Target Name	HIV-1 protease
Target TTD ID	TTDS00319

Target Species	Human immunodeficiency virus 1
Chemical Type	N-Aryl Heteroarylisopropanolamines
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{50} = -4.284 - (0.659)^{*}\text{Sfit} + (0.010)^{*}\text{Dip-mom} - (0.340)^{*}\text{HOMO} + (0.008)^{*}\text{MW} + (0.008)^{*}\text{Volume} - (0.053)^{*}\text{G\_CDS\_aq}$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Parameter - description: Sfit - Steric fit between ligand and receptor; Dip-Mom - Dipole moment (AMSOL); HOMO - HOMO ligand energy (AMSOL); MW - Molecular weight (AMSOL); Volume - Molecular volume (AMSOL); G_CDS_aq - Cavity-dispersion-solvent free energy (AMSOL).
Reference	Design, Synthesis and QSAR Studies on N-Aryl Heteroarylisopropanolamines, a New Class of Non-Peptidic HIV-1 Protease Inhibitors. *Bioorganic & Medicinal Chemistry* 10 (2002) 2511–2526

Target Species	Human immunodeficiency virus 1
Chemical Type	Six-membered cyclic ureas
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/K_i) = 2.139(\pm 0.740) + 0.167(\pm 0.018)\ {}^{1}SIC$

	$R^2 = 0.646;\ \ R^2_{cv} = 0.617;\ \ s = 0.750;\ F = 90.$
QSAR Model 2	$\log(1/K_i) = 2.168(\pm 0.535) + 0.108(\pm 0.010)\,{}^2SIC + 12.750(\pm 1.848)\,{}^{HD}FPSA^{(2)}$ $R^2 = 0.816;\ \ R^2_{cv} = 0.792;\ \ s = 0.545;\ F = 107$
QSAR Model 3	$\log(1/K_i) = 15.901(\pm 0.917) + 261.881(\pm 24.823)\,{}^{HD}FCPSA^{(2)} - 160.948(\pm 36.184)I^A - 5.708(\pm 0.746)J$ $R^2 = 0.855;\ \ R^2_{cv} = 0.832;\ \ s = 0.489;\ F = 92$
QSAR Model 4	$\log(1/K_i) = 42.585(\pm 8.445) + 15.601(\pm 1.776)\,{}^{HD}FPSA^{(2)} - 141.775(\pm 34.923)I^A - 6.204(\pm 0.732)J - 0.234(\pm 0.073)E^{\min}_{e-n}(O-H)$ $R^2 = 0.873;\ \ R^2_{cv} = 0.847;\ \ s = 0.463;\ F = 79$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Structural information content of order 1 (^{1}SIC) accounts for both molecular constitutional and structural diversity. ^{HD}FPSA$^{(2)}$ (fractional positive surface area of hydrogen donors). ^{H}FPSA$^{(2)}$ (fractional positive surface area of hydrogen donor species). The hydrogen bond descriptor ^{HD}FCPSA$^{(2)}$ which is a charge weighted analogue of ^{HD}FPSA$^{(2)}$ (weighted by Zefirov's atomic charges). First moment of inertia (I^A). Balaban topological index J, ameasure of molecular 'centricity'. The minimum electronuclear attraction energy for O–H bond, E^{min}_{e-n} (O_H), which may be regarded as an immediate scale of the bond strength.
Reference	Six-Membered Cyclic Ureas as HIV-1 Protease Inhibitors: A QSAR Study Based on CODESSA PRO Approach. *Bioorganic & Medicinal Chemistry Letters* 12 (2002) 3453–3457

