Target Name	Nicotinic acetylcholine receptor
Target TTD ID	TTDS00303

Target Species	Human
Chemical Type	Caracurine V analogues
Mode of Action	Ligand
QSAR Model 1	$\hat{pK_i} = 3.0387 + 0.1025 \cdot \mathrm{DsDs_3} - 0.0032 \cdot \mathrm{AA_9} - 0.0164 \cdot \mathrm{DsH_3} + 0.0202 \cdot \mathrm{DsDs_4}$ $R^2_{\mathrm{CV}-1} = 0.73,\quad \mathrm{RMSEP}_{\mathrm{CV}-1} = 0.39,\ R^2_{\mathrm{CV}-40\%} = 0.69,\quad \mathrm{RMSEP}_{\mathrm{CV}-40\%} = 0.42,\quad R^2 = 0.77,$ $\mathrm{RMSEC} = 0.38,\quad m = 33,\quad \mathrm{LV} = 3$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** R^2_{CV-1} (also known as q^2) and $R^2_{CV-40\%}$ are the leave-one-out and leave-40%-out cross-validated squared multiple correlation coefficients, and $RMSEP_{CV-1}$ and $RMSEP_{CV-40\%}$ are the respective root-mean squared errors of prediction. R^2 is the coefficient of determination, RMSEC is the root mean squared error of calibration (also known as s), m is the number of molecules and LV is the number of principal components. *'Ds'*, *'A'* and *'H'*, describe surface points with strong H-bond donor, H-bond acceptor and hydrophilic properties, respectively. $DsDs_3$ and $DsDs_4$ describe the presence or absence of the allyl alcohol group and DsH_3 discriminates between compounds with one and two allyl alcohol moieties.
Reference	Bisquaternary caracurine V and iso-caracurine V salts as ligands for the muscle type of nicotinic acetylcholine receptors: SAR and QSAR studies. *Bioorganic & Medicinal Chemistry* 12 (2004) 6277–6285

Target Species	Human
Chemical Type	Iso-caracurine V analogues
Mode of Action	Ligand
QSAR Model 1	$\hat{pK_i} = 3.0387 + 0.1025 \cdot \mathrm{DsDs_3} - 0.0032 \cdot \mathrm{AA_9} - 0.0164 \cdot \mathrm{DsH_3} + 0.0202 \cdot \mathrm{DsDs_4}$ $R^2_{\mathrm{CV}-1} = 0.73, \quad \mathrm{RMSEP_{CV}}_{-1} = 0.39, \; R^2_{\mathrm{CV}-40\%} = 0.69, \quad \mathrm{RMSEP_{CV}}_{-40\%} = 0.42, \quad R^2 = 0.77,$ $\mathrm{RMSEC} = 0.38, \quad m = 33, \quad \mathrm{LV} = 3$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** R^2_{CV-1} (also known as q^2) and $R^2_{CV-40\%}$ are the leave-one-out and leave-40%-out cross-validated squared multiple correlation coefficients, and $RMSEP_{CV-1}$ and $RMSEP_{CV-40\%}$ are the respective root-mean squared errors of prediction. R^2 is the coefficient of determination, RMSEC is the root mean squared error of calibration (also known as s), m is the number of molecules and LV is the number of principal components. *'Ds'*, *'A'* and *'H'*, describe surface points with strong H-bond donor, H-bond acceptor and hydrophilic properties, respectively. $DsDs_3$ and $DsDs_4$ describe the presence or absence of the allyl alcohol group and DsH_3 discriminates between compounds with one and two allyl alcohol moieties.
Reference	Bisquaternary caracurine V and iso-caracurine V salts as ligands for the muscle type of nicotinic acetylcholine receptors: SAR and QSAR studies. *Bioorganic & Medicinal Chemistry* 12 (2004) 6277–6285