

Birgit SchiÄ,tt

List of Publications by Year in descending order

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131
papers

4,474
citations

87843

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128225

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141
all docs

141
docs citations

141
times ranked

5560
citing authors

#	ARTICLE	IF	CITATIONS
1	Enantioselective Hydrosilylation of Ketones with a Chiral Titanocene Catalyst. <i>Journal of the American Chemical Society</i> , 1994, 116, 11667-11670.	6.6	190
2	The influence of cholesterol on membrane protein structure, function, and dynamics studied by molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2015, 1848, 1783-1795.	1.4	144
3	On the electronic nature of low-barrier hydrogen bonds in enzymatic reactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1998, 95, 12799-12802.	3.3	136
4	P-type ATPases as drug targets: Tools for medicine and science. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2009, 1787, 207-220.	0.5	129
5	Peptide Aggregation and Pore Formation in a Lipid Bilayer: A Combined Coarse-Grained and All Atom Molecular Dynamics Study. <i>Biophysical Journal</i> , 2008, 95, 4337-4347.	0.2	127
6	Ion Pathways in the Sarcoplasmic Reticulum Ca ²⁺ -ATPase. <i>Journal of Biological Chemistry</i> , 2013, 288, 10759-10765.	1.6	125
7	Binding of Serotonin to the Human Serotonin Transporter. <i>Molecular Modeling and Experimental Validation. Journal of the American Chemical Society</i> , 2008, 130, 3853-3865.	6.6	123
8	Characterization of the Short Strong Hydrogen Bond in Benzoylacetone by ab Initio Calculations and Accurate Diffraction Experiments. Implications for the Electronic Nature of Low-Barrier Hydrogen Bonds in Enzymatic Reactions. <i>Journal of the American Chemical Society</i> , 1998, 120, 12117-12124.	6.6	120
9	Mutual adaptation of a membrane protein and its lipid bilayer during conformational changes. <i>Nature Communications</i> , 2011, 2, 304.	5.8	108
10	Substrate Binding and Formation of an Occluded State in the Leucine Transporter. <i>Biophysical Journal</i> , 2008, 94, 1600-1612.	0.2	89
11	Conformational Dynamics of the Estrogen Receptor $\hat{\pm}$: Molecular Dynamics Simulations of the Influence of Binding Site Structure on Protein Dynamics. <i>Biochemistry</i> , 2007, 46, 1743-1758.	1.2	85
12	Binding and Orientation of Tricyclic Antidepressants within the Central Substrate Site of the Human Serotonin Transporter. <i>Journal of Biological Chemistry</i> , 2010, 285, 8363-8374.	1.6	85
13	A direct interaction of cholesterol with the dopamine transporter prevents its out-to-inward transition. <i>PLoS Computational Biology</i> , 2018, 14, e1005907.	1.5	81
14	The Two Enantiomers of Citalopram Bind to the Human Serotonin Transporter in Reversed Orientations. <i>Journal of the American Chemical Society</i> , 2010, 132, 1311-1322.	6.6	79
15	Mechanistic Investigation of the 2,5-Diphenylpyrrolidine-Catalyzed Enantioselective $\hat{\pm}$ -Chlorination of Aldehydes. <i>Chemistry - A European Journal</i> , 2005, 11, 7083-7090.	1.7	76
16	Understanding the Phase Behavior of Coarse-Grained Model Lipid Bilayers through Computational Calorimetry. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1551-1569.	1.2	73
17	The Charge Density Distribution in a Model Compound of the Catalytic Triad in Serine Proteases. <i>Chemistry - A European Journal</i> , 2001, 7, 3756-3767.	1.7	71
18	Reaction Mechanism of Soluble Epoxide Hydrolase: Insights from Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2002, 124, 14558-14570.	6.6	69

