Gerald Monard

List of Publications by Year in Descending Order

50 papers	1,468 citations	19 h-index	38 g-index
59 ext. papers	1,593 ext. citations	4.5 avg, IF	4.23 L-index

#	Paper	IF	Citations
50	Using Atomic Charges to Describe the p of Carboxylic Acids. *Journal of Chemical Information and Modeling*, **2021**, 61, 2733-2743	6.1	3
49	Elucidation of the atroposelectivity in the synthesis of axially chiral thiohydantoin derivatives. *Organic and Biomolecular Chemistry*, **2020**, 18, 2233-2241	3.9	2
48	Dendrigraft of Poly-l-lysine as a Promising Candidate To Reverse Heparin-based Anticoagulants in Clinical Settings. *ACS Medicinal Chemistry Letters*, **2019**, 10, 917-922	4.3	9
47	Semi-Empirical Born-Oppenheimer Molecular Dynamics (SEBOMD) within the Amber Biomolecular Package. *Journal of Chemical Information and Modeling*, **2019**, 59, 206-214	6.1	2
46	Biotinylation enhances the anticancer effects of 15d-PGJ2 against breast cancer cells. *International Journal of Oncology*, **2018**, 52, 1991-2000	4.4	1
45	Synthesis and evaluation of new designed multiple ligands directed towards both peroxisome proliferator-activated receptor- and angiotensin II type 1 receptor. *European Journal of Medicinal Chemistry*, **2018**, 158, 334-352	6.8	2
44	Solvent Effects in Quantum Chemistry **2017**, 727-739		1
43	Computational insights into substrate binding and catalytic mechanism of the glutaminase domain of glucosamine-6-phosphate synthase (GlmS). *RSC Advances*, **2017**, 7, 29626-29638	3.7	3
42	Assessing protein-ligand binding modes with computational tools: the case of PDE4B. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 563-575	4.2	0
41	Pretransfer Editing in Threonyl-tRNA Synthetase: Roles of Differential Solvent Accessibility and Intermediate Stabilization. *ACS Catalysis*, **2017**, 7, 3102-3112	13.1	6
40	Digitizing Poly-l-lysine Dendrigrafts: From Experimental Data to Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2017**, 57, 2173-2180	6.1	13
39	Molecular dynamics simulations of apo, holo, and inactivator bound GABA-at reveal the role of active site residues in PLP dependent enzymes. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 875-91	4.2	3
38	Hydration Effect on Amide I Infrared Bands in Water: An Interpretation Based on an Interaction Energy Decomposition Scheme. *Journal of Physical Chemistry B*, **2015**, 119, 9056-67	3.4	14
37	Why does Asn71 deamidate faster than Asn15 in the enzyme triosephosphate isomerase? Answers from microsecond molecular dynamics simulation and QM/MM free energy calculations. *Biochemistry*, **2015**, 54, 1429-39	3.2	13
36	Solvent Effects in Quantum Chemistry **2015**, 1-13		
35	AlgoGen: A tool coupling a linear-scaling quantum method with a genetic algorithm for exploring non-covalent interactions. *Computational and Theoretical Chemistry*, **2014**, 1028, 7-18	2	13
34	Water interactions with hydrophobic groups: assessment and recalibration of semiempirical molecular orbital methods. *Journal of Chemical Physics*, **2014**, 141, 034106	3.9	15

