Supporting information

Nanostructured lipopeptide-based membranomimetics for stabilizing bacteriorhodopsin

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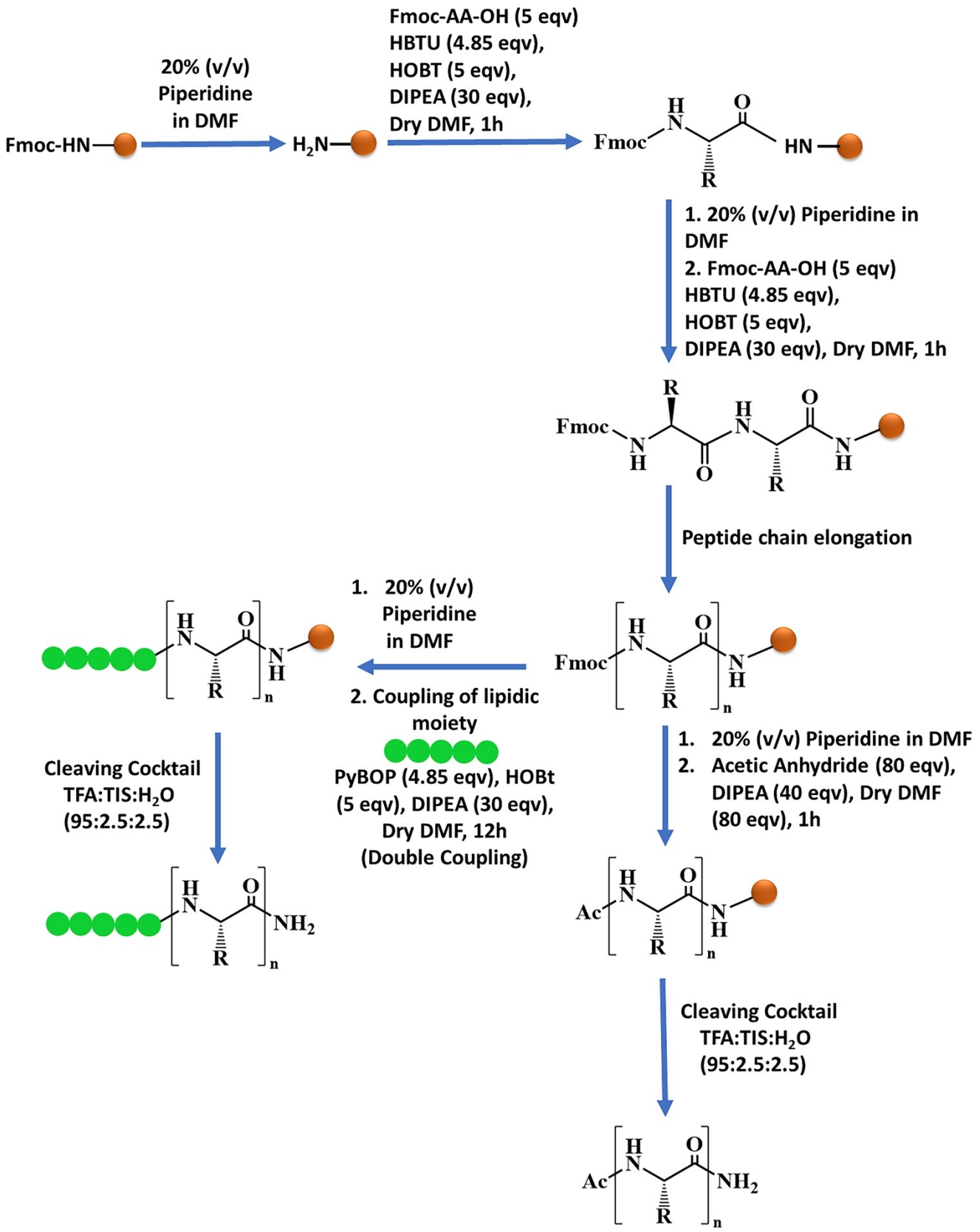


Figure S1. Synthesis of linear detergent peptides (by solid phase peptide synthesis protocol – general scheme).

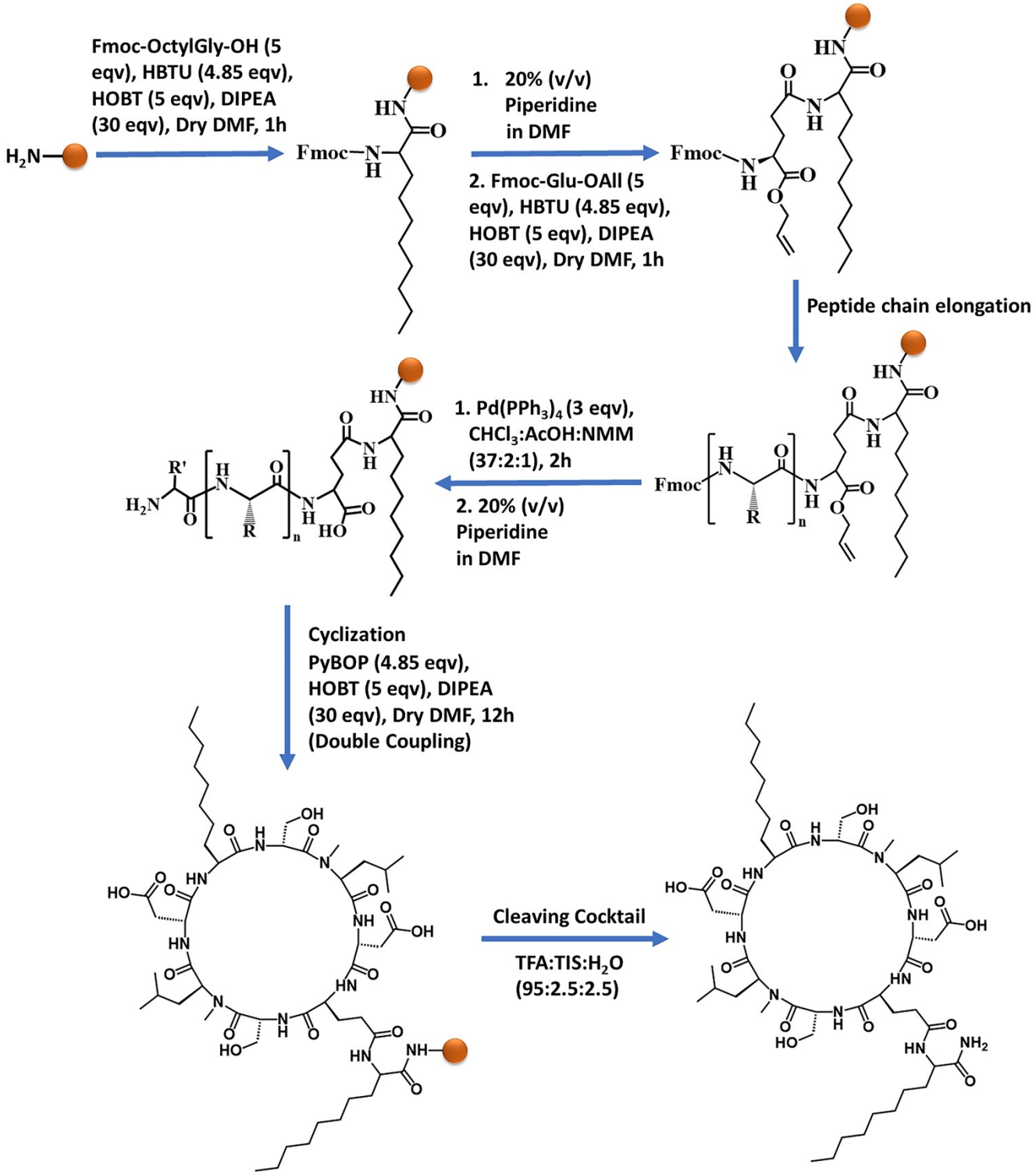


Figure S2. Synthesis of cyclic detergent peptides (by solid phase peptide synthesis protocol – general scheme).

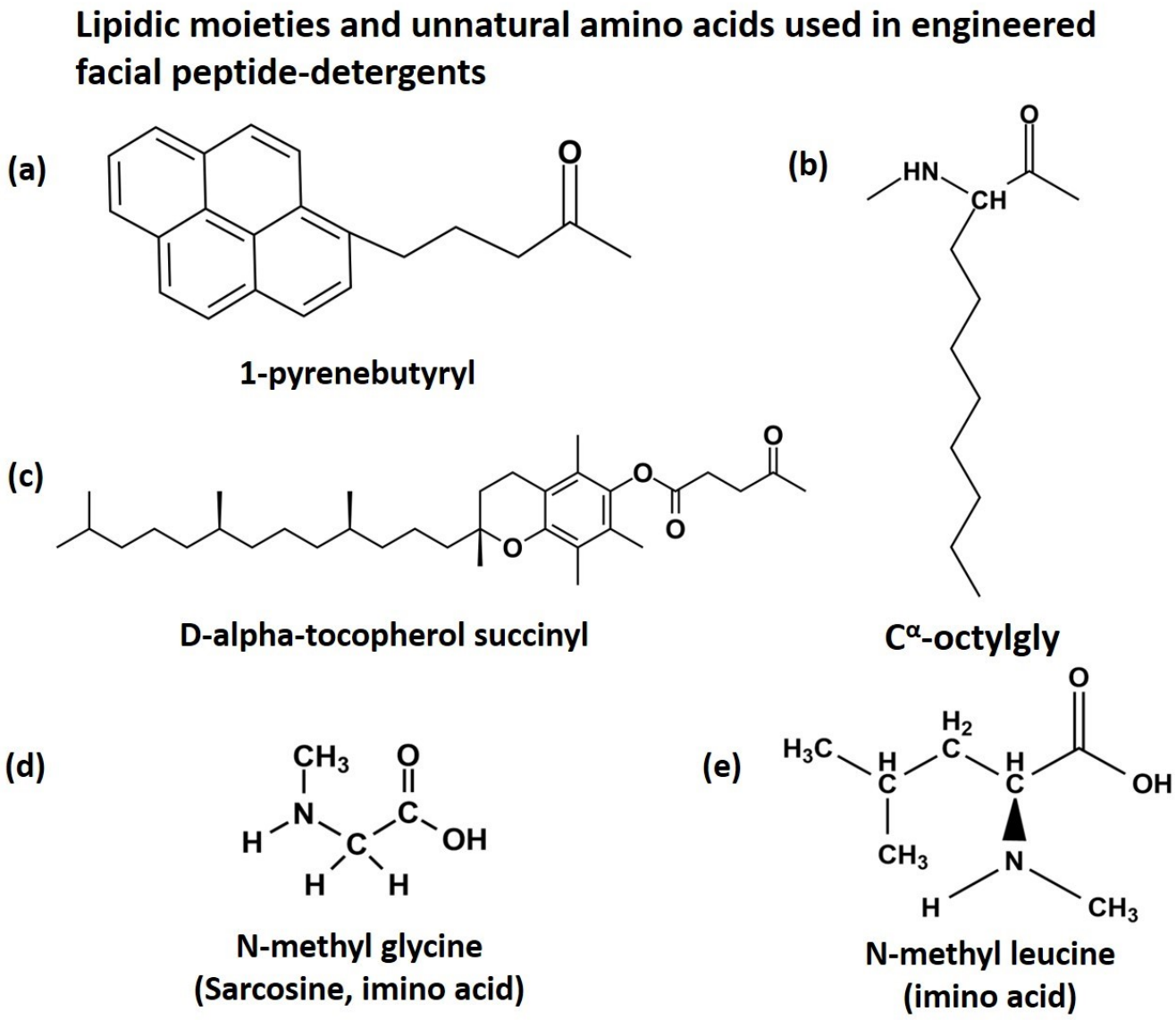


Figure S3. Different lipidic chains (a-c) and unnatural amino acids (d-e) used in our engineered facial peptide-detergents.

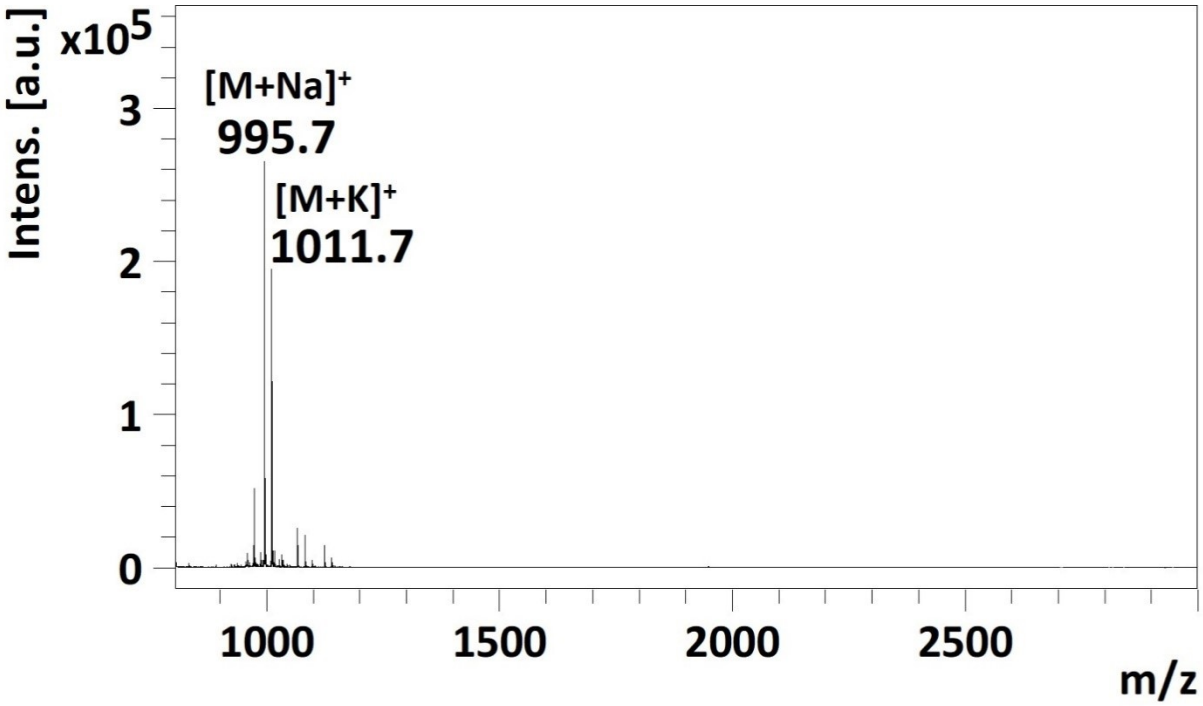


Figure S4. MALDI-TOF mass spectrum of peptide 1. Calculated mass: 972.1 Da; Observed mass: 995.7 Da ($[M+Na]^+$)and 1011.7 Da ($[M+K]^+$)

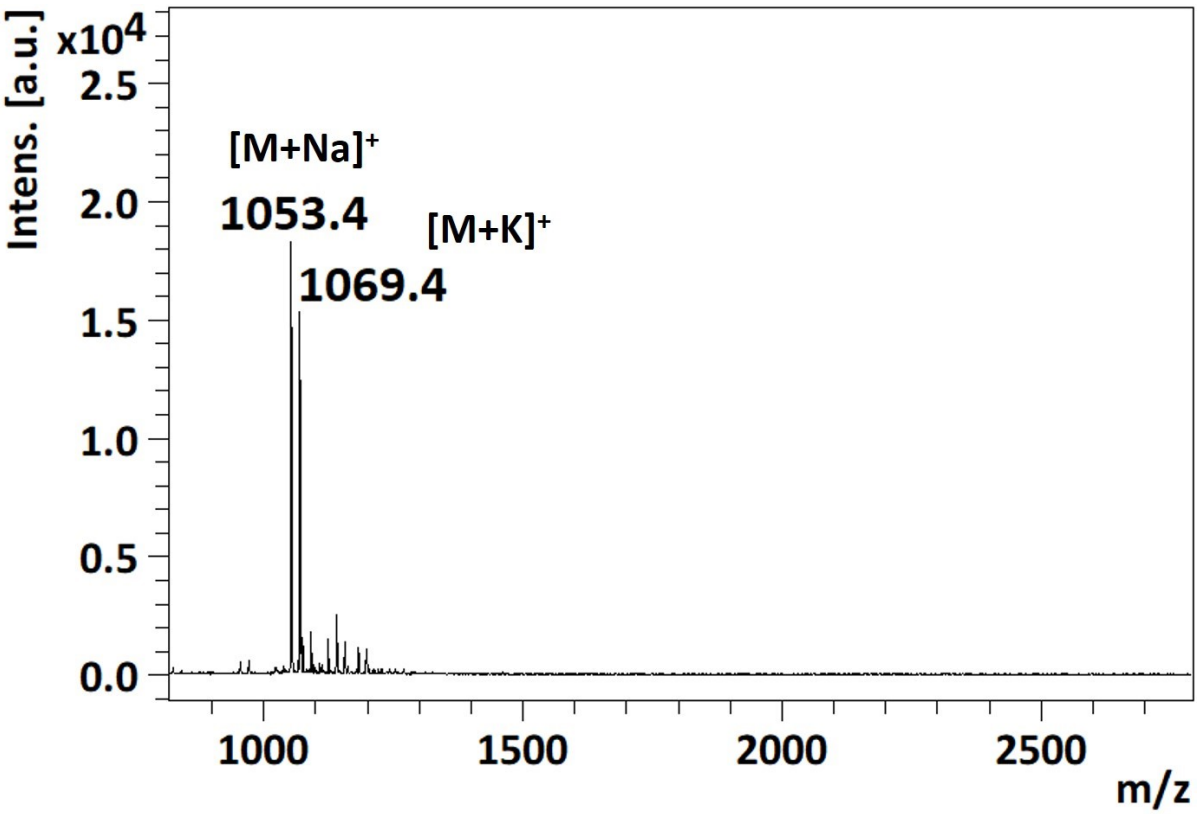


Figure S5. MALDI-TOF mass spectrum of peptide 2. Calculated mass:1030.3Da; Observed mass: 1053.4 Da ($[M+Na]^+$) and 1069.4 Da ($[M+K]^+$)

