Supplement to

The Structure of Bioactive Gastrin-17 Analogs of the N-Terminal Region

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Figure 1S. ECD spectra of G17(1-6)-NH_2 in various solvents.

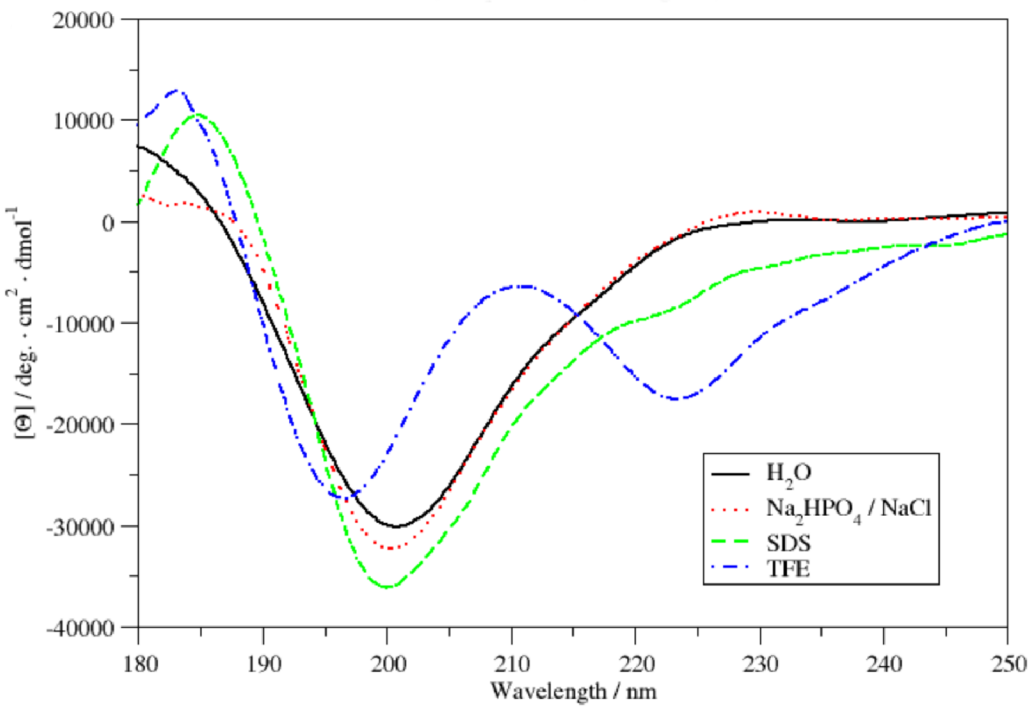

Figure 2S. ECD spectra of G17(1-6) in various solvents.

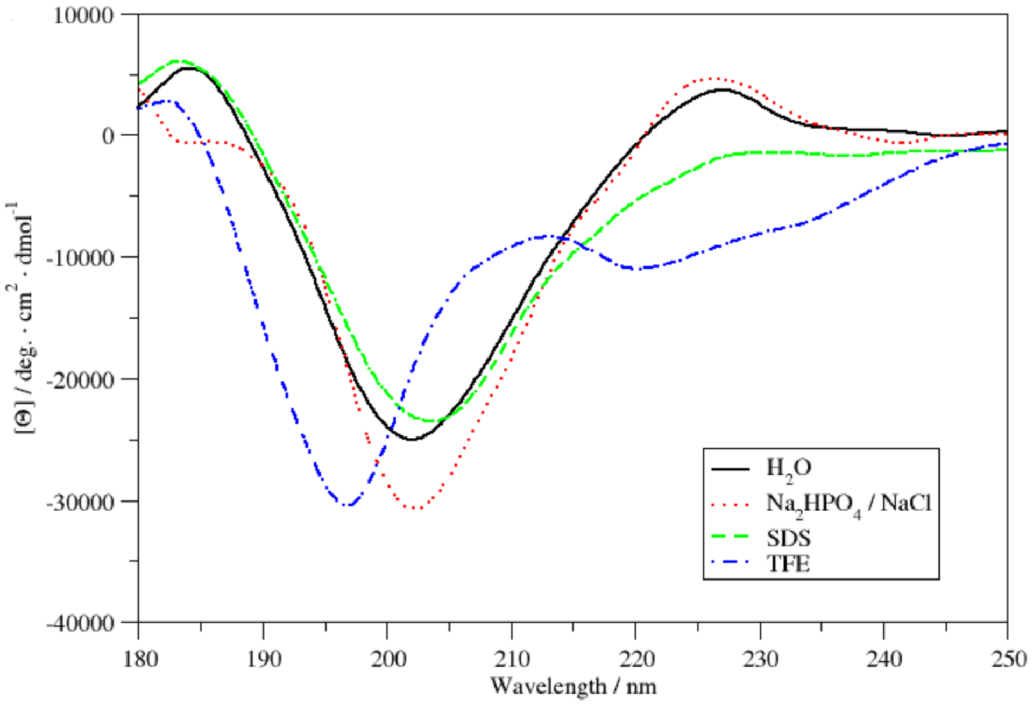

Figure 3S. ECD spectra of G17(1-5)-NH_2 in various solvents.

