

Supporting Information

Searching for New Leads to Treat Epilepsy. Target-based Virtual Screening for the Discovery of Anticonvulsant Agents.

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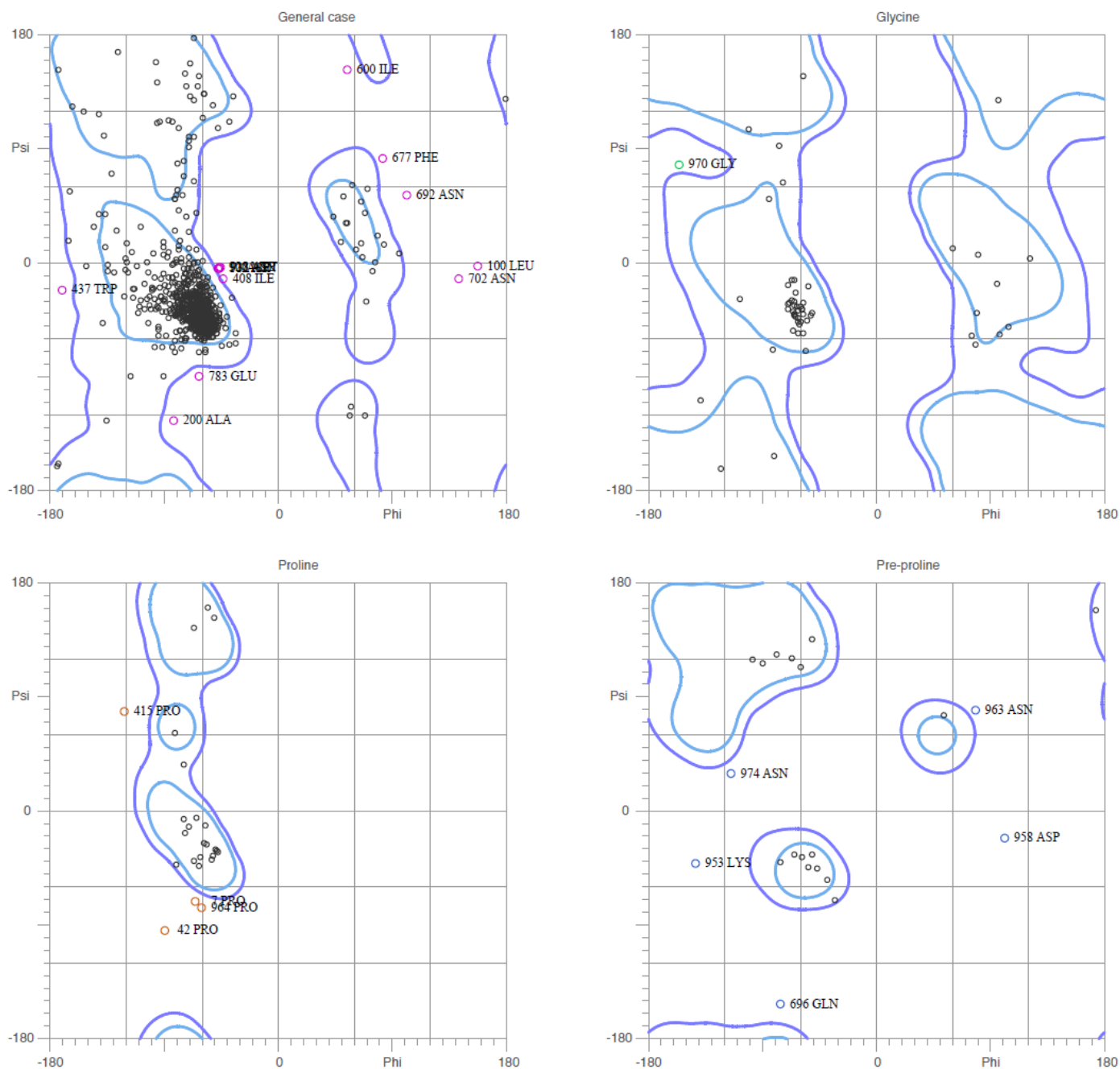
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MolProbity Ramachandran analysis

nav12cerrado.pdb, model 1



90.6% (884/976) of all residues were in favored (98%) regions.
97.6% (953/976) of all residues were in allowed (>99.8%) regions.

