

Ligand-Binding Affinity Estimates Supported by Quant

Chemical Reviews

116, 5520-5566

DOI: [10.1021/acs.chemrev.5b00630](https://doi.org/10.1021/acs.chemrev.5b00630)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Converging ligand-binding free energies obtained with free-energy perturbations at the quantum mechanical level. <i>Journal of Computational Chemistry</i> , 2016, 37, 1589-1600.	1.5	46
2	Effective representation of amide III, II, I, and A modes on local vibrational modes: Analysis of ab initio quantum calculation results. <i>Journal of Chemical Physics</i> , 2016, 145, 164113.	1.2	4
3	Screened exchange hybrid density functional for accurate and efficient structures and interaction energies. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15519-15523.	1.3	49
4	QM/MM Calculations on Proteins. <i>Methods in Enzymology</i> , 2016, 577, 119-158.	0.4	75
5	The electron's spin and molecular chirality – how are they related and how do they affect life processes?. <i>Chemical Society Reviews</i> , 2016, 45, 6478-6487.	18.7	194
6	Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK _a corrections. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 1087-1100.	1.3	27
7	An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4988-4997.	1.4	15
8	Efficient Geometry Optimization of Large Molecular Systems in Solution Using the Fragment Molecular Orbital Method. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9794-9804.	1.1	12
9	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 989-1006.	1.3	24
10	Towards full Quantum-Mechanics-based Protein-Ligand Binding Affinities. <i>ChemPhysChem</i> , 2017, 18, 898-905.	1.0	46
11	Computing converged free energy differences between levels of theory via nonequilibrium work methods: Challenges and opportunities. <i>Journal of Computational Chemistry</i> , 2017, 38, 1376-1388.	1.5	28
12	Recent advances in dynamic docking for drug discovery. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1320.	6.2	55
13	Full QM Calculation of RNA Energy Using Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method. <i>Journal of Physical Chemistry A</i> , 2017, 121, 2503-2514.	1.1	21
14	Comparison of QM/MM Methods To Obtain Ligand-Binding Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2245-2253.	2.3	45
15	On-the-Fly QM/MM Docking with Attracting Cavities. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 73-84.	2.5	42
16	Can System Truncation Speed up Ligand-Binding Calculations with Periodic Free-Energy Simulations?. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2865-2873.	2.5	0
17	How Many Conformations Need To Be Sampled To Obtain Converged QM/MM Energies? The Curse of Exponential Averaging. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5745-5752.	2.3	70
18	New generation of docking programs: Supercomputer validation of force fields and quantum-chemical methods for docking. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 78, 139-147.	1.3	37

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20	Electrostatics Explains the Position-Dependent Effect of G-U Wobble Base Pairs on the Affinity of RNA Kissing Complexes. <i>ChemPhysChem</i> , 2017, 18, 2782-2790.	1.0	5
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35	Fragment-based quantum mechanical calculation of protein-protein binding affinities. <i>Journal of Computational Chemistry</i> , 2018, 39, 1617-1628.	1.5	23
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