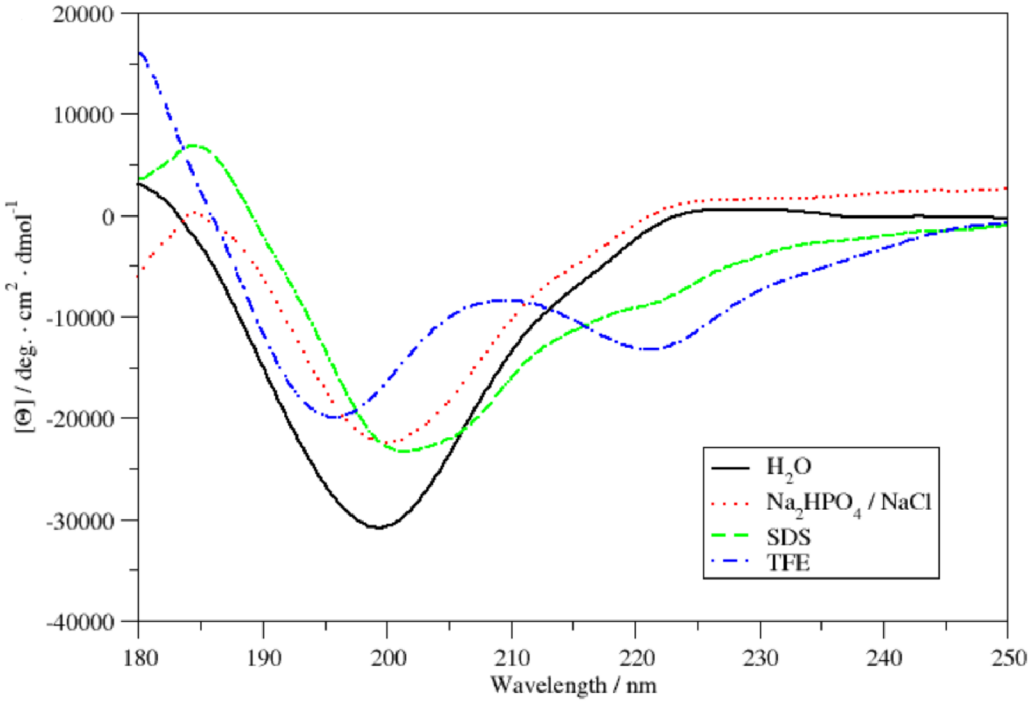

Figure 4S. ECD spectra of G17(1-5) in various solvents.

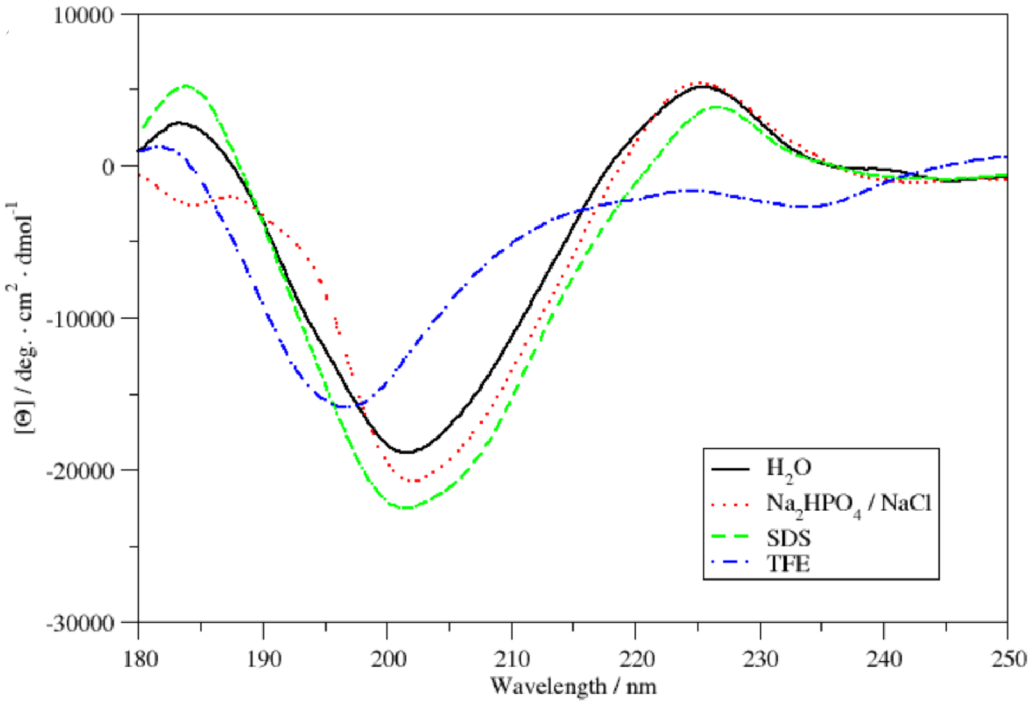

Figure 5S. ECD spectra of G17(1-4)-NH_2 in various solvents.

