Target Name	GABA-A receptor alpha 3
Target TTD ID	TTDR01178

Target Species	Human
Chemical Type	Phthalazines
Mode of Action	Modulator
QSAR Model 1	$pK_i = 8.14817 - 0.06079*\text{"PEOE\_VSA\_PPOS"} + 0.016144*\text{"Slog P\_VSA9"}\ 0.017353*\text{"PEOE VSA-0"}$ $+ 0.000235*\text{"weinerPath"} + 0.010737*\text{"PEOE\_VSA\_POS"} - 0.056294*\text{"PEOE\_VSA}$ $+ 3\text{"} - 1.00127*<-6.82572 - \text{"log S"} > -0.016909*<\text{"PEOE\_VSA} + 0\text{"} - 85.5211>$ $N_{training} = 86$, $N_{test} = 17$, optimal number of components (ONC) = 4, $R^2 = 0.742$, adjusted R^2 (R^2_{adj}) = 0.721, Bs R^2 = 0.748, R^2_{cv} (q^2) = 0.687, randomized $R^2 = 0.383$, PRESS = 8.764, $R^2_{pred} = 0.671$, LOF = 0.234, F test = 28.171, $(R^2 - R^2_O) / R^2 = 0$, and $k = 1$.
QSAR Model 2	$pK_i = 8.50466 + 0.230131*<\text{"Kier1"} - 20.5959> + 0.014112*\text{"S log P\_VSA9"} - 0.964241*<-6.87042 - \text{"log S"}>$ $-0.01636*\text{"PEOE\_VSA-0"} - 0.136879*<33.9457 - \text{"vsa\_pol"}> + 0.071594*<23.3534 - \text{"PEOE\_VSA\_PPOS"}>$ $-0.046163*\text{"PEOE\_VSA + 3"}$ $N_{training} = 86$, $N_{test} = 17$, ONC = 3, $R^2 = 0.770$, adjusted R^2 (R^2_{adj}) = 0.761, Bs R^2 = 0.754, R^2_{cv} (q^2) = 0.692, randomized $R^2 = 0.362$, PRESS = 8.764, $R^2_{pred} = 0.679$, $(R^2 - R^2_O) / R^2 = 0$, and $k = 1$.
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Descriptors used in the study represent physical properties, subdivided surface areas, atom and bond counts, Kier and Hall connectivity and kappa shape indices, adjacency and distance matrix descriptors, and partial charge descriptors.

Reference	Combinatorial Library Enumeration and Lead Hopping using Comparative Interaction Fingerprint Analysis and Classical 2D QSAR Methods for Seeking Novel GABAA r3 Modulators. *J. Chem. Inf. Model.* 2009, *49*, 2498–2511

Target Species	Human
Chemical Type	Phthalazine core-based derivatives
Mode of Action	Modulator
QSAR Model 1	$pK_i = 8.14817 - 0.06079*\text{"PEOE\_VSA\_PPOS"} + 0.016144*\text{"Slog P\_VSA9"}\ 0.017353*\text{"PEOE VSA-0"} + 0.000235*\text{"weinerPath"} + 0.010737*\text{"PEOE\_VSA\_POS"} - 0.056294*\text{"PEOE\_VSA} + 3\text{"} - 1.00127*<-6.82572 - \text{"log S"}> - 0.016909*<\text{"PEOE\_VSA} + 0\text{"} - 85.5211>$ $N_{training} = 86$, $N_{test} = 17$, optimal number of components (ONC) = 4, $R^2 = 0.742$, adjusted R^2 (R^2_{adj}) = 0.721, Bs R^2 = 0.748, R^2_{cv} (q^2) = 0.687, randomized R^2 = 0.383, PRESS = 8.764, R^2_{pred} = 0.671, LOF = 0.234, F test = 28.171, $(R^2 - R^2_O) / R^2$ = 0, and $k = 1$.
QSAR Model 2	$pK_i = 8.50466 + 0.230131*<\text{"Kier1"} - 20.5959> + 0.014112*\text{"S log P\_VSA9"} - 0.964241*<-6.87042 - \text{"log S"}> - 0.01636*\text{"PEOE\_VSA-0"} - 0.136879*<33.9457 - \text{"vsa\_pol"}> + 0.071594*<23.3534 - \text{"PEOE\_VSA\_PPOS"}> - 0.046163*\text{"PEOE\_VSA + 3"}$ $N_{training} = 86$, $N_{test} = 17$, ONC = 3, $R^2 = 0.770$, adjusted R^2 (R^2_{adj}) = 0.761, Bs R^2 = 0.754, R^2_{cv} (q^2) = 0.692, randomized R^2 = 0.362, PRESS = 8.764, R^2_{pred} = 0.679, $(R^2 - R^2_O) / R^2 = 0$, and $k = 1$.
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Descriptors used in the study represent physical properties, subdivided surface areas, atom and bond counts, Kier and Hall connectivity and kappa shape indices, adjacency and distance matrix descriptors, and partial charge descriptors.
Reference	Combinatorial Library Enumeration and Lead Hopping using Comparative Interaction Fingerprint Analysis and Classical 2D QSAR Methods for Seeking Novel GABAA r3 Modulators. *J. Chem. Inf.*

	Model. 2009, *49*, 2498–2511