RJC

RASĀYAN *J. Chem.*
Vol. 15 | No. 2 |1503-1508| April - June | 2022
ISSN: 0974-1496 | e-ISSN: 0976-0083 | CODEN: RJCABP
http://www.rasayanjournal.com
http://www.rasayanjournal.co.in

MOLECULAR DOCKING AND BIOLOGICAL ACTIVITY OF N-(4-METHOXY)-BENZOYL-N'-PHENYLTHIOUREA AND N-(4-TRIFLUORO)-BENZOYL-N'-PHENYLTHIOUREA AS ANTI-BREAST CANCER CANDIDATES

D. Kesuma[1], Siswandono[2] and A. Kirtishanti[3,]✉

[1]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Universitas Surabaya, Surabaya, Indonesia, 60293.

[2]Department of Medicinal Chemistry, Faculty of Pharmacy, Universitas Airlangga, Surabaya, Indonesia, 60286.

[3]Department of Clinical and Community Pharmacy, Faculty of Pharmacy, Universitas Surabaya, Surabaya, Indonesia, 60293.

✉Corresponding Author: aguslina@staff.ubaya.ac.id

ABSTRACT

Current breast cancer therapy does not always work optimally, and cases of resistance have been reported. Therefore, it is imperative to develop new effective drugs with minimal side effects through predictions of the epidermal growth factor receptor (EGFR) signalling pathway inhibition. Among chemicals with the potential as anticancer candidates for breast cancer are phenylthiourea derivatives. In this study, two phenylthiourea derivatives were synthesized: N-(4-methoxy)-benzoyl-N'-phenylthiourea and N-(4-trifluoromethyl)-benzoyl-N'-phenylthiourea. These compounds were docked with the EGFR receptor (code: 1M17.pdb) to predict their cytotoxic activity *in silico* using AutoDock tools. Furthermore, the microculture tetrazolium technique (MTT) was used to investigate *in vitro* cytotoxicity against MCF-7 cells. The *in silico* test revealed that the compounds N-(4-trifluoromethyl)-benzoyl-N'-phenylthiourea and N-(4-methoxy)-benzoyl-N'-phenylthiourea had a binding score of -8.2 and -7.3 kcal/mol, respectively, and the *in vitro* cytotoxic activity testing showed IC_{50} values of 0.37 mM and 0.38 mM, demonstrating significant EGFR inhibitory activity in MCF-7 cells. Therefore, it can be concluded that N-(4-trifluoromethyl)-benzoyl-N'-phenylthiourea has better cytotoxic activity than N-(4-methoxy)-benzoyl-N'-phenylthiourea.

Keywords: Molecular Docking, Cytotoxic Activity, Breast Cancer, Phenylthiourea.

RASĀYAN *J. Chem.*, Vol. 15, No.2, 2022

INTRODUCTION

Breast cancer is the most prevalent cancer in the world, which, together with lung cancer and colorectal cancer, is among the top five leading causes of cancer-related mortality.[1] The increasing number of new breast cancer cases is a health problem that needs immediate attention. Breast cancer treatment is generally a combination of radiotherapy, surgery, and chemotherapy. Therapy options depend on the cancer stage: radiotherapy and surgery for early-stage cancers and chemotherapy for advanced cancers. However, because drug options and undesirable side effects are known limiting factors of chemotherapy[2,3], it is thereby necessary to develop novel chemotherapy drugs with higher anticancer activity and minimal side effects. The development of anticancer drugs is currently towards growth factor receptor (GFR)-targeted therapy. Epidermal growth factor receptor (EGFR)/HER1 plays an essential role in delivering signals needed in cell proliferation. Changes in the EGFR regulatory system and a mutation in the EGFR gene can cause overexpression of EGFR, resulting in uncontrolled cell growth, as seen in several types of cancer, including breast cancer.[4,5] EGFR overexpression in approximately 40% of breast cancer patients correlates with a poor clinical prognosis.[6] Chemotherapeutic agents that have been developed for breast cancer therapy include thiourea and phenylthiourea derivatives. After synthesizing several phenylthiourea derivatives, Li discovered that N-(5-Chloro-2-hydroxybenzyl)-N-(4hydroxybenzyll)-N'-phenylthiourea inhibits the enzymatic activity of EGFR (IC_{50} = 0.08 mM) and HER-2 (IC_{50} =0.35 mM). In addition, these compounds

http://doi.org/10.31788/RJC.2022.1526836

can inhibit the proliferation of MCF-7 cells.[7] In a different study, Huang synthesized thiourea-derived compounds and observed their cytotoxic activity against the NCl-H460, A549, HepG3, and SKOV3 cell lines. The results indicated that thiourea-derived compounds have greater anticancer activity than 5-fluorouracil.[8] In this study, two phenylthiourea derivatives were synthesized, namely N-(4-methoxy)-benzoyl-N'-phenylthiourea (4-OCH_3-BPTU) and N-(4-trifluoromethyl)-benzoyl-N'-phenylthiourea (4-CF_3-BPTU). Before the synthesis, their cytotoxic activity was predicted *in silico* (molecular docking) using the AutoDock Vina 1.2.program. The phenylthiourea derivatives were docked with EGFR (PDB: 1M17) with the erlotinib as the original ligand.[9] A smaller Binding Score (BS) obtained from the molecular docking indicates lower binding energy of the docked compounds, which means that the ligand-receptor bonds are more stable and produce greater activity.[10] Infrared (IR), ^{1}H-NMR, ^{13}C-NMR, and mass spectrometers were used to identify the two synthesized compounds.[11,12,13] To determine the *in vitro* cytotoxic activity of the two compounds against MCF-7 cells, the microculture tetrazolium technique (MTT) was used.[14,15] The IC_{50} values derived from this process were then compared with those of hydroxyurea (HU, the simplest compound first synthesized from urea) and erlotinib. Here, erlotinib was selected as a comparison compound because it has been used clinically to stop the growth of cancer cells. In addition, the selectivity of the synthesized compounds for cancer cells was observed using normal cells, namely Vero cells. This study was designed to obtain new compounds derived from phenylthiourea as anticancer candidates for breast cancer by predicting whether or not and to what extent they inhibited EGFR signalling.

EXPERIMENTAL

Molecular Docking

MarvinSketch v. 19.17.0 was used to draw the chemical structures of 4-OCH_3-BPTU and 4-CF_3-BPTU. Afterward, Avogadro v. 1.2.0 was used to convert the derived 2D sketches into 3D form for docking. Finally, the geometric structures of both compounds were optimized using the Merck molecular force field (MMFF94) and then stored in mol2 file format.

Prediction of *In Silico* Cytotoxic Activity

The compounds, 4-OCH_3-BPTU and 4-CF_3-BPTU, were docked with EGFR receptor (PDB: 1M17) in the AutoDock Vina 1.2.0 program to predict the *in silico* cytotoxicity activity. Furthermore, the binding scores generated by the docking were observed for any similarity with those of HU and erlotinib for comparison.

Synthesis

N-phenylthiourea was reacted with triethylamine (TEA) and 4-methoxy or 4-trifluorobenzoyl chloride in tetrahydrofuran (THF). In a water bath, the mixture was refluxed, then the sample was applied on thin-layer chromatography (TLC) plate. TLC was performed every hour until a spot appeared on the plate. This process was followed by THF evaporation and then recrystallization[16] IR, ^{1}H-NMR, ^{13}C-NMR, and HRMS spectroscopy techniques were used to identify the structure of the synthesized compound.[11,12]

Cytotoxic Activity against MCF-7 Cells

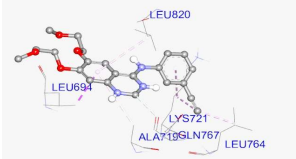
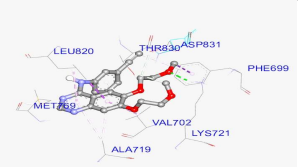
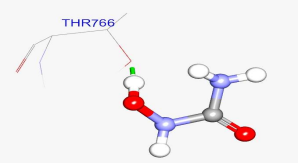
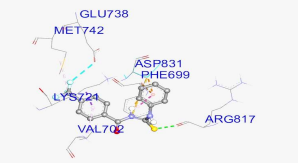
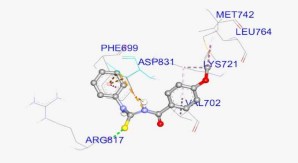
Cultures of MCF-7 breast cancer cells and normal cells, i.e., Vero cells, were grown on 96-well plates for a 24-hour incubation in a CO_2 incubator. Afterward, various concentrations of the test compounds, HU and erlotinib were added to the 96-well plates. A culture medium that did not contain MCF-7 and Vero cells was used as a control. The microplate to which the test compounds, HU and erlotinib were added was then re-incubated for 24 hours. The next step was inverting the microplate at 180°C to remove the media in the wells and washing each well with 100 µL of PBS; in this process, the PBS was discarded. Then, the microplate was added with the MTT reagent (100 µL, 0.5 mg/mL) and incubated for 4 hours. Following the incubation was the addition of 100 µL of 10% SDS in 0.01 n HCl into each well to dissolve the formed formazan crystals, stopping the MTT reaction. After wrapping the microplate in a paper, it was incubated at 37°C for 24 hours; finally, the absorbance was measured and read at 595 nm using an ELISA reader and the surviving fraction was calculated.[17,18] Probit analysis was used to determine the IC_{50} values of the two synthesized compounds, HU and erlotinib for MCF-7 cells and Vero cells.[14] The selectivity of the synthesized compounds for cancer cells was calculated as a ratio of the IC_{50} for normal cells to the IC_{50} for cancer cells.

