Ã–dÃ¶n Farkas

List of Publications by Year
in descending order

45 papers	1,922 citations	304743 22 h-index	265206 42 g-index
46 all docs	46 docs citations	46 times ranked	1865 citing authors

#	Article	IF	Citations
1	Geometry optimization with QM/MM, ONIOM, and other combined methods. I. Microiterations and constraints. Journal of Computational Chemistry, 2003, 24, 760-769.	3.3	560
2	Methods for optimizing large molecules. II. Quadratic search. Journal of Chemical Physics, 1999, 111, 10806-10814.	3.0	169
3	Effects of the Protein Environment on the Structure and Energetics of Active Sites of Metalloenzymes. ONIOM Study of Methane Monooxygenase and Ribonucleotide Reductase. Journal of the American Chemical Society, 2002, 124, 192-193.	13.7	124
4	Methods for optimizing large molecules. Part III. An improved algorithm for geometry optimization using direct inversion in the iterative subspace (GDIIS). Physical Chemistry Chemical Physics, 2002, 4, 11-15.	2.8	114
5	Methods for geometry optimization of large molecules. I. An O(N2) algorithm for solving systems of linear equations for the transformation of coordinates and forces. Journal of Chemical Physics, 1998, 109, 7100-7104.	3.0	65
6	Toward a computed peptide structure database: The role of a universal atomic numbering system of amino acids in peptides and internal hierarchy of database. International Journal of Quantum Chemistry, 2002, 90, 933-968.	2.0	54
7	Peptide models. XXXIII. Extrapolation of low-level Hartree-Fock data of peptide conformation to large basis set SCF, MP2, DFT, and CCSD(T) results. The Ramachandran surface of alanine dipeptide computed at various levels of theory. Journal of Computational Chemistry, 2003, 24, 1026-1042.	3.3	54
8	Peptide Models. 18. Hydroxymethyl Side-Chain Induced Backbone Conformational Shifts of l-Serine Amide. All ab Initio Conformers of For-l-Ser-NH2. Journal of the American Chemical Society, 1996, 118, 7809-7817.	13.7	49
9	Peptide models XXIV: An ab initio study on N-formyl-L-prolinamide with trans peptide bond. The existence or non-existence of Î±L and ÏµL conformations. Computational and Theoretical Chemistry, 1999, 465, 79-91.	1.5	48
10	Phenylalanine Ammoniaâ€Lyaseâ€Catalyzed Deamination of an Acyclic Amino Acid: Enzyme Mechanistic Studies Aided by a Novel Microreactor Filled with Magnetic Nanoparticles. ChemBioChem, 2015, 16, 2283-2288.	2.6	46
11	Peptide models XXII. A conformational model for aromatic amino acid residues in proteins. A comprehensive analysis of all the RHF/6â€“31+G* conformers of For-L-Pheâ€“NH2. Computational and Theoretical Chemistry, 1998, 455, 303-314.	1.5	44
12	Peptide models XX. Aromatic side-chainâ€“backbone interaction in phenylalanine-containing diamide model system. A systematic search for the identification of all the ab initio conformers of N-formyl-L-phenylalanine-amide. Canadian Journal of Chemistry, 1997, 75, 1120-1130.	1.1	43
13	Peptide models XIX: Side-chain conformational energy surface and amide I vibrational frequencies of N-formyl-l-phenylalaninamide (For-Phe-NH2) in its Î³L or Î³inv or C7eq backbone conformation. Computational and Theoretical Chemistry, 1996, 369, 105-114.	1.5	41
14	Peptide models XVI. The identification of selected HCO?L?SER?NH2 conformers via a systematic grid search usingab initio potential energy surfaces. Journal of Computational Chemistry, 1996, 17, 821-834.	3.3	37
15	Peptide models XXIII. Conformational model for polar side-chain containing amino acid residues: A comprehensive analysis of RHF, DFT, and MP2 properties of HCO-L-SER-NH2. Journal of Computational Chemistry, 2000, 21, 626-655.	3.3	37
16	Mechanism of the Tyrosine Ammonia Lyase Reactionâ€”Tandem Nucleophilic and Electrophilic Enhancement by a Proton Transfer. Chemistry - A European Journal, 2012, 18, 7793-7802.	3.3	37
17	Mechanism for the Oxidation of Sulfides and Sulfoxides with Periodates: Reactivity of the Oxidizing Species. European Journal of Organic Chemistry, 2009, 2009, 2102-2111.	2.4	35
18	Characteristics of Ramachandran maps of L-alanine diamides as computed by various molecular mechanics, semiempirical and ab initio MO methods.. Computational and Theoretical Chemistry, 1998, 455, 275-301.	1.5	34

