Paul G Seybold

List of Publications by Year
in descending order

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62 papers	3,065 citations	361413 20 h-index	155660 55 g-index
62 all docs	62 docs citations	62 times ranked	3740 citing authors

#	Article	IF	Citations
1	Computational Estimation of the Acidities of Pyrimidines and Related Compounds. Molecules, 2022, 27, 385.	3.8	4
2	Computational Estimation of the Aqueous Acidities of Alcohols, Hydrates, and Enols. Journal of Physical Chemistry A, 2021, 125, 3600-3605.	2.5	9
3	The many faces of fluorine: Some noncovalent interactions of fluorine compounds. Journal of Chemical Thermodynamics, 2021, 156, 106382.	2.0	21
4	A general model for the solubilities of gases in liquids. Journal of Molecular Modeling, 2020, 26, 244.	1.8	2
5	Computational Estimation of the Gas-Phase and Aqueous Acidities of Carbon Acids. Journal of Physical Chemistry A, 2020, 124, 2152-2159.	2.5	9
6	Computational estimation of the acidities of purines and indoles. Journal of Molecular Modeling, 2019, 25, 12.	1.8	9
7	A stochastic cellular automata model of tautomer equilibria. Molecular Physics, 2018, 116, 746-751.	1.7	2
8	Modeling molecular boiling points using computed interaction energies. Journal of Molecular Modeling, 2018, 24, 21.	1.8	4
9	Anesthetic activity and the electrostatic potential (revisited). Journal of Molecular Modeling, 2018, 24, 19.	1.8	3
10	Combining Chemical Information Literacy, Communication Skills, Career Preparation, Ethics, and Peer Review in a Team-Taught Chemistry Course. Journal of Chemical Education, 2016, 93, 439-443.	2.3	28
11	Computational estimation of pK_a values. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 290-297.	14.6	85
12	Intuitive and counterintuitive noncovalent interactions of aromatic Ï€ regions with the hydrogen and the nitrogen of HCN. Journal of Computational Science, 2015, 10, 209-216.	2.9	83
13	Quantum chemical estimation of the acidities of some inorganic oxoacids. Molecular Physics, 2015, 113, 232-236.	1.7	12
14	Cellular Automata Modeling of Complex Biochemical Systems. , 2015, , 1-23.		1
15	Theoretical estimation of the aqueous pK_as of thiols. Molecular Physics, 2014, 112, 340-348.	1.7	5
16	Quantum Chemicalâ€QSPR Estimation of the Acidities and Basicities of Organic Compounds. Advances in Quantum Chemistry, 2012, , 83-104.	0.8	16
17	Charge competition in halogenated hydrocarbons. International Journal of Quantum Chemistry, 2012, 112, 219-229.	2.0	12
18	Theoretical estimation of the acidities of alcohols and azoles in gas phase, DMSO, and water. International Journal of Quantum Chemistry, 2012, 112, 3769-3776.	2.0	16

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19	Correlations Involving the Solubility of Gases in Water at 298.15 K and 101325 Pa. Journal of Chemical & Engineering Data, 2011, 56, 727-732.	1.9	12
20	The O₂/N₂ Ratio Gas Solubility Mystery. Journal of Chemical & Engineering Data, 2011, 56, 5036-5044.	1.9	18
21	A Class Project Combining Organic Chemistry, Quantum Chemistry, and Statistics. Annual Reports in Computational Chemistry, 2011, 7, 237-249.	1.7	4
22	Quantum chemical study of the energetics and directionality of acidâ€catalyzed aromatic epoxide ring openings. International Journal of Quantum Chemistry, 2010, 110, 2931-2937.	2.0	2
23	On the Role of Solute Polarizability in Determining the Solubilities of Gases in Liquids. Journal of Chemical & Engineering Data, 2010, 55, 37-40.	1.9	13
24	Quantum chemical analysis of the energetics of the anti and gauche conformers of ethanol. Structural Chemistry, 2009, 20, 43-48.	2.0	24
25	Conformational analysis of anilinonaphthalenesulfonate derivatives. I. 2-anilino-6-naphthalenesulfonate. International Journal of Quantum Chemistry, 2009, 18, 115-122.	2.0	0
26	Topological influences on the carcinogenicity of aromatic hydrocarbons. I. The bay region geometry. International Journal of Quantum Chemistry, 2009, 24, 95-101.	2.0	1
27	Topological influences on the carcinogenicity of aromatic hydrocarbons. II. Substituent effects. International Journal of Quantum Chemistry, 2009, 24, 103-108.	2.0	0
28	Correlations between quantum chemical indices and the pK_as of a diverse set of organic phenols. International Journal of Quantum Chemistry, 2009, 109, 3679-3684.	2.0	19
29	Analysis of the pK_as of aliphatic amines using quantum chemical descriptors. International Journal of Quantum Chemistry, 2008, 108, 2849-2855.	2.0	26
30	Solubility Correlations. Part 1. Chemistry and Biodiversity, 2007, 4, 2547-2554.	2.1	2
31	Relationships between aqueous acidities and computed surface-electrostatic potentials and local ionization energies of substituted phenols and benzoic acids. Journal of Molecular Modeling, 2004, 10, 235.	1.8	33
32	Synergistic interactions among QSAR descriptors. International Journal of Quantum Chemistry, 2004, 96, 1-9.	2.0	35
33	First-order stochastic cellular automata simulations of the lindemann mechanism. International Journal of Chemical Kinetics, 2004, 36, 230-237.	1.6	12
34	Absolute pKa Determinations for Substituted Phenols. Journal of the American Chemical Society, 2002, 124, 6421-6427.	13.7	519
35	Comparison of different atomic charge schemes for predicting pKa variations in substituted anilines and phenols. International Journal of Quantum Chemistry, 2002, 90, 445-458.	2.0	182
36	Substituent effects on the electronic structure and pKa of benzoic acid. International Journal of Quantum Chemistry, 2002, 90, 1396-1403.	2.0	136

