Christofer S Tautermann

List of Publications by Year
in descending order

71	2,932	159525 30	175177 52
papers	citations	h-index	g-index

72	72	72	3897
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Covalent inhibitor reactivity prediction by the electrophilicity indexâ€"in and out of scope. Journal of Computer-Aided Molecular Design, 2021, 35, 531-539.	1.3	7
2	Proteinâ€"ligand free energies of binding from full-protein DFT calculations: convergence and choice of exchangeâ€"correlation functional. Physical Chemistry Chemical Physics, 2021, 23, 9381-9393.	1.3	20
3	BIreactive: A Machine-Learning Model to Estimate Covalent Warhead Reactivity. Journal of Chemical Information and Modeling, 2020, 60, 2915-2923.	2.5	27
4	Current and Future Challenges in Modern Drug Discovery. Methods in Molecular Biology, 2020, 2114, 1-17.	0.4	10
5	A Fast Ab Initio Predictor Tool for Covalent Reactivity Estimation of Acrylamides. Journal of Chemical Information and Modeling, 2019, 59, 3565-3571.	2.5	27
6	Second M 3 muscarinic receptor binding site contributes to bronchoprotection by tiotropium. British Journal of Pharmacology, 2019, 176, 2864-2876.	2.7	7
7	Enhancing Drug Residence Time by Shielding of Intra-Protein Hydrogen Bonds: A Case Study on CCR2 Antagonists. ACS Medicinal Chemistry Letters, 2019, 10, 324-328.	1.3	15
8	Allosteric Activation of Striatal-Enriched Protein Tyrosine Phosphatase (STEP, PTPN5) by a Fragment-like Molecule. Journal of Medicinal Chemistry, 2019, 62, 306-316.	2.9	29
9	Crystal Structure of CC Chemokine Receptor 2A in Complex with an Orthosteric Antagonist Provides Insights for the Design of Selective Antagonists. Structure, 2019, 27, 427-438.e5.	1.6	37
10	Multiple Binding Sites Contribute to the Mechanism of Mixed Agonistic and Positive Allosteric Modulators of the Cannabinoid CB1 Receptor. Angewandte Chemie, 2018, 130, 2610-2615.	1.6	11
11	Identifying Functional Hotspot Residues for Biased Ligand Design in G-Protein-Coupled Receptors. Molecular Pharmacology, 2018, 93, 288-296.	1.0	42
12	Multiple Binding Sites Contribute to the Mechanism of Mixed Agonistic and Positive Allosteric Modulators of the Cannabinoid CB1 Receptor. Angewandte Chemie - International Edition, 2018, 57, 2580-2585.	7.2	43
13	Lateâ€Stage Functionalization of Drugâ€Like Molecules Using Diversinates. ChemMedChem, 2018, 13, 983-987.	1.6	32
14	GPCR Homology Model Generation for Lead Optimization. Methods in Molecular Biology, 2018, 1705, 115-131.	0.4	3
15	Engineering Salt Bridge Networks between Transmembrane Helices Confers Thermostability in G-Protein-Coupled Receptors. Journal of Chemical Theory and Computation, 2018, 14, 6574-6585.	2.3	10
16	Development of a ¹³C NMR Chemical Shift Prediction Procedure Using B3LYP/cc-pVDZ and Empirically Derived Systematic Error Correction Terms: A Computational Small Molecule Structure Elucidation Method. Journal of Organic Chemistry, 2017, 82, 5135-5145.	1.7	58
17	Editorial overview: New technologies: GPCR drug design and function â€" exploiting the current (of) structures. Current Opinion in Pharmacology, 2016, 30, vii-x.	1.7	7
18	Impact, determination and prediction of drugâ€"receptor residence times for GPCRs. Current Opinion in Pharmacology, 2016, 30, 22-26.	1.7	24