There were 23 outliers (phi, psi):

- 7 PRO (-66.3, -71.1)
- 42 PRO (-90.9, -94.8)
- 73 ASP (-48.5, -4.1)
- 100 LEU (157.9, -2.2)
- 102 ASN (-47.9, -4.6)
- 200 ALA (-83.6, -124.1)
- 408 ILE (-44.9, -12.2)
- 415 PRO (-122.4, 79.7)
- 437 TRP (-172.0, -21.9)

- 600 ILE (54.5, 153.4)
- 677 PHE (82.5, 83.0)
- 692 ASN (101.4, 54.6)
- 696 GLN (-76.2, -152.0)
- 702 ASN (142.6, -12.0)
- 783 GLU (-63.6, -89.0)
- 918 ASP (-46.0, -3.8)
- 920 MET (-47.9, -3.2)
- 953 LYS (-143.9, -41.1)
- 958 ASP (101.0, -21.7)
- 963 ASN (78.1, 80.2)
- 964 PRO (-61.9, -76.8)
- 970 GLY (-156.5, 78.1)
- 974 ASN (-115.5, 30.7)

<http://kinemage.biochem.duke.edu>

Lovell, Davis, et al. Proteins 50:437 (2003)

Figure S1. Ramachandran plots of the overall architecture of the final Nav1.2 close model.

