Target Name	HIV-1 reverse transcriptase
Target TTD ID	TTDS00317

Target Species	Human immunodeficiency virus 1
Chemical Type	2-amino-6-arylsulfonylbenzonitriles
Mode of Action	Inhibitor
QSAR Model 1	$pC_1 = 0.573(\pm0.377)S_4 - 0.129(\pm0.043)S_C - 6.281 \times (\pm5.091)S_{15} + 0.992(\pm0.643)I_{o-OMe} - 0.921(\pm0.589)I_{m-CF_3} + 1.546(\pm0.698) \times [^1\chi^v]_{ma} + 2.680(\pm0.813)[^1\chi^v]_{mb} - 0.530 \times (\pm0.408)[^1\chi^v]^2_{ma} + 58.024(\pm46.265)$ $n = 64, Q^2 = 0.724, R^2_a = 0.775, R^2 = 0.804, R = 0.897, F = 28.2(df 8, 55), s = 0.461,$ $AVRES = 0.339, SDEP = 0.508, S_{PRESS} = 0.548, PRESS = 16.5, Pres_{av} = 0.404$
QSAR Model 2	$pC_1 = 0.572(\pm0.356)S_4 - 0.132(\pm0.040)S_C - 5.656 \times (\pm4.841)S_{15} + 0.942(\pm0.610)I_{o-OMe} - 0.840(\pm0.561)I_{m-CF_3} + 1.354(\pm0.675) \times [^1\chi^v]_{ma} + 2.767(\pm0.772)[^1\chi^v]_{mb} - 0.492 \times (\pm0.387)[^1\chi^v]^2_{ma} + 52.376(\pm43.989)$ $n = 63, Q^2 = 0.750, R^2_a = 0.794, R^2 = 0.821, R = 0.906, F = 30.9(df 8, 54), s = 0.437,$ $AVRES = 0.326, SDEP = 0.477, S_{PRESS} = 0.515, PRESS = 14.3, Pres_{av} = 0.388$
QSAR Model 3	$pC_1 = 0.605(\pm0.342)S_4 - 0.134(\pm0.039)S_C - 5.350 \times (\pm4.644)S_{15} + 0.906(\pm0.585)I_{o-OMe} - 0.825(\pm0.538)I_{m-CF_3} + 1.431(\pm0.650) \times [^1\chi^v]_{ma} + 2.651(\pm0.746)[^1\chi^v]_{mb} - 0.539 \times (\pm0.373)[^1\chi^v]^2_{ma} + 49.566(\pm42.201)$ $n = 62, Q^2 = 0.770, R^2_a = 0.811, R^2 = 0.836, R = 0.914, F = 33.7(df 8, 53), s = 0.418,$ $AVRES = 0.314, SDEP = 0.457, S_{PRESS} = 0.495, PRESS = 13.0, Pres_{av} = 0.374$
QSAR Model 4	$pC_1 = 0.681(\pm0.228)S_4 + 1.109(\pm0.206)I + 0.635(\pm0.479)I_{o-OMe} + 0.411(\pm0.457) + 1.193(\pm0.524)[^1\chi^v]_{ma} + 2.102(\pm0.510)[^1\chi^v]_{mb} - 0.639(\pm0.292)[^1\chi^v]^2_{ma}$

