New J. Chem.

Supplementary information

Propensities to form β-turn and β-hairpin structures of D-Pro-Gly and Aib-D-Ala containing peptides: A computational study

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Table S1 Torsion angles (°) and thermodynamic properties (kcal mol^{-1}) of local minima of Ac-D-Pro-Gly-NHMe optimized in CH_2Cl_2[a]

Conf.	Turn[b]	D-Pro					Gly			DSD-PBEP86-D3BJ/def2-TZVP			M06-2X/cc-pVTZ		
		ω_0	ϕ_1	ψ_1	ω_1	χ_1^1	ϕ_1	ψ_2	ω_2	ΔE_e	ΔH	ΔG	ΔE_e	ΔH	ΔG
dPG-1	I'(d)	174.2	60.4	27.9	-179.1	29.8	82.2	0.3	-179.4	0.57	0.56	0.00	0.69	0.67	0.00
dPG-2	II'(d)	-179.5	54.8	-131.9	179.8	27.2	-78.5	-0.6	177.4	0.00	0.00	0.13	0.00	0.00	0.02
dPG-3	I'(u)	173.6	68.9	17.9	-173.8	-26.1	80.5	2.8	-179.8	0.52	0.50	0.44	0.59	0.56	0.39
dPG-4	ext	-177.6	66.9	-149.9	-177.6	-30.3	-179.1	175.8	179.6	3.99	3.82	1.76	3.71	3.53	1.36
dPG-5		-7.6	89.2	6.3	178.7	-34.1	-178.9	175.9	178.4	3.31	3.18	1.82	3.37	3.24	1.77
dPG-6		176.0	79.6	12.4	-179.8	-31.1	-179.1	175.9	178.3	3.09	2.99	1.98	3.10	3.00	1.87
dPG-7		2.7	74.3	-160.2	-176.1	-33.8	178.6	176.8	179.9	4.61	4.39	1.99	4.35	4.13	1.61
dPG-8	II'(u)	-178.7	60.7	-134.2	176.7	-26.8	-80.7	1.4	178.1	0.28	0.58	2.03	0.11	0.41	1.74
dPG-9		176.1	66.9	24.5	-179.7	26.3	175.6	176.5	178.0	3.73	3.56	2.16	3.79	3.62	2.10
dPG-10		-6.3	87.7	8.4	170.6	-33.5	-63.7	151.6	178.3	3.46	3.34	2.22	3.51	3.38	2.15
dPG-11		-4.5	66.5	26.9	176.9	25.9	-178.4	-177.9	-179.4	4.54	4.22	2.45	4.61	4.29	2.40
dPG-12		-178.5	58.8	-145.1	-170.0	25.1	64.9	-151.6	-178.3	4.08	3.96	2.50	4.27	4.15	2.57
dPG-13	ext	-178.4	58.1	-141.9	-179.0	24.9	-177.7	-178.7	-178.8	4.05	3.97	2.54	3.96	3.89	2.33
dPG-14		-7.1	87.5	8.0	-178.6	-33.1	-83.8	59.3	179.6	3.39	3.34	2.56	3.76	3.70	2.81
dPG-15		-177.3	68.0	-151.6	-167.5	-30.9	64.7	-153.8	-177.5	3.95	3.87	2.74	3.89	3.80	2.56
dPG-16		174.2	84.4	-68.1	169.9	-33.7	-63.7	153.1	176.9	3.03	3.15	2.81	2.89	3.00	2.55
dPG-17		-8.5	86.3	10.2	178.1	-31.9	83.6	-60.9	179.2	3.38	3.44	2.89	3.71	3.77	3.11
dPG-18		3.1	57.3	-147.1	-177.5	26.2	83.1	-61.8	178.8	5.27	5.27	3.00	5.47	5.47	3.09
dPG-19		171.5	86.4	-67.6	176.0	-32.2	-80.9	-7.1	-179.8	2.37	2.56	3.15	2.41	2.61	3.08
dPG-20		171.9	87.0	-61.6	179.1	-33.4	179.8	178.7	179.8	4.34	4.16	3.18	3.70	3.51	2.42
dPG-21		171.5	85.7	-63.8	175.4	-33.0	86.1	7.0	179.8	2.68	2.11	3.33	2.70	2.14	3.24
dPG-22		174.6	67.8	23.7	179.7	26.7	-84.5	60.3	179.9	3.88	3.94	3.34	4.19	4.26	3.54
dPG-23		175.2	67.9	23.4	173.6	26.1	-67.5	147.1	177.3	4.10	4.10	3.36	4.31	4.31	3.46
dPG-24		3.5	57.2	-143.5	-177.8	25.5	-177.3	179.1	-179.4	5.00	4.95	3.53	4.76	4.71	3.18
dPG-25		-4.6	71.0	22.6	177.8	24.8	-84.2	58.5	-179.8	4.59	4.66	3.57	4.95	5.02	3.82
dPG-26		2.9	71.3	-154.9	175.2	-32.5	-63.2	151.9	178.6	4.70	4.68	3.60	4.58	4.55	3.35
dPG-27		174.8	66.0	27.2	176.4	27.5	83.8	-61.5	176.4	3.77	3.79	3.60	4.17	4.20	3.89
dPG-28		-8.4	85.7	8.7	-172.6	-32.5	65.8	-157.7	-177.9	3.38	3.39	3.69	3.30	3.31	3.49
dPG-29		172.6	84.9	-63.2	174.9	-32.9	84.9	-59.3	179.5	3.33	3.37	3.72	3.30	3.34	3.57
dPG-30		172.6	83.3	-71.5	172.9	16.3	86.6	6.8	-179.9	4.02	4.21	3.82	4.38	4.57	4.06
dPG-31		-2.9	68.5	24.4	167.7	24.8	-63.7	150.8	178.7	4.63	4.62	3.83	4.75	4.74	3.83
dPG-32		1.4	74.8	-157.1	-177.8	-32.6	82.9	-58.5	-179.2	4.70	4.71	3.93	4.92	4.93	4.03
dPG-33		2.1	70.6	-152.4	-176.4	-31.8	-84.4	63.2	-177.7	4.36	4.37	3.93	4.48	4.49	3.93
dPG-34		172.8	83.0	-73.1	173.1	16.8	85.4	-60.1	179.9	4.80	4.92	3.95	5.11	5.23	4.15
dPG-35		171.5	85.3	-65.3	-176.7	-32.3	-83.0	55.0	178.2	3.23	3.38	4.01	3.25	3.40	3.92
dPG-36		4.2	57.1	-148.1	-168.2	25.7	64.6	-153.2	-178.5	5.15	5.16	4.07	5.20	5.21	4.00
dPG-37		-1.5	67.7	-153.1	-171.9	-30.6	-83.2	-7.9	178.0	4.42	4.70	4.18	4.54	4.82	4.18

dPG-38	-5.5	67.1	26.6	175.7	27.2	83.8	-63.4	177.4	4.45	4.55	4.39	4.69	4.79	4.51
dPG-39	-0.9	74.1	24.8	170.2	23.3	106.5	-3.1	179.9	4.39	4.56	4.65	4.91	5.08	5.05
dPG-40	173.2	83.5	-79.2	176.9	16.4	176.7	-173.8	-178.7	5.60	5.52	4.65	5.40	5.32	4.33
dPG-41	3.1	57.1	-142.4	-176.0	26.3	-83.5	67.7	-176.0	4.70	4.98	4.93	4.76	5.04	4.88

[a] Calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) and M06-2X/cc-pVTZ//SMD M06-2X/6-31+G(d) levels of theory in CH_2Cl_2. The torsion angles listed are for the D-Pro-Gly segment as defined in Fig. 1a. ΔE_e, ΔH, and ΔG are the relative electronic energy, enthalpy, and Gibbs free energy, respectively. ΔH and ΔG were calculated at 25℃ and 1 atm. Only the conformers with $\Delta G < 5$ kcal mol^{-1} at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory are listed. [b] The turn types of the D-Pro-Gly tripeptide are designated depending on Pro puckering, *e.g.*, II′(d) is the type II′ β-turn with a down-puckered D-Pro residue. Extended structures are denoted by "ext".

Table S2 Torsion angles (°) and thermodynamic properties (kcal mol^{-1}) of local minima of Ac-D-Pro-Gly-NHMe optimized in water[a]

Conf.	Turn[b]	D-Pro					Gly			DSD-PBEP86-D3BJ/def2-TZVP			M06-2X/cc-pVTZ		
		ω_0	ϕ_1	ψ_1	ω_1	χ_1^1	ϕ_1	ψ_2	ω_2	ΔE_e	ΔH	ΔG	ΔE_e	ΔH	ΔG
dPG-2	II'(d)	-178.8	52.1	-138.5	179.2	29.5	-75.9	-1.5	177.9	0.00	0.00	0.00	0.00	0.00	0.00
dPG-7	ext	2.6	67.7	-150.7	-175.0	-31.3	178.8	178.8	-178.8	3.68	3.76	0.28	3.56	3.64	0.17
dPG-4	ext	-176.6	61.5	-147.3	-176.4	-29.1	-180.0	-178.4	-177.8	2.96	2.89	0.63	2.76	2.69	0.43
dPG-33		1.9	74.5	-157.5	-170.8	-33.0	-84.5	-7.5	-179.6	2.28	2.48	0.66	2.72	2.93	1.10
dPG-36		9.6	53.6	-149.9	-169.8	23.6	59.1	-151.9	-176.9	2.72	2.91	0.70	2.82	3.01	0.80
dPG-1	I'(d)	178.7	59.0	26.5	-177.6	25.9	73.8	8.5	-179.4	0.94	0.94	0.78	1.11	1.12	0.96
dPG-12		-176.5	53.8	-145.5	-167.4	24.6	59.1	-152.6	-176.9	1.58	1.81	0.84	1.70	1.94	0.97
dPG-15		-175.5	59.9	-149.0	-170.8	-28.3	59.2	-153.9	-177.5	1.41	1.68	0.86	1.38	1.66	0.83
dPG-6		179.6	72.6	15.6	178.1	-31.0	-179.9	179.2	178.5	3.15	3.07	0.95	3.17	3.09	0.97
dPG-23		178.4	64.1	25.7	171.1	23.0	-61.1	153.7	176.7	2.81	2.82	1.19	2.94	2.95	1.32
dPG-8	II'(u)	-176.4	57.2	-140.1	177.3	-27.6	-75.5	-0.8	178.5	0.39	0.74	1.27	0.17	0.52	1.05
dPG-3	I'(u)	179.4	62.6	26.2	-175.8	-27.6	80.5	3.1	-179.6	0.68	0.18	1.35	0.77	0.27	1.44
dPG-28		-1.9	84.8	9.5	-176.1	-34.6	62.0	-156.4	-176.3	2.57	2.65	1.47	2.66	2.74	1.56
dPG-5		1.7	80.2	10.8	179.2	-34.4	177.6	179.1	178.5	3.61	3.50	1.69	3.74	3.63	1.83
dPG-10		-0.7	85.4	4.8	173.7	-35.3	-62.0	153.9	176.1	2.37	2.52	1.92	2.50	2.65	2.05
dPG-26		4.7	68.1	-156.2	-177.2	-32.4	-64.9	150.3	173.8	2.19	2.57	2.02	2.21	2.59	2.04
dPG-37		4.8	64.0	-157.0	-173.8	-32.4	-79.7	-8.4	178.2	2.36	2.67	2.16	2.56	2.87	2.35
dPG-22		178.5	65.3	25.8	177.6	23.3	-79.2	-10.4	-179.3	2.75	2.82	2.23	3.28	3.35	2.76
dPG-13	ext	-178.9	53.7	-146.2	-178.0	28.8	179.6	-170.0	-177.6	2.67	2.87	2.27	2.70	2.90	2.31
dPG-16		176.1	81.6	-80.4	164.6	-30.7	-60.3	157.8	176.0	3.10	3.29	2.55	2.86	3.05	2.31
dPG-14		0.1	79.2	18.7	-179.8	-32.1	-78.2	-7.1	179.4	2.48	2.61	2.55	2.90	3.02	2.97
dPG-24		5.8	56.4	-149.4	-176.2	26.2	-179.6	-174.8	-178.3	3.92	4.09	2.70	3.79	3.96	2.57
dPG-25		6.1	68.4	20.8	176.6	18.6	-85.8	-6.6	-179.2	4.18	3.36	2.94	4.75	3.93	3.51
dPG-31		4.2	71.2	19.7	171.4	18.1	-61.1	152.7	176.0	3.98	4.01	2.95	4.21	4.25	3.19
dPG-19		174.4	83.0	-73.6	176.3	-32.1	-76.1	-13.3	-179.2	2.99	3.10	3.03	3.04	3.16	3.09
dPG-21		170.4	86.1	-62.2	178.3	-33.0	76.5	10.5	179.9	3.54	3.45	3.08	3.55	3.45	3.08
dPG-18		1.7	57.7	-150.8	-172.5	28.5	78.6	8.1	178.6	2.72	2.94	3.19	3.05	3.28	3.53
dPG-32		4.0	70.9	-156.0	-173.1	-33.1	82.5	-57.1	178.8	4.00	4.20	3.54	4.24	4.45	3.79
dPG-39		3.4	67.4	20.4	172.1	21.5	77.8	13.9	178.9	3.84	3.89	3.55	4.33	4.38	4.04
dPG-41		3.9	52.2	-150.5	-179.6	29.2	-82.2	74.9	-169.9	4.50	4.62	3.64	4.61	4.73	3.75
dPG-11		1.9	65.6	24.8	-178.8	21.4	173.3	174.3	177.1	4.90	4.95	3.80	5.08	5.13	3.99
dPG-40		171.7	81.2	-80.8	176.5	21.6	-175.7	-163.8	-177.6	5.97	6.04	4.14	5.91	5.98	4.08
dPG-30		171.6	81.8	-55.9	178.8	19.8	77.1	11.7	179.5	5.22	5.33	4.17	5.53	5.64	4.48
dPG-38		0.5	58.8	27.1	-174.2	25.5	80.3	-79.4	170.3	5.58	5.58	4.39	5.69	5.68	4.50

