Stephen D Pickett

List of Publications by Year in Descending Order

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	Structural variation of protein-ligand complexes of the first bromodomain of BRD4. *Organic and Biomolecular Chemistry*, **2021**, 19, 5632-5641	3.9	1
40	Guidelines for Recurrent Neural Network Transfer Learning-Based Molecular Generation of Focused Libraries. *Journal of Chemical Information and Modeling*, **2020**, 60, 5699-5713	6.1	17
39	A Turing Test for Molecular Generators. *Journal of Medicinal Chemistry*, **2020**, 63, 11964-11971	8.3	17
38	BRADSHAW: a system for automated molecular design. *Journal of Computer-Aided Molecular Design* , **2020**, 34, 747-765	4.2	17
37	De Novo Molecule Design by Translating from Reduced Graphs to SMILES. *Journal of Chemical Information and Modeling*, **2019**, 59, 1136-1146	6.1	25
36	Nuisance Compounds, PAINS Filters, and Dark Chemical Matter in the GSK HTS Collection. *SLAS Discovery*, **2018**, 23, 532-545	3.4	23
35	Structurally Diverse Mitochondrial Branched Chain Aminotransferase (BCATm) Leads with Varying Binding Modes Identified by Fragment Screening. *Journal of Medicinal Chemistry*, **2016**, 59, 2452-67	8.3	14
34	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, 8189-206	8.3	134
33	An analysis of the attrition of drug candidates from four major pharmaceutical companies. *Nature Reviews Drug Discovery*, **2015**, 14, 475-86	64.1	713
32	The Discovery of in Vivo Active Mitochondrial Branched-Chain Aminotransferase (BCATm) Inhibitors by Hybridizing Fragment and HTS Hits. *Journal of Medicinal Chemistry*, **2015**, 58, 7140-63	8.3	22
31	CHAPTER 4:Current Status and Future Direction of Fragment-Based Drug Discovery: A Computational Chemistry Perspective. *RSC Drug Discovery Series*, **2015**, 73-100	0.6	2
30	Increasing small molecule drug developability in sub-optimal chemical space. *MedChemComm*, **2013** , 4, 673	5	46
29	QSAR workbench: automating QSAR modeling to drive compound design. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 321-36	4.2	29
28	USING CHEMOINFORMATICS TOOLS TO ANALYZE CHEMICAL ARRAYS IN LEAD OPTIMIZATION **2013**, 179-204		
27	The developability of heteroaromatic and heteroaliphatic rings □do some have a better pedigree as potential drug molecules than others?. *MedChemComm*, **2012**, 3, 1062	5	128
26	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, 164-71	8.8	286
25	Molecular clinical safety intelligence: a system for bridging clinically focused safety knowledge to early-stage drug discovery - the GSK experience. *Drug Discovery Today*, **2011**, 16, 646-53	8.8	9

24	Automated Lead Optimization of MMP-12 Inhibitors Using a Genetic Algorithm. *ACS Medicinal Chemistry Letters*, **2011**, 2, 28-33	4.3	38
23	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, 1872-86	6.1	105
22	Analysis of neighborhood behavior in lead optimization and array design. *Journal of Chemical Information and Modeling*, **2009**, 49, 195-208	6.1	25
21	Evolving interpretable structure-activity relationship models. 2. Using multiobjective optimization to derive multiple models. *Journal of Chemical Information and Modeling*, **2008**, 48, 1558-70	6.1	27
20	Evolving interpretable structure-activity relationships. 1. Reduced graph queries. *Journal of Chemical Information and Modeling*, **2008**, 48, 1543-57	6.1	22
19	Computer-Aided Molecular Diversity Analysis and Combinatorial Library Design. *Reviews in Computational Chemistry*, **2007**, 1-51		15
18	Contemporary QSAR classifiers compared. *Journal of Chemical Information and Modeling*, **2007**, 47, 219-27	6.1	109
17	Methods for mining HTS data. *Drug Discovery Today*, **2006**, 11, 694-9	8.8	46
16	Training similarity measures for specific activities: application to reduced graphs. *Journal of Chemical Information and Modeling*, **2006**, 46, 577-86	6.1	25
15	Discovery of novel low molecular weight inhibitors of IMPDH via virtual needle screening. *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 1691-4	2.9	39
14	Optimizing the size and configuration of combinatorial libraries. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 381-90		41
13	Combinatorial Library Design, Molecular Similarity, and Diversity Applications **2003**, 187-242		3
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, 2173-84	8.3	77
11	Computational methods for the prediction of 'drug-likeness' *Drug Discovery Today*, **2000**, 5, 49-58	8.8	475
10	Classification of kinase inhibitors using BCUT descriptors. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1431-40		58
9	Enhancing the hit-to-lead properties of lead optimization libraries. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 263-72		108
8	Pharmacophore Pattern Application in Virtual Screening. Library Design and QSAR. *Methods and Principles in Medicinal Chemistry*, **2000**, 131-159	0.4	10
7	GRid-INdependent descriptors (GRIND): a novel class of alignment-independent three-dimensional molecular descriptors. *Journal of Medicinal Chemistry*, **2000**, 43, 3233-43	8.3	419

6	Diversity Profiling and Design Using 3D Pharmacophores: Pharmacophore-Derived Queries (PDQ). *Journal of Chemical Information and Computer Sciences*, **1996**, 36, 1214-1223		138
5	Partition-based selection. *Journal of Computer - Aided Molecular Design*, **1996**, 7-8, 85-114		29
4	Empirical scale of side-chain conformational entropy in protein folding. *Journal of Molecular Biology* , **1993**, 231, 825-39	6.5	249
3	Evaluation of the sequence template method for protein structure prediction. Discrimination of the (beta/alpha)8-barrel fold. *Journal of Molecular Biology*, **1992**, 228, 170-87	6.5	32
2	Computational-chemical assessments of well characterised uniform catalysts. *Faraday Discussions of the Chemical Society*, **1989**, 87, 79		6
1	Quantification of Molecular Similarity and Its Application to Combinatorial Chemistry135-156		8