Supporting Information for

Mapping the sequence–structure relationships of simple cyclic hexapeptides

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To verify that 100 ns BE-META simulation was sufficient to provide converged structural descriptions of the CPs studied, two sets of simulations were performed for all 27 CPs starting from two different initial configurations, S1 and S2 (structure 1 and structure 2). These two sets of simulations were used to monitor simulation convergence. To describe the convergence behavior of each set of BE-META simulations, we monitored the overlap of probability density with the final converged reference results as a function of simulation time. The normalized integrated product (NIP)[1] of the population densities in the 2D principal subspace is calculated as:

$$\text{NIP} = \frac{2\sum_i \rho_i \rho_{i,ref}}{\sum_i \rho_i^2 + \sum_i \rho_{i,ref}^2}$$

where ρ_{i} and $\rho_{\text{i,ref}}$ are the population density of grid point *i* and its reference value, respectively. The summation is over all the grid points in the 3D principal subspace. The NIP value ranges from 0 (no overlap) to 1 (perfect overlap). For each S1 simulation, the population density calculated from the last 25 ns of the S2 simulation was used as the reference, and vice versa.

Table S1. **(A)** G_nA_{6-n} and **(B)** G_nV_{6-n} cyclic hexapeptides. Populations and turn types are shown for the top 3 most populated conformations. Residues forming type I, I', II, II' β turns are colored red, orange, green, and blue respectively; γ turn is colored cyan.

(A) G_nA_{6-n}

G_6		G_5A_1		G_4A_2					
GGGGGG		AGGGGG (A−1)		AAGGGG (A−2)		AGAGGG (A−3)		AGGAGG (A−4)	
32.5±0.3	GGGGGG	20.9±0.3	AGGGGG	16.8±0.3	AAGGGG	15.1±0.4	AGAGGG	31.6±0.4	AGGAGG
20.8±0.4	GGGGGG	10.7±0.2	AGGGGG	15.5±0.2	AAGGGG	9.3±0.3	AGAGGG	20.8±0.2	AGGAGG
19.2±0.2	GGGGGG	8.7±0.4	AGGGGG	12.3±0.2	AAGGGG	8.2±0.2	AGAGGG	9.8±0.1	AGGAGG

G_3A_3							
AAAGGG (A−5)		AAGAGG (A−6)		AAGGAG (A−7)		AGAGAG (A−8)	
16.5±0.2	AAAGGG	25.0±0.2	AAGAGG	19.6±0.5	AAGGAG	41.4±0.4	AGAGAG
12.6±0.2	AAAGGG	11.6±0.1	AAGAGG	10.7±0.4	AAGGAG	20.8±0.3	AGAGAG
8.0±0.3	AAAGGG	5.8±0.2	AAGAGG	8.0±0.1	AAGGAG	5.4±0.2	AGAGAG

G_2A_4						G_1A_5		A_6	
AAAAGG (A−9)		AAAGAG (A−10)		AAGAAG (A−11)		AAAAAG (A−12)		AAAAAA (A−13)	
21.3±0.3	AAAAGG	26.6±0.2	AAAGAG	28.4±0.3	AAGAAG	19.0±0.4	AAAAAG	22.5±0.3	AAAAAA
16.6±0.3	AAAAGG	17.5±0.3	AAAGAG	7.2±0.3	AAGAAG	13.5±0.2	AAAAAG	20.5±0.3	AAAAAA
11.9±0.3	AAAAGG	8.4±0.2	AAAGAG	3.5±0.1	AAGAAG	13.3±0.2	AAAAAG	15.4±0.2	AAAAAA

(B) G_nV_{6-n}

G_6		G_5V_1		G_4V_2					
GGGGGG		VGGGGG (V−1)		VVGGGG (V−2)		VGVGGG (V−3)		VGGVGG (V−4)	
32.5±0.3	GGGGGG	38.5±0.3	VGGGGG	18.7±0.3	VVGGGG	14.7±0.2	VGVGGG	45.6±0.6	VGGVGG
20.8±0.4	GGGGGG	9.8±0.3	VGGGGG	10.0±0.4	VVGGGG	12.2±0.2	VGVGGG	9.2±0.2	VGGVGG
19.2±0.2	GGGGGG	7.8±0.3	VGGGGG	8.8±0.2	VVGGGG	8.3±0.2	VGVGGG	7.3±0.2	VGGVGG

G_3V_3							
VVVGGG (V−5)		VVGVGG (V−6)		VVGGVG (V−7)		VGVGVG (V−8)	
29.7±0.6	VVVGGG	37.2±0.2	VVGVGG	81.8±0.4	VVGGVG	36.0±0.3	VGVGVG
15.5±0.2	VVVGGG	21.9±0.4	VVGVGG	1.3±0.1	VVGGVG	10.5±0.3	VGVGVG
10.2±0.1	VVVGGG	5.0±0.1	VVGVGG	0.3±0.1	VVGGVG	5.2±0.2	VGVGVG

G_2V_4						G_1V_5		V_6	
VVVVGG (V−9)		VVVGVG (V−10)		VVGVVG (V−11)		VVVVVG (V−12)		VVVVVV (V−13)	
47.3±0.4	VVVVGG	47.6±0.3	VVVGVG	34.5±0.4	VVGVVG	18.7±0.4	VVVVVG	22.3±0.2	VVVVVV
33.2±0.2	VVVVGG	7.9±0.1	VVVGVG	8.7±0.3	VVGVVG	14.5±0.1	VVVVVG	17.6±0.3	VVVVVV
0.7±0.1	VVVVGG	6.2±0.2	VVVGVG	7.9±0.2	VVGVVG	14.1±0.3	VVVVVG	11.7±0.1	VVVVVV

Table S2. Cumulative variance associated to the first three eigenvectors of **(A)** G_nA_{6-n} and **(B)** G_nV_{6-n} cyclic hexapeptides.

(A)

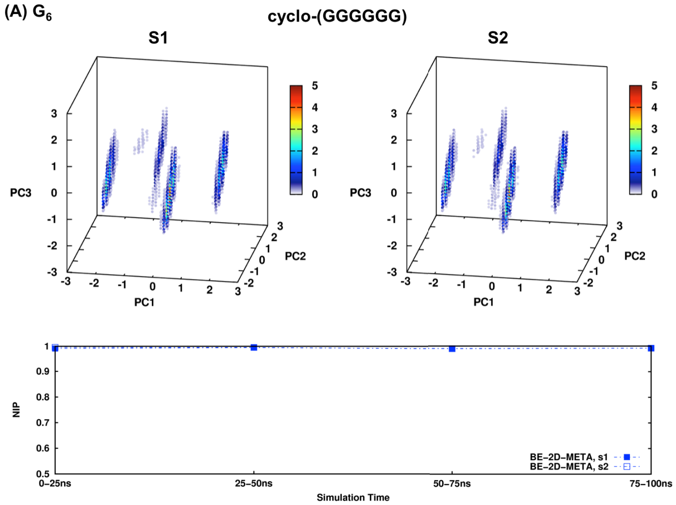
Sequence	% Variance of first 3 PC's
GGGGGG	65.8
AGGGGG	53.0
AAGGGG	60.6
AGAGGG	59.5
AGGAGG	63.5
AAAGGG	64.5
AAGAGG	59.8
AAGGAG	63.6
AGAGAG	59.7
AAAAGG	64.7
AAAGAG	68.5
AAGAAG	68.4
AAAAAG	64.0
AAAAAA	71.4

(B)

Sequence	% Variance of first 3 PC's
GGGGGG	65.8
VGGGGG	56.9
VVGGGG	63.5
VGVGGG	64.1
VGGVGG	58.5
VVVGGG	63.9
VVGVGG	61.3
VVGGVG	65.5
VGVGVG	58.1
VVVVGG	67.0
VVVGVG	68.6
VVGVVG	65.9
VVVVVG	62.4
VVVVVV	64.2

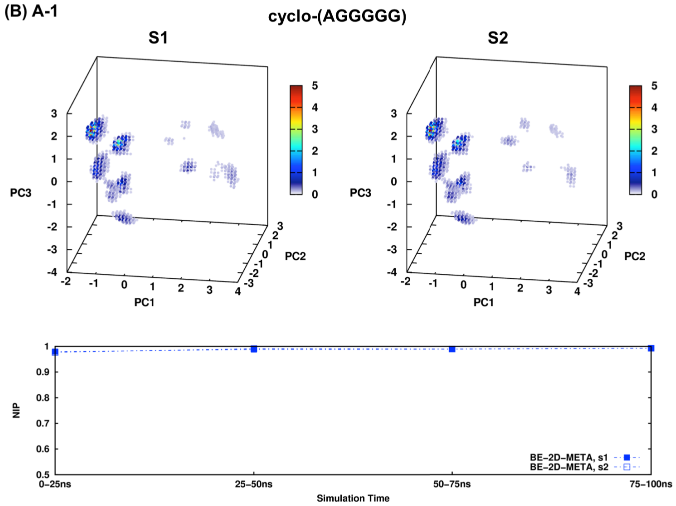
(A) G_6

cyclo-(GGGGGG)



