Irene T Weber

List of Publications by Year
in descending order

117 papers	5,123 citations	76196 40 h-index	102304 66 g-index
173 all docs	173 docs citations	173 times ranked	2681 citing authors

#	Article	IF	Citations
1	Novel bis-Tetrahydrofuranylurethane-Containing Nonpeptidic Protease Inhibitor (PI) UIC-94017 (TMC114) with Potent Activity against Multi-PI-Resistant Human Immunodeficiency Virus In Vitro. Antimicrobial Agents and Chemotherapy, 2003, 47, 3123-3129.	1.4	355
2	Design of HIV Protease Inhibitors Targeting Protein Backbone: An Effective Strategy for Combating Drug Resistance. Accounts of Chemical Research, 2008, 41, 78-86.	7.6	236
3	High Resolution Crystal Structures of HIV-1 Protease with a Potent Non-peptide Inhibitor (UIC-94017) Active Against Multi-drug-resistant Clinical Strains. Journal of Molecular Biology, 2004, 338, 341-352.	2.0	205
4	Structure-Based Design of Novel HIV-1 Protease Inhibitors To Combat Drug Resistance. Journal of Medicinal Chemistry, 2006, 49, 5252-5261.	2.9	144
5	Ultra-high Resolution Crystal Structure of HIV-1 Protease Mutant Reveals Two Binding Sites for Clinical Inhibitor TMC114. Journal of Molecular Biology, 2006, 363, 161-173.	2.0	136
6	Effectiveness of Nonpeptide Clinical Inhibitor TMC-114 on HIV-1 Protease with Highly Drug Resistant Mutations D30N, I50V, and L90M. Journal of Medicinal Chemistry, 2006, 49, 1379-1387.	2.9	132
7	Enhancing Protein Backbone Bindingâ€"A Fruitful Concept for Combating Drugâ€Resistant HIV. Angewandte Chemie - International Edition, 2012, 51, 1778-1802.	7.2	131
8	HIV-1 Protease: Structural Perspectives on Drug Resistance. Viruses, 2009, 1, 1110-1136.	1.5	128
9	Structural implications of drug-resistant mutants of HIV-1 protease: High-resolution crystal structures of the mutant protease/substrate analogue complexes. Proteins: Structure, Function and Bioinformatics, 2001, 43, 455-464.	1.5	125
10	Bis-Tetrahydrofuran: a Privileged Ligand for Darunavir and a New Generation of HIV Protease Inhibitors That Combat Drug Resistance. ChemMedChem, 2006, 1, 939-950.	1.6	116
11	Amprenavir complexes with HIVâ€1 protease and its drugâ€resistant mutants altering hydrophobic clusters. FEBS Journal, 2010, 277, 3699-3714.	2.2	116
12	Structural and kinetic analysis of drug resistant mutants of HIV-1 protease. FEBS Journal, 1999, 263, 238-244.	0.2	115
13	Kinetic and modeling studies of S3-S3' subsites of HIV proteinases. Biochemistry, 1992, 31, 4793-4800.	1.2	113
14	Comparative analysis of the sequences and structures of HIV-1 and HIV-2 proteases. Proteins: Structure, Function and Bioinformatics, 1991, 10, 325-339.	1.5	102
15	Atomic resolution crystal structures of HIV-1 protease and mutants V82A and I84V with saquinavir. Proteins: Structure, Function and Bioinformatics, 2007, 67, 232-242.	1.5	84
16	Effect of Flap Mutations on Structure of HIV-1 Protease and Inhibition by Saquinavir and Darunavir. Journal of Molecular Biology, 2008, 381, 102-115.	2.0	81
17	HIV-1 Protease with 20 Mutations Exhibits Extreme Resistance to Clinical Inhibitors through Coordinated Structural Rearrangements. Biochemistry, 2012, 51, 2819-2828.	1.2	78
18	Studies on the role of the S4substrate binding site of HIV proteinases. FEBS Letters, 1991, 279, 356-360.	1.3	71

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19	Crystal structures of HIV protease V82A and L90M mutants reveal changes in the indinavir-binding site. FEBS Journal, 2004, 271, 1516-1524.	0.2	71
