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Structure and Stability of Cyclic Peptide Based Nanotubes: An Molecular Dynamics Study of the Influence of Amino Acid Composition

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Electronic Supplementary Information

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Table S1: The average distance (in Å) and standard deviation of the centre of mass distance between Cα planes of consecutive chains in various CPNTs.

CP unit	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
	mean	SD	mean	SD	mean	SD	mean	SD	mean	SD	mean	SD	mean	SD	mean	SD
CP1-CP2	4.76	0.07	4.76	0.06	4.74	0.06	4.76	0.05	4.76	0.06	4.76	0.06	4.87	0.07	4.84	0.06
CP2- CP3	4.78	0.06	4.88	0.07	4.85	0.07	4.81	0.06	4.81	0.06	4.85	0.06	4.84	0.06	4.84	0.06
CP3- CP4	4.78	0.06	4.77	0.06	4.76	0.06	4.76	0.05	4.77	0.05	4.77	0.05	4.90	0.07	4.85	0.06
CP4- CP5	4.78	0.06	4.84	0.07	4.87	0.08	4.81	0.06	4.82	0.06	4.86	0.06	4.84	0.06	4.82	0.06
CP5- CP6	4.78	0.06	4.75	0.06	4.75	0.06	4.76	0.06	4.77	0.05	4.76	0.05	4.88	0.06	4.90	0.07
CP6- CP7	4.78	0.06	4.87	0.07	4.85	0.07	4.82	0.06	4.82	0.06	4.87	0.06	4.85	0.06	4.83	0.06
CP7- CP8	4.76	0.07	4.76	0.06	4.74	0.07	4.75	0.06	4.75	0.06	4.78	0.06	4.84	0.08	4.86	0.07

Table S2: The average diameter of each CP unit (in Å) and the standard deviation (SD) with respect to the longest Cα-Cα distance.

CP unit	Cα-Cα distance	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
		mean	SD	mean	SD	mean	SD	mean	SD	mean	SD	mean	SD	mean	SD	mean	SD
CP1	1	9.74	0.44	9.65	0.40	9.72	0.38	9.68	0.41	9.72	0.39	9.43	0.40	10.38	0.38	9.40	0.48
	2	9.79	0.68	9.92	0.57	10.22	0.55	9.77	0.52	10.09	0.49	10.18	0.51	10.46	0.37	9.82	0.43
	3	9.73	0.44	9.75	0.40	9.48	0.38	9.71	0.41	9.58	0.39	9.86	0.38	8.90	0.40	10.09	0.40
	4	9.81	0.67	9.63	0.59	9.59	0.65	9.98	0.52	9.74	0.51	9.69	0.56	9.38	0.40	10.09	0.43
CP2	1	9.81	0.40	9.79	0.37	9.79	0.36	9.77	0.37	9.83	0.37	9.85	0.30	9.78	0.29	9.98	0.29
	2	9.79	0.41	10.03	0.32	9.72	0.33	9.83	0.37	9.71	0.39	10.02	0.35	9.90	0.29	10.22	0.27
	3	9.75	0.40	9.72	0.37	9.57	0.36	9.77	0.37	9.76	0.37	9.62	0.30	10.00	0.30	9.80	0.32
	4	9.74	0.41	9.87	0.34	10.26	0.32	9.86	0.37	9.92	0.39	10.06	0.31	9.63	0.30	9.50	0.31
CP3	1	9.77	0.38	9.74	0.36	9.69	0.33	9.74	0.36	9.77	0.35	9.71	0.27	9.87	0.29	9.79	0.34

