Supplementary information

Helix foldamers of γ-peptides based on 2-aminocyclopentylacetic acid

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Table S1 Backbone torsion angles for the optimized helical and extended structures of oligopeptides composed of γAc$_5$a (**1**) and γAc$_5$a (**2**)[a]

Dipeptides

H$_1$	ϕ	θ	ζ	ψ	**H$_2$**	ϕ	θ	ζ	ψ
H$_1$-14	–89.0	56.0	73.0	–159.7	**H$_2$**-14	–86.4	82.0	54.7	–152.6
	–130.0	51.4	58.2	–114.8		–138.2	65.1	45.5	–105.1
av.	–109.5	53.7	65.6	–137.2	av.	–112.3	73.5	50.1	–128.8
H$_1$-12	81.8	50.0	–72.9	173.8	**H$_2$**-12	57.1	75.3	–67.2	137.1
	81.9	45.1	–62.6	126.9		66.2	87.6	–61.6	106.3
av.	81.8	47.5	–67.8	150.4	av.	61.6	81.4	–64.4	121.7
H$_1$-9	–98.7	56.0	84.7	–90.7	**H$_2$**-9	–97.8	72.8	70.3	–91.1
	–98.6	54.8	84.5	–85.2		–95.0	67.2	76.1	–84.4
av.	–98.7	55.4	84.6	–87.9	av.	–96.4	70.0	73.2	–87.7
H$_1$-7	87.4	40.9	52.8	87.9	**H$_2$**-7	61.9	58.9	41.1	95.6
	81.3	37.1	56.4	108.8		59.4	57.7	44.3	104.6
av.	84.4	39.0	54.6	98.4	av.	60.7	58.3	42.7	100.1
E$_1$[b]	–92.2	50.9	175.6	157.4	**E$_2$**[b]	–93.9	68.0	179.8	–144.6
	–90.3	51.0	174.7	158.3		–95.5	67.1	–178.9	–148.5
av.	–91.2	51.0	175.1	157.8	av.	–94.7	67.6	–179.6	–146.5

Tetrapeptides

H$_1$	ϕ	θ	ζ	ψ	**H$_2$**	ϕ	θ	ζ	ψ
H$_1$-14	–94.0	55.0	77.5	–139.1	**H$_2$**-14	–93.4	83.5	54.4	–133.1
	–165.9	53.9	64.8	–127.3		–175.4	68.3	51.3	–104.4
	–127.8	50.1	71.4	–164.6		–150.9	74.0	50.4	–142.1
	–112.6	51.9	59.4	–143.0		–114.5	64.1	44.8	–138.4
av.	–135.4	52.0	65.2	–144.9	av.	–146.9	68.8	48.9	–128.3
H$_1$-12	84.9	50.4	–67.7	160.2	**H$_2$**-12	56.3	81.1	–64.0	127.2
	92.1	50.3	–72.3	165.1		59.4	103.1	–65.3	124.9
	87.2	50.1	–73.7	175.3		59.8	97.9	–67.2	122.9
	80.9	43.2	–63.8	132.4		68.9	92.4	–63.0	107.2
av.	86.3	48.5	–69.4	158.3	av.	61.1	93.6	–64.9	120.5
H$_1$-9	–98.1	56.1	84.2	–93.0	**H$_2$**-9	–98.1	71.9	70.8	–90.5
	–98.1	55.0	84.2	–88.4		–97.5	70.9	71.0	–88.9
	–99.0	55.7	83.7	–89.5		–97.4	71.6	70.2	–89.2
	–99.0	53.7	85.2	–83.2		–95.7	67.2	75.5	–86.2
av.	–98.6	55.1	84.3	–88.5	av.	–97.2	70.4	71.9	–88.7
H$_1$-7	86.8	40.3	53.3	89.4	**H$_2$**-7	61.9	59.2	39.9	95.1
	83.4	38.8	53.6	89.7		60.7	60.2	39.6	96.5
	83.9	39.5	52.2	90.1		61.6	59.7	39.3	96.2
	83.2	37.9	55.4	107.2		59.5	57.8	43.5	103.7
av.	84.3	39.1	53.6	94.1	av.	61.0	59.2	40.6	97.9
E$_1$[b]	–92.3	51.3	173.8	163.3	**E$_2$**[b]	–93.8	68.1	179.7	–145.1

	–90.4	50.3	175.5	153.2		–94.5	66.8	179.7	–152.6
	–90.4	50.1	175.3	151.6		–95.8	67.1	–180.0	–145.5
	–91.0	51.0	175.3	154.9		–94.8	67.1	–178.2	–148.3
av.	–91.0	50.6	175.0	155.7	av.	–94.7	67.3	–179.7	–147.9

Hexapeptides

H$_1$	ϕ	θ	ζ	ψ	**H$_2$**	ϕ	θ	ζ	ψ
H$_1$-14	–90.6	53.4	72.7	–159.5	**H$_2$**-14	–96.6	77.9	56.7	-164.3
	–144.1	53.0	70.2	–115.5		–131.8	69.7	56.9	-115.8
	–161.0	53.3	66.7	–125.4		–166.6	67.9	51.6	-102.4
	–142.5	53.2	69.2	–162.3		–166.4	69.2	51.0	-115.5
	–96.1	48.8	74.4	–162.5		–145.4	74.4	49.0	-134.2
	–129.3	53.4	61.7	–112.4		–127.8	67.5	41.5	-123.9
av.	–134.6	52.4	68.4	–135.6	av.	–147.6	69.7	50.0	-118.4
H$_1$-12	85.6	51.2	–67.3	157.6	**H$_2$**-12	55.4	82.1	-62.7	125.5
	93.1	50.8	–68.0	156.2		60.1	102.6	-65.3	125.2
	93.5	51.7	–68.4	156.8		59.8	97.3	-66.2	122.4
	92.9	51.8	–70.8	162.8		68.7	95.1	-66.4	124.0
	88.3	49.7	–74.2	176.0		61.3	98.4	-68.2	124.7
	80.9	43.0	–64.3	132.9		69.3	90.3	-62.7	107.3
av.	89.0	49.7	–68.8	157.0	av.	62.4	94.3	–65.2	121.5
H$_1$-9	–99.0	55.8	84.3	–90.2	**H$_2$**-9	–98.0	72.3	70.5	-89.5
	–97.8	54.7	84.2	–87.3		–96.6	71.1	70.8	-89.6
	–98.5	54.6	83.9	–86.7		–97.4	71.1	70.4	-89.8
	–98.0	55.4	83.6	–89.3		–97.9	69.9	71.2	-88.2
	–98.1	55.0	84.1	–88.0		–97.8	71.2	70.1	-88.9
	–98.7	54.2	85.0	–83.3		–95.6	67.1	75.3	-84.2
av.	–98.4	55.0	84.2	–87.5	av.	–97.2	70.5	71.4	-88.4
H$_1$-7	85.8	40.1	53.6	89.8	**H$_2$**-7	59.5	59.1	39.0	94.0
	83.5	39.1	53.1	89.1		61.5	60.4	38.8	96.7
	83.3	38.9	52.6	90.4		61.6	60.0	38.9	95.8
	84.3	39.2	52.4	87.4		61.3	59.7	38.7	97.3
	82.6	38.1	53.5	91.2		62.4	59.3	39.2	97.0
	82.0	36.6	56.8	107.2		60.0	57.9	43.1	103.5
av.	83.6	38.7	53.7	92.5	av.	61.1	59.4	39.6	97.4
E$_1$[b]	–92.5	51.2	174.2	164.4	**E$_2$**[b]	–93.7	68.0	179.7	-146.3
	–89.8	50.9	174.6	161.7		–95.0	66.7	179.7	-153.6
	–90.6	50.8	173.9	163.4		–96.0	66.8	-178.7	-154.7
	–89.7	50.7	175.0	161.1		–95.8	66.8	-179.3	-155.0
	–90.3	50.9	174.0	163.8		–95.9	67.3	-179.8	-145.9
	–89.8	50.6	176.2	153.9		–94.8	67.0	-177.9	-148.7
av.	–90.4	50.8	174.7	161.4	av.	–95.2	67.1	-179.4	-150.7

Octapeptides

H$_1$	ϕ	θ	ζ	ψ	**H$_2$**	ϕ	θ	ζ	ψ
H$_1$-14	–90.0	54.1	72.7	–157.7	**H$_2$**-14	–93.0	82.6	54.0	–145.4
	–150.5	53.1	69.0	–118.5		–157.9	66.3	55.2	–99.3