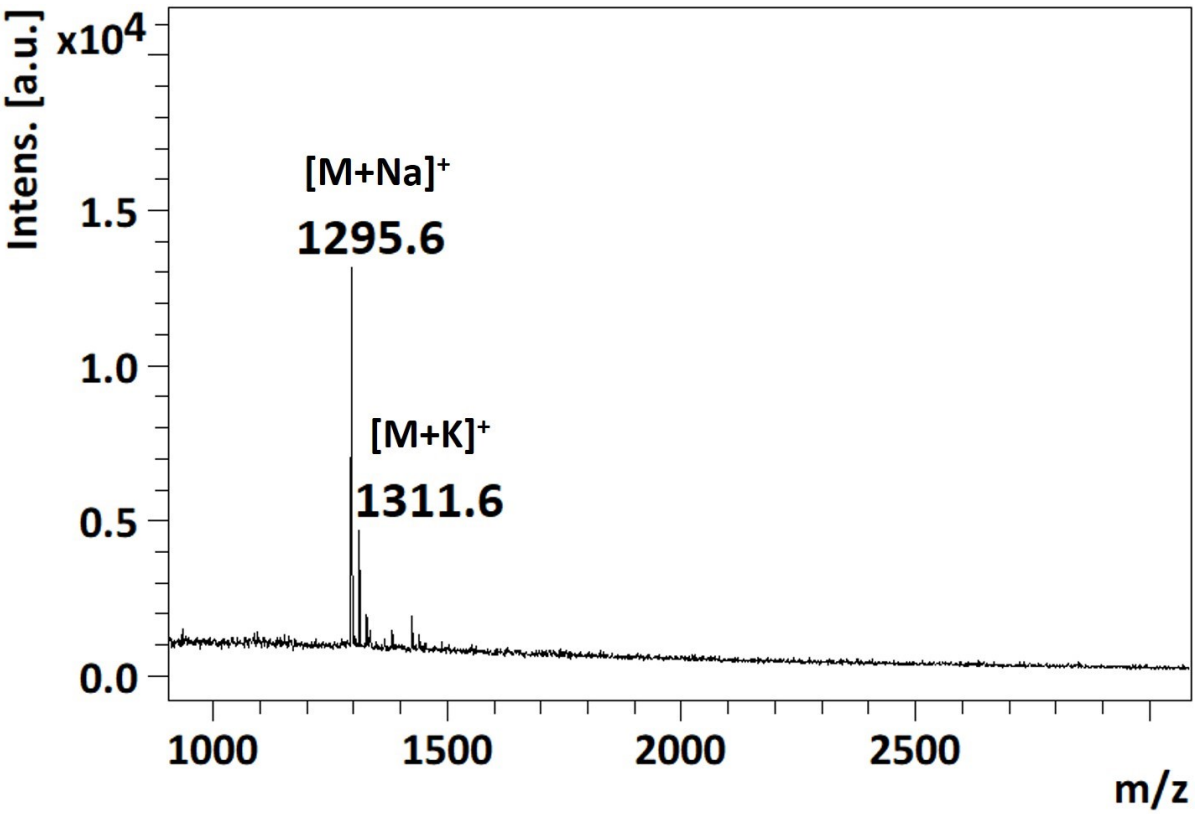


Figure S6. MALDI-TOF mass spectrum of peptide 3. Calculated mass: 1273.6 Da; Observed mass: 1295.6 Da ($[M+Na]^+$) and 1311.6 Da ($[M+K]^+$).

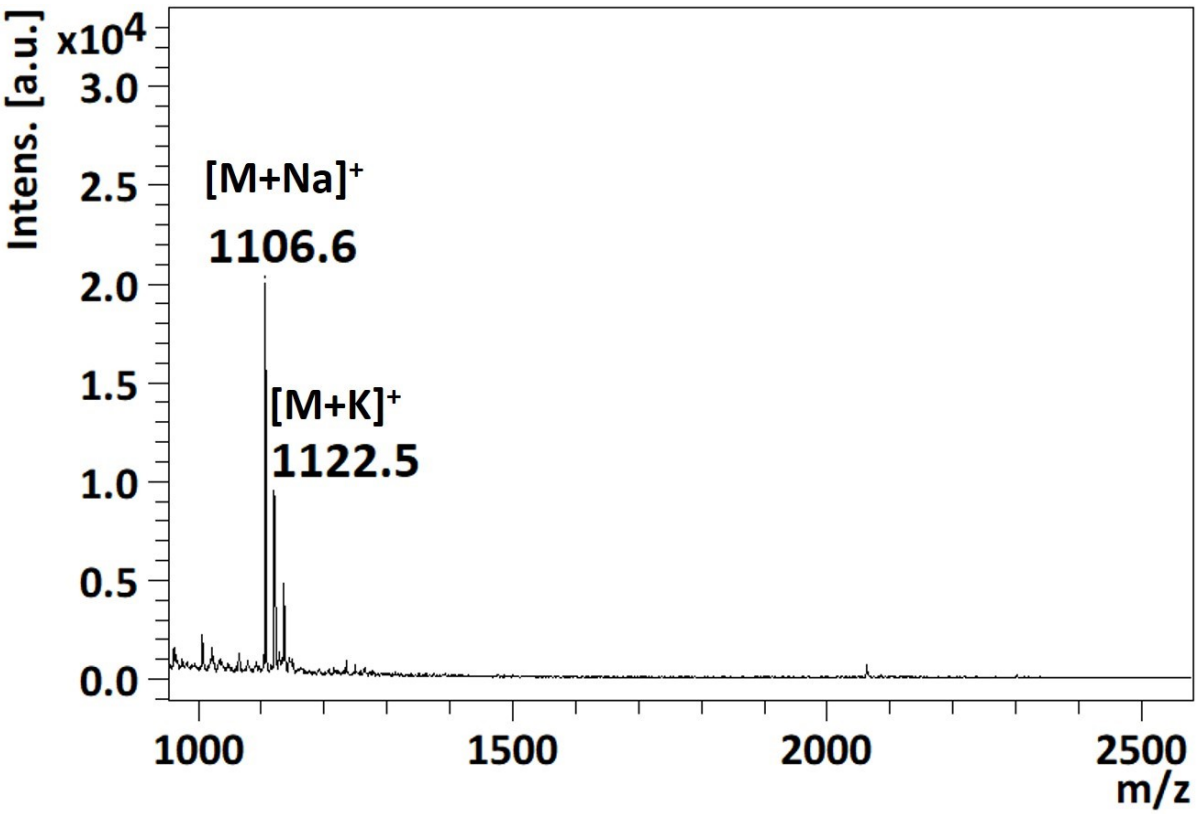


Figure S7. MALDI-TOF mass spectrum of peptide 4. Calculated mass: 1084.4 Da; Observed mass: 1106.6 Da ($[M+Na]^+$) and 1122.5 Da ($[M+K]^+$).

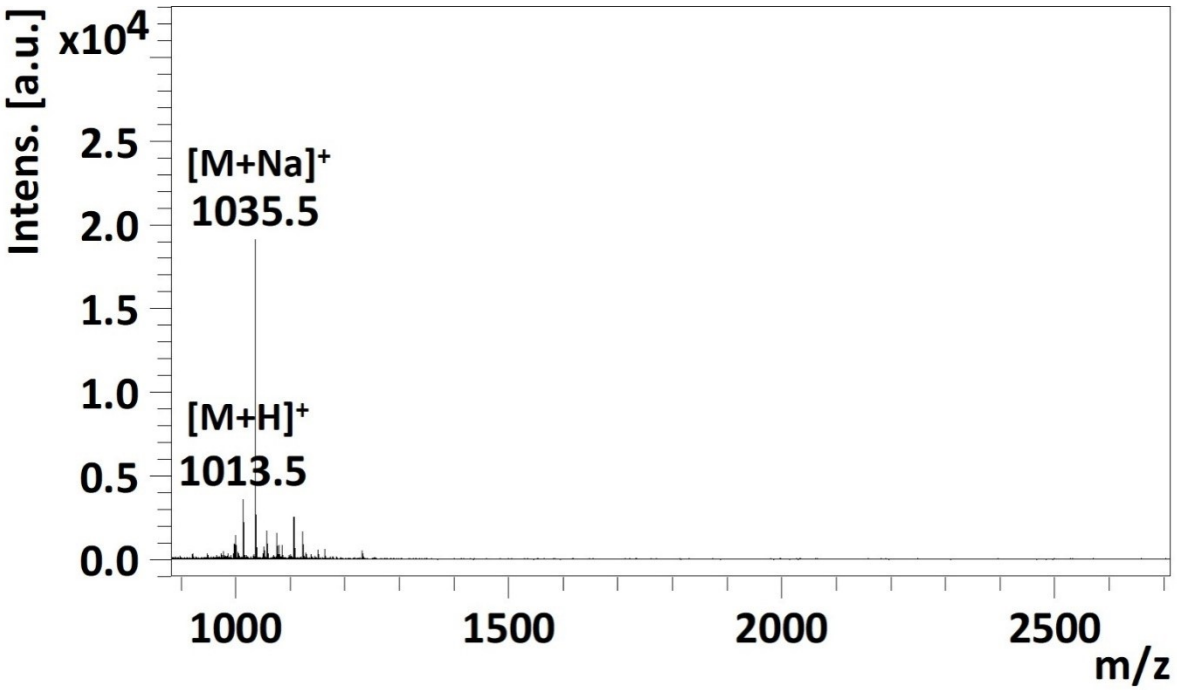


Figure S8. MALDI-TOF mass spectrum of peptide 5. Calculated mass: 1012.5 Da; Observed mass: 1013.5 Da ($[M+H]^+$) and 1035.5 Da ($[M+Na]^+$)

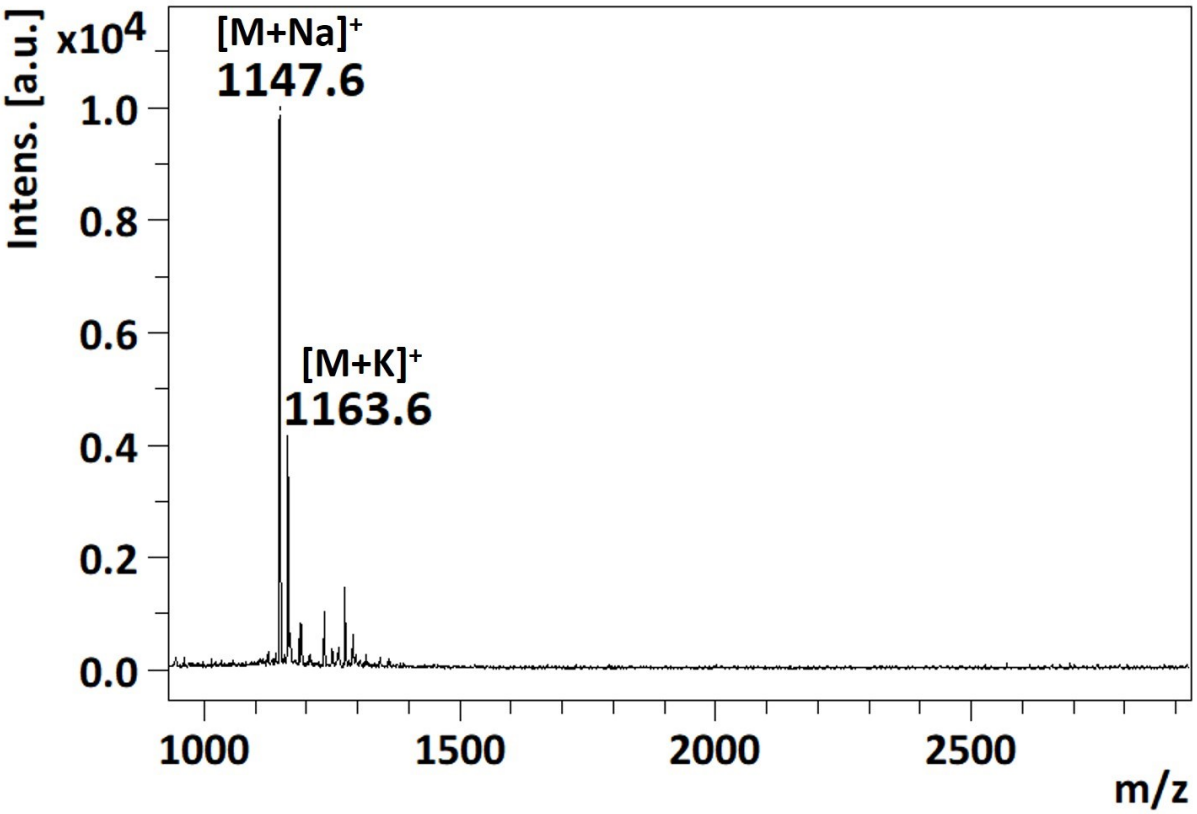


Figure S9. MALDI-TOF mass spectrum of peptide 6. Calculated mass: 1125.4 Da; Observed mass: 1147.6 Da ($[M+Na]^+$) and 1163.6 Da ($[M+K]^+$)

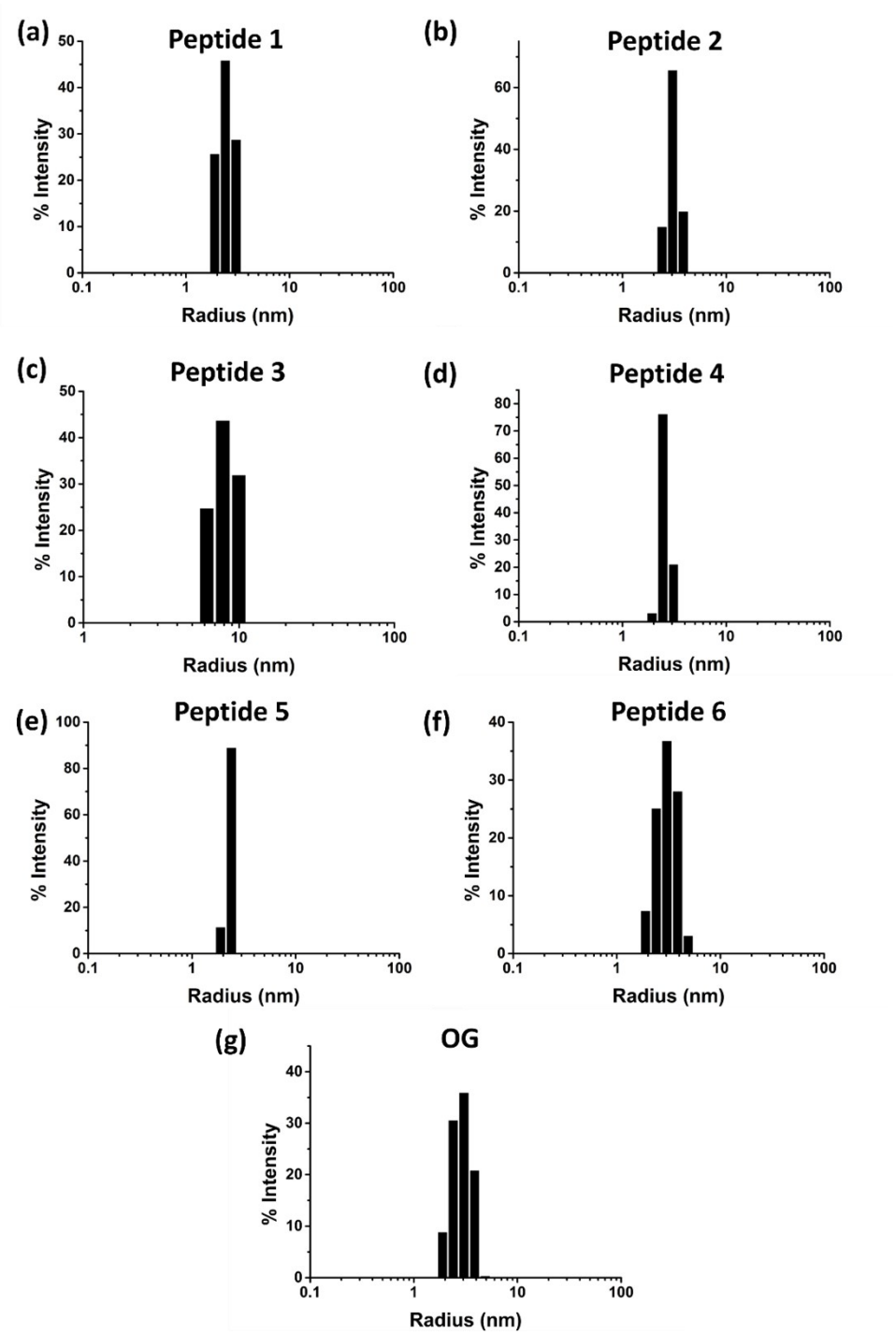


Figure S10. Histogram of particle size distributions of self-assembled detergent peptides 1 - 6 and OG (Octyl-β-D-Glucopyranoside, commercial detergent) obtained from DLS studies in buffer (100 mM Tris and 40 mM NaCl, pH 7.4). The average hydrodynamic radius of self-assembled peptides 1 – 6 and OG are 2.3±0.3 nm, 2.8±0.9 nm, 8.1±0.1 nm, 1.8±0.6 nm, 1.7±0.9 nm, 2.6±0.7 nm and 2.7±0.1 nm, respectively. The hydrodynamic radius of self-assembled peptides 1, 2 and 6 are having comparable values with commercial detergent, OG. The hydrodynamic radius of self-assembled peptide 3 has large value. The average radius are mean ± SD of triplicate samples.

