| | |
|---|---|
| **Target Name** | $\sigma_1$ receptor |
| **Target TTD ID** | TTDS00129 |

| | |
|---|---|
| **Target Species** | Guinea Pigs |
| **Target Location** | Brain |
| **Chemical Type** | N-(3-phenylpropyl)-N'-benzylpiperazines |
| **Mode of Action** | Ligand |
| **QSAR Model 1** | $\mathrm{Log}(1/K_i) = -0.63(\pm 0.47) - 1.54(\pm 1.45)(\pi_x)^2 + 1.26(\pm 1.01)(\pi_x) + 0.96(\pm 0.79)\mathrm{MR} + 0.62(\pm 0.37)\sigma_{m,p}$, $n = 9;\ r^2 = 0.89;\ F_{4,8} = 7.93;\ s = 0.13;\ q^2 = 0.43;\ 0.01 < P < 0.05$ |
| **Molecular Descriptor** | Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**<br>*n* is the number of compounds; r, the correlation coefficient; s, the standard deviation; F, F-ratio; MR, molar refractivity; $\pi_x$, hydrophobicity and $\sigma_{m,p}$, sigma Hammett constant values for the corresponding meta and para-substituted compounds. |
| **Reference** | Synthesis and structure–activity relationships of N-(3-phenylpropyl)-N'-benzylpiperazines: Potent ligands for $\sigma_1$ and $\sigma_2$ receptors. *Bioorganic & Medicinal Chemistry* 16 (2008) 755–761 |