Supporting Information

Cytotoxic Activity of Rearranged Drimane Meroterpenoids against Colon Cancer Cells via Down-Regulation of β-Catenin Expression

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Figure S1. LC-MS analysis of the combined extract of the three sponges *Smenospongia aurea*, *S. cerebriformis*, and *Verongula rigida* for the detection of unreported mass signals (*m/z* 384.2 and 398.2)

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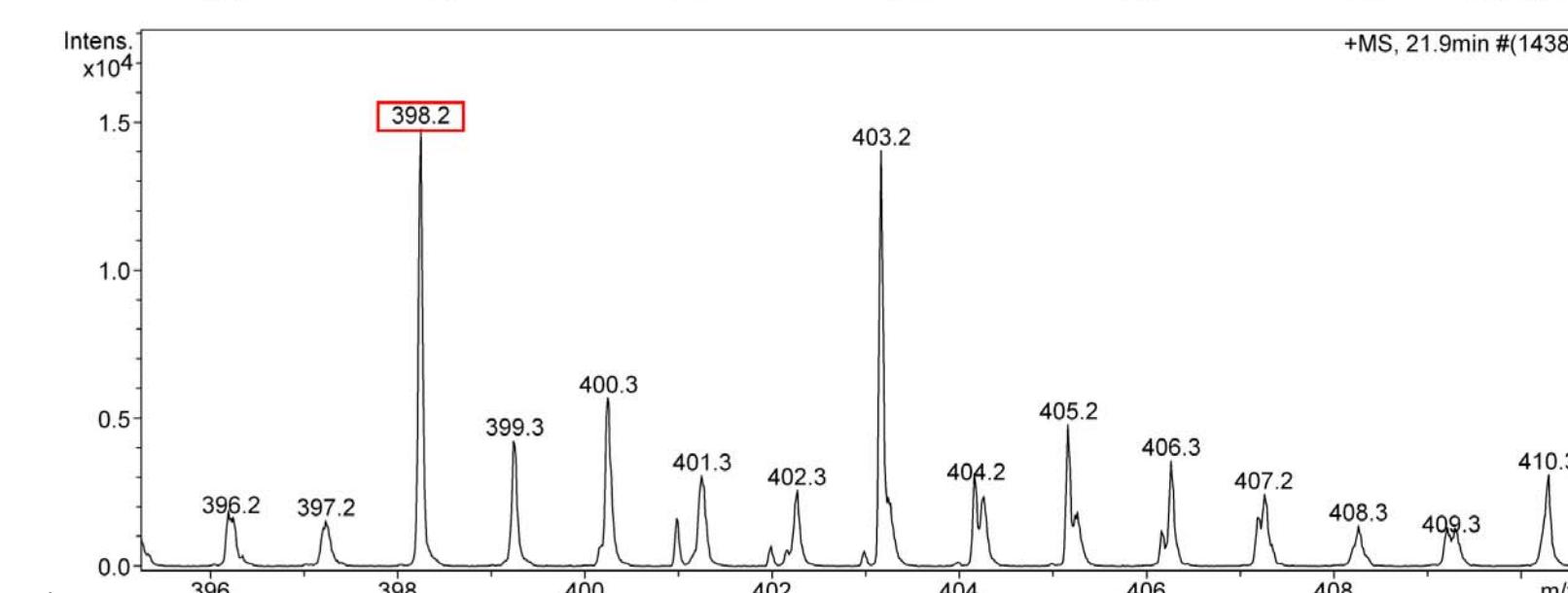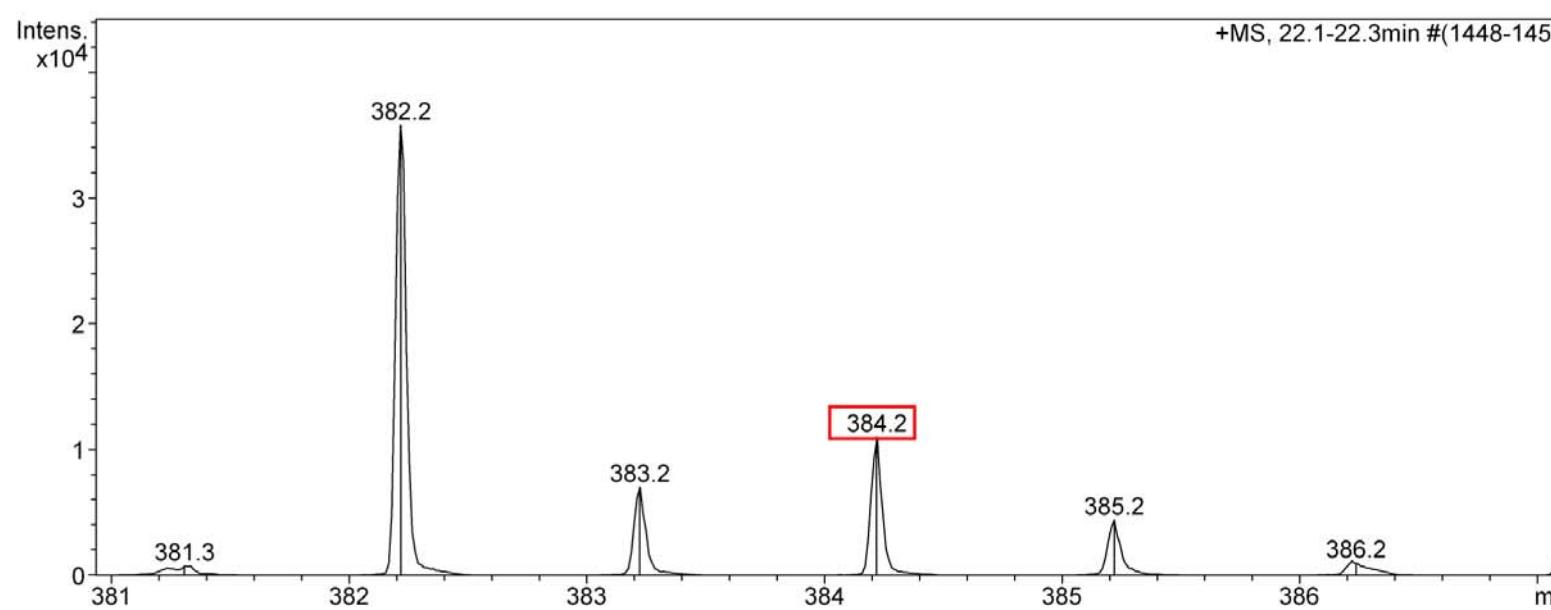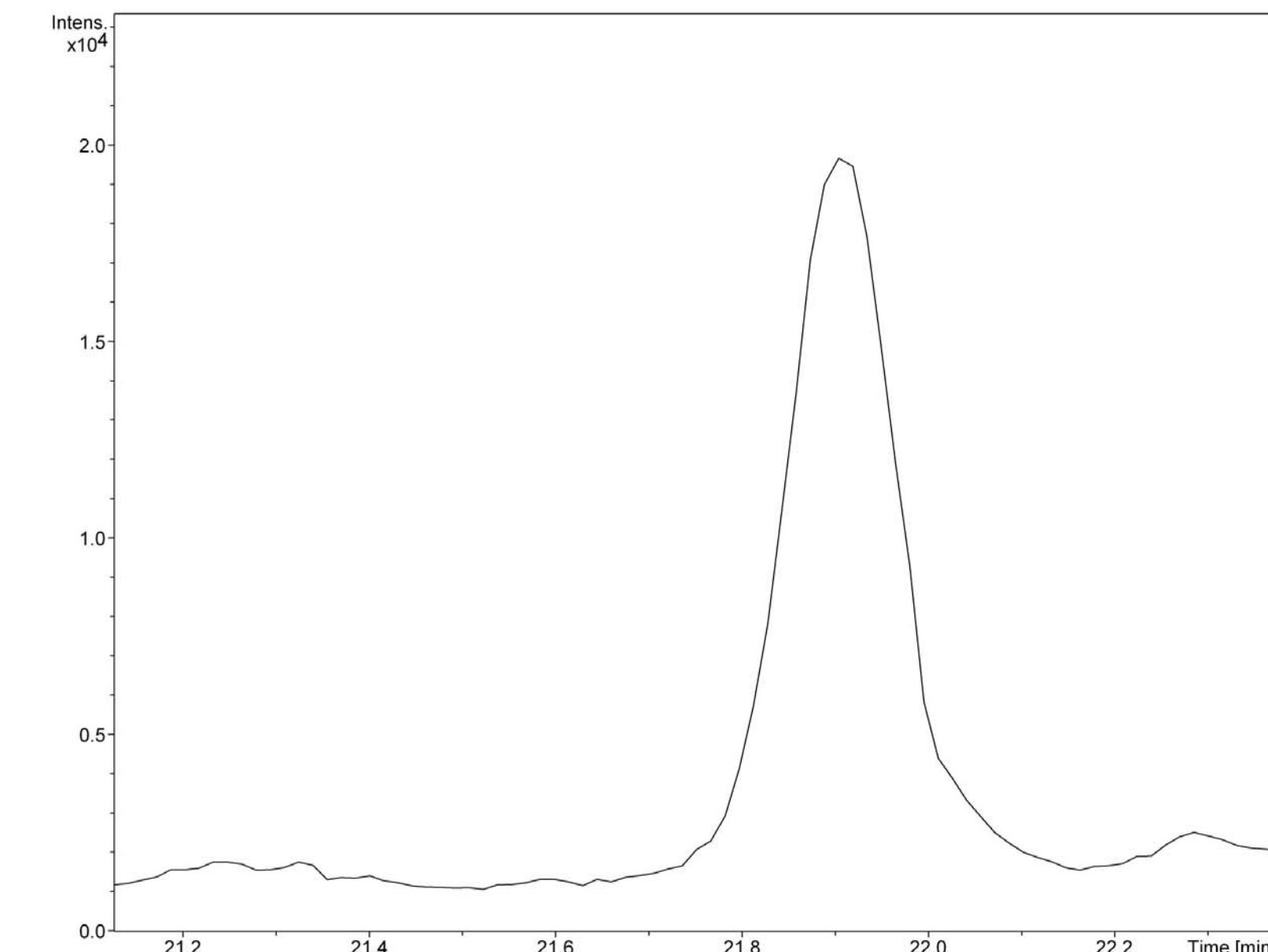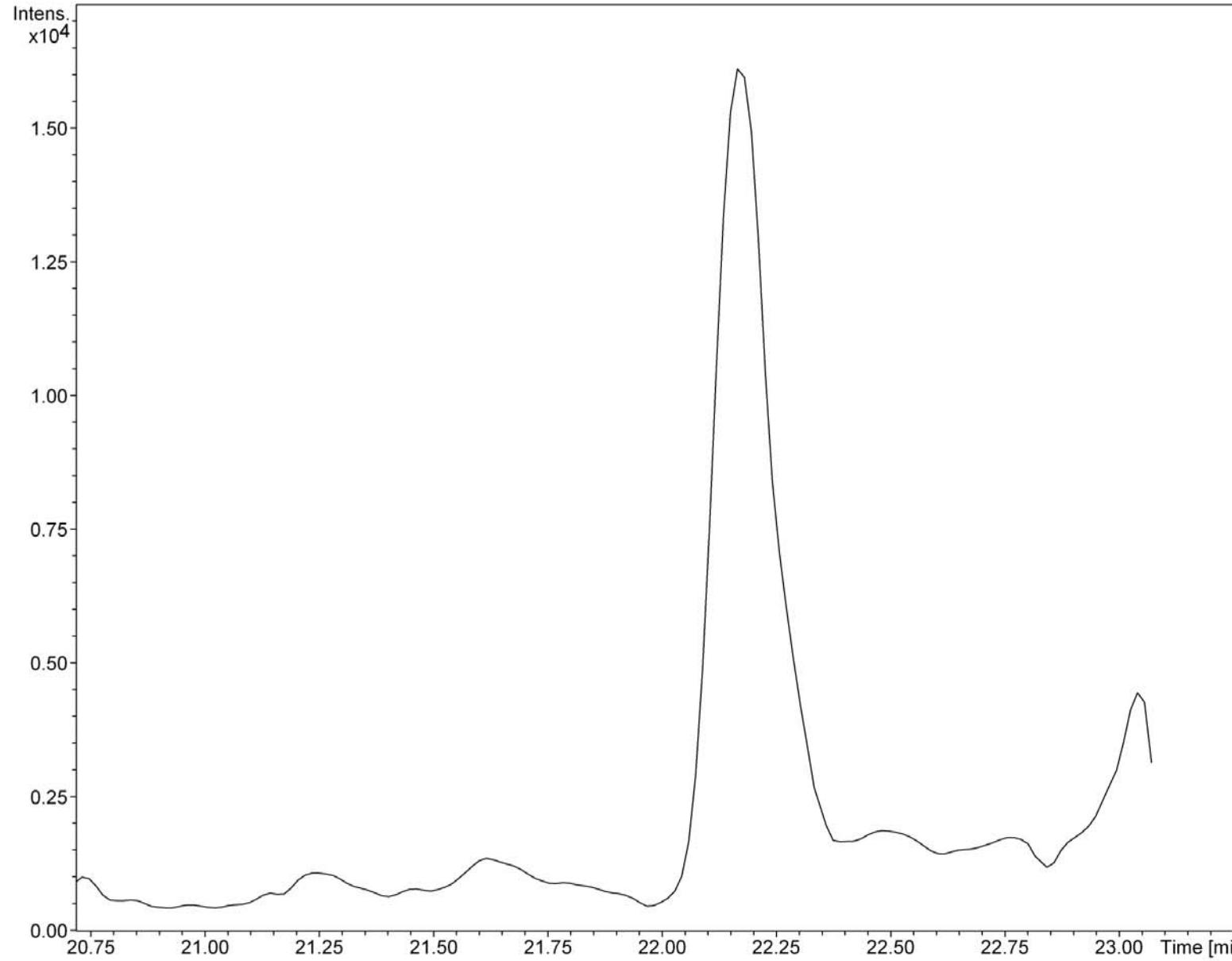
Table S1. The Major Conformers of Compounds 1–4 and Diastereomers I-IV (see Figures 1 and 5 in the main text) Identified by Conformational Searches in MMFF94 Force Field Using the Macromodel

