



UNIVERSITY OF CALCUTTA

FACULTY ACADEMIC PROFILE/ CV



1. **Full name of the faculty member:** Dr. Achintya Saha

2. **Designation:** Professor

3. **Specialization:** Pharmaceutical Technology

4. **Contact information:**

Department of Chemical Technology, University of Calcutta, 92, A.P.C. Road, Kolkata
700 009, India

Email: achintya_saha@yahoo.com

Mobile: +919433134636

5. **Academic qualifications:**

College/ university from which the degree was obtained	Abbreviation of the degree
Jadavpur University	B. Pharmacy
Jadavpur University	M. Pharmacy
Jadavpur University	Ph.D.

6. **Positions held/ holding:** Head of the Department (May'2015-April'2017)

7. **Research interests:**

- Computer aided drug design: 2D & 3D QSAR studies, Pharmacophore mapping, and Receptor based docking, dynamics and de novo design
- Ethno-pharmacology: Estrogenic/contraceptive activities, dual therapy for metabolic disorders from herbal resources

8. **Research guidance:**

Number of researchers awarded Ph.D degrees: 19
Number of researchers pursuing Ph.D: 08
Number of researchers awarded M. Tech. degrees: 16
Number of researchers awarded MD (Ayurvedic) degrees: 08

9. Projects (Last 10 years):

Completed projects:

- 1) DST SERB Scheme, “**Design and development of novel PPAR modulators for adjuvant therapy of metabolic syndrome**”, Financial Assistance (2013) as Principal Investigator for four years of Rs. 36.00 Lakhs.
- 2) University Potential of Excellence (UPE) II Scheme Research Project, “**Chemometric modeling on drug design and development of selective LRRK2 inhibitors for therapeutic application of Parkinson’s disease**”, Financial Assistance (2017) as Principal Investigator for five years of Rs. 15 Lakhs.
- 3) UGC DRS1 Program, “**Small Molecular Drug Discovery and Delivery Design Against Infectious Diseases**” – Financial Assistance (2017) as Coordinator for five years of Rs. 1.41 Cr.
- 4) DST SERB MATRICS Scheme, “**Understanding the unique structural dynamics of dengue viral proteins through large scale molecular simulations**” – Financial Assistance (2020) as Principal Investigator for three years of Rs. 6.60 Lakhs.

10. Select list of publications:

a) *Journals*: **180 (List attached 2019-2024)**

b) *Books/book chapters* : **10**

- Application of Computation in the Biosynthesis of Phytochemicals, **Achintya Saha**, Megha Jethwa, Aditi Gangopadhyay, Book Chapter In *Computational Phytochemistry*, 2nd Edn., ED: Lutfun Nahar and Satya D. Sarker, Elsevier, USA, **Chapter 10**, 321-347, 2024. ISBN: 9780443161032. <https://www.elsevier.com>
- Business Perspectives of Essential Oils from Herbs, Spices, and Oilseeds: Opportunities, Challenges and Applications, Gourab Chatterjee, Priyanka Saha, Asit Kumar Saha, Anjan Mishra, **Achintya Saha**, Book Chapter In *Business Trends, Transformations and Way Ahead*, Series II, ED: Arunangshu Giri, Wendrila Biswas, Sourabh Bhattacharya, Excel India Publishers, Ned Delhi, **Chapter 17**, 321-355, 2024. ISBN: 978-93-89947-77-9. <https://www.grouppexcelindia.com>
- “Nanoemulsion Delivery of Herbal Products: Prospects and Challenges”, Hemanga Hazarika, Harshita Krishnatreyya, Pronobesh Chattopadhyay, Achintya Saha, Yashwant V. Pathak, Md Kamaruz Zaman, Book Chapter In *Nano Medicine and Nano Safety: Recent Trends and Clinical Evidences*, Ed: Malay K. Das, Yashwant V. Pathak, Springer, Singapore, **Chapter 11**, 267-288, 2021. ISBN: 978-981-15-6254-9, <https://doi.org/10.1007/978-981-15-6255-6>, <https://link.springer.com>
- “QSAR and QAAR Studies on Mixtures of 3-(Benzylidene)indolin-2-one Isomers as Leads to Develop PET Radiotracers for Detection of Parkinson’s Disease: QSAR and QAAR Studies to Develop PET Radiotracers”, Sagar S. Bhayye, Achintya Saha, Book Chapter In *Research Anthology on Diagnosing and Treating Neurocognitive Disorders*, Ed: Mehdi Khosrow-Pour IGI Global, Hershey PA (USA), **Chapter 19**, 366-384, 2021. ISBN: 9781799834427, www.igi-global.com

