

Birgit Schitt

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

120
papers

3,646
citations

35
h-index

56
g-index

141
ext. papers

4,071
ext. citations

5.5
avg, IF

5.26
L-index

#	Paper	IF	Citations
120	The Effect of Cholesterol on Membrane-Bound Islet Amyloid Polypeptide. <i>Frontiers in Molecular Biosciences</i> , 2021 , 8, 657946	5.6	3
119	Effect of cholesterol on the dimerization of C99-A molecular modeling perspective. <i>Biointerphases</i> , 2021 , 16, 031002	1.8	1
118	General Protocol for Constructing Molecular Models of Nanodiscs. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2869-2883	6.1	1
117	Effect of palmitoylation on the dimer formation of the human dopamine transporter. <i>Scientific Reports</i> , 2021 , 11, 4164	4.9	0
116	Molecular mechanism of sugar transport in plants unveiled by structures of glucose/H symporter STP10. <i>Nature Plants</i> , 2021 , 7, 1409-1419	11.5	3
115	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	3.4	5
114	Benevolent and Malevolent Effects of Cations on Bufadienolide Binding to Na,K-ATPase. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 976-986	6.1	2
113	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations. <i>ELife</i> , 2020 , 9,	8.9	20
112	Novel nescapine derivatives stabilize the native state of insulin against fibrillation. <i>International Journal of Biological Macromolecules</i> , 2020 , 147, 98-108	7.9	7
111	Simulating Multiple Substrate-Binding Events by β -Glutamyltransferase Using Accelerated Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 10104-10116	3.4	1
110	Capturing Biologically Complex Tissue-Specific Membranes at Different Levels of Compositional Complexity. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 7819-7829	3.4	15
109	A Photoswitchable Inhibitor of the Human Serotonin Transporter. <i>ACS Chemical Neuroscience</i> , 2020 , 11, 1231-1237	5.7	6
108	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	2.3	5
107	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	6.1	6
106	Substrate and inhibitor binding to the serotonin transporter: Insights from computational, crystallographic, and functional studies. <i>Neuropharmacology</i> , 2019 , 161, 107548	5.5	8
105	Molecular modeling of neurological membrane proteins - from binding sites to synapses. <i>Neuroscience Letters</i> , 2019 , 700, 38-49	3.3	2
104	Membrane Interactions of IAPP. <i>Biophysical Journal</i> , 2019 , 116, 491a	2.9	2

103	Structure and Dynamics of Cinnamycin-Lipid Complexes: Mechanisms of Selectivity for Phosphatidylethanolamine Lipids. <i>ACS Omega</i> , 2019 , 4, 18889-18899	3.9	7
102	Conformational Changes in the 5-HT Receptor Extracellular Domain Measured by Voltage-Clamp Fluorometry. <i>Molecular Pharmacology</i> , 2019 , 96, 720-734	4.3	1
101	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	5.4	33
100	Dimer Interface of the Human Serotonin Transporter and Effect of the Membrane Composition. <i>Scientific Reports</i> , 2018 , 8, 5080	4.9	22
99	Insight into the molecular mechanism behind PEG-mediated stabilization of biofluid lipases. <i>Scientific Reports</i> , 2018 , 8, 12293	4.9	7
98	A direct interaction of cholesterol with the dopamine transporter prevents its out-to-inward transition. <i>PLoS Computational Biology</i> , 2018 , 14, e1005907	5	51
97	On the effect of mutations in bovine or camel chymosin on the thermodynamics of binding to caseins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018 , 86, 75-87	4.2	0
96	Modeling and Mutational Analysis of the Binding Mode for the Multimodal Antidepressant Drug Vortioxetine to the Human 5-HT Receptor. <i>Molecular Pharmacology</i> , 2018 , 94, 1421-1434	4.3	7
95	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. <i>Journal of Membrane Biology</i> , 2018 , 251, 609-631	2.3	26
94	Simulations of membrane-bound diglycosylated human prion protein reveal potential protective mechanisms against misfolding. <i>Journal of Neurochemistry</i> , 2017 , 142, 171-182	6	8
93	How a short pore forming peptide spans the lipid membrane. <i>Biointerphases</i> , 2017 , 12, 02D405	1.8	3
92	Ligand Binding in the Extracellular Vestibule of the Neurotransmitter Transporter Homologue LeuT. <i>ACS Chemical Neuroscience</i> , 2017 , 8, 619-628	5.7	9
91	Reactive Center Loop Insertion in α_1 -Antitrypsin Captured by Accelerated Molecular Dynamics Simulation. <i>Biochemistry</i> , 2017 , 56, 634-646	3.2	16
90	Identification of Key Interactions in the Initial Self-Assembly of Amylin in a Membrane Environment. <i>Biochemistry</i> , 2017 , 56, 4884-4894	3.2	19
89	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	3.4	4
88	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	5.7	14
87	A conserved leucine occupies the empty substrate site of LeuT in the Na(+)-free return state. <i>Nature Communications</i> , 2016 , 7, 11673	17.4	44
86	A direct view of the complex multi-pathway folding of telomeric G-quadruplexes. <i>Nucleic Acids Research</i> , 2016 , 44, 11024-11032	20.1	43