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19	Conformational Flexibility of Chitosan: A Molecular Modeling Study. <i>Biomacromolecules</i> , 2010, 11, 3196-3207.	2.6	67
20	Molecular Docking with Ligand Attached Water Molecules. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 909-917.	2.5	67
21	Electron Density Distributions of Redox Active Mixed Valence Carboxylate Bridged Trinuclear Iron Complexes. <i>Journal of the American Chemical Society</i> , 2003, 125, 11088-11099.	6.6	66
22	Strong Nâ~Hâ€¦â€¦â€¦O Hydrogen Bonding in a Model Compound of the Catalytic Triad in Serine Proteases. <i>Angewandte Chemie - International Edition</i> , 1999, 38, 1239-1242.	7.2	62
23	Incorporation of Antimicrobial Peptides into Membranes: A Combined Liquid-State NMR and Molecular Dynamics Study of Alamethicin in DMPC/DHPC Bicelles. <i>Journal of Physical Chemistry B</i> , 2009, 113, 6928-6937.	1.2	62
24	Monoamine transporters: insights from molecular dynamics simulations. <i>Frontiers in Pharmacology</i> , 2015, 6, 235.	1.6	60
25	Comparative Modeling of the Human Monoamine Transporters: Similarities in Substrate Binding. <i>ACS Chemical Neuroscience</i> , 2013, 4, 295-309.	1.7	59
26	A direct view of the complex multi-pathway folding of telomeric G-quadruplexes. <i>Nucleic Acids Research</i> , 2016, 44, 11024-11032.	6.5	59
27	A conserved leucine occupies the empty substrate site of LeuT in the Na ⁺ -free return state. <i>Nature Communications</i> , 2016, 7, 11673.	5.8	58
28	Exploring Interactions of Endocrine-Disrupting Compounds with Different Conformations of the Human Estrogen Receptor ð± Ligand Binding Domain: A Molecular Docking Study. <i>Chemical Research in Toxicology</i> , 2008, 21, 2195-2206.	1.7	57
29	Cholesterol binding to a conserved site modulates the conformation, pharmacology, and transport kinetics of the human serotonin transporter. <i>Journal of Biological Chemistry</i> , 2018, 293, 3510-3523.	1.6	55
30	Unbiased Simulations Reveal the Inward-Facing Conformation of the Human Serotonin Transporter and Na ⁺ Ion Release. <i>PLoS Computational Biology</i> , 2011, 7, e1002246.	1.5	54
31	Molecular Basis for Selective Serotonin Reuptake Inhibition by the Antidepressant Agent Fluoxetine (Prozac). <i>Molecular Pharmacology</i> , 2014, 85, 703-714.	1.0	54
32	Formation of maleic anhydride on a vanadyl pyrophosphate surface: a theoretical study of the mechanism. <i>The Journal of Physical Chemistry</i> , 1991, 95, 2297-2307.	2.9	52
33	Molecular Dynamics Simulations of Ground and Transition States for the Hydride Transfer from Formate to NAD ⁺ in the Active Site of Formate Dehydrogenase. <i>Journal of the American Chemical Society</i> , 1999, 121, 8164-8173.	6.6	52
34	Ligand Induced Conformational Changes of the Human Serotonin Transporter Revealed by Molecular Dynamics Simulations. <i>PLoS ONE</i> , 2013, 8, e63635.	1.1	49
35	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations. <i>ELife</i> , 2020, 9, .	2.8	49
36	Capturing Biologically Complex Tissue-Specific Membranes at Different Levels of Compositional Complexity. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7819-7829.	1.2	47

