Target Name	Carbonic anhydrase IX
Target TTD ID	TTDR00211

Target Species	Human
Chemical Type	Aromatic sulfonamides
Mode of Action	Inhibitor
QSAR Model 1	$\log K_I(\text{hCA IX}) = 2.3511 - 0.1223(\pm 0.0287)^2\chi + 0.4905(\pm 0.1122)I_3$ $n = 32,\quad \text{Se} = 0.3085,\quad R = 0.7150,\quad R^2_A = 0.47746,\quad F = 15.1629,\quad Q = 2.3176$
QSAR Model 2	$\log K_I(\text{hCA IX}) = 2.6141 - 0.3804(\pm 0.1258)^1\chi + 0.5025(\pm 0.2425)^2\chi^v + 0.4879(\pm 0.1070)\text{I}_3$ $n = 32,\quad \text{Se} = 0.2955,\quad R = 0.7529,\quad \text{R}^2_A = 0.5204,\quad \text{F} = 12.2126,\quad \text{Q} = 2.5478$
QSAR Model 3	$\log K_I(\text{hCA IX}) = 2.4664 - 0.3643(\pm 0.1193)^1\chi + 0.5092(\pm 0.2291)^2\chi^v + 0.2962(\pm 0.1434)I_2 + 0.3930(\pm 0.1112)I_3$ $n = 32,\quad \text{Se} = 0.2796,\quad R = 0.7933,\quad R^2_A = 0.5705,\quad F = 11.2945,\quad Q = 2.8372$
QSAR Model 4	$\log K_I(\text{hCA IX}) = 3.7804 - 0.7091(\pm 0.3046)^1\chi + 0.5123(\pm 0.2270)^2\chi^v + 0.00462 \times (\pm 0.0038)I_1 + 0.3119(\pm 0.1427)I_2 + 0.3520(\pm 0.1151)\text{I}_3$ $n = 32,\quad \text{Se} = 0.2770,\quad R = 0.8040,\quad R^2_A = 0.5785,\quad F = 9.5077,\quad Q = 2.9025$
QSAR Model 5	$\log K_I(\text{hCA IX}) = 3.9171 - 0.5583(\pm 0.3274)^1\chi - 0.1447(\pm 0.1212)^2\chi + 0.4171(0.2403)^2\chi^v + 0.0053(\pm 0.0038)\text{PI} + 0.3771(\pm 0.1517)I_2 + 0.3480(\pm 0.1142)I_3$ $n = 32,\quad \text{Se} = 0.2748,\quad R = 0.8158,\quad R^2_A = 0.5852,\quad F = 8.2903,\quad Q = 2.9687$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Topological indices used being: Wiener (W)-, Szeged (Sz)-, PI (Padmakar–Ivan)-, Randic

	connectivity ($^0\chi$, $^1\chi$, $^2\chi$)-, and Kier and Hall's valence connectivity ($^0\chi^v$, $^1\chi^v$, $^2\chi^v$)-indices. The indicator parameters: I_1, I_2, I_3 assumes the value 1 when heterocyclic, halogens, and –NH2 group para to –SO2NH2 are, respectively, present in the compounds used. In absence of which the values of indicator parameters are zero. n is the number of the compounds, R is the correlation co-efficient, Se is the standard error of estimation, F is the Fischer F -ratio and Q is the quality factor. log *K*, logarithm of binding constant (*K*); ^2x, Randic connectivity index; I_3, indicator parameter for the presence (=1) or absence (=0) of $–NH_2$ group para to $–SO_2NH_2$; *n*, number of compounds; Se, standard error of estimation; *R*, multiple correlation coefficient; R_A^2, adjustable R^2; *F*, Fishers F-ratio; *Q*, quality factor
Reference	Carbonic anhydrase inhibitors: the first QSAR study on inhibition of tumor-associated isoenzyme IX with aromatic and heterocyclic sulfonamides. *Bioorganic & Medicinal Chemistry Letters* 14 (2004) 3283–3290

