Target Name	Vitamin D receptor (VDR)
Target TTD ID	TTDS00251

Target Species	Human
Chemical Type	Analogues of 1α,25-dihydroxyvitamin D_3
Mode of Action	Binder
QSAR Model 1	$-\log(\text{VDR}) = -3.648 - 7.853 \cdot L2m + 36.997 \cdot P1m - 8.645 \cdot L1v + 25.155 \cdot E1v - 24.251 \cdot E1e + 3.245 \cdot P2s + 7.603 \cdot Tu + 70.642 \cdot Dm$ $N = 86 \quad R = 0.857 \quad S = 0.734 \quad F_{\text{exp}} = 26.72 \quad p < 10^{-5} \quad q^2_{\text{LOO}} = 0.675$ $S_{\text{LOO}} = 0.813 \quad q^2_{\text{LGO}} = 0.653 \quad S_{\text{LGO}} = 0.849.$
QSAR Model 2	$-\log(\text{VDR}) = -1.032 - 0.358 \cdot {}^{1}\Omega L2m - 0.714 \cdot {}^{2}\Omega E1e - 0.273 \cdot {}^{3}\Omega L1v + 0.459 \cdot {}^{5}\Omega Dm + 0.631 \cdot {}^{4}\Omega E1v$ $N = 86 \quad R = 0.847 \quad S = 0.744 \quad F_{\text{exp}} = 40.537 \quad p < 10^{-5} \quad q^2 = 0.679 \quad S_{\text{cv}} = 0.793$ $q^2_{\text{LGO}} = 0.652 \quad S_{\text{LGO}} = 0.841$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *E*1*v*, *E*1*e*, *Dm*, variables encoding atomic distribution; *L*2*m* and *L*1*v*, variables encoding size; *N*, number of compounds used; *R*, correlation coefficient; *S*, standard deviation of regression; *F*exp, Fisher ratio at 95% confidence level; *p*, significance of the variables in the model; q^2_{LOO}, S_{LOO}, q^2_{LGO}, $S_{LGO,}$ square of correlation coefficient and standard deviation of the leave-one-out and leave-group-out crossvalidation respectively; BCUT, Galvez topological charge indices, 2D autocorrelations, and WHIM descriptors. *N* is the number of compounds used, *R* is the correlation coefficient, *S* is the standard deviation of the regression, F_{exp} is the Fisher ratio at the 95% confidence level, *p* is the significance of the variables in the model, q^2_{LOO}, S_{LOO} and q^2_{LGO}, S_{LGO} are the square of the correlation coefficient and the standard

	deviation of the leave-one-out and leave-group-out cross-validation, respectively; Descriptors: P1m, P2s, Tu, L1v; Atomic distribution (E1v, E1e, and Dm) and size (L1v and L2m)
Reference	Quantitative structure–activity relationship studies of vitamin D receptor affinity for analogues of 1α,25-dihydroxyvitamin D3.1: WHIM descriptors. *Bioorganic & Medicinal Chemistry Letters* 15 (2005) 5165–5169

