Dr. Nilanjan Adhikari

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Department of Pharmaceutical Technology,

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Previous position

Research Associate

Council of Scientific and Industrial Research

New Delhi, India

Academic Qualifications:

Sl. No.	Degree	Year	Subject	University/Institution
1.	B. Pharm.	2007	Pharmacy	Jadavpur University, Kolkata
2.	M. Pharm.	2009	Pharmaceutical Chemistry	Jadavpur University, Kolkata
3.	Ph.D	2018	Pharmacy	Jadavpur University, Kolkata

Awards/Honors/Fellowships:

Sl. No.	Name of Award	Awarding Agency	Year
1	Research Associateship (RA)	Council of Scientific and Industrial Research (CSIR), New Delhi, India	2019
2	Research Fellowship	University Grants Commission (UGC), New Delhi, India	2015
3	Project Fellowship	Council of Scientific and Industrial Research (CSIR), New Delhi, India	2012

4	Post graduate Research Fellowship	Ministry of Human Resource and Development (MHRD), New Delhi, India	2007

Positions/Employments (in chronological order):

S. No.	Positions held	Name of the Institute	From	To
1.	Post Graduate Research Fellow	Jadavpur University, Kolkata	08/2007	07/2009
2.	Assistant Professor	Guru Nanak Institute of Pharmaceutical Science and Technology, Kolkata	07/2009	04/2012
3.	Project Fellow	CSIR sponsored project at Jadavpur University, Kolkata	04/2012	02/2015
4.	Research Fellow (RGNF, UGC)	Jadavpur University, Kolkata	03/2015	07/2018
5.	Assistant Professor	Adamas University, Kolkata	08/2018	05/2019
6.	Research Associate (RA), CSIR	Jadavpur University, Kolkata	05/2019	02/2021
7.	Assistant Professor	Jadavpur University, Kolkata	02/2021	Continuing

Professional Activity:

1. PhD. Supervision: **02**; M. Pharm. Supervision: **02**
2. **Reviewer** of ***European Journal of Medicinal Chemistry*** (Elsevier), **Impact Factor: 6.514**; ***Journal of Molecular Structure*** (Elsevier), **Impact Factor: 3.196**; ***Current Pharmaceutical Design*** (Bentham Science); **Impact Factor: 3.116**; ***SAR and QSAR in Environmental Research*** (Taylor and Francis), **Impact Factor: 3.681**; ***Structural Chemistry*** (Springer), **Impact Factor: 1.887**; ***Journal of Biomolecular Structure and Dynamics*** (Taylor and Francis).
3. Acting as **Program Officer** of **National Service Scheme (NSS), Jadavpur University**.

4. Acted as the **Joint Treasurer** in the Two Day National Seminar on **"Advances in Pharmaceutical Technology: Opportunities and Challenges"** held in School of Pharmaceutical Technology**,** Adamas University, Kolkata on **22th – 23th February, 2019.**
5. Acted as the **Paper/Poster Evaluator** in the two days "**National Conference: NATCONPH**" (Conference Theme: "Collaborative Health Sciences - Visions for the Future") organized by NSHM Knowledge Campus, Kolkata on 14th - 15th February, 2019 at Science City Auditorium, Kolkata.
6. Acted as the **Volunteered of the Hospitality Committee Member** in the 2nd International Conference on "**Current Trends in Higher Education (ICCTHE 2019)**" held in Adamas University, Kolkata on 21st - 22nd January, 2019.
7. Acted as the **Committee Member** of a day long workshop on "**GMP NORMS: GLOBAL QUALITY MANAGEMENT IN PHARMACEUTICALS**" was held in School of Pharmaceutical Technology**,** Adamas University, Kolkata on **18th August 2018**.

Area of Research:

My research is involved in the exploration and understanding of biological systems at the molecular level with a tool set offered by modern chemistry. My work resides in the interface of designing newer compounds through modern molecular modeling techniques followed by synthesis through organic chemistry and subsequently conduct cell biology and manipulation of cellular activity with these newer bioactive small molecules.
I also believe that not only discovery of right bioactive molecules but also the delivery of the molecules to the particular site of action is equally challenging.

Major Focus of Research:

- Drug designing of different bioactive molecules through rigorous computational modeling techniques and large scale quantitative structure-activity relationship (QSAR) analysis.
- Design and development of selective small molecule matrix metalloproteinase inhibitors (MMPIs) as potential anticancer agents.
- Design and development of subtype specific histone deacetylase (HDAC) inhibitors as epigenetic modulators acted as potential anticancer agents.

- Design and development of dual acting MMP-2 and HDAC8 inhibitors and evaluating their anticancer properties.