	–150.1	49.3	67.2	–156.5		–160.8	66.5	43.9	–144.4
	–103.0	**50.0**	**76.2**	**–152.4**		**–96.7**	**63.4**	**56.6**	**–160.1**
	–142.4	53.8	70.2	–118.1		–154.5	67.2	58.6	–100.4
	–159.7	52.4	66.1	–153.8		–176.4	67.7	50.0	–112.2
	–99.9	49.1	75.4	–164.8		–141.7	71.1	51.2	–143.8
	–126.7	53.7	60.0	–118.1		–118.5	65.8	43.1	–130.5
av.	–133.2	51.6	69.2	–140.3	av.	–143.8	66.9	51.2	–127.2
H$_1$-12	85.8	50.5	–67.0	157.8	**H**$_2$-12	56.0	82.4	–63.2	123.9
	93.4	50.6	–67.8	155.7		60.4	103.7	–65.4	124.7
	93.9	51.9	–67.5	155.0		59.3	97.7	–65.9	121.7
	94.3	51.4	–67.3	155.1		69.0	95.1	–66.9	125.6
	94.0	51.7	–68.3	156.4		62.4	94.9	–66.7	125.8
	92.6	51.9	–69.2	160.0		69.3	91.4	–65.3	120.5
	89.4	51.1	–71.7	168.6		60.7	103.3	–67.6	123.0
	84.2	45.1	–63.4	129.9		69.4	90.5	–64.0	107.1
av.	90.9	50.5	–67.8	154.8	av.	63.3	94.9	–65.6	121.5
H$_1$-9	–99.2	55.7	84.1	–90.3	**H**$_2$-9	–98.4	71.9	70.6	–90.2
	–97.8	54.9	84.1	–86.9		–97.4	70.2	71.2	–89.5
	–98.5	54.8	83.7	–86.8		–98.0	69.8	70.8	–88.0
	–98.2	54.5	84.2	–85.8		–98.4	70.5	70.3	–89.5
	–98.7	54.9	83.5	–87.1		–98.1	69.7	71.0	–88.3
	–98.5	54.9	83.7	–89.0		–98.4	70.2	70.8	–88.3
	–98.7	54.9	84.2	–89.5		–97.9	71.1	70.2	–89.0
	–99.9	54.3	84.4	–83.3		–95.7	67.2	75.2	–85.0
av.	–98.7	54.9	84.0	–87.3	av.	–97.8	70.1	71.3	–88.5
H$_1$-7	86.8	40.1	53.8	89.2	**H**$_2$-7	62.0	59.0	39.5	95.2
	83.2	38.2	53.1	92.2		60.9	60.2	38.5	96.7
	84.7	39.2	52.9	88.9		62.3	59.6	38.5	96.7
	83.4	38.7	52.9	89.9		61.4	59.7	38.6	96.6
	84.5	39.2	52.5	89.9		62.0	59.8	38.0	97.1
	84.2	39.4	52.1	91.3		62.4	59.5	38.1	96.4
	85.5	39.6	53.2	92.8		62.4	59.4	39.3	97.7
	83.5	38.0	54.7	107.4		60.7	57.8	42.1	102.8
av.	84.5	39.0	53.2	92.7	av.	61.8	59.4	39.1	97.4
E$_1$[b]	–92.1	51.1	174.5	163.3	**E**$_2$[b]	–93.5	68.0	179.9	–146.8
	–90.9	50.6	173.6	159.3		–95.2	66.8	–179.6	–154.6
	–90.4	50.4	176.7	154.2		–96.1	66.9	–178.9	–155.0
	–90.7	50.3	175.7	150.7		–96.2	66.8	–178.8	–156.3
	–90.9	50.2	175.1	154.7		–96.2	66.8	–178.9	–154.8
	–90.1	50.6	175.5	156.8		–95.8	66.8	–179.2	–155.4
	–91.0	50.2	176.1	152.7		–95.9	67.3	–179.8	–146.3
	–91.1	50.8	175.1	157.7		–94.9	66.9	–177.8	–152.3
av.	–90.9	50.5	175.3	156.2	av.	–95.5	67.0	–179.1	–152.7

[a] Optimized at the M06-2X/6-31+G(d) level of theory in the gas phase. Backbone torsion angles in γAc$_5$a residues **1** and **2** are defined in Fig. 2 of the text. Torsion angles for the first residues of the **H**$_1$-14 and **H**$_2$-14 foldamers for tetra- to octapeptides are excluded in calculating the mean values. [b] Extended structure.

Table S2 Mean distances (Å) and angles (°) for the C=O···H–N H-bonds of the helix foldamers of Ac-(γAc_5a)$_n$-NHMe

		γAc$_5$a (**1**)		γAc$_5$a (**2**)	
n	Helix type	*d*(C=O···H–N)	∠N–H···O	*d*(C=O···H–N)	∠N–H···O
4	**H**-14	2.00	169.1	2.04	172.0
	H-12	2.00	168.0	1.93	153.4
	H-9	1.87	170.8	1.88	171.1
	H-7	2.09	133.4	2.39	118.7
6	**H**-14	1.97	167.6	1.95	169.4
	H-12	1.99	168.0	1.91	151.5
	H-9	1.85	171.9	1.86	171.8
	H-7	2.09	133.9	2.36	119.5
8	**H**-14	1.95	168.4	1.98	168.8
	H-12	1.99	169.4	1.90	152.3
	H-9	1.85	172.5	1.86	171.8
	H-7	2.07	134.5	2.34	119.9

Table S3 Helical parameters for the helix foldamers of oligo-γAc$_5$a peptides

n	Foldamer	*m*[a]	□*p*[b]	□*d*[c]	*r*[d]	Foldamer	*m*[a]	□*p*[b]	□*d*[c]	*r*[d]
4	**H$_1$**-14	2.5	5.1	2.1	2.9	**H$_2$**-14	2.4	5.1	2.1	2.8
	H$_1$-12	2.5	5.7	2.3	2.8	**H$_2$**-12	2.4	5.7	2.4	2.3
	H$_1$-9	2.6	8.8	3.4	1.9	**H$_2$**-9	2.6	8.9	3.5	1.8
	H$_1$-7	2.5	9.5	3.8	1.5	**H$_2$**-7	2.3	8.8	3.8	1.5
6	**H$_1$**-14	2.5	5.1	2.1	2.9	**H$_2$**-14	2.5	5.0	2.0	2.8
	H$_1$-12	2.5	5.7	2.3	2.8	**H$_2$**-12	2.4	5.6	2.4	2.3
	H$_1$-9	2.6	8.8	3.5	1.8	**H$_2$**-9	2.6	8.8	3.4	1.9
	H$_1$-7	2.4	9.3	3.8	1.5	**H$_2$**-7	2.4	8.8	3.8	1.5
8	**H$_1$**-14	2.5	5.1	2.1	2.9	**H$_2$**-14	2.5	4.9	2.0	2.9
	H$_1$-12	2.5	5.7	2.3	2.8	**H$_2$**-12	2.4	5.6	2.4	2.3
	H$_1$-9	2.6	8.8	3.4	1.8	**H$_2$**-9	2.6	8.8	3.4	1.8
	H$_1$-7	2.5	9.5	3.8	1.5	**H$_2$**-7	2.3	8.8	3.8	1.5

[a] Number of residues per turn. [b] Rise per turn (pitch) (Å). [c] Rise per residue (Å). [d] Radius of helix (Å).

Conformational analysis of the γAc$_5$a (1) dipeptide

A conformational analysis of the γAc$_5$a (**1**) dipeptide, Ac-[γAc$_5$a (**1**)]$_2$-NHMe, has been carried out to determine which helical structures are preferred in the gas phase and in solution. All DFT calculations have been carried out using the hybrid-meta-GGA M06-2X functional[1] and the Solvation Model based on Density (SMD) method[2] implemented in the Gaussian 09 program.[3]

From the extended structure of Ac-[γAc$_5$a (**1**)]$_2$-NHMe, 147 initial structures for optimization were generated by the systematic search of the Discovery Studio package[4] using the CHARMm force field with the maximum systematic conformations = 1000 and the energy threshold = 40 kcal mol^{-1}. First, these initial structures were optimized at the HF/3-21G(d) level of theory and reoptimized at the M06-2X/6-31G(d) level of theory in the gas phase and followed by further optimization at the M06-2X/6-31+G(d) level of theory in the gas phase. We obtained 25 local minima with ΔE_e < 10 kcal mol^{-1} at the M06-2X/6-31+G(d) level of theory. Next, for all local minima at the M06-2X/6-31+G(d) level of theory, the single-point energies and solvation free energies were calculated at M06-2X/cc-pVTZ and SMD M06-2X/6-31+G(d) levels of theory, respectively. The torsion angles and relative electronic energies of the 25 local minima and two helix foldamers **H**$_d$-9 and **H**$_d$-12 at the M06-2X/cc-pVTZ//M06-2X/6-31+G(d) level of theory in the gas phase and the SMD M06-2X/6-31+G(d) level of theory in chloroform and water are listed in Table S4.

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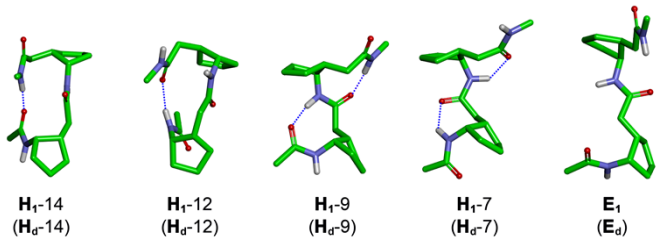
4 *Discovery Studio* (*Version 2.5*), Accelrys Software, Inc., San Diego, CA, 2009.

