Lance M Westerhoff

List of Publications by Year
in descending order

15	524	933447 10	1199594 12
papers	citations	h-index	g-index

15	15	15	674
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The role of quantum mechanics in structure-based drug design. Drug Discovery Today, 2007, 12, 725-731.	6.4	226
2	Quantum mechanical/quantum mechanical methods. I. A divide and conquer strategy for solving the SchrÃ¶dinger equation for large molecular systems using a composite density functionalâ€“semiempirical Hamiltonian. Journal of Chemical Physics, 2000, 113, 5604-5613.	3.0	77
3	Accurate macromolecular crystallographic refinement: incorporation of the linear scaling, semiempirical quantum-mechanics programDivConinto thePHENIXrefinement package. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 1233-1247.	2.5	46
4	Pairwise Decomposition of Residue Interaction Energies Using Semiempirical Quantum Mechanical Methods in Studies of Proteinâ^'Ligand Interaction. Journal of the American Chemical Society, 2005, 127, 6583-6594.	13.7	40
5	A Critical Assessment of the Performance of Proteinâ^'Ligand Scoring Functions Based on NMR Chemical Shift Perturbations. Journal of Medicinal Chemistry, 2007, 50, 5128-5134.	6.4	35
6	High-throughput quantum-mechanics/molecular-mechanics (ONIOM) macromolecular crystallographic refinement withPHENIX/DivCon: the impact of mixed Hamiltonian methods on ligand and protein structure. Acta Crystallographica Section D: Structural Biology, 2018, 74, 1063-1077.	2.3	18
7	Computational alanine scanning with linear scaling semiempirical quantum mechanical methods. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2329-2337.	2.6	17
8	Quantum Mechanical Pairwise Decomposition Analysis of Protein Kinase B Inhibitors: Validating a New Tool for Guiding Drug Design. Journal of Chemical Information and Modeling, 2010, 50, 651-661.	5.4	17
9	The critical role of QM/MM X-ray refinement and accurate tautomer/protomer determination in structure-based drug design. Journal of Computer-Aided Molecular Design, 2021, 35, 433-451.	2.9	15
10	XModeScore: a novel method for accurate protonation/tautomer-state determination using quantum-mechanically driven macromolecular X-ray crystallographic refinement. Acta Crystallographica Section D: Structural Biology, 2016, 72, 586-598.	2.3	15
11	Quantum mechanical description of the interactions between DNA and water. Journal of Molecular Graphics and Modelling, 2006, 24, 440-455.	2.4	10
12	MovableType Software for Fast Free Energy-Based Virtual Screening: Protocol Development, Deployment, Validation, and Assessment. Journal of Chemical Information and Modeling, 2020, 60, 5437-5456.	5.4	7
13	Fast, Routine Free Energy of Binding Estimation Using MovableType. ACS Symposium Series, 0, , 247-265.	0.5	1
14	Accurate Determination of Tautomeric/Protonation States in Quantum-Mechanic Driven Macromolecular Crystallographic Refinement. Biophysical Journal, 2015, 108, 620a.	0.5	0
15	The Impact of Experimental, Protein Structure on our Ability to Model Protein Function. Biophysical Journal, 2016, 110, 544a.	0.5	0