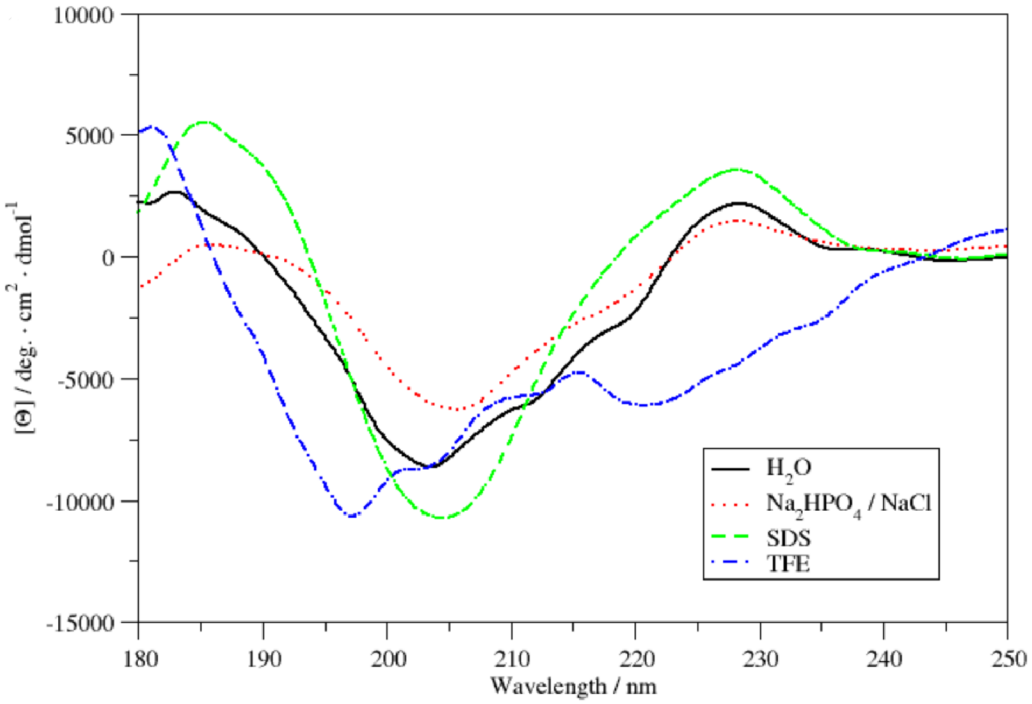

Figure 6S. ECD spectra of G17(1-4) in various solvents.

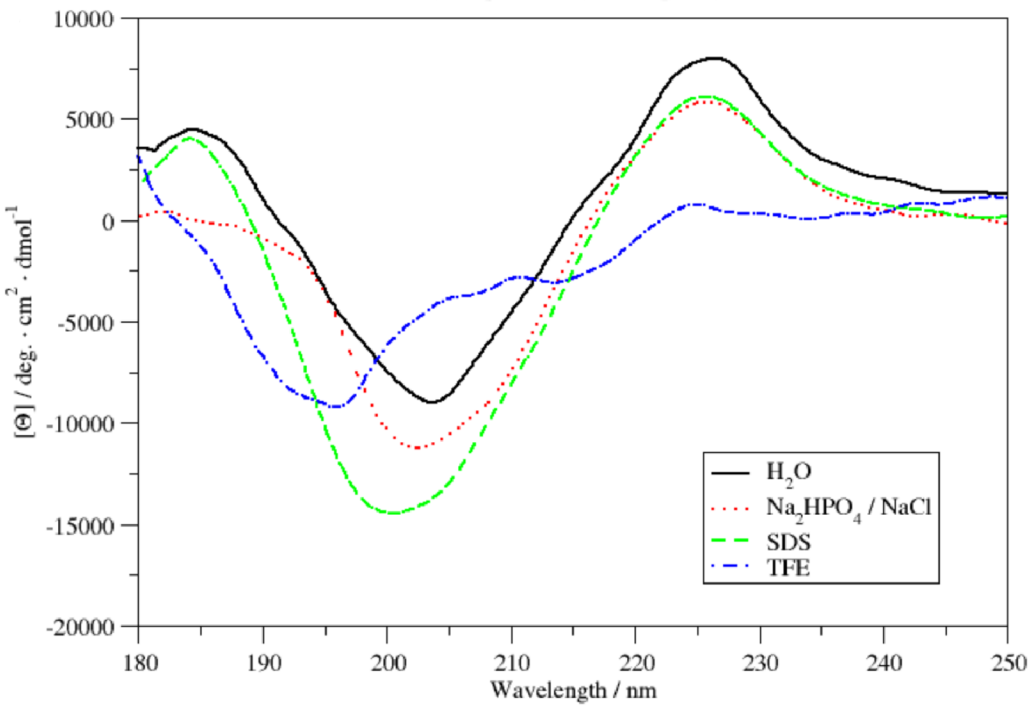

Figure 7S. – DSSP-calculated secondary structure of G17(1-12) as function of time during REMD simulations in different solvents. **A**, H_2O; **B**, DMSO; **C**, TFE.