Conformers[a]	Relative energy (kJ/mol)	Boltzmann population (%)[b]
Compound **1**_1	0	56.037729
Compound **1**_2	0.602	43.962271
Compound **2**_1	0	51.543966
Compound **2**_2	0.153	48.456034
Compound **3**_1	0	51.336713
Compound **3**_2	2.144	21.612859
Compound **3**_3	3.226	13.973626
Compound **3**_4	4.368	8.814366
Compound **3**_5	7.604	2.388533
Compound **3**_6	8.206	1.873902
Compound **4**_1	0	36.700324
Compound **4**_2	0.072	35.646713
Compound **4**_3	1.408	20.795324
Compound **4**_4	5.792	3.54697
Compound **4**_5	5.963	3.310669
Compound **7**_1/Diastereomer **I**_1	0	36.804449
Compound **7**_2/Diastereomer **I**_2	0.695892	27.795755
Compound **7**_3/Diastereomer **I**_3	2.145233	15.489979
Compound **7**_4/Diastereomer **I**_4	4.882416	5.134409
Compound **7**_5/Diastereomer **I**_5	5.186493	4.541669
Compound **7**_6/Diastereomer **I**_6	5.698822	3.693638
Compound **7**_7/Diastereomer **I**_7	6.940643	2.238126
Compound **7**_8/Diastereomer **I**_8	7.630707	1.694275
Compound **7**_9/Diastereomer **I**_9	9.045135	0.957575
Compound **7**_10/Diastereomer **I**_10	9.136536	0.92291
Compound **7**_11/Diastereomer **I**_11	9.727264	0.727214
Compound **6**_1/Diastereomer **II**_1	0	32.017963
Compound **6**_2/Diastereomer **II**_2	0.62851	24.8472
Compound **6**_3/Diastereomer **II**_3	2.079132	13.839654
Compound **6**_4/Diastereomer **II**_4	4.072021	6.193936
Compound **6**_5/Diastereomer **II**_5	4.595612	5.014557
Compound **6**_6/Diastereomer **II**_6	4.980194	4.29391
Compound **6**_7/Diastereomer **II**_7	5.464386	3.532006
Compound **6**_8/Diastereomer **II**_8	5.539764	3.426218
Compound **6**_9/Diastereomer **II**_9	5.844849	3.029448
Compound **6**_10/Diastereomer **II**_10	7.599854	1.492392
Compound **6**_11/Diastereomer **II**_11	8.657684	0.973977
Compound **6**_12/Diastereomer **II**_12	9.555878	0.677927
Compound **6**_13/Diastereomer **II**_13	9.619263	0.660812
Diastereomer **III**_1	0	24.280092
Diastereomer **III**_2	0.323029	21.313512
Diastereomer **III**_3	2.124298	10.305491

Diastereomer **III**_4	2.359467	9.372742
Diastereomer **III**_5	3.464508	6.001516
Diastereomer **III**_6	3.737854	5.374898
Diastereomer **III**_7	4.721985	3.613669
Diastereomer **III**_8	4.868011	3.406937
Diastereomer **III**_9	5.125763	3.070475
Diastereomer **III**_10	5.14682	3.044502
Diastereomer **III**_11	5.94339	2.207779
Diastereomer **III**_12	6.095245	2.076587
Diastereomer **III**_13	6.950897	1.470409
Diastereomer **III**_14	7.093628	1.388134
Diastereomer **III**_15	7.535187	1.161634
Diastereomer **III**_16	8.289703	0.856794
Diastereomer **III**_17	9.347809	0.559106
Diastereomer **III**_18	9.646057	0.495724
Diastereomer **IV**_1	0	21.777569
Diastereomer **IV**_2	0.665497	16.649949
Diastereomer **IV**_3	1.509735	11.844058
Diastereomer **IV**_4	2.216461	8.905957
Diastereomer **IV**_5	2.646759	7.486718
Diastereomer **IV**_6	2.693665	7.346382
Diastereomer **IV**_7	3.550049	5.200357
Diastereomer **IV**_8	4.857391	3.068908
Diastereomer **IV**_9	5.165039	2.710712
Diastereomer **IV**_10	5.188477	2.685203
Diastereomer **IV**_11	5.197205	2.675764
Diastereomer **IV**_12	5.463776	2.402946
Diastereomer **IV**_13	6.76709	1.420367
Diastereomer **IV**_14	6.771423	1.417886
Diastereomer **IV**_15	7.26001	1.164233
Diastereomer **IV**_16	7.793915	0.938639
Diastereomer **IV**_17	8.447083	0.721211
Diastereomer **IV**_18	8.856262	0.611467
Diastereomer **IV**_19	9.142761	0.544726
Diastereomer **IV**_20	9.746643	0.426949

[a]See Computational Details regarding the procedures for conformational search processes. [b]Calculated populations based on the relative MMFF94 potential energy of each conformer

Table S2. Experimental (Exp.) and Calculated (Cal.) Chemical Shift Values (CS, δ) of Compounds 1 and 2

	Exp. CS of **1**	Cal. CS of **1**	Exp. CS of **2**	Cal. CS of **2**
C-1	23.4	25.39	23	26.49
C-2	28.9	30.48	25.3	27.68
C-3	33.2	35.15	32.2	34.79
C-4	160.5	156.5	153.9	150.81
C-5	40.6	45.38	39.6	43.84
C-10	49.4	49.64	47.6	48.22
C-9	43.1	50.2	44.5	51.15
C-8	37.4	38.63	38.7	40.16
C-7	28.2	30.8	28	30.11
C-6	36.5	37.1	37.8	39.53
C-11	102.7	102.34	105.8	104.92
C-15	34.6	35.22	34.7	35.16
C-16	109.2	106.31	109.4	106.35
C-17	143.7	140.76	143.6	140.73
C-18	144.6	138.09	144.5	138.03
C-19	98.8	97.22	98.8	97.11
C-20	132.3	127.74	132.5	127.49
C-21	146.6	142.63	146.7	142.97
C-22	162	158.47	162	158.57
C-23	14.6	14.63	14.6	14.45
C-14	17.7	20.73	19	21.4
C-13	18.5	21.1	18.8	21.46
C-12	20.7	21.46	33.2	32.96
OCH_3	56.6	53.75	56.7	53.72
H-1a	2.27	2.49	1.94	2.1
H-1b	1.51	1.69	2.3	2.62
H-2a	1.87	1.78	1.82	1.97
H-2b	1.22	1.38	1.68	1.6
H-3a	2.33	2.47	2.11	2.13
H-3b	2.02	1.95	2.44	2.58
H-10	0.92	1.33	1.4	1.62
H-8	1.4	1.63	1.33	1.52
H-7a	1.39	1.42	1.17	1.16
H-7b	1.39	1.59	1.5	1.85
H-6a	1.19	1.27	0.93	0.99
H-6b	1.43	1.49	1.92	2.03
H-15a	2.89	3.04	2.83	3.05
H-15b	2.8	3.01	2.96	3.09
H-19	6.98	6.84	6.98	6.82
H-23a	2.54	2.34	2.54	2.41
H-23b	2.54	2.41	2.54	2.4
H-23c	2.54	2.46	2.54	2.4
H-14a	0.91	0.86	0.95	1.03
H-14b	0.91	1.2	0.95	1.59
H-14c	0.91	1.11	0.95	0.89
H-13a	1.04	0.76	1.01	0.85
H-13b	1.04	0.86	1.01	1.93
H-13c	1.04	1.97	1.01	0.79
OCH_3	3.9	3.76	3.91	3.9
OCH_3	3.9	4.04	3.91	3.77
OCH_3	3.9	3.77	3.91	3.91
H-11a	4.32	4.37	4.66	4.83
H-11b	4.36	4.61	4.69	5.03
H-12a	1.04	0.43	0.98	1.16
H-12b	1.04	1.43	0.98	0.5
H-12c	1.04	1.74	0.98	1.37

Table S3. Experimental (Exp.) and Calculated (Cal.) CS Values (δ) of Compounds 3 and 4