Target Species	Human immunodeficiency virus 1

Chemical Type	Alkyl substituted P2/P2' 3-aminoindazoles
Mode of Action	Inhibitor
QSAR Model 1	$\text{Log}\,1/K_i = -0.39(\pm 0.22)\text{C}\log P + 13.33(\pm 1.79)$ $n = 6, \quad r^2 = 0.858, \quad q^2 = 0.475, \quad s = 0.256$
QSAR Model 2	$\text{Log}\,1/K_i = -0.53(\pm 0.25)\text{CMR} + 20.72(\pm 4.97)$ $n = 7, \quad r^2 = 0.860, \quad q^2 = 0.708, \quad s = 0.306$
QSAR Model 3	$\text{Log}\,1/\text{IC}_{90} = 0.49(\pm 0.21)\text{C}\log P + 3.01(\pm 1.74)$ $n = 7, \quad r^2 = 0.874, \quad q^2 = 0.733, \quad s = 0.276$
QSAR Model 4	$\text{Log}\,1/\text{IC}_{90} = 0.56(\pm 0.29)\text{CMR} + 4.12(\pm 5.82)$ $n = 6, \quad r^2 = 0.875, \quad q^2 = 0.576, \quad s = 0.307$
QSAR Model 5	$\text{Log}\,1/T = 0.95(\pm 0.16)\text{C}\log P - 10.67(\pm 1.28)$ $n = 7, \quad r^2 = 0.979, \quad q^2 = 0.945, \quad s = 0.203$
QSAR Model 6	$\text{Log}\,1/T = 0.98(\pm 0.17)\text{CMR} - 22.75(\pm 3.55)$ $n = 7, \quad r^2 = 0.976, \quad q^2 = 0.939, \quad s = 0.219$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Clog P range = 5.45–9.15; CMR range = 17.85 – 21.28; Clog P versus CMR (r^2 = 0.922); ClogP is the calculated partition coefficient in octanol/water and is a measure of hydrophobicity; CMR is the calculated molar refractivity for the whole molecule, and is a measure of volume and polarizability; MR is calculated as follows : (n^2-1/n^2+2) (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance; L is the Verloop's sterimol parameter that defines substituents' length.

Reference	A mechanistic study of 3-aminoindazole cyclic urea HIV-1 protease inhibitors using comparative QSAR. *Bioorganic & Medicinal Chemistry* 12 (2004) 5819–5831

Target Species	Human immunodeficiency virus 1
Chemical Type	P1/P1' substituted symmetrical aminoindazole analogs of cyclic urea
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{Log}\,1/K_i = -0.35(\pm 0.12)\mathrm{C}\log P + 12.95(\pm 0.95)$ $n = 10, \quad r^2 = 0.851, \quad q^2 = 0.780, \quad s = 0.202, \ \text{outlier}: 4\text{-}CH_3$
QSAR Model 2	$\mathrm{Log}\,1/K_i = -0.37(\pm 0.11)\mathrm{CMR} + 17.62(\pm 2.28)$ $n = 10, \quad r^2 = 0.877, \quad q^2 = 0.825, \quad s = 0.184, \ \text{outlier}: 4\text{-}CH_3$
QSAR Model 3	$\mathrm{Log}\,1/\mathrm{IC}_{90} = 0.28(\pm 0.11)\mathrm{C}\log P + 4.28(\pm 0.83)$ $n = 10, \quad r^2 = 0.813, \quad q^2 = 0.659, \quad s = 0.181, \ \text{outlier}: 3\text{-}C(CH_3)_3$
QSAR Model 4	$\mathrm{Log}\,1/\mathrm{IC}_{90} = 0.29(\pm 0.10)\mathrm{CMR} + 0.47(\pm 2.08)$ $n = 10, \quad r^2 = 0.844, \quad q^2 = 0.728, \quad s = 0.166, \ \text{outlier}: 3\text{-}C(CH_3)_3$
QSAR Model 5	$\mathrm{Log}\,1/T = 0.56(\pm 0.16)\mathrm{C}\log P - 8.15(\pm 1.30)$ $n = 11, \quad r^2 = 0.867, \quad q^2 = 0.776, \quad s = 0.302$
QSAR Model 6	$\mathrm{Log}\,1/T = 0.59(\pm 0.16)\mathrm{CMR} - 15.50(\pm 3.29)$ $n = 11, \quad r^2 = 0.878, \quad q^2 = 0.793, \quad s = 0.290$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**

	Clog P range = 5.45–9.62; CMR range = 17.85 – 21.56; Clog P versus CMR (r^2 = 0.986); ClogP is the calculated partition coefficient in octanol/water and is a measure of hydrophobicity; CMR is the calculated molar refractivity for the whole molecule, and is a measure of volume and polarizability; MR is calculated as follows : (n^2-1/n^2+2) (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance; L is the Verloop's sterimol parameter that defines substituents' length.
Reference	A mechanistic study of 3-aminoindazole cyclic urea HIV-1 protease inhibitors using comparative QSAR. *Bioorganic & Medicinal Chemistry* 12 (2004) 5819–5831

