Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Simplified and Enhanced VCD Analysis of Cyclic Peptides Guided by Artificial Intelligence

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Electronic Supplementary File

Summary

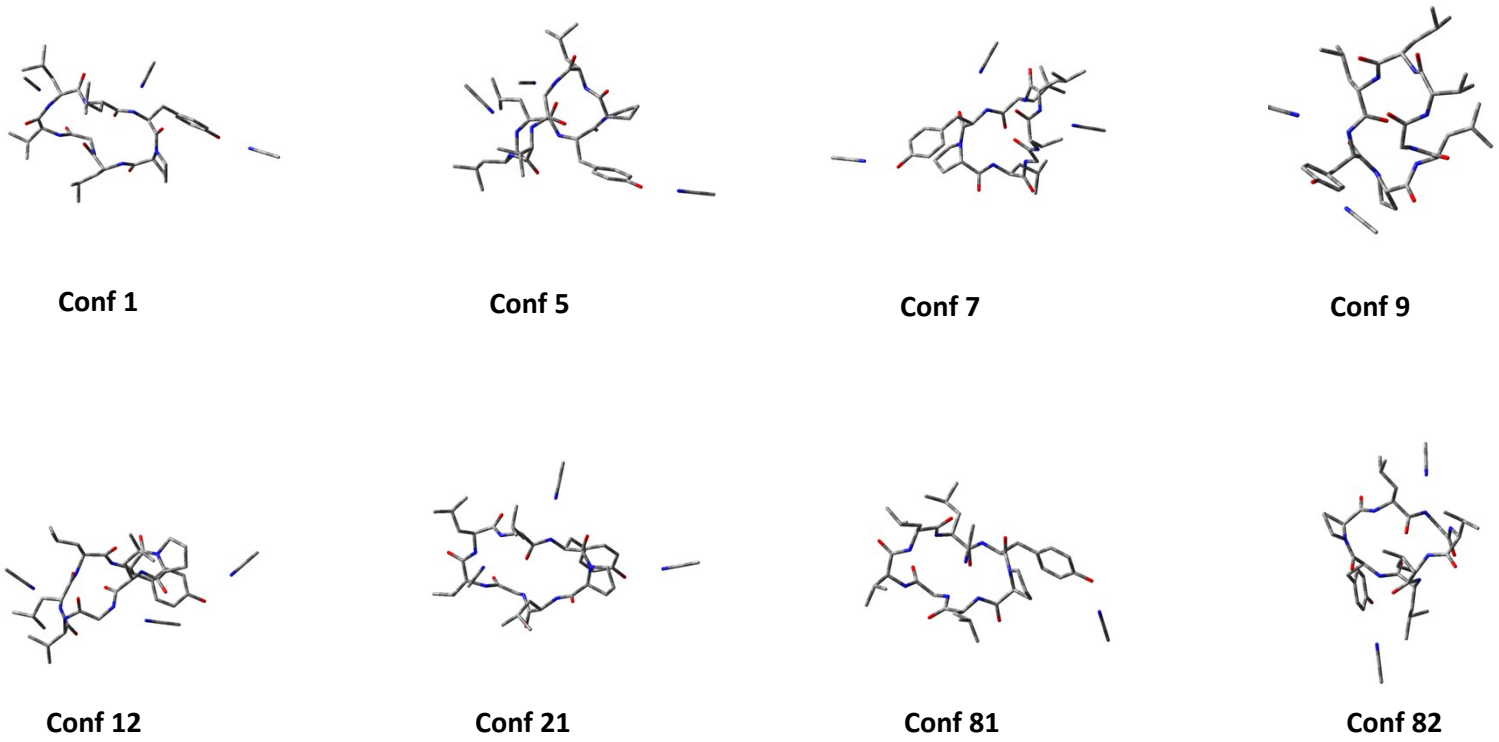

Figure S1: Structures of the main conformers identified for all-L cyclic (molecular complex) at the B3LYP/PCM(ACN)/6-31G(d) level using the GA-VCD protocol. Hydrogens are omitted for clarity.

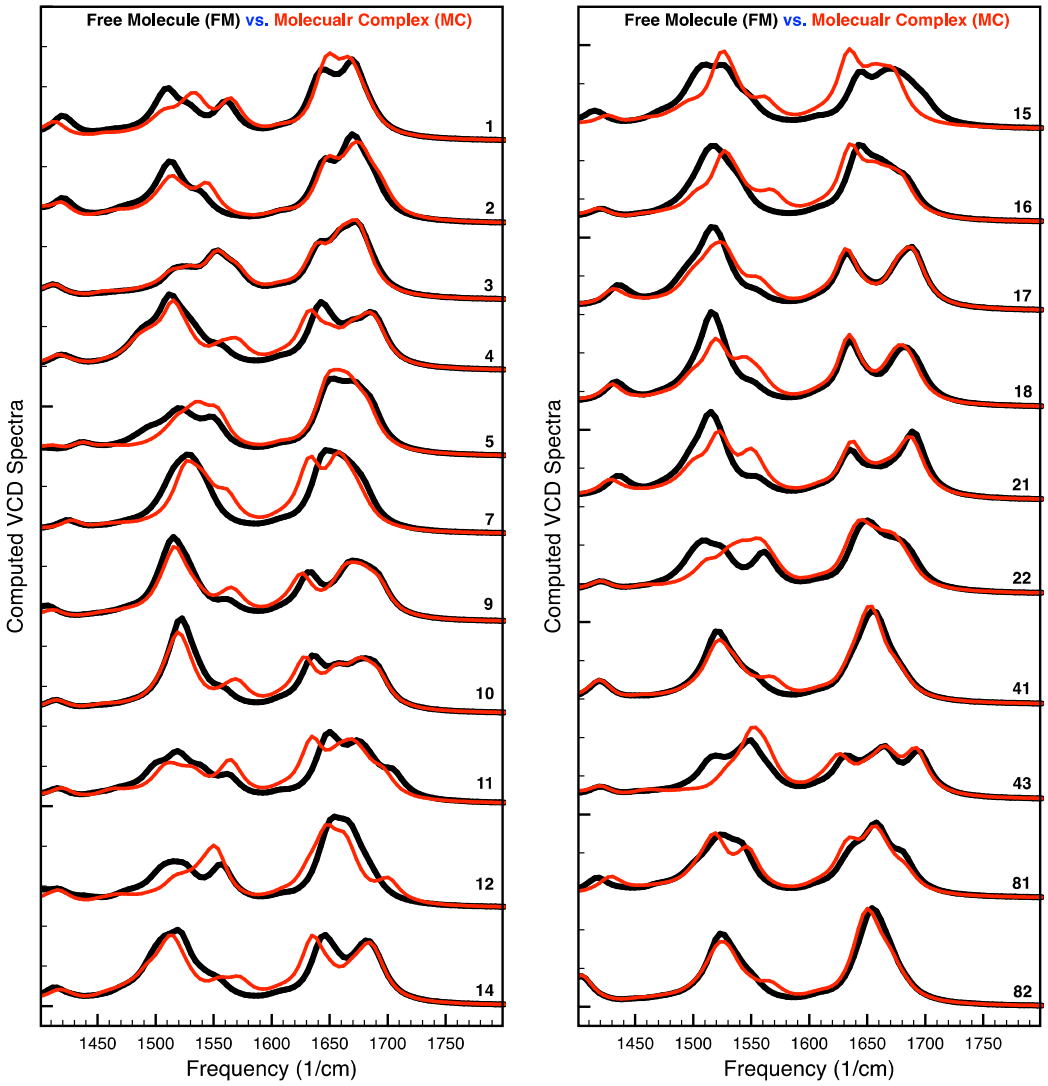

Figure S2. Comparison of the IR spectra computed for free molecule and for the molecular complex. The spectra of all the 21 conformers are shown. The numeric labels indicate the numbering of the considered low-energy conformers.

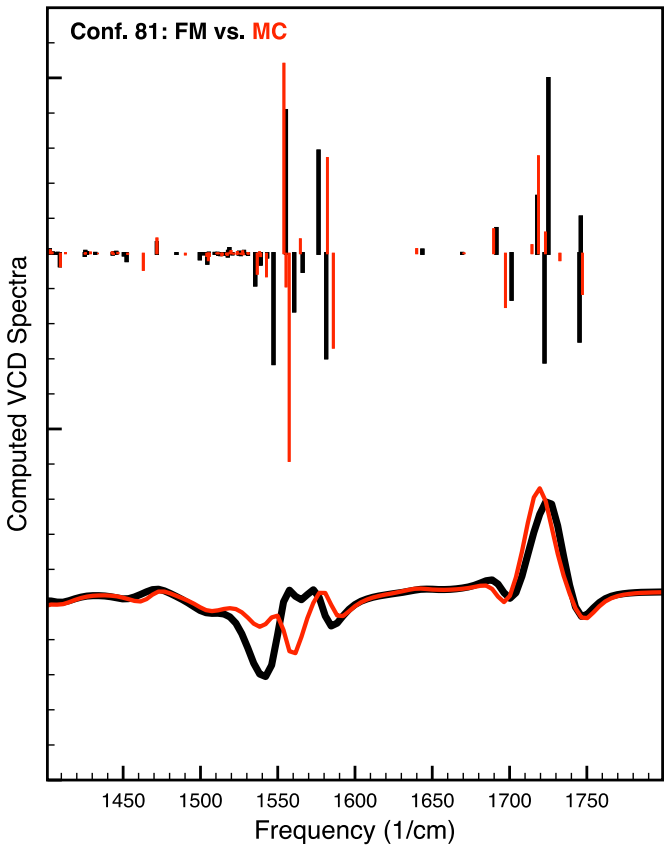

Figure S3: Comparison of the VCD spectra computed for the free molecule (black) and molecular complex (red) associated with conformer 81 of the cyclic peptide. The position of the normal modes is indicated by the vertical bars.

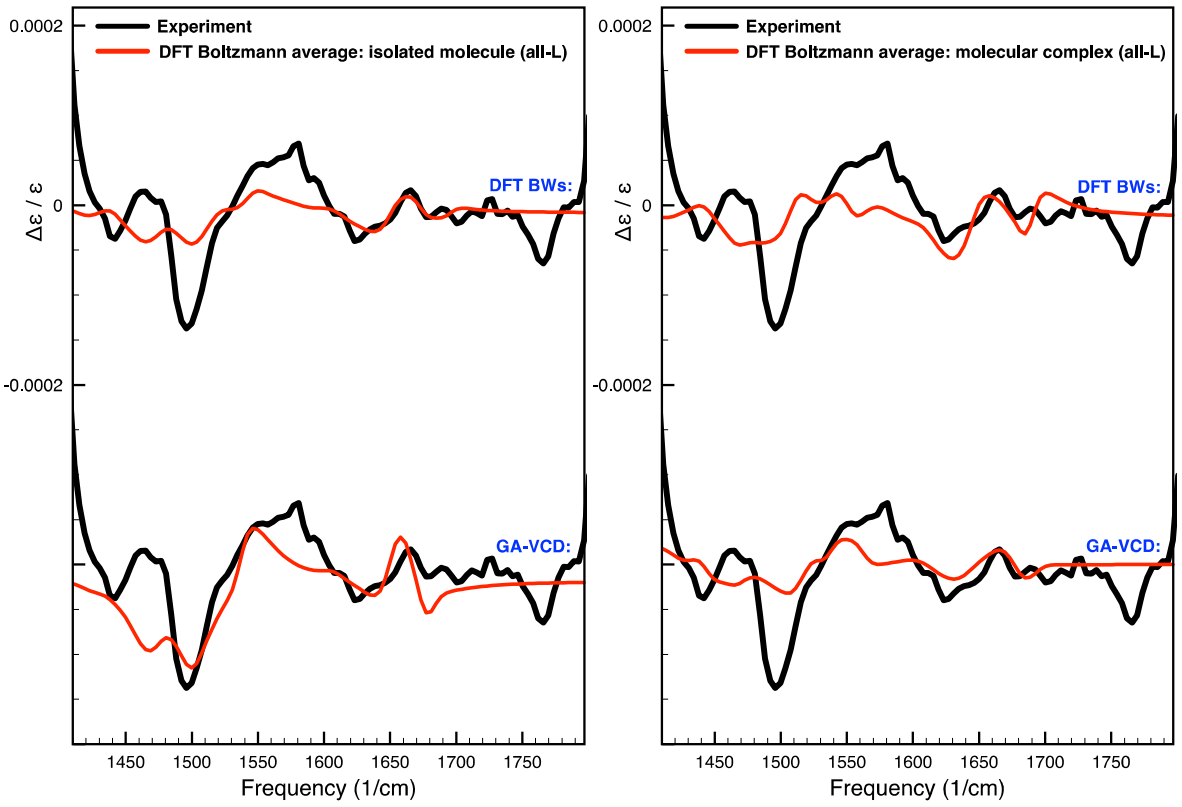

Figure S4: Comparison of experimental and calculated vibrational dissymmetry factor (VDF) spectra for FM and MC ensembles using both the standard Boltzmann weighting (BW) and the GA-VCD protocol.

Table S1: Normal mode (NM) analysis for conformer 81 of the (all-L) cyclic peptide: decomposition of the normal modes of the molecular complex (MC) into modes of the free molecule (FM). Only the modes (in the amide I and II modes spectra interval) that have VCD intensities larger than 100 × 10^{-44} $esu^2 \cdot cm^2$ (absolute values) have been considered. The frequencies of the normal modes (Freq.), the rotational strengths (R.S.) and the dipole strength (D.S.) are also given. Units: Freq. (cm^{-1}), R.S.(10^{-44} $esu^2 \cdot cm^2$) and D.S.(10^{-40} $esu^2 \cdot cm^2$). The overlap values (6th column) are obtain by computing a scalar product between the normalised nuclear displacement vectors of the FM and of the MC. The similarity values (7th column) are obtained by taking the square of the Overlap values (6th column). We considered conformer 81 because this conformer exhibits some of the largest changes in the VCD spectra when going from FM to MC.

	NM	Freq.	D.S.	R.S.	Overlap	Similarity
MC	288	1536.7	183.7	-117.0		
FM	260	1535.4	381.2	-180.2	0.97	0.94
MC	291	1542.7	520.8	-131.7		
FM	261	1538.5	232.0	-59.8	0.32	0.10
FM	263	1543.1	187.7	-21.0	0.79	0.63
MC	292	1554.0	1662.6	1082.1		
FM	263	1543.1	187.7	-21.0	0.31	0.10
FM	265	1555.3	1057.7	815.1	-0.86	0.75
MC	293	1555.4	53.1	-188.7		
FM	264	1547.3	351.1	-628.5	-0.94	0.89
MC	294	1557.4	1276.0	-1183.6		
FM	266	1560.6	940.7	-328.4	0.60	0.36
FM	267	1566.2	979.4	-102.8	0.73	0.54
MC	296	1582.1	651.2	544.9		
FM	268	1576.4	515.1	584.0	-0.97	0.93
MC	297	1586.0	1714.9	-538.2		
FM	269	1581.3	1645.7	-595.6	0.97	0.94
MC	300	1689.7	534.7	139.1		
FM	272	1691.5	511.2	143.1	0.98	0.96
MC	301	1697.3	1979.2	-307.1		
FM	273	1701.3	1477.7	-261.7	0.95	0.91
MC	303	1718.7	1339.7	554.4		
FM	274	1717.9	1486.3	326.1	0.62	0.39
FM	275	1722.6	909.1	-619.3	-0.71	0.51
MC	304	1723.2	1235.5	120.1		
FM	276	1725.1	1029.3	997.2	0.94	0.89
MC	306	1747.1	911.9	-232.4		
FM	277	1745.3	1311.0	-500.3	-0.60	0.35
FM	278	1746.1	286.1	207.9	0.77	0.59

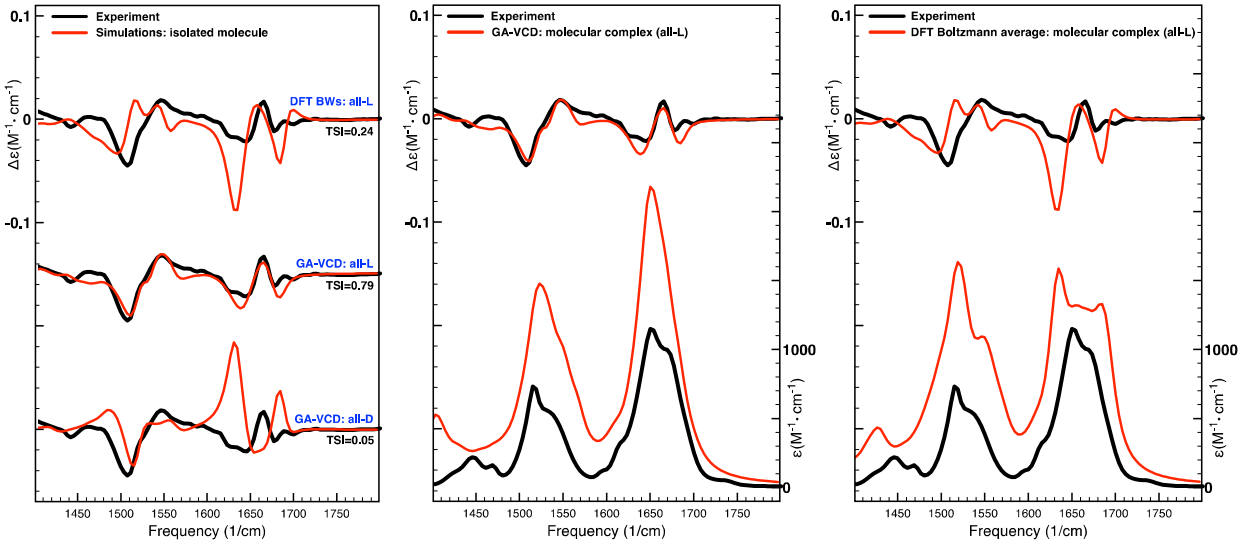

Figure S5: GA-VCD analysis for the molecular complex. **Left panel:** comparison between experimental and simulated VCD spectra. The simulated spectra are obtained as Boltzmann averages using factors optimised with a genetic algorithm. The experimental spectrum was fitted using calculations for the all-L (GA-VCD: all-L) configuration and also with calculations for the the all-D (GA-VCD: all-D) configuration. **Middle panel:** comparison between the experimental and GA-VCD IR and VCD spectra. **Right panel:** comparison between the experimental and the DFT Boltzmann averaged IR and VCD spectra.

