Edward Arnold

List of Publications by Year
in descending order

78 papers	4,432 citations	136950 32 h-index	106344 65 g-index
86 all docs	86 docs citations	86 times ranked	4361 citing authors

#	Article	IF	Citations
1	Structure and Function of HIV-1 Reverse Transcriptase: Molecular Mechanisms of Polymerization and Inhibition. Journal of Molecular Biology, 2009, 385, 693-713.	4.2	426
2	Structure and functional implications of the polymerase active site region in a complex of HIV-1 RT with a double-stranded DNA template-primer and an antibody fab fragment at 2.8 Å... resolution. Journal of Molecular Biology, 1998, 284, 1095-1111.	4.2	317
3	High-resolution structures of HIV-1 reverse transcriptase/TMC278 complexes: Strategic flexibility explains potency against resistance mutations. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 1466-1471.	7.1	310
4	Structures of influenza A proteins and insights into antiviral drug targets. Nature Structural and Molecular Biology, 2010, 17, 530-538.	8.2	292
5	HIV-1 reverse transcriptase complex with DNA and nevirapine reveals non-nucleoside inhibition mechanism. Nature Structural and Molecular Biology, 2012, 19, 253-259.	8.2	176
6	Structures of HIV-1 RTâ€“DNA complexes before and after incorporation of the anti-AIDS drug tenofovir. Nature Structural and Molecular Biology, 2004, 11, 469-474.	8.2	157
7	Structure of HIV-1 Reverse Transcriptase with the Inhibitor Î²-Thujaplicinol Bound at the RNase H Active Site. Structure, 2009, 17, 1625-1635.	3.3	135
8	HIV-1 Reverse Transcriptase Structure with RNase H Inhibitor Dihydroxy Benzoyl Naphthyl Hydrazone Bound at a Novel Site. ACS Chemical Biology, 2006, 1, 702-712.	3.4	132
9	Taking aim at a moving target: designing drugs to inhibit drug-resistant HIV-1 reverse transcriptases. Current Opinion in Structural Biology, 2004, 14, 716-730.	5.7	130
10	Structural Basis of Mycobacterium tuberculosis Transcription and Transcription Inhibition. Molecular Cell, 2017, 66, 169-179.e8.	9.7	130
11	Review of HIV-1 reverse transcriptase three-dimensional structure: Implications for drug design. Journal of Computer - Aided Molecular Design, 1993, 1, 129-150.	1.0	127
12	HIV-1 reverse transcriptase and antiviral drug resistance. Part 1. Current Opinion in Virology, 2013, 3, 111-118.	5.4	126
13	Structural basis of HIV-1 resistance to AZT by excision. Nature Structural and Molecular Biology, 2010, 17, 1202-1209.	8.2	115
14	Touching the heart of HIV-1 drug resistance: the fingers close down on the dNTP at the polymerase active site. Chemistry and Biology, 1999, 6, R137-R146.	6.0	107
15	Crystal engineering of HIV-1 reverse transcriptase for structure-based drug design. Nucleic Acids Research, 2008, 36, 5083-5092.	14.5	91
16	Snapshot of the equilibrium dynamics of a drug bound to HIV-1 reverse transcriptase. Nature Chemistry, 2013, 5, 174-181.	13.6	88
17	HIV-1 reverse transcriptase and antiviral drug resistance. Part 2. Current Opinion in Virology, 2013, 3, 119-128.	5.4	83
18	Trapping HIV-1 Reverse Transcriptase Before and After Translocation on DNA. Journal of Biological Chemistry, 2003, 278, 16280-16288.	3.4	79