Table S4 Backbone torsion angles (°) and relative electronic energies (kcal mol^{-1}) of Ac-[γAc$_5$a(**1**)]$_2$-NHMe

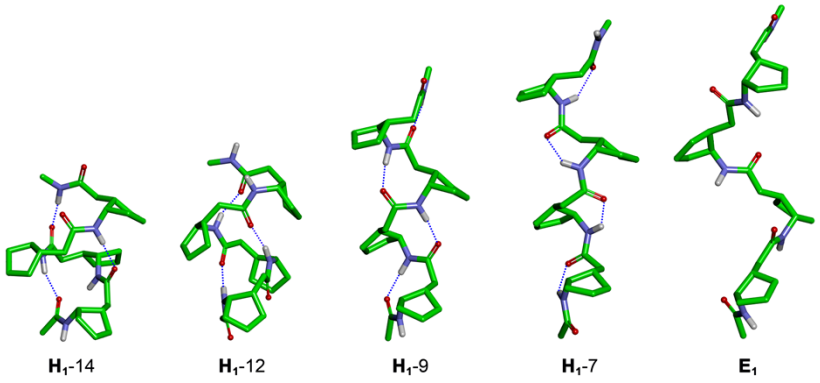
Conf.	Backbone torsion angles[a]								Relative energies[b]		
	ϕ_1	θ_1	ζ_1	ψ_1	ϕ_2	θ_2	ζ_2	ψ_2	ΔE_0	ΔE_c	ΔE_w
d1	–111.6	–46.3	80.6	79.2	65.6	10.8	60.3	175.8	0.00	2.17	2.01
H$_d$-9[c]	–98.7	56.0	84.7	–90.7	–98.6	54.8	84.5	–85.2	1.73	0.00	0.00
d2	–101.4	52.5	86.1	–82.0	–115.7	8.0	63.8	9.0	1.76	2.53	2.21
d3	66.3	13.8	60.1	–172.6	–92.7	44.5	66.5	16.8	3.34	2.97	1.55
H$_d$-14[d]	–89.0	56.0	73.0	–159.7	–130.0	51.4	58.2	–114.8	4.51	2.16	0.96
d4	–72.7	–47.1	66.4	56.9	–99.1	55.2	84.7	–87.6	4.61	2.94	1.53
d5	–99.3	56.1	84.0	–91.5	–91.7	52.2	–160.3	–74.9	5.28	3.58	1.16
d6	–103.5	55.2	85.0	–88.7	–168.2	54.1	–165.6	102.5	5.47	2.07	1.52
d7	–161.4	46.8	55.0	–146.6	–96.0	52.1	174.5	150.5	5.50	2.80	0.23
d8	–97.9	51.5	71.7	–146.2	–156.2	50.2	–88.5	–143.1	5.78	4.77	3.42
d9	84.1	39.6	69.9	175.3	–112.5	19.9	52.2	43.6	6.54	5.79	5.25
d10	–99.6	56.2	84.3	–92.8	–89.7	52.1	175.0	164.1	6.64	3.77	1.64
d11	–73.0	–46.4	67.4	55.0	–99.3	–16.0	61.5	38.8	6.95	6.16	3.64
d12	–78.8	11.6	–69.4	–82.2	–91.3	44.8	63.9	22.2	6.97	5.69	2.71
d13	–136.3	50.9	66.9	–83.8	92.0	40.3	45.4	67.0	7.20	6.98	6.64
d14	–178.7	47.9	62.4	173.9	–112.4	16.6	51.0	44.1	7.36	5.90	4.53
d15	85.8	39.7	56.4	95.3	–101.4	55.1	84.8	–88.1	7.75	5.74	5.67
d16	–90.6	50.5	176.1	104.1	–89.1	28.1	–64.2	150.4	7.75	6.34	5.04
d17	–133.3	20.5	50.4	28.3	–177.2	44.3	–93.5	–102.5	7.89	6.20	4.19
d18	–73.5	–47.6	64.8	57.0	–94.4	51.5	174.5	162.4	7.96	5.75	2.70
d19	–170.5	53.4	–94.6	–124.6	–102.7	54.2	84.7	–88.0	8.04	4.59	3.73
d20	–161.0	8.3	54.0	51.5	82.0	35.3	55.8	114.8	8.08	7.85	6.21
H$_d$-7[e]	87.4	40.9	52.8	87.9	81.3	37.1	56.4	108.8	8.26	8.68	8.54
d21	–162.2	33.1	–90.9	–120.2	87.1	39.0	55.2	108.8	8.47	7.06	7.36
d22	–86.2	29.4	–65.9	164.2	–105.5	20.6	53.5	46.2	8.71	7.88	5.66
E$_d$[f]	–92.2	50.9	175.6	157.4	–90.3	51.0	174.7	158.3	11.61	7.53	4.69
H$_d$-12[g]	81.8	50.0	–72.9	173.8	81.9	45.1	–62.6	126.9	15.73	14.66	12.18

[a] Backbone torsion angles in the γAc$_5$a (**1**) residue are defined in Fig. 1h of the text and optimized at the M06-2X/6-31+G(d) level of theory in the gas phase. [b] Relative energies at the M06-2X/cc-pVTZ//M06-2X/6-31+G(d) level of theory in the gas phase (ΔE_0), chloroform (ΔE_c), and water (ΔE_w). [c] **H$_1$**-9 structure. [d] **H$_1$**-14 structure. [e] **H$_1$**-7 structure. [f] Extended structure. [g] **H$_1$**-12 structure.

(a)



(b)



(c)

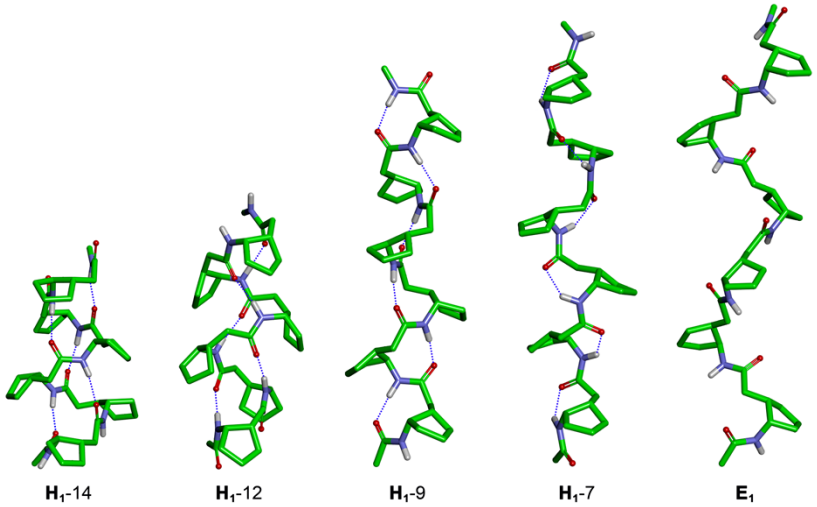
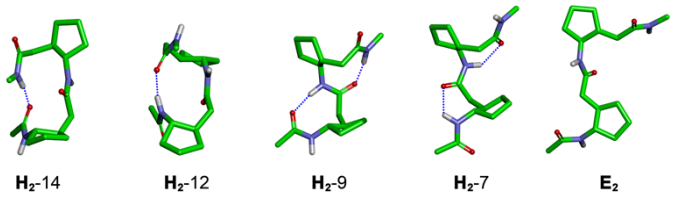
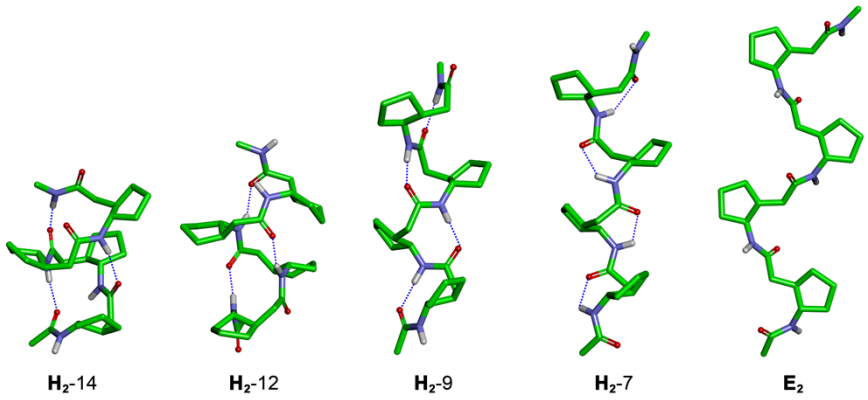


Fig. S1 The optimized helical and extended structures of oligopeptides composed of γAc$_5$a (**1**): (a) dipeptide, (b) tetrapeptide, and (c) hexapeptide.

