Dr. Amit Kumar Halder

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PROFESSIONAL EXPERIENCE

(28.08.2021-Present)

Associate Professor
Dr. B. C. Roy College of Pharmacy and Allied Health Sciences, Durgapur, West Bengal, India Pin713206
https://bcrcp.ac.in/

(01.08.2017 to 31.07.2021)

Post-doctoral investigator
Prof. Natália Cordeiro, LAQV/REQUIMTE, Faculty of Sciences, University of Porto,
Rua do Campo Alegre, s/n, 4169-007 Porto, Portugal
www.fc.up.pt

- The development and application of advanced software tools employing machine learning techniques for prediction of the toxicity and/or biological activity of a wide variety of chemicals and nanomaterials.

(30.06.2016 to 29.06.2017)

Post-doctoral researcher
Dr. Bahareh Honarparvar, School of Health Sciences, University of KwaZulu-Natal, Durban, 4001, South Africa
https://www.ukzn.ac.za/

- Understanding molecular alteration in drug susceptibility against subtype B and South African subtype-C (C-SA) HIV-1 proteases through molecular dynamics simulations studies.

(01.08.2008 to 30.04.2011)

Assistant Professor
Dr. B. C. Roy College of Pharmacy and Allied Health Sciences, West Bengal, India
https://bcrcp.ac.in/

- Teaching of undergraduate pharmacy students

EDUCATION

(01.05.2011 to 30.05.2016) **PhD degree** (Doctor of Philosophy in Pharmacy)

Prof. Tarun Jha, Jadavpur University, Kolkata, INDIA (http://www.jaduniv.edu.in/)

Prof. Achintya Saha, University of Calcutta, Kolkata, India (https://www.caluniv.ac.in/)

Dr. Krishna Das Saha, CSIR-Indian Institute of Chemical Biology, Kolkata, India (https://www.iicb.res.in/)

Teaching of undergraduate pharmacy students

(01.07.2006-30.06.2008)

Master degree (Master of Pharmacy)

(01.06.2002-30.05.2006) Jadavpur University, Kolkata, INDIA (http://www.jaduniv.edu.in/)

Bachelor degree (Bachelor of Pharmacy)

Jadavpur University, Kolkata, INDIA (http://www.jaduniv.edu.in/)

Post-doctoral research (2017-2021)

Topic: Development and application of advanced *in silico* tools towards the prediction of the properties of chemical species

Advisor: Prof. Maria Natalia D. S. Cordeiro, LAQV/REQUIMTE, Faculty of Sciences, University of Porto, Portugal

Main objective: Development and application of advanced software tools employing machine learning and molecular modeling techniques for prediction of the toxicity/biological activity/physicochemical property of a wide variety of chemicals (i.e., pharmaceuticals, nanomaterials, deep eutectic solvents).

Other involvements: Development of chemometric softwares (Java and Python based), web-based applications (FLASK).

Github repository: My developed Python-based tools are available at https://github.com/ncordeirfcup/

Post-doctoral research (2016-2017)

Topic: Molecular modeling - mechanistic studies

Advisors: Prof. Gert Kruger, School of Health Sciences, University of Kwazulu-Natal, South Africa
Dr. Bahareh Honarparvar, School of Health Sciences, University of Kwazulu-Natal, South Africa

Main objective: Understanding molecular alteration in drug susceptibility against subtype B and South African subtype-C HIV-1 proteases through molecular dynamics simulations studies.

Ph.D. research (2011-2016)

Title: Rational design of derivatives and analogs of phenylacetyl isoglutamine: Synthesis, biological activity and molecular modeling**.**

Advisors: Prof. Tarun Jha, Department of Pharmaceutical Technology, Jadavpur University, India
Prof. Achintya Saha, Department of Chemical Technology, University of Calcutta, India
Dr. Krishna Das Saha, CSIR-Indian Institute of Chemical Biology, Kolkata, India

Main objective: Rational design of derivatives and analogs of phenylacetyl isoglutamine as potential inhibitors of matrix metalloproteinases and histone deacetylases through computer-aided drug design, synthetic chemistry and enzymatic assays. The most potent compounds were investigated and reported with anti-migratory, anti-invasive and anti-proliferative properties through *in vitro* assay techniques, Work of Ph.D. thesis was published in Bioorganic & Medicinal

Chemistry (2016), RSC advances (2015), Journal of Pharmacy and Pharmacology (2013) and Future Medicinal Chemistry (2019).