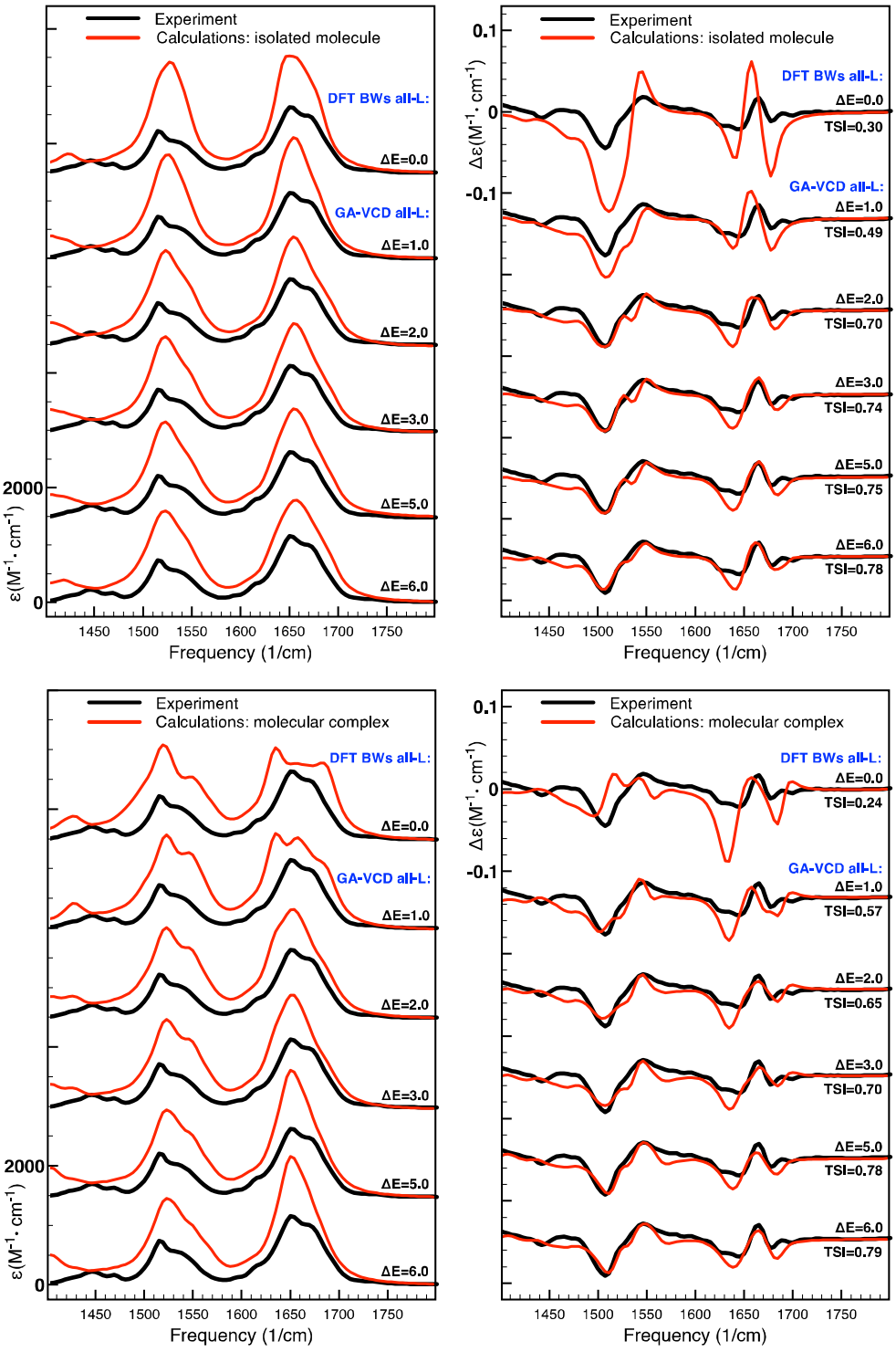

Figure S6: Dependence of the IR and VCD simulated spectra on the energy uncertainty (ΔE) value used when applying the GA-VCD protocol (see Table S2 for more details).

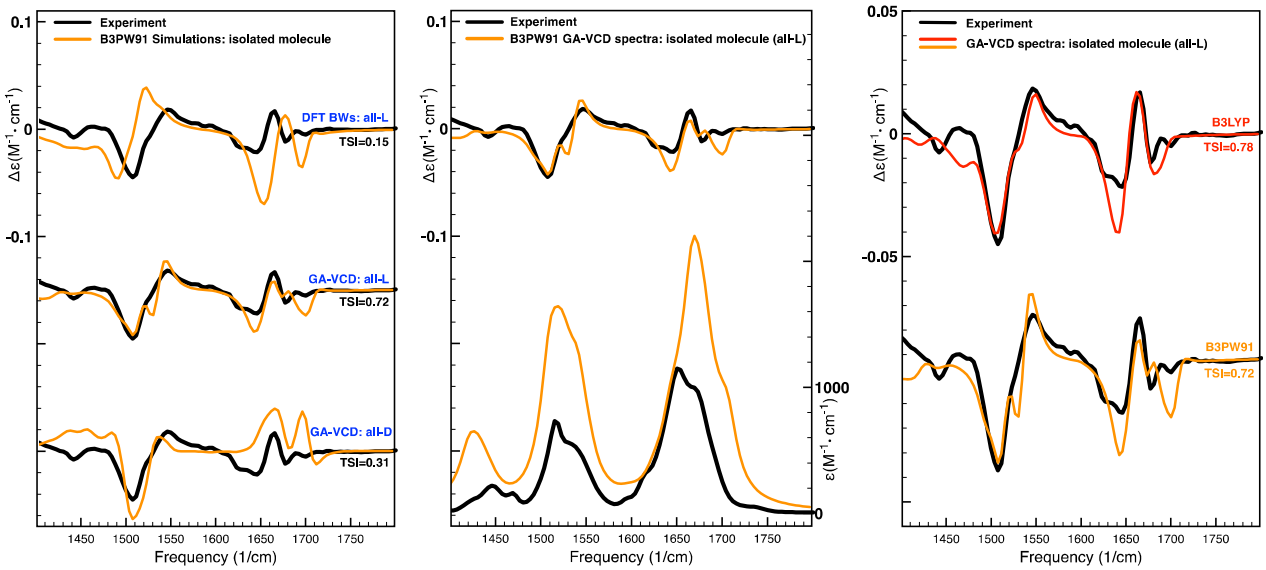

Figure S7: GA-VCD analysis for the free molecule using the simulated spectra obtained from B3PW91/PCM(ACN)/cc-pVDZ calculations. **Left panel**: comparison between experimental and simulated VCD spectra. The simulated spectra are obtained as Boltzmann averages using factors optimised with a genetic algorithm. The experimental spectrum was fitted using calculations for the all-L (GA-VCD: all-L) configuration and also with calculations for the the all-D (GA-VCD: all-D) configuration. **Middle panel:** comparison between the experimental and GA-VCD IR and VCD spectra. **Right panel:** comparison of the experimental VCD spectrum and GA-VCD spectra obtained from B3PW91/PCM(ACN)/cc-pVDZ and B3LYP/PCM(ACN)/6-31G(d) calculations.

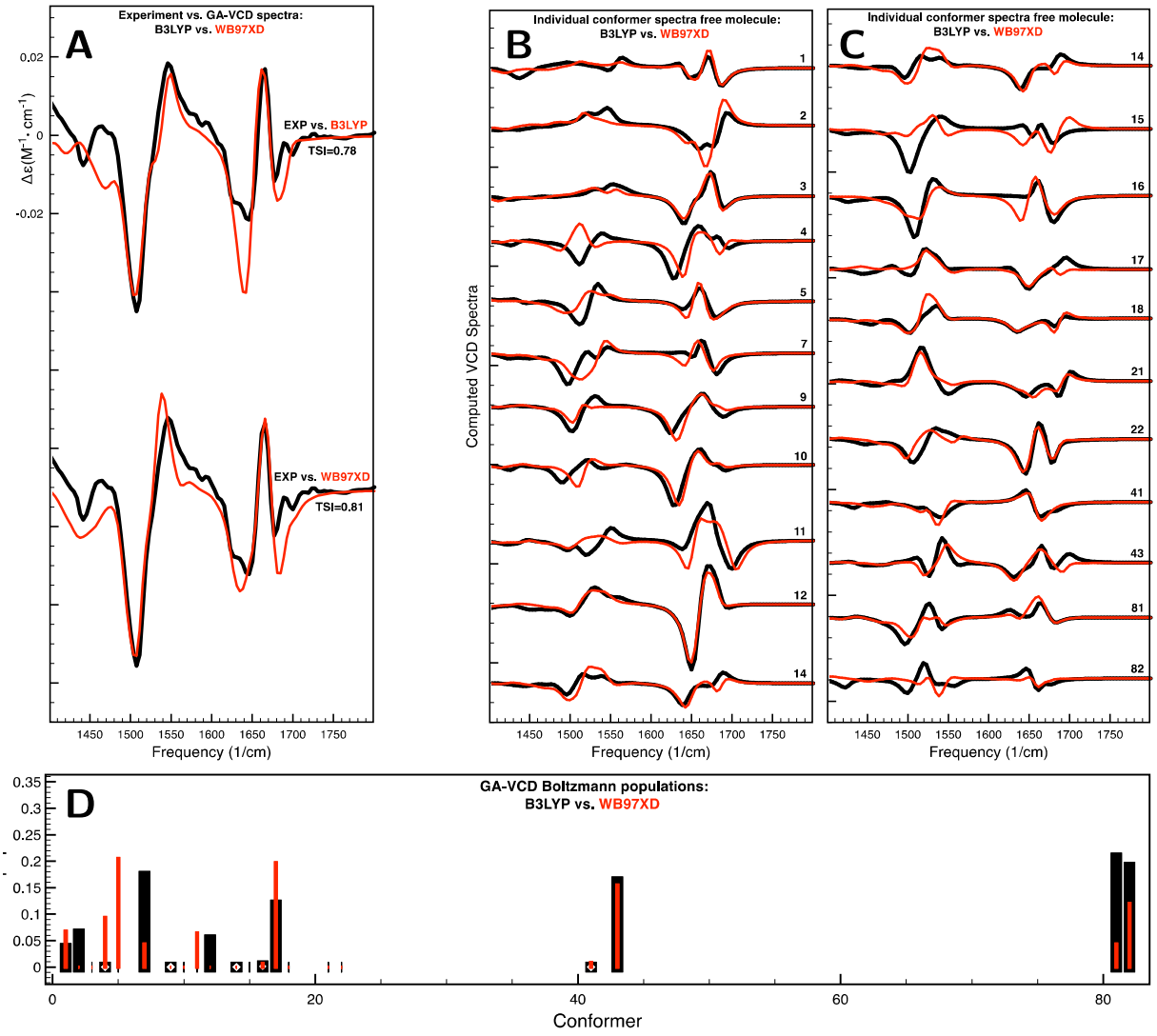

Figure S8: Comparison of the VCD spectra and GA-VCD Boltzmann populations predicted for the free molecule using the wB97X-D/PCM(ACN)/6-31G(d) and B3LYP/PCM(ACN)/6-31G(d) levels of theory. **Panel A**: comparison between experimental and simulated VCD spectra. The simulated spectra are obtained as Boltzmann averages using factors optimised with a genetic algorithm. The experimental spectrum was fitted using calculations for the all-L (GA-VCD: all-L) configuration. **Panels B and C:** Comparison of the VCD spectra computed for the free molecule at the wB97X-D/PCM(ACN)/6-31G(d) and B3LYP/PCM(ACN)/6-31G(d) levels. The spectra of all the 21 conformers are shown. The numeric labels indicate the numbering of the considered low-energy conformers. (The frequencies of the B3LYP/PCM(ACN)/6-31G(d) normal modes were scaled with 0.976 in the 1200–1650 cm^{-1} frequency interval and with 0.963 in the 1650–1900 cm^{-1} region. The frequencies of the wB97X-D/PCM(ACN)/6-31G(d) normal modes were scaled with 0.9565 in the 1200–1650 cm^{-1} frequency interval and with 0.9370 in the 1650–1900 cm^{-1} region.) **Panel D:** Comparison of the conformer Boltzmann factors optimized by the GA-VCD protocol at the wB97X-D/PCM(ACN)/6-31G(d) (red bars) and B3LYP/PCM(ACN)/6-31G(d) (black bars) levels.

Table S2: Comparison of the dihedral angles defining the backbone of the 21 low-energy conformer structures predicted with the B3LYP and wB97X-D exchange-correlation functions.

		Pro_1	Pro_1	Leu_2	Leu_2	Gly_3	Gly_3	Val_4	Val_4	Leu_5	Leu_5	Leu_6	Leu_6	Tyr_7	Tyr_7
Conf.	Calc.	Φ	Ψ	Φ	Ψ	Φ	Ψ	Φ	Ψ	Φ	Ψ	Φ	Ψ	Φ	Ψ
1	B3LYP	-84.7	-6.5	-81.4	81.8	-77.9	38.7	-135.1	57.6	-146.8	40.1	-103.4	-151.1	-152.3	125.9
	WB97XD	-77.9	-9.6	-80.3	85.8	-78.9	37.8	-131.7	54.3	-143.4	38.8	-110.4	-145.8	-157.0	133.7
2	B3LYP	-86.9	-8.4	-85.0	78.4	-72.3	164.5	-112.9	133.4	-120.1	13.7	-73.5	171.9	-141.7	125.9
	WB97XD	-80.3	-5.9	-84.3	72.6	-110.2	150.2	-58.2	146.9	-111.6	0.2	-104.1	-163.6	-146.6	129.2
3	B3LYP	-86.4	-4.4	-84.2	77.1	-76.1	44.4	-141.7	52.5	-138.7	15.7	-85.7	71.4	-46.1	127.6
	WB97XD	-81.7	-8.9	-82.8	68.2	-81.5	48.3	-134.5	49.3	-130.2	17.1	-85.6	59.4	-48.9	130.2
4	B3LYP	-98.9	6.0	-70.4	-44.7	109.7	-13.5	-115.1	-0.1	-155.5	-56.4	-126.7	150.3	-66.9	135.9
	WB97XD	-90.7	-5.5	-67.9	-31.8	86.8	-55.7	-67.8	-27.9	-103.2	-78.5	-136.3	158.6	-52.9	137.5
5	B3LYP	-108.5	29.4	-64.4	-46.5	120.7	127.7	-94.9	-59.8	-73.6	-46.7	-84.9	67.2	-72.2	133.5
5	WB97XD	-92.9	14.9	-60.1	-48.5	142.7	138.3	-113.2	-66.8	-54.0	-38.4	-111.3	32.1	-46.0	132.6
7	B3LYP	-101.7	10.7	-76.1	-41.7	-147.9	177.7	-66.5	-28.4	-104.5	1.9	-139.5	61.4	-64.5	133.4
7	WB97XD	-94.7	3.9	-64.2	-41.5	-156.2	179.9	-60.9	-37.8	-86.6	-9.1	-130.3	36.2	-61.6	132.8
9	B3LYP	-83.9	-9.5	-71.1	-28.9	91.4	-50.0	-70.5	-25.7	-111.6	-74.6	-130.7	155.5	-61.0	144.1
	WB97XD	-72.2	-23.4	-58.6	-42.2	90.6	-51.2	-67.2	-27.4	-101.5	-77.2	-135.3	147.0	-59.8	146.7
10	B3LYP	-90.8	-5.1	-72.2	-27.2	89.8	-53.2	-72.9	-23.9	-109.7	-75.9	-133.1	158.0	-57.6	136.2
	WB97XD	-85.8	-11.9	-61.0	-36.6	86.9	-55.5	-65.9	-28.8	-102.4	-77.7	-135.0	151.9	-53.3	138.5
11	B3LYP	-94.3	-6.9	-69.7	-40.4	79.8	165.0	-86.8	-18.3	-107.7	-19.9	-125.5	115.2	-73.3	138.1
	WB97XD	-80.7	-5.8	-74.4	-30.5	71.4	176.2	-76.9	-20.4	-112.3	11.6	-124.1	160.4	-131.2	132.5
12	B3LYP	-93.2	12.5	-93.7	-145.3	-146.3	174.0	-75.4	-40.6	-113.0	-4.3	-84.4	63.1	-56.5	133.0
	WB97XD	-87.9	8.1	-91.1	-150.3	-153.5	178.2	-70.4	-40.6	-113.1	2.2	-86.1	55.3	-56.1	134.8
14	B3LYP	-100.6	7.1	-64.1	-40.6	107.5	-5.6	-108.0	-69.3	-114.0	-9.0	-142.1	157.2	-95.8	131.5
	WB97XD	-97.3	11.1	-59.7	-35.4	75.3	21.9	-149.2	-60.9	-108.8	-15.1	-149.5	170.9	-97.2	131.5
15	B3LYP	-86.8	0.4	-62.6	-41.7	-145.8	-141.8	-115.2	4.7	-107.0	-88.6	-63.5	140.8	-138.1	134.0
	WB97XD	-90.8	1.2	-65.8	-38.0	-160.6	-177.3	-60.6	-38.6	-105.4	12.0	-134.2	28.6	-62.8	133.0
16	B3LYP	-101.5	9.7	-70.8	-40.0	-159.1	-176.1	-64.3	-33.4	-82.9	-31.1	-130.3	81.1	-69.2	134.0
	WB97XD	-95.4	5.3	-62.7	-44.1	-157.9	179.5	-59.0	-41.6	-65.7	-32.8	-123.2	41.8	-60.6	132.7
17	B3LYP	-82.6	122.4	-175.8	-51.6	130.7	-15.3	-138.3	-63.4	-76.8	-40.0	-134.4	170.5	-127.9	131.1
	WB97XD	-75.7	123.1	-178.6	-52.1	96.6	10.0	-134.3	-61.1	-111.1	-10.3	-146.3	172.4	-137.8	135.2
18	B3LYP	-83.8	119.4	179.1	-49.6	-168.3	-149.9	-83.9	-31.3	-88.9	-40.3	-128.6	138.2	-136.9	136.1
	WB97XD	-78.4	118.4	175.5	-52.6	-172.9	-159.5	-74.1	-38.0	-83.2	-44.7	-126.1	130.8	-142.5	139.6
21	B3LYP	-82.8	116.7	-170.6	-58.3	123.6	-24.1	-89.0	-25.0	-162.7	-63.3	-69.3	157.9	-138.9	133.6
	WB97XD	-72.7	116.2	-175.1	-59.5	107.0	-20.6	-74.1	-32.6	-179.8	-59.4	-62.0	158.8	-151.8	139.1
22	B3LYP	-100.9	9.4	-69.7	-45.7	-138.1	-171.3	-70.3	-32.0	-89.4	-63.9	-81.5	71.2	-74.0	134.1
	WB97XD	-98.6	2.9	-59.6	-49.1	-128.1	172.6	-60.6	-39.5	-77.0	-53.6	-83.1	61.3	-75.6	133.9
41	B3LYP	-92.4	-4.8	-114.1	124.8	-61.4	-26.5	-59.5	-28.4	-112.3	30.0	74.9	-67.7	-152.0	135.0
	WB97XD	-80.3	-22.3	-80.2	121.1	-63.3	-29.5	-61.5	-27.5	-103.9	24.6	73.2	-70.2	-157.5	141.5
82	B3LYP	-89.9	-8.2	-113.8	147.3	-63.1	-27.4	-63.2	-22.5	-116.7	24.1	71.8	-67.3	-134.5	146.2
	WB97XD	-86.2	-4.0	-108.4	145.7	-63.1	-30.3	-65.3	-20.0	-105.6	8.4	66.6	-67.7	-135.3	146.2
43	B3LYP	-91.0	11.5	-82.7	67.0	55.5	-135.3	-79.2	-19.5	-87.1	61.3	74.3	104.1	-59.8	140.9
	WB97XD	-91.9	18.5	-78.9	76.0	56.6	-131.9	-101.4	-2.2	-89.5	70.9	70.3	74.0	-52.6	138.8
81	B3LYP	-100.1	8.3	-117.8	10.1	82.7	-58.1	-68.4	-21.8	-116.4	32.7	70.6	-76.3	-135.9	130.7
	WB97XD	-98.1	6.5	-112.6	-1.3	83.1	-58.9	-63.5	-22.1	-108.4	15.1	69.7	-78.9	-125.0	133.3
		Pro_1	Pro_1	Leu_2	Leu_2	Gly_3	Gly_3	Val_4	Val_4	Leu_5	Leu_5	Leu_6	Leu_6	Tyr_7	Tyr_7

