Target Name	Carbonic anhydrase II
Target TTD ID	TTDS00306

Target Species	Human
Chemical Type	Benzene sulfonamides
Mode of Action	Inhibitor
QSAR Model 1	$\log K = 2.1443 + 0.4220(\pm 0.0623)\,{}^{0}\chi^{v} + 2.4495(\pm 0.1959)\mathrm{IP_1}$ $n = 29,\ \mathrm{Se} = 0.5010,\ R = 0.9394,\ R_{\mathrm{A}}^2 = 0.8735,\ F = 97.666,\ Q = 1.8751$
QSAR Model 2	$\log K = 3.5111 - 0.0215(\pm 0.0084)W + 0.0200(\pm 0.0069)\mathrm{Sz} + 1.9486(\pm 0.2289)\mathrm{IP_1}$ $n = 29,\ \mathrm{Se} = 0.4545,\ R = 9488,\ R_{\mathrm{A}}^2 = 0.8866,\ F = 73.942,\ Q = 1.9979$
QSAR Model 3	$\log K = 1.9828 - 0.0238(\pm 0.00813)W + 0.0199(\pm 0.0066)\mathrm{Sz} + 0.8407(\pm 0.4450)^2\chi^{v} + 1.9132(\pm 0.2190)\mathrm{IP_1}$ $n = 29,\ \mathrm{Se} = 0.4525,\ R = 0.9548,\ R_{\mathrm{A}}^2 = 0.8968,\ F = 61.855,\ Q = 2.1100$
QSAR Model 4	$\log K = 4.8219 + 0.6748(\pm 0.0979)\log P + 2.4335(\pm 0.1937)\mathrm{IP_1}$ $n = 29,\ \mathrm{Se} = 0.4955,\ R = 0.9408,\ R_{\mathrm{A}}^2 = 0.8763,\ F = 100.197,\ Q = 1.8987$
QSAR Model 5	$\log K = 2.2096 + 0.4347(\pm 0.0987)\log P + 0.4226(\pm 0.1060)^2\chi + 2.5167(\pm 0.1559)\mathrm{IP_1}$ $n = 29,\ \mathrm{Se} = 0.3952,\ R = 0.9642,\ R_{\mathrm{A}}^1 = 0.9213,\ F = 110.276,\ Q = 2.4400$
QSAR Model 6	$\log K = 1.6434 + 0.4033(\pm 0.0546)\log P + 0.4350(\pm 0.0585)^2\chi + 3.0451(\pm 0.1104)\mathrm{IP_1} + 1.0549(\pm 0.1383)\mathrm{IP_2}$ $n = 29,\ \mathrm{Se} = 0.2180,\ R = 0.9897,\ R_{\mathrm{A}}^2 = 0.9761,\ F = 286.500,\ Q = 4.5400$

Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** log *K*, logarithm of binding constant (*K*) to human CA-II; ${}^{0}x^{v}$, zero-order Kier and Hall's valence connectivity index; ${}^{2}x^{v}$, second-order Kier and Hall's valence connectivity index; log *P*, lipophilicity (hydrophobic parameter); *W*, Wiener index; *Sz*, Szeged index; IP_1, indicator parameter for the presence (=2) or absence (=0) of substitution at 4-position; *n*, number of compounds; Se, standard error of estimation; *R*, multiple correlation coefficient; R_A^2, adjustable R^2; *F*, Fishers statistics; *Q*, quality factor
Reference	QSAR studies on benzene sulfonamide carbonic anhydrase inhibitors: need of hydrophobic parameter for topological modeling of binding constants of sulfonamides to human CA-II. *Bioorganic & Medicinal Chemistry Letters* 15 (2005) 923–930

