

# Birgit SchiÄ,tt

## List of Publications by Year in descending order

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131  
papers

4,474  
citations

87843

38  
h-index

128225

60  
g-index

141  
all docs

141  
docs citations

141  
times ranked

5560  
citing authors

#	ARTICLE	IF	CITATIONS
1	Binding and Activation of Serotonergic G-Protein Coupled Receptors by the Multimodal Antidepressant Vortioxetine. ACS Chemical Neuroscience, 2022, 13, 1129-1142.	1.7	1
2	Effect of palmitoylation on the dimer formation of the human dopamine transporter. Scientific Reports, 2021, 11, 4164.	1.6	8
3	The Effect of Cholesterol on Membrane-Bound Islet Amyloid Polypeptide. Frontiers in Molecular Biosciences, 2021, 8, 657946.	1.6	7
4	Effect of cholesterol on the dimerization of C99A molecular modeling perspective. Biointerphases, 2021, 16, 031002.	0.6	4
5	General Protocol for Constructing Molecular Models of Nanodiscs. Journal of Chemical Information and Modeling, 2021, 61, 2869-2883.	2.5	11
6	Molecular mechanism of sugar transport in plants unveiled by structures of glucose/H <sup>+</sup> symporter STP10. Nature Plants, 2021, 7, 1409-1419.	4.7	27
7	Interaction of Amyloid- $\beta$ -(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.	1.2	13
8	Beneficent and Maleficent Effects of Cations on Bufadienolide Binding to Na <sup>+</sup> ,K <sup>+</sup> -ATPase. Journal of Chemical Information and Modeling, 2021, 61, 976-986.	2.5	2
9	Novel nospapine derivatives stabilize the native state of insulin against fibrillation. International Journal of Biological Macromolecules, 2020, 147, 98-108.	3.6	15
10	A Generic Protocol for Constructing Molecular Models of Nanodiscs in Silico. Biophysical Journal, 2020, 118, 385a.	0.2	0
11	Simulating Multiple Substrate-Binding Events by $\hat{1}^3$ -Glutamyltransferase Using Accelerated Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 10104-10116.	1.2	2
12	Capturing Biologically Complex Tissue-Specific Membranes at Different Levels of Compositional Complexity. Journal of Physical Chemistry B, 2020, 124, 7819-7829.	1.2	47
13	Allosteric Network Analysis in the NMDA Receptor. Biophysical Journal, 2020, 118, 417a.	0.2	0
14	Folding Kinetics of Multiple G-Quadruplex Telomeric DNA Structures. Biophysical Journal, 2020, 118, 335a.	0.2	0
15	A Photoswitchable Inhibitor of the Human Serotonin Transporter. ACS Chemical Neuroscience, 2020, 11, 1231-1237.	1.7	14
16	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations. ELife, 2020, 9, .	2.8	49
17	Molecular modeling of neurological membrane proteins $\hat{1}$ from binding sites to synapses. Neuroscience Letters, 2019, 700, 38-49.	1.0	3
18	Membrane Interactions of IAPP. Biophysical Journal, 2019, 116, 491a.	0.2	3