20	Molecular basis for substrate recognition and drug resistance from 1.1 to 1.6 A resolution crystal structures of HIV-1 protease mutants with substrate analogs. FEBS Journal, 2005, 272, 5265-5277.	2.2	71
21	Comparison of inhibitor binding in HIV-1 protease and in non-viral aspartic proteases: the role of the flap. FEBS Letters, 1990, 269, 269-272.	1.3	70
22	Kinetic, Stability, and Structural Changes in High-resolution Crystal Structures of HIV-1 Protease with Drug-resistant Mutations L24I, I50V, and G73S. Journal of Molecular Biology, 2005, 354, 789-800.	2.0	68
23	A Novel Bis-Tetrahydrofuranylurethane-Containing Nonpeptidic Protease Inhibitor (PI), GRL-98065, Is Potent against Multiple-PI-Resistant Human Immunodeficiency Virus In Vitro. Antimicrobial Agents and Chemotherapy, 2007, 51, 2143-2155.	1.4	66
24	Effect of sequence polymorphism and drug resistance on two HIV-1 Gag processing sites. FEBS Journal, 2002, 269, 4114-4120.	0.2	64
25	Design and Development of Highly Potent HIV-1 Protease Inhibitors with a Crown-Like Oxotricyclic Core as the P2-Ligand To Combat Multidrug-Resistant HIV Variants. Journal of Medicinal Chemistry, 2017, 60, 4267-4278.	2.9	64
26	Inhibition of autoprocessing of natural variants and multidrug resistant mutant precursors of HIV-1 protease by clinical inhibitors. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 9072-9077.	3.3	63
27	Joint X-ray/Neutron Crystallographic Study of HIV-1 Protease with Clinical Inhibitor Amprenavir: Insights for Drug Design. Journal of Medicinal Chemistry, 2013, 56, 5631-5635.	2.9	61
28	Comparison of the substrate specificity of the human T-cell leukemia virus and human immunodeficiency virus proteinases. FEBS Journal, 2000, 267, 6287-6295.	0.2	59
29	Highly resistant HIV-1 proteases and strategies for their inhibition. Future Medicinal Chemistry, 2015, 7, 1023-1038.	1.1	55
30	Machine learning methods accurately predict host specificity of coronaviruses based on spike sequences alone. Biochemical and Biophysical Research Communications, 2020, 533, 553-558.	1.0	52
31	Drug-Resistant HIV-1 Proteases Identify Enzyme Residues Important for Substrate Selection and Catalytic Rate. Biochemistry, 1998, 37, 13835-13845.	1.2	51
32	Human Immunodeficiency Virus, Type 1 Protease Substrate Specificity Is Limited by Interactions between Substrate Amino Acids Bound in Adjacent Enzyme Subsites. Journal of Biological Chemistry, 1996, 271, 4709-4717.	1.6	49
33	Mechanism of Drug Resistance Revealed by the Crystal Structure of the Unliganded HIV-1 Protease with F53L Mutation. Journal of Molecular Biology, 2006, 358, 1191-1199.	2.0	48
34	Probing Multidrugâ€Resistance and Proteinâ€“Ligand Interactions with Oxatricyclic Designed Ligands in HIVâ€1 Protease Inhibitors. ChemMedChem, 2010, 5, 1850-1854.	1.6	47
35	Narrow Substrate Specificity and Sensitivity toward Ligand-binding Site Mutations of Human T-cell Leukemia Virus Type 1 Protease. Journal of Biological Chemistry, 2004, 279, 27148-27157.	1.6	45
36	HIV Protease: Historical Perspective and Current Research. Viruses, 2021, 13, 839.	1.5	45

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37	Structural Evidence for Effectiveness of Darunavir and Two Related Antiviral Inhibitors against HIV-2 Protease. Journal of Molecular Biology, 2008, 384, 178-192.	2.0	44
38	Highly Potent HIV-1 Protease Inhibitors with Novel Tricyclic P2 Ligands: Design, Synthesis, and Proteinâ€“Ligand X-ray Studies. Journal of Medicinal Chemistry, 2013, 56, 6792-6802.	2.9	42