Target Species	Human immunodeficiency virus 1
Chemical Type	Nonsymmetrical 3-aminoindazoles
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{Log}\,1/K_i = -0.73(\pm 0.31)\mathrm{C}\log P + 15.26(\pm 2.04)$ $n = 5,\ r^2 = 0.950,\ q^2 = 0.859,\ s = 0.091$ outliers: CH_2-2-naphthyl, CH_2-cy-C_3H_5
QSAR Model 2	$\mathrm{Log}\,1/K_i = -0.78(\pm 0.76)\mathrm{CMR} + 22.79(\pm 12.0)$ $n = 5,\ r^2 = 0.780,\ q^2 = 0.210,\ s = 0.200$ outliers: CH_2-2-naphthyl, $CH_2C_6H_5$
QSAR Model 3	$\mathrm{Log}\ 1/\mathrm{IC}_{90} = 1.27(\pm 0.64)\mathrm{C}\log P + 15.35(\pm 4.21)$ $n = 5,\ r^2 = 0.930,\ q^2 = 0.800,\ s = 0.189$ outliers: CH_2-2-naphthyl, CH_2-cy-C_3H_5
QSAR Model 4	$\mathrm{Log}\,1/\mathrm{IC}_{90} = 0.22(\pm 0.36)\mathrm{CMR} + 3.56(\pm 5.95)$ $n = 5,\ r^2 = 0.553,\ q^2 = -0.234,\ s = 0.274$ outliers: CH_2-cy-C_4H_7, C_6H_{13}
QSAR Model 5	$\mathrm{Log}\,1/T = 0.15(\pm 0.13)\mathrm{C}\log P - 6.05(\pm 2.18)$ $n = 5,\ r^2 = 0.814,\ q^2 = 0.516,\ s = 0.100$ outliers: CH_2-cy-C_4H_7, C_6H_{13}
QSAR Model 6	$\mathrm{Log}\,1/T = 0.31(\pm 0.37)\mathrm{CMR} - 5.50(\pm 2.46)$ $n = 5,\ r^2 = 0.708,\ q^2 = 0.136,\ s = 0.182$ outliers: CH_2-cy-C_4H_7, C_5H_{11}

Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Clog P range = 5.63–7.52; CMR range = 15.32 – 18.26; Clog P versus CMR (r^2 = 0.669)ClogP is the calculated partition coefficient in octanol/water and is a measure of hydrophobicity; CMR is the calculated molar refractivity for the whole molecule, and is a measure of volume and polarizability; MR is calculated as follows : (n^2-1/n^2+2) (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance; L is the Verloop's sterimol parameter that defines substituents' length.
Reference	A mechanistic study of 3-aminoindazole cyclic urea HIV-1 protease inhibitors using comparative QSAR. *Bioorganic & Medicinal Chemistry* 12 (2004) 5819–5831

Target Species	Human immunodeficiency virus 1
Chemical Type	Nonsymmetrical P2/P2' substituted 3-aminoindazole cyclic urea compounds
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{Log}\,1/K_i = -0.47(\pm 0.15)\mathrm{C}\log P + 13.50(\pm 1.09)$ $n = 8,\ \ r^2 = 0.900,\ \ q^2 = 0.819,\ \ s = 0.121$ outliers: $R_1 = 4\text{-}C_2H_5,\ \ R_2 = CH_2C_6H_5;\ \ R_1 = 4\text{-}C_2H_5,\ \ R_2 = C_4H_9$
QSAR Model 2	$\mathrm{Log}\,1/K_i = -0.30(\pm 0.14)\mathrm{CMR} + 15.32(\pm 2.42)$ $n = 8,\ \ r^2 = 0.813,\ \ q^2 = 0.651,\ \ s = 0.142$ outliers: $R_1 = 4\text{-}C_2H_5,\ \ R_2 = CH_2C_6H_5;\ R_1 = 3,5\text{-di-}CH_3,\ \ R_2 = C_4H_9$
QSAR Model 3	$\mathrm{Log}\,1/\mathrm{IC}_{90} = 0.23(\pm 0.15)\mathrm{C}\log P + 4.72(\pm 1.10)$ $n = 6,\ \ r^2 = 0.822,\ \ q^2 = 0.530,\ \ s = 0.111$ outliers: $R_1 = 4\text{-}CH_3,\ R_2 = CH_2C_6H_5;\ R_1 = 3,5\text{-di-}CH_3,\ R_2 = CH_2C_6H_5;$ $R_1 = 3\text{-}CH_3,\ R_2 = C_4H_9$
QSAR Model 4	$\mathrm{Log}\,1/\mathrm{IC}_{90} = 0.32(\pm 0.16)\mathrm{CMR} + 1.03(\pm 2.69)$

