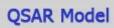
## **Therapeutic Targets Database**





Target Name	Estrogen receptor
Target TTD ID	TTDS00242

Target Species	Human
Chemical Type	Tetrahydroisoquinoline derivatives
Mode of Action	Modulator
QSAR Model 1	$[pIC_{50}]_{\alpha}^{RLB} = 0.586(\pm 0.369)S_1 - 0.096(\pm 0.079)S_{15} + 2.764$ $- 0.158(\pm 0.091) \log P$ $n = 21,  R_a^2 = 0.613,  R^2 = 0.671,  R = 0.819,$ $F = 11.6 \text{ (df } 3, 17),  s = 0.112,  \text{AVRES} = 0.087,$ $Q^2 = 0.512,  \text{SDEP} = 0.122,  S_{PRESS} = 0.136,  \text{Pres}_{av} = 0.107$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: MoDel and e-dragon Hydrophobicity (log $P$ ) and molar refractivity (MR), Electrotopological state (E-state), mathematically defined as: $S_i = I_i + \Delta I_i$ $I = \left[\left(\frac{2}{N}\right)^2 \delta^V + 1\right]/\delta \text{ and } \Delta I_i = \sum (I_i - I_j)/r_{ij}^2$ $I$ is the intrinsic state of an atom, $\Delta I_i$ is the perturbation effect, $N$ is the principal quantum number, $\delta$ is the number of sigma electrons on the atom (excluding those bonding to hydrogen), $\delta^V$ is the number of valence electrons (excluding those bonding to hydrogen), $i$ and $i$ are serial numbers of atoms and $i$ is the shortest graph distance between two atoms $i$ and $i$ plus one.
Reference	QSAR of estrogen receptor modulators: exploring selectivity requirements for $ER_{\alpha}$ versus $ER_{\beta}$

binding of tetrahydroisoquinoline derivatives using E-state and physicochemical parameters.	
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