Target Name	Estrogen receptor
Target TTD ID	TTDS00242

Target Species	Human
Chemical Type	Tetrahydroisoquinoline derivatives
Mode of Action	Modulator
QSAR Model 1	$[\mathrm{pIC}_{50}]_{\alpha}^{\mathrm{RLB}} = 0.586(\pm 0.369)S_1 - 0.096(\pm 0.079)S_{15} + 2.764 - 0.158(\pm 0.091)\log P$ $n = 21, \quad R_a^2 = 0.613, \quad R^2 = 0.671, \; R = 0.819,$ $F = 11.6 \; (\mathrm{df} \; 3, 17), \quad s = 0.112, \quad \mathrm{AVRES} = 0.087,$ $Q^2 = 0.512, \; \mathrm{SDEP} = 0.122, \; S_{\mathrm{PRESS}} = 0.136, \quad \mathrm{Pres}_{\mathrm{av}} = 0.107$
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: $S_i = I_i + \Delta I_i$ $I = \left[\left(\frac{2}{N}\right)^2 \delta^V + 1\right]/\delta$ and $\Delta I_i = \sum(I_i - I_j)/r_{ij}^2$ I is the intrinsic state of an atom, ΔI_i is the perturbation effect, N is the principal quantum number, δ is the number of sigma electrons on the atom (excluding those bonding to hydrogen), δ^V is the number of valence electrons (excluding those bonding to hydrogen), i and j are serial numbers of atoms and r_{ij} is the shortest graph distance between two atoms i and j plus one.
Reference	QSAR of estrogen receptor modulators: exploring selectivity requirements for ER_α versus ER_β

	binding of tetrahydroisoquinoline derivatives using E-state and physicochemical parameters. *Bioorganic & Medicinal Chemistry Letters* 15 (2005) 957–961