	$n = 63, Q^2 = 0.823, R_a^2 = 0.840, R^2 = 0.856, R = 0.925, F = 55.4(df6, 56), s = 0.385,$ $AVRES = 0.275, SDEP = 0.402, S_{\text{PRESS}} = 0.426, PRESS = 10.2, \text{Pr}es_{\text{av}} = 0.308$
QSAR Model 5	$pC_2 = -0.111(\pm0.050)S_C - 1.231(\pm0.604)I_{\text{m}-\text{CF}_3} + 1.615(\pm0.863)[^1\chi^v]_{\text{ma}}$ $+ 2.431(\pm0.769)[^1\chi^v]_{\text{mb}} - 0.796(\pm0.480)[^1\chi^v]^2_{\text{ma}} + 2.209(\pm0.490)$ $n = 51, Q^2 = 0.603, R_a = 0.660, R^2 = 0.694, R = 0.833, F = 20.4(df5, 45), s = 0.583,$ $AVRES = 0.470, SDEP = 0.624, S_{\text{PRESS}} = 0.664, PRESS = 19.9, \text{Pr}es_{\text{av}} = 0.535$
QSAR Model 6	$pC_2 = 0.904(\pm0.300)I - 1.095(\pm0.536)I_{\text{m}-\text{CF}_3} + 1.747(\pm0.772)[^1\chi^v]_{\text{ma}}$ $+2.430(\pm0.685)[^1\chi^v]_{\text{mb}} - 0.879(\pm0.430)[^1\chi^v]^2_{\text{ma}} + 1.695(\pm0.458)$ $n = 51, Q^2 = 0.685, R_a^2 = 0.730, R^2 = 0.757, R = 0.870, F = 28.0(df5, 45), s = 0.520,$ $AVRES = 0.415, SDEP = 0.556, S_{\text{PRESS}} = 0.591, PRESS = 15.7, \text{Pr}es_{\text{av}} = 0.467$
QSAR Model 7	$pC_2 = 0.853(\pm0.284)I - 0.819(\pm0.544)I_{\text{m}-\text{CF}_3} + 1.669(\pm0.727)[^1\chi^v]_{\text{ma}}$ $+2.601(\pm0.655)[^1\chi^v]_{\text{mb}} - 0.852(\pm0.404)[^1\chi^v]^2_{\text{ma}} + 1.719(\pm0.425)$ $n = 50, Q^2 = 0.731, R_a^2 = 0.763, R^2 = 0.787, R = 0.887, F = 32.5(df5, 44), s = 0.487,$ $AVRES = 0.396, SDEP = 0.514, S_{\text{PRESS}} = 0.548, PRESS = 13.2, \text{Pr}es_{\text{av}} = 0.452$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** First order valence molecular connectivity ($^1\chi^v$)= $\sum_{i<j}(\delta_i^v \delta_{ji}^v)^{-0.5}$ δ_i^v stands for valence δ value of atom i. **Parameter** - definition: $\mathbf{I_p}$ - Indicator variable having value 1 if para substituent is present, value 0 otherwise; **I** - Indicator variable having value 1 for sullfonyl compounds, value 0 otherwise; $\mathbf{I_{2m\text{-}Me}}$ - Indicator variable having value 1 if bi-meta-methyl substituents are present, value 0 otherwise; $\mathbf{I_{o\text{-}OMe}}$ - Indicator variable having value 1 if ortho-methoxy substituent is present, value 0 otherwise; $\mathbf{I_{m\text{-}CF3}}$ - Indicator variable having value 1 if meta-trifluoromethyl substituent is present, value 0 otherwise.
Reference	QSAR modeling of HIV-1 reverse transcriptase inhibitor 2-amino-6-arylsulfonylbenzonitriles and congeners using molecular connectivity and E-state parameters. *Bioorganic & Medicinal Chemistry* 12 (2004) 745–754

Target Species	Human immunodeficiency virus 1
Chemical Type	Quinazolinones
Mode of Action	Inhibitor
Activity Type	Wild-type HIV-1 inhibitory activity study
QSAR Model 1	$pIC_{90} = 6.114(\pm0.3) - 0.0738(\pm0.008)\ Rww + 6.437(\pm1)\ LDip + 1.408(\pm0.2)\ Mor21m + 1.000(\pm0.2)\ Mor31u + 1.242(\pm0.3)\ Mor32m - 1.210(\pm0.3)\ MATS5e - 0.768(\pm0.2)\ DISPe$ $N = 154,\ R = 0.7866,\ S = 0.419,\ F = 33.861\quad R_{loo} = 0.7592,\ S_{loo} = 0.431$ $R_{l\text{-}20\%\text{-}o} = 0.6667,\ S_{l\text{-}20\%\text{-}o} = 0.496$
QSAR Model 2	$pIC_{90} = 5.936(\pm0.6) - 0.638(\pm0.09)\ AECC + 2.289(\pm0.5)\ BELe2 + 0.211(\pm0.05)\ TE2 + 0.121(\pm0.03)\ RDF090v + 1.651(\pm0.3)\ Mor21v - 0.658(\pm0.1)\ nCq - 0.366(\pm0.07)\ nHDon$ $N = 154,\ R = 0.7953,\ S = 0.412,\ F = 35.892\quad R_{loo} = 0.7682,\ S_{loo} = 0.423$ $R_{l\text{-}20\%\text{-}o} = 0.7129,\ S_{l\text{-}20\%\text{-}o} = 0.467$
QSAR Model 3	$pIC_{90} = 0.747(\pm1) - 0.204(\pm0.02)\ MDDD + 0.364(\pm0.06)\ TE2 + 1.846(\pm0.3)\ Mor23e - 3.612(\pm0.5)\ Mor23v + 0.539(\pm0.1)\ Mor16e + 0.730(\pm0.2)\ Mor21m + 0.972(\pm0.2)\ MAXDP$ $N = 154,\ R = 0.7991,\ S = 0.408,\ F = 36.856\ R_{loo} = 0.7760,\ S_{loo} = 0.417$
QSAR Model 4	$pIC_{90} = 0.598(\pm1) - 0.199(\pm0.03)\ MDDD + 0.331(\pm0.08)\ TE2 + 1.876(\pm0.4)\ Mor23e - 3.578(\pm0.6)\ Mor23v + 0.588(\pm0.2)\ Mor16e + 0.737(\pm0.3)\ Mor21m + 1.013(\pm0.3)\ MAXDP$ $N = 100,\ R = 0.7918,\ S = 0.421,\ F = 22.093\ R_{loo} = 0.7700,\ S_{loo} = 0.430$ $N = 54,\ R_{val} = 0.8095,\ S_{val} = 0.421$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**