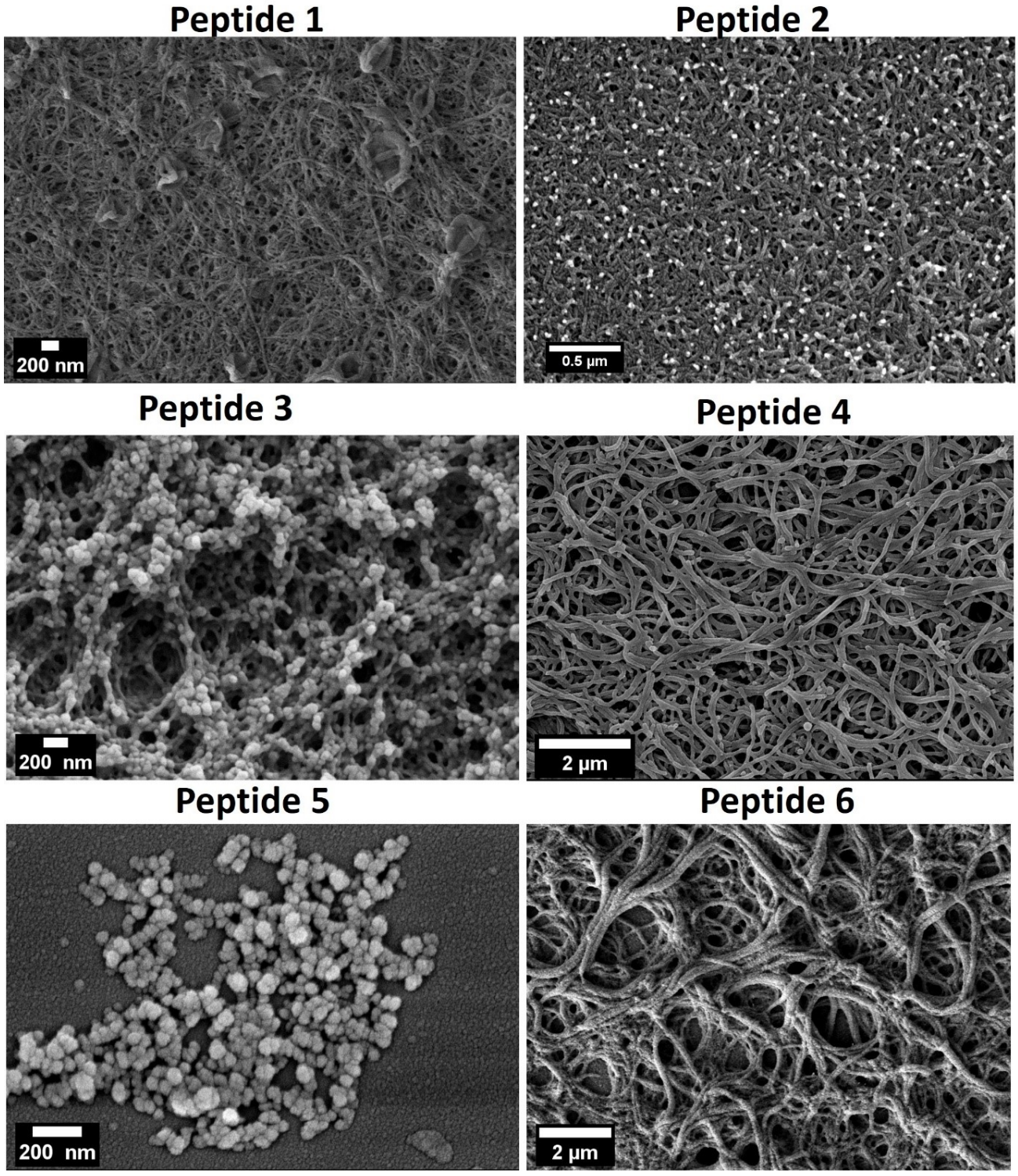


Figure S11. FE-SEM images of self-assembled detergent peptides. The average width of fibrillar peptides are as follows; Peptide 1: 48.6±8.4 nm, Peptide 2: 31.9±4.1 nm, Peptide 3: 41.8±11.4 nm, Peptide 4: 75.5±16.8 nm, Peptide 5: 41.9±5.4 nm, and Peptide 6: 78.8±13.6 nm. The average diameters are mean ± SD of triplicate samples.

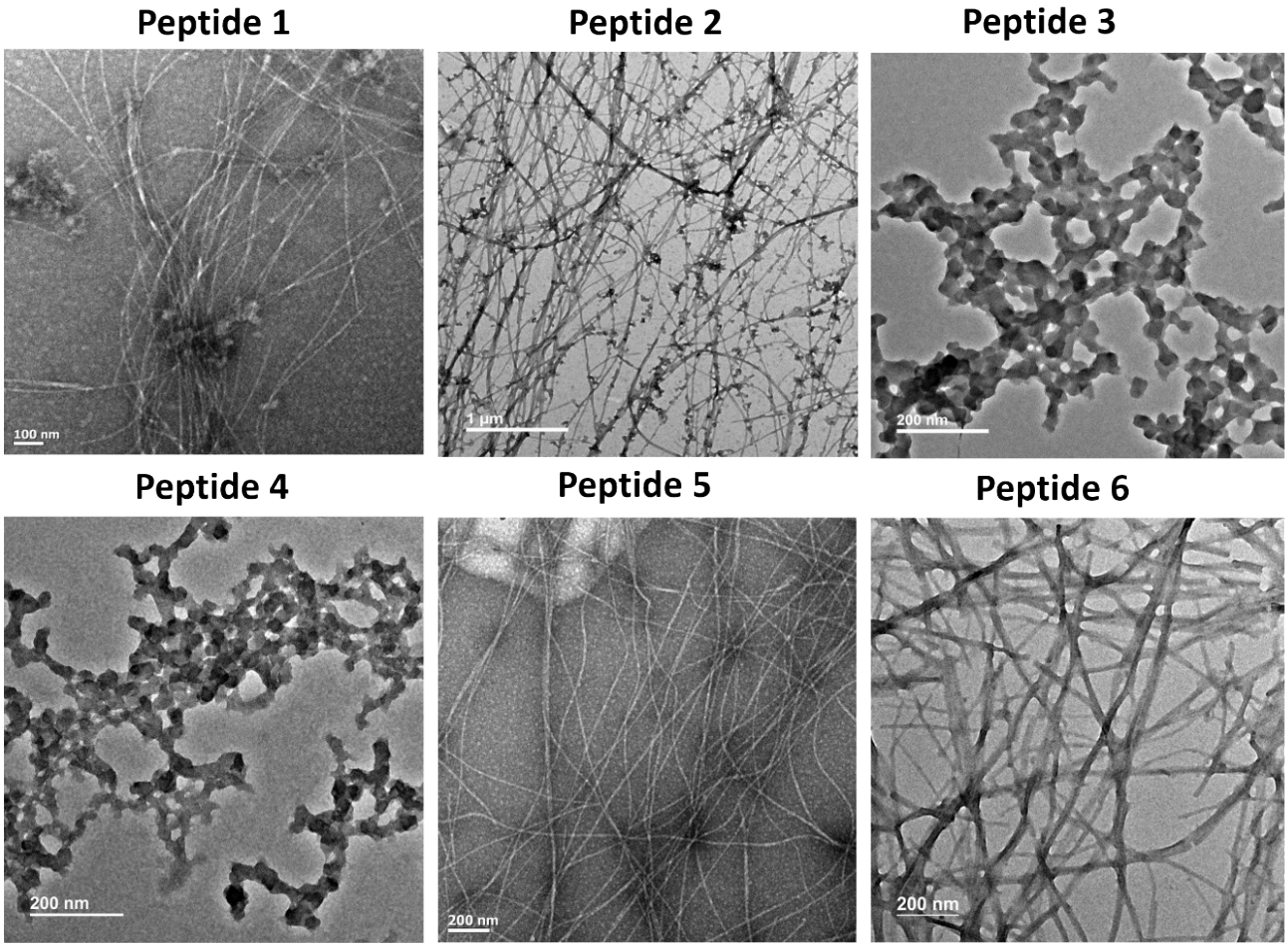


Figure S12. HR-TEM images of self-assembled detergent peptides. The average width of fibrillar peptides are as follows; peptide 1: 15.5±4.2 nm, peptide 2: 43.6±11.7 nm, peptide 3: 38.7±11.9 nm, peptide 4: 28.3±5.4 nm, peptide 5: 14.7±2.2 nm and peptide 6: 26.3±6.2 nm. The average diameters are mean ± SD of triplicate samples.

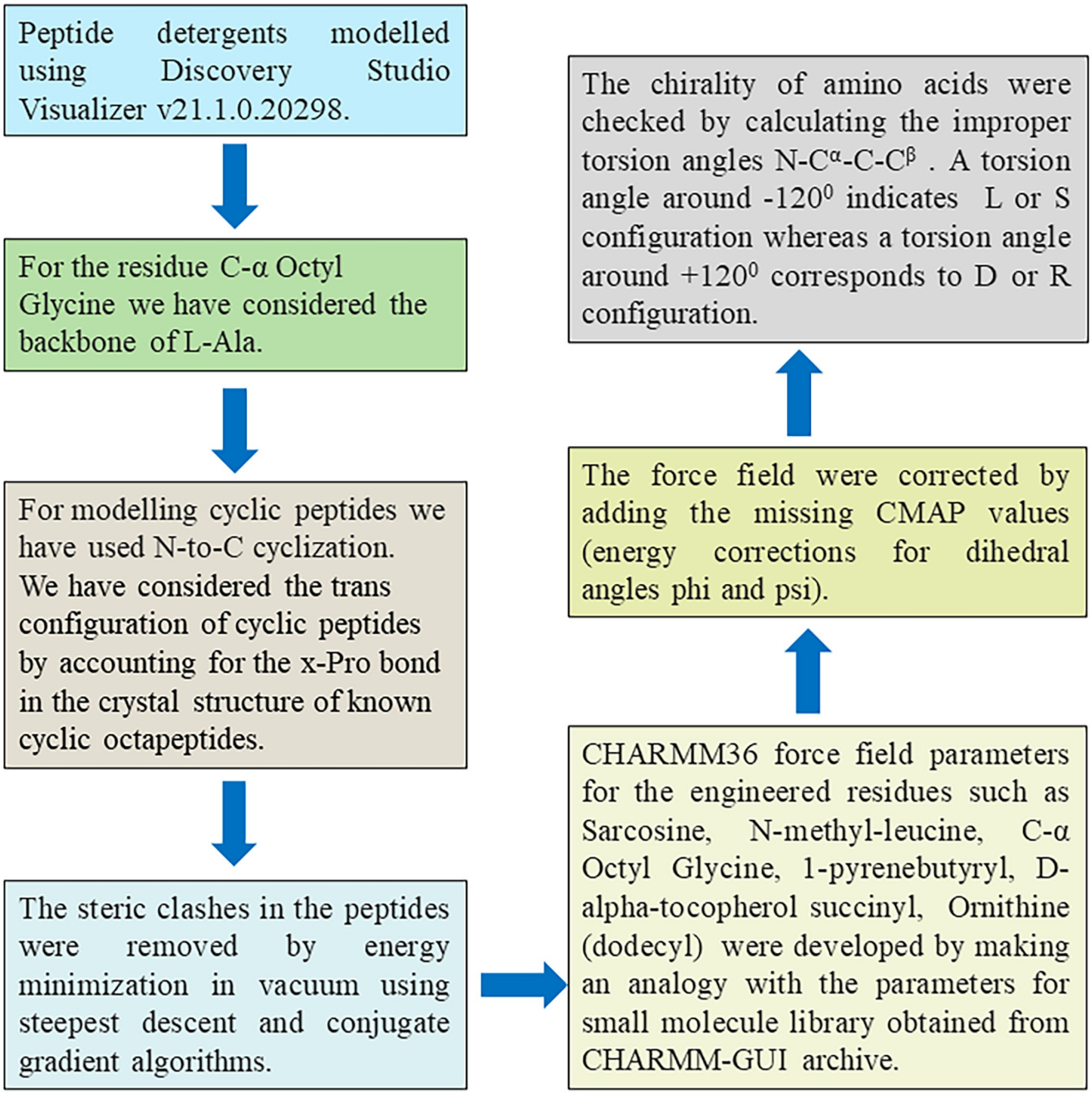


Figure S13. Flowchart depicting the strategies involved in the development of CHARMM36 force field parameters for unnatural amino acid residues

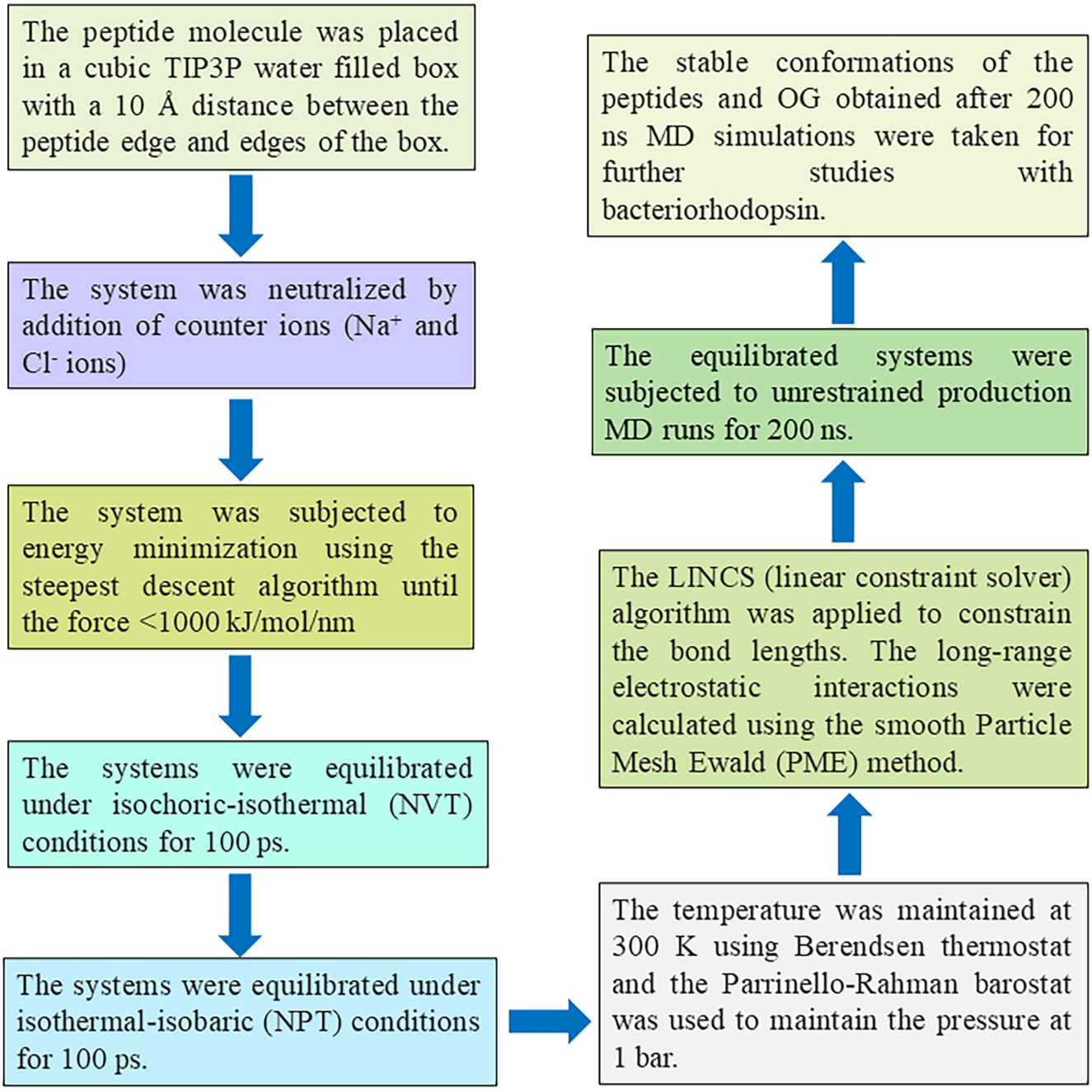
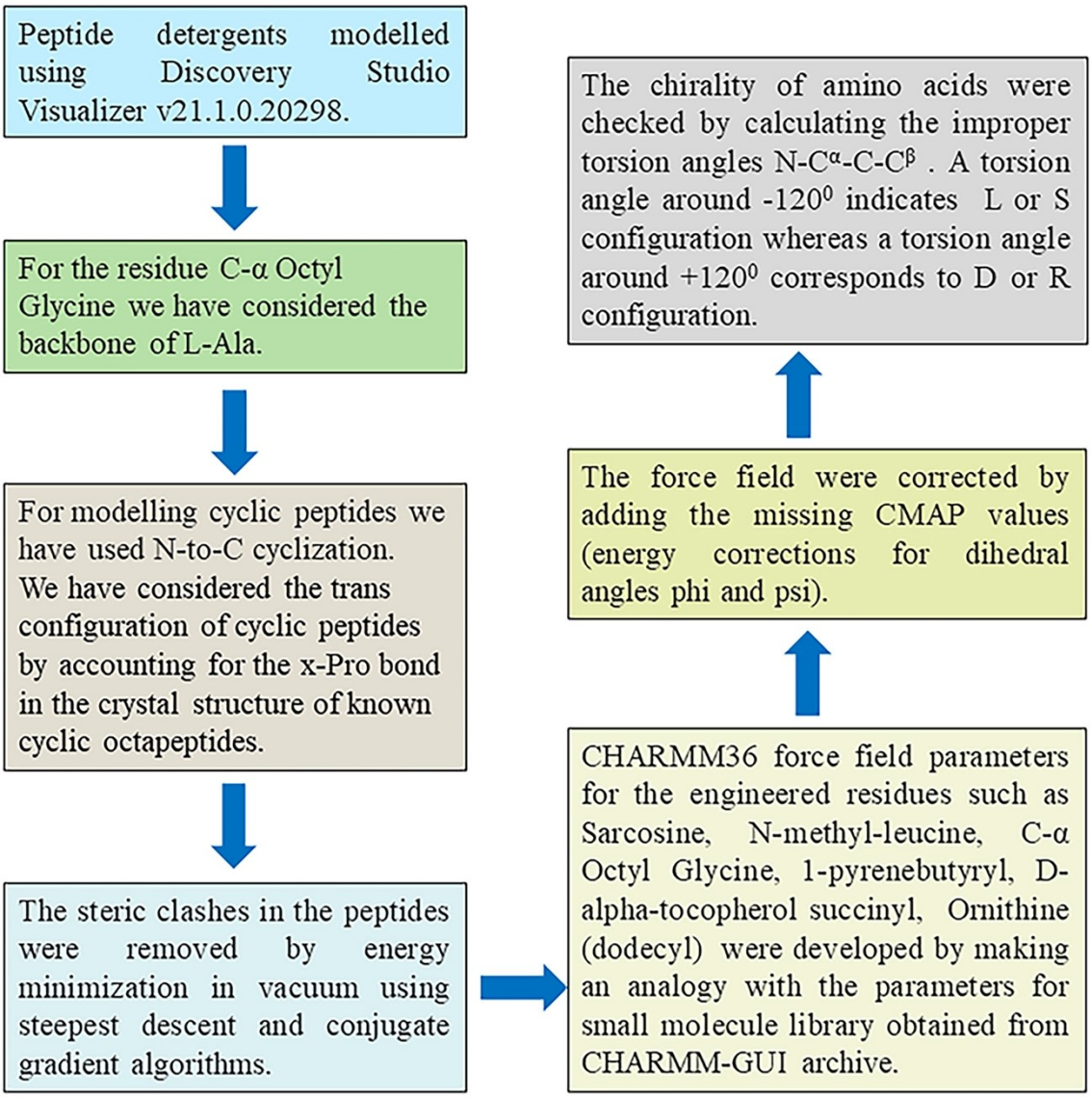


Figure S14. Flowchart showing the step-wise protocol for MD simulation of detergent peptides.



