

Dvir Doron

List of Publications by Year in descending order

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11
papers

294
citations

933447

10
h-index

1281871

11
g-index

11
all docs

11
docs citations

11
times ranked

290
citing authors

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