Thomas H Keller

List of Publications by Year
in descending order

100 papers	6,984 citations	87888 38 h-index	60623 81 g-index
109 all docs	109 docs citations	109 times ranked	8105 citing authors

#	Article	IF	Citations
1	Spiroindolones, a Potent Compound Class for the Treatment of Malaria. Science, 2010, 329, 1175-1180.	12.6	1,031
2	PA-824 Kills Nonreplicating Mycobacterium tuberculosis by Intracellular NO Release. Science, 2008, 322, 1392-1395.	12.6	568
3	Structural basis for the activation of flaviviral NS3 proteases from dengue and West Nile virus. Nature Structural and Molecular Biology, 2006, 13, 372-373.	8.2	478
4	Spirotetrahydro Î²-Carbolines (Spiroindolones): A New Class of Potent and Orally Efficacious Compounds for the Treatment of Malaria. Journal of Medicinal Chemistry, 2010, 53, 5155-5164.	6.4	381
5	An adenosine nucleoside inhibitor of dengue virus. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20435-20439.	7.1	323
6	A practical view of â€˜druggabilityâ€™. Current Opinion in Chemical Biology, 2006, 10, 357-361.	6.1	257
7	A chemical genetic screen in Mycobacterium tuberculosis identifies carbon-source-dependent growth inhibitors devoid of in vivo efficacy. Nature Communications, 2010, 1, 57.	12.8	250
8	A Small-Molecule Dengue Virus Entry Inhibitor. Antimicrobial Agents and Chemotherapy, 2009, 53, 1823-1831.	3.2	190
9	Peptide inhibitors of dengue virus NS3 protease. Part 1: Warhead. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 36-39.	2.2	152
10	Small Molecule Inhibitors That Selectively Block Dengue Virus Methyltransferase. Journal of Biological Chemistry, 2011, 286, 6233-6240.	3.4	147
11	Peptide inhibitors of dengue virus NS3 protease. Part 2: SAR study of tetrapeptide aldehyde inhibitors. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 40-43.	2.2	142
12	Inhibition of Dengue Virus Polymerase by Blocking of the RNA Tunnel. Journal of Virology, 2010, 84, 5678-5686.	3.4	104
13	Structureâ^'Activity Relationships of Antitubercular Nitroimidazoles. 1. Structural Features Associated with Aerobic and Anaerobic Activities of 4- and 5-Nitroimidazoles. Journal of Medicinal Chemistry, 2009, 52, 1317-1328.	6.4	101
14	NMR Analysis of a Novel Enzymatically Active Unlinked Dengue NS2B-NS3 Protease Complex. Journal of Biological Chemistry, 2013, 288, 12891-12900.	3.4	93
15	Lipiarmycin targets RNA polymerase and has good activity against multidrug-resistant strains of Mycobacterium tuberculosis. Journal of Antimicrobial Chemotherapy, 2008, 62, 713-719.	3.0	92
16	A fluorescence quenching assay to discriminate between specific and nonspecific inhibitors of dengue virus protease. Analytical Biochemistry, 2009, 395, 195-204.	2.4	92
17	Imidazolopiperazines: Hit to Lead Optimization of New Antimalarial Agents. Journal of Medicinal Chemistry, 2011, 54, 5116-5130.	6.4	91
18	The Identification of Indacaterol as an Ultralong-Acting Inhaled Î²₂-Adrenoceptor Agonist. Journal of Medicinal Chemistry, 2010, 53, 3675-3684.	6.4	90

