Target Name	Benzodiazepine receptor
Target TTD ID	TTDS00374

Target Species	Human
Chemical Type	Phenylimidazopyridines
Mode of Action	Binder
QSAR Model 1	$\log(1/IC_{50}) = 2.051(\pm 0.929)\pi_X - 1.320(\pm 1.087)(\pi_X)^2 - 1.650(\pm 0.376)I_Z + 1.054(\pm 0.290)I_R + 5.028$ $n = 22,\ r = 0.936,\ s = 0.26,\ F_{4,17} = 29.92\ (4.67),\ (\pi_X)_0 = 0.78$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** π_X refers to the hydrophobic constant of X-substituent and I_Z and I_R are two indicator parameters used for Z- and R-substituents. I_Z takes a value of 1 for Z=Cl and zero for any other substituent. Similarly, I_R takes a value of 1 for R=an alkylamine group and zero for others. π_{R7} refers to the hydrophobic role of R7-substituent. σ is Hammett's electronic constant. $V_{w,R3}$ is the van der Waals volume of R3-substituent.
Reference	Quantitative Structure-Activity Relationship Studies on Some Nonbenzodiazepine Series of Compounds Acting at the Benzodiazepine Receptor. *Bioorganic & Medicinal Chemistry* 6 (1998) 2213-2218

Target Species	Human
Chemical Type	Imidazobenzothiazoles

Mode of Action	Binder
QSAR Model 1	$\log(1/IC_{50}) = 3.549(\pm1.089)\pi_{R7} - 5.169(\pm1.290)(\pi_{R7})^2 + 7.123$ $n = 14,\ r = 0.945,\ s = 0.23,\ F_{3,11} = 46.16\ (6.22),\ (\pi_{R7})_0 = 0.34$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** π_X refers to the hydrophobic constant of X-substituent and I_Z and I_R are two indicator parameters used for Z- and R-substituents. I_Z takes a value of 1 for Z=Cl and zero for any other substituent. Similarly, I_R takes a value of 1 for R=an alkylamine group and zero for others. π_{R7} refers to the hydrophobic role of R7-substituent. σ is Hammett's electronic constant. $V_{w,R3}$ is the van der Waals volume of R3-substituent.
Reference	Quantitative Structure-Activity Relationship Studies on Some Nonbenzodiazepine Series of Compounds Acting at the Benzodiazepine Receptor. *Bioorganic & Medicinal Chemistry* 6 (1998) 2213-2218

Target Species	Human
Chemical Type	Oxadiazoles
Mode of Action	Binder
QSAR Model 1	$\log(1/IC_{50}) = 2.574(\pm0.477)D - 1.850(\pm0.985)\pi_{R2} + 3.362(\pm1.914)\sigma_{R2} + 1.784(\pm1.573)\sigma_{R1} - 1.148(\pm0.469)V_{w,R3} + 6.220$ $n = 34,\ r = 0.923,\ s = 0.43,\ F_{5,28} = 32.32\ (3.76)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** π_X refers to the hydrophobic constant of X-substituent and I_Z and I_R are two indicator parameters used for Z- and R-substituents. I_Z takes a value of 1 for Z=Cl and zero for any other substituent. Similarly, I_R takes a value of 1 for R=an alkylamine group and zero for others. π_{R7} refers to the

	hydrophobic role of R7-substituent. σ is Hammett's electronic constant. $V_{w,R3}$ is the van der Waals volume of R3-substituent.
Reference	Quantitative Structure-Activity Relationship Studies on Some Nonbenzodiazepine Series of Compounds Acting at the Benzodiazepine Receptor. *Bioorganic & Medicinal Chemistry* 6 (1998) 2213-2218

Target Species	Human
Chemical Type	8 substituted, 2-phenyl congeners
Mode of Action	Ligand
QSAR Model 1	$\mathrm{pIC}_{50} = -0.32(\pm 0.10)vW + 9.63(\pm 0.28)$ $n = 9,\ r^2 = 0.883,\ Q^2 = 0.745,\ s = 0.208, F = 52.77$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Hammett (σ) and Hansch (π) substituent constants, the molar refractivity (MR), the van der Waals volume (vW) and the STERIMOL Verloop parameters L, B_1, and B_5 were employed to model bulkiness and polarizability effects. *n* is the number of compounds, r and Q are the correlation coefficient and the cross-validated correlation coefficient, respectively; s is the standard deviation; F is the F statistic.
Reference	High Affinity Central Benzodiazepine Receptor Ligands: Synthesis and Structure-Activity Relationship Studies of a New Series of Pyrazolo[4,3-c]quinolin-3-ones. *Bioorganic & Medicinal Chemistry* 6 (1998) 389±399

Target Species	Human
Chemical Type	6 substituted, 2-phenyl congeners

Mode of Action	Ligand
QSAR Model 1	$\mathrm{pIC}_{50} = -2.63(\pm 0.47)vW + 9.35(\pm 0.45)$ $n = 5,\ r^2 = 0.912,\ Q^2 = 0.801,\ s = 0.543,\ F = 31.23$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Hammett (σ) and Hansch (π) substituent constants, the molar refractivity (MR), the van der Waals volume (vW) and the STERIMOL Verloop parameters L, B_1, and B_5 were employed to model bulkiness and polarizability effects. *n* is the number of compounds, r and Q are the correlation coefficient and the cross-validated correlation coefficient, respectively; s is the standard deviation; F is the F statistic.
Reference	High Affinity Central Benzodiazepine Receptor Ligands: Synthesis and Structure-Activity Relationship Studies of a New Series of Pyrazolo[4,3-c]quinolin-3-ones. *Bioorganic & Medicinal Chemistry* 6 (1998) 389±399

Target Species	Human
Chemical Type	8-OCF3; 2-phenyl substituted congeners
Mode of Action	Ligand
QSAR Model 1	$\mathrm{pIC}_{50} = -1.40(\pm 0.29)\sigma - 1.55(\pm 0.42)MR + 9.46(\pm 0.24)$ $n = 15,\ r^2 = 0.803,\ Q^2 = 0.723,\ s = 0.418,\ F = 24.51$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Hammett (σ) and Hansch (π) substituent constants, the molar refractivity (MR), the van der Waals volume (vW) and the STERIMOL Verloop parameters L, B_1, and B_5 were employed to model bulkiness and polarizability effects. *n* is the number of compounds, r and Q are the correlation coefficient and the cross-validated

	correlation coefficient, respectively; s is the standard deviation; F is the F statistic.
Reference	High Affinity Central Benzodiazepine Receptor Ligands: Synthesis and Structure-Activity Relationship Studies of a New Series of Pyrazolo[4,3-c]quinolin-3-ones. *Bioorganic & Medicinal Chemistry* 6 (1998) 389±399