Table S3: Dependence of the Boltzmann populations optimised using the genetic algorithm on the energy uncertainty (Δ*E*). The 2nd column (DFT) list the Boltzmann factors predicted with DFT (i.e., Δ*E* = 0.0). The Δ*E* values are given in kcal/mol.

Conf.	DFT	GA-VCD Boltzmann factors					
1	0.0000	0.0000	0.0000	0.0004	0.0248	0.0357	0.0353
2	0.0000	0.0000	0.0000	0.0000	0.0001	0.0035	0.0636
3	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000
4	0.0009	0.0120	0.0002	0.0001	0.0002	0.0002	0.0001
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.8598	0.3827	0.1453	0.1450	0.1508	0.1581	0.1713
9	0.0016	0.0214	0.0003	0.0001	0.0003	0.0003	0.0002
10	0.0001	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000
12	0.0001	0.0008	0.0085	0.0776	0.0719	0.0699	0.0519
14	0.0011	0.0148	0.1642	0.0001	0.0002	0.0002	0.0002
15	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
16	0.0240	0.0107	0.0040	0.0018	0.0042	0.0044	0.0028
17	0.0000	0.0000	0.0000	0.0000	0.0004	0.0112	0.1160
18	0.0001	0.0009	0.0096	0.1246	0.1132	0.1105	0.0000
21	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
22	0.0001	0.0012	0.0000	0.0000	0.0000	0.0000	0.0000
41	0.0026	0.0012	0.0004	0.0002	0.0005	0.0005	0.0003
43	0.0028	0.0361	0.2110	0.1853	0.1753	0.1679	0.1647
81	0.0798	0.1654	0.0977	0.1280	0.1287	0.1252	0.2050
82	0.0270	0.3510	0.3581	0.3367	0.3167	0.3125	0.1885
ΔE	0.0	1.0	2.0	3.0	4.0	5.0	6.0

Table S4. Dihedral angles (in degrees) of main conformers identified for all-L cyclic at the B3LYP/PCM(ACN)/6-31G(d) level using the GA-VCD protocol.

Confs	Pro_1		Leu_2		Gly_3		Val_4		Leu_5		Leu_6		Tyr_7	
	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ	ϕ	ψ
1	-84	-6	-81	81	-77	38	-135	57	-146	40	-103	-151	-152	126
2	-87	-8	-85	78	-72	165	-113	133	-120	13	-73	171	-141	126
7	-102	13	-79	-42	-145	178	-64	-32	-93	-15	-130	63	-64	133
12	-93	12	-93	-145	-146	173	-75	-40	-113	-4	-84	63	-56	133
20	-83	119	-169	-53	133	-18	-130	-69	-81	-32	-133	166	-130	130
43	-91	11	-82	67	55	-135	-79	-19	-87	61	74	104	-60	141
81	-100	8	-118	10	83	-58	-68	-21	-116	32	70	-76	-136	130
82	-90	-8	-113	147	-63	-27	-63	-22	-116	24	71	-67	-134	146
Lit*	-74	-15	-63	-27	-172	177	-56	-39	-82	-8	-157	71	-64	144

* Auvin-Guette et al., *Tetrahedron* 1999, **55**, 11495 (assigned by NMR in DMSO-d_6)

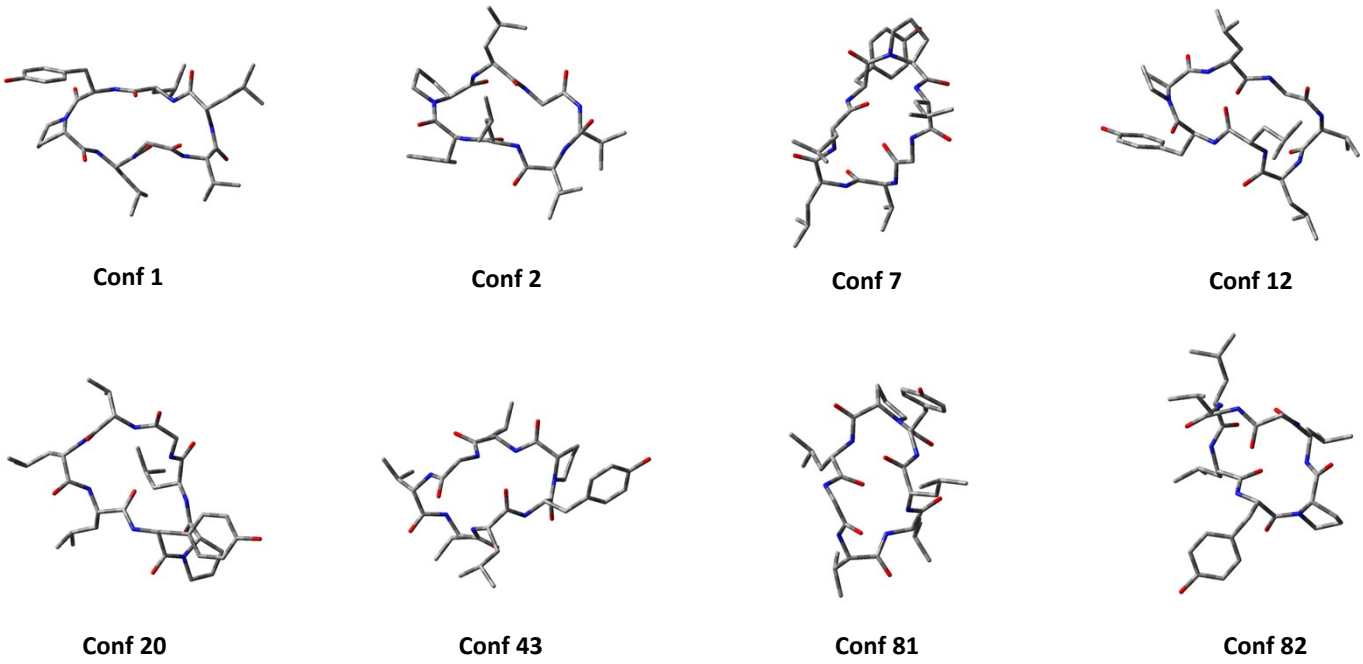

Figure S9: Structures of the main conformers identified for all-L cyclic (free molecules) at the B3LYP/PCM(ACN)/6-31G(d) level using the GA-VCD protocol. Hydrogens are omitted for clarity.

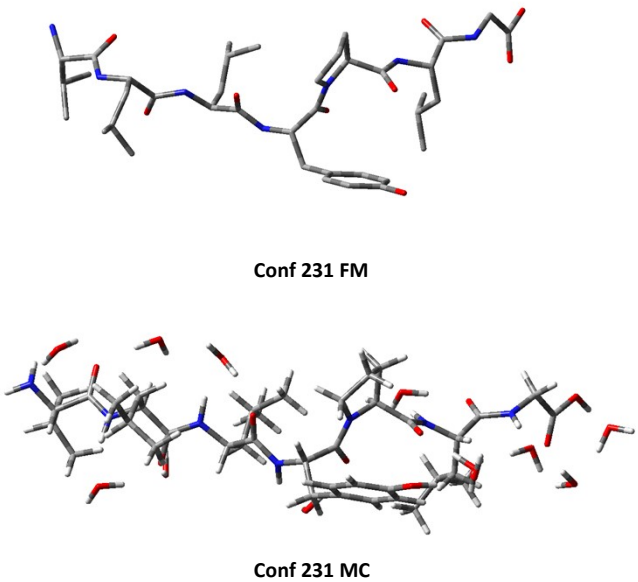

Figure S10: Structure of one of the main conformers identified for all-L linear (free molecule and molecular complex) at the B3LYP/PCM(DMSO)/6-31G(d) level using the GA-VCD protocol.

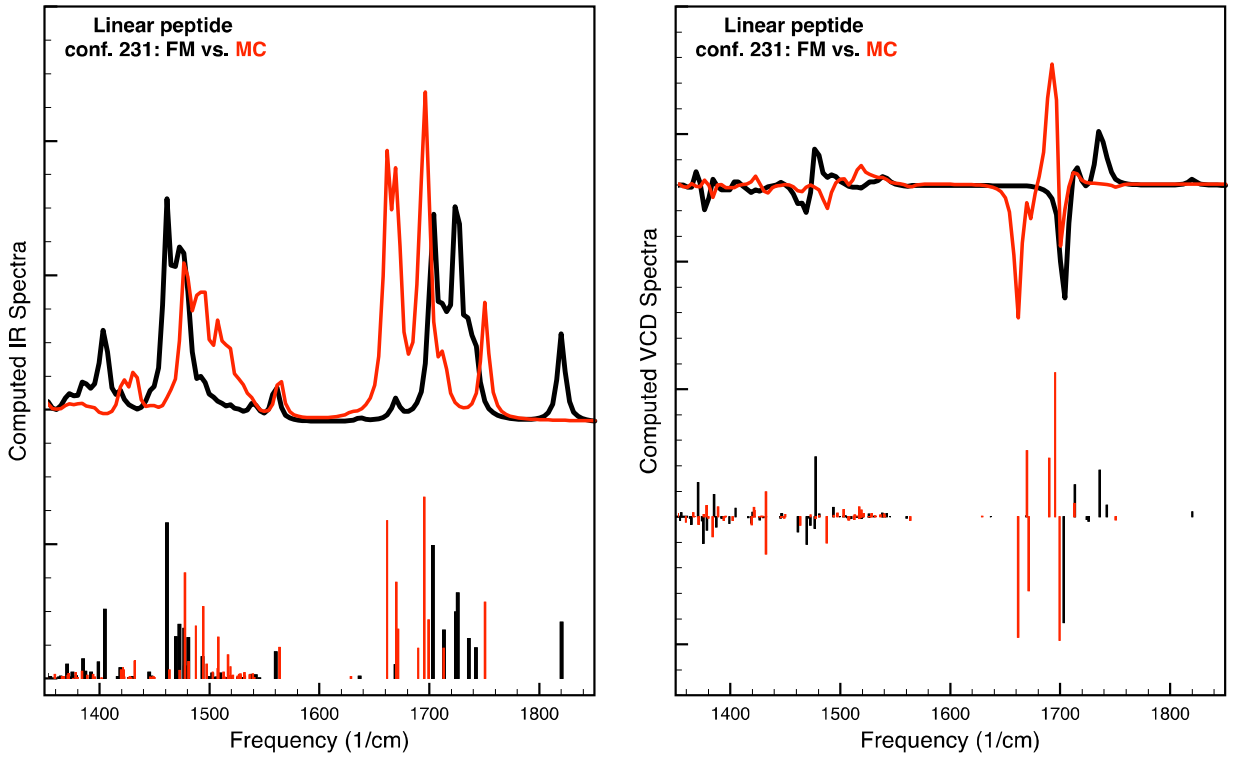

Figure S11: Comparison of the IR (left) and VCD (right) spectra computed for the free molecule (black) and molecular complex (red) associated with conformer 231 of the linear peptide. The position of the normal modes is indicated by the vertical bars.

Table S5: Normal mode (NM) analysis for conformer 231 of the (all-L) linear peptide: decomposition of the normal modes of the molecular complex (MC) into modes of the free molecule (FM). Only the modes (in the amide I and II modes spectra interval) that have VCD intensities larger than 100 × 10^{-44} $esu^{2}\cdot cm^{2}$ (absolute values) have been considered. The frequencies of the normal modes (Freq.), the rotational strengths (R.S.) and the dipole strength (D.S.) are also given. Units: Freq. (cm^{-1}), R.S.(10^{-44} $esu^{2}\cdot cm^{2}$) and D.S.(10^{-40} $esu^{2}\cdot cm^{2}$). The overlap values (6th column) are obtained by computing a scalar product between the normalised nuclear displacement vectors of the FM and of the MC. The similarity values (7th column) are obtain by taking the square of the Overlap values (6th column).

