

Effect on the Conformation of a Terminally Blocked, (*E*) β,γ -Unsaturated δ -Amino Acid Residue Induced by Carbon Methylation

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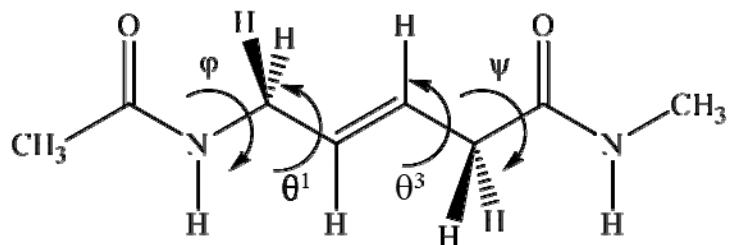
SUPPORTING INFORMATION

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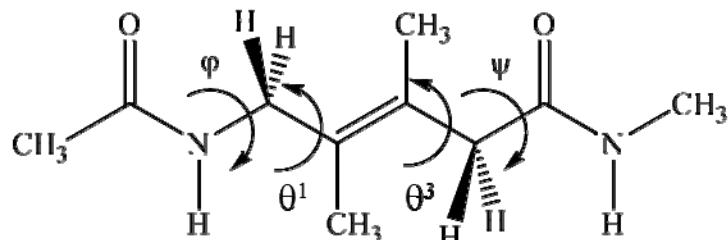
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Table S1. Values obtained for the torsion angles (in degrees) of compound A in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



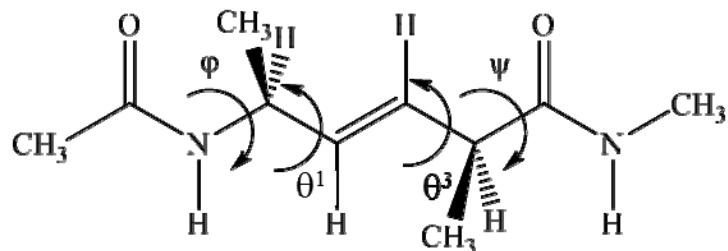
ΔG (kcal/mol)	d(N-H···O) (Å)	$\langle \text{N-H} \cdots \text{O} \rangle$ (°)	ϕ (°)	θ^1 (°)	θ^3 (°)	ψ (°)	Population (T=298 K)
0.0	2.17	155.5	-69.0	-6.0	-104.0	13.7	50.0
0.1	2.08	160.6	-66.1	116.0	105.0	-11.0	41.2
1.5	-	-	121.6	122.9	-111.0	25.4	3.8
1.6	-	-	97.8	119.8	-132.4	132.1	3.4
2.4	-	-	99.3	124.9	112.8	-26.5	0.8
2.7	-	-	99.1	120.2	130.5	-139.7	0.6
3.3	-	-	85.6	-110.9	111.9	-20.3	0.2
3.8	-	-	81.5	-103.9	117.2	66.7	0.0
4.3	-	-	130.3	123.3	-106.2	-95.7	0.0

Table S2. Values obtained for the torsion angles (in degrees) of compound **B** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



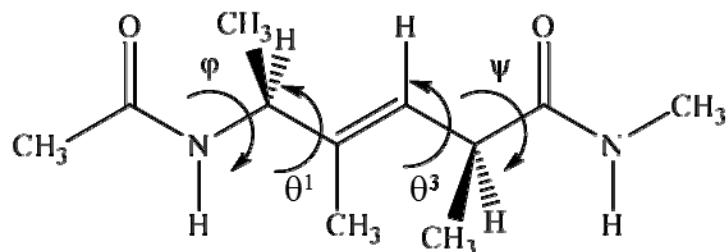
ΔG (kcal/mol)	d(N-H···O) (Å)	\angle N-H···O (°)	ϕ (°)	θ^1 (°)	θ^3 (°)	ψ (°)	Population (T=298 K)
0.0	2.07	157.7	61.6	-124.3	-95.2	14.1	93.4
1.8	2.11	152.3	51.3	56.2	91.0	-27.7	2.4
2.9	2.10	140.1	-106.8	-109.9	98.1	-96.6	0.8
3.3			-105.2	-101.6	-93.1	24.8	0.4
3.3			-85.9	108.9	-87.1	12.4	0.4
3.6			-104.9	-123.0	95.5	-21.7	0.2
3.7			-164.8	-81.9	-89.9	-159.6	0.2
4.6			-87.1	109.9	-84.7	-95.7	0.0
4.8		117.3	110.9	-92.5	-118.5		0.0

Table S3. Values obtained for the torsion angles (in degrees) of compound **C** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



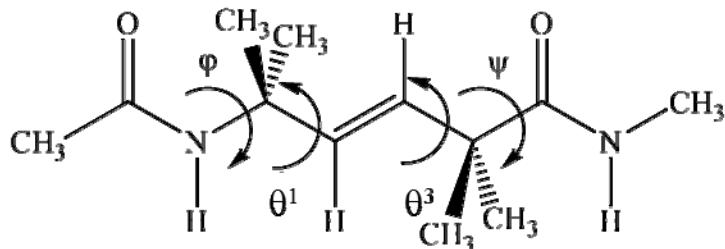
ΔG (kcal/mol)	d(N-H···O) (Å)	$\langle N\text{-}H \cdots O \rangle$ (°)	ϕ (°)	θ^1 (°)	θ^3 (°)	ψ (°)	Population (T=298 K)
0.0	2.07	159.6	-65.7	115.3	105.6	-12.1	76.9
1.0	2.16	154.2	-68.5	-5.6	-110.4	17.1	13.8
1.9	2.10	155.2	63.0	13.3	103.2	-15.3	3.1
2.2	-	-	-93.3	-125.7	111.4	-33.4	1.8
2.3	-	-	-145.1	-126.5	109.9	-29.3	1.5
2.4	2.06	156.7	59.4	-127.5	-107.7	25.4	1.3
2.8	-	-	-148.4	12.3	121.6	-116.1	0.7
3.8	-	-	-87.4	1.3	-9.8	-82.1	0.1
3.8	-	-	-149.4	-124.5	-115.2	-92.7	0.1
3.8	-	-	-81.8	103.5	-119.4	25.1	0.1
3.9	-	-	-148.8	-130.5	-122.0	23.1	0.1
3.9	-	-	-160.7	118.0	-3.7	-97.0	0.1
4.1	-	-	-150.8	-127.2	-9.9	-93.5	0.1
4.2	-	-	-160.9	121.0	-116.1	26.7	0.1
4.3	-	-	-160.5	113.2	119.8	-108.5	0.1
4.4	-	-	-75.2	100.4	-12.9	-96.2	0.0
5.0	-	-	62.5	123.4	-116.0	32.7	0.0
5.3	-	-	-160.8	107.7	95.1	107.7	0.0
5.5	-	-	62.6	-130.3	116.5	-28.9	0.0
5.9	-	-	61.4	127.0	5.5	-80.2	0.0
6.0	-	-	71.2	1.2	-118.9	28.5	0.0
6.2	-	-	61.6	-134.7	125.0	-111.0	0.0
6.7	-	-	70.7	-1.6	-21.4	-92.9	0.0

Table S4. Values obtained for the torsion angles (in degrees) of compound **D** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



ΔG (kcal/mol)	d(N-H···O) (Å)	$\langle N\text{-}H\cdots O \rangle$ (°)	ϕ (°)	θ^1 (°)	θ^3 (°)	ψ (°)	Population (T=298 K)
0.0	2.07	154.0	-57.9	131.3	89.4	-13.5	98.6
2.8	2.12	151.6	52.8	55.4	93.2	-28.7	0.8
3.4	2.14	162.5	-60.1	-31.9	-51.1	-31.5	0.3
3.8	2.09	158.1	65.3	10.3	94.4	-4.3	0.1
4.3			54.7	-132.1	-49.7	-32.8	0.1
4.9			-103.1	-119.1	106.0	-85.5	0.0
4.9			-63.7	-30.3	149.5	-133.3	0.0
5.5			-79.5	105.6	-49.1	-41.1	0.0
5.7			-101.9	-123.1	-49.8	-37.2	0.0
6.2			61.6	-135.2	101.9	-21.0	0.0
6.5			-158.6	107.53	86.31	100.2	0.0
7.0			-162.37	106.5	109.7	-98.6	0.0
7.3			-159.5	110.2	-49.1	-41.2	0.0
7.4			57.5	-135.1	149.0	-133.2	0.0
7.7			84.3	129.2	-52.0	-34.0	0.0
7.9			83.1	116.8	99.7	-90.7	0.0
8.0			-160.9	-34.2	-49.2	-37.6	0.0
9.4			74.2	0.6	-55.8	-36.3	0.0

Table S5. Values obtained for the torsion angles (in degrees) of compound **E** in the minimum energy conformations calculated at the M06L/6-31+G(d,p) level and their corresponding free energies (ΔG) at 298K. H-Bonding parameters for the conformations with this type of specific interaction are included. Populations have been calculated according to a Boltzmann distribution of minima



ΔG (kcal/mol)	d(N-H···O) (Å)	$\langle N\text{-H} \cdots O \rangle$ (°)	ϕ (°)	θ^1 (°)	θ^3 (°)	ψ (°)	Population (T=298 K)
0.0	2.04	155.7	58.1	-125.8	-107.4	23.8	74.2
0.6	2.05	157.3	-61.5	-14.0	-109.9	15.8	25.4
3.9	-	-	-176.7	-126.1	112.5	-28.7	0.3
4.2	-	-	-59.4	-125.2	113.1	-32.4	0.1
4.4	-	-	-63.3	-13.3	115.8	-28.5	0.0
4.4	-	-	-59.8	-119.7	-113.8	32.4	0.0
4.5	-	-	61.1	-126.0	116.3	-27.7	0.0
4.7	-	-	58.9	122.9	-126.6	117.4	0.0
4.8	-	-	177.4	-25.5	113.3	-29.7	0.0
4.9	-	-	-176.5	-126.5	-117.8	23.7	0.0
5.2	-	-	-178.5	19.2	115.1	-33.7	0.0
5.6	-	-	-176.4	-122.2	-1.0	99.0	0.0
5.7	-	-	-176.5	-117.8	-104.3	-103.2	0.0
5.8	-	-	58.3	120.4	127.7	-117.9	0.0
5.9	-	-	-179.3	21.0	126.8	-124.9	0.0
6.0	-	-	-61.3	-13.3	130.7	-122.3	0.0
6.1	-	-	-178.7	16.8	-131.2	120.2	0.0
6.4	-	-	60.5	-130.7	128.7	-120.3	0.0
6.5	-	-	65.6	7.4	-32.4	-45.9	0.0
6.7	-	-	-177.4	19.4	-29.3	-51.5	0.0
6.7	-	-	-176.8	-124.0	-8.6	-96.8	0.0
6.9	-	-	61.7	-111.5	22.5	56.6	0.0
7.0	-	-	179.2	-19.1	-19.9	-58.8	0.0

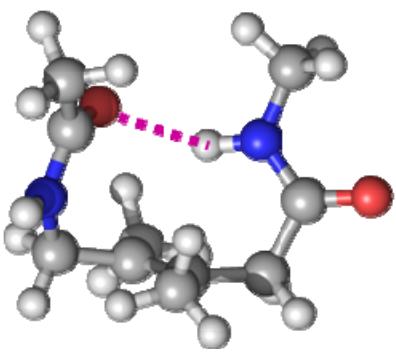


Figure S1. Minimum energy structure of compound **B** destabilized by 1.8 kcal/mol with respect to the global minimum (Table S2). Despite the high ΔG value, this structure presents a C_{10} H-bonded ring.

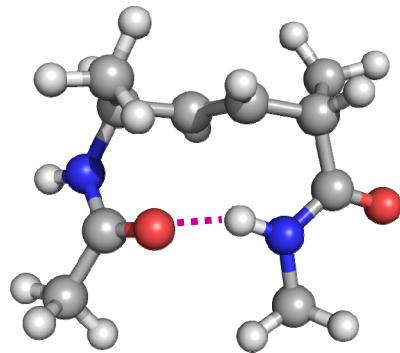


Figure S2. Minimum energy structure of compound **C** destabilized by 2.4 kcal/mol with respect to the global minimum (Table S3). Despite the high ΔG value, this structure presents a C_{10} H-bonded ring.

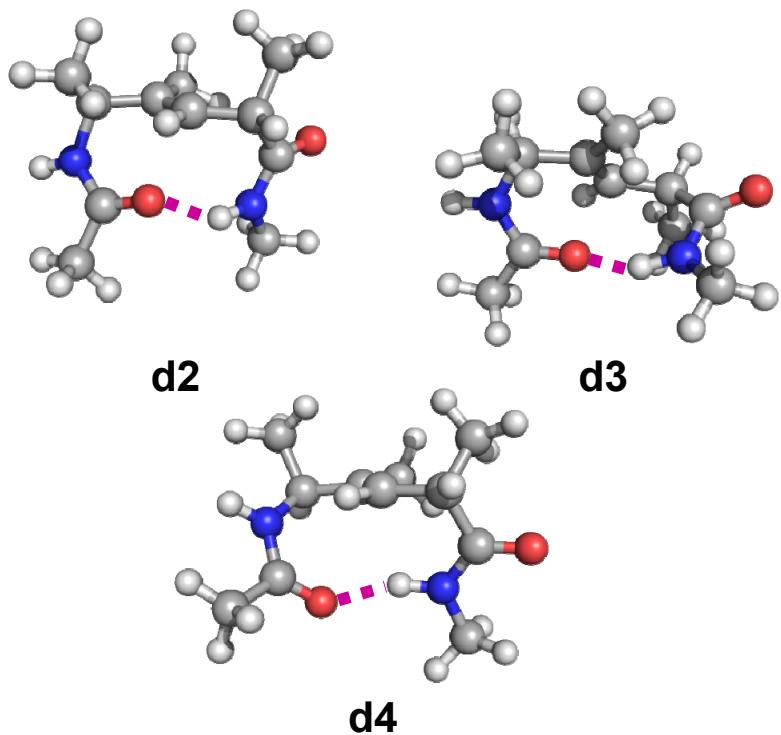


Figure S3. Minimum energy structures of compound **D** destabilized by 2.8 (**d2**), 3.4 (**d3**) and 3.8 (**d4**) kcal/mol with respect to the global minimum (Table S4). Despite the high ΔG values, each structure presents a C₁₀ H-bonded ring.

Table S6. Crystal data and structure refinement parameters for Boc-5-amino-pent-3-(E)-enoyl-NH*i*Pr (**6**)

Identification code	mc309B2
Empirical formula	C ₁₃ H ₂₄ N ₂ O ₃
Formula weight	256.34
Temperature	293(2) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	C 2/c
Unit cell dimensions	a = 54.6587(11) Å α= 90°. b = 5.86885(11) Å β= 99.241(2)°. c = 29.3845(4) Å γ = 90°.
Volume	9303.7(3) Å ³
Z	24
Density (calculated)	1.098 Mg/m ³
Absorption coefficient	0.630 mm ⁻¹
F(000)	3360
Crystal size	0.10 × 0.10 × 0.02 mm ³
Theta range for data collection	3.047 to 72.173°.
Index ranges	-66 ≤ h ≤ 62, -5 ≤ k ≤ 7, -36 ≤ l ≤ 34
Reflections collected	32059
Independent reflections	9073 [R(int) = 0.0244]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.78404
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9073 / 405 / 502
Goodness-of-fit on F ²	1.044
Final R indices [I>2sigma(I)]	R ₁ = 0.0548, wR ₂ = 0.1502
R indices (all data)	R ₁ = 0.0821, wR ₂ = 0.1660
Extinction coefficient	n/a
Largest diff. peak and hole	0.299 and -0.173 e.Å ⁻³
CCDC deposition no.	1948908

Table S7. Crystal data and structure refinement parameters for Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**10**)

Identification code	mc92p2
Empirical formula	C ₁₇ H ₃₂ N ₂ O ₃
Formula weight	312.44
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	$a = 5.990(2)$ Å $\alpha = 88.95(5)^\circ$. $b = 8.937(2)$ Å $\beta = 87.04(8)^\circ$. $c = 17.928(3)$ Å $\gamma = 80.67(7)^\circ$.
Volume	945.7(5) Å ³
Z	2
Density (calculated)	1.097 Mg/m ³
Absorption coefficient	0.594 mm ⁻¹
F(000)	344
Crystal size	0.55 × 0.35 × 0.10 mm ³
Theta range for data collection	4.940 to 60.001°.
Index ranges	-6 ≤ h ≤ 6, -10 ≤ k ≤ 10, 0 ≤ l ≤ 20
Reflections collected	2793
Independent reflections	2793 [R(int) = 0.000]
Completeness to theta = 60.001°	99.9 %
Absorption correction	none
Refinement method	full-matrix least-squares on F ²
Data / restraints / parameters	2793 / 0 / 200
Goodness-of-fit on F ²	1.059
Final R indices [I>2sigma(I)]	R ₁ = 0.0692, wR ₂ = 0.1924
R indices (all data)	R ₁ = 0.0736, wR ₂ = 0.2017
Extinction coefficient	0.026(4)
Largest diff. peak and hole	0.612 and -0.336 e.Å ⁻³
CCDC deposition no.	1948909

Table S8. Crystal data and structure refinement parameters for Azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-N*i*Pr (**11**)

Identification code	mc310	
Empirical formula	C ₁₃ H ₂₃ N ₅ O ₂	
Formula weight	281.36	
Temperature	293(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.1653(3) Å b = 9.4255(3) Å c = 10.5148(3) Å	α= 107.580(3)°. β= 91.726(3)°. γ = 106.465(3)°.
Volume	823.73(5) Å ³	
Z	2	
Density (calculated)	1.134 Mg/m ³	
Absorption coefficient	0.645 mm ⁻¹	
F(000)	304	
Crystal size	0.50 × 0.40 × 0.20 mm ³	
Theta range for data collection	4.447 to 72.814°.	
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -13 ≤ l ≤ 10	
Reflections collected	13055	
Independent reflections	3269 [R(int) = 0.0168]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.80313	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3269 / 44 / 203	
Goodness-of-fit on F ²	1.079	
Final R indices [I>2sigma(I)]	R ₁ = 0.0523, wR ₂ = 0.1533	
R indices (all data)	R ₁ = 0.0550, wR ₂ = 0.1567	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.303 and -0.217 e.Å ⁻³	
CCDC deposition no.	1952416	

Table S9. Backbone torsion angles ($^{\circ}$) for the three independent molecules in the X-ray diffraction structure of Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**)

Molecule	ω^N	ϕ	θ^1	θ^2	θ^3	ψ	ω^C
1	174.7(2)	141.8(2)	119.8(3)	178.5(2)	-121.2(3)	-123.2(2)	179.3(2)
2	174.96(19)	140.2(2)	125.6(2)	178.7(2)	-117.9(3)	-142.2(2)	-178.4(2)
3	-167.41(16)	87.9(2)	127.4(2)	-178.39(18)	-107.4(2)	-138.7(2)	-178.8(2)

Table S10. Intermolecular H-bond parameters [\AA and $^{\circ}$] in the X-ray diffraction structure of Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**)

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
N_1-H0_1...O0_3#1	0.86	2.13	2.982(2)	170.5
NT_1-HT_1...O_3#2	0.86	2.13	2.967(2)	163.1
N_2-H0_2...O0_1	0.86	2.12	2.9545(19)	163.7
NT_2-HT_2...O_1	0.86	2.07	2.905(2)	164.7
N_3-H0_3...O0_2	0.86	2.20	2.9459(19)	145.1
NT_3-HT_3...O_2	0.86	2.05	2.898(2)	169.9

Symmetry transformations used to generate equivalent atoms:

#1 x, -y+1, z-1/2 #2 x, -y, z-1/2

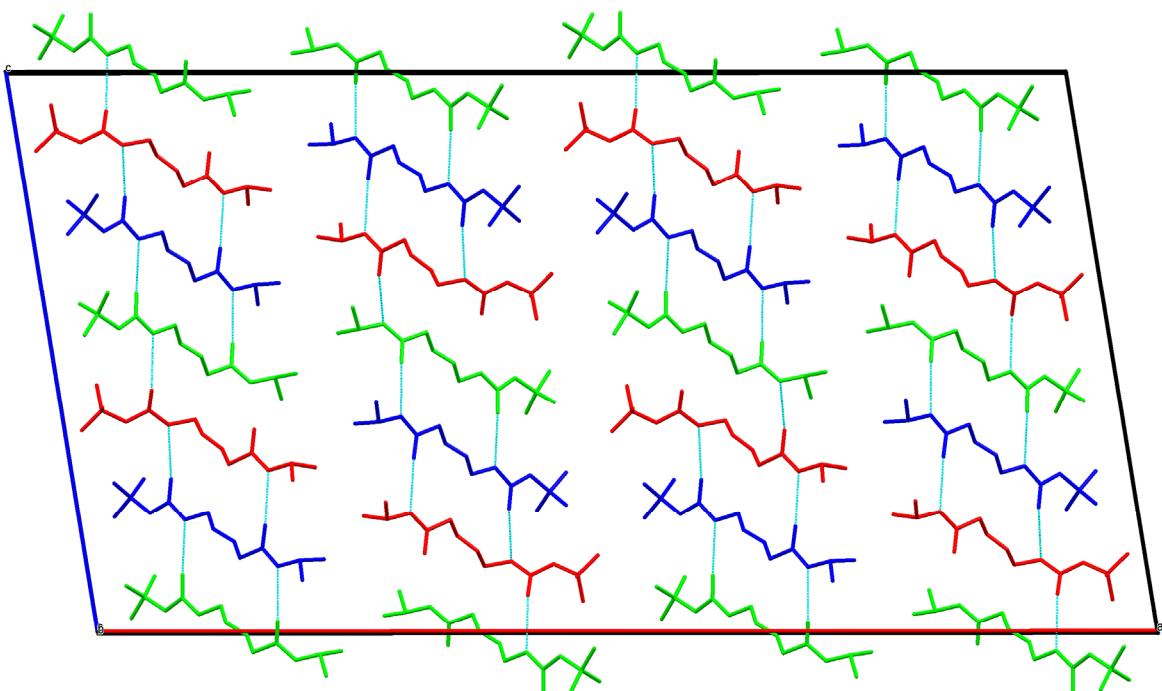


Figure S4. Packing mode of Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**) as viewed nearly down the *b* direction. Each of the three independent molecules is shown in a different color. Intermolecular H-bonds are indicated by dashed lines.

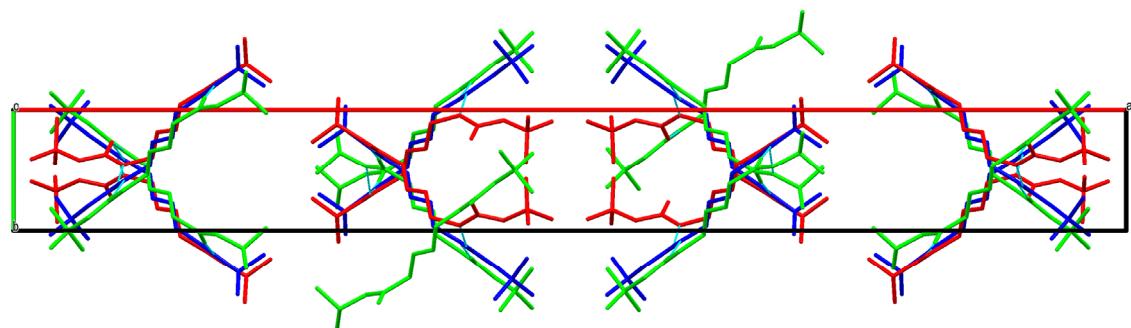


Figure S5. Packing mode of Boc-5-amino-pent-3-(*E*)-enoyl-NH*i*Pr (**6**) as viewed down the *c* direction. Each of the three independent molecules is shown in a different color.

Table S11. Backbone torsion angles ($^{\circ}$) in the X-ray diffraction structure of Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-N*i*Pr (**10**)

ω^N	ϕ	θ^1	θ^2	θ^3	ψ	ω^C
178.29(18)	60.4(3)	8.9(4)	-175.3(2)	98.7(3)	-3.3(3)	-177.9(2)

Table S12. Intra- and interermolecular H-bond parameters [\AA and $^{\circ}$] in the X-ray diffraction structure of Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-N*i*Pr (**10**)

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
NT-HT...O0	0.86	2.30	3.120(3)	160.6
N1-H1...O1#1	0.86	2.14	2.988(3)	166.9

Symmetry transformations used to generate equivalent atoms:

#1 $x, y-1, z$

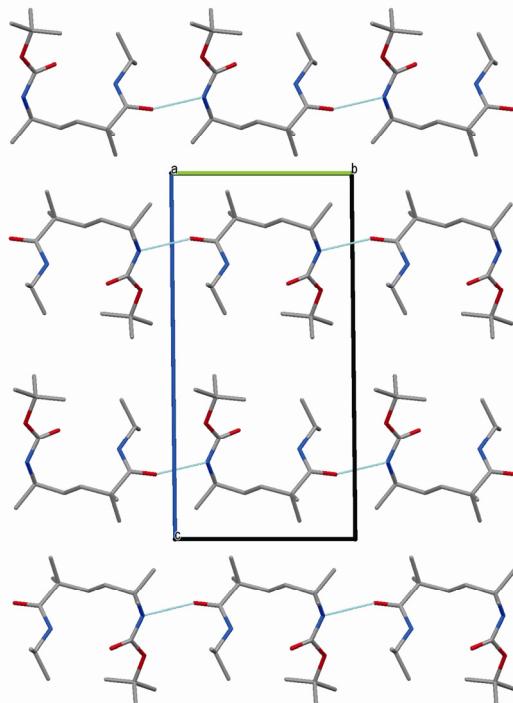


Figure S6. Packing mode of Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-N*i*Pr (**10**) as viewed down the *a* direction. Intermolecular H-bonds are represented by dashed lines.

Table S13. Backbone torsion angles ($^{\circ}$) in the X-ray diffraction structure of azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**)

ω^N	ϕ	θ^1	θ^2	θ^3	ψ	ω^C
176.09(14)	50.7(2)	-130.52(15)	177.94(12)	-110.48(15)	32.42(17)	177.21(14)

Table S14. Intra- and interermolecular H-bond parameters [\AA and $^{\circ}$] in the X-ray diffraction structure of azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**)

D-H...A	d(D-H)	d(H...A)	d(D...A)	\angle (DHA)
NT-HT...O0	0.86	2.25	3.0641(15)	158.7
N1-H1...O1#1	0.86	2.05	2.8694(15)	159.3

Symmetry transformations used to generate equivalent atoms:

#1 $x, y-1, z$

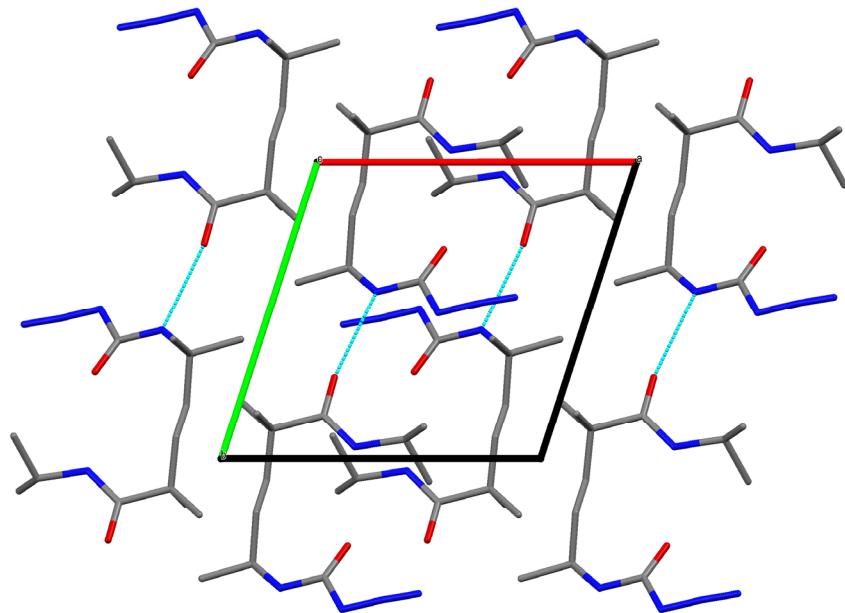


Figure S7. Packing mode of azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**) as viewed down the *c* direction. Intermolecular H-bonds are represented by dashed lines.

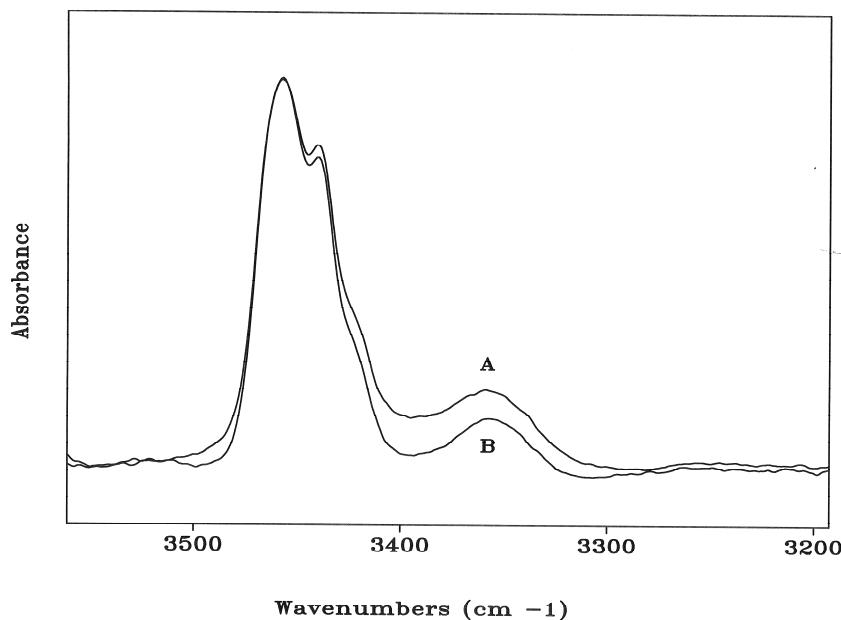


Figure S8. FT-IR absorption spectra in CDCl_3 solution of compound (Boc)A **6** in the 3500-3200 cm^{-1} wavenumber (N-H stretching) region in CDCl_3 solution at the concentrations of 1.0 mM (A) and 0.1 mM (B).

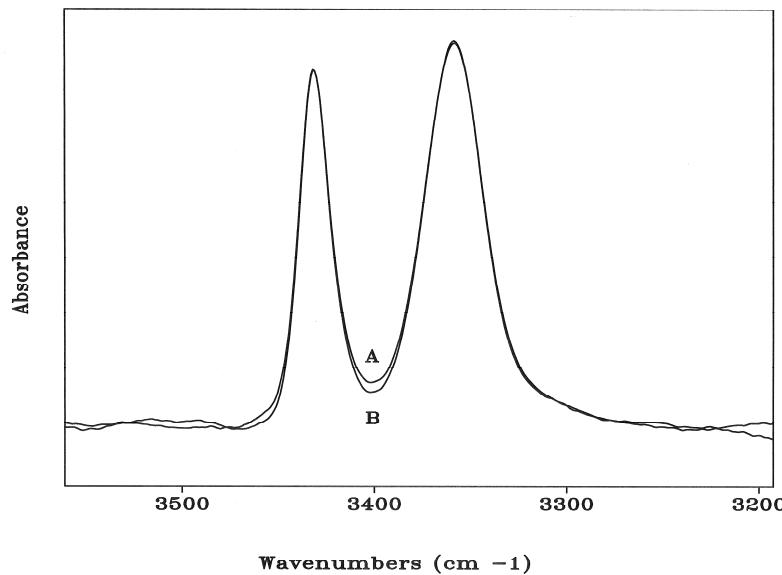
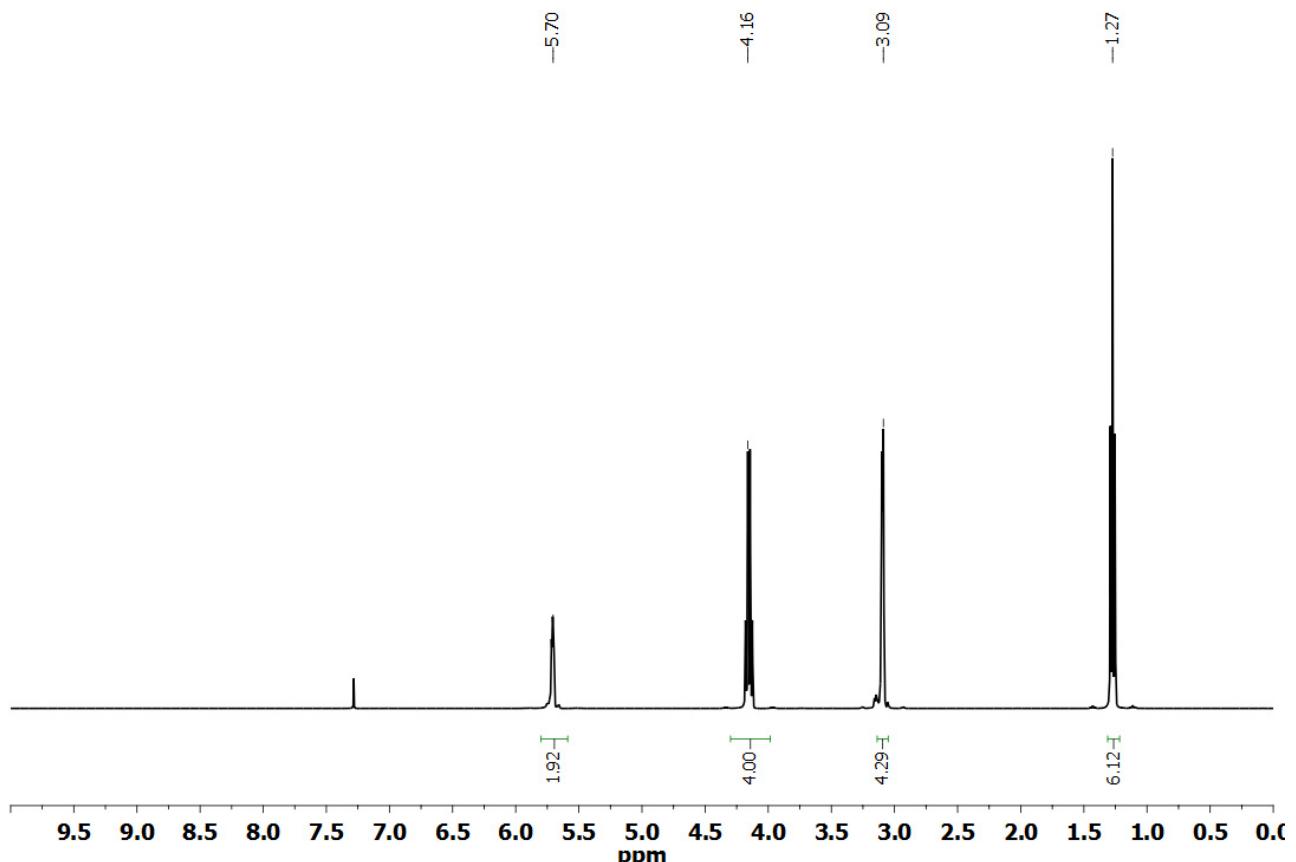
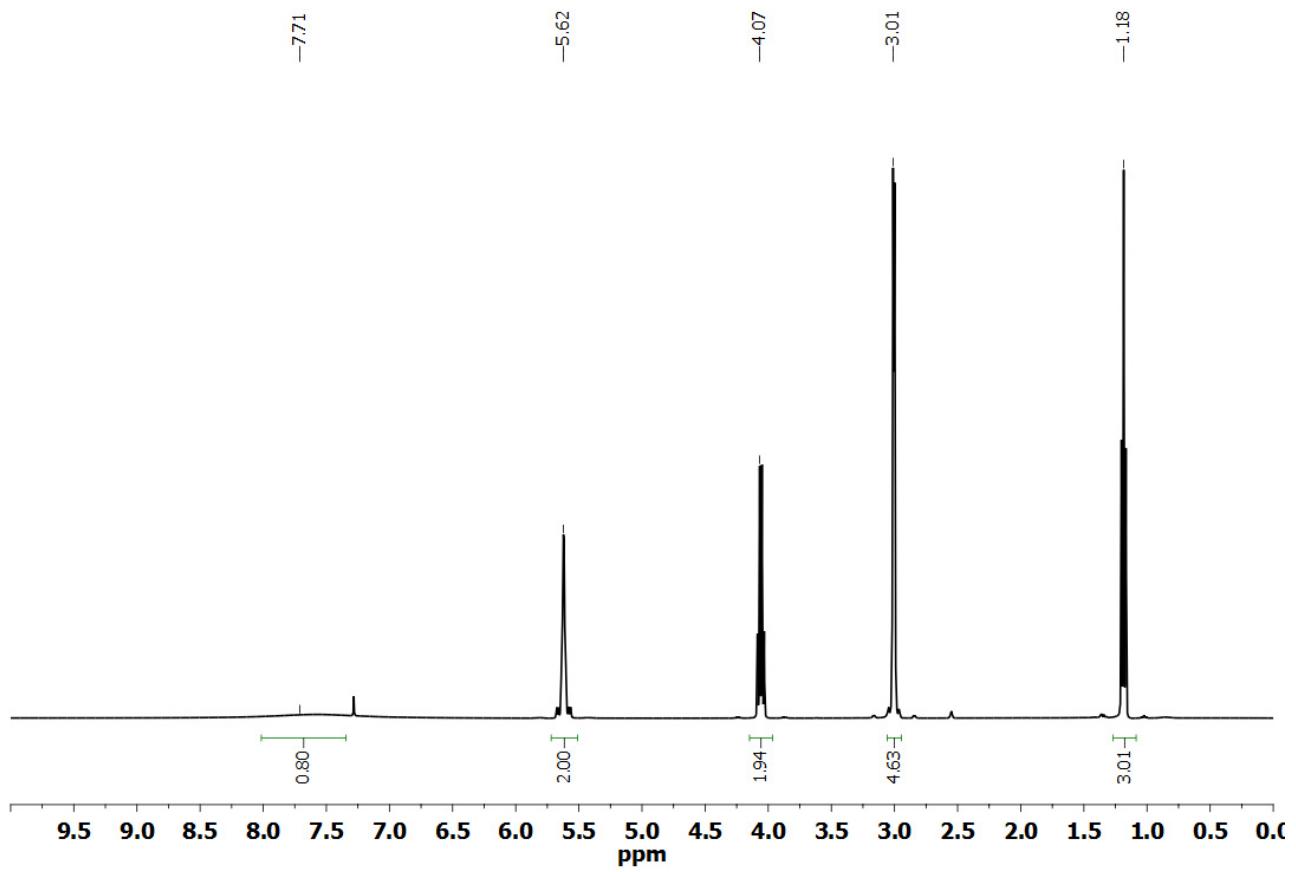
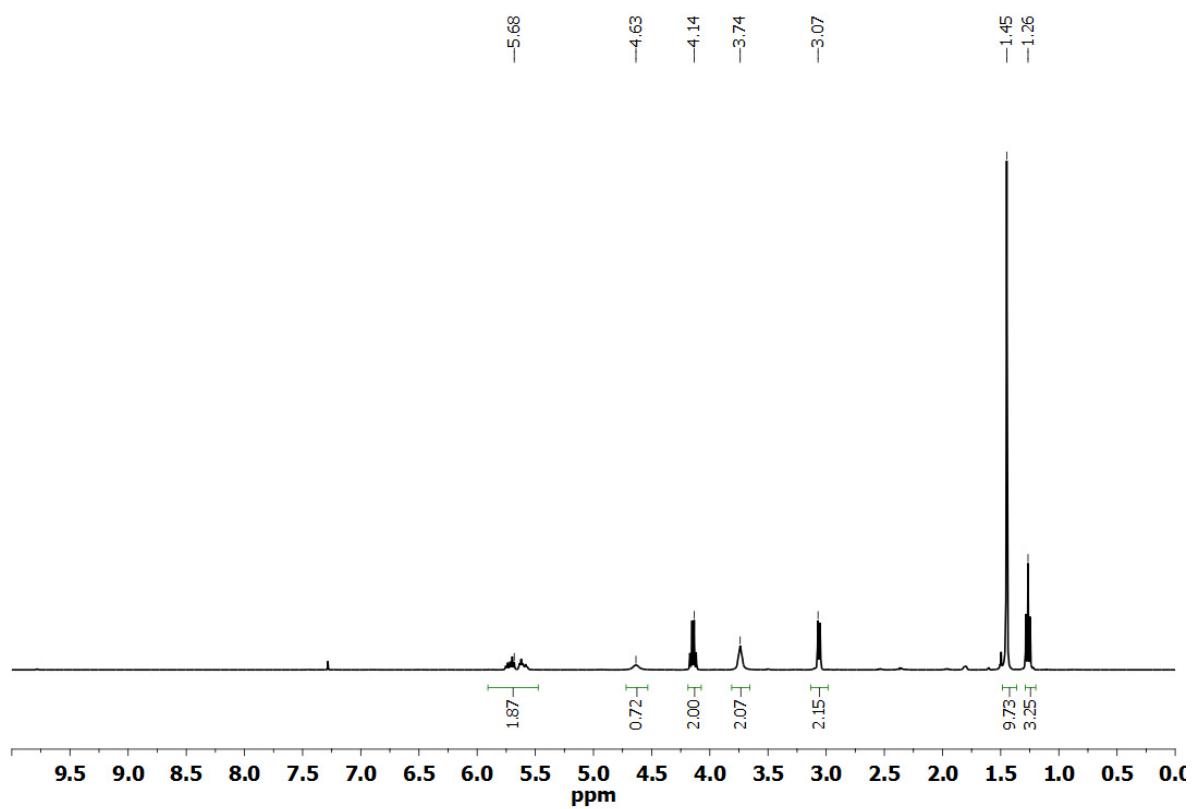
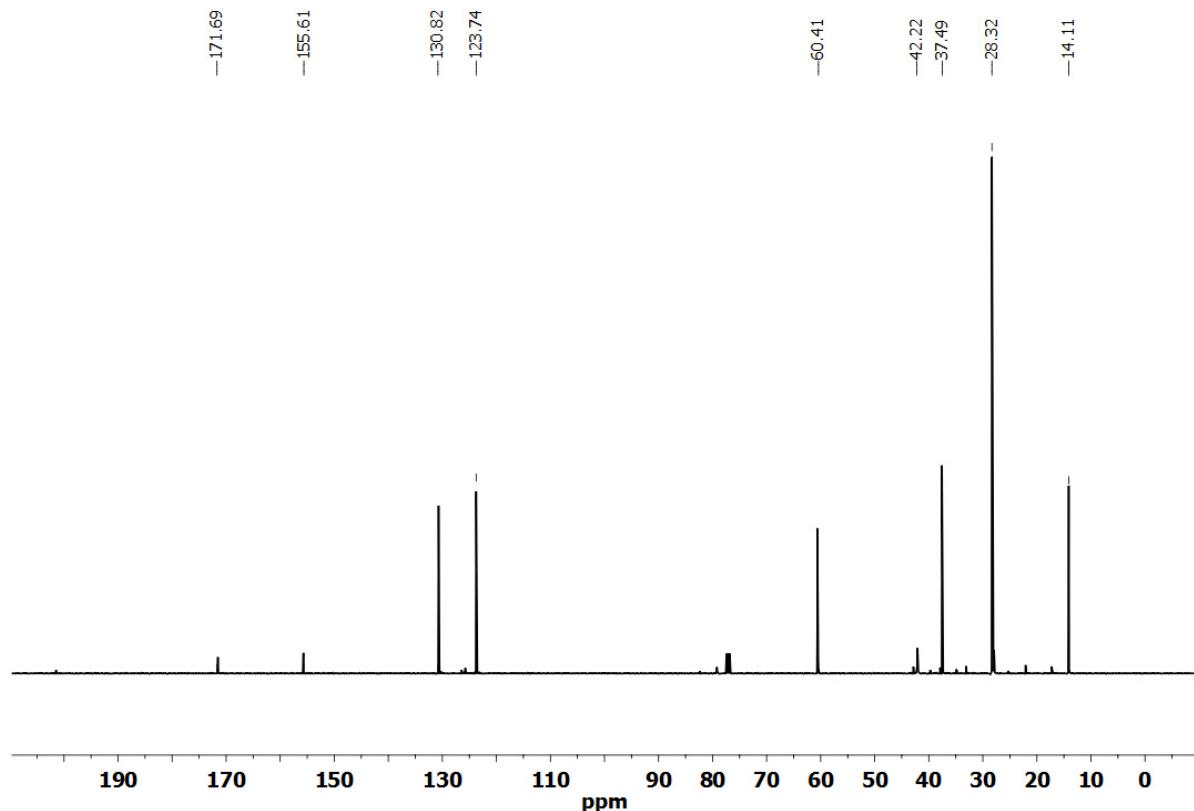