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19	Global Bayesian Models for the Prioritization of Antitubercular Agents. Journal of Chemical Information and Modeling, 2008, 48, 2362-2370.	5.4	89
20	Pharmacological profile of PKF242â€484 and PKF241â€466, novel dual inhibitors of TNFâ€Î± converting enzyme and matrix metalloproteinases, in models of airway inflammation. British Journal of Pharmacology, 2002, 135, 1655-1664.	5.4	83
21	Structural Dynamics of Zika Virus NS2B-NS3 Protease Binding to Dipeptide Inhibitors. Structure, 2017, 25, 1242-1250.e3.	3.3	83
22	Structureâ^'Activity Relationships of Antitubercular Nitroimidazoles. 2. Determinants of Aerobic Activity and Quantitative Structureâ^'Activity Relationships. Journal of Medicinal Chemistry, 2009, 52, 1329-1344.	6.4	82
23	Zika Virus Protease: An Antiviral Drug Target. Trends in Microbiology, 2017, 25, 797-808.	7.7	80
24	Peptide Inhibitors of West Nile NS3 Protease:â€‰ SAR Study of Tetrapeptide Aldehyde Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 6585-6590.	6.4	79
25	Discovery of a Non-Peptidic Inhibitor of West Nile Virus NS3 Protease by High-Throughput Docking. PLoS Neglected Tropical Diseases, 2009, 3, e356.	3.0	71
26	Structural Insights into the Inhibition of Zika Virus NS2B-NS3 Protease by a Small-Molecule Inhibitor. Structure, 2018, 26, 555-564.e3.	3.3	70
27	Diastereocontrolled nickel(0)- and palladium(0) catalyzed â€œmetallo-ene-typeâ€• cyclizations/carbonylations. Tetrahedron Letters, 1989, 30, 5883-5886.	1.4	68
28	Inhibition of Dengue Virus RNA Synthesis by an Adenosine Nucleoside. Antimicrobial Agents and Chemotherapy, 2010, 54, 2932-2939.	3.2	65
29	Synthesis and antitubercular activity of 7-(R)- and 7-(S)-methyl-2-nitro-6-(S)-(4-(trifluoromethoxy)benzyloxy)-6,7-dihydro-5H-imidazo[2,1-b][1,3]oxazines, analogues of PA-824. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 2256-2262.	2.2	62
30	Functionalization of Peptides and Proteins by Mukaiyama Aldol Reaction. Journal of the American Chemical Society, 2010, 132, 9546-9548.	13.7	61
31	Fragment-Based Ligand Design of Novel Potent Inhibitors of Tankyrases. Journal of Medicinal Chemistry, 2013, 56, 4497-4508.	6.4	59
32	N-Sulfonylanthranilic Acid Derivatives as Allosteric Inhibitors of Dengue Viral RNA-Dependent RNA Polymerase. Journal of Medicinal Chemistry, 2009, 52, 7934-7937.	6.4	54
33	Inhibition of Dengue Virus by an Ester Prodrug of an Adenosine Analog. Antimicrobial Agents and Chemotherapy, 2010, 54, 3255-3261.	3.2	48
34	Development of isoform selective PI3-kinase inhibitors as pharmacological tools for elucidating the PI3K pathway. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5445-5450.	2.2	46
35	A Translation Inhibitor That Suppresses Dengue Virus In Vitro and In Vivo. Antimicrobial Agents and Chemotherapy, 2011, 55, 4072-4080.	3.2	43
36	The use of porcupine inhibitors to target Wnt-driven cancers. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5472-5476.	2.2	43

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37	The Crystal Structures of the SH2 Domain of p56lckComplexed with Two Phosphonopeptides Suggest a Gated Peptide Binding Site. Journal of Molecular Biology, 1995, 246, 344-355.	4.2	41
38	Palladium(0)- and nickel(0) catalyzed â€œmetallo-ene-typeâ€•cyclizations: Stereodirecting resident chirality.. Tetrahedron Letters, 1990, 31, 1265-1268.	1.4	39
39	Structureâ€“Activity Relationships of Antitubercular Nitroimidazoles. 3. Exploration of the Linker and Lipophilic Tail of ((S)-2-Nitro-6,7-dihydro-5H-imidazo[2,1-b][1,3]oxazin-6-yl)-(4-trifluoromethoxybenzyl)amine (6-Amino PA-824).. Journal of Medicinal Chemistry, 2011, 54, 5639-5659.	6.4	38
40	Peptide deformylase inhibitors of Mycobacterium tuberculosis: Synthesis, structural investigations, and biological results. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 6568-6572.	2.2	37
41	Conformational analysis of 14-membered macrolides using x-ray crystallography and molecular mechanics calculations. Journal of the American Chemical Society, 1988, 110, 7858-7868.	13.7	35
42	NMR study of complexes between low molecular mass inhibitors and the West Nile virus NS2Bâ€“NS3 protease. FEBS Journal, 2009, 276, 4244-4255.	4.7	35
43	Discovery and Optimization of a Porcupine Inhibitor. Journal of Medicinal Chemistry, 2015, 58, 5889-5899.	6.4	35
44	Structural characterization of the linked <scp>NS</scp>2Bâ€<scp>NS</scp>3 protease of Zika virus. FEBS Letters, 2017, 591, 2338-2347.	2.8	35
45	Structural and ligand-binding analysis of the YAP-binding domain of transcription factor TEAD4. Biochemical Journal, 2018, 475, 2043-2055.	3.7	35
46	Finding New Medicines for Flaviviral Targets. Novartis Foundation Symposium, 2008, , 102-119.	1.1	34
47	Structural and Functional Analyses of an Allosteric EYA2 Phosphatase Inhibitor That Has On-Target Effects in Human Lung Cancer Cells. Molecular Cancer Therapeutics, 2019, 18, 1484-1496.	4.1	34
48	Exploring the binding of peptidic West Nile virus NS2Bâ€“NS3 protease inhibitors by NMR. Antiviral Research, 2013, 97, 137-144.	4.1	33
49	Enantiodivergent Synthesis of (R)- and (S)-Rolipram. Molecules, 1998, 3, 107-119.	3.8	31
50	A new orally bioavailable dual adenosine A2B/A3 receptor antagonist with therapeutic potential. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3081-3085.	2.2	31
51	Mechanistic Study of the Spiroindolones: A New Class of Antimalarials. Molecules, 2012, 17, 10131-10141.	3.8	31
52	Drug Design For Flavivirus Proteases: What Are We Missing?. Current Pharmaceutical Design, 2014, 20, 3422-3427.	1.9	30
53	Yellow fever virus NS3 protease: peptide-inhibition studies. Journal of General Virology, 2007, 88, 2223-2227.	2.9	29
54	Synthesis and hybridization properties of oligonucleotides containing 2'-O-modified ribonucleotides. Nucleic Acids Research, 1993, 21, 4499-4505.	14.5	28