	Molecular descriptor - Type - Description: Rww - Topological - Reciprocal hyper-detour index; LDip – Charge - Local dipole index; Mor21m - 3D-MoRSE - 3D-MoRSE—signal 21/weighted by atomic masses; Mor21m - 3D-MoRSE - 3D-MoRSE—signal 21/unweighted; Mor32m - 3D-MoRSE - 3D-MoRSE—signal 32/weighted by atomic masses; MATS5e - 2D Autocorrelations - Moran autocorrelation—lag 5/weighted by atomic Sanderson electronegativities; DISPe - Geometrical - D COMMA2 value/weighted by atomic Sanderson electronegativities; AECC - Topological - Average eccentricity; BELe2 – BCUT - Lowest eigenvalue no. 2 of Burden matrix/weighted by atomic Sanderson electronegativities; TE2 - Charge - Topographic electronic descriptor (bond restricted); RDF090v - RDF - Radial distribution function—9.0 weighted by atomic van der Waals volumes; Mor21v - 3D-MoRSE - 3D-MoRSE—signal 21/weighted by atomic Van der Waals volumes; nCq - Functional groups - Number of total quaternary C(sp^3); nHDon - Functional groups - Number of donor atoms for H-bonds (with N and O); MDDD - Topological - Mean distance degree deviation; Mor23e - 3D-MoRSE - 3D-MoRSE—signal 23/weighted by atomic Sanderson electronegativities; Mor23v - 3D-MoRSE - 3D-MoRSE—signal 23/weighted by atomic Van der Waals volumes; Mor16e - 3D-MoRSE - 3D-MoRSE—signal 16/weighted by atomic Sanderson electronegativities; MAXDP - Topological - Maximal electrotopological positive variation; De – WHIM - D total accessibility index/weighted by atomic Sanderson electronegativities; SRW05 - Molecular walk counts - Self-returning walk count of order 05; RDF115u - RDF - Radial distribution function—11.5 unweighted; Mor02e - 3D-MoRSE - 3D-MoRSE—signal 23/weighted by atomic Sanderson electronegativities; H-051 - Atom-centred fragments - H-attached to alfa-C; H3v - GETAWAY - H autocorrelation of lag 3/weighted by atomic van der Waals volumes; H8e - GETAWAY - H autocorrelation of lag 8/weighted by atomic Sanderson electronegativities; GATS1v - 2D - Autocorrelations Geary autocorrelation—lag 1/weighted by atomic van der Waals volumes; SPAM - Geometrical - Average span R; RDF065u – RDF - Radial distribution function—6.5 unweighted; Mor21u - 3D-MoRSE - 3D-MoRSE—signal 21/unweighted; E2e - WHIM - 2nd component accessibility directional WHIM index/weighted by atomic Sanderson electronegativities; HATS8v - GETAWAY - Leverage-weighted autocorrelation of lag 8/weighted by atomic van der Waals volumes; N-072 - Atom-centred fragments - RCO-N< / >N-X=X; Mor11u - 3D-MoRSE - 3D-MoRSE—signal 11/unweighted; Mor14u - 3D-MoRSE - 3D-MoRSE—signal 14/unweighted; RDF045p - RDF - Radial distribution function—4.5 weighted by atomic polarizabilities; Dp - WHIM - D total accessibility index/weighted by atomic polarizabilities; H8m - GETAWAY - H autocorrelation of lag 8/weighted by atomic masses; BELe4 - BCUT - Lowest eigenvalue no. 4 of Burden matrix/weighted by atomic Sanderson electronegativities.

