Supplementary information

Helix preferences of cyclopentane-containing β/γ-hybrid peptides

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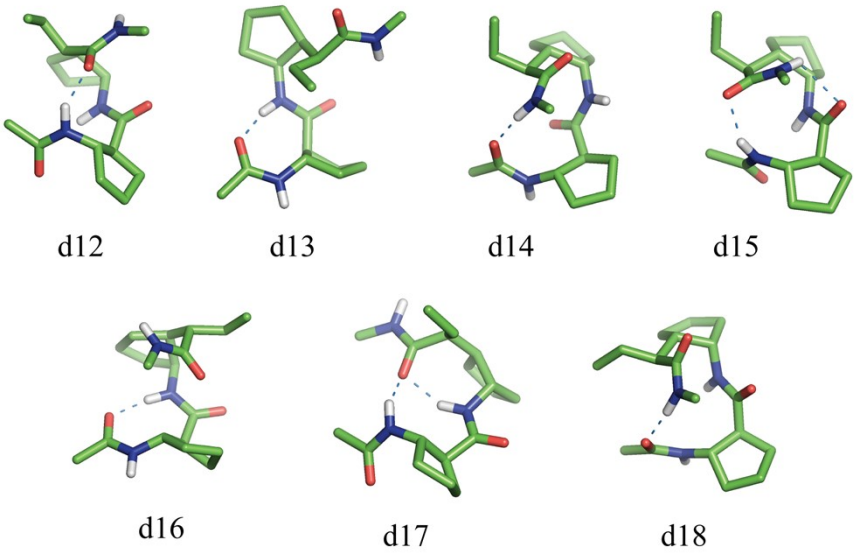

Fig. S1 Conformers d12–d18 of Ac-βAc$_5$a-γ(Et)Ac$_5$a-NHMe optimized at the PCM M06-2X/6-31+G(d) level of theory in chloroform. For clarity, all non-polar hydrogen atoms are omitted. All H-bonds are represented by dotted lines.

Table S1 H-bond types and torsion angles (deg) of 16 local minima of the pentamer composed of βAc$_5$a-γ(Et)Ac$_5$a dimeric units optimized at the PCM M06-2X/6-31+G(d) level of theory in chloroform[a]

Conf.	H-bond type[b]	Residues	ϕ	θ	ζ	ψ	χ^1
p01	H_{13} ($H_{13}^{I'}$)	β1	-63	113		-143	-20
		γ2	-152	51	57	-111	-27
		β3	-127	111		-93	-20
		γ4	-137	51	58	-128	-27
		β5	-96	92		-108	-2
p02	$C_{8/9}$-ribbon ($C_{8/9}^{IV'}$)	β1	-74	128		-62	-33
		γ2	-98	58	79	-94	-36
		β3	-70	128		-62	-33
		γ4	-98	59	79	-94	-36
		β5	-70	129		-63	-33
p03	$2C_{8/13}$	β1	-73	127		-83	-31
		γ2	-172	50	52	-111	-24
		β3	-72	126		-81	-30
		γ4	-171	50	52	-112	-25
		β5	-71	127		-65	-32
p04	$2C_{13}$, $C_{13/17}$ ($H_{18/17}^{I}$)	β1	-118	110		-105	-19
		γ2	-111	43	54	-146	-19
		β3	-86	104		-117	-13
		γ4	180	55	69	-101	-31
		β5	-148	67		-98	34
p05	$C_{8/9}$-ribbon ($C_{8/9}^{IV'}$)	β1	-71	131		-69	13
		γ2	-97	59	79	-91	-36
		β3	-67	131		-68	13
		γ4	-97	59	80	-91	-36
		β5	-67	132		-70	13
p06	$H_{11/13}$	β1	65	82		-83	42
		γ2	-145	39	45	54	-13
		β3	71	94		-108	36
		γ4	-131	44	42	58	-21
		β5	61	101		-100	-15
p07	C_{17}, C_{18}, C_{13} ($H_{18/17}^{II'}$)	β1	-157	98		-157	-12
		γ2	-140	50	57	-106	-26
		β3	-161	123		-167	-29
		γ4	-168	51	57	-100	-23
		β5	-120	92		-108	-4
p08	$H_{13/11}$ ($H_{13/11}^{II'}$)	β1	-150	66		65	22
		γ2	77	35	60	-151	-35
		β3	-111	71		99	43
		γ4	67	17	57	-148	-34
		β5	-75	68		74	41
p09	$2C_8C_9$, C_8 ($C_{8/9}^{II'}$)	β1	-108	70		5	34
		γ2	-101	57	78	-111	-39
		β3	-104	62		33	36
		γ4	-89	62	68	-126	-36