Masters research (2006-2008)

Title: Rational Design of 1,5-N,N'-Disubstituted-2-(Substituted Naphthalenesulphonyl) Gluatamamides by Synthesis, Biological Evaluation and QSAR study.
Advisors: Prof. Tarun Jha, Department of Pharmaceutical Technology, Jadavpur University, India
Main objective: Rational design of derivatives and analogs of 1,5-N,N'-Disubstituted-2-(Substituted Naphthalenesulphonyl) Gluatamamides as potential antitumor agents through synthetic chemistry, in vivo assay and QSAR. Thesis work was published in *European Journal of Medicinal Chemistry* (2010).

Research interests

Computational chemistry

Keywords: 2D-QSAR (linear and classification analyses), 3D-QSAR (CoMFA, CoMSIA, MFA), pharmacophore mapping (ligand- and structure-based), molecular docking (rigid, semi-rigid, flexible, induced-fit), molecular dynamics simulation, homology modeling, fragment-based lead identification and modification, virtual screening etc.

Cancer biology

Keywords: *In vitro* cytotoxicity assay, enzyme inhibition assay, flow cytometry, confocal microscopy, western blotting, invasion and migration assay.

Synthetic chemistry

Syntheses, purification and characterization of organic compounds.

Technical skills

- Experienced user of molecular modeling packages: Biovia Discovery Studio, Schrodinger, MOE, Tripos, Hyperchem, Gaussian, Amber, Desmond, Scikit-Learn, RDKit.
- Visualization of structures and molecules: GaussView, VMD, Chimera, Pymol, Discovery Studio Visualizer,
- Plotting: Plotly, Xmgrace, Matplotlib
- Programming Languages: Python, R, FLASK, Java, HTML, CSS, SQL
- Use of parallel clusters and high performance computing
- Experienced in all main Operating Systems - Unix/Linux, Windows, OX S.

Publications

1. Mitra, S., Halder, A. K., Koley, A., Ghosh, N., Panda, P., Mandal, S. C., Cordeiro, M. N. D. S. Unveiling structural determinants for FXR antagonism in 1,3,4-trisubstituted-Pyrazol amide derivatives: A multi-scale in silico modelling approach. Computers in Biology and Medicine,2024, 180, 108991
2. Mishra, P., Nandi, S., Chatterjee, A., Nayek, T., Basak, S., Halder, A. K., Mukherjee, A. Development of 2D and 3D QSAR models of pyrazole derivatives as acetylcholine esterase inhibitors. Journal of Serbian Chemical Society. In Press. 2024. Doi: 10.2298/JSC230221039M
3. Banerjee, T., Sarkar, A., Ali, S. Z., Bhowmik, R., Karmakar, S., Halder, A. K., Ghosh, N., Bioprotective role of phytocompounds against the pathogenesis of non-alcoholic fatty liver disease to non-alcoholic steatohepatitis: unraveling underlying molecular mechanisms. Planta Medica. In Press. 2024. DOI: 10.1055/a-2277-4805.