dPG-17	-0.6	83.3	12.5	175.2	-33.3	84.6	-56.3	179.6	4.42	4.59	4.50	4.77	4.93	4.84
dPG-27	-174.8	50.7	43.9	-158.8	25.8	86.7	-120.6	176.1	4.24	4.50	4.82	4.25	4.51	4.83
dPG-29	172.0	85.2	-61.7	175.6	-33.2	85.0	-46.7	-178.3	5.09	4.45	4.83	4.97	4.33	4.71
dPG-34	172.0	82.3	-58.8	174.4	19.8	84.1	-43.0	-177.7	6.74	6.75	4.85	6.89	6.90	5.00

[a] Calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) and M06-2X/cc-pVTZ//SMD M06-2X/6-31+G(d) levels of theory in water. The torsion angles listed are for the D-Pro-Gly segment as defined in Fig. 1a. ΔE_e, ΔH, and ΔG are the relative electronic energy, enthalpy, and Gibbs free energy, respectively. ΔH and ΔG were calculated at 25℃ and 1 atm. Only the conformers with $\Delta G < 5$ kcal mol^{-1} at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory are listed. [b] The turn types of the D-Pro-Gly tripeptide are designated depending on Pro puckering, *e.g.*, II′(d) is the type II′ β-turn with a down-puckered D-Pro residue. Extended structures are denoted by "ext".

Table S3 Torsion angles (°) and thermodynamic properties (kcal mol^{-1}) of local minima of Ac-Aib-D-Ala-NHMe optimized in CH_2Cl_2[a]

Conf.	Turn[b]	Aib			D-Ala			DSD-PBEP86-D3BJ/def2-TZVP			M06-2X/cc-pVTZ		
		ϕ_1	ψ_1	ω_1	ϕ_1	ψ_2	ω_2	ΔE_e	ΔH	ΔG	ΔE_e	ΔH	ΔG
BdA-1	I'	58.0	33.2	176.0	73.7	12.0	-179.3	0.00	0.00	0.00	0.00	0.00	0.00
BdA-2	II	-52.8	132.5	177.5	79.0	3.4	-177.6	0.58	0.76	0.27	0.43	0.61	0.12
BdA-3		56.9	38.6	179.7	82.6	-72.0	172.9	2.80	2.79	0.91	2.81	2.80	0.92
BdA-4		-58.8	-34.9	176.5	88.2	-67.5	177.5	2.99	2.90	0.99	2.98	2.89	0.98
BdA-5		76.0	-57.6	-180.0	76.6	17.2	178.6	3.48	3.48	1.00	3.84	3.84	1.36
BdA-6	I	-56.8	-35.6	-176.2	-61.4	-23.5	179.9	1.98	2.02	1.11	1.58	1.62	0.71
BdA-7		-77.0	57.9	178.0	74.6	17.9	179.1	3.67	3.53	1.25	4.17	4.03	1.75
BdA-8		58.4	38.6	-176.4	-62.5	-31.4	178.6	5.00	4.92	1.40	4.61	4.53	1.00
BdA-9		-58.3	-35.6	-179.3	163.4	-157.3	-176.0	3.15	3.07	1.44	2.89	2.82	1.19
BdA-10		-58.4	-36.9	176.5	81.3	14.8	179.1	3.14	3.14	1.52	3.40	3.39	1.77
BdA-11		-179.1	-179.0	178.9	75.4	18.3	178.9	4.30	4.37	1.60	4.24	4.31	1.54
BdA-12		-52.2	140.8	178.7	159.2	-161.8	-177.3	4.14	4.02	1.85	4.00	3.88	1.72
BdA-13		-76.5	55.0	174.4	84.7	-68.7	177.5	3.97	4.06	1.88	4.33	4.42	2.24
BdA-14		53.0	-136.1	179.3	166.5	-161.0	-175.2	4.15	4.05	2.26	3.79	3.69	1.90
BdA-15	II'	52.3	-131.1	-176.8	-61.6	-22.4	178.7	2.62	2.67	2.61	2.01	2.06	2.00
BdA-16		-171.4	36.9	174.2	159.5	-159.9	-176.3	6.77	6.71	2.63	6.40	6.34	2.27
BdA-17		51.3	-137.6	178.4	87.3	-69.9	175.1	3.90	3.89	2.64	3.93	3.92	2.67
BdA-18	ext	-179.3	-179.0	179.1	161.0	-161.2	-175.9	4.17	3.51	2.85	3.88	3.21	2.56
BdA-19		-78.9	43.6	176.3	156.2	-158.6	-177.6	5.44	5.38	2.85	5.37	5.32	2.79
BdA-20		76.3	-55.4	177.4	86.0	-69.1	176.2	3.87	4.08	2.97	4.15	4.36	3.25
BdA-21		171.0	-37.6	-174.8	159.9	-164.8	-177.4	6.89	6.77	3.05	6.55	6.43	2.70
BdA-22		-74.4	65.6	-171.8	60.2	-144.7	-177.9	3.97	4.08	3.06	4.24	4.35	3.33
BdA-23		76.8	-61.7	179.6	160.3	-163.3	-176.0	5.36	4.58	3.94	5.32	4.54	3.89
BdA-24		-59.7	-35.5	-172.0	-75.1	54.2	179.9	5.02	4.25	4.09	5.31	4.54	4.38
BdA-25		-179.5	-178.7	177.6	85.5	-69.2	177.6	4.55	4.92	4.22	4.37	4.74	4.04
BdA-26		77.1	-55.5	-172.3	-75.9	53.7	177.9	6.00	6.16	4.39	6.51	6.67	4.89
BdA-27		59.3	36.0	176.6	-56.1	135.8	-178.2	5.68	5.66	4.47	5.27	5.24	4.05
BdA-28		77.2	-54.8	-174.4	-60.4	-33.5	179.5	5.59	5.70	4.71	5.59	5.70	4.71
BdA-29		-52.2	138.8	-175.6	-77.5	51.2	177.0	5.95	6.07	4.74	6.04	6.16	4.83
BdA-30		-76.7	58.4	-176.7	-59.8	-34.2	178.2	5.40	5.45	4.81	5.35	5.39	4.76
BdA-31		72.6	-63.8	173.4	175.4	36.7	175.9	7.28	7.41	4.82	7.16	7.29	4.69
BdA-32		-76.7	55.8	-174.4	-76.8	49.9	177.0	5.93	5.51	4.96	6.37	5.95	5.40

[a] Calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) and M06-2X/cc-pVTZ//SMD M06-2X/6-31+G(d) levels of theory in CH_2Cl_2. The torsion angles listed are for the Aib-D-Ala segment as defined in Fig. 1b. ΔE_e, ΔH, and ΔG are the relative electronic energy, enthalpy, and Gibbs free energy, respectively. ΔH and ΔG were calculated at 25℃ and 1 atm. Only the conformers with ΔG < 5 kcal mol^{-1} at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory are listed. [b] Extended structures are denoted by "ext".

Table S4 Torsion angles (°) and thermodynamic properties (kcal mol^{-1}) of local minima of Ac-Aib-D-Ala-NHMe optimized in water[a]

Conf.	Turn[b]	Aib			D-Ala			DSD-PBEP86-D3BJ/def2-TZVP			M06-2X/cc-pVTZ		
		ϕ_1	ψ_1	ω_1	ϕ_1	ψ_2	ω_2	ΔE_e	ΔH	ΔG	ΔE_e	ΔH	ΔG
BdA-1	I'	54.6	37.3	175.7	69.6	16.2	-179.1	0.00	0.37	0.00	0.00	0.53	0.00
BdA-5		77.6	-48.9	-174.2	69.1	21.6	179.6	3.73	4.02	0.40	4.09	4.53	0.75
BdA-12		-52.6	140.4	176.2	159.4	-158.7	-176.5	2.91	2.97	0.90	2.92	3.13	0.90
BdA-10		-57.6	-37.3	-173.6	69.2	24.9	179.5	1.75	2.09	1.22	2.02	2.51	1.48
BdA-9		-53.4	-40.0	174.2	164.5	-152.9	-175.2	2.87	2.95	1.44	2.62	2.85	1.18
BdA-14		52.2	-137.3	178.0	166.0	-157.2	-175.9	2.70	3.04	1.53	2.41	2.90	1.24
BdA-6	I	-54.0	-39.6	-175.2	-61.9	-25.0	-179.3	2.10	2.18	1.53	1.75	1.99	1.19
BdA-3		52.3	44.0	-172.2	78.4	-89.2	170.7	2.62	2.67	1.62	2.62	2.83	1.62
BdA-2	II	-52.6	134.5	176.5	69.0	15.7	-178.2	0.15	0.00	1.75	0.00	0.00	1.60
BdA-18	ext	178.8	-179.5	-178.5	159.8	-156.5	-174.7	5.26	5.40	2.09	5.03	5.32	1.85
BdA-4		-54.6	-43.1	179.1	86.0	-67.7	177.5	3.41	3.66	2.35	3.47	3.88	2.41
BdA-19		-77.5	47.6	174.8	160.0	-154.7	-175.4	5.13	5.32	2.50	5.25	5.59	2.61
BdA-11		-178.7	-174.5	-175.2	70.3	21.7	177.7	4.04	4.35	2.69	4.02	4.48	2.65
BdA-8		52.5	43.7	-177.9	-59.0	-36.7	178.0	3.44	3.57	2.85	3.14	3.42	2.54
BdA-27		52.8	43.3	-177.0	-55.7	140.2	178.5	3.55	3.76	3.02	3.22	3.58	2.69
BdA-17		52.6	-141.8	-179.2	85.5	-66.9	179.1	3.22	3.62	3.02	3.33	3.89	3.14
BdA-16		-170.7	42.8	172.7	163.0	-154.0	-175.4	7.54	7.59	3.17	7.30	7.49	2.92
BdA-30		-77.5	56.3	177.0	-56.5	-36.3	-177.9	5.84	6.01	3.35	5.77	6.09	3.28
BdA-2		-50.6	137.6	-178.7	80.3	-78.9	169.5	2.49	2.99	3.39	2.59	3.24	3.48
BdA-40		-49.5	139.3	179.8	-56.0	142.7	177.9	3.39	3.81	3.58	3.06	3.63	3.25
BdA-15	II'	52.4	-132.9	-176.1	-60.4	-23.3	179.5	2.20	2.58	3.74	1.66	2.19	3.19
BdA-7		-74.8	65.3	-176.4	69.8	23.1	177.6	3.82	4.34	4.03	4.27	4.95	4.48
BdA-20		77.2	-51.5	178.9	86.3	-65.9	177.2	5.53	5.87	4.31	5.80	6.29	4.57
BdA-38		54.2	39.6	174.5	151.2	65.4	179.6	5.96	6.29	4.33	6.44	6.92	4.81
BdA-22		-72.0	74.9	-163.3	55.0	-146.6	-175.3	3.75	4.41	4.39	3.73	4.55	4.37
BdA-23		76.1	-63.7	176.4	162.3	-154.4	-175.1	5.16	5.48	4.62	5.36	5.83	4.81
BdA-29		-49.7	140.2	-173.1	-77.4	33.7	175.2	5.15	4.92	4.78	5.14	5.06	4.76
BdA-42		-175.9	64.8	-154.5	55.8	-155.4	-175.6	6.52	6.89	4.98	6.27	6.80	4.73

[a] Calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) and M06-2X/cc-pVTZ//SMD M06-2X/6-31+G(d) levels of theory in water. The torsion angles listed are for the Aib-D-Ala segment as defined in Fig. 1b. ΔE_e, ΔH, and ΔG are the relative electronic energy, enthalpy, and Gibbs free energy, respectively. ΔH and ΔG were calculated at 25℃ and 1 atm. Only the conformers with ΔG < 5 kcal mol^{-1} at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory are listed. [b] Extended structures are denoted by "ext".

