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Research and Professional Experience

- **Associate Professor** [Dec 16, 2022 - Till], Department of Chemistry, Hansraj College University Enclave, University of Delhi, Delhi-110007.
- **Assistant Professor** [Dec 15, 2014 – Dec. 15, 2022], Department of Chemistry, Hansraj College University Enclave, University of Delhi, Delhi-110007.
- **Research Collaborator** [July 2021-] Mayo Clinic Florida USA (Employee ID, 309707; Person ID, 309707).
- **Assistant Professor - Affiliate** [October 1, 2018 – September 30, 2021], Department of Medicine, Stritch School of Medicine, University of Loyola, Chicago, United States of America.
- **Affiliate Professor** [September 1, 2019 – August 30, 2022], Department of Pharmaceutical Chemistry, University of Debrecen, Debrecen, Hungary.
- **Post-Doctoral Researcher** [August 1, 2016 - July 31, 2017], Department of Chemistry, Massachusetts Institute of Technology (M.I.T.), 77 Massachusetts Avenue, Cambridge, MA 02139 United States of America (Advisor: Prof. Alexander M Klibanov).
- **Assistant Professor (Ad-hoc)** [Aug 5, 2010-Dec 14, 2014], Department of Chemistry, Sri Venkateswara College, University of Delhi, New Delhi-110021.
- **Principal Investigator** [2011 - 2014], Department of Chemistry, University of Delhi, *Title of the Project: "*Novel functionalized tetrahedral activated small peptidomimetic inhibitors of malarial aspartic proteases, plasmepsin I and plasmepsin II" *Funding Agency*: Department of Science and Technology, Ministry of Science and Technology, Government of India.
- **Ph. D. in Chemistry** [2004 – 2010], Department of Chemistry, University of Delhi, Delhi- 110007 India. Title of the Thesis: **"Synthesis, Conformational Features and Reactivity Studies of *Sym N,N',N*"-Triarylguanidines"**. Advisor**:** Prof. Natesan Thirupathi**.**
- **M. Sc. in Organic Chemistry** [2001 - 2003]: Division: First
- **B. Sc.** [1999 - 2001]: Division: First

Patent (International) – Granted

- **Brijesh Rathi**, Snigdha Singh, Neha Sharma, Poonam, Agam P Singh, Ravi Durvasula, Prakasha Kempaiah "Hydroxyethylamine-based piperazine compounds, and methods of producing and using the same for treating disease" (US Patent App. 11485714; 1 Nov. 2022) **Granted.**
- Zoltner Martin, Zahedifard Farnaz, **Brijesh Rathi**, Neha Sharma, Meenakshi Bansal "Phthalimide-based substances with antiprotozoal activity and their use in therapy" (Czech Patent App. PV 2021-408; 15 August 2023) **Granted**.

Patent (Indian) - Filed

- Brijesh Rathi, Prakasha Kempaiah, Agam P Singh, Snigdha Singh, Yash Gupta, Neha Sharma, Poonam, Ravi Durvasula, "Hydroxyethylamine-based Piperazine Compounds, and Methods of Producing and Using the Same for Treating Disease" Application No. *INDIA Patent No: 202011056923* was filed on Apr 29, 2021.
- Neha Sharma, Brijesh Rathi, Agam P Singh "Novel Antiparasitic Agents Based on Piperazine and Uses thereof" (Patent Filed; Application No. 202011043767; 08 October 2020).

Research Publications (Citation: 2454; h-index: 26)

1. Bege; M.; Singh, V.; Sharma, N.; Debreczeni, N.; Bereczki, I.; Poonam; Herczegh, P.; **Rathi, B**.*; Singh, S.*; Borbás, A*. "In vitro and in vivo antiplasmodial evaluation of sugar-modified nucleoside analogues" *Sci. Rep.* **2023**, *13*, 12228 (IF, 4.996; Nature Group Publications, Netherland; ISSN: 2045-2322).
2. Bansal, M.; Kumar, S.; Rathi, B.* "Synthesis of novel phthalimide-based piperazine conjugated analogs as anti-malarial agents" *Chem. Biol. Lett.* **2023**, *10*, 627 (Scopus Indexed; ISSN, 2347-9825).
3. Sharma, H.; Kumar, M.; Sethi, A.; Poonam; **Rathi, B.*** "Metal-free construction of aminated isoquinoline frameworks from 2-(2-oxo-2-arylethyl) benzonitrile in an aqueous medium" *Green Chem.* **2023**, 25**,** 167 (IF, 9.8; RSC London; ISSN, 1463-9270).
4. Kumar; M.; Verma, S.; Sharma, M.; Poonam;* Rathi, B*. "Metal-Catalyzed Synthesis of Benzofused Five-Membered N/O/S Heterocycles, a Progressive Area in Synthetic Chemistry" *Eur. J. Org. Chem.* **2023** Accepted DOI: 10.1002/ejoc.202300877 (IF: 2.8; Wiley; ISSN:1099-0690).
5. Silva, R.; Lima, S. C.; Reis, W. P.; Magalhães, J. F.; Magalhães, R.; **Rathi, B.**; Kohl, A.; Bezerra, M. C.; Pena, L. "Comparison of DNA extraction methods for COVID-19 host genetics studies" *Plos ONE* **2023**, 18, e0287551 (IF: 3.24; Plos Publications; ISSN: eISSN-1932-6203).

6. Wang, Z.; Sharma, P. P.; **Rathi, B.**; Xie, M.; Clercq, E. D.; Pannecouque, C.; Kang, D.; Zhan, P.; Liu, X. "Escaping from Flatland: Multiparameter Optimization Leads to the Discovery of Novel Tetrahydropyrido[4,3- d]pyrimidine Derivatives as HIV-1 NNRTIs with Superior Antiviral Activities against NNRTI-Resistant Variants and Favorable Drug-Like Profiles" *J. Med. Chem.* **2023**, 66, 13, 8643–8665 (IF, 8.04; American Chemical Society; ISSN, 1520-4804).
7. Souza, R.M.C.; Pimentel, L.M.L.M.; Ferreira, L.K.M.; Hernandes, V.P.; Santos, A.C.D.S.; Dantas, W.M.; Silva, C.J.O.; Brito, R.M.M.; Andrade, J.L.; Andrade-Neto, V.F.; Fujiwara, R.T.; Bueno, L.L.; Junior, V.S.; Pena, L.; Camara, C.A.; **Rathi, B.**; Oliveira, R.N. "Biological activity of 1, 2, 3-triazole-2-Amino-1, 4-Naphthoquinone derivatives and their evaluation as therapeutic strategy for malaria control" *Eur. J. Med. Chem.* **2023**, 255, 115400 (IF: 7.088; Elsevier, Netharlands; ISSN, 0223-5234).
8. Hooda, A.; Singh, D.; Nehra, K.; Dalal, A.; Kumar, S.; Malik, R.S.; **Rathi, B.**; Kumar, P. "Luminescent Tb (III) complexes with Lewis bases for displays: Synthesis and spectral investigation" *Inorg. Chem. Comm.* **2023**, *151*, 110583 (IF, 3.428; Elsevier, Netharlands; ISSN, 1879-0259).
9. Shaikh, A. S.; Sethi, A.; Makhal, P. N.; **Rathi, B.**; Kaki, V. R. "Quest for selective MMP9 inhibitors: a computational approach" *J. Biomol. Struct. Dyn.* **2023**, DOI: 10.1080/07391102.2023.2186710 (IF,5.235; Elsevier; ISSN, 1538-0254).
10. Kumar, S.; Yadav, D.; Singh, D.; Shakya, K.; **Rathi, B.***; Poonam* "Recent developments on Junin virus, a causative agent for Argentine haemorrhagic fever" *Rev. Med. Virol*., **2023**, 33, e2419 (IF, 11.043; Wiley; ISSN, 1099-1654).
11. Upadhyay, C., Bhattacharya, S., Kumar, S., Kumar, D., Bhadula, N., Rathi, B., Singh, A. P., & Singh, P. "Novel fluorinated piperazine based-amino acid derivatives as antiplasmodial agents: Synthesis, bioactivity and computational studies. *Chem. Biol. Lett.* **2023**, *10*, 543 (Scopus Indexed; ISSN, 2347-9825).
12. Jee, B.; Sharma, P. P.; Goel, V. K.; Kumar, S.; Singh, Y.; Rathi, B. "Natural Metabolite Ursolic Acid as an Inhibitor of Dormancy Regulator DosR of Mycobacterium tuberculosis: Evidence from Molecular Docking, Molecular Dynamics Simulation, and Free Energy Analysis" *Curr. Comput. Aided Drug Des.* **2023** *In Press* DOI: 10.2174/1573409919666230201100543 (IF, 1.63; Bentham Science Publishers; ISSN, 1875-6697).
13. Raj, S.; Rathi, B.; Mehra, P.; Asthana, S.; Kumar, D. "Deciphering the role of c-MET in Metabolic reprogramming of Head and Neck squamous cell Carcinoma via In Silico analysis" *Chem. Biol. Lett.* **2023**, *10*, 532 (Scopus Indexed; ISSN, 2347-9825).
14. Maurya, S.; Srivastava, R.; Arfin, S.; Hawthorne, S.; Jha, N. K.; Agrawal, K.; Raj, S.; **Rathi, B.**; Kumar, A.; Raj, R.; Agrawal, S.; Paiva-Santos, A. C.; Malik, A. A.; Dua, K.; Rana, R.; Ojha, S.; Jha, S. K.; Sharma, A.; Kumar, D.; El-Zahaby, S. A.; Nagar, A. "Exploring state of the art advances in targeted nanomedicines for managing acute and chronic inflammatory lung diseases" *Nanomedicine* **2023,** *17*, 2245 (IF, 6.096; Future Medicine; ISSN, 1748-6963).
15. Sujata Maurya, Sibi Raj, Nihar Ranjan Bhoi, Neel Mani, Brijesh Rathi, Dhruv Kumar "Morphological analysis of metabolically dysregulated spermatozoa using

Artificial Intelligence based approach" *J. Integrat. Sci. Technol.* **2023**, 2, 532 (Indian Science Publications; ISSN, 2321-4635).

