Target Name	Influenza neuraminidase
Target TTD ID	TTDS00174

Target Species	Influenza virus
Chemical Type	Benzoic acids
Mode of Action	Inhibitor
QSAR Model 1	$\log 1/C = 0.10(\pm 0.05)\mathrm{NVE} - 7.15(\pm 5.90)$ $n = 6, \quad r^2 = 0.886, \quad s = 0.585, \quad q^2 = 0.713$ $outlier : \mathrm{X} = \mathrm{NHC(=NH)NH_2}, \ \mathrm{Y} = \mathrm{H}, \ \mathrm{Z} = \mathrm{CH_2NH_2}$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** C is the molar concentration of a compound. ClogP is the calculated octanol/water partition coefficient. Cπ and π are the calculated and experimentally obtained hydrophobic parameters for the substituents. MR is the molar refractivity and is defined by the Lorentz–Lorenz equation: $MR = n^2 - 1/n^2 + 2(MW/\delta)$, where n = refractive index, δ = density, and MW = molecular weight. CMR is the calculated molar refractivity. Molar refractivity (MR) has a strong correlation with the molecular polarizability. Number of valence electrons (NVE) is a parameter that was found to be another approach to understanding polarizability and calculated by simply summing up the valence electrons in a molecule, for example, H = 1, C = 4, Si = 4, N = 5, P = 5, O = 6, S = 6, and halogens = 7. There are three commonly encountered electronic parameters: σ, σ^-, and σ^+ that account for specific electronic effects of substituents on aromatic systems. These parameters are known as the Hammett parameters and their application has been illustrated. MgVol is the molar volume calculated by C-QSAR Program using the method of Abraham and McGowan. I is an indicator variable that takes the value of 1 or 0 for structural features that cannot be defined by the normal parameters. In QSAR equation, n is the number of data points, r is the correlation coefficient, r^2 is the goodness of fit, q^2 is

	the goodness of prediction, and *s* is the standard deviation.
Reference	A QSAR study on influenza neuraminidase inhibitors. *Bioorganic & Medicinal Chemistry* 14 (2006) 982–996

Target Species	Influenza virus
Chemical Type	Carbocyclic derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log 1/\mathrm{C} = 8.84(\pm 3.14)\mathrm{MgVol} - 11.29(\pm 6.49)$ $n = 6, \quad r^2 = 0.938, \quad s = 0.352, \quad q^2 = 0.875$ $outliers : \mathrm{X} = \text{cyclohexyl; phenyl}$
QSAR Model 2	$\log 1/C = 0.63(\pm 0.21)C\log P - 0.74(\pm 0.39)\text{bilin } C\log P$ $+ 2.15(\pm 0.27)I + 7.15(\pm 0.40)$ $n = 20, \quad r^2 = 0.965, \quad s = 0.263, \quad q^2 = 0.945$ $optimum\ value = 0.384$
QSAR Model 3	$\log 1/C = 0.72(\pm 0.42)C\pi_{\mathrm{X}} - 1.20(\pm 0.44)I$ $+ 6.59(\pm 0.33)$ $n = 11, \quad r^2 = 0.944, \quad s = 0.225, \quad q^2 = 0.861$ $outliers : \mathrm{X} = \mathrm{Me}, \mathrm{Y} = \mathrm{CH}(C_2\mathrm{H}_5)_2;$ $\mathrm{X} = \mathrm{H}, \mathrm{Y} = \mathrm{CH}(C_2\mathrm{H}_5)_2$