		β5	-66	127		-64	-33
p10	$2C_{8/13}$, C_8	β1	-76	134		-81	12
		γ2	-177	48	47	-135	-18
		β3	-81	131		-80	13
		γ4	-176	52	52	-131	-28
		β5	-80	127		-60	15
p11	$3C_8$	β1	-74	128		-60	15
		γ2	-143	51	54	65	-26
		β3	-75	130		-68	14
		γ4	-122	42	44	47	-17
		β5	-74	132		-69	13
p12	$3C_8$	β1	-73	129		-61	-34
		γ2	-155	42	46	48	-15
		β3	-94	110		-46	-22
		γ4	-121	32	41	45	-3
		β5	-86	122		-60	-30
p13	$3C_8$	β1	-81	122		-54	-31
		γ2	66	5	50	37	-31
		β3	-77	124		-58	-31
		γ4	66	2	46	44	-29
		β5	-76	129		-65	-34
p14	$H_{15/16}$ ($H_{15/16}^{II'}$)	β1	-165	111		-128	-21
		γ2	-147	49	-84	96	-18
		β3	67	75		-165	20
		γ4	-115	56	-64	-76	-43
		β5	-121	90		78	38
p15	C_{20}, C_{22}, $2C_7$ ($H_{20/22}^{V}$)	β1	60	112		-139	-23
		γ2	-148	52	-84	-150	-18
		β3	58	106		-132	-19
		γ4	-119	3	-74	-121	-26
		β5	66	73		179	42
p16	$3C_8$, $C_{9/18}$	β1	32	62		-109	35
		γ2	-104	59	75	-75	-37
		β3	42	63		-106	39
		γ4	-113	48	62	-157	-30
		β5	33	64		-108	42

[a] Torsion angles are defined in Fig. 3. [b] C*n* and C*n*/*m* represent an *n*-membered H-bond and a bifurcated H-bond with *n*- and *m*-membered pseudorings, respectively. The helical structure with C_n (or $C_{n/m}$) H-bonds was represented by H_n (or $H_{n/m}$). The initial structures for optimization were shown in parentheses, taken from ref. s1. The primed type of H-bond stands for the enantiomer of the corresponding helical structure in ref. s1.