	Exp. CS of **3**	Cal. CS of **3**	Exp. CS of **4**	Cal. CS of **4**
C-1	23	25.19	22.7	26.23
C-2	28.8	30.31	25.2	27.52
C-3	33.2	35.03	32.2	34.7
C-4	161	156.88	153.7	150.4
C-5	40.5	45.45	39.6	43.97
C-10	50	50.66	47.8	49.23
C-9	42.9	50.28	44.2	51.17
C-8	38.1	39.25	39.1	41.04
C-7	28.1	30.64	28	30.17
C-6	36.9	37.42	38.2	39.92
C-11	102.4	102.18	105.8	105.2
C-15	32.7	34.67	32.5	34.61
C-16	110.3	114.23	110.1	114.11
C-17	181.59	179.12	181.57	178.99
C-18	158.9	154.8	158.9	154.57
C-19	96.92	106.96	96.89	106.75
C-20	155.6	155.77	155.6	155.74
C-21	161.4	159.11	161.5	159.04
C-22	116.24	114.66	116.19	114.68
C-23	25.9	27.58	25.8	27.55
C-14	17.5	20.35	19	21.09
C-13	18	20.78	18.4	21.21
C-12	20.7	21.43	33.3	33.25
OC*H₃*	56.4	57.32	56.5	57.22
H-1a	2.13	2.39	1.85	1.98
H-1b	1.42	1.58	2.19	2.44
H-2a	1.84	1.72	1.77	1.91
H-2b	1.2	1.32	1.65	1.57
H-3a	2.29	2.47	2.1	2.12
H-3b	2.04	1.95	2.42	2.55
H-10	0.8	1.12	1.17	1.47
H-8	1.22	1.38	1.11	1.28
H-7a	1.36	1.43	1.15	1.19
H-7b	1.36	1.61	1.46	1.83
H-6a	1.3	1.42	1.01	1.14
H-6b	1.47	1.62	1.97	2.13
H-15a	2.53	2.71	2.47	2.54
H-15b	2.37	2.43	2.51	2.69
H-19	6.14	6.36	6.16	6.36
H-23a	1.58	1.05	1.61	1.83
H-23b	1.58	1.82	1.61	1.69
H-23c	1.58	1.7	1.61	1.06
H-14a	0.81	0.74	0.85	0.94
H-14b	0.81	1.12	0.85	1.51
H-14c	0.81	1.03	0.85	0.77
H-13a	0.97	0.76	0.95	0.68
H-13b	0.97	1.79	0.95	0.76
H-13c	0.97	0.7	0.95	1.86
OC*H₃*	3.83	3.61	3.84	3.51
OC*H₃*	3.83	3.95	3.84	4.61
OC*H₃*	3.83	4.38	3.84	3.82
H-11a	4.38	4.48	4.65	4.87
H-11b	4.4	4.68	4.68	5.05
H-12a	1.01	1.42	1.01	0.5
H-12b	1.01	1.75	1.01	0.79
H-12c	1.01	0.47	1.01	2.01
C-24	26	27.82	25.8	27.61
H-24a	1.6	1.83	1.61	1.83
H-24b	1.6	1.08	1.61	1.07
H-24c	1.6	1.67	1.61	1.72

Figure S2. CP3 analysis of compounds 1 (B) and 2 (A)

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Assignment of stereochemistry and structure using NMR and CP3

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highlights:
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  CP3: NMR data
  DP4: NMR data
  force field
    evaluation
  InChIKey collision
  RInChI project
  solubility challenge

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Please select version of database to use:
CP3-original
CP3-database2
CP3-database3

Enter two 1H and 13C experimental spectra then two calculated spectra:

13C Expt A 23.00,25.30,32.20,153.90,39.60,47.60,44.50,38.70,28.00,37.80,105.80,3
13C Expt B 3.70,144.60,98.80,132.30,146.60,162.00,14.60,17.70,18.50,56.60,20.70
13C Calc A 26.49,27.68,34.79,150.81,43.84,48.22,51.15,40.16,30.11,39.53,104.92,3
13C Calc B 0.76,138.09,97.22,127.74,142.63,158.47,14.63,20.73,21.10,53.75,21.46
1H Expt A 54,0.95,0.95,0.95,1.01,1.01,1.01,3.91,3.91,3.91,4.66,4.69,0.98,0.98,0.98
1H Expt B 54,0.91,0.91,0.91,1.04,1.04,1.04,3.90,3.90,3.90,4.32,4.36,1.04,1.04,1.04
1H Calc A 40,1.03,1.59,0.89,0.85,1.93,0.79,3.90,3.77,3.91,4.83,5.03,1.16,0.50,1.37
1H Calc B 46,0.86,1.20,1.11,0.76,0.86,1.97,3.76,4.04,3.77,4.37,4.61,0.43,1.43,1.74

Assign resonances
Calculate
Re-read input
Clear text

CP3 thinks ExpA goes with CalcA and ExpB with CalcB:

ExpA with CalcA and ExpB with CalcB: 100.0%
ExpA with CalcB and ExpB with CalcA: 0.0%

CP3 values:

	C data	H data	All data
ExpA-CalcA & ExpB-CalcB	0.69	0.66	0.67
ExpA-CalcB & ExpB-CalcA	-0.86	-0.94	-0.90

Probabilities:

	C data	H data	All data
ExpA-CalcA & ExpB-CalcB	100.0%	99.9%	100.0%
ExpA-CalcB & ExpB-CalcA	0.0%	0.1%	0.0%

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Figure S3. CP3 analysis of compounds 3 (B) and 4 (A)

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highlights:
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CP3: NMR data
DP4: NMR data
force field
  evaluation
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Assignment of stereochemistry and structure using NMR and CP3

Please select version of database to use:
CP3-original
CP3-database2
CP3-database3

Enter two 1H and 13C experimental spectra then two calculated spectra:

13C Expt A 58.90,96.89,155.60,161.50,116.19,25.80,19.00,18.40,56.50,33.30,25.80

13C Expt B 58.90,96.92,155.60,161.40,116.24,25.90,17.50,18.00,56.40,20.70,26.00

13C Calc A 4.57,106.75,155.74,159.04,114.68,27.55,21.09,21.21,57.22,33.25,27.61

13C Calc B 4.80,106.96,155.77,159.11,114.66,27.58,20.35,20.78,57.32,27.58,21.43

1H Expt A 1.85,2.19,1.77,1.65,2.10,2.42,1.17,1.11,1.15,1.46,1.01,1.97,2.47,2.51,6.1

1H Expt B 2.13,1.42,1.84,1.20,2.29,2.04,0.80,1.22,1.36,1.36,1.30,1.47,2.53,2.37,6.1

1H Calc A 77,0.68,0.76,1.86,3.51,4.61,3.82,4.87,5.05,0.50,0.79,2.01,1.83,1.07,1.72

1H Calc B 03,0.76,1.79,0.70,3.61,3.95,4.38,4.48,4.68,1.42,1.75,0.47,1.83,1.08,1.67

CP3 thinks ExpA goes with CalcA and ExpB with CalcB:

 ExpA with CalcA and ExpB with CalcB: 100.0%
 ExpA with CalcB and ExpB with CalcA: 0.0%

CP3 values:

	C data	H data	All data
ExpA-CalcA & ExpB-CalcB	0.36	0.58	0.47
ExpA-CalcB & ExpB-CalcA	-0.68	-0.99	-0.84

Probabilities:

	C data	H data	All data
ExpA-CalcA & ExpB-CalcB	100.0%	99.9%	100.0%
ExpA-CalcB & ExpB-CalcA	0.0%	0.1%	0.0%

Assign resonances

Calculate

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Table S4. Calculated (Cal.) CS Values (δ) of Diastereomers I-IV Shown in Figure 5

	Cal. CS of I	Cal. CS of II	Cal. CS of III	Cal. CS of IV
C-1	26.1	24.1	25.42	24.74
C-2	27.64	26.78	27.28	26.92
C-3	34.86	34.37	34.72	34.57
C-4	151.46	150.47	151.15	150.3
C-5	44.31	43.89	44.1	43.92
C-10	49.09	47.93	49.8	49.2
C-9	48.74	48.61	48.93	49.01
C-8	40.42	40.16	40.73	41.2
C-7	29.64	30.01	29.76	29.89
C-6	40.29	39.8	40.32	40.29
C-11	104.79	105.3	104.83	105.54
C-15	39.4	39.29	38.17	37.96
C-16	54.13	54.31	48.44	48.86
C-20	199.66	199.17	202.52	202.56
C-19	150.29	150.46	149.45	149.16
C-14	21.06	21.16	20.93	21.02
C-13	18.64	19.66	19.44	19.2
OCH₃	55.51	55.56	55.29	55.38
H-1a	2.28	1.6	2.25	1.81
H-1b	2.41	1.94	2.26	1.82
H-2a	1.81	1.8	1.87	1.88
H-2b	1.58	1.46	1.58	1.49
H-3a	2.11	2.11	2.13	2.12
H-3b	2.6	2.62	2.61	2.55
H-10	1.66	1.77	1.71	1.16
H-8	1.59	1.43	1.16	1.48
H-7a	1.2	1.29	1.13	1.26
H-7b	1.9	1.87	1.89	1.89
H-6a	1.34	1.38	1.23	1.24
H-6b	2.24	2.21	2.21	2.21
H-15a	2.06	2.16	2.26	2.41
H-15b	1.18	1.2	1.78	1.86
H-14a	0.67	0.83	0.76	0.86
H-14b	1.59	1.6	1.57	1.56
H-14c	0.61	0.46	0.7	0.62
H-13a	0.67	0.78	0.6	0.77
H-13b	1.01	1.87	0.83	1.72
H-13c	0.76	0.64	0.81	0.71
OCH₃	4.08	4.1	3.58	4.27
OCH₃	4.48	3.53	4.32	4
OCH₃	3.55	4.46	4.14	3.79
H-11a	4.85	4.92	4.85	4.91
H-11b	5.02	5.03	5.04	5.05
C-12	33.14	32.88	33.15	33.14
H-12a	0.68	0.75	0.65	0.55
H-12b	0.89	0.84	0.82	0.82
H-12c	2.08	2.07	2.16	2.01
C-18	132.16	132.17	133.42	133.59
C-17	82.99	82.98	77.75	77.86
C-21	174.22	174.35	175.78	176.01
OCH₂CH₃	60.78	60.86	60.59	60.89
OCH₂CH₃	15.69	15.62	15.75	15.81
H-16	2.81	2.74	2.57	2.64
H-18	6.03	6.01	6.1	6.06
OCH₂aCH₃	4.26	4.29	4.35	4.31
OCH₂bCH₃	4.15	4.15	4.16	4.2
OCH₂CH₃a	0.94	1.35	1.04	1.1
OCH₂CH₃b	1.31	1.31	1.38	1.29
OCH₂CH₃c	1.33	0.94	1.34	1.42

Figure S4. DP4 analysis of compound 7 with diastereomers I–IV[a]

[a]Isomers 1–4 in the analysis are structurally equivalent to diastereomers **I–IV** (see Figure 5) and experimental CS data shown here are for compound **7.**

Figure S5. DP4 analysis of compound 6 with diastereomers I–IV*[a]*

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instructions
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  step 3
  step 4
applet source code

Other NMR
  parameters:
  CP3

Assignment of stereochemistry and structure using NMR and DP4

Please select version of database to use:

DP4-original
DP4-database2

Select probability distribution:

◉ t distribution (recommended)
○ normal distribution

13C Calc:

C1,C2,C3,C4,C5,C6,C7,C8,C9,C10,C11,C12,C13,(
26.10,27.64,34.86,151.46,44.31,49.09,48.74,40.42
24.10,26.78,34.37,150.47,43.89,47.93,48.61,40.16
25.42,27.28,34.72,151.15,44.10,49.80,48.93,40.73
24.74,26.92,34.57,150.30,43.92,49.20,49.01,41.20

1H Calc:

H29,H30,H31,H32,H33,H34,H35
2,0.68,0.89,2.08,2.81,6.03,4.26,4.15,0.94,1.31,1.33
3,0.75,0.84,2.07,2.74,6.01,4.29,4.15,1.35,1.31,0.94
4,0.65,0.82,2.16,2.57,6.10,4.35,4.16,1.04,1.38,1.34
5,0.55,0.82,2.01,2.64,6.06,4.31,4.20,1.10,1.29,1.42

13C Expt:

21.62(C1),24.73(C2),32.07(C3),153.50(C4),39.44((

1H Expt:

26(H31),4.17(H32),1.21(H33),1.21(H34),1.21(H35)

[Read Data] [Show Assignments] [Calculate] [Clear]

WARNING: One or more of the carbon shifts have large errors (largest error 11.6 ppm).
DP4 calculation has been attempted anyway, but you may wish to check the input data.
To check the assignments, click Show Assignments.

