CURRICULUM VITAE OF SANDIPAN CHAKRABORTY

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4. Date of Birth : 13/04/1981

5. Gender (M/F/T) : M

6. Category Gen/SC/ST/OBC : Gen

7. Whether differently abled (Yes/No) : No

8. Academic Qualification (Undergraduate Onwards)

	Degree	**Year**	**Subject**	**University/Institution**
1.	B. Sc.	2003	Chemistry	University of Calcutta
2.	M. Sc.	2006	Bioinformatics	West Bengal University of Technology
3.	Ph. D.	2016	Biophysics and bioinformatics	University of Calcutta

9. Work experience (in chronological order)

S. No.	Positions held	Name of the Institute	From	To
1.	Research Assistant	Laboratory of Computational Biophysics & Bioengineering, Department of Physics, Tougaloo College, Mississippi, U.S.A	2011	2012
2.	Postdoctoral Fellow	Department of Physical Chemistry, Indian Associations for the Cultivation of Science, India	2015	2020
3.	Assistant Professor	Amity University, Kolkata	2020	2022
4.	Associate Principal Research Scientist	Dr. Reddys Institute of Life Sciences	2022	Present

10. Professional Recognition/ Award/ Prize/ Certificate, Fellowship received by the applicant.

S. No.	Name of the award	Awarding Agency	Year
1.	Silver Medal for 1st Class 2nd in M.Sc.	West Bengal University of Technology	2006
2.	Overseas research consultancy	Laboratory of Computational Biophysics & Bioengineering, Department of Physics, Tougaloo College, Mississippi	2014-2015
3.	Outstanding reviewer recognition	Molecular Biosystems (Royal Society of Chemistry)	2015-2016
4.	Outstanding reviewer recognition	Journal of Luminescence (Elsevier)	2016
5.	Outstanding reviewer recognition	Journal of Molecular Structure (Elsevier)	2018
6.	Associate Editorial Board Members	Mini-reviews in Medicinal Chemistry	2019-till date
7.	Academic Editor	PLOS ONE	2021-till date
7.	Postdoctoral Fellowship	Indian Associations for the Cultivation of Science, India	2016-2018
8.	Postdoctoral Fellowship	Indian Associations for the Cultivation of Science, India	2018-2020
9.	World's top 2% of Scientists List (Chemical Physics category)	Stanford university ranking	2022,2023

11. Publications (List of papers published in SCI Journals, in year wise descending order).
H-index: 24, Total citation: 1618; * indicate corresponding author

2024

1. Antiviral Flavonoids: A Natural Scaffold with Prospects as Phytomedicines against SARS-CoV2. Chiranjeet Saha, Roumi Naskar, **Sandipan Chakraborty.* Mini Reviews in Medicinal Chemistry** (2024) 24, 39-59. DOI: https://doi.org/10.2174/1389557523666230503105053 (**I.F. 3.8**)

2023

2. A multi-tier computational screening framework to effectively search the mutational space of SARS-CoV-2 receptor binding motif to identify mutants with enhanced ACE2 binding abilities. **Sandipan Chakraborty***, Chiranjeet Saha. **Molecular Informatics** (2023) 42, 2300055. DOI: https://doi.org/10.1002/minf.202300055 (**I.F. 3.6**)
3. Design, synthesis and evaluation of 2-aryl quinoline derivatives against 12R-lipoxygenase (12R-LOX): Discovery of first inhibitor of 12R-LOX. Harshavardhan Bhuktar, Sharda Shukla, Kumar Reddy Kakularam, Srikanth Battu, Manupati Srikanth, Susmita Srivastava, Raghavender Medishetti, Pooja Ram, PC Jagadish, Mahaboobkhan Rasool, **Sandipan Chakraborty**, Nooruddin Khan, Pallu Reddanna, Srinivas Oruganti, Manojit

Pal. **Bioorganic Chemistry** (2023) 138, 106606. DOI: https://doi.org/10.1016/j.bioorg.2023.106606 (**I.F. 5.1**)

4. Preferential ordering and organization of hydration water favor nucleation of ice by ice-nucleating proteins over antifreeze proteins. Rahul Aich, Prasun Pal, Sandipan Chakraborty*, Biman Jana*. **The Journal of Physical Chemistry B** (2023), 127, 6038–6048. DOI: https://doi.org/10.1021/acs.jpcb.3c01641 (**I.F. 3.466)**