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55	Solubility-Driven Optimization of Phosphodiesterase-4 Inhibitors Leading to a Clinical Candidate. Journal of Medicinal Chemistry, 2012, 55, 7472-7479.	6.4	27
56	Probing the specificity of the S1 binding site of subtilisin Carlsberg with boronic acids. Bioorganic and Medicinal Chemistry, 1994, 2, 35-48.	3.0	26
57	Preclinical Evaluation of the Antifolate QN254, 5-Chloro-Nâ€²6â€²-(2,5-Dimethoxy-Benzyl)-Quinazoline-2,4,6-Triamine, as an Antimalarial Drug Candidate. Antimicrobial Agents and Chemotherapy, 2010, 54, 2603-2610.	3.2	25
58	A General Method for the Synthesis of 2â€²-O-Modified Ribonucleosides. Helvetica Chimica Acta, 1993, 76, 884-892.	1.6	24
59	Indium mediated allylation in peptide and protein functionalization. Chemical Communications, 2011, 47, 9066.	4.1	24
60	Synthesis and biological properties of novel glucocorticoid androstene C-17 furoate esters. Bioorganic and Medicinal Chemistry, 2004, 12, 5213-5224.	3.0	23
61	Anti-infectives: Can cellular screening deliver?. Current Opinion in Chemical Biology, 2011, 15, 529-533.	6.1	23
62	Fragment-Based Drug Discovery of Potent Protein Kinase C Iota Inhibitors. Journal of Medicinal Chemistry, 2018, 61, 4386-4396.	6.4	23
63	Pharmacophore Model for Wnt/Porcupine Inhibitors and Its Use in Drug Design. Journal of Chemical Information and Modeling, 2015, 55, 1435-1448.	5.4	21
64	Finding new medicines for flaviviral targets. Novartis Foundation Symposium, 2006, 277, 102-14; discussion 114-9, 251-3.	1.1	21
65	Discovery of Irreversible Inhibitors Targeting Histone Methyltransferase, SMYD3. ACS Medicinal Chemistry Letters, 2019, 10, 978-984.	2.8	20
66	CGH2466, a combined adenosine receptor antagonist, p38 mitogen-activated protein kinase and phosphodiesterase type 4 inhibitor with potent in vitro and in vivo anti-inflammatory activities. British Journal of Pharmacology, 2005, 144, 1002-1010.	5.4	19
67	Scaffold Hopping and Optimization of Maleimide Based Porcupine Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 6678-6692.	6.4	19
68	Diastereoselective reduction of 9-oxo-13-tetradecanolide and 10,10-dimethyl-9-oxo-13-tetradecanolide. Journal of the American Chemical Society, 1990, 112, 450-452.	13.7	18
69	New Highly Potent and Selective Adenosine A3 Receptor Antagonists. Current Topics in Medicinal Chemistry, 2004, 4, 863-870.	2.1	18
70	Impact of non-profit organizations on drug discovery: opportunities, gaps, solutions. Drug Discovery Today, 2008, 13, 347-352.	6.4	17
71	Structureâ€“Activity Relationship Studies of Mitogen Activated Protein Kinase Interacting Kinase (MNK) 1 and 2 and BCR-ABL1 Inhibitors Targeting Chronic Myeloid Leukemic Cells. Journal of Medicinal Chemistry, 2016, 59, 3063-3078.	6.4	16
72	Escherichia coli Topoisomerase IV E Subunit and an Inhibitor Binding Mode Revealed by NMR Spectroscopy. Journal of Biological Chemistry, 2016, 291, 17743-17753.	3.4	15

