Birgit Schitt

List of Publications by Citations

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	Enantioselective Hydrosilylation of Ketones with a Chiral Titanocene Catalyst. *Journal of the American Chemical Society*, **1994**, 116, 11667-11670	16.4	153
119	On the electronic nature of low-barrier hydrogen bonds in enzymatic reactions. *Proceedings of the National Academy of Sciences of the United States of America*, **1998**, 95, 12799-802	11.5	120
118	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. *Journal of the American Chemical Society*, **1998**, 120, 12117-12124	16.4	115
117	Peptide aggregation and pore formation in a lipid bilayer: a combined coarse-grained and all atom molecular dynamics study. *Biophysical Journal*, **2008**, 95, 4337-47	2.9	113
116	P-type ATPases as drug targets: tools for medicine and science. *Biochimica Et Biophysica Acta - Bioenergetics*, **2009**, 1787, 207-20	4.6	109
115	Binding of serotonin to the human serotonin transporter. Molecular modeling and experimental validation. *Journal of the American Chemical Society*, **2008**, 130, 3853-65	16.4	109
114	Ion pathways in the sarcoplasmic reticulum Ca2+-ATPase. *Journal of Biological Chemistry*, **2013**, 288, 10759-65	5.4	106
113	The influence of cholesterol on membrane protein structure, function, and dynamics studied by molecular dynamics simulations. *Biochimica Et Biophysica Acta - Biomembranes*, **2015**, 1848, 1783-95	3.8	105
112	Mutual adaptation of a membrane protein and its lipid bilayer during conformational changes. *Nature Communications*, **2011**, 2, 304	17.4	89
111	Substrate binding and formation of an occluded state in the leucine transporter. *Biophysical Journal* , **2008**, 94, 1600-12	2.9	87
110	Binding and orientation of tricyclic antidepressants within the central substrate site of the human serotonin transporter. *Journal of Biological Chemistry*, **2010**, 285, 8363-74	5.4	79
109	Conformational dynamics of the estrogen receptor alpha: molecular dynamics simulations of the influence of binding site structure on protein dynamics. *Biochemistry*, **2007**, 46, 1743-58	3.2	76
108	The two enantiomers of citalopram bind to the human serotonin transporter in reversed orientations. *Journal of the American Chemical Society*, **2010**, 132, 1311-22	16.4	74
107	Mechanistic investigation of the 2,5-diphenylpyrrolidine-catalyzed enantioselective alpha-chlorination of aldehydes. *Chemistry - A European Journal*, **2005**, 11, 7083-90	4.8	73
106	The charge density distribution in a model compound of the catalytic triad in serine proteases. *Chemistry - A European Journal*, **2001**, 7, 3756-67	4.8	68
105	Understanding the phase behavior of coarse-grained model lipid bilayers through computational calorimetry. *Journal of Physical Chemistry B*, **2012**, 116, 1551-69	3.4	62
104	Conformational flexibility of chitosan: a molecular modeling study. *Biomacromolecules*, **2010**, 11, 3196-207	5.4	61

103	Incorporation of antimicrobial peptides into membranes: a combined liquid-state NMR and molecular dynamics study of alamethicin in DMPC/DHPC bicelles. *Journal of Physical Chemistry B*, **2009**, 113, 6928-37	3.4	60
102	Electron density distributions of redox active mixed valence carboxylate bridged trinuclear iron complexes. *Journal of the American Chemical Society*, **2003**, 125, 11088-99	16.4	60
101	Reaction mechanism of soluble epoxide hydrolase: insights from molecular dynamics simulations. *Journal of the American Chemical Society*, **2002**, 124, 14558-70	16.4	59
100	Molecular docking with ligand attached water molecules. *Journal of Chemical Information and Modeling*, **2011**, 51, 909-17	6.1	58
99	Strong N-H???O Hydrogen Bonding in a Model Compound of the Catalytic Triad in Serine Proteases. *Angewandte Chemie - International Edition*, **1999**, 38, 1239-1242	16.4	57
