Supplementary information

Helix foldamers of γ-peptides based on 2-aminocyclohexylacetic acid: a computational study

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Table S1 Backbone torsion angles for optimized helical and extended structures of oligopeptides of γAc$_6$a residues **1** and **2**[a]

Dipeptides

$\mathbf{H}_1$	ϕ	θ	ζ	ψ	$\mathbf{H}_2$	ϕ	θ	ζ	ψ
$\mathbf{H}_1$-14	−93.2	62.0	71.1	−155.6	$\mathbf{H}_2$-14	−161.5	54.3	50.4	−152.4
	−139.8	56.7	52.6	−112.7		−97.2	57.8	58.6	−164.1
av.	−116.5	59.4	61.8	−134.2	av.	−129.3	56.0	54.5	−158.2
$\mathbf{H}_1$-12	82.5	51.6	−79.4	−178.2	$\mathbf{H}_2$-12	65.0	61.2	−84.4	174.1
	78.3	46.8	−69.5	137.4		65.6	65.7	−63.7	120.0
av.	80.4	49.2	−74.5	159.6	av.	65.3	63.5	−74.1	147.0
$\mathbf{H}_1$-9	−100.2	63.0	81.0	−97.6	$\mathbf{H}_2$-9	−103.5	61.6	79.2	−90.9
	−100.6	61.4	81.3	−93.4		−108.6	58.2	80.2	−82.2
av.	−100.4	62.2	81.1	−95.5	av.	−106.1	59.9	79.7	−86.6
$\mathbf{H}_1$-7	137.6	50.5	44.0	80.3	$\mathbf{H}_2$-7	63.5	49.9	45.9	94.4
	133.4	49.4	44.1	89.9		63.9	48.2	51.5	104.5
av.	135.5	49.9	44.1	85.1	av.	63.7	49.1	48.7	99.4
$\mathbf{E}_1$[b]	−95.9	57.5	167.1	157.5	$\mathbf{E}_2$[b]	−97.3	58.2	−176.3	−142.2
	−93.5	57.1	168.4	150.0		−100.3	57.6	−175.0	−135.3
av.	−94.7	57.3	167.7	153.7	av.	−98.8	57.9	−175.6	−138.8

Tetrapeptides

$\mathbf{H}_1$	ϕ	θ	ζ	ψ	$\mathbf{H}_2$	ϕ	θ	ζ	ψ
$\mathbf{H}_1$-14	−94.9	60.8	69.6	−158.6	$\mathbf{H}_2$-14	−91.3	61.7	60.8	−171.4
	−146.4	56.7	66.8	−131.6		−147.4	60.0	66.1	−115.4
	−140.6	56.4	67.1	−144.9		−170.0	58.4	59.4	−113.8
	−141.4	57.9	54.4	−124.0		−147.8	56.7	50.7	−143.7
av.	−142.8	57.0	62.8	−133.5	av.	−155.1	58.4	58.7	−124.3
$\mathbf{H}_1$-12	−160.6	62.6	−76.3	175.8	$\mathbf{H}_2$-12	65.4	61.9	−85.1	179.2
	83.6	53.8	−77.2	167.7		66.6	63.1	−84.5	174.2
	83.1	55.6	−74.4	168.9		76.7	56.1	−87.0	176.7
	79.6	52.0	−66.1	129.8		63.1	67.4	−58.6	116.5
av.	82.1	53.8	−72.6	155.5	av.	67.9	62.1	−78.8	161.7
$\mathbf{H}_1$-9	−100.5	62.6	80.9	−98.3	$\mathbf{H}_2$-9	−103.5	61.3	79.3	−90.7
	−100.1	61.8	81.3	−95.1		−111.6	59.2	75.8	−86.4
	−99.9	61.6	81.9	−94.3		−109.0	60.4	75.6	−86.9
	−100.9	60.7	81.6	−93.6		−104.7	59.7	80.0	−83.6
av.	−100.4	61.7	81.4	−95.3	av.	−107.2	60.1	77.7	−86.9
$\mathbf{H}_1$-7	137.1	50.4	43.7	80.2	$\mathbf{H}_2$-7	63.2	50.1	46.2	93.8
	135.6	51.0	42.2	82.2		65.2	51.3	45.6	98.5
	138.6	51.5	41.9	81.5		65.0	50.9	45.7	96.5
	136.7	50.3	42.9	88.6		64.4	47.8	50.9	104.1
av.	137.0	50.8	42.7	83.1	av.	64.4	50.0	47.1	98.2
$\mathbf{E}_1$[b]	−96.1	57.3	169.2	142.1	$\mathbf{E}_2$[b]	−97.7	58.1	−173.5	−145.6
	−94.4	56.9	170.5	145.0		−99.3	57.4	−176.7	−145.2
	−95.1	56.6	168.1	147.1		−100.5	57.8	−171.6	−149.4
	−94.9	57.1	168.5	152.8		−99.4	56.9	−176.0	−136.7
av.	−95.1	57.0	169.1	146.7	av.	−99.2	57.5	−174.4	−144.2

Hexapeptides

$\mathbf{H_1}$	ϕ	θ	ζ	ψ	$\mathbf{H_2}$	ϕ	θ	ζ	ψ
$\mathbf{H_1}$-14	−95.0	60.6	69.5	−159.2	$\mathbf{H_2}$-14	−91.9	60.8	61.8	−171.8
	−142.8	56.1	65.3	−127.6		−143.9	58.0	66.6	−118.6
	−149.6	56.7	65.2	−133.2		−165.7	58.4	59.1	−110.9
	−145.0	57.9	66.7	−133.9		−158.4	57.5	53.7	−153.1
	−147.2	58.8	66.8	−130.9		−97.7	58.1	63.3	−161.2
	−150.2	58.1	56.9	−125.5		−132.1	61.7	53.1	−113.5
av.	−147.0	57.5	64.2	−130.2	av.	−139.6	58.7	59.2	−131.5
$\mathbf{H_1}$-12	−159.1	61.4	−76.3	175.7	$\mathbf{H_2}$-12	65.4	62.4	−82.1	172.7
	88.4	53.4	−76.4	162.5		64.6	67.9	−75.2	168.9
	89.5	54.9	−74.5	161.0		73.4	58.4	−89.1	−176.3
	90.4	55.6	−76.0	165.0		65.9	62.4	−80.8	171.2
	85.8	55.5	−77.7	174.1		75.6	58.4	−84.3	169.2
	75.8	51.4	−66.5	132.5		64.9	69.1	−56.8	112.0
av.	86.0	54.2	−74.2	159.0	av.	68.3	63.1	−78.0	163.0
$\mathbf{H_1}$-9	−100.3	62.8	80.6	−98.6	$\mathbf{H_2}$-9	−101.8	59.4	81.8	−89.8
	−99.9	61.8	81.3	−94.6		−116.0	57.9	73.6	−85.3
	−99.4	61.7	81.3	−95.6		−106.7	60.7	77.6	−88.2
	−99.9	62.2	80.6	−95.6		−111.2	59.2	75.0	−87.4
	−99.8	61.8	81.7	−95.0		−106.9	61.7	75.5	−89.7
	−101.3	61.6	80.7	−95.6		−104.7	58.9	79.9	−82.9
av.	−100.1	62.0	81.0	−95.8	av.	−107.9	59.7	77.2	−87.2
$\mathbf{H_1}$-7	141.1	51.1	42.4	80.0	$\mathbf{H_2}$-7	63.9	50.2	45.2	95.6
	135.5	50.1	42.3	83.2		66.6	52.7	43.3	96.9
	138.3	51.1	41.3	80.8		65.1	51.5	44.8	97.7
	135.9	50.3	42.0	82.8		65.7	51.7	44.0	96.3
	138.3	51.4	41.9	81.2		65.8	51.4	45.1	97.4
	133.1	49.0	44.0	91.2		64.5	47.7	50.5	104.0
av.	137.0	50.5	42.3	83.2	av.	65.3	50.9	45.5	98.0
$\mathbf{E_1}$[b]	−96.4	57.4	165.6	168.3	$\mathbf{E_2}$[b]	−98.8	58.2	−172.5	−151.5
	−94.6	57.1	166.6	162.5		−101.2	57.4	−172.4	−148.8
	−94.0	57.1	167.7	154.5		−99.8	56.6	−173.8	−154.4
	−95.8	55.8	168.4	139.4		−101.4	57.8	−174.2	−145.4
	−95.6	56.2	169.3	148.0		−99.1	57.3	−175.8	−145.7
	−96.2	57.2	165.9	165.4		−99.7	57.5	−174.5	−138.1
av.	−95.4	56.8	167.3	156.3	av.	−100.0	57.5	−173.9	−147.3

Octapeptides

$\mathbf{H_1}$	ϕ	θ	ζ	ψ	$\mathbf{H_2}$	ϕ	θ	ζ	ψ
$\mathbf{H_1}$-14	−96.0	60.6	70.4	−156.7	$\mathbf{H_2}$-14	−92.6	60.5	62.3	−170.8
	−145.2	56.1	64.7	−127.3		−145.4	58.0	64.0	−121.1
	−147.7	56.2	66.1	−139.1		−159.3	57.0	56.5	−118.5
	−137.1	56.9	66.4	−139.5		−151.9	58.6	56.7	−122.8
	−141.8	57.1	66.8	−130.6		−153.0	59.7	58.7	−115.9
	−151.3	57.9	65.2	−134.5		−160.5	61.1	55.1	−121.7
	−141.2	58.5	67.1	−143.5		−147.2	60.4	55.1	−134.8
	−134.8	55.9	52.3	−129.3		−135.4	59.0	46.2	−126.4
av.	−142.7	56.9	64.1	−134.8	av.	−150.4	59.1	56.0	−123.0

