Target Name	Sodium channel
Target TTD ID	TTDS00155

Target Species	Human
Chemical Type	3-(4-phenoxyphenyl)pyrazoles
Mode of Action	Blocker
QSAR Model 1	$\log(1/K_i) = 2.860(\pm1.419)\text{ClogP} - 0.282(\pm0.190)(\text{ClogP})^2 + 1.138(\pm 0.516)I_1 - 0.604(\pm2.368)$ $n = 15,\ r = 0.975,\ r_{cv}^2 = 0.90,\ s = 0.33,\ F_{3,11} = 70.32\ (6.22),\ (\text{ClogP})_o = 5.07$
QSAR Model 2	$\log(1/K_r) = 2.155(\pm0.981)\text{ClogP} - 0.211(\pm0.132)(\text{Clog P})^2 + 0.600(\pm0.357)I_1 - 0.708\ (\pm1.637)$ $n = 15,\ r = 0.975,\ r_{cv}^2 = 0.88,\ s = 0.23,\ F_{3,11} = 70.25\ (6.22),\ (\text{ClogP})_o = 5.11$
QSAR Model 3	$\log(1/K_i) = 4.819(\pm1.859)\text{ClogP} - 0.540(\pm0.252)(\text{ClogP})^2 - 3.629(\pm3.242)$ $n = 15,\ r = 0.919,\ r_{cv}^2 = 0.73,\ s = 0.57,\ F_{2,12} = 32.55(6.93),\ (\text{ClogP})_0 = 4.46$
QSAR Model 4	$\log(1/K_r) = 3.187(\pm1.086)\text{ClogP} - 0.348(\pm0.147)(\text{ClogP})^2 - 2.303(\pm1.895)$ $n = 15,\ r = 0.943,\ r_{cv}^2 = 0.67,\ s = 0.33,\ F_{2,12} = 47.90(6.93),\ (\text{ClogP})_o = 4.58$
QSAR Model 5	$\log(1/K_i) = 1.406(\pm 0.200)\log(1/K_r) + 0.099(\pm 0.871)$ $n = 15,\ r = 0.972,\ r_{cv}^2 = 0.81,\ s = 0.33,\ F_{1,13} = 219.75(9.07)$
QSAR Model 6	$\log(1/IC_{50}) = 0.423(\pm0.139)\text{ClogP} + 4.257(\pm0.981)$ $n = 12,\ r = 0.906,\ r_{cv}^2 = 0.74,\ s = 0.28,\ F_{1,10} = 45.75(10.04)$

Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** n is the number of data points; r, the correlation coefficient; r_{cv}^2 is the square of the crossvalidated correlation coefficient; s, the standard deviation; ClogP, the calculated hydrophobicity and F, F-ratio between the variances of calculated and observed activities. ClogP and CMR refer to calculated hydrophobicity and calculated molar refractivity. Pol referring to the polarizability of the molecule; Indicator variables I's which have been used to account for the effect of some specific features of the compounds; n is the number of data points, r is the correlation coefficient, r_{CV}^2 is the square of the cross-validated correlation coefficient obtained from leave-one-out jackknife procedure, whose value greater than 0.6 indicates excellent predictive ability of the equation, s is the standard deviation, and F is the F-ratio between the variances of calculated and observed activities; An indicator variable I1 which has been used for an amide group (CONH2) present in the compound. For a compound that has an amide group, I1 has been assigned a value of unity and for others its value is zero; Indicator variable I2 has been used for compounds that have symmetrical groups on both sides of the linker chain.
Reference	A QSAR Study on Some Series of Sodium and Potassium Channel Blockers. *Medicinal Chemistry*, 2009, *5*, 570-576

Target Species	Human
Chemical Type	2-alkyl-4-arylimidazoles
Mode of Action	Blocker
QSAR Model 1	$\log(1/K_i) = 2.860(\pm1.419)\text{ClogP} - 0.282(\pm0.190)(\text{ClogP})^2 + 1.138(\pm 0.516)I_1 - 0.604(\pm2.368)$ $n = 15,\ r = 0.975,\ r_{cv}^2 = 0.90,\ s = 0.33,\ F_{3,11} = 70.32\ (6.22),\ (\text{ClogP})_o = 5.07$
QSAR Model 2	$\log(1/K_r) = 2.155(\pm0.981)\text{ClogP} - 0.211(\pm0.132)(\text{Clog P})^2 + 0.600(\pm0.357)I_1 - 0.708\ (\pm1.637)$ $n = 15,\ r = 0.975,\ r_{cv}^2 = 0.88,\ s = 0.23,\ F_{3,11} = 70.25\ (6.22),\ (\text{ClogP})_o = 5.11$

QSAR Model 3	$\log(1/K_i) = 4.819(\pm1.859)ClogP - 0.540(\pm0.252)(ClogP)^2 - 3.629(\pm3.242)$ $n = 15,\ r = 0.919,\ r_{cv}^2 = 0.73,\ s = 0.57,\ F_{2,12} = 32.55(6.93),\ (ClogP)_0 = 4.46$
QSAR Model 4	$\log(1/K_r) = 3.187(\pm1.086)ClogP - 0.348(\pm0.147)(ClogP)^2 - 2.303(\pm1.895)$ $n = 15,\ r = 0.943,\ r_{cv}^2 = 0.67,\ s = 0.33,\ F_{2,12} = 47.90(6.93),\ (ClogP)_o = 4.58$
QSAR Model 5	$\log(1/K_i) = 1.406(\pm 0.200)\log(1/K_r) + 0.099(\pm 0.871)$ $n = 15,\ r = 0.972,\ r_{cv}^2 = 0.81,\ s = 0.33,\ F_{1,13} = 219.75(9.07)$
QSAR Model 6	$\log(1/IC_{50}) = 0.423(\pm0.139)ClogP + 4.257(\pm0.981)$ $n = 12,\ r = 0.906,\ r_{cv}^2 = 0.74,\ s = 0.28,\ F_{1,10} = 45.75(10.04)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** n is the number of data points; r, the correlation coefficient; r_{cv}^2 is the square of the crossvalidated correlation coefficient; s, the standard deviation; ClogP, the calculated hydrophobicity and F, F-ratio between the variances of calculated and observed activities. ClogP and CMR refer to calculated hydrophobicity and calculated molar refractivity. Pol referring to the polarizability of the molecule; Indicator variables I's which have been used to account for the effect of some specific features of the compounds; n is the number of data points, r is the correlation coefficient, r_{CV}^2 is the square of the cross-validated correlation coefficient obtained from leave-one-out jackknife procedure, whose value greater than 0.6 indicates excellent predictive ability of the equation, s is the standard deviation, and F is the F-ratio between the variances of calculated and observed activities; An indicator variable I1 which has been used for an amide group (CONH2) present in the compound. For a compound that has an amide group, I1 has been assigned a value of unity and for others its value is zero; Indicator variable I2 has been used for compounds that have symmetrical groups on both sides of the linker chain.
Reference	A QSAR Study on Some Series of Sodium and Potassium Channel Blockers. *Medicinal Chemistry*, 2009, *5*, 570-576