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2023-24

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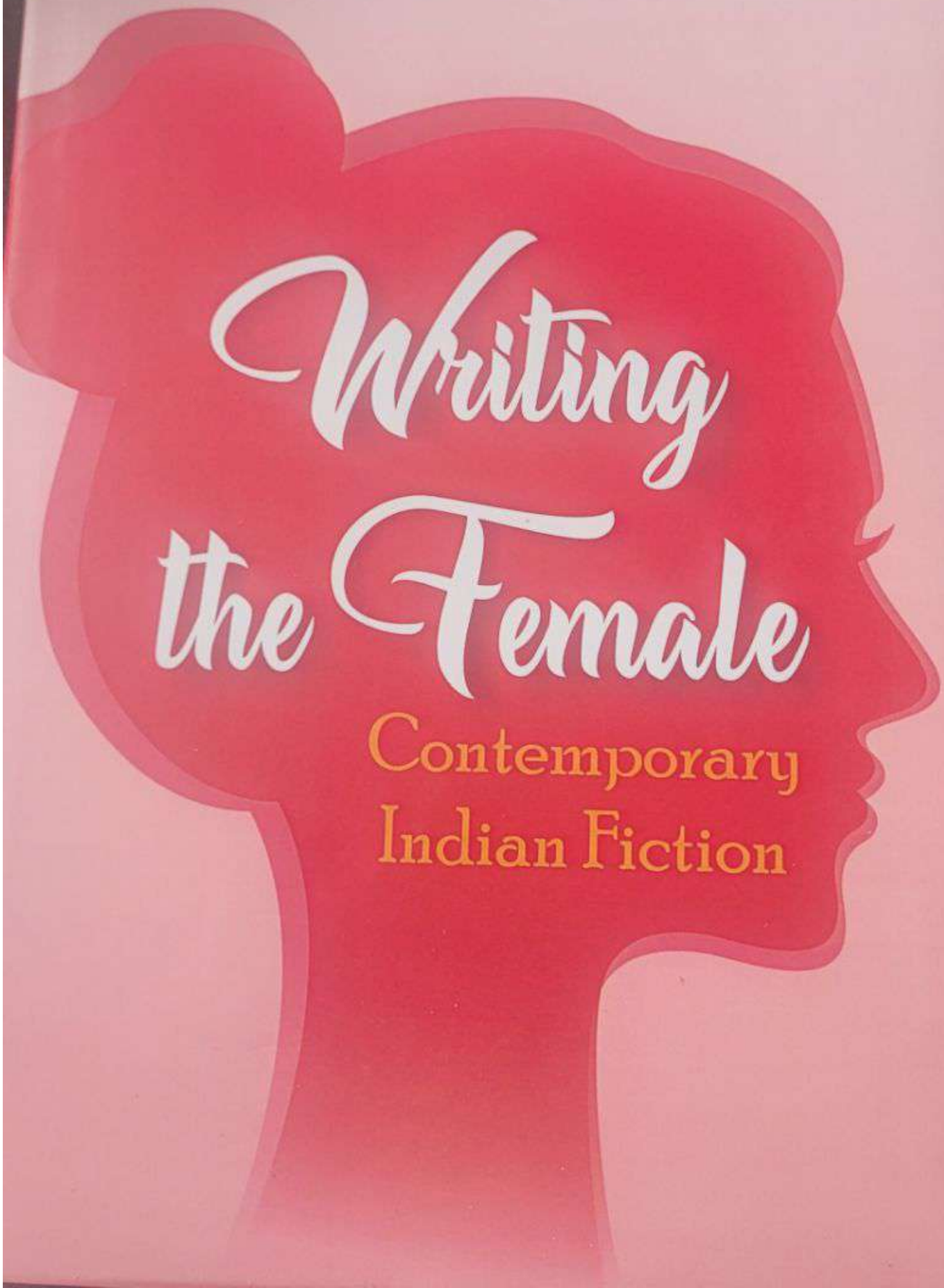

Writing the Female

Contemporary Indian Fiction

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CHAPTER

7

Affirming the Woman's Word/World: Food Thoughts on *Alphabet Soup for Lovers*

Jyothimol P.

A little altered line from Shakespeare would render the thrust of this paper. "If Food is the music of love, then feast on." Food signifies many things for many people. For women especially Indian women, it is not just physical sustenance that the world of food provides. It is aphrodisiac, a creative spirit and very much a woman's discourse as far as the Indian domestic culinary space is concerned. It has been an attempt to catch back that aspect of woman's sphere, often a restrictive space that has been part of the woman's movements in Kerala. Many tried to liberate women from the restrictive kitchen; but at a later stage attempts have been made to catch that space back too in an altered reading of the notions of feminism.

> Gender norms strongly affect food preparation behaviors, in ways ranging from division of this labor to holding women responsible for the health of their families and whether they

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www.co-textpublishers.com
Essays

ISBN 978-81-952253-1-6

PRICE ₹ 799

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AUTHORS PRESS

Worldwide Circulation through Authorspress Global Network
First Published in 2023
by
Authorspress
Q-2A Hauz Khas Enclave, New Delhi-110 016 (India)
Phone: (0) 9818049852
E-mail: authorspressgroup@gmail.com
Website: www.authorspressbooks.com

Tales Unraveled: Sufferings and Pangs of the Downtrodden in the Short Stories of K. V. Dominic

ISBN 978-93-5529-890-4

Printed in India at Thomson Press (India) Limited

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Responding Responsibly: A Levinasian Ethical Reading of *Sanchita Karma and Other Tales of Ethics and Choice from India*

DR. KAVITHA GOPALAKRISHNAN

ABSTRACT

This paper aims to extend the ethics of Levinas to understanding the characters portrayed in Dominican short stories. His stories exude Levinasian spirit. As conceived by Levinas, the subject is not the egocentric subject in traditional philosophy but rather an ethical subject based on—the other. The paper also delves into Levinas'—responsibility for the other as portrayed in the select short story collection. Levinas asserts that the nonintegrable alterity, infinity, and transcendence of the other give us an inescapable and infinite responsibility for the other. The responsibility for the other will appear when we encounter face to face with the other.

Keywords: Emmanuel Levinas, ethical subject, responsibility for the other, the face

> Dear friend, what harm have I done to you that you should kill me? See how I became your saviour just now! What harm have this forest and its animals done to you? Haven't you felled thousands of trees and hunted hundreds of animals? You and your people survive only because of our presence. ("World Environment Day", 8)

This conversation between the tree and Kaatturaja changes the latter's self and conscience forever. This face-to-face encounter made Kaaturaaja promise the tree that he would "devote (his) life to the preservation of this forest" (8). According to Levinas, the concept of the "face" can be identified, though it is not confined solely to facial features, as a significant realm for engaging with others. Be it humans, the planet, animals, or plants, all existence embodies this notion of the face, encapsulating a fragility and susceptibility that compellingly emphasizes the sheer distinct nature of the non-human realm.The paper tries to elaborate how through the stories in *Sanchita Karma*, Dr. K. V. Dominic elucidates Levinas' concept of the pre-cognitive, face-to-face interaction with the profound otherness of another individual, as an

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നാളെ ചരിത്രമായേക്കാവുന്ന വാർത്തകളാണ് മാധ്യമങ്ങൾ ഇന്ന് റിപ്പോർട്ട് ചെയ്യുന്നത്. വസ്തുനിഷ്ഠമായും നൈതികമായും അല്ല അതു നിർവ്വഹിക്കുന്നതെങ്കിൽ ചരിത്രവും വികലമാക്കപ്പെടും. സാംസ്കാരിക, സാമൂഹിക വിപ്ലവങ്ങൾ സംഭവിക്കുമ്പോൾ അവ സത്യസന്ധമായും പക്ഷപാത രഹിതമായും റിപ്പോർട്ട് ചെയ്യേണ്ടത് ഒരു സമൂഹത്തിന്റെ സാംസ്കാരിക ഉടർച്ചയ്ക്ക് അനിവാര്യമാണ്.

എഡിറ്റർ

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മാളൂബൻ പ്രസിദ്ധീകരണം
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വില: ₹ 1000

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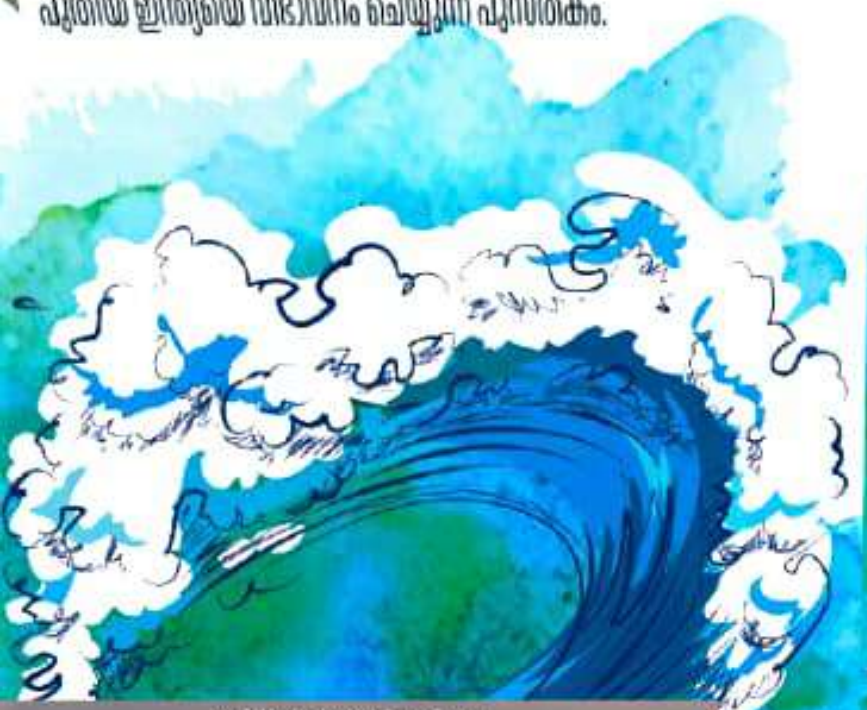

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രാമചരിതം: നാല്പത്തിയെട്ടാം പടലം

വ്യാഖ്യാ: ഡോ. മഞ്ജുഷ വി. പണിക്കർ

രാമചരിതം: നാല്പത്തിയെട്ടാം പടലം
വ്യാഖ്യാതാവ്: ഡോ. മഞ്ജുഷ വി. പണിക്കർ
(മലയാളം: കവിത)

The electronic versions have been created by making use of the production infrastructure of River Valley Technologies.

The electronic versions were generated from sources marked up in LaTeX in a computer running GNU/LINUX operating system. PDF was typeset using XeTeX from TeXLive 2020 and the cloud framework, Ithal (ഇതൾ). The base font used was traditional script of Rachana, contributed by KH Hussain, et al. and maintained by Rachana Institute of Typography. The font used for Latin script was Linux Libertine developed by Philipp H. Poll.

Page from a Ramayana Series, a painting by Annonymous. The image is taken from Wikimedia Commons and is gratefully acknowledged.

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രാമചരിതം:
നാല്പത്തിയെട്ടാം പടലം

സംഗ്രഹം

രാവണപുത്രനായ ഇന്ദ്രജിത്ത് വാനരന്മാരിൽ മിക്കവരെയും രാമലക്ഷ്മണന്മാരെയും വീഴ്ത്തിയതുകണ്ട് ശേഷിച്ച വാനരസേന 'ഈ യുദ്ധത്തിൽ ജയിക്കുക നമ്മാൽ അസാധ്യ'മെന്ന ചിന്തിച്ച് യുദ്ധഭൂമിയിൽനിന്ന പിന്മാറാൻ ഭാവിക്കുന്നു. ഇതുകണ്ട വിഭീഷണൻ അവരെ തടഞ്ഞുനിർത്തി സമാധാനിപ്പിക്കുന്നു. പിന്നീട് ഹനുമാനെ കണ്ടുപിടിച്ച്, അവർ ഇരുവരും ചേർന്ന് ജാംബവാനെ അന്വേഷിച്ച കണ്ടെത്തുന്നു. വിഭീഷണന്റെ ശബ്ദംകേട്ട ജാംബവാൻ "ഹനുമാൻ ജീവിച്ചിരിപ്പുണ്ടോ?" എന്ന് അന്വേഷിക്കുന്നു. ഇതുകേട്ട് ജാംബവാന്റെ കാല്ക്കൽവീണ് നമസ്കരിക്കുന്ന ഹനുമാനോട് "നീയുണ്ടെങ്കിൽ വാനരന്മാരെയും രാമലക്ഷ്മണന്മാരെയും ജീവിപ്പിക്കാൻ കഴിയും" എന്ന ജാംബവാൻ പറയുന്നു.

പാട്ട് 1

അകമഴന്റു കവിവീരർ പടൈയാളികളുടെ
യറുതികണ്ടുമുടനേയരചന്മാർ തിരുവുട-
മ്പകിലവും മറൈയുമാറൊളികൊള്ളത്തിരംകളേ
റ്റവർകിടന്തപടികണ്ടുമതികം ചപലരായ്
ഇകലില് വെല്വതു നമുക്കരുതെൻറും
നിനൈവിനോടിടർ
മുഴുത്തു മതികെട്ടു കുലൈയിൻറ പടൈപോ-
യകലും മുമ്പവർകളെത്തടൈന്തുകൊണ്ടണൈവവർ
ക്കമുതവാരിതി വിപീഴണനിവണ്ണം മൊഴിന്താൻ

പടയാളികളുടെ നാശംകണ്ടും രാമലക്ഷ്മണന്മാരുടെ തിരുവുടൽ മറയുമാറ് അസ്ത്രങ്ങളേറ്റ് അവർ കിടക്കുന്ന മട്ടുകണ്ടും ഏറെ ചപലരായി, മനസ്സവെന്ത് 'യുദ്ധത്തിൽ ജയിക്കുവാൻ നമുക്കു സാധ്യമല്ല' എന്ന ചിന്തയോടെ യുദ്ധം അവസാനിപ്പിച്ച് വാനരപ്പട യുദ്ധഭൂമിവിട്ടു പോകാൻ തുടങ്ങി. അവരെ തടഞ്ഞുകൊണ്ട്, ആശ്രിതർക്ക് അമൃതവാരിധിയായ വിഭീഷണൻ ഇപ്രകാരം പറഞ്ഞു.

കുറിപ്പ്

അകമഴന്റു — ഉള്ളുവെന്ത്
വെല്വതു — ജയിക്കുക എന്നത്
കുലൈയിന്റ — തളർന്ന, ക്ഷീണിച്ച
അമുതവാരിതി — അമൃതവാരിധി

പാട്ട് 2

ഇവണ്ണമേയിവനൊരിക്കല്
മുന്നമത്തിരംകളാ-
ലിവരെല്ലാരെയുമിമണ്മിചൈ
നിരത്തിയികലില്-
ച്ചവൈപ്പിറന്തരിയ വെറ്റിയുമിയറ്റിനകരില്-
ച്ചുരുതിപെറ്റിരുന്ത നേരമരനാഴികയിൻ മു-
മ്പവനിനായകരും വാനരകുലംകളുമെഴ-
ന്തടല് തൊട്ടത്തനരരക്കർ മുടിയുംപടിയട്ട-
ത്തിവിടയും വരുമവ്വണ്ണമിനിയെന്റഴകുതാ-
യിതു തെളിന്തറിക നിങ്കളിരുകൂറില്ലിതിനേ

വിഭീഷണൻ പറയുന്നു: "ഇപ്രകാരം മുമ്പൊരിക്കൽ ഇന്ദ്രജിത്ത് അസ്ത്രങ്ങൾകൊണ്ട് ഇവരെയെല്ലാരെയും നിലംപതിപ്പിച്ച, ജയവുംനേടി രാജധാനിയിൽ കീർത്തികേട്ടിരുന്നു. എന്നാൽ അരനാഴികതികയുംമുമ്പ് രാജാക്കന്മാരും വാനരകുലവും എഴുന്നേറ്റ് രാക്ഷസർ നശിക്കുംവണ്ണം യുദ്ധംചെയ്തു. അടുത്തതായി ഇവിടെയും അപ്രകാരം വരുമെന്ന് നിങ്ങൾ ഭംഗിയായി തെളിഞ്ഞറിയുക. ഇതിനു രണ്ടുപക്ഷമില്ല."

കുറിപ്പ്

ചവൈപ്പിറന്ത് — രസം ജനിച്ച്
ചുരുതി — ശ്രുതി, കീർത്തി
ഇരുകൂറ് — രണ്ടുപക്ഷം

പാട്ട് 3

ഇതുതെളിന്തവർകളോടുമുരൈചെയ്തു വിരൈവോ-
ടടലിലാരുയിർ വിടാതവർകളെൻററിവുതെ-
ന്റതികമമ്പൊടു വിപീഴണൻ വരിന്റളവിലേ
അയനുള്ളത്തിരംകളേറ്റിടലവുന്തളർന്തുപോ-
യതിനെയാതരവു ചെയ്തുലകില് വീഴ്ന്തവനുണർ-
ന്തളവില്ലാതെ വെലമീട്ടും മാരുതിയെഴ-
ന്തുതകവോരാരൊരു തുരത്തിനിനിയെ-
ൻറുയിരുള്ളോരെയവൻവിനവുമാറു ചമൈന്താൻ

ഇത് അവരോടു തെളിഞ്ഞു പറഞ്ഞശേഷം, വേഗത്തിൽ 'യുദ്ധത്തിൽ ആരാണ് ജീവൻ നഷ്ടപ്പെടാത്തവർ എന്നറിയണം' എന്ന് പറഞ്ഞു വിഭീഷണൻ അന്വേഷിച്ച വരുന്നു. ബ്രഹ്മാസ്ത്രമേറ്റ് ശരീരം തളർന്നു നിലത്തുവീണ അമിതബലവാനായ മാരുതി എഴുന്നേറ്റ് 'ഒരു കാര്യത്തിനിനി ഉതകുന്നവർ ആര്' എന്ന് അതിജീവിച്ചവരെ അന്വേഷിക്കുവാൻ തുടങ്ങി.

കുറിപ്പ്

അയനുള്ളത്തിരം — ബ്രഹ്മാസ്ത്രം
തുരം — കാര്യം, ഭാരം
വിനവുമാറ് — അന്വേഷിക്കുമാറ്

പാട്ട് 4

വിനവിനോരുതരമേ വളർകരംകളിലൊരോ-
വിമലചൂരിയനു നേരൊളികൊൾ കൊള്ളികളിര-
ണ്ടിനിയവായുള്ളവും വീചി നടകൊണ്ടളവു ക-
ണ്ടിരുവരും തമ്മിലണൈന്തിടുർന്തഴകുതായ്
മുനിവർതേടും മറഞാനപ്പൊരുളേഴുലകിനും
മുതല്വനാന മതുചൂതനനന്തനുമൊരോ
മനുചരായിവർ വീഴ്ന്തമയും വാനരകുലം
മലൈകൾനേർ കിടന്തവാറുമവർ പാർത്തനരെങ്കും.

വിഭീഷണനും ഹനുമാനും ദീർഘങ്ങളായ കരങ്ങളിൽ തിളക്കമുള്ള വിറകിൻകൊള്ളികളും വീശി പടക്കളത്തിലൂടെ അന്വേഷിച്ച നടന്നു. അപ്പോൾ മുനിമാർ തേടുന്ന വേദസാരവും ഏഴുലകിനും ആദിമൂലവുമായ മധുസൂദനന്റെയും അനന്തന്റെയും മനുഷ്യാവതാരങ്ങളായ രാമലക്ഷ്മണന്മാർ വീണുകിടക്കുന്നതും വാനരന്മാർ മലകൾപോലെ വീണു കിടക്കുന്നതും അവർ കണ്ടു.

കുറിപ്പ്

മറഞാനപ്പൊരുൾ — വേദസാരം
മുതല്വനാന — ആദിമൂലമായ
മതുചൂതനൻ — മധുസൂദനൻ

പാട്ട് 5

അവനിമീതു തുടൈ തോൾ കര മുരഞ്ചിരംകൾ കാ-
ലവയവേയരിന്തു വേറുചെയ്തു ചോരിയുമിഴ്-
ന്തുവരിമീതെങ്കമെഴിന്റ തിരൈമാലൈകൾ തിളൈ-
ത്തുയരുംവണ്ണമിടകെട്ടിയുയിർവിട്ടുടനടൻ
കവികൾ നായകർ കിടന്തവരെല്ലാരെയുമുള്ളില്
കനിവുപൂണ്ടവർകൾ നോക്കിനരന്നോക്കിൻ വഴിയേ
നിവിരനീള നടകൊണ്ടളവു കണ്ടലംകളാല്
നിറൈന്ത ചോകമൊടു കണ്ടനർ കിടന്തവടിവേ.

തുട, തോൾ, കരം, ശിരസ്സ്, കാല് തുടങ്ങി ഒരോന്നും അരിഞ്ഞു വേർപെട്ട്, ഉയരുന്ന തിരമാലകൾ തിളച്ചുവരുംപോലെ ചോരയൊഴുകി, ശ്വാസനാളി അടഞ്ഞ് ഉയിരറ്റ് ഭൂമിയിൽ അടുത്തടുത്തു കിടക്കുന്ന വാനരനായകന്മാരെയും ഉള്ളിൽ കനിവുപൂണ്ട് അവൻ നോക്കി. വീക്ഷണവഴിയിലൂടെ നടന്നപ്പോൾ അവർ കിടക്കുന്നത് കണ്ണുകളിൽ നിറഞ്ഞ ശോകത്തോടുകൂടി അവൻ കണ്ടു.

കുറിപ്പ്

ഉമിഴ്ന്തു — വമിച്ച്, പുറത്തേക്കൊഴുകി
ഇടകെട്ടി — ശ്വാസനാളിയടഞ്ഞ്
നോക്കിൻവഴി — വീക്ഷണമാർഗ്ഗം
കണ്ടലം — കൺതലം

പാട്ട് 6

വടിവുമിക്കചരവൻ, കെവയനംകതൻ വെയ്യോ-
ൻറനയനത്തിമുകനും തെതിമുകൻ തുമുകനും
കൊടിയ കേതരി ചുഴേണനനിലോമൻ വിവിതൻ,
കുമുതമൈന്തനൊടുതുർമ്മുകന്നളൻ കിരതനൻ
ഇടവന്നീലനൊടു താരനും തെംപനലക-
ത്തെതിരില്ലാത കെച കോമുക ചുവേതനൊളിവാർ
തടിലിടൈന്തകിറനോടു വളർപാവകവിലോ-
ചനൻ കെവാക്കൻ നല്ല വേകതെരിചിപ്പെയരിനാൻ.

അവിടെ കണ്ട വാനരന്മാരുടെ പേരുകളാണ് ഈ പാട്ടിൽ സൂചിപ്പിക്കുന്നത്. ശരഭൻ, ഗവയൻ, സുഗ്രീവൻ, അസ്ഥിമുഖൻ, ദധിമുഖൻ, സുമുഖൻ, കേസരി, സുഷേണൻ, ലോമൻ, വിവിധൻ, കുമുദൻ, മൈന്ദൻ, ദുർമ്മുഖൻ, നളൻ, കൃഥനൻ, ഇടവൻ, നീലൻ, താരൻ, ദംഭൻ, ഗജൻ, ഗോമുഖൻ, സുവേദൻ, വിദ്യുദ്ദംഷ്ട്രൻ, ഗവാക്ഷൻ, വേഗദർശി എന്നവരെയെല്ലാം കാണുന്നു.

കുറിപ്പ്

വെയ്യോൻറനയൻ — സൂര്യപുത്രനായ സുഗ്രീവൻ
അത്തിമുകൻ — അസ്ഥിമുഖൻ
ഒളിവാർതടിലിടൈന്തെകിറൻ — മിന്നലിനു തുല്യം മനോഹരമായ ദംഷ്ട്രയുള്ളവൻ, വിദ്യുദ്ദംഷ്ട്രൻ
വേകതെരിചിപ്പെയരിനാൻ — വേഗദർശിയെന്ന പേരോടുകൂടിയവൻ

പാട്ട് 7

പെരിയരുരൈപ്പതിനുടനടക്കുകിലൊടുക്കമില്ലെങ്കും
പെരിയതക്കനൊടു ചോതിമുകനുംവിനതനും
ചെയല്മികുത്ത പിരതാപിയിങ്ങനെയുമികലില്
ത്തിറമിയൻറ പനതൻ ചതവെലിപ്പെയരിനാൻ
തുയില് കൊള്ളിന്റപടി തുമ്മിരതന്നാതരവും
ചുരുതിമിക്കെഴമിയക്കനുമ്മറ്റുമിങ്ങനെ
നയമിയന്റ കവിമന്നർതമ്മന്നവനെയും
നലമെഴം പരിച്ചു കണ്ടനർ നടന്തനർ പിന്നും.

പിന്നീടു കണ്ട വാനരന്മാരെയാണ് ഈ പാട്ടിൽ പരാമർശിക്കുന്നത്. പേരുകൾ പറയാൻ തുടങ്ങിയാൽ അവസാനമുണ്ടാകുകയില്ല. തക്ഷൻ, ജ്യോതിർമ്മുഖൻ, വിനതൻ, പനസൻ, ശതബലി, യക്ഷൻ എന്നിങ്ങനെ നയമേറിയ കപിമന്നവരുടെ മന്നവനെയും നന്നായിട്ടുകണ്ട് അവർ പിന്നെയും നടന്നു.

കുറിപ്പ്

ഉരൈപ്പതിനടക്കുകിൽ — പറയാൻ തുടങ്ങിയാൽ
തക്കൻ — തക്ഷൻ
ചെയൽ — സാമർത്ഥ്യം
ചതവെലി — ശതബലി
തുയിൽകൊള്ളുന്നപടി — ഉറങ്ങുന്നമാതിരിയുള്ള
ഇയക്കൻ — യക്ഷൻ
കപിമന്നർതമ്മന്നവർ — കപിമന്നവരുടെ മന്നവൻ

പാട്ട് 8

നടന്തനേരമിടകൂട നടന്തൊരളവിലേ
നളിനമാതിന്മണവാളനൊരു മണിയുരുവ-
മുടൈയനായിരന്തു മൂവടിയമ്മാവലിതന്നോ-
ടുതകമേറ്റുലകമീരടിയളക്കുമകമേ
മുടിയുമാറളന്തനാളളന്തുകൂട്ടും മുന്നമേ
മുഴംകുമൊൺപറൈ മുഴക്കിന കവിക്കരചനെ-
ക്കൊടിയ ചാംപവനെയംപിട തുടർന്തുടലെല്ലാം
കുലൈന്തവന്തന്നൈയണൈന്തനരറിന്തിരുവരും.

മഹാവിഷ്ണു വാമനരൂപം ധരിച്ച മഹാബലിയോട് ഉദകപൂർവ്വം മൂന്നടിയിരന്നു വാങ്ങി. ഉലകം രണ്ടടി അളക്കുന്നതിനുള്ളിൽ അവസാനിക്കുമാറ് അളന്നപ്പോൾ, അളന്നുതീരുംമുമ്പ് ഭംഗിയുള്ള പെരുമ്പറ മുഴക്കിയ ജാംബവാനെ ഉടലിലെല്ലാം ഇടതൂർന്ന് അമ്പുകളേറ്റ തളർന്നവനായി കണ്ട് ഇരുവരും അടുത്തെത്തി.

കുറിപ്പ്

നളിനമാതിൻമണവാളൻ — മഹാവിഷ്ണു
മാണിയുരുവം — വടുരൂപം
ഉതകമേറ്റ — ജലമേറ്റ്
ഒൺപറൈ — ഭംഗിയുള്ള പറ

പാട്ട് 9

ഇരുവർ നായകരണൈന്തതില് വിപീഴണനുതിർ-
ന്തികലില് നിൻറുയിർ പിരിന്തുതില്ലയോയെനമൊഴി-
ന്തരികില് നിൻറളവുമിണ്ണമിണ്ണചെം കുരുതിയാ-
ലയനു നന്തനനിയം പിനനയെന്തമൊഴിയാല്
അരുതു കാണമതു കണ്ണിണൈയില്
വെൺകണൈകൾപ-
യ്ന്തരികില് നിൻറതു മകൻറവുമാകിലും നിന്ന-
ക്കരുതിനേനിതു വിപീഴണനെന്മേടമൊഴിയ-
ക്കനിവുനുണ്മൈയുമിയൻറപടി കണ്ടഴകുതായ്.

വിഭീഷണൻ മുന്നോട്ടുചെന്ന് "യുദ്ധത്തിൽ നിന്റെ പ്രാണൻ പിരിഞ്ഞില്ലല്ലോ?" എന്ന ചോദിച്ച് അരികിൽ നിന്നപ്പോൾ ചെഞ്ചോര വമിച്ചുവമിച്ച് ബ്രഹ്മപുത്രനായ ജാംബവാൻ തളർന്ന മൊഴിയാൽ പറഞ്ഞു: "കണ്ണിണയിൽ വെൺകണകൾ പാഞ്ഞതുകൊണ്ട് അരികിലുള്ളതും അകലെയുള്ളതും കാണുവാൻ സാധ്യമല്ല. എങ്കിലും നിന്നെ വിഭീഷണനെന്നു കരുതുന്നു" എന്ന പറയുമ്പോൾ അദ്ദേഹത്തിന്റെ കനിവും സൂക്ഷ്മതയും അഴകോടെ കണ്ടു.

കുറിപ്പ്

ഉമിണ്ണമിണ്ണ് — വമിച്ച വമിച്ച്
ആയനുനന്തനൻ — അജനു നന്ദനൻ, ബ്രഹ്മപുത്രൻ, ജാംബവാൻ
നുണ്മൈ — കൂർമ്മ, ഇന്ദ്രിയങ്ങളുടെ സൂക്ഷ്മത

പാട്ട് 10

അഴകുതായ് മുടിന്തുപോയ കവിവീരരില് നമ-
ക്കനിലനന്തനനനുമനുളനോയെൻറുമേടം
മൊഴിന്ത ചാംപവനോടെന്തവനില് നിങ്കനിവുപോയ്
മുഴുവനായിതു കഴിത്തിനിയ വേന്തരെയെല്ലാം
അഴിവിനോടിതു വിപീഴണനുരൈത്തളവിലേ-
യയനുനന്തനനൊഴിന്തനനവന്നിടരില്ലാ-
തൊഴികിലോ മുടിന്തതും മുടിന്തുതല്ലവന്നമ-
ക്കുളനല്ലാതൊഴികിലോയിനിയങ്കുള്ളോൻറുമില്ലേ

"വല്ലാതെ നശിച്ചുപോയ കപിവീരന്മാരിൽ വായുപുത്രനായ ഹനുമാനുണ്ടോ?" എന്ന ചോദിച്ച ജാംബവാനോട്, "ഉത്കൃഷ്ടരായ രാജാക്കന്മാരെപ്പോലും അന്വേഷിക്കാതെ നിന്റെ ശ്രദ്ധ മുഴുവൻ അവനിലായതെന്ത്?" എന്ന വിഭീഷണൻ ചോദിച്ചപ്പോൾ "അവൻ ആപത്തില്ലാതെ ശേഷിക്കുകയാണെങ്കിൽ നശിച്ചതൊന്നും നശിച്ചതല്ല: അവൻ നമുക്കില്ലെങ്കിൽ ഇനിയിങ്ങുള്ളതും ഇല്ല" എന്ന് ജാംബവാൻ മറുപടി പറഞ്ഞു.

കുറിപ്പ്

ഉളനോ — ഉണ്ടോ
എൻറുമേടം — എന്ന വിവരം

പാട്ട് 11

അതു ചൊന്നോരളവില് മാരുതി വിരണൈവനുടേ
യടിപണിന്തനനനുമനെന്നും നാമമുരൈ ചെ-
യ്തതിതമമ്പിനൊടു ചാംപവൻ മൊഴിന്തനനഴി-
ന്തരചർ നായകരെ വാനരവരേന്തിരരേയും
ചതിയിനാലടലിലിന്നിചിചരാതിപതിതൻ
തനയനാല് മുടിവുവന്ത പടൈയോടുമതികം
മതിയില്ലാത വിരൈവോടിനിയുണർത്തുമതിനാം
വഴിയുഴൈപ്പതിനു നീയൊഴികിലാവവരില്ലേ.

ജാംബവാൻ ഇപ്രകാരം പറഞ്ഞപ്പോൾ ഹനുമാൻ തന്റെ പേരുച്ചരിച്ച് ജാംബവാന്റെ കാൽക്കൽ വന്ദിച്ചു. അധികം വാത്സല്യത്തോടുകൂടി ജാംബവാൻ പറഞ്ഞു: "നാശം സംഭവിച്ച രാജാധിരാജന്മാരെയും വാനരശ്രേഷ്ഠന്മാരെയും ചതികൊണ്ട് രാവണപുത്രനായ ഇന്ദ്രജിത്തു യുദ്ധത്തിൽ നശിപ്പിച്ച പടയോടുകൂടി വേഗത്തിൽ ഉണർത്തുന്നതിന് വേണ്ട പ്രകാരം പരിശ്രമിക്കുന്നതിന് സാധിക്കുന്നവർ നീയൊഴികെ മറ്റാരുമില്ല."

കുറിപ്പ്

മതിയില്ലാതവിരൈവ് — മതിവരാത്തവേഗം
ആംവഴി — ആകുന്നപ്രകാരം
ഉഴൈപ്പതിന്ന് — പരിശ്രമിക്കുന്നതിന്

ഡോ. മഞ്ജുഷ വി. പണിക്കർ

അസിസ്റ്റന്റ് പ്രൊഫസർ, മലയാള വിഭാഗം, ബസേലിയസ് കോളജ്, കോട്ടയം.

പിൻകുറിപ്പ്

- മുപ്പതു മുതൽ നാല്പതു മിനിട്ടിനകം വായിച്ചു തീർക്കാവുന്ന ഉള്ളടക്കമാണ് സായാഹ്ന പുറത്തിറക്കുന്ന ഈ ഫോൺ പിഡിഎഫുകളിൽ ഉള്ളത്. ഇതു വായിക്കുവാനായി ഒരിക്കലും ഒരു കമ്പ്യൂട്ടറോ ഡെസ്ക്ടോപ് ആപ്ലിക്കേഷനുകളൊ ആവശ്യമില്ല.
- ആധുനിക മനുഷ്യന്റെ സന്തതസഹചാരിയായ സ്മാർട്ട് ഫോണുകളുടെ സ്ക്രീനിൽ തന്നെ വായിക്കുവാൻ തക്ക രീതിയിലാണ ഈ പിഡിഎഫുകൾ വിന്യസിച്ചിരിക്കുന്നത്. ഫോണിന്റെ വീതിക്കു നിജപ്പെടുത്തിയ രീതിയിലാണ് മാർജിനുകൾ ചിട്ടപ്പെടുത്തിയിരിക്കുന്നത്.
- പിഡിഎഫ് പ്രമാണങ്ങൾ വായിക്കുവാനുള്ള പ്രയോഗങ്ങൾ എല്ലാതരം സ്മാർട്ട്ഫോണുകളിലും ഇന്നു ലഭ്യമാണ്. എന്നിരിക്കിലും സൗജന്യമായി കിട്ടുന്ന അഡോബി അക്രോബാറ്റ് റീഡർ ആണ് ഇവയിൽ ഏറ്റവും മുന്തിയത്. അതുകൊണ്ട് അഡോബി റീഡർ ഇൻസ്റ്റാൾ ചെയ്യുകയും അതിൽ ഈ ഫോൺ പിഡിഎഫുകൾ വായിക്കുകയും ചെയ്യുക.
- സ്വതന്ത്രപ്രസാധനം ആഗ്രഹിക്കുന്ന/ഇഷ്ടപ്പെടുന്ന ആർക്കുവേണമെങ്കിലും സായാഹ്നയിലൂടെ സ്വന്തം കൃതികൾ പ്രസാധനം ചെയ്യാവുന്നതാണ്. 30 മുതൽ 60 മിനിട്ടുകൾക്കകം വായിച്ചുതീർക്കാവുന്ന ഉള്ളടക്കം – കഥകൾ, അനുഭവക്കുറിപ്പുകൾ, ലേഖനങ്ങൾ, അഭിമുഖങ്ങൾ, സിനിമാനിരൂപണങ്ങൾ, കവിതകൾ – എന്നു തുടങ്ങി എന്തുവേണമെങ്കിലും അയയ്ക്കാവുന്നതാണ്. അയയ്ക്കേണ്ട വിലാസം: <editors@sayahna.org>.
- പ്രതികരണങ്ങൾ <editors@sayahna.org> എന്ന ഇമെയിലിലേയ്ക്ക് അയയ്ക്കുകയോ, ഈ വെബ് പേജിൽ കമന്റുകളായി ചേർക്കുകയോ ചെയ്യുക. നിർദ്ദേശങ്ങളും വിമർശനങ്ങളും എപ്പോഴും സ്വീകാര്യമാണ്. അവ സായാഹ്നപ്രവർത്തകർക്ക് കൂടുതൽ ഉത്തേജനം നൽകുന്നതാണ്.

സായാഹ്ന ഫൗണ്ടേഷൻ, ജഗതി, തിരുവനന്തപുരം
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14

High-k Dielectrics Based on Two-Dimensional Nanomaterials-Filled Polymer Nanocomposites

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Abstract

In sophisticated electronics and electric power systems, higher electrical energy concentrations in adaptable dielectric compounds are essential. It displayed great promise in terms of developing energy storage applications. Among many dielectric compounds, the two-dimensional (2D) materials-filled polymers are emerging as the preferred dielectric for high energy density capacitors due to its high breakdown strength and elegant failure mechanism. The excellent mechanical, thermal, and electric properties of 2D materials allow them to be used in a variety of fields and polymer nanocomposites-filled 2D materials have significantly improved properties, indicating a great deal of promise in dielectric and energy storage applications. More emphasis is being paid to inorganic-polymer nanocomposites, which combine the advantages of inorganic nanoparticles' higher dielectric constant and polymers' sky-scraping breakdown strength. In conductor-insulator systems, features like higher surface area and conductivity of 2D nanomaterials substantially boost density of polarization and its interfacial interphases. The development of conductive channels in a matrix is a difficult challenge to solve. The inclusion of additional nanoparticle, surface fabrication, sandwich configuration, and core-shell design have all been proven to be effective in reducing dielectric loss and increasing breakdown strength. This extraordinary demonstration of energy storage capability sheds new light on the evolution of high-efficiency dielectric materials.

In this chapter, we will be discussing high-k dielectrics 2D materials, opportunities, challenges, and the enhancement of its dielectric mechanisms. Their applications in different fields are also highlighted.

***Keywords*:** 2D nanofillers, polymer dielectrics, dielectric constant, dielectric tangent loss, breakdown strength

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Mayank Pandey, Kalim Deshmukh and Chaudhery Mustansar Hussain (eds.) Two-Dimensional Nanomaterials-Based Polymer Nanocomposites: Processing, Properties and Applications, (509–540)

Nanomaterials in Environmental Analysis

Edited by
Suresh Kumar Kailasa
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ELSEVIER

Nanomaterials in Environmental Analysis

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Elsevier
Radarweg 29, PO Box 211, 1000 AE Amsterdam, Netherlands
125 London Wall, London EC2Y 5AS, United Kingdom
50 Hampshire Street, 5th Floor, Cambridge, MA 02139, United States

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ISBN: 978-0-12-820643-0

Publisher: Candice G. Janco
Acquisitions Editor: Anita Koch
Editorial Project Manager: Lindsay C. Lawrence
Production Project Manager: Bharatwaj Varatharajan
Cover Designer: Christian J. Bilbow

Typeset by MPS Limited, Chennai, India

CHAPTER

1 NANOMATERIALS IN MEASUREMENT OF POLLUTANTS IN ENVIRONMENTAL SAMPLES

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1.1 INTRODUCTION

The societal and technological impact of nanostructured materials is enormous and continually growing in all the research areas [1–5]. The integration of nanostructured materials for chemical analyses offers outstanding analytical features such as selectivity, rapidity, sensitivity, and miniaturization [6–9]. Further, the integration of nanoscale materials with analytical tools has triggered the development of straightforward analytical strategies for the detection and quantification of trace-level target analytes even at the single molecule level. In recent years, numerous research papers have described the outstanding applications of nanostructured materials in the development of analytical method for chemical analysis and identification [10–13]. Importantly, nanomaterials were modified with specific ligand chemistry, thereby allowing them to measure multiple targets in various sample matrices [11–13]. Nanostructured materials possess unique optical, electrical, magnetic, and physicochemical properties and offer specific surfaces for effective functionalization for the development of colorimetric/fluorescence probes [3,8,11] and extracting probes [14–17]. Many types of nanomaterials, such as metal nanoparticles, semiconductor quantum dots (QDs), metal nanoclusters (NCs), carbon dots, graphene oxide, MXenes, perovskite, carbon nitride, and boron nitrides, have been used as probes for assaying numerous analytes (inorganic, organic, pesticides, drugs, and biomolecules) [1–11]. These nanostructured materials have gained fundamental interest in recognizing molecular species without any sample preparation.

Several nanostructured materials have been used in electrochemical analytical strategies for the analysis of a wide variety of analytes with adequate selectivity and sensitivity [18,19]. Analytical features of UV–visible, fluorescence, Raman, mass spectrometric, and electroanalytical techniques have been greatly improved by integrating nanostructured materials for the analysis of various chemicals. To explore the promising applications of nanostructured materials in analytical chemistry, various types of nanostructured materials (metal nanoparticles, QDs, metal NCs, carbon dots, graphene oxide, perovskite, carbon nitride, boron nitrides, and MXenes) have successfully been integrated with optical spectroscopic and mass spectrometric techniques for assaying of various target analytes. This chapter provides a detailed summary of nanomaterials-based analytical strategies for chemical analysis. This chapter mainly focuses on (1) nanomaterials-based colorimetric and fluorescence analytical strategies, (2) nanomaterials-based mass spectrometric tools for the

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00001-8

CHAPTER

METAL NANOPARTICLES FOR VISUAL DETECTION OF ORGANIC POLLUTANTS

2

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2.1 INTRODUCTION

Chemical sensors that respond to particular analytes through obvious color changes are more eminent due to their simplicity and low-cost [1]. Importantly, no sophisticated or luxurious analytical instruments are required. Additionally, colorimetric sensors could be useful in developing point-of-care testing (POCT) devices. Coupling a dye or chromogenic singling unit with a receptor moiety is important to develop the colorimetric chemical sensors [2]. Recently, nanoparticle-based materials have been explored for this purpose due to their high selectivity, sensitivity, biocompatibility, and suitability for practical applications. Among nanoparticles, noble metal nanoparticles such as silver and gold provide characteristic physicochemical and optical properties, display higher extinction coefficients than organic molecules, and display beautiful color changes with analytes that can be visualized through the eyes [3].

Organic pollutants are toxic chemicals that adversely affect human health and the environment around them. Most organic pollutants are highly toxic and cannot be degraded. Organic pollutants are major responsible for bio-magnification due to their accumulation in the ecosystem. Generally, pesticides, polychlorinated biphenyls, aromatic hydrocarbons, dioxins, phenols, bisphenol-A, surfactants, linear alkylbenzene sulfonates, alkanes, polycyclic aromatic hydrocarbons, antibiotics, toxins, and amines are considered as an organic pollutant. The presence of organic pollutants above the permissible levels in soil and water bodies induces severe problems for human health as it enters the food chain and impacts the country's economy. Therefore, to monitor organic pollutants, the development of new strategies and sensing methods is highly desirable; it would greatly benefit to human health and the environment.

Chemical sensors are advantageous as compared to sophisticated analytical instruments such as atomic absorption spectroscopy (AAS), atomic emission spectroscopy (AES), mass spectroscopy (ms), and chromatography methods. Because they are very cheap and no need for any specific lab space and trained persons to handle the instrument. Among chemical sensors, colorimetric sensing methods depend on the color change of a sensing probe upon interaction with a specific analyte, it can be used by common people, who have no prior knowledge of science. Moreover, compared to traditional organic dye-based colorimetric sensing systems, nanoparticle-based sensors have their advantages. Here in this chapter, we present an overview of the application of silver (Ag), gold

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00002-X

CHAPTER

FLUORESCENT METAL NANOPARTICLES FOR ASSAYING OF TOXIC CHEMICAL SPECIES

3

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3.1 INTRODUCTION

Toxic chemical species (TCS) are ubiquitous, predominantly released into the environment by various anthropogenic activities and natural sources, and pose a serious threat to human health and the environment worldwide [1,2]. These released TCS are nondegradable and persistent and can lead to accumulation in the food chain. Some of the TCSs are easily transported and persistent in the environment and are readily absorbed by the gastrointestinal tract and tissue and target the central nervous system that leads to death [3]. Currently, the most important concerns for everyone about water, food, and environmental safety issues are caused by the consumption of contaminated water, food, and the environment. Therefore it is very important to monitor the toxic species in the environment, drinking water, food, and even biological fluids. Further, the selective detection and quantification of these chemicals are extremely essential. Therefore materials capable of high sensitivity and selectivity are significantly important.

In this regard, fluorescence-based detection methods have received significant attention in a wide range of research areas due to their high sensitivity, low detection limits, indestructibility, and low cost [4–6]. Fluorescent metal nanoparticles (FMNPs), quantum dots (QDs), and upconversion nanoparticles (UCNPs) have emerged as promising fluorescent nanomaterials due to their potential application in various fields such as optoelectronic devices, sensors, and biomedicine. The unique features of fluorescent nanomaterials include good photostability, high photoluminescence, and biocompatibility [7,8]. The fluorescence emission properties of these can be tuned by controlling their particle size and composition. Further, the nature of fluorescent nanoparticles depends on the functionalization of the surface with different biomolecules and organic ligands to make them water-soluble and increase their biocompatibility. These surface ligands can alter the selectivity and sensitivity of these materials for various analytes. Thus fluorescent nanomaterials have emerged as promising optical materials due to their exceptional characteristics such as physicochemical and optical properties, composition, high tunable shape, size, and surface functionalization [9,10]. Moreover, these FNMs can be decorated with multiple functional groups that target specific chemical species owing to selective interaction into a measurable optical signal. All these characteristic properties of nanomaterials have greatly enhanced the knowledge and extended the horizon of material in various potential applications such as the detection of

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00004-3

CHAPTER

4 FLUORESCENT CARBON NANOPARTICLES FOR CHEMICAL SPECIES IDENTIFICATION

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4.1 INTRODUCTION

Environmental contamination is a major subject that has drawn global caution for decades. The observation and inspection of various environmental contaminants are ever time of primary importance to nature and human beings. To this intention, the researchers have long been committed to exploring sensitive and efficient analytical approaches for the accurate sensing of emerging contaminants in environmental specimens. Some transition elements, such as Cu, Fe, or Zn, are requisite for human metabolism and are rarely harmful to human health when at their optimal level [1,2]. On the other hand, other metals, such as Hg^{2+}, Pb^{2+}, As^{3+}, Cd^{2+}, and so on, are dangerous to humans, even at trace levels. The mentioned toxic elements are readily preconcentrated in the body and arranged with biological fragments, such as nucleic acids and enzymes, inhibiting normal biological reactions and functions [3–5]. Conventional methods for the sensing of metal ions in water are tedious and time-consuming. Thus, there exists a need to develop novel sensing technologies for more sensitive and rapid detection. While optical-based assays using fluorescent nanomaterials have been reported, they are typically dependent on the changes to the signal intensity, which brings about several disadvantages for potential environmental monitoring. Moreover, most of these sensing systems only demonstrate selectivity and sensitivity to one cation.

Nanoscience is an emerging field of science that is anticipated to benefit outstandingly from environmental monitoring. With the development of nanotechnology, various nanostructured materials have been examined in-depth for their potential of providing new resolutions or improving the current resolutions to the plenty of urgent environmental issues from water pollution to air pollution [6,7]. Nanostructured architectures such as carbon-based nanomaterials, metallic nanoparticles, and metal-organic frameworks have versatile implementations in contaminant sensing [2,8–10]. In the past few years, scientists have witnessed a surging interest in the fabrication of carbon dot (CD)-based fluorescent probes. Fluorescence methods have the advantages of high sensitivity, high accuracy, and relative simplicity. However, macroscopic or conventional carbon architecture lacks the appropriate bandgap, making it difficult to act as a potent fluorescent material. But CDs (besides, called carbon quantum dots) (CDs or CQDs), as an emerging star in carbon-based architectures are generally smaller than 10 nm in size and are described as zero-dimensional and spherical-like carbon architectures. In addition, the fluorescence (FL) quantum yield (QY) of CDs can be increased

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00006-7

CHAPTER

GRAPHENE QUANTUM DOTS IN ENVIRONMENTAL POLLUTION CONTROL

5

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5.1 INTRODUCTION

Graphene quantum dots (GQDs), a novel type of zero-dimensional (0D) nanomaterial, are derivatives of graphene/graphite and other graphitic materials having layered structures and varying in size from 1 to 100 nm [1,2]. As a result of the predominance of the prominent quantum confinement, edge impacts, and abundant surface functionality, GQDs exhibit excellent optical and electrical characteristics [3]. In addition to the low toxicity and high water solubility, GQDs possess other noteworthy advantages such as low cost, good biocompatibility, high surface area, chemically stable, robust, inert, tunable bandgap, and the excellent photoluminescence (PL) property [4–8]. Due to the high electron movement with a high-speed reaction, GQDs are considered a good sensing material for sensing applications. Moreover, GQDs display prominent peroxidase mimetic activity originating from their aromatic structure [9]. These unique properties make GQDs a promising material in catalysis, sensors, bioimaging, medical optoelectronics, diagnosis, and energy storage devices [10–12].

In recent years, environmental pollution caused by the contamination of industrial and agricultural sewage and domestic wastage has become the main focus of the world's attention. In particular, contamination of harmful chemicals in the environment may cause serious issues to the environment as well as the health of living beings and also hinders the sustainable development of both society and the economy. Different nonbiological hazardous substances including inorganic heavy metal ions are found in urban areas which are mainly released by different human activities [13]. In addition to these contaminants, the presence of microorganisms in tap and drinking water also poses serious threats to humans and the entire water ecosystem [14]. In recent years, the utilization of different nanomaterials has been studied in depth for their potential in many applications related to environmental problems from water pollution to air pollution. The most promising solution for these problems is nanomaterial-based catalysis, and it has attracted much attention since

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00007-9

CHAPTER

TWO-DIMENSIONAL CARBON NANOMATERIALS IN ENVIRONMENTAL ANALYSIS

6

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6.1 INTRODUCTION

An increase in the population of the world, combined with the rapid growth of factories and industries, has resulted in an energy crisis and pollution. Pollution has emerged as the most pressing environmental issue due to growing urbanization and an increasing population. Furthermore, technological innovation has resulted in the emergence of new contaminants, which are increasing at an alarming rate and are beyond the ability of the environment to self-remediate. Environmental pollution is regarded as a worldwide public concern that poses a major threat to human health and the natural environment. Improving the quality of soil, water, and air is a challenge. There is an urgent need to develop methods that can quickly and easily reduce pollution levels to risk-free levels [1,2].

Nanotechnology is one of the most promising research fields at present since it studies and exploits the novel properties of materials at the nanoscale (10^{-9} m) [3,4]. Nanomaterials, due to their small size and larger surface area to volume ratio than their bulk counterparts, exhibit several unique properties that have drawn interest in the scientific community in recent decades. Nanoparticles have a large surface area and high surface energy, allowing them to absorb significant amounts of pollutants or catalyze reactions at a much faster rate, lowering energy consumption during degradation or preventing contaminants from being released [5]. Carbon nanomaterials are among the most often used tools in this field due to their unique features, including attractive optical properties, high conductivity, high mechanical strength, chemical versatility, etc. [6]. Carbon nanomaterials are classified into one of three classes based on the dimensionality of their structure: zero-dimensional (0D), one-dimensional (1D), or two-dimensional materials (2D) (Fig. 6.1).

0D nanomaterials are usually spherical or quasi-spherical nanoparticles having a diameter of less than 100 nm, compared with bulk high-dimensional nanomaterials [7]. Fullerenes, carbon dots, and nanodiamonds are the most famous 0D carbon nanomaterials with unique electrical and optical properties, including low cost, low toxicity, good solubility, good photostability, and chemical inertness [8–10]. The 1D materials have two dimensions within the nanoscale, that is, materials whose only one dimension is above 100 nm. Carbon nanotubes, carbon nanofibers, and carbon nanohorns are the most well-known 1D carbon nanomaterials with interesting properties [11]. The 1D carbon nanomaterials have unique features such as a high surface-to-volume ratio, high electrocatalytic properties, high thermal capacity, and excellent electrochemical properties. The 2D carbon

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00008-0

CHAPTER

7 NANOMATERIALS-BASED ELECTROANALYTICAL TECHNIQUES FOR THE IDENTIFICATION OF POLLUTANTS

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7.1 INTRODUCTION

Industrialization and unplanned urbanization helped mankind in attaining comfort, as well as advancement, and as a bonus, it also yielded unwanted and lethal environmental pollution. Since the last two decades, the degree of increase in environmental pollution is immeasurable. The consequences of environmental pollution like global warming, climate change, and serious health issues to human and animal populations are overwhelming. In order to checkmate the degree of environmental pollution, various environmental pollution agencies started working on it by performing various possible awareness programs for humans in order to slow down the rate of environmental pollution. The industries let down their effluents enriched with various pollutants based on the type of industrial operations into the open environment. The pollutants-rich effluents reach water streams, thereby entering into soil followed by food crops and finally into the food chain. The common pollutants present in the polluted environmental matrix (water, soil sediments, and air) are classified into organic, inorganic, and nuclear waste. The organic pollutants include dyes, drugs, antibiotics, pesticides, insecticides, and aromatic nitro compounds. The inorganic pollutants include the heavy metal ions (Pb^{2+}, Hg^{2+}, Cd^{2+}, Cr^{6+}, As^{3+}, and As^{5+}) and anions like chloride, bromide, nitrite, nitrate, sulfate, sulfite, and sulfides. The nuclear waste includes the radioactive heavy metal uranium along with other trace substances. The above-mentioned pollutant levels should be minimum in water, soil, or air, i.e., below microgram levels, in order to have a safer environment. However, day by day, the levels of pollutants increased like anything in several orders, as it was proved by climate change and global warming that occurred in recent years. In order to protect our environment from pollution, government agencies of different nations set the permissible limits or threshold limits of various pollutants in water and air medium. The permissible limits of various pollutants in drinking water are given in Table 7.1. The preliminary step, in combating environmental pollution, is to monitor the level of pollutants in the matrix. This needs a very accurate technique. The electroanalytical techniques are proven to be better compared to all other instrumental-based techniques because of their simple instrumentation, cost-effectiveness, miniaturization, and field portability and also can be used in digital online monitoring systems. The electroanalytical

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00009-2

CHAPTER

8 NANOMATERIALS IN ASSAYING OF POLLUTANTS BY SURFACE-ENHANCED RAMAN SPECTROSCOPY

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8.1 INTRODUCTION

Raman spectroscopy is an emerging spectroscopic analytical technique employed from the past few decades to obtain structural information of the molecules. It identifies the vibrational modes of molecules and records the inelastic scattering of incident light by the molecules present in the medium. "The Raman effect" which is the root of "Raman spectroscopy" has a series of research works in its history. Sir Raman's quest about the deep blue color of the sea on his way to Europe was "the beginning" of the discovery of a fundamental yet crucial phenomenon. Sir Raman explained the quantized nature of light involved in the scattering phenomenon in a monograph "Molecular Diffraction of Light" in 1922 [1]. In April 1923, K. R. Ramanathan noticed the absolute conversion of violet incident wavelengths of sunlight into a green beam as a scattered ray [2]. In 1925, a similar observation was made by another student, Krishnan, while studying molecular scattering in 65 liquids [3]. In 1928 S. Venkateswaran observed that the scattered light was green, unlike the expected blue color which was true for other samples. Sir Raman along with his students designed several experiments to analyze the unusual scattering in liquids and vapors. He observed a weak prismatic pattern when the complementary filter was mounted in between the source and observer for a series of around 80 organic and inorganic liquids which implied that the observed phenomenon is not fluorescence and is ubiquitous. Sir Raman conveyed to Krishnan that their observations have relevance to the Kramers−Heisenberg formulation. On March 31, 1928, they published their findings to *Nature* in an article "A New Type of Secondary Radiation" [4]. Students Krishnan and Venkateswaran witnessed a first-line spectrum of modified radiation on February 28, 1928, and Sir Raman published the results in *Nature* on March 8, 1928 [5].

Sir Raman's discovery was signified by German physicist and mathematician, Max Born, in a note titled "On the Theory of Raman Effect" published in *Naturwissenschaften* in August 1928 [6] and later reviewed in an article "The Raman Effect, a New Radiation Effect Discovered by C. V. Raman" [7]. In this article, Sir Raman's discovery was christened as "Raman effect" and the

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00010-9

CHAPTER

9 FUNCTIONAL NANOMATERIALS FOR THE SENSING OF VOLATILE ORGANIC COMPOUNDS

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9.1 INTRODUCTION

As technology advances and people's living conditions improve around the world, we now live in an environment where we are exposed to harmful gases and chemicals. Almost every aspect of daily living, such as cooking, using automobiles, pesticides, and even simple breathing, releases organic molecules into the environment. These volatile and nonvolatile compounds such as carbonyls, alkanes, alkenes, aromatics, and either have lowered the air quality. As a result of such circumstances, the human being is exposed to a large number of risk factors [1,2].

Volatile organic compounds (VOCs) are organic compounds that are liquid or solid under normal temperature and pressure conditions but quickly evaporate at room temperature. These include acetone ($(CH_3)_2CO$), ethanol (C_2H_5OH), formaldehyde (HCHO), carbon disulfide (CS_2), and many more. VOCs are emitted by a variety of sources, including vent gases, industrial waste water, petrochemical processes, and paints. The concentration of VOCs is significantly higher in indoor spaces including homes and workplaces, offices, schools, and commercial buildings due to the usage of various consumers and personal care products such as perfumes and sprays. Exposure to these volatile compounds is considered highly hazardous and carcinogenic by nature and may pose both short and long-term risk to human as well the as ecosystem, even at a lower concentration of sub-ppb level. Various health problems related to kidney, liver, and stomach, neurological system, respiratory system, cardiovascular system, and other disorders such as cough, eye irritation, and headache are caused among humans due to the exposure to these VOCs. As a result, it is highly essential to measure and monitor the presence of these toxic compounds into the atmosphere.

In addition to various safety-related applications, it is critical to design equipment that can detect VOCs for monitoring poisonous, explosive gases, and indoor pollutants. One of the most essential requirements is progress in the breath analysis approach for illness identification in the field of medical diagnostics. Exhaled gases are made up of a variety of gases, some of which are used as exhale breath markers (EBMs), such as ammonia, acetone, nitrogen monoxide, isoprene, and others, and any changes in their concentration can cause a variety of diseases and treatment efficacy. As a result, they can be used as a noninvasive health monitoring tool. Acetone can be used to properly evaluate the body's fat-burning rate, isoprene can be used to detect high blood

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00011-0

CHAPTER

NANOMATERIALS IN SAMPLE PREPARATION

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10.1 INTRODUCTION

The analytical process usually contains important steps, including sampling, sample preparation, isolation of the targeted analyte, identification, quantification, and data interpretation. Sample preparation is an important step during the qualitative and quantitative analysis. Sample preparation is a term that refers to all of the things that happen to samples before the instrumental analysis. The main objective of sample preparation is the selective isolation of the targeted analyte from the complex matrix and the pretreatment of the targeted analyte before analysis. The sample preparation is a crucial step when the sample contains complex coexistent materials, or direct analysis is not practically possible; it may be due to the low selectivity and sensitivity, and a trace amount of analyte may be present in the complex sample. Several potentially coexistent materials and trace levels of analyte make an earlier extraction process, which generally contains isolation and pretreatment of targeted analytes. The key objects in this research are the advancement in the extraction methods and the enhancement of present techniques employing new adsorbent materials. The extraction and pre-concentration of analytes from the matrix were performed using a number of traditional methods, including solid-phase extraction (SPE) [1−3], liquid−liquid extraction (LLE) [4−7], and solvent extraction [8,9]. Dispersive liquid−liquid microextraction [10−12], hollow fiber liquid-phase microextraction [13,14], single-drop liquid microextraction [15,16], in-syringe dispersive liquid−liquid microextraction [17], headspace solid-phase microextraction (HS-SPME) [15,16], and solid-phase microextraction (SPME) [18,19] are examples of microextraction methods. The SPE is a sample preparation and pre-concentration method that differs from LLE because it requires less solvent. For the last decades, it has been used to pre-concentrate or clean target analytes from a complex matrix. The performance and evaluation of sample preparation methods traditionally focus on complete extraction and recoveries. SPE and LLE have been utilized to extract and pre-concentrate analytes [20]. The comprehensive advancement of an analytical method based on the adsorptive extraction process includes several intermediary processes between the collection of specimens and the final report of results, such as sample preparation, adsorption, desorption, and analysis. These methods begin with the obtained biological and environmental samples such as food,

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00012-2

CHAPTER

NANOMATERIALS FOR REMOVAL OF TOXIC CHEMICAL SPECIES 11

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11.1 INTRODUCTION

Environmental pollution is a big problem in the modern world. Due to industrialization and development, a large quantity of toxic pollutants are released into the environment, and they cause toxic effects on the environment and harm the ecosystem. Toxic pollutants are a serious problem in the modern world [1]. There are a number of sources that cause environmental pollution, such as industrialization, growth in population, urbanization, mining, and exploration, which are the leading causes of environmental contamination in both developing and developed countries [2]. Industries are the key source of toxic pollutants because untreated industrial waste is dumped into the environment, and several pollutants may be released into the ecosystem, such as pesticides, herbicides, chlorinated compounds, hydrocarbons, and heavy metals. They may threaten the ecosystem [3]. Pesticides are widely used in agriculture, and animal farming contributes to soil contamination, posing considerable health risks to humans. Chemical pollution is not just a problem in developing countries but also in developed countries [4]. The discharge of toxic pollutants into the ecosystem causes bioaugmentation and bioaccumulation in humans, resulting in major health issues such as cancer, skin problems, liver and kidney damage, muscle weakness, headaches, dysentery, stomach problems, and brain diseases [5]. Industrial effluents, farm wastes, chemical substances, biological agents, and anthropogenic contaminants are the main types of pollutants [6]. The current problem is to keep these harmful compounds from surpassing their limits. Several traditional methods have been reported to minimize the pollutants from the ecosystem such as adsorption [7], chemical precipitation [8], membrane filtration [9], ion exchange [10], coagulation and flocculation [11], reverse osmosis, irradiation [12], flotation and extraction [13], biosorption processes [14], and electrochemical treatment techniques [15]. These reported methods have some limitations, such as being time-consuming, pH-dependent, needing extra instrumental protocols, and needing a large amount of volatile organic liquids. The researcher focused on improving the adsorption process to eliminate toxic chemicals. The adsorption method is easy, simple, and economically friendly because it depends on the quality of the adsorbent material. Several adsorbent materials have been reported to eliminate the toxins from the ecosystem such as clay minerals [16], activated carbons [17], chelating compounds [18], polymers [19–24], and chitosan/natural zeolites [25].

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00013-4

CHAPTER

NANOMATERIALS FOR TRACING HEAVY METAL SPECIES FROM WATER SYSTEMS

12

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12.1 INTRODUCTION

Water is known as an essential substance required by living organisms to maintain their survivability. The availability of clean water is important for drinking, bathing, agriculture, and many other irrigating purposes that ensure a healthy quality of life. However, due to the increasing global developments, the demand for clean water by the population increases annually. This worsens when potential water sources have been compromised with various pollutions [1]. Among these contaminants found in water sources include the presence of heavy metals [2,3]. Although several heavy metals are essential for human health, an excess amount of these metals can have an undesirable effect on humans [4]. Through past studies, the reports have shown that heavy metals in drinking water sources, such as surface water, groundwater, and seawater, were focused extensively on a few issues including [5–7]:

1. Types and quantities of heavy metals.
2. Factors that affect metal concentration sources.
3. Effect on human exposure.
4. Health risks toward human exposure.
5. Remediation process in treating heavy metal contaminants.