	2	9.82	0.39	9.99	0.31	9.82	0.36	9.72	0.39	9.77	0.36	10.00	0.30	10.13	0.30	9.86	0.27
	3	9.77	0.38	9.73	0.35	9.59	0.33	9.77	0.35	9.73	0.35	9.77	0.27	9.88	0.30	9.76	0.28
	4	9.76	0.39	9.96	0.31	10.15	0.38	9.97	0.38	9.91	0.35	10.08	0.29	9.58	0.28	9.86	0.28
CP4	1	9.78	0.38	9.74	0.33	9.68	0.35	9.76	0.36	9.73	0.35	9.65	0.30	9.91	0.28	9.99	0.26
	2	9.80	0.38	9.73	0.34	10.35	0.36	9.84	0.36	9.81	0.38	10.03	0.33	10.00	0.31	10.14	0.26
	3	9.79	0.38	9.82	0.33	9.63	0.34	9.78	0.36	9.77	0.36	9.84	0.29	9.93	0.26	9.81	0.28
	4	9.76	0.38	9.82	0.36	9.56	0.47	9.83	0.36	9.95	0.36	10.01	0.37	9.67	0.30	9.62	0.29
CP5	1	9.76	0.39	9.70	0.34	9.50	0.34	9.83	0.37	9.75	0.35	9.74	0.34	9.42	0.27	10.04	0.29
	2	9.76	0.38	9.91	0.33	10.11	0.49	9.67	0.39	9.84	0.36	9.84	0.41	10.21	0.30	9.52	0.30
	3	9.79	0.39	9.84	0.33	9.73	0.35	9.75	0.37	9.72	0.35	9.55	0.34	10.32	0.27	9.71	0.31
	4	9.80	0.38	9.77	0.33	9.92	0.50	9.93	0.37	9.93	0.35	10.24	0.36	9.37	0.35	9.92	0.31
CP6	1	9.78	0.40	9.80	0.35	9.59	0.33	9.70	0.36	9.76	0.35	9.63	0.33	9.70	0.27	9.69	0.25
	2	9.79	0.39	9.92	0.32	10.09	0.37	9.98	0.36	9.76	0.39	9.67	0.36	9.78	0.27	9.91	0.26
	3	9.78	0.39	9.71	0.34	9.58	0.33	9.75	0.36	9.77	0.35	9.81	0.32	9.98	0.26	9.84	0.25
	4	9.77	0.39	9.96	0.31	10.09	0.37	9.83	0.38	9.90	0.38	10.28	0.32	10.16	0.25	10.06	0.28
CP7	1	9.81	0.40	9.78	0.36	9.67	0.36	9.75	0.38	9.76	0.36	9.80	0.41	9.93	0.29	9.70	0.40
	2	9.78	0.41	9.79	0.36	10.12	0.34	9.78	0.38	9.88	0.34	9.77	0.33	9.29	0.34	9.61	0.32
	3	9.74	0.40	9.77	0.36	9.56	0.36	9.79	0.38	9.70	0.36	9.56	0.35	9.82	0.30	10.05	0.31
	4	9.77	0.41	10.01	0.33	10.10	0.34	9.91	0.39	9.92	0.35	10.17	0.40	10.24	0.38	9.95	0.32
CP8	1	9.75	0.46	9.74	0.40	9.61	0.41	9.69	0.40	9.70	0.40	9.62	0.44	10.27	0.36	9.65	0.36
	2	9.80	0.65	9.78	0.53	10.16	0.62	9.84	0.53	9.89	0.54	10.17	0.44	10.46	0.43	9.72	0.50
	3	9.75	0.46	9.65	0.40	9.50	0.40	9.63	0.40	9.62	0.41	9.82	0.42	9.15	0.40	9.76	0.36
	4	9.78	0.65	9.85	0.55	9.75	0.66	9.96	0.52	9.92	0.53	9.59	0.45	9.30	0.52	10.15	0.46
1-8[a]		9.78	0.43	9.81	0.37	9.81	0.40	9.80	0.39	9.80	0.38	9.85	0.36	9.84	0.32	9.84	0.33

[a]average over all the chains

Table S3: Various energy contributions (in kcal/mol) to the free energy of binding of each CP unit of different model systems.

ΔE_{vdW}																
CP unit	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD
CP1	-19.69	2.22	-33.02	3.10	-26.18	2.38	-26.78	2.90	-28.34	2.57	-37.23	3.37	-50.21	3.24	-48.45	3.04
CP2	-37.60	3.26	-66.58	4.14	-54.64	3.36	-52.66	3.91	-53.90	3.63	-75.53	3.97	-96.30	3.92	-93.85	3.69
CP3	-37.90	3.41	-68.41	4.36	-57.12	3.24	-55.13	3.80	-53.94	4.15	-79.11	4.09	-102.75	4.17	-99.96	4.11
CP4	-38.37	2.97	-61.00	3.76	-57.42	3.21	-54.23	3.63	-55.85	3.67	-79.09	4.14	-102.45	3.84	-98.17	4.11
CP5	-38.29	3.27	-59.76	3.75	-56.32	3.28	-54.32	3.56	-56.08	3.62	-77.88	4.05	-106.78	4.02	-93.90	4.25
CP6	-37.95	3.12	-65.51	4.28	-57.44	3.39	-56.17	3.82	-54.78	3.66	-75.49	3.97	-107.85	3.58	-94.81	4.81
CP7	-37.70	3.44	-63.40	4.03	-54.75	3.77	-52.09	3.61	-51.10	3.48	-74.69	4.18	-95.26	3.78	-94.65	4.25
CP8	-19.65	2.29	-31.34	2.98	-24.79	2.48	-24.90	2.41	-24.77	2.36	-38.83	3.16	-45.41	2.89	-48.65	3.35