- “Big Leaf Mahogany seeds: *Swietenia macrophylla* seeds offer possible phytotherapeutic intervention against diabetic pathophysiology”, Saikat Dewanjee, Paramita Paul, Tarun K. Dua, Shovonlal Bhowmick, Achintya Saha, Book Chapter In *Nuts and Seeds in Health and Disease Prevention*, Ed: Victor R Preedy, Ronald Ross Watson, Second Edition, Academic Press, Elsevier, USA, Section 6 Extracts from Nuts and Seeds in Health, **Chapter 38**, 543-565, 2020. ISBN: 978-0-12-818553-7. <https://www.elsevier.com>
- “Application of computation in the study of biosynthesis of phytochemicals”, Nilanjan Adhikari, Sk. Abdul Amin, Tarun Jha, Achintya Saha, Book Chapter In *Computational Phytochemistry*, ED: Satya D. Sarker and Lutfun Nahar, Elsevier, USA, **Chapter 9**, 255-276, 2018. ISBN: 978-0-12-812364-5. <https://www.elsevier.com>
- “Structural Insight into the Viral 3C-like Protease Inhibitors: Comparative SAR/QSAR Approaches”, Nilanjan Adhikari, Sandip Kumar Baidya, Achintya Saha, Nahid Ali, Tarun Jha, Book Chapter 11, In *Viral Proteases and Their Inhibitors*, 1st Edn., Ed: S. P. Gupta, Academic Press, USA, p. 317-409 , 2017. ISBN: 9780128097120, <https://www.elsevier.com>
- “Design and Development of Matrix Metalloproteinase Inhibitors Containing Zinc-Binding Groups, without Zinc-Binding Groups, and Mechanism-Based”, Nilanjan Adhikari, Sandip Kumar Baidya, Achintya Saha, Nahid Ali, Tarun Jha, Book Chapter In *Advances in Studies on Enzyme Inhibitors as Drugs*, Ed: S. P. Gupta, Nova Science Publishers, Inc., Hauppauge, NY, USA, **Vol. 2, Chapter 6**, p. 135-207, 2016. ISBN: 9781536105216, <https://www.novapublishers.com>
- “Design and Development of Some Selective Enzyme Inhibitors for Parkinson’s and Alzheimer’s Diseases Based on Molecular Modeling and Dynamics Studies”, Achintya Saha, Sagar S. Bhayye, Tabassum Hossain, Book Chapter In *Advances in Studies on Enzyme Inhibitors as Drugs*, Ed: S. P. Gupta, Nova Science Publishers Inc., Hauppauge, NY, USA, **Vol. 2, Chapter 3**, p. 51-89, 2016. ISBN: 9781536105216, <https://www.novapublishers.com>
- “Ligand and Structure Based Drug Design of Non-Steroidal Aromatase Inhibitors (NSAIs) in Breast Cancer”, Tarun Jha, Nilanjan Adhikari, Amit K. Halder, **Achintya Saha**, Book Chapter In *Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment*, IGI Global, Pennsylvania (USA), **Chapter 11**, 400-470, 2015. ISBN: 9781466681361, www.igi-global.com

c) **Conference/seminar volumes: 97 (List attached 2019-2024)**

11. **Membership of Learned Societies:**

1. The Asiatic Society
2. Fellow of Indian Chemical Society.
3. Fellow of Institute of Chemists.
4. Indian Society for Technical Education.
5. Indian Pharmaceutical Association.
6. Indian Pharmacy Graduates Association.
7. Indian Science Congress Association.
8. Indian Society of Pharmacognosy.
9. Indian Association for Cancer Research.
10. Indian Institute of Chemical Engineers.

