Zhenquan Hu

List of Publications by Year
in descending order

42	1,184	516215 16	414034 32
papers	citations	h-index	g-index

42	42	42	1675
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Using <scp>PyMOL</scp> as a platform for computational drug design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1298.	6.2	348
2	Ligand recognition and allosteric regulation of DRD1-Gs signaling complexes. Cell, 2021, 184, 943-956.e18.	13.5	94
3	OpenVirtualToxLabâ€"A platform for generating and exchanging in silico toxicity data. Toxicology Letters, 2015, 232, 519-532.	0.4	89
4	W246^{6.48} Opens a Gate for a Continuous Intrinsic Water Pathway during Activation of the Adenosineâ€...A_{2A} Receptor. Angewandte Chemie - International Edition, 2015, 54, 556-559.	7.2	64
5	Mechanism of host substrate acetylation by a YopJ family effector. Nature Plants, 2017, 3, 17115.	4.7	50
6	Discovery of N -(5-((5-chloro-4-((2-(isopropylsulfonyl)phenyl)amino)pyrimidin-2-yl)amino)-4-methoxy-2-(4-methyl-1,4-diazepan-1-yl)phenyl)acrylamide (CHMFL-ALK/EGFR-050) as a potent ALK/EGFR dual kinase inhibitor capable of overcoming a variety of ALK/EGFR associated drug resistant mutants in NSCLC. European Journal of Medicinal Chemistry, 2017, 139, 674-697.	2.6	38
7	Discovery of 1-(4-(4-Amino-3-(4-(2-morpholinoethoxy)phenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl)phenyl)-3-(5-(tert-butyl)isoxazol- (CHMFL-FLT3-213) as a Highly Potent Type II FLT3 Kinase Inhibitor Capable of Overcoming a Variety of FLT3 Kinase Mutants in FLT3-ITD Positive AML. Journal of Medicinal Chemistry, 2017, 60, 8407-8424.	2.9	32
8	Discovery of 4-((((4-(5-chloro-2-(((1s,4s)-4-((2-methoxyethyl)amino)cyclohexyl)amino)pyridin-4-yl)thiazol-2-yl)amino)methyl)tetrahydro-2H-pyran-4-car (JSH-150) as a novel highly selective and potent CDK9 kinase inhibitor. European Journal of Medicinal Chemistry, 2018, 158, 896-916.	2.6	32
9	Implementing WebGL and HTML5 in Macromolecular Visualization and Modern Computer-Aided Drug Design. Trends in Biotechnology, 2017, 35, 559-571.	4.9	30
10	Discovery of N-(4-(6-Acetamidopyrimidin-4-yloxy)phenyl)-2-(2-(trifluoromethyl)phenyl)acetamide (CHMFL-FLT3-335) as a Potent FMS-like Tyrosine Kinase 3 Internal Tandem Duplication (FLT3-ITD) Mutant Selective Inhibitor for Acute Myeloid Leukemia. Journal of Medicinal Chemistry, 2019, 62, 875-892.	2.9	20
11	NF-Î°B Inhibitory and Antibacterial Helvolic and Fumagillin Derivatives from Aspergillus terreus. Journal of Natural Products, 2020, 83, 730-737.	1.5	20
12	Discovery of N-(3-(5-((3-acrylamido-4-(morpholine-4-carbonyl)phenyl)amino)-1-methyl-6-oxo-1,6-dihydropyridin-3-yl)-2-methylphenyl)-4-(tert-butyl)ber (CHMFL-BTK-01) as a highly selective irreversible Bruton's tyrosine kinase (BTK) inhibitor. European Journal of Medicinal Chemistry, 2017, 131, 107-125.	2.6	18
13	Discovery of 2-((3-Amino-4-methylphenyl)amino)-N-(2-methyl-5-(3-(trifluoromethyl)benzamido)phenyl)-4-(methylamino)pyrimidine-5-carboxam (CHMFL-ABL-053) as a Potent, Selective, and Orally Available BCR-ABL/SRC/p38 Kinase Inhibitor for Chronic Myeloid Leukemia. Journal of Medicinal Chemistry, 2016, 59, 1984-2004.	2.9	17
14	Discovery of 2-((3-Acrylamido-4-methylphenyl)amino)-N-(2-methyl-5-(3,4,5-trimethoxybenzamido)phenyl)-4-(methylamino)pyrimidine-5-carbox (CHMFL-BMX-078) as a Highly Potent and Selective Type II Irreversible Bone Marrow Kinase in the X Chromosome (BMX) Kinase Inhibitor. Journal of Medicinal Chemistry, 2017, 60, 1793-1816.	2.9	17
15	Two new tricycloalternarenes from Hawaiian endophytic fungus Didymella sp. FT433. Tetrahedron Letters, 2018, 59, 3381-3383.	0.7	17
16	Discovery of 2-(4-Chloro-3-(trifluoromethyl)phenyl)-N-(4-((6,7-dimethoxyquinolin-4-yl)oxy)phenyl)acetamide (CHMFL-KIT-64) as a Novel Orally Available Potent Inhibitor against Broad-Spectrum Mutants of c-KIT Kinase for Gastrointestinal Stromal Tumors. Journal of Medicinal Chemistry, 2019, 62, 6083-6101.	2.9	17
17	Structure-activity relationship investigation for benzonaphthyridinone derivatives as novel potent Bruton's tyrosine kinase (BTK) irreversible inhibitors. European Journal of Medicinal Chemistry, 2017, 137, 545-557.	2.6	16
18	Discovery of 4-((N-(2-(dimethylamino)ethyl)acrylamido)methyl)-N-(4-methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)phenyl)benzamide (CHMFL-PDGFR-159) as a highly selective type II PDGFRÎ± kinase inhibitor for PDGFRÎ± driving chronic eosinophilic leukemia. European Journal of Medicinal Chemistry, 2018, 150, 366-384.	2.6	16

