Target Name	Nav1.4 channel
Target TTD ID	TTDS00416

Target Species	Human
Chemical Type	Tocainide analogues
Mode of Action	Blocker
QSAR Model 1	$pEC_{50} = 3.174(\pm 1.17)C\ Log\ D - 3.629(\pm 1.50)\log(\beta C\ Log\ D + 1) + 3.161(\pm 0.59)\log\beta$ $= -0.905; n = 20; r^2 = 0.734; s = 0.402; F = 14.749$
QSAR Model 2	$pEC_{50} = 1.401(\pm 0.62)C\ Log\ D - 1.894(\pm 1.08)\log(\beta C\ Log\ D + 1) + 3.798(\pm 0.46)\log\beta$ $= -1.489; n = 20; r^2 = 0.666; s = 0.394; F = 10.632$
QSAR Model 3	$pEC_{50} = 0.465(\pm 0.11)C\ Log\ D + 0.431(\pm 0.10)pK_a + 0.487(\pm 0.89)$ $n = 22; r^2 = 0.589; s = 0.514; F = 13.62$
QSAR Model 4	$pEC_{50} = 0.568(\pm 0.10)C\ Log\ D + 0.616(\pm 0.16)pK_a - 1.286(\pm 1.43)$ $n = 20; r^2 = 0.677; s = 0.376; F = 17.83$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Lipophilic and basic molecular properties for VGSCs blocking activity were calculated as C Log D (pH¼ 7.42) and pKa using the Advanced Chemistry Development (ACD) software
Reference	2D- and 3D-QSAR of Tocainide and Mexiletine analogues acting as $Na_V1.4$ channel blockers. *European Journal of Medicinal Chemistry* 44 (2009) 1477–1485

Target Species	Human

Chemical Type	Mexiletine analogues
Mode of Action	Blocker
QSAR Model 1	$pEC_{50} = 3.174(\pm 1.17)C\ Log\ D - 3.629(\pm 1.50)\log(\beta C\ Log\ D + 1) + 3.161(\pm 0.59)\log\beta$ $= -0.905; n = 20; r^2 = 0.734; s = 0.402; F = 14.749$
QSAR Model 2	$pEC_{50} = 1.401(\pm 0.62)C\ Log\ D - 1.894(\pm 1.08)\log(\beta C\ Log\ D + 1) + 3.798(\pm 0.46)\log\beta$ $= -1.489; n = 20; r^2 = 0.666; s = 0.394; F = 10.632$
QSAR Model 3	$pEC_{50} = 0.465(\pm 0.11)C\ Log\ D + 0.431(\pm 0.10)pK_a + 0.487(\pm 0.89)$ $n = 22; r^2 = 0.589; s = 0.514; F = 13.62$
QSAR Model 4	$pEC_{50} = 0.568(\pm 0.10)C\ Log\ D + 0.616(\pm 0.16)pK_a - 1.286(\pm 1.43)$ $n = 20; r^2 = 0.677; s = 0.376; F = 17.83$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Lipophilic and basic molecular properties for VGSCs blocking activity were calculated as C Log D (pH¼ 7.42) and pKa using the Advanced Chemistry Development (ACD) software
Reference	2D- and 3D-QSAR of Tocainide and Mexiletine analogues acting as $Na_V1.4$ channel blockers. *European Journal of Medicinal Chemistry* 44 (2009) 1477–1485