11. Association of Pharmaceutical Teachers of India.
 12. Association of Chemistry Teachers in India.
 13. International Society for Computational Biology
 14. Senior Member of Asia-Pacific Chemical, Biological & Environmental Engineering Society (APCBEEES)
12. **Invited lectures delivered:**
- Fourth International Conference on “Advances in Bio-Informatics and Environmental Engineering – ICABEE 2016”, Rome, Italy, August, 2016.
 - International Conference on “Cheminformatics and Computational Chemical Biology” and “11th Asia Pacific Diabetes Conference and Expo”, Brisbane, Australia, July, 2016.
 - 23rd CCTCC, Conference on Current Trends in Computational Chemistry 2015, Interdisciplinary Centre for Nanotoxicity, Jackson State University, Jackson, Mississippi, USA, November, 2015.
 - Plenary Lecturer at International Conference on “Updates on Natural Products in Medicine and Healthcare Systems” Biotechnology & Genetic Engineering Discipline, Khulna University, Bangladesh, July, 2013.
13. **Awards:**
- DST Fast Track Young Scientist, 2006.
 - DST BOYSCAST Fellow, 2008.
 - SAARC Fellow, 2013, Dept. of Pharmaceutical Technology, Dhaka University.
14. **Other notable activities:**
- Participated **Seven Orientation/Refresher Courses**, organised by **Jadavpur University, IISc, Bangalore, IIT, Kharagpur and Nagpur College of Pharmacy, Nagpur.**
 - **Organised** 6 four weeks “**Orientation Courses**” for the College Teachers, conducted by UGC-Academic Staff College, University of Calcutta, on February’2001 (42nd Orientation Course), December’2002 (53rd Orientation Course), June’2005 (63rd Orientation Course), July’2006 (68th Orientation Course), July’2010 (85th Orientation Course) and January’2014 (103rd Orientation Course) as **Course Coordinator..**

List of Publication (2019-2024)

Research Articles:

1. A comprehensive review of ultraviolet radiation and functionally modified textile fabric with special emphasis on UV protection, Buddhadeb Saha, Achintya Saha, Parikshit Das, Ajay Kakati, Amartya Banerjee, Pronobesh Chattopadhyay, *Heliyon*, e40027 **10 (22)**, 2024. www.cell.com/heliyon (<https://doi.org/10.1016/j.heliyon.2024.e40027>)
2. Antimicrobial activity, Phytochemical screening by HPTLC, FTIR and GC-MS of the extracts of *Cissus quadrangularis* (L.), Shubham Paul, Sakshar Saha, Srijan Panigrahi, Dipanjan Sengupta, Sreya Das, Atanu Chatterjee, Ranabir Sahu, Gouranga Nandi, Achintya Saha, Aditi Gangopadhyay, Ritu Khanra, *Afr. J. Biomed. Res.*, 1203-1220, **27(1s)**, 2024. <https://africanjournalofbiomedicalresearch.com> (<https://doi.org/10.53555/AJBR.v27i1S.1212>)
3. Novel ACE inhibitory peptides from enzymatic hydrolysate of *Channa punctata* protein: In vitro and In silico assay of structure-activity relationship, Madhushrita Das, Aditi Gangopadhyay, Achintya Saha, Niloy Chatterjee, Pubali Dhar, *Food Bioscience*, (Published