Heavy metals can be considered metallic elements in the periodic table except for those in groups 1 and 2 [8]. These metals are the elements possessing a density values of more than 4 ± 1 g/cm^3 or have density five times higher than water [9]. The issue of heavy metal contamination is a growing concern, particularly in developing regions. Inadequate water and wastewater treatment efforts, coupled with increased industrial activity, have led to increased heavy metal contamination in rivers, lakes, and other water sources in developing countries. These contaminants can absorb in the sediment (an important component in the riverine ecosystems), which serves as both a sink and a source of heavy metals [10,11]. Most heavy metals can quickly deposit into the sediment after entering rivers, making them more concentrated in the sediment than in the water body of riverine

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00014-6

CHAPTER

13 NANOMATERIALS AS PROMISING ADSORBENTS FOR THE REMOVAL OF RADIOACTIVE ELEMENTS

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13.1 INTRODUCTION

With the fast growth of the economy and the rapidly growing population, the world's energy claims continue to grow. The extended utilization of fossil energy has caused severe threats to the environment, and on the other side, traditional fossil fuels are likewise confronting the shortage issues [1,2]. Nuclear power plant plays an important role in overcoming energy shortage and reducing environmental problems such as climate change. The extensive usage of nuclear energy and additional application of nuclear power, namely, mining industry, weapon testing, water pollution, and medical research by various types of radioisotopes (such as ^{237}U, ^{137}Cs, ^{131}I, ^{129}I, ^{60}Co, ^{99}Mo, ^{241}Am) lasts an incredible concern around the world. Furthermore, the nuclear accident, such as Fukushima disaster in 2011, with the consequent series of difficulties, has increased genuine concern on human beings of present and people of future [3]. Among these radioactive elements, uranium (U(VI)) is a critical actinide radioactive element, which is mostly used in nuclear power plant. U(VI) and its isotopes produced a high level of nuclear waste, and it released in aquatic system during the nuclear process [4]. By WHO, the limit of U(VI) in portable water is 30 ppb. Above this limit causes numerous health problems in the living organisms. In the aqueous bodies, U(VI) mostly exists in uranyl ions, which are extremely toxic and portable. Unnecessary exposure to U (VI) may damage DNA and lead to serious health complications such as lung cancer and liver disease [5]. Hence, the removal of these ions from the water bodies is essential for the human health and the environment. Thorium generally exists in the tetravalent form Th(IV), which is generated by the α-decay of U(VI). Th(IV) is used as nuclear fuel and it is not self-fissile. Thus, after absorption of neutrons, it generated atom of U-233, which is fissile fuel material. Moreover, Th(IV) reactors produce hazardous waste when it mixed with ground water and lived long as radioactive products, which poses a human life and the aquatic system [6,7]. Among the various radioactive elements, radioactive iodine mostly ^{129}I and ^{131}I are the toxic species [8]. This radioactive iodine has been mostly used in the medical science foe the diagnosis and treatment of thyroid cancer [9]. The medical use of ^{129}I with 15.7×10^6 years of half-life and ^{131}I with 8 days half-life is observed

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00015-8

CHAPTER

NANOSTRUCTURE MEMBRANES FOR THE REMOVAL OF TOXIC CHEMICAL SPECIES

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14.1 INTRODUCTION

Major water contamination from ever-increasing industrial activity is a severe challenge to human welfare and the whole environment, resulting in a renewed focus on creating highly effective and reliable water treatment (WT) technology. Toxic wastewater (WW) discharged into the atmosphere can include a range of organic and inorganic contaminants [1,2]. Heavy metals (HMs) (such as mercury, nickel, manganese, cadmium, lead, zinc, chromium, copper, arsenic, and iron) are the most toxic pollutants present in WW, and their generation is accelerating, leading to fast industrialization activities [3,4]. A few of the leading causes of groundwater pollution by HMs include the coal industry, electroplating, oil refining, mineral smelting, mining, batteries industries, electronics manufacturing, fertilizer and pesticide industries, nuclear energy generation, chemical processing, and reprocessing and reuse of solid waste [3,5].

HMs can have severely adverse effects on human health and the whole ecosystem due to their poisonous and cancerous nature [6]. Because of the harmful effects of HMs, academic and commercial researchers have made efforts to improve the productive and long-term process to remove toxic HMs from urban and industrial wastewater, potable water, and other freshwater bodies and seawater [3,6]. Various methods that have been used to separate or recover HMs from wastewater are adsorption [7], ion exchange [8], membrane-based techniques [9], solvent extraction [10], precipitation [11], coagulation and flocculation [5], flotation [9], and bioremediation [12]. Fig. 14.1 indicates the distribution of the total publications regarding existing technologies applied to remove toxic metals from WW for the last five years (2018–22). From Fig. 14.1, we can see that the HM separation from WW has received a lot of attention, using various approaches.

The key objectives of wastewater treatment (WWT) are removing hazardous contaminants and bioremediation for sustainable disposal and/or reuse. These eliminated and absorbed pollutants may be recovered and frequently termed value-added products (VAPs) [13]. These kinds of VAPs may be recycled and reused from WW and employed as raw materials for various manufacturing processes or used for a variety of uses in the condition in which they have been recovered [9,13].

This book chapter presents a brief idea about HM removal and recovery from WW. In brief, the chapter describes the various sources of HMs in WW and their toxic effects on the human,

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00016-X

CHAPTER

NANOSTRUCTURE MATERIALS FOR WASTEWATER TREATMENT 15

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15.1 INTRODUCTION

Water is one of the world's most precious natural resources, necessary for the survival of all living things as well as human life. Nowadays, rapid world population growth, thriving industrialization, civilization, urbanization, different agricultural activities, and also environmental, global, and geological changes are giving rise to continual contamination of water resources, which is an important issue of worldwide concern [1]. The main sources of wastewater are industrial waste, commercial waste, hospital discharge, domestic wastewater, and agricultural wastewater [1].

Wastewater is a complicated matrix constituting 99.9% water, and the remaining 0.1% contains suspended solids, inorganic solids, dissolved biodegradable organics, organic compounds like body waste, various microorganisms, micropollutants, heavy metals, nutrients, particulate stuff, etc. [1]. These pollutants are classified as inorganic, organic, gaseous, and biological. Inorganic contaminants contain harmful and toxic metals, for example, Mn, Fe, Cu, Zn, Co, Mo, Ni, Cd, Hg, etc., fertilizers, free and total chlorine, phosphorus, sulfate, nitrogen, and other industrial wastes. Organic contaminants include agricultural chemicals (organic herbicides, pesticides, insecticides, etc.), dyes, pharmaceuticals, polycyclic aromatic hydrocarbons, organic solvents, detergents, personal care products, phenolic compounds, oils, food processing wastes, plasticizers, greases, and other persistent organic pollutants. Also, wastewater includes high microorganism concentrations such as bacteria, protozoa, and viruses. Some of these pollutants are resistible to degradation with chemical, light, biological, thermal, and other degradative factors owing to their complex molecular structure. These properties make them very inconvenient to degrade, so they can be accumulated in the food chain and living tissues and ultimately affect humans and other living species [2,3]. When their concentration exceeds the permissible limit, these pollutants can cause serious health problems due to their carcinogenicity, mutagenicity, and teratogenicity properties. To decrease negative effects on nature, the emissions of toxic pollutants into water, soil, and air must be controlled and followed [4]. For this reason, the removal of pollutants from effluents before their discharge into the environment is one of the most important topics in terms of environmental protection.

Among these pollutants, one of the significant issues of the industry is the production of a huge quantity of colored waste from its process in plastic, textile, leather, rubber, paper, printing,

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00017-1

CHAPTER

APPLICATIONS OF BIOMATERIALS IN ENVIRONMENTAL ANALYSIS 16

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16.1 INTRODUCTION

Changes in lifestyle, increasing use of technology, industrialization, excessive use of resources, and the lack of waste management create many problems. The world is facing the biggest challenges in meeting the rising requirements for a clean environment. According to a WHO report, more than 1 billion people do not have access to safe and clean water and nearly 1.6 million people die every year because of living or non-living water contaminants [1]. It is very necessary to maintain human health and sustainable development of society and economy. Anthropogenic activities have an adverse effect on the environment by polluting drinking water, clean air, and fertile soil [2]. Even trace amount of pollutants enter the human body and creates harmful condition. Detection of such trace pollutants become an eagerly solved problem. Nanotechnology provides solutions to detect such trace quantities of biotic or abiotic molecules simply by the application of nanomaterials. Due to its role, nanotechnology is considered an applied technology in various areas such as life sciences, engineering, medicine, and environment Bayda et al. [3]. Nanotechnology can synthesize nanomaterials and construct devices by controlling their unique properties. It offers many advantages to improving existing environmental technologies and creates new technologies, which are better than the current technologies. Due to their smaller size and larger surface area, nanoparticles show higher reactivity [4].

Heavy metals are naturally occurring elements having a density greater than 5 g/cm^3 and atomic weights in the range of 63.5−200.6 g/mol [5]. Heavy metal pollution becomes an important component of manmade activities such as metal mining, steelmaking, metal-dependent industries, metal leaching from dumped landfills, excretion, domesticated poultry, fertilizers, and automobile industries. In addition to anthropogenic activities, natural resources such as weathering of metal-bearing rocks, forest fires, and volcanic eruptions also add heavy metals to the environment. Heavy metals such as mercury, chromium, lead, arsenic, cadmium, nickel, copper, and zinc are considered environmental pollutants. Ions of heavy metals are nonbiodegradable and can be accumulated in the food chain, which ultimately affects human beings [6]. Heavy metals can be absorbed via the gastrointestinal tract, inhalation of metal fumes, and skin exposure. They are transported in the blood through specific chaperons and in cells by selective and nonselective channels as they do not cross lipid membranes. Even for aquatic organisms, they are directly or indirectly affecting them.

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00018-3

CHAPTER

2D NANOMATERIALS FOR REMOVAL OF GAS MOLECULES 17

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17.1 INTRODUCTION

Nanomaterials, having exactly similar chemical structures, can be classified according to the dimensions that show quite different properties. Among zero, one, two, and three dimensions (0D, 1D, 2D, and 3D), limited attention has been paid to 2D nanomaterials by the researchers. Strong in-plane bonds and weak van der Waals (vdW) forces exist between the layers. After the extraction of 2D nanodimension graphene by the Geim Group from Manchester University, United Kingdom, in 2004, there was a great interest generated among the researchers on the study of 2D nanomaterials [1].

Fig. 17.1 depicts representative 2D nanomaterials such as graphene, hexagonal boron nitride (h-BN), transition metal dichalcogenides (TMDs), and metal organic frameworks (MOFs)

17.2 GENERAL PROPERTIES OF 2D NANOMATERIALS

2D nanomaterials, being the thinnest nanomaterial with a layered structure, have strong in-plane bonds and weak van der Waals forces. Having such unique structural features, they exhibit many satisfactory properties which facilitate their widespread use in the areas of electronics, catalysts, energy storage devices, sensors, and, of course, the composites, etc. Both graphene oxide (GO) and reduced graphene oxide (rGO) exhibit low adsorption capacity for gases such as CO_2, H_2 and

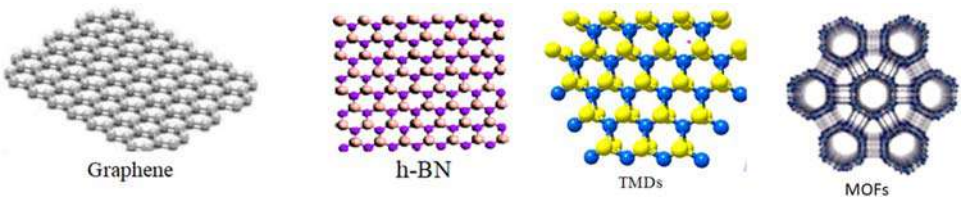

FIGURE 17.1

Representative pictures of 2D nanomaterials.

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00020-1

CHAPTER

18 NANOMATERIALS FOR HUMIDITY AND TEMPERATURE SENSING APPLICATIONS

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18.1 INTRODUCTION

Humidity and temperature sensor have received attention, which can be used in indoor or outdoor applications. Humidity measurement is important for the balance of the environment. It has received awareness due to these vapors are reactive dipolar molecules that can condense and evaporate even with slight changes in ambient temperature. Almost all environmental phenomena are controlled by humidity caused by electron-negativity differences of hydrogen and oxygen atoms [1]. Humidity control has been used in our daily life like the use of air conditioning in the living room and in the field of agriculture to store the seed, meteorology to monitor the environment industrial in chemical storage, electronic processing [2,3]. Temperature sensors define as a device that can detect and react to the changes of heat in the surroundings [4]. The fundamental concept comes out from the second law of thermodynamics in terms of the rate of change of energy with entropy. Generally, conventional contact thermometer (such as thermocouple) needs a direct heat transfer and thermal equilibrium between the measured object and the sensor [5]. These properties might cause a long time and change the actual temperature of sample during measurement, especially the size of the sample is small as compared to the sensor head.

Sensing materials are an important part that plays a vital role in detecting small changes that occur in humidity or temperature. Metal oxide [6,7], carbon-based materials [8,9] and polymers [1,10] are among the most widely used sensing materials as moisture sensors. As for temperature sensing, most of the materials used are carbon [11,12], fluorescent [13,14] and ceramic [15,16]. Each of these materials has its own characteristics according to the specific needs of the application.

In humidity detection, the sensing element reacts to different atmospheric humidity conditions, which it adsorbs or desorbs the water molecules. These small changes will be interpreted in physical properties especially in electrical properties. The units that are frequent in humidity measurement are relative humidity (RH), dew/frost point (D/F PT), and parts per million (PPM) [1].

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00021-3

CHAPTER

19 FUTURE TRENDS OF NANOMATERIALS IN ENVIRONMENTAL ANALYSIS

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19.1 INTRODUCTION

Environmental problems and controversies are becoming the main point of scientific and political concern due to the rapid increase in world population, widespread agricultural activities, urbanization, industrial activities, global climate change, and contamination of water, air, and soils [1]. The environmental contaminants are a great group of compounds that arose from industrial, domestic, agricultural, commercial, and hospital wastes involving pharmaceuticals, personal care products, dyes, heavy metals, free and total chlorine, sulfate, fertilizers, agrochemicals, phosphorus, polycyclic aromatic hydrocarbons, plasticizers, phenolic compounds, organic solvents, greases, detergents, oils, food processing wastes, several microorganisms, human and animal fecal waste, and other persistent contaminants [1].

Environmental contaminants display diverse negative health impacts such as infant mortality, perinatal disorders, respiratory disorders, malignancies, allergy, cardiovascular disorders, endothelial dysfunction, increase in oxidative stress, mental diseases, etc. Furthermore, many investigations have shown that exposure to environmental pollution has been connected to an incremented venture of mortality and morbidity from many organ disorders, diseases, cancers, and other chronic diseases [2]. Thus the development of accurate and reliable analytical methods for determining various pollutants is crucial for environmental security and public health.

Nanotechnology can be described as producing matter at the atomic and molecular levels to generate a novel structure, device, and system with excellent optical, electronic, magnetic, mechanical, and conductive properties [3]. Nowadays, nanomaterials have received global attention because of their unique size, shape, and special chemical characteristics. Nanoparticles in a wide range of chemical structures are routinely designed, synthesized, and manufactured in various areas such as chemical synthesis and purification, energy harvesting and storage, electronics and optics, medical therapeutics and diagnostics, textiles, construction, etc. [4]. The implementation of nanotechnology holds great promise to improve water, air, and soil quality. Many types of nanomaterials, including graphene, graphene oxide, carbon nanotubes, magnetic nanoparticles, metal and metal oxide nanoparticles, and quantum dots, have been employed in sample preparation, electrochemical sensing, colorimetric detection, fluorescent detection, mass spectrometry, and surface-enhanced Raman scattering for environmental analysis [5].

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00022-5

CHAPTER

NANOMATERIALS: CHALLENGES AND ENVIRONMENTAL TOXICITY 20

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20.1 INTRODUCTION

Nanotechnology continues to offer new nanoscale material with unique physicochemical properties, leading to great anticipation over the potential uses of nanomaterials (NMs) to create significant advances in the chemical, electronics, construction, cosmetics, medicine, and other industries [1]. As nanotechnology and nanoscience have become one of the fastest-growing research and technology areas, attracting an international gold rush, the exposed population to nanomaterials continues to increase [2]. The nanotechnology products database includes 9422 nanoenabled products in 2021, and the top five categories were "electronics," "medicine," "construction," "cosmetics," and "textiles." However, with the growth of the manufactured nanomaterials industry less than a few decades ago, concern has been raised over their possible discharge into the aquatic and terrestrial environments. Most importantly, their ever-increasing demands and consumption in our day-to-day activity could lead to unique impacts on the biological systems because of their unique physicochemical properties and thus create concerns over potential environmental safety. However, because of their complexities, NMs have not normally been considered in conventional safety assessments of chemicals and therefore generated uncertainty in the reliability of standard tests of safety. In particular, NMs can change their size, morphologies, chemical form, and dissolution characteristics once discharged into the aquatic and terrestrial environments, and thus NMs require different regulations from that equivalent micrometer-sized materials [3]. The fate of NMs through a safety experiment in research laboratories under controlled reaction conditions can differ significantly as compared to the real environment, largely because of their characteristic changes in properties and bioavailability after the interaction with natural nanoparticles and colloidal materials available in the environment. Thus generalizations of hazard based on any one aspect across NMs is not possible, while risk assessment for new and complex NMs also remains difficult because of the lack of information on specific molecular interactions of NMs and organisms. In the past few years, many researchers focused their attention on assessing the hazard of NMs [4–6], and thus substantial advancements have been made in how we envisage about NMs and their interactions with the environment and organisms. The NMs Environmental Health and Safety (nanoEHS) [7,8] is an important concern for their acceptance, development, and approval into the market. However,

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00023-7

CHAPTER

NANOSTRUCTURED SENSORS FOR DETECTION OF EMERGING ORGANIC POLLUTANTS

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21.1 INTRODUCTION

"Emerging pollutant" is a term used to refer to substances released in the environment, which can be synthetic or naturally obtained, and are characterized to be not included in conventional regulations due to multiple reasons. Typically, the low concentrations, novelty in the environment, or the scarcity of knowledge around them are arguments used in order to include the concept of emerging pollution in many studies. However, at present, the recognition of the occurrence of these substances has permitted the advance in regulations, politics, and laws around them [1–4]. Emerging pollutants can be identified as inorganic and organic compounds obtained in typical processes from pharmaceuticals and personal care products industries, but also, these have been recognized in a much broader industrial spectrum, which includes the manufacture or use of substances such as preservatives, nanomaterials, metals for use in electronic devices, and flame retardants, among others [1,5–8].

The causes of this denomination within what is conventionally established as a contaminant and an emerging pollutant can be many. However, from an analytical chemistry perspective, the two main reasons are: (1) the improvement in the sensitivity of analytical technologies applied to environmental monitoring, and (2) a greater awareness of the risks and consequently greater requirements in the control and monitoring of the composition of systems (i.e., water, air, and soil) and mass consumption products (e.g., food, personal care products) [9–12]. With this last point, it was widely accepted by society in general that the environment can be visualized as an "infinite" reservoir, meaning "infinite," that its capacity to absorb all wastes from cities was very great with respect to the number of substances released in relatively small amounts. From this point of view, for example, discharges of wastewater from a hospital are considered negligible compared to discharges from the entire city, and the same logic was applied to animal production farms, metal–mechanic industries, and beauty centers, among others. However, under this approach it was not taken into account that the prevalence of some substances, their high bioactivity, their chemo- and biotransformation, and their continuous discharges can mean a risk to health and the environment in the long term. Thus many well-known substances have been identified in quantities and places where initially they were not expected, and

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00024-9

CHAPTER

NANO-ZEROVALENT IRON FOR WATER AND WASTEWATER TREATMENT

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22.1 INTRODUCTION

Rapid industrialization and urbanization have increased the discharge of waste containing different types of organic and inorganic contaminants into water bodies. Some of these pollutants are detrimental to human health even at small concentrations, and some of them are persistent in the environment. It is therefore important to reduce or remove these pollutants from industrial and other waste streams before discharging them into water bodies. A large number of different physicochemical and biological techniques such as adsorption, ion exchange, precipitation, oxidation−reduction process, and membrane processes are commonly used for reducing the concentrations of different classes of pollutants [1,2].

Nanomaterials have shown great potential for the treatment of water/wastewater because they possess various physical and chemical properties such as faster kinetics, excellent adsorption capacity, and high photocatalytic activity. Therefore, nanomaterials are the best candidates for environmental remediation purposes. Nanostructured adsorbents are used to remove pollutants from water/wastewater as they have higher efficiency and a faster reaction rate. Nanofiltration and green nanotechnology are other techniques employed for environmental remediation purposes [3]. Heavy metals can be removed effectively using nanoadsorbents such as carbon nanotubes (CNTs), TiO_2, ZnO, MgO, and Fe_3O_4. Nanocatalysts such as silver (Ag), Fe_3O_4, and TiO_2 have also shown excellent removal efficiency against different toxic pollutants. Nanomembranes such as multiwalled CNTs and sodium titanate nanobelt (Na-TNB) have been highly effective in reducing foulants, heavy metals, and dyes from wastewater [4].

In the last few decades, the application of nanotechnology in the treatment of different waste streams has increased, and nanoparticles have been widely investigated for the treatment of a variety of organic and inorganic pollutants in water/wastewater. These particles, because of their small size and high reactivity, have shown high efficacy in eliminating different pollutants from water/wastewater. Among the different classes of nanoparticles, nanoscale zerovalent iron (nZVI) is one of the most commonly investigated materials. Iron is one of the most widely distributed and abundant elements in the earth's crust. In the last two decades, a great deal of research has been conducted on engineered nZVI for environmental remediation purposes. Due to its high reductive capacity, non-hazardous and environmentally benign nature, and relatively low cost, it has shown good potential for the removal of different classes of contaminants from groundwater and industrial effluents [5].

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00025-0

CHAPTER

23 CARBON DOTS ASSEMBLY ON METAL NANOSTRUCTURES FOR SENSING APPLICATIONS IN ENVIRONMENTAL ANALYSIS

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23.1 INTRODUCTION

Sensing is the technique where biomolecules, viruses, and bacteria are detected. The world is currently fighting with a deadly pandemic, and the detection of SARS-CoV-2 virus is impossible without the sensing technology. The SARS-CoV-2 is detected in minutes making easy the livelihood of human being. Like corona virus only, the insulin in human body, blood tests, urine tests, antimicrobial tests, some cancerous cells, and pregnancy, these all are done by sensing. Metal nanomaterials (NMs) are famous because of their physicochemical characteristics. The benefits of inorganic nanomaterials are simply produced, the plausibility of diverse surface modification cations, catalysis of chemical reactions, accelerating the transfer of electron, bio-availability/compatibility, and improved immobilization of enzyme [1]. Gold, platinum, silver, palladium, TiO_2, iron oxide, zeolites, aluminosilicates, doped inorganic nanomaterials, nanowires, nanorods, quantum dots, transition metal nanoparticles, CNTs, GQDs, carbon dots, etc. are vastly used for sensing application [2–4] (Fig. 23.1).

Carbon dots falls under the class of zero-dimensional carbon material with a diameter less than 10 nm. Carbon dots. Carbon dot generally composed of SP^3 and SP^2 hybridized carbon cores of amorphous carbon or lattice of graphite. These were first found during electrophoresis of single walled carbon nanotubes back in 2004. Carbon molecules are considered as having very low solubility that is why the carbon dots came into consideration because of rich surface functional groups (amine, hydroxyl, and carbonyl groups), which gives rise to tremendous water solubility and their favorable luminescent properties, very low toxicity, high chemical stability, and easy surface functionalization [4,5]. Carbon dots are classified in two specific groups – graphene quantum dots (GQDs) and carbon nanodots (CDs). Graphene quantum dots are small particles of graphene with hexagonal lamellar rings, which are rich in oxygen containing functional groups at the edge, and this results in the quantum property and edge effects resulting in exceptional photoluminescence functionality. On the other hand, the amorphous carbon (CDs) is synthesized by partly

Nanomaterials in Environmental Analysis. DOI: https://doi.org/10.1016/B978-0-12-820643-0.00026-2

Nanomaterials in Environmental Analysis

Edited by **Suresh Kumar Kailasa, Tae Jung Park, Rakesh Kumar Singhal**

Quick reference providing promising applications of nanoparticles in detection techniques and in the removal of chemical species from the environment

In todays' world with its widespread usage of personal-care products, pharmaceuticals, surfactants, flame retardants, plasticizers, various industrial additives, metals and metalloids, pesticides, and pesticide metabolites, environmental contaminants are an increasing sources of pollution with a severe effect on the ecological system. Industries that produce these contaminants must find answers to remediate this.

Nanomaterials in Environmental Analysis contributes to solving this problem by providing researchers in industry and academia with promising applications of nanoparticles in detection techniques and in the removal of chemical species from the environment. Each chapter covers an aspect of using nanoparticles in detecting, measuring and remediating toxic chemical species in the environment.

Key Features:

- Explores the application of nanoparticles for the identification and quantification of pollutants from various environments
- Serves as a quick reference and source of knowledge on nanoparticles-based techniques for environmental applications
- Takes foundational knowledge for application to research in the area
- Provides future trends

Editors:

Suresh Kumar Kailasa, Associate Professor, Department of Chemistry, S. V. National Institute of Technology, Surat, Gujarat, India

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ISBN 978-0-12-820643-0

9 780128 206430

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Vol. 2

2024

Teresian Book of Research in Chemistry

Department of Chemistry and

Centre for Research

Published by
Teresian Publishing House
St. Teresa's College (Autonomous), Ernakulam
Kerala - India

Teresian Book of Research in Chemistry

April 2024
Vol. 2

Proceedings of the International Seminar on Chemical Science for Sustainable Future

Teresian Publishing House

TERESIAN BOOK OF RESEARCH IN CHEMISTRY

Vol. 2, 2024

Proceedings of the International Seminar on Chemical Science for Sustainable Future

February 23, 2024

Editor:

Dr. Saritha Chandran A.
Head - Department of Chemistry and Centre for Research
St. Teresa's College (Autonomous), Ernakulam-682011

Publisher:

Teresian Publishing House
St. Teresa's College, Ernakulam, Kerala-682011
Tel: +91 484 2351870, E-mail: teresianrnd@gmail.com

Designed & Paginated by:

Johnson E.V.

Distributors:

Sooryagatha Publishers, T. D. Road, Ernakulam.

ISBN: 9 788172 551797

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 1-10

Qualitative and Quantitative Determination of Phytochemicals in *Cynanchum viminale(L.)L.*

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Abstract:

Since ancient times, the phytoconstituents present in medicinal plants have been pivotal in the treatment of various diseases worldwide. *Cynanchum viminale(L.)L.* is a part of traditional medicine widely used by folk people for treatment of various diseases. The current study reports the phytogenic chemi-cal compounds in *Cynanchum viminale(L.)L.* to prove its use in folklore medicines. Preliminary phytochemical investigation reflected the presence of carbohydrates, reducing sugars, starch, proteins, alkaloids, phenolic compounds, saponins and flavonoids. The quantitative analysis revealed high content of total phenolics(32.731mg/g) followed by flavonoids (26.2106mg/g) and alkaloids(9.2581mg/g).

Keywords: Phytochemicals, *Cynanchum viminale(L.)L.*

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 11-18

Exploring the Biological Activities of N-Substituted Pyrroles Synthesized via a Novel Solvent-Free Protocol: A Molecular Docking Study

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Abstract:

This study presents the synthesis of N-substituted pyrroles using a novel solvent-free protocol catalyzed by manganese (II) under microwave irradiation. Sixteen compounds were synthesized and characterized. Subsequently, molecular docking studies were conducted using AutoDock Vina and LibDock to explore the potential biological activities of the synthesized compounds. Docking simulations revealed promising binding affinities and interactions with protein targets relevant to various therapeutic areas. The results suggest potential applications of the synthesized N-substituted pyrroles in drug discovery. In particular, compound 3c displayed the highest binding affinity (LibDock score: 118.117), indicating its potential as a potent inhibitor. Integration of computational docking with experimental synthesis offers a powerful approach to develop sustainable and effective drug candidates, highlighting the importance of green chemistry principles in pharmaceutical research.

Keywords: N-substituted pyrroles, Solvent-free synthesis, Manganese (II) catalysis, Molecular docking, Drug discovery, Green chemistry.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 19-34

A Comprehensive Study on Efficacy of Chitosan-Metal oxide Nanocomposites as α-amylase Carriers

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Abstract:

Chitosan-Fe_3O_4 (CSM) and chitosan-TiO_2 (CST) were the two chitosan-metal oxide nanocomposites synthesized and investigated in this study for the suitable support for immobilization of starch hydrolyzing enzyme, α-amylase. The α-amylase is an industrial enzyme which has wide implementation in food, detergent, paper and textile industry. The significance of the study is to allow the enzyme for industrial usage by improving its properties and stabilities. The immobilized enzyme, CSTE has shown better immobilization efficiency of 84.30%, while CSME imparts gentle and rapid separation from the reaction system due to its magnetic property. The efficiency of immobilized enzymes was evaluated based on their stability and activity. Both of the immobilized enzymes demonstrated adequate thermal stability compared to the free enzyme. The immobilized enzymes have exhibited enhanced stability over 6 months of storage and retained more than 50% of their initial activities after 10 cycles of reuses.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 35-48

ZnO-GO Composites: An Efficient Photocatalyst for Degradation of Methylene Blue

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Abstract:

Everyday a huge amount of waste water containing various toxic organic dyes is directly dumped into water bodies from industries including textile related industries. These dyes pose a huge threat to all organisms including humans. Therefore, it is necessary to find alternatives to tackle this situation. In the present work, ZnO, GO and the composites has been synthesized, characterized and tested for photocatalytic activity. The results shows that the photodegradation efficiency of the composite is much more improved when compared to ZnO as photocatalyst alone.

Keywords: Zinc oxide, GO, Composite, Photocatalytic degradation, Methylene blue.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 49-54

Unlocking Nature's Power: Discovery of a Novel Antioxidant Sulphated Pyruvylated Polysaccharide from Red Seaweed Macroalgaes

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Abstract:

Unearthing Astonishing Antioxidant Benefits in Alkali-Free Methods from Red Seaweed Species *Gracilaria salicornia* and *Gelidium pusillum*. Against traditional beliefs, our research uncovers heightened biochemical activity and more insightful NMR spectra without relying on alkali treatment. These unforeseen results not only defy established norms but stress the importance of tailoring extraction techniques to unveil the unique antioxidant potential of each algal species. This revelation prompts a reassessment of extraction protocols, highlighting substantial enhancements in both bioactivity and precise spectroscopic characterization, all achieved without the need for alkali treatment.

Keywords:

Biochemical activity, Nuclear Magnetic Resonanse (NMR), Bioactivity enhancement.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 55-64

Green Synthesis of Copper Oxide Nanoparticles

Alisha Susan Joshy, Amritha E.A., Ashmi Theresa Joseph, Mishma Benny, & Linto Anto*

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Abstract:

Green synthesis of Coleus Amboinicus plant mediated copper oxide nanoparticles were developed and characterized by various spectroscopic techniques like Infrared spectroscopy, Scanning electron microscopy, X-ray diffraction spectroscopy. This study was conducted by eco-friendly means and their antibacterial properties were evaluated showing promising results against antibacterial strain. It shows the production of bio-compatible nanoparticles with significant antibacterial activity.

Keywords:

Coleus Amboinicus, Spectroscopic techniques, Biocompatible nanoparticle, Antibacterial.

Teresian Book of Research in Chemistry
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Bacopa Monnieri Extract Mediated Green Synthesis, Characterisation and Applications of Zinc Oxide Nanoparticles

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Abstract:

Green synthesis of Bacopa Monnieri plant mediated zinc oxide nanoparticles were developed and characterized by various spectroscopic techniques like UV visible absorption spectroscopy, X-ray diffraction spectroscopy, Scanning and electron microscopy. This study was conducted by eco-friendly means and their antibacterial properties were evaluated showing promising results against antibacterial strain. It shows the production of bio-compatible nanoparticles with significant antibacterial activity.

Introduction

Nanochemistry is the combination of chemistry and nano-science that deals with the designing and synthesis of materials of nanoscale of different shape, size and structural composition. This study discusses the potential ability of Bacopa monnieri extract for the preparation of Zinc oxide nanoparticles through green synthesis.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 74-82

Caffeine Extraction and Comparative Quantification in Chosen Brands of Tea, Coffee and Green Tea

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Abstract:

This study explores the caffeine content in popular tea, coffee, and green tea brands consumed widely in India. Caffeine, a key ingredient in these beverages, influences various physiological processes and has both positive and negative health impacts. The aim was to analyze and compare the caffeine levels across eight selected brands: Kannan Devan, AVT, 3 Roses, Red Label (tea); Bru, Nescafe (coffee); Ripple, Lipton (green tea). Through this comparative analysis, the study aims to raise awareness among consumers about their daily caffeine intake and its potential health effects. Understanding these caffeine levels can empower consumers to make informed choices regarding beverage consumption for better health outcomes.

Keywords:

Caffeine; comparative analysis; consumer awareness; TLC.

Teresian Book of Research in Chemistry
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Design, Synthesis, and Evaluation of Schiff base Derivatives of Quercetin as Anti-Inflammatory Agents

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Abstract:

To develop new medications for problems associated with inflammation and unfavorable side effects of current drugs, further research is required. Quercetin is a naturally occurring flavonoid that is known to have a wide range of biological functions which include anti-inflammatory properties. However, quercetin's low solubility and poor bioavailability have restricted its applicability. This current study synthesized and investigated a new quercetin Schiff base by acid-catalyzed condensation of quercetin and 4-aminophenol. And it is studied using various spectroscopic techniques which include, NMR, UV, FTIR, and CHNS. The anti-inflammatory effect of this Schiff base is studied using the **HRBC membrane stabilization method**. And the study shows that it has a better IC50 value than commonly used Ibuprofen. Hence, synthesized quercetin Schiff base can take action as a promising anti-inflammatory agent.

Keywords: Schiff base, Quercetin, Inflammation, Anti-Inflammatory Agents, Spectral studies.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 96-112

Microwave Assisted Synthesis And Spectroscopic Studies of N-Ethyl Derivative of 1,8-Naphthalimide

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Abstract:

Today, fluorescent probes based on small organic molecules have become indispensable tools in modern biology because they can provide information on the localization and quantity of the molecules of interest without the aid of genetic engineering. Keeping this in mind, the photophysical properties of organic molecules can be tuned by introducing an electron rich donor and an electron deficient acceptor to a π linker. This π linkage between the donor and acceptor results in the formation of a D-π-A system.1,8-naphthalimide and its derivatives form one such class of compounds which exhibit excellent fluorescent properties.

Keywords:

Fluorescence, sensors, naphthalimides, pH sensors.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 113-123

Study of the Effect of Solvents on Electronic Spectra of Aromatic Azo Compounds by Experimental and DFT Calculations

Luduveena Francis, Rameesa Latheef, Roseben Paulson, S. Neha Devu, & Maria Linsha P. L.*

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Abstract:

Two azo derivatives NAR and NAP with donor group nitro aniline and acceptor groups - Resorcinol and Salicylic acid were synthesized and characterized using IR, UV and ^{1}H-NMR spectroscopic methods. The absorption maxima values of azo compounds in different solvents such as Chloroform, dichloromethane and Acetone with increasing order of solvent polarity were identified both experimentally and computational methods. The present work provides a concise overview of the inter-twined dynamics between azo compounds, solvatochromism and theoretical calculations, highlighting the synergy between experimental observations and theoretical insights.

Keywords:

Azo compounds, Solvatochromism, DFT calculations.

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Vol. 2 (2024), Pages 124-133

Synthesis, Characterization, and Photoluminescence Studies of Zn (II) Based Zeolite Imidazolate Frameworks (ZIFS)

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Abstract:

This study delves into the synthesis of Zinc (II) based Zeolite Imidazolate Frameworks (ZIFs) using hydrothermal methods, recognized for their cost-effectiveness and efficiency. Employing the hydrothermal approach, four distinct compounds were synthesized through two different methodologies. Characterization was conducted employing various techniques to validate the structural integrity and properties of the synthesized compounds. The findings of this study indicate the potential application of ZIFs in luminescence, expanding their utility beyond conventional roles. ZIFs exhibit versatile applications, including catalysis, gas storage, and sequestration of small metals.

Keywords:

ZIFs, MOFs, Imidazole 4,5 dicarboxylic acid, n-butyl amine, photoluminescence, LMCT.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 134-142

Voltammetric Sensor for the Antioxidant - BHA

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Abstract:

Butylated Hydroxyanisole (BHA), is a synthetic antioxidant used in various food products[1]. However adverse health effects can occur upon excess intake of BHA. Herein, a voltametric sensor for BHA based on Multiwalled carbon nanotube modified Platinum electrode [MWCNT/Pt E] has been developed. Excellent electrocatalytic activity towards the electro-oxidation of BHA was observed with the MWCNT/Pt E compared with the bare Pt E. The oxidation peak current of BHA increased with concentrations in the linear range 11.0×10^{-6} to 1.0×10^{-7} M with a detection limit 9.49×10^{-8} M. Interference of various co-existing species on the electro-chemical response of BHA at the modified electrode was examined. The sensor was also utilised for the determination of BHA in commercially available vegetable oil sample.

Keywords:

Voltammetry, Multiwalled carbon nanotube, BHA.

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Green Polymer Nanocomposite Sensor film for Detection and Removal of Hg(II) from Aquatic System

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Abstract:

The development of a green polymer nanocomposite sensor for both removal and detection of the nanomolar concentration of Mercury (Hg2+) from the aquatic system has a significant attraction in the recent research community. The incorporation of green synthesized silver nanoparticles (AgNP) into the polymer blend results in polymer silver nanocomposite film. The green synthesized AgNP which improves the properties of the polymers. In the colorimetric detection, a linear decrease in the intensity of the absorption peak of AgNP present in the composite film by the addition of Hg (II) solution. The sensing mechanism, AgNP in the composite film undergoes a rapid redox-favored reaction, i.e. the Ag (0) from AgNP gets oxidized to Ag+ ions in the presence of Hg2+ ions, and that reduced to Hg(0) the deposited on the Ag surface results in Ag-Hg alloy.

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Study of Water Quality Parameters of Different Water Sources in Kumbalangi Panchayat, Kerala Region

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Abstract:

After air, water is arguably the most valuable natural resource. This paper is an evaluation of water quality of the tap, well and other water resources found in Kumbalangi Panchayat. Water quality is a major issue we are facing in this developing world. Water quality analysis was carried out in Kumbalangi panchayat which is an island village in the outskirts of Kochi city in the state of Kerala, India, by using the parameters like ammonia, pH, alkalinity, hardness, chlorine and E.coli, in tap water, well water, bore well water, pond water and Backwater samples. Samples were collected randomly from 8 wards out of 17 wards in Kumbalangi panchayat. The wards chosen were 1, 2, 3, 4, 7, 14, 16 and 17. Based on the analysis of the water samples, we found that some of these unsafe attributes were detected in a few of the Kumbalangi Panchayat ward.

Keywords:

Water Quality, E.coli, pH, Drinking water.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 160-166

Novel Aldehyde Promoted Synthesis of Highly Substituted Furanones and Quinolines - Computational & Biological Evaluation

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Abstract

We had recently developed a highly efficient method for the synthesis of 3(2*H*)-furanones and quinolines by the reaction between aldonitrones and dibenzoylacetylene (DBA). Aldonitrones are synthesized by the reaction between aldehydes and phenyl-hydroxylamine (Scheme 1). Close examination of the reaction sequence depicted in Scheme 1 reveals that phenylhydxoxylamine and DBA are the stoichiometric reagents here with one molecule of aldehyde liberated per molecule of furanone/quinoline formed. In principle, aldehyde liberated in this reaction can be recycled to generate aldonitrones *in situ* leading to tremendous improvement in the atom efficiency of furanone/quinoline forming reaction. We propose to develop a greener protocol for the generation of target furanone/quinoline by using benzal-dehyde as a "promoter." The ratio of products formed by geometry optimisation by DFT analysis. Explore the tumor suppressing potential of 3(2*H*)-furanones was carried out by MTT assay.

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Nanoparticle Based Electrochemical Sensor for Synthetic Food Colourant Sunset Yellow

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Abstract:

Two electrochemical sensors were developed utilizing the electrocatalytic characteristics of multiwalled carbon nanotubes (MWCNTs) and gold nanoparticles (AuNPs) to detect the synthetic food colourant, sunset yellow (SY). First, Glassy carbon electrode (GCE) modified with AuNP was used to study the electrochemical oxidation of SY. On further modification of AuNP/GCE with MWCNT, the nanocomposite film modified electrode shown exceptional electron transfer ability towards the oxidation of SY with great sensitivity and stability with. The electrode modified by nanocomposite film exhibited a linear response, with a detection limit of 4.03×10^{-8} M., in the concentration range of 1.00×10^{-5} to 1.00×10^{-6} M under optimum conditions. The sensors were also utilized for the quantification of SY in commercially available soft drink samples.

Key words:

Electrochemical Sensor, Sunset Yellow, Food colourant.

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Effect of Solvent in the Fluorescence Intensity of Blue Fluorecent Carbon Dots (CDs) Derived From Luffa Cylindrica Fiber (Peechinga) as Natural Precursor

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Abstract:

A simple, eco-friendly, and economic method for the preparation of water-soluble, blue-fluorescent Carbon Dots (CDs) have been developed via hydrothermal process using *Luffa Cylindrica Fiber* (LCF) (Peechinga) as a carbon source. The use of LCF opens the possibility of use biodiversity in obtaining new materials. The synthesized C-Dots were chara-cterized by Scanning Electron Microscope (SEM), Dynamic Light Scattering Method (DLS), Fluorescence spectrophoto-meter; UV-Visible absorption spectra as well as Fourier transform infrared spectroscopy (FTIR). The results reveal that the as-prepared CDs were spherical shape with an average diameter of 2.5nm and emit bright blue photoluminescence (PL). The surface of the C-Dots was rich in hydroxyl and carboxyl groups and presented various merits including high fluorescent quantum yield, excellent photostability, low toxicity and satisfactory solubility. The PL emission spectrum of the CDs was recorded at progressively increasing excitation wavelengths shows that,

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 185-189

Novel Class of Cytotoxic Metal Complexes

Sneha Jose Eeetinilkunnathil,[a*] & Puzhavoorparambil Velayudhan Mohanan[b]

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Abstract:

Metal complexes have raised much attention for several decades due to the relevance of metal ions in biological reactions. Significant side effects and drug resistance by metal based drugs limits their clinical applications. Low toxicity against normal cell lines is the preliminary criteria for successful development of metal based drugs. Better DNA binding, enzyme inhibitory and antibacterial properties of the synthesized complexes prompted us to check toxicity level of selected compounds against normal 3T3-L1 cells. Assay selected for the cell viability study is the sensitive, quantitative and reliable MTT colorimetric assay. Compounds were found to be non toxic to the normal cells which make them better candidates for its development as good thera-peutic agents.

Keywords:

2-methoxy-4-chromanones, mononuclear complexes, cytotoxicity.

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 190-200

Density Functional Theory Studies of 3-Formyl Chromone Hydrazones

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Abstract

The two 3-formyl chromone hydrazones were synthesized. Calculations of the synthesized molecules were made with the Gaussian package program at B3LYP, HF, and M062X levels on 6-31++g(d,p) basis sets. DE, Dh, and DG values were calculated using the thermodynamic parameters obtained from the calculations. Finally, ADME/T analysis was performed to examine the effects of the molecules on human metabolism.

Keywords:

DFT, Molecular docking, ADME/T.

1. Introduction

It is very important to be very fast in order to compare the activities of molecules with theoretical calculations and to have preliminary information about the properties of molecules [1,2]. Theoretical studies are an important guide to experimental studies. In this study, molecules were calculated with the Gaussian package program at B3LYP, HF, and M062X levels on 6-31++g(d,p) basis sets [3-5]. DE, Dh, and DG values

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 201-212

Sugarcane Bagasse-Derived Cellulose Nanocrystals: Versatile Applications in Biocomposite films and Antibacterial Solutions

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Abstract:

In pursuit of sustainable antibacterial solutions, this study explores the potential of harnessing sugarcane bagasse for cellulose nanocrystals (CNCs) production and subsequent development of CNC-ZnS nanocomposites. With approximately 1.9 billion tonnes of sugarcane bagasse generated annually as a by-product of the sugar industry, addressing environmental distress caused by its disposal is imperative. Utilizing an acid-hydrolysis method, CNCs were successfully extracted from sugarcane bagasse. FTIR and XRD studies of raw material, chemically purified cellulose(CPC) and CNC revealed successful extraction of cellulose and removal of non-celluloisic components. Transmission electron microscope(TEM) revealed rod-like CNCs with diameters ranging from 2-7 nm. A nanocomposite of CNC with Zinc Sulphide (ZnS) was fabricated and it exhibited enhanced antibacterial properties against *Escherichia coli*, as validated by the agar-well diffusion method. Bio-

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 213-227

Synthesis and Characterization of Nanocrystalline Cellulose Derived from Pineapple Crown Fibers

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Abstract:

Sustainable alternatives are being explored to replace conventional materials, driven by the need to reduce environmental impact. Cellulose nanocrystals (CNCs) extracted from various sources have high mechanical strength and are biocompatible and biodegradable. Research is focusing on utilizing cellulosic-rich wastes for the extraction of CNCs for pharmaceutical applications and composite materials. Pineapple, by-products, like leaves, contribute to pollution and land issues, with approximately 3 billion tons generated annually. Pineapple crown leaves are rich in cellulose, hemicellulose, and lignin, with cellulose making up 79-83%. Recently, pineapple crown leaves have been used in textiles, paper, and as reinforcement in polymers. Cellulose, a renewable and biodegradable material, can be processed into nanocrystalline cellulose (NCC) with unique properties offers benefits like biocompatibility, non-

Teresian Book of Research in Chemistry
Vol. 2 (2024), Pages 228-244

Synthesis and Characterization of Activated Carbon from Human Hair Waste and Adsorption Studies using Methyl Orange as Model Dye

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Abstract

This study focuses on the effective adsorption capacity of Human Hair Activated Carbon. Activated carbon is an appealing tool for remediation applications because of its huge surface area, porous structure, ease of synthesis, and low cost. Activated carbon is used to remediate contaminants from a variety of industries, including fertiliser plants, automobiles, petroleum, pharmaceutics, cosmetics, and textiles. It also removes organic and inorganic pollutants as well as colours from effluent streams. This study addresses a crucial environmental concern and contributes to the development of sustainable solutions for water treatment in industrial settings by the adsorption of methyl orange, a dye found in industrial effluents. The characterisation of the activated carbon is done using SEM, FTIR, CHNS and XRD.

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The Department of Chemistry started functioning with the very inception of the college and is celebrating its Diamond Jubilee this year. In 1969 the degree course in Chemistry was introduced. It became a Post Graduate department in 1984 when M. Sc. in Pure Chemistry was started and was elevated as Research Centre of the Mahatma Gandhi University in 2019. The department's illustrious history is punctuated by the notable achievements of its alumni, who have become distinguished figures both nationally and internationally.

PREFACE

The Department of Chemistry was established in 1969 and became a Post graduate department in 1984. The department has highly qualified and dedicated faculty. The Department of Chemistry and Centre for Research, Baselius College, Kottayam is very pleased to release the Book of the National conference on Exploring Frontiers in Chemical Innovation, EFCI-2023 conducted during December 14-15, 2023. This is an account of most of the contributions presented at the conference.

EFCI 2023 conference hosted by Department of Chemistry and Centre for Research, Baselius College with a view to provide a platform for young researchers and science aspirants to communicate with National experts. This event is very rich with eminent scientists and will inspire the younger generation to develop research interest to match the emerging need of the society.

We would like to thank all the academicians, delegates and participants for their contributions to the conference. We are much grateful to the sponser of the programme KSCSTEC. From the teachers, students and research scholars are encouraging. This proceedings is a compilation of the abstracts of invited lectures and presented papers.

We thank all those who have contributed to the successful organization of the seminar.

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IL1

Advancement of Surface-Enhanced Raman Spectroscopy in Cancer Diagnostic Applications

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Abstract

Surface-enhanced Raman scattering (SERS) was investigated as a highly sensitive spectroscopic modality where the signal intensity of molecular vibration is enhanced up to 10^8 –10^{14} folds compared to simple Raman spectra. Multiplexing capability of Raman fingerprints, molecular specificity, high sensitivity, and capability to fish out complex biological compositions at the molecular level augmented SERS as a potential diagnostic modality in biology and medicine. While assessing all the merits of classical Raman spectroscopy, SERS provides a more sensitive and selective detection and quantification platform. Non-invasive, chemically specific, and spatially resolved analysis facilitates the exploration of SERS-based nanoprobes in diagnostic and theranostic applications with improved clinical outcomes compared to the currently available so-called state-of-the-art technologies. Adequate knowledge of the mechanism and properties of SERS-based nanoparticle probes is inevitable in utilizing the full potential of this modality for biomedical applications. The safety and efficiency of metal nanoparticles and Raman reporters must be critically evaluated for the successful translation of SERS into clinics. On the other hand, the advancement of nanotechnology holds great promise for both diagnosis and therapy in several communicable and non-communicable diseases, including cancer, neurodegenerative disorders, and infectious diseases, which are coined as nanotheranostics. Exploration of a sensitive diagnostic nanoprobe, especially with the aim of point-of-care treatment, is another challenging task for early and accurate detection of cancer biomarkers, which facilitates efficacious therapy by reducing mortality and morbidity. Recently, we have fabricated programmable nanoparticles that feature a label-free SERS-based detection and grading of cervical cancer. We also developed SERS-nanoprobes which are conjugated with target-specific antibodies for the multiplex detection of breast and lung cancer biomarkers, which furnished a semi-quantitative evaluation of biomarkers through both modalities. In another approach, we have developed a gold nanorod (GNR)--based therapeutic nanoprobe for targeting metastatic

melanoma by combining PTT, PDT, and chemotherapy along with SERS imaging for better treatment and an effective follow-up therapeutic response. We believe that this proof-of-concept will provide a blueprint for the diagnosis and differential staging of cancer into various histological subtypes based on the differential expression of the antigens. Recently, we are progressing SERS with artificial intelligence (AI) screening/prevalence of multiple cancers from clinical blood samples. Therefore, SERS techniques are being explored as an upcoming molecular diagnostic modality, ranging from simple detection platforms to complicated clinical applications.

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5. *M. M. Joseph & K K Maiti et.al.*, Biomaterials**, 2018**, 140-181.

IL2

The Role of Speciality Polymers for Aerospace Application

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The need for high performance and capability to design materials to meet specific requirements has made polymers a first choice for many aerospace applications. Such materials can be tailored to give high strength coupled with relatively low weight, corrosion resistance and offer long-term durability under severe environmental conditions. Composite materials, mainly fiber-reinforced polymers, are used in aerospace industry over other conventional metallic materials due to their specific strength properties with weight saving of 20-40%. The polymer composites constitute up to 80% of modern launch vehicles comprised of several vital components like the honey comb structures, equipment panels, support structures, solar array substrates, antennas, etc. Most of aerospace resins are developed from thermosetting resins as they cure permanently by irreversible cross-linking at elevated temperatures, thus making them highly desirable for structural

applications. The resins offer good mechanical and thermal properties and bind the fibres together into a firm matrix. The most common resins are epoxies, phenolics, silicone, polyurethanes, polymides, cyanate ester resins etc and the section of the resin is application dependent. Polymers also find extensive application as adhesive to produce high strength, durable joints without the need for mechanical fasteners, specialty coatings, thermal protection systems, sealants etc. Advances in polymer materials including nanotechnology, 3D printing, robust manufacturing technologies etc will enhance the role of polymers as an enabling technology leading to advanced polymer materials with vast applications such as thin films or ultra-light aero structures, smart materials for space deployable spacecrafts, electrochromic polymers for thermo-optical uses and electroactive polymers for futuristic missions.

IL3

Kinetics of self-assembly of L-histidine from real time NMR spectroscopy

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Abstract

L-Histidine is an essential amino acid with unique biochemical and physiological properties. Histidinemia is a disease condition caused by the elevated level of l-histidine in our blood. Mutations in the histidase, an enzyme for the breakdown of histidine, is the cause of the rise in histidine concentration. To our knowledge, no research has been done on why a high concentration of histidine causes histidinemia. In this study, we provide a potential explanation why the elevated levels of histidine in the human body causes histidinemia. Inthis study we have found that l-histidine self-assembled in water to form nano sheet structures at physiological pH and temperature, using 1D ^{1}H NMR spectroscopy, difusion ordered spectroscopy (DOSY) and scanning electron microscope (SEM) techniques. The kinetics of self-assembly has been studied using real time NMR spectroscopy. We observed that both thearomatic ring and aliphatic part are equally contributing to the self-assembly of l-histidine. The symptoms of histidinemia, neurological deficits and speech delays, are similar to that of the neurodegenerative diseases caused by the self-assembly of peptides and proteins. We speculate that the self-assembly of l-histidine might be the cause of histidinemia.

Reference

Ajitha Ajikumar, Anakha Premkumar and Sunilkumar Puthenpurackal Narayanan, The self-assembly of L-histidine might be the cause of histidinemia, *Nature Scientific Reports*, **2023**, 13, 17461. https://doi.org/10.1038/s41598-023-44749-5.

IL4

Unlocking Catalyst Secrets: Path to Enhancement

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Abstract: It is necessary, continually, to devise, develop and deploy new techniques of investigation to understand how and why certain molecules transform readily and others do not when they impinge upon an active site. This is why a detailed understanding of the atomic architecture of the catalytically active center is important to improve existing catalysts or design superior new ones.[1]The active site of many biological systems operates *via*a chemical switching mechanism, in which a stable resting state to be protected from decomposition transforms into its active form only when a triggering signal is present. To mimic the enzyme activity, chemists have shown significant effort in the design and control of artificial catalysts for remote tunning of its activity with external stimuli such as light, pH, or metal coordination.[2] However, the control of the properties of active metal centers by a well-defined ligand system is an ultimate goal, by which one can tune its reactivity for the activation of a particular substrate. To get superior activity in a catalyst one has to understand the mode of activation of the pre-catalyst, it's binding mode, and the important step of the catalytic cycle.The presentation is aiming to understand the active catalysts, involved in dehydrogenation, hydrogenation, and tandem (de)hydrogenation reactions.[3] In particular, a few analysis tools such as NMR spectroscopy, UV-vis study, initial rate kinetics, and control studies will be discussed with a few selected examples to understand the catalysts for their betterment.

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ABSTRACTS OF POSTER PRESENTATION

PP1

A DFT Investigation on the Mechanism of Ligand Assisted Manganese Catalyzed Ullmann Coupling Reaction.

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Abstract

Ullmann coupling reactions are one of the most widely employed transition metal-catalyzed coupling reactions for C-O bond coupling. These reactions have great significance and extensive applications in the pharmaceutical and biological fields. The high cost, low abundance, and toxicity created a strong demand to search for an alternative to the traditional copper metal catalyst. Manganese-catalyzed cross-coupling reactions have been recently relevant because of their sustainable and eco-friendly properties. In this work, we discuss a detailed Density Functional Theory (DFT) study of the Mn (II) catalyzed Ullmann coupling reaction between aryl halides and phenols by employing DMEDA (Dimethyl ethylene diamine) as ligands. All calculations discussed in the work are performed at the DFT level, using the hybrid B3LYP functional augmented with CPCM solvation model using acetonitrile as the solvent. The Mn and I atoms are described using (LANL2DZ) and the C, H, N and O atoms were described by a 6-31+G(d) basis set. We have identified that the active catalyst species is a three-coordinated DMEDA ligated Mn (II)-phenoxide complex. The proposed mechanism proceeds via a σ bond metathesis, involving a single transition state. The activation barrier 25.92 kcal/mol concords well with the experimental temperature requirement (110° C). This study primarily investigates the relevance of enhancing the mechanisms of cross-coupling reactions through both theoretical and experimental methodologies[1].

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PP2

Asymmetric Plasmonic Nanostructure for Temperature and Magnetic Field Detection

Lakshmi S[1], Simitha S,[1] Devika Mohan,[1,2] Jesly Jacob*[2], Vibin Ipe Thomas*[1]

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Abstract

Many diverse technological applications, such as soft robotics and flexible electronics, demand the development of intelligent sensors that can simultaneously detect different physical parameters. Taking advantage of plasmonic optical structures, which can experience minute variations of physical parameters in their close contact, a dual channel-based silver nanostructure of concentric square rings and disks on SiO_2 substrate is proposed for synchronized detection of magnetic field (H) and temperature (T). The thermometric PDMS and ferromagnetic Fe_3O_4 were placed in two channels of the nanostructure, forming the sensor. The structure modeling and electromagnetic study were carried out using finite element method (FEM). The concurrent detection of H and T was realized through the sensing matrix, which again solved the problem of cross-sensitivity caused by temperature variation. The impact of structural asymmetry on sensor performance is studied by tuning the geometrical parameters, such as disk length and ring length, separately and together. Asymmetry and channel size significantly enhance performance, where disk optimization raises temperature and magnetic field sensitivity to about 760 and 8319 times using 70% and 80% asymmetric systems, respectively. Also, the smallest ΔW (5 nm) provides a sufficiently high channel separation factor of about 7.47 µm during multiparameter sensing. The asymmetric sensing toward the solo parameter was also tested by placing PDMS/ Fe3O4 on both channels. The multiple peaks displayed with higher sensitivity and CH-factor, making the detection more specific. Thus system holding narrow channels and unique channel asymmetry combination reveals excellent multi and solo sensing in temperature and magnetic field detection.

Keywords: Plasmonic nanostructure, Magnetic Fluid, PDMS, multifunctional

Reference: [1] S. Simitha, D. Mohan, S.M. Francis, A. Ramachandran, J. Jacob, V.I. Thomas, Phys. Chem. Chem. Phys. 2023, 25, 21981-21992.

PP3

Mechanistic insight into ligand free manganese catalysed Ullman type cross coupling reaction: A Computational study.

Nayanthara S[a] , Parvathi Santhoshkumar[a] , C Rajalakshmi[a] , Vibin Ipe-Thomas*[a]

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Abstract

The manganese catalyzed O-arylation reaction outweighs owing to their economical and ecological benefits over the traditional metal catalyzed Ullmann coupling reactions. In the present work, a detailed theoretical investigation into the mechanism of ligand-free manganese catalyzed C-O coupling of phenols with aryl halides has been carried out for the first time with the aid of Density Functional Theory techniques using Becke3LYP-D3. In our study a solvent coordinated manganese complex is found to be the active catalyst and the reaction proceeds via sigma bond metathesis mechanism. Further we have investigated the electronic effect of functional group on the feasibility of the reaction[1].

1.K. Rohit, S. Saranya, N. A. Harry and G. Anilkumar, *Chemistry Select*, **2019**, *4*, 5150–5154.

PP4

A Detailed Computational Investigation into the Mechanism of Iron Catalyzed Csp^2-Csp Cross-Coupling Reaction

John B Kottooran[a], Shilpa Sara Mathew[a], Parvathi Santhoshkumar[a], C. Rajalakshmi[a], Binuja Varghese[a], Vibin Ipe Thomas*[a]

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Abstract

There are multifarious methods for carbon-carbon bond-forming reactions in organic synthesis. Among these reactions for C-C bond-forming reactions, Sonogashira coupling reactions have a prominent position for constructing Csp2-Csp bonds. These reactions are deemed to be versatile tools for the fabrication of molecules like biaryl acetylenes that have biological and pharmaceutical importance. Palladium which is traditionally used for these reactions is limited due to its high cost, low abundance and

was characterized by UV Visible, ^{1}H NMR , FTIR and LCMS studies. By analysing the results we could predict the possible structure of the compound.

Keywords: *plectranthus rotundifolius,* UV Visible, ^{1}H NMR , FTIR and LCMS.

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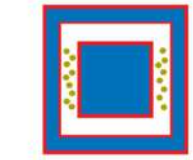

Keywords: Plasmonic nanostructure, finite element method, Refractive Index, Cancer detection.

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OP4

Unveiling the Novel Mechanistic Trends in Transition Metal Catalyzed Cross-Coupling Reactions

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Abstract

Employing 3d- transition metals as catalysts for cross-coupling reactions is a captivating research area that is recently garnering interest due to its viability, sustainability, and affordability. However, a comprehensive understanding of the underlying mechanism in this context has yet to be established. With the aid of density functional theory, we herein report a general mechanism for the cross-coupling reactions catalyzed by 3d-transition metals. The catalytic cycle initiates with the activation of the nucleophilic coupling partner via transmetalation processes followed by the activation of the electrophilic coupling partner (organic halide). Remarkably, all the post-transmetalation processes follow a concerted pathway liberating the cross-coupled product in a single step in all the investigated reactions. The mechanisms thereby adopt a non-redox mechanistic route contrary to the conventional paths seen in Pd catalysis. Notably, the activation of the electrophilic partner is found to be the rate-determining step in all the cases irrespective of the substrates, ligands, and catalytic metal center employed. Establishing a general mechanism for first-row transition metal-catalyzed cross-coupling reactions will thus aid in developing efficient sustainable synthetic protocols.

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OP8

Investigation on the Synthesis of NIR Reflective Nano Pigments

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Abstract

The utilization of near infra-red (NIR) reflecting inorganic pigments has garnered widespread application across industries including defense, construction, plastics, and ink [1]. Notably, the application of NIR reflective pigments on external building surfaces, such as walls and roofs, has been recognized for its capacity to diminish energy consumption by reducing interior temperatures [2]. These pigments possess the capability to absorb light within the visible spectrum while reflecting the NIR segment of incident radiation. However, numerous inorganic pigments used for colouring purposes, such as chromium green, cobalt blue, cadmium yellow, nickel titanate yellow, and lead chromate, contain toxic metal ions, leading to restrictions on their usage. This paper specifically focuses on the yellow pigment derived from Bi_2O_3, detailing the synthesis of both Bi_2O_3 and Nd-doped Bi_2O_3 via a low-temperature solvothermal method. The synthesized materials underwent comprehensive characterization using techniques such as powder X-ray diffraction (PXRD), Fourier-transform infrared spectroscopy (FT-IR), Ultraviolet-Diffuse reflectance spectroscopy (UV-DRS), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and analysis of CIE-L*a*b* colour values. The colorimetric analysis provided quantifiable data on pigment colour, notably revealing a significant improvement in the yellow hue component (b*) values, reaching 50.72 in Nd-doped Bi_2O_3 compared to undoped Bi_2O_3 (17.96), alongside increased NIR reflectance. Furthermore, this study comprehensively examines the impact of metal substitution on structural, optical, and morphological properties. The findings underscore the potential of Nd-doped Bi_2O_3 as a promising cool pigment, offering a viable alternative to toxic pigments in various applications.

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OP9

Self-assembly of L-histidine might be the cause of histidinemia

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Scientific Reports **volume 13**, Article number: 17461 (2023)

Abstract

L-histidine is an essential amino acid with unique biochemical and physiological properties. Histidinemia is a disease condition caused by the elevated level of L-histidine in the blood (1). Mutations in the HAL gene, which gives instructions for producing the enzyme known as histidase (an enzyme for the breakdown of histidine), are the cause of the rise in histidine concentration and subsequently histidinemia(1). The two main symptoms of this condition are neurological deficits and speech delays(2). No research has been done on why a high concentration of histidine causes histidinemia, despite the fact that the molecular mechanism of the increase in histidine concentration has been well researched. In this study, we provide a potential explanation for the unusually elevated levels of histidine in the human body that characterize the histidinemia illness condition. It was reported that the amino acid L-histidine self-assembled in water-methanol medium, but not in water alone medium(3). In this study we have found that L-histidine self-assembled in water to form nano sheet structures at 25mM and 50mM concentrations, pH 7-8 (physiological pH) and temperatures of 20ºC and 37ºC (physiological temperature) using NMR spectroscopy and Scanning Electron Microscope techniques. The kinetics of self-assembly has been studied using real time NMR spectroscopy. We observed that both the aromatic ring and aliphatic part are equally contributing to the self-assembly of L-histidine. The symptoms of histidinemia are similar to that of the neurodegenerative diseases caused by the amyloid fibril formation from peptides and proteins. We speculate that amyloid fibril formation by the self-assembly of L-histidine might be the cause of histidinemia.

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OP10

Kaolin- carboxyl graphene incorporated graphitic carbon nitride: An efficient photocatalyst for the degradation of cefepime under sunlight.