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37	Identification of a Common Binding Mode for Imaging Agents to Amyloid Fibrils from Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2013, 135, 15114-15128.	6.6	42
38	Protofibrillar Assembly Toward the Formation of Amyloid Fibrils. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2385-2390.	2.1	39
39	Thermodynamic and structural investigation of the specific SDS binding of <i>Humicola insolens</i> cutinase. <i>Protein Science</i> , 2014, 23, 1023-1035.	3.1	39
40	Importance of C α -N Bond Rotation in N-Acyl Oxazolidinones in their SmI ₂ -Promoted Coupling to Acrylamides. <i>Journal of the American Chemical Society</i> , 2009, 131, 10253-10262.	6.6	37
41	Protonation States of Important Acidic Residues in the Central Ca ²⁺ Ion Binding Sites of the Ca ²⁺ -ATPase: A Molecular Modeling Study. <i>Biochemistry</i> , 2011, 50, 11109-11120.	1.2	37
42	Bicelles and Other Membrane Mimics: Comparison of Structure, Properties, and Dynamics from MD Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15831-15843.	1.2	37
43	Residue-Specific Information about the Dynamics of Antimicrobial Peptides from ¹⁵ N and ² H Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2009, 131, 18335-18342.	6.6	35
44	Short Strong Hydrogen Bonds in 2-Acetyl-1,8-dihydroxy-3,6-dimethylnaphthalene: An Outlier to Current Hydrogen Bonding Theory?. <i>Journal of Physical Chemistry A</i> , 2007, 111, 345-351.	1.1	34
45	Modeling the Self-Assembly and Stability of DHPC Micelles Using Atomic Resolution and Coarse Grained MD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1556-1569.	2.3	33
46	Mutation in transforming growth factor beta induced protein associated with granular corneal dystrophy type 1 reduces the proteolytic susceptibility through local structural stabilization. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 2812-2822.	1.1	33
47	The Importance of Being Capped: Terminal Capping of an Amyloidogenic Peptide Affects Fibrillation Propensity and Fibril Morphology. <i>Biochemistry</i> , 2014, 53, 6968-6980.	1.2	33
48	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. <i>Journal of Membrane Biology</i> , 2018, 251, 609-631.	1.0	33
49	Theoretical Investigation of the Hydride Transfer from Formate to NAD ⁺ and the Implications for the Catalytic Mechanism of Formate Dehydrogenase. <i>Journal of the American Chemical Society</i> , 1998, 120, 7192-7200.	6.6	32
50	Dimer Interface of the Human Serotonin Transporter and Effect of the Membrane Composition. <i>Scientific Reports</i> , 2018, 8, 5080.	1.6	32
51	Binding of the Amphetamine-like 1-Phenyl-piperazine to Monoamine Transporters. <i>ACS Chemical Neuroscience</i> , 2012, 3, 693-705.	1.7	28
52	<i>In Vitro</i> Effects of the Endocrine Disruptor p,p'-DDT on Human Follitropin Receptor. <i>Environmental Health Perspectives</i> , 2016, 124, 991-999.	2.8	28
53	Bovine Chymosin: A Computational Study of Recognition and Binding of Bovine β -Casein. <i>Biochemistry</i> , 2010, 49, 2563-2573.	1.2	27
54	Synthesis of uronic-Noeurostegine a potent bacterial β -glucuronidase inhibitor. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 7807.	1.5	27

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55	Binding of the Multimodal Antidepressant Drug Vortioxetine to the Human Serotonin Transporter. ACS Chemical Neuroscience, 2015, 6, 1892-1900.	1.7	27
56	Conformational Dynamics of the Human Islet Amyloid Polypeptide in a Membrane Environment: Toward the Aggregation Prone Form. Biochemistry, 2016, 55, 2031-2042.	1.2	27
57	Identification of Key Interactions in the Initial Self-Assembly of Amylin in a Membrane Environment. Biochemistry, 2017, 56, 4884-4894.	1.2	27
58	Molecular mechanism of sugar transport in plants unveiled by structures of glucose/H ⁺ symporter STP10. Nature Plants, 2021, 7, 1409-1419.	4.7	27
59	The Low-Barrier Hydrogen Bond of Deuterated Benzoylacetone Probed by Very Low Temperature Neutron and X-ray Diffraction Studies and Theoretical Calculations. Chemistry - A European Journal, 2007, 13, 5539-5547.	1.7	26
60	Initial Stage of Cheese Production: A Molecular Modeling Study of Bovine and Camel Chymosin Complexed with Peptides from the Chymosin-Sensitive Region of β -Casein. Journal of Agricultural and Food Chemistry, 2011, 59, 5636-5647.	2.4	26
61	Properties of an Inward-Facing State of LeuT: Conformational Stability and Substrate Release. Biophysical Journal, 2015, 108, 1390-1399.	0.2	26
62	Coadsorption of carbon monoxide and hydrogen on the nickel(100) surface: a theoretical investigation of site preferences and surface bonding. The Journal of Physical Chemistry, 1990, 94, 1554-1564.	2.9	25
63	The oxidative species on a vanadyl pyrophosphate surface. Catalysis Today, 1993, 16, 79-90.	2.2	25
64	Tracing Cytoplasmic Ca ²⁺ Ion and Water Access Points in the Ca ²⁺ -ATPase. Biophysical Journal, 2012, 102, 268-277.	0.2	25
65	Structural Basis for Simvastatin Competitive Antagonism of Complement Receptor 3. Journal of Biological Chemistry, 2016, 291, 16963-16976.	1.6	25
66	Regioselective monoepoxidation of 1,3-dienes catalysed by transition-metal complexes. Journal of the Chemical Society Chemical Communications, 1992, , 1072-1074.	2.0	24
67	Cofactor Activation and Substrate Binding in Pyruvate Decarboxylase. Insights into the Reaction Mechanism from Molecular Dynamics Simulations. Biochemistry, 2005, 44, 14792-14806.	1.2	24
68	Water-Mediated Interactions Influence the Binding of Thapsigargin to Sarco/Endoplasmic Reticulum Calcium Adenosinetriphosphatase. Journal of Medicinal Chemistry, 2013, 56, 3609-3619.	2.9	23
69	Insights to ligand binding to the monoamine transporters from homology modeling to LeuBAT and dDAT. Frontiers in Pharmacology, 2015, 6, 208.	1.6	23
70	Binding of Mazindol and Analogs to the Human Serotonin and Dopamine Transporters. Molecular Pharmacology, 2014, 85, 208-217.	1.0	22
71	Binding-Induced Fluorescence of Serotonin Transporter Ligands: A Spectroscopic and Structural Study of 4-(4-(Dimethylamino)phenyl)-1-methylpyridinium (APP ⁺) and APP ⁺ Analogues. ACS Chemical Neuroscience, 2014, 5, 296-304.	1.7	21
72	Comparative MD analysis of the stability of transthyretin providing insight into the fibrillation mechanism. Biopolymers, 2007, 86, 73-82.	1.2	20

