Xinyong Liu

List of Publications by Year in Descending Order

98 papers	2,753 citations	28 h-index	48 g-index
106 ext. papers	3,536 ext. citations	6.9 avg, IF	5.42 L-index

#	Paper	IF	Citations
98	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	6.8	1
97	Contemporary Medicinal Chemistry Strategies for the Discovery and Development of Novel HIV-1 Non-nucleoside Reverse Transcriptase Inhibitors.. *Journal of Medicinal Chemistry*, **2022**,	8.3	6
96	Novel RNase H inhibitors blocking RNA-directed strand displacement DNA synthesis by HIV-1 reverse transcriptase.. *Journal of Molecular Biology*, **2022**, 167507	6.5	0
95	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	6.8	2
94	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	8.3	11
93	SARS-CoV-2 Entry inhibitors targeting virus-ACE2 or virus-TMPRSS2 interactions. *Current Medicinal Chemistry*, **2021**,	4.3	1
92	An insight on medicinal aspects of novel HIV-1 capsid protein inhibitors. *European Journal of Medicinal Chemistry*, **2021**, 217, 113380	6.8	6
91	Design, synthesis, and biological evaluation of piperidinyl-substituted [1,2,4]triazolo[1,5-a]pyrimidine derivatives as potential anti-HIV-1 agents with reduced cytotoxicity. *Chemical Biology and Drug Design*, **2021**, 97, 67-76	2.9	5
90	Design, synthesis, and evaluation of "dual-site"-binding diarylpyrimidines targeting both NNIBP and the NNRTI adjacent site of the HIV-1 reverse transcriptase. *European Journal of Medicinal Chemistry*, **2021**, 211, 113063	6.8	5
89	Discovery of highly potent and selective influenza virus neuraminidase inhibitors targeting 150-cavity. *European Journal of Medicinal Chemistry*, **2021**, 212, 113097	6.8	3
88	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 Fsp values and favorable drug-like properties. *European Journal of Medicinal Chemistry*, **2021**, 213, 113051	6.8	4
87	Recent developments in the medicinal chemistry of single boron atom-containing compounds. *Acta Pharmaceutica Sinica B*, **2021**, 11, 3035-3059	15.5	28
86	Medicinal chemistry strategies for discovering antivirals effective against drug-resistant viruses. *Chemical Society Reviews*, **2021**, 50, 4514-4540	58.5	30
85	Boronic acid-containing diarylpyrimidine derivatives as novel HIV-1 NNRTIs: Design, synthesis and biological evaluation. *Chinese Chemical Letters*, **2021**,	8.1	4
84	Discovery of Novel Dihydrothiopyrano[4,3-]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	8.3	2
83	Medicinal chemistry strategies towards the development of effective SARS-CoV-2 inhibitors. *Acta Pharmaceutica Sinica B*, **2021**,	15.5	5
82	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	8.3	1

81	Design, synthesis, and antiviral activity of phenylalanine derivatives as HIV-1 capsid inhibitors. *Bioorganic and Medicinal Chemistry*, **2021**, 48, 116414	3.4	0
80	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	6.8	3
79	Design, synthesis, and mechanism study of dimerized phenylalanine derivatives as novel HIV-1 capsid inhibitors. *European Journal of Medicinal Chemistry*, **2021**, 226, 113848	6.8	4
78	Discovery of potential dual-target prodrugs of HIV-1 reverse transcriptase and nucleocapsid protein 7. *Bioorganic and Medicinal Chemistry Letters*, **2020**, 30, 127287	2.9	
77	Inhibitors of SARS-CoV-2 Entry: Current and Future Opportunities. *Journal of Medicinal Chemistry*, **2020**, 63, 12256-12274	8.3	111
76	Targeting the entry step of SARS-CoV-2: a promising therapeutic approach. *Signal Transduction and Targeted Therapy*, **2020**, 5, 98	21	13
75	New techniques and strategies in drug discovery. *Chinese Chemical Letters*, **2020**, 31, 1695-1708	8.1	45
74	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	6.8	11
73	Structure-Activity Relationship Exploration of NNIBP Tolerant Region I Leads to Potent HIV-1 NNRTIs. *ACS Infectious Diseases*, **2020**, 6, 2225-2234	5.5	8
72	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	6.8	37
71	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	8.3	20
70	Structure-Based Bioisosterism Yields HIV-1 NNRTIs with Improved Drug-Resistance Profiles and Favorable Pharmacokinetic Properties. *Journal of Medicinal Chemistry*, **2020**, 63, 4837-4848	8.3	20
69	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	6.8	12
68	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	6.8	3
67	Fsp: A new parameter for drug-likeness. *Drug Discovery Today*, **2020**, 25, 1839-1845	8.8	52
66	Novel Human Urate Transporter 1 Inhibitors as Hypouricemic Drug Candidates with Favorable Druggability. *Journal of Medicinal Chemistry*, **2020**, 63, 10829-10854	8.3	8
65	Exploring the hydrophobic channel of NNIBP leads to the discovery of novel piperidine-substituted thiophene[3,2-]pyrimidine derivatives as potent HIV-1 NNRTIs. *Acta Pharmaceutica Sinica B*, **2020**, 10, 878-894	15.5	26
64	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	8.3	18