H_1-12	−161.7	62.3	−74.9	173.0	**H_2-12**	65.4	62.8	−87.4	176.8
	88.6	52.9	−78.3	168.5		75.3	54.7	−92.4	−174.7
	83.9	54.9	−73.6	163.1		64.6	65.4	−84.2	172.1
	88.0	55.3	−75.3	164.0		77.3	54.4	−92.4	−175.1
	88.4	54.5	−77.0	168.2		65.6	64.6	−88.8	178.7
	84.6	54.0	−77.1	170.1		71.1	57.0	−90.9	−175.9
	82.7	54.2	−79.0	177.3		66.5	62.8	−88.8	−177.7
	74.0	51.2	−65.8	131.1		65.7	60.2	−72.5	131.3
av.	84.3	53.9	−75.2	163.2	av.	68.9	60.2	−87.2	174.4
H_1-9	−100.3	62.6	80.7	−98.3	**H_2-9**	−103.3	60.4	80.3	−89.3
	−99.5	62.0	81.0	−95.7		−112.3	58.6	75.1	−86.1
	−99.5	61.9	80.6	−96.3		−107.0	61.6	75.7	−89.2
	−100.1	61.7	81.1	−95.7		−107.9	59.2	77.2	−86.9
	−100.3	61.7	81.0	−95.7		−110.6	60.1	74.9	−88.7
	−100.1	61.7	81.1	−95.4		−105.7	60.1	77.8	−86.8
	−99.9	61.8	81.5	−94.5		−111.1	59.1	75.3	−87.7
	−100.6	61.3	81.0	−94.5		−105.2	59.3	80.1	−82.8
av.	−100.1	61.8	81.0	−95.8	av.	−107.9	59.8	77.1	−87.2
H_1-7	139.8	50.4	43.3	81.2	**H_2-7**	63.6	50.6	44.8	94.7
	138.7	51.2	41.0	80.4		65.5	52.1	44.1	96.6
	135.9	50.4	42.9	81.7		66.1	52.1	42.9	95.8
	134.2	49.8	42.5	82.7		65.3	52.1	44.0	96.9
	138.9	51.5	40.7	81.2		66.2	51.2	43.4	96.9
	135.9	50.7	41.8	81.5		65.8	52.4	43.0	94.2
	136.3	50.9	41.9	82.6		65.3	51.7	44.8	96.7
	134.1	48.8	43.9	90.4		64.1	48.8	48.4	101.1
av.	136.7	50.5	42.3	82.7	av.	65.2	51.4	44.4	96.6
E_1[b]	−96.4	57.6	166.9	163.7	**E_2**[b]	−96.9	57.7	−174.6	−146.3
	−93.9	57.6	165.5	159.5		−98.9	56.4	−171.7	−156.2
	−93.0	56.3	169.8	150.4		−100.9	56.4	−172.5	−156.2
	−94.0	57.6	167.4	159.2		−101.4	57.2	−174.6	−147.1
	−94.0	56.4	167.0	156.7		−99.6	57.1	−174.5	−146.0
	−93.1	57.0	168.1	151.7		−99.6	57.2	−176.1	−145.6
	−94.0	56.9	168.2	154.3		−100.1	58.4	−174.1	−141.4
	−93.9	57.1	167.7	155.6		−99.1	57.0	−175.9	−136.4
av.	−94.0	57.1	167.6	156.4	av.	−99.6	57.2	−174.2	−146.9

[a] Optimized at the M06-2X/6-31+G(d) level of theory in the gas phase. Backbone torsion angles in γ-amino acid residues are defined in Fig. 1c of the text. Torsion angles for the first residue of the **H_1**-14, **H_1**-12, and **H_2**-14 foldamers are excluded in calculating the mean values. [b] Extended structure.

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Table S2 Mean distances (Å) and angles (°) for the C=O···H–N H-bonds of helix foldamers of Ac-(γAc$_6$a)$_n$-NHMe

		Residue **1**		Residue **2**	
n	Helix type	*d*(C=O···H–N)	∠N–H···O	*d*(C=O···H–N)	∠N–H···O
4	**H**-14	1.98	167.0	1.93	169.3
	H-12	2.05	158.5	1.93	161.3
	H-9	1.90	167.2	1.87	172.0
	H-7	2.07	139.1	2.26	121.7
6	**H**-14	1.97	168.8	1.95	165.9
	H-12	2.05	160.9	1.91	158.5
	H-9	1.89	167.1	1.87	171.0
	H-7	2.05	140.0	2.22	123.1
8	**H**-14	1.96	170.4	1.93	167.0
	H-12	2.06	159.7	1.90	156.7
	H-9	1.89	167.2	1.86	171.8
	H-7	2.04	140.1	2.19	124.1

Table S3 Helical parameters for helix foldamer of oligo-γAc$_6$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	5.2	2.1	2.9	**H$_2$**-14	2.5	5.3	2.1	2.9
	H$_1$-12	2.5	5.8	2.3	2.9	**H$_2$**-12	2.4	5.0	2.1	2.7
	H$_1$-9	2.5	8.6	3.4	1.9	**H$_2$**-9	2.5	8.1	3.3	2.0
	H$_1$-7	3.2	13.5	4.2	1.7	**H$_2$**-7	2.3	8.7	3.8	1.6
6	**H$_1$**-14	2.5	5.2	2.1	2.9	**H$_2$**-14	2.5	5.1	2.0	2.9
	H$_1$-12	2.5	5.7	2.3	2.9	**H$_2$**-12	3.1	5.9	1.9	2.9
	H$_1$-9	2.5	8.6	3.4	1.9	**H$_2$**-9	2.5	8.1	3.2	2.1
	H$_1$-7	3.1	12.9	4.2	1.7	**H$_2$**-7	2.3	8.7	3.8	1.6
8	**H$_1$**-14	2.5	5.2	2.1	2.9	**H$_2$**-14	2.5	5.0	2.0	2.9
	H$_1$-12	2.5	5.7	2.3	2.9	**H$_2$**-12	2.4	5.2	2.1	2.7
	H$_1$-9	2.5	8.6	3.4	1.9	**H$_2$**-9	2.4	8.1	3.3	2.0
	H$_1$-7	3.0	12.7	4.3	1.6	**H$_2$**-7	2.3	8.7	3.8	1.6

^{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$_6$a (1) dipeptide in the gas phase

Conformational analysis of the γAc$_6$a (**1**) dipeptide, Ac-[γAc$_6$a (**1**)]$_2$-NHMe, has been carried out to confirm whether the helical structures are preferred in the gas phase. All DFT calculations have been carried out using the hybrid-meta-GGA M06-2X functional[1] implemented in the Gaussian 09 program.[2]

From the extended structure of Ac-[γAc$_6$a (**1**)]$_2$-NHMe, the 200 initial structures for optimization were generated by the systematic search of the Discovery Studio package[3] using the CHARMm force field with the maximum systematic conformations = 1000 and the energy threshold = 20 kcal/mol. 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 the 30 local minima with ΔE_e < 12 kcal mol^{-1} at the M06-2X/6-31+G(d) level of theory. Then, at the M06-2X/cc-pVTZ level of theory, the single-point energies were calculated for all local minima at the M06-2X/6-31+G(d) level of theory. The torsion angles and relative electronic energies of the 30 local minima and two helix foldamers **H**$_d$-7 and **H**$_d$-12 at the M06-2X/cc-pVTZ//M06-2X/6-31+G(d) level of theory in the gas phase are listed in Table S4.

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3 *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$_6$a (**1**)]$_2$-NHMe

	Backbone torsion angles[a]								
Conf.	ϕ_1	θ_1	ζ_1	ψ_1	ϕ_2	θ_2	ζ_2	ψ_2	ΔE_0[b]
H$_d$-9[c]	−100.2	63.0	81.0	−97.6	−100.6	61.4	81.3	−93.4	0.00
d1	−103.1	61.0	81.5	−95.3	−126.2	47.9	36.8	49.9	2.01
H$_d$-14[d]	−93.2	62.0	71.1	−155.6	−139.8	56.7	52.6	−112.7	2.10
d2	−105.9	62.2	80.1	−102.2	−157.3	60.4	−168.7	102.1	3.50
d3	−101.8	62.7	81.3	−94.2	−94.8	58.1	−170.3	−73.2	3.80
d4	−101.1	62.3	82.2	−95.9	−93.0	58.4	168.5	158.2	4.68
d5	−100.7	64.2	80.3	−98.1	−161.0	54.8	55.8	−148.4	5.13
d6	−102.8	60.6	83.3	−91.5	−96.0	62.8	−104.5	−108.7	5.26
d7	−102.9	61.6	68.4	−179.1	−153.2	57.8	−72.8	131.8	5.29
d8	−160.7	58.2	−97.6	−126.8	−104.4	61.7	80.8	−96.7	5.98
d9	−95.7	58.0	168.4	156.6	−99.8	62.3	80.5	−98.1	6.39
d10	−117.9	45.8	36.3	53.0	−104.4	61.8	81.2	−97.1	6.65
d11	−162.6	58.7	−95.4	−129.0	−97.5	61.2	68.0	−145.7	6.66
d12	−97.0	58.0	161.3	−171.8	−101.9	62.2	80.8	−96.2	6.74
d13	−100.5	62.4	81.1	−97.1	−150.4	55.0	157.4	−100.5	7.06
d14	−92.1	55.5	178.3	112.8	−145.7	59.8	−63.9	132.8	7.08
d15	−94.9	55.8	170.6	129.5	−139.1	60.0	−63.9	130.0	7.35
d16	−127.9	60.6	−67.6	−73.8	−162.9	56.4	49.8	71.9	7.44
d17	−127.0	48.0	39.7	57.3	−162.5	57.1	−96.3	−119.2	8.15
d18	−121.7	46.9	35.7	54.4	−110.8	61.3	−75.4	120.8	8.20
d19	−160.8	57.7	−96.5	−122.4	−95.7	58.0	168.7	155.0	8.32
d20	−104.3	63.5	−90.8	114.5	−97.9	57.7	168.3	152.0	8.41
d21	−153.4	59.3	68.4	−174.6	−147.2	52.6	33.8	69.4	8.62
d22	−151.2	50.4	55.3	9.9	172.1	61.6	−95.8	−107.3	8.85
d23	−160.1	59.1	−108.3	93.2	−157.1	57.9	−93.7	−131.2	9.30
d24	−157.5	58.6	−176.3	−54.6	−154.8	60.3	−91.1	−151.1	9.46
E$_d$[e]	−95.9	57.5	167.1	157.5	−93.5	57.1	168.4	150.0	9.69
d25	−155.7	57.2	163.3	162.2	−156.4	57.3	−95.9	−126.3	9.92
d26	152.9	53.7	58.5	174.2	−126.4	46.2	27.2	59.1	10.29
d27	−130.5	49.5	39.3	61.4	126.8	45.5	47.2	89.3	10.38
H$_d$-7[f]	137.6	50.5	44.0	80.3	133.4	49.4	44.1	89.9	13.50
H$_d$-12[g]	82.5	51.6	−79.4	−178.2	78.3	46.8	−69.5	137.4	21.34

[a] Backbone torsion angles in γ-amino acid residues are defined in Fig. 1c 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. [c] **H$_1$**-9 structure. [d] **H$_1$**-14 structure. [e] Extended structure. [f] **H$_1$**-7 structure. [g] **H$_1$**-12 structure.