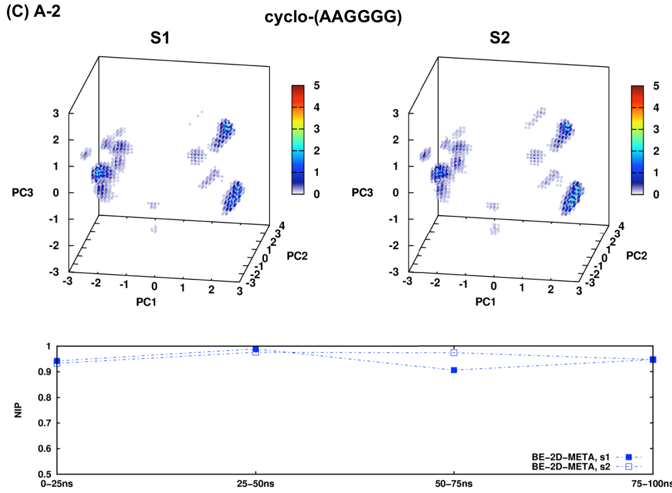
(B) A-1

cyclo-(AGGGGG)



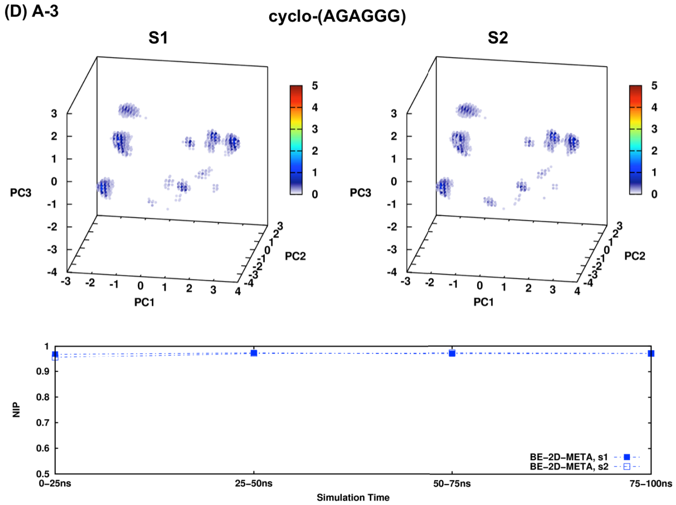
(C) A-2

cyclo-(AAGGGG)



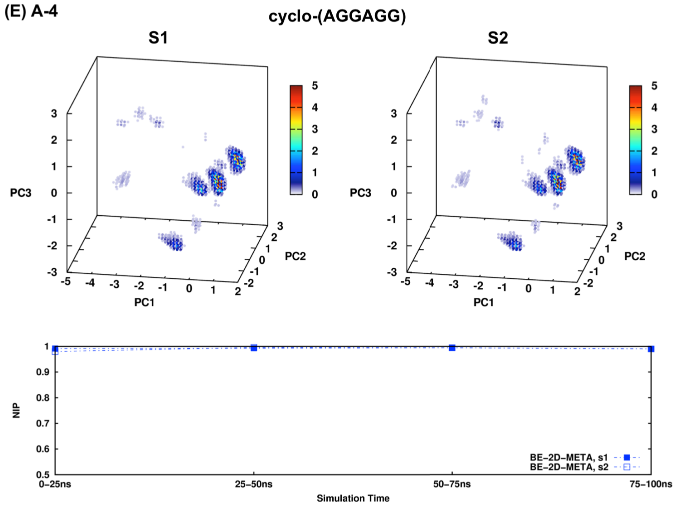
(D) A-3

cyclo-(AGAGGG)



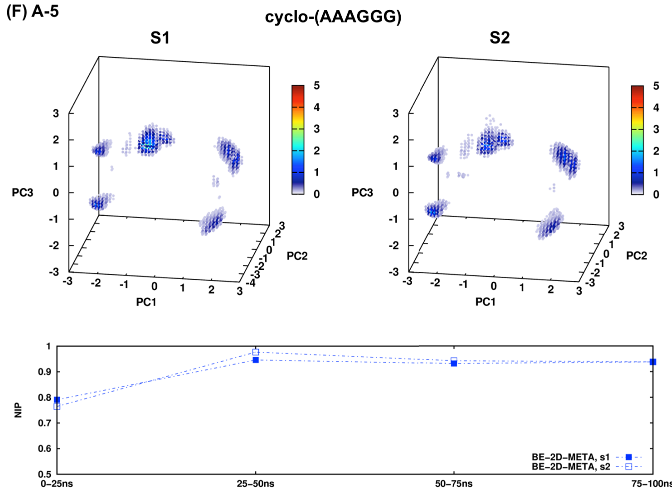
(E) A-4

cyclo-(AGGAGG)



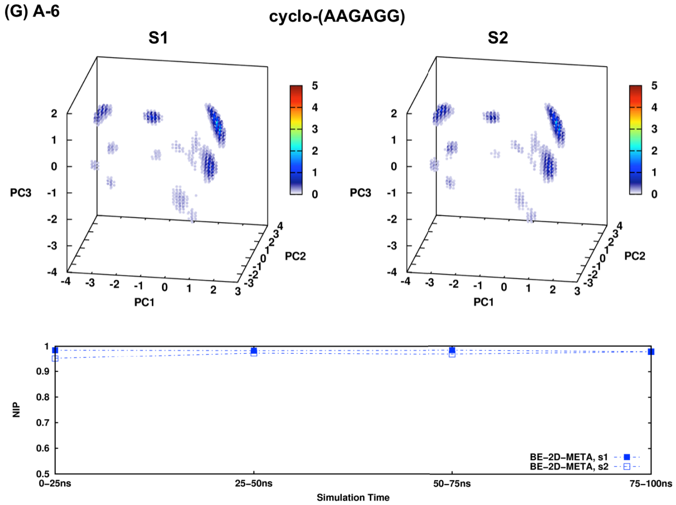
(F) A-5

cyclo-(AAAGGG)



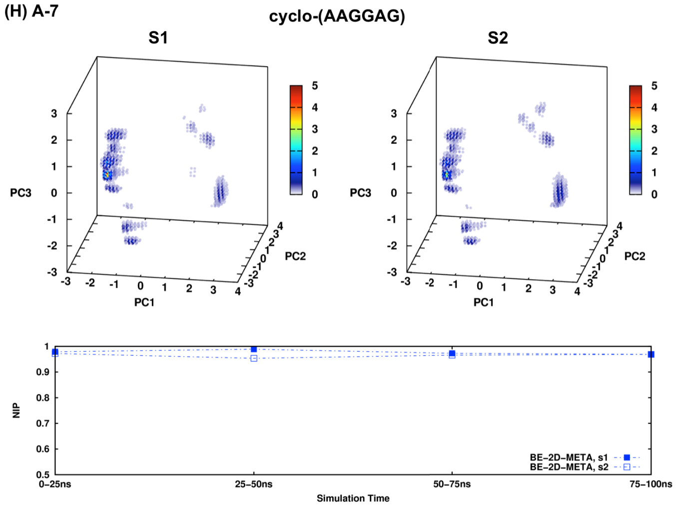
(G) A-6

cyclo-(AAGAGG)



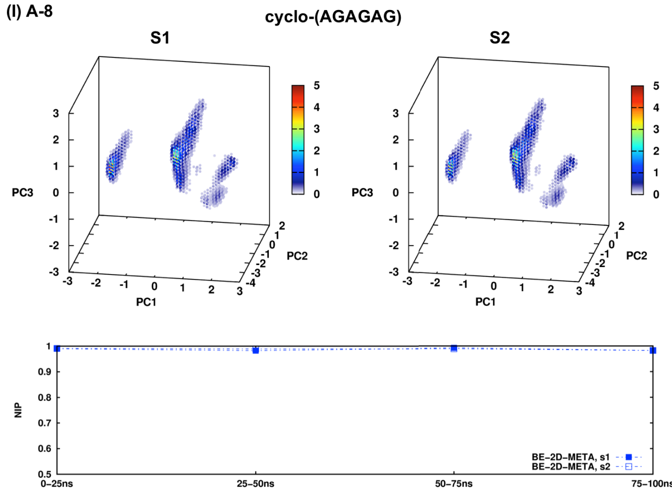
(H) A-7

cyclo-(AAGGAG)

