Casper Steinmann

List of Publications by Year
in descending order

28 papers	705 citations	516710 16 h-index	552781 26 g-index
35 all docs	35 docs citations	35 times ranked	788 citing authors

#	Article	IF	Citations
1	Supramolecular Complexes of Plant Neurotoxin Veratridine with Cyclodextrins and Their Antidote-like Effect on Neuro-2a Cell Viability. Pharmaceutics, 2022, 14, 598.	4.5	2
2	The augâ€ccâ€pVTZâ€¦ basis set for the pâ€block fourthâ€row elements Ga, Ge, As, Se, and Br. Magnetic Resonance in Chemistry, 2021, 59, 1134-1145.	1.9	6
3	Cost-Effective Potential for Accurate Polarizable Embedding Calculations in Protein Environments. Journal of Chemical Theory and Computation, 2020, 16, 1162-1174.	5.3	12
4	Combining polarizable embedding with the Frenkel exciton model: applications to absorption spectra with overlapping soluteâ€“solvent bands. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	0
5	Response properties of embedded molecules through the polarizable embedding model. International Journal of Quantum Chemistry, 2019, 119, e25717.	2.0	37
6	Structure-guided approach identifies a novel class of HIV-1 ribonuclease H inhibitors: binding mode insights through magnesium complexation and site-directed mutagenesis studies. MedChemComm, 2018, 9, 562-575.	3.4	18
7	Improving solvation energy predictions using the SMD solvation method and semiempirical electronic structure methods. Journal of Chemical Physics, 2018, 149, 104102.	3.0	39
8	Relative Ligand-Binding Free Energies Calculated from Multiple Short QM/MM MD Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3228-3237.	5.3	23
9	Computational Approach to Evaluation of Optical Properties of Membrane Probes. Journal of Chemical Theory and Computation, 2017, 13, 719-726.	5.3	11
10	An averaged polarizable potential for multiscale modeling in phospholipid membranes. Journal of Computational Chemistry, 2017, 38, 601-611.	3.3	12
11	Mapping Interaction Energies in Chorismate Mutase with the Fragment Molecular Orbital Method. Journal of Physical Chemistry A, 2017, 121, 1797-1807.	2.5	9
12	Automated Fragmentation Polarizable Embedding Density Functional Theory (PE-DFT) Calculations of Nuclear Magnetic Resonance (NMR) Shielding Constants of Proteins with Application to Chemical Shift Predictions. Journal of Chemical Theory and Computation, 2017, 13, 525-536.	5.3	18
13	Modeling Electronic Circular Dichroism within the Polarizable Embedding Approach. Journal of Chemical Theory and Computation, 2017, 13, 4442-4451.	5.3	12
14	Computational Approach for Studying Optical Properties of DNA Systems in Solution. Journal of Chemical Theory and Computation, 2016, 12, 5050-5057.	5.3	26
15	Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. Journal of Physical Chemistry A, 2015, 119, 5344-5355.	2.5	78
16	Electronic Energy Transfer in Polarizable Heterogeneous Environments: A Systematic Investigation of Different Quantum Chemical Approaches. Journal of Chemical Theory and Computation, 2015, 11, 4283-4293.	5.3	17
17	A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+. PeerJ, 2014, 2, e449.	2.0	46
18	Nuclear Magnetic Shielding Constants from Quantum Mechanical/Molecular Mechanical Calculations Using Polarizable Embedding: Role of the Embedding Potential. Journal of Chemical Theory and Computation, 2014, 10, 981-988.	5.3	37

#	Article	IF	Citations
19	Hybrid RHF/MP2 Geometry Optimizations with the Effective Fragment Molecular Orbital Method. PLoS ONE, 2014, 9, e88800.	2.5	11
20	Inhibitor Ranking through QM Based Chelation Calculations for Virtual Screening of HIV-1 RNase H Inhibition. PLoS ONE, 2014, 9, e98659.	2.5	17
21	Fully Integrated Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2013, 9, 2235-2249.	5.3	56
22	Mapping Enzymatic Catalysis Using the Effective Fragment Molecular Orbital Method: Towards all ab initio Biochemistry. PLoS ONE, 2013, 8, e60602.	2.5	33
23	Interface of the Polarizable Continuum Model of Solvation with Semi-Empirical Methods in the GAMESS Program. PLoS ONE, 2013, 8, e67725.	2.5	13
24	A computational method for the systematic screening of reaction barriers in enzymes: searching forBacillus circulansxylanase mutants with greater activity towards a synthetic substrate. PeerJ, 2013, 1, e111.	2.0	7
25	The Effective Fragment Molecular Orbital Method for Fragments Connected by Covalent Bonds. PLoS ONE, 2012, 7, e41117.	2.5	28
26	FragIt: A Tool to Prepare Input Files for Fragment Based Quantum Chemical Calculations. PLoS ONE, 2012, 7, e44480.	2.5	39
27	Effective Fragment Molecular Orbital Method: A Merger of the Effective Fragment Potential and Fragment Molecular Orbital Methods^{â€}. Journal of Physical Chemistry A, 2010, 114, 8705-8712.	2.5	80
28	Using a genetic algorithm to find molecules with good docking scores. PeerJ Physical Chemistry, 0, 3, e18.	0.0	13