- Online), **42**, 2024. <https://www.journals.elsevier.com> (IF: 4.8) (<https://doi.org/10.1016/j.fbio.2024.104765>)
4. Structure-guided screening of protein-protein interaction for the identification of Myc-Max heterodimer complex modulators, Shovonlal Bhowmick, Kunal Roy, Achintya Saha, *Journal of Biomolecular Structure & Dynamics*, (Published Online), **42**, 2024. <http://www.tandfonline.com> (IF: 5.235) (<https://doi.org/10.1080/07391102.2023.2294174>)
 5. Investigation of Bio-active Amaryllidaceae Alkaloidal Small Molecules as Putative SARS-CoV-2 Main Protease and Host TMPRSS2 Inhibitors: Interpretation by *in-silico* Simulation Study, Shovonlal Bhowmick, Tapan Kumar Mistri, Mohammad Rizwan Rizwan Khan, Pritee Chunarkar Patil, Rosa Busquets, Abu Md Ashif Iqbal, Ankita Chudhury, Dilip Kumar Roy, Partha Palit, Achintya Saha, *Journal of Biomolecular Structure & Dynamics*, (Published Online), **42**, 2024. <http://www.tandfonline.com> (IF: 5.235) (<https://doi.org/10.1080/07391102.2023.2238065>)
 6. Optimization and establishment of laboratory rearing conditions for *Cimex lectularius* L. against variable temperature and relative humidity, Amartya Banerjee, Achintya Saha, Parikshit Das, Ajay Kakati, Buddhadeb Saha, Danswring Goyary, Yangchen D. Bhutia, Sanjeev Karmakar, Sumit Kishor, Saidur Rahaman, Pronobesh Chattopadhyay, *Scientific Reports*, 9163-9171, **14**, 2024. www.nature.com/srep (IF: 4.60) (<https://doi.org/10.1038/s41598-024-59728-7>)
 7. Identification of potential therapeutic dual inhibitors of EGFR/HER2 in breast cancer, Megha Jethwa, Aditi Gangopadhyay, Achintya Saha, *European Journal of Medicinal Chemistry Reports*, 100143, **11**, 2024. (IF: 1.3) <https://www.sciencedirect.com/> (<https://doi.org/10.1016/j.ejmcr.2024.100143>)
 8. Raman Spectroscopic Insights of Phase Separated Insulin Aggregates, Sandip Dolui, Anupam Roy, Uttam Pal, Shubham Kundu, Esha Pandit, Bhisma N. Ratha, Ranit Pariary, Achintya Saha, Anirban Bhunia, Nakul Maiti, *ACS Physical Chemistry Au*, 268–280, **4 (3)**, 2024. (IF: 2.944) <https://pubs.acs.org> (<https://doi.org/10.1021/acspchemau.3c00065>)
 9. “Role of biomarkers and molecular signalling pathways in acute lung injury”, Pakter Niri, Achintya Saha, Subramanyam Polopalli, Mohit Kumar, Sanghita Das, Pronobesh Chattopadhyay, *Fundamental & Clinical Pharmacology*, 640–657, **38 (4)**, 2024. <https://onlinelibrary.wiley.com> (IF: 2.9) (<https://doi.org/10.1111/fcp.12987>)
 10. Identification of potential 3CLpro inhibitors-modulators for human norovirus infections through an advanced virtual screening approach, Shovonlal Bhowmick, Tapan Kumar Mistri, Mohammad K. Okla, Ibrahim A. Saleh, Achintya Saha, Pritee Chunarkar Patil, *Research Square*, (Preprint), 2023. <https://www.researchsquare.com> (<http://dx.doi.org/10.21203/rs.3.rs-3614758/v1>)
 11. Anti-Parkinson potential of Indian *Ocimum* species in relation to active components as revealed using metabolites profiling, *in vitro* and *in silico* enzyme inhibition studies, Sreerupa Sarkar, Jhelam Chatterjee, Aditi Gangopadhyay, Mohammed Sheashea, Mohamed A. Farag, Achintya Saha, Susmita Das, Bratati De, *Free Radicals and Antioxidants*, 74-85, **13 (2)**, 2023. <https://www.antiox.org> (IF: 0.5) (<https://doi.org/10.5530/fra.2023.2.13>)
 12. Rock Inhibitors as an Alternative Therapy for Corneal Grafting: A Systematic Review, Subramanyam Polopalli, Achintya Saha, Pakter Niri, Mohit Kumar, Parikshit Das, Dev Vrat Kamboj, Pronobesh Chattopadhyay, *Journal of Ocular Pharmacology and Therapeutics*, 585–599, **39(9)**, 2023. <https://www.liebertpub.com> (IF: 2.3) (doi: <https://doi.org/10.1089/jop.2023.0040>)
 13. Toxicological Evaluation of a Nonlethal Riot Control Combinational Formulation upon Dermal Application Using Animal Models, Sanghita Das, Achintya Saha, Amartya Banerjee, Danswring Goyary, Sanjeev Karmakar, Sanjal Kumar Dwivedi, Pronobesh Chattopadhyay,