	NM	Freq.	D.S.	R.S.	Overlap	Similarity
MC	362	1661.6	2348.5	-942.5		
FM	280	1713.4	721.9	251.6	0.64	0.41
FM	281	1724.1	989.5	-19.6	-0.44	0.20
FM	283	1735.9	594.6	366.6	0.44	0.20
MC	363	1669.8	1435.0	516.8		
FM	192	1204.8	37.4	-18.9	0.31	0.09
FM	193	1205.3	31.3	19.8	0.45	0.20
FM	278	1669.4	205.1	5.8	-0.78	0.60
FM	279	1703.2	1978.0	-829.1	0.59	0.35
MC	364	1671.3	732.6	-578.7		
FM	192	1204.8	37.4	-18.9	-0.36	0.13
FM	193	1205.3	31.3	19.8	-0.39	0.15
FM	278	1669.4	205.1	5.8	0.76	0.58
FM	279	1703.2	1978.0	-829.1	0.63	0.40
MC	365	1689.9	447.8	457.4		
FM	281	1724.1	989.5	-19.6	-0.53	0.28
FM	283	1735.9	594.6	366.6	-0.43	0.19
MC	366	1695.4	2699.6	1129.7		
FM	282	1725.8	1277.7	-34.7	0.88	0.77
MC	367	1699.4	874.6	-968.8		
FM	280	1713.4	721.9	251.6	0.56	0.32
FM	281	1724.1	989.5	-19.6	0.35	0.12
FM	283	1735.9	594.6	366.6	-0.61	0.37
MC	368	1713.1	449.8	103.8		
FM	284	1742.4	455.4	89.7	0.94	0.88

Section S1. Cartesian coordinates

Free molecule (B3LYP/PCM(ACN)/6-31G(d))
Conformer 1

Symbol	X	Y	Z
N	-1.71884	-1.67947	1.090373
C	-2.97122	-1.36376	0.410607
H	-2.71618	-0.74987	-0.45329
C	-3.83994	-0.61805	1.435292
O	-4.03338	-1.13719	2.539682
C	-3.69809	-2.64577	-0.08004
H	-2.98248	-3.19457	-0.70089

H	-3.91816	-3.26129	0.798526
C	-4.96216	-2.35702	-0.86035
C	-6.21328	-2.3154	-0.23024
H	-6.28409	-2.52234	0.834872
C	-4.9132	-2.09154	-2.23857
H	-3.95779	-2.12809	-2.75742
C	-7.37658	-2.01651	-0.94108
H	-8.33822	-1.99652	-0.43306
C	-6.06416	-1.79052	-2.96295
H	-6.01885	-1.59169	-4.02946
C	-7.30383	-1.75021	-2.3129
O	-8.40313	-1.45253	-3.06936
H	-9.19215	-1.45347	-2.50296
N	-4.35729	0.599027	1.120938
C	-4.31246	1.285729	-0.18268
H	-4.40163	0.575911	-1.00793
C	-3.02418	2.088652	-0.4419
O	-2.84198	2.608087	-1.54901
C	-5.54658	2.215202	-0.12796
H	-6.42502	1.653054	-0.46132
H	-5.42566	3.08139	-0.78187
C	-5.664	2.565328	1.363117
H	-6.66399	2.907836	1.640477
H	-4.95241	3.355595	1.626998
C	-5.29176	1.25536	2.067098
H	-4.80985	1.398077	3.03726
H	-6.16151	0.605401	2.215996
N	-2.145	2.194622	0.579692
H	-2.33593	1.697026	1.439889
C	-0.87311	2.914903	0.459067
H	-1.06049	3.762906	-0.20515
C	0.140879	1.96884	-0.22301
O	0.961202	1.304578	0.432459
C	-0.40454	3.395624	1.834893
H	-1.24327	3.925181	2.305822
H	-0.18847	2.514168	2.450852
C	0.832679	4.316845	1.822458
H	1.639725	3.794178	1.291314
C	0.567356	5.65114	1.10758
H	0.298116	5.516653	0.053797
H	-0.24916	6.199504	1.595251
H	1.459598	6.287076	1.136307
C	1.306352	4.562259	3.263065

H	0.531737	5.074588	3.848446
H	1.543076	3.620266	3.771507
H	2.205312	5.189005	3.278686
N	0.041305	1.9233	-1.56787
H	-0.75362	2.422009	-1.96144
C	0.630212	0.877957	-2.40995
H	0.125217	0.913667	-3.37523
H	0.43366	-0.10364	-1.95917
C	2.134381	0.95031	-2.69744
O	2.575479	0.560432	-3.78039
N	2.92316	1.34829	-1.66803
H	2.471464	1.523649	-0.77395
C	4.382785	1.265225	-1.72061
H	4.615331	0.543527	-2.51291
C	4.873517	0.681585	-0.37933
O	5.620395	1.293552	0.382964
C	5.029977	2.610078	-2.1401
H	4.561418	2.825208	-3.11079
C	4.702384	3.78301	-1.20488
H	5.167338	3.649813	-0.22509
H	5.070167	4.720423	-1.63839
H	3.620236	3.887462	-1.06416
C	6.539645	2.465243	-2.3831
H	6.754243	1.646507	-3.08144
H	6.941918	3.386713	-2.81927
H	7.073719	2.267555	-1.44983
N	4.386274	-0.54969	-0.01502
H	4.76034	-0.84416	0.881911
C	3.872	-1.63009	-0.8628
H	3.399655	-1.17146	-1.73616
C	2.739986	-2.39798	-0.12687
O	2.643581	-3.62404	-0.20917
C	4.962574	-2.59314	-1.37274
H	4.441782	-3.36856	-1.9425
H	5.590778	-2.04508	-2.08696
C	5.85854	-3.25152	-0.29197
H	5.287384	-3.30677	0.645683
C	6.206067	-4.69348	-0.6929
H	6.846987	-5.17023	0.058447
H	5.298556	-5.29775	-0.80133
H	6.742747	-4.71462	-1.6506
C	7.14553	-2.45024	-0.02936
H	7.770458	-2.42386	-0.93181

H	6.946389	-1.41315	0.260616
H	7.736076	-2.9134	0.770116
C	0.709645	-2.1673	1.255104
H	0.80884	-3.25588	1.194072
C	-0.55001	-1.82125	0.419645
O	-0.48586	-1.70658	-0.80718
C	0.659337	-1.72776	2.733183
C	1.921754	-2.05276	3.557322
H	2.772139	-1.54911	3.078552
C	1.774095	-1.48168	4.975742
H	0.938358	-1.95615	5.506582
H	2.683028	-1.65516	5.563375
H	1.587346	-0.40128	4.955221
C	2.224875	-3.55847	3.602992
H	1.378064	-4.11657	4.024628
H	2.438256	-3.96587	2.609081
H	3.098747	-3.75502	4.235181
H	-1.77992	-1.84284	2.086551
H	0.47181	-0.64661	2.774183
H	-0.19213	-2.21955	3.22346
N	1.881378	-1.62714	0.584194
H	1.940764	-0.61579	0.510102

Conformer 2

Symbol	X	Y	Z
N	-1.31122	-1.35769	1.550438
C	-2.51517	-1.49596	0.739914
H	-2.2969	-1.01974	-0.21535
C	-3.64666	-0.79683	1.508021
O	-3.8514	-1.11057	2.685207
C	-2.86663	-2.98938	0.499729
H	-1.98052	-3.45615	0.056271
H	-3.03015	-3.45455	1.47789
C	-4.07272	-3.19329	-0.39227
C	-5.36172	-3.31418	0.144822
H	-5.49743	-3.2868	1.223191
C	-3.93762	-3.23884	-1.78923
H	-2.94828	-3.15735	-2.23391
C	-6.47999	-3.47232	-0.67523
H	-7.47071	-3.56967	-0.23663
C	-5.04292	-3.39494	-2.62236
H	-4.93002	-3.43457	-3.70156

C	-6.32231	-3.51164	-2.06522
O	-7.3728	-3.66712	-2.92645
H	-8.19695	-3.739	-2.41775
N	-4.37881	0.166831	0.888297
C	-4.3618	0.515257	-0.54447
H	-4.19749	-0.36804	-1.16484
C	-3.28624	1.539228	-0.94962
O	-3.11282	1.793751	-2.14792
C	-5.78148	1.084183	-0.77793
H	-6.46036	0.253279	-0.99604
H	-5.80392	1.775614	-1.62289
C	-6.1371	1.728636	0.570195
H	-7.21381	1.855046	0.708477
H	-5.6689	2.715305	0.658038
C	-5.53855	0.759159	1.596045
H	-5.21202	1.242522	2.520086
H	-6.23848	-0.04028	1.865071
N	-2.59671	2.13968	0.043729
H	-2.75735	1.841791	0.997388
C	-1.60519	3.193626	-0.20809
H	-1.95195	3.720759	-1.10317
C	-0.24412	2.529256	-0.53426
O	0.666607	2.421418	0.29024
C	-1.53453	4.163958	0.978838
H	-2.53237	4.204851	1.432869
H	-0.84892	3.75517	1.730803
C	-1.11803	5.604875	0.613925
H	-1.83673	5.97045	-0.13576
C	-1.2361	6.506686	1.851983
H	-2.25014	6.485993	2.269059
H	-0.54305	6.182557	2.639223
H	-0.99459	7.546702	1.603522
C	0.288867	5.704779	0.005187
H	1.045469	5.339221	0.709708
H	0.392672	5.123873	-0.91709
H	0.524793	6.749356	-0.23171
N	-0.15106	2.057675	-1.79777
H	-0.97639	2.093205	-2.38701
C	1.037701	1.361895	-2.23906
H	0.82306	0.883435	-3.19984
H	1.273509	0.573525	-1.51957
C	2.217055	2.332637	-2.41651
O	2.049885	3.54788	-2.50297

N	3.468591	1.799345	-2.51206
H	4.202563	2.499226	-2.51241
C	3.940157	0.425039	-2.34965
H	3.072078	-0.22122	-2.22031
C	4.817553	0.421501	-1.07675
O	5.606611	1.347951	-0.88671
C	4.692593	-0.04296	-3.6366
H	3.956225	0.098804	-4.43899
C	5.925482	0.807916	-3.97644
H	6.701239	0.719645	-3.20955
H	6.348457	0.471215	-4.92925
H	5.676547	1.86842	-4.08737
C	5.057472	-1.53306	-3.59347
H	4.180332	-2.16624	-3.41635
H	5.491616	-1.83738	-4.55189
H	5.80264	-1.74707	-2.81813
N	4.65934	-0.55389	-0.12965
H	5.277353	-0.40351	0.661908
C	4.050126	-1.88189	-0.21306
H	3.622221	-1.99145	-1.2129
C	2.853635	-2.07357	0.750086
O	2.406062	-3.20198	0.957822
C	5.072242	-3.02285	-0.0175
H	4.502712	-3.94969	-0.12526
H	5.791387	-2.99063	-0.8438
C	5.825361	-3.02758	1.341437
H	5.240467	-2.44589	2.070396
C	5.932367	-4.45855	1.891674
H	6.46724	-4.47505	2.848625
H	4.938629	-4.89286	2.047358
H	6.478097	-5.10511	1.192242
C	7.224504	-2.39533	1.237369
H	7.860204	-2.98451	0.56406
H	7.201232	-1.37176	0.846176
H	7.713327	-2.36511	2.217906
C	1.071526	-1.00561	2.02873
H	1.073447	-1.92352	2.624291
C	-0.08776	-1.13163	1.007686
O	0.089617	-1.03542	-0.20674
C	0.906571	0.223733	2.945905
C	2.007645	0.398785	4.011201
H	2.974195	0.470671	3.493374
C	1.784715	1.715781	4.770647

H	0.834084	1.696689	5.319683
H	2.585895	1.889234	5.49845
H	1.758941	2.572025	4.086256
C	2.079904	-0.78543	4.98633
H	1.121637	-0.9254	5.504015
H	2.328975	-1.72453	4.479699
H	2.847746	-0.6117	5.749221
H	-1.42402	-1.48294	2.549128
H	0.857444	1.119286	2.314106
H	-0.06353	0.148398	3.453885
N	2.338444	-0.95753	1.321528
H	2.651295	-0.05953	0.973356

Conformer 7

Symbol	X	Y	Z
N	0.426113	-0.51302	-1.95217
C	1.639886	-1.10027	-1.38802
H	1.603703	-0.96937	-0.30334
C	2.87834	-0.41263	-2.00632
O	2.925218	-0.25752	-3.22727
C	1.635274	-2.60911	-1.73966
H	0.682578	-3.02162	-1.38536
H	1.642732	-2.68961	-2.83243
C	2.78094	-3.4048	-1.15325
C	3.937403	-3.66738	-1.89869
H	4.014555	-3.29587	-2.91745
C	2.712558	-3.912	0.15423
H	1.820064	-3.73756	0.751127
C	4.995571	-4.40401	-1.36411
H	5.880556	-4.60304	-1.96431
C	3.760042	-4.6466	0.704286
H	3.697672	-5.04117	1.713868
C	4.909132	-4.89633	-0.05685
O	5.902412	-5.63185	0.525982
H	6.633679	-5.74194	-0.10366
N	3.889239	-0.00752	-1.18036
C	4.09413	-0.32806	0.24444
H	3.522685	-1.21476	0.523138
C	3.690802	0.78749	1.231107
O	4.022379	0.696481	2.415653
C	5.626062	-0.62065	0.367329
H	5.795905	-1.63338	0.740109

H	6.073786	0.069695	1.08556
C	6.200973	-0.42468	-1.05132
H	6.269483	-1.38615	-1.57041
H	7.196288	0.028631	-1.04072
C	5.164872	0.457765	-1.75408
H	5.307532	1.518292	-1.51023
H	5.132202	0.348365	-2.83694
N	2.995987	1.836697	0.733536
H	2.6092	1.773381	-0.20455
C	2.590942	2.950529	1.586957
H	3.415752	3.14614	2.274455
C	1.389669	2.622805	2.497581
O	1.342331	3.032386	3.660344
C	2.318005	4.188462	0.705403
H	3.234112	4.386134	0.13195
H	1.540372	3.926071	-0.02339
C	1.901179	5.472576	1.449027
H	0.976028	5.263171	2.003961
C	2.959253	5.939505	2.460311
H	3.92917	6.097366	1.970168
H	2.660364	6.889138	2.919717
H	3.095207	5.21015	3.264836
C	1.593017	6.578664	0.428241
H	0.815732	6.265929	-0.27931
H	1.245344	7.488744	0.930793
H	2.488225	6.839106	-0.15158
N	0.388539	1.914119	1.922947
H	0.49133	1.564404	0.974563
C	-0.76903	1.476023	2.669421
H	-1.58618	2.21114	2.63062
H	-0.49269	1.367869	3.723377
C	-1.27303	0.148182	2.107876
O	-0.77034	-0.36336	1.100374
N	-2.33146	-0.4149	2.740923
H	-2.62962	-0.01457	3.623142
C	-2.72735	-1.79893	2.451907
H	-1.82857	-2.42467	2.480214
C	-3.25747	-1.9944	1.016584
O	-3.13434	-3.0911	0.471409
C	-3.6977	-2.30948	3.553286
H	-3.18075	-2.09812	4.500606
C	-5.04761	-1.57579	3.57461
H	-5.63919	-1.8057	2.681617

H	-5.62832	-1.893	4.447196
H	-4.93692	-0.48682	3.633844
C	-3.89434	-3.82951	3.469859
H	-4.50807	-4.16947	4.310871
H	-4.39618	-4.11806	2.541392
H	-2.93625	-4.35887	3.513102
N	-3.85187	-0.92732	0.414658
H	-3.95758	-0.07288	0.948796
C	-4.32251	-0.96054	-0.96571
H	-4.27096	-2.00891	-1.27029
C	-3.40973	-0.19711	-1.95655
O	-3.72401	-0.12174	-3.14609
C	-5.76985	-0.44986	-1.10723
H	-5.80837	0.595765	-0.7686
H	-5.99766	-0.43786	-2.17872
C	-6.84321	-1.26345	-0.36074
H	-6.60684	-1.23744	0.712147
C	-8.21563	-0.59894	-0.55043
H	-8.99009	-1.12948	0.015531
H	-8.20564	0.444085	-0.21202
H	-8.51106	-0.60496	-1.60772
C	-6.88448	-2.73438	-0.80217
H	-7.05975	-2.81424	-1.88328
H	-5.95272	-3.26203	-0.57073
H	-7.69734	-3.26586	-0.29354
C	-1.34067	1.162105	-2.21313
H	-1.4622	0.864323	-3.25975
C	0.082266	0.772589	-1.75724
O	0.848047	1.588835	-1.22366
C	-1.56582	2.676309	-2.06197
C	-2.89603	3.220447	-2.61664
H	-3.71788	2.644465	-2.16908
C	-3.06698	4.686976	-2.18942
H	-2.26522	5.312018	-2.60435
H	-4.02183	5.091398	-2.54534
H	-3.04168	4.792989	-1.09814
C	-2.99777	3.086091	-4.1438
H	-3.93104	3.532321	-4.50803
H	-2.16633	3.605629	-4.63858
H	-2.98972	2.038221	-4.45763
H	-0.25769	-1.14136	-2.35489
H	-1.48619	2.924897	-0.99645
H	-0.73253	3.190031	-2.55848

N	-2.28975	0.361588	-1.43676
H	-2.04906	0.158585	-0.4716

Conformer 12

Symbol	X	Y	Z
N	-0.75659	-1.03499	1.470524
C	-2.02935	-1.33533	0.815137
H	-1.9933	-0.95619	-0.21058
C	-3.18188	-0.68245	1.613871
O	-3.22073	-0.81071	2.839492
C	-2.19306	-2.87602	0.805216
H	-1.29616	-3.29862	0.33701
H	-2.20401	-3.20686	1.850075
C	-3.42768	-3.37645	0.087609
C	-4.63566	-3.56541	0.772458
H	-4.68406	-3.36035	1.839066
C	-3.40018	-3.66301	-1.28645
H	-2.4733	-3.53781	-1.84173
C	-5.78131	-4.01609	0.115348
H	-6.70667	-4.16257	0.667923
C	-4.53444	-4.11303	-1.95796
H	-4.50453	-4.33666	-3.02003
C	-5.73317	-4.29022	-1.25628
O	-6.81546	-4.73889	-1.96022
H	-7.57704	-4.81761	-1.36261
N	-4.1365	0.023416	0.945339
C	-4.42237	0.04132	-0.50416
H	-4.12822	-0.90498	-0.96527
C	-3.72221	1.150111	-1.32249
O	-4.09084	1.358166	-2.48243
C	-5.95379	0.213974	-0.54649
H	-6.42982	-0.76408	-0.41894
H	-6.27474	0.638008	-1.49913
C	-6.23324	1.110796	0.667616
H	-7.2729	1.068336	1.003071
H	-5.9997	2.155214	0.42998
C	-5.2666	0.573198	1.729158
H	-4.90917	1.337421	2.424948
H	-5.71444	-0.23209	2.322302
N	-2.72772	1.82662	-0.70845
H	-2.39904	1.514803	0.205309
C	-1.8196	2.695934	-1.43957

H	-2.31228	2.913204	-2.39274
C	-0.56133	1.872882	-1.82332
O	-0.66382	0.691997	-2.1615
C	-1.55412	4.007887	-0.67952
H	-0.98266	3.78271	0.230432
H	-0.92644	4.654825	-1.30807
C	-2.81649	4.804522	-0.29049
H	-3.42754	4.164029	0.359709
C	-2.41609	6.05009	0.514218
H	-1.81026	6.734001	-0.09467
H	-3.30238	6.600656	0.850615
H	-1.82909	5.782845	1.401055
C	-3.66805	5.192424	-1.50897
H	-4.05711	4.314326	-2.03571
H	-4.52758	5.798995	-1.20033
H	-3.08247	5.785582	-2.22421
N	0.627323	2.525996	-1.8307
H	0.733351	3.430349	-1.38868
C	1.861178	1.848911	-2.16132
H	2.098375	1.952021	-3.23056
H	1.738907	0.777868	-1.97314
C	3.005593	2.450625	-1.34378
O	2.831325	3.448531	-0.6418
N	4.219729	1.841526	-1.44187
H	4.964387	2.322742	-0.9501
C	4.55055	0.669175	-2.25338
H	4.023607	0.742499	-3.2088
C	4.016875	-0.64974	-1.64387
O	3.497963	-1.4948	-2.37085
C	6.069891	0.647387	-2.59132
H	6.257445	1.617807	-3.07029
C	6.997003	0.536065	-1.37034
H	6.896058	-0.43445	-0.87208
H	8.038135	0.629929	-1.6958
H	6.828468	1.321182	-0.62347
C	6.383828	-0.45218	-3.61645
H	5.762578	-0.35383	-4.51316
H	7.433196	-0.38597	-3.92186
H	6.218314	-1.45153	-3.19943
N	4.11958	-0.79189	-0.28965
H	4.674438	-0.11976	0.226405
C	3.568205	-1.93631	0.429486
H	3.138228	-2.58648	-0.33575