This calculation will use the DP4-database2 version of the database and the t distribution.
(To change these options select the desired database and distribution from the menus at the
top of the applet and then click Calculate).

Results of DP4 using both carbon and proton data:
  Isomer 1: 20.8%
  Isomer 2: 79.2%
  Isomer 3: 0.0%
  Isomer 4: 0.0%

(c) Jonathan M Goodman and Steven G Smith

*[a]*Isomers 1–4 in the DP4 result are indicating diastereomers **I–IV** (see Figure 5) and experimental CS data shown in the analysis are corresponding to those for compound **6.**

Figure S6. DP4 analysis of compound 6 with diastereomers II–IV[a]

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Assignment of stereochemistry and structure using NMR and DP4

Please select version of database to use:

| DP4-original |
| DP4-database2 |

Select probability distribution:

◉ t distribution (recommended)
○ normal distribution

13C Calc:

C1,C2,C3,C4,C5,C6,C7,C8,C9,C10,C11,C12,C13,(
24.10,26.78,34.37,150.47,43.89,47.93,48.61,40.16
25.42,27.28,34.72,151.15,44.10,49.80,48.93,40.73
24.74,26.92,34.57,150.30,43.92,49.20,49.01,41.20

1H Calc:

H1, H2, H3, H4, H5, H6, H7, H8, H9, H10, H11, H12
1.60,1.94,1.80,1.46,2.11,2.62,1.77,1.43,1.29,1.87,1
2.25, 2.26, 1.87, 1.58, 2.13, 2.61, 1.71, 1.16, 1.13, 1
1.81,1.82,1.88,1.49,2.12,2.55,1.16,1.48,1.26,1.89,1

13C Expt:

21.62(C1),24.73(C2),32.07(C3),153.50(C4),39.44((

1H Expt:

1.54(H1),1.81(H2),1.72(H3),1.61(H4),2.09(H5),2.44

[Read Data] [Show Assignments] [Calculate] [Clear]

WARNING: One or more of the carbon shifts have large errors (largest error 11.6 ppm).
DP4 calculation has been attempted anyway, but you may wish to check the input data.
To check the assignments, click Show Assignments.

This calculation will use the DP4-database2 version of the database and the t distribution.
(To change these options select the desired database and distribution from the menus at the top of the applet and then click Calculate).

Results of DP4 using both carbon and proton data:
  Isomer 1: 100.0%
  Isomer 2: 0.0%
  Isomer 3: 0.0%

Results of DP4 using the carbon data only:

(c) Jonathan M Goodman and Steven G Smith

[a]The structures of Isomers **1**–**3** in the analysis are identical to those of diastereomers **II**–**IV** (see Figure 5) and experimental CS data of compound **6** are used for this DP4 analysis.

Figure S7. ^{1}H NMR spectrum of compound **1** in CDCl$_3$ (600 MHz)
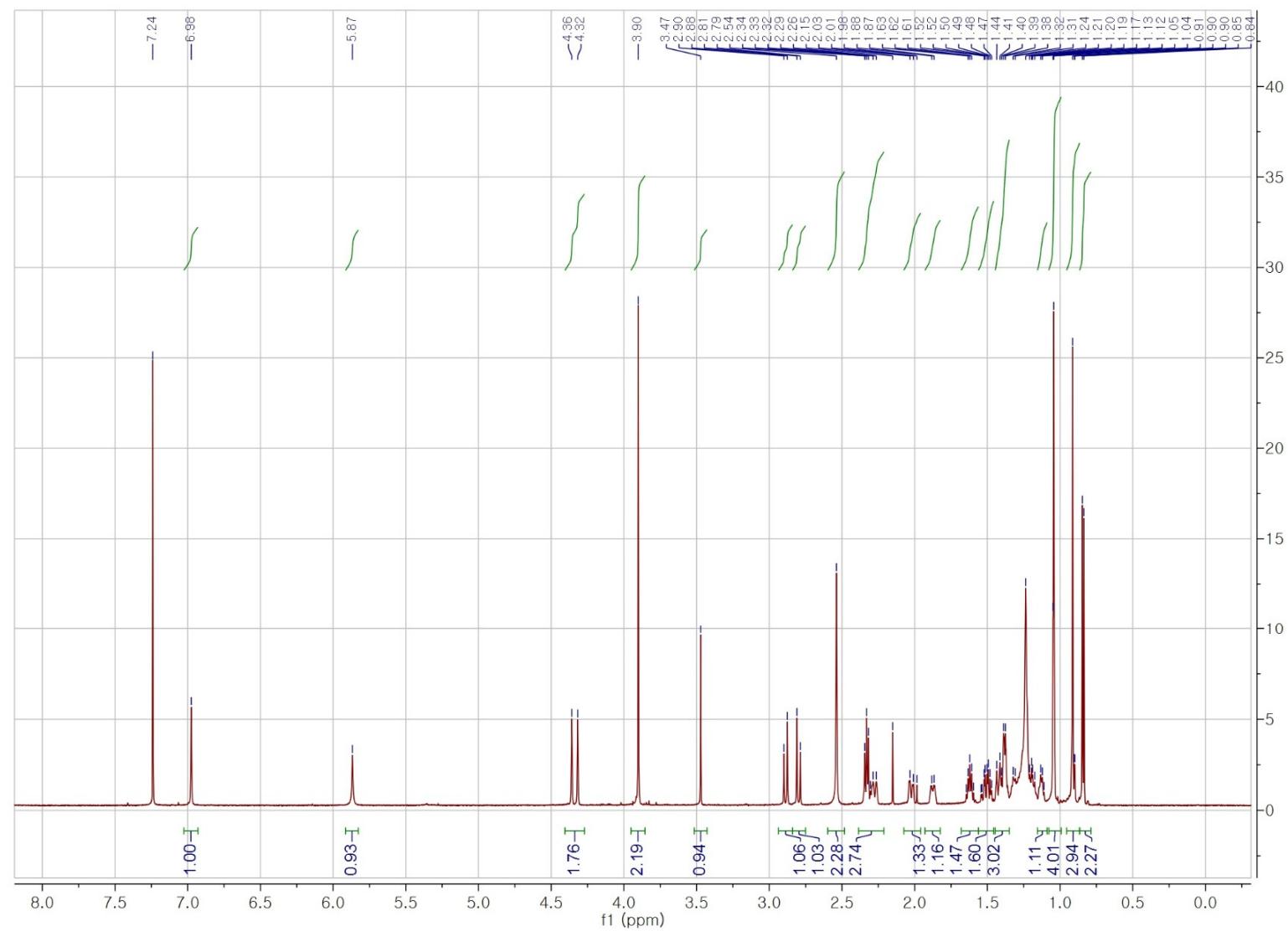
Figure S8. ^{13}C NMR spectrum of compound 1 in CDCl$_3$ (150 MHz)