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73	Interrogating the Molecular Basis for Substrate Recognition in Serotonin and Dopamine Transporters with High-Affinity Substrate-Based Bivalent Ligands. <i>ACS Chemical Neuroscience</i> , 2016, 7, 1406-1417.	1.7	20
74	Reactive Center Loop Insertion in α -1-Antitrypsin Captured by Accelerated Molecular Dynamics Simulation. <i>Biochemistry</i> , 2017, 56, 634-646.	1.2	20
75	Addition of a carbonyl functionality to titanium carbenes. A study of the mechanism and intermediates in the Tebbe reaction. <i>Journal of the Chemical Society Dalton Transactions</i> , 1993, , 337-344.	1.1	19
76	Resolution Enhancement in Solid-State NMR of Oriented Membrane Proteins by Anisotropic Differential Linebroadening. <i>Journal of the American Chemical Society</i> , 2008, 130, 5028-5029.	6.6	17
77	Inhibition of plasminogen activator inhibitor-1 binding to endocytosis receptors of the low-density-lipoprotein receptor family by a peptide isolated from a phage display library. <i>Biochemical Journal</i> , 2006, 399, 387-396.	1.7	16
78	Synthesis and inhibitory evaluation of 3-linked imipramines for the exploration of the S2 site of the human serotonin transporter. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 2725-2738.	1.4	16
79	Lipid Dynamics Studied by Calculation of ^{31}P Solid-State NMR Spectra Using Ensembles from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5119-5129.	1.2	15
80	Insight into the molecular mechanism behind PEG-mediated stabilization of biofluid lipases. <i>Scientific Reports</i> , 2018, 8, 12293.	1.6	15
81	Substrate and inhibitor binding to the serotonin transporter: Insights from computational, crystallographic, and functional studies. <i>Neuropharmacology</i> , 2019, 161, 107548.	2.0	15
82	Novel noscapine derivatives stabilize the native state of insulin against fibrillation. <i>International Journal of Biological Macromolecules</i> , 2020, 147, 98-108.	3.6	15
83	A DFT study of solvation effects on the tautomeric equilibrium and catalytic ylide generation of thiamin models. <i>Journal of Computational Chemistry</i> , 2008, 29, 1037-1047.	1.5	14
84	Modeling and Mutational Analysis of the Binding Mode for the Multimodal Antidepressant Drug Vortioxetine to the Human 5-HT _{3A} Receptor. <i>Molecular Pharmacology</i> , 2018, 94, 1421-1434.	1.0	14
85	Molecular Modeling Investigation of the Interaction between <i>Humicola insolens</i> Cutinase and SDS Surfactant Suggests a Mechanism for Enzyme Inactivation. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1977-1987.	2.5	14
86	Structure and Dynamics of Cinnamycin-Lipid Complexes: Mechanisms of Selectivity for Phosphatidylethanolamine Lipids. <i>ACS Omega</i> , 2019, 4, 18889-18899.	1.6	14
87	A Photoswitchable Inhibitor of the Human Serotonin Transporter. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1231-1237.	1.7	14
88	Hot-Spot Mapping of the Interactions between Chymosin and Bovine β -Casein. <i>Journal of Agricultural and Food Chemistry</i> , 2013, 61, 7949-7959.	2.4	13
89	Interaction of Amyloid- β -(1-42) Peptide and Its Aggregates with Lipid/Water Interfaces Probed by Vibrational Sum-Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11208-11218.	1.2	13
90	Dynamics of Fluorescent Dyes Attached to G-Quadruplex DNA and their Effect on FRET Experiments. <i>ChemPhysChem</i> , 2015, 16, 2562-2570.	1.0	12