Scopus H-index: 24

Total Number of Citations: **1531**

Total number of Paper Publication: 105

Total number of Book Chapter publication: 08

Publications:

A] Research Articles/Papers published in Referred Journals as Notified by UGC

1. S.K. Baidya, S. Banerjee, **N. Adhikari**, T. Jha, Selective inhibitors of medium-size S1' pocket matrix metalloproteinases: A stepping stone of future drug discovery, ***Journal of Medicinal Chemistry***, 2022, 65, 16, 10709-10754. **I.F: 8.039**
2. S. Pulya, T. Patel, M. Paul, **N. Adhikari**, S. Banerjee, G. Routholla, S. Biswas,T. Jha, B. Ghosh, Selective inhibition of histone deacetylase 3 by novel hydrazide based small molecules as therapeutic intervention for the treatment of cancer, ***European Journal of Medicinal Chemistry***, 2022, 238, 114470. **I.F: 7.088**
3. S. Banerjee, S.K. Baidya, B. Ghosh, **N. Adhikari**, T. Jha, First Report on Predictive Comparative Ligand-based Multi-QSAR Modeling Analysis of 4-pyrimidinone and 2-pyridinone based APJ inhibitors, ***New Journal of Chemistry***, 2022, 46, 11591-11607. **I.F: 3.925**
4. **N. Adhikari**, S. Banerjee, S.K. Baidya, B. Ghosh, T. Jha, Ligand-based quantitative structural assessments of SARS-CoV-2 3CLpro inhibitors: An analysis in light of structure-based multi-molecular modeling evidences, ***Journal of Molecular Structure***, 2022, 1251, 132041. **I.F: 3.196**
5. S. Das, S.A. Amin, S. Datta, **N. Adhikari**, T. Jha, Synthesis, biological activity, structure activity relationship study and liposomal formulation development of some arylsulfonyl pyroglutamic acid derivatives. ***Journal of Molecular Structure***, 2022, 1248, 131512. **I.F: 3.196**

6. S. Datta, A.K. Halder, **N. Adhikari**, S.A. Amin, S. Das, T. Jha, Synthesis, anticancer activity, SAR and binding mode of interaction studies of substituted pentanoic acids: Part II. ***Future Medicinal Chemistry***, 2022, 14, 17–34. **I.F: 3.808**
7. V. Yadav, S. Banerjee, S.K. Baidya, **N. Adhikari**, T. Jha, Applying comparative molecular modelling techniques on diverse hydroxamate-based HDAC2 inhibitors: an attempt to identify promising structural features for potent HDAC2 inhibition, ***SAR and QSAR in Environmental Researc***h, 2022, 33, pp. 1–22. **I.F: 3.000**
8. G. Routholla, S. Pulya, T. Patel, **N. Adhikari**, S.A. Amin, M. Paul, S. Bhagavatula, S. Biswas, T. Jha, B. Ghosh, Design, synthesis and binding mode of interaction of novel small molecule o-hydroxy benzamides as HDAC3-selective inhibitors with promising antitumor effects in 4T1-Luc breast cancer xenograft model, ***Bioorganic Chemistry***. 2021, 117, 105446. **I.F: 5.275**
9. S. Sanyal, S.A. Amin, **N. Adhikari**, T. Jha, Ligand-based design of anticancer MMP2 inhibitors: a review. ***Future Medicinal Chemistry***, 2021, 13, 1987-2013. **I.F: 3.808**
10. S.A. Amin, P. Trivedi, **N. Adhikari**, G. Routholla, D. Vijayasarathi, S. Das, B. Ghosh, T. Jha, Quantitative activity–activity relationship (QAAR) driven design to develop hydroxamate derivatives of pentanoic acids as selective HDAC8 inhibitors: synthesis, biological evaluation and binding mode of interaction studies, ***New Journal of Chemistry***. 2021, 45, 17149-62. **I.F: 3.591**
11. G. Routholla, S. Pulya, T. Patel, S.A. Amin, **N. Adhikari**, S. Biswas, T. Jha, B. Ghosh, Synthesis, biological evaluation, and molecular docking analysis of novel linker-less benzamide based potent and selective HDAC3 inhibitors. ***Bioorganic Chemistry***, 2021, 114, 105050. **I.F: 5.275**
12. **N. Adhikari**, T. Jha, B. Ghosh, Dissecting Histone Deacetylase 3 in Multiple Disease Conditions: Selective Inhibition as a Promising Therapeutic Strategy. ***Journal of Medicinal Chemistry***, 2021, 64, 8827-8869. **I.F: 7.446**
13. T.K. Patel, **N. Adhikari**, S.A. Amin, S. Biswas, T. Jha, B. Ghosh, Small molecule drug conjugates (SMDCs): an emerging strategy for anticancer drug design and discovery. ***New Journal of Chemistry***, 2021, 45, 5291-5321. **I.F: 3.591**
14. S. Guti, S.K. Baidya, S. Banerjee, **N. Adhikari**, T. Jha, A robust classification-dependent multi-molecular modelling study on some biphenyl sulphonamide based MMP-8 inhibitors. ***SAR and QSAR in Environmental Research***, 2021, 32, 835-861. **I.F: 3.000**
15. **N. Adhikari**, S. Banerjee, S.K. Baidya, B. Ghosh, T. Jha, Robust classification-based molecular modelling of diverse chemical entities as potential SARS-CoV-2 3CLpro