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73	Structural model of human PORCN illuminates disease-associated variants and drug-binding sites. Journal of Cell Science, 2021, 134, .	2.0	15
74	Probing the specificity of the S1 binding site of subtilisin Carlsberg with boronic acids. Biochemical and Biophysical Research Communications, 1991, 176, 401-405.	2.1	14
75	Application of Fragmentâ€Based Drug Discovery against DNA Gyraseâ€...B. ChemPlusChem, 2015, 80, 1250-1254.	2.8	14
76	Conformationally controlled reductions of 14-membered macrolides. Tetrahedron Letters, 1990, 31, 6307-6310.	1.4	12
77	Synthesis and Structure-Activity Relationship of N-Arylrolipram Derivatives as Inhibitors of PDE4 Isozymes.. Chemical and Pharmaceutical Bulletin, 2001, 49, 1009-1017.	1.3	12
78	Discovery and Optimization of 4-(8-(3-Fluorophenyl)-1,7-naphthyridin-6-yl)transcyclohexanecarboxylic Acid, an Improved PDE4 Inhibitor for the Treatment of Chronic Obstructive Pulmonary Disease (COPD). Journal of Medicinal Chemistry, 2015, 58, 6747-6752.	6.4	12
79	NMR structural characterization of the Nâ€terminal active domain of the gyrase B subunit fromPseudomonas aeruginosa and its complex with an inhibitor. FEBS Letters, 2015, 589, 2683-2689.	2.8	12
80	The importance of molecular complexity in the design of screening libraries. Journal of Computer-Aided Molecular Design, 2013, 27, 783-792.	2.9	11
81	Use of difference NOE experiments to assign the geometry of trimethylsilyl enol ethers. Journal of Organic Chemistry, 1987, 52, 1870-1872.	3.2	10
82	N-Arylrolipram derivatives as potent and selective PDE4 inhibitors. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 3229-3234.	2.2	10
83	Potent and selective xanthine-based inhibitors of phosphodiesterase 5. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2376-2379.	2.2	10
84	Peptidomimetic ethyl propenoate covalent inhibitors of the enterovirus 71 3C protease: a P2â€“P4 study. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 332-339.	5.2	10
85	Discovery of dual GyrB/ParE inhibitors active against Gram-negative bacteria. European Journal of Medicinal Chemistry, 2018, 157, 610-621.	5.5	10
86	Targeting EYA2 tyrosine phosphatase activity in glioblastoma stem cells induces mitotic catastrophe. Journal of Experimental Medicine, 2021, 218, .	8.5	9
87	Design and synthesis of a library of chemokine antagonists. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 6249-6252.	2.2	7
88	Characterization of the interaction between Escherichia coli topoisomerase IV E subunit and an ATP competitive inhibitor. Biochemical and Biophysical Research Communications, 2015, 467, 961-966.	2.1	7
89	Fragment-based Discovery of a Small-Molecule Protein Kinase C-iota Inhibitor Binding Post-kinase Domain Residues. ACS Medicinal Chemistry Letters, 2019, 10, 318-323.	2.8	7
90	Stepwise Evolution of Fragment Hits against MAPK Interacting Kinases 1 and 2. Journal of Medicinal Chemistry, 2020, 63, 621-637.	6.4	7

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91	Fragment-based lead discovery of indazole-based compounds as AXL kinase inhibitors. Bioorganic and Medicinal Chemistry, 2021, 49, 116437.	3.0	7
92	Synthesis of N-Arylrolipram Derivatives - Potent and Selective Phosphodiesterase-IV Inhibitors - by Copper Catalyzed Lactam-Aryl Halide Coupling. Heterocycles, 1998, 48, 2225.	0.7	6
93	Biophysical Studies of Bacterial Topoisomerases Substantiate Their Binding Modes to an Inhibitor. Biophysical Journal, 2015, 109, 1969-1977.	0.5	6
94	Probing biological mechanisms with chemical tools. Pharmacological Research, 2020, 153, 104656.	7.1	4
95	Structureâ€“activity relationship studies of allosteric inhibitors of <scp>EYA2</scp> tyrosine phosphatase. Protein Science, 2022, 31, 422-431.	7.6	4
96	Dengue Drug Discovery. Topics in Medicinal Chemistry, 2011, , 243-275.	0.8	2
97	Backbone resonance assignments for the SET domain of human methyltransferase NSD3 in complex with its cofactor. Biomolecular NMR Assignments, 2017, 11, 225-229.	0.8	2
98	Artificial Neural Network Analysis of Pharmacokinetic and Toxicity Properties of Lead Molecules for Dengue Fever, Tuberculosis and Malaria. Current Computer-Aided Drug Design, 2016, 12, 52-61.	1.2	2
99	Dual Specific Inhibitors Of The BCR-ABL and MNK Kinases As Potential Therapeutics For Blast Crisis Chronic Myeloid Leukemia. Blood, 2013, 122, 2702-2702.	1.4	1
100	State of the art technologies in drug discovery 2011. Current Opinion in Chemical Biology, 2011, 15, 461-462.	6.1	0