Irene T Weber

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	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
3	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
4	HIV Protease: Historical Perspective and Current Research. Viruses, 2021, 13, 839.	1.5	45
5	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
6	Revertant mutation V48C alters conformational dynamics of highly drug resistant HIV protease PRS17. Journal of Molecular Graphics and Modelling, 2021, 108, 108005.	1.3	1
7	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
8	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
9	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
10	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
11	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
12	Evolution of drug resistance in HIV protease. BMC Bioinformatics, 2020, 21, 497.	1.2	10
13	Potent HIVâ€l 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
14	Potent antiviral HIV-1 protease inhibitor combats highly drug resistant mutant PR20. Biochemical and Biophysical Research Communications, 2019, 519, 61-66.	1.0	13
15	Highly Drug-Resistant HIV-1 Protease Mutant PRS17 Shows Enhanced Binding to Substrate Analogues. ACS Omega, 2019, 4, 8707-8719.	1.6	16
16	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
17	Steric hindrance controls pyridine nucleotide specificity of a flavinâ€dependent NADH:quinone oxidoreductase. Protein Science, 2019, 28, 167-175.	3.1	6
18	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

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19	Crystal structure of yeast nitronate monooxygenase from Cyberlindnera saturnus. Proteins: Structure, Function and Bioinformatics, 2018, 86, 599-605.	1.5	8
20	Drug Resistance Mutation L76V Alters Nonpolar Interactions at the Flap–Core Interface of HIV-1 Protease. ACS Omega, 2018, 3, 12132-12140.	1.6	19
21	Analysis of drug resistance in HIV protease. BMC Bioinformatics, 2018, 19, 362.	1.2	16
22	Design and Synthesis of Potent HIV-1 Protease Inhibitors Containing Bicyclic Oxazolidinone Scaffold as the P2 Ligands: Structure–Activity Studies and Biological and X-ray Structural Studies. Journal of Medicinal Chemistry, 2018, 61, 9722-9737.	2.9	24
23	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
24	Design and Synthesis of Highly Potent HIV-1 Protease Inhibitors Containing Tricyclic Fused Ring Systems as Novel P2 Ligands: Structure–Activity Studies, Biological and X-ray Structural Analysis. Journal of Medicinal Chemistry, 2018, 61, 4561-4577.	2.9	31
25	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
26	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
27	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
28	Design, synthesis, X-ray studies, and biological evaluation of novel macrocyclic HIV-1 protease inhibitors involving the P1′-P2′ ligands. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4925-4931.	1.0	7
29	Decoding HIV resistance: from genotype to therapy. Future Medicinal Chemistry, 2017, 9, 1529-1538.	1.1	9
30	Design, Synthesis, Biological Evaluation, and Xâ€ray Studies of HIVâ€1 Protease Inhibitors with Modified P2′ Ligands of Darunavir. ChemMedChem, 2017, 12, 1942-1952.	1.6	8
31	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
32	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
33	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
34	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
35	Automated prediction of HIV drug resistance from genotype data. BMC Bioinformatics, 2016, 17, 278.	1.2	22
36	In vitro heme biotransformation by the HupZ enzyme from Group A streptococcus. BioMetals, 2016, 29, 593-609.	1.8	27

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37	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
38	Tackling the problem of HIV drug resistance. Postepy Biochemii, 2016, 62, 273-279.	0.5	12
39	Identifying representative drug resistant mutants of HIV. BMC Bioinformatics, 2015, 16, S1.	1.2	13
40	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
41	Can we design drugs for HIV/AIDS that are less susceptible to resistance?. Future Medicinal Chemistry, 2015, 7, 2301-2304.	1.1	1
42	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
43	Structure-Based Design of Potent HIV-1 Protease Inhibitors with Modified P1-Biphenyl Ligands: Synthesis, Biological Evaluation, and Enzyme–Inhibitor X-ray Structural Studies. Journal of Medicinal Chemistry, 2015, 58, 5334-5343.	2.9	21
44	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
45	Highly resistant HIV-1 proteases and strategies for their inhibition. Future Medicinal Chemistry, 2015, 7, 1023-1038.	1.1	55
46	Design of HIV-1 Protease Inhibitors with Amino-bis-tetrahydrofuran Derivatives as P2-Ligands to Enhance Backbone-Binding Interactions: Synthesis, Biological Evaluation, and Protein–Ligand X-ray Studies. Journal of Medicinal Chemistry, 2015, 58, 6994-7006.	2.9	13
47	Conformational variation of an extreme drug resistant mutant of HIV protease. Journal of Molecular Graphics and Modelling, 2015, 62, 87-96.	1.3	22
48	Design of <i>gem</i> â€Difluoroâ€ <i>bis</i> â€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
49	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
50	Identifying representative drug resistant mutants of HIV reverse transcriptase. , 2014, , .		0
51	Prediction of HIV drug resistance from genotype with encoded three-dimensional protein structure. BMC Genomics, 2014, 15, S1.	1.2	27
52	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
53	Highly Potent HIV-1 Protease Inhibitors with Novel Tricyclic P2 Ligands: Design, Synthesis, and Protein–Ligand X-ray Studies. Journal of Medicinal Chemistry, 2013, 56, 6792-6802.	2.9	42
54	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