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37	Fluorescence Quantum Yields and Their Relation to Lifetimes of Rhodamine 6G and Fluorescein in Nine Solvents: Improved Absolute Standards for Quantum YieldsÂ¶. Photochemistry and Photobiology, 2002, 75, 327-334.	2.5	114
38	Halogens in molecular structure-property relationships. Advances in Quantitative Structure - Property Relationships, 2002, , 109-136.	1.0	4
39	Comparison of Quantum Chemical Parameters and Hammett Constants in Correlating pKaValues of Substituted Anilines. Journal of Organic Chemistry, 2001, 66, 6919-6925.	3.2	158
40	Cellular Automata Models of Aqueous Solution Systems. Reviews in Computational Chemistry, 2001, , 205-254.	1.5	18
41	Molecular structureâ€“property relationships for alkenes. Journal of Molecular Graphics and Modelling, 2001, 20, 36-53.	2.4	12
42	Substituent effects on the physical properties and pKa of phenol. International Journal of Quantum Chemistry, 2001, 85, 569-579.	2.0	155
43	Cellular automata models of kinetically and thermodynamically controlled reactions. International Journal of Chemical Kinetics, 2000, 32, 529-534.	1.6	16
44	Substituent effects on the physical properties and pKa of aniline. International Journal of Quantum Chemistry, 2000, 80, 1107-1115.	2.0	108
45	Solvent Dependence of the Fluorescence Lifetimes of Xanthene Dyes. Photochemistry and Photobiology, 1999, 70, 737-744.	2.5	480
46	Aurora borealis: Stochastic cellular automata simulations of the excited-state dynamics of oxygen atoms. International Journal of Quantum Chemistry, 1999, 75, 751-756.	2.0	9
47	Stochastic Cellular Automata Models of Molecular Excited-State Dynamics. Journal of Physical Chemistry A, 1998, 102, 886-891.	2.5	14
48	A Cellular Automata Model of Acid Dissociation. Journal of Chemical Information and Computer Sciences, 1998, 38, 271-275.	2.8	13
49	Simulation of First-Order Chemical Kinetics Using Cellular Automata. Journal of Chemical Information and Computer Sciences, 1997, 37, 386-391.	2.8	28
50	A simple model for the chromatographic retentions of polyhalogenated biphenyls. Analytical Chemistry, 1993, 65, 1631-1634.	6.5	18
51	Molecular modeling of the physical properties of alkanes. Journal of the American Chemical Society, 1988, 110, 4186-4194.	13.7	292
52	Modeling the tissue solubilities and metabolic rate constant (Vmax) of halogenated methanes, ethanes, and ethylenes. Toxicology Letters, 1988, 43, 235-256.	0.8	82
53	Molecular structure: Property relationships. Journal of Chemical Education, 1987, 64, 575.	2.3	141
54	Theperi effect in aromatic hydrocarbon carcinogenesis: An empirical force field examination. International Journal of Quantum Chemistry, 1987, 31, 847-853.	2.0	8

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55	The search for active substructures in structure-activity studies. International Journal of Quantum Chemistry, 1987, 32, 245-260.	2.0	5
56	Topological determinants in organic chemistry. International Journal of Quantum Chemistry, 1983, 23, 1683-1683.	2.0	0
57	Relationships between carcinogenicity, mutagenicity, and theoretical reactivity indices for polycyclic aromatic hydrocarbons. International Journal of Quantum Chemistry, 1981, 20, 401-408.	2.0	2
58	A molecular orbital study of the metabolism and carcinogenicity of the phenols of benzo(a)pyrene. International Journal of Quantum Chemistry, 1980, 18, 261-270.	2.0	0
59	Substituent effects in chemical carcinogenesis: Methyl derivatives of the benzacridines. Journal of Heterocyclic Chemistry, 1979, 16, 421-425.	2.6	24
60	Methylbenz[a]anthracenes: Correlations between theoretical reactivity indices and carcinogenicity. International Journal of Quantum Chemistry, 1978, 14, 311-320.	2.0	1
61	Why are there four bases in DNA?. International Journal of Quantum Chemistry, 1976, 10, 39-43.	2.0	1
62	Computational estimation of the acidities of some inorganic nitrogen acids. Molecular Physics, 0, , 1-4.	1.7	3