(a)

(b)

(c)

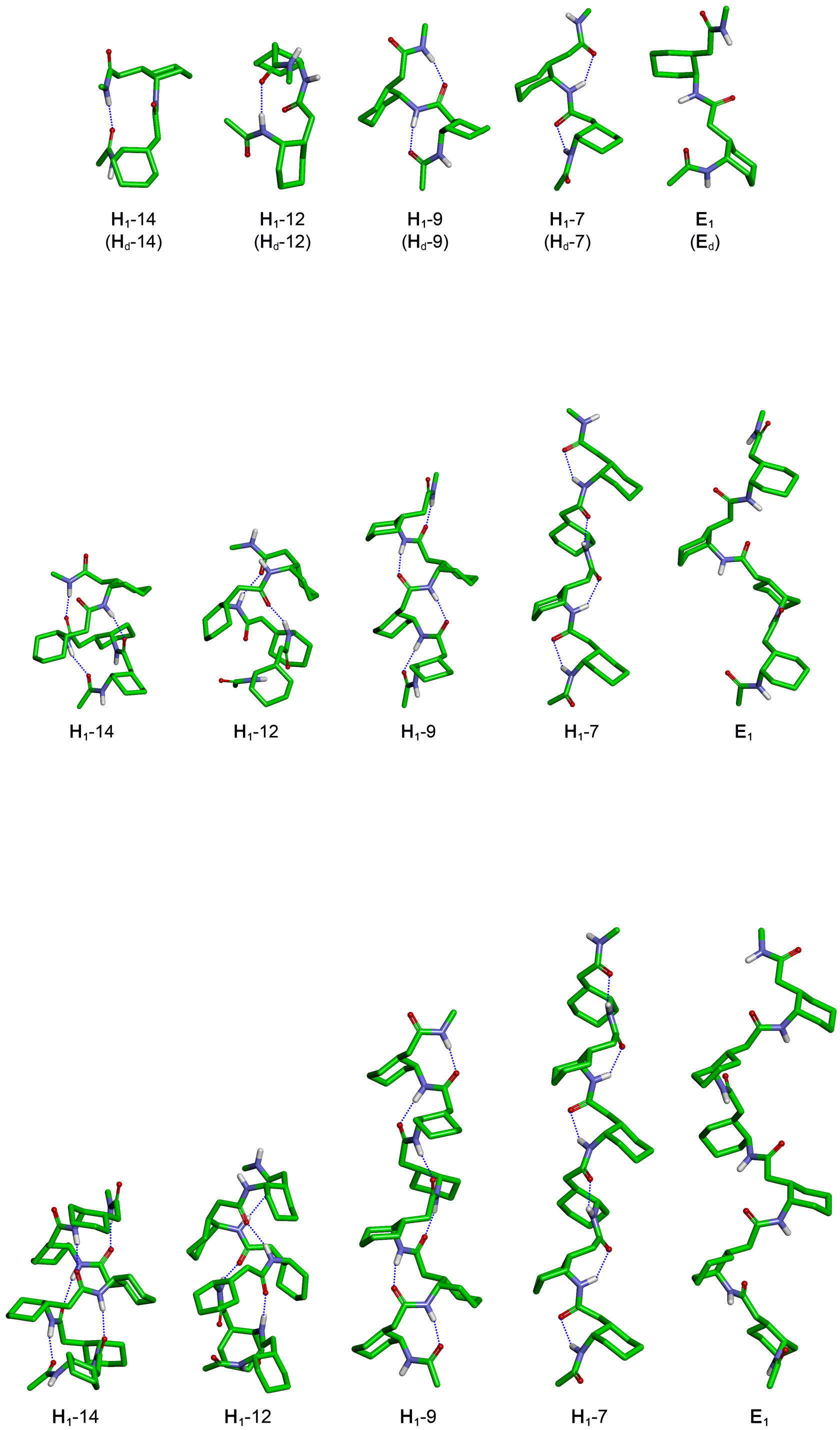
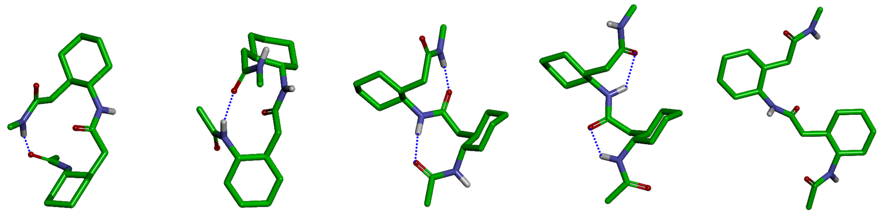


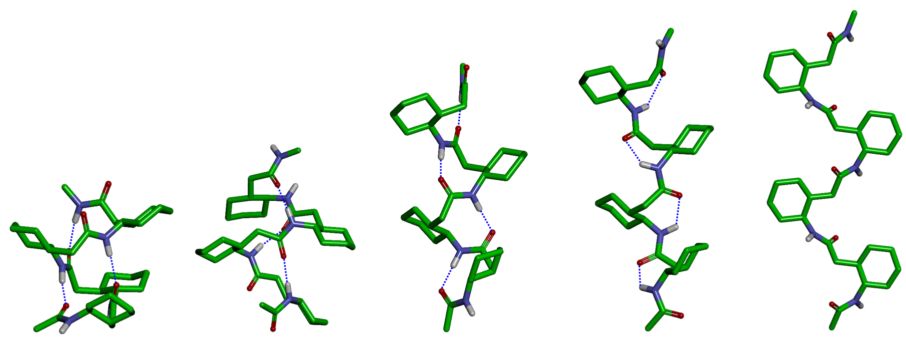
Fig. S1 The optimized helical and extended structures of oligopeptides with γAc$_6$a (**1**) residues: (a) dipeptide, (b) tetrapeptide, and (c) hexapeptide.

(a)



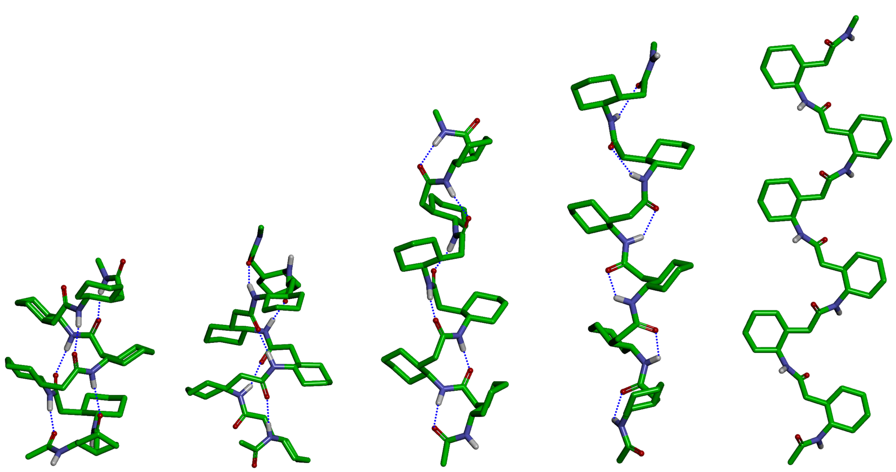
H_2-14 H_2-12 H_2-9 H_2-7 E_2

(b)



H_2-14 H_2-12 H_2-9 H_2-7 E_2

(c)



H_2-14 H_2-12 H_2-9 H_2-7 E_2

(d)

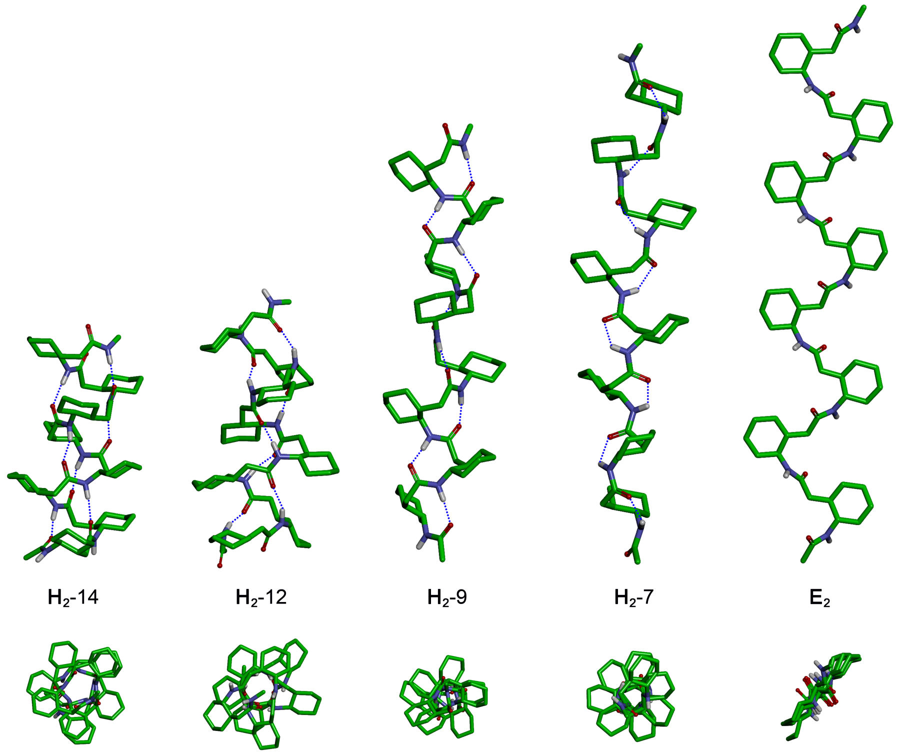


Fig. S2 The optimized helical and extended structures of oligopeptides with γAc$_6$a (**2**) residues: (a) dipeptide, (b) tetrapeptide, (c) hexapeptide, and (d) octapeptide.