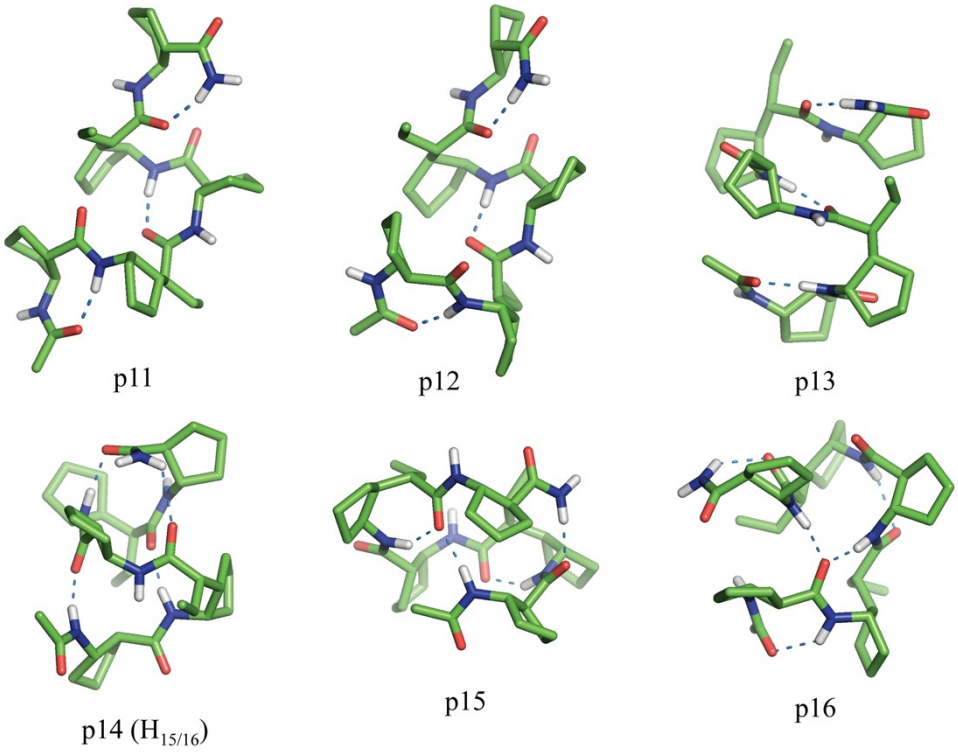

Fig. S2 Conformers p11–p16 of the pentamer composed of βAc_5a-$\gamma(Et)Ac_5a$ dimeric units optimized at the PCM M06-2X/6-31+G(d) level of theory in chloroform. For clarity, all non-polar hydrogen atoms are omitted. All H-bonds are represented by dotted lines.

Table S2 Torsion angles (deg) and relative thermodynamic properties (kcal/mol), and populations (%) for H_{13}-helical and $C_{8/9}$-ribbon structures of the tetramer composed of βAc_5a-$\gamma(Et)Ac_5a$ dimeric units optimized at the PCM M06-2X/6-31+G(d) level of theory in chloroform[a]

Conf.	Residues	ϕ	θ	ζ	ψ	ΔE_0[b]	ΔE_s[c]	ΔH_s[d]	ΔG_s[e]	ω[f]
H_{13}	β1	-63	114		-141	0.00	0.00	0.00	0.00	0.1
	γ2	-154	51	57	-113					
	β3	-116	109		-99					
	γ4	-137	51	60	-124					
C_8C_9-ribbon	β1	-73	129		-63	0.49	3.82	4.16	4.32	99.9
	γ2	-99	58	79	-94					
	β3	-70	128		-62					
	γ4	-95	58	81	-96					

[a] Torsion angles are defined in Fig. 3. Calculated at the M06-2X/def2-TZVP//PCM M06-2X/6-31+G(d) level of theory in chloroform at 25 °C. [b] Relative energies calculated at the M06-2X/def2-TZVP level of theory in the gas phase. [c] Relative energies in chloroform. [d] Relative enthalpies in chloroform at 25 °C. [e] Relative Gibbs free energies in chloroform at 25 °C. [f] Populations calculated by ΔG_s values in chloroform at 25 °C.

Table S3 Backbone torsion angles (deg) of other helical structures of β/γ-hybrid peptides[a]

Peptides	Helix type[b]	Residues	ϕ	θ	ζ	ψ
βCaa$_{(x)}$-γCaa$_{(x)}$ pentamer (NMR)[c]	(*M*)-H$_{11/13}^{III'}$	β	145	68		-8
		γ	123	-84	63	-106
βLeu-γAdb hexamer (NMR)[d]	(*P*)-H$_{11}^{II}$	β1	68	52		34
		γ2	101	79	-62	145
		β3	65	47		63
		γ4	91	75	-60	135
		β5	63	54		82
		γ6	136	-77	71	79
*t*ACBC-γAbu hexamer (DFT)[e]	C$_{8/9}$-ribbon	β1	89	-101		32
		γ2	-99	68	74	-89
		β3	88	-101		33
		γ4	100	-69	-73	95
		β5	88	-100		28
		γ6	-86	-56	-67	170
*t*ACBC-γAbu hexamer (DFT)[f]	C$_{8/9}$-ribbon	β1	91	-99		25
		γ2	-99	67	76	-90
		β3	91	-100		27
		γ4	-99	67	76	-91
		β5	92	-100		27
		γ6	-92	56	63	13
βAla-γAbu octamer (HF)[g]	(*M*)-H$_{11/13}^{III'}$	β	-86	61		16
		γ	94	-81	72	-151
	(*P*)-H$_{11}^{II}$	β	79	47		68
		γ	81	80	-72	138
	C$_{8/9}^{IV}$-ribbon	β	72	-132		64
		γ	98	-69	-75	98

