Target Name	CCK-A receptor
Target TTD ID	TTDC00082

Target Species	Human
Chemical Type	1,4-benzodiazepine derivatives
Mode of Action	Antagonists
QSAR Model 1	$\log(1/IC_{50})_{CCK\text{-}A} = 2.642(\pm1.896)ClogP - 0.337(\pm0.265)(ClogP)^2 + 1.531 + 0.842(\pm0.556)I_{R1} + 1.464(\pm0.626)I_{R2} - 1.093(\pm0.955)I_X - 0.750(\pm0.620)I_R$ $n = 30, r = 0.901, s = 0.69, F_{6,23} = 16.54(3.71), (ClogP)_o = 3.92$
QSAR Model 2	$\log(1/IC_{50})_{CCK\text{-}A} = 3.229(\pm1.669)ClogP - 0.429(\pm0.235)(ClogP)^2 + 0.932 + 0.723(\pm0.491)I_{R1} + 1.268(\pm0.552)I_{R2} - 1.121(\pm0.817)I_X - 0.909(\pm0.541)I_R$ $n = 29, r = 0.926, s = 0.59, F_{6,22} = 22.16(3.76), (ClogP)_o = 3.76$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** I_{R1}, I_{R2}, and I_X stand, with a value of unity each, for the substituents R^1=CH_3, R^2=NHCO-*p*-chlorophenyl or NHCO-2-indolyl, and X=C1, respectively, and are zero in each case for the other substituents. The variable I_R is meant for the stereospecificity of R^2-substituents. n is the number of data points used to derive the equation, r is the correlation coefficient, s is the standard deviation, and F is the F-ratio between the variances of calculated and observed activities. LogP values of the compounds (P=octanol/water partition coefficient).
Reference	Quantitative Structure-Activity Relationship Study on Some Nonpeptidal Cholecystokinin Antagonists. *Bioorganic & Medicinal Chemistry* 7 (1999) 1127-1130