Stephen D Roughley

List of Publications by Year
in descending order

24 papers	3,540 citations	489802 18 h-index	685536 24 g-index
27 all docs	27 docs citations	27 times ranked	5114 citing authors

#	Article	IF	Citations
1	Rapid optimisation of fragments and hits to lead compounds from screening of crude reaction mixtures. Communications Chemistry, 2020, 3, .	2.0	11
2	Design and Synthesis of 56 Shapeâ€Diverse 3D Fragments. Chemistry - A European Journal, 2020, 26, 8969-8975.	1.7	38
3	Five Years of the KNIME Vernalis Cheminformatics Community Contribution. Current Medicinal Chemistry, 2020, 27, 6495-6522.	1.2	10
4	Establishing Drug Discovery and Identification of Hit Series for the Anti-apoptotic Proteins, Bcl-2 and Mcl-1. ACS Omega, 2019, 4, 8892-8906.	1.6	35
5	Application of Off-Rate Screening in the Identification of Novel Pan-Isoform Inhibitors of Pyruvate Dehydrogenase Kinase. Journal of Medicinal Chemistry, 2017, 60, 2271-2286.	2.9	22
6	Dynamic undocking and the quasi-bound state as tools for drug discovery. Nature Chemistry, 2017, 9, 201-206.	6.6	68
7	Fragment-Based Lead Discovery. Annual Reports in Medicinal Chemistry, 2017, , 371-439.	0.5	14
8	Off-Rate Screening (ORS) By Surface Plasmon Resonance. An Efficient Method to Kinetically Sample Hit to Lead Chemical Space from Unpurified Reaction Products. Journal of Medicinal Chemistry, 2014, 57, 2845-2850.	2.9	52
9	Intramolecular nitrone dipolar cycloadditions: control of regioselectivity and synthesis of naturally-occurring spirocyclic alkaloids. Organic and Biomolecular Chemistry, 2012, 10, 8963.	1.5	17
10	Targeting conserved water molecules: Design of 4-aryl-5-cyanopyrrolo[2,3-d]pyrimidine Hsp90 inhibitors using fragment-based screening and structure-based optimization. Bioorganic and Medicinal Chemistry, 2012, 20, 6770-6789.	1.4	40
11	Fatty acid amide hydrolase inhibitors. 3: Tetra-substituted azetidine ureas with in vivo activity. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 901-906.	1.0	10
12	How Well Can Fragments Explore Accessed Chemical Space? A Case Study from Heat Shock Protein 90. Journal of Medicinal Chemistry, 2011, 54, 3989-4005.	2.9	74
13	Hsp90 Inhibitors and Drugs from Fragment and Virtual Screening. Topics in Current Chemistry, 2011, 317, 61-82.	4.0	29
14	The Medicinal Chemistâ€™s Toolbox: An Analysis of Reactions Used in the Pursuit of Drug Candidates. Journal of Medicinal Chemistry, 2011, 54, 3451-3479.	2.9	1,969
15	Fatty acid amide hydrolase inhibitors. 2. Novel synthesis of sterically hindered azabenzhydryl ethers and an improved synthesis of VER-156084. Tetrahedron Letters, 2010, 51, 5191-5194.	0.7	4
16	Drug discovery chemistry: a primer for the non-specialist. Drug Discovery Today, 2009, 14, 731-744.	3.2	39
17	Fatty acid amide hydrolase inhibitors. Surprising selectivity of chiral azetidine ureas. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4241-4244.	1.0	29
18	Combining Hit Identification Strategies: Fragment-Based and in Silico Approaches to Orally Active 2-Aminothieno[2,3-d]pyrimidine Inhibitors of the Hsp90 Molecular Chaperone. Journal of Medicinal Chemistry, 2009, 52, 4794-4809.	2.9	157

#	Article	IF	Citations
19	4,5-Diarylisoxazole Hsp90 Chaperone Inhibitors: Potential Therapeutic Agents for the Treatment of Cancer. Journal of Medicinal Chemistry, 2008, 51, 196-218.	2.9	386
20	Novel, Potent Small-Molecule Inhibitors of the Molecular Chaperone Hsp90 Discovered through Structure-Based Design. Journal of Medicinal Chemistry, 2005, 48, 4212-4215.	2.9	232
21	Drug-like Annotation and Duplicate Analysis of a 23-Supplier Chemical Database Totalling 2.7 Million Compounds. Journal of Chemical Information and Computer Sciences, 2004, 44, 643-651.	2.8	126
22	Structure-based design of agents targeting the bacterial ribosome. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 2455-2458.	1.0	32
23	Nitrone dipolar cycloaddition routes to piperidines and indolizidines. Part 9.Part 8. See Ref. 22. Formal synthesis of (â€“)-pinidine and total synthesis of (â€“)-histrionicotoxin, (+)-histrionicotoxin and (â€“)-histrionicotoxin 235AThis manuscript is dedicated to the sixtieth birthday of Professor L. Tietze.. Journal of the Chemical Society, Perkin Transactions 1, 2002, , 1494-1514.	1.3	56
24	Synthesis of (â˜)-Histrionicotoxin by a Tandem Process. Journal of the American Chemical Society, 1999, 121, 4900-4901.	6.6	90