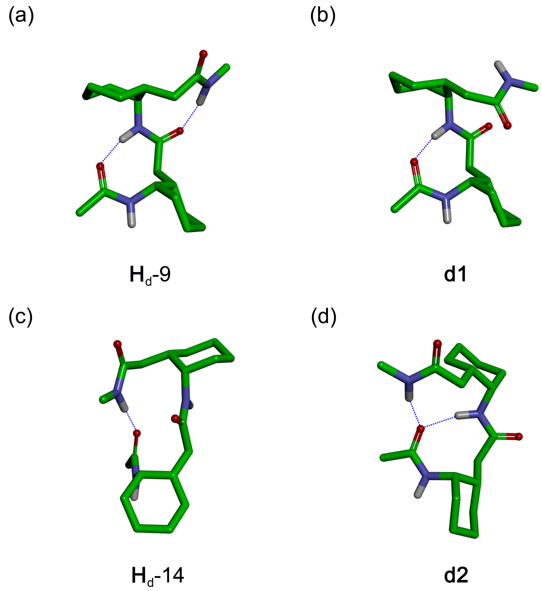


Fig. S3 Representative optimized structures of the γAc_6a (**1**) dipeptide at the M06-2X/6-31+G(d) level of theory.

Electronic Supplementary Material (ESI) for New Journal of Chemistry

Cartesian coordinates of helical and extended structures of octa-γAc$_6$a (1) peptide optimized at the M06-2X/6-31+G(d) level of theory:

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

E_e = -3788.64561449 Hartrees

H	-7.93065700	-2.43181200	3.28241000
H	-8.89282500	-0.99635800	2.92430200
H	-9.33741400	-2.56496600	2.19999900
C	-8.50464900	-1.92496300	2.50045700
C	-7.56371100	-1.58868600	1.36653300
O	-6.67624300	-0.74266400	1.50784900
N	-7.73470300	-2.26438200	0.21098300
H	-8.47549900	-2.95191200	0.17138300
C	-6.81914600	-2.16699500	-0.92973600
C	-7.29349100	-1.14776900	-1.98256500
C	-8.59567800	-1.61808100	-2.63746100
C	-8.42391900	-3.00057800	-3.27475400
C	-7.92751000	-4.03088800	-2.25665900
C	-6.64766500	-3.55227100	-1.56152400
H	-5.86661900	-1.82617400	-0.51817200
H	-6.50852800	-1.12246400	-2.75120100
H	-9.39918900	-1.64950600	-1.88502100
H	-8.91051200	-0.89119300	-3.39583800
H	-9.36630100	-3.33458500	-3.72237900
H	-7.69242000	-2.92539400	-4.09137700
H	-7.74389800	-4.99409900	-2.74435000
H	-8.72050900	-4.22037600	-1.51608100
H	-5.84139700	-3.48177000	-2.30304900
H	-6.32091600	-4.26738100	-0.79706700
C	-7.40356700	0.26398200	-1.41392100
H	-8.04466600	0.28369200	-0.52436900
H	-7.87869500	0.91546700	-2.16096300
C	-6.04840900	0.89227500	-1.10958800
O	-5.03321200	0.56030500	-1.72844600
N	-6.05164400	1.87904700	-0.19101300
H	-6.91122400	2.04510100	0.31612500
C	-4.88088500	2.70663400	0.09899400
C	-4.82040700	3.08179400	1.58936400
C	-4.87300000	3.96352700	-0.78283800
H	-4.01231600	2.08423600	-0.14700700
C	-5.93069600	4.07106500	1.96662600
H	-3.85375900	3.58470000	1.73409500
C	-4.83458400	1.84691500	2.49036300
C	-5.98769500	4.93889000	-0.39916500
H	-3.89630300	4.45440100	-0.66839800
H	-4.96131100	3.66625800	-1.83403900
C	-5.90240000	5.31805600	1.08044700
H	-6.91735100	3.58594400	1.88457100
H	-5.82111800	4.34772600	3.02213900
H	-5.74174700	1.25391500	2.33541700
H	-4.82032600	2.17133700	3.53862000
C	-3.59429300	0.99285600	2.29671700
H	-5.93173600	5.83372900	-1.02843600
H	-6.96559100	4.47788800	-0.60298200
H	-6.72053200	5.99453900	1.35176300
H	-4.96509200	5.86281300	1.26114200
O	-2.46790200	1.49231300	2.40097100
N	-3.80244000	-0.31187900	2.03458000
H	-4.76827500	-0.62141100	1.94159500
C	-2.71579500	-1.29060300	2.05041100
C	-2.95307400	-2.41492000	1.02922900
C	-2.53718600	-1.86452400	3.46404900
H	-1.81076500	-0.74207600	1.76555400
C	-4.11782600	-3.32262700	1.44490700
H	-2.03396300	-3.01735600	1.02699200
C	-3.14326900	-1.85882500	-0.37890500
C	-3.71724500	-2.75172800	3.86700100
H	-1.60729700	-2.45049400	3.48382200
H	-2.41068900	-1.03906000	4.17361000
C	-3.92358700	-3.88230200	2.85622100
H	-5.06478900	-2.76207900	1.40303700
H	-4.21029600	-4.13987100	0.71764800
H	-3.96881700	-1.14102800	-0.40817900
H	-3.39040600	-2.67825900	-1.06902300
C	-1.88256200	-1.20181100	-0.91340800
H	-3.55220700	-3.16027900	4.87002400
H	-4.63121800	-2.14114000	3.92325100
H	-4.78316000	-4.50056500	3.14112000
H	-3.04258000	-4.53939000	2.86420000
O	-0.77497500	-1.72006500	-0.73652200
N	-2.07084600	-0.05556100	-1.59421000
H	-3.03078000	0.26945200	-1.70919000
C	-0.98481200	0.62619500	-2.29558700
C	-1.04264300	2.14550300	-2.06387700
C	-1.01752500	0.29942000	-3.79515400
H	-0.06041000	0.23629600	-1.85733300
C	-2.26238500	2.75658600	-2.75917100
H	-0.13475500	2.55952300	-2.52440400
C	-0.99764600	2.49272800	-0.57713200
C	-2.23283100	0.92402500	-4.48534200
H	-0.09320100	0.68488300	-4.24857100
H	-1.01039400	-0.78884000	-3.92654900
C	-2.27788100	2.43672900	-4.25512300
H	-3.18468100	2.36773600	-2.30243300
H	-2.26797500	3.84245000	-2.59851800
H	-1.81749200	2.01425000	-0.02933200
H	-1.11388700	3.57871400	-0.45367400
C	0.33851000	2.12867600	0.05138400
H	-2.20795600	0.69929800	-5.55757500
H	-3.15442900	0.47184800	-4.09042000
H	-3.17053800	2.86699100	-4.72414400
H	-1.40637200	2.90489900	-4.73480100

O	1.39314900	2.35116800	-0.55402400
N	0.28811200	1.58752200	1.28309700
H	-0.62934100	1.49678600	1.72138600
C	1.49428500	1.37750200	2.08429300
C	1.42665800	0.05786300	2.87018800
C	1.72268700	2.56486300	3.03156100
H	2.31917700	1.32158300	1.36620800
C	0.36623100	0.12761800	3.97324700
H	2.41156600	-0.06547700	3.34295500
C	1.21212800	-1.14121800	1.94674900
C	0.66175400	2.62335100	4.13358600
H	2.72008000	2.45665100	3.48122300
H	1.73284200	3.49268000	2.44808800
C	0.61277200	1.30853100	4.91560700
H	-0.63158100	0.23515400	3.52450900
H	0.36128500	-0.81684100	4.53310000
H	0.30265300	-1.02422400	1.34759700
H	1.09691500	-2.04906900	2.55469100
C	2.41137100	-1.38040900	1.04560400
H	0.87154700	3.46247000	4.80672000
H	-0.32507300	2.81357700	3.68783500
H	-0.17008100	1.35076400	5.68208500
H	1.56830200	1.16046300	5.43925400
O	3.55003700	-1.43873900	1.52246400
N	2.15155000	-1.53486400	-0.26742200
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C	2.93589800	-1.43123300	-2.61552400
C	3.26378800	-3.51332400	-1.21819000
H	4.13187700	-1.57143200	-0.82283500
C	1.69081200	-2.06498700	-3.24557400
H	3.81119500	-1.72647400	-3.21084200
C	2.87562400	0.09587800	-2.63325600
C	2.01601600	-4.13544800	-1.84934000
H	4.15846200	-3.80837100	-1.78516000
H	3.40164000	-3.87523000	-0.19279600
C	1.78689300	-3.59287500	-3.26194400
H	0.79171900	-1.77057800	-2.68453400
H	1.56542800	-1.67624900	-4.26490600
H	2.08703700	0.47569500	-1.97443500
H	2.64967000	0.43593200	-3.65329500
C	4.21609500	0.70756400	-2.25881800
H	2.11359300	-5.22712500	-1.86839800
H	1.13701900	-3.90557200	-1.22988100
H	0.87579600	-4.02421500	-3.69369800
H	2.62358600	-3.89567000	-3.90806400
O	5.25852300	0.28260600	-2.76824300
N	4.18021900	1.72068600	-1.37493000
H	3.26812900	2.00411500	-1.01779200
C	5.37278900	2.48187600	-1.00398100
C	5.36402200	2.81598000	0.49518300
C	5.48181600	3.75681100	-1.85056600
H	6.23120400	1.83493400	-1.20839600
C	4.25328700	3.81670100	0.83040200
H	6.33269100	3.29036600	0.70347000
C	5.29897300	1.54564500	1.33726400