2022

5. Number of Hydrogen Bonds per Unit Solvent Accessible Surface Area: A Descriptor of Functional States of Proteins. Prasun Pal, **Sandipan Chakraborty*** and Biman Jana*. **The Journal of Physical Chemistry B** (2022), 126, 10822–10833. DOI: https://doi.org/10.1021/acs.jpcb.2c05367 **(I.F. 3.466)**
6. Molecular Factors of Ice Growth Inhibition for Hyperactive and Globular Antifreeze Proteins: Insights from Molecular Dynamics Simulation. Prasun Pal, Rahul Aich, **Sandipan Chakraborty* and** Biman Jana*. **Langmuir** (2022), 38, 15132–15144. DOI: https://doi.org/10.1021/acs.langmuir.2c02149 **(I.F. 4.331)**
7. *In silico* investigation of the role of vitamins in cancer therapy through inhibition of MCM7 oncoprotein. Sunny Mukherjee, Sucharita Das, Navneeth Sriram, **Sandipan Chakraborty*** and Mahesh Kumar Sah*. **RSC Advance** (2022), 12**,** 31004-31015. DOI: 10.1039/D2RA03703C (**I.F. 4.036**)
8. Ultrafast Relaxation Dynamics of Conjugated Polymer Nanoparticles by Tuning Their Interchain Interactions. Srijon Ghosh, **Sandipan Chakraborty,** Arnab Ghosh, Kritiman Marjit, Goutam Ghosh and Amitava Patra*. **The Journal of Physical Chemistry C** (2022), 126, 18177–18187. DOI: https://doi.org/10.1021/acs.jpcc.2c06093 **(I.F. 4.177)**
9. Decoding the effects of spike receptor binding domain mutations on antibody escape abilities of omicron variants. **Sandipan Chakraborty*,** Aditi Saha, Chiranjeet Saha, Sanjana Ghosh and Trisha Mondal. **Biochemical and Biophysical Research Communications** (2022), 627,168-175. DOI: https://doi.org/10.1016/j.bbrc.2022.08.050 **(I.F. 3.322)**
10. Decoding Molecular Factors Shaping Human Angiotensin Converting Enzyme 2 Receptor Usage by Spike Glycoprotein in Lineage B Beta-coronaviruses. **Sandipan Chakraborty,*** Sanjana Ghosh and Trisha Mondal. **BBA - Molecular Basis of Disease,** (2022, 1868, 166514) DOI: https://doi.org/10.1016/j.bbadis.2022.166514 **(I.F. 6.633)**
11. Self-Assembled Nanomaterials of Naphthalene Monoimide in Aqueous Medium for Multimodal Detection of Picric Acid. Sucharita Dey, Ankita Saha, Prince Kumar, Chirantan Kar, **Sandipan Chakraborty*** and Pradip K Sukul*. **Journal of Photochemistry and Photobiology A: Chemistry,** (2022, 423, 113599), DOI: https://doi.org/10.1016/j.jphotochem.2021.113599 (**I.F. 5.141**)
12. Flavonoid: A Natural Scaffold with Modulatory Activities on Diverse Cellular Signaling Pathways Related to Complex Diseases. **Sandipan Chakraborty. Current Topics in Medicinal Chemistry** (2022, 22**,** 734-734) DOI: 10.2174/1568026622092205271415 34 **(I.F. 3.570)**
13. E484K and N501Y SARS-CoV 2 Spike Mutants Increase ACE2 Recognition but Reduce Affinity for Neutralizing Antibody. **Sandipan Chakraborty.* International Immunopharmacology,** (2022, 102, 108424) DOI: https://doi.org/10.1016/j.intimp.2021.108424 (**I.F. 5.714**)

2021

14. Molecular Insight into the Effect of a Single-Nucleotide Polymorphic Variation on the Structure and Dynamics of Methionine Synthase Reductase and Its Association with Neural Tube Defects. Susanta Sadhukhan[1], Subhajit Maity[1], **Sandipan Chakraborty[1]**, Silpita Paul, Dinesh Munian, Arup Kumar Pattanayak, Biman Jana* and Madhusudan Das*. **ACS Omega.** (2021, 6, 26372–26380) DOI: https://doi.org/10.1021/acsomega.1c03563 **(I.F. 4.132)** (1: Equal contribution)
15. Differential Hydration of Ice-Binding Surface of Globular and Hyperactive Antifreeze Proteins. Prasun Pal, **Sandipan Chakraborty*** and Biman Jana*. **Advanced Theory and Simulations.** (2021), 4, 2100090. DOI: https://doi.org/10.1002/adts.202100090 (**I.F. 4.105**)
16. Multi-target inhibition ability of neohesperidin dictates its neuroprotective activity: Implication in Alzheimer's disease therapeutics. **Sandipan Chakraborty***, Jyotirmoy Rakshit*, Jaya Bandyopadhyay* and Soumalee Basu*. **International Journal of Biological Macromolecules**. (2021), 176, 315-324. DOI: https://doi.org/10.1016/j.ijbiomac.2021.02.073 (**I.F. 8.025**)
17. Evolutionary and structural analysis elucidates mutations on SARS-CoV2 spike protein with altered human ACE2 binding affinity. **Sandipan Chakraborty***. **Biochemical and Biophysical Research Communications.** (2021), 538, 97-103. DOI: https://doi.org/10.1016/j.bbrc.2021.01.035 (**I.F. 3. 322**)
18. Combined Structure and Ligand-Based Design of Selective Acetylcholinesterase Inhibitors. Horacio Pérez-Sánchez, Helena den Haan, Alfonso Pérez-Garrido, Jorge Peña-García, **Sandipan Chakraborty**, Ilkay Erdogan Orhan, Fatma Sezer Senol Deniz, and José Manuel Villalgordo. **Journal of Chemical Information and Modeling**, (2020), 61, 467-480. DOI: https://doi.org/10.1021/acs.jcim.0c00463 (**I.F. 6.162**)

2020

19. Phylogenomics Analysis of SARS-CoV2 Genomes Reveals Distinct Selection Pressure on Different Viral Strains. Sanjana Ghosh and **Sandipan Chakraborty***. **BioMed Research International,** (2020), Article ID: 5746461. DOI: https://doi.org/10.1155/2020/5746461 (**I.F. 3.411**)
20. Scope of β-Secretase (BACE1)-Targeted Therapy in Alzheimer's Disease: Emphasizing the Flavonoid Based Natural Scaffold for BACE1 Inhibition. Sucharita Das, Swaha Sengupta and **Sandipan Chakraborty*. ACS Chemical Neuroscience,** (2020), 11, 3510-3522. DOI: 10.1021/acschemneuro.0c00579 (**I.F. 5.780**)
21. Structural insight into the effect of polymorphic variation on the functional dynamics of methionine synthase reductase: Implications in neural tube defects. Susanta Sadhukhan,[1] Subhajit Maity,[1] **Sandipan Chakraborty**,[1] Silpita Paul, Dinesh Munian, Arup Kumar Pattanayak, Biman Jana, Madhusudan Das. **Chemical Biology and Drug Design,** (2020), 97, 283-292. DOI: 10.1111/cbdd.13780. (**I.F. 2.873**).
22. Novel mechanism of Cholesterol transport by ABCA5 in Macrophages and its Role in Dyslipidemia. Aleepta Guha Ray, Kamalika Roy Choudhury, **Sandipan Chakraborty**, Devasmita Chakravarty, Vivek Chander, Biman Jana, Khawer N. Siddiqui and Arun Bandyopadhyay. **Journal of Molecular Biology**, (2020), 432, 4922-4941. DOI:10.1016/j.jmb.2020.07.006. (**I.F. 6.151**).
23. Deciphering the Role of the Non-ice-binding Surface in the Antifreeze Activity of Hyperactive Antifreeze Proteins. Prasun Pal, **Sandipan Chakraborty*** and Biman Jana*. **Journal of Physical Chemistry B**, (2020), 124, 4686–4696. DOI: 10.1021/acs.jpcb.0c01206 (**I.F. 3.466**).