16
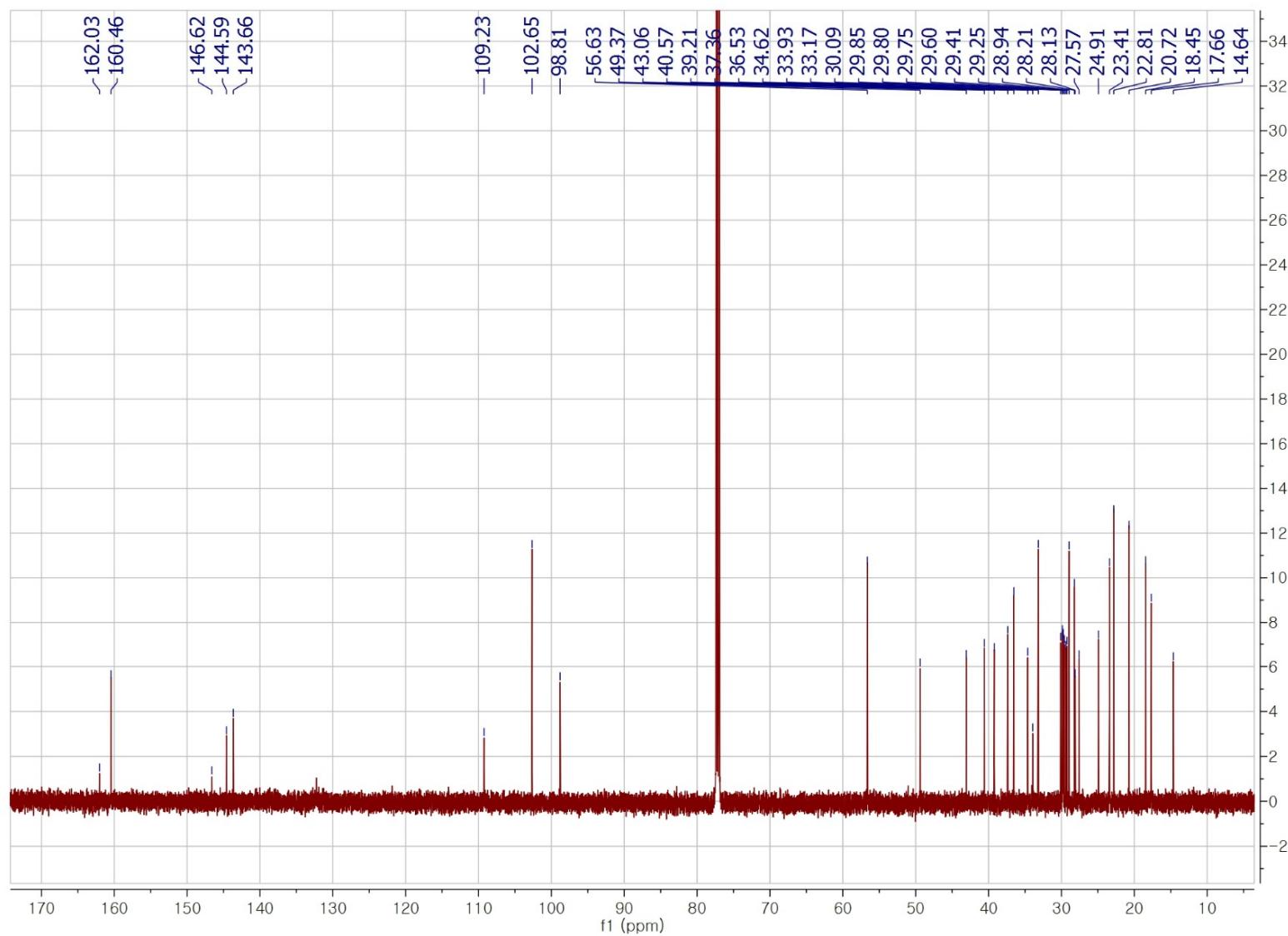
Figure S9. HSQC spectrum of compound 1 in CDCl₃
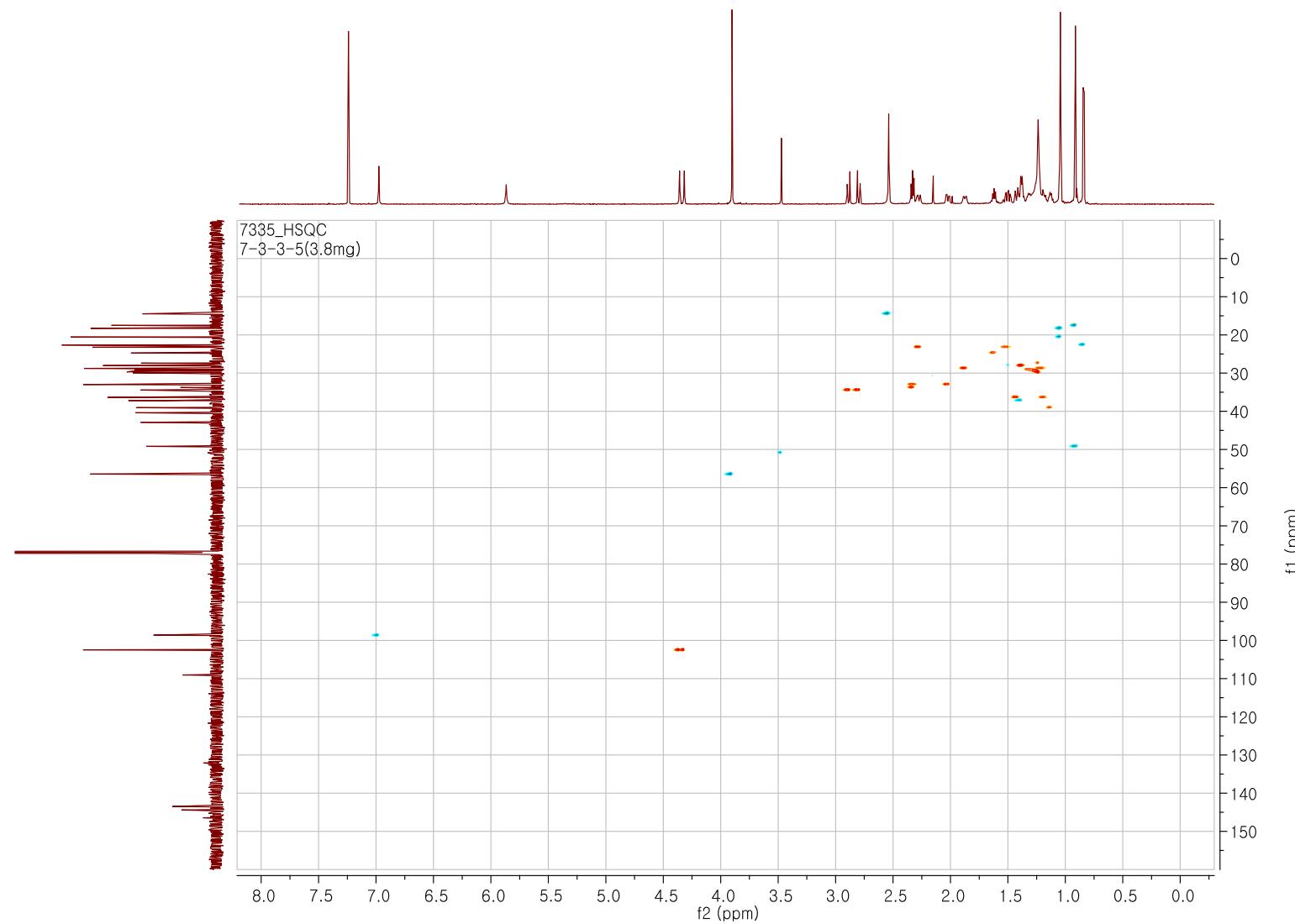
Figure S10. HMBC spectrum of compound 1 in CDCl₃ and its inspection
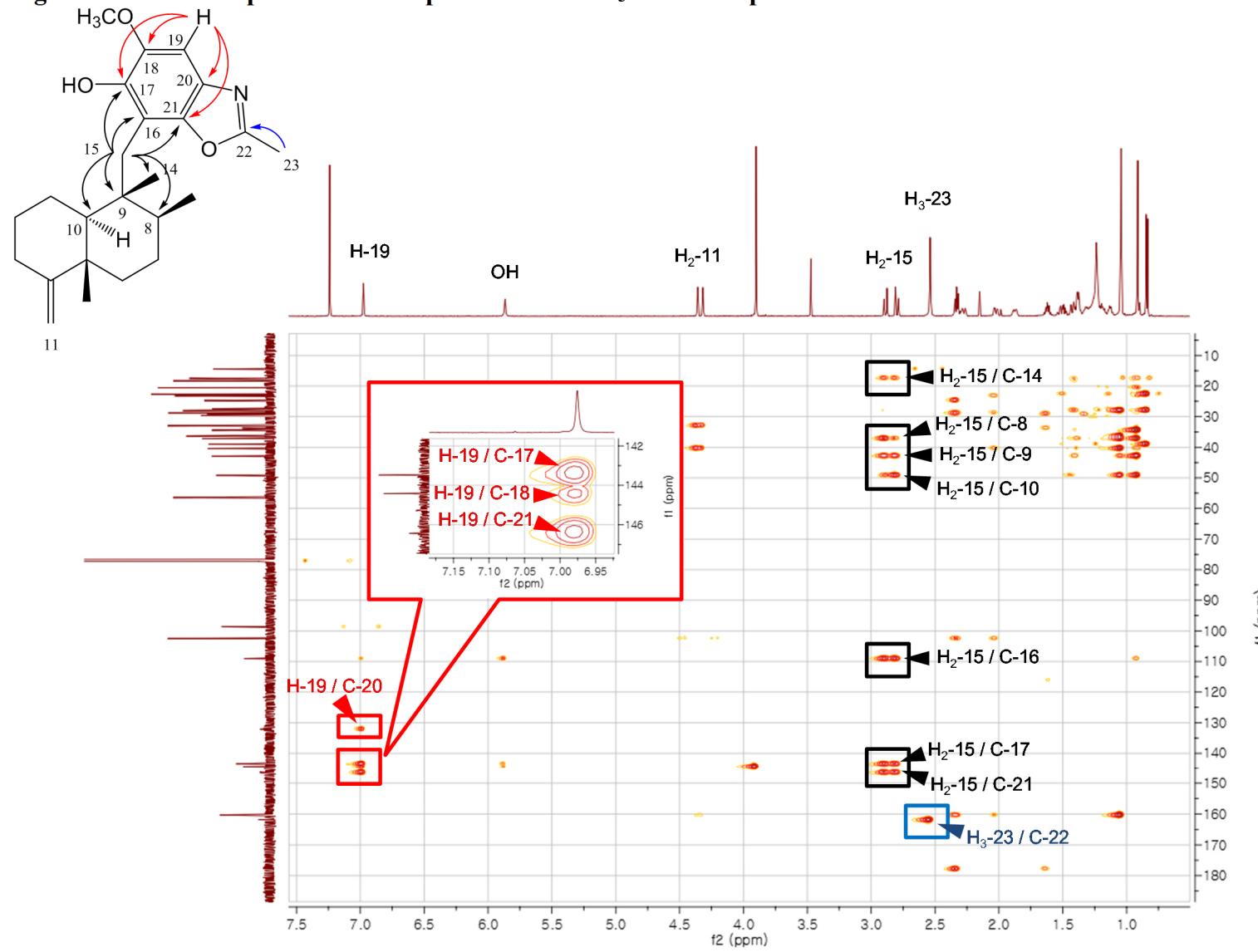
Figure S11. COSY spectrum of compound 1 in CDCl₃