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Abstract

Kaolin-carboxyl graphene incorporated graphitic carbon nitride (g-C_3N_4/KG) was successfully synthesized and utilized for the photocatalytic degradation of pharmaceutical compound, ‘cefepime’. The structural and optical properties of g-C_3N_4/KG were thoroughly investigated using various characterization techniques including FT-IR, XRD, TEM, SEM, EDX, BET, DRS and PL. Photoluminescence studies revealed that g-C_3N_4/KG catalyst exhibits a pronounced charge separation and electron flow. Furthermore, DRS studies demonstrated an enhanced capacity for visible light absorption. The investigation on the active radical species revealed that superoxide and hydroxy radicals play a significant role in the photocatalytic degradation of both cefepime and dye pollutants. g-C_3N_4/KG gave complete removal of MB and 85% degradation of cefepime within 75 minutes and 135 minutes of solar light irradiation, respectively. Moreover, a plausible mechanism for the breakdown of the antibiotic cefepime was proposed, along with the identification of the intermediates formed during the degradation process. Overall, this study highlights the potential of this innovative photocatalyst for the removal of dyes and medical waste from water under solar light.

Key words: kaolin-carboxyl graphene, g-C_3N_4, Degradation, Methylene blue, Cefepime, Solar light

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OP11

Sustainable Synthesis of Chitosan-Polyacrylic Acid Modified Natural Fibers for Enhanced Methylene Blue Dye Adsorption

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Abstract

In this study, we explored the adsorption capabilities of cost-effective adsorbent materials derived from natural fibers, specifically Jute fiber and sugarcane fiber sourced from jute stems and sugarcane bagasse, respectively. To enhance their adsorption

properties, a novel adsorbent was synthesized through a layer-by-layer (Lbl) deposition method, involving the application of chitosan (CHI) and polyacrylic acid (PAA) onto these natural fibers. Characterization techniques such as Fourier-transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FE-SEM), and X-ray diffraction (XRD) were employed to assess the functional groups, surface morphology, thermal stability, crystal structure, and mechanical properties of the modified fibers.The resulting fibers exhibited significantly improved adsorption properties for the removal of methylene blue dye from water. Systematic experiments were conducted to evaluate various adsorption parameters, revealing that 10Lbl fibers demonstrated the highest adsorption capacity compared to 1Lbl and 5Lbl fibers. The optimal conditions for maximum adsorption were found to be at pH 9 and temperatures of 30°C (for Jute) and 50°C (for Bagasse) using 0.05g of fiber. The adsorption data were effectively described by the Pseudo 2nd Order and Langmuir isotherms, with high correlation coefficients (R^2=1), indicating a successful fit to the models. Thermodynamic studies suggested that the adsorption process is endothermic and spontaneous. This research underscores the potential of utilizing agricultural waste-derived materials as a sustainable and cost-effective strategy for efficiently removing dyes from water. The findings offer a promising solution to address challenges associated with water pollution, emphasizing the importance of repurposing natural fibers for environmental remediation.

OP12

A Facile Chemical Recycling of Aluminum from Food Packaging Covers to Synthesize Alumina

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Abstract

This work reports the chemical recycling of food packaging covers to recover the coated aluminum and its purification and chemical conversion into alumina through series of reaction. Food packaging covers coated with aluminum is widely used to preserve the food[1]. However, these covers after use are reaching landfills without processing. Such unprocessed waste covers are serious threat to the environment as they can release aluminum[2]. Hence, processing such covers are vital for the safety of the environment[3].

OP13

Highly Selective and Sensitive Detection of Fluoroquinolones Using *Sauropus Androgynus* Derived Carbon Dots

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Abstract

Carbon Dots (CDs) are a recently introduced form of fluorescent carbon nanoparticle in the family of carbon nanoparticles. This discovery was made possible by the work of Xu et al. in 2004[1,2]. CDs are typically less than 10 nm in diameter and therefore can exist as discrete, quasi-spherical, nanocrystalline, or amorphous carbon structures. In this work, a green synthetic approach for synthesizing fluorescent carbon dots using *Sauropus androgynus* leaves as the carbon source by one- step hydrothermal mediated synthesis is presented. To the best of our knowledge, it is the first attempt to synthesize carbon dots from *Sauropus androgynus* leaves. This methodology is simple, eco-friendly, cost-effective, less time-consuming, and requires only water as a solvent without the addition of any other chemical reagents. The as-prepared carbon dots were characterized using different analytical techniques, which confirmed that they were biocompatible, highly stable over a wide range of pH values and at high ionic strengths and exhibit strong blue fluorescence. Furthermore, it was revealed that the developed carbon dots have selective and sensitive photoluminescence response to the drug levofloxacin (a fluoroquinolone drug), evident from the enhanced fluorescence spectra, and a broad range was observed in the linear correlation between the intensity of fluorescence and concentration of levofloxacin. The detection limit of the developed fluorescence probe was found to be 0.67 µM over a linear range of 0-30 µM. This opens up the possibility of using it as a prospective candidate in sensing applications.

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OP14

A New green Multicomponent synthetic Protocol for the synthesis of *β*-acetamido ketone derivatives

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Abstract

A simple and efficient multicomponent protocol for the synthesis of *β*-acetamido ketones *via* the one-pot condensation of aryl aldehydes, enolizable aryl ketones, acetyl chloride and acetonitrile using $Zncl_2$ is described. The current method offers many advantages such as short reaction times, easy workup procedures and good-to-excellent yields of products.

Key Words: Multicomponent reaction, Green chemistry, *β*-Acetamido ketone, Zinc Chloride, Nontoxic catalyst

OP15

Anti-Snake Venom Activity of Various Flavonoids on Phospholipase a2: *In Silico* Evaluation

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Abstract

Molecular docking simulations were performed using the ligands Naringenin, Quercetin, Kaempferol, Rutin, Vitexin, and Apigenin against the receptor 2ARM, Phospholipase A2 enzymes found in the venom of Russell's viper (Daboia russelii). Studies revealed that all ligands have favorable binding affinities with the target molecule, as evidenced by the negative binding energies. Among the tested ligands, Vitexin exhibits the highest binding affinity, with a binding energy of -8.9 Kcal/mol, followed by Rutin with a binding energy of -8.1 Kcal/mol. Naringenin, Quercetin, Kaempferol and Apigenin also show relatively strong binding affinities, with binding energies ranging from -7.2 to -8.0 Kcal/mol. These results provide useful information for the development of potential drug candidates or for the design of experiments to further investigate the binding interactions between these ligands and the target molecule.

OP16

Facile fabrication of Ni coated MnO_2 incorporated high performance Al-Zn alloy metal matrix composites as efficient sacrificial anodes

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Abstract

In Al-based metal matrix composites (MMCs), the ceramic composites play a key role to attain enhancement in various metallurgical and galvanic characteristics. The metallic coating on ceramic composites were often used to improve better bonding and wettability between metal matrix and composites. In this work, nickel coated MnO_2 was prepared by electroless nickel coating method and was beneficially explored into Al-Zn alloy anode matrix to achieve synergistic activation enhancement. The incorporation of MnO_2-Ni into Al-Zn alloy anodes was micro-structurally and electrochemically characterized. The metallurgical and galvanic characteristics of the anode were improved substantially by uniform dispersion of MnO_2-Ni into the Al-Zn alloy matrix. The effective dispersion of MnO_2-Ni in the alloy matrix can provide numerous lattice activation centers and intercalation channels, facilitated effective destruction of the passive alumina film. Very high galvanic efficiency of was achieved by fine tuning of MnO_2-Ni composite into the Al-Zn alloy metal matrix. The anode exhibited active open circuit potential, very low polarization and non-columbic metal loss during prolonged galvanic exposure studies.

OP17

Physicochemical characterization and fatty acid profiles of Coconut oil and Coconut testa oils from *Cocos nucifera* L.

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Abstract

Cocos nucifera L. is also known as coconut palm tree which is a major plantation crop in several parts of the world and are widely used for edible and non-edible purposes. The culinary nature of the plant is widely known from the ancient period onwards. The oil derived from the seed has a potential source of nutrients and is

FULL PAPERS

OP10

Kaolin- carboxyl graphene incorporated graphitic carbon nitride: An efficient photocatalyst for the degradation of cefepime under sunlight.

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Abstract

Kaolin-carboxyl graphene incorporated graphitic carbon nitride (g-C_3N_4/KG) was successfully synthesized and utilized for the photocatalytic degradation of pharmaceutical compound, 'cefepime'. The structural and optical properties of g-C_3N_4/KG were thoroughly investigated using various characterization techniques including XRD, SEM, EDX, BET, DRS and PL. Photoluminescence studies revealed that g-C_3N_4/KG catalyst exhibits a pronounced charge separation and electron flow. Furthermore, DRS studies demonstrated an enhanced capacity for visible light absorption. g-C_3N_4/KG gave complete removal of MB and 85% degradation of cefepime within 75 minutes and 135 minutes of solar light irradiation, respectively. This study highlights the potential of this innovative photocatalyst for the removal of dyes and medical waste from water under solar light.

Key words: kaolin-carboxyl graphene, g-C_3N_4, Degradation, Methylene blue, Cefepime, Solar light

1. Introduction

In the contemporary era, the expeditious progression of the agricultural and industrial sectors has engendered a noteworthy societal quandary: the pervasiveness of water contamination arising from the discharge of organic pollutants such as organic dyes, pesticides, and other deleterious organic substances like pharmaceuticals into aquatic reservoirs. Pharmaceuticals, especially antibiotics, are crucial for human health and veterinary medicine. However, excessive consumption and improper disposal of pharmaceutical waste into the aquatic sources contribute to antimicrobial resistance and global health threats. From this vantage point, guaranteeing the well-being and survival of living organisms necessitates the critical undertaking of purifying water. Multiple methodologies, encompassing biological treatment, membrane filtration, and catalytic

310-380 nm the highest intensity peak was observed at a wavelength of 340 nm (**Fig. 1b**) [6].Fourier transform infrared (FTIR) spectroscopy analysis was used to investigate the surface functional groups of the as-prepared CDs. The broad peak at 3260 cm^{-1} indicates the presence of hydroxyl group and the absorption at 2961 cm^{-1} is attributed to C-H stretching vibration. The peaks at1639 cm^{-1} and 1452 cm^{-1} corresponds to C=O and C=C stretching vibrations respectively.The band at 1391cm^{-1} and1077 cm^{-1} could be assigned to bending vibrations of C-H and C-O bonds [12]. The FTIR study suggests that the CDs have a hydroxy group on their surface and have negatively charged moieties, which account for their water solubility (**Fig. 1c).**

Morphological features of the synthesized CDs were investigated using transmission electron microscopy. Well dispersed and spherical carbon dots with a diameter of 9.3 nm was obtained as shown in **Fig. 2** (a and b). The charge of the surface functionalities on carbon dots was investigated using zeta potential analysis and it was found to be -11.4 mV. This also indicates the stability of CDs in aqueous dispersion.

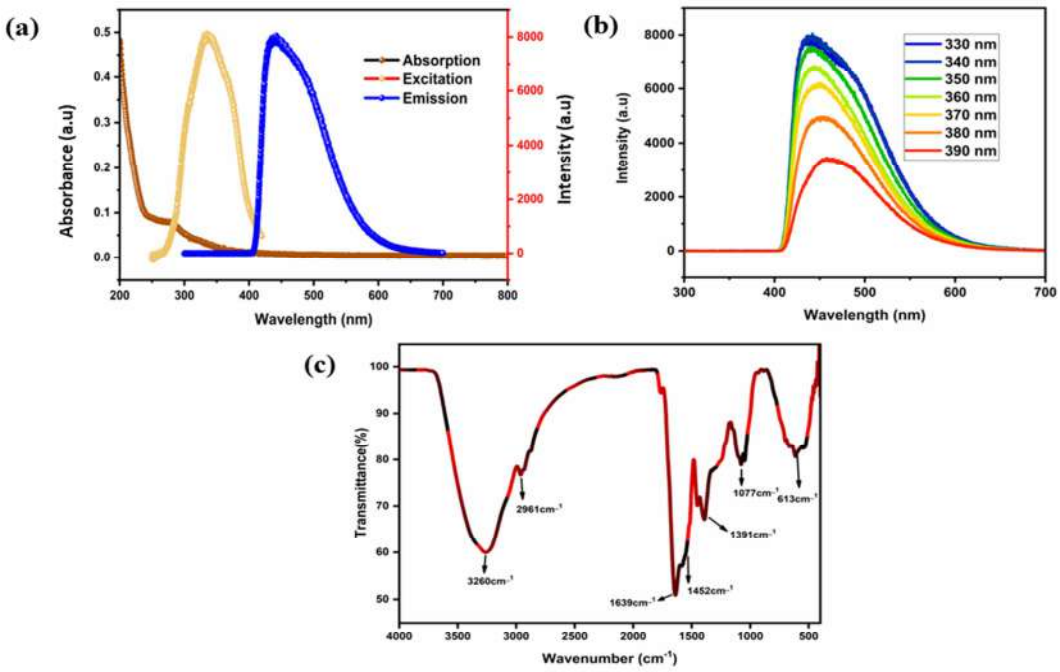

Figure 1: (a) Absorption, excitation and emission spectrum, (b) emission spectrum at different excitation wavelengths, and (c) FT-IR spectrum of CDs

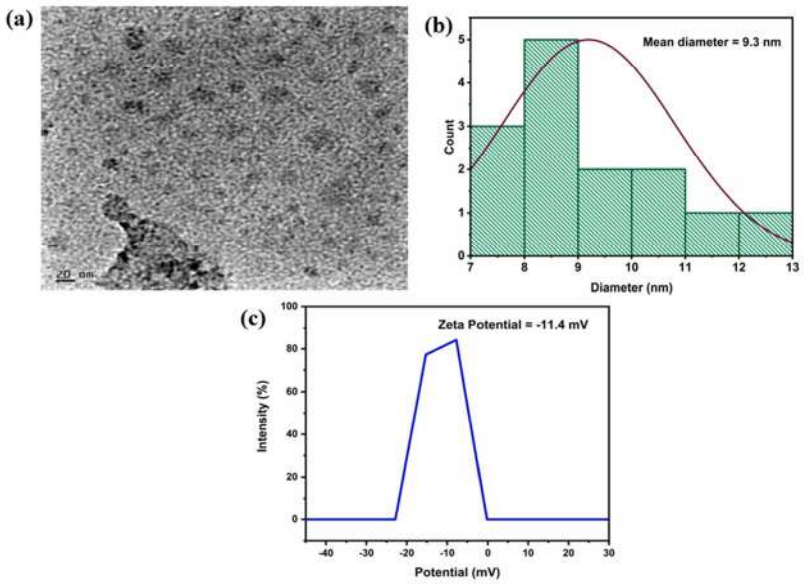

Figure 2: (a) TEM image, (b) size distribution histogram, and (c) zeta potential curve of CDs

3.2 Stability analysis

The ionic strength of solution is a crucial factor so their effect of emission intensity of as-prepared CDs was investigated at different concentrations of potassium chloride (0.1-0.9M). **Fig. 3a** shows no obvious change of emission intensity of CDs under these ionic concentrationsimplying thatthe synthesised CDs possess remarkable stability to highly ionic solutions.The luminescent property of the as-prepared CDs in different pH solutions was explored [13]. The results reveal that the CDs displays almost stable photoluminescence within 3-12 pH range (**Fig. 3b**). The stability of CDs under photoirradiation was also investigated and it was found that the CDs were stable upon continuous irradiation (**Fig. 3c**).

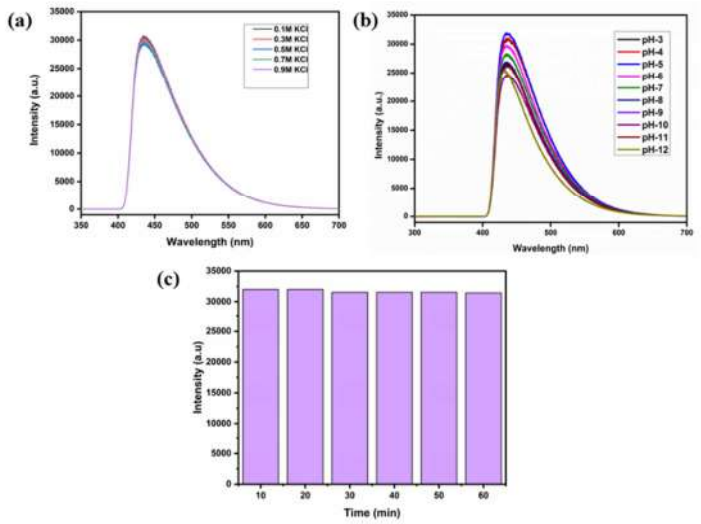

Figure 3: Stability of CDs at (a) different ionic strengths, (b) different pH and (c) photoirradiation time

3.3 Detection of levofloxacin using fluorescence spectroscopy

In recent years, the development of fluorescence-based sensors for selective and sensitive detection of drugs has been pursued by various researchers [14-17]. To determine the ability of CDs obtained from *Sauropusandrogynus* for analytical purposes, their fluorescence intensity in the presence of various drugs were studied.It was observed that levofloxacin enhanced the fluorescence of CDs, thereby showing higher selectivity of the as-prepared CDs toward levofloxacin than other drugs (**Fig.4a**). Thus, from the above observations, the as-prepared CDs can be utilized as a fluorescent sensor for sensitive and selective detection of levofloxacin.

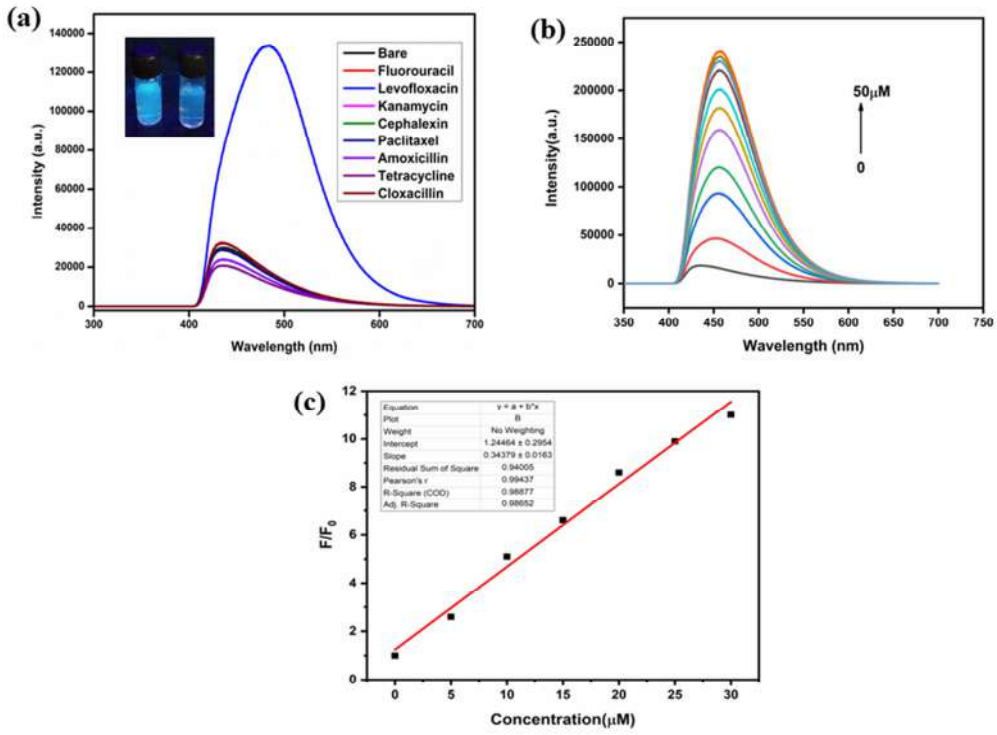

Figure 4: (a) Fluorescence response of CDs in the presence of different antibiotics, (b) different concentrations of levofloxacin, and (c) linear relation between F/F_0 and levofloxacin concentrations

Fig. 4b shows the change in the PL intensity of the CDs at different concentration of levofloxacin (0-50 μM). It was observed that with increase in the concentration of levofloxacin the fluorescence intensity has gradually enhanced.The fluorescence enhancement efficiency can further be described by the Stern–Volmer plot depicting a perfect linear behaviour [6].**Fig. 4c**shows the relative fluorescence response as (F/F_0) as a function of levofloxacinconcentration in the range of 0-30μM. The linear equation was, F/F_0 = 1.24464+0.34379 [levofloxacin] (F and F_0 were the PL intensity in the presence and absence of levofloxacin, respectively), which suggests that by using the as-prepared CDs the detection of levofloxacin is completely feasible. The limit of detection (LOD) was calculated by using the equation 3σ/m (where σ is the standard deviation of blank signal (n=3) and m is the slope of the linear fit) and was found to be 0.67 μM.

Different factors, including pH and experimental period, were tuned to improve the antibiotics' fluorescence response.

Influence of pH: The impact of the pH (3-12) on the emission intensity of the probe was tested, and it was determined that the mechanism was pH-dependent. Fluorescence enhancement rose with pH for levofloxacin, but after attaining a maximum at pH 4, enhancement efficiency dropped (**Fig. 5a**). Therefore, pH 4 was selected as the working pH for levofloxacin detection.

Influence of experimental period: The reaction time was tuned to ensure that the reaction was completed. After 5 minutes of incubation, there were no discernible alterations in the F/F_0 signals (**Fig. 5b**).

Interference studies were also performed to confirm the practicability of the sensor in the presence of other drugs in the same concentration. As shown if **Fig. 5c**, the presence of other drugs does not impart any changes in the fluorescence enhancement of CDs using levofloxacin.

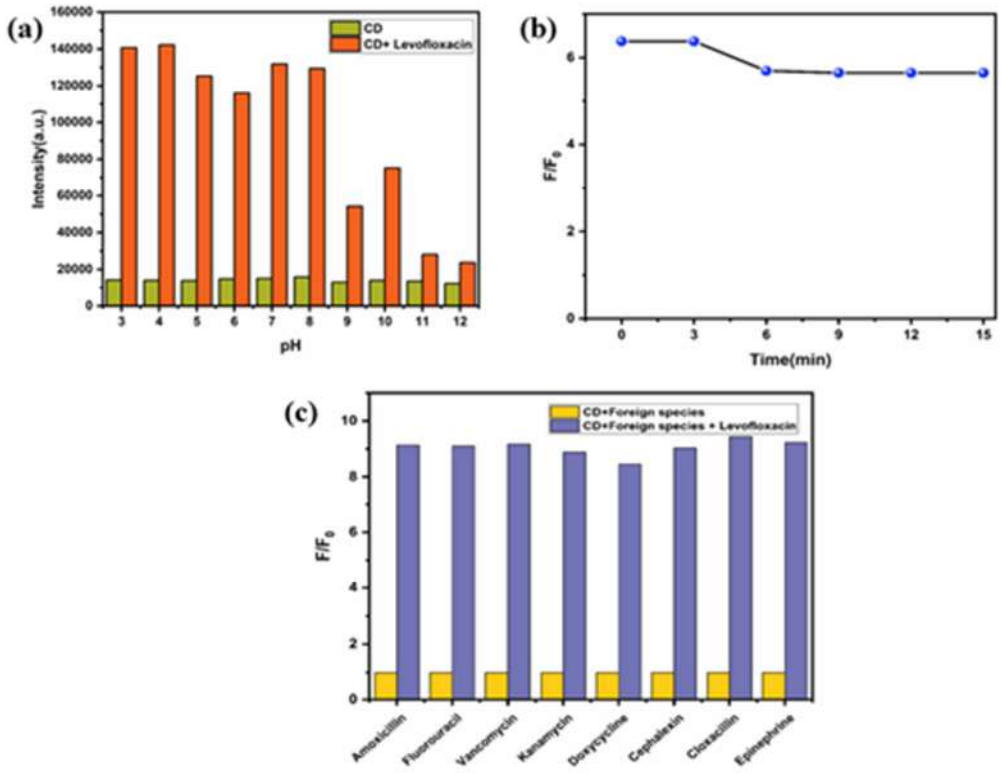

Figure 5: Optimization of (a) pH and (b) time for the detection of levofloxacin, (c) interference studies in the presence of different antibiotics

3.4 Mechanism for the fluorescence sensing of levofloxacin

The surface of the as-prepared CDs is abundantly covered in hydrophilic groups, including carboxylic and hydroxyl groups, according to FTIR and XPS measurements. Both the ability to form hydrogen bonds with levofloxacin and water solubility are provided by these functional groups [18,19]. The nonradiative decay would be further reduced by increasing the distance between the CDs, which would be caused by the electrostatic repulsion between the levofloxacin absorbed on the surface of the CDs. Additionally, the levofloxacin attached may change the surface defects of the CDs, resulting in the enhancement of the PL intensity [20-22]. Despite this, more research is necessary to determine the precise mechanism of fluorescence enhancement.

3.5 Real sample analysis

When it comes to guaranteeing a sensor's function in environmental protection, the sensor's practicability is always crucial. The proposed sensor exhibits high selectivity and sensitivity for levofloxacin fluorescence detection. This allowed for a direct examination of levofloxacin in real water samples. For this objective, tap water and river water samples were collected. Before being spiked with different analyte concentrations, these samples were pre-processed. For the determination of levofloxacin in water samples, fluorescence intensity measurements were utilized to compute recovery percentages and RSD values (**Table 1**). The acquired RSD values demonstrate the precision and accuracy of the experiment, which was repeated three times.

Table 1. The sensing of levofloxacin in real samples through fluorescence analysis

Sample	Analyte	Measured(μM)	Added (μM)	Found (μM)	Recovery (%)	RSD (%) n=3
Tap water	**Levofloxacin**	-	10	11	110	2.7
			20	19.5	97.5	5.1
			30	32.16	107.2	2.3
River water	**Levofloxacin**	-	10	10.5	105	2.5
			20	22	110	1.6
			30	35	116.6	1.4

4. Conclusions

In this work, we successfully synthesized CDs from *Sauropusandrogynus*leaves by hydrothermal method. Optical and physicochemical properties of as-synthesized CDs were thoroughly characterized using various analytical techniques. CDs exhibited strong fluorescence, which is stable to various effects like pH, ionic strength, and continuous irradiation. Real sample analysis was also found successful for the detection of levofloxacin. With all of the advantages of the CDs developed in this study, a quick response, stable, highly sensitive, and selective detecting approach for the quantitative detection of trace amounts of levofloxacin has been formulated.

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OP14

A New greenMulticomponent synthetic Protocol for the synthesis of

β-acetamido ketone derivatives

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Abstract

A simple and efficient multicomponent protocol for the synthesis of β-acetamido ketones via the one-pot condensation of aryl aldehydes, enolizable aryl ketones, acetyl chloride and acetonitrile using $ZnCl_2$ is described. The current method offers many advantages such as short reaction times, easy workup procedures and good-to-excellent yields of products.

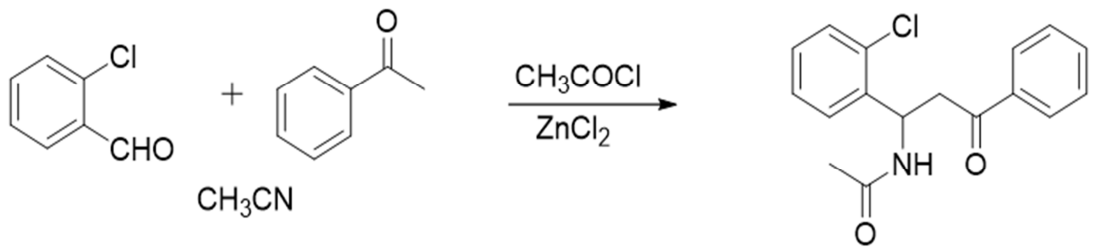
Key Words: Multicomponent reaction,Green chemistry,*β*-Acetamido ketone, Zinc Chloride, Nontoxic catalyst

1. Introduction

Multicomponent reactions (MCRs) are one-pot reactions which involve three or more components and they show high atom economy and excellent selectivity, they have an outstanding status in modern organic synthesis and medicinal chemistry.[1]MCRs have become effective tools for drug discovery and have a significant impact on the convergent synthesis of important and complex organic molecules from simple and easily accessible starting components.[2-12] *β*-Acetamido ketones are expedient building blocks for a number of biologically and pharmaceutically valuable scaffolds.[13-17] They are building blocks for compounds like 1,3-amino alcohols and the structural scaffolds of naturally occurring nucleoside peptide antibiotics like neopolyoxins and nikkomycins and β-acetamido ketones can act as aglucosidase inhibitors.[18] A number of methods have been reported for the synthesis of β-acetamido ketones through multicomponent reactions, used catalysts such as montmorillonite K10,[19]selectfluorTM,[20] H6P2W18O62,[21] H3PW12O40,[22]$Zr(HSO_4)_4$,[23] $Mg(HSO_4)_2$,[24] $BiCl_3$,[25] silica sulfuric acid,[26] ZnO,[27] TMSCl,[28]I_2,[29] sulfamicacid,[30]$CoCl_2$,[31-33] and $ZrOCl_2.8H_2O$.[34] Most of these methods suffer from some disadvantages such as, low yield, high reaction

temperature, expensive reagent,performance of the reaction under certain special conditions etc.Therefore, it is still important to find a practical, affordable, easy-to-use, and non-polluting process for synthesising *β*-acetamido carbonyl compounds.

In recent years, the applications of environmentally benign, green catalysts have received significant interest. Green chemistry is the usage of a set of principles that reduces the generation of hazardous substances in the synthesis and application of chemical products. Hence, using Zinc chloride ($ZnCl_2$), which is green, inexpensive and less toxic, has found more attention.We report herein $ZnCl_2$catalysed one-pot multicomponent reaction of acetophenones, arylaldehydes, and acetyl chloride in acetonitrile for the synthesis of *β*-acetamido ketones (Scheme 1).



Scheme 1. Zncl$_2$catalysed synthesis of *β*-acetamido ketones

2. Experimental

All the chemicals were purchased from Aldrich, Merck, and Fluka. TLC was used to monitor the reactions. Using a Perkin Elmer Infrared FTIR spectrophotometer, the IR was measured. JEOL (JNM-ECZ400s) DMSO-D6 was used to record the ^{1}H and ^{13}C NMR spectra, with TMS functioning as the internal standard. mass spectra (MS) was recorded using Shimadzu LCMS-8045 spectrometer.

2.1 General procedure for the preparation of *β*-acetamidoketones(2a-2c):

A mixture of aryl aldehydes (1 mmol),enolizable aryl ketones (1 mmol), acetyl chloride (1 ml), acetonitrile (2 mL) and Zncl$_2$ (25 mol %) was stirred at room temperature. After completion of reaction (monitored by TLC), the reaction mixture was added to ice water. The product was filtered, washed with diethylether and recrystallized from ethanol to give compounds (2a-2c) in high yields. FT-IR,^{1}H NMR,^{13}C NMR, and Mass spectra are used to identify isolated products.

3. Results and discussion

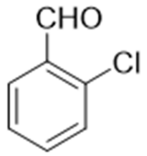
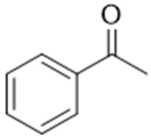
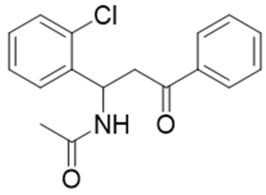
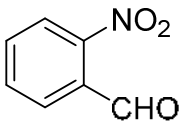
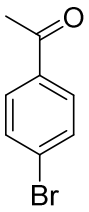
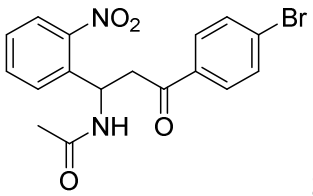
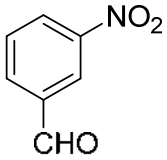
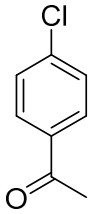
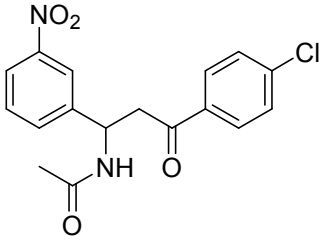
We started our studies by employing $ZnCl_2$ as a catalyst to synthesise the *β*-acetamido ketone. For the optimizations, 2-chlorobenzaldehyde and acetophenone was selected as the reaction.Using acetonitrile as the solvent, reactions were optimised with respect to quantity of catalyst, reaction time, and temperature.We decided to conduct the screening experiments at room temperature and observed that a highest yield of 89% is obtained from a reaction containing 25mol% of the catalyst, and no noticeable variation in the yield was seen after addingadditional mole of catalyst.

Table 1. Optimization of catalyst for the synthesis of *β*-acetamido ketone derivatives.

Entry	Catalyst (mole%)	Temperature (^{o}C)	Time (min)	Yield (%)
1	No Catalyst	Rt	120	-
2	No Catalyst	80	60	-
3	5	80	60	33
4	10	80	60	55
5	5	Rt	60	33
6	10	Rt	60	55
7	15	Rt	60	72
8	20	Rt	60	84
9	25	Rt	60	89
10	30	Rt	60	89

To show the efficiency of this catalyst, a variety of aryl aldehydes were reacted with substituted aromatic ketones, acetyl chloride, and acetonitrile to generate various substituted *β*-acetamido ketone derivatives under the optimal reaction conditions. All desired products were obtained in good to excellent yield. Detailed list of synthesized compounds are given in Table 2.

Table 2. Synthesis of substituted *β* acetamido ketone derivatives using $Zncl_2$ as catalyst

Entry	Aldehyde	ketone	Product	Yield (%)
1			 **2a**	**91**
2			 **2b**	**90**
3			 **2c**	**92**

Synthesised compounds were identified by their FT-IR,^{1}H NMR,^{13}C NMR, and Mass spectra. Spectral data for isolated *β*- acetamido ketone derivatives are given below.

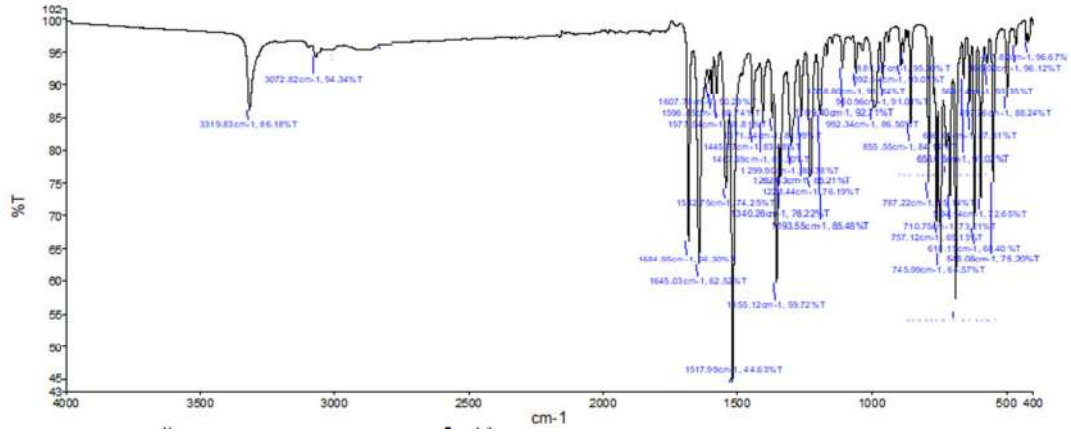


Figure 1: FTIR Spectra ofN-(1-(2-chlorophenyl)-3-oxo-3-phenylpropyl) acetamide**2a**

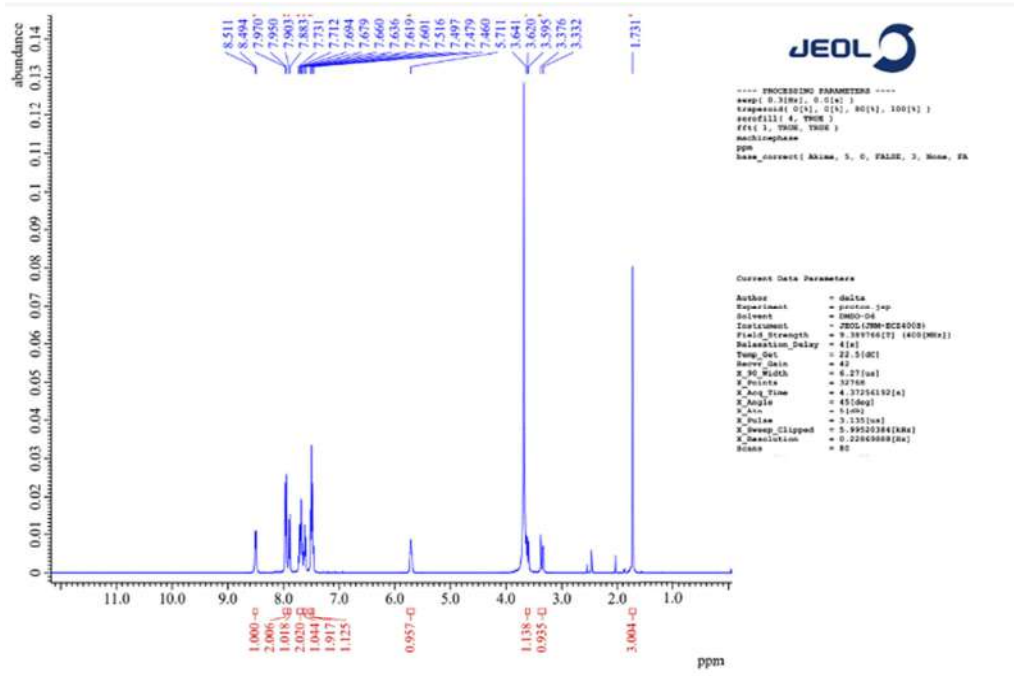


Figure 2: [I]H NMR Spectra of N-(1-(2-chlorophenyl)-3-oxo-3-phenylpropyl) acetamide **2a**

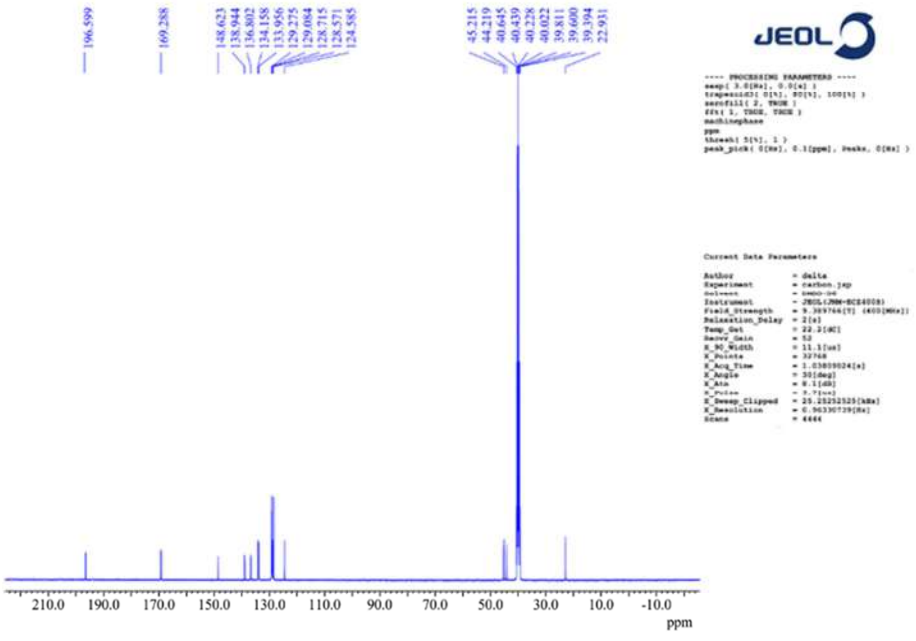


Figure 3: [13]C NMR Spectra ofN-(1-(2-chlorophenyl)-3-oxo-3-phenylpropyl) acetamide **2a**

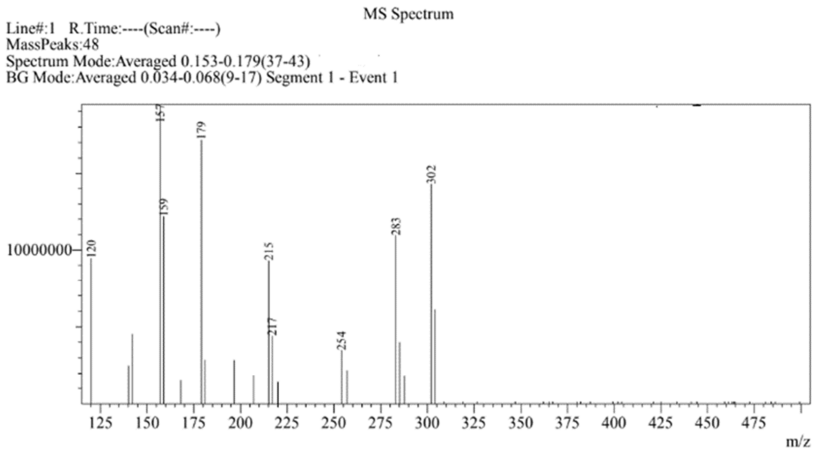


Figure 4: Mass Spectra ofN-(1-(2-chlorophenyl)-3-oxo-3-phenylpropyl) acetamide **2a**

4. Conclusion

In conclusion, we describeanexpedient and efficient method for the synthesis of *β*-acetamido ketones through the condensation of an aryl aldehyde, an acetophenone, acetyl chloride, and acetonitrile in the presence of $Zncl_2$ as a catalyst at room temperature. This method offers many advantages such as easy to perform, short reaction time, low cost, and non-toxic catalyst.These $Zncl_2$-catalyzed reactions provided the desired *β*-acetamido ketones in excellent yield.

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OP15

Anti-Snake Venom Activity of Various Flavonoids on Phospholipase A2: *In Silico* Evaluation

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Abstract

Molecular docking simulations were performed using the ligands Naringenin, Quercetin, Kaempferol, Rutin, Vitexin, and Apigenin against the receptor 2ARM, Phospholipase A2 enzymes found in the venom of Russell's viper (Daboia russelii). Studies revealed that all ligands have favorable binding affinities with the target molecule, as evidenced by the negative binding energies. Among the tested ligands, Vitexin exhibits the highest binding affinity, with a binding energy of -8.9 Kcal/mol, followed by Rutin with a binding energy of -8.1 Kcal/mol. Naringenin, Quercetin, Kaempferol and Apigenin also show relatively strong binding affinities, with binding energies ranging from -7.2 to -8.0 Kcal/mol. These results provide useful information for the development of potential drug candidates or for the design of experiments to further investigate the binding interactions between these ligands and the target molecule.

1. Introduction

Russell's Viper (Daboia russelii) is a major contributor to snakebite morbidity and mortality spanning over 10 South-East Asian countries, including the Indian subcontinent. The venom of Russell's Viper consists primarily of a complex mixture of bioactive components, with proteins and peptides being the predominant elements [1]. These venom components have the potential to influence on various stages of blood coagulation, contributing to the severity of envenomation [2]. Snake venom contains numerous proteases which interfere with the haemostatic system of victims; however, phospholipase A2 (PLA2) is documented as one of the major anticoagulant components in venom of Viperidae family of snakes including Russell's Viper [3]. Venom PLA2 plays a significant role in pathogenesis of snakebite by interfering with the blood coagulation process either by hydrolyzing the phospholipids of plasma

and/or platelets membranes [4]. Therefore, any compound capable of inhibiting this activity holds promise as a potential lead molecule for antivenom development. In this study, the inhibitory effect of various flavonoids is evaluated against a major phospholipase A2 (PLA2), *viz* 2ARM by molecular docking studies [5].

1.1. Docking

Docking is a computational method which predicts the preferred orientation of one molecule with another when bound to form a stable complex with overall minimum energy [6]. It is used to analyze the binding mode and strength of ligand (small molecule) to a receptor (macromolecule such as a protein) [7]. The process involves simulating the interaction between the ligand and receptor to determine how they fit together and whether they form stable complexes and is widely used in drug discovery and also in fields of biochemistry and biophysics [8].

1.2. Flavonoids

Flavonoids are a group of natural compounds found in plants that have been shown to have various health benefits, including anti-oxidant, anti- inflammatory and anti- viral properties [9]. Flavonoids are the most common group of polyphenolic compounds in the human diet. They are secondary metabolites, meaning they are organic compounds that have no direct involvement with the growth or development of plants. The selected flavonoids for study are: Naringenin, Quercetin, Kaempferol, Rutin, Vitexin, Apigenin [10].

2. Experimental Methods

2.1. Protein preparation

The 3D crystal protein-structures of 2ARM were extracted from the RCSB PDB database (https://www.rcsb.org/). The 3D crystal structures of 2ARM were prepared for molecular dockingusing Discovery Studio software to remove all ligands, non-protein parts and water molecules.

2.2. Molecular Docking

Molecular docking simulation was carried out to analyze the protein-ligand interaction mechanism to obtain information about the binding affinity and ligand activity. In the present work, we performed the molecular docking analysis using AutoDock Tools and AutoDock 4.2 software, to analyze docked conformations and the

interaction between the ligand and the protein [11]. The 3D grid was generated by the AUTOGRID algorithm to evaluate the ligand-receptor. interaction energy. The defined coordinates of the 2ARM -phospholipase A2 binding site region are located on the active site of Ala 18, Tyr 22, His 48 and Asp 49 [12]. The grid maps were constructed with a value of 60 Å in all directions (X, Y, Z axes), with a default grid spacing of 0.375 Å, the Grid Coordinates for the main protease binding site determined as (x = 12.18, y = 0.65, z = 4.66). The established interaction analysis as well as the 2D and 3D visualizations were exploited using the BIOVIA Discovery Studio Visualizer 2020.

3. Results and Discussions

3.1. Analysis of the binding modes of the flavonoids with 2ARM

The 2D visualization of the best active compounds, based on the number of hydrogen bondswith the important amino acids of the 2ARM -phospholipase A2, were presented in Figure 1. Figure 1shows that Naringenin, Quercetin, Kaempferol, Rutin , Vitexin , Apigenin formed several hydrogen bonding interactions with the residues Ala 18 , Tyr 22, His 48 and Asp 49 inthe deepest regions of the 2ARM -phospholipase A2 active site. As a result, they are able to cover the receptor binding pocket of this protein, which prevents phospholipase A2 and transcription. Furthermore, we observed a strong correlation between the best interactions formed with 2ARM -phospholipase A2 and the high docking score observed for these compounds. However, the high docking score does not reflect the position and formation of strong interactionswith the active site of 2ARM -phospholipase A2. These results indicate that these ligands could be studied as a potential therapeutic solution against phospholipase by inhibiting virus replicationand transcription.

3.1.a. 2D visualization of binding modes of the flavonoids with 2ARM

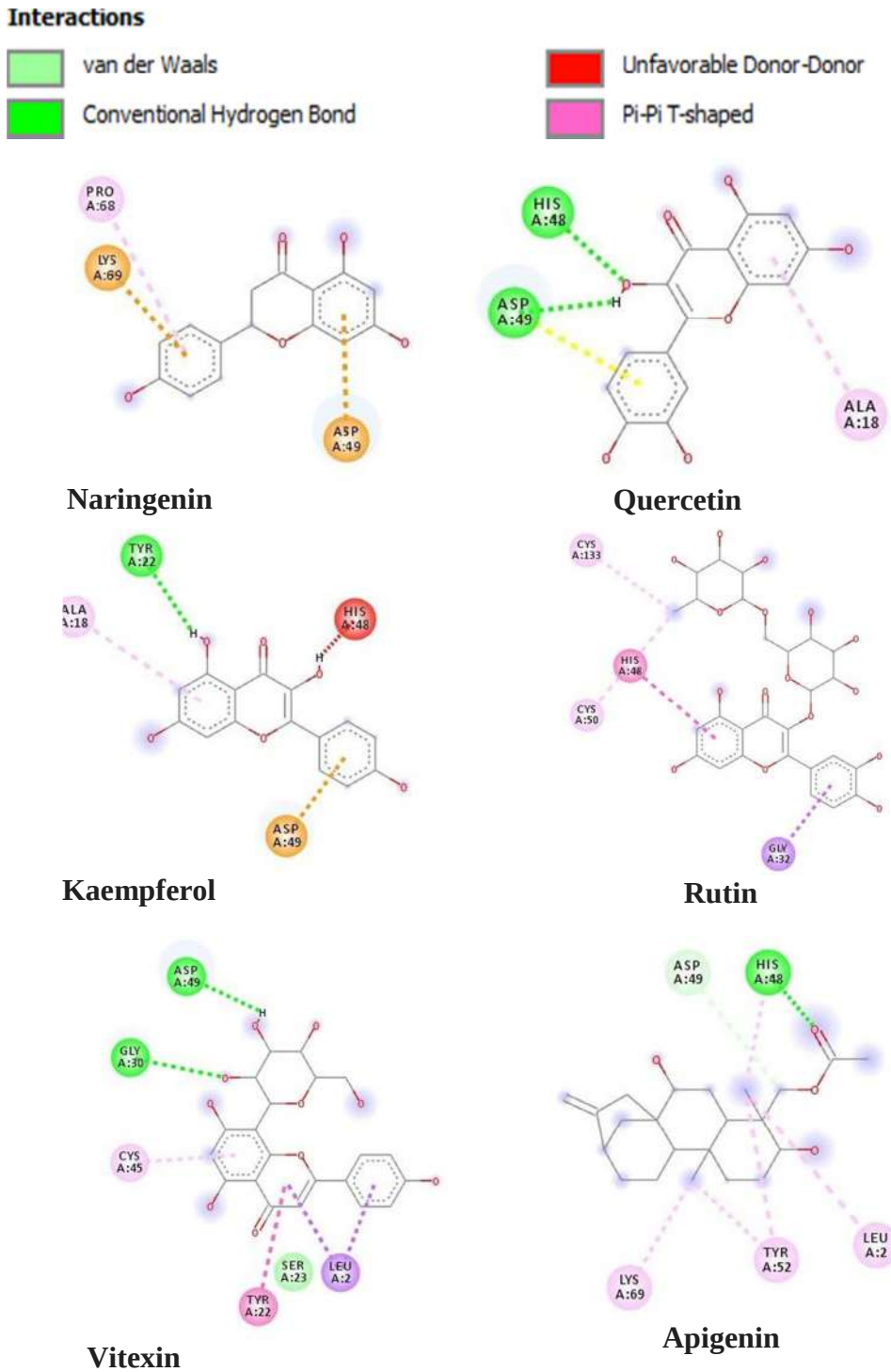

Figure 1: 2D visualization of binding modes of the flavonoids with 2ARM

3.1.b. 3D visualization of binding modes of the flavonoids with 2ARM

The 3 D visualization of the best active compounds, based on the number of hydrogenbonds with the important amino acids of the 2ARM -phospholipase A2 were presented in Figure

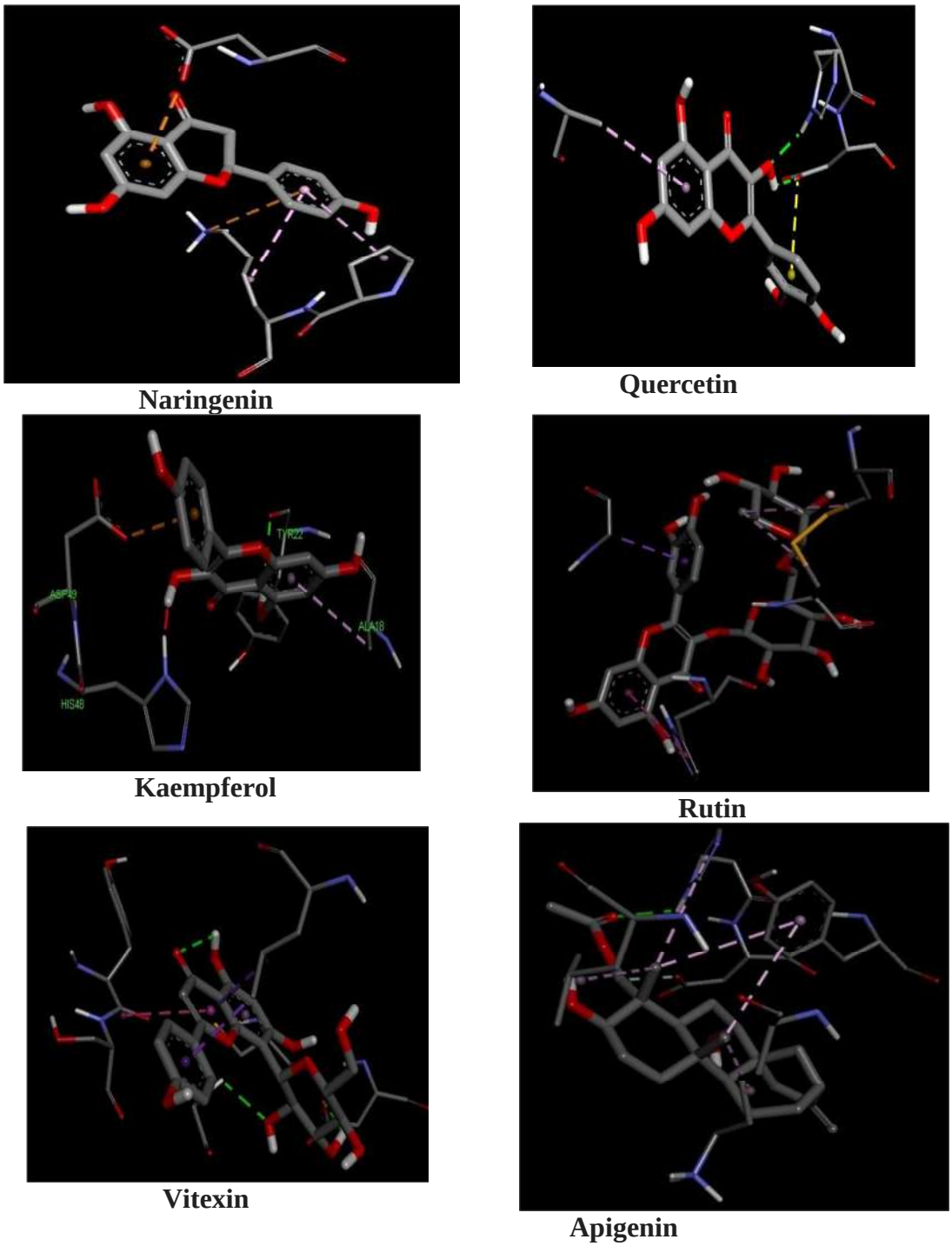

Figure 2: 3D visualization of binding modes of the flavonoids with 2ARM

Molecular docking simulations typically evaluate the strength of interactions between the ligand and the target molecule, including van der Waals interactions, hydrogen bonding, and electrostatic interactions. In the case of Vitexin, its chemical structure may have allowed for favorable interactions with the binding site of the target molecule, leading to a high binding affinity.

3.2. Analysis of the binding modes of the flavonoids with 2ARM

The computer-aided drug design (CADD) approach is a dynamic research area. Computational screening of compounds has been extensively employed in recent years, includingscreening, design, identification of new drugs against phospholipase A2. Therefore, we performedmolecular docking of the studied ligands with 2ARM - phospholipase A2. Table 1 shows the results of the calculated binding affinities of each ligand.

Table 1: Binding affinity of 2ARM with Ligands.

Ligands	**Binding Energy ((Kcal/mol)**
Naringenin	-7.2 Kcal/mol
Quercetin	-7.9 Kcal/mol
Kaempferol	-8.0 Kcal/mol
Rutin	-8.1 Kcal/mol
Vitexin	-8.8 Kcal/mol
Apigenin	-7.6 Kcal/mol

Studies revealed that all ligands have favorable binding affinities with the target molecule, as evidenced by the negative binding energies. Among the tested ligands, Vitexin exhibits the highest binding affinity, with a binding energy of -8.9 Kcal/mol, followed by Rutin with a binding energy of -8.1 Kcal/mol. Naringenin, Quercetin, Kaempferol and Apigenin also show relatively strong binding affinities, with binding energies ranging from -7.2 to -8.0 Kcal/mol. These results provide useful information for the development of potential drug candidates or for the design of experiments to further investigate the binding interactions between these ligands and the target molecule.

4. Conclusion

Molecular docking simulations were performed using the ligands Naringenin, Quercetin, Kaempferol, Rutin, Vitexin, and Apigenin against the receptor 2ARM - phospholipase A2 . The results of the docking simulations are summarized as follows:

Based on the data provided, molecular docking simulations suggest that all of the tested ligands have favorable binding affinities with the target molecule, as evidenced by the negative binding energies. Among the tested ligands, Vitexin exhibits the highest binding affinity, with a binding energy of -8.9 Kcal/mol, followed by Rutin with a binding energy of -8.1 Kcal/mol. Naringenin, Quercetin, Kaempferol and

Apigenin also show relatively strong binding affinities, with binding energies ranging from -7.2 to -8.0 Kcal/mol. These results provide useful information for the development of potential drug candidates .Naringenin, Quercetin , Kaempferol , Rutin , Vitexin , Apigenin formed several hydrogen bonding interactions with the residues Ala 18 , Tyr 22, His 48 and Asp 49 in the deepest regions of the 2ARM active site. Asa result, they are able to cover the receptor binding pocket of this protein, which prevents 2ARMand transcription.

Vitexin exhibits the highest binding affinity among the tested ligands, with a binding energyof -8.8 Kcal/mol, because it has a favorable chemical structure that can form strong interactions with the target molecule. Molecular docking simulations typically evaluate the strength of interactions between the ligand and the target molecule, including van der Waals interactions, hydrogen bonding, and electrostatic interactions. In the case of Vitexin, its chemical structure may have allowed for favorable interactions with the binding site of the target molecule, leading to a high binding affinity. Additionally, the presence of functional groups such as hydroxyl groups, which are known to be important for ligand binding, may have contributed to Vitexin's strong binding affinity.

In conclusion, molecular docking simulations suggest that all tested ligands have the potential to bind to the target molecule, with some showing stronger binding affinities than others.These results provide useful information for the development of potential drug candidates or for the design of experiments to further investigate the binding interactions between these ligands andthe target molecule.

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OP16

Facile fabrication of Ni coated MnO_2 incorporated high performance Al-Zn alloy metal matrix composites as efficient sacrificial anodes

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Abstract

In Al-based metal matrix composites (MMCs), the ceramic composites play a key role to attain enhancement in various metallurgical and galvanic characteristics. The metallic coating on ceramic composites were often used to improve better bonding and wettability between metal matrix and composites. In this work, nickel coated MnO_2 was prepared by electroless nickel coating method and was beneficially explored into Al-Zn alloy anode matrix to achieve synergistic activation enhancement. The incorporation of MnO_2-Ni into Al-Zn alloy anodes was micro-structurally and electrochemically characterized. The metallurgical and galvanic characteristics of the anode were improved substantially by uniform dispersion of MnO_2-Ni into the Al-Zn alloy matrix. The effective dispersion of MnO_2-Ni in the alloy matrix can provide numerous lattice activation centers and intercalation channels, facilitated effective destruction of the passive alumina film. Very high galvanic efficiency of was achieved by fine tuning of MnO_2-Ni composite into the Al-Zn alloy metal matrix. The anode exhibited active open circuit potential, very low polarization and non-columbic metal loss during prolonged galvanic exposure studies.

1 Introduction

Aluminum is one of the most effective and economical substrate for cathodic protection of steel due to its high current capacity, low density, inherent negative potential and reasonable cost [1,2]. However, pure Al supports nano range protective oxide film, which make it useless as sacrificial anode. The addition of alloying elements like In, Ga, Ce, Hg, La, Se and Zn shifts open circuit potential (OCP) from –1.18 to –1.10 V versus saturated calomel electrode (SCE), an operating potential from –1.12 to –1.05 V versus SCE, a current efficiency of more than 85 %, and an anode capacity of more than 2600h Kg^{-1} [3], causing so-called activation of Al alloy sacrificial anode. Most of the works in the field were carried out on Al-rich Zn sacrificial anode where Zn destabilize the Al_2O_3

layer due to the formation of $ZnAl_2O_4$ spinel, and the concentration of Zn has been optimized to 5 Wt % due to high improvement in metallurgical and electrochemical properties of the alloy through the formation of beta-phase [4].

Discontinuously reinforced aluminum metal matrix composites exhibits blending properties of both composites and matrix leads to substantial improvement in physicochemical and galvanic characteristics [5]. The incorporation of metal composites can also improve grain boundaries, suppressing grain boundary corrosion of the metal. The composites of Al and Mn have been used for the fabrication of high wear resistant sacrificial anode. The inclusion of CeO_2, SiO_2, ZrO_2, and TiO_2 in the Al matrix can effectively suppress the non-columbic metal loss leading to considerable improvement in galvanic characteristics [6]. It is well known that the fabrication and performance of metal matrix composites are strongly influenced by the composite-matrix interface and the wetting nature of the composites with molten metal [7]. The most important metals used to coat the composites are copper and nickel. Nickel and copper coatings on carbon fiber and graphite prior to dispersion, enhanced the wettability with molten aluminum. The incorporation of optimum amount of nickel in to manganese oxide remarkably enhances its capacitive performance, high power property, good cycling stability and moreover the presence of MnO_2 in aluminum matrix can form $MnAl_6$ which in turn significantly improves both psychochemical and metallurgical characteristics of aluminum metal matrix. In this context, the present study beneficially explores nickel deposited MnO_2 for developing high performance Al-Zn alloy matrix sacrificial anodes with a view of its enhanced wettability.

2 Experimental methods

2.1 Electroless nickel deposition

Commercially available MnO_2 (Merck India, assay-99.90%,) with average grain size from 7 to 10 □m were used, were initially ball-milled for 2 h to break up agglomerates. For nickel deposition, the bath was selected which has the following composition: Nickel sulphate- 35 g L^{-1}, sodium hypophosphite- 20 g L^{-1}, sodium citrate- 15 g L^{-1}, sodium acetate- 5 g L^{-1}, and 0.5 g L^{-1} tetra butyl ammonium bromide (TBAB).

2.2 Fabrication of the anode

Commercially available Al (99.75 %) and Zn (99.95 %) ingots were used for casting Al + 5% Zn alloy sacrificial anode. The alloy ingots were cut, weighed and melted

in a graphite crucible, kept in muffle furnace at 700□ C. Different amounts of nickel coated MnO_2 particles were added to the melt and stirred using a SiC rod to homogenize it. The melt was again kept in muffle furnace for 15 min at the same temperature and poured in to a preheated graphite die of dimension 5.5 x 3.5 x 0.5 cm.

2.3 Electrochemical characterization

2.3.1 OCP, CCP and Potentiodynamic polarization evaluation

The open circuit potential (OCP) versus time up to 60 days was interpreted in terms of the electrode-electrolyte interphase. The closed circuit potential (CCP) of the test anodes with respect to SCE was continuously monitored when the anode was coupled with mild steel cathode. Linear sweep voltammetry (LSV) was carried out using an Autolab 80 plus FRA2 corrosion system. The electrolyte used was aerated 3% NaCl solution. Ag/AgCl, Pt and the anodes having 1 cm^2 exposed area were used as reference, counter and working electrodes respectively.

3 Results and discussion

3.1 Interfacial Wettability

To initiate the activation process of composite incorporated metal alloy anodes, the composite should effectively wet the alloy melt. Effective wetting, which is the measurement of liquid metal / solid interface, can be described in terms of contact angle (θ) and surface tension of liquid [8]. The magnitude of contact angle describes the wettability as $\theta = 0^o$, for perfect wetting; $\theta = 180^o$, no wetting and $0^o < \theta < 180^o$ for partial wettability. This means that a low contact angle was indicative of good wettability. The correlation between the wt % of MnO_2, MnO_2-Ni composite and the contact angle in molten Al-Zn alloy is shown in Fig.1. Al-Zn anode showed significant decrease in contact angles with MnO_2-Ni when compared to pure MnO_2. This revealed a decrease in solid/ liquid interfacial energy due to proper modification of the composite with nickel coated interface [9]. There were no marked differences in contact angle with low concentrations of composite (0.01 wt %) due to increase of surface energy.

