UNIVERSITY OF CALCUTTA

FACULTY ACADEMIC PROFILE/ CV

1. **Full name of the faculty member**: Dr. AchintyaSaha
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, duel 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:	13
Number of researchers awarded MD (Ayurvedic) degrees:	08

9. **Projects (Last 10 years):**

Completed projects:

1) UGC Major Research Project, "**Molecular Modeling Studies on selective enzymes' inhibitors for therapeutic applications of mutagenic diseases**", Financial Assistance (2012) as Principal Investigator for three years of Rs. 10.06 Lakhs.

2) 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.

3) 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.

Current projects:

1) 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.
2) 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:*** **160 (List attached 2017-2022)**

b) ***Books/ book chapters :*** **08**

- "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 Inihibitors: 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 2017-2022)**

11. **Membership of Learned Societies**:
    1. Fellow of Indian Chemical Society.
    2. Fellow of Institute of Chemists.
    3. Indian Society for Technical Education.
    4. Indian Pharmaceutical Association.
    5. Indian Pharmacy Graduates Association.
    6. Indian Science Congress Association.
    7. Indian Society of Pharmacognosy.
    8. Indian Association for Cancer Research.
    9. Indian Institute of Chemical Engineers.
    10. Association of Pharmaceutical Teachers of India.
    11. Association of Chemistry Teachers in India.
    12. International Society for Computational Biology
    13. Senior Member of Asia-Pacific Chemical, Biological & Environmental Engineering Society (APCBEES)

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 (2017-2023)

Research Articles:

1. 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, Achintya Saha, Souvik Basak, *Molecular Simulation*, (Published online), **49**, 2023. https://www.tandfonline.com/ (IF: 2.178) (https://doi.org/10.1080/08927022.2023.2185079)
2. 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***, (Published online), **36**, 2023. http://www.akademiai.com (IF: 1.088) (https://doi.org/10.1007/s00764-023-00228-1)
3. 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*****,** (Published online), **18**, 2023. https://benthamscience.com (IF: 1.639) (doi: 10.2174/1573409919666230112170025)
4. 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***, (Published online), **44**, 2023. http://www.tandfonline.com (doi: 10.1080/07391102.2022.2080764)
5. 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)

6. 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)
7. Fatty acid β-oxidation targeted metastatic growth inhibition in triple negative breast cancer exploiting biotin-functionalized copolymer, Bhuban Ruidas, Neha Choudhury, Sutapa Som Chaudhury, Tapas Kumar Sur, Sovonlal Bhowmick, Achintya Saha, Pritha Das, Priyadarsi De, Chitrangada Das**,** ***Authorea,*** (Preprint), April 2022. (DOI: 10.22541/au.164922125.58119911/v1)
8. Modelling and Molecular dynamics simulation of novel anticancer ligand for restructuring mutant P53 into wild type, Ashik Chhetri, Moloy Roy\, Aditi Gangopadhyay, Achintya Saha, Puja Mishra, Amit Kumar Haldar, 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)
9. 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)
10. Structure-based identification of Galectin-1 selective modulators in dietary food polyphenols – A pharmacoinformatics approach, Shovonlal Bhowmick, Achintya Saha, Sameh Mohamed Osman, Fatmah Ali Alasmary, Tahani Mazyad Almutairi, Md Ataul Islam, ***Molecular Diversity***, 1697–1714, 25, 2022. http://www.springerlink.com (doi: 10.1007/s11030-021-10297-1)
11. 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)
12. 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)
13. 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)
14. 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, Danswrang Goyary, Sanjeev Karmakar, Pronobesh Chattopadhyay, ***Toxicology Research***, 1129–1143, **10 (6)**, 2021. https://academic.oup.com DOI: 10.1093/toxres/tfab095
15. 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)

16. 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)
17. 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)
18. 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 Alasmary, 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)
19. 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)
20. 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
21. *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)
22. 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)
23. 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
24. 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)
25. 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)
26. 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)
27. 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)