inhibitors: theoretical justification in light of experimental evidences, ***SAR and QSAR in Environmental Research***. 2021, 32, 473-493. **I.F: 3.000**

16. S. Pulya, S.A. Amin, **N. Adhikari**, S. Biswas, T. Jha, B. Ghosh, HDAC6 as privileged target in drug discovery: A perspective. ***Pharmacological research***, 2021, 163, 105274. **I.F: 7.658**
17. **N. Adhikari**, S.K. Baidya, T. Jha, Effective anti-aromatase therapy to battle against estrogen-mediated breast cancer: Comparative SAR/QSAR assessment on steroidal aromatase inhibitors. ***European Journal of Medicinal Chemistry***, 2020, 208, 112845. **I.F: 6.514**
18. S. Banerjee, S.A. Amin, S.K. Baidya, **N. Adhikari**, T. Jha, Exploring the structural aspects of ureido-amino acid-based APN inhibitors: a validated comparative multi-QSAR modelling study. ***SAR and QSAR in Environmental Research***, 2020, 31, 325-345. **I.F: 3.000**
19. S. Mondal, **N. Adhikari**, S. Banerjee, S. A. Amin, T. Jha, Matrix metalloproteinase-9 (MMP-9) and its inhibitors in cancer: A minireview. ***European Journal of Medicinal Chemistry***, 2020, 194, 112260. **I.F: 4.833**
20. R. Sarkar, S. Banerjee, S. A. Amin, **N. Adhikari**, T. Jha, Histone deacetylase-3 (HDAC3) inhibitors as anticancer agents: A review. ***European Journal of Medicinal Chemistry***, 2020, 192, p. 112171. **I.F: 4.833.**
21. S. Jain, B. Bhardwaj, S. A. Amin, **N. Adhikari**, T. Jha, S. Gayen, Exploration of good and bad structural fingerprints for inhibition of indoleamine-2,3-dioxygenase enzyme in cancer immunotherapy using Monte Carlo optimization and Bayesian classification QSAR modeling. ***Journal of Biomolecular Structure and Dynamics***, 2020, 38, 1683-1696. **I.F: 3.310**
22. S. Banerjee, **N. Adhikari**, S. A. Amin, T. Jha, Structural exploration of tetrahydroisoquinoline derivatives as HDAC8 inhibitors through multi-QSAR modeling study, ***Journal of Biomolecular Structure and Dynamics***, 2020, 38, 1551-1564. **I.F: 3.310**
23. S. Jain, S. A. Amin, **N. Adhikari**, T. Jha, S. Gayen, Good and Bad Molecular fingerprints for human rhinovirus 3C protease inhibition: Identification, validation and application in designing of new inhibitors through Monte Carlo-based QSAR study, ***Journal of Biomolecular Structure and Dynamics***, 2020, 38, 66-77. **I.F: 3.310**
24. S. Banerjee, S. A. Amin, **N. Adhikari**, T. Jha, Essential elements regulating HDAC8 inhibition: a classification based structural analysis and enzyme-inhibitor interaction

study of hydroxamate based HDAC8 inhibitors. ***Journal of Biomolecular Structure and Dynamics***, 2020, 38, 5513-5525. **I.F: 3.310**

