Target Name	Carbonic anhydrase I
Target TTD ID	TTDR01224

Target Species	Human
Chemical Type	Ureido derivatives of aromatic/heterocyclic sulfonamides
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{p}K_\mathrm{i} = -0.0054(\pm 0.0012)W + 0.0037(\pm 8.9737\times 10^{-4})Sz + 1.2519(\pm 0.1542)J + 0.8344(\pm 0.2559)Ip_1 + 1.2944(\pm 0.1577)Ip_2 - 0.3717$ $n = 39,\ \mathrm{SE} = 0.3725,\ R = 0.9171,\ Q = 2.4620,\ F = 34.917$
QSAR Model 2	$\mathrm{p}K_\mathrm{i} = -0.0037(\pm 0.0012)W + 0.0034(\pm 7.8340\times 10^{-4})Sz - 0.4551(\pm 0.1326)B + 1.3288(\pm 0.1358)J + 0.5245(\pm 0.2399)\mathrm{I}p_1 + 1.3779(\pm 0.11390)Ip_2 - 2.4643$ $n = 39,\ \mathrm{SE} = 0.3235,\ R = 0.9401,\ Q = 2.9067,\ F = 40.559$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** K_i, inhibition constant; p K_i, logarithmic transformation of K_i; ${}^0x^v$, zero-order connectivity index; ${}^1x^v$, first-order connectivity indices; *W*, Wiener index; *Sz*, Szeged index; *B*, branching index; *J*, Balaban index; Ip_1 and Ip_2, indicator parameters
Reference	QSAR Studies on Carbonic Anhydrase Inhibitors: A Case of Ureido and Thioureido Derivatives of Aromatic/Heterocyclic Sulfonamides. *Bioorganic & Medicinal Chemistry* 10 (2002) 2993–2999

Target Species	Human
Chemical Type	Thioureido derivatives of aromatic/heterocyclic sulfonamides

Mode of Action	Inhibitor
QSAR Model 1	$pK_i = -0.0054(\pm 0.0012)W + 0.0037(\pm 8.9737\times 10^{-4})Sz + 1.2519(\pm 0.1542)J + 0.8344(\pm 0.2559)Ip_1 + 1.2944(\pm 0.1577)Ip_2 - 0.3717$ $n = 39,\ \mathrm{SE} = 0.3725,\ R = 0.9171,\ Q = 2.4620,\ F = 34.917$
QSAR Model 2	$pK_i = -0.0037(\pm 0.0012)W + 0.0034(\pm 7.8340\times 10^{-4})Sz - 0.4551(\pm 0.1326)B + 1.3288(\pm 0.1358)J + 0.5245(\pm 0.2399)Ip_1 + 1.3779(\pm 0.11390)Ip_2 - 2.4643$ $n = 39,\ \mathrm{SE} = 0.3235,\ R = 0.9401,\ Q = 2.9067,\ F = 40.559$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** K_i, inhibition constant; p K_i, logarithmic transformation of K_i; ${}^0x^v$, zero-order connectivity index; ${}^1x^v$, first-order connectivity indices; *W*, Wiener index; *Sz*, Szeged index; *B*, branching index; *J*, Balaban index; Ip_1 and Ip_2, indicator parameters
Reference	QSAR Studies on Carbonic Anhydrase Inhibitors: A Case of Ureido and Thioureido Derivatives of Aromatic/Heterocyclic Sulfonamides. *Bioorganic & Medicinal Chemistry* 10 (2002) 2993–2999

Target Species	Human
Chemical Type	Sulfonamides incorporating β-alanyl moieties
Mode of Action	Inhibitor
QSAR Model 1	$\log K_I(\mathrm{hCA\,I}) = 6.4759 - 0.4563(\pm 0.0558)\ {}^1\chi$ $n = 49$, S.E. = 0.7814, $r = -0.7664$, $F = 66.885$
QSAR Model 2	$\log K_I(\mathrm{hCA\,I}) = 6.5421 - 0.4148(\pm 0.0377)\ {}^1\chi - 1.2582(\pm 0.1636)\mathrm{IP}_2$ $n = 49$, S.E. = 0.5225, $R = 0.9052$, $F = 104.363$
QSAR Model 3	$\log K_I(\mathrm{hCA\,I}) = 6.7621 - 0.4239(\pm 0.0361)\ {}^1\chi - 0.4307(\pm 0.1795)\mathrm{IP}_1 - 1.4046(\pm 0.1673)\mathrm{IP}_2$