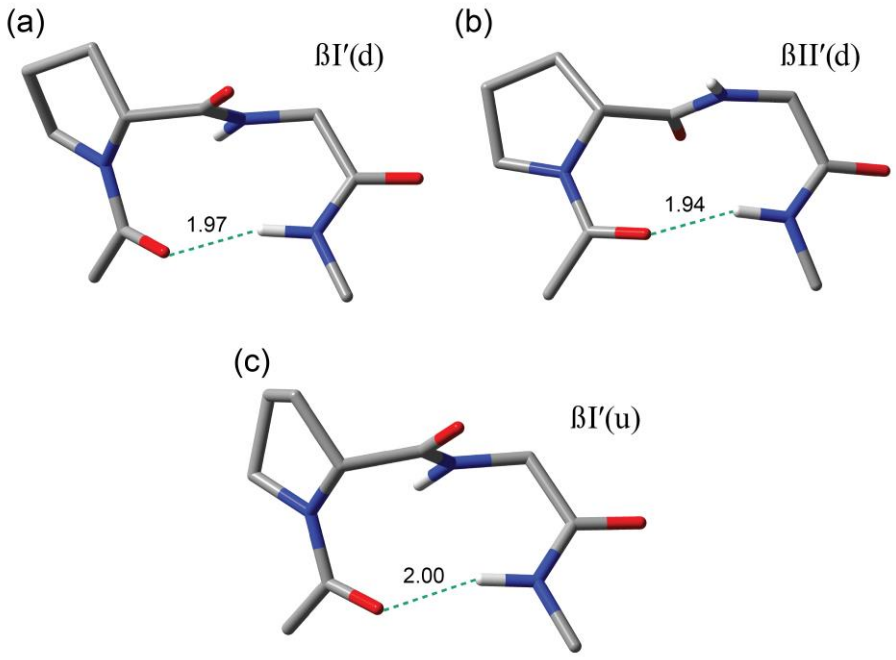

Fig. S1 Preferred conformations of Ac-D-Pro-Gly-NHMe optimized in CH_2Cl_2: (a) dPG-1 (βI′(d); Δ*G* = 0.00), (b) dPG-2 (βII′(d); Δ*G* = 0.13), and (c) dPG-3 (βI′(u); Δ*G* = 0.44). The values of Δ*G* were calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in CH_2Cl_2. All Δ*G* values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å.

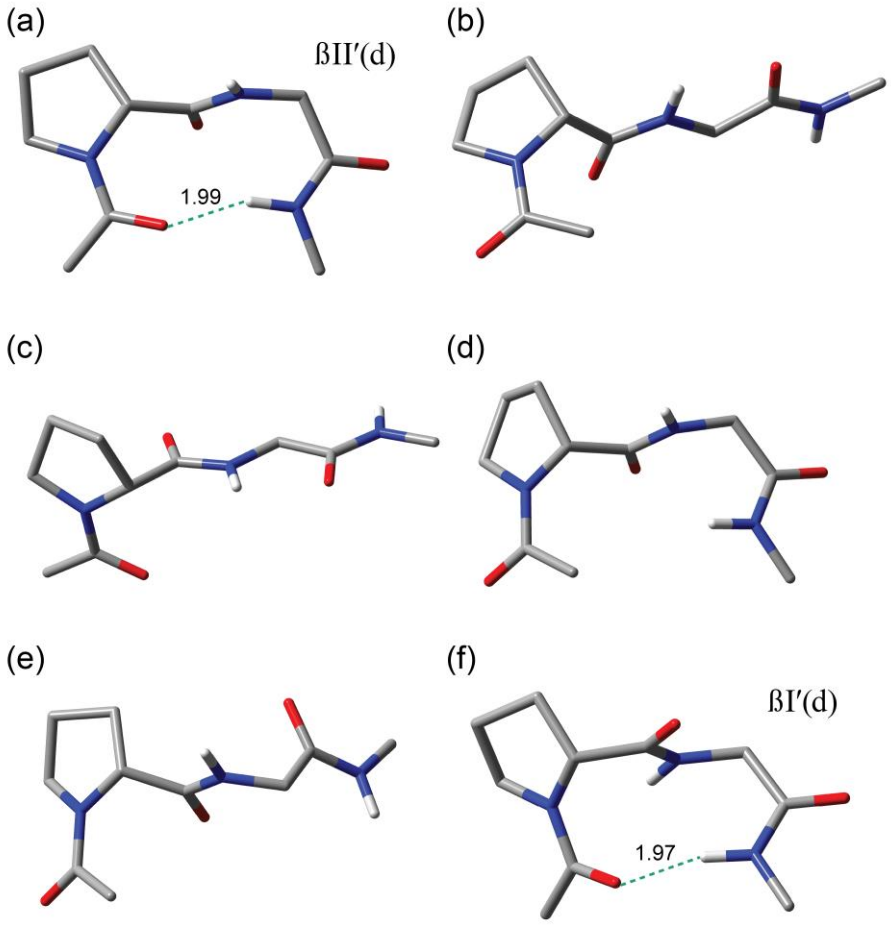

Fig. S2 Preferred conformations of Ac-D-Pro-Gly-NHMe optimized in water: (a) dPG-2 (βII′(d); Δ*G* = 0.00), (b) dPG-7 (ext; Δ*G* = 0.28), (c) dPG-4 (ext; Δ*G* = 0.63), (d) dPG-33 (Δ*G* = 0.66), (e) dPG-36 (Δ*G* = 0.70), and (f) dPG-1 (βI′(d); Δ*G* = 0.78). The values of Δ*G* were calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water. All Δ*G* values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å.

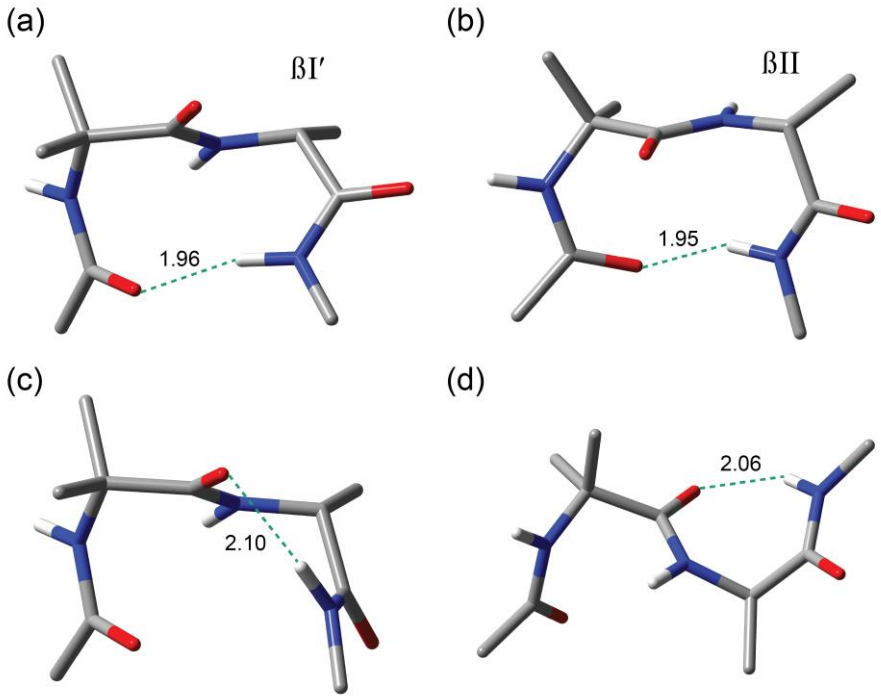

Fig. S3 Preferred conformations of Ac-Aib-D-Ala-NHMe optimized in CH_2Cl_2: (a) BdA-1 (βI′; ΔG = 0.00), (b) BdA-2 (βII; ΔG = 0.27), (c) BdA-3 (ΔG = 0.91), and (d) BdA-4 (ΔG = 0.99). The values of ΔG were calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in CH_2Cl_2. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

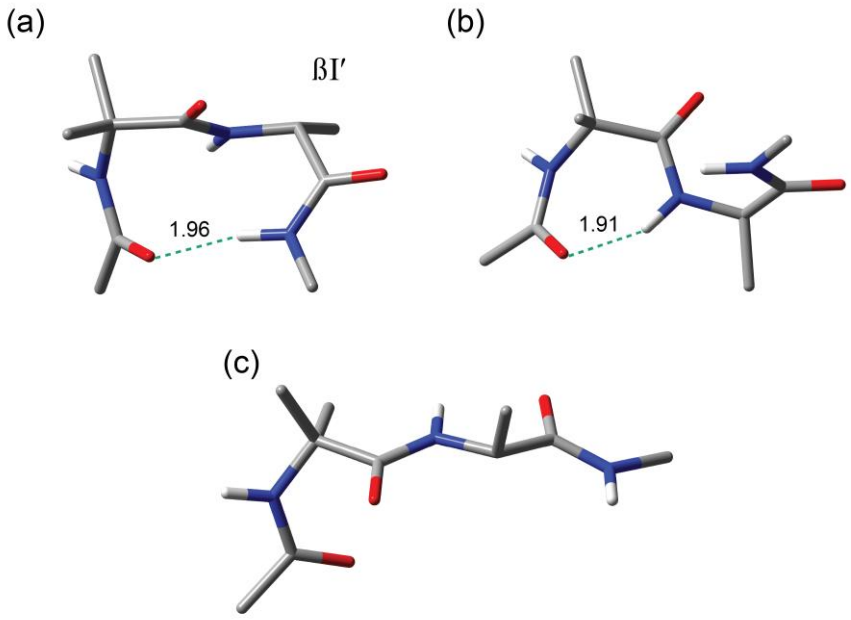

Fig. S4 Preferred conformations of Ac-Aib-D-Ala-NHMe optimized in water: (a) BdA-1 (βI′; ΔG = 0.00), (b) BdA-5 (ΔG = 0.40), and (c) BdA-12 (ΔG = 0.90). The values of ΔG were calculated at the DSD-PBEP86-D3BJ/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å.