24. Molecular insight into silk fibroin based delivery vehicle for amphiphilic drugs: Synthesis, characterization and molecular dynamics studies. Mercedes G. Montalbán, **Sandipan Chakraborty**, Jorge Peña-García, Hugo Verli, Gloria Villora, Horacio Pérez-Sánchez, F. Guillermo Díaz-Baños. **Journal of Molecular Liquids**, (2020), 299, 112156. DOI:10.1016/j.molliq.2019.112156 **(I.F 6.633)**
25. Ionophore constructed from non-covalent assembly of a G-quadruplex and liponucleoside transports K+-ion across biological membranes. Manish Debnath, **Sandipan Chakraborty**, Y Pavan Kumar, Ritapa Chaudhuri, Biman Jana and Jyotirmayee Dash. **Nature Communications,** (2020), 11, 469. DOI:10.1038/s41467-019-13834-7 (Selected as Editor's choice article in Therapeutics area) **(I.F 17.7)**

2019

26. Calcium ion implicitly modulates the adsorption ability of ion-dependent type II antifreeze proteins on an ice/water interface: A structural insight. **Sandipan Chakraborty** and Biman Jana. **Metallomics**, (2019), 11, 1387-1400. DOI:10.1039/C9MT00100J **(I.F 4.636)**
27. Structural Insight and Ultrafast Dynamics of 2D-Porphyrin Nanostructures. Rajesh Bera, **Sandipan Chakraborty**, Sandip Kumar Nayak, Biman Jana and Amitava Patra. **Journal of Physical Chemistry C**, (2019), 123, 15815-15826. DOI:10.1021/acs.jpcc.9b03112. **(I.F 4.177)**
28. Molecular dynamics study of PrP conversion. Lyudmyla Dorosh, Min Wu, **Sandipan Chakraborty**, Holger Wille and Maria Stepanova. **PRION**, (2019), 13 (Supply 1), 119-119. DOI:10.1080/2F19336896.2019.1615197. **(I.F: 2.547)**
29. Encapsulation of Triclosan within 2-Hydroxypropyl–β–Cyclodextrin cavity and its application in the chemisorption of Rhodamine B dye. Munisamy Maniyazagan, **Sandipan Chakraborty**, Horacio Pérez-Sánchez, Thambusamy Stalin. **Journal of Molecular Liquids**, (2019), 282, 235-243. DOI:10.1016/j.molliq.2019.02.113. **(I.F: 6.633)**
30. Antifreeze Proteins: An Unusual Tale of Structural Evolution, Hydration and Function. **Sandipan Chakraborty** and Biman Jana*. **Proceedings of the Indian National Science Academy,** (2019), 85, 169-187. DOI:10.16943/ptinsa/2018/49553.
31. Molecular structure of a hyperactive antifreeze protein adsorbed to ice. Konrad Meister, Carolyn Moll, **Sandipan Chakraborty**, Biman Jana, Arthur DeVries, Hans Ramløv, Huib Bakker. **Journal of Chemical Physics**, (2019), 150, 131101. DOI:10.1063/1.5090589 (JCP Editor's choice collection 2019, highlighted in international media). **(I.F 4.304)**
32. Hybrid approach to sieve out natural compounds against dual targets in Alzheimer's Disease. Sucharita Das, **Sandipan Chakraborty** and Soumalee Basu. **Scientific Reports**, (2019), 9, 1-15, Article no. 3714. DOI:10.1038/s41598-019-40271-9 **(I.F: 4.996)**
33. Targeted DNA oxidation and trajectory of radical DNA using DFT based QM/MM dynamics**.** Pradip Biswas and **Sandipan Chakraborty**. **Nucleic Acids Research**, (2019), 47, 2757-2765. DOI:10.1093/nar/gkz089 **(I.F: 19.160)**
34. Ordered hydration layer mediated ice adsorption of a globular antifreeze protein: Mechanistic insight. **Sandipan Chakraborty** and Biman Jana. **Physical Chemistry Chemical Physics**, (2019), 21, 19298-19310. DOI:10.1039/C9CP03135A **(I.F: 3.945)**

2018

35. Importance of the hydroxyl substituents in the B–ring of plant flavonols on their preferential binding interactions with VEGF G–quadruplex DNA: Multi-spectroscopic and molecular modeling studies. Snehasish Bhattacharjee, **Sandipan Chakroborty**, Erik Chorell, Pradeep K. Sengupta and Sudipta Bhowmik. **International Journal of Biological Macromolecule**, (2018), 118, 629-639. DOI:10.1016/j.ijbiomac.2018.06.115. **(I.F 8.025)**
36. Molecular insight into the inclusion of the dietary plant flavonol fisetin and its chromophore within a chemically modified γ-cyclodextrin: Multi-spectroscopic, molecular docking and solubility studies. Biswapathik Pahari[$], **Sandipan Chakraborty[$]**, Pradeep K. Sengupta. **Food Chemistry**, (2018), 260, 221-230. DOI:10.1016/j.foodchem.2018.03.128. **($: Equal contribution**) **(I.F: 9.231)**
37. Multi-functional neuroprotective activity of neohesperidin dihydrochalcone: a novel scaffold for Alzheimer's disease therapeutics identified via drug repurposing screening. **Sandipan Chakraborty***, Jyotirmoy Rakshit, Jaya Bandyopadhyay* and Soumalee Basu*. **New Journal of Chemistry**, (2018), 42, 11755-11769. DOI:10.1039/C8NJ00853A **(I.F 3.925)**
38. Optimum number of anchored clathrate water and its instantaneous fluctuations dictate ice plane recognition specificities of insect antifreeze protein. **Sandipan Chakraborty**, Biman Jana. **The Journal of Physical Chemistry B**, (2018), 122, 3056-3067. DOI: 10.1021/acs.jpcb.8b00548. **(I.F 3.466)**