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19	Detecting Allosteric Sites of HIV-1 Reverse Transcriptase by X-ray Crystallographic Fragment Screening. Journal of Medicinal Chemistry, 2013, 56, 2738-2746.	6.4	78
20	Crystallographic Fragment Screening and Structure-Based Optimization Yields a New Class of Influenza Endonuclease Inhibitors. ACS Chemical Biology, 2013, 8, 2501-2508.	3.4	76
21	Advantages of crystallographic fragment screening: Functional and mechanistic insights from a powerful platform for efficient drug discovery. Progress in Biophysics and Molecular Biology, 2014, 116, 92-100.	2.9	73
22	Transcription inhibition by the depsipeptide antibiotic salinamide A. ELife, 2014, 3, e02451.	6.0	71
23	Molecular modeling studies of HIVâ€1 reverse transcriptase nonnucleoside inhibitors: Total energy of complexation as a predictor of drug placement and activity. Protein Science, 1995, 4, 2203-2222.	7.6	66
24	Structures of HIV-1 RT-RNA/DNA ternary complexes with dATP and nevirapine reveal conformational flexibility of RNA/DNA: insights into requirements for RNase H cleavage. Nucleic Acids Research, 2014, 42, 8125-8137.	14.5	60
25	Phenyl Substituted 4-Hydroxypyridazin-3(2H)-ones and 5-Hydroxypyrimidin-4(3H)-ones: Inhibitors of Influenza A Endonuclease. Journal of Medicinal Chemistry, 2014, 57, 8086-8098.	6.4	50
26	Mutations in HIV-1 Reverse Transcriptase Affect the Errors Made in a Single Cycle of Viral Replication. Journal of Virology, 2014, 88, 7589-7601.	3.4	46
27	Linear Interaction Energy (LIE) Models for Ligand Binding in Implicit Solvent:â€‰ Theory and Application to the Binding of NNRTIs to HIV-1 Reverse Transcriptase. Journal of Chemical Theory and Computation, 2007, 3, 256-277.	5.3	45
28	3-Hydroxyquinolin-2(1H)-ones As Inhibitors of Influenza A Endonuclease. ACS Medicinal Chemistry Letters, 2013, 4, 547-550.	2.8	44
29	Evolving understanding of HIV-1 reverse transcriptase structure, function, inhibition, and resistance. Current Opinion in Structural Biology, 2020, 61, 113-123.	5.7	43
30	Conformational States of HIV-1 Reverse Transcriptase for Nucleotide Incorporation vs Pyrophosphorolysisâ€”Binding of Foscarnet. ACS Chemical Biology, 2016, 11, 2158-2164.	3.4	38
31	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.	6.4	37
32	Structure of a Dihydroxycoumarin Active-Site Inhibitor in Complex with the RNase H Domain of HIV-1 Reverse Transcriptase and Structureâ€“Activity Analysis of Inhibitor Analogs. Journal of Molecular Biology, 2014, 426, 2617-2631.	4.2	36
33	Structure of <scp>HIV</scp>â€1 reverse transcriptase bound to a novel 38â€mer hairpin templateâ€primer <scp>DNA</scp> aptamer. Protein Science, 2016, 25, 46-55.	7.6	33
34	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.	6.4	33
35	Effects of the Î”67 Complex of Mutations in Human Immunodeficiency Virus Type 1 Reverse Transcriptase on Nucleoside Analog Excision. Journal of Virology, 2004, 78, 9987-9997.	3.4	31
36	Evolution of the <scp>SARSâ€CoV</scp>â€2 proteome in three dimensions (3D) during the first 6 months of the <scp>COVID</scp>â€19 pandemic. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1054-1080.	2.6	31