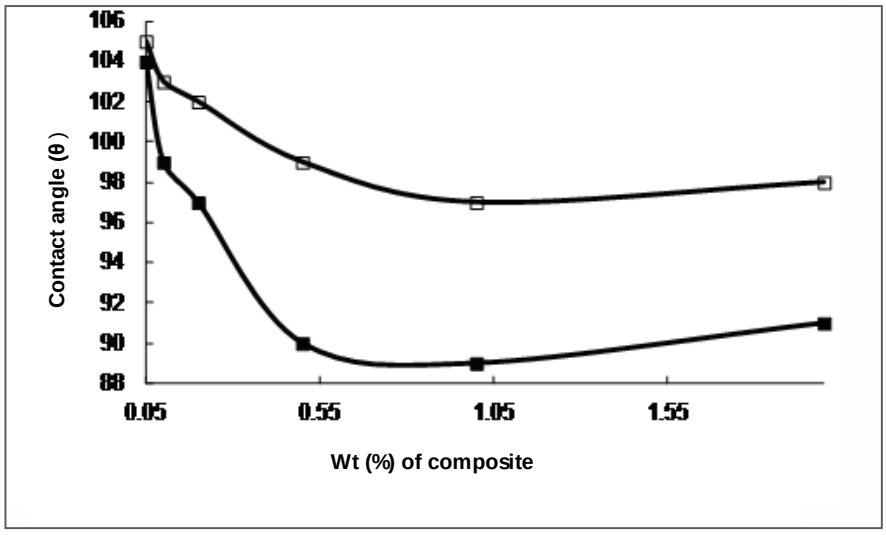

Figure 1: Correlation of wt.% of the composite (□) MnO_2, (■) MnO_2-Ni with contact angle.

Several other important parameters such as surface finish of the solid, purity of the melt, composition, temperature and pressure have significant influence on the contact angle (θ) measurement. Also, it was often difficult to control these parameters and the literature contains many contradictions and inaccuracies attributable to error in measuring the angle.

3.2 *Morphological and microstructural characteristics*

Figure 2 (A) and B demonstrated the morphology of MnO_2 incorporated Al-Zn and MnO_2-Ni with Al-Zn anode. During this analysis a variation in morphology was evident. Spangles-like finish during casting of the aluminium anode resembled many other composite incorporated alloy anodes commonly reported in literature.

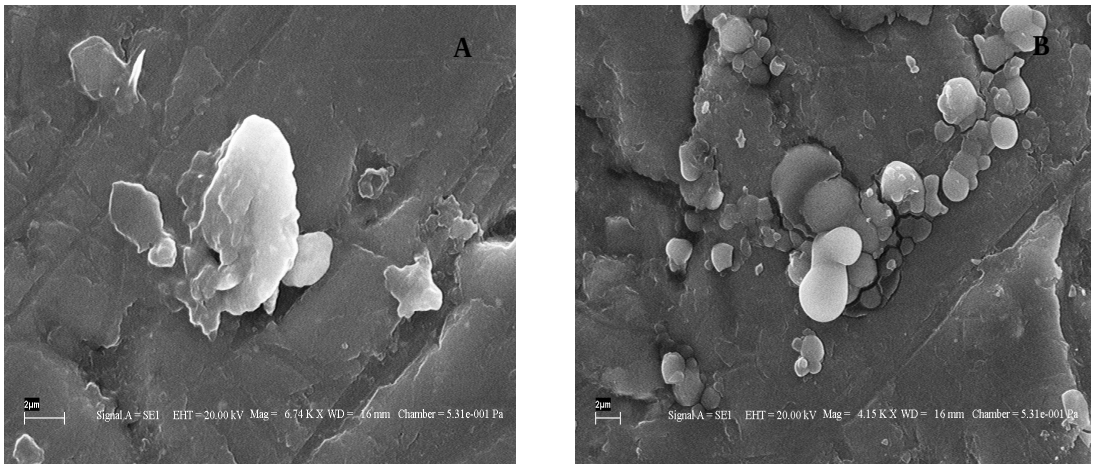

Figure 2: SEM micrographs of Al-Zn incorporated with nano MnO_2 (A), MnO_2-Ni (B)

Intermetallic particles appeared to be bright in image because of higher atomic number in comparison with the Al matrix as shown in Fig. 2. The large particles (μm), called the constituent particles are seen in both MnO_2-NiandMnO_2incorporated anodes. There was also a large number of fine particles (50-200nm white dots of <0.5μm) also called the dispersoids present in nano MnO_2 incorporated anode compared to that of MnO_2-Ni incorporated one. The size of intermetallic particles is larger in MnO_2incorporated Al-Zn anode and also their distribution is not uniform than MnO_2-Ni incorporated anode. Generally, the large micrometer sized inter-metallic particles present causes localized dissolution, initiating on the particle-matrix boundary regions and resulted in higher non-columbic metal loss of the anode [10]. Hence, the presence of smaller intermetallic particles and their uniform distribution can have significant effect on the galvanic and metallurgical performance of anode.

Fig. 3 (A) and (B) depicts the concurrent AFM topography of MnO_2incorporated Al-Zn anode and Fig. 3 (C) and (D)for MnO_2-Ni with Al-Zn anode. A note-worthy variation in topographies of two anodes was evident during the analysis. Generally, both the anodes exhibited the constituent particles (>0.5μm). However, MnO_2-Ni incorporated anode has well defined smaller dispersoid in the matrix compared to MnO_2incorporated anode. This result was in well accordance with morphological characterization by SEM micrograph. Hence it was inferred that MnO_2-Ni incorporation resulting in formation of fine inter-metallics of uniform size than that of MnO_2 incorporation, a favorable criterion for effective metallurgical enhancement of the anode.

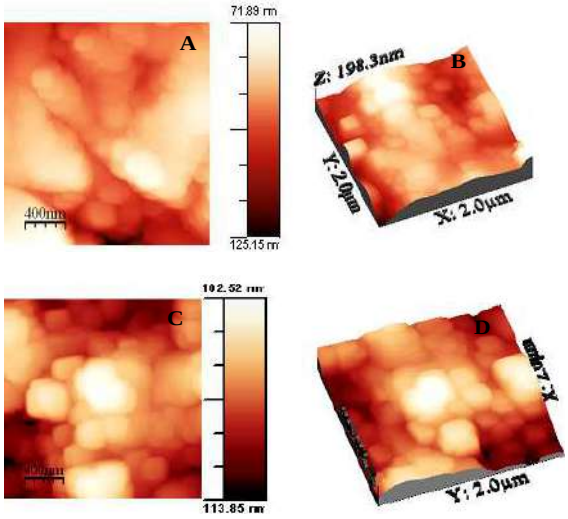

Figure 3: AFM micrographs of Al-Zn + MnO_2(A), Al-Zn + MnO_2-Ni (C); (B) and (D) are 3-D view

3.3 OCP decay

The initial OCP values of MnO_2-Ni incorporated anodes were in -0.960 to -0.989Vrange which shifted to -0.947 to -0.981V following two months of immersion as shown in Fig. 4. The 0.5% MnO_2-Ni incorporated anode exhibits high OCP shift of -0.042V in negative direction as compared to the pure Al-Zn anode. Even after two months of performance review, such a high cathodic change in OCP seemed to be constant. This may be caused by the anode's uneven corrosion, notably pitting in sacrificial anodes. [11].

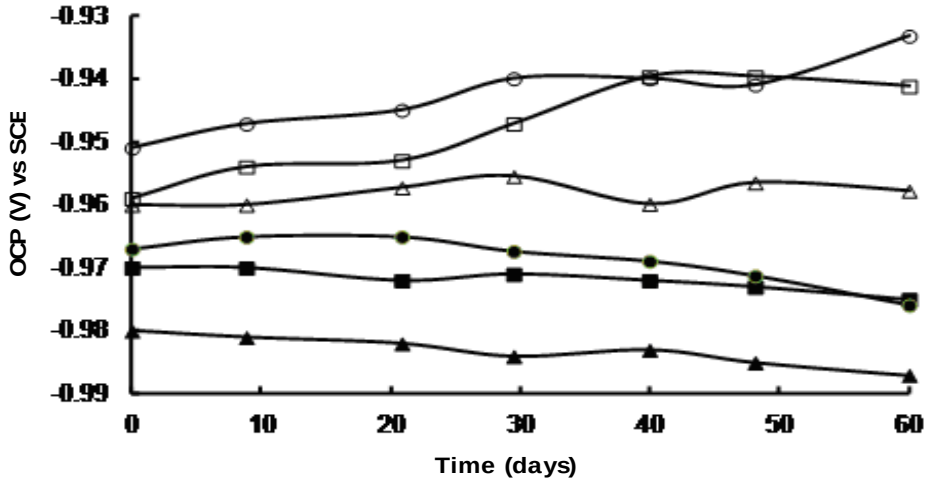

Figure 4: OCP decay of Al-Zn anode incorporated with different MnO_2-Ni (O) concentration: 0%, (Δ) - 0.05%, (□) - 0.1%, (●) - 0.2%, (▲) - 0.5%, (■) - 1%

In sharp contrast, Due to the development of a passive alumina coating on surface of ananode and subsequent ennoblement of the pure Al-Zn anode displayed substantial anodic OCP shift. Moreover, owing to the enrichment of hydrodynamic alumina layer on the anode surface, there was a significant decrease in the rate of diffusion of dissolved oxygen to cathode which in-turn suppresses the anodic dissolution reaction of Al-Zn anode. The best anode could not be determined only by the fact that all of the composite-incorporated anodes showed greater OCP value than pure Al-Zn anode. An in-depth evaluation of anode performance was carried out in this setting, as such.

3.4 Potentio-dynamic polarization

For MnO_2 and MnO_2-Ni incorporated Al-Zn alloy sacrificial anodes, the potentio-dynamic polarization curves are shown in Fig. 5. The incorporation of MnO_2-Ni into Al-Zn anode resulted in changes in the corrosion potential to negative values than MnO_2 incorporated Al-Zn anode [E_{corr} (Corrosion Potential) shifted from -0.968 to -0.894V vs.

Ag/AgCl], desirable factor for an effective system of cathodic protection. The anode with MnO2 showed a lower E_{corr} value and a wider passive zone in the polarization curve. The metal surface has formed oxide layers to prevent further corrosion. I_{corr} of the anodes varied from 3.141 to 3.106 A cm^{-2}. Generally, increasing I_{corr} means that the Al-Zn anode is of sacrificial active/action nature. Since the MnO2-Ni-included Al-Zn anode had a greater current density than the MnO2-integrated Al-Zn anode, this proved the Al-Zn anode was much more active than the MnO2 incorporated Al-Zn anode. It was hypothesized that any intermetallic phases generated during anode production would serve as extra cathodic sites, amplifying the corrosive attack.

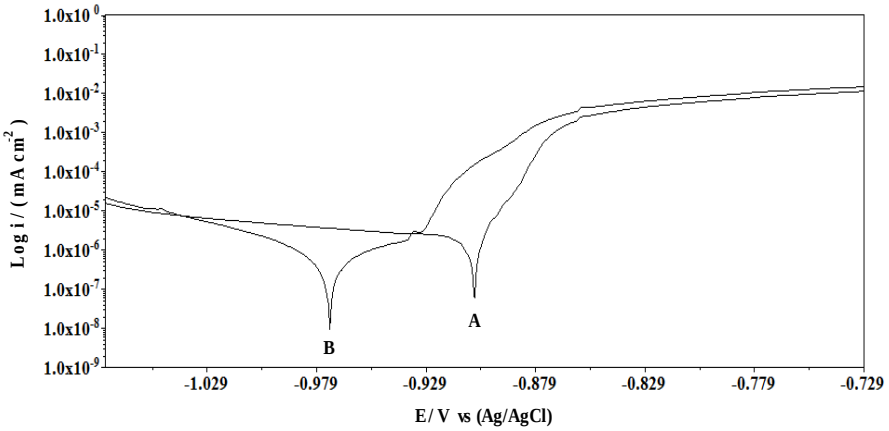

Figure 5: Potentiodynamic polarization behavior of Al-Zn anode incorporated with MnO_2 (A) and MnO_2-Ni (B) in 3 % NaCl solution

3.5 Self corrosion rate

Since non-columbic metal loss was primary shortcoming of Al-Zn sacrificial anodes, its self-corrosion values were estimated. Fig. 6 depicts the self-corrosion values of anodes for two months of exposure in 3% NaCl. All anodes incorporate with composited show self-corrosion values in 13.880 to 6.994 µg cm^{-2} h^{-1}range, and with bare Al-Zn anode, shows low self-corrosion. According to the findings of OCP decay and polarization investigations, 0.5% of the composite integrated anodes had the lowest self-corrosion values. Reduction in the values of self-corrosion for an anode can be because of reduction in grain-boundary corrosion owing to better refinement of grains [12]. A suitable metallic coating on composite can act as wetting promotion agent as well as in-situ hybridizing agent [8], provides enhanced mechanical strength to the matrix. An intermetallic phase, if formed between in the coating and matrix, would strengthen the Al-Zn matrix, which effectively suppresses the non-columbic metal loss. That is the dissolved nickel coating in

the Al-Zn matrix can form a second hybridized reinforcement by reacting with nickel coated MnO_2 composite material. This means of adding a second reinforcement in the matrix can be termed in-situ hybridization of composites; effectively reduces self-corrosion rate of Al-Zn anode. Low self-corrosion rate is a need for an effective sacrificial anode for preventing frequent anode material replacement.

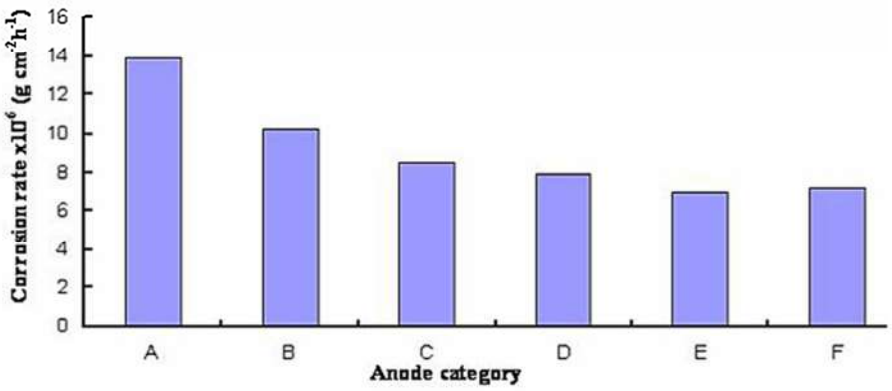

Figure 6: Comparison self-corrosion rates of the MnO $_2$-Niwith Al-Zn:(A) 0%, (B) 0.05%,(C) 0.1%, (D) 0.2%, (E) 0.5% (F)1%.

4 CONCLUSIONS

The incorporation of MnO_2-Ni composite in to Al-Zn alloy anode yielded high metallurgical and galvanic characteristics due to enhanced wettability. Physicochemical and electrochemical results revealed that the nickel coating provides not only the wetting promotion agent but also in-situ alloying element. An incorporated anode with 0.5% optimum quantity MnO_2-Ni showed highly active OCP due to local passive oxide layer thinning on the surface of the anode; also resist severe polarization during galvanic exposure studies. The optimum concentration of MnO_2-Ni was significant for effective activation of anode as other combinations had adverse or negligible effect. A high galvanic efficiency of was achieved during long-term evaluation owing to the effective suppression of non-columbic metal loss.

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OP17

Physicochemical characterization and fatty acid profiles of Coconut oil and Coconut testa oils from *Cocos nucifera* L.

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Abstract

Cocos nucifera L. is also known as coconut palm tree which is a major plantation crop in several parts of the world and are widely used for edible and non-edible purposes. The culinary nature of the plant is widely known from the ancient period onwards. The oil derived from the seed has a potential source of nutrients and is widely used for cooking and food for special dietary use. The benefit of the oil is not limited to the food and pharmaceutical industry but also used in several industries including in cosmetics. This study was carried out with coconut oil and Testa oil. The coconut oil was obtained from the inner white layer of coconut which is dried and crushed by the pulveriser known as expeller pressing. The Coconut Testa oil was obtained by the brown portion of the coconut generally known as copra covering the coconut kernel and it is the by-product during the preparation of Desiccated Coconut Powder and Virgin Coconut Oil. Both coconut oil and coconut testa oils were collected from the local market and the parameters of Butyro-refractometer reading at 40^0C and Refractive Index at 40^0 C and fatty acid profile are analysed. Major fatty acids present in the coconut oil and testa oil were detected as Lauric Acid (C12:0) and minor oil was Caproic Acid (C6:0).

1. Introduction

Cocos nucifera (L.) is also known as Coconut. Its belongs to the family of Arecaceae widely found in Malaysisa, India, Indonesia, Philipines and some islands of Indian pacific ocean region. It's a monocotyledon tree of around 15 to 25 meter in height with a dense canopy family. Nowadays, hybrid verities of *Cocos nucifera* (L.) with less height below 10 meters are also available with good yield. *Cocos nucifera* (L.) belongs to the Palm family. All parts of the plant is used for several purposes. Some part of this plant having culinary effects and used as a medicine.

The coconut fruit has three areas known as outer epicarp, a mesocarp, and inner endocarp. The epicarp, is the outer skin of the fruit, and the mesocarp, which is heavy, fibrous, and tanned when dry, have many industrial uses. The endocarp is the hard dark core. Inside is a solid white albumen of varied thickness, depending on the age of the fruit,

and with an oily pulp consistency and a liquid albumen called coconut water that is thick, sweet, and slightly acidic [1,2]. Testa is the , by product from the coconut processing industry from coconut This coconut testa is dried, roasted and crushed to get the coconut testa oil. Since the process of manufacturing is exactly the same as that of coconut oil, coconut testa oil can be used as a cooking source.

1.2 Phytochemistry

Phytochemical studies of the coconut fiber (mesocarp) ethanolic extract revealed that the presence of phenols, tannins, leucoanthocyanidins, flavonoids, triterpenes, steroids, and alkaloids [3], while a butanol extract recovered triterpenes, saponins, and condensed tannins [4]. Notably, compounds like flavonoids having antioxidant action are widely distributed in edible vegetables, fruits, and many herbs [5–7]. Condensed tannins are reported to possess antihelminthic activity by binding to proteins present in the cuticle, oral cavity, esophagus, and cloaca of nematodes, thus intensifying the physical and chemical damage in helminth [8].

The lyophilized extract and fractions, as well as ethyl acetate extracts, from the *C. nucifera* fiber are rich in polyphenols, compounds such as catechins, epicatechins, tannins, and flavonoids [3,9–11].

The constituents of the liquid albumen were identified as vitamin B, nicotinic acid (B3, 0.64 µg/mL), pantothenic acid (B5, 0.52 µg/mL), biotin (0.02 µg/mL), riboflavin (B2, <0.01 ng/mL), folic acid (0.003 µg/mL), with trace quantities of vitamins B1, B6, and C, pyridoxine, thiamine, folic acid, amino acids, L-arginine, plant hormones (auxin, 1,3-diphenylurea, cytokinin), enzymes (acid phosphatase, catalase, dehydrogenase, diastase, peroxidase, RNA polymerases), and growth-promoting factors [12–13]. Furthermore, oil extracted from the solid albumen is primarily lauric acid and alpha tocopherol [14, 15]. Root phenolic compounds were identified as flavonoids and saponins [16]. Other compounds identified in leaf epicuticular wax were lupeol methylether, skimmiwallin, [3b-methoxy-25-ethyl-9,19-cyclolanost-24(241)-ene], and isoskimmiwallin [3b-methoxy-24-ethyl-9,19-cyclolanost-25(251)-ene] [17].

2. Materials and Method

Wet coconut whole (WCW) and copra whole (CW) were purchased from the local market. The white kernel and testa of wet coconut and copra were separated manually to get wet coconut white kernel (WCWK) and wet coconut testa (WCT); copra white kernel

(CWK) and copra testa (CT). Standard gallic acid, cholesterol, FAME mix, toc-opherols, hydroxybenzoic acid, chlorogenic acid, vanillic acid, syringic acid, coumaric acid, caffeic acid, ferulic acid and cinnamic acid were procured from Sigma Chemica. Wet coconut whole (WCW) and copra whole (CW) were purchased from the local market. The white kernel and testa of wet coconut and copra were separated manually toget wet coconut white kernel (WCWK) and wet coconut testa (WCT); copra white kernel (CWK) and copra testa (CT). Standard gallic acid, cholesterol, FAME mix, toc-opherols, hydroxybenzoic acid, chlorogenic acid, vanillic acid, syringic acid, coumaric acid, caffeic acid, ferulic acid and cinnamic acid were procured from Sigma Chemica. Wet coconut whole (WCW) and copra whole (CW) were purchased from the local market. The white kernel and testa of wet coconut and copra were separated manually to get wet coconut white kernel (WCWK) and wet coconut testa (WCT); copra white kernel (CWK) and copra testa (CT). Standard gallic acid, cholesterol, FAME mix, toc-opherols, hydroxybenzoic acid, chlorogenic acid, vanillic acid, syringic acid, coumaric acid, caffeic acid, ferulic acid and cinnamic acid were procured from Sigma Chemica. The coconut oil and the testa coconut oil were purchased from the local market. The Standard were procured from Sigma Chemicals.

2.1 Apparatus

(1) Gas liquid chromatograph with the following characteristics:

a) Injection system heated to a temperature of 20 – 50°C higher than the column.

b) Oven – capable of heating the column to at least 220°C and maintaining the temperature to within ±1°C. If temperature programming is to be employed, twin columns are recommended.

c) Packed column - may be glass or stainless steel. However glass is preferred as steel may decompose polyunsaturated fatty acids having more than 3 double bonds.

2.2 Column packing with column length, internal diameter and operating temperature are as follows

i) 12- 15 % ethylene glycol succinate on 100 / 120 mesh gas chrom P (2m x 4 mm, at 180 degree C)

ii) 2- 10 % Apizon –L on 80/ 100 mesh Chromosorb W or Celite (2 m x 4 mm at 220 degree C)

iii) 10 % Butan-1-4 diol succinate on 80 / 100 mesh Chromosorb W or celite (2 m x 4 mm at 175 degree C)

iv) 3 % SE – 30 on 100 / 120 mesh Chromosorb –G silanised (2m x 3mm at 190 ° C) Condition the newly prepared column by disconnecting the detector and heating the column in the oven to the normal operating temperature for 16 hours while running the carrier gas at a rate of 20 – 60 mL/minutes

v) Detector – Flame ionization detector – capable of being heated to a temperature above that of the column

Syringe – 10 μL graduated in 1/10th of a microlitre

Recorder – electronic with high precision with rate of response below 1.5 second, width of paper 25cm, paper speed 25-150 cm/hours

Integrator for carrying out rapid and accurate calculations.

Other Glasswares

a. 50 and 100 mL boiling flasks

b. Reflux condenser

c. Graduated pipette – 10 mL

d. Test tubes with ground stoppers

e. 250 mL Separating funnels

Reagents:

(1) Carrier Gas – Inert gas (nitrogen, helium, argon) thoroughly dried and containing less than 10 mg / kg of oxygen

(2) Auxillary gas Hydrogen 99.9 % minimum purity. Free from organic impurities, air or oxygen

(3) Reference standards – a mixture of methyl esters or methyl esters of oils of known purity preferably similar to the fatty matter being analysed

(4) Methanolic Sodium hydroxide solution - approx 0.5 N. Dissolve 2 gm of Sodium Hydroxide in 100 mL methanol containing not more than 0.5 % m/m water. When the solution has to be stored for considerable time, a small amount of white ppt of

Sodium Carbonate may be formed. This has no effect on the preparation of the methyl esters OILS AND FATS 2016 49

(5) Methanolic solution of Boron trifloride – 12 - 15 % m/m, 14 and 50 % solutions are commercially available. The metahnolic solution of boron trifloride should be stored in a refrigerator

(6) Heptane- Chromatographic quality

(7) Redistilled petroleum Ether 40 – 60°C

(8) Anhydrous Sodium sulphate.

(9) Saturated solution of Sodium chloride.

(10) Methyl red – 1 gm / litre in 60 % alcohol

The methyl esters of fatty acids are formed using boron trifluoride or methanol and alkali and separated by gas – liquid chromatography using a flame ionization detector. The elution pattern of methyl esters can be compared with authentic oils for identification

2.3 Procedure

Prepare the methyl esters of the fatty acids. The method using boron trifluoride gives good results and is preferable to alternative methods which may be used when boron trifluoride is not available. Because of the toxic character of boron trifluoride various operations must be performed under a ventilated hood. All glass ware must be washed with water immediately after use. If the oil or fatty acids include fatty acids containing more than 2 double bonds it is advisable to purge the air from the methanol and the flask by passing a stream of nitrogen into the methanol for a few minutes. Transfer about 350 mg of clear oil to a 50 mL conical flask, and add 6 mL of 0.5 N methanolic sodium hydroxide solution, 7 mL of boron trifluoride solution and a boiling chip. Fit the condenser to the flask. Boil under reflux until the droplets of oil disappear (5- 10 minutes). Add the appropriate amount of boron trifluoride solution with a bulb or automatic pipette through the top of the condenser. Continue boiling for 2 minutes. Add 2- 5 mL of heptane to the boiling mixture through the top of the condenser. Continue boiling for 1 minute. Withdraw the source of heat and then remove the condenser. Add a small amount of saturated Sodium Chloride solution to the flask in order to bring the level of liquid into the neck of the flask. Transfer about 1 mL of the upper layer (Heptane solution) into a test tube with a ground glass neck and add a little anhydrous Sodium Sulphate to remove any

trace of water. This solution will contain about 5 – 10 % of methyl esters and may be injected directly into the column of gas liquid chromatograph.

3. Result and Discussion

Fatty acid profile, Composistion and Properties of Coconut Oil and and coconut testa oil was analysed by FAME Method. The Significance differences among the two were found eventhough it was the derivatives of the same species. The coconut oil contains lauric acid (46.23%), myristic acid (19.78 %) caprylic acid (9.04 %) Palmitic acid (8029%), Oleic acid (6.08 %) and other fatty acids like caproic acid, Stearic acid, Linoleic acid are represented less. The total fatty acid of coconut oil is shown in Table 1 below, the lauric acid content of is the highest with 46.23% in both coconut oil and coconut testa oil and the composition of caproic acid is less in both oils. Both oils contain palmitic acid which is commonly found in palm family tree oils.

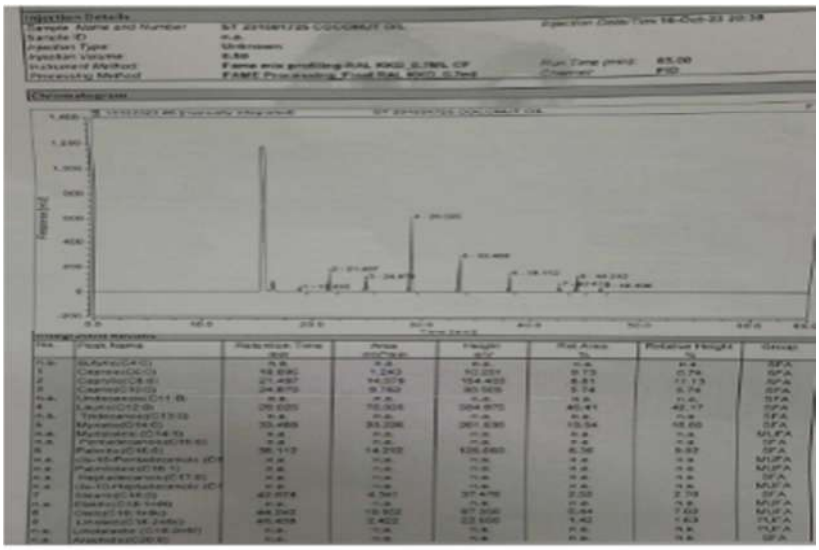
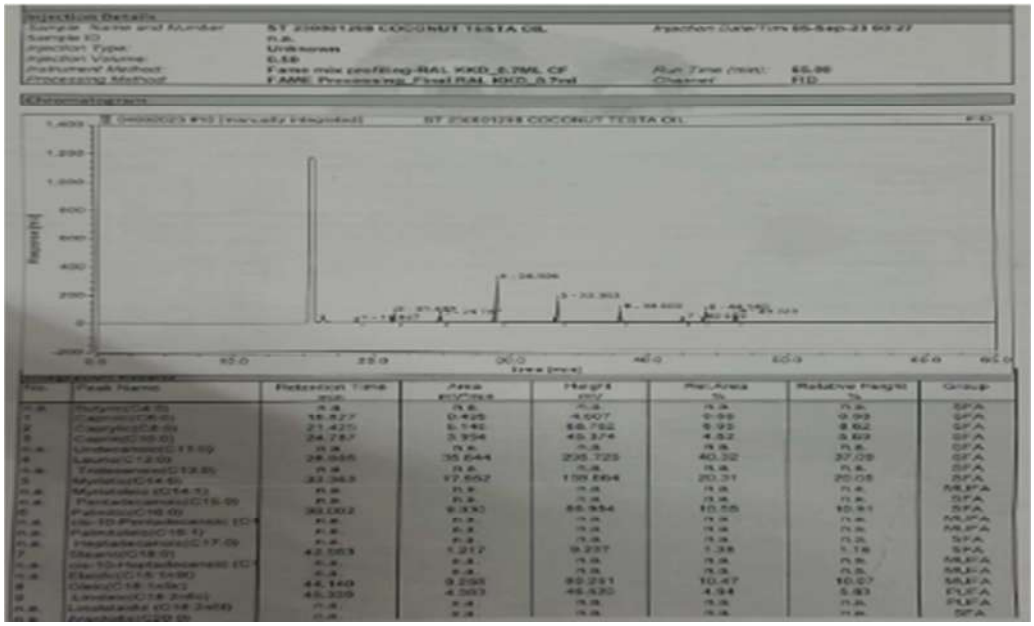
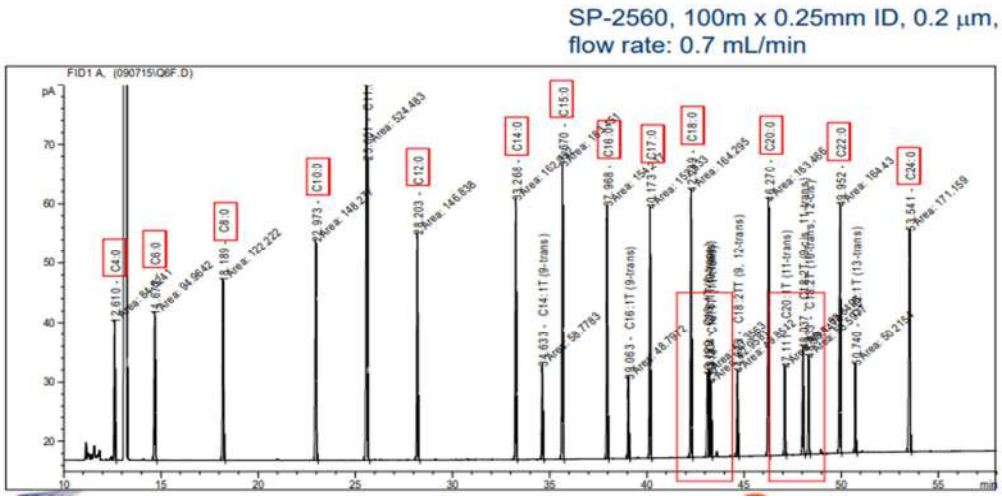


Table 1: The composition of fatty acids in Testa oil and coconut oil

Sl.No	Fatty Acid present		Testa Oil Composition (%)	Coconut oil Composition (%)
1	Caproic acid	C6:0		0.72
2	Caprylic acid	C8:0		9.04
3	Capric acid	C10:0		5.83
4	Lauric acid	C12:0		46.23
5	Myristic acid	C14:0		19.78
6	Palmitic acid	C16:0		8.29
7	Stearic acid	C18:0		2.57
8	Oleic acid	C18:1		6.08
9	Linoleic acid	C18:2		1.46





4. Conclusion

Cocos nucifera L oil is widely used plant oil that has important culinary effects. Compared with coconut oil and coconut testa oil both have higher content of lauric acid. The coconut oil contains 92.46% of saturated fatty acids and 6.08 % of mono saturated fatty acids and 1.46 % of Poly saturated fatty acids whereas the coconut testa oil have 84.59 % of saturated fatty acid, 10.47 % of monosaturated fatty acids and 4.94 % poly saturated fatty acids. Compare with both oils the coconut testa oil is rich in Poly unsaturated fatty acids and monounsaturated fatty acids compare to coconut oil.

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OP18

Insilico Study of the Bioactivity of Eugenol using Molecular Docking

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Abstract

Eugenol is a bioactive component which is frequently found in variety of medicinal plants. Eugenol has attained considerable attention because of its pharmaceutical applications including antibacterial, antioxidant, anti-inflammatory and anticancer properties. This article focuses on the insilico analysis of possible interactions between eugenol and some relevant proteins by using molecular docking tool. Docking study is carried out between Eugenol and proteins like MCR-1, COX-2 and 5-LOX. The bioactivities of eugenol against the mentioned proteins are verified by measuring the binding energies of eugenol with them and it shows higher affinity towards 5-LOX.

1. Introduction

In the field of molecular modelling, molecular docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex [1]. Molecular docking is a common method used for the structure-based drug design. The molecular docking approach can be used to model the interaction between a small molecule and a protein at the atomic level, which allows us to characterize the behavior of small molecules in the binding site of target proteins as well as to elucidate fundamental biochemical processes.[2] The aim of molecular docking is to achieve an optimized conformation for both the protein and ligand and relative orientation between protein and ligand so that the free energy of the overall system is minimized. Molecular recognition plays a key role in promoting fundamental biomolecular events such as enzyme-substrate, drug-protein and drug-nucleic acid interactions. [3,4] The docking process involves two basic steps: prediction of the ligand conformation as well as its position and orientation within these sites (usually referred to as pose) and assessment of the binding affinity. [5]

There are two types of docking, Lock and Key or rigid docking and Induced fit or Flexible Docking. In rigid docking, both the internal geometry of the receptor and ligand is kept fixed during docking. In Induced fit model, both the ligand and side chain of the protein is kept flexible and the energy for different conformations of the ligand fitting into the protein is calculated. For induced fit docking, the main chain is also moved to incorporate the conformational changes of the protein upon ligand binding. This method can evaluate many different possible conformations which make it more exhaustive and possibly simulate real life phenomenon and hence trustworthy.

To date, many software and tools for docking have been employed. AutoDock Vina (in UCSF [University of California, San Francisco] Chimera) is one of the computationally fastest and most accurate software employed in docking. The first step involved in using UCSF chimera is the retrieval of target protein ID from the protein database, the second step involves visualization of the protein structure in UCSF Chimera, the third step involves preparation of the target protein for docking, the fourth step involves preparation of the ligand for docking, the fifth step involves docking of the ligand and the target protein as Mol.2 files in Chimera by using AutoDock Vina, and the final step involves interpretation and analysis of the docking results. Another important factor is that evaluation by visualisation to check whether the docking solutions for known ligands

match crystallographic conformations. This is important to check whether docking stimulations can reproduce external data.

AutoDock is a collection of command-line programs that can be employed to predict binding conformations of a small flexible ligand to a macromolecular target whose structure is known. This technique combines the rapid grid-based method used for energy evaluation with conformation searching and simulated annealing. The UCSF (University of California, San Francisco) Chimera software is used for visualization as well as analysis of density maps, 3D microscopy, molecular structures, and the associated data [6]. The challenges in the scope, size, and types of data used with the experimental cutting-edge methods are addressed by this software. It provides advanced options for high-quality rendering (reliable calculations of the molecular surface, interactive ambient occlusion, etc) and provides professional approaches to the design and distribution of the software. Chimera is freely available software for non-commercial use and shows advances particularly in its performance, extensibility, visualization, and usability.

This study has used the software UCSF chimera and Autodock vina to carry out the molecular docking studies to find the binding energies that indicates the extent of binding between a chosen ligand and a particular protein. The ligand used here is Eugenol and its binding with various proteins are studied. This study would give information about the antimicrobial property of the ligand towards the corresponding protein.

The ligand, Eugenol is a phenolic component that can be obtained from a wide range of plant sources including clove oil, nutmeg oil, cinnamon extract and many other plants. It owns strong health promoting functions that make it a versatile natural ingredient. Eugenol was firstly extracted from the leaves and buds of Eugenia caryophyllata commonly named as clove. Currently, eugenol can also be synthesized by allylation of guaiacol with allyl chloride having the similar kind of functional property. Eugenol is present in significant amount in the extracts of numerous medicinal herbs so it has fascinated the attention of several researchers and opened up the gateway of research regarding its utilization as a medicine to cure various diseases. Eugenol is avowed to possess certain pharmacological properties including anaesthetic activity, antioxidant potential, antimicrobial role, anti-inflammatory action, anti-carcinogenic effects, neuroprotective ability, hypolipidemic efficiency and anti-diabetic effectiveness. Eugenol

is declared as GRAS (generally recognized as safe) by World Health Organization (WHO) and is considered as non-mutagenic.

As a result of its wide spectrum of biological and functional properties, eugenol is still proclaimed as the priority of research. Therefore, it is of significant worth to rationally confederate the research findings related to the therapeutic potential of eugenol to elucidate its importance for human health and mechanisms involved in the functionality of eugenol to obviate several lifestyle related indispositions. [7]

1.1 Antibacterial Activity of Eugenol

Clove oil polyphenol eugenol illustrates potent antibacterial potential against numerous strains of Gram-positive (*Entero-coccus faecalis, Staphylococcus epidermidis, Streptococcus pyo-genes, Staphylococcus aureus, Streptococcus pneumonia, Listeria monocytogenes, Bacillus cereus, Bacillus subtilis) and Gram-negative (E. coli, Proteus vulgaris, Salmonella choleraesuis, Salmonella typhi, Pseudomonas aeruginosa, Helicobacter pylori and Yersinia enterocolitica*) bacteria. Eugenol damages cell membrane and cell wall, inducing cell-lysis in Gram negative and Gram positive bacteria resulting in leakage of intracellular fluid along with lipid and protein contents. [8.9]

E coli is a Gram negative, facultative anaerobic, rod shaped, coliform bacterium of the genus Escherichia that is commonly found in the lower intestine of warm-blooded organisms (endotherms). Most *E. coli* strains are harmless, but some serotypes (EPEC, ETEC etc.) can cause serious food poisoning in their hosts, and are occasionally responsible for food contamination incidents that prompt product recalls. Most *E. coli* strains do not cause disease, naturally living in the gut, but virulent strains can cause gastroenteritis, urinary tract infections, neonatal meningitis, hemorrhagic colitis, and Crohn's disease. This article focuses on the antibacterial activity of Eugenol against E.coli.

1.2 Antioxidant Activity of Eugenol

Many human related disorders like cancer, diabetes, arthritis, Parkinson's disease, AIDS and Alzheimer's complications are prompted and exaggerated due to redundant group of the free radicals. Reports have indicated that fruits and vegetables containing cache of phytonutrients like polyphenols, flavonoids and anthocyanin are observed to be efficacious in scavenging the free radical.[10] Eugenol, a potent phenolic component in clove oil is chiefly responsible for its antioxidant and free radical scavenging activity.

Antioxidant power of eugenol can be elucidated by forming complexes with reduced metals. Potent inhibitory effect on lipid peroxidation by isoeugenol and eugenol is administrated to be due to eradication of free radical and formation of iron–oxygen chelate complex, by keeping iron and copper at a reduced state respectively. [11]

In order to understand the possible mechanism behind the anti-oxidant activity of eugenol, molecular docking studies were examined using human peroxiredoxin 5 enzyme (PDB: 1HD2) which has a broader activity against ROS and was mostly involved in stress protection mechanisms and in cell differentiation. From docking results it can be suggested that all the ligands interact favourably with the target proteins.[12]

The anti-oxidant property of P.cubeba fruit's essential oil can be determined using this method. Eugenol and methyl eugenol were identified as the two major constituents of this oil. The high content of methyleugenol/eugenol (75.26%) associated with other constituents (major and minor components) also could have been responsible for their bioactivities. Eugenol possesses the ability to transfer electron or hydrogen atoms by neutralizing free radicals, which can block the oxidative process.[13,14] The presence of methyleugenol/eugenol as the principal chemotype of this oil gives him better antioxidant potency, and therefore good DNA damage protective effects, which can be manifested via direct trapping of the free radicals or inhibiting the propagation of radical chain reactions through transfers of hydrogen or electrons. The eugenol and methyl eugenol are the main contributors of antioxidant activity, sharing common residues with the human peroxiredoxin 5 active sites.

1.3 Anti-inflammatory and Anticancer Activity

Eugenol have many antimicrobial, antioxidant, anti-inflammatory and anticancer properties. Numerous diseases such as osteoarthritis, Crohn's disease, colon cancer, breast cancer and prostate cancer are associated with the progression of chronic inflammation with activation of pro inflammatory mediators such as interleukins and intracellular enzymes such as COX and LOX [15,16]. COX is the main enzyme in catalysing the metabolic conversion of arachidonic acid to prostaglandins, which mediates homeostatic functions in different physiological systems [17-18]. COX-2 is responsible for the high production of prostaglandins during the inflammatory process and pathogenic stimuli and cancer progress. Lipoxygenases (LOXs) form a heterogeneous class of enzymes that catalyze the peroxidation of polyunstaturated fatty acids [19-20]. The 5-LOX enzyme is a

lipoxygenase isoform associated with inflammation, bronchoconstriction, hypersensitivity, anaphylaxis, and asthma [21]. Compounds that have dual COX-2/5-LOX inhibitors can be used in cancer chemotherapy. [22] COX-2 and 5-LOX inhibitors can down regulate the progression of colorectal cancer, reducing the capacity for invasion and proliferation in cells of mouse colorectal cancer cell lines (CT26 cells) and human colorectal cancer (HCA7cells), through supply of the PI3K/AKT pathway. [23] The combination of celecoxib (COX-2 inhibitor) with MK886 (5-LOX inhibitor) can suppress the growth of pancreatic tumour cells [24]. Docking studies revealed that the eugenol interacts in the active site of COX-2 as well as with 5-LOX. The possibility of molecular fitting of eugenol with dual activity of COX-2/5-LOX, demonstrating its potential as an anti-inflammatory agent to act in the composition or synthesis of new selective drugs to fight diseases that need to inhibit inflammatory processes such as: osteoarthritis, Crohn's disease and cancer. Various activities of Eugenol can be studied using Molecular docking.

1.4 Molecular Docking

Docking requires the following: (1) Windows 7, 8, or 10 or Mac operating system and Linux, and (2) UCSF Chimera 1.12. UCSF Chimera is an extensible program that is meant mainly for visualization and analysis of the molecular structures. However, in this paper, we are operating Autodock Vina in Chimera for docking purposes. Docking was done by taking MCR-1 protein of E Coli, Human peroxiredoxin enzyme, COX-2 and 5-LOX as the Receptor proteins and Eugenol as ligand.

Table 1 -Enzyme/Protein and PDB ID

SI No.	Enzyme/Protein	PBD/ID
1	MCR-1	5GRR
2	COX-2	4OJT
3	5-LOX	3V99

2. Results and Discussion

2.1 Docking between MCR-1 and Eugenol

Eugenol can be used against E coli bacteria. Eugenol is combined with colistin against a collection of clinical E.Coli isolates and interactions between eugenol and MCR-1 give the anti-bacterial activity. MCR-1 is a colistin resistant gene. MCR-1 is regarded as a

phosphoethanolamine transferase via sequence alignment. MCR-1 homologues LptA and EptC can catalyze modification of the 1′ and 4′ phosphoryl groups of lipid A(moiety of lipopolysaccharides) using phosphoethanolamine (PEA) as a substrate to transfer positive charges, which will hinder the interaction and reduce affinity of colistin to lipid A therefore confers colistin resistance to host bacteria. [25-27]

To obtain better insight into interactions of eugenol and MCR-1 protein, molecular docking analysis was performed. The results indicated that phenolic hydroxyl group in eugenol could bind with zinc atom of MCR-1 protein in the form of metal ion coordination bond, which could further elucidate phenolic hydroxyl as an important functional group. In addition, catalytic amino acid Ser284, which is in the active pocket of MCR-1 protein was found to hydrogen bond with methoxy in ortho-position of MCR-1 protein, thus stabilizing the docked structures. This is the first study to evaluate antimicrobial property of eugenol against colistin-resistant E. coli.[28-29] The optimal interaction and relative affinity parameters were used to elucidate the spatial conformation among the MCR-1 protein and bioactive group of eugenol after docking. MCR-1 protein binding contribute to the potential efficacy of eugenol to treat clinical colistin-resistant bacteria.

The results of docking for the first experiment explained above that are the docking between MCR-1 protein and Eugenol is obtained as in Figure 1

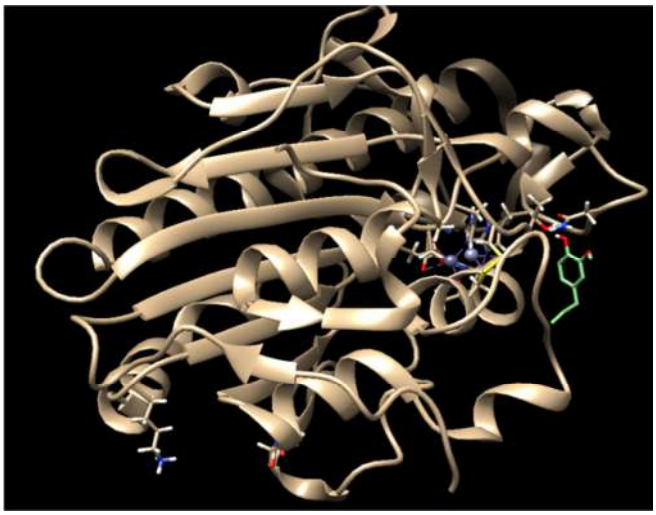

Figure 1: Binding of Eugenol with MCR-1 protein of E. coli

The result of docking is shown below. Docking was performed to study the possible interaction between eugenol and MCR-1. The binding energy between the

receptor and ligand is -5.5 kcal/mol. Crystal structure of MCR-1 (PDB ID: 5GRR), is adapted from Protein Data Bank was obtained in PDB format.

Weighting parameters of scoring function include spatial interaction, hydrophobic interaction, hydrogen-bonding energy and number of rotatable keys in ligand. Affinity was measured to assess docking. The lower the parameter is, the ligand is more likely to bind with the active pocket. The results showed that free energy of binding was – 5.5 kcal/mol, which indicating a possible bind between MCR-1 protein and eugenol.

The results indicated that phenolic hydroxyl group in eugenol could bind with zinc atom of MCR-1 protein in the form of metal ion coordination bond, which could further elucidate phenolic hydroxyl as an important functional group. In addition, catalytic amino acid Ser284, which is in the active pocket of MCR-1 protein was found to hydrogen bond with methoxy in ortho-position of MCR-1 protein, thus stabilizing the docked structures. A metal ion coordination bond with catalytic zinc atom and a hydrogen bond with crucial amino acid residue Ser284 of MCR-1 were observed after molecular docking, indicating antibacterial activity and direct molecular interactions of eugenol with MCR-1 protein. Eugenol exhibited synergistic effect with colistin and enhanced its antimicrobial activity. This might further contribute to the antibacterial actions against colistin-resistant E. coli strains. [30]

2.2 Docking between COX-2 and Eugenol

Docking between COX-2 (pdb id: 4OJT) and Eugenol (PubChem id: 3314) was carried out in the same manner as above. The results obtained are given in Figure 2.

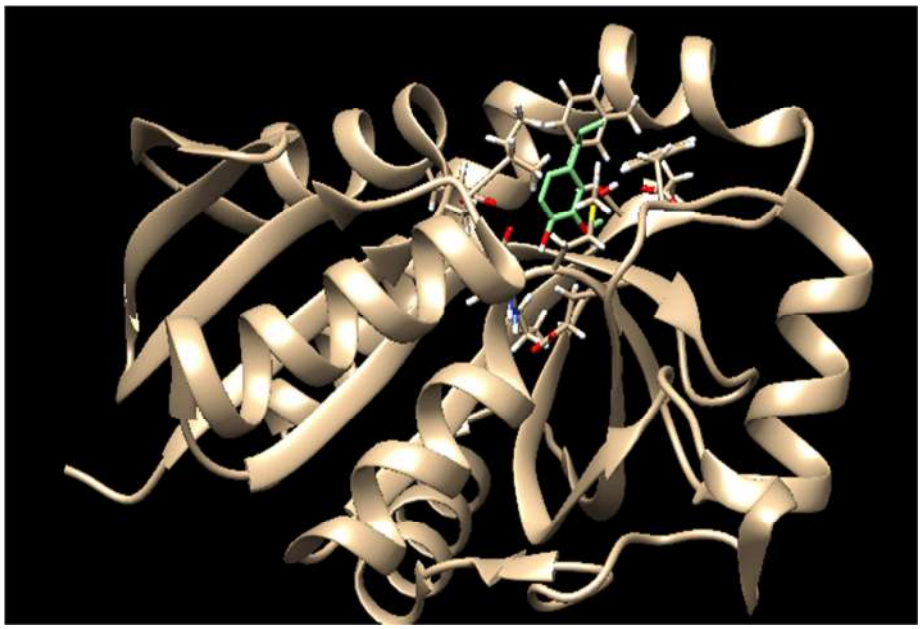

Figure 2: Docking between Eugenol and COX-2

The result obtained of docking between Eugenol and COX-2 is shown below. The binding energy between the Eugenol and COX-2 is -6.2 kcal/mol. COX-2 is responsible for the high production of prostaglandins during the inflammatory process and pathogenic stimuli and cancer progress. Eugenol also occupies an orientation very similar to the binding mode of arachidonic acid in the COX-2 active site. According to the computational analysis, eugenol interacts with regions of the active site of COX-2 into the hydrophobic pocket. Ser 530 and Tyr 385 are the key amino-acid fragments that contribute considerably in the inhibition of the protein by the interaction protein–ligand of the active pocket of the enzyme. Eugenol has also been shown to act on the inhibition of the active site in which peroxidase is responsible for converting prostaglandin to G2 into prostaglandin H2 by the interaction with the group with the lateral methyl radicals of the pyrrole rings of the heme group [31]. Eugenol acts as an inhibitor of COX-2. So, it has anti-inflammatory and anticancer properties.

2.3 **Docking between 5-LOX and Eugenol**

Docking between 5-LOX (pdb id: 3V99) and Eugenol (PubChem id: 3314) was carried out. The image obtained after docking is given in Figure 3

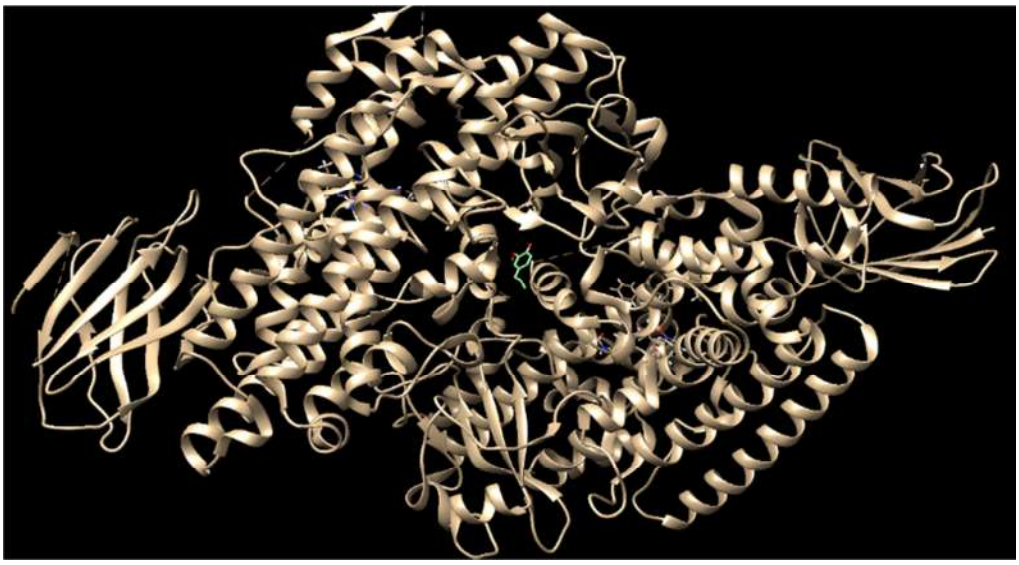

Figure 3: Binding of Eugenol with 5-LOX

The binding energy of Eugenol with 5-LOX is -6.3 kcal/mol. The binding energy of eugenol with the active sites of 5-LOX, suggests the interaction between eugenol and 5-LOX. Eugenol had shown better interaction stabilized of with the active site amino acids of 5-LOX targets respectively the fragments coordinated with $^{Fe3+}$ His 367 by van der Waals interactions, His 372 by π-π T-shaped, and Ile 673 by H-bonds besides other fragments close to the group coordinated to iron ion as Tr 364 by van der Waals interactions.

The possibility of molecular fitting of eugenol with dual activity of 5-LOX, demonstrating its potential as an anti-inflammatory agent to act in the composition or synthesis of new selective drugs to fight diseases that need to inhibit inflammatory processes such as: osteoarthritis, Crohn's disease and cancer. [32]

3. Conclusion

In this study we have highlighted the pharmacological properties of Eugenol. Eugenol is a naturally occurring product from cloves. Eugenol have various pharmacological properties including antimicrobial activity, antioxidant activity, anti-inflammatory action, anticarcinogenic effects etc. The therapeutic potential of eugenol that highlights its importance as one of the principal bioactive components having several health promoting functions.

Here with help of molecular docking using USCF Chimera and Autodock Vina we have found out the binding energies between Eugenol and various other receptor sites that

led to inhibition of the activity of that particular enzyme. Through this study we have found that Eugenol possess antibacterial activity by the binding with MCR-1 protein against colistin-resistant E.coli. It shows antioxidant property by binding with the human peroxiredoxin 5 enzyme. The docking studies shows that Eugenol is a main contributor of antioxidant activity, sharing many common residues with the active site of human peroxiredoxin 5 enzyme which has a broader activity against ROS. Eugenol shows anti-inflammatory and anticancer activities by binding with COX-2 and 5-LOX enzymes. The binding of eugenol inhibits the activities of both COX-2 and 5-LOX enzymes. The possibility of molecular fitting of eugenol with COX-2/5-LOX has been explored, demonstrating its potential as an anti-inflammatory agent to act in the composition or synthesis of new selective drugs to fight diseases that need to inhibit inflammatory processes such as cancer. The medicinal activities of Eugenol and its derivatives have in particular, attracted a lot of attention recently. The studies shown that eugenol can act against a number of different microorganisms of different origin. Eugenol can act as a therapeutic tool against a wide variety of diseases. It is one of the principal bioactive components having several health promoting functions. Further studies are needed to determine the functions of Eugenol in human health and diseases.

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OP19

Trimyristin Isolation, Essential Oil Analysis and Radical Scavenging Potential of *Myristica Fragrans*

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Abstract

Myristica fragrans, which is commonly known as Nutmeg, belongs to the family Myristicaceae. GC -MS analysis of nutmeg showed the presence of terpene hydrocarbons (sabinene and pinene), myrcene, phellandrene, camphene, limonene, terpinene, myrcene, pcymene and other terpene derivatives. Nutmeg also yields nutmeg butter which contains

25 to 40 % fixed oil and is a semi-solid reddish-brown fat having the aroma of nutmeg. Isolation, purification, recrystallisation and saponification of trimyristin was carried out. Eugenol and terpinen- 4-ol from nutmeg were the most active principles and it was compared with the sample. Antioxidant studies The reducing power of Myristica fragrans extracted by ethanol is determined by this method using reducing power method was also performed and found to inhibit in a dose dependent manner

1. Introduction

Myristica fragrans, which is commonly known as Nutmeg, belongs to the family Myristicaceae is indigenous to Banda islands in the Moluccas in east Indonesia. All parts of the plant are aromatic. The major chemical constituents of *Myristica fragrans* are alkyl benzene derivatives (myristicin, elemicin, safrole) myristic acid, alpha-pinene, terpenes, beta-pinene and trimyristin. Nutmeg contains about 10% essential oil, chiefly composed of terpene hydrocarbons (sabinene and pinene), myrcene, phellandrene, camphene, limonene, terpinene, myrcene, pcymene and other terpene derivatives. Nutmeg also yields nutmeg butter which contains 25 to 40 % fixed oil and is a semi-solid reddish-brown fat having the aroma of nutmeg. Therapeutic efficacy of Munzij wa Mushil-e-Balgham (Poly Herbal Formulation) and Dalk (Massage) with Roghan-e-Farfiyun in The Management of Irqunnasa (Sciatica): An Open Labelled Clinical Trial in 2017. It has been reported for significant analgesic e□ect similar to morphine and aspirin; relaxant e□ect due to inhibitory e□ect on muscarinic receptors and anti- inflammatory action by inhibitory effect on prostaglandin synthesis [1].

Eugenol and isoeugenol from nutmeg were the most active principles on rabbit platelet function **[**2**]**. Some activity was also shown by safrole, myristicin, elemicin, limonene, alpha-terpineol, terpinene-4-01 and linalool **[**3**]**. When the effects of dietary administration (3.9 mg days for 17 months) of essential oil on the polyunsaturated fatty acid composition of the retina of aged rats were studied, their levels were increased. Thus there is a possible relationship between the antioxidant properties and the prevention of age related macular degeneration.

The most active constituent as inhibitors of platelet aggregation from nutmeg oil. It showed that, medicinally, nutmeg oil and nutmeg powder could be replaced by eugenol and isoeugenol. Flavonoids from several plants including *M. fragrans* were found to have

hypolipidaemic activity [5]**.** The possible insulin function effects of several herbs, spices and medicinal plants were evaluated.

2. Experimental

2.1 Materials

2.1.1 Collection of plant materials

The seed of *Myristica fragrans* was collected from locality of Meenadom, Kottayam district. 500 g of raw and ripe seeds of *Myristica fragrans* were shade dried during the month of March 2016 and it was powdered in a grinder.

2.1.2 Gas Chromatography

In gas chromatography, there are two phases, a stationary liquid phase and a mobile gaseous phase that is usually nitrogen, hydrogen or helium. When the sample is injected into the GC, the mobile phase takes the sample to the column packed with the stationery phase. The components of the oil emerge from the column depending upon their volatility. Nature of the stationary phase, temperature of the column and the programme of the run also affect the separation of the components. Compounds are detected by a flame ionization detector (FID). Here, as the various components in the sample come out of the column, they pass through a hydrogen flame where it is burnt producing a charged particle that is detected by a pair of electrodes. The magnitude of the response produced is proportional to the number of oxidizable carbons in the molecule. The quantitative response from the detector is amplified and visualized as a series of peaks on the graph. The area of each peak will give a good indication of the percentage contribution of that particular component. Thus the gas chromatography is the most reliable method for confirming the oil composition.

2.1.3 Thin Layer Chromatography

Thin-layer chromatography is a chromatographic technique used to separate non-volatile mixtures. This layer of adsorbent is known as the stationary phase. After the sample has been applied on the plate, a solvent or solvent mixture (known as the mobile phase) is drawn up the plate via capillary action.

2.1.4 Isolation, purification and recrystallization of trimyristin

To a 100 mL round-bottom flask, 20 g of ground nutmeg was added. To this 100 mL of chloroform was added and refluxed for two hours in a heating mantle attached with a reflux condenser. Then the solution was cooled to room temperature. The solution is decanted and the brown solid part is allowed to remain in the RB flask and the chloroform is allowed to evaporate leaving a yellow solid. After complete evaporation ethanol is added to it and is cooled in ice cold solution. The white precipitate formed was filtered and transferred to a tared watch glass, and allow it to dry completely before determining the mass of product. To determine the melting point, trimyristin was purified and IR analysis was done on it.

The crude trimyristin is air dried and dissolved in alcohol and recrystallized sample was obtained as white crystalline precipitate. Melting point and yield of the substance is noted.

2.1.5 Saponification of trimyristin.

To a 100 mL round-bottom flask, 30 mL of 95% ethanol and 3N NaOH are added. This solution is stirred and 1.0 g of trimyristin was added to it. A condenser ia attached to it as before, and refluxed for 1 hour. The mixture is cooled to room temperature, and 20 mL of distilled water and 20 mL of saturated NaCl solution are added. Vacuum filter was used collect the solid and is washed with 25 mL of cold water. The solution of sodium myristateis transferred to a tared watch glass, and allow it to dry thoroughly, weighed and the percent yield is determined.

2.1.6 Extraction of essential oil

15g of crushed nutmeg was taken in a Clevenger apparatus and 100 ml distilled water is added and it is refluxed for 6 hours and the essential oil was extracted and collected. The essential oil thus obtained is dried over anhydrous sodium sulphate. It is weighed and stored in a sealed vial in dark at 4^0c and GC analysis was carried to know its composition.

2.1.7 Determination of Antioxidant activity

Principle

The reducing power of *Myristica fragrans* extracted by ethanol is determined by this method. Substances, which reduction potential, react with potassium ferricyanide

(Fe^{3+}) to form potassium ferrocyanide (Fe^{2+}), which then reacts with ferric chloride to form ferric ferrous complex that has an absorption maximum at 700 nm.(6)

Procedure

Ferric reducing power was determined as follows. 100µl of the extract (100-500µg/ml) were mixed with 2.5 ml of 200 mmol/L phosphate buffer (p^H 6.6) and 2.5 ml 1% potassium ferricyanide and incubated at 50^0c for 20 minutes. Then 2.5 ml 10% CCl_3COOH was added. Centrifuge for 10 minutes. 5 ml upper layer is taken and is mixed with 5 ml water and 1 ml 1% $FeCl_3$. The absorbance of the mixture was then measured at 700 nm. Ascorbic acid is used as a positive control.

3. Result and Discussion

Yield of the isolated compound was found to be 9.39%. The purity was checked by TLC and R_f was compared with standard. Trimyristin produced a distinct spot at R_f 0.836. Melting point of the isolated compound=53.6^0C. Yield of the essential oil =1.1 mL

The IR Spectra of Trimyristin is shown below in the Figures 1 (a) and (b).

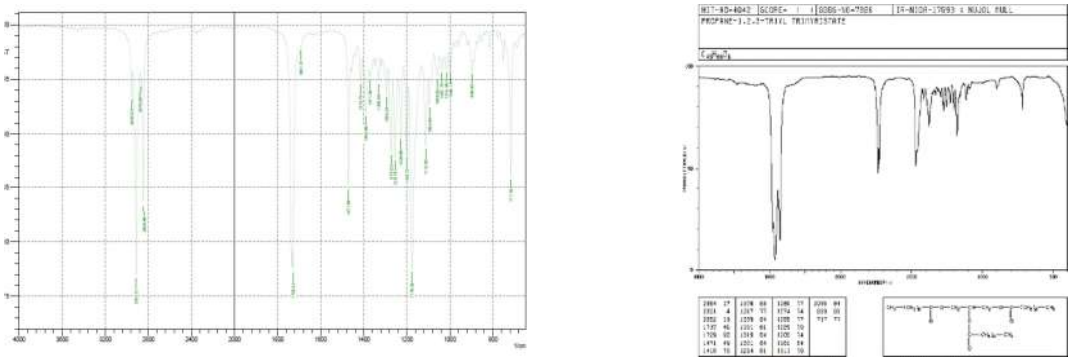


Figure 1: (a) IR spectra of the Isolated trimyristin and (b) IR spectra of the standard Trimyristin

The key peaks characteristic of trimyristin were compared with IR spectra of pure compound. The main functional groups on trimyristin are the C=O and the C-O bonds of the ester functional group and the associated peaks of the bonds are comparable with the IR spectrum. A sharp peak at 1728 cm^{-1} & 1176 cm^{-1} is seen in the isolated compound also. Two peaks at 2912 cm^{-1} and 2848 cm^{-1} represents the aliphatic hydrogens of the trimyristin's long hydrophobic chains, they are less defining than the previous two peaks, as all IR spectra contain a peak within the 2900 cm^{-1} 2800 cm^{-1} region. The standard showed two peaks at 2890 cm^{-1} and 2917cm^{-1} representing the aliphatic C-H chains, a

peak at 1750 cm^{-1} representing the carbonyl C=O bond, and a peak at 1150 cm^{-1}, representing the C-O ester bond. IR data and melting point supports the results.

Saponification of trimyristin gave positive test for the soap formation which again confirmed the formation of trimyristin.

The chromatogram of standards and essential oil composition of *Myristica fragrans* is shown in the Figure 2 below. Chromatogram showing the essential oil composition of Myristica fragrans and the relative abundance of the components with retention time of myristic acid is shown in Figure 3.