39	Longâ€Range Electrostaticsâ€Induced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. Angewandte Chemie - International Edition, 2016, 55, 4924-4927.	7.2	42
40	Molecular dynamics simulations of HIV-1 protease with peptide substrate. Protein Engineering, Design and Selection, 1994, 7, 1353-1363.	1.0	41
41	Structural Basis for Specificity of Retroviral Proteasesâ€. Biochemistry, 1998, 37, 4518-4526.	1.2	41
42	Studies on the substrate specificity of the proteinase of equine infectious anemia virus using oligopeptide substrates. Biochemistry, 1993, 32, 3347-3353.	1.2	40
43	Crystallographic Analysis of Human Immunodeficiency Virus 1 Protease with an Analog of the Conserved CA-p2 Substrate. Interactions with Frequently Occurring Glutamic Acid Residue at P2' Position of Substrates. FEBS Journal, 1997, 249, 523-530.	0.2	39
44	Structural Studies of a Rationally Selected Multi-Drug Resistant HIV-1 Protease Reveal Synergistic Effect of Distal Mutations on Flap Dynamics. PLoS ONE, 2016, 11, e0168616.	1.1	39
45	Analysis of comparative modeling predictions for CASP2 targets 1, 3, 9, and 17. Proteins: Structure, Function and Bioinformatics, 1997, 29, 68-73.	1.5	38
46	Critical differences in HIVâ€1 and HIVâ€2 protease specificity for clinical inhibitors. Protein Science, 2012, 21, 339-350.	3.1	38
47	Design of Highly Potent, Dualâ€Acting and Centralâ€Nervousâ€Systemâ€Penetrating HIVâ€1 Protease Inhibitors with Excellent Potency against Multidrugâ€Resistant HIVâ€1 Variants. ChemMedChem, 2018, 13, 803-815.	1.6	36
48	Extreme Multidrug Resistant HIV-1 Protease with 20 Mutations Is Resistant to Novel Protease Inhibitors with P1â€²-Pyrrolidinone or P2-Tris-tetrahydrofuran. Journal of Medicinal Chemistry, 2013, 56, 4017-4027.	2.9	34
49	Molecular dynamics simulations of 14 HIV protease mutants in complexes with indinavir. Journal of Molecular Modeling, 2004, 10, 373-381.	0.8	33
50	Structure of choline oxidase in complex with the reaction product glycine betaine. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 405-413.	2.5	32
51	Molecular mechanics analysis of drug-resistant mutants of HIV protease. Protein Engineering, Design and Selection, 1999, 12, 469-474.	1.0	31
52	Design of HIV-1 Protease Inhibitors with C3-Substituted Hexahydrocyclopentafuranyl Urethanes as P2-Ligands: Synthesis, Biological Evaluation, and Proteinâ€“Ligand X-ray Crystal Structure. Journal of Medicinal Chemistry, 2011, 54, 5890-5901.	2.9	31
53	Design and Synthesis of Highly Potent HIV-1 Protease Inhibitors Containing Tricyclic Fused Ring Systems as Novel P2 Ligands: Structureâ€“Activity Studies, Biological and X-ray Structural Analysis. Journal of Medicinal Chemistry, 2018, 61, 4561-4577.	2.9	31
54	Prediction of HIV drug resistance from genotype with encoded three-dimensional protein structure. BMC Genomics, 2014, 15, S1.	1.2	27

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55	In vitro heme biotransformation by the HupZ enzyme from Group A streptococcus. BioMetals, 2016, 29, 593-609.	1.8	27
56	Conformational Changes and Substrate Recognition in Pseudomonas aeruginosa <scp>d</scp>-Arginine Dehydrogenase[,]. Biochemistry, 2010, 49, 8535-8545.	1.2	26
57	Design, Synthesis, and X-ray Structure of Substituted Bis-tetrahydrofuran (Bis-THF)-Derived Potent HIV-1 Protease Inhibitors. ACS Medicinal Chemistry Letters, 2011, 2, 298-302.	1.3	26
58	Novel P2 Tris-tetrahydrofuran Group in Antiviral Compound 1 (GRL-0519) Fills the S2 Binding Pocket of Selected Mutants of HIV-1 Protease. Journal of Medicinal Chemistry, 2013, 56, 1074-1083.	2.9	26