[a] Torsion angles are defined in Fig. 3. [b] (*M*)- and (*P*)-H$_n$ stand for the left- and right-handed helices with repeated C$_n$ pseudocyles. H$_{11/13}^{III'}$ is an enantiomer of the H$_{11/13}^{III}$ structures of Ac-(βAla-γAbu)$_4$-NHMe (peptide **1**) optimized at the HF/6-31G(d) level of theory taken from ref. s1. [c] Mean values deduced from ^{1}H NMR spectrum of Boc-[βCaa$_{(x)}$-γCaa$_{(x)}$]$_2$-βCaa$_{(x)}$-OMe (peptide **4**) in $CDCl_3$ taken from ref. s2. βCaa and γCaa$_{(x)}$ stand for C-linked carbo-β- and γ-amino acids of D-xylose, respectively. [d] Deduced from ^{1}H NMR spectrum of Boc-[βLeu-γAdb]$_3$-OBn (peptide **5**) in $CDCl_3$ taken from ref. s3. γAdb stands for 4-amino-3,3-dimethylbutanoic acid. [e] Boc-[(*R*, *R*)-*t*ACBC-γAbu]$_3$-OBn (peptide **6**) optimized at the B3LYP/6-311G(d,p) level of theory in chloroform taken from ref. s4. [f] Ac-[(*R*,*R*)-*t*ACBC-γAbu]$_3$-OMe optimized at the PCM M06-2X/6-31+G(d) level of theory in chloroform (this work). [g] Mean values from H$_{11/13}^{III'}$, H$_{11}^{II}$, and C$_{8/9}^{IV}$-ribbon structures of Ac-(βAla-γAbu)$_4$-NHMe (peptide **1**) optimized at the HF/6-31G(d) level of theory taken from ref. s1.

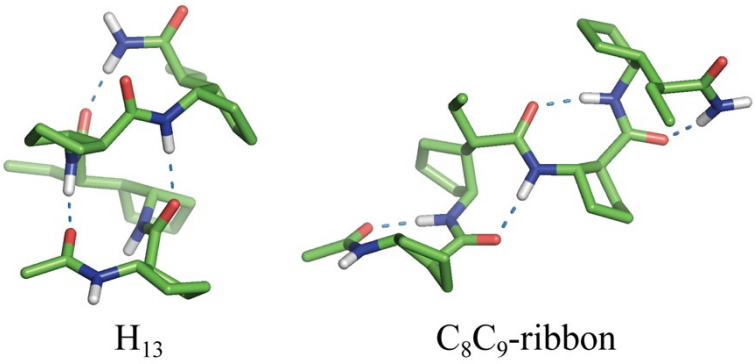

Fig. S3 H_{13}-helical and $C_{8/9}$-ribbon structures of the tetramer composed of βAc_5a-$\gamma(Et)Ac_5a$ dimeric units optimized at the PCM M06-2X/6-31+G(d) level of theory in chloroform. For clarity, all non-polar hydrogen atoms are omitted. All H-bonds are represented by dotted lines.

Conformational study of $C_{8/9}$-ribbon structures for Boc-[(*R*,*R*)-*t*ACBC-γAbu]$_3$-OMe

Aitken and his colleagues reported the most preferred $C_{8/9}$-ribbon structure for Boc-[(*R*,*R*)-*t*ACBC-γAbu]$_3$-OBn (peptide **6**) by the conformational search and DFT calculation at the B3LYP/6-311G(d,p) level of theory in chloroform (ref. s4). Although the conformations of three (*R*,*R*)-*t*ACBC residues are similar, those of three γAbu residues are quite different from each other. The torsion angles of the second γAbu residue are quite similar to those of the C_9^I structure for the H_9^I helical structure of Ac-(γAbu)$_6$-NHMe optimized at the HF/6-31G(d) level of theory (ref. s1). The first γAbu residue adopted the $C_9^{I'}$ structure, i.e., the enantiomer of the C_9^I structure. However, the third γAbu residue exhibited the unusual C_9 structure, which is denoted as C_9^N structure.

To check the feasibility of other structures, we calculated the four possible structures of Boc-[(*R*,*R*)-*t*ACBC-γAbu]$_3$-OMe by considering the combination of C_9^I and $C_9^{I'}$ structures for γAbu residues; i.e., $C_9^{I'}C_9^{I'}C_9^{I'}$, $C_9^{I'}C_9^IC_9^N$, $C_9^IC_9^IC_9^I$, and $C_9^{I'}C_9^IC_9^{I'}$. The torsion angles and thermodynamic properties calculated at the M06-2X/def2-TZVP//PCM M06-2X/6-31+G(d) level of theory in chloroform at 25 °C are shown in Table S4 and the corresponding structures are depicted in Fig. S4.

