3.4.5 Bibliometrics of the Publications during the last five years based on average Citation Index in Scopus/ Web of Science

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doi: 10.22199/issn.0717-6279-2020-01-0003

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Journal of Mathematics

ISSN 0717-6279 (On line)

Z_k-Magic Labeling of Star of Graphs

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Received: November 2018 | Accepted: April 2019

Abstract:

For any non-trivial abelian group A under addition a graph G is said to be A-magic if there exists a labeling $f : E(G) \to A - \{0\}$ such that, the vertex labeling $f+$ defined as $f+(v) = Pf(uv)$ taken over all edges uv incident at v is a constant. An A-magic graph G is said to be Zk-magic graph if the group A is Zk, the group of integers modulo k and these graphs are referred to as k-magic graphs. In this paper we prove that the graphs such as star of cycle, flower, double wheel, shell, cylinder, gear, generalised Jahangir, lotus inside a circle, wheel, closed helm graph are Zk-magic graphs.

Keywords: A-magic labeling; Flower; Double wheel; Shell; Cylinder; Gear; Generalised Jahangir; Lotus inside a circle; Wheel; Closed helm graph.

MSC (2010): 05C78.

Cite this article as (IEEE citation style):

P. Jeyanthi and K. Jeya Daisy, "Z_k-Magic Labeling of Star of Graphs", *Proyecciones (Antofagasta, On line)*, vol. 39, no. 1, pp. 31-50, Feb. 2020, doi: 10.22199/issn.0717-6279-2020-01-0003. [Accessed dd-mm-yyyy].

Scopus Preview

Source details

Advances in Mathematics: Scientific Journal

Scopus coverage years: from 2019 to 2021

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Subject area: Mathematics: General Mathematics

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ISSN: 1857-8365 (printed); 1857-8438 (electronic)
https://doi.org/10.37418/amsj.9.4.15 Spec. Issue on NCFCTA-2020

RESULTS ON RELATIVELY PRIME DOMINATION NUMBER OF VERTEX SWITCHING OF COMPLEMENT GRAPHS

C. JAYASEKARAN[1] AND A. JANCY VINI

ABSTRACT. Let G be a non-trivial graph. A set $S \subseteq V$ is said to be a relatively prime dominating set if it is a dominating set with at least two elements and for every pair of vertices u and v in S such that $(d(u), d(v)) = 1$. The minimum cardinality of a relatively prime dominating set is called a relatively prime domination number and it is denoted by $\gamma_{\text{rpd}}(G)$. For a finite undirected graph $G(V, E)$ and a subset $\sigma \subseteq V$, the switching of G by σ is defined as the graph $G^{\sigma}(V, E')$ which is obtained from G by removing all edges between σ and its complement $V - \sigma$ and adding as edges all non-edges between σ and $V - \sigma$. In this paper we compute the relatively prime domination number of vertex switching of complement of path P_n, cycle C_n, star $K_{1,n}$ and complete bipartite graph $K_{m,n}$.

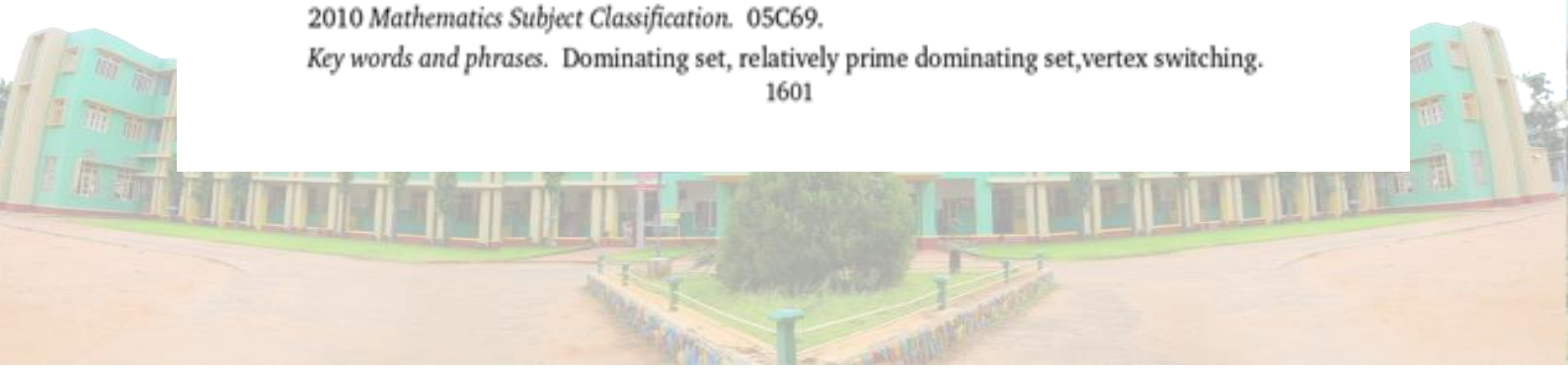
1. INTRODUCTION

By a graph $G = (V, E)$ we mean a finite undirected simple graph. The order and size of G are denoted by p and q respectively. For graph theoretical terms, we refer to Harary [2] and for terms related to domination we refer to Haynes [3]. A subset S of V is said to be a dominating set in G if every vertex not in S is adjacent to at least one member of S. The domination number $\gamma(G)$ is the number of vertices in a smallest dominating set for G.

[1]*corresponding author*

2010 *Mathematics Subject Classification.* 05C69.

Key words and phrases. Dominating set, relatively prime dominating set,vertex switching.



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https://doi.org/10.37418/amsj.9.6.93 Spec. Issue on ICIGA-2020

OPERATIONS ON SOME STAR RELATED PERFECT MEAN CORDIAL GRAPHS

A. ANNIE LYDIA[1] AND M. K. ANGEL JEBITHA

ABSTRACT. A vertex labeling $h : V(G) \to \{0,1,2,3\}$ is said to be perfect mean cordial labeling of a graph G if it induces an edge labeling h^* defined as follows:

$$h^*(wz) = \begin{cases} 1 & \text{if } 2|(h(w)+h(z)) \\ 0 & \text{otherwise} \end{cases},$$

with the condition that $|e_h(0) - e_h(1)| \leq 1$ and $|v_h(\alpha) - v_h(\beta)| \leq 1$ for all $\alpha, \beta \in \{0,1,2,3\}$,where $e_h(\delta)$ is number of edges label with $\delta(\delta = 0,1)$ and $v_h(\lambda)$ denote the number of vertices labeled with λ $(\lambda = 0,1,2,3)$. A graph G is said to be perfect mean cordial graph if it admits a perfect mean cordial labeling. In this paper, we prove that operations on some star related perfect mean cordial graphs are perfect mean cordial graphs.

1. INTRODUCTION

In the present era, graph theory has become a highly challenging and interesting area for the study of numerous mathematicians and computer experts. Since it has many applications and scope for various researches, it has attracted the attention of the erudite scholars who have the overwhelming desire for updating the field of mathematics. Particularly graph labeling has become a widely popular and area of concern,since it offers wide range of applications. A graph labeling is an assignment of integers to the nodes or the links, or both, subject to certain conditions.

[1]*corresponding author*

2010 *Mathematics Subject Classification.* 05C78.

Key words and phrases. Perfect mean cordial graph, perfect mean cordial labeling.

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THE DOMINATION UNIFORM SUBDIVISION NUMBER OF $G \circ K_1$

T. BERJIN MAGIZHA[1] AND M. K. ANGEL JEBITHA

ABSTRACT. Let $G = (V, E)$ be an undirected and simple graph. A dominating set D of G is a set of vertices of G such that every vertex in $V - D$ is adjacent to at least one vertex in D. The domination number of G, denoted by $\gamma(G)$, is the minimum cardinality taken over all dominating sets of G. The domination uniform subdivision number of G is the least positive integer k such that the subdivision of any k edges from G results in a graph having domination number greater than that of G and is denoted by $usd_{\gamma}(G)$. In this paper, we discuss the domination uniform subdivision number for a standard graph operation namely corona of graphs.

1. INTRODUCTION

Let $G = (V, E)$ be a simple undirected graph of order n and size m. If $v \in V(G)$, then the neighborhood of v is the set $N(v)$ consisting of all vertices u which are adjacent to v. The closed neighborhood is $N[v] = N(v) \cup \{v\}$. The degree of v in G is $|N(v)|$ and is denoted by $deg(v)$. The maximum degree of G is $max\{deg(v) : v \in V(G)\}$ and is denoted by $\Delta(G)$. A vertex v is said to be full vertex if $deg(v) = n - 1$. A vertex v is said to be pendant vertex if $deg(v) = 1$. An edge incident with pendant vertex is called leaf or pendent edge. A path, a cycle and a complete graph on n vertices are denoted by P_n, C_n and K_n respectively.

[1]*corresponding author*

2010 *Mathematics Subject Classification.* 05C69.

Key words and phrases. Domination number, domination uniform subdivision number, domination subdivision stable set.

Scopus Preview

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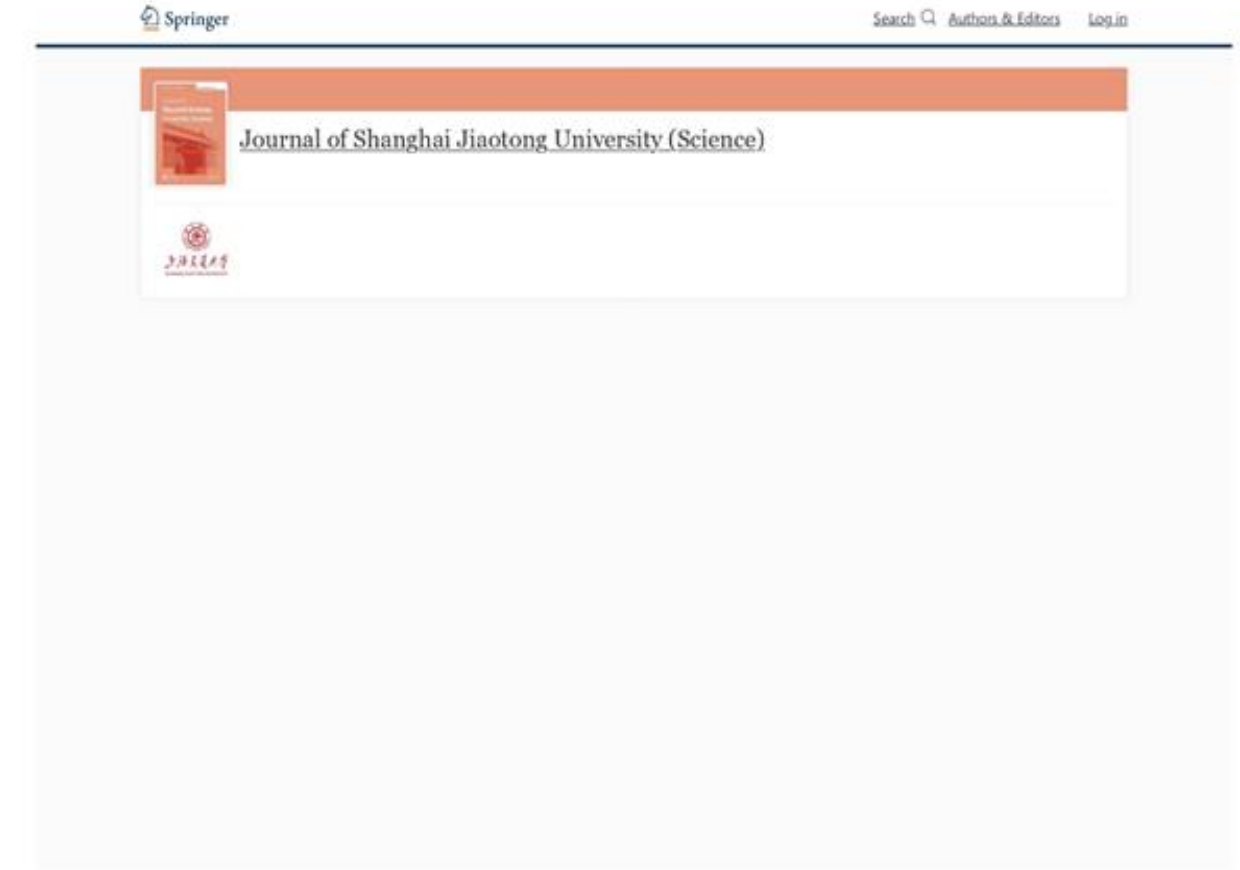
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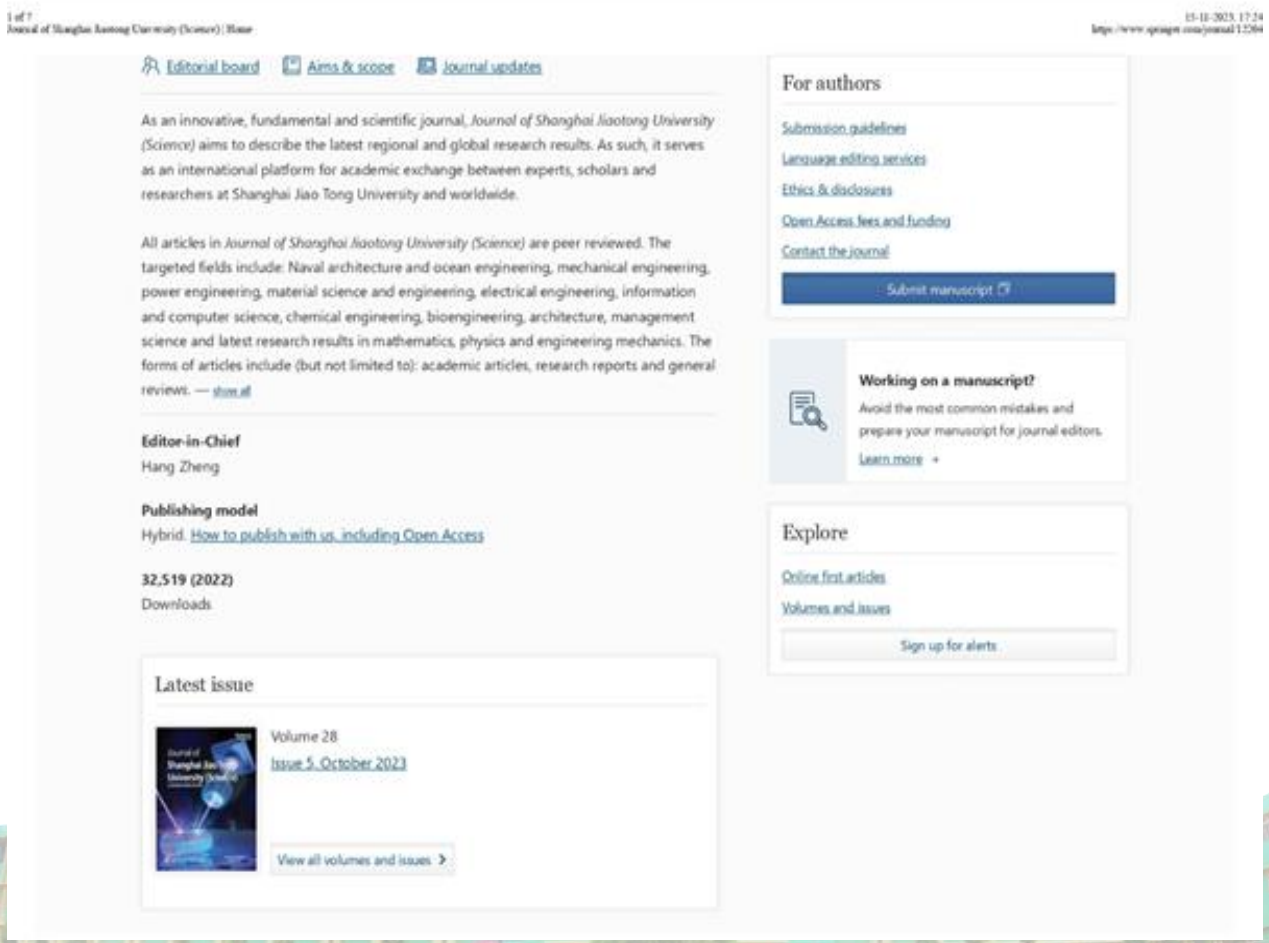
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2-DOMINATING SETS AND 2- DOMINATION POLYNOMIAL OF PATHS

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[1, 2, 3] *Affiliated to Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli - 627 012, Tamil Nadu, India.*

Abstract: *Let G be a simple connected graph of order n. Let $D_2(G, i)$ be the family of 2-dominating sets in G with cardinality i. The polynomial $D_2(G, x) = \sum_{i=\gamma_2(G)}^{n} d_2(G, i)x^i$ is called the 2-domination polynomial of G. In this paper we obtain a recursive formula for $d_2(P_n, i)$. Using this recursive formula we construct the 2-domination polynomial, $D_2(P_n, x) = \sum_{i=\lceil \frac{n+1}{2} \rceil}^{n} d_2(P_n, i)x^i$, where $d_2(P_n, i)$ is the number of 2-dominating sets of P_n of cardinality i and some properties of this polynomial have been studied.*

Keywords: **Path, 2-dominating set, 2-domination number, 2-domination polynomial.**

1. INTRODUCTION

Let G = (V, E) be a simple graph of order n. For any vertex v∈ V, the open neighbourhood of V is the set N(v) = {u∈ V / uv∈ E} and the closed neighbourhood of V is the set N[v] = N(v) ∪ {v}. For a set S ⊆V, the open neighbourhood of S is $N(S) = \cup_{v \in S} N(v)$ and the closed neighbourhood of S is N[S] = N(S) ∪ S.

