M Katharine Holloway

List of Publications by Year
in descending order

38 papers	3,086 citations	270111 25 h-index	406436 35 g-index
38 all docs	38 docs citations	38 times ranked	2797 citing authors

#	Article	IF	Citations
1	Molecular Simulations Identify Binding Poses and Approximate Affinities of Stapled Î±-Helical Peptides to MDM2 and MDMX. Journal of Chemical Theory and Computation, 2017, 13, 863-869.	2.3	49
2	The evolution of drug design at Merck Research Laboratories. Journal of Computer-Aided Molecular Design, 2017, 31, 255-266.	1.3	12
3	P2â€Quinazolinones and Bisâ€Macrocycles as New Templates for Nextâ€Generation Hepatitisâ€…C Virus NS3/4a Protease Inhibitors: Discovery of MKâ€2748 and MKâ€6325. ChemMedChem, 2015, 10, 727-735.	1.6	22
4	High-Throughput Screen of GluK1 Receptor Identifies Selective Inhibitors with a Variety of Kinetic Profiles Using Fluorescence and Electrophysiology Assays. Journal of Biomolecular Screening, 2015, 20, 708-719.	2.6	7
5	Discovery of MK-5172, a Macrocyclic Hepatitis C Virus NS3/4a Protease Inhibitor. ACS Medicinal Chemistry Letters, 2012, 3, 332-336.	1.3	181
6	Development of potent macrocyclic inhibitors of genotype 3a HCV NS3/4A protease. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 7201-7206.	1.0	6
7	Development of macrocyclic inhibitors of HCV NS3/4A protease with cyclic constrained P2â€“P4 linkers. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 7207-7213.	1.0	9
8	Discovery of MK-1220: A Macrocyclic Inhibitor of Hepatitis C Virus NS3/4A Protease with Improved Preclinical Plasma Exposure. ACS Medicinal Chemistry Letters, 2011, 2, 207-212.	1.3	30
9	Thermodynamics of Ligand Binding and Efficiency. ACS Medicinal Chemistry Letters, 2011, 2, 433-437.	1.3	141
10	Structure-based design of novel P2-P4 macrocyclic inhibitors of hepatitis C NS3/4A protease. , 2010, , 209-214.		0
11	Discovery of Vaniprevir (MK-7009), a Macrocyclic Hepatitis C Virus NS3/4a Protease Inhibitor. Journal of Medicinal Chemistry, 2010, 53, 2443-2463.	2.9	166
12	Structure and modeling in the design of Î²â€•and Î³â€‰secretase inhibitors. Drug Development Research, 2009, 70, 70-93.	1.4	23
13	Discovery of aminoheterocycles as a novel Î²-secretase inhibitor class: pH dependence on binding activity part 1. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 2977-2980.	1.0	59
14	PLâ€‰100, a novel HIVâ€‰1 protease inhibitor displaying a high genetic barrier to resistance: An in vitro selection study. Journal of Medical Virology, 2008, 80, 2053-2063.	2.5	20
15	Molecular Modeling Based Approach to Potent P2â^'P4 Macrocyclic Inhibitors of Hepatitis C NS3/4A Protease. Journal of the American Chemical Society, 2008, 130, 4607-4609.	6.6	137
16	Discovery and X-ray Crystallographic Analysis of a Spiropiperidine Iminohydantoin Inhibitor of Î²-Secretaseâ€¡. Journal of Medicinal Chemistry, 2008, 51, 6259-6262.	2.9	59
17	Structure-guided design of Î²-secretase (BACE-1) inhibitors. Expert Opinion on Drug Discovery, 2007, 2, 1129-1138.	2.5	9
18	Evaluating scoring functions for docking and designing Î²-secretase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 823-827.	1.0	23

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19	Î²-Secretase (BACE-1) inhibitors: Accounting for 10s loop flexibility using rigid active sites. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 1117-1121.	1.0	47
20	Discovery and SAR of isonicotinamide BACE-1 inhibitors that bind Î²-secretase in a N-terminal 10s-loop down conformation. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 1788-1792.	1.0	56
21	Macrocyclic Inhibitors of Î²-Secretase:â€‰ Functional Activity in an Animal Model. Journal of Medicinal Chemistry, 2006, 49, 6147-6150.	2.9	91
22	Conformationally biased P3 amide replacements of Î²-secretase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 641-644.	1.0	74
23	BACE-1 inhibition by a series of Ï^[CH2NH] reduced amide isosteres. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 3635-3638.	1.0	61
24	Rational design and synthesis of selective BACE-1 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 601-604.	1.0	45
25	A naphthyridine carboxamide provides evidence for discordant resistance between mechanistically identical inhibitors of HIV-1 integrase. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 11233-11238.	3.3	328
26	Identification of a Small Molecule Nonpeptide Active Site Î²-Secretase Inhibitor That Displays a Nontraditional Binding Mode for Aspartyl Proteases. Journal of Medicinal Chemistry, 2004, 47, 6117-6119.	2.9	124
27	Structure-Based Design of Potent and Selective Cell-Permeable Inhibitors of Human Î²-Secretase (BACE-1). Journal of Medicinal Chemistry, 2004, 47, 6447-6450.	2.9	274
28	A Priori Prediction of Ligand Affinity by Energy Minimization. , 2002, , 63-84.		2
29	4-Aryl-2,4-dioxobutanoic Acid Inhibitors of HIV-1 Integrase and Viral Replication in Cells. Journal of Medicinal Chemistry, 2000, 43, 4923-4926.	2.9	218
30	A priori prediction of ligand affinity by energy minimization. Journal of Computer - Aided Molecular Design, 1998, 9/11, 63-84.	1.0	7
31	An Orally Bioavailable Pyrrolinone Inhibitor of HIV-1 Protease:â€‰ Computational Analysis and X-ray Crystal Structure of the Enzyme Complex. Journal of Medicinal Chemistry, 1997, 40, 2440-2444.	2.9	64
32	A priori prediction of activity for HIV-1 protease inhibitors employing energy minimization in the active site. Journal of Medicinal Chemistry, 1995, 38, 305-317.	2.9	240
33	The Development of Cyclic Sulfolanes as Novel and High-Affinity P2 Ligands for HIV-1 Protease Inhibitors. Journal of Medicinal Chemistry, 1994, 37, 1177-1188.	2.9	56
34	3'-Tetrahydrofuranylglycine as a novel, unnatural amino acid surrogate for asparagine in the design of inhibitors of the HIV protease. Journal of the American Chemical Society, 1993, 115, 801-803.	6.6	42
35	Potent HIV protease inhibitors: the development of tetrahydrofuranylglycines as novel P2-ligands and pyrazine amides as P3-ligands. Journal of Medicinal Chemistry, 1993, 36, 2300-2310.	2.9	76
36	Synthesis and antiviral activity of a series of HIV-1 protease inhibitors with functionality tethered to the P1 or P1' phenyl design. Journal of Medicinal Chemistry, 1992, 35, 1685-1701.	2.9	187

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37	X-ray crystal structure of the HIV protease complex with L-700,417, an inhibitor with pseudo C2 symmetry. Journal of the American Chemical Society, 1991, 113, 9382-9384.	6.6	140
38	Virtual Fragment Scanning: Current Trends, Applications and Web-Based Tools. , 0, , 223-244.		1