Target Species	Human
Chemical Type	Heterocyclic sulfonamides
Mode of Action	Inhibitor
QSAR Model 1	$\log K_I(\text{hCA IX}) = 2.3511 - 0.1223(\pm 0.0287)^2\chi + 0.4905(\pm 0.1122)I_3$ $n = 32, \quad \text{Se} = 0.3085, \quad R = 0.7150, \quad R_A^2 = 0.47746, \quad F = 15.1629, \quad Q = 2.3176$
QSAR Model 2	$\log K_I(\text{hCA IX}) = 2.6141 - 0.3804(\pm 0.1258)^1\chi + 0.5025(\pm 0.2425)^2\chi^v + 0.4879(\pm 0.1070)I_3$ $n = 32, \quad \text{Se} = 0.2955, \quad R = 0.7529, \quad R_A^2 = 0.5204, \quad F = 12.2126, \quad Q = 2.5478$
QSAR Model 3	$\log K_I(\text{hCA IX}) = 2.4664 - 0.3643(\pm 0.1193)^1\chi + 0.5092(\pm 0.2291)^2\chi^v + 0.2962(\pm 0.1434)I_2 + 0.3930(\pm 0.1112)I_3$ $n = 32, \quad \text{Se} = 0.2796, \quad R = 0.7933, \quad R_A^2 = 0.5705, \quad F = 11.2945, \quad Q = 2.8372$

QSAR Model 4	$\log K_I(\text{hCA IX}) = 3.7804 - 0.7091(\pm 0.3046)^1\chi + 0.5123(\pm 0.2270)^2\chi^v + 0.00462 \times (\pm 0.0038)I_1 + 0.3119(\pm 0.1427)I_2 + 0.3520(\pm 0.1151)I_3$ $n = 32, \quad \text{Se} = 0.2770, \quad R = 0.8040, \quad R^2_A = 0.5785, \quad F = 9.5077, \quad Q = 2.9025$
QSAR Model 5	$\log K_I(\text{hCA IX}) = 3.9171 - 0.5583(\pm 0.3274)^1\chi - 0.1447(\pm 0.1212)^2\chi + 0.4171(0.2403)^2\chi^v + 0.0053(\pm 0.0038)\text{PI} + 0.3771(\pm 0.1517)I_2 + 0.3480(\pm 0.1142)I_3$ $n = 32, \quad \text{Se} = 0.2748, \quad R = 0.8158, \quad R^2_A = 0.5852, \quad F = 8.2903, \quad Q = 2.9687$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Topological indices used being: Wiener (W)-, Szeged (Sz)-, PI (Padmakar–Ivan)-, Randic connectivity ($^0\chi$, $^1\chi$, $^2\chi$)-, and Kier and Hall's valence connectivity ($^0\chi^v$, $^1\chi^v$, $^2\chi^v$)-indices. The indicator parameters: I_1, I_2, I_3 assumes the value 1 when heterocyclic, halogens, and –NH2 group para to –SO2NH2 are, respectively, present in the compounds used. In absence of which the values of indicator parameters are zero. n is the number of the compounds, R is the correlation co-efficient, Se is the standard error of estimation, F is the Fischer F -ratio and Q is the quality factor. log *K*, logarithm of binding constant (*K*); ^2x, Randic connectivity index; I_3, indicator parameter for the presence (=1) or absence (=0) of $–NH_2$ group para to $–SO_2NH_2$; *n*, number of compounds; Se, standard error of estimation; *R*, multiple correlation coefficient; R^2_A, adjustable R^2; *F*, Fishers F-ratio; *Q*, quality factor
Reference	Carbonic anhydrase inhibitors: the first QSAR study on inhibition of tumor-associated isoenzyme IX with aromatic and heterocyclic sulfonamides. *Bioorganic & Medicinal Chemistry Letters* 14 (2004) 3283–3290