BR-detergent complexes	Cubic box dimension (nm)	No. of detergent molecules	Total number of atoms
BR-Peptide 1	16.98	90	483837
BR-Peptide 2	17.06	90	492891
BR-Peptide 3	16.35	90	436956
BR-Peptide 4	17.44	90	525342
BR-Peptide 5	17.06	90	492768
BR-Peptide 6	16.79	90	469863
BR-BP-1	17.35	90	510780
BR-LPD12	18.31	90	617304
BR-PD1	18.50	90	633663
BR-A6D	16.79	90	470487
BR-A6K	16.55	90	450699
BR-OG	16.01	90	408657

Figure S15. Flowchart showing the step-wise protocol for MD simulation of detergent encased BR systems.

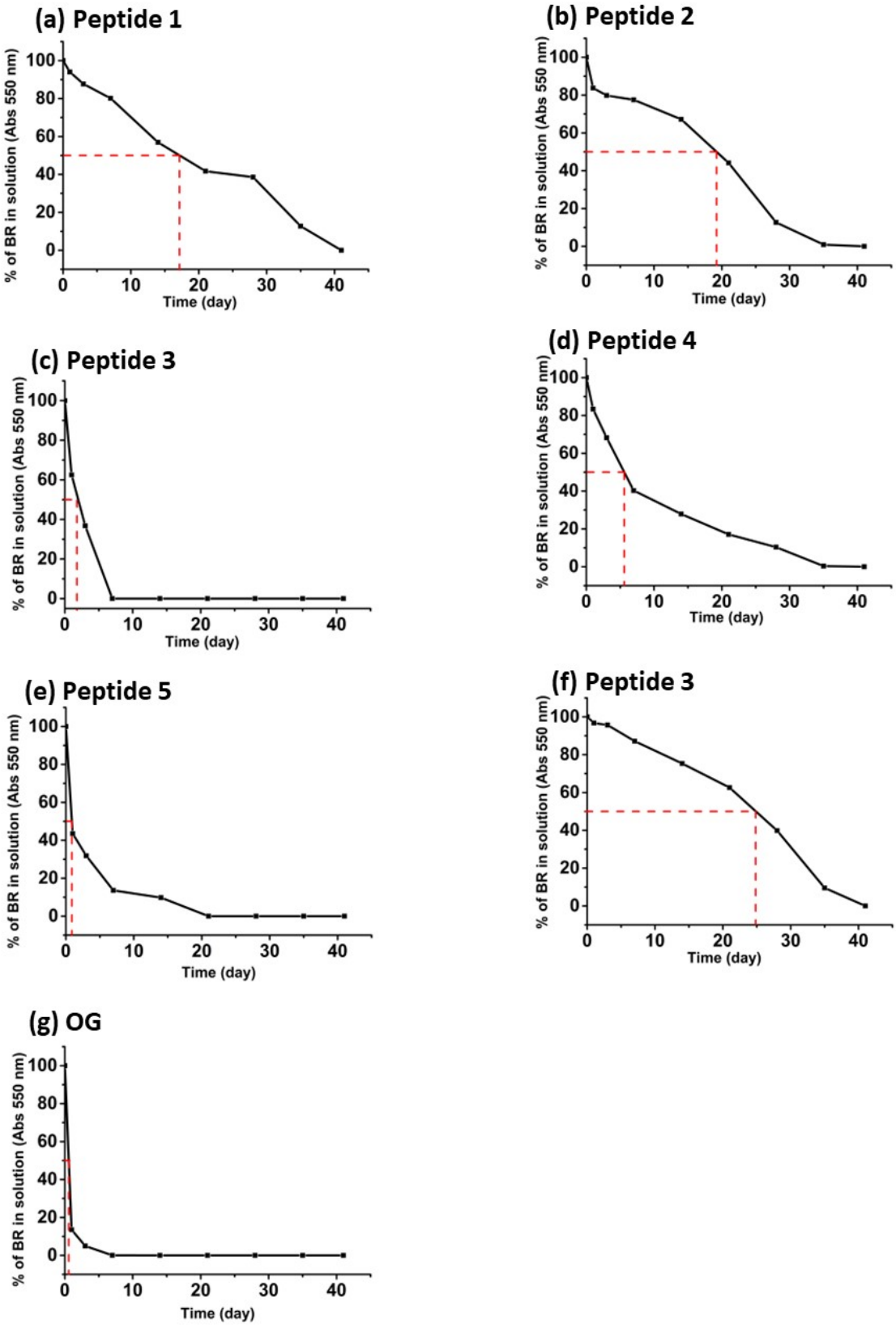


Figure S16. Plot of half-life determination of BR in presence of peptide detergents 1-6 and commercial detergent (OG).

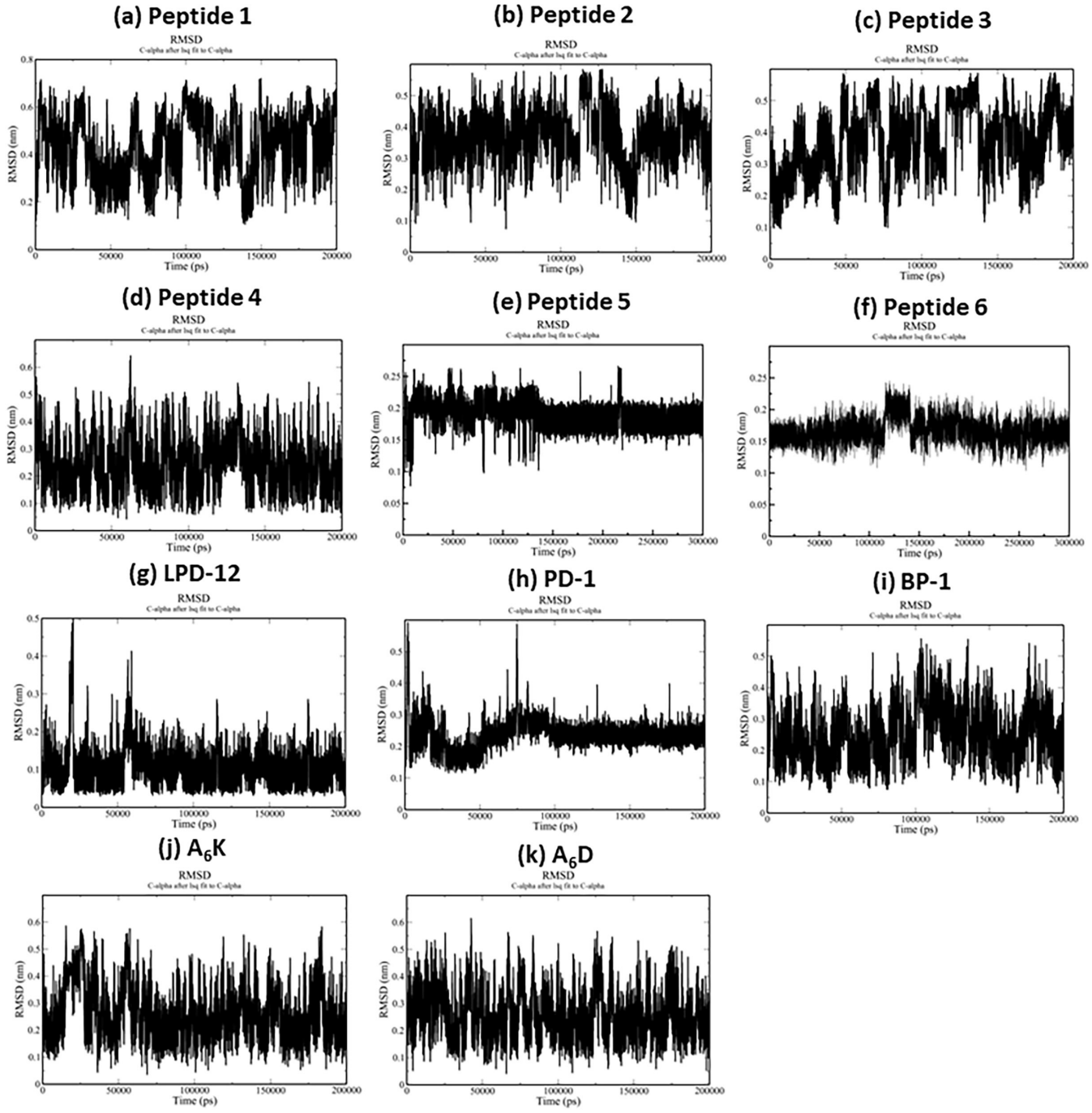


Figure S17. RMSD Plot of Cα atoms of peptide detergents. Peptides 1-6 are our engineered peptide detergents whereas peptides D1-D5 are peptides reported by other groups.

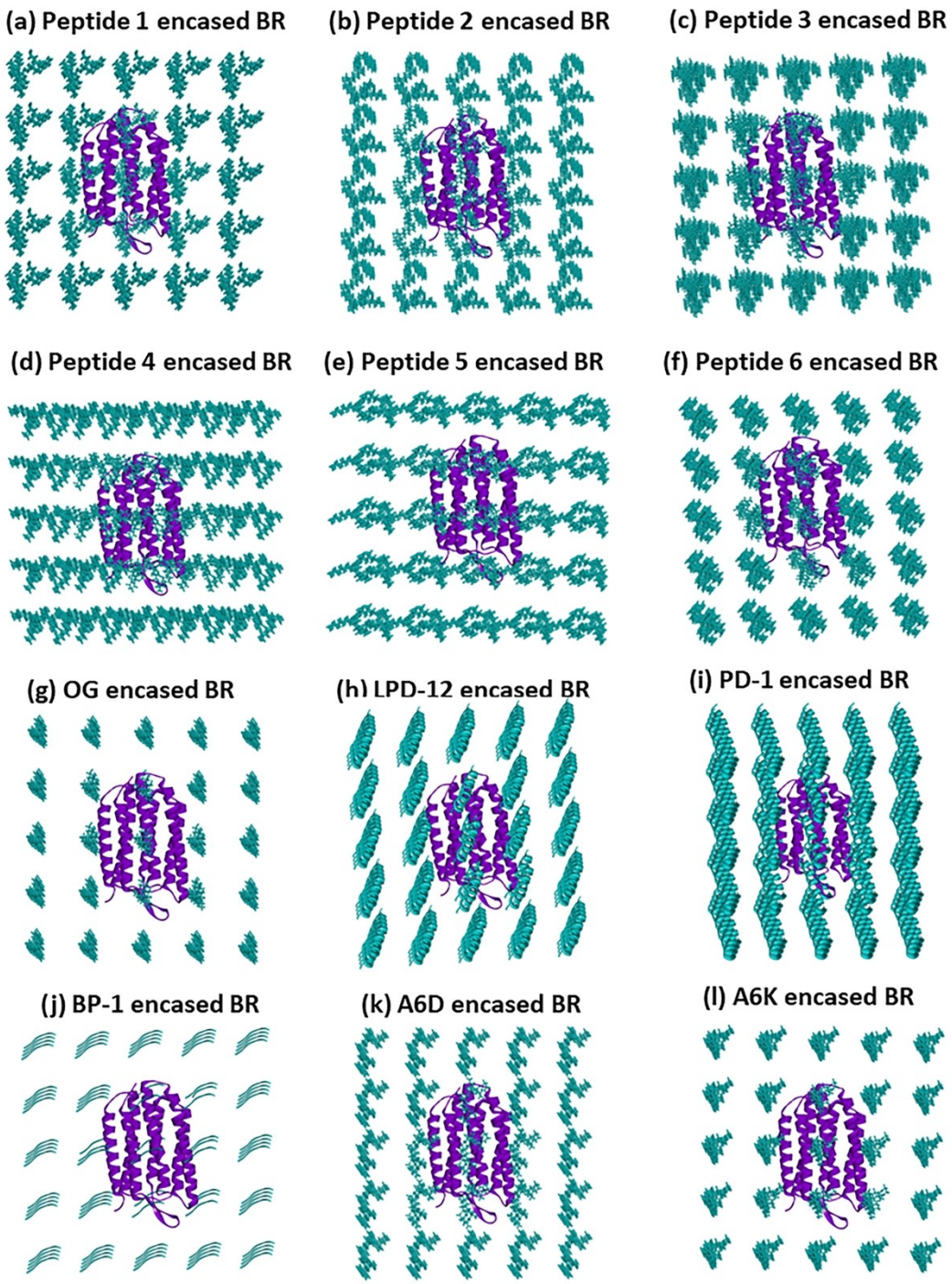
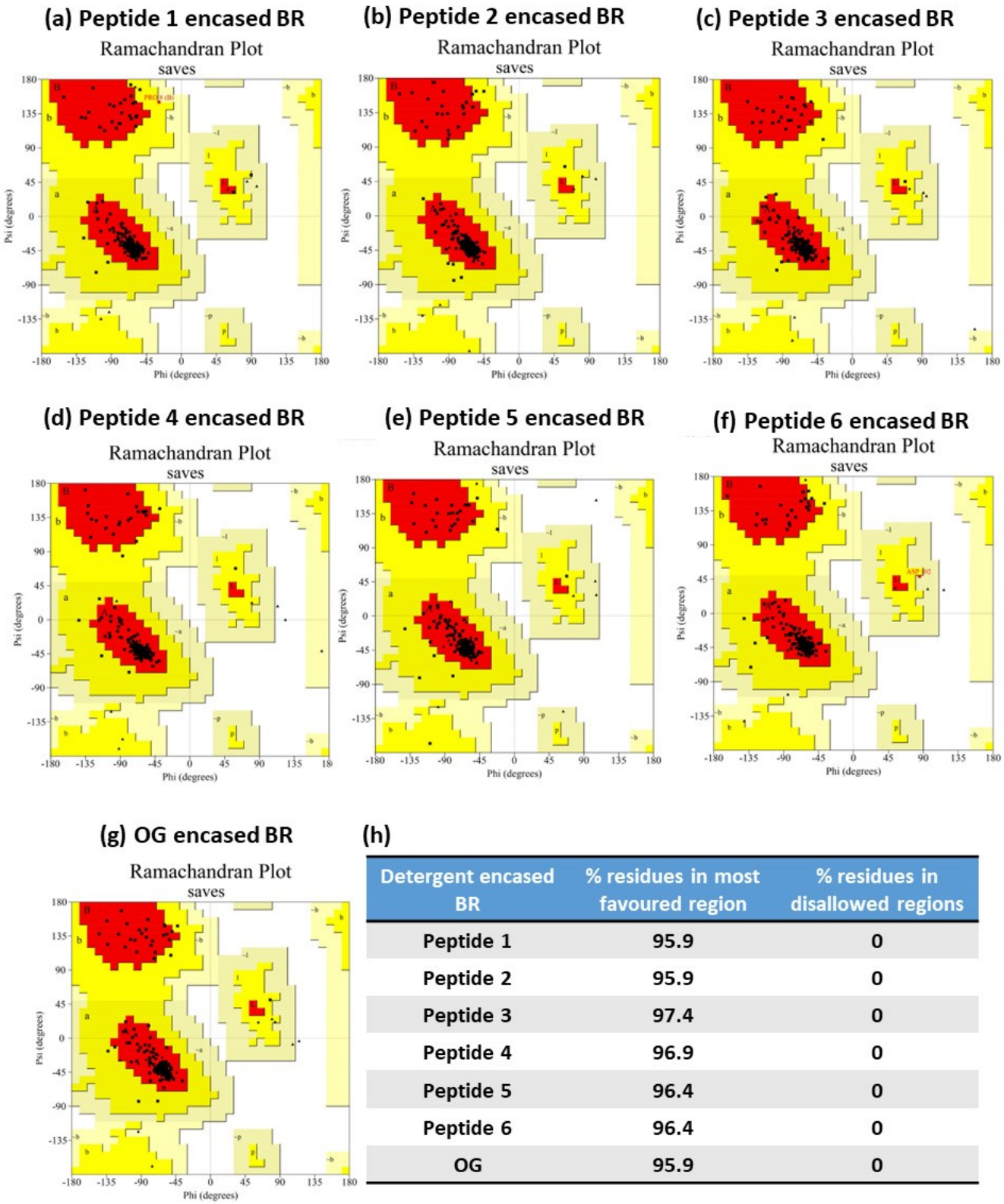


Figure S18. Initial models of detergent-encased BR systems at time t=0 ns of MD simulations. Each box contains ninety detergent molecules, wherein each detergent molecule is 20 Å apart from the other and BR is positioned at the centre of the box. The detergent molecules are displayed as green stick and ribbon models while BR is represented as purple ribbons. Note that (a) to (f) represents our designed facial lipopeptide detergents encasing BR. (g) OG is the commercial detergent encasing BR and (h) to (l) corresponds to control group detergent peptides reported by other groups.