16. Dalal, A.; Nehra, K.; Hooda, A.; Singh, D.; Kumar, P.; Kumar, S.; Malik, R. S.; Rathi, B. "Luminous lanthanide diketonates: Review on synthesis and optoelectronic characterizations, *Inorg. Chim. Acta* **2023**, 550, 121406 (IF, 2.8; Elsevier; ISSN, 0020-1693).
17. Anjani, Kumar, S.; Rathi, B.; Poonam "Recent updates on the biological efficacy of approved drugs and potent synthetic compounds against SARS-CoV-2" *RSC Adv.*, **2023**, 13, 3677-3687 (IF: 4.036; Royal Society of Chemistry UK; ISSN, 2046-2069).
18. Sharma, N.; Sharma, H.; Kumar, M.; Grishina, M.; Pandit, U.; Poonam and **B. Rathi*** "Solvent-free mechanochemical grinding facilitates clean synthesis of *N*-substituted amines" *Org. Biomol. Chem.*, **2022**, 20, 6673-6679 (IF, 3.89; ISSN, 1477-0539; Royal Society of Chemistry London).
19. Jiang, X.; Sharma, P. P.; **Rathi, B.**; Ji, X.; Hu, L.; Kang, G.D.; Wang, Z.; Xie, M.; Xu, S.; Zhang, X.; Clercq, E. D.; Cocklin, S.; Pannecouque, C.; Dick, A.; Liu, L.; Zhan, P. "Discovery of novel 1,2,4-triazole phenylalanine derivatives targeting an unexplored region within the interprotomer pocket of the HIV capsid protein". *J. Med. Virol.* **2022**, 94, 5975 (IF, 12.7; Wiley Germany; ISSN, 1096-9071;).
20. Pant, P.; Sharma, P.P.; **Rathi, B.**; Sharma, S. "Mycobacterium tuberculosis Dormancy Regulon proteins Rv2627c and Rv2628 as Toll Like Receptor agonist and as potential adjuvant" *Int. Immunopharmacol.* **2022**, *112*, 109238 (IF, 5.714; Elsevier Netherlands; ISSN, 1567-5769).
21. Ji, X.; Li, J.; Sharma, P. P.; Jiang, X.; Rathi, B.; Gao, Z.; Hu, L.; Kang, D.; Clercq, E.; Cocklin, S.; Liu, C.; Pannecouque, C.; Dick, A.; Zhan, P.; Liu, X. Design, synthesis and structure-activity relationships of phenylalanine-containing peptidomimetics as novel HIV-1 capsid binders based on Ugi four-component reaction. *Molecules* **2022,** *27*, 5995 (IF, 4.411; MDPI Switzerland; ISSN, 1420-3049).
22. Kumar, S.; Sharma, N.; Dantas, W.; Nascimento, J.C.F.; Maus, H.; Oliveira, R. N.; Pandit, U.; Singh, A.; Schirmeister, T.; Hazari, P. P.; Pena, L.; Poonam*, **Rathi, B.*** "A potent candidate against Zika virus infection: Synthesis, bioactivity, radiolabeling and biodistribution studies" *New J. Chem.* **2022,** 46, 18764 (IF: 3.93; Royal Society of Chemistry; ISSN, 1396-9261).
23. Sharma, P. P.; Bhardwaj, S.; Sethi, A.; Poonam; Rathi, B. Chitosan based architectures as biomedical carriers *Carbohydr. Res.* **2022** Accepted (IF, 2.975; Elsevier; ISSN, 1873-426X).
24. Nehra, K.; Dalal, A.; Hooda, A.; Bhagwan, S.; Jakhar, K.; Singh, D.; Malik, R. S.; Kumar, S.; **Rathi, B.** "Synthesis, thermal and photoluminescence investigation of Tb (III) β-diketonates with 1, 10-phenanthroline derivatives" *J. Lumin.* **2022**, *251*, 1192333 (If, 4.171; Elsevier; ISSN, 1872-7883).
25. Gupta, Y.; Sharma, N.; Singh, S.; Romero, J.G.; Rajendran, V.; Mogire, R.M.; Kashif, M.; Beach, J.; Jeske, W.; Poonam, Ogutu, B.; Kanzok, S.M.; Akala, H.M.; Legac, J.; Rosenthal, P.J.; Rademacher, D.J.; Durvasula, R.; Singh, A.P.; **Rathi**,

B.* and Kempaiah, P. The multistage antimalarial compound Calxinin perturbates P. falciparum Ca^{2+} homeostasis by targeting a unique ion channel. *Pharmaceutics* **2022**, 14, 1371 (IF, 6.525; ISSN, 1999-4923; MDPI Switzerland).

26. Singh, V.; Hada, R.S.; Jain, R.; Vashistha, M.; Kumari, G.; Singh, S.; Sharma, N.; Bansal, M.; Poonam, Zoltner, M.; Caffrey, C.R.; **Rathi, B*** and Singh, S. "Designing and development of phthalimides as potent anti-tubulin hybrid molecules against malaria". *Eur. J. Med. Chem.* **2022**, 239, 114534 (IF: 7.088; Elsevier, Netharlands; ISSN, 0223-5234).
27. Arfin, S.; Chauhan, S.; Mani, N.; **Rathi, B.;** Kumar, D. "In Silico analysis of Ceruloplasmin alteration in Oral Squamous Cell Carcinoma" *Chem. Biol. Lett.* **2022**, 9, 342 (Scopus Indexed; ISSN, 2347-9825).
28. Kumar, K.; Kovalenko, S.; Bhardwaj, S.; Sethi, A.; Gorobets, N.; Desenko, S. M.; Poonam, **Rathi, B.*** "Drug Repurposing against SARS-CoV-2 using Computational Approaches" *Drug Discov. Today* **2022**, 27, 2015-2027 (IF, 8.369; Elsevier Netherland; ISSN, 1359-6446).
29. Raj, S.; Kesari, K. K.; Kumar, A.; **Rathi, B.**; Sharma, A.; Gupta, P.K.; Jha, S. K.; Jha, N. K.; Slama, P.; Roychoudhury, S.; Kumar, D. "Molecular Mechanism(s) of regulation(s) of c-MET/HGF Signalling in Head and Neck Cancer" *Mol. Cancer* **2022**, *21*, 31 (**IF, 41.444**; BMC Springer Nature; ISSN, 1476-4598).
30. Gupta, Y.; Goicoechea, S.; Pearce, C.; Mathur, R.; Romero, J.; Kwofie, S.; Weyenberg, M.; Daravath, B.; Sharma, N.; Poonam, Akala, H.; Kanzok, S.; Durvasula, R.; **Rathi, B.**; Kempaiah, P. "The emerging paradigm of calcium homeostasis as a new therapeutic target for Protozoan Parasites" *Med. Res. Rev.* **2022,** 42, 56-82 (IF, **12.994**; Wiley-VCH Verlag GmbH & Co. KGaA, Germany; ISSN: 1098-1128).
31. Sharma, P. P.; Sethi, A.; Diwedi, B.; Grishina, M.; **Rathi, B.**; Singh, G. "Novel Inhibitors of malarial aspartyl proteases, plasmepsin II and IV: In silico design and validation studies" *Chem. Biol. Lett.* **2022**, *9*, 315 (Scopus Indexed; ISSN, 2347-9825).
32. Sharma, N.; Kashif, M.; Singh, V.; Fontinha, D.; Mukherjee, B.; Kumar, D.; Singh, S.; Prudêncio, M.; Singh, A.*; **Rathi, B.*** "Novel antiplasmodial compounds leveraged with multistage potency against Parasite *Plasmodium falciparum*: In vitro, in vivo evaluations and pharmacokinetic studies" *J. Med. Chem.* **2021**, *64*, 8666 (IF, 8.04; American Chemical Society; ISSN, 1520-4804).
33. Mehta, J.; Rolta, R.; Salaria, D.; Awofisayo, O.; Fadare, O.A.; Sharma, P. P.; **Rathi, B.**; Chopra, A.; Kaushik, N.; Choi, E. H.; Kaushik, N. K. "Phytocompounds from North Western Himalayan medicinal plants as potential drug to treat multidrug resistant *Salmonella typhimurium*: an in silico approach" *Biomedicine* **2021**, *9*, 1402 (IF, 6.08; MDPI Switzerland; ISSN: 2227-9059).
34. Li, J.; Jiang, X.; Dick, A.; Sharma, P. P.; Chen, C.-H.; **Rathi, B.**; Kang, D.; Wang, Z.; Ji, X.; Lee, K.-H.; Cocklin, S.; Liu.; Zhan, P.; "Design, Synthesis, and Antiviral Activity of Phenylalanine Derivatives as HIV-1 Capsid Inhibitors" *Bioorg. Med. Chem.* **2021**, *48*, 116414 (IF: 3.641; Elsevier; ISSN: 0968-0896).