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37	Molecular dynamics of HIV-1 reverse transcriptase indicates increased flexibility upon DNA binding. Proteins: Structure, Function and Bioinformatics, 2001, 45, 176-182.	2.6	30
38	Phenyl substituted 3-hydroxypyridin-2(1H)-ones: Inhibitors of influenza A endonuclease. Bioorganic and Medicinal Chemistry, 2013, 21, 6435-6446.	3.0	30
39	Developing and Evaluating Inhibitors against the RNase H Active Site of HIV-1 Reverse Transcriptase. Journal of Virology, 2018, 92, .	3.4	30
40	Alpha-carboxy nucleoside phosphonates as universal nucleoside triphosphate mimics. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3475-3480.	7.1	29
41	Drug Resistance in Non-B Subtype HIV-1: Impact of HIV-1 Reverse Transcriptase Inhibitors. Viruses, 2014, 6, 3535-3562.	3.3	27
42	Rapid experimental SAD phasing and hot-spot identification with halogenated fragments. IUCrJ, 2016, 3, 51-60.	2.2	27
43	Structure of HIV-1 RT/dsRNA initiation complex prior to nucleotide incorporation. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7308-7313.	7.1	26
44	Epistasis and entrenchment of drug resistance in HIV-1 subtype B. ELife, 2019, 8, .	6.0	25
45	Buried surface analysis of HIV-1 reverse transcriptase p66/p51 heterodimer and its interaction with dsDNA template/primer. Journal of Molecular Recognition, 1994, 7, 157-161.	2.1	24
46	Binding interface and impact on protease cleavage for an RNA aptamer to HIV-1 reverse transcriptase. Nucleic Acids Research, 2020, 48, 2709-2722.	14.5	22
47	A New Class of Allosteric HIV-1 Integrase Inhibitors Identified by Crystallographic Fragment Screening of the Catalytic Core Domain. Journal of Biological Chemistry, 2016, 291, 23569-23577.	3.4	20
48	Structural Basis of HIV-1 Inhibition by Nucleotide-Competing Reverse Transcriptase Inhibitor INDOPY-1. Journal of Medicinal Chemistry, 2019, 62, 9996-10002.	6.4	20
49	Negative-Strand RNA Virus L Proteins: One Machine, Many Activities. Cell, 2015, 162, 239-241.	28.9	17
50	Exploring the role of the Î±-carboxyphosphonate moiety in the HIV-RT activity of Î±-carboxy nucleoside phosphonates. Organic and Biomolecular Chemistry, 2016, 14, 2454-2465.	2.8	17
51	Structural Insights into HIV Reverse Transcriptase Mutations Q151M and Q151M Complex That Confer Multinucleoside Drug Resistance. Antimicrobial Agents and Chemotherapy, 2017, 61, .	3.2	16
52	Human endogenous retrovirus-K (HERV-K) reverse transcriptase (RT) structure and biochemistry reveals remarkable similarities to HIV-1 RT and opportunities for HERV-Kâ€“specific inhibition. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	16
53	Non-Nucleoside Reverse Transcriptase Inhibitors Join Forces with Integrase Inhibitors to Combat HIV. Pharmaceuticals, 2020, 13, 122.	3.8	13
54	Revealing the Structural Plasticity of SARS-CoV-2 nsp7 and nsp8 Using Structural Proteomics. Journal of the American Society for Mass Spectrometry, 2021, 32, 1618-1630.	2.8	13

