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| **Target Name** | $\beta_3$-adrenergic receptor |
| **Target TTD ID** | TTDC00184 |

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| **Target Species** | Human |
| **Chemical Type** | Thiazole benzenesulfonamide substituted 3-pyridylethanolamines |
| **Mode of Action** | Agonist |
| **QSAR Model 1** | $\mathrm{pEC_{50}} = 0.782(\pm 0.121)\log \mathrm{P(o/w)} - 0.463(\pm 0.120)\mathrm{chi1v\_C} - 0.042(\pm 0.013)\mathrm{vsa\_pol} + 0.169(\pm 0.688)$<br>$n = 16,\ \ r^2 = 0.881,\ \ \mathrm{SE} = 0.187,\ \ F = 29.599$ |
| **QSAR Model 2** | $\mathrm{pEC_{50}} = 3.670(\pm 1.003)\mathrm{a\_ICM} - 0.012(\pm 0.004)\mathrm{PEOE\_VSA} - 0 + 0.694(\pm 0.084)\mathrm{SlogP} - 9.832(\pm 1.888)$<br>$n = 16,\ \ r^2 = 0.877,\ \ \mathrm{SE} = 0.190,\ \ F = 28.643$ |
| **QSAR Model 3** | $\mathrm{pEC_{50}} = 2.404(\pm 0.963)\mathrm{a\_ICM} + 35.991(\pm 15.289)\mathrm{E\_ele} + 0.640(\pm 0.089)\mathrm{SlogP} - 7.443(\pm 2.129)$<br>$n = 16,\ \ r^2 = 0.865,\ \ \mathrm{SE} = 0.199,\ \ F = 25.549$ |
| **QSAR Model 4** | $\mathrm{pEC_{50}} = 0.014(\pm 0.002)\mathrm{PEOE\_VSA\_NEG} + 92.891(\pm 15.324)\mathrm{E\_ele} - 0.028(\pm 0.006)\mathrm{SlogP\_VSA0} + 0.006(\pm 0.843)$<br>$n = 16,\ \ r^2 = 0.872,\ \ \mathrm{SE} = 0.194,\ \ F = 27.214$ |

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| **QSAR Model 5** | $$\mathrm{pEC}_{50} = 0.266(\pm 0.039)\mathrm{chi0} + 88.998(\pm 14.954)\mathrm{E\_ele} - 0.030(\pm 0.006)\mathrm{SlogP\_VSA0} - 3.880(\pm 1.234)$$ $$n = 16,\ \ r^2 = 0.876,\ \ \mathrm{SE} = 0.191,\ \ F = 28.303$$ |
| **QSAR Model 6** | $$\mathrm{pEC}_{50} = 45.869(\pm 15.591)\mathrm{E\_ele} + 0.558(\pm 0.071)\mathrm{SlogP} - 0.003(\pm 0.001)\mathrm{SlogP\_VSA8} - 2.526(\pm 0.777)$$ $$n = 16,\ \ r^2 = 0.864,\ \ \mathrm{SE} = 0.200,\ \ F = 25.364$$ |
| **Molecular Descriptor** | Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**<br><br>2D-descriptors based on atoms and connection information of the molecules; i3D-descriptors used three-dimensional coordinate information about each molecule, which are invariant to rotations and translations of the conformation; and x3D descriptors which were supported by three-dimensional coordinate information require an absolute frame of reference using QuaSAR module; observed squared correlation coefficient ($r^2$); Calculated values of descriptors: E_ele; Chi0; SlogP_VSA0; SlogP; SlogP_VSA8. |
| **Reference** | QSAR analysis of thiazole benzenesulfonamide substituted 3-pyridylethanolamines as b3-adrenergic receptor agonist. Bioorganic & Medicinal Chemistry Letters 15 (2005) 3167–3173 |