35. Gupta, Y.; Kumar, S.; Zak, S.; Jones, K.; Upadhyay, C.; Sharma, N.; Azizi, S-A.; Kathayat, R.; Poonam; Herbert, A.; Durvasula, R.; Dickinson, B.; Dye, J.; **Rathi, B.***; Kempaiah, P.* "Antiviral Evaluation of Hydroxyethylamine Analogs: Inhibitors of SARS-CoV-2 Main Protease (3CLpro), A Virtual Screening and Simulation Approach" *Bioorg. Med. Chem.* **2021**, *47*, 116393 (IF: 3.641; Elsevier; ISSN: 0968-0896).
36. Sharma, P. P.; Bansal, M.; Sethi, A.; Poonam, Pena, L.; Grishina, M.; Chaturvedi, S.; Kumar, D.; **Rathi, B.*** "Computational methods directed towards drug repurposing for COVID-19: advantages and limitations" *RSC Adv.* **11**, 36181 (IF: 4.036; Royal Society of Chemistry, UK; ISSN: 2046-2069).
37. Kumar, S.; Gupta, Y.; Zak, S.; Jones, K.; Upadhyay, C.; Sharma, N.; Herberty, A.; Durvasula, R.; Potemkin, V.; Dye, J.; Poonam; Kempaiah, P.*; **Rathi , B.***; "A novel compound active against SARS-CoV-2 targeting Uridylate-specific endoribonuclease (NendoU/NSP15): *In silico* and *in vitro* investigations" *RSC Med. Chem.* **2021**, 12, 1757-1764 (IF, 3.47; Royal Society of Chemistry UK; ISSN, 2632-8682).
38. Dantas, W. M.; Oliveira, V. N.; Santos, D. A. L.; Seabra, G.; Sharma, P. P.; **Rathi, B.**; Pena, L.; Oliveira, R. "Searching Anti-Zika Virus Activity in 1H-1,2,3-triazole based compounds" *Molecules* **2021**, *26*, 5869 (IF, 4.411; MDPI Switzerland; ISSN, 1420-3049).
39. Bansal, M.; Upadhyaya, C.; Poona; Kumar, S.; **Rathi, B.*** 'Phthalimide Analogs for Antimalarial Drug Discovery' *RSC Med. Chem.* **2021**, *12*, 1854 (IF, 3.47; Royal Society of Chemistry UK; ISSN, 2632-8682).
40. Oliveira, V.N.; Moura, C.; Peixoto, A.; Ferreira, VPS.; Araújo, H.M.; Pimentel, L.M.L.; Pessoa, C.; Nicolete, R.; Anjos, J.; Sharma, P. P.; **Rathi, B.**; Pena, L.; Rollin, P.; Tatibouët, A.; Oliveira, R. "Synthesis of alkynylated 1,2,4-oxadiazole/1,2,3-1H-triazole glycoconjugates: discovering new drug candidates for use in chemotherapy against lung carcinoma and *Mycobacterium tuberculosis*" *Eur J. Med. Chem.* **2021**, *220*, 113472 (IF: 7.088; Elsevier, Netharlands; ISSN, 0223-5234).
41. Rolta, R.; Salaria, D.; Sharma, P. P.; Sharma, B.; Kumar, V.; **Rathi, B.**; Verma, M.; Sourirajan, A.; Baumler, D. A.; Dev, K. "Phytocompounds of Rheum emodi, Thymus serpyllum, and Artemisia annua Inhibit Spike Protein of SARS-CoV-2 Binding to ACE2 Receptor: In Silico Approach" *Curr. Pharmacol. Rep.* **2021**, *7*, 135 (IF, 1.52; Springer International Publishing Switzerland; ISSN, 2198641X).
42. Chandel,V.; Kumar, A.; Kumar, A.; **Rathi, B.**; Kumar, D. Role of Monocarboxylate Transporters in Head and Neck Squamous Cell Carcinoma. *Life Sci.* **2021**, *279*, 119709 (IF, 5.037; Elsevier; ISSN, 0024-3205).
43. Chandel, V.; Tripathi, G.; Nayar, S. A.; **Rathi, B.**; Kumar, A.; Kumar, D. "In silico identification and validation of triarylchromones as potential inhibitor against main protease of severe acute respiratory syndrome coronavirus 2" *J. Biomol. Struct. Dyn.* **2021** Accepted https://doi.org/10.1080/07391102.2021.1918255 (IF,5.235; Elsevier; ISSN, 1538-0254).
44. Feng, D.; Wei, F.; Sun, Y.; Sharma, P.; Zhang, T.; Lin, H.; **Rathi, B.**; Clercq, E.; Pannecouque, C.; Kang, D.; Zhan, P.; Liu, X. "Boronic acid-containing

diarylpyrimidine derivatives as novel HIV-1 NNRTIs: design, synthesis, and biological evaluation" *Chin. Chem. Lett.* **2021**, *32*, 4053 (IF, 6.779; Elsevier; ISSN 1001-8417).

45. Raj, S.; Mathur, A.; **Rathi, B.**; Kumar, N.; Jha, S. K.; Kumar, D. "Mutational Heterogeneity in Spike Glycoproteins of Severe Acute Respiratory Syndrome Coronavirus 2" *3 Biotech* **2021**, *11***,** 236 (IF, 1.798; Springer; ISSN, 2190-5738).
46. Arfin, S.; Jha, N. K.; Jha, S. K.; Kesari, K.; Ruokolianen, J.; Roychoudhury, S.; **Rathi, B**.; Kumar, D. "Oxidative Stress in Cancer Cell Metabolism" *Antioxidants* **2021**, *10*, 642 (IF, 6.312; MDPI Switzerland; ISSN: 2076-3921).
47. Gupta Y.; Maciorowski, D.; Zak, S.; Jones, K.; Kathayat, R.; Azizi, S.; Mathur, R.; Pearce, C.; Ilc, J.; Husein, H.; Herbert, A.; Bharti, A.; **Rathi, B**.; Durvasula, R.; Becker, D.; Dickinson, B.; Dye, J.; Kempaiah, P. "Bisindolylmaleimide IX: A novel anti-SARS-CoV2 agent targeting viral main protease 3CLpro demonstrated by virtual screening pipeline and in-vitro validation assays" *Methods* **2021**, *195*, 57-71 (IF, 3.608; Elsevier; ISSN, 1095-9130).
48. Kumar, S.; Upadhyaya, C.; Kempaiah, P.; **Rathi, B.**; Poonam "Multi-targeting approach for nsp3, nsp9, nsp12 and nsp15 proteins of SARS-CoV-2 by Diosmin as illustrated by Molecular Docking and Molecular Dynamics simulation methodologies" *Methods* **2021**, *195*, 44-56 (IF, 3.608; Elsevier; ISSN, 1095-9130).
49. Sharma, P.; Kumar, S.; Srivastava, S.; Srivastava, M.; Jee, B.; Gorobets, N.; Kumar, D.; Kumar, M.; Asthana, S.; Zhang, P.; Poonam, Zoltner, M.; **Rathi, B**.* "Computational study of novel inhibitory molecule, 1-(4-((2S,3S)-3-amino-2-hydroxy-4-phenylbutyl)piperazin-1-yl)-3-phenylurea, with high potential to competitively block ATP binding to the RNA dependent RNA polymerase of SARS-CoV-2 virus" *J. Biomol. Struct. Dyn.* **2021** *Accepted* https://doi.org/10.1080/07391102.2021.1940281 (IF, 5.235; Taylor & Francis; ISSN, 1538-0254).
50. Chandel, V.; Sharma, P. P.; Kumar, N.; Jha, N.; **Rathi, B**.; Kumar, D. "In silico identification of potential inhibitor for TP53-induced glycolysis and apoptosis regulator in head and neck squamous cell carcinoma" *3Biotech* **2021**, 11, 117 (IF, 2.406; Springer; ISSN, 2190-5738).
51. Sharma, P.; Kumar, S; Kumar K.; Singh, A.; Singh, I.; Grishina, M.; Pandey, K.; Singh, P.; Potemkin, V.; Poonam, Singh, G.; **Rathi, B.*** "In silico Validation of Novel Inhibitors of Malarial Aspartyl Protease, Plasmepsin V and Antimalarial Efficacy Prediction" *J. Biomol. Struct. Dyn.* **2022**, 40, 8352 (IF, 5.235; Taylor & Francis; ISSN, 1538-0254).
52. Sharma, N.; Gupta, Y.; Bansal, M.; Singh, S.; Pathak, P.; Shahbaaz, M.; Mathur, R.; Singh, J.; Kashif, M.; Grishina, M.; Potemkin, V.; Rajendran, V.; Poonam; Kempaiah, P.; Singh, A.; **Rathi, B.*** "Multistage Antiplasmodial Activity of Hydroxyethylamine Compounds, *In vitro* and *In vivo* Evaluations" *RSC Adv.* **2020**, 10, 35516-35530 (IF: 4.036; Royal Society of Chemistry, UK; ISSN: 2046-2069).
53. Raj, S.; Chandel, V.; **Rathi, B.** and Kumar, D. "Understanding the Molecular Mechanism(s) of SARS-CoV2 Infection and Propagation in Human to Discover

Potential Preventive and Therapeutic Approach", *Coronaviruses*, **2020**,1, 73-81 (ISSN, 2666-7975).

