Xinyong Liu

List of Publications by Year in descending order

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		109264	128225
106	4,306	35	60
papers	citations	h-index	g-index

106	106	106	3561
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anti-HIV Drug Discovery and Development: Current Innovations and Future Trends. Journal of Medicinal Chemistry, 2016, 59, 2849-2878.	2.9	260
2	Inhibitors of SARS-CoV-2 Entry: Current and Future Opportunities. Journal of Medicinal Chemistry, 2020, 63, 12256-12274.	2.9	183
3	Conformational restriction: an effective tactic in 'follow-on'-based drug discovery. Future Medicinal Chemistry, 2014, 6, 885-901.	1.1	163
4	HIVâ€1 NNRTIs: structural diversity, pharmacophore similarity, and impliations for drug design. Medicinal Research Reviews, 2013, 33, E1-72.	5.0	161
5	Fsp3: A new parameter for drug-likeness. Drug Discovery Today, 2020, 25, 1839-1845.	3.2	156
6	Discovery of bioactive molecules from CuAAC click-chemistry-based combinatorial libraries. Drug Discovery Today, 2016, 21, 118-132.	3.2	138
7	The Journey of HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) from Lab to Clinic. Journal of Medicinal Chemistry, 2019, 62, 4851-4883.	2.9	124
8	Strategies for the Design of HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors: Lessons from the Development of Seven Representative Paradigms. Journal of Medicinal Chemistry, 2012, 55, 3595-3613.	2.9	115
9	Overview of Recent Strategic Advances in Medicinal Chemistry. Journal of Medicinal Chemistry, 2019, 62, 9375-9414.	2.9	108
10	Design, Synthesis, and Evaluation of Thiophene[3,2-d]pyrimidine Derivatives as HIV-1 Non-nucleoside Reverse Transcriptase Inhibitors with Significantly Improved Drug Resistance Profiles. Journal of Medicinal Chemistry, 2016, 59, 7991-8007.	2.9	107
11	Design Strategies of Novel NNRTIs to Overcome Drug Resistance. Current Medicinal Chemistry, 2009, 16, 3903-3917.	1.2	92
12	Recent Advances in DAPYs and Related Analogues as HIV-1 NNRTIs. Current Medicinal Chemistry, 2011, 18, 359-376.	1.2	92
13	Medicinal chemistry strategies for discovering antivirals effective against drug-resistant viruses. Chemical Society Reviews, 2021, 50, 4514-4540.	18.7	84
14	New techniques and strategies in drug discovery. Chinese Chemical Letters, 2020, 31, 1695-1708.	4.8	82
15	Structure-Based Optimization of Thiophene[3,2-d]pyrimidine Derivatives as Potent HIV-1 Non-nucleoside Reverse Transcriptase Inhibitors with Improved Potency against Resistance-Associated Variants. Journal of Medicinal Chemistry, 2017, 60, 4424-4443.	2.9	79
16	Fused heterocycles bearing bridgehead nitrogen as potent HIV-1 NNRTIs. Part 3: Optimization of [1,2,4]triazolo[1,5-a]pyrimidine core via structure-based and physicochemical property-driven approaches. European Journal of Medicinal Chemistry, 2015, 92, 754-765.	2.6	76
17	Identification of Dihydrofuro[3,4-d]pyrimidine Derivatives as Novel HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors with Promising Antiviral Activities and Desirable Physicochemical Properties. Journal of Medicinal Chemistry, 2019, 62, 1484-1501.	2.9	70
18	Recent developments in the medicinal chemistry of single boron atom-containing compounds. Acta Pharmaceutica Sinica B, 2021, 11, 3035-3059.	5.7	70

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19	Targeting the entrance channel of NNIBP: Discovery of diarylnicotinamide 1,4-disubstituted 1,2,3-triazoles as novel HIV-1 NNRTIs with high potency against wild-type and E138K mutant virus. European Journal of Medicinal Chemistry, 2018, 151, 339-350.	2.6	68