QSAR Model 4	$\log 1/C = -0.44(\pm 0.28)\text{CMR-Y} - 1.12(\pm 0.40)I + 7.86(\pm 0.64)$ $n = 9, \quad r^2 = 0.906, \quad s = 0.231, \quad q^2 = 0.819$ $outlier : \text{X} = \text{H}, \text{Y} = C_4\text{H}_9$
QSAR Model 5	$\log 1/C = 0.84(\pm 0.22)C\log P - 1.48(\pm 0.46)\text{IS} + 9.34(\pm 0.53)$ $n = 9, \quad r^2 = 0.967, \quad s = 0.231, \quad q^2 = 0.946$ $outlier : \text{CH}(C_2\text{H}_5)_2$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** C is the molar concentration of a compound. ClogP is the calculated octanol/water partition coefficient. Cπ and π are the calculated and experimentally obtained hydrophobic parameters for the substituents. MR is the molar refractivity and is defined by the Lorentz–Lorenz equation: $MR = n^2 - 1/n^2 + 2(MW/\delta)$, where n = refractive index, δ = density, and MW = molecular weight. CMR is the calculated molar refractivity. Molar refractivity (MR) has a strong correlation with the molecular polarizability. Number of valence electrons (NVE) is a parameter that was found to be another approach to understanding polarizability and calculated by simply summing up the valence electrons in a molecule, for example, H = 1, C = 4, Si = 4, N = 5, P = 5, O = 6, S = 6, and halogens = 7. There are three commonly encountered electronic parameters: σ, σ^-, and σ^+ that account for specific electronic effects of substituents on aromatic systems. These parameters are known as the Hammett parameters and their application has been illustrated. MgVol is the molar volume calculated by C-QSAR Program using the method of Abraham and McGowan. *I* is an indicator variable that takes the value of 1 or 0 for structural features that cannot be defined by the normal parameters. In QSAR equation, n is the number of data points, r is the correlation coefficient, r^2 is the goodness of fit, q^2 is the goodness of prediction, and s is the standard deviation.
Reference	A QSAR study on influenza neuraminidase inhibitors. *Bioorganic & Medicinal Chemistry* 14 (2006) 982–996

Target	Influenza virus

Species	
Chemical Type	Cyclopentanes
Mode of Action	Inhibitor
QSAR Model 1	$\log 1/C = -42.35(\pm 12.30)\mathrm{MgVol} + 7.46(\pm 2.17)\mathrm{MgVol}^2 + 65.21(\pm 17.20)$ $n = 11, \quad r^2 = 0.889, \quad s = 0.216, \quad q^2 = 0.815$ *inversion point* : 2.84(2.80–2.88) *outliers* : $CH(CH_3)C_2H_5$; $CH(C_2H_5)_2$; $CH(C_2H_5)CH_2OCH_3$
QSAR Model 2	$\log 1/C = -17.58(\pm 9.42)\mathrm{MgVol} + 2.96(\pm 1.67)\mathrm{MgVol}^2 + 30.80(\pm 13.25)$ $n = 10, \quad r^2 = 0.838, \quad s = 0.163, \quad q^2 = 0.708$ *inversion point* : 2.97(2.88–3.18) *outliers* : C_4H_9, $CH(C_2H_5)_2$, $CH(CH_3)CH_2CH(CH_3)_2$; $(CH_2)_2C_6H_5$
QSAR Model 3	$\log 1/C = -0.05(\pm 0.02)\mathrm{NVE} + 1.64(\pm 0.44)C\pi_X + 12.09(\pm 3.22)$ $n = 10, \quad r^2 = 0.924, \quad s = 0.232, \quad q^2 = 0.843$ *outliers* : $X = CH_3, Y = CH(CH_3)_2$; $X = C_2H_5, Y = C_2H_5$; $X = C_2H_5, Y = CH_2CH_2OH$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** C is the molar concentration of a compound. ClogP is the calculated octanol/water partition coefficient. Cπ and π are the calculated and experimentally obtained hydrophobic parameters for the substituents. MR is the molar refractivity and is defined by the Lorentz–Lorenz equation: $MR = n^2 - 1/n^2 + 2(MW/\delta)$, where n = refractive index, δ = density, and MW = molecular weight. CMR is the

	calculated molar refractivity. Molar refractivity (MR) has a strong correlation with the molecular polarizability. Number of valence electrons (NVE) is a parameter that was found to be another approach to understanding polarizability and calculated by simply summing up the valence electrons in a molecule, for example, H = 1, C = 4, Si = 4, N = 5, P = 5, O = 6, S = 6, and halogens = 7. There are three commonly encountered electronic parameters: σ, σ^-, and σ^+ that account for specific electronic effects of substituents on aromatic systems. These parameters are known as the Hammett parameters and their application has been illustrated. MgVol is the molar volume calculated by C-QSAR Program using the method of Abraham and McGowan. *I* is an indicator variable that takes the value of 1 or 0 for structural features that cannot be defined by the normal parameters. In QSAR equation, *n* is the number of data points, *r* is the correlation coefficient, r^2 is the goodness of fit, q^2 is the goodness of prediction, and *s* is the standard deviation.
Reference	A QSAR study on influenza neuraminidase inhibitors. *Bioorganic & Medicinal Chemistry* 14 (2006) 982–996