RESULTS AND DISCUSSION

In Silico Cytotoxic Activity

Table-1 shows the *in silico* test outcome of the compounds 4-OCH_3-BPTU, 4-CF_3-BPTU, HU, and erlotinib. The method validation obtained a root-mean-square deviation (RMSD) value of 1.02 A^0, which meets the validation requirements[21]. As seen in Table-1, 4-OCH_3-BPTU (-7.3 kcal/mol) and 4-CF_3-BPTU (-8.2 kcal/mol) had a lower binding score (BS) than HU (-3.8 Kcal/mol). Compared with erlotinib (-7.5 kcal/mol), 4-CF_3-BPTU had a lower BS, while 4-OCH_3-BPTU had a slightly higher BS. The -OCH_3 group at the para position has low lipophilic and electronic properties but can substantially boost electrons; thus, adding the -OCH_3 group results in BS that is only slightly higher than or almost similar to erlotinib but smaller than HU. On the contrary, the –CF_3 group at the para position has high lipophilic and electronic properties and high electron-withdrawing capabilities. Therefore, with the addition of the –CF_3 group, the resultant *in silico* cytotoxic activity was proven greater than the compound added with the -OCH_3 group.

Table-1: *In Silico* Test Results: Binding Scores and Interaction Binding of 4-OCH_3-BPTU, 4-CF_3-BPTU, HU, and Erlotinib

Substituents	Binding Scores (kcal/mol)	Interaction Binding
1M17 (Ligand: AQ4)	-7.5	
Erlotinib	-7.5	
Hydroxyurea (HU)	-3.8	
4-CF_3-BPTU	-8.2	
4-OCH_3-BPTU	-7.3	

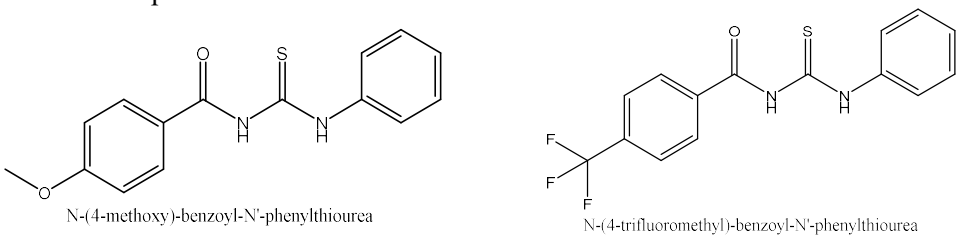
Synthesis

The compounds 4-OCH_3-BPTU and 4-CF_3-BPTU were synthesized from 4-methoxy and 4-trifluorobenzoyl chloride with N-phenylthiourea, producing shiny white, water-insoluble crystals. Figure-1 shows the structure of the synthesized compounds, with the details presented in Table-2.

In vitro Cytotoxic Activity

As presented in Table3, the compounds 4-OCH_3-BPTU and 4-CF_3-BPTU had an IC_{50} value of 0.38 and 0.37 mM, respectively, indicating higher cytotoxic activities than HU (IC_{50} = 9.76 mM) and erlotinib (IC_{50} = 0.92 mM). The table also shows that 4-CF_3-BPTU had a slightly lower IC_{50} value than 4-OCH_3-BPTU, which means that the former has a higher cytotoxic activity than the latter. This result also corresponds to

the *in silico* activity prediction in which 4-CF_3-BPTU was found to have a smaller BS than 4-OCH_3-BPTU. Based on the physicochemical quality, the –CF_3 group at the para position has high lipophilic and electronic properties, allowing it to penetrate the cancer cell membrane. For these reasons, it is predicted to inhibit the phosphorylation of EGFR in the intracellular domain, resulting in the inhibition of intracellular signalling, which is involved in cell proliferation.



(a) (b)

Fig.-1: Structures of 4-OCH_3-BPTU (a) and 4-CF_3-BPTU (b)

Table-2: Characterization of N-(4-methoxy)-benzoyl-N'-phenylthiourea (4-OCH_3-BPTU) and N-(4-trifluoromethyl)-benzoyl-N'-phenylthiourea (4-CF_3-BPTU)

Characteristics and Methods	N-(4-methoxy)-benzoyl-N'-phenylthiourea (4-OCH_3-BPTU)	N-(4-trifluoromethyl)-benzoyl-N'-phenylthiourea (4-CF3-BPTU)
Appearance	White crystal	White crystal
Yield (%)	70	67
m.p. (ºC)	108–109	125–126
^{1}H-NMR (DMSO-d6, 500 MHz)	δ 3.90 (s, 3H, OCH3); δ 7.02 (d, *J*=8.9 Hz, 2H, Ar-H); δ 7.29 (t, *J*=7.6 Hz, 1H, Ar-H); δ 7.43 (t, *J*=7.6 Hz, 2H, Ar-H); δ 7.72 (d, *J*=7.6 Hz, 2H, Ar-H); δ 7.88 (d, *J*=8.9 Hz, 2H, Ar-H); δ 9.07 (s, 1H,O=C-NH-C=S); δ 12.68 (s, 1H,S=C-NH-Ar).	δ 7.31 (t, *J*=7.8 Hz, 2H, Ar-H); δ 7.43 (t, *J*=7.8 Hz, 1H, Ar-H); δ 7.70 (d, *J*=8.0 Hz, 2H, Ar-H); δ 7.81 (d, *J*=7.8 Hz, 2H, Ar-H); δ 8.02 (d, *J*=8.0 Hz, 2H, Ar-H); δ 9.19 (s, 1H,O=C-NH-C=S); δ 12.45 (s, 1H,S=C-NH-Ar).
^{13}C-NMR (DMSO-d6, 125 MHz)	δ 55.8 (1C, OCH3); δ 114.6 (2C, Ar); δ 123.6 (2C, Ar); δ 124.3 (1C, Ar); δ 127.0 (2C, Ar); δ 129.0 (1C, Ar); δ 129.8 (2C, Ar); δ 137.8 (1C, Ar); δ 164.2 (1C, Ar); δ 166.5 (1C, C=O); δ 178.7 (1C, C=S).	δ 124.4 (1C, CF_3); δ 126.4 (2C, Ar); δ 126.4 (2C, Ar); δ 127.3 (2C, Ar); δ 128.2 (1C, Ar); δ 129.1 (2C, Ar); δ 135.1 (1C, Ar); δ 135.4 (1C, Ar); δ 137.5 (1C, Ar); δ 165.8 (1C, C=O); δ 178.1 (1C, C=S).
IR (KBr), ν_{max} (cm^{-1})	1661 (C=O amide); 1593 and 1505 (C=C aromatic); 3300 and 1593 (NH stretch secondary amides); 1075 and 805 (C=S).	1671 (C=O amide); 1600 and 1497 (C=C aromatic); 3269 and 1600 (NH stretch secondary amides); 1082 and 838 (C=S).
HRMS (m/z)	$C_{15}H_{13}N_2O_2S$: $(M-H)^-$ = 285.0692	$C_{15}H_{10}N_2OSF_3$: $(M-H)^-$ = 323.0472
Calc. Mass	285.0698	323.0466

Table-3: IC_{50} Values of the Test and Comparison Compounds for MCF-7 and Vero Cells and Their Selectivity Index Values

Compounds	IC_{50} (mM) MCF-7 Cells	IC_{50} (mM) Vero Cells	Selectivity Index (SI)
4-OCH_3-BPTU	0.38	22.59	59.45
4-CF_3-BPTU	0.37	37.28	100.76
HU	9.76	-	
Erlotinib	0.92	-	

In addition to cytotoxic activity, the test compounds were examined on their selectivity for MCF-7 cancer cells using Vero cells (normal cells). A Selectivity Index (SI) is a selectivity parameter that measures the safety of a drug. SI was calculated using the formula below:

$$\textit{Selectivity Index (SI)} = \frac{IC_{50} \text{ normal cells}}{IC_{50} \text{ cancer cells}}$$

Based on Table-3, the compounds 4-OCH_3-BPTU and 4-CF_3-BPTU each had an SI value of 59.45 and 100.76, indicating high selectivity for MCF-7 cancer cells (SI > 2).[20,21] Also, 4-CF_3-BPTU had a higher SI value or, thus, better selectivity than 4-OCH_3-BPTU. Nevertheless, according to the SI values, the two test compounds can kill cancer cells with little or no impact on normal cells.

CONCLUSION

The test compounds 4-CF_3-BPTU and 4-OCH_3-BPTU generally exhibit higher *in silico* and *in vitro* cytotoxic activity than hydroxyurea (HU) and erlotinib, except 4-OCH_3-BPTU which has lower *in silico* cytotoxic activity than erlotinib. Overall, 4-CF_3-BPTU has a higher cytotoxic activity than 4-OCH_3-BPTU both *in silico* and *in vitro*.

ACKNOWLEDGEMENT

The authors would like to thank Indonesia's Doctorate General of Resources for Science, Technology and Higher Education at the Ministry of Research, Technology and Higher Education (KEMENRISTEK DIKTI) for funding this study through the Ph.D. programme scholarship scheme at the University of Airlangga, Surabaya, Indonesia.