59	Structure-based design, synthesis, X-ray studies, and biological evaluation of novel HIV-1 protease inhibitors containing isophthalamide-derived P2-ligands. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4903-4909.	1.0	26
60	Structural alignment of retroviral protease sequences. Gene, 1989, 85, 565-566.	1.0	25
61	Programming the Rous Sarcoma Virus Protease to Cleave New Substrate Sequences. Journal of Biological Chemistry, 1996, 271, 10538-10544.	1.6	25
62	The L76V Drug Resistance Mutation Decreases the Dimer Stability and Rate of Autoprocessing of HIV-1 Protease by Reducing Internal Hydrophobic Contacts. Biochemistry, 2011, 50, 4786-4795.	1.2	25
63	Room Temperature Neutron Crystallography of Drug Resistant HIV-1 Protease Uncovers Limitations of X-ray Structural Analysis at 100 K. Journal of Medicinal Chemistry, 2017, 60, 2018-2025.	2.9	25
64	Molecular mechanics calculations on rous sarcoma virus protease with peptide substrates. Protein Science, 1997, 6, 2365-2374.	3.1	24
65	Design and Synthesis of Potent HIV-1 Protease Inhibitors Containing Bicyclic Oxazolidinone Scaffold as the P2 Ligands: Structureâ€“Activity Studies and Biological and X-ray Structural Studies. Journal of Medicinal Chemistry, 2018, 61, 9722-9737.	2.9	24
66	Steady-State Kinetic Mechanism and Reductive Half-Reaction of <scp>d</scp>-Arginine Dehydrogenase from Pseudomonas aeruginosa. Biochemistry, 2010, 49, 9542-9550.	1.2	23
67	Sparse Representation for HIV-1 Protease Drug Resistance Prediction. , 2013, 2013, 342-349.		23
68	Caspase-3 binds diverse P4 residues in peptides as revealed by crystallography and structural modeling. Apoptosis: an International Journal on Programmed Cell Death, 2009, 14, 741-752.	2.2	22
69	Autocatalytic maturation, physical/chemical properties, and crystal structure of group N HIVâ€1 protease: Relevance to drug resistance. Protein Science, 2010, 19, 2055-2072.	3.1	22
70	Conformational variation of an extreme drug resistant mutant of HIV protease. Journal of Molecular Graphics and Modelling, 2015, 62, 87-96.	1.3	22
71	Automated prediction of HIV drug resistance from genotype data. BMC Bioinformatics, 2016, 17, 278.	1.2	22
72	Molecular model of equine infectious anemia virus proteinase and kinetic measurements for peptide substrates with single amino acid substitutions. Biochemistry, 1993, 32, 3354-3362.	1.2	21

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73	Mutational Analysis of the Substrate Binding Pocket of Murine Leukemia Virus Protease and Comparison with Human Immunodeficiency Virus Proteases. Journal of Biological Chemistry, 1995, 270, 29162-29168.	1.6	21
74	Structure-Based Design of Potent HIV-1 Protease Inhibitors with Modified P1-Biphenyl Ligands: Synthesis, Biological Evaluation, and Enzymeâ€"Inhibitor X-ray Structural Studies. Journal of Medicinal Chemistry, 2015, 58, 5334-5343.	2.9	21
75	Binding of Clinical Inhibitors to a Model Precursor of a Rationally Selected Multidrug Resistant HIV-1 Protease Is Significantly Weaker Than That to the Released Mature Enzyme. Biochemistry, 2016, 55, 2390-2400.	1.2	21
76	Characterization of the murine leukemia virus protease and its comparison with the human immunodeficiency virus type 1 protease. Journal of General Virology, 2006, 87, 1321-1330.	1.3	20
77	Design of gemâ€Difluoroâ€bisâ€Tetrahydrofuran as P2 Ligand for HIVâ€1â€...Protease Inhibitors to Improve Brain Penetration: Synthesis, Xâ€ray Studies, and Biological Evaluation. ChemMedChem, 2015, 10, 107-115.	1.6	20
