Target Name	5-Lipoxygenase
Target TTD ID	TTDS00112

Target Species	Human
Chemical Type	1-phenyl[2H]-tetrahydro-triazine-3-one analogues
Mode of Action	Inhibitor
QSAR Model 1	$\log 1/IC_{50} = 5.7242\times10^{-4}\ (\pm 1.6440\times10^{-4})\ W - 0.6957\ (\pm 0.1504)\ MR_2 + 0.8529\ (\pm 0.1409)\ \pi_{3'} + 0.4773\ (\pm 0.0746)\ \pi_{5'} + 0.3533\ (\pm 0.0530)\ \pi_5 + 0.4473\ (\pm 0.1587)\ \Sigma\sigma_m - 0.6256\ (\pm 0.0421)\ \Sigma\sigma_p + 0.8187\ (\pm 0.1136)\ Ip_3 + 4.4393$ $n = 60,\ SE = 0.2316,\ R_A^2 = 0.7247,\ R = 0.8729,\ F = 20.414$
QSAR Model 2	$IC_{50} = 4.0849\times10^{-4}\ (\pm 2.0780\times10^{-4})\ W - 0.6496\ (\pm 0.1537)\ MR_2 + 0.0847\ (\pm 0.0683)\ MR_4 + 0.8699\ \pi_{3'} + 0.5021\ (\pm 0.0766)\ \pi_{5'} + 0.3739\ (\pm 0.0551)\ \pi_5 + 0.4751\ (\pm 0.1592)\ \Sigma\sigma_m - 0.6786\ (\pm 0.4117)\ \Sigma\sigma_p + 0.7406\ (\pm 0.1284)\ Ip_3 + 4.4582$ $n = 60,\ SE = 0.2302,\ R_A^2 = 0.7281,\ R = 0.8772,\ F = 18.551$
QSAR Model 3	$\log 1/IC_{50} = 0.0010\ (\pm 7.9403\times10^{-4})\ logRB - 0.6349\ (\pm 0.1524)\ MR_2 + 0.1269\ (\pm 0.0693)\ MR_4 + 0.8734\ (\pm 0.1131)\ \pi_5 + 0.4885\ (\pm 0.1552)\ \Sigma\sigma_m - 0.7100\ (\pm 0.4014)\ \Sigma\sigma_p + 0.6954\ (\pm 0.1256)\ Ip_3 - 0.2767\ (\pm 0.1352)\ Ip_4 + 4.50$ $n = 60,\ SE = 0.2242,\ R_A^2 = 0.7421,\ R = 0.8865,\ F = 17.981$
QSAR Model 4	$\log 1/IC_{50} = 2.8515\times10^{-4}\ (\pm 1.8793\times10^{-4})\ W - 0.6603\ (\pm 0.1341)\ MR_2 + 0.0929\ (\pm 0.0621)\ MR_4 + 0.7483\ (\pm 0.1272)\ \pi_{3'} + 0.6403\ (\pm 0.0754)\ \pi_{5'} + 0.5321(\pm 0.1017)\ \pi_5 + 0.6685\ (\pm 0.1471)\ \Sigma\sigma_m - 0.78\ (\pm 0.3588)\ \Sigma\sigma_p - 0.2792\ (\pm 0.0771)\ Ip_2 + 0.6501\ (\pm 0.1138)\ Ip_3 - 0.3088\ (\pm 0.1214)\ Ip_4 + 4.6535$ $n = 60,\ SE = 0.2007,\ R_A^2 = 0.7944,\ R = 0.9126,\ F = 21, 728$

QSAR Model 5	$\log 1/IC_{50} = 4.2510\times10^{-4}\ (\pm 1.2756\times10^{-4})\ W - 0.5156(\pm 0.0997)\ MR_2 + 0.0732\ (\pm 0.0415)\ MR_4 + 0.7097\ (\pm 0.0859)\ \pi_{3'} + 0.6150\ (\pm 0.0524)\ \pi_{5'} + 0.5351(\pm 0.0679)\ \pi_5 + 0.8970\ (\pm 0.1059)\ \Sigma\sigma_m - 0.9132\ (\pm 0.2396)\ \Sigma\sigma_p - 0.2670\ (\pm 0.0518)\ Ip_2 + 0.6715\ (\pm 0.0762)\ Ip_3 - 0.3648\ (\pm 0.0821)\ Ip_4 + 4.5975$ $n = 54,\ SE = 0.1325,\ R_A^2 = 0.9060, R = 0.9620,\ F = 47.446$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Molar refractivity (MR) of 2- and 4- substituents (MR_2 and MR_4), lipophilic effects of 3'-, 5'- and 5-substituents ($\pi_{3'}$, $\pi_{5'}$ and $\pi_{5'}$),sum of Hammett σ_m value for the 3'-, 5'-phenyl or α-pyridyl substituents ($\sum\sigma_m$) and sum of Hammett σ_P $^{\sigma_p}$ value for the 3'- and 5'-α--pyridyl substituents ($\sum\sigma_P$). Ip_1 is 1 when phenyl group is attached with N, Ip_2 and Ip_4 are 1 when hydrogen is not present at R_4 and $R_{5'}$. When $C = O$ is present at R_4 the indicator parameter is Ip_3 having the value of unity.
Reference	QSAR Study on 5-Lipoxygenase Inhibitors Using Distance-Based Topological Indices. *Bioorganic & Medicinal Chemistry* 11 (2003) 5519–5527

Target Species	Human
Chemical Type	2,6-di-*tert*-Butylphenol derivatives
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{50}(LOX) = 47.25(\pm 7.21)EHOMO + 19.57(\pm 2.20)$ $n = 14\ r^2 = 0.784\ Q^2 = 0.695\ s = 0.489\ F = 42.88$
QSAR Model 2	$pIC_{50}(LOX) = -37.09(\pm 7.13)Q_{ox} - 17.47(\pm 4.35)$ $n = 14\ r^2 = 0.693\ Q^2 = 0.626\ s = 0.589\ F = 27.08$
QSAR Model 3	$pIC_{50}(LOX) = 38.82(\pm 8.01)EHOMO + 0.16(\pm 0.08)ClogP + 16.25(\pm 2.70)$ $n = 14\ r^2 = 0.833\ Q^2 = 0.745\ s = 0.440\ F = 27.46$
QSAR Model 4	$pIC_{50}(LOX) = -0.13(\pm 0.02)Fe3^+ + 2.79(\pm 0.34)$ $n = 14\ r^2 = 0.823\ Q^2 = 0.792\ s = 0.440\ F = 55.88$

Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Atomic charges and the energies of the highest-occupied (EHOMO) and lowest unoccupied molecular (ELUMO) orbital. Hydrophobicity, the ClogP parameter20
Reference	QSAR Study of Dual Cyclooxygenase and 5-Lipoxygenase Inhibitors 2,6-di-tert-Butylphenol Derivatives. *Bioorganic & Medicinal Chemistry* 11 (2003) 4207–4216