#	Article	IF	Citations
19	A â€œStepping Stoneâ€•Approach for Obtaining Quantum Free Energies of Hydration. Journal of Physical Chemistry B, 2015, 119, 7030-7040.	1.2	34
20	GPCR structure, function, drug discovery and crystallography: report from Academia-Industry International Conference (UK Royal Society) Chicheley Hall, 1â€“2 September 2014. Naunyn-Schmiedeberg's Archives of Pharmacology, 2015, 388, 883-903.	1.4	34
21	Energy decomposition analysis approaches and their evaluation on prototypical proteinâ€“drug interaction patterns. Chemical Society Reviews, 2015, 44, 3177-3211.	18.7	284
22	Rodent selectivity of piperidine-4-yl-1H-indoles, a series of CC chemokine receptor-3 (CCR3) antagonists: Insights from a receptor model. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 229-235.	1.0	1
23	What can we learn from molecular dynamics simulations for GPCR drug design?. Computational and Structural Biotechnology Journal, 2015, 13, 111-121.	1.9	60
24	SKINK: a web server for string kernel based kink prediction in Î±-helices. Bioinformatics, 2014, 30, 1769-1770.	1.8	1
25	Computational Method To Identify Druggable Binding Sites That Target Proteinâ€“Protein Interactions. Journal of Chemical Information and Modeling, 2014, 54, 1391-1400.	2.5	22
26	Heteroaromatic Ï€-Stacking Energy Landscapes. Journal of Chemical Information and Modeling, 2014, 54, 1371-1379.	2.5	144
27	GPCR structures in drug design, emerging opportunities with new structures. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4073-4079.	1.0	116
28	Density functional theory calculations on entire proteins for free energies of binding: Application to a model polar binding site. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3335-3346.	1.5	34
29	Largeâ€scale DFT calculations in implicit solventâ€”A case study on the T4 lysozyme L99A/M102Q protein. International Journal of Quantum Chemistry, 2013, 113, 771-785.	1.0	34
30	Free Energies of Binding from Large-Scale First-Principles Quantum Mechanical Calculations: Application to Ligand Hydration Energies. Journal of Physical Chemistry B, 2013, 117, 9478-9485.	1.2	41
31	Molecular Basis for the Long Duration of Action and Kinetic Selectivity of Tiotropium for the Muscarinic M3 Receptor. Journal of Medicinal Chemistry, 2013, 56, 8746-8756.	2.9	85
32	Economical and Accurate Protocol for Calculating Hydrogen-Bond-Acceptor Strengths. Journal of Chemical Information and Modeling, 2013, 53, 3262-3272.	2.5	14
33	Target Based Virtual Screening by Docking into Automatically Generated GPCR Models. Methods in Molecular Biology, 2012, 914, 255-270.	0.4	1
34	The Implication of the First Agonist Bound Activated GPCR X-ray Structure on GPCR in Silico Modeling. ACS Medicinal Chemistry Letters, 2011, 2, 414-418.	1.3	10
35	First Principles-Based Calculations of Free Energy of Binding: Application to Ligand Binding in a Self-Assembling Superstructure. Journal of Chemical Theory and Computation, 2011, 7, 1102-1108.	2.3	19
36	The use of G-protein coupled receptor models in lead optimization. Future Medicinal Chemistry, 2011, 3, 709-721.	1.1	15

#	Article	IF	Citations
37	String Kernels and High-Quality Data Set for Improved Prediction of Kinked Helices in Î±-Helical Membrane Proteins. Journal of Chemical Information and Modeling, 2011, 51, 3017-3025.	2.5	15
38	Electrostatic embedding in large-scale first principles quantum mechanical calculations on biomolecules. Journal of Chemical Physics, 2011, 135, 224107.	1.2	52
39	Developing Chemical Genetic Approaches to Explore G Protein-Coupled Receptor Function: Validation of the Use of a Receptor Activated Solely by Synthetic Ligand (RASSL). Molecular Pharmacology, 2011, 80, 1033-1046.	1.0	56
40	Dispersion dominated halogenâ€“Ï€ interactions: energies and locations of minima. Physical Chemistry Chemical Physics, 2010, 12, 14941.	1.3	73
41	An improved treatment of spectator mode vibrations in reduced dimensional quantum dynamics: Application to the hydrogen abstraction reactions Î¼+CH4, H+CH4, D+CH4, and CH3+CH4. Journal of Chemical Physics, 2009, 131, 044111.	1.2	31
42	G-protein-coupled receptor-focused drug discovery using a target class platform approach. Drug Discovery Today, 2009, 14, 231-240.	3.2	160
43	Use of 5-hydroxy-4H-benzo[1,4]oxazin-3-ones as Î²2-adrenoceptor agonists. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6640-6644.	1.0	31
44	Revisiting Automated G-Protein Coupled Receptor Modeling: The Benefit of Additional Template Structures for a Neurokinin-1 Receptor Model. Journal of Medicinal Chemistry, 2009, 52, 3166-3173.	2.9	30
45	Sharpening the Toolbox of Computational Chemistry: A New Approximation of CriticalF-Values for Multiple Linear Regression. Journal of Chemical Information and Modeling, 2009, 49, 28-34.	2.5	13
46	Theoretical Prediction of Hydrogen Bond Strength for Use in Molecular Modeling. Journal of Chemical Information and Modeling, 2009, 49, 2067-2076.	2.5	37
47	Comparative study of cluster- and supercell-approaches for investigating heterogeneous catalysis by electronic structure methods: Tunneling in the reaction N + H â† NH on Ru(0001). Physical Chemistry Chemical Physics, 2006, 8, 1437.	1.3	21
48	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192
49	Modeling the heterogeneous reaction probability for chlorine nitrate hydrolysis on ice. Journal of Geophysical Research, 2006, 111, .	3.3	3
50	Rates of the reaction C2H3+H2â†'C2H4+H. Molecular Physics, 2006, 104, 151-158.	0.8	7
51	The thermodesorption mechanism of ammonia from Ru(0001). Surface Science, 2006, 600, 1054-1059.	0.8	3
52	Reaction rates of all hydrogenation steps in ammonia synthesis over a Ru(0001) surface. Journal of Catalysis, 2006, 244, 199-207.	3.1	14
53	The importance of tunneling in the first hydrogenation step in ammonia synthesis over a Ru(0001) surface. Journal of Chemical Physics, 2005, 122, 134702.	1.2	19
54	Sulfurous acid (H2SO3) on Io?. Icarus, 2004, 169, 242-249.	1.1	20