- Cutaneous and Ocular Toxicology*, 118-130, **42 (3)**, 2023. <https://www.tandfonline.com> (IF: 1.974) (doi: <https://doi.org/10.1080/15569527.2023.2220393>)
14. Coomassie brilliant blue G-250 acts as a potential chemical chaperone to stabilize therapeutic insulin, Ranit Pariary, Sandip Dolui, Gourav Shome, Sk Abdul Mohid, Achintya Saha, Bhisma Ratha, Amaravadhi Harikishore, Kuladip Jana, Nakul Maiti, Anirban Bhunia, *ChemComm*, 8095–8098, **52**, 2023. <https://pubs.rsc.org> (IF: 6.065) (doi: <https://doi.org/10.1039/D3CC01791E>)
 15. Drug repurposing against the RNA-dependent RNA polymerase domain of dengue serotype 3 by virtual screening and molecular dynamics simulations, Aditi Gangopadhyay, Achintya Saha, *Journal of Biomolecular Structure & Dynamics*, 5152-5165, **41 (11)**, 2023. <http://www.tandfonline.com> (IF: 5.235) (doi: 10.1080/07391102.2022.2080764)
 16. Exploring potential non-steroidal aromatase inhibitors for therapeutic application against estrogen dependent breast cancer, Khushboo Pandey, Kiran Bharat Lokhande, Achintya Saha, Arvind Goja, K Venkateswara Swamy, Shuchi Nagar, *Current Computer-Aided Drug Design*, 243–257, **19 (4)**, 2023. <https://benthamscience.com> (IF: 1.639) (doi: 10.2174/1573409919666230112170025)
 17. Exploring Allosteric Hits of the NS2B-NS3 Protease of DENV2 by Structure-guided Screening, Aditi Gangopadhyay, Achintya Saha, *Computational Biology and Chemistry*, 107876, **104**, 2023. <https://www.journals.elsevier.com> (IF: 3.737) (doi: <https://doi.org/10.1016/j.compbiolchem.2023.107876>)
 18. 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, Ashik Chhetri, Moloy Roy, Puja Mishra, Amit Kumar Halder, Souvik Basak, Aditi Gangopadhyay, Achintya Saha, Plaban Bhattacharya, *Molecular Simulation*, 678–689, **49**, 2023. <https://www.tandfonline.com/> (IF: 2.178) (<https://doi.org/10.1080/08927022.2023.2185079>)
 19. Analytical method development for exploring pharmacokinetic profile of ursolic acid in rat tissues by high-performance thin-layer chromatography, Plaban Bhattacharya, Achintya Saha, Souvik Basak, *Journal of Planar Chromatography - Modern TLC*, 9–19, **36**, 2023. <http://www.akademai.com> (IF: 1.088) (<https://doi.org/10.1007/s00764-023-00228-1>)
 20. Search for potentially biased epidermal growth factor receptor (EGFR) inhibitors through pharmacophore modelling, molecular docking, and molecular dynamics (MD) simulation approaches, Megha Jethwa, Aditi Gangopadhyay, Achintya Saha, *Journal of Biomolecular Structure & Dynamics*, 1681–1689, **41 (5)**, 2023. <http://www.tandfonline.com> (doi: <https://doi.org/10.1080/07391102.2021.2023644>)
 21. Multi-target QSAR modeling for the identification of novel inhibitors against Alzheimer's disease, Vinay Kumar, Achintya Saha, Kunal Roy, *Chemometrics and Intelligent Laboratory Systems*, 104734, **233**, 2023. <https://www.journals.elsevier.com> (doi: <https://doi.org/10.1016/j.chemolab.2022.104734>)
 22. Fatty acid β -oxidation targeted metastatic growth inhibition in triple negative breast cancer exploiting biotin-functionalized copolymer, Bhuvan Ruidas, Neha Choudhury, Sutapa Som Choudhury, Tapas Kumar Sur, Sovonlal Bhowmick, Achintya Saha, Pritha Das, Priyadarsi De, Chitragada Das, *Authorea*, (Preprint), April 2022. (DOI: 10.22541/au.164922125.58119911/v1)
 23. Modelling and Molecular dynamics simulation of novel anticancer ligand for restructuring mutant P53 into wild type, Ashik Chhetri, Moloy Roy¹, Aditi Gangopadhyay, Achintya Saha, Puja Mishra, Amit Kumar Halder, Souvik Basak, *International Journal of Computational Biology and Drug Design*, 77–95, **15 (2)**, 2022. <https://www.inderscience.com> (doi: 10.1504/IJCBDD.2022.10051973)