Nav1.2 Close model

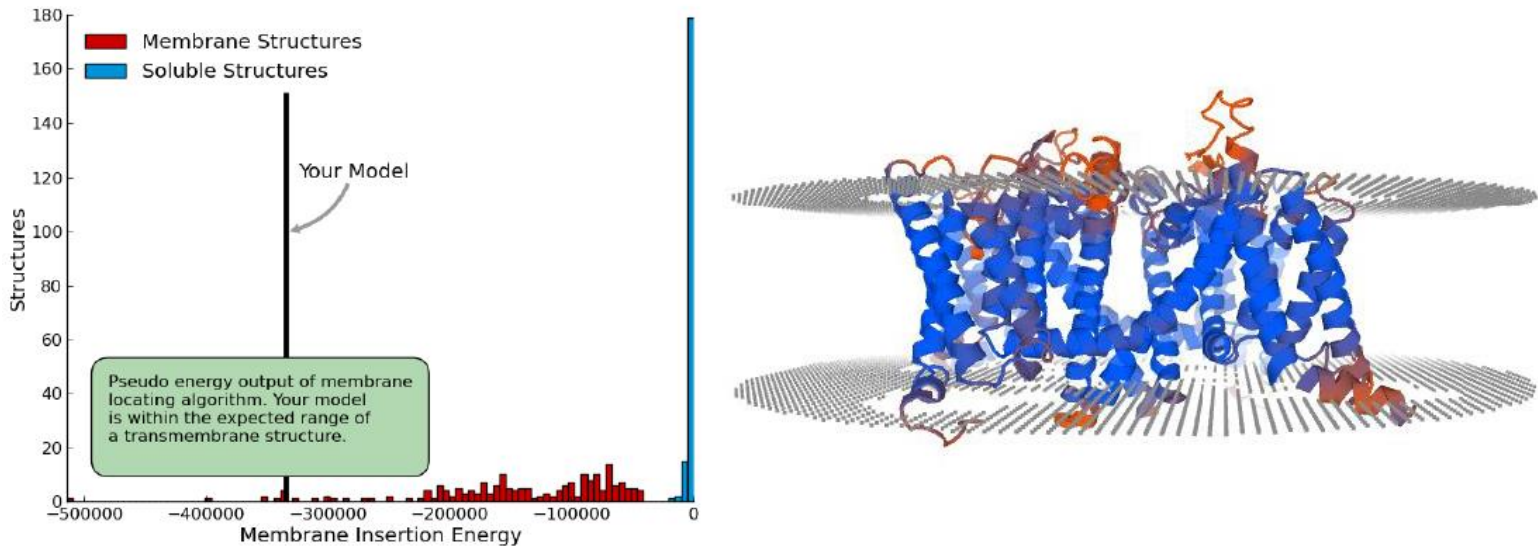


Figure S2. Results of QMEANbrane software for Nav1.2 close model.

Red: NaK closed-pore (2AHY)
Green: NaK opened-pore (3E86)

Blue: NavAb (3RVY)
Orange: NaK (3E86)

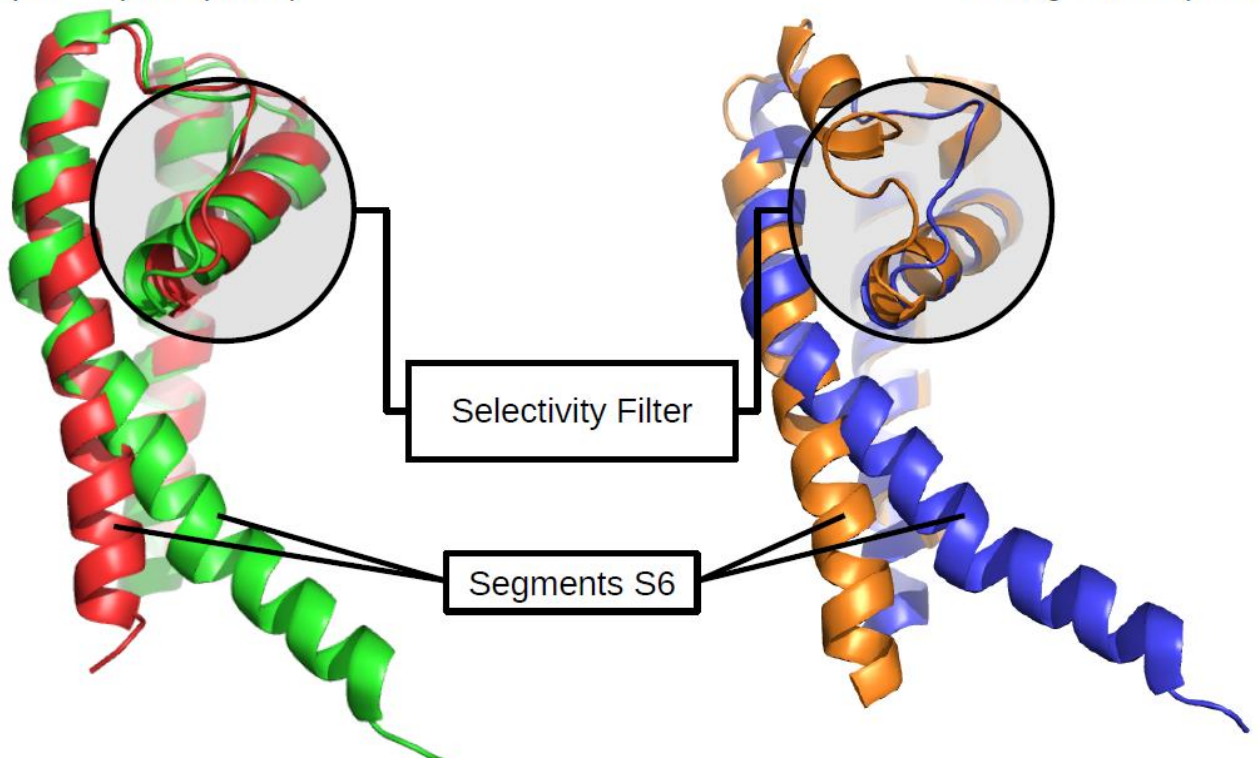


Figure S3. Comparison between open and closed experimental conformations of the NaK pore (PDB entries: 3E86 and 2AHY) and between this open conformation with the NavAb template (PDB entry: RVY).