C	4.36538500	4.74888400	-1.51347200
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H	5.46094000	3.48408300	-2.91250800
C	4.36832400	5.08594900	-0.01922900
H	3.26693600	3.36176100	0.65915000
H	4.30161400	4.06686200	1.89859200
H	4.42783600	0.93362800	1.07661700
H	5.20376100	1.80965800	2.40036400
C	6.57855200	0.72451700	1.20243400
H	4.47931800	5.66065000	-2.11170900
H	3.39243200	4.31255000	-1.78245800
H	3.54723300	5.77364000	0.21670900
H	5.30420400	5.60623200	0.23225000
O	7.67346700	1.27349600	1.12296900
N	6.40670500	-0.62060000	1.20462400
H	5.45776000	-0.97483700	1.31654600
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H	8.59186700	-2.61810800	2.85965700
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H	6.26307800	-4.46564900	-0.05092700
H	6.36036000	-1.74867800	-1.30888900
H	7.44345900	-3.06111600	-1.80356500
C	8.45344900	-1.21398100	-1.44344800
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H	5.53206100	-2.47503000	3.08454400
H	5.56493500	-4.83165500	2.32836100
H	7.32488500	-4.79112000	2.18547500
O	9.62857500	-1.46172200	-1.17893000
N	8.05617800	-0.05214300	-1.99856000
H	7.07341800	0.08874700	-2.22191400
C	8.99980100	1.02273800	-2.21940400
H	9.84815000	0.67377400	-2.81598700
H	8.48878600	1.82825000	-2.75227700
H	9.37720000	1.40055200	-1.26288000

(2) **H$_1$**-12

E_e = -3788.51401879 Hartrees

H	-8.85950700	0.11103500	2.30151200
H	-8.76528400	-1.27045300	3.43794600
H	-7.28065600	-0.45539800	2.87774900
C	-8.28836000	-0.77600500	2.59081600
C	-8.14799500	-1.76662300	1.45297500
O	-8.00120800	-2.96815100	1.65206300
N	-8.15737500	-1.22272100	0.21156600
H	-8.17163300	-0.21152600	0.11593900
C	-7.76646700	-2.00948700	-0.95045700
C	-7.42079900	-1.09904700	-2.14040300
C	-8.66415500	-0.40267200	-2.71741800
C	-9.73879100	-1.42443200	-3.09612100
C	-10.10379700	-2.29567900	-1.89251000
C	-8.86899500	-3.00630100	-1.34068300
H	-6.86861900	-2.57994700	-0.67511500
H	-7.07060500	-1.79617200	-2.91789800
H	-9.06711000	0.30747900	-1.98963500
H	-8.36726600	0.18691000	-3.59481500
H	-10.62614900	-0.91102900	-3.48432500
H	-9.36396900	-2.06868400	-3.90543800
H	-10.87037800	-3.02940200	-2.16707900
H	-10.53323400	-1.66285800	-1.10469100
H	-8.46497800	-3.68576300	-2.10489700
H	-9.11212300	-3.60839200	-0.46150000
C	-6.22729800	-0.16252000	-1.89759300
H	-5.91384100	0.24196300	-2.87097600
H	-5.36720000	-0.73176500	-1.52655600
C	-6.42971700	1.05698300	-1.00031800
O	-7.54056900	1.43902100	-0.62990900
N	-5.28742300	1.72725100	-0.73229700
H	-4.42680300	1.22154400	-0.93559100
C	-5.13195400	2.96957900	0.03264300
C	-4.93680300	2.76403100	1.54385400
C	-6.19180200	4.06256900	-0.23387300
H	-4.18538100	3.37387800	-0.34572900
C	-6.26988700	2.51553100	2.25505200
H	-4.57876300	3.74516800	1.89956900
C	-3.80256200	1.79933600	1.89264600
C	-7.45003700	4.06234800	0.65027500
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H	-6.47360800	4.03910400	-1.29251500
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H	-6.76655900	1.65029500	1.80861900
H	-6.08756500	2.27721200	3.31117600
H	-3.54116100	1.95407700	2.94956400
H	-2.89849800	2.06111400	1.32666500
C	-4.05089900	0.29652900	1.76787100
H	-7.93202000	5.04395100	0.56176400
H	-8.14921900	3.31524500	0.27840300
H	-8.08688400	3.63400500	2.66999200
H	-6.62642700	4.61551500	2.58360700
O	-5.17045100	-0.19396100	1.69486100
N	-2.89486200	-0.41693000	1.86422800
H	-2.04497100	0.11952500	1.70909900
C	-2.70998100	-1.86662200	1.98661200
C	-2.72738800	-2.63628000	0.65653300
C	-3.60667600	-2.56312100	3.03102800
H	-1.68707100	-1.94956200	2.36988400
C	-4.15771900	-2.86696400	0.16177900
H	-2.33642100	-3.63377800	0.92029200
C	-1.71246300	-2.10821700	-0.36050800
C	-4.97234600	-3.05846800	2.54092500
H	-3.02896400	-3.43261200	3.37609900
H	-3.72216900	-1.90086600	3.89754400
C	-4.89722700	-3.74630300	1.17581300
H	-4.67215900	-1.90666700	0.06513800
H	-4.13877100	-3.34101800	-0.82966800
H	-1.63233700	-2.84574200	-1.17300500
H	-0.71678200	-2.07129800	0.10299700
C	-1.96646600	-0.78447800	-1.07421200
H	-5.39084500	-3.74987000	3.28114900
H	-5.65999700	-2.21973400	2.46248200
H	-5.91785300	-3.96279200	0.84608100
H	-4.36834900	-4.70848500	1.26290000
O	-3.08529700	-0.29644500	-1.21117500
N	-0.84091200	-0.28280400	-1.64590800
H	0.03280600	-0.67128500	-1.29883600
C	-0.70320900	0.79719000	-2.62742700
C	-0.57794300	2.20495300	-2.02639600
C	-1.73323100	0.78708900	-3.77594600
H	0.26360000	0.58206600	-3.09531600
C	-1.94186500	2.74173500	-1.58851400
H	-0.26042300	2.83277800	-2.87584000
C	0.56714500	2.33515400	-1.01967800
C	-3.04626600	1.54559400	-3.53772300
H	-1.22075900	1.25318100	-4.62874900
H	-1.93891000	-0.25023900	-4.06413900
C	-2.84286700	2.88537600	-2.82109800
H	-2.37755300	2.05122600	-0.86014500
H	-1.81910200	3.71045100	-1.08549500
H	0.74527400	3.40626700	-0.84417600
H	1.49481900	1.95007200	-1.46500300
C	0.40752600	1.73901000	0.37566300
H	-3.53179200	1.71723100	-4.50598900
H	-3.71484100	0.92262400	-2.94656500
H	-3.82108900	3.29754600	-2.54567700
H	-2.37899300	3.60848300	-3.50812400
O	-0.68575600	1.50880100	0.88478700
N	1.59383800	1.62051600	1.02474800
H	2.41943200	1.64485900	0.43093900
C	1.84678800	1.30998300	2.43437300
C	1.94960100	-0.19020300	2.74469300

C	0.92569200	2.01611500	3.45174200
H	2.84708200	1.72636400	2.60152800
C	0.56357700	-0.83003300	2.82620700
H	2.36733900	-0.22858700	3.76468700
C	2.98473400	-0.92458600	1.88940900
C	-0.37930500	1.29981400	3.82932800
H	1.53081500	2.11938100	4.36292300
H	0.71613600	3.03268000	3.09996400
C	-0.20556200	-0.21345700	3.99942200
H	0.03988100	-0.66268000	1.87964400
H	0.65956800	-1.91660900	2.95557600
H	3.19496600	-1.89058100	2.37069300
H	3.93521200	-0.37294200	1.90557800
C	2.65559300	-1.27691900	0.44041200
H	-0.75674000	1.73274100	4.76340300
H	-1.12810000	1.48989800	3.06227200
H	-1.19259200	-0.67788000	4.10951800
H	0.34670400	-0.42487300	4.92679100
O	1.51367600	-1.28933300	-0.00926000
N	3.75241900	-1.68766900	-0.24592300
H	4.64236900	-1.43545000	0.17438400
C	3.84201300	-2.26884400	-1.58870800
C	3.88751900	-1.23831200	-2.72809900
C	2.82706700	-3.38791000	-1.89888300
H	4.82578200	-2.75479400	-1.57732300
C	2.49158300	-0.70131800	-3.04864900
H	4.19953800	-1.82428600	-3.60865100
C	4.99275100	-0.19307800	-2.56531800
C	1.47533900	-2.95767200	-2.48483800
H	3.32429300	-4.03505300	-2.63423100
H	2.67864000	-3.99588100	-0.99915700
C	1.60813400	-1.85378300	-3.53924400
H	2.07254100	-0.24199800	-2.14844400
H	2.56178700	0.08298300	-3.81477700
H	5.14348700	0.29277300	-3.53935300
H	5.94325900	-0.69522200	-2.33952400
C	4.81561000	0.95851700	-1.57776700
H	0.99404500	-3.83565000	-2.93142700
H	0.82700500	-2.61239900	-1.68111400
H	0.60879500	-1.49377600	-3.81230400
H	2.05276600	-2.26689000	-4.45639000
O	3.73848000	1.27241300	-1.07745500
N	5.97025800	1.65044900	-1.41319400
H	6.80415200	1.16784800	-1.73387400
C	6.22129800	2.90121600	-0.69668300
C	6.42518900	2.75421100	0.82161400
C	5.23535600	4.05071400	-0.99403200
H	7.18720800	3.22650500	-1.10865000
C	5.09059600	2.58910400	1.55326700
H	6.82770800	3.73183600	1.13395400
C	7.51772200	1.75742800	1.21805700
C	3.96777200	4.11533000	-0.13186200
H	5.80459300	4.97568500	-0.82962300
H	4.97541500	4.02867000	-2.05752900
C	4.24325600	3.85008500	1.35155000
H	4.57795100	1.70690000	1.15907700