Target Species	Human
Chemical Type	Sulfonamides incorporating β-alanyl moieties
Mode of Action	Inhibitor
QSAR Model 1	$\log K_I(\text{hCA II}) = 2.2447 - 0.1593(\pm 0.0219)\ {}^{1}\chi + 0.3728(\pm 0.1656)J - 0.5423(\pm 0.1140)\ IP_1 - 0.9305(\pm 0.1018)IP_2 + 0.1013(\pm 0.1799)IP_3$ $n = 49,\ \text{S.E.} = 0.2700,\ R = 0.9166,\ R^2A = 0.8215,\ F = 45.172$
QSAR Model 2	$\log K_I(\text{hCA II}) = 2.1843 - 0.1580(\pm 0.0216)\ {}^{1}\chi + 0.3955(\pm 0.1573)J - 0.5805(\pm 0.1122)\ IP_1 - 0.9073(\pm 0.0923)IP_2$ $n = 49,\ \text{S.E.} = 0.2679,\ R = 0.9159,\ R^2_A = 0.8242,\ F = 57.275$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** log *K*, logarithm of binding constant (*K*); ${}^{1}x$, 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; R_A^2, adjustable R^2; *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	$pKi = [2.4909(\pm1.4516)] + E_{HOMO}\ [0.4819\ (\pm0.1325)] + E_{LUMO}\ [-1.0320\ (\pm0.3441)] + PMI\text{-}X\ [-0.0022\ (\pm0.0022)]$ n = 16, r = 0.9741, r^2 =0.9302, S =.1561, F=53.3471
QSAR Model 2	$pKi = 3.1137\ [(\pm1.6949)] + E_{HOMO}\ [0.4731\ (\pm0.1404)] + E_{LUMO}\ [-0.9739\ (\pm0.3651)] + CSEV\ [-0.0052\ (\pm0.0067)]$ n = 16, r = 0.9600, r^2 = 0.9216, S = 0.1655, F= 47.0310
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

Target Species	Human
Chemical Type	Benzenesulphonamide derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log Kc = 31.4072 - 9.6189\ (\pm 0.5809)\ J$ $n = 29,\ \ Se = 0.4287,\ \ r = -0.9541,\ \ F = 274.192,\ \ Q = 2.2256.$
QSAR Model 2	$\log Kc = 25.8505 - 7.6003\ (\pm 0.6591)\ J + 0.805\ (\pm 0.190)\ I$ $n = 29,\ \ Se = 0.336,\ \ r = 0.9731,\ \ F = 232.104,\ \ Q = 2.8961.$
QSAR Model 3	$\log Kc = 20.3759 - 6.1371\ (\pm 0.6623)\ J + 0.194\ (\pm 0.0514)\ {}^1\chi + 1.1330\ (\pm 0.1775)\ I$ $n = 29,\ \ Se = 0.2736,\ \ r = 0.9829,\ \ F = 238.138,\ \ Q = 3.5925.$
QSAR Model 4	$\log Kc = 18.3126 - 6.538\ (\pm 0.6004)\ J + 0.7504\ (\pm 0.1999)\ {}^1\chi$ $- 0.0025\ (\pm 8.6322 \times 10^{-4})\ W + 1.2837\ (\pm 0.1651)\ I$ $n = 29,\ \ Se = 0.2412,\ \ r = 0.9873,\ \ F = 231.859,\ \ Q = 4.0933.$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *n* is the number of data point, Se is the standard error of estimation, r is the correlation coefficient, F is the F ratio and Q is the quality factor. J: Balaban index; ^{1}X: First-order Randic connectivity index; Wiener (W) index accounts for the size, shape and branching of the molecule. **Wiener index (W).** W=W(G) of G is defined as the half sum of the elements of the distance matrix:

	$$W - W(G) = 1/2\sum_{i=1}, \sum_{j-1}(D_{ij})$$ Where $(D)_{ij}$ is the *ij*th element of the distance matrix which denotes the shortest graph-theoretical distance between sites *i and j* of G. **The first-order connectivity index (χ).** The first-order connectivity index $\chi = \chi(G)$ of G is defined as: $$^1\chi^1\chi(G) = \sum_{i,j}[d(i).d(j)]^{-0.5}$$ **Balaban index (J).** The Balaban index J=J(G) of G is defined as: $$J = M/\mu + 1\sum_{\text{bonds}}(d_i.d_j)^{-0.5}$$ Where *M* is the number of bonds in G, μ is the cyclomatic number of G, and d_i (*i*= 1, 2, 3, ……N; N is the number of vertices in G) is the distance sum. The cyclomatic number $\mu = \mu(G)$ of a cyclic graph G is equal to the minimum number of edges necessary to be erased from G in order to transform it into the related acyclic graph. In case of monocyclic graph $\mu=1$ otherwise it is calculated by means of the following expression. $$\grave{\imath} = M - N + 1$$ **Szeged index (Sz).** The Szeged index, Sz=Sz(G), is calculated according to the following expression: $$\text{Sz} = \text{Sz}(G)\sum_{\text{edges}} n_u.n_v$$ Where n_u is the number of vertices lying closer to one end of the edge e=uv; the meaning of n_v is analogous. Edges equidistance from both ends of an edge, e= uv are not taken into account.
Reference	QSAR study on benzenesulphonamide carbonic anhydrase inhibitors: topological approach using Balaban index. *Bioorganic & Medicinal Chemistry* 12 (2004) 789–793