ΔE_{ele}																
CP unit	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD
CP1	-41.35	4.53	-43.03	4.25	-44.12	3.67	-49.21	7.48	-47.34	5.57	-57.70	7.68	-40.05	4.32	-43.67	6.14
CP2	-84.85	5.84	-79.41	5.99	-82.91	5.42	-98.33	9.22	-93.35	7.82	-107.71	10.99	-84.66	5.23	-89.59	7.68
CP3	-86.56	5.44	-78.94	6.26	-82.68	6.05	-100.06	10.04	-93.19	7.74	-116.13	11.11	-87.78	5.15	-92.84	7.17
CP4	-85.91	5.88	-85.71	5.77	-80.49	6.46	-98.43	9.27	-97.19	7.90	-115.76	11.03	-89.61	6.16	-97.17	7.28
CP5	-85.84	5.44	-85.82	5.85	-81.01	6.44	-99.13	9.26	-98.78	9.18	-111.12	11.62	-88.20	5.36	-94.19	8.24
CP6	-85.99	5.21	-81.02	5.68	-81.49	6.24	-100.78	12.11	-99.13	8.39	-115.34	10.45	-86.06	5.45	-90.56	8.22
CP7	-83.45	6.72	-81.72	5.65	-81.56	6.27	-96.03	11.37	-97.30	7.39	-108.21	11.01	-87.61	5.91	-89.34	7.42
CP8	-39.98	5.31	-43.45	3.84	-44.93	4.05	-46.68	6.80	-46.35	5.18	-54.48	7.48	-43.28	4.58	-43.04	5.32

ΔE_{MM}

CP unit	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD
CP1	-61.04	3.36	-76.05	3.66	-70.30	3.15	-75.99	6.80	-75.68	5.29	-94.93	7.02	-90.26	4.22	-92.11	5.51
CP2	-122.44	4.27	-145.99	4.73	-137.56	4.71	-150.99	8.41	-147.25	7.01	-183.24	10.07	-180.96	5.13	-183.43	7.08
CP3	-124.45	3.96	-147.36	4.72	-139.80	4.70	-155.19	8.78	-147.14	6.71	-195.24	11.01	-190.53	5.13	-192.80	6.77
CP4	-124.29	4.53	-146.71	4.66	-137.91	5.38	-152.66	8.53	-153.04	7.14	-194.85	10.01	-192.06	5.64	-195.34	6.44
CP5	-124.13	4.06	-145.58	4.91	-137.33	5.13	-153.45	8.51	-154.85	8.39	-188.99	10.79	-194.98	5.46	-188.09	8.34
CP6	-123.94	3.98	-146.53	4.68	-138.93	4.73	-156.94	11.18	-153.91	7.64	-190.82	9.44	-193.91	5.03	-185.37	8.69
CP7	-121.15	5.08	-145.12	4.65	-136.31	4.99	-148.13	10.28	-148.41	6.47	-182.90	9.37	-182.86	5.49	-184.00	6.60
CP8	-59.63	4.29	-74.79	3.27	-69.71	3.43	-71.58	6.25	-71.12	4.97	-93.31	6.72	-88.70	4.32	-91.69	4.97

ΔG_{pol}

CP unit	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD
CP1	35.79	2.16	39.98	2.10	38.59	1.77	43.85	4.81	43.83	3.72	52.61	4.37	43.90	1.94	47.28	3.21
CP2	72.65	2.44	75.73	2.66	72.81	2.51	89.77	6.09	87.40	4.59	98.70	6.50	88.95	2.56	94.09	4.16
CP3	73.49	2.21	75.99	2.85	73.67	2.42	91.25	6.32	86.68	4.65	106.38	6.93	93.16	2.53	96.47	3.66
CP4	73.28	2.37	79.12	2.66	73.38	2.66	89.18	6.54	91.32	5.23	106.64	6.24	95.69	2.88	99.31	4.03
CP5	73.39	2.15	78.38	2.65	74.02	2.67	91.09	6.33	92.27	5.57	102.25	7.22	95.61	2.61	96.79	5.08
CP6	73.21	2.09	76.16	2.62	72.25	2.87	93.86	7.90	90.88	5.70	104.36	6.04	93.69	2.80	93.02	5.41
CP7	71.97	2.89	76.54	2.62	71.26	2.75	88.35	7.09	88.68	4.57	99.00	6.51	89.55	2.77	92.98	4.17
CP8	35.08	2.64	39.94	2.08	39.46	1.65	41.43	4.64	41.34	3.72	50.74	4.86	43.59	2.02	46.29	3.15