C	2.39696	-1.55548	1.356689
O	1.782173	-2.43628	1.973228
C	4.631742	-2.71454	1.231828
H	5.091808	-2.03117	1.959271
H	4.098606	-3.47638	1.812165
C	5.736712	-3.38754	0.395281
H	6.258456	-2.60714	-0.17702
C	6.762516	-4.04077	1.334613
H	7.588789	-4.48219	0.765731
H	7.187017	-3.31152	2.034879
H	6.297662	-4.84106	1.924835
C	5.180599	-4.41356	-0.60401
H	4.54229	-3.9462	-1.36146
H	5.999147	-4.91763	-1.13087
H	4.591633	-5.18376	-0.08883
C	1.079921	0.297672	2.368585
H	1.071915	-0.35373	3.248994
C	-0.32595	0.215365	1.7239
O	-0.98849	1.230633	1.47293
C	1.438725	1.736916	2.753554
C	2.737574	1.891067	3.570341
H	3.535738	1.334779	3.057837
C	3.152993	3.36969	3.608642
H	3.307482	3.7632	2.596817
H	2.38117	3.9819	4.093221
H	4.084781	3.502015	4.170684
C	2.603077	1.323438	4.991317
H	2.353033	0.256445	4.990802
H	3.541897	1.439756	5.545091
H	1.818243	1.851226	5.548591
H	-0.13656	-1.80412	1.722356
H	1.508885	2.328998	1.831281
H	0.597711	2.156886	3.316411
N	2.093829	-0.24413	1.459153
H	2.581083	0.407141	0.858971

Conformer 20

Symbol	X	Y	Z
N	1.220311	1.707319	-1.3357
C	2.515193	1.045954	-1.20411
H	2.357408	0.181352	-0.5642
C	3.467012	2.084959	-0.58165

O	3.51656	3.21046	-1.09535
C	3.045646	0.585293	-2.58843
H	2.273917	-0.05431	-3.03005
H	3.136108	1.474747	-3.22159
C	4.366473	-0.15155	-2.52183
C	5.584552	0.536106	-2.61071
H	5.582013	1.61446	-2.7495
C	4.410923	-1.54441	-2.35082
H	3.481655	-2.10688	-2.292
C	6.805761	-0.13358	-2.52923
H	7.738729	0.419897	-2.60698
C	5.621445	-2.22897	-2.26758
H	5.647689	-3.30733	-2.14343
C	6.826994	-1.52229	-2.35661
O	7.987069	-2.24104	-2.2756
H	8.744709	-1.63974	-2.36448
N	4.224597	1.754115	0.488073
C	4.308539	0.4461	1.167061
H	4.289265	-0.36008	0.430461
C	3.1643	0.283978	2.193788
O	3.035468	1.053401	3.145399
C	5.684748	0.515516	1.863969
H	6.448829	0.184802	1.152612
H	5.735113	-0.13256	2.742736
C	5.861862	2.006128	2.196708
H	6.912484	2.286327	2.310931
H	5.335324	2.245643	3.122947
C	5.205849	2.728111	1.012665
H	4.701297	3.655706	1.295319
H	5.924638	2.966347	0.220137
N	2.325925	-0.75578	1.941604
H	2.608164	-1.40834	1.222137
C	1.227495	-1.18761	2.828336
H	1.646452	-1.40055	3.815457
C	0.719211	-2.5378	2.293748
O	0.666663	-3.53032	3.017458
C	0.13366	-0.09894	2.95857
H	0.663376	0.819387	3.225928
H	-0.31671	0.067262	1.973956
C	-0.97562	-0.33848	4.0126
H	-1.47154	0.637218	4.117697
C	-2.05852	-1.33467	3.566023
H	-1.66549	-2.3522	3.469016

H	-2.87327	-1.36705	4.299224
H	-2.49322	-1.03783	2.603332
C	-0.41765	-0.71321	5.395364
H	0.365304	-0.01508	5.715614
H	-1.21385	-0.69302	6.14847
H	0.008183	-1.72354	5.395162
N	0.366826	-2.55299	0.971687
H	0.43744	-1.6932	0.426851
C	0.188939	-3.80686	0.257717
H	0.165074	-4.60292	1.007086
H	1.040502	-4.00331	-0.40342
C	-1.05963	-3.94131	-0.6136
O	-1.10146	-4.82818	-1.46636
N	-2.07971	-3.07604	-0.37794
H	-1.95928	-2.39288	0.358214
C	-3.31194	-3.1289	-1.16647
H	-3.03943	-3.67466	-2.07107
C	-3.68169	-1.72598	-1.68869
O	-3.56937	-1.45246	-2.8818
C	-4.44487	-3.95069	-0.48497
H	-4.00742	-4.95325	-0.38672
C	-4.85122	-3.50286	0.926946
H	-5.4527	-2.58576	0.921257
H	-5.47372	-4.27598	1.390478
H	-3.98334	-3.35231	1.578605
C	-5.66406	-4.05708	-1.41286
H	-5.38353	-4.43173	-2.40394
H	-6.40579	-4.7435	-0.99056
H	-6.15308	-3.08402	-1.54595
N	-4.10971	-0.79819	-0.78121
H	-4.32127	-1.08803	0.164345
C	-4.60344	0.509493	-1.21928
H	-5.12528	0.368526	-2.16837
C	-3.46708	1.505455	-1.52314
O	-3.62622	2.403437	-2.35279
C	-5.57234	1.061398	-0.15006
H	-6.34801	0.298908	0.007667
H	-5.02302	1.155831	0.79695
C	-6.25943	2.404411	-0.46747
H	-5.48068	3.16514	-0.60759
C	-7.09742	2.347618	-1.75334
H	-6.47172	2.170341	-2.6334
H	-7.85085	1.550623	-1.69876

H	-7.62654	3.295158	-1.90854
C	-7.12393	2.827385	0.730442
H	-7.92721	2.101315	0.911354
H	-6.52883	2.904214	1.648303
H	-7.59045	3.802441	0.549078
C	-1.14643	2.148451	-0.92552
H	-1.20374	2.654812	-1.89343
C	0.052056	1.180734	-0.91892
O	-0.07165	0.017963	-0.5072
C	-0.97256	3.190363	0.211226
C	-2.05967	4.278984	0.29156
H	-3.0364	3.778763	0.345526
C	-1.8779	5.091983	1.583204
H	-1.91955	4.450114	2.47131
H	-0.90964	5.609517	1.589268
H	-2.66167	5.852311	1.679655
C	-2.05963	5.200223	-0.93732
H	-1.08238	5.684986	-1.06355
H	-2.29723	4.651077	-1.85329
H	-2.80992	5.991696	-0.823
H	1.258605	2.674133	-1.63935
H	-0.93807	2.641454	1.16193
H	0.005651	3.675945	0.096887
N	-2.35297	1.357323	-0.76734
H	-2.24036	0.492431	-0.25103

Conformer 43

Symbol	X	Y	Z
N	-1.67277	-1.09187	0.222023
H	-1.91819	-2.07187	0.287533
C	-2.4233	-0.26037	-0.70684
H	-1.69958	0.358631	-1.24228
C	-3.39854	0.63462	0.090284
O	-3.98446	0.202832	1.083643
C	-3.13739	-1.14297	-1.77034
H	-3.74563	-0.4802	-2.39645
H	-2.35064	-1.54819	-2.41584
C	-3.98605	-2.27878	-1.23646
C	-5.30808	-2.07744	-0.81389
H	-5.7447	-1.08439	-0.86584
C	-3.46891	-3.5822	-1.1639
H	-2.45675	-3.77783	-1.51228

C	-6.08214	-3.12827	-0.32663
H	-7.10692	-2.94997	-0.00845
C	-4.22801	-4.64421	-0.67362
H	-3.81889	-5.64868	-0.62426
C	-5.54106	-4.41806	-0.24969
O	-6.24858	-5.48915	0.219811
H	-7.13658	-5.19654	0.482826
N	-3.57328	1.920067	-0.32875
C	-3.13281	2.53276	-1.59197
H	-3.10482	1.795392	-2.39957
C	-1.73837	3.194666	-1.5821
O	-1.41143	3.885109	-2.56179
C	-4.2279	3.587895	-1.8589
H	-5.08235	3.100796	-2.34066
H	-3.86467	4.380729	-2.51415
C	-4.60339	4.058693	-0.44649
H	-5.58493	4.537678	-0.40329
H	-3.86306	4.777208	-0.07643
C	-4.55841	2.767985	0.380592
H	-4.24716	2.923289	1.417231
H	-5.52688	2.25543	0.397334
N	-0.9244	2.977283	-0.53059
H	-1.15125	2.256316	0.157235
C	0.434421	3.537988	-0.47327
H	0.389645	4.496146	-0.99922
C	1.405471	2.627924	-1.26463
O	2.303827	1.967312	-0.73196
C	0.896753	3.734343	0.973303
H	0.960101	2.752662	1.453999
H	1.921153	4.12738	0.9386
C	0.020252	4.674403	1.823789
H	-1.00251	4.271638	1.833553
C	0.530769	4.683355	3.27285
H	0.545882	3.672194	3.696309
H	1.551869	5.083412	3.326389
H	-0.1056	5.307865	3.910861
C	-0.03948	6.102791	1.261501
H	0.96592	6.539377	1.195412
H	-0.48664	6.137166	0.261582
H	-0.64114	6.749772	1.910691
N	1.178598	2.607653	-2.599
H	0.365254	3.110602	-2.94961
C	1.879608	1.67295	-3.45515

H	2.945086	1.923328	-3.50163
H	1.469555	1.766432	-4.46432
C	1.680991	0.222927	-2.98215
O	0.581282	-0.21752	-2.654
N	2.814917	-0.52572	-2.96735
H	3.692558	-0.08177	-3.20582
C	2.849739	-1.90644	-2.50543
H	1.914764	-2.38503	-2.81236
C	2.877198	-2.0036	-0.96487
O	2.581104	-3.07129	-0.40564
C	4.043306	-2.64757	-3.1783
H	4.95641	-2.09557	-2.90796
C	4.21043	-4.09815	-2.70289
H	5.048322	-4.5587	-3.23801
H	4.407438	-4.16675	-1.63161
H	3.310835	-4.68754	-2.91679
C	3.890237	-2.61573	-4.70892
H	2.990428	-3.1629	-5.01707
H	3.815756	-1.59802	-5.10296
H	4.753544	-3.09677	-5.18107
N	3.267068	-0.90633	-0.2791
H	3.252461	0.000504	-0.73979
C	3.505072	-0.91693	1.169104
H	3.822383	-1.93556	1.414671
C	2.196814	-0.64476	1.966363
O	2.08918	0.308165	2.734685
C	4.59747	0.091843	1.540005
H	4.241649	1.094517	1.272836
H	4.696149	0.087388	2.632035
C	5.976978	-0.15497	0.899017
H	5.848595	-0.17904	-0.19251
C	6.91886	1.012086	1.232796
H	7.089669	1.081031	2.315187
H	7.894207	0.881986	0.749377
H	6.501605	1.96976	0.899257
C	6.599732	-1.49186	1.330094
H	6.717385	-1.53492	2.421021
H	5.992001	-2.35092	1.024348
H	7.592842	-1.61869	0.883178
N	1.238586	-1.58733	1.745495
H	1.483943	-2.3101	1.069419
C	-0.17788	-1.50948	2.126561
H	-0.57159	-2.5147	1.949723

C	-0.89637	-0.53281	1.176059
O	-0.7376	0.69196	1.259033
C	-0.44499	-1.12652	3.592349
H	-0.16753	-0.08009	3.729544
H	-1.53189	-1.19884	3.745488
C	0.272845	-1.99186	4.64449
H	1.352964	-1.90385	4.467007
C	-0.01613	-1.43899	6.048731
H	0.526764	-2.00582	6.814368
H	-1.08675	-1.50179	6.284296
H	0.28308	-0.38737	6.131996
C	-0.10698	-3.4776	4.557368
H	0.182665	-3.92182	3.598355
H	0.391344	-4.05213	5.347155
H	-1.18977	-3.6141	4.679073

Conformer 81

Symbol	X	Y	Z
N	1.18134	2.097721	0.027398
H	0.830429	2.438114	0.920801
C	2.473104	1.424003	-0.00565
H	2.50325	0.863742	-0.93876
C	2.57519	0.520459	1.229237
O	2.310595	0.990852	2.338831
C	3.61527	2.481721	0.008265
H	3.429601	3.152404	-0.83784
H	3.501968	3.072448	0.923876
C	5.014257	1.910268	-0.07492
C	5.763218	1.65122	1.083618
H	5.332972	1.871602	2.057628
C	5.605208	1.622913	-1.31363
H	5.056248	1.825347	-2.2306
C	7.051112	1.123927	1.014928
H	7.627624	0.935293	1.915554
C	6.892181	1.091434	-1.40087
H	7.332074	0.880753	-2.37306
C	7.621517	0.841756	-0.23235
O	8.890678	0.334239	-0.24534
H	9.172134	0.195368	-1.16449
N	2.959136	-0.78022	1.081656
C	3.5302	-1.41119	-0.1233

H	3.965227	-0.66521	-0.79035
C	2.533021	-2.23188	-0.97031
O	2.951222	-2.9036	-1.91165
C	4.6352	-2.31983	0.456126
H	5.533696	-1.71586	0.617435
H	4.881526	-3.13461	-0.2267
C	4.049164	-2.78349	1.798238
H	4.818475	-3.09795	2.508193
H	3.373396	-3.63244	1.648392
C	3.276779	-1.55716	2.30809
H	2.360542	-1.81476	2.846481
H	3.883151	-0.92805	2.967192
N	1.213954	-2.15217	-0.63136
H	0.993054	-1.66805	0.231753
C	0.217227	-3.06459	-1.18529
H	0.760826	-3.69762	-1.89413
C	-0.87717	-2.37678	-2.02022
O	-1.86574	-3.03107	-2.39077
C	-0.43782	-3.94043	-0.09659
H	-0.9433	-3.2784	0.621555
H	-1.22402	-4.52285	-0.58762
C	0.50384	-4.88957	0.66688
H	1.274915	-4.28369	1.163014
C	-0.28683	-5.6183	1.764736
H	-1.07544	-6.24506	1.3286
H	-0.76443	-4.90949	2.45157
H	0.36964	-6.26865	2.354012
C	1.209278	-5.89506	-0.25593
H	1.824727	-6.58769	0.329855
H	0.477518	-6.49193	-0.81612
H	1.868879	-5.4014	-0.97773
N	-0.72144	-1.07711	-2.34226
H	0.0965	-0.55923	-2.03832
C	-1.63925	-0.39789	-3.2536
H	-1.1264	0.474356	-3.65421
H	-1.90283	-1.08005	-4.06909
C	-2.92321	0.100708	-2.57304
O	-3.23392	1.299133	-2.57093
N	-3.6705	-0.8455	-1.95643
H	-3.36843	-1.81437	-2.06182
C	-4.92992	-0.50966	-1.2994
H	-5.49865	0.143626	-1.96993
C	-4.74684	0.355687	-0.03147

O	-5.68081	1.045647	0.376506
C	-5.79146	-1.76592	-1.0152
H	-6.67504	-1.37977	-0.49217
C	-6.26461	-2.41862	-2.32317
H	-5.42785	-2.83314	-2.89793
H	-6.95422	-3.2416	-2.10625
H	-6.78709	-1.697	-2.96129
C	-5.10345	-2.78658	-0.09418
H	-4.80295	-2.33857	0.859238
H	-5.791	-3.60986	0.126785
H	-4.21075	-3.22553	-0.55686
N	-3.5251	0.310163	0.563442
H	-2.83712	-0.31619	0.163197
C	-3.08851	1.214452	1.623737
H	-3.92624	1.900155	1.78761
C	-1.88762	2.071735	1.138439
O	-1.00728	2.446843	1.922975
C	-2.74667	0.483593	2.931762
H	-1.92969	-0.2234	2.732025
H	-2.34321	1.227639	3.627402
C	-3.91644	-0.26595	3.596545
H	-4.30887	-0.99608	2.873808
C	-3.40254	-1.04824	4.815102
H	-4.20929	-1.62876	5.277638
H	-2.60326	-1.74537	4.535926
H	-3.00135	-0.36813	5.57787
C	-5.06861	0.66959	3.995583
H	-4.7147	1.461467	4.669094
H	-5.53114	1.141853	3.122781
H	-5.85165	0.111268	4.522282
N	-1.9021	2.375922	-0.17817
H	-2.63345	1.980827	-0.76176
C	-0.86129	3.099382	-0.92128
H	-1.24913	3.166297	-1.93999
C	0.400588	2.217829	-1.06952
O	0.666822	1.674622	-2.15147
C	-0.54911	4.525139	-0.416
H	-0.41525	4.513716	0.670416
H	0.419846	4.807509	-0.8482
C	-1.57494	5.609829	-0.80966
H	-1.72243	5.546389	-1.89879
C	-2.94484	5.440963	-0.13461
H	-3.43146	4.502266	-0.41467