#	Article	IF	Citations
55	The ground-state tunneling splitting of various carboxylic acid dimers. Journal of Chemical Physics, 2004, 120, 631-637.	1.2	71
56	On the Formation of the Sulfonate Ion from Hydrated Sulfur Dioxide. Journal of Physical Chemistry A, 2004, 108, 3859-3864.	1.1	35
57	Double hydrogen tunneling revisited: The breakdown of experimental tunneling criteria. Journal of Chemical Physics, 2004, 120, 11650-11657.	1.2	54
58	Mechanism of the Cisâ˜Trans Isomerization of Bis(glycinato)copper(II). Journal of Physical Chemistry B, 2004, 108, 2098-2102.	1.2	27
59	Extended method for adiabatic mode reordering. Journal of Computational Chemistry, 2003, 24, 386-395.	1.5	1
60	Reactions of HOBr + HCl + nH2O and HOBr + HBr + nH2O. Chemical Physics Letters, 2003, 372, 569-576.	1.2	7
61	The ground state tunneling splitting of the 2-pyridone2-hydroxypyridine dimer. Chemical Physics, 2003, 292, 47-52.	0.9	26
62	About the Kinetic Feasibility of the Lipscomb Mechanism in Human Carbonic Anhydrase II. Journal of Physical Chemistry B, 2003, 107, 12013-12020.	1.2	27
63	Modeling Anhydrous and Aqua Copper(II) Amino Acid Complexes:Â A New Molecular Mechanics Force Field Parametrization Based on Quantum Chemical Studies and Experimental Crystal Data. Inorganic Chemistry, 2003, 42, 2268-2279.	1.9	69
64	Toward elimination of discrepancies between theory and experiment: The gas-phase reaction of N2O5 with H2O. Physical Chemistry Chemical Physics, 2003, 5, 487-495.	1.3	27
65	Influence of Backbone Conformations of Human Carbonic Anhydrase II on Carbon Dioxide Hydration:â€‰ Hydration Pathways and Binding of Bicarbonate. Journal of the American Chemical Society, 2003, 125, 8921-8927.	6.6	28
66	The optimal tunneling path for the proton transfer in malonaldehyde. Journal of Chemical Physics, 2002, 117, 1962-1966.	1.2	80
67	An accurate semiclassical method to predict ground-state tunneling splittings. Journal of Chemical Physics, 2002, 117, 1967-1974.	1.2	47
68	Reactions of HOCl + HCl +nH2O and HOCl + HBr +nH2O. Journal of Physical Chemistry A, 2002, 106, 7850-7857.	1.1	19
69	Towards the Experimental Decomposition Rate of Carbonic Acid (H2CO3) in Aqueous Solution. Chemistry - A European Journal, 2002, 8, 66-73.	1.7	84
70	About the Stability of Sulfurous Acid (H2SO3) and Its Dimer. Chemistry - A European Journal, 2002, 8, 5644-5651.	1.7	43
71	On the Surprising Kinetic Stability of Carbonic Acid (H2CO3). Angewandte Chemie - International Edition, 2000, 39, 891-894.	7.2	152