Target Name	Estrogen receptor beta
Target TTD ID	TTDS00250

Target Species	Human
Chemical Type	Tetrahydroisoquinoline derivatives
Mode of Action	Modulator
QSAR Model 2	$[\mathrm{pIC}_{50}]_{\beta}^{\mathrm{RLB}} = -0.629(\pm 0.637)S_1 - 0.057(\pm 0.013)\mathrm{MR} + 8.192$ $n = 21, \quad R_a^2 = 0.796, \quad R^2 = 0.817, \quad R = 0.904,$ $F = 40.1 \ (\mathrm{df}\ 2, 18), \quad s = 0.205, \quad \mathrm{AVRES} = 0.147,$ $Q^2 = 0.768, \quad \mathrm{SDEP} = 0.213, \quad S_{\mathrm{PRESS}} = 0.231, \quad \mathrm{Pres}_{\mathrm{av}} = 0.169$
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