2017

39. Chiral Alkylated-Aniline as a Noninvasive Fluorescence Sensor: Spectroscopic and molecular modeling studies. Bidisha Sengupta, Chirantan Sen Mukherjee, **Sandipan Chakraborty**, Maria Jones Muhammad, Willium Gladney Jr, George Armstrong. **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, (2017), 187, 23-29. DOI:10.1016/j.saa.2017.06.008. **(I.F 4.831)**
40. Multi-functional activities of citrus flavonoid narirutin in Alzheimer's disease therapeutics: An integrated screening approach and in vitro validation. **Sandipan Chakraborty***, Soumalee Basu.* **International Journal of Biological Macromolecules**, (2017), 103, 733-743. DOI:10.1016/j.ijbiomac.2017.05.110. **(I.F 8.025)**
41. Exciton dynamics and formation mechanism of MEH-PPV polymer-based Nanostructures. Arnab Ghosh, Bikash Jana, **Sandipan Chakraborty**, Sourav Maiti, Biman Jana, Hirendra N. Ghosh and Amitava Patra. **The Journal of Physical Chemistry C**, (2017), 121, 21062-21072. DOI:10.1021/acs.jpcc.7b08336. **(I.F: 4.177)**
42. The human VGF-derived bioactive peptide TLQP-21 binds heat shock 71 kDa protein 8 (HSPA8) on the surface of SH-SY5Y cells. Shamim Akhter, **Sandipan Chakraborty**, Daniela Moutinho, Elia Álvarez-Coiradas, Isaac Rosa, Juan Viñuela, Eduardo Domínguez, Angel García and Jesús R. Requena. **PLOS ONE**, (2017), 12, e0185176. DOI:10.1371/journal.pone.0185176. **(I.F 3.752)**
43. Lycopene prevents mitochondrial dysfunction during D-galactosamine/lipopolysaccharide-induced fulminant hepatic failure in albino rats. Sheik

Abdulazeez Sheriff, Shaikhussain Shaik Ibrahim, Thiruvengadam Devaki, **Sandipan Chakraborty**, Subhash Agarwal and Horacio Pérez-Sánchez. **Journal of Proteome Research**, (2017), 16, 3190-3199. DOI:10.1021/acs.jproteome.7b00176. **(I.F 5.370)**

44. Molecular insight into the adsorption of Spruce Budworm antifreeze protein to an ice surface: A clathrate-mediated recognition mechanism. **Sandipan Chakraborty** and Biman Jana. **Langmuir**, (2017), 33, 7202-7214. DOI:10.1021/acs.langmuir.7b01733. **(I.F 4.331)**
45. Modulation of the conformational dynamics of Apo-Adenylate kinase through a π-cation interaction. Ritaban Halder, Rabindra Nath Manna, **Sandipan Chakraborty** and Biman Jana; **The Journal of Physical Chemistry B**, (2017), 121, 5699-5708. DOI:10.1021/acs.jpcb.7b01736. **(I.F 3.466)**
46. Environment sensitive fluorescent analogue of biologically active oxazoles differentially recognizes human serum albumin and bovine serum albumin: photophysical and molecular modeling studies. Jyotirmay Maiti, Suman Biswas, Ankur Chaudhuri, **Sandipan Chakraborty**, Sibani Chakraborty and Ranjan Das. **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy**, (2017), 175, 191-199. DOI:10.1016/j.saa.2016.12.032. **(I.F 4.831)**
47. Dual inhibition of BACE1 and Aβ aggregation by β-ecdysone: Application of a Phytoecdysteroid scaffold in Alzheimer's disease therapeutics. **Sandipan Chakraborty* and** Soumalee Basu*. **International Journal of Biological Macromolecules**, (2017), 95, 281-287. DOI:10.1016/j.ijbiomac.2016.11.061.
(I.F 8.025)
48. Multi-potent Natural Scaffolds Targeting Amyloid Cascade: In Search of Alzheimer's disease Therapeutics. **Sandipan Chakraborty.* Current Topics in Medicinal Chemistry**, (2017, 17, 3336-3348), DOI:10.2174/1568026618666180116122921. **(I.F 3.570)**
49. A sensitive fluorescent probe for the polar solvation dynamics at protein-surfactant interfaces. Priya Singh, Susobhan Choudhury, Subhankar Singha, Yonwoong Jun, **Sandipan Chakraborty,** Jhimli Sengupta, Ranjan Das, Kyo-Han Ahn, Samir Kumar Pal. **Physical Chemistry Chemical Physics**, (2017, 19, 12237-12245), DOI:10.1039/C6CP08804J. **(I.F 3.945)**
50. Conformational and hydration properties modulate ice recognition ability of type I antifreeze protein and its mutants. **Sandipan Chakraborty and** Biman Jana**. Physical Chemistry Chemical Physics**, (2017, 19, 11678-11689), DOI:10.1039/C7CP00221A. (**Highlighted in New Frontiers in Indian Research-themed collection published by RSC**) **(I.F 3.945)**
51. Hepatoprotective activity of chrysin is mediated through TNF-α in chemically-induced acute liver damage: An in vivo study and molecular modeling. Anca Hermenean, Teodora Mariasiu, Inmaculada Navarro-González, Josefina Vegara-Meseguer, Eftimie Miuțescu, **Sandipan Chakraborty** and Horacio Pérez-Sánchez. **Experimental and Therapeutic Medicine**, (2017, 13, 1671-1680), DOI: 10.3892/etm.2017.4181. **(I.F 2.751)**
52. Critical insight into the interaction of naringenin with human haemoglobin: A combined spectroscopic and computational modeling approaches. Subhajit Maity, **Sandipan Chakraborty and** Abhay Sankar Chakraborti. **Journal of Molecular Structure**, (2017, 1129, 256-262), DOI:10.1016/j.molstruc.2016.09.085. **(I.F 3.841)**