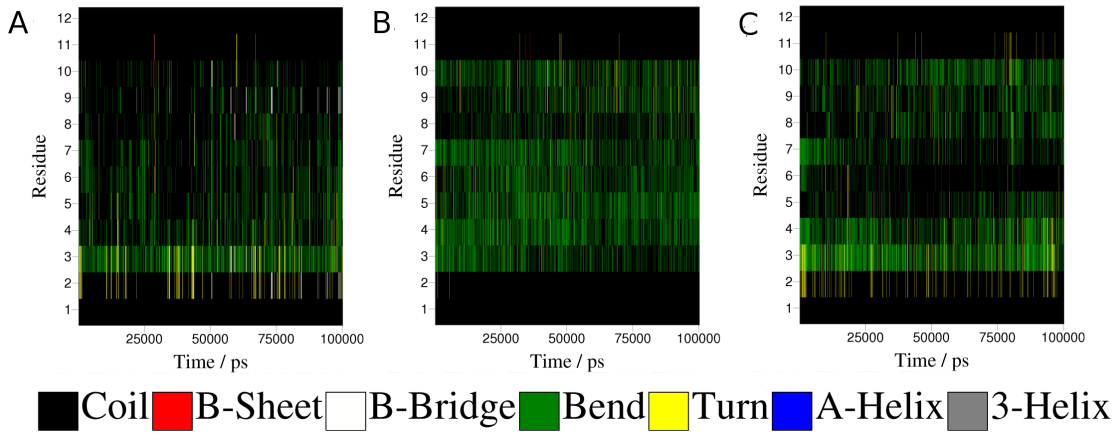

Table 1S. Cluster analysis of G17(1-12) REMD simulations.

Peptide	Solvent	Structures in cluster number					Total number of clusters	Total number of structures	Cluster 1% of total structures
		1	2	3	4	5			
G17(1-12)	H_2O	37	13	10	10	8	1581	2003	1.8
	DMSO	85	54	39	34	34	1268	2003	4.2
	TFE	61	27	21	19	17	997	2003	3.0

Figure 8S. DSSP-calculated secondary structure of G17(1-6)-NH_2 as function of time during REMD simulations in different solvents. **A**, H_2O; **B**, DMSO; **C**, TFE.

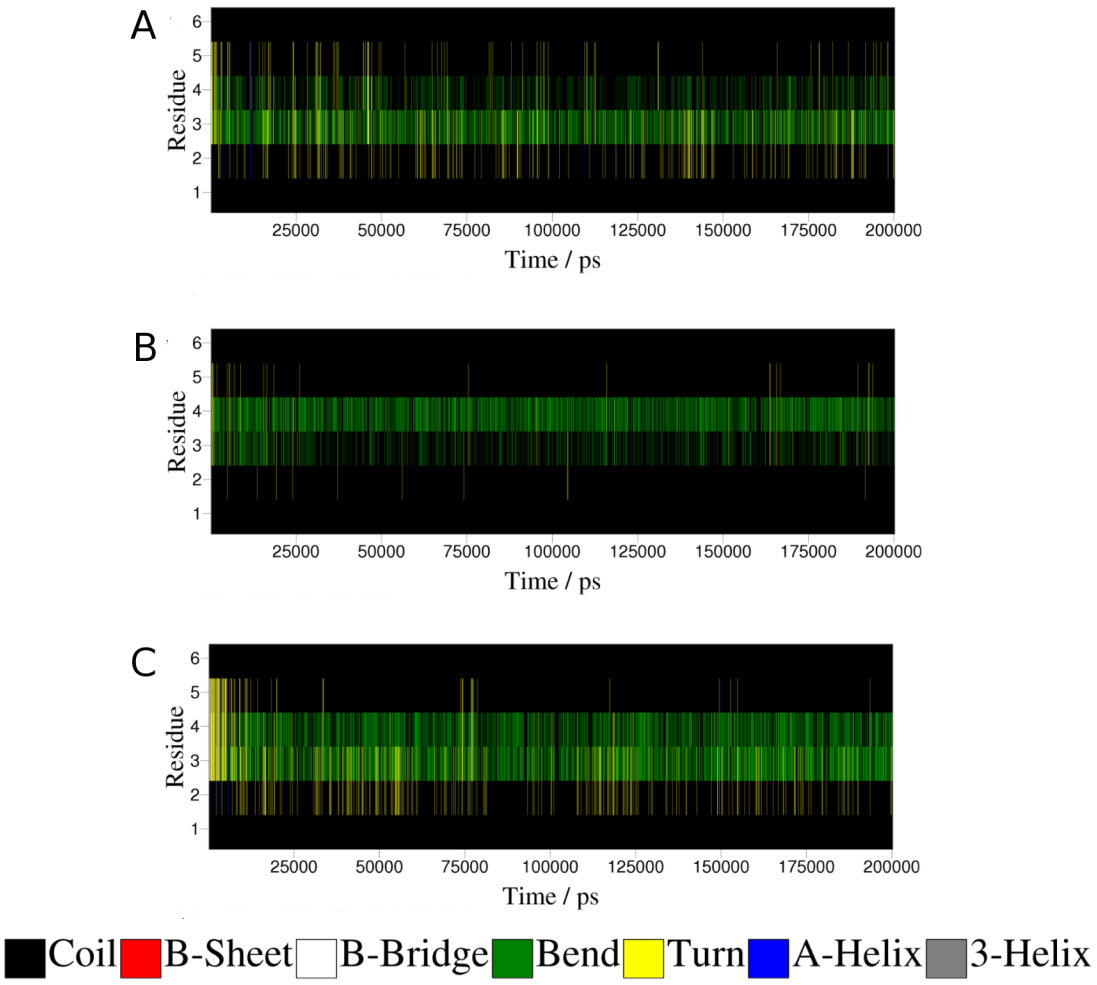

Figure 9S. DSSP-calculated secondary structure of G17(1-6) as function of time during REMD simulations in different solvents. **A**, H_2O; **B**, DMSO; **C**, TFE.

