Stephen D Pickett

List of Publications by Year
in descending order

40 papers	4,386 citations	201385 27 h-index	288905 40 g-index
44 all docs	44 docs citations	44 times ranked	5621 citing authors

#	Article	IF	Citations
1	An analysis of the attrition of drug candidates from four major pharmaceutical companies. Nature Reviews Drug Discovery, 2015, 14, 475-486.	21.5	996
2	Computational methods for the prediction of â€˜drug-likenessâ€™. Drug Discovery Today, 2000, 5, 49-58.	3.2	552
3	GRid-INdependent Descriptors (GRIND):â€‰ A Novel Class of Alignment-Independent Three-Dimensional Molecular Descriptors. Journal of Medicinal Chemistry, 2000, 43, 3233-3243.	2.9	466
4	The impact of aromatic ring count on compound developability: further insights by examining carbo- and hetero-aromatic and -aliphatic ring types. Drug Discovery Today, 2011, 16, 164-171.	3.2	333
5	Empirical Scale of Side-Chain Conformational Entropy in Protein Folding. Journal of Molecular Biology, 1993, 231, 825-839.	2.0	263
6	Design Principles for Fragment Libraries: Maximizing the Value of Learnings from Pharma Fragment-Based Drug Discovery (FBDD) Programs for Use in Academia. Journal of Medicinal Chemistry, 2016, 59, 8189-8206.	2.9	182
7	Diversity Profiling and Design Using 3D Pharmacophores:â€‰ Pharmacophore-Derived Queries (PDQ). Journal of Chemical Information and Computer Sciences, 1996, 36, 1214-1223.	2.8	165
8	The developability of heteroaromatic and heteroaliphatic rings â€“ do some have a better pedigree as potential drug molecules than others?. MedChemComm, 2012, 3, 1062.	3.5	144
9	Contemporary QSAR Classifiers Compared. Journal of Chemical Information and Modeling, 2007, 47, 219-227.	2.5	122
10	Enhancing the Hit-to-Lead Properties of Lead Optimization Librariesâ€. Journal of Chemical Information and Computer Sciences, 2000, 40, 263-272.	2.8	117
11	Lead Optimization Using Matched Molecular Pairs: Inclusion of Contextual Information for Enhanced Prediction of hERG Inhibition, Solubility, and Lipophilicity. Journal of Chemical Information and Modeling, 2010, 50, 1872-1886.	2.5	113
12	An Algorithm-Directed Two-Component Library Synthesized Via Solid-Phase Methodology Yielding Potent and Orally Bioavailable p38 MAP Kinase Inhibitors. Journal of Medicinal Chemistry, 2002, 45, 2173-2184.	2.9	82
13	Increasing small molecule drug developability in sub-optimal chemical space. MedChemComm, 2013, 4, 673.	3.5	67
14	Classification of Kinase Inhibitors Using BCUT Descriptors. Journal of Chemical Information and Computer Sciences, 2000, 40, 1431-1440.	2.8	63
15	Methods for mining HTS data. Drug Discovery Today, 2006, 11, 694-699.	3.2	54
16	De Novo Molecule Design by Translating from Reduced Graphs to SMILES. Journal of Chemical Information and Modeling, 2019, 59, 1136-1146.	2.5	50
17	Optimizing the Size and Configuration of Combinatorial Libraries. Journal of Chemical Information and Computer Sciences, 2003, 43, 381-390.	2.8	45
18	Automated Lead Optimization of MMP-12 Inhibitors Using a Genetic Algorithm. ACS Medicinal Chemistry Letters, 2011, 2, 28-33.	1.3	43

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19	Nuisance Compounds, PAINS Filters, and Dark Chemical Matter in the GSK HTS Collection. SLAS Discovery, 2018, 23, 532-544.	1.4	42
20	Discovery of novel low molecular weight inhibitors of IMPDH via virtual needle screening. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 1691-1694.	1.0	41
21	Partition-based selection. Journal of Computer - Aided Molecular Design, 1996, 7-8, 85-114.	1.0	39
22	Guidelines for Recurrent Neural Network Transfer Learning-Based Molecular Generation of Focused Libraries. Journal of Chemical Information and Modeling, 2020, 60, 5699-5713.	2.5	36
23	Evaluation of the sequence template method for protein structure prediction. Journal of Molecular Biology, 1992, 228, 170-187.	2.0	33
24	QSAR workbench: automating QSAR modeling to drive compound design. Journal of Computer-Aided Molecular Design, 2013, 27, 321-336.	1.3	33
25	BRADSHAW: a system for automated molecular design. Journal of Computer-Aided Molecular Design, 2020, 34, 747-765.	1.3	33
26	Computer-Aided Molecular Diversity Analysis and Combinatorial Library Design. Reviews in Computational Chemistry, 2007, , 1-51.	1.5	29
27	The Discovery of in Vivo Active Mitochondrial Branched-Chain Aminotransferase (BCATm) Inhibitors by Hybridizing Fragment and HTS Hits. Journal of Medicinal Chemistry, 2015, 58, 7140-7163.	2.9	29
28	Evolving Interpretable Structureâ"Activity Relationship Models. 2. Using Multiobjective Optimization To Derive Multiple Models. Journal of Chemical Information and Modeling, 2008, 48, 1558-1570.	2.5	28
29	Training Similarity Measures for Specific Activities:Â Application to Reduced Graphs. Journal of Chemical Information and Modeling, 2006, 46, 577-586.	2.5	27
30	Analysis of Neighborhood Behavior in Lead Optimization and Array Design. Journal of Chemical Information and Modeling, 2009, 49, 195-208.	2.5	26
31	Evolving Interpretable Structureâ"Activity Relationships. 1. Reduced Graph Queries. Journal of Chemical Information and Modeling, 2008, 48, 1543-1557.	2.5	23
32	Structurally Diverse Mitochondrial Branched Chain Aminotransferase (BCATm) Leads with Varying Binding Modes Identified by Fragment Screening. Journal of Medicinal Chemistry, 2016, 59, 2452-2467.	2.9	23
33	A Turing Test for Molecular Generators. Journal of Medicinal Chemistry, 2020, 63, 11964-11971.	2.9	23
34	Computational-chemical assessments of well characterised uniform catalysts. Faraday Discussions of the Chemical Society, 1989, 87, 79.	2.2	11
35	Molecular clinical safety intelligence: a system for bridging clinically focused safety knowledge to early-stage drug discovery â€" the GSK experience. Drug Discovery Today, 2011, 16, 646-653.	3.2	10
36	Quantification of Molecular Similarity and Its Application to Combinatorial Chemistry. , 0, , 135-156.		10

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37	Alchemical Free Energy Methods Applied to Complexes of the First Bromodomain of BRD4. Journal of Chemical Information and Modeling, 2022, 62, 1458-1470.	2.5	8
38	Structural variation of proteinâ€“ligand complexes of the first bromodomain of BRD4. Organic and Biomolecular Chemistry, 2021, 19, 5632-5641.	1.5	6
39	CHAPTER 4. Current Status and Future Direction of Fragment-Based Drug Discovery: A Computational Chemistry Perspective. RSC Drug Discovery Series, 2015, , 73-100.	0.2	2
40	Optimizing the Size and Configuration of Combinatorial Libraries.. ChemInform, 2003, 34, no.	0.1	0