Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information 2

Coarse-grained molecular dynamics studies of the structure and stability of peptide-drug amphiphile filaments for drug delivery

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Parameters

Table S2-1. Atom parameters.

Index	Residue	Atom name	Atom type	CG type reference*	Mass	Charge
1	MC	Z4B	Z4B	SER*	28	0
2	MC	Z3A	Z3A	LYS2*	28	0
3	MC	Z2A	Z2A	CT2**	25	0
4	MC	Z2B	Z2B	LYS2*	26	0
5	MC	Z4A	Z4A	CT2**	25	0
6	MC	Z1C	Z1C	CT2**	35	0
7	MC	Z1A	Z1A	CT2**	26	0
8	MC	Z1B	Z1B	CT2**	36	0
9	MC	Z5B	Z5B	EO**	42	0
10	MC	Z5D	Z5D	SER*	28	0
11	MC	Z5A	Z5A	EO**	40	0
12	MC	Z5C	Z5C	CT2**	29	0
13	MC	LA	LA	OA**	56	0
14	MC	LB	LB	CYS*	46	0
15	MC	LE	LE	SER*	43	0
16	MC	LD	LD	GBB*	56	0
17	MC	LC	LC	CYS*	46	0
18	MC	G1	G1	GBB*	56	0
19	MC	G2	G2	GBB*	55	0
20	MC	V2	V2	VAL*	43	0
21	MC	G3	G3	GBB*	55	0
22	MC	Q3	Q3	GLN*	72	0
23	MC	G4	G4	GBB*	55	0
24	MC	I4	I4	ILE*	54	0
25	MC	G5	G5	GBB*	55	0
26	MC	V5	V5	VAL*	43	0
27	MC	G6	G6	GBB*	55	0
28	MC	Y6A	Y6A	TYR1*	52	0
29	MC	Y6B	Y6B	TYR2*	54	0
30	MC	G7	G7	GBB*	55	0
31	MC	L7A	L7A	LYS1*	42	0
32	MC	L7B	L7B	LYS2*	31	0.1118
33	MC	G8	G8	GBB*	55	0

34	MC	L8A	L8A	LYS1*	42	0
35	MC	L8B	L8B	LYS2*	31	0.1118

* R. DeVane, W. Shinoda, P. B. Moore and M. L. Klein, *J. Chem. Theory Comput.*, 2009, **5**, 2115-2124.
** W. Shinoda, R. DeVane and M. L. Klein, *Mol. Simulat*., 2007, 33, 27-36.

Table S2-2. Bond parameters.

Atom1	**Atom2**	**k_b**	**b_0 (rad)**
7	8	443.3	1.39
7	6	198.7	2.4
8	6	159.4	2.78
6	4	154.89	2.37
8	3	151.1	2.42
3	4	160.4	2.84
3	2	130.45	2.62
4	5	158.4	2.5
2	5	192.2	2.34
2	1	143.96	2.52
5	1	231.6	2.42
5	11	112.8	3.8
1	9	385.5	1.48
11	9	172.6	2.5
9	10	95.7	2.86
11	10	331.4	1.55
11	12	304.3	1.57
11	13	109.2	2.5
13	14	65.4	3.9
14	17	37.2	3
17	16	59	2.8
18	19	54.3	3.7
19	20	92	2.5
19	21	31.9	3.6
21	22	86.3	2.5
21	23	35.3	3.6
23	24	90.4	2.5
23	25	20.4	3.6
25	26	91.3	2.5
25	27	24	3.6
27	28	6.7	4.7
28	29	296.8	3
27	30	20.4	3.6

30	31	87.9	2.5
31	32	54.5	3.9
30	33	31.6	3.7
33	34	85.2	2.5
34	35	55.7	3.9
16	15	125.7	2.5
16	18	117.4	2.5

Table S2-3. Angle parameters.

Atom1	**Atom2**	**Atom3**	**k_0**	**θ_0 (rad)**
8	7	6	273.4	1.57
7	6	8	1642.2	0.52
6	8	7	400.6	1.05
6	8	3	407.5	1.57
8	6	4	443.3	1.59
6	4	3	410.1	1.56
8	3	4	470.2	1.55
4	3	2	453.2	1.48
3	4	5	450.25	1.46
4	5	2	370.5	1.73
3	2	5	362.1	1.6
5	2	1	603.4	1.04
2	5	1	464.96	1.12
5	1	2	638.2	0.99
5	1	9	311.8	1.47
1	5	11	522.2	1.21
1	9	10	50.3	2.93
5	11	10	108.5	2.25
5	11	9	771.8	0.79
5	11	12	31.9	1.8
9	10	11	335.25	1.07
9	11	12	7.37	2.1
10	11	12	84.6	1.92
11	13	14	22.5	2.8
13	14	17	9.8	2.5
14	17	16	9.9	2.1
18	19	21	7.7	2.6
20	19	21	32.3	1.1
19	21	22	7.9	2.4
19	21	23	2.1	2.6
22	21	23	40.4	1.1
21	23	24	5.9	2.4
21	23	25	9.5	2.6

