

Casper Steinmann

List of Publications by Year in descending order

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28
papers

705
citations

516215

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times ranked

788
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#	ARTICLE	IF	CITATIONS
1	Supramolecular Complexes of Plant Neurotoxin Veratridine with Cyclodextrins and Their Antidote-like Effect on Neuro-2a Cell Viability. <i>Pharmaceutics</i> , 2022, 14, 598.	2.0	2
2	The aug-cc-pVTZ basis set for the p-block fourth-row elements Ga, Ge, As, Se, and Br. <i>Magnetic Resonance in Chemistry</i> , 2021, 59, 1134-1145.	1.1	6
3	Cost-Effective Potential for Accurate Polarizable Embedding Calculations in Protein Environments. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1162-1174.	2.3	12
4	Combining polarizable embedding with the Frenkel exciton model: applications to absorption spectra with overlapping solute-solvent bands. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	0
5	Response properties of embedded molecules through the polarizable embedding model. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25717.	1.0	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. <i>MedChemComm</i> , 2018, 9, 562-575.	3.5	18
7	Improving solvation energy predictions using the SMD solvation method and semiempirical electronic structure methods. <i>Journal of Chemical Physics</i> , 2018, 149, 104102.	1.2	39
8	Relative Ligand-Binding Free Energies Calculated from Multiple Short QM/MM MD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3228-3237.	2.3	23
9	Computational Approach to Evaluation of Optical Properties of Membrane Probes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 719-726.	2.3	11
10	An averaged polarizable potential for multiscale modeling in phospholipid membranes. <i>Journal of Computational Chemistry</i> , 2017, 38, 601-611.	1.5	12
11	Mapping Interaction Energies in Chorismate Mutase with the Fragment Molecular Orbital Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1797-1807.	1.1	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. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 525-536.	2.3	18
13	Modeling Electronic Circular Dichroism within the Polarizable Embedding Approach. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4442-4451.	2.3	12
14	Computational Approach for Studying Optical Properties of DNA Systems in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5050-5057.	2.3	26
15	Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5344-5355.	1.1	78
16	Electronic Energy Transfer in Polarizable Heterogeneous Environments: A Systematic Investigation of Different Quantum Chemical Approaches. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4283-4293.	2.3	17
17	A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+. <i>PeerJ</i> , 2014, 2, e449.	0.9	46
18	Nuclear Magnetic Shielding Constants from Quantum Mechanical/Molecular Mechanical Calculations Using Polarizable Embedding: Role of the Embedding Potential. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 981-988.	2.3	37

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19	Hybrid RHF/MP2 Geometry Optimizations with the Effective Fragment Molecular Orbital Method. PLoS ONE, 2014, 9, e88800.	1.1	11
20	Inhibitor Ranking through QM Based Chelation Calculations for Virtual Screening of HIV-1 RNase H Inhibition. PLoS ONE, 2014, 9, e98659.	1.1	17
21	Fully Integrated Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2013, 9, 2235-2249.	2.3	56
22	Mapping Enzymatic Catalysis Using the Effective Fragment Molecular Orbital Method: Towards all ab initio Biochemistry. PLoS ONE, 2013, 8, e60602.	1.1	33
23	Interface of the Polarizable Continuum Model of Solvation with Semi-Empirical Methods in the GAMESS Program. PLoS ONE, 2013, 8, e67725.	1.1	13
24	A computational method for the systematic screening of reaction barriers in enzymes: searching for <i>Bacillus circulans</i> xylanase mutants with greater activity towards a synthetic substrate. PeerJ, 2013, 1, e111.	0.9	7
25	The Effective Fragment Molecular Orbital Method for Fragments Connected by Covalent Bonds. PLoS ONE, 2012, 7, e41117.	1.1	28
26	FragIt: A Tool to Prepare Input Files for Fragment Based Quantum Chemical Calculations. PLoS ONE, 2012, 7, e44480.	1.1	39
27	Effective Fragment Molecular Orbital Method: A Merger of the Effective Fragment Potential and Fragment Molecular Orbital Methods. Journal of Physical Chemistry A, 2010, 114, 8705-8712.	1.1	80
28	Using a genetic algorithm to find molecules with good docking scores. PeerJ Physical Chemistry, 0, 3, e18.	0.0	13