H	5.27149200	2.41498400	2.62282300
H	7.82787700	1.98512100	2.24721600
H	8.40984300	1.92408300	0.59532000
C	7.21949900	0.25831800	1.19526900
H	3.51813300	5.10804200	-0.24997100
H	3.24380500	3.39074400	-0.50067800
H	3.29050300	3.77122400	1.88828400
H	4.77933700	4.70472000	1.78916100
O	6.11929600	-0.22065400	0.96067600
N	8.32275700	-0.47289800	1.52014300
H	9.16342900	0.07225100	1.65085300
C	8.51537700	-1.92729500	1.63215500
C	8.57395800	-2.65374800	0.27506400
C	7.56818400	-2.65069100	2.60717900
H	9.51840500	-2.00032100	2.07140400
C	7.17957300	-2.89773900	-0.31024200
H	8.99169700	-3.64655800	0.50506300
C	9.58046700	-2.01502400	-0.69431800
C	6.21026900	-3.06760300	2.03419100
H	8.10178900	-3.55817100	2.92060300
H	7.44198400	-2.03496400	3.50389700
C	6.34626100	-3.73887200	0.66418100
H	6.69746300	-1.93717200	-0.50995000
H	7.27759700	-3.41743700	-1.27240600
H	9.63118300	-2.63579200	-1.59772200
H	10.57915800	-2.03627700	-0.23902600
C	9.26577200	-0.60918400	-1.17549000
H	5.73062700	-3.75825700	2.73700000
H	5.56551100	-2.19203500	1.95438200
H	5.34938900	-3.93063500	0.25034600
H	6.82962600	-4.71925800	0.78394900
O	8.18174800	-0.28961500	-1.65012700
N	10.28620500	0.28805500	-1.08825100
H	11.20598700	-0.05861200	-0.85798800
C	10.19080000	1.57196000	-1.76238700
H	9.28174800	2.08723500	-1.44469000
H	11.05459100	2.18004400	-1.49299700
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(3) **H$_1$**-9

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H	15.63431500	1.10761300	-0.17457300
C	14.83416900	1.75917800	0.18410200
C	13.44842400	1.20300900	-0.05379900
O	12.45039800	1.82631000	0.30955300
N	13.37734400	0.00357800	-0.67535700
H	14.24822800	-0.42884500	-0.95221800
C	12.13234800	-0.64342900	-1.09779900
C	11.68244900	-1.73907200	-0.10800600
C	12.71071100	-2.87423500	-0.07146700
C	12.91432800	-3.47954600	-1.46406000
C	13.31480700	-2.41613900	-2.48995000
C	12.32565200	-1.24433800	-2.49666700
H	11.37927300	0.15200900	-1.13634500
H	10.74758000	-2.15990400	-0.50984500
H	13.66591000	-2.49517500	0.32281500
H	12.37131500	-3.64664500	0.62791100
H	13.66716400	-4.27459100	-1.42778000
H	11.97348400	-3.94813500	-1.78519400
H	13.37089400	-2.85374500	-3.49242900
H	14.33261400	-2.06011400	-2.26797000
H	11.34926500	-1.60285000	-2.84669800
H	12.64988800	-0.46103600	-3.19117500
C	11.36781800	-1.18152100	1.29083400
H	12.13376500	-0.46322000	1.60269100
H	11.35417000	-2.00369600	2.01294100
C	9.97539300	-0.57444100	1.31284600
O	8.98731400	-1.31495600	1.40819700
N	9.89313200	0.75911600	1.17276700
H	10.76457700	1.26213200	1.00215200
C	8.63401900	1.50238300	1.13118700
C	8.22598700	1.84260000	-0.31970900
C	8.76982000	2.78811400	1.95636300
H	7.87953800	0.85112600	1.58610600
C	9.25645900	2.78708600	-0.94910800
H	7.27203700	2.39031400	-0.26131000
C	7.98210800	0.58685000	-1.17730300
C	9.76739800	3.76886200	1.33081800
H	7.77941900	3.26004800	2.01156400
H	9.06370900	2.53143800	2.98031000
C	9.40651500	4.07081000	-0.12664600
H	10.23038700	2.28080600	-1.02303500
H	8.94511700	3.02925300	-1.97234300
H	8.76146500	-0.16231500	-0.99468900
H	8.00899000	0.86111700	-2.23644800
C	6.59443500	0.02704700	-0.91879500
H	9.78527400	4.69486800	1.91629600
H	10.78439900	3.35729500	1.37309700
H	10.16736300	4.71825200	-0.57645700
H	8.45669200	4.62435400	-0.15756800
O	5.61748400	0.52388500	-1.49644300
N	6.50003600	-0.96558600	-0.01822100
H	7.35842600	-1.23278000	0.46897900
C	5.23805200	-1.58004500	0.39301100
C	4.74145700	-1.00693000	1.73919200
C	5.41381500	-3.09999000	0.50217000
H	4.51378100	-1.34892800	-0.39609700
C	5.72447000	-1.36129300	2.86056200
H	3.78923800	-1.51227900	1.96609800
C	4.45377300	0.50393900	1.67008500
C	6.36002800	-3.48903800	1.64321200
H	4.42365900	-3.54051800	0.68203900
H	5.77442000	-3.49248000	-0.45534000
C	5.90881400	-2.87755900	2.97283200
H	6.69835800	-0.88698400	2.67014600
H	5.35127700	-0.95504100	3.80827200
H	5.25244800	1.02378300	1.12801200
H	4.40695400	0.91044000	2.68514600
C	3.09212200	0.76013200	1.04911300
H	6.40326000	-4.58122600	1.72493800
H	7.38130200	-3.15308800	1.42209800
H	6.63634400	-3.10954800	3.75859600
H	4.95341200	-3.32993900	3.27683900
O	2.07295500	0.66425200	1.74776800
N	3.06658700	1.03882500	-0.26511200
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C	1.83919300	1.27495300	-1.02322000
C	1.41338100	0.02126600	-1.81836800
C	2.04041100	2.46074600	-1.97593600
H	1.06825300	1.52341600	-0.28543300
C	2.46270400	-0.30862200	-2.88654700
H	0.48105000	0.28119700	-2.34460900
C	1.10661200	-1.18280700	-0.90896600
C	3.05844600	2.14534900	-3.07693300
H	1.06878200	2.69520200	-2.43223900
H	2.34821900	3.33952200	-1.39810500
C	2.67207900	0.87389600	-3.83756500
H	3.41802300	-0.56679600	-2.40628900
H	2.13840500	-1.19244500	-3.44910200
H	1.86133000	-1.27295300	-0.11875200
H	1.12295800	-2.10021900	-1.50529600
C	-0.29490200	-1.07426200	-0.33536900
H	3.12593000	2.99423300	-3.76698800
H	4.05817200	2.01432500	-2.64334000
H	3.44302800	0.62913900	-4.57676000
H	1.73953000	1.05199500	-4.39308300
O	-1.26589100	-1.43440100	-1.01614200
N	-0.40825200	-0.53427600	0.88989300
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C	-1.68541800	-0.31259200	1.56544000
C	-2.13712500	1.16048800	1.45406100

C	-1.56926700	-0.71721600	3.04043300
H	-2.41205200	-0.96192500	1.06484400
C	-1.14975900	2.07138100	2.19238100
H	-3.10584700	1.23660900	1.97282100
C	-2.36199300	1.60057200	-0.00457000
C	-0.61565200	0.19931300	3.81372000
H	-2.57236800	-0.65947900	3.48514900
H	-1.24519400	-1.76220000	3.10435900
C	-1.02010600	1.66870300	3.66507600
H	-0.16238200	2.02123400	1.71050100
H	-1.49126400	3.11066300	2.11437300
H	-1.55368300	1.23201100	-0.64744800
H	-2.36948900	2.69376300	-0.05601400
C	-3.72462400	1.14374100	-0.49468000
H	-0.61066700	-0.08691800	4.87179900
H	0.41239400	0.07144800	3.45117500
H	-0.28866100	2.31256800	4.16610000
H	-1.98686000	1.83196200	4.16380400
O	-4.73102200	1.81020500	-0.21459800
N	-3.76729400	-0.01146600	-1.17995400
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C	-5.00097300	-0.61838200	-1.67715400
C	-5.48338400	-1.75973500	-0.75500400
C	-4.77832900	-1.14957000	-3.09909000
H	-5.74951600	0.18121200	-1.69632600
C	-4.46731200	-2.90772900	-0.75633300
H	-6.41709200	-2.14772100	-1.19219400
C	-5.81130200	-1.27154800	0.66804300
C	-3.79025200	-2.32076500	-3.12473200
H	-5.74942200	-1.48189700	-3.49101000
H	-4.43142100	-0.33125000	-3.74023300
C	-4.23222000	-3.43733800	-2.17463200
H	-3.51306000	-2.56393900	-0.33144800
H	-4.83451000	-3.71287200	-0.10844600
H	-5.04309400	-0.57400200	1.02201900
H	-5.83601600	-2.12854000	1.34822600
C	-7.19741800	-0.65275900	0.71296600
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H	-2.78799600	-1.97985000	-2.83496700
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H	-6.39416200	1.18063100	0.39778900
C	-8.52431300	1.43176300	0.54574300
C	-8.92713500	1.79204800	-0.90186200
C	-8.39013000	2.70631900	1.38849700
H	-9.28340000	0.77830900	0.98928300
C	-7.89387000	2.74464800	-1.51420000
H	-9.88114700	2.33925000	-0.83906100
C	-9.16942700	0.54805200	-1.77710100
C	-7.39046400	3.69533700	0.77975400
H	-9.38119100	3.17677700	1.44824800
H	-8.09828400	2.43472900	2.40940600
C	-7.74813300	4.01756700	-0.67431200
H	-6.91865800	2.24187300	-1.58990800
H	-8.20147700	3.00001100	-2.53551500
H	-8.39520600	-0.20703500	-1.59627400
H	-9.13050900	0.83459500	-2.83260000
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H	-6.37460500	3.28115800	0.81640300
H	-6.98570000	4.67131000	-1.11282600
H	-8.69889600	4.57033400	-0.70030100
O	-11.52958200	0.49030500	-2.13116400
N	-10.67099900	-0.99347300	-0.63022100
H	-9.81841700	-1.26456900	-0.13570600
C	-11.94120800	-1.59011800	-0.21993800
C	-12.42339800	-1.02478500	1.13502200
C	-11.79027900	-3.11459500	-0.13217300
H	-12.66453300	-1.33551700	-1.00152000
C	-11.44719200	-1.41781000	2.24993900
H	-13.38771300	-1.50894300	1.35416600
C	-12.67249200	0.49260700	1.08998100
C	-10.84615100	-3.53496000	0.99933800
H	-12.78625800	-3.54234200	0.04635400
H	-11.43844600	-3.49924700	-1.09634700
C	-11.28781600	-2.93846800	2.33890000
H	-10.46454400	-0.95811200	2.06850300
H	-11.81378100	-1.02029500	3.20415500
H	-11.86061300	0.99615600	0.55004600
H	-12.69632600	0.88538700	2.11140200
C	-14.03114300	0.81306100	0.48264000
H	-10.81563300	-4.62922400	1.06359000
H	-9.82149500	-3.20679100	0.78170000
H	-10.56428900	-3.19573200	3.12109700
H	-12.25124600	-3.37989600	2.63464700
O	-15.05196600	0.79459600	1.16658300
N	-14.04991800	1.08210000	-0.84141700
H	-13.19303400	0.97289200	-1.38342100
C	-15.30796100	1.31640900	-1.51862300
H	-15.84263600	2.14542700	-1.04626300
H	-15.10193200	1.56309800	-2.56138700
H	-15.95433000	0.43264400	-1.47440700