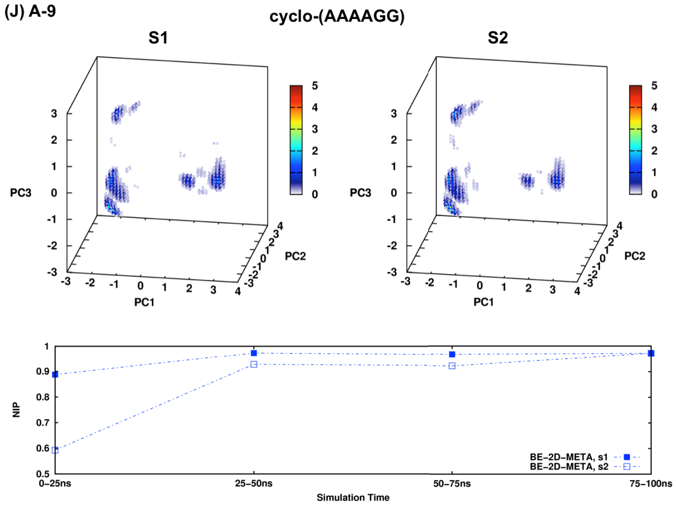


(I) A-8

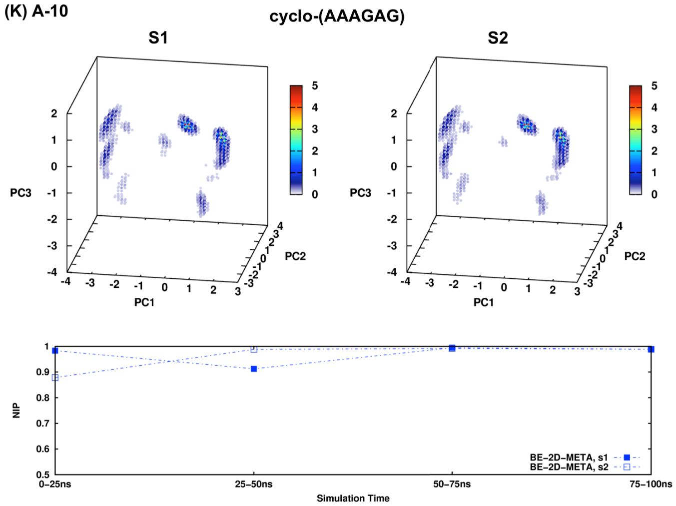
cyclo-(AGAGAG)



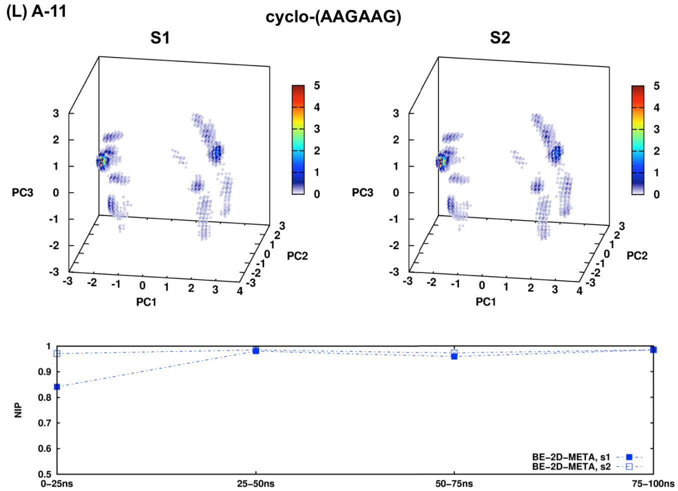
(J) A-9 cyclo-(AAAAGG)



(K) A-10 cyclo-(AAAGAG)



(L) A-11 cyclo-(AAGAAG)



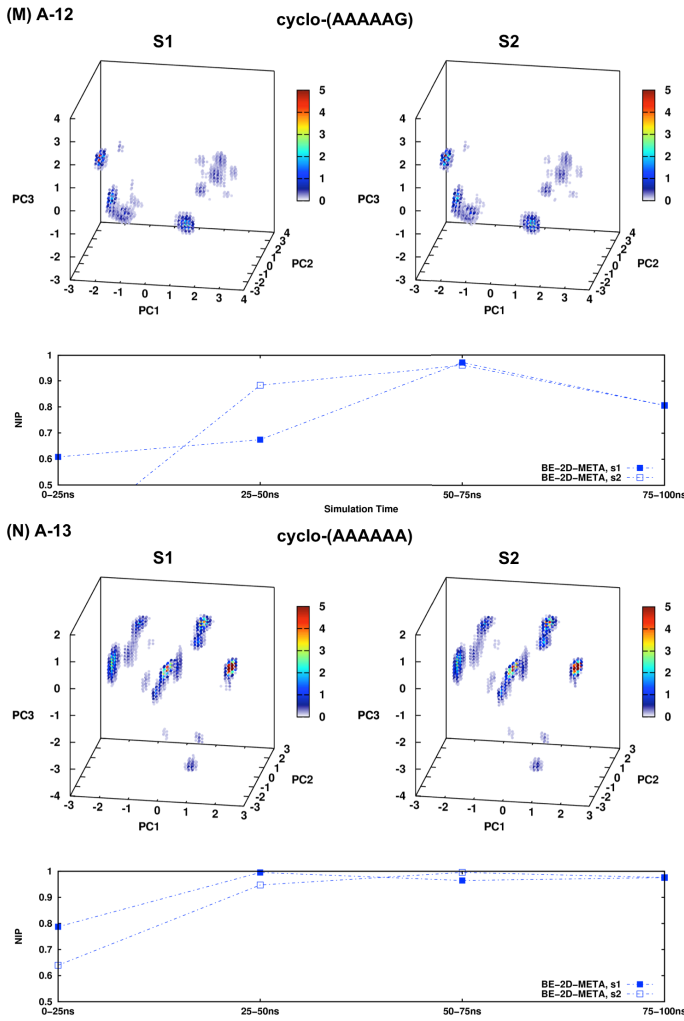
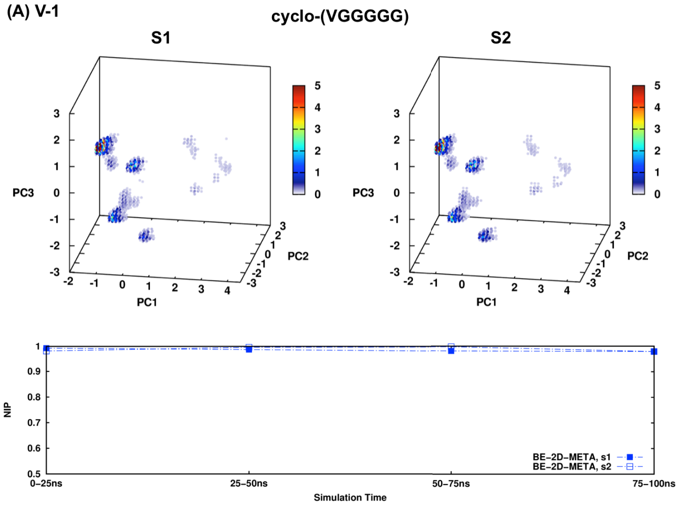


Figure S1. Conformational density profiles as a function of the first three largest principal components for S1 and S2, along with the NIP figures of all $G_nA_{6\text{-}n}$ cyclic hexapeptides (**A-N**).

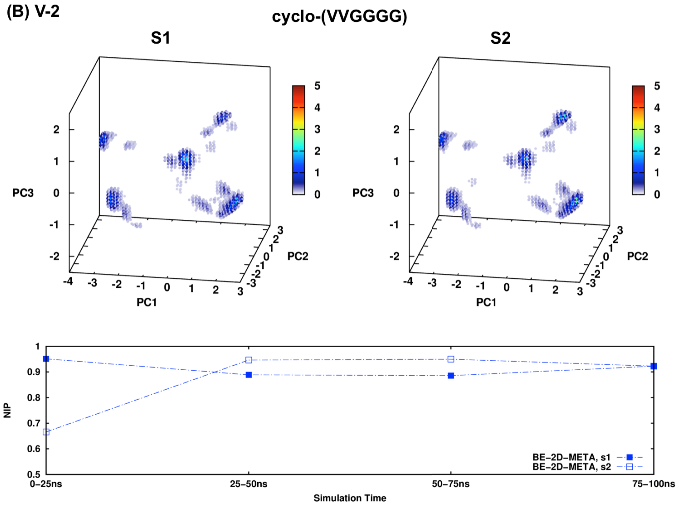
(A) V-1

cyclo-(VGGGGG)



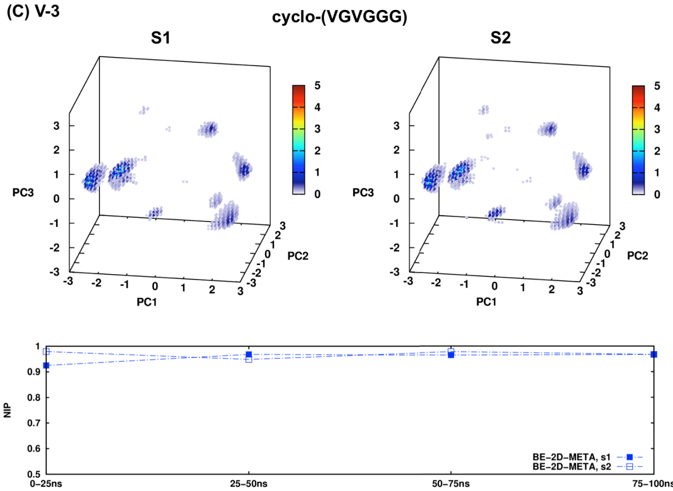
(B) V-2

cyclo-(VVGGGG)