7335_COSY
7-3-3-5(3.8mg)
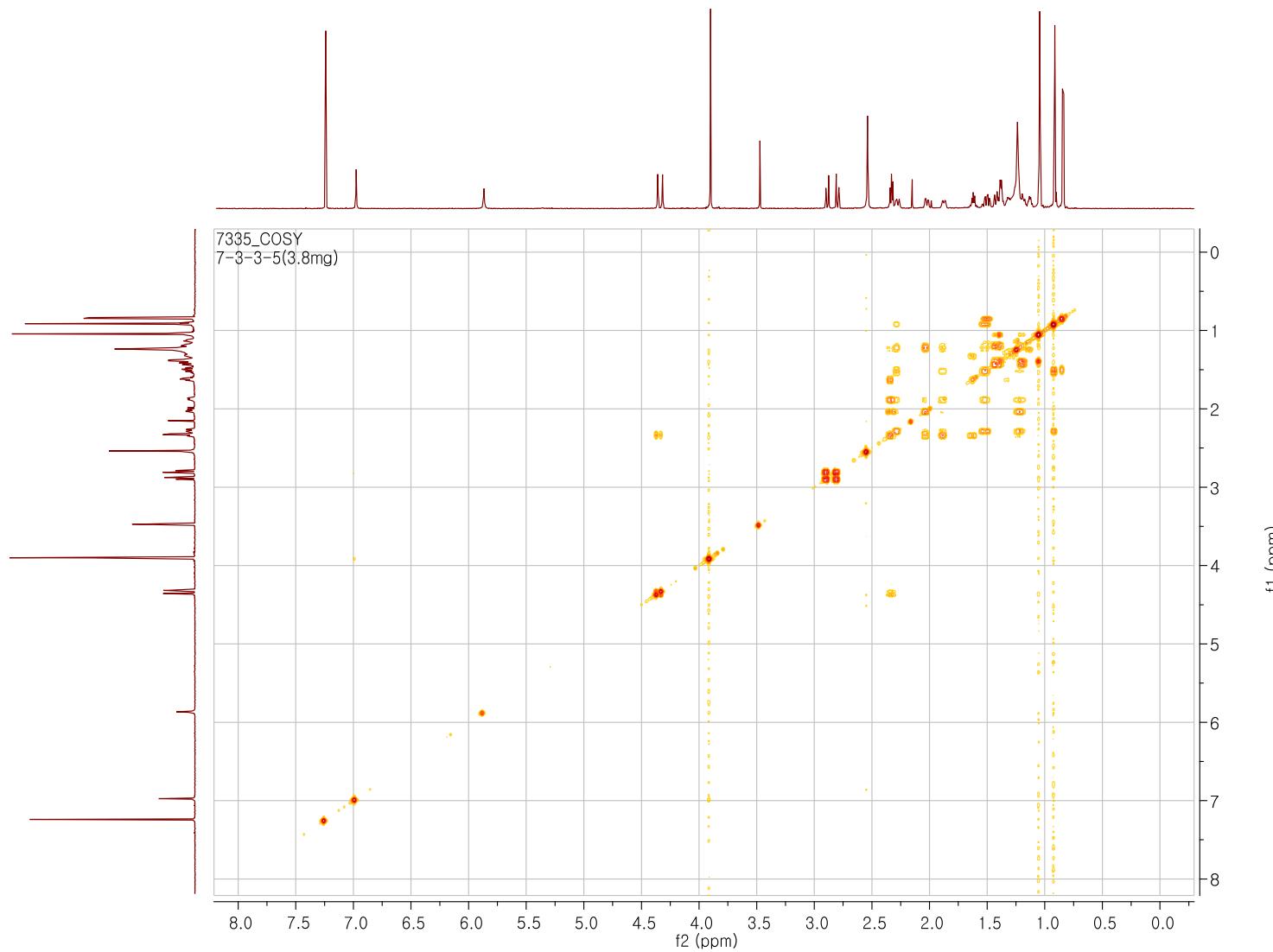
Figure S12. HRFABMS analysis of compound 1
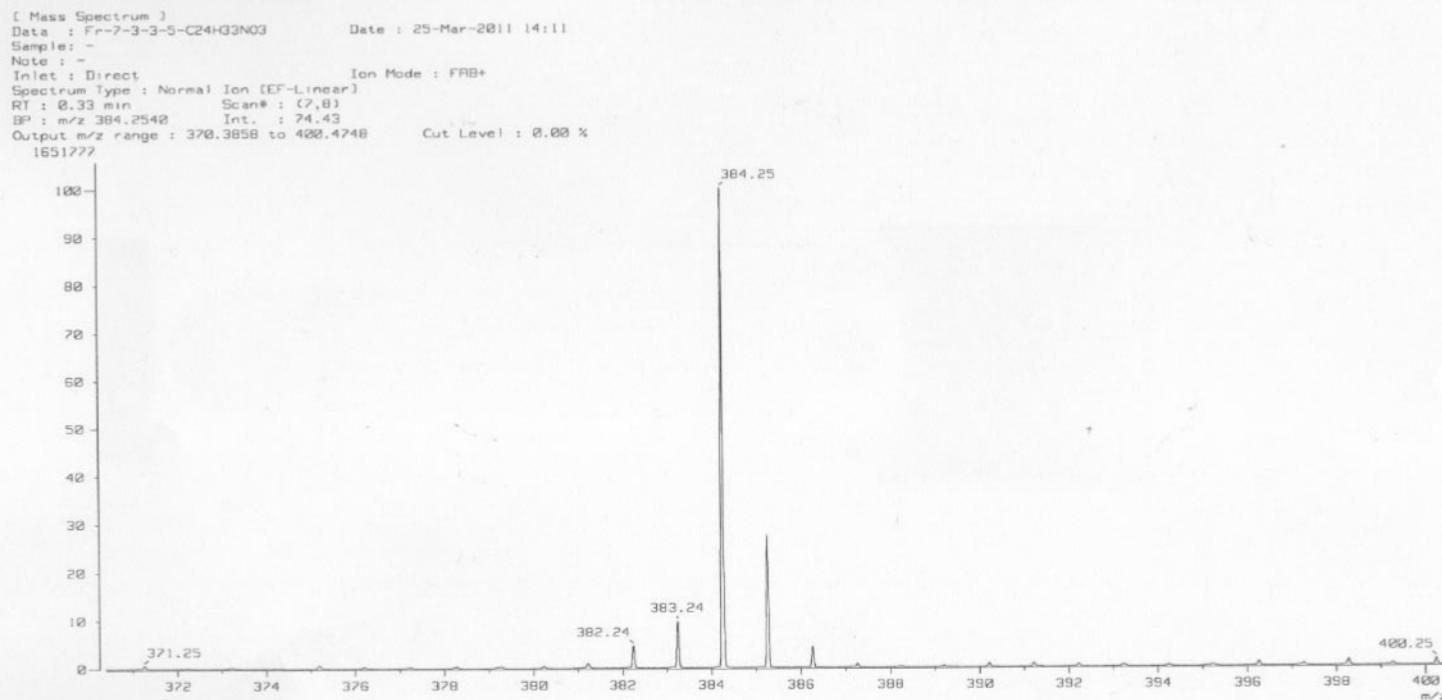
[Mass Spectrum]
Data : Fr-7-3-3-5-C24H33NO3   Date : 25-Mar-2011 14:11
Sample: -
Note : -
Inlet : Direct   Ion Mode : FAB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.33 min   Scan# : (7,8)
BP : m/z 384.2540   Int. : 74.43
Output m/z range : 370.3858 to 400.4748   Cut Level : 0.00 %

```
[ Elemental Composition ]                                        Page: 1
Data  : Fr-7-3-3-5-C24H33NO3        Date : 25-Mar-2011 14:11
Sample: -
Note : -
Inlet : Direct                      Ion Mode : FAB+
RT : 0.33 min                       Scan#: (7,8)
Elements : C 24/0, H 34/1, O 3/1, N 1/1
Mass Tolerance      : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z  Int%   Err[ppm / mmu]   U.S.  Composition
  384.2540    100.0    +0.4 /  +0.2    8.5  C 24 H 34 O 3 N

  385.2570     27.5

  405.2285     15.7

  406.2357     26.2
```