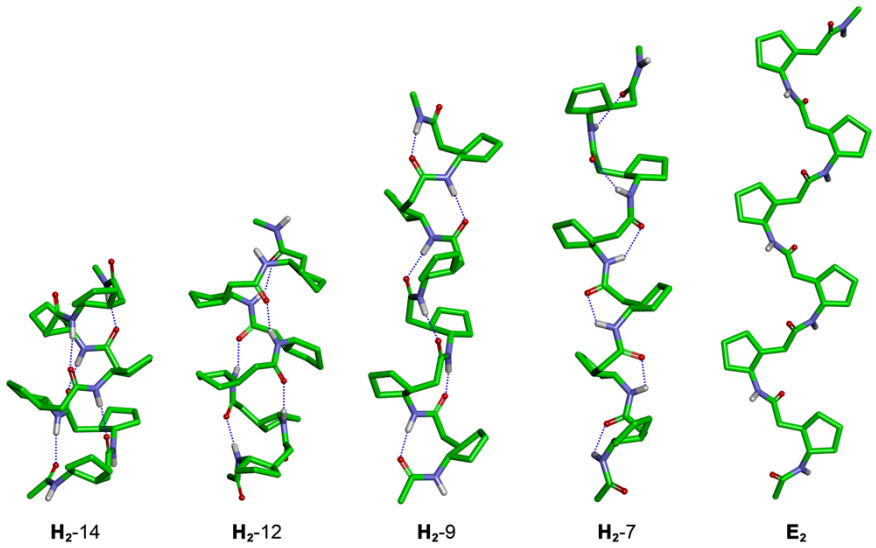
(a)



(b)



(c)



(d)

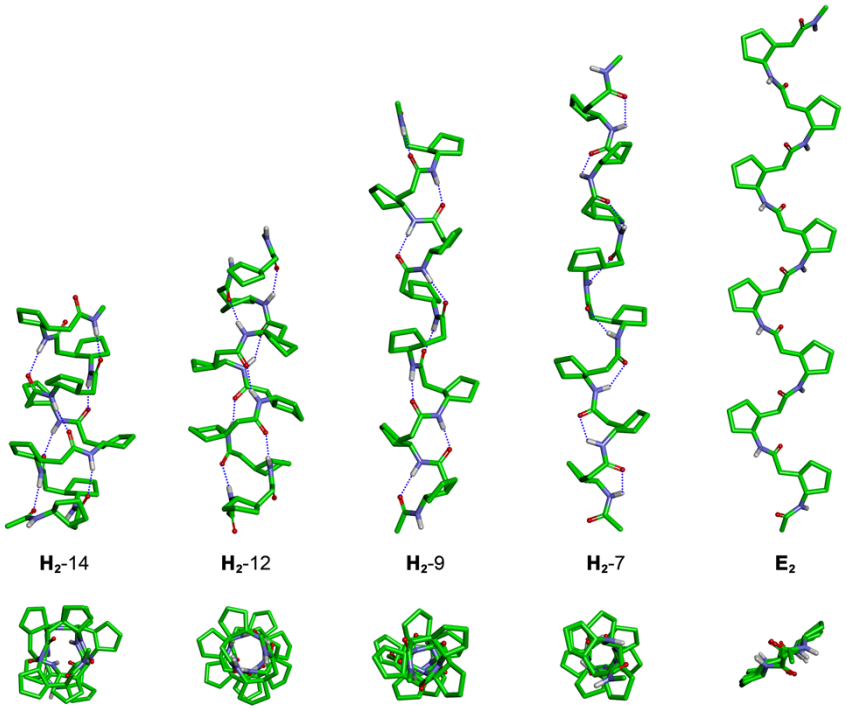


Fig. S2 The optimized helical and extended structures of oligopeptides composed of γAc$_5$a (**2**): (a) dipeptide, (b) tetrapeptide, (c) hexapeptide, and (d) octapeptide.

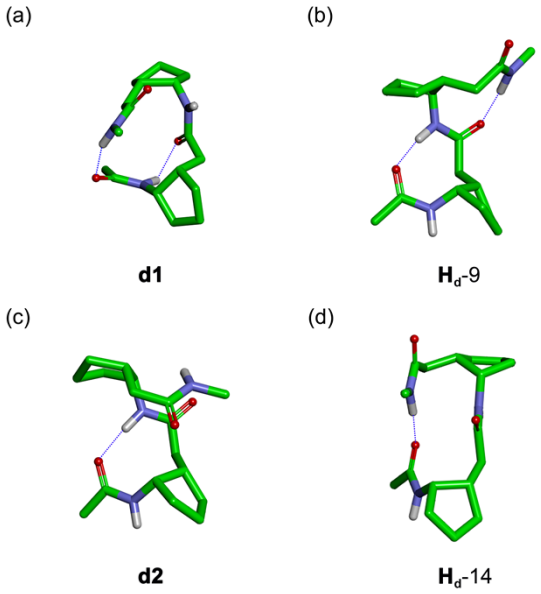


Fig. S3 Representative optimized structures of the γAc_5a (**1**) dipeptide at the M06-2X/6-31+G(d) level of theory in the gas phase.

Cartesian coordinates of the helical and extended structures of the octa-γAc$_5$a (1) peptide optimized at the M06-2X/6-31+G(d) level of theory:

(1) **H$_1$**-14

E_e = -3474.2033902 Hartrees

H	-7.36776500	-3.05247900	2.94956700
H	-8.31287200	-1.56056900	2.89852400
H	-8.91655800	-3.02541200	2.07717400
C	-8.02580700	-2.44223200	2.32252200
C	-7.24644400	-2.00294200	1.10451100
O	-6.38125500	-1.12641300	1.17649800
N	-7.52581800	-2.63069100	-0.05648600
H	-8.23377000	-3.35411200	-0.04788800
C	-6.74599800	-2.44543000	-1.28457000
C	-7.27919000	-1.29523700	-2.15705900
C	-8.58887400	-1.87176400	-2.71935200
C	-8.32826300	-3.39185500	-2.88239500
C	-6.96249200	-3.65566800	-2.19699200
H	-5.70308500	-2.29418000	-0.99490500
H	-6.55469100	-1.17873200	-2.97285000
H	-9.40489800	-1.69465900	-2.00679200
H	-8.87450300	-1.38828500	-3.65804200
H	-9.12803800	-3.97815700	-2.41707500
H	-8.30046000	-3.69033300	-3.93342100
H	-6.15934600	-3.67095200	-2.94010800
H	-6.91855500	-4.60594400	-1.65463200
C	-7.42699300	0.05709100	-1.47816600
H	-8.00978700	-0.02853100	-0.55307400
H	-7.98694800	0.73002900	-2.14348100
C	-6.08956200	0.73495600	-1.20902300
O	-5.09422900	0.48775800	-1.89383500
N	-6.09080300	1.66486600	-0.23178000
H	-6.94138800	1.78292100	0.30435400
C	-4.95900800	2.54650200	0.03984900
C	-4.89994000	2.94334600	1.52073400
C	-5.14686800	3.90807700	-0.64157000
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C	-6.04457300	3.96344700	1.66245800
H	-3.94505800	3.46815600	1.65513300
C	-4.91978700	1.77459000	2.49989500
C	-6.15664800	4.64552200	0.27052700
H	-4.18290600	4.43063500	-0.65366500
H	-5.48406600	3.80966200	-1.67787800
H	-6.98190600	3.45367500	1.92661600
H	-5.84685500	4.67543000	2.46874700
H	-5.78204800	1.12180000	2.32004400
H	-4.98553400	2.15762900	3.52504100
C	-3.61901600	0.99420300	2.40311900
H	-7.17273300	4.55074700	-0.12615000
H	-5.93941100	5.71549200	0.32120500
O	-2.54067400	1.54643900	2.64762300
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H	-4.65454100	-0.66156400	1.83759700
C	-2.58855500	-1.21008500	2.06093000
C	-2.69541500	-2.29486000	0.97994600
C	-2.61025300	-2.04194000	3.34912100
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C	-3.72376700	-3.30016800	1.54786400
H	-1.70958600	-2.77452700	0.94832200
C	-3.00025900	-1.77402900	-0.41537100
C	-3.73060100	-3.06834400	3.08434700
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H	-2.78086600	-1.42818200	4.23894800
H	-4.71794900	-3.11622000	1.12128700
H	-3.45022500	-4.32679500	1.28536400
H	-3.91675500	-1.17077800	-0.42321900
H	-3.16219600	-2.61737300	-1.10212100
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H	-4.69317100	-2.64567400	3.39783200
H	-3.58747200	-3.99269000	3.65042400
O	-0.68493900	-1.14590500	-0.58037700
N	-2.15301200	-0.06762600	-1.93165800
H	-3.14087700	0.12065500	-2.10327000
C	-1.14282600	0.78669500	-2.54835000
C	-1.20469600	2.22418900	-1.99678000
C	-1.43165500	0.98991900	-4.03823100
H	-0.17703600	0.31516700	-2.36076800
C	-2.44266200	2.80443300	-2.70467200
H	-0.30526000	2.73714500	-2.36024000
C	-1.21772400	2.32614100	-0.47667100
C	-2.50278700	2.10673900	-4.08831900
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H	-1.74439300	0.06286000	-4.52754600
H	-3.34663800	2.55665400	-2.13910800
H	-2.39471700	3.89607700	-2.77748700
H	-1.94509700	1.63204300	-0.03688700
H	-1.52708500	3.33706200	-0.17178900
C	0.15630300	2.08758400	0.14067200
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H	-2.30676900	2.80365700	-4.90793800
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N	0.15773300	1.59445000	1.39352500
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C	1.39894400	0.22003500	3.04603900
C	1.39555900	2.58855600	3.27432100
H	2.21437000	1.54791000	1.50065600
C	0.37554400	0.51489300	4.15764600
H	2.40049500	0.17184400	3.49484000
C	1.18684000	-1.07376300	2.26753300
C	0.42479300	2.05560100	4.35774600

