

Peter Gedeck

List of Publications by Year in descending order

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52
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citations

257101

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43
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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.	1.6	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.	2.5	26
3	Capturing mixture composition: an open machine-readable format for representing mixed substances. Journal of Cheminformatics, 2019, 11, 33.	2.8	14
4	Development of a Cytopathic Effect-Based Phenotypic Screening Assay against <i>Cryptosporidium</i> . ACS Infectious Diseases, 2018, 4, 635-645.	1.8	9
5	Shared Consensus Machine Learning Models for Predicting Blood Stage Malaria Inhibition. Journal of Chemical Information and Modeling, 2017, 57, 445-453.	2.5	15
6	A <i>Cryptosporidium</i> PI(4)K inhibitor is a drug candidate for cryptosporidiosis. Nature, 2017, 546, 376-380.	13.7	144
7	Developing Collaborative QSAR Models Without Sharing Structures. Journal of Chemical Information and Modeling, 2017, 57, 1847-1858.	2.5	7
8	Mutations in the <i>Plasmodium falciparum</i> Cyclic Amine Resistance Locus (PfCARL) Confer Multidrug Resistance. MBio, 2016, 7, .	1.8	49
9	UDP-galactose and acetyl-CoA transporters as <i>Plasmodium</i> multidrug resistance genes. Nature Microbiology, 2016, 1, 16166.	5.9	102
10	Benefit of Retraining pK_a Models Studied Using Internally Measured Data. Journal of Chemical Information and Modeling, 2015, 55, 1449-1459.	2.5	17
11	FOCUS " Development of a Global Communication and Modeling Platform for Applied and Computational Medicinal Chemists. Journal of Chemical Information and Modeling, 2015, 55, 896-908.	2.5	18
12	Matched Molecular Pair Analysis: Significance and the Impact of Experimental Uncertainty. Journal of Medicinal Chemistry, 2014, 57, 3786-3802.	2.9	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.	2.3	35
14	Deriving Static Atomic Multipoles from the Electrostatic Potential. Journal of Chemical Information and Modeling, 2013, 53, 3410-3417.	2.5	25
15	Comparability of Mixed IC50 Data " A Statistical Analysis. PLoS ONE, 2013, 8, e61007.	1.1	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.	1.0	46
17	The Experimental Uncertainty of Heterogeneous Public pK_a Data. Journal of Medicinal Chemistry, 2012, 55, 5165-5173.	2.9	183
18	Atomic multipoles: Electrostatic potential fit, local reference axis systems, and conformational dependence. Journal of Computational Chemistry, 2012, 33, 1673-1688.	1.5	56