Target Species	Human
Chemical Type	1α,25-dihydroxyvitamin D_3
Mode of Action	Binder
QSAR Model 1	$-\log(\mathrm{VDR}) = 0.2666 \times \mathrm{RDF140m} - 0.236 \times \mathrm{RDF055m} + 0.119 \times \mathrm{RDF095e} + 0.095 \times \mathrm{RDF035m} - 0.268 \times \mathrm{RDF095m} - 1.547$ $N = 31, R^2 = 0.70, S = 0.49, F(5, 25) = 11.54, p < 10^{-5}$, AIC = 0.36, FIT = 1.03, $Q^2_{\mathrm{LOO}} = 0.56$, $S_{\mathrm{LOO}} = 0.54$, $q^2_{\mathrm{BOOT}} = 0.50$, $a(R^2) = 0.12$, $a(Q^2) = -0.37$, $R^2_{\mathrm{EXT}} = 0.33$
QSAR Model 2	$-\log(\mathrm{VDR}) = 0.337 \times \mathrm{RDF140m} - 0.205 \times \mathrm{RDF055m} + 0.160 \times \mathrm{RDF095e} + 0.427 \times \mathrm{RDF035m} - 0.241 \times \mathrm{RDF035v} - 0.311 \times \mathrm{RDF095m} - 1.648$ $N = 31, R^2 = 0.78, S = 0.42, F(6, 24) = 14.42, p < 10^{-5}$, AIC = 0.29, FIT = 1.29, $Q^2_{\mathrm{LOO}} = 0.67$, $S_{\mathrm{LOO}} = 0.57$, $q^2_{\mathrm{BOOT}} = 0.65$, $a(R^2) = 0.14$, $a(Q^2) = -0.45$, and $R^2_{\mathrm{EXT}} = 0.66$.
QSAR Model 3	$-\log(\mathrm{VDR}) = 1.119 - 0.181 \times {}^{1}\Omega\mathrm{RDF055m} + 0.128 \times {}^{2}\Omega\mathrm{RDF140m} - 0.315 \times {}^{6}\Omega\mathrm{RDF095m} - 0.171 \times {}^{5}\Omega\mathrm{RDF035v}$ $N = 31, R^2 = 0.75, S = 0.44, F(4, 26) = 19.73, p < 10^{-5}$, AIC = 0.26, FIT = 1.67, $Q^2_{\mathrm{LOO}} = 0.66$, $S_{\mathrm{LOO}} = 0.59$, $q^2_{\mathrm{BOOT}} = 0.64$, $a(R^2) = 0.08$, $a(Q^2) = -0.31$, and $R^2_{\mathrm{EXT}} = 0.73$.
QSAR Model 4	$-\log(\mathrm{VDR}) = 0.864 - 0.160 \times {}^{1}\Omega\mathrm{RDF055m} + 0.096 \times {}^{2}\Omega\mathrm{RDF140m} - 0.311 \times {}^{6}\Omega\mathrm{RDF095m} - 0.170 \times {}^{5}\Omega\mathrm{RDF035v}$

	$N = 30, R^2 = 0.80, S = 0.35, F(4, 25) = 24.91, p < 10^{-5}$, AIC = 0.17, FIT = 2.16, $Q^2_{\mathrm{LOO}} = 0.72$ $S_{\mathrm{LOO}} = 0.54$, $q^2_{\mathrm{BOOT}} = 0.70$, $a(\bar{R}^2) = 0.07$, $a(\bar{Q}^2) = -0.38$, $R^2_{\mathrm{EXT}} = 0.79$.
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ^{1}ΩRDF055m, ^{6}Ω RDF095m, and ^{2}Ω RDF140m, Radial Distribution Function weighted by atomic masses at 5.5, 9.5 and 14.0 A respectively; ^{5}Ω RDF035v, Radial Distribution Function weighted by atomic van der Waals volumes at 3.5 A; *N*, number of compounds included in the model; R^2, square of correlation coefficient; *S*, standard deviation of the regression; *F*, Fisher ratio; *p*, significance of the model; ρ, ratio between number of cases and adjustable parameter numbers; AIC, Akaike's information criterion; FIT, Kubinyi function; q^2_{LOO} and S_{LOO}, cross-validated squared regression coefficient and standard deviation of the LOO procedures respectively; q^2_{BOOT}, cross-validated squared regression coefficient of the Bootstarpping procedures; R^2_{EXT}, square of correlation coefficient of the external set. RDF descriptors: RDF035m, RDF055m, RDF095m, RDF140m, RDF035v, RDF095e; Constitutional descriptors: Ss, Ms, nBM, nCIR, RBF, nH; Geometrical descriptors: H3D, SPAN, SPAM, ASP, L/Bw, SEig; WHIM descriptors: G2u, E3e, P1p, G1p, Kp, Ds; GETAWAY descriptors: HGM, H8v, H8p, RARS, R4m+, R6e.
Reference	Radial Distribution Function descriptors for predicting affinity for vitamin D receptor. *European Journal of Medicinal Chemistry* 43 (2008) 1360-1365