4. Mondal, I., Halder, A. K., Pattanayak, N., Mandal, S. K., Cordeiro, M. N. D. S. Shaping the future of obesity treatment: in silico multi-modeling of ip6k1 inhibitors for obesity and metabolic dysfunction. Pharmaceuticals, 2024, 17, 263.
5. Halder, A. K.,, Mishra, P., Basak, S., Roy, D., Das, A., Karmakar, S., Mondal, R., Banerjee, S., De, P., Chatterjee, A., Mallick, S., Hazra, A. Structural insights into the interactions of repositioning and known drugs for Alzheimer's disease with hen egg white lysozyme by MM-GBSA. Journal of Biomolecular Structure and Dynamics, 2024, 18, 1-19.
6. Sar, S., Mitra, S., Panda, P., Mandal, S. C., Ghosh, N., Halder, A. K., Cordeiro, M. N. D. S. In Silico Modeling and Structural Analysis of Soluble Epoxide Hydrolase Inhibitors for Enhanced Therapeutic Design. Molecules, 2023, 28(17), 6379
7. Mitra, S., Chatterjee, S., Bose, S., Panda, P., Basak, S., Ghosh, N., Mandal, S. C., Singhmura, S., Halder, A. K. Finding structural requirements of structurally diverse α-glucosidase and α-amylase inhibitors through validated and predictive 2D-QSAR and 3D-QSAR analyses. Journal of Molecular Graphics and Modelling, 2024, 124, 108640.
8. Halder, A. K., Moura, A. S., Cordeiro, M. N. D. S. Predicting the ecotoxicity of endocrine disruptive chemicals: Multitasking in silico approaches towards global models, Science of the Total Environment, 2023,889, 164337
9. Halder, A. K., Mitra, S., Cordeiro, M. N. D. S. Designing multi-target drugs for the treatment of major depressive disorder. Expert Opinion in Drug Discovery, 2023, 18, 643-658.
10. Mitra, S., Halder, A. K., Ghosh, N., Mandal., S.C., Cordeiro, M. N. D. S. Multi-model in silico characterization of 3-benzamidobenzoic acid derivatives as partial agonists of Farnesoid X receptor in the management of NAFLD. Computers in Biology and Medicine, 2023, 157, 106789.
11. Chetri, A., Roy, M., Mishra, P., Halder, A,K., Basak, S., Gangopadhyay, A., Saha A., Bhattacharya, P. Genetic algorithm-de novo, molecular dynamics and MMGBSA based modelling of a novel Benz-pyrazole based anticancer ligand to functionally revert mutant P53 into wild type P53. Molecular Simulation. 2023, 49, 678–689
12. Ghosh, A., Panda, P., Halder, A. K., Cordeiro, M. N. D. S. In silico characterization of aryl benzoyl hydrazide derivatives as potential inhibitors of RdRp enzyme of H5N1 influenza virus, Frontiers in Pharmacology. 2022, 13, 1004255
13. Chhetri, A., Roy, M., Gangopadhyay, A., Saha, A., Mishra, P., Halder, A. K., Basak, S. Modelling and Molecular dynamics simulation of novel anticancer ligand for restructuring mutant P53 into wild type. International Journal of Computational Biology and Drug Design, 2022, 15, 77-95.
14. Pramanik, S. D., Halder,A. K., Mukherjee, U., Kumar,D., Dey,Y.N., Rajagopal, M. Potential of Histone deacetylase Inhibitors in the control and regulation of Prostate, Breast and Ovarian cancer. Frontiers in Chemistry, 2022, 10, 948217.
15. Halder, A.K., Haghbakhsh, R., Voroshylova, I. V., Duarte, A. R. C., Cordeiro, M. N. D. S. Predicting the Surface Tension of Deep Eutectic Solvents: A Step Forward in the Use of Greener Solvents. Molecules 2022, 27(15), 4896.
16. Halder, A. K., Moura, A. S. Cordeiro, M. N. D. S. Moving Average-Based Multitasking In Silico Classification Modeling: Where Do We Stand and What Is Next? International Journal of Molecular Sciences, 2022, 23,4937.
17. Gupta, S., Dey, Y. N., Kannojiaa, P., Halder, A. K., Sharma, D., Wanjari, M. M., Chouule, S., Pawar, S., Kaushik, A., Gaidhani, S. N., Gurav, S. Analgesic and Anti-inflammatory Activities of Trayodashang Guggulu, an Ayurvedic Formulation. Phytomedicine Plus, 2022, 2, 100281
18. Halder, A. K., Ambure, P., Perez, Y., Cordeiro, M. N. D. S. Turning deep-eutectic solvents into value-added products for CO2 capture: A desirability-based virtual screening study. Journal of CO2 Utilization, 2022, 58, 101926
19. Halder, A. K., Delgado, A. H. S., Codeiri, M. N.D.S, First multi-target QSAR model for predicting the cytotoxicity of acrylic acid-based dental monomers, Dental Materials, 2022, 38, 333-346.
20. Halder, A. K., Cordeiro, M.N. D. S. Multi-target in silico prediction of inhibitors for mitogen-activated protein kinase-interacting kinases. Biomolecules, 2021, 11, 1670.
21. Datta, S, Halder,A.K., Adhikari,N., Amin, S. A., Das, S. Jha, T. Synthesis, anticancer activity, SAR and binding mode of interaction studies of substituted pentanoic acids: Part II. Future Medicinal Chemistry, 2022, 14, 17-34
22. Halder, A.K., Haghbakhsh, R., Voroshylova, I. V., Duarte, A. R. C., Cordeiro, M. N. D. S. Density of deep eutectic solvents: the path forward cheminformatics-driven reliable predictions for mixtures. Molecules. 2021, 26, 5779

