Target Name	Potassium channel
Target TTD ID	TTDR00174

Target Species	Human
Chemical Type	Khellinone derivatives
Mode of Action	Blocker
QSAR Model 1	$\log(1/K_d) = 1.700(\pm1.310)\text{ClogP} - 0.155(\pm0.138)(\text{ClogP})^2 - 0.755(\pm0.431)\text{CMR} + 0.242(\pm0.101)\text{Pol} - 1.705(\pm0.962)I_2 - 0.327(\pm2.078)$ $n = 22,\ r = 0.937,\ r_{cv}^2 = 0.82,\ s = 0.29,\ F_{5,16} = 22.96\ (4.44),\ (\text{ClogP})_o = 5.48$
QSAR Model 2	$\log(1/K_d) = 0.760(\pm1.573)\text{ClogP} - 0.057(\pm0.166)(\text{ClogP})^2 + 0.083(\pm0.057)\text{Pol} - 2.333(\pm1.175)I_2 + 0.813(\pm2.597)$ $n = 22,\ r = 0.879,\ s = 0.38,\ F_{4,17} = 14.44(4.67)$
QSAR Model 3	$\log(1/K_d) = 1.330(\pm2.033)\text{ClogP} - 0.103(\pm0.213)(\text{ClogP})^2 + 0.182(\pm0.289)\text{CMR} - 1.628(\pm1.502)I_2 + 0.627(\pm3.188)$ $n = 22,\ r = 0.824,\ s = 0.45,\ F_{4,17} = 9.01(4.67)$
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	Benzopyrans
Mode of Action	Activator
QSAR Model 1	$pEC_{50} = 3.1471(\pm 0.8480)J + 1.3840$ $n = 28, \quad S.E. = 0.7267, \quad R = -0.5918, \quad F = 14.011, \quad Q = 0.8143.$
QSAR Model 2	$pEC_{50} = 2.0694(\pm 0.4385)J + 1.3247(\pm 0.1495)IP_1 + 3.5646$ $n = 28, S.E. = 0.3641, R = 0.9182, F = 67.167, Q = 2.5218.$
QSAR Model 3	$pEC_{50} = 2.7548(\pm 0.4761)J + 4.9137(\pm 1.8983)MRI - 1.1747(\pm 0.1468)I_{P1} + 0.5055$ $n = 28, S.E. = 0.3286, R = 0.9367, F = 57.220, Q = 2.8505.$
QSAR Model 4	$pEC_{50} = 3.7015(\pm 0.9099)J + 5.2400(\pm 1.8987)MRI + 2.184\ 0 \times 10^{-4}(\pm 1.795\ 5 \times 10^{-4})W$ $- 1.2294(\pm 0.1522)I_{p1} - 1.4982$ $n = 28, S.E. = 0.3254, R = 0.9406, F = 44.143, Q = 2.8905.$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *n* is the number of compounds; Se, standard error of estimation; *R*, the multiple correlation coefficient; F, the F-ratio; Q is the quality factor (Q=R/S.E) and J is the Balaban index (the average

	distance sum connectivity index); Wiener index (W) is a widely used topological index; Sz is Szeged index; $^1\chi$ is First-order connectivity index; N is Molecular negentropy; MRI is Molecular redundancy index.
Reference	QSAR studies on benzopyran potassium channel activators. *European Journal of Medicinal Chemistry* 41 (2006) 360–366

Target Species	Human
Target Location	Heart
Chemical Type	Khellinone derivatives
Mode of Action	Blocker
QSAR Model 1	$\log(1/EC_{50}) = 2.661(\pm0.851)\Sigma\pi - 0.541(\pm0.171)(\Sigma\pi)^2 + 0.119(\pm0.041)st - 3.178(\pm2.544)$ $n = 12,\ r = 0.942,\ r_{cv}^2 = 0.67,\ s = 0.14,\ F_{3,8} = 20.86(7.59)\ ,\ \Sigma\pi_0 = 2.46$
QSAR Model 2	$\log(1/EC_{50}) = 0.696(\pm0.392)B_1 + 0.290(\pm0.186)I_P - 0.137(\pm0.061)L + 5.205(\pm0.665)$ $n = 19,\ r = 0.852,\ r_{cv}^2 = 0.43,\ s = 0.17,\ F_{3,15} = 13.20(5.42)$
QSAR Model 3	$\log(1/EC_{50}) = 1.001(\pm0.453)B_1 - 0.173(\pm0.064)L - 0.325(\pm0.258)I_0 + 5.111(\pm0.811)$ $n = 16,\ r = 0.915,\ r_{cv}^2 = 0.71,\ s = 0.17,\ F_{3,12} = 20.58(5.95)$
QSAR Model 4	$\log(1/IC_{50}) = 0.760(\pm0.226)\ \pi_X + 5.441(\pm0.263)$ $n = 17,\ r = 0.880,\ s = 0.42,\ F_{1.15} = 51.53(8.68)$
QSAR Model 5	$\log(1/IC_{50}) = 0.514(\pm0.203)\ \pi_X - 0.732(\pm0.453)\ I_{CN} + 0.585(\pm0.312)\ I_{Cf} + 5.642(\pm0.268)$

	$n = 17, r = 0.961, r_{cv}^2 = 0.87, s = 0.26, F_{3,13} = 52.80(5.74)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *n* is the number of compounds; r, is the correlation coefficient; r_{cv}^2, is the square of cross-validated correlation coefficient obtained from leave-one-out (Loo) jackknife procedure; s, the standard deviation; π ,hydrophobic constant; $\sum \pi$, the sum of π -values of R1- and R2-substituents; st, surface tension parameter; F is the F-ratio between the variances of calculated and observed activities; hydrophobic constant π; Verloop's STERIMOL parameters B and L, and the surface tension parameter st
Reference	A Quantitative Structure-Activity Relationship Study on Some Series of Potassium Channel Blockers. *Medicinal Chemistry*, 2008, *5*, 87-92

Target Species	Rat
Target Location	Aorta artery
Chemical Type	6-subsituted benzopyran-4-carbothioamides
Mode of Action	Opener
QSAR Model 1	$pEC_{50} = 4.067\ (\pm 1.352)\ \sigma_m + 0.791\ (\pm 0.331)\ \pi - 0.347\ (\pm 0.275)\ \pi^2 + 1.756\ (\pm 1.825)\ L - 0.234\ (\pm 0.224)\ L^2 + 2.794$ $n = 13,\ r = 0.957,\ s = 0.393,\ \text{ideal}\ \pi = 1.14,\ \text{ideal}\ L = 3.75$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *n* is the number of compounds; r, the correlation coefficient; s, the standard deviation; π, hydrophobic parameter and L, steric parameter.
Reference	Structure-activity relationships of 6-substituted benzopyran-4-carbothioamide potassium channel openers. *Bioorgmic &Medicinal Chemirrry Letters*. Volume 3, Issue 8, August 1993, Pages 1659-1662