

S.No.	Paper Title	Author list (Dep. of L.S author in bold)	Journal Name	Year
1	In silico identification of chikungunya virus replication inhibitor validated using biochemical and cell-based approaches	Meenakshi Chaudhary1,* , Akash Kumar1, Kiran Bala Sharma2, Sudhanshu Vrat2 and <b>Deepak Sehgal1</b>	FEBS Journal	2024
2	Exploring the role of TLK2 mutation in tropical calcific pancreatitis: an insilico and molecular dynamics simulation study	Ashish Srivastava, <b>Sri krishna Jayadev Magani</b> , Kiran Bharat Lokhande, Madhusudan Chitakhindi, <b>Ashutosh Singh</b>	Journal of Biomolecular structure and dynamics	2024
3	Complete mitogenome of <i>Lepidopygopsis typus</i> , an evolutionarily-distinct, endangered cyprinid fish from the Western Ghats Biodiversity Hotspot: phylogenetic relationships and implications for conservation.	Chandra, S., Abhilash, R., Sidharthan, A., Raghavan, R. & <b>Dahanukar, N.</b> (corresponding author)	Gene	2024
4	The loach genus <i>Lepidocephalichthys</i> (Telesotei: Cobitidae) in Sri Lanka and peninsular India: Multiple colonizations and unexpected species diversity.	Sudasinghe, H., <b>Dahanukar, N.</b> , Raghavan, R., Ranasinghe, T., Wijesooriya, K., Pethiyagoda, R., Rüber, L. & Meegaskumbura, M.	Hydrobiologia	2024
5	Altered neuroepithelial morphogenesis and migration defects in iPSC-derived cerebral organoids and 2D neural stem cells in familial bipolar disorder.	Phalnikar, K., Srividya, M., Mythri, S.V., Vasavi, N.S., Ganguly, A., Kumar, A., Padmaja, S., Kalia, K., Mishra, S.S., Dhanya, S.K., Paul, P., Holla, B., Ganesh, S., <b>Reddy, P.C.</b> , Sud, R., Viswanath, B., and Muralidharan, B.	Oxford Open Neuroscience	2024
6	LSD1 Regulates Neurogenesis in Human Neural Stem Cells Through the Repression of Human-Enriched Extracellular Matrix and Cell Adhesion Genes.	Channakkar, A.S., D'Souza, L., Kumar, A., Kalia, K., Prabhu, S., Phalnikar, K., <b>Reddy, P.C.</b> and Muralidharan, B.,	Oxford Stem Cells	2024

7	High-pressure microfluidisation positively impacts structural properties and improves functional characteristics of almond proteins obtained from almond meal	T.P. Sari, Amresh H. Dhamane, <b>Kamlesh Pawar</b> , Mudit Bajaj, Prarabdh C. Badgujar, Ayon Tarafdar, Vikrant Bodana, Sunil Pareek	Food Chemistry	2024
8	Characterization of genetic and molecular tools for studying the endogenous expression of Lactate dehydrogenase in Drosophila melanogaster	Madhulika Rai, Sarah M. Carter, Shefali A. Shefali, <b>Geetanjali Chawla</b> , Jason M. Tennesen	PLOS One	2024
9	Autoacetylation of lysine 187 is critical for TIP60's phase separation and functions	Dubey S, Gupta H and <b>Gupta A</b>	BioRxiv	2023
10	Exploring potential of Plasmodium RUVBL proteins as anti-malarial drug target	Khurana J, Shrivastava A, Singh A and <b>Gupta A</b>	Journal of Biomolecular Structure and Dynamics	2023
11	Methotrexate, an anti-inflammatory drug, inhibits Hepatitis E viral replication	Akash Kumar, Preeti Hooda, Anindita Puri, Radhika Khatter, Mohammed S.Al-Dosari, Neha Sinha, Mohammad K. Parvez & <b>Deepak Sehgal</b>	Journal of Enzyme Inhibition and Medicinal Chemistry	2023
12	Inhibition of HEV Replication by FDA-Approved RdRp Inhibitors	Preeti Hooda, Mohammed Al-Dosari, Neha Sinha, Mohammad K. Parvez,* and <b>Deepak Sehgal*</b>	ACS Omega Publications	2023
13	Identification of a novel inhibitor of SARS-CoV-2 main protease: an in silico, biochemical, and cell-based approach	Aditya Trivedi <sup>1</sup> Vandana Kardam , Krishna Kishore Inampudi, Sudhanshu Vrati, Dharmender Gupta <sup>4</sup> , Aekagra Singh , Sarala Rani Kayampeta <sup>5</sup> , Mohan Appaiahgari, and <b>Deepak Sehgal</b>	FEBS Journal	2023
14	Immunoinformatics-based multi-epitope containing fused polypeptide vaccine design against visceral leishmaniasis with high	Kumar, P., Kumar, P., Shrivastava, A., Dar, M. A., Lokhande, K. B., Singh, N., <b>Singh, Ashutosh.</b> , Velayutham, R., & Mandal, D	International journal of biological macromolecules	2023

