Supplementary information

Conformational preferences of β-sheet structures in cyclopropane-containing γ-peptides

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Table S1 Geometric parameters and strengths of inter-strand H-bonds of β-sheets of the Ac-(γAmc$_3$-**1**)$_2$-NHMe peptide[a]

	N–H···O H-bonds				C–H···O H-bonds			
Type[b]	HB[c]	*d*(NH···O)	*θ*(N–H···O)	ΔE_2[d]	HB[c]	*d*(CH···O)	*θ*(C–H···O)	ΔE_2[d]
p	I_a	1.92	173.6	8.64	II_a	2.64	140.9	0.17
	I_b	1.91	161.4	9.15	II_b	2.42	135.4	0.68
	I_c	1.93	167.5	6.18	II_c	2.47	139.2	0.94
	av.	1.92	167.5	23.97[e]	av.	2.51	138.5	1.79[e]
ap	I_a'	1.94	167.0	6.94	II_a'	2.47	138.5	0.75
	I_b'	2.01	160.4	6.56	II_b'	2.31	141.8	1.27
	I_c'	2.07	152.0	2.32	II_c'	2.76	110.0	0.03
	av.	2.01	159.8	15.82[e]	av.	2.51	130.1	2.05[e]

[a] Optimized at the M06-2X/6-31+G(d) level of theory; all distances and angles are in Å and degrees, respectively. [b] **p** and **ap** denote parallel and antiparallel β-sheets, respectively. [c] Defined in Fig. 3a. [d] The second perturbation energy (kcal mol^{-1}) of the lone pair orbitals of the carbonyl oxygen with the corresponding N–H (or C–H) antibonding orbital calculated at the M06-2X/cc-pVTZ level of theory. [e] The sum of ΔE_2 values in each strand.

Table S2 Geometric parameters and strengths of inter-strand H-bonds of β-sheets of the Ac-(γAmc$_3$-**1**)$_4$-NHMe peptide[a]

	N–H···O H-bonds				C–H···O H-bonds			
Type[b]	HB[c]	d(NH···O)	θ(N–H···O)	ΔE_2[d]	HB[c]	d(CH···O)	θ(C–H···O)	ΔE_2[d]
p	I_a	1.93	172.2	8.58	II_a	2.61	140.1	0.17
	I_b	1.90	164.2	8.36	II_b	2.51	134.6	0.55
	I_c	1.93	164.1	7.81	II_c	2.45	138.2	0.70
	I_d	1.93	161.5	8.37	II_d	2.37	138.9	0.84
	I_e	1.93	167.6	6.26	II_e	2.48	139.0	0.90
	av.	1.92	165.9	39.38[e]	av.	2.48	138.2	3.16[e]
ap	I_a'	1.96	166.2	6.44	II_a'	2.50	136.7	0.29
	I_b'	1.95	161.9	7.83	II_b'	2.28	143.8	1.37
	I_c'	1.99	170.5	5.83	II_c'	2.59	138.4	0.17
	I_d'	1.99	161.7	5.54	I_d'	2.30	143.7	1.43
	I_e'	1.98	162.3	6.41	II_e'	2.48	140.1	0.27
	av.	1.97	164.5	32.05[e]	av.	2.43	140.6	3.53[e]

[a] Optimized at the M06-2X/6-31+G(d) level of theory; all distances and angles are in Å and degrees, respectively. [b] **p** and **ap** denote parallel and antiparallel β-sheets, respectively. [c] Defined in Fig. 3b. [d] The second perturbation energy (kcal mol^{-1}) of the lone pair orbitals of the carbonyl oxygen with the corresponding N–H (or C–H) antibonding orbital calculated at the M06-2X/cc-pVTZ level of theory. [e] The sum of ΔE_2 values in each strand.

Table S3 Geometric parameters and strengths of inter-strand H-bonds of β-sheets of the Ac-(γAmc$_3$-**1**)$_6$-NHMe peptide[a]

	N–H···O H-bonds				C–H···O H-bonds			
Type[b]	HB[c]	d(NH···O)	θ(N–H···O)	ΔE_2[d]	HB[c]	d(CH···O)	θ(C–H···O)	ΔE_2[d]
p	I_a	1.93	171.2	8.31	II_a	2.59	139.8	0.18
	I_b	1.90	164.7	8.31	II_b	2.50	135.3	0.59
	I_c	1.93	164.0	7.86	II_c	2.44	138.6	0.70
	I_d	1.93	163.6	7.69	II_d	2.45	138.0	0.71
	I_e	1.93	163.6	7.66	II_e	2.44	138.4	0.74
	I_f	1.92	161.8	8.55	II_f	2.36	139.2	0.88
	I_g	1.93	166.9	6.16	II_g	2.46	139.5	0.97
	av.	1.93	165.1	54.54[e]	av.	2.46	138.4	4.77[e]
ap	I_a'	1.95	167.1	6.32	II_a'	2.48	138.4	0.26
	I_b'	1.99	162.8	5.58	II_b'	2.37	143.2	1.04
	I_c'	2.01	158.6	5.51	II_c'	2.31	141.3	1.28
	I_d'	2.02	161.1	6.25	II_d'	2.30	144.3	0.60
	I_e'	2.02	165.5	5.39	II_e'	2.43	143.2	0.28
	I_f'	2.02	159.0	4.72	II_f'	2.31	139.4	1.29
	I_g'	1.99	161.8	6.46	II_g'	2.46	139.3	0.31
	av.	2.00	162.3	40.23[e]	av.	2.38	141.3	5.06[e]

[a] Optimized at the M06-2X/6-31+G(d) level of theory; all distances and angles are in Å and degrees, respectively. [b] **p** and **ap** denote parallel and antiparallel β-sheets, respectively. [c] Defined in Fig. 3c. [d] The second perturbation energy (kcal mol^{-1}) of the lone pair orbitals of the carbonyl oxygen with the corresponding N–H (or C–H) antibonding orbital calculated at the M06-2X/cc-pVTZ level of theory. [e] The sum of ΔE_2 values in each strand.

Table S4 Deformation energies (kcal mol^{-1}) of β-sheets of Ac-(γAmc$_3$-**1**)$_n$-NHMe peptides[a]

n	Type[b]	$\Delta E_{def,A}$[c]	$\Delta E_{def,B}$[c]	ΔE_{def}[d]
2	**p**	1.24	0.80	2.04
	ap	0.33	0.97	1.29
4	**p**	2.20	1.72	3.92
	ap	2.57	1.27	3.84
6	**p**	3.11	2.94	6.06
	ap	3.66	2.36	6.02

[a] Calculated at the M06-2X/cc-pVTZ level of theory without BSSE corrections. [b] **p** and **ap** denote parallel and antiparallel β-sheets, respectively. [c] Relative deformation energies of each strand of β-sheets. [d] The sum of $\Delta E_{def,A}$ and $\Delta E_{def,B}$.