23. Halder, A.K., Cordeiro, M. N. D. S. QSAR-Co-X: An open access toolkit for multitarget QSAR modelling. Journal of Cheminformatics, 2021, 13, 29.
24. Halder, A.K., Cordeiro, M. N. D. S. AKT inhibitors: The road ahead to computational modelling guided discovery. International Journal of Molecular Sciences, 2021, 44, 8944.
25. Jha, T., Samanta, S., Halder, A. K., Adhikari, N., Abdul Amin, S. K., Sanyal, A., Mukherjee, T. Synthesis, biological evaluation, and enzyme assay of some 5-N-substituted-2-N-(arylsulphonyl)-L(+)glutamines as potential anticancer agents. Journal of Indian Chemical Society, 2020, 97, 1259-1264.
26. Halder, A. K., Melo, A., Cordeiro, M.N.D.S. A unified in silico model based on perturbation theory for assessing the genotoxicity of metal oxide nanoparticles. Chemosphere, 2020,244,125489.
27. Halder, A. K., Cordeiro, M. N. D. S. Advanced in silico methods for the development of anti-leishmaniasis and anti-trypanosomiasis agents. Current Medicinal Chemistry, 2020, 27, 697-718.
28. Halder, A. K., Giri, A. K., Cordeiro, M.N.D.S. Multi-Target Chemometric Modelling, Fragment Analysis and Virtual Screening with ERK Inhibitors as Potential Anticancer Agents. Molecules, 2019, 24, 3909.
29. Halder, A. K., Cordeiro, M. N. D. S. Development of Multi-Target Chemometric Models for the Inhibition of Class I PI3K Enzyme Isoforms: A Case Study Using QSAR-Co Tool. International Journal of Molecular Sciences, 2019, 20, 4191.
30. Halder, A. K., Cordeiro, M. N. D. S. Probing the environmental toxicity of deep eutectic solvents and their components: An in silico modeling approach. ACS Sustainable Chemistry and Engineering, 2019, 7, 10649-10660.
31. Moura, A. S., Halder, A. K., Cordeiro, M. N. D. S. From biomedicinal to in silico models and back to therapeutics: A review on the advancement of peptidic modelling. Future Medicinal Chemistry, 2019, 11, 2313–2331.
32. Ambure, P., Halder, A. K., Gonzalez-Diaz, H., Cordeiro, M.N.D.S. QSAR-Co: An Open Source Software for Developing Robust Multi-tasking or Multi-target Classification-Based QSAR Models. Journal of Chemical Information and Modeling, 2019, 59(6):2538-2544.
33. Dutta, S., Halder, A. K., Adhikari, N., Amin, S. A., Das, S., Saha, A., Jha, T. Synthesis, anticancer activity, SAR and binding mode of interaction studies of substituted pentanoic acids. Future Medicinal Chemistry,2019, 11(14), 1679-1702.
34. Halder, A. K., Cordeiro, M.N.D.S. Development of predictive linear and non-linear QSTR models for Aliivibriofischeri toxicity of Deep Eutectic Solvents. International Journal of Quantitative Structure Property Relationships, 2019, 4, 50-69.
35. Halder, A. K., Honarparvar, B. Molecular alteration in drug susceptibility against subtype B and C-SA HIV-1 proteases: MD study. Structural Chemistry, 2019, 30, 1715–1727.
36. Tolufashe, G. F., Govender, T., Halder, A. K., Ibeji, C. U, Lawal, M. M., Ntombela, T., Maquire, G. M., Lamichhane, G., Kruger, H. G., Honarparvar, B. Inhibition of Mycobacterium tuberculosis L,D-transpeptidase 5 by carbapenems: MD and QM/MM Mechanistic Studies. ChemistrySelect,2018, 3, 13603– 13612.
37. Halder, A. K., Moura, A. S., Cordeiro, M. N. D. S. QSAR modelling: a therapeutic patent review 2010-present. Expert Opinion in Therapeutic Patents, 2018, 28, 467-476.
38. Halder, A. K. Finding the structural requirements of diverse HIV-1 protease inhibitors using multiple QSAR modelling for lead identification. SAR and QSAR in Environmental Research, 2018, 29, 911-933.
39. Maphumulo, S. I., Halder, A. K., Govender, T., Maseko, S., Maguire, G.E.M., Honarparvar, B. Kruger, H. G. Exploring the flap dynamics of the South African HIV C-SA protease in presence of FDA-approved inhibitors: MD study Chemical Biology and Drug Design, 2018, 92, 1899-1913.
40. Sengupta, D., Majumdar, Z. H., Mukherjee, A., Sharma, D., Halder, A. K.,Basu, S., Jha, T. Benzamide porphyrins with directly conjugated and distal pyridyl or pyridinium groups substituted to the porphyrin macrocycles: Study of the photosensitizing abilities as inducers of apoptosis in cancer cells under photodynamic conditions. Journal of Photochemistry and Photobiology:B, 2017, 178, 228-236.