63	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	8.3	47
62	Design, synthesis and biological evaluation of "Multi-Site"-binding influenza virus neuraminidase inhibitors. *European Journal of Medicinal Chemistry*, **2019**, 178, 64-80	6.8	18
61	Molecular design opportunities presented by solvent-exposed regions of target proteins. *Medicinal Research Reviews*, **2019**, 39, 2194-2238	14.4	16
60	Overview of Recent Strategic Advances in Medicinal Chemistry. *Journal of Medicinal Chemistry*, **2019**, 62, 9375-9414	8.3	53
59	Discovery of novel anti-influenza agents via contemporary medicinal chemistry strategies (2014-2018 update). *Future Medicinal Chemistry*, **2019**, 11, 375-378	4.1	5
58	Discovery of novel indolylarylsulfones as potent HIV-1 NNRTIs via structure-guided scaffold morphing. *European Journal of Medicinal Chemistry*, **2019**, 182, 111619	6.8	7
57	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	3.4	7
56	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,	6.3	15
55	Novel urate transporter 1 (URAT1) inhibitors: a review of recent patent literature (2016-2019). *Expert Opinion on Therapeutic Patents*, **2019**, 29, 871-879	6.8	20
54	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	3.9	28
53	Discovery of novel 1,4-disubstituted 1,2,3-triazole phenylalanine derivatives as HIV-1 capsid inhibitors. *RSC Advances*, **2019**, 9, 28961-28986	3.7	24
52	Design, synthesis, and biologic evaluation of novel galloyl derivatives as HIV-1 RNase H inhibitors. *Chemical Biology and Drug Design*, **2019**, 93, 582-589	2.9	8
51	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	3.4	12
50	Contemporary medicinal-chemistry strategies for the discovery of selective butyrylcholinesterase inhibitors. *Drug Discovery Today*, **2019**, 24, 629-635	8.8	24
49	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	8.3	41
48	Discovery of potent HIV-1 non-nucleoside reverse transcriptase inhibitors by exploring the structure-activity relationship of solvent-exposed regions I. *Chemical Biology and Drug Design*, **2019**, 93, 430-437	2.9	8
47	Efficient drug discovery by rational lead hybridization based on crystallographic overlay. *Drug Discovery Today*, **2019**, 24, 805-813	8.8	15
46	The Journey of HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors (NNRTIs) from Lab to Clinic. *Journal of Medicinal Chemistry*, **2019**, 62, 4851-4883	8.3	74

