Target Name	CCK-B receptor
Target TTD ID	TTDS00043

Target Species	Human
Chemical Type	1,4-benzodiazepine derivatives
Mode of Action	Antagonists
QSAR Model 1	$\log(1/IC_{50})_{CCK\text{-}B} = 0.932(\pm 0.855)ClogP + 2.773(\pm 1.024)D_{R2} + 1.521$ $n = 12, r = 0.922, s = 0.67, F_{2,9} = 25.64$
QSAR Model 2	$\log(1/IC_{50})_{gastrin} = 1.281(\pm 0.820)ClogP + 1.912(\pm 0.963)D_{R2} + 0.292$ $n = 11, r = 0.921, s = 0.60, F_{2,8} = 22.49$
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