A set D ⊆V is a dominating set of G if N[D] = V or equivalently, every vertex in V – D is adjacent to at least one vertex in D.

The domination number of a graph G is defined as the minimum cardinality taken over all dominating sets D of vertices in G and is denoted by γ(G).

We use the notation $\lceil x \rceil$ for the smallest integer greater than or equal to x and $\lfloor x \rfloor$ for the largest integer less than or equal to x. Also, we denote the set {1,2,3,…,n} by [n], throughout this paper.

2. 2 - DOMINATING SETS OF PATHS

In this section, we state the 2-domination number of path and some of its properties.

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Advances in Mathematics: Scientific Journal

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IDEAL THEORY IN NEAR-SEMIRINGS AND ITS APPLICATION TO AUTOMATA

C. JENILA[1] AND P. DHEENA

ABSTRACT. In this paper we develop ideal theory in near-semirings. We use the ideal theory to find the necessary and sufficient conditions for a linear sequential machine to be minimal.

1. INTRODUCTION

It has been shown that a homomorphic group-automaton $\mathcal{A} = (Q, A, B, F, G)$, where Q is a state set, A is an input set and B is an output set are groups and $F : Q \times A \to Q$ and $G : Q \times A \to B$, the state-transition function and output function respectively, are homomorphisms, is minimal if and only if the $N(\mathcal{A})$-group Q is generated by 0 and does not contain non-zero ideals which are annihilated by g_0 where $g_0 : Q \to B$ ([3], Theorem 9.259). Pilz [3] considered linear sequential machines in which the state set forms a group.

Krishna and Chatterjee [2] considered a generalized linear sequential machine $\mathcal{M} = (Q, A, B, F, G)$ where Q, A, B are semigroups and R-semimodules for some semiring R and $F : Q \times A \to Q$ and $G : Q \times A \to B$ are R-homomorphisms. They have obtained a necessary condition for the above generalized sequential machine to be minimal. So naturally one is interested to find a necessary and sufficient conditions for the above generalized linear sequential machine to be minimal. To achieve that, we develop ideal theory in a

[1]*corresponding author*

2010 *Mathematics Subject Classification.* 16Y30, 16Y60.

Key words and phrases. Near-semiring, ideal, linear sequential machine.

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Journal of Drug Delivery Science and Technology

Formerly known as: S.T.P. Pharma Sciences

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Publisher: Editions de Sante

ISSN: 1773-2247 E-ISSN: 2588-8943

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$$8.0 = \frac{26{,}884 \text{ Citations to date}}{3{,}361 \text{ Documents to date}}$$

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CiteScore rank 2022

Category	Rank	Percentile
Pharmacology, Toxicology and Pharmaceutics — Pharmaceutical Science	#32/171	81st

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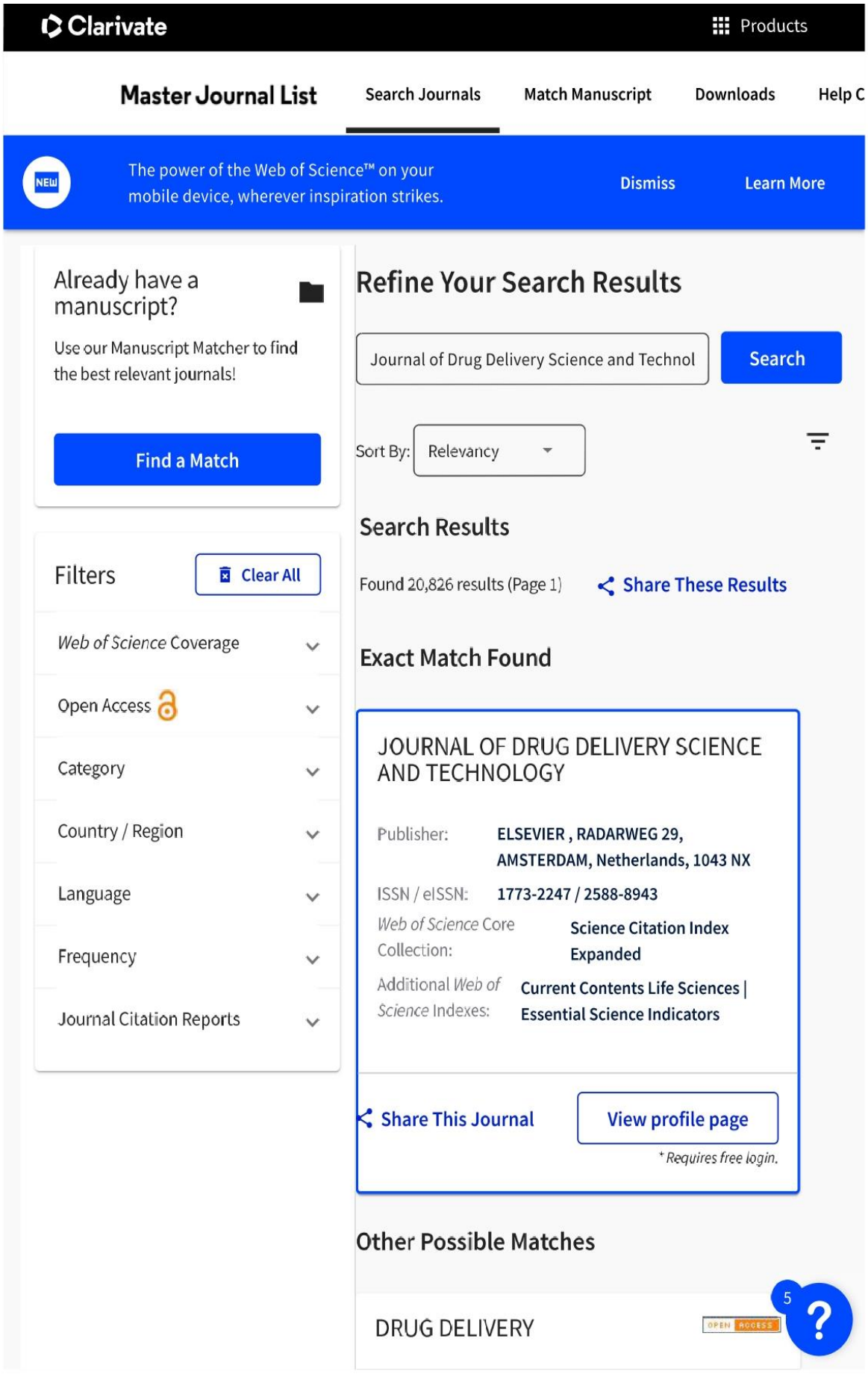
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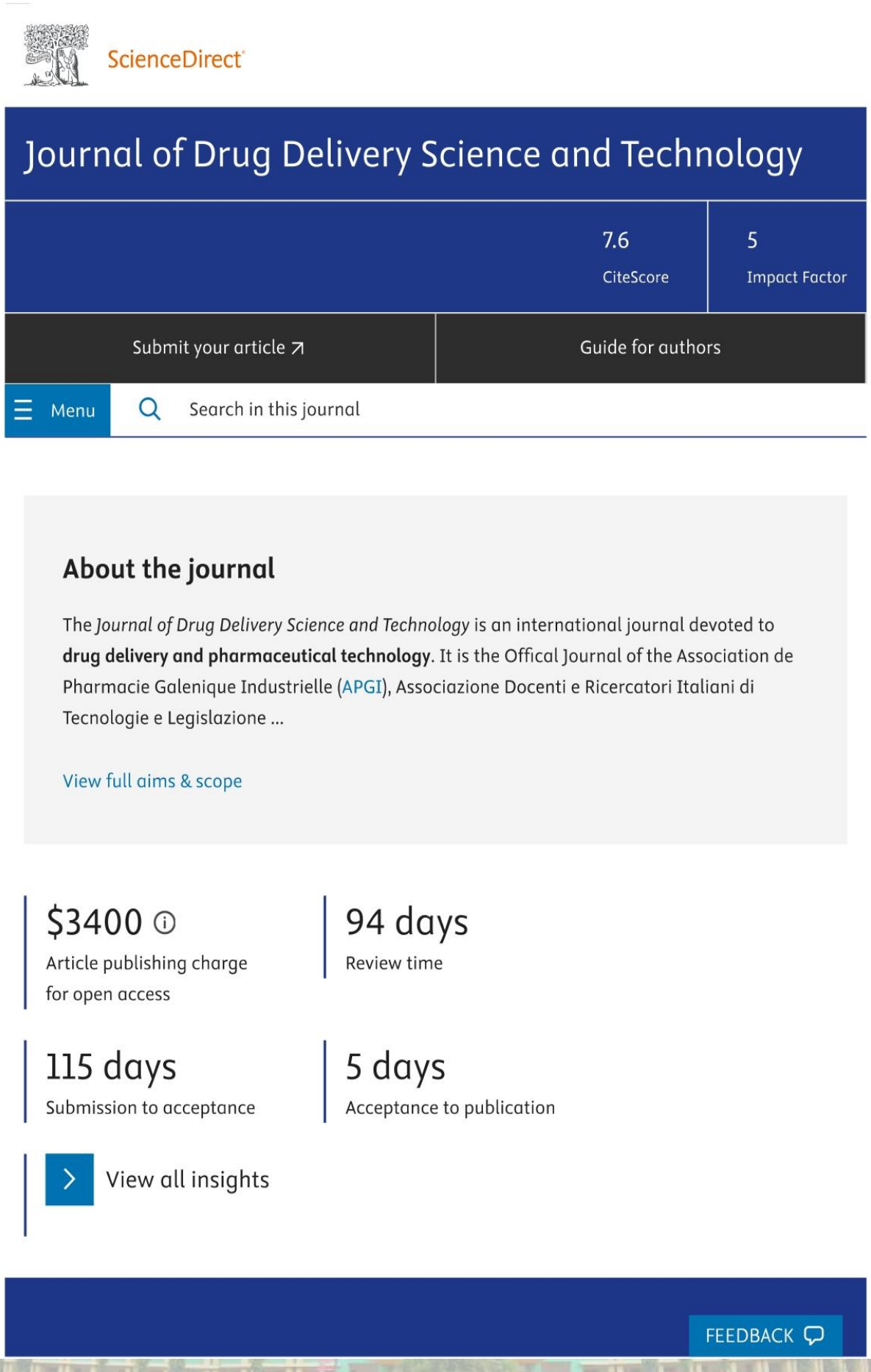
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Volume 57, June 2020, 101752

Curcumin-encased hydroxyapatite nanoparticles as novel biomaterials for antimicrobial, antioxidant and anticancer applications: A perspective of nano-based drug delivery

Saleth Sebastiammal [a b], Arul Sigamani Lesly Fathima [a], Sandhanasamy Devanesan [c d], Mohamad S. AlSalhi [c d], Johnson Henry [e], Marimuthu Govindarajan [f g], Baskaralingam Vaseeharan [h]

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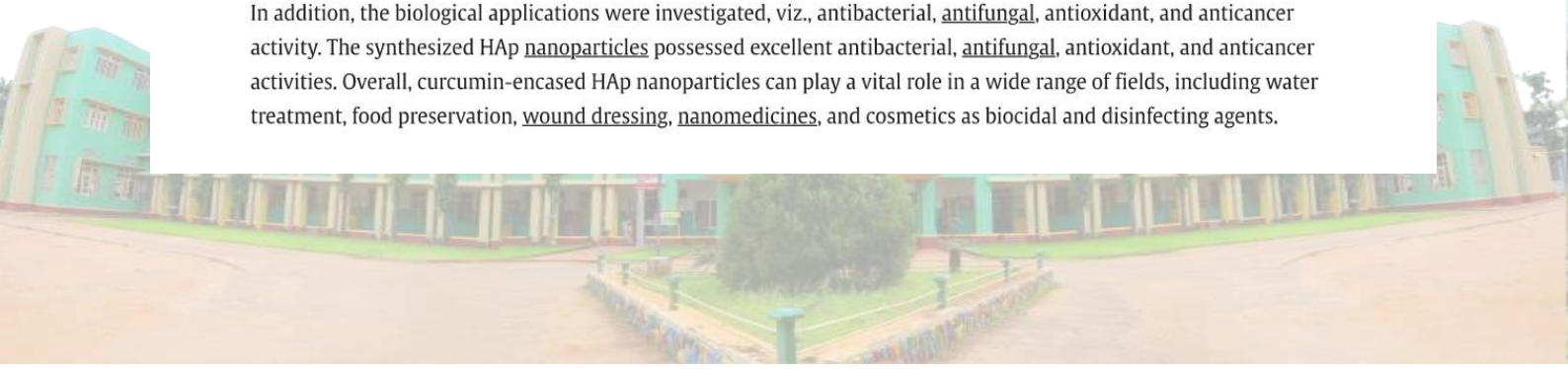
Highlights

- Pure, surfactant-assisted, and curcumin-mediated HAp NPs were synthesized.
- Pure, surfactant-assisted, and curcumin-mediated HAp NPs were characterized.
- HAp NPs possess excellent antibacterial and antifungal properties.
- HAp NPs exhibit free radical quenching activity as effective antioxidants.
- HAp NPs kill HeLa cells and are effective anticancer agents.

Abstract

Hydroxyapatite (HAp) is an important biological molecule and principal mineral component found in bones that is used in various clinical applications to significantly enhance the biological activity and biocompatibility of man-made biological molecule. Several analyses have been performed to control the structural properties of HAp by varying the processing parameters. This study described the synthesis of HAp nanoparticles (NPs) via the sol-gel method, that would be effective for biomedical applications, such as bone graft substitution. It also examined the effects of pure HAp, surfactant (PEG and CTAB)-assisted HAp NPs, and curcumin-mediated HAp NPs. The synthesized HAp NPs were analyzed using XRD, FTIR, RAMAN, FESEM, TEM, EDAX, UV-DRS, and PL analysis. From the XRD analysis, it was found that the prepared HAp NPs have a hexagonal structure with nanosize distribution. From FESEM and TEM analyses, it was found that the synthesized HAp NPs were rod-like in shape and the elemental analysis was conducted using EDAX. In addition, the biological applications were investigated, viz., antibacterial, antifungal, antioxidant, and anticancer activity. The synthesized HAp nanoparticles possessed excellent antibacterial, antifungal, antioxidant, and anticancer activities. Overall, curcumin-encased HAp nanoparticles can play a vital role in a wide range of fields, including water treatment, food preservation, wound dressing, nanomedicines, and cosmetics as biocidal and disinfecting agents.