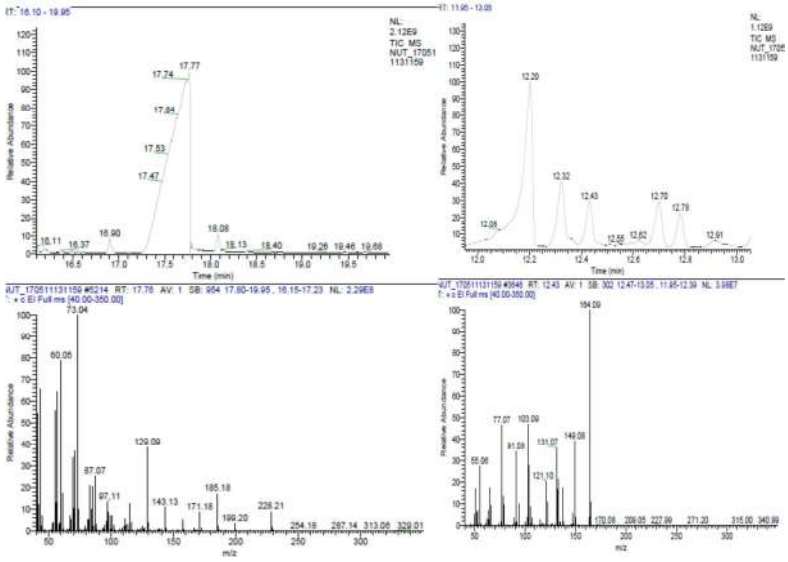


Figure 2: Chromatogram showing the relative abundance of the components with retention time (*trans* iso eugenol & terpinen- 4-ol)

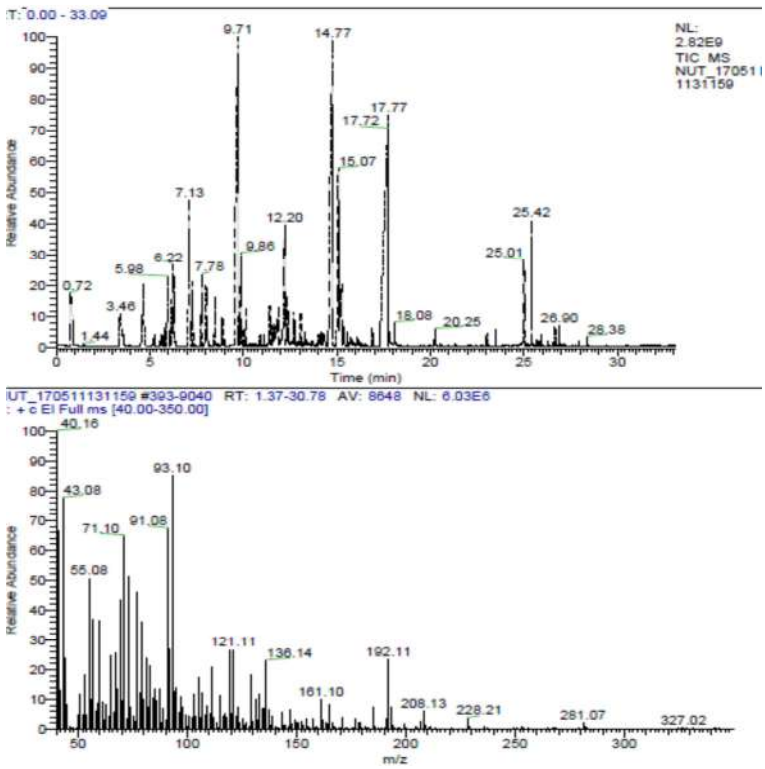


Figure 3: Chromatogram showing the essential oil composition of Myristica fragrans and the relative abundance of the components with retention time of myristic acid

Table1: Essential oil composition of *Myristica fragrans*

Essential oil Components	**R_t**	**Essential oil components**	**R_t**
+-4-carene	7.78	a-pinene	5.78
Asarone	15.07	α' copaene	12.70
1,4 cyclohexadiene 1-methyl-4-(1-methylethyl)	7.13	1,3 benzodioxole 4- methoxy-6-2-propenyl	14.77
1-methyl-4-(methylethyl)-E cyclohexanol	8.49	Cyclohexanol methyl-4-(1-methylethenyl)cis	7.31
α' cyclogeraniol acetate	23.49	16 heptadecen 2,5,8 trione	28.38
4(10) Thujene	4.66	Dipivaloyl menthane	27.94
3,7 nonadien 2 one 4,8,dimethyl	12.20	p-menth 1 en-8-ol acetate	12.32
2,6 octadien-1-ol,3,7 dimethyl propanoate,Z	26.26	2 isopropenyl 5 methyl cyclohexyl acetate	25.42
Isobutyl 2-(4-methylcyclohex -3-enyl)propan-2 yl carbonate	25.01	3 ethyl phenol tert –butyl dimethyl silyl ether	18.08
Geranyl acetate	12.78	L-α' terpineol	9.86
Trans iso eugenol	12.43	2 pentylcyclopentanone	10.13
p-menth-1-en-3-ol, trans	10.13	2 pentylcyclopentanone	10.13
methyleugenol	13.07	methyl tetra decanoate	16.90
Myristic acid	17.76	o-cymene	6.22
p-cymen-8-ol	9.76	pulegone	26.90
safrole	11.41	terpinen- 4-ol	9.71

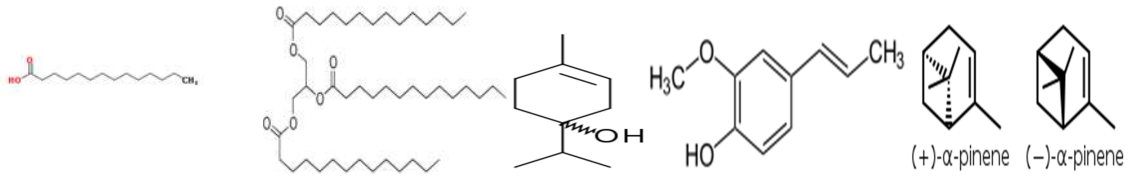
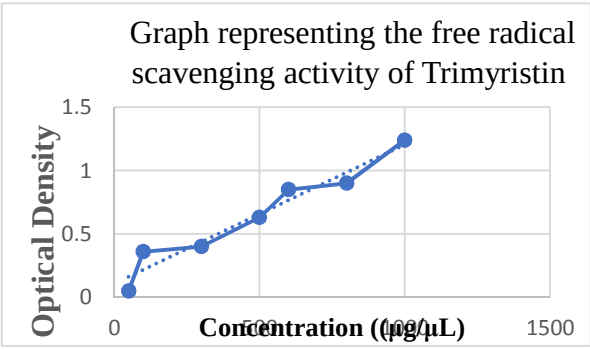


Figure 4: Structure of active compounds from *Myristica fragrans*

The yield of the essential oil was found to be 8.8% which plays an important role in determining the properties. Thirty-two chemical constituents were identified. Most of these compounds are monoterpenes or phenylpropanoids. Myristic acid, trans isoeugenol, methyleugenol, terpinen- 4-ol etc were found to be the major components.

Table 2: showing the free radical scavenging capacity of trimyristin

Concentration (µg/µL)	Absorbance
0	0.05
100	0.36
300	0.40
500	0.63
600	0.85
800	0.90
1000	1.24



Trimyristin showed 405 µg/µL radical scavenging activity at a concentration of 1mg/mL concentration which shows that this pure compound possesses only moderate free radical scavenging capacity. The presence of reductants in the plant causes the reduction of Fe^{3+}/ferricyanide complex to ferrous form by donating an electron. The amount of Fe^{2+} complex can be monitored by measuring the formation Prussian blue at 700nm wavelength. Increase in absorbance at 700nm reflects an increase in reducing ability.

4. Conclusion

The percent recovery of trimyristin and the percent yield of sodium myristate were noticable, suggesting that the isolation, purification, and reflux reactions were effective. subsequent validation of activity and the mechanism of action. *Myristica fragrans* is a resource of medicinally

active compounds and has diverse pharmacological effects; hence, this drug encourages researchers to explore its various novel therapeutic uses for the benefit of mankind. The reducing power of a compound is reflected by its potential antioxidant activity.

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OP20

Bioactive Compounds in *Glycosmis Pentaphylla* Leaf Extract: Phytochemical Analysis and Antimicrobial Studies

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Abstract

Glycosmis pentaphylla which belongs to the family *Rutaceae.* It is commonly known as Orange berry (English).is a medium-sized tree. It is a shrub and the leaves usually have 3 to 5 pinnately arranged leaflets, though these are sometimes reduced to one or two, all forms being often found on the same plant. The leaves of the plant were under investigation. The leaves of Glycosmis pentaphylla were collected, and an ethyl acetate extract was obtained. GC-MS analysis identified the components. Antibacterial screening using the disc diffusion method revealed significant antimicrobial activity against four pathogenic bacterial strains, encompassing both gram-positive and gram-negative organisms. The observed antibacterial effects are attributed to the active components present in the ethyl acetate extract.

Key Words: *Glycosmis pentaphylla*, GC-MS, Antibacterial activity, Disc diffusion method,

Introduction

Glycosmis pentaphylla (Retz.) Correa belongs to *Rutaceae* family. It is commonly known as Orange berry (English). It is a shrub growing 1 to 5 meters high. Leaves usually have 3 to 5 pinnately arranged leaflets, though these are sometimes reduced to one or two, all forms being often found on the same plant. Leaflets are oblong, 5 to 18 centimeters long, and 2 to 7 centimeters wide. Flowers are small, white, about 6 millimeters in diameter, born in axillary, solitary or paired. Fruit is fleshy, pink or reddish, rounded, 1 centimeter in diameter, and contains a single nearly spherical seed which is about 4 millimeters in diameter. Mesocarp is fleshy and sweet. *Glycosmis pentaphylla* has a long history of usage in traditional medicine against various ailments around the world [1]. In ayurvedic and other traditional medicinal practices the plant has been used against

diseases like bilious complaints, cough, worms, jaundice, fever, inflammation, rheumatism, anaemia and vermifuge. Phytochemicals like alkaloids, flavonoids, terpenes and sterols have been isolated from this plant. Important pharmacological activities such as hepatoprotective, anti-inflammatory, anti-tumor, antioxidant, antibacterial, antiviral, anti-ulcer, chemo protective and antiseptic properties were also discovered [2].

Glycosmis pentaphylla contains carbohydrates, alkaloids, flavonoids, tannins and phenolic acids, glycosmin, and a crystalline glycoside present in traces throughout the plant. Leaves also yield tannin, traces of salicin, and about 2.1 percent of sugars (reducing and non-reducing). From the leaves, study isolated glycolone, a quinolone alkaloid. From the root bark study, isolated carbazole and 3-methylcarbazole. Stem extract yielded a new naphthoquine, glycoquinone, a new acridone alkaloid, and glycocitrine along with 12 known compounds [2].

Various medicinal uses include bitter juice of leaves used for fevers, liver complaints and intestinal worms, especially in children, paste of leaves, with a bit of ginger, applied to eczema and other skin diseases; also, applied over the navel for worms and other bowel disorders [3], infusion of leaves given to women after delivery to induce appetite, wood is used for snake bites [4]. It is used for cough, jaundice, inflammation, rheumatism and anemia. In Bangladesh, it is used to reduce blood sugar and to relieve pain. A study on *Glycosmis pentaphylla* suggests that the berry may aid in the reduction of certain kinds of tumors [5].

Orange berry has been shown to reduce toxicity in some individuals. According to an Indian research study, the berry was found to possess free radical seeking properties that act as an antioxidant. The 1935 study concludes that the berry may help to prevent or slow the progression of degenerative disease [6].

There is some research that suggests that *Glycosmis pentaphylla* can aid in the reduction of harmful enzymes released during liver disease. The plant emits a protective chemical that helps to shield the liver from extensive damage caused by liver disease in rats which suggests that the plant could provide similar effects to human beings. More research is needed to verify these liver enhancing effects [7].

Plant materials have shown to posses potential for the development as new drugs. Hence the chemical compounds present in them are likely to be biologically active even at

lower concentrations. No work had been reported on the ethyl acetate extract of the leaves of *Glycosmis pentaphylla* collected from Thrissur district, Kerala. The present work reports the components present in the ethyl acetate extract of leaves of *Glycosmis pentaphylla* and its antimicrobial activity.

Materials and Methods

Plant material

Leaves of *Glycosmis pentaphylla* plant was collected in the month of November 2014 from different areas of Thrissur district, Kerala. Leaves was collected from the plant were shade dried. After drying the plant materials were powdered. Powdered leaves were used for extraction in ethyl acetate. Fifty gram of powder was used for extraction.

Method of extraction

The leaves collected were shade dried. Coarsely powdered 50g of the plant material was extracted with 500 mL of ethyl acetate. The extraction was carried out in a round bottom flask by boiling the material in the solvent with a water condenser. Refluxed the material until the solvent started to boil and the hot content was left standing overnight. Then filtered and collected the extract and added fresh solvent to residue. The process is repeated three times to complete the extraction. The combined extract collected was reduced to 20 ml.

Identification

GC-MS analysis of this extract was conducted to identify the components present in it. GC/MS analyses were carried out using a Perkin Elmer Clarus 500 GC equipped with a Clarus 500 mass spectrometer, capillary column (0.32μm film thickness). 1μL of each sample was diluted with 300μL of Et_2O and injected (0.5μL) in the "split" mode (1:30) with a column temperature program of 40°C for 5 min, then increased to 250°C at 4°C/min and finally held at this temperature for 10min. Injector and detector were set at 150 and 270°C, respectively, and the carrier gas was He with a head pressure of 12.0 psi. Mass spectra were acquired over 40-500amu range at 1scan/sec with ionizing electron energy 70eV, ion source 230^{o}C. The transfer line was set at 250^{o}C, while the carrier gas was He at 1.0mL/min.

Biological activity

The antibacterial screening of the extract was carried out by determining the zone of inhibition using standard method [8]. The extract was tested against four pathogenic bacterial strains of gram positive and gram negative organism by disc diffusion method [9]. The test microorganisms of gram positive bacteria: *Staphylococcus aureus, Bacillus subtilis, Streptococcus faecalis, Staphylococcus albus* gram negative bacteria: *Escherichia coli, Pseudomonas aeruginosa, Protieus vulgaris, Klebsiella aerogenes.* Previously prepared paper discs were dispensed onto the surface of the inoculated agar plate. Each disc was pressed down firmly to ensure complete contact with the agar surface. The discs were placed on the medium suitably apart and the plates were incubated at 5°C for 1h to permit good diffusion and then transferred to incubator at 37°C for 24 hours. After completion of 24h, the plates were inverted and placed in an incubator set to 37°C for 24 hours.

Results and Discussion

Large numbers of spots were observed on TLC examination of *Glycosmis pentaphylla*, hence it was subjected to GC-MS analysis. From the earlier reports of *Glycosmis pentaphylla,* contains monoterpenes, sesquiterpenes, diterpenes, alkane and alkene, fatty acids. On GC-MS analysis of this fraction different compounds were present. The components were identified by library search spectrum. The results of GC-MS analysis of *Glycosmis pentaphylla* is given in Table 1.

From the GC-MS analysis of *Glycosmis pentaphylla* leaves extract(ethyl acetate) were shown that the major components are Bicyclo [5.2.0] nonane, 2-methylene-4,8,8-trimethyl-4-vinyl(10.93%) and 1,19-Eicosadiene (9.84%). The activity of each compound against the microorganism under study can be concluded from their respective zone of inhibition diameter which is given in Table 2. It was observed that all the extract exhibit biological activity, hampering the growth of one or the other organism. Table 3 shows the minimal inhibitory concentration. It is found from the antibacterial study using the disc diffusion method, the ethyl acetate extract of the leaves of Glycosmis *pentaphylla* shows activity towards both gram positive and gram negative bacteria are given in the Table 2.

The maximum activity shown by *Staphylococcus aureus* at 5mg/l, *Bacillus subtilis* at 5mg/l and *Protieus vulgaris* at 5mg/l. The antimicrobial activity in ethyl acetate extract may

be due to the presence of components present or due to the synergistic effect of the major and minor components. Usually the major components are responsible for the antimicrobial activity of plant extract, but the minor components also play major role making the whole oil more active than the combination of major components in synergism.

Conclusion

In the present study GC-MS analysis of *Glycosmis pentaphylla* leaves extract(ethyl acetate) were shown that the major components are Bicyclo [5.2.0] nonane, 2-methylene-4,8,8-trimethyl-4-vinyl(10.93%) and 1,19-Eicosadiene (9.84%). Therefore, the leaves extract of *Glycosmis pentaphylla* in ethyl acetate solvent, a potentially useful antimicrobial agent. This antimicrobial activity can be attributed to the compounds present in the extract. Hence it can be used as a potential antimicrobial agent.

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Table 1. GC-MS analysis of leaves ethyl acetate extract of *Glycosmis pentaphylla*

Sl.No.	Compound	%
1.	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl	10.93
2.	1,19-Eicosadiene	9.84
3.	1,6-Cyclodecadiene,1-methyl-5-methylene-8-(1-methylethyl)-,[S(E,E)]-	4.63
4.	Naphthalene,1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-(1S-cis)	1.53
5.	Cyclohexane,1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-[1S-(1alpha,2beta,4beta)]-	1.23
6.	Cyclohexane,1-ethenyl-1-methyl-2-(1-methyethenyl)-4-(1-methylethylidene)-	1.05
7.	1,5,5-Trimethyl-6-methylene-cyclohexene	0.9
8.	Bicyclo[5.2.0]nonane	0.8
9.	1H-Cycloprop[e]azulene, decahydro 1,1,7-trimethyl-4- methylene-	4.03
10.	4,7-Methanoazulene,1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-[1S-(1alpha,4alpha,7alpha)]-	2.11
11.	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene-	4.97

Table 2. Antimicrobial screening of extract

Sl.No.	**Test organisms**	**Diameter of zone of inhibition (mm) at different concentrations**			
		Glycosmis pentaphylla			**STD**
	Gram +ve bacteria	**1 mg/l**	**2.5 mg/l**	**5 mg/l**	**2µg/disc**
1	*Staphylococcus aureus*	11	12	13	20
2	*Bacillus subtilis*	10	12	14	19
3	*Streptococcus faecalis*	11	12	13	19
4	*Staphylococcus albus*	10	12	14	18
	Gram-ve bacteria	**1 mg/l**	**2.5 mg/l**	**5 mg/l**	**2µg/disc**
1	*Escherichia coli*	09	10	10	18
2	*Pseudomonas aeruginosa*	10	11	11	19
3	*Klebsiella aerogenes*	10	11	12	19
4	*Protieus vulgaris*	11	13	14	19
Standard (STD) – Ciprofloxacin 2µg/disc Solvent – DMSO (Shows nil effect against the micro organisms under test)					

Table 3. Minimal inhibitory concentration

MIC - DETERMINATION : µg/ml							
Sl.No.	**Tested organism**	**Diameter of zone of inhibition (mm) at different concentrations**					
		Glycosmis pentaphylla					**STD***
	Gram +ve bacteria	800	600	400	200	100	
1	*Staphylococcus aureus*	07	07	06	06	06	20
2	*Bacillus subtilis*	07	07	05	05	04	19
3	*Streptococcus faecalis*	08	07	07	06	06	19
4	*Staphylococcus albus*	07	07	06	06	06	18
	Gram –ve bacteria	800	600	400	200	100	
1	*Escherichia coli*	07	06	NI	NI	NI	18
2	*Pseudomonas aeruginosa*	07	05	03	NI	NI	19
3	*Klebsiellaaerogenes*	07	06	04	NI	NI	19
4	*Protieus vulgaris*	08	05	04	04	03	19
*Standard (STD) – Ciprofloxacin 2µg/disc							

OP21

Preparation, characterization of Co/TiO_2 nanoparticles and a theoretical investigation on its application for photocatalytic degradation of methylene blue

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[a]M. Sc student, Baselius College, Kottayam, [b,*] Assistant Professor, Baselius College, Kottayam

Abstract

To improve the photocatalytic property of titanium dioxide, titanous sulfate as the titanium source, cobalt carbonate as the cobalt source $(Co)_x(TiO_2)_x$ with x=0.1%wt, 0.2%wt, 0.3%wt , and 0.5%wt Co^{2+}- doped titania nanoparticles were prepared via coprecipitation method. Based on the degradation rate of methylene blue, the effects of the co-doped rate on photocatalytic activities of the sample were researched. The result showed that doping cobalt could improve the photocatalytic performance of the titanium dioxide nanotubes under the visible light. The experimental and theoretical studies of the adsorption of methylene blue (MB) on TiO2 were established. The geometry of methylene blue was optimized by density functional theory (DFT) at the B3LYP/LanL2DZ level of theory using Gaussian software 09W. The binding energy of methylene blue with TiO_2 in the presence

and absence of Co has been computed. The composition and structure of the samples were characterized by X-ray diffraction and UV-visible spectroscopy.

1. Introduction

Environmental cleaning using TiO_2 photocatalysts has attracted a great deal of attention due to the increase in the level of environmental pollutions in the world [1]. TiO_2 is considered as one of the most promising materials due to its high stability and environmental safety. However, the application of TiO_2 in water and air purification is restricted as its intrinsic wide band gap (3.2 eV) requires high energy excitation such as UV irradiation, which only composes 5% of solar irradiation. Thus, the major portion of solar energy (visible light) could not be used for photocatalytic reaction. Besides, high recombination rate of photo-excited carriers is another limitation for the applicable fields of TiO_2. Due to the short life of photo-excited carriers, only a small part of electrons and vacancies can move to its surface, which leads to further reduction of photocatalytic efficiency [2]. For more than a decade, studies have mainly concentrated on the suspension of TiO_2 fine powder because of its higher photocatalytic activity compared with TiO2 thin films [3]. From among the three principal crystalline forms of titania, rutile does absorb some visible light, while anatase absorbs only in the UV region. Unfortunately, rutile is not a good photocatalyst. It is also known that optimal photocatalytic efficiency is obtained with a mixture of anatase and a small percentage of rutile [4]. Many attempts have been made to sensitize titanium dioxide to the whole visible region, such as doping with transition metals [5–16], transition metal ions [17–23], nonmetal atoms [13, 24] and organic materials. Introduction of dopants allows titania to absorb in the visible region but this does not necessarily mean that the doped catalyst has a better photocatalytic activity. When the doping level exceeds an optimal limit, which usually lies at very low dopant concentration and low visible light absorption, the dopant causes recombination of sites and has undesirable effects on photocatalysis.

Co-precipitation method is an attractive method for synthesis of TiO_2, and it is becoming increasingly important to distribute materials and precursors used in a reaction to produce a required material. The aim in co-precipitation is to prepare multicomponent materials through the formation of intermediate precipitates, usually hydrous oxides or oxalates, so that an intimate mixture of components is formed during precipitation and chemical homogeneity is maintained on calcination [10].

Metal is carried out in solution, this permits tailoring of certain desired structural characteristics such as compositional homogeneity, grain size, particle morphology and porosity. Preparation of transition metal-doped TiO_2 nanoparticles by co-precipitation method, characterization and investigation of their photocatalytic activity have been reported in recent literature.

The paper presents the theoretical and computational study of application of TiO_2 nanoparticles containing different amounts of cobalt for heterogeneous photocatalytic degradation of methylene blue (MB). MB is the most commonly used substance for dying cotton, wood and silk. It can cause eye burns, which may be responsible for permanent injury to the eyes of human and animals. Although MB is seen in some medical uses in large quantities, it can also be widely used in colouring paper, dyeing cottons, wools, coating for paper stocks, etc. Though MB is not strongly hazardous, it can cause some harmful effects. Theoretical studies aim at studying the interaction of neutral and protonated forms of MB dye with TiO_2 molecule. Density functional theory (DFT) calculations at the B3LYP/LanL2DZ level were used to understand the electronic properties of these forms and its interaction with the TiO_2 nanoparticle.

Cobalt doped nanoparticles synthesised by coprecipitation method was characterized by X-ray diffraction (XRD). Moreover, the photo-catalytic performance of the prepared samples in degrading MB dye was estimated using UV–Vis spectrophotometry.

2. Methods

2.1 Experimental

Meta form of liquid tiatanyl hydroxide was collected From TTPL plant washed and filtered and post leach cake was obtained. About 1000 g of cake is taken in the beaker and about 150 ml of water of added to it. It is then trangerd to gravity bottle (100 ml) and made the gravity to 1.30. After the entire checking it was then transferred to the heater provided with an electric stirrer, then 826 ml of H_2SO_4 was added and stirred cooled for half an hour and measured the transferred to 3 necked round bottomed flask for half an hour. Its colour fades and volume and thus tiatanyl Sulphate was prepared $TiOSO_4$, and volume was found to be 1379 ml. From 1370 ml $TiOSO_4$, 600 ml was transferred to RB flask provided with mechanical stirrer to reduce 162 g TiO_2 to 50 g/L TiO_2. This ortho form of titanyl hydroxide was prepared. To it liquid ammonia was added to obtain pH in the range 5.5 -6. Since $TiOSO_4$ is acidic in nature .PH of the solution is measured using

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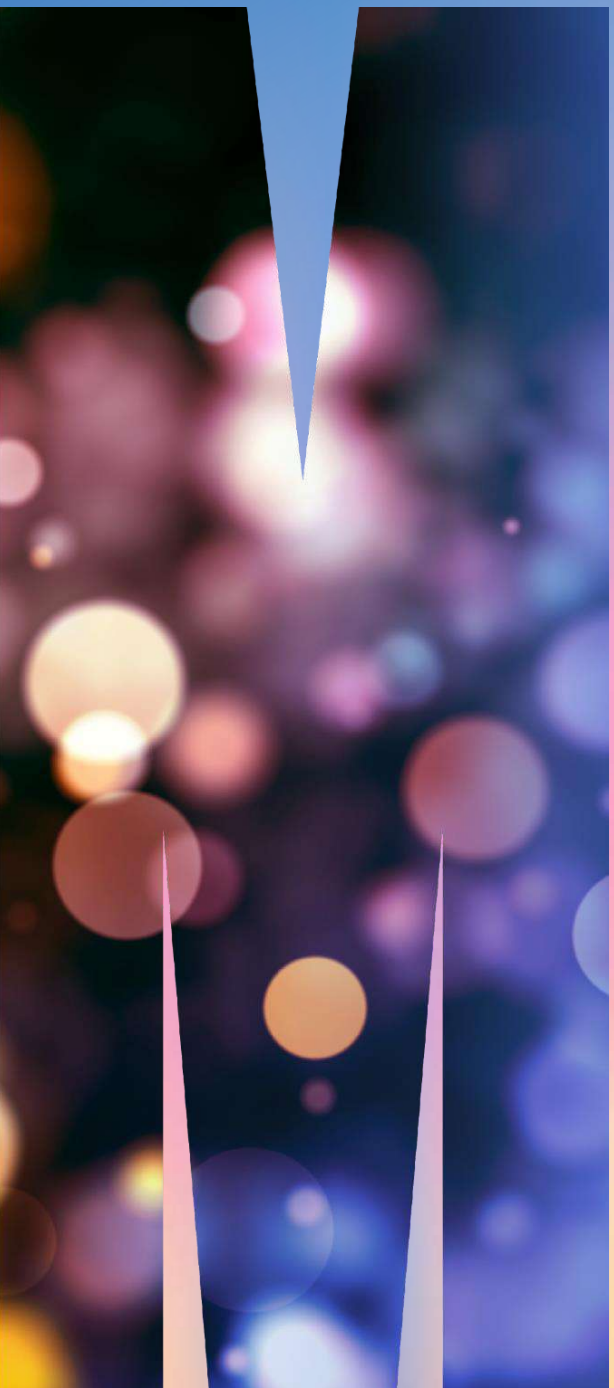

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10.10am	**Tea Break and Poster Viewing [Exhibition foyer]**
10.30am	**Keynote Speaker:** **Prof. Datin. Paduka Dr Khatijah Mohamad Yusoff** **Universiti Putra Malaysia (UPM), Malaysia** Topic: Harnessing the Potential of Newcastle Disease Virus: An Encouraging Strategy for Cancer Treatment
11.20am	**Plenary Speaker:** **Dr Kamal Dua** **University of Technology Sydney, Australia** Topic: Integration of Biological and Technological Advances in Developing Novel Therapeutic Interventions for Lung Diseases
12.10pm	**Plenary Speaker:** **Mdm Rosliza Lajis, Head of New Drug Product Section** **National Pharmaceutical Regulatory Agency (NPRA)** **Ministry of Health, Malaysia** Topic: The Evolution of Pharmaceutical Product Registration in Malaysia

Agenda: Day 1

Time (MYT)	DAY 1 – 25 OCTOBER 2023, WEDNESDAY Auditorium 5114
1.00pm	Sponsor talk
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2.00pm	Oral Presentation [Kindly refer to the Oral Presentation Schedule]
3.40pm	Tea break and poster viewing [Exhibition foyer]
4:00pm	Poster evaluation [Exhibition foyer] *ALL presenters please standby at your poster
	End of Day 1

Agenda: Day 2

Time (MYT)	DAY 2 – 26 OCTOBER 2023, THURSDAY Auditorium 5114
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9.00am	**Keynote Speaker:** **Professor Chris Bain** **Monash University Australia** Topic: Digital Health and its Relationship to Precision Health and Wellness
10.10am	**Tea Break and Poster Viewing [Exhibition foyer]**
10.30am	**Plenary Speaker:** **Associate Professor Dr Daniel Malone,** **Monash Institute of Pharmaceutical Sciences** **Monash University Australia** Topic: Exploring Ways to Better Prepare Pharmacy Students for Practice
11.20am	**Plenary Speaker:** **Dr Janattul Ain Jamal, Faculty of Pharmacy,** **Universiti Teknologi MARA (UiTM), Malaysia** Topic: Optimizing Antimicrobial Therapy: Dosing, Therapeutic Drug Monitoring, Challenges, and Opportunities
12.10pm	**Poster evaluation [Exhibition foyer]** ***ALL presenters please standby at your poster**

Agenda: Day 2

Time (MYT)	DAY 2 – 26 OCTOBER 2023, THURSDAY Auditorium 5114
1.00pm	**Lunch break and poster viewing [Exhibition foyer]**
2.00pm	**Oral Presentation [Kindly refer to the Oral Presentation Schedule]**
3.40pm	**Tea break and poster viewing [Exhibition foyer]**
4:00pm	**Invited Speaker:** **Dr Daniel Wright** **The Oxford Vaccine Group** **University of Oxford, United Kingdom** Topic: Developing Vaccines Against Emerging Pathogens
4.50pm	**AWARD PRESENTATION AND CLOSING CEREMONY**
5.30pm	**Adjourn**
	End of MONASH INITIATE 2023

Oral Presentation Schedule Day 1 – 25 Oct 2023 (Wed)

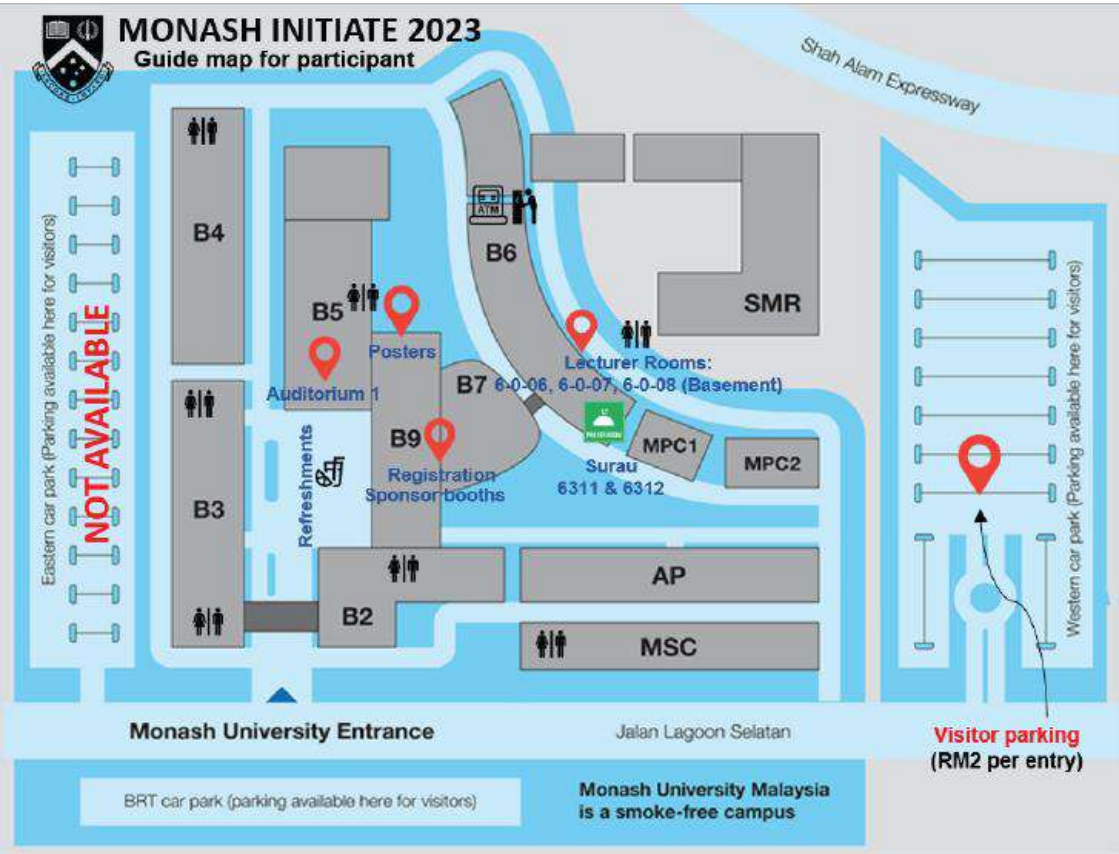
Time Start (pm)	Time End (pm)	Drug delivery (DD)	Drug discovery and synthesis (DS)	Life Sciences (LS)	Clinical Pharmacy (CP) + Digital Health (DH)
Venue		**Lecture theatre 6006**	**Auditorium 5114**	**Lecture theatre 6007**	**Lecture theatre 6008**
2.00	2.15	OP-DD-05	OP-DS-01	OP-LS-01	OP-CP-01
2.15	2.30	OP-DD-06	OP-DS-03	OP-LS-02	OP-CP-03
2.30	2.45	OP-DD-08	OP-DS-04	OP-LS-03	OP-CP-04
2.45	3.00	OP-DD-09	OP-DS-05	OP-LS-04	OP-CP-05
3.00	3.15	OP-DD-10	OP-DS-06	OP-LS-05	OP-CP-06
3.15	3.30	OP-DD-12	OP-DS-09	OP-LS-06	OP-CP-07
3.30	3.45	OP-DD-13	OP-DS-12	OP-LS-08	OP-DH-03
3.45	4.00	OP-DD-11	Tea break and poster viewing		
4.00	4.15	-	OP-DS-15	OP-LS-09	OP-DH-04
4.15	4.30	-	OP-DS-19	OP-LS-21	OP-DH-05
4.30	4.45	-	OP-DS-20	OP-LS-07	
4.45	5.00	-		OP-LS-14	

Oral Presentation Schedule Day 2 – 26 Oct 2023 (Thurs)

Time Start (pm)	Time End (pm)	Drug delivery (DD)	Drug discovery and synthesis (DS)	Life Sciences (LS)	Public Health (PH)
Venue		**Lecture theatre 6006**	**Auditorium 5114**	**Lecture theatre 6007**	**Lecture theatre 6008**
2.00	2.15	OP-DD-15	OP-DS-13	OP-LS-10	OP-PH-01
2.15	2.30	OP-DD-19	OP-DS-21	OP-LS-11	OP-PH-02
2.30	2.45	OP-DD-16	OP-DS-22	OP-LS-16	OP-PH-04
2.45	3.00	-	OP-DS-23	OP-LS-17	OP-PH-05
3.00	3.15	-	OP-DS-24	OP-LS-18	OP-PH-06
3.15	3.30	-	OP-DS-25	OP-LS-19	OP-PH-07
3.30	3.45	-	-	OP-LS-20	OP-PH-03

All abstracts will be published in the Monash INITIATE 2023 e-book which will be available for view and download on 25 October 2023.

VENUE MAP



Building index

Building 2 (B2)
School of Arts and Social Sciences
School of Information Technology
Admissions
Counselling Services
External Relations, Development and Alumni
Facilities Management
Finance
Future Students
General Studies
International Student Support
Marketing & Media
Monash Abroad
Plenary Theatre
Scholarships and Study Loans
Security
Student Services

Building 3 (B3)
Jeffrey Cheah School of Medicine and Health Sciences
Brain Research Institute Monash Sunway (BRIMS)

Building 4 (B4)
School of Science
Jeffrey Cheah School of Medicine and Health Sciences
Teaching and Research Labs
Plant House

Building 5 (B5)
School of Engineering
Engineering Laboratories

Building 6 (B6)
School of Business

Facilities Management (Mail Room)
ATM
Cafeteria
MUPA Lounge

Building 7 (B7)
Bookshop
Learning Skills
Library and Learning Commons
Monash University English Language Centre

Building 9 (B9)
Computer Laboratories

MPC 1 & MPC 2
(Multi-purpose Court)

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(Monash Sports Centre)
Monash University Student Association

AP
(Emergency Assembly Point)

SMR
(Sunway Monash Residence)

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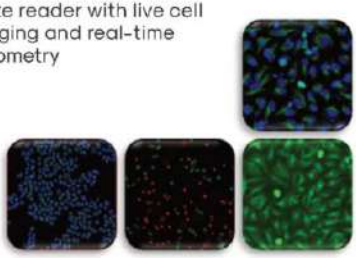

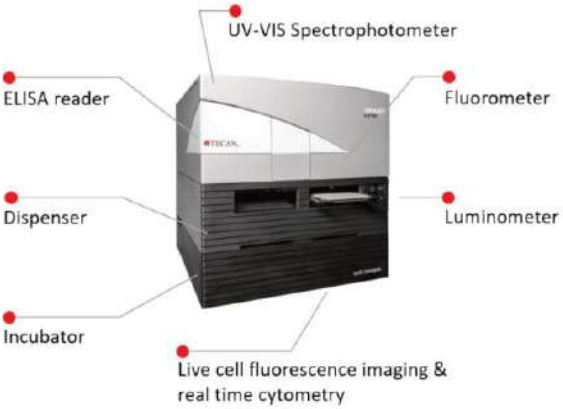

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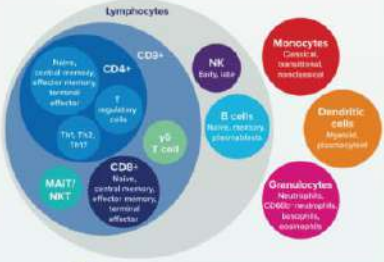

1 tube

CD3	CD28	CD161
CD4	CD38	CD294
CD8	CD45	CCR4
CD11c	CD45RA	CCR6
CD14	CD45RO	CCR7
CD16	CD56	CXCR3
CD19	CD57	CXCR5
CD20	CD66b	HLA-DR
CD25	CD123	IgD
CD27	CD127	TCRγδ

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37 cell populations

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Apoptosis
Metabolism
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Cytokine production
Transcription factors

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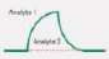
Pure or complex.
Small or large.

Affinity
Reflects the binding strength.

Kinetics
How fast/slow a complex forms and dissociates.

Concentration
Determine concentration of active analyte.

Specificity
Is the molecule specific for its target?



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✓ How highly efficient is it?
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Application


Food Sanitation


Public Places


Personal Hygiene


Air Deodorisation


Pet Disinfectant


Healthcare Hygiene


Children Disinfectant

Disinfectant Contact Time

TEST ORGANISM	CHLORINE DIOXIDE	ALCOHOL 70%	QUATERNARY	AMPHOTERIC SURFACTANT	HYPOCHLORITE
STAPHYLOCOCCUS AUREUS	5 mins	5 mins	5 mins	5 mins	5 mins
CANDIDA ALBICANS	5 mins	5 mins	15 mins	15 mins	5 mins
ENTEROCOCCUS HIRAE	5 mins	5 mins	5 mins	5 mins	5 mins
PSEUDOMONAS AERUGINOSA	5 mins	5 mins	5 mins	5 mins	5 mins
ESCHERICHIA COLI	5 mins	5 mins	5 mins	5 mins	5 mins
BACILLUS CEREUS	5 mins				5 mins
ASPERGILLUS BRASILIENSIS	5 mins				15 mins

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PPE	STERILE COVERALL • STERILE BOOT COVER • STERILE GOWN • COVERALL • BOOT COVER • GOWN • NON WOVEN CAP • FACE MASK • RESPIRATOR MASK • SAFETY GOGGLE • FACE SHIELD • NITRILE GLOVE • LATEX GLOVE • SHOE COVER
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PREPARED MEDIA	STERIPACK TRIPLE WRAPPED MEDIA • PREPARED PLATED MEDIA • PREPARED TUBED MEDIA • TRANSCULTSWAB • CHROMOGENIC AGAR
LABORATORY	BEAKER • JUG • CYLINDER • FUNNEL • GLASS STIRRING ROD • FORCEP • SPATULA • STIRRER BAR • WASH BOTTLE • STAINLESS STEEL SCISSORS • DECON 90
TRAINING	DEMONSTRATION ASEPTIC GOWNING • DEMONSTRATION GLOVING TECHNIQUE • CLEANROOM INTRODUCTION AND CONTAMINATION IN CLEANROOM • DEISINFECTANT SELECTION • CLEANING PROGRAMME

PRESENTERS DRUG DISCOVERY & SYNTHESIS

Oral Presenters		
Date: 25 October 2023 (Wednesday)		
ID	**Presenters**	**Time**
OP-DS-01	**Associate Professor Dr B. R. Prashantha Kumar** Novel Derivatives of Eugenol as Potent Anti-Inflammatory Agents via PPARγ Agonism: Rational Design, Synthesis, Analysis, PPARγ Protein Binding Assay and Computational Studies	2:00 PM
OP-DS-03	**Indhumathi Thirugnanasambandham** Innovative Approaches to Unveil Potential PAD4 Inhibitors for Rheumatoid Arthritis Treatment	2:15 PM
OP-DS-04	**Dr Prabitha P** Novel Glitazones Derivatives with Neuroprotective and Anti-Inflammatory Potential for PGC-1α Activation via PPAR-γ Binding in LPS-Induced SHSY5Y Cells	2:30 PM
OP-DS-05	**Associate Professor Dr T. Tamilanban** Attenuation of *N*-Nitrosodiethylamine and Phenobarbitone Induced Hepatocellular Carcinoma by Posterior Salivary Gland Toxin from Cuttlefish *Sepia pharaonis* in Male Rats	2:45 PM
OP-DS-06	**Dr Honnavalli Yogish Kumar** Design and Synthesis of Novel *N*-[3-(benzimidazol-2-ylamino)phenyl]amine and *N*-[3-(benzoxazol-2-ylamino)phenyl]amine Derivatives as Potential Anticancer Agents	3:00 PM

Oral Presenters		
Date: 25 October 2023 (Wednesday)		
ID	**Presenters**	**Time**
OP-DS-09	**Ms Deepthy Varghese** Development and Evaluation of Novel β-Diketonates as Potential Antiangiogenic Agents by Inhibition of MMP9: A Computational and Experimental Approach	3:15 PM
OP-DS-12	**Ms Mustika Furi** Principal Component Analysis, Total Phenolic Content, In Vitro Antioxidant, Tyrosinase Inhibitory and Antimalarial Activities of Terap (*Artocarpus odoratissimus* Blanco) Leaves	3:30 PM
OP-DS-15	**Ms Rahayu Utami** Phytochemical Profile and Antioxidant Capacity of Leaves Extract of *Sauropus androgynus* Originated from Riau Province, Indonesia	4:00 PM
OP-DS-19	**Ms Jing Yi Wong** Protective Effect of Atorvastatin Against NMDA-Induced Excitotoxic Retinal Injury in Rats: A Dose-Response Study	4:15 PM
OP-DS-20	**Ms Jannelle Manarang** Determination of Sedative and Anxiolytic Effect of *Clitoria ternatea* Flower Extract on Male Albino Mice	4:30 PM

Oral Presenters		
Date: 26 October 2023 (Thursday)		
ID	**Presenters**	**Time**
OP-DS-13	**Dr Srikanth Jeyabalan** *In silico* and *In vivo* Evaluation of 4-Hydroxy Benzoic Acid against Mercury Chloride Induced Alzheimer Disease in Zebrafish (Danio rerio)	2:00 PM
OP-DS-21	**Ms Nina Angela B. Lazaro** Antibacterial Activity of Oral Spray containing *Graptophyllum pictum* (L.) Griff Leaf Extract against *Streptococcus mutans*	2:15 PM
OP-DS-22	**Ms Yoghinni A/P Manogaran** Synthesis and Evaluation of Anticancer Potential of Novel Imino Analogues	2:30 PM
OP-DS-23	**Ms Dharshini Jagadeesan** Discovery of New Quinoline Analogues for Oral Squamous Cell Carcinoma Treatment	2:45 PM
OP-DS-24	**Ms Darssheela A/P Ramasamy** In vitro Antiviral Activity of *Coriander sativum L.* Crude Extract against Respiratory Syncytial Virus	3:00 PM
OP-DS-25	**Dr Sivananthan Manoharan** Tripeptide GVR Blocked Catalytic Site of C-domain of Somatic ACE and Chymase Enzymes Simultaneously Then Reduced High Blood Pressure in Strictly Fasted Spontaneously Hypertensive Rats	3:15 PM

Novel Derivatives of Eugenol as Potent Anti-Inflammatory Agents via PPARγ Agonism: Rational Design, Synthesis, Analysis, PPARγ Protein Binding Assay and Computational Studies

Noor Fathima Anjum, Madhusudan N. Purohit, B.R. Prashantha Kumar
Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Mysuru 570 015, India. JSS Academy of Higher Education & Research, Mysuru 570 015, India.
Correspondence: Dr. B.R. Prashantha Kumar
(email: brprashanthkumar@jssuni.edu.in)

Introduction: Eugenol, a natural product abundantly found in clove buds, is known for its pharmacological properties such as anti-inflammatory, antidiabetic, antioxidant, and anticancer activities. It is well known from the literature that peroxisome proliferator-activated receptors (PPARγ) have been reported to regulate inflammatory responses. **Objective:** This work aimed to search for new potent semi-synthetic anti-inflammatory PPARγ agonists. **Methodology:** We applied a computational approach to design semi-synthetic derivatives of eugenol, synthesize, purify, and analyze them as potential anti-inflammatory agents and PPARγ agonists. Compounds were screened for PPARγ protein binding by time-resolved fluorescence (TR-FRET) assay. **Results:** The biochemical assay identified one potent compound (1C), which exhibited significant binding affinity with an IC_{50} value of 10.65 µM as compared to the standard pioglitazone. In addition to the protein binding studies, the synthesized eugenol derivatives were screened for in vitro anti-inflammatory activity at concentrations ranging from 6.25 µM to 400 µM. Among four compounds tested, 1C shows reasonably good anti-inflammatory activity with an IC_{50} value of 133.8 µM compared to a standard Diclofenac sodium IC_{50} value of 54.32 µM. Structure-activity relationships are derived based on computational studies. Additionally, molecular dynamics simulations were performed to examine the stability of the protein-ligand complex, the dynamic behavior, and the binding affinity of newly synthesized molecules. **Conclusion:** We identified novel eugenol derivatives as PPARγ agonists with anti-inflammatory properties.

Keywords: Eugenol derivatives; peroxisome proliferator-activated receptor gamma (PPARγ); molecular dynamics; anti-inflammatory activity.

Innovative Approaches to Unveil Potential PAD4 Inhibitors for Rheumatoid Arthritis Treatment

Indhumathi Thirugnanasambandham[1], Gowthamarajan Kuppusamy[1], Srikanth Jupudi[2]

[1]Department of Pharmaceutics, JSS College of Pharmacy, JSS Academy of Higher Education & Research, Ooty, Nilgiris, Tamil Nadu, India; [2]Department of Pharmaceutical Chemistry, JSS College of Pharmacy, JSS Academy of Higher Education & Research, Ooty, Nilgiris, Tamil Nadu, India.

Correspondence: Gowthamarajan Kuppusamy (email: gowthamsang@jssuini.edu.in)

Introduction: Rheumatoid arthritis (RA) is an autoimmune disease characterized by persistent impairment, functional limitations, and mobility restrictions. Dysregulation of peptidylarginine deiminase 4 (PAD4) affects impaired citrullination and excessive NETosis, contributing to RA development. Targeting PAD4 with specific inhibitors is of great interest due to the unique expression profile and diverse functions of this enzyme. **Objective:** Our objective was to identify potential PAD4 inhibitors with innovative approaches and techniques. **Methodology:** Virtual screening of 30 FDA-approved drug molecules was performed using molecular docking. The top-ranked compounds were subjected to an enzymatic bio-assay. Stability analysis of the inhibitors within the catalytic pocket was conducted through molecular dynamics simulations. Structural changes of PAD4 were examined using nuclear magnetic resonance (NMR) spectroscopy and electrospray ionization mass-spectrometry (ESI/MS-TOF). The binding affinity between PAD4 and the selected inhibitor was determined using an in vitro binding assay. **Results:** Saquinavir (SQV) emerged as a potential PAD4 inhibitor based on the enzymatic bio-assay. Molecular dynamics simulations revealed a stable binding conformation of SQV within the catalytic pocket of PAD4. Analysis of PAD4 structural changes using NMR and ESI/MS-TOF provided insights into the protein-inhibitor interaction. The in vitro binding assay confirmed significant binding affinity between PAD4 and SQV. **Conclusion:** SQV shows promise as a potential drug candidate for RA treatment. Its inhibitory properties, stable binding conformation, and significant binding affinity with PAD4 highlight its potential as a targeted therapeutic option. This study contributes to drug discovery and synthesis efforts, emphasizing the importance of developing PAD4-specific inhibitors for RA treatment.

Keywords: Rheumatoid arthritis; peptidyl arginine deiminase 4; drug repositioning; biophysical characterization.

Novel Glitazones Derivatives with Neuroprotective and Anti-Inflammatory Potential for PGC-1α Activation via PPAR-γ Binding in LPS-Induced SHSY5Y Cells

Prabitha P, Prashantha Kumar BR
Department of Pharmaceutical Chemistry, JSS College of Pharmacy, Mysuru 570015, JSS Academy of Higher Education & Research, Mysuru, Karnataka, India.
Correspondence: Dr.Prabitha P (email: pprabitha@jssuni.edu.in)

Introduction: Glitazones, also known as thiazolidinediones (TZD) have received a lot of attention due to their biological activities. In the present study, fifteen novel glitazones were designed and synthesized for their neuroprotective and anti-inflammatory potential. **Methodology:** We designed compounds using *in silico c*omputational approaches and analyzed their binding affinity to activate PGC-1α via PPAR-γ binding. The molecular dynamic simulation was done to study the conformational changes in molecular interactions with the active site of the protein. The proposed fifteen novel glitazones were synthesized by Knoevenagel condensation and screened for TR-FRET PPAR-γ competitive binding assay to arrive at a selective PPAR-γ ligand. The PPAR-γ transcriptional activity in SHSY5Y cells was measured with an ELISA-based PPARγ transcription factor assay kit. To evaluate the effect of these compounds on the mitochondrial membrane potential of cells, JC-1 staining studies were performed. The neuroprotective effects of synthesized glitazones were tested in Lipopolysaccharide (LPS) intoxicated SHSY5Y neuroblastoma cell lines. To explore the anti-inflammatory potential of synthesized glitazones, the level of cytokines (TNF-α, NF-kB, and IL-6) was estimated using flow cytometry. **Results:** Three compounds with the best binding affinity were selected based on the lowest CDOCKER interaction energy. Interestingly, three compounds PP001, PP002, and PP010 from the synthesized series were found to have more significant neuroprotective and anti-inflammatory activity than the standard drug pioglitazone based on the reduced levels of IL-6, TNF-α, and NF-kB expression in SHSY5Y cell lines. **Conclusion:** This study showed the potential neuroprotective effect of novel glitazones PP001, PP002, and PP010 under neuroinflammatory conditions; The effect could involve activation of central PGC-1α signaling via the PPAR- γ receptor.

Keywords: Glitazones; PPAR-γ; PGC-1α; TZDs; Neuroprotective; Anti-inflammatory; Docking; Molecular Dynamic Simulation.

Attenuation of *N*-Nitrosodiethylamine and Phenobarbitone Induced Hepatocellular Carcinoma by Posterior Salivary Gland Toxin from Cuttlefish *Sepia pharaonis* in Male Rats

K Sandhanam, Arunkumar Subramanian, T Tamilanban
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Correspondence: T Tamilanban (email: tamilant@srmist.edu.in)

Introduction: Hepatocellular Carcinoma (HCC) is a life-threatening disease and is the third leading cause of death around the globe. *Sepia pharaonis* is a type of marine cuttlefish species that belongs to the squid family, and recent research has shown that the active ingredients in sepia ink (SIP) may have several potential medical uses. **Objectives:** The goal of the current study was to assess the zoochemical status, antioxidant potential, and anticancer activity of SIP and its polysaccharides in *N*-nitrosodiethylamine (DEN) induced HCC. **Methodology:** HCC was induced by single i.p injection of DEN at a dose of 200 mg/kg used as an initiator and phenobarbitone (PB) 0.05% in drinking water p.o. used as a promoter. The SIP treatment was received for 90 days after 14 days of development of HCC and continued for the entire study period, whereas the other three groups were given normal saline, 5-FU (20mg/kg) i.p. **Results:** The results showed that the injection of DEN+PB led to the development of liver tumors in rats. Significant escalation of the serum biochemical parameters like SGOT, SGPT, ALP, urea, creatinine, and tumor markers was observed with depletion of endogenous antioxidants SOD, CAT, GPX, GSH, and LPO thereby leading to higher lipid peroxidation. Intraperitoneal administration of SIP at a high dose of 400 mg/kg/bw to DEN- and PB-treated rats compared to control, returned the aforementioned variables to around normal levels. The biochemical results supported histological findings that SIP has a significant dose-dependent hepatoprotective effect. **Conclusion:** Our findings demonstrated that SIP therapy reduced liver damage in DEN-induced hepatocellular carcinoma, preserved the antioxidant defense system, and had anti-carcinogenic activity.

Keywords: Hepatocellular Carcinoma; N-Nitrosodiethylamine; Fucoidan; Sepia ink Polysaccharides; Sepia pharaonis.

Design and Synthesis of Novel *N*-[3-(benzimidazol-2-ylamino)phenyl]amine and *N*-[3-(benzoxazol-2-ylamino)phenyl]amine Derivatives as Potential Anticancer Agents

Honnavalli Yogish Kumar[1,2,3], P. R. Murumkar[1], B. P. Srinivasan[2], Vijay Pawar[1], M. R. Yadav[1]

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Introduction: Chronic myeloid leukemia (CML) is a clonal cancer in which cells of the myeloid family undergo aggressive cellular multiplication. Imatinib mesylate is a blockbuster drug approved by the US FDA for targeting the BCR-ABL, the integral protein responsible for the development of CML. This drug paved the way to explore interests in the area of molecular targeted therapies. **Objectives:** Various substituted benzimidazolyl derivatives were designed utilizing knowledge-based drug design approach. The structure of the well-known marketed drug imatinib was used as the prototype. The pyridopyrimidine system of imatinib was isosterically replaced with benzimidazolyl and benzoxazolyl moieties and the modelled compounds were synthesized and screened using an *in vitro* cell-based assay. **Methodology:** The thiourea intermediates were synthesized by reacting various *o*-phenylenediamine or *o*-aminophenol with *m*-nitrophenyl isothiocyanates. The subsequent cyclisation of the thiourea intermediates was performed using dicyclohexylcarbodiimide as the cyclodesulfurising agent. The thiourea derivatives were synthesized from different isothiocyanates. **Results:** *In vitro* cytotoxicity assay of twenty-six selected compounds was carried out at National Cancer Institute (NCI), USA and **NSC D-762842/1** and **NSC D-764942/1** have shown remarkable cytotoxicity with GI_{50} values ranging between 0.589-14.3 µM and 0.276-12.3 µM respectively, in the representative nine subpanels of human tumour cell lines. Further, flow cytometry analysis demonstrated that **NSC D-762842/1** exerted cell cycle arrest at G2/M phase and showed dose-dependent enhancement in apoptosis in K-562 leukaemic cells. **Conclusion:** Overall, amide derivatives of *N*-(benzimidazol-2-yl)phenyl-1,3-diamine were found to possess moderate to good anticancer activity. Considering their *in vitro* cytotoxicity profiles, these compounds are likely to act as new lead chemotherapeutics and therefore, this piece of work needs to be further taken up for *in vivo* and mechanistic investigations.

Keywords: Imatinib; Cell lines; Leukemia; Cytotoxicity.

Development and Evaluation of Novel β-Diketonates as Potential Antiangiogenic Agents by Inhibition of MMP9: A Computational and Experimental Approach

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Introduction: Gelatinase A (MMP2) and B (MMP9) have been proven to be involved in cancer angiogenesis, metastasis and are therefore good targets in drug discovery. It is also reported that MMP9 cleaves the effector T cell chemoattractants such as CXCL-9, -10, -11 thereby making it a good target to promote antitumor immunity in lymphoma models. **Objective:** This study aims to design, synthesize, and characterize a series of novel Knovenagel condensates of β-diketonates and tested for their antiangiogenic potentials by the inhibition of MMP9. **Methodology:** Several molecules were designed and screened for their binding affinity towards MMP9 by molecular docking studies. Out of these ligands, molecules that showed higher binding affinity were complexed with receptors and subjected to MD simulation studies. using GROMACS 5.7.4 package. The ADME properties of ligands that were stable in the MD simulation studies were predicted using SwissADME. The compounds were then synthesized using Knovenagel condensation and subjected to CAM assay to evaluate their antiangiogenic potential. **Results:** Eighteen compounds were designed for molecular docking studies and seven of these showed strong affinity to MMP9 and were used for MD simulation and ADMET computational studies. None of the compounds elicited significant toxicity in the ADMET studies, and one (viz. BH2), when complexed with MMP9, showed remarkable stability of the complex with the receptor in the MD simulation studies. The radius of gyration, RMSD, and RMSF of this protein-ligand complex in the 10ns MD simulation analysis further validated the stability of their interaction in the solvated, charge-neutralized system. BH2 was therefore synthesized by a modified Knovenagel condensation and its structure was confirmed by IR, ^{1}HNMR,^{13}C NMR, MS spectroscopy and elemental analysis. BH2 was used in the CAM assay to prove its antiangiogenic potential by the inhibition of MMP9. **Conclusion:** The Knovenagel condensates of β-diketonates can therefore be considered as a novel class of MMP9 inhibitors. Further preclinical studies are required to promote them as clinical drugs.

Keywords: Angiogenesis; beta-diketonates; MMP9.

Principal Component Analysis, Total Phenolic Content, In Vitro Antioxidant, Tyrosinase Inhibitory and Antimalarial Activities of Terap (*Artocarpus odoratissimus* Blanco) Leaves

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Introduction: Terap is a species belonging to the *Artocarpus* genus which is rich in phenolic compounds including flavonoids. In Riau, Terap leaves are widely used as traditional medicine. Flavonoids are important for human health because of their pharmacological activity such as antioxidant, tyrosinase inhibitory and antimalarial activities. **Objectives:** The present study explored antioxidant, tyrosinase inhibitory and antimalarial activities of the leaves of *Artocarpus odoratissimus* Blanco. **Methodology:** The leaves of *A. odoratissimus* were extracted using the maceration technique using ethanol and subsequently fractionated using hexane, ethyl acetate, and butanol. The capability of the extract to scavenge radicals was evaluated using the DPPH (2,2-diphenyl-1-picryl-hydrazyl) assay. The phenolic content (TPC) was assessed using the Folin-Ciocalteau method. The antimalarial activity was assessed using the hematin polymerization inhibition method. The tyrosinase inhibitor assay was conducted using tyrosinase from mushroom. The chemical composition analysis of the extract and fractions was performed using the Fourier transform infrared (FTIR) method, chemometrics analysis using Principal Component Analysis (PCA). **Results:** Results showed that the ethanol extract and the fractions prepared with n-hexane, ethyl acetate, and n-butanol contain phenolic compounds and flavonoids. The ethyl acetate fraction showed the highest radical scavenging activity with IC_{50} 42.9 µg/mL in the DPPH assay. Meanwhile, for tyrosinase inhibitory activity, the ethyl acetate fraction showed the highest activity with IC_{50} 18.85 µg/mL. These results were in accordance with the total phenolic content (TPC) of the extract, in which the highest TPC was obtained from the ethanol extract [154 mg gallic acid equivalent (GAE/g)] and the ethyl acetate fraction [106 mg gallic acid equivalent (GAE/g)]. The ethanol extract at 1000 µg/mL showed highest antimalaria activity with 89.9% inhibition. IR spectrum profiles combined with chemometrics PCA suggested that phenolic compounds were present in the extract and fractions of Terap leaves. **Conclusion:** This study revealed that the ethanol extract and the ethyl acetate fraction of the leaves of *A. odoratissimus* could be used as natural antimalarial, sunscreen, and antioxidant agents.

Keywords: *Artocarpus odoratissimus* Blanco; Terap; antimalarial activity; antioxidant activity; PCA; tyrosinase inhibitory activity.

In silico and *In vivo* Evaluation of 4-Hydroxy Benzoic Acid against Mercury Chloride Induced Alzheimer Disease in Zebrafish (Danio rerio)

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Introduction: Alzheimer's disease (AD) is a progressive neurodegenerative disorder characterized by memory loss and cognitive decline. The neurotoxic effects of mercury chloride ($HgCl_2$) have been linked to AD-like symptoms in various organisms, including zebrafish, making it an essential model for evaluating potential therapeutics. **Objectives:** In this study, we investigated the neuroprotective effects of 4-hydroxy benzoic acid (4-HBA) using molecular docking and simulation techniques and *in vivo* evaluation against $HgCl_2$-induced Alzheimer's-like pathology in zebrafish model. **Methodology:** *In silico* analysis was done using AutoDock and molecular simulations in GROMACS software. ADME and toxicity profiling were predicted using SwissADME and Pro-Tox databases. Molecular docking simulations involved assessment of the binding affinity of 4-HBA with acetylcholinesterase (AChE), a key enzyme associated with AD pathogenesis. For the *in vivo* evaluation, adult zebrafish were exposed to $HgCl_2$ to induce AD-like symptoms. Subsequently, the treatment group received 4-HBA regimen, while a control group remained untreated. Behavioural assessments were conducted to measure memory and cognitive function, while histological analyses were performed to assess neurodegeneration formation in zebrafish brains. **Results:** The molecular docking and dynamic simulation results revealed favorable interactions between 4-HBA and AChE, suggesting a potential inhibitory effect on AChE activity. Treatment with 4-HBA significantly ameliorated the memory deficits and cognitive impairments induced by $HgCl_2$ exposure. Histological analysis revealed a reduction in neurodegeneration in 4-HBA-treated zebrafish compared to the untreated group. Furthermore, spectrophotometer analysis showed a decrease in AChE activity in the brains of 4-HBA-treated zebrafish, confirming the potential mechanism of action. **Conclusion:** Our findings demonstrate the neuroprotective effects of 4-HBA against $HgCl_2$-induced Alzheimer's-like pathology in zebrafish. 4-HBA holds promise as a therapeutic candidate for Alzheimer's disease and warrants further investigation for its potential use in human AD management. The zebrafish model is a valuable platform for preclinical drug screening and underscores the translational potential of this research.

Keywords: Alzheimer's disease; Mercury chloride; Molecular simulations; Acetylcholinesterase; Zebrafish.

