Target Name	PPAR-α
Target TTD ID	TTDS00340

Target Species	Human
Chemical Type	2-Alkoxydihydrocinnamates
Mode of Action	Agonist
QSAR Model 1	pEC_{50}= [-0.502(± 0.409)] + σ_p [1.855(± 1.588)] + $\mathcal{R}$ [- 3.366(± 2.129)] n=13, r=0.812, r^2=0.660, SEE =0.444, F=9.698, Q^2=0.405, SPRESS = 0.587, SDEP=0.515
QSAR Model 2	pEC_{50}= [-4.640(± 1.450)] +HOF [-0.006(± 0.002)] +DI [- 0.347(± 0.136)] n=13, r=0.934, r^2=0.873, SEE=0.271, F=34.415, Q^2=0.776, SPRESS=0.360, SDEP=0.316
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *n* is the number of compounds; r, the correlation coefficient; SEE, standard error of estimation; Q^2, cross-validated squared correlation coefficient; SPRESS, predictive residual sum of square; SDEP, standard error of predictivity; F, F-ratio; D1, dipole moment of X-axis and D3, dipole moment of Z-axis; σ_p, Harmett's constant. structural indicator variable I_1 expresses 1 for presence of two carbon spacer between biphenyloxy and the central ring, I2 expresses 1 for presence of methyl and ethyl group at R2 and 0 for its absence. hydrophobic (π), steric (molar refractivity or MR) hydrogen acceptor (HA), hydrogen Donor (HD) and electronic (field effect or $\mathcal{F}$, resonance effect or $\mathcal{R}$ and Hammett's constant or σ_p); Logarithmic partition coefficient (LogP); Connolly accessible area (CAA), Connolly molecular area (CMA), Connolly solvent excluded volume (CSEV), exact mass (EM), molecular weight (MW), principal moment of inertia X-axis (PMIX); Electronic energy (EE), highest occupied molecular orbital energy

	(HOMO), lowest unoccupied molecular orbital energy (LUMO), dipole moment of X-axis (D1), dipole moment of Y-axis (D2), dipole moment of Z-axis (D3), resultant dipole (D4), repulsion energy (RE), VDW-1, 4-energy (E14), Non-1, 4-VDW energy (EV) and total energy (TE)
Reference	Quantitative Structure Activity Analysis of 2-Alkoxydihydrocinnamates as PPAR α/γ Dual Agonist. *Medicinal Chemistry*, 2008, *4*, 273-277