Target Name	Cyclooxygenase (COX)
Target TTD ID	TTDS00039

Target Species	Human
Chemical Type	4',5 di-substiuted biphenyl acetic acid molecules
Mode of Action	Inhibitor
QSAR Model 1	$\log CPE\% = -0.266 - 0.0085 f_3^N + 0.0488 f_{10}^E + 0.0429 \frac{\mu_k^+}{\mu_k^-} (k=3)$ $r^2 = 0.854 \quad q^2 = 0.776 \quad F = 27.257 \quad \sigma = 0.127$
QSAR Model 2	$\log CPE\% = 6.806 - 0.01474 f_3^N + 0.050 f_{10}^E + 0.634\,NICS(1) + 0.024 \frac{\mu_k^+}{\mu_k^-} (k=3)$ $r^2 = 0.916 \quad q^2 = 0.867 \quad F = 35.041 \quad \sigma = 0.100$
QSAR Model 3	$\log CPE\% = 9.762 - 0.019 f_3^N + 0.036 f_{10}^E + 0.818\,NICS(1)$ $r^2 = 0.895 \quad q^2 = 0.774 \quad F = 38.818 \quad \sigma = 0.108$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Chemical potential (μ): a useful global index of reactivity in atoms, molecules and clusters. f_k^a: a single value around each atomic site that characterize the atomic contribution in a molecule. logCPE% refers to the anti-inflammatory activity. f_3^N, f_{10}^E and $\frac{\mu_k^+}{\mu_k^-}$ (k=3): weighted nucleophilic frontier electron densities on atom 3, weighted electrophilic frontier electron densities on atom 10 and relative nucleophilic chemical potential on atom 3, respectively. r^2: the correlation coefficient. q^2: the cross-

	validated correlation coefficient using leave-one-out (LOO) method. σ: the standard error. F: F-test value.
Reference	Towards the design of Cyclooxygenase (COX) inhibitors based on 4′,5 di-substituted biphenyl acetic acid molecules: a QSAR study with a new DFT based descriptor – nucleus independent chemical shift. *J Mol Model* (2009) 15:1221–1228