Dvir Doron

List of Publications by Year
in descending order

11	294	933447 10	1281871 11
papers	citations	h-index	g-index

11	11	11	290
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Challenges in computational studies of enzyme structure, function and dynamics. Journal of Molecular Graphics and Modelling, 2014, 54, 62-79.	2.4	50
2	Hybrid Quantum and Classical Simulations of the Dihydrofolate Reductase Catalyzed Hydride Transfer Reaction on an Accurate Semi-Empirical Potential Energy Surface. Journal of Chemical Theory and Computation, 2011, 7, 3420-3437.	5.3	45
3	Collective Reaction Coordinate for Hybrid Quantum and Molecular Mechanics Simulations: A Case Study of the Hydride Transfer in Dihydrofolate Reductase. Journal of Chemical Theory and Computation, 2012, 8, 2484-2496.	5.3	35
4	Path-Integral Calculations of Nuclear Quantum Effects in Model Systems, Small Molecules, and Enzymes via Gradient-Based Forward Corrector Algorithms. Journal of Chemical Theory and Computation, 2011, 7, 1273-1286.	5.3	31
5	Hybrid Quantum and Classical Simulations of the Formate Dehydrogenase Catalyzed Hydride Transfer Reaction on an Accurate Semiempirical Potential Energy Surface. Journal of Chemical Theory and Computation, 2012, 8, 4786-4796.	5.3	25
6	Quantum and Classical Simulations of Orotidine Monophosphate Decarboxylase: Support for a Direct Decarboxylation Mechanism. Biochemistry, 2013, 52, 4382-4390.	2.5	22
7	How Accurate Are Transition States from Simulations of Enzymatic Reactions?. Journal of Chemical Theory and Computation, 2014, 10, 1863-1871.	5.3	21
8	Momentum Distribution as a Fingerprint of Quantum Delocalization in Enzymatic Reactions: Open-Chain Path-Integral Simulations of Model Systems and the Hydride Transfer in Dihydrofolate Reductase. Journal of Chemical Theory and Computation, 2012, 8, 1223-1234.	5.3	20
9	Simulations of remote mutants of dihydrofolate reductase reveal the nature of a network of residues coupled to hydride transfer. Journal of Computational Chemistry, 2014, 35, 1411-1417.	3.3	20
10	Free Energy Simulations of Active-Site Mutants of Dihydrofolate Reductase. Journal of Physical Chemistry B, 2015, 119, 906-916.	2.6	20
11	Multiscale Quantumâ€Classical Simulations of Enzymes. Israel Journal of Chemistry, 2014, 54, 1108-1117.	2.3	5