The $C_{8/9}$ conformation with the $C_9^{I'}C_9^{I'}C_9^{I'}$ structure for γAbu residues were found to be the most preferred (populated at 93.2%) and the conformation with the $C_9^{I'}C_9^IC_9^N$ structure suggested by Aitken and his colleagues was populated only at 5.9% with ΔG_s = 1.63 kcal/mol in chloroform.

References

s1. C. Baldauf, R. Günther and H.-J. Hofmann, *J. Org. Chem*., 2006, **71**, 1200–1208.
s2. G. V. M. Sharma, V. B. Jadhav, K. V. S. Ramakrishna, P. Jayaprakash, K. Narsimulu, V. Subash and A. C. Kunwar, *J. Am. Chem. Soc.*, 2006, **128**, 14657–14668.
s3. R. Misra, G. George, R. M. Reja, S. Dey, S. Raghothama and H. N. Gopi, *Chem. Commun*., 2020, **56**, 2171–2173.
s4. C. M. Grison, S. Robinab and D. J. Aitken, *Chem. Commun*., 2015, **51**, 16233–16236.

Table S4 Torsion angles (deg) and relative thermodynamic properties (kcal/mol), and populations (%) for the four $C_{8/9}$-ribbon structures of Boc-[(*R*,*R*)-*t*ACBC-γAbu]$_3$-OMe in chloroform[a]

Conf.[b]	Residues	ϕ	θ	ζ	ψ	ΔE_s[c]	ΔH_s[d]	ΔG_s[e]	ω[f]
$C_9^{I'}C_9^{I'}C_9^{I'}$	β1	91	-99		25	1.94	1.42	0.00	93.2
	γ2	-99	67	76	-90				
	β3	91	-100		27				
	γ4	-99	67	76	-91				
	β5	92	-100		27				
	γ6	-92	56	63	13				
$C_9^{I'}C_9^{I}C_9^{N}$	β1	90	-99		24	0.00	0.00	1.63	5.9
	γ2	-99	67	77	-90				
	β3	92	-99		26				
	γ4	100	-68	-75	95				
	β5	88	-98		17				
	γ6	-80	-45	-60	178				
$C_9^{I}C_9^{I}C_9^{I}$	β1	92	-99		27	0.73	0.86	3.07	0.5
	γ2	100	-67	-76	95				
	β3	89	-99		28				
	γ4	101	-68	-75	95				
	β5	91	-102		38				
	γ6	119	-38	-44	-43				
$C_9^{I'}C_9^{I}C_9^{I'}$	β1	91	-99		25	1.68	1.73	3.30	0.4
	γ2	-98	67	76	-91				
	β3	91	-101		30				
	γ4	100	-67	-76	94				
	β5	89	-99		27				
	γ6	-92	56	64	12				

[a] Torsion angles are defined in Fig. 3. Calculated at the M06-2X/def2-TZVP//PCM M06-2X/6-31+G(d) level of theory in chloroform at 25 °C. [b] Conformations are represented only by the structures of the γAbu residue. The $C_9^{I'}$ structure is the enantiomer of the C_9^{I} structure for the H_9^{I} helical structure of Ac-(γAbu)$_6$-NHMe optimized at the HF/6-31G(d) level of theory (ref. s1). [c] Relative energies in chloroform. [d] Relative enthalpies in chloroform at 25 °C. [e] Relative Gibbs free energies in chloroform at 25 °C. [f] Populations calculated by ΔG_s values in chloroform at 25 °C.

