Ming-Ju Huang

List of Publications by Year
in descending order

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54	1,098	489802 18	466096 32
papers	citations	h-index	g-index

54	54	54	1467
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Using experimental data of Escherichia coli to develop a QSAR model for predicting the photo-induced cytotoxicity of metal oxide nanoparticles. Journal of Photochemistry and Photobiology B: Biology, 2014, 130, 234-240.	1.7	85
2	Theoretical Comparative Study of Oxygen Adsorption on Neutral and Anionic Ag_n and Au_n Clusters (n = 2â€“25). Journal of Physical Chemistry C, 2014, 118, 21911-21927.	1.5	58
3	Effects of local protein environment on the binding of diatomic molecules to heme in myoglobins. DFT and dispersion-corrected DFT studies. Journal of Molecular Modeling, 2013, 19, 3307-3323.	0.8	6
4	Binding of O₂ and NO to Heme in Heme-Nitric Oxide/Oxygen-Binding (H-NOX) Proteins. A Theoretical Study. Journal of Physical Chemistry B, 2013, 117, 10103-10114.	1.2	18
5	Factors that distort the heme structure in Heme-Nitric Oxide/OXygen-Binding (H-NOX) protein domains. A theoretical study. Journal of Inorganic Biochemistry, 2013, 118, 28-38.	1.5	3
6	Assessment of dispersion corrections in DFT calculations on large biological systems. Molecular Physics, 2012, 110, 3061-3076.	0.8	8
7	Theoretical study of triatomic silver (Ag3) and its ions with coupled-cluster methods and correlation-consistent basis sets. Physical Chemistry Chemical Physics, 2012, 14, 6849.	1.3	19
8	FeP(Im)â^'AB bonding energies evaluated with a large number of density functionals (Pâ€‰=â€‰porphine,) Tj ETQq0 0 0 rgBT /Overloc	0.8	13
9	Theoretical Characterization of the F₂O₃ Molecule by Coupled-Cluster Methods. Journal of Physical Chemistry A, 2010, 114, 10197-10201.	1.1	4
10	Iron Porphyrins with Different Imidazole Ligands. A Theoretical Comparative Study. Journal of Physical Chemistry A, 2010, 114, 9554-9569.	1.1	47
11	Computational modeling of inclusion complexes of Î²â€cyclodextrin with enantiomers of salsolinol, Nâ€methylâ€salsolinol, and 1â€benzylâ€tetrahydroisoquinoline. International Journal of Quantum Chemistry, 2009, 109, 81-90.	1.0	27
12	Supramolecular interactions of fullerenes with (Cl)Fe- and Mn porphyrins. A theoretical study. Physical Chemistry Chemical Physics, 2009, 11, 6072.	1.3	5
13	Dispersion-corrected DFT calculations on C60-porphyrin complexes. Physical Chemistry Chemical Physics, 2009, 11, 4365.	1.3	23
14	Electronic structure, absorption spectra, and hyperpolarisabilities of some novel pushâ€“pull zinc porphyrins. A DFT/TDDFT study. Molecular Physics, 2008, 106, 147-160.	0.8	14
15	STRUCTURE AND PROPERTIES OF PERFLUOROALKYLATED PHTHALOCYANINES: A THEORETICAL STUDY. Journal of Theoretical and Computational Chemistry, 2008, 07, 541-563.	1.8	9
16	ASSESSMENT OF SOME RECENTLY DEVELOPED DENSITY FUNCTIONALS FOR CALCULATIONS ON IRON PORPHYRINS. Journal of Theoretical and Computational Chemistry, 2008, 07, 615-628.	1.8	2
17	QSAR study of the structural and conformational requirements for the binding of anandamide analogs to the cannabinoid receptor CB1. Molecular Physics, 2008, 106, 1847-1852.	0.8	2
18	Interaction of Metal Porphyrins with Fullerene C60:Â A New Insight. Journal of Physical Chemistry B, 2007, 111, 4374-4382.	1.2	25