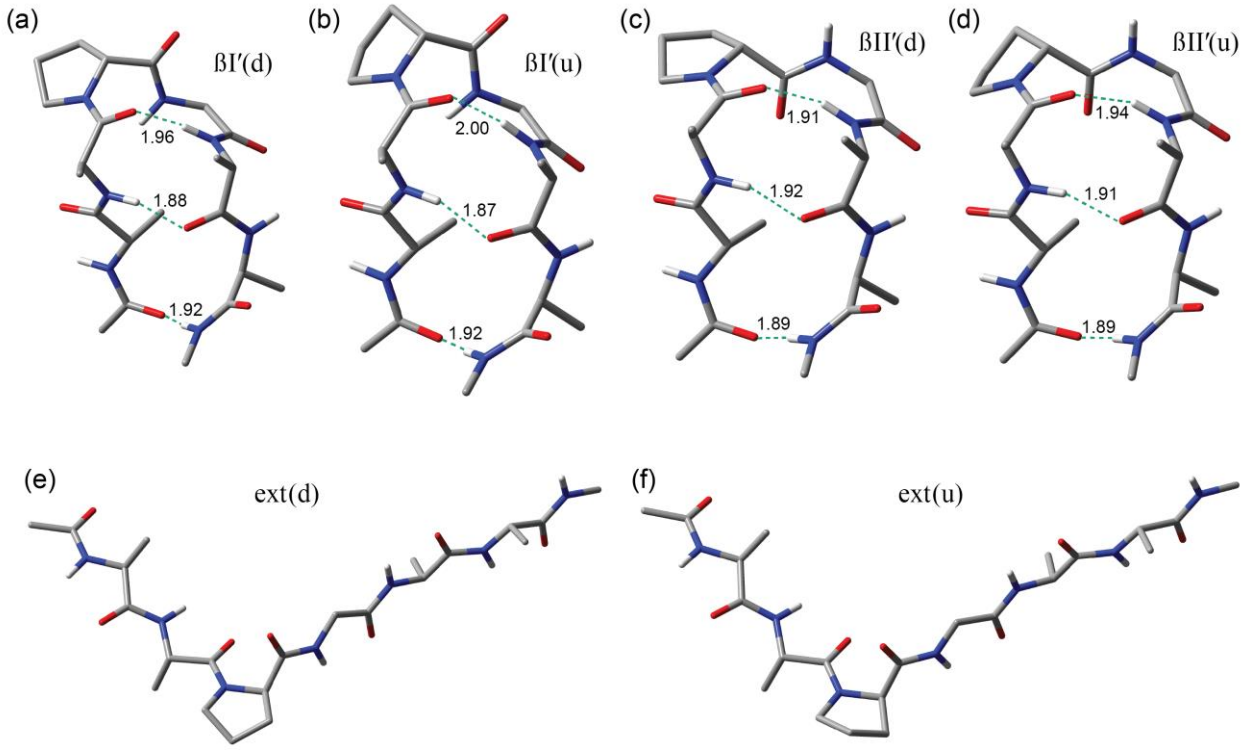

Fig. S5 β-Hairpin and extended structures of Ac-Ala-Ala-D-Pro-Gly-Ala-Ala-NHMe (**hp**$_{dPG}$-**1**) optimized in CH_2Cl_2: (a) βI′(d) (ΔG = 0.00), (b) βI′(u) (ΔG = 1.04), (c) βII′(d) (ΔG = 0.15), (d) βII′(u) (ΔG = 0.47), (e) ext(d) (ΔG = 4.24), and (f) ext(u) (ΔG = 4.53). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in CH_2Cl_2. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

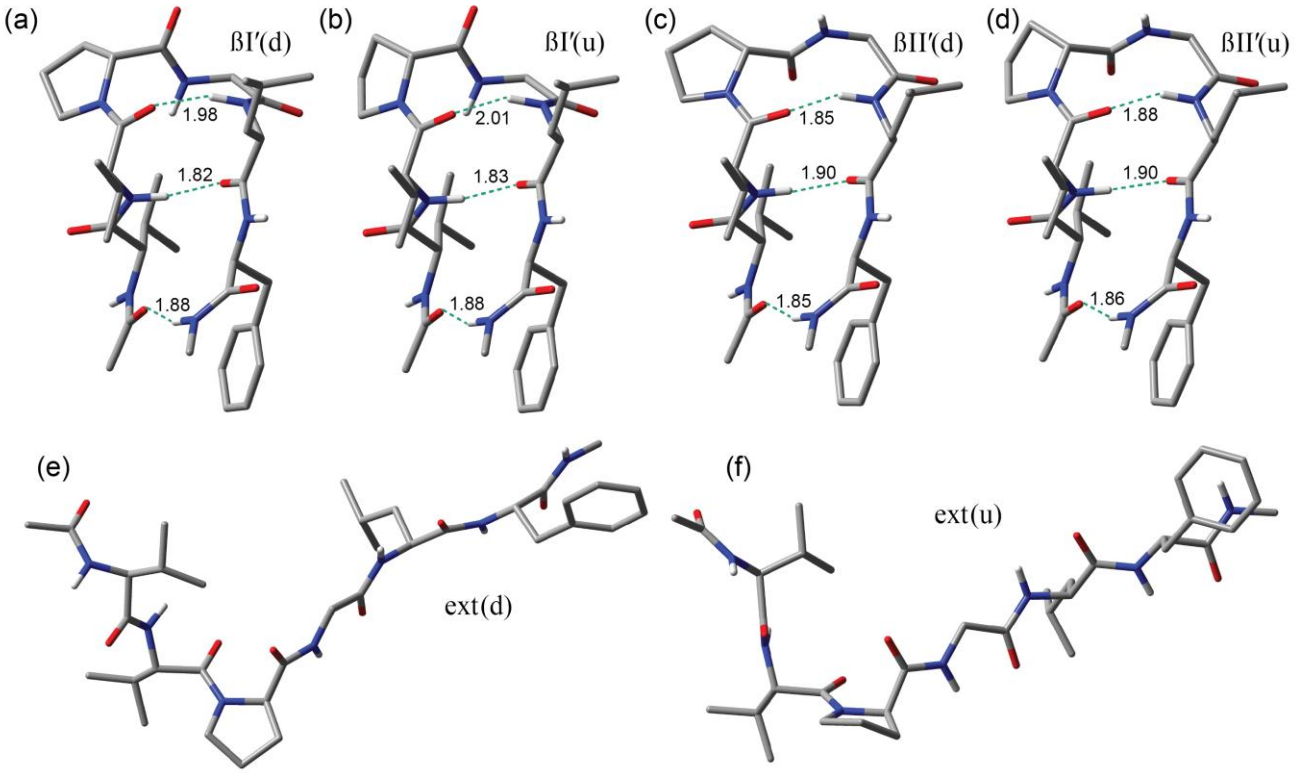

Fig. S6 β-Hairpin and extended structures of Ac-Val-Val-D-Pro-Gly-Leu-Phe-NHMe (**hp**$_{dPG}$-**2**) optimized in CH_2Cl_2: (a) βI′(d) (ΔG = 1.42), (b) βI′(u) (ΔG = 0.33), (c) βII′(d) (ΔG = 1.91), (d) βII′(u) (ΔG = 0.00), (e) ext(d) (ΔG = 1.76), and (f) ext(u) (ΔG = 1.49). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in CH_2Cl_2. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

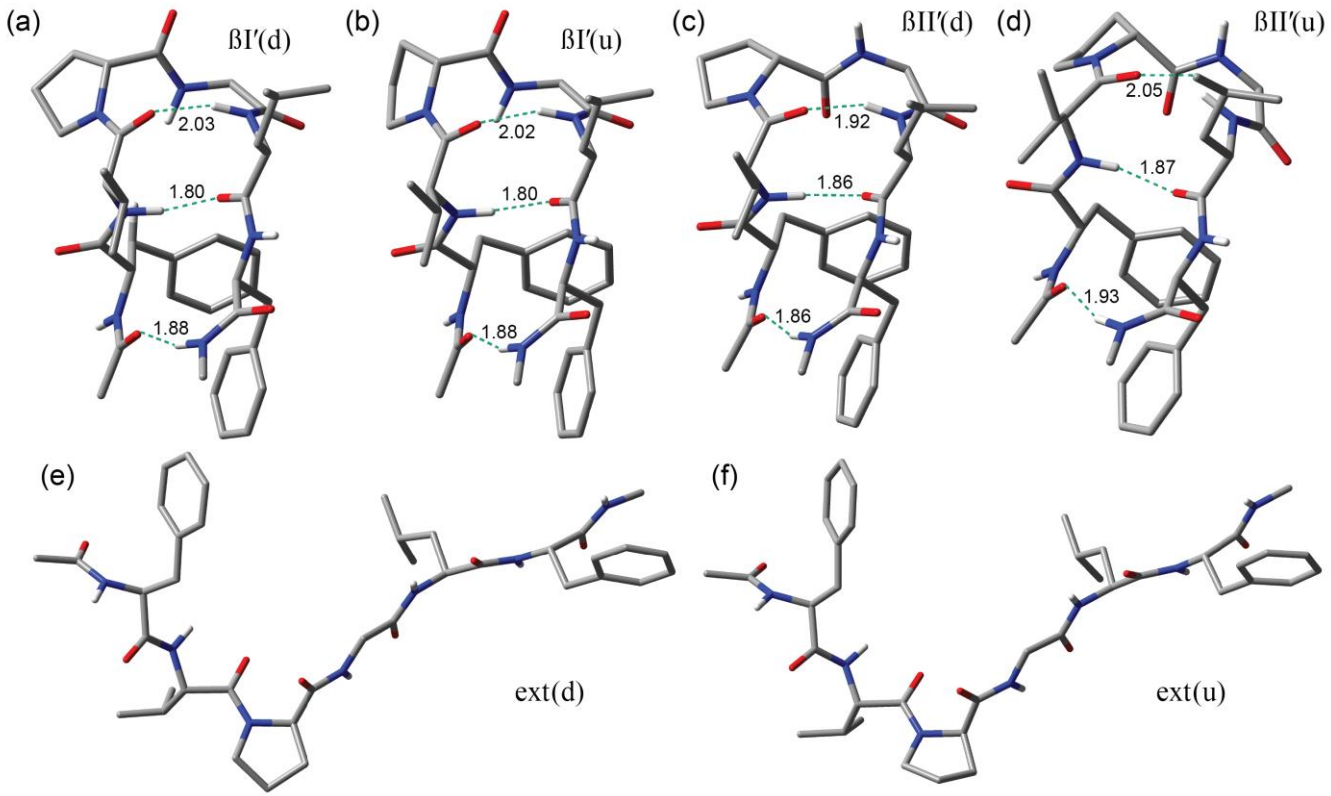

Fig. S7 β-Hairpin and extended structures of Ac-Phe-Val-D-Pro-Gly-Leu-Phe-NHMe (**hp**$_{dPG}$-**3**) optimized in CH_2Cl_2: (a) βI′(d) (ΔG = 4.15), (b) βI′(u) (ΔG = 2.15), (c) βII′(d) (ΔG = 1.37), (d) βII′(u) (ΔG = 0.00), (e) ext(d) (ΔG = 7.43), and (f) ext(u) (ΔG = 3.51). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in CH_2Cl_2. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

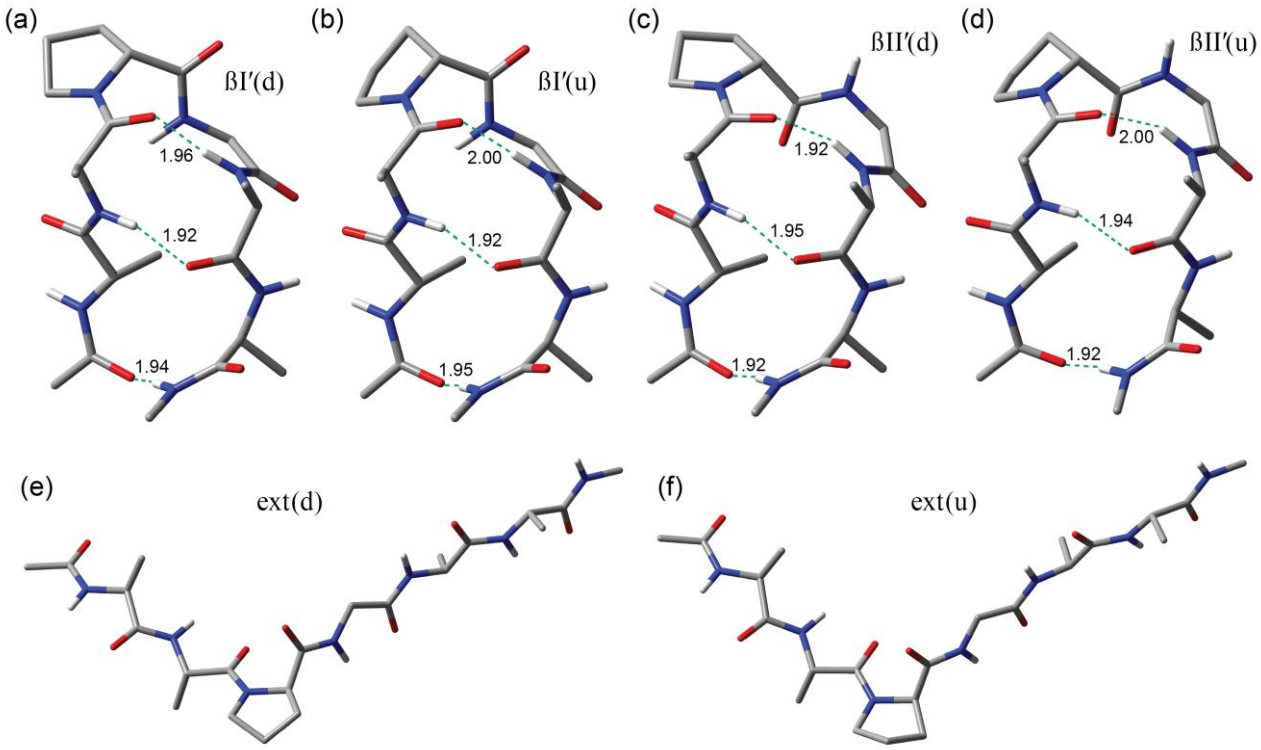

Fig. S8 β-Hairpin and extended structures of Ac-Ala-Ala-D-Pro-Gly-Ala-Ala-NHMe (**hp**$_{dPG}$-**1**) optimized in water: (a) βI′(d) (ΔG = 0.00), (b) βI′(u) (ΔG = 2.04), (c) βII′(d) (ΔG = 2.16), (d) βII′(u) (ΔG = 4.01), (e) ext(d) (ΔG = 10.09), and (f) ext(u) (ΔG = 7.91). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in water. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