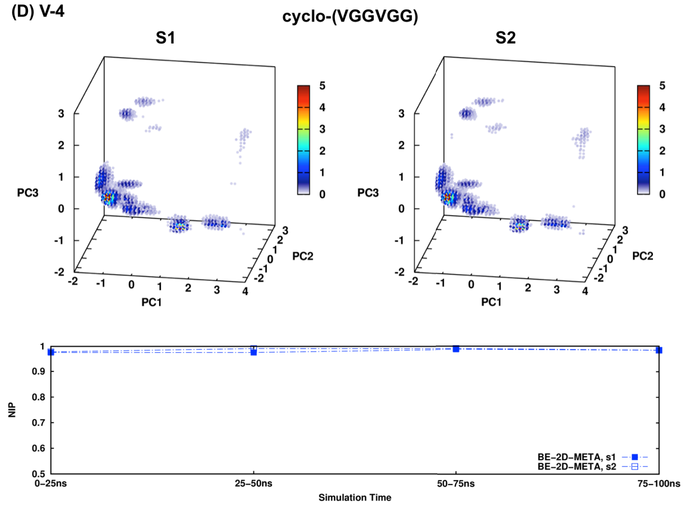
(C) V-3

cyclo-(VGVGGG)



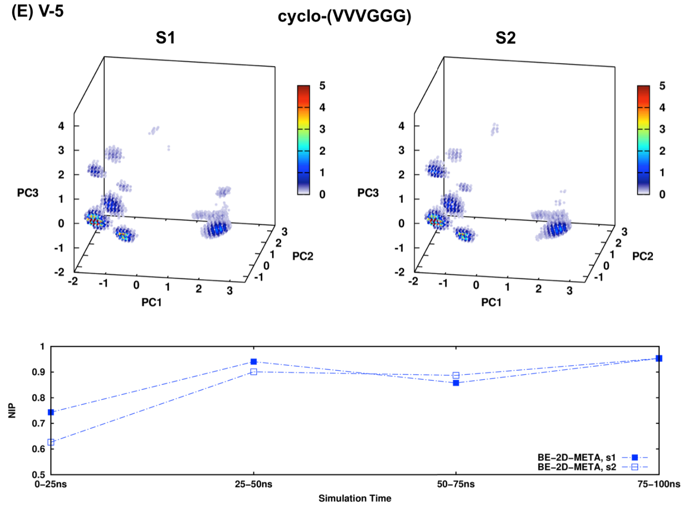
(D) V-4

cyclo-(VGGVGG)



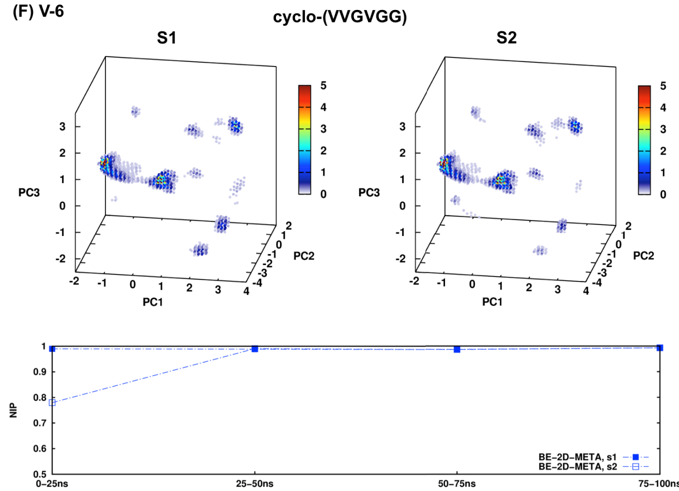
(E) V-5

cyclo-(VVVGGG)



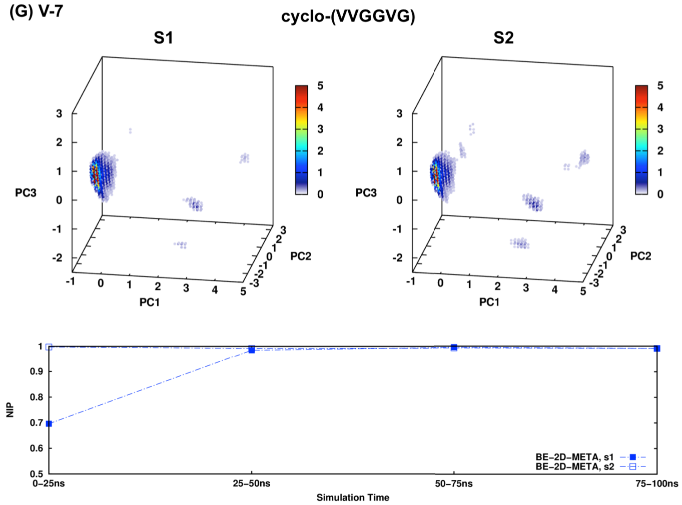
(F) V-6

cyclo-(VVGVGG)



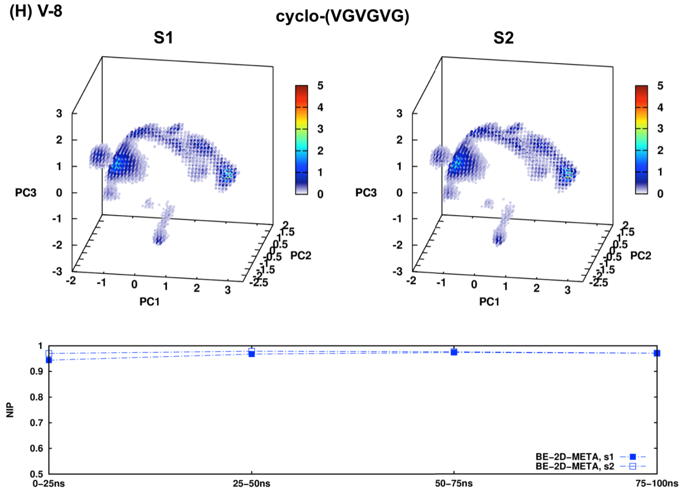
(G) V-7

cyclo-(VVGGVG)



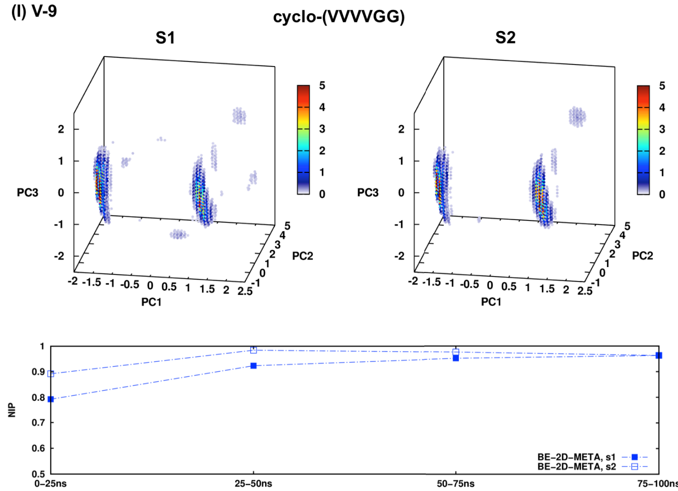
(H) V-8

cyclo-(VGVGVG)



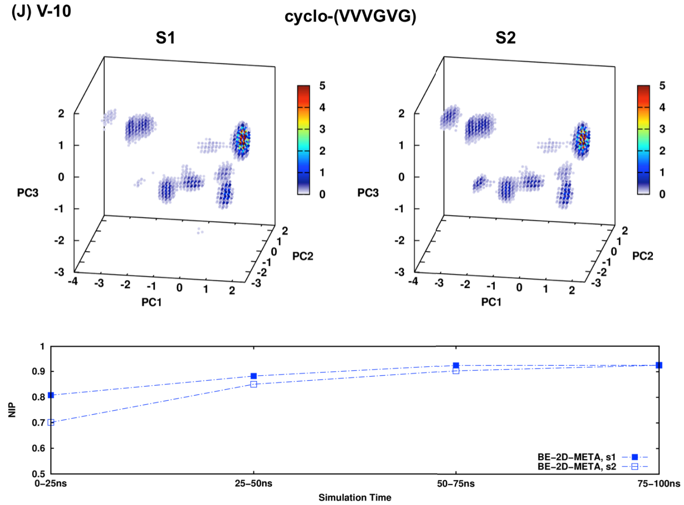
(I) V-9

cyclo-(VVVVGG)



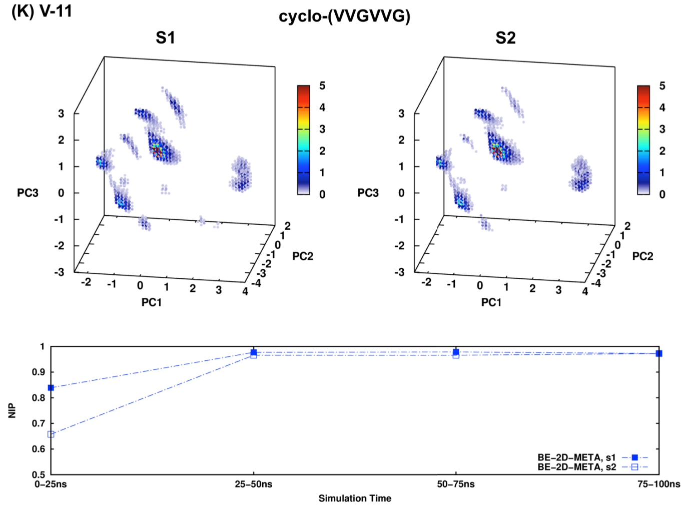
(J) V-10

cyclo-(VVVGVG)