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19	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
20	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
21	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
22	Substrate and inhibitor binding to the serotonin transporter: Insights from computational, crystallographic, and functional studies. <i>Neuropharmacology</i> , 2019, 161, 107548.	2.0	15
23	Structure and Dynamics of Cinnamycin-Lipid Complexes: Mechanisms of Selectivity for Phosphatidylethanolamine Lipids. <i>ACS Omega</i> , 2019, 4, 18889-18899.	1.6	14
24	Conformational Changes in the 5-HT <sub>3A</sub> Receptor Extracellular Domain Measured by Voltage-Clamp Fluorometry. <i>Molecular Pharmacology</i> , 2019, 96, 720-734.	1.0	7
25	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
26	On the effect of mutations in bovine or camel chymosin on the thermodynamics of binding $\hat{\rho}$ -caseins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 75-87.	1.5	1
27	Modeling and Mutational Analysis of the Binding Mode for the Multimodal Antidepressant Drug Vortioxetine to the Human 5-HT <sub>3A</sub> Receptor. <i>Molecular Pharmacology</i> , 2018, 94, 1421-1434.	1.0	14
28	Understanding Conformational Dynamics of Complex Lipid Mixtures Relevant to Biology. <i>Journal of Membrane Biology</i> , 2018, 251, 609-631.	1.0	33
29	Dimer Interface of the Human Serotonin Transporter and Effect of the Membrane Composition. <i>Scientific Reports</i> , 2018, 8, 5080.	1.6	32
30	Insight into the molecular mechanism behind PEG-mediated stabilization of biofluid lipases. <i>Scientific Reports</i> , 2018, 8, 12293.	1.6	15
31	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
32	Simulations of membrane-bound diglycosylated human prion protein reveal potential protective mechanisms against misfolding. <i>Journal of Neurochemistry</i> , 2017, 142, 171-182.	2.1	10
33	How a short pore forming peptide spans the lipid membrane. <i>Biointerphases</i> , 2017, 12, 02D405.	0.6	6
34	Mapping Cholesterol Binding Sites on the Human Dopamine Transporter. <i>Biophysical Journal</i> , 2017, 112, 339a.	0.2	0
35	Ligand Binding in the Extracellular Vestibule of the Neurotransmitter Transporter Homologue LeuT. <i>ACS Chemical Neuroscience</i> , 2017, 8, 619-628.	1.7	10
36	Reactive Center Loop Insertion in $\hat{\rho}$ -1-Antitrypsin Captured by Accelerated Molecular Dynamics Simulation. <i>Biochemistry</i> , 2017, 56, 634-646.	1.2	20

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37	Identification of Key Interactions in the Initial Self-Assembly of Amylin in a Membrane Environment. <i>Biochemistry</i> , 2017, 56, 4884-4894.	1.2	27
38	<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
39	Structural Basis for Simvastatin Competitive Antagonism of Complement Receptor 3. <i>Journal of Biological Chemistry</i> , 2016, 291, 16963-16976.	1.6	25
40	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
41	Probing the Folding Dynamics of Human Telomeric G-Quadruplex with Single-Molecule FRET. <i>Biophysical Journal</i> , 2016, 110, 406a.	0.2	0
42	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
43	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
44	A conserved leucine occupies the empty substrate site of LeuT in the Na <sup>+</sup> -free return state. <i>Nature Communications</i> , 2016, 7, 11673.	5.8	58
45	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
46	Conformational Dynamics of the Human Islet Amyloid Polypeptide in a Membrane Environment: Toward the Aggregation Prone Form. <i>Biochemistry</i> , 2016, 55, 2031-2042.	1.2	27
47	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
48	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
49	Insights to ligand binding to the monoamine transporters" from homology modeling to LeuBAT and dDAT. <i>Frontiers in Pharmacology</i> , 2015, 6, 208.	1.6	23
50	Monoamine transporters: insights from molecular dynamics simulations. <i>Frontiers in Pharmacology</i> , 2015, 6, 235.	1.6	60
51	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
52	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
53	Properties of an Inward-Facing State of LeuT: Conformational Stability and Substrate Release. <i>Biophysical Journal</i> , 2015, 108, 1390-1399.	0.2	26
54	Binding of the Multimodal Antidepressant Drug Vortioxetine to the Human Serotonin Transporter. <i>ACS Chemical Neuroscience</i> , 2015, 6, 1892-1900.	1.7	27