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19	Electronic Structure of Some Substituted Iron(II) Porphyrins. Are They Intermediate or High Spin?. Journal of Physical Chemistry A, 2007, 111, 5927-5935.	1.1	45
20	Assessment of the performance of density-functional methods for calculations on iron porphyrins and related compounds. Journal of Computational Chemistry, 2006, 27, 1577-1592.	1.5	78
21	Nuclear magnetic resonance spectral analysis and molecular properties of berberine. International Journal of Quantum Chemistry, 2005, 105, 396-409.	1.0	15
22	Application of quantitative structure activity relationship (QSAR) models to predict ozone toxicity in the lung. Environmental Toxicology, 2005, 20, 441-448.	2.1	4
23	Effects of Peripheral Substituents and Axial Ligands on the Electronic Structure and Properties of Cobalt Porphyrins. Journal of Physical Chemistry A, 2005, 109, 11996-12005.	1.1	29
24	Effects of Peripheral Substituents on the Electronic Structure and Properties of Unligated and Ligated Metal Phthalocyanines, Metal = Fe, Co, Zn. Journal of Chemical Theory and Computation, 2005, 1, 1201-1210.	2.3	46
25	DFT Study of Unligated and Ligated ManganeseIIPorphyrins and Phthalocyanines. Inorganic Chemistry, 2005, 44, 1941-1949.	1.9	78
26	Ab Initio Study of Prednisolone, 6Â-Fluoroprednisolone, 9Â-Fluoroprednisolone, and 6Â,9Â-Difluoroprednisolone. Structural Chemistry, 2004, 15, 487-492.	1.0	1
27	Ab initio studies of tamoxifen and related compounds. International Journal of Quantum Chemistry, 2004, 96, 374-379.	1.0	4
28	Theoretical study of the hydrophobic character of the dimerization of dexanabinol. International Journal of Quantum Chemistry, 2004, 96, 426-431.	1.0	1
29	Capillary electrophoretic separation and theoretical study of inclusion complexes of sulfobutyl ether ?-cyclodextrin with estrogens. International Journal of Quantum Chemistry, 2004, 100, 746-752.	1.0	15
30	Theoretical AM1 studies of inclusion complexes of heptakis(2-O-hydroxypropyl)-?-cyclodextrins with alkylated phenols. International Journal of Quantum Chemistry, 2004, 100, 771-778.	1.0	9
31	An ab initio theoretical study of the stereoisomers of tetrahydrocannabinols. , 2001, 15, 323-333.		3
32	Toxicity Assessment of Atrazine and Related Triazine Compounds in the Microtox Assay, and Computational Modeling for Their Structure-Activity Relationship. International Journal of Molecular Sciences, 2000, 1, 63-74.	1.8	51
33	Theoretical study of the stereoisomers of tetrahydrocannabinols. International Journal of Quantum Chemistry, 1997, 61, 127-135.	1.0	2
34	Theoretical studies of inclusion complexes of ?-cyclodextrin with methylated benzoic acids. International Journal of Quantum Chemistry, 1997, 64, 711-719.	1.0	47
35	Theoretical studies of inclusion complexes of ?- and ?-cyclodextrin with benzoic acid and phenol. International Journal of Quantum Chemistry, 1997, 65, 1135-1152.	1.0	47
36	AM1-based model system for estimation of brain / blood concentration ratios. International Journal of Quantum Chemistry, 1996, 60, 1775-1787.	1.0	9

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37	Theoretical am1 studies of inclusion complexes of ?- and ?-cyclodextrins with methylated benzoic acids and phenol, and ?-cyclodextrin with buckminsterfullerene. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 1996, 25, 97-102.	1.6	16
38	Computational Approaches to the Design of Safer Drugs and Their Molecular Properties. Computational Chemistry - Reviews of Current Trends, 1996, , 219-266.	0.4	3
39	Theoretical AM1 Studies of Inclusion Complexes of Î±- And Î²-Cyclodextrins with Methylated Benzoic Acids and Phenol, and Î³-Cyclodextrin With Buckminsterfullerene. , 1996, , 209-214.		3
40	Relative reactivity of 1,4- and 1,6-dihydronicotinic acid derivatives to radically mediated oxidation?a theoretical and experimental evaluation. International Journal of Quantum Chemistry, 1995, 56, 161-170.	1.0	1
41	Nitrogen radical cations as intermediates in enzymatically mediated oxidative deaminations?application of molecular parametric models. International Journal of Quantum Chemistry, 1995, 56, 171-179.	1.0	4
42	Solubilization and electrochemical stabilization of substituted phenols through the use of 2-hydroxypropyl-Î²-cyclodextrin. Supramolecular Chemistry, 1994, 4, 69-76.	1.5	4
43	Stability of the 1,3-substituted 1,4-dihydropyridines: Substituent effects on the acid catalyzed hydration and oxidation reactions. International Journal of Quantum Chemistry, 1994, 52, 173-180.	1.0	0
44	Quantitative structure-inhibitory activity relationships of substituted phenols onbacillus subtilis spore germination. International Journal of Quantum Chemistry, 1994, 52, 181-185.	1.0	2
45	Neural network studies. Computational and Theoretical Chemistry, 1994, 309, 259-266.	1.5	41
46	Hydroxyl stretching in substituted phenols: An AM1 study. International Journal of Quantum Chemistry, 1993, 48, 7-15.	1.0	1
47	A theoretical study of the dithionite reduction of pyridinium salts. International Journal of Quantum Chemistry, 1993, 48, 17-24.	1.0	0
48	A theoretical study of prednisolone, 6Î±-fluoroprednisolone, 9Î±-fluoroprednisolone, 6Î±,9Î±-difluoroprednisolone and related compounds. Computational and Theoretical Chemistry, 1993, 279, 59-69.	1.5	1
49	Intermolecular interactions of methyl acetate, ?-propiolactone, ethyl acetate, and ?-butyrolactone: AnAM1 semiempirical study. International Journal of Quantum Chemistry, 1992, 44, 81-89.	1.0	2
50	Vibrational calculations on water with improved force fields. International Journal of Quantum Chemistry, 1992, 44, 427-434.	1.0	9
51	Neural network studies. 4. An extended study of the aqueous solubility of organic compounds. International Journal of Quantum Chemistry, 1992, 44, 853-867.	1.0	15
52	An Extended Version of a Novel Method for the Estimation of Partition Coefficients. Journal of Pharmaceutical Sciences, 1992, 81, 272-281.	1.6	106
53	Predicting partition coefficients for isomeric diastereoisomers of some tripeptide analogs. Journal of Computational Chemistry, 1991, 12, 1182-1186.	1.5	21
54	Reactivity of biologically important reduced pyridines. VIII. A semiempirical (AM1) study of the oxidation of 3-substituted-1-methyl-1,4-dihydropyridines. Journal of Computational Chemistry, 1991, 12, 1278-1282.	1.5	17