45	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	2.9	8
44	Discovery of Novel Diarylpyrimidine Derivatives as Potent HIV-1 NNRTIs Targeting the "NNRTI Adjacent" Binding Site. *ACS Medicinal Chemistry Letters*, **2018**, 9, 334-338	4.3	25
43	Further Exploring Solvent-Exposed Tolerant Regions of Allosteric Binding Pocket for Novel HIV-1 NNRTIs Discovery. *ACS Medicinal Chemistry Letters*, **2018**, 9, 370-375	4.3	21
42	Discovery of C-1 modified oseltamivir derivatives as potent influenza neuraminidase inhibitors. *European Journal of Medicinal Chemistry*, **2018**, 146, 220-231	6.8	21
41	Discovery of novel diarylpyrimidines as potent HIV-1 NNRTIs by investigating the chemical space of a less explored "hydrophobic channel". *Organic and Biomolecular Chemistry*, **2018**, 16, 1014-1028	3.9	18
40	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	6.8	44
39	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	2.9	8
38	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	6.8	21
37	Update on Recent Developments in Small Molecular HIV-1 RNase H Inhibitors (2013-2016): Opportunities and Challenges. *Current Medicinal Chemistry*, **2018**, 25, 1682-1702	4.3	30
36	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	8.3	24
35	Structural basis for potent and broad inhibition of HIV-1 RT by thiophene[3,2-]pyrimidine non-nucleoside inhibitors. *ELife*, **2018**, 7,	8.9	41
34	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	6.8	36
33	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	8.3	32
32	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	6.8	17
31	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	6.8	16
30	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	8.3	65
29	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	3.4	16
28	Discovery of Thiophene[3,2-]pyrimidine Derivatives as Potent HIV-1 NNRTIs Targeting the Tolerant Region I of NNIBP. *ACS Medicinal Chemistry Letters*, **2017**, 8, 1188-1193	4.3	21

27	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	3.4	12
26	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	6.8	5
25	The development of an effective synthetic route of lesinurad (RDEA594). *Chemistry Central Journal*, **2017**, 11, 86		8
24	An improved synthesis approach of the HIV-1 inhibitor RDEA427, a pyrrolo[2,3-d]pyrimidine derivative. *Arkivoc*, **2017**, 2016, 45-51	0.9	3
23	Discovery of bioactive molecules from CuAAC click-chemistry-based combinatorial libraries. *Drug Discovery Today*, **2016**, 21, 118-132	8.8	101
22	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	8.3	84
21	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, 857-71	6.2	26
20	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	6.8	16
19	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, 281-9	6.8	19
18	Anti-HIV Drug Discovery and Development: Current Innovations and Future Trends. *Journal of Medicinal Chemistry*, **2016**, 59, 2849-78	8.3	199
17	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	6.8	20
16	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	3.4	7
15	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, 330-7	6.8	37
14	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, 754-65	6.8	69
13	"Old Dogs with New Tricks": exploiting alternative mechanisms of action and new drug design strategies for clinically validated HIV targets. *Molecular BioSystems*, **2014**, 10, 1998-2022		24
12	Discovery of N-substituted oseltamivir derivatives as potent and selective inhibitors of H5N1 influenza neuraminidase. *Journal of Medicinal Chemistry*, **2014**, 57, 8445-58	8.3	50
11	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, 5290-7	3.4	9
10	Conformational restriction: an effective tactic in 'follow-on'-based drug discovery. *Future Medicinal Chemistry*, **2014**, 6, 885-901	4.1	104

9	Recent progress in the research of small molecule HIV-1 RNase H inhibitors. *Current Medicinal Chemistry*, **2014**, 21, 1956-67	4.3	30
8	HIV-1 NNRTIs: structural diversity, pharmacophore similarity, and implications for drug design. *Medicinal Research Reviews*, **2013**, 33 Suppl 1, E1-72	14.4	147
7	Multivalent Agents: A Novel Concept and Preliminary Practice in Anti-HIV Drug Discovery. *Current Medicinal Chemistry*, **2013**, 20, 815-832	4.3	20
6	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, 5527-36	3.4	12
5	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, 3595-613	8.3	107
4	Recent advances in DAPYs and related analogues as HIV-1 NNRTIs. *Current Medicinal Chemistry*, **2011**, 18, 359-76	4.3	86
3	Design strategies of novel NNRTIs to overcome drug resistance. *Current Medicinal Chemistry*, **2009**, 16, 3903-17	4.3	83
2	Designed multiple ligands: an emerging anti-HIV drug discovery paradigm. *Current Pharmaceutical Design*, **2009**, 15, 1893-917	3.3	57
1	Recent advances in the research of HIV-1 RNase H inhibitors. *Mini-Reviews in Medicinal Chemistry*, **2008**, 8, 1243-51	3.2	16