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55	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
56	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
57	Sparse Representation for HIV-1 Protease Drug Resistance Prediction. , 2013, 2013, 342-349.		23
58	Capturing the Reaction Pathway in Near-Atomic-Resolution Crystal Structures of HIV-1 Protease. Biochemistry, 2012, 51, 7726-7732.	1.2	13
59	Potent Antiviral HIV-1 Protease Inhibitor GRL-02031 Adapts to the Structures of Drug Resistant Mutants with Its P1′-Pyrrolidinone Ring. Journal of Medicinal Chemistry, 2012, 55, 3387-3397.	2.9	13
60	Reaction Intermediates Discovered in Crystal Structures of Enzymes. Advances in Protein Chemistry and Structural Biology, 2012, 87, 57-86.	1.0	7
61	Critical differences in HIVâ€1 and HIVâ€2 protease specificity for clinical inhibitors. Protein Science, 2012, 21, 339-350.	3.1	38
62	HIV-1 Protease with 20 Mutations Exhibits Extreme Resistance to Clinical Inhibitors through Coordinated Structural Rearrangements. Biochemistry, 2012, 51, 2819-2828.	1.2	78
63	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
64	Enhancing Protein Backbone Binding—A Fruitful Concept for Combating Drugâ€Resistant HIV. Angewandte Chemie - International Edition, 2012, 51, 1778-1802.	7.2	131
65	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
66	Design of HIV-1 Protease Inhibitors with C3-Substituted Hexahydrocyclopentafuranyl Urethanes as P2-Ligands: Synthesis, Biological Evaluation, and Protein–Ligand X-ray Crystal Structure. Journal of Medicinal Chemistry, 2011, 54, 5890-5901.	2.9	31
67	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
68	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
69	Conformational Changes and Substrate Recognition in <i>Pseudomonas aeruginosa</i> <scp>d</scp> -Arginine Dehydrogenase [,] . Biochemistry, 2010, 49, 8535-8545.	1.2	26
70	Probing Multidrugâ€Resistance and Protein–Ligand Interactions with Oxatricyclic Designed Ligands in HIVâ€l Protease Inhibitors. ChemMedChem, 2010, 5, 1850-1854.	1.6	47
71	Autocatalytic maturation, physical/chemical properties, and crystal structure of group N HIV \hat{e} protease: Relevance to drug resistance. Protein Science, 2010, 19, 2055-2072.	3.1	22
72	Amprenavir complexes with HIVâ€1 protease and its drugâ€resistant mutants altering hydrophobic clusters. FEBS Journal, 2010, 277, 3699-3714.	2.2	116

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73	Steady-State Kinetic Mechanism and Reductive Half-Reaction of <scp>d</scp> -Arginine Dehydrogenase from <i>Pseudomonas aeruginosa</i> . Biochemistry, 2010, 49, 9542-9550.	1.2	23
74	HIV-1 Protease: Structural Perspectives on Drug Resistance. Viruses, 2009, 1, 1110-1136.	1.5	128
75	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
76	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
77	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
78	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
79	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
80	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
81	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
82	Structure-Based Design of Novel HIV-1 Protease Inhibitors To Combat Drug Resistance. Journal of Medicinal Chemistry, 2006, 49, 5252-5261.	2.9	144
83	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
84	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
85	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
86	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
87	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
88	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
89	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
90	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

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91	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
92	Molecular dynamics simulations of 14 HIV protease mutants in complexes with indinavir. Journal of Molecular Modeling, 2004, 10, 373-381.	0.8	33
93	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
94	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
95	Identification of Protein Folding Cores Using Charge Center Model of Protein Structure. Scientific World Journal, The, 2002, 2, 84-86.	0.8	2
96	Effect of sequence polymorphism and drug resistance on two HIV-1 Gag processing sites. FEBS Journal, 2002, 269, 4114-4120.	0.2	64
97	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
98	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
99	Molecular mechanics analysis of drug-resistant mutants of HIV protease. Protein Engineering, Design and Selection, 1999, 12, 469-474.	1.0	31
100	Improved Parameters for Generating Partial Charges: Correlation with Observed Dipole Moments. Journal of Molecular Modeling, 1999, 5, 143-152.	0.8	18
101	Structural and kinetic analysis of drug resistant mutants of HIV-1 protease. FEBS Journal, 1999, 263, 238-244.	0.2	115
102	Drug-Resistant HIV-1 Proteases Identify Enzyme Residues Important for Substrate Selection and Catalytic Rate. Biochemistry, 1998, 37, 13835-13845.	1.2	51
103	Structural Basis for Specificity of Retroviral Proteasesâ€. Biochemistry, 1998, 37, 4518-4526.	1.2	41
104	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
105	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
106	Molecular mechanics calculations on rous sarcoma virus protease with peptide substrates. Protein Science, 1997, 6, 2365-2374.	3.1	24
107	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
108	Programming the Rous Sarcoma Virus Protease to Cleave New Substrate Sequences. Journal of Biological Chemistry, 1996, 271, 10538-10544.	1.6	25

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109	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
110	Molecular dynamics simulations of HIV-1 protease with peptide substrate. Protein Engineering, Design and Selection, 1994, 7, 1353-1363.	1.0	41
111	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
112	Studies on the substrate specificity of the proteinase of equine infectious anemia virus using oligopeptide substrates. Biochemistry, 1993, 32, 3347-3353.	1.2	40
113	Kinetic and modeling studies of S3-S3' subsites of HIV proteinases. Biochemistry, 1992, 31, 4793-4800.	1.2	113
114	Studies on the role of the S4substrate binding site of HIV proteinases. FEBS Letters, 1991, 279, 356-360.	1.3	71
115	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
116	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
117	Structural alignment of retroviral protease sequences. Gene, 1989, 85, 565-566.	1.0	25