Figure S9. FT-IR absorption spectra in CDCl_3 solution (1.0 mM concentration) of compound (Boc)E **10** in the 3500-3200 cm^{-1} wavenumber (N-H stretching) region in CDCl_3 solution at the concentrations of 1.0 mM (A) and 0.1 mM (B).

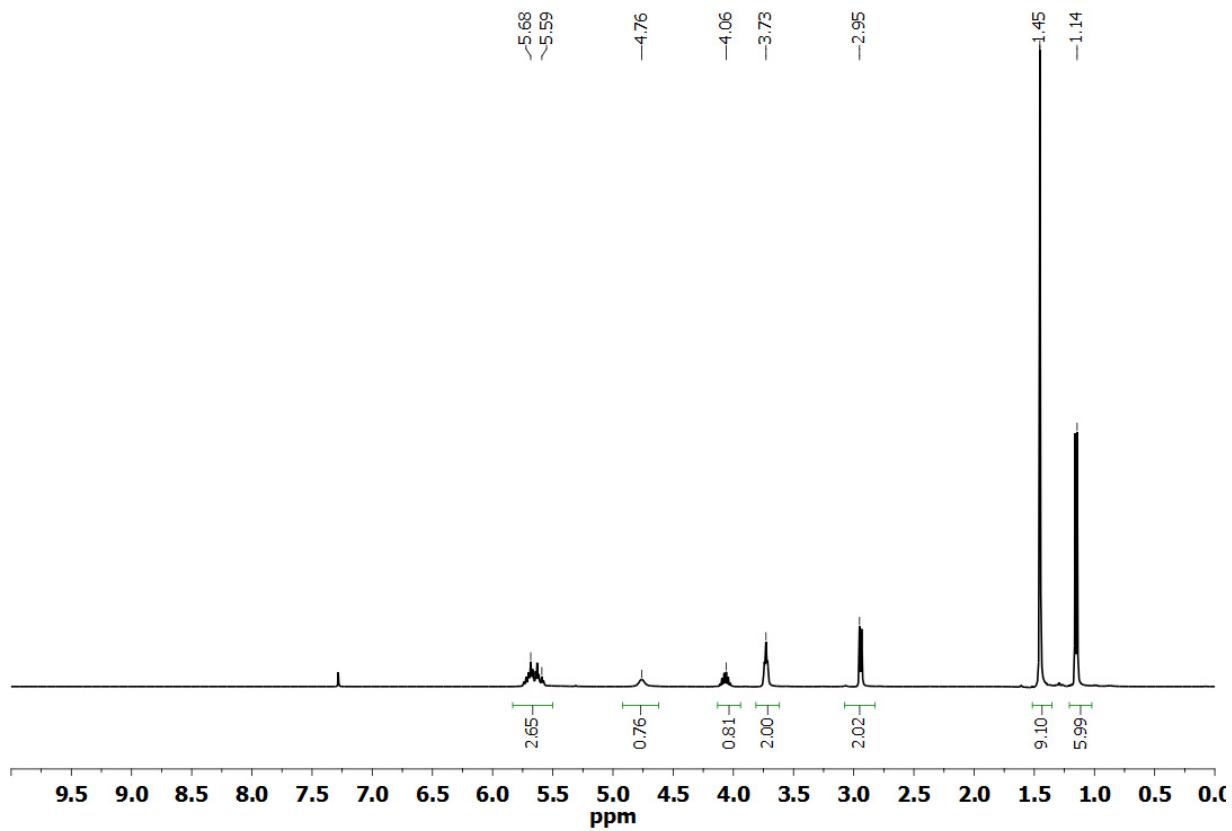




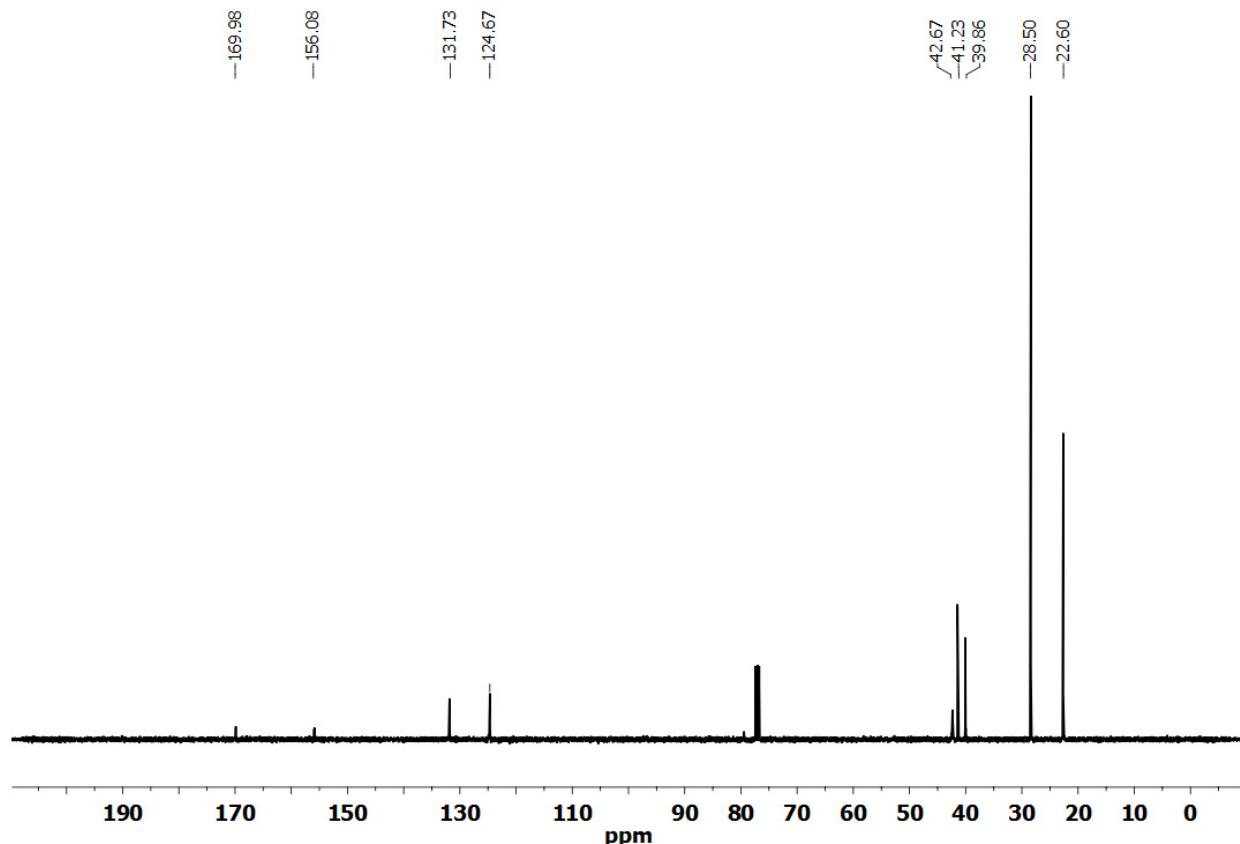
¹H NMR (400 MHz, CDCl₃) of compound 4.



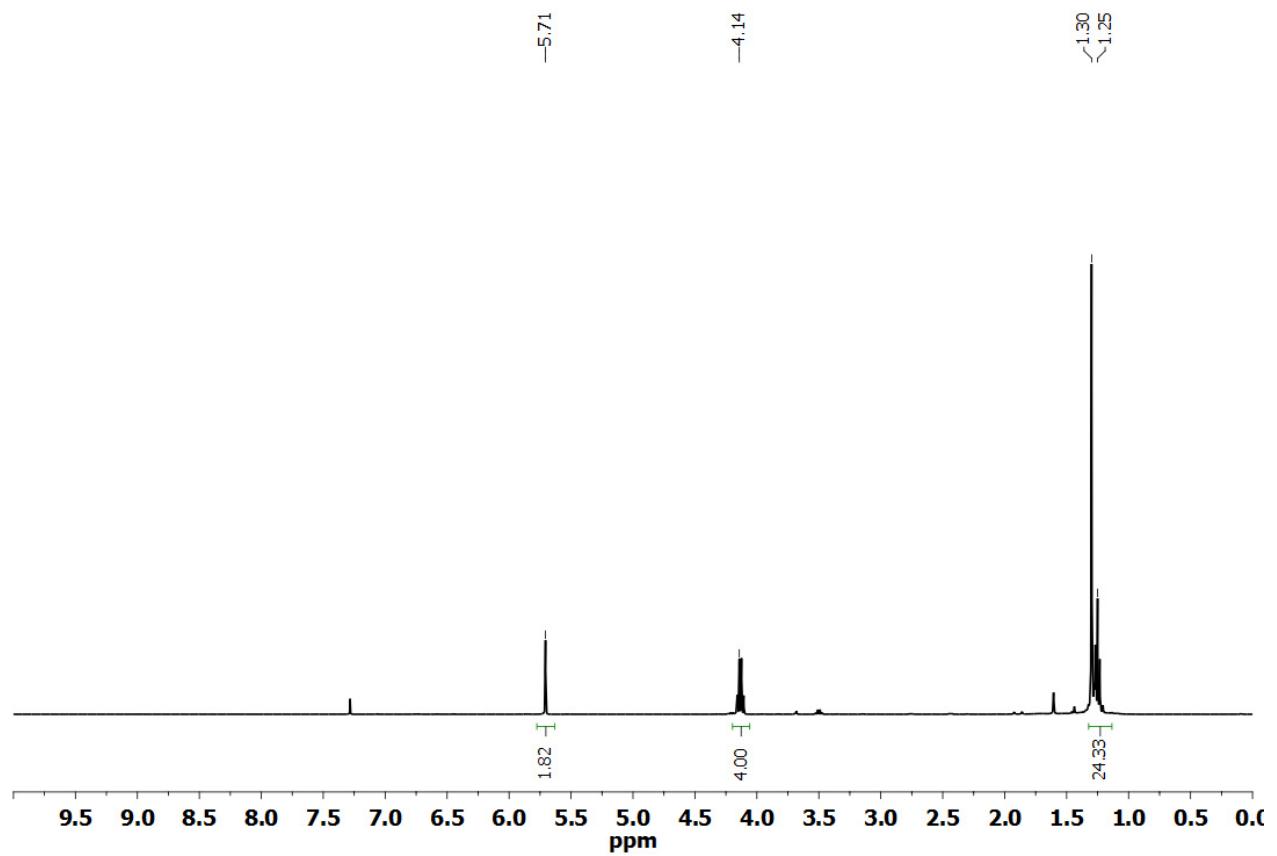
¹³C NMR (101 MHz, CDCl₃) of compound 4.



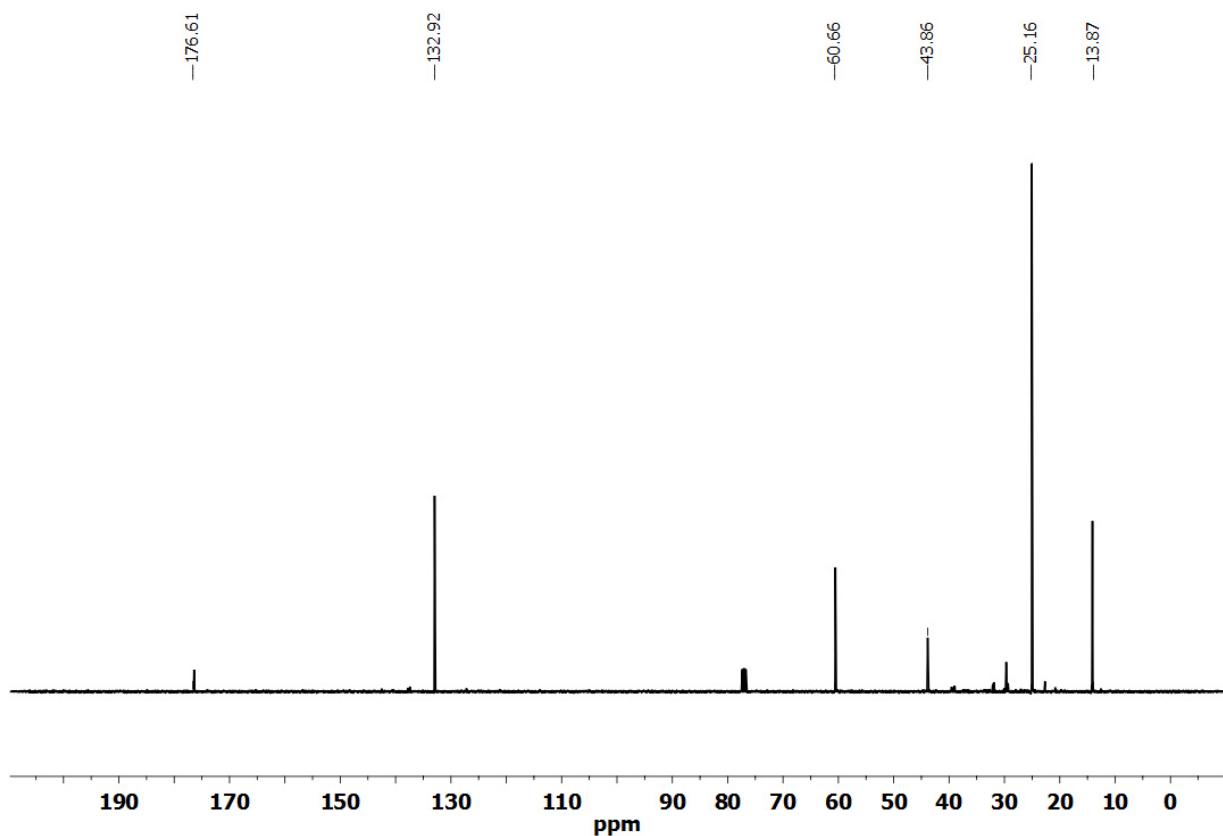
¹H NMR (400 MHz, CDCl₃) of compound 6.



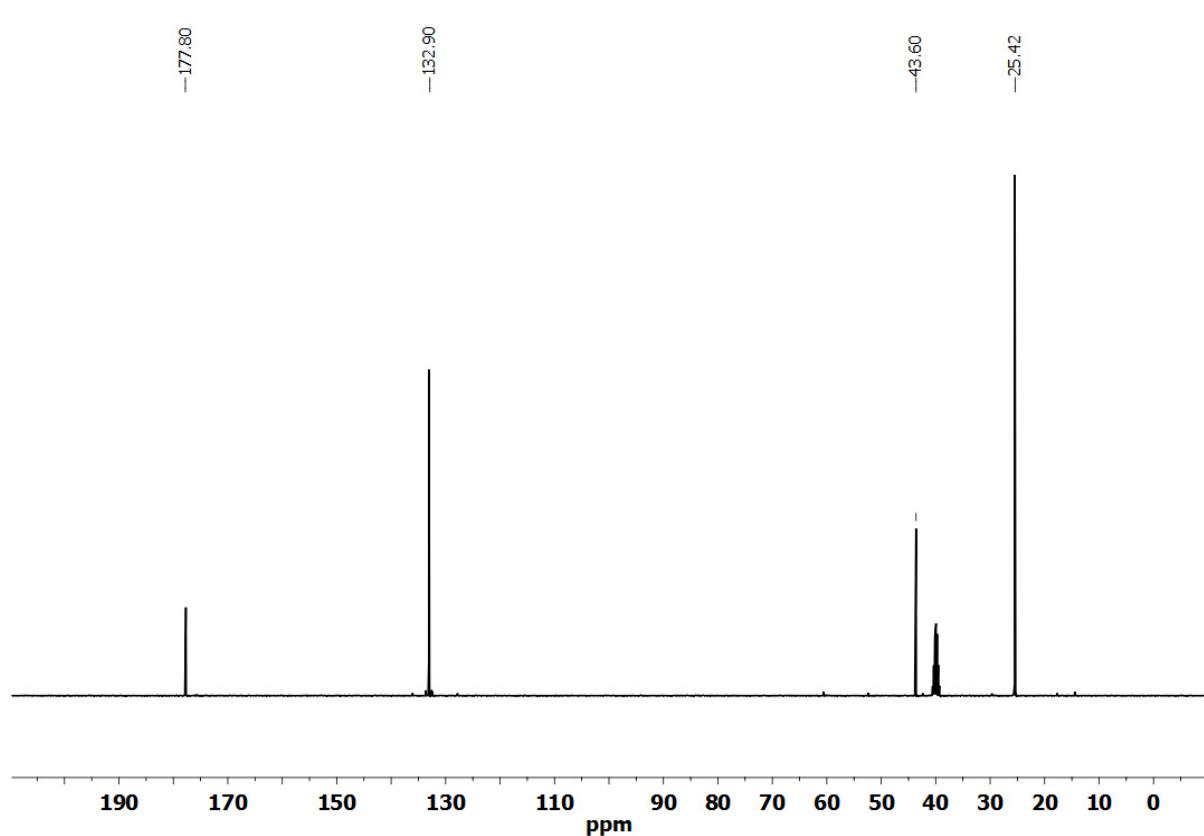
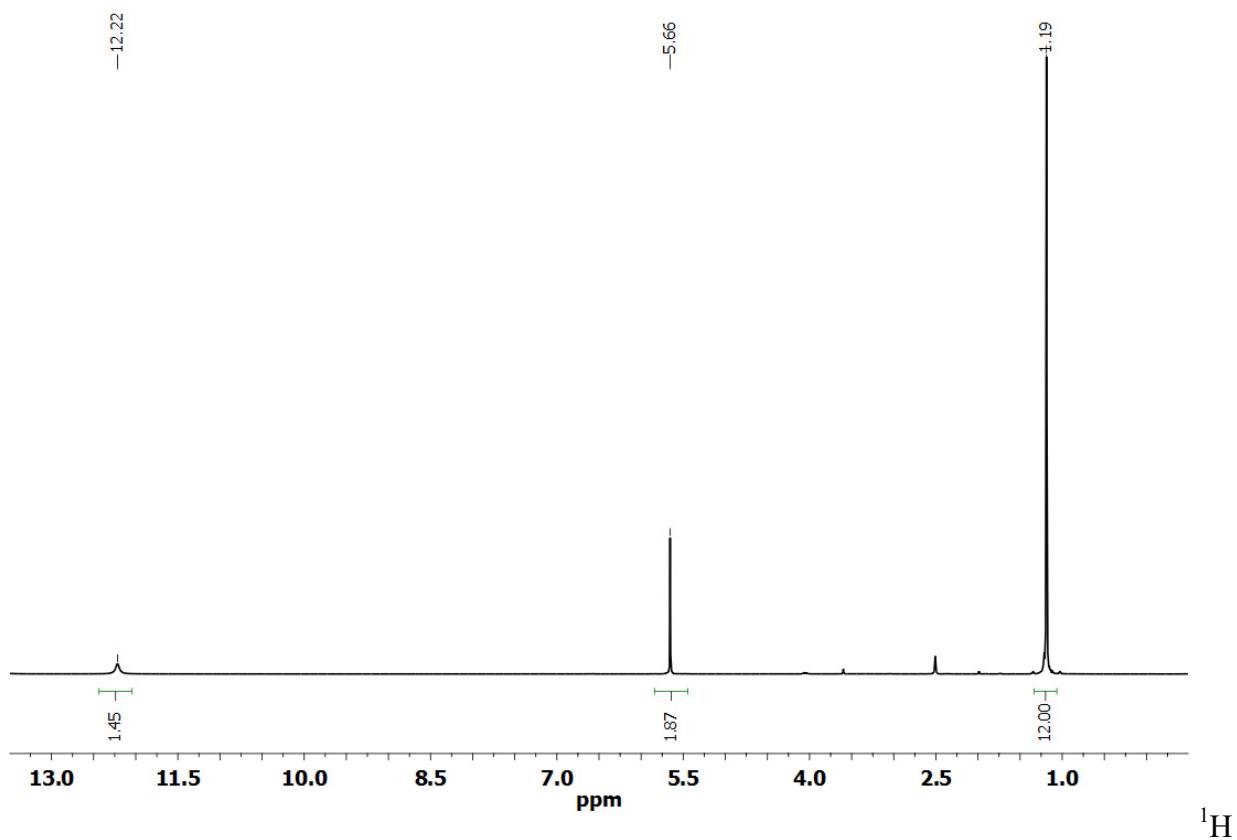
¹³C NMR (101 MHz, CDCl₃) of compound 6.

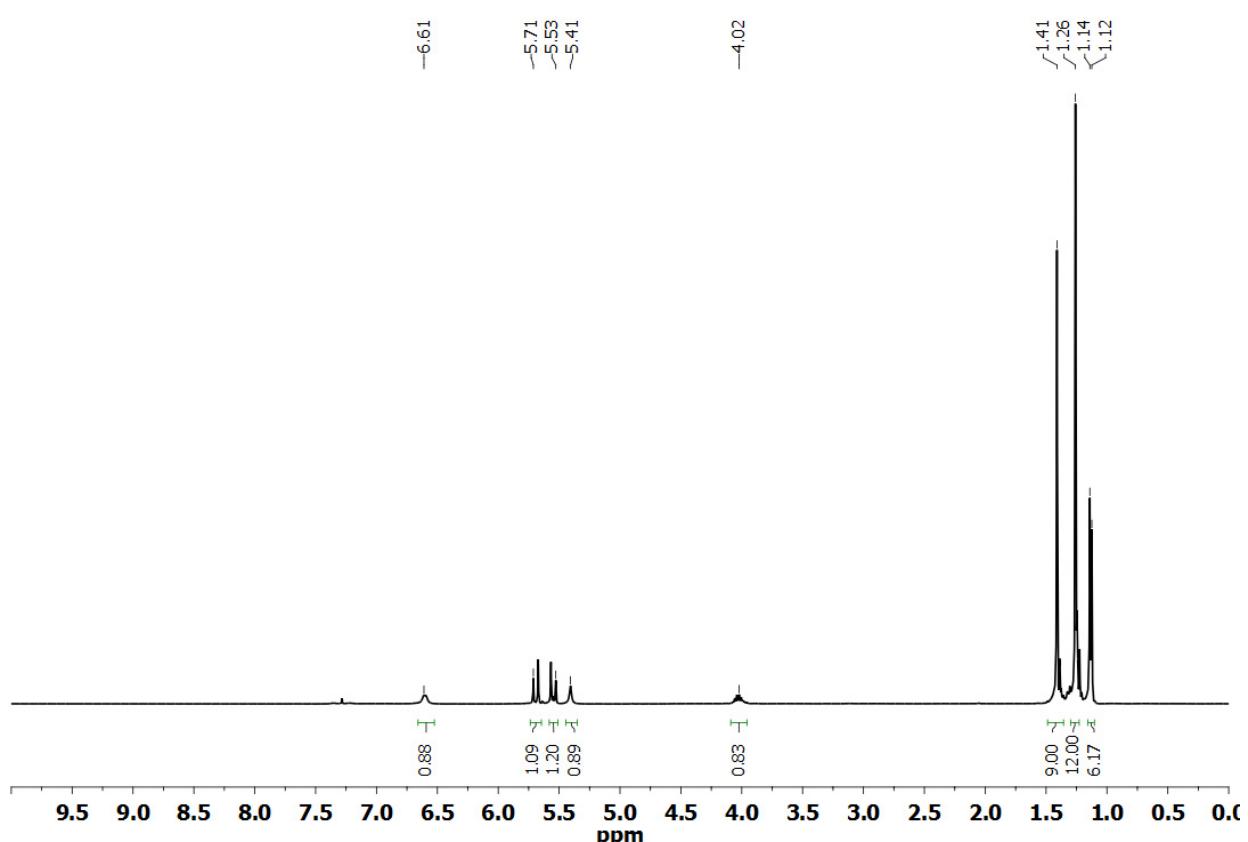
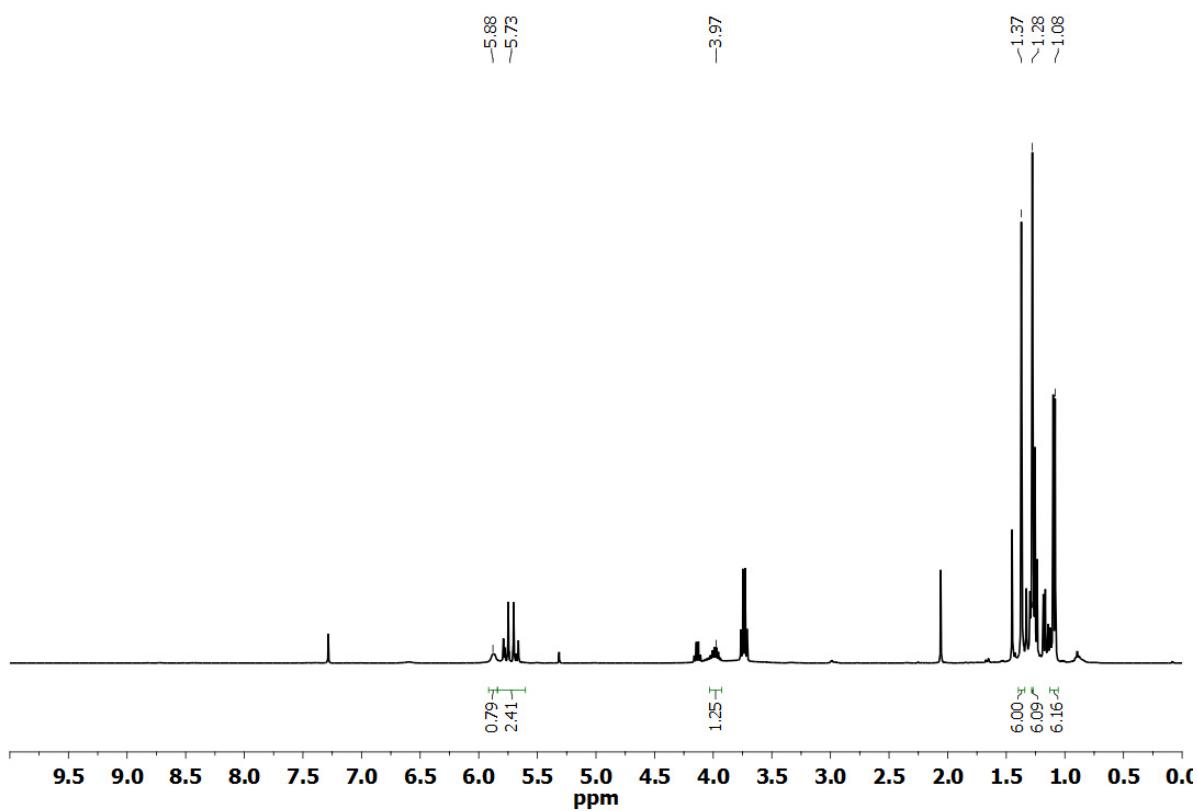


¹H NMR (400 MHz, CDCl₃) of compound 7.

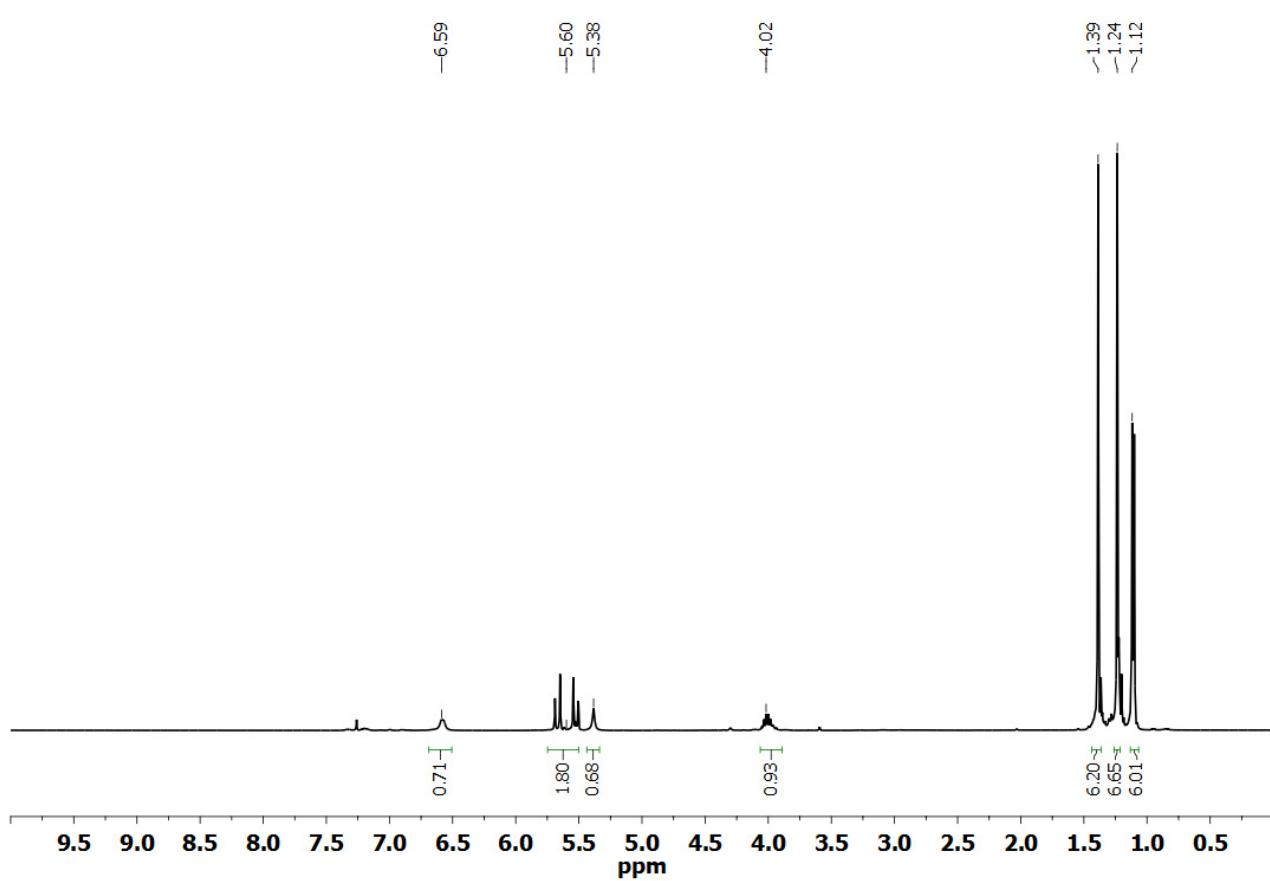
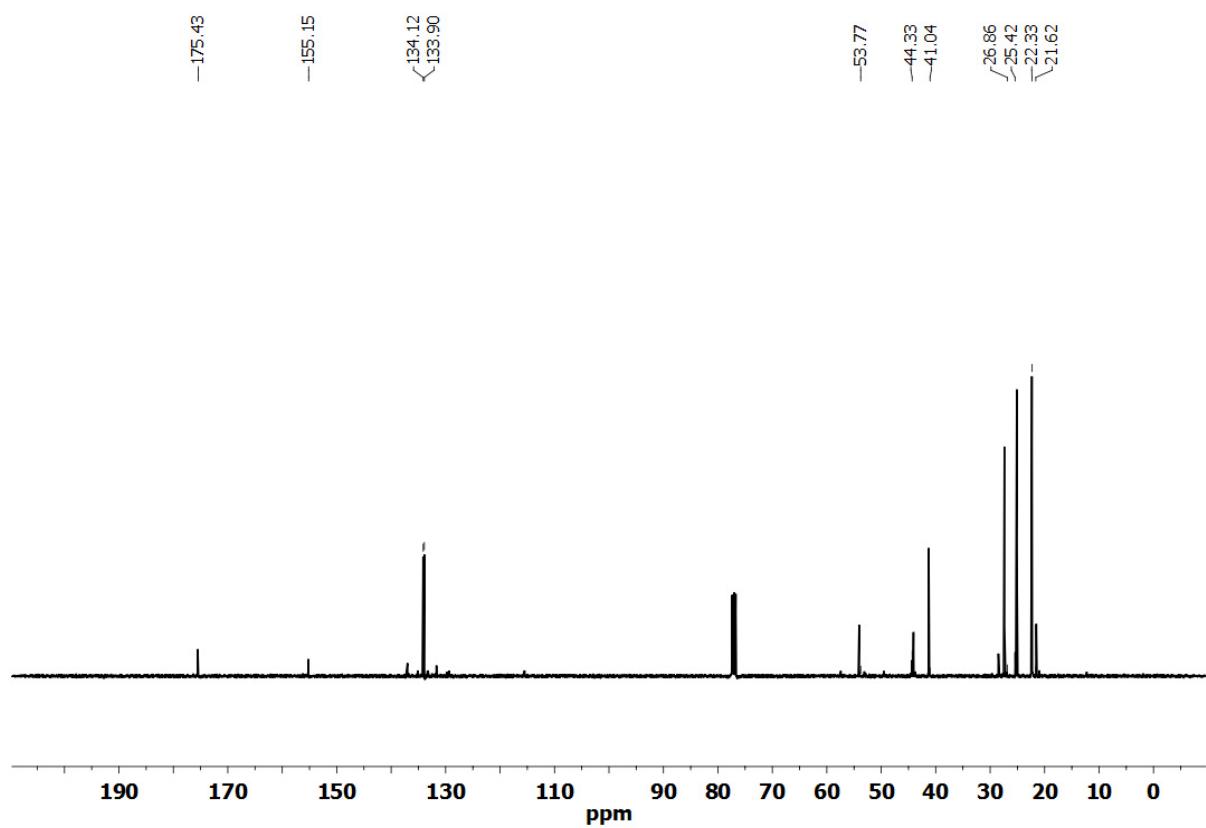


¹³C NMR (101 MHz, CDCl₃) of compound 7.

