

# Gerald Monard

## List of Publications by Citations

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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	Combined Quantum Mechanical/Molecular Mechanical Methodologies Applied to Biomolecular Systems. <i>Accounts of Chemical Research</i> , <b>1999</b> , 32, 904-911	24.3	304
49	Hybrid classical quantum force field for modeling very large molecules. <i>International Journal of Quantum Chemistry</i> , <b>1996</b> , 58, 153-159	2.1	124
48	Deamidation of asparagine residues: direct hydrolysis versus succinimide-mediated deamidation mechanisms. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 1111-20	2.8	88
47	Insights in the Peptide Hydrolysis Mechanism by Thermolysin: A Theoretical QM/MM study. <i>Journal of Molecular Modeling</i> , <b>2000</b> , 6, 527-538	2	72
46	Modeling of Peptide Hydrolysis by Thermolysin. A Semiempirical and QM/MM Study. <i>Journal of the American Chemical Society</i> , <b>1998</b> , 120, 8825-8833	16.4	68
45	Complexed and ligand-free high-resolution structures of urate oxidase (Uox) from <i>Aspergillus flavus</i> : a reassignment of the active-site binding mode. <i>Acta Crystallographica Section D: Biological Crystallography</i> , <b>2004</b> , 60, 453-62		66
44	Simulation of liquid water using semiempirical Hamiltonians and the divide and conquer approach. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 3425-32	2.8	58
43	Oxygen pressurized X-ray crystallography: probing the dioxygen binding site in cofactorless urate oxidase and implications for its catalytic mechanism. <i>Biophysical Journal</i> , <b>2008</b> , 95, 2415-22	2.9	53
42	Computational study on nonenzymatic peptide bond cleavage at asparagine and aspartic acid. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 8752-61	2.8	51
41	Reaction mechanism of deamidation of asparaginyl residues in peptides: effect of solvent molecules. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 8354-65	2.8	50
40	Determination of enzymatic reaction pathways using QM/MM methods. <i>International Journal of Quantum Chemistry</i> , <b>2003</b> , 93, 229-244	2.1	49
39	Rationalization of the pKa values of alcohols and thiols using atomic charge descriptors and its application to the prediction of amino acid pKa's. <i>Journal of Chemical Information and Modeling</i> , <b>2014</b> , 54, 2200-13	6.1	46
38	Theoretical investigation of the monomer reactivity in polyindole derivatives. <i>Synthetic Metals</i> , <b>1999</b> , 101, 115-116	3.6	37
37	Theoretical study of the reduction mechanism of sulfoxides by thiols. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 7628-36	2.8	31
36	Theoretical study of indole polymerization. <i>Computational and Theoretical Chemistry</i> , <b>1998</b> , 434, 129-134		28
35	Linear scaling algorithm for the coordinate transformation problem of molecular geometry optimization. <i>Journal of Chemical Physics</i> , <b>2000</b> , 113, 5598-5603	3.9	26
34	Vibrational energy relaxation of the amide I mode of N-methylacetamide in D <sub>2</sub> O studied through Born-Oppenheimer molecular dynamics. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 6186-97	3.4	25

