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|---|---|
| **Target Name** | CYP19 |
| **Target TTD ID** | TTDS00252 |

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|---|---|
| **Target Species** | Human |
| **Chemical Type** | Benzcyclo derivatives |
| **Mode of Action** | Inhibitor |
| **QSAR Model 1** | $\mathrm{pIC50} = 3.875(\pm 0.425)\mathrm{HC}_2 - 0.285(\pm 0.033)S_4 + 4.504(\pm 0.632)C_5 - 0.334(\pm 0.085)R'_{13} + 0.252(\pm 0.095)\log P + 2.455(\pm 0.317)$<br>$n = 36;\ R^2 = 0.874;\ EV = 85.3\%;\ F = 41.710;\ df = 5, 30;$<br>$s = 0.213;\ \mathrm{AVRES} = 0.173;\ \mathrm{PRESS} = 1.910;\ Q^2 = 0.824$ |
| **Molecular Descriptor** | Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**<br><br>$\mathrm{HC}_2$ is Huckel charge at atom C2. $S_4$ is electrotopological state index of atom$\mathrm{C}_4$. $R'_{13}$ is electronic charge at atom $R'_{13}$. log P denotes hydrophobicity of the molecule. The independent variables used in the model are not intercorrelated (R < 0.5). |
| **Reference** | Exploring benzcyclo derivatives as potent aromatase inhibitors using ligand-based modeling studies. *European Journal of Medicinal Chemistry* 45 (2010) 4307-4315 |