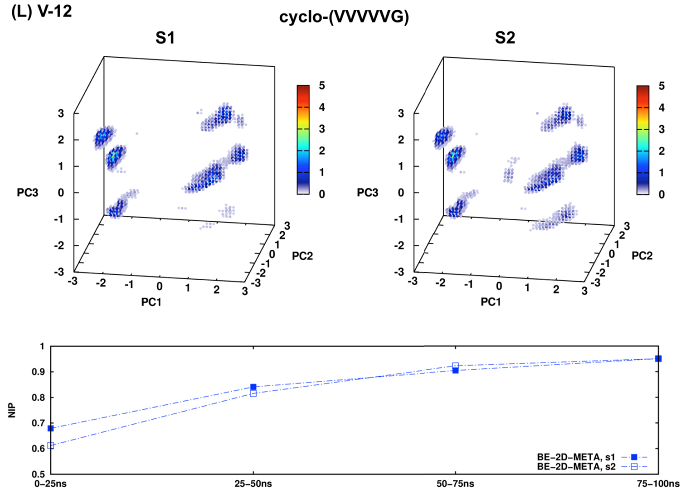
(K) V-11

cyclo-(VVGVVG)



(L) V-12

cyclo-(VVVVVG)



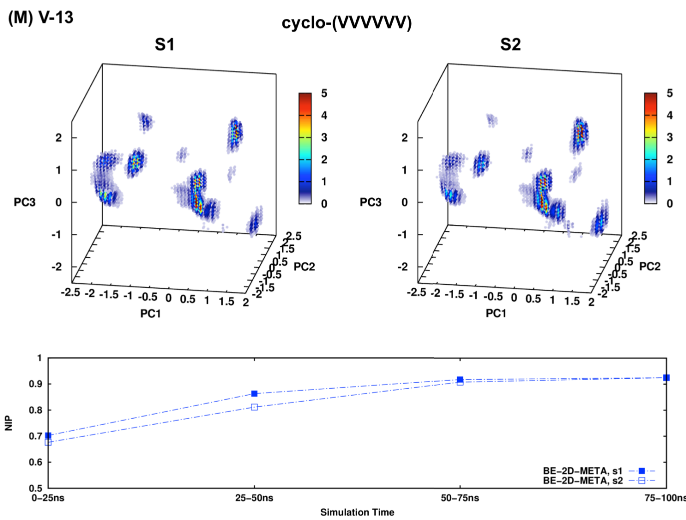
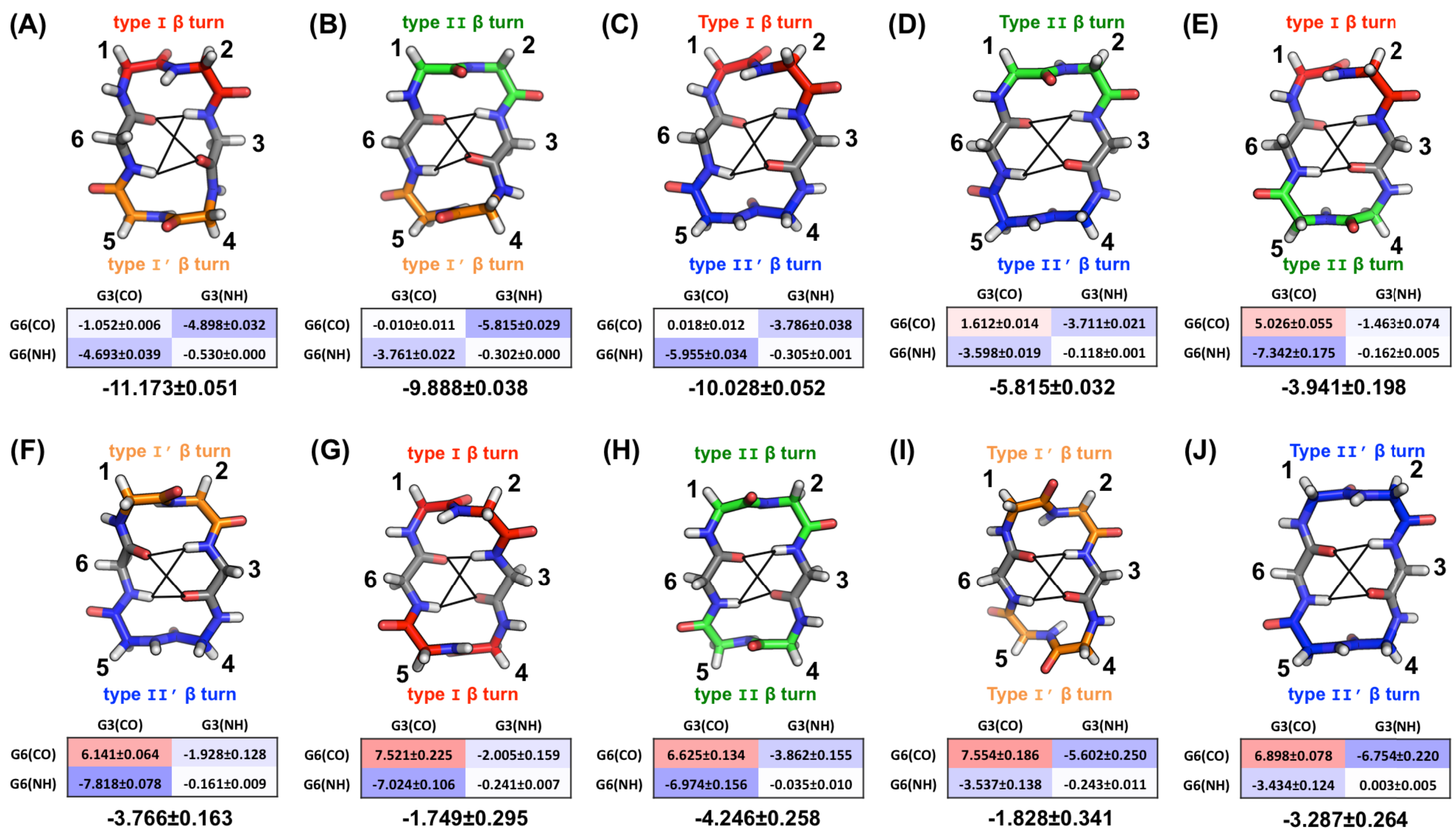


Figure S2. Conformational density profiles as a function of the first three largest principal components for S1 and S2, along with the NIP figures of all G_nV_{6-n} cyclic hexapeptides (**A-M**).



(A)

	G3(CO)	G3(NH)
G6(CO)	-1.052±0.006	-4.898±0.032
G6(NH)	-4.693±0.039	-0.530±0.000

-11.173±0.051

(B)

	G3(CO)	G3(NH)
G6(CO)	-0.010±0.011	-5.815±0.029
G6(NH)	-3.761±0.022	-0.302±0.000

-9.888±0.038

(C)

	G3(CO)	G3(NH)
G6(CO)	0.018±0.012	-3.786±0.038
G6(NH)	-5.955±0.034	-0.305±0.001

-10.028±0.052

(D)

	G3(CO)	G3(NH)
G6(CO)	1.612±0.014	-3.711±0.021
G6(NH)	-3.598±0.019	-0.118±0.001

-5.815±0.032

(E)

	G3(CO)	G3(NH)
G6(CO)	5.026±0.055	-1.463±0.074
G6(NH)	-7.342±0.175	-0.162±0.005

-3.941±0.198

(F)

	G3(CO)	G3(NH)
G6(CO)	6.141±0.064	-1.928±0.128
G6(NH)	-7.818±0.078	-0.161±0.009

-3.766±0.163

(G)

	G3(CO)	G3(NH)
G6(CO)	7.521±0.225	-2.005±0.159
G6(NH)	-7.024±0.106	-0.241±0.007

-1.749±0.295

(H)

	G3(CO)	G3(NH)
G6(CO)	6.625±0.134	-3.862±0.155
G6(NH)	-6.974±0.156	-0.035±0.010

-4.246±0.258

(I)

	G3(CO)	G3(NH)
G6(CO)	7.554±0.186	-5.602±0.250
G6(NH)	-3.537±0.138	-0.243±0.011

-1.828±0.341

(J)

	G3(CO)	G3(NH)
G6(CO)	6.898±0.078	-6.754±0.220
G6(NH)	-3.434±0.124	0.003±0.005

-3.287±0.264

Figure S3. Structure and Coulombic interaction (kJ/mol) between C=O and NH of the two non-turning residues (residues 3 and 6) for configurations with (**A**) type I β turn + type I' β turn, (**B**) II+I', (**C**) I+II', (**D**) II+II', (**E**) I+II, (**F**) I'+II', (**G**) I+I, (**H**) II+II, (**I**) I'+I' and (**J**) II'+II' in cyclo-G_6. The C=O bonds of the two non-turning residues point toward different sides of the CP plane in **A–D**, but the same side in **E–J**. Solid black lines within structures highlight the interactions found in the accompanying tables. It is noted that due to their low populations in the structural ensemble of cyclo-G_6, configurations **F–J** were not identified as one of the clusters in the cluster analysis. Instead, structures containing turns whose dihedrals were within 30° of the ideal value for a given type of β turn were extracted from the neutral replica of the BE-META simulation for analysis.