	immunogenicity and TLR binding.			
15	Leveraging ChatGPT and Bard: What does it convey for water treatment, desalination and harvesting sectors?"	SS, Ray., Pranav, RT., Verma, R.K, Harish, P., Kim, B., <b>Ashutosh Singh</b> , Young,N. K	Desalination	2023
16	Terpenoid phytocompounds from mangrove plant <i>Xylocarpus moluccensis</i> as possible inhibitors against SARS-CoV-2	Kale, A., Shahakar, B., Shrivastava, A., Nawani, N., Swamy, K. V., <b>Singh, Ashutosh.</b> , Pawar, S.V.	Computational Biology and Chemistry	2023
17	Pharmacoinformatics approach for the screening of Kovidra ( <i>Bauhinia variegata</i> ) phytoconstituents against tumor suppressor protein in triple negative breast cancer	More-Adate, P., Lokhande, K. B., Shrivastava, A., Doiphode, S., Nagar, S., <b>Singh, Ashutosh.</b> , & Baheti, A.	Journal of Biomolecular Structure and Dynamics	2023
18	Screening of potential phytomolecules against MurG as drug target in nosocomial pathogen <i>Pseudomonas aeruginosa</i> : perceptions from computational campaign.	Kiran Bharat Lokhande, Sarika Vishnu Pawar, Smriti Madkaiker, Ashish Shrivastava, Swamy K. Venkateswara, Neelu Nawani, Minal Wani, Payel Ghosh & <b>Ashutosh Singh</b>	Journal of Biomolecular Structure and Dynamics	2023
19	In silico discovery of potent inhibitors against monkeypox's major structural proteins	Lokhande, K. B., Shrivastava, A., <b>Singh, Ashutosh.</b>	Journal of Biomolecular Structure and Dynamics	2023
20	Identification of potential drug candidates as TGR5 agonist to combat type II diabetes using in silico docking and molecular dynamics simulation studies	Bhimanwar, R. S., Lokhande, K. B., Shrivastava, A., <b>Singh, Ashutosh.</b> , Chitlange, S. S., & Mittal, A.	Journal of Biomolecular Structure and Dynamics	2023
21	Dysregulated Metabolites and Lipids in Serum of Patients with Acute Hepatitis E: A Longitudinal Study	Shaheen Khan, Yashwant Kumar, Charu Sharma, Sonu Kumar Gupta, Amit Goel, Rakesh Aggarwal, <b>Naga Suresh Veerapu</b>	Journal of Viral Hepatitis	2023

