David J Diller

List of Publications by Year
in descending order

31 papers	1,338 citations	471061 17 h-index	476904 29 g-index
32 all docs	32 docs citations	32 times ranked	1789 citing authors

#	Article	IF	Citations
1	Rigorous Computational and Experimental Investigations on MDM2/MDMX-Targeted Linear and Macrocyclic Peptides. Molecules, 2019, 24, 4586.	1.7	4
2	Inhibiting IL-2 signaling and the regulatory T-cell pathway using computationally designed peptides. Investigational New Drugs, 2019, 37, 9-16.	1.2	5
3	Identification and initial optimization of inhibitors of Clostridium difficile (C. difficile) toxin B (TcdB). Bioorganic and Medicinal Chemistry Letters, 2018, 28, 756-761.	1.0	6
4	Development of a Simple Electron Transfer and Polarization Model and Its Application to Biological Systems. Journal of Chemical Theory and Computation, 2017, 13, 329-339.	2.3	0
5	A combined cheminformatic and bioinformatic approach to address the proteolytic stability challenge in peptideâ€based drug discovery. Biopolymers, 2015, 104, 775-789.	1.2	2
6	Avalanche for shape and feature-based virtual screening with 3D alignment. Journal of Computer-Aided Molecular Design, 2015, 29, 1015-1024.	1.3	9
7	Rational, computer-enabled peptide drug design: principles, methods, applications and future directions. Future Medicinal Chemistry, 2015, 7, 2173-2193.	1.1	35
8	A structural informatics approach to mine kinase knowledge bases. Drug Discovery Today, 2010, 15, 203-209.	3.2	7
9	Computational alanine scanning with linear scaling semiempirical quantum mechanical methods. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2329-2337.	1.5	17
10	Insights for Predicting Blood-Brain Barrier Penetration of CNS Targeted Molecules Using QSPR Approaches. Journal of Chemical Information and Modeling, 2010, 50, 1123-1133.	2.5	59
11	Edtiorial [Hot Topic: In Silico ADME/Tox Models: Progress and Challenges (Guest Editors: Robert K.) Tj ETQq1 1 0.784314 rgBT /Overlock	0.8	0
12	In Silico hERG Modeling: Challenges and Progress. Current Computer-Aided Drug Design, 2009, 5, 106-121.	0.8	21
13	2-Benzimidazolyl-9-(chroman-4-yl)-purinone derivatives as JAK3 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6788-6792.	1.0	14
14	Characterization of Chemical Libraries for Luciferase Inhibitory Activity. Journal of Medicinal Chemistry, 2008, 51, 2372-2386.	2.9	180
15	Technique for Generating Three-Dimensional Alignments of Multiple Ligands from One-Dimensional Alignments. Journal of Chemical Information and Modeling, 2008, 48, 1041-1054.	2.5	22
16	Library Fingerprints:â€‰ A Novel Approach to the Screening of Virtual Libraries. Journal of Chemical Information and Modeling, 2007, 47, 1354-1365.	2.5	16
17	Understanding hERG inhibition with QSAR models based on a one-dimensional molecular representation. Journal of Computer-Aided Molecular Design, 2007, 21, 379-393.	1.3	17
18	Improved NaÃ¯ve Bayesian Modeling of Numerical Data for Absorption, Distribution, Metabolism and Excretion (ADME) Property Prediction. Journal of Chemical Information and Modeling, 2006, 46, 1945-1956.	2.5	101

#	Article	IF	Citations
19	Successful Screening of Large Encoded Combinatorial Libraries Leading to the Discovery of Novel p38 MAP Kinase Inhibitors. Combinatorial Chemistry and High Throughput Screening, 2006, 9, 351-358.	0.6	5
20	Discovery and Characterization of Triaminotriazine Aniline Amides as Highly Selective p38 Kinase Inhibitors. Journal of Pharmacology and Experimental Therapeutics, 2006, 318, 495-502.	1.3	16
21	The Discovery of Novel Chemotypes of p38 Kinase Inhibitors. Current Topics in Medicinal Chemistry, 2005, 5, 953-965.	1.0	40
22	Fast Small Molecule Similarity Searching with Multiple Alignment Profiles of Molecules Represented in One-Dimension. Journal of Medicinal Chemistry, 2005, 48, 6980-6990.	2.9	21
23	Deriving Knowledge through Data Mining High-Throughput Screening Data. Journal of Medicinal Chemistry, 2004, 47, 6373-6383.	2.9	45
24	Kinases, Homology Models, and High Throughput Docking. Journal of Medicinal Chemistry, 2003, 46, 4638-4647.	2.9	129
25	Use of Catalyst Pharmacophore Models for Screening of Large Combinatorial Libraries. Journal of Chemical Information and Computer Sciences, 2002, 42, 1204-1211.	2.8	70
26	Computation of the physio-chemical properties and data mining of large molecular collections. Journal of Computational Chemistry, 2002, 23, 172-183.	1.5	56
27	Can we separate active from inactive conformations?. Journal of Computer-Aided Molecular Design, 2002, 16, 105-112.	1.3	37
28	High throughput docking for library design and library prioritization. Proteins: Structure, Function and Bioinformatics, 2001, 43, 113-124.	1.5	283
29	An accurate numerical model for calculating the equilibration rate of a hanging-drop experiment. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 656-663.	2.5	10
30	A critical evaluation of several global optimization algorithms for the purpose of molecular docking. Journal of Computational Chemistry, 1999, 20, 1740-1751.	1.5	43
31	The Role of Waters in Docking Strategies with Incremental Flexibility for Carbohydrate Derivatives:Â Heat-Labile Enterotoxin, a Multivalent Test Case. Journal of Medicinal Chemistry, 1999, 42, 1778-1788.	2.9	67