28. 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)
29. 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/jpcbfk (doi: 10.1021/acs.jpcb.9b09139)
30. Exploring QSAR, docking and pharmacophore mapping for prediction of Beta-secretase 1 (BACE1) inhibitory activity against Alzheimer's disease, Vinay Kumar, Probir Kumar Ojha, Achintya Saha, Kunal Roy, ***SAR and QSAR in Environmental Research***, 87–133, **31 (2)**, 2020. https://www.tandfonline.com (DOI: 10.1080/1062936X.2019.1695226)
31. Supramolecular assembly of amino acid based cationic polymer for efficient gene transfection efficiency in triple negative breast cancer, Rima Saha, Sagar Bhayye, Shuvam Ghosh, Achintya Saha, Kishor Sarkar, ***ACS Applied Bio Materials***, 5349-5365, **2 (12)**, 2019. https://pubs.acs.org/journal/aabmcb
32. Carnosic Acid Attenuates Cadmium Induced Nephrotoxicity by Inhibiting Oxidative Stress, Promoting Nrf2/HO-1 Signalling and Impairing TGF-B1/Smad/Collagen IV Signalling, Sonjit Das, SaikatDewanjee, Tarun K. Dua, SwarnalataJoardar, Pratik Chakraborty, Shovonlal Bhowmick, Achintya Saha, Simanta Bhattacharjee, Vincenzo De Feo, ***Molecules***, 4176, **24 (22)**, 2019. https://www.mdpi.com/journal/molecules
33. Synthesis, Anticancer Activity, SAR and Binding Mode of Interaction Studies of Substituted Pentanoic Acids, Sanchita Datta, Amit K Halder, Nilanjan Adhikari, Sk. Abdul Amin, Sanjib, Achintya Saha, Tarun Jha, ***Future Medicinal Chemistry***, 1679-1702, **11 (14)**, 2019. http://www.future-science.com/loi/fmc
34. Discovery of Nano-PiperolactamA: A Non-Steroidal Contraceptive Lead Acting Through Down-Regulation of Interleukins, Plaban Bhattacharya, Achintya Saha, Souvik Basak, ***Nanomedicine: Nanotechnology, Biology, and Medicine***, 347–358, **18**, 2019.. www.sciencedirect.com/journal/nanomedicine-nanotechnology-biology-and-medicine/
35. Rosmarinic Acid Attenuates Cadmium-Induced Nephrotoxicity via Inhibition of Oxidative Stress, Apoptosis, Inflammation, and Fibrosis, SwarnalataJoardar, SaikatDewanjee, Shovonlal Bhowmick, Tarun K. Dua, Sonjit Das, Achintya Saha, Vincenzo De Feo, ***International Journal of Molecular Sciences***, 2027, **20 (8)**, 2019. https://www.mdpi.com/journal/ijms/sections/bioactives
36. Fundamental Pharmacological Expressions on Ocular Exposure to Capsaicin, The Principal Constituent in Pepper Sprays, Harshita Krishnatreyya, Hemanga Hazarika,Achintya Saha, Pronobesh Chattopadhyay, ***Scientific Reports***, Article number: 12153, **8**, 2018. www.nature.com/srep
37. Synthesis of Novel Tricyclic Pyrazolo(1,4)oxathiinopyrazines and Evaluation of Their Competency towards the Inhibition of Lactate Dehydrogenase Activity, Prasun Mukherjee, Asish R. Das, Raghwendra Mishra, ShovonlalBhowmick, Achintya Saha, Asish R Das, ***Drug Research***, 653-660, **68 (11)**, 2018. https://www.thieme.com