	$n = 7, \quad r^2 = 0.840, \quad q^2 = -0.705, \quad s = 0.116$ outliers: $R_1 = 4\text{-}C_2H_5, \quad R_2 = CH_2C_6H_5$; $R_1 = 3,5\text{-di-}CH_3, \quad R_2 = CH_2C_6H_5$
QSAR Model 5	$\text{Log}\,1/T = 0.52(\pm 0.21)\text{C}\log P - 7.69(\pm 1.55)$ $n = 9, \quad r^2 = 0.808, \quad q^2 = 0.695, \quad s = 0.215$
QSAR Model 6	$\text{Log}\,1/T = 0.44(\pm 0.18)\text{CMR} - 11.37(\pm 3.02)$ $n = 9, \quad r^2 = 0.807, \quad q^2 = 0.697, \quad s = 0.215$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Clog P range = 6.34–8.40; CMR range = 15.45 – 18.43; Clog P versus CMR (r^2 = 0.665); ClogP is the calculated partition coefficient in octanol/water and is a measure of hydrophobicity; CMR is the calculated molar refractivity for the whole molecule, and is a measure of volume and polarizability; MR is calculated as follows : (n^2-1/n^2+2) (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance; L is the Verloop's sterimol parameter that defines substituents' length.
Reference	A mechanistic study of 3-aminoindazole cyclic urea HIV-1 protease inhibitors using comparative QSAR. *Bioorganic & Medicinal Chemistry* 12 (2004) 5819–5831

Target Species	Human immunodeficiency virus 1
Chemical Type	3-aminoindazole cyclic urea derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\text{Log}\,1/K_i = -0.34(\pm 0.07)\text{C}\log P + 12.82(0.53)$ $n = 28, \quad r^2 = 0.801, \quad q^2 = 0.771, \quad s = 0.195$ outliers: $R_1 = H, \quad R_2/R_3 = 3\text{-NH-}(CH_2)_4\text{-indazole}$; $R_1 = 4\text{-}CH_3, \quad R_2/R_3 = 3\text{-}NH_2\text{-indazole}$; $R_1 = H, \quad R_2 = CH_2\text{-2-naphthyl}$, $R_3 = 3\text{-}NH_2\text{-indazole}$; $R_1 = H, \quad R_2 = C_6H_{13}$, $R_3 = 3\text{-}NH_2\text{-indazole}$

QSAR Model 2	$\mathrm{Log}\,1/\mathrm{IC}_{90} = 0.46(\pm0.11)\mathrm{C}\log P + 1.23(\pm0.28)I_1 - 0.19(\pm0.10)L_4 + 3.61(\pm0.78)$ $n = 27, \quad r^2 = 0.833, \quad q^2 = 0.773, \quad s = 0.234$ outliers: $\mathrm{R}_1 = 3\text{-}\mathrm{CMe}_3, \quad \mathrm{R}_2/\mathrm{R}_3 = 3\text{-}\mathrm{NH}_2\text{-indazole}; \ \mathrm{R}_1 = \mathrm{H}, \quad \mathrm{R}_2 = \mathrm{C}_5\mathrm{H}_{11}, \ \mathrm{R}_3 = 3\text{-}\mathrm{NH}_2\text{-indazole}; \ \mathrm{R}_1 = \mathrm{H}, \quad \mathrm{R}_2 = \mathrm{C}_6\mathrm{H}_{13}, \ \mathrm{R}_3 = 3\text{-}\mathrm{NH}_2\text{-indazole}; \ \mathrm{R}_1 = 3,5\text{-di-Me}, \quad \mathrm{R}_2 = \mathrm{CH}_2\mathrm{C}_6\mathrm{H}_5, \ \mathrm{R}_3 = 3\text{-}\mathrm{NH}_2\text{-indazole}$
QSAR Model 3	$\mathrm{Log}\,1/T = 0.78(\pm0.15)\mathrm{C}\log P + 1.17(\pm0.40)I_1 - 9.56(\pm1.25)$ $n = 27, \quad r^2 = 0.808, \quad q^2 = 0.750, \quad s = 0.360$ outliers: $\mathrm{R}_1 = 4\text{-}\mathrm{C}_4\mathrm{H}_9, \quad \mathrm{R}_2/\mathrm{R}_3 = 3\text{-}\mathrm{NH}_2\text{-indazole}; \ \mathrm{R}_1 = 3\text{-}(\mathrm{CH}_3)_3, \quad \mathrm{R}_2/\mathrm{R}_3 = 3\text{-}\mathrm{NH}_2\text{-indazole}; \ \mathrm{R}_1 = \mathrm{H}, \quad \mathrm{R}_2 = \mathrm{C}_6\mathrm{H}_{13}, \ \mathrm{R}_3 = 3\text{-}\mathrm{NH}_2\text{-indazole}; \ \mathrm{R}_1 = 4\text{-}\mathrm{C}_2\mathrm{H}_5, \quad \mathrm{R}_2 = \mathrm{C}_6\mathrm{H}_5, \ \mathrm{R}_3 = 3\text{-}\mathrm{NH}_2\text{-indazole}$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ClogP is the calculated partition coefficient in octanol/water and is a measure of hydrophobicity; CMR is the calculated molar refractivity for the whole molecule, and is a measure of volume and polarizability; MR is calculated as follows : $(n^2\text{-}1/n^2\text{+}2)$ (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance; L is the Verloop's sterimol parameter that defines substituents' length.
Reference	A mechanistic study of 3-aminoindazole cyclic urea HIV-1 protease inhibitors using comparative QSAR. *Bioorganic & Medicinal Chemistry* 12 (2004) 5819–5831