25. S. A. Amin, S. Banerjee, **N. Adhikari**, T. Jha, Discriminations of active from inactive HDAC8 inhibitors Part II: Bayesian classification study to find molecular fingerprints. ***SAR and QSAR in Environmental Research***, 2020, 31, 245-260. **I.F: 2.287**
26. S. A. Amin, **N. Adhikari**, T. Jha, Exploration of histone deacetylase 8 inhibitors through classification QSAR study: Part II. ***Journal of molecular Structure***, 2020, 1204, 127529. **I.F: 2.120**
27. A. T. K. Baidya, K. Ghosh, S. A. Amin, N. Adhikari, J. Nirmal, T. Jha, S. Gayen, In silico modelling, identification of crucial molecular fingerprints, and prediction of new possible substrates of human organic cationic transporters 1 and 2. ***New Journal of chemistry***, 2020, 44, 4129-4143. **I.F: 3.069**
28. S. Banerjee, S. A. Amin, S. K. Baidya, **N. Adhikari**, T. Jha, Exploring the structural aspects of ureido-amino acid-based APN inhibitors: a validated comparative multi-QSAR modelling study. ***SAR and QSAR in Environmental Research***, 2020, 31, 325-345. **I.F: 2.287**
29. S. A. Amin, **N. Adhikari**, T. Jha, Development of decision trees to discriminate HDAC8 inhibitors and non-inhibitors using recursive partitioning. ***Journal of Biomolecular Structure and Dynamics***, 2021, 39, 1-8. **I.F: 3.123**
30. S. A. Amin, **N. Adhikari**, S. Gayen, T. Jha, Reliable structural information for rational design of benzoxazole type potential cholesteryl seter transfer protein (CETP) inhibitors through multiple validated modelling techniques. ***Journal of Biomolecular Structure and Dynamics***, 2019, 37, 4528-4541. **I.F: 3.123**
31. S. A. Amin, **N. Adhikari**, B. Ghosh, T. Jha, Designing potential HDAC3 inhibitors to improve memory and learning. ***Journal of Biomolecular Structure and Dynamics***, 2019, 37, 2133-2142. **I.F: 3.123**
32. S. A. Amin, **N. Adhikari**, S. Baidya, S. Gayen, T. Jha, Structural refinement and prediction of potential CCR2 antagonists through validated multi-QSAR modeling, ***Journal of Biomolecular Structure and Dynamics***, 2019, 37, 75-94. **I.F: 3.123**
33. P. Trivedi, **N. Adhikari**, S. A. Amin, Y. Bobde, R. Ganesh, T. Jha, B. Ghosh, Design, synthesis, biological evaluation and molecular docking study of arylcarboxamido piperidine and piperazine-based hydroxamates as potential HDAC8 inhibitors with promising anticancer activity. ***European Journal of Pharmaceutical Sciences***, 2019, 138, 105046. **I.F: 3.532**

34. B. Bhardwaj, A. T. K. Baidya, S. A. Amin, **N. Adhikari**, T. Jha, S. Gayen, Insight into structural features of phenyltetrazole derivatives as ABCG2 inhibitors for the treatment of multidrug resistance in cancer, ***SAR and QSAR in Environmental Research***, 2019, 30, 457-475. **I.F: 2.227**
35. S. Dutta, A. K. Halder, **N. Adhikari**, S. A. Amin, S. Das, A. Saha, T. Jha, Synthesis, anticancer activity, structure–activity relationship and binding mode of interaction studies of substituted pentanoic acids, Future Medicinal Chemistry, 2019, 11, 1679-1702. **I.F: 3.969**
36. S. Sanyal, S. A. Amin, **N. Adhikari**, T. Jha, QSAR modelling on a series of arylsulfonamide-based hydroxamates as potent MMP-2 inhibitors, ***SAR and QSAR in Environmental Research***, 30, 2019, 247-263. **I.F: 2.227**
37. S. K. Baidya, S. A. Amin, S. Banerjee, **N. Adhikari**, T. Jha, Structural exploration of arylsulfonamide-based ADAM17 inhibitors through validated comparative multi-QSAR modelling studies, ***Journal of Molecular Structure***, 2019, 1185, 128-142. **I.F: 2.011**
38. S. A. Amin, **N. Adhikari**, S. Kotagiri, T. Jha, B. Ghosh, Histone deacetylase 3 inhibitors in learning and memory processes with special emphasis on benzamides. ***European Journal of Medicinal Chemistry***, 2019, 166, 369-380. **I.F: 4.816**
39. S. Banerjee, **N. Adhikari**, S. A. Amin, Tarun Jha, Histone deacetylase 8 (HDAC8) and its inhibitors with selectivity to other isoforms: An overview. ***European Journal of Medicinal Chemistry***, 2019, 164, 214-240. **I.F: 4.816**
40. **N. Adhikari**, S. A. Amin, Tarun Jha, Selective and noonselective HDAC8 inhibitors: a therapeutic patent review. ***Pharmaceutical Patent Analyst***, 2018, 7, 259-276.
41. **N. Adhikari**, S. A. Amin, P. Trivedi, T. Jha, B. Ghosh, HDAC3 is a potential validated target for cancer: An overview on the benzamide-based selective HDAC3 inhibitors through comparative SAR/QSAR/QAAR approaches. ***European Journal of Medicinal Chemistry***, 2018, 157, 1127-1142. **I.F: 4.816**
42. P. Trivedi, **N. Adhikari**, S. A. Amin, T. Jha, B. Ghosh, Design, synthesis and biological screening of 2-aminobenzamides as selective HDAC3 inhibitors with promising anticancer effects. ***European Journal of Pharmaceutical Sciences***, 2018, 124, 165-181. **I.F: 3.466**
43. R. Gaikwad, S. Ghorai, S. A. Amin, **N. Adhikari**, T. Patel, K. Das, T. Jha, S. Gayen, Monte Carlo based modelling approach for designing and predicting cytotoxicity of 2-phenylindole derivatives against breast cancer cell line MCF7. ***Toxicology in Vitro***, 2018, 52, 23-32. **I.F: 3.105**