Figure S13. ^{1}H NMR spectrum of compound 2 in CDCl$_3$ (600 MHz)
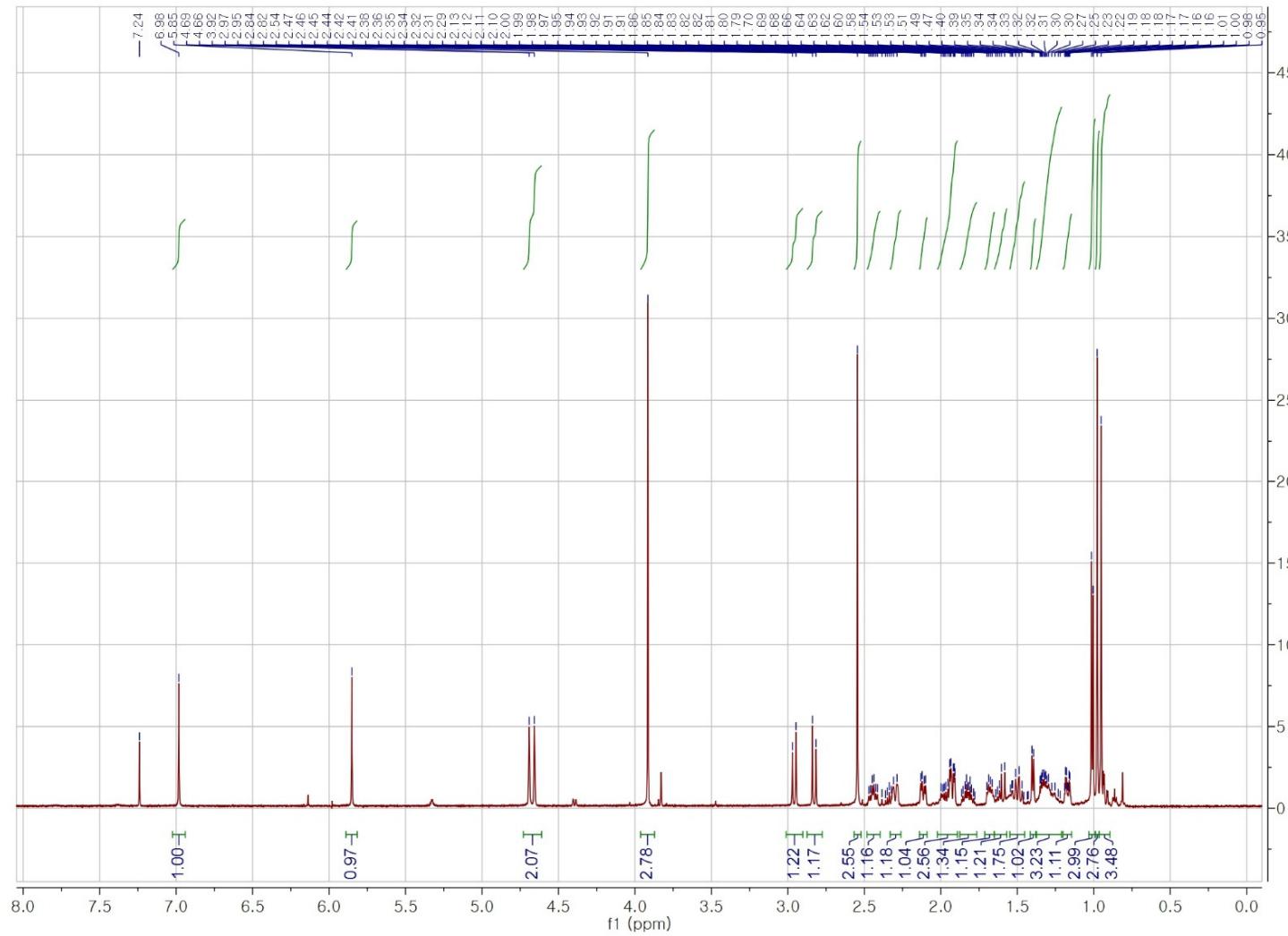
Figure S14. ^{13}C NMR spectrum of compound 2 in CDCl$_3$ (150 MHz)
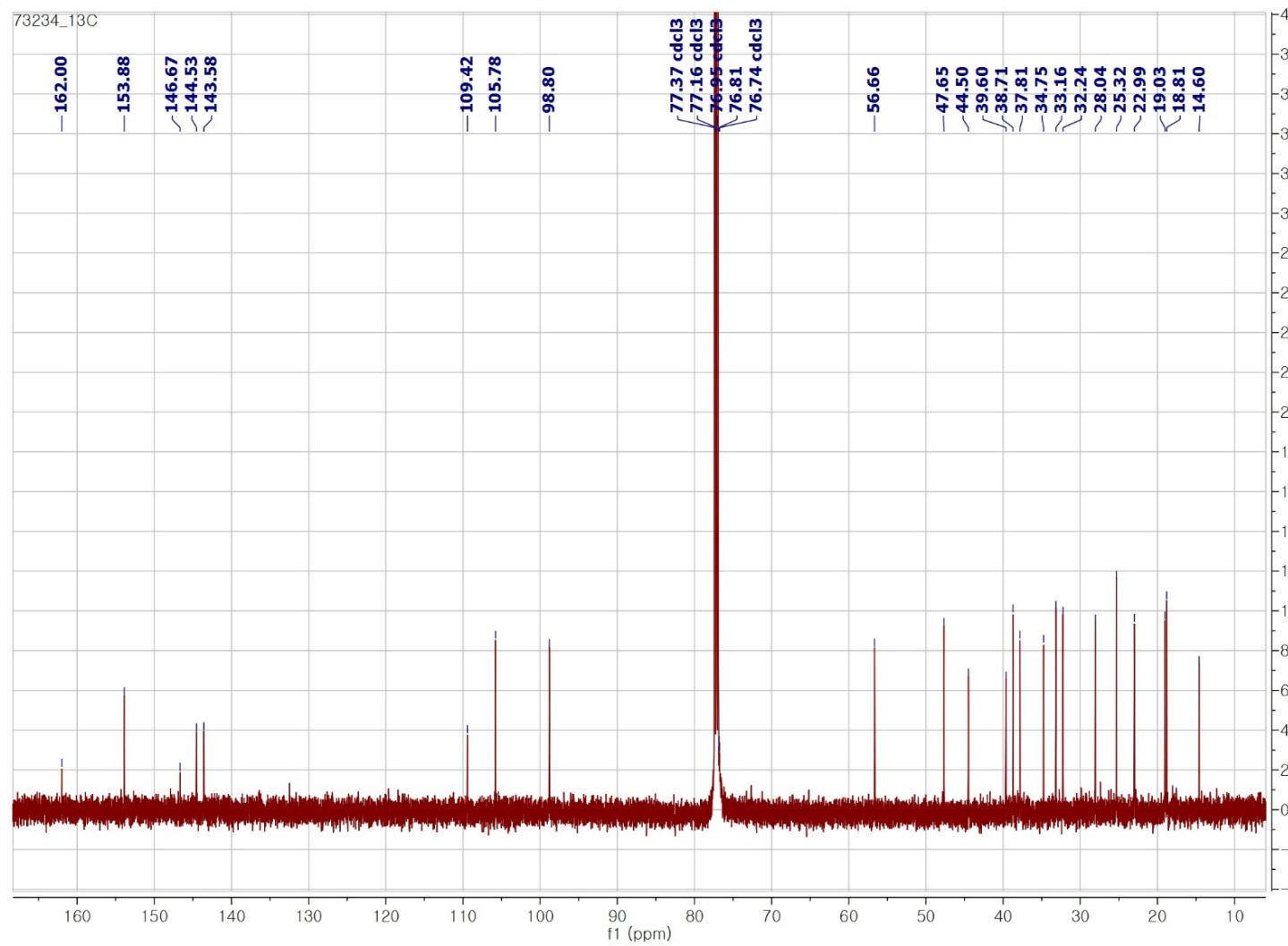
Figure S15. HSQC spectrum of compound 2 in CDCl₃
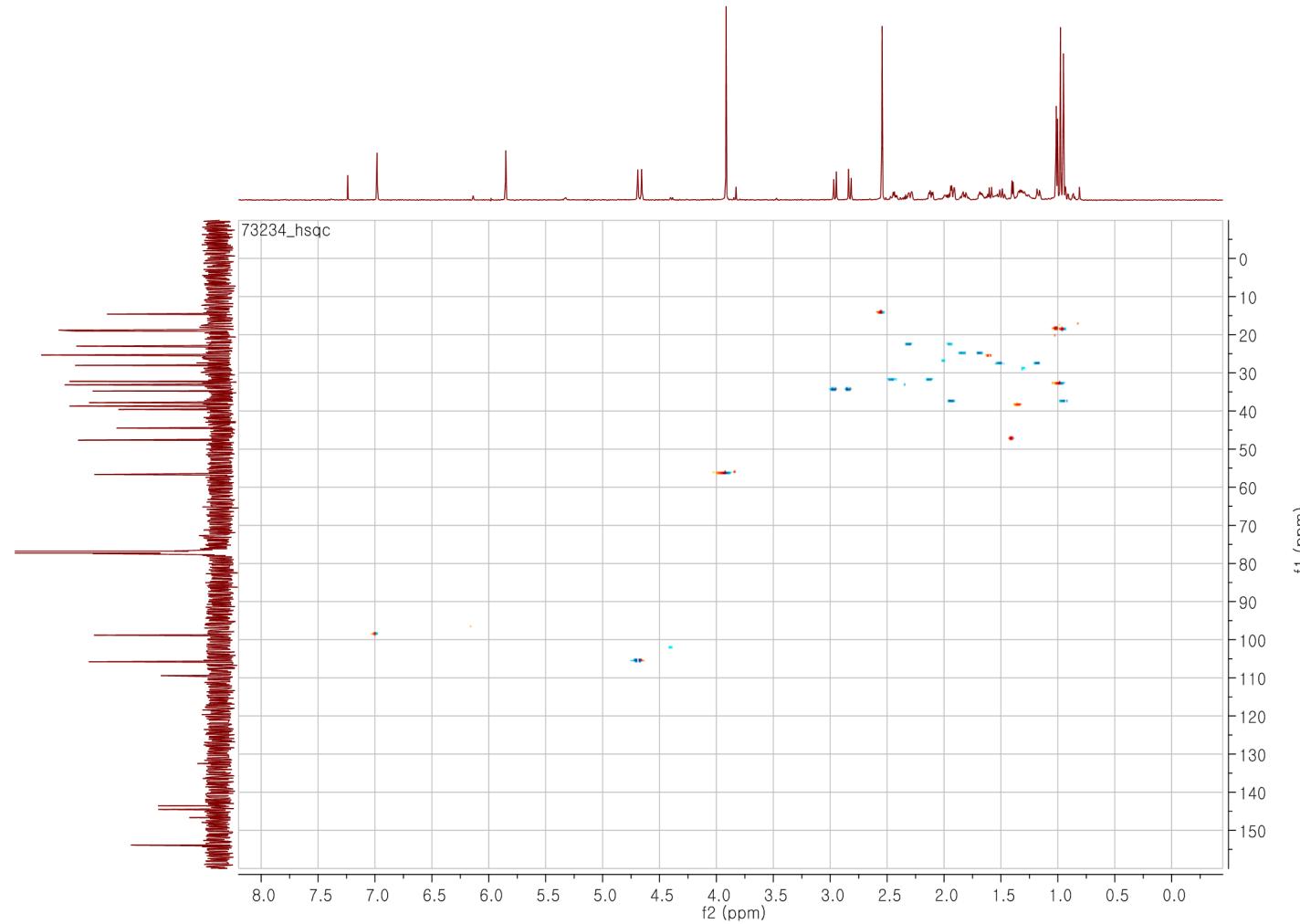
Figure S16. HMBC spectrum of compound 2 in CDCl3 and its interpretation
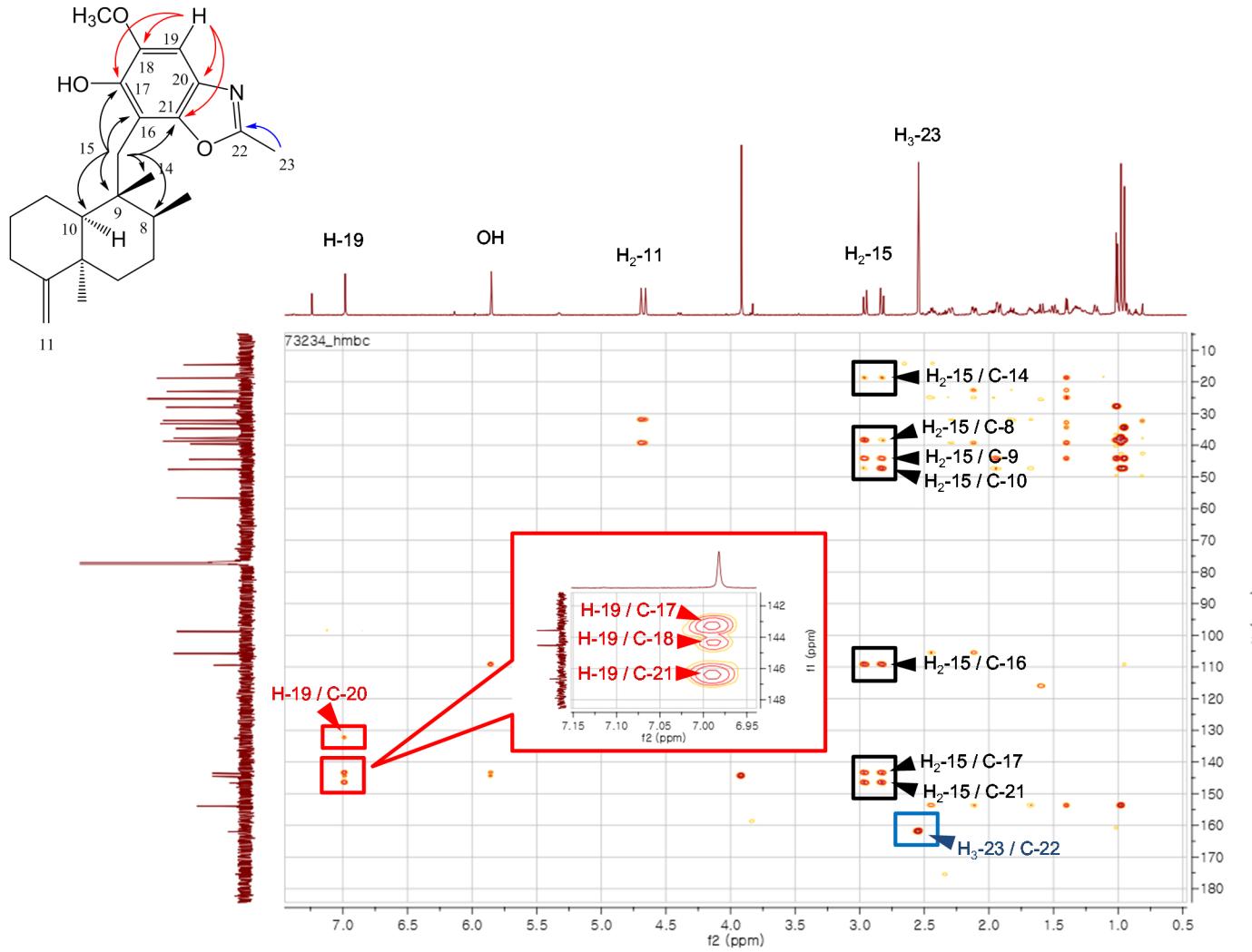
Figure S17. COSY spectrum of compound 2 in CDCl₃