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19	Conformations of ethylbenzene (CH3î—¸CH2î—¸Ph). An ab initio study. Computational and Theoretical Chemistry, 1996, 367, 25-31.	1.5	32
20	Mechanism of nucleophilic substitutions at phenacyl bromides with pyridines. A computational study of intermediate and transition state. Journal of Physical Organic Chemistry, 2008, 21, 988-996.	1.9	28
21	Concerted S_N2 mechanism for the hydrolysis of acid chlorides: comparisons of reactivities calculated by the density functional theory with experimental data. Journal of Physical Organic Chemistry, 2011, 24, 480-491.	1.9	26
22	A DFT study of transition structures and reactivity in solvolyses of tertâ€butyl chloride, cumyl chlorides, and benzyl chlorides. Journal of Physical Organic Chemistry, 2008, 21, 53-61.	1.9	25
23	Molecular modelling of xylose isomerase catalysis: the role of electrostatics and charge transfer to metals. Protein Engineering, Design and Selection, 1995, 8, 925-933.	2.1	21
24	Effect of Substituents on Activation Parameters in Aliphatic SN2 Reactions. A DFT Study. Journal of Organic Chemistry, 2006, 71, 3409-3416.	3.2	21
25	Peptide models. XIV. Ab initio study on the role of side-chain backbone interaction stabilizing the building unit of right- and left-handed helices in peptides and proteins. International Journal of Quantum Chemistry, 1997, 61, 797-814.	2.0	20
26	Peptide models XXI. Side-chain/backbone conformational interconversions in HCO-l-Ser-NH2. Tracing relaxation paths by ab initio modeling. An exploratory study. Computational and Theoretical Chemistry, 1998, 455, 315-338.	1.5	16
27	Computational Study of Reactivity and Transition Structures in Nucleophilic Substitutions on Benzyl Bromides. European Journal of Organic Chemistry, 2006, 2006, 5570-5580.	2.4	16
28	Peptide models XII Topological features of molecular mechanics and ab-initio 8D-Ramachandran maps. Conformational data for Ac-(l-Ala)4-NHMe and For-(l-Ala)4-NH2. Computational and Theoretical Chemistry, 1995, 331, 11-26.	1.5	15
29	Peptide models VII The ending of the right-handed helices in oligopeptides [For-(Ala)n-NH2 for 2 â©½ n â©½ 4] and in proteins. Computational and Theoretical Chemistry, 1995, 331, 5-10.	1.5	14
30	Conformational effects of one glycine residue on the other glycine residues in the Ac-Gly-Gly-Gly-NHMe tripeptide motif: an ab initio exploratory study. Computational and Theoretical Chemistry, 2002, 588, 187-200.	1.5	14
31	Exploration of the Four-Dimensional-Conformational Potential Energy Hypersurface ofN-Acetyl-l-aspartic AcidNâ€˜-Methylamide with Its Internally Hydrogen Bonded Side-Chain Orientation. Journal of Physical Chemistry A, 2002, 106, 6999-7009.	2.5	13
32	Generation and analysis of the conformational potential energy surfaces of N-acetyl-N-methyl-l-alanine-Nâ€²-methylamide. An exploratory ab initio study. Computational and Theoretical Chemistry, 2003, 625, 121-136.	1.5	11
33	Mechanism of the Gibbs Reaction. 3. Indophenol Formation via Radical Electrophilic Aromatic Substitution (SREAr) on Phenols. Journal of Organic Chemistry, 1994, 59, 6543-6557.	3.2	10
34	Reverse turn conformation of N-thioacetyl thioprolyl glycine Nâ€²-methylamide in the crystal and in solution. Tetrahedron, 1993, 49, 6661-6668.	1.9	9
35	Geometry optimization of Kringle 1 of plasminogen using the PM3 semiempirical method. International Journal of Quantum Chemistry, 2000, 77, 82-89.	2.0	9
36	Mechanism for the reactions of sulfides and sulfoxides with hypochlorites: racemization and oxygen exchange of oxysulfonium salts and sulfoxides. Journal of Physical Organic Chemistry, 2012, 25, 1086-1096.	1.9	9

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37	Antibody Recognition and Conformational Flexibility of a Plaque-Specific Î²-Amyloid Epitope Modulated by Non-native Peptide Flanking Regions. Journal of Medicinal Chemistry, 2008, 51, 1150-1161.	6.4	6
38	Quantum chemical (QM:MM) investigation of the mechanism of enzymatic reaction of tryptamine and N,N-dimethyltryptamine with monoamine oxidase A. Organic and Biomolecular Chemistry, 2020, 18, 9660-9674.	2.8	6
39	Mechanism for the reactions of sulfides with hypochlorous acid and N â€chlorosulfonâ€amides: Formation of solvated chlorosulfonium cation and Î» 4 â€sulfane intermediates. Journal of Physical Organic Chemistry, 2019, 32, e4005.	1.9	4
40	Parameter-free linear relationship (PFLR) and its application to 3D QSAR. Journal of Mathematical Chemistry, 2009, 45, 598-606.	1.5	2
41	Helix compactness and stability: Electron structure calculations of conformer dependent thermodynamic functions. Chemical Physics Letters, 2013, 563, 80-87.	2.6	2
42	An exploratory study on the oxo-enol tautomerization of selected dioxopiperazines and their sulphur-containing analogues. Computational and Theoretical Chemistry, 1993, 286, 131-148.	1.5	1
43	Peptide models. XIV. Ab initio study on the role of side-chain backbone interaction stabilizing the building unit of right- and left-handed helices in peptides and proteins. , 1997, 61, 797.		1
44	Synthesis, structure and conformational analysis of imidazo-thiazines. Journal of Molecular Structure, 1996, 377, 277-288.	3.6	0
45	Quantum chemical study of the hydrolysis of oxidized endogenous psychedelic N,N-dimethyltryptamine. Computational and Theoretical Chemistry, 2022, , 113789.	2.5	0