78	Drug Resistance Mutation L76V Alters Nonpolar Interactions at the Flapâ€"Core Interface of HIV-1 Protease. ACS Omega, 2018, 3, 12132-12140.	1.6	19
79	Structure-Based Design of Highly Potent HIV-1 Protease Inhibitors Containing New Tricyclic Ring P2-Ligands: Design, Synthesis, Biological, and X-ray Structural Studies. Journal of Medicinal Chemistry, 2020, 63, 4867-4879.	2.9	19
80	Improved Parameters for Generating Partial Charges: Correlation with Observed Dipole Moments. Journal of Molecular Modeling, 1999, 5, 143-152.	0.8	18
81	Structural studies of antiviral inhibitor with HIV-1 protease bearing drug resistant substitutions of V32I, I47V and V82I. Biochemical and Biophysical Research Communications, 2019, 514, 974-978.	1.0	18
82	Bovine leukemia virus protease: comparison with human T-lymphotropic virus and human immunodeficiency virus proteases. Journal of General Virology, 2007, 88, 2052-2063.	1.3	17
83	Substituent effects on P2-cyclopentyltetrahydrofuranyl urethanes: Design, synthesis, and X-ray studies of potent HIV-1 protease inhibitors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 2308-2311.	1.0	17
84	Novel complex MAD phasing and RNase H structural insights using selenium oligonucleotides. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 354-361.	2.5	17
85	Design of novel HIV-1 protease inhibitors incorporating isophthalamide-derived P2-P3 ligands: Synthesis, biological evaluation and X-ray structural studies of inhibitor-HIV-1 protease complex. Bioorganic and Medicinal Chemistry, 2017, 25, 5114-5127.	1.4	16
86	Analysis of drug resistance in HIV protease. BMC Bioinformatics, 2018, 19, 362.	1.2	16
87	Potent HIVâ€1 Protease Inhibitors Containing Carboxylic and Boronic Acids: Effect on Enzyme Inhibition and Antiviral Activity and Proteinâ€Ligand Xâ€ray Structural Studies. ChemMedChem, 2019, 14, 1863-1872.	1.6	16
88	Highly Drug-Resistant HIV-1 Protease Mutant PRS17 Shows Enhanced Binding to Substrate Analogues. ACS Omega, 2019, 4, 8707-8719.	1.6	16
89	Probing Lipophilic Adamantyl Group as the P1-Ligand for HIV-1 Protease Inhibitors: Design, Synthesis, Protein X-ray Structural Studies, and Biological Evaluation. Journal of Medicinal Chemistry, 2016, 59, 6826-6837.	2.9	15
90	Capturing the Reaction Pathway in Near-Atomic-Resolution Crystal Structures of HIV-1 Protease. Biochemistry, 2012, 51, 7726-7732.	1.2	13

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91	Potent Antiviral HIV-1 Protease Inhibitor GRL-02031 Adapts to the Structures of Drug Resistant Mutants with Its P1â€²-Pyrrolidinone Ring. Journal of Medicinal Chemistry, 2012, 55, 3387-3397.	2.9	13
92	Identifying representative drug resistant mutants of HIV. BMC Bioinformatics, 2015, 16, S1.	1.2	13
93	Design of HIV-1 Protease Inhibitors with Amino-bis-tetrahydrofuran Derivatives as P2-Ligands to Enhance Backbone-Binding Interactions: Synthesis, Biological Evaluation, and Proteinâ€“Ligand X-ray Studies. Journal of Medicinal Chemistry, 2015, 58, 6994-7006.	2.9	13
94	Potent antiviral HIV-1 protease inhibitor combats highly drug resistant mutant PR20. Biochemical and Biophysical Research Communications, 2019, 519, 61-66.	1.0	13
95	Tackling the problem of HIV drug resistance. Postepy Biochemii, 2016, 62, 273-279.	0.5	12
96	Design, synthesis, biological evaluation and X-ray structural studies of HIV-1 protease inhibitors containing substituted fused-tetrahydropyranyl tetrahydrofuran as P2-ligands. Organic and Biomolecular Chemistry, 2015, 13, 11607-11621.	1.5	10
