Accelerating QM/MM Free Energy Computations via Int

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Citation Report

#	Article	IF	Citations
1	Force matching as a stepping stone to QM/MM CB[8] host/guest binding free energies: a SAMPL6 cautionary tale. Journal of Computer-Aided Molecular Design, 2018, 32, 983-999.	2.9	21
2	Prediction of CB[8] hostâ€“guest binding free energies in SAMPL6 using the double-decoupling method. Journal of Computer-Aided Molecular Design, 2018, 32, 1059-1073.	2.9	13
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4	Use of Interaction Energies in QM/MM Free Energy Simulations. Journal of Chemical Theory and Computation, 2019, 15, 4632-4645.	5.3	21
5	The Good, the Bad, and the Ugly: â€œHiPenâ€ a New Dataset for Validating (S)QM/MM Free Energy Simulations. Molecules, 2019, 24, 681.	3.8	9
6	Accelerated Computation of Free Energy Profile at Ab Initio Quantum Mechanical/Molecular Mechanics Accuracy via a Semiempirical Reference Potential. 3. Gaussian Smoothing on Density-of-States. Journal of Chemical Theory and Computation, 2020, 16, 6814-6822.	5.3	11
7	Free energy level correction by Monte Carlo resampling with weighted histogram analysis method. Chinese Journal of Chemical Physics, 2020, 33, 183-195.	1.3	2
8	What Does the BrÃ¸nsted Slope Measure in the Phosphoryl Transfer Transition State?. ACS Catalysis, 2020, 10, 13932-13945.	11.2	3
9	On the faithfulness of molecular mechanics representations of proteins towards quantum-mechanical energy surfaces. Interface Focus, 2020, 10, 20190121.	3.0	13
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13	Making free-energy calculations routine: Combining first principles with machine learning. Physical Review B, 2020, 101, .	3.2	35
14	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of waterâ€“octanol partition coefficients in the SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 471-483.	2.9	7
15	Alchemical Hydration Free-Energy Calculations Using Molecular Dynamics with Explicit Polarization and Induced Polarity Decoupling: An Onâ€“theâ€“Fly Polarization Approach. Journal of Chemical Theory and Computation, 2020, 16, 1146-1161.	5.3	14
16	Self-Parametrizing System-Focused Atomistic Models. Journal of Chemical Theory and Computation, 2020, 16, 1646-1665.	5.3	22
17	Biomolecular QM/MM Simulations: What Are Some of the â€œBurning Issuesâ€?. Journal of Physical Chemistry B, 2021, 125, 689-702.	2.6	68
18	Accelerated Computation of Free Energy Profile at Ab Initio Quantum Mechanical/Molecular Mechanics Accuracy via a Semiempirical Reference Potential. 4. Adaptive QM/MM. Journal of Chemical Theory and Computation, 2021, 17, 1318-1325.	5.3	13

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19	ParaMol: A Package for Automatic Parameterization of Molecular Mechanics Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 2026-2047.	5.4	22
20	A replica exchange umbrella sampling (REUS) approach to predict hostâ€“guest binding free energies in SAMPL8 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 667-677.	2.9	5
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