Table S3. Thermodynamic decomposition of all 14 G_nA_{6-n} cyclic hexapeptides (A–N).

(A) G_6

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
GGGGGG 32.5±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GGGGGG 20.8±0.4%	1.12±0.05	1.53±0.76	-0.41±0.73	3.33±0.17	-0.29±0.80	-1.50±0.34	2.43±0.27	-2.84±0.94	-0.10±0.04	6.19±0.12	-0.39±0.07	-1.65±0.12	-0.30±0.03	-0.41±0.02	1.01±1.07	-1.31±1.80	-0.07±0.14	-1.43±0.45
GGGGGG 19.2±0.2%	1.31±0.04	0.75±0.99	0.56±0.99	2.37±0.29	-0.92±1.05	-0.70±0.33	4.19±0.21	-3.63±0.94	-0.17±0.04	5.64±0.22	-0.43±0.02	-1.74±0.03	-0.51±0.08	-0.42±0.02	0.51±1.35	-1.43±1.73	0.03±0.07	-0.72±0.27

(B) A-1

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
AGGGGG 20.9±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AGGGGG 10.7±0.2%	1.67±0.09	2.03±1.98	-0.36±1.95	-3.17±0.14	-1.14±1.87	6.34±0.27	12.56±0.50	-12.93±2.18	-0.22±0.08	-9.19±0.17	0.28±0.08	1.67±0.09	4.02±0.04	0.28±0.02	-1.41±0.54	0.28±1.58	0.13±0.17	6.21±0.34
AGGGGG 8.7±0.4%	2.19±0.16	4.08±0.81	-1.89±0.84	0.66±0.24	-6.39±1.06	9.81±0.45	11.41±1.62	-13.30±1.66	1.40±0.05	1.71±0.27	-0.35±0.10	-1.51±0.12	-0.38±0.08	-0.21±0.02	2.27±0.81	-8.66±1.78	0.52±0.12	9.29±0.47

(C) A-2

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
AAGGGG 16.8±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAGGGG 15.5±0.2%	0.20±0.03	-3.55±1.02	3.74±1.00	0.90±0.18	1.68±0.90	-6.13±0.28	-2.93±0.09	6.67±1.05	-0.01±0.03	-4.68±0.19	0.16±0.07	0.79±0.15	4.44±0.05	0.20±0.03	-2.35±1.54	4.02±1.52	-0.68±0.09	-5.45±0.36
AAGGGG 12.3±0.2%	0.78±0.09	0.15±1.09	0.63±1.09	3.73±0.30	1.75±1.28	-5.34±0.36	0.23±0.83	0.40±1.34	-0.53±0.04	0.47±0.19	-0.59±0.04	-1.40±0.12	5.93±0.09	-0.15±0.05	0.70±0.90	1.05±1.58	-1.04±0.16	-4.30±0.46

(D) A-3

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
AGAGGG 15.1±0.4%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AGAGGG 9.3±0.3%	1.20±0.13	-0.24±1.61	1.45±1.68	-3.96±0.36	1.71±1.45	2.01±0.31	17.17±1.30	-15.72±1.40	-2.27±0.10	-8.94±0.33	-0.01±0.07	1.26±0.11	5.88±0.07	0.11±0.05	-1.97±1.39	3.68±2.11	-0.70±0.17	2.71±0.37
AGAGGG 8.2±0.2%	1.53±0.09	-1.40±0.96	2.93±0.90	-10.66±0.28	-10.24±0.88	19.50±0.52	21.15±1.05	-18.22±1.56	-1.54±0.05	-10.05±0.27	-0.07±0.09	0.41±0.13	0.56±0.07	0.03±0.03	1.42±0.74	-11.66±1.34	0.94±0.18	18.56±0.64

(E) A-4

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
AGGAGG 31.6±0.4%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AGGAGG 20.8±0.2%	1.05±0.05	2.09±0.73	-1.04±0.74	-1.28±0.14	1.35±0.75	2.02±0.41	4.98±0.23	-6.02±0.77	-0.32±0.03	-5.91±0.10	0.41±0.04	1.21±0.02	3.07±0.03	0.25±0.01	-1.19±1.08	2.54±1.67	0.27±0.10	1.75±0.40
AGGAGG 9.8±0.1%	2.93±0.04	6.02±1.47	-3.10±1.50	-6.96±0.08	-11.67±1.22	24.65±0.31	12.58±0.36	-15.68±1.15	0.93±0.03	-5.86±0.12	-0.72±0.03	-3.81±0.14	2.45±0.03	0.06±0.02	0.12±0.61	-11.79±0.89	-2.95±0.16	27.60±0.33

(F) A-5

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
AAAGGG 16.5±0.2%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAAGGG 12.6±0.2%	0.67±0.06	0.54±0.48	0.13±0.45	-21.02±0.32	-30.25±0.72	51.81±0.56	-1.38±0.49	1.50±0.65	4.20±0.06	-20.79±0.24	0.54±0.15	-0.06±0.13	-4.95±0.10	0.04±0.03	2.06±1.18	-32.30±1.82	-1.71±0.08	53.52±0.52
AAAGGG 8.0±0.3%	1.79±0.11	-0.03±1.35	1.82±1.40	-2.16±0.35	-10.14±1.50	12.27±0.42	12.40±1.40	-10.58±1.40	3.89±0.09	-8.52±0.19	0.92±0.19	2.86±0.08	-1.45±0.08	0.14±0.03	1.59±1.28	-11.73±2.55	-2.28±0.16	14.55±0.41

(G) A-6

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
AAGAGG 25.0±0.2%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAGAGG 11.6±0.1%	1.92±0.04	4.46±0.71	-2.54±0.73	8.74±0.28	5.08±0.62	-9.36±0.49	8.15±0.36	-10.69±0.64	0.08±0.07	10.17±0.38	-0.68±0.11	-3.47±0.12	2.78±0.05	-0.14±0.03	3.11±1.37	1.97±1.77	-2.38±0.03	-6.98±0.49
AAGAGG 5.8±0.2%	3.65±0.07	-0.32±1.84	3.98±1.88	-21.77±0.29	-31.16±1.82	52.61±0.41	42.07±1.67	-38.09±1.51	-4.81±0.12	-13.34±0.22	-0.87±0.09	-6.12±0.19	3.38±0.05	-0.01±0.02	5.66±1.47	-36.82±2.90	1.93±0.09	50.67±0.43

Colour scale (kJ/mol): (A) 8, 4, 0, −4, −8; (B) 20, 10, 0, −10, −20; (C) 10, 5, 0, −5, −10; (D) 30, 15, 0, −15, −30; (E) 30, 15, 0, −15, −30; (F) 60, 30, 0, −30, −60; (G) 60, 30, 0, −30, −60.

(H) A-7

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
AAGGAG 19.6±0.5%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAGGAG 10.7±0.4%	1.51±0.09	-2.62±2.61	4.12±2.62	15.09±0.23	14.50±2.81	-32.21±0.48	13.63±0.93	-9.50±2.71	0.53±0.09	10.81±0.15	0.72±0.10	5.38±0.14	-2.18±0.09	-0.17±0.02	1.17±0.95	13.32±3.00	2.05±0.09	-34.25±0.44
AAGGAG 8.0±0.1%	2.24±0.08	0.61±2.86	1.62±2.87	22.29±0.15	26.24±2.58	-47.92±0.70	19.22±0.63	-17.60±2.68	-2.31±0.10	17.62±0.32	0.04±0.06	0.65±0.15	6.40±0.08	-0.10±0.03	-1.41±1.64	27.64±1.80	1.55±0.24	-49.46±0.69

Color scale (kJ/mol): 50, 25, 0, −25, −50

(I) A-8

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
AGAGAG 41.4±0.4%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AGAGAG 20.8±0.3%	1.71±0.06	-1.89±0.87	3.61±0.91	24.55±0.15	26.99±0.84	-53.43±0.24	10.73±0.11	-7.12±0.92	-2.91±0.05	23.49±0.09	0.09±0.03	-0.21±0.09	4.12±0.10	-0.03±0.03	-2.67±1.09	29.66±1.35	0.07±0.08	-53.50±0.28
AGAGAG 5.4±0.2%	5.11±0.10	1.90±2.79	3.21±2.83	5.21±0.16	-2.53±2.62	-0.78±0.50	49.91±2.29	-46.71±3.46	-1.22±0.09	3.34±0.25	0.73±0.06	1.04±0.14	0.96±0.06	0.36±0.03	-3.27±1.60	0.74±2.68	0.00±0.15	-0.78±0.65