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91	Ethylidyne on the rhodium(100) surface: a theoretical investigation. <i>Langmuir</i> , 1990, 6, 806-816.	1.6	11
92	The influence of solvation on short strong hydrogen bonds: a density functional theory study of the Asp-His interaction in subtilisins. <i>Chemical Communications</i> , 2004, , 498-499.	2.2	11
93	QSAR studies and pharmacophore identification for arylsubstituted cycloalkenecarboxylic acid methyl esters with affinity for the human dopamine transporter. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 5262-5274.	1.4	11
94	Solvent Binding Analysis and Computational Alanine Scanning of the Bovine Chymosinâ€“Bovine Î²-Casein Complex Using Molecular Integral Equation Theory. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5706-5717.	2.3	11
95	Mutants and molecular dockings reveal that the primary L-thyroxine binding site in human serum albumin is not the one which can cause familial dysalbuminemic hyperthyroxinemia. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2016, 1860, 648-660.	1.1	11
96	General Protocol for Constructing Molecular Models of Nanodiscs. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2869-2883.	2.5	11
97	Simulations of membraneâ€“bound diglycosylated human prion protein reveal potential protective mechanisms against misfolding. <i>Journal of Neurochemistry</i> , 2017, 142, 171-182.	2.1	10
98	Ligand Binding in the Extracellular Vestibule of the Neurotransmitter Transporter Homologue LeuT. <i>ACS Chemical Neuroscience</i> , 2017, 8, 619-628.	1.7	10
99	Testing theory beyond molecular structure: Electron density distributions of complex molecules. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 23-31.	1.0	9
100	Enantioselective Proteins: Selection, Binding Studies and Molecular Modeling of Antibodies with Affinity towards Hydrophobic BINOL Derivatives. <i>ChemBioChem</i> , 2007, 8, 1974-1980.	1.3	9
101	Revealing a Dual Role of Ganglioside Lipids in the Aggregation of Membrane-Associated Islet Amyloid Polypeptide. <i>Journal of Membrane Biology</i> , 2019, 252, 343-356.	1.0	8
102	Effect of palmitoylation on the dimer formation of the human dopamine transporter. <i>Scientific Reports</i> , 2021, 11, 4164.	1.6	8
103	Allosteric-Activation Mechanism of Bovine Chymosin Revealed by Bias-Exchange Metadynamics and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10453-10462.	1.2	7
104	Conformational Changes in the 5-HT _{3A} Receptor Extracellular Domain Measured by Voltage-Clamp Fluorometry. <i>Molecular Pharmacology</i> , 2019, 96, 720-734.	1.0	7
105	The Effect of Cholesterol on Membrane-Bound Islet Amyloid Polypeptide. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 657946.	1.6	7
106	Stepwise or concerted addition of 1,3-butadiene to oxygen adsorbed on the silver (110) surface?. <i>The Journal of Physical Chemistry</i> , 1993, 97, 10738-10741.	2.9	6
107	Early Events in the Amyloid Formation of the A546T Mutant of Transforming Growth Factor Î²-Induced Protein in Corneal Dystrophies Compared to the Nonfibrillating R555W and R555Q Mutants. <i>Biochemistry</i> , 2015, 54, 5546-5556.	1.2	6
108	How a short pore forming peptide spans the lipid membrane. <i>Biointerphases</i> , 2017, 12, 02D405.	0.6	6

