

Target Name	Carbonic anhydrase IV
Target TTD ID	TTDR00209

Target Species	Human
Chemical Type	Sulfonamides incorporating β -alanyl moieties
Mode of Action	Inhibitor
QSAR Model 1	$\log K_1(\text{hCAIV}) = 2.7452 - 0.1811(\pm 0.0250) {}^1\chi + 0.5123(\pm 0.1866) J - 0.8039(\pm 0.1300) IP_1 - 0.9189(\pm 0.1161) IP_2 + 0.2796(\pm 0.2052) IP_3$ $n = 49, \text{ S.E.} = 0.3080, R = 0.9077, R_A^2 = 0.8034, F = 40.223$
Molecular Descriptor 1	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>$\log K$, logarithm of binding constant (K); ${}^1\chi$, 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</p>
Reference	<p>QSAR study on carbonic anhydrase inhibitors: water-soluble sulfonamides incorporating β-alanyl moieties, possessing long lasting-intra ocular pressure lowering properties—a molecular connectivity approach. <i>European Journal of Medicinal Chemistry</i> 40 (2005) 1002–1012</p>