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| **Target Name** | Calcium channel |
| **Target TTD ID** | TTDS00163 |

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| **Target Species** | Human |
| **Target Location** | Heart |
| **Chemical Type** | 1,4-dihydropyridines |
| **Mode of Action** | Blocker |
| **QSAR Model 1** | $\log(1/IC_{50}) = 0.44(\pm0.26)\pi + 1.47(\pm0.93)\sigma_m - 0.032(\pm0.011)V_w - 1.65(\pm0.53)F_5^{(e)} - 6.5(\pm1.9)\varepsilon_{rot} + 0.217(\pm0.071)B1p + 17.4(\pm3.2)$<br>$n = 45, r = 0.95, s = 0.49, F_{6,38} = 54.69$ |
| **QSAR Model 2** | $\log(1/IC_{50}) = 0.179(\pm0.075)\varepsilon_{rot} - 0.256(\pm0.094)Pol - 1.820(\pm0.466)Ip + 0.556(\pm0.382)I_{ew} + 13.241(\pm2.633)$<br>$n = 40, r = 0.921, r_{cv}^2 = 0.78, s = 0.25, F_{4,35} = 48.73(3.91)$ |
| **Molecular Descriptor** | Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**<br><br>$\pi$ refers to hydrophobic parameter of X-substituent, $\sigma_m$ is the electronic parameter (Hammett constant) of the Xsubstituent at meta position, $V_w$ refers to van der Waals volume of the whole molecule, $F_5^{(e)}$ refers to the frontier electron density at the 5-position of the phenyl ring, $\varepsilon_{rot}$ is the energy barrier of the rotate in of the phenyl ring, and B1p is the STERIMOL width parameter for the X-substituent at para-position. Pol refers to the polarizablity of the molecule and Ip and Iew are the two indicator variables used with a value of 1 each for an X-substituent being at para-position and for that being electron-withdrawing in nature. |
| **Reference** | QSAR Studies on some Calcium Channel Blockers. *Letters in Drug Design & Discovery*, 2008, 5, |

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| **Target Species** | Human |
| **Target Location** | Heart |
| **Chemical Type** | Benzazepinone analogs |
| **Mode of Action** | Blocker |
| **QSAR Model 1** | $\log(1/IC_{50}) = 2.719(\pm0.842)\sigma_{R1} + 0.878(\pm0.376)I_X + 0.376(\pm0.357)I_{R2} + 5.479(\pm0.385)$<br>$n = 14, r = 0.920, r_{cv}^2 = 0.70, s = 0.24, F_{3,10} = 18.30(6.55)$ |
| **QSAR Model 2** | $\log(1/IC_{50}) = 2.848(\pm0.791)\sigma_{R1} + 0.788(\pm0.472)I_X + 0.480(\pm0.353)I_{R2} + 5.410(\pm0.365)$<br>$n = 13, r = 0.941, r_{cv}^2 = 0.70, s = 0.21, F_{3,9} = 23.15(6.99)$ |
| **QSAR Model 3** | $\log(1/EC_{50}) = -0.889(\pm0.845)^1\chi^v + 0.066(\pm0.044)(^1\chi^v)^2 - 0.218\ st - 1.004(\pm0.413)\ I_1 + 20.363(\pm3.552)$<br>$n = 17, r = 0.953, r_{cv}^2 = 0.82, s = 0.25, F_{4,12} = 29.56(5.41), {}^1\chi^v_{opt} = 6.73$ |
| **Molecular Descriptor** | Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**<br><br>$\pi$ refers to hydrophobic parameter of X-substituent, $\sigma_m$ is the electronic parameter (Hammett constant) of the Xsubstituent at meta position, $V_w$ refers to van der Waals volume of the whole molecule, $F_5^{(e)}$ refers to the frontier electron density at the 5-position of the phenyl ring, $\varepsilon_{rot}$ is the energy barrier of the rotate in of the phenyl ring, and B1p is the STERIMOL width parameter for the X-substituent at para-position. Pol refers to the polarizablity of the molecule and Ip and Iew are the two indicator variables used with a value of 1 each for an X-substituent being at para-position and for that being electron-withdrawing in nature. |

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| | $\sigma_{R1}$ stands for the Hammett constants of $R_1$- substituent and $I_X$ and $I_{R2}$ are the two indicator variables, used with a value of 1 each, for X = S in the 7-membered ring and R2 = OMe, respectively. $^1\chi^V$ is Kier's first-order valence molecular connectivity index of the molecule, stands for surface tension of the molecule, and $I_1$ is an indicator parameter, used with a value of 1, for compounds bearing 3,5-dmethyl group at the phenyl ring. 1ℵv is a measure of molecular size |
| **Reference** | QSAR Studies on some Calcium Channel Blockers. *Letters in Drug Design & Discovery*, 2008, 5, 307-312 |

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| **Target Species** | Human |
| **Target Location** | Heart |
| **Chemical Type** | Quinolizidinyl derivatives |
| **Mode of Action** | Blocker |
| **QSAR Model 1** | $\log(1/IC_{50}) = 2.719(\pm0.842)\sigma_{R1} + 0.878(\pm0.376)I_X + 0.376(\pm0.357)I_{R2} + 5.479(\pm0.385)$<br>$n = 14, r = 0.920, r_{cv}^2 = 0.70, s = 0.24, F_{3,10} = 18.30(6.55)$ |
| **QSAR Model 2** | $\log(1/IC_{50}) = 2.848(\pm0.791)\sigma_{R1} + 0.788(\pm0.472)I_X + 0.480(\pm0.353)I_{R2} + 5.410(\pm0.365)$<br>$n = 13, r = 0.941, r_{cv}^2 = 0.70, s = 0.21, F_{3,9} = 23.15(6.99)$ |
| **QSAR Model 3** | $\log(1/EC_{50}) = -0.889(\pm0.845)^1\chi^v + 0.066(\pm0.044)(^1\chi^v)^2 - 0.218\ st - 1.004(\pm0.413)\ I_1 + 20.363(\pm3.552)$<br>$n = 17, r = 0.953, r_{cv}^2 = 0.82, s = 0.25, F_{4,12} = 29.56(5.41), {}^1\chi^v_{opt} = 6.73$ |
| **Molecular Descriptor** | Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**<br>$\pi$ refers to hydrophobic parameter of X-substituent, $\sigma_m$ is the electronic parameter (Hammett |

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| | constant) of the Xsubstituent at meta position, $V_w$ refers to van der Waals volume of the whole molecule, $F_5^{(e)}$ refers to the frontier electron density at the 5-position of the phenyl ring, $\varepsilon_{rot}$ is the energy barrier of the rotate in of the phenyl ring, and B1p is the STERIMOL width parameter for the X-substituent at para-position. Pol refers to the polarizablity of the molecule and Ip and Iew are the two indicator variables used with a value of 1 each for an X-substituent being at para-position and for that being electron-withdrawing in nature.<br><br>$\sigma_{R1}$ stands for the Hammett constants of $R_1$- substituent and $I_X$ and $I_{R2}$ are the two indicator variables, used with a value of 1 each, for X = S in the 7-membered ring and R2 = OMe, respectively. $^1\chi^V$ is Kier's first-order valence molecular connectivity index of the molecule, stands for surface tension of the molecule, and $I_1$ is an indicator parameter, used with a value of 1, for compounds bearing 3,5-dmethyl group at the phenyl ring. 1ℵv is a measure of molecular size |
| **Reference** | QSAR Studies on some Calcium Channel Blockers. *Letters in Drug Design & Discovery*, 2008, 5, 307-312 |