Target Species	Human immunodeficiency virus 1
Chemical Type	Nonsymmetrical 3-aminoindazole cyclic urea
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{Log}\,1/\mathrm{IC}_{90} = 8.46(\pm3.17)\mathrm{C}\log P - 0.58(\pm0.22)\mathrm{C}\log P^2 - 23.23(\pm11.54)$

	$n = 8, \quad r^2 = 0.906, \quad q^2 = 0.721, \quad s = 0.119$ optimum $C\log P = 7.315$ (7.181–7.437) outliers: $R_1 = 3\text{-}CH_3, \quad R_2 = C_4H_9$; $R_1 = 4\text{-}C_2H_5, \quad R_2 = C_4H_9$
QSAR Model 2	$\text{Log}\,1/IC_{90} = 0.082(\pm 0.020)C\log P + 5.90(\pm 0.14)$ $n = 4, \quad r^2 = 0.994, \quad q^2 = 0.977, \quad s = 0.008$ outliers: $R_1 = 3\text{-}CH_3, \quad R_2 = CH_2C_6H_5$; $R_1 = 4\text{-}C_2H_5, \quad R_2 = CH_2C_6H_5$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ClogP is the calculated partition coefficient in octanol/water and is a measure of hydrophobicity; CMR is the calculated molar refractivity for the whole molecule, and is a measure of volume and polarizability; MR is calculated as follows : $(n^2\text{-}1/n^2\text{+}2)$ (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance; L is the Verloop's sterimol parameter that defines substituents' length.
Reference	A mechanistic study of 3-aminoindazole cyclic urea HIV-1 protease inhibitors using comparative QSAR. *Bioorganic & Medicinal Chemistry* 12 (2004) 5819–5831

Target Species	Human immunodeficiency virus 1
Chemical Type	3-(S-$(CH_2)_n$-C6H5), 6-C_6H_5, 6'-R (hydrophobic) substituted 4-hydroxy-5,6-dihydro pyran-2-ones
Mode of Action	Inhibitor
QSAR Model 1	$\text{Log}(1/IC_{50}) = 1.41(\pm 0.36)C\log P - 0.62(\pm 0.24)B5_R - 1.16(\pm 0.51)I_0 + 1.38(\pm 1.08)$ $n = 28, \quad r = 0.901, \quad r^2 = 0.812, \quad q^2 = 0.715, \quad s = 0.287$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ClogP is the calculated partition coefficient in octanol/water and is a measure of the hydrophobicity of the molecule. It explains: (a) hydrophobic interactions between ligand and receptor, and (b)

	random walk process in movement of the drug molecule in the organism from site of injection to sites of action. CMR is the calculated molar refractivity for the whole molecule and is a measure of volume and polarizability. MR is calculated as follows : (n^2 _ $1/n^2$ + 2) (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance. B5 is the Verloop's sterimol parameter that defines maximum width of the substituents. The indicator variable I is assigned the value of 1 or 0 for special affects that cannot be parameterized and has been explained wherever used.
Reference	From SAR to comparative QSAR: role of hydrophobicity in the design of 4-hydroxy-5,6-dihydropyran-2-ones HIV-1 protease inhibitors. *Bioorganic & Medicinal Chemistry* 13 (2005) 4078–4084.

