Target Name	Cannabinoid receptor 2
Target TTD ID	TTDC00314

Target Species	Human
Chemical Type	Indole-carbaldehyde derivatives
Mode of Action	Agonist
QSAR Model 1	Activity_1 = 4.41587 – 0.044168 * "Vm" + 0.288075 * "Shadow-Ylength" – 8.61825 * "CHI-V-3_C" + 0.10173 * "S_sCl" + 3.8733 *CHI-V-3_P" + 0.143023 * "Atype_C_25"
QSAR Model 2	Activity_2 = 4.23864 – 0.061214 * "Jurs-WPSA-3" - 0.578218 * "Kappa-1" + 3.43232 * "CHI-V-3_P" - 7.9442 * "CHI-V-3_C" + 0.28685 * "Shadow-Ylength" - 0.003465 * "Jurs-WNSA-2"
QSAR Model 3	Activity_3 = 3.4148 + 0.382564 * "Shadow-nu" + 0.60716 * "Kappa-1" + 3.34357 * "CHI-V-3_P" + 7.60251 * "CHI-V-3_C" + 0.421722 * "Shadow-Ylength" + 0.022095 * "MR"
QSAR Model 4	Activity_4 = 3.13947 – 0.415564 * "Kappa-1" + 3.24785 * "CHI-V-3_P" – 8.18443 * "CHI-V-3_C" + 0.374616 * "Shadow-Ylength" - 0.008721 * "MR" – 0.068866 * "Jurs-WPSA-3"
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Molar volume (Vm) is a steric descriptor or size descriptor representing the volume of the molecule. Atype_C_25 is one of the various atom type AlogP descriptors that are used to estimate the logP of molecule which characterizes the lipophilicity. Shadow indices (Shadow_Ylength) are a set of 3 dimensional geometric descriptors that help to characterize the size and shape of the molecules. The descriptors are calculated by projecting the molecular surface on three mutually perpendicular planes, XY, YZ, and XZ and van der waals radii for the atoms. Topological indices are 2 dimensional descriptors based on graph theory concepts. Kier & Hall valence-modified connectivity index (CHIV): This index is a refinement of the molecular connectivity index, where a vertex subgraph valence d is enhanced to dv to take into account electron

	configuration of the atom represented by the vertex: $$\delta^V = (Z^V - h)/(Z - Z^V - 1)$$ Where Z^V is the number of valence electrons in the atom, Z is its atomic number, and h is the number of hydrogens bound to it. This formula is designed to reproduce the unmodified molecular connectivity index for saturated hydrocarbons, for which $d^V = d$. However, d^V distinguishes between multiple and single bonds. The denominator introduces further distinction between element rows due to the presence of the atomic number Z. CHI-V-3 is a Kier & Hall valence-modified connectivity index of order 3. The connectivity indices are single valued parameters that can be calculated from the 2D graph representation of molecules. They characterize structures according to their size, degree of branching and overall shape. CHI-V-3_P has positive coefficient and CHI-V-3_C has negative coefficient. The atom-type E-state indices are molecular descriptors encoding topological and electronic information related to particular atom types in the molecule. They are calculated by summing the E-state values of all atoms of the same atom type in the molecule. S sCl is the sum of E-state indices for chlorine atoms with a single bond. Thus it is clear that the chlorine atoms and the electronic environment surrounding them are critical for CB2 agonistic activity.
Reference	QSAR Studies on some Calcium Channel Blockers. *Letters in Drug Design & Discovery*, 2008, 5, 307-312