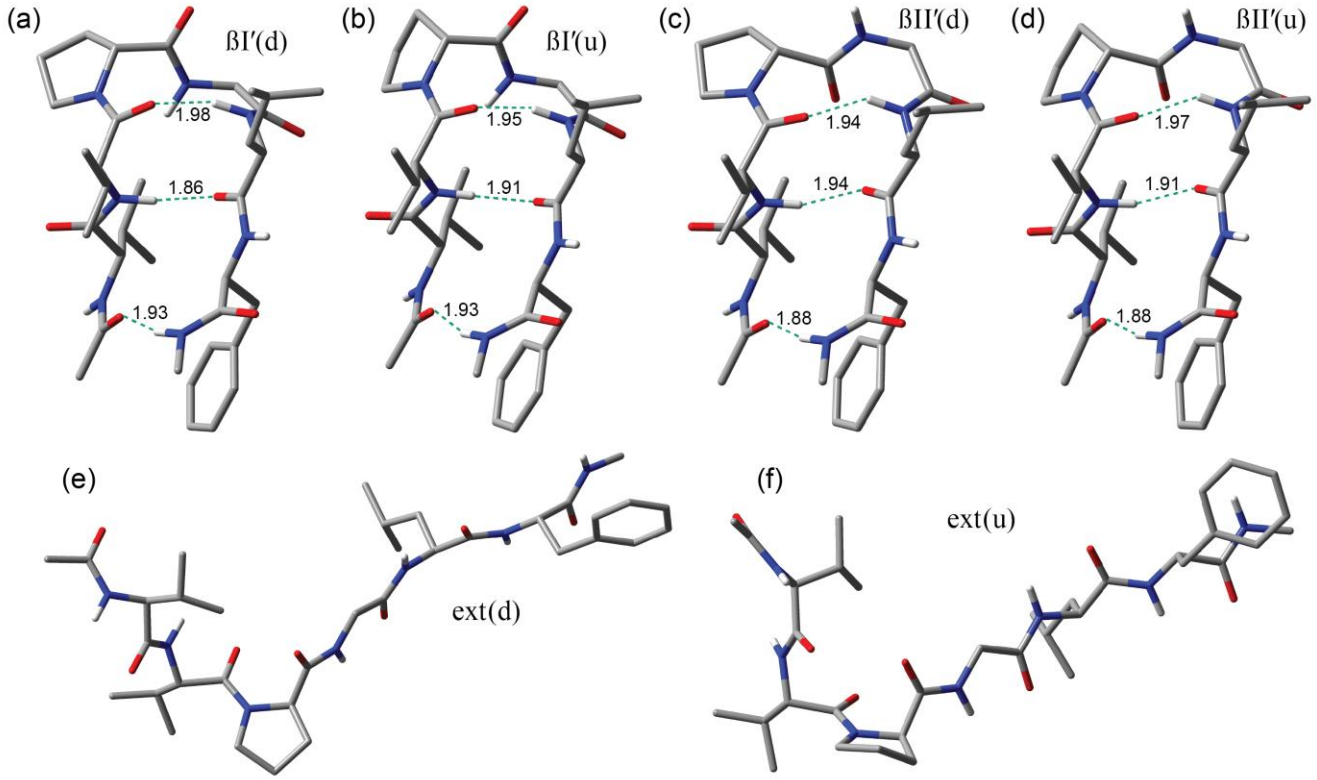

Fig. S9 β-Hairpin and extended structures of Ac-Val-Val-D-Pro-Gly-Leu-Phe-NHMe (**hp**$_{dPG}$-**2**) optimized in water: (a) βI′(d) (ΔG = 0.88), (b) βI′(u) (ΔG = 0.00), (c) βII′(d) (ΔG = 2.17), (d) βII′(u) (ΔG = 0.47), (e) ext(d) (ΔG = 6.74), and (f) ext(u) (ΔG = 6.60). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in water. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

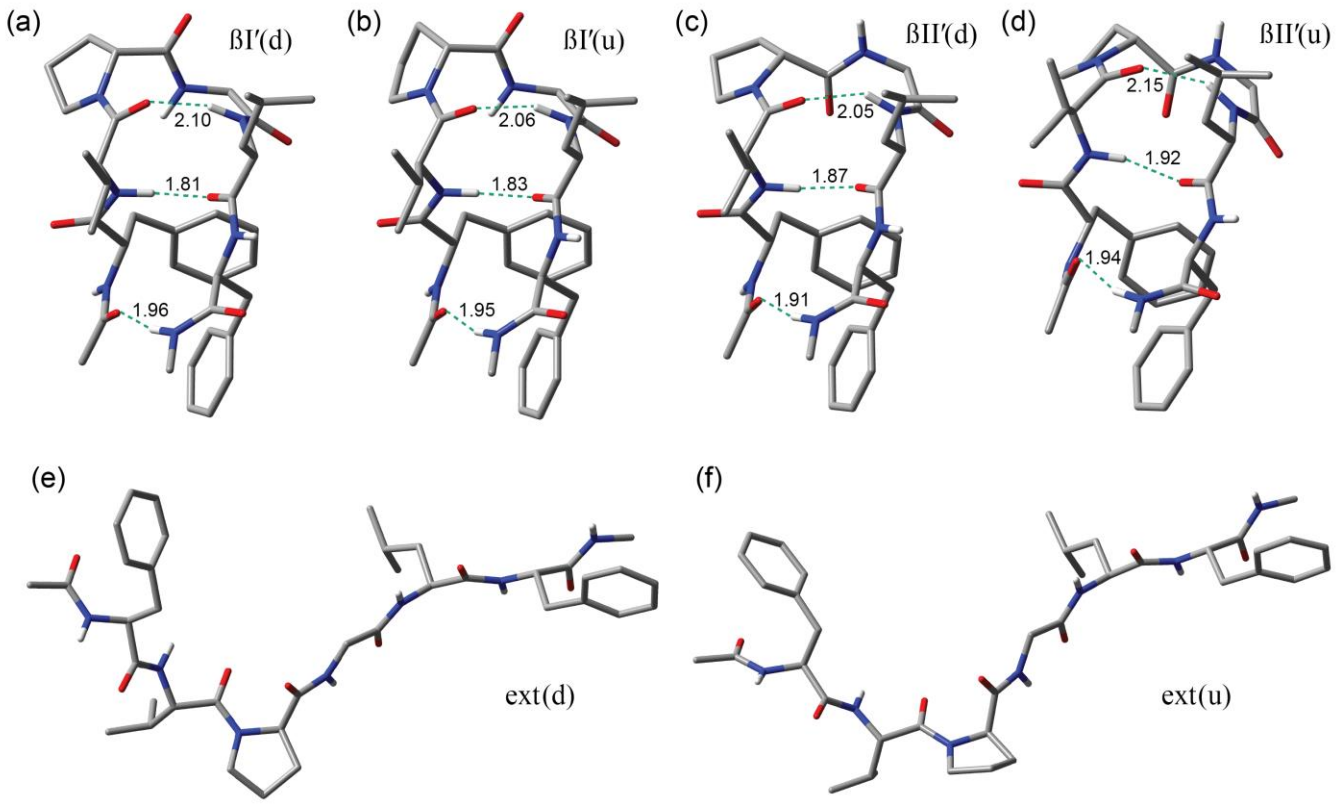

Fig. S10 β-Hairpin and extended structures of Ac-Phe-Val-D-Pro-Gly-Leu-Phe-NHMe (**hp**$_{dPG}$-**3**) optimized in water: (a) βI′(d) (ΔG = 3.45), (b) βI′(u) (ΔG = 2.19), (c) βII′(d) (ΔG = 0.00), (d) βII′(u) (ΔG = 0.40), (e) ext(d) (ΔG = 8.26), and (f) ext(u) (ΔG = 6.11). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in water. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

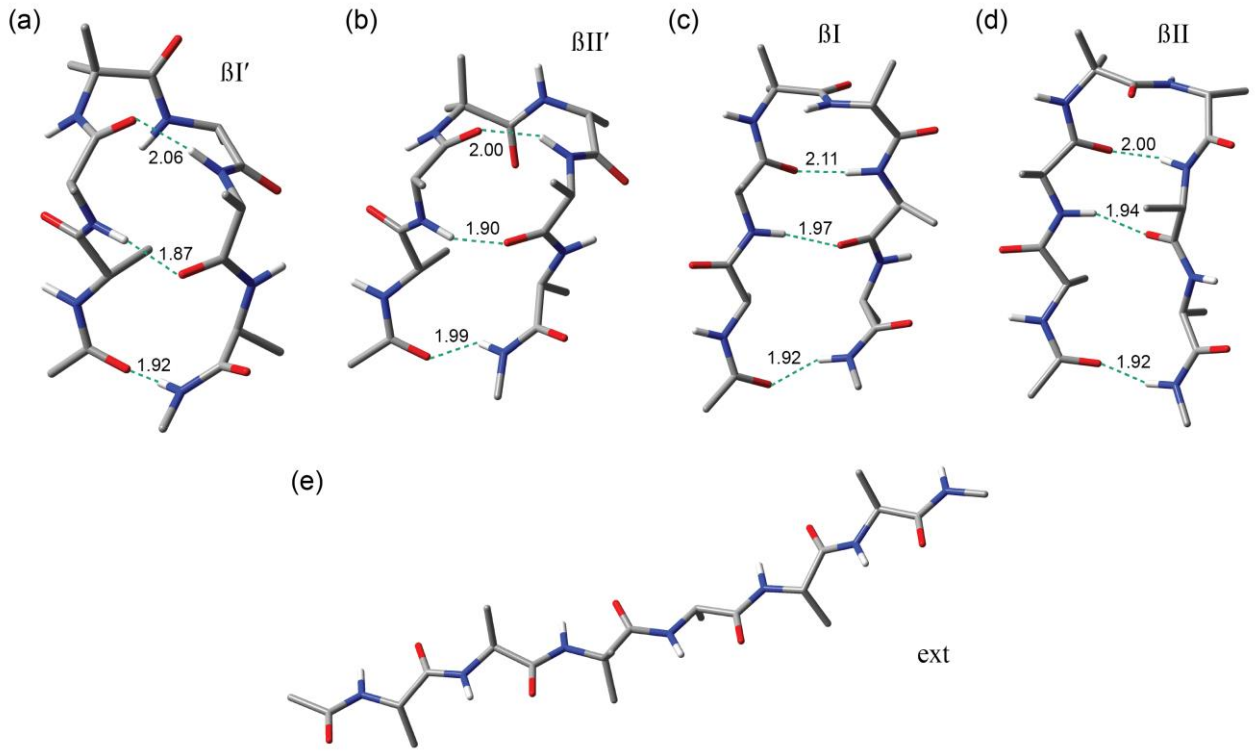

Fig. S11 β-Hairpin and extended structures of Ac-Ala-Ala-Aib-D-Ala-Ala-Ala-NHMe (**hp**$_{BdA}$-**1**) optimized in CH_2Cl_2: (a) βI′ (ΔG = 0.00), (b) βII′ (ΔG = 1.56), (c) βI (ΔG = 2.07), (d) βII (ΔG = 0.93), and (e) ext (ΔG = 2.48). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in CH_2Cl_2. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

