

Target Name	Melanocortin-4 receptor
Target TTD ID	TTDC00072

Target Species	Human
Chemical Type	Trans-4-(4-chlorophenyl) pyrrolidine-3-carboxamides of piperazinecyclohexanes
Mode of Action	Binder
QSAR Model 1	$pK_i = -16.251(\pm 4.498) + 47.465(\pm 12.437)MSD + 12.540(\pm 1.759)BELe5$ $- 286.790(\pm 64.271)JGI9 - 0.125(\pm 0.027)RDF040m - 0.908(\pm 0.170)N-075$ $- 0.213(\pm 0.089)RDF010e + 0.439(\pm 0.138)C-008 + 0.462(\pm 0.110)C-026$
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>MSD is one of the topological descriptors, and it is the mean square distance index also called Balaban; BELe5 is the lowest eigenvalue n. 5 of Burden matrix/weighted by atomic Sanderson electro-negativities; JGI9 is the mean topological charge index of order 9; DF040m and RDF010e belong to the radial distribution function (RDF) descriptors; In these descriptors (RDF040m and RDF010e) weighting schemes are the atomic masses and the atomic Sanderson electro-negativities respectively, that show the mass and the electro-negativity of the molecules play a main role in these descriptors; (C-008, C-026, N-075) belong to the atom-centred fragment descriptors that describe each atom by its own atom type and the bond types and atom types of its first neighbours; The C-008, C-026 and N-075 descriptors, represent CHR_2X, $R-CX-R$ and $R-N-R/R-N-X$ respectively.</p>
Reference	QSAR study on melanocortin-4 receptors by support vector machine. <i>European Journal of Medicinal Chemistry</i> 45 (2010) 1087–1093