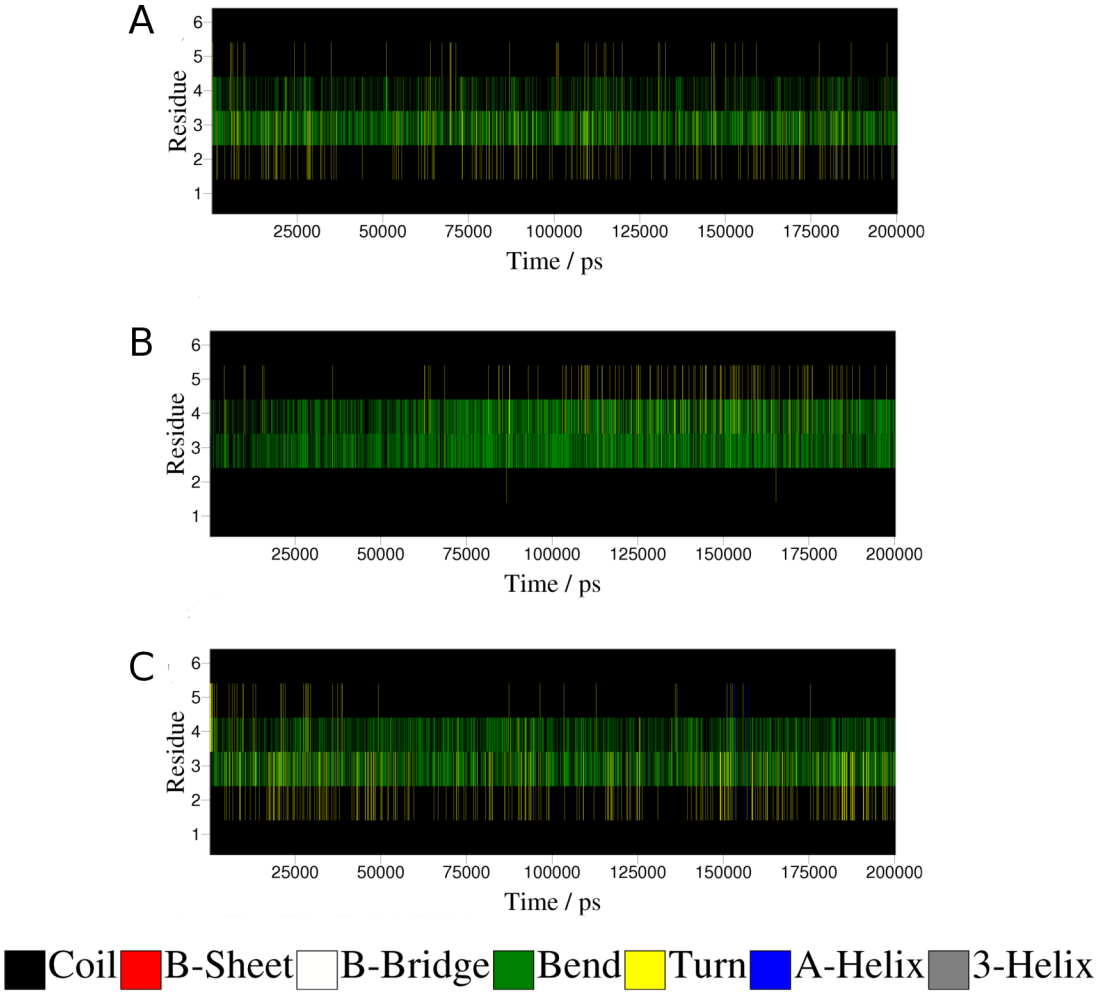

Table 2S. Cluster analysis of G17(1-6)-NH_2 and G17(1-6) REMD simulations.

Peptide	Solvent	Structures in cluster number					Total number of clusters	Total number of structures	Cluster 1% of total structures
		1	2	3	4	5			
G17(1-6)-NH_2	H_2O	882	383	250	240	169	151	4003	22
	DMSO	1100	761	194	193	169	115	4003	27.5
	TFE	865	334	301	237	206	151	4003	21.6
G17(1-6)	H_2O	1051	528	292	222	194	89	4003	26.2
	DMSO	1851	523	407	134	117	67	4003	46.2
	TFE	561	548	385	251	202	98	4003	14

Figure 10S. DSSP-calculated secondary structure of G17(1-5)-NH_2 as function of time during REMD simulations in different solvents. **A**, H_2O; **B**, DMSO; **C**, TFE.