85	Conformational Dynamics of the Human Islet Amyloid Polypeptide in a Membrane Environment: Toward the Aggregation Prone Form. <i>Biochemistry</i> , 2016 , 55, 2031-42	3.2	21
84	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, 648-60	4	9
83	In Vitro Effects of the Endocrine Disruptor p,pSDDT on Human Follitropin Receptor. <i>Environmental Health Perspectives</i> , 2016 , 124, 991-9	8.4	20
82	Structural Basis for Simvastatin Competitive Antagonism of Complement Receptor 3. <i>Journal of Biological Chemistry</i> , 2016 , 291, 16963-76	5.4	15
81	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, 2725-38	3.4	15
80	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, 1783-95	3.8	105
79	Properties of an inward-facing state of LeuT: conformational stability and substrate release. <i>Biophysical Journal</i> , 2015 , 108, 1390-1399	2.9	21
78	Binding of the multimodal antidepressant drug vortioxetine to the human serotonin transporter. <i>ACS Chemical Neuroscience</i> , 2015 , 6, 1892-900	5.7	19
77	Early Events in the Amyloid Formation of the A546T Mutant of Transforming Growth Factor β -Induced Protein in Corneal Dystrophies Compared to the Nonfibrillating R555W and R555Q Mutants. <i>Biochemistry</i> , 2015 , 54, 5546-56	3.2	4
76	Dynamics of fluorescent dyes attached to G-quadruplex DNA and their effect on FRET experiments. <i>ChemPhysChem</i> , 2015 , 16, 2562-70	3.2	9
75	Insights to ligand binding to the monoamine transporters-from homology modeling to LeuBAT and dDAT. <i>Frontiers in Pharmacology</i> , 2015 , 6, 208	5.6	21
74	Monoamine transporters: insights from molecular dynamics simulations. <i>Frontiers in Pharmacology</i> , 2015 , 6, 235	5.6	51
73	Bicelles and Other Membrane Mimics: Comparison of Structure, Properties, and Dynamics from MD Simulations. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 15831-43	3.4	31
72	Thermodynamic and structural investigation of the specific SDS binding of Humicola insolens cutinase. <i>Protein Science</i> , 2014 , 23, 1023-35	6.3	26
71	The importance of being capped: Terminal capping of an amyloidogenic peptide affects fibrillation propensity and fibril morphology. <i>Biochemistry</i> , 2014 , 53, 6968-80	3.2	25
70	Molecular basis for selective serotonin reuptake inhibition by the antidepressant agent fluoxetine (Prozac). <i>Molecular Pharmacology</i> , 2014 , 85, 703-14	4.3	47
69	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, 5119-29	3.4	13
68	Binding-induced fluorescence of serotonin transporter ligands: A spectroscopic and structural study of 4-(4-(dimethylamino)phenyl)-1-methylpyridinium (APP(+)) and APP(+) analogues. <i>ACS Chemical Neuroscience</i> , 2014 , 5, 296-304	5.7	14