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E-ISSN: 1984-6428

Subject area: Materials Science: Materials Science (miscellaneous) | Chemical Engineering: General Chemical Engineering | Chemistry: General Chemistry

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Chemistry		

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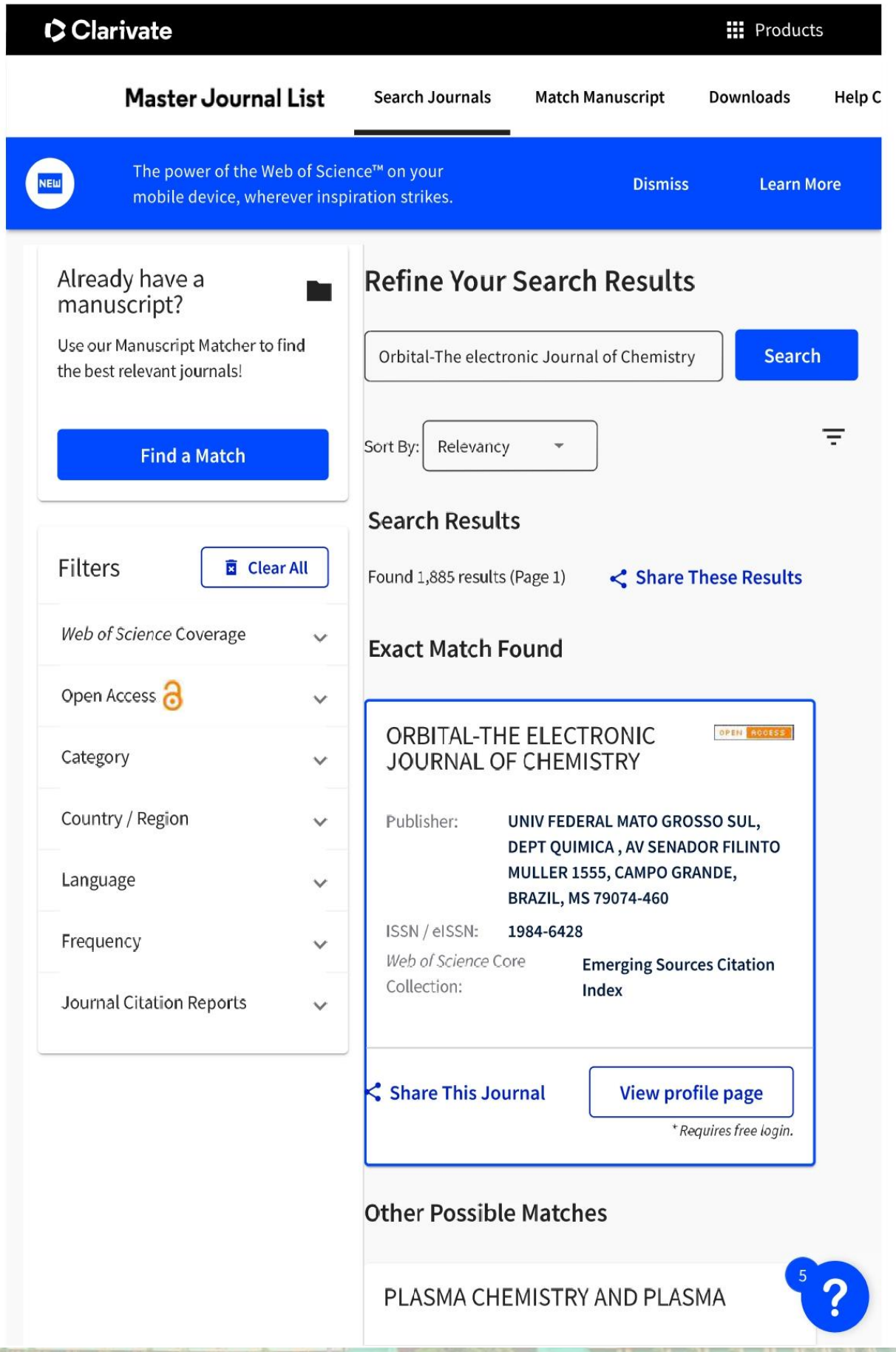
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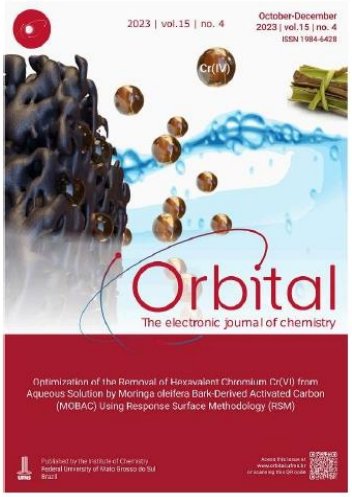

FULL PAPERS

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| Vol 12 | | No. 2 | | April-June 2020 |

FULL PAPER

Electronic Band Structure, Density of States, Phase Transitions, Metallization and Superconducting Transition of KBr under High Pressure

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Article history: Received: 11 April 2019; revised: 09 November 2019; accepted: 06 April 2020. Available online: 28 June 2020. DOI: http://dx.doi.org/10.17807/orbital.v12i2.1401

Abstract:

The results of a full potential linear muffin-tin orbital (FP-LMTO) study on the electronic properties of ionic insulator potassium bromide (KBr) under pressure is presented. The phase transition pressure at which the compound undergoes structural phase transition from NaCl to CsCl structure is predicted from the total energy calculations. The ground state properties and band gap values are compared with the experimental results. At normal pressure KBr is a direct band gap insulator. In KBr, the metallization occurs through indirect closing of the band gap between Γ and H points at the reduced volume V/Vo=0.45 (CsCl structure), the corresponding metallization pressure is 1.274 Mbar. On further increase of pressure, KBr becomes superconductor, and this material comes under the class of electron-phonon-mediated high pressure superconductor. The superconducting transition temperatures (Tc) of KBr is obtained as a function of pressure for both NaCl and CsCl structures. The highest Tc estimated is 5.911 K and the corresponding pressure is 5 Mbar in the NaCl structure and 0.897 K in the CsCl structure. It is also confirmed that the metallization, structural phase transition and onset of superconductivity do not occur simultaneously in ionic compounds.

Keywords: band structure; density of states; phase transition; metallization; superconductivity

1. Introduction

Ionic compounds are ubiquitous materials and are characterized by their highly crystalline nature, high melting points and strong miscibility in polar media. Potassium bromide (KBr) is a large band gap ionic insulator with energy gap = 7.4 eV and its ionic crystalline structure produces its unique high ultraviolet transmissivity. The transition of an insulator to a metal (metallization) at high compression is generally the result of the pressure induced closure of the band gap. Potassium chloride is expected to have a uniquely high metallization pressure among large bandgap solid insulators [1]. Under strong shock compression, the insulating –conducting transition is enhanced by the thermal promotion of electrons across band gap. This is a result of high temperature produced by high pressure (>1 Mbar) shock waves [1]. Recently, ramp compression has been used to compress materials to pressures above 8 Mbar while keeping the temperature low compared to that of shock waves [2]. Band structure calculations reveal that alkali halide compounds are wide-gap insulators that explain their optical transparency [3]. Ionic salts have gained substantial importance recently due to the ability of ionic liquids to dissolve a variety of organic substance including cellulose. Ionic crystals are probably the simplest system to understand, since the interactions among the ions are purely electrostatic in origin. Hence the description of their ground state energies is exact within the limit of calculation [3].

The physical properties of materials undergo a variety of changes when they are subjected to

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Scopus Preview

Source details

Progress in Organic Coatings

Scopus coverage years: from 1972 to Present

Publisher: Elsevier

ISSN: 0300-9440

Subject area: Chemistry: Organic Chemistry | Materials Science: Materials Chemistry | Materials Science: Surfaces, Coatings and Films | Chemical Engineering: General Chemical Engineering

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$$11.4 = \frac{23{,}738 \text{ Citations to date}}{2{,}087 \text{ Documents to date}}$$

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Chemistry Organic Chemistry	#13/197	93rd
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Materials Science		

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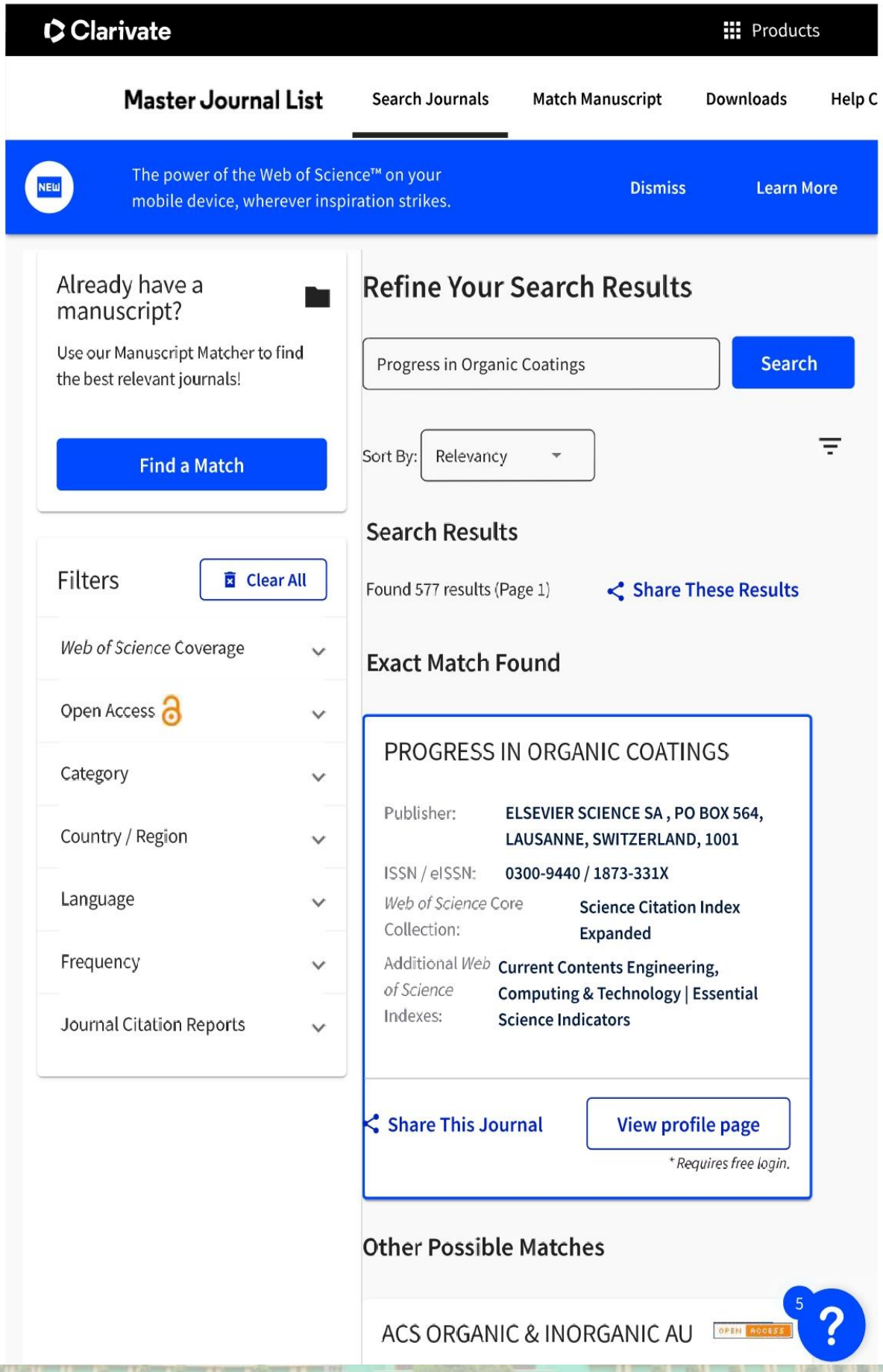
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Fabrication and modeling of prototype bike silencer using hybrid glass and chicken feather fiber/hydroxyapatite reinforced epoxy composites

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ARTICLE INFO

Keywords:
Chicken feather fiber
Hybrid composites
Emission characteristics
Sound absorption
Heat releasing nature

ABSTRACT

Recently, the significant development and advantages of bioactive natural composite materials have been employed in modern engineering constructions, aerospace, packing industries, automotive fields, and more. The fiber materials are derived from natural plant materials (e.g., coir, jute, and bamboo) and animal waste products which show excellent physico-chemical, thermal, and mechanical properties compared to man-made fibers. In this study, the replacement of man-made fiber materials with polymer matrix composites using natural waste chicken feather fiber (CFF) based reinforced lightweight epoxy hybrid composite materials were prepared for the development of a prototype bike silencer. The hybrid composites were prepared from epoxy resin reinforced with synthetic inorganic glass fibers (GF) and natural organic CFFs (with 5, 10, and 20 % composition) together with 3 % of nano-hydroxyapatite (nHA) as a catalytic filler. The 3D modeling, design, and fabrication of a prototype bike silencer were undertaken, using Suzuki Samurai as a reference model specimen. The hybrid 82 G F/15CFF/3HA composite material showed optimum tensile strength and yield strength values of 167.00 and 58.10 MPa, respectively. The observed von-Mises stress, maximum displacement, Young's modulus, and Poisson's ratio values were 6.9260 MPa, 0.8661 mm, 13.90 GPa, and 0.39, respectively. Further, the presence of voids in the hybrid 82 G F/15CFF/3nHA composite bike silencer showed higher absorption capacity with effective reduction of toxic CO, HC, O_2, and CO_2 pollutants as well as remarkable heat releasing capacity, as compared to the steel silencer. The fabricated hybrid 82 G F/15CFF/3nHA composite material may effectively be utilized for the development of renewable, eco-friendly biocomposites with exceptional performances.

1. Introduction

Fibers are firmly considered as fundamental components in composite materials as they bear the main loading and have been widely used in aerospace, automotive, construction, and sporting industries [1–4]. Glass fibers (GF) are one of the most widely used reinforcements, owing to their strength and competitive price [5–7]. Recently, environment-friendly natural fibers derived from animal wastes have been used in various applications in the place of glass or synthetic fibers. This is because they show exceptional mechanical properties like high tensile strength, flame retardant nature, lightweight, high thermal stability, and prominent stiffness. The natural fibers derived from animal sources are an attractive reinforcement for the development of bio-composites. In this regard, chicken feather fibers (CFFs) are

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[1] Authors have equal contribution to this work.

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Scopus Preview

Source details

Inorganic and Nano-Metal Chemistry

Formerly known as: Synthesis and Reactivity in Inorganic, Metal-Organic and Nano-Metal Chemistry

Scopus coverage years: from 2017 to Present

Publisher: Taylor & Francis

ISSN: 2470-1556 E-ISSN: 2470-1564

Subject area: Chemistry: Inorganic Chemistry | Chemistry: Physical and Theoretical Chemistry

Source type: Journal

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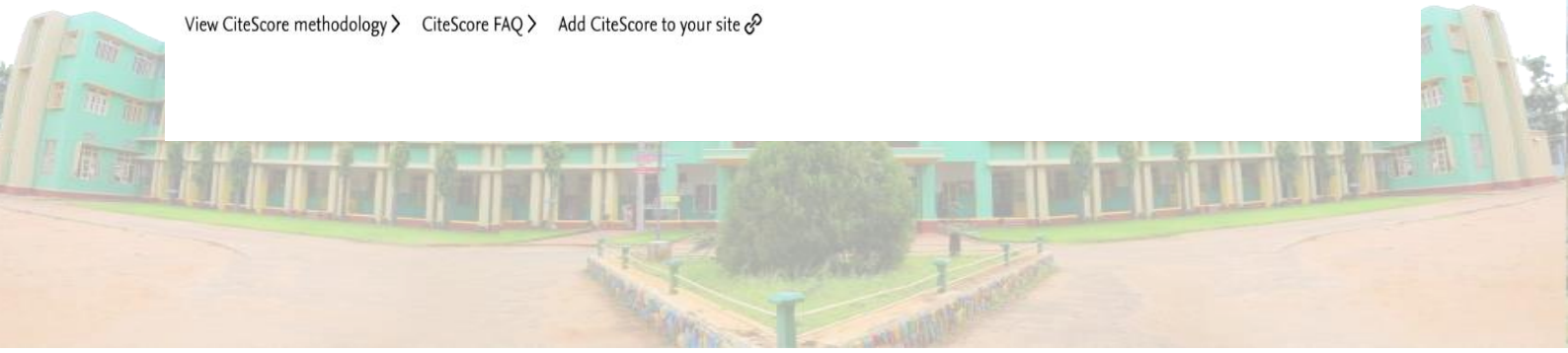