Electronic Supplementary Material (ESI) for New Journal of Chemistry
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(4) **H_1-7**

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H	18.08759700	0.67332900	2.26217600
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H	16.52635000	1.45705800	2.60580500
C	17.32322200	1.34814800	1.86589900
C	16.84795300	0.79941700	0.52915800
O	17.60259300	0.78486500	-0.43454500
N	15.57623600	0.31096000	0.54786000
H	15.02702700	0.57240400	1.36370800
C	14.72373700	-0.12744700	-0.56414400
C	13.94522500	-1.40007400	-0.15336500
C	14.85689900	-2.63062100	-0.13066300
C	15.54183800	-2.85543700	-1.47873700
C	16.33616900	-1.61364600	-1.88526600
C	15.44571400	-0.37009700	-1.89546300
H	13.98627300	0.67491500	-0.72762000
H	13.18159500	-1.54540800	-0.93436000
H	15.62161700	-2.48118300	0.64541500
H	14.27144100	-3.51191800	0.16159800
H	16.19799700	-3.73219300	-1.42684400
H	14.77907400	-3.07365900	-2.24108300
H	16.77914600	-1.75042300	-2.87872900
H	17.16650100	-1.45134000	-1.18858100
H	14.65272800	-0.50670300	-2.64593500
H	16.02142800	0.51220000	-2.17792500
C	13.21615000	-1.26767900	1.19906800
H	13.93755200	-1.34109300	2.01924800
H	12.50761300	-2.09805000	1.30327400
C	12.51187600	0.07337400	1.34015600
O	13.07578200	1.01373600	1.90259300
N	11.30902400	0.13033300	0.72253900
H	10.90796300	-0.77475500	0.47936800
C	10.31547100	1.20956600	0.66914800
C	9.74247800	1.31105400	-0.76469400
C	10.81538600	2.58496200	1.12599900
H	9.49368300	0.91215300	1.33928400
C	10.76061600	1.92982100	-1.72779100
H	8.87681200	1.98789900	-0.68790400
C	9.23981200	-0.03403100	-1.32985400
C	11.80843100	3.22346000	0.15340500
H	9.92068800	3.22204400	1.19043200
H	11.24504400	2.51708000	2.12640200
C	11.22488600	3.30813400	-1.25715100
H	11.62796200	1.25550100	-1.79665600
H	10.32281300	1.98812400	-2.73258900
H	10.08900300	-0.64190400	-1.65953600
H	8.61240400	0.16292100	-2.20708500
C	8.49051000	-0.84651100	-0.28464600
H	12.07949800	4.22185400	0.51601300
H	12.73249400	2.63271600	0.14411300
H	11.96533200	3.71488500	-1.95535100
H	10.36883700	3.99903400	-1.26291500
O	9.08702400	-1.70372500	0.37070300
N	7.20688900	-0.46361900	-0.10079400
H	6.81294000	0.10710100	-0.84826800
C	6.17068600	-0.99480200	0.79435000
C	5.42547300	0.17715700	1.47681200
C	6.66535400	-1.98692000	1.85395300
H	5.44903600	-1.52256400	0.15173300
C	6.28068000	0.82866000	2.56727800
H	4.54056800	-0.27504500	1.95262000
C	4.93108300	1.25489300	0.49004900
C	7.49377700	-1.33469700	2.96252500
H	5.75925100	-2.42429500	2.29876400
H	7.22300400	-2.79649700	1.38046000
C	6.73107500	-0.18462800	3.61960100
H	7.16484600	1.28233900	2.09359100
H	5.71613300	1.64729400	3.03162500
H	5.77077800	1.87870400	0.16596000
H	4.21548000	1.90532000	1.00652800
C	4.31562500	0.64030700	-0.75764800
H	7.75976900	-2.09290000	3.70829300
H	8.43660400	-0.96697700	2.53987500
H	7.35438700	0.30762700	4.37500400
H	5.84739600	-0.57810500	4.14336700
O	5.00753800	0.45729300	-1.76220200
N	3.03201600	0.25054100	-0.59781900
H	2.55814200	0.63994800	0.21697900
C	2.08748400	-0.36869300	-1.53591000
C	1.36855500	-1.54954900	-0.84035500
C	2.68977700	-0.82937900	-2.86871800
H	1.33116600	0.39923500	-1.76034200
C	2.29191500	-2.76422600	-0.70855600
H	0.53273800	-1.81888500	-1.50582700
C	0.77762400	-1.19067700	0.53902800
C	3.57650500	-2.07026500	-2.74929600
H	1.83321500	-1.06816000	-3.51630300
H	3.23653400	-0.00894600	-3.33684100
C	2.83409100	-3.21719300	-2.06429900
H	3.13295700	-2.49328000	-0.05152300
H	1.75197000	-3.58002300	-0.21145900
H	1.57702800	-1.14547600	1.28631600
H	0.08488500	-1.98391400	0.84363700
C	0.09157300	0.16742500	0.53488300
H	3.91116200	-2.37232500	-3.74848600
H	4.47821300	-1.81588800	-2.17975800
H	3.49672000	-4.08084300	-1.93610000
H	1.99721300	-3.54897500	-2.69637400
O	0.72283900	1.17759600	0.85561200
N	-1.17648800	0.14497400	0.06887500
H	-1.60945400	-0.77767900	0.04428100
C	-2.16589300	1.22296600	-0.05623200
C	-2.91439800	1.07677400	-1.40269400

C	-1.60555700	2.64394100	0.07334300
H	-2.89610700	1.07380300	0.75391800
C	-2.02172200	1.47862100	-2.58115200
H	-3.75786200	1.78294400	-1.34660800
C	-3.49582300	-0.33268900	-1.64365300
C	-0.73485200	3.06078800	-1.11289600
H	-2.48117900	3.30791300	0.12295800
H	-1.05864100	2.75052100	1.01121200
C	-1.48830400	2.90368600	-2.43387500
H	-1.17653100	0.77492700	-2.63288200
H	-2.58325200	1.36794000	-3.51760200
H	-2.70192100	-1.01604800	-1.96360700
H	-4.23124600	-0.27755100	-2.45480900
C	-4.10740200	-0.91882600	-0.37984000
H	-0.41044600	4.09908000	-0.97790900
H	0.17469700	2.44779200	-1.12277100
H	-0.83685800	3.15128100	-3.27980700
H	-2.33078300	3.61022200	-2.46494800
O	-3.43043300	-1.64726500	0.34934400
N	-5.35919400	-0.48251600	-0.11785600
H	-5.84352500	-0.05387900	-0.90603200
C	-6.27219500	-0.80213900	0.98721000
C	-6.92956300	0.50030500	1.50346400
C	-5.64389600	-1.56705200	2.15816100
H	-7.06561000	-1.43575200	0.56162100
C	-5.93973400	1.34161500	2.31506200
H	-7.73987400	0.17407000	2.17462500
C	-7.55687500	1.36552700	0.39029100
C	-4.68248200	-0.72289800	2.99689900
H	-6.48549900	-1.88151600	2.79296900
H	-5.14948800	-2.46991700	1.79623300
C	-5.35499900	0.55850000	3.49003800
H	-5.12532400	1.66290100	1.64748900
H	-6.43946300	2.25398300	2.66468000
H	-6.77285400	1.90756400	-0.14919200
H	-8.21625400	2.11047400	0.85085100
C	-8.30445700	0.52370100	-0.63235300
H	-4.32674400	-1.31846200	3.84562100
H	-3.79907100	-0.47745800	2.39493400
H	-4.63980000	1.18073100	4.04017300
H	-6.16254500	0.30565300	4.19286000
O	-7.73226000	0.14612600	-1.65739000
N	-9.55316800	0.17448800	-0.25067100
H	-9.94245900	0.72445400	0.51429700
C	-10.58025200	-0.61520900	-0.94139700
C	-11.22571000	-1.60222600	0.06042000
C	-10.10083200	-1.37706800	-2.18277400
H	-11.35616800	0.09700600	-1.26260300
C	-10.27810900	-2.75996000	0.39156200
H	-12.10769800	-2.01282000	-0.45638200
C	-11.70919900	-0.93853000	1.36628800
C	-9.18344800	-2.55769600	-1.85875600
H	-11.01148900	-1.75806200	-2.66844900
H	-9.61742100	-0.69301900	-2.88195000
C	-9.84052100	-3.51400800	-0.86380600
H	-9.39132200	-2.35058800	0.89983400
H	-10.76609000	-3.43781200	1.10345500
H	-10.85461300	-0.73807300	2.02125800
H	-12.37122300	-1.63568700	1.89294600
C	-12.39796900	0.39462400	1.11658400
H	-8.93101000	-3.08429700	-2.78632900
H	-8.24037600	-2.17659800	-1.44892000
H	-9.15221200	-4.32409200	-0.59696300
H	-10.71996800	-3.98430100	-1.32789700
O	-11.74834800	1.44089000	1.16429300
N	-13.69961000	0.28692200	0.76355400
H	-14.12429200	-0.62034200	0.95185000
C	-14.71327600	1.31942800	0.51150700
C	-15.48669700	0.98790400	-0.78757000
C	-14.19042600	2.76070400	0.45667400
H	-15.42214400	1.25557200	1.35015300
C	-14.65119400	1.29668400	-2.03409200
H	-16.36375200	1.65433400	-0.78657700
C	-15.99328200	-0.46795200	-0.86272900
C	-13.39449400	3.08497700	-0.80893100
H	-15.08270300	3.40287500	0.48661400
H	-13.60167600	2.97843900	1.34945200
C	-14.19821300	2.75566500	-2.06631600
H	-13.76708100	0.64094200	-2.03220300
H	-15.22933600	1.04649500	-2.93284900
H	-15.15345800	-1.13564400	-1.08402300
H	-16.70300300	-0.55212900	-1.69413200
C	-16.61274000	-0.95347700	0.43263700
H	-13.11549800	4.14479700	-0.79794600
H	-12.45992200	2.51218700	-0.80325600
H	-13.60109700	2.94520900	-2.96539600
H	-15.08093600	3.40916300	-2.12705700
O	-15.92961900	-1.45335000	1.32675300
N	-17.94218300	-0.76326200	0.58541500
H	-18.47868500	-0.38464200	-0.18128800
C	-18.61583200	-1.15957600	1.81059500
H	-18.15446200	-0.66499400	2.66904500
H	-19.66520600	-0.87101500	1.74434700
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(5) **E$_1$**