41. Halder, A. K., Amin, S. A., Jha, T., Gayen, S. Insight into the structural requirements of pyrimidine-based phosphodiesterase 10A (PDE10A) inhibitors by comparative 3D QSAR approaches. SAR and QSAR in Environmental Research,2017, 28, 253-273.
42. Jha, T., Basu, S., Halder, A. K., Adhikari, N., Samanta, S. Possible Anticancer Agents: Synthesis, Pharmacological Activity and Molecular Modeling Studies on some 5-N-Substituted-2-N-(Substituted Benzenesulphonyl)-L(+)Glutamines. Medicinal Chemistry Research, 2017, 26, 1437–1458.
43. Halder, A. K., Saha, A., Jha, T. Predictive quantitative structure toxicity relationship study on avian toxicity of some diverse agrochemical pesticides by Monte Carlo method: QSTR on pesticides. International Journal of Quantitative Structure Property Relationship, 2017, 2, 19-34.
44. Adhikari, N., Halder, A. K.#, Mallick, S., Saha, A., Saha, K. D., Jha, T. Robust design of some selective matrix metalloproteinase-2 inhibitors over matrix metalloproteinase-9 through in silico /fragment-based lead identification and de novo lead modification: Syntheses and biological assays. Bioorganic and Medicinal Chemistry, 2016, 24, 4291-4309.
45. Halder, A. K., Mukherjee, A., Adhikari, N., Saha, A., Jha, T.Development of nitric oxide synthase (NOS) inhibitors for cancer angiogenesis. Current Enzyme Inhibition, 2016, 12, 49-66.
46. Halder, A. K., Mallick, S., Shikha, D., Saha, A., Saha, K. D., Jha, T. Design of dual MMP-2/HDAC-8 inhibitors by pharmacophore mapping, molecular docking, synthesis and biological activity. RSC Advances, 2015, 5, 72373 – 72386.
47. Adhikari, N., Halder, A. K., Saha, A., Saha, K. D., Jha, T. Structural findings of phenylindoles as cytotoxic antimitotic agents in human breast cancer cell lines through multiple validated QSAR studies. Toxicology In Vitro, 2015, 29, 1392-1404.
48. Hazra, A., Mondal, C., Chakraborty, D., Halder, A. K., Bharitkar, Y. P., Mondal, S. K., Banerjee, S., Jha, T., Mondal, N. B. Towards the development of anticancer drugs from andrographolode: Semisynthesis, bioevaluation, QSAR analysis and pharmaceutical studies. Current Topics in Medicinal Chemistry, 2015, 15, 1013-1026.
49. Halder, A. K., Saha, A., Jha, T. Stepwise development of structure activity relationship of diverse PARP-1 inhibitors through comparative and validated in silico modeling techniques and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1756-1779.
50. Mondal, C., Halder, A. K.#, Adhikari, N., Saha, A., Saha, K. D., Gayen, S., Jha, T. Comparative validated molecular modeling of p53-HDM2 inhibitors as antiproliferative agents. European Journal of Medicinal Chemistry, 2015, 90, 860-875.
51. Halder, A. K., Goodarzi, M. Recent advances in multi-task QSAR modeling for drug design. Pharmaceutical Sciences, 2015, 21, 175-177.
52. Mondal, C., Adhikari, N., Halder, A. K., Jha, T. Structural exploration of 2,6,9-trisubstituted as potent CDK2 inhibitors in cancer through validated molecular modelling studies. Journal of Engineering, Science, Management and Education, 2014,7, 166-176
53. Mondal, C., Halder, A. K., Adhikari, N., Jha, T. Structural findings of cinnolines as anti-schizophrenic PDE10A inhibitors through comparative chemometric modelling. Molecular Diversity, 2014, 18, 655–671.
54. Adhikari, N, Halder, A. K., Mondal, C., Jha, T.Structural findings of quinolone carboxylic acids in cytotoxic, antiviral, and anti-HIV-1 integrase activity through validated comparative molecular modeling studies. Medicinal Chemistry Research, 2014, 23, 3096-3127.
55. Halder, A. K., Saha, A., Jha, T. Exploration of structural and physicochemical requirements and search of virtual hits for aminopeptidase N inhibitors. Molecular Diversity, 2013, 17, 123-137.
56. Halder, A. K., Saha, A., Jha, T. The Role of 3D Pharmacophore Mapping Based Virtual Screening for Identification of Novel Anticancer Agents: An Overview. Current Topics in Medicinal Chemistry, 2013, 9, 417-432.