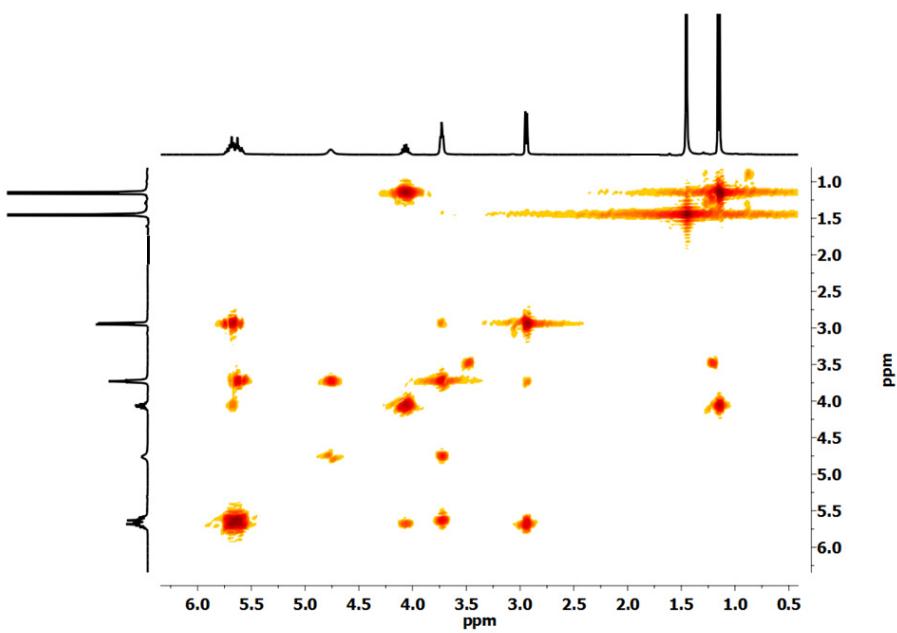




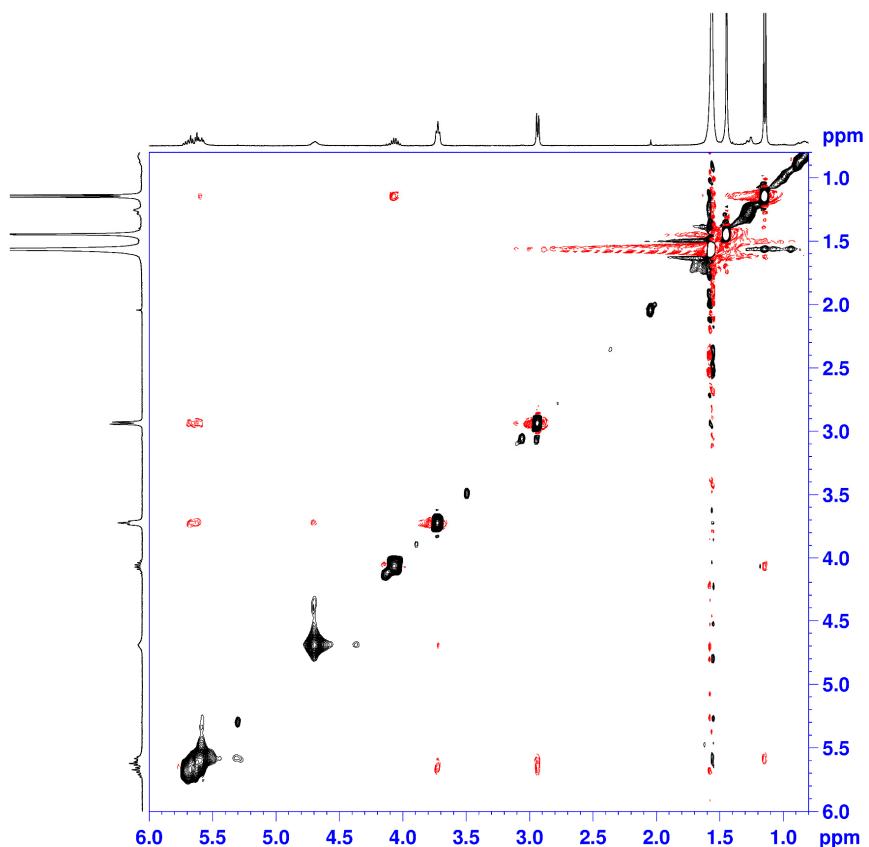
¹H NMR (400 MHz, CDCl₃) of compound **10**.



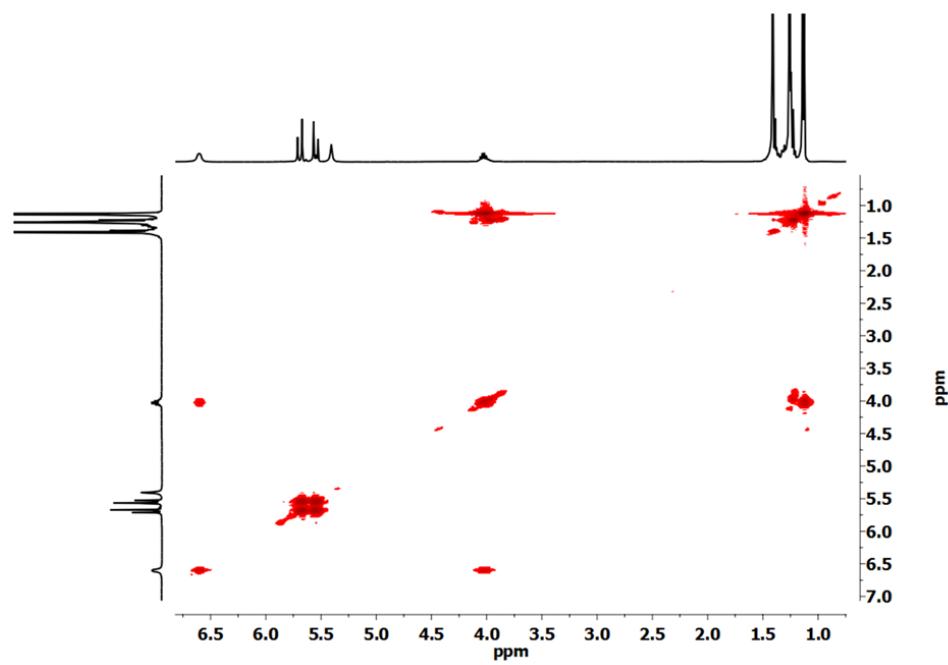
¹H NMR (400 MHz, CDCl₃) of compound **11**.



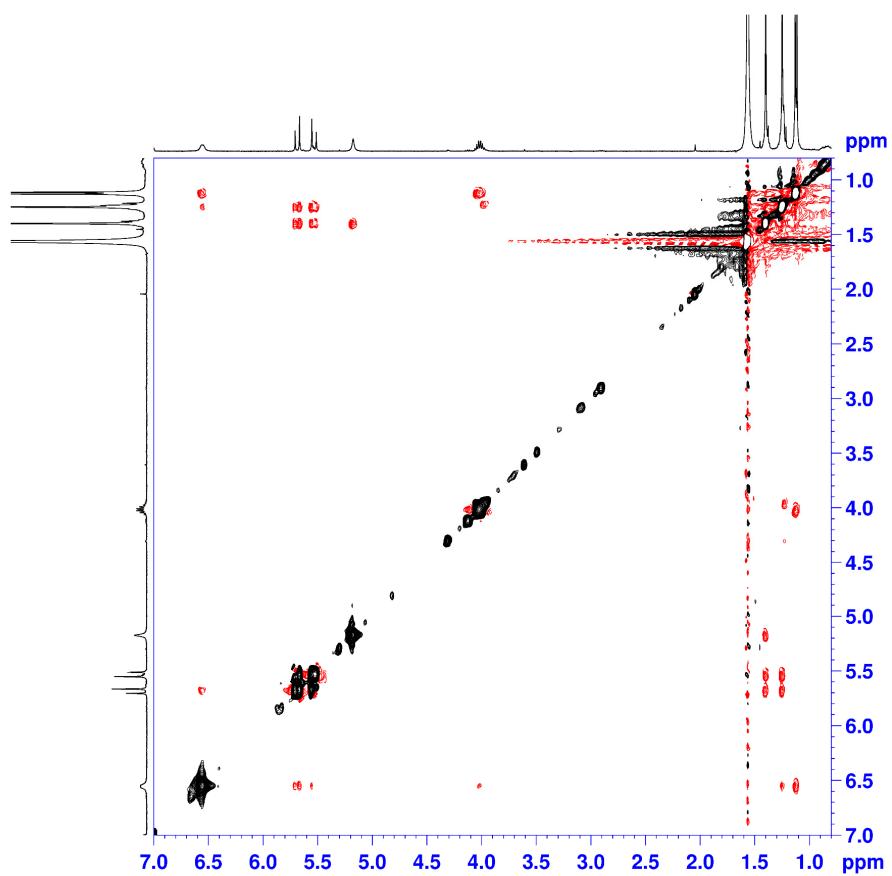
2D-COSY NMR (400 MHz, CDCl_3) of compound **6**.



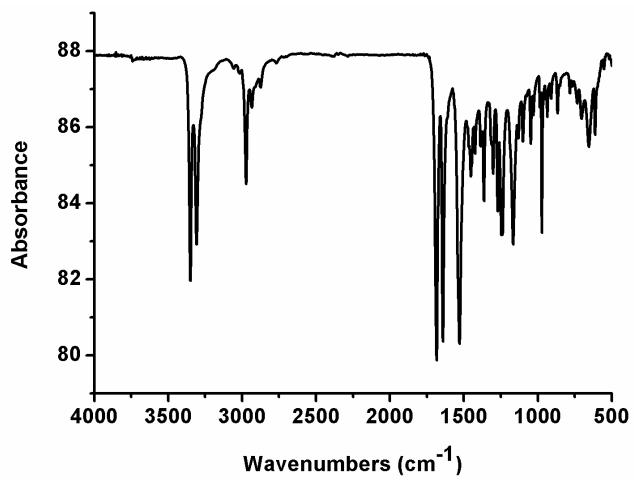
2D-NOESY NMR (400 MHz, CDCl_3) of compound **6**.



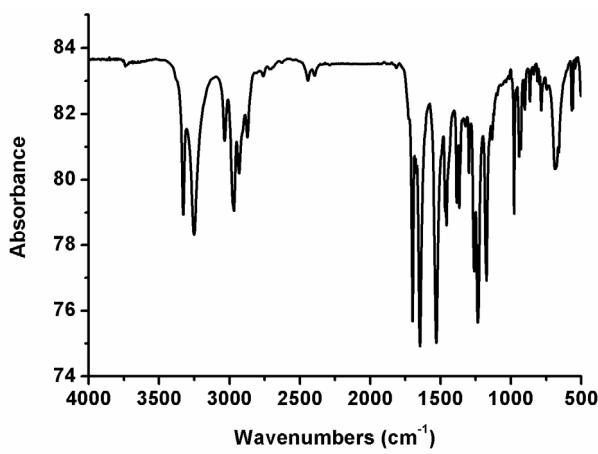
2D-COSY NMR (400 MHz, CDCl_3) of compound **10**.



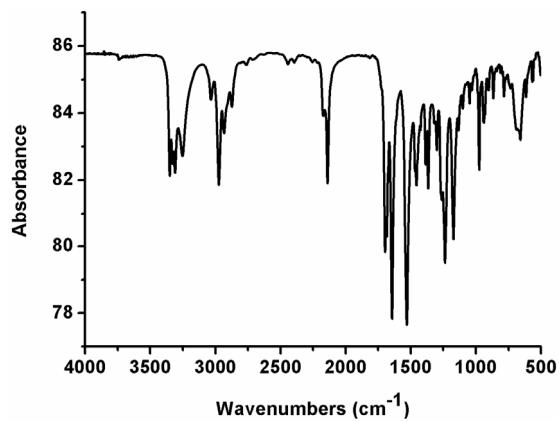
2D-NOESY NMR (400 MHz, CDCl_3) of compound **10**.



FT-IR (KBr) spectrum of compound **6**.



FT-IR (KBr) spectrum of compound **10**.



FT-IR (KBr) spectrum of compound **11**.

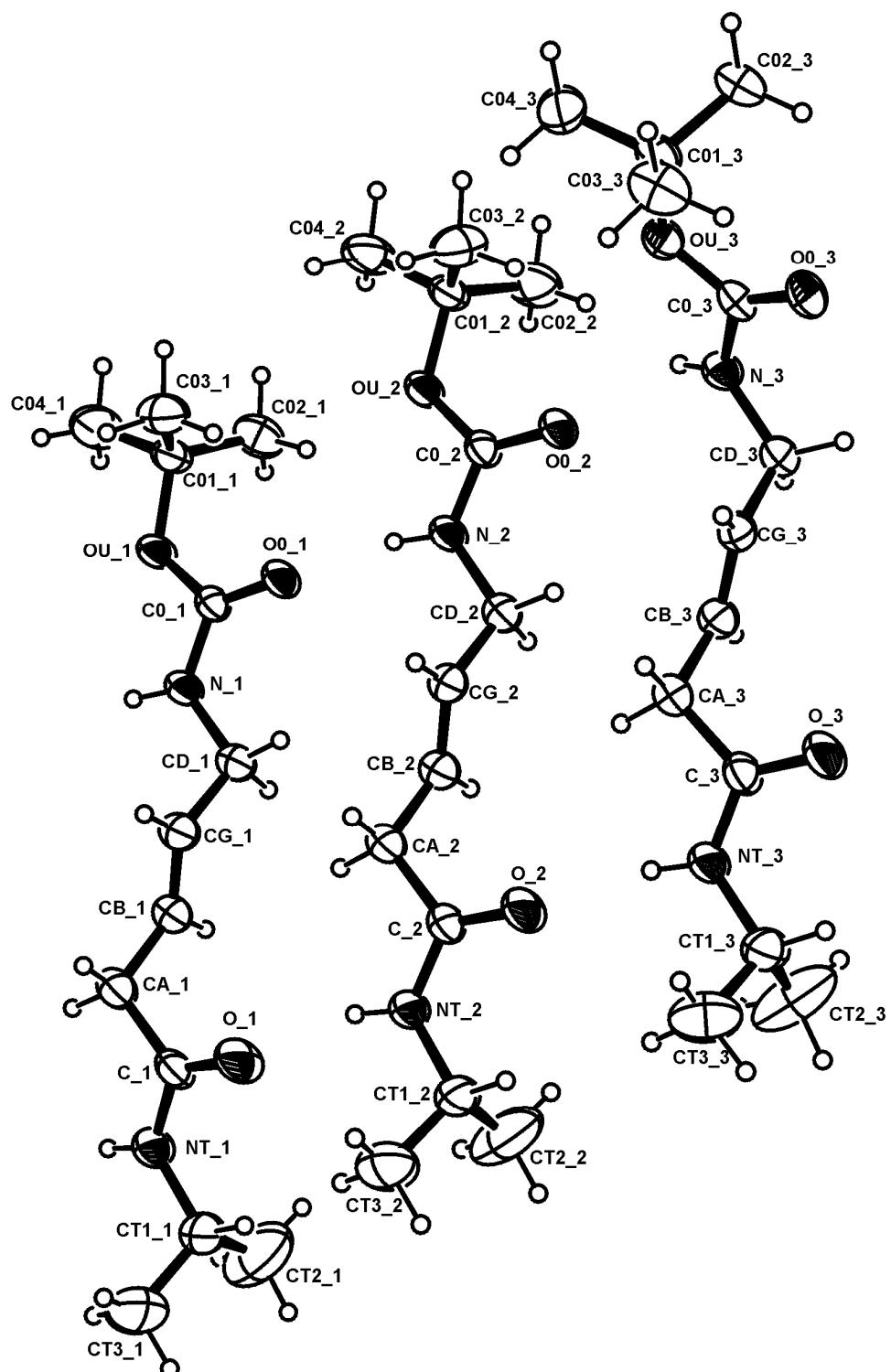


Figure S10 – ORTEP drawing of the X-Ray diffraction structure of Boc-5-aminopent-3-(*E*)-enoyl-NH*i*Pr (**6**). Anisotropic displacement ellipsoids for the non-H atoms are drawn at the 30% probability level.

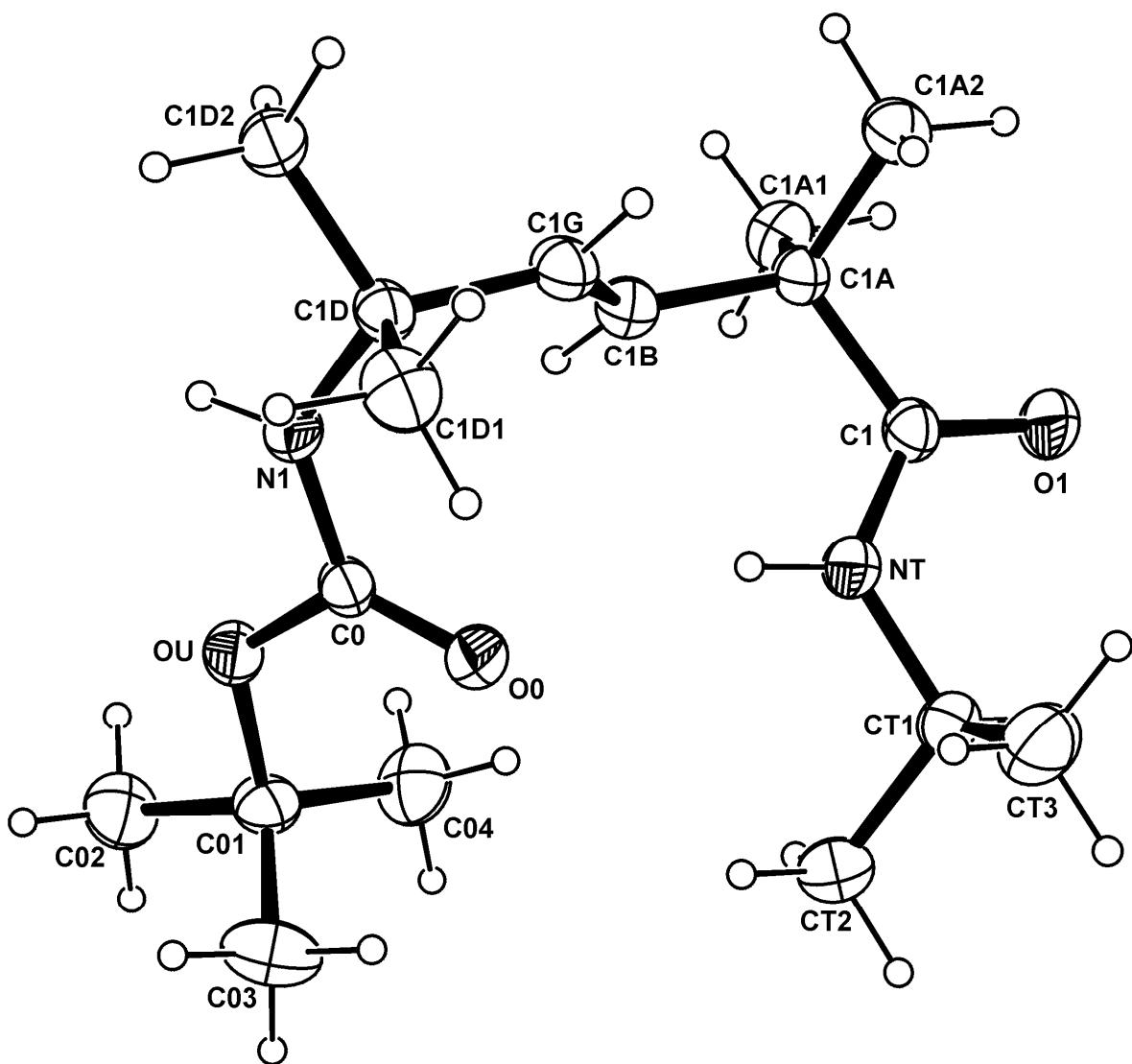


Figure S11 – ORTEP drawing of the X-Ray diffraction structure of Boc-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**10**). Anisotropic displacement ellipsoids for the non-H atoms are drawn at the 30% probability level.

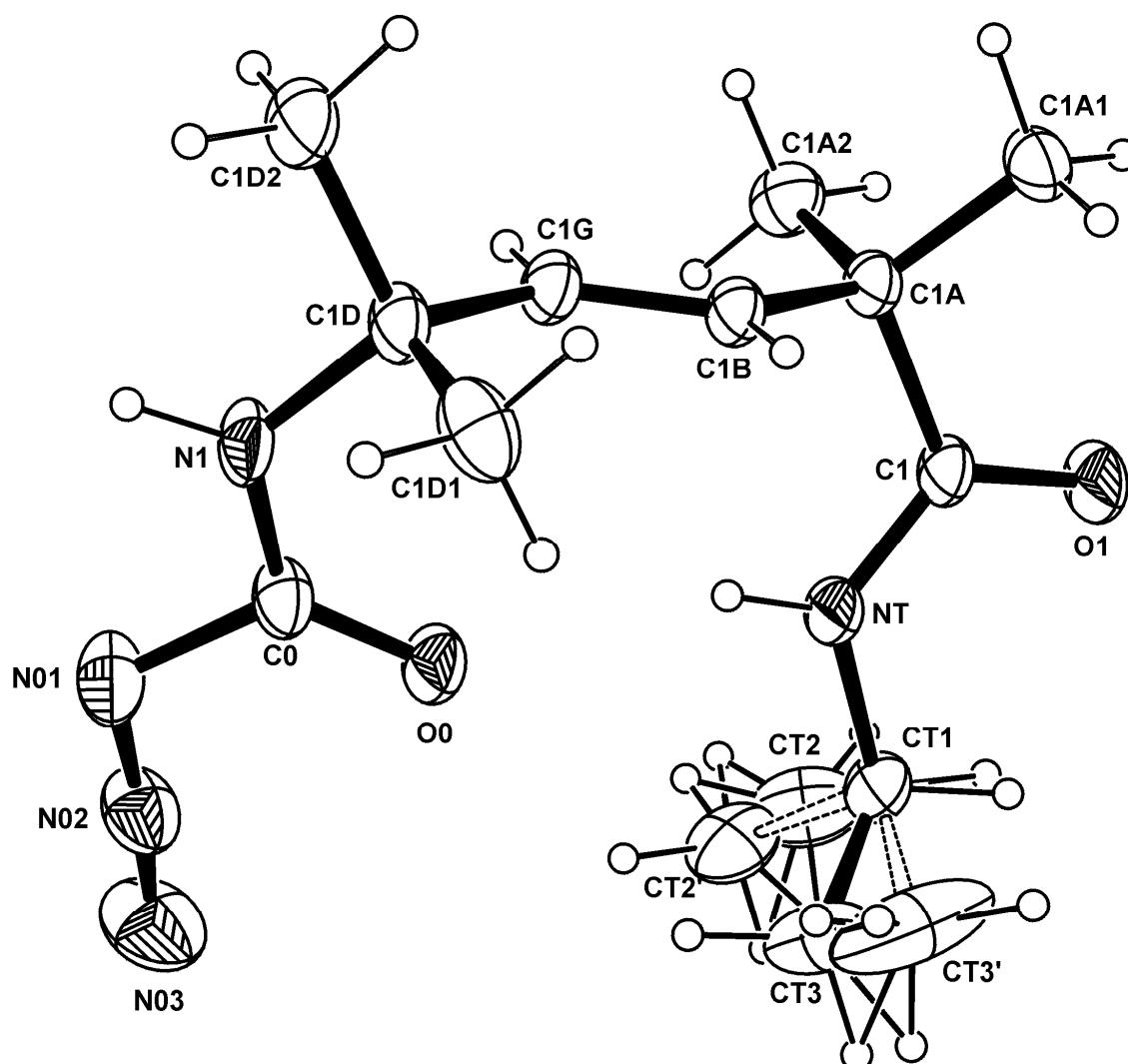


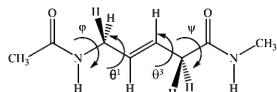
Figure S12 – ORTEP drawing of the X-Ray diffraction structure of azidocarbonyl-5-amino-2,2,5,5-tetramethyl-pent-3-(*E*)-enoyl-NH*i*Pr (**11**). Anisotropic displacement ellipsoids for the non-H atoms are drawn at the 30% probability level. The second position for the methyl groups of the disordered C-terminal isopropyl group (atoms CT2' and CT3') is highlighted by dashed bonds.

Coordinates files

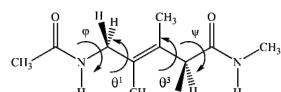
Per each studied compound several conformational minima were generated. This file contains a list of all minimal energy structures in pdb format per each studied compound (i.e. named *A*, *B*, *C*, *D* and *E*, see below).

In the first row of each coordinates set, the name of the compound and the energy ranking position in the corresponding Table *Sn* is included (being 1 the absolute minimum and the subsequent less stable conformers listed as n > 1).

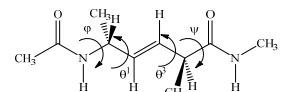
All used energy components to characterize each studied structure are included as well, as part of following rows of the header.



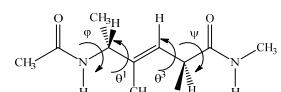
Compound A **Table S1**



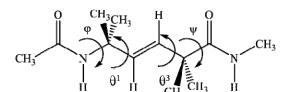
Compound B **Table S2**



Compound C **Table S3**

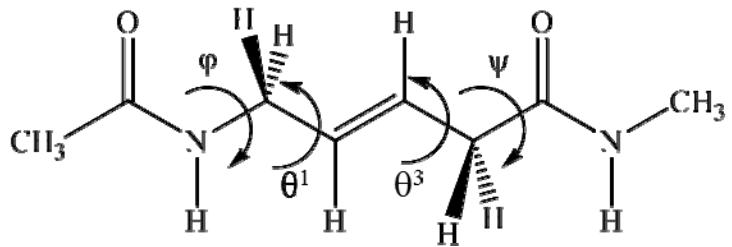


Compound D **Table S4**



Compound E **Table S5**

COMPOUND A



REMARK Compound A structure 01
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.994743
 REMARK Sum of electronic and thermal Energies= -572.980690
 REMARK Sum of electronic and thermal Enthalpies= -572.979746
 REMARK Sum of electronic and thermal Free Energies= -573.036492
 REMARK 0 Virtual frequencies used

ATOM							
ATOM	1	H	RES	1	3.247	2.569	0.520
ATOM	2	C	RES	1	2.817	1.716	1.049
ATOM	3	H	RES	1	2.038	2.109	1.706
ATOM	4	H	RES	1	3.592	1.250	1.663
ATOM	5	C	RES	1	2.189	0.784	0.048
ATOM	6	O	RES	1	1.364	1.169	-0.779
ATOM	7	N	RES	1	2.581	-0.520	0.117
ATOM	8	H	RES	1	3.214	-0.808	0.846
ATOM	9	C	RES	1	2.025	-1.520	-0.774
ATOM	10	H	RES	1	2.655	-2.415	-0.712
ATOM	11	H	RES	1	2.121	-1.147	-1.802
ATOM	12	C	RES	1	0.582	-1.843	-0.528
ATOM	13	H	RES	1	0.109	-2.451	-1.301
ATOM	14	C	RES	1	-0.157	-1.380	0.482
ATOM	15	H	RES	1	0.324	-0.753	1.236
ATOM	16	C	RES	1	-1.635	-1.515	0.585
ATOM	17	H	RES	1	-2.009	-2.283	-0.101
ATOM	18	H	RES	1	-1.956	-1.818	1.588
ATOM	19	C	RES	1	-2.411	-0.230	0.271
ATOM	20	O	RES	1	-3.602	-0.125	0.549
ATOM	21	N	RES	1	-1.699	0.757	-0.329
ATOM	22	H	RES	1	-0.726	0.613	-0.574
ATOM	23	C	RES	1	-2.317	2.008	-0.697
ATOM	24	H	RES	1	-2.848	1.939	-1.653
ATOM	25	H	RES	1	-3.044	2.292	0.067
ATOM	26	H	RES	1	-1.546	2.777	-0.778
TER							

REMARK Compound A structure 02
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.994614
 REMARK Sum of electronic and thermal Energies= -572.980617
 REMARK Sum of electronic and thermal Enthalpies= -572.979673
 REMARK Sum of electronic and thermal Free Energies= -573.036310
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	3.577	2.403	0.223
ATOM	2	C	RES	1	3.205	1.745	-0.564
ATOM	3	H	RES	1	4.055	1.347	-1.123
ATOM	4	H	RES	1	2.600	2.360	-1.234
ATOM	5	C	RES	1	2.329	0.688	0.055
ATOM	6	O	RES	1	1.350	0.974	0.744
ATOM	7	N	RES	1	2.689	-0.602	-0.188
ATOM	8	H	RES	1	3.488	-0.786	-0.773
ATOM	9	C	RES	1	1.912	-1.729	0.324
ATOM	10	H	RES	1	1.816	-1.625	1.411
ATOM	11	H	RES	1	2.502	-2.631	0.129
ATOM	12	C	RES	1	0.553	-1.802	-0.295
ATOM	13	H	RES	1	0.512	-1.915	-1.381
ATOM	14	C	RES	1	-0.576	-1.651	0.403
ATOM	15	H	RES	1	-0.492	-1.501	1.482
ATOM	16	C	RES	1	-1.937	-1.525	-0.182
ATOM	17	H	RES	1	-1.944	-1.848	-1.230
ATOM	18	H	RES	1	-2.668	-2.155	0.336
ATOM	19	C	RES	1	-2.517	-0.107	-0.156
ATOM	20	O	RES	1	-3.696	0.096	-0.430
ATOM	21	N	RES	1	-1.651	0.883	0.174
ATOM	22	H	RES	1	-0.672	0.684	0.352
ATOM	23	C	RES	1	-2.082	2.261	0.206
ATOM	24	H	RES	1	-2.142	2.696	-0.799
ATOM	25	H	RES	1	-3.077	2.325	0.652
ATOM	26	H	RES	1	-1.374	2.841	0.800

TER

REMARK Compound A structure 03
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.990026
 REMARK Sum of electronic and thermal Energies= -572.975651
 REMARK Sum of electronic and thermal Enthalpies= -572.974707
 REMARK Sum of electronic and thermal Free Energies= -573.034083
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.311	-0.568	-1.410
ATOM	2	C	RES	1	5.039	-0.602	-0.353
ATOM	3	H	RES	1	5.884	-0.196	0.207
ATOM	4	H	RES	1	4.890	-1.645	-0.060
ATOM	5	C	RES	1	3.835	0.276	-0.128
ATOM	6	O	RES	1	3.836	1.470	-0.406
ATOM	7	N	RES	1	2.745	-0.354	0.410
ATOM	8	H	RES	1	2.793	-1.343	0.602
ATOM	9	C	RES	1	1.497	0.337	0.678
ATOM	10	H	RES	1	1.670	1.370	0.354
ATOM	11	H	RES	1	1.296	0.360	1.758
ATOM	12	C	RES	1	0.347	-0.278	-0.048
ATOM	13	H	RES	1	0.449	-0.350	-1.133
ATOM	14	C	RES	1	-0.761	-0.743	0.543
ATOM	15	H	RES	1	-0.840	-0.671	1.630
ATOM	16	C	RES	1	-1.927	-1.340	-0.171
ATOM	17	H	RES	1	-1.677	-1.517	-1.224
ATOM	18	H	RES	1	-2.192	-2.315	0.250
ATOM	19	C	RES	1	-3.220	-0.524	-0.159
ATOM	20	O	RES	1	-4.312	-1.056	-0.310
ATOM	21	N	RES	1	-3.055	0.819	-0.001
ATOM	22	H	RES	1	-2.114	1.176	0.078
ATOM	23	C	RES	1	-4.161	1.744	-0.037
ATOM	24	H	RES	1	-4.121	2.388	-0.921
ATOM	25	H	RES	1	-5.079	1.157	-0.074
ATOM	26	H	RES	1	-4.177	2.375	0.857

TER

REMARK Compound A structure 04
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.988756
 REMARK Sum of electronic and thermal Energies= -572.974281
 REMARK Sum of electronic and thermal Enthalpies= -572.973337
 REMARK Sum of electronic and thermal Free Energies= -573.033943
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.193	0.609	1.612
ATOM	2	C	RES	1	-5.064	-0.115	0.805
ATOM	3	H	RES	1	-5.973	-0.083	0.200
ATOM	4	H	RES	1	-4.965	-1.114	1.236
ATOM	5	C	RES	1	-3.895	0.305	-0.050
ATOM	6	O	RES	1	-3.845	1.404	-0.592
ATOM	7	N	RES	1	-2.910	-0.632	-0.196
ATOM	8	H	RES	1	-2.942	-1.464	0.372
ATOM	9	C	RES	1	-1.683	-0.349	-0.925
ATOM	10	H	RES	1	-1.930	0.477	-1.599
ATOM	11	H	RES	1	-1.416	-1.218	-1.537
ATOM	12	C	RES	1	-0.551	0.024	-0.023
ATOM	13	H	RES	1	-0.712	0.909	0.596
ATOM	14	C	RES	1	0.597	-0.653	0.059
ATOM	15	H	RES	1	0.757	-1.533	-0.565
ATOM	16	C	RES	1	1.742	-0.287	0.946
ATOM	17	H	RES	1	1.561	0.678	1.434
ATOM	18	H	RES	1	1.845	-1.033	1.746
ATOM	19	C	RES	1	3.062	-0.312	0.191
ATOM	20	O	RES	1	3.385	-1.265	-0.508
ATOM	21	N	RES	1	3.853	0.784	0.371
ATOM	22	H	RES	1	3.503	1.544	0.932
ATOM	23	C	RES	1	5.144	0.923	-0.262
ATOM	24	H	RES	1	5.338	0.003	-0.813
ATOM	25	H	RES	1	5.157	1.763	-0.964
ATOM	26	H	RES	1	5.936	1.068	0.479

TER

REMARK Compound A structure 05
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.988527
 REMARK Sum of electronic and thermal Energies= -572.974228
 REMARK Sum of electronic and thermal Enthalpies= -572.973284
 REMARK Sum of electronic and thermal Free Energies= -573.032592
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.161	1.582	-0.016
ATOM	2	C	RES	1	-4.122	1.630	-0.348
ATOM	3	H	RES	1	-3.613	2.428	0.199
ATOM	4	H	RES	1	-4.140	1.885	-1.410
ATOM	5	C	RES	1	-3.492	0.271	-0.180
ATOM	6	O	RES	1	-3.945	-0.732	-0.718
ATOM	7	N	RES	1	-2.385	0.234	0.626
ATOM	8	H	RES	1	-2.009	1.100	0.980
ATOM	9	C	RES	1	-1.635	-0.991	0.849
ATOM	10	H	RES	1	-2.327	-1.805	0.603
ATOM	11	H	RES	1	-1.380	-1.076	1.911
ATOM	12	C	RES	1	-0.407	-1.084	0.003
ATOM	13	H	RES	1	-0.569	-1.017	-1.076
ATOM	14	C	RES	1	0.831	-1.263	0.478
ATOM	15	H	RES	1	0.969	-1.328	1.561
ATOM	16	C	RES	1	2.062	-1.388	-0.357
ATOM	17	H	RES	1	2.614	-2.301	-0.111
ATOM	18	H	RES	1	1.794	-1.470	-1.417
ATOM	19	C	RES	1	3.075	-0.250	-0.245
ATOM	20	O	RES	1	4.262	-0.417	-0.493
ATOM	21	N	RES	1	2.547	0.955	0.115
ATOM	22	H	RES	1	1.550	1.006	0.266
ATOM	23	C	RES	1	3.341	2.156	0.195
ATOM	24	H	RES	1	4.379	1.875	0.017
ATOM	25	H	RES	1	3.041	2.889	-0.561
ATOM	26	H	RES	1	3.262	2.619	1.184

TER

REMARK Compound A structure 06
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.988426
 REMARK Sum of electronic and thermal Energies= -572.974151
 REMARK Sum of electronic and thermal Enthalpies= -572.973206
 REMARK Sum of electronic and thermal Free Energies= -573.032239
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.342	1.606	0.535
ATOM	2	C	RES	1	-4.300	1.756	0.245
ATOM	3	H	RES	1	-3.790	2.306	1.040
ATOM	4	H	RES	1	-4.307	2.367	-0.661
ATOM	5	C	RES	1	-3.683	0.417	-0.069
ATOM	6	O	RES	1	-4.141	-0.326	-0.931
ATOM	7	N	RES	1	-2.593	0.082	0.685
ATOM	8	H	RES	1	-2.190	0.776	1.297
ATOM	9	C	RES	1	-1.843	-1.142	0.455
ATOM	10	H	RES	1	-2.531	-1.810	-0.073
ATOM	11	H	RES	1	-1.594	-1.602	1.418
ATOM	12	C	RES	1	-0.604	-0.910	-0.349
ATOM	13	H	RES	1	-0.758	-0.485	-1.343
ATOM	14	C	RES	1	0.630	-1.185	0.079
ATOM	15	H	RES	1	0.780	-1.594	1.079
ATOM	16	C	RES	1	1.873	-0.971	-0.718
ATOM	17	H	RES	1	2.322	-1.943	-0.970
ATOM	18	H	RES	1	1.643	-0.479	-1.670
ATOM	19	C	RES	1	2.933	-0.216	0.070
ATOM	20	O	RES	1	3.158	-0.454	1.251
ATOM	21	N	RES	1	3.622	0.720	-0.646
ATOM	22	H	RES	1	3.370	0.874	-1.609
ATOM	23	C	RES	1	4.689	1.504	-0.071
ATOM	24	H	RES	1	4.451	2.572	-0.080
ATOM	25	H	RES	1	4.810	1.180	0.963
ATOM	26	H	RES	1	5.632	1.348	-0.605