44. S. A. Amin, **N. Adhikari**, T. Jha, Design of Aminopeptidase N (APN) inhibitors as Anticancer Agents. ***Journal of Medicinal Chemistry***, 2018, 61, 6468-6490. **I.F: 6.253**
45. S. A. Amin, **N. Adhikari**, T. Jha, S. Gayen, A review on camptothecin analogs with promising cytotoxic profile. ***Anti-cancer Agents in Medicinal Chemistry***, 2018, 13, 1796-1814. **I.F: 2.556**
46. S. A. Amin, **N. Adhikari**, S. Bhargava, T. Jha, S. Gayen, Structural exploration of hydroxyethylamines as HIV-1 protease inhibitors: new features identified. ***SAR and QSAR in Environmental Research***, 2018, 229, 385-408. **I.F: 2.227**
47. S. A. Amin, **N. Adhikari**, T. Jha, Structure-activity relationships of HDAC8 inhibitors: Non-hydroxamates as anticancer agent. ***Pharmacological Research***, 2018, 131, 128-142. **I.F: 4.897**
48. **N**. **Adhikari**, S. A. Amin, A. Saha, T. Jha, Structural exploration for the refinement of anticancer matrix metalloproteinase-2 inhibitor designing approaches through robust validated multi-QSARs. ***Journal of Molecular Structure***, 2018, 1156, 501-515. **I.F: 2.011**
49. S. A. Amin, S. Bhargava, **N. Adhikari**, S. Gayen, T. Jha, Exploring pyrazolo[3,4-d]pyrimidine phosphodiesterase 1 (PDE1) inhibitors: a predictive approach combining comparative validated multiple molecular modelling techniques. ***Journal of Biomolecular Structure and Dynamics***, 2018, 36, 590-608. **I.F: 3.107**
50. R. Gaikwad, S. A. Amin, **N. Adhikari**, S. Ghorai, T. Patel, K. Das, T. Jha, S. Gayen, Identification of molecular fingerprints of phenylindole derivatives as cytotoxic agents: a multi-QSAR approach. ***Structural Chemistry***, 2018, 29, 1095-1107. **I.F: 2.019**
51. **N**. **Adhikari**, S. A. Amin, A. Saha, T. Jha, Exploring *in-house* glutamate inhibitors of matrix metalloproteinase-2 through validated robust chemico-biological quantitative approaches. ***Structural Chemistry***, 2018, 29, 285-295. **I.F: 2.019**
52. S. A. Amin, **N. Adhikari**, S. Gayen, T. Jha, Integrin antagonists: a special emphasis on structural requirements of N-benzoyl-L-biphenylalanines as α4β7 and α4β1 antagonists. ***Current Signal Transduction Therapy***, 2018, 13, 105-118.
53. S. A. Amin, **N. Adhikari**, S. Gayen, T. Jha, An integrated QSAR modeling approach to explore the structure-property and selectivity relationships of N-benzoyl-l-biphenylalanines as integrin antagonists. ***Molecular Diversity***, 2018, 22, 129-158. **I.F: 2.229**