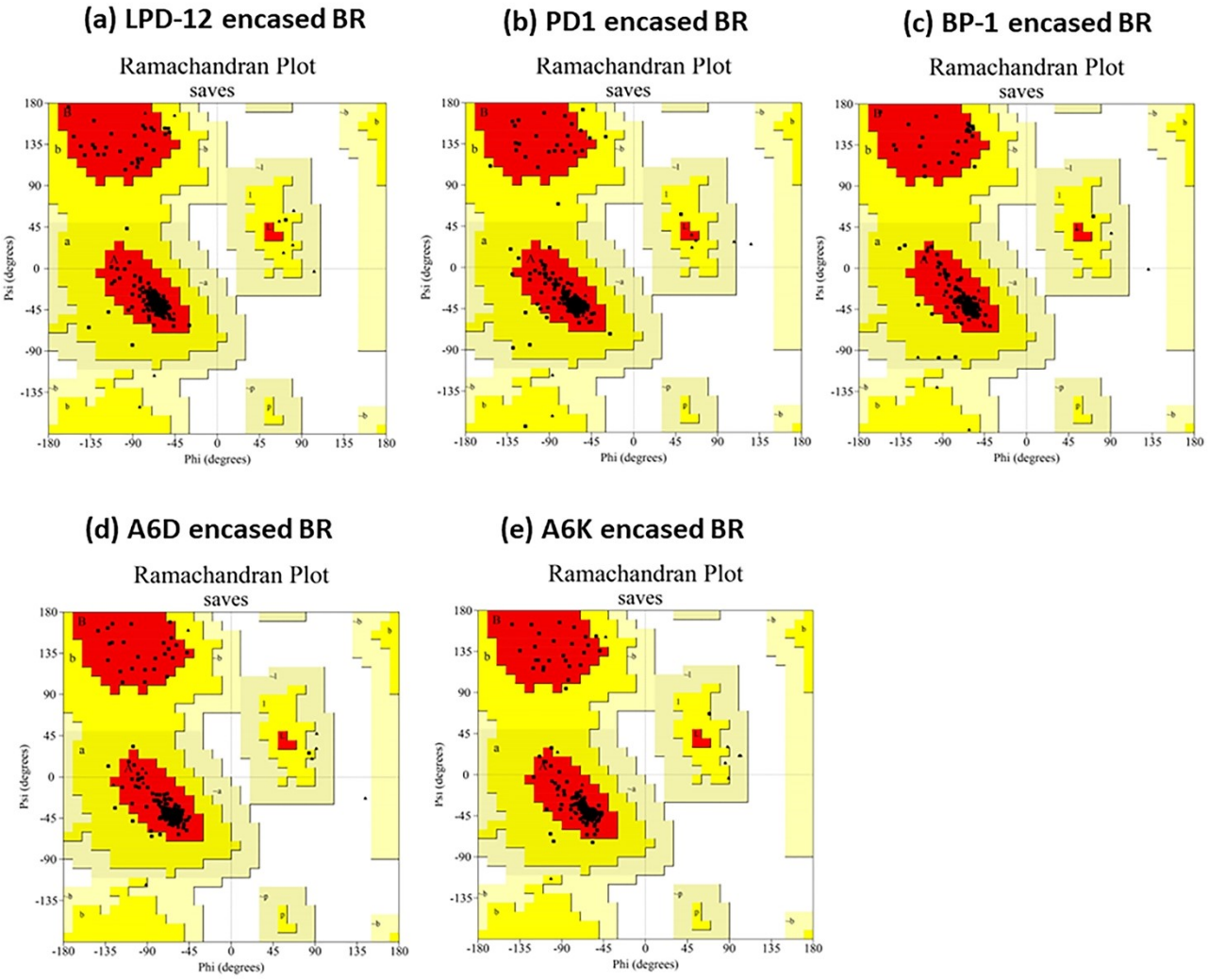


(h)

Detergent encased BR	% residues in most favoured region	% residues in disallowed regions
Peptide 1	95.9	0
Peptide 2	95.9	0
Peptide 3	97.4	0
Peptide 4	96.9	0
Peptide 5	96.4	0
Peptide 6	96.4	0
OG	95.9	0

Figure S19. Analyses of secondary structure changes in BR by monitoring backbone dihedral angles- phi and psi of our engineered detergent encased BR systems. Figures (a) to (g) show the Ramachandran map of BR encased by detergent molecules. most favored regions (red), additionally allowed regions (yellow),

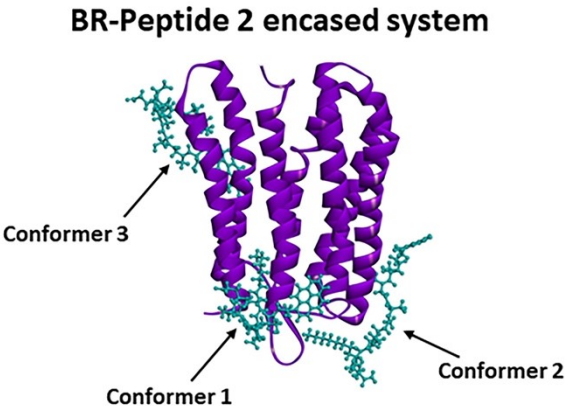
generously allowed regions (beige) and disallowed regions (white). Figure (h) shows the distribution of residues in the favored and disallowed regions of Ramachandran map.



(f)

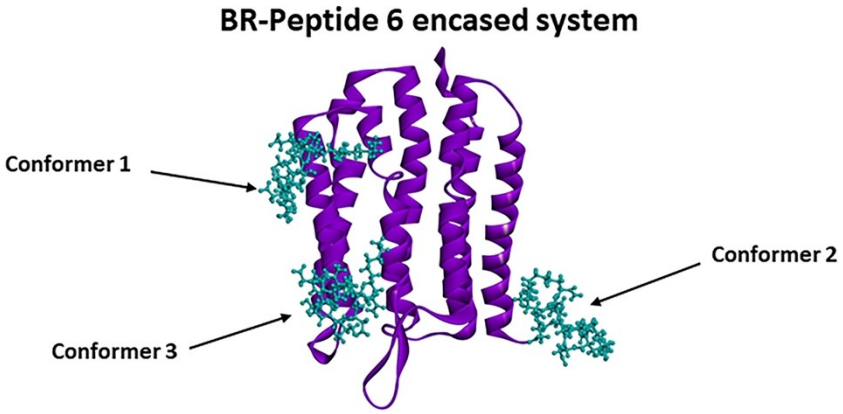
Peptide detergent encased BR	% residues in most favoured region	% residues in disallowed regions
LPD-12	97.4	0
PD1	93.3	0
BP-1	96.4	0
A6D	95.9	0
A6K	97.4	0

Figure S20. Analyses of secondary structure changes in BR by monitoring backbone dihedral angles-phi and psi of reported detergent encased BR systems. Figures (a) to (g) show the Ramachandran map of BR encased by detergent molecules. most favored regions (red), additionally allowed regions (yellow), generously allowed regions (beige) and disallowed regions (white). Figure (h) shows the distribution of residues in the favored and disallowed regions of Ramachandran map.



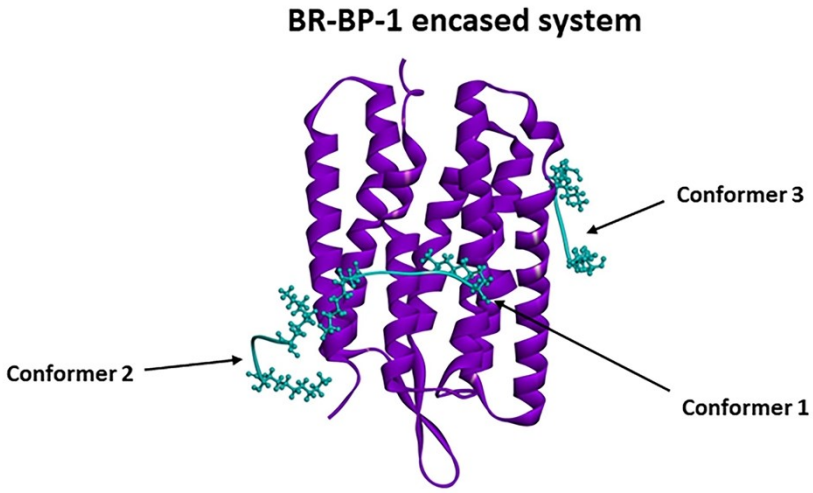
Residues	Dihedral angles of Conformer 1			Dihedral angles of Conformer 2			Dihedral angles of Conformer 3		
	ϕ	ψ	ω	ϕ	ψ	ω	ϕ	ψ	ω
PYRENEBUTYRYL-1	NA	NA	NA	NA	NA	NA	NA	NA	NA
SER-2	NA	125.49	NA	NA	147.14	NA	NA	156.59	NA
SAR-3	73.60	17.03	-178.35	-39.30	144.39	179.59	98.35	179.69	-179.49
SER-4	-157.76	154.45	-177.67	-151.99	148.08	-176.32	-139.71	162.20	164.20
SAR-5	-63.27	-46.67	-171.95	114.15	141.50	-173.79	59.95	-176.25	-172.57
GLU-6	-79.40	-24.44	-175.95	-145.21	164.47	-169.41	-44.15	149.21	176.56
OCTYLGLY-7	-90.60	-39.49	-178.64	-109.33	1.22	-168.60	-94.77	77.67	164.64
GLU-8	-83.06	NA	174.39	-83.72	NA	-174.25	-76.31	NA	-169.53

Figure S21. The dihedral angles of BR-Peptide 2 encased system. Note that we have tabulated the dihedral angles of Peptide 2 in three different conformations (conformer 1, conformer 2 and conformer 3).



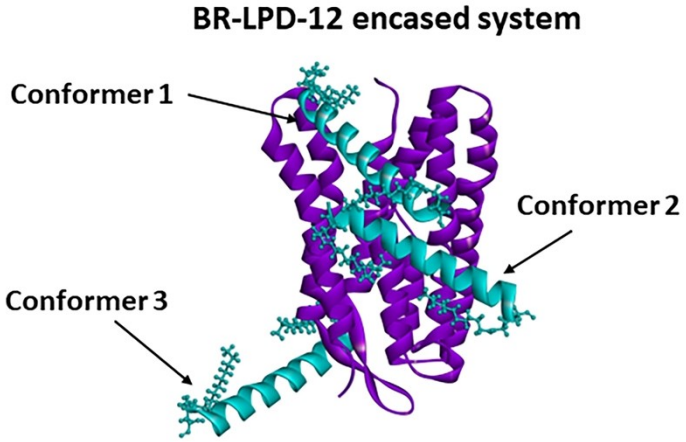
Residues	Dihedral angles of Conformer 1			Dihedral angles of Conformer 2			Dihedral angles of Conformer 3		
	ϕ	ψ	ω	ϕ	ψ	ω	ϕ	ψ	ω
D-SER-1	112.72	-168.67	172.05	81.40	-134.75	152.19	72.04	-158.33	167.51
N-ME-LEU-2	-82.64	20.07	-176.40	-85.45	48.62	178.51	-61.86	137.28	176.02
D-ASP-3	103.44	174.55	-170.93	59.34	44.95	-170.99	105.04	-20.24	177.50
OCTYLGLY-4	-56.86	131.79	-166.31	-157.13	-178.51	179.29	-99.57	-18.34	179.66
D-SER-5	143.27	80.26	169.34	51.72	61.13	-177.42	64.25	39.55	-177.30
N-ME-LEU-6	-88.52	16.78	159.17	-94.07	16.41	175.97	-113.22	119.89	-156.19
D-ASP-7	79.33	19.05	166.36	71.02	28.87	-177.40	106.59	-125.76	-175.13
GLU-8	-91.05	-48.11	-175.77	-114.21	170.73	166.37	-79.08	61.34	-172.09

Figure S22. The dihedral angles of BR-Peptide 6 encased system. Note that we have tabulated the dihedral angles of Peptide 6 in three different conformations (conformer 1, conformer 2 and conformer 3).



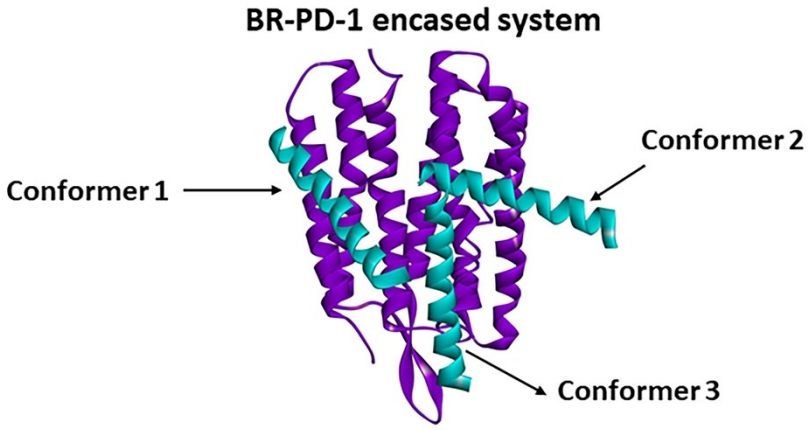
Residues	Dihedral angles of Conformer 1				Dihedral angles of Conformer 1				Dihedral angles of Conformer 1		
	ϕ	ψ	ω		ϕ	ψ	ω		ϕ	ψ	ω
OCTGLY-1	NA	137.58	NA		NA	148.59	NA		NA	161.82	NA
SER-2	-161.15	156.44	-175.42		-108.50	131.16	-175.74		-91.06	17.25	-173.83
LEU-3	-133.01	124.72	-158.37		-107.70	10.04	-176.92		-160.55	172.03	178.69
SER-4	-83.49	136.06	171.17		-106.82	137.41	154.85		-159.46	141.43	177.36
N-ME-LEU-5	-94.14	83.95	-176.01		-113.43	113.62	162.50		-94.86	179.62	167.22
ASP-6	-137.12	125.80	-165.75		-99.90	132.00	171.15		-88.64	93.24	168.44
OCTGLY-7	-104.23	2.77	-179.64		-77.95	-20.56	-178.00		-171.40	160.72	179.58
ASP-8	-104.03	NA	-167.44		-68.83	NA	177.32		-100.89	NA	172.44

Figure S23. The dihedral angles of BR-BP-1 encased system. Note that we have tabulated the dihedral angles of BP-1 in three different conformations (conformer 1, conformer 2 and conformer 3).



Residues	Dihedral angles of Conformer 1			Dihedral angles of Conformer 2			Dihedral angles of Conformer 3		
	ϕ	ψ	ω	ϕ	ψ	ω	ϕ	ψ	ω
ALA-1	NA	145.04	NA	NA	-41.05	NA	NA	148.23	NA
ORL-2	-65.62	-37.78	-168.59	-64.89	-41.04	-178.96	-52.78	-45.19	170.57
ALA-3	-63.11	-39.90	173.81	-65.54	-43.02	175.83	-58.10	-42.22	176.09
GLU-4	-65.78	-39.97	178.55	-65.78	-39.97	178.55	-61.73	-46.22	172.76
ALA-5	-64.59	-36.28	171.09	-66.91	-37.57	175.89	-58.87	-43.85	169.76
ALA-6	-56.68	-49.66	162.66	-55.67	-37.71	172.45	-65.55	-39.80	177.86
GLU-7	-66.92	-41.71	-177.63	-70.33	-43.53	-179.84	-49.47	-48.91	168.90
LYS-8	-67.65	-39.54	172.75	-58.09	-37.15	172.70	-62.17	-46.39	-179.56
ALA-9	-58.87	-38.01	167.57	-66.47	-52.10	171.23	-52.16	-42.39	169.67
ALA-10	-63.93	-42.38	171.03	-56.09	-39.52	179.33	-67.29	-45.85	-174.80
LYS-11	-58.58	-49.11	168.88	-72.27	-30.03	176.40	-58.42	-40.95	170.82
TYR-12	-58.82	-44.41	177.84	-73.31	-43.72	175.94	-50.53	-50.90	177.39
ALA-13	-59.00	-47.67	174.65	-54.56	-46.97	174.96	-80.90	-29.44	-170.44
ALA-14	-63.49	-42.40	-177.29	-61.54	-42.70	176.39	-63.62	-59.18	178.19
GLU-15	-72.99	-35.46	-176.26	-67.30	-29.34	168.25	-56.68	-45.78	170.21
ALA-16	-61.59	-41.25	168.86	-61.59	-41.25	168.86	-58.30	-43.36	176.11
ALA-17	-61.94	-38.89	173.83	-66.45	-40.80	176.05	-61.08	-41.77	171.81
GLU-18	-62.80	-47.72	172.04	-65.81	-43.58	178.44	-62.80	-47.72	172.04
LYS-19	-59.66	-43.25	174.36	-60.93	-42.76	170.66	-61.25	-38.45	174.55
ALA-20	-62.90	-43.30	171.61	-59.17	-40.94	170.67	-66.85	-45.40	177.71
ALA-21	-64.30	-43.66	174.57	-65.97	-40.53	173.25	-64.30	-43.66	174.57
LYS-22	-83.10	-17.79	-172.16	-78.24	-22.32	-175.23	-64.13	-40.58	164.01
ALA-23	-66.67	-36.85	174.46	-84.56	-20.29	171.54	-62.88	-24.97	179.94
ORL-24	-95.27	-14.26	176.79	-89.01	-15.57	165.63	-67.81	-37.02	172.29
ALA-25	-70.17	NA	176.33	-77.48	NA	162.86	-83.76	NA	-179.91

Figure S24. The dihedral angles of BR-LPD-12 encased system. Note that we have tabulated the dihedral angles of LPD-12 in three different conformations (conformer 1, conformer 2 and conformer 3).