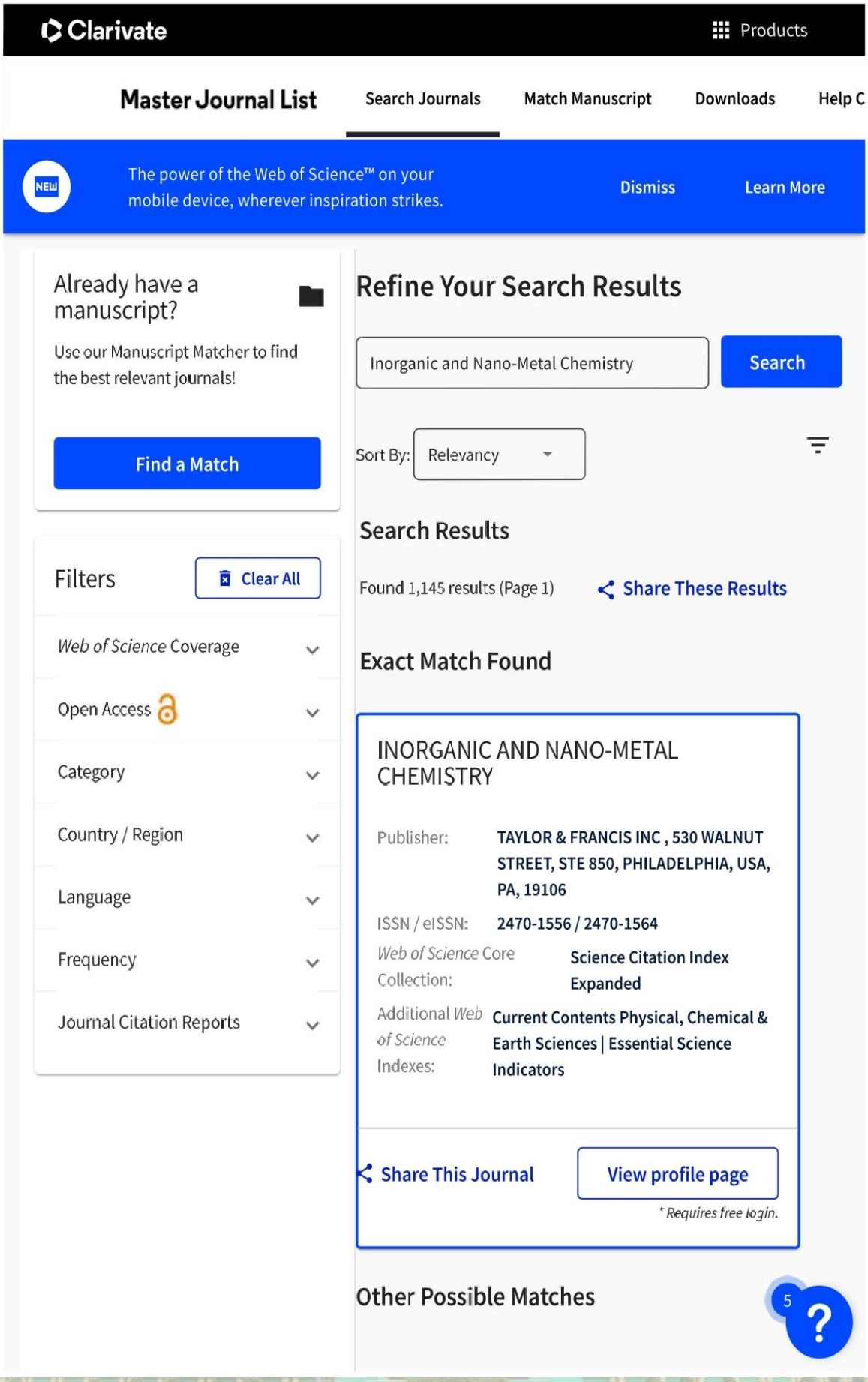
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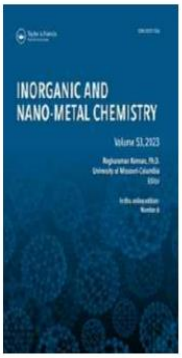

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Article

Synthesis, growth mechanism and photocatalytic properties of nickel oxide (NiO) nanoflower: a hydrothermal process

S. Virgin Jeba, S. Sebastiammal, S. Sonia & A. Lesly Fathima

Pages 1431-1441 | Received 26 May 2020, Accepted 07 Sep 2020, Published online: 27 Oct 2020

Cite this article | https://doi.org/10.1080/24701556.2020.1837163 | Check for updates

Abstract

The present report explores the synthesis strategy of flower like Nickel Oxide (NiO) nanostructures from nanosheets as their building blocks in the presence of citric acid as surfactant. An easy and inexpensive hydrothermal technique was designed for the synthesis of NiO nanoparticles. The structural, morphological and compositional analyses were done by the techniques such as X-ray Diffraction, Field Emission Scanning Electron Microscopy and Energy Dispersive X-ray Analysis respectively and growth mechanism of the NiO nanostructure was also dealt in detail. Diffraction pattern confirms that the prepared NiO is belongs to the face cantered cubic structure. The average crystalline size was obtained by Debye Scherrer formula and the values (8 nm, 9 nm, 7 nm and 7.5 nm for NiO nanoflowers synthesized with 0.5 g, 1 g, 1.5 g and 2 g of citric acid respectively) are comparable with the size obtained by the Williamson Hall plot method. Morphological analysis confirms the formation of nanosheets constituted floral microspheres with a diameter ranging from 750 nm to 850 nm. Elemental analysis proves the presence of Ni and O and its purity. The 750 nm sized, regularly arranged NiO nanoflowers were subjected to photocatalytic degradation of Methylene Blue (MB) and Rhodamine 6G (Rh 6G) under Ultra Violet irradiation and bestow the effective degradation efficiency (76.5% and 92.6%

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ISSN: 2405-8300 E-ISSN: 2405-8300

Subject area: Chemistry: General Chemistry

Source type: Journal

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Category	Rank	Percentile
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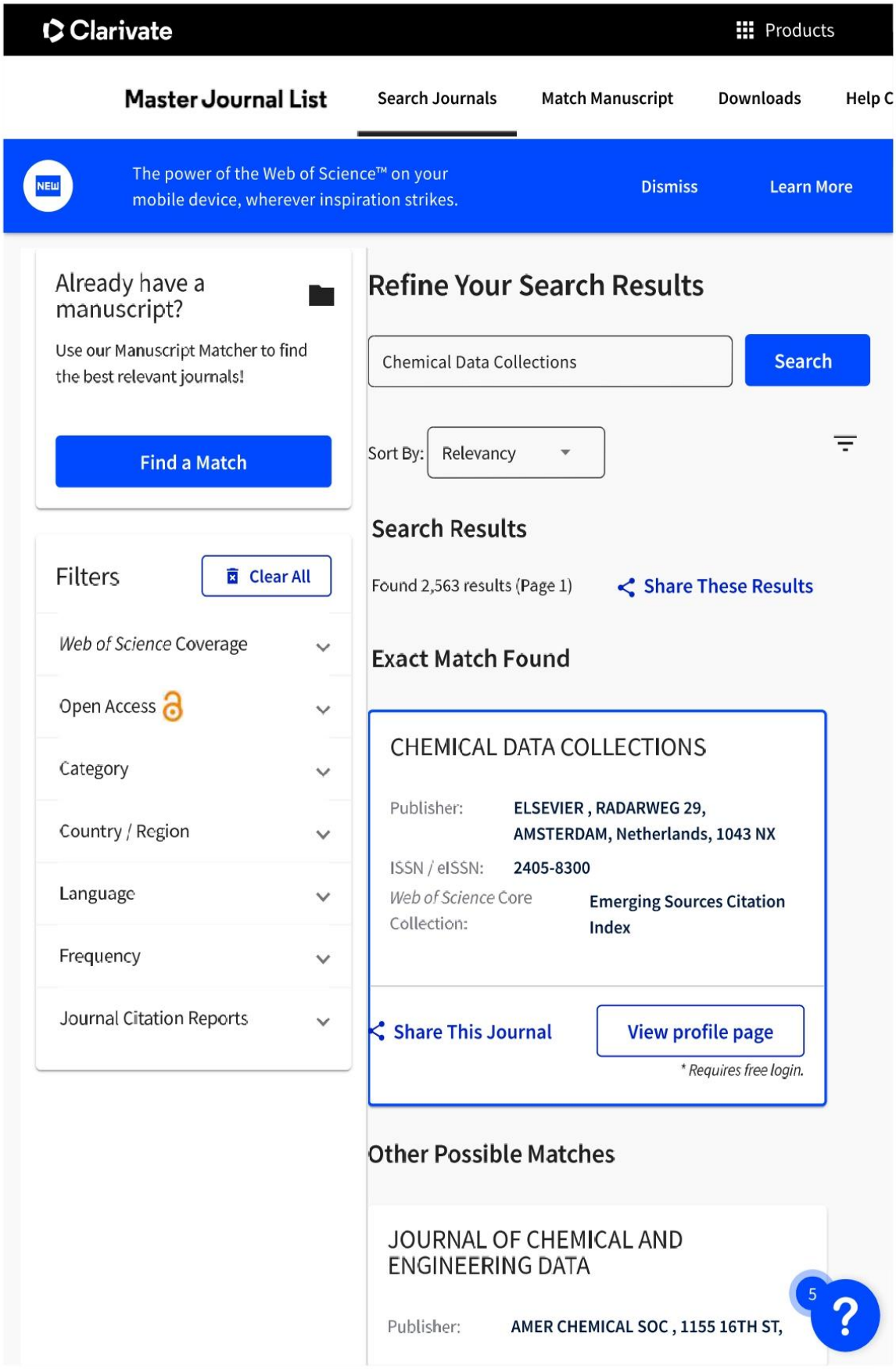
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Data Article

Quantum chemical insight into molecular structure, spectroscopic (FT–IR, FT–Raman, UV-vis, NMR), and molecular docking of 3,5-di-tert-butyl-2-hydroxybenzaldehyde

S.J. Jenepha Mary, C. James[†,*]

Department of Physics and Research Centre, Scott Christian College (Autonomous), Nagercoil- 629003, Tamil Nadu, India (Affiliated to Manonmaniam Sundarnar University, Abishekapatti, Tirunelveli 627012, India)

ARTICLE INFO

Article history:
Received 1 May 2020
Revised 23 June 2020
Accepted 27 August 2020
Available online 29 August 2020

Keywords:
NBO
Chemical shift
FT-IR
Raman
Influenza virus

ABSTRACT

The molecule of therapeutic interest 3,5-Di-tert-butyl-2-hydroxybenzaldehyde, a salicylaldehyde derivative has been subjected to FT-IR, FT- Raman, UV-Visible and NMR spectral studies, along with quantum chemical computations using density functional theory. The title molecule has been optimized at B3LYP level of theory and 6-311G+(d,p) basis set. NBO analysis has been performed to study donor acceptor interactions and stability of the molecule arising from hyperconjugative interactions. Spectral analysis has been carried out and the vibrational assignments have been made on potential energy difference. To explain bioactivity several molecular electronic parameters such as frontier molecular orbitals, ESP, charge analysis have been discussed. Antiviral activity of 3,5-Di-tert-butyl-2-hydroxybenzaldehyde has been carried out against influenza viral proteins of type A, type B, type C, and type D. Molecular docking simulations shows it has a good binding affinity toward influenza type D virus.

Specifications Table

Subject area	Spectroscopy and Computational Chemistry
Compound	3,5-Di-tert-butyl-2-hydroxybenzaldehyde
Data category	Computational simulations, Natural bond orbital analysis, vibrational analysis, NMR chemical shift and molecular docking.
Data acquisition format	FT-IR, FT-Raman, NMR, UV-Vis
Data type	Experimental and theoretical
Procedure	Experimental: Sample has been purchased from sigma Aldrich. FT-IR spectrum has been recorded using Perkin-Elmer FT-IR spectrophotometer, FT Raman spectrum has been recorded using BRUKER RFS 27, UV-visible spectrum has been measured using JASCO (V-570) UV/VIS/NIR spectrometer. Computations: Geometry optimization and NBO analysis have been carried out using Gaussian 09 program package and visualized using Gauss view 5.0,Vibrational analysis using MOLVIB 7.0 and molecular docking simulation using AutoDock 4.2 and PYMOL.
Data accessibility	Data is available within the article

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† Register number: 18113162132001

https://doi.org/10.1016/j.cdc.2020.100530
2405-8300/

Scopus Preview

Source details

Spectroscopy Letters

Scopus coverage years: from 1968 to Present

Publisher: Taylor & Francis

ISSN: 0038-7010 E-ISSN: 1532-2289

Subject area: Physics and Astronomy: Atomic and Molecular Physics, and Optics | Chemistry: Analytical Chemistry | Chemistry: Spectroscopy

Source type: Journal

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SJR 2022
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Chemistry		

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SPECTROSCOPY LETTERS

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Molecular structure elucidation, charge transfer interactions, electronic properties, vibrational spectral investigation and molecular docking of the antiviral active molecule (E)-4-[1-(2-carbamothioylhydrazinylidene)ethyl]-phenyl benzoate dimer - aided by density functional theory

S. J. Jenepha Mary* and C. James

Department of Physics and Research Centre, Scott Christian College (Autonomous), Manonmaniam Sundarnar University, Nagercoil, India

ABSTRACT

The molecular structure of the novel thiosemicarbazide (E)-4-[1-(2-carbamothioylhydrazinylidene) ethyl] - phenyl benzoate has been synthesized and subjected to Raman and Fourier transform infrared spectral studies. Optimized parameters of (E)-4-[1-(2-carbamothioylhydrazinylidene) ethyl] - phenyl benzoate monomer and dimer have been compared with X-ray diffraction data. The existence of hydrogen bonded intramolecular interactions, intermolecular interactions and the hyperconjugative energy leading to the stabilization of the system have been revealed by natural bond orbital analysis. Charge transfer interactions from highest occupied molecular orbital to lowest unoccupied molecular orbital and the observed low energy gap predict the molecule to be more reactive. Molecular electrostatic potential image shows the potential binding site is around the sulfur atom. The spectra have been analyzed and the assignments of the normal modes of vibrations have been carried out with the help of normal coordinate analysis following the scaled quantum chemical force field methodology. The observed spectral shift substantiates the spectral evidence of the intermolecular hydrogen bonding. Molecular docking scores reveal good binding affinity and the inhibition activity of the molecule against dengue viral protein 4c11.

ARTICLE HISTORY
Received 4 April 2020
Accepted 22 August 2020

KEYWORDS
Fourier transform infrared; molecular docking; molecular electrostatic potential; natural bond analysis; normal coordinate analysis; Raman

Introduction

Thiosemicarbazones have fascinated appreciable attention owing to their distinguished bonding modes, ion-sensing abilities and structural diversity.[1,2] In search of promising therapeutic agents of pharmacological importance, the compound (E)-4-[1-(2-carbamothioylhydrazinylidene) ethyl] - phenyl benzoate (CAPB) has been chosen. Thiosemicarbazone derivatives possess a prominent class of biologically active molecules by virtue of their antibacterial, antiviral, antifungal and antitumor activities.[3,4] Thiosemicarbazones were the first compound to act in the human body by inhibiting the genetic expression of a wide variety of viruses.[5] Acetophenone thiosemicarbazones have been found to be potent inhibitor against influenza and parainfluenza viruses.[6] The title compound (E)-4-[1-(2-carbamothioylhydrazinylidene) ethyl] - phenyl benzoate, which shows the presence of the acetophenone thiosemicarbazone has the capability to destroy protozoal parasites by inhibiting cysteine proteases.[7] Also, the attachment of the methyl and the phenyl group in the thiosemicarbazone moiety of the title compound provides high hydrophobicity, promotes the disruption of the mitochondrial potential prior to the death of K562 cells and lowers the toxicity for peripheral blood mononuclear cells (PBMN) indicates that the title molecule has potential therapeutic property.[8] Bz-Trp-TSC, a thiosemicarbazone derivative is used in the treatment of dengue fever.[9] Spectral analysis and reactive sites of (E)-1-(5-bromo-2- hydroxybenzylidene)semicarbazide has been reported.[10]

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*Register number: 18113162132001

Supplemental data for this article can be accessed here.