54. S. A. Amin, **N. Adhikari**, S. Gayen, T. Jha, First report on the validated classification-based chemometric modeling of human rhinovirus 3C protease (HRV 3Cpro) inhibitors. ***International Journal of Quantitative Structure-Property Relationships***, 2018, 3, 1-20.
55. T. Jha, **N**. **Adhikari**, A. Saha, S. A. Amin, Multiple molecular modelling studies on some derivatives and analogues of glutamic acid as matrix metalloproteinase-2 inhibitors. ***SAR and QSAR in Environmental Research***, 2018, 29, 43-68. **I.F: 2.227**
56. S. A. Amin, **N. Adhikari**, T. Jha, Diverse classes of HDAC8 inhibitors: In search of molecular fingerprints that regulate activity. ***Future Medicinal Chemistry***, 2018, 10, 1589-1602. **I.F: 3.969**
57. **N. Adhikari**, S. A. Amin, B. Ghosh, T. Jha, Shedding light on designing potential meprin β inhibitors through ligand-based robust validated computational approaches: A proposal to chemists!. ***Journal of Biomolecular Structure and Dynamics***, 2018, 36, 3003-3022. **I.F: 3.107**
58. S. Bhargava, **N. Adhikari**, S. A. Amin, K. Das, S. Gayen, T. Jha, Hydroxyethylamine derivatives as HIV-1 protease inhibitors: a predictive QSAR modelling study based on Monte Carlo optimization. ***SAR and QSAR in Environmental Research***, 2017, 28, 973-990. **I.F: 1.642**
59. A. Mukherjee, **N. Adhikari**, T. Jha, A pentanoic acid derivative targeting matrix metalloproteinase-2 (MMP-2) induces apoptosis in a chronic myeloid leukemia cell line. ***European Journal of Medicinal Chemistry***, 2017, 141, 37-50. **I.F: 4.519**
60. S. A. Amin, **N**. **Adhikari**, T. Jha, S. Gayen, An integrated multi-QSAR modeling approach for designing Knoevenagel-type indoles with enhancing cytotoxic profiles. ***Current Computer-Aided Drug Design***, 2017, 13, 336-345. **I.F: 0.77**
61. S. A. Amin, **N. Adhikari**, S. Gayen, T. Jha, An integrated ligand-based modelling approach to explore the structure-property relationships of influenza endonuclease inhibitors. ***Structural Chemistry***, 2017, 28, 1663-1678. **I.F: 1.582**
62. S. A. Amin, **N**. **Adhikari**, T. Jha, Structure-activity relationships of hydroxamate-based HDAC-8 inhibitors: reality behind anticancer drug discovery. ***Future Medicinal Chemistry***, 2017, 9, 2211-2237. **I.F: 3.556**
63. S. A. Amin, **N. Adhikari**, S. Gayen, T. Jha, Homoisoflavonoids as potential antiangiogenic agents for retinal neovascularisation. ***Biomedicine and Pharmacotherapy***, 2017, 95, 818-827. **I.F: 3.457**

64. S. A. Amin, **N**. **Adhikari**, S. Gayen, T. Jha, First report on the structural exploration and prediction of new BPTES analogs as glutaminase inhibitors. ***Journal of Molecular Structure***, 2017, 1143, 49-64. **I.F: 1.753**
65. S. A. Amin, **N**. **Adhikari**, T. Jha, Is dual inhibition of metalloenzymes HDAC-8 and MMP-2 a potential pharmacological target to combat hematological malignancies? ***Pharmacological Research***, 2017, 122, 8-19. **I.F: 4.48**
66. T. Jha, S. Basu, A. K. Halder, **N. Adhikari**, S. Samanta, 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. **I.F: 1.607**
67. S. A. Amin, **N**. **Adhikari**, R. Agarwal, T. Jha, S. Gayen, Possible binding mode analysis of pyrazolo-triazole hybrids as potential anticancer agents through validated molecular docking and 3D-QSAR modelling approaches. ***Letters in Drug Design and Discovery***, 2017, 14, 515-527. **I.F: 1.170**
68. S. A. Amin, **N**. **Adhikari**, S. Bhargava, T. Jha, S. Gayen, Designing potential antitrypanosomal thiazol-2-ethylamines through predictive regression based and classification based QSAR analyses. ***Current Drug Discovery Technologies***, 2017, 14, 39-52.
69. S. A. Amin, **N. Adhikari**, V. Shukla, T. Jha, S. Gayen, Structural findings of pyrazolo[1,5-a]pyrimidine compounds for their Pim-1/2 kinase inhibition as potential anticancer agents. ***Indian Journal of Biochemistry and Biophysics***, 2017, 54, 32-46. **I.F: 0.385**
70. **N**. **Adhikari**, S. A. Amin, A. Saha, T. Jha, Combating breast cancer with non-steroidal aromatase inhibitors (NSAIs): Understanding the chemico-biological interactions through comparative SAR/QSAR study. ***European Journal of Medicinal Chemistry***, 2017, 137, 365-438. **I.F: 4.816**
71. **N**. **Adhikari**, S. A. Amin, A. Saha, T. Jha, Understanding chemico-biological interactions of glutamate MMP-2 inhibitors through rigorous alignment-dependent 3D-QSAR analyses. ***ChemistrySelect***, 2017, 2, 7888-7898. **I.F: 1.505**
72. **N. Adhikari**, S. A. Amin, T. Jha, S. Gayen, Integrating regression and classification-based QSARs with molecular docking analyses to explore the structure-antiaromatase activity relationships of letrozole-based analogs. ***Canadian Journal of Chemistry***, 2017, 95, 1285-1295. **I.F: 1.08**