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55	Early Events in the Amyloid Formation of the A546T Mutant of Transforming Growth Factor $\beta$ -Induced Protein in Corneal Dystrophies Compared to the Nonfibrillating R555W and R555Q Mutants. <i>Biochemistry</i> , 2015, 54, 5546-5556.	1.2	6
56	Binding of Mazindol and Analogs to the Human Serotonin and Dopamine Transporters. <i>Molecular Pharmacology</i> , 2014, 85, 208-217.	1.0	22
57	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
58	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
59	Molecular Basis for Selective Serotonin Reuptake Inhibition by the Antidepressant Agent Fluoxetine (Prozac). <i>Molecular Pharmacology</i> , 2014, 85, 703-714.	1.0	54
60	Lipid Dynamics Studied by Calculation of $^{31}\text{P}$ Solid-State NMR Spectra Using Ensembles from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5119-5129.	1.2	15
61	Binding-Induced Fluorescence of Serotonin Transporter Ligands: A Spectroscopic and Structural Study of 4-(4-(Dimethylamino)phenyl)-1-methylpyridinium (APP <sup>+</sup> ) and APP <sup>+</sup> Analogues. <i>ACS Chemical Neuroscience</i> , 2014, 5, 296-304.	1.7	21
62	Aggregation of Transforming Growth Factor $\beta$ Induced Protein Studied by Protein-Protein Docking. <i>Biophysical Journal</i> , 2014, 106, 681a.	0.2	0
63	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
64	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
65	Hot-Spot Mapping of the Interactions between Chymosin and Bovine $\beta$ -Casein. <i>Journal of Agricultural and Food Chemistry</i> , 2013, 61, 7949-7959.	2.4	13
66	Comparative Modeling of the Human Monoamine Transporters: Similarities in Substrate Binding. <i>ACS Chemical Neuroscience</i> , 2013, 4, 295-309.	1.7	59
67	Conformational Stability and Substrate Translocation - A Computational Study of the Leucine Transporter. <i>Biophysical Journal</i> , 2013, 104, 407a-408a.	0.2	0
68	Water-Mediated Interactions Influence the Binding of Thapsigargin to Sarco/Endoplasmic Reticulum Calcium Adenosinetriphosphatase. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 3609-3619.	2.9	23
69	Solvent Binding Analysis and Computational Alanine Scanning of the Bovine Chymosin $\beta$ -Casein Complex Using Molecular Integral Equation Theory. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5706-5717.	2.3	11
70	Ion Pathways in the Sarcoplasmic Reticulum $\text{Ca}^{2+}$ -ATPase. <i>Journal of Biological Chemistry</i> , 2013, 288, 10759-10765.	1.6	125
71	Ligand Induced Conformational Changes of the Human Serotonin Transporter Revealed by Molecular Dynamics Simulations. <i>PLoS ONE</i> , 2013, 8, e63635.	1.1	49
72	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

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73	Binding of the Amphetamine-like 1-Phenyl-piperazine to Monoamine Transporters. ACS Chemical Neuroscience, 2012, 3, 693-705.	1.7	28
74	Tracing Cytoplasmic Ca <sup>2+</sup> Ion and Water Access Points in the Ca <sup>2+</sup> -ATPase. Biophysical Journal, 2012, 102, 268-277.	0.2	25
75	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, 1556-1569.	2.3	33
76	Protofibrillar Assembly Toward the Formation of Amyloid Fibrils. Journal of Physical Chemistry Letters, 2011, 2, 2385-2390.	2.1	39
77	Protonation States of Important Acidic Residues in the Central Ca <sup>2+</sup> Ion Binding Sites of the Ca <sup>2+</sup> -ATPase: A Molecular Modeling Study. Biochemistry, 2011, 50, 11109-11120.	1.2	37
78	Identifying Calcium ion Access Points and Transport Pathways in SERCA. Biophysical Journal, 2011, 100, 467a.	0.2	0
79	Molecular Docking with Ligand Attached Water Molecules. Journal of Chemical Information and Modeling, 2011, 51, 909-917.	2.5	67
80	Initial Stage of Cheese Production: A Molecular Modeling Study of Bovine and Camel Chymosin Complexed with Peptides from the Chymosin-Sensitive Region of Î²-Casein. Journal of Agricultural and Food Chemistry, 2011, 59, 5636-5647.	2.4	26
81	Understanding the Phase Changes of Coarse-Grained Model Bilayers Through Computational Calorimetry. Biophysical Journal, 2011, 100, 332a-333a.	0.2	0
82	Mutual adaptation of a membrane protein and its lipid bilayer during conformational changes. Nature Communications, 2011, 2, 304.	5.8	108
83	Synthesis of uronic-Noeurostegine " a potent bacterial Î²-glucuronidase inhibitor. Organic and Biomolecular Chemistry, 2011, 9, 7807.	1.5	27
84	Unbiased Simulations Reveal the Inward-Facing Conformation of the Human Serotonin Transporter and Na <sup>+</sup> Ion Release. PLoS Computational Biology, 2011, 7, e1002246.	1.5	54
85	Binding and Orientation of Tricyclic Antidepressants within the Central Substrate Site of the Human Serotonin Transporter. Journal of Biological Chemistry, 2010, 285, 8363-8374.	1.6	85
86	Modeling the Membrane Role in Ca <sup>2+</sup> -ATPase Catalytic Cycle. Biophysical Journal, 2010, 98, 487a.	0.2	0
87	A Coarse Grained Molecular Dynamics Study of the Formation and Structure of Bicelles. Biophysical Journal, 2010, 98, 569a.	0.2	0
88	Ca <sup>2+</sup> -ATPase: Lipid-Protein Interaction As Observed in Crystals and MD Simulations. Biophysical Journal, 2010, 98, 20a.	0.2	0
89	Bovine Chymosin: A Computational Study of Recognition and Binding of Bovine Î²-Casein. Biochemistry, 2010, 49, 2563-2573.	1.2	27
90	The Two Enantiomers of Citalopram Bind to the Human Serotonin Transporter in Reversed Orientations. Journal of the American Chemical Society, 2010, 132, 1311-1322.	6.6	79