Scopus Preview

Source details

Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy

Formerly known as Spectrochimica Acta - Part A: Molecular Spectroscopy

Years currently covered by Scopus: from 1995 to 2024

Publisher: Elsevier

ISSN: 1386-1425

Subject areas: Physics and Astronomy (Instrumentation) | Chemistry (Spectroscopy) | Chemistry (Analytical Chemistry) | Physics and Astronomy (Atomic and Molecular Physics, and Optics)

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CiteScore rank 2023

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Chemistry (Spectroscopy)	#8/276	97th
Chemistry		

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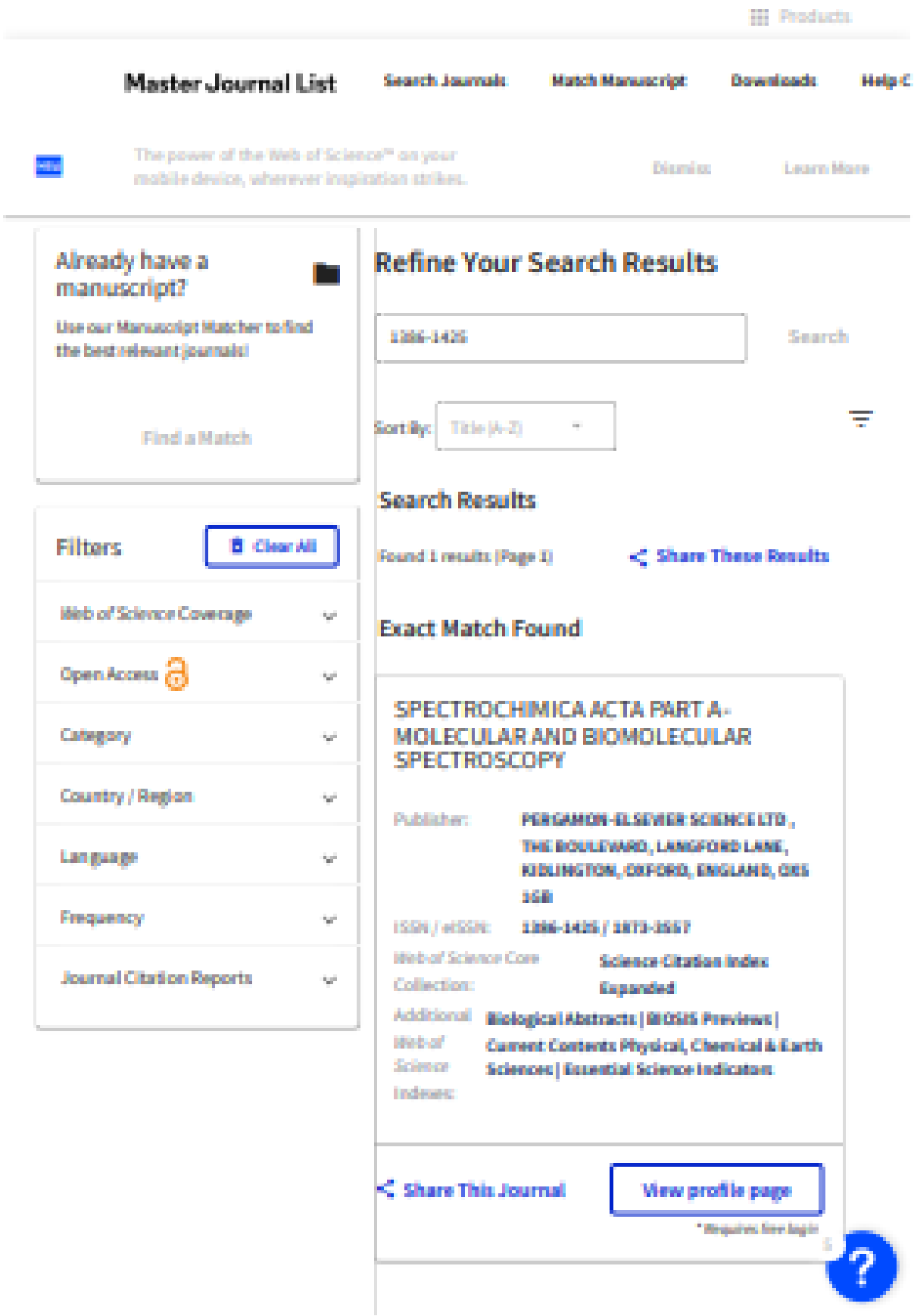
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Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

Volume 228, 5 March 2020, 117832

Spectroscopic investigation of supramolecular organometallic compound L-threonine cadmium acetate monohydrate

Abila Jeba Queen M [a b], Bright K.C [c], Mary Delphine S [a], Aji Udhaya P [a]

[a] Research department of Physics, Holy Cross College (Autonomous), Nagercoil 629004, India

[b] Register No: 12514, Manonmanium Sundaranar University, Abishekapatti, Tirunelveli, India

[c] Department of Physics, St. John's College, Anchal, Kollam 691306, Kerala, India

Received 10 October 2019, Revised 14 November 2019, Accepted 14 November 2019, Available online 15 November 2019, Version of Record 7 February 2020.

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Highlights

- A new [Cd $(C_2H_3O_2)$ $(C_4H_9NO_3)$ (H_2O)] H_2O crystal prepared by the chemical reaction between L-Threonine and Cadmium acetate.
- The asymmetric structural unit tends to increase the ionic polarization, which results better dielectric material.

Scopus Preview

Source details

Drug Invention Today

Scopus coverage years: from 2012 to 2020
(coverage discontinued in Scopus)
Publisher: JPR Solutions
ISSN: 0975-7619 E-ISSN: 0975-7619
Subject area: Pharmacology, Toxicology and Pharmaceutics: Drug Discovery
Source type: Journal

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Pharmacology, Toxicology and Pharmaceutics — Drug Discovery	#143/143	0th

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Antidiabetic activity of chelating tris n-methylethylenediamine iron complex.

- **Source:** Drug Invention Today . 1/15/2020, Vol. 14 Issue 1, p121-126. 6p. 7 Charts, 7 Graphs.

- **Author(s):** Brabha, M. Jaya; Malbi, M. Anitha

- **Abstract:** Polydentate ligand whose structure permits the attachment of their two or more donor atoms to the same metal ion simultaneously and thus produces one or more rings is called chelate. Chelates are used for the elimination of harmful radioactive and heavy metal toxicity from the body. Some of the chelating agents such as ethylenediaminetetraacetic acid, ethylenediamine, and 1,2-trans-cyclohexylenedinitrilotetraacetic acid are used in the elimination of harmful radioactive metals from the body. Chelates used in food preservation. Fruit, fruit juice, foodstuffs, etc., are now preserved with the help of chelating compounds. Supplementation of essential trace elements is an area of increasing interest in the field of human and veterinary pharmacology. In the present work synthesis of tris N-methyl ethylene diamine iron complex and confirm their application by anti-diabetic activity. The synthesized complex was characterized by elemental analysis, energy dispersive X-ray analysis, ultraviolet-visible, magnetic susceptibility, Fourier transform-infrared, thermogravimetric analysis and differential thermal analysis, and X-ray diffraction. Applications of the complex were studied by its antidiabetic activity.

Scopus Preview

Source details

Materials Today: Proceedings

Scopus coverage years: 2005, from 2014 to Present

E-ISSN: 2214-7853

Subject area: Materials Science: General Materials Science

Source type: Conference Proceeding

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$4.9 = \frac{108{,}812 \text{ Citations to date}}{22{,}228 \text{ Documents to date}}$

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CiteScore rank 2022

Category	Rank	Percentile
Materials Science General Materials Science	#259/453	42nd

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Materials Today: Proceedings

Volume 21, Part 1, 2020, Pages 514-518

An investigation on host-guest complexation of Metformin hydrochloride with hydroxypropyl-α-cyclodextrin for enhanced oral bioavailability

S. Lizy Roselet [a], J. Prema Kumari [b]

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https://doi.org/10.1016/j.matpr.2019.06.650

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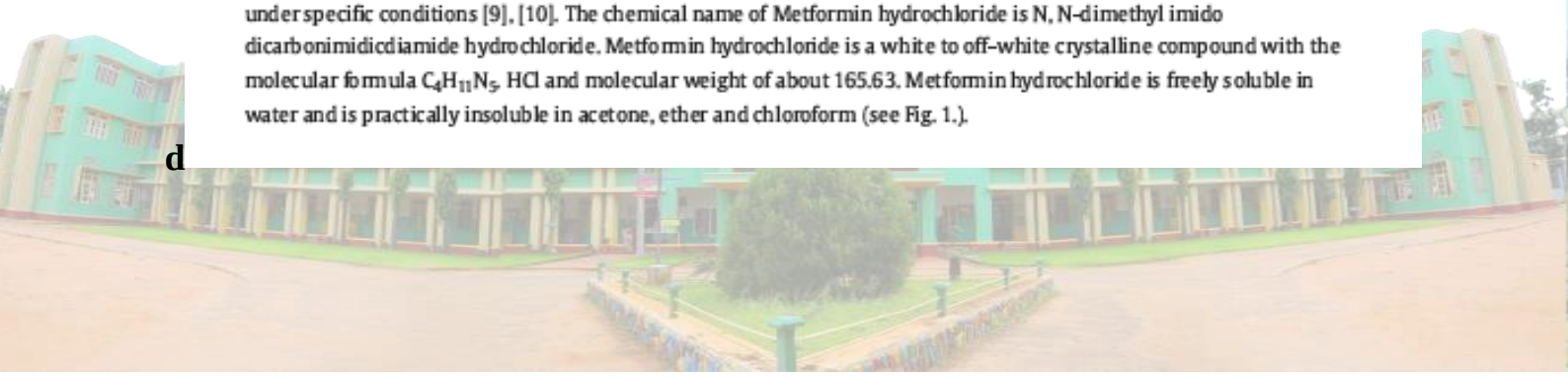
Abstract

Metformin hydrochloride is an orally administered biguanide which is an oral anti-hyperglycemic agent. It shows incomplete absorption from the gastrointestinal tract and the absolute bioavailability is 50–60% with relatively short plasma half-life of 1.5–4.5 h. In this study the host-guest complexation of hydroxypropyl-α-cyclodextrin with Metformin hydrochloride is discussed. Inclusion complexes of Metformin hydrochloride with hydroxypropyl-α-cyclodextrin were prepared in solid and liquid state and they are characterized using spectrophotometry, fluorimetry, ^{1}H NMR and phase solubility studies. The subsistence of host–guest interaction makes hydroxypropyl-α-cyclodextrin a suitable candidate for the enhancement of bioavailability of Metformin hydrochloride.

Introduction

Metformin is widely used for the treatment of type-II diabetes. Chemically, metformin is a hydrophilic base [1]. However, is usually present in oral dosage forms in its hydrochloride salt form. Metformin HCl has acid dissociation constant values (pKa) of 2.8 and 11.5 and, therefore, exists very large as the hydrophilic cationic species at physiological pH values (>99.9%) [2]. The lipid solubility of the unionized species is low as shown by its low water-oil partition coefficient value (log P = 1.43) [3]. This chemical parameter indicates low lipophilicity and, therefore, rapid passive diffusion of metformin trough cell membranes is unlikely [2]. Based on these properties, metformin HCl is defined as class III (low permeability, high solubility) by the Biopharmaceutics Classification System (BCS). Poor wettability of drug leads to poor dissolution and hence, shows variation in bioavailability. Metformin has poor flow properties. Cyclodextrins are used to form host-guest inclusion complexes with various drugs in solution or a solid state have been recognized as pharmaceutical excipients [4], [5], [6], [7]. Inclusion complexes formed with a host-guest molecule may exhibit improved chemical orbiological properties compared to the host molecule alone. Such inclusion may: (i) improve aqueous solubility, dissolution, and bioavailability [8]. Inclusion compounds of cyclodextrins with hydrophobic molecules are able to penetrate body tissues, these can be used to release biologically active compounds under specific conditions [9], [10]. The chemical name of Metformin hydrochloride is N, N-dimethyl imido dicarbonimidicdiamide hydrochloride. Metformin hydrochloride is a white to off-white crystalline compound with the molecular formula $C_4H_{11}N_5$. HCl and molecular weight of about 165.63. Metformin hydrochloride is freely soluble in water and is practically insoluble in acetone, ether and chloroform (see Fig. 1.).



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Source details

Research Journal of Chemistry and Environment

Scopus coverage years: from 2007 to Present

Publisher: International Congress of Chemistry and Environment

ISSN: 0972-0626

Subject area: Earth and Planetary Sciences: General Earth and Planetary Sciences; Chemical Engineering: General Chemical Engineering; Environmental Science: General Environmental Science; Chemistry: General Chemistry; View all

Source type: Journal

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SNIP 2022
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Category	Rank	Percentile
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Chemical Engineering General Chemical	#249/272	8th

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Indexed in: **SCOPUS, Chemical Abstracts, UGC, NAAS, Indian Citation Index etc.**
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Research Journal of Chemistry and Environment_____Vol. 24 (10) October (2020)
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Vegetable Peel Extract mediated Synthesis of Silver nanoparticles and its antimicrobial activities

Nandhini S. and Daniel Sheeba*
Department of Chemistry, Holy Cross College (Autonomous), Nagercoil-629004, Tamil Nadu, INDIA
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Abstract

Green synthesis of nanoparticles using plant extract has been proposed as a cost effective, environmental friendly and a reliable alternative to chemical and physical methods for the production of nanoparticles. The present study focuses on the green synthesis of silver nanoparticles (AgNPs) using vegetable peel extracts of Pumpkin (Cucurbita pepo) and Snake gourd (Trichosanthes cucumerina). This peel extracts acts as a reducing and stabilizing agent for the production of silver nanoparticles. The aqueous peel extracts of these vegetables are added separately to 1 mM silver nitrate solution and the formation of silver nanoparticles is primarily detected by the change of colour from colourless to reddish-brown.

The reduction of Ag^+ to Ag^0 is confirmed by UV-Visible spectrum. FT-IR spectroscopy is performed to detect the bioactive molecules liable for reduction and capping of biogenic silver nanoparticles. The nature of the particle is determined from the X-ray diffraction analysis. The antimicrobial activities of the synthesised nanoparticles are tested against human pathogens and show toxic effects on Staphylococcus aureus, Klebsiella pneumonia, Escherichia coli, Pseudomonas aerogenisa, Aspergillus and Candida albicans.

Keywords: Green synthesis, Vegetable peel extracts, Silver nanoparticles, Characterization, Antimicrobial Activities.

Introduction

Nanobiotechnology is one of the most promising areas in modern nanoscience and technology which interlaces various disciplines of science such as physics, chemistry, biology and material science. Nanoparticles are synthesized using top-down and bottom-up strategies.[1] Owing to their high surface-to-volume ratio, surface energy, spatial confinement and reduced imperfections, metal nanoparticles have characteristic physical, chemical, electrical, magnetic, thermal, optical and biological properties in contrast to the bulk materials.[2] Recent advancements in nanotechnology have led to the expansive growth in the synthesis of nanosized particles, wires, and tubes for potential applications in different fields. Due to their Surface Plasmon Resonance, Enhanced Rayleigh Scattering and Surface Enhanced Raman Scattering in metal nanoparticles, nanoparticles are considered as building blocks for the next generation of optoelectronic, electronics and various chemical and biochemical sensors.[3]

Nanoparticle synthesis are usually carried out by various physical and chemical methods like laser ablation, pyrolysis, lithography, chemical vapour deposition, sol-gel technique and electro deposition which are very expensive and hazardous.[4,5] In the traditional wet method for the synthesis of nanoparticles, hazardous substances such as sodiumborohydride, tetrakishydroxymethyl-phosphonium chloride (THPC), poly-N-vinyl pyrrolidone (PVP) and hydroxylamine have been used.

Other dry methods such as UV irradiation, aerosol and lithography are also not considered as eco-friendly. The use of toxic chemicals and non-polar solvents for the synthesis of nanoparticles limits their applications in clinical fields. Therefore, the biosynthesis of clean, bio-compatible, non-toxic and eco-friendly nanoparticles produced from both extracellularly and intracellularly deserves merit.[6]

Among noble metal nanoparticles, silver nanoparticles (AgNPs) have received considerable attention due to their attractive physiochemical properties. The use of environmentally benign materials like plant extracts, bacteria and fungi for the synthesis of AgNPs offers numerous benefits for pharmaceutical, biomedical and agricultural applications. The role of AgNPs as an anticancer agent should open new door in the field of medicine. AgNPs should serve as one of the best ways of treating diseases that involve cell proliferation and cell death.[7]

Green synthesis of AgNPs by various plants and microorganisms has been reported. However, the potential of plants as biological materials for the synthesis of nanoparticles and their compatibility to biological systems is yet to be fully explored. Researchers have achieved success in the biosynthesis of AgNPs using extracts obtained from *Anacardium occidentale, Gloriosa superba, Hibiscus cannabinus, Malva parviflora, Ocimum tenuiflorum, Sesbania grandiflora, Mangifera indica, Prosopis juliflora* and *Cocculus hirsutus*.[8-16]

Investigations on the biosynthesis of AgNPs with plant extracts have been made so far, the present study concentrates on the biosynthesis of AgNPs using vegetable peel extracts of Pumpkin (*Cucurbita pepo*) and Snake gourd (*Trichosanthes cucumerina*). Pumpkin is an excellent source of vitamin A and beta-carotene. Vitamin C is present in moderate content but no other nutrients are in significant amount. The colour of the flesh varies from golden-yellow to orange depending up on the polyphenolic pigments in it. Pumpkin peel and seeds are rich source of protein, minerals, vitamins, and omega-3 fatty acids.[17]

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Invitro Study of Ruthenium(II)-Phenanthroline-Phendione Complex on SK-MEL-28 and L6 Cell Lines

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Abstract- The *invitro* antiproliferative and cytotoxic effects of $[Ru(phen)_2(phendione)]^{2+}$ (phen = 1,10-phenanthroline and phendione= 1,10-phenanthroline-5,6-dione) complex is evaluated on SK-MEL-28 melanoma and normal L6 cell lines using MTT assay and double staining method. The antiproliferative and cytotoxic effects determined using MTT assay method on both the cell lines decreases with increase in concentration of the complex. The IC_{50} value of this complex against the SK-MEL-28 cell and normal living L6 cell line is found to be 52.648 and 90.974 µg/mL respectively. Apoptosis determination using double staining method followed by fluorescent microscopic images predicts that the synthesized $[Ru(phen)_2(phendione)]^{2+}$complex shows late apoptotic effect when treated on SK-MEL-28 cells and exhibit early apoptotic effect on normal L6 cells. The apoptotic character of $[Ru(phen)_2(phendione)]^{2+}$ complex is due to the chromatin condensation of both cancerous and normal cells by the DNA binding dyes. The results revealed that the synthesized $[Ru(phen)_2(phendione)]^{2+}$ complex shows good anti-skin cancer effect on SK-MEL-28 cell line and no cytotoxicity on L6 cell line. Thus the synthesized complex can be therefore suggested as an effective anti-skin cancer drug.