Target Species	Human
Chemical	Para-substituted aromatic sulfonamides

Type	
Mode of Action	Inhibitor
QSAR Model 1	$\log K_1 = -0.96(\pm 0.40)^1 \chi_{\text{inf}} - 0.6852(\pm 0.15) N - rings + 4.57(\pm 0.85)$ $n = 47,\ R = 0.8149,\ R^2 = 0.6642,\ R^2_{adj} = 0.6773,\ RMS = 0.2773,\ F = 33.18$
QSAR Model 2	$\log K_1 = -0.93(\pm 0.39)^1 \chi_{\text{inf}} - 0.56(\pm 0.51)^0 \chi^v_{\text{inf}} - 0.79(\pm 0.17) N - rings + 5.79(\pm 1.38)$ $n = 47,\ R = 0.8356,\ R^2 = 0.6984,\ R^2_{adj} = 0.6773,\ RMS = 0.2773,\ F = 33.18$
QSAR Model 3	$\log K_1 = -0.94(\pm 0.37)^1 \chi_{\text{inf}} - 1.00(\pm 0.64)^0 \chi^v_{\text{inf}} + 0.71(\pm 0.66)^1 \chi^v_{\text{inf}} - 0.85(\pm 0.17) N - rings + 4.98(\pm 1.52)$ $n = 47,\ R = 0.8534,\ R^2 = 0.7283,\ R^2_{adj} = 0.7024,\ RMS = 0.2632,\ F = 28.14$
QSAR Model 4	$\log K_1 = -0.71(\pm 0.67)^0 \chi_{\text{inf}} - 0.30(\pm 1.37)^1 \chi^v_{\text{inf}} - 0.90(\pm 0.41)^0 \chi^v_{\text{inf}} - 1.01(\pm 0.65)^1 \chi^v_{\text{inf}} - 0.87(\pm 0.21) N - rings + 5.49(\pm 2.77)$ $n = 47,\ R = 0.8541,\ R^2 = 0.7296,\ R^2_{adj} = 0.6966,\ RMS = 0.2625,\ F = 22.12$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Calculated descriptors include: 1. Kappa[1]; 2. Kappa[2]; 3. Kappa[3]; 4. Mean Wiener; 5. Wiener information index; 6. Polarity; 7. Gordon; 8. Balaban; 9. Schultz; 10. Quadratic index; 11. Zagreb[1]; 12. Zagreb2; 13. Wiener; 14. Number of rings; 15. Number of branches; 16. Topological diameter; 17. Topological radius; 18. Xu[1]; 19. Xu[2]; 20. Xu[3]; 21. Kier-Hall[0] ($^0\chi^v$); 22. Kier-Hall[1] ($^1\chi^v$); 23. Kier-Hall[inf,0] ($^0\chi^v_{inf}$); 24. Kier-Hall[inf,1] ($^1\chi^v_{inf}$); 25. Randic[0] ($^0\chi$); 26. Randic[1] ($^1\chi$); 27. Randic[inf,0] ($^0\chi_{inf}$); 28. Randic[inf,1] ($^1\chi_{inf}$); 29. Modified Randic index.
Reference	QSAR study on para-substituted aromatic sulfonamides as carbonic anhydrase II inhibitors using topological information indices. *Bioorganic & Medicinal Chemistry* 14 (2006) 1108–1114