| | |
|---|---|
| **Target Name** | 5-$HT_6$ receptor |
| **Target TTD ID** | TTDC00185 |

| | |
|---|---|
| **Target Species** | Human |
| **Chemical Type** | 1-(azacyclyl)-3-arylsulfonyl-1H-pyrrolo[2,3-b] pyridines |
| **Mode of Action** | Ligand |
| **QSAR Model 1** | $pK_i = 30.04(\pm4.99) - 43.67(\pm11.52) \times \chi 1A - 0.43(\pm0.06) \times \mathrm{AECC} - 1.84(\pm0.41) \times \mathrm{Mor28}v + 0.20(\pm0.07) \times L2\,m$ |
| **QSAR Model 2** | $pK_i = 10.49(\pm1.12) + 0.47(\pm0.14) \times \text{Total Energy } (a.u.) - 0.0007(\pm0.0002) \times \text{Isolated Atomic Energy } \left(\text{kcal mol}^{-1}\right) + 0.14(\pm0.05) \times \text{Dipole Moment (debye)} + 0.22(\pm0.04) \times \text{Hydration energy } \left(\text{kcal mol}^{-1}\right) - 0.09(\pm0.04) \times \log P$<br>$r = 0.726,\ S = 0.284,\ p < 10^{-4} \quad r_{loo} = 0.616,\ S_{loo} = 0.329,$<br>$r_{l-25\%-o} = 0.324,\ S_{l-25\%-o} = 0.465,\ S_{\text{rand}} = 0.343$<br>$r_{\text{test}} = 0.653,\ S_{\text{test}} = 417$ |
| **Molecular Descriptor** | Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**<br><br>χ1A (topological descriptor indicating the average connectivity index chi-1), AECC (topological descriptor indicating average eccentricity), Mor28v (3D-MoRSE descriptor-signal 28 weighted by atomic van der Waals volumes), and L2m (the 2nd component size directional WHIM index/weighted by atomic masses).<br><br>The chemical descriptors, calculated using the PM3 method and HyperChem program, were Hydration energy, Dipole Moment, Binding Energy, CoreeCore Interaction, Total Energy, Isolated Atomic Energy, LogP, Heat of Formation, Electronic Energy, Polarizability, Refractivity, Volume, |

| | |
|---|---|
| | and Mass. |
| **Reference** | QSAR studies of bioactivities of 1-(azacyclyl)-3-arylsulfonyl-1H-pyrrolo[2,3-b] pyridines as 5-HT6 receptor ligands using physicochemical descriptors and MLR and ANN-modeling. *European Journal of Medicinal Chemistry* 45 (2010) 3911-3915 |