Mark A Murcko

List of Publications by Year in Descending Order

56 papers	9,927 citations	35 h-index	62 g-index
62 ext. papers	10,783 ext. citations	11.2 avg, IF	6.03 L-index

#	Paper	IF	Citations
56	Applications of Deep Learning in Molecule Generation and Molecular Property Prediction. *Accounts of Chemical Research*, **2021**, 54, 263-270	24.3	39
55	Critical assessment of AI in drug discovery. *Expert Opinion on Drug Discovery*, **2021**, 16, 937-947	6.2	7
54	Assessing the impact of generative AI on medicinal chemistry. *Nature Biotechnology*, **2020**, 38, 143-145	44.5	61
53	What Makes a Great Medicinal Chemist? A Personal Perspective. *Journal of Medicinal Chemistry*, **2018**, 61, 7419-7424	8.3	16
52	Preclinical activity of VX-787, a first-in-class, orally bioavailable inhibitor of the influenza virus polymerase PB2 subunit. *Antimicrobial Agents and Chemotherapy*, **2015**, 59, 1569-82	5.9	126
51	Accurate and reliable prediction of relative ligand binding potency in prospective drug discovery by way of a modern free-energy calculation protocol and force field. *Journal of the American Chemical Society*, **2015**, 137, 2695-703	16.4	633
50	Discovery and Development of Telaprevir (Incivek) A Protease Inhibitor to Treat Hepatitis C Infection **2015**, 195-212		3
49	Discovery of a novel, first-in-class, orally bioavailable azaindole inhibitor (VX-787) of influenza PB2. *Journal of Medicinal Chemistry*, **2014**, 57, 6668-78	8.3	145
48	Envisioning the Future: Medicine in the Year 2050. *Disruptive Science and Technology*, **2012**, 1, 89-99		2
47	What do medicinal chemists actually make? A 50-year retrospective. *Journal of Medicinal Chemistry*, **2011**, 54, 6405-16	8.3	268
46	The Discovery of VX-745: A Novel and Selective p38 Kinase Inhibitor. *ACS Medicinal Chemistry Letters*, **2011**, 2, 758-63	4.3	46
45	Kinase-likeness and kinase-privileged fragments: toward virtual polypharmacology. *Journal of Medicinal Chemistry*, **2008**, 51, 1214-22	8.3	83
44	Inhibitors of hepatitis C virus NS3.4A protease. Effect of P4 capping groups on inhibitory potency and pharmacokinetics. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 3406-11	2.9	16
43	Inhibitors of hepatitis C virus NS3.4A protease. Part 3: P2 proline variants. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 1939-42	2.9	45
42	Toward a pharmacophore for kinase frequent hitters. *Journal of Medicinal Chemistry*, **2004**, 47, 5616-9	8.3	55
41	Prediction of drug-likeness *Advanced Drug Delivery Reviews*, **2002**, 54, 255-71	18.5	307
40	Guiding molecules towards drug-likeness. *Current Opinion in Drug Discovery & Development*, **2002**, 5, 540-9		21

39	Chemogenomic approaches to drug discovery. *Current Opinion in Chemical Biology*, **2001**, 5, 464-70	9.7	151
38	Chapter 29. Structure-Based Drug Design. *Annual Reports in Medicinal Chemistry*, **1999**, 34, 297-306	1.6	13
37	Recognizing molecules with drug-like properties. *Current Opinion in Chemical Biology*, **1999**, 3, 384-7	9.7	235
36	The SHAPES strategy: an NMR-based approach for lead generation in drug discovery. *Chemistry and Biology*, **1999**, 6, 755-69		230
35	Designing libraries with CNS activity. *Journal of Medicinal Chemistry*, **1999**, 42, 4942-51	8.3	255
34	Properties of known drugs. 2. Side chains. *Journal of Medicinal Chemistry*, **1999**, 42, 5095-9	8.3	277
33	Consensus scoring: A method for obtaining improved hit rates from docking databases of three-dimensional structures into proteins. *Journal of Medicinal Chemistry*, **1999**, 42, 5100-9	8.3	612
32	Virtual screening□n overview. *Drug Discovery Today*, **1998**, 3, 160-178	8.8	769
31	Hepatitis C virus NS3 RNA helicase domain with a bound oligonucleotide: the crystal structure provides insights into the mode of unwinding. *Structure*, **1998**, 6, 89-100	5.2	556
30	Design, syntheses, and activity of new 3-[(sulfonylaryl)-amino]-1,4-benzodiazepin-2-one derivatives as □-thrombin inhibitors. *European Journal of Medicinal Chemistry*, **1998**, 33, 471-488	6.8	5
29	Can we learn to distinguish between "drug-like" and "nondrug-like" molecules?. *Journal of Medicinal Chemistry*, **1998**, 41, 3314-24	8.3	469
28	Conformational analysis of carbonic anhydrase inhibitors using ab initio molecular orbital methods. 1. Rotational isomerism in methane sulfonamide anion, CH3-SO2-NH□*Theoretical Chemistry Accounts*, **1997**, 96, 56-60	1.9	13
27	The structural basis for the specificity of pyridinylimidazole inhibitors of p38 MAP kinase. *Chemistry and Biology*, **1997**, 4, 423-31		250
26	Structure-based design of non-peptidic pyridone aldehydes as inhibitors of interleukin-1□ converting enzyme. *Bioorganic and Medicinal Chemistry Letters*, **1997**, 7, 2181-2186	2.9	27
25	The properties of known drugs. 1. Molecular frameworks. *Journal of Medicinal Chemistry*, **1996**, 39, 2887-93	8.3	1403
24	CONCERTS: dynamic connection of fragments as an approach to de novo ligand design. *Journal of Medicinal Chemistry*, **1996**, 39, 1651-63	8.3	98
23	Structure and mechanism of inosine monophosphate dehydrogenase in complex with the immunosuppressant mycophenolic acid. *Cell*, **1996**, 85, 921-30	56.2	358
22	FK506-binding protein mutational analysis: defining the active-site residue contributions to catalysis and the stability of ligand complexes. *Protein Engineering, Design and Selection*, **1996**, 9, 173-80	1.9	66