20	Exploiting the Tolerant Region I of the Non-Nucleoside Reverse Transcriptase Inhibitor (NNRTI) Binding Pocket: Discovery of Potent Diarylpyrimidine-Typed HIV-1 NNRTIs against Wild-Type and E138K Mutant Virus with Significantly Improved Water Solubility and Favorable Safety Profiles. Journal of Medicinal Chemistry, 2019, 62, 2083-2098.	2.9	66
21	Designed Multiple Ligands: An Emerging Anti-HIV Drug Discovery Paradigm. Current Pharmaceutical Design, 2009, 15, 1893-1917.	0.9	65
22	Discovery of N-Substituted Oseltamivir Derivatives as Potent and Selective Inhibitors of H5N1 Influenza Neuraminidase. Journal of Medicinal Chemistry, 2014, 57, 8445-8458.	2.9	65
23	Design, synthesis and structure-activity relationships of 4-phenyl-1H-1,2,3-triazole phenylalanine derivatives as novel HIV-1 capsid inhibitors with promising antiviral activities. European Journal of Medicinal Chemistry, 2020, 190, 112085.	2.6	65
24	Structural basis for potent and broad inhibition of HIV-1 RT by thiophene[3,2-d]pyrimidine non-nucleoside inhibitors. ELife, 2018, 7, .	2.8	57
25	Discovery of phenylalanine derivatives as potent HIV-1 capsid inhibitors from click chemistry-based compound library. European Journal of Medicinal Chemistry, 2018, 158, 478-492.	2.6	51
26	Structure-Based Bioisosterism Yields HIV-1 NNRTIs with Improved Drug-Resistance Profiles and Favorable Pharmacokinetic Properties. Journal of Medicinal Chemistry, 2020, 63, 4837-4848.	2.9	50
27	Optimization of N-Substituted Oseltamivir Derivatives as Potent Inhibitors of Group-1 and -2 Influenza A Neuraminidases, Including a Drug-Resistant Variant. Journal of Medicinal Chemistry, 2018, 61, 6379-6397.	2.9	46
28	Discovery of novel 1,4-disubstituted 1,2,3-triazole phenylalanine derivatives as HIV-1 capsid inhibitors. RSC Advances, 2019, 9, 28961-28986.	1.7	42
29	Fused heterocycles bearing bridgehead nitrogen as potent HIV-1 NNRTIs. Part 4: Design, synthesis and biological evaluation of novel imidazo[1,2-a]pyrazines. European Journal of Medicinal Chemistry, 2015, 93, 330-337.	2.6	41
30	Design, Synthesis, and Mechanism Study of Benzenesulfonamide-Containing Phenylalanine Derivatives as Novel HIV-1 Capsid Inhibitors with Improved Antiviral Activities. Journal of Medicinal Chemistry, 2020, 63, 4790-4810.	2.9	41
31	Update on Recent Developments in Small Molecular HIV-1 RNase H Inhibitors (2013-2016): Opportunities and Challenges. Current Medicinal Chemistry, 2018, 25, 1682-1702.	1.2	41
32	Discovery of novel anti-HIV agents via Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC) click chemistry-based approach. Expert Opinion on Drug Discovery, 2016, 11, 857-871.	2.5	39
33	Novel urate transporter 1 (URAT1) inhibitors: a review of recent patent literature (2016â€“2019). Expert Opinion on Therapeutic Patents, 2019, 29, 871-879.	2.4	39
34	Targeting the hydrophobic channel of NNIBP: discovery of novel 1,2,3-triazole-derived diarylpyrimidines as novel HIV-1 NNRTIs with high potency against wild-type and K103N mutant virus. Organic and Biomolecular Chemistry, 2019, 17, 3202-3217.	1.5	39
35	Exploring the hydrophobic channel of NNIBP leads to the discovery of novel piperidine-substituted thiophene[3,2-d]pyrimidine derivatives as potent HIV-1 NNRTIs. Acta Pharmaceutica Sinica B, 2020, 10, 878-894.	5.7	39