57. Halder, A. K., Saha, A., Jha, T. Exploring QSAR and pharmacophore mapping of structurally diverse selective matrix metalloproteinase-2 inhibitors. Journal of Pharmacy and Pharmacology, 2013, 65, 1541-1554.
58. Adhikari, N., Halder, A. K., Mondal, C., Jha, T. Exploring structural requirements of aurone derivatives as antimalarials by validated DFT based QSAR, HQSAR and COMFA-COMSIA approach. Medicinal Chemistry Research, 2013, 22, 6029-6045.
59. Mondal, C., Halder, A. K., Adhikari, N., Jha, T. Cholesteryl ester transfer protein inhibitors in coronary heart disease-Part II: Validated comparative chemometric modeling of N, N-disubstituted trifluoro-3-amino-2-propanols. Computers in Biology and Medicine, 2013, 43, 1545-1555.
60. Adhikari, N., Halder, A. K., Mondal, C., Jha, T. Ligand based validated comparative chemometric modeling and pharmacophore mapping of aurone derivatives as antimalarial agents. Current Computer Aided Drug Design, 2013, 9, 417-432.
61. Adhikari, N., Jana, D., Halder, A. K., Mondal, C., Maiti, M. K., Jha, T. Chemometric modeling of 5-phenylthiophenecarboxylic acid derivatives as antirheumatic agents, Current Computer Aided Drug Design, 2012, 8, 182-195.
62. Jana, D., Halder, A. K., Adhikari, N., Maiti, M. K., Mondal, C., Jha, T. Chemometric modeling and pharmacophore mapping in coronary heart disease: 2-arylbenzoxazoles as cholesteryl ester transfer protein inhibitors, MedChemComm, 2011, 2, 840-852.
63. Halder, A. K., Jha, T. Validated predictive QSAR modeling of N-aryl-oxazolidinone-5-carboxamides for anti-HIV protease activity, Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6082-6087.
64. Halder, A. K., Adhikari, N., Maity, M. K., Jha, T. Synthesis, pharmacological activity and comparative QSAR modeling of 1,5-N,N' -Disubstituted-2-(substituted naphthalenesulphonyl) glutamamide compounds as possible anticancer agents. European Journal of Medicinal Chemistry,2010, 45, 1760-1771.
65. Halder, A. K., Adhikari, N. Jha. T. Structural findings of 2-Phenylindole-3-Carbaldehyde Derivatives for antimitotic activity by FA-sMLR QSAR Analysis. Chemical Biology and Drug Design, 2010, 75, 204-213.
66. Jha, T., Chakrabortty, P., Adhihari, N., Halder, A. K., Maity, M. K. QSAR study on coumarins as antimeningoencephalitic agents.Internet Electronic Journal of Molecular Design, 2009, 8, 1-13.
67. Halder, A. K., Adhikari, N., Jha, T. Comparative QSAR modeling of 2-phenylindole-3-carbaldehyde derivatives as potential antimitotic agents Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1737-1739.
68. Alam, S. M., Samanta, S., Halder, A. K., Jha, T. QSAR modelling of KATP-pβ channel opener R/S-3,4-dihydro-2,2-dimethyl-6-halo-4-(substituted phenyl aminocarbonyl- amino)-2H-1-benzopyrans using MLR-FA techniques. European Journal of Medicinal Chemistry, 2009, 44, 359-364.
69. Jha, T., Samanta, S., Basu, S., Halder, A. K., Adhihari, N., Maity, M. K. QSAR Study On Some Orally Active Uracil Derivatives as Human-Gonadotropin-Releasing-Hormone Receptor Antagonists. Internet Electronic Journal of Molecular Design, 2008, 7, 234-250.
70. Alam, S. M., Samanta, S., Halder, A. K., Basu, S., Jha, T. Structural finding of R/S-3,4-dihydro-2,2-dimethyl-6-halo-4-(substituted phenylaminocarbonylamino)-2H-1-benzopyrans as selective pancreatic β-cells KATP-pβ channel openers, Canadian Journal of Chemistry, 2007, 85,1053-1063.