21	Computational methods to predict binding free energy in ligand-receptor complexes. *Journal of Medicinal Chemistry*, **1995**, 38, 4953-67	8.3	345
20	The synthesis and evaluation of peptidyl aspartyl aldehydes as inhibitors of ice.. *Bioorganic and Medicinal Chemistry Letters*, **1994**, 4, 2359-2364	2.9	24
19	Structure and mechanism of interleukin-1 beta converting enzyme. *Nature*, **1994**, 370, 270-5	50.4	782
18	GroupBuild: a fragment-based method for de novo drug design. *Journal of Medicinal Chemistry*, **1993**, 36, 1700-10	8.3	175
17	CONCEPTS: New dynamic algorithm for de novo drug suggestion. *Journal of Computational Chemistry*, **1993**, 14, 1184-1193	3.5	67
16	Conformational analysis of HIV protease inhibitors. I. Rotation of the amide group adjacent to the P?1 decahydroisoquinoline ring system in ro 31-8959 and related systems. *Journal of Computational Chemistry*, **1993**, 14, 1446-1453	3.5	4
15	Inhibition of carbonic anhydrase. [Erratum to document cited in CA115(3):24912t]. *Journal of the American Chemical Society*, **1992**, 114, 1128-1128	16.4	2
14	Ab initio molecular orbital conformational analysis of prototypical organic systems. 1. Ethylene glycol and 1,2-dimethoxyethane. *Journal of the American Chemical Society*, **1992**, 114, 10010-10018	16.4	93
13	New isomeric classes of topically active ocular hypotensive carbonic anhydrase inhibitors: 5-substituted thieno[2,3-b]thiophene-2-sulfonamides and 5-substituted thieno[3,2-b]thiophene-2-sulfonamides. *Journal of Medicinal Chemistry*, **1991**, 34, 1805-18	8.3	98
12	cDNA encoding murine FK506-binding protein (FKBP): nucleotide and deduced amino acid sequence. *Gene*, **1991**, 109, 255-8	3.8	25
11	Inhibition of carbonic anhydrase. *Journal of the American Chemical Society*, **1991**, 113, 4484-4490	16.4	45
10	Thienothiopyran-2-sulfonamides: novel topically active carbonic anhydrase inhibitors for the treatment of glaucoma. *Journal of Medicinal Chemistry*, **1989**, 32, 2510-3	8.3	186
9	Rotational barriers. 4. Dimethoxymethane. The anomeric effect revisited. *Journal of the American Chemical Society*, **1989**, 111, 4821-4828	16.4	128
8	Barriers to rotation adjacent to double bonds. 4. Effect of basis set on structures, and of electron correlation on relative energies. *Journal of Computational Chemistry*, **1988**, 9, 488-494	3.5	25
7	Rotational barriers. 2. Energies of alkane rotamers. An examination of gauche interactions. *Journal of the American Chemical Society*, **1988**, 110, 8029-8038	16.4	140
6	Bond bending and hybridization. *Computational and Theoretical Chemistry*, **1988**, 169, 355-365		12
5	Rotational barriers. *Computational and Theoretical Chemistry*, **1988**, 163, 1-17		33
4	An ab initio study of diazoethene, a propadienone isoelectronic with a bent structure. *Journal of the American Chemical Society*, **1988**, 110, 364-368	16.4	7

3	Nonbonded interactions. 1. Anisotropic hydrogen-hydrogen interactions. *Journal of Computational Chemistry*, **1987**, 8, 1124-1130	3.5	20
2	Enthalpies of hydration of alkenes. 3. Cycloalkenes. *Journal of the American Chemical Society*, **1985**, 107, 6019-6022	16.4	18
1	Evaluation guidelines for machine learning tools in the chemical sciences. *Nature Reviews Chemistry*,	34.6	3