Index Terms- $[Ru(phen)_2(phendione)]^{2+}$complex, SK-MEL 28 cell line, L6 cell line, *Invitro*-antiproliferative effect, Cytotoxicity.

I. INTRODUCTION

Melanoma is a type of skin cancer with an increasing incidence and mortality rate [1]. The increased risk of melanoma is mainly related to UV exposure [2]. Melanoma can be cured by surgical excision at the early stage, however, later stages with distant metastasis is currently incurable. The development of agents capable of triggering cancer cell apoptosis may represent a novel therapeutic approach for melanoma treatment. An anticancer agent without affecting normal cells become effective and novel cytotoxic drug with low side effects on immune system induces apoptosis in cancer cells. Therefore, the search for new agents with a potential anti-melanoma effect is encouraged [3].

Ruthenium(II)-polypyridyl complexes are active against some cisplatin resistant cell lines and shows low side effects due to their higher selectivity for cancer cells compared with normal cells. Ruthenium can mimic iron in binding to some biological molecules [4]. Ruthenium (II) complexes with polypyridine ligands is of great interest due to their therapeutic values, DNA intercalation, protein binding and pharmacological applications. A series of octahedral ruthenium(II)-polypyridyl complexes containing N,N-chelating ligands, such as 2,2′-bipyridine (bpy), 1,10-phen anthroline (phen) etc are investigated based on their structure-activity relationships in DNA-binding properties and *invitro* cytotoxic effects toward human cancer cells. Therefore, Ru(II) complexes is used as an alternative to platinum complexes in cancer therapies possessing several favourable physico-chemical properties and biological applications [5,6].

Phendione a versatile bis-chelating ligand and organic linker focus mainly on the assembly of metal organic materials. The unique properties of phendione, as chelating agents plays a major role in complex chemistry. The diketone functionality can be easily transformed to other chelating groups such as a diamine or dioxime. Phendione act as redox active species due to the presence of quinonoid functionality and also act as a Lewis base due to the presence of diiminic nitrogen atoms. The *ortho*-quinone moiety of the phendione ligand may enhance the interaction with DNA *via* intercalation and hydrogen-bonding interactions [7,8].

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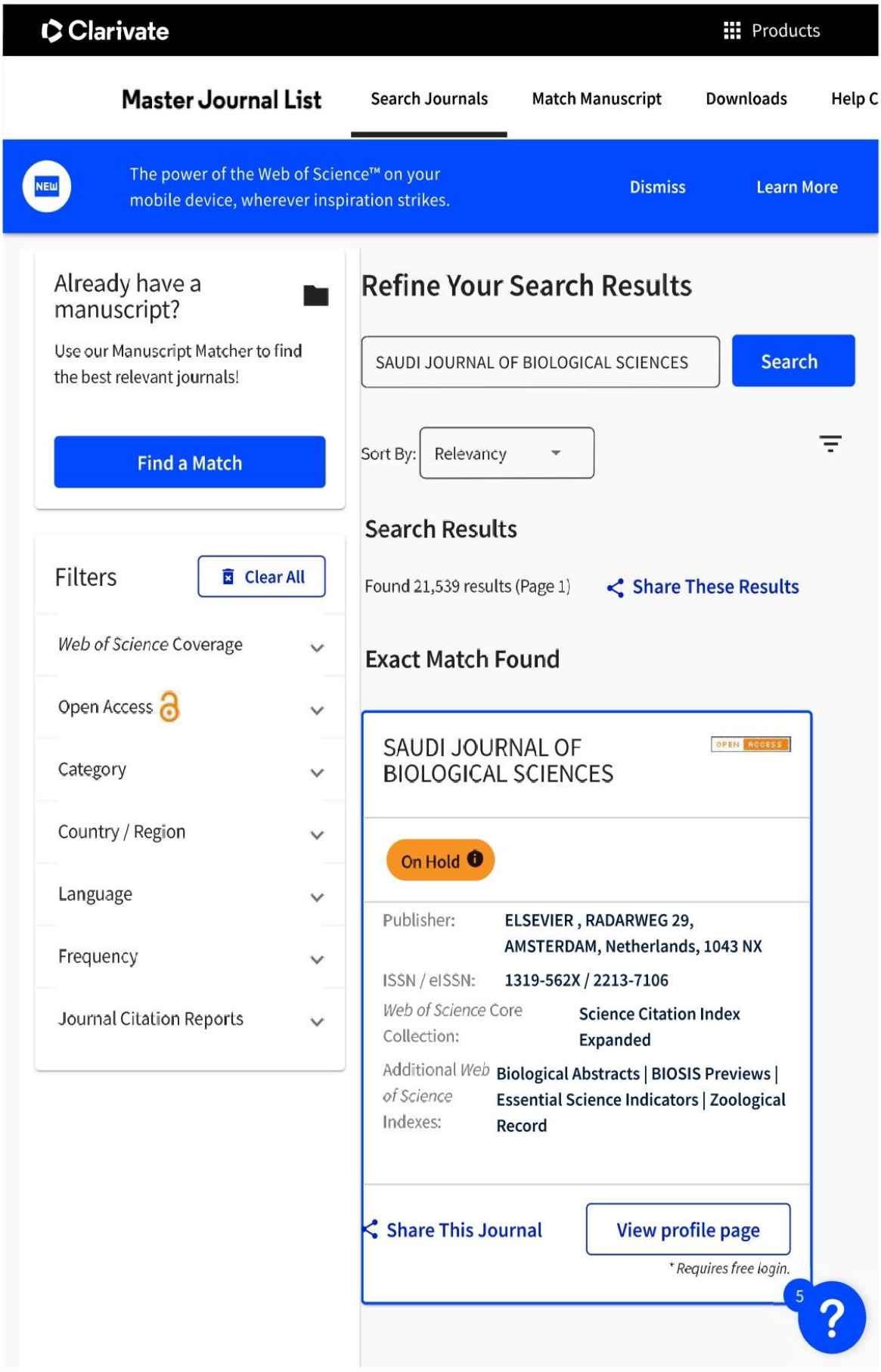
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Original article

In-vitro antibacterial, antioxidant potentials and cytotoxic activity of the leaves of *Tridax procumbens*

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ABSTRACT

The present study explored the phytochemicals, antibacterial, antioxidant and cytotoxic effect of *Tridax procumbens* leaves. The leaves were dried and extracted with various organic solvents. The leaves contained the phytochemicals such as alkaloids, carbohydrates, polyphenols and tannins respectively. Antimicrobial potentials of the extracts were determined by performing the disc diffusion techniques. Results revealed that different organic solvents extracts namely methanol, ethanol and ethyl acetate extracts documented comparatively good activity against the studied microbial strains. The methanol extract of leaves of *T. procumbens* showed combatively better antioxidant potential. The tested plant leaf extract showed high activity against human lung cancer cells than breast cancer cell lines. 250 μg/ml plants extract showed 84 ± 2.8% toxicity against human lung cancer cells.

1. Introduction

Pathogenic bacteria always developing resistance against various antibacterial drugs used presently to control many diseases (Al-Dhabi et al., 2015; Al-Dhabi and Arasu, 2016; Barathikannan et al., 2016). For this reason, biologist, chemist and pharmacologist always were trying to explore novel compounds from various natural sources. The increasing availability of medicinal plants throughout the world attracted much more attention, because these medicinal plants have various useful metabolites (Bonjar and Farrokhi, 2004; Cuong et al., 2017; Elango et al., 2017). The parts of medicinal plants such as, root, stem, flowers, leaves possess various antimicrobial properties (Elango et al., 2016; Fowsiya et al., 2016 Glorybai et al., 2015; Haritha et al., 2016). It is widely used in traditional medicine system, as insect repellent, anticoagulant, antifungal and antibacterial agent (Helan et al., 2016; Ilavenil et al., 2017; Park et al., 2016a). Also, this medicinal plant promotes growth of hairs and showed wound healing property (Park et al., 2016b). The leaf extract showed antiparasitic activity and insecticidal properties (Ravikumar et al., 2005; Park etal., 2017). This medicinal plant showed the presence of phytochemical compounds such as, β-amyron, β-amyrin, stigma sterol, lupeol, luteolin, campasterol, arachidic acid, fucosterol, palmatic acid and lauric acid (Surendra et al., 2016a; Surendra et al., 2016b; Gurusamy et al., 2019). The knowledge of traditional medicine system and combined efforts between traditional healers and modern researchers are very important to validate existing knowledge of medicinal plants in a particular geographical location (Hamill et al., 2000). In under developing and developing countries, people frequently used traditional medicine system, however, little information is available on biological role and chemical composition of medicinal plants (Tabuti et al., 2003). Herbal medicines have been used in various countries to meet health care needs (Awe and Omojalasola, 2003; Surendra et al., 2016c; Roopan et al., 2019). Medicinal plants showed various activities, including, antimicrobial activities (Abo et al., 1999). *Tridax procumbens* has immense antibacterial and antifungal potential (Ali et al., 2001; Rajkumari et al., 2019; Valsalam et al., 2019a; Valsalam et al., 2019b) This medicinal plant is widely distributed in Asia, Africa and Australia and available in almost all seasons in almost all part of the country. Traditinally, *Tridax procumbens* has been used to treat typhoid fever, fever, cough, epilepsy, asthma, and diarrhoea

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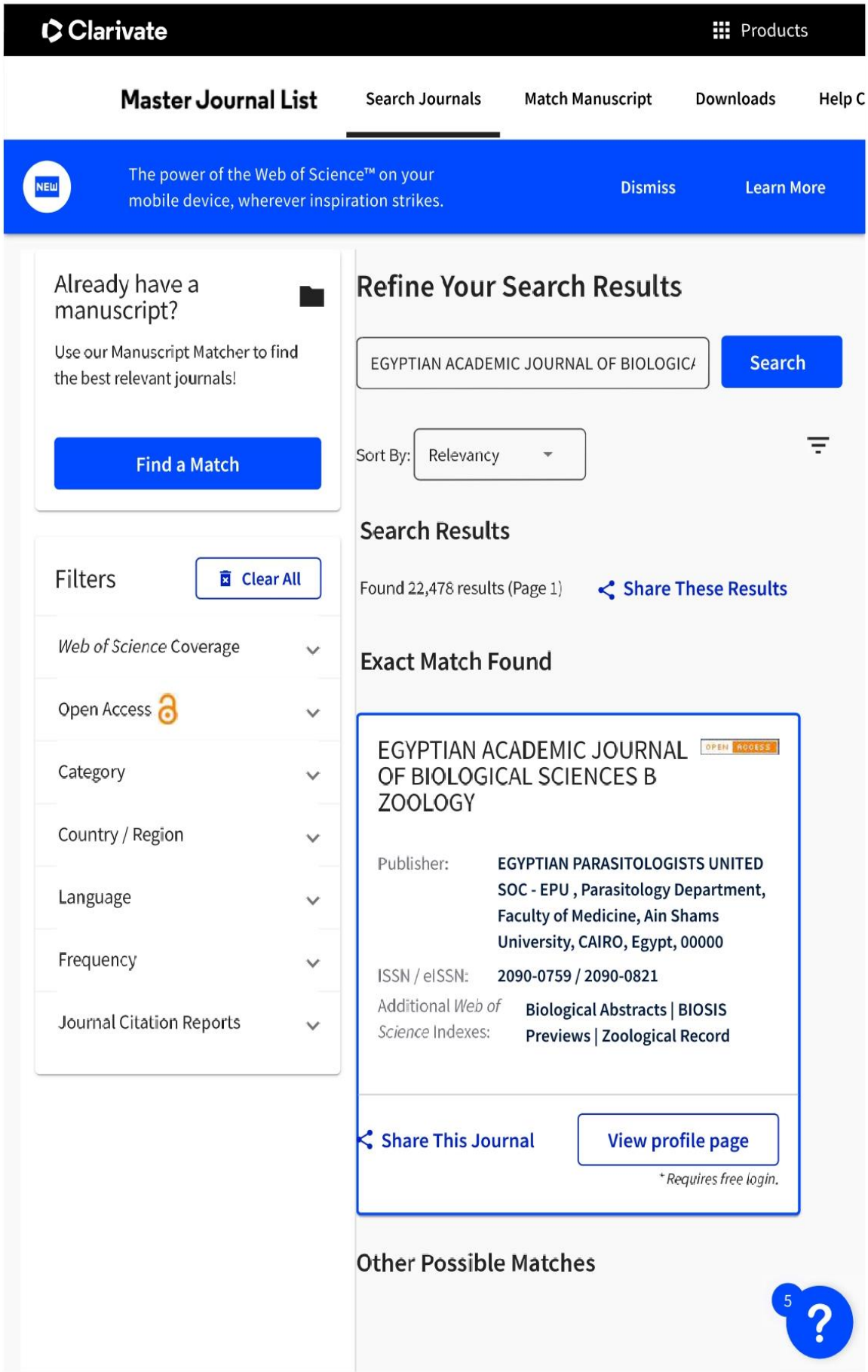
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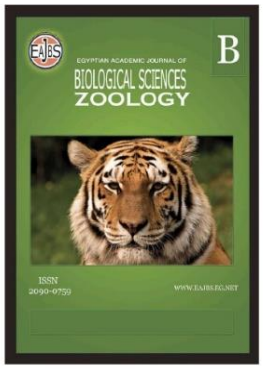

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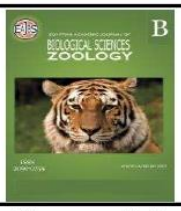

In Vivo Toxic and Teratogenic Effects of Biologically Synthesized Silver Nanoparticles in The Embryos of the Zebrafish, *Danio rerio*.

P.C. Jeba Preethi Jansi[1,*], Jeni Chandar Padua[2] and R. Regis Freeda[2]

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ABSTRACT

In the current study, AgNPs synthesized using *Bacopa monnieri* were characterized by FTIR, UV-Spectrophotometry, XRD, and SEM measurements and subjected to diverse antimicrobial and toxicity assays. FTIR spectrum confirmed the involvement of amines, phenols, alkenes, amides, aromatic, and nitro compounds in the capping and reduction of AgNPs while XRD characterized the crystalline particles presenting a spherical structure around 24nm. SEM measurements showed a spherical and polygonal structure with size ranging from 35-45 nm indicating polydispersity. Comparative toxicity assays of *Bacopa monnieri* leaf extracts with nanosynthesized AgNPs on *Danio rerio* embryos, confirmed that mortality, hatchability, heartbeat rate, teratogenicity, and embryogenicity were concentration-dependent. Lethal effects were pronounced in nanosynthesised AgNPs whereas sub lethal and teratogenic toxicity effects like lordosis, scoliosis, edema and growth retardation were expressed in 84% of the exposed models. The incidence of scoliosis was found to be higher in all concentrations suggesting a possible alteration in the WNT Genes. The antimicrobial study confirmed the toxic effect of AgNPs of *B. monnieri*. This study gives newer dimensions in the furtherance of toxicity studies on green synthesized nanoparticles.