Residues	Dihedral angles of Conformer 1			Dihedral angles of Conformer 2			Dihedral angles of Conformer 3		
	ϕ	ψ	ω	ϕ	ψ	ω	ϕ	ψ	ω
GLU-1	NA	-42.66	NA	NA	-24.81	NA	NA	-45.42	NA
GLU-2	-53.28	-52.69	-179.70	-55.03	-42.48	157.91	-70.95	-41.49	-179.07
LEU-3	-64.51	-38.27	169.48	-68.61	-44.28	178.77	-55.68	-43.21	-178.85
LEU-4	-65.17	-36.13	167.11	-69.61	-30.03	178.94	-61.68	-42.43	170.19
LYS-5	-65.24	-37.43	164.69	-65.81	-36.96	164.61	-58.94	-44.34	174.65
GLN-6	-65.71	-36.62	168.62	-62.87	-45.68	172.46	-63.15	-44.83	170.12
ALA-7	-60.94	-50.15	168.95	-59.89	-42.89	175.57	-61.39	-38.37	175.87
LEU-8	-62.83	-40.90	177.66	-66.78	-39.63	178.27	-69.70	-35.46	174.82
GLN-9	-72.06	-32.69	179.51	-63.43	-48.23	174.51	-68.37	-30.87	177.76
GLN-10	-75.31	-23.21	175.63	-64.82	-33.56	-178.07	-71.28	-32.94	177.60
ALA-11	-64.11	-38.53	172.14	-64.26	-38.54	169.78	-60.51	-36.20	167.69
GLN-12	-66.64	-43.13	163.57	-57.43	-39.00	171.92	-65.75	-43.39	174.26
GLN-13	-68.47	-35.80	177.21	-60.60	-42.73	-179.80	-68.71	-35.95	-173.69
LEU-14	-62.81	-37.81	171.44	-52.53	-38.52	178.37	-63.27	-42.46	167.18
LEU-15	-65.39	-40.06	178.46	-84.24	-20.52	-171.03	-71.59	-44.21	-176.67
GLN-16	-62.07	-46.47	176.25	-66.96	-48.79	165.04	-64.33	-46.53	172.85
GLN-17	-51.19	-44.03	166.51	-61.55	-46.80	-171.44	-62.32	-36.66	-179.92
ALA-18	-65.39	-34.91	174.38	-62.10	-41.50	179.43	-63.53	-37.79	175.76
GLN-19	-65.45	-37.15	167.31	-60.41	-49.46	174.25	-71.54	-40.60	177.02
GLU-20	-63.95	-37.13	177.20	-59.69	-40.11	170.79	-63.95	-37.13	177.20
LEU-21	-62.89	-49.17	165.85	-61.91	-44.70	169.42	-62.89	-49.17	165.85
ALA-22	-54.73	-39.58	-177.76	-51.53	-39.93	174.09	-70.09	-34.93	168.09
LYS-23	-69.02	-34.40	171.75	-97.33	-37.01	-177.46	-97.33	-37.01	-177.46
LYS-24	-78.55	NA	-179.81	-106.46	NA	-168.54	-91.38	NA	-161.24

Figure S25. The dihedral angles of BR-PD-1 encased system. Note that we have tabulated the dihedral angles of PD-1 in three different conformations (conformer 1, conformer 2 and conformer 3).

Table S1. Dihedral angle values of Peptide 1.

Residues	**Initial Dihedral angles for Peptide 1**				**Dihedral angles for Peptide 1 after 200 ns MD simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
OctylGly-1	NA	-179.97	NA		NA	155.02	NA
Ser-2	179.96	179.98	-179.97		-123.38	144.24	-179.01
Sar-3	-179.97	179.99	-179.94		36.55	-148.05	171.92
Ser-4	180.00	-179.95	179.98		-97.23	137.62	-175.76
Sar-5	180.00	-179.98	-179.93		104.29	130.70	-164.58
Glu-6	179.96	180.00	179.99		-131.76	62.08	-174.95
OctylGly-7	180.00	179.96	-179.98		-157.80	159.83	179.26
Glu-8	-179.98	NA	179.99		-85.69	NA	-174.91

Table S2. Dihedral angle values of Peptide 2.

Residues	**Initial Dihedral angles for Peptide 2**				**Dihedral angles for Peptide 2 after 200 ns MD simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
Pyrenebutyryl-1	NA	NA	NA		NA	NA	NA
Ser-2	NA	176.47	NA		NA	166.71	NA
Sar-3	-152.27	173.26	165.94		-50.33	152.98	-177.43
Ser-4	-164.81	171.66	-178.30		-147.38	142.46	173.03
Sar-5	165.95	150.75	172.31		72.34	148.54	-164.66
Glu-6	-149.76	173.25	-172.10		-75.61	133.78	172.59
OctylGly-7	-164.21	165.49	-172.07		-178.07	149.38	172.06
Glu-8	-171.08	-	177.74		-59.28	NA	176.23

Table S3. Dihedral angle values of Peptide 3.

Residues	**Initial Dihedral angles for Peptide 3**				**Dihedral angles for Peptide 3 after 200 ns MD simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
D-alpha-tocopherol succinyl-2	NA	NA	NA		NA	NA	NA
Ser-2	NA	119.18	NA		NA	150.07	NA
Sar-3	-122.25	-174.20	162.25		-66.19	-166.38	-171.80
Ser-4	-170.36	164.31	179.68		-171.50	113.25	-157.75
Sar-5	154.27	133.62	168.56		-68.99	-28.30	-176.71
Glu-6	-150.31	-175.95	-171.49		-47.40	-48.84	169.30
OctylGly-7	-179.79	179.24	178.74		-82.29	-31.28	-173.88
Glu-8	-161.37	NA	-176.14		-84.61	NA	-178.97

Table S4. Dihedral angle values of Peptide 4.

Residues	**Initial Dihedral angles for Peptide 4**				**Dihedral angles for Peptide 4 after 200 ns MD simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
OctylGly-1	NA	-179.97	NA		NA	149.49	NA
Ser-2	179.96	179.98	-179.97		-121.44	124.23	-176.10
N-Me-Leu-3	-179.97	179.99	-179.94		-101.34	128.01	-163.24
Ser-4	-180.00	-179.95	-179.94		-116.34	139.54	171.83
N-Me-Leu-5	180.00	-179.98	-179.93		-86.73	120.05	178.34
Glu-6	179.96	180.00	179.99		-108.44	164.30	-171.74
OctylGly-7	180.00	179.96	-179.98		-58.12	149.34	178.24
Glu-8	-179.98	NA	179.99		-86.48	NA	-174.97

Table S5. Dihedral angle values of Peptide 5.

Residues	**Initial Peptide 5 Dihedral angles**				**Peptide 5 Dihedral angles after 300 ns MD Simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
^{D}Ser-1	172.12	128.28	-179.30		86.68	-154.23	-172.48
Sar-2	-179.11	-102.62	174.00		83.94	-72.16	-179.93
^{D}Asp-3	109.83	89.59	169.50		71.75	32.92	-179.40
OctylGly-4	-91.46	-166.28	169.82		-113.75	5.71	-173.94
^{D}Ser-5	34.28	-176.04	149.77		146.23	-136.13	-167.59
Sar-6	-103.94	174.24	-174.36		-89.61	-165.57	-178.97
^{D}Asp-7	57.16	18.16	176.65		92.76	-147.93	-178.35
Glu-8	-76.44	-126.43	-179.75		-116.06	98.94	-176.24

Table S6. Dihedral angle values of Peptide 6.

Residues	**Initial Peptide 6 Dihedral angles**				**Peptide 6 Dihedral angles after 300 ns MD Simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
^{D}Ser-1	172.12	128.28	-179.30		74.62	65.81	-174.14
N-Me-Leu-2	-179.11	-102.62	174.00		-118.52	107.62	169.76
^{D}Asp-3	109.83	89.59	169.50		62.78	-143.96	177.02
OctylGly-4	-91.46	-166.28	169.82		-133.03	129.75	-173.41
^{D}Ser-5	34.28	-176.04	149.77		160.72	-124.12	-177.42
N-Me-Leu-6	-103.94	174.24	-174.36		-103.02	143.01	-177.36
^{D}Asp-7	57.16	18.16	176.65		73.74	-153.78	173.54
Glu-8	-76.44	-126.43	-179.75		-123.61	172.89	-176.31

Table S7. Dihedral angle values of Peptide BP-1.

Residues	**Initial BP-1 Dihedral angles**				**BP-1 Dihedral angles after 200 ns MD Simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
OctylGly-1	NA	120.06	NA		NA	143.08	NA
Ser-2	-120.06	119.97	-179.98		-102.15	110.85	-170.09
Leu-3	-119.96	119.97	-179.99		-111.58	155.90	-177.35
Ser-4	-119.95	120.00	-180.00		-89.19	139.73	-174.47
N-Me-Leu-5	-120.05	120.05	-180.00		-98.95	85.00	-163.72
Asp-6	-120.00	120.03	-179.97		-68.75	133.45	-174.62
OctylGly-7	-120.01	119.94	-179.95		-64.02	131.41	-170.98
Asp-8	-119.95	NA	-179.96		-64.66	NA	170.47

Table S8. Dihedral angle values of Peptide LPD-12.

Residues	Initial LPD-12 Dihedral angles				LPD-12 Dihedral angles after 200 ns MD Simulation		
	φ	ψ	ω		φ	ψ	ω
Ala-1	NA	-43.28	NA		NA	-52.41	NA
Orl-2	-63.83	-45.90	-175.86		-70.16	-24.72	175.17
Ala-3	-63.86	-43.40	177.92		-60.11	-47.84	158.08
Glu-4	-62.10	-42.39	179.73		-58.37	-39.77	171.79
Ala-5	-64.22	-40.36	178.89		-65.22	-30.21	-179.93
Ala-6	-64.22	-39.44	177.80		-74.19	-37.19	179.76
Glu-7	-62.65	-46.78	178.97		-67.87	-43.94	169.88
Lys-8	-61.05	-44.87	-179.10		-58.20	-45.56	176.85
Ala-9	-65.20	-42.93	-179.52		-50.63	-48.56	176.62
Ala-10	-64.66	-40.02	179.06		-69.52	-47.37	178.93
Lys-11	-62.87	-39.82	176.56		-57.07	-41.22	159.99
Tyr-12	-60.89	-45.01	177.66		-60.17	-49.29	179.40
Ala-13	-60.71	-41.58	177.45		-62.35	-36.77	170.56
Ala-14	-60.59	-44.69	177.58		-62.08	-47.56	168.78
Glu-15	-62.53	-40.44	177.06		-64.38	-45.34	-179.77
Ala-16	-64.17	-41.30	177.23		-59.70	-41.21	176.57
Ala-17	-64.55	-42.01	177.41		-62.45	-45.44	172.80
Glu-18	-58.20	-45.98	176.72		-53.55	-43.07	169.11
Lys-19	-60.12	-40.04	179.81		-61.87	-40.46	176.92
Ala-20	-65.52	-41.79	178.22		-76.78	-41.35	170.11
Ala-21	-59.40	-45.24	179.78		-56.16	-36.83	171.29
Lys-22	-65.92	-40.18	179.82		-70.40	-26.03	175.20
Ala-23	-65.20	-41.85	-178.98		-79.13	-19.0	174.03
Orl-24	-63.66	-30.17	-179.04		-75.49	-36.18	176.61
Ala-25	-72.48	NA	179.92		-75.34	NA	166.86

Table S9. Dihedral angle values of Peptide PD-1.

Residues	Initial PD-1 Dihedral angles				PD-1 Dihedral angles after 200 ns MD Simulation		
	φ	ψ	ω		φ	ψ	ω
Glu-1	NA	-47.06	NA		NA	-38.41	173.22
Glu-2	-56.97	-46.97	-180.00		-73.86	-27.24	169.02
Leu-3	-57.03	-46.94	-179.99		-66.10	-38.95	169.02
Leu-4	-57.04	-46.99	-179.98		-57.31	-39.04	169.71
Lys-5	-57.04	-46.98	-179.95		-60.69	-45.81	167.37
Gln-6	-57.03	-46.99	-179.96		-67.09	-36.07	-178.55
Ala-7	-56.94	-47.06	179.99		-57.80	-46.13	169.64
Leu-8	-56.99	-46.97	-179.97		-61.39	-47.63	176.68
Gln-9	-57.05	-46.96	-179.96		-64.06	-42.74	-179.76
Gln-10	-57.02	-46.99	-179.95		-61.43	-36.53	175.59
Ala-11	-57.01	-47.04	-179.97		-60.45	-44.65	168.63
Gln-12	-56.96	-46.99	-180.00		-64.20	-41.43	173.73
Gln-13	-56.98	-47.01	-179.99		-57.20	-49.76	167.32
Leu-14	-57.01	-47.04	-179.99		-60.42	-44.55	175.33
Leu-15	-56.97	-46.98	-179.98		-64.50	-42.55	171.35
Gln-16	-57.04	-47.00	-179.95		-50.70	-46.87	163.69
Gln-17	-56.99	-47.00	-179.96		-66.21	-39.55	-176.93
Ala-18	-56.98	-46.94	179.98		-58.20	-43.62	175.84
Gln-19	-57.06	-46.99	-179.96		-65.29	-39.80	169.39
Glu-20	-57.04	-46.94	179.98		-58.48	-50.85	168.91
Leu-21	-57.03	-47.00	-179.98		-54.06	-42.64	175.62
Ala-22	-57.01	-47.00	-179.98		-63.11	-39.15	171.70
Lys-23	-56.97	-119.99	-179.97		-58.99	-44.79	170.12
Lys-24	-120.05	NA	-179.96		-95.69	NA	-169.01

Table S10. Dihedral angle values of detergent-like Peptide A_6D.

Residues	**Initial A_6D Dihedral angles**				**A_6D Dihedral angles after 200 ns MD Simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
Ala-1	NA	51.67	NA		NA	-179.97	NA
Ala-2	-107.47	-12.74	-177.37		-179.96	179.99	-179.98
Ala-3	-79.86	177.63	171.54		-179.98	180.00	-179.94
Ala-4	-78.63	149.59	-174.91		-179.99	179.95	179.98
Ala-5	-60.55	141.99	-173.54		-180.00	179.98	-179.93
Ala-6	-79.89	137.22	175.11		-179.96	180.00	179.99
Asp-7	-62.58	NA	-177.43		-179.99	NA	-179.97

Table S11. Dihedral angle values of detergent-like Peptide A_6K.

Residues	**Initial A_6K Dihedral angles**				**A_6K Dihedral angles after 200 ns MD Simulation**		
	φ	**ψ**	**ω**		**φ**	**ψ**	**ω**
Ala-1	NA	-179.97	NA		NA	128.41	NA
Ala-2	-179.96	179.99	-179.98		-111.30	-9.85	179.89
Ala-3	-179.98	180.00	-179.94		-116.78	152.26	170.68
Ala-4	-179.99	179.95	179.98		-96.12	127.84	176.81
Ala-5	-180.00	179.98	-179.93		-54.79	152.60	166.49
Ala-6	-179.96	180.00	179.99		-51.20	129.45	-177.37
Lys-7	-179.99	NA	-179.97		-79.92	NA	-178.78

Table S12. The half-life period of BR in the presence of peptides 1-6 and OG.

Detergent used for stabilising BR	**Time taken for decaying (100% to 50%) (day)**
Peptide 1	17.18 ± 0.14 ≈17
Peptide 2	19.22 ± 0.004 ≈19
Peptide 3	1.97 ± 0.039 ≈2
Peptide 4	5.60 ± 0.02 ≈5.6
Peptide 5	0.88 ± 0.0001 ≈1
Peptide 6	24.87 ± 0.053 ≈25
OG	0.57 ± 0.001 ≈0.6

Table S13. Important parameters of detergent encased BR systems obtained from MD simulations.

BR-detergent Complexes	C^{α}-atom RMSD of BR (nm)	% Covered Area	van der Waals energy (kJ/mol)	Electrostatic energy (kJ/mol)	Total energy[a] (kJ/mol)
BR-Peptide 1	0.32±0.03	65.3±4.4	-1382.5±113.1	-3044.6±599.4	-4427.1±576.0
BR-Peptide 2	0.29±0.02	71.8±2.6	-1708.0±84.6	-1793.6±428.3	-3501.6±414.4
BR-Peptide 3	0.25±0.03	75.7±6.2	-1678.7±164.7	-2337.4±482.6	-4016.1±491.4
BR-Peptide 4	0.24±0.02	84.9±3.9	-1846.7±117.5	-2626.6±499.5	-4473.3±571.7
BR-Peptide 5	0.19±0.01	57.8±2.6	-1171.8±242.6	-928.7±564.6	-2100.5±710.1
BR-Peptide 6	0.26±0.02	89.9±1.9	-2057.3±67.2	-2913.7±518.0	-4971.0±506.3
BR-BP-1	0.21±0.02	70.8±3.1	-1384.5±215.3	-1710.0±643.9	-3094.5±825.6
BR-LPD-12	0.26±0.02	86.4±3.4	-1798.4±76.3	-2073.6±508.5	-3872.0±537.4
BR-PD-1	0.25±0.01	86.1±2.7	-1711.6±58.0	-2364.7±507.4	-4076.3±520.1
BR-A_6D	0.20±0.03	43.3±5.9	-571.6±210.5	-1487.9±1544.5	-2059.5±1557.0
BR-A_6K	0.23±0.02	53.9±4.6	-1024.0±203.3	-1229.7±425.1	-2253.7±546.2
BR-OG	0.34±0.03	89.9±4.5	-2215.6±115.1	-473.3±122.0	-2688.9±190.5

[a]Total energy= van der Waals energy+ Electrostatic energy

Table S14. Molecular interactions in Peptide 1 encased BR system.

Peptide1	**BR**	**Bond-length (Å)**	**Types of interactions**
GLU6:OE2	GLY6:H3	1.63	Hydrogen Bond; Electrostatic
GUN8:OE2	ARG7:NH1	4.25	Electrostatic
GLU6:OE1	LYS30:NZ	4.56	Electrostatic
GUN8:HNL2	GLY33:O	2.82	Hydrogen Bond
GUN8:OE1	ARG7:HH11	1.80	Hydrogen Bond
GUN8:OK	TRP10:HE1	1.76	Hydrogen Bond
GUN8:OE1	SER169:HG1	1.63	Hydrogen Bond
GLK7:O	ASN176:HD21	1.81	Hydrogen Bond
GUN8:OK	ASN176:HD22	2.32	Hydrogen Bond

Table S15. Molecular interactions in Peptide 2 encased BR system.