Phytochemical Profile and Antioxidant Capacity of Leaves Extract of *Sauropus androgynus* Originated from Riau Province, Indonesia

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Introduction: *Sauropus androgynus* is a plant from Euphorbiaceae family which contains high levels of phenolic, flavonoid as well as antioxidant properties. **Objectives:** This present study aims to determine phenolic and flavonoid content, antioxidant activity and FTIR spectrum profile of leaves extract of *Sauropus androgynus* originated from Riau Province, Indonesia. **Methodology:** The plant samples were collected from five different regency in Riau Province, Indonesia namely Pekanbaru (PKU), Pelalawan (PLN), Kampar (KMP), Rokan Hulu (RHU) and Kepulauan Meranti (KMI) regency. The dried-bulk leaves were extracted by maceration method using ethanol as solvent. The determination of total phenolic and flavonoid content was conducted by colorimetry method using Folin Ciocalteu and $AlCl_3$ as reagents, respectively. As for antioxidant capacity was evaluated using the DPPH free radical scavenging method. The chemometric analysis on the FTIR spectrum dataset of the ethanol extracts using principal component analysis (PCA). **Results:** The result showed that ethanol extract KMI afforded the highest total phenolic and flavonoid content among others with values of 79.536 ± 0.349 mgGAE/g extract and 67.780 ± 2.295 mgQE/g extract, respectively. The ethanol extract KMI also gave the most potential antioxidant capacity and significantly different from three other extracts (PKU, PLN and KMP) with an IC_{50} value of 32.7 ± 6.43 µg/mL. The three extracts (KMI, RHU and PLN) can be grouped based on FTIR spectrum data using PCA with a total variance of 99.1% at wavelength range of 2800-3300 cm^{-1}. **Conclusion:** These obtained results revealed that geographic origin provides different antioxidant capacity as well as the phytochemical profiles.

Keywords: Antioxidant; leaves; PCA; Riau; *Sauropus androgynus*.

Protective Effect of Atorvastatin Against NMDA-Induced Excitotoxic Retinal Injury in Rats: A Dose-Response Study

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Introduction: Excitotoxicity is caused by glutamate-mediated NMDA receptor stimulation resulting in Ca^{2+} overload and neuronal apoptosis, such as in diseases like glaucoma, a leading cause of irreversible blindness. None of the existing treatments directly target mechanisms underlying neuronal apoptosis in glaucoma. Atorvastatin (ATV), primarily known as a cholesterol-lowering agent, exhibits potential benefits for neurodegenerative disorders due to its pleiotropic effects including modulation of synaptic transmission. However, it remains uncertain whether ATV can provide protection against excitotoxic neuronal apoptosis. **Objectives:** To determine whether ATV prevents NMDA-induced neuronal apoptosis and to identify the optimal dose of its anti-apoptotic effect in rat retinas. **Methodology:** Seven groups of rats (n=9 per group, total=63), aged 6-8 weeks, were treated intravitreally. Group 1 received no treatment, while group 2 was administered DMSO 24 hours before NMDA (160 mM) exposure. Groups 3 to 7 received atorvastatin dissolved in DMSO at five doses (0.1, 0.5, 1.0, 20, 100 µM) 24 hours before NMDA exposure. Seven days post-injection, rats were sacrificed, and their retinas were isolated. Retinal cell apoptosis was assessed using Bax and Bcl-2 ELISA kits with Bcl-2/Bax ratio being analysed. **Results:** In NMDA-treated group, the Bax protein expression was higher by 2.00-fold compared to the untreated group ($P \leq 0.0001$). In ATV-treated groups 3-7, the same was lower by 1.73, 2.10, 1.80, 2.93, and 1.91-folds, respectively, compared to the NMDA-treated group ($P \leq 0.0001$). Conversely, in NMDA-treated rats, the mean Bcl-2 protein level remained comparable to untreated rats. However, in ATV-treated groups 3-7, the same was significantly higher by 2.35, 1.87, 2.01, 3.86, and 2.27-folds, respectively, compared to the NMDA-treated group. Notably, among the ATV-treated groups, the group receiving 20 µM showed a significantly higher Bcl-2/Bax ratio than other ATV-treated groups. **Conclusions:** ATV protects against NMDA-induced retinal cell apoptosis in rats with 20 µM emerging as the optimal dose. Dose optimisation can be useful for future studies to determine protective mechanisms involved in ATV on retinal cell apoptosis by using other markers.

Keywords: Atorvastatin; dose optimization; retina; excitotoxic retinal injury; neuroprotection.

Determination of Sedative and Anxiolytic Effect of *Clitoria ternatea* Flower Extract on Male Albino Mice

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Introduction: The *Clitoria ternatea* flower has gained a great deal of interest recently due to its medical benefits in treating issues like stress, anxiety, depression, and many more. **Objectives:** To look for potential sedative and anxiolytic effects of *C. ternatea* flower extract in different concentrations (20, 200, and 2000 mg/kg) in male albino mice and to compare the effects of *C. ternatea* to diazepam. **Methodology:** The flower of *C. ternatea* was macerated with distilled water, infused for 2 hours, lyophilized and reconstituted. Administered to the mice through oral gavage then mice initially underwent a right reflex test for 0, 15, 30, and 60 minutes after administration and then placed in a hole board test for 5 minutes. **Results:** The result showed anthocyanins and alkaloids in the *C. ternatea* flower. In the right reflex test, one-way ANOVA indicated statistically significant differences between groups at intervals of 0, 30, and 60 minutes (p 0.05) and no statistically significant differences in the 15-minute interval. In the hole board test, one-way ANOVA showed statistically significant differences among the tested groups, in which number of head dipping ($F = 3.193$, $p < 0.030$), time of dipping ($F = 4.392$, $p < 0.008$), and rearing ($F = 4.123$, $p < 0.011$) were significantly ($p < 0.05$) found in mice treated with 2000, 200, and 20 mg/kg, which is similar to the group treated with diazepam (1 mg/kg, p.o). **Conclusion:** This study has proven that the flower extract of *C. ternatea* has sedative properties at 2000 mg/kg from 0 to 60 minutes and at 200 mg/kg from a 30- to 60-minute observation time. Thus, the flower extracts of *C. ternatea* (2000 and 200 mg/kg) and diazepam (1 mg/kg) have the same action when taken orally, which has a similar effect to diazepam.

Keywords: *Clitoria ternatea*; sedative; anxiolytic.

Antibacterial Activity of Oral Spray containing *Graptophyllum pictum* (L.) Griff Leaf Extract against *Streptococcus mutans*

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Introduction: The need for more alternatives to current oral health care products arises as strains of *Streptococcus mutans* start to become resistant to fluoride-containing products. To combat these, the study aims to evaluate the antibacterial activity of an oral spray containing extracts from the leaves of *Graptophyllum pictum* (L.) Griff. **Objectives:** The study aims to evaluate the antibacterial activity of herbal oral spray formulation containing *Graptophyllum pictum* (L.) Griff (Purple Caricature Plant) leaf extract against *Streptococcus mutans*. **Methods:** A disk diffusion test was performed to determine the optimal concentration of *G. pictum* (L.) Griff leaf extract to be used in the formulation of the oral spray. Linear regression method was used to identify what concentration has the highest antibacterial property. A final disk diffusion test was performed to determine the significant difference between the oral spray containing *G. pictum* (L.) Griff leaf extract and the commercially available product (cetylpyridinium chloride + sodium fluoride) against *Streptococcus mutans*. **Results:** In determining the optimal concentration, only the 0.50% concentration among eight concentrations obtained a p-value of 0.033, showing its significant effect against the bacterial sample. In the antibacterial activity test using the oral spray solution, it obtained a t stat value of 5.291502 (>t-Crit two-tail value of 4.302653). This may suggest that the solution is as effective compared to the cetylpyridinium chloride + sodium fluoride oral spray. **Conclusion:** Based on the results, this study showed that the formulated oral spray from *G. pictum* (L.) Griff leaf extract has significant antibacterial activity against *S. mutans* and it may be a useful adjunct in the prevention of dental caries. This indicates the potential of *G. pictum* (L.) Griff leaf extract formulations to combat fluoride-resistant cariogens.

Keywords: *Graptophyllum pictum*, purple caricature plant, oral spray, Streptococcus mutans, antimicrobial susceptibility test

Synthesis and Evaluation of Anticancer Potential of Novel Imino Analogues

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Introduction: Breast cancer is the major of cause of deaths in female cancer patients. The safety of commercially available chemotherapeutic drugs is always major concern for the investigators. Benzopyrans and imines are known to offer high anticancer potential. **Objective**: Present study was intended to carry out the synthesis, characterization and anticancer activity of some new imino analogues (NIA). **Methodology:** Study involved synthesis of new imino analogues (NIAs), by hydrazination of benzotetronic acid ester (1), followed by Schiff reaction with different aldehydes to offer NIA (4a-d). Synthesized NIA were characterized based on the 1H-NMR, 13C-NMR, FTIR, and mass spectrometric data. Synthesized compounds were investigated for their cell viability against HEK-293 (normal cells) and anticancer potential against MCF-7 cancer cell lines using MTT assay and invitro scratch assay. **Results:** The study revealed that structures of NIA were in full agreement with their spectral data. Appearance of the new IR signal at 2926 and 1698 cm^{-1} indicated the C-H and C=O stretching confirmed the presence of ester group in the structure of NIA (2). Absence of IR signal at 2926 cm^{-1} related to C-H stretching and appearance of new IR doublet signal at 3267 cm^{-1} related N-H stretching, confirmed the presence of hydrazide group in NIA (3). Absence of IR doublet signal at 3267 and appearance of new IR signals between 1594-1582 confirmed the presence of C=N group in the NIA (4a-d). Appearance of new 1H-NMR signal between 9.33-9.35 confirmed the presence of N=CH protons in the NIA 4a-d. Appearance of new ^{13}C-NMR signal at 151.37-152.09 confirmed the presence of N=C group in the NIA (4a-d). The parent ion peaks of all NIAs were in full agreement with respective molecular ion peak in their respective mass spectra. The cell viability study, MTT and invitro scratch assay of NIAs, revealed compound 4d to possess highest activity and safety when compared with standard (irinotecan). **Conclusion:** Present study concludes that among all synthesized compounds, the compound 4d possess highest anticancer potential and more safety when compared with irinotecan. It was observed that incorporation of electron donating group (*p*-methoxy) in the NIA offered maximum safety and anticancer activity. However, further clinical studies are required to further establish its clinical significance.

Keywords: Benzopyran; Imino analogues; Anticancer; Cytotoxicity; Synthesis.

Discovery of New Quinoline Analogues for Oral Squamous Cell Carcinoma Treatment

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Introduction: Among oral cancer, the oral squamous cell carcinoma (OSCC) is considered as the 6th most common cancer worldwide. Although there are several chemotherapeutics available, but the associated side effects with the current anticancer drugs offers a major challenge. **Objective:** Hence based on the severity of OSCC and side-effects of existing chemotherapeutic, an effort was made to develop new anticancer for OSCC treatment. In this study, new quinoline analogues (NQA) were synthesized, characterized, and evaluated for the anticancer properties in OSCC. **Methodology:** The synthesis experiment involved treatment of substituted quinoline (1) with ethyl chloroacetate to offer ester derivative (2), that on reaction with hydrazine hydrate yielded hydrazide analogue (3), which was finally cyclized into oxadiazole analogues (4) using aromatic acid. The chemical structures of synthesized NQA were characterized based on the FTIR, NMR and mass spectral data. The synthesized NQA were further evaluated for their antiproliferative potential (IC50) using CAL27, OSCC cell line followed by cell cycle analysis. **Result:** The antiproliferative study of NQA revealed NQA3 to exhibit the lowest IC50 value (3.26µg/mL). Whereas cell cycle analysis revealed that all NQA1-4 causes cell arrest in cell synthesis 'S-phase'. **Discussion:** A lower IC50 value gives the confidence of less toxicity in the OSCC cell line. The active metabolite in NQA gives the ability to arrest the cells in the S-phase, preventing the cells from going through the mitotic phase and halting the progression of cancer. **Conclusion:** The ability of NQA to arrest the cells in the S-phase, sheds light on hope for the application of NQA in OSCC treatment, however further investigation to study the molecular activity of NQAs is currently under active study.

Keywords: Quinoline analogues; Irinotecan; Synthesis; Oxadiazole; Hydrazide; Ester; Anticancer activity.

In vitro Antiviral Activity of *Coriander sativum L.* Crude Extract against Respiratory Syncytial Virus

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Introduction: Human respiratory syncytial virus (RSV) is a leading cause of childhood acute lower respiratory infection worldwide. Recently, vaccines for RSV have been approved, however their usage is restricted to elderly individuals. To date, only one antiviral drug is used to treat RSV, namely ribavirin. Ribavirin is a broad spectrum nucleoside analogue which has been shown to cause side effects and is costly. Hence, there is a need to develop a safe yet cheap antivirals against RSV. *Coriander sativum L.* is a culinary and medicinal herb that has been shown to exert antiviral activities against dengue, hepatitis A, Newcastle disease and Human immunodeficiency virus infections. **Objectives:** This study aims to determine whether seed extract from *Coriander sativum L.* have antiviral properties against RSV in vitro. **Methodology:** Methanolic crude extract from dried coriander seeds was prepared using maceration method. Maximum non-toxic concentration (MNTC) of seed extract was determined using MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) tetrazolium reduction assay, which was 125 µg/mL. The antiviral activity of the methanolic seed extract was examined using normal human bronchial epithelial cell line BEAS-2B cells as RSV-infection model. Ribavirin was used as a positive control. Viral load post treatment was quantified using Median Tissue Culture Infectious Dose (TCID-50)-MTT assay and end point PCR analysis. Finally, a gas chromatography-mass spectrometry (GC-MS) analysis was performed to identify the bioactive compounds present in the extract. **Results:** Treatment of RSV-infected BEAS2B cells with *Coriander sativum L.* seed crude extract at 125 µg/mL significantly reduced RSV-induced cell death or cytopathic effect and viral replication. The GC-MS analysis revealed that methanolic seed extract contains high amounts of bioactive compounds including n-Hexadecanoic acid, 5-Hydroxymethylfurfural, and linalool. **Conclusion:** Collectively, the results suggest that methanolic extract of *Coriander sativum L.* seed could be a natural source of an antiviral drug candidate against RSV infection.

Keywords: Respiratory syncytial virus; *Coriander sativum* L.; antiviral; plant extracts; active compounds.

Tripeptide GVR Blocked Catalytic Site of C-domain of Somatic ACE and Chymase Enzymes Simultaneously Then Reduced High Blood Pressure in Strictly Fasted Spontaneously Hypertensive Rats

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Introduction: Hypertension is one of the most common chronic diseases affecting millions of people worldwide. Angiotensin-I-converting enzyme (ACE) is one of the enzymes responsible for causing high blood pressure. When ACE is inhibited (e.g. by ACE inhibitors), chymase enzymes will be activated to carry out ACE's task which is to convert angiotensin-I to angiotensin-II and cause an increase in blood pressure. ACE is composed of 2 domains i.e. the C-domain and N-domain. Selective inhibition of the C-domain of ACE and chymase enzyme simultaneously is an important therapeutic goal to reduce systolic blood pressure in hypertensive patients and reduce chronic dry cough, which is the main side effect of ACE inhibitors. The dry cough is due to accumulation of bradykinins (another substrate of ACE) which forces doctors to change ACE inhibitors to other antihypertensive medications. **Methods:** We first carried out *in silico* studies, followed by *in vitro* and *in vivo* experiments. For the *in silico* methodology, the crystal structure of the enzymes were downloaded from the protein data bank and then docked with ligand; tripeptide glycine-valine-arginine (GVR) through molecular docking analysis. Later, the peptide was synthesised and tested *in vitro* through enzyme kinetic studies. Subsequently, *in vivo* toxicity and efficacy of the peptide was tested in spontaneously hypertensive rats (SHRs). **Results:** Based on the molecular docking studies, GVR competitively inhibited C-domain but not N-domain of somatic ACE and chymase. The molecular docking studies were validated using enzyme-kinetic analysis where tripeptide GVR was found to be a competitive inhibitor and was able to bound at the catalytic and active sites of both enzymes. In long-term toxicity studies, the lethal dose (LD_{50}) of GVR was >2000 mg/kg b.w. Based on *in vivo* experiments which lasted for 3 weeks, at the dosage of 100 mg/kg b.w, tripeptide GVR significantly reduced the systolic blood pressure in strictly fasted spontaneously hypertensive rats (SHRs). Interestingly, based on lipid profile studies, triglyceride was significantly reduced ($p<0.05$) in tripeptide GVR treated SHRs when compared to negative and positive control (captopril), respectively. Based on the histopathologist's review, tripeptide GVR did not produce any toxic effect in the liver and kidney tissues and these findings are in line with the *in vivo* toxicity study. Through metabolomic studies, GVR affected ACE pathways. **Conclusion:** Based on our results, the tripeptide GVR could be developed as an antihypertensive agent which could target both ACE and chymase enzymes with reduced side effects. GVR may reduce coughing frequency in patients and improve patients' quality of life.

Keywords: *In silico*; *In vitro*; *In vivo*; Peptide; Renin angiotensin system.

Poster Presenters	
ID	**Presenters**
PP-DS-01	**Mr Arunkumar Subramanian**
	Computational Investigation and Neuroprotective Potential of Pterostilbene against Sleep Deprivation Induced Alzheimer's Disease Using Zebrafish Model
PP-DS-04	**Ms Aathira Sujathan Nair**
	Unraveling Nature's Secrets: Virtual Screening and Molecular Docking of Coumarin Derivatives to Unlock ER-alpha Receptor Potential
PP-DS-05	**Mr Shadisvaaran Saminathan**
	The Protective Effect of Annatto Tocotrienol on Hypertension and Periodontitis in Animal Model
PP-DS-06	**Ms Kavesha Parameswaran**
	In-vitro Antiviral Activity of Linalool against Respiratory Syncytial Virus

Poster Presenters	
ID	**Presenters**
PP-DS-07	**Dr Sri Devi Sukumaran** 2′-Hydroxychalcone Analogues With Modified C4-Substituents for the Treatment of Alzheimer's Disease: Biological Evaluation and Molecular Modelling Studies
PP-DS-08	**Dr. apt. Hariyanti** Characterization and Antioxidant Activity of Gelatin, and the Derived Peptides from Barramundi (*Lates calcarifer*) Scales
PP-DS-09	**How Wan Leong** *In silico* Pharmacokinetic and Molecular Docking Studies of Labdane Diterpenes of *Alpinia* Genus against Butyrylcholinesterase, A Therapeutic Target for Alzheimer's Disease

Computational Investigation and Neuroprotective Potential of Pterostilbene against Sleep Deprivation Induced Alzheimer's Disease Using Zebrafish Model

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Introduction: The depletion of oxidizing enzymes and the formation of β-amyloid plaques that cause neurodegeneration in Alzheimer's disease have frequently been linked to sleep cycle disruptions. A growing body of scientific evidence suggests that healthy sleep patterns can facilitate the synthesis and activity of anti-oxidant enzymes and can promote the clearance of β-amyloid plaques out of the brain. **Methods:** Using *in-silico* tools like Molinspiration, SwissADME, and PreADMET, the bioactivity score, molecular properties, and pharmacokinetic parameters of pterostilbene were assessed. The binding affinity and interactions of pterostilbene with the selected six receptors were predicted using Autodock 4.2 software. To further confirm its neuroprotective potential, *in vitro* assays on acetylcholinesterase enzyme level, lipid peroxidation activity, and catalase activity were performed. *In vivo* neurobehavioral analysis of zebrafish treated with pterostilbene was carried out using T-maze, Y-maze, and inhibitory avoidance apparatus. **Results:** Pterostilbene complies with Lipinski's rule and has significant blood-brain barrier penetration and bioavailability. *In silico* studies reveal that pterostilbene has good binding affinity and interactions with different receptors which supports pterostilbene's multi-target potential. *In vitro* assays show that pterostilbene exhibits cholinesterase inhibition and potent antioxidant properties. *In vivo* neurobehavioral analysis reveals that pterostilbene supports greater memory retention in zebrafish, and histopathological studies reveal significant amelioration and reduction of amyloid deposits on zebrafish brains against sleep deprivation-induced AD. **Conclusion:** Further exploration with respect to preclinical and clinical aspects of pterostilbene is required to confirm the therapeutic potential of pterostilbene for the treatment of Alzheimer's disease.

Keywords: Pterostilbene; Alzheimer's Disease; Anti-oxidant; Sleep deprivation.

Unraveling Nature's Secrets: Virtual Screening and Molecular Docking of Coumarin Derivatives to Unlock Estrogen Receptor Alpha Potential

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Introduction: Breast cancer is the second leading cause of cancer mortality worldwide. In Malaysia, the prevalence of developing breast cancer is 1 in 20. It is the most prevalent cancer seen in women. The estrogen receptor alpha (ER-alpha) is the focus of our work to battle breast cancer. A ligand with high ER-alpha affinity is still sought after despite extensive studies. The pharmacological effects of coumarins have been the subject of substantial research. The pharmacological value of coumarins in treating different cancers has received a lot of attention and thus, we focus on coumarins as a potential target against ER-alpha. **Objectives:** To virtually screen libraries of coumarin compounds based on their physicochemical properties; evaluate their binding affinity towards the ER-alpha using different softwares; and evaluate the molecular dynamics of the top 10 best compounds. **Methodology:** Virtual screening of coumarin compounds obtained from databases like ChemBL, BindingDB based on physicochemical properties of compounds using Datawarrior; evaluation of binding affinity of the virtually screened compounds and filtering out the top ten against ER-alpha (PDB ID: 1R5K) using AutoDock, YASARA, and Discovery Studio; and evaluation of the best hit compound using Molecular Dynamics. **Results:** The top 10 hits were chosen using the Autodock Vina and YASARA tools from 509 compounds. These hits were chosen for Molecular Dynamics modelling after being further examined and shown to have the highest binding affinity. Compound **3** has the greatest binding affinity of -11.47 kcal/mol. Compound **3** attained equilibrium during molecular dynamics simulations at 55 ns and remained stable, demonstrating RMSD variations between 4.0 and 5.5 from 55 to 100 ns. **Conclusion:** Notably, compounds **1, 2,** and **3** stood out due to their strong binding affinities. MD simulations of the **1R5K-compound 3 complex** revealed equilibrium at 55 ns, with stability maintained up to 100 ns. RMSD variations between 4.0 and 5.5 from 55 to 100 ns were observed. These findings enhance our grasp of drug-receptor interactions, suggesting potential advancements in ER-alpha-targeted breast cancer therapies.

Keywords: Virtual screening; molecular dynamics; binding affinity; estrogen receptor-alpha; coumarins.

The Protective Effect of Annatto Tocotrienol on Hypertension and Periodontitis in Animal Model

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Introduction: Periodontitis is a common chronic inflammatory disease which damages the tooth supporting structure in the oral cavity. Recent findings show periodontitis is linked to blood pressure elevation. Adults in Malaysia are greatly affected by hypertension (HT) and periodontitis (PD), but combating these conditions is cost prohibitive. Annatto tocotrienol (AT) from *Bixa orellana* was shown to have protective effects on diseases mediated by inflammation based on recent studies. **Objectives**: To explore the protective effects of annatto tocotrienol on periodontitis and hypertension in rats. **Methodology**: 12-week-old male Wistar rats were divided into 7 groups. Hypertension was induced in the rats using NG-nitro-l-arginine methyl ester (L-NAME) (40 mg/kg) intraperitoneally for 2 weeks. After 14 days, on the rats' left maxillary second molar, an orthodontic wire was ligated for 4 weeks to induce periodontitis. The rats were then treated with AT (60 mg/kg/day, oral) for 4 weeks. After 4 weeks the plasma and the maxilla were collected for further analysis. Plasma pro-inflammatory cytokines were analyzed using ELISA whereas micro-computed tomography was used to determine alveolar bone loss and percentage of bone remaining. **Results**: Bone loss was established in the rats with ligation as significant difference was observed comparing sham group to PD group ($p<0.05$). Alveolar bone loss was severe in rats with both PD + HT group compared to PD group ($p<0.001$). Percentage of bone remaining was significantly higher in the PD group compared to PD + HT ($p<0.001$). AT treatment significantly reduced periodontitis-induced alveolar bone loss and improved percentage of bone remaining in rats with hypertension ($p<0.05$). However, circulating IL-6, IL-1β and TNF-α showed no significant difference among groups. **Conclusion**: This study shows the association of hypertension in exacerbating periodontitis in rats. Furthermore, treatment of AT showed protective effects against periodontitis and hypertension concurrently.

Keywords: Annatto tocotrienol; hypertension; periodontitis; computed tomography.

In-vitro Antiviral Activity of Linalool against Respiratory Syncytial Virus

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Introduction: Human respiratory syncytial virus (RSV) was found to be one of the most prevalent respiratory pathogen which caused acute respiratory tract illnesses among children between the years 2015 to 2019 in Malaysia. The absence of RSV-specific antiviral drug and vaccine, especially for children, coupled with the risk of re-infections has raised the need for the development of antiviral targeting RSV. Essential oils are secondary metabolites of aromatic plants and are composed of various compounds. They are being used extensively in numerous industries for their biological properties. Linalool; one of the compounds found in essential oils, has been shown to exert antiviral activity against influenza virus, adenovirus and herpes simplex virus. **Objectives:** In this study, we sought to explore the potential inhibitory effects of linalool against RSV infection in human lung epithelial cells. **Methodology:** The antiviral property of linalool was assessed in vitro using normal human bronchial epithelial cell line BEAS-2B cells as RSV-infection model. BEAS-2B cells were infected with RSV at multiplicity of infection (MOI) 0.1 for 2 hours before being treated with linalool at various non-toxic concentrations which was determined prior to the antiviral assay. Ribavirin; non-RSV specific antiviral drug, was used as positive control. The inhibitory effect of linalool was assessed by end-point PCR. **Results:** The maximum non-toxic concentration of linalool on BEAS-2B cells was determined to be 100 µg/mL. Linalool at 20 µg/mL showed slight antiviral activity against RSV compared to treatment at 40 µg/mL and 100 µg/mL. The control drug ribavirin showed the most significant antiviral activity against RSV. **Conclusion:** To conclude, linalool exhibited mild antiviral activity against RSV. Despite the differences between in antiviral potency between linalool and ribavirin, linalool remains to be a viable candidate for potential therapeutic application against RSV infection considering the high costs, side effects and challenging administration method associated with ribavirin.

Keywords: Antiviral effect; respiratory syncytial virus; natural compound; linalool.

2′-Hydroxychalcone Analogues With Modified C4-Substituents for the Treatment of Alzheimer's Disease: Biological Evaluation and Molecular Modelling Studies

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Introduction: Alzheimer's disease (AD) is characterised as a progressive neurodegenerative disorder and is typically managed with cholinesterase inhibitors as the first line of treatment. **Objectives:** This study aims to determine the efficacy of C4-substituted tertiary nitrogen-bearing 2′-hydroxychalcones as a therapeutic candidate for the treatment of AD. **Methodology:** The target compounds were designed and synthesised on the basis of a previously developed mixed type acetylcholinesterase (AChE) inhibitor. Subsequently, the anticholinesterase activity of these compounds was examined and molecular docking experiments were carried out. **Results:** The study found that the majority of the 2′-hydroxychalcone analogues inhibited AChE more effectively than butyrylcholinesterase (BuChE). Among them, compound 4c was identified to be the one with the highest AChE inhibitor potency (IC_{50}: 3.3 μM) and best AChE selectivity over BuChE (ratio >30:1). According to molecular docking analyses, compound 4c interacts with both the peripheral anionic site (PAS) and catalytic anionic site (CAS) regions of AChE. Additionally, ADMET analysis supported the therapeutic value of compound 4c based on its blood–brain barrier penetration properties. **Conclusion:** Overall, the findings reveal that this 2′-hydroxychalcone merits further investigation as a potential AD treatment approach.

Keywords: Alzheimer's disease; acetylcholinesterase; butyrylcholinesterase; chalcones; molecular modelling.

Characterization and Antioxidant Activity of Gelatin, and the Derived Peptides from Barramundi (*Lates calcarifer*) Scales

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Introduction: Fish gelatin hydrolysate includes a wide extent of benefits in pharmaceutical and food applications include Barramundi scales. The gelatin extraction method using autoclave was selected with the best product yield. **Objectives:** The purpose of this study to determine the antioxidant activity of gelatin hydrolysate of Barramundi scales and its characteristics. **Methodology:** Gelatin was extracted using acetic acid 5% with autoclave method. Hydrolysis was carried out with 1% Protease, followed by fractionation with a molecular weight cut off sieve. The antioxidant activity of Barramundi scale gelatin hydrolysate was determined using the 2,2-diphenyl-1-picrylhydrazil (DPPH) and Ferric Reducing Antioxidant Power (FRAP) methods. **Results:** Gelatin hydrolysis results obtained a yield of 94.4% with pH value 5,21. The obtained gelatin hydrolysate was then fractionated using the Molecular Weight Cut-Off ultrafiltration technique of 50 KDa, producing the highest yield of 60.04% of <50 KDa fraction. The highest protein content was found in the gelatin sample, namely 40.59 %. The best antioxidant activity from the DPPH method was found in gelatin hydrolysate. Meanwhile, the best antioxidant activity from the DPPH method was found in fraction < 50 KDa of gelatin hydrolysate. **Conclusion:** Antioxidant activities of these peptide were higher than those before hydrolysis.

Keywords: *Lates calcarifer*; Barramundi scales; autoclave; gelatine hydrolysate; Antioxidant activity.

In silico Pharmacokinetic and Molecular Docking Studies of Labdane Diterpenes of *Alpinia* Genus against Butyrylcholinesterase, A Therapeutic Target for Alzheimer's Disease

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Introduction: Labdane diterpenes are phytochemicals which have been reported effective against acetylcholinesterase inhibition. Butyrylcholinesterase (BChE) is another enzyme involved in hydrolysis of acetylcholine in the brain. Both enzymes are regarded as important therapeutic targets for Alzheimer's disease. Nonetheless, study on the effect of labdane diterpenes towards BChE inhibition is scarce. In view of their versatility in displaying various biological activities found in previous studies, the present project has been designed to explore the potential of such scaffold against the BChE through computational methods. **Objectives**: This project aimed to study the pharmacokinetic profiles of labdane diterpenes of *Alpinia* genus via *in silico* methods and to evaluate their binding interactions in the active site of butyrylcholinesterase through molecular docking. **Methodology**: A series of 30 labdane diterpenes (Refer to Appendix 1) from *Alpinia* genus were investigated for physicochemical properties using Molinspiration server and pharmacokinetic profiles using pkCSM. Docking systems consisting of butyrylcholinesterase protein (PDB ID: 4DBS) and labdane diterpenes were subjected to docking studies using AutoDockTools (ADT4.2). Protein-Ligand Interaction Profiler (PLIP) was used to analyze the docking outputs; LigPlot+ program was used to illustrate the binding interaction between butyrylcholinesterase protein and labdane diterpenes. **Results**: A total of 20 labdane diterpenes met the requirement of Lipinski's rule and complied to Veber rule. Some of these compounds have shown high volume of distribution (steady state) and can readily cross the blood-brain barrier. Most compounds were predicted to be metabolized directly in the liver. Molecular docking studies have identified ten compounds with comparatively good binding energy ranging from -10.48 kcal/mol to -17.70 kcal/mol. Hydrogen bonding was found as the main binding interaction between the binding site residues and labdane diterpenes. **Conclusion**: Several labdane diterpenes in the present study have exhibited drug likeness, good oral bioavailability as well as considerable drug distribution and blood-brain-barrier penetration based on *in silico* prediction. Ten compounds were shown to have relatively good binding within the binding site of BChE from the docking studies.

Keywords: Labdane diterpenes; butyrylcholinesterase; Alzheimer's disease; molecular docking; *in silico* pharmacokinetics.

MONASH INITIATE 2023

25 - 26 October 2023

Translating Research into Practice: Revolutionizing healthcare delivery and outcomes

PRESENTERS DRUG DELIVERY

Oral Presenters		
Date: 25 October 2023 (Wednesday)		
ID	**Presenters**	**Time**
OP-DD-05	**Mr Mohammed Semol Ahmed** Evaluation of Protective Effect of Drugs in Diabetes-Induced Cognitive Impairment in Rats	2:00 PM
OP-DD-06	**Mr Gabriele De Rubis** Berberine-Loaded Nanoparticles Attenuate TGF-β-Induced Remodelling Features in Human Bronchial Epithelial Cells	2:15 PM
OP-DD-08	**Ms Deni Anggraini** Preparation and Hair Growth Activity Test of Microemulsion Ethanol Extract of Cayenne Pepper (Capsicum Frutenscens L)	2:30 PM
OP-DD-09	**Mr Hazem Choukaife** Preparation and Characterization of Alginate Beads and Microbeads Using Dripping and Electrospray Method	2:45 PM
OP-DD-10	**Ms Gressy Novita** Improving Mechanical Properties of Ibuprofen via Multicomponent Crystal	3:00 PM
OP-DD-12	**Ms Nur Zahirah Binti Mohamad Zin** Optimizing Doxorubicin-Loaded Solid Lipid Nanoparticles via Solvent-Diffusion Method	3:15 PM

Oral Presenters		
Date: 25 October 2023 (Wednesday)		
ID	**Presenters**	**Time**
OP-DD-13	**Dr Keshav Raj Paudel** Zerumbone Liquid Crystalline Nanoparticles Protect Against Oxidative Stress, Inflammation and Senescence Induced by Cigarette Smoke Extract In Vitro	3:30 PM
OP-DD-11	**Ms Wira Noviana Suhery** Utilization of Pregelatinized Sweet Potato Starch of White, Yellow, and Purple Varieties as Suspending Agent in The Formulation of Ibuprofen Suspension	4:00 PM

Oral Presenters		
Date: 26 October 2023 (Thursday)		
ID	**Presenters**	**Time**
OP-DD-15	**Dr Rajesh Dodiya** Porous Swellable Hypromellose Composite Fortified with Bioactive Extracted from Eucalyptus camaldulensis Leaf to Mitigate Dermal Wound Infections	2:00 PM
OP-DD-19	**Dr. D. Senthil Rajan** Pharmaceutical Optimization of Polyelectrolyte Complexing Topical Formulation of Loratadine With Vitamin-C for Rheumatoid Arthritis	2:15 PM
OP-DD-16	**Associate Professor Dr. Rohan Krishna Barse** Formulation Development, Optimization and Evaluation of a Novel *In Situ* Gel for the Treatment of Glaucoma	2:30 PM

Evaluation of Protective Effect of Drugs in Diabetes-Induced Cognitive Impairment in Rats

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Introduction: Diabetes mellitus causes deficits in remembering, learning new things, concentration or decision making and poor glycemic control has been associated with progression of cognitive dysfunction. Cognitive dysfunction with its wide range from mild cognitive impairment to dementia is one of the chronic complications of diabetes mellitus. **Objectives:** The study was designed to evaluate the protective effect of allantoin, β-cyclodextrin and gelucire 44/14 and the combinations of allantoin + β-cyclodextrin and allantoin + gelucire 44/14 in diabetes induced cognitive impairment in rats. **Methodology:** Diabetes was induced in male rats by administrating streptozotocin (53mg/kg,i.p). A total number of 54 male wistar rats were divided into 7 different groups. 5 groups of diabetic rats were treated with allantoin (200mg/kg,p.o), β-cyclodextrin (31.5mg/kg,p.o) and gelucire 44/14 (200mg/kg,p.o) and treatment with the combination drugs of allantoin (200mg/kg,p.o) + β-cyclodextrin (31.5mg/kg,p.o) and allantoin (200mg/kg,p.o) + gelucire 44/14 (200mg/kg,p.o) for eight weeks. After eight weeks, degree of cognitive impairment was determined using Barnes maze, T-maze, Elevated plus maze, and Passive avoidance test. Glycosylated haemoglobin, brain levels of dopamine, serotonin, GABA, nor-adrenaline was measured by spectrofluorimeter whereas anti-cholinesterase by spectrophotometer and antioxidants by UV-Visible spectrophotometer. And calculated using One Way Analysis of Variance (ANOVA) followed by Dunnet multiple comparison test. **Results:** Treatment with allantoin, β-cyclodextrin and gelucire 44/14 and combinations of allantoin + β-cyclodextrin and allantoin + gelucire 44/14 significantly improved memory and learning performances when compared with diabetic and control rats. The treated rats also showed a significant decrease in glycosylated haemoglobin and significantly elevated body weight, anti-oxidant status compared to diabetic and control rats. Also significantly corrected the altered neurotransmitters levels in the brain when compared to diabetic & control rats. **Conclusion:** Allantoin, β-cyclodextrin and gelucire 44/14 provides beneficial effects on cognitive deficits seen in diabetic rats and can be used to delay onset / prevent progression of the diabetes induced cognitive impairment.

Keywords: Diabetes, cognitive impairment, allantoin, β-cyclodextrin and gelucire 44/14, behavioural studies, neurotransmitters.

Berberine-Loaded Nanoparticles Attenuate TGF-β-Induced Remodelling Features in Human Bronchial Epithelial Cells

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Introduction: Pathologic airway remodelling, characterized by aberrant activation of epithelial reparation and migration, extracellular matrix (ECM) deposition, and epithelial-to-mesenchymal transition (EMT), is a common pathophysiological feature of respiratory diseases such as chronic obstructive pulmonary disease (COPD) and asthma. The main activator of remodelling is Transforming Growth Factor-β (TGF-β). Current treatments available for asthma and COPD have limited efficacy and do not target airway remodelling. Berberine is a phytochemical with multifaceted therapeutic activity, whose clinical application is hampered by poor solubility and unfavourable pharmacokinetics. **Objectives:** To encapsulate berberine in monoolein-based liquid crystalline nanoparticles (BM-LCNs) and to test its potential in inhibiting *in vitro* remodelling features exerted by stimulating human BEAS-2B bronchial epithelial cells with TGF-β. **Methodology:** BEAS-2B cells were stimulated with 5 ng/mL recombinant human TGF-β for 48 h and co-incubated with 0.5 µM BM-LCNs for 24 or 48 h. The *in vitro* activity of BM-LCNs was assessed by measuring: inhibition of TGF-β-induced cell migration (wound healing migration assay); changes in the levels of remodelling-related proteins (Human XL Cytokine Array); measurement of nitric oxide (NO) levels (Griess reagent). **Results:** Stimulation of BEAS-2B cells with TGF-β significantly increased their migration by 25% (24 h) and 40% (48 h). Treatment with BM-LCNs reduced the migration to levels comparable to the untreated group at both time points. Furthermore, BM-LCNs significantly reduced the expression of TGF-β-induced effector proteins (endoglin, basic FGF, myeloperoxidase, thrombospondin, VEGF), and restored the production of Cystatin C and NO, two negative regulators of remodelling downregulated by TGF-β, to levels comparable to the untreated group. **Conclusion:** We demonstrate potent *in vitro* therapeutic efficacy of BM-LCNs in counteracting TGF-β-induced epithelial remodelling. This study supports the suitability of berberine-loaded drug delivery systems to target airway remodelling, with potential application as treatment strategy against pathologies characterized by aberrant tissue remodelling such as COPD and asthma.

Keywords: Airway remodelling; COPD; asthma; berberine; nanoparticles

Preparation and Hair Growth Activity Test of Microemulsion Ethanol Extract of Cayenne Pepper (*Capsicum Frutenscens L*)

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Introduction: Cayenne pepper contains capsaicin which has activity as a hair growth agent. Microemulsion is an oil and water dispersion system with a particle size of 10-200 nm which can be used topically as a drug delivery system through the scalp. **Objectives**: The aim of this study was to prepare a microemulsion formulation as a topical preparation that is physically and chemically stable and has good hair growth activity. **Methodology**: Microemulsion was made with olive oil and tween 80 as surfactants and using a magnetic stirrer at 1000 rpm for 3 minutes. Three variations of the concentration of ethanol extract of cayenne pepper made in microemulsions were 0.1%, 0.2% and 0.3%. Microemulsion tests included organoleptic tests, specific gravity, pH, viscosity, freezing and thawing stability tests and hair growth activity tests on rabbits. **Results**: The results showed that microemulsion ethanol extract of cayenne pepper 0.1%, 0.2% and 0.3% was quite stable with a clear appearance and a particle size range of 27,7 nm – 167,8 nm. Hair growth length of 1.27 cm for 30 days. A two-way ANOVA statistical test showed that the hair length of rabbits using microemulsion was significantly different from the hair length of negative control animals at $p<0.05$. **Conclusion**: The ethanol extract of cayenne pepper can be formulated into a microemulsion to form a stable microemulsion during storage. Cayenne pepper ethanol extract microemulsion 0.2% can help hair growth with hair growth length of 1.27 cm after 30 days.

Keywords: Capsicum; hair growth; microemulsion

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Preparation and Characterization of Alginate Beads and Microbeads Using Dripping and Electrospray Method

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Introduction: The hydrogelling ability of alginate has garnered significant attention from pharmaceutical scientists due to its useful applications as hydrogel carriers for targeted drug delivery systems. Understanding the physical properties of alginate hydrogel particles is critical to facilitate the manufacturing process and overcome limitations associated with the final product. The electrospray technique is a novel method capable of producing particles within a controlled size range. In comparison with the dripping method, electrospray formulates monodisperse droplets in the range of nano- to millimeter range by applying electric field. **Objectives:** This study aims to investigate the effects of applying high voltage on the characteristics of alginate beads fabricated using the dripping method. Additionally, it examines how voltage affects other process parameters, such as alginate concentration, $CaCl_2$ concentration, and needle gauge, in relation to various particle characteristics. **Methodology:** Alginate beads and microbeads were prepared using the dripping and electrospray methods, respectively. The alginate solution was pumped through a dispensing needle at a constant flow rate with and without applying voltage on the tip of the stainless-steel needle. The extruded drops were received in $CaCl_2$ solution as a curing bath. Afterward, the formed beads/microbeads underwent two rounds of washing with distilled water, followed by drying at 40°C for 14 hours in a laboratory oven. **Results:** The outcomes of the central composite design demonstrated the factors that have a significant effect on alginate beads/microbeads characteristics. Applying voltage from 12 Kv reduced the size from 1.1 mm to 0.5 mm using the same parameter levels. The application of a high-power voltage significantly influenced water uptake, swelling, and erosion behaviors. Specifically, the results revealed a favorable impact on both swelling and water uptake, while concurrently inducing an adverse effect on the erosion of the microbeads. **Conclusion:** The electrospray technique is a valuable preparation method that provides greater control over the characteristics of resulting particles compared to the conventional dripping method. The application of voltage enables the production of controlled particles with a wide size range, thereby enhancing the versatility of this technique in various manufacturing processes.

Keywords: Alginate, Electrospray, ionic gelation, Beads, Microbeads

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Improving Mechanical Properties of Ibuprofen via Multicomponent Crystal

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Introduction: Ibuprofen is a non-steroidal anti-inflammatory analgesic (NSAID) that belongs to BCS class II. Generally, ibuprofen has a bad flowability because of a high cohesiveness. Another problem in manufacturing is the high tendency for sticking to the punches. Besides these detrimental properties, ibuprofen indicates bad dissolution behavior because of its hydrophobic structure. **Objectives**: To improve the properties of ibuprofen can be used co-crystallization method for multicomponent crystal with nicotinamide as co-former. **Methodology**: Ibuprofen-nicotinamide cocrystal formation by Solvent Drop Grinding (SDG) and Solvent Evaporation (SE). The characterization of the co-crystal formation included crystal morphology, powder X-ray diffractogram, and thermal behavior. The mechanical properties testing including flowability (angles of repose and compressibility index), solubility and dissolution rate were conducted on ibuprofen-nicotinamide multicomponent crystal and pure ibuprofen. **Results**: By forming the cocrystal, we demonstrated that the flow ability, compressibility index of the multicomponent crystal was improved from the parent drug. The multicomponent crystal of ibuprofen-nicotinamide in this case shows an improved solubility in water and buffer phosphate pH 7.2 media and a better dissolution profile in buffer phosphate pH 7.2. However, the dissolution rate in buffer phosphate pH 7.2 media was found to be essentially indifference. **Conclusion**: It can be concluded that the multicomponent crystal of ibuprofen-nicotinamide by the SDG and SE method can improve the mechanical properties of ibuprofen.

Keywords: Ibuprofen, Nicotinamide, Cocrystal, Mechanical Properties

Utilization of Pregelatinized Sweet Potato Starch of White, Yellow, and Purple Varieties as Suspending Agent in The Formulation of Ibuprofen Suspension

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Introduction: Research on the utilization of white, yellow, and purple sweet potato pregelatinized starch as a suspending agent has been carried out. Sweet potato starch contains amylose and amylopectin which can function as suspending agents. **Objectives**: The study aimed to determine the potential of sweet potato pregelatinized starch from white, yellow, and purple varieties as a suspending agent for better drug delivery in an ibuprofen suspension formula. **Methodology**: The stages of the research consisted of preparing pregelatinized starch, examining the physical and microscopic properties of pregelatinized starch (determination of starch moisture content, measurement of gelatination temperature, microscopic examination using SEM, and examination of the polarization properties of starch using a polarizing microscope), formulation and evaluation of ibuprofen suspension. The use of sweet potato pregelatinized starch as a suspending agent was 5% w/v, 10% w/v, and 15% w/v for each variety (F1-F9). **Results**: The results showed that on examination of the physical properties of sweet potato starch, the highest starch yields were respectively produced by white sweet potato starch, yellow sweet potato starch, and purple sweet potato. The microscopic form of white, yellow, or purple sweet potato starch using a polarizing microscope and SEM shows almost the same shape, namely the presence of several starch granules that have an irregular surface with a larger particle size compared to native starch which is spherical, oval and polygonal in shape. The resulting suspensions were evaluated for their sedimentation volume, viscosity and rheology, re-dispersibility, and stability studies were performed for 2 months. The results of the suspension preparation evaluation showed that there were no significant differences in the suspension evaluation results using variations of pregelatinized sweet potato starch such as sedimentation volume, redispersion time, and suspension viscosity. **Conclusion**: The use of sweet potato pregelatinized starch as a suspending agent at a concentration of 15% w/v has produced an ibuprofen suspension that meets the requirements and is stable during storage.

Keywords: Ibuprofen; *Ipomoea batatas*; Pregelatinized starch; Suspending agent.

Optimizing Doxorubicin-Loaded Solid Lipid Nanoparticles via Solvent-Diffusion Method

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Introduction: Breast cancer treatment remains an active focus of research, aiming to enhance outcomes through innovative approaches. This study explores solid lipid nanoparticles (SLNs) as carriers for the potent anticancer drug doxorubicin. SLNs show great promise as drug delivery systems, offering improved drug encapsulation and controlled release, potentially enhancing cancer therapy effectiveness. **Objectives:** The primary goal of this study is to investigate the formulation and preparation of SLNs containing doxorubicin, using the nanoprecipitation method through two mixing techniques: conventional mixing and static mixing. Additionally, we aim to assess the impact of different surfactants and lipid compositions on the size and uniformity of SLNs. Furthermore, we seek to evaluate the feasibility of using SLNs as drug carriers for targeted breast cancer therapy using the solvent-diffusion technique. **Methodology:** The study utilized the nanoprecipitation method via two mixing processes to prepare SLNs. Glycerol Monostearate (F23) was the focus due to its favorable characteristics. A static mixer and two syringe pumps facilitated the continuous mixing of lipids in an organic phase solution, followed by rapid mixing with a surfactant in a non-solvent solution to fabricate nanoparticles. **Results:** Among the formulations tested, Glycerol Monostearate (F23) exhibited the most promising results with a particle size of 302.6 nm, zeta potential of -17 mV, encapsulation efficiency of 90.67%, and drug loading of 22.35%. The research emphasized the significant influence of the mixing method, surfactant choice, and lipid composition on the size and uniformity of SLNs. **Conclusion:** The findings suggest that SLNs hold potential as drug delivery systems for improved breast cancer therapy. The nanoprecipitation method offers advantages of reproducibility, scalability, and efficiency compared to traditional batch processes. Efficiently encapsulating doxorubicin within SLNs opens new avenues for targeted drug delivery, revolutionizing breast cancer treatment and potentially benefiting other diseases.

Keywords: Breast cancer therapy, Solid lipid nanoparticles (SLNs), Doxorubicin, Nanoprecipitation, Drug delivery systems.

Zerumbone Liquid Crystalline Nanoparticles Protect Against Oxidative Stress, Inflammation and Senescence Induced By Cigarette Smoke Extract *In Vitro*

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Introduction: Cigarette smoke is among the main risk factors for chronic obstructive pulmonary disease (COPD), causing oxidative stress, inflammation and cellular senescence that exacerbate disease progression. The main cells responsible for the release of oxidative stress and inflammatory mediators are broncho-epithelial cells and alveolar macrophages. Although many treatment lines are available for COPD, these present important side effects as limitations. Alternative treatment strategies, such as those involving natural products, are hampered by issues such as poor solubility, poor bioavailability, and difficult drug targeting. **Objectives:** In this study we encapsulated zerumbone in liquid crystalline nanoparticles (ZER-LCNs) in order to increase its effectiveness against COPD hallmarks. **Methodology:** The nanoparticle formulation was subjected to *in-vitro* biological studies to understand the anti-inflammatory, antioxidant, and anti-senescence activity on cigarette smoke extract-treated RAW264.7 macrophage and BCi-NS1.1 basal epithelial cell lines. **Results:** The ZER-LCNs successfully reduced the expression of pro-inflammatory markers including IL-6, IL-1β, and TNF-α, as well as production of nitric oxide. Additionally, ZER-LCNs successfully reduced oxidative stress through reduction of reactive oxygen species levels and regulation of genes including Gpx2 and GCLC. Anti-senescence activity was also obtained, with reduction of SIRT1, CDKN1A and CDKN2A expression. **Conclusion:** This study demonstrates the *in vitro* strong activity of ZER-LCNs as anti-inflammatory, anti-oxidative stress, and anti-senescence therapeutic agents, highlighting the potential of this innovative formulation as suitable treatment for COPD.

Keywords: Zerumbone; liquid crystalline nanoparticles; monoolein; P407; anti-inflammatory; antioxidant

Porous Swellable Hypromellose Composite Fortified with Bioactive Extracted from *Eucalyptus Camaldulensis* Leaf to Mitigate Dermal Wound Infections

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Introduction: Wound healing after injuries and infection remains challenging due to the complexity of wound healing processes, cell-signaling events, and biochemical cataracts. Several conventional therapies include synthetic and natural healing promoters with the inclusion of gauze dressing; however, these treatments require multiple components and are mostly inadequate for complete healing. Therefore, effective treatment of injured skin and wounds requires comprehensive dressing with antibacterial, antioxidant, anti-inflammatory, and hemostasis effects. **Method:** Composite fortified with a phenolic rich Eucalyptus camaldulensis green extract (ECG) and Eucalyptus camaldulensis yellow extract (ECY) was prepared using a freeze-drying process. In brief, HPMC with glycerol as the composite forming fluid was prepared in de-ionized water. The porous composite with or without phenolic-rich extract at low and high content concerning composite forming fluid were Fabricated by cryodesiccation using a Lyophilizer. The test composites fabricated were denoted with low and high content of ECG and ECY extracts as ECGLC (Eucalyptus camaldulensis green low content), ECGHC (Eucalyptus camaldulensis green high content), ECYLC(Eucalyptus camaldulensis yellow low content), and ECYHC(Eucalyptus camaldulensis yellow high content), respectively, and the control composite was denoted as HPMCC(Hydroxy propyl methyl cellulose control). **Results and Discussions**; Infrared spectroscopy and thermal analysis of ECG and ECY fortified composite indicated significant hydrogen bonding-based cross-linking, while scanning electron microscopy image showed a porous structure. The chromatography profiling demonstrated 0.022±0.02 and 0.027±0.01 µg/mg of quercetin for the ECG and ECY fortified composite, respectively. The antibacterial and antioxidant activity of extract incorporated composite was significantly (p <0.001) higher than that of control. Biocompatibility results revealed that composites were compatible with >80% viability of HaCaT and RAW 264.7 cells. The results of the blood-coagulation and clotting kinetics showed time and dose-dependent hemostasis. *Eucalyptus camaldulensis* leaf hydrophilic extract incorporated composite significantly (p <0.001) attenuated the nitrite production against lipopolysaccharides-stimulated macrophage cells. Moreover, the HaCaT cell showed 48.12±1.85 (%) of migration treated with ECY incorporated composite after 24 h. Overall, the hydrophilic extract-incorporated composites showed multifarious biological properties, suggesting their potential for comprehensive wound healing dressing.

Keywords: Anti-inflammatory, *Eucalyptus camaldulensis*, Quercetin, Hypromellose, a phenolic rich Eucalyptus camaldulensis leaf hydrophobic extract (ECG), a phenolic rich Eucalyptus camaldulensis leaf hydrophilic extract (ECY)

Formulation Development, Optimization and Evaluation of A Novel *In Situ* Gel for the Treatment of Glaucoma

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Introduction: Glaucoma is the leading cause of blindness worldwide and affects around 80 million patients. Vision loss occurs in some glaucoma patients due to excessive intraocular pressure. Issues with the use of eyedrops for glaucoma treatment include short residence time, poor bioavailability and rapid precorneal drainage. **Methods:** The present work described formulation development (cold method) for dorzolamide-hydrochloride loaded poloxamer/HPMC based polymer matrix novel *in situ* gel for enhanced ocular retention. A 3^2 factorial study (resulting in formulation batches F1 to F9) was used and the optimal formulation was selected via evaluation of gelling capacity, viscosity and % cumulative drug release. The optimized batch was further evaluated via *ex vivo,* histopathology*, in vivo* and gamma scintigraphy studies. **Results:** Optimized formulation (F4) successfully sustained release of drug up to 5 hours in *ex vivo* goat corneal permeability study. Histopathology on goat cornea proved the presence of normal ocular surface structures. Comparative *in vivo* experiments in normotensive rabbits showed that the optimized formulation (F4) sustained therapeutic effect for up to 8 h with 31.22 ± 3.65% reduction in intraocular pressure whereas a marketed formulation showed immediate release effect with 18.22 ± 4.42% reduction in intraocular pressure for up to 2-3 h. Gamma scintigraphy revealed an increase in ocular residence for the *in situ* gel formulation (F4) compared to marketed eye drops. **Discussion and conclusion**: Our developed non-irritant *in situ* gel is a new viable alternative for glaucoma treatment which should be further evaluated for human use via clinical studies.

Keywords: *in situ* gel, poloxamer, *in vivo, glaucoma*

Pharmaceutical Optimization of Polyelectrolyte Complexing Topical Formulation of Loratadine With Vitamin-C for Rheumatoid Arthritis

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Introduction: The aim of this study was to develop and evaluate topical administration of poorly soluble drug Loratadine with Vitamin adjuvant by developing the Loratadine - Ascorbic acid polyelectrolyte complexing nanoparticles gel (LA-Gel). **Methods:** LA-Gel was prepared by polyelectrolyte complex (PEC) technique using chitosan & Sodium alginate. LA-Gel was characterized by measuring the morphology, particle size, Polydispersity index, zeta potential, encapsulation efficiency (% EE), and FTIR Compatibility studies. In-vitro and In-vivo studies were carried out to demonstrate anti-arthritic activity. **Results:** LA-G F3 and LA-G F2 possessed better result when compared to LA-G F1 , here the LA-G F3 shows PS of 45.59± 0.5 nm, PDI of 0.06 ± 0.02, ZP of - 7.3 ± 0.36 mV, % EE of 85.4 ± 1.5, pH of 6.28 ± 0.3, viscosity of 5556 ± 14 cP, and drug content of 93.49 ± 0.48%. LA-G F3 showed a zero order controlled release manner within 8 hrs by following Higuchi Kinetics Model. The LA-G F2 and LA-G F3 revealed note worthy results Characterization study, In-*vitro* activity anti inflammatory activity and In-vivo study showed the inhibition of paw thickness, arthritis score, reduced elevated level WBC, ESR , Reduction of paw thickness were observed in at the end of treatment period on Day 15. **Discussion and Conclusion:** In-vitro and In-vivo studies of LA-G F2 and LA-G F3 shows encouraging results to demonstrate anti-arthritic activity by comparing with standard gel against induced arthritis in wistar rats. The LA-G F3 exhibited better anti-arthritic activity when compared with Standard formulation. Polyelectrolyte Complexing Topical Formulation of Loratadine with Ascorbic acid can be an effective controlled release system of combined therapy that administered topically on the skin surface for the treatment of Rheumatoid arthritis.

Keywords: Polyelectrolyte complex, Loratadine, L-Ascorbic acid, Rheumatoid arthritis.

Poster Presenters	
ID	**Presenters**
PP-DD-01	**Ms Berlian Sarasitha Hariawan**
	Characterization of Amniotic Mesenchymal Stem Cell Metabolite Products Liposome Loaded to Bone-Scaffold
PP-DD-02	**Ms Devy Maulidya Cahyani**
	Biopharmaceutical Study of Ursolic Acid Prepared into Niosome Coated with Chitosan
PP-DD-03	**Ms Rifda Tarimi Octavia**
	Dissolving Microneedle Patch for Delivery of Amniotic Mesenchymal Stem Cells Metabolite Products as an Antiaging Product
PP-DD-04	**Prof Dr Gowthamarajan K**
	Management of Atherosclerosis by Formulating and Optimizing Nanotheranostic Particles using the Design of Experiment Approach
PP-DD-05	**Mr Prajyod Deepak Haryan**
	pH Responsive Ofloxacin Loaded Carbomer Based Sol-Gel Composite Formulation and Evaluation for the Management of Periodontitis
PP-DD-06	**Mr Mohamad Siddiq Bin Mohamad**
	Assessing the Potential of Nano-Delivery Systems Containing 18b-Glycyrrhetinic Acid in Mitigating Lung Cancer.
PP-DD-08	**Dr Fith Khaira Nursal**
	Design of Mometasone Furoate Loaded Niosomal System as Drug Delivery Carrier

Characterization of Amniotic Mesenchymal Stem Cell Metabolite Products Liposome Loaded to Bone-Scaffold

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Introduction: Xenograft is a bone scaffold obtained from a different species used in another. Xenograft is widely used due to its 3D structure and has properties similar to human bone. Xenograft has good biocompatibility properties but lacks osteoconductive, osteoinductive, and osteoconductive properties. Amniotic Mesenchymal Stem Cells Metabolite Products (AMSC-MP) is a secretome extracted from human placenta tissue that contains growth hormone and cytokines that can be used for bone regeneration therapy. Liposome is a vesicular bilayer that can deliver both lipophilic and hydrophilic drugs. Liposomes can avoid AMSC-MP burst release growth factors from the scaffold and enhance osteogenesis activity. **Objectives:** This study aims to evaluate the effect of different phospholipids on the physical characteristics of AMSC-MP liposome loaded to scaffold and its biocompatibility in vitro. **Methodology:** The thin layer hydration method was used to create the AMSC-MP liposome. AMSC-MP liposomes were composed of L-α-fosfatidilcoline (PC) as unsaturated, hydrogenated soybean (HSPC) as a saturated phospholipid, and three types of a charged phospholipid, which were cationic surfactant i.e 1,2-dioleoyltrimethylammoniumpropane (DOTAP), and anionic phospholipid i.e. 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (DOPE) dan non-ionic phospholipid i.e dipalmitoyl-phosphatidylglycerol (DPPG). Liposome AMSC-MP was embedded in the scaffold by incubating for 24 hours. MTT assay was conducted to determine biocompatibility in vitro. **Results:** The results showed that the liposomes with saturated phospholipids, HSPC-DOTAP (132.35±2.75), HSPC-DPPG (148.35±19.86) and HSPC-DOTAP (152.85±5.86) have larger particle sizes than the liposomes with saturated phospholipids, PC-DOTAP (139.355±2.75), PC-DPPG (99.05±1.90) and PC-DOTAP (91.85±0.07). Cationic phospholipids caused an increase in zeta potential. Moreover, based on the MTT viability test against 7f2 cells and MSC, the result shows that all the formulas have good biocompatibility in vitro. **Conclusion:** Different phospholipid types could affect the liposome's particle size and zeta potential; however, it does not affect biocompatibility in vitro.

Keywords: Bone regeneration, stem cell, scaffold, liposome.

Biopharmaceutical Study of Ursolic Acid Prepared into Niosome Coated with Chitosan

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Introduction: Ursolic Acid (UA) is a pentacyclic triterpenoid compound that effectively inhibits tumor growth through modulation of apoptosis, inhibition of cell cycle, and autophagy. However, UA has poor water solubility and permeability. Niosomes have been reported to improve the bioavailability of low water-soluble drugs. **Objectives:** This study aimed to evaluate the biopharmaceutic and in vivo oral absorption of UA niosome modified with chitosan layers. **Methodology:** UA niosomes were prepared using a thin layer hydration method, then chitosan was added by vortexing the mixtures. Biopharmaceutics study was then determined for solubility and permeability compared to free UA. The in vivo oral absorption was then determined in mice's gastric, duodenum, jejunum, ileum, and liver after 30 minutes, 1 hour, 2 hours, and 4 hours of oral administration of UA. **Results:** The results showed the addition of chitosan layers increase the solubility and permeability of UA niosome. Niosome coated with a chitosan layer produced higher absorption gastrointestinal tract, with the highest absorption in the duodenum. Moreover, the photomicrographs of the organs revealed that UA niosomes with the chitosan layer were highly accumulated in the liver after 4 hours of oral administration. **Conclusion:** It can be concluded that the chitosan layer successfully improved oral absorption of UA niosomes through enhanced permeability of UA.

Keywords: Ursolic acid, niosome, chitosan, absorption.

Dissolving Microneedle Patch for Delivery of Amniotic Mesenchymal Stem Cells Metabolite Products as an Antiaging Product

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Introduction: Microneedles have emerged as a promising technology for enhancing the delivery of Amniotic Mesenchymal Stem Cell Metabolite Product (AMSC-MP) in skin rejuvenation and aging management. AMSC-MP contains Growth Factors (GF) that regulate cellular activities, but its hydrophilic nature and high molecular weight (>75 kDa) pose challenges to effective delivery. **Objective:** This study aimed to develop and evaluate the characteristics and effectiveness AMSC-MP-loaded microneedle patches as a solution to overcome these barriers, compared to the previously developed transfersome. **Methodology:** Microneedles were fabricated using the double-casting method with three different formulations varying in AMSC-MP concentration. The physicochemical evaluation involved scanning electron microscopy (SEM), TA-TX2 Texture Analyzer, and EX-101 optical coherence tomography (OCT) microscopy, respectively, to assess microneedle morphology, mechanical resistance, and insertion properties on Parafilm® M layer and full-thickness neonatal porcine skin. In vivo effectiveness was evaluated by quantifying collagen fibroblast cell count and conducting a skin irritation study, then comparing the result with the transfersome system previously developed. **Results:** The AMSC-MP microneedles exhibited a pyramidal shape with sharp tips and a height of 500µm per needle. Mechanical resistance evaluation revealed sufficient strength and the highest insertion depths were observed in formulation 1 (F1) on Parafilm® M layer at 447.44 ± 37.21 and formulation 2 (F2) on full-thickness porcine skin at 717.92 ± 25.40 µm. These findings demonstrate the successful penetration of microneedles through the stratum corneum and viable epidermis. Collagen levels were higher in all microneedle formulations compared to the transfersome formulation, with F1 exhibiting the highest quantity of fibroblast cells. Evaluation of inflammatory cell count indicated minimal presence in microneedle formulations, suggesting no irritative effects. **Conclusion:** Microneedle patches have shown favorable characteristics, including good mechanical strength, effective delivery of AMSC-MP, and minimal irritation. Therefore, they hold potential as a technology for delivering anti-aging agents and promoting skin rejuvenation.

Keywords: Microneedle, AMSC-MP, anti-aging, drug delivery

Management of Atherosclerosis by Formulating and Optimizing Nanotheranostic Particles using the Design of Experiment Approach

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Introduction: Atherosclerosis is one of the leading causes of death due to non-communicable diseases. The progression of atherosclerosis might lead to several other complications, such as myocardial infarctions, stroke and congestive heart failure. Lipid-based nanotheranostic particles with suitable drug and imaging agents can be implemented to study the extent of the atherosclerotic plaques, and based on the imaging, the treatment can be altered. Design of Experiments (DoE) is implemented to study the effect of different concentrations of different lipids and the homogenization speed on the particle size of the lipid-based nanotheranostic particle with the help of a central composite design(CCD). **Objectives:** To develop a nanotheranostic particle for the imaging and therapy of atherosclerosis using the DoE method. **Methodology:** The methodology is initiated by identifying a suitable target. Once the target was identified, in-silico docking studies were carried out with a few drug molecules and the promising ones were chosen. Blank lipid-based nanoparticles were optimized using the CCD model with different lipid ratios as the factors. After optimization, they are loaded with the drug of choice and tagged with an imaging agent and the nanotheranostic particle is subjected to characterization and evaluation tests. **Results:** The target has been identified as the LOX-1 receptor, and for that, Ligand binding studies were conducted with different molecules. The promising molecules have been shortlisted, and the same is being studied for in-vitro results. **Conclusion:** The docking studies show promising results, and the same is expected in the in-vitro studies. If the results are favourable, the promising molecules can be used to develop a nanotheranostic particle for managing atherosclerosis.

