## Michelle A Sahai

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Case study: Biochemistry without borders: a case study utilising infographics. Essays in Biochemistry, 2022, 66, 65-73.	4.7	3
2	The fine art of preparing membrane transport proteins for biomolecular simulations: Concepts and practical considerations. Methods, 2021, 185, 3-14.	3.8	6
3	Molecular Mechanisms of Action of Stimulant Novel Psychoactive Substances (NPS) that target the High-affinity Transporter for Dopamine. Neuronal Signaling, 2021, 5, NS20210006.	3.2	3
4	The Role of Dopamine in the Stimulant Characteristics of Novel Psychoactive Substances (NPS)—Neurobiological and Computational Assessment Using the Case of Desoxypipradrol (2-DPMP). Frontiers in Pharmacology, 2020, 11, 806.	3.5	6
5	Mechanistic Insights into the Stimulant Properties of Novel Psychoactive Substances (NPS) and Their Discrimination by the Dopamine Transporter—In Silico and In Vitro Exploration of Dissociative Diarylethylamines. Brain Sciences, 2018, 8, 63.	2.3	15
6	Combined in vitro and in silico approaches to the assessment of stimulant properties of novel psychoactive substances – The case of the benzofuran 5-MAPB. Progress in Neuro-Psychopharmacology and Biological Psychiatry, 2017, 75, 1-9.	4.8	17
7	Identification of a nucleoside analog active against adenosine kinase–expressing plasma cell malignancies. Journal of Clinical Investigation, 2017, 127, 2066-2080.	8.2	7
8	Computational Modeling of the N-Terminus of the Human Dopamine Transporter (hDAT). Biophysical Journal, 2015, 108, 252a.	0.5	2
9	Computational modeling of the N-terminus of the human dopamine transporter and its interaction with PIP <sub>2</sub> -containing membranes. Proteins: Structure, Function and Bioinformatics, 2015, 83, 952-969.	2.6	47
10	Spontaneous Inward Opening of the Dopamine Transporter Is Triggered by PIP <sub>2</sub> -Regulated Dynamics of the N-Terminus. ACS Chemical Neuroscience, 2015, 6, 1825-1837.	3.5	95
11	Abstract 4496: Genomics-based resistome analysis revealed endogenous adenosine kinase levels as a chief determinant of specificity for a novel nucleoside analog lymphoma inhibitor. , 2015, , .		0
12	ESCRT-II/Vps25 Constrains Digit Number by Endosome-Mediated Selective Modulation of FGF-SHH Signaling. Cell Reports, 2014, 9, 674-687.	6.4	12
13	Missense dopamine transporter mutations associate with adult parkinsonism and ADHD. Journal of Clinical Investigation, 2014, 124, 3107-3120.	8.2	129
14	De novo mutation in the dopamine transporter gene associates dopamine dysfunction with autism spectrum disorder. Molecular Psychiatry, 2013, 18, 1315-1323.	7.9	181
15	Path Searching Towards the Symmetric Inward Open Structure of LeuT. Biophysical Journal, 2013, 104, 57a.	0.5	0
16	Drosophila melanogaster: a novel animal model for the behavioral characterization of autism-associated mutations in the dopamine transporter gene. Molecular Psychiatry, 2013, 18, 1235-1235.	7.9	9
17	Quantifying Water-Mediated Protein–Ligand Interactions in a Glutamate Receptor: A DFT Study. Journal of Physical Chemistry B, 2011, 115, 7085-7096.	2.6	16
18	A comparative analysis of the role of water in the binding pockets of ionotropic glutamate receptors. Physical Chemistry Chemical Physics, 2010, 12, 14057.	2.8	15

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19	Transition State Infrared Spectra for the Trans→Cis Isomerization of a Simple Peptide Model. Journal of Physical Chemistry A, 2007, 111, 8384-8389.	2.5	6
20	Quantifying the Intrinsic Effects of Two Point Mutation Models of Pro-Pro-Pro Triamino Acid Diamide. A First-Principle Computational Study. Journal of Physical Chemistry B, 2007, 111, 13135-13142.	2.6	14
21	Quantifying the Intrinsic Effects of Two Point Mutation Models of Prolineâ <sup>~,</sup> Proline Diamino Acid Diamide: A First-Principle Computational Study. Journal of Physical Chemistry B, 2007, 111, 11592-11602.	2.6	15
22	First-Principle Computational Study on the Full Conformational Space of I-Threonine Diamide, the Energetic Stability of Cis and Trans Isomers. Journal of Physical Chemistry A, 2006, 110, 11527-11536.	2.5	14
23	Selenocysteine derivatives I. Sidechain conformational potential energy surface of N-acetyl-l-selenocysteine-N-methylamide (MeCO-l-Sec-NH-Me) in its βl backbone conformation. Computational and Theoretical Chemistry, 2005, 725, 111-125.	1.5	4
24	First Principle Computational Study on the Full Conformational Space ofl-Proline Diamides. Journal of Physical Chemistry A, 2005, 109, 2660-2679.	2.5	29
25	A modular numbering system of selected oligopeptides for molecular computations: using pre-computed amino acid building blocks. Computational and Theoretical Chemistry, 2003, 666-667, 169-218.	1.5	11
26	An ab initio exploratory study of the full conformational space of MeCO-l-threonine-NH-Me. Computational and Theoretical Chemistry, 2003, 666-667, 251-267.	1.5	7
27	An ab initio exploratory study on the conformational features of the dipeptide MeCO-Ala-Ala-NH-Me in its four different configurations: determination of the behaviour of d-enantiomer amino acids within a peptide chain. Computational and Theoretical Chemistry, 2003, 666-667, 291-301.	1.5	8
28	A model study of the IgA hinge region: an exploratory study of selected backbone conformations of MeCO-I-Pro-I-Thr-NH-Me. Computational and Theoretical Chemistry, 2003, 666-667, 311-319.	1.5	5
29	An ab initio exploratory study on selected conformational features of MeCO-I-Ala-I-Ala-I-Ala-NH-Me as a XxxYyyZzz tripeptide motif within a protein structure. Computational and Theoretical Chemistry, 2003, 666-667, 327-336.	1.5	4
30	Toward a computed peptide structure database: The role of a universal atomic numbering system of amino acids in peptides and internal hierarchy of database. International Journal of Quantum Chemistry, 2002, 90, 933-968.	2.0	54
31	Ab initio quantum mechanical characterization of platinum, palladium, and nickel complexes ofL-ascorbic acid. International Journal of Quantum Chemistry, 2002, 90, 882-887.	2.0	4
32	Albert Szent-Györgyi—The Scientist Who Discovered Vitamin C. Frontiers for Young Minds, 0, 8, .	0.8	1