Peter Gedeck

List of Publications by Year in descending order

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52 papers	2,016 citations	257450 24 h-index	254184 43 g-index
56 all docs	56 docs citations	56 times ranked	2834 citing authors

#	Article	IF	Citations
1	Using Machine Learning to Parse Chemical Mixture Descriptions. ACS Omega, 2021, 6, 22400-22409.	3.5	2
2	Prediction of pK_a Using Machine Learning Methods with Rooted Topological Torsion Fingerprints: Application to Aliphatic Amines. Journal of Chemical Information and Modeling, 2019, 59, 4706-4719.	5.4	26
3	Capturing mixture composition: an open machine-readable format for representing mixed substances. Journal of Cheminformatics, 2019, 11, 33.	6.1	14
4	Development of a Cytopathic Effect-Based Phenotypic Screening Assay against Cryptosporidium. ACS Infectious Diseases, 2018, 4, 635-645.	3.8	9
5	Shared Consensus Machine Learning Models for Predicting Blood Stage Malaria Inhibition. Journal of Chemical Information and Modeling, 2017, 57, 445-453.	5.4	15
6	A Cryptosporidium PI(4)K inhibitor is a drug candidate for cryptosporidiosis. Nature, 2017, 546, 376-380.	27.8	144
7	Developing Collaborative QSAR Models Without Sharing Structures. Journal of Chemical Information and Modeling, 2017, 57, 1847-1858.	5.4	7
8	Mutations in the Plasmodium falciparum Cyclic Amine Resistance Locus (PfCARL) Confer Multidrug Resistance. MBio, 2016, 7, .	4.1	49
9	UDP-galactose and acetyl-CoA transporters as Plasmodium multidrug resistance genes. Nature Microbiology, 2016, 1, 16166.	13.3	102
10	Benefit of Retraining pKa Models Studied Using Internally Measured Data. Journal of Chemical Information and Modeling, 2015, 55, 1449-1459.	5.4	17
11	FOCUS â€" Development of a Global Communication and Modeling Platform for Applied and Computational Medicinal Chemists. Journal of Chemical Information and Modeling, 2015, 55, 896-908.	5.4	18
12	Matched Molecular Pair Analysis: Significance and the Impact of Experimental Uncertainty. Journal of Medicinal Chemistry, 2014, 57, 3786-3802.	6.4	62
13	Multipole-Based Force Fields from ab Initio Interaction Energies and the Need for Jointly Refitting All Intermolecular Parameters. Journal of Chemical Theory and Computation, 2013, 9, 1499-1511.	5.3	35
14	Deriving Static Atomic Multipoles from the Electrostatic Potential. Journal of Chemical Information and Modeling, 2013, 53, 3410-3417.	5.4	25
15	Comparability of Mixed IC50 Data â€" A Statistical Analysis. PLoS ONE, 2013, 8, e61007.	2.5	211
16	Development of isoform selective PI3-kinase inhibitors as pharmacological tools for elucidating the PI3K pathway. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5445-5450.	2.2	46
17	The Experimental Uncertainty of Heterogeneous Public K_i Data. Journal of Medicinal Chemistry, 2012, 55, 5165-5173.	6.4	183
18	Atomic multipoles: Electrostatic potential fit, local reference axis systems, and conformational dependence. Journal of Computational Chemistry, 2012, 33, 1673-1688.	3.3	56