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19	Global Free Energy Scoring Functions Based on Distance-Dependent Atom-Type Pair Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 707-720.	2.5	26
20	Three Descriptor Model Sets a High Standard for the CSAR-NRC HiQ Benchmark. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2139-2145.	2.5	7
21	Design and synthesis of a library of chemokine antagonists. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 6249-6252.	1.0	7
22	Avoidance of the Ames test liability for arylamines via computation. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 3173-3182.	1.4	29
23	Synthesis and evaluation of two series of 4 ϵ -aza-carbocyclic nucleosides as adenosine A2A receptor agonists. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 1219-1224.	1.0	10
24	A physical properties based approach for the exploration of a 4-hydroxybenzothiazolone series of β 2-adrenoceptor agonists as inhaled long-acting bronchodilators. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 5302-5307.	1.0	25
25	Leave-Cluster-Out Cross-Validation Is Appropriate for Scoring Functions Derived from Diverse Protein Data Sets. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1961-1969.	2.5	84
26	Computational Analysis of Structure-Activity Relationships. <i>Progress in Medicinal Chemistry</i> , 2010, 49, 113-160.	4.1	20
27	Insight into the Mechanism of Inactivation and pH Sensitivity in Potassium Channels from Molecular Dynamics Simulations. <i>Biochemistry</i> , 2008, 47, 7414-7422.	1.2	50
28	Exploiting QSAR models in lead optimization. <i>Current Opinion in Drug Discovery & Development</i> , 2008, 11, 569-75.	1.9	14
29	Drug block of the hERG potassium channel: Insight from modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 568-580.	1.5	100
30	QSAR - How Good Is It in Practice? Comparison of Descriptor Sets on an Unbiased Cross Section of Corporate Data Sets. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1924-1936.	2.5	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. <i>British Journal of Pharmacology</i> , 2005, 144, 1002-1010.	2.7	19
32	Use Of The R-Group Descriptor for Alignment-Free QSAR. <i>QSAR and Combinatorial Science</i> , 2005, 24, 611-619.	1.5	17
33	Computational Chemistry at Novartis. <i>Chimia</i> , 2005, 59, 545-549.	0.3	7
34	Long-chain formoterol analogues: an investigation into the effect of increasing amino-substituent chain length on the β 2-adrenoceptor activity. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 4705-4710.	1.0	42
35	New Highly Potent and Selective Adenosine A3 Receptor Antagonists. <i>Current Topics in Medicinal Chemistry</i> , 2004, 4, 863-870.	1.0	18
36	Calculation of Intersubstituent Similarity Using R-Group Descriptors.. <i>ChemInform</i> , 2003, 34, no.	0.1	0

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37	Calculation of Intersubstituent Similarity Using R-Group Descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 406-411.	2.8	49
38	The Reaction Mechanism of Bovine Lens Leucine Aminopeptidase. <i>Journal of Physical Chemistry B</i> , 2002, 106, 8815-8830.	1.2	25
39	Analysis for pharmaceutical scientists. <i>Trends in Biotechnology</i> , 2002, 20, 360.	4.9	0
40	Visual and computational analysis of structure-activity relationships in high-throughput screening data. <i>Current Opinion in Chemical Biology</i> , 2001, 5, 389-395.	2.8	54
41	Additive NDDO-based atomic polarizability model. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 473-497.	1.0	33
42	New Multicentre Point Charge Models for Molecular Electrostatic Potentials from Semiempirical MO-Calculations. <i>Journal of Molecular Modeling</i> , 2000, 6, 452-466.	0.8	8
43	Numerical self-consistent reaction field study of the excited-state properties of p-(dimethylamino)-benzonitrile derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 1999, 121, 7-15.	2.0	16
44	A Semiempirical QM/MM Implementation and its Application to the Absorption of Organic Molecules in Zeolites. <i>Journal of Molecular Modeling</i> , 1999, 5, 1-7.	0.8	23
45	Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 17-31.	1.0	37
46	Fast Long-Range Adiabatic Electron Transfer in a Model Polyglycine α -Helix. <i>Journal of the American Chemical Society</i> , 1999, 121, 1379-1380.	6.6	10
47	Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 17.	1.0	2
48	Numerical self-consistent reaction field study of intramolecular charge transfer in p-(dimethylamino)-benzonitrile. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 1997, 105, 165-181.	2.0	44
49	Semi-Empirical Mo Calculations on Enzyme Reaction Mechanisms. , 1997, , 307-317.		5
50	1,5-hydrogen transfer - a hitherto ignored decay channel in the photodegradation of poly(2,6-dimethyl-1,4-phenylene oxide). <i>Chemical Physics Letters</i> , 1996, 257, 616-621.	1.2	4
51	Photophysics and Photochemistry of Intramolecular Stilbene-Amine Exciplexes. <i>Journal of the American Chemical Society</i> , 1995, 117, 660-669.	6.6	46
52	A COMPARISON OF PHYCOCYANINS FROM THREE DIFFERENT SPECIES OF CYANOBACTERIA EMPLOYING RESONANCE-ENHANCED COHERENT ANTI-STOKES RAMAN SPECTROSCOPY. <i>Photochemistry and Photobiology</i> , 1993, 57, 56-62.	1.3	10