67	Binding of mazindol and analogs to the human serotonin and dopamine transporters. <i>Molecular Pharmacology</i> , 2014 , 85, 208-17	4.3	18
66	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, 15114-28	16.4	38
65	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, 2812-22	4	28
64	Hot-spot mapping of the interactions between chymosin and bovine κ casein. <i>Journal of Agricultural and Food Chemistry</i> , 2013 , 61, 7949-59	5.7	10
63	Comparative modeling of the human monoamine transporters: similarities in substrate binding. <i>ACS Chemical Neuroscience</i> , 2013 , 4, 295-309	5.7	49
62	Water-mediated interactions influence the binding of thapsigargin to sarco/endoplasmic reticulum calcium adenosinetriphosphatase. <i>Journal of Medicinal Chemistry</i> , 2013 , 56, 3609-19	8.3	23
61	Solvent Binding Analysis and Computational Alanine Scanning of the Bovine Chymosin-Bovine κ Casein Complex Using Molecular Integral Equation Theory. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 5706-17	6.4	11
60	Ion pathways in the sarcoplasmic reticulum Ca^{2+} -ATPase. <i>Journal of Biological Chemistry</i> , 2013 , 288, 10759-65	5.4	106
59	Ligand induced conformational changes of the human serotonin transporter revealed by molecular dynamics simulations. <i>PLoS ONE</i> , 2013 , 8, e63635	3.7	43
58	Understanding the phase behavior of coarse-grained model lipid bilayers through computational calorimetry. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 1551-69	3.4	62
57	Binding of the amphetamine-like 1-phenyl-piperazine to monoamine transporters. <i>ACS Chemical Neuroscience</i> , 2012 , 3, 693-705	5.7	26
56	Tracing cytoplasmic Ca^{2+} ion and water access points in the Ca^{2+} -ATPase. <i>Biophysical Journal</i> , 2012 , 102, 268-77	2.9	22
55	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, 1556-69	6.4	28
54	Molecular docking with ligand attached water molecules. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 909-17	6.1	58
53	Initial stage of cheese production: a molecular modeling study of bovine and camel chymosin complexed with peptides from the chymosin-sensitive region of κ casein. <i>Journal of Agricultural and Food Chemistry</i> , 2011 , 59, 5636-47	5.7	22
52	Mutual adaptation of a membrane protein and its lipid bilayer during conformational changes. <i>Nature Communications</i> , 2011 , 2, 304	17.4	89
51	Synthesis of uronic-noeurostegine--a potent bacterial β -glucuronidase inhibitor. <i>Organic and Biomolecular Chemistry</i> , 2011 , 9, 7807-13	3.9	21
50	Protofibrillar Assembly Toward the Formation of Amyloid Fibrils. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 2385-2390	6.4	34

49	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, 11109-20	3.2	32
48	Unbiased simulations reveal the inward-facing conformation of the human serotonin transporter and Na(+) ion release. <i>PLoS Computational Biology</i> , 2011 , 7, e1002246	5	44
47	Binding and orientation of tricyclic antidepressants within the central substrate site of the human serotonin transporter. <i>Journal of Biological Chemistry</i> , 2010 , 285, 8363-74	5.4	79
46	Bovine chymosin: a computational study of recognition and binding of bovine kappa-casein. <i>Biochemistry</i> , 2010 , 49, 2563-73	3.2	21
45	The two enantiomers of citalopram bind to the human serotonin transporter in reversed orientations. <i>Journal of the American Chemical Society</i> , 2010 , 132, 1311-22	16.4	74
44	Conformational flexibility of chitosan: a molecular modeling study. <i>Biomacromolecules</i> , 2010 , 11, 3196-207	6.1	61
43	P-type ATPases as drug targets: tools for medicine and science. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2009 , 1787, 207-20	4.6	109
42	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, 6928-37	3.4	60
41	Importance of C-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, 10253-62	16.4	37
40	Residue-specific information about the dynamics of antimicrobial peptides from (1)H-(15)N and (2)H solid-state NMR spectroscopy. <i>Journal of the American Chemical Society</i> , 2009 , 131, 18335-42	16.4	32
39	Substrate binding and formation of an occluded state in the leucine transporter. <i>Biophysical Journal</i> , 2008 , 94, 1600-12	2.9	87
38	Binding of serotonin to the human serotonin transporter. Molecular modeling and experimental validation. <i>Journal of the American Chemical Society</i> , 2008 , 130, 3853-65	16.4	109
37	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, 4337-47	2.9	113
36	Exploring interactions of endocrine-disrupting compounds with different conformations of the human estrogen receptor alpha ligand binding domain: a molecular docking study. <i>Chemical Research in Toxicology</i> , 2008 , 21, 2195-206	4	54
35	Resolution enhancement in solid-state NMR of oriented membrane proteins by anisotropic differential linebroadening. <i>Journal of the American Chemical Society</i> , 2008 , 130, 5028-9	16.4	16
34	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, 1037-47	3.5	12
33	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, 345-51	2.8	32
32	Enantioselective proteins: selection, binding studies and molecular modeling of antibodies with affinity towards hydrophobic BINOL derivatives. <i>ChemBioChem</i> , 2007 , 8, 1974-80	3.8	8