36	Discovery and Characterization of Fluorine-Substituted Diarylpyrimidine Derivatives as Novel HIV-1 NNRTIs with Highly Improved Resistance Profiles and Low Activity for the hERG Ion Channel. Journal of Medicinal Chemistry, 2020, 63, 1298-1312.	2.9	37

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37	Structure-Based Optimization of N-Substituted Oseltamivir Derivatives as Potent Anti-Influenza A Virus Agents with Significantly Improved Potency against Oseltamivir-Resistant N1-H274Y Variant. Journal of Medicinal Chemistry, 2018, 61, 9976-9999.	2.9	35
38	Contemporary medicinal-chemistry strategies for the discovery of selective butyrylcholinesterase inhibitors. Drug Discovery Today, 2019, 24, 629-635.	3.2	35
39	Recent Progress in the Research of Small Molecule HIV-1 RNase H Inhibitors. Current Medicinal Chemistry, 2014, 21, 1956-1967.	1.2	35
40	2,4,5-Trisubstituted Pyrimidines as Potent HIV-1 NNRTIs: Rational Design, Synthesis, Activity Evaluation, and Crystallographic Studies. Journal of Medicinal Chemistry, 2021, 64, 4239-4256.	2.9	33
41	Medicinal chemistry strategies towards the development of effective SARS-CoV-2 inhibitors. Acta Pharmaceutica Sinica B, 2022, 12, 581-599.	5.7	33
42	Contemporary Medicinal Chemistry Strategies for the Discovery and Development of Novel HIV-1 Non-nucleoside Reverse Transcriptase Inhibitors. Journal of Medicinal Chemistry, 2022, 65, 3729-3757.	2.9	33
43	Discovery of Novel Diarylpyrimidine Derivatives as Potent HIV-1 NNRTIs Targeting the â€œNNRTI Adjacentâ€• Binding Site. ACS Medicinal Chemistry Letters, 2018, 9, 334-338.	1.3	32
44	5-Hydroxypyrido[2,3-b]pyrazin-6(5H)-one derivatives as novel dual inhibitors of HIV-1 reverse transcriptase-associated ribonuclease H and integrase. European Journal of Medicinal Chemistry, 2018, 155, 714-724.	2.6	31
45	Discovery of uracil-bearing DAPYs derivatives as novel HIV-1 NNRTIs via crystallographic overlay-based molecular hybridization. European Journal of Medicinal Chemistry, 2017, 130, 209-222.	2.6	30
46	Discovery of Thiophene[3,2-d]pyrimidine Derivatives as Potent HIV-1 NNRTIs Targeting the Tolerant Region I of NNIBP. ACS Medicinal Chemistry Letters, 2017, 8, 1188-1193.	1.3	30
47	Novel Human Urate Transporter 1 Inhibitors as Hypouricemic Drug Candidates with Favorable Druggability. Journal of Medicinal Chemistry, 2020, 63, 10829-10854.	2.9	30
48	Further Exploring Solvent-Exposed Tolerant Regions of Allosteric Binding Pocket for Novel HIV-1 NNRTIs Discovery. ACS Medicinal Chemistry Letters, 2018, 9, 370-375.	1.3	28
49	Molecular design opportunities presented by solventâ€exposed regions of target proteins. Medicinal Research Reviews, 2019, 39, 2194-2238.	5.0	28
50	Structural optimization of pyridine-type DAPY derivatives to exploit the tolerant regions of the NNRTI binding pocket. European Journal of Medicinal Chemistry, 2016, 121, 352-363.	2.6	27
51	Discovery of C-1 modified oseltamivir derivatives as potent influenza neuraminidase inhibitors. European Journal of Medicinal Chemistry, 2018, 146, 220-231.	2.6	26
52	Discovery of novel diarylpyrimidines as potent HIV-1 NNRTIs by investigating the chemical space of a less explored â€œhydrophobic channelâ€• Organic and Biomolecular Chemistry, 2018, 16, 1014-1028.	1.5	26
53	â€œOld Dogs with New Tricksâ€• exploiting alternative mechanisms of action and new drug design strategies for clinically validated HIV targets. Molecular BioSystems, 2014, 10, 1998.	2.9	25
54	Discovery of piperidine-substituted thiazolo[5,4-d]pyrimidine derivatives as potent and orally bioavailable HIV-1 non-nucleoside reverse transcriptase inhibitors. Communications Chemistry, 2019, 2, .	2.0	24