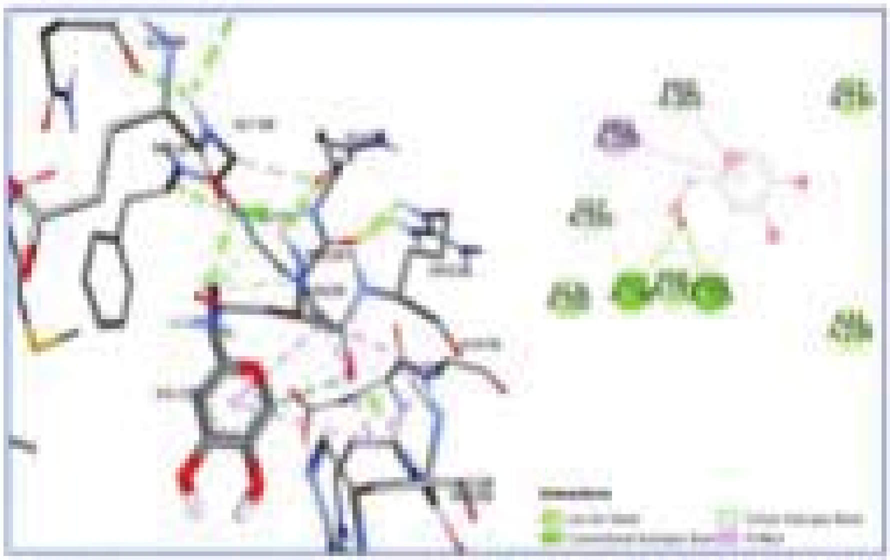
REFERENCES

1. https://www.who.int/cancer/PRGlobocanFinal.pdf
2. V.N. Dange, S.J. Shid, C.S. Magdum and S.K. Mohite, *Asian Journal of Pharmaceutical Research*, **7(1)**, 49(2017), https://doi.org/10.5958/2231-5691.2017.000089
3. Siswandono and B. Soekardjo, Medicinal Chemistry, Airlangga University Press, Indonesia, p. 255-288, p. 304-305 (2008)
4. N. Yamashita, M. Kondo, S. Zhao, W. Li, K. Koike, K. Nemoto and Y. Kanno, *Bioorganic & Medicinal Chemistry Letters*, **231**, 3(2017), https://doi.org/10.1016/j.bmcl.2017.03.061
5. A.A. Zulkifli, F.H. Tan, T.L. Putoczki, S.S. Stylli and R.B. Luwor, *Molecular and Cellular Endocrinology*, **451**, 15(2017), https://doi.org/10.1016/j.mce.2017.01.010
6. I.O. Alanazi and Z. Khan, *Asian Pacific Journal of Cancer Prevention*, **17**, 445(2016), https://doi.org/10.7314/APJCP.2016.17.2.445
7. H.Q. Li, T. Yan, Y. Yang, L. Shi, C.F. Zhou and H.L. Zhu, *Bioorganic & Medicinal Chemistry*, **18 (1)**, 305(2009), https://doi.org/10.1016/j.bmc.2009.10.054
8. X.C. Huang, M. Wang, Y.M. Pan, G.Y. Yao, H.S. Wang, X.Y. Tian, J.K. Qin and Y. Zhang, *European Journal of Medicinal Chemistry*, **69C**, 508(2013), https://doi.org/10.1016/j.ejmech.2013.08.055
9. W. Yang, Y. Hu, Y.S. Yang, F. Zhang, Y.B. Zhang, X.L. Wang, J.F. Tang, W.Q. Zhong and H.L. Zhu, *Bioorganic & Medicinal Chemistry*, **21(5)**, 1050(2013), https://doi.org/10.1016/j.bmc.2013.01.013
10. A. Hinchliffe, Molecular Modelling for Beginners 2nd ed, John Wiley and Sons Ltd, United Kingdom (2008)
11. V. Murugan, S. Revathi, K. Sumathi, K.M. Geetha and K. Divekar, *Asian Journal of Research in Chemistry*, **3(2)**, 496(2010)
12. D.L. Pavia, G.M. Lampman, G.S. Kriz, R. James and J.R. Vyvyan, Spectroscopy 4th ed, Brooks/Cole, France, p. 851-886 (2009)
13. P.A. Patil, R.P. Bhole, R.V. Chikhale, K.P. Bhusari and A. Chandekar, *Asian Journal of Research in Chemistry*, **3(3)**, 531(2010)
14. https://ccrc.farmasi.ugm.ac.id/?page_id=240
15. V.A. Kangralkar and A.R. Kulkarni, *Research Journal of Pharmacy and Technology*, **6(11)**, 1240-1241 (2013)

16. D. Kesuma, A.L. Nasyanka, M. Rudyanto, Siswandono, B.T. Purwanto and I.G.A. Sumartha, *Rasayan Journal of Chemistry*, **13(3)**, 1914(2020), https://doi.org/10.31788/RJC.2020.1335694
17. D. Satria, J. Silalahi, G. Haro, S. Ilyas and P.A.Z. Hasibuan, *Rasāyan Journal of Chemistry*, **12(2)**, 803 (2019), https://doi.org/10.31788/RJC.2019.1225180
18. V. Venkataramireddy, M. Shankaraiah, A.T. Rao, Ch. Kalyani, M.L. Narasu, R. Varala and A. Jayashree, *Rasayan Journal of Chemistry*, **9(1)**, 31(2016)
19. R.B. Badisa, S.F. Darling-Reed, P. Joseph, J.S. Cooperwood, L.M. Latinwo and C.B. Goodman, *Anticancer Research*, **29(8)**, 2993(2009)
20. M. Rashidi, A. Seghatoleslam, M. Namavari, A. Amiri, M.A. Fahmidehkar, A. Ramezani, E. Eftekhar, A. Hosseini, N. Erfani and S. Fakher, *International Journal of Cancer Management*, **10(5)**, 1(2017), https://doi.org/10.5812/ijcm.8633
21. B.T. Purwanto, Siswandono, D. Kesuma, T. Widiandani and I. Siswanto, *Rasayan Journal of Chemistry*, **14 (2)**, 1341(2021), https://doi.org/10.31788/RJC.2021.1426196

[RJC-6836/2021]

RASĀYAN
Journal of Chemistry
(An International Quarterly Research Journal of Chemical Sciences)



Rasayan J. Chem.
ISSN (Print): 0974-1496
ISSN (Online): 0976-0083
CODEN: RJCABP

Abstracted in: Scopus, 2008
ELSEVIER
SCOPUS

Editorial Board

Editor-in-Chief:

Sanjay K. SHARMA, FRSC

Professor, Department of Chemistry &
Dean(Research), JECRC University, Jaipur, India

Contact: +91 9001699997

Email: editor@rasayanjournal.com,

Research Interest: Green Chemistry, Organic Chemistry and Water treatment

Editorial Office:

Pratima SHARMA

Publisher and Managing Editor,
RASĀYAN Journal of Chemistry,
23 'Anukampa', Janakpuri, Opp. Heerapura Power Stn.,Ajmer Road, Jaipur-302024 (India)

Contact: 9414202678

Email: rasayanjournal@gmail.com

Bassiim H. Hammadii

Department of Chemical Engineering,College of Engineering, Qatar University, P.O. Box 2713,Doha, Qatar

Contact: +97440434142

Email: b.hammadi@qu.edu.qa

Research Interest: Reaction Engineering, Adsorption Technology

Florent ALLAIS

Director, R&D Unit of Industrial Agro-Biotechnologies URD ABI- AgroParis Tech, Pomacle, France

Contact: +33 633 698 126

Email: Florent.allais@agroparistech.fr

Research Interest: Green Chemistry, Bio-based Polymers

Goutam BRAHMACHARI

Professor, Chemistry Department, Visva-Bharati University, Santiniketan-731235, India.

Contact: +91 943485744

Email: goutam.brahmachari@visva-bhartai.ac.in

Research Interest: Organic Synthesis; Green Chemistry; Natural products, Medicinal Chemistry

Ishmael MASESANE

Professor, Department of Chemistry, University of Botswana, Botswana

Contact: 26772874348

Email: MASESANE@UB.AC.BW

Research Interest: Organic synthesis, Natural product Chemistry, Medicinal Chemistry

Marei Maiiowd EL-AJAILY

University of Benghazi, Faculty of Science , Department of Chemistry, Benghazi, Libya

Contact: 00218918315683

Email: melajaily@gmail.com

Research Interest: Mixed ligand complexes, Drugs, Applications, Corrosion inhibition, Molecular docking, DFT studies

Eno E. EBENSO

Professor, North-West University Gauteng, South Africa

Contact: +27825387286

Email: Eno.Ebenso@nwu.ac.za

Research Interest:

Giusy LOFRANO

Department of Environment, University of Salerno, Salerno, Italy

Contact: 0039 347 90 60 670

Email: glofrano@unisa.it

Research Interest: nanotechnologies, wastewater treatment, advanced oxidation processes

Hakan ARSLAN

Department of Chemistry, Faculty of Arts and Science, Mersin University, Mersin, TR-33343, Turkey

Contact: +90.532.7073122

Email: hakan.arslan@mersin.edu.tr

Research Interest: Coordination chemistry, Hetrocyclic Chemistry, Kinetic Studies, X-ray diffraction studies, Spectroscopy

Ime Bassey OBOT

Center of Research Excellence in Corrosion Research Institute, King Fahd University of Petroleum and Minerals (KFUPM), P.O. Box 489, Dhahran, 31262, Saudi Arabia

Contact: +966 13 860-8283

Email: obot@kfupm.edu.sa

Research Interest: Corrosion and Scale Inhibition, Chemo-informatics, Computational Chemistry.