31	The low-barrier hydrogen bond of deuterated benzoylacetone probed by very low temperature neutron and X-ray diffraction studies and theoretical calculations. <i>Chemistry - A European Journal</i> , 2007 , 13, 5539-47	4.8	23
30	Comparative MD analysis of the stability of transthyretin providing insight into the fibrillation mechanism. <i>Biopolymers</i> , 2007 , 86, 73-82	2.2	19
29	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, 5262-74	3.4	9
28	Conformational dynamics of the estrogen receptor alpha: molecular dynamics simulations of the influence of binding site structure on protein dynamics. <i>Biochemistry</i> , 2007 , 46, 1743-58	3.2	76
27	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, 387-96	3.8	15
26	Cofactor activation and substrate binding in pyruvate decarboxylase. Insights into the reaction mechanism from molecular dynamics simulations. <i>Biochemistry</i> , 2005 , 44, 14792-806	3.2	23
25	Mechanistic investigation of the 2,5-diphenylpyrrolidine-catalyzed enantioselective alpha-chlorination of aldehydes. <i>Chemistry - A European Journal</i> , 2005 , 11, 7083-90	4.8	73
24	Testing theory beyond molecular structure: Electron density distributions of complex molecules. <i>International Journal of Quantum Chemistry</i> , 2004 , 96, 23-31	2.1	8
23	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	2.1	5
22	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 , 498-9	5.8	11
21	Electron density distributions of redox active mixed valence carboxylate bridged trinuclear iron complexes. <i>Journal of the American Chemical Society</i> , 2003 , 125, 11088-99	16.4	60
20	Reaction mechanism of soluble epoxide hydrolase: insights from molecular dynamics simulations. <i>Journal of the American Chemical Society</i> , 2002 , 124, 14558-70	16.4	59
19	The charge density distribution in a model compound of the catalytic triad in serine proteases. <i>Chemistry - A European Journal</i> , 2001 , 7, 3756-67	4.8	68
18	Starke N-H...O-Wasserstoffbrückenbindungen in einer Modellverbindung für die katalytische Triade in Serinproteasen. <i>Angewandte Chemie</i> , 1999 , 111, 1321-1324	3.6	5
17	Strong N-H...O Hydrogen Bonding in a Model Compound of the Catalytic Triad in Serine Proteases. <i>Angewandte Chemie - International Edition</i> , 1999 , 38, 1239-1242	16.4	57
16	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	16.4	44
15	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	16.4	28
14	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	16.4	115

13	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, 12799-802	11.5	120
12	Enantioselective Hydrosilylation of Ketones with a Chiral Titanocene Catalyst. <i>Journal of the American Chemical Society</i> , 1994 , 116, 11667-11670	16.4	153
11	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		13
10	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		5
9	The oxidative species on a vanadyl pyrophosphate surface. <i>Catalysis Today</i> , 1993 , 16, 79-90	5.3	21
8	Regioselective monoepoxidation of 1,3-dienes catalysed by transition-metal complexes. <i>Journal of the Chemical Society Chemical Communications</i> , 1992 , 1072-1074		13
7	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	3.8	4
6	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		48
5	Coadsorption of carbon monoxide and hydrogen on the nickel(100) surface: a theoretical investigation of site preferences and surface bonding. <i>The Journal of Physical Chemistry</i> , 1990 , 94, 1554-1564		22
4	Ethylidyne on the rhodium(100) surface: a theoretical investigation. <i>Langmuir</i> , 1990 , 6, 806-816	4	10
3	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
2	Molecular mechanism of high affinity sugar transport in plants unveiled by structures of glucose/H ⁺ symporter STP10		1
1	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations		1