98	Exploring interactions of endocrine-disrupting compounds with different conformations of the human estrogen receptor alpha ligand binding domain: a molecular docking study. *Chemical Research in Toxicology*, **2008**, 21, 2195-206	4	54
97	A direct interaction of cholesterol with the dopamine transporter prevents its out-to-inward transition. *PLoS Computational Biology*, **2018**, 14, e1005907	5	51
96	Monoamine transporters: insights from molecular dynamics simulations. *Frontiers in Pharmacology*, **2015**, 6, 235	5.6	51
95	Comparative modeling of the human monoamine transporters: similarities in substrate binding. *ACS Chemical Neuroscience*, **2013**, 4, 295-309	5.7	49
94	Formation of maleic anhydride on a vanadyl pyrophosphate surface: a theoretical study of the mechanism. *The Journal of Physical Chemistry*, **1991**, 95, 2297-2307		48
93	Molecular basis for selective serotonin reuptake inhibition by the antidepressant agent fluoxetine (Prozac). *Molecular Pharmacology*, **2014**, 85, 703-14	4.3	47
92	A conserved leucine occupies the empty substrate site of LeuT in the Na(+)-free return state. *Nature Communications*, **2016**, 7, 11673	17.4	44
91	Unbiased simulations reveal the inward-facing conformation of the human serotonin transporter and Na(+) ion release. *PLoS Computational Biology*, **2011**, 7, e1002246	5	44
90	Molecular Dynamics Simulations of Ground and Transition States for the Hydride Transfer from Formate to NAD+in the Active Site of Formate Dehydrogenase. *Journal of the American Chemical Society*, **1999**, 121, 8164-8173	16.4	44
89	A direct view of the complex multi-pathway folding of telomeric G-quadruplexes. *Nucleic Acids Research*, **2016**, 44, 11024-11032	20.1	43
88	Ligand induced conformational changes of the human serotonin transporter revealed by molecular dynamics simulations. *PLoS ONE*, **2013**, 8, e63635	3.7	43
87	Identification of a common binding mode for imaging agents to amyloid fibrils from molecular dynamics simulations. *Journal of the American Chemical Society*, **2013**, 135, 15114-28	16.4	38
86	Importance of C-N bond rotation in N-acyl oxazolidinones in their SmI2-promoted coupling to acrylamides. *Journal of the American Chemical Society*, **2009**, 131, 10253-62	16.4	37

85	Protofibrillar Assembly Toward the Formation of Amyloid Fibrils. *Journal of Physical Chemistry Letters*, **2011**, 2, 2385-2390	6.4	34
84	Cholesterol binding to a conserved site modulates the conformation, pharmacology, and transport kinetics of the human serotonin transporter. *Journal of Biological Chemistry*, **2018**, 293, 3510-3523	5.4	33
83	Protonation states of important acidic residues in the central Ca□+ ion binding sites of the Ca□+-ATPase: a molecular modeling study. *Biochemistry*, **2011**, 50, 11109-20	3.2	32
82	Residue-specific information about the dynamics of antimicrobial peptides from (1)H-(15)N and (2)H solid-state NMR spectroscopy. *Journal of the American Chemical Society*, **2009**, 131, 18335-42	16.4	32
81	Short strong hydrogen bonds in 2-acetyl-1,8-dihydroxy-3,6-dimethylnaphthalene: an outlier to current hydrogen bonding theory?. *Journal of Physical Chemistry A*, **2007**, 111, 345-51	2.8	32
80	Bicelles and Other Membrane Mimics: Comparison of Structure, Properties, and Dynamics from MD Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 15831-43	3.4	31
79	Mutation in transforming growth factor beta induced protein associated with granular corneal dystrophy type 1 reduces the proteolytic susceptibility through local structural stabilization. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2013**, 1834, 2812-22	4	28
78	Modeling the Self-Assembly and Stability of DHPC Micelles Using Atomic Resolution and Coarse Grained MD Simulations. *Journal of Chemical Theory and Computation*, **2012**, 8, 1556-69	6.4	28
77	Theoretical Investigation of the Hydride Transfer from Formate to NAD+and the Implications for the Catalytic Mechanism of Formate Dehydrogenase. *Journal of the American Chemical Society*, **1998**, 120, 7192-7200	16.4	28