Keywords: Nanotheranostics, atherosclerosis, molecular docking, Design of Experiments

pH Responsive Ofloxacin Loaded Carbomer Based Sol-Gel Composite: Formulation and Evaluation for the Management of Periodontitis

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Introduction: Gingival recession is characterized as periodontal disease also known as gum disease. Antibacterial medicine is necessary for the treatment of this persistent infection. The in situ forming system is initially in the form of a sol, and when gradually supplied, it transforms into a gel or solid depot. **Objectives:** Treatment of periodontitis using in situ gel. **Methodology:** Cold Method : This method involved slow addition of polymer in cold solvent with continuous stir. The formed mixtures were stored overnight at 4°C and studied for their gelation temperature to select optimum concentration of Polymer grades for effective in situ gel formulation. **Results:** In situ gel exhibited a pseudoplastic flow pattern. The optimized batch consist of 0.105 gm of Carbopol 934 and 0.125 gm of HPMC K 100 which is having desired gelation time of 1.30 min, 90% drug release at 4 hours and drug content was found to be 90.50%. The viscosity of the optimized batch was found to be 3312 centipoise. **Conclusion:** Ofloxacin-loaded pH-sensitive in situ gel was successfully formulated by a combination of Carbopol 934 and HPMC K-100. FTIR study indicates no sign of incompatibility between drug and excipients, likely to be the best candidate for in situ gel. Selected polymers were likely to be proper for periodontal in situ gel. The formulation remains in a liquid state at non-physiologic conditions (at pH 3-4) and forms gel at physiologic conditions (at pH 6-7.5). The developed formulation shows acceptable gelation time and drug release results, which were dependent on concentrations of Carbopol 934 and HPMC K-100.Amongst the various formulations (F1-F4) assorted, optimized batch consists of 0.105g of Carbopol 934 and 0.125g of HPMC K-100, which has having desired gelation time of 1.30min, 90% drug release at 4 hr, and drug content is found to be 90.50%.The viscosity of the optimized batch was found to be 3312 centipoise. Antimicrobial studies indicate that ofloxacin retained its antimicrobial activity when formulated as in situ gel delivery for the treatment of periodontitis

Keywords: Periodontitis, in situ gel, pH sensitive, ofloxacin

Assessing the Potential of Nano-Delivery Systems Containing 18b-Glycyrrhetinic Acid in Mitigating Lung Cancer

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Introduction: 18β-Glycyrrhetinic acid (18β-Gly), a naturally occurring substance extracted from the licorice plant, has shown promising anti-cancer potential. However, the clinical application of free 18β-Gly is hindered by its poor physicochemical characteristics, such as limited bioavailability and low water solubility. This study aims to formulate nano-delivery system using Polylactic-co-glycolic acid (PLGA) for 18β-Gly to overcome these challenges. **Methods:** In this research, we formulate PLGA encapsulated 18β-Gly nano-formulation using adapted emulsion-evaporation method producing 18β-Gly-PLGA. After preparing the nano-formulation, we examined the physicochemical properties of nanoparticles and its anti-cancer effects on A549 lung cancer cells, comparing the effects of nano-formulation to free 18β-Gly. **Results:** Our study has yielded significant results, demonstrating that 18β-Gly-PLGA nano-formulation exhibits favourable physicochemical properties, including sustained in vitro drug release and high entrapment efficiency. Moreover, 18β-Gly-PLGA nano-formulation effectively inhibits the proliferation and migration of A549 cells. Underlying mechanisms of 18β-Gly-PLGA's anti-cancer effects involve the significant down-regulation of oncogenes such as KRT18, EGFR, BRAF, and KRAS. Furthermore, 18β-Gly-PLGA nano-formulation significantly reduces the expression of proteins associated with cancer proliferation and migration such as ErbB2, Survivin, M-CSF, and Mesothelin. **Discussion and Conclusion:** The nano-formulation of 18β-Gly-PLGA demonstrates an improved physicochemical profile and robust anti-cancer activities compared to free 18β-Gly.

Keywords: 18β-Glycyrrhetinic Acid, PLGA nanoparticle, A549 lung cancer cells

Design of Mometasone Furoate Loaded Niosomal System as Drug Delivery Carrier: optimization formula

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Introduction: Some topical applications of compounds combined with glucocorticoids and vitamin D can treat mild to moderate psoriasis, while systemic treatment is needed for severe psoriasis. Mometasone furoate (MF) is a steroidal anti-inflammatory compound that is reported to have clinical indications for treating psoriasis. Transdermal psoriasis therapy can be done by forming MF in the niosomal system, namely a nanovesicles so that the penetration power through the skin layers is higher and will increase the bioavailability of the drug. **Objectives:** This research aimed to develop a niosome formula containing MF, through optimization of surfactant combination (Tween 80 and Span 60), as well as the amount of cholesterol. **Methodology:** Optimization was designed using the Box Behnken experimental approach, and niosomes were made using the thin-layer hydration method. Evaluation of particle size, polydispersion index, zeta potential, and entrapment efficiency were used as the research's response variables. **Results:** The niosomes produced have the appearance of a cloudy liquid (dispersion), milky white in color, and odorless. The size of niosomal vesicles varies around 336.1 nm. In general, a zeta potential greater than ±30 mV is a good indicator of stability. All formulations have good stability so the tendency for aggregate formation or flocculation is lower. Measurement of entrapment efficiency was carried out spectrophotometrically by measuring free drug and drug entrapped in vesicles and obtained EE results ± 87%. The results show that MF can be formed using the niosomes system at MF concentration 1.396 mg/mL, cholesterol 0.5 M, and surfactant (combination) HLB value 4.7. **Conclusion:** This result indicated the formula can be developed for a transdermal drug delivery system.

Keywords: Niosomes, nanovesicle, mometasone furoat, surfactant.

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Oral Presenters		
Date: 25 October 2023 (Wednesday)		
ID	**Presenters**	**Time**
OP-LS-01	**Dr Mohammad Anas Shamsi** Repurposing Drugs for Bruton's Tyrosine Kinase Inhibition: A Combined Virtual Screening and Molecular Dynamics Study	2:00 PM
OP-LS-02	**Dr Saleha Anwar** Synthesis and Biological Activity of Bisindole Derivatives as Novel Mark4 Inhibitors	2:15 PM
OP-LS-03	**Ms Amanda Shen Yee Kong** In-silico analysis of nsSNPs in BCL-2 family proteins and their implications for colorectal cancer treatments	2:30 PM
OP-LS-04	**Mr Mohammad Yusuf Hasan** Protective Role of microRNA-21 as an Anti-Inflammatory Switch through α7nAChR Activation in Preventing Cerebral Ischemic Reperfusion (I/R) Injury	2:45 PM
OP-LS-05	**Ms Liyana Shafiqah Binti Sahul Hamid** Investigating the effects of 6-gingerol and 6-gingerol standardized *Zingiber Officinale* extract on chronic nicotine addiction in mice	3:00 PM
OP-LS-06	**Ms Nur Syahidah Binti Nor Hisam** In-Vitro Study: A Novel Action of Navitoclax on IL-3-Induced Human Endothelial Cells Angiogenesis Through PI3-AKT Signalling	3:15 PM

Oral Presenters		
Date: 25 October 2023 (Wednesday)		
ID	**Presenters**	**Time**
OP-LS-08	**Hui Yan Liew** Investigation of Cellular Traction Force as a Drug Testing Readout for In Vitro Cancer Metastasis	3:30 PM
OP-LS-09	**Dr Karniza Khalid** Alpha-1-Antitrypsin Deficiency: A Population-Based Study on Diagnosis, Clinical Manifestations, and Phenotypic Variations	4:00 PM
OP-LS-21	**En Li Soh** A systematic review: The ability of fermented herbal extract compounds in skin anti-ageing	4:15 PM
OP-LS-07	**Ms Hui Nee Hon** Development of 3D In Vitro Model using Organ-on-Chip to Modulate Breast Cancer Metastasis	4:30 PM
OP-LS-14	**Ms Kevina A/P N Yanasegaran** Single Nucleotide Polymorphisms Associated with Type 2 Diabetes Mellitus Control Among Malay Population: rs6265 Brain-Derived Neurotrophic Factor	4:45 PM

Oral Presenters		
Date: 26 October 2023 (Thursday)		
ID	**Presenters**	**Time**
OP-LS-10	**Mr Ludwig Hoon** minSNPs: From Derivation of Resolution-Optimised SNP Sets to Analysis of Nanopore Whole Genome	2:00 PM
OP-LS-11	**Ms Sofia Kokkinis** Curcumin-Loaded Liposomes Inhibit Cigarette Smoke Induced Senescence in Human Bronchial Epithelial Cells	2:15 PM
OP-LS-16	**Dr Sivaraman Dhanasekaran** Neurocognitive Investigation of Nano tailored therapeutics against Amyloid Beta Induced Neuropathological Implications	2:30 PM
OP-LS-17	**Dr Sufia Islam** Multidrug resistance isolates of Staphylococcus aureus in young children of Dhaka, Bangladesh	2:45 PM
OP-LS-18	**Mr Kian Christian J. Elman** Molecular Identification of *Campylobacter jejuni* and *C. coli* in the Raw Milk of Philippine Carabaos (*Bubalus bubalis*)	3:00 PM
OP-LS-19	**Ms Ira Oktaviani Rz** Physicochemical Analysis of Pangasius hypopthalmus Bone Gelatin Extract Using Organic Waste	3:15 PM
OP-LS-20	**Ms Rahimatul Uthia** Examining the Effects of Chia Seed Consumption on Body Weight and Cholesterol Reduction in Coturnix coturnix	3:30 PM

Repurposing Drugs for Bruton's Tyrosine Kinase Inhibition: A Combined Virtual Screening and Molecular Dynamics Study

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Introduction: Bruton's tyrosine kinase (BTK) is a protein kinase that plays a crucial role in various biological processes, including immune system function and cancer development and its overexpression is directly related to cancer progression and development. Thus, inhibition of BTK has been proposed as a therapeutic strategy for various diseases. Our study focuses on identification of new BTK inhibitors that can be implicated in cancer therapeutics. **Methods:** In this study, we aimed to identify potential inhibitors of BTK by using a drug repurposing approach. To identify potential inhibitors, we performed a molecular docking-based virtual screening using a library of repurposed drugs from DrugBank. We then used various filtrations followed by molecular dynamics (MD) simulations, principal component analysis (PCA), and Molecular Mechanics Poisson Boltzmann Surface Area (MM-PBSA) to further evaluate the binding interactions and stability of the top-ranking compounds.**Results:** Molecular docking-based virtual screening approach identified several repurposed drugs as potential BTK inhibitors, including Eltrombopag and Alectinib which have already been approved for human use. MD simulations provided insights into the binding interactions and stability of the identified compounds, which will be helpful for further experimental validation and optimization. **Discussion and Conclusion:** The study results demonstrate that drug repurposing is a promising approach to identifying potential inhibitors of BTK. The molecular docking-based virtual screening approach identified several repurposed drugs as potential BTK inhibitors, including Eltrombopag and Alectinib, which have already been approved for human use. This highlights the potential for drug repurposing in the discovery of new treatments for diseases, as it allows for the re-evaluation of existing drugs for new indications. This approach can save time and resources compared to traditional drug discovery methods, as these drugs have already undergone extensive safety and efficacy testing. Overall, our study demonstrates the importance of computational methods in drug discovery.

Keywords: Bruton's tyrosine kinase; drug repurposing; Eltrombopag; Alectinib; Virtual screening.

Synthesis and Biological Activity of Bisindole Derivatives as Novel MARK4 Inhibitors

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Introduction: Microtubule affinity regulating kinase 4 (MARK4) is a serine/threonine kinase that is directly associated with different types of cancer. Despite interest for pharmacological inhibition of MARK4, a small number of MARK4 inhibitors are currently available with most of them display low selectivity or bioavailability. Thus, we targeted the synthesis, structural characterization and evaluation of inhibitory effects of new bisindole derivatives as potent MARK4 inhibitors that can function with improved efficacy and selectivity. **Methods:** A series of bisindole derivatives were envisioned and synthesized. The actual binding affinity was measured with both fluorescence quenching and ITC. Enzyme inhibition assays investigated the effect of these bisindoles on the MARK4 functionality. Molecular docking was also performed to rationalise the molecular interactions within the catalytic site of MARK4. Cell proliferation assays were performed to check the effect of these bisindoles on inhibition of different cancer cell lines. **Results:** Bisindoles were found to bind with MARK4 with a significant affinity, depicted by fluorescence quenching and ITC. Enzyme inhibition assays established these as MARK4 inhibitors with IC50 values in the low micromolar range. Molecular docking revealed critical residues involved in the binding process. The antiproliferative activity of derivatives 18, 26, 33 and 20 was evaluated against A549, MCF7 and OVCAR-3 cancer cells. Among the tested compounds, 20 displayed the best cytotoxic activity against OVCAR-3 cells with GI50 = 7 ± 0.5 μM, TGI = 10 ± 0.8 μM and IC50 = 20 ± 1.2 μM and A549 cancer cells with GI50 = 4 ± 0.52 μM, TGI= 12.5± 0.8 μM and IC50= 32.5± 2.4 μM. In addition, compounds 18 and 26 induce apoptosis in A549 cells and deviated the cells from early to late apoptotic events. **Conclusion:** Overall, new bisindole derivatives possess significant antiproliferative properties, yet a non-selective cytotoxic effect was observed on normal MRC5 cells.

Keywords: MARK4; kinase inhibitors; Cell viability assays; cancer therapeutics; Molecular docking

In-silico Analysis of nsSNPs in *BCL-2* Family Proteins and their Implications for Colorectal Cancer Treatments

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Introduction: Colorectal cancer (CRC) is a complex disease characterized by abnormal cell proliferation in the colon and rectum. While the involvement of *BCL-2* family proteins in CRC development is acknowledged, the precise impact of genetic variations, particularly nonsynonymous single nucleotide polymorphisms (nsSNPs) within these proteins remains elusive. To unravel the pathogenic mechanisms underlying these nsSNPs in *BCL-2* family proteins, we conducted an *in-silico* study employing structure-based bioinformatic tools, aiming to uncover their molecular role in CRC pathogenesis. **Objectives**: We aim to identify pathogenic nsSNPs in *BCL-2* family proteins associated with CRC and explore potential molecular targets for anticancer treatment. **Methodology**: We retrieved nsSNPs of pro- and anti-apoptotic *BCL-2* genes (OMIM: 151430) from the NCBI genome database (GRCh37.p13). Pathogenicity was assessed using SIFT, PolyPhen-2, SNPs&GO, PhD-SNP, PANTHER, and Condel. Amino acid substitutions' impact on protein stability was evaluated through MutPred, PredictSNP, and I-Mutant2.0. Evolutionary conservation analysis utilized ConSurf, while Mutation3D and HOPE employed for protein functional analysis. Homology modelling with SWISS-Model and molecular docking analyses using AutoDock generated 3D structures of wild-type and mutated *BCL-2* family proteins and investigated their ligand interactions. **Results**: Ninety-four nsSNPs of *BCL-2* genes predicted as pathogenic; 31 nsSNPs showed decreased protein stability. Conservation analysis identified rs960653284, rs758817904, rs1466732626, rs569276903, rs746711568, rs764437421, rs779690846, and rs2038330314 as highly functional and exposed, while rs376149674, rs1375767408, rs1582066443, rs367558446, rs367558446, rs1319541919, and rs1370070128 were considered structural and buried. Molecular docking revealed lower binding affinity of G233D, R102C, and R102P towards d-Alpha-Tocopherol and Tocotrienol, indicating less favorable protein-ligand interactions, while R127C, R88C, R127P, G175D, and V34G exhibited higher binding affinity towards d-Alpha-Tocopherol. **Conclusion**: Our findings illuminate the role of pathogenic nsSNPs in *BCL-2* family proteins associated with CRC, elucidating their effects on protein stability, conservation, and function. Molecular docking analysis with Fluorouracil, d-Alpha-Tocopherol, and Tocotrienol revealed diverse binding patterns and interactions, indicating potential for targeted therapeutic interventions.

Keywords: Colorectal cancer, BCL-2 apoptosis regulators, Molecular docking, protein stability, targeted therapeutic.

Protective Role of microRNA-21 as an Anti-Inflammatory Switch through α7nAChR Activation in Preventing Cerebral Ischemic Reperfusion (I/R) Injury

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Introduction: Ischemic stroke is characterized by a sudden loss of blood flow in an artery leading to the brain. The activation of the α7-Nicotinic Acetylcholine Receptor (α7nAChR), which is found in immune cells such as microglia, has shown promising results in improving inflammatory profiles in stroke-induced rats but its exact mechanism of neuroprotection remains controversial. Analysis of known key microRNA's is an interesting avenue for the investigation to unravel the neuroprotection basis of α7nAchR activation. **Objectives:** To investigate the role of microRNA-21 in mediating inflammation via α7nAChR activation in preventing cerebral ischemia-reperfusion injury. **Methodology:** The mouse BV2 microglia cells were preconditioned with PNU-120596 (α7nAchR agonist) and then kept in hypoxia chamber (Oxygen-glucose-deprived) to mimic ischemic injury. Later the protein and gene expression of M1 (pro-inflammatory) and M2 (anti-inflammatory) markers as well as other downstream signalling pathways (NF-kB and STAT3) was measured by qRT-PCR and ELISA. Antagomir of microRNA-21 was transfected to investigate the protective role of microRNA-21. **Results:** The optimum time point of OGD was finalized after measuring cell viability at different time points (1,2,4,6,8 hour) using MTT assay. 4 hours was finalized as the optimum time as it showed more than 80% cell viability as well as successful inflammation.The activation of α7nAChR by an agonist PNU 282987 inhibited the OGD/R-induced elevation of pro-inflammatory markers (TNF-a, IL-6) while increasing the expression of the anti-inflammatory marker IL-10. It was also discovered that after OGD/R, NFkB-p65 levels increased significantly, whereas α7nAChR activation by agonist significantly reduced its expression. We have also reported that microRNA-21 regulates α7nAChR activation by switching proinflammatory M1 cytokines to anti-inflammatory M2 cytokines. **Conclusion:** The results demonstrated that activation of α7nAChRs inhibits the transformation of M1 microglia and promotes the M2 phenotype regulated by NFkB and STAT3 pathways and microRNA-21 provides a key role in this process.

Keywords: Ischemic Stroke; microRNA-21; a7nAChR; microglia; I/R injury.

Investigating the effects of 6-gingerol and 6-gingerol standardized *Zingiber Officinale* extract on chronic nicotine addiction in mice

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Introduction: Genetic studies have shown the interaction of serotonin subtype 3 receptor (5-HT3R) genetic variants and their association with nicotine-induced effects. Thus, we aim to further evaluate the implications of 5-HT3R antagonists; palonosetron (PAL), 6-gingerol (6G) and 6G-standardized ginger extracts (GE) on chronic nicotine addiction in mice. **Methods:** Swiss albino mice were divided into saline (SAL) and nicotine (NIC) groups, with the latter continuously administered with nicotine for 28 days to induce chronic nicotine addiction. Nicotine preferences were observed using the conditioned place preference (CPP) test (Test 2). Mice that developed preference were treated with PAL, 6G, bupropion (BUP), different doses of GE (70mg/kg, 100mg/kg, and 130mg/kg) and the CPP score was analyzed (Test 3). The mice brains were sectioned, and the prefrontal cortex was used to study genes involved in the pathophysiology of nicotine addiction such as serotonin receptor genes (*Htr3a, Htr3b, Htr2a, Htr2c*), acetylcholine nicotinic receptor genes (*Chrna4, Chrna7, Chrnb2*) and dopamine receptors genes (*Drd1, Drd2*) using RT² Profiler PCR array. **Results:** Mice treated with BUP, 6G and GE 100 showed significantly decreased nicotine preference on post-test 3. We found that mice receiving NIC showed increased trend of gene expression in *Htr3a*, *Htr2c, Chrnb2* and *Drd2* and reduced trends in some genes (*Htr3b, Htr2a, Chrna7* and *Drd1*). Increased trend of certain gene expression is seen in treatment groups; BUP [*Htr3a*, *Htr3b, Htr2c*], PAL (*Chrna4, Chrna7* and *Drd2*), 6G (*Htr2a, Htr2c, Chrna4*) and GE 100 [*Chrna4* ($p<0.05$), *Chrna7, Chrnb2* and *Htr3b*] when compared to NIC. **Conclusion:** Behavioural analysis shows that nicotine-addicted mice treated with 6G and GE100 effectively diminished nicotine preference, suggesting their potential use as a treatment to address nicotine dependency. The insight into gene expression levels may aid in a deeper understanding of the molecular mechanism involved in nicotine addiction.

Keywords: *Nicotine, Zingiber Officinale, Gingerol, 5-HT3; Conditioned Place Preference*

In-Vitro Study: A Novel Action of Navitoclax on IL-3-Induced Human Endothelial Cells Angiogenesis Through PI3-AKT Signalling.

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Introduction: Pathogenesis of cancer metastasis is comparable to intraplaque neovascularization in atherosclerosis which is predominantly contributed by endothelial cell activation modulated by interleukin such as interleukin-3 (IL-3). Navitoclax is well known as an apoptotic agent in solid and non-solid tumours. Hence, it is postulated that navitoclax can be developed as a novel therapeutic drug for intraplaque angiogenesis by regulating endothelial cell activation. However, limited evidence of the navitoclax effect on endothelial cell activity has been identified. **Objectives:** This study investigates the navitoclax effect on IL-3-induced endothelial cell angiogenesis that involves proliferative and migratory activities through the PI3K-AKT mechanism. **Methodology:** Primary endothelial cells isolated from human umbilical veins were utilized. Initially, MTT assay was conducted to determine the navitoclax safety concentration. Three groups which include; i) control; ii) 25ng/ml IL-3; iii) 25ng/ml IL-3 with 0.9µM navitoclax, were applied for subsequent experiments. BrdU colorimetric assay was done to examine cell proliferation after 24 hours of treatment. Then, cell migration at 0, 12 and 24 hours was monitored through scratch wound assay. Next, endothelial cells were seeded on Matrigel to observe the tube formation for 8 hours of treatment. Protein expression of CXCL-8, MMP-3, PI3K and p-AKT in cell lysate after 24 hours of treatment was analysed. **Results:** MTT assay showed 0.9µM navitoclax for 24 hours of treatment did not decrease cell viability significantly. Furthermore, only 3% of proliferating cells were inhibited by the navitoclax as compared to the control. However, navitoclax notably reduced cell migration and tube formation, which is consistent with CXCL-8 released and MMP-3 expressions that are associated with angiogenic and migratory mechanisms. Lastly, navitoclax also downregulated PI3K and p-AKT expressions significantly. **Conclusion:** These findings showed a novel effect of navitoclax as an anti-angiogenic agent by modulating cell motility through MMP-3 activity and PI3K-AKT signalling in IL-3-induced human endothelial cells.

Keywords: ABT-263, cell survival, HUVEC, motility, tube formation

Development of 3D In Vitro Model Using Organ-on-Chip to Modulate Breast Cancer Metastasis

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Introduction: Breast cancer continues to be the primary cancer influencing women globally, with metastasis being responsible for 90% of deaths. The initiation of breast cancer metastasis has been found to be influenced by increased extracellular matrix (ECM) rigidity. However, the current two-dimensional (2D) *in vitro* models for cancer metastasis cannot recapitulate the complex three-dimensional (3D) tumor microenvironment, thereby limiting comprehensive research on cancer metastasis. **Objectives:** Therefore, we seek to develop a 3D *in vitro* metastasis model utilizing an organ-on-chip (OoC) system, which is capable of housing 3D breast tumor spheroids embedded within a 3D ECM comprised of Alginate and Matrigel. This 3D model aims to investigate the influence of ECM rigidity on breast cancer metastasis, closely replicating the physiological conditions of the tumor microenvironment. **Methodology:** We first fabricated an OoC comprising a spheroids compartment and a chemoattractant compartment, interconnected by invasion channels. Next, we formed 3D breast tumor spheroids using MDA-MB-231 cells and embedded them into stiff (50kPa) and soft (25kPa) alginate/Matrigel matrices before seeding them into the OoC. Subsequently, we introduced 20% fetal bovine serum (FBS) as a chemoattractant to trigger metastasis. Live-imaging was then performed to observe the morphological changes of the spheroids, marking the initial stage of the invasion in metastasis. **Results:** Our result showed that MDA-MB-231 spheroids in the stiff ECM exhibited a significant decrease (68.94%) in circularity, whereas spheroids in the soft hydrogel showed a relatively smaller decrease of 29.92% from Day 0 to Day 2. This finding indicates that ECM with higher rigidity initiates cancer invasion on Day 2. **Conclusion:** Our OoC demonstrates a valuable 3D *in vitro* model to modulate breast cancer metastasis as it can accommodate 3D cultures and facilitate live-imaging of morphological changes in spheroids and invasion under different ECM rigidities, making it highly advantageous for comprehensive cancer metastasis research.

Keywords: Breast cancer metastasis, extracellular matrix rigidity, 3D spheroids culture, organ-on-chip

Investigation of Cellular Traction Force as a Drug Testing Readout for In Vitro Cancer Metastasis

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Introduction: Metastasis causes 90% of cancer-related deaths in solid tumours. While current in vitro models mainly focus on the antiproliferative effects of anticancer drugs, the impact of metastasis potential has always been neglected and remains unexplored. This is mainly due to the complexity and challenges associated with studying the intricate processes of metastasis, where cells migrate from the primary tumour to secondary sites, involving actin-myosin machinery to generate sufficient force for cell migration and invasion. **Objectives:** In this study, we aim to explore the use of cellular traction force as a drug testing readout for in vitro cancer metastasis models. **Methodology:** We first established invasive and non-invasive in vitro breast cancer models using MDA-MB-231 and MCF-7 cell lines, respectively. Subsequently, cisplatin and 5-fluorouracil(5FU) were selected as paradigm antimetastatic and non-antimetastatic drugs to evaluate the ability of in vitro cellular traction force to identify positive and negative metastatic drugs. We then conducted characterization of cell morphology, invasion assay, and traction force measurement after drug treatment on both in vitro cancer models. **Results:** Our results demonstrated that the invasive cancer model, MDA-MB-231, exhibited an elongated spindle-like morphology, compared to the more spherical shape of the non-invasive cell model, MCF-7. We also found that the MDA-MB-231 showed a higher average magnitude of force compared to MCF-7. When subjected to drug treatment, significant differences in the average cellular traction force of MDA-MB-231 in response to both antimetastatic and non-metastatic drugs were observed. By comparing cellular traction force with cell morphology and invasion assay, we demonstrated its potential to directly quantify the forces accountable for cell movement and assess the antimetastatic activity of drugs. **Conclusion:** Our findings suggest the immense potential of cellular traction force measurement in the context of drug testing for cancer metastasis and facilitating our understanding of cancer cell behaviour during metastasis.

Keywords: Breast cancer metastasis, cellular traction force, MCF-7, MDA-MB-231, drug testing readout

Alpha-1-Antitrypsin Deficiency: A Population-Based Study on Diagnosis, Clinical Manifestations, and Phenotypic Variations

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Introduction: Alpha-1-antitrypsin (AAT) deficiency is an inherited condition characterised by a deficiency in primary lung antiprotease, alpha-1 antitrypsin. This deficiency results in heightened protease-mediated tissue damage, leading to emphysema in adults. Additionally, the abnormal build-up of alpha-1-antitrypsin in the liver can lead to liver disease in both children and adults. A confirmed diagnosis is made when the serum alpha-1 antitrypsin is below 0.9 µmol/L. **Objectives:** We aimed to describe the clinical, biochemical, polymorphic, and pathological variances of AAT deficiency in a Malaysian population. **Methodology:** A retrospective analysis was performed using the database from the Special Protein Unit of the Institute for Medical Research, Kuala Lumpur, Malaysia. Clinical and biochemical data of samples sent for AAT phenotyping from January 1st, 2018, till December 31st, 2022, were collated. Data were presented descriptively, while presence of associations were tested with univariate analysis. **Results:** The study included 344 patients. Majority were infants (mean age 2.6±1.93 months), male (57.8%), and were Malays (57.5%). The overall mean AAT was 1.5±0.40 µmol/L. Hyperbilirubinemia/prolonged jaundice was the commonest reason for AAT phenotyping referral for neonates (30/43) and infants (121/186), hepatosplenomegaly for toddler/older paediatric age group (16/49), and respiratory symptoms for adults (15/66). Protease inhibitor (Pi) MM was the commonest normal variant found (70.7%). Nine were identified as AAT deficient; rare deficient variants included FM (1/9), and IM (1/9). There was a statistically significant difference in AAT value between different age groups ($F(3, 340)=13.08$, $p<0.001$). Post-hoc analysis determined that mean AAT was significantly lower in neonates vs. adults (95%CI:-0.458,-0.001, $p=0.049$), infants vs. toddler/older paediatric groups (95%CI:-0.354,-0.032, $p=0.012$), and infants vs. adults (95%CI: -0.497,-0.168, $p<0.001$). **Conclusion:** The epidemiology of this condition remains unknown in many countries as it often goes undiagnosed. We recommend the establishment of a more comprehensive patient registry to support future endeavours in AAT deficiency research and improved patient tracking.

Keywords: Alpha-1-antitrypsin, rare diseases, precision medicine, diagnostic, Malaysia

minSNPs: From Derivation of Resolution-Optimised SNP Sets to Analysis of Nanopore Whole Genome Sequence Data

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Introduction: Nanopore DNA sequencing technology is increasingly used in public health genomic surveillance. This is because it is portable and can generate long-read sequence data in real time. This, coupled with the large volume of publicly available sequencing data, allow for the development of optimised tools for genomic surveillance of microbial pathogens. **Objectives:** The objective was to develop a method to utilise resolution-optimised SNP sets and Nanopore sequencer-generated data to quickly assign microbial genomes into lineage within the relevant species. **Methodology:** We used minSNPs, an R package we created to derive SNP sets optimised for identifying the major lineages of *Staphylococcus aureus* with publicly available geographically diverse genomic data. We then extended minSNPs to do SNP calling with Nanopore-generated sequence data with short search strings. We also created a similar approach to determine the presence/absence of antibiotic-resistance (mecA) and virulence (lukS-PV, lukF-PV) genes. **Results:** The approach was tested with 24 isolates belonging to different major lineages, including a combination of antibiotic-resistant and virulence strains. These were previously sequenced with Illumina short-read sequencing. We performed DNA extraction with PureLink Mini Kit (Thermo Fisher), barcoded them with Rapid Barcoding Kit 96 and multiplex sequenced with Mk1C using R9 chemistry flow cell. Besides 2 failed sequencing, 5000 reads were sufficient for assigning samples to major lineages and detecting the tested genes irrespective of the basecalling method. **Conclusion:** minSNPs is an efficient and flexible tool for mining resolution-optimised sets of SNP markers that is applicable for microbial surveillance for biological entities for which there is extensive known genomic diversity. Extending minSNPs to make use of Nanopore sequencer provided a simple and quick way to make use of the surveillance markers.

Keywords: Nanopore sequencing, SNP mining, Microbial genomics

Curcumin-Loaded Liposomes Inhibit Cigarette Smoke Induced Senescence in Human Bronchial Epithelial Cells

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Introduction: Chronic obstructive pulmonary disease (COPD) is known to be one of the most common diseases caused by cigarette smoke. COPD causes an increase of goblet cells, mucus gland hyperplasia and fibrosis making the airways to become blocked reducing airflow. The wall lining begins to collapse and thicken due to the inflammation. Curcumin is derived from turmeric or *Curcuma longa* extract and has been used in traditional medicine for years. The anti-inflammatory properties make it a great dietary supplement. Curcumin has poor bioavailability due to its hydrophobic nature. The poor solubility of curcumin has called for new delivery systems to be implemented allowing the stomach to absorb a higher dose of the active. Liposomes can be used to encapsulate the curcumin within the lipid bilayer and protect it from the harsh conditions in the stomach and allow it to be absorbed by the stomach lining. **Objectives:** To assess the therapeutic potential of curcumin-loaded liposomes in inhibiting cigarette smoke-induced senescence *in vitro* in human broncho epithelial cells (BCiNS1.1). **Methodology:** The optimal safe concentration of curcumin liposome for BCiNS1.1 was identified with MTT assay. To induce senescence, the cells were exposed for 24 hours to 5% cigarette smoke extract (CSE). The anti-senescence effect of the curcumin liposomes was evaluated through X-gal staining and immunocytochemistry of key senescence markers; p16 and p21. **Results:** Pre-treatment with 2.5 µM of curcumin liposome for 24 hours before stimulation with 5% CSE significantly reduced X-gal positive cells compared to 5% CSE alone. Consistently, the protein expressions of p21 and p16 were significantly decreased (38.6% and 39.2% respectively), compared to CSE alone. **Conclusion:** The curcumin-loaded liposomes significantly protected BCiNS1.1 cells from CSE-induced senescence by targeting p16 and p21 expression. This highlights the promising potential of curcumin-loaded liposomes in reducing cigarette smoke-induced broncho-epithelial senescence in COPD.

Keywords: Curcumin, Liposomes, COPD, senescence

Single Nucleotide Polymorphisms Associated with Type 2 Diabetes Mellitus Control Among Malay Population: rs6265 Brain-Derived Neurotrophic Factor

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Background: Type 2 Diabetes Mellitus (T2DM) is a common polygenic lifestyle disease in Malaysia. Despite numerous studies linking specific genes and lifestyle factors to T2DM, information associated with single nucleotide polymorphisms (SNPs) and T2DM control in the Malay population is still limited. So, this study aimed to determine the potential genetic loci that influence or limit T2DM control, as indicated by HbA1c values, among Malays, by considering their physical activity level.

Methods: Participants were recruited from Universiti Kebangsaan Malaysia (UKM), Bangi by simple random sampling with informed consent. Socio-demographic data, anthropometric and biochemical blood measurements were collected. Disease status and physical activity level were determined by self-reported questionnaires and global physical activity questionnaires (GPAQ) respectively. Genotyping was performed using the MassARRAY System (Agena Bioscience). All descriptive data were reported in mean and standard deviations (mean ± SD) with simple regression analysis performed for SNP associations.

Results: Amongst the 363 T2DM individuals recruited, 67.8% participants were obese based on their body mass index (BMI) whilst 83.5% and 86.8% participants had been diagnosed with hypertension and hyperlipidaemia respectively. Males, increasing age, higher levels of waist-hip ratio, systolic and diastolic pressure, total cholesterol, triglyceride and low-density lipoprotein were associated with higher Hba1c values ($p<0.05$). Amongst the 17 T2DM associated SNPs analysed, rs6265 of brain-derived neurotrophic factor (BDNF) gene showed a positive correlation with HbA1c levels [adjusted β 95% (CI) = 0.240 (0.052, 0.429); $p<0.013$]. However, among those who are active (n=104), the heterozygous allele, CT of SNP rs6265 was associated with higher HbA1c level [OR 95% (CI) = 0.368 (0.131, 0.606); $p<0.003$].

Discussion and conclusion: BDNF gene regulates glucose metabolism and energy homeostasis, thus rs6265 of BDNF gene maybe a limiting factor for HbA1c control [1]. Further data validation in a larger cohort can be performed in association with dietary and exercise patterns.

Keywords: Type 2 Diabetes Mellitus; BDNF gene; SNP rs6265; Malay; HbA1c

Acknowledgment: This study was supported by the research university grants scheme (GUP), GUP-2021-009.

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Neurocognitive Investigation of Nano tailored therapeutics against Amyloid Beta Induced Neuropathological Implications

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Background: Neurodegenerative disorders have become a greater challenge for healthcare providers in recent years since they have a detrimental influence on the socioeconomic well-being of societies all over the world. WHO forecast predicts that 75% of the people with dementia aged above 60 years may likely to reside in developing countries by the year 2025. Researchers attempting a versatile therapeutic approach to effectively combat the pathological complications associated with AD, wherein the shift of strategy towards nano-tailored therapeutics through novel delivery renders beneficial results. **Methods**: The present investigation aimed at the pre-clinical investigation on the neurocognitive potential of liposome-encapsulated neurotherapeutics (LENT) on (Amyloid beta) Aβ25-35-induced neuroinflammation and oxidative stress in mice. Animals were subjected to pretreatment with Liposome encapsulated hesperidin and chlorogenic acid through nasal drug delivery for the periods of 3 weeks dose-dependently, then received a single intra cerebro ventricular (i.c.v.) injection of Aβ25-35 (10µg/mouse) subsequent treatment for one-week post ICV injection. Cognitive behavioral changes were evaluated using different types of memory tasks, including short-term, long-term, exploratory, and working memory in the experimental animals. Quantification of brain level neurotransmitters, including metabolic enzymes, was ascertained using spectrometric techniques followed by estimation of pro-inflammatory cytokines. Brain histological investigation proceeded with immunohistochemistry and differential staining to advocate the neuromorphological changes between treatment groups. **Results**: The study findings revealed some promising outcomes, including a remarkable decrease in the level of inflammatory cytokine, which justifies the ameliorative and neuroprotective potential of the plant derived components like hesperidin and chlorogenic acid. **Discussion and Conclusion**: In conclusion, phytotherapeutics-loaded liposomes with targeted drug delivery advocate a novel strategy in the clinical management of AD and its complications.

Keywords: Neuroinflammation, Alzheimer's disease, Amyloid beta, Liposomes, Neurotherapeutics, Neurotransmitters.

Multidrug Resistance Isolates of *Staphylococcus aureus* in Young Children of Dhaka, Bangladesh

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Introduction: *Staphylococcus aureus* (*S. aureus)* is one of the causes of illness and mortality in children. Both continuous and intermittent nasal carriage of *S. aureus* can act as a reservoir for internal infections as well as external transmission to other people. Its systemic invasion from the nasopharynx increases the risk of infection in children. Therefore, the identification of *S. aureus* in the nasal carriage is essential. **Objective:** This study was conducted to determine the prevalence of *S. aureus* among Bangladeshi children of various age groups with antibiotic susceptibility profiles. **Methodology:** 163 schoolchildren, 5 to 15 years old, who were randomly chosen, had their nasopharynx sampled. The identification of bacterial isolates was done using conventional microbiological techniques. Antibiotic susceptibility testing was conducted using the disk diffusion method. The VITEK® 2 system (BioMerieux) was used to further confirm the multidrug-resistant (MDR) isolates, and isolates that were resistant to 30 g of cefoxitin were labelled as methicillin-resistant *S. aureus* (MRSA). **Results:** Out of 44 participants, 27% had *S. aureus* nasal carriage. Cefixime was 100% resistant, followed by ampicillin and penicillin (95.5% and 90.9%) respectively. Six or more antibiotics were resistant to about 57% of MDR isolates. Among 42 MDR strains, 40 samples were tested for methicillin-resistant *S. aureus* (MRSA), and 47.5% of them tested positive for MRSA. The MRSA strains exhibited 100% cefixime and ampicillin resistance. **Conclusions:** Multidrug-resistant *S. aureus* strains were found in the children's nasopharyngeal samples. Antibiotic usage with caution and regular antimicrobial resistance (AMR) testing should be encouraged throughout the country. The national AMR) surveillance program should be properly established in order to monitor and regulate the usage of antibiotics.

Keywords: *S. aureus*, multidrug resistance, antimicrobial resistance, methicillin-resistant *S. aureus*.

Molecular Identification of *Campylobacter jejuni* and *C. coli* in the Raw Milk of Philippine Carabaos (*Bubalus bubalis)*

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Introduction: *Campylobacter* is an important cause of food-borne diseases worldwide. In the Philippines, several studies on the prevalence of *Campylobacter* spp. in chicken meat and dog feces have been conducted but there are no studies yet on its presence in carabao's milk. As such, this study was the first to investigate *Campylobacter* spp., specifically, *C. jejuni* and *C. coli*, in raw carabao's milk. **Objectives**: To optimize a PCR amplification protocol that was used in the molecular detection of *Campylobacter* spp., particularly *C. jejuni* and *C. coli* in raw carabao's milk. **Methodology**: We collected 49 raw milk samples (100 ml each) from backyard farms associated with the Provincial Veterinary Office of Nueva Ecija, Philippines. Accordingly, we determined the presence of *C. jejuni* and *C. coli* by utilizing two methods, (1) using the traditional culture-based method, boiling lysis, to extract *Campylobacter* DNA and (2) using milk bacterial DNA isolation kit from Norgen Biotek. Extracted DNA were then amplified using primers for genes that encode the Lipid A markers. **Results**: For *C. coli,* results show a 4% prevalence rate using the traditional culture-based method and 14.2% using the milk bacterial DNA kit. No *C. jejuni* was detected from the 49 samples. **Discussion/Conclusion**: Results revealed that raw milk of carabaos from backyard farms can become a source of food-borne infection which necessitates the creation of protocols for its handling and storage. It also revealed a discrepancy in the results when traditional method of isolation is used and when milk bacterial isolation kit is utilized emphasizing the difficulty in isolating and culturing *Campylobacter* from milk using the traditional method. The difficulty arose from the presence of competing microflora in milk, and this can pose a problem in the surveillance efforts of the country.

Keywords: Conventional PCR, *lpxA*, *lpxa-RKK2m*, culture-based methods, and Lipid A markers.

Physicochemical Analysis of *Pangasius hypophthalmus* Bone Gelatin Extract Using Organic Waste

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Introduction: The utilization of gelatin derived from fish bones shows potential development, but has not been extensively employed yet. Organic waste of pineapples serves as a natural ingredient to hydrolyze gelatin. **Objective:** This study aims to assess the physicochemical characteristics of the bone gelatin from *Pangasius hypopthalmus* obtained through the use of pineapple waste under the prescribed standards for gelatin quality. **Methodology:** This experimental study encompassed multiple stages. The process started with preparing the pineapple waste liquid extract followed by gelatin extraction (comprising pre-treatment and main extraction stages). During the initial phase of the treatment, the bones were immersed in a solution consisting of pineapple waste liquid in a ratio of 1:5 (mass/volume). This process was divided into three durations; 24, 48, and 72 hours. In the primary extraction process, the ossein was subjected to water immersion at a temperature of 75°C for five hours. **Results:** The analysis revealed the following results: the yields of the three treatments were 2.55%, 2.56%, and 2.77%. The pH values were 4.58, 4.99, and 4.34. The water contents were 11.66%, 11.42%, and 11.02%. The ash contents were 17.71%, 17.71%, and 20.97%. The crude fat contents were 0.17%, 0.42%, and 0.05%. The protein contents were 64.71%, 63.37%, and 58.04%. **Conclusion:** Based on the analysis of various physicochemical characteristics of the gelatin, the samples examined met the predetermined quality standards for gelatin. Notably, the optimal immersing time for achieving desirable gelatin characteristics was 24 hours of immersion.

Keywords: Gelatin; *Pangasius hypopthalmus* Bone; Pineapple Waste

Examining the Effects of Chia Seed Consumption on Body Weight and Cholesterol Reduction in *Coturnix coturnix*

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Introduction: In the Riau Health Polytechnic under the Indonesian Health Ministry, employees consume chia seed (*Salvia hispanica*) as a drink to decrease body weight. Chia seeds contain phenolic compounds such as flavonols and phenolic acids (myricetin, quercetin, kaempferol, and caffeic acid). These compounds are primary and synergistic antioxidants that confer antioxidant activity to chia seeds. Antioxidants reduce cholesterol levels by inhibiting cholesterol absorption in the intestine and increasing the formation of bile acids from cholesterol which is excreted in feces. Besides that, chia seeds contain a relatively high protein which can reduce appetite. The high fiber content in chia seeds can also prolong satiety. **Objectives:** This study aims to evaluate the effect of chia seeds consumption on weight and cholesterol reduction in the common quail (*Coturnix coturnix)*. **Methodology:** Animals were divided into five groups; positive controls, negative controls and three treatment groups given chia seeds at different concentrations (n = 6 animals in each group). In treatment groups, chia seeds were administered once, twice, or thrice a day at 1.8 mg/200 g body weight for 30 days. Body weight and cholesterol levels were measured at baseline and the last day of treatment. Data was collected and analyzed using a one way ANOVA, Kruskal-Wallis, and Post Hoc tests. **Results:** The difference in average body weight from baseline in the five groups; negative controls, positive controls, thrice a day feeding, twice a day feeding, and once a day feeding were 42.93, 52.26, 44.16, 45.33, and 46.25 grams respectively. The average cholesterol levels in each group was 173.67, 333.17, 202.67, 210.00, and 240.00 mg/dL respectively. It was found that administration of chia seed thrice a day (1.8 mg/200 g BW) confers the most significant reduction of body weight and cholesterol levels ($p<0.05$). **Conclusion:** Administration of chia seeds thrice a day at 1.8 mg/200 g body weight can decrease weight and cholesterol levels in *Coturnix coturnix.*

Keywords: Chia seeds, bodyweight, cholesterol levels.

A systematic review: The ability of fermented herbal extract compounds in skin anti-ageing

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Introduction: Skin ageing is a multifactorial process where the environment (extrinsic factors) and genetics (intrinsic factors) both play a part in this complicated biological process. Existing reviews on the efficacy of herbal extracts for skin anti-ageing focus mainly on in vitro studies of unfermented extracts. Whereas reviews regarding in vivo comparative study of fermented versus unfermented herbal compounds or compared to placebo is scarce. This systematic review is conducted to determine the viability of the use of fermented herbal compounds as a topical formulation and oral administration in skin anti ageing by focusing on in vivo studies both in humans and animals. **Objective**: To determine the viability of the use of fermented herbal compounds as topical formulation and oral administration in preventing and reversing the signs of skin ageing by focusing on in vivo studies. **Methodology**: For this systematic review, the following online databases: Cochrane Central Register of controlled trials, Ovid Medline, and Embase via Ovid databases were searched and retrieved from Jan 2012 until Dec 2022. The articles generated were rigorously screened for eligibility using the Covidence software and manually as well. Data from eligible studies were then extracted and collated for synthesis and descriptive analysis. **Results**: After the final data extraction process, 9 studies satisfied the inclusion and exclusion criterias and were included in this review. The main findings from this systematic review are that fermented herbal extracts from pomegranate, honeybush, papaya, red grape, soybean, and S-equol from soy germ have shown promising skin anti-ageing results. These fermented herbal extracts could be utilized as a source of active ingredients for the development and production of effective products for preventing and reversing skin ageing. Fermented versions of the honeybush extract have been shown to be more effective than the unfermented honeybush extract in terms of reversing skin ageing caused by UVB irradiation. **Conclusion**: Our review of the 9 in vivo fermented herbal compounds studies suggests that fermented herbal compounds may have a beneficial effect on skin anti-ageing in women and men. However, this area still requires further research as other formulations such as topical formulations have not fully been explored and compared and the side-effect profile also needs to be explored. This is to ensure the safety and efficacy of the fermented herbal compounds if women and men would like to use these compounds in the future.

Keywords: Fermented, Herbal, Anti-Ageing, Topical routes and Oral routes

Poster Presenters	
ID	**Presenters**
PP-LS-01	**Hetvi Saurin Shah** Insight into Kisspeptin and its Transcriptional Regulation in MDA-MB-231 Breast Cancer Cell Line
PP-LS-02	**Assistant Professor Leyon Varghese** Silibinin is a Strong Inhibitor of Bacterial Metalloproteinase (BEMPs): An In Silico and In Vitro Approach
PP-LS-03	**Dr Nor Syafinaz binti Yaakob** Investigating the Effects of 6-gingerol Standardised Ginger Extracts on Nicotine-Induced Toxicity in Mice Heart and Kidney
PP-LS-04	**Nursyamila binti Shamsuddin** Evaluation of 3'Untranslated Region of MIR497HG in Transiently Expressed Luciferase Reporter Vector for microRNA-lncRNA Interaction Study
PP-LS-05	**Hin Yee Thew** Exploring the Neuroprotective Effects of Xanthone in Alzheimer's Disease Models: An In-Vitro and Computational Investigations
PP-LS-06	**Jeena John** Deciphering the Role of NAMPT and SIRT1 in Chemotherapy-Induced Cognitive Impairment
PP-LS-07	**Amelia Suhana binti Zamri** Identification of a Novel Bruton's Tyrosine Kinase Gene Mutation in X-Linked Agammaglobulinemia

Poster Presenters	
ID	**Presenters**
PP-LS-08	**Ms Ai Sze Wee** Chemical Constituents and Anti-Cholinesterase Profile of Essential Oil from *Murraya koenigii* Leaves
PP-LS-09	**Dr Suraiami Binti Mustar** Potential Neuroprotective Effects of Honey in the Treatment of Neurodegenerative Disorders
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Insight into Kisspeptin and its Transcriptional Regulation in MDA-MB-231 Breast Cancer Cell Line

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Introduction: The KISS-1 gene, encoding the kisspeptin hormone, has been primarily studied for its influence on the hypothalamic-pituitary-gonadal axis (HPG). However, recent studies suggest a significant role for KISS-1 in suppression of metastasis in various cancers. Kisspeptin-10 (KP-10) is a short fragment of Kisspeptin which shows anti-tumour effects. Also, there are various signaling molecules and transcriptional factors associated with Kisspeptin which helps in suppression of metastasis.Objectives: The study mainly focuses on to elucidate the effect of how exogenous kisspeptin (KP-10) stimulated the intracellular signalling pathway of breast cancer MDA-MB-231 cell line and its effect with the interacting signalling molecules and transcriptional factors. **Methodology:** The study comprises dual methods as in vitro and in silico techniques. The MDA-MB-231 cells are cultured exogenous treatment of Kisspeptin-10 (KP-10) (Merck: K2644) is given at various concentration (10, 25, 50, 100,200,500, 1000 nM). Further cell viability assay (MTT Assay) and cell migration analysis is done. Concurrently, in silico analysis, docking experiments via HADDOCK, the interacting signalling molecules and transcriptional factors involved in breast cancer metastasis were identified. For MDA-MB-231 cell lines, RNA would be isolated by Trizol method (Invitrogen) and cDNA would be prepared and further RT-PCR. **Results:** Cell viability showcased the IC-50 to be 100 nM, further cell migration analysis confirmed that KP-10 inhibited the mobility of breast cancer cells. HADDOCK analysis confirmed: SP1, NMYC, PKC, Kiss1, Kiss1R as the transcriptional regulators and hence gene expression analysis of the same was done. **Conclusion:** Hence, the present study would provide a comprehensive understanding of the role KISS-1 in breast cancer. Our findings will likely provide information in the development of new therapeutic approaches, harnessing the potential of Kisspeptin as a target for breast cancer treatment.

Keywords: Kisspeptin, KP-10, MDA-MB-231, metastasis

Silibinin is a Strong Inhibitor of Bacterial Metalloproteinase (BEMPs): An In Silico and In Vitro Approach

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Introduction: Metalloproteinase are important in cell invasion and tissue remodeling; and are therefore promising drug targets in managing enteroinvasive pathogens. Silibinin a widely used dietary supplement with well known hepatoprotective roles have also projected for its anticancer properties. Here we examined the inhibitory potential of silibinin towards bacterial metalloproteinase (BEMPs) through a combination of in silico and in vitro approach. **Objective:** Study the binding affinity of silibinin towards different BEMPs and its validation using in vitro systems. **Methodology:** Molecular docking studies were conducted using silibinin as the ligand and different BEMPs as receptors. To analyze the stability of this silibinin-BEMP interactions, molecular dynamic (MD) simulation studies using GROMACS 5.7.4 package were performed. In vitro gelatinolytic activity assays including zymography were also conducted to validate the in silico findings. **Results:** Molecular docking studies showed strong binding affinity between silibinin and BEMPs such as coccolysin (-9.5 kcal/mol) and fragilysin (-9.3 kcal/mol). In the MD simulations studies, Root Mean Square Deviation of protein-ligand complexes were within 0.25nm throughout the simulation and the Root Mean Square Fluctuation also showed minimal residue fluctuation. The compactness of complex as well as the number of hydrogen bonds between them were also found consistent through the simulation time. To confirm these observation in vitro, spent fermentation broth of E. faecalis was mixed with silibinin to observe the inhibition of gelatinolytic activity. Further the gelatinase was separated on a gelatine-PAGE and its treatment with silibinin inhibited the gelatinolytic activity. **Conclusion:** Our results are clearly indicative of the direct inhibitory potential of silibinin towards different tissue remodeling gelatinase of enterobacteria. Since BEMPs are important in bacterial invasion and hence in its virulence, role of silibinin in the bacterial invasion can be explored further to determine if its supplementation will help reduce the occasional virulence of gut microbial species.

Keywords: Enteroinvasive, Gelatinase, Molecular Docking, MD Simulation, Virulence

Investigating the Effects of 6-Gingerol Standardised Ginger Extracts on Nicotine-Induced Toxicity in Mice Heart and Kidney

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Background: Our current studies are exploring the potential of natural products for smoking cessation. We have shown that 6-gingerol (6G, a bioactive compound in ginger) reduced nicotine addiction in mice models. As ginger extracts were shown to possess antioxidant properties, and it is well-known that chronic smoking can lead to nicotine-induced toxicity in vital organs, we aim to explore whether the ginger extract and compound possibly have concurrent effects in reducing nicotine addiction and nicotine-induced oxidative injuries. **Methodology:** Concentrations of 6G in soil-based and soilless ginger ethanolic extracts (GE) were quantified by HPLC. Mice with chronic nicotine addiction were divided into control groups [nicotine (Nic 1mg/kg) and normal saline] and treatment groups [(6G+Nic, 6G-standardised soilless ginger extracts with 3 doses (GE70+Nic, GE100+Nic, GE130+Nic)]. Mice were euthanized for heart and kidney harvest. Oxidative stress markers [total protein (TP), oxidation protein product (AOPP), malondialdehyde (MDA)] and antioxidant markers [glutathione (GSH), superoxide dismutase (SOD) and catalase (CAT)] were analysed to assess effects of the treatments on nicotine-induced organ toxicity. **Results:** The concentrations of 6G were similar in both ginger extracts, therefore the soilless GE was utilised downstream. For oxidative stress markers, TP concentration in the kidney remained consistent but was significantly reduced in heart tissues of Nic and 6G+Nic groups. Nic treatment induced AOPP and MDA increase that is not significantly affected by most treatments in both renal and heart tissues except in the 6G+Nic group where the MDA level in the heart was reduced. For antioxidant markers, the GE100+Nic group exhibited a significant increase of GSH content (vs Nic group) in renal tissue whereas no significant changes were observed in heart tissue for all groups.No significant changes were observed for SOD and CAT activities in both renal and heart tissues. **Discussion and Conclusion:** In parallel with our studies in exploring potential of 6G and GE to treat chronic nicotine addiction, these findings are essential in understanding their concurrent effects on vital organs, particularly the heart and kidney.

Keywords: Nicotine, Zingiber Officinale, Oxidative stress, Antioxidant, Mice

Evaluation of 3' Untranslated Region of MIR497HG in Transiently Expressed Luciferase Reporter Vector for microRNA-lncRNA Interaction Study

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Introduction: Sequence elements in the 3'untranslated region (3'UTR) of long non-coding RNA (lncRNA) can be used as a target site for multiple regulatory molecules such as microRNA (miRNA). However, little is known about the post-transcriptional mechanism that possibly regulate the lncRNA, microRNA-195-497 cluster host gene (MIR497HG) in hepatocellular carcinoma. Dual-luciferase assay is a sensitive and convenient way to examine the transcriptional activity of MIR497HG. The dual-luciferase assay system relies on Firefly luciferase (Fluc) as a primary reporter to monitor the transcriptional activity and Renilla luciferase (Rluc) as a control reporter for normalization. **Objectives**: This study aims to describe in detail step-by-step for miRNA and 3'UTR of MIR497HG target validation and application of reporter vector system through the measurement of dual-luciferase assay to monitor miRNA-lncRNA interaction. **Methodology:** A 1.5kb fragment of 3'UTR of MIR497HG was amplified by Polymerase Chain Reaction (PCR) from genomic DNA of human hepatocellular carcinoma cell line (HepG2 cell). To generate luciferase reporter plasmid, the purified PCR product was inserted into multiple cloning site (MCS) of pmirGLO Dual-Luciferase miRNA target expression vector. Restriction enzyme digestion was performed to further validate the ligation of insert. The ligated product was transformed into competent Escherichia coli, DH5α using heat-shock method. Positive clones were isolated from ampicillin agar plates and desired clone was confirmed by DNA sequencing. The HepG2 cells were transiently transfected with 40ng, 100ng and 200ng of pmirGLO-3'UTR MIR497HG construct or pmirGLO vector alone using the Fugene HD transfection reagent for 24 h. Later, the luciferase activity was detected by measuring the activity of the dual-luciferase reporter assay system. **Results:** Restriction enzyme digestion and DNA sequencing result confirmed that the luciferase reporter vector was successfully inserted by 3'UTR of MIR497HG. This recombinant plasmid was termed as pmirGLO_3'UTR MIR497HG. There was a significant decrease in the relative luciferase activity for the pmirGLO_3'UTR MIR497HG ($P<0.001$) compared to cells transfected with pmirGLO empty vector. **Conclusion:** This study demonstrates that 3'UTR of MIR497HG is a target for active miRNA in HCC cell lines. Taken together, this study highlights the post-transcriptional regulation of 3'UTR MIR497HG region by certain miRNAs in HCC cells. Computational analysis and quantitative Real-time Polymerase Chain Reaction (RT-qPCR) are required to identify this endogenous miRNA.

Keywords: Long non-coding RNA, MIR497HG, 3'untranslated region, microRNA, luciferase

Exploring the Neuroprotective Effects of Xanthone in Alzheimer's Disease Models: An In-Vitro and Computational Investigations

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Introduction: Alzheimer's disease (AD) is characterized by amyloid-β (Aβ) protein aggregation, leading to neuronal cell death. **Objectives**: This study explores the potential neuroprotective effects of α-mangosteen (α-M), a natural compound from Garcinia mangostana, against Aβ42-induced neurotoxicity, with α-M extracted through a solvent-based method. **Methodology**: The research comprises in-vitro experiments assessing α-M's impact on Aβ42 aggregation and toxicity, along with computational analyses employing molecular docking and dynamics simulations to investigate α-M's effects on Aβ42 aggregation and structure. **Results**: The in-vitro cell-based experiments showed that a 0.1 μM α-M pre-treatment significantly protected up to 21.09±3.39% of SH-SY5Y cells from Aβ42-induced neurotoxicity. Additionally, dot blot assays demonstrated a decrease in Aβ42 aggregation when exposed to 0.5 and 1.0 μM α-M, indicating its potential to mitigate Aβ42 oligomer formation. Furthermore, computational studies revealed interactions between α-M and the N-terminus and C-terminus regions of Aβ42, crucial for fibril formation. The molecular interaction between the Aβ42-α-M complex, with a binding energy of -6.55 kcal/mol, was verified through molecular docking and visualization. A hydrogen bond formed with the Gln15 residue of Aβ42, securing the Aβ42 monomer and inhibiting Aβ42 oligomer development. Molecular dynamics simulations of the Aβ42-α-M complex revealed a tightening of the C-terminal Aβ42 region, reducing the Rg value. Additionally, α-M's interaction with Gly33 and Gly37 residues at the N-terminus of Aβ42 disrupted the formation of surface features on the amyloid, diminishing Aβ42 aggregation. Principal component analysis (PCA) results further affirmed these computational findings, with a low root-mean-square deviation (RMSD) compared to Aβ42. **Conclusion**: The study suggests that α-M could serve as a lead compound for further exploration, facilitating the development of novel therapeutic agents targeting Alzheimer's disease more effectively. These valuable insights into α-M's neuroprotective properties open avenues for potential advancements in future AD therapies.

Keywords: Alzheimer’s disease, neuroprotection, mangosteen

Deciphering the Role of NAMPT and SIRT1 in Chemotherapy-Induced Cognitive Impairment

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Introduction: Chemotherapy-induced cognitive impairment(CICI)/chemobrain is defined by the long/short-term effects on cognition in cancer patients/survivors. However, heterogeneity in cancer and chemotherapy is a hurdle to understanding the molecular mechanisms underlying CICI. Chemotherapy inhibits nicotinamide phosphoribosyl transferase(NAMPT), which leads to a decrease in nicotinamide adenine dinucleotide(NAD+) levels, resulting in the susceptibility of cancer cells to oxidative damage and death, which may also suppress non-cancerous cells, particularly those found in the brain tissues. In general, dyscognition may be caused by the downregulation of the NAMPT-mediated NAD+/Sirtuin 1(SIRT1) pathway from the suppression by chemotherapy. **Objectives**: To evaluate the role of NAMPT and SIRT1 in CICI using in vitro and in vivo studies. **Methodology:** Differentiated SHSY5Y cell lines were treated with quercetin and its derivatives against Methotrexate and 5-Fluorouracil, which were selected after the insilico drug screening followed by subjecting to cytotoxicity assay, flow cytometry, and PCR analysis. For the in vivo study, Cyclophosphamide, Methotrexate, 5-Fluorouracil(CMF) along with the test drugs was administered to tumor-bearing mice for a 21-day chemotherapy cycle, followed by the assessment of cognition by Morris Water Maze, estimation of NAMPT, SIRT1 markers by western blotting. **Results:** Differentiated SHSY5Y cells were protected by the phytochemicals against MF toxicity, evidenced by cytotoxicity and flow cytometric analysis. PCR studies showed decreased mRNA expression of NAMPT and SIRT1 markers in MF-treated cells and increased in test-drug-treated cells. In the in vivo study, chemotherapy negatively affected spatial learning ability and reduced the expression of NAMPT and SIRT1 proteins. The test drugs ameliorated these cognitive impairments and enhanced the targeted proteins. **Conclusion:** The treatment of phytochemicals proved its possible ability to alleviate CICI and could pave the way for identifying treatment strategies to combat chemobrain. NAMPT and SIRT1 may be ideal candidates for resolving the molecular complexity in chemobrain by NAD+ regulation due to their neuroprotective functions.

Keywords: Cancer, Cognition, Chemobrain

Identification Of A Novel Bruton's Tyrosine Kinase Gene Mutation In X-Linked Agammaglobulinemia: A Case Report

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Introduction: X-linked agammaglobulinemia (XLA) is an X-linked recessive disease characterized by a profound deficiency of immunoglobulin isotypes and very low or absent B cells, resulting in recurrent bacterial infections. It has been associated with mutations in the Bruton's tyrosine kinase (*BTK*) gene that encodes a cytoplasmic protein crucial in B cell maturation. Its mutation blocks B cell differentiation at the pre-B cell stage leading to failure of immunoglobulins production, and is responsible for XLA. **Methodology:** In this report, a five-year-old boy suspected with XLA was studied. He was admitted at birth for presumed sepsis that required ventilation. At 4 months old, he had multiple admissions for otitis media, respiratory tract infections with persistent cough and frequent fever, followed by recurrent pneumonia at 26 months old. In between admission, he required several courses of antibiotics. BTK protein expression test by flow cytometry and immunoglobulins level test were carried out. Then, the blood samples from the patient, mother, and control were sent for *BTK* full gene analysis. **Results:** The patient had absent B cells and markedly reduced serum immunoglobulin G (IgG) and immunoglobulin A (IgA). Flow cytometric analysis showed he had only 3% of monocytes expressing BTK protein as compared to the control's (87.9%). Genetic analysis revealed a novel mutation at the exon 11 of *BTK* gene (NM_000061.3:c.953_956delCTGT;p.Ser318Cysfs*12). The four-nucleotide deletion resulted in a frameshift and premature termination, hence disrupting the protein structure. However, the mother did not carry the mutation and had normal BTK protein expression. **Conclusion:** Taken together, these findings confirmed the diagnosis of XLA in the patient. We concluded that this *BTK* gene mutation in our patient is a sporadic case and emphasizes the reliability and importance of *BTK* gene sequencing to diagnose XLA in not only inherited cases, but also in sporadic cases.