73234_cosy
7-3-2-3-4
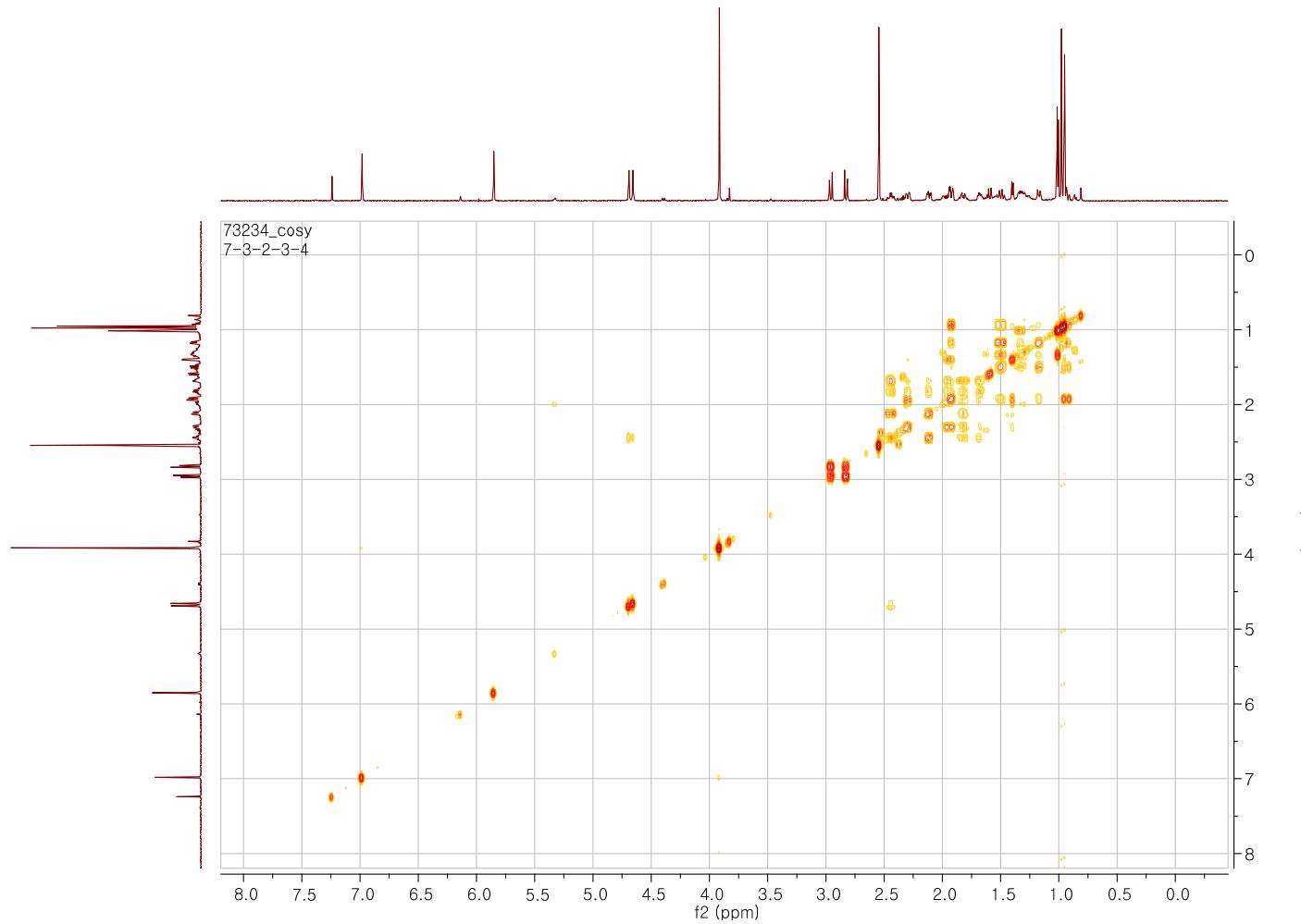
Figure S18. HRFABMS analysis of compound 2

[Mass Spectrum]
Data : Fr-7-3-2-3-4-C24H33NO3   Date : 25-Mar-2011 14:06
Sample: -
Note : -
Inlet : Direct   Ion Mode : FAB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.43 min   Scan# : (9,10)
BP : m/z 384.2542   Int. : 90.81
Output m/z range : 371.2760 to 397.9822   Cut Level : 0.00 %

```
[ Elemental Composition ]                                         Page: 1
Data  : Fr-7-3-2-3-4-C24H33NO3      Date : 25-Mar-2011 14:06
Sample: -
Note : -
Inlet : Direct                      Ion Mode : FAB+
RT : 0.43 min                       Scan#: (9,10)
Elements : C 24/0, H 34/1, O 3/1, N 1/1
Mass Tolerance      : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z Int%   Err[ppm / mmu]   U.S.  Composition
  383.2462   13.6    +0.4 /  +0.1    9.0   C 24 H 33 O 3 N

  384.2542  100.0    +0.7 /  +0.3    8.5   C 24 H 34 O 3 N

  385.2605   28.0

  398.2696   10.4
```

Figure S19. ^{1}H NMR spectrum of a mixture of compounds 3 and 4 in CDCl$_3$ (600 MHz)
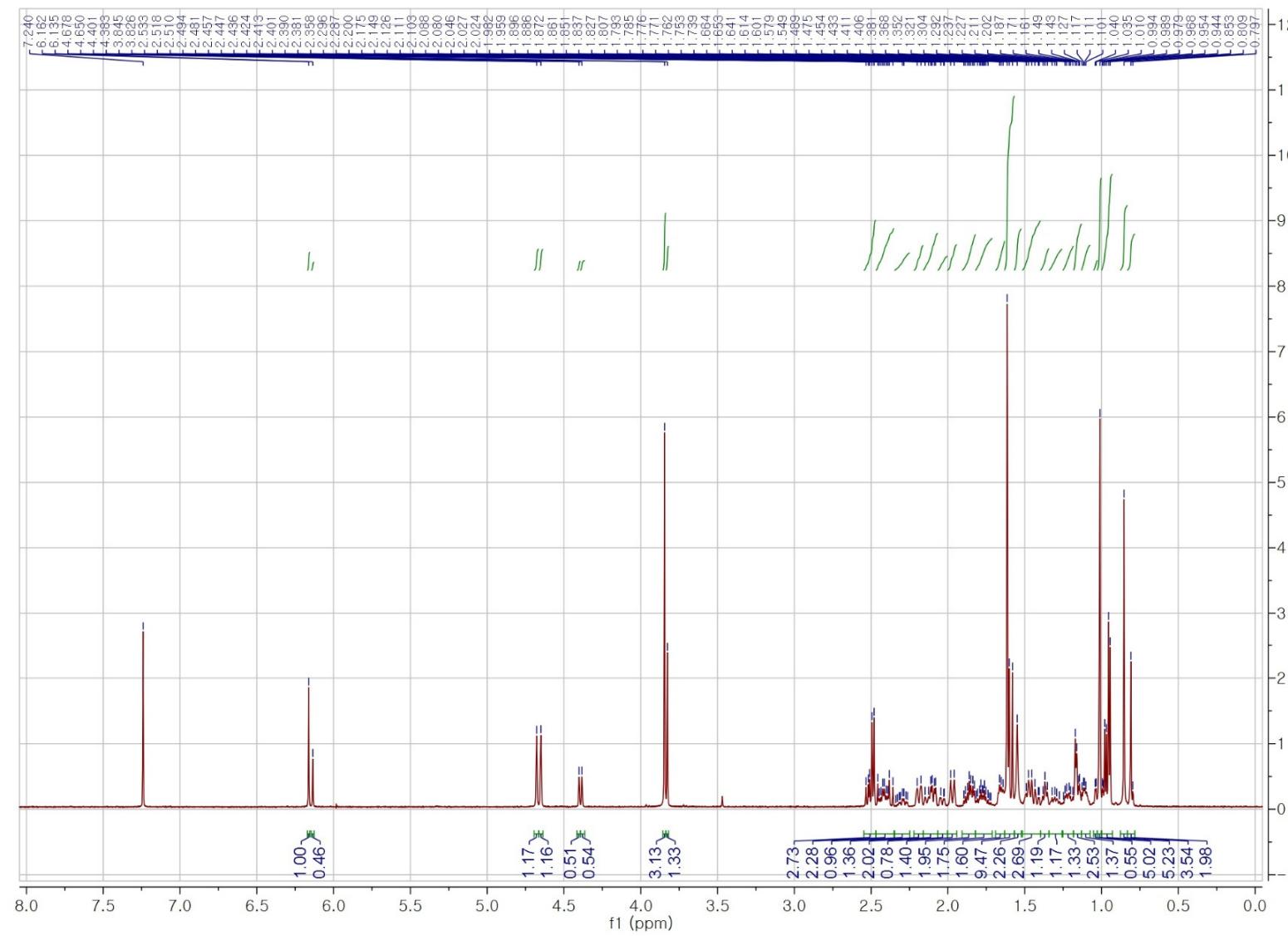
Figure S20. ^{13}C NMR spectrum of a mixture of compounds **3** and **4** in CDCl$_3$ (150 MHz)
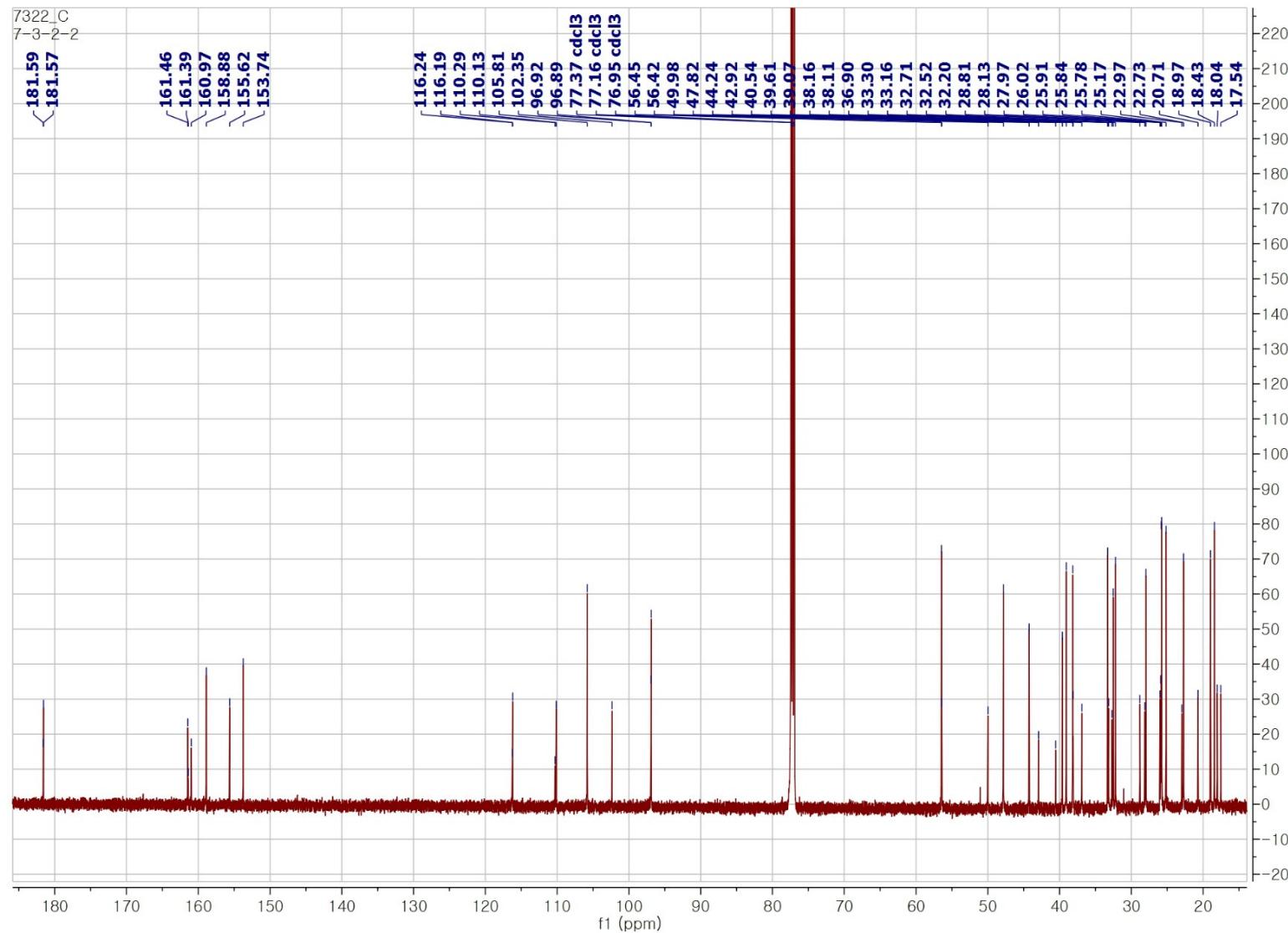
Figure S21. HSQC spectrum of a mixture of compounds 3 and 4 in CDCl₃

7322_HSQC
7-3-2-2