Target Species	Influenza virus
Chemical Type	Isoquinolines
Mode of Action	Inhibitor
QSAR Model 1	$\log 1/C = 0.28(\pm 0.08)\pi + 0.16(\pm 0.09)\sigma^+ + 2.62(\pm 0.06)$ $n = 14, \quad r^2 = 0.868, \quad s = 0.079, \quad q^2 = 0.728$ *outliers* : 4-Br; 4-CN
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** C is the molar concentration of a compound. ClogP is the calculated octanol/water partition coefficient. Cπ and π are the calculated and experimentally obtained hydrophobic parameters for the substituents. MR is the molar refractivity and is defined by the Lorentz–Lorenz equation: $MR = n^2 - 1/n^2 + 2(MW/\delta)$, where *n* = refractive index, δ = density, and MW = molecular weight. CMR is the calculated molar refractivity. Molar refractivity (MR) has a strong correlation with the molecular

	polarizability. Number of valence electrons (NVE) is a parameter that was found to be another approach to understanding polarizability and calculated by simply summing up the valence electrons in a molecule, for example, H = 1, C = 4, Si = 4, N = 5, P = 5, O = 6, S = 6, and halogens = 7. There are three commonly encountered electronic parameters: σ, σ^-, and σ^+ that account for specific electronic effects of substituents on aromatic systems. These parameters are known as the Hammett parameters and their application has been illustrated. MgVol is the molar volume calculated by C-QSAR Program using the method of Abraham and McGowan. *I* is an indicator variable that takes the value of 1 or 0 for structural features that cannot be defined by the normal parameters. In QSAR equation, *n* is the number of data points, *r* is the correlation coefficient, r^2 is the goodness of fit, q^2 is the goodness of prediction, and *s* is the standard deviation.
Reference	A QSAR study on influenza neuraminidase inhibitors. *Bioorganic & Medicinal Chemistry* 14 (2006) 982–996

Target Species	Influenza virus
Chemical Type	Pyrrolidines
Mode of Action	Inhibitor
QSAR Model 1	$\log 1/C = -27.72(\pm 17.70)\mathrm{MgVol} + 6.88(\pm 4.10)\mathrm{MgVol}^2 + 32.33(\pm 18.82)$ $n = 9, \quad r^2 = 0.896, \quad s = 0.236, \quad q^2 = 0.768$ *inversion point* : 2.02(1.80–2.09) *outliers* : $\mathrm{CON(C_2H_5)CH(CH_3)_2}$; $\mathrm{CON[CH(CH_3)_2]_2}$; $\mathrm{CON[(CH_2)_3OH]CH(CH_3)_2}$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** C is the molar concentration of a compound. ClogP is the calculated octanol/water partition coefficient. Cπ and π are the calculated and experimentally obtained hydrophobic parameters for the substituents. MR is the molar refractivity and is defined by the Lorentz–Lorenz equation: $MR = n^2 -$

	$1/n^2 + 2(MW/\delta)$, where n = refractive index, δ = density, and MW = molecular weight. CMR is the calculated molar refractivity. Molar refractivity (MR) has a strong correlation with the molecular polarizability. Number of valence electrons (NVE) is a parameter that was found to be another approach to understanding polarizability and calculated by simply summing up the valence electrons in a molecule, for example, H = 1, C = 4, Si = 4, N = 5, P = 5, O = 6, S = 6, and halogens = 7. There are three commonly encountered electronic parameters: σ, σ^-, and σ^+ that account for specific electronic effects of substituents on aromatic systems. These parameters are known as the Hammett parameters and their application has been illustrated. MgVol is the molar volume calculated by C-QSAR Program using the method of Abraham and McGowan. *I* is an indicator variable that takes the value of 1 or 0 for structural features that cannot be defined by the normal parameters. In QSAR equation, n is the number of data points, r is the correlation coefficient, r^2 is the goodness of fit, q^2 is the goodness of prediction, and s is the standard deviation.
Reference	A QSAR study on influenza neuraminidase inhibitors. *Bioorganic & Medicinal Chemistry* 14 (2006) 982–996