Keywords: X-linked agammaglobulinemia; *BTK* mutation; novel mutation; sporadic XLA

Chemical Constituents and Anti-Cholinesterase Profile of Essential Pil from *Murraya koenigii* Leaves

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Introduction: Traditionally, *Murraya koenigii* (L.) Spreng has been utilized as an ingredient in medicinal formulations. As of the present, several studies have reported on the potential of the leaves of *M. koenigii* to enhance learning and memory functions in animal models. However, these investigations have been limited, as they lack the identification of specific chemical fingerprints associated with the observed effects. **Objectives:** This study was aimed to identify the chemical constituents and anti-cholinesterase activity of the essential oil extracted from the leaves of *M. koenigii*. **Methodology:** The leaves of *M. koenigii* were collected from Air Itam, Penang. A voucher specimen (KLU50161) was deposited in the Herbarium at University Malaya. The chemical composition of the essential oil isolated by steam distillation of the leaves of *M. koenigii* was analysed by gas chromatography-mass spectrometry. Cholinesterase inhibitory activity was assessed using the Ellman's method with modification. Rivastigmine and donepezil served as the reference standards. **Results:** Forty-one compounds constituting 97.34% of the essential oil isolated from the leaves of *M. koenigii* were identified, with β-phellandrene (35.42%), β-caryophyllene (16.79%) and α-pinene (17.75%) as the major constituents. The essential oil of the leaves of *M. koenigii* showed inhibitory activity against the cholinesterase enzymes, particularly towards the acetylcholinesterase (AChE), with IC_{50} value of 36.89 ± 1.98 µg/mL. **Discussion and conclusion:** The results of the present study revealed that the essential oil of the leaves of *Murraya koenigii* have the anti-acetylcholinesterase potential and could hold significance in the endeavour to discover novel cholinesterase inhibitors.

Keywords: *Murraya koenigii*; essential oil composition; anti-acetylcholinesterase; Rutaceae.

Potential Neuroprotective Effects of Honey in the Treatment of Neurodegenerative Disorders

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The global rise in neurodegenerative disorders among the elderly has spurred heightened research efforts to address this issue. As pharmaceutical treatments often come with complex complications, natural products have emerged as promising alternatives for alleviating neurodegenerative diseases. Among these natural remedies, honey has garnered significant attention for its potential neuroprotective properties. Hence, the objective of this work is to provide a comprehensive overview of studies conducted in the last 10 years that explore the neuroprotective effects of honey. In this narrative review, the terms "honey" and "neurodegenerative" were used to search for articles published between January 2012 to December 2022 from three databases (PubMed, ScienceDirect, and Scopus). The selected articles were written in English and comprised research articles related to honey and its related compounds. Review articles and articles on other bee products such as propolis, beebread, beeswax and melittin were excluded. Sixteen articles were chosen out of 1,167, with six in vitro, eight in vivo, one combined research, and one clinical intervention. Most in vitro studies investigate the effect of honey/compounds on the inhibition of acetylcholinesterase and butyrylcholinesterase. For in vivo studies, rats were used as the animal model, comparing the neuroinflammation makers of the control group with the honey intervention group. The Tualang and Thyme honey were both found to be the best antioxidant, anti-inflammatory and anticholinesterase activity among the types of honey investigated, contributing to the deterrence and treatment of numerous neurological conditions including Alzheimer's disease. The high polyphenol content of honey, specifically quercetin and gallic acid in Tualang and Thyme, is found to be largely responsible for its neuroprotective effects. The exact mechanism of action causing its anti-neurodegenerative features is still unknown, but polyphenols show the potential to prevent and disintegrate the formation of protein clumps or aggregates in the brain, thus attenuating its neurotoxicity effects. In conclusion, honey appears to be an effective natural product to attenuate neurodegenerative diseases. To further verify these findings, more clinical research is needed.

Keywords: Honey, neurodegenerative, Alzheimer’s disease, polyphenol

Molecular Identification of Competing Microflora for the Optimization of Campylobacter Isolation from Raw Carabaos' Milk

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Introduction: Campylobacter sp. is one of the leading causes of milk-borne diarrhea and detecting their presence in milk is a necessary step in preventing outbreaks of diseases caused by this microorganism. However, detection and isolation of Campylobacter is difficult because of the presence of other microflora in milk. As a fastidious organism, Campylobacter are usually outgrown by other microorganisms, identifying the competing organisms will help in the successful isolation of Campylobacters. **Objectives:** This study aims to identify the non-Campylobacter colonies that grew on Modified charcoal-cefoperazone-deoxycholate agar (mCCDA) by using molecular methods in order that proper adjustment in the protocol for the isolation of Campylobacter can be done. **Methodology:** Forty six (46) non-Campylobacter colonies were picked from Modified charcoal-cefoperazone-deoxycholate agar (mCCDA) which was streaked with milk samples collected from 15 carabaos raised in backyard farms in an agricultural area in the Philippines. DNA were extracted using boiling lysis and amplified using 16S rRNA. The amplicons were sequenced with SeqStudio Genetic Analyzer and BLAST was used to compare the sequences to the those in the database and identify the microorganisms. **Results:** Results show that 61% of the isolates are Acinetobacter baumanii and 28% are *Pseudomonas aeruginosa*, two of the most significant pathogens in terms of multidrug resistance.
Klebsiella sp. and Pseudoroseomonas sp. are also identified from the isolates. **Conclusion:** Findings from this study will help in determining the antibiotics that can be added to the culture media to prevent the growth of unwanted microflora. It is therefore recommended that
antibiotic susceptibility testing should be conducted to identify the antibiotics that can be added to the culture media to suppress the growth of the competing microflora of Campylobacter.

Keywords: 16s rRNA; Acinetobacter sp; gene sequencing; Modified charcoal-cefoperazone-deoxycholate agar (mCCDA)

Effect of Hypothyroidism with Obesity in Male Infertility

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Introduction: Worldwide, nearly 48 million (15%) couples and 186 million people suffer from infertility. Infertility is commonly assumed to be a feminine issue, although 30% of infertility is due to male reproductive system issues. Few studies have found that hypothyroidism and obesity affect male fertility individually, but none have examined male infertility in hypothyroidism with obesity condition. **Objectives:** The objective of this study is to investigate the effect of hypothyroidism and obesity on male reproductive functions and whether thyroxine replacement reverses the effect. **Methodology:** ICR male mice have been divided into five groups i.e., Control, Hypothyroidism, Obese, Hypothyroidism with obese, and Hypothyroidism with obese group supplemented with thyroxine. Mice's body weight was measured. Hypothyroidism and obesity have been confirmed by serum thyroxine and leptin level evaluation. Mice were sacrificed and cauda epididymis and testis were collected for further analysis. **Results:** Mice body weight and serum leptin levels were significantly increased in the Obese and hypothyroid obese groups whereas serum thyroxine levels significantly decreased in hypothyroid, obesity with the hypothyroid group. Sperm count between groups was not significant, but abnormal sperm morphology, vitality, HOS, and DNA integrity have been found affected in the hypothyroid, obese, and hypothyroid obese groups, but thyroxine administration could reverse the effect. Altered levels of spermatogenic and steroidogenic markers have also been found in groups in comparison to control and surprisingly, the effects have been restored upon administration of thyroxine. **Conclusion:** Our findings suggested that hypothyroidism and obesity condition adversely affect sperm quality which may lead to infertility. Moreover, altered spermatogenic and steroidogenic marker expression indicates that hypothyroidism with obesity not only affects sperm quality but also affects spermatogenesis. Administration of thyroxine may improve the condition.

Keywords: Male infertility, hypothyroidism, obesity, thyroxine, sperm quality

Antiviral Activity of Polysaccharide Fraction Isolated from Medicinal Mushroom *Ganoderma neo-japonicum* Imazeki Against Enterovirus A71

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Introduction: Enterovirus A71 (EV-A71)-associated hand, foot and mouth disease (HFMD) outbreaks have been frequently reported in the Asia Pacific countries. Following the near-complete eradication of poliovirus, EV-A71 has been recognized as an important neurotropic enterovirus that causes fatal neurological complications. To date, there are still no licensed antiviral agents available to ameliorate EV-A71 infection. We have previously reported a crude aqueous *Ganoderma neo-japonicum* Imazeki (GNJI) extract (S2) demonstrated potent antiviral activity against EV-A71. GNJI is a medicinal mushroom that can be found in several Asian countries, including Malaysia. Recently, polysaccharides isolated from other *Ganoderma* species mushrooms were reported with antiviral activity. Therefore, we hypothesized that polysaccharide is one of the bioactive components present in S2. **Objectives:** This study aims (1) To identify the antiviral activity of the S2 polysaccharide fraction, and (2) To determine the bioactive composition of S2 and the polysaccharide fraction. **Methodology:** The crude polysaccharide fraction (S2-PG) was obtained by precipitating from S2 with 90% ethanol. A post-infection treatment antiviral assay was performed to compare the antiviral activity of S2-PG and S2 on human primary oral fibroblast (HPOF) cells. The total glucan, phenolic (TPC), carbohydrate and protein content of S2 and S2-PG were determined using standard biochemical assays. **Results:** S2-PG (1.25 mg/ml and 2.5 mg/ml) significantly reduced the virus titer of EV-A71-infected HPOF cells in a concentration-dependent manner. The S2-PG fraction has a higher total amount of carbohydrate (45.78 ± 1.871 g/100g) and glucan (19.5% w/w) than S2. β-glucan is the major glucan component as compared to the α-glucan. The total protein and TPC were significantly lower in the S2-PG fraction compared to S2. **Conclusion:** In conclusion, our findings have suggested that β-glucan polysaccharide could be one of the vital bioactive compounds responsible for the antiviral activity demonstrated by S2. This GNJI could be further developed into a promising antiviral agent against EV-A71.

Keywords: Hand, foot, and mouth disease, *Ganoderma neo-japonicum* Imazeki, antiviral, enterovirus A71, polysaccharide

Comparative Analysis of HPLC-UV-DAD Methods for Rapid, Effective and Economical Fucoxanthin Quantitation

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Fucoxanthin, a unique marine carotenoid found in brown algae, holds promise as a health supplement for improving conditions of metabolic syndrome through enhancing insulin sensitivity and secretion. However, existing quantification methods for this pigment lack technical and techno-economic optimization. This study aims to identify a high-performance liquid chromatography (HPLC) method that efficiently and economically quantifies fucoxanthin. Five HPLC methods from literature were adapted and customized for quantification using standards and samples from various algae species. Comparative analysis focused on performance aspects (linearity, repeatability, time efficiency) and cost-effectiveness. The findings reveal that a simple isocratic method utilising aqueous methanol, outperforms other approaches in terms of both performance and cost, enabling fucoxanthin identification within 5 min. Notably, this method demonstrates superior separation of fucoxanthin from other compounds, utilizes minimal organic solvents, and incurs a low cost of RM5.70 per HPLC analysis sample. This study offers a refined method that can be employed by the functional food industry to produce cost-effective, high-quality fucoxanthin products for consumers.

Keywords: Fucoxanthin, quantitation, HPLC-DAD, method performances, economical evaluation, quality assurance and control.

What Phytochemicals Contribute Significantly to the Antioxidant and Anti-inflammatory Activity of Tiger Milk Mushroom, *Lignosus rhinoceros*?

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Tiger milk mushroom, Lignosus rhinocerus supplementation is proven to effectively improve respiratory health by halting the prolonged inflammation and improving antioxidant status. However, the main contributors to the antioxidant and anti-inflammatory properties of this medicinal mushroom are not well validated yet. The current study is aimed to isolate and identify the primary bioactive compounds that contribute to the antioxidant and anti-inflammatory properties of Lignosus rhinocerus. The percentage of yield of derived fractions from crude ethanolic extract (CEE) prepared by 70% ethanol, i.e. aqueous fraction (AQF), ethyl acetate fraction (EAF) and butanol fraction (BUF) was ranged from AQF>BUF>EAF. The total phenolic content was significantly higher in BUF while EAF exhibited the highest total saponin content ($p < 0.05$). Through multiple antioxidant assays, EAF and BUF exhibited higher antioxidant activity than CEE and AQF, except for iron chelating activity. This study shows that the antioxidant activity of Lignosus rhinocerus is highly contributed by the phenolic composition and saponin ($p<0.05$). While for anti-inflammatory assay, all fractions show no significant difference in inhibiting heat-induced protein denaturation, suggesting that there is a synergistic effect between different compounds that contributes to the anti-inflammatory properties ($p < 0.05$).

Keywords: Tiger milk mushroom, Lignosus rhinoceros, saponins, phenolic compounds, antioxidant, anti-inflammatory

MONASH INITIATE 2023

25 - 26 October 2023

Translating Research into Practice: Revolutionizing healthcare delivery and outcomes

PRESENTERS CLINICAL PHARMACY & PHARMACY PRACTICE

Oral Presenters		
Date: 25 October 2023 (Wednesday)		
ID	**Presenters**	**Time**
OP-CP-01	**Ms Roheena Zafar** Comparative Analysis of Potential Drug-Drug Interactions in Public and Private Hospitals Among Chronic Kidney Disease Patients in Khyber Pakhtunkhwa: A Retrospective Cross-Sectional Study	2:00 PM
OP-CP-03	**Dr Maseera Ahmedi** A Study On Usage Pattern Of Insulin Among Diabetic Patients With Or Without Thyroid Disorders	2:15 PM
OP-CP-04	**Mohd Farizh Che Pa** Predictors of Virological Failure among Patients on Antiretroviral Therapy	2:30 PM
OP-CP-05	**Fina Aryani** A Study on Behavioral Analysis of Drug Information Provision by Pharmacy Staff on Gastritis Self-Medication in Pharmacies in Pekanbaru	2:45 PM
OP-CP-06	**Mr Sunil Shrestha** Impact of Pharmacist-Led Intervention on Pain-Related Outcomes: An Umbrella Review of Published Systematic Reviews	3:00 PM
OP-CP-07	**Ms Nur Shahirah Mohd Yasin** Investigation into Educational Content in Developing of an Interactive multimedia-based application for Type II Diabetes Mellitus Patients	3:15 PM

Comparative Analysis of Potential Drug-Drug Interactions in Public and Private Hospitals Among Chronic Kidney Disease Patients in Khyber Pakhtunkhwa: A Retrospective Cross-Sectional Study

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Introduction: Chronic kidney disease (CKD) is a significant public health challenge due to its rising incidence, mortality, and morbidity. Patients with kidney diseases often suffer from various comorbid conditions, multiple prescribers and concomitant use of several drugs is often imposing increased risk of drug drug interactions making them susceptible to potential drug-drug interactions. Inappropriate prescriptions for CKD patients and their consequences in the form of potential drug-drug interactions are a major challenge in Pakistan. **Objective:** To compare the incidence of potential drug-drug interactions (pDDIs) and their risk factors among public and private sector hospitals in Khyber Pakhtunkhwa, Pakistan. **Method:** A retrospective cross-sectional study design was conducted to compare potential drug-drug interactions among public and private sector hospitals from January 2022 to December 2022. All adult patients aged 18 years and above, of both genders, who currently been diagnosed with chronic kidney disease (including all stages of CKD) were included. Data of the CKD patients admitted to the nephrology units of public sector hospital was obtained from manual medication orders while in private sector hospital, data was extracted from electronic medication order and administration record (MOAR). The evaluation of pDDIs was carried out with the help of Lexicomp UpToDate®, which classifies pDDIs, based on interaction risk rating, level of severity, reliability rating and level of documentation based on the availability of scientific evidences.

Results: A total of 358 patients' data was retrieved; with n=179 from each hospital. However, due to incomplete data, n=4 patients (n=2 in each hospital) were excluded from the final analysis. The majority of patients in the public hospital were male (74%), while in the private hospital, 58.8% were male. The highest percentage of patients in the public hospital (46.9%) were in the age group of 41-60 years, whereas in the private hospital, 48.0% were in the age group of more than 60 years. The maximum hospital stay in the public hospital was higher compared to the private hospital, with 57.1% staying for 3-4 days, while in the private hospital, 40.1% stayed for less than 2 days. The prevalence of pDDIs was found to be significantly higher in private hospitals (84.7%) than in public hospitals (26.6%) and patients in public hospitals having more comorbidities compared to those in private hospitals. The majority of pDDIs (79.0%) were of moderate severity, and a significant number of patients also experienced major pDDIs. In the private hospital, univariate analysis revealed a statistically significant association between pDDIs and patients aged 41–60 years (OR= 5.6; p=0.008), a hospital stay of 3-4 days (OR= 2.9; p=0.038), and a hospital stay of >4 days (OR=3.2; p=0.048). Patients admitted to the private hospital were also significantly more likely to be prescribed a higher number of drugs (OR=1.2; p=0.009). Most pDDIs had fair documentation in both public and private hospitals. An increase in the number of prescribed drugs was identified as an independent risk factor for pDDIs in both private and public hospitals. **Conclusion:** The prevalence of pDDIs was higher among CKD patients at private hospitals, while most of the pDDIs were of moderate severity. A considerable number of patients also experienced major pDDIs. The risk of experiencing pDDIs was found to be higher in older patients and among those prescribed a higher number of drugs.

Keywords: Comparative analysis; Drug-drug interaction; Private and public hospital; Polypharmacy; Documentation of drug interactions.

A Study On Usage Pattern Of Insulin Among Diabetic Patients With Or Without Thyroid Disorders

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Introduction: Thyroid dysfunction and diabetes mellitus are closely linked. Several studies have documented the increased prevalence of thyroid disorders in patients with diabetes mellitus and vice versa. Untreated thyroid dysfunction can impair the metabolic control of diabetic patients, and this association can have significant repercussions on the outcome of both disorders. **Objectives**: To study the prevalence of thyroid disorders among diabetic patients and evaluate insulin usage patterns among diabetes mellitus patients. During the study, it was also intended to report any drug-related effects among these two populations. **Methodology**: A cross-sectional observational study with simple random sampling was conducted in a tertiary care hospital over 6 months. In this study, Diabetic patients with or without thyroid disorders of both genders of all age groups were included and those patients not willing to participate or who have discontinued insulin and are on OHA's were excluded. **Results**: A total of 190 diabetic patients were included in this study out of which 149 patients did not have thyroid. In our study, patients were predominantly (117) females. About 21.85% of insulin was prescribed to thyroid patients compared to 78.1% of insulin to non-thyroid patients. About 24.6% of thyroid patients have more than 10% HbA1c values compared to 75.3% of non-thyroid patients. This shows that thyroid patients are better at maintaining their HbA1c values. On the day of admission (DOA), a high GRBS level of more than 200 mg/dl was observed in a larger proportion of non-thyroid patients (55.78%) compared to thyroid patients (15.78%). Similarly, on the day of discharge (DOD), a higher incidence of GRBS levels exceeding 200 mg/dl was predominantly seen in non-thyroid patients (38.42%) compared to thyroid patients (8.42%). **Conclusion**: Overall, during the study, it was observed that thyroid patients were better at maintaining their sugar levels.

Keywords: Diabetes Mellitus, Thyroid disorders, Insulin usage pattern

Predictors of Virological Failure among Patients on Antiretroviral Therapy

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Introduction: Virological failure among the patients on antiretroviral therapy is a significant challenge in treating HIV patients. **Objective**: To identify predictors of virological failure among HIV patients started on antiretroviral therapy. **Methods**: A multicentre retrospective cohort study was conducted in Hospital Sungai Buloh, Selangor and Hospital Tuanku Ja'afar, Seremban, Negeri Sembilan. Adult patients aged 18 years and above were selected using a simple random sampling method. Data from January 2010 to December 2020 were retrieved from patient's medical record. Patients with viral load result >1000 copies/ml in two consecutive results at least 3 months apart were categorized as virological failure. The model fitted and multivariate logistic regression analysis were performed with 95% confidence level and p values < 0.05 were taken as statically significant. **Results**: From the total of 355 patients were recruited in this study, 92 patients (25.9%) were considered virological failure. Virological failure was predicted by history of non-adherence (odds ratio (OR) = 14.046, 95% confidence interval (CI): 4.130-47.776), history of missed appointment (OR = 4.909, 95% CI: 1.984-12.150), social support (OR = 0.247, 95% CI: 0.065-0.937 and use of reminder (OR = 0.100, 95% CI: 0.038-0.264). **Conclusion**: Predictors of antiretroviral virological failure were patients with history of non-adherence, history of missed appointment, poor social support and not using reminder. Continuous patient education is important factors in delaying HIV virological failure.

Keywords: HIV, antiretroviral, predictors, virological failure.

A Study on Behavioral Analysis of Drug Information Provision by Pharmacy Staff on Gastritis Self-Medication in Pharmacies in Pekanbaru

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Introduction: The provision of drug information by pharmacy staff in self-medication is very important to prevent the occurrence of medication errors so that it could achieve the rational self-medication practices. **Objectives:** This study aims to analyze the provision of drug information behavior by pharmacy staff including pharmacists and pharmacy technicians in gastritis self-medication service at retail pharmacies in Pekanbaru, Indonesia. **Methodology:** This research was observational. The study population consisted of 90 pharmacy staff members, comprising 45 pharmacists and 45 pharmacy technicians. The sampling procedure employed was purposive sampling, guided by the criteria of individuals involved in providing care to gastritis patients, as delineated by the study scenario. The assessment tool utilized for data collection was a drug information provision checklist. This checklist was developed in accordance with the regulations set forth by the Ministry of Health of the Republic of Indonesia. The assessment of drug information provision was carried out using a Likert scale evaluation approach. The category of providing of drug information is divided into 5, very poor (0-20%), poor (21-40%), good enough (41-60%), good (61-80%) and very good (81-100%). **Results:** The results showed that there were no differences in the provision of drug information between pharmacists and pharmacist technicians with p value=0.00 ($p<0.05$). Based on the drug information provision checklist, it was known that pharmacists and pharmacist technicians provided of drug information only when asked by patients. The category of drug information by pharmacists are 46% (good enough) and pharmacy technicians are 37% (poor). **Conclusion:** The provision of drug information in gastritis self-medication service by pharmacist at retail pharmacies in Pekanbaru, Indonesia was found better than pharmacy technicians.

Keywords: Gastritis, Pharmaceutical technicinas, Pharmacist, Providing drug information, Self-medication

Impact of Pharmacist-Led Intervention on Pain-Related Outcomes: An Umbrella Review of Published Systematic Reviews

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Introduction: Pain is a pervasive and challenging healthcare issue, affecting millions worldwide. Addressing pain management effectively is becoming increasingly important in contemporary healthcare delivery. **Objective**: To systematically review published systematic reviews (SRs) examining the impact of pharmacist interventions on pain-related clinical, humanistic and economic outcomes. **Methods**: A review was conducted by searching the literature from six electronic databases [APA PsycINFO, Ovid MEDLINE(R), Embase, Cochrane Central Register of Controlled Trials, CINAHL, Scopus and DARE] from their inception to June 2023. Only review articles published in English were included. Two independent reviewers screened the titles and abstracts of the studies for selection based on the inclusion/exclusion criteria. The methodological quality of the studies was also assessed. **Results**: From a total of 2055 titles retrieved, 11 SRs reporting on the effectiveness of pharmacist-led pain management interventions were included. They covered a range of strategies, including educational sessions, medication reviews and adjustments, and multi-component interventions aimed at addressing various facets of pain management. The findings indicated that pharmacist-led interventions were effective in clinical outcomes (decreasing pain intensity and achieving pain relief, better pain medication management and adherence, identification and counteracting adverse drug reactions and drug-related problems, improved physical functioning and mental health, decreased length of stay and increased) and humanistic outcomes (better confidence among healthcare providers, healthcare utilization and quality of life, patient satisfaction as well as chemotherapy knowledge of cancer patients). The economic impact of pharmacist-led interventions was also investigated in four SRs. Two reviews reported statistically significant cost savings associated with pharmacist-led interventions. However, one study reported that pharmacist-led interventions were more expensive than usual care. **Conclusions**: Our findings suggest that pharmacist-led pain management interventions effectively improve clinical, humanistic, and economic outcomes, which can significantly reduce the burden of pain management on healthcare systems.

Keywords: Pharmacist, pain, Systematic review, umbrella reviews

Investigation into Educational Content in Developing of an Interactive multimedia-based application for Type II Diabetes Mellitus Patients

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Introduction: The development of interactive multimedia-based applications has become increasingly important in providing effective health education to Type 2 Diabetes Mellitus (T2DM) patients. Understanding the educational content required for such applications is crucial for designing a user-friendly and impactful tool for T2DM management. **Objectives:** This study aims to investigate the educational content necessary for developing an interactive multimedia-based application specifically tailored for T2DM patients. **Methods**: Semi-structured interviews were carried out with a sample of T2DM outpatients (n=16) at a tertiary referral university hospital in Kuala Lumpur between October 2022 and January 2023. The interviews were recorded, transcribed, and subjected to thematic analysis. **Results**: The majority of participants had been diagnosed with T2DM for less than ten years. The thematic analysis identified several key aspects related to the educational content required for the multimedia-based application. These include preference for educational material, essential content and interactive features. They proposed a discussion area that would allow them to communicate and receive immediate advice from healthcare professionals, thus eliminating the need for frequent hospital visits. **Conclusion**: The findings of this study highlight the significance of interactive multimedia-based applications in providing health education for T2DM patients. The identified essential content areas, such as insulin dose modification, hypoglycaemia management, and dietary recommendations, can inform the development of effective educational materials. The app developers should also include doctors, pharmacists, nutritionists, and psychologists who are experts in their fields to add more behavioural modification techniques in applications that assist patients.

Keywords: Educational material, diabetes mellitus, multimedia applications, health education, patient communication

Poster Presenters	
ID	**Presenters**
PP-CP-01	**Prof Dr Sajeeth C. I.**
	Quality of Life Among Women with Vulvovaginal Candidiasis in a Tertiary Care Centre in India
PP-CP-02	**Dr Wei Wen Chong**
	Development and Validation of an Instrument to Measure Patient-Centered Communication among Malaysian Hospital Pharmacists

Quality of Life Among Women with Vulvovaginal Candidiasis in a Tertiary Care Centre in India

Dr. C. I. Sajeeth[1], Dr. V.Karthikeyan[1], Irene V.R[2*], Dr. Sabitha.J[3]

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Introduction: Vulvovaginal candidiasis (VVC) is a frequent, irritating, and recurrent infection. These infections create a danger to the well-being of the women and have a detrimental impact on their quality of life (QoL). **Objective:** The aim of this study is to assess the quality of life (QoL), among women with VVC.The study design: prospective study design. **Methodology**: Study site: Paalana hospital of medical sciences, Study duration: 7month.The sample size n=130. Severity of VVC is determined by using VSQ questionnaire (Vulvovaginal symptom questionnaire) and Vulvar disease quality of life index (VDQoL questionnaire) used to assess the quality of life. Statistical analysis was carried out by using Graphpad prism software, un-paired student t-test to determine P-value between pre-treatment and post-treatment. **Result & Discussion**: In this study, 130 cases were collected; among the collected data; VVC was more common in women in the reproductive age range. Quality of life (QoL) is determined by VDQoL with sub-domains like (Nil effect, Mild, Moderate and Severe, Very severe effect). After the course of treatment, their QoL is determined by administering the same questionnaire to the patients. By comparing the Pre-test and Post-test, patients with Nil effect (p-value 0.66), Mild effect ($p<0.0001$), & Moderate effect ($p<0.0001$). **Conclusion**: Based on the findings of the study, it can be concluded that vulvovaginal candidiasis have a negative impact on the patient's quality of life. The majority of women having a mild effect of VVC on their QoL.

Keywords: Vulvovaginal Candidiasis (VVC), Prevalence, Candida albicans, VSQ, VDQoL

Development and Validation of an Instrument to Measure Patient-Centered Communication among Malaysian Hospital Pharmacists

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Introduction: Effective communication that prioritizes patient-centered care is important in all healthcare settings, including pharmacy. Currently, there is a lack of comprehensive tools to measure patient-centered communication (PCC) among pharmacists in Malaysia. **Objectives**: To develop an instrument that can measure PCC in Malaysian hospital pharmacists, and to establish the validity and reliability of the instrument. **Methodology**: A multi-step process was utilized to develop and validate the communication assessment instrument. Firstly, a comprehensive literature search was conducted to determine the core elements of the PCC instrument. Face and content validity were established by an expert panel of healthcare communication experts and hospital pharmacists. Pilot testing was then conducted using previous audio data of pharmacist-simulated patient communication. The resulting scores were compared to the Four Habits Coding Scheme (FHCS) to establish concurrent validity. Internal consistency, intra-rater reliability and inter-rater reliability were also assessed. **Results**: The final instrument consisted of 29 items rated on a three-point scale, covering six core elements: Building rapport, Exploring patient perspectives, Empathy and compassion, Shared decision-making, Patient education, and Self-efficacy. The total scores from the instrument and FHCS scores were significantly correlated ($p<0.05$). High internal consistency was demonstrated with a calculated Cronbach's alpha of 0.834. Furthermore, intra-rater reliability and inter-rater reliability, assessed using intra-class correlation, were deemed acceptable at 0.673 and 0.679, respectively. **Conclusion**: The developed instrument represents a valid and reliable tool for assessing PCC among hospital pharmacists in Malaysia. It may be useful in identifying communication gaps and evaluating the impact of communication training interventions on pharmacist-patient interactions.

Keywords: Healthcare communication, patient-centered, pharmacist-patient interaction

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LABORATORY ONE STOP SOLUTION

01 Site Assessments
Check site condition & take site measurement

02 Design, Planning & Consultation
Identify client's needs, provide design, planning, consultation, drawing & proposal

03 Furniture Manufacturing
Produce lab furniture, cabinets, fume hoods & many more

04 Supply, Install & Renovation
- Lab Furniture - Custom Item, Gas Piping
- M&E (Electrical and plumbing according to lab requirement)
- Lab Renovation – Flooring, ceiling, partition (PIR, PU, Gypsum), lighting

05 Site Inspection
Ensure everything is in order and project handover

06 After Sales Service & Maintenance
- LEV/ DOE (local authorities submission)
- Consultation on ISO and GMP
- Fume Hood Maintenance
- Any maintenance queries for your lab

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PRESENTERS DIGITAL HEALTH

Oral Presenters		
Date: 25 October 2023 (Wednesday)		
ID	**Presenters**	**Time**
OP-DH-03	**Ms Sharmila Sathianathan** Approaches Used to Identify Health Misinformation on Social Media and Challenges Faced; a Qualitative Study	3:30 PM
OP-DH-04	**Ms Defin Allevia Yumnanisha** Comparing Mobile Teledermoscopy and Self-Screening Applications as the Future Skin Cancer Screening Tools: A Meta-Analysis of Diagnostic Accuracy Studies	4:00 PM
OP-DH-05	**Mr Muhammad Candrika Agyawisnu Yuwono** Delving into the Effects of Digital Meditation: Nurturing Adolescent Mental Health via Mindfulness App and Website Interventions: A Systematic Review and Meta-Analysis	4:15 PM

Approaches Used to Identify Health Misinformation on Social Media and Challenges Faced; a Qualitative Study

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Introduction: Health misinformation, a component of information disorder is information that is not true but is not constructed to ruin or cause harm. Social media caused half of the spread of health misinformation. It is still unclear how the general public identify health misinformation on social media and challenges faced in regards to this. **Objectives**: To explore the approaches employed by the general public in identifying health misinformation on social media and challenges faced in regards to this. **Methodology**: This was an exploratory qualitative study. Individual, semi-structured interviews were conducted with 22 people from the general public in Malaysia. Audio-taped interviews were transcribed verbatim and imported into Atlas Ti software. A thematic analysis method was used to identify themes from the qualitative data. **Results**: Respondents described the approaches they used to identify health misinformation on social media were looking at the characteristics of messages and the source of the message. They deemed messages were misinformation if they were illogical and exaggerated. Respondents believed in messages from the government and questioned messages that contradicted credible sources. Respondents perceived that anyone could spread misinformation with a tendency from older people, those with lower education background and from rural areas. Messages that were viral on social media and were long posed a difficulty in accuracy determination. Furthermore, misinformation that contained anecdotes and testimonials were challenging to differentiate especially if they contained academicians or health care workers endorsing them. **Conclusion**: This study allows us to understand the areas that pose a challenge in identification of health misinformation on social media faced by the general public. Interventions can be designed that allows a targeted approach to this problem.

Keywords: Approaches, health misinformation, social media

Comparing Mobile Teledermoscopy and Self-Screening Applications as the Future Skin Cancer Screening Tools: A Meta-Analysis of Diagnostic Accuracy Studies

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Introduction: Despite being one of the fastest-growing cancer cases worldwide, especially in Asia, skin cancer remains being frequently misdiagnosed or left untreated due to society's lack of awareness. Teledermatology tools, including mobile teledermoscopy and self-screening applications, are utilized to address this gap. This research aims to provide crucial insights into the effectiveness of aforementioned tools, offering valuable information to healthcare professionals, policymakers, and the public. Ultimately, the study's findings may precede the widespread adoption of innovative technologies, transforming how skin cancer is screened, diagnosed, and managed, thus contributing to the early detection and improved prognosis of this life-threatening disease. **Methodology**: The study systematically reviewed relevant clinical trials within the past 10 years from five databases (PubMed, Embase, ScienceDirect, Wiley, ProQuest) according to the PRISMA guideline. Included documents were assessed for risk of bias using QUADAS-2 and statistically analyzed with Meta-DiSc. The diagnostic accuracy for skin cancer was reported using sensitivity, specificity, true positive, true negative, false positive, and false negative. **Results**: The authors screened 805 titles and abstract, with eleven studies included in the analysis. The overall study quality assessed by the QUADAS-2 resulted in six "unclear" and five "low" risks of bias studies. Among 7.863 skin lesions, mobile teledermoscopy exhibited strong potential for detecting skin cancer, with a sensitivity of 94% (95% CI: 91-96%), specificity of 91% (95% CI: 90-91%), and Area Under the Curve (AUC) of 0.9605. In comparison, self-screening applications had lower sensitivity of 89% (95%CI: 0.86-0.92), specificity of 73% (95%CI: 0.70-0.76), and an AUC of 0.903 than mobile teledermoscopy. **Conclusion**: Mobile teledermoscopy showed higher accuracy in detecting skin cancer compared to self-screening applications. However, further research is required to evaluate other teledermatology methods, such as real-time consultations without dermoscopy, and to compare the cost-effectiveness and applicability of each tool.

Keywords: Teledermoscopy, mobile application, skin cancer

Delving into the Effects of Digital Meditation: Nurturing Adolescent Mental Health via Mindfulness App and Website Interventions: A Systematic Review and Meta-Analysis

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Introduction: Over 50% of adolescents undergo depression, stress, and anxiety. This is associated with some factors, including, age, separation from parents and friends, academic and organizational demands, and financial issues. Neglecting these concerns can lead to further physical and psychological issues. Mindfulness meditation refers to various types of mindfulness based psychotherapy, which are effective treatments to reduce stress and depression. Unfortunately, this solution may be costly and time-consuming. Therefore, mindfulness meditations, which are accessible through apps and websites, provide affordability, adaptability, and enhanced privacy. **Objective**: To evaluate the effect of mindfulness app and website interventions on adolescent mental health. **Methodology**: This study followed the Preferred Reporting Item for Systematic Review and Meta-analysis (PRISMA). We systematically searched through PubMed, Scopus, Cochrane, Wiley, and ProQuest until August 22, 2023. Critical appraisal of included studies was performed with Cochrane Risk of Bias 2.0. Pooled mean, SD, and p-value were analyzed using a random-effects model. **Results**: Thirty-seven randomized studies yielding 5667 participants are included. Mindfulness app and website interventions showed a beneficial effect on depression (SMD: -0.71[0.93,-0.49], p<0.001), anxiety (SMD: -3.29 [-4.15, -2.43], p<0.001), stress (SMD: -0.72 [-0.98, -0.45], p<0.001), mindfulness (SMD: 1.20 [0.84, 1.56], p<0.001), and self-compassion (SMD: 0.98 [0.61, 1.34], p<0.001). We further assess a subgroup analysis to find the best duration of intervention and effect differences of intervention before and after COVID-19. **Conclusion**: Despite COVID-19 pandemic challenges, our meta-analysis indicates that digital mental health interventions for adolescents significantly reduce depression, anxiety, and stress while boosting mindfulness and self-compassion. Optimized intervention durations and best mindfulness practices should be implemented in today's 2 million mental health apps.

Keywords: Application, website, mental health, mindfulness

Poster Presenters	
ID	**Presenters**
PP-DH-01	**Dr Adliah Binti Mhd Ali**
	Machine Learning Methods in Determining Chronic Disease Patients' Belief Towards Medication and Associations with Medication Wastage

Machine Learning Methods in Determining Chronic Disease Patients' Belief Towards Medication and Associations with Medication Wastage

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Introduction: In Malaysia, the public healthcare system is heavily subsidize by the government and led to unnecessary cost spent. The study employs data analytics techniques to predict patients' related factor who were more likely to waste their subsidized medication and is important to evaluate the applicability of this method in the future. This study evaluate the suitability of machine learning methods in elucidating the high-risk group of chronic disease patients who were more likely to waste their subsidized medications.

Methodology: One thousand questionnaires were distributed to chronic disease patients receiving subsidize medications in six government healthcare settings in Malaysia. The questionnaire consist of patients' demographic characteristics and validated questionnaire on Belief about Medicines Questionnaire (BMQ) by Horne et al and Return and Disposal of Unused Medications (ReDiUM) by Sim et al. Data analytics used for this study were stacked ensemble learning (EL) and Support Vector Machine (SVM). Random Forest (RF), eXtreme Gradient Boosting (XGB) and Naive Bayes (NB) were use as base learners. The test error estimate is define by the root mean square error (RMSE) for evaluation of metric performance. Algorithms tested using the same validation data and SVM variable importance with backward elimination was use to select and rank important variables.

Results: Machine learning models constructed using the selected variables reported RMSE values of 5.144 ($p=0.359$) for best individual base learner (SVM) and 5.246 ($p=0.506$) for stacked EL model. The lower the RMSE, the better the model and its predictions. The Wilcoxon signed ranked test reported that there was no significant difference ($p<0.05$) between the predictions of the machine learning models and the actual scores. The significant variables identified from the SVM variable importance method were education, disease hypertension, BMQ Total Necessity, BMQ Total Concern and BMQ Total Harm. SVM is a set of supervised learning methods used for classification, regression and outlier detection.

Conclusion: Based on the result predicted using machine learning, this promising method may be use in the future to predict high–risk group of chronic disease patients' who were more likely to waste their medications compared to the conventional method.

Keywords: Chronic disease patients, medication wastage, prediction, machine learning

MONASH INITIATE 2023

25 - 26 October 2023

Translating Research into Practice: Revolutionizing healthcare delivery and outcomes

Oral Presenters Date: 26 October 2023 (Thursday)		
ID	**Presenters**	**Time**
OP-PH-01	**Dr Kavita Jetly A/P Jagjit Kumar Jetly** The Mechanism Linking Cigarette Pack Factors, Point-of-Sale Marketing, and Individual Factors with Smoking Intention among School-Going Adolescents	2:00 PM
OP-PH-02	**Ye Shing Lourdes Loh** Price Control and Public Opinion: Investigating External Reference Pricing Perceptions	2:15 PM
OP-PH-04	**Dr Huysean Huot** Knowledge, Attitude and Practice of Antibiotics and Their Associated Factors Among People Living in Phnom Penh, Cambodia	2:30 PM

Oral Presenters		
Date: 26 October 2023 (Thursday)		
ID	**Presenters**	**Time**
OP-PH-05	**Ms Vottey Nara** The Prevalence of Stress, Anxiety, Depression, and Antipsychotic Drug's Use Among University Students in Phnom Penh, Cambodia	2:45 PM
OP-PH-06	**Ms Sidra Sabir** A Comparative Study of Physical Activity in Obese and Non-obese Individuals with Knee Osteoarthritis	3:00 PM
OP-PH-07	**Ms Sydney Tjandra** Where Is Health Fair? A Bibliometric Study Quantifying Global Health Disparities	3:15 PM
OP-PH-03	**Ms Zi Rong Chia** Interview to Understand the Demands That Lead to Burnout and Motivations Among Malaysian Community Pharmacists: A Cross-Sectional Study	3:30 PM

The Mechanism Linking Cigarette Pack Factors, Point-of-Sale Marketing, and Individual Factors with Smoking Intention among School-Going Adolescents

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Introduction: One of the most preventable causes of death is diseases caused by tobacco usage. In Malaysia, cigarette smoking among adolescents has not reduced over the years. Exposure to nicotine during adolescence can affect brain development and cause many health risks. **Objectives:** This study aimed to explore mechanisms linking cigarette pack factors, point-of-sale marketing, and individual factors (psychological reactant trait) to predict smoking intention among school-going adolescents. **Methodology:** This was a cross-sectional study conducted among six urban secondary schools in Selangor. A multi-stage simple random sampling procedure was done to select district education offices, schools, classrooms, and adolescents aged 13 to 16. A pre-tested and validated self-administered questionnaire consisted of personal factors (demographic status), family factors (parent education, parent smoking), social factors (peer smoking), psychological factors (psychological reactant trait), recall exposure to the point-of-sale marketing, cigarette pack factors (pack appraisal of the conventional pack, pack receptivity of conventional pack, pictorial warning negative affect) and the smoking intention was used. Data analysis for structural equation modelling was done using SMART-PLS v3.2.8. **Results:** A total of 386 adolescents fulfilling the inclusion criteria participated. The structural model controlled by personal, family, and social factors showed pictorial warning message reactance (β=0.153, *p*=<0.001), pack receptivity of conventional pack (β=0.297, *p*=0.004), and psychological reactant trait (β=0.174, *p*=<0.001) was positively related to smoking intention. Pictorial warning negative affect (β=-0.153, *p*=0.001) was negatively related to smoking intention. Psychological reactant trait was positively related to pictorial warning message reactance (β=0.340, *p*=<0.001). Pictorial warning message reactance also positively mediates the relationship between psychological reactant traits and smoking intention (β=0.05, *p*=0.001). The model has strong predictive power.—**Conclusion:** The finding revealed cigarette pack factors and psychological reactant trait is essential in predicting smoking intention. Hence, policymakers should consider these factors in developing smoking combat policies among adolescents.

Keywords: Cigarette pack factors, point-of-sale marketing, smoking intention

Price Control and Public Opinion: Investigating External Reference Pricing Perceptions

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Introduction: The Malaysian government conducted two public consultations in 2021 on the implementation of External Reference Pricing (ERP). ERP is a pricing system that sets local pharmaceutical prices by comparing them with international market rates from a selection of countries. However, certain aspects of stakeholders such as views of the general public in both public consultations were absent. This research is part of a larger study on medicine price controls that aims to analyse the views of key stakeholders which are greatly underrepresented in the policy evaluation process. **Methods:** Data were collected via 16 semi-structured interviews with pharmacists (n=2), medical doctors (n=2), policymakers (n=1), academicians (n=2), NGO policy advisors (n=1), pharmaceutical representatives (n=2), and the general public (n=6). Thematic analysis using NVivo v.12 informed by a theoretical perspective of interpretivism was conducted to capture the key themes derived from transcribed data. **Results**: Our findings are categorised into (i) public sentiments on the implementation of ERP, (ii) the challenges and shortfalls of the current Malaysian healthcare system, and (iii) recommendations from key stakeholders in addressing the said challenges. The results demonstrated mixed reactions to the implementation of ERP. Both policymakers and medical doctors have maintained a stance of neutrality, yet advocates for the implementation of ERP should recognise the potential complexities and challenges associated with the adoption of ERP. The general public together with academicians and NGO policy advisors, has shown great support for ERP. In contrast, pharmaceutical representatives and pharmacists are less enthusiastic about the policy, as ERP may affect the industry's profitability and the subsequent R&D into new drugs. **Discussions and Conclusion**: Implementing medicine price controls has remained a significant challenge in Malaysia, and its negotiation has reached an impasse. As such, the ERP policy entails pharmaceutical companies to make necessary concessions to improve the affordability of medicines. It is essential for the government to implement adaptable pricing structures and facilitate transparent communication between the pharmaceutical industry and the general public. Therefore, there is a need to revise the current policy practices and involve necessary stakeholders in designing a feasible health policy for all.

Keywords: Public Health, Health Policy, Pharmaceutical Pricing Policy, External Reference Pricing

Interview to Understand the Demands That Lead to Burnout and Motivations Among Malaysian Community Pharmacists: A Cross-Sectional Study

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Introduction: Malaysian community pharmacists experience burnout that leads to reduced job satisfaction and compromised patient care. There is currently no research on burnout among Malaysian community pharmacists, emphasizing the need for urgent attention. **Objective**: Our main objectives are to identify the factors that contribute to burnout, motivations, and engagement among Malaysian community pharmacists. The secondary aim includes examining the burnout status and job satisfaction level of the participants. **Methodology**: Between January to April 2023, a mixed-methods cross-sectional study was conducted among 30 selected Malaysian community pharmacists using purposive sampling. This approach involved both qualitative and quantitative data collection. The Jobs-Demands Resources (JDR) model was used to identify the factors contributing to burnout and motivation among participants. Participants were asked to rate the burnout status and job satisfaction on a likert scale of 1 to 5. Thematic analysis with both inductive and deductive approaches was performed on the interview data by using the NVivo software to derive codes, themes, and domains. Intercoder reliability tests (ICR) using Cohen's kappa were used to assess the agreement between 2 coders, to achieve kappa value >0.75. Data analysis is continued until data saturation, marked by 0% new information. **Results**: Data saturation reached at the 12th interview with a total of 36 codes. The analysis revealed three domains: job demands, job resources, and personal resources. The codes 'Multitasking and heavy workload', 'Undersupport, underappreciation from government', 'Colleagues and management support', 'Hobby and leisure activities' appear the most which are in 11 files out of 12 transcripts. Besides, Malaysian community pharmacists experience moderate burnout (mean score: 2.33, 95% CI: 1.77 to 2.89) but report high job satisfaction (mean score: 3.67, 95% CI: 3.33 to 4.01). **Conclusion**: Burnout among Malaysian community pharmacists is a prevalent issue and warrants urgent action. Future research could involve conducting larger quantitative studies with validated tools to enhance comprehension of our study.

Keywords: Burnout, Malaysian community pharmacists, semi-structured interview

Knowledge, Attitude and Practice of Antibiotics and Their Associated Factors Among People Living in Phnom Penh, Cambodia

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Introduction: The inappropriate use of antibiotics is one of the most global health concerns and a major cause of antibiotics resistance. **Objectives:** The aim of this study was to determine the knowledge, attitude and practice (KAP) of antibiotics among people living in Phnom Penh, Cambodia and their associated factors. **Methodology:** A cross-sectional survey was conducted within different area in Phnom Penh, Cambodia by using a convenient sampling in between May 2023 to July 2023. A total 250 respondents were enrolled in this study. The cut-off for the score of attitudes were categorized as negative (0.00-2.50), and positive (2.51-5.00). Knowledge and practice were categorized as low or poor (0.00-0.33), moderate (0.34-0.66), and high or good (0.67-1.00). The data collection was analyzed and reported as the descriptive results. Chi-square test was used to determine the association between sociodemographic and KAP. **Results:** The majority of respondents were male (n=132; 52.8%) and female (n=118; 47.2%). Most participants are from 18 to 28 years old (n=117; 46.8%), the level of education is in bachelor degree (n=149; 59.6%) and university students (n=111; 44.4%). Most participants have moderate knowledge (n=165; 66%), positive attitude toward antibiotics (n=240; 96%), and high practice of antibiotics (n=118; 47.2%). The Chi-square test showed significant relationship between education and attitude, education and practice, and occupation and practice toward antibiotics use, all with a p-value <0.01. **Conclusion:** These results demonstrate the ongoing need to enhance understanding and improve awareness of people living in Phnom Penh toward taking antibiotics in order to avoid antibiotic resistance, which is a public health risk. People with low KAP should also be given preferential attention in community engagement programs.

Keywords: Knowledge, Attitude, Practice, Antibiotics

The Prevalence of Stress, Anxiety, Depression, and Antipsychotic Drug's Use Among University Students in Phnom Penh, Cambodia

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Introduction: Mental health was deemed essential to human health by the World Health Organization. Stress, depression and anxiety (SAD) are common mental health disorders which are reported to be increased among college/university students and they can interfere with learning ability, affect academic performance and impair practice performance. **Objectives**: This study aims to determine the prevalence of SAD and its associated factors, and to improve awareness of health management toward SAD among medical students and non-medical students within 2 universities in Phnom Penh. **Methodology**: An online survey questionnaire was circulated to medical and non-medical students by using google forms. The questionnaire was divided into three parts, including demographic information, potential associated factors and the 21-item Depression, Anxiety, and Stress Scales (DASS-21). A total of 201 respondents were enrolled in this study. Descriptive data and chi-square tests were performed in the study. **Results**: It is found that among 201 university students participated in this survey was female (112, 55.7%), single (191, 95%), and Buddhism (190, 94.5%). The ages were ranged from 17 to 40 years old, with an average of 21.46 ± 2.74. Approximately, students were unemployed (141, 70.1%). Most are from bachelor degree (185, 92%) including pharmacy (42, 20.9%), dentist (34, 16.9%) and bachelor of English (25, 12.4%). Notably, the prevalence of severe and extremely severe depression was 28 cases (13.9%) and 36 cases (17%), respectively. Noteworthy also is the significant prevalence of extremely severe anxiety, recorded at 68 cases (33.8%). Listen to music (47, 23.4%), hanging out with friends (33, 16.4%) and play sports (29, 14.4%) were likely to do in order to manage the mental health problem. Stress was found associated with age ($p<0.05$) and education ($p<0.05$) while depression was only associated with students who have outside work ($p<0.05$). However, only 13 participants (6.46%) were using medication to deal with SAD including psychotic drugs (sleeping pills) (3, 6.03%) and nonpsychotic drugs (10, 20.1%). **Conclusion**: Notably, about one out of seven respondents had severe depression, while one out of three had severe anxiety. This finding suggests the need - of having mental health/support services and mental health prevention intervention at universities.

Keywords: Stress, depression, anxiety, antipsychotic drugs

A Comparative Study of Physical Activity in Obese and Non-obese Individuals with Knee Osteoarthritis

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Introduction: Knee osteoarthritis (KOA) is a debilitating musculoskeletal disease that affects a large proportion of the population. Obesity is a well-known risk factor for KOA and is associated with decreased physical activity. However, there is limited and insufficient data on the impact of obesity on physical activity levels among the KOA population. This study was carried out to comprehensively assess and compare physical activity levels in obese and non-obese individuals with KOA. **Methods:** A cross-sectional study was conducted involving 80 participants recruited from two physiotherapy clinics. Participants were divided into obese and non-obese groups based on their BMI (≥ 23 kg/m² and ≤ 22.9 kg/m², respectively). Physical activity level was measured using the Malay version of International Physical Activity Questionnaire (IPAQ). Both categorical and continuous scores were obtained. Pain severity was included as a covariate and measured using the Visual Analogue Scale (VAS). A one-way ANCOVA was employed to compare the results between the two groups. **Results:** The categorical scoring for the overall study population (N=80) showed that a greater proportion of participants (63.75%) had moderate level of physical activity, while the continuous scoring yielded a mean score of 1974.45 metabolic equivalent of task (MET) min/week**.** A Significant difference in the mean IPAQ scores was found between obese and non-obese groups**.** The adjusted mean score for the obese group (n = 53) was 1720.90 (MET) min/week, and 2472.15 MET min/week for the non-obese group (n=27). **Conclusion**: The considerable discrepancy in mean IPAQ scores between the two groups highlights the potential influence of BMI on activity levels in the KOA population. Further research is needed to unravel the complex relationship between BMI, physical activity, and KOA and provide valuable insights for tailored interventions and improved patient outcomes.

Keywords: Knee osteoarthritis, Physical activity level, Comparative Study

Where Is Health Fair? A Bibliometric Study Quantifying Global Health Disparities

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Introduction: Despite the massive progress in health, various determinants of health, such as income inequality, have led to worse health status. Inequity escalates the likelihood of premature mortality and heightened morbidity. Health is enhanced in equitable societies due to their elevated social cohesion, positive social relationships, and reduced stress levels. The presence of health disparities both among and within countries has led to a focus on enhancing the creation and utilization of global health inequality research in order to enhance the ability to take effective actions. **Objective:** This bibliometric analysis aims to visually represent how knowledge has developed in health inequality research to understand the research landscape and emerging trends regarding health inequalities. **Methodology:** This research utilized bibliometric analysis using metadata from published literature in the Scopus database. The search was conducted on August 27th, 2022, employing the keyword 'Health inequality' and its synonyms. The data was categorized into publication years: pre-COVID-19 (2017–2019) and during COVID-19 (2020–2022). VOSviewer and Biblioshiny were employed for network visualization analysis. Two independent reviewers carried out the selection of frequently occurring keywords and clusters of keyword co-occurrence. **Results:** Metadata from a total of 52761 publications were included for bibliometric analysis, comprised of two groups of datasets namely pre-COVID-19 (n=15842) and during COVID-19 (n=36919). Health disparities, social determinants of health, and health equity were among the top-occurring keywords in studies. Post-COVID-19, a marked rise in health services and systems research calls for governments to reform pandemic preparedness infrastructure and robust systems with more resilience. Studies on health inequalities were mostly reported by authors from the United States (n=28626), United Kingdom (n=5154), and Canada (n=3824); HIC inequity niches including sexual orientation are also identified. **Conclusion:** The dominance of HICs calls for more research from LMICs and LICs, considering their different trends in health inequality.

Keywords: Bibliometric, COVID-19, health inequality, health disparities, lower-middle-income countries

Poster Presenters	
ID	**Presenters**
PP-PH-02	**Ms Nur Khairah Badaruddin**
	Researching Virtual Clinics Implementation: Navigating the Stakeholder Engagement Experience
PP-PH-04	**Dr Carl Lexter B. Tan**
	The COVID 19 Pandemic Effect on Pre-Medical and Medical Students' on Pursuing the MD dream: A Scoping Review
PP-PH-05	**Dr Nurul Aain Binti Ahmad Fauzi**
	Characteristic Profiling in Rheumatoid Arthritis patients achieving low disease activity (LDA)/remission within 12 months of Biologic DMARDs treatment

Researching Virtual Clinics Implementation: Navigating the Stakeholder Engagement Experience

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Introduction: A research study was conducted to assess the implementation of virtual clinics (VC) in public primary healthcare in Malaysia. Engaging stakeholders to secure site approval, establishing rapport, and becoming familiar with the local system are crucial steps preceding the initiation of data collection. Identifying and addressing issues in the early stages of stakeholder engagement ensures a smooth data collection process. **Objectives**: This study aims to reflect on issues encountered by investigators at the early stage of stakeholder engagement at the research sites. **Methodology**: Qualitative content analysis of the observation notes gathered from all the investigators involved in VC research was done. All the investigators were female and possessed > 5 years of research experience. They are medical doctors, research officers or nurses with age between 29 to 50 years old. The data source encompassed discussion and reflective notes from researchers during their engagements with stakeholders from each healthcare facility under three different health state departments. The data were analysed thematically in an Excel sheet. **Results**: Investigators encountered significant challenges in conducting research at multiple sites due to variations in Standard Operating Procedures. Two main themes emerged namely communication (technical instruction) and bureaucratic structure. Under the bureaucratic structure, researchers had to establish tailored arrangements and direct communication with district health offices and clinics, which caused unforeseen delays. Furthermore, communication issues were observed, which were exacerbated by staff turnover at the study sites, resulting in a loss of accountability that disrupted the engagement process. **Conclusion**: This research has identified the communication issues within a bureaucratic structure during stakeholder engagement. Creating a transparent communication platform via a designated liaison can overcome these challenges by promoting synergy between researchers and stakeholders, facilitating the study's feasibility. This study's insights are valuable to guide future research strategies.

Keywords: Virtual clinic, reflective, challenges, engagement, site approval.

The COVID 19 Pandemic Effect on Pre-Medical and Medical Students' on Pursuing the MD dream: A Scoping Review

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Introduction: The COVID-19 pandemic has significantly affected the lives of the population. The pandemic affects not only the healthcare workers but also the potential future healthcare workers, the premedical and medical students. Even though healthcare professionals are in shortage, there has yet to be research on whether this subset of the population wants to pursue the MD dream. **Objectives:** This scoping review aimed to explore whether premedical students still want to continue pursuing their medical degree, as presented in the literature. **Methodology**: The scoping review was guided by JBI methodology on scoping review. A comprehensive search about enrollment, attrition rate, and dropouts of premedical or medical students was conducted in PubMed, Google Scholar, EBSCO host, Cochrane, and Web of Science, following a set of inclusion criteria that is free and available full articles written in English from December 2019 to December 2022. The initial search yielded twenty-six articles (Studies from China = 9; USA = 2; Pakistan = 1; UAE = 1). Thirteen papers were not included (No desired population = 2; No desired concept = 8; Not relevant = 1; Not accessible = 1; Not in English = 1), wherein thirteen journals were accepted, appraised using Critical Appraisal Skills Programme (CASP) checklist for qualitative research, and included in the scoping review. **Results**: Thirteen articles were categorized into different themes (motivators or demotivators) to subthemes (Psychological, Humanitarian, Societal, Scientific, or Extrinsic factors). Common primary motivators in pursuing medicine are helping others and benefiting society (10/13 articles). On the other hand, the main demotivators are fear of contracting the disease and mental stressors (7/13 articles). **Conclusion:** The scoping review showed that motivating factors outnumbered the demotivating factors, as exhibited by 10 of the 13 studies in this scoping review. Thus, even if the pandemic exposed the grueling side of the medical profession, premedical students still want to pursue medicine for the service and benefit of others. Although the results are reassuring, further research on the topic is needed.

Keywords: *COVID-19 pandemic, pre-medical student; medical student; enrollment; dropout; attrition*

Characteristic Profiling in Rheumatoid Arthritis patients achieving low disease activity (LDA)/remission within 12 months of Biologic DMARDs treatment

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Introduction: Biologic DMARDs is a cornerstone of rheumatoid arthritis therapy. This study profiled the characteristics of RA patients treated with biologic DMARDs and achieved low disease activity/remission within 12 months duration. **Methods**: Fifty-five RA patients enrolled between March 2022 to May 2023 were included. Subjects were categorised according to bDMARDs received, i.e., JAKi (Baricitinib, Tofacitinib) or non-JAKi (Adalimumab, Etanercept, Golimumab, Tocilizumab). Subjects were prospectively follow-up at baseline, 1-month, 3-month, 6-month, and 12-month, with HAQ-DI, clinical and laboratory assessment data collected. Thirty-six patients completed for one year duration while nineteen patients dropped out due to adverse events and/or inefficacy. **Results**: Our data demonstrated a median disease duration of 12.5 years (IQR 10.0) with 52.8% subjects was biologic-naïve. Median DAS28-CRP and HAQ-DI scores at baseline were 4.40 (IQR 1.29) and 1.313 (IQR 1.13). Our preliminary analyses showed that at one month of treatment initiation, DAS28-CRP LDA or remission was significantly achieved by the JAKi users (59.1%) as compared to the non-JAKi users (15.4%) ($p<0.05$). At 12 months of treatment however, no significant difference was observed ($p>0.05$) between these groups. A Wilcoxon-signed rank test showed that at 12 months of treatment, the non-JAKi group elicited a statistically significant improvement in all parameters measured: 28-TJC, 28-SJC, VAS (mm), PGA (mm), EGA (mm), HAQ-DI and DAS-28-CRP ($p<0.05$). Similar improvements are noted at completion among JAKi users, except CRP level ($p=0.07$). Comparisons of baseline, 1-month, 3-month, 6-month and 12-month values among JAKi and Non-JAKi users showed that most significant improvements in parameters measured occur only for the first month of treatment. **Conclusion**: We observed significant clinical improvement in term of clinical composite measures and DAS-28-CRP in RA patients treated with JAKi within one month of treatment. However, the clinical improvement was comparable after 12-month treatment in this RA population irrespective of biologic received.

Keywords: RA, bDMARDs, remission, disease activity

Multidisciplinary National Seminar Proceedings

"Recent Trends of Collecting, Analyzing and Sharing Qualitative Research Data"

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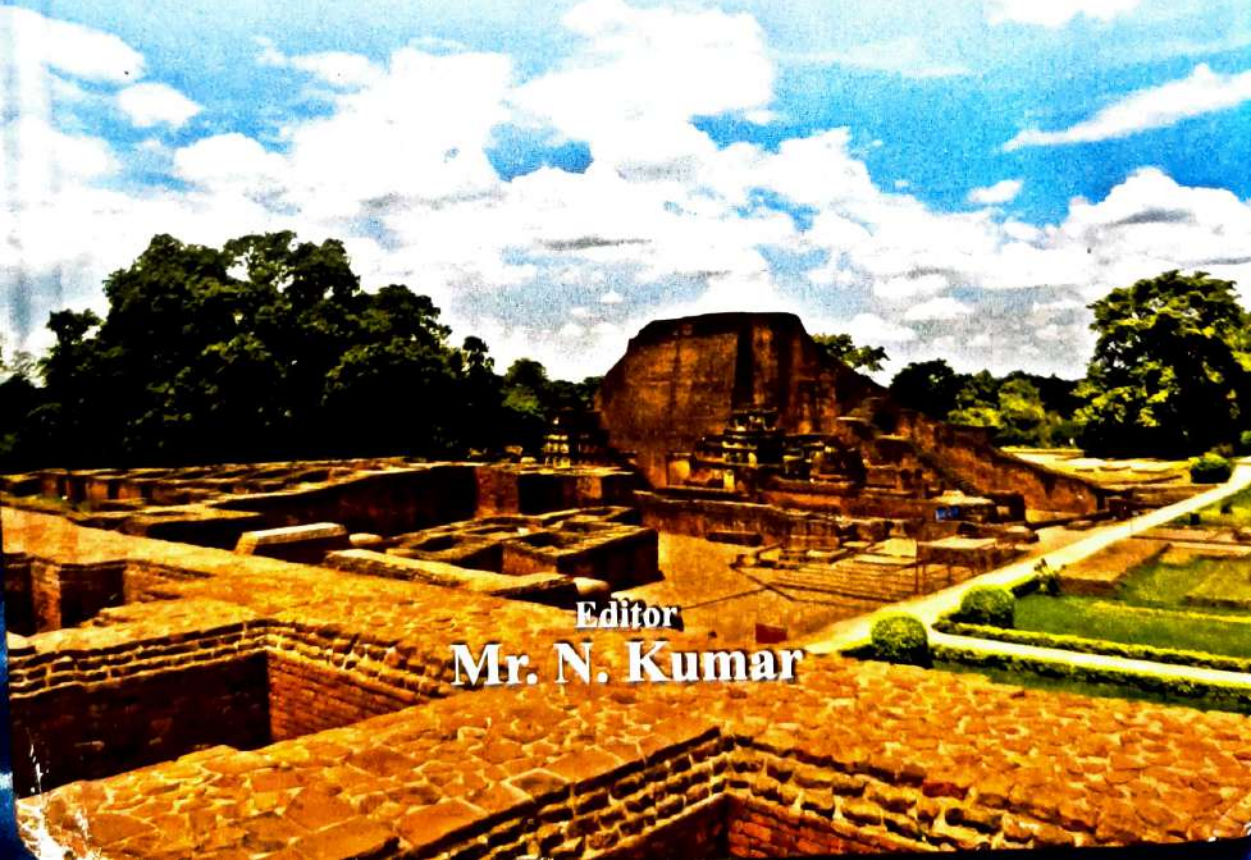

Editor

Mr. N. Kumar

Branch Place of Institution
International Centre for Scientific Research and Development (ICSRD)
80 Feet Road, Opposite NGV Indoor Stadium
Koramangala, 8th Block Bangalore,
Karnataka-560095 India

Edition: 2023

ISBN: 978-81-963779-8-4

Printed at: Shahdara, Delhi-110032

Contents

Work-Life Balance of Women IT Professionals in the Post-COVID Era: A Study on Remote Work Experiences

*Prof. Dr Manoj Narayanan K S
**Dr Mishel Elizabeth Jacob
***Mr. Akhil T S

Abstract

The COVID-19 pandemic reshaped the work landscape, making Work from Home (WFH) a common practice, especially in the IT sector in India. The primary objective of this research is to examine the work-life balance of women employees in the IT sector while working from home during the post-COVID era. Additionally, the study aims to investigate the influence of age, marital status, place and type of residence, and the number of children on work-life balance.This research employed a structured questionnaire to collect data from 80 women IT professionals in Kerala. Statistical tests, including the Kruskal Wallis H test and Mann-Whitney U test, were utilized to analyze the

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