2016

53. Multi-target screening mines hesperidin as a multi-potent inhibitor: Implication in Alzheimer's disease therapeutics. **Sandipan Chakraborty***, Jaya Bandyopadhyay, Sourav Chakraborty, and Soumalee Basu*. **European Journal of Medicinal Chemistry**, (2016, 121, 810-822), DOI:10.1016/j.ejmech.2016.03.057. **(I.F 7.088)**
54. Designer interface peptide grafts target estrogen receptor alpha dimerization. **Sandipan Chakraborty**, B.K. Asare, Pradip K. Biswas and R.V. Rajnarayanan. **Biochemical and Biophysical Research Communications**, (2016, 478, 116-122), DOI:10.1016/j.bbrc.2016.07.083. **(I.F 3.322)**
55. Exploring the interactions of the dietary plant flavonoids Fisetin and Naringenin with G-Quadruplex and duplex DNA, showing contrasting binding behavior: Spectroscopic and molecular modeling approaches. Snehasish Bhattacharjee, **Sandipan Chakraborty**, Pradeep K. Sengupta, Sudipta Bhowmik. **Journal of Physical Chemistry B**, (2016, 120, 8942-8952), DOI:10.1021/acs.jpcb.6b06357. **(I.F 3.466)**
56. Oral delivery of quercetin to diabetic animals using novel pH responsive carboxypropionylated chitosan/alginate microparticles. Piyasi Mukhopadhyay, Subhajit Maity, **Sandipan Chakraborty**, Ruchira Rudra, Hiral Ghodadara, Manisha Solanki, Abhay Sankar Chakraborti, A. K. Prajapati and P. P. Kundu. **RSC advances**, (2016, 6, 73210-73221), DOI:10.1039/C6RA12491G. **(I.F 4.036)**
57. Molecular recognition of aromatic carboxylic acids by hydroxypropyl-γ-cyclodextrin: experimental and theoretical evidence. Irina Terekhova, Roman Kumeev, Gennady Alper, **Sandipan Chakraborty**, Horacio Pérez-Sánchez, Estrella Núñez-Delicado. **RSC advances**, (2016), 6, 49567-49577. DOI:10.1039/C6RA06340C. **(I.F 4.036)**
58. Molecular insight into the differential anti-androgenic activity of resveratrol and its natural analogs: *in silico* approach to understand biological actions. **Sandipan Chakraborty**, Avinash Kumar, Nasir A. Butt, Liangfen Zhang, Raquema Williams, Agnes M. Rimando, Pradip K. Biswas, and Anait S. Levenson. **Molecular BioSystems**, (2016), 12, 1702-1709. DOI:10.1039/C6MB00186F. **(I.F: 3.743, citation: 15)**

2015

59. Probing the conformational dynamics of the bioactive peptide TLQP-21 in solution: A Molecular Dynamics study. **Sandipan Chakraborty***, Shamim Akhter, Jesús R. Requena and Soumalee Basu. **Chemical Biology & Drug Design**, (2015), 86, 938-944. DOI:10.1111/cbdd.12541. **(I.F 2.873)**
60. Structural insight into the mechanism of amyloid precursor protein recognition by β-secretase 1: A molecular dynamics study. **Sandipan Chakraborty*** and Soumalee Basu*. **Biophysical Chemistry**, (2015), 202, 1-12. DOI:10.1016/j.bpc.2015.03.006. **(I.F 3.628)**
61. Photophysical study of a charge transfer oxazole dye in micelles: Role of surfactant headgroups. Jyotirmay Maiti, Yeasmin Sarkar, Partha Pratim Parui, **Sandipan Chakraborty**, Suman Biswas and Ranjan Das. **Journal of Luminescence**, (2015), 163, 21–27. DOI:10.1016/j.jlumin.2015.02.054. **(I.F 4.171)**
62. Fragment-based designing for the generation of novel leads against BACE1. Sucharita Das, **Sandipan Chakraborty**, Soumalee Basu. **Central Nervous System Agents in Medicinal Chemistry (Formerly Current Medicinal Chemistry-Central Nervous System Agents).** (2015), 15, 52-64. DOI: 10.2174/1871524915666150127122546.
63. Ground and excited state proton transfer of the bioactive plant flavonol Robinetin in a protein environment: Spectroscopic and molecular modeling studies. Biswa Pathik Pahari,

Sudip Chaudhuri, **Sandipan Chakraborty** and Pradeep K. Sengupta. **Journal of Physical Chemistry B**, (2015), 119, 2533-2545 DOI:10.1021/jp508410v. **(I.F 3.466)**