ΔG_{np}																
CP unit	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD
CP1	-1.92	0.05	-3.23	0.21	-2.50	0.11	-2.67	0.15	-2.66	0.13	-3.53	0.20	-4.50	0.28	-4.48	0.17
CP2	-4.84	0.06	-7.46	0.18	-6.34	0.11	-6.37	0.18	-6.24	0.17	-8.28	0.17	-9.37	0.19	-9.27	0.21
CP3	-4.84	0.06	-7.37	0.17	-6.49	0.10	-6.47	0.17	-6.15	0.17	-8.68	0.19	-9.92	0.25	-9.63	0.18
CP4	-4.84	0.06	-6.70	0.20	-6.50	0.10	-6.32	0.19	-6.36	0.19	-8.67	0.17	-9.70	0.15	-9.41	0.17
CP5	-4.83	0.06	-6.55	0.22	-6.40	0.11	-6.34	0.17	-6.37	0.15	-8.50	0.16	-9.94	0.20	-9.00	0.24
CP6	-4.84	0.07	-7.12	0.19	-6.58	0.11	-6.63	0.17	-6.26	0.15	-8.28	0.17	-9.97	0.14	-9.11	0.29
CP7	-4.85	0.07	-7.21	0.20	-6.45	0.12	-6.27	0.16	-6.00	0.16	-8.11	0.17	-9.14	0.16	-9.32	0.18
CP8	-1.93	0.06	-3.07	0.18	-2.40	0.12	-2.41	0.16	-2.34	0.15	-3.58	0.13	-3.76	0.17	-4.22	0.21

ΔG_{solv}																
CP unit	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD
CP1	33.86	2.18	36.75	2.12	36.09	1.79	41.17	4.76	41.17	3.69	49.09	4.34	39.40	1.87	42.81	3.17
CP2	67.81	2.45	68.26	2.66	66.47	2.53	83.40	6.04	81.17	4.55	90.41	6.47	79.58	2.50	84.82	4.09
CP3	68.66	2.21	68.61	2.87	67.18	2.44	84.78	6.27	80.52	4.60	97.70	6.86	83.23	2.46	86.84	3.63
CP4	68.44	2.37	72.42	2.65	66.88	2.67	82.87	6.45	84.96	5.15	97.97	6.19	85.99	2.84	89.90	4.04
CP5	68.55	2.16	71.83	2.62	67.63	2.67	84.75	6.32	85.90	5.50	93.75	7.16	85.68	2.58	87.79	4.98
CP6	68.37	2.09	69.04	2.61	65.67	2.87	87.23	7.86	84.62	5.65	96.08	5.98	83.72	2.78	83.91	5.24
CP7	67.12	2.90	69.32	2.65	64.81	2.75	82.09	7.05	82.68	4.54	90.89	6.48	80.41	2.72	83.66	4.10
CP8	33.16	2.65	36.88	2.10	37.06	1.66	39.02	4.59	39.00	3.67	47.16	4.83	39.83	2.01	42.08	3.08

	TΔS															
CP unit	AA		AF		AL		AQ		QAEA		QL		WL		WL3QL	
	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD	AVG	SD
CP1	-16.42	1.34	-20.38	4.08	-18.41	1.29	-18.33	1.15	-18.56	1.37	-23.62	1.55	-26.46	1.51	-25.92	1.96
CP2	-17.18	3.10	-21.35	4.90	-17.75	2.88	-18.31	2.94	-20.18	1.20	-26.06	2.41	-26.35	2.02	-29.40	2.31
CP3	-19.06	3.07	-21.88	3.36	-20.03	1.53	-18.04	1.91	-19.57	2.82	-26.31	0.95	-25.49	1.54	-24.93	1.26
CP4	-18.75	1.53	-21.59	3.65	-21.54	4.00	-17.84	1.42	-20.36	3.95	-25.75	1.62	-28.09	2.60	-27.86	2.09
CP5	-17.75	3.15	-21.50	5.49	-20.79	4.60	-19.02	3.27	-19.02	3.47	-25.62	4.79	-22.86	3.49	-27.21	2.50
CP6	-19.14	3.42	-20.05	5.00	-20.80	3.67	-19.98	2.95	-19.63	2.59	-24.11	2.93	-26.43	2.40	-26.29	2.11
CP7	-19.18	5.06	-19.98	3.53	-20.41	1.87	-20.32	1.65	-20.50	1.74	-24.48	4.01	-25.41	2.21	-26.36	0.90
CP8	-16.38	1.06	-19.57	2.48	-18.21	1.94	-18.78	2.02	-18.08	0.66	-23.22	1.82	-23.53	0.95	-24.99	2.71

ΔE_{vdW} and ΔE_{ele} represent the van der Waals and electrostatic interactions, respectively. ΔE_{MM} results from the addition of ΔE_{vdW} and ΔE_{ele} energy components. ΔG_{pol} and ΔG_{np} denote the polar and non-polar contributions to salvation. ΔG_{solv} is obtained from the addition of ΔG_{pol} and ΔG_{np}. $T\Delta S$ denotes the addition of $T\Delta S_{translational}$, $T\Delta S_{rotational}$, and $T\Delta S_{vibrational}$.