H	-3.61387	6.262498	-0.41758
H	-2.84533	5.454064	0.958693
C	-0.99547	6.99911	-0.49741
H	-0.0435	7.163582	-1.01619
H	-0.81439	7.114867	0.57924
H	-1.68847	7.790921	-0.80491

Conformer 82

Symbol	X	Y	Z
N	-2.0846	-0.45459	0.84728
H	-1.69771	-0.88851	1.686388
C	-2.41265	0.962719	0.931388
H	-2.26941	1.383013	-0.06576
C	-1.48419	1.60369	1.978908
O	-1.1802	0.967445	2.991134
C	-3.87508	1.216845	1.408622
H	-3.97555	0.764707	2.401518
H	-3.9985	2.299608	1.547043
C	-4.96083	0.69575	0.493494
C	-5.25311	1.326453	-0.72645
H	-4.68089	2.19855	-1.03486
C	-5.73518	-0.41261	0.854474
H	-5.54252	-0.91595	1.798749
C	-6.27046	0.868279	-1.55799
H	-6.491	1.364426	-2.49845
C	-6.76271	-0.88531	0.034368
H	-7.35399	-1.74575	0.339694
C	-7.03186	-0.24472	-1.17846
O	-8.02365	-0.65091	-2.02925
H	-8.47416	-1.42307	-1.64962
N	-1.06352	2.888807	1.805477
C	-1.43074	3.824357	0.730024
H	-2.44313	3.639859	0.364846
C	-0.51545	3.778534	-0.51145
O	-0.81138	4.441291	-1.50638
C	-1.34197	5.200828	1.426706
H	-2.28361	5.395305	1.950993
H	-1.17736	6.005376	0.706851
C	-0.19396	5.013357	2.430275
H	-0.22558	5.736048	3.249477
H	0.773218	5.119999	1.926679
C	-0.38164	3.574719	2.930506

H	0.558373	3.071738	3.171639
H	-1.02345	3.523718	3.817061
N	0.603389	3.020651	-0.40062
H	0.672902	2.403367	0.400235
C	1.449257	2.68054	-1.53508
H	1.039485	3.20482	-2.40089
C	1.335518	1.161922	-1.7339
O	1.199417	0.408066	-0.76327
C	2.928133	3.072415	-1.31855
H	3.313536	2.492228	-0.46942
H	3.494253	2.75034	-2.204
C	3.181831	4.571419	-1.06878
H	2.612514	4.860359	-0.1742
C	4.671706	4.799775	-0.77123
H	5.291576	4.533636	-1.6373
H	5.007955	4.195488	0.079743
H	4.865164	5.852328	-0.53432
C	2.713099	5.452653	-2.23664
H	3.203897	5.156671	-3.17343
H	1.629614	5.393313	-2.38374
H	2.96356	6.503207	-2.04836
N	1.425096	0.701645	-3.00609
H	1.438048	1.376572	-3.7603
C	1.040439	-0.66607	-3.33863
H	0.001093	-0.85175	-3.04833
H	1.119242	-0.78314	-4.42284
C	1.872587	-1.76023	-2.67212
O	1.367165	-2.86973	-2.45946
N	3.145827	-1.46636	-2.33556
H	3.505357	-0.54613	-2.55693
C	4.013606	-2.4425	-1.67933
H	3.981942	-3.36865	-2.26243
C	3.498313	-2.86423	-0.28228
O	3.858459	-3.94321	0.193788
C	5.478896	-1.92512	-1.67433
H	5.67011	-1.61537	-2.7116
C	5.690979	-0.70411	-0.76546
H	5.57379	-0.97138	0.290763
H	6.704547	-0.31146	-0.89886
H	4.993053	0.113302	-0.98185
C	6.475177	-3.04313	-1.33751
H	6.366635	-3.89176	-2.02211
H	7.49994	-2.66588	-1.42501

H	6.330214	-3.41295	-0.31836
N	2.656717	-2.00672	0.35114
H	2.384782	-1.1419	-0.1127
C	1.977983	-2.32853	1.603348
H	2.287652	-3.34666	1.859566
C	0.43653	-2.35732	1.427112
O	-0.30821	-2.1792	2.401133
C	2.353879	-1.36414	2.743608
H	2.066641	-0.34686	2.442453
H	1.724818	-1.61703	3.603681
C	3.833974	-1.37292	3.16592
H	4.442531	-1.12595	2.284447
C	4.075868	-0.28038	4.219143
H	5.133931	-0.23443	4.502616
H	3.783604	0.708317	3.845204
H	3.494679	-0.47818	5.129346
C	4.292745	-2.74322	3.688683
H	5.330435	-2.69389	4.039917
H	4.24451	-3.5133	2.911939
H	3.671166	-3.06825	4.533774
N	-0.00929	-2.59524	0.177148
H	0.673372	-2.70208	-0.56726
C	-1.40683	-2.55367	-0.27854
H	-1.34961	-2.8486	-1.32689
C	-1.94077	-1.09971	-0.33921
O	-2.21854	-0.58939	-1.42921
C	-2.31896	-3.54996	0.464109
H	-1.82982	-4.53252	0.405813
H	-2.36189	-3.28398	1.523909
C	-3.75004	-3.66348	-0.09779
H	-4.23212	-2.68063	-0.00568
C	-3.78375	-4.06648	-1.58064
H	-4.81777	-4.20441	-1.91811
H	-3.25077	-5.0124	-1.74552
H	-3.33011	-3.30404	-2.22284
C	-4.55777	-4.6554	0.753211
H	-5.59885	-4.70827	0.413404
H	-4.56233	-4.36378	1.810361
H	-4.13341	-5.66591	0.687222

Molecular complex (B3LYP/PCM(ACN)/6-31G(d))
Conformer 1

Symbol	X	Y	Z
N	1.450341	1.624819	0.121483
C	2.729843	1.028705	-0.25105
H	2.484022	0.139794	-0.82939
C	3.479794	0.688975	1.049588
O	3.760618	1.592721	1.840742
C	3.583054	1.984108	-1.1222
H	2.963766	2.280054	-1.97628
H	3.787697	2.886007	-0.53548
C	4.876033	1.356143	-1.59902
C	6.070339	1.508179	-0.88119
H	6.07432	2.108083	0.02569
C	4.911011	0.573292	-2.76446
H	4.002887	0.444005	-3.34979
C	7.257506	0.906634	-1.30123
H	8.172149	1.044433	-0.73114
C	6.086561	-0.03485	-3.19782
H	6.104671	-0.6332	-4.10415
C	7.273094	0.127427	-2.46736
O	8.393893	-0.48331	-2.93621
H	9.15962	-0.28969	-2.35269
N	3.795269	-0.61066	1.326098
C	3.756026	-1.75876	0.401914
H	3.908531	-1.44359	-0.63217
C	2.446937	-2.56903	0.427993
O	2.299862	-3.51383	-0.35748
C	4.937655	-2.63182	0.884082
H	5.858964	-2.26268	0.421381
H	4.806291	-3.67844	0.602026
C	4.958901	-2.38652	2.399883
H	5.922512	-2.62781	2.855646
H	4.192165	-2.99241	2.895495
C	4.626023	-0.89473	2.522699
H	4.079546	-0.64149	3.434879
H	5.523132	-0.26678	2.486436
N	1.520211	-2.22098	1.347382
H	1.68714	-1.39989	1.915547
C	0.262234	-2.95662	1.52171
H	0.492109	-4.00662	1.319254
C	-0.74105	-2.46203	0.453637
O	-1.60902	-1.6138	0.718737
C	-0.25781	-2.78272	2.951389

H	0.569506	-3.00833	3.637239
H	-0.52089	-1.72779	3.095299
C	-1.47282	-3.65961	3.318102
H	-2.26069	-3.47401	2.575862
C	-1.14255	-5.16042	3.307871
H	-0.8186	-5.51175	2.321854
H	-0.34376	-5.38986	4.025182
H	-2.02282	-5.74943	3.589911
C	-2.01806	-3.23709	4.69091
H	-1.2649	-3.38717	5.475511
H	-2.30377	-2.17859	4.698233
H	-2.90185	-3.82686	4.960104
N	-0.57555	-3.02485	-0.76201
H	0.263249	-3.59592	-0.85058
C	-1.0816	-2.46732	-2.02214
H	-0.54951	-2.96902	-2.83011
H	-0.83445	-1.39909	-2.05726
C	-2.57513	-2.59206	-2.34465
O	-2.93579	-2.7536	-3.51298
N	-3.43708	-2.38152	-1.31967
H	-3.03552	-2.155	-0.4114
C	-4.87406	-2.20464	-1.53547
H	-4.98509	-1.87296	-2.5752
C	-5.36505	-1.06505	-0.61457
O	-6.2097	-1.24819	0.26429
C	-5.65092	-3.54117	-1.41172
H	-5.16537	-4.18764	-2.15628
C	-5.50422	-4.22749	-0.0461
H	-5.99622	-3.6506	0.740471
H	-5.95483	-5.22654	-0.07864
H	-4.44864	-4.35025	0.222893
C	-7.12086	-3.38805	-1.83
H	-7.20679	-2.9266	-2.82199
H	-7.60461	-4.37046	-1.87837
H	-7.67214	-2.76988	-1.11636
N	-4.79337	0.169386	-0.76687
H	-5.17578	0.856276	-0.11522
C	-4.05613	0.713678	-1.91147
H	-3.54186	-0.11771	-2.40135
C	-2.93041	1.664112	-1.41294
O	-2.74547	2.7711	-1.9239
C	-4.94281	1.393929	-2.97435
H	-4.25702	1.807959	-3.72061

H	-5.52042	0.609649	-3.48167
C	-5.90615	2.502191	-2.47954
H	-5.47713	2.957701	-1.57766
C	-6.0338	3.609824	-3.53724
H	-6.7232	4.395948	-3.20604
H	-5.06141	4.072679	-3.74039
H	-6.41975	3.206647	-4.48311
C	-7.29565	1.946747	-2.12421
H	-7.7781	1.521361	-3.01442
H	-7.24765	1.16061	-1.36437
H	-7.94727	2.7415	-1.74118
C	-1.00794	1.856992	0.130819
H	-1.03507	2.876081	-0.2657
C	0.280616	1.185314	-0.41038
O	0.23927	0.296644	-1.26462
C	-1.05343	1.885323	1.676205
C	-2.30004	2.55885	2.282609
H	-3.18595	2.008441	1.941354
C	-2.24514	2.458663	3.814786
H	-1.386	3.012409	4.216016
H	-3.15161	2.876582	4.268316
H	-2.15452	1.416591	4.144918
C	-2.45452	4.021118	1.836549
H	-1.56204	4.607482	2.091226
H	-2.61655	4.104545	0.756306
H	-3.31405	4.486399	2.333572
H	1.474374	2.453692	0.711995
H	-0.99226	0.849758	2.03667
H	-0.16346	2.403773	2.049482
N	-2.17291	1.173166	-0.40292
H	-2.29536	0.207308	-0.11256
C	12.95069	0.466479	-0.00496
H	13.72927	-0.23811	-0.31111
H	13.29654	1.486036	-0.19777
H	12.76531	0.349297	1.06657
C	11.72587	0.208084	-0.75208
N	10.75305	0.001932	-1.34685
C	1.955876	6.979752	2.055036
H	1.337571	7.245546	2.917299
H	3.00862	7.123865	2.314652
H	1.702405	7.638554	1.219489
C	1.720532	5.589152	1.682764
N	1.533502	4.483239	1.387077

C	-7.33403	3.82309	2.884932
H	-7.61633	3.263847	3.781585
H	-6.7349	4.689238	3.180258
H	-8.2414	4.172953	2.384183
C	-6.56634	2.968716	1.985523
N	-5.95556	2.28919	1.270809

Conformer 5

Symbol	X	Y	Z
N	0.163304	-1.31736	-1.95129
C	1.444093	-1.00168	-1.32136
H	1.247821	-0.40482	-0.42661
C	2.341841	-0.24647	-2.32141
O	2.457291	-0.6781	-3.47202
C	2.093126	-2.35204	-0.92044
H	1.342374	-2.90105	-0.34024
H	2.275874	-2.91203	-1.84523
C	3.368043	-2.24068	-0.11528
C	4.625724	-2.23217	-0.73254
H	4.690746	-2.3064	-1.81585
C	3.324236	-2.16257	1.286119
H	2.35998	-2.19741	1.788675
C	5.803084	-2.14111	0.011777
H	6.768273	-2.14604	-0.48728
C	4.488779	-2.06723	2.043256
H	4.447571	-2.01301	3.127328
C	5.741028	-2.05498	1.410664
O	6.846608	-1.97077	2.197393
H	7.660503	-1.97432	1.647934
N	3.008539	0.869431	-1.91645
C	3.18756	1.40353	-0.55165
H	2.915714	0.662081	0.201633
C	2.371328	2.687979	-0.25763
O	2.803552	3.520946	0.544404
C	4.6917	1.725573	-0.52256
H	5.252083	0.798543	-0.36668
H	4.932927	2.428926	0.274718
C	4.939124	2.285924	-1.93241
H	5.986216	2.221669	-2.24058
H	4.645384	3.34068	-1.97293
C	4.027572	1.434171	-2.8343
H	3.550538	2.01308	-3.63145

H	4.56197	0.603893	-3.305
N	1.198362	2.855519	-0.90847
H	0.815331	2.112467	-1.49024
C	0.448802	4.100361	-0.74918
H	1.163629	4.917449	-0.87382
C	-0.09564	4.364092	0.674409
O	0.060716	5.487529	1.164126
C	-0.63153	4.209738	-1.84635
H	-0.11529	4.12315	-2.81281
H	-1.30714	3.349056	-1.7859
C	-1.46681	5.505807	-1.84149
H	-1.97772	5.582127	-0.87121
C	-0.60811	6.76702	-2.02032
H	-0.01509	6.710708	-2.9429
H	-1.24306	7.658512	-2.08758
H	0.075541	6.908553	-1.17819
C	-2.54644	5.421914	-2.93168
H	-2.09251	5.353268	-3.929
H	-3.18706	4.542317	-2.79525
H	-3.18703	6.311375	-2.91787
N	-0.75768	3.404588	1.374613
H	-1.07222	3.715353	2.293483
C	-1.26615	2.113737	0.957557
H	-1.0599	1.935894	-0.09816
H	-2.35605	2.100249	1.078838
C	-0.62476	0.947403	1.725221
O	0.596747	0.822238	1.822169
N	-1.51697	0.061304	2.247575
H	-2.50369	0.237715	2.098774
C	-1.10127	-1.18798	2.880293
H	-0.01818	-1.10975	2.981158
C	-1.30795	-2.38849	1.930742
O	-0.38287	-3.16811	1.693517
C	-1.69343	-1.36417	4.306035
H	-1.36501	-0.46757	4.848826
C	-3.2278	-1.40955	4.370113
H	-3.5518	-1.41283	5.416538
H	-3.69399	-0.54017	3.892141
H	-3.62657	-2.31553	3.900155
C	-1.07886	-2.59085	4.997359
H	-1.37282	-3.52266	4.499815
H	0.015836	-2.54299	5.000719
H	-1.41878	-2.64825	6.03699

N	-2.54533	-2.52928	1.376265
H	-3.25155	-1.82267	1.550284
C	-2.81461	-3.49544	0.312783
H	-2.19579	-4.37058	0.511925
C	-2.32645	-2.96373	-1.05104
O	-1.63472	-3.66749	-1.79799
C	-4.3069	-3.87859	0.309973
H	-4.53655	-4.297	1.299059
H	-4.90824	-2.96485	0.208186
C	-4.73496	-4.88089	-0.78067
H	-4.52782	-4.42866	-1.76144
C	-3.96362	-6.20708	-0.70054
H	-4.34227	-6.9166	-1.44542
H	-2.89505	-6.0669	-0.89211
H	-4.0777	-6.66951	0.288735
C	-6.24966	-5.12035	-0.69062
H	-6.51726	-5.58237	0.268529
H	-6.80948	-4.18158	-0.7781
H	-6.58723	-5.79014	-1.48962
C	-2.16923	-0.99869	-2.55436
H	-2.0092	-1.76753	-3.31497
C	-0.78792	-0.39733	-2.19512
O	-0.59482	0.822604	-2.09182
C	-3.14902	0.063143	-3.05707
C	-4.52375	-0.46747	-3.50949
H	-4.98107	-0.99684	-2.66168
C	-5.43702	0.713318	-3.87289
H	-5.02923	1.277168	-4.72189
H	-6.43725	0.364027	-4.15386
H	-5.54582	1.408479	-3.03154
C	-4.42022	-1.45307	-4.68352
H	-3.9226	-0.98644	-5.54379
H	-3.85909	-2.35666	-4.42038
H	-5.41748	-1.7719	-5.0082
H	-0.09302	-2.29637	-2.05682
H	-3.2872	0.81426	-2.26879
H	-2.66804	0.588156	-3.89182
N	-2.68886	-1.69567	-1.37025
H	-3.16177	-1.12986	-0.67237
C	11.67161	-1.90247	-0.43921
H	12.27146	-2.76356	-0.13075
H	11.53436	-1.93372	-1.52387
H	12.20279	-0.984	-0.17329

C	10.37523	-1.93635	0.226654
N	9.345868	-1.96312	0.757965
C	-2.78471	4.340784	6.627932
H	-3.2623	5.324135	6.665243
H	-3.50661	3.582869	6.945513
H	-1.93487	4.332519	7.316522
C	-2.32926	4.058879	5.271083
N	-1.96818	3.832573	4.192541
C	-6.77616	1.213755	0.779838
H	-6.87038	1.625849	-0.22898
H	-7.60369	0.522637	0.963653
H	-6.82333	2.030309	1.506047
C	-5.50708	0.51081	0.909737
N	-4.49514	-0.04868	1.01239