2014

64. Insight into the anti-amyloidogenic activity of polyphenols and its application in virtual screening of phytochemical database. **Sandipan Chakraborty*** and Soumalee Basu*. **Medicinal Chemistry Research**, (2014), 23, 5141-5148. DOI:10.1007/s00044-014-1081-2. (**I.F 2.351**)
65. Mechanistic insight into the radical scavenging activity of polyphenols and its application in virtual screening of phytochemical library: an in silico approach. **Sandipan Chakraborty*** and Soumalee Basu*. **European Food Research and Technology**, (2014), 239, 885-893. DOI:10.1007/s00217-014-2285-x. **(I.F 3.498)**
66. Structural insights into selective agonist actions of tamoxifen on human estrogen receptor alpha. **Sandipan Chakraborty and** Pradip K. Biswas. **Journal of Molecular Modeling**, (2014), 20, 1-12 Article no. 2338. DOI:10.1007/s00894-014-2338-x. **(I.F 2.172)**
67. Effect of β-cyclodextrin on the molecular properties of myricetin upon nano-encapsulation: Insight from optical spectroscopy and quantum chemical studies. **Sandipan Chakraborty**, Soumalee Basu and Soumen Basak. **Carbohydrate Polymers**, (2014), 99, 116-125. DOI:10.1016/j.carbpol.2013.08.008. **(I.F 10.723)**
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72. Pinpointing Proline substitution to be responsible for the loss of amyloidogenesis in IAPP. **Sandipan Chakraborty*,** Barnali Mukherjee and Soumalee Basu*****. **Chemical Biology and Drug Design**, (2013), 82, 446-452. DOI:10.1111/cbdd.12172. **(I.F 2.873)**

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75. Characterization of diadzein–hemoglobin binding using optical spectroscopy and molecular dynamics simulations. Bidisha Sengupta, **Sandipan Chakraborty**, Maurice Crawford, Jasmine M. Taylor, Laura E. Blackmon, Pradip K. Biswas and Wolfgang H. Kramer. **International Journal of Biological Macromolecules**, (2012), 51, 250–258. DOI:10.1016/j.ijbiomac.2012.05.013. **(I.F 8.025)**
76. Elucidation of the mechanistic pathways of the hydroxyl radical scavenging reaction by Daidzein using hybrid QM/MM dynamics. **Sandipan Chakraborty** and P. K. Biswas. **Journal of Physical Chemistry A**, (2012), 116, 8775-8785. DOI:10.1021/jp303543z. **(I.F 2.944)**
77. In silico design of peptidic inhibitors targeting estrogen receptor alpha dimer interface. **Sandipan Chakraborty**, Shawn Cole, Nicholas Rader, Candace King, R. Rajnarayanan and P. K. Biswas. **Molecular Diversity**, (2012), 16, 441–451. DOI:10.1007/s11030-012-9378-x. **(I.F 3.364)**
78. Insight into estrogen receptor beta–beta and alpha–beta homo- and heterodimerization: A combined molecular dynamics and sequence analysis study. **Sandipan Chakraborty**, Hadassah Willett and P.K. Biswas. **Biophysical Chemistry**, (2012), 170, 42-50. DOI:10.1016/j.bpc.2012.09.002. **(I.F 3.628)**
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80. A critical study on the interactions of hesperitin with human hemoglobin: Fluorescence spectroscopic and molecular modeling approach. **Sandipan Chakrabarty,** Sudip Chaudhuri, Biswapathik Pahari, Jasmine Taylor, Pradeep K. Sengupta and Bidisha Sengupta. **Journal of Luminescence**, (2012), 132, 1522–1528. DOI:10.1016/j.jlumin.2012.01.021. **(I.F 4.171)**
81. Mechanistic Insight into the Structure and Dynamics of Entangled and Hydrated λ-Phage DNA. **Sandipan Chakraborty**, Takashi Uematsu, Christer Svanberg, Per Jacobsson, Jan Swenson, Michael Zäch, Rajendar Trehan, George Armstrong and Bidisha Sengupta. **Journal of Physical Chemistry A**, (2012), 116, 4274-4284. DOI:10.1021/jp2108363. **(I.F 2.944)**
82. Binding and antioxidant properties of therapeutically important plant flavonoids in biomembranes: Insights from spectroscopic and quantum chemical studies. Biswapathik Pahari^, **Sandipan Chakraborty**^, Sudip Chaudhuri, Bidisha Sengupta and Pradeep K. Sengupta. **Chemistry and Physics of Lipids**, (2012), 165, 488-496. DOI:10.1016/j.chemphyslip.2011.10.006. (^Equal contribution). **(I.F 3.57)**

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83. Encapsulation of 3-hydroxyflavone in γ-cyclodextrin nanocavities: Excited state proton transfer fluorescence and molecular docking studies. Biswapathik Pahari, **Sandipan Chakraborty** and Pradeep K. Sengupta. **Journal of Molecular Structure**, (2011), 1006, 483–488. DOI:10.1016/j.molstruc.2011.09.055. **(I.F 3.841)**
84. Conformational transition in the substrate binding domain of β-secretase exploited by NMA and its implication in inhibitor recognition: BACE1–myricetin a case study. **Sandipan Chakraborty**, Sanjay Kumar and Soumalee Basu. N**eurochemistry International**, (2011), 58, 914–923. DOI:10.1016/j.neuint.2011.02.021. **(I.F 4.297)**
85. Probing the interactions of hemoglobin with antioxidant flavonoids via fluorescence spectroscopy and molecular modeling studies. Sudip Chaudhuri, **Sandipan Chakraborty** and Pradeep K. Sengupta. **Biophysical Chemistry**, (2011), 154, 26-34. DOI:10.1016/j.bpc.2010.12.003. **(I.F 3.628)**

2010

86. Inclusion of chrysin in β-cyclodextrin nanocavity and its effect on antioxidant potential of chrysin: A spectroscopic and molecular modeling approach. **Sandipan Chakraborty,** Soumalee Basu, Ansuman Lahiri and Soumen Basak. **Journal of Molecular Structure**, (2010), 977, 180-188. DOI:10.1016/j.molstruc.2010.05.030. **(I.F 3.841)**
87. Encapsulation of serotonin in β-cyclodextrin nano-cavities: Fluorescence spectroscopic and molecular modeling studies. Sudip Chaudhuri, **Sandipan Chakraborty** and Pradeep K. Sengupta. **Journal of Molecular Structure**, (2010), 975, 160-165. DOI:10.1016/j.molstruc.2010.04.014. **(I.F 3.841)**