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91	Conformational Flexibility of Chitosan: A Molecular Modeling Study. <i>Biomacromolecules</i> , 2010, 11, 3196-3207.	2.6	67
92	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
93	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
94	Importance of C $\alpha$ -N Bond Rotation in N-Acyl Oxazolidinones in their SmI <sub>2</sub> -Promoted Coupling to Acrylamides. <i>Journal of the American Chemical Society</i> , 2009, 131, 10253-10262.	6.6	37
95	Residue-Specific Information about the Dynamics of Antimicrobial Peptides from <sup>1</sup> H $\alpha$ and <sup>15</sup> N and <sup>2</sup> H Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2009, 131, 18335-18342.	6.6	35
96	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
97	Substrate Binding and Formation of an Occluded State in the Leucine Transporter. <i>Biophysical Journal</i> , 2008, 94, 1600-1612.	0.2	89
98	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
99	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
100	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, 2195-2206.	1.7	57
101	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
102	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, 1743-1758.	1.2	85
103	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
104	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
105	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, 5539-5547.	1.7	26
106	Comparative MD analysis of the stability of transthyretin providing insight into the fibrillation mechanism. <i>Biopolymers</i> , 2007, 86, 73-82.	1.2	20
107	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
108	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

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109	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
110	Cofactor Activation and Substrate Binding in Pyruvate Decarboxylase. Insights into the Reaction Mechanism from Molecular Dynamics Simulations. <i>Biochemistry</i> , 2005, 44, 14792-14806.	1.2	24
111	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
112	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
113	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
114	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
115	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
116	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
117	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.	7.2	62
118	Molecular Dynamics Simulations of Ground and Transition States for the Hydride Transfer from Formate to NAD <sup>+</sup> in the Active Site of Formate Dehydrogenase. <i>Journal of the American Chemical Society</i> , 1999, 121, 8164-8173.	6.6	52
119	Theoretical Investigation of the Hydride Transfer from Formate to NAD <sup>+</sup> 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
120	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
121	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
122	Enantioselective Hydrosilylation of Ketones with a Chiral Titanocene Catalyst. <i>Journal of the American Chemical Society</i> , 1994, 116, 11667-11670.	6.6	190
123	The oxidative species on a vanadyl pyrophosphate surface. <i>Catalysis Today</i> , 1993, 16, 79-90.	2.2	25
124	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
125	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
126	Regioselective monoepoxidation of 1,3-dienes catalysed by transition-metal complexes. <i>Journal of the Chemical Society Chemical Communications</i> , 1992, , 1072-1074.	2.0	24



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127	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.	1.1	5
128	Formation of maleic anhydride on a vanadyl pyrophosphate surface: a theoretical study of the mechanism. The Journal of Physical Chemistry, 1991, 95, 2297-2307.	2.9	52
129	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
130	Ethylidyne on the rhodium(100) surface: a theoretical investigation. Langmuir, 1990, 6, 806-816.	1.6	11
131	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.	1.1	1