Reference	QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase. *Bioorganic & Medicinal Chemistry* 14 (2006) 5876–5889

Target Species	Human immunodeficiency virus 1
Chemical Type	Quinazolinones
Mode of Action	Inhibitor
Activity Type	HIV-1 reverse transcriptase mutant K-103N inhibitory acitivity
QSAR Model 1	$pIC_{90} = 1.576(\pm1) + 1.118(\pm0.1)$ N-072 $- 1.007(\pm0.1)$ Mor11u $- 1.081(\pm0.2)$ Mor14u $+ 0.116(\pm0.02)$ RDF045p $+ 7.756(\pm2)$ Dp $- 4.096(\pm0.9)$ H8m $- 2.040(\pm0.7)$ BELe4
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Molecular descriptor - Type - Description: Rww - Topological - Reciprocal hyper-detour index; LDip – Charge - Local dipole index; Mor21m - 3D-MoRSE - 3D-MoRSE—signal 21/weighted by atomic masses; Mor21m - 3D-MoRSE - 3D-MoRSE—signal 21/unweighted; Mor32m - 3D-MoRSE - 3D-MoRSE—signal 32/weighted by atomic masses; MATS5e - 2D Autocorrelations - Moran autocorrelation—lag 5/weighted by atomic Sanderson electronegativities; DISPe - Geometrical - D COMMA2 value/weighted by atomic Sanderson electronegativities; AECC - Topological - Average eccentricity; BELe2 – BCUT - Lowest eigenvalue no. 2 of Burden matrix/weighted by atomic Sanderson electronegativities; TE2 - Charge - Topographic electronic descriptor (bond restricted); RDF090v - RDF - Radial distribution function—9.0 weighted by atomic van der Waals volumes; Mor21v - 3D-MoRSE - 3D-MoRSE—signal 21/weighted by atomic Van der Waals volumes; nCq - Functional groups - Number of total quaternary C(sp^3); nHDon - Functional groups - Number of donor atoms for H-bonds (with N and O); MDDD - Topological - Mean distance degree deviation; Mor23e - 3D-MoRSE - 3D-MoRSE—signal 23/weighted by atomic Sanderson electronegativities; Mor23v - 3D-MoRSE - 3D-MoRSE—signal 23/weighted by atomic Van der Waals volumes; Mor16e - 3D-MoRSE - 3D-MoRSE—signal 16/weighted by atomic Sanderson electronegativities;

	MAXDP - Topological - Maximal electrotopological positive variation; De – WHIM - D total accessibility index/weighted by atomic Sanderson electronegativities; SRW05 - Molecular walk counts - Self-returning walk count of order 05; RDF115u - RDF - Radial distribution function—11.5 unweighted; Mor02e - 3D-MoRSE - 3D-MoRSE—signal 23/weighted by atomic Sanderson electronegativities; H-051 - Atom-centred fragments - H-attached to alfa-C; H3v - GETAWAY - H autocorrelation of lag 3/weighted by atomic van der Waals volumes; H8e - GETAWAY - H autocorrelation of lag 8/weighted by atomic Sanderson electronegativities; GATS1v - 2D - Autocorrelations Geary autocorrelation—lag 1/weighted by atomic van der Waals volumes; SPAM - Geometrical - Average span R; RDF065u – RDF - Radial distribution function—6.5 unweighted; Mor21u - 3D-MoRSE - 3D-MoRSE—signal 21/unweighted; E2e - WHIM - 2nd component accessibility directional WHIM index/weighted by atomic Sanderson electronegativities; HATS8v - GETAWAY - Leverage-weighted autocorrelation of lag 8/weighted by atomic van der Waals volumes; N-072 - Atom-centred fragments - RCO-N< / >N-X=X; Mor11u - 3D-MoRSE - 3D-MoRSE—signal 11/unweighted; Mor14u - 3D-MoRSE - 3D-MoRSE—signal 14/unweighted; RDF045p - RDF - Radial distribution function—4.5 weighted by atomic polarizabilities; Dp - WHIM - D total accessibility index/weighted by atomic polarizabilities; H8m - GETAWAY - H autocorrelation of lag 8/weighted by atomic masses; BELe4 - BCUT - Lowest eigenvalue no. 4 of Burden matrix/weighted by atomic Sanderson electronegativities.
Reference	QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase. *Bioorganic & Medicinal Chemistry* 14 (2006) 5876–5889

