Target Name	3-Hydroxy-anthranilic acid dioxygenase (3-HAO)
Target TTD ID	TTDR01339

Target Species	Human
Target Location	Brain
Chemical Type	4,5-, 4,6-disubstituted and 4,5,6-trisubstituted 3-hydroxyanthranilic acid derivatives
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{50}(nM) = -1.0617(\pm 0.0903)^{0}\chi^{v} + 1.3269(\pm 0.1779)\mathrm{Ip}_5 + 5.6907$ *n=16*, Se = 0.3472, R_A^2=0. 9150, R^2 = 0.9264, R = 0.9625, F = 81.758, $p = 4.330 \times 10^{-8}$
QSAR Model 2	$pIC_{50}(nM) = -1.3468(\pm 0.1846)^{0}\chi^{v} + -0.4144(\pm 0.2389)^{1}\chi^{v} + 1.4243(\pm 0.1748)\mathrm{Ip}_5 + 6.0887$ *n=16*, Se = 0.3231, R_A^2=0. 9264, R^2 = 0.9411, R = 0.9701, F = 63.928
QSAR Model 3	$pIC_{50}(nM) = -1.1512(\pm 0.1084)^{0}\chi^{v} + -1.4397(\pm 0.2389)Ip_5 + 0.2974(\pm 0.2163)\mathrm{Ip}_6 + 6.1027$ *n=16*, Se = 0.3359, R_A^2=0. 9205, R^2 = 0.9363, R = 0.9677, F = 58.867
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *n* is the number of compounds; Se, standard error of estimation; R_A^2, adjustable R^2; R^2, coefficient of determination; R, correlation coefficient; F, F-ratio, *p*, probability; χ^V, molecular connectivity indices The connectivity index $\chi = \chi(G)$ of a graph G is defined by Randic[2] as under: $\chi = \chi(G) = \sum_{ij}[d_i\, d_j]^{-0.5}$ Where d_i is the valence of a vertex i, equal to the number of bonds connected to the atom i, in G, representing the graph of a compound. Meaning of d_j is analogous. In the case of hetero-systems the connectivity is given in terms of valence delta values δ_i^V and δ_j^V of

	atoms *i* and *j* and is denoted by χ^V. This version of the connectivity index is called the valence connectivity index and defined as under: $\chi^V = \chi^V(G) = \sum_{ij}[\delta_i^V\ \delta_j^V]^{-0.5}$ Where the sum is taken over all bonds *i–j* of the molecule. Valence delta values are given by $\delta_i^V = \frac{Z_i^V - H_i}{Z_i - Z_j - 1}$ Where Z_i is the atomic number of atom *i*, Z_i^V is the number of valence electron of the atom *i* and H_i is number of hydrogen atoms attached to atom *i*. δ_i^V values are available in books of Kier and Hall.
Reference	QSAR Study on Inhibition of Brain 3-Hydroxy-anthranilic Acid Dioxygenase (3-HAO):A Molecular Connectivity Approach. *Bioorganic & Medicinal Chemistry* 9 (2001) 3295–3299