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55	Design, synthesis and biological evaluation of â€œMulti-Siteâ€•binding influenza virus neuraminidase inhibitors. European Journal of Medicinal Chemistry, 2019, 178, 64-80.	2.6	24
56	Design, synthesis and biological evaluation of novel acetamide-substituted doravirine and its prodrugs as potent HIV-1 NNRTIs. Bioorganic and Medicinal Chemistry, 2019, 27, 447-456.	1.4	24
57	Discovery of novel DAPY-IAS hybrid derivatives as potential HIV-1 inhibitors using molecular hybridization based on crystallographic overlays. Bioorganic and Medicinal Chemistry, 2017, 25, 4397-4406.	1.4	23
58	In situ click chemistry-based rapid discovery of novel HIV-1 NNRTIs by exploiting the hydrophobic channel and tolerant regions of NNIBP. European Journal of Medicinal Chemistry, 2020, 193, 112237.	2.6	23
59	An insight on medicinal aspects of novel HIV-1 capsid protein inhibitors. European Journal of Medicinal Chemistry, 2021, 217, 113380.	2.6	23
60	Novel fused pyrimidine and isoquinoline derivatives as potent HIV-1 NNRTIs: a patent evaluation of WO2016105532A1, WO2016105534A1 and WO2016105564A1. Expert Opinion on Therapeutic Patents, 2017, 27, 383-391.	2.4	22
61	Efficient drug discovery by rational lead hybridization based on crystallographic overlay. Drug Discovery Today, 2019, 24, 805-813.	3.2	22
62	Multivalent Agents: A Novel Concept and Preliminary Practice in Anti-HIV Drug Discovery. Current Medicinal Chemistry, 2013, 20, 815-832.	1.2	21
63	Design, synthesis and evaluation of novel HIV-1 NNRTIs with dual structural conformations targeting the entrance channel of the NNRTI binding pocket. European Journal of Medicinal Chemistry, 2016, 115, 53-62.	2.6	21
64	Novel diarylpyrimidines and diaryltriazines as potent HIV-1 NNRTIs with dramatically improved solubility: a patent evaluation of US20140378443A1. Expert Opinion on Therapeutic Patents, 2016, 26, 281-289.	2.4	21
65	Discovery of novel 1,2,3-triazole oseltamivir derivatives as potent influenza neuraminidase inhibitors targeting the 430-cavity. European Journal of Medicinal Chemistry, 2020, 187, 111940.	2.6	21
66	Recent Advances in the Research of HIV-1 RNase H Inhibitors. Mini-Reviews in Medicinal Chemistry, 2008, 8, 1243-1251.	1.1	19
67	Arylazolyl(azinyl)thioacetanilides. Part 10: Design, synthesis and biological evaluation of novel substituted imidazopyridinylthioacetanilides as potent HIV-1 inhibitors. Bioorganic and Medicinal Chemistry, 2012, 20, 5527-5536.	1.4	17
68	Targeting the entry step of SARS-CoV-2: a promising therapeutic approach. Signal Transduction and Targeted Therapy, 2020, 5, 98.	7.1	17
69	1-Hydroxypyrido[2,3-d]pyrimidin-2(1H)-ones as novel selective HIV integrase inhibitors obtained via privileged substructure-based compound libraries. Bioorganic and Medicinal Chemistry, 2017, 25, 5779-5789.	1.4	16
70	Design, synthesis, and antiviral evaluation of novel hydrazone-substituted thiophene[3,2-d]pyrimidine derivatives as potent human immunodeficiency virus-1 inhibitors. Chemical Biology and Drug Design, 2018, 92, 2009-2021.	1.5	16
71	Discovery of novel indolylarylsulfones as potent HIV-1 NNRTIs via structure-guided scaffold morphing. European Journal of Medicinal Chemistry, 2019, 182, 111619.	2.6	16