Color scale (kJ/mol): 60, 30, 0, −30, −60

(J) A-9

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
AAAAGG 21.3±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAAAGG 16.6±0.3%	0.62±0.03	-0.18±1.24	0.80±1.24	-17.59±0.17	-14.85±1.14	32.26±0.33	8.28±0.25	-7.48±1.23	-4.37±0.01	-13.84±0.13	0.09±0.06	-2.59±0.11	3.02±0.03	0.09±0.02	1.03±1.00	-15.88±1.78	2.34±0.10	29.92±0.34
AAAAGG 11.9±0.3%	1.45±0.07	-3.15±1.25	4.60±1.24	4.92±0.08	6.53±1.25	-14.61±0.19	18.13±0.62	-13.53±1.56	-0.71±0.03	1.61±0.12	0.10±0.04	2.94±0.10	0.83±0.04	0.17±0.04	-0.77±2.68	7.30±3.62	2.94±0.14	-17.55±0.20

Color scale (kJ/mol): 40, 20, 0, −20, −40

(K) A-10

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
AAAGAG 26.6±0.2%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAAGAG 17.5±0.3%	1.04±0.06	-1.74±1.85	2.78±1.84	40.16±0.14	42.71±2.10	-84.60±0.50	6.21±0.46	-3.43±1.89	1.05±0.07	38.90±0.25	-0.41±0.06	0.41±0.12	0.33±0.13	-0.13±0.03	-4.85±1.32	47.56±3.40	0.18±0.14	-84.78±0.57
AAAGAG 8.4±0.2%	2.88±0.06	-1.83±0.83	4.71±0.87	16.27±0.10	17.67±0.88	-35.76±0.45	30.14±0.92	-25.43±0.71	3.38±0.10	7.32±0.11	1.05±0.08	7.65±0.07	-3.10±0.08	-0.03±0.03	-0.23±0.70	17.89±1.03	-0.34±0.13	-35.42±0.41

Color scale (kJ/mol): 90, 45, 0, −45, −90

(L) A-11

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
AAGAAG 28.4±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAGAAG 7.2±0.3%	3.42±0.12	3.71±1.63	-0.29±1.62	36.71±0.14	37.90±1.65	-70.90±0.36	23.24±2.12	-23.53±2.56	0.38±0.04	40.44±0.10	-1.29±0.09	-2.14±0.12	-0.56±0.10	-0.12±0.03	-6.82±0.88	44.72±1.65	1.54±0.23	-72.44±0.41
AAGAAG 3.5±0.1%	5.25±0.12	5.47±3.51	-0.22±3.52	34.28±0.27	32.06±3.36	-60.87±0.46	78.78±4.79	-79.00±5.35	2.21±0.07	23.26±0.22	0.11±0.08	5.12±0.21	3.64±0.10	-0.06±0.05	-7.13±1.72	39.19±3.68	-2.04±0.12	-58.83±0.50

Color scale (kJ/mol): 80, 40, 0, −40, −80

(M) A-12

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
AAAAAG 19.0±0.4%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAAAAG 13.5±0.2%	0.85±0.09	-2.04±1.00	2.89±1.03	0.19±0.27	3.45±1.11	-5.68±0.57	11.12±0.74	-8.24±0.88	-5.22±0.05	6.53±0.20	-1.12±0.08	-4.08±0.10	4.04±0.10	0.04±0.02	-0.27±1.15	3.72±2.18	0.95±0.09	-6.64±0.56
AAAAAG 13.3±0.2%	0.89±0.07	-4.68±0.50	5.56±0.50	-18.98±0.25	-26.02±0.60	40.31±0.23	17.31±0.53	-11.75±0.75	1.60±0.10	-12.52±0.12	0.42±0.10	-0.94±0.12	-7.58±0.13	0.04±0.03	3.29±1.74	-29.31±2.14	-0.93±0.12	41.24±0.33

Color scale (kJ/mol): 50, 25, 0, −25, −50

(N) A-13

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
AAAAAA 22.5±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
AAAAAA 20.5±0.3%	0.24±0.06	7.51±1.70	-7.27±1.70	9.57±0.19	22.74±1.79	-24.80±0.35	-4.53±0.25	-2.74±1.69	-3.48±0.07	2.24±0.05	-1.26±0.08	0.20±0.17	11.88±0.08	-0.01±0.02	-1.49±0.80	24.23±2.58	1.12±0.08	-25.92±0.39
AAAAAA 15.4±0.2%	0.96±0.04	4.38±1.32	-3.42±1.32	18.11±0.09	23.95±1.34	-37.68±0.30	1.23±0.21	-4.65±1.28	-0.15±0.06	12.73±0.15	-0.17±0.05	0.79±0.16	4.97±0.08	-0.06±0.02	-3.25±1.14	27.19±1.94	0.84±0.17	-38.52±0.42

Color scale (kJ/mol): 40, 20, 0, −20, −40

Table S4. Thermodynamic decomposition of all 13 G_nV_{6-n} cyclic hexapeptides (**A–M**).

(A) V-1

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
VGGGGG 38.5±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VGGGGG 9.8±0.3%	3.41±0.07	1.13±1.72	2.28±1.71	2.96±0.15	-8.74±1.90	6.91±0.20	15.35±1.03	-13.07±2.24	1.35±0.05	3.02±0.09	-0.35±0.08	-0.94±0.09	0.14±0.08	-0.27±0.01	0.98±1.26	-9.72±2.82	0.67±0.14	6.24±0.29
VGGGGG 7.8±0.3%	4.01±0.11	2.81±2.00	1.20±2.01	2.79±0.33	-0.47±2.29	0.49±0.38	29.24±1.79	-28.04±2.75	-0.39±0.03	-5.30±0.20	0.79±0.07	2.05±0.14	5.31±0.10	0.32±0.03	-2.24±2.22	1.77±4.09	0.16±0.08	0.33±0.33

30 15 0 −15 −30 kJ/mol

(B) V-2

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
VVGGGG 18.7±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVGGGG 10.0±0.4%	1.55±0.12	-3.77±0.68	5.32±0.58	-19.46±0.40	-21.08±0.67	36.77±0.90	27.62±1.38	-22.30±1.91	-2.89±0.09	-4.36±0.39	-0.25±0.07	-0.91±0.11	-10.78±0.07	-0.28±0.03	3.03±2.32	-24.10±2.67	0.45±0.09	36.32±0.87
VVGGGG 8.8±0.2%	1.88±0.09	-2.78±2.30	4.67±2.24	23.28±0.34	24.18±2.44	-50.24±0.71	28.28±1.05	-23.61±2.97	-2.15±0.10	30.08±0.32	-0.48±0.12	-1.56±0.18	-2.20±0.09	-0.40±0.02	-1.38±2.21	25.56±4.23	3.39±0.06	-53.63±0.68

50 25 0 −25 −50 kJ/mol

(C) V-3

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
VGVGGG 14.7±0.2%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VGVGGG 12.2±0.2%	0.28±0.04	-1.22±1.50	1.50±1.49	16.99±0.24	16.19±1.73	-34.40±0.44	-3.30±0.52	4.80±1.82	4.22±0.08	10.87±0.20	-0.26±0.09	0.45±0.09	1.83±0.17	-0.12±0.03	1.56±1.93	14.63±3.53	-0.65±0.18	-33.76±0.38
VGVGGG 8.3±0.2%	1.26±0.06	-0.31±1.52	1.58±1.47	35.01±0.34	33.00±1.79	-68.31±0.88	5.94±1.06	-4.37±2.42	7.50±0.08	29.29±0.49	-0.19±0.17	-0.53±0.16	-0.94±0.16	-0.12±0.03	-2.27±1.00	35.26±2.46	-2.30±0.17	-66.01±0.95

70 35 0 −35 −70 kJ/mol

(D) V-4

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
VGGVGG 45.6±0.6%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VGGVGG 9.2±0.2%	3.99±0.07	4.38±1.38	-0.39±1.35	22.56±0.15	21.43±1.63	-39.60±0.40	28.71±0.86	-29.10±1.83	-1.48±0.02	18.06±0.14	0.45±0.11	0.88±0.16	4.62±0.06	0.03±0.02	-2.75±1.55	24.18±2.96	0.66±0.06	-40.26±0.43
VGGVGG 7.3±0.2%	4.58±0.09	-2.75±1.74	7.33±1.66	-6.99±0.39	-4.58±1.74	8.81±0.46	50.43±1.33	-43.10±2.96	-10.34±0.12	-5.69±0.16	0.44±0.13	2.07±0.21	6.38±0.07	0.15±0.03	0.32±1.54	-4.90±1.90	6.79±0.09	2.02±0.40

50 25 0 −25 −50 kJ/mol

(E) V-5

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
VVVGGG 29.7±0.6%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVVGGG 15.5±0.2%	1.62±0.05	6.89±1.53	-5.27±1.48	-14.86±0.17	-14.50±1.62	36.24±0.40	9.36±0.41	-14.63±1.84	0.05±0.08	-11.49±0.19	0.60±0.10	0.25±0.09	-4.47±0.08	0.21±0.01	-1.03±1.67	-13.47±2.86	-1.26±0.06	37.51±0.41
VVVGGG 10.2±0.1%	2.68±0.05	6.20±1.91	-3.53±1.88	-6.62±0.30	-3.92±1.57	16.75±0.69	26.31±0.26	-29.83±1.75	0.47±0.04	-14.35±0.31	0.52±0.12	2.94±0.21	3.39±0.10	0.40±0.03	-2.08±0.82	-1.83±1.76	-0.71±0.12	17.45±0.75