54. Srivastava, S.; Verma, S.; Kamthania, S.; Agarwal, D.;Saxena, A.; Kolbe, M.; **Rathi, B**.;Nayar, A.; Shin, H.; Vashisht, K.; Pandey, K. C. "Computationally validated SARS-CoV-2 CTL and HTL Multi-Patch Vaccines designed by reverse epitomics approach, shows potential to cover large ethnically distributed human population worldwide" *J. Biomol. Struct. Dyn.* **2022**, *40*, 2369 (IF, 5.235; Taylor & Francis; ISSN, 1538-0254).
55. Chandel, V.; Sharma, P. P.; Raj, S.; Choudhari, R.; **Rathi, B.**; Kumar, D. "Structure-based drug repurposing for targeting Nsp9 replicase and spike proteins of severe acute respiratory syndrome coronavirus 2" *J. Biomol. Struct. Dyn.* **2022**, *40*, 249 (IF, 5.235; Taylor & Francis; ISSN, 1538-0254).
56. Kumar, S.; Goicoechea, S.; Kumar, S.; Pearce, C. M.; Durvasula, R.; Kempaiah, P.; **Rathi, B.***; Poonam* "Oseltamivir analogs with potent anti-influenza virus activity" *Drug Discov. Today.* **2020**, *25, 1389-1402* (IF, 8.369; Elsevier Netherland; ISSN, 1359-6446).
57. Kumar, S.; Sharma, P. P.; Shankar, U.; Kumar, D.; Joshi, S. K.; Pena, L.; Durvasula, R.; Kumar, A.; Kempaiah, P.; Poonam; **Rathi, B.*** "Discovery of New Hydroxyethylamine Analogs Against 3CLpro Protein Target of SARS-CoV-2: Molecular Docking, Molecular Dynamics Simulation and Structure-Activity Relationship Studies" *J. Chem. Inf. Model.* **2020** 60, *12,* 5754 (IF, 6.162; American Chemical Society; ISSN, 1549-9596).
58. Kumar, S.; Upadhyay, C.; Bansal, M.; Grishina, M.; Potemkin, V.; **Rathi, B.***; Poonam* "Experimental and computational studies of microwave assisted, facile ring opening of epoxide with less reactive aromatic amines in nitromethane" *ACS Omega* **2020**, 5, 30, 18746–18757 (IF, 4.132; American Chemical Society; ISSN, 2470-1343).
59. Kumar, S.; Poonam, **Rathi, B.** "Coronavirus Disease COVID-19: A New Threat to Public Health**"** *Curr. Topics Med. Chem.* **2020**, 20, 599-600 (IF: 3.442; Bentham Science Publishers, UAE; ISSN, 1568-0266).
60. Chhikara, BS.; **Rathi, B.**; Singh, J.; Poonam "Corona virus SARS-CoV-2 disease COVID-19: Infection, prevention and clinical advances of the prospective chemical drug therapeutics" *Chem. Biol. Lett.* 2020, 7, 63-72 (Scopus Indexed; ISSN, 2347-9825).
61. Singh, S.; El-Sakkary, N.; Skinner, D. E.; Sharma, P. P.; Ottilie, S.; Antonova-Koch, Y.; Kumar, P.; Winzeler, E.; Poonam; Caffrey, C. R.*; and **Rathi, B.*** "Synthesis and bioactivity of phthalimide analogs as potential drugs to treat schistosomiasis, a neglected disease of poverty" *Pharmaceuticals*, **2020,** 13, 25 (IF, 5. 215; MDPI Switzerland; ISSN, 1424-8247).
62. Upadhyay, C.; Monika; Oliveira**,** R.; Borbas, A.; Kempaiah, P.; Poonam; **Rathi, B.*** "Fluorinated scaffolds for antimalarial drug discovery" *Expert Opin Drug Dis* **2020**, *15*, 705 (IF, 7.05; Taylor & Francis UK; ISSN, 1746-045X).
63. Kelemen, V.; Csávás, M.; Péter, M.; Herczeg, M.; Poonam, **Rathi, B.**; Jain, N.; Borbás, A. "Photoinitiated Thiol-Ene Reactions of Various 2,3-Unsaturated O-, C-S- and N- Glycosides - Scope and Limitations Study" *Chem. Asian J. 2020, 15*,

87610 (IF, 4.568; Wiley-VCH Verlag GmbH & Co. KGaA, Germany; ISSN, 1861-471X).

64. Zhang, S.; Xiao, M.; Zhang, Y.; Li, Y.; Liu, H.; Han, G.; **Rathi, B.**; Wu, L.; "Mimicking Neuromelanin Nanoparticles As a Selective Pb2+ Probe" *Analytica Chim. Acta.* **2020,** 1105, 208-213 (IF, 6.911; Elsevier Netherlands; ISSN, 1873-4324).
65. Kwofie, S.; Emmanuel, B.; Dankwa, B.; Enninful, K.; Teye, J.; Davidson, C.; Nimely, J.; **Rathi, B.**; Miller, W. "Review of Atypical Organometallic Compounds As Antimalarial Drugs" *J. Chem.* **2020,** *2020*, 9; Article ID 9414093 (IF, 1.727; Hindawi Publishers London, ISSN, 2090-9071).
66. Kwofie, SK; Broni,……**Rathi, B.**; Miller, W. A.; Yaya, A.; Wilson, M. D. "Outwitting an Old Neglected Nemesis: A Review on Leveraging Integrated Data-Driven Approaches to Aid in Unraveling of Leishmanicides of Therapeutic Potential" *Curr. Topics Med. Chem*. **2020**, *20*, 349-366 (IF: 3.295; Bentham Science Publishers, UAE; ISSN, 1568-0266).
67. Singh, S.; Achieng, A. O.; Vandana: Pant, A.; Nasamu, A. S.; Pandit, M.; Singh, J.; Quadri, A.; Gupta, N.; Poonam; Ghosh, P. C.; Singh, B. K.; Latha, N.; Kempaiah, P.; Chandra, R.; Dunn, B. M.; Pandey, K. C.; Goldberg, D. E.; Singh, A.*; and **Rathi, B.*** "Fast-acting small molecules targeting malarial aspartyl proteases, plasmepsins, inhibit malaria infection at multiple life stages". *ACS Infect. Dis.* **2019**, *5,* 184-198 (IF: 5.084; American Chemical Society; ISSN, 2373-8227).
68. Chistov, A. A.; Orlov, A. A.; Streshnev, P. P.; Slesarchuk, N. A.; Aparin, I.O.; **Rathi, B.**; Brylev, V. A.; Kutyakov, S. V.; Mikhura, I. V.; Ustinov, A. V.; Westman, G.; Palyulin, V.A.; Jain, N.; Osolodkin, D.I.; Kozlovskaya, L. I.; Korshun, V. A. Compounds based on 5- (perylen-3-ylethynyl)uracil scaffold: high activity against tick-borne encephalitis virus and non-specific activity against enterovirus A." *Eur. J. Med. Chem.* **2019**, *171*, 93-103 (IF: 7.088; Elsevier, Netherlands; ISSN, 0223-5234).
69. Wu, L.; Xu, Z.; Meng, Q.; Xiao, Y.; Cao, Q.; **Rathi, B.**; Liu, H.; Han, G.; Zhang, J.; Yan, J. "A New Aptamer/Black Phosphorous Interdigital Electrode for Malachite Green Detection" *Analytica Chim. Acta.* **2020**, 1099, 39-45 (IF: 6.558; Elsevier Netherlands; ISSN, 1873- 4324).
70. Poonam, Kumari, P.; Grishina, M.; Potemkin, V.; Verma, A.; **Rathi, B.** Oxygen mediated highly efficient cobalt(II) porphyrin-catalyzed reduction of functional chromones: Experimental and Computational studies. *New J. Chem.*, **2019**, *43*, 5228-5238 (IF: 3.9; Royal Society of Chemistry; ISSN, 1396-9261).
71. Kumar, S.; Wu, L.; Sharma, N.; Ayushee; Kaushik, K.; Grishina, M.; Chhikara, BS.; Poonam; Potemkin, V.; **Rathi, B.*** "Theoretical and experimental studies of an oseltamivir–triazole-based thermoresponsive organogel" *RSC Adv*., **2019**, *9*, 21031 (IF: 4.036; Royal Society of Chemistry, UK; ISSN: 2046-2069).
72. Chhikara, B.S.; **Rathi, B.**; Keykavous, P. "Critical Evaluation of Pharmaceutical Rational Design of Nano-Delivery Systems for Doxorubicin in Cancer Therapy. *J. Mat. NanoSci.* **2019**, *6*, 47-66 (Indian Science Publishers; ISSN: 2394-0867).