TER

REMARK Compound A structure 07
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.987842
 REMARK Sum of electronic and thermal Energies= -572.973553
 REMARK Sum of electronic and thermal Enthalpies= -572.972609
 REMARK Sum of electronic and thermal Free Energies= -573.031235
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.538	-0.491	0.557
ATOM	2	C	RES	1	-4.773	-0.657	-0.203
ATOM	3	H	RES	1	-5.106	-0.210	-1.143
ATOM	4	H	RES	1	-4.686	-1.737	-0.338
ATOM	5	C	RES	1	-3.457	-0.119	0.299
ATOM	6	O	RES	1	-2.967	-0.468	1.365
ATOM	7	N	RES	1	-2.853	0.806	-0.511
ATOM	8	H	RES	1	-3.249	1.000	-1.417
ATOM	9	C	RES	1	-1.533	1.330	-0.190
ATOM	10	H	RES	1	-1.478	1.402	0.900
ATOM	11	H	RES	1	-1.466	2.344	-0.600
ATOM	12	C	RES	1	-0.422	0.464	-0.702
ATOM	13	H	RES	1	-0.314	0.393	-1.788
ATOM	14	C	RES	1	0.393	-0.248	0.082
ATOM	15	H	RES	1	0.252	-0.189	1.164
ATOM	16	C	RES	1	1.488	-1.135	-0.407
ATOM	17	H	RES	1	1.396	-2.140	0.018
ATOM	18	H	RES	1	1.421	-1.259	-1.495
ATOM	19	C	RES	1	2.918	-0.691	-0.109
ATOM	20	O	RES	1	3.855	-1.479	-0.154
ATOM	21	N	RES	1	3.067	0.634	0.174
ATOM	22	H	RES	1	2.244	1.218	0.158
ATOM	23	C	RES	1	4.356	1.231	0.427
ATOM	24	H	RES	1	4.625	1.954	-0.350
ATOM	25	H	RES	1	4.376	1.734	1.398
ATOM	26	H	RES	1	5.094	0.428	0.427

TER

REMARK Compound A structure 08
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.986046
 REMARK Sum of electronic and thermal Energies= -572.971526
 REMARK Sum of electronic and thermal Enthalpies= -572.970582
 REMARK Sum of electronic and thermal Free Energies= -573.030504
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.216	1.352	-0.436
ATOM	2	C	RES	1	4.602	0.523	-0.794
ATOM	3	H	RES	1	5.177	-0.404	-0.719
ATOM	4	H	RES	1	4.387	0.716	-1.847
ATOM	5	C	RES	1	3.306	0.503	-0.024
ATOM	6	O	RES	1	2.603	1.499	0.103
ATOM	7	N	RES	1	2.971	-0.699	0.535
ATOM	8	H	RES	1	3.529	-1.511	0.323
ATOM	9	C	RES	1	1.684	-0.879	1.198
ATOM	10	H	RES	1	1.483	0.043	1.751
ATOM	11	H	RES	1	1.795	-1.689	1.926
ATOM	12	C	RES	1	0.566	-1.154	0.241
ATOM	13	H	RES	1	0.529	-2.146	-0.215
ATOM	14	C	RES	1	-0.344	-0.239	-0.103
ATOM	15	H	RES	1	-0.267	0.751	0.350
ATOM	16	C	RES	1	-1.459	-0.468	-1.071
ATOM	17	H	RES	1	-1.384	0.252	-1.899
ATOM	18	H	RES	1	-1.401	-1.472	-1.498
ATOM	19	C	RES	1	-2.839	-0.335	-0.435
ATOM	20	O	RES	1	-3.599	-1.286	-0.306
ATOM	21	N	RES	1	-3.149	0.929	-0.019
ATOM	22	H	RES	1	-2.468	1.661	-0.150
ATOM	23	C	RES	1	-4.388	1.247	0.648
ATOM	24	H	RES	1	-4.948	2.015	0.105
ATOM	25	H	RES	1	-4.983	0.334	0.681
ATOM	26	H	RES	1	-4.217	1.595	1.672

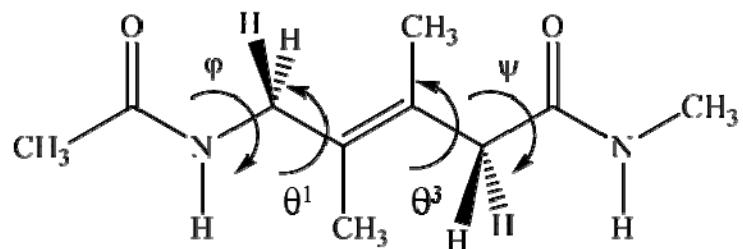
TER

REMARK Compound A structure 09
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -572.985956
 REMARK Sum of electronic and thermal Energies= -572.971669
 REMARK Sum of electronic and thermal Enthalpies= -572.970725
 REMARK Sum of electronic and thermal Free Energies= -573.029642
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.569	-0.393	1.203
ATOM	2	C	RES	1	-5.146	-0.654	0.231
ATOM	3	H	RES	1	-5.923	-0.471	-0.514
ATOM	4	H	RES	1	-4.898	-1.719	0.227
ATOM	5	C	RES	1	-3.972	0.251	-0.049
ATOM	6	O	RES	1	-4.073	1.472	-0.039
ATOM	7	N	RES	1	-2.793	-0.390	-0.316
ATOM	8	H	RES	1	-2.769	-1.398	-0.315
ATOM	9	C	RES	1	-1.561	0.324	-0.603
ATOM	10	H	RES	1	-1.780	1.376	-0.388
ATOM	11	H	RES	1	-1.314	0.258	-1.672
ATOM	12	C	RES	1	-0.423	-0.175	0.221
ATOM	13	H	RES	1	-0.557	-0.139	1.304
ATOM	14	C	RES	1	0.723	-0.640	-0.284
ATOM	15	H	RES	1	0.851	-0.660	-1.369
ATOM	16	C	RES	1	1.892	-1.083	0.538
ATOM	17	H	RES	1	1.600	-1.173	1.587
ATOM	18	H	RES	1	2.246	-2.066	0.200
ATOM	19	C	RES	1	3.025	-0.063	0.478
ATOM	20	O	RES	1	3.039	0.934	1.187
ATOM	21	N	RES	1	3.989	-0.333	-0.452
ATOM	22	H	RES	1	3.927	-1.189	-0.979
ATOM	23	C	RES	1	5.111	0.546	-0.682
ATOM	24	H	RES	1	6.059	0.069	-0.414
ATOM	25	H	RES	1	5.158	0.864	-1.728
ATOM	26	H	RES	1	4.969	1.424	-0.051

TER

COMPOUND B



REMARK Compound B structure 01
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.566852
 REMARK Sum of electronic and thermal Energies= -651.549664
 REMARK Sum of electronic and thermal Enthalpies= -651.548720
 REMARK Sum of electronic and thermal Free Energies= -651.612528
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	2.859	2.528	-1.042
ATOM	2	C	RES	1	3.356	1.899	-0.299
ATOM	3	H	RES	1	3.635	2.549	0.532
ATOM	4	H	RES	1	4.262	1.481	-0.744
ATOM	5	C	RES	1	2.380	0.862	0.192
ATOM	6	O	RES	1	1.350	1.171	0.793
ATOM	7	N	RES	1	2.701	-0.431	-0.071
ATOM	8	H	RES	1	3.543	-0.630	-0.586
ATOM	9	C	RES	1	1.821	-1.538	0.308
ATOM	10	H	RES	1	1.722	-1.548	1.397
ATOM	11	H	RES	1	2.347	-2.456	0.020
ATOM	12	C	RES	1	0.477	-1.463	-0.367
ATOM	13	C	RES	1	0.546	-1.310	-1.857
ATOM	14	H	RES	1	1.380	-1.886	-2.276
ATOM	15	H	RES	1	0.717	-0.263	-2.144
ATOM	16	H	RES	1	-0.364	-1.632	-2.365
ATOM	17	C	RES	1	-0.667	-1.457	0.347
ATOM	18	C	RES	1	-0.679	-1.507	1.855
ATOM	19	H	RES	1	-1.691	-1.358	2.240
ATOM	20	H	RES	1	-0.049	-0.721	2.288
ATOM	21	H	RES	1	-0.324	-2.466	2.248
ATOM	22	C	RES	1	-2.010	-1.243	-0.283
ATOM	23	H	RES	1	-2.041	-1.547	-1.334
ATOM	24	H	RES	1	-2.782	-1.835	0.220
ATOM	25	C	RES	1	-2.513	0.205	-0.248
ATOM	26	O	RES	1	-3.682	0.476	-0.509
ATOM	27	N	RES	1	-1.592	1.149	0.063
ATOM	28	H	RES	1	-0.636	0.894	0.287
ATOM	29	C	RES	1	-1.962	2.544	0.124
ATOM	30	H	RES	1	-2.332	2.897	-0.844
ATOM	31	H	RES	1	-2.759	2.707	0.856
ATOM	32	H	RES	1	-1.086	3.125	0.410

TER

REMARK Compound B structure 02
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.565562
 REMARK Sum of electronic and thermal Energies= -651.548817
 REMARK Sum of electronic and thermal Enthalpies= -651.547873
 REMARK Sum of electronic and thermal Free Energies= -651.609718
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	1.472	2.649	-1.228
ATOM	2	C	RES	1	2.397	2.255	-0.794
ATOM	3	H	RES	1	2.817	3.042	-0.167
ATOM	4	H	RES	1	3.093	2.031	-1.606
ATOM	5	C	RES	1	2.050	1.066	0.063
ATOM	6	O	RES	1	1.410	1.180	1.109
ATOM	7	N	RES	1	2.453	-0.144	-0.403
ATOM	8	H	RES	1	2.925	-0.189	-1.292
ATOM	9	C	RES	1	2.062	-1.393	0.248
ATOM	10	H	RES	1	2.587	-1.464	1.209
ATOM	11	H	RES	1	2.446	-2.204	-0.381
ATOM	12	C	RES	1	0.571	-1.530	0.490
ATOM	13	C	RES	1	0.208	-1.706	1.931
ATOM	14	H	RES	1	0.504	-0.817	2.502
ATOM	15	H	RES	1	0.750	-2.554	2.368
ATOM	16	H	RES	1	-0.857	-1.876	2.099
ATOM	17	C	RES	1	-0.315	-1.434	-0.524
ATOM	18	C	RES	1	0.104	-1.248	-1.954
ATOM	19	H	RES	1	1.131	-1.567	-2.148
ATOM	20	H	RES	1	0.021	-0.197	-2.264
ATOM	21	H	RES	1	-0.551	-1.817	-2.622
ATOM	22	C	RES	1	-1.801	-1.365	-0.314
ATOM	23	H	RES	1	-2.338	-1.822	-1.150
ATOM	24	H	RES	1	-2.120	-1.910	0.580
ATOM	25	C	RES	1	-2.375	0.050	-0.180
ATOM	26	O	RES	1	-3.539	0.298	-0.483
ATOM	27	N	RES	1	-1.526	0.988	0.311
ATOM	28	H	RES	1	-0.596	0.727	0.621
ATOM	29	C	RES	1	-1.976	2.335	0.569
ATOM	30	H	RES	1	-2.646	2.384	1.436
ATOM	31	H	RES	1	-1.106	2.965	0.760
ATOM	32	H	RES	1	-2.528	2.716	-0.293

TER

REMARK Compound B structure 03
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.559594
 REMARK Sum of electronic and thermal Energies= -651.542202
 REMARK Sum of electronic and thermal Enthalpies= -651.541258
 REMARK Sum of electronic and thermal Free Energies= -651.608228
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.830	0.042	-0.003
ATOM	2	C	RES	1	-4.955	0.048	0.651
ATOM	3	H	RES	1	-5.133	-0.699	1.427
ATOM	4	H	RES	1	-4.874	1.033	1.119
ATOM	5	C	RES	1	-3.743	-0.353	-0.151
ATOM	6	O	RES	1	-3.672	-1.434	-0.727
ATOM	7	N	RES	1	-2.739	0.574	-0.197
ATOM	8	H	RES	1	-2.824	1.412	0.357
ATOM	9	C	RES	1	-1.487	0.348	-0.906
ATOM	10	H	RES	1	-1.305	1.184	-1.584
ATOM	11	H	RES	1	-1.665	-0.541	-1.521
ATOM	12	C	RES	1	-0.333	0.102	0.033
ATOM	13	C	RES	1	-0.432	-1.232	0.714
ATOM	14	H	RES	1	-0.161	-2.043	0.025
ATOM	15	H	RES	1	-1.466	-1.437	1.013
ATOM	16	H	RES	1	0.191	-1.325	1.606
ATOM	17	C	RES	1	0.671	0.987	0.217
ATOM	18	C	RES	1	0.795	2.315	-0.468
ATOM	19	H	RES	1	0.798	3.123	0.274
ATOM	20	H	RES	1	0.005	2.527	-1.189
ATOM	21	H	RES	1	1.759	2.383	-0.985
ATOM	22	C	RES	1	1.847	0.699	1.123
ATOM	23	H	RES	1	2.170	1.623	1.614
ATOM	24	H	RES	1	1.598	-0.023	1.905
ATOM	25	C	RES	1	3.029	0.211	0.296
ATOM	26	O	RES	1	3.776	0.980	-0.298
ATOM	27	N	RES	1	3.160	-1.147	0.240
ATOM	28	H	RES	1	2.468	-1.714	0.705
ATOM	29	C	RES	1	4.149	-1.798	-0.585
ATOM	30	H	RES	1	4.819	-1.025	-0.964
ATOM	31	H	RES	1	4.730	-2.521	-0.007
ATOM	32	H	RES	1	3.692	-2.312	-1.437

TER

REMARK Compound B structure 04
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.560502
 REMARK Sum of electronic and thermal Energies= -651.543359
 REMARK Sum of electronic and thermal Enthalpies= -651.542414
 REMARK Sum of electronic and thermal Free Energies= -651.607198
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.850	1.610	-0.911
ATOM	2	C	RES	1	-3.801	1.754	-0.645
ATOM	3	H	RES	1	-3.768	2.554	0.098
ATOM	4	H	RES	1	-3.253	2.074	-1.536
ATOM	5	C	RES	1	-3.277	0.484	-0.024
ATOM	6	O	RES	1	-3.757	0.012	1.000
ATOM	7	N	RES	1	-2.234	-0.105	-0.686
ATOM	8	H	RES	1	-1.864	0.338	-1.513
ATOM	9	C	RES	1	-1.620	-1.350	-0.239
ATOM	10	H	RES	1	-1.572	-2.046	-1.080
ATOM	11	H	RES	1	-2.318	-1.768	0.493
ATOM	12	C	RES	1	-0.275	-1.130	0.406
ATOM	13	C	RES	1	-0.383	-0.591	1.802
ATOM	14	H	RES	1	-0.846	-1.326	2.472
ATOM	15	H	RES	1	-1.050	0.279	1.825
ATOM	16	H	RES	1	0.572	-0.288	2.236
ATOM	17	C	RES	1	0.894	-1.359	-0.233
ATOM	18	C	RES	1	1.010	-1.814	-1.658
ATOM	19	H	RES	1	1.680	-1.144	-2.212
ATOM	20	H	RES	1	0.062	-1.850	-2.199
ATOM	21	H	RES	1	1.466	-2.809	-1.718
ATOM	22	C	RES	1	2.234	-1.131	0.415
ATOM	23	H	RES	1	2.195	-1.277	1.500
ATOM	24	H	RES	1	2.963	-1.860	0.047
ATOM	25	C	RES	1	2.881	0.236	0.192
ATOM	26	O	RES	1	4.092	0.395	0.292
ATOM	27	N	RES	1	2.015	1.251	-0.091
ATOM	28	H	RES	1	1.029	1.033	-0.122
ATOM	29	C	RES	1	2.449	2.617	-0.250
ATOM	30	H	RES	1	2.076	3.256	0.557
ATOM	31	H	RES	1	3.540	2.621	-0.223
ATOM	32	H	RES	1	2.116	3.030	-1.207

TER

REMARK Compound B structure 05
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.560446
 REMARK Sum of electronic and thermal Energies= -651.543158
 REMARK Sum of electronic and thermal Enthalpies= -651.542213
 REMARK Sum of electronic and thermal Free Energies= -651.607388
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.585	-0.413	0.116
ATOM	2	C	RES	1	-4.760	-0.012	0.708
ATOM	3	H	RES	1	-4.708	-0.605	1.625
ATOM	4	H	RES	1	-4.985	1.024	0.973
ATOM	5	C	RES	1	-3.474	-0.185	-0.060
ATOM	6	O	RES	1	-3.111	-1.271	-0.497
ATOM	7	N	RES	1	-2.740	0.953	-0.248
ATOM	8	H	RES	1	-3.057	1.818	0.159
ATOM	9	C	RES	1	-1.445	0.911	-0.918
ATOM	10	H	RES	1	-1.289	1.896	-1.376
ATOM	11	H	RES	1	-1.531	0.184	-1.726
ATOM	12	C	RES	1	-0.305	0.594	0.018
ATOM	13	C	RES	1	0.001	1.719	0.964
ATOM	14	H	RES	1	-0.886	1.989	1.553
ATOM	15	H	RES	1	0.291	2.624	0.414
ATOM	16	H	RES	1	0.804	1.500	1.668
ATOM	17	C	RES	1	0.360	-0.583	0.011
ATOM	18	C	RES	1	0.081	-1.720	-0.924
ATOM	19	H	RES	1	-0.722	-1.536	-1.636
ATOM	20	H	RES	1	-0.211	-2.607	-0.351
ATOM	21	H	RES	1	0.991	-1.995	-1.474
ATOM	22	C	RES	1	1.495	-0.866	0.963
ATOM	23	H	RES	1	1.330	-0.420	1.948
ATOM	24	H	RES	1	1.568	-1.943	1.147
ATOM	25	C	RES	1	2.900	-0.436	0.542
ATOM	26	O	RES	1	3.888	-0.818	1.159
ATOM	27	N	RES	1	2.968	0.397	-0.534
ATOM	28	H	RES	1	2.100	0.676	-0.968
ATOM	29	C	RES	1	4.218	0.908	-1.039
ATOM	30	H	RES	1	4.304	1.990	-0.892
ATOM	31	H	RES	1	5.021	0.416	-0.488
ATOM	32	H	RES	1	4.332	0.689	-2.105

TER

REMARK Compound B structure 06
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.560747
 REMARK Sum of electronic and thermal Energies= -651.543715
 REMARK Sum of electronic and thermal Enthalpies= -651.542771
 REMARK Sum of electronic and thermal Free Energies= -651.606743
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.988	-0.624	1.619
ATOM	2	C	RES	1	-4.916	0.008	0.731
ATOM	3	H	RES	1	-4.917	1.055	1.042
ATOM	4	H	RES	1	-5.809	-0.183	0.132
ATOM	5	C	RES	1	-3.700	-0.397	-0.061
ATOM	6	O	RES	1	-3.564	-1.528	-0.515
ATOM	7	N	RES	1	-2.766	0.586	-0.241
ATOM	8	H	RES	1	-2.898	1.474	0.219
ATOM	9	C	RES	1	-1.510	0.356	-0.941
ATOM	10	H	RES	1	-1.380	1.131	-1.700
ATOM	11	H	RES	1	-1.650	-0.598	-1.462
ATOM	12	C	RES	1	-0.345	0.266	0.008
ATOM	13	C	RES	1	-0.517	-0.796	1.064
ATOM	14	H	RES	1	-1.228	-1.558	0.730
ATOM	15	H	RES	1	-0.916	-0.385	2.000
ATOM	16	H	RES	1	0.422	-1.299	1.312
ATOM	17	C	RES	1	0.748	1.059	-0.056
ATOM	18	C	RES	1	0.999	2.110	-1.097
ATOM	19	H	RES	1	0.224	2.187	-1.860
ATOM	20	H	RES	1	1.948	1.915	-1.614
ATOM	21	H	RES	1	1.112	3.096	-0.631
ATOM	22	C	RES	1	1.871	0.931	0.938
ATOM	23	H	RES	1	2.295	1.915	1.161
ATOM	24	H	RES	1	1.521	0.537	1.898
ATOM	25	C	RES	1	3.065	0.064	0.533
ATOM	26	O	RES	1	4.153	0.184	1.084
ATOM	27	N	RES	1	2.816	-0.853	-0.442
ATOM	28	H	RES	1	1.883	-0.889	-0.829
ATOM	29	C	RES	1	3.816	-1.784	-0.906
ATOM	30	H	RES	1	3.544	-2.818	-0.670
ATOM	31	H	RES	1	3.966	-1.699	-1.986
ATOM	32	H	RES	1	4.750	-1.541	-0.397

TER

REMARK Compound B structure 07
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.559519
 REMARK Sum of electronic and thermal Energies= -651.542174
 REMARK Sum of electronic and thermal Enthalpies= -651.541230
 REMARK Sum of electronic and thermal Free Energies= -651.606709
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.152	2.564	-0.826
ATOM	2	C	RES	1	3.577	2.250	0.047
ATOM	3	H	RES	1	2.626	2.789	0.056
ATOM	4	H	RES	1	4.154	2.537	0.929
ATOM	5	C	RES	1	3.428	0.749	0.022
ATOM	6	O	RES	1	4.393	-0.009	0.003
ATOM	7	N	RES	1	2.148	0.284	0.021
ATOM	8	H	RES	1	1.363	0.920	0.041
ATOM	9	C	RES	1	1.856	-1.145	-0.014
ATOM	10	H	RES	1	2.114	-1.604	0.949
ATOM	11	H	RES	1	2.523	-1.604	-0.753
ATOM	12	C	RES	1	0.409	-1.335	-0.381
ATOM	13	C	RES	1	0.178	-1.472	-1.854
ATOM	14	H	RES	1	0.614	-0.615	-2.383
ATOM	15	H	RES	1	-0.873	-1.523	-2.141
ATOM	16	H	RES	1	0.681	-2.363	-2.249
ATOM	17	C	RES	1	-0.564	-1.232	0.544
ATOM	18	C	RES	1	-0.316	-0.967	1.998
ATOM	19	H	RES	1	-0.722	0.015	2.276
ATOM	20	H	RES	1	0.739	-0.970	2.275
ATOM	21	H	RES	1	-0.833	-1.703	2.627
ATOM	22	C	RES	1	-2.019	-1.195	0.179
ATOM	23	H	RES	1	-2.232	-1.763	-0.733
ATOM	24	H	RES	1	-2.628	-1.656	0.970
ATOM	25	C	RES	1	-2.497	0.239	-0.054
ATOM	26	O	RES	1	-1.731	1.158	-0.325
ATOM	27	N	RES	1	-3.847	0.405	0.044
ATOM	28	H	RES	1	-4.414	-0.399	0.266
ATOM	29	C	RES	1	-4.501	1.667	-0.211
ATOM	30	H	RES	1	-3.721	2.405	-0.401
ATOM	31	H	RES	1	-5.155	1.613	-1.087
ATOM	32	H	RES	1	-5.092	1.989	0.651

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REMARK Compound B structure 08
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.558345
 REMARK Sum of electronic and thermal Energies= -651.541047
 REMARK Sum of electronic and thermal Enthalpies= -651.540103
 REMARK Sum of electronic and thermal Free Energies= -651.605328
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.612	-0.671	-0.216
ATOM	2	C	RES	1	4.830	-0.042	-0.647
ATOM	3	H	RES	1	4.777	-0.284	-1.711
ATOM	4	H	RES	1	5.121	1.006	-0.539
ATOM	5	C	RES	1	3.512	-0.383	0.000
ATOM	6	O	RES	1	3.060	-1.525	0.001
ATOM	7	N	RES	1	2.861	0.656	0.599
ATOM	8	H	RES	1	3.246	1.584	0.524
ATOM	9	C	RES	1	1.541	0.480	1.196
ATOM	10	H	RES	1	1.450	1.219	2.002
ATOM	11	H	RES	1	1.535	-0.508	1.656
ATOM	12	C	RES	1	0.411	0.668	0.212
ATOM	13	C	RES	1	0.230	2.096	-0.201
ATOM	14	H	RES	1	1.183	2.536	-0.526
ATOM	15	H	RES	1	-0.124	2.698	0.646
ATOM	16	H	RES	1	-0.500	2.240	-0.997
ATOM	17	C	RES	1	-0.360	-0.351	-0.220
ATOM	18	C	RES	1	-0.214	-1.781	0.206
ATOM	19	H	RES	1	-1.084	-2.106	0.795
ATOM	20	H	RES	1	0.689	-1.982	0.780
ATOM	21	H	RES	1	-0.172	-2.433	-0.674
ATOM	22	C	RES	1	-1.514	-0.124	-1.175
ATOM	23	H	RES	1	-1.301	0.675	-1.887
ATOM	24	H	RES	1	-1.687	-1.039	-1.755
ATOM	25	C	RES	1	-2.775	0.279	-0.425
ATOM	26	O	RES	1	-2.986	1.434	-0.074
ATOM	27	N	RES	1	-3.630	-0.751	-0.146
ATOM	28	H	RES	1	-3.391	-1.675	-0.469
ATOM	29	C	RES	1	-4.844	-0.568	0.612
ATOM	30	H	RES	1	-4.922	0.494	0.848
ATOM	31	H	RES	1	-5.724	-0.869	0.036
ATOM	32	H	RES	1	-4.823	-1.137	1.547

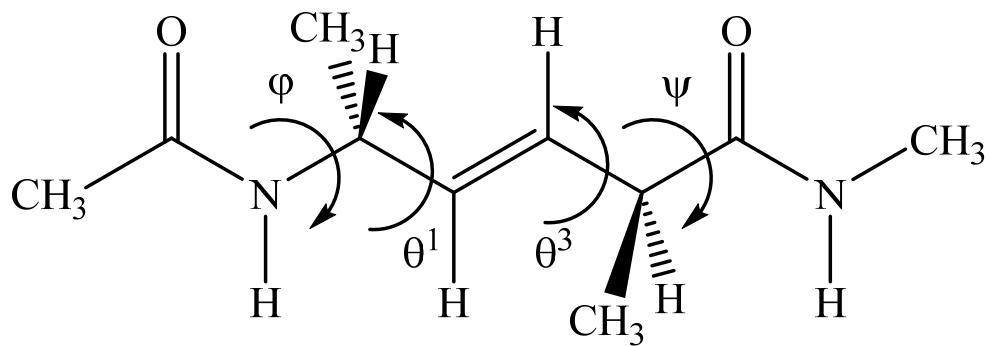
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REMARK Compound B structure 09
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.557408
 REMARK Sum of electronic and thermal Energies= -651.540157
 REMARK Sum of electronic and thermal Enthalpies= -651.539213
 REMARK Sum of electronic and thermal Free Energies= -651.605070
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.366	-0.564	1.352
ATOM	2	C	RES	1	5.072	0.283	0.728
ATOM	3	H	RES	1	5.939	0.543	0.117
ATOM	4	H	RES	1	4.829	1.131	1.373
ATOM	5	C	RES	1	3.945	-0.145	-0.179
ATOM	6	O	RES	1	4.058	-1.084	-0.959
ATOM	7	N	RES	1	2.798	0.592	-0.069
ATOM	8	H	RES	1	2.748	1.315	0.632
ATOM	9	C	RES	1	1.592	0.304	-0.833
ATOM	10	H	RES	1	1.856	-0.544	-1.475
ATOM	11	H	RES	1	1.366	1.146	-1.493
ATOM	12	C	RES	1	0.438	-0.063	0.062
ATOM	13	C	RES	1	0.605	-1.409	0.701
ATOM	14	H	RES	1	0.048	-1.527	1.633
ATOM	15	H	RES	1	1.661	-1.609	0.910
ATOM	16	H	RES	1	0.255	-2.197	0.024
ATOM	17	C	RES	1	-0.641	0.729	0.232
ATOM	18	C	RES	1	-0.861	2.053	-0.440
ATOM	19	H	RES	1	-1.726	2.008	-1.115
ATOM	20	H	RES	1	-0.012	2.406	-1.026
ATOM	21	H	RES	1	-1.094	2.829	0.301
ATOM	22	C	RES	1	-1.818	0.308	1.075
ATOM	23	H	RES	1	-1.525	-0.411	1.845
ATOM	24	H	RES	1	-2.235	1.182	1.594
ATOM	25	C	RES	1	-2.888	-0.376	0.233
ATOM	26	O	RES	1	-2.663	-1.407	-0.388
ATOM	27	N	RES	1	-4.101	0.253	0.216
ATOM	28	H	RES	1	-4.222	1.082	0.775
ATOM	29	C	RES	1	-5.234	-0.270	-0.509
ATOM	30	H	RES	1	-6.016	-0.635	0.166
ATOM	31	H	RES	1	-5.664	0.488	-1.169
ATOM	32	H	RES	1	-4.877	-1.106	-1.113

TER

COMPOUND C



REMARK Compound C structure 01
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.563040
 REMARK Sum of electronic and thermal Energies= -651.546084
 REMARK Sum of electronic and thermal Enthalpies= -651.545140
 REMARK Sum of electronic and thermal Free Energies= -651.608291
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	9.578	-7.725	-7.655
ATOM	2	C	RES	1	10.237	-6.715	-9.377
ATOM	3	H	RES	1	10.750	-7.596	-9.773
ATOM	4	H	RES	1	9.241	-6.554	-9.796
ATOM	5	H	RES	1	10.773	-5.796	-9.646
ATOM	6	H	RES	1	8.835	-2.552	-7.786
ATOM	7	C	RES	1	9.028	-3.275	-6.990
ATOM	8	H	RES	1	8.074	-3.619	-6.585
ATOM	9	H	RES	1	9.574	-2.747	-6.204
ATOM	10	C	RES	1	9.898	-4.380	-7.533
ATOM	11	O	RES	1	10.987	-4.150	-8.060
ATOM	12	N	RES	1	9.403	-5.641	-7.410
ATOM	13	H	RES	1	8.516	-5.776	-6.949
ATOM	14	C	RES	1	10.140	-6.830	-7.859
ATOM	15	C	RES	1	11.491	-6.886	-7.208
ATOM	16	H	RES	1	11.499	-6.959	-6.117
ATOM	17	C	RES	1	12.639	-6.789	-7.882
ATOM	18	H	RES	1	12.590	-6.690	-8.970
ATOM	19	C	RES	1	14.000	-6.702	-7.277
ATOM	20	H	RES	1	14.684	-7.321	-7.858
ATOM	21	C	RES	1	14.600	-5.284	-7.357
ATOM	22	O	RES	1	15.783	-5.085	-7.091
ATOM	23	N	RES	1	13.752	-4.289	-7.710
ATOM	24	H	RES	1	12.778	-4.481	-7.919
ATOM	25	C	RES	1	14.214	-2.923	-7.789
ATOM	26	H	RES	1	14.481	-2.532	-6.801
ATOM	27	H	RES	1	15.104	-2.853	-8.420
ATOM	28	H	RES	1	13.419	-2.309	-8.214
ATOM	29	C	RES	1	13.889	-7.114	-5.813
ATOM	30	H	RES	1	14.569	-7.953	-5.626
ATOM	31	H	RES	1	12.877	-7.484	-5.624
ATOM	32	H	RES	1	14.158	-6.256	-5.195

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REMARK Compound C structure 02
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.561816
 REMARK Sum of electronic and thermal Energies= -651.545003
 REMARK Sum of electronic and thermal Enthalpies= -651.544059
 REMARK Sum of electronic and thermal Free Energies= -651.606675
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	18.289	10.480	8.527
ATOM	2	C	RES	1	18.511	9.589	9.116
ATOM	3	H	RES	1	17.629	9.318	9.702
ATOM	4	H	RES	1	19.319	9.854	9.803
ATOM	5	C	RES	1	18.995	8.498	8.197
ATOM	6	O	RES	1	19.902	8.681	7.386
ATOM	7	N	RES	1	18.379	7.291	8.328
ATOM	8	H	RES	1	17.673	7.172	9.039
ATOM	9	C	RES	1	18.765	6.133	7.531
ATOM	10	H	RES	1	18.092	5.274	7.657
ATOM	11	C	RES	1	20.191	5.707	7.753
ATOM	12	H	RES	1	20.544	4.948	7.053
ATOM	13	C	RES	1	21.029	6.221	8.655
ATOM	14	H	RES	1	20.651	6.991	9.331
ATOM	15	C	RES	1	22.495	5.950	8.760
ATOM	16	H	RES	1	22.835	5.101	8.185
ATOM	17	C	RES	1	23.344	7.178	8.375
ATOM	18	O	RES	1	24.570	7.136	8.435
ATOM	19	N	RES	1	22.660	8.270	7.949
ATOM	20	H	RES	1	21.648	8.250	7.887
ATOM	21	C	RES	1	23.346	9.465	7.519
ATOM	22	H	RES	1	23.663	9.402	6.471
ATOM	23	H	RES	1	22.679	10.321	7.635
ATOM	24	H	RES	1	24.241	9.608	8.129
ATOM	26	C	RES	1	18.607	6.717	6.129
ATOM	27	H	RES	1	19.103	7.688	6.036
ATOM	28	H	RES	1	19.133	6.005	5.489
ATOM	29	H	RES	1	17.586	6.807	5.744
ATOM	30	C	RES	1	22.813	5.699	10.225
ATOM	31	H	RES	1	23.608	4.946	10.243
ATOM	32	H	RES	1	21.902	5.241	10.622
ATOM	33	H	RES	1	23.112	6.514	10.886

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REMARK Compound C structure 03
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.560331
 REMARK Sum of electronic and thermal Energies= -651.543472
 REMARK Sum of electronic and thermal Enthalpies= -651.542528
 REMARK Sum of electronic and thermal Free Energies= -651.605270
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	1.856	-2.108	2.296
ATOM	2	C	RES	1	2.693	-1.717	1.711
ATOM	3	H	RES	1	3.356	-1.159	2.377
ATOM	4	H	RES	1	3.233	-2.578	1.313
ATOM	5	C	RES	1	2.146	-0.907	0.563
ATOM	6	O	RES	1	1.433	-1.416	-0.302
ATOM	7	N	RES	1	2.481	0.413	0.564
ATOM	8	H	RES	1	3.070	0.751	1.308
ATOM	9	C	RES	1	2.072	1.366	-0.471
ATOM	10	H	RES	1	2.523	2.321	-0.166
ATOM	11	C	RES	1	2.653	0.997	-1.835
ATOM	12	H	RES	1	3.742	0.918	-1.784
ATOM	13	H	RES	1	2.401	1.767	-2.570
ATOM	14	H	RES	1	2.249	0.044	-2.181
ATOM	15	C	RES	1	0.580	1.546	-0.542
ATOM	16	H	RES	1	0.227	2.033	-1.454
ATOM	17	C	RES	1	-0.317	1.144	0.360
ATOM	18	H	RES	1	0.030	0.644	1.269
ATOM	19	C	RES	1	-1.798	1.225	0.188
ATOM	20	H	RES	1	-2.014	1.859	-0.685
ATOM	21	C	RES	1	-2.499	1.818	1.405
ATOM	22	H	RES	1	-2.268	1.240	2.307
ATOM	23	H	RES	1	-2.182	2.851	1.576
ATOM	24	H	RES	1	-3.581	1.791	1.264
ATOM	25	C	RES	1	-2.438	-0.137	-0.154
ATOM	26	O	RES	1	-3.653	-0.304	-0.077
ATOM	27	N	RES	1	-1.589	-1.110	-0.562
ATOM	28	H	RES	1	-0.590	-0.942	-0.598
ATOM	29	C	RES	1	-2.079	-2.419	-0.926
ATOM	30	H	RES	1	-2.757	-2.801	-0.158
ATOM	31	H	RES	1	-1.228	-3.094	-1.029
ATOM	32	H	RES	1	-2.633	-2.393	-1.871

REMARK Compound C structure 04
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.556939
 REMARK Sum of electronic and thermal Energies= -651.539714
 REMARK Sum of electronic and thermal Enthalpies= -651.538770
 REMARK Sum of electronic and thermal Free Energies= -651.604785
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.789	-0.112	-0.766
ATOM	2	C	RES	1	-4.853	-0.649	-0.936
ATOM	3	H	RES	1	-4.881	-1.590	-0.381
ATOM	4	H	RES	1	-4.802	-0.869	-2.004
ATOM	5	C	RES	1	-3.700	0.248	-0.564
ATOM	6	O	RES	1	-3.544	1.355	-1.069
ATOM	7	N	RES	1	-2.853	-0.249	0.389
ATOM	8	H	RES	1	-2.949	-1.214	0.671
ATOM	9	C	RES	1	-1.636	0.455	0.793
ATOM	10	H	RES	1	-1.829	1.497	0.507
ATOM	11	C	RES	1	-1.452	0.365	2.297
ATOM	12	H	RES	1	-2.334	0.754	2.811
ATOM	13	H	RES	1	-0.584	0.945	2.622
ATOM	14	H	RES	1	-1.296	-0.670	2.622
ATOM	15	C	RES	1	-0.472	-0.046	-0.017
ATOM	16	H	RES	1	-0.628	-0.010	-1.098
ATOM	17	C	RES	1	0.681	-0.530	0.458
ATOM	18	H	RES	1	0.845	-0.575	1.538
ATOM	19	C	RES	1	1.810	-1.044	-0.384
ATOM	20	H	RES	1	1.485	-1.023	-1.436
ATOM	21	C	RES	1	2.179	-2.476	-0.013
ATOM	22	H	RES	1	2.472	-2.541	1.040
ATOM	23	H	RES	1	1.331	-3.146	-0.173
ATOM	24	H	RES	1	3.028	-2.818	-0.607
ATOM	25	C	RES	1	3.062	-0.150	-0.336
ATOM	26	O	RES	1	4.193	-0.608	-0.446
ATOM	27	N	RES	1	2.808	1.182	-0.205
ATOM	28	H	RES	1	1.844	1.475	-0.140
ATOM	29	C	RES	1	3.850	2.179	-0.238
ATOM	30	H	RES	1	4.807	1.656	-0.250
ATOM	31	H	RES	1	3.808	2.823	0.646
ATOM	32	H	RES	1	3.782	2.806	-1.133