Mam SINGH

Professor and Dean, school of Chemical sciences, Gujrat central University, Gandhinagar, Gujrat, India

Contact: +91 9408635094

Email: mansingh50@hotmail.com

Research Interest: Surface Chemistry, Physical Chemistry

Archive Issue

Volume 15, Number 2, 738-1587, April- June(2022)

PALM SHELL-DERIVED ACTIVATED CARBON ADSORBENT IS BETTER THAN THAT OF COCONUT SHELL: COMPARATIVE STUDIES OF COD ADSORPTION FROM PALM OIL MILL EFFLUENT
— I. Mustafa, Fathurrahmi, Suriarah, M. Farida and K. Ahmad

ANTIBACTERIAL ACTIVITIES TEST AND BRINE SHRIMP LETHALITY TEST OF Simargaolgaol (Aglaonema modestum Schott ex Engl.) LEAVES FROM NORTH SUMATERA, INDONESIA
— Saronom Silaban, Bajoka Nainggolan, Murniaty Simorangkir, TiurmaSolomasi Zega, Putri Mandaoni Pakpahan and Kasta Gurning

CHARACTERISTICS TEST OF POLYPROPYLENE MEMBRANE AS A CR2016 TYPE LITHIUM-ION COIN CELL BATTERY SEPARATOR
— A. Suprabawati, I. Rahayu, A. Rostika, A. Anggraini and K. Wulandhari

THREE-STEP SYNTHESIS OF VARIOUS-1H-1,2,3-TRIAZOL-4- YL) METHYL) PYRIDO[2,3-B]PYRAZIN-2(1H)-ONES VIA C-N JUNCTION AND THEIR ANTI-PROLIFERATIVE ACTIVITY
— Pavani .V and Jagadeesh Kumar Ega

Au-TiO2NANOSPHERES CATALYZED ONE-POT-MCR SYNTHESIS, CHARACTERIZATION AND ANTIPROLIFERATION ACTIVITY OF INDOLYL-IMIDAZOLOPYRIDINES CARBOXYLIC ACID HYBRIDS
— Prasad Boda, Jagadeesh Kumar Ega, Kavitha Siddoju

SYNTHESIS, SPECTRAL CHARACTERIZATION, BIOLOGICAL ACTIVITY OF MACROCYCLIC LIGANDS AND METAL COMPLEXES DERIVED FROM 3,4- DIAMINOBENZOPHENONE AND DIKETONES
— A. Palaniammal and S. Vedanayaki

APPLICATION OF IMAGE ANALYSIS USING TEXTURES OF Py14BA:nFA FOR MESOGEN PARAMETERS
— Ch. Kamalakar, C.J. Sreelatha, K. Mallika, A.V.N. Ashok Kumar and S. Sreehari Sastry

ISOLATION AND CHARACTERIZATION OF CHITOSAN FROM SEA AND FRESHWATER WASTE, NORTH SUMATERA PROVINCE, INDONESIA
— Ridwanto, A.S. Daulay and K. Gurning

BIOCHEMICAL CHARACTERIZATION, ANTIPROLIFERATIVE AND CYTOTOXICITY EFFECT OF PURIFIED L-ASPARAGINASE, AN ANTI-LEUKEMIA ENZYME ISOLATED FROM NEW BACTERIA Myroides Gitamensis
— V.S.S.L. Prasad Talluri, S.S. Lanka, B.Mutaliyeva, A. Sharipova, A. Suigenbayeva and A. Tleuova

PHYTOCHEMICAL SCREENING AND ANTIDYSLIPIDEMIC ACTIVITY OF CORIANDER LEAF ETHANOL EXTRACT (Coriandrum sativum L.) IN WISTAR MALE RATS
— S.M. Sinaga, H. Cintya, M. Batubara, I. Zilena and H.D. Syahputra

OPTIMIZATION OF CONTINUOUS MICROWAVE INACTIVATOR FOR POLYPHENOL OXIDASE INACTIVATION ON GREEN TEA PROCESSING USING RESPONSE SURFACE METHODOLOGY
— S.U. Handayani, Sutrisno, D. Ariwibowo, R. Amalia and M.E Yulianto

SPREAD PREDICTION OF COVID-19 IN ANDHRA PRADESH BASED ON ENVIRONMENTAL CHEMISTRY
— Habibulla Mohammad, Ch Gangadhar, Riazuddin Mohammed and K. Phani Rama Krishna

EFFECT OF HYBRID Mg(OH)2/CHITOSAN ON THE HYDROPHILICITY AND ANTIFOULING OF POLYETHERSULFONE (PES) MEMBRANE
— U. Fathanah, I. Machdar, M. Riza, N. Arahman, M. Y. Wahab, S. Muchtar, C. M. Rosnelly, S Mulyati, Y. Syamsuddin, S. Juned and F. Razi

PHASE FORMATION BEHAVIOR ON MECHANICALLY ACTIVATED ANNEALING OF Al-RICH PERITECTIC Al-Cr COMPOSITIONS
— K.Y. Karuna, J. Joardar, A.V.L.N.S.H. Hariharan and K. Ram Mohan Rao

APPLICATION OF JENGKOL PEEL (Pithecollobium jiringa) AS IRON CORROSION INHIBITORS IN HYDROCHLORIC ACID MEDIUM
— Rondang Tambun, Melani D. Fitri, Rafika Husna and Vikram Alexander

ANTIMICROBIAL STUDY AND SYNTHESIS OF MIXED LIGAND COMPLEX OF Ni(II) ION DERIVED FROM ISATIN SCHIFF BASE AND HISTIDINE
— Shobhana Sharma, Poonam Yadav, Seema, Suman Kumari and Mamta Ranka

AN ECO-FRIENDLY PREPARATION OF 2,6- DIARYLPIPERIDIN-4-ONES USING A GLUCOSE-CHOLINE CHLORIDE DEEP EUTECTIC SOLVENT
— K. Hemalatha and D. Ilangeswaran

ISOLATION OF SECONDARY METABOLITE COMPOUNDS FROM Elaeocarpus mastersii KING STEM BARK AND THEIR BIOLOGICAL ACTIVITY EVALUATION
— Tia Okselni, Adlis Santoni and Mai Efdi

THE ROLE OF NATURAL PRODUCTS AGAINST COVID-19: A REVIEW
— D. Dutta, B. R. Chhetri, J. Biswas and N. K. Bhattacharyya

MOLECULAR DOCKING AND DYNAMICS SIMULATIONS OF FENOLIC CONTENTS ON HENNA PLANT (Lawsonia inermis L.) AS ANTIDIBETIC THROUGH INHIBITION OF DIGESTIVE ENZYME α-AMYLASE
— Mus Ifaya, Ida Musfiroh, Sahidin, Gofarana Wilar, Yasmiwar Susilawati, Syawal abdurrahman and Dwi Syah Fitra Ramadhan

BIOETHANOL PRODUCTION USING TARO ROOTS WASTE (Colocasia esculenta) FROM BOGOR INDONESIA AND ANALYSIS OF CHEMICAL COMPOUNDS
— Rosalina1, Askal Maimulyanti, Anita Herawati Permana, Maman Sukiman, Henny Rochaeny and Nurdiani

THE DESIGN, SYNTHESIS AND BIOLOGICAL EVALUATION OF THE PEPTIDE DERIVATIVES CONTAINING GUANIDINE MOIETY WITH 5-CHLORO-THIOPHENE-2-CARBOXYLIC ACID CONJUGATES
— Sunil Tivari, Siddhant V. Kokate, Uttam B. Shelar and Yashwantsinh Jadeja

FUNCTIONALIZATION OF SILICA FROM BAGASSE ASH WITH PRIMARY AMINES: FTIR ANALYSIS
— N.A. Rahman, W. Widiyastuti and S.P.A. Anggraini

ACID AND BIO-ACTIVATION OF CARBON PREPARED FROM CORNCOB FOR ADSORPTION OF Cd(II) FROM AQUEOUS SOLUTION
— A. A. Ojo, I. Osasona, A.O. Olawole and J.A. Johnson

SELECTED INDIAN MEDICINAL PLANTS FOR MITIGATING POLYCYSTIC OVARIAN SYNDROME: A REVIEW
— K. Shalini, V. Chitra and K. Ilango

CURCUMINOID NANOEMULSION FROM Curcuma xanthorrhiza EXTRACT AND ITS ACTIVITY AS ANTIOXIDANT, ANTIBACTERIAL AND ANTIFUNGAL
— S. Atun, A. Sinardekawati, A.C. Purpratama, N. Aznam and A. Sangal

RESEARCH OF THE PROCESS OF SYNTHESIS OF DIAMMONIUM PHOSPHATE FROM EXTRACTIVE PHOSPHORIC ACID FROM BALANCED PHOSPHATESILICON SHAPES OF THE KARATAU BASIN
— K.T Zhantasov, A.A. Kadirbayeva, N.D. Torebay, G.S. Shaimerdenova, Z.A. Makhanova, K.U. Nyshanbayeva, A.B. Seitkhanova and E.B. Mussirepova

THE POTENTIAL OF GARLIC AND VIRGIN COCONUT OIL AS SARS-CoV-2 ANTIVIRAL: A REVIEW
— Suryana, J. Kusmoro, B. Mayawatie, Y. Deawati and A.R. Noviyanti

THE IDENTIFICATION OF MOLECULAR MECHANISMS FROM BIOACTIVE COMPOUNDS IN Sansevieria trifasciata PLANT AS ANTI-ALOPECIA: In-Silico APPROACH
— Henny Kasmawati, Resmi Mustarichie, Eli Halimah, Ruslin and Arfan

PHYTOCHEMICAL CONSTITUENTS AND CYTOTOXIC ACTIVITY FROM Scoparia dulcis LINN OF INDONESIA ORIGIN
— Hasnawati, S. Wahyuono, R. A. Susidarti and D. Santosa