24. Quercetin: A Silent Retarder of Fatty Acid Oxidation in Breast Cancer Metastasis Through Steering of Mitochondrial CPT1, Bhuban Ruidas, Tapas Kumar Sur, Chitrangada Das Mukhopadhyay, Koel Sinha, Sutapa Som Chaudhury, Pramita Sharma, Sovonlal Bhowmick, Achintya Saha, Rabindranath Majumder, *Breast Cancer*, 748–760, **29**, 2022. <https://www.springer.com> (<https://doi.org/10.1007/s12282-022-01356-y>)
25. Structure-based identification of Galectin-1 selective modulators in dietary food polyphenols – A pharmacoinformatics approach, Shovonlal Bhowmick, Achintya Saha, Sameh Mohamed Osman, Fatmah Ali Alasmay, Tahani Mazyad Almutairi, Md Ataul Islam, *Molecular Diversity*, 1697–1714, **25**, 2022. <http://www.springerlink.com> (doi: 10.1007/s11030-021-10297-1)
26. Carnosic acid attenuates doxorubicin-induced cardiotoxicity by decreasing oxidative stress and its concomitant pathological consequences, Prasenjit Manna, Saikat Dewanjee, Swarnalata Joardar, Pratik Chakraborty, Hiranmoy Bhattacharya, Shrestha Bhanja, Chiranjib Bhattacharyya, Manas Bhowmik, Shovonlal Bhowmick, Achintya Saha, Joydeep Das, Parames C. Sil, *Food and Chemical Toxicology*, (Published online, 113205), **166**, 2022. <https://www.journals.elsevier.com> (doi: <https://doi.org/10.1016/j.fct.2022.113205>)
27. Exploring CIP2A modulators using multiple molecular modeling approaches, Shovonlal Bhowmick, Kunal Roy, Achintya Saha, *Journal of Biomolecular Structure & Dynamics*, 1048–1063, **40 (3)**, 2022. <http://www.tandfonline.com> (doi: 10.1080/07391102.2020.1821781)
28. Identification of potent food constituents as SARS-CoV-2 papain-like protease modulators through advanced pharmacoinformatics approaches, Shovonlal Bhowmick, Achintya Saha, Nora Abdullah AlFaris, Jozaa Zaidan ALTamimi, Zeid A. ALOthman, Tahany Saleh Aldayel, Saikh Mohammad Wabaidur, Md Ataul Islam, *Journal of Molecular Graphics and Modelling*, 108113, **111**, 2022. <http://www.springerlink.com> (<https://doi.org/10.1016/j.jmgm.2021.108113>)
29. Assessment of toxicological consequences upon acute inhalation exposure to chemically improvised nonlethal riot control combinational formulation (NCF) containing oleoresin capsicum and skatole Sanghita Das, Achintya Saha, Pompy Patowary, Pakter Niri, Danswring Goyary, Sanjeev Karmakar, Pronobesh Chattopadhyay, *Toxicology Research*, 1129–1143, **10 (6)**, 2021. <https://academic.oup.com> DOI: 10.1093/toxres/tfab095
30. Dabrafenib, Idelalisib and Nintedanib Act as Significant Allosteric Modulator for Dengue NS3 Protease, R.V.Sriram Uday, Rajdip Misra, Annaram Harika, Sandip Dolui, Achintya Saha, Uttam Pal, V. Ravichandiran, Nakul c Maiti, *PLoS ONE*, e0257206, **16 (9)**, 2021. <https://plos.org> (doi: 10.1371/journal.pone.0257206)
31. Anti-Alzheimer's Potential of Different Varieties of Piper betle Leaves and Molecular Docking Analyses of Metabolites, Mamita Debnath, Susmita Das, Shovonlal Bhowmick, Swagata Karak, Achintya Saha, Bratati De, *Free Radicals and Antioxidants*, 13-18, **11 (1)**, 2021. <https://www.antiox.org> (DOI: <https://doi.org/10.5530/fra.2021.1.3>)
32. Insight into the Screening of Potential Beta-Lactamase Inhibitors as Anti-Bacterial Chemical Agents through Pharmacoinformatics Study, Pratap Parida, Shovonlal Bhowmick, Achintya Saha, Md. Ataul Islam, *Journal of Biomolecular Structure & Dynamics*, 923-942, **39 (3)**, 2021. <http://www.tandfonline.com> (doi: 10.1080/07391102.2020.1720819)
33. Structure-based identification of SARS-CoV-2 main protease inhibitors from anti-viral specific chemical libraries – An exhaustive computational screening approach, Shovonlal Bhowmick, Achintya Saha, Sameh Mohamed Osman, Fatmah Ali Alasmay, Tahani Mazyad Almutairi, Md Ataul Islam, *Molecular Diversity*, 1979-1997, **25 (3)**, 2021. <http://www.springerlink.com> (<https://doi.org/10.1007/s11030-021-10297-1>)
34. Myricitrin, a glycosyloxyflavone in Myrica esculenta bark ameliorates diabetic nephropathy via improving glycemic status, reducing oxidative stress, and suppressing inflammation, Tarun

