Target Name	Mu-type opioid receptor
Target TTD ID	TTDS00126

Target Species	Human
Chemical Type	4-phenylpiperidine derivatives
Mode of Action	Agonist
QSAR Model 1	$-\log ED_{50} = 20.637 - 48.722*CN + 0.585*DNO + 0.004*T_{O-4-3-N} + 0.373*PHI$ $N = 38, S = 0.598, R^2 = 0.647 q^2 = 0.577$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** **Descriptor**: Molecular descriptors (***Number of descriptors***) **Constitutional descriptors**: Molecular weight, number of atoms, number of non-H atoms, number of heteroatoms, number of multiple bonds, number of aromatic bonds, number of functional groups, number of rings, number of H-bond donors, etc. (***48***) **Topological descriptors**: Zagreb index, Quadratic index, Narumi simple topological index, Pogliani index, polarity number, Wiener W index, Balaban-type index, Kier symmetry index, Kier flexibility index, Randic shape index, etc. (***119***) **Connectivity indices**: Average valence connectivity index, salvation connectivity index, modified Randic connectivity index, reciprocal distance Randic-type index, etc. (***33***) **Geometrical descriptors**: 3D-Wiener index, 3D-Harary index, average geometric distance, gravitational index, HOMA total, aromaticity index, etc. (***74***) **Chemical parameters**: ClogP, molecular refractivity, polarizability, hydration energy, atomic charge, interatomic distance, etc. (***18***)
Reference	QSAR study of 4-phenylpiperidine derivatives as μ opioid agonists by neural network method.

	European Journal of Medicinal Chemistry 41 (2006) 226–232