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19	Salviachinensines Aâ€“F, Antiproliferative Phenolic Derivatives from the Chinese Medicinal Plant Salvia chinensis. Journal of Natural Products, 2018, 81, 2531-2538.	1.5	16
20	Discovery of (E)-N¹-(3-Fluorophenyl)-N³-(3-(2-(pyridin-2-yl)vinyl)-1H-indazol-6-yl)malonamide (CHMFL-KIT-033) as a Novel c-KIT T670I Mutant Selective Kinase Inhibitor for Gastrointestinal Stromal Tumors (GISTs). Journal of Medicinal Chemistry, 2019, 62, 5006-5024.	2.9	15
21	Clavukoellians Aâ€“F, Highly Rearranged Nardosinane Sesquiterpenoids with Antiangiogenic Activity from Clavularia koellikeri. Journal of Natural Products, 2019, 82, 1331-1337.	1.5	15
22	Circumdatin M, a new benzodiazepine alkaloid with a unique pyrimidone-4-pyrone moiety from a Hawaiian marine fungus Aspergillus sp. FM242. Tetrahedron Letters, 2019, 60, 1724-1726.	0.7	14
23	Discovery of N-((1-(4-(3-(3-((6,7-Dimethoxyquinolin-3-yl)oxy)phenyl)ureido)-2-(trifluoromethyl)phenyl)piperidin-4-yl)methyl)propionamide (CHMFL-KIT-8140) as a Highly Potent Type II Inhibitor Capable of Inhibiting the T670I â€œGatekeeperâ€•Mutant of cKIT Kinase. Journal of Medicinal Chemistry, 2016, 59, 8456-8472.	2.9	13
24	Repurposing cabozantinib to GISTs: Overcoming multiple imatinib-resistant cKIT mutations including gatekeeper and activation loop mutants in GISTs preclinical models. Cancer Letters, 2019, 447, 105-114.	3.2	13
25	Discovery of 6â€²-chloro-N-methyl-5â€™-(phenylsulfonamido)-[3,3â€²-bipyridine]-5-carboxamide (CHMFL-PI4K-127) as a novel Plasmodium falciparum PI(4)K inhibitor with potent antimalarial activity against both blood and liver stages of Plasmodium. European Journal of Medicinal Chemistry, 2020, 188, 112012.	2.6	13
26	Secondary Metabolites from the Leather Coral-Derived Fungal Strain Xylaria sp. FM1005 and Their Glycoprotein IIb/IIIa Inhibitory Activity. Journal of Natural Products, 2021, 84, 466-473.	1.5	13
27	Discovery of 4-Methyl-N-(4-((4-methylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)-3-((1-nicotinoylpiperidin-4-yl)oxy)benzamide (CHMFL-ABL/KIT-155) as a Novel Highly Potent Type II ABL/KIT Dual Kinase Inhibitor with a Distinct Hinge Binding. Journal of Medicinal Chemistry, 2017, 60, 273-289.	2.9	12
28	Discovery of (E)-N-(4-methyl-5-(3-(2-(pyridin-2-yl)vinyl)-1H-indazol-6-yl)thiazol-2-yl)-2-(4-methylpiperazin-1-yl)acetamide (IHMT-TRK-284) as a novel orally available type II TRK kinase inhibitor capable of overcoming multiple resistant mutants. European Journal of Medicinal Chemistry, 2020, 207, 112744.	2.6	12
29	Discovery of (S)-2-(1-(4-Amino-3-(3-fluoro-4-methoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl)propyl)-3-cyclopropyl-5-fluoroqu (IHMT-PI3Kΐ-372) as a Potent and Selective PI3Kΐ Inhibitor for the Treatment of Chronic Obstructive Pulmonary Disease. Journal of Medicinal Chemistry, 2020, 63, 13973-13993.	2.9	12
30	Tryptoquivalines W and X, two new compounds from a Hawaiian fungal strain and their biological activities. Tetrahedron Letters, 2020, 61, 151730.	0.7	11
31	Fungal Epithiodiketopiperazines Carrying Î±,Î²â€²-Polysulfide Bridges from Penicillium steckii YE, and Their Chemical Interconversion. ChemBioChem, 2021, 22, 416-422.	1.3	11
32	Discovery ofN-(3-((1-Isonicotinoylpiperidin-4-yl)oxy)-4-methylphenyl)-3-(trifluoromethyl)benzamide (CHMFL-KIT-110) as a Selective, Potent, and Orally Available Type II c-KIT Kinase Inhibitor for Gastrointestinal Stromal Tumors (GISTs). Journal of Medicinal Chemistry, 2016, 59, 3964-3979.	2.9	10
33	Discovery and characterization of a novel potent type II native and mutant BCR-ABL inhibitor (CHMFL-074) for Chronic Myeloid Leukemia (CML). Oncotarget, 2016, 7, 45562-45574.	0.8	10
34	Antibacterial kaneoheoic acids A-F from a Hawaiian fungus Fusarium sp. FM701. Phytochemistry, 2021, 181, 112545.	1.4	9
35	Discovery of (S)-2-amino-N-(5-(6-chloro-5-(3-methylphenylsulfonamido)pyridin-3-yl)-4-methylthiazol-2-yl)-3-methylbutanamide (CHMFL-PI3KD-317) as a potent and selective phosphoinositide 3-kinase delta (PI3Kΐ) inhibitor. European Journal of Medicinal Chemistry, 2018, 156, 831-846.	2.6	8
36	Aspochalasin H1: A New Cyclic Aspochalasin from Hawaiian Plant-Associated Endophytic Fungus Aspergillus sp. FT1307. Molecules, 2021, 26, 4239.	1.7	8