33	Importance of Polarization and Charge Transfer Effects to Model the Infrared Spectra of Peptides in Solution. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 1840-9	6.4	24
32	An approach based on Density Functional Theory (DFT) calculations to assess the Candida antarctica lipase B selectivity in rutin, isoquercitrin and quercetin acetylation. <i>Journal of Molecular Catalysis B: Enzymatic</i> , <b>2010</b> , 66, 325-331		19
31	An efficient method for the coordinate transformation problem of massively three-dimensional networks. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 9747-9753	3.9	17
30	Peptide binding to $\beta$ -cyclodextrins: structure, dynamics, energetics, and electronic effects. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 11810-7	2.8	16
29	Water interactions with hydrophobic groups: assessment and recalibration of semiempirical molecular orbital methods. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 034106	3.9	15
28	Comparative semiempirical and ab initio study of the structural and chemical properties of uric acid and its anions. <i>International Journal of Quantum Chemistry</i> , <b>2007</b> , 107, 172-181	2.1	15
27	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. <i>Theoretical Chemistry Accounts</i> , <b>2002</b> , 107, 147-153	1.9	15
26	Hydration Effect on Amide I Infrared Bands in Water: An Interpretation Based on an Interaction Energy Decomposition Scheme. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 9056-67	3.4	14
25	X-ray, ESR, and quantum mechanics studies unravel a spin well in the cofactor-less urate oxidase. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2011</b> , 79, 1964-76	4.2	14
24	AlgoGen: A tool coupling a linear-scaling quantum method with a genetic algorithm for exploring non-covalent interactions. <i>Computational and Theoretical Chemistry</i> , <b>2014</b> , 1028, 7-18	2	13
23	Digitizing Poly-l-lysine Dendrigrafts: From Experimental Data to Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 2173-2180	6.1	13
22	Why does Asn71 deamidate faster than Asn15 in the enzyme triosephosphate isomerase? Answers from microsecond molecular dynamics simulation and QM/MM free energy calculations. <i>Biochemistry</i> , <b>2015</b> , 54, 1429-39	3.2	13
21	Combining a genetic algorithm with a linear scaling semiempirical method for protein-ligand docking. <i>Computational and Theoretical Chemistry</i> , <b>2009</b> , 898, 31-41		12
20	Intrinsic reactivity of uric acid with dioxygen: Towards the elucidation of the catalytic mechanism of urate oxidase. <i>Bioorganic Chemistry</i> , <b>2009</b> , 37, 111-25	5.1	12
19	Reduction mechanism in class A methionine sulfoxide reductases: a theoretical chemistry investigation. <i>Theoretical Chemistry Accounts</i> , <b>2011</b> , 129, 93-103	1.9	11
18	Dendrigraft of Poly-l-lysine as a Promising Candidate To Reverse Heparin-based Anticoagulants in Clinical Settings. <i>ACS Medicinal Chemistry Letters</i> , <b>2019</b> , 10, 917-922	4.3	9
17	Quantum computations of the UV-visible spectra of uric acid and its anions. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 761, 203-207		9
16	Computer simulation of reactions in beta-cyclodextrin molecular reactors: transition state recognition. <i>Organic and Biomolecular Chemistry</i> , <b>2010</b> , 8, 4346-55	3.9	8

15	What is the effective dielectric constant in a Cyclodextrin cavity? Insights from Molecular Dynamics simulations and QM/MM calculations. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 968, 71-76	2	7
14	Pretransfer Editing in Threonyl-tRNA Synthetase: Roles of Differential Solvent Accessibility and Intermediate Stabilization. <i>ACS Catalysis</i> , <b>2017</b> , 7, 3102-3112	13.1	6
13	Solvent Effects in Quantum Chemistry <b>2012</b> , 561-571		5
12	Theoretical Approach to the Wear and Tear Mechanism in Triosephosphate Isomerase: A QM/MM Study. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 3925-3934	3.4	5
11	Computational insights into substrate binding and catalytic mechanism of the glutaminase domain of glucosamine-6-phosphate synthase (GlmS). <i>RSC Advances</i> , <b>2017</b> , 7, 29626-29638	3.7	3
10	Initiation of the reaction of deamidation in triosephosphate isomerase: investigations by means of molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , <b>2012</b> , 116, 6288-301	3.4	3
9	Using Atomic Charges to Describe the p of Carboxylic Acids. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 2733-2743	6.1	3
8	Molecular dynamics simulations of apo, holo, and inactivator bound GABA-at reveal the role of active site residues in PLP dependent enzymes. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2016</b> , 84, 875-91	4.2	3
7	Elucidation of the atroposelectivity in the synthesis of axially chiral thiohydantoin derivatives. <i>Organic and Biomolecular Chemistry</i> , <b>2020</b> , 18, 2233-2241	3.9	2
6	Semi-Empirical Born-Oppenheimer Molecular Dynamics (SEBOMD) within the Amber Biomolecular Package. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 206-214	6.1	2
5	Synthesis and evaluation of new designed multiple ligands directed towards both peroxisome proliferator-activated receptor- $\alpha$ and angiotensin II type 1 receptor. <i>European Journal of Medicinal Chemistry</i> , <b>2018</b> , 158, 334-352	6.8	2
4	Solvent Effects in Quantum Chemistry <b>2017</b> , 727-739		1
3	Biotinylation enhances the anticancer effects of 15d-PGJ2 against breast cancer cells. <i>International Journal of Oncology</i> , <b>2018</b> , 52, 1991-2000	4.4	1
2	Assessing protein-ligand binding modes with computational tools: the case of PDE4B. <i>Journal of Computer-Aided Molecular Design</i> , <b>2017</b> , 31, 563-575	4.2	0
1	Solvent Effects in Quantum Chemistry <b>2015</b> , 1-13		