BSA ADSORPTION, ANTIBIOFILM, AND ANTIBIOFOULING BEHAVIOR OF POLY (N-TERT-AMYLACRYLAMIDE-COACRYLAMIDE/AMPSNa) HYDROGELS
— K. Jayanthi and P. Pazhanisamy

SYNTHESIS, CHARACTERISATION AND ANTIMICROBIAL EVALUATIONS OF ACETYLOXYPHENYL-1,2,3-TRIAZOLOTETRAMETHYL HEXAHYDROACRIDINEDIONES
— P. Shanmugasundaram, R. Sujatha, M. Vijey Aanandhi, K. Saravanan and P. Subbramaniyan

MODIFICATION OF GELATIN/CARBONATED HYDROXYAPATITE MEMBRANE WITH CHITOSAN TO IMPROVE THE TENSILE STRENGTH
— M. Mahmudi, B. Pidhatika, S. Suyanta and N. Nuryono

In-vitro EVALUATION OF THE A-GLUCOSIDASE INHIBITORY, ANTI-CHOLESTEROL, AND DPPH SCAVENGING POTENTIAL OF LEAVE EXTRACTS OF Rhaphidophora pinnata
— Masfria, Y.M Permata and Faizar

POTENTIOMETRIC DETERMINATION OF STABILITY CONSTANTS OF METFORMIN COMPLEXES WITH METALS IN AQUEOUS MEDIA
— Ahmed Zain A. Thabet, Mohammad Mohsin, Fahd Saleh T. Saleh and Mohamad Asif

RP-HPLC ANALYTICAL METHOD DEVELOPMENT AND VALIDATION FOR NEWLY SYNTHESIZED ISOEUGENOLINDOLE-3-ACETIC ACID
— A. Nishad, R. R. Badekar, S. K. Sharma, R. S. Lokhande and V. R. Patil

INFLUENCE OF STRUCTURAL AND MOLECULAR FEATURES OF CHRYSOTILE ON INTERACTION WITHIN ACID-CHRYSOTILE SYSTEM
— A.K. Dikanbayeva, A.P. Auyeshov, M.S. Satayev, I.V. Pirminova, Ch.Z. Yeskibayeva and K.T. Arynov

THE EFFECT OF KAEMPFEROL, ETHYL-pMETHOXYCINNAMATE, AND THE ETHANOL EXTRACT OF Kaempferia galanga RHIZOME ON THE PRODUCTION OF PROSTAGLANDIN BY In-vitro AND In-silico STUDY
— I. S. Wahyuni, I. Sufiawati, W. Nittayananta, N. M. Saptarini and J. Levita

CAMBRIDGE STRUCTURE DATABASE ANALYSIS OF MOLECULAR INTERACTION ENERGIES IN BROMINESUBSTITUTED COUMARIN STRUCTURES
— Jigmat Stondus and Rajni Kant

CARBON NANOTUBES (MWCNTs) ADDED BIODIESEL BLENDS: AN ENGINE ANALYSIS
— Chiranjeeva Rao. Seela

POLYANILINE/CARBOXYMETHYL GUAR GUM NANOCOMPOSITES: AS BIODEGRADABLE, CONDUCTIVE FILM
— J. Meena, S. K. Verma, R. Rameshwari and D. K. Verma

BIOETHANOL PRODUCTION FROM CASSAVA AND BAGASSE BY THERMAL HYDROLYSIS PROCESS AND LOCAL YEAST FERMENTATION
— F. M. Djuned, R.F. Adinda, H. Kamila and M. Faisal

IDENTIFICATION AND ANTIOXIDANT ACTIVITY TEST FOR FRACTIONATED COMPOUND FROM ETHANOL EXTRACT OF THE SINGKUT RHIZOME (Molineria latifolia Dryand)
— D. Roza, R. Selly, D.Z. Hayati and G. Fadhilah

THE KINETIC RELEASE AND In-vivo STUDY OF ALGINATECHITOSAN ENCAPSULATED METFORMIN AGAINST TYPE II DIABETES MELLITUS
— Sari Edi Cahyaningrum, Amaria and Fitriari Izzatunnisa Muhaimin

EVALUATION OF ACTIVATED CARBONS OBTAINED FROM COLOMBIAN MINERAL COALS FOR ADSORPTION OF CAFFEIN
— S. Ortiz-Home, H. CÃ³rdoba-Bueno, D. GÃ³mez-RÃos, H. RamÃrez-MaluleÂ and J. Guerrero-PÃ©rez

MICROWAVE-ASSISTED SYNTHESIS OF 4-METHYL COUMARINS, THEIR ANTIOXIDANT AND ANTIBACTERIAL ACTIVITIES
— D. U. C. Rahayu, R. S. Al-Laily, D. A. Khalwani, A. Anjani, S. Handayani, E. Saepudin, H. Dianhar and P. Sugita

GREEN SOLVENT ENHANCED MECHANICAL EXTRACTION OF PALM KERNEL OIL
— E.K. Sitepu, A. Candra, E.F. Zaidar, A. Vika, F. Sebayang, F.R. Dewi, J.A. Karo-karo and J.Br. Tarigan

DITIZHONE-IMMOBILIZED NICKEL SLAG FOR THE ADSORPTION OF SILVER(I) ION
— N. H. Aprilita, M. Luqman and A. Suratman

IN SILICO DOCKING STUDIES OF PHYTOSTEROL COMPOUNDS SELECTED FROM Ficus religiosa AS POTENTIAL CHEMOPREVENTIVE AGENT
— H.D. Syahputra, M. Masfria, P.A.Z Hasibuan and I. Iksen

BIOCHEMICAL CHARACTERIZATION, ANTIPROLIFERATIVE AND CYTOTOXICITY EFFECT OF PURIFIED L-ASPARAGINASE, AN ANTI-LEUKEMIA ENZYME ISOLATED FROM NEW BACTERIA Myroides Gitamensis
— VSSL Prasad Talluri, S. S. Lanka, B. Mutaliyeva, A. Sharipova, A. Suigenbayeva and A. Tleuova

CHEMICAL COMPOUNDS CONTAINED Saurauia vulcani (Korth.) AND ITS ANTIBACTERIAL ACTIVITY AGAINST Staphylococcus aureus AND Escherichia coli
— Eka Kartika Silalahi, Tamrin, Lamek Marpaung and Rikson Siburian

EFFICIENT SYNTHESIS OF 2-AMINO-4-(2-CHLORO-5-(4- SUBSTITUTEDPHENYL) PYRIDIN-3-YL)-1-(4-SUBSTITUTED PHENYL)-7,7-DISUBSTITUTED-5-OXO-1,4,5,6,7,8- HEXAHYDROQUINOLINE-3-CARBONITRILE DERIVATIVES AND THEIR MICROBIAL SCREENING
— K. V. Goswami,S. P. Vyas, K. P. Damor, Kokila A. Parmar and Sarju N. Parajapati

ADSORPTIVE MICELLAR FLOCCULATION AND CLOUD POINT EXTRACTION AS PRE-CONCENTRATION METHODS FOR THE DETERMINATION OF PHENOSAFRANINE DYE IN AQUEOUS SOLUTIONS

— K. Arunakumari, P. Shyamala, SK. Ameerkhan and D. B. N. S. Varma

APPROACHES, CHALLENGES, AND PROSPECTS OF LIFE CYCLE ASSESSMENT APPLIED IN NANO BIOREMEDIATION OF CONTAMINATED SITES

— G. Pandey, S. Bajpai, S. Tripathi, Reeta Chauhan and Pratima Sharma

COMBINATION OF COCONUT COIR AND BENTONITE AS A BIOSORBENT FOR REMOVAL OF LEAD (Pb) IN WASTEWATER

— I. P. Bako, M. Iqbal, S. Muchtar and Mariana

COMPUTATIONAL EXAMINATION OF FLAVONOID COMPOUNDS: UTILIZATION OF MOLECULAR SIMULATION TO DISCOVER DRUG CANDIDATES FOR COVID-19

— Rafi Firdaus Wisnumurti , Solmaz Aslanzadeh and Arli Aditya Parikesit

THE EFFECT OF CALCINATION TEMPERATURE ON SILICAALUMINA CHARACTER FROM LAPINDO MUD EXTRACT BY TEMPLATE CATFISH BONES GELATIN

— R. Nuryanto, D.S. Widodo, A. Suseno, W. Trisunaryanti and Triyono

ADSORPTIVE REMOVAL OF HEXAVALENT CHROMIUM USING RESPONSE SURFACE METHODOLOGY AND ARTIFICIAL NEURAL NETWORK

— P. Roy

INVESTIGATION OF ENHANCING THE PERFORMANCE AND DEPOSITION CHARACTERISTICS OF COPPER (II) METHANE SULPHONATE SALT COMPLEXED WITH DMANNITOL BATH

— S. Jothilakshmi, S. Rekha, A. Alvin Kalicharan and R. Ranjani

BIO-MICROBEADS FROM BACTERIAL CELLULOSE INCORPORATED WITH ANTIMICROBIAL OF CHITOSAN AND MORINGA LEAVES FLAVONOID

— S. Silviana, V. F. Giraldi, L. A. Purnomo, A. N. Saâ€™adah and F. Dalanta

BIOCATALYTIC EFFECT OF Simarouba glauca LEAF PHYTOCHEMICALS ON BIOLOGICALLY ACTIVE SILVER NANOPARTICLES YIELD AND ABTS ANTIOXIDANT ACTIVITY: GREEN SYNTHESIS

— D. Sivaselvi, N. Vijayakumar, R. Jayaprakash, V. Amalan, R. Rajeswari and M. Reddi Nagesh