72	Design, synthesis, and biological evaluation of piperidinylâ€substituted [1,2,4]triazolo[1,5â€a]pyrimidine derivatives as potential antiâ€HIVâ€1 agents with reduced cytotoxicity. Chemical Biology and Drug Design, 2021, 97, 67-76.	1.5	16

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73	Boronic acid-containing diarylpyrimidine derivatives as novel HIV-1 NNRTIs: Design, synthesis and biological evaluation. Chinese Chemical Letters, 2021, 32, 4053-4057.	4.8	16
74	Design, synthesis, and evaluation of â€œdual-siteâ€•binding diarylpyrimidines targeting both NNIBP and the NNRTI adjacent site of the HIV-1 reverse transcriptase. European Journal of Medicinal Chemistry, 2021, 211, 113063.	2.6	15
75	Exploiting the tolerant region I of the non-nucleoside reverse transcriptase inhibitor (NNRTI) binding pocket. Part 2: Discovery of diarylpyrimidine derivatives as potent HIV-1 NNRTIs with high Fsp3 values and favorable drug-like properties. European Journal of Medicinal Chemistry, 2021, 213, 113051.	2.6	15
76	Design, synthesis, and mechanism study of dimerized phenylalanine derivatives as novel HIV-1 capsid inhibitors. European Journal of Medicinal Chemistry, 2021, 226, 113848.	2.6	15
77	Newly Emerging Strategies in Antiviral Drug Discovery: Dedicated to Prof. Dr. Erik De Clercq on Occasion of His 80th Anniversary. Molecules, 2022, 27, 850.	1.7	15
78	Design, synthesis, and biologic evaluation of novel galloyl derivatives as <scp>HIV</scp>â€1 <scp>RN</scp>ase H inhibitors. Chemical Biology and Drug Design, 2019, 93, 582-589.	1.5	14
79	Medicinal chemistry strategies of targeting HIV-1 capsid protein for antiviral treatment. Future Medicinal Chemistry, 2020, 12, 1281-1284.	1.1	14
80	Discovery of Novel Dihydrothiopyrano[4,3-d]pyrimidine Derivatives as Potent HIV-1 NNRTIs with Significantly Reduced hERG Inhibitory Activity and Improved Resistance Profiles. Journal of Medicinal Chemistry, 2021, 64, 13658-13675.	2.9	14
81	First discovery of a potential carbonate prodrug of NNRTI drug candidate RDEA427 with submicromolar inhibitory activity against HIV-1 K103N/Y181C double mutant strain. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 1348-1351.	1.0	13
82	Discovery of potent <scp>HIV</scp>â€1 nonâ€nucleoside reverse transcriptase inhibitors by exploring the structureâ€“activity relationship of solventâ€exposed regions I. Chemical Biology and Drug Design, 2019, 93, 430-437.	1.5	13
83	Discovery of highly potent and selective influenza virus neuraminidase inhibitors targeting 150-cavity. European Journal of Medicinal Chemistry, 2021, 212, 113097.	2.6	13
84	Arylazolyl(azinyl)thioacetanilides. Part 20: Discovery of novel purinylthioacetanilides derivatives as potent HIV-1 NNRTIs via a structure-based bioisosterism approach. Bioorganic and Medicinal Chemistry, 2016, 24, 4424-4433.	1.4	12
85	Design, synthesis and biological evaluation of 3-hydroxyquinazoline-2,4(1H,3H)-diones as dual inhibitors of HIV-1 reverse transcriptase-associated RNase H and integrase. Bioorganic and Medicinal Chemistry, 2019, 27, 3836-3845.	1.4	12
86	Discovery of novel anti-influenza agents via contemporary medicinal chemistry strategies (2014â€“2018) Tj ETQq0 0 0 rgBT /Overlock 1	1.1	12
87	Structureâ€“Activity Relationship Exploration of NNIBP Tolerant Region I Leads to Potent HIV-1 NNRTIs. ACS Infectious Diseases, 2020, 6, 2225-2234.	1.8	12
88	Identification of C5-NH₂ Modified Oseltamivir Derivatives as Novel Influenza Neuraminidase Inhibitors with Highly Improved Antiviral Activities and Favorable Druggability. Journal of Medicinal Chemistry, 2021, 64, 17992-18009.	2.9	12
