Target Name	K_{ATP} channel
Target TTD ID	TTDS00331

Target Species	Human
Target Location	Pancreatic β-cell
Chemical Type	R/S-3,4-dihydro-2,2-dimethyl-6-halo-4-(substituted phenylaminocarbonylamino)-2*H*-1-benzopyrans
Mode of Action	Opener
QSAR Model 1	$\log \mathrm{PRIS} = 2.001(\pm 0.042) + 0.730(\pm 0.189) q_{18} - 0.408(\pm 0.055) I\_\mathrm{ClR}_2 - 0.326(\pm 0.059) I\_\mathrm{ClR}_3$ $n = 23,\ R = 0.926,\ R^2 = 0.857,\ R^2_{\mathrm{A}} = 0.835,\ F_{(3,19)} = 38.099,\ p < 0.00001,$ $s = 0.074,\ R^2_{\mathrm{cv}} = 0.843,\ \mathrm{SSY} = 0.725,\ \mathrm{PRESS} = 0.171,\ \mathrm{SDEP} = 0.075,\ S_{\mathrm{PRESS}} = 0.081.$
QSAR Model 2	$\log \mathrm{PRIS} = 1.887(\pm 0.037) - 0.237(\pm 0.081) q_{17} - 0.477(\pm 0.152) q_{19} - 0.415(\pm 0.051) I\_\mathrm{ClR}_2 - 0.286(\pm 0.059) I\_\mathrm{ClR}_3$ $n = 23,\ R = 0.941,\ R^2 = 0.885,\ R^2_{\mathrm{A}} = 0.859,\ F_{(4,18)} = 34.609,\ p < 0.00001,$ $s = 0.068,\ R^2_{\mathrm{cv}} = 0.805,\ \mathrm{SSY} = 0.725,\ \mathrm{PRESS} = 0.212,\ \mathrm{SDEP} = 0.084,\ S_{\mathrm{PRESS}} = 0.092.$
QSAR Model 3	$\log \mathrm{PRIS} = 1.769(\pm 0.083) - 0.515(\pm 0.236) q_{11} - 0.292(\pm 0.074) q_{17} - 0.237(\pm 0.069) q_{21} - 0.448(\pm 0.048) I\_\mathrm{ClR}_2 - 0.350(\pm 0.049) I\_\mathrm{ClR}_2$ $n = 23,\ R = 0.953,\ R^2 = 0.908,\ R^2_{\mathrm{A}} = 0.881,\ F_{(5,17)} = 33.452,\ p < 0.00001,$ $s = 0.063,\ R^2_{\mathrm{cv}} = 0.795,\ \mathrm{SSY} = 0.725,\ \mathrm{PRESS} = 0.223,\ \mathrm{SDEP} = 0.086,\ S_{\mathrm{PRESS}} = 0.096.$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Semi-empirical quantum chemical descriptors (WangeFord charges e q_x), partition coefficient (log P), molar refractivity (MR), the principle moment of inertia (PMX, PMY and PMZ) and indicator parameters are used as the predictor variables. WangeFord charges (q_x), partition coefficient (log P),

	molar refractivity (MR) and the principle moment of inertia (PMX, PMY and PMZ)
Reference	QSAR modelling of pancreatic β-cell K_{ATP} channel openers R/S-3,4-dihydro-2,2-dimethyl-6-halo-4-(substituted phenylaminocarbonylamino)-2*H*-1-benzopyrans using MLR-FA techniques. *European Journal of Medicinal Chemistry* 44 (2009) 359-364