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H	0.27983300	-1.02307100	1.65645000
H	1.08774600	-1.91036800	2.97090300
C	2.39342000	-1.37710200	1.39546800
H	-0.57429600	2.48110600	4.22046900
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N	2.17444100	-1.41620100	0.06694000
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H	1.78790500	-2.42839600	-3.85125800
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H	1.90136100	-4.46271800	-2.59354200
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N	3.89024900	2.09567000	-1.60056700
H	2.95426800	2.38013400	-1.31384100
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C	5.14406000	2.87665600	0.39136800
C	4.80544600	4.37001200	-1.44700800
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C	4.04318600	3.86251600	0.84063600
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C	5.06680900	1.49797400	1.02927800
C	3.83117700	4.84053200	-0.34542900
H	5.76648400	4.88809100	-1.35210600
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H	3.10917900	3.32786300	1.04062700
H	4.32581600	4.37542200	1.76621900
H	4.21359500	0.92604400	0.63603900
H	4.89460200	1.59364100	2.11202600
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(2) $\mathbf{H_1}$-12

E_e = -3474.1155693 Hartrees

H	-9.17565900	1.39111200	1.62430100
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H	-7.96669700	0.50697100	2.58887700
C	-8.96886100	0.45670300	2.15579500
C	-9.14037800	-0.68099200	1.16917200
O	-10.25736600	-1.00131500	0.77800900
N	-7.98570500	-1.30124500	0.80184500
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C	-7.83748000	-2.35072400	-0.20415600
C	-7.66517000	-1.82864000	-1.64518700
C	-9.10660900	-1.54909100	-2.08771200
C	-9.88999000	-2.75724300	-1.53608800
C	-9.05548300	-3.28899300	-0.33924800
H	-6.95199700	-2.91926000	0.10112700
H	-7.32143600	-2.70890800	-2.21620900
H	-9.45731300	-0.62045300	-1.63274900
H	-9.18827900	-1.44908300	-3.17699900
H	-10.89094000	-2.46435700	-1.21491800
H	-9.98917700	-3.53525000	-2.30327000
H	-8.67761200	-4.29576100	-0.55376700
H	-9.63338300	-3.33807800	0.58434700
C	-6.60245000	-0.75875400	-1.89316600
H	-6.54517000	-0.58425700	-2.97856600
H	-5.61459600	-1.14140300	-1.60900400
C	-6.79273100	0.63112700	-1.28903300
O	-7.89065700	1.11646000	-1.04238100
N	-5.61551900	1.30835200	-1.16594100
H	-4.76683100	0.75318300	-1.25631000
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C	-6.62243600	3.62846400	-1.20805900
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H	-4.86090000	4.05027300	0.68984900
C	-4.17581000	2.18867400	1.39141600
C	-7.44199500	3.79831000	0.09971800
H	-6.22135900	4.59425200	-1.53681800
H	-7.21741600	3.21974400	-2.02562300
H	-7.02134800	1.98279100	1.21691700
H	-6.74934400	3.44712000	2.17615100
H	-4.08348500	2.60111800	2.40777300
H	-3.19321500	2.33746000	0.92597800
C	-4.39732200	0.69392700	1.61082000
H	-8.45543600	3.40985600	-0.01998700
H	-7.51045300	4.85867000	0.37143300
O	-5.51093700	0.18313700	1.73156000
N	-3.23295800	0.01808100	1.78650800
H	-2.38331300	0.52128700	1.53631700
C	-3.04138800	-1.35043900	2.26718200
C	-2.94172600	-2.39551000	1.14154700
C	-4.19298400	-1.90184600	3.13434200
H	-2.11281800	-1.32158300	2.84601000
C	-4.41343200	-2.64427200	0.80069500
H	-2.57567000	-3.30886900	1.64150300
C	-1.93730800	-2.14107700	0.01852000
C	-5.06420800	-2.77520600	2.19104300
H	-3.75196200	-2.51520400	3.92792600
H	-4.76281300	-1.10385200	3.61107900
H	-4.81241700	-1.77459200	0.27219700
H	-4.55909600	-3.52765600	0.16715900
H	-1.91986000	-3.03363700	-0.62499400
H	-0.92761400	-2.06545400	0.44121200
C	-2.16040200	-0.98173100	-0.94734800
H	-6.10778300	-2.45279400	2.19596300
H	-5.04208200	-3.82213700	2.51712800
O	-3.28021200	-0.57646000	-1.26024400
N	-1.00749500	-0.54019500	-1.50954700
H	-0.14650000	-0.86547200	-1.07265000
C	-0.83504000	0.36133100	-2.64938800
C	-0.65373800	1.83733000	-2.25229700
C	-2.03173500	0.42062300	-3.62232100
H	0.05536700	-0.00678800	-3.16860700
C	-2.09770500	2.29369000	-2.03109000
H	-0.30434100	2.33241800	-3.17457500
C	0.40954500	2.17132700	-1.20764300
C	-2.82607100	1.70313400	-3.25271300
H	-1.63411500	0.49592900	-4.64018300
H	-2.64370100	-0.48033000	-3.57317600
H	-2.47492000	1.85496400	-1.10291500
H	-2.18952600	3.38394500	-1.95597800
H	0.47649200	3.26749900	-1.13475900
H	1.39203300	1.84212600	-1.56916700
C	0.23005000	1.70608000	0.23350800
H	-3.87697800	1.48323600	-3.05238500
H	-2.79551200	2.41760200	-4.08399000
O	-0.87335300	1.56855900	0.76346300
N	1.41122900	1.58548900	0.88948800
H	2.24567400	1.59307900	0.30542500
C	1.65003300	1.40659800	2.32132900
C	1.79803600	-0.06689200	2.74052400
C	0.51305200	1.90507800	3.23837400
H	2.57280200	1.95891500	2.52671200
C	0.33957300	-0.51727500	2.85387200
H	2.19541700	-0.02530200	3.76902400
C	2.79876600	-0.92976700	1.97354100
C	-0.30618000	0.64583600	3.63048200
H	0.96733900	2.35992900	4.12506500
H	-0.09679800	2.66709300	2.75237700
H	-0.08965100	-0.60164600	1.85123100
H	0.23313700	-1.48682200	3.35494500
H	2.86988500	-1.89994800	2.48826200

H	3.79785200	-0.48182000	2.05341500
C	2.53525500	-1.29383700	0.51516300
H	-1.36797000	0.76930100	3.40534000
H	-0.22290500	0.46241100	4.70833100
O	1.40379700	-1.41199900	0.04380900
N	3.67490800	-1.59498000	-0.15512600
H	4.54075800	-1.31845500	0.30088400
C	3.83106400	-2.19850600	-1.47853200
C	3.95601200	-1.16790100	-2.61364100
C	2.64080200	-3.06664300	-1.93756500
H	4.74254500	-2.80345700	-1.40820700
C	2.49510800	-0.79758600	-2.88003700
H	4.29447600	-1.75373200	-3.48491200
C	5.00220500	-0.06540500	-2.46217700
C	1.79998800	-2.17295300	-2.88993500
H	3.03925000	-3.93355500	-2.47489600
H	2.06074100	-3.43959200	-1.09277300
H	2.12273400	-0.17904700	-2.05802700
H	2.36597100	-0.24058200	-3.81571700
H	5.06144700	0.47507900	-3.41839700
H	5.99002300	-0.52388800	-2.32486700
C	4.82324300	1.02889100	-1.41381500
H	0.75533000	-2.12117400	-2.57436800
H	1.81242200	-2.58723400	-3.90482700
O	3.72844000	1.38072100	-0.97297700
N	5.99470300	1.64443500	-1.11653400
H	6.83458400	1.17478900	-1.44478500
C	6.21834100	2.85159200	-0.32603900
C	6.41792100	2.60082000	1.18134900
C	5.04658600	3.85711900	-0.34641800
H	7.11889100	3.30663400	-0.75720000
C	4.98122400	2.48124000	1.69544200
H	6.81054600	3.55591900	1.56867600
C	7.45025100	1.56045900	1.61343400
C	4.27897300	3.65686900	0.98871100
H	5.45944700	4.86921700	-0.40574900
H	4.41032300	3.70852500	-1.21967300
H	4.56178000	1.52446300	1.37166800
H	4.91947900	2.53670600	2.78884700
H	7.61530500	1.67863900	2.69416700
H	8.41571500	1.79619200	1.14103700
C	7.17893000	0.07217700	1.40404800
H	3.21600200	3.46937400	0.81893900
H	4.35472400	4.55893900	1.60663200
O	6.07867900	-0.40163400	1.14568000
N	8.29244100	-0.68443400	1.61372700
H	9.13931400	-0.16856800	1.81264600
C	8.43515900	-2.14420900	1.58171800
C	8.65360100	-2.70068800	0.15987000
C	7.19972000	-2.91999500	2.09090700
H	9.30837300	-2.34953000	2.21050600
C	7.22662400	-2.87289100	-0.37168000
H	9.06981400	-3.71074700	0.29910100
C	9.66881400	-1.95078600	-0.71023800
C	6.49055500	-3.48606000	0.83240700
H	7.53668500	-3.73026500	2.74451300
H	6.54693500	-2.27533300	2.68134400
H	6.80983300	-1.89512600	-0.62738000
H	7.19087100	-3.50514900	-1.26604000
H	9.75585400	-2.47544000	-1.67035600
H	10.65705000	-2.00085400	-0.23436200
C	9.33546300	-0.51137000	-1.05730800
H	5.42158700	-3.25717400	0.83153400
H	6.58631100	-4.57743100	0.80743500
O	8.26311800	-0.17603100	-1.55330700
N	10.31529000	0.40469400	-0.83206700
H	11.23306400	0.07570200	-0.56810900
C	10.18455700	1.76232100	-1.33607200
H	9.29826500	2.23796000	-0.90808500
H	11.06728800	2.33294700	-1.04586400
H	10.08279000	1.77011900	-2.42591300