Book chapters

1. Banerjee, T., Sar, S., Saha, S., Baidya, A., Sarkar, A., Karmakar, S., Halder, A. K., Ghosh, N. Herbal Medicines for the Treatment of Liver Cirrhosis. In: Dhara, A.K., Mandal, S.C. (eds) Role of Herbal Medicines. Springer, Singapore. https://doi.org/10.1007/978-981-99-7703-1_10.

2. Sar, S., Banerjee, T., Kumar, Baidya,A., Saha, S., Mondal, J., Chaki, R., Halder,A. K., Ghosh, N. Role of Natural Polysaccharides in the Management of Lifestyle Diseases. In: Dhara, A.K., Mandal, S.C. (eds) Role of Herbal Medicines. Springer, Singapore. https://doi.org/10.1007/978-981-99-7703-1_10.
3. Sar, S., Banerjee, T., Baidya, A., Saha, S., Kumar,A., Halder, A. K., Ghosh, M., Nasare, V. D., Ghosh, N., Pharmacovigilance of Herbal Medicines for Lifestyle Diseases. In: Dhara, A.K., Mandal, S.C. (eds) Role of Herbal Medicines. Springer, Singapore. https://doi.org/10.1007/978-981-99-7703-1_10.
4. Mitra, S., Nandi, S., Halder, A. K., Cordeiro, M. N. D. S. SMILES-Based Bioactivity Descriptors to Model the Anti-dengue Virus Activity: A Case Study. In: QSPR/QSAR Analysis Using SMILES and Quasi-SMILES. Challenges and Advances in Computational Chemistry and Physics, vol 33. Springer, Cham. 2023
5. Halder, A. K., Cordeiro, M. N. D. S. Chemometric modelling of Daphnia toxicity. In: Chemometrics and cheminformatics in aquatic toxicology. (Edn. Roy, K.) Wiley, 2021, Chapter 15. pp. 293-317
6. Halder, A. K., Moura, A. S., Cordeiro, M. N. D. S. Advanced chemometric modeling approaches for the design of multitarget drugs against neurodegenerative diseases. In: Methods in Pharmacology and Toxicology: Multi-Target Drug Design Using Chem-Bioinformatic Approaches,(Edn. Roy, K.)Springer Protocols, 2018, Chapter 3, pp. 155-186.
7. Jha, T., Adhikari, N., Halder, A. K., Saha, A. Ligand Based & Structure Based Drug Design of Non-Steroidal Aromatase Inhibitors (NSAIs) in Breast Cancer, In: Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment. (Edn. Roy, K.), IGI Global, 2015, Chapter 11, pp. 400-470.
8. Jha, T., Halder, A. K., Adhikari, N. Epstein–Barr virus and treatment of its infection, In: Cancer causing viruses and their inhibitors. (Edn. Gupta, S. P.), CRC Press, 2014, pp. 157-205.

Conference presentations (Oral/Poster)