76	Thermodynamic and structural investigation of the specific SDS binding of Humicola insolens cutinase. *Protein Science*, **2014**, 23, 1023-35	6.3	26
75	Binding of the amphetamine-like 1-phenyl-piperazine to monoamine transporters. *ACS Chemical Neuroscience*, **2012**, 3, 693-705	5.7	26
74	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. *Journal of Membrane Biology*, **2018**, 251, 609-631	2.3	26
73	The importance of being capped: Terminal capping of an amyloidogenic peptide affects fibrillation propensity and fibril morphology. *Biochemistry*, **2014**, 53, 6968-80	3.2	25
72	Water-mediated interactions influence the binding of thapsigargin to sarco/endoplasmic reticulum calcium adenosinetriphosphatase. *Journal of Medicinal Chemistry*, **2013**, 56, 3609-19	8.3	23
71	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, 5539-47	4.8	23
70	Cofactor activation and substrate binding in pyruvate decarboxylase. Insights into the reaction mechanism from molecular dynamics simulations. *Biochemistry*, **2005**, 44, 14792-806	3.2	23
69	Dimer Interface of the Human Serotonin Transporter and Effect of the Membrane Composition. *Scientific Reports*, **2018**, 8, 5080	4.9	22
68	Tracing cytoplasmic Ca(2+) ion and water access points in the Ca(2+)-ATPase. *Biophysical Journal*, **2012**, 102, 268-77	2.9	22

67	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. *Journal of Agricultural and Food Chemistry*, **2011**, 59, 5636-47	5.7	22
66	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		22
65	Properties of an inward-facing state of LeuT: conformational stability and substrate release. *Biophysical Journal*, **2015**, 108, 1390-1399	2.9	21
64	Conformational Dynamics of the Human Islet Amyloid Polypeptide in a Membrane Environment: Toward the Aggregation Prone Form. *Biochemistry*, **2016**, 55, 2031-42	3.2	21
63	Insights to ligand binding to the monoamine transporters-from homology modeling to LeuBAT and dDAT. *Frontiers in Pharmacology*, **2015**, 6, 208	5.6	21
62	Synthesis of uronic-noeurostegine--a potent bacterial β-glucuronidase inhibitor. *Organic and Biomolecular Chemistry*, **2011**, 9, 7807-13	3.9	21
61	Bovine chymosin: a computational study of recognition and binding of bovine kappa-casein. *Biochemistry*, **2010**, 49, 2563-73	3.2	21
60	The oxidative species on a vanadyl pyrophosphate surface. *Catalysis Today*, **1993**, 16, 79-90	5.3	21
59	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations. *ELife*, **2020**, 9,	8.9	20
58	In Vitro Effects of the Endocrine Disruptor p,pSDDT on Human Follitropin Receptor. *Environmental Health Perspectives*, **2016**, 124, 991-9	8.4	20
57	Binding of the multimodal antidepressant drug vortioxetine to the human serotonin transporter. *ACS Chemical Neuroscience*, **2015**, 6, 1892-900	5.7	19
56	Identification of Key Interactions in the Initial Self-Assembly of Amylin in a Membrane Environment. *Biochemistry*, **2017**, 56, 4884-4894	3.2	19
55	Comparative MD analysis of the stability of transthyretin providing insight into the fibrillation mechanism. *Biopolymers*, **2007**, 86, 73-82	2.2	19
54	Binding of mazindol and analogs to the human serotonin and dopamine transporters. *Molecular Pharmacology*, **2014**, 85, 208-17	4.3	18
53	Reactive Center Loop Insertion in α1-Antitrypsin Captured by Accelerated Molecular Dynamics Simulation. *Biochemistry*, **2017**, 56, 634-646	3.2	16
52	Resolution enhancement in solid-state NMR of oriented membrane proteins by anisotropic differential linebroadening. *Journal of the American Chemical Society*, **2008**, 130, 5028-9	16.4	16
51	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. *Biochemical Journal*, **2006**, 399, 387-96	3.8	15
50	Capturing Biologically Complex Tissue-Specific Membranes at Different Levels of Compositional Complexity. *Journal of Physical Chemistry B*, **2020**, 124, 7819-7829	3.4	15

49	Structural Basis for Simvastatin Competitive Antagonism of Complement Receptor 3. *Journal of Biological Chemistry*, **2016**, 291, 16963-76	5.4	15