(3) **H_1**-9

E_e = -3474.1894947 Hartrees

H	15.07829700	-2.63714300	-0.10173300
H	14.96655100	-1.73171700	-1.61179900
H	15.73177500	-0.98272000	-0.18549700
C	14.92747700	-1.63987700	-0.52419400
C	13.55006400	-1.15960200	-0.12815800
O	12.53956600	-1.73380200	-0.53540000
N	13.49497400	-0.08856100	0.69619800
H	14.37113100	0.31161900	1.00700000
C	12.26436600	0.42983300	1.29623800
C	11.70720100	1.64677100	0.52786000
C	12.73336500	2.74172300	0.85781900
C	13.17927200	2.45049300	2.31411100
C	12.59904100	1.05188700	2.65642800
H	11.55481100	-0.40137200	1.35454100
H	10.75762100	1.91465000	1.01540700
H	13.58087000	2.66693500	0.16429000
H	12.30819800	3.74139400	0.73427300
H	14.27082500	2.46499400	2.40369300
H	12.80461200	3.20565100	3.00970000
H	11.67146300	1.15327300	3.22836000
H	13.27723400	0.42645800	3.24501500
C	11.43515800	1.44720900	-0.96745900
H	12.23228200	0.84757400	-1.42226900
H	11.40774000	2.42032400	-1.46655400
C	10.06549400	0.82118900	-1.16938300
O	9.06073100	1.54159300	-1.24054900
N	10.01933300	-0.51954900	-1.19757300
H	10.89725500	-1.02535600	-1.06026700
C	8.79135700	-1.29821300	-1.32611500
C	8.28341600	-1.79223300	0.04692600
C	9.10971700	-2.62038600	-2.03529500
H	8.06070100	-0.68265200	-1.85956600
C	9.32443600	-2.86151500	0.41331900
H	7.32330100	-2.29891100	-0.13480700
C	8.06467700	-0.71803600	1.11991700
C	9.71278400	-3.52756500	-0.93019600
H	8.17557300	-3.04534400	-2.41727200
H	9.77935700	-2.47341000	-2.88760600
H	10.20302600	-2.38012400	0.86328000
H	8.93197700	-3.57085900	1.14779000
H	8.86883000	0.02722100	1.07361800
H	8.07855500	-1.18084000	2.11120500
C	6.69532900	-0.08033300	0.95992200
H	10.80005500	-3.59530100	-1.02441100
H	9.31571100	-4.54376500	-1.00455400
O	5.71601300	-0.55911300	1.54928000
N	6.61537900	0.95808800	0.11398300
H	7.47237900	1.24580100	-0.36902900
C	5.37607900	1.65508400	-0.21389200
C	4.78047900	1.16041400	-1.55102500
C	5.69341800	3.12079300	-0.53701400
H	4.69138000	1.53321900	0.63101700
C	5.76889800	1.73347800	-2.57848100
H	3.81658600	1.67664600	-1.67947700
C	4.53427100	-0.34857200	-1.67205500
C	6.19857000	3.10633900	-2.00457000
H	4.77046900	3.70428900	-0.45278500
H	6.41812300	3.54304000	0.16499700
H	6.64030900	1.07012700	-2.65940300
H	5.32076300	1.80413700	-3.57400000
H	5.36405900	-0.90377200	-1.21662100
H	4.47299900	-0.62621400	-2.72843600
C	3.19938500	-0.71971100	-1.05043400
H	7.28512600	3.21737500	-2.04957100
H	5.76032300	3.93241200	-2.57189000
O	2.17138100	-0.72092700	-1.74285600
N	3.20272100	-0.97475200	0.26709500
H	4.09323200	-0.89002700	0.76810200
C	2.00792000	-1.29442600	1.04101000
C	1.45757100	-0.05544300	1.78188700
C	2.39470800	-2.21044900	2.20908000
H	1.27994600	-1.74285300	0.35784400
C	2.51182900	0.16368600	2.87865500
H	0.51993100	-0.36789800	2.26707500
C	1.16400600	1.18145000	0.92418600
C	2.96855500	-1.25748500	3.29145100
H	1.49149500	-2.71037000	2.57483200
H	3.10105100	-2.98604200	1.89908800
H	3.35988400	0.72648000	2.46628800
H	2.10968400	0.74648900	3.71283400
H	1.94674100	1.30886600	0.16587300
H	1.15088500	2.07265900	1.55836000
C	-0.21476000	1.08113100	0.29576700
H	4.05959800	-1.31378800	3.32742700
H	2.59236900	-1.52751800	4.28243700
O	-1.20044300	1.55381600	0.88036200
N	-0.29230600	0.41378600	-0.86578400
H	0.57438100	0.01966500	-1.24624100
C	-1.53051000	0.18178400	-1.60167100
C	-2.10082000	-1.22903800	-1.33389700
C	-1.21548700	0.11058200	-3.10183000
H	-2.22954800	0.98259900	-1.34094600
C	-1.09770600	-2.12961300	-2.06973800
H	-3.06449100	-1.28686200	-1.86324000
C	-2.33735200	-1.60259600	0.13438000
C	-0.68919400	-1.33140900	-3.33240100
H	-2.14196900	0.27801700	-3.66147600
H	-0.50152600	0.88274000	-3.40309300
H	-0.22049800	-2.29924700	-1.43152300
H	-1.52732800	-3.10950500	-2.29874100
H	-1.51001500	-1.23423300	0.75409500

H	-2.38284000	-2.69129700	0.23230000
C	-3.67920200	-1.07227200	0.60884500
H	0.39666000	-1.33962900	-3.45693200
H	-1.12755700	-1.76203100	-4.23737800
O	-4.69728000	-1.77012500	0.49613000
N	-3.69020500	0.18260300	1.08406600
H	-2.80489800	0.69991700	1.07890200
C	-4.88857300	0.87910100	1.54039000
C	-5.45540800	1.81849400	0.45225700
C	-4.50181000	1.87541600	2.64168600
H	-5.60789600	0.12337800	1.87095300
C	-4.40895000	2.94190200	0.41644700
H	-6.39192800	2.23730700	0.85170800
C	-5.75902300	1.17948700	-0.90779700
C	-3.95328900	3.11510100	1.88600300
H	-5.40194700	2.13591700	3.20859400
H	-3.78131600	1.44469900	3.34307700
H	-3.55876400	2.63357700	-0.20607100
H	-4.81617100	3.85928000	-0.01922900
H	-4.96874200	0.46581900	-1.17323200
H	-5.79410800	1.95634100	-1.67756400
C	-7.13074300	0.52712800	-0.89155900
H	-2.86302400	3.16407400	1.94624800
H	-4.34857200	4.03797300	2.32055900
O	-8.13535000	1.18927500	-1.18688900
N	-7.17869300	-0.75287300	-0.49094000
H	-6.30195500	-1.18902400	-0.18831000
C	-8.41049500	-1.52384300	-0.35821600
C	-8.89911400	-1.57164900	1.10662500
C	-8.10998900	-3.00274800	-0.63465200
H	-9.14716000	-1.09268000	-1.04300600
C	-7.85598200	-2.48618900	1.76681800
H	-9.86443700	-2.10074600	1.10206400
C	-9.09755800	-0.21967600	1.80085400
C	-7.50152300	-3.53979100	0.68853300
H	-9.05174600	-3.51369900	-0.86176500
H	-7.44758000	-3.12765000	-1.49628200
H	-6.96386600	-1.90124400	2.02657900
H	-8.23725300	-2.92802100	2.69240700
H	-8.29196100	0.47025900	1.51897500
H	-9.06953600	-0.35796500	2.88589200
C	-10.46903500	0.34570600	1.47280200
H	-6.41723300	-3.65323300	0.60730500
H	-7.91747900	-4.52134500	0.93427800
O	-11.44659600	0.04341500	2.16795100
N	-10.54831500	1.11997500	0.37666300
H	-9.70104600	1.23961900	-0.18639700
C	-11.79655600	1.67630400	-0.13244800
C	-12.34893800	0.85108500	-1.31633200
C	-11.51326800	3.02793700	-0.79934800
H	-12.49448400	1.74155300	0.70635400
C	-11.35551400	1.19072700	-2.43998200
H	-13.32611800	1.28561100	-1.57523900
C	-12.54336200	-0.64967000	-1.07330300
C	-10.95063700	2.66718500	-2.19899000
H	-12.45789800	3.57456600	-0.89354500
H	-10.83130000	3.64145800	-0.20315200
H	-10.47179900	0.54398200	-2.35917900
H	-11.79437900	1.02075900	-3.42790600
H	-11.70718600	-1.04258200	-0.47924300
H	-12.55642400	-1.17667500	-2.03210300
C	-13.88304800	-0.93710300	-0.40969600
H	-9.86231500	2.77123200	-2.22528600
H	-11.36157700	3.33054500	-2.96590500
O	-14.87634700	-1.22644000	-1.07264300
N	-13.92264100	-0.80273400	0.93394500
H	-13.08182700	-0.52548600	1.44084500
C	-15.17000600	-0.97656000	1.64775800
H	-15.56399300	-1.98701000	1.49966600
H	-14.98839400	-0.81001500	2.71074300
H	-15.92510800	-0.26826800	1.29094800

