Pharmacological characterisation of the highly $Na_V1.7$ selective spider venom peptide Pn3a

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Supplementary Table 1: Energy and structural statistics of the 20 lowest energy structures of μ-TRTX-Pn3a calculated using a simulated annealing procedure with CNS

	μ-TRTX-Pn3a	**STDEV**
Energies:		
Overall (kcal/mol)	-1344	39.9
Bonds (kcal/mol)	22.6	1.48
Angles (kcal/mol)	58.6	4.08
Improper (kcal/mol)	20.6	2.70
Dihedral (kcal/mol)	169	2.99
Van Der Wall (kcal/mol)	-154	6.18
NOE (kcal/mol)	0.33	0.03
cDih (kcal/mol)	0.29	0.19
Electrostatic	-1461	45.8
RMSD:		
Bonds (Å)	1.28e-2	4.53e-4
Angles (°)	1.375	0.0436
Improper (Å)	1.43	0.1166
Dihedral (Å)	41.3	0.199
NOE (Å)	2.53e-2	1.15e-3
cDih (Å)	0.189	0.0671
Pairwise RMSD (Residues 2-31)		
Backbone atoms (Å)	0.33	0.07
Heavy atoms (Å)	116	0.12
Experimental Data:		
Distance Restraints:		
Intra-residue (i- j=0)	111	
Sequential (i-j = 1)	160	
Medium range (i-j <5)	67	

Long range (i-j ≥ 5)	149
Dihedral restraints	43 backbone / 19 side chain
Hydrogen bond restraints	34 (for 17 hbonds)
NOE violations >0.3 Å	0
cDih violations> 3.0°	1

Ramachandran statistics

Residues in most favoured regions (%)	92
Residues in additionally allowed regions (%)	8