

Indian Journal of Biochemistry & Biophysics

<http://www.niscpr.res.in>; <http://nopr.niscpr.res.in>

VOLUME 63	NUMBER 9	SEPTEMBER 2026
CODEN: IJBBBQ 63 (9) 991-1120 (2026)		ISSN: 0301-1208 (Print); 0975-0959 (Online)

CONTENTS

Papers

- | | |
|--|------|
| <i>In silico</i> characterization unveils <i>Helicobacter pylori</i> protein HP0973 as a novel EGFR-interacting virulence factor
Debabrata Dash, Debashis Barik, Aditya Kumar Panda & Sushil Kumar Pathak* | 995 |
| Development of an efficient chemo-enzymatic process for the synthesis of Nilotinib
Sagar Narayan Tarate†, Saurav Subhash Gite†, Ravinder Reddy Patlolla, Kethavath Anjali Priya Naik, Kethavath Santhosh Nayak, KRS Sambasiva Rao & Linga Banoth* | 1013 |
| Neuroprotective role of hydroxychloroquine and trimebutine in alzheimer's disease: Network pharmacology and molecular simulations
Renukaradhya Maharudraiah, Krishna Kant, Madhusudhan Reddy Alimeneti, Roma Kumari Gupta, Sunil Kumar Kurmi, Santosh Prasad Chaudhary Kurmi, Aleesha Mujeeb Shaheen & Mahalakshmi Suresha Biradar* | 1020 |
| Design, synthesis, <i>in silico</i> study, and anti-psoriatic activity of some novel Fumaric acid ester derivatives
Priyanka Sharma, Hemlata Bisht, Niyaz Alam, Shikha Shukla, Azhar Danish Khan & Anurag Agrawal* | 1036 |
| Computational and experimental studies supporting the anti-breast cancer potential of N-hydroxyphthalimide
Karthik Nallasamy, Sumathi Sivaraman, Manu Vashishtha & Jeyavijayan Subbiah* | 1047 |
| <i>In silico</i> evaluation of black seed oil from <i>Nigella sativa</i> as a therapeutic agent for rheumatoid arthritis: Molecular docking and structural analysis
Madhavi Patel, Muthu Kumaradoss Mohan Maruga Raja & Ravi Manne* | 1062 |
| Computational identification of potential tissue plasminogen activator (tPA) inhibitors from <i>Paris polyphylla</i> phytoconstituents through molecular docking and molecular dynamics simulations for anti-inflammatory therapy
Ghassan Adel Jassim Alkhalifah, Sibghatullah Muhammad Ali Sangi, Vijayanandhan Venkatesan, Sreeharsha Nagaraja, Mahalakshmi Suresha Biradar, Shankar Mani*, Mohammed Monirul Islam, Afzal Haq Asif & Veeriah Chowdary Jasthi* | 1075 |
| Integrated GC-MS phytochemical profiling, network pharmacology, and molecular docking to elucidate the molecular mechanisms of <i>Nymphoides hydrophyllum</i> against Helminthiasis
Afsona Khatun, Nabanita Banik, Somali Gorai, Ankan Pradhan, Monika Sekar, Sujay Chakraborty & Thirumal Margesan* | 1086 |
| Synthesis of imidazole derivatives and <i>in silico/in vitro</i> evaluation of potential antidiabetic activity
Sanjana Mareguddi, Prabitha Prabhakaran, Ammar Abdul Razzak Mahmood, Saleem Javid, Nina Bhagyanath & Somashekar Mahadevappa Metri* | 1099 |

Facile synthesis, characterization, biological studies of novel schiff base ligand and its metal complexes 1112

Perka Sailaja, Kotte Kamalakar, Mandapati Venkateswara Reddy, Aedudodla Ramakrishna Reddy
& Sunkari Jyothi*

Instructions to Authors 1118

*Author for correspondence

Author Index

Agrawal A	1036	Jyothi S	1112	Pathak SK	995
Alam N	1036	Kamalakar K	1112	Patlolla RR	1013
Alimeneti MR	1020	Kant K	1020	Prabhakaran P	1099
Alkhalifah GAJ	1075	Khan AD	1036	Pradhan A	1086
Asif AH	1075	Khatun A	1086	Raja MKMM	1062
Banik N	1086	Kurmi SK	1020	Rao KRSS	1013
Banoth L	1013	Kurmi SPC	1020	Reddy AR	1112
Barik D	995	Maharudraiah R	1020	Reddy MV	1112
Bhagyanath N	1099	Mahmood AAR	1099	Sailaja P	1112
Biradar MS	1020, 1075	Mani S	1075	Sangi SMA	1075
Bisht H	1036	Manne R	1062	Sekar M	1086
Chakraborty S	1086	Mareguddi S	1099	Shaheen AM	1020
Dash D	995	Margesan T	1086	Sharma P	1036
Gite SS	1013	Metri SM	1099	Shukla S	1036
Gorai S	1086	Nagaraja S	1075	Sivaraman S	1047
Gupta RK	1020	Naik KAP	1013	Subbiah J	1047
Islam MM	1075	Nallasamy K	1047	Tarate SN	1013
Jasthi VC	1075	Nayak KS	1013	Vashishtha M	1047
Javid S	1099	Panda AK	995	Venkatesan V	1075
		Patel M	1062		

Keyword Index

ADMET studies	1062	<i>Helicobacter pylori</i>	995	Nilotinib	1013
Alzheimer's disease	1020	HP0973	995	Nimesulide	1075
Anthelmintic efficacy	1086	Human intestinal absorption	1047	Nitrilase	1013
Anti-inflammatory activity	1075	(HIA)		Orthokeratosis	1036
<i>Bacillus amylolique faciens</i>	1112	Hydroxychloroquine	1020	Oxidative stress	1086
Biocatalysis	1013	Hypothetical protein	995	<i>Paris polyphylla</i>	1075
Biological processes (BP)	1062	Imidazole derivatives	1099	Phthalimide derivative	1047
Black seed oil	1062	Immunological modulation	1086	Protein structure modeling	995
Cellular components (CC)	1062	Ketoconazole	1099	Protein-protein interaction	995
Dacarbazine	1099	Losartan	1099	Psoriasis	1036
Density functional theory	1047	<i>Macrophomina phaseolina</i>	1112	Receptor tyrosine kinase	995
(DFT)		MD Simulation	1020	Rheumatoid arthritis	1062
Disoglucose	1075	Metal complexes	1112	Schiff base	1112
Docking	1020	Mitogen-activated protein	1036	<i>Sclerotium rolfsii</i>	1112
Erythematous plaques	1036	kinase		Signalling pathways	1086
Frontier molecular orbitals	1047	MM-GBSA analysis	1075	Sustainable manufacturing	1013
(FMOs)		Molecular functions (MF)	1062	Synthesis	1036
Fumaric acid ester (FAE)	1036	Mouse tail model	1036	tPA Inhibitor	1075
Green Chemistry	1013	N-Hydroxyphthalimide (NHP)	1047	Trimebutine	1020
				α -Amylase inhibition	1099