Target Species	Human immunodeficiency virus 1
Target Location	Brain
Chemical Type	Pyridinone derivatives
Mode of Action	Inhibitor
QSAR Model 1	pIC_{50}= [1.68606(± 0.831985)] +πR [1.16113(± 0.385725)] +*MRR* [-0.156878(± 0.0788598)] +*FL* [-2.82229(± 3.63907)]

	n=15, r=0.896721, r^2=0.804108, variance=0.251497, std=0.501495, F=15.0511, r^2_{bs}=0.842882, Q^2 =0.643468, Spress =0.676562, SDEP=0.579373, TEST r^2pred=0.431562
QSAR Model 2	pIC_{50}= [1.8662(± 0.596524)] + *πR* [1.20788(± 0.2731)] + *MRR* [-0.166236(± 0.0558207)] + *FL* [-1.90143(± 2.6264)] n=14, r=0.954098, r^2=0.910303, variance=0.120888, std= 0.347689, F=33.82, r^2_{bs}=0.671036, Q^2=0.700404, Spress= 0.635435, SDEP=0.537041,TEST r^2pred =0.628856
QSAR Model 3	pIC_{50}= [1.06046(± 1.29273)] + *πR* [0.953597(± 0.450673)] + *MRR*[-0.115622(± 0.0915389)] +*BiR* [0.179027(± 0.329464)] n=15, r=0.883302, r^2=0.780222, variance=0.282164, std= 0.531191, F=13.0168, r^2_{bs}=0.826314, Q^2=0.609694, Spress=0.707882, SDEP= 0.606194, TEST r^2pred=0.814872
QSAR Model 4	pIC_{50}= [1.05834 (± 1.31004)] +*πR* [0.956304 (± 0.450923)] + *MRR* [-0.116159(± 0.0915962)] + *LR* [0.091635 (±0.171746)] n =15, r=0.882774, r^2=0.779291, variance = 0.28336, std=0.532315,F=12.9464, r^2_{bs},=0.814349, Q^2= 0.608752, Spress=0.708736, SDEP=0.606926, TEST r^2pred =0.818346
QSAR Model 5	pIC_{50}= [0.5653(± 2.03912)] + *πR* [-0.117623(± 3.79305)] + *σpR* [-2.38755(± 2.22205)] +*IVo/s* [-0.365691(± 1.03479)] + *BiR* [1.45512(± 2.27845)] +*BiiR* [-0.87684 (± 1.9205)] n=30, r=0.763969, r^2 = 0.583649 , std=0.732199, F=5.37364, Q^2=0.376359, Spress=0.896122 , SDEP=0.78464
QSAR Model 6	pIC_{50}= [0.528215(± 1.79612)] + *πR* [-0.250969(± 3.34209)]+*σpR* [-2.69733(± 1.97052)] +*IVo/s* [-0.365023(± 0.911366)]+*BiR* [1.31597(± 2.00935)] +*BiiR* [-0.721829(± 1.69535)] n=29, r=0.793441, r^2 = 0.629548, variance=0.413455, std=0.643005, F=6.23115
QSAR Model 7	pIC_{50}= [0.4947(± 1.60288)] + *πR* [-0.37148 (± 2.98367)]+*σpR* [-2.97729 (± 1.77249)] + *IVo/s* [-0.36442(± 0.8132)]+*BiR* [1.19021(± 1.79574)] +*BiiR* [-0.581739(± 1.51689)] n = 28 , r= 0.820661 , r^2 = 0.673485 std = 0.572094, F=7.21925, Q^2 = 0.427777, Spress=0.757353, SDEP=0.655887 , TEST r^2 = 0.673485
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Terms and Definition of Indicator Variables: *πR*: Hydrophobic constant for substituent at R position; *σpR*: Electronic parameter sigma at para

	position of substituent R; IVo/s: Indicator parameter having 1 if oxygen is present at X position of pyridinone ring, value 0 otherwise; BiR: STERIMOL constant for substituent at R position (width parameter); MRL: Molar refractivity (steric parameter) for substituent at L position; LR: STERIMOL constant for substituent at R position (Length parameter); $BiiR$: STERIMOL constant for substituent at R position (width parameter); FL: Field effect for substituent at L position. n is number of compounds, r is correlation coefficient, std, F, r^2_{bs}, Q^2, Spress, SDEP are standard deviation, probability factor related to F-ratio, bootstrapping squared correlation coefficient,
Reference	QSAR Study on Pyridinone Derivatives as HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitor: A Mixed Approach. *Medicinal Chemistry*, 2007, *3*, 227-232 227