<u>Book chapters:</u>

1. Translating the knowledge of functional dynamics toward designing inhibitors of BACE1, a key Aspartate protease in Alzheimer's disease. **Sandipan Chakraborty**, Soumalee Basu. **Book title: Protease in human disease**. ISBN: 978-981-10-3161-8, (2017), 171-193, DOI: 10.1007/978-981-10-3162-5_9.
2. Proteases—The Sharp Scissors in Human Diseases. **Sandipan Chakraborty**, Soumalee Basu. **Book title: Pathophysiological aspects of proteases**. ISBN: 978-981-10-6140-0, (2017), 635-645, DOI: https://doi.org/10.1007/978-981-10-6141-7_27.
3. Encapsulation of pharmaceutically active dietary polyphenols in cyclodextrin-based nanovehicles: Insights from spectroscopic studies. Pradeep K Sengupta, Snehasish Bhattacharya, **Sandipan Chakraborty**, Sudipta Bhowmik. **Book title: Design of nanostructures for versatile therapeutic applications for Pharmaceutical Nanotechnology**. ISBN: 978-0-12-813667-6 (2018) 623-645, DOI:10.1016/B978-0-12-813667-6.00015-2.

<u>12. Conference presentations:</u>

1. "Encapsulation of serotonin in beta-cyclodextrin nano cavity: Spectroscopic and theoretical studies" in **International Conference on Soft System 2008**. Sudip Choudhury, **Sandipan Chakraborty**, Biswapathik Pahari, Pradeep K. Sengupta
2. "Encapsulation of 7-HF in beta-cyclodextrin nano cavity: Spectroscopic and theoretical studies" in **national symposium organized by Indian Photobiologyl Society**, 09th Aug, 2008. Koushik Basu, **Sandipan Chakraborty**, Biswapathik Pahari, Pradeep K. Sengupta.

3. "Encapsulation of chrysin into β-cyclodextrin nanocavity enhances its antioxidant potential: A spectroscopic and ab initio molecular modelling study" In **International Conference on Physics Biology Interface**, December 13-16, 2009. **Sandipan Chakraborty**, Ansuman Lahiri, Soumen Basak, Soumalee Basu
4. "Hybrid molecular dynamics study of DNA damage pathways arising from hydrogen abstractions by OH radicals" **Current trend in computational Chemistry (CCTCC)** 2012, Jackson, Mississippi, USA, 2012. Pradip K. Biswas and **Sandipan Chakraborty**.
5. "Ligand selective conformational changes of Estrogen Receptor alpha homo-dimer: A new insight into agonist action of tamoxifen" in **Institutional Development Award (IDEA 2012) in Washington DC, USA. Sandipan Chakraborty** and P. K. Biswas
6. "The role of Resveratrol in prevention and therapy of hormone-dependent cancers: in silico studies" in **Mississippi Academy of Science, 30th Southern Biomedical Engineering Conference 2014,** Gulfport, MS, April 10-13, 2014. Chakraborty S, Zhang L, Lin SY, Rimando AM, Biswas PK and Levenson AS.
7. "Conformational Dynamics of BACE1 and Its Application in Inhibitor Screening" **DBT-CU IPLS conference**, 10-12 January, 2014. **Sandipan Chakraborty**, Soumalee Basu. (Oral presentation).
8. "Effect of structure and hydration on the Ice recognition Mechanism of Antifreeze Protein: A Clathrate Mediated Ice Adsorption. 15th **Indian Theoretical Chemistry Symposium, Hyderabad**, (DEC 14-16) 2016. **Sandipan Chakraborty**, Biman Jana,

13. Seminar/workshop:

1. QIP short term courses on "Approaches to the Screening of Bioactive Molecules from Natural Resources", 13-17th July 2009, Indian Institute of Technology, Guwahati, India.
2. Participation in the webinar on "Renin Angiotensin System– SARS-CoV2 Drug Repurposing and Discovery Opportunities. 29 April, 2020, organized by Amity Institute of Indian System of Medicine, Health & Allied Sciences Domain, Amity University Uttar Pradesh, Noida (INDIA).
3. Participation in the webinar on the topic "How to write a good Research Grant Proposal and Research Project Management" organized by Amity Science, Technology & Innovation Foundation (ASTIF) on August 06, 2020.
4. Participation in the webinar on Green Computing organized by Department of Computer Science and Engineering, Amity School of Engineering and Technology, Amity University, Uttar Pradesh, Noida on 15th May 2020.
5. Participation in the webinar Lecture Series on the topic of "Why Antimicrobial Stewardship", held on 16 June, 2020, organized by Amity International Society for Natural Products, Health & Allied Sciences Domain, Amity University Uttar Pradesh, Noida (INDIA).
6. Participation in the webinar Lecture Series on the topic of "Phytochemistry by design" delivered, held on 19 August, 2020, organized by Amity International Society for Natural Products, Health & Allied Sciences Domain, Amity University Uttar Pradesh, Noida (INDIA).
7. Participation in the Bilateral Indo-US Webinar on COVID Biology, dated August 16-19, 2020 organized by Indian Institute of Science education and Research Kolkata, India in collaboration with IISc, Bangalore, India, University of Pennsylvania, and the University of Colorado, School of Medicine, USA.

8. Participated in five days Faculty development program on "Teaching, Research and Innovation in India: A Biologist's view during 4th -8th July, 2020 organised by Amity Institute of Biotechnology, Amity University Kolkata.