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REMARK Compound C structure 05
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.557536
 REMARK Sum of electronic and thermal Energies= -651.540350
 REMARK Sum of electronic and thermal Enthalpies= -651.539406
 REMARK Sum of electronic and thermal Free Energies= -651.604573
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.481	-0.462	-1.685
ATOM	2	C	RES	1	-5.057	-0.770	-0.727
ATOM	3	H	RES	1	-5.858	-0.700	0.013
ATOM	4	H	RES	1	-4.734	-1.811	-0.800
ATOM	5	C	RES	1	-3.956	0.188	-0.349
ATOM	6	O	RES	1	-4.139	1.398	-0.267
ATOM	7	N	RES	1	-2.735	-0.380	-0.116
ATOM	8	H	RES	1	-2.645	-1.385	-0.113
ATOM	9	C	RES	1	-1.589	0.415	0.323
ATOM	10	H	RES	1	-1.776	1.409	-0.107
ATOM	11	C	RES	1	-1.555	0.556	1.837
ATOM	12	H	RES	1	-2.496	0.985	2.189
ATOM	13	H	RES	1	-0.742	1.216	2.155
ATOM	14	H	RES	1	-1.413	-0.414	2.325
ATOM	15	C	RES	1	-0.345	-0.154	-0.289
ATOM	16	H	RES	1	-0.378	-0.269	-1.375
ATOM	17	C	RES	1	0.763	-0.526	0.363
ATOM	18	H	RES	1	0.806	-0.426	1.451
ATOM	19	C	RES	1	1.993	-1.084	-0.283
ATOM	20	H	RES	1	1.780	-1.225	-1.354
ATOM	21	C	RES	1	2.386	-2.429	0.318
ATOM	22	H	RES	1	2.566	-2.335	1.394
ATOM	23	H	RES	1	1.592	-3.165	0.170
ATOM	24	H	RES	1	3.308	-2.795	-0.136
ATOM	25	C	RES	1	3.198	-0.126	-0.248
ATOM	26	O	RES	1	4.352	-0.539	-0.260
ATOM	27	N	RES	1	2.883	1.199	-0.246
ATOM	28	H	RES	1	1.907	1.454	-0.256
ATOM	29	C	RES	1	3.887	2.234	-0.306
ATOM	30	H	RES	1	4.861	1.756	-0.198
ATOM	31	H	RES	1	3.753	2.959	0.502
ATOM	32	H	RES	1	3.862	2.767	-1.263

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REMARK Compound C structure 06
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.560267
 REMARK Sum of electronic and thermal Energies= -651.543637
 REMARK Sum of electronic and thermal Enthalpies= -651.542693
 REMARK Sum of electronic and thermal Free Energies= -651.604461
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-2.667	-9.643	-8.259
ATOM	2	C	RES	1	-2.155	-10.164	-10.231
ATOM	3	H	RES	1	-1.968	-11.210	-9.972
ATOM	4	H	RES	1	-3.145	-9.979	-10.653
ATOM	5	H	RES	1	-1.477	-9.831	-11.028
ATOM	6	H	RES	1	-2.303	-5.777	-11.730
ATOM	7	C	RES	1	-2.020	-5.865	-10.679
ATOM	8	H	RES	1	-2.850	-5.520	-10.059
ATOM	9	H	RES	1	-1.164	-5.203	-10.522
ATOM	10	C	RES	1	-1.597	-7.286	-10.403
ATOM	11	O	RES	1	-0.702	-7.834	-11.046
ATOM	12	N	RES	1	-2.269	-7.922	-9.406
ATOM	13	H	RES	1	-2.978	-7.419	-8.894
ATOM	14	C	RES	1	-1.957	-9.297	-8.991
ATOM	15	C	RES	1	-0.556	-9.379	-8.460
ATOM	16	H	RES	1	-0.350	-8.809	-7.550
ATOM	17	C	RES	1	0.425	-10.047	-9.069
ATOM	18	H	RES	1	0.187	-10.584	-9.992
ATOM	19	C	RES	1	1.861	-10.051	-8.661
ATOM	20	H	RES	1	2.431	-10.826	-9.152
ATOM	21	C	RES	1	2.549	-8.690	-8.885
ATOM	22	O	RES	1	3.697	-8.493	-8.494
ATOM	23	N	RES	1	1.815	-7.737	-9.509
ATOM	24	H	RES	1	0.867	-7.926	-9.817
ATOM	25	C	RES	1	2.364	-6.422	-9.742
ATOM	26	H	RES	1	2.522	-5.881	-8.803
ATOM	27	H	RES	1	3.331	-6.492	-10.247
ATOM	28	H	RES	1	1.669	-5.859	-10.367
ATOM	29	C	RES	1	1.966	-10.435	-7.192
ATOM	30	H	RES	1	2.922	-10.942	-7.019
ATOM	31	H	RES	1	1.127	-11.083	-6.920
ATOM	32	H	RES	1	1.974	-9.527	-6.585

TER

REMARK Compound C structure 07
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.556076
 REMARK Sum of electronic and thermal Energies= -651.538761
 REMARK Sum of electronic and thermal Enthalpies= -651.537816
 REMARK Sum of electronic and thermal Free Energies= -651.603832
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.100	2.702	-0.208
ATOM	2	C	RES	1	-3.737	1.961	-0.922
ATOM	3	H	RES	1	-4.537	1.801	-1.649
ATOM	4	H	RES	1	-2.865	2.366	-1.441
ATOM	5	C	RES	1	-3.470	0.668	-0.193
ATOM	6	O	RES	1	-4.322	0.117	0.496
ATOM	7	N	RES	1	-2.212	0.158	-0.345
ATOM	8	H	RES	1	-1.578	0.591	-1.000
ATOM	9	C	RES	1	-1.835	-1.126	0.222
ATOM	10	H	RES	1	-2.456	-1.231	1.122
ATOM	11	C	RES	1	-2.187	-2.278	-0.718
ATOM	12	H	RES	1	-3.256	-2.267	-0.941
ATOM	13	H	RES	1	-1.943	-3.242	-0.261
ATOM	14	H	RES	1	-1.631	-2.200	-1.659
ATOM	15	C	RES	1	-0.387	-1.153	0.610
ATOM	16	H	RES	1	0.001	-2.148	0.839
ATOM	17	C	RES	1	0.438	-0.106	0.694
ATOM	18	H	RES	1	0.077	0.902	0.482
ATOM	19	C	RES	1	1.883	-0.185	1.087
ATOM	20	H	RES	1	2.147	-1.239	1.253
ATOM	21	C	RES	1	2.153	0.613	2.364
ATOM	22	H	RES	1	1.907	1.666	2.204
ATOM	23	H	RES	1	1.544	0.235	3.190
ATOM	24	H	RES	1	3.206	0.556	2.655
ATOM	25	C	RES	1	2.727	0.390	-0.050
ATOM	26	O	RES	1	2.637	1.567	-0.385
ATOM	27	N	RES	1	3.569	-0.496	-0.654
ATOM	28	H	RES	1	3.565	-1.453	-0.338
ATOM	29	C	RES	1	4.418	-0.131	-1.763
ATOM	30	H	RES	1	4.293	0.939	-1.933
ATOM	31	H	RES	1	4.139	-0.667	-2.676
ATOM	32	H	RES	1	5.469	-0.335	-1.542

TER

REMARK Compound C structure 08
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.555343
 REMARK Sum of electronic and thermal Energies= -651.538026
 REMARK Sum of electronic and thermal Enthalpies= -651.537082
 REMARK Sum of electronic and thermal Free Energies= -651.602276
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-3.835	-1.835	-1.615
ATOM	2	C	RES	1	-4.156	-1.096	-0.877
ATOM	3	H	RES	1	-5.069	-0.638	-1.262
ATOM	4	H	RES	1	-4.387	-1.612	0.059
ATOM	5	C	RES	1	-3.091	-0.036	-0.748
ATOM	6	O	RES	1	-2.742	0.659	-1.696
ATOM	7	N	RES	1	-2.548	0.102	0.499
ATOM	8	H	RES	1	-2.816	-0.543	1.228
ATOM	9	C	RES	1	-1.474	1.041	0.775
ATOM	10	H	RES	1	-1.624	1.861	0.059
ATOM	11	C	RES	1	-1.606	1.582	2.193
ATOM	12	H	RES	1	-2.571	2.075	2.336
ATOM	13	H	RES	1	-0.816	2.306	2.405
ATOM	14	H	RES	1	-1.512	0.777	2.931
ATOM	15	C	RES	1	-0.103	0.469	0.531
ATOM	16	H	RES	1	0.717	1.156	0.749
ATOM	17	C	RES	1	0.167	-0.758	0.082
ATOM	18	H	RES	1	-0.662	-1.438	-0.125
ATOM	19	C	RES	1	1.538	-1.335	-0.165
ATOM	20	H	RES	1	1.544	-1.729	-1.193
ATOM	21	C	RES	1	1.833	-2.485	0.792
ATOM	22	H	RES	1	1.910	-2.109	1.815
ATOM	23	H	RES	1	1.039	-3.236	0.751
ATOM	24	H	RES	1	2.780	-2.972	0.545
ATOM	25	C	RES	1	2.612	-0.256	-0.065
ATOM	26	O	RES	1	3.270	-0.062	0.952
ATOM	27	N	RES	1	2.768	0.489	-1.199
ATOM	28	H	RES	1	2.090	0.368	-1.936
ATOM	29	C	RES	1	3.605	1.666	-1.225
ATOM	30	H	RES	1	4.354	1.560	-0.440
ATOM	31	H	RES	1	3.034	2.583	-1.033
ATOM	32	H	RES	1	4.105	1.758	-2.191

TER

REMARK Compound C structure 09
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.555571
 REMARK Sum of electronic and thermal Energies= -651.538508
 REMARK Sum of electronic and thermal Enthalpies= -651.537564
 REMARK Sum of electronic and thermal Free Energies= -651.602269
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.996	1.502	1.600
ATOM	2	C	RES	1	-4.401	0.598	1.746
ATOM	3	H	RES	1	-3.659	0.788	2.526
ATOM	4	H	RES	1	-5.084	-0.181	2.090
ATOM	5	C	RES	1	-3.806	0.181	0.425
ATOM	6	O	RES	1	-4.501	-0.129	-0.538
ATOM	7	N	RES	1	-2.442	0.162	0.372
ATOM	8	H	RES	1	-1.904	0.484	1.163
ATOM	9	C	RES	1	-1.724	-0.171	-0.859
ATOM	10	H	RES	1	-2.365	-0.911	-1.358
ATOM	11	C	RES	1	-1.604	1.038	-1.774
ATOM	12	H	RES	1	-2.599	1.434	-1.988
ATOM	13	H	RES	1	-1.135	0.767	-2.725
ATOM	14	H	RES	1	-1.007	1.831	-1.311
ATOM	15	C	RES	1	-0.429	-0.824	-0.482
ATOM	16	H	RES	1	-0.532	-1.692	0.170
ATOM	17	C	RES	1	0.788	-0.426	-0.862
ATOM	18	H	RES	1	0.883	0.452	-1.503
ATOM	19	C	RES	1	2.088	-1.065	-0.453
ATOM	20	H	RES	1	2.664	-1.259	-1.372
ATOM	21	C	RES	1	1.936	-2.362	0.322
ATOM	22	H	RES	1	1.444	-2.176	1.280
ATOM	23	H	RES	1	1.348	-3.089	-0.244
ATOM	24	H	RES	1	2.912	-2.803	0.537
ATOM	25	C	RES	1	2.868	-0.042	0.384
ATOM	26	O	RES	1	2.692	0.084	1.590
ATOM	27	N	RES	1	3.737	0.733	-0.327
ATOM	28	H	RES	1	3.853	0.547	-1.311
ATOM	29	C	RES	1	4.522	1.782	0.281
ATOM	30	H	RES	1	4.243	1.827	1.334
ATOM	31	H	RES	1	4.320	2.752	-0.184
ATOM	32	H	RES	1	5.594	1.573	0.209

TER

REMARK Compound C structure 10
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.555434
 REMARK Sum of electronic and thermal Energies= -651.538244
 REMARK Sum of electronic and thermal Enthalpies= -651.537300
 REMARK Sum of electronic and thermal Free Energies= -651.602264
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.236	1.296	-1.000
ATOM	2	C	RES	1	4.530	1.291	-0.168
ATOM	3	H	RES	1	5.029	0.896	0.721
ATOM	4	H	RES	1	4.252	2.331	0.021
ATOM	5	C	RES	1	3.298	0.521	-0.571
ATOM	6	O	RES	1	2.693	0.751	-1.613
ATOM	7	N	RES	1	2.905	-0.461	0.297
ATOM	8	H	RES	1	3.373	-0.546	1.187
ATOM	9	C	RES	1	1.653	-1.193	0.100
ATOM	10	H	RES	1	1.544	-1.291	-0.985
ATOM	11	C	RES	1	1.763	-2.563	0.747
ATOM	12	H	RES	1	2.611	-3.123	0.344
ATOM	13	H	RES	1	0.854	-3.145	0.576
ATOM	14	H	RES	1	1.894	-2.479	1.833
ATOM	15	C	RES	1	0.487	-0.404	0.629
ATOM	16	H	RES	1	0.394	-0.363	1.718
ATOM	17	C	RES	1	-0.374	0.264	-0.146
ATOM	18	H	RES	1	-0.222	0.221	-1.226
ATOM	19	C	RES	1	-1.529	1.097	0.321
ATOM	20	H	RES	1	-1.427	2.093	-0.131
ATOM	21	C	RES	1	-1.611	1.272	1.836
ATOM	22	H	RES	1	-1.750	0.309	2.341
ATOM	23	H	RES	1	-0.697	1.728	2.227
ATOM	24	H	RES	1	-2.457	1.912	2.094
ATOM	25	C	RES	1	-2.895	0.608	-0.178
ATOM	26	O	RES	1	-3.858	1.364	-0.239
ATOM	27	N	RES	1	-2.967	-0.717	-0.487
ATOM	28	H	RES	1	-2.127	-1.271	-0.399
ATOM	29	C	RES	1	-4.190	-1.350	-0.917
ATOM	30	H	RES	1	-4.961	-0.579	-0.954
ATOM	31	H	RES	1	-4.505	-2.131	-0.218
ATOM	32	H	RES	1	-4.083	-1.791	-1.913

TER

REMARK Compound C structure 11
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.555700
 REMARK Sum of electronic and thermal Energies= -651.538720
 REMARK Sum of electronic and thermal Enthalpies= -651.537776
 REMARK Sum of electronic and thermal Free Energies= -651.602088
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.019	-0.827	-2.006
ATOM	2	C	RES	1	-4.392	-1.319	-1.259
ATOM	3	H	RES	1	-5.050	-1.953	-0.659
ATOM	4	H	RES	1	-3.663	-1.952	-1.770
ATOM	5	C	RES	1	-3.776	-0.269	-0.369
ATOM	6	O	RES	1	-4.449	0.559	0.234
ATOM	7	N	RES	1	-2.411	-0.295	-0.285
ATOM	8	H	RES	1	-1.901	-1.040	-0.734
ATOM	9	C	RES	1	-1.680	0.621	0.591
ATOM	10	H	RES	1	-2.283	1.540	0.583
ATOM	11	C	RES	1	-1.634	0.104	2.021
ATOM	12	H	RES	1	-2.650	-0.081	2.375
ATOM	13	H	RES	1	-1.170	0.834	2.691
ATOM	14	H	RES	1	-1.067	-0.831	2.090
ATOM	15	C	RES	1	-0.347	0.918	-0.027
ATOM	16	H	RES	1	-0.392	1.239	-1.069
ATOM	17	C	RES	1	0.839	0.850	0.590
ATOM	18	H	RES	1	0.868	0.538	1.636
ATOM	19	C	RES	1	2.171	1.187	-0.012
ATOM	20	H	RES	1	2.638	1.955	0.620
ATOM	21	C	RES	1	2.107	1.728	-1.437
ATOM	22	H	RES	1	1.676	0.991	-2.124
ATOM	23	H	RES	1	1.494	2.632	-1.488
ATOM	24	H	RES	1	3.112	1.969	-1.789
ATOM	25	C	RES	1	3.182	0.032	0.019
ATOM	26	O	RES	1	4.386	0.241	-0.074
ATOM	27	N	RES	1	2.647	-1.219	0.107
ATOM	28	H	RES	1	1.642	-1.303	0.153
ATOM	29	C	RES	1	3.458	-2.412	0.085
ATOM	30	H	RES	1	3.270	-3.011	-0.812
ATOM	31	H	RES	1	3.274	-3.033	0.967
ATOM	32	H	RES	1	4.502	-2.098	0.083

TER

REMARK Compound C structure 12
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.554623
 REMARK Sum of electronic and thermal Energies= -651.537266
 REMARK Sum of electronic and thermal Enthalpies= -651.536321
 REMARK Sum of electronic and thermal Free Energies= -651.602059
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.846	-1.524	1.431
ATOM	2	C	RES	1	-4.362	-0.559	1.598
ATOM	3	H	RES	1	-5.153	0.161	1.820
ATOM	4	H	RES	1	-3.705	-0.639	2.468
ATOM	5	C	RES	1	-3.655	-0.137	0.334
ATOM	6	O	RES	1	-4.248	0.011	-0.731
ATOM	7	N	RES	1	-2.314	0.077	0.451
ATOM	8	H	RES	1	-1.848	-0.138	1.320
ATOM	9	C	RES	1	-1.491	0.431	-0.710
ATOM	10	H	RES	1	-1.824	-0.204	-1.542
ATOM	11	C	RES	1	-1.706	1.892	-1.096
ATOM	12	H	RES	1	-2.764	2.075	-1.294
ATOM	13	H	RES	1	-1.135	2.138	-1.996
ATOM	14	H	RES	1	-1.378	2.557	-0.290
ATOM	15	C	RES	1	-0.057	0.143	-0.394
ATOM	16	H	RES	1	0.374	0.715	0.432
ATOM	17	C	RES	1	0.697	-0.739	-1.054
ATOM	18	H	RES	1	0.241	-1.311	-1.866
ATOM	19	C	RES	1	2.140	-1.071	-0.783
ATOM	20	H	RES	1	2.704	-0.885	-1.711
ATOM	21	C	RES	1	2.294	-2.546	-0.417
ATOM	22	H	RES	1	1.817	-2.739	0.547
ATOM	23	H	RES	1	1.829	-3.184	-1.174
ATOM	24	H	RES	1	3.348	-2.826	-0.334
ATOM	25	C	RES	1	2.706	-0.188	0.324
ATOM	26	O	RES	1	2.526	-0.432	1.512
ATOM	27	N	RES	1	3.400	0.903	-0.112
ATOM	28	H	RES	1	3.451	1.072	-1.104
ATOM	29	C	RES	1	3.918	1.904	0.790
ATOM	30	H	RES	1	3.863	1.498	1.801
ATOM	31	H	RES	1	3.330	2.829	0.754
ATOM	32	H	RES	1	4.959	2.139	0.555

TER

REMARK Compound C structure 13
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.554694
 REMARK Sum of electronic and thermal Energies= -651.537411
 REMARK Sum of electronic and thermal Enthalpies= -651.536467
 REMARK Sum of electronic and thermal Free Energies= -651.601829
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.092	-1.513	-0.892
ATOM	2	C	RES	1	4.190	-1.805	-0.349
ATOM	3	H	RES	1	3.549	-2.387	-1.016
ATOM	4	H	RES	1	4.509	-2.441	0.479
ATOM	5	C	RES	1	3.530	-0.569	0.210
ATOM	6	O	RES	1	4.090	0.165	1.017
ATOM	7	N	RES	1	2.263	-0.325	-0.237
ATOM	8	H	RES	1	1.869	-0.906	-0.961
ATOM	9	C	RES	1	1.523	0.873	0.165
ATOM	10	H	RES	1	1.837	1.051	1.204
ATOM	11	C	RES	1	1.936	2.081	-0.662
ATOM	12	H	RES	1	3.016	2.222	-0.587
ATOM	13	H	RES	1	1.450	2.991	-0.299
ATOM	14	H	RES	1	1.673	1.950	-1.717
ATOM	15	C	RES	1	0.059	0.557	0.155
ATOM	16	H	RES	1	-0.228	-0.312	0.750
ATOM	17	C	RES	1	-0.884	1.254	-0.486
ATOM	18	H	RES	1	-0.599	2.138	-1.059
ATOM	19	C	RES	1	-2.366	0.984	-0.461
ATOM	20	H	RES	1	-2.713	0.947	-1.506
ATOM	21	C	RES	1	-3.106	2.115	0.251
ATOM	22	H	RES	1	-2.839	2.117	1.310
ATOM	23	H	RES	1	-2.842	3.084	-0.181
ATOM	24	H	RES	1	-4.190	1.989	0.176
ATOM	25	C	RES	1	-2.674	-0.353	0.204
ATOM	26	O	RES	1	-2.792	-0.473	1.418
ATOM	27	N	RES	1	-2.779	-1.408	-0.657
ATOM	28	H	RES	1	-2.634	-1.240	-1.640
ATOM	29	C	RES	1	-2.979	-2.764	-0.204
ATOM	30	H	RES	1	-3.174	-2.724	0.868
ATOM	31	H	RES	1	-2.093	-3.385	-0.376
ATOM	32	H	RES	1	-3.835	-3.225	-0.705

TER

REMARK Compound C structure 14
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.555207
 REMARK Sum of electronic and thermal Energies= -651.538010
 REMARK Sum of electronic and thermal Enthalpies= -651.537066
 REMARK Sum of electronic and thermal Free Energies= -651.601663
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.864	0.545	0.377
ATOM	2	C	RES	1	5.034	1.000	-0.169
ATOM	3	H	RES	1	4.739	1.919	0.344
ATOM	4	H	RES	1	5.409	1.255	-1.163
ATOM	5	C	RES	1	3.923	-0.010	-0.305
ATOM	6	O	RES	1	4.084	-1.096	-0.854
ATOM	7	N	RES	1	2.721	0.357	0.228
ATOM	8	H	RES	1	2.603	1.292	0.588
ATOM	9	C	RES	1	1.539	-0.499	0.106
ATOM	10	H	RES	1	1.531	-0.888	-0.921
ATOM	11	C	RES	1	1.625	-1.679	1.071
ATOM	12	H	RES	1	2.543	-2.244	0.893
ATOM	13	H	RES	1	0.773	-2.352	0.931
ATOM	14	H	RES	1	1.619	-1.333	2.110
ATOM	15	C	RES	1	0.307	0.317	0.347
ATOM	16	H	RES	1	0.229	0.775	1.337
ATOM	17	C	RES	1	-0.686	0.467	-0.536
ATOM	18	H	RES	1	-0.577	-0.012	-1.513
ATOM	19	C	RES	1	-1.968	1.212	-0.322
ATOM	20	H	RES	1	-2.103	1.902	-1.165
ATOM	21	C	RES	1	-2.023	2.024	0.969
ATOM	22	H	RES	1	-1.948	1.379	1.851
ATOM	23	H	RES	1	-1.206	2.750	1.012
ATOM	24	H	RES	1	-2.969	2.565	1.029
ATOM	25	C	RES	1	-3.216	0.317	-0.380
ATOM	26	O	RES	1	-4.315	0.780	-0.663
ATOM	27	N	RES	1	-3.017	-0.989	-0.047
ATOM	28	H	RES	1	-2.082	-1.278	0.203
ATOM	29	C	RES	1	-4.095	-1.945	0.026
ATOM	30	H	RES	1	-4.260	-2.289	1.052
ATOM	31	H	RES	1	-3.894	-2.815	-0.608
ATOM	32	H	RES	1	-5.000	-1.450	-0.327

TER

REMARK Compound C structure 15
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.554103
 REMARK Sum of electronic and thermal Energies= -651.536733
 REMARK Sum of electronic and thermal Enthalpies= -651.535789
 REMARK Sum of electronic and thermal Free Energies= -651.601448
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.018	-2.187	-0.418
ATOM	2	C	RES	1	3.980	-2.220	-0.082
ATOM	3	H	RES	1	3.376	-2.709	-0.851
ATOM	4	H	RES	1	3.957	-2.830	0.824
ATOM	5	C	RES	1	3.525	-0.822	0.257
ATOM	6	O	RES	1	4.122	-0.115	1.063
ATOM	7	N	RES	1	2.407	-0.390	-0.396
ATOM	8	H	RES	1	1.874	-1.049	-0.943
ATOM	9	C	RES	1	1.788	0.902	-0.075
ATOM	10	H	RES	1	1.798	0.997	1.019
ATOM	11	C	RES	1	2.595	2.049	-0.673
ATOM	12	H	RES	1	3.627	2.010	-0.319
ATOM	13	H	RES	1	2.163	3.011	-0.382
ATOM	14	H	RES	1	2.597	1.990	-1.767
ATOM	15	C	RES	1	0.373	0.907	-0.566
ATOM	16	H	RES	1	0.244	0.915	-1.654
ATOM	17	C	RES	1	-0.705	0.944	0.220
ATOM	18	H	RES	1	-0.583	0.944	1.306
ATOM	19	C	RES	1	-2.123	0.996	-0.266
ATOM	20	H	RES	1	-2.115	0.986	-1.366
ATOM	21	C	RES	1	-2.830	2.258	0.229
ATOM	22	H	RES	1	-2.870	2.255	1.321
ATOM	23	H	RES	1	-2.297	3.153	-0.101
ATOM	24	H	RES	1	-3.858	2.308	-0.143
ATOM	25	C	RES	1	-2.863	-0.237	0.255
ATOM	26	O	RES	1	-3.144	-0.367	1.441
ATOM	27	N	RES	1	-3.160	-1.173	-0.691
ATOM	28	H	RES	1	-2.901	-0.989	-1.647
ATOM	29	C	RES	1	-3.833	-2.411	-0.376
ATOM	30	H	RES	1	-4.004	-2.425	0.700
ATOM	31	H	RES	1	-3.223	-3.278	-0.649
ATOM	32	H	RES	1	-4.798	-2.484	-0.887

TER

REMARK Compound C structure 16
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.554408
 REMARK Sum of electronic and thermal Energies= -651.537223
 REMARK Sum of electronic and thermal Enthalpies= -651.536279
 REMARK Sum of electronic and thermal Free Energies= -651.601288
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.818	1.407	0.904
ATOM	2	C	RES	1	3.889	1.006	1.313
ATOM	3	H	RES	1	4.126	0.265	2.082
ATOM	4	H	RES	1	3.359	1.838	1.785
ATOM	5	C	RES	1	3.043	0.466	0.188
ATOM	6	O	RES	1	2.841	1.099	-0.843
ATOM	7	N	RES	1	2.524	-0.784	0.387
ATOM	8	H	RES	1	2.600	-1.198	1.305
ATOM	9	C	RES	1	1.528	-1.341	-0.534
ATOM	10	H	RES	1	1.875	-1.070	-1.538
ATOM	11	C	RES	1	1.490	-2.851	-0.378
ATOM	12	H	RES	1	2.474	-3.294	-0.553
ATOM	13	H	RES	1	0.782	-3.291	-1.085
ATOM	14	H	RES	1	1.161	-3.134	0.629
ATOM	15	C	RES	1	0.189	-0.700	-0.298
ATOM	16	H	RES	1	-0.349	-1.018	0.599
ATOM	17	C	RES	1	-0.296	0.278	-1.066
ATOM	18	H	RES	1	0.302	0.609	-1.917
ATOM	19	C	RES	1	-1.554	1.070	-0.827
ATOM	20	H	RES	1	-2.123	1.093	-1.770
ATOM	21	C	RES	1	-1.196	2.507	-0.445
ATOM	22	H	RES	1	-0.712	2.513	0.535
ATOM	23	H	RES	1	-0.507	2.941	-1.174
ATOM	24	H	RES	1	-2.088	3.138	-0.388
ATOM	25	C	RES	1	-2.417	0.428	0.251
ATOM	26	O	RES	1	-2.218	0.602	1.448
ATOM	27	N	RES	1	-3.413	-0.379	-0.221
ATOM	28	H	RES	1	-3.476	-0.528	-1.216
ATOM	29	C	RES	1	-4.266	-1.149	0.651
ATOM	30	H	RES	1	-4.126	-0.771	1.665
ATOM	31	H	RES	1	-4.008	-2.215	0.640
ATOM	32	H	RES	1	-5.316	-1.038	0.370

TER

REMARK Compound C structure 17
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.553968
 REMARK Sum of electronic and thermal Energies= -651.536871
 REMARK Sum of electronic and thermal Enthalpies= -651.535927
 REMARK Sum of electronic and thermal Free Energies= -651.600310
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.624	0.460	0.502
ATOM	2	C	RES	1	4.818	0.928	-0.066
ATOM	3	H	RES	1	4.756	1.967	0.266
ATOM	4	H	RES	1	5.079	0.911	-1.127
ATOM	5	C	RES	1	3.520	0.231	0.263
ATOM	6	O	RES	1	3.106	0.138	1.414
ATOM	7	N	RES	1	2.852	-0.295	-0.806
ATOM	8	H	RES	1	3.191	-0.080	-1.730
ATOM	9	C	RES	1	1.536	-0.943	-0.704
ATOM	10	H	RES	1	1.283	-1.241	-1.730
ATOM	11	C	RES	1	1.599	-2.199	0.162
ATOM	12	H	RES	1	2.383	-2.875	-0.192
ATOM	13	H	RES	1	0.643	-2.728	0.118
ATOM	14	H	RES	1	1.810	-1.940	1.201
ATOM	15	C	RES	1	0.486	0.017	-0.222
ATOM	16	H	RES	1	0.687	0.480	0.744
ATOM	17	C	RES	1	-0.638	0.283	-0.896
ATOM	18	H	RES	1	-0.794	-0.213	-1.860
ATOM	19	C	RES	1	-1.748	1.190	-0.456
ATOM	20	H	RES	1	-1.968	1.887	-1.275
ATOM	21	C	RES	1	-1.432	2.006	0.795
ATOM	22	H	RES	1	-1.256	1.360	1.661
ATOM	23	H	RES	1	-0.536	2.616	0.648
ATOM	24	H	RES	1	-2.267	2.668	1.033
ATOM	25	C	RES	1	-3.077	0.455	-0.232
ATOM	26	O	RES	1	-4.156	1.012	-0.404
ATOM	27	N	RES	1	-2.960	-0.825	0.223
ATOM	28	H	RES	1	-2.030	-1.195	0.358
ATOM	29	C	RES	1	-4.102	-1.628	0.584
ATOM	30	H	RES	1	-4.105	-1.867	1.653
ATOM	31	H	RES	1	-4.126	-2.564	0.016
ATOM	32	H	RES	1	-4.996	-1.049	0.351

TER

REMARK Compound C structure 18
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.552926
 REMARK Sum of electronic and thermal Energies= -651.535731
 REMARK Sum of electronic and thermal Enthalpies= -651.534787
 REMARK Sum of electronic and thermal Free Energies= -651.599868
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.895	2.102	0.746
ATOM	2	C	RES	1	3.881	2.150	0.341
ATOM	3	H	RES	1	3.213	2.540	1.113
ATOM	4	H	RES	1	3.906	2.853	-0.494
ATOM	5	C	RES	1	3.494	0.787	-0.175
ATOM	6	O	RES	1	4.131	0.213	-1.053
ATOM	7	N	RES	1	2.394	0.227	0.407
ATOM	8	H	RES	1	1.816	0.790	1.013
ATOM	9	C	RES	1	1.842	-1.047	-0.072
ATOM	10	H	RES	1	1.856	-1.011	-1.170
ATOM	11	C	RES	1	2.702	-2.218	0.391
ATOM	12	H	RES	1	3.729	-2.093	0.042
ATOM	13	H	RES	1	2.311	-3.159	-0.006
ATOM	14	H	RES	1	2.707	-2.283	1.484
ATOM	15	C	RES	1	0.432	-1.157	0.415
ATOM	16	H	RES	1	0.304	-1.317	1.489
ATOM	17	C	RES	1	-0.652	-1.038	-0.353
ATOM	18	H	RES	1	-0.532	-0.865	-1.426
ATOM	19	C	RES	1	-2.063	-1.063	0.161
ATOM	20	H	RES	1	-2.045	-1.479	1.176
ATOM	21	C	RES	1	-2.969	-1.918	-0.717
ATOM	22	H	RES	1	-2.943	-1.596	-1.766
ATOM	23	H	RES	1	-2.635	-2.959	-0.706
ATOM	24	H	RES	1	-4.009	-1.901	-0.376
ATOM	25	C	RES	1	-2.512	0.391	0.373
ATOM	26	O	RES	1	-2.041	1.064	1.283
ATOM	27	N	RES	1	-3.419	0.881	-0.518
ATOM	28	H	RES	1	-3.790	0.268	-1.226
ATOM	29	C	RES	1	-3.918	2.235	-0.449
ATOM	30	H	RES	1	-3.389	2.739	0.360
ATOM	31	H	RES	1	-4.991	2.257	-0.237
ATOM	32	H	RES	1	-3.733	2.772	-1.385

TER

REMARK Compound C structure 19
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.553124
 REMARK Sum of electronic and thermal Energies= -651.536008
 REMARK Sum of electronic and thermal Enthalpies= -651.535064
 REMARK Sum of electronic and thermal Free Energies= -651.599447
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.468	-0.849	0.080
ATOM	2	C	RES	1	-4.758	-0.690	-0.735
ATOM	3	H	RES	1	-4.682	-1.634	-1.279
ATOM	4	H	RES	1	-5.160	0.073	-1.408
ATOM	5	C	RES	1	-3.407	-0.353	-0.152
ATOM	6	O	RES	1	-2.812	-1.118	0.598
ATOM	7	N	RES	1	-2.897	0.861	-0.522
ATOM	8	H	RES	1	-3.456	1.459	-1.109
ATOM	9	C	RES	1	-1.605	1.372	-0.042
ATOM	10	H	RES	1	-1.488	2.333	-0.565
ATOM	11	C	RES	1	-1.626	1.643	1.455
ATOM	12	H	RES	1	-2.450	2.315	1.707
ATOM	13	H	RES	1	-0.693	2.117	1.776
ATOM	14	H	RES	1	-1.755	0.712	2.011
ATOM	15	C	RES	1	-0.490	0.471	-0.499
ATOM	16	H	RES	1	-0.524	0.206	-1.559
ATOM	17	C	RES	1	0.482	-0.040	0.260
ATOM	18	H	RES	1	0.503	0.180	1.330
ATOM	19	C	RES	1	1.530	-0.993	-0.226
ATOM	20	H	RES	1	1.350	-1.179	-1.296
ATOM	21	C	RES	1	1.443	-2.323	0.517
ATOM	22	H	RES	1	1.602	-2.178	1.590
ATOM	23	H	RES	1	0.456	-2.772	0.381
ATOM	24	H	RES	1	2.214	-3.009	0.161
ATOM	25	C	RES	1	2.961	-0.443	-0.157
ATOM	26	O	RES	1	3.937	-1.176	-0.045
ATOM	27	N	RES	1	3.062	0.912	-0.277
ATOM	28	H	RES	1	2.208	1.442	-0.369
ATOM	29	C	RES	1	4.332	1.596	-0.310
ATOM	30	H	RES	1	5.110	0.851	-0.138
ATOM	31	H	RES	1	4.392	2.361	0.470
ATOM	32	H	RES	1	4.509	2.071	-1.281

TER

REMARK Compound C structure 20
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.552282
 REMARK Sum of electronic and thermal Energies= -651.535106
 REMARK Sum of electronic and thermal Enthalpies= -651.534162
 REMARK Sum of electronic and thermal Free Energies= -651.598853
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.489	-1.597	-1.301
ATOM	2	C	RES	1	-3.653	-0.995	-1.665
ATOM	3	H	RES	1	-3.070	-1.631	-2.335
ATOM	4	H	RES	1	-4.047	-0.151	-2.236
ATOM	5	C	RES	1	-2.787	-0.599	-0.495
ATOM	6	O	RES	1	-2.357	-1.424	0.305
ATOM	7	N	RES	1	-2.526	0.739	-0.388
ATOM	8	H	RES	1	-2.781	1.327	-1.166
ATOM	9	C	RES	1	-1.584	1.301	0.592
ATOM	10	H	RES	1	-1.580	2.382	0.402
ATOM	11	C	RES	1	-2.064	1.068	2.022
ATOM	12	H	RES	1	-3.086	1.436	2.150
ATOM	13	H	RES	1	-1.413	1.600	2.721
ATOM	14	H	RES	1	-2.047	0.004	2.266
ATOM	15	C	RES	1	-0.197	0.773	0.361
ATOM	16	H	RES	1	-0.120	-0.314	0.328
ATOM	17	C	RES	1	0.880	1.549	0.214
ATOM	18	H	RES	1	0.754	2.635	0.251
ATOM	19	C	RES	1	2.298	1.096	-0.030
ATOM	20	H	RES	1	2.889	1.353	0.865
ATOM	21	C	RES	1	2.899	1.824	-1.227
ATOM	22	H	RES	1	2.366	1.550	-2.139
ATOM	23	H	RES	1	2.835	2.908	-1.092
ATOM	24	H	RES	1	3.949	1.555	-1.366
ATOM	25	C	RES	1	2.369	-0.416	-0.231
ATOM	26	O	RES	1	2.433	-0.933	-1.340
ATOM	27	N	RES	1	2.345	-1.143	0.925
ATOM	28	H	RES	1	2.136	-0.650	1.780
ATOM	29	C	RES	1	2.168	-2.578	0.911
ATOM	30	H	RES	1	2.557	-2.952	-0.036
ATOM	31	H	RES	1	1.110	-2.862	0.983
ATOM	32	H	RES	1	2.718	-3.038	1.735

TER

REMARK Compound C structure 21
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.552223
 REMARK Sum of electronic and thermal Energies= -651.535062
 REMARK Sum of electronic and thermal Enthalpies= -651.534118
 REMARK Sum of electronic and thermal Free Energies= -651.598740
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-2.736	2.792	-1.414
ATOM	2	C	RES	1	-3.294	2.293	-0.619
ATOM	3	H	RES	1	-3.219	2.891	0.293
ATOM	4	H	RES	1	-4.339	2.264	-0.935
ATOM	5	C	RES	1	-2.786	0.877	-0.478
ATOM	6	O	RES	1	-2.787	0.090	-1.415
ATOM	7	N	RES	1	-2.322	0.551	0.768
ATOM	8	H	RES	1	-2.356	1.259	1.484
ATOM	9	C	RES	1	-1.821	-0.769	1.146
ATOM	10	H	RES	1	-1.678	-0.711	2.235
ATOM	11	C	RES	1	-2.846	-1.874	0.888
ATOM	12	H	RES	1	-3.795	-1.641	1.379
ATOM	13	H	RES	1	-2.479	-2.824	1.288
ATOM	14	H	RES	1	-3.024	-1.991	-0.182
ATOM	15	C	RES	1	-0.488	-1.109	0.535
ATOM	16	H	RES	1	-0.136	-2.113	0.778
ATOM	17	C	RES	1	0.245	-0.330	-0.264
ATOM	18	H	RES	1	-0.137	0.660	-0.516
ATOM	19	C	RES	1	1.560	-0.689	-0.889
ATOM	20	H	RES	1	1.477	-0.516	-1.970
ATOM	21	C	RES	1	1.992	-2.138	-0.677
ATOM	22	H	RES	1	2.130	-2.363	0.387
ATOM	23	H	RES	1	1.244	-2.830	-1.074
ATOM	24	H	RES	1	2.940	-2.325	-1.185
ATOM	25	C	RES	1	2.717	0.223	-0.459
ATOM	26	O	RES	1	3.699	0.395	-1.172
ATOM	27	N	RES	1	2.591	0.774	0.782
ATOM	28	H	RES	1	1.763	0.551	1.314
ATOM	29	C	RES	1	3.627	1.579	1.382
ATOM	30	H	RES	1	4.105	1.067	2.224
ATOM	31	H	RES	1	3.230	2.536	1.733
ATOM	32	H	RES	1	4.382	1.766	0.617

