

Table S1. Occupancy of the main-chain hydrogen bonds as a function of time from the beginning to the end of the 20 ns long MD trajectories of THP peptide and MS-8 peptomer.

THP			MS-8		
donor	acceptor	occupancy (%)	donor	acceptor	occupancy (%)
GLY19	ILE17	99.72	GLY22	GLN20	99.56
GLY22	GLN20	99.26	GLY19	SAR17	98.85
GLY28	LEU26	99.08	GLY25	VAL23	98.02
GLY16	PRO14	98.40	GLY16	PRO14	98.01
GLY25	VAL23	98.16	GLY22	VAL23	95.25
GLY16	ILE17	94.56	GLY19	GLN20	93.36
GLY31	PRO29	92.24	GLY16	SAR17	90.81
GLY25	LEU26	91.86	GLY7	PRO5	90.44
GLY13	PRO11	91.46	GLY13	PRO11	90.19
GLY34	PRO32	90.62	GLY10	PRO8	90.04
GLY19	GLN20	90.56	GLY31	PRO29	86.62
GLY37	PRO35	90.52	GLY37	PRO35	86.19
GLY10	PRO8	88.88	GLY34	PRO32	86.06
GLY7	PRO5	87.78	GLY4	PRO2	81.99
GLY22	VAL23	86.60	GLY34	PRO35	79.98
GLY28	PRO29	80.46	GLY13	PRO14	79.23
GLY13	PRO14	79.44	GLY10	PRO11	78.81
GLY37	PRO38	77.48	GLY31	PRO32	78.46
GLY34	PRO35	77.40	GLY37	PRO38	77.37
GLY31	PRO32	76.82	GLY28	PRO29	74.92
GLY10	PRO11	76.78	GLY25	NLE26	74.72
GLY4	PRO2	76.60	GLY7	PRO8	74.16
GLY7	PRO8	73.86	GLY4	PRO5	69.65
GLY4	PRO5	70.28	GLY28	NLE26	67.92
GLY1	PRO2	27.52	GLY1	PRO2	31.63

The H-bond selection criteria are described in the Experimental Section. Residues 17 and 26 are bolded for comparison.