33	Rationalization of the pKa values of alcohols and thiols using atomic charge descriptors and its application to the prediction of amino acid pKaS. *Journal of Chemical Information and Modeling*, **2014**, 54, 2200-13	6.1	46
32	Vibrational energy relaxation of the amide I mode of N-methylacetamide in DD studied through Born-Oppenheimer molecular dynamics. *Journal of Physical Chemistry B*, **2014**, 118, 6186-97	3.4	25
31	Initiation of the reaction of deamidation in triosephosphate isomerase: investigations by means of molecular dynamics simulations. *Journal of Physical Chemistry B*, **2012**, 116, 6288-301	3.4	3
30	Solvent Effects in Quantum Chemistry **2012**, 561-571		5
29	What is the effective dielectric constant in a Ecyclodextrin cavity? Insights from Molecular Dynamics simulations and QM/MM calculations. *Computational and Theoretical Chemistry*, **2011**, 968, 71-76	2	7
28	Importance of Polarization and Charge Transfer Effects to Model the Infrared Spectra of Peptides in Solution. *Journal of Chemical Theory and Computation*, **2011**, 7, 1840-9	6.4	24
27	Reduction mechanism in class A methionine sulfoxide reductases: a theoretical chemistry investigation. *Theoretical Chemistry Accounts*, **2011**, 129, 93-103	1.9	11
26	X-ray, ESR, and quantum mechanics studies unravel a spin well in the cofactor-less urate oxidase. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1964-76	4.2	14
25	Peptide binding to Ecyclodextrins: structure, dynamics, energetics, and electronic effects. *Journal of Physical Chemistry A*, **2011**, 115, 11810-7	2.8	16
24	Computer simulation of reactions in beta-cyclodextrin molecular reactors: transition state recognition. *Organic and Biomolecular Chemistry*, **2010**, 8, 4346-55	3.9	8
23	An approach based on Density Functional Theory (DFT) calculations to assess the Candida antarctica lipase B selectivity in rutin, isoquercitrin and quercetin acetylation. *Journal of Molecular Catalysis B: Enzymatic*, **2010**, 66, 325-331		19
22	Combining a genetic algorithm with a linear scaling semiempirical method for proteinligand docking. *Computational and Theoretical Chemistry*, **2009**, 898, 31-41		12
21	Intrinsic reactivity of uric acid with dioxygen: Towards the elucidation of the catalytic mechanism of urate oxidase. *Bioorganic Chemistry*, **2009**, 37, 111-25	5.1	12
20	Deamidation of asparagine residues: direct hydrolysis versus succinimide-mediated deamidation mechanisms. *Journal of Physical Chemistry A*, **2009**, 113, 1111-20	2.8	88
19	Oxygen pressurized X-ray crystallography: probing the dioxygen binding site in cofactorless urate oxidase and implications for its catalytic mechanism. *Biophysical Journal*, **2008**, 95, 2415-22	2.9	53
18	Computational study on nonenzymatic peptide bond cleavage at asparagine and aspartic acid. *Journal of Physical Chemistry A*, **2008**, 112, 8752-61	2.8	51
17	Comparative semiempirical and ab initio study of the structural and chemical properties of uric acid and its anions. *International Journal of Quantum Chemistry*, **2007**, 107, 172-181	2.1	15
16	Theoretical study of the reduction mechanism of sulfoxides by thiols. *Journal of Physical Chemistry A*, **2006**, 110, 7628-36	2.8	31

15	Reaction mechanism of deamidation of asparaginyl residues in peptides: effect of solvent molecules. *Journal of Physical Chemistry A*, **2006**, 110, 8354-65	2.8	50
14	Quantum computations of the UV–visible spectra of uric acid and its anions. *Computational and Theoretical Chemistry*, **2006**, 761, 203-207		9
13	Simulation of liquid water using semiempirical Hamiltonians and the divide and conquer approach. *Journal of Physical Chemistry A*, **2005**, 109, 3425-32	2.8	58
12	Complexed and ligand-free high-resolution structures of urate oxidase (Uox) from Aspergillus flavus: a reassignment of the active-site binding mode. *Acta Crystallographica Section D: Biological Crystallography*, **2004**, 60, 453-62		66
11	Theoretical Approach to the Wear and Tear Mechanism in Triosephoshate Isomerase: A QM/MM Study. *Journal of Physical Chemistry B*, **2004**, 108, 3925-3934	3.4	5
10	Determination of enzymatic reaction pathways using QM/MM methods. *International Journal of Quantum Chemistry*, **2003**, 93, 229-244	2.1	49
9	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. *Theoretical Chemistry Accounts*, **2002**, 107, 147-153	1.9	15
8	An efficient method for the coordinate transformation problem of massively three-dimensional networks. *Journal of Chemical Physics*, **2001**, 114, 9747-9753	3.9	17
7	Insights in the Peptide Hydrolysis Mechanism by Thermolysin: A Theoretical QM/MM study. *Journal of Molecular Modeling*, **2000**, 6, 527-538	2	72
6	Linear scaling algorithm for the coordinate transformation problem of molecular geometry optimization. *Journal of Chemical Physics*, **2000**, 113, 5598-5603	3.9	26
5	Combined Quantum Mechanical/Molecular Mechanical Methodologies Applied to Biomolecular Systems. *Accounts of Chemical Research*, **1999**, 32, 904-911	24.3	304
4	Theoretical investigation of the monomer reactivity in polyindole derivatives. *Synthetic Metals*, **1999**, 101, 115-116	3.6	37
3	Theoretical study of indole polymerization. *Computational and Theoretical Chemistry*, **1998**, 434, 129-134		28
2	Modeling of Peptide Hydrolysis by Thermolysin. A Semiempirical and QM/MM Study. *Journal of the American Chemical Society*, **1998**, 120, 8825-8833	16.4	68
1	Hybrid classical quantum force field for modeling very large molecules. *International Journal of Quantum Chemistry*, **1996**, 58, 153-159	2.1	124