Target Name	ATP-sensitive potassium channel
Target TTD ID	TTDS00150

Target Species	Human
Chemical Type	Cromakalim analogs
Mode of Action	Openers
Activity Type	Vasorelexant activity
QSAR Model 1	$\log(1/IC_{50}) = 14.990(\pm3.257) - 1.093(\pm0.387)\ {}^{1}\chi^{v}$ $n = 12,\ r = 0.893,\ s = 0.28,\ F_{1,10} = 39.52(10.04)$
QSAR Model 2	$\log(1/IC_{50}) = 16.866(\pm3.154) - 1.330(\pm0.382)\ {}^{1}\chi^{v} + 0.461(\pm0.414)\ I_1$ $n = 12,\ r = 0.939,\ s = 0.23,\ F_{2,9} = 33.53(8.02)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Structural parameter ${}^{1}\chi^{v}$ is Kier's first-order valence molecular connectivity index, which is calculated as: $${}^{1}\chi^{v} = \sum(\delta_i^v\ \delta_j^v)^{-1/2}$$ Where δ_i^v and δ_j^v are vertex connectivity indices of atoms I and j, respectively, and the summation extends to all bonded pairs of non-hydrogenic atoms in the group or molecule. A unified definition of δ^v was given as: $$\delta_i^v = (Z_i^v - h_i)/(Z_i - Z_i^v - 1)$$ Where Z_i^v is the number of valence electrons of atom i, h_i is the number of hydrogen atoms attached to it, and Z_i is its atomic number. ClogP is the calculated hydrophobicity parameter of the

	compounds.
Reference	A QSAR Study on some Series of ATP-Sensitive Potassium Channel Openers. *Letters in Drug Design & Discovery*, 2008, 5, 173-177

Target Species	Human
Chemical Type	Benzopyran derivatives
Mode of Action	Openers
Activity Type	Vasorelexant activity
QSAR Model 1	$\log (1/IC_{50}) = 6.021(\pm 1.381) - 0.288(\pm 0.275)\ {}^{1}\chi^{v}$ $n = 8,\ r = 0.723,\ s = 0.43,\ F_{1,6} = 6.57(13.74)$
QSAR Model 2	$\log (1/IC_{50}) = 6.436(\pm 0.607) - 0.318(\pm 0.116)\ {}^{1}\chi^{v} - 0.725(\pm 0.325)I_2$ $n = 8,\ r = 0.968,\ s = 0.17,\ F_{2,5} = 37.18(13.27)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Structural parameter ${}^{1}\chi^{v}$ is Kier's first-order valence molecular connectivity index, which is calculated as: $${}^{1}\chi^{v} = \sum(\delta_i^v\ \delta_j^v)^{-1/2}$$ Where δ_i^v and δ_j^v are vertex connectivity indices of atoms I and j, respectively, and the summation extends to all bonded pairs of non-hydrogenic atoms in the group or molecule. A unified definition of δ^v was given as: $$\delta_i^v = (Z_i^v - h_i)/(Z_i - Z_i^v - 1)$$ Where Z_i^v is the number of valence electrons of atom i, h_i is the number of hydrogen atoms attached to it, and Z_i is its atomic number. ClogP is the calculated hydrophobicity parameter of the

	compounds.
Reference	A QSAR Study on some Series of ATP-Sensitive Potassium Channel Openers. *Letters in Drug Design & Discovery*, 2008, 5, 173-177

Target Species	Human
Chemical Type	1,4-benzothiazine derivatives
Mode of Action	Openers
Activity Type	Vasorelexant activity
QSAR Model 1	$\log(1/IC_{50}) = 0.916(\pm0.474)ClogP - 1.098(\pm1.012)I_3 - 2.743(\pm1.014)I_4 + 7.653(\pm1.508)$ $n = 15, r = 0.946, r_{cv}^2 = 0.80, s = 0.84, F_{3,11} = 31.35(6.22)$
QSAR Model 2	$\log(1/IC_{50}) = 1.393(\pm0.909)ClogP + 4.640(\pm2.326)$ $n = 15, r = 0.667, s = 1.78, F_{1,13} = 10.42(9.07)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Structural parameter $^1\chi^v$ is Kier's first-order valence molecular connectivity index, which is calculated as: $$^1\chi^v = \sum(\delta_i^v\ \delta_j^v)^{-1/2}$$ Where δ_i^v and δ_j^v are vertex connectivity indices of atoms I and j, respectively, and the summation extends to all bonded pairs of non-hydrogenic atoms in the group or molecule. A unified definition of δ^v was given as: $$\delta_i^v = (Z_i^v - h_i)/(Z_i - Z_i^v - 1)$$ Where Z_i^v is the number of valence electrons of atom i, h_i is the number of hydrogen atoms attached to it, and Z_i is its atomic number. ClogP is the calculated hydrophobicity parameter of the

	compounds.
Reference	A QSAR Study on some Series of ATP-Sensitive Potassium Channel Openers. *Letters in Drug Design & Discovery*, 2008, 5, 173-177