E_e = -3788.53657067 Hartrees

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H	-18.16280800	-0.35598400	-0.98590700
C	-17.80016500	0.39195200	-0.27584300
C	-16.48228300	0.01856800	0.37401600
O	-15.82037400	0.83994100	0.99434400
N	-16.09994600	-1.28083700	0.23459700
H	-16.70698100	-1.90480900	-0.27884600
C	-14.92051600	-1.83982600	0.89468300
C	-13.68631100	-1.85035700	-0.02701700
C	-13.86969100	-2.84570200	-1.17796700
C	-14.16213700	-4.25490200	-0.65747000
C	-15.38896500	-4.26310100	0.25718800
C	-15.22857400	-3.25434300	1.40046100
H	-14.72136400	-1.17819400	1.74468400
H	-12.83624200	-2.19355500	0.57979800
H	-14.70055300	-2.50854600	-1.81862200
H	-12.96730000	-2.84962300	-1.79800500
H	-14.30623900	-4.94926300	-1.49303200
H	-13.28977000	-4.61410000	-0.09329100
H	-15.55744100	-5.26398600	0.67016900
H	-16.28550000	-4.02886900	-0.33765600
H	-14.39214500	-3.57261200	2.03632000
H	-16.12349200	-3.22960100	2.03326000
C	-13.35356400	-0.44850900	-0.52825900
H	-13.38031400	0.26792500	0.30409400
H	-14.11650500	-0.10792500	-1.24126600
C	-11.97501400	-0.36954000	-1.17134400
O	-11.11100200	-1.22071300	-0.99261900
N	-11.76514400	0.73745900	-1.93433500
H	-12.52070200	1.40556500	-2.01472800
C	-10.50775700	1.01019100	-2.62808800
C	-9.55795700	1.89766700	-1.80217000
C	-10.79499300	1.65411500	-3.99001600
H	-10.03928600	0.03101400	-2.77384100
C	-10.11471200	3.31797200	-1.65917400
H	-8.61314500	1.96151900	-2.36053000
C	-9.24194700	1.27136600	-0.44756900
C	-11.33644100	3.08169700	-3.85732000
H	-9.85313300	1.68559900	-4.55342900
H	-11.48873600	1.01993800	-4.55435700
C	-10.39155100	3.95184300	-3.02477400
H	-11.04590400	3.28398500	-1.07129800
H	-9.40223000	3.92920100	-1.09407900
H	-9.00122800	0.20666300	-0.57153100
H	-10.12285300	1.30622600	0.20763200
C	-8.05213700	1.93248500	0.23420400
H	-11.48249900	3.51498900	-4.85317300
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H	-9.44002600	4.06655700	-3.56312900
O	-7.19697100	2.55206400	-0.38781400
N	-7.98414500	1.74169800	1.58009600
H	-8.71604100	1.19717400	2.01729200
C	-6.86939300	2.21065600	2.40060800
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C	-7.38663400	2.68973600	3.76224400
H	-6.44101000	3.05565400	1.85135800
C	-6.28960800	-0.02440000	3.44791000
H	-4.94081500	1.60431800	3.10231900
C	-5.26448800	0.63737200	1.22964100
C	-7.87944300	1.53365500	4.63889100
H	-6.55958700	3.19508000	4.27821800
H	-8.17649200	3.43413800	3.60976600
C	-6.79021400	0.47202600	4.80669600
H	-7.10636300	-0.54375900	2.92123800
H	-5.48442600	-0.75486400	3.58500300
H	-4.99878000	1.49125300	0.59234000
H	-6.05533600	0.09296400	0.69712600
C	-4.02844400	-0.23761600	1.37275600
H	-8.19680300	1.91929900	5.61426700
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H	-7.16363400	-0.36670100	5.40527600
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N	-3.87926400	-1.18395700	0.40655300
H	-4.59302700	-1.24464500	-0.30729700
C	-2.74505700	-2.10320100	0.34610000
C	-1.61560000	-1.58045300	-0.56201600
C	-3.22029300	-3.48283300	-0.12523200
H	-2.37116000	-2.17197200	1.37332000
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C	-3.64244000	-3.48274300	-1.59855800
H	-2.38920700	-4.18866100	0.00348900
H	-4.03885100	-3.82539900	0.51850800
C	-2.51955900	-2.94931000	-2.49114300
H	-2.87381200	-0.83884300	-2.15567700
H	-1.22229500	-1.21943100	-2.65189300
H	-0.94076100	-0.22093000	0.98266200
H	-1.88101300	0.55346100	-0.27895500
C	0.18751300	0.18264000	-0.78224000
H	-3.92735500	-4.49692200	-1.90043500
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H	-1.66734900	-3.64247500	-2.45090000
O	0.95331500	-0.64132400	-1.27013400
N	0.45780200	1.51626500	-0.77581500
H	-0.21645900	2.13408400	-0.34308300
C	1.66171800	2.09220200	-1.37226400
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C	1.32329600	3.42828500	-2.04418800
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C	2.46135500	3.36740900	0.66821200
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C	3.14496700	0.95256900	0.33563900
C	1.00113500	4.52998900	-1.02852000
H	2.19600700	3.73778000	-2.63428200
H	0.49365000	3.28318400	-2.74595800
C	2.14153000	4.69538500	-0.02182400
H	1.59586200	3.04820900	1.27079000
H	3.30328100	3.49093900	1.35841500
H	3.24496300	0.15493500	-0.41278500
H	2.32727600	0.64252600	1.00018200
C	4.45422300	1.02311100	1.10767600
H	0.80931500	5.47196900	-1.55451600
H	0.07218600	4.29261600	-0.48754600
H	1.88700000	5.46005900	0.72095200
H	3.03912600	5.04945000	-0.54863800
O	5.34583900	1.81452600	0.82261900
N	4.57849500	0.10942300	2.10888100
H	3.80346700	-0.51986100	2.27143100
C	5.79181700	-0.04583300	2.90860000
C	6.73388000	-1.12096800	2.33351500
C	5.42326300	-0.37210300	4.36072200
H	6.29456200	0.92613900	2.86443300
C	6.12335900	-2.51968800	2.47410600
H	7.65692000	-1.09438600	2.92966400
C	7.11577700	-0.81317900	0.88795000
C	4.82890500	-1.77687400	4.51095100
H	6.33944500	-0.31156400	4.96278100
H	4.73328900	0.38965400	4.74155800
C	5.76950900	-2.83511300	3.92966600
H	5.21688500	-2.58211200	1.85095300
H	6.82904400	-3.26261000	2.08582600
H	7.43542300	0.23387500	0.79818000
H	6.24239200	-0.92201600	0.23112300
C	8.25911600	-1.68891500	0.39673200
H	4.62562600	-1.98013000	5.56838700
H	3.85503500	-1.83706300	4.00161100
H	5.31693500	-3.83035400	4.00594600
H	6.69396000	-2.85949700	4.52368200
O	9.12590100	-2.11805700	1.14993900
N	8.26854500	-1.92693400	-0.94279500
H	7.52560600	-1.52440100	-1.49871500
C	9.31366900	-2.69503400	-1.61600000
C	10.42888800	-1.79367600	-2.17926600
C	8.69621200	-3.55061000	-2.72848200
H	9.73973200	-3.34428000	-0.84371500
C	9.91626700	-0.94441700	-3.34746000
H	11.21505100	-2.45740500	-2.56633900
C	11.05645900	-0.93425600	-1.08539200
C	8.19532300	-2.70566800	-3.90449400
H	9.46965000	-4.23947800	-3.09323600
H	7.88811000	-4.16241800	-2.31089200
C	9.31136700	-1.81351900	-4.45262000
H	9.15718700	-0.23704200	-2.97673700
H	10.74239700	-0.34531900	-3.74624700
H	11.30479900	-1.55570200	-0.21449100
H	10.33642800	-0.18597300	-0.72819000
C	12.33650000	-0.25413800	-1.55029200
H	7.80476100	-3.36238700	-4.69012000
H	7.34775400	-2.07697900	-3.59097900
H	8.93280500	-1.18577700	-5.26740900
H	10.10118400	-2.44760100	-4.88011100
O	13.05051600	-0.72828900	-2.42672000
N	12.64812800	0.89599800	-0.89398600
H	12.00849400	1.21977800	-0.18067000
C	13.85062100	1.67991600	-1.17149800
C	15.02019600	1.30877600	-0.23987400
C	13.53168200	3.17636300	-1.06768000
H	14.12676800	1.43185800	-2.20190800
C	14.73156800	1.73835300	1.20240600
H	15.89995600	1.86827200	-0.58787100
C	15.36077800	-0.17568000	-0.33114600
C	13.26391000	3.61881400	0.37508800
H	14.39768600	3.73191500	-1.45112600
H	12.68075000	3.41407200	-1.71666800
C	14.42870200	3.23594600	1.29103400
H	13.87245400	1.16432800	1.58513900
H	15.59161800	1.48747200	1.83278000
H	15.43414800	-0.48344100	-1.38257300
H	14.55483400	-0.77902100	0.10797900
C	16.68586900	-0.50395600	0.34154700
H	13.08977900	4.70045400	0.40262500
H	12.33899300	3.15643700	0.75270900
H	14.20817500	3.52045400	2.32626900
H	15.32358100	3.79856200	0.98991700
O	17.57961100	0.32012600	0.47933700
N	16.80922700	-1.79596100	0.75836400
H	16.05105300	-2.43324600	0.55871700
C	18.04131500	-2.32452300	1.30809800
H	18.67527800	-1.47652900	1.56959000
H	17.83523600	-2.91240500	2.20653400
H	18.57135900	-2.95033800	0.58159300