(4) **H_1-7**

E_e = -3474.1328149 Hartrees

H	-16.07287300	-1.71338200	0.22804100
H	-17.30108200	-0.42998000	0.41808000
H	-17.14179800	-1.27408800	-1.12471100
C	-16.58334100	-0.88412600	-0.26837000
C	-15.63882300	0.19820900	-0.76307600
O	-16.06950000	1.28491800	-1.13300400
N	-14.32937400	-0.16118400	-0.78824900
H	-14.06692700	-1.02240700	-0.31573200
C	-13.17865600	0.66312200	-1.15813700
C	-12.62492200	1.46894700	0.03744900
C	-13.50620800	2.72352100	0.04634700
C	-13.69717600	3.06963500	-1.44336200
C	-13.45900500	1.74615000	-2.21685400
H	-12.43022200	-0.04967900	-1.52362200
H	-11.59582500	1.76542800	-0.22392500
H	-14.47582300	2.48033700	0.49673900
H	-13.05985700	3.53988300	0.62449900
H	-14.69995500	3.45873400	-1.62858100
H	-12.97232000	3.82941700	-1.75662200
H	-12.57078700	1.82988000	-2.85320300
H	-14.30247400	1.47620100	-2.85373000
C	-12.59534100	0.70213000	1.36448800
H	-13.61838800	0.46798500	1.67493900
H	-12.13612400	1.32524700	2.14001600
C	-11.84914900	-0.61487200	1.20828500
O	-12.43610300	-1.64379300	0.85939400
N	-10.51972900	-0.53559500	1.43488700
H	-10.12821700	0.39727300	1.54911300
C	-9.49985500	-1.56153200	1.21239900
C	-9.00414900	-1.60954900	-0.25097900
C	-9.96233700	-3.00526800	1.48675800
H	-8.67969000	-1.28280000	1.88366100
C	-10.00812500	-2.54396500	-0.93637100
H	-8.01953000	-2.10470300	-0.23527800
C	-8.85890700	-0.24349200	-0.93180300
C	-10.31071200	-3.63183300	0.11192800
H	-9.13061700	-3.54468500	1.95282100
H	-10.80296300	-3.02890800	2.18207900
H	-10.92257200	-1.98407800	-1.16521300
H	-9.61959900	-2.94919700	-1.87675000
H	-9.84681700	0.21790600	-1.03496100
H	-8.44198200	-0.37882400	-1.93589000
C	-7.99807700	0.70201300	-0.10566200
H	-11.35892200	-3.93402200	0.07060600
H	-9.69523300	-4.51986300	-0.06931300
O	-8.49113600	1.38830500	0.79560400
N	-6.68503000	0.68872400	-0.41712400
H	-6.36937500	-0.02936600	-1.06700000
C	-5.58545800	1.36460800	0.27512600
C	-5.04314800	0.54435100	1.46681700
C	-5.94848900	2.72227400	0.90501300
H	-4.81229900	1.48645400	-0.49157000
C	-5.96489600	0.95120500	2.62220800
H	-4.03057500	0.92400600	1.67972100
C	-4.96066300	-0.96605100	1.21749700
C	-6.20468000	2.45878400	2.41162900
H	-5.09316000	3.39429100	0.77510900
H	-6.80619200	3.17780700	0.40806700
H	-6.91366400	0.40781600	2.53628900
H	-5.53101800	0.71716300	3.60019200
H	-5.96928700	-1.37404400	1.09284000
H	-4.49915800	-1.45688800	2.08146000
C	-4.18414900	-1.26059800	-0.05889200
H	-7.22064800	2.73926800	2.69564200
H	-5.50971400	3.04434400	3.02336800
O	-4.75409900	-1.31920100	-1.15354000
N	-2.85307100	-1.39580200	0.11499100
H	-2.48402400	-1.16833100	1.03652100
C	-1.81165600	-1.50930500	-0.90835700
C	-1.35861900	-0.13502800	-1.45201300
C	-2.22783000	-2.28430300	-2.17317400
H	-0.98208800	-2.01225600	-0.39950500
C	-2.35941000	0.14581200	-2.57862600
H	-0.36245200	-0.28293800	-1.89920600
C	-1.26401500	0.97370100	-0.39732900
C	-2.58144200	-1.22383600	-3.24833500
H	-1.37466800	-2.88949100	-2.49776000
H	-3.05703700	-2.96300400	-1.96786700
H	-3.30037800	0.50365100	-2.14409400
H	-1.99729000	0.91081900	-3.27358600
H	-2.26318000	1.19452800	-0.00690900
H	-0.87017800	1.88632500	-0.85816900
C	-0.40092200	0.53776300	0.77898400
H	-3.61297600	-1.33329700	-3.58906600
H	-1.92557400	-1.33191800	-4.11906800
O	-0.89237500	-0.06668100	1.73841500
N	0.91077200	0.82487600	0.65051300
H	1.21931600	1.18558500	-0.25081200
C	2.01949900	0.40506400	1.51080000
C	2.55568600	-0.99625900	1.14157200
C	1.67106100	0.27927700	3.00593600
H	2.79181000	1.16613900	1.35447200
C	1.63994800	-1.93955700	1.92982500
H	3.57258000	-1.06773000	1.56055300
C	2.62279100	-1.28560900	-0.36277100
C	1.42152800	-1.22716700	3.27794600
H	2.53007200	0.63469300	3.58511100
H	0.81318600	0.89945500	3.26935800
H	0.68367400	-2.03681200	1.40193600
H	2.06876900	-2.94150700	2.03638500
H	1.60936400	-1.31719700	-0.77723900

H	3.08641000	-2.26454200	-0.52715300
C	3.38373200	-0.18855200	-1.09545800
H	0.41246900	-1.39997800	3.65694100
H	2.13051000	-1.60099200	4.02462200
O	2.80325700	0.82058900	-1.50968700
N	4.71209700	-0.39969700	-1.19818700
H	5.09508600	-1.19028600	-0.68242000
C	5.74344600	0.52110400	-1.68205100
C	6.23854000	1.48568300	-0.58036200
C	5.29518200	1.46428200	-2.81378800
H	6.55830100	-0.12996300	-2.01736100
C	5.22765800	2.63645600	-0.64515200
H	7.21998900	1.86414900	-0.90910300
C	6.39343300	0.85615000	0.80941500
C	4.94575600	2.82092600	-2.14867200
H	6.13488900	1.58348400	-3.50687300
H	4.45941800	1.04503400	-3.37597200
H	4.30770000	2.33470000	-0.12970600
H	5.60074800	3.54554400	-0.16178100
H	5.40823100	0.57035200	1.19331200
H	6.82403100	1.59076900	1.49867200
C	7.24290700	-0.40617600	0.75129400
H	3.90193800	3.08845600	-2.32290400
H	5.57282100	3.61935500	-2.55989200
O	6.73303000	-1.50394400	0.50181600
N	8.56279200	-0.20966600	0.94761900
H	8.89047500	0.75320400	1.00109000
C	9.65302800	-1.17793000	0.80832900
C	10.16713100	-1.28079300	-0.64521200
C	9.28572800	-2.63086900	1.16345000
H	10.44054700	-0.80206000	1.47074200
C	9.21755200	-2.30308000	-1.27954300
H	11.17401400	-1.72665400	-0.59373100
C	10.25722600	0.05349500	-1.39556900
C	8.98475600	-3.35295700	-0.17566000
H	10.15245500	-3.08578800	1.65534000
H	8.44855600	-2.67490300	1.86141500
H	8.27118400	-1.80714100	-1.52698300
H	9.62270800	-2.72986300	-2.20301100
H	9.25141700	0.46604000	-1.52884900
H	10.68959700	-0.11115700	-2.38855500
C	11.06987500	1.06619900	-0.60083700
H	7.96069000	-3.72957000	-0.20058100
H	9.66099600	-4.20427300	-0.30954300
O	10.54296300	1.75057900	0.28282700
N	12.38292000	1.10160800	-0.90568900
H	12.73332400	0.40618600	-1.55914500
C	13.45445200	1.83103300	-0.22570400
C	14.00802400	1.06724600	0.99924100
C	13.04279600	3.19722800	0.35671000
H	14.23041500	1.94904400	-0.98654500
C	13.06922900	1.49139200	2.13590700
H	15.01005200	1.47971600	1.19649700
C	14.11984500	-0.45319800	0.83797900
C	12.77902700	2.98028200	1.86889200
H	13.87605600	3.89240900	0.20999200
H	12.17628000	3.60730800	-0.16420300
H	12.13909800	0.91395700	2.06623000
H	13.50367700	1.30842100	3.12470900
H	13.11490900	-0.87289800	0.71077300
H	14.54086500	-0.88615400	1.75299000
C	14.93247500	-0.85378700	-0.38056800
H	11.74968300	3.23152800	2.13111000
H	13.44320900	3.61330900	2.46700000
O	14.50817000	-0.70772000	-1.52707100
N	16.16504700	-1.36093500	-0.15218200
H	16.48360300	-1.48335100	0.79739100
C	17.02653400	-1.74933700	-1.25556600
H	17.95115200	-2.16225900	-0.85130800
H	16.53091600	-2.50072200	-1.87597000
H	17.25759200	-0.88443300	-1.88337400

