Peter Gedeck

List of Publications by Year in descending order

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52 papers	2,016 citations	257101 24 h-index	253896 43 g-index
56 all docs	56 docs citations	56 times ranked	2834 citing authors

#	Article	IF	Citations
1	Comparability of Mixed IC50 Data â€“ A Statistical Analysis. PLoS ONE, 2013, 8, e61007.	1.1	211
2	The Experimental Uncertainty of Heterogeneous Public K_i Data. Journal of Medicinal Chemistry, 2012, 55, 5165-5173.	2.9	183
3	A Cryptosporidium PI(4)K inhibitor is a drug candidate for cryptosporidiosis. Nature, 2017, 546, 376-380.	13.7	144
4	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.	2.5	135
5	UDP-galactose and acetyl-CoA transporters as Plasmodium multidrug resistance genes. Nature Microbiology, 2016, 1, 16166.	5.9	102
6	Drug block of the hERG potassium channel: Insight from modeling. Proteins: Structure, Function and Bioinformatics, 2007, 68, 568-580.	1.5	100
7	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.	2.5	84
8	Matched Molecular Pair Analysis: Significance and the Impact of Experimental Uncertainty. Journal of Medicinal Chemistry, 2014, 57, 3786-3802.	2.9	62
9	Atomic multipoles: Electrostatic potential fit, local reference axis systems, and conformational dependence. Journal of Computational Chemistry, 2012, 33, 1673-1688.	1.5	56
10	Visual and computational analysis of structureâ€“activity relationships in high-throughput screening data. Current Opinion in Chemical Biology, 2001, 5, 389-395.	2.8	54
11	Insight into the Mechanism of Inactivation and pH Sensitivity in Potassium Channels from Molecular Dynamics Simulations. Biochemistry, 2008, 47, 7414-7422.	1.2	50
12	Calculation of Intersubstituent Similarity Using R-Group Descriptors. Journal of Chemical Information and Computer Sciences, 2003, 43, 406-411.	2.8	49
13	Mutations in the Plasmodium falciparum Cyclic Amine Resistance Locus (PfCARL) Confer Multidrug Resistance. MBio, 2016, 7, .	1.8	49
14	Photophysics and Photochemistry of Intramolecular Stilbene-Amine Exciplexes. Journal of the American Chemical Society, 1995, 117, 660-669.	6.6	46
15	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
16	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.	2.0	44
17	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.	1.0	42
18	Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods. International Journal of Quantum Chemistry, 1999, 75, 17-31.	1.0	37

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19	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
20	Additive NDDO-based atomic polarizability model. International Journal of Quantum Chemistry, 2000, 77, 473-497.	1.0	33
21	Avoidance of the Ames test liability for arylâ€“amines via computation. Bioorganic and Medicinal Chemistry, 2011, 19, 3173-3182.	1.4	29
22	Global Free Energy Scoring Functions Based on Distance-Dependent Atom-Type Pair Descriptors. Journal of Chemical Information and Modeling, 2011, 51, 707-720.	2.5	26
23	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
24	The Reaction Mechanism of Bovine Lens Leucine Aminopeptidase. Journal of Physical Chemistry B, 2002, 106, 8815-8830.	1.2	25
25	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.	1.0	25
26	Deriving Static Atomic Multipoles from the Electrostatic Potential. Journal of Chemical Information and Modeling, 2013, 53, 3410-3417.	2.5	25
27	A Semiempirical QM/MM Implementation and its Application to the Absorption of Organic Molecules in Zeolites. Journal of Molecular Modeling, 1999, 5, 1-7.	0.8	23
28	Computational Analysis of Structureâ€“Activity Relationships. Progress in Medicinal Chemistry, 2010, 49, 113-160.	4.1	20
29	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.	2.7	19
30	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.	2.5	18
31	New Highly Potent and Selective Adenosine A3 Receptor Antagonists. Current Topics in Medicinal Chemistry, 2004, 4, 863-870.	1.0	18
32	Use Of The R-Group Descriptor for Alignment-Free QSAR. QSAR and Combinatorial Science, 2005, 24, 611-619.	1.5	17
33	Benefit of Retraining pKa Models Studied Using Internally Measured Data. Journal of Chemical Information and Modeling, 2015, 55, 1449-1459.	2.5	17
34	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.	2.0	16
35	Shared Consensus Machine Learning Models for Predicting Blood Stage Malaria Inhibition. Journal of Chemical Information and Modeling, 2017, 57, 445-453.	2.5	15
36	Capturing mixture composition: an open machine-readable format for representing mixed substances. Journal of Cheminformatics, 2019, 11, 33.	2.8	14

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37	Exploiting QSAR models in lead optimization. Current Opinion in Drug Discovery & Development, 2008, 11, 569-75.	1.9	14
38	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.	1.3	10
39	Fast Long-Range Adiabatic Electron Transfer in a Model Polyglycine Î±-Helix. Journal of the American Chemical Society, 1999, 121, 1379-1380.	6.6	10
40	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.	1.0	10
41	Development of a Cytopathic Effect-Based Phenotypic Screening Assay against Cryptosporidium. ACS Infectious Diseases, 2018, 4, 635-645.	1.8	9
42	New Multicentre Point Charge Models for Molecular Electrostatic Potentials from Semiempirical M0-Calculations. Journal of Molecular Modeling, 2000, 6, 452-466.	0.8	8
43	Three Descriptor Model Sets a High Standard for the CSAR-NRC HiQ Benchmark. Journal of Chemical Information and Modeling, 2011, 51, 2139-2145.	2.5	7
44	Design and synthesis of a library of chemokine antagonists. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 6249-6252.	1.0	7
45	Developing Collaborative QSAR Models Without Sharing Structures. Journal of Chemical Information and Modeling, 2017, 57, 1847-1858.	2.5	7
46	Computational Chemistry at Novartis. Chimia, 2005, 59, 545-549.	0.3	7
47	Semi-Empirical Mo Calculations on Enzyme Reaction Mechanisms. , 1997, , 307-317.		5
48	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.	1.2	4
49	Using Machine Learning to Parse Chemical Mixture Descriptions. ACS Omega, 2021, 6, 22400-22409.	1.6	2
50	Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods. International Journal of Quantum Chemistry, 1999, 75, 17.	1.0	2
51	Analysis for pharmaceutical scientists. Trends in Biotechnology, 2002, 20, 360.	4.9	0
52	Calculation of Intersubstituent Similarity Using R-Group Descriptors.. ChemInform, 2003, 34, no.	0.1	0