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37	Assessing the Performance of Traveling-salesman based Automated Path Searching (TAPS) on Complex Biomolecular Systems. Journal of Chemical Theory and Computation, 2021, 17, 5301-5311.	2.3	8
38	Discovery of (E)-N-(4-((4-methylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)-3-((3-(2-(pyridin-2-yl)vinyl)-1H-indazol-6-yl)thio)propanamide (CHMFL-ABL-121) as a highly potent ABL kinase inhibitor capable of overcoming a variety of ABL mutants including T315I for chronic myeloid leukemia. European Journal of Medicinal Chemistry, 2018, 160, 61-81.	2.6	7
39	Discovery and characterization of a novel highly potent and selective type II native and drug-resistant V299L mutant BCR-ABL inhibitor (CHMFL-ABL-039) for Chronic Myeloid Leukemia (CML). Cancer Biology and Therapy, 2019, 20, 877-885.	1.5	6
40	Discovery of a highly potent kinase inhibitor capable of overcoming multiple imatinib-resistant ABL mutants for chronic myeloid leukemia (CML). European Journal of Pharmacology, 2021, 897, 173944.	1.7	6
41	Molecular mechanisms of endocrine and metabolic disruption: An in silico study on antitrypanosomal natural products and some derivatives. Toxicology Letters, 2016, 252, 29-41.	0.4	4
42	Axitinib overcomes multiple imatinib resistant cKIT mutations including the gatekeeper mutation T670I in gastrointestinal stromal tumors. Therapeutic Advances in Medical Oncology, 2019, 11, 175883591984975.	1.4	3