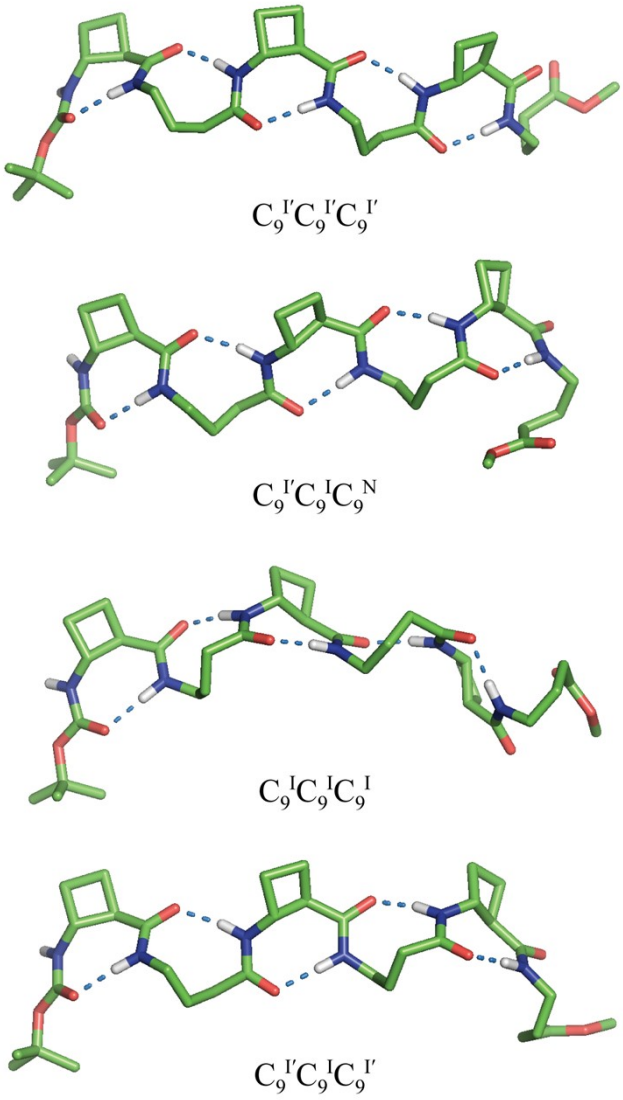

Fig. S4 Four possible structures of Boc-[(*R*,*R*)-*t*ACBC-γAbu]$_3$-OMe by considering the combination of C_9^{I} and $C_9^{I'}$ structures for γAbu residues optimized at the PCM M06-2X/6-31+G(d) level of theory in chloroform. For clarity, all non-polar hydrogen atoms are omitted. All H-bonds are represented by dotted lines.

Cartesian coordinates of the H_{13} helical structures of the pentamer composed of βAc_5a-$\gamma(Et)Ac_5a$ dimeric units and its analog with two pyrrolidines at the first and fourth residues optimized at the PCM M06-2X/6-31+G(d) level of theory in chloroform**:**