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55	Structure of HIVâ€1 reverse transcriptase/d4TTP complex: Novel DNA crossâ€linking site and pHâ€dependent conformational changes. Protein Science, 2019, 28, 587-597.	7.6	11
56	Pronounced Inhibition Shift from HIV Reverse Transcriptase to Herpetic DNA Polymerases by Increasing the Flexibility of Î±-Carboxy Nucleoside Phosphonates. Journal of Medicinal Chemistry, 2015, 58, 8110-8127.	6.4	9
57	Guanine Î±-carboxy nucleoside phosphonate (G-Î±-CNP) shows a different inhibitory kinetic profile against the DNA polymerases of human immunodeficiency virus (HIV) and herpes viruses. Biochemical Pharmacology, 2017, 136, 51-61.	4.4	9
58	Analysis of the Zidovudine Resistance Mutations T215Y, M41L, and L210W in HIV-1 Reverse Transcriptase. Antimicrobial Agents and Chemotherapy, 2015, 59, 7184-7196.	3.2	8
59	Integrative structural biology studies of HIV-1 reverse transcriptase binding to a high-affinity DNA aptamer. Current Research in Structural Biology, 2020, 2, 116-129.	2.2	8
60	Identification of a pharmacophore for nucleoside analog inhibitors directed at HIV-1 reverse transcriptase. Journal of Molecular Recognition, 1994, 7, 211-214.	2.1	7
61	Pivot residue: an analysis of domain motion in proteins. The Protein Journal, 1999, 18, 807-811.	1.1	6
62	Factors influencing the efficacy of rilpivirine in HIV-1 subtype C in low- and middle-income countries. Journal of Antimicrobial Chemotherapy, 2016, 71, 367-371.	3.0	6
63	Alpha-carboxynucleoside phosphonates: direct-acting inhibitors of viral DNA polymerases. Future Medicinal Chemistry, 2019, 11, 137-154.	2.3	6
64	X-ray crystal structure of MTH938 fromMethanobacterium thermoautotrophicumat 2.2 Ã... resolution reveals a novel tertiary protein fold. Proteins: Structure, Function and Bioinformatics, 2001, 45, 486-488.	2.6	5
65	Differential Isotopic Enrichment To Facilitate Characterization of Asymmetric Multimeric Proteins Using Hydrogen/Deuterium Exchange Mass Spectrometry. Analytical Chemistry, 2015, 87, 4015-4022.	6.5	4
66	Aryl and Arylalkyl Substituted 3â€Hydroxypyridinâ€2(1 H)â€ones: Synthesis and Evaluation as Inhibitors of Influenzaâ€…A Endonuclease. ChemMedChem, 2019, 14, 1204-1223.	3.2	4
67	Crystal Structure of a Retroviral Polyprotein: Prototype Foamy Virus Protease-Reverse Transcriptase (PR-RT). Viruses, 2021, 13, 1495.	3.3	4
68	HIV-1 gp120 Antagonists Also Inhibit HIV-1 Reverse Transcriptase by Bridging the NNRTI and NRTI Sites. Journal of Medicinal Chemistry, 2021, 64, 16530-16540.	6.4	4
69	Structural basis of HIV inhibition by L-nucleosides: Opportunities for drug development and repurposing. Drug Discovery Today, 2022, 27, 1832-1846.	6.4	4
70	Reply to: Is one solution good enough?. Nature Structural and Molecular Biology, 2006, 13, 185-185.	8.2	3
71	Fragment Screening for Drug Discovery: Efficient Approaches for Exploring Chemical Space. Progress in Biophysics and Molecular Biology, 2014, 116, 81.	2.9	3
72	Michael G. Rossmann (1930â€“2019). Nature Structural and Molecular Biology, 2019, 26, 660-662.	8.2	3

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73	Co-crystallization with diabodies: A case study for the introduction of synthetic symmetry. Structure, 2021, 29, 598-605.e3.	3.3	3
74	HIV-1 Reverse Transcriptase Mutations Found in a Drug-Experienced Patient Confer Reduced Susceptibility to Multiple Nucleoside Reverse Transcriptase Inhibitors. Antiviral Therapy, 2002, 6, 231-238.	1.0	1
75	Michael G. Rossmann (1930â€“2019), pioneer in macromolecular and virus crystallography: scientist, mentor and friend. Acta Crystallographica Section D: Structural Biology, 2019, 75, 523-527.	2.3	0
76	Structures of Wildâ€Type and AZTâ€Resistant HIVâ€1 Reverse Transcriptase Complexed with AZTppppA Yield Insights into the Nucleotide Excision Mechanism. FASEB Journal, 2007, 21, A640.	0.5	0
77	Spectroscopic Studies of Rilpivirine (TMC278/R278474) in Complex with HIVâ€1 Reverse Transcriptase. FASEB Journal, 2007, 21, A630.	0.5	0
78	Pingry School SMART Team Project: Modeling Current Strategies in HIVâ€1 Reverse Transcriptase Inhibitors. FASEB Journal, 2012, 26, lb240.	0.5	0