Target Species	Human immunodeficiency virus 1
Chemical Type	3-(S-$(CH_2)_n$-C6H5), 6-C_6H_5, 6'-R (polar) substituted 4-hydroxy-5,6-dihydro pyran-2-ones
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{Log}(1/\mathrm{IC}_{50}) = 2.47(\pm 1.21)\mathrm{CMR} + 1.58(\pm 0.84)I_{\mathrm{COOH}} - 23.03(\pm 14.33)$ $n = 6,\ r = 0.972,\ r^2 = 0.945,\ q^2 = 0.661,\ s = 0.276$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ClogP is the calculated partition coefficient in octanol/water and is a measure of the hydrophobicity of the molecule. It explains: (a) hydrophobic interactions between ligand and receptor, and (b) random walk process in movement of the drug molecule in the organism from site of injection to sites of action. CMR is the calculated molar refractivity for the whole molecule and is a measure of volume and polarizability. MR is calculated as follows : (n^2 _ $1/n^2$ + 2) (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance. B5 is the Verloop's sterimol parameter that defines maximum width of the substituents. The

	indicator variable I is assigned the value of 1 or 0 for special affects that cannot be parameterized and has been explained wherever used.
Reference	From SAR to comparative QSAR: role of hydrophobicity in the design of 4-hydroxy-5,6-dihydropyran-2-ones HIV-1 protease inhibitors. *Bioorganic & Medicinal Chemistry* 13 (2005) 4078–4084

Target Species	Human immunodeficiency virus 1
Chemical Type	3-(S-(2R',5R''-C_6H_5)), 6-C_6H_5, 6'-R (hydrophobic) substituted 4-hydroxy-5,6-dihydro-pyran-2-ones
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{Log}(1/\mathrm{IC}_{50}) = -0.28(\pm 0.23)\mathrm{Clog}P + 0.73(\pm 0.24)B5_{\mathrm{R}'} - 0.92(0.40)I_{\mathrm{R}} + 7.67(\pm 1.45)$ $n = 17,\ r = 0.892,\ r^2 = 0.797,\ q^2 = 0.654,\ s = 0.255$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ClogP is the calculated partition coefficient in octanol/water and is a measure of the hydrophobicity of the molecule. It explains: (a) hydrophobic interactions between ligand and receptor, and (b) random walk process in movement of the drug molecule in the organism from site of injection to sites of action. CMR is the calculated molar refractivity for the whole molecule and is a measure of volume and polarizability. MR is calculated as follows : (n^2 _ $1/n^2$ + 2) (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance. B5 is the Verloop's sterimol parameter that defines maximum width of the substituents. The indicator variable I is assigned the value of 1 or 0 for special affects that cannot be parameterized and has been explained wherever used.
Reference	From SAR to comparative QSAR: role of hydrophobicity in the design of 4-hydroxy-5,6-dihydropyran-2-ones HIV-1 protease inhibitors. *Bioorganic & Medicinal Chemistry* 13 (2005) 4078–4084

Target Species	Human immunodeficiency virus 1
Chemical Type	3-S-R'', 6-C_6H_5, 6'-R substituted 4-hydroxy-5,6-dihydro-pyran-2-ones
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{Log}(1/\mathrm{IC}_{50}) = 0.82(\pm 0.60)\mathrm{Clog}P - 0.07(\pm 0.06)\mathrm{Clog}P^2 + 0.47(\pm 0.19)\mathrm{CMR} - 1.28(\pm 2.93)$ $n = 57,\ r = 0.850,\ r^2 = 0.722,\ q^2 = 0.676,\ s = 0.436$ Optimum $\mathrm{Clog}P\ (\log P_0) = 6.345$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ClogP is the calculated partition coefficient in octanol/water and is a measure of the hydrophobicity of the molecule. It explains: (a) hydrophobic interactions between ligand and receptor, and (b) random walk process in movement of the drug molecule in the organism from site of injection to sites of action. CMR is the calculated molar refractivity for the whole molecule and is a measure of volume and polarizability. MR is calculated as follows : (n^2 _ $1/n^2$ + 2) (MW/d), where n is the refractive index, MW is the molecular weight, and d is the density of a substance. B5 is the Verloop's sterimol parameter that defines maximum width of the substituents. The indicator variable I is assigned the value of 1 or 0 for special affects that cannot be parameterized and has been explained wherever used.
Reference	From SAR to comparative QSAR: role of hydrophobicity in the design of 4-hydroxy-5,6-dihydropyran-2-ones HIV-1 protease inhibitors. *Bioorganic & Medicinal Chemistry* 13 (2005) 4078–4084