38. Exploration of Structural and Physicochemical Properties of Small Molecules to Inhibit NMDA Functionality, Tabasum Hossain, Arup Mukherjee, Achintya Saha, ***Structural Chemistry***, 1175–1187, **29**, 2018. https://link.springer.com
39. Carnosic Acid, A Natural Diterpene, Attenuates Arsenic Induced Hepatotoxicity via Reducing Oxidative Stress, MAPK Activation, and Apoptotic Cell Death Pathway, Sonjit Das, Swarnalata Joardar, Prasenjit Manna, Tarun K. Dua, Niloy Bhattacharya, Ritu Khanra, Shovonlal Bhowmick, Jatin Kalita, Achintya Saha, Supratim Ray, Vincenzo De Feo, SaikatDewanjee, ***Oxidative Medicine and Cellular Longevity***, Article ID 1421438, **2018**, 2018. https://www.hindawi.com/
40. *In silico* modelling of azole derivatives with tyrosinase inhibition ability: Application of the models for activity prediction of new compounds, Biplab De, Indrani Adhikari, Ashis Nandy, Achintya Saha, BinoyBehari Goswami, ***Computational Biology and Chemistry***, 105–114, **74**, 2018. https://www.sciencedirect.com
41. Exploring Molecular Structural Requirement for AChE Inhibition Through Multi-Chemometric and Dynamics Simulation Analyses, Tabasum Hossain, Arup Mukherjee, Achintya Saha, ***Journal of Biomolecular Structure & Dynamics***, 1274-1285, **36 (5)**, 2018. http://www.tandfonline.com
42. Molecular Dynamics Simulation Study Reveals Polar Nature of Pathogenic Mutations Responsible For Stabilizing Active Conformation of Kinase Domain in Leucine Rich Repeat Kinase II, Sagar S. Bhayye, Achintya Saha, Kunal Roy, ***Structural Chemistry***, 657–666, **29 (3)**, 2018. https://link.springer.com
43. Structural Insight of Amyloidogenic Intermediates of Human Insulin, Sandip Dolui, Anupam Roy, Uttam Pal, Achintya Saha, Nakul C. Maiti, ***ACS Omega***, 2452–2462, 3, 2018. http://pubs.acs.org
44. Exploring *in house* Glutamate Inhibitors of Matrix Metalloproteinase-2 Through Validated Robust Chemico-biological Quantitative Approaches, Nilanjan Adhikari, Sk. Abdul Amin, Achintya Saha, Tarun Jha, ***Structural Chemistry***, 285–297, **29 (1)**, 2018. https://link.springer.com
45. A Comparative Study on Selective PPAR Modulators through Quantitative Structure-Activity Relationship, Pharmacophore and Docking Analyses, Ashis Nandi, Kunal Roy, Achintya Saha, ***Current Computer-Aided Drug Design***, 54–67, **14 (1)**, 2018. http://benthamscience.com
46. Multiple molecular modeling studies on some derivatives and analogs of glutamic acid as matrix metalloproteinase-2 inhibitors, Tarun Jha, Nilanjan Adhikari, Achintya Saha, Sk. Abdul Amin, ***SAR and QSAR in Environmental Research***, 43-68, **29 (1)**, 2018. http://www.tandfonline.com
47. Structural exploration for the refinement of anticancer matrix metalloproteinase-2 inhibitor designing approaches through robust validated multi-QSARs, Nilanjan Adhikari, Sk. Abdul Amin, Achintya Saha, Tarun Jha, ***Journal of Molecular Structure***, 501-515, **1156**, 2018. https://www.sciencedirect.com
48. Capsaicin, the Primary Constituent of Pepper Sprays and its Pharmacological Effects on Mammalian Ocular Tissues, Harshita Krishnatreyya, Achintya Saha, Pronobesh

Chattopadhyay, ***European Journal of Pharmacology***, 114-121, **819**, 2018. https:// sciencedirect.com

49. Understanding Chemico-Biological Interactions of Glutamate MMP-2 Inhibitors through Rigorous Alignment-Dependent 3D-QSAR Analyses, Nilanjan Adhikari, Sk. Abdul Amin, Achintya Saha, Tarun Jha, ***ChemistrySelect***, 7888–7898, **2 (26)**, 2017. http://onlinelibrary.wiley.com
50. Fabrication of β-Cyclodextrin-mediated Single Bimolecular Inclusion Complex: Characterization, Molecular Docking, *in-vitro* Release and Bioavailability Studies for Gefitinib and Simvastatin Conjugate, Souvik Basak, Sandip Mondal, Suddhasattya Dey, Plaban Bhattacharya, Achintya Saha, Vinay Deep Punetha, Ali Abbas, Nanda Gopal Sahoo, ***Journal of Pharmacy and Pharmacology***, 1304–1317, **69 (10)**, 2017. http://onlinelibrary.wiley.com
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