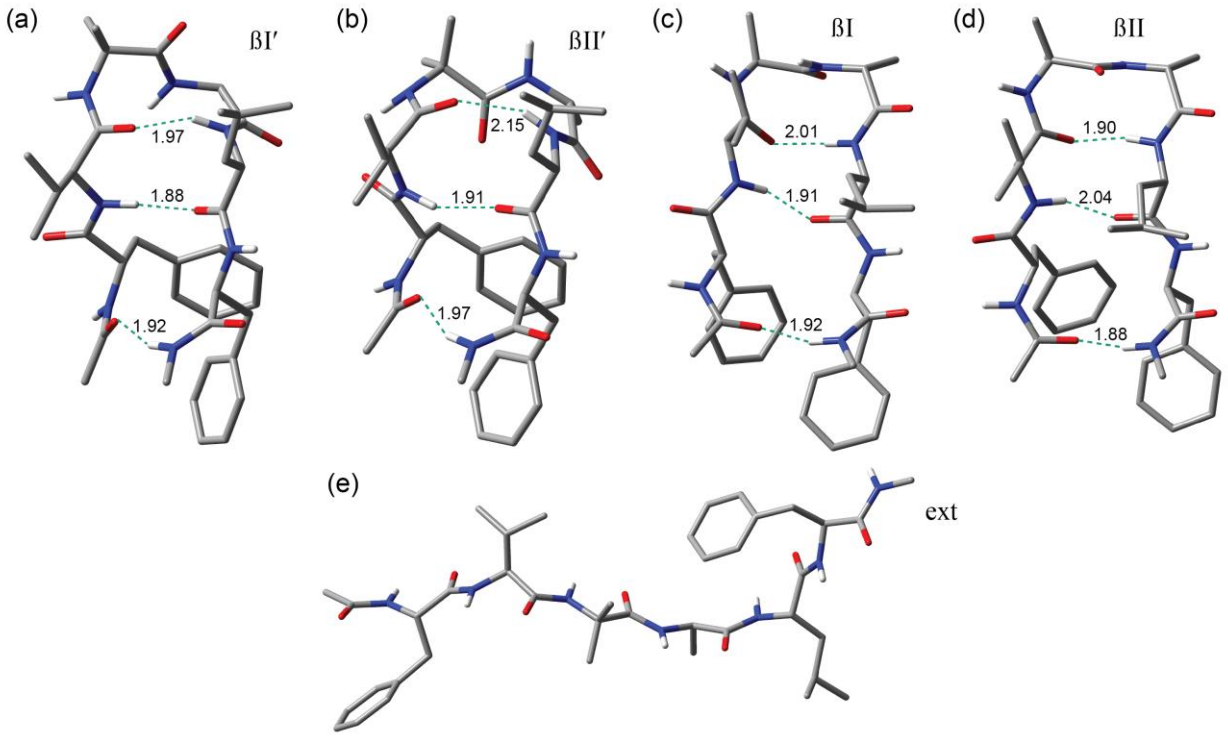

Fig. S12 β-Hairpin and extended structures of Ac-Phe-Val-Aib-D-Ala-Leu-Phe-NHMe (**hp**$_{BdA}$**-2**) optimized in CH_2Cl_2: (a) βI′ (ΔG = 0.00), (b) βII′ (ΔG = 6.96), (c) βI (ΔG = 16.38), (d) βII (ΔG = 9.50), and (e) ext (ΔG = 6.40). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in CH_2Cl_2. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

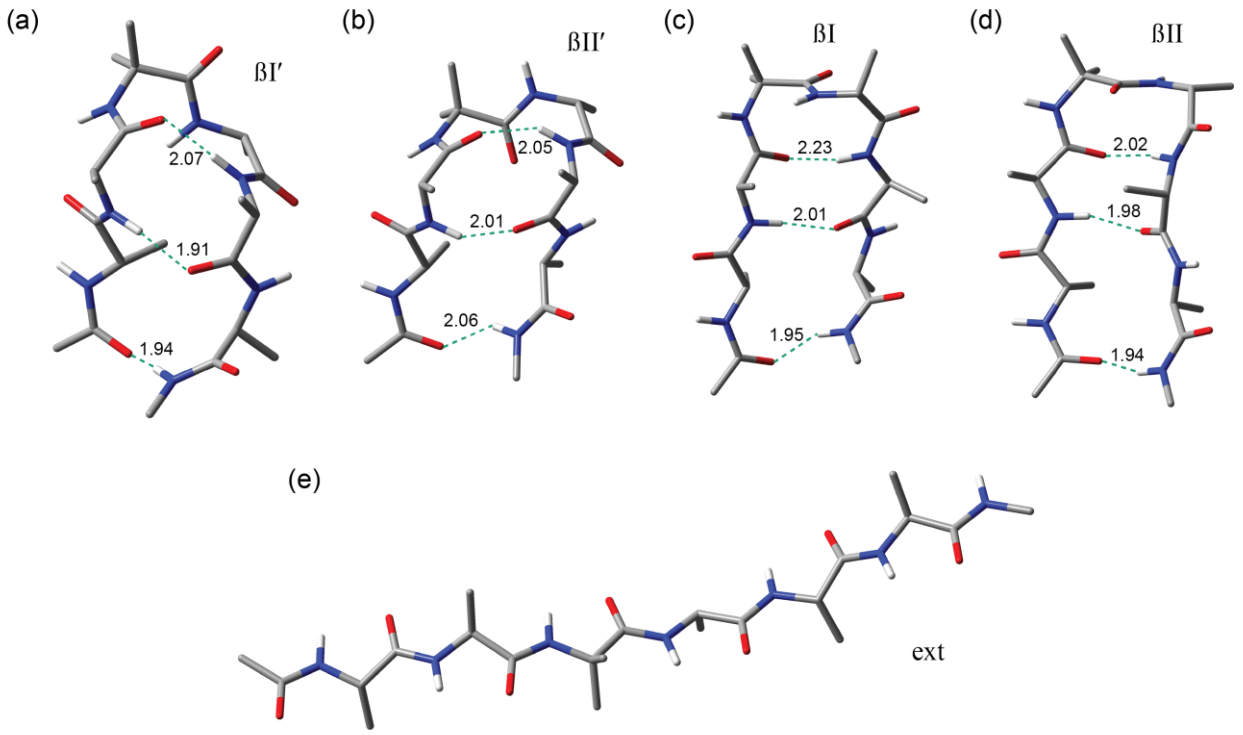

Fig. S13 β-Hairpin and extended structures of Ac-Ala-Ala-Aib-D-Ala-Ala-Ala-NHMe (**hp**$_{BdA}$-**1**) optimized in water: (a) βI′ (ΔG = 0.00), (b) βII′ (ΔG = 6.10), (c) βI (ΔG = 5.46), (d) βII (ΔG = 3.35), and (e) ext (ΔG = 9.20). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in water. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

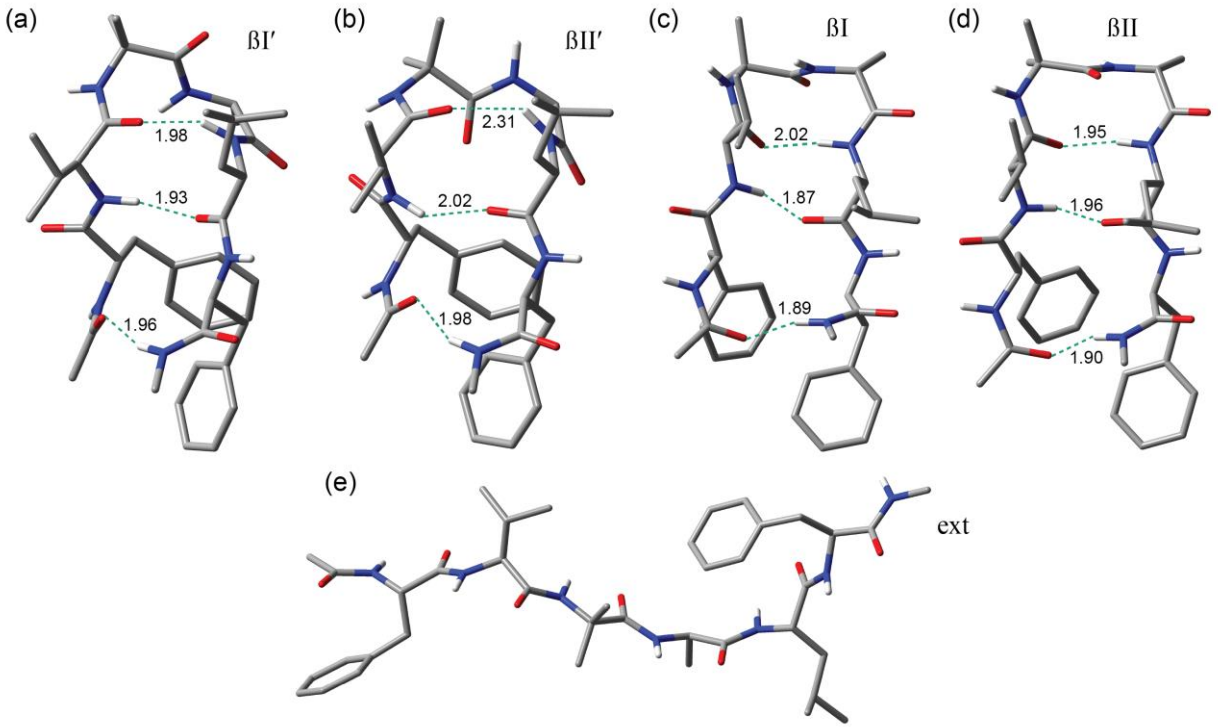

Fig. S14 β-Hairpin and extended structures of Ac-Phe-Val-Aib-D-Ala-Leu-Phe-NHMe (**hp**$_{BdA}$-**2**) optimized in water: (a) βI′ (ΔG = 0.00), (b) βII′ (ΔG = 5.95), (c) βI (ΔG = 16.59), (d) βII (ΔG = 8.14), and (e) ext (ΔG = 9.55). The values of ΔG were calculated at the M06-2X/cc-pVTZ//SMD M06-2X/6-31G(d) level of theory in water. All ΔG values are in kcal mol^{-1}. Intramolecular H-bonds are represented by dotted lines and all non-H-bonded hydrogen atoms are omitted for clarity. All distances are in units of Å .

Table S5 H-bond energies (kcal mol^{-1}) in β-hairpins of the D-Pro-Gly-containing heptapeptides in CH_2Cl_2 and water[a]

Peptide	Turn type	H-Bond	CH_2Cl_2			Water		
			d	ΔE_2	$\Delta E_{2,s}$	*d*	ΔE_2	$\Delta E_{2,s}$
hp$_{dPG}$-1	I′(d)	HB1	1.96	4.09	19.73	1.96	3.69	17.87
		HB2	1.88	8.97		1.92	7.83	
		HB3	1.92	6.67		1.94	6.35	
	I′(u)	HB1	2.00	3.30	19.37	2.00	3.27	16.99
		HB2	1.87	9.45		1.92	7.83	
		HB3	1.92	6.62		1.95	5.89	
	II′(d)	HB1	1.91	7.13	21.95	1.92	6.50	19.74
		HB2	1.92	6.72		1.95	5.92	
		HB3	1.89	8.10		1.92	7.32	
	II′(u)	HB1	1.94	6.29	21.60	2.00	5.04	17.37
		HB2	1.91	7.15		1.94	5.13	
		HB3	1.89	8.16		1.92	7.20	
hp$_{dPG}$-2	I′(d)	HB1	1.98	4.63	22.62	1.98	4.50	19.03
		HB2	1.82	9.13		1.86	7.17	
		HB3	1.88	8.86		1.93	7.36	
	I′(u)	HB1	2.01	4.33	22.65	1.95	4.96	16.67
		HB2	1.83	9.25		1.91	4.68	
		HB3	1.88	9.07		1.93	7.03	
	II′(d)	HB1	1.85	9.81	26.60	1.94	7.04	22.99
		HB2	1.90	6.76		1.94	6.91	
		HB3	1.85	10.03		1.88	9.04	
	II′(u)	HB1	1.88	8.39	24.91	1.97	6.31	22.91
		HB2	1.90	6.69		1.91	7.82	
		HB3	1.86	9.83		1.88	8.78	
hp$_{dPG}$-3	I′(d)	HB1	2.03	3.38	22.00	2.10	2.41	16.31
		HB2	1.80	9.85		1.81	7.77	
		HB3	1.88	8.77		1.96	6.13	
	I′(u)	HB1	2.02	3.93	21.06	2.06	3.23	16.66
		HB2	1.80	8.76		1.83	7.15	
		HB3	1.88	8.37		1.95	6.28	
	II′(d)	HB1	1.92	6.76	23.39	2.05	4.11	18.57
		HB2	1.86	7.32		1.87	7.03	
		HB3	1.86	9.31		1.91	7.43	
	II′(u)	HB1	2.05	4.15	17.65	2.15	2.83	14.43
		HB2	1.87	6.57		1.92	5.24	
		HB3	1.93	6.93		1.94	6.36	

[a] Each β-hairpin had three H-bonds between C=O and H–N groups of backbones in the turn motif and antiparallel β-strands, which were designated by HB1, HB2, and HB3, respectively [HB1 between C=O(2) and H–N(5); HB2 between N–H(2) and O=C(5); HB3 between C=O(Ac) and H–N(NHMe)]. $\Delta E_{2,s}$ is the sum of the second perturbation energy (ΔE_2) of each H-bond between the lone pair orbitals of the carbonyl oxygen with the corresponding N–H antibonding orbital.