73. Sharma, N., Verma, A.; Poonam, Kempaiah, P., and **Rathi, B.*** "Chemical libraries targeting Liver Stage Malarial infection. *Chem. Biol. Lett*., **2019**, *6*, 14-22 (Scopus Indexed; ISSN, 2347-9825).
74. Kotnala, K.; Verma, K.; Sharma, A.; Parashar, S.; **Rathi, B.**; **Kumar, R.**; Chhikara, B. S.; Singh, J. "Indian Medicinal Plants for skin care and cosmeceuticals: A review" *J. Biomed. Ther. Sci.* 2019, 6(2), 24-60 (Indian Science Pub.; ISSN: 2394-2274).
75. Poonam; Gupta, Y.; Singh, S.; Wu, L.; Rawat, M. and **Rathi, B.*** "Multistage Inhibitors of Malaria Parasite: Emerging Hope for Chemoprotection and Malaria Eradication" *Med. Res. Rev.* **2018**, *38*, 1511-1535 (IF, **12.99**; Wiley-VCH Verlag GmbH & Co. KGaA, Germany; ISSN: 1098-1128).
76. Singh, S.; Sharma, N.; Upadhyay, C.; Kumar, S.; **Rathi, B.**; Poonam "Small Molecules Effective against Liver and Blood Stage Malarial Infection" *Curr. Topics Med. Chem.* **2018**, *18*, 2008-202 (IF: 3.295; Bentham Science Publishers, UAE; ISSN: 1568-0266).
77. Wu, L.; **Rathi, B.**; Chen, Y.; Wu, X.; Liu, H.; Li, J.; Ming, A.; Han, G.; "Characterization of immobilized Tyrosinase--an enzyme that is stable in organic solvent at 100 oC" *RSC Adv.* **2018**, *8*, 39529-39535 (IF: 4.036; Royal Society of Chemistry, UK; ISSN: 2046-2069).
78. Singh, S.; Singh, A.; **Rathi, B**.; Tomar, V.; Chandra, R. "Modern Advancement in the Area of Antimalarial Drug Development" *Indian J. Heterocyclic Chem.* **2018**, *28*, 185-194 (IF, 0.33; ISSN, 2456-4311).
79. Singh, A. K.; Rajendran, V.; Singh, S.; Kumar, P.; Kumar, Y.; Singh, A.; Miller, W.; Potemkin, V. Poonam; Grishina, M.; Gupta, N.; Kempaiah, P.; Durvasula, R., Singh, B.; Dunn, B. M. and **Rathi, B.*** "Antiplasmodial activity of hydroxyethylamine analogs: Synthesis, biological activity and structure activity relationship of plasmepsin inhibitors" *Bioorg. Med. Chem.* **2018**, *26*, 3837-3844 (IF: 3.641; Elsevier; ISSN: 0968-0896).
80. Miller, W. A.; Teye, J.; Achieng, A.O.; Mogire, R. M.; Akala, H.; Ong'cha, J. M.; **Rathi, B.**; Durvasula, R.; Kempaiah, P.; Kwofie, S. K. "Antimalarials: Review of Plasmepsins as Drug Targets and HIV Protease Inhibitors Interactions". *Curr. Topics Med. Chem.* **2018***, 18,* 2022-2028. (IF: 3.295; Bentham Science Publishers, UAE; ISSN: 1568-0266).
81. Kumari, V.; Singh, A. P.; Singh J.; Sharma, R.; Akhter, M.; Mishra, P. K.; Saxena, A. K.; Dixit, R.; **Rathi, B.**; Katyal, A. and Pandey, K. C. "Biochemical Characterization of 2017 Unusual Cysteine Protease of P. falciparum, Metacaspase-2 (MCA-2)" *Mol. Biochem. Parasitol.* **2018**, *220*, 28-41 (IF: 2.536; Elsevier; ISSN: 0166-6851).
82. Kumar, P.; Achieng, A. O.; Rajendran, V.; Ghosh, P.; Singh, B.K.; Rawat, M.; Perkins, Douglas J.; Kempaiah,P.; **Rathi, B**.* "Synergistic blending of high-valued heterocycles inhibits growth of *Plasmodium falciparum* in culture and P. berghei infection in mouse model" *Sci. Rep.* **2017**, *7*, 6724 (IF, 4.379; Nature Group Publications, Netherland; ISSN: 2045-2322).

83. Gorobets, N.; Yuriy S.; Singh B.; Poonam and **Rathi, B.*** "An Overview of Currently Available Antimalarials" *Curr. Topics Med. Chem.* **2017**, 17, 2143-2157 (IF: 3.295; Bentham Science Publishers, UAE; ISSN: 1568-0266).
84. Editorial: **Rathi, B.**; Yaroslav, F.; Latha, N.; Poonam "New Avenues in Controlling Infectious Diseases" *Curr. Topics Med. Chem.* **2017**, *17*, 2113 (IF: 3.295; Bentham Science Publishers, UAE; ISSN: 1568-0266).
85. Singh, A.; Bhardwaj, J.; Olival, A.; Kumar, Y.; Podder, A.; Maheshwari, A.; Latha, N.; Singh, B. K.; Tomás, H.; Rodrigues, J.; **Rathi, B.*** "Design, Synthesis and Biological Evaluation of Arylpiperazine Based Novel Phthalimides: Active Inducers of Testicular Germ Cell Apoptosis" *J. Chem. Sci.* **2016**, *128,* 1245-1263 (IF: 1.254; Springer; ISSN: 0973- 7103).
86. Meet Our Editorial Board Member**,** *Curr. Topics Med. Chem.,* **2016***, 16,* 895-896 (IF: 2.9; ISSN: 1568-0266).
87. Singh, A.; Medviediev, V. V.; Shishkin, O.; Bahadur, V.; Singh, T.; Singh, B. K.; Vijayan, N.; Balachandran, V.; Gorobets, Yu N. and **Rathi, B.*** "Functionalized Organic Frameworks Explored As Second Order NLO Agents" *J. Chem. Sci.* **2016**, 128, 297-309 (IF: 1.254; Springer; ISSN: 0973-7103).
88. Gupta, N.; Gupta, C.; Sharma, S.; **Rathi, B**.; Sharma, R. K. and Bohidar, H. B. "Magnetic iron oxide nanoparticles encapsulating horseradish peroxidase (HRP): synthesis, characterization and carrier for the generation of free radicals for potential applications in cancer therapy" *RSC Adv.* **2016**, 6, 111099 (IF: 4.036; Royal Society of Chemistry, UK; ISSN: 2046-2069).
89. Chhikara, B. S., Kumar, R., **Rathi, B.**, Krishnamoorthy, S., & Kumar, A. "Prospects of Applied Nanomedicine: potential clinical and (bio)medical interventions via nanoscale research advances" *Chem. Biol. Lett.* **2016**, 3, 50-56 (Scopus Indexed; ISSN, 2347-9825).

90. Singh, A. K.; Rathore, S.; Tang, Y.; Goldfarb, N. E.; Dunn, B. M.; Rajendran, V.; Ghosh, P. C.; Latha, N.; Singh, B. K. and **Rathi, B.*** "Hydroxyethylamine Based Phthalimides As New Class of Plasmepsin Hits: Design, Synthesis and Antimalarial Evaluation" *Plos ONE* **2015**, *10*, e0139347 (IF: 3.24; Plos; ISSN: eISSN-1932-6203).

91. Singh, A. K.; Rajendran, V.; Ghosh, P. C.; Singh, N.; Latha, N.; Garg, S.; Pandey, K. C.; Singh, B. K.; **Rathi, B**.* "Design, Synthesis and Biological Evaluation of Functionalized Phthalimides: A New Class of Antimalarials and Inhibitors of Falcipain-2, a Major Hemoglobinase of Malaria Parasite" *Bioorg. Med. Chem.* **2015**, *23*, 1817–1827 (IF: 3.641; Elsevier; ISSN: 0968-0896).

92. Editorial: Rodrigues, J. and **Rathi, B**. "Self-assembled Organic Nanostructures in Medicinal Chemistry: Advances and Applications" *Curr. Topics Med. Chem.* **2015**, *15*, 1161-1161 (IF: 2.90; ISSN: 1568-0266).
93. Sharma, P.; **Rathi, B**.; Rodrigues, J.; Gorobets, Yu. N. "Self-Assembled Peptide Nanoarchitectures: Applications and Future Aspects" *Curr. Topics Med. Chem.* **2015**, *15*, 1268-1289 (IF: 3.40; ISSN: 1568-0266).