(1) Ac-[βAc_5a-$\gamma(Et)Ac_5a$]$_2$-βAc_5a-NH_2

C	-4.276169	-3.999129	1.872544
C	-3.952005	-2.844703	0.957254
O	-3.035159	-2.055187	1.211226
N	-4.694933	-2.703468	-0.156209
C	-4.404426	-1.668038	-1.138820
C	-4.542572	-0.224368	-0.575300
C	-3.201594	0.480953	-0.510465
O	-2.380517	0.369469	-1.428655
N	-2.994969	1.291324	0.547047
C	-1.872670	2.224997	0.622334
C	-1.458389	2.484327	2.078652
C	-1.216938	1.223184	2.911636
C	-0.141976	0.398538	2.211707
O	1.026251	0.810447	2.158484
N	-0.551492	-0.753052	1.661037
C	0.305944	-1.712347	0.991870
C	-0.209210	-2.074784	-0.443412
C	0.749088	-1.495730	-1.467497
O	1.776555	-2.108193	-1.792014
N	0.432986	-0.273419	-1.929154
C	1.241501	0.458781	-2.899187
C	1.365221	1.941595	-2.506406
C	1.804957	2.183611	-1.063486
C	3.151062	1.502714	-0.829540
O	4.113449	1.706984	-1.573176
N	3.204472	0.688896	0.245172
C	4.418057	0.031705	0.682210
C	4.568724	-1.429386	0.164441
C	5.332883	-1.445510	-1.147901
O	6.542922	-1.216658	-1.185328
N	4.602996	-1.723074	-2.247472
H	-4.426337	-3.615133	2.884282
H	-3.414272	-4.672641	1.895163
H	-5.159489	-4.559788	1.561321
H	-5.428247	-3.372595	-0.353700
H	-3.372592	-1.798554	-1.485272
H	-5.000000	-0.248583	0.418657
H	-3.733563	1.361433	1.237127
H	-1.062587	1.790858	0.031246
H	-0.506240	3.030562	2.026750
H	-2.145503	0.635523	2.953995
H	-1.533839	-1.012137	1.726970
H	1.301003	-1.260685	0.926937
H	-1.201169	-1.637152	-0.584731
H	-0.491171	0.092445	-1.690579
H	2.213617	-0.036771	-2.948499
H	2.138476	2.364798	-3.161477
H	1.068351	1.737134	-0.379624
H	2.395341	0.656701	0.868640
H	5.269161	0.621749	0.322447
H	3.564991	-1.840523	0.007615
H	3.590009	-1.827402	-2.198372
H	5.047487	-1.633938	-3.151995
C	-5.355965	-1.743878	-2.338305
H	-5.042422	-2.495308	-3.068371
H	-6.367164	-2.001014	-1.992474
C	-5.446925	0.524094	-1.596649
H	-6.479006	0.524011	-1.229173
H	-5.145698	1.567500	-1.737192
C	-5.353555	-0.313169	-2.877142
H	-4.408211	-0.108513	-3.393010
H	-6.173403	-0.117618	-3.573614
C	-2.285015	3.622592	0.149061
H	-1.377338	4.210038	-0.035620
H	-2.861084	3.592169	-0.781210
C	-2.548972	3.443023	2.601141
H	-2.154156	4.123275	3.360221
H	-3.357200	2.875541	3.082787
C	-3.072922	4.198856	1.347108
H	-2.938263	5.279925	1.433340
H	-4.145994	4.023837	1.215359
C	0.394695	-3.052930	1.741897
H	-0.582220	-3.266441	2.195969
H	1.143971	-3.021816	2.539648
C	-0.251235	-3.614318	-0.487655
H	-1.273669	-3.946075	-0.266589
H	0.034538	-4.006602	-1.466869
C	0.689839	-4.065275	0.636910
H	1.730302	-3.969005	0.304023
H	0.523596	-5.101254	0.947338

C	0.530345	0.542241	-4.254398
H	1.258803	0.856274	-5.010911
H	0.114333	-0.421100	-4.564095
C	-0.005216	2.534762	-2.896565
H	-0.693702	2.498401	-2.041647
H	0.079264	3.584914	-3.191712
C	-0.540804	1.636381	-4.045980
H	-0.720416	2.202544	-4.964230
H	-1.493583	1.184490	-3.750906
C	4.494551	-0.105275	2.204185
H	4.686823	0.853781	2.695517
H	3.539039	-0.495296	2.584626
C	5.306582	-2.189183	1.298006
H	4.649049	-2.968851	1.697451
H	6.217078	-2.671574	0.933733
C	5.605047	-1.138608	2.385280
H	6.575947	-0.667111	2.191874
H	5.636359	-1.568308	3.390823
C	-0.775872	1.542098	4.344841
H	0.127335	2.162743	4.304177
H	-1.559676	2.139983	4.824852
C	-0.509728	0.282572	5.167610
H	-1.396264	-0.361850	5.194899
H	0.315853	-0.299111	4.742114
H	-0.243726	0.534150	6.198490
C	1.921438	3.678502	-0.733254
H	0.935809	4.138811	-0.877694
H	2.602678	4.148785	-1.454246
C	2.406685	3.930400	0.694041
H	2.355658	4.993888	0.947561
H	1.799561	3.369998	1.415799
H	3.445579	3.605375	0.820237