40 20 0 −20 −40 kJ/mol

(F) V-6

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
VVGVGG 37.2±0.2%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVGVGG 21.9±0.4%	1.32±0.05	-0.39±0.93	1.71±0.93	-9.04±0.17	-11.94±0.87	20.59±0.30	6.48±0.33	-4.77±0.81	-0.31±0.07	-0.38±0.15	-1.07±0.09	-3.82±0.13	-3.81±0.03	0.35±0.01	0.16±1.21	-12.09±1.86	2.70±0.14	17.89±0.36
VVGVGG 5.0±0.1%	4.99±0.06	1.02±2.12	3.97±2.07	14.18±0.08	13.84±2.48	-27.00±0.42	73.16±1.96	-69.19±3.93	-2.82±0.11	13.79±0.11	0.23±0.14	1.48±0.26	1.47±0.09	0.02±0.03	0.17±3.23	13.67±5.04	4.32±0.13	-31.32±0.54

70 35 0 −35 −70 kJ/mol

(G) V-7

	ΔG	ΔH	$-T\Delta S$	ΔH_{P}	ΔH_{W}	ΔH_{PW}	$-T\Delta S_{\mathrm{P}}^{\mathrm{conf}}$	$-T\Delta S_{\mathrm{W}}$	$\Delta H_{\mathrm{P}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{P}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{P}}^{\mathrm{bond}}$	$\Delta H_{\mathrm{P}}^{\mathrm{angle}}$	$\Delta H_{\mathrm{P}}^{\mathrm{dih.}}$	$\Delta H_{\mathrm{P}}^{\mathrm{imp.}}$	$\Delta H_{\mathrm{W}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{W}}^{\mathrm{EE}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{LJ}}$	$\Delta H_{\mathrm{PW}}^{\mathrm{EE}}$
VVGGVG 81.8±0.4%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVGGVG 1.3±0.1%	10.32±0.08	-0.15±3.00	10.47±3.03	52.07±0.88	34.75±3.43	-86.97±1.13	337.23±10.71	-326.75±10.13	3.78±0.14	44.76±0.62	-0.12±0.27	0.98±0.35	2.70±0.24	-0.04±0.06	-0.97±3.88	35.71±6.13	5.18±0.49	-92.15±1.32
VVGGVG 0.3±0.1%	13.96±0.19	16.56±6.84	-2.60±6.67	58.42±1.16	59.64±8.77	-101.50±2.42	1016.51±36.68	-1019.11±42.59	4.25±0.39	40.23±0.84	0.39±0.58	1.78±0.64	11.96±0.34	-0.18±0.14	-5.94±10.57	65.58±12.53	-0.12±0.40	-101.38±2.61

80 40 0 −40 −80 kJ/mol

(H) V-8

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
VGVGVG 36.0±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VGVGVG 10.5±0.3%	3.02±0.09	1.45±1.94	1.57±1.94	-0.88±0.32	-4.51±1.86	6.85±0.51	32.09±1.27	-30.52±2.09	-7.08±0.09	8.82±0.23	0.45±0.07	0.91±0.12	-4.10±0.09	0.12±0.03	1.95±1.05	-6.46±2.90	2.49±0.16	4.36±0.56
VGVGVG 5.2±0.2%	4.69±0.10	-0.46±1.26	5.15±1.31	40.90±0.64	36.47±1.83	-77.83±1.33	65.38±3.13	-60.23±2.69	-2.38±0.12	36.23±0.54	0.36±0.15	0.62±0.25	6.05±0.11	0.01±0.04	0.67±1.79	35.80±3.54	-0.44±0.17	-77.39±1.30

(I) V-9

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
VVVVGG 47.3±0.4%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVVVGG 33.2±0.2%	0.88±0.03	0.49±0.14	0.39±0.14	40.29±0.14	41.77±0.21	-81.58±0.20	-3.26±0.24	3.66±0.30	-1.32±0.11	39.65±0.04	0.23±0.08	-1.49±0.11	3.35±0.11	-0.13±0.02	-3.43±1.11	45.20±1.11	0.39±0.10	-81.96±0.13
VVVVGG 0.7±0.1%	10.68±0.19	7.17±5.52	3.51±5.63	12.90±1.14	4.85±5.53	-10.58±1.17	700.76±38.40	-697.26±35.34	-7.07±0.47	8.23±0.70	0.51±0.28	2.25±0.83	9.10±0.18	-0.11±0.10	-7.72±5.15	12.57±10.58	2.75±0.40	-13.33±1.11

(J) V-10

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
VVVGVG 47.6±0.3%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVVGVG 7.9±0.1%	4.49±0.05	5.28±2.63	-0.79±2.65	-38.12±0.35	-39.48±2.81	82.88±0.49	48.35±0.99	-49.14±2.33	-4.63±0.17	-25.87±0.43	0.28±0.12	1.12±0.21	-9.07±0.07	0.03±0.01	1.89±0.24	-41.37±2.93	0.76±0.06	82.12±0.47
VVVGVG 6.2±0.2%	5.09±0.08	11.29±2.44	-6.20±2.49	-63.30±0.30	-64.70±2.44	139.29±0.36	59.44±2.09	-65.64±1.92	-5.32±0.18	-60.52±0.30	-0.00±0.14	1.88±0.23	0.61±0.11	0.05±0.03	3.49±1.90	-68.19±3.94	0.89±0.06	138.41±0.32

(K) V-11

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
VVGVVG 34.5±0.4%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVGVVG 8.7±0.3%	3.44±0.07	-0.10±1.20	3.54±1.25	30.87±0.25	27.89±0.74	-58.87±0.54	38.00±1.74	-34.46±1.32	-0.85±0.11	22.50±0.30	0.43±0.10	2.95±0.21	5.41±0.07	0.44±0.01	-2.66±1.90	30.55±2.56	1.43±0.16	-60.30±0.64
VVGVVG 7.9±0.2%	3.67±0.10	0.78±1.33	2.88±1.39	54.43±0.71	48.13±1.16	-101.78±1.69	41.93±1.89	-39.05±1.56	-1.23±0.11	39.80±0.79	1.27±0.10	7.06±0.12	7.63±0.14	-0.11±0.02	-0.75±0.52	48.88±1.65	-2.54±0.21	-99.24±1.81

(L) V-12

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
VVVVVG 18.7±0.4%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVVVVG 14.5±0.1%	0.64±0.06	4.57±1.39	-3.93±1.38	-34.87±0.21	-37.26±1.65	76.69±0.35	10.10±0.72	-14.03±1.68	5.14±0.17	-40.40±0.22	-0.08±0.12	3.47±0.21	-2.96±0.07	-0.04±0.03	3.49±2.01	-40.75±3.53	-2.05±0.11	78.74±0.26
VVVVVG 14.1±0.3%	0.70±0.06	0.07±1.49	0.63±1.50	-14.02±0.17	-27.19±1.61	41.28±0.44	5.04±0.66	-4.41±1.38	4.91±0.23	-27.99±0.22	0.28±0.09	6.36±0.27	2.00±0.04	0.42±0.02	3.43±2.43	-30.61±3.03	-5.01±0.14	46.29±0.34

(M) V-13

	ΔG	ΔH	$-T\Delta S$	ΔH_P	ΔH_W	ΔH_{PW}	$-T\Delta S_P^{conf}$	$-T\Delta S_W$	ΔH_P^{LJ}	ΔH_P^{EE}	ΔH_P^{bond}	ΔH_P^{angle}	$\Delta H_P^{dih.}$	$\Delta H_P^{imp.}$	ΔH_W^{LJ}	ΔH_W^{EE}	ΔH_{PW}^{LJ}	ΔH_{PW}^{EE}
VVVVVV 22.3±0.2%	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
VVVVVV 17.6±0.3%	0.59±0.04	2.92±0.71	-2.34±0.71	21.04±0.26	26.65±0.67	-44.77±0.32	18.93±0.75	-21.27±1.25	-5.97±0.10	23.66±0.15	-0.13±0.06	-3.75±0.30	7.11±0.14	0.12±0.02	-1.21±2.53	27.87±2.11	1.25±0.11	-46.02±0.26
VVVVVV 11.7±0.1%	1.60±0.03	-3.86±1.07	5.46±1.06	50.35±0.40	45.22±1.14	-99.43±0.34	8.31±0.90	-2.85±0.38	-1.44±0.10	65.67±0.07	0.65±0.15	-1.11±0.13	-13.40±0.10	-0.03±0.01	-3.31±0.48	48.52±1.54	2.78±0.13	-102.21±0.39

Color scale (kJ/mol): (H)–(J), (L): 80, 40, 0, −40, −80; (K): 60, 30, 0, −30, −60; (M): 70, 35, 0, −35, −70

References

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