94. Sharma, A.; Sharma, S.; Sharma, K.; Chetri, S.; Vashishtha, A.; Singh, P.; Kumar, R.; **Rathi**, **B**; and Agarwal, V. "Algae as crucial organisms in advancing nanotechnology: a systematic review" *J. Appl. Phycol*. **2015**, *28*, 1759-1774 (IF: 3.215; Citation: 1; Springer, ISSN: 1573-5176).
95. Rani, R.; Thukral, K.; Krishna, A.; Vijayan, N. **Rathi, B.** "Synthesis and nucleation studies on L-leucine hydrobromide: a promising nonlinear optical material" *J. Appl. Crystallogr.* **2014**, *47*, 1966-1974 (IF: 3.215; ISSN: 1600-5767).
96. Singh, A.; Balachandran, V.; Vijayan, N.; Bahadur, V.; Tiwari, H.; Singh, B. and **Rathi, B.*** "Synthesis, Structural Aspects and Nonlinear Optical Properties of Novel Phthalimide Derivatives: Theoretical and Experimental Approach" *J. Phys. Org. Chem.* **2014**, *27*, 490- 497 (IF: 2.39; John Wiley & Sons; ISSN: 1099-1395).
97. Vijayan, V.; Philip, J.; Haranath, V.; **Rathi, B**.; Bhagavannarayana, G.; Halder, S.; Roy, N.; Jayalakshmy, M. S. and Verma, S. "Bulk growth of ninhydrin single crystals by solvent evaporation method and its characterization for SHG and THG applications" *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* **2014**, 122, 309- 314 (IF: 4.098; Elsevier; ISSN: 1386-1425).
98. Sharma, P. P.; Kumar, R.; Singh, A.; Singh, B. K.; Kumar, A and **Rathi B.*** "Potentials of Hydrogels in Cancer Therapy" *Curr. Cancer Ther. Rev.* **2014**, *10*, 246-270 (Bentham Science Publications; Citation: 1; ISSN: 1875-6301).
99. **Rathi, B**.; Sharma, P.; Singh, R. P. "Tetrahedral Hydroxyethylamine: A Privileged Scaffold in Development of Antimalarial Agents" *Chem. Biol. Lett.* **2014**, 1, 11-13 (Indian Science Publications; ISSN: 2347–9825).
100. **Rathi, B.***; Singh, A.; Kishan, R.; Latha, N.; Pandey, K. C. Tiwari, H. and Singh, B. K. 'Functionalized hydroxyethylamine based peptide nanostructures as potential inhibitors of falcipain-3, an essential proteases of *Plasmodium falciparum' Bioorg. Med. Chem.* **2013**, 21, 5503–5509 (IF: 3.441; Elsevier; ISSN: 0968-0896).
101. Singh, A.; Kishan, R.; Vijayan, N.; Balachandran, V.; Tiwari, H.; Singh, B. and **Rathi, B.*** "Entry of Chiral Phthalimides With Significant Second Order Nonlinear Optical and Piezoelectric Properties' *RSC Adv.*, **2013**, 3, 14750-14756 (IF: 4.036; Royal Society of Chemistry, UK; ISSN: 2046-2069).
102. Kishan, R.; Vijayan, N.; Rupini, B.; Singh, R.; Kumar, Y. and **Rathi, B.*** "Structural Aspects, Biological and Nonlinear Optical Response of New *N,N'*–Di(2- tolyl)formamidinium Tosylate" *Adv. Chem. Lett.* **2013**, *1*, 134-139 (American Scientific Publishers, USA; ISSN: 2326-7488).
103. Rupini, B.; Sharda, P.; **Rathi, B.*** "Asymmetric Reductive Amination of Carbonyl Compounds by Using *N,N,N*-Tributylpropanaminium Based Novel Chiral Ionic Liquid" *Int. J. Org. Chem.*, **2013**, *3*, 190-193. (IF: 0.57; Scientific Research Publishers, USA; ISSN: 2161-4695).
104. Rani, N.; Vijayan, N.; Riscob, B.; Jat, S. K.; Das, S.; Bhagwannarayan, G.; **Rathi, B.**; Wahab, M. A. "Single Crystal Growth of Ninhydrin by Unidirectional Sankaranarayanan- Ramasamy (SR) Method by Using Glass Ampoule For Non-

linear Optical Applications" *CrystEngComm*, **2013**, 15, 2127–2132 (IF: 4.069 for five years; Royal Society of Chemistry, UK; ISSN: 1466-8033).

105. Vijayan, N.; Rani, N.; Madhurambal, G.; Bhagavannarayana, G.; **Rathi, B.**; Philip, R.; Safakath, K.; Mojumdar, S. C. 'Synthesis, growth, and characterization of iminodiacetic acid monohydrochloride' *J. Thernal Analysis and Calorimetry* **2013**, 112, 1113-1119; (IF: 1.604; Springer; ISSN: 1572-8943).
106. Vijayan, N.; Bhagwannarayan, G.; Halder, S. K.; Verma, S.; Philip, J.; **Rathi, B.** "X-ray Topography, Photopyroelectric and Two-photon Absorption Studies on Solution Grown Benzimidazole Single Crystal" *Appl. Phys. A* **2013**, *110*, 55-58 (IF: 1.630; Springer; ISSN: 1432-0630).
107. Rani, N.; Vijayan, N.; **Rathi, B**.; Bhagavannarayana, G. "Studies on the effect of polymer coating on solution grown hygroscopic non-linear optical single crystal of L-lysine monohydrochloride" *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* **2012**. *97*, 871-875 (IF: 4.098; Elsevier; ISSN: 1386-1425).
108. Vijayan, N.; Bhagavannarayana, G.; Maurya, K. K.; Haranath, D.; **Rathi, B**.; Balamurgan, N.; Sharma, Y. K.; Ramasamy, P. "Effect of Annealing on Bridgman Grown Organic Scintillation Material of *trans*-Stilbene" *MatChemPhys* **2012***, 132,* 453-457. (IF: 4.09; Elsevier; ISSN: 0254-0584).
109. Renuka, N.; Vijayan, N.; **Rathi, B**.; Nagarajan, K.; Ramesh Babu, R.; Bhagavannarayana, G. "Synthesis, Growth and Optical Properties of Semi Organic Non-linear Optical Single Crystal: L-Arginine Acetate" *OPTIK* **2012**, *123*, 189-192. (IF: 2.44; Elsevier; ISSN: 0030- 4026).
110. Gopi, K.; **Rathi, B**.; Natesan, T. "Synthesis and Conformational Features of *N*,*N*′,*N*″-Triarylguanidines" *J. Chem. Sci.* **2010**, *122*, 157-167 (IF,1.57; ISSN, 0973-7103).
111. Mahapatra, S. C.; Tiwari, H. K.; Singla, M.; **Rathi, B**.; Sharma, A.; Mahiya, K.; Kumar, M.; Sinha, S.; Chauhan, S. S. "Antimalarial Evaluation of Copper(II) Nanohybrid Solids: Inhibition of Plasmepsin II, A Hemoglobin-degrading Malarial Aspartic Protease from *Plasmodium falciparum* " *J. Biol. Inorg. Chem.* 2010, 15, 373-385 (IF, 3.358; Springer; ISSN, 1432-1327).

**Corresponding/co-corresponding Author*

Books

Edited Books

Singh, A., Rathi, B., Verma, A. K., & Singh, I. K. (Eds.). (2023). *Natural Product Based Drug Discovery Against Human Parasites: Opportunities and Challenges*. Springer (ISBN: 9789811996047).

Book Chapter(s)

- Saniya Arfin, Kirti Agrawal, Ashok Kumar, Arun Kumar, Brijesh Rathi, Dhruv Kumar, Chapter 1 - Metabolic dysregulation in cancer progression, Editor(s): Dhruv Kumar, Shailendra Asthana, Autophagy and Metabolism, Academic Press, 2022, Pages 1-39, ISBN 9780323998796, https://doi.org/10.1016/B978-0-323-99879-6.00008-0.
- Tejveer Singh, Arun Sidram Kharat, Brijesh Rathi, Dhruv Kumar, Chapter 11 - Designing metabolic target-specific inhibitors for cancer therapy, Editor(s): Dhruv Kumar, Shailendra Asthana, Autophagy and Metabolism, Academic Press, 2022, Pages 239-280, ISBN 9780323998796, https://doi.org/10.1016/B978-0-323-99879-6.00011-0
- Sujata Maurya, Kavindra Kumar Kesari, Shubhadeep Roychoudhury, Jayaramulu Kolleboyina, Niraj Kumar Jha, Saurabh Kumar Jha, Ankur Sharma, Arun Kumar, Brijesh Rathi & Dhruv Kumar (2022). Metabolic Dysregulation and Sperm Motility in Male Infertility. In: Kesari, K.K., Roychoudhury, S. (eds) Oxidative Stress and Toxicity in Reproductive Biology and Medicine. Advances in Experimental Medicine and Biology, vol 1358. Springer, Cham. https://doi.org/10.1007/978-3-030-89340-8_12
- Maurya, S., Mishra, M.K., Rathi, B., Kumar, D. (2022). Lipid Nanocarriers: Applications in Biomedical Research and in Drug Delivery. In: Gopi, S., Balakrishnan, P., Mubarak, N.M. (eds) Nanotechnology for Biomedical Applications. Materials Horizons: From Nature to Nanomaterials. Springer, Singapore. https://doi.org/10.1007/978-981-16-7483-9_2.
- Raj, S.; Mishra, M.K.; Harihar, S.; Kumar, A.; Roychoudhury, S.; Kumar, A.; **Rathi, B.**; Kumar, D. (**2022**) The Author(s), under exclusive license to Springer Nature Switzerland AG 2021 43 K. K. Kesari, N. K. Jha (eds.), Free Radical Biology and Environmental Toxicity, Molecular and Integrative Toxicology, https://doi.org/10.1007/978-3-030-83446-3 Regulation of Glucose Transporters in Cancer Progression. Springer P. 191-208 (ISBN, 978-3-030-83446-3 (eBook).
- Kumar S., Kumari P., Rathee G., Rathi B. (2021) Nanomaterials for Early Cancer Diagnostics. In: Malik A., Afaq S., Tarique M. (eds) Nanomedicine for Cancer Diagnosis and Therapy. Springer, Singapore. p.p. 97-114. https://doi.org/10.1007/978-981-15-7564-8_5 (ISBN, 978-981-15-7564-8)
- **Brijesh Rathi** and Poonam (**2018**) "Chemical Therapeutics for the treatment of alcoholism" ALCOHOLISM: Causes, Symptoms Effects and Treatment. Page: 237-248 Manakin Press, New Delhi India (ISBN: 9789-38667-7488).
- Renuka, N.; Babu, R.; Vijayan, N.; **Rathi, B.**; Thukral, K. "Effect of Oxygen Ion Irradiation on the Structural and Optical Properties of L-Arginine Acetate Single Crystals" *Recent Trends in Material Science and Application* **2017**, 511-519 (Springer, ISBN: 978-3-319- 44890-9).