97	Evolution of drug resistance in HIV protease. BMC Bioinformatics, 2020, 21, 497.	1.2	10
98	Decoding HIV resistance: from genotype to therapy. Future Medicinal Chemistry, 2017, 9, 1529-1538.	1.1	9
99	Highly drugâ€resistant HIVâ€1 protease reveals decreased intraâ€subunit interactions due to clusters of mutations. FEBS Journal, 2020, 287, 3235-3254.	2.2	9
100	Substituted Bis-THF Protease Inhibitors with Improved Potency against Highly Resistant Mature HIV-1 Protease PR20. Journal of Medicinal Chemistry, 2015, 58, 5088-5095.	2.9	8
101	Design, Synthesis, Biological Evaluation, and Xâ€ray Studies of HIVâ€1 Protease Inhibitors with Modified P2â€² Ligands of Darunavir. ChemMedChem, 2017, 12, 1942-1952.	1.6	8
102	Crystal structure of yeast nitronate monooxygenase from Cyberlindnera saturnus. Proteins: Structure, Function and Bioinformatics, 2018, 86, 599-605.	1.5	8
103	Reaction Intermediates Discovered in Crystal Structures of Enzymes. Advances in Protein Chemistry and Structural Biology, 2012, 87, 57-86.	1.0	7
104	Design, synthesis, X-ray studies, and biological evaluation of novel macrocyclic HIV-1 protease inhibitors involving the P1â€²-P2â€² ligands. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4925-4931.	1.0	7
105	A Single-Point Mutation in <scp>d</scp>-Arginine Dehydrogenase Unlocks a Transient Conformational State Resulting in Altered Cofactor Reactivity. Biochemistry, 2021, 60, 711-724.	1.2	7
106	Longâ€Range Electrostaticsâ€Induced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. Angewandte Chemie, 2016, 128, 5008-5011.	1.6	6
107	Steric hindrance controls pyridine nucleotide specificity of a flavinâ€dependent NADH:quinone oxidoreductase. Protein Science, 2019, 28, 167-175.	3.1	6
108	Design, Synthesis, and X-ray Studies of Potent HIV-1 Protease Inhibitors with P2-Carboxamide Functionalities. ACS Medicinal Chemistry Letters, 2020, 11, 1965-1972.	1.3	6

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109	Design, synthesis, and X-ray studies of potent HIV-1 protease inhibitors incorporating aminothiochromane and aminotetrahydronaphthalene carboxamide derivatives as the P2 ligands. European Journal of Medicinal Chemistry, 2018, 160, 171-182.	2.6	4
110	Proton transfer and drug binding details revealed in neutron diffraction studies of wild-type and drug resistant HIV-1 protease. Methods in Enzymology, 2020, 634, 257-279.	0.4	4
111	Novel HIV PR inhibitors with C4-substituted bis-THF and bis-fluoro-benzyl target the two active site mutations of highly drug resistant mutant PRS17. Biochemical and Biophysical Research Communications, 2021, 566, 30-35.	1.0	3
112	Identification of Protein Folding Cores Using Charge Center Model of Protein Structure. Scientific World Journal, The, 2002, 2, 84-86.	0.8	2
113	Design, Synthesis and Xâ€Ray Structural Studies of Potent HIVâ€1 Protease Inhibitors Containing Câ€4 Substituted Tricyclic Hexahydroâ€Furofuran Derivatives as P2 Ligands. ChemMedChem, 2022, 17, .	1.6	2
114	Can we design drugs for HIV/AIDS that are less susceptible to resistance?. Future Medicinal Chemistry, 2015, 7, 2301-2304.	1.1	1
115	Revertant mutation V48G alters conformational dynamics of highly drug resistant HIV protease PRS17. Journal of Molecular Graphics and Modelling, 2021, 108, 108005.	1.3	1
116	Discovery of a new flavin N5-adduct in a tyrosine to phenylalanine variant of d-Arginine dehydrogenase. Archives of Biochemistry and Biophysics, 2022, 715, 109100.	1.4	1
117	Identifying representative drug resistant mutants of HIV reverse transcriptase. , 2014, , .		0