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19	Global Free Energy Scoring Functions Based on Distance-Dependent Atom-Type Pair Descriptors. Journal of Chemical Information and Modeling, 2011, 51, 707-720.	5.4	26
20	Three Descriptor Model Sets a High Standard for the CSAR-NRC HiQ Benchmark. Journal of Chemical Information and Modeling, 2011, 51, 2139-2145.	5.4	7
21	Design and synthesis of a library of chemokine antagonists. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 6249-6252.	2.2	7
22	Avoidance of the Ames test liability for arylâ€“amines via computation. Bioorganic and Medicinal Chemistry, 2011, 19, 3173-3182.	3.0	29
23	Synthesis and evaluation of two series of 4â€²-aza-carbocyclic nucleosides as adenosine A2A receptor agonists. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 1219-1224.	2.2	10
24	A physical properties based approach for the exploration of a 4-hydroxybenzothiazolone series of Î²2-adrenoceptor agonists as inhaled long-acting bronchodilators. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5302-5307.	2.2	25
25	Leave-Cluster-Out Cross-Validation Is Appropriate for Scoring Functions Derived from Diverse Protein Data Sets. Journal of Chemical Information and Modeling, 2010, 50, 1961-1969.	5.4	84
26	Computational Analysis of Structureâ€“Activity Relationships. Progress in Medicinal Chemistry, 2010, 49, 113-160.	10.4	20
27	Insight into the Mechanism of Inactivation and pH Sensitivity in Potassium Channels from Molecular Dynamics Simulations. Biochemistry, 2008, 47, 7414-7422.	2.5	50
28	Exploiting QSAR models in lead optimization. Current Opinion in Drug Discovery & Development, 2008, 11, 569-75.	1.9	14
29	Drug block of the hERG potassium channel: Insight from modeling. Proteins: Structure, Function and Bioinformatics, 2007, 68, 568-580.	2.6	100
30	QSAR â˜’ How Good Is It in Practice? Comparison of Descriptor Sets on an Unbiased Cross Section of Corporate Data Sets. Journal of Chemical Information and Modeling, 2006, 46, 1924-1936.	5.4	135
31	CGH2466, a combined adenosine receptor antagonist, p38 mitogen-activated protein kinase and phosphodiesterase type 4 inhibitor with potent in vitro and in vivo anti-inflammatory activities. British Journal of Pharmacology, 2005, 144, 1002-1010.	5.4	19
32	Use Of The R-Group Descriptor for Alignment-Free QSAR. QSAR and Combinatorial Science, 2005, 24, 611-619.	1.4	17
33	Computational Chemistry at Novartis. Chimia, 2005, 59, 545-549.	0.6	7
34	Long-chain formoterol analogues: an investigation into the effect of increasing amino-substituent chain length on the Î²2-adrenoceptor activity. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4705-4710.	2.2	42
35	New Highly Potent and Selective Adenosine A3 Receptor Antagonists. Current Topics in Medicinal Chemistry, 2004, 4, 863-870.	2.1	18
36	Calculation of Intersubstituent Similarity Using R-Group Descriptors.. ChemInform, 2003, 34, no.	0.0	0

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37	Calculation of Intersubstituent Similarity Using R-Group Descriptors. Journal of Chemical Information and Computer Sciences, 2003, 43, 406-411.	2.8	49
38	The Reaction Mechanism of Bovine Lens Leucine Aminopeptidase. Journal of Physical Chemistry B, 2002, 106, 8815-8830.	2.6	25
39	Analysis for pharmaceutical scientists. Trends in Biotechnology, 2002, 20, 360.	9.3	0
40	Visual and computational analysis of structureâ€“activity relationships in high-throughput screening data. Current Opinion in Chemical Biology, 2001, 5, 389-395.	6.1	54
41	Additive NDDO-based atomic polarizability model. International Journal of Quantum Chemistry, 2000, 77, 473-497.	2.0	33
42	New Multicentre Point Charge Models for Molecular Electrostatic Potentials from Semiempirical M0-Calculations. Journal of Molecular Modeling, 2000, 6, 452-466.	1.8	8
43	Numerical self-consistent reaction field study of the excited-state properties of p-(dimethylamino)-benzonitrile derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 1999, 121, 7-15.	3.9	16
44	A Semiempirical QM/MM Implementation and its Application to the Absorption of Organic Molecules in Zeolites. Journal of Molecular Modeling, 1999, 5, 1-7.	1.8	23
45	Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods. International Journal of Quantum Chemistry, 1999, 75, 17-31.	2.0	37
46	Fast Long-Range Adiabatic Electron Transfer in a Model Polyglycine Î±-Helix. Journal of the American Chemical Society, 1999, 121, 1379-1380.	13.7	10
47	Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods. International Journal of Quantum Chemistry, 1999, 75, 17.	2.0	2
48	Numerical self-consistent reaction field study of intramolecular charge transfer in p-(dimethylamino)-benzonitrile. Journal of Photochemistry and Photobiology A: Chemistry, 1997, 105, 165-181.	3.9	44
49	Semi-Empirical Mo Calculations on Enzyme Reaction Mechanisms. , 1997, , 307-317.		5
50	1,5-hydrogen transfer â€" a hitherto ignored decay channel in the photodegradation of poly(2,6-dimethyl-1,4-phenylene oxide). Chemical Physics Letters, 1996, 257, 616-621.	2.6	4
51	Photophysics and Photochemistry of Intramolecular Stilbene-Amine Exciplexes. Journal of the American Chemical Society, 1995, 117, 660-669.	13.7	46
52	A COMPARISON OF PHYCOCYANINS FROM THREE DIFFERENT SPECIES OF CYANOBACTERIA EMPLOYING RESONANCE-ENHANCED COHERENT ANTI-STOKES RAMAN SPECTROSCOPY. Photochemistry and Photobiology, 1993, 57, 56-62.	2.5	10