Doctoral/Master Thesis Supervision

- **Neha Sharma,** Date of Award: 8th June 2023); University of Delhi; Role: Supervisor.
- **Dr. Prem P Sharma** (Reg No. 18001907001; Date of Award: 20.07.2022); DCRUST, Murthal; Role: Co-supervisor.
- **Dr. Pramila Gupta (**MUR1403063; Date of Award: 20.02.2021; Mewar University Rajasthan); Role: Co-supervisor.
- **Shivani Jaiswal** (Enrolments No.: A14587820006; Amity University) 'In-silico Screening of Phytochemicals Against ERK2 Using Structure-Based Drug Designing Approach".

Professional Editing/editor services

- **Guest Editor:** Frontiers in Drug Discovery (DOI: 10.3389/fddsv.2023.1223140).
- **Associate Editor (Guest):** Frontiers in Cellular and Infection Microbiology (doi: 10.3389/fcimb.2023.1175996).

Administrative Committees

Coordinator DST PAC, 17-18 August, 2023.
Coordinator DST PAC, 16-17 December, 2022.
Coordinator DST PAC, 15 December, 2022.
Coordinator DST PAC, 29-30 December, 2022.
Convener (Founder), Research Committee of Hansraj College, 2018-2021.
Convenor, Research Committee, Hansraj College, University of Delhi, 2018-2021.
Co-convenor, Research Committee, Hansraj College, University of Delhi, 2021 onwards.
Convenor (Founder), Institutional Innovation Cell (IIC), A Unit of MHRD-Innovation Cell, Hansraj College, University of Delhi, 2018 onwards.
Coordinator, Centre for Global Health Study Site, a unit of Global Health Center Loyola University Chicago, USA (2018-2019).
Coordinator, Laboratory For Translational Chemistry and Drug Discovery, Hansraj College, University of Delhi (2017 onwards).
Member of Hostel Committee, 2015-16.
Editorial Member, Brochure Committee of University of Delhi 2022.

Research Interest

Medicinal Chemistry and Drug Discovery

Research Projects (Total funding secured >3.5 Cr Rupees)

1. Title of the project: “Small Molecule Drug Discovery for Rare Genetic Disorder Therapy [DST/TDT/RARE/2022/21(G)/2]”
   Funding Agency: DST, Government of India
   Duration: Three Years (2023-2026)
   Project Cost: Rs. 1,02,12,522/-
   Role: PI
2. Title of the project: “To Synthesize Noble Metabolic Pathways Inhibitors for the Development of Broad-spectrum Antiviral Therapy”
   Funding Agency: INMAS-DRDO, Government of India
   Duration: Three Years (2023-2025)
   Project Cost: Rs. 23,90,774/-
   Role: PI
3. Title of the project: “Target Based Screening and Development of Hydroxyethylamine Derivatives as Novel Antimalarials” (CRD/2022/000580)”
   Funding Agency: SERB, Government of India (ASEAN-India R&D Project).
   Duration: Two Years (2023-2025)
   Project Cost: Rs. 34,00,000/-
   Role: PI
4. Title of the project: “Molecular theranostic probes based on optically active amines for targeting SARS-CoV-2”
   Funding Agency: DRDO, Government of India
   Duration: Three Years (2021-2024)
   Project Cost: 49.04 Lakh
   Role: PI
5. Title of the project: “Repurposing of Drugs and Validation of Lead Compounds Against Main Protease and RNA Dependent RNA Polymerase of SARS-CoV-2”
   Funding Agency: BRICS - DST, Government of India
   Duration: Three Years (2021-2023)
   Project Cost: 42.87 Lakh
   Role: Co-PI
6. Title of the project: “Design and Synthesis of Novel Bioactive DOTA Conjugates”
   Funding Agency: INMAS-DRDO, Government of India
   Duration: Three Years (2021-2022)
   Project Cost: 8.90 Lakh
   Role: PI
7. Title of the Project: “Lead Optimization of Potent Multistage Antimalarials”
   Funding Agency: SERB, Government of India
   Duration: Three Years (2020-2023)
   Project Cost: 46.41 Lakh
   Role: PI

8. Title of the Project: “Development of Nanoantenna Sensor for Infrared Detection”
   Funding Agency: DST, Government of India
   Duration: 2019-2021
   Cost: 63.08 Lakh
   Role: PI
9. Title of the Project: "Design and Catalytic Large-Scale Synthesis of New Functionalized Perfluorinated Ketones/Ethers as Potential Fire Extinguishants"
   Funding Agency: DRDO, Government of India
   Project Cost: 48.2 Lakh
   Duration: 2017-2020
   Role: PI
10. Title of the Project: *“*A New Class of Anti-malarials: Constituting New Avenues for Anti-malarial Therapy*”*
    Funding Agency: SERB, Government
    of India Duration: 2016-2019
    Cost: 32.89 Lakh
    Role: PI
11. Title of the Project: *“*Novel functionalized tetrahedral activated small peptidomimetic inhibitors of malarial aspartic proteases, plasmepsin I and II*”*
    Funding Agency: DST, Government of India
    Project Cost: 10 Lakh
    Duration: 2011-2014
    Role: PI
12. Title of the project: “Contributions to bioinformatics and nanomedicine: computational, biochemical and biophysical evaluation of new small peptide and fatty acid derivatives as well as their self-assembled nano structures as molecular weapons against against infectious diseases” (INT/BLR/P-4/2014).
    Funding Agency: DST, Government of India
    Project cost: 5 Lakh
    Duration: 2014-2016
    Role: Co-PI
13. Title of the project: “Functionalized Nano-antimalarials: Design, Synthesis and Structural Aspects of Novel Metal Complexes as Inhibitors of Plasmepsin I and Plasmepsin II” (INT/PORTUGAL/P-17/2013)
    Funding Agency: DST, Government of India
    Project cost: 5 Lakh
    Duration: 2014-2017
    Role: Co-PI
14. Title of the Project: “Thio-click approach for the synthesis of stable glycomimetics and chiral oxathiacrown ethers”

Funding Agency: Department of Science and Technology, Ministry of Science and Technology, Government of India
Project Cost: 38 Lakh
Duration: 2017-2020
Role: Co-PI In collaboration with IIT Delhi

15. Title of the Project: *"*Conjugates and Analogues of Antiviral Compound AUY11 (INT/RUS/RFBR/P-194/2015)*"*
Funding Agency: Department of Science and Technology, Ministry of Science and Technology, Government of India
Project Cost: 24.28 Lakh
Duration: 2015-2017
Role: Co-PI In collaboration with IIT Delhi

16. Title of the Project: "Survey of Tree Species in Delhi Region and Screening of Selected Medicinal Plants for Anti-Cancer Activity" (SVC-101)
Funding: University of Delhi
Project Cost: 10 Lakh
Duration: One Year (2012-2013).

17. Title of the Project: "Engineered Biocompatible Organic Nanoarchitectures: A New Paradigm for Disinfections" (HRC-308)
Funding Agency: University of Delhi
Project Cost: 6 Lakh
Duration: One Year (2015-2016).

Research Collaboration

- **Dr. Agam P Singh,** Scientist, National Institute of Immunology (NII), New Delhi**.**
- **Prof. Conor R Caffrey,** University of California, San Diego, USA.
- **Dr. Prakasha Kempaiah,** Infectious Disease Division, Mayo Clinic, Florida, USA.
- **Dr. Martin Zoltner**, BioCev, Charles University of Prague, Czech Republic.
- **Dr. Lindomar Pena,** Department of Virology, Aggeu Magalhaes, Institute (IAM), Oswaldo Cruz Foundation (Fiocruz), Recife 50670-420, Pernambuco, Brazil.

Conferences/Seminar/workshop Organized.