Conformer 7

Symbol	X	Y	Z
N	-0.6274	-0.66116	1.641755
C	-1.90983	-0.60721	0.942252
H	-1.71521	-0.2453	-0.0702
C	-2.87827	0.327983	1.701925
O	-2.98346	0.208586	2.923958
C	-2.48341	-2.04497	0.890569
H	-1.71024	-2.68482	0.44929
H	-2.62707	-2.37895	1.923899
C	-3.77435	-2.1899	0.114495
C	-5.01599	-2.19788	0.763673
H	-5.05387	-2.0958	1.845836
C	-3.76679	-2.33639	-1.28205
H	-2.81775	-2.35167	-1.81411
C	-6.2102	-2.34217	0.055984
H	-7.16021	-2.35521	0.583043
C	-4.9486	-2.47672	-2.00502
H	-4.93224	-2.59628	-3.08441
C	-6.1841	-2.48233	-1.33964
O	-7.3063	-2.63512	-2.09057
H	-8.10532	-2.63289	-1.51932
N	-3.58955	1.25948	0.998881
C	-3.77202	1.377197	-0.45774
H	-3.45222	0.463425	-0.96052
C	-2.98236	2.538616	-1.1064
O	-3.29503	2.940391	-2.22986

C	-5.30638	1.585517	-0.64522
H	-5.74854	0.714524	-1.13434
H	-5.47981	2.448502	-1.29063
C	-5.88102	1.783396	0.778408
H	-6.38837	0.872689	1.111799
H	-6.59915	2.606744	0.829579
C	-4.65121	2.0369	1.6609
H	-4.37054	3.097895	1.662851
H	-4.75342	1.70068	2.691462
N	-1.96141	3.05856	-0.3868
H	-1.66254	2.580595	0.459586
C	-1.1361	4.146973	-0.90168
H	-1.78329	4.771323	-1.51942
C	-0.01438	3.677513	-1.85192
O	0.276805	4.331998	-2.85779
C	-0.57401	4.958945	0.286102
H	-1.43345	5.303752	0.87723
H	-0.00398	4.275876	0.929536
C	0.309202	6.169937	-0.0729
H	1.166271	5.809383	-0.65828
C	-0.43612	7.210268	-0.92299
H	-1.34148	7.560592	-0.40971
H	0.199778	8.083892	-1.10921
H	-0.72865	6.799765	-1.89432
C	0.855646	6.805449	1.214671
H	1.418265	6.078791	1.813025
H	1.524426	7.643099	0.984852
H	0.039126	7.191968	1.838622
N	0.644318	2.554715	-1.4819
H	0.356348	2.039846	-0.65231
C	1.704511	1.988097	-2.28359
H	2.694605	2.344349	-1.96371
H	1.570301	2.308429	-3.32127
C	1.689802	0.464539	-2.17787
O	0.946003	-0.13104	-1.38895
N	2.577571	-0.19209	-2.95882
H	3.122827	0.337637	-3.62747
C	2.561448	-1.65125	-3.07413
H	1.532401	-1.96377	-3.2825
C	2.89955	-2.37571	-1.75422
O	2.460695	-3.51326	-1.56866
C	3.445436	-2.09009	-4.27494
H	3.111281	-1.46115	-5.1129

C	4.94524	-1.83546	-4.05744
H	5.355073	-2.51162	-3.29889
H	5.49232	-2.01259	-4.98951
H	5.15894	-0.80817	-3.7402
C	3.183078	-3.55056	-4.66706
H	3.76272	-3.80495	-5.56115
H	3.47048	-4.23671	-3.865
H	2.123781	-3.71917	-4.89064
N	3.673691	-1.71781	-0.85102
H	4.057677	-0.80277	-1.08228
C	3.983797	-2.28221	0.457216
H	3.605902	-3.30781	0.437909
C	3.241407	-1.59245	1.627018
O	3.4753	-1.94128	2.789775
C	5.498349	-2.29323	0.751281
H	5.861749	-1.25642	0.748541
H	5.622541	-2.66662	1.773674
C	6.36063	-3.1315	-0.21014
H	6.244424	-2.71662	-1.22092
C	7.84113	-2.99892	0.17915
H	8.48284	-3.54209	-0.52441
H	8.161192	-1.95001	0.186101
H	8.021217	-3.41002	1.181159
C	5.938219	-4.60801	-0.25235
H	5.975862	-5.05561	0.749943
H	4.922256	-4.73368	-0.64169
H	6.612236	-5.18323	-0.89816
C	1.595952	0.151038	2.288857
H	1.49919	-0.4824	3.175541
C	0.189976	0.400201	1.700437
O	-0.14293	1.519858	1.273961
C	2.266295	1.48859	2.651946
C	3.606359	1.399244	3.406894
H	4.277518	0.735888	2.845461
C	4.259908	2.789481	3.45833
H	3.620441	3.505529	3.991499
H	5.223625	2.752156	3.980022
H	4.436925	3.186169	2.451071
C	3.444654	0.823462	4.821577
H	4.407862	0.810727	5.345887
H	2.750802	1.43304	5.415777
H	3.070031	-0.2039	4.796124
H	-0.34938	-1.54178	2.074934

H	2.406435	2.053343	1.722785
H	1.555268	2.06765	3.256507
N	2.360256	-0.61928	1.301147
H	2.152373	-0.46419	0.318953
C	-12.0801	-2.74314	0.626848
H	-12.6916	-1.89281	0.311603
H	-12.6007	-3.67083	0.372399
H	-11.9394	-2.69892	1.710622
C	-10.7867	-2.70024	-0.04415
N	-9.75949	-2.66649	-0.57921
C	2.166617	-4.69563	3.962764
H	2.103348	-4.80589	5.049248
H	2.158503	-5.68809	3.502892
H	3.092269	-4.17453	3.701107
C	1.0461	-3.90394	3.471124
N	0.16649	-3.26218	3.070283
C	6.719601	3.106442	-0.80893
H	7.757481	2.761109	-0.81103
H	6.567502	3.781947	-1.6556
H	6.52755	3.651111	0.120062
C	5.815966	1.966318	-0.91285
N	5.096078	1.060071	-0.99524

Conformer 9

Symbol	X	Y	Z
N	-1.86847	-1.77366	-0.17943
C	-2.76021	-1.20645	0.827773
H	-2.40367	-0.20167	1.061284
C	-2.72075	-2.09234	2.09537
O	-2.58963	-3.31119	1.984267
C	-4.20207	-1.1057	0.274543
H	-4.52119	-2.10411	-0.04468
H	-4.8604	-0.8249	1.105737
C	-4.3475	-0.11159	-0.86141
C	-4.22411	1.267267	-0.63443
H	-4.02995	1.637905	0.370213
C	-4.61379	-0.53523	-2.17044
H	-4.71449	-1.59716	-2.37789
C	-4.35288	2.191822	-1.67017
H	-4.25848	3.255247	-1.46881
C	-4.74913	0.37535	-3.21691
H	-4.95671	0.035928	-4.2276

C	-4.61787	1.749076	-2.97593
O	-4.75975	2.596355	-4.02933
H	-4.65259	3.527976	-3.73773
N	-2.84308	-1.48431	3.31466
C	-3.19956	-0.07288	3.575756
H	-4.00184	0.251505	2.906658
C	-2.08136	0.974008	3.458622
O	-2.37625	2.169251	3.519194
C	-3.71829	-0.08168	5.045185
H	-4.54083	0.624468	5.174211
H	-2.91056	0.218446	5.721613
C	-4.10448	-1.54226	5.306921
H	-5.10166	-1.75609	4.905841
H	-4.10211	-1.79288	6.37129
C	-3.05017	-2.32011	4.518713
H	-2.11111	-2.4073	5.079233
H	-3.36071	-3.31825	4.21069
N	-0.80597	0.528506	3.373511
H	-0.63932	-0.4531	3.185666
C	0.326531	1.450656	3.366895
H	0.153978	2.187311	4.155581
C	0.427838	2.289026	2.07599
O	0.938363	3.417212	2.095134
C	1.619392	0.656895	3.657148
H	1.425279	0.042677	4.547202
H	1.791084	-0.04021	2.826068
C	2.892418	1.490795	3.899947
H	3.054327	2.135455	3.026595
C	2.776428	2.396496	5.13521
H	2.559749	1.806751	6.035627
H	3.716408	2.933692	5.307103
H	1.986921	3.146551	5.021397
C	4.101814	0.551953	4.027257
H	4.220158	-0.07305	3.133904
H	5.027177	1.123083	4.164027
H	3.991585	-0.11648	4.891107
N	-0.05141	1.721163	0.947584
H	-0.2707	0.726265	0.959065
C	-0.19293	2.454437	-0.30002
H	-0.37072	3.506743	-0.0534
H	-1.05906	2.072428	-0.84299
C	1.010531	2.371078	-1.24537
O	0.886013	2.067872	-2.43014

N	2.218761	2.659602	-0.68062
H	2.211959	3.083999	0.24404
C	3.409755	2.76552	-1.52164
H	3.140139	3.314855	-2.43047
C	3.879485	1.39088	-2.04526
O	4.557906	1.318912	-3.07138
C	4.524359	3.563777	-0.79054
H	4.022064	4.46688	-0.41546
C	5.125837	2.82064	0.4121
H	4.361828	2.478205	1.118992
H	5.701656	1.945533	0.090468
H	5.805767	3.482867	0.958733
C	5.622109	4.018774	-1.7626
H	6.350275	4.645631	-1.23619
H	6.151734	3.16363	-2.19267
H	5.204156	4.605766	-2.58819
N	3.521551	0.309708	-1.30189
H	2.910555	0.483948	-0.513
C	3.734928	-1.06946	-1.74485
H	4.20367	-0.99396	-2.72559
C	2.37317	-1.7521	-2.01097
O	1.982431	-1.96178	-3.15981
C	4.634467	-1.88007	-0.79119
H	4.176385	-1.91461	0.206911
H	4.656027	-2.9172	-1.15501
C	6.08083	-1.36727	-0.64577
H	6.03364	-0.33339	-0.27628
C	6.823184	-2.20555	0.406445
H	7.837331	-1.82214	0.567972
H	6.30107	-2.19351	1.370909
H	6.909534	-3.25193	0.085555
C	6.846027	-1.36071	-1.97818
H	6.401292	-0.66819	-2.69986
H	7.886007	-1.05118	-1.82049
H	6.862403	-2.36303	-2.42658
C	0.311861	-2.64024	-0.93026
H	-0.06223	-2.54165	-1.95134
C	-0.54252	-1.80414	0.032262
O	-0.00604	-1.2099	0.987235
C	0.265949	-4.12282	-0.47758
C	1.099546	-5.10438	-1.3233
H	2.138157	-4.74536	-1.32802
C	1.08675	-6.49062	-0.65987

H	1.464208	-6.44762	0.368806
H	0.068841	-6.90053	-0.62612
H	1.711504	-7.19686	-1.21906
C	0.618723	-5.19089	-2.77966
H	1.2017	-5.93829	-3.33121
H	-0.43638	-5.48947	-2.82717
H	0.731025	-4.23448	-3.29969
H	-2.27087	-2.382	-0.89282
H	0.609415	-4.16422	0.564989
H	-0.78329	-4.44427	-0.47329
N	1.661709	-2.09527	-0.90542
H	1.992378	-1.82767	0.0136
C	-4.24725	7.939792	-2.83481
H	-4.24083	8.103385	-1.75334
H	-3.31267	8.318494	-3.25847
H	-5.08582	8.488147	-3.27347
C	-4.38094	6.516567	-3.12048
N	-4.48751	5.385521	-3.34844
C	-4.20507	-5.63971	-3.6552
H	-3.55986	-6.52126	-3.70964
H	-5.16735	-5.92858	-3.22275
H	-4.36918	-5.2557	-4.66611
C	-3.57657	-4.61482	-2.82997
N	-3.07532	-3.79956	-2.1747

Conformer 12

Symbol	X	Y	Z
N	0.694952	-1.26411	-1.70175
C	2.000153	-1.18982	-1.04631
H	1.87369	-0.70959	-0.071
C	2.990324	-0.39624	-1.92499
O	3.173898	-0.72997	-3.09683
C	2.52587	-2.63027	-0.83674
H	1.743802	-3.19723	-0.31687
H	2.654635	-3.0795	-1.82733
C	3.815761	-2.70078	-0.04762
C	5.063069	-2.67771	-0.68705
H	5.10564	-2.6246	-1.77225
C	3.801616	-2.77644	1.354216
H	2.849132	-2.80883	1.879175
C	6.25528	-2.72226	0.036641
H	7.210418	-2.70981	-0.48122

C	4.981773	-2.82097	2.092213
H	4.960803	-2.88481	3.176274
C	6.221944	-2.79314	1.437439
O	7.343192	-2.84314	2.203787
H	8.14634	-2.82504	1.639385
N	3.659615	0.654642	-1.37149
C	3.806861	1.002443	0.055945
H	3.756783	0.104751	0.678308
C	2.762359	1.985158	0.636334
O	2.973354	2.483551	1.748822
C	5.220983	1.616687	0.11006
H	5.958402	0.810111	0.182362
H	5.333928	2.271691	0.975073
C	5.339446	2.331696	-1.24298
H	6.373884	2.535171	-1.53223
H	4.804207	3.288191	-1.21521
C	4.652854	1.361174	-2.21075
H	4.156088	1.856391	-3.05002
H	5.355556	0.629895	-2.62665
N	1.658207	2.230149	-0.09899
H	1.505187	1.73554	-0.98005
C	0.559788	3.048345	0.398487
H	0.95498	3.629572	1.232792
C	-0.58365	2.156073	0.917095
O	-0.94931	1.133168	0.326356
C	0.017362	3.987145	-0.7001
H	-0.35741	3.365234	-1.52192
H	-0.84776	4.524092	-0.28734
C	1.034982	5.003128	-1.25412
H	1.886941	4.437725	-1.6574
C	0.402788	5.790348	-2.41232
H	-0.45304	6.382798	-2.06285
H	1.126892	6.482383	-2.85822
H	0.044787	5.120844	-3.20357
C	1.568286	5.958513	-0.17565
H	2.121114	5.429386	0.608179
H	2.249167	6.696035	-0.61676
H	0.746791	6.50788	0.303047
N	-1.18381	2.580632	2.049992
H	-0.83479	3.394514	2.548018
C	-2.28004	1.823213	2.607236
H	-2.48753	2.200979	3.61333
H	-1.97708	0.776939	2.698806

C	-3.55977	1.939978	1.756117
O	-3.73771	2.87281	0.978025
N	-4.50517	0.97258	1.943125
H	-5.30161	1.054152	1.319735
C	-4.39018	-0.22503	2.768944
H	-3.73765	0.007046	3.612154
C	-3.67144	-1.40255	2.066987
O	-2.9598	-2.15318	2.738948
C	-5.76243	-0.60256	3.406753
H	-6.07561	0.315843	3.92148
C	-6.86017	-0.96878	2.397635
H	-6.60957	-1.87608	1.836909
H	-7.79799	-1.15881	2.930943
H	-7.05687	-0.17164	1.673653
C	-5.60473	-1.70215	4.467424
H	-4.85465	-1.4308	5.21851
H	-6.55891	-1.85801	4.982262
H	-5.30186	-2.65514	4.021856
N	-3.84286	-1.54813	0.722032
H	-4.52575	-0.9737	0.230613
C	-3.24662	-2.66524	-0.00512
H	-2.6111	-3.18532	0.714974
C	-2.31544	-2.24941	-1.15776
O	-1.73025	-3.12997	-1.80695
C	-4.30652	-3.64667	-0.56046
H	-5.00177	-3.07873	-1.19456
H	-3.78266	-4.34928	-1.21792
C	-5.10604	-4.43894	0.490581
H	-5.60273	-3.72347	1.160602
C	-6.2033	-5.25638	-0.20914
H	-6.81682	-5.79588	0.521697
H	-6.86802	-4.6133	-0.79829
H	-5.76546	-5.99819	-0.88968
C	-4.2135	-5.34859	1.348898
H	-3.5005	-4.77383	1.949047
H	-4.82252	-5.94188	2.04124
H	-3.64759	-6.04829	0.719771
C	-1.42416	-0.46654	-2.60647
H	-1.42033	-1.30183	-3.313
C	0.0488	-0.1971	-2.22135
O	0.585041	0.902675	-2.39751
C	-2.08041	0.766932	-3.23472
C	-3.46899	0.525864	-3.85761

H	-4.11802	0.0899	-3.08611
C	-4.08445	1.867775	-4.28296
H	-4.16778	2.555231	-3.43281
H	-3.46917	2.357066	-5.04965
H	-5.0872	1.725578	-4.70316
C	-3.42083	-0.44576	-5.04727
H	-3.06387	-1.441	-4.75924
H	-4.4185	-0.57147	-5.48434
H	-2.75725	-0.06624	-5.83555
H	0.174829	-2.13628	-1.63399
H	-2.15158	1.546562	-2.46565
H	-1.39867	1.155815	-4.00029
N	-2.19174	-0.93535	-1.44779
H	-2.43235	-0.24825	-0.74001
C	12.13025	-2.78566	-0.50658
H	12.65651	-1.85065	-0.29394
H	12.74039	-3.62496	-0.16068
H	11.98205	-2.87392	-1.58662
C	10.84121	-2.79555	0.174013
N	9.817893	-2.80339	0.717531
C	-7.91065	0.979154	-2.46391
H	-8.81802	1.223525	-1.90417
H	-7.58996	1.860225	-3.02705
H	-8.13199	0.16917	-3.16477
C	-6.85713	0.567143	-1.54419
N	-6.01978	0.245423	-0.8081
C	2.821315	4.195319	4.556517
H	2.859183	3.730083	5.545862
H	3.283875	3.532423	3.819098
H	3.365905	5.143552	4.588656
C	1.436351	4.425357	4.163684
N	0.33537	4.594846	3.835269