	$n = 49$, S.E. = 0.4974, $R = 0.9165$, $F = 78.695$
QSAR Model 4	$\log K_I(\text{hCAI}) = 3.7166 - 0.3551(\pm 0.0330)\ {}^1\chi + 1.1389(\pm 0.2402)J - 0.8425(\pm 0.1713)\ IP_1 - 1.2586(\pm 0.1410)IP_2$ $n = 49$, S.E. = 0.4092, $R = 0.9455$, $F = 92.817$.
QSAR Model 5	$\log K_I(\text{hCAI}) = 4.0181 - 0.3617(\pm 0.0323)\ {}^1\chi + 1.0254(\pm 0.2407)J - 0.8013(\pm 0.1678)\ IP_1 - 1.3744(\pm 0.1498)IP_2 + 0.5054(\pm 0.2647)IP_3$ $n = 49$, S.E. = 0.3974, $R = 0.9499$, $F = 79.447$.
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** log *K*, logarithm of binding constant (*K*); ${}^1x$, Randic connectivity index; *J*, Balaban index; IP_1, IP_2 and IP_3, indicator parameter for the presence (=1) or absence (=0) of halogen, five-member ring and methyl group respectively; *n*, number of compounds; S.E., standard error of estimation; R, multiple correlation coefficient; *F*, Fishers statistics
Reference	QSAR study on carbonic anhydrase inhibitors: water-soluble sulfonamides incorporating b-alanyl moieties, possessing long lasting-intra ocular pressure lowering properties—a molecular connectivity approach. *European Journal of Medicinal Chemistry* 40 (2005) 1002–1012

Target Species	Human
Chemical Type	Sulfamide derivatives
Mode of Action	Inhibitior
QSAR Model 1	$pKi = [2.6911(\pm 1.1075)] + E_{HOMO}\ [0.5005\ (\pm 0.1112)] + E_{LUMO}\ [-0.8299\ (\pm 0.2725)] + NVDW\ [-0.0378\ (\pm 0.0313)]$ n = 16, r = 0.9741, r^2 = 0.9436, S = 0.1219, F= 67.0453
QSAR Model 2	$pKi = [2.6265(\pm 1.2956)] + E_{HOMO}\ [0.4548\ (\pm 0.1182)] + E_{LUMO}\ [-0.7881\ (\pm 0.3071)] + PMI\text{-}X\ [-0.0014\ (\pm 0.0020)]$

	n = 16, r = 0.9625, r^2 = 0.9264, S =0.1393, F=50.4040
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** BP: Thermodynamic descriptor-Boiling Point (Kelvin) CP: Thermodynamic descriptor-Critical Pressure (Kelvin) CT: Thermodynamic descriptor-Critical Temperature (bar) HF: Thermodynamic descriptor-Heat of formation (Kcal/mole) HLC: Thermodynamic descriptor-Henrys Law Constant IGTC: Thermodynamic descriptor-Ideal Gas Thermal Capacity Log P: Thermodynamic descriptor-Logarithmic Partition Coefficient MP: Thermodynamic descriptor-Melting Point (Kelvin) MR: Thermodynamic descriptor-Molar Refractivity (cm3/mole) SGP: Thermodynamic descriptor-Standard Gibb's Free Energy (kJ/mole) VDW: Thermodynamic descriptor-Van der Waals Force (kcal/mole) PC: Thermodynamic descriptor-Partition Coefficient For Water / Octanol NVDW: Thermodynamic descriptor-Non-1,4-Van der Waals Force (kcal/mole) SE: Thermodynamic descriptor-Stretch Energy (kcal/mole) SBE: Thermodynamic descriptor-Stretch Bend Energy (kcal/mole) TORE: Thermodynamic descriptor-Torsion Energy (kcal/mole) ET: Thermodynamic descriptor-Total Energy (kcal/mole) CAA: Steric descriptor-Connolly Accessible Surface Area (Å) CMA: Steric descriptor-Connolly Molecular Surface Area (Å) CSEV: Steric descriptor-Connolly Solvent- Excluded Volume (Å) EM: Steric descriptor-Exact Mass (g/mole) MW: Steric descriptor-Molecular Weight (atomic mass units) OVAL: Steric descriptor-Ovality

	PMI-X: Steric descriptor-Principal Moments of Inertia at x axis (g/moles Å) PMI-Y: Steric descriptor-Principal Moments of Inertia at y axis (g/moles Å) PMI-Z: Steric descriptor-Principal Moments of Inertia at z axis (g/moles Å) DIPOLE-X: Electronic descriptor-Dipole Moment-X axis (Debye) DIPOLE-Y: Electronic descriptor-Dipole Moment-Y axis (Debye) DIPOLE-Z: Electronic descriptor-Dipole Moment-Z axis (Debye) EE: Electronic descriptor-Electronic Energy (Ev) EHOMO: Electronic descriptor-Energy of Highest Occupied Molecular Orbital (eV) ELUMO: Electronic descriptor-Energy of Lowest Unoccupied Molecular Orbital (eV) RE: Electronic descriptor-Repulsion Energy (eV) BE: Electronic descriptor-Bending Energy (kcal/mole) DDE: Electronic descriptor-Dipole-Dipole Energy (kcal/mole) K_i, inhibition constant; p K_i, logarithmic transformation of K_i; $E_{HOMO,}$ Energy of Highest Occupied Molecular Orbital (eV); E_{LUMO}, Energy of Lowest Unoccupied Molecular Orbital (eV); NVDW, Non-1,4-Van der Waals Force (kcal/mole); *n*, number of compounds; r, simple correlation coefficient; r^2, squared correlation coefficient; S, standard deviation; *F*, Fisher value
Reference	Quantitative Structure Activity Relationship Studies of Sulfamide Derivatives as Carbonic Anhydrase Inhibitor: As Antiglaucoma Agents. *Medicinal Chemistry*, 2007, 3, 379-386