POTENTIAL OF Navicula salinicola EXTRACT, A MICROALGAE FROM MALUKU ISLANDS, AS AN ANTIINFLAMMATORY AGENT USING THE HUMAN RED BLOOD CELLS (HRBC) METHOD

— D. Kurnia, Idar, V. J. Angraeni, I. Musfiroh , R. Hendriani , A. Asnawi and Z. Nurachman

MOLECULAR DOCKING STUDY, ANTIOXIDANT ACTIVITY, PROXIMATE CONTENT, AND TOTAL PHENOL OF Lemna perpusilla Torr. GROWN IN SUMEDANG, WEST JAVA, INDONESIA

— Y. Andriani, Y. Mulyani, Iskandar, S. Megantar and J. Levita

DFT STUDY ON THE CONFORMATIONAL CHANGE IN π-π STACKING INTERACTION OF NAPHTHALENE, α - NAPHTHOL AND β-NAPHTHOL SYSTEMS

— Ibrahim Ali, Benzir Ahmed, Mrinal J Bezbaruah, Pratyashee Barukial, Madhab Upadhyaya, and Bipul Bezbaruah

COBALT(II) AND NICKEL(II) COMPLEXES OF A SCHIFF BASE: SYNTHESIS, CHARACTERISATION AND ANTIMICROBIAL INVESTIGATIONS

— Jesna K. Sebastian , M. K. Muraleedharan Nair and Sreesha Sasi

ACTIVATION OF ZINC-PHOSPHATE WITH SILVER FOR ENHANCED ANTIMICROBIAL ACTIVITY

— A.L. Arunachalam, P.S. Raghavan, S. Induja and V. Parthasarathy

PHYTOCHEMICAL AND ANTIOXIDANT ACTIVITY OF SOURSOP (Annona muricata L.) LEAVES KOMBUCHA ENRICHED WITH GALACTOMANNAN FROM ENDOSPERM OF Arenga pinnata

— A.Candra, B.E. Prasetyo, J.B. Tarigan, E. Zaidar and A. Hasibuan

EFFECT OF GOLD MODIFICATION ON THE PROPERTIES AND PHOTOACTIVITY OF Fe3O4/SiO2/TiO2 IN THE DEGRADATION OF NITROBENZENE

— K. Mauludi, N. Nuryono, R. Roto, M.I.D. Mardjan and E.S. Kunarti

INTEGRATED EXTRACTION BY PERCOLATION, DISTILLATION, AND SOXHLET EXTRACTION TO SEPARATE BIOACTIVE AND BIOENERGY COMPOUNDS FROM SPENT COFFEE GROUND

— Askal Maimulyanti and Anton Restu Prihadi

NEW DECAHYDROACRIDINE-1,8-DIONES DERIVED FROM 3-AMINOCYCLOHEX-2-EN-1-ONE: SYNTHESIS, CHARACTERIZATION, ANTIOXIDANT, In-vitro, AND In-silico ANTI-INFLAMMATORY ACTIVITY

— I. P. Sari, H. Hariyanti, A. Yanuar and H. Hayun

CHARACTERIZATION OF NANOPARTICLES FROM Polymesoda Erosa CLAMSHELL POWDER FOR MATERIAL APPLICATION

— J. Cahyadi, M. Lubis, M.H.S Ginting and G.E. Ayu

CHEMICAL NUTRIENT CONTENT OF SARGASSUM LIQUID FERTILIZER PRODUCED FROM SHIPHON-CONNECTED DECOMPOSERS

— Nurhayati, F. Huslina and A.P. Asmara

In-silico SCREENING OF FLAVONOIDS AS AgrA INHIBITORS BY MOLECULAR DOCKING, NORMAL MODE ANALYSIS, AND ADMET STUDY

— Hriday Kumar Basak, Uttam Paswan, Sujoy Karmakar and AbhikChatterjee

DESIGNING AND VIRTUAL SCREENING OF QUINAZOLINONE ANALOGUES AS POTENTIAL PHARMACOPHORES FOR ANTITUBERCULAR ACTIVITY

— Susmita Dhar, Samaresh Datta and Soumya Ranjan Pradhan

INVESTIGATION OF THE CONVERSION PROCESS OF CALCIUM CHLORIDE OF SODA PRODUCTION DISTILLER LIQUID IN THE PRESENCE OF MIRABILITE AND THENARDITE

— A.A. Anarbayev, G.M. Ormanova, B.N. Kabylbekova, B. Kh. Kucharov, and M. B. Kenzhekhanova

ANTIBACTERIAL PEPTIDE FROM SOLID PHASE EXTRACTION (SPE) FRACTIONATION ON TRYPSIN HYDROLYSIS OF JATROPHA (Ricinus communis) SEED PROTEIN ACID EXTRACT

— D. R. Atmawati, Z. Andriana, R. T. Swasono and T. J. Raharjo

DEVELOPMENT OF MOLECULARLY IMPRINTED POLYMER MICROSPHERES MADE BY SURFACE IMPRINTING FOR PURIFICATION OF ANDROGRAPHOLIDE

— W. Winingsih, S. Ibrahim and S. Damayanti

INVESTIGATION OF TOTAL PHENOLIC CONTENT, FLAVONOID CONTENT, AND HEMOSTATIC ACTIVITY OF BEETROOT (Beta vulgaris. L) EXTRACT IN HEPARININDUCED THROMBOCYTOPENIA RAT

— S.E. Nugraha, E. Suwarso, Yuandani and R.A. Syahputra

STUDIES ON GLASS FIBRE REINFORCEMENT OF COMMERCIAL VINYL ESTER/FURAN RESIN HYBRID MATRIX RESIN SYSTEM

— Priyanka Bhargava, H.C. Kataria, and Sandesh Kumar Jain

STATISTICAL OPTIMIZATION OF PROCESS PARAMETERS FOR HYDROGEN PRODUCTION IN Halobacterium salinarium IMMOBILIZED WITH CALCIUM ALGINATE AND Escherichia coli

— Brijesh, R.R. Sivakiran and Jagadish H. Patil

GREEN SYNTHESIS OF CHROMIUM OXIDE NANOPARTICLES USING CHROMIUM (III) COMPLEX AS A SINGLE ROUTE PRECURSOR: ANTI-OXIDANT ACTIVITY

— Richa Kothari and Anjali Soni

PREPARATION AND CHARACTERIZATION OF CHITOSAN FROM GOLDFISH SCALES FOR ANTI-DANDRUFF SHAMPOO

— Eldi Firmansyah, Rini Hardiyanti, Artha Klara Samosir, Minanda Payungta Beru Sitepu and Nurmiahayati Boru Siagian

SYNTHESIS AND IN VITRO CYTOTOXIC EVALUATION OF NOVEL TRIAZOLE-BENZIMIDAZOLE EMBODIED PYRAZOLE DERIVATIVES AGAINST BREAST CANCER

— Bala Narsimha Dhoddi, Ravi Kurapati, Govardhan Reddy Kundur, Sampath Bitla, Balaswamy Puligilla, and Jalapathi Pochampally

MOLECULAR DOCKING AND MOLECULAR DYNAMIC STUDIES: SCREENING PHYTOCHEMICALS OF Acalypha indica AGAINST BRAF KINASE RECEPTORS FOR POTENTIAL USE IN MELANOCYTIC TUMOURS

— A. Asnawi, L.O. Aman, Nursamsiar, A. Yuliantini, and E. Febrina

THE MOLECULAR APPROACH OF NATURAL PRODUCTS AS PANCREATIC CANCER TREATMENT: A REVIEW

— M. F. Lubis, P. A. Z. Hasibuan, U. Harahap, D. Satria, H. Syahputra, M. Muhammad and R. Astyka

Papuacerdrus papuana (f. Muell) h.l.li., A NEW SOURCE FOR TWO BIOACTIVE DITERPENES: FERRUGINOL AND transCOMMUNIC ACID THAT VIRTUALLY ACTIVE AGAINST SARS-COV-2

— A. Agusta, D. Wulansari, Praptiwi, A. Fathoni, L. Oktavia and A.P. Keim

QUANTITATIVE ANALYSIS OF AMLODIPINE BESYLATE AND VALSARTAN IN TABLET DOSAGE FORM BY ABSORPTION FACTOR SPECTROPHOTOMETRY METHOD

— S. M. Sinaga, N.N. Pertiwi and Muchlisyam

SYNTHESIS AND CHARACTERISATION OF SOME Pb(II) MACROCYCLIC COMPLEXES

— Arpit Srivastava, Ashish Rajak, Ramakant, Subhash Chandra Shrivastava, Rafat Saba and Shekhar Srivastava

NEW METHOD DEVELOPMENT AND VALIDATION FOR HYDRAZINE IN PANTOPRAZOLE SODIUM SESQUIHYDRATE USING RP-HPLC

— SudharshanaCharyulu S., T. Krishnamohan, N. Sundara Rao, V.V.K.P.L.N.Murty, Y.L.N. Murthy and J. V. Shanmukha Kumar

WOOD VINEGAR AS A SUPPORTING ACTIVE INGREDIENT AND NEEM OIL DISPERSANT IN A NANOEMULSION SYSTEM AND THEIR BIOACTIVITY

— A. H. Prianto, Y. Yulizar, Budiawan and P. Simanjuntak

In-silico ANALYSIS AND MOLECULAR DOCKING STUDIES OF NOVEL THIAZOLIDINEDIONE DERIVATIVES AGAINST PPAR-γ

— B. Geetha, N. Harikrishnan, P. Sharmili, E. Esther Rani, A. Haripriya and C. N. Hemalatha