- "National Seminar on Climate Change Tunnel Vision?' organized by Hansraj College & British Council, UK, Prof. Alison Greig (Anglia Ruskin University), Friday 25th August 2023. **Role: Convener.**

- "2nd Indo-US Symposium on Chemical Biology and Drug Discovery" Jointly organized by Hansraj College, University of Delhi and Mayo Clinic Florida USA on 27th June 2023**. Role: Convener.**
- "2nd International conference on Integrative Chemistry, Biology and Translational Medicine (ICBTM-2022)" December 6-8, 2023, Jointly organised by Hansraj College University of Delhi, Delhi, India & Mayo Clinic Florida USA, INMAS-DRDO Delhi and Miranda House Delhi. **Role: Convener**
- "1st International conference on Integrative Chemistry, Biology and Translational Medicine (ICBTM-2019)" Feb 25-26, 2019, Jointly organised by Centre for Global Health, Hansraj College University of Delhi, Delhi, India & Loyola University Stritch School of Medicine Maywood, Chicago USA. **Role: Convener**
- Indo-US Colloquium on Recent developments in interdisciplinary research, July 2, 2018, Jointly organised by IQAC, Department of Chemistry, Hansraj College University of Delhi, Delhi, India & Loyola University Stritch School of Medicine Maywood, IL USA. **Role: Convener**
- "Indo-Portuguese workshop on Nanotechnology in Chemistry and Biology (INCB- 2016)" jointly organized by Department of Chemistry, Hansraj College and CQM, University of Madeira, Portugal (February 12-13, 2016). **Role: National Coordinator**.
- India International Science Festival (IISF-2015) organized by Ministry of Science & Technology, Govt. of India during December 4-8, 2015 (**Role: Coordinator**).
- MHRD funded "National Workshop on Role of Technical Terminology in Higher Education" (23-24 July, **2015**) in Hansraj College, University of Delhi (**Role: Coordinator**).
- "1st International conference on emerging trends of nanotechnology in drug discovery" was organized (May 26-27, **2014**) by Sri Venkateswara College & Department of Biochemistry, University of Delhi South Campus in association with Centro de Química da Madeira, Universidade da Madeira, Portugal (**Role: National coordinator and organizing secretary**).
- "A National Symposium on Recent Trends in Innovative Research at Under-graduation: Science and Society" was organized (28th Feb-2nd March **2013)** by Sri Venkateswara College, University of Delhi (**Role: Organizing secretary**).
- A national seminar on Recent Trends in Chemistry" was organized (March 20-22, **2012**) by Department of Chemistry, Sri Venkateswara College, University of Delhi (**Role: Treasurer**)**.**
- A national conference on "Convergence of Science and Spirituality" was organized (5- 6th Nov **2011**) by Sri Venkateswara College in association with Institute for Science and Spirituality, A Study Wing of ISKCON Delhi (**Role: Coordinator**).

Invited Lectures

- Invited Lecture on “Medicinal Chemistry: Scope & Future Aspects” J. C. Bose University of Science and Technology, YMCA Faridabad; 29th March 2023.
- “Identification and optimization of novel *N*-substituted amines as therapeutic agents for the management of various diseases” during International Conference on Interdisciplinary Research in Cancer Biology (IC-IRCB-2022), 22-23 September 2022 organized by School of Health Sciences & Technology, UPES University, Dehradun, Uttarakhand, India.
- “Hydroxyethylamine Pharmacophore Based Novel Multistage Antimalarials” during Interdisciplinary Research in Biomedical Sciences" CONIAPS XXVII organized by Amity University Uttar Pradesh, Noida in association with International Academy of physical Sciences (AIPS), Prayagraj; from 26 to 28 October 2021.
- “Computer Aided Drug Design”, National Workshop on Bioinformatics: Resources, Tools, and its applications (19-27 July 2021), Zakir Husain Delhi College, University of Delhi, New Delhi.
- “Discovery of next-generation antimalarials” Amity University Noida, Friday, 11 June 2021.
- “Understanding the therapeutic developments for novel coronavirus COVID-19 management” DiSTAP (Singapore-MIT Alliance for Research and Technology (SMART) Centre) Biweekly seminar, Thursday, 23rd April 2020.
- “Design of multistage inhibitors of malaria parasite; malarial aspartic proteases as crucial drug targets to achieve multistage activity” VI Forum PPGDITM (UFRPE-UFPB-UFRN-UFC), Recife, capital of Pernambuco State, in the campus of the Federal Rural University of Pernambuco, Brazil, 28th November's 2019.
- “Multistage Antimalarials Targeting Malarial Proteases” during International Workshop on Chemistry and Chemical Biology of Carbohydrates, Nucleic Acids and Antibiotics (22-24, May **2019**) organized by University of Debrecen, Hungary.
- “New Antimalarials: Multistage Inhibitors of Malaria Parasite as Emerging Hope for the Malaria Eradication” Department of Pharmaceutical Chemistry, University of Debrecen, Hungary (June 12, **2018**).
- Invited Speaker for the workshop “How to get published research paper in the right journals” organized by Grace India Educational Charitable Trust, Delhi at Hansraj College, University of Delhi (October 27, **2018**).
- "Discovery of Multistage Antimalarials: Synergistic Fusion of Privileged Bioactive Scaffolds Triggers Growth Inhibition of Malaria Parasite Plasmodium Falciparum" Drug Discovery & Therapy World Congress (DDTWC-2017) July 10-13, **2017**, Boston, MA United States of America.
- "Functionalized Small Molecules As Potential Antimalarial Agents" National conference on Frontiers in Research & Development on Agriculture, Bio-medicinal, Chemical and Pharmaceutical sciences (4th March, **2016**), Mewar University, Rajasthan.

Awards/Fellowships/Recognitions Availed

2023 (July) – "Mahatma Hansraj Research Excellence Award" Hansraj College, University of Delhi.
2023 (June) – Appointed "Scientific Advisor", Delhi High Court, New Delhi.
2022 (June) – "Institute of Eminence Fellow Award" by University of Delhi.
2021 (October) – Best Paper Presentation Award by International Conference of International Academy of Physical Sciences and Amity University, Noida.
2021 (July) - Scientists join hands targeting to synthesize compounds to inhibit maturation & propagation of COVID 19 virus – a story about our research published on DST, Govt. of India website.
2019 – "CAPES-Print Fellowship" from Coordenação de Aperfeiçoamento de Pessoal de Nível Superior, Ministry of Education, Brazil.
2018 - The prestigious "Excellence Awards for In Service Teachers" by University of Delhi. This award is given to highly deserving individuals for their contribution to academic activities.
2018 - "Best Young Teacher award" by Grace India Award-2018 Function on the occasion of 87th Birth Anniversary of Bharat Ratna Dr. APJ Abdul Kalam celebrated at Hansraj College University of Delhi.
2016-2017 "UGC-Raman International Fellowship" by UGC, Ministry of Human Recourses and Development, Govt. of India.
2016 – "Early Career Research Award" by Science & Engineering Research Board (SERB), Ministry of Science of Technology, Govt. of India.
2011-2014 – "Young Scientist Fellowship" by DST, Ministry of Science of Technology, Govt. of India.
2017 – "International Reviewer for Russian Science Foundation (RSF)" – on recommendations of Russian International Affairs Council (RIAC), Russia.
2018 - Ambassador for Bentham Science Publishers.

Short Course(s)/ Resource person.

- Four Credit Course on "Antimalarial Drug Discovery Towards Malaria Eradication" Federal Rural University of Pernambuco, Recife, Brazil, 27 November, 2019.
- Antimalarial drugs: Preclinical and Clinical Aspects (14 credit PhD elective course and undergarduate elective course) 7-16 October 2019, University of Debrecen, Hungary.

International Visits

- Visiting Fellow [June 11-18, 2018], Department of Pharmaceutical Chemistry, University of Debrecen, Hungary.
- Visiting Fellow [June 6-16, 2016], Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Moscow, Russia.

- ❖ Visiting Fellow [June 30 –July 7, 2016], Belarussian State University, Minsk, Belarus.
- ❖ Visiting Fellow [Oct. 2014], Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal.

Honorary Positions (Editing/Review/Membership of Scientific Bodies)

- **Life Member,** Chemical Research Society of India (CRSI) - LM 3495.
- **Advisory Board Member**, Avishkaran, The BIONEST of NIPER Hyderabad.
- **Section Editor**, Current Topics in Medicinal Chemistry (IF: 3.37).
- **Associate Editor,** Chemical Biology Letters, Indian Science Publishers.
- **Life Member** (L32926), The Indian Science Congress Association, Kolkata.
- **Editorial Review Board Member,** ARKIVOC, Arkat USA.
- **Jury Member**, DST Inspire 2015.
- **Reviewer,** Journal of Medicinal Chemistry (ACS); Chemical Science (RSC); Annals of Medicine; RSC Interface; Biochemistry; Plos ONE, RSC Advances; Computational and Structural Biotechnology Journal; Toxicology Research; Physical Chemistry Chemical Physics; Microbial Pathogenesis; Journal of Chemical Physics; Journal of Heterocyclic Chemistry; Bioorganic Medicinal Chemistry; ARKIVOC; Journal of Molecular Liquids; Frontiers Molecular Biosciences.

Certificate Courses Pursued at Massachusetts Institute of Technology (M. I. T.)

- EHS Representative Orientation, MIT Training course from Massachusetts Institute of Technology (M. I. T.), Cambridge, United State of America.
- Chemist Chem Hygiene & Safety, MIT Training course from Massachusetts Institute of Technology (M. I. T.), Cambridge, United State of America.
- Chemist Lab Spec Chem Hygiene, MIT Training course from Massachusetts Institute of Technology (M. I. T.), Cambridge, United State of America.
- Managing Hazardous Waste, MIT Training course from Massachusetts Institute of Technology (M. I. T.), Cambridge, United State of America.
- Managing Your Time , from Massachusetts Institute of Technology (M. I. T.), Cambridge, United State of America.

Personal Details

Father's Name: Sh. Mangey Ram
Date of Birth: June 5, 1981
Sex: M
Languages Known: English, Hindi
Nationality: Indian