Nav1.2 Open model

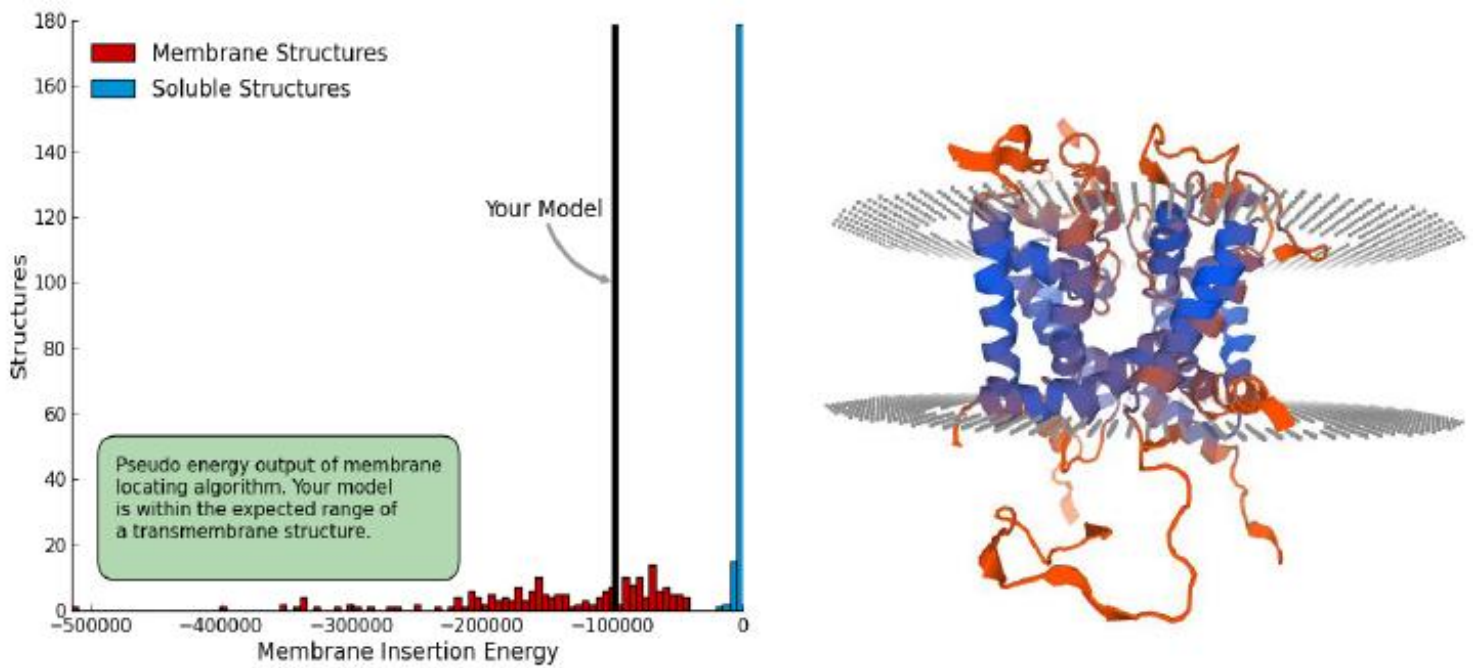


Figure S5. Results of QMEANbrane software for Nav1.2 open model.

Table S1: Value of the scores achieved for each domain of the closed and open models of Nav1.2.

	Domain I	Domain II	Domain III	Domain IV
Close Model				
C-score	-2.47	-0.59	-0.81	-0.82
TM-score	0.43	0.64	0.61	0.61
Open Model				
DOPE score	1.42	1.39	0.90	1.68