Target Species	Influenza virus
Chemical Type	Miscellaneous compounds
Mode of Action	Inhibitor
QSAR Model 1	$\log 1/C = 0.41(\pm 0.10)C\log P + 5.58(\pm 0.22)$ $n = 6, \quad r^2 = 0.972, \quad s = 0.141, \quad q^2 = 0.945$
QSAR Model 2	$\log 1/C = 2.24(\pm 1.12)\mathrm{CMR} - 10.00(\pm 8.1)$ $n = 5, \quad r^2 = 0.931, \quad s = 0.755, \quad q^2 = 0.724$
QSAR Model 3	$\log 1/C = 0.12(\pm 0.03)\mathrm{NVE} - 7.23(\pm 3.69)$ $n = 5, \quad r^2 = 0.981, \quad s = 0.249, \quad q^2 = 0.953$

QSAR Model 4	$\log 1/C = 0.11(\pm 0.05)\mathrm{NVE} - 5.96(\pm 6.55)$ $n = 7, \quad r^2 = 0.846, \quad s = 0.619, \quad q^2 = 0.774$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** C is the molar concentration of a compound. ClogP is the calculated octanol/water partition coefficient. Cπ and π are the calculated and experimentally obtained hydrophobic parameters for the substituents. MR is the molar refractivity and is defined by the Lorentz–Lorenz equation: $MR = n^2 - 1/n^2 + 2(MW/\delta)$, where n = refractive index, δ = density, and MW = molecular weight. CMR is the calculated molar refractivity. Molar refractivity (MR) has a strong correlation with the molecular polarizability. Number of valence electrons (NVE) is a parameter that was found to be another approach to understanding polarizability and calculated by simply summing up the valence electrons in a molecule, for example, H = 1, C = 4, Si = 4, N = 5, P = 5, O = 6, S = 6, and halogens = 7. There are three commonly encountered electronic parameters: σ, σ^-, and σ^+ that account for specific electronic effects of substituents on aromatic systems. These parameters are known as the Hammett parameters and their application has been illustrated. MgVol is the molar volume calculated by C-QSAR Program using the method of Abraham and McGowan. *I* is an indicator variable that takes the value of 1 or 0 for structural features that cannot be defined by the normal parameters. In QSAR equation, n is the number of data points, r is the correlation coefficient, r^2 is the goodness of fit, q^2 is the goodness of prediction, and s is the standard deviation.
Reference	A QSAR study on influenza neuraminidase inhibitors. *Bioorganic & Medicinal Chemistry* 14 (2006) 982–996

Target Species	Influenza virus
Chemical Type	Thiourea analogues
Mode of Action	Inhibitor

QSAR Model 1	$pIC_{50} = 3.2747 + 3.5165 * \text{shadow\_XYfrac} - 0.9702 * \text{Atype\_C\_25} + 0.0098 * \text{shadow\_XY} + 0.1182 * \text{Atype\_H\_47} - 0.6835 * \text{Atype\_C\_5}$ $N = 24;\ \text{LOF} = 0.106;\ r^2 = 0.854;\ r^2_{\text{adj}} = 0.814;\ F\text{-test} = 21.081;$ $\text{LSE} = 0.036;\ r = 0.924;\ q^2 = 0.748$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** **Descriptor type** (Descriptors): **Structural** (Molecular weight, number of chiral centers, number of rotatable bonds, number of hydrogen-bond acceptors, number of hydrogen-bond donors); **Electronic (**Sum of atomic polarizabilities, sum of partial charges, sum of formal charges, dipole moment, energy of highest ccupied orbital (HOMO), energy of lowest unoccupied orbital (LUMO), superdelocalizability); **Topological (**Kier and Hall molecular connectivity index, Wiener index, Zagreb index, Hosoya index, Balaban indices); **E-state indices** (Electrotopological-state indices); **Spatial** (Jurs descriptors, radius of gyration, PMI, area, shadow indices, density, Vm); **Thermodynamic** (Molar refractivity, heat of formation, log of the partition coefficient, log of the partition coefficient atom type value, desolvation free energy of water, desolvation free energy of octanol). N is number of compounds in training set, LOF is lack of fit score, r^2 is squared correlation coefficient, r^2_{adj} is square of adjusted correlation coefficient, F-test is a variance related static which compares two models differing by one or more variables to see if the more complex model is more reliable than the less complex one, the model is supposed to be good if the F-test is above a threshold value, LSE is least square error, r is correlation coefficient, q^2 is the square of the correlation coefficient of the cross validation.
Reference	Quantitative structure activity relationship studies on thiourea analogues as influenza virus neuraminidase inhibitors. *European Journal of Medicinal Chemistry* 43 (2008) 293-299