GREEN SYNTHESIS AND EVALUATION OF In-vitro ANTICANCER (MCF-7) AND MOLECULAR DOCKING STUDIES OF V2+ AND CO2+ COMPLEXES OF SCHIFF BASE

— R. Geetha, K. Rajasekar and S. Balasubramaniyan

PURIFICATION OF UNDERGROUND WATER USING SORBENT BASED ON SILICONY ROCK-FLASK OF WEST KAZAKHSTAN

— S.A. Montaev, S.S. Satayeva, K.A. Narikov, A.F. Urazova , G. Zh. Sdikova, M.B. Mambetova, and D.S. Nazarova

STRUCTURE MODIFICATION: EFFECT OF LIPOPHILIC, ELECTRONIC, AND STERIC PARAMETERS OF N-BENZOYLN'-PHENYLTHIOUREA COMPOUNDS ON ANTIVIRAL ACTIVITY OF COVID-19 BY IN SILICO

— D. Kesuma, C.H.A. Makayasa, F. Suhud, Azminah, T. A. Yuniarta, I. G. A. Sumartha, R. R. Risthanti and F. F. Dani

QSAR STUDY OF PYRAZOLE-UREA HYBRID COMPOUNDS AS ANTIMALARIAL AGENT VIA PROLYL-tRNA SYNTHETASE INHIBITION

— I. G. A. Sumartha, T.A. Yuniarta and D. Kesuma

APPLICATION OF TARTARIC ACID DERIVATIVES IN ENANTIOSEPARATION OF RS-IBUPROFEN

— D.N. Jadhav, P. Nag, R. S. Lokhande, J. G. Chandorkar, and S. K. Sharma

A COMPREHENSIVE ANALYTICAL APPROACH FOR QUALITY EVALUATION OF FLAVONOID-RICH EXTRACT OF Glycyrrhiza glabra (GutGard®)

— Vineet Kumar Singh, Rojison Koshy, Deepak Mundkinajeddu and Jothie Richard Edwin

EFFICIENT PHOTOCATALYTIC ACTIVITY AND DEFLUORIDATION STUDIES OF METAL OXIDE/CLAY NANOCOMPOSITES

— P. Mariselvi and T. AnanthaKumar

THE MORPHOLOGICAL AND CHEMICAL CHARACTERIZATION OF ENCAPSULATED POWDER IN RODENT TUBER MUTANT PLANT (Typhonium flagelliforme) EXTRACT

— N. F. Sianipar, S. Yuliani, K. Assidqi and R. Purnamaningsih

MOLECULAR DOCKING AND BIOLOGICAL ACTIVITY OF N- (4-METHOXY)-BENZOYL-N'-PHENYLTHIOUREA AND N-(4-TRIFLUORO)-BENZOYL-N'-PHENYLTHIOUREA AS ANTIBREAST CANCER CANDIDATES

— D. Kesuma, Siswandono and A. Kirtishanti

MULTIPLE RESPONSE OPTIMIZATION OF THE GREEN TEA DE-CAFFEINATED PROCESS FOR STIMULATING THE HUMAN ANTIBODY

— V. Paramita, M.E. Yulianto, I. Hartati, E. Yohana, D. Rohdiana, S. Shabri, D. Ariwibowo, T. Sutrisno and B. Wijayanto

SCREENING OF GENETIC VARIANTS, PHYTOCHEMICAL ANALYSIS, CHARACTERIZATION AND ANTIMICROBIAL ACTIVITY OF Physalis minima FRUITS EXTRACT

— Sobiya Pradeepkumar, Suriyavathana Muthukrishnan, Anandhi Eswaran, Nirubama Kumar, Thamaraiselvi Ganesan and R. Jayaprakash

UPLC-MS/MS METHOD FOR SIMULTANEOUS DETERMINATION OF METFORMIN AND GLIMEPIRIDE IN HUMAN PLASMA: A GREEN APPROACH TO ENVIRONMENT

— Chung Duong Dinh, Yen Nguyen Thi Ngoc and Dung Phan Thanh

DETERMINATION OF PHENOLIC, FLAVONOID CONTENT, ANTIOXIDANT AND ANTIBACTERIAL ACTIVITIES OF SERI (Muntingia calabura L.) LEAVES ETHANOL EXTRACT FROM NORTH SUMATERA, INDONESIA

— Suharni P. Sinaga, Damson A. Lumbangaol, Iksen , R.F.R. Situmorang and K. Gurning

INHIBITORY ACTIVITY, METABOLITE CONTENTS DETERMINATION, AND IN SILICO PREDICTION OF PARSLEY LEAVES FRACTION (Petrocelinum crispum MILL) AS ANTIFUNGAL AGENT OF Malassezia furfur

— S. Hasanuddin, Erisman, E. Meilanda, D.S.F. Ramadhan, D. Gozali, M. Arba and R. Mustarichie

STRUCTURE AND RHEOLOGICAL PROPERTIES OF WATER SOLUTIONS OF SODIUM CARBOXYMETHYL STARCH OBTAINED IN SOLID PHASE

— S.S. Saparov, M.A. Makhkamov, N.A. Abdullaeva, U. Mirzakulov and I.B. Gulomova

ANTIOXIDANT ACTIVITY OF ALKALOID FRACTIONS AND COMPOUNDS FROM Litsea cubeba Lour. Fruits

— A.Dalimunthe, P.A.Z. Hasibuan, H. Nufus, M. Muhammad and D. Satria

EVALUATION OF MICRONUTRIENT STATUS WITH PHYSICO-CHEMICAL PROPERTIES OF SOME AGRICULTURAL SOILS OF SELECTED AREAS OF PENDURTHI MANDAL, VISAKHAPATNAM DISTRICT, ANDHRA PRADESH

— Syeda Bano and Anima S. Dadhich

ANTIOXIDANT AND CELL PROLIFERATION INDUCTION ACTIVITIES COMBINATION OF HYDROALCOHOL EXTRACT OF Artocarpus lacucha Buch. Ham. LEAVES AND Anredera cordifolia (Ten) Steenis. LEAVES

— Nazliniwaty, O.A Hanafiah, D. Pertiwi, M. M

Volume- 15 | Number- 1 | XXX - XXX | January - March | 2022
www.rasayanjournal.com | www.rasayanjournal.co.in

RASĀYAN Journal of Chemistry

Rasayan Journal of Chemistry

COUNTRY

India

Universities and research institutions in India

SUBJECT AREA AND CATEGORY

Biochemistry, Genetics and Molecular Biology
- Biochemistry

Chemical Engineering
- Chemical Engineering (miscellaneous)

Chemistry
- Chemistry (miscellaneous)

Energy
- Energy (miscellaneous)

Pharmacology, Toxicology and Pharmaceutics
- Pharmacology, Toxicology and Pharmaceutics (miscellaneous)

PUBLISHER

Rasayan Journal

H-INDEX

24

PUBLICATION TYPE

Journals

ISSN

09741496, 09760083

COVERAGE

2008-2021

INFORMA

Homepag

How to publish ir this journ

editor@ra anjournal in

SCOPE

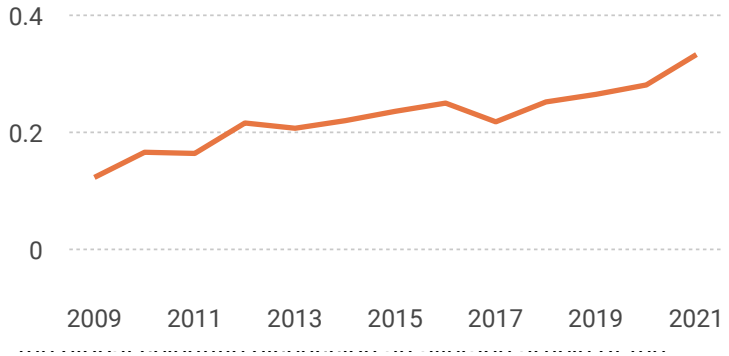
RASĀYAN Journal of Chemistry (RJC) signifies a confluence of diverse streams of Chemistry to st the cerebral powers of its contributors and readers. By introducing the journal by this name, we humbly intend to provide an open platform to all researchers, academicians and readers to showc their ideas and research findings among the people of their fraternity and to share their vast repos of knowledge and information. The journal seeks to embody the spirit of inquiry and innovation to augment the richness of existing chemistry literature and theories. We also aim towards making th journal an unparalleled reservoir of information and in process aspire to inculcate and expand the research aptitude. RASĀYAN Journal of Chemistry (RJC) widely covers all branches of Chemistry including: Organic, Inorganic, Physical, Analytical, Biological, Pharmaceutical, Industrial, Environm Agricultural & Soil, Petroleum, Polymers, Nanotechnology, Green Chemistry, Forensic, Phytochemis Synthetic Drugs, Computational, as well as Chemical Physics and Chemical Engineering.

