GÃ¡bor NÃ¡ray-SzabÃ³

List of Publications by Year
in descending order

15	385	1039880 9	1372474 10
papers	citations	h-index	g-index

15	15	15	408
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Conservative evolution and industrial metabolism in Green Chemistry. Green Chemistry, 2018, 20, 2171-2191.	4.6	45
2	Editorial (Thematic Issue: Chemistry Towards Biology: Proceedings of the Katowice Conference). Current Protein and Peptide Science, 2016, 17, 94-94.	0.7	0
3	Quantum Mechanical Modeling: A Tool for the Understanding of Enzyme Reactions. Biomolecules, 2013, 3, 662-702.	1.8	21
4	Quantum mechanical studies on the existence of a trigonal bipyramidal phosphorane intermediate in enzymatic phosphate ester hydrolysis. Theoretical Chemistry Accounts, 2007, 118, 129-134.	0.5	22
5	Predicting Anti-HIV-1 Activities of HEPT-analog Compounds by Using Support Vector Classification. QSAR and Combinatorial Science, 2005, 24, 1021-1025.	1.5	12
6	Energy decomposition scheme for combined ab initio quantum mechanical / molecular mechanical methods. International Journal of Quantum Chemistry, 2005, 104, 328-334.	1.0	1
7	Comparative redox and pK a calculations on cytochrome c 3 from several Desulfovibrio species using continuum electrostatic methods. Journal of Biological Inorganic Chemistry, 1999, 4, 73-86.	1.1	37
8	Application of neural networks in structure-activity relationships. , 1999, 19, 249-269.		55
9	Electrostatic modulation of electron transfer in the active site of heme peroxidases. Journal of Biological Inorganic Chemistry, 1997, 2, 135-138.	1.1	27
10	Crystallization and preliminary diffraction analysis of Ca2+-calmodulin-drug and apocalmodulin-drug complexes. , 1997, 28, 131-134.		5
11	Role of electrostatics at the catalytic metal binding site in xylose isomerase action: Ca2+-inhibition and metal competence in the double mutant D254E/D256E. , 1997, 28, 183-193.		19
12	NDDO fragment self-consistent field approximation for large electronic systems. Journal of Computational Chemistry, 1992, 13, 830-837.	1.5	85
13	Bond orbital framework for rapid calculation of environmental effects on molecular potential surfaces. Chemical Physics Letters, 1983, 96, 499-501.	1.2	42
14	Conformational analysis by bond orbitals with delocalization corrections: Rotation of the ser-195 side chain in Î±-chymotrypsin. International Journal of Quantum Chemistry, 1982, 22, 929-938.	1.0	13
15	A wavefunction model to chemical bonding. International Journal of Quantum Chemistry, 0, , e26686.	1.0	1