TER

REMARK Compound C structure 22
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.551920
 REMARK Sum of electronic and thermal Energies= -651.534787
 REMARK Sum of electronic and thermal Enthalpies= -651.533843
 REMARK Sum of electronic and thermal Free Energies= -651.598478
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.519	-0.887	-0.091
ATOM	2	C	RES	1	-4.799	-0.666	-0.882
ATOM	3	H	RES	1	-4.709	-1.567	-1.492
ATOM	4	H	RES	1	-5.197	0.142	-1.503
ATOM	5	C	RES	1	-3.459	-0.362	-0.256
ATOM	6	O	RES	1	-2.863	-1.181	0.436
ATOM	7	N	RES	1	-2.960	0.882	-0.521
ATOM	8	H	RES	1	-3.530	1.523	-1.049
ATOM	9	C	RES	1	-1.691	1.381	0.029
ATOM	10	H	RES	1	-1.571	2.371	-0.435
ATOM	11	C	RES	1	-1.765	1.563	1.538
ATOM	12	H	RES	1	-2.608	2.205	1.803
ATOM	13	H	RES	1	-0.851	2.030	1.917
ATOM	14	H	RES	1	-1.894	0.597	2.030
ATOM	15	C	RES	1	-0.548	0.523	-0.439
ATOM	16	H	RES	1	-0.575	0.268	-1.501
ATOM	17	C	RES	1	0.447	0.056	0.315
ATOM	18	H	RES	1	0.486	0.271	1.384
ATOM	19	C	RES	1	1.538	-0.841	-0.188
ATOM	20	H	RES	1	1.424	-0.955	-1.276
ATOM	21	C	RES	1	1.446	-2.215	0.479
ATOM	22	H	RES	1	1.602	-2.115	1.556
ATOM	23	H	RES	1	0.459	-2.653	0.310
ATOM	24	H	RES	1	2.208	-2.898	0.091
ATOM	25	C	RES	1	2.892	-0.208	0.126
ATOM	26	O	RES	1	3.305	-0.097	1.275
ATOM	27	N	RES	1	3.590	0.233	-0.962
ATOM	28	H	RES	1	3.173	0.128	-1.873
ATOM	29	C	RES	1	4.866	0.896	-0.850
ATOM	30	H	RES	1	5.145	0.888	0.204
ATOM	31	H	RES	1	4.812	1.935	-1.191
ATOM	32	H	RES	1	5.638	0.376	-1.425

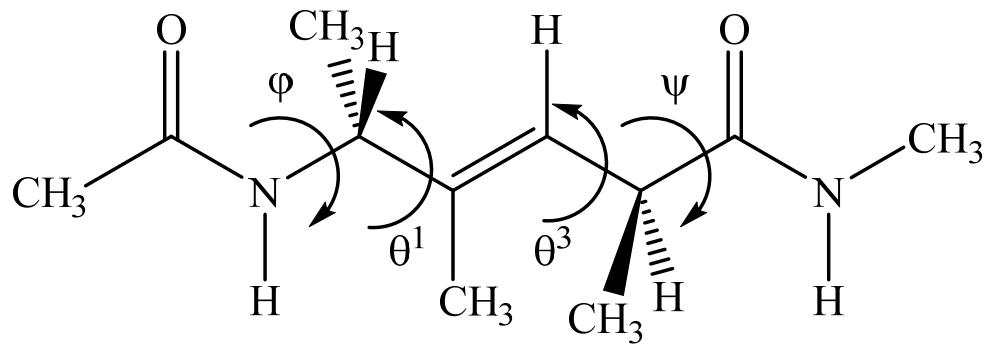
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REMARK Compound C structure 23
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -651.550456
 REMARK Sum of electronic and thermal Energies= -651.533131
 REMARK Sum of electronic and thermal Enthalpies= -651.532187
 REMARK Sum of electronic and thermal Free Energies= -651.597687
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-3.944	-1.946	-1.353
ATOM	2	C	RES	1	-4.180	-0.904	-1.126
ATOM	3	H	RES	1	-4.316	-0.360	-2.064
ATOM	4	H	RES	1	-5.127	-0.905	-0.581
ATOM	5	C	RES	1	-3.102	-0.340	-0.229
ATOM	6	O	RES	1	-2.832	-0.844	0.855
ATOM	7	N	RES	1	-2.460	0.762	-0.723
ATOM	8	H	RES	1	-2.731	1.093	-1.634
ATOM	9	C	RES	1	-1.409	1.501	-0.024
ATOM	10	H	RES	1	-1.234	2.390	-0.648
ATOM	11	C	RES	1	-1.871	1.997	1.347
ATOM	12	H	RES	1	-2.781	2.597	1.253
ATOM	13	H	RES	1	-1.094	2.620	1.799
ATOM	14	H	RES	1	-2.072	1.155	2.011
ATOM	15	C	RES	1	-0.105	0.761	0.080
ATOM	16	H	RES	1	0.677	1.309	0.610
ATOM	17	C	RES	1	0.148	-0.469	-0.366
ATOM	18	H	RES	1	-0.650	-1.034	-0.850
ATOM	19	C	RES	1	1.431	-1.236	-0.170
ATOM	20	H	RES	1	1.649	-1.770	-1.108
ATOM	21	C	RES	1	1.260	-2.266	0.946
ATOM	22	H	RES	1	1.140	-1.749	1.901
ATOM	23	H	RES	1	0.370	-2.878	0.773
ATOM	24	H	RES	1	2.130	-2.924	1.020
ATOM	25	C	RES	1	2.596	-0.301	0.132
ATOM	26	O	RES	1	2.858	0.090	1.265
ATOM	27	N	RES	1	3.309	0.089	-0.966
ATOM	28	H	RES	1	2.997	-0.223	-1.872
ATOM	29	C	RES	1	4.378	1.055	-0.893
ATOM	30	H	RES	1	4.600	1.216	0.162
ATOM	31	H	RES	1	4.093	2.014	-1.340
ATOM	32	H	RES	1	5.277	0.687	-1.395

TER

COMPOUND D



REMARK Compound D structure 01
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.850519
 REMARK Sum of electronic and thermal Energies= -690.831929
 REMARK Sum of electronic and thermal Enthalpies= -690.830985
 REMARK Sum of electronic and thermal Free Energies= -690.898529
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	24.700	2.565	5.823
ATOM	2	C	RES	1	24.177	2.185	4.942
ATOM	3	H	RES	1	23.786	3.052	4.407
ATOM	4	H	RES	1	23.341	1.564	5.272
ATOM	5	C	RES	1	25.164	1.466	4.060
ATOM	6	O	RES	1	26.134	2.046	3.568
ATOM	7	N	RES	1	24.922	0.143	3.855
ATOM	8	H	RES	1	24.107	-0.270	4.281
ATOM	9	C	RES	1	25.775	-0.715	3.026
ATOM	10	H	RES	1	25.601	-1.767	3.282
ATOM	11	C	RES	1	27.243	-0.402	3.228
ATOM	12	C	RES	1	27.705	-0.260	4.643
ATOM	13	H	RES	1	27.889	-1.233	5.113
ATOM	14	H	RES	1	26.944	0.242	5.254
ATOM	15	H	RES	1	28.620	0.331	4.724
ATOM	16	C	RES	1	28.026	-0.225	2.153
ATOM	17	H	RES	1	27.550	-0.295	1.170
ATOM	18	C	RES	1	29.466	0.171	2.136
ATOM	19	H	RES	1	29.798	0.500	1.152
ATOM	20	C	RES	1	29.816	1.248	3.185
ATOM	21	O	RES	1	30.986	1.484	3.477
ATOM	22	N	RES	1	28.776	1.878	3.779
ATOM	23	H	RES	1	27.819	1.698	3.493
ATOM	24	C	RES	1	29.012	2.884	4.788
ATOM	25	H	RES	1	29.574	2.468	5.630
ATOM	26	H	RES	1	29.595	3.719	4.387
ATOM	27	H	RES	1	28.049	3.254	5.142
ATOM	29	C	RES	1	25.437	-0.488	1.623
ATOM	30	H	RES	1	24.414	-0.874	1.644
ATOM	31	H	RES	1	25.406	0.535	1.246
ATOM	32	H	RES	1	26.015	-1.089	0.908
ATOM	33	C	RES	1	30.295	-1.094	2.407
ATOM	34	H	RES	1	29.696	-1.968	2.688
ATOM	35	H	RES	1	30.764	-0.726	3.328
ATOM	36	H	RES	1	31.101	-1.435	1.753

TER

REMARK Compound D structure 02
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.845900
 REMARK Sum of electronic and thermal Energies= -690.827615
 REMARK Sum of electronic and thermal Enthalpies= -690.826671
 REMARK Sum of electronic and thermal Free Energies= -690.892524
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	20.614	-1.737	-1.337
ATOM	2	C	RES	1	20.546	-1.626	-0.251
ATOM	3	H	RES	1	19.534	-1.303	0.002
ATOM	4	H	RES	1	21.254	-0.849	0.038
ATOM	5	C	RES	1	20.952	-2.930	0.385
ATOM	6	O	RES	1	22.106	-3.360	0.306
ATOM	7	N	RES	1	19.967	-3.623	1.012
ATOM	8	H	RES	1	19.046	-3.219	1.062
ATOM	9	C	RES	1	20.191	-4.941	1.632
ATOM	10	C	RES	1	21.581	-5.014	2.273
ATOM	11	C	RES	1	21.682	-4.787	3.747
ATOM	12	H	RES	1	21.545	-5.713	4.317
ATOM	13	H	RES	1	20.904	-4.090	4.079
ATOM	14	H	RES	1	22.648	-4.366	4.032
ATOM	15	C	RES	1	22.635	-5.230	1.469
ATOM	16	H	RES	1	22.434	-5.345	0.400
ATOM	17	C	RES	1	24.089	-5.237	1.824
ATOM	18	H	RES	1	24.721	-5.401	0.955
ATOM	19	C	RES	1	24.536	-3.956	2.561
ATOM	20	O	RES	1	25.176	-4.005	3.610
ATOM	21	N	RES	1	24.148	-2.785	2.000
ATOM	22	H	RES	1	23.607	-2.780	1.144
ATOM	23	C	RES	1	24.431	-1.521	2.637
ATOM	24	H	RES	1	25.473	-1.493	2.967
ATOM	25	H	RES	1	24.250	-0.718	1.920
ATOM	26	H	RES	1	23.802	-1.357	3.519
ATOM	28	H	RES	1	19.397	-5.096	2.374
ATOM	29	C	RES	1	20.099	-5.990	0.554
ATOM	30	H	RES	1	20.322	-6.962	1.003
ATOM	31	H	RES	1	19.180	-6.094	-0.028
ATOM	32	H	RES	1	20.912	-5.734	-0.128
ATOM	33	C	RES	1	24.359	-6.448	2.719
ATOM	34	H	RES	1	25.273	-6.943	2.371
ATOM	35	H	RES	1	23.534	-7.150	2.553
ATOM	36	H	RES	1	24.455	-6.298	3.795

TER

REMARK Compound D structure 03
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.846859
 REMARK Sum of electronic and thermal Energies= -690.828829
 REMARK Sum of electronic and thermal Enthalpies= -690.827885
 REMARK Sum of electronic and thermal Free Energies= -690.892021
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-2.036	16.465	-8.597
ATOM	2	C	RES	1	-1.859	15.387	-8.565
ATOM	3	H	RES	1	-2.073	15.000	-9.564
ATOM	4	H	RES	1	-2.556	14.938	-7.853
ATOM	5	C	RES	1	-0.410	15.140	-8.241
ATOM	6	O	RES	1	0.499	15.521	-8.980
ATOM	7	N	RES	1	-0.162	14.483	-7.075
ATOM	8	H	RES	1	-0.935	14.181	-6.504
ATOM	9	C	RES	1	1.197	14.168	-6.644
ATOM	10	H	RES	1	1.289	14.393	-5.582
ATOM	11	C	RES	1	2.254	14.955	-7.400
ATOM	12	C	RES	1	3.490	14.166	-7.692
ATOM	13	H	RES	1	3.425	13.736	-8.699
ATOM	14	H	RES	1	3.598	13.321	-6.998
ATOM	15	H	RES	1	4.407	14.755	-7.641
ATOM	16	C	RES	1	2.033	16.211	-7.811
ATOM	17	H	RES	1	1.068	16.657	-7.565
ATOM	18	C	RES	1	2.968	17.036	-8.656
ATOM	19	C	RES	1	2.181	18.189	-9.259
ATOM	20	H	RES	1	1.736	18.783	-8.455
ATOM	21	H	RES	1	1.363	17.785	-9.860
ATOM	22	H	RES	1	2.860	18.840	-9.812
ATOM	23	C	RES	1	3.645	16.239	-9.787
ATOM	24	O	RES	1	4.840	16.368	-10.043
ATOM	25	N	RES	1	2.827	15.441	-10.522
ATOM	26	H	RES	1	1.901	15.216	-10.175
ATOM	27	C	RES	1	3.371	14.600	-11.561
ATOM	28	H	RES	1	3.958	15.195	-12.263
ATOM	29	H	RES	1	4.033	13.826	-11.153
ATOM	30	H	RES	1	2.548	14.119	-12.090
ATOM	32	C	RES	1	1.434	12.694	-6.860
ATOM	33	H	RES	1	0.570	12.060	-6.631
ATOM	34	H	RES	1	1.727	12.497	-7.895
ATOM	35	H	RES	1	2.272	12.396	-6.221
ATOM	36	H	RES	1	3.709	17.589	-8.082

TER

REMARK Compound D structure 04
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.845165
 REMARK Sum of electronic and thermal Energies= -690.827151
 REMARK Sum of electronic and thermal Enthalpies= -690.826207
 REMARK Sum of electronic and thermal Free Energies= -690.891357
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	1.574	2.494	2.759
ATOM	2	C	RES	1	2.403	2.312	2.070
ATOM	3	H	RES	1	3.229	1.866	2.629
ATOM	4	H	RES	1	2.716	3.284	1.685
ATOM	5	C	RES	1	1.906	1.466	0.926
ATOM	6	O	RES	1	1.074	1.891	0.123
ATOM	7	N	RES	1	2.415	0.206	0.861
ATOM	8	H	RES	1	3.066	-0.080	1.574
ATOM	9	C	RES	1	2.059	-0.767	-0.173
ATOM	10	H	RES	1	2.509	-0.486	-1.128
ATOM	11	C	RES	1	0.562	-1.023	-0.274
ATOM	12	C	RES	1	0.107	-1.514	-1.614
ATOM	13	H	RES	1	0.892	-1.399	-2.371
ATOM	14	H	RES	1	-0.760	-0.948	-1.976
ATOM	15	H	RES	1	-0.180	-2.567	-1.593
ATOM	16	C	RES	1	-0.269	-0.812	0.758
ATOM	17	H	RES	1	0.161	-0.448	1.693
ATOM	18	C	RES	1	-1.760	-0.901	0.755
ATOM	19	C	RES	1	-2.153	-2.267	0.217
ATOM	20	H	RES	1	-1.430	-3.007	0.548
ATOM	21	H	RES	1	-2.237	-2.225	-0.873
ATOM	22	H	RES	1	-3.123	-2.550	0.631
ATOM	23	C	RES	1	-2.437	0.175	-0.120
ATOM	24	O	RES	1	-3.631	0.086	-0.403
ATOM	25	N	RES	1	-1.657	1.196	-0.545
ATOM	26	H	RES	1	-0.680	1.250	-0.276
ATOM	27	C	RES	1	-2.201	2.260	-1.355
ATOM	28	H	RES	1	-3.207	2.510	-1.007
ATOM	29	H	RES	1	-1.554	3.135	-1.273
ATOM	30	H	RES	1	-2.278	1.974	-2.410
ATOM	32	C	RES	1	2.780	-2.080	0.100
ATOM	33	H	RES	1	3.584	-1.972	0.834
ATOM	34	H	RES	1	1.999	-2.729	0.501
ATOM	35	H	RES	1	3.208	-2.551	-0.791
ATOM	36	H	RES	1	-2.170	-0.852	1.762

TER

REMARK Compound D structure 05
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.845956
 REMARK Sum of electronic and thermal Energies= -690.828142
 REMARK Sum of electronic and thermal Enthalpies= -690.827198
 REMARK Sum of electronic and thermal Free Energies= -690.890930
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	3.035	-2.574	0.927
ATOM	2	C	RES	1	3.543	-1.739	0.437
ATOM	3	H	RES	1	4.272	-1.317	1.132
ATOM	4	H	RES	1	4.069	-2.150	-0.426
ATOM	5	C	RES	1	2.504	-0.755	-0.040
ATOM	6	O	RES	1	1.662	-1.067	-0.883
ATOM	7	N	RES	1	2.549	0.474	0.541
ATOM	8	H	RES	1	3.282	0.657	1.206
ATOM	9	C	RES	1	1.624	1.576	0.215
ATOM	10	H	RES	1	1.819	2.322	1.000
ATOM	11	C	RES	1	1.979	2.190	-1.129
ATOM	12	H	RES	1	3.031	2.485	-1.142
ATOM	13	H	RES	1	1.378	3.082	-1.327
ATOM	14	H	RES	1	1.814	1.473	-1.938
ATOM	15	C	RES	1	0.186	1.127	0.380
ATOM	16	C	RES	1	-0.094	0.396	1.659
ATOM	17	H	RES	1	0.310	-0.624	1.630
ATOM	18	H	RES	1	0.384	0.898	2.509
ATOM	19	H	RES	1	-1.160	0.312	1.876
ATOM	20	C	RES	1	-0.742	1.358	-0.560
ATOM	21	H	RES	1	-0.441	1.883	-1.464
ATOM	22	C	RES	1	-2.177	0.899	-0.509
ATOM	23	H	RES	1	-2.579	0.992	-1.528
ATOM	24	C	RES	1	-3.055	1.761	0.396
ATOM	25	H	RES	1	-2.696	1.750	1.429
ATOM	26	H	RES	1	-3.053	2.800	0.054
ATOM	27	H	RES	1	-4.080	1.386	0.399
ATOM	28	C	RES	1	-2.347	-0.594	-0.177
ATOM	29	O	RES	1	-3.345	-1.017	0.402
ATOM	30	N	RES	1	-1.360	-1.407	-0.639
ATOM	31	H	RES	1	-0.478	-0.997	-0.927
ATOM	32	C	RES	1	-1.363	-2.820	-0.348
ATOM	33	H	RES	1	-2.395	-3.173	-0.313
ATOM	34	H	RES	1	-0.897	-3.042	0.622
ATOM	35	H	RES	1	-0.815	-3.355	-1.126

TER

REMARK Compound D structure 06
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.842324
 REMARK Sum of electronic and thermal Energies= -690.823884
 REMARK Sum of electronic and thermal Enthalpies= -690.822940
 REMARK Sum of electronic and thermal Free Energies= -690.890171
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.070	-0.088	-1.797
ATOM	2	C	RES	1	4.947	0.307	-0.786
ATOM	3	H	RES	1	5.849	0.044	-0.230
ATOM	4	H	RES	1	4.870	1.396	-0.839
ATOM	5	C	RES	1	3.761	-0.363	-0.138
ATOM	6	O	RES	1	3.705	-1.578	0.020
ATOM	7	N	RES	1	2.759	0.478	0.256
ATOM	8	H	RES	1	2.837	1.464	0.057
ATOM	9	C	RES	1	1.530	0.014	0.903
ATOM	10	H	RES	1	1.748	-1.033	1.154
ATOM	11	C	RES	1	1.301	0.795	2.184
ATOM	12	H	RES	1	2.163	0.685	2.846
ATOM	13	H	RES	1	0.414	0.437	2.713
ATOM	14	H	RES	1	1.161	1.865	1.989
ATOM	15	C	RES	1	0.380	0.015	-0.090
ATOM	16	C	RES	1	0.593	-0.904	-1.253
ATOM	17	H	RES	1	1.554	-0.708	-1.740
ATOM	18	H	RES	1	0.645	-1.948	-0.919
ATOM	19	H	RES	1	-0.186	-0.825	-2.014
ATOM	20	C	RES	1	-0.717	0.766	0.099
ATOM	21	H	RES	1	-0.781	1.384	0.995
ATOM	22	C	RES	1	-1.940	0.848	-0.771
ATOM	23	H	RES	1	-1.747	0.351	-1.730
ATOM	24	C	RES	1	-2.345	2.295	-1.023
ATOM	25	H	RES	1	-2.596	2.785	-0.079
ATOM	26	H	RES	1	-1.530	2.846	-1.502
ATOM	27	H	RES	1	-3.228	2.353	-1.664
ATOM	28	C	RES	1	-3.076	0.099	-0.062
ATOM	29	O	RES	1	-3.880	0.661	0.672
ATOM	30	N	RES	1	-3.095	-1.245	-0.299
ATOM	31	H	RES	1	-2.346	-1.642	-0.846
ATOM	32	C	RES	1	-4.002	-2.137	0.383
ATOM	33	H	RES	1	-4.761	-1.523	0.869
ATOM	34	H	RES	1	-3.493	-2.732	1.150
ATOM	35	H	RES	1	-4.489	-2.815	-0.324

TER

REMARK Compound D structure 07
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.841331
 REMARK Sum of electronic and thermal Energies= -690.822699
 REMARK Sum of electronic and thermal Enthalpies= -690.821755
 REMARK Sum of electronic and thermal Free Energies= -690.889586
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-3.676	3.082	-0.034
ATOM	2	C	RES	1	-2.892	2.537	-0.560
ATOM	3	H	RES	1	-3.098	2.549	-1.634
ATOM	4	H	RES	1	-1.950	3.068	-0.388
ATOM	5	C	RES	1	-2.771	1.149	0.014
ATOM	6	O	RES	1	-2.881	0.914	1.213
ATOM	7	N	RES	1	-2.504	0.158	-0.891
ATOM	8	H	RES	1	-2.277	0.415	-1.841
ATOM	9	C	RES	1	-2.123	-1.166	-0.425
ATOM	10	H	RES	1	-2.904	-1.474	0.283
ATOM	11	C	RES	1	-2.105	-2.132	-1.602
ATOM	12	H	RES	1	-3.086	-2.195	-2.082
ATOM	13	H	RES	1	-1.823	-3.135	-1.273
ATOM	14	H	RES	1	-1.367	-1.816	-2.348
ATOM	15	C	RES	1	-0.805	-1.176	0.336
ATOM	16	C	RES	1	-0.738	-2.209	1.413
ATOM	17	H	RES	1	-1.416	-1.935	2.231
ATOM	18	H	RES	1	-1.069	-3.191	1.052
ATOM	19	H	RES	1	0.262	-2.331	1.836
ATOM	20	C	RES	1	0.162	-0.295	0.053
ATOM	21	H	RES	1	-0.013	0.457	-0.717
ATOM	22	C	RES	1	1.459	-0.116	0.780
ATOM	23	H	RES	1	1.779	-1.061	1.240
ATOM	24	C	RES	1	1.292	0.933	1.891
ATOM	25	H	RES	1	0.971	1.885	1.458
ATOM	26	H	RES	1	0.524	0.612	2.600
ATOM	27	H	RES	1	2.228	1.102	2.434
ATOM	28	C	RES	1	2.536	0.368	-0.186
ATOM	29	O	RES	1	2.346	1.305	-0.954
ATOM	30	N	RES	1	3.727	-0.292	-0.101
ATOM	31	H	RES	1	3.804	-1.061	0.546
ATOM	32	C	RES	1	4.874	0.061	-0.903
ATOM	33	H	RES	1	4.581	0.895	-1.541
ATOM	34	H	RES	1	5.192	-0.773	-1.536
ATOM	35	H	RES	1	5.719	0.373	-0.280

TER

REMARK Compound D structure 08
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.841206
 REMARK Sum of electronic and thermal Energies= -690.822763
 REMARK Sum of electronic and thermal Enthalpies= -690.821819
 REMARK Sum of electronic and thermal Free Energies= -690.888678
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.161	1.910	1.153
ATOM	2	C	RES	1	4.413	0.928	0.746
ATOM	3	H	RES	1	5.307	1.057	0.132
ATOM	4	H	RES	1	4.647	0.255	1.575
ATOM	5	C	RES	1	3.278	0.453	-0.126
ATOM	6	O	RES	1	2.941	1.046	-1.145
ATOM	7	N	RES	1	2.655	-0.691	0.289
ATOM	8	H	RES	1	2.939	-1.121	1.157
ATOM	9	C	RES	1	1.486	-1.224	-0.413
ATOM	10	H	RES	1	1.672	-1.035	-1.476
ATOM	11	C	RES	1	1.393	-2.720	-0.161
ATOM	12	H	RES	1	2.289	-3.234	-0.521
ATOM	13	H	RES	1	0.526	-3.144	-0.675
ATOM	14	H	RES	1	1.280	-2.944	0.906
ATOM	15	C	RES	1	0.232	-0.470	-0.018
ATOM	16	C	RES	1	-0.298	-0.735	1.359
ATOM	17	H	RES	1	-0.777	-1.721	1.426
ATOM	18	H	RES	1	0.514	-0.733	2.096
ATOM	19	H	RES	1	-1.034	0.004	1.684
ATOM	20	C	RES	1	-0.309	0.404	-0.882
ATOM	21	H	RES	1	0.206	0.542	-1.833
ATOM	22	C	RES	1	-1.492	1.303	-0.621
ATOM	23	H	RES	1	-1.839	1.674	-1.596
ATOM	24	C	RES	1	-1.097	2.517	0.217
ATOM	25	H	RES	1	-0.758	2.211	1.211
ATOM	26	H	RES	1	-0.279	3.058	-0.265
ATOM	27	H	RES	1	-1.947	3.189	0.352
ATOM	28	C	RES	1	-2.717	0.604	-0.019
ATOM	29	O	RES	1	-3.429	1.132	0.829
ATOM	30	N	RES	1	-2.995	-0.622	-0.552
ATOM	31	H	RES	1	-2.290	-1.044	-1.139
ATOM	32	C	RES	1	-4.088	-1.435	-0.077
ATOM	33	H	RES	1	-4.787	-0.781	0.445
ATOM	34	H	RES	1	-3.753	-2.209	0.625
ATOM	35	H	RES	1	-4.602	-1.918	-0.912

TER

REMARK Compound D structure 09
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.841437
 REMARK Sum of electronic and thermal Energies= -690.823143
 REMARK Sum of electronic and thermal Enthalpies= -690.822199
 REMARK Sum of electronic and thermal Free Energies= -690.888621
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	3.705	-2.641	0.532
ATOM	2	C	RES	1	3.967	-1.804	-0.119
ATOM	3	H	RES	1	5.043	-1.650	-0.022
ATOM	4	H	RES	1	3.740	-2.079	-1.153
ATOM	5	C	RES	1	3.248	-0.568	0.359
ATOM	6	O	RES	1	3.438	-0.095	1.475
ATOM	7	N	RES	1	2.371	-0.019	-0.533
ATOM	8	H	RES	1	2.244	-0.461	-1.432
ATOM	9	C	RES	1	1.585	1.184	-0.247
ATOM	10	H	RES	1	2.050	1.586	0.663
ATOM	11	C	RES	1	1.752	2.186	-1.374
ATOM	12	H	RES	1	2.811	2.410	-1.520
ATOM	13	H	RES	1	1.233	3.121	-1.151
ATOM	14	H	RES	1	1.354	1.805	-2.322
ATOM	15	C	RES	1	0.159	0.810	0.108
ATOM	16	C	RES	1	0.048	-0.124	1.276
ATOM	17	H	RES	1	0.362	-1.140	1.003
ATOM	18	H	RES	1	0.720	0.189	2.082
ATOM	19	H	RES	1	-0.965	-0.193	1.678
ATOM	20	C	RES	1	-0.899	1.292	-0.567
ATOM	21	H	RES	1	-0.716	1.984	-1.388
ATOM	22	C	RES	1	-2.353	1.035	-0.249
ATOM	23	H	RES	1	-2.935	1.340	-1.132
ATOM	24	C	RES	1	-2.838	1.878	0.929
ATOM	25	H	RES	1	-2.285	1.631	1.839
ATOM	26	H	RES	1	-2.689	2.941	0.724
ATOM	27	H	RES	1	-3.896	1.693	1.124
ATOM	28	C	RES	1	-2.732	-0.438	-0.045
ATOM	29	O	RES	1	-3.602	-0.787	0.746
ATOM	30	N	RES	1	-2.091	-1.321	-0.865
ATOM	31	H	RES	1	-1.279	-0.982	-1.361
ATOM	32	C	RES	1	-2.286	-2.745	-0.742
ATOM	33	H	RES	1	-1.545	-3.208	-0.077
ATOM	34	H	RES	1	-2.229	-3.225	-1.722
ATOM	35	H	RES	1	-3.274	-2.915	-0.315

TER

REMARK Compound D structure 10
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.839553
 REMARK Sum of electronic and thermal Energies= -690.820953
 REMARK Sum of electronic and thermal Enthalpies= -690.820008
 REMARK Sum of electronic and thermal Free Energies= -690.888270
 REMARK 0 Virtual frequencies used

ATOM							
ATOM	1	H	RES	1	-4.776	-1.093	-1.579
ATOM	2	C	RES	1	-4.792	-0.391	-0.742
ATOM	3	H	RES	1	-5.177	0.569	-1.096
ATOM	4	H	RES	1	-5.484	-0.797	-0.001
ATOM	5	C	RES	1	-3.411	-0.320	-0.137
ATOM	6	O	RES	1	-2.838	-1.311	0.301
ATOM	7	N	RES	1	-2.839	0.921	-0.128
ATOM	8	H	RES	1	-3.383	1.703	-0.453
ATOM	9	C	RES	1	-1.521	1.195	0.467
ATOM	10	H	RES	1	-1.342	2.255	0.223
ATOM	11	C	RES	1	-1.565	1.056	1.980
ATOM	12	H	RES	1	-2.379	1.660	2.388
ATOM	13	H	RES	1	-0.632	1.400	2.436
ATOM	14	H	RES	1	-1.730	0.014	2.264
ATOM	15	C	RES	1	-0.433	0.404	-0.237
ATOM	16	C	RES	1	-0.510	0.443	-1.734
ATOM	17	H	RES	1	-1.287	-0.237	-2.103
ATOM	18	H	RES	1	-0.782	1.444	-2.090
ATOM	19	H	RES	1	0.431	0.165	-2.213
ATOM	20	C	RES	1	0.522	-0.250	0.442
ATOM	21	H	RES	1	0.482	-0.240	1.531
ATOM	22	C	RES	1	1.639	-1.074	-0.127
ATOM	23	H	RES	1	1.429	-1.291	-1.184
ATOM	24	C	RES	1	1.757	-2.408	0.604
ATOM	25	H	RES	1	1.952	-2.250	1.670
ATOM	26	H	RES	1	0.830	-2.979	0.513
ATOM	27	H	RES	1	2.586	-2.991	0.198
ATOM	28	C	RES	1	3.009	-0.376	-0.154
ATOM	29	O	RES	1	4.053	-1.010	-0.264
ATOM	30	N	RES	1	2.971	0.985	-0.096
ATOM	31	H	RES	1	2.068	1.421	0.020
ATOM	32	C	RES	1	4.159	1.800	-0.154
ATOM	33	H	RES	1	5.016	1.128	-0.217
ATOM	34	H	RES	1	4.261	2.420	0.743
ATOM	35	H	RES	1	4.157	2.453	-1.033

TER

REMARK Compound D structure 11
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.839966
 REMARK Sum of electronic and thermal Energies= -690.821378
 REMARK Sum of electronic and thermal Enthalpies= -690.820434
 REMARK Sum of electronic and thermal Free Energies= -690.887910
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.704	-2.398	0.547
ATOM	2	C	RES	1	-3.652	-2.403	0.253
ATOM	3	H	RES	1	-3.046	-2.685	1.118
ATOM	4	H	RES	1	-3.541	-3.167	-0.520
ATOM	5	C	RES	1	-3.299	-1.058	-0.332
ATOM	6	O	RES	1	-3.896	-0.585	-1.295
ATOM	7	N	RES	1	-2.280	-0.395	0.286
ATOM	8	H	RES	1	-1.731	-0.882	0.980
ATOM	9	C	RES	1	-1.755	0.869	-0.249
ATOM	10	H	RES	1	-1.707	0.751	-1.340
ATOM	11	C	RES	1	-2.703	2.020	0.066
ATOM	12	H	RES	1	-3.680	1.828	-0.380
ATOM	13	H	RES	1	-2.314	2.959	-0.341
ATOM	14	H	RES	1	-2.833	2.141	1.146
ATOM	15	C	RES	1	-0.360	1.080	0.290
ATOM	16	C	RES	1	-0.250	1.445	1.740
ATOM	17	H	RES	1	-0.526	2.494	1.904
ATOM	18	H	RES	1	-0.945	0.855	2.349
ATOM	19	H	RES	1	0.751	1.271	2.137
ATOM	20	C	RES	1	0.691	0.929	-0.530
ATOM	21	H	RES	1	0.495	0.648	-1.567
ATOM	22	C	RES	1	2.147	1.071	-0.169
ATOM	23	H	RES	1	2.241	1.747	0.688
ATOM	24	C	RES	1	2.944	1.649	-1.334
ATOM	25	H	RES	1	2.802	1.069	-2.254
ATOM	26	H	RES	1	2.607	2.664	-1.557
ATOM	27	H	RES	1	4.016	1.693	-1.117
ATOM	28	C	RES	1	2.643	-0.277	0.366
ATOM	29	O	RES	1	2.380	-0.635	1.510
ATOM	30	N	RES	1	3.344	-1.053	-0.508
ATOM	31	H	RES	1	3.533	-0.699	-1.432
ATOM	32	C	RES	1	3.828	-2.369	-0.161
ATOM	33	H	RES	1	3.548	-2.558	0.876
ATOM	34	H	RES	1	4.917	-2.428	-0.250
ATOM	35	H	RES	1	3.379	-3.139	-0.796

TER

REMARK Compound D structure 12
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.839101
 REMARK Sum of electronic and thermal Energies= -690.820450
 REMARK Sum of electronic and thermal Enthalpies= -690.819506
 REMARK Sum of electronic and thermal Free Energies= -690.887452
 REMARK 0 Virtual frequencies used

ATOM							
ATOM	1	H	RES	1	-4.706	-2.433	0.286
ATOM	2	C	RES	1	-3.684	-2.378	-0.093
ATOM	3	H	RES	1	-3.014	-2.843	0.634
ATOM	4	H	RES	1	-3.656	-2.954	-1.021
ATOM	5	C	RES	1	-3.351	-0.938	-0.400
ATOM	6	O	RES	1	-4.027	-0.260	-1.167
ATOM	7	N	RES	1	-2.257	-0.435	0.247
ATOM	8	H	RES	1	-1.628	-1.091	0.688
ATOM	9	C	RES	1	-1.719	0.895	-0.082
ATOM	10	H	RES	1	-1.691	0.971	-1.178
ATOM	11	C	RES	1	-2.641	1.988	0.448
ATOM	12	H	RES	1	-3.618	1.911	-0.030
ATOM	13	H	RES	1	-2.222	2.976	0.233
ATOM	14	H	RES	1	-2.780	1.898	1.530
ATOM	15	C	RES	1	-0.307	0.994	0.452
ATOM	16	C	RES	1	-0.177	1.139	1.938
ATOM	17	H	RES	1	-0.551	2.113	2.275
ATOM	18	H	RES	1	-0.779	0.389	2.467
ATOM	19	H	RES	1	0.853	1.047	2.288
ATOM	20	C	RES	1	0.722	0.947	-0.409
ATOM	21	H	RES	1	0.494	0.827	-1.470
ATOM	22	C	RES	1	2.191	1.021	-0.105
ATOM	23	H	RES	1	2.339	1.283	0.951
ATOM	24	C	RES	1	2.882	2.060	-0.983
ATOM	25	H	RES	1	2.788	1.779	-2.035
ATOM	26	H	RES	1	2.433	3.046	-0.840
ATOM	27	H	RES	1	3.949	2.127	-0.753
ATOM	28	C	RES	1	2.793	-0.363	-0.364
ATOM	29	O	RES	1	3.063	-0.756	-1.492
ATOM	30	N	RES	1	2.960	-1.132	0.753
ATOM	31	H	RES	1	2.730	-0.734	1.650
ATOM	32	C	RES	1	3.466	-2.483	0.698
ATOM	33	H	RES	1	3.655	-2.717	-0.351
ATOM	34	H	RES	1	2.741	-3.200	1.095
ATOM	35	H	RES	1	4.403	-2.583	1.256

TER

REMARK Compound D structure 13
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.840061
 REMARK Sum of electronic and thermal Energies= -690.821760
 REMARK Sum of electronic and thermal Enthalpies= -690.820816
 REMARK Sum of electronic and thermal Free Energies= -690.886837
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.596	-0.547	1.004
ATOM	2	C	RES	1	-4.750	-1.098	0.588
ATOM	3	H	RES	1	-4.289	-1.690	1.382
ATOM	4	H	RES	1	-5.154	-1.775	-0.169
ATOM	5	C	RES	1	-3.808	-0.125	-0.076
ATOM	6	O	RES	1	-4.178	0.660	-0.944
ATOM	7	N	RES	1	-2.513	-0.166	0.357
ATOM	8	H	RES	1	-2.225	-0.932	0.947
ATOM	9	C	RES	1	-1.471	0.630	-0.306
ATOM	10	H	RES	1	-1.653	0.552	-1.386
ATOM	11	C	RES	1	-1.585	2.098	0.094
ATOM	12	H	RES	1	-2.558	2.489	-0.206
ATOM	13	H	RES	1	-0.806	2.690	-0.399
ATOM	14	H	RES	1	-1.477	2.221	1.176
ATOM	15	C	RES	1	-0.115	0.043	0.010
ATOM	16	C	RES	1	0.381	0.224	1.414
ATOM	17	H	RES	1	0.711	1.257	1.586
ATOM	18	H	RES	1	-0.413	0.039	2.147
ATOM	19	H	RES	1	1.222	-0.428	1.658
ATOM	20	C	RES	1	0.588	-0.571	-0.957
ATOM	21	H	RES	1	0.122	-0.649	-1.940
ATOM	22	C	RES	1	1.947	-1.210	-0.803
ATOM	23	H	RES	1	2.349	-1.361	-1.815
ATOM	24	C	RES	1	1.867	-2.580	-0.134
ATOM	25	H	RES	1	1.470	-2.497	0.882
ATOM	26	H	RES	1	1.209	-3.244	-0.701
ATOM	27	H	RES	1	2.858	-3.032	-0.061
ATOM	28	C	RES	1	2.991	-0.329	-0.103
ATOM	29	O	RES	1	3.813	-0.785	0.684
ATOM	30	N	RES	1	2.974	0.984	-0.474
ATOM	31	H	RES	1	2.194	1.304	-1.029
ATOM	32	C	RES	1	3.860	1.961	0.110
ATOM	33	H	RES	1	4.659	1.422	0.620
ATOM	34	H	RES	1	3.346	2.593	0.845
ATOM	35	H	RES	1	4.295	2.603	-0.661

