A computational study of the resistance of HIV-1 aspartic protease to the inhibitors ABT-538 and VX-478 and design of new analogues

DOI: 10.1006/bbrc.1997.8008
Biochemical and Biophysical Research Communications, 1998, 242, 545-51.

#	Paper	IF	Citations
22	Aspartic protease inhibitors. An integrated approach for the design andsynthesis of diaminodiol-based peptidomimetics. *FEBS Journal*, **2000**, 267, 1715-22		22
21	Computational design of new cyclic urea inhibitors for improved binding of HIV-1 aspartic protease. *Biochemical and Biophysical Research Communications*, **2000**, 268, 384-9	3.4	4
20	Amprenavir: a new human immunodeficiency virus type 1 protease inhibitor. *Clinical Therapeutics*, **2000**, 22, 549-72	3.5	44
19	Computational studies on HIV-1 protease inhibitors: influence of calculated inhibitor-enzyme binding affinities on the statistical quality of 3D-QSAR CoMFA models. *Journal of Medicinal Chemistry*, **2000**, 43, 4446-51	8.3	64
18	Design and synthesis of novel [60]fullerene derivatives as potential HIV aspartic protease inhibitors. *Organic Letters*, **2000**, 2, 3955-8	6.2	98
17	Molecular dynamics studies on HIV-1 protease: Drug resistance and folding pathways. *Proteins: Structure, Function and Bioinformatics*, **2001**, 43, 365-372	4.2	33
16	Homology modeling of the estrogen receptor subtype beta (ER-beta) and calculation of ligand binding affinities. *Journal of Molecular Graphics and Modelling*, **2001**, 20, 155-67	2.8	23
15	Kinetic and molecular modeling of nucleoside and nucleotide inhibition of malate dehydrogenase. *Nucleosides, Nucleotides and Nucleic Acids*, **2002**, 21, 813-23	1.4	3
14	The solution structures of the HIV protease inhibitor DG35-VIII. *Molecular Simulation*, **2002**, 28, 827-843	2	1
13	Computational studies on tetrahydropyrimidine-2-one HIV-1 protease inhibitors: improving three-dimensional quantitative structure-activity relationship comparative molecular field analysis models by inclusion of calculated inhibitor- and receptor-based properties. *Journal of Medicinal Chemistry*, **2002**, 45, 973-83	8.3	58
12	Inhibition of Candida albicans secreted aspartic protease by a novel series of peptidomimetics, also active on the HIV-1 protease. *Biochemical and Biophysical Research Communications*, **2002**, 297, 1350-3	3.4	21
11	Comparative study of some energetic and steric parameters of the wild type and mutants HIV-1 protease: a way to explain the viral resistance. *Journal of Cellular and Molecular Medicine*, **2002**, 6, 251-60	5.6	5
10	Computational studies of the resistance patterns of mutant HIV-1 aspartic proteases towards ABT-538 (ritonavir) and design of new derivatives. *Journal of Molecular Graphics and Modelling*, **2002**, 21, 171-9	2.8	11
9	Synthesis and evaluation of 17alpha-20E-21-(4-substituted phenyl)-19-norpregna-1,3,5(10),20-tetraene-3,17beta-diols as probes for the estrogen receptor alpha hormone binding domain. *Journal of Medicinal Chemistry*, **2003**, 46, 2865-76	8.3	27
8	Molecular modeling of the binding of 5-substituted 2adeoxyuridine substrates to thymidine kinase of herpes simplex virus type-1. *Nucleosides, Nucleotides and Nucleic Acids*, **2004**, 23, 555-65	1.4	5
7	Synthesis and evaluation of (17alpha,20Z)-21-(4-substituted-phenyl)-19-norpregna-1,3,5(10),20-tetraene-3,17beta-diols as ligands for the estrogen receptor-alpha hormone binding domain: comparison with 20E-isomers. *Journal of Medicinal Chemistry*, **2005**, 48, 4300-11	8.3	15
6	Evaluation of a neural networks QSAR method based on ligand representation using substituent descriptors. Application to HIV-1 protease inhibitors. *Journal of Molecular Graphics and Modelling*, **2006**, 25, 37-45	2.8	5

5	Synthesis and evaluation of isomeric (17alpha,20E)-11beta-methoxy-21-(trifluoromethylphenyl)-19-norpregna-1,3,5(10),20-tetraene-3,17beta-diols as ERalpha-hormone binding domain ligands: effect of the methoxy group on receptor binding and uterotrophic growth. *Journal of Medicinal Chemistry*, **2007**, 50, 472-9	8.5	10
4	Catalytic contributions from remote regions of enzyme structure. *Chemical Reviews*, **2011**, 111, 7595-624	68.1	59
3	Synthesis and evaluation of 17E(dimethylphenyl)vinyl estradiols as probes of the estrogen receptor-ligand binding domain. *Steroids*, **2012**, 77, 471-6	2.8	11
2	An in silico pharmacological approach toward the discovery of potent inhibitors to combat drug resistance HIV-1 protease variants. *Journal of Cellular Biochemistry*, **2019**, 120, 9063-9081	4.7	10
1	Inhibitors of the Human Immunodeficiency Virus Protease. 113-135		