Quartiles

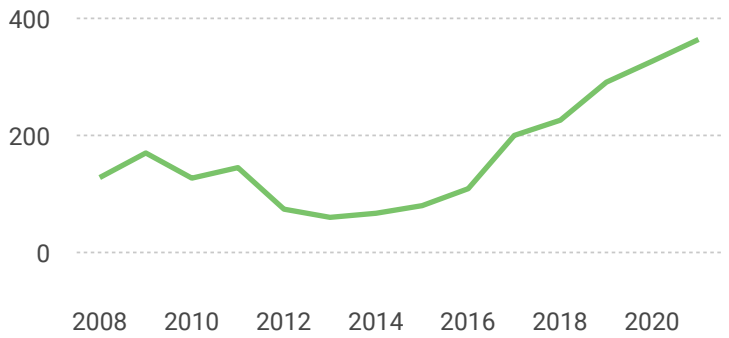
FIND SIMILAR JOURNALS

1	2	3
Asian Journal of Chemistry	**Oriental Journal of Chemistry**	**Arabian Journal of**
IND	IND	SAU
16% similarity	16% similarity	16% similarity

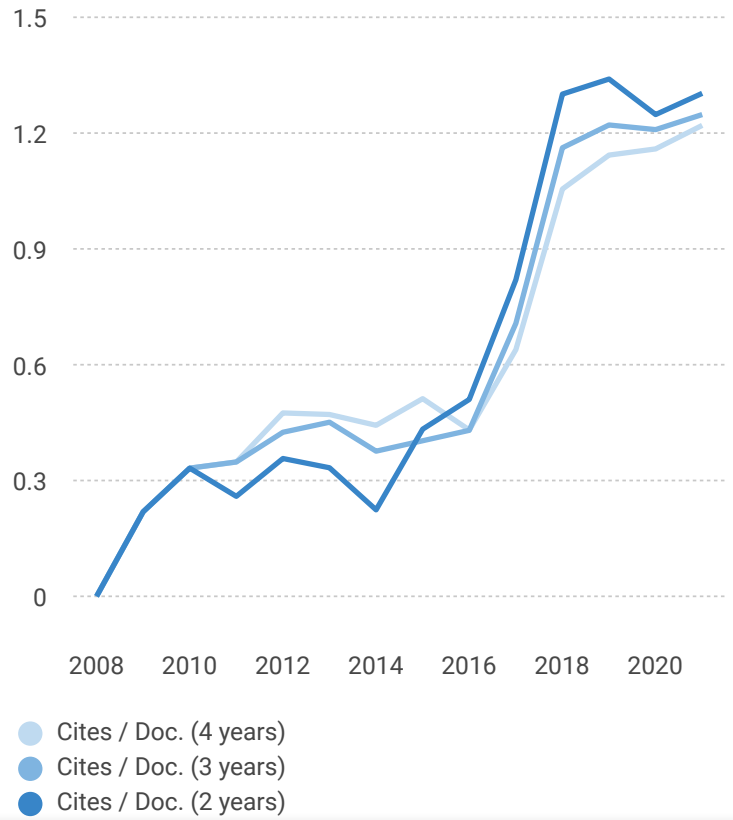
SJR

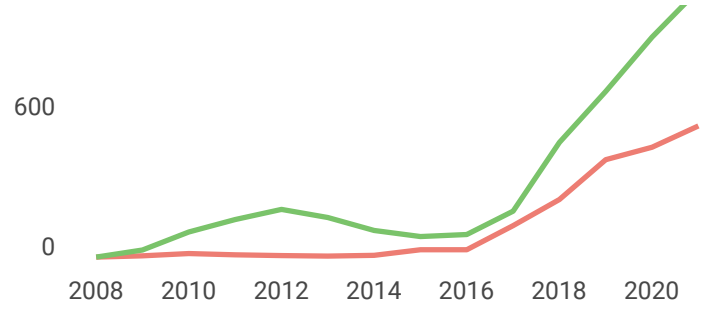


Total Documents



Citations per document

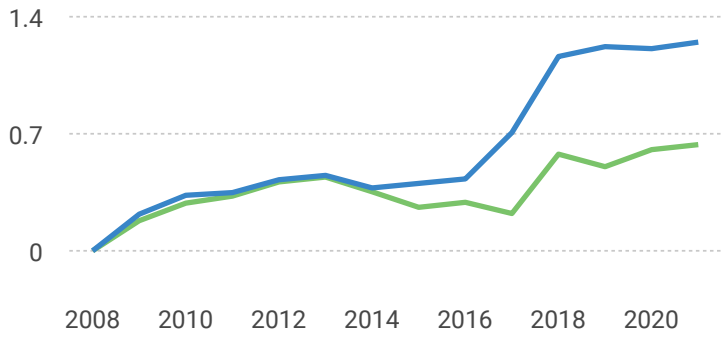




us® data as of April 2022

A

Ex[illegible]tes per Doc Cites per Doc



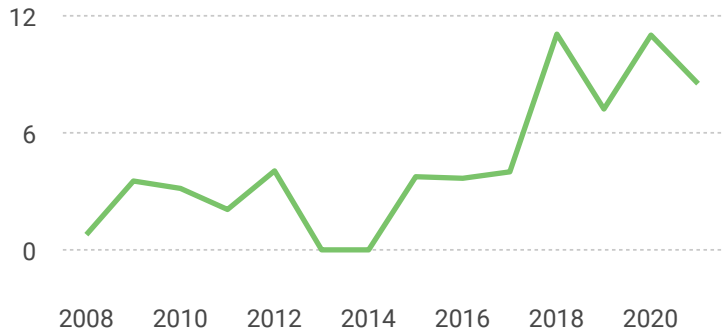
IVES AS POTENTIAL ANTIDIABETIC AGENTS"
g/10.31788/RJC.2021.1456665 in Scopus.

SCImago Team

Melanie Ortiz 3 months ago

% Interna

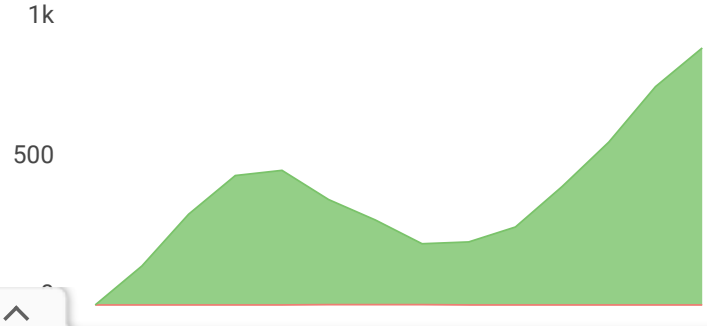
Dear Abhishek,



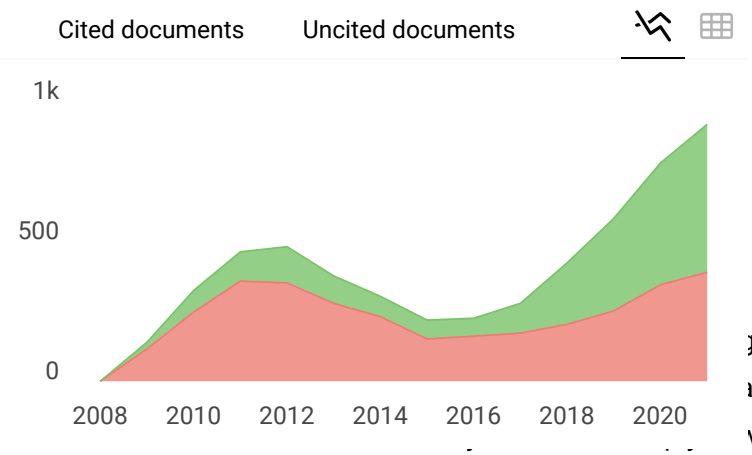
nent, unfortunately we cannot help you with your
copus support team:
nswers/detail/a_id/14883/kw/scimago

C

Citable documents Non-citable documents



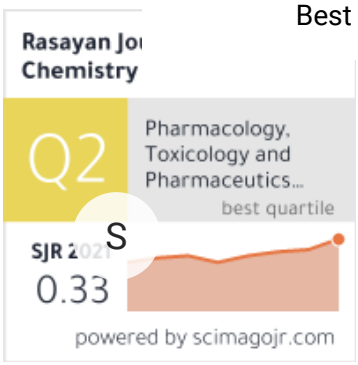
RE 20 DAYS . KINDLY GIVE ME STATUS OF



SCImago Team

go Journal & Country Rank is not a journal. SJR
ators of journals indexed in Elsevier/Scopus.
vith your request, we suggest you contact the
journal's editorial staff , so they could inform you more deeply.

Best Regards, SCImago Team



your own website

Just copy the code below and paste within your html code:

<a href="https://www.scima

?

SCImago Graphica

Explore, visually communicate and make sense of data with our **new data visualization tool**.

on Scopus in 2020 or not?

Thank you

reply

SCImago Team

Melanie Ortiz 3 years ago

Source details

Rasayan Journal of Chemistry

Scopus coverage years: from 2008 to Present
Publisher: Rasayan Journal
ISSN: 0974-1496 E-ISSN: 0976-0083

Subject area: Pharmacology, Toxicology and Pharmaceutics: General Pharmacology, Toxicology and Pharmaceutics | Energy: General Energy | Chemistry: General Chemistry | Chemical Engineering: General Chemical Engineering | Biochemistry, Genetics and Molecular Biology: Biochemistry

Source type: Journal

View all documents > | Set document alert | Save to source list

CiteScore | CiteScore rank & trend | Scopus content coverage

CiteScore 2021

$$2.0 = \frac{2{,}423 \text{ Citations } 2018 - 2021}{1{,}207 \text{ Documents } 2018 - 2021}$$

Calculated on 05 May, 2022

CiteScoreTracker 2022

$$1.7 = \frac{1{,}953 \text{ Citations to date}}{1{,}117 \text{ Documents to date}}$$

Last updated on 06 June, 2022 • Updated monthly

CiteScore rank 2021

Category	Rank	Percentile
Pharmacology, Toxicology and Pharmaceutics	#36/74	52nd
└ General Pharmacology, Toxicology and Pharmaceutics		
Energy	#38/68	44th
└ General Energy		