Table S2: RMSD between the designed models and X-ray crystal structures of the 9-11 residue macrocycles. Related to Figure 3.

Design Name	RMSD (CA only) (Å)	RMSD backbone (C+N+CA+O+CN) (Å)	RMSD All Heavy atoms (Å)
D9.1	2.36	2	3.03
D9.8	0.39	0.33	0.88
D9.24	0.89	1.2	2.1
D9.29	0.78	1.11	1.66
D9.30	2.54	2.49	4.07
D9.30_LE0*	0.78	0.78	1.47
D10.1	0.27	0.27	0.47
D10.21	0.38	0.9	1.19
D10.22	0.75	0.82	1.58
D10.23	0.38	0.41	1.28
D10.31	0.47	0.45	0.84
D10.65	1.74	1.67	2.47
D11.1	0.43	0.43	1.11
D11.3	0.4	0.43	0.93
D11.4	0.51	0.54	0.93
D11.25	0.63	0.87	1.47

*Structure prediction runs for D9.30 identified conformation LE0 with lower energy than the design model. For more details, please see the methods section on computational design of structured membrane-permeable peptides.