Target Name	Type I fatty acid synthase (FAS)
Target TTD ID	TTDS00386

Target Species	Human
Chemical Type	3-aryl-4-hydroxyquinolin-2(1H)-one derivatives
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{50} = 1.418(MATS6e) + 13.117(AROM) + 0.073(Dx) + 3.658(qB5) + 0.054(DISPm) - 6.039$ $n = 15;\ R^2 = 0.878;\ SEC = 0.244;\ PRESS_{cal} = 0.715;\ F_{(2,12)} = 42.999(cF = 3.885);$ $Q^2_{LOO} = 0.796;\ SEV = 0.282;\ PRESS_{val} = 1.194(SS_Y = 5.842)$
QSAR Model 2	$pIC_{50} = 1.449(MATS6e) + 13.882(AROM) + 0.055(Dx) + 3.774(qB5) + 0.059(DISPm) - 6.799$ $n = 10;\ R^2 = 0.898;\ SEC = 0.256;\ PRESS_{cal} = 0.457;\ F_{(2,7)} = 30.982(cF = 4.737);$ $Q^2_{LOO} = 0.659;\ SEV = 0.392;\ PRESS_{val} = 1.535(SS_Y = 4.502)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** BIC5 - bond information content – neighborhood symmetry of 5-order, LP1 - Lovasz-Pelikan index,MATS1p –Moran autocorrelation lag 1 weighted by atomic polarizability, RNCG - relative negative charge, RDF125p - Radial Distribution Function 12.5 weighted by atomic polarizability, and E2u - 2nd component accessibility directionalWHIMindex unweighted, MATS6e - Moran autocorrelation lag 6 weighted by atomic Sanderson electronegativity, AROM - aromaticity index, DISPm - dCOMMA2 value weighted by atomic masses, Dx - dipole moment along the x-axis, and qB5 - partial Mulliken Charge of carbon 5 of the ring B
Reference	Multivariate SAR/QSAR of 3-aryl-4-hydroxyquinolin-2(1*H*)-one derivatives as type I fatty acid synthase (FAS) inhibitors. *European Journal of Medicinal Chemistry* 45 (2010) 5817-5826