INTRODUCTION

Nanoparticles (NPs) display a wide range of applications (Krishnasamyet *et al*., 2015; Shankar *et al*; 2016; Edison *et al*., 2019; Edison *et al*., 2012) which continue to proliferate on various fronts due to their enhanced characteristics based on size, bio-distribution, and morphology (Rajeshkumar *et al*., 2015). Plant-based NPs are found to be biocompatible, swift, and, inexpensive (Huang *et al*., 2007; Edison et al., 2018; Edison *et al*., 2016). Among the huge array of metal nanoparticles, silver (Ag) nanoparticles are found to exhibit potential properties due to their high reactivity. Silver ions attach to tissue proteins causing structural alterations in the bacterial cell wall and nuclear membrane ultimately leading to cellular deformation and death (Castellano *et al*., 2007; Alsammarraie *et al*., 2018). The present study pivots around the synthesis and characterization of AgNPs using *Bacopa monnieri*, a potent medicinal plant used for cardiac, respiratory and neuropharmacological disorders (Ghosh *et al*., 2007), evaluating its antibacterial efficacy, toxicity and possible teratogenic effects using the zebrafish, *Danio rerio* preferred for its small size, transparency, rapid embryogenesis, continuous reproduction (Choi *et al*., 2016) and suitability for *in vivo* high-throughput screening (Zhao *et al*., 2009; Scown *et al*., 2010).

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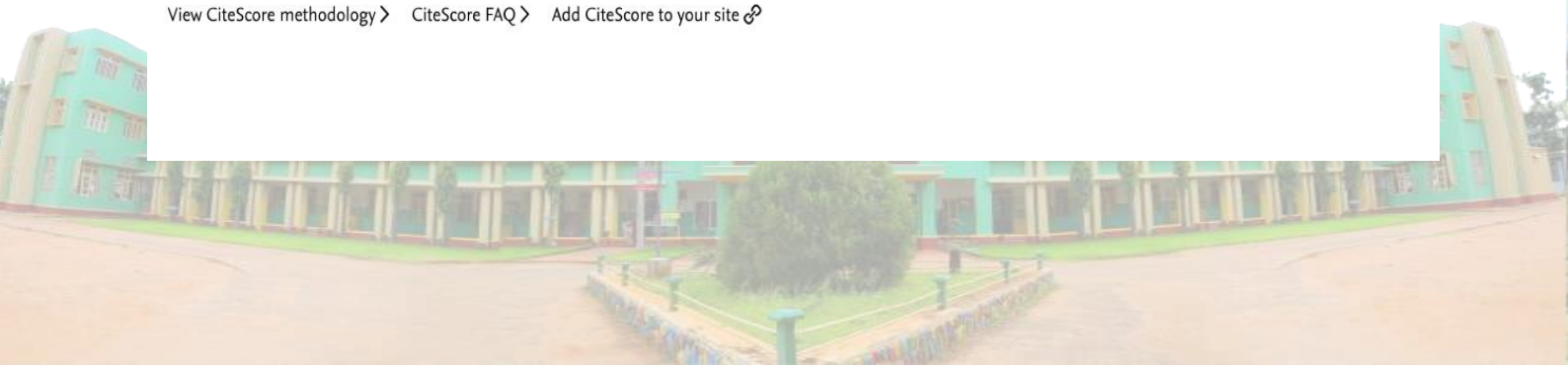

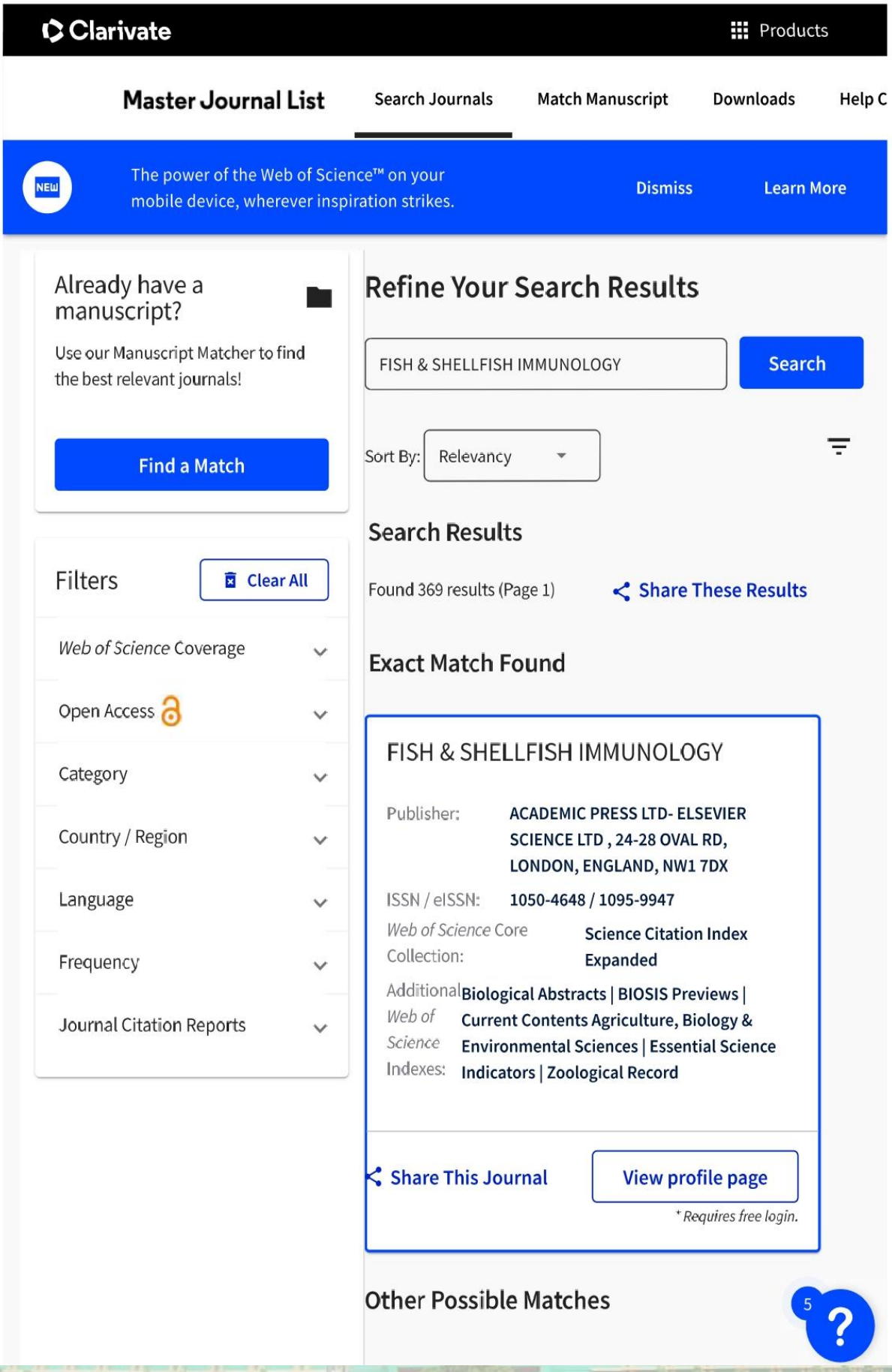
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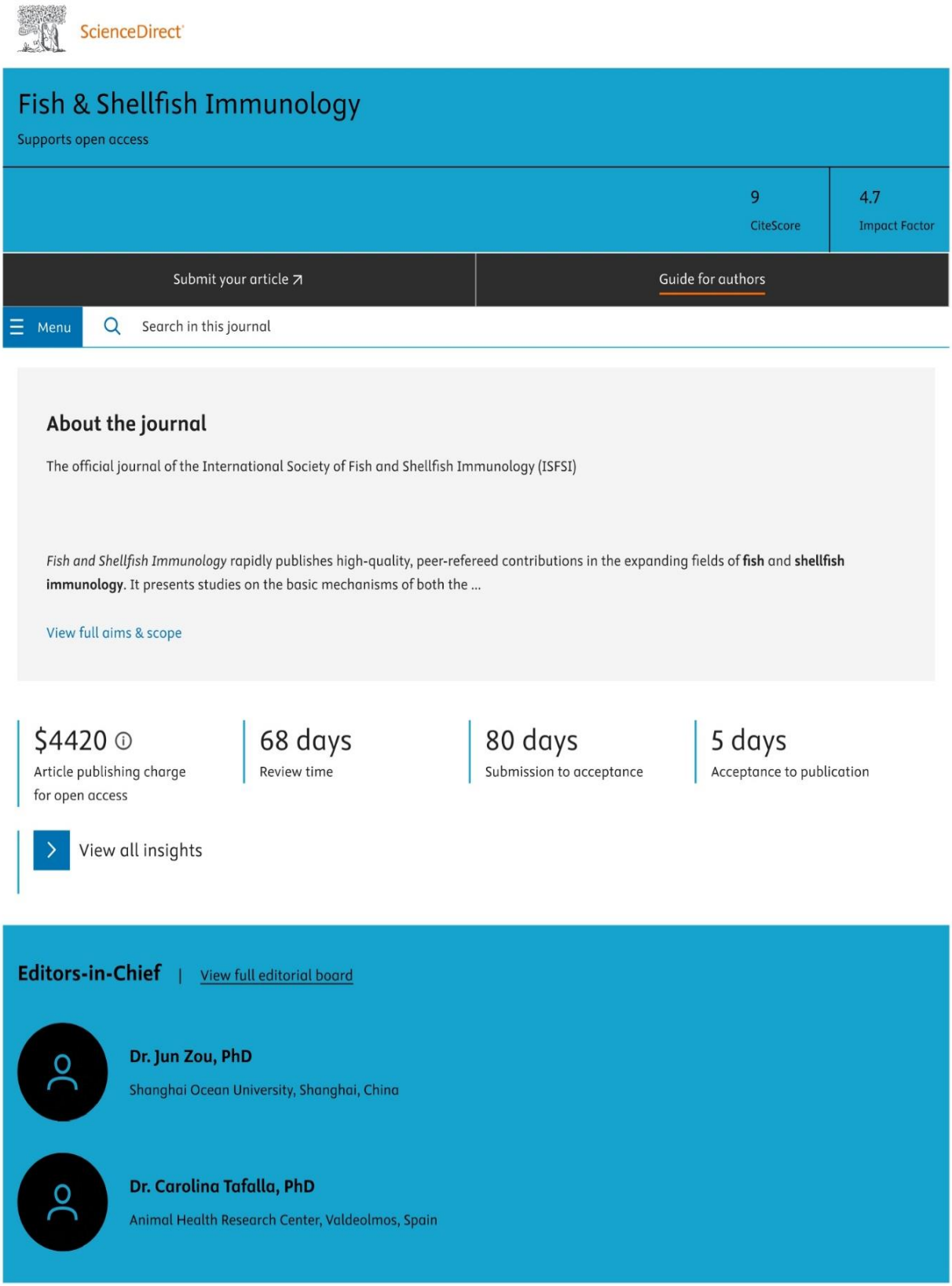

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Full length article

Characterization of a novel O-acetyl sialic acid specific lectin from the hemolymph of the marine crab, *Atergatis integerrimus* (Lamarck, 1818)

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ARTICLE INFO

Keywords:
C-type lectin
Hemolymph
Malignant cells
Sialic acid

ABSTRACT

An O-acetyl sialic acid specific lectin was purified from the hemolymph of the marine crab *Atergatis integerrimus* by affinity chromatography using BSM (Bovine Submaxillary Mucin) coupled to cyanogen bromide activated Sepharose 4B and biospecific adsorption using formalinized buffalo erythrocytes. The purified AiL (*Atergatis integerrimus* lectin) showed an 1218 fold increase in specific activity when compared to the crude hemolymph agglutinin. The lectin, on non - denaturing PAGE showed a single band of 216 kDa and when subjected to SDS - PAGE, the lectin resolved into three subunits of molecular weight 70, 72 and 74 kDa. Physico chemical characterization revealed the lectin as pH and temperature sensitive, calcium dependent and sensitive to calcium chelators. Based on the calcium dependency of the lectin, AiL could be classified as a C-type lectin. The purified lectin agglutinated buffalo erythrocytes with greater avidity and was inhibited by the glycoproteins BSM, thyroglobulin, fetuin, PSM, and sugars raffinose, trehalose, L - fucose, α - Lactose, melibiose and GluNAc suggesting the affinity of the lectin to sialic acid. Reduction in HA with asialo buffalo erythrocytes and HAI titer with desialylated BSM, confirms the sialic acid specificity of the lectin. The reduction in HAI following de - O - acetylation confirms the specificity of the lectin for O - acetyl sialic acid. FTIR analysis confirms the purified lectin as a glycoprotein with spectral bands corresponding to amide bands and saccharides. Thus this study paves way to assess the therapeutic application of this lectin that could be targeted to modified sialic acid moieties that are expressed on the malignant cells and pathogenic microbes and also deduce the crystal structure of the lectin.

1. Introduction

Lectins are ubiquitous glycoproteins of non - immune origin that recognize specific carbohydrate structures and agglutinate a variety of animal cells by binding to cell surface glycoproteins and glycolipids [1]. Lectin - carbohydrate interaction represents a ligand - receptor interaction that is universal in all living organisms [2] and such interactions aid in different biological roles like cellular and tissue transport of carbohydrates, glycoproteins and calcium [3], cytolytic and cytotoxic [4] and cell adhesion, migration and apoptosis [5]. They are capable of inducing cell proliferation, cell arrest or apoptosis and have been implicated in organ morphogenesis, tumor cell metastasis, leukocyte trafficking, immune response and inflammation, as well as recognition of extracellular matrix [6]. Lectins isolated from animal tissues were investigated as apoptotic agents, immunomodulatory, antiviral and importance owing to its function which includes induction of apoptosis, negative regulation of B cell signaling, induction of cytokine secretion [8] and inhibition of bacterial and viral sialidases by altering the immunopotency of sialoconjugates expressed on the microbial surface [9]. Sialic acids are a family of sugars with more than twenty derivatives which differs only in the acyl substitution of the C-5 amino group and O-substituted sialic acids exhibit species and tissue specific distribution [10]. O-acetylation of sialic acids may change with transformation or alteration in the environment of the cell [11] and modified sialic acids such as 9-O-acetyl sialic acid, N-glycolyl neuraminic acid and α-2,6 sialic acids have been detected in human malignant cells [12]. Among arthropods, crustaceans were found to be rich source of sialic acid specific lectins. Lectins have been purified from many brachyuran crabs that are sialic acid specific [13,14]. A 9-O-acetyl and 4-O acetyl sialic acid specific lectin was purified from the hemolymph of marine crab *Cancer*

Scopus Preview

Source details

Annals of Tropical Medicine and Public Health

Scopus coverage years: from 2009 to 2020
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ISSN: 1755-6783 E-ISSN: 0974-6005
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Category	Rank	Percentile
Medicine Public Health, Environmental and Occupational Health	#466/516	9th

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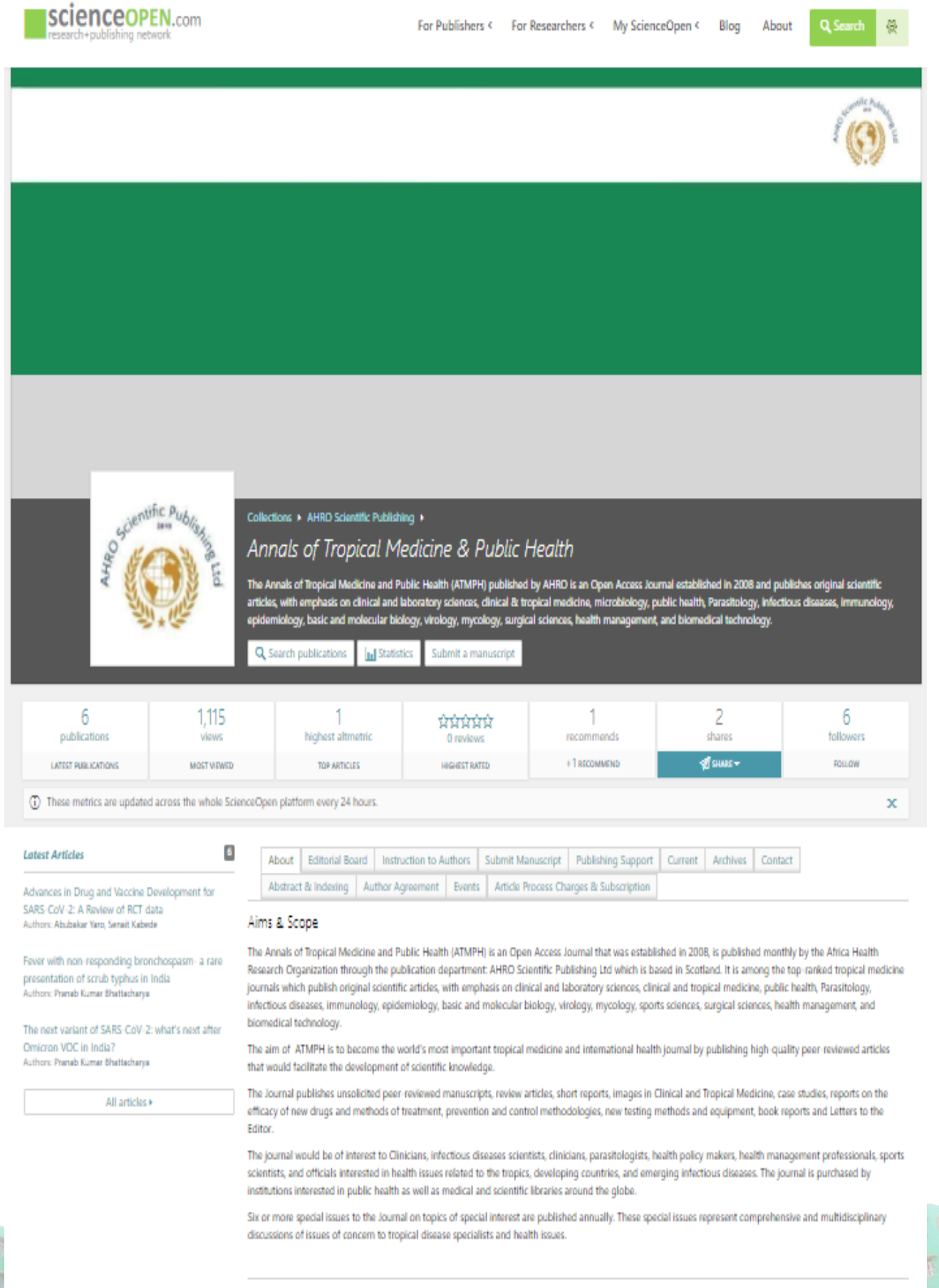
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Bai & Rose (2020): Purification and characterization of hemolymph lectin April 2020 Vol. 23 Issue 7