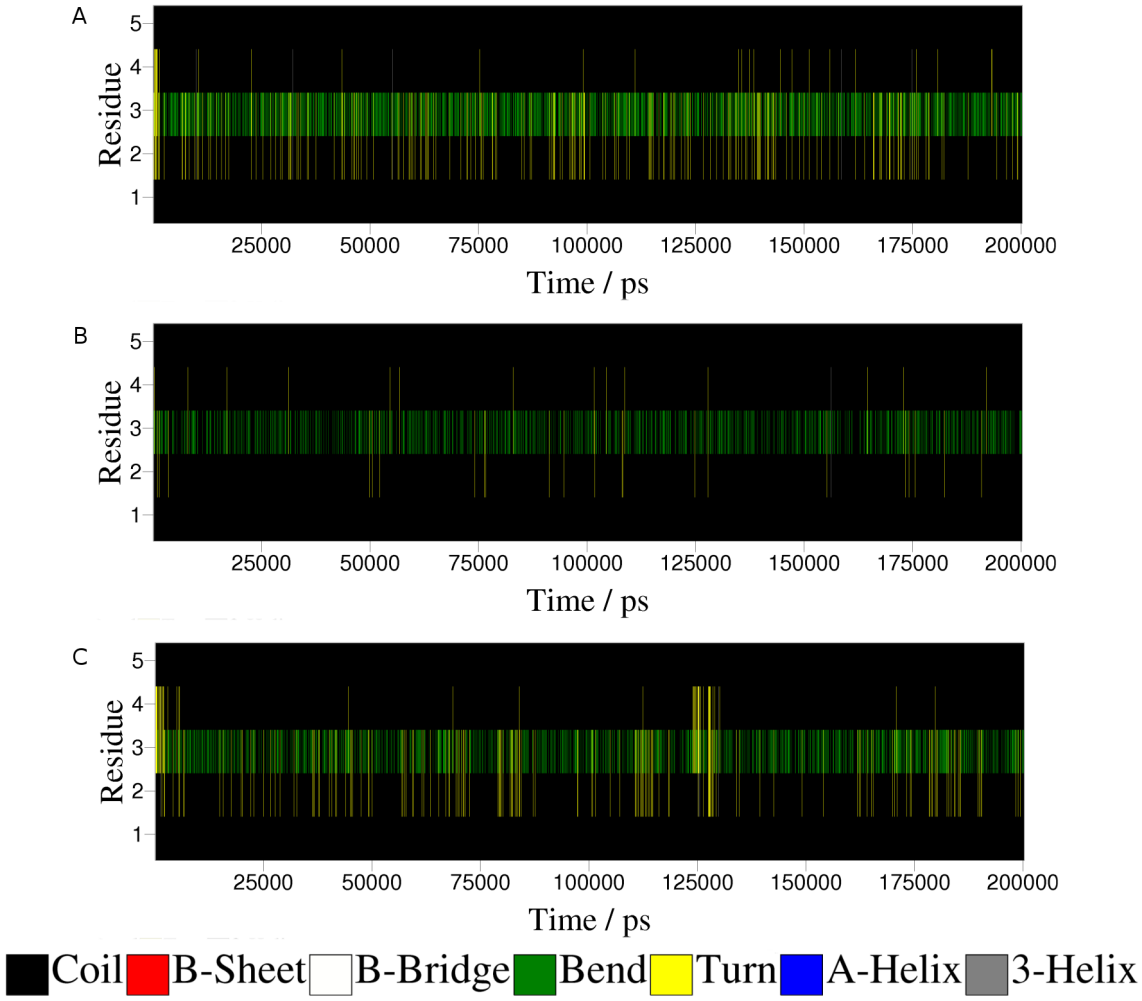

Figure 11S. DSSP-calculated secondary structure of G17(1-5) as function of time during REMD simulations in different solvents. **A**, H_2O; **B**, DMSO; **C**, TFE.

