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	Absolute pKa Determinations for Substituted Phenols. Journal of the American Chemical Society, 2002, 124, 6421-6427.	13.7	519
2	Solvent Dependence of the Fluorescence Lifetimes of Xanthene Dyes. Photochemistry and Photobiology, 1999, 70, 737-744.	2.5	480
3	Molecular modeling of the physical properties of alkanes. Journal of the American Chemical Society, 1988, 110, 4186-4194.	13.7	292
4	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
5	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
6	Substituent effects on the physical properties and pKa of phenol. International Journal of Quantum Chemistry, 2001, 85, 569-579.	2.0	155
7	Molecular structure: Property relationships. Journal of Chemical Education, 1987, 64, 575.	2.3	141
8	Substituent effects on the electronic structure and pKa of benzoic acid. International Journal of Quantum Chemistry, 2002, 90, 1396-1403.	2.0	136
9	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
10	Substituent effects on the physical properties and pKa of aniline. International Journal of Quantum Chemistry, 2000, 80, 1107-1115.	2.0	108
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	Modeling the tissue solubilities and metabolic rate constant (Vmax) of halogenated methanes, ethanes, and ethylenes. Toxicology Letters, 1988, 43, 235-256.	0.8	82
14	Synergistic interactions among QSAR descriptors. International Journal of Quantum Chemistry, 2004, 96, 1-9.	2.0	35
15	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
16	Simulation of First-Order Chemical Kinetics Using Cellular Automata. Journal of Chemical Information and Computer Sciences, 1997, 37, 386-391.	2.8	28
17	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
18	Analysis of the pK_as of aliphatic amines using quantum chemical descriptors. International Journal of Quantum Chemistry, 2008, 108, 2849-2855.	2.0	26

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19	Substituent effects in chemical carcinogenesis: Methyl derivatives of the benzacridines. Journal of Heterocyclic Chemistry, 1979, 16, 421-425.	2.6	24
20	Quantum chemical analysis of the energetics of the anti and gauche conformers of ethanol. Structural Chemistry, 2009, 20, 43-48.	2.0	24
21	The many faces of fluorine: Some noncovalent interactions of fluorine compounds. Journal of Chemical Thermodynamics, 2021, 156, 106382.	2.0	21
22	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
23	A simple model for the chromatographic retentions of polyhalogenated biphenyls. Analytical Chemistry, 1993, 65, 1631-1634.	6.5	18
24	Cellular Automata Models of Aqueous Solution Systems. Reviews in Computational Chemistry, 2001, , 205-254.	1.5	18
25	The O₂/N₂ Ratio Gas Solubility Mystery. Journal of Chemical & Engineering Data, 2011, 56, 5036-5044.	1.9	18
26	Cellular automata models of kinetically and thermodynamically controlled reactions. International Journal of Chemical Kinetics, 2000, 32, 529-534.	1.6	16
27	Quantum Chemicalâ€QSPR Estimation of the Acidities and Basicities of Organic Compounds. Advances in Quantum Chemistry, 2012, , 83-104.	0.8	16
28	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
29	Stochastic Cellular Automata Models of Molecular Excited-State Dynamics. Journal of Physical Chemistry A, 1998, 102, 886-891.	2.5	14
30	A Cellular Automata Model of Acid Dissociation. Journal of Chemical Information and Computer Sciences, 1998, 38, 271-275.	2.8	13
31	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
32	Molecular structureâ€“property relationships for alkenes. Journal of Molecular Graphics and Modelling, 2001, 20, 36-53.	2.4	12
33	First-order stochastic cellular automata simulations of the lindemann mechanism. International Journal of Chemical Kinetics, 2004, 36, 230-237.	1.6	12
34	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
35	Charge competition in halogenated hydrocarbons. International Journal of Quantum Chemistry, 2012, 112, 219-229.	2.0	12
36	Quantum chemical estimation of the acidities of some inorganic oxoacids. Molecular Physics, 2015, 113, 232-236.	1.7	12

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37	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
38	Computational estimation of the acidities of purines and indoles. Journal of Molecular Modeling, 2019, 25, 12.	1.8	9
39	Computational Estimation of the Gas-Phase and Aqueous Acidities of Carbon Acids. Journal of Physical Chemistry A, 2020, 124, 2152-2159.	2.5	9
40	Computational Estimation of the Aqueous Acidities of Alcohols, Hydrates, and Enols. Journal of Physical Chemistry A, 2021, 125, 3600-3605.	2.5	9
41	Theperi effect in aromatic hydrocarbon carcinogenesis: An empirical force field examination. International Journal of Quantum Chemistry, 1987, 31, 847-853.	2.0	8
42	The search for active substructures in structure-activity studies. International Journal of Quantum Chemistry, 1987, 32, 245-260.	2.0	5
43	Theoretical estimation of the aqueous pK_as of thiols. Molecular Physics, 2014, 112, 340-348.	1.7	5
44	A Class Project Combining Organic Chemistry, Quantum Chemistry, and Statistics. Annual Reports in Computational Chemistry, 2011, 7, 237-249.	1.7	4
45	Modeling molecular boiling points using computed interaction energies. Journal of Molecular Modeling, 2018, 24, 21.	1.8	4
46	Halogens in molecular structure-property relationships. Advances in Quantitative Structure - Property Relationships, 2002, , 109-136.	1.0	4
47	Computational Estimation of the Acidities of Pyrimidines and Related Compounds. Molecules, 2022, 27, 385.	3.8	4
48	Computational estimation of the acidities of some inorganic nitrogen acids. Molecular Physics, 0, , 1-4.	1.7	3
49	Anesthetic activity and the electrostatic potential (revisited). Journal of Molecular Modeling, 2018, 24, 19.	1.8	3
50	Relationships between carcinogenicity, mutagenicity, and theoretical reactivity indices for polycyclic aromatic hydrocarbons. International Journal of Quantum Chemistry, 1981, 20, 401-408.	2.0	2
51	Solubility Correlations. Part 1. Chemistry and Biodiversity, 2007, 4, 2547-2554.	2.1	2
52	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
53	A stochastic cellular automata model of tautomer equilibria. Molecular Physics, 2018, 116, 746-751.	1.7	2
54	A general model for the solubilities of gases in liquids. Journal of Molecular Modeling, 2020, 26, 244.	1.8	2

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55	Methylbenz[a]anthracenes: Correlations between theoretical reactivity indices and carcinogenicity. International Journal of Quantum Chemistry, 1978, 14, 311-320.	2.0	1
56	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
57	Why are there four bases in DNA?. International Journal of Quantum Chemistry, 1976, 10, 39-43.	2.0	1
58	Cellular Automata Modeling of Complex Biochemical Systems. , 2015, , 1-23.		1
59	Topological determinants in organic chemistry. International Journal of Quantum Chemistry, 1983, 23, 1683-1683.	2.0	0
60	Conformational analysis of anilinonaphthalenesulfonate derivatives. I. 2-anilino-6-naphthalenesulfonate. International Journal of Quantum Chemistry, 2009, 18, 115-122.	2.0	0
61	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
62	Topological influences on the carcinogenicity of aromatic hydrocarbons. II. Substituent effects. International Journal of Quantum Chemistry, 2009, 24, 103-108.	2.0	0