(5) **E_1**

E_e = -3474.1894947 Hartrees

H	-18.44598700	0.54898600	1.76548000
H	-17.64347400	1.60017400	0.59815500
H	-18.36833000	0.06469700	0.05356600
C	-17.82581200	0.55676000	0.86489100
C	-16.49856100	-0.09871000	1.19024700
O	-15.71441700	0.40171100	1.98565000
N	-16.23769800	-1.27264300	0.55330000
H	-16.94168500	-1.65680000	-0.06273800
C	-15.05693800	-2.08160500	0.85169900
C	-13.86384700	-1.73869200	-0.05795200
C	-14.24643100	-2.37711300	-1.40578100
C	-15.12449200	-3.60602000	-1.05089700
C	-15.32845000	-3.54260900	0.48284500
H	-14.82488400	-1.93254500	1.91054500
H	-12.99143700	-2.27118000	0.34357300
H	-14.82096900	-1.65498800	-2.00120400
H	-13.35759100	-2.63711200	-1.98452100
H	-16.08475600	-3.56414900	-1.57772900
H	-14.65323700	-4.54739700	-1.34622900
H	-14.58557400	-4.16765400	0.98897100
H	-16.31670700	-3.88249600	0.81024100
C	-13.51791400	-0.26034700	-0.13252100
H	-13.36984100	0.14652000	0.87629200
H	-14.35362200	0.30326100	-0.56806100
C	-12.25135700	-0.01146800	-0.93904800
O	-11.43541700	-0.89385800	-1.18073400
N	-12.07181200	1.27289800	-1.34880300
H	-12.78001000	1.95622800	-1.11153700
C	-10.91542900	1.70212500	-2.13081500
C	-9.74837200	2.18048400	-1.24926000
C	-11.26382400	2.97123100	-2.91318600
H	-10.63211200	0.85906600	-2.76750400
C	-10.20829300	3.56791200	-0.76284600
H	-8.88017600	2.31257100	-1.90838600
C	-9.34993200	1.22273400	-0.13762800
C	-11.13634000	4.11621600	-1.87954600
H	-10.52347100	3.09885100	-3.70961900
H	-12.24925500	2.91388100	-3.38712700
H	-10.76354000	3.46070000	0.17845500
H	-9.35377300	4.21735500	-0.55882000
H	-9.15261800	0.22469600	-0.55116400
H	-10.17557900	1.10076200	0.57610400
C	-8.09603300	1.68486300	0.59004800
H	-12.11662300	4.38817200	-1.47148800
H	-10.73429200	5.02197100	-2.34148300
O	-7.28009100	2.44619600	0.08328800
N	-7.92287700	1.15974700	1.83291500
H	-8.63260400	0.53440400	2.19322500
C	-6.75065100	1.44143200	2.65653300
C	-5.61507100	0.42679000	2.42626200
C	-7.08771400	1.21378800	4.13262400
H	-6.44242600	2.46619200	2.43117700
C	-6.10663300	-0.83369700	3.16145200
H	-4.72684100	0.80970900	2.94560100
C	-5.24448800	0.19812800	0.96878600
C	-6.99393600	-0.31969400	4.32591200
H	-6.32901100	1.71752200	4.74050400
H	-8.06079800	1.63265200	4.40880100
H	-6.69896800	-1.45194700	2.47344100
H	-5.26735900	-1.44540700	3.50062100
H	-4.97158400	1.14902300	0.49256800
H	-6.10920500	-0.18853100	0.41376400
C	-4.06556600	-0.75350900	0.83113400
H	-7.98726600	-0.78168900	4.29193900
H	-6.57300700	-0.56770900	5.30411700
O	-3.21271400	-0.87674200	1.70293100
N	-4.00311400	-1.43629700	-0.34359900
H	-4.74785000	-1.30521300	-1.01607600
C	-2.94319900	-2.39388200	-0.64667800
C	-1.73948200	-1.74276300	-1.35055700
C	-3.43124600	-3.38737900	-1.70478800
H	-2.66005900	-2.86605600	0.29865900
C	-2.24082700	-1.51565600	-2.78855600
H	-0.93712700	-2.49170900	-1.37502400
C	-1.19287200	-0.49443400	-0.67412000
C	-3.28192400	-2.63565100	-3.05007100
H	-2.77244400	-4.26171900	-1.68567600
H	-4.44923200	-3.74068600	-1.50992200
H	-2.71471500	-0.52756800	-2.85960500
H	-1.41268100	-1.52716100	-3.50159600
H	-0.92805400	-0.71521600	0.36800000
H	-1.96275300	0.28739800	-0.63877500
C	0.05519700	0.01816300	-1.37601700
H	-4.23924100	-2.20969600	-3.37111000
H	-2.96515700	-3.31416900	-3.84687800
O	0.84002700	-0.73100700	-1.94693700
N	0.26221800	1.36003300	-1.29799600
H	-0.42544800	1.92635600	-0.81802000
C	1.42430500	2.01612500	-1.89111100
C	2.60570600	2.11925700	-0.91010800
C	1.10545600	3.48794400	-2.16545700
H	1.68320000	1.44974100	-2.79015200
C	2.18115200	3.25025500	0.04484200
H	3.47780600	2.45539100	-1.48602000
C	2.97507100	0.81748600	-0.21582000
C	1.27977500	4.19204300	-0.79671300
H	1.83858900	3.87119700	-2.88265800
H	0.11301000	3.62554900	-2.60676700
H	1.61374700	2.82554100	0.88393700
H	3.05093500	3.75740800	0.46917900
H	3.17010300	0.03413400	-0.96008000

H	2.13422500	0.46102300	0.39354500
C	4.22108600	0.96818200	0.64328700
H	0.31147100	4.34553600	-0.30703600
H	1.72321900	5.18392600	-0.91883200
O	5.09083000	1.79827900	0.40355600
N	4.32339200	0.09036400	1.67695600
H	3.56659300	-0.56411000	1.82865800
C	5.46480400	0.06651400	2.58720900
C	6.58478400	-0.87259500	2.10293300
C	5.05619000	-0.58244300	3.91240300
H	5.81009500	1.09892700	2.69405800
C	6.02664100	-2.27612600	2.40075000
H	7.45477400	-0.69834200	2.74952000
C	7.01994100	-0.66444900	0.66062000
C	5.10717000	-2.10595800	3.63851100
H	5.79767200	-0.31052200	4.67093400
H	4.08149600	-0.23207100	4.26731700
H	5.44563800	-2.62766600	1.53741700
H	6.83173100	-2.99675400	2.56152600
H	7.31501300	0.38072500	0.49852800
H	6.17907600	-0.85523500	-0.01909500
C	8.20002900	-1.55247500	0.29404800
H	4.10588900	-2.50408300	3.43871900
H	5.48548500	-2.64882000	4.50906400
O	8.98690200	-1.98285300	1.12960100
N	8.34333600	-1.80983200	-1.03382500
H	7.65366700	-1.43701600	-1.67376500
C	9.41638100	-2.64552100	-1.56552400
C	10.66946800	-1.83241500	-1.93778800
C	8.99697200	-3.22428900	-2.91990100
H	9.62898400	-3.40874400	-0.81141800
C	10.26760200	-1.13309800	-3.24948200
H	11.46935900	-2.55199300	-2.15584200
C	11.16988300	-0.88790100	-0.85535400
C	9.24476800	-2.07865500	-3.93206300
H	9.64695900	-4.07565500	-3.14709100
H	7.96548700	-3.59163200	-2.91645800
H	9.80045800	-0.16591500	-3.01965100
H	11.14206500	-0.92721200	-3.87152300
H	11.36206500	-1.44175600	0.07275200
H	10.39917600	-0.14311800	-0.61748000
C	12.46104000	-0.19783100	-1.26940700
H	8.31401100	-1.54675200	-4.15948900
H	9.61637100	-2.46838100	-4.88364700
O	13.26468900	-0.71434200	-2.03757900
N	12.67865600	1.01978100	-0.70415500
H	11.97215900	1.39519300	-0.08450600
C	13.87284500	1.81649900	-0.97321200
C	15.00830400	1.53280000	0.02660500
C	13.57746400	3.29537000	-0.70929800
H	14.16902300	1.60663200	-2.00496800
C	14.54484000	2.24945900	1.30799300
H	15.90576100	2.04013300	-0.35110000
C	15.34685600	0.06178100	0.21104500
C	13.68694100	3.45000900	0.82776900
H	14.34953300	3.89354100	-1.20428300
H	12.60975900	3.60881500	-1.11453200
H	13.93754400	1.56285600	1.91285900
H	15.39709300	2.55035000	1.92137500
H	15.57203100	-0.39868800	-0.75962200
H	14.48227300	-0.48033400	0.61687800
C	16.55172300	-0.12961700	1.11906100
H	12.69600500	3.43300100	1.29602900
H	14.13688100	4.41007800	1.09528400
O	17.39829900	0.73619800	1.29756000
N	16.64625900	-1.34849400	1.71619100
H	15.96441800	-2.05848200	1.49254100
C	17.80562200	-1.69254900	2.51649400
H	17.94653500	-0.94708900	3.30289000
H	17.64395600	-2.67124700	2.97073400
H	18.71435300	-1.71918000	1.90619900