TER

REMARK Compound D structure 14
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.838395
 REMARK Sum of electronic and thermal Energies= -690.819782
 REMARK Sum of electronic and thermal Enthalpies= -690.818838
 REMARK Sum of electronic and thermal Free Energies= -690.886699
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.298	0.812	-1.186
ATOM	2	C	RES	1	-4.810	0.887	-0.212
ATOM	3	H	RES	1	-4.780	1.948	0.048
ATOM	4	H	RES	1	-5.417	0.363	0.530
ATOM	5	C	RES	1	-3.395	0.373	-0.331
ATOM	6	O	RES	1	-2.603	0.834	-1.146
ATOM	7	N	RES	1	-3.059	-0.617	0.548
ATOM	8	H	RES	1	-3.778	-0.982	1.151
ATOM	9	C	RES	1	-1.747	-1.286	0.563
ATOM	10	H	RES	1	-1.777	-1.900	1.477
ATOM	11	C	RES	1	-1.600	-2.210	-0.635
ATOM	12	H	RES	1	-2.446	-2.901	-0.682
ATOM	13	H	RES	1	-0.684	-2.802	-0.570
ATOM	14	H	RES	1	-1.574	-1.630	-1.561
ATOM	15	C	RES	1	-0.629	-0.278	0.752
ATOM	16	C	RES	1	-0.889	0.747	1.813
ATOM	17	H	RES	1	-1.552	1.536	1.440
ATOM	18	H	RES	1	-1.388	0.305	2.684
ATOM	19	H	RES	1	0.026	1.232	2.162
ATOM	20	C	RES	1	0.486	-0.321	0.012
ATOM	21	H	RES	1	0.588	-1.063	-0.777
ATOM	22	C	RES	1	1.617	0.662	0.056
ATOM	23	H	RES	1	1.688	1.122	1.052
ATOM	24	C	RES	1	1.373	1.774	-0.976
ATOM	25	H	RES	1	1.322	1.344	-1.980
ATOM	26	H	RES	1	0.420	2.272	-0.777
ATOM	27	H	RES	1	2.175	2.520	-0.961
ATOM	28	C	RES	1	2.933	-0.033	-0.274
ATOM	29	O	RES	1	3.056	-0.769	-1.247
ATOM	30	N	RES	1	3.966	0.257	0.571
ATOM	31	H	RES	1	3.787	0.858	1.359
ATOM	32	C	RES	1	5.295	-0.275	0.387
ATOM	33	H	RES	1	5.277	-0.887	-0.516
ATOM	34	H	RES	1	5.598	-0.902	1.232
ATOM	35	H	RES	1	6.032	0.524	0.258

TER

REMARK Compound D structure 15
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.838489
 REMARK Sum of electronic and thermal Energies= -690.819989
 REMARK Sum of electronic and thermal Enthalpies= -690.819045
 REMARK Sum of electronic and thermal Free Energies= -690.886307
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.463	0.175	-0.942
ATOM	2	C	RES	1	-4.564	0.795	-0.929
ATOM	3	H	RES	1	-4.390	1.121	-1.957
ATOM	4	H	RES	1	-4.751	1.674	-0.308
ATOM	5	C	RES	1	-3.395	-0.049	-0.480
ATOM	6	O	RES	1	-3.115	-1.107	-1.032
ATOM	7	N	RES	1	-2.694	0.461	0.578
ATOM	8	H	RES	1	-2.945	1.387	0.889
ATOM	9	C	RES	1	-1.489	-0.113	1.192
ATOM	10	H	RES	1	-1.447	0.339	2.191
ATOM	11	C	RES	1	-1.589	-1.625	1.385
ATOM	12	H	RES	1	-2.545	-1.896	1.842
ATOM	13	H	RES	1	-0.785	-1.948	2.053
ATOM	14	H	RES	1	-1.512	-2.165	0.441
ATOM	15	C	RES	1	-0.217	0.283	0.466
ATOM	16	C	RES	1	-0.174	0.021	-1.006
ATOM	17	H	RES	1	-0.397	-1.028	-1.233
ATOM	18	H	RES	1	-0.950	0.599	-1.520
ATOM	19	H	RES	1	0.784	0.279	-1.460
ATOM	20	C	RES	1	0.804	0.791	1.179
ATOM	21	H	RES	1	0.634	0.955	2.245
ATOM	22	C	RES	1	2.158	1.196	0.653
ATOM	23	H	RES	1	2.813	1.342	1.524
ATOM	24	C	RES	1	2.111	2.519	-0.109
ATOM	25	H	RES	1	1.464	2.441	-0.987
ATOM	26	H	RES	1	1.716	3.313	0.530
ATOM	27	H	RES	1	3.108	2.798	-0.455
ATOM	28	C	RES	1	2.884	0.127	-0.180
ATOM	29	O	RES	1	3.657	0.425	-1.085
ATOM	30	N	RES	1	2.669	-1.163	0.210
ATOM	31	H	RES	1	1.904	-1.334	0.846
ATOM	32	C	RES	1	3.219	-2.278	-0.524
ATOM	33	H	RES	1	4.084	-1.919	-1.083
ATOM	34	H	RES	1	2.498	-2.695	-1.238
ATOM	35	H	RES	1	3.535	-3.069	0.161

TER

REMARK Compound D structure 16
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.838605
 REMARK Sum of electronic and thermal Energies= -690.820194
 REMARK Sum of electronic and thermal Enthalpies= -690.819250
 REMARK Sum of electronic and thermal Free Energies= -690.885956
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-3.618	-2.859	0.106
ATOM	2	C	RES	1	-3.780	-2.067	-0.628
ATOM	3	H	RES	1	-3.360	-2.381	-1.588
ATOM	4	H	RES	1	-4.861	-1.955	-0.740
ATOM	5	C	RES	1	-3.210	-0.775	-0.091
ATOM	6	O	RES	1	-3.560	-0.322	0.995
ATOM	7	N	RES	1	-2.304	-0.165	-0.911
ATOM	8	H	RES	1	-2.009	-0.677	-1.728
ATOM	9	C	RES	1	-1.576	1.088	-0.647
ATOM	10	H	RES	1	-1.223	1.408	-1.635
ATOM	11	C	RES	1	-2.483	2.189	-0.111
ATOM	12	H	RES	1	-3.354	2.315	-0.760
ATOM	13	H	RES	1	-1.928	3.131	-0.093
ATOM	14	H	RES	1	-2.850	1.971	0.892
ATOM	15	C	RES	1	-0.342	0.856	0.205
ATOM	16	C	RES	1	-0.567	0.324	1.585
ATOM	17	H	RES	1	-1.382	0.846	2.094
ATOM	18	H	RES	1	-0.876	-0.728	1.554
ATOM	19	H	RES	1	0.327	0.395	2.211
ATOM	20	C	RES	1	0.863	1.128	-0.322
ATOM	21	H	RES	1	0.903	1.481	-1.355
ATOM	22	C	RES	1	2.211	0.972	0.325
ATOM	23	H	RES	1	2.089	0.900	1.413
ATOM	24	C	RES	1	3.129	2.140	-0.008
ATOM	25	H	RES	1	3.306	2.182	-1.085
ATOM	26	H	RES	1	2.683	3.085	0.313
ATOM	27	H	RES	1	4.102	2.034	0.479
ATOM	28	C	RES	1	2.823	-0.341	-0.179
ATOM	29	O	RES	1	3.488	-0.406	-1.206
ATOM	30	N	RES	1	2.534	-1.430	0.592
ATOM	31	H	RES	1	1.938	-1.304	1.395
ATOM	32	C	RES	1	2.926	-2.769	0.222
ATOM	33	H	RES	1	3.603	-2.688	-0.629
ATOM	34	H	RES	1	2.064	-3.378	-0.074
ATOM	35	H	RES	1	3.445	-3.269	1.044

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REMARK Compound D structure 17
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.839466
 REMARK Sum of electronic and thermal Energies= -690.821629
 REMARK Sum of electronic and thermal Enthalpies= -690.820685
 REMARK Sum of electronic and thermal Free Energies= -690.885733
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.997	-1.045	-1.686
ATOM	2	C	RES	1	4.116	-1.529	-1.256
ATOM	3	H	RES	1	3.415	-1.755	-2.064
ATOM	4	H	RES	1	4.456	-2.465	-0.807
ATOM	5	C	RES	1	3.546	-0.642	-0.178
ATOM	6	O	RES	1	4.188	-0.324	0.817
ATOM	7	N	RES	1	2.271	-0.202	-0.389
ATOM	8	H	RES	1	1.738	-0.589	-1.153
ATOM	9	C	RES	1	1.575	0.598	0.613
ATOM	10	H	RES	1	1.801	0.145	1.589
ATOM	11	C	RES	1	2.115	2.030	0.635
ATOM	12	H	RES	1	3.184	2.021	0.857
ATOM	13	H	RES	1	1.609	2.623	1.403
ATOM	14	H	RES	1	1.950	2.511	-0.333
ATOM	15	C	RES	1	0.075	0.592	0.413
ATOM	16	C	RES	1	-0.702	0.710	1.687
ATOM	17	H	RES	1	-0.619	-0.209	2.281
ATOM	18	H	RES	1	-0.292	1.513	2.311
ATOM	19	H	RES	1	-1.764	0.916	1.536
ATOM	20	C	RES	1	-0.488	0.544	-0.807
ATOM	21	H	RES	1	0.168	0.526	-1.679
ATOM	22	C	RES	1	-1.963	0.624	-1.118
ATOM	23	H	RES	1	-2.094	0.278	-2.154
ATOM	24	C	RES	1	-2.483	2.059	-1.050
ATOM	25	H	RES	1	-2.374	2.466	-0.041
ATOM	26	H	RES	1	-1.923	2.702	-1.734
ATOM	27	H	RES	1	-3.543	2.096	-1.308
ATOM	28	C	RES	1	-2.863	-0.310	-0.297
ATOM	29	O	RES	1	-3.999	0.009	0.036
ATOM	30	N	RES	1	-2.338	-1.542	-0.035
ATOM	31	H	RES	1	-1.353	-1.674	-0.208
ATOM	32	C	RES	1	-3.042	-2.516	0.764
ATOM	33	H	RES	1	-4.100	-2.252	0.756
ATOM	34	H	RES	1	-2.697	-2.522	1.805
ATOM	35	H	RES	1	-2.917	-3.518	0.347

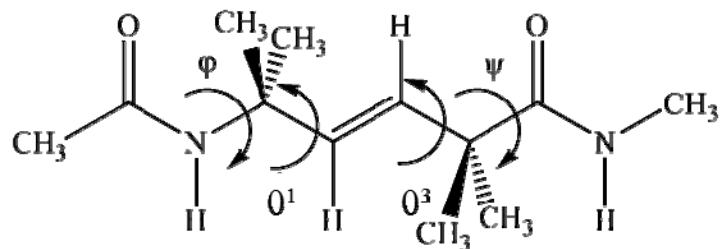
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REMARK Compound D structure 18
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -690.836565
 REMARK Sum of electronic and thermal Energies= -690.818162
 REMARK Sum of electronic and thermal Enthalpies= -690.817217
 REMARK Sum of electronic and thermal Free Energies= -690.883614
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.989	1.217	1.175
ATOM	2	C	RES	1	-3.945	1.206	1.496
ATOM	3	H	RES	1	-3.632	2.248	1.592
ATOM	4	H	RES	1	-3.884	0.727	2.476
ATOM	5	C	RES	1	-3.111	0.541	0.425
ATOM	6	O	RES	1	-3.075	0.963	-0.724
ATOM	7	N	RES	1	-2.407	-0.556	0.840
ATOM	8	H	RES	1	-2.445	-0.797	1.817
ATOM	9	C	RES	1	-1.525	-1.349	-0.012
ATOM	10	H	RES	1	-1.286	-2.241	0.589
ATOM	11	C	RES	1	-2.251	-1.846	-1.265
ATOM	12	H	RES	1	-3.220	-2.269	-0.991
ATOM	13	H	RES	1	-1.668	-2.628	-1.758
ATOM	14	H	RES	1	-2.419	-1.029	-1.968
ATOM	15	C	RES	1	-0.199	-0.678	-0.336
ATOM	16	C	RES	1	0.695	-1.499	-1.217
ATOM	17	H	RES	1	0.739	-2.542	-0.876
ATOM	18	H	RES	1	0.314	-1.526	-2.244
ATOM	19	H	RES	1	1.718	-1.121	-1.265
ATOM	20	C	RES	1	0.132	0.535	0.134
ATOM	21	H	RES	1	-0.604	1.061	0.739
ATOM	22	C	RES	1	1.396	1.298	-0.181
ATOM	23	H	RES	1	1.423	2.168	0.491
ATOM	24	C	RES	1	1.404	1.829	-1.613
ATOM	25	H	RES	1	1.390	1.007	-2.334
ATOM	26	H	RES	1	0.521	2.446	-1.793
ATOM	27	H	RES	1	2.304	2.417	-1.800
ATOM	28	C	RES	1	2.704	0.554	0.123
ATOM	29	O	RES	1	3.719	0.708	-0.548
ATOM	30	N	RES	1	2.676	-0.234	1.238
ATOM	31	H	RES	1	1.770	-0.439	1.633
ATOM	32	C	RES	1	3.803	-1.052	1.615
ATOM	33	H	RES	1	4.706	-0.588	1.217
ATOM	34	H	RES	1	3.734	-2.068	1.205
ATOM	35	H	RES	1	3.881	-1.116	2.703

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COMPOUND E



REMARK Compound E structure 01
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.130470
 REMARK Sum of electronic and thermal Energies= -730.111038
 REMARK Sum of electronic and thermal Enthalpies= -730.110094
 REMARK Sum of electronic and thermal Free Energies= -730.177310
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-2.874	2.847	1.595
ATOM	2	C	RES	1	-3.383	2.255	0.832
ATOM	3	H	RES	1	-3.720	2.951	0.061
ATOM	4	H	RES	1	-4.257	1.776	1.281
ATOM	5	C	RES	1	-2.396	1.291	0.222
ATOM	6	O	RES	1	-1.364	1.691	-0.318
ATOM	7	N	RES	1	-2.730	-0.025	0.317
ATOM	8	H	RES	1	-3.610	-0.255	0.753
ATOM	9	C	RES	1	-1.943	-1.150	-0.245
ATOM	10	C	RES	1	-1.957	-1.070	-1.769
ATOM	11	H	RES	1	-1.493	-0.144	-2.117
ATOM	12	H	RES	1	-2.987	-1.101	-2.134
ATOM	13	H	RES	1	-1.417	-1.916	-2.204
ATOM	14	C	RES	1	-2.645	-2.427	0.218
ATOM	15	H	RES	1	-3.681	-2.461	-0.140
ATOM	16	H	RES	1	-2.650	-2.504	1.311
ATOM	17	H	RES	1	-2.125	-3.303	-0.176
ATOM	18	C	RES	1	-0.556	-1.103	0.349
ATOM	19	H	RES	1	-0.544	-1.072	1.440
ATOM	20	C	RES	1	0.592	-1.076	-0.331
ATOM	21	H	RES	1	0.556	-1.085	-1.423
ATOM	22	C	RES	1	1.973	-0.930	0.241
ATOM	23	C	RES	1	2.009	-1.079	1.764
ATOM	24	H	RES	1	1.637	-2.065	2.065
ATOM	25	H	RES	1	1.402	-0.317	2.265
ATOM	26	H	RES	1	3.037	-0.973	2.120
ATOM	27	C	RES	1	2.906	-1.961	-0.397
ATOM	28	H	RES	1	2.881	-1.899	-1.489
ATOM	29	H	RES	1	2.610	-2.974	-0.105
ATOM	30	H	RES	1	3.935	-1.780	-0.077
ATOM	31	C	RES	1	2.535	0.484	-0.070
ATOM	32	O	RES	1	3.745	0.704	-0.051
ATOM	33	N	RES	1	1.619	1.453	-0.303
ATOM	34	H	RES	1	0.626	1.248	-0.289
ATOM	35	C	RES	1	2.030	2.821	-0.511
ATOM	36	H	RES	1	2.703	2.901	-1.370
ATOM	37	H	RES	1	1.141	3.426	-0.691
ATOM	38	H	RES	1	2.565	3.212	0.360

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REMARK Compound E structure 02
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.129525
 REMARK Sum of electronic and thermal Energies= -730.110094
 REMARK Sum of electronic and thermal Enthalpies= -730.109150
 REMARK Sum of electronic and thermal Free Energies= -730.176300
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	1.580	2.842	1.952
ATOM	2	C	RES	1	2.448	2.462	1.407
ATOM	3	H	RES	1	3.168	2.064	2.127
ATOM	4	H	RES	1	2.896	3.313	0.891
ATOM	5	C	RES	1	1.978	1.460	0.383
ATOM	6	O	RES	1	1.214	1.783	-0.527
ATOM	7	N	RES	1	2.440	0.191	0.551
ATOM	8	H	RES	1	3.059	0.017	1.328
ATOM	9	C	RES	1	2.145	-0.948	-0.337
ATOM	10	C	RES	1	2.897	-2.152	0.233
ATOM	11	H	RES	1	2.572	-2.370	1.255
ATOM	12	H	RES	1	3.980	-1.978	0.229
ATOM	13	H	RES	1	2.700	-3.039	-0.374
ATOM	14	C	RES	1	2.654	-0.645	-1.750
ATOM	15	H	RES	1	3.732	-0.454	-1.734
ATOM	16	H	RES	1	2.148	0.228	-2.166
ATOM	17	H	RES	1	2.469	-1.501	-2.406
ATOM	18	C	RES	1	0.666	-1.257	-0.386
ATOM	19	H	RES	1	0.385	-1.916	-1.209
ATOM	20	C	RES	1	-0.270	-0.803	0.448
ATOM	21	H	RES	1	0.038	-0.136	1.258
ATOM	22	C	RES	1	-1.750	-1.037	0.360
ATOM	23	C	RES	1	-2.129	-2.078	-0.696
ATOM	24	H	RES	1	-1.666	-3.045	-0.468
ATOM	25	H	RES	1	-1.814	-1.776	-1.700
ATOM	26	H	RES	1	-3.214	-2.207	-0.711
ATOM	27	C	RES	1	-2.276	-1.485	1.728
ATOM	28	H	RES	1	-2.004	-0.771	2.513
ATOM	29	H	RES	1	-1.858	-2.461	1.995
ATOM	30	H	RES	1	-3.366	-1.555	1.702
ATOM	31	C	RES	1	-2.502	0.266	-0.023
ATOM	32	O	RES	1	-3.723	0.343	0.104
ATOM	33	N	RES	1	-1.758	1.276	-0.530
ATOM	34	H	RES	1	-0.751	1.194	-0.621
ATOM	35	C	RES	1	-2.382	2.511	-0.946
ATOM	36	H	RES	1	-3.025	2.902	-0.152
ATOM	37	H	RES	1	-1.602	3.237	-1.174
ATOM	38	H	RES	1	-3.009	2.364	-1.832

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REMARK Compound E structure 03
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.122837
 REMARK Sum of electronic and thermal Energies= -730.103095
 REMARK Sum of electronic and thermal Enthalpies= -730.102150
 REMARK Sum of electronic and thermal Free Energies= -730.171091
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.658	-0.984	-1.168
ATOM	2	C	RES	1	-4.953	-1.301	-0.397
ATOM	3	H	RES	1	-4.444	-2.207	-0.737
ATOM	4	H	RES	1	-5.540	-1.539	0.493
ATOM	5	C	RES	1	-4.026	-0.151	-0.080
ATOM	6	O	RES	1	-4.453	0.941	0.279
ATOM	7	N	RES	1	-2.696	-0.423	-0.234
ATOM	8	H	RES	1	-2.433	-1.377	-0.432
ATOM	9	C	RES	1	-1.594	0.512	0.093
ATOM	10	C	RES	1	-1.637	0.869	1.575
ATOM	11	H	RES	1	-1.514	-0.020	2.201
ATOM	12	H	RES	1	-2.598	1.331	1.809
ATOM	13	H	RES	1	-0.843	1.579	1.826
ATOM	14	C	RES	1	-1.726	1.780	-0.762
ATOM	15	H	RES	1	-2.657	2.302	-0.539
ATOM	16	H	RES	1	-1.710	1.532	-1.828
ATOM	17	H	RES	1	-0.887	2.453	-0.554
ATOM	18	C	RES	1	-0.324	-0.193	-0.318
ATOM	19	H	RES	1	-0.305	-0.497	-1.368
ATOM	20	C	RES	1	0.746	-0.417	0.451
ATOM	21	H	RES	1	0.715	-0.104	1.497
ATOM	22	C	RES	1	2.043	-1.061	0.036
ATOM	23	C	RES	1	2.372	-2.186	1.021
ATOM	24	H	RES	1	1.619	-2.977	0.955
ATOM	25	H	RES	1	2.393	-1.820	2.052
ATOM	26	H	RES	1	3.355	-2.605	0.798
ATOM	27	C	RES	1	2.003	-1.624	-1.388
ATOM	28	H	RES	1	1.808	-0.847	-2.135
ATOM	29	H	RES	1	1.223	-2.388	-1.478
ATOM	30	H	RES	1	2.964	-2.086	-1.629
ATOM	31	C	RES	1	3.212	-0.043	0.064
ATOM	32	O	RES	1	4.372	-0.407	0.224
ATOM	33	N	RES	1	2.866	1.254	-0.161
ATOM	34	H	RES	1	1.889	1.467	-0.305
ATOM	35	C	RES	1	3.843	2.311	-0.268
ATOM	36	H	RES	1	3.873	2.731	-1.279
ATOM	37	H	RES	1	3.633	3.116	0.441
ATOM	38	H	RES	1	4.819	1.881	-0.039

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REMARK Compound E structure 04
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.122548
 REMARK Sum of electronic and thermal Energies= -730.102951
 REMARK Sum of electronic and thermal Enthalpies= -730.102006
 REMARK Sum of electronic and thermal Free Energies= -730.170583
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.515	-0.900	-0.936
ATOM	2	C	RES	1	-4.707	-1.265	-0.299
ATOM	3	H	RES	1	-4.516	-2.301	-0.588
ATOM	4	H	RES	1	-5.042	-1.246	0.742
ATOM	5	C	RES	1	-3.466	-0.446	-0.565
ATOM	6	O	RES	1	-3.004	-0.323	-1.696
ATOM	7	N	RES	1	-2.915	0.145	0.535
ATOM	8	H	RES	1	-3.297	-0.097	1.437
ATOM	9	C	RES	1	-1.658	0.930	0.542
ATOM	10	C	RES	1	-1.471	1.421	1.972
ATOM	11	H	RES	1	-1.359	0.590	2.677
ATOM	12	H	RES	1	-2.329	2.027	2.277
ATOM	13	H	RES	1	-0.579	2.048	2.051
ATOM	14	C	RES	1	-1.798	2.134	-0.397
ATOM	15	H	RES	1	-2.658	2.746	-0.107
ATOM	16	H	RES	1	-1.936	1.810	-1.430
ATOM	17	H	RES	1	-0.899	2.755	-0.336
ATOM	18	C	RES	1	-0.526	0.050	0.061
ATOM	19	H	RES	1	-0.707	-0.389	-0.920
ATOM	20	C	RES	1	0.618	-0.192	0.711
ATOM	21	H	RES	1	0.783	0.257	1.694
ATOM	22	C	RES	1	1.761	-1.048	0.231
ATOM	23	C	RES	1	2.108	-2.065	1.322
ATOM	24	H	RES	1	1.269	-2.749	1.479
ATOM	25	H	RES	1	2.329	-1.569	2.273
ATOM	26	H	RES	1	2.992	-2.638	1.036
ATOM	27	C	RES	1	1.444	-1.787	-1.074
ATOM	28	H	RES	1	1.227	-1.098	-1.897
ATOM	29	H	RES	1	0.574	-2.439	-0.943
ATOM	30	H	RES	1	2.297	-2.405	-1.367
ATOM	31	C	RES	1	3.022	-0.194	-0.048
ATOM	32	O	RES	1	4.154	-0.650	0.076
ATOM	33	N	RES	1	2.778	1.070	-0.494
ATOM	34	H	RES	1	1.815	1.354	-0.602
ATOM	35	C	RES	1	3.832	1.958	-0.922
ATOM	36	H	RES	1	4.781	1.510	-0.627
ATOM	37	H	RES	1	3.834	2.094	-2.010
ATOM	38	H	RES	1	3.736	2.938	-0.447

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REMARK Compound E structure 05
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.121925
 REMARK Sum of electronic and thermal Energies= -730.102115
 REMARK Sum of electronic and thermal Enthalpies= -730.101171
 REMARK Sum of electronic and thermal Free Energies= -730.170374
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	2.468	-2.260	-2.385
ATOM	2	C	RES	1	3.187	-1.516	-2.033
ATOM	3	H	RES	1	3.321	-0.762	-2.814
ATOM	4	H	RES	1	4.133	-2.037	-1.879
ATOM	5	C	RES	1	2.708	-0.963	-0.712
ATOM	6	O	RES	1	2.594	-1.669	0.283
ATOM	7	N	RES	1	2.402	0.371	-0.721
ATOM	8	H	RES	1	2.503	0.872	-1.590
ATOM	9	C	RES	1	1.890	1.125	0.432
ATOM	10	C	RES	1	1.750	2.580	-0.026
ATOM	11	H	RES	1	1.072	2.661	-0.884
ATOM	12	H	RES	1	2.723	2.999	-0.304
ATOM	13	H	RES	1	1.340	3.193	0.781
ATOM	14	C	RES	1	2.883	1.054	1.596
ATOM	15	H	RES	1	3.857	1.446	1.287
ATOM	16	H	RES	1	3.008	0.026	1.938
ATOM	17	H	RES	1	2.521	1.661	2.432
ATOM	18	C	RES	1	0.536	0.622	0.884
ATOM	19	H	RES	1	0.233	1.001	1.862
ATOM	20	C	RES	1	-0.270	-0.201	0.212
ATOM	21	H	RES	1	0.069	-0.583	-0.754
ATOM	22	C	RES	1	-1.602	-0.739	0.660
ATOM	23	C	RES	1	-1.552	-2.268	0.577
ATOM	24	H	RES	1	-0.793	-2.657	1.262
ATOM	25	H	RES	1	-1.295	-2.602	-0.434
ATOM	26	H	RES	1	-2.527	-2.692	0.829
ATOM	27	C	RES	1	-1.963	-0.318	2.089
ATOM	28	H	RES	1	-2.036	0.770	2.192
ATOM	29	H	RES	1	-1.207	-0.678	2.794
ATOM	30	H	RES	1	-2.928	-0.748	2.369
ATOM	31	C	RES	1	-2.757	-0.243	-0.241
ATOM	32	O	RES	1	-3.799	-0.877	-0.365
ATOM	33	N	RES	1	-2.554	0.969	-0.831
ATOM	34	H	RES	1	-1.676	1.435	-0.656
ATOM	35	C	RES	1	-3.568	1.630	-1.616
ATOM	36	H	RES	1	-3.932	2.540	-1.126
ATOM	37	H	RES	1	-3.191	1.893	-2.609
ATOM	38	H	RES	1	-4.402	0.936	-1.726

TER

REMARK Compound E structure 06
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.122230
 REMARK Sum of electronic and thermal Energies= -730.102595
 REMARK Sum of electronic and thermal Enthalpies= -730.101651
 REMARK Sum of electronic and thermal Free Energies= -730.170317
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-3.274	3.044	0.912
ATOM	2	C	RES	1	-3.753	2.247	0.340
ATOM	3	H	RES	1	-3.821	2.554	-0.707
ATOM	4	H	RES	1	-4.764	2.135	0.738
ATOM	5	C	RES	1	-2.995	0.959	0.562
ATOM	6	O	RES	1	-2.798	0.513	1.689
ATOM	7	N	RES	1	-2.560	0.340	-0.573
ATOM	8	H	RES	1	-2.743	0.791	-1.457
ATOM	9	C	RES	1	-1.812	-0.942	-0.623
ATOM	10	C	RES	1	-1.594	-1.246	-2.099
ATOM	11	H	RES	1	-1.001	-0.468	-2.593
ATOM	12	H	RES	1	-2.557	-1.329	-2.614
ATOM	13	H	RES	1	-1.071	-2.197	-2.223
ATOM	14	C	RES	1	-2.652	-2.053	0.014
ATOM	15	H	RES	1	-3.612	-2.150	-0.503
ATOM	16	H	RES	1	-2.843	-1.841	1.067
ATOM	17	H	RES	1	-2.121	-3.007	-0.061
ATOM	18	C	RES	1	-0.520	-0.787	0.149
ATOM	19	H	RES	1	-0.670	-0.554	1.202
ATOM	20	C	RES	1	0.715	-0.929	-0.342
ATOM	21	H	RES	1	0.851	-1.169	-1.400
ATOM	22	C	RES	1	2.007	-0.798	0.423
ATOM	23	C	RES	1	1.791	-0.602	1.927
ATOM	24	H	RES	1	1.254	-1.457	2.351
ATOM	25	H	RES	1	1.213	0.302	2.148
ATOM	26	H	RES	1	2.756	-0.518	2.432
ATOM	27	C	RES	1	2.851	-2.053	0.186
ATOM	28	H	RES	1	3.021	-2.224	-0.881
ATOM	29	H	RES	1	2.342	-2.930	0.597
ATOM	30	H	RES	1	3.828	-1.949	0.662
ATOM	31	C	RES	1	2.820	0.427	-0.063
ATOM	32	O	RES	1	4.044	0.454	-0.015
ATOM	33	N	RES	1	2.073	1.485	-0.490
ATOM	34	H	RES	1	1.067	1.394	-0.459
ATOM	35	C	RES	1	2.661	2.750	-0.856
ATOM	36	H	RES	1	3.740	2.605	-0.923
ATOM	37	H	RES	1	2.285	3.092	-1.825
ATOM	38	H	RES	1	2.460	3.525	-0.108

TER

REMARK Compound E structure 07
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.121583
 REMARK Sum of electronic and thermal Energies= -730.101919
 REMARK Sum of electronic and thermal Enthalpies= -730.100975
 REMARK Sum of electronic and thermal Free Energies= -730.170183
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.348	-1.320	0.297
ATOM	2	C	RES	1	-4.650	-1.156	-0.526
ATOM	3	H	RES	1	-5.105	-0.462	-1.239
ATOM	4	H	RES	1	-4.504	-2.120	-1.017
ATOM	5	C	RES	1	-3.329	-0.688	0.037
ATOM	6	O	RES	1	-2.670	-1.378	0.806
ATOM	7	N	RES	1	-2.931	0.555	-0.370
ATOM	8	H	RES	1	-3.530	1.067	-1.001
ATOM	9	C	RES	1	-1.674	1.208	0.054
ATOM	10	C	RES	1	-1.696	1.449	1.560
ATOM	11	H	RES	1	-1.774	0.505	2.103
ATOM	12	H	RES	1	-2.552	2.075	1.824
ATOM	13	H	RES	1	-0.787	1.968	1.881
ATOM	14	C	RES	1	-1.621	2.546	-0.687
ATOM	15	H	RES	1	-2.488	3.168	-0.436
ATOM	16	H	RES	1	-1.598	2.401	-1.772
ATOM	17	H	RES	1	-0.722	3.098	-0.403
ATOM	18	C	RES	1	-0.515	0.354	-0.404
ATOM	19	H	RES	1	-0.543	0.116	-1.469
ATOM	20	C	RES	1	0.474	-0.121	0.357
ATOM	21	H	RES	1	0.464	0.096	1.427
ATOM	22	C	RES	1	1.600	-1.019	-0.082
ATOM	23	C	RES	1	1.590	-2.263	0.813
ATOM	24	H	RES	1	0.650	-2.807	0.685
ATOM	25	H	RES	1	1.685	-1.993	1.869
ATOM	26	H	RES	1	2.429	-2.915	0.559
ATOM	27	C	RES	1	1.481	-1.447	-1.549
ATOM	28	H	RES	1	1.497	-0.590	-2.231
ATOM	29	H	RES	1	0.547	-1.995	-1.709
ATOM	30	H	RES	1	2.315	-2.102	-1.811
ATOM	31	C	RES	1	2.979	-0.333	0.057
ATOM	32	O	RES	1	4.011	-0.981	0.188
ATOM	33	N	RES	1	2.965	1.026	-0.041
ATOM	34	H	RES	1	2.070	1.479	-0.161
ATOM	35	C	RES	1	4.169	1.820	-0.029
ATOM	36	H	RES	1	4.310	2.351	-0.977
ATOM	37	H	RES	1	4.155	2.553	0.784
ATOM	38	H	RES	1	5.009	1.142	0.121

TER

REMARK Compound E structure 08
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.120691
 REMARK Sum of electronic and thermal Energies= -730.100973
 REMARK Sum of electronic and thermal Enthalpies= -730.100029
 REMARK Sum of electronic and thermal Free Energies= -730.169870
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	5.610	-1.133	-0.502
ATOM	2	C	RES	1	4.789	-1.254	0.208
ATOM	3	H	RES	1	5.098	-0.852	1.176
ATOM	4	H	RES	1	4.614	-2.327	0.312
ATOM	5	C	RES	1	3.549	-0.608	-0.365
ATOM	6	O	RES	1	3.106	-0.930	-1.464
ATOM	7	N	RES	1	2.980	0.349	0.422
ATOM	8	H	RES	1	3.364	0.486	1.344
ATOM	9	C	RES	1	1.738	1.097	0.106
ATOM	10	C	RES	1	1.932	1.885	-1.194
ATOM	11	H	RES	1	2.101	1.213	-2.037
ATOM	12	H	RES	1	2.793	2.556	-1.106
ATOM	13	H	RES	1	1.041	2.487	-1.395
ATOM	14	C	RES	1	1.520	2.065	1.261
ATOM	15	H	RES	1	2.377	2.739	1.355
ATOM	16	H	RES	1	1.382	1.540	2.212
ATOM	17	H	RES	1	0.633	2.678	1.087
ATOM	18	C	RES	1	0.600	0.116	-0.068
ATOM	19	H	RES	1	0.782	-0.617	-0.852
ATOM	20	C	RES	1	-0.544	0.115	0.619
ATOM	21	H	RES	1	-0.730	0.856	1.397
ATOM	22	C	RES	1	-1.694	-0.851	0.441
ATOM	23	C	RES	1	-1.442	-1.863	-0.671
ATOM	24	H	RES	1	-0.566	-2.472	-0.433
ATOM	25	H	RES	1	-1.240	-1.389	-1.639
ATOM	26	H	RES	1	-2.291	-2.546	-0.781
ATOM	27	C	RES	1	-1.912	-1.599	1.767
ATOM	28	H	RES	1	-2.110	-0.894	2.577
ATOM	29	H	RES	1	-1.024	-2.188	2.015
ATOM	30	H	RES	1	-2.767	-2.280	1.695
ATOM	31	C	RES	1	-2.941	0.036	0.226
ATOM	32	O	RES	1	-3.315	0.809	1.103
ATOM	33	N	RES	1	-3.582	-0.080	-0.971
ATOM	34	H	RES	1	-3.216	-0.713	-1.663
ATOM	35	C	RES	1	-4.736	0.719	-1.310
ATOM	36	H	RES	1	-5.000	1.306	-0.430
ATOM	37	H	RES	1	-4.522	1.402	-2.138
ATOM	38	H	RES	1	-5.586	0.088	-1.586

TER

REMARK Compound E structure 09
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.121757
 REMARK Sum of electronic and thermal Energies= -730.102173
 REMARK Sum of electronic and thermal Enthalpies= -730.101228
 REMARK Sum of electronic and thermal Free Energies= -730.169713
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.134	0.361	-2.869
ATOM	2	C	RES	1	3.877	-0.465	-2.203
ATOM	3	H	RES	1	4.777	-1.073	-2.088
ATOM	4	H	RES	1	3.099	-1.069	-2.677
ATOM	5	C	RES	1	3.491	0.099	-0.856
ATOM	6	O	RES	1	4.251	0.822	-0.220
ATOM	7	N	RES	1	2.237	-0.240	-0.427
ATOM	8	H	RES	1	1.767	-0.978	-0.928
ATOM	9	C	RES	1	1.701	0.069	0.909
ATOM	10	C	RES	1	1.702	1.587	1.144
ATOM	11	H	RES	1	1.174	2.097	0.333
ATOM	12	H	RES	1	2.722	1.971	1.194
ATOM	13	H	RES	1	1.191	1.814	2.086
ATOM	14	C	RES	1	2.534	-0.629	1.987
ATOM	15	H	RES	1	3.570	-0.287	1.942
ATOM	16	H	RES	1	2.514	-1.715	1.855
ATOM	17	H	RES	1	2.138	-0.401	2.982
ATOM	18	C	RES	1	0.269	-0.408	0.980
ATOM	19	H	RES	1	-0.084	-0.578	1.998
ATOM	20	C	RES	1	-0.575	-0.569	-0.044
ATOM	21	H	RES	1	-0.221	-0.367	-1.060
ATOM	22	C	RES	1	-2.021	-0.988	0.029
ATOM	23	C	RES	1	-2.246	-2.171	-0.915
ATOM	24	H	RES	1	-1.673	-3.040	-0.575
ATOM	25	H	RES	1	-1.932	-1.931	-1.936
ATOM	26	H	RES	1	-3.306	-2.429	-0.949
ATOM	27	C	RES	1	-2.456	-1.375	1.446
ATOM	28	H	RES	1	-2.348	-0.544	2.152
ATOM	29	H	RES	1	-1.860	-2.216	1.816
ATOM	30	H	RES	1	-3.507	-1.675	1.442
ATOM	31	C	RES	1	-2.960	0.163	-0.414
ATOM	32	O	RES	1	-4.066	-0.061	-0.891
ATOM	33	N	RES	1	-2.493	1.420	-0.178
ATOM	34	H	RES	1	-1.577	1.518	0.235
ATOM	35	C	RES	1	-3.280	2.601	-0.443
ATOM	36	H	RES	1	-4.175	2.288	-0.981
ATOM	37	H	RES	1	-3.586	3.100	0.483
ATOM	38	H	RES	1	-2.723	3.314	-1.058