Peptide	BR	Bond length (Å)	Type of interactions
GUN8:OE1	LYS172:HZ3	1.56	Hydrogen Bond;Electrostatic
GLU6:OE2	LYS40:NZ	5.13	Electrostatic
GLU6:OE2	ARG225:NH1	3.64	Electrostatic
GLU6:OE1	ARG225:NH2	5.38	Electrostatic
SER2:HG	GLY73:O	1.93	Hydrogen Bond
GUN8:HN	TYR64:OH	2.51	Hydrogen Bond
GLU6:O	TRP12:HE1	1.97	Hydrogen Bond
GLK7:O	LYS40:HZ1	2.52	Hydrogen Bond
GLK7:O	LYS40:HZ2	2.31	Hydrogen Bond
SER2:O	GLY73:HN	1.91	Hydrogen Bond
SER2:O	GLN75:HE21	2.97	Hydrogen Bond
SAR5:O	TYR133:HH	1.88	Hydrogen Bond
SER2:OG	TYR150:HH	2.05	Hydrogen Bond
GUN8:OK	ASN202:HD21	2.19	Hydrogen Bond
GLU6:O	ASN202:HD22	2.54	Hydrogen Bond
PYR1	ARG175:NH2	4.44	Electrostatic
PYR1	ARG175:NH2	4.45	Electrostatic
PYR1	TYR64:HB2	2.91	Hydrophobic
PYR1	TYR64	5.90	Hydrophobic
PYR1	TYR64	4.83	Hydrophobic
PYR1	PHE88	5.00	Hydrophobic
PYR1	TYR147	4.81	Hydrophobic
PYR1	TRP80	5.52	Hydrophobic
PYR1	PHE153	5.00	Hydrophobic
PYR1	PHE153	4.96	Hydrophobic
PYR1	PHE153	5.19	Hydrophobic
PYR1	GLY72:C,O;GLY73:N	4.74	Hydrophobic
PYR1	GLY72:C,O;GLY73:N	4.19	Hydrophobic
PYR1	GLY72:C,O;GLY73:N	3.80	Hydrophobic
PYR1	GLY72:C,O;GLY73:N	5.04	Hydrophobic
PYR1	ILE140	5.19	Hydrophobic
PYR1	PRO70	5.07	Hydrophobic
PYR1	MET32	4.96	Hydrophobic
PYR1	ALA139	4.42	Hydrophobic
PYR1	VAL199	4.78	Hydrophobic
PYR1	VAL199	5.40	Hydrophobic
PYR1	ILE203	4.49	Hydrophobic

PYR1	ILE203	4.89	Hydrophobic
PYR1	ALA139	5.29	Hydrophobic
PYR1	PRO70	5.14	Hydrophobic
PYR1	LEU48	5.16	Hydrophobic
PYR1	LEU48	5.20	Hydrophobic
PYR1	ALA51	5.30	Hydrophobic
PYR1	ILE52	4.82	Hydrophobic
PYR1	ILE52	5.45	Hydrophobic
PYR1	ILE52	4.26	Hydrophobic
PYR1	ALA114	5.43	Hydrophobic
PYR1	LEU28	5.26	Hydrophobic
PYR1	ALA44	4.83	Hydrophobic
PYR1	ALA51	4.86	Hydrophobic
PYR1	ALA84	5.15	Hydrophobic
PYR1	LEU109	5.21	Hydrophobic
PYR1	ALA110	4.87	Hydrophobic
PYR1	ALA110	4.87	Hydrophobic
PYR1	ALA110	3.63	Hydrophobic
PYR1	VAL177	5.18	Hydrophobic
PYR1	VAL177	4.98	Hydrophobic
PYR1	VAL179	5.34	Hydrophobic

Table S16. Molecular interactions in Peptide 3 encased BR system.

Peptide 3	BR	Bond length (Å)	Type of interaction
GUN8:OE2	LYS41:HZ2	1.72	Hydrogen Bond;Electrostatic
SER2:HG	ALA110:O	1.90	Hydrogen Bond
GUN8:HN	THR107:OG1	2.10	Hydrogen Bond
GUN8:HNL2	LEU28:O	2.72	Hydrogen Bond
GLK7:O	GLY6:HN1	2.57	Hydrogen Bond
GLK7:O	GLY6:HN3	2.70	Hydrogen Bond
GUN8:OK	ARG7:HN	2.52	Hydrogen Bond
GUN8:OE1	TYR26:HH	1.79	Hydrogen Bond
TOC1	TYR26	5.73	Hydrophobic
TOC1	LEU123	5.38	Hydrophobic
TOC1:C16	LEU127	4.95	Hydrophobic
TOC1:C27	ALA84	4.46	Hydrophobic
TOC1:C27	LEU87	4.10	Hydrophobic
TOC1:C27	LEU123	4.92	Hydrophobic
TOC1	PRO70	4.66	Hydrophobic
TOC1	LYS129	5.48	Hydrophobic
TOC1:C17	VAL130	4.74	Hydrophobic
TOC1:C16	PRO70	4.30	Hydrophobic
TOC1:C16	VAL130	4.47	Hydrophobic
TOC1:C28	VAL130	5.10	Hydrophobic
TOC1	ILE11	5.09	Hydrophobic
TOC1	LEU15	4.76	Hydrophobic
TOC1:C16	ALA14	4.07	Hydrophobic
TOC1:C15	LEU15	4.85	Hydrophobic
TOC1:C15	ALA18	3.96	Hydrophobic
TOC1:C27	LEU15	4.89	Hydrophobic
TOC1:C28	ILE11	5.11	Hydrophobic
TOC1:C2	LEU22	4.91	Hydrophobic
TOC1	PRO186	4.83	Hydrophobic
TOC1	LEU146	4.58	Hydrophobic
TOC1	PRO186	5.42	Hydrophobic
TOC1:C17	PRO186	4.47	Hydrophobic
TOC1:C17	VAL187	4.54	Hydrophobic
TOC1:C16	LEU146	4.56	Hydrophobic
TOC1:C16	PRO186	4.34	Hydrophobic
TOC1:C15	ALA143	4.34	Hydrophobic

TOC1:C15	LEU146	5.47	Hydrophobic
TOC1:C28	PRO186	5.24	Hydrophobic
TOC1:C28	LEU190	4.41	Hydrophobic
TOC1:C29	LEU190	5.02	Hydrophobic
TOC1	ILE140	5.01	Hydrophobic
TOC1:C28	ILE117	4.92	Hydrophobic
TOC1:C28	ILE140	4.87	Hydrophobic
TOC1:C29	ILE117	5.10	Hydrophobic
TOC1:C16	ALA18	4.18	Hydrophobic
TOC1:C16	LEU22	4.63	Hydrophobic
TOC1:C15	ALA14	3.92	Hydrophobic
TOC1:C15	ALA18	4.24	Hydrophobic
TOC1:C28	LEU58	5.13	Hydrophobic
TOC1	VAL217	5.12	Hydrophobic
TOC1	LEU221	4.88	Hydrophobic
TOC1	VAL213	5.21	Hydrophobic
TOC1	VAL217	5.49	Hydrophobic
TOC1:C17	VAL217	4.98	Hydrophobic
TOC1:C17	LEU221	4.26	Hydrophobic
TOC1:C16	VAL217	4.34	Hydrophobic
TOC1:C29	LEU22	4.36	Hydrophobic
TOC1	LEU146	5.26	Hydrophobic
TOC1:C17	LEU146	5.48	Hydrophobic
TOC1:C16	LEU146	4.65	Hydrophobic
TOC1:C15	ALA143	4.14	Hydrophobic
TOC1:C15	ALA144	4.34	Hydrophobic
TOC1:C2	ALA114	4.40	Hydrophobic
TOC1:C2	LEU25	4.78	Hydrophobic
TOC1	LEU15	4.68	Hydrophobic
TOC1	ALA18	4.54	Hydrophobic
TOC1	ALA18	4.73	Hydrophobic
TOC1	LEU123	5.49	Hydrophobic
TOC1	ALA143	4.97	Hydrophobic
TOC1	LEU190	5.04	Hydrophobic
TOC1	LEU15	5.09	Hydrophobic
TOC1	LEU190	4.60	Hydrophobic
TOC1:C28	TRP12	4.81	Hydrophobic
TOC1:C29	TRP12	4.87	Hydrophobic
TOC1	TYR26	4.29	Hydrophobic
TOC1:C27	TYR26	5.07	Hydrophobic
TOC1:C17	PHE27	4.47	Hydrophobic
TOC1:C17	PHE54	4.61	Hydrophobic
TOC1:C28	PHE54	4.81	Hydrophobic
TOC1	TRP80	5.13	Hydrophobic
TOC1	TRP80	5.32	Hydrophobic
TOC1:C2	TRP80	5.21	Hydrophobic

TOC1:C28	TYR131	5.18	Hydrophobic
TOC1:C29	TYR131	4.76	Hydrophobic
TOC1:C29	PHE135	5.22	Hydrophobic
TOC1	TRP137	5.10	Hydrophobic
TOC1:C17	TRP137	5.32	Hydrophobic
TOC1:C28	TRP138	5.11	Hydrophobic
TOC1	TYR147	5.35	Hydrophobic
TOC1:C29	TRP189	5.48	Hydrophobic

Table S17. Molecular interactions in Peptide 4 encased BR system.

Peptide	BR	Bond length (Å)	Type of interaction
GLU6:OE1	LYS30:HZ1	1.72	Hydrogen Bond;Electrostatic
GUN8:OE2	GLY6:N	3.55	Electrostatic
GUN8:HNL1	TYR147:OH	2.92	Hydrogen Bond
SER2:HN	LEU224:O	3.04	Hydrogen Bond
GUN8:OE1	GLY6:HT2	1.84	Hydrogen Bond
GLK7:O	TRP10:HE1	1.95	Hydrogen Bond
GLU6:OE2	TYR26:HH	1.58	Hydrogen Bond
GLK1:O	LYS30:HZ2	1.86	Hydrogen Bond
ACE0:O	GLN105:HE21	2.97	Hydrogen Bond
ACE0:O	GLN105:HE22	3.06	Hydrogen Bond
GLK7:O	TYR131:HH	1.92	Hydrogen Bond
GLK7:O	TYR147:HH	2.80	Hydrogen Bond
GLK7:O	ARG225:HE	3.07	Hydrogen Bond
SER4:OG	ARG225:HH11	2.87	Hydrogen Bond
GLU6:O	ARG225:HH11	1.90	Hydrogen Bond
GUN8:OK	ARG225:HH12	3.04	Hydrogen Bond
GLK7:O	ARG225:HH21	2.40	Hydrogen Bond

Table S18. Molecular interactions in Peptide 5 encased BR system.

Peptide	BR	Bond Length (Å)	Type of interaction
DAS7:OD1	LYS129:HZ1	1.75	Hydrogen Bond; Electrostatic
DAS3:OD2	LYS172:HZ2	1.77	Hydrogen Bond; Electrostatic
DAS3:OD2	GLY6:N	4.76	Electrostatic
DAS7:OD2	LYS129:NZ	2.84	Electrostatic
DAS3:OD1	LYS172:NZ	4.74	Electrostatic
GON8:HI	SER59:OG	1.87	Hydrogen Bond
GON8:HI	LEU127:O	1.88	Hydrogen Bond
GON8:HX2	THR55:OG1	1.96	Hydrogen Bond
GON8:HX1	SER214:O	2.58	Hydrogen Bond
DAS3:O	TRP10:HE1	1.89	Hydrogen Bond
DAS7:O	THR67:HG1	2.90	Hydrogen Bond
GON8:O	TRP80:HE1	3.00	Hydrogen Bond
GON8:OL	LYS129:HN	2.08	Hydrogen Bond

Table S19. Molecular interactions in Peptide 6 encased BR system.

Peptide	BR	Bond Length (Å)	Type of interaction
DAS3:OD1	LYS30:HZ3	1.59	Hydrogen Bond; Electrostatic
DAS3:OD2	LYS40:HZ3	1.58	Hydrogen Bond; Electrostatic
DAS3:OD2	GLY6:N	5.52	Electrostatic
DAS3:OD2	LYS30:NZ	3.27	Electrostatic
DAS3:OD1	LYS40:NZ	4.47	Electrostatic
DAS3:OD2	ARG225:NH2	5.03	Electrostatic
GON8:HI	ASN176:OD1	1.78	Hydrogen Bond
DSN5:HN	ILE198:O	1.91	Hydrogen Bond
GON8:HX2	SER158:OG	2.00	Hydrogen Bond
GON8:HX2	SER158:O	3.06	Hydrogen Bond
GON8:HX1	SER162:OG	2.50	Hydrogen Bond
DAS7:O	GLY6:HN1	1.99	Hydrogen Bond
LEN6:O	TRP10:HE1	2.10	Hydrogen Bond
DAS3:OD2	TYR26:HH	1.60	Hydrogen Bond
GON8:OL	LYS159:HZ1	2.86	Hydrogen Bond
DAS3:OD1	ASN176:HD22	1.98	Hydrogen Bond
GON8:OE2	ARG225:HH12	1.85	Hydrogen Bond
LEN2:O	ARG225:HH22	2.09	Hydrogen Bond
DSN1:C,O;LEN2:N	TRP12	4.84	Hydrophobic

Table S20. Molecular interactions in OG encased BR system.

OG	BR	Bond Length (Å)	Type of interaction
LIG239:O5	THR67:HG1	1.91	Hydrogen Bond
LIG269:O6	TRP137:HE1	2.83	Hydrogen Bond
LIG257:O5	ARG225:HH21	2.99	Hydrogen Bond
LIG277:O6	ARG227:HE	1.93	Hydrogen Bond
LIG277:O6	ARG227:HH21	2.95	Hydrogen Bond
LIG232:H23	SER183:OG	2.94	Hydrogen Bond
LIG238:H23	GLY21:O	1.78	Hydrogen Bond
LIG239:H14	MET68:O	2.85	Hydrogen Bond
LIG241:H23	SER214:OG	1.95	Hydrogen Bond
LIG245:H23	THR55:OG1	1.91	Hydrogen Bond
LIG251:H18	TYR131:OH	2.10	Hydrogen Bond
LIG257:H18	TYR26:OH	2.47	Hydrogen Bond
LIG272:H15	LEU28:O	2.78	Hydrogen Bond
LIG272:H23	PHE27:O	2.98	Hydrogen Bond
LIG272:H23	THR47:OG1	2.04	Hydrogen Bond
LIG277:H18	ASP96:OD2	2.30	Hydrogen Bond
LIG277:H23	SER226:OG	1.90	Hydrogen Bond
LIG278:H18	SER59:OG	1.74	Hydrogen Bond
LIG300:H23	SER169:O	2.30	Hydrogen Bond
LIG261:C13	ALA44	4.08	Hydrophobic
LIG272	ALA44	4.12	Hydrophobic
LIG238:C13	ALA51	4.42	Hydrophobic
LIG260	ALA51	4.71	Hydrophobic
LIG282:C13	ALA81	4.27	Hydrophobic
LIG259	ALA84	4.65	Hydrophobic
LIG316	ALA114	4.79	Hydrophobic
LIG269	VAL136	4.50	Hydrophobic
LIG269:C13	ALA139	4.11	Hydrophobic
LIG312	ALA139	4.47	Hydrophobic
LIG295:C13	ALA143	4.03	Hydrophobic
LIG315:C13	ALA143	4.18	Hydrophobic
LIG316:C13	ALA143	4.38	Hydrophobic
LIG281	VAL177	4.86	Hydrophobic
LIG281	VAL180	4.49	Hydrophobic
LIG305:C13	ALA196	3.98	Hydrophobic

LIG314	VAL199	4.54	Hydrophobic
LIG236	ILE117	4.75	Hydrophobic
LIG237:C13	LEU146	4.65	Hydrophobic
LIG238	LEU28	5.06	Hydrophobic
LIG238:C13	LEU48	4.92	Hydrophobic
LIG239	LEU127	5.46	Hydrophobic
LIG241:C13	LEU207	5.26	Hydrophobic
LIG241:C13	VAL210	5.42	Hydrophobic
LIG241:C13	LEU211	4.88	Hydrophobic
LIG247:C13	LEU206	4.90	Hydrophobic
LIG250:C13	LEU22	5.25	Hydrophobic
LIG252:C13	LEU19	4.77	Hydrophobic
LIG254	ILE11	5.08	Hydrophobic
LIG256:C13	VAL210	4.07	Hydrophobic
LIG258	ILE117	5.20	Hydrophobic
LIG258:C13	ILE140	4.74	Hydrophobic
LIG259:C13	LEU87	4.74	Hydrophobic
LIG261	LEU92	4.39	Hydrophobic
LIG264:C13	VAL187	5.29	Hydrophobic
LIG265:C13	LEU190	4.25	Hydrophobic
LIG273:C13	LEU25	4.37	Hydrophobic
LIG277	LEU93	5.42	Hydrophobic
LIG277	LEU223	5.06	Hydrophobic
LIG277:C13	LEU48	4.53	Hydrophobic
LIG277:C13	VAL49	5.12	Hydrophobic
LIG278	LEU58	4.65	Hydrophobic
LIG282:C13	MET56	4.95	Hydrophobic
LIG286:C13	LEU58	5.18	Hydrophobic
LIG286:C13	LEU62	4.67	Hydrophobic
LIG287:C13	LEU87	4.21	Hydrophobic
LIG290:C13	ILE222	5.32	Hydrophobic
LIG294:C13	LEU149	4.81	Hydrophobic
LIG295:C13	LEU146	5.30	Hydrophobic
LIG308:C13	LEU207	4.73	Hydrophobic
LIG310:C13	ILE198	4.39	Hydrophobic
LIG318:C13	VAL213	5.48	Hydrophobic
LIG320:C13	LEU61	4.56	Hydrophobic
LIG320:C13	LEU62	5.00	Hydrophobic
LIG320	TRP10	5.38	Hydrophobic
LIG254	TRP12	4.99	Hydrophobic
LIG250	TYR26	4.65	Hydrophobic
LIG309:C13	TRP80	4.50	Hydrophobic
LIG259	TRP80	5.09	Hydrophobic
LIG282:C13	TRP80	4.13	Hydrophobic
LIG243:C13	PHE88	4.64	Hydrophobic
LIG260:C13	PHE88	5.17	Hydrophobic

LIG251	PHE135	4.32	Hydrophobic
LIG283	TRP137	4.89	Hydrophobic
LIG316	TYR147	4.67	Hydrophobic
LIG237:C13	TYR150	5.26	Hydrophobic
LIG306	TYR150	4.87	Hydrophobic
LIG294	PHE153	4.61	Hydrophobic
LIG294	PHE154	5.35	Hydrophobic
LIG306	PHE154	4.08	Hydrophobic

Table S21. Molecular interactions in BP-1 encased BR system.