48	Synthesis and inhibitory evaluation of 3-linked imipramines for the exploration of the S2 site of the human serotonin transporter. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 2725-38	3.4	15
47	Interrogating the Molecular Basis for Substrate Recognition in Serotonin and Dopamine Transporters with High-Affinity Substrate-Based Bivalent Ligands. *ACS Chemical Neuroscience*, **2016**, 7, 1406-1417	5.7	14
46	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	5.7	14
45	Lipid dynamics studied by calculation of 31P solid-state NMR spectra using ensembles from molecular dynamics simulations. *Journal of Physical Chemistry B*, **2014**, 118, 5119-29	3.4	13
44	Addition of a carbonyl functionality to titanium carbenes. A study of the mechanism and intermediates in the Tebbe reaction. *Journal of the Chemical Society Dalton Transactions*, **1993**, 337-344		13
43	Regioselective monoepoxidation of 1,3-dienes catalysed by transition-metal complexes. *Journal of the Chemical Society Chemical Communications*, **1992**, 1072-1074		13
42	A DFT study of solvation effects on the tautomeric equilibrium and catalytic ylide generation of thiamin models. *Journal of Computational Chemistry*, **2008**, 29, 1037-47	3.5	12
41	Solvent Binding Analysis and Computational Alanine Scanning of the Bovine Chymosin-Bovine □Casein Complex Using Molecular Integral Equation Theory. *Journal of Chemical Theory and Computation*, **2013**, 9, 5706-17	6.4	11
40	The influence of solvation on short strong hydrogen bonds: a density functional theory study of the Asp-His interaction in subtilisins. *Chemical Communications*, **2004**, 498-9	5.8	11
39	Hot-spot mapping of the interactions between chymosin and bovine □casein. *Journal of Agricultural and Food Chemistry*, **2013**, 61, 7949-59	5.7	10
38	Ethylidyne on the rhodium(100) surface: a theoretical investigation. *Langmuir*, **1990**, 6, 806-816	4	10
37	Ligand Binding in the Extracellular Vestibule of the Neurotransmitter Transporter Homologue LeuT. *ACS Chemical Neuroscience*, **2017**, 8, 619-628	5.7	9
36	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. *Biochimica Et Biophysica Acta - General Subjects*, **2016**, 1860, 648-60	4	9
35	Dynamics of fluorescent dyes attached to G-quadruplex DNA and their effect on FRET experiments. *ChemPhysChem*, **2015**, 16, 2562-70	3.2	9
34	QSAR studies and pharmacophore identification for arylsubstituted cycloalkenecarboxylic acid methyl esters with affinity for the human dopamine transporter. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 5262-74	3.4	9
33	Simulations of membrane-bound diglycosylated human prion protein reveal potential protective mechanisms against misfolding. *Journal of Neurochemistry*, **2017**, 142, 171-182	6	8
32	Substrate and inhibitor binding to the serotonin transporter: Insights from computational, crystallographic, and functional studies. *Neuropharmacology*, **2019**, 161, 107548	5.5	8

31	Enantioselective proteins: selection, binding studies and molecular modeling of antibodies with affinity towards hydrophobic BINOL derivatives. *ChemBioChem*, **2007**, 8, 1974-80	3.8	8
30	Testing theory beyond molecular structure: Electron density distributions of complex molecules. *International Journal of Quantum Chemistry*, **2004**, 96, 23-31	2.1	8
29	Insight into the molecular mechanism behind PEG-mediated stabilization of biofluid lipases. *Scientific Reports*, **2018**, 8, 12293	4.9	7
28	Novel noscapine derivatives stabilize the native state of insulin against fibrillation. *International Journal of Biological Macromolecules*, **2020**, 147, 98-108	7.9	7
27	Structure and Dynamics of Cinnamycin-Lipid Complexes: Mechanisms of Selectivity for Phosphatidylethanolamine Lipids. *ACS Omega*, **2019**, 4, 18889-18899	3.9	7
26	Modeling and Mutational Analysis of the Binding Mode for the Multimodal Antidepressant Drug Vortioxetine to the Human 5-HT Receptor. *Molecular Pharmacology*, **2018**, 94, 1421-1434	4.3	7
