Target Name	Thyrotropin-releasing hormone receptor
Target TTD ID	TTDR01197

Target Species	Human
Chemical Type	Thyrotropin-releasing hormone analogs
Mode of Action	Agonist
QSAR Model 1	$pEC_{50} = 40.8522 - 1.35 \times \langle C\text{-}038 \rangle - 0.67 \times \langle nCt \rangle - 12.71 \times \langle BEHm7 \rangle + 5.00 \times \langle GATS4P \rangle$ $N = 24$, LOF = 0.298, $r^2 = 0.954$, $r^2_{adj} = 0.945$, F-test = 99.265, LSE = 0.132, $q^2 = 0.929$, BS $r^2 = 0.955$, BS error = 0.000, $r^2_{pred} = 0.887$
QSAR Model 2	$pEC_{50} = -22.5786 - 30.2063 \times \langle MATS1p \rangle - 4.72172 \times \langle EEig14x \rangle + 155.38 \times \langle G2p \rangle + 2.97646 \times \langle H3u \rangle$ $N = 24$, LOF = 0.215, $r^2 = 0.960$, $r^2_{adj} = 0.952$, F-test = 115.220, LSE = 0.995, $q^2 = 0.961$, BS $r^2 = 0.961$, BS error = 0.000, $r^2_{pred} = 0.729$.
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** nCt, number of total tertiary C(sp3); BEHm7, highest Eigen value n.7 of burden matrix/weighted by atomic masses; GATS4p, Geary autocorrelation-lag 4/weighted by atomic polarizabilites; *N*, number of compounds in training set; LOF, lack of fit; r^2, squared correlation coefficient; r^2_{adj}, square of adjusted correlation coefficient; *F*-test, variance related statistic that determines whether the more complex model is more reliable than the less complex one; LSE, least-square error; q^2, square of the correlation coefficient of the cross-validation; r^2_{pred}, r^2-like statistic based on test set predictions derived from predicted sum of squared residuals (PRESS). ACI: (MATS1p) Moran autocorrelation-lag 1/weighted by atomic polarizabilites; AE: (EEIig14x) Eigen value 14 from edge adjacency matrix weighted by edge degrees; W/P(C): (G2p) Second component symmetry directional WHIM index/weighted by atomic polarizabilties; H: (H3u) H autocorrelation of lag 3/unweighted; C: (C-038) Al–C(=X)–Al where ‘‘X’’ = any electronegative

	atom (N, O, S, P, Se, and halogens); ‘‘Al’’ = aliphatic group; ‘‘=’’ = double bond; NX: (nCt) No. of total tertiary C(sp3); B: (BEHm7) Highest Eigen value n.7 of burden matrix/weighted by atomic masses; ACI: (GATS4p) Geary autocorrelation-lag 4/weighted by atomic polarizabilites.
Reference	Selectivity-based QSAR approach for screening and evaluation of TRH analogs for TRH-R1 and TRH-R2 receptors subtypes. *Journal of Molecular Graphics and Modelling* 27 (2008) 309–320