Target Name	Follicle stimulating hormone receptor
Target TTD ID	TTDS00438

Target Species	Human
Chemical Type	6-amino-4-phenyltetrahydroquinoline derivatives
Mode of Action	Antagonist
QSAR Model 1	$$_{P}IC_{50} = 1.300(\pm 0.283) I_{NH\text{–}(CO)[X\text{–}Y]} + 6.267(\pm 0.234),$$ $$n = 19,\ r = 0.744,\ r^2 = 0.554,\ r^2_{Adj} = 0.527,\ s = 0.574,\ F = 21.077,$$ $$p = 0.000,\ q^2 = 0.432,\ S_{press} = 0.647,\ SDEP = 0.612,\ DW = 1.440.$$
QSAR Model 2	$$_{P}IC_{50} = 1.501(\pm 0.253) I_{NH\text{–}(CO)[X\text{–}Y]} - 0.871(\pm 0.323)\, I_{sub[R_1]} + 6.267(\pm 0.200),$$ $$n = 19,\ r = 0.833,\ r^2 = 0.693,\ r^2_{Adj} = 0.655,\ s = 0.490,\ F = 18.08,\ p = 0.000,$$ $$q^2 = 0.567,\ S_{press} = 0.583,\ SDEP = 0.535,\ DW = 1.795.$$
QSAR Model 3	$$_{P}IC_{50} = 0.304(\pm 0.081) C\log P + 1.621(\pm 0.190)\, I_{NH\text{–}(CO)[X\text{–}Y]} - 1.079(\pm 0.245) I_{sub[R_1]} + 4.168(\pm 0.576),$$ $$n = 19,\ r = 0.918,\ r^2 = 0.843,\ r^2_{Adj} = 0.811,\ s = 0.363,\ F = 26.76,\ p = 0.000,$$ $$q^2 = 0.754,\ S_{press} = 0.453,\ SDEP = 0.403,\ DW = 2.576.$$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ClogP is the calculated partition coefficient of compounds in octanol/water and a measure of the hydrophobicity of compounds. CMR is the calculated molar refractivity based on the Lorentz–Lorentz equation, MR = $(n^2 - 1)/(n^2 + 2)$ MW/d, where n is the index of refraction, MW represents molecular

	weight of the compound and *d* is the density. An indicator variable designated as I with a relevant subscript was assigned 1.0 when a particular substituent or chemical feature is present and 0 if absent.
Reference	First QSAR report on FSH receptor antagonistic activity: Quantitative investigations on physico-chemical and structural features among 6-amino-4-phenyltetrahydroquinoline derivatives. *Bioorganic & Medicinal Chemistry Letters* 15 (2005) 4496–4501