25	Molecular Modeling Investigation of the Interaction between Humicola insolens Cutinase and SDS Surfactant Suggests a Mechanism for Enzyme Inactivation. *Journal of Chemical Information and Modeling*, **2019**, 59, 1977-1987	6.1	6
24	A Photoswitchable Inhibitor of the Human Serotonin Transporter. *ACS Chemical Neuroscience*, **2020**, 11, 1231-1237	5.7	6
23	Revealing a Dual Role of Ganglioside Lipids in the Aggregation of Membrane-Associated Islet Amyloid Polypeptide. *Journal of Membrane Biology*, **2019**, 252, 343-356	2.3	5
22	Possible involvement of collective domain movement in the catalytic reaction of soluble epoxide hydrolase. *International Journal of Quantum Chemistry*, **2004**, 99, 61-69	2.1	5
21	Starke N□???O-Wasserstoffbr□kenbindungen in einer Modellverbindung f□ die katalytische Triade in Serinproteasen. *Angewandte Chemie*, **1999**, 111, 1321-1324	3.6	5
20	Stepwise or concerted addition of 1,3-butadiene to oxygen adsorbed on the silver (110) surface?. *The Journal of Physical Chemistry*, **1993**, 97, 10738-10741		5
19	Interaction of Amyloid-□-(1-42) Peptide and Its Aggregates with Lipid/Water Interfaces Probed by Vibrational Sum-Frequency Generation Spectroscopy. *Journal of Physical Chemistry B*, **2021**, 125, 11208-11218	3.4	5
18	Early Events in the Amyloid Formation of the A546T Mutant of Transforming Growth Factor □-Induced Protein in Corneal Dystrophies Compared to the Nonfibrillating R555W and R555Q Mutants. *Biochemistry*, **2015**, 54, 5546-56	3.2	4
17	Allosteric-Activation Mechanism of Bovine Chymosin Revealed by Bias-Exchange Metadynamics and Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 10453-10462	3.4	4
16	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. *Organometallics*, **1992**, 11, 4213-4221	3.8	4
15	How a short pore forming peptide spans the lipid membrane. *Biointerphases*, **2017**, 12, 02D405	1.8	3
14	The Effect of Cholesterol on Membrane-Bound Islet Amyloid Polypeptide. *Frontiers in Molecular Biosciences*, **2021**, 8, 657946	5.6	3

13	Molecular mechanism of sugar transport in plants unveiled by structures of glucose/H symporter STP10. *Nature Plants*, **2021**, 7, 1409-1419	11.5	3
12	Molecular modeling of neurological membrane proteins - from binding sites to synapses. *Neuroscience Letters*, **2019**, 700, 38-49	3.3	2
11	Membrane Interactions of IAPP. *Biophysical Journal*, **2019**, 116, 491a	2.9	2
10	Beneficent and Maleficent Effects of Cations on Bufadienolide Binding to Na,K-ATPase. *Journal of Chemical Information and Modeling*, **2021**, 61, 976-986	6.1	2
9	Studies of the oxidative addition of some substrates containing carbon–heteroatom bonds to some tungsten and platinum complexes. *Journal of the Chemical Society Dalton Transactions*, **1989**, 2099-2107		1
8	Molecular mechanism of high affinity sugar transport in plants unveiled by structures of glucose/H+ symporter STP10		1
7	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations		1
6	Simulating Multiple Substrate-Binding Events by γ-Glutamyltransferase Using Accelerated Molecular Dynamics. *Journal of Physical Chemistry B*, **2020**, 124, 10104-10116	3.4	1
5	Effect of cholesterol on the dimerization of C99-A molecular modeling perspective. *Biointerphases*, **2021**, 16, 031002	1.8	1
4	General Protocol for Constructing Molecular Models of Nanodiscs. *Journal of Chemical Information and Modeling*, **2021**, 61, 2869-2883	6.1	1
3	Conformational Changes in the 5-HT Receptor Extracellular Domain Measured by Voltage-Clamp Fluorometry. *Molecular Pharmacology*, **2019**, 96, 720-734	4.3	1
2	Effect of palmitoylation on the dimer formation of the human dopamine transporter. *Scientific Reports*, **2021**, 11, 4164	4.9	0
1	On the effect of mutations in bovine or camel chymosin on the thermodynamics of binding to κ-caseins. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 75-87	4.2	0