Target Name	Proto-oncogene tyrosine-protein kinase LCK
Target TTD ID	TTDS00407

Target Species	Human
Chemical Type	Flavonoid derivatives
Mode of Action	Inhibitors
QSAR Model 1	$\log 1/IC_{50} = 0.1586(\pm 0.0784)\log P - 0.0799(\pm 0.0268)He + 0.6499 \times (\pm 0.2148)I_{NH} + 2.3047$ $n = 31,\ r = 0.8257,\ Se = 0.4067,\ F = 19.283,\ Q = 2.030$
QSAR Model 2	$\log 1/IC_{50} = 0.2071(\pm 0.0895)\log P - 0.1231(\pm 0.0473)He - 0.3169(\pm 0.2866)I_1 + 2.0029 + 0.5420(\pm 0.2351)I_{NH}$ $n = 31,\ r = 0.8343,\ Se = 0.4050,\ F = 14.887,\ Q = 2.06$
QSAR Model 3	$\log 1/IC_{50} = 0.1537(\pm 0.0940)\log P - 0.0803(\pm 0.0165)He - 0.4602(\pm 0.1711)I_3 + 2.8095$ $n = 39,\ r = 0.7948,\ Se = 0.4815,\ F = 17.125,\ Q = 1.650$
QSAR Model 4	$\log 1/IC_{50} = 0.1436(\pm 0.0942)\log P - 0.0739 \times (\pm 0.0174)He - 0.4184(\pm 0.1748)I_3 + 2.7485 + 0.2110(\pm 0.1930)I_{OH}$ $n = 39,\ r = 0.8036,\ Se = 0.48,\ F = 13.677,\ Q = 1.674$
QSAR Model 5	$\log 1/IC_{50} = 0.2214(\pm 0.0385)\log P - 0.0901(\pm 0.0102)He - 0.4746(\pm 0.1252)I_3 + 2.8080$ $n = 70,\ r = 0.7896,\ Se = 0.4603,\ F = 34.225,\ Q = 1.710$
QSAR Model 6	$\log 1/IC_{50} = 0.2360(\pm 0.0375)\log P - 0.0924(\pm 0.0098)He - 0.3664(\pm 0.1283)I_3 + 2.6814 + 0.3205(\pm 0.1309)I_{NH}$ $n = 70,\ r = 0.8107,\ Se = 0.4428,\ F = 29.238,\ Q = 1.83$
QSAR Model 7	$\log 1/IC_{50} = 0.0497(\pm 0.0068)He - 0.9622(\pm 0.1159)I_{NO_2} - 0.4557(\pm 0.1172)I_{OMe} + 2.9154$ $n = 104,\ r = 0.7783,\ Se = 0.4611,\ F = 48.148,\ Q = 1.688$

QSAR Model 8	$\log 1/IC_{50} = 0.1221(\pm 0.0292)\text{logP} - 0.0595(\pm 0.0077)\text{He} + 0.5677(\pm 0.1215)\text{I}_{\text{OH}} + 2.4257 + 0.7633(\pm 0.1145)\text{I}_{\text{NH}}$ $n = 104,\ r = 0.8032,\ \text{Se} = 0.4398,\ F = 42.267,\ Q = 1.826$
QSAR Model 9	$\log 1/\text{IC}_{50} = 0.1300(\pm 0.0291)\text{logP} - 0.0568(\pm 0.0077)\text{He} - 0.188(\pm 0.0999)\text{I}_3 + 2.5666 + 0.5591(\pm 0.1199)\text{I}_{\text{OH}} + 0.7137(\pm 0.1159)\text{I}_{\text{NH}}$ $n = 104,\ r = 0.8115,\ \text{Se} = 0.4337,\ F = 35.485,\ Q = 1.870$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** I1 is used for presence of –OH group at any position by 1; I3, indicates presence of substituents at R3position by I3=1 otherwise zero; INH indicates presence of amino group by INH=1, otherwise 0; I1 indicates presence of –OH group at any position by I1=1, otherwise 0; IOH indicates presence of –OH group on phenyl ring by IOH=1 otherwise 0; INO2 indicates presence of nitro group by INO2 =1, otherwise 0; IOMe indicates presence of methoxy group by IOMe=1, otherwise 0; Hydrophobic parameter (logP) and hydration energy (He); n is the number of compounds; Se is the standard error of estimation; r is the correlation coefficient; F is the F-static and Q is the quality factor=R/Se.
Reference	QSAR study of flavonoid derivatives as p56lck tyrosin kinase inhibitors. *Bioorganic & Medicinal Chemistry* 12 (2004) 1209–1214