Peptide	BR	Bond Length (Å)	Type of interaction
ASP6:OD2	LYS30:NZ	5.42	Electrostatic
GLK1:HN	LEU62:O	2.28	Hydrogen Bond
ASA8:HNL1	ILE198:O	2.80	Hydrogen Bond
ASP6:O	TYR64:HH	1.85	Hydrogen Bond
ASP6:O	THR107:HG1	1.69	Hydrogen Bond
LEU3:O	ASN176:HD21	1.61	Hydrogen Bond
LEN5:HB2	PHE153	2.84	Hydrophobic
LEU3:C,O;SER4:N	TYR147	4.06	Hydrophobic
LEU3	LEU62	5.42	Hydrophobic
LEU3	LEU206	5.15	Hydrophobic
LEU3	LEU221	5.25	Hydrophobic
LEU3	ALA18	4.53	Hydrophobic
LEU3	ALA114	5.26	Hydrophobic
LEU3	LYS172	5.02	Hydrophobic
LEU3	VAL177	5.46	Hydrophobic
LEU3	VAL187	4.99	Hydrophobic
LEU3	VAL210	4.76	Hydrophobic
LEU3	VAL210	5.08	Hydrophobic
LEU3	TYR147	5.17	Hydrophobic

Table S22. Molecular interactions in LPD-12 encased BR system.

Peptide	BR	Bond Length (Å)	Type of interaction
LYS11:HZ2	ASP115:OD1	1.55	Hydrogen Bond;Electrostatic
LYS19:HZ1	ASP104:OD1	1.69	Hydrogen Bond;Electrostatic
LYS22:HZ3	GLY231:OT2	1.79	Hydrogen Bond;Electrostatic
GLU4:OE2	LYS30:HZ1	1.81	Hydrogen Bond;Electrostatic
GLU7:OE2	LYS30:HZ2	2.89	Hydrogen Bond;Electrostatic
GLU7:OE1	LYS30:HZ3	1.76	Hydrogen Bond;Electrostatic
GLU7:OE2	ARG225:HH12	1.80	Hydrogen Bond;Electrostatic
GLU4:OE1	LYS129:NZ	4.02	Electrostatic
GLU4:OE2	ARG225:NH2	4.72	Electrostatic
GLU7:OE1	ARG225:NH2	3.02	Electrostatic
LYS8:HZ1	THR67:OG1	2.14	Hydrogen Bond
LYS8:HZ1	MET68:O	2.67	Hydrogen Bond
LYS8:HZ2	MET68:O	2.21	Hydrogen Bond
LYS11:HZ2	LYS11:HZ2	2.51	Hydrogen Bond
TYR12:HH	TYR12:HH	1.58	Hydrogen Bond
ORL24:HE	TYR150:OH	2.78	Hydrogen Bond
ALN25:HNL2	SER158:O	2.13	Hydrogen Bond
GLU4:OE2	TYR26:HH	1.89	Hydrogen Bond
ALA23:O	THR55:HG1	1.96	Hydrogen Bond
ORL24:OI	GLY65:HN	2.39	Hydrogen Bond
ORL24:OI	LEU66:HN	1.88	Hydrogen Bond
ALA13:O	GLY106:HN	2.06	Hydrogen Bond
ORL24:O	LYS159:HZ1	2.14	Hydrogen Bond
ALA23:O	SER162:HG	1.73	Hydrogen Bond
TYR12	TYR131	5.99	Hydrophobic
ALA5	VAL136	4.96	Hydrophobic
ALA1	LEU25	5.01	Hydrophobic
ALA16	ILE11	4.82	Hydrophobic

ALA9	VAL124	5.09	Hydrophobic
ALA13	LEU123	4.93	Hydrophobic
ALA13	LEU127	5.43	Hydrophobic
ALA6	LEU190	5.10	Hydrophobic
ALA6	ILE191	5.28	Hydrophobic
ALA10	ILE191	4.38	Hydrophobic
ALA10	ILE198	4.57	Hydrophobic
ALA10	VAL199	4.73	Hydrophobic
ALA13	ILE203	5.22	Hydrophobic
ALA17	ILE203	4.36	Hydrophobic
ALA17	LEU206	5.43	Hydrophobic
ALA3	VAL217	4.87	Hydrophobic
ALA3	LEU221	5.01	Hydrophobic
ALA6	LEU19	4.95	Hydrophobic
LYS19	LEU48	5.38	Hydrophobic
ALA23	LEU48	5.05	Hydrophobic
ALA23	ALA51	3.91	Hydrophobic
ALA13	LEU146	4.50	Hydrophobic
ALA14	LEU146	5.30	Hydrophobic
ALA17	LEU146	4.71	Hydrophobic
ALA20	ILE229	5.05	Hydrophobic
TYR12	LEU15	5.31	Hydrophobic
ALA1	TYR26	3.57	Hydrophobic
ALN25:CB	TYR64	4.16	Hydrophobic
ALA17	TRP80	4.12	Hydrophobic
ALA21	TRP80	5.06	Hydrophobic
ALA14	TRP80	4.91	Hydrophobic
ALA17	TRP80	4.03	Hydrophobic
LYS22	PHE88	5.24	Hydrophobic
ALA1	TYR133	5.45	Hydrophobic
ALA5	TYR133	5.01	Hydrophobic
ALA6	TYR147	4.32	Hydrophobic
ALA9	TYR147	4.89	Hydrophobic
ALA9	TYR150	4.22	Hydrophobic

Table S23. Molecular interactions in PD-1 encased BR system.

Peptide	BR	Bond Length (Å)	Type of interaction
LYS23:HZ2	ASP96:OD2	1.93	Hydrogen Bond;Electrostatic
LYA24:HZ2	ASP38:OD2	1.82	Hydrogen Bond;Electrostatic
LYS23:NZ	ASP102:OD2	2.95	Electrostatic
GLU1:OE1	GLY6:N	4.22	Electrostatic
GLU1:OE1	LYS30:NZ	5.11	Electrostatic
GLN13:HE22	THR128:OG1	1.74	Hydrogen Bond
GLN6:HE22	GLY113:O	2.72	Hydrogen Bond
GLN13:HE22	GLY113:O	2.39	Hydrogen Bond
GLU2:OE1	GLY72:HN	2.04	Hydrogen Bond
GLU2:OE2	GLY73:HN	2.17	Hydrogen Bond
GLU1:OE2	TYR79:HH	1.57	Hydrogen Bond
GLU1:OE1	TYR131:HN	1.65	Hydrogen Bond
GLU2:O	SER132:HG	3.01	Hydrogen Bond
GLN9:OE1	ARG225:HH12	1.78	Hydrogen Bond
GLN9:OE1	ARG225:HH22	2.30	Hydrogen Bond
ALA7	ILE11	4.90	Hydrophobic
ALA7	LEU15	4.03	Hydrophobic
LEU3	LEU206	5.47	Hydrophobic
LEU3	LEU207	4.76	Hydrophobic
LEU4	LEU207	5.34	Hydrophobic
ALA7	VAL199	4.05	Hydrophobic
LEU8	ILE191	5.35	Hydrophobic
ALA11	ILE191	4.68	Hydrophobic
ALA11	ILE198	4.24	Hydrophobic
ALA11	VAL199	5.13	Hydrophobic
LEU4	LEU190	5.06	Hydrophobic
ALA7	ALA196	3.65	Hydrophobic
LEU4	LEU25	4.71	Hydrophobic
ALA7	LEU22	4.29	Hydrophobic
LEU8	LEU22	4.94	Hydrophobic
ALA11	LEU19	5.02	Hydrophobic
ALA11	LEU22	5.22	Hydrophobic
LEU15	MET209	5.31	Hydrophobic
ALA22	ILE203	5.33	Hydrophobic
ALA22	LEU206	5.05	Hydrophobic

LEU4	MET32	5.04	Hydrophobic
ALA7	MET32	5.37	Hydrophobic
LEU8	MET32	4.29	Hydrophobic
ALA11	LEU28	5.12	Hydrophobic
ALA18	LEU58	4.89	Hydrophobic
LEU21	LEU58	5.43	Hydrophobic
ALA22	LEU61	5.18	Hydrophobic
LYS5	LEU109	5.32	Hydrophobic
ALA7	PRO165	4.46	Hydrophobic
ALA11	PRO165	5.08	Hydrophobic
LYS23	LYS41	4.37	Hydrophobic
LYS23	ILE45	5.46	Hydrophobic
LEU3	ALA14	4.69	Hydrophobic
LEU4	ALA18	3.91	Hydrophobic
LEU4	VAL29	5.00	Hydrophobic
LEU8	PRO165	5.34	Hydrophobic
LEU14	LYS172	5.39	Hydrophobic
LEU4	ALA184	5.02	Hydrophobic
LEU4	VAL187	5.31	Hydrophobic
LEU4	ALA196	5.20	Hydrophobic
LEU3	VAL210	4.94	Hydrophobic
LEU15	VAL210	5.34	Hydrophobic
LEU8	VAL217	5.33	Hydrophobic
LEU14	TRP12	5.45	Hydrophobic
ALA11	TRP12	4.36	Hydrophobic
LEU14	TRP12	5.47	Hydrophobic
LYS5	TYR26	4.74	Hydrophobic
ALA18	PHE54	4.81	Hydrophobic

Table S24. Molecular interactions in A_6D encased BR system.

Peptide	BR	Bond Length (Å)	Type of interaction
ASP7:OD1	LYS40:HZ1	1.84	Hydrogen Bond; Electrostatic
ASP7:OD1	LYS129:HZ3	1.67	Hydrogen Bond; Electrostatic
ASP7:OD1	LYS172:NZ	4.71	Electrostatic
ALA4:HN	ASN176:O	1.99	Hydrogen Bond
ALA1:HN	THR55:OG1	1.84	Hydrogen Bond
ALA6:HN	LEU127:O	1.86	Hydrogen Bond
ALA1:HN	SER59:OG	2.89	Hydrogen Bond
ALA2:HN	SER59:OG	2.00	Hydrogen Bond
ALA3:O	TRP10:HN	2.73	Hydrogen Bond
ALA4:O	TYR64:HH	1.76	Hydrogen Bond
ALA6:O	LYS129:HN	2.72	Hydrogen Bond
ALA1:O	TYR147:HH	1.80	Hydrogen Bond
ASP7:OT2	LYS172:HZ3	1.72	Hydrogen Bond
ALA6:O	ASN176:HD22	1.98	Hydrogen Bond
ALA6:O	ARG225:HH12	2.08	Hydrogen Bond
ASP7:OT1	ARG225:HH12	2.72	Hydrogen Bond
ALA1:C,O;ALA2:N	TYR64	5.00	Hydrophobic
ALA2	ALA184	3.39	Hydrophobic
ALA2	VAL188	5.04	Hydrophobic
ALA2	LEU207	4.39	Hydrophobic
ALA3	VAL180	4.11	Hydrophobic
ALA3	ALA184	4.31	Hydrophobic
ALA5	VAL180	4.48	Hydrophobic
ALA2	LEU15	4.52	Hydrophobic
ALA2	LEU19	4.96	Hydrophobic
ALA2	MET209	4.91	Hydrophobic
ALA3	VAL210	4.41	Hydrophobic
ALA3	VAL213	4.12	Hydrophobic
ALA5	VAL217	4.94	Hydrophobic
ALA5	LEU221	4.69	Hydrophobic
ALA1	VAL177	4.34	Hydrophobic
ALA3	VAL177	4.64	Hydrophobic
ALA4	VAL179	4.33	Hydrophobic
ALA4	VAL180	4.85	Hydrophobic
ALA1	LEU58	5.09	Hydrophobic

ALA2	ALA51	4.12	Hydrophobic
ALA4	ALA44	4.06	Hydrophobic
ALA5	MET32	4.47	Hydrophobic
ALA5	LYS40	4.65	Hydrophobic
ALA5	VAL69	4.18	Hydrophobic
ALA5	LYS129	4.66	Hydrophobic
ALA6	VAL124	4.40	Hydrophobic
ALA6	LEU127	5.42	Hydrophobic
ALA4	ILE52	4.99	Hydrophobic
ALA1	LEU109	4.28	Hydrophobic
ALA2	ALA110	3.89	Hydrophobic
ALA2	LEU206	4.49	Hydrophobic
ALA2	VAL210	5.23	Hydrophobic
ALA4	LEU206	5.33	Hydrophobic
ALA4	ILE198	3.88	Hydrophobic
ALA5	ILE191	4.86	Hydrophobic
ALA5	ILE198	4.89	Hydrophobic
ALA1	VAL151	3.99	Hydrophobic
ALA2	LEU58	5.35	Hydrophobic
ALA2	LEU61	4.37	Hydrophobic
ALA2	LEU62	4.39	Hydrophobic
ALA1	PRO77	4.59	Hydrophobic
ALA4	ARG7	3.68	Hydrophobic
ALA1	ALA14	4.36	Hydrophobic
ALA1	LEU61	5.24	Hydrophobic
ALA3	ILE11	4.34	Hydrophobic
ALA3	ALA14	4.30	Hydrophobic
ALA3	LEU15	4.88	Hydrophobic
ALA3	ALA3	5.37	Hydrophobic
ALA4	ALA4	4.28	Hydrophobic
ALA4	ALA4	4.83	Hydrophobic
ALA1	ALA1	4.88	Hydrophobic
ALA2	ALA2	4.46	Hydrophobic
ALA3	ALA3	4.29	Hydrophobic
ALA1	ALA1	5.03	Hydrophobic
ALA2	ALA2	4.69	Hydrophobic
ALA3	ALA3	5.46	Hydrophobic
ALA3	ALA3	4.58	Hydrophobic

Table S25. Molecular interactions in A_6K encased BR system.

Peptide	BR	Bond Length (Å)	Type of interactions
LYA7:HZ2	ASP115:OD1	1.78	Hydrogen Bond;Electrostatic
LYA7:HZ3	ASP96:OD1	1.64	Hydrogen Bond;Electrostatic
LYA7:HZ3	GLU74:OE1	1.85	Hydrogen Bond;Electrostatic
LYA7:HZ3	VAL112:O	1.83	Hydrogen Bond
ALA1:HN	GLY21:O	2.26	Hydrogen Bond
ALA6:HN	SER183:OG	1.89	Hydrogen Bond
ALA3:HN	ALA44:O	2.72	Hydrogen Bond
LYA7:HNL1	ALA143:O	2.96	Hydrogen Bond
ALA3:HN	ALA110:O	2.09	Hydrogen Bond
ALA1:HN	SER214:OG	2.00	Hydrogen Bond
LYA7:HNL2	SER158:OG	1.99	Hydrogen Bond
ALA4:O	LYS129:HN	2.34	Hydrogen Bond
ACE0:O	TYR147:HH	1.85	Hydrogen Bond
ALA6:O	ARG225:HH12	2.50	Hydrogen Bond
ALA6:O	ARG225:HH22	1.73	Hydrogen Bond
ALA2:HA	PHE54	2.93	Hydrophobic
ALA1	LEU207	4.68	Hydrophobic
ALA3	VAL180	4.89	Hydrophobic
ALA3	ALA184	4.15	Hydrophobic
ALA4	LEU181	5.45	Hydrophobic
ALA4	VAL210	5.23	Hydrophobic
ALA4	LEU211	5.19	Hydrophobic
ALA1	LEU87	4.39	Hydrophobic
ALA2	ILE52	5.05	Hydrophobic
ALA2	MET56	5.39	Hydrophobic
ALA3	ILE52	3.83	Hydrophobic
ALA1	VAL180	4.75	Hydrophobic
ALA1	LEU181	4.60	Hydrophobic
ALA3	VAL173	4.78	Hydrophobic
ALA1	LEU25	4.72	Hydrophobic
ALA3	ALA51	4.44	Hydrophobic
ALA6	ALA51	4.32	Hydrophobic
ALA2	VAL173	4.44	Hydrophobic
ALA6	PRO165	3.71	Hydrophobic

ALA5	VAL136	4.38	Hydrophobic
ALA5	ALA139	4.39	Hydrophobic
ALA3	VAL179	4.70	Hydrophobic
ALA3	VAL180	5.39	Hydrophobic
ALA6	VAL187	4.89	Hydrophobic
ALA2	LEU48	4.51	Hydrophobic
ALA3	ALA44	4.35	Hydrophobic
ALA5	LYS41	4.52	Hydrophobic
ALA5	ALA44	3.75	Hydrophobic
ALA5	ILE45	4.67	Hydrophobic
ALA6	LYS41	5.17	Hydrophobic
ALA1	ALA144	3.95	Hydrophobic
ALA2	ALA110	4.12	Hydrophobic
ALA2	ALA114	4.14	Hydrophobic
ALA1	LEU66	5.03	Hydrophobic
ALA1	PRO77	4.39	Hydrophobic
ALA2	ARG7	4.79	Hydrophobic
ALA5	MET68	5.19	Hydrophobic
ALA5	PRO77	3.68	Hydrophobic
ALA4	ALA18	4.28	Hydrophobic
ALA2	VAL217	4.12	Hydrophobic
ALA2	LEU221	5.13	Hydrophobic
ALA4	VAL217	4.26	Hydrophobic
ALA6	LEU19	5.33	Hydrophobic
ALA6	LEU22	4.13	Hydrophobic
ALA6	LYS159	4.69	Hydrophobic
ALA3	PHE54	4.39	Hydrophobic
ALA5	TYR64	4.10	Hydrophobic
ALA1	TYR79	5.21	Hydrophobic
ALA3	PHE88	3.94	Hydrophobic
ALA5	PHE88	4.54	Hydrophobic
ALA1	TYR133	4.04	Hydrophobic
ALA6	TYR133	5.26	Hydrophobic
ALA1	TRP137	4.58	Hydrophobic
ALA1	TRP137	5.45	Hydrophobic
ALA1	TYR147	4.10	Hydrophobic
ALA4	TYR150	4.86	Hydrophobic
ALA5	TYR150	3.83	Hydrophobic
ALA2	TYR150	4.54	Hydrophobic
ALA5	PHE156	4.55	Hydrophobic