73. **N. Adhikari**, A. Mukherjee, A. Saha, T. Jha, Arylsulfonamides and selectivity of matrix metalloproteinase-2: An overview. ***Europran Journal of Medicinal Chemistry***, 2017, 129, 72-109. **I.F: 4.519**
74. S. A. Amin, **N. Adhikari**, T. Jha, S. Gayen, First molecular modeling report on novel arylpyrimidine kynurenine monooxygenase inhibitors through multi-QSAR analysis against Huntington's disease: A proposal to chemists!. ***Bioorganic and Medicinal Chemistry Letters***, 2016, 23, 5712-5718. **I.F: 2.454**
75. S. A. Amin, **N. Adhikari**, S. Gayen, T. Jha, Insight into the structural requirements of theophylline-based aldehyde dehydrogenase 1A1 (ALDH1A1) inhibitors through multi-QSAR modeling and molecular docking approaches. ***Current Drug Discovery Technologies***, 2016, 13, 84-100.
76. S. A. Amin, **N. Adhikari**, T. Jha, S. Gayen, Exploring structural requirements of unconventional Knoevenagel-type indole derivatives as cytotoxic agents through comparative QSAR modeling approaches. ***Canadian Journal of Chemistry***, 2016, 94, 637-644. **I.F: 1.08**
77. **N. Adhikari**, A. K. Halder, S. Mallick, A. Saha, K. D. Saha, T. Jha, 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. **I.F: 2.930**
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regression, PCRA, FA-MLR and PLS techniques. ***European Journal of Medicinal Chemistry***, 2010, 45, 1119-1127. **I.F: 3.193**

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B] Book Chapters

1. **N. Adhikari**, S.A. Amin, T. Jha, Dissecting the Drug Development Strategies Against SARS-CoV-2 Through Diverse Computational Modeling Techniques. In: ***In Silico Modeling of Drugs Against Coronaviruses***, ***Methods in Pharmacology and Toxicology*.** Ed. K. Roy, Humana, New York, 2021, pp. 329-431
2. **N. Adhikari**, S. A. Amin, T. Jha. Collagenases, Gelatinases and Their Inhibitors in Cancer. In: ***Cancer Leading Proteases***, Ed. S. P. Gupta, Elsevier, Netherlands, 2019, pp. 265-294.
3. S. A. Amin, **N. Adhikari**, B. Ghosh, T. Jha. Histone Deacetylase 3 and Its Inhibitors. In: ***Advances in Medicine and Biology***, Volume 145, (Ed. Leon V. Berhardt). Nova Science Publishers, New York, 2019, p. 131-202.
4. **N. Adhikari**, S. A. Amin, T. Jha, A. Saha. Application of computation in the biosynthesis of phytochemicals. In: ***Computational Phytochemistry***. **(**Eds. S. D. Sarkar and L. Nahar). Elsevier, Netherlands, 2018, p. 256-263.

5. **N. Adhikari**, S. Baidya, A. Saha, T. Jha. Structural insight into the viral 3C-like protease inhibitors: Comparative SAR/QSAR approaches. In: ***Viral Proteases and their inhibitors***. (Ed S. P. Gupta). Academic Press, USA, 2017, p. 317-402.
6. **N. Adhikari**, S. Baidya, A. Saha, N. Ali, T. Jha. Design and development of matrix metalloproteinase inhibitors containing zinc-binding groups, without zinc-binding groups, and mechanism-based. In: ***Advances in studies on enzyme inhibitors as drugs. Volume 2: Miscellaneous drugs***. (Ed S. P. Gupta). Nova Science Publishers, New York, 2017, p. 135-208.
7. T. Jha, **N. Adhikari**, A. K. Halder, A. Saha. 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***. (Ed. K. Roy). IGI Global, Hershey PA, USA, 2015, p. 400-470.
8. T. Jha, A. K. Halder, **N. Adhikari**. Epstein–Barr Virus and Treatment of Its Infection, In: ***Cancer causing viruses and their inhibitors***. (Ed S. P. Gupta). CRC Press, Boca Raton, 2014, p. 157-205.