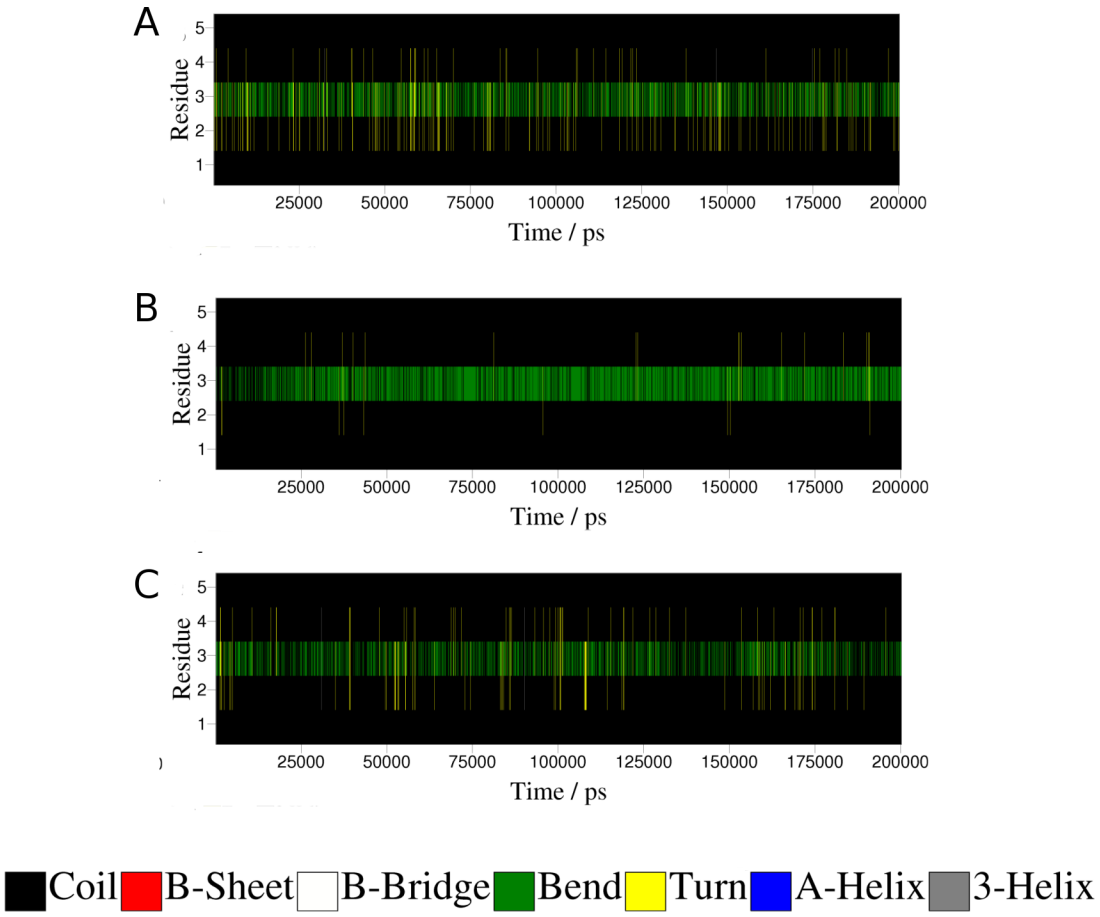

Table 3S. Cluster analysis of G17(1-5)-NH_2 and G17(1-5) REMD simulations.

Peptide	Solvent	Structures in cluster number					Total number of clusters	Total number of structures	Cluster 1% of total structures
		1	2	3	4	5			
G17(1-5)-NH_2	H_2O	1605	790	362	207	191	47	4003	40.1
	DMSO	1100	1031	346	246	233	45	4003	27.5
	TFE	1641	584	539	299	207	41	4003	41
G17(1-5)	H_2O	1754	714	357	315	188	28	4003	43.8
	DMSO	2479	599	464	168	66	24	4003	61.9
	TFE	1343	688	549	241	240	34	4003	33.5

Figure 12S. DSSP-calculated secondary structure of G17(1-4)-NH_2 as function of time during REMD simulations in different solvents. **A**, H_2O; **B**, DMSO; **C**, TFE.