(2) The analog with two pyrrolidines

C	-4.370186	-4.162980	1.603839
C	-3.984561	-2.957543	0.783686
O	-3.055817	-2.214890	1.120551
N	-4.687923	-2.718248	-0.340987
C	-4.333191	-1.622158	-1.225289
C	-4.525317	-0.221252	-0.586887
C	-3.213772	0.526687	-0.504389
O	-2.418345	0.502826	-1.451306
N	-2.999962	1.264157	0.603007
C	-1.881301	2.196647	0.722823
C	-1.469961	2.379429	2.190919
C	-1.240413	1.075309	2.961579
C	-0.174104	0.277556	2.219121
O	1.001835	0.670036	2.209083
N	-0.594332	-0.823515	1.578573
C	0.264440	-1.743371	0.856995
C	-0.229235	-1.998303	-0.607611
C	0.737890	-1.337112	-1.571172
O	1.801453	-1.894965	-1.874792
N	0.389808	-0.113133	-2.008087
C	1.224899	0.686910	-2.894279
C	1.411867	2.117525	-2.357327
C	1.822008	2.215390	-0.891043
C	3.161002	1.506957	-0.694608
O	4.129642	1.752038	-1.417384
N	3.198674	0.627022	0.326330
C	4.401368	-0.071737	0.729983
C	4.548553	-1.489325	0.099791
C	5.346136	-1.411140	-1.190181
O	6.562812	-1.218143	-1.181325
N	4.634071	-1.563404	-2.325624
H	-4.595148	-3.840177	2.623276
H	-3.510058	-4.837099	1.649028
H	-5.227032	-4.702713	1.196070
H	-5.446684	-3.337492	-0.596442
H	-3.282379	-1.733918	-1.511761
H	-4.989565	-0.303438	0.400148
H	-3.720063	1.270264	1.315711
H	-1.071481	1.794530	0.108792
H	-0.514120	2.921324	2.169019
H	-2.174709	0.495061	2.978533
H	-1.577327	-1.084258	1.626801
H	1.265376	-1.300440	0.838055
H	-1.224041	-1.561734	-0.726769
H	-0.550777	0.224656	-1.789983
H	2.173622	0.160873	-3.015068
H	2.207112	2.573703	-2.961494
H	1.070131	1.712832	-0.265727
H	2.384607	0.566917	0.940957
H	5.262089	0.539268	0.434184
H	3.543215	-1.867897	-0.116304
H	3.617786	-1.632927	-2.301216
H	5.098335	-1.397520	-3.209011
C	-5.208365	-1.589172	-2.497887
H	-4.797647	-2.190767	-3.311456
H	-6.215976	-1.962144	-2.265128

C	-5.455499	0.512503	-1.602764	H	0.167627	3.845257	-2.907915
H	-6.494516	0.421369	-1.267150	N	-0.411551	2.053369	-3.920215
H	-5.223736	1.575594	-1.711867	H	-0.508146	2.680588	-4.710914
N	-5.312709	-0.184872	-2.878766	C	4.448044	-0.330205	2.237412
H	-4.435822	0.106248	-3.311714	H	4.643833	0.583606	2.807387
C	-2.297629	3.615001	0.321081	H	3.480713	-0.736008	2.568440
H	-1.392199	4.216114	0.172722	C	5.245146	-2.348886	1.186105
H	-2.868510	3.630829	-0.612559	H	4.563359	-3.142131	1.511561
C	-2.557194	3.316383	2.760904	H	6.153353	-2.822381	0.804991
H	-2.154535	3.965129	3.543107	C	5.540345	-1.391907	2.356513
H	-3.361169	2.730366	3.227244	H	6.522055	-0.923636	2.217695
C	-3.093133	4.122659	1.543990	H	5.545743	-1.898658	3.326030
H	-2.976280	5.200545	1.680854	C	-0.794682	1.323308	4.406910
H	-4.163048	3.935928	1.403265	H	0.117616	1.931536	4.392263
C	0.334398	-3.134182	1.510615	H	-1.569518	1.911112	4.913002
H	-0.653945	-3.380500	1.920541	C	-0.546862	0.025821	5.174084
H	1.062891	-3.161267	2.327486	H	-1.443276	-0.605200	5.177597
C	-0.254858	-3.531564	-0.769711	H	0.268786	-0.549455	4.721887
H	-1.279120	-3.886438	-0.599637	H	-0.274258	0.229834	6.213743
H	0.057605	-3.846396	-1.768533	C	1.935704	3.675055	-0.423757
C	0.661595	-4.061115	0.341374	H	0.948356	4.144521	-0.524710
H	1.709745	-3.938969	0.042511	H	2.614182	4.212747	-1.098876
H	0.491168	-5.117468	0.569745	C	2.419364	3.800421	1.020621
C	0.523371	0.954315	-4.227310	H	2.354999	4.836156	1.368372
H	1.275875	1.238053	-4.976774	H	1.820030	3.169140	1.687932
H	-0.009835	0.068853	-4.587506	H	3.462818	3.479588	1.116223
C	0.069547	2.770857	-2.721105				
H	-0.655772	2.642949	-1.903046				