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109	Addition of aldehydes to tantalum-carbene complexes and the reduction of epoxides by unsaturated tantalum complexes. Theoretical study of the reaction mechanism and product structures. <i>Organometallics</i> , 1992, 11, 4213-4221.	1.1	5
110	Possible involvement of collective domain movement in the catalytic reaction of soluble epoxide hydrolase. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 61-69.	1.0	5
111	Effect of cholesterol on the dimerization of C99 – A molecular modeling perspective. <i>Biointerphases</i> , 2021, 16, 031002.	0.6	4
112	Molecular modeling of neurological membrane proteins – from binding sites to synapses. <i>Neuroscience Letters</i> , 2019, 700, 38-49.	1.0	3
113	Membrane Interactions of IAPP. <i>Biophysical Journal</i> , 2019, 116, 491a.	0.2	3
114	Simulating Multiple Substrate-Binding Events by \hat{I}^3 -Glutamyltransferase Using Accelerated Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10104-10116.	1.2	2
115	Beneficent and Maleficent Effects of Cations on Bufadienolide Binding to Na ⁺ ,K ⁺ -ATPase. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 976-986.	2.5	2
116	Studies of the oxidative addition of some substrates containing carbon-heteroatom bonds to some tungsten and platinum complexes. <i>Journal of the Chemical Society Dalton Transactions</i> , 1989, , 2099-2107.	1.1	1
117	On the effect of mutations in bovine or camel chymosin on the thermodynamics of binding \hat{I}^2 -caseins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 75-87.	1.5	1
118	Investigating C99 in Amyloid Formation using Molecular Dynamics: From Simple to Complex Neuronal Models. <i>Biophysical Journal</i> , 2019, 116, 493a-494a.	0.2	1
119	Binding and Activation of Serotonergic G-Protein Coupled Receptors by the Multimodal Antidepressant Vortioxetine. <i>ACS Chemical Neuroscience</i> , 2022, 13, 1129-1142.	1.7	1
120	Modeling the Membrane Role in Ca ²⁺ -ATPase Catalytic Cycle. <i>Biophysical Journal</i> , 2010, 98, 487a.	0.2	0
121	A Coarse Grained Molecular Dynamics Study of the Formation and Structure of Bicelles. <i>Biophysical Journal</i> , 2010, 98, 569a.	0.2	0
122	Ca ²⁺ -ATPase: Lipid-Protein Interaction As Observed in Crystals and MD Simulations. <i>Biophysical Journal</i> , 2010, 98, 20a.	0.2	0
123	Identifying Calcium ion Access Points and Transport Pathways in SERCA. <i>Biophysical Journal</i> , 2011, 100, 467a.	0.2	0
124	Understanding the Phase Changes of Coarse-Grained Model Bilayers Through Computational Calorimetry. <i>Biophysical Journal</i> , 2011, 100, 332a-333a.	0.2	0
125	Conformational Stability and Substrate Translocation - A Computational Study of the Leucine Transporter. <i>Biophysical Journal</i> , 2013, 104, 407a-408a.	0.2	0
126	Aggregation of Transforming Growth Factor \hat{I}^2 Induced Protein Studied by Protein-Protein Docking. <i>Biophysical Journal</i> , 2014, 106, 681a.	0.2	0

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127	Probing the Folding Dynamics of Human Telomeric G-Quadruplex with Single-Molecule FRET. Biophysical Journal, 2016, 110, 406a.	0.2	0
128	Mapping Cholesterol Binding Sites on the Human Dopamine Transporter. Biophysical Journal, 2017, 112, 339a.	0.2	0
129	A Generic Protocol for Constructing Molecular Models of Nanodiscs in Silico. Biophysical Journal, 2020, 118, 385a.	0.2	0
130	Allosteric Network Analysis in the NMDA Receptor. Biophysical Journal, 2020, 118, 417a.	0.2	0
131	Folding Kinetics of Multiple G-Quadruplex Telomeric DNA Structures. Biophysical Journal, 2020, 118, 335a.	0.2	0