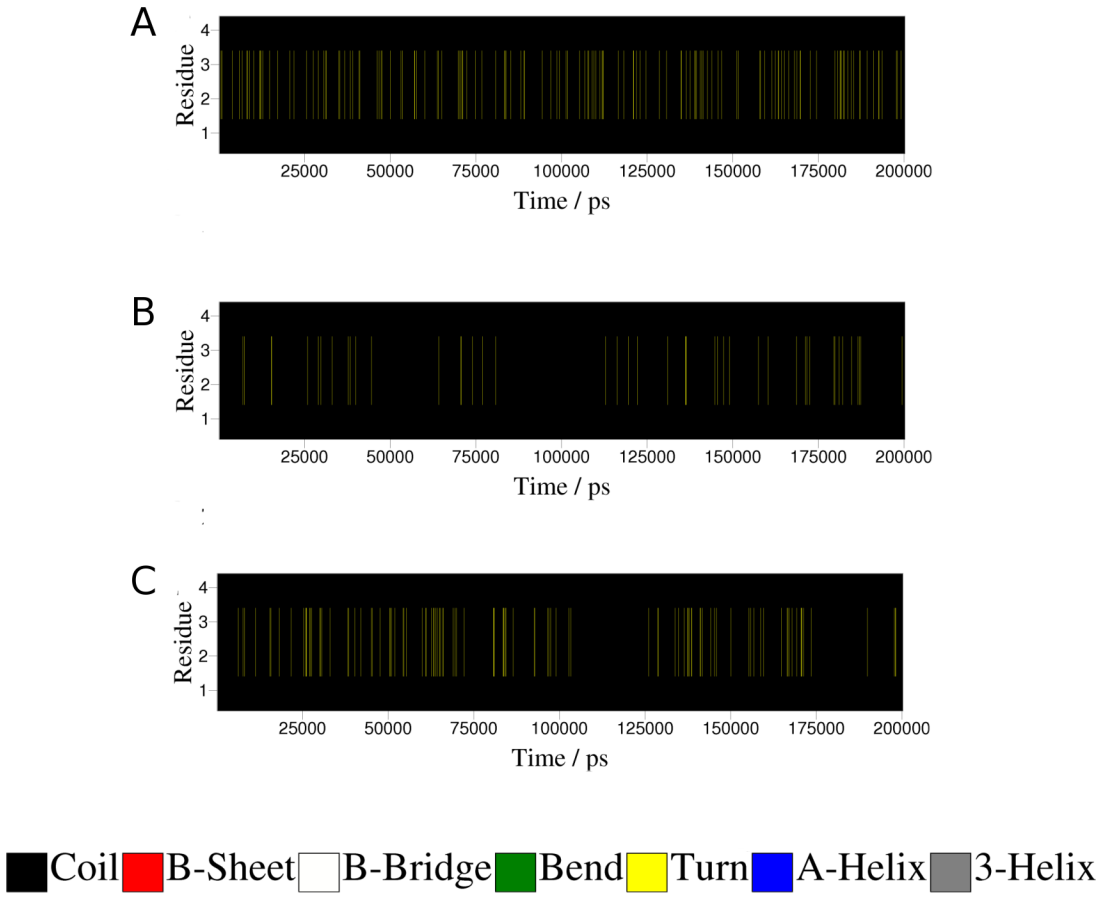

Figure 13S. DSSP-calculated secondary structure of G17(1-4) as function of time during REMD simulations in different solvents. **A**, H_2O; **B**, DMSO; **C**, TFE.

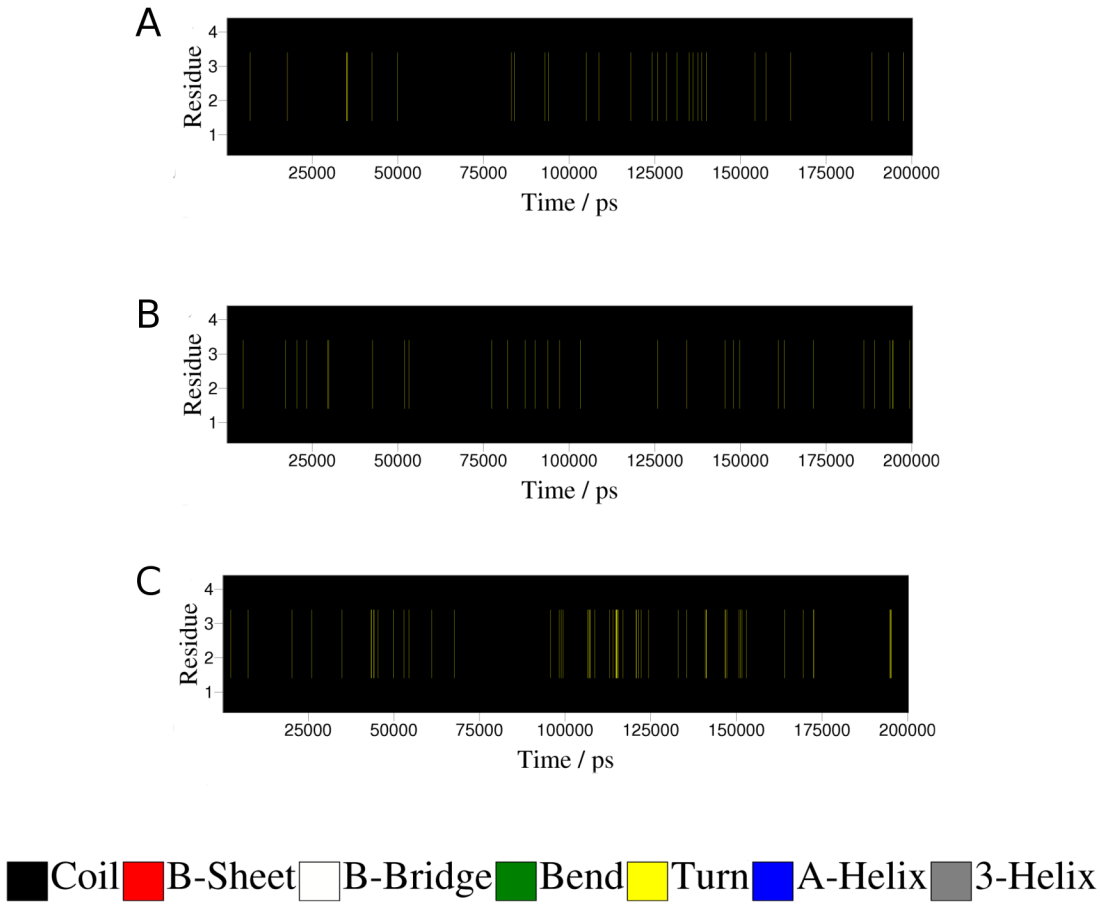

Table 4S. Cluster analysis of G17(1-4)-NH_2 and G17(1-4) REMD simulations.

Peptide	Solvent	Structures in cluster number					Total number of clusters	Total number of structures	Cluster 1% of total structures
		1	2	3	4	5			
G17(1-4)-NH_2	H_2O	2402	989	374	85	51	12	4003	60
	DMSO	2388	713	530	161	137	12	4003	59.7
	TFE	2523	721	447	123	79	13	4003	63
G17(1-4)	H_2O	2828	805	302	37	19	8	4003	70.6
	DMSO	2855	848	144	124	18	7	4003	71.3
	TFE	2781	580	521	76	26	9	4003	69.5