Table S6 H-bond energies (kcal mol^{-1}) in β-hairpins of the Aib-D-Ala-containing heptapeptides in CH_2Cl_2 and water[a]

Peptide	Turn type	H-Bond	CH_2Cl_2			Water		
			d	ΔE_2	$\Delta E_{2,s}$	*d*	ΔE_2	$\Delta E_{2,s}$
hp$_{BdA}$-1	I′	HB1	2.06	2.16	19.02	2.07	2.08	16.75
		HB2	1.87	9.50		1.91	7.64	
		HB3	1.92	7.36		1.94	7.03	
	II′	HB1	2.00	4.79	18.99	2.05	4.15	14.71
		HB2	1.90	7.26		2.01	5.28	
		HB3	1.99	6.94		2.06	5.28	
	I	HB1	2.11	1.36	15.12	2.23	0.55	12.36
		HB2	1.97	5.17		2.01	4.10	
		HB3	1.92	8.59		1.95	7.71	
	II	HB1	2.00	4.25	19.55	2.02	4.22	16.88
		HB2	1.95	8.56		1.98	6.75	
		HB3	1.92	6.74		1.94	5.91	
hp$_{BdA}$-2	I′	HB1	1.97	5.79	18.08	1.98	5.54	15.54
		HB2	1.88	5.39		1.93	4.32	
		HB3	1.92	6.90		1.96	5.68	
	II′	HB1	2.15	2.75	14.64	2.31	1.46	11.65
		HB2	1.91	5.32		2.02	3.80	
		HB3	1.97	6.57		1.98	6.39	
	I	HB1	2.01	3.17	21.56	2.02	2.68	23.64
		HB2	1.91	11.24		1.87	12.93	
		HB3	1.92	7.15		1.89	8.03	
	II	HB1	1.90	6.77	21.17	1.95	5.60	22.69
		HB2	2.04	6.87		1.96	8.46	
		HB3	1.88	7.53		1.90	8.63	

[a] Each β-hairpin had three H-bonds between C=O and H–N groups of backbones in the turn motif and antiparallel β-strands, which were designated by HB1, HB2, and HB3, respectively [HB1 between C=O(2) and H–N(5); HB2 between N–H(2) and O=C(5); HB3 between C=O(Ac) and H–N(NHMe)]. $\Delta E_{2,s}$ is the sum of the second perturbation energy (ΔE_2) of each H-bond between the lone pair orbitals of the carbonyl oxygen with the corresponding N–H antibonding orbital.

Cartesian coordinates of the most preferred β-hairpin structures of the **hp**$_{dPG}$**-1**, **hp**$_{dPG}$**-2**, **hp**$_{dPG}$**-3**, **hp**$_{BdA}$**-1**, and **hp**$_{BdA}$**-2** heptapeptides optimized at the SMD M06-2X/6-31G(d) level of theory in water**:**

(1) **hp**$_{dPG}$**-1** with the βI′(d) motif

E_e = -1769.9478575 Hartrees

C	-3.375738	4.502750	-1.742745
C	-2.931730	3.141120	-1.280678
O	-3.725959	2.185254	-1.244255
N	-1.648428	3.021500	-0.915143
C	-1.083102	1.765159	-0.466696
C	0.153236	2.084005	0.365059
O	0.798633	3.118077	0.165530
C	-0.673489	0.865220	-1.637031
N	0.476908	1.157598	1.281547
C	1.686680	1.240014	2.090877
C	1.396483	0.822884	3.524787
C	-0.287643	-2.958569	0.477685
C	-1.467448	-1.984141	0.460307
O	-1.493670	-0.991290	1.203867
C	0.148972	-3.245387	1.903832
N	-2.444560	-2.239818	-0.415879
C	-3.536719	-1.304069	-0.632621
C	-4.231521	-0.990437	0.692119
O	-4.524041	-1.882036	1.496752
C	-4.542796	-1.920570	-1.597541
N	-4.559498	0.293825	0.868988
C	-5.263676	0.717996	2.064491
H	-4.207587	4.829862	-1.113459
H	-3.745974	4.419838	-2.768097
H	-2.575088	5.242991	-1.704053
H	-1.021606	3.817265	-0.964893
H	-1.822175	1.248821	0.151895
H	-1.523771	0.709560	-2.306981
H	0.142498	1.328980	-2.201601
H	-0.083631	0.302705	1.339798
H	2.023374	2.275119	2.055886
H	0.973465	-0.185464	3.554216
H	-0.569680	-3.882258	-0.033041
H	0.993372	-3.938812	1.903647
H	0.449733	-2.321084	2.404356
H	-2.333287	-3.013994	-1.062186
H	-3.140383	-0.372801	-1.053363
H	-4.972745	-2.829251	-1.166269
H	-5.347467	-1.209972	-1.800045
H	-4.219000	0.989648	0.205881
H	-6.226282	0.206203	2.147018
H	-4.678186	0.500232	2.962751
H	-5.437205	1.791822	2.004166
H	-0.340170	-0.105214	-1.258037
H	0.683103	1.518731	3.972017
H	2.316562	0.831276	4.115301
H	-0.676165	-3.694371	2.462557
H	-4.054051	-2.171669	-2.543242
C	2.708738	0.300126	1.454051
O	2.589597	-0.929024	1.604656
N	3.673715	0.803802	0.672841
C	4.016956	2.215613	0.413382
C	4.573682	-0.120812	-0.025475
C	5.466920	2.113849	-0.051454
H	3.369092	2.620380	-0.370596
H	3.904098	2.813783	1.317741
H	5.143064	-0.703968	0.704247
C	5.484339	0.807962	-0.848592
C	3.843203	-1.130622	-0.901016
H	5.767941	2.978687	-0.644989
H	6.126580	2.035509	0.818217
H	5.048665	0.970254	-1.839822
H	6.479997	0.380606	-0.972513
O	4.331584	-2.241155	-1.104057
N	2.697359	-0.714011	-1.485774
H	2.314528	0.193416	-1.237725
C	1.914812	-1.588163	-2.326333
H	1.428427	-1.006901	-3.113025
H	2.582533	-2.308472	-2.805497
C	0.819888	-2.378286	-1.620982
O	0.011700	-3.021714	-2.297112
N	0.799482	-2.346078	-0.276761
H	1.439542	-1.737945	0.235398

(2) **hp**$_{dPG}$**-2** with the βI′(u) motif

E_e = -2275.9683047 Hartrees

C	4.887488	-2.638696	1.125271
C	3.551080	-2.057160	0.754289
O	3.154436	-0.976941	1.220851
N	2.771003	-2.780616	-0.063260
C	1.438086	-2.335176	-0.422467
C	0.557431	-2.330257	0.833914
O	0.607634	-3.253248	1.650952
C	0.846021	-3.262737	-1.500386
C	1.672508	-3.183837	-2.783988
C	-0.608572	-2.899449	-1.800299
N	-0.279798	-1.282911	0.940159
C	-1.199957	-1.104468	2.055648
C	-0.739019	-0.004363	3.021498
C	0.625356	-0.363139	3.604884
C	-1.761561	0.183338	4.142201
C	-1.555542	2.584810	-1.059430
C	-0.224770	1.828003	-0.908009
O	-0.123476	0.642550	-1.261031
C	-1.929875	3.366616	0.206772
N	0.808713	2.491971	-0.378898
C	2.100031	1.843608	-0.219705
C	2.881858	2.615171	0.831655
O	2.914688	3.852989	0.796279
C	2.879429	1.842003	-1.554144
C	4.126262	0.997000	-1.495161
C	5.296974	1.481293	-0.901471
C	6.431012	0.677481	-0.808682
C	6.411046	-0.621596	-1.316917
C	5.251686	-1.111051	-1.915767
C	4.117489	-0.305354	-2.000694
N	3.531548	1.885940	1.742277
C	4.477880	2.516607	2.645557
C	-3.357956	3.920423	0.190259
C	-3.618605	4.780255	-1.044908
C	-3.609778	4.714713	1.470017
H	5.612557	-1.828279	1.218185
H	3.111486	-3.664686	-0.423717
H	1.496217	-1.314351	-0.824411
H	0.883391	-4.285642	-1.101634
H	2.732743	-3.399315	-2.617340
H	1.589797	-2.181761	-3.221445
H	1.295756	-3.903154	-3.517463
H	-1.260996	-3.078229	-0.938638
H	-0.982944	-3.502417	-2.633259
H	-0.683756	-1.841526	-2.085390
H	-0.228312	-0.543855	0.236316
H	-1.239567	-2.053675	2.597858
H	-0.653183	0.927337	2.444890
H	0.982363	0.442309	4.254722
H	1.375244	-0.526571	2.825790
H	0.555238	-1.277143	4.207103
H	-1.403739	0.927567	4.860184
H	-1.908111	-0.759684	4.682665
H	-2.731500	0.518094	3.764406
H	-1.445221	3.270816	-1.905516
H	-1.803454	2.717483	1.081870
H	0.738857	3.476039	-0.140111
H	1.931394	0.814695	0.110574
H	2.203036	1.455643	-2.322658
H	3.119703	2.882043	-1.802134
H	5.320205	2.499973	-0.517596
H	7.333139	1.067859	-0.347058
H	7.295828	-1.247628	-1.248747
H	5.229097	-2.120742	-2.317389
H	3.211225	-0.689731	-2.464586
H	3.541389	0.872086	1.637194
H	3.983628	3.300376	3.223756
H	-4.049859	3.067691	0.176444
H	-4.625308	5.209803	-1.010384
H	-3.535381	4.202829	-1.972341
H	-2.900638	5.608585	-1.095455
H	-3.427213	4.101675	2.359457
H	-4.643119	5.074317	1.511309
H	-2.947766	5.587779	1.519672
H	-1.230300	4.204663	0.319867
H	4.786900	-3.126434	2.100577
H	5.240411	-3.373572	0.398938
H	4.865839	1.761467	3.327985
H	5.310693	2.964008	2.092076
C	-2.567338	-0.793082	1.445479
O	-2.915806	0.376360	1.214455
N	-3.357635	-1.827506	1.119805
C	-3.064205	-3.265661	1.266936
C	-4.680894	-1.581297	0.541649
C	-4.033492	-3.896270	0.271452
H	-2.016093	-3.479050	1.048204
H	-3.281364	-3.585221	2.292054
H	-5.277660	-0.960292	1.214201
C	-5.268953	-2.997220	0.379397
C	-4.650240	-0.824753	-0.783043
H	-3.610026	-3.847199	-0.737770
H	-4.246810	-4.939581	0.509310
H	-5.936712	-3.062223	-0.482398
H	-5.840028	-3.247309	1.277495
O	-5.626532	-0.156104	-1.122319
N	-3.556931	-0.979717	-1.559644
H	-2.751479	-1.459790	-1.169644
C	-3.374013	-0.236914	-2.786539
H	-2.825115	-0.844542	-3.508633
H	-4.355589	-0.011172	-3.210982
C	-2.605175	1.071733	-2.633048
O	-2.091027	1.597076	-3.621973
N	-2.574854	1.613937	-1.398740
H	-2.868713	1.027043	-0.619332