Paper Presentation in Conferences/Seminars:

A] International:

1. **N. Adhikari**, S. Banerjee, S. A. Amin, T. Jha, "**Exploring Structural Requirements of Diarylurea Derivatives as VEGFR-2 inhibitors Through Comparative QSAR Modeling Study**" at **International Conference on Drug Discovery (ICDD) 2020** held in BITS-Hyderabad, India from 29th Feb-2nd Mar 2020.
2. **N. Adhikari**, S. A. Amin, B. Ghosh, T. Jha, "**DFT-based quantum chemical descriptors and alignment dependent 3D field calculations of metalloenzyme meprin β inhibitors: a quantitative SAR assessment**" at the **4th Annual Conference of Society for the Study of XENOBIOTICS (SSX), INDI**A (Theme: Exploring impact of ADMET and modelling science and technology in drug discovery and development) from 19th to 21st September 2019, in IISC Bangalore.
3. **N. Adhikari**, A. K. Halder, S. Mullick, A. Saha, K. D. Saha, T. Jha, "**Fragment-based *De Novo* Lead Generation, Synthesis and Biological Screening of Selective Matrix Metalloproteinase-2 Inhibitors**"-23rd CCTCC Conference on Current Trends in Computational Chemistry 2015, Interdisciplinary Centre for Nanotoxicity, Jackson State University, Jackson, Mississippi, USA, November 2015, p. 36.

4. **N. Adhikari**, C. Mondal, A. K. Halder, T. Jha, Volunteered, Participated, and presented a poster entitled "**Structural exploration of phenylindoles as antimitotic agents in human breast cancer cells through validated comparative chemometric modelling"** in 2nd Pharm. Tech. IAPST International Conference on "**New Insights into Disease and Recent Therapeutic Approaches**" in Jadavpur University, Kolkata, on 17th – 19th January, 2014.

   This poster was awarded 3rd in this poster session event.
5. **N. Adhikari**, C. Mondal, A. K. Halder, T. Jha, Participated and presented a poster entitled "**Structural exploration of carboxamides as CCR5 antagonists having potent anti-HIV-1 activity by validated comparative chemometric tools"** in the "**Recent Advances in Computational Drug Design**" at JN Tata Auditorium in IISC, Bangalore on 16th -17th September, 2013.
6. **N. Adhikari**, D. Jana, M. K. Maiti, A. K. Halder, T. Jha, Participated and presented a poster entitled "**Exploring structural prediction of Aurone derivatives and designing new potent antimalarials by validated QSAR modeling**" in International Conference on "**Recent Advances in Drug Discovery"** in University College of Pharmaceutical Sciences, Kakatiya University, Warangal, India on 22th-24th October, 2010.

B] National:

1. **N. Adhikari**, C. Mondal, A. K. Halder, T. Jha, Participated and presented a poster entitled "**Structural exploration of 2, 6, 9-trisubstituted purine derivatives as potent CDK2 inhibitors in cancer through validated molecular modeling studies"** in DST sponsored seminar and workshop in "**Recent Advances in Clinical Research With A Special Emphasis on BA/BE Study**" in Bioequivalence Study Centre, Jadavpur University, Kolkata, on 11th -15th September, 2014.
2. **N. Adhikari**, A. K. Halder, C. Mondal, T. Jha, Participated and presented a poster entitled "**Structural findings of quinolone carboxylic acids as HIV-1 integrase inhibitors through validated robust Chemometric modelling and docking study**" in the National Conference on "**New Trends in Bioinformatics**" at the Supercomputing Facility for Bioinformatics & Computational Biology in IIT Delhi on 30th-31th July, 2012.

Relevant Information:

1. Become the top 2% scientist of world based on the single year data of 2020 as per the August 2021 data-update for "Updated science-wide author databases of standardized citation indicators" by Stanford University.

(https://journals.plos.org/plosbiology/article?id=10.1371/journal.pbio.3000918)

2. Participated in the workshop and training in flow cytometry conducted by 5th annual meeting of the Cytometry Society India & 13th INDO-US cytometry workshop on advanced flow cltometry techniques in Centre of Research in Nanoscience & Nanotechnology, Kolkata, India.

3. Participated in the 6th INDO-US workshop on drug design conducted by Mathematical Chemistry, Kolkata (IUWMC-KOLKATA) on 8th – 10th January, 2010 at Heritage Institute of Technology, Kolkata, India.

Other information:

1. Authored one Bengali poetry book "Bayosandhi" comprising 42 poems published by one of the reputed publishing house "Patrolekha" in Kolkata in 2007.

2. Trained as a vocalist of "Vocal Classical" from "Pracheen Kala Kendra", Chandigarh, India.

I hereby declare that all of the abovementioned information is true and correct to the best of my knowledge and belief.

Signature

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