TER

REMARK Compound E structure 10
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.121500
 REMARK Sum of electronic and thermal Energies= -730.101947
 REMARK Sum of electronic and thermal Enthalpies= -730.101002
 REMARK Sum of electronic and thermal Free Energies= -730.169451
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-5.028	1.651	1.593
ATOM	2	C	RES	1	-4.172	1.931	0.975
ATOM	3	H	RES	1	-3.408	2.381	1.615
ATOM	4	H	RES	1	-4.525	2.683	0.266
ATOM	5	C	RES	1	-3.705	0.716	0.208
ATOM	6	O	RES	1	-4.460	0.091	-0.530
ATOM	7	N	RES	1	-2.395	0.380	0.400
ATOM	8	H	RES	1	-1.842	0.971	1.001
ATOM	9	C	RES	1	-1.696	-0.752	-0.253
ATOM	10	C	RES	1	-1.702	-0.561	-1.767
ATOM	11	H	RES	1	-1.187	0.361	-2.054
ATOM	12	H	RES	1	-2.732	-0.510	-2.126
ATOM	13	H	RES	1	-1.207	-1.401	-2.263
ATOM	14	C	RES	1	-2.392	-2.069	0.117
ATOM	15	H	RES	1	-3.423	-2.066	-0.239
ATOM	16	H	RES	1	-2.396	-2.213	1.202
ATOM	17	H	RES	1	-1.859	-2.908	-0.339
ATOM	18	C	RES	1	-0.308	-0.763	0.340
ATOM	19	H	RES	1	-0.292	-0.837	1.431
ATOM	20	C	RES	1	0.848	-0.745	-0.331
ATOM	21	H	RES	1	0.820	-0.697	-1.423
ATOM	22	C	RES	1	2.234	-0.822	0.252
ATOM	23	C	RES	1	2.234	-0.976	1.776
ATOM	24	H	RES	1	1.712	-1.892	2.072
ATOM	25	H	RES	1	1.747	-0.131	2.274
ATOM	26	H	RES	1	3.262	-1.034	2.141
ATOM	27	C	RES	1	2.964	-2.013	-0.380
ATOM	28	H	RES	1	2.967	-1.945	-1.472
ATOM	29	H	RES	1	2.474	-2.950	-0.097
ATOM	30	H	RES	1	4.003	-2.033	-0.044
ATOM	31	C	RES	1	3.061	0.451	-0.050
ATOM	32	O	RES	1	4.286	0.438	-0.006
ATOM	33	N	RES	1	2.340	1.578	-0.305
ATOM	34	H	RES	1	1.334	1.507	-0.313
ATOM	35	C	RES	1	2.961	2.862	-0.529
ATOM	36	H	RES	1	4.041	2.709	-0.531
ATOM	37	H	RES	1	2.659	3.285	-1.492
ATOM	38	H	RES	1	2.709	3.575	0.264

TER

REMARK Compound E structure 11
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.120837
 REMARK Sum of electronic and thermal Energies= -730.101167
 REMARK Sum of electronic and thermal Enthalpies= -730.100223
 REMARK Sum of electronic and thermal Free Energies= -730.169039
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.058	2.033	-2.141
ATOM	2	C	RES	1	3.442	2.181	-1.251
ATOM	3	H	RES	1	2.472	2.581	-1.558
ATOM	4	H	RES	1	3.952	2.923	-0.632
ATOM	5	C	RES	1	3.364	0.878	-0.491
ATOM	6	O	RES	1	4.372	0.293	-0.109
ATOM	7	N	RES	1	2.097	0.407	-0.283
ATOM	8	H	RES	1	1.335	1.030	-0.504
ATOM	9	C	RES	1	1.768	-0.777	0.525
ATOM	10	C	RES	1	2.215	-0.561	1.976
ATOM	11	H	RES	1	1.714	0.308	2.415
ATOM	12	H	RES	1	3.295	-0.402	2.016
ATOM	13	H	RES	1	1.970	-1.438	2.583
ATOM	14	C	RES	1	2.453	-2.022	-0.055
ATOM	15	H	RES	1	3.538	-1.923	0.008
ATOM	16	H	RES	1	2.167	-2.161	-1.101
ATOM	17	H	RES	1	2.143	-2.909	0.505
ATOM	18	C	RES	1	0.276	-1.006	0.492
ATOM	19	H	RES	1	-0.068	-1.679	1.279
ATOM	20	C	RES	1	-0.608	-0.535	-0.393
ATOM	21	H	RES	1	-0.262	0.104	-1.210
ATOM	22	C	RES	1	-2.088	-0.820	-0.437
ATOM	23	C	RES	1	-2.445	-1.341	-1.831
ATOM	24	H	RES	1	-1.944	-2.296	-2.016
ATOM	25	H	RES	1	-2.137	-0.637	-2.610
ATOM	26	H	RES	1	-3.525	-1.477	-1.919
ATOM	27	C	RES	1	-2.529	-1.839	0.618
ATOM	28	H	RES	1	-2.313	-1.499	1.637
ATOM	29	H	RES	1	-2.022	-2.796	0.464
ATOM	30	H	RES	1	-3.607	-2.008	0.543
ATOM	31	C	RES	1	-2.914	0.464	-0.176
ATOM	32	O	RES	1	-4.019	0.635	-0.678
ATOM	33	N	RES	1	-2.350	1.350	0.691
ATOM	34	H	RES	1	-1.458	1.108	1.098
ATOM	35	C	RES	1	-3.044	2.528	1.154
ATOM	36	H	RES	1	-3.926	2.659	0.526
ATOM	37	H	RES	1	-3.371	2.426	2.195
ATOM	38	H	RES	1	-2.409	3.415	1.071

TER

REMARK Compound E structure 12
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.119858
 REMARK Sum of electronic and thermal Energies= -730.100133
 REMARK Sum of electronic and thermal Enthalpies= -730.099189
 REMARK Sum of electronic and thermal Free Energies= -730.168433
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.854	2.112	1.138
ATOM	2	C	RES	1	4.258	1.288	1.536
ATOM	3	H	RES	1	3.500	1.694	2.210
ATOM	4	H	RES	1	4.936	0.653	2.110
ATOM	5	C	RES	1	3.697	0.490	0.383
ATOM	6	O	RES	1	4.425	0.009	-0.482
ATOM	7	N	RES	1	2.340	0.352	0.381
ATOM	8	H	RES	1	1.825	0.722	1.166
ATOM	9	C	RES	1	1.563	-0.426	-0.613
ATOM	10	C	RES	1	1.979	-1.893	-0.566
ATOM	11	H	RES	1	1.804	-2.321	0.425
ATOM	12	H	RES	1	3.041	-1.980	-0.801
ATOM	13	H	RES	1	1.414	-2.475	-1.300
ATOM	14	C	RES	1	1.800	0.150	-2.015
ATOM	15	H	RES	1	2.854	0.075	-2.286
ATOM	16	H	RES	1	1.502	1.202	-2.055
ATOM	17	H	RES	1	1.202	-0.403	-2.746
ATOM	18	C	RES	1	0.116	-0.202	-0.246
ATOM	19	H	RES	1	-0.182	0.849	-0.240
ATOM	20	C	RES	1	-0.783	-1.139	0.058
ATOM	21	H	RES	1	-0.484	-2.190	0.065
ATOM	22	C	RES	1	-2.239	-0.925	0.411
ATOM	23	C	RES	1	-3.096	-1.745	-0.564
ATOM	24	H	RES	1	-2.889	-2.811	-0.431
ATOM	25	H	RES	1	-2.878	-1.518	-1.614
ATOM	26	H	RES	1	-4.165	-1.592	-0.383
ATOM	27	C	RES	1	-2.480	-1.442	1.836
ATOM	28	H	RES	1	-1.917	-0.849	2.559
ATOM	29	H	RES	1	-2.172	-2.489	1.914
ATOM	30	H	RES	1	-3.541	-1.380	2.098
ATOM	31	C	RES	1	-2.550	0.581	0.394
ATOM	32	O	RES	1	-2.245	1.307	1.336
ATOM	33	N	RES	1	-3.147	1.066	-0.731
ATOM	34	H	RES	1	-3.323	0.440	-1.500
ATOM	35	C	RES	1	-3.397	2.476	-0.920
ATOM	36	H	RES	1	-3.337	2.959	0.056
ATOM	37	H	RES	1	-2.654	2.938	-1.580
ATOM	38	H	RES	1	-4.392	2.637	-1.342

TER

REMARK Compound E structure 13
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.119684
 REMARK Sum of electronic and thermal Energies= -730.100073
 REMARK Sum of electronic and thermal Enthalpies= -730.099129
 REMARK Sum of electronic and thermal Free Energies= -730.168218
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.817	2.063	1.438
ATOM	2	C	RES	1	-3.992	2.217	0.739
ATOM	3	H	RES	1	-3.162	2.685	1.275
ATOM	4	H	RES	1	-4.350	2.903	-0.031
ATOM	5	C	RES	1	-3.646	0.895	0.095
ATOM	6	O	RES	1	-4.468	0.265	-0.565
ATOM	7	N	RES	1	-2.371	0.461	0.319
ATOM	8	H	RES	1	-1.730	1.095	0.774
ATOM	9	C	RES	1	-1.775	-0.767	-0.260
ATOM	10	C	RES	1	-1.763	-0.669	-1.783
ATOM	11	H	RES	1	-1.195	0.204	-2.119
ATOM	12	H	RES	1	-2.787	-0.578	-2.150
ATOM	13	H	RES	1	-1.314	-1.566	-2.222
ATOM	14	C	RES	1	-2.581	-1.993	0.186
ATOM	15	H	RES	1	-3.604	-1.939	-0.187
ATOM	16	H	RES	1	-2.610	-2.059	1.278
ATOM	17	H	RES	1	-2.109	-2.903	-0.198
ATOM	18	C	RES	1	-0.398	-0.852	0.349
ATOM	19	H	RES	1	-0.401	-0.948	1.437
ATOM	20	C	RES	1	0.766	-0.809	-0.300
ATOM	21	H	RES	1	0.770	-0.702	-1.387
ATOM	22	C	RES	1	2.140	-0.852	0.331
ATOM	23	C	RES	1	2.104	-1.250	1.806
ATOM	24	H	RES	1	1.611	-2.219	1.927
ATOM	25	H	RES	1	1.579	-0.502	2.402
ATOM	26	H	RES	1	3.121	-1.333	2.202
ATOM	27	C	RES	1	3.000	-1.856	-0.443
ATOM	28	H	RES	1	2.985	-1.675	-1.524
ATOM	29	H	RES	1	2.611	-2.867	-0.293
ATOM	30	H	RES	1	4.040	-1.851	-0.097
ATOM	31	C	RES	1	2.664	0.605	0.262
ATOM	32	O	RES	1	2.227	1.467	1.018
ATOM	33	N	RES	1	3.588	0.878	-0.702
ATOM	34	H	RES	1	3.953	0.123	-1.260
ATOM	35	C	RES	1	4.143	2.199	-0.887
ATOM	36	H	RES	1	5.191	2.246	-0.570
ATOM	37	H	RES	1	4.078	2.505	-1.934
ATOM	38	H	RES	1	3.564	2.890	-0.275

TER

REMARK Compound E structure 14
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.120344
 REMARK Sum of electronic and thermal Energies= -730.100941
 REMARK Sum of electronic and thermal Enthalpies= -730.099997
 REMARK Sum of electronic and thermal Free Energies= -730.168020
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	3.169	3.314	0.164
ATOM	2	C	RES	1	3.734	2.459	-0.212
ATOM	3	H	RES	1	4.737	2.529	0.215
ATOM	4	H	RES	1	3.809	2.536	-1.300
ATOM	5	C	RES	1	3.083	1.186	0.277
ATOM	6	O	RES	1	2.962	0.946	1.476
ATOM	7	N	RES	1	2.658	0.340	-0.703
ATOM	8	H	RES	1	2.709	0.666	-1.657
ATOM	9	C	RES	1	1.936	-0.939	-0.483
ATOM	10	C	RES	1	2.821	-1.890	0.327
ATOM	11	H	RES	1	3.025	-1.483	1.319
ATOM	12	H	RES	1	3.775	-2.053	-0.186
ATOM	13	H	RES	1	2.318	-2.856	0.439
ATOM	14	C	RES	1	1.684	-1.525	-1.865
ATOM	15	H	RES	1	2.635	-1.692	-2.382
ATOM	16	H	RES	1	1.061	-0.868	-2.481
ATOM	17	H	RES	1	1.176	-2.489	-1.786
ATOM	18	C	RES	1	0.663	-0.657	0.284
ATOM	19	H	RES	1	0.841	-0.203	1.257
ATOM	20	C	RES	1	-0.576	-0.924	-0.133
ATOM	21	H	RES	1	-0.751	-1.372	-1.112
ATOM	22	C	RES	1	-1.854	-0.670	0.635
ATOM	23	C	RES	1	-2.557	-2.019	0.868
ATOM	24	H	RES	1	-1.926	-2.669	1.480
ATOM	25	H	RES	1	-2.760	-2.513	-0.085
ATOM	26	H	RES	1	-3.512	-1.877	1.386
ATOM	27	C	RES	1	-1.604	0.006	1.978
ATOM	28	H	RES	1	-1.062	0.953	1.881
ATOM	29	H	RES	1	-0.993	-0.639	2.617
ATOM	30	H	RES	1	-2.544	0.186	2.511
ATOM	31	C	RES	1	-2.755	0.135	-0.326
ATOM	32	O	RES	1	-3.115	-0.349	-1.396
ATOM	33	N	RES	1	-3.112	1.390	0.065
ATOM	34	H	RES	1	-2.773	1.745	0.944
ATOM	35	C	RES	1	-3.927	2.253	-0.758
ATOM	36	H	RES	1	-3.379	3.152	-1.060
ATOM	37	H	RES	1	-4.202	1.692	-1.651
ATOM	38	H	RES	1	-4.838	2.557	-0.233

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REMARK Compound E structure 15
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.119667
 REMARK Sum of electronic and thermal Energies= -730.100099
 REMARK Sum of electronic and thermal Enthalpies= -730.099155
 REMARK Sum of electronic and thermal Free Energies= -730.167849
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	3.975	2.694	-1.425
ATOM	2	C	RES	1	3.379	2.557	-0.520
ATOM	3	H	RES	1	2.385	2.979	-0.686
ATOM	4	H	RES	1	3.875	3.120	0.275
ATOM	5	C	RES	1	3.378	1.091	-0.156
ATOM	6	O	RES	1	4.423	0.475	0.033
ATOM	7	N	RES	1	2.141	0.519	-0.074
ATOM	8	H	RES	1	1.346	1.141	-0.087
ATOM	9	C	RES	1	1.885	-0.856	0.383
ATOM	10	C	RES	1	2.369	-1.027	1.827
ATOM	11	H	RES	1	1.847	-0.336	2.497
ATOM	12	H	RES	1	3.442	-0.836	1.887
ATOM	13	H	RES	1	2.178	-2.048	2.173
ATOM	14	C	RES	1	2.603	-1.857	-0.533
ATOM	15	H	RES	1	3.685	-1.729	-0.465
ATOM	16	H	RES	1	2.291	-1.714	-1.571
ATOM	17	H	RES	1	2.346	-2.879	-0.236
ATOM	18	C	RES	1	0.401	-1.127	0.317
ATOM	19	H	RES	1	0.094	-1.977	0.929
ATOM	20	C	RES	1	-0.502	-0.476	-0.419
ATOM	21	H	RES	1	-0.201	0.356	-1.056
ATOM	22	C	RES	1	-1.983	-0.766	-0.502
ATOM	23	C	RES	1	-2.330	-1.112	-1.960
ATOM	24	H	RES	1	-1.801	-2.019	-2.267
ATOM	25	H	RES	1	-2.044	-0.295	-2.626
ATOM	26	H	RES	1	-3.406	-1.284	-2.076
ATOM	27	C	RES	1	-2.406	-1.917	0.404
ATOM	28	H	RES	1	-2.173	-1.731	1.458
ATOM	29	H	RES	1	-1.883	-2.833	0.116
ATOM	30	H	RES	1	-3.477	-2.123	0.309
ATOM	31	C	RES	1	-2.682	0.579	-0.197
ATOM	32	O	RES	1	-2.417	1.579	-0.858
ATOM	33	N	RES	1	-3.592	0.590	0.816
ATOM	34	H	RES	1	-3.756	-0.254	1.339
ATOM	35	C	RES	1	-4.307	1.786	1.198
ATOM	36	H	RES	1	-4.027	2.575	0.500
ATOM	37	H	RES	1	-5.389	1.632	1.147
ATOM	38	H	RES	1	-4.044	2.103	2.212

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REMARK Compound E structure 16
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.119944
 REMARK Sum of electronic and thermal Energies= -730.100389
 REMARK Sum of electronic and thermal Enthalpies= -730.099445
 REMARK Sum of electronic and thermal Free Energies= -730.167818
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-3.709	3.074	-0.394
ATOM	2	C	RES	1	-2.924	2.495	-0.883
ATOM	3	H	RES	1	-2.017	3.106	-0.876
ATOM	4	H	RES	1	-3.206	2.312	-1.924
ATOM	5	C	RES	1	-2.666	1.237	-0.087
ATOM	6	O	RES	1	-2.614	1.243	1.137
ATOM	7	N	RES	1	-2.478	0.110	-0.841
ATOM	8	H	RES	1	-2.430	0.227	-1.842
ATOM	9	C	RES	1	-2.039	-1.188	-0.310
ATOM	10	C	RES	1	-1.978	-2.148	-1.501
ATOM	11	H	RES	1	-1.278	-1.788	-2.262
ATOM	12	H	RES	1	-2.968	-2.270	-1.955
ATOM	13	H	RES	1	-1.633	-3.133	-1.175
ATOM	14	C	RES	1	-3.055	-1.711	0.710
ATOM	15	H	RES	1	-4.045	-1.789	0.250
ATOM	16	H	RES	1	-3.119	-1.048	1.572
ATOM	17	H	RES	1	-2.758	-2.709	1.050
ATOM	18	C	RES	1	-0.668	-1.105	0.329
ATOM	19	H	RES	1	-0.408	-1.981	0.926
ATOM	20	C	RES	1	0.188	-0.091	0.209
ATOM	21	H	RES	1	-0.088	0.779	-0.386
ATOM	22	C	RES	1	1.532	0.048	0.880
ATOM	23	C	RES	1	1.456	1.259	1.829
ATOM	24	H	RES	1	0.689	1.089	2.590
ATOM	25	H	RES	1	1.199	2.163	1.273
ATOM	26	H	RES	1	2.417	1.425	2.328
ATOM	27	C	RES	1	1.919	-1.192	1.678
ATOM	28	H	RES	1	1.955	-2.098	1.061
ATOM	29	H	RES	1	1.182	-1.372	2.467
ATOM	30	H	RES	1	2.887	-1.061	2.173
ATOM	31	C	RES	1	2.529	0.426	-0.237
ATOM	32	O	RES	1	2.351	1.431	-0.920
ATOM	33	N	RES	1	3.597	-0.402	-0.417
ATOM	34	H	RES	1	3.687	-1.218	0.164
ATOM	35	C	RES	1	4.599	-0.162	-1.429
ATOM	36	H	RES	1	4.643	-0.984	-2.150
ATOM	37	H	RES	1	4.326	0.754	-1.953
ATOM	38	H	RES	1	5.591	-0.033	-0.983

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REMARK Compound E structure 17
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.119380
 REMARK Sum of electronic and thermal Energies= -730.099719
 REMARK Sum of electronic and thermal Enthalpies= -730.098774
 REMARK Sum of electronic and thermal Free Energies= -730.167573
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.107	-2.997	0.084
ATOM	2	C	RES	1	-3.787	-2.226	0.787
ATOM	3	H	RES	1	-2.926	-2.597	1.349
ATOM	4	H	RES	1	-4.617	-2.061	1.479
ATOM	5	C	RES	1	-3.525	-0.949	0.024
ATOM	6	O	RES	1	-4.380	-0.443	-0.697
ATOM	7	N	RES	1	-2.276	-0.423	0.194
ATOM	8	H	RES	1	-1.697	-0.833	0.911
ATOM	9	C	RES	1	-1.832	0.868	-0.351
ATOM	10	C	RES	1	-2.688	2.002	0.226
ATOM	11	H	RES	1	-2.598	2.042	1.316
ATOM	12	H	RES	1	-3.737	1.847	-0.038
ATOM	13	H	RES	1	-2.365	2.966	-0.180
ATOM	14	C	RES	1	-1.939	0.860	-1.883
ATOM	15	H	RES	1	-2.982	0.775	-2.192
ATOM	16	H	RES	1	-1.372	0.023	-2.300
ATOM	17	H	RES	1	-1.525	1.790	-2.286
ATOM	18	C	RES	1	-0.386	1.099	0.014
ATOM	19	H	RES	1	-0.078	2.134	-0.143
ATOM	20	C	RES	1	0.508	0.203	0.438
ATOM	21	H	RES	1	0.235	-0.846	0.565
ATOM	22	C	RES	1	1.957	0.470	0.780
ATOM	23	C	RES	1	2.380	1.899	0.459
ATOM	24	H	RES	1	1.797	2.608	1.054
ATOM	25	H	RES	1	2.224	2.159	-0.594
ATOM	26	H	RES	1	3.432	2.064	0.713
ATOM	27	C	RES	1	2.161	0.209	2.283
ATOM	28	H	RES	1	1.882	-0.816	2.536
ATOM	29	H	RES	1	1.549	0.900	2.870
ATOM	30	H	RES	1	3.210	0.353	2.565
ATOM	31	C	RES	1	2.761	-0.619	0.036
ATOM	32	O	RES	1	2.559	-1.806	0.273
ATOM	33	N	RES	1	3.683	-0.198	-0.873
ATOM	34	H	RES	1	3.794	0.788	-1.042
ATOM	35	C	RES	1	4.482	-1.122	-1.646
ATOM	36	H	RES	1	4.218	-2.131	-1.328
ATOM	37	H	RES	1	4.279	-1.024	-2.717
ATOM	38	H	RES	1	5.550	-0.962	-1.473

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REMARK Compound E structure 18
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.119065
 REMARK Sum of electronic and thermal Energies= -730.099540
 REMARK Sum of electronic and thermal Enthalpies= -730.098596
 REMARK Sum of electronic and thermal Free Energies= -730.167056
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.604	-2.127	-1.064
ATOM	2	C	RES	1	-4.734	-1.166	-0.560
ATOM	3	H	RES	1	-5.415	-1.336	0.277
ATOM	4	H	RES	1	-5.202	-0.464	-1.255
ATOM	5	C	RES	1	-3.398	-0.710	-0.022
ATOM	6	O	RES	1	-2.716	-1.422	0.706
ATOM	7	N	RES	1	-3.017	0.545	-0.406
ATOM	8	H	RES	1	-3.654	1.084	-0.973
ATOM	9	C	RES	1	-1.772	1.214	0.034
ATOM	10	C	RES	1	-1.810	1.441	1.542
ATOM	11	H	RES	1	-1.866	0.490	2.075
ATOM	12	H	RES	1	-2.685	2.043	1.805
ATOM	13	H	RES	1	-0.918	1.980	1.875
ATOM	14	C	RES	1	-1.734	2.557	-0.698
ATOM	15	H	RES	1	-2.611	3.166	-0.447
ATOM	16	H	RES	1	-1.706	2.417	-1.784
ATOM	17	H	RES	1	-0.842	3.116	-0.407
ATOM	18	C	RES	1	-0.594	0.382	-0.417
ATOM	19	H	RES	1	-0.642	0.097	-1.470
ATOM	20	C	RES	1	0.433	-0.001	0.341
ATOM	21	H	RES	1	0.466	0.272	1.395
ATOM	22	C	RES	1	1.592	-0.869	-0.087
ATOM	23	C	RES	1	1.550	-2.152	0.763
ATOM	24	H	RES	1	0.606	-2.679	0.595
ATOM	25	H	RES	1	1.631	-1.908	1.824
ATOM	26	H	RES	1	2.378	-2.820	0.501
ATOM	27	C	RES	1	1.527	-1.246	-1.563
ATOM	28	H	RES	1	1.504	-0.371	-2.224
ATOM	29	H	RES	1	0.617	-1.819	-1.761
ATOM	30	H	RES	1	2.373	-1.882	-1.846
ATOM	31	C	RES	1	2.868	-0.105	0.323
ATOM	32	O	RES	1	3.072	0.185	1.498
ATOM	33	N	RES	1	3.740	0.227	-0.672
ATOM	34	H	RES	1	3.518	-0.019	-1.623
ATOM	35	C	RES	1	4.959	0.957	-0.417
ATOM	36	H	RES	1	5.051	1.078	0.662
ATOM	37	H	RES	1	5.832	0.411	-0.789
ATOM	38	H	RES	1	4.940	1.948	-0.882

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REMARK Compound E structure 19
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.118615
 REMARK Sum of electronic and thermal Energies= -730.098716
 REMARK Sum of electronic and thermal Enthalpies= -730.097772
 REMARK Sum of electronic and thermal Free Energies= -730.167027
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-3.568	-2.345	-1.357
ATOM	2	C	RES	1	-4.003	-1.403	-1.012
ATOM	3	H	RES	1	-4.905	-1.657	-0.452
ATOM	4	H	RES	1	-4.284	-0.807	-1.884
ATOM	5	C	RES	1	-3.025	-0.724	-0.083
ATOM	6	O	RES	1	-2.688	-1.227	0.982
ATOM	7	N	RES	1	-2.542	0.475	-0.531
ATOM	8	H	RES	1	-2.852	0.796	-1.435
ATOM	9	C	RES	1	-1.573	1.321	0.179
ATOM	10	C	RES	1	-2.096	1.675	1.576
ATOM	11	H	RES	1	-2.217	0.778	2.185
ATOM	12	H	RES	1	-3.061	2.184	1.499
ATOM	13	H	RES	1	-1.393	2.349	2.075
ATOM	14	C	RES	1	-1.427	2.603	-0.645
ATOM	15	H	RES	1	-2.379	3.143	-0.701
ATOM	16	H	RES	1	-1.085	2.382	-1.663
ATOM	17	H	RES	1	-0.693	3.268	-0.184
ATOM	18	C	RES	1	-0.217	0.662	0.300
ATOM	19	H	RES	1	0.480	1.216	0.934
ATOM	20	C	RES	1	0.178	-0.476	-0.271
ATOM	21	H	RES	1	-0.539	-1.037	-0.873
ATOM	22	C	RES	1	1.503	-1.171	-0.057
ATOM	23	C	RES	1	1.356	-2.125	1.133
ATOM	24	H	RES	1	0.525	-2.816	0.958
ATOM	25	H	RES	1	1.147	-1.573	2.052
ATOM	26	H	RES	1	2.276	-2.696	1.281
ATOM	27	C	RES	1	1.864	-1.983	-1.312
ATOM	28	H	RES	1	1.944	-1.349	-2.201
ATOM	29	H	RES	1	1.095	-2.740	-1.502
ATOM	30	H	RES	1	2.819	-2.500	-1.176
ATOM	31	C	RES	1	2.678	-0.211	0.213
ATOM	32	O	RES	1	3.536	-0.448	1.056
ATOM	33	N	RES	1	2.749	0.866	-0.623
ATOM	34	H	RES	1	1.948	1.062	-1.205
ATOM	35	C	RES	1	3.803	1.847	-0.534
ATOM	36	H	RES	1	4.571	1.444	0.128
ATOM	37	H	RES	1	4.243	2.040	-1.516
ATOM	38	H	RES	1	3.448	2.796	-0.116

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REMARK Compound E structure 20
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.118170
 REMARK Sum of electronic and thermal Energies= -730.098450
 REMARK Sum of electronic and thermal Enthalpies= -730.097506
 REMARK Sum of electronic and thermal Free Energies= -730.166615
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	4.868	1.606	-1.482
ATOM	2	C	RES	1	4.370	1.642	-0.510
ATOM	3	H	RES	1	3.695	2.501	-0.493
ATOM	4	H	RES	1	5.150	1.789	0.241
ATOM	5	C	RES	1	3.692	0.315	-0.261
ATOM	6	O	RES	1	4.318	-0.740	-0.274
ATOM	7	N	RES	1	2.343	0.389	-0.048
ATOM	8	H	RES	1	1.961	1.307	0.130
ATOM	9	C	RES	1	1.500	-0.745	0.361
ATOM	10	C	RES	1	1.944	-1.264	1.733
ATOM	11	H	RES	1	1.851	-0.484	2.495
ATOM	12	H	RES	1	2.984	-1.595	1.688
ATOM	13	H	RES	1	1.323	-2.113	2.038
ATOM	14	C	RES	1	1.582	-1.873	-0.679
ATOM	15	H	RES	1	2.584	-2.301	-0.706
ATOM	16	H	RES	1	1.332	-1.491	-1.674
ATOM	17	H	RES	1	0.865	-2.660	-0.422
ATOM	18	C	RES	1	0.065	-0.292	0.432
ATOM	19	H	RES	1	-0.576	-0.984	0.986
ATOM	20	C	RES	1	-0.493	0.779	-0.138
ATOM	21	H	RES	1	0.125	1.472	-0.715
ATOM	22	C	RES	1	-1.948	1.182	-0.028
ATOM	23	C	RES	1	-2.117	2.131	1.162
ATOM	24	H	RES	1	-1.460	2.999	1.045
ATOM	25	H	RES	1	-1.868	1.629	2.100
ATOM	26	H	RES	1	-3.150	2.479	1.234
ATOM	27	C	RES	1	-2.373	1.908	-1.315
ATOM	28	H	RES	1	-2.230	1.287	-2.205
ATOM	29	H	RES	1	-1.783	2.822	-1.444
ATOM	30	H	RES	1	-3.428	2.194	-1.268
ATOM	31	C	RES	1	-2.887	-0.028	0.166
ATOM	32	O	RES	1	-3.758	-0.050	1.028
ATOM	33	N	RES	1	-2.724	-1.033	-0.743
ATOM	34	H	RES	1	-1.909	-1.003	-1.338
ATOM	35	C	RES	1	-3.501	-2.248	-0.701
ATOM	36	H	RES	1	-4.319	-2.093	0.003
ATOM	37	H	RES	1	-3.916	-2.483	-1.686
ATOM	38	H	RES	1	-2.905	-3.102	-0.360

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REMARK Compound E structure 21
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.118350
 REMARK Sum of electronic and thermal Energies= -730.098676
 REMARK Sum of electronic and thermal Enthalpies= -730.097731
 REMARK Sum of electronic and thermal Free Energies= -730.166561
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.668	2.544	0.081
ATOM	2	C	RES	1	-4.041	2.083	-0.685
ATOM	3	H	RES	1	-3.210	2.757	-0.912
ATOM	4	H	RES	1	-4.659	1.971	-1.578
ATOM	5	C	RES	1	-3.615	0.714	-0.208
ATOM	6	O	RES	1	-4.438	-0.146	0.093
ATOM	7	N	RES	1	-2.267	0.520	-0.137
ATOM	8	H	RES	1	-1.666	1.264	-0.458
ATOM	9	C	RES	1	-1.602	-0.741	0.273
ATOM	10	C	RES	1	-1.989	-1.864	-0.684
ATOM	11	H	RES	1	-1.690	-1.632	-1.711
ATOM	12	H	RES	1	-3.071	-2.008	-0.661
ATOM	13	H	RES	1	-1.509	-2.802	-0.387
ATOM	14	C	RES	1	-2.017	-1.097	1.706
ATOM	15	H	RES	1	-3.095	-1.260	1.760
ATOM	16	H	RES	1	-1.746	-0.295	2.398
ATOM	17	H	RES	1	-1.501	-2.008	2.023
ATOM	18	C	RES	1	-0.124	-0.434	0.270
ATOM	19	H	RES	1	0.167	0.379	0.941
ATOM	20	C	RES	1	0.818	-1.086	-0.412
ATOM	21	H	RES	1	0.532	-1.922	-1.056
ATOM	22	C	RES	1	2.311	-0.833	-0.387
ATOM	23	C	RES	1	2.993	-1.996	0.345
ATOM	24	H	RES	1	2.717	-2.948	-0.119
ATOM	25	H	RES	1	2.698	-2.012	1.395
ATOM	26	H	RES	1	4.083	-1.899	0.298
ATOM	27	C	RES	1	2.817	-0.793	-1.836
ATOM	28	H	RES	1	2.272	-0.074	-2.457
ATOM	29	H	RES	1	2.675	-1.772	-2.304
ATOM	30	H	RES	1	3.886	-0.560	-1.880
ATOM	31	C	RES	1	2.600	0.457	0.398
ATOM	32	O	RES	1	2.636	0.466	1.625
ATOM	33	N	RES	1	2.764	1.593	-0.341
ATOM	34	H	RES	1	2.730	1.532	-1.345
ATOM	35	C	RES	1	2.991	2.884	0.265
ATOM	36	H	RES	1	3.038	2.737	1.344
ATOM	37	H	RES	1	3.934	3.322	-0.075
ATOM	38	H	RES	1	2.178	3.582	0.038

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REMARK Compound E structure 22
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.118463
 REMARK Sum of electronic and thermal Energies= -730.098877
 REMARK Sum of electronic and thermal Enthalpies= -730.097933
 REMARK Sum of electronic and thermal Free Energies= -730.166334
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.648	-1.727	-1.337
ATOM	2	C	RES	1	-3.805	-1.152	-1.723
ATOM	3	H	RES	1	-4.187	-0.303	-2.297
ATOM	4	H	RES	1	-3.252	-1.809	-2.398
ATOM	5	C	RES	1	-2.904	-0.766	-0.573
ATOM	6	O	RES	1	-2.471	-1.597	0.216
ATOM	7	N	RES	1	-2.619	0.570	-0.482
ATOM	8	H	RES	1	-2.948	1.171	-1.223
ATOM	9	C	RES	1	-1.652	1.154	0.476
ATOM	10	C	RES	1	-2.122	0.905	1.905
ATOM	11	H	RES	1	-2.211	-0.162	2.113
ATOM	12	H	RES	1	-3.102	1.367	2.057
ATOM	13	H	RES	1	-1.419	1.350	2.617
ATOM	14	C	RES	1	-1.630	2.655	0.195
ATOM	15	H	RES	1	-2.623	3.096	0.332
ATOM	16	H	RES	1	-1.293	2.865	-0.827
ATOM	17	H	RES	1	-0.941	3.156	0.881
ATOM	18	C	RES	1	-0.288	0.576	0.174
ATOM	19	H	RES	1	0.107	0.860	-0.806
ATOM	20	C	RES	1	0.406	-0.265	0.943
ATOM	21	H	RES	1	-0.021	-0.583	1.896
ATOM	22	C	RES	1	1.694	-0.965	0.580
ATOM	23	C	RES	1	2.599	-1.057	1.819
ATOM	24	H	RES	1	2.099	-1.633	2.605
ATOM	25	H	RES	1	2.844	-0.072	2.229
ATOM	26	H	RES	1	3.538	-1.564	1.576
ATOM	27	C	RES	1	1.338	-2.379	0.110
ATOM	28	H	RES	1	0.755	-2.347	-0.813
ATOM	29	H	RES	1	0.740	-2.887	0.872
ATOM	30	H	RES	1	2.244	-2.960	-0.081
ATOM	31	C	RES	1	2.468	-0.245	-0.541
ATOM	32	O	RES	1	2.835	-0.812	-1.564
ATOM	33	N	RES	1	2.773	1.061	-0.277
ATOM	34	H	RES	1	2.304	1.499	0.502
ATOM	35	C	RES	1	3.429	1.905	-1.245
ATOM	36	H	RES	1	3.910	1.257	-1.979
ATOM	37	H	RES	1	2.721	2.556	-1.774
ATOM	38	H	RES	1	4.188	2.529	-0.766

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REMARK Compound E structure 23
 REMARK ALL ENERGIES ARE EXPRESSED IN HARTREES
 REMARK Sum of electronic and zero-point Energies= -730.117827
 REMARK Sum of electronic and thermal Energies= -730.098098
 REMARK Sum of electronic and thermal Enthalpies= -730.097153
 REMARK Sum of electronic and thermal Free Energies= -730.166196
 REMARK 0 Virtual frequencies used

ATOM	1	H	RES	1	-4.936	-1.957	-0.831
ATOM	2	C	RES	1	-4.194	-1.346	-1.350
ATOM	3	H	RES	1	-4.718	-0.828	-2.157
ATOM	4	H	RES	1	-3.437	-2.004	-1.785
ATOM	5	C	RES	1	-3.645	-0.321	-0.385
ATOM	6	O	RES	1	-4.382	0.433	0.241
ATOM	7	N	RES	1	-2.283	-0.317	-0.264
ATOM	8	H	RES	1	-1.764	-0.852	-0.945
ATOM	9	C	RES	1	-1.517	0.685	0.493
ATOM	10	C	RES	1	-1.931	0.665	1.971
ATOM	11	H	RES	1	-1.807	-0.337	2.388
ATOM	12	H	RES	1	-2.972	0.971	2.080
ATOM	13	H	RES	1	-1.296	1.352	2.541
ATOM	14	C	RES	1	-1.748	2.081	-0.098
ATOM	15	H	RES	1	-2.808	2.340	-0.045
ATOM	16	H	RES	1	-1.427	2.120	-1.144
ATOM	17	H	RES	1	-1.179	2.830	0.462
ATOM	18	C	RES	1	-0.049	0.349	0.414
ATOM	19	H	RES	1	0.597	1.184	0.695
ATOM	20	C	RES	1	0.514	-0.821	0.096
ATOM	21	H	RES	1	-0.119	-1.683	-0.134
ATOM	22	C	RES	1	1.992	-1.145	0.116
ATOM	23	C	RES	1	2.304	-1.913	1.403
ATOM	24	H	RES	1	1.676	-2.807	1.469
ATOM	25	H	RES	1	2.123	-1.292	2.282
ATOM	26	H	RES	1	3.353	-2.219	1.423
ATOM	27	C	RES	1	2.333	-2.031	-1.093
ATOM	28	H	RES	1	2.080	-1.553	-2.045
ATOM	29	H	RES	1	1.780	-2.975	-1.036
ATOM	30	H	RES	1	3.401	-2.269	-1.111
ATOM	31	C	RES	1	2.869	0.122	0.072
ATOM	32	O	RES	1	3.713	0.369	0.925
ATOM	33	N	RES	1	2.673	0.918	-1.021
ATOM	34	H	RES	1	1.861	0.735	-1.593
ATOM	35	C	RES	1	3.343	2.187	-1.176
ATOM	36	H	RES	1	4.217	2.184	-0.524
ATOM	37	H	RES	1	3.667	2.329	-2.210
ATOM	38	H	RES	1	2.702	3.030	-0.889

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