24	23	25	24.2	1.1
23	25	26	4.1	2.5
23	25	27	5.1	2.6
26	25	27	34.4	1.1
25	27	28	2.8	2.5
25	27	30	3.9	2.7
27	28	29	4.3	2.7
28	27	30	15.2	0.9
27	30	33	8.4	2.6
27	30	31	3.6	2.5
30	31	32	17.6	2.9
31	30	33	33.2	1.1
30	33	34	6.3	2.5
33	34	25	16.9	2.9
17	16	18	9.5	1.5
17	16	15	27.6	2.9
15	16	18	53.3	1.4
10	9	11	201.1	1.5
10	11	13	66.8	2.3
12	11	13	54	1.7
16	18	19	0.6	3.3
18	19	20	3.2	2.8
1	9	11	174.7	2.7
5	11	13	43.7	1.5
9	11	13	223.8	1.5
9	11	13	12	2.9
10	9	11	1112.1	0.6
10	11	13	60	2.3
12	11	13	64.5	2.3

Table S2-4. Dihedral angle parameters.

Atom1	Atom2	Atom3	Atom4	k_Φ	n	δ (degree)	Weighting factor
10	11	13	14	0.2	2	0	0
12	11	13	14	0.2	2	59	0
11	13	14	17	0.1	2	81	0
13	14	17	16	0.1	1	13	0
14	17	16	15	0.1	2	313	0
14	17	16	18	0.3	1	0	0
17	16	18	19	0.4	2	343	0
15	16	18	19	0.4	1	143	0
15	18	19	20	0.3	1	149	0
18	19	21	23	0.4	1	47	0
18	19	21	22	1.1	1	165	0
19	21	23	25	0.4	1	28	0
19	21	23	24	1	1	146	0
21	23	25	26	1	1	137	0
21	23	25	27	0.5	2	248	0
23	25	27	30	0.3	1	24	0
23	25	27	28	0.7	1	134	0
25	27	30	31	0.8	1	140	0
25	27	28	29	0.3	1	132	0
27	30	31	32	0.4	1	186	0
25	27	30	33	0.9	1	32	0
27	30	33	34	0.8	1	143	0
30	33	34	35	0.3	1	104	0
5	11	13	14	0.3	2	155	0
9	11	13	14	0.3	2	235	0
12	11	13	14	0.2	2	0	0
10	11	13	14	0.3	1	62	0

Table S2-5 LJ 9-6 Parameters

Aatom	**ε (kcal/mol)**	**σ (Å)**
B1	0.85	3
B2	0.82	4
B3	0.82	4
B4	0.82	4
B5	0.82	4
B6	0.82	4
B7	0.82	4
B8	0.82	4
B9	0.82	4
R1a	0.36	4.44
R1b	0.469	4.58
R1b	0.469	4.58
R1c	0.405	4.25
R2a	0.405	4.25
R2b	0.36	4.44
R3	0.405	4.25
R4a	0.82	4
R4b	0.4491	3.7
CC1	0.85	3
CC2	0.405	4.25
CC3	0.69	3.7
CC4	0.58	4.1
CC5	0.69	3.7
CC6	0.58	4.1

Table S2-6 LJ 12-4 Parameters

Atom1	**Atom2**	**ε (kcal/mol)**	**σ (Å)**
W	W	0.895	4.371
CC1	W	1.2	3.685
CC3	W	0.776	4.0355
CC2	W	0.92	4.31
CC4	W	0.51	4.23
CC5	W	0.776	4.0355
CC6	W	0.51	4.23
R1a	W	0.37	4.4
R1b	W	0.364	4.476
R1c	W	0.92	4.31
R2a	W	0.92	4.31
R2b	W	0.37	4.4
R3	W	0.92	4.31
R4a	W	0.39	4.1855
R4b	W	0.7	3.95
B1	W	0.39	4.1855
B2	W	0.39	4.1855
B3	W	0.39	4.1855
B4	W	0.39	4.1855
B5	W	0.39	4.1855
B6	W	0.39	4.1855
B7	W	0.39	4.1855
B8	W	0.39	4.1855
B9	W	0.39	4.1855