

Supplementary Materials

Computational Design of High-Affinity Blockers for Sodium Channel NaV1.2 from μ -Conotoxin KIIIA

Sequence alignment used in homology modelling

Table S1. Sequence alignment of the target and uploaded template. The missing residues in the template are indicated by the dashes.

The template contained no ligands.

Target	DVMILTVFCLSVFALIGLQLFMGNLRNKCLQWPPDNSSFEINITSSFFNNSLDGNG
template_upload. 1. Å	DVMILTVFCLSVFALIGLQLFMGNLRNKCLQWPPD-----
Target	TTFNRTVSIFNWDEYIEDKSHFYFLEGQNDALLCGNSSDAGQCPEGYICVKAGR
template_upload. 1. Å	-----FNWDEYIEDKSHFYFLEGQNDALLCGNSSDAGQCPEGYICVKAGR
Target	PNYGYTSFDIFSWAFLSLFRLMTQDFWENLYQLTLRAAGKTYMIFVVLVIFLG
template_upload. 1. Å	PNYGYTSFDIFSWAFLSLFRLMTQDFWENLYQLTLRAAGKTYMIFVVLVIFLG
Target	YLINLILAVVAMAYEEQNQATLEEAEITLVLAIIVFIFAVVGMQLFGKSYKECVC
template_upload. 1. Å	YLINLILAVVAMAYEEQNQATLEEAEITLVLAIIVFIFAVVGMQLFGKSYKECVC
Target	KISNDCELPRWHMHDFHFSFLIVFRVLCGEWETMWDCEVAGQTMCLTVFMMVM
template_upload. 1. Å	KISNDCELPRWHMHDFHFSFLIVFRVLCGEWETMWDCEVAGQTMCLTVFMMVM
Target	VIGNLVVLNLFALLLIPSIMNVLLVCLIFWLIFSIMGVNLFAGKFYHCINYTTG
template_upload. 1. Å	VIGNLVVLNLFALLLIPSIMNVLLVCLIFWLIFSIMGVNLFAGKFYHCINYTTG
Target	EMFDVSVVNNYSECKALIESNQATARWKNVKVNFNDVGLGYLSLLQVATFKGWMDI
template_upload. 1. Å	EMFDVSVVNNYSECKALIESNQATARWKNVKVNFNDVGLGYLSLLQVATFKGWMDI
Target	MYAAVDSRNVELQPKYEDNLYMYLYFVIFIIFGSFFTLNLFIGVIIDNFNQKKK
template_upload. 1. Å	MYAAVDSRNVELQPKYEDNLYMYLYFVIFIIFGSFFTLNLFIGVIIDNFNQKKK
Target	IRTLFALMMSLPALFNIGLLFLVMFIYAIFGMSNFAYVKREVGIDDMFNFE
template_upload. 1. Å	IRTLFALMMSLPALFNIGLLFLVMFIYAIFGMSNFAYVKREVGIDDMFNFE
Target	GNSMICLFQITTSAGWDGLLAPILNSGPPDCDPDKDHPGSSVKGDCGNPSVG
template_upload. 1. Å	GNSMICLFQITTSAGWDGLLAPILNSGPPDCDPDKDHPGSSVKGDCGNPSVG
Target	FVSYIIISFLVWVNMVIAVILENFSVA
template_upload. 1. Å	FVSYIIISFLVWVNMVIAVILENFSVA

Time series of the R14 contacts with the channel residues

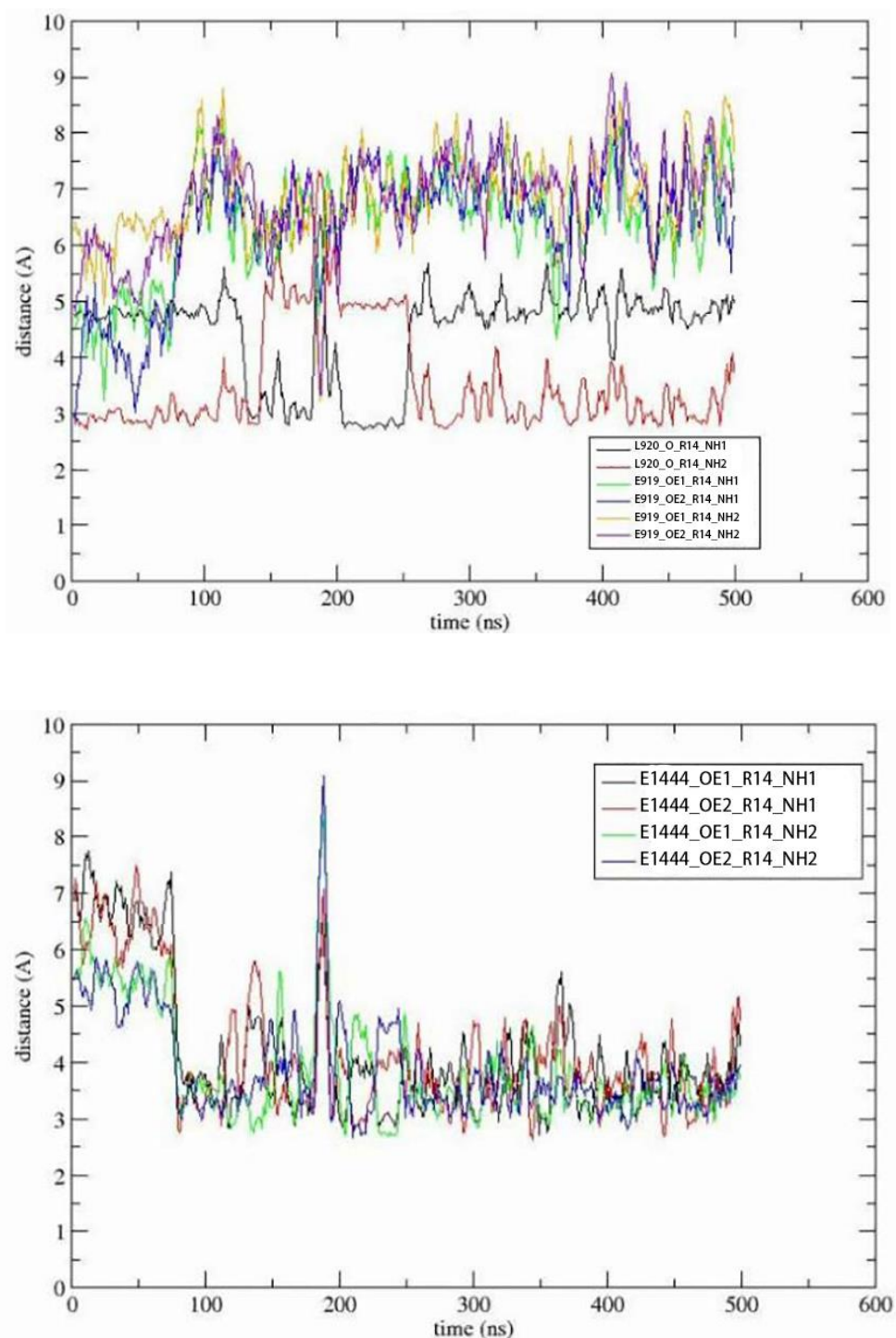


Figure S1. The toxin residue R14 makes contact with the channel residues E919, L920 and E1444. The time series of the E919/L920–R14 and E1444–R14 pair distances in the Nav1.2–KIIIA complex are shown at the top and bottom graphs, respectively. After about 100 ns, R14 is seen to switch from E919 to E1414. The E1444–R14 contact is preserved during the rest of the MD simulations.