Neil John Bruce

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3705229/publications.pdf

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17	537	840585 11	887953 17
papers	citations	h-index	g-index

19	19	19	971
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Brownian Dynamics Simulations of Proteins in the Presence of Surfaces: Long-Range Electrostatics and Mean-Field Hydrodynamics. Journal of Chemical Theory and Computation, 2021, 17, 3510-3524.	2.3	7
2	Simulation of the Positive Inotropic Peptide S100A1ct in Aqueous Environment by Gaussian Accelerated Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 4654-4666.	1.2	3
3	The Effect of Force-Field Parameters on Cytochrome P450-Membrane Interactions: Structure and Dynamics. Scientific Reports, 2020, 10, 7284.	1.6	22
4	KBbox: A Toolbox of Computational Methods for Studying the Kinetics of Molecular Binding. Journal of Chemical Information and Modeling, 2019, 59, 3630-3634.	2.5	15
5	Regulation of adenylyl cyclase 5 in striatal neurons confers the ability to detect coincident neuromodulatory signals. PLoS Computational Biology, 2019, 15, e1007382.	1.5	16
6	Differing Membrane Interactions of Two Highly Similar Drug-Metabolizing Cytochrome P450 Isoforms: CYP 2C9 and CYP 2C19. International Journal of Molecular Sciences, 2019, 20, 4328.	1.8	11
7	Influence of Transmembrane Helix Mutations on Cytochrome P450-Membrane Interactions and Function. Biophysical Journal, 2019, 116, 419-432.	0.2	23
8	Identification of Rare Lewis Oligosaccharide Conformers in Aqueous Solution Using Enhanced Sampling Molecular Dynamics. Journal of Physical Chemistry B, 2018, 122, 2462-2474.	1.2	28
9	New approaches for computing ligandâ€“receptor binding kinetics. Current Opinion in Structural Biology, 2018, 49, 1-10.	2.6	122
10	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	1.5	148
11	Comparative electrostatic analysis of adenylyl cyclase for isoform dependent regulation properties. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1844-1858.	1.5	13
12	Free Energy Calculations using a Swarmâ€Enhanced Sampling Molecular Dynamics Approach. ChemPhysChem, 2015, 16, 3233-3241.	1.0	10
13	webSDA: a web server to simulate macromolecular diffusional association. Nucleic Acids Research, 2015, 43, W220-W224.	6.5	12
14	<scp>SDA</scp> 7: A modular and parallel implementation of the simulation of diffusional association software. Journal of Computational Chemistry, 2015, 36, 1631-1645.	1.5	64
15	Exploring Protein Kinase Conformation Using Swarm-Enhanced Sampling Molecular Dynamics. Journal of Chemical Information and Modeling, 2014, 54, 2764-2775.	2.5	12
16	Ab Initio Protein Folding Using a Cooperative Swarm of Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2010, 6, 1925-1930.	2.3	7
17	Molecular dynamics simulations of AÎ² fibril interactions with Î²-sheet breaker peptides. Peptides, 2010, 31, 2100-2108.	1.2	23