- K. Dua, Swarnalata Joardar, Pratik Chakraborty, Shovonlal Bhowmick, Achintya Saha, Vincenzo De Feo, Saikat Dewanjee, *Molecules*, 258, **26**, 2021. <https://www.mdpi.com/journal/molecules> (doi: 10.3390/molecules26020258)
35. Mechanistic Studies of the Stabilization of Insulin Helical Structure by Coomassie Brilliant Blue, Sandip Dolui, Ranit Pariary, Achintya Saha, Bhisma N Ratha, Amaravadhi Harikishore, Susmita Saha, Snehasikta Swarnakar, Anirban Bhunia, Nakul C Maiti, **bioRxiv267799**, <https://doi.org/10.1101/2020.08.26.267799>
 36. *In silico* modeling for dual inhibition of acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) enzymes in Alzheimer's disease, Vinay Kumar, Achintya Saha, Kunal Roy, *Computational Biology and Chemistry*, 107355, **88**, 2020. <https://www.journals.elsevier.com> (doi: 10.1016/j.compbiolchem.2020.107355)
 37. Cheminformatic modelling of β -amyloid aggregation inhibitory activity against Alzheimer's disease, Vinay Kumar, Probir K Ojha, Achintya Saha, Kunal Roy, *Computers in Biology and Medicine*, 103658, **118**, 2020. <https://www.journals.elsevier.com> (doi: 10.1016/j.compbiomed.2020.103658)
 38. Pharmacognostical, phytochemical and pharmacological potentials of Cannabis sativa L., Sudipta Baroi, Achintya Saha, Ritesh Bachar, Sitesh C Bachar, *Asian Journal of Pharmacognosy*, 14-23, **4(2)**, 2020. <http://www.pharmacognosyasia.com>
 39. A Multi-layered Variable Selection Strategy for QSAR Modeling of Butyrylcholinesterase Inhibitors, Binoy Kumar, Priyanka De, Probir Ojha, Achintya Saha, Kunal Roy, *Current Topics in Medicinal Chemistry*, 1601-1627, **20 (18)**, 2020. <https://benthamscience.com/journals> (DOI: 10.2174/1568026620666200616142753)
 40. Chemometric modeling of structurally diverse carbamates for the inhibition of acetylcholinesterase enzyme (AChE) in Alzheimer's disease, Vinay Kumar, Achintya Saha, *International Journal of Quantitative Structure-Property Relationships*, 6-60, **5 (3)**, 2020. www.igi-global.com (DOI: 10.4018/IJQSPR.2020070102)
 41. Cannabinoid as Potential Aromatase Inhibitor Through Molecular Modeling and Screening for Anti-Cancer Activity, Sudipta Baroi, Achintya Saha, Ritesh Bachar, Sitesh C Bachar, *Dhaka Univ. J. Pharm. Sci.*, 47-58, **19 (1)**, 2020. <https://www.banglajol.info/index.php/JPharma> (DOI: <https://doi.org/10.3329/dujps.v19i1.47818>)
 42. Amelioration from the Ocular Irritant Capsaicin: Development and Assessment of a Capsazepine *in situ* Gel System for Ocular Delivery, Harshita Krishnatreyya, Hemanga Hazarika, Achintya Saha, Pronobesh Chattopadhyay, *Expert Opinion on Drug Delivery*, 863–880, **17 (6)**, 2020. <https://www.tandfonline.com/loi/iedd20> (doi: 10.1080/17425247.2020.1754396)
 43. Simultaneous pharmacokinetics estimation of Nateglinide and Pioglitazone by RP-HPLC: Computational study to unlock the synergism, Suddhasattya Dey, Souvik Basak, Anjan De, Shahreja Parvez Alam, Tabassum Hossain, Achintya Saha, Manik Ghosh, Tanushree Karmakar, *Journal of Chromatographic Science*, 309-322, **58 (4)**, 2020. <https://academic.oup.com/chromsci> (doi: 10.1093/chromsci/bmz116)
 44. Order, Disorder and Re-Order State of Lysozyme: Aggregation Mechanism by Raman Spectroscopy, Sandip Dolui, Animesh Mondal, Anupam Roy, Uttam Pal, Supriya Das, Achintya Saha, Nakul Maiti, *The Journal of Physical Chemistry Part B*, 50-60, **124 (1)**, 2020. <https://pubs.acs.org/journal/jpcbfb> (doi: 10.1021/acs.jpcb.9b09139)
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