14. Sanctioned projects:

1. Name of the awarding body: **Microsoft Inc. (AI for health)**
   Title of project: Probing the evolution of SARS-CoV2 spike protein during disease outbreak and its impact on human ACE2 recognition (grant - ID:00011000243)
   Amounts awarded: Computational resource usage of 35000 USD
   Start and end dates: 11.07.2020-31.07.2021

2. Name of the awarding body: **Microsoft Inc. (AI for health)**
   Title of project: Identification of therapeutics targeting novel druggable allosteric sites of SARS-CoV-2 Polymerase-Exonuclease multi-protein complex using drug repurposing (grant - ID: AI4H-001288-X7Q6P1-2021022407)
   Amounts awarded: Computational resource usage of 75000 USD
   Start and end dates: 2021-2024

3. Name of the awarding body: **COVID-19 HPC Consortium**
   Title of project: Predicting future SARS-CoV2 spike RBD variants with pandemic potential (grant - ID: CHE210070)
   Amounts awarded: Computational resource usage of 140000 USD
   Start and end dates: 2021-2022

4. Name of the awarding body: **Science and Engineering Research Board (SERB) Core Research Grant**
   Title of project: Molecular Insights into Ligand-selective and Cholesterol-specific Activation of the GPCR Serotonin1A Receptor with GPU-enabled High-performance Computing (grant - ID: CRG/2021/003804)
   Co-PI: Prof. Amitabha Chattopadhyay, CSIR-Centre for Cellular & Molecular Biology, India
   Amounts awarded: 48.2 lacs
   Start and end dates: 2021-2024

5. Name of the awarding body: **Indian Council of Medical Research (ICMR)**
   Title of project: Prediction of Idiosyncratic Drug Induced Liver Injury (iDILI): A comprehensive in silico, in vitro and in vivo based multi-tier screening approach (grant - ID: IIRP-2023-1414/F1)
   Co-PI: Dr. Kishore Parsa and Dr. Kiranam Chatti, DR, Reddy's Institute of Life Sciences, India
   Amounts awarded: 64.91 lacs
   Start and end dates: 2023-2026

6. Name of the awarding body: **AMD's High Performance Compute Fund**
   Title of project: Probing the Altered Microheterogeneity of Alzheimer's Brain using Computational Lipidomics
   Amounts awarded: 14400 node-hours allocation on AMD HPC and supercomputers
   Start and end dates: 2024-2025

15. Other professional activities:

Academic Editor: PLOS ONE (Impact Factor: 3.24)

Editorial Advisory board: Mini Reviews in Medicinal Chemistry (Impact Factor: 3.862)

Guest Editor: Current Topics in Medicinal Chemistry (Impact factor: 3.295)

Best reviewer recognition: Molecular Biosystems (Royal Society of Chemistry), Journal of Luminescence (Elsevier), Journal of Molecular Structure (Elsevier)

Reviewer of the journals: PLOS Computational Biology (PLOS), Molecular Biosystems (RSC publishing), Journal of Luminescence (Elsevier), International Journal of Biological Macromolecule (Elsevier), Journal of Molecular Structure (Elsevier). Combinatorial Chemistry and High throughput Screening (Bentham Science), The Natural Product Journal (Bentham Science), Molecular informatics (Wiley), Current Topics in Medicinal Chemistry (Bentham Science), Bioorganic Chemistry (Elsevier), Computers in Biology and Chemistry (Elsevier), International Immunopharmacology (Elsevier), RSC Advance (RSC), Scientific Reports (Nature), Oxidative Medicine and Cellular Longevity (Hindawi), Journal of Clinical Medicine (MDPI), Current Microbology (Springer), Applied Biochemistry and Biotechnology (Springer) and many more

16. Current Collaborations:

1. Prof. Amitabha Chattopadhyay, CSIR Bhatnagar Fellow, SERB Distinguished Fellow, FTWAS, FRSB, FRSC, FNA, FNASc, FASc, CSIR-Centre for Cellular & Molecular Biology, India

2. Prof. Arun Bandyopadhyay, Director, CSIR-Indian Institute of Chemical Biology, FNASc, FAScT

3. Prof. Horacio Pérez-Sánchez, Principal investigator, BIO-HPC group, Universidad Católica San Antonio de Murcia (UCAM), Spain.

4. Dr. P. K. Biswas, Associate Professor & Chair, Department of Physics, Laboratory of Computational Biophysics & Bioengineering, Tougaloo College, USA.

5. Prof. Jesus Requena, Leader, Prion Lab, Center for Research in Molecular Medicine and Chronic Diseases (CiMUS), Universidade de Santiago de Compostela, Barcelona

6. Prof. Bidisha Sengupta, Assistant Professor, Department of Chemistry and Biochemistry, Stephen F. Austin State University, USA

7. Prof. Pradeep K. Sengupta, Ex-Senior Professor, Saha Institute of Nuclear Physics, UGC Emeritus Fellow, Dept. of Biophysics, Molecular Biology & Bioinformatics, University of Calcutta.

8. Dr. Jaya Bandyopadhyay, Associate Professor & Head, Department of Biotechnology, MAKAUT, India

9. Dr. Anindita Seal, Associate Professor, Dr. B. C Guha Centre for Genetic Engineering and Biotechnology, University of Calcutta

10. Dr. Mahesh Kumar Sah, Assistant Professor, Dept of Biotechnology, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, INDIA

11. Dr. Somsubhra Nath, Scientist, Dept. of Basic and Translational Research, Technical Director, Molecular Diagnostics Laboratory, Saroj Gupta Cancer Centre and Research Institute (SGCC & RI), Thakurpukur, Kolkata, India

I declare that the above particulars are correct to the best of my knowledge and belief.

Sandipan Chakraborty

Place: Kolkata.

Sandipan Chakraborty

Date: 26.04.2023