Purification and Characterization of Hemolymph Lectin of Freshwater Crab, Lamella Lamellifrons (Alcock, 1909)

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ABSTRACT

Lectins offer novel biomaterials useful in therapeutics and understanding animal lectins is of high value in the field of protein chemistry and designing new drugs on the principle of protein-carbohydrate or protein-protein interaction. The objective of this study was to isolate and characterise a brachyuran crab lectin. A 68 kDa O-acetyl sialic acid specific lectin, lamellin was purified from the hemolymph of the freshwater crab, *Lamella lamellifrons* using single step affinity chromatography. Lamellin strongly agglutinated rabbit and buffalo erythrocytes and was inhibited by BSM followed by bovine and porcine thyroglobulin. The optimum activity of the lectin was achieved between pH 7-7.5 and temperature 30-40^{0}C. The purified lectin was calcium dependent, sensitive to EDTA and had marked specificity to the O-acetyl group of sialic acid which was validated with a range of assays such as hemagglutination (HA), hemagglutination inhibition (HAI), de-O-acetylation and neuraminidase treatment of the glycoprotein inhibitors. Purification of a sialic acid-specific lectin with a strong affinity for O-acetyl group will find immense application in recognising pathogens and tumor cells.

Key words: affinity purification, agglutinin, hemagglutination, glycocalyx, sialic acid

How to cite this article: Mai SMM, Rose MRB (2020): Purification and characterization of hemolymph lectin of freshwater crab, lamella lamellifrons (Alcock, 1909), Ann Trop & Public Health; 23 (7): 1174-1187. DOI: http://doi.org/10.36295/ASRO.2020.23743

INTRODUCTION

The invertebrate immune system relies on non-self-recognition molecules to ensure efficient defense responses against infectious pathogens that continuously threaten their survival. Lectins are ubiquitous molecules found in nature among an array of non-self-recognition molecules. They are a class of carbohydrate - binding proteins, known to play crucial roles in cell - cell recognition events, triggering several important cellular processes, encompassing different members that are diverse in their protein structures, carbohydrate affinities and specificities (Laija et al., 2010) and known for their larger biological roles and potential applications (Dharmendra Kumar and Yashoda Mittal, 2011; Rabia Hamid et al., 2013; Chernikov et al., 2013; Debjani Datta et al., 2016). Because of their diagnostic potentials (Pramanik et al., 2010; Yu-Chieh Wang et al., 2011) and therapeutic applications (Na et al., 2011; Liqin Wu et al., 2014; Breitenbach Barroso Coelho, 2018) there is a marked interest in identifying lectins with diverse specificity.

The unique feature of brachyuran crab lectins is its property to interact with diverse species of sialic acids (Mercy and Ravindranath, 1993). Sialic acids form the glycocalyx on vertebrate cell surfaces and secreted glycan molecules (Varki, 2007) and get altered on neoplastic transformation. Altered expression of sialic acid types or their linkages can have prognostic significance clinically as these altered expression can alter cell-cell and cell-extra cellular matrix (ECM) interaction, thereby affecting cell adhesion and migration, and can contribute to tumor development and malignancy (Maria Hedlund et al., 2008). Considering the importance of sialic acids in cell sociology (Lloyd, 1975), a lectin which specifically recognizes terminal sialic acid residues is likely to be a useful analytical tool in studying the biological functions of sialoglycoconjugates.

Sialic acid specific lectins are reported in the hemolymph of a number of brachyuran crabs (Ravindranath et al., 1985; Fragkiadakis and Stratakis, 1997; Kongtawelert, 1998; Maghil Denis et al., 2003; Kim et al., 2006; Na et al.,

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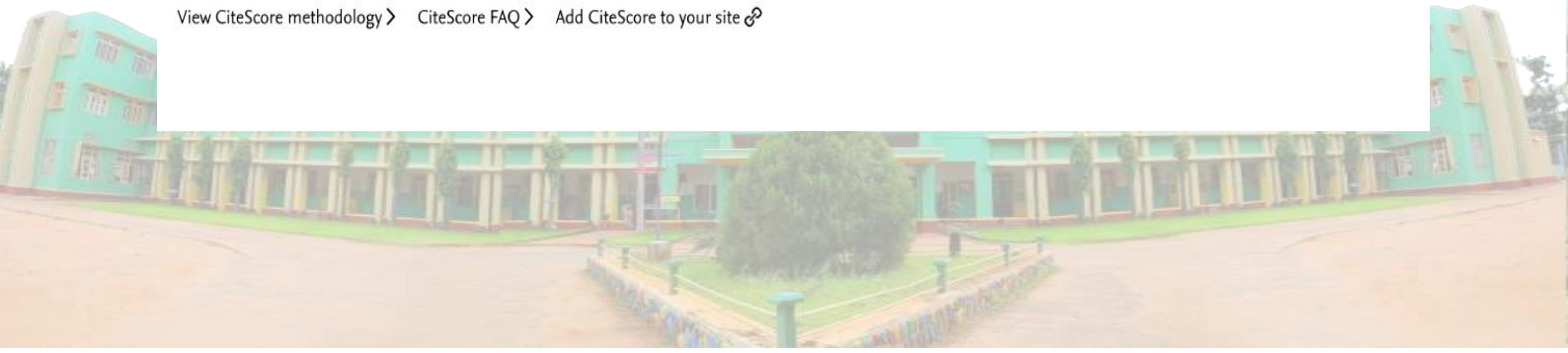

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Dystopian Society: Thwarted Life in Mahesh Dattani's *Clearing the Rubble*

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Research Supervisor, P. G. and Research Dept. of English,

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Abstract

The paper entitled, "Dystopian Society: Thwarted Life in Mahesh Dattani's *Clearing the Rubble*." vividly pictures the social discrimination prevailing in India with reference to Mahesh Dattani's radio play, *Clearing the Rubble*. This paper exemplifies the unfair treatment received by the economic and religious minorities, even at the time of natural calamities. This play is set up at the backdrop of the terrible earthquake in Bhuj, Gujarat in January 2001. This paper also aims at exhibiting the various kinds of class, religious and economic discriminations found in the Indian society and also traces the reason why rescue fails. This study further shows that religion and poverty has become a torturous weapon against the people more than the natural trauma.

Keywords: Discrimination, hindu, muslim, powerless, victim, voiceless

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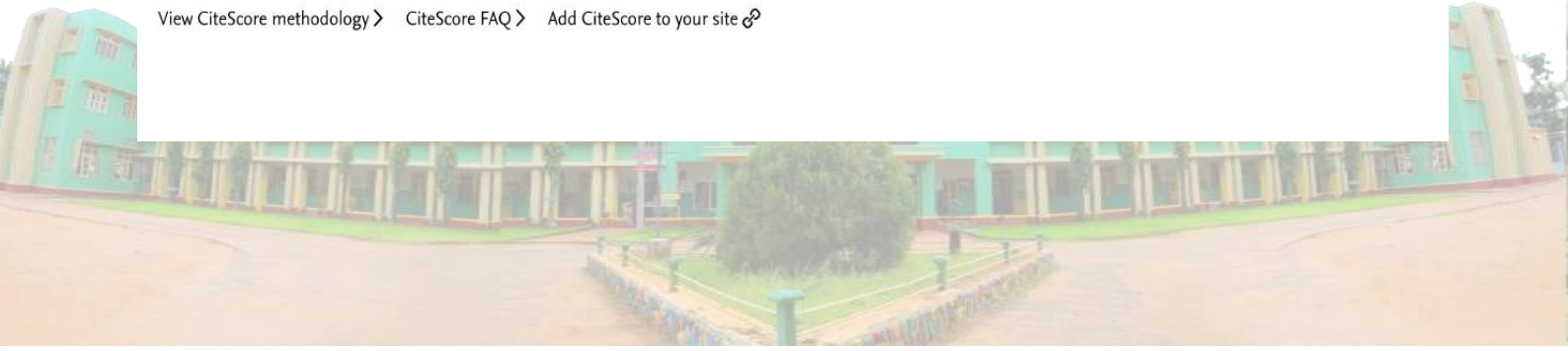

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Destructive Desire in Kazuo Ishiguro's *When We Were Orphans*

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Abstract

The paper entitled "Destructive Desire in Kazuo Ishiguro's *When We Were Orphans*" takes a gander at ways by which desire is been ruinous. Christopher Banks, the central character is a detective who comes up short at discovering his parents and simultaneously narrates his own life in a way better to analyse. As an orphan, Banks couldn't achieve in characterising himself through his past and his nationality which he seems to be associated with his past as well. Likewise, he is an untrustworthy storyteller whose memory is the main access to his story which is set in the midst of many grieved past experiences. This paper also highlights the ways in which Banks' own desire turns to be a great hindrance for him to gain a fulfilled living.

Keywords: Desire, discovering, untrustworthy, experiences, hindrance.

"Desire is the kind of thing that eats you and leaves you starving." -Nayyirah Waheed

Desire is a key idea in contemporary way of thinking about mind or psyche, which is fascinatingly understudied. There is nothing extraordinary about human wants. Human want is

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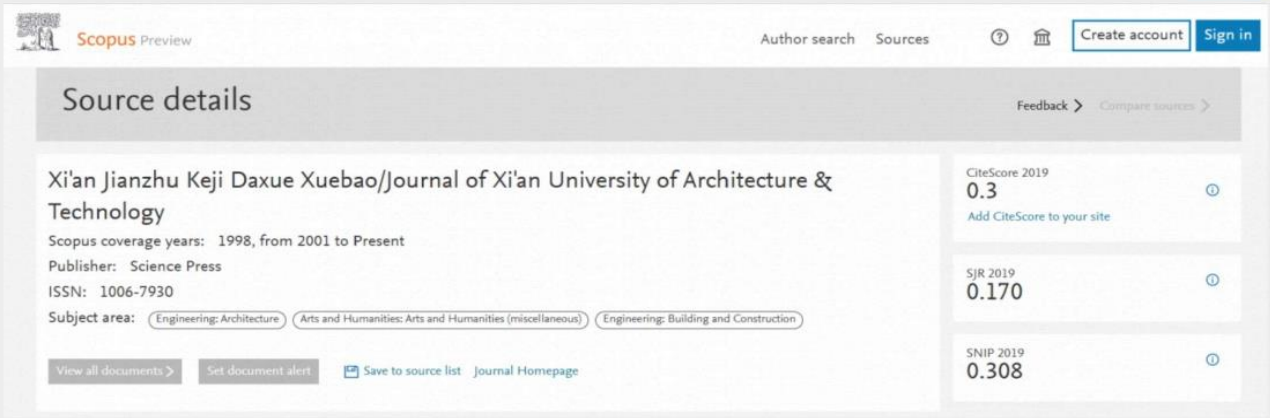

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ORIGINAL RESEARCH PAPERS – WAYS AND MEANS TO HONE THE ART OF WRITING

Dr. R. Abilasha, Assistant Professor of English, Holy Cross College (Autonomous), Nagercoil, Tamilnadu, India.

Dr. M. Ilankumaran, Professor of English, Noorul Islam Centre for Higher Education, Kumaracoil, Thuckalay, Tamilnadu, India.

Abstract

Writing is a personal activity but a public service. Writing academic papers is a hard task requiring the vocabulary skill. It involves a high level of language command and a careful scrutiny. Writing an essay is different from that of an Original Research Paper (ORP). Writing ORP is an academic activity that includes a variety of sources to support the point of writing. It becomes a troublesome one if the preparation and expertise on the topic are insufficient. An essay simply reveals the knowledge and perception of the writer who simply supports or opposes the arguments on the topic. In ORP, sources play a vital role and they form a part of course work. Personal interpretation and arguments ought to be based on works of different authors through their books, articles and theses. The writer has to evaluate and synthesize the works taken from the sources. The students at college level are expected to write at least one research paper before they graduate. It can be a daunting one if they have not done it before. This paper has been penned to aim at providing a lead to the research aspirants and others in finding ways to enhance their skills in writing ORPs by developing the vocabulary pertaining to the academic writing.

Keywords: Topic, Tools, Sources, Strategy, Activities, Writer's Block, Procedures, Methodology, Writing Instructions.

Introduction

Writing a research paper is a frightening process for many beginners. One of the stumbling blocks is about how to start writing a paper. Writing Original Research Paper has to present the ideas earned through the information or data collected from various sources. The way the materials are gathered will open up avenues to make up-to-date findings and judgments in terms of original interpretations. It is nothing but a process of interaction between the data collected in

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Journal of Critical Reviews

Scopus coverage years: from 2019 to 2020

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GREEN PACKAGING: A PRACTICE OF SUSTAINABLE MANAGEMENT IN CONSUMER PERSPECTIVE

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ABSTRACT

The present situation of the planet pushes forward everyone to be more eco friendly. It urges us to be more eco conscious person. Due to various environmental issues like global warming, marine pollution, extinction of species, destruction of ozone layer, climatic changes and other natural disaster everyone as a consumer and as a manufacturer are aspire to practice sustainable management concept in all walk of life. Therefore green packaging is one of the ways to attain sustainability. So the consumers in general are conscious of their health and wellbeing. Hence they look for green products and services which are free them from hazards to their health and provide them an eco friendly ambience. For such benefits they are willing to pay an extra premium to green products and services. Hence it is the prime responsibility of the manufacturers and consumers to produce and consume the products which have environmental benefits to the society at large. Therefore this research paper focuses on addressing the consumers, manufactures and policy makers about the extent of pollution in and around coastal villages which affect the human and the living creatures. The data was collected with the help of an interview schedule. Proportionate stratified random sampling method was used to represent 395 respondents from the population of three taluk in Kanyakumari district, India. The result of the analysis indicates that the income group between₹10,001- ₹20,000 respondents having more concern for future generation. Which shows that even the low income group has more concern for future generation and safety of the environment, thus it reflects in their behaviour. This paper too offers few suggestions to the policymakers, manufactures and the end consumers to follow the practice of sustainable management by way of green packaging.

Key words: green packaging, sustainable packaging, eco-friendly packaging, green consumers, Global consumers, sustainable development, sustainable management.

Introduction

There is a globally link between these three concepts 'Green packaging', 'sustainable management' and 'the consumer'. The word sustainable management is the ability to maintain the economic viability and nourishing the needs of the present and future generations by limiting resources. This application can be practiced in three categories that are businesses, agriculture and society. Society which comprises of people that is consumers and they are the king of every business. As ever growing environmental issues such as global warming, pollution and the depletion of natural resources threatening the very existence of humankind, the consumers must learn to reduce, reuse and recycle in order to protect our planet. Green packaging is the practice of sustainable management in day today life of every consumer to avoid such issues. Using non green packaging is unsustainable because it creates pollutants, but using green packaging which is biodegradable can solve the problem of pollution. This