Conformer 21

Symbol	X	Y	Z
N	0.618026	1.793576	0.321189
C	1.862974	1.09687	0.015884
H	1.641688	0.03298	0.053595
C	2.893436	1.519202	1.079609
O	3.03114	2.722869	1.326595
C	2.362782	1.478318	-1.40623
H	1.536113	1.275649	-2.09592

H	2.537289	2.560071	-1.4142
C	3.606587	0.737224	-1.84722
C	4.887891	1.243225	-1.58715
H	4.992035	2.199469	-1.07947
C	3.515371	-0.49384	-2.51667
H	2.534968	-0.90689	-2.74601
C	6.038309	0.551877	-1.96883
H	7.020712	0.967479	-1.76214
C	4.652864	-1.19757	-2.90509
H	4.571572	-2.14597	-3.42821
C	5.927635	-0.67982	-2.63173
O	7.00464	-1.40377	-3.03513
H	7.838315	-0.94944	-2.78352
N	3.63372	0.578211	1.715296
C	3.68947	-0.87037	1.4343
H	3.643823	-1.04253	0.356644
C	2.55048	-1.62327	2.154773
O	2.450603	-1.64089	3.380964
C	5.071516	-1.27468	1.99387
H	5.82106	-1.12014	1.210482
H	5.102875	-2.32569	2.292447
C	5.299179	-0.30282	3.162466
H	6.357603	-0.18428	3.409855
H	4.7712	-0.65985	4.049572
C	4.677773	1.008329	2.668853
H	4.23378	1.608165	3.467645
H	5.403623	1.639541	2.142351
N	1.675768	-2.24126	1.317483
H	1.928782	-2.2885	0.339287
C	0.56053	-3.10058	1.756614
H	0.969031	-3.91828	2.356482
C	-0.00188	-3.75512	0.47953
O	-0.01821	-4.97467	0.328159
C	-0.49441	-2.31384	2.582478
H	0.03803	-1.52324	3.116259
H	-1.19312	-1.81707	1.899258
C	-1.28339	-3.14113	3.624074
H	-1.98425	-2.42685	4.080135
C	-2.12142	-4.27141	3.007608
H	-1.49053	-5.03051	2.53213
H	-2.72038	-4.77057	3.778428
H	-2.81456	-3.88892	2.248211
C	-0.38774	-3.67299	4.755319

H	0.217964	-2.8723	5.193754
H	-0.99927	-4.11382	5.551249
H	0.297207	-4.45436	4.403888
N	-0.43299	-2.87297	-0.47107
H	-0.39097	-1.86883	-0.28746
C	-0.72575	-3.28696	-1.83147
H	-0.55218	-4.36575	-1.89104
H	-0.04731	-2.79695	-2.53709
C	-2.14549	-3.00773	-2.32832
O	-2.37582	-2.9231	-3.53311
N	-3.11289	-2.89031	-1.37849
H	-2.85608	-3.0653	-0.41512
C	-4.52126	-2.78817	-1.75106
H	-4.65222	-3.35544	-2.67685
C	-4.93811	-1.34759	-2.11257
O	-5.89747	-1.1432	-2.85809
C	-5.43036	-3.41962	-0.65735
H	-4.96908	-4.39223	-0.43667
C	-5.48009	-2.60747	0.64684
H	-5.97692	-1.64236	0.497784
H	-6.04261	-3.15956	1.407216
H	-4.48457	-2.40788	1.061043
C	-6.84564	-3.68778	-1.1893
H	-6.82121	-4.32254	-2.0822
H	-7.44045	-4.20049	-0.42534
H	-7.35502	-2.75609	-1.45298
N	-4.22206	-0.35346	-1.5247
H	-3.34566	-0.6157	-1.08619
C	-4.44644	1.071115	-1.82594
H	-4.4526	1.205344	-2.91277
C	-3.21626	1.829818	-1.30295
O	-2.47852	2.482132	-2.03992
C	-5.79781	1.563317	-1.24902
H	-6.52376	0.77467	-1.46469
H	-5.72817	1.643689	-0.15564
C	-6.33654	2.883893	-1.83783
H	-6.31747	2.786192	-2.93401
C	-7.80145	3.074281	-1.41242
H	-8.42389	2.227715	-1.72532
H	-7.8834	3.165474	-0.32133
H	-8.22243	3.984945	-1.85422
C	-5.50704	4.120804	-1.45739
H	-5.45776	4.237584	-0.36664

H	-4.48374	4.066866	-1.83945
H	-5.96562	5.02867	-1.86704
C	-1.76545	2.15803	0.652445
H	-1.54654	3.162645	0.283291
C	-0.60156	1.227265	0.237193
O	-0.80981	0.050947	-0.09645
C	-1.89741	2.174884	2.189393
C	-3.0216	3.065679	2.75788
H	-3.98023	2.70855	2.3558
C	-3.07232	2.911608	4.28583
H	-3.2138	1.864376	4.578472
H	-2.14117	3.265605	4.747062
H	-3.89768	3.494847	4.709968
C	-2.86466	4.540832	2.362363
H	-1.89772	4.93708	2.697367
H	-2.92853	4.685642	1.278536
H	-3.65362	5.147043	2.822422
H	0.690672	2.79348	0.511357
H	-2.04539	1.141801	2.534929
H	-0.93581	2.502709	2.603036
N	-3.00311	1.714838	0.03654
H	-3.57128	1.059161	0.557888
C	11.9213	0.686103	-1.75154
H	11.83531	1.704199	-1.36118
H	12.38471	0.050604	-0.99147
H	12.55639	0.698144	-2.6419
C	10.60045	0.171212	-2.09072
N	9.551238	-0.23954	-2.36087
C	0.764731	7.502339	0.242369
H	0.854251	7.784021	-0.81074
H	-0.09781	8.016818	0.675624
H	1.668802	7.816068	0.772104
C	0.594295	6.058456	0.359348
N	0.458524	4.910454	0.452858

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Symbol	X	Y	Z
N	0.588725	2.05663	0.192132
H	0.118035	2.460432	0.996537
C	1.923888	1.493384	0.364271
H	2.103428	0.868417	-0.50812
C	1.96359	0.699628	1.673408

O	1.57518	1.245721	2.712693
C	2.979881	2.637068	0.406229
H	2.847667	3.218825	-0.51278
H	2.722339	3.289367	1.247807
C	4.412293	2.163615	0.526027
C	5.031038	2.025566	1.778571
H	4.475349	2.278584	2.678548
C	5.164488	1.836388	-0.61149
H	4.718901	1.945382	-1.59824
C	6.343957	1.574883	1.895931
H	6.816337	1.478949	2.869296
C	6.479951	1.38238	-0.51266
H	7.044667	1.140699	-1.40884
C	7.080946	1.247468	0.748219
O	8.359365	0.818537	0.917156
H	8.772237	0.617245	0.048951
N	2.441297	-0.57327	1.667968
C	3.136623	-1.25723	0.562537
H	3.623803	-0.53816	-0.09812
C	2.266363	-2.15123	-0.34662
O	2.826236	-2.78822	-1.24066
C	4.200956	-2.10181	1.298364
H	5.070528	-1.46801	1.500416
H	4.524659	-2.95157	0.695015
C	3.503813	-2.49029	2.609571
H	4.208948	-2.75407	3.402138
H	2.844923	-3.35163	2.452982
C	2.685293	-1.24316	2.969871
H	1.738238	-1.47547	3.461111
H	3.241511	-0.55553	3.615719
N	0.921004	-2.18798	-0.13461
H	0.533009	-1.73663	0.692624
C	0.084802	-3.17552	-0.81571
H	0.773748	-3.76848	-1.42675
C	-0.90165	-2.57846	-1.83578
O	-1.79468	-3.29303	-2.32131
C	-0.65786	-4.09812	0.1715
H	-1.31856	-3.48231	0.794224
H	-1.30208	-4.7509	-0.42693
C	0.238155	-4.95702	1.08322
H	0.870642	-4.28091	1.675902
C	-0.63985	-5.74801	2.065084
H	-1.29818	-6.44325	1.527859

H	-1.27307	-5.08101	2.662038
H	-0.02468	-6.3369	2.755361
C	1.159384	-5.90108	0.29523
H	1.735864	-6.5354	0.978881
H	0.575189	-6.56189	-0.35905
H	1.875867	-5.3552	-0.32782
N	-0.72863	-1.29721	-2.21804
H	0.000519	-0.72892	-1.80134
C	-1.44853	-0.72251	-3.35149
H	-0.8853	0.142352	-3.69592
H	-1.50726	-1.46866	-4.15196
C	-2.86573	-0.23533	-3.01664
O	-3.20564	0.943163	-3.18854
N	-3.70712	-1.17017	-2.51677
H	-3.35293	-2.12612	-2.46092
C	-5.10276	-0.85371	-2.22929
H	-5.52606	-0.34248	-3.10095
C	-5.26462	0.182791	-1.09639
O	-6.2672	0.895744	-1.05818
C	-5.945	-2.12883	-1.96969
H	-6.94563	-1.75271	-1.72224
C	-6.06226	-2.98007	-3.24358
H	-5.09235	-3.38932	-3.55025
H	-6.73651	-3.82609	-3.07156
H	-6.46016	-2.39345	-4.07923
C	-5.44355	-2.96521	-0.78104
H	-5.39826	-2.37756	0.141989
H	-6.12216	-3.80711	-0.60788
H	-4.44632	-3.38415	-0.96396
N	-4.25751	0.248055	-0.18593
H	-3.48694	-0.40032	-0.29477
C	-4.13242	1.297634	0.822653
H	-4.91924	2.022536	0.587478
C	-2.77917	2.038852	0.635477
O	-2.0892	2.407264	1.59432
C	-4.31781	0.781826	2.255843
H	-3.56935	0.001765	2.440702
H	-4.0864	1.606599	2.939792
C	-5.71724	0.224323	2.581027
H	-5.94721	-0.56615	1.852056
C	-5.70364	-0.41813	3.976909
H	-6.67896	-0.85752	4.216718
H	-4.95011	-1.21195	4.045966

H	-5.4755	0.327883	4.749602
C	-6.81912	1.290929	2.485337
H	-6.60347	2.138597	3.149457
H	-6.92955	1.670576	1.464788
H	-7.78669	0.871703	2.786307
N	-2.45764	2.273959	-0.6566
H	-3.03361	1.857673	-1.38341
C	-1.2739	2.986981	-1.1521
H	-1.42471	3.044672	-2.23248
C	-0.00107	2.11728	-1.02341
O	0.456974	1.534818	-2.01697
C	-1.08828	4.419691	-0.60486
H	-1.21428	4.422181	0.482644
H	-0.04525	4.700964	-0.79996
C	-1.9925	5.497365	-1.2416
H	-1.87155	5.428046	-2.33355
C	-3.48482	5.325937	-0.91754
H	-3.88822	4.386354	-1.306
H	-4.06702	6.146025	-1.35467
H	-3.65203	5.339924	0.167505
C	-1.51082	6.890644	-0.80602
H	-0.46011	7.054165	-1.07354
H	-1.60333	7.014244	0.28096
H	-2.10693	7.677845	-1.28212
C	11.08586	-0.46361	-3.67959
H	11.75365	0.358041	-3.95384
H	11.68248	-1.36111	-3.49273
H	10.39988	-0.65784	-4.50905
C	10.33105	-0.11166	-2.48313
N	9.732502	0.168034	-1.53127
C	-1.10696	0.540304	4.24333
H	-1.74538	0.138241	5.035057
H	-0.11998	0.780612	4.645156
H	-1.55705	1.447136	3.82938
C	-0.95856	-0.43214	3.168269
N	-0.84314	-1.19808	2.303159

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Symbol	X	Y	Z
N	1.77613	-0.258	-1.05676
H	1.568246	-0.98838	-1.73826
C	1.70607	1.118849	-1.52935

H	1.406847	1.734093	-0.67862
C	0.688966	1.172506	-2.68407
O	0.625776	0.232817	-3.48132
C	3.062219	1.633078	-2.10305
H	3.322245	0.985466	-2.94793
H	2.887707	2.633741	-2.52175
C	4.212077	1.6842	-1.12221
C	4.284562	2.671993	-0.12689
H	3.492358	3.413007	-0.0432
C	5.263138	0.763235	-1.19898
H	5.242908	-0.00661	-1.96696
C	5.35557	2.734449	0.75921
H	5.403323	3.50455	1.52382
C	6.348345	0.811731	-0.32081
H	7.154202	0.088015	-0.40607
C	6.399721	1.800963	0.670215
O	7.424706	1.910852	1.558101
H	8.092212	1.208813	1.398248
N	-0.08089	2.284841	-2.85066
C	-0.04483	3.53714	-2.07832
H	0.954867	3.737102	-1.68698
C	-0.99529	3.579364	-0.8625
O	-0.97794	4.559535	-0.11631
C	-0.44778	4.597218	-3.126
H	0.438314	4.884011	-3.70233
H	-0.85555	5.493335	-2.65366
C	-1.45048	3.845199	-4.01483
H	-1.5651	4.298198	-5.00278
H	-2.43749	3.823812	-3.5397
C	-0.86752	2.427674	-4.10055
H	-1.63015	1.646921	-4.16422
H	-0.19493	2.305638	-4.95666
N	-1.82757	2.520293	-0.71863
H	-1.65718	1.707674	-1.2997
C	-2.61273	2.275055	0.482937
H	-2.42758	3.109071	1.16238
C	-2.08398	0.968893	1.095904
O	-1.67583	0.055002	0.364346
C	-4.12452	2.145563	0.190437
H	-4.27361	1.268344	-0.45372
H	-4.63263	1.929472	1.140583
C	-4.77751	3.376606	-0.46656
H	-4.26089	3.559205	-1.41936

C	-6.25026	3.073325	-0.78162
H	-6.81952	2.888746	0.138826
H	-6.35	2.187423	-1.42014
H	-6.72025	3.91698	-1.3002
C	-4.64884	4.642955	0.39386
H	-5.08711	4.488311	1.388892
H	-3.60355	4.942307	0.523162
H	-5.17785	5.4808	-0.07558
N	-2.11891	0.872308	2.442979
H	-2.38064	1.694586	2.988975
C	-1.40042	-0.1933	3.129682
H	-0.33187	-0.15232	2.893092
H	-1.51794	-0.03667	4.206002
C	-1.85382	-1.61289	2.793698
O	-1.05044	-2.5519	2.867018
N	-3.13976	-1.78855	2.421618
H	-3.75141	-0.982	2.401382
C	-3.66487	-3.10612	2.069645
H	-3.39118	-3.80091	2.87044
C	-2.99559	-3.70711	0.810556
O	-3.03448	-4.92679	0.630655
C	-5.21575	-3.05344	1.985505
H	-5.52848	-2.53257	2.901612
C	-5.73411	-2.2532	0.780361
H	-5.50533	-2.76481	-0.16132
H	-6.82208	-2.14506	0.844011
H	-5.30861	-1.2442	0.724453
C	-5.83471	-4.45774	2.022111
H	-5.516	-5.00948	2.913612
H	-6.92739	-4.38134	2.043673
H	-5.54734	-5.04285	1.143846
N	-2.38419	-2.84213	-0.03914
H	-2.36952	-1.84762	0.183209
C	-1.59008	-3.275	-1.1851
H	-1.61818	-4.36915	-1.17483
C	-0.10136	-2.86087	-1.04159
O	0.62029	-2.76883	-2.04469
C	-2.1471	-2.74804	-2.52148
H	-2.12227	-1.64975	-2.49431
H	-1.44686	-3.05019	-3.30755
C	-3.56744	-3.21478	-2.88659
H	-4.24714	-2.89684	-2.08349
C	-4.02024	-2.52137	-4.18106

H	-5.04973	-2.79851	-4.43686
H	-3.97871	-1.42941	-4.08688
H	-3.37819	-2.80801	-5.02428
C	-3.67453	-4.74185	-3.02174
H	-4.68149	-5.02968	-3.3471
H	-3.47637	-5.25057	-2.07274
H	-2.96374	-5.11944	-3.76902
N	0.329382	-2.62755	0.214491
H	-0.33922	-2.70118	0.975664
C	1.640153	-2.08756	0.605672
H	1.614954	-2.10074	1.69582
C	1.755416	-0.58014	0.26285
O	1.831844	0.254806	1.169186
C	2.82556	-2.9504	0.130092
H	2.620206	-3.98095	0.452227
H	2.851106	-2.96385	-0.9629
C	4.20176	-2.51481	0.672797
H	4.396602	-1.49026	0.327529
C	4.269596	-2.51511	2.208196
H	5.28269	-2.27025	2.548529
H	4.011103	-3.50221	2.614504
H	3.590635	-1.7774	2.648989
C	5.295613	-3.41703	0.08124
H	6.29122	-3.09137	0.404873
H	5.275819	-3.40272	-1.01517
H	5.163367	-4.45811	0.404245
C	11.40405	-1.84646	0.966785
H	12.26379	-1.5522	1.575596
H	11.05473	-2.82976	1.29457
H	11.71332	-1.90871	-0.08051
C	10.33492	-0.8659	1.111234
N	9.485924	-0.08582	1.226831
C	-3.30284	5.526455	5.396459
H	-4.23355	5.990114	5.05733
H	-3.38552	5.300241	6.46339
H	-2.47876	6.229357	5.244324
C	-3.05516	4.301036	4.646216
N	-2.8586	3.325509	4.051669