22	“Immobilization of laccase on poly-L-lysine modified silver nanoparticles formed by green synthesis for enhanced stability, suppressed estrogenic activity of 17 $\beta$ -estradiol, biocompatibility and anti-cancer action: An in vitro and in silico study”.	Syeda Fauzia Farheen Zofair a, Md Amiruddin Hashmi a, Irfanul Haq Faridi a, Fayyaz Rasool b, <b>Sri Krishna Jayadev Magani</b> b, Masood Alam Khan c, Hina Younus	Journal of Molecular Liquids	2023
23	“Role of Identified proteins in the proteome profiles of CDK4/6 inhibitor-resistant breast cancer cell lines	Binayak Kumar, Peeyush Prasad, Ragini Singh, Ram Krishna Sahu, Ashutosh Singh, <b>Srikrishna Jayadev Magani</b> and Suresh Hedau	Molecular Omics	2023
24	A Systematic Design and Synthesis of PET-based Fluorescent Probes for Monitoring pH During Mitophagy	Rashmi Yadav , Subrata Munan , Mudassar Ali , <b>Koyeli Mapa</b> , Animesh Samanta.	Chem Asian J	2023
25	Bacterial Transcription Factors and the Cell Cycle	Morigen Morigen, Monika Glinkowska, Jianping Xie, <b>Richa Priyadarshini</b> and Kazutoshi Kasho.	Front Microbiol.	2023
26	Metal-free synthesis and study of glycine betaine derivatives in water for antimicrobial and anticancer applications	Suchismita Rath; Debajit Maiti; Malvika Modi; Parul Pal; Subrata Munan; Biswajit Mohanty; Anjani Bhatia; Rohit Bhowal; <b>Richa Priyadarshini</b> ; Animesh Samanta; Parthapratim Munshi; Subhabrata Sen.	iScience	2023
27	Benzoxazine-grafted-chitosan biopolymer films with inherent disulfide linkage: Antimicrobial properties.	Sangeeta Sahu , Rashmi Niranjana , <b>Richa Priyadarshini*</b> , Bimlesh Lochab*	Chemosphere	2023
28	Next-generation membrane-active glycopeptide antibiotics that also inhibit bacterial cell division.	Paramita Sarkar, Kathakali De, Malvika Modi, Geetika Dhanda, <b>Richa Priyadarshini</b> , Julia E. Bandow, Jayanta Haldar*	Chem. Sci.	2023
29	Criegee Intermediate-Mediated Oxidation of Dimethyl Disulfide: Effect	Gowtham Babu, Arijit Das, <b>Anindita Chakrabarty</b> , Goutam	<i>ACS J of Phys. Chem. A.</i>	2023

	of Formic Acid and Its Atmospheric Relevance.	Chowdhury and Mausumi Goswami*		
30	Unravelling the molecular mechanism underlying drought stress response in chickpea via integrated multi-omics analysis.	MEMORANDUM OF UNDERSTANDING Singh V, Gupta K, Singh S, Jain M, <b>Garg R.</b>	Frontiers in Plant Sciences	2023
31	Unravelling Differential DNA Methylation Patterns in Genotype Dependent Manner under Salinity Stress Response in Chickpea	Gupta K, <b>Garg R</b>	IJMS	2023
32	Biogeography and evolutionary history of <i>Puntius sensu lato</i> (Teleostei: Cyprinidae) in Sri Lanka	Sudasinghe, H., Ranasinghe, T., <b>Dahanukar, N.</b> , Raghavan, R., Rüber, L., Pethiyagoda, R. & Meegaskumbura, M.	Scientific Reports	2023
33	The world's largest cave fish from Meghalaya, Northeast India, is a new species, <i>Neolissochilus pnar</i> (Cyprinidae, Torinae).	<b>Dahanukar, N.</b> , Sundar, R.L., Rangad, D., Proudlove, G. & Raghavan, R.	Vertebrate Zoology	2023
34	Evolution in the dark: Unexpected genetic diversity and morphological stasis in the blind, aquifer-dwelling catfish <i>Horaglanis</i> .	Raghavan, R., Sundar, R.L., Arjun, C.P., Britz, R. & <b>Dahanukar, N.</b> (corresponding author)	Vertebrate Zoology	2023
35	Regulation of chromatin accessibility and gene expression in the developing hippocampal primordium by LIM-HD transcription factor LHX2	Suresh, V., Muralidharan, B., Pradhan, S.J., Bose, M., D'Souza, L., Parichha, A., <b>Reddy, P.C., Galande, S.</b> and Tole, S.	PLoS genetics	2023
36	Multifunctional Multicomponent Highly Biocompatible pH-Responsive Iron-Oxide Embedded Nanodiamond Cargo for Artesunate to Inhibit Cancer Growth	Mishra, V. S., Patil, S., <b>Reddy, P. C.</b> , & Lochab, B.	ACS Materials Letters	2023
37	OXR1 maintains the retromer to delay brain	Kapahi P , Wilson K , Bar S , Dammer E , Hodge B , Carrera E	Nature Communications	2023

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