(3) **hp**$_{dPG}$**-3** with the βII′(d) motif

E_e = -2428.3460371 Hartrees

C	4.838107	-1.112636	2.472671
C	3.441374	-0.912960	1.954976
O	2.837687	0.163441	2.094985
N	2.836412	-1.962881	1.376511
C	1.489524	-1.823937	0.869920
C	0.506254	-1.580081	2.018188
O	0.617455	-2.126996	3.116890
C	1.065088	-3.061306	0.060010
C	1.736513	-3.053189	-1.290762
C	2.987561	-3.643127	-1.489634
C	3.649446	-3.506647	-2.710100
C	3.063354	-2.783849	-3.747272
C	1.805368	-2.208799	-3.563988
C	1.147722	-2.343288	-2.343952
N	-0.497454	-0.755163	1.679069
C	-1.627975	-0.438714	2.538747
C	-1.578689	1.007099	3.042598
C	-0.302110	1.228142	3.851338
C	-2.813871	1.322650	3.883845
C	-2.156998	2.150591	-1.547536
C	-0.801913	1.596238	-1.080777
O	-0.597243	0.379106	-0.981612
C	-2.751987	3.112770	-0.509332
C	-4.164280	3.603208	-0.843764
C	-4.229515	4.251845	-2.225076
C	-4.626786	4.579099	0.236522
N	0.137737	2.502056	-0.777687
C	1.473959	2.099334	-0.369460
C	2.120389	3.283277	0.334397
O	2.040921	4.417121	-0.158347
C	2.323679	1.698493	-1.597455
C	3.704024	1.211125	-1.233224
C	3.979789	-0.157326	-1.193735
C	5.243220	-0.621375	-0.830126
C	6.248986	0.283821	-0.497919
C	5.986365	1.653837	-0.539486
C	4.724524	2.112897	-0.909485
N	2.785110	3.010674	1.459871
C	3.638482	4.013270	2.071542
H	5.413803	-0.202997	2.291426
H	3.344086	-2.829950	1.245976
H	1.455671	-0.952982	0.201918
H	1.303907	-3.965680	0.630873
H	-0.021835	-3.016411	-0.069421
H	3.449358	-4.209359	-0.683444
H	4.624478	-3.964645	-2.848283
H	3.579692	-2.674756	-4.696048
H	1.335887	-1.653837	-4.370965
H	0.171111	-1.885701	-2.198792
H	-0.487890	-0.330155	0.748266
H	-1.591916	-1.114915	3.396832
H	-1.560822	1.663940	2.162229
H	0.594699	1.001494	3.266321
H	-0.295595	0.589413	4.742933
H	-0.237470	2.269314	4.182605
H	-3.737582	1.228379	3.305746
H	-2.760330	2.345548	4.269341
H	-2.874247	0.643581	4.742976
H	-1.981608	2.681462	-2.489039
H	-2.090206	3.983355	-0.422877
H	-2.763000	2.614710	0.467936
H	-4.839091	2.737334	-0.831784
H	-5.227642	4.661620	-2.411950
H	-4.008348	3.538134	-3.026241
H	-3.509013	5.076417	-2.296398
H	-4.575122	4.124001	1.231847
H	-5.659223	4.898421	0.060980
H	-3.994152	5.474990	0.243255
H	-0.013973	3.489077	-0.962305
H	1.388562	1.253373	0.318399
H	1.777848	0.910781	-2.128233
H	2.384190	2.574174	-2.253557
H	3.194605	-0.863923	-1.453538
H	5.436834	-1.691132	-0.805258
H	7.232948	-0.073954	-0.209452
H	6.768011	2.365820	-0.291116
H	4.528542	3.183060	-0.954226
H	2.902504	2.034167	1.729042
H	3.062786	4.910493	2.308383
H	4.782586	-1.276663	3.553876
H	5.336820	-1.966834	2.010085
H	4.050057	3.602998	2.992973
H	4.461684	4.290762	1.403540
C	-2.845149	-0.733277	1.662856
O	-3.366193	0.158568	0.976305
N	-3.264525	-2.007876	1.584650
C	-2.630675	-3.189825	2.187827
C	-4.162514	-2.384338	0.487200
C	-3.684233	-4.265051	1.949697
H	-1.693175	-3.425572	1.667145
H	-2.420708	-3.025772	3.245411
H	-5.144878	-1.924427	0.627955
C	-4.213254	-3.926545	0.552592
C	-3.534954	-1.935881	-0.828082
H	-3.266734	-5.271683	2.009902
H	-4.478648	-4.168661	2.695706
H	-3.541896	-4.343365	-0.204480
H	-5.220471	-4.301294	0.366545
O	-2.330858	-2.096958	-1.037610
N	-4.358779	-1.409168	-1.752117
H	-5.320889	-1.206964	-1.507453
C	-3.823402	-0.939245	-3.010789
H	-3.234661	-1.725930	-3.487683
H	-4.655339	-0.687332	-3.671793
C	-2.920233	0.286359	-2.905225
O	-2.160362	0.564074	-3.835700
N	-3.066250	1.056934	-1.811602
H	-3.542333	0.663256	-1.002728

(4) **hp**$_{BdA}$-**1** with the βI′ motif

E_e = -1771.1555245 Hartrees

C	-3.477581	4.462578	-1.635926
C	-3.008383	3.109078	-1.176267
O	-3.761310	2.121234	-1.209881
N	-1.747647	3.032603	-0.726071
C	-1.156394	1.777348	-0.303511
C	0.055846	2.104369	0.556217
O	0.772132	3.076163	0.285511
C	-0.686566	0.939397	-1.497007
N	0.296998	1.262391	1.572570
C	1.504951	1.377904	2.381667
C	1.285146	0.798883	3.766417
C	-0.010486	-2.837828	0.721855
C	-1.279137	-1.982082	0.636633
O	-1.484615	-1.038120	1.413545
C	0.433150	-3.014679	2.161261
N	-2.134795	-2.301927	-0.341469
C	-3.272967	-1.457417	-0.668691
C	-4.136947	-1.218710	0.568611
O	-4.446857	-2.141508	1.330272
C	-4.116472	-2.142873	-1.737787
N	-4.595446	0.030724	0.704934
C	-5.492221	0.377932	1.791745
H	-4.349406	4.749771	-1.042242
H	-3.794863	4.386539	-2.679319
H	-2.706265	5.228886	-1.545057
H	-1.141359	3.844970	-0.758312
H	-1.895001	1.221873	0.280864
H	-1.506092	0.794364	-2.206258
H	0.132774	1.454677	-2.009664
H	-0.268591	0.413393	1.659263
H	1.746920	2.440893	2.450827
H	0.982040	-0.249880	3.711922
H	-0.203932	-3.808121	0.256941
H	1.341319	-3.620955	2.200210
H	0.636065	-2.043254	2.618450
H	-1.827932	-2.984466	-1.028718
H	-2.917407	-0.490848	-1.042800
H	-4.514120	-3.087348	-1.355539
H	-4.950546	-1.498422	-2.025276
H	-4.249100	0.761650	0.084139
H	-6.419507	-0.198158	1.727296
H	-5.027700	0.179295	2.762030
H	-5.726938	1.439439	1.720348
H	-0.335880	-0.040842	-1.156667
H	0.505092	1.362572	4.283142
H	2.209255	0.861312	4.346627
H	-0.350785	-3.513623	2.736215
H	-3.510452	-2.344186	-2.625865
C	2.631751	0.658610	1.637925
O	2.861544	-0.547129	1.802689
N	3.301549	1.410016	0.750289
H	2.999413	2.370434	0.609985
C	4.392901	0.883781	-0.070753
C	4.701252	1.917155	-1.157887
C	5.628330	0.621469	0.786489
C	3.955408	-0.418202	-0.771520
H	3.802026	2.174480	-1.725974
H	5.099709	2.826854	-0.698763
H	5.450717	1.516843	-1.845664
H	6.446940	0.252097	0.165225
H	5.938012	1.556902	1.259665
H	5.416921	-0.118041	1.562184
O	4.728665	-1.366991	-0.888693
N	2.716122	-0.408870	-1.311187
H	2.135678	0.417665	-1.195084
C	2.194005	-1.504811	-2.105817
C	1.750751	-1.042310	-3.488975
H	3.012397	-2.225349	-2.207845
C	1.062484	-2.251856	-1.393134
H	0.944216	-0.305862	-3.416196
H	2.595211	-0.588207	-4.012291
H	1.392112	-1.893518	-4.069860
O	0.253103	-2.927081	-2.037490
N	1.033093	-2.172895	-0.050560
H	1.685726	-1.567099	0.445613

(5) **hp**$_{BdA}$-**2** with the βI′ motif

E_e = -2429.5478772 Hartrees

C	4.415928	-0.652711	3.140405
C	3.085426	-0.556869	2.447309
O	2.492110	0.529112	2.324877
N	2.536568	-1.695272	1.994991
C	1.252655	-1.670291	1.324779
C	0.131894	-1.403599	2.333543
O	0.129932	-1.931751	3.447898
C	0.978391	-2.998921	0.600728
C	1.913946	-3.185047	-0.567904
C	3.117648	-3.880886	-0.422971
C	4.025050	-3.960213	-1.479038
C	3.733264	-3.350027	-2.697330
C	2.528067	-2.666290	-2.856424
C	1.625724	-2.582712	-1.798319
N	-0.849383	-0.605082	1.878065
C	-2.057241	-0.328842	2.642115
C	-3.201188	-0.312331	1.633089
O	-3.303606	0.616543	0.820144
C	-2.003640	1.006679	3.399916
C	-0.828238	1.035894	4.372123
C	-3.327145	1.236250	4.128681
N	-4.039108	-1.358404	1.635880
C	-5.194309	-1.439094	0.736833
C	-4.742964	-1.215943	-0.721084
O	-5.446079	-0.592281	-1.517266
C	-6.247339	-0.401785	1.120189
C	-5.770797	-2.853603	0.840919
N	-3.577654	-1.791912	-1.079540
C	-3.047993	-1.757404	-2.433715
C	-2.187705	-0.512197	-2.705835
O	-1.321186	-0.521786	-3.584218
C	-2.256001	-3.026582	-2.715237
N	-2.485006	0.588388	-1.987547
C	-1.585203	1.722049	-1.980391
C	-0.255760	1.290041	-1.347587
O	-0.123577	0.166516	-0.844127
C	-2.187699	2.883047	-1.173117
C	-3.632920	3.234556	-1.539839
C	-3.748779	3.685946	-2.993956
C	-4.143906	4.315807	-0.589453
N	0.732341	2.194303	-1.326776
C	2.027258	1.858235	-0.759338
C	2.698294	3.126111	-0.258514
O	2.797635	4.116789	-0.995947
C	2.931842	1.183556	-1.810668
C	4.256602	0.768686	-1.223906
C	4.382716	-0.475700	-0.601619
C	5.585594	-0.858732	-0.011692
C	6.676553	0.009550	-0.027204
C	6.557013	1.258408	-0.637194
C	5.355118	1.633843	-1.234704
N	3.191089	3.073048	0.981351
C	4.031253	4.141321	1.490792
H	5.083469	0.108202	2.728853
H	3.028627	-2.573669	2.110892
H	1.263925	-0.865858	0.584102
H	1.071232	-3.820692	1.320307
H	-0.059528	-2.973329	0.249851
H	3.345138	-4.361284	0.526611
H	4.959586	-4.497827	-1.348336
H	4.439086	-3.410260	-3.520160
H	2.290699	-2.193538	-3.805191
H	0.695718	-2.031592	-1.925154
H	-0.756817	-0.193010	0.948296
H	-2.187974	-1.146821	3.358469
H	-1.866519	1.797658	2.651033
H	0.128523	0.905769	3.856359
H	-0.924690	0.242579	5.122252
H	-0.799627	1.996177	4.896787
H	-4.172071	1.294328	3.432945
H	-3.295456	2.173382	4.692309
H	-3.522658	0.422255	4.837038
H	-3.929820	-2.078553	2.342377
H	-5.852294	0.612423	1.025260
H	-6.553565	-0.573148	2.155687
H	-7.122193	-0.498823	0.473817
H	-5.009223	-3.609559	0.629511
H	-6.591008	-2.968874	0.127695
H	-6.161598	-3.016827	1.850020
H	-3.026336	-2.264586	-0.370244
H	-3.903352	-1.690968	-3.115586
H	-2.904441	-3.900893	-2.626607
H	-1.426575	-3.128603	-2.006566
H	-1.844475	-2.994879	-3.724839
H	-3.029785	0.465033	-1.136759
H	-1.389840	2.029113	-3.012873
H	-1.557515	3.768219	-1.324657
H	-2.135514	2.626054	-0.108258
H	-4.257375	2.341541	-1.398104
H	-4.780537	3.963713	-3.233114
H	-3.445896	2.899906	-3.693665
H	-3.112503	4.561311	-3.173906
H	-4.096942	3.976476	0.451484
H	-5.183017	4.576272	-0.815762
H	-3.540295	5.227309	-0.677063
H	0.632388	3.085018	-1.804807
H	1.858206	1.173418	0.074483
H	2.393127	0.308506	-2.191960
H	3.074743	1.888595	-2.636617
H	3.528747	-1.149498	-0.585787
H	5.668566	-1.836111	0.457744
H	7.615511	-0.285150	0.431880
H	7.403449	1.938625	-0.652706
H	5.261306	2.609203	-1.708214
H	3.107919	2.203235	1.507298
H	3.506475	5.097961	1.437744
H	4.263969	-0.433169	4.201672
H	4.873573	-1.638526	3.039607
H	4.275066	3.925306	2.530234
H	4.958172	4.216656	0.912144