1. Halder, A. K., Cordeiro, M. N. D. S., Understanding the environmental toxicity of deep eutectic solvents and their components: a multitasking quantitative structure-toxicity relationship modelling approach. XXIV Encontro Luso Galego de Quimica, University of Porto, Portugal, 21-23 November 2018.
2. Halder, A. K., Samanta, S., Mukherjee, T., Bandopadhaya, S.,Jha, T. Possible anticancer agents: Synthesis, biological evaluation and modelcular modeling of 5-N-siubstituted-2-(substituted benzenesulphonyl)-L(+) glutamines. (Abstract published in J. Cancer Res. Therapeut.,2012, 8, Suppl1, S23 and paper presented in 31st Annual Convention of the Indian Association for Cancer Research and International Symposium on 'Cancer Genomics and its Impact in Clinics' organized in ACTREC, Tata Memorial Centre, Kharghar, Navi Mumbai, INDIA), 26-29th January 2012.
3. Halder, A. K., Mondal, C., Adhikari, N., Saha, A., Jha, T. Finding structural requirements and novel leads for active and selective Polo-like kinase-1 inhibitors. National Conference on 'New Trends in Bioinformatics', IIT Delhi, India, July 30-31, 2012.
4. Halder, A. K., Jha, T., Structural findings of carboxamide antiprotease compounds by validated predictive QSAR modeling based on internal and external predictabilities, International Conference on Recent Advances in Drug Discovery, University College of Pharmaceutical Sciences, Kakatiya University, Warangal, A. P., India, 22nd-24th October 2010.
5. Halder, A. K., Alam, S. M., Samanta, S., Basu, S., Jha, T., QSAR modeling of N-aryl-oxazolidone-5-carboxamides as HIV protease inhibitors. International Conference on the Interface of Chemistry-Biology in Biomedical Research, BITS Pilani, 22-24th February 2008.

Referee/Reviewer

International Journal of Molecular Sciences, Molecules, Molecular Diversity, Environmental Science-Nano, Chemosphere, Journal of Molecular Structure and Dynamics, SAR & QSAR in Environmental Research,etc

Fellowship/Awards

- **2019,** Fellowship obtained for the project UID/QUI/50006/2019, with financial support from FCT/MEC through national funds.
- **2018.** Fellowship obtained for the project Interreg Sudoe NanoDesk-SOE1/P1/E02015
- **2017,** Fellowship obtained for the project UID/QUI/50006, with financial support from FCT/MEC through national funds and co-financed by European Regional Development Find (ERDF) POCI-01-0145-FEDER-007265 within the framework of Partnership agreement PT2020.
- **2016,** Post-Doctoral Fellowship awarded by University of Kwazulu-Natal, Durban, South Africa.
- **2014,** International Travel Grant sanctioned by Scientific and Engineering Research Board (SERB), New Delhi for attending International Conference in San Francisco, USA..
- **2011-2015,** Senior Research Fellowship- Council of Scientific and Industrial Research (CSIR), New Delhi, India for Ph.D. program.
- **2006-2008,** Fellowship for Post-Graduate program in Pharmacy (GATE fellowship), University Grants Commission (UGC), Govt. of India
- **2006**, Qualified National Graduate Aptitude Test in Engineering (GATE)

M. Pharm. Dissertation

- Preclinical evaluation of thrombocytogenic activity of hydro-alcoholic extract of Psidium guajava fruits of Wistar rats with in silico modeling on Dengue virus protease inhibitors. Student name: Soumik Bhattacharjee. Year: 2021-22,
- Evaluation of effect of donepezil on metoprolol associated memory consolidation on Swiss albino mice with in silico modeling on 5HT2a antagonists. Student name: Koushik Pal. Year: 2021-22
- In vivo and in silico studies on the effect of ibuprofen on wound healing process. Student name: Sachin Karmakar. Year 2022-23

Granted Project

Title: Design and development of drug-like candidates in form of biphenyl sulfonamide derivatives as FXR partial agonists for therapeutic management of non-alcoholic fatty liver disease.
Duration (in months): 36 Total
Granting agency: Science & Technology and Biotechnology Department, Government of West Bengal, India
Amount sanctioned: Rs. 26,10,000

Personal details

Date of Birth: 02.08.1983
Gender: Male
Languages known: English (fluent), Hindi (fleunt), Bengali (mother tongue), Portuguese (beginner)
Nationality: Indian
Home address: B-2/444, KALYANI, NADIA, WEST BEGAL, PIN 741235, INDIA

RESUME

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Personal Information

Fathers Name : Somnath Banerjee
Date of Birth : 25/01/1975

Educational Qualification

1. **Completed MBA from Sikkim Manipal University in the year 2008**
2. **Completed MCA from Bangalore University in the year 2001**
3. **Completed B.Sc from Burdwan University in the year 1996**

Experience

Teaching experience of 20 years from Dr.B.C.Roy College of Pharmacy & AHS, Durgapur (from Sept 2005 to date).

Hobbies/ Interests

Programming, story book reading etc

I hereby declare that all the above mentioned information are correct and true to the best of my knowledge and belief.

12/12/24

(Soumen Banerjee)
Date : 12/12/2024
Durgapur - 12

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