

# Stephen D Pickett

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

41  
papers

3,589  
citations

25  
h-index

44  
g-index

44  
ext. papers

4,006  
ext. citations

7.5  
avg, IF

5.1  
L-index

#	Paper	IF	Citations
41	An analysis of the attrition of drug candidates from four major pharmaceutical companies. <i>Nature Reviews Drug Discovery</i> , <b>2015</b> , 14, 475-86	64.1	713
40	Computational methods for the prediction of Tdrug-likenessT <i>Drug Discovery Today</i> , <b>2000</b> , 5, 49-58	8.8	475
39	GRid-INdependent descriptors (GRIND): a novel class of alignment-independent three-dimensional molecular descriptors. <i>Journal of Medicinal Chemistry</i> , <b>2000</b> , 43, 3233-43	8.3	419
38	The impact of aromatic ring count on compound developability: further insights by examining carbo- and hetero-aromatic and -aliphatic ring types. <i>Drug Discovery Today</i> , <b>2011</b> , 16, 164-71	8.8	286
37	Empirical scale of side-chain conformational entropy in protein folding. <i>Journal of Molecular Biology</i> , <b>1993</b> , 231, 825-39	6.5	249
36	Diversity Profiling and Design Using 3D Pharmacophores: Pharmacophore-Derived Queries (PDQ). <i>Journal of Chemical Information and Computer Sciences</i> , <b>1996</b> , 36, 1214-1223		138
35	Design Principles for Fragment Libraries: Maximizing the Value of Learnings from Pharma Fragment-Based Drug Discovery (FBDD) Programs for Use in Academia. <i>Journal of Medicinal Chemistry</i> , <b>2016</b> , 59, 8189-206	8.3	134
34	The developability of heteroaromatic and heteroaliphatic rings Do some have a better pedigree as potential drug molecules than others?. <i>MedChemComm</i> , <b>2012</b> , 3, 1062	5	128
33	Contemporary QSAR classifiers compared. <i>Journal of Chemical Information and Modeling</i> , <b>2007</b> , 47, 219-271	8.1	109
32	Enhancing the hit-to-lead properties of lead optimization libraries. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2000</b> , 40, 263-72		108
31	Lead optimization using matched molecular pairs: inclusion of contextual information for enhanced prediction of HERG inhibition, solubility, and lipophilicity. <i>Journal of Chemical Information and Modeling</i> , <b>2010</b> , 50, 1872-86	6.1	105
30	An algorithm-directed two-component library synthesized via solid-phase methodology yielding potent and orally bioavailable p38 MAP kinase inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2002</b> , 45, 2173-84	8.2	77
29	Classification of kinase inhibitors using BCUT descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2000</b> , 40, 1431-40		58
28	Increasing small molecule drug developability in sub-optimal chemical space. <i>MedChemComm</i> , <b>2013</b> , 4, 673	5	46
27	Methods for mining HTS data. <i>Drug Discovery Today</i> , <b>2006</b> , 11, 694-9	8.8	46
26	Optimizing the size and configuration of combinatorial libraries. <i>Journal of Chemical Information and Computer Sciences</i> , <b>2003</b> , 43, 381-90		41
25	Discovery of novel low molecular weight inhibitors of IMPDH via virtual needle screening. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2003</b> , 13, 1691-4	2.9	39

24	Automated Lead Optimization of MMP-12 Inhibitors Using a Genetic Algorithm. <i>ACS Medicinal Chemistry Letters</i> , <b>2011</b> , 2, 28-33	4.3	38
23	Evaluation of the sequence template method for protein structure prediction. Discrimination of the (beta/alpha) <sub>8</sub> -barrel fold. <i>Journal of Molecular Biology</i> , <b>1992</b> , 228, 170-87	6.5	32
22	QSAR workbench: automating QSAR modeling to drive compound design. <i>Journal of Computer-Aided Molecular Design</i> , <b>2013</b> , 27, 321-36	4.2	29
21	Partition-based selection. <i>Journal of Computer - Aided Molecular Design</i> , <b>1996</b> , 7-8, 85-114		29
20	Evolving interpretable structure-activity relationship models. 2. Using multiobjective optimization to derive multiple models. <i>Journal of Chemical Information and Modeling</i> , <b>2008</b> , 48, 1558-70	6.1	27
19	Analysis of neighborhood behavior in lead optimization and array design. <i>Journal of Chemical Information and Modeling</i> , <b>2009</b> , 49, 195-208	6.1	25
18	Training similarity measures for specific activities: application to reduced graphs. <i>Journal of Chemical Information and Modeling</i> , <b>2006</b> , 46, 577-86	6.1	25
17	De Novo Molecule Design by Translating from Reduced Graphs to SMILES. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 1136-1146	6.1	25
16	Nuisance Compounds, PAINS Filters, and Dark Chemical Matter in the GSK HTS Collection. <i>SLAS Discovery</i> , <b>2018</b> , 23, 532-545	3.4	23
15	The Discovery of in Vivo Active Mitochondrial Branched-Chain Aminotransferase (BCATm) Inhibitors by Hybridizing Fragment and HTS Hits. <i>Journal of Medicinal Chemistry</i> , <b>2015</b> , 58, 7140-63	8.3	22
14	Evolving interpretable structure-activity relationships. 1. Reduced graph queries. <i>Journal of Chemical Information and Modeling</i> , <b>2008</b> , 48, 1543-57	6.1	22
13	Guidelines for Recurrent Neural Network Transfer Learning-Based Molecular Generation of Focused Libraries. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 5699-5713	6.1	17
12	A Turing Test for Molecular Generators. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 11964-11971	8.3	17
11	BRADSHAW: a system for automated molecular design. <i>Journal of Computer-Aided Molecular Design</i> , <b>2020</b> , 34, 747-765	4.2	17
10	Computer-Aided Molecular Diversity Analysis and Combinatorial Library Design. <i>Reviews in Computational Chemistry</i> , <b>2007</b> , 1-51		15
9	Structurally Diverse Mitochondrial Branched Chain Aminotransferase (BCATm) Leads with Varying Binding Modes Identified by Fragment Screening. <i>Journal of Medicinal Chemistry</i> , <b>2016</b> , 59, 2452-67	8.3	14
8	Pharmacophore Pattern Application in Virtual Screening. Library Design and QSAR. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2000</b> , 131-159	0.4	10
7	Molecular clinical safety intelligence: a system for bridging clinically focused safety knowledge to early-stage drug discovery - the GSK experience. <i>Drug Discovery Today</i> , <b>2011</b> , 16, 646-53	8.8	9

6	Quantification of Molecular Similarity and Its Application to Combinatorial Chemistry	135-156	8
5	Computational-chemical assessments of well characterised uniform catalysts. <i>Faraday Discussions of the Chemical Society</i> , <b>1989</b> , 87, 79		6
4	Combinatorial Library Design, Molecular Similarity, and Diversity Applications	<b>2003</b> , 187-242	3
3	CHAPTER 4: Current Status and Future Direction of Fragment-Based Drug Discovery: A Computational Chemistry Perspective. <i>RSC Drug Discovery Series</i> , <b>2015</b> , 73-100		0.6 2
2	Structural variation of protein-ligand complexes of the first bromodomain of BRD4. <i>Organic and Biomolecular Chemistry</i> , <b>2021</b> , 19, 5632-5641		3.9 1
1	USING CHEMOINFORMATICS TOOLS TO ANALYZE CHEMICAL ARRAYS IN LEAD OPTIMIZATION	<b>2013</b> , 179-204	