89	Discovery of Novel Bicyclic Imidazolopyridine-Containing Human Urate Transporter 1 Inhibitors as Hypouricemic Drug Candidates with Improved Efficacy and Favorable Druggability. Journal of Medicinal Chemistry, 2022, 65, 4218-4237.	2.9	12
90	Arylazolyl(azinyl)thioacetanilides. Part 16: Structure-based bioisosterism design, synthesis and biological evaluation of novel pyrimidinylthioacetanilides as potent HIV-1 inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 5290-5297.	1.4	11

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91	The development of an effective synthetic route of lesinurad (RDEA594). Chemistry Central Journal, 2017, 11, 86.	2.6	11
92	Design, synthesis, and mechanistic investigations of phenylalanine derivatives containing a benzothiazole moiety as HIV-1 capsid inhibitors with improved metabolic stability. European Journal of Medicinal Chemistry, 2022, 227, 113903.	2.6	11
93	Targeting dual tolerant regions of binding pocket: Discovery of novel morpholine-substituted diarylpyrimidines as potent HIV-1 NNRTIs with significantly improved water solubility. European Journal of Medicinal Chemistry, 2020, 206, 112811.	2.6	10
94	Structure-Based Design and Discovery of Pyridyl-Bearing Fused Bicyclic HIV-1 Inhibitors: Synthesis, Biological Characterization, and Molecular Modeling Studies. Journal of Medicinal Chemistry, 2021, 64, 13604-13621.	2.9	10
95	Development of Novel Dihydrofuro[3,4-d]pyrimidine Derivatives as HIV-1 NNRTIs to Overcome the Highly Resistant Mutant Strains F227L/V106A and K103N/Y181C. Journal of Medicinal Chemistry, 2022, 65, 2458-2470.	2.9	10
96	Novel diaryltriazines with a picolinonitrile moiety as potent HIV-1 RT inhibitors: a patent evaluation of WO2016059647(A2). Expert Opinion on Therapeutic Patents, 2017, 27, 9-15.	2.4	9
97	Discovery, optimization, and target identification of novel coumarin derivatives as HIV-1 reverse transcriptase-associated ribonuclease H inhibitors. European Journal of Medicinal Chemistry, 2021, 225, 113769.	2.6	9
98	Novel RNase H Inhibitors Blocking RNA-directed Strand Displacement DNA Synthesis by HIV-1 Reverse Transcriptase. Journal of Molecular Biology, 2022, 434, 167507.	2.0	9
99	HIV-1 capsid inhibitors: a sword to destroy the virus. Future Medicinal Chemistry, 2022, 14, 605-607.	1.1	8
100	Identification of novel potent HIV-1 inhibitors by exploiting the tolerant regions of the NNRTIs binding pocket. European Journal of Medicinal Chemistry, 2021, 214, 113204.	2.6	6
101	SARS-CoV-2 Entry Inhibitors Targeting Virus-ACE2 or Virus-TMPRSS2 Interactions. Current Medicinal Chemistry, 2022, 29, 682-699.	1.2	5
102	Design, synthesis, and antiviral activity of phenylalanine derivatives as HIV-1 capsid inhibitors. Bioorganic and Medicinal Chemistry, 2021, 48, 116414.	1.4	4
103	Design, synthesis, and biological evaluation of novel double-winged galloyl derivatives as HIV-1 RNase H inhibitors. European Journal of Medicinal Chemistry, 2022, 240, 114563.	2.6	4
104	An improved synthesis approach of the HIV-1 inhibitor RDEA427, a pyrrolo[2,3-d]pyrimidine derivative. Arkivoc, 2017, 2016, 45-51.	0.3	3
105	Discovery of potential dual-target prodrugs of HIV-1 reverse transcriptase and nucleocapsid protein 7. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127287.	1.0	3
106	Discovery of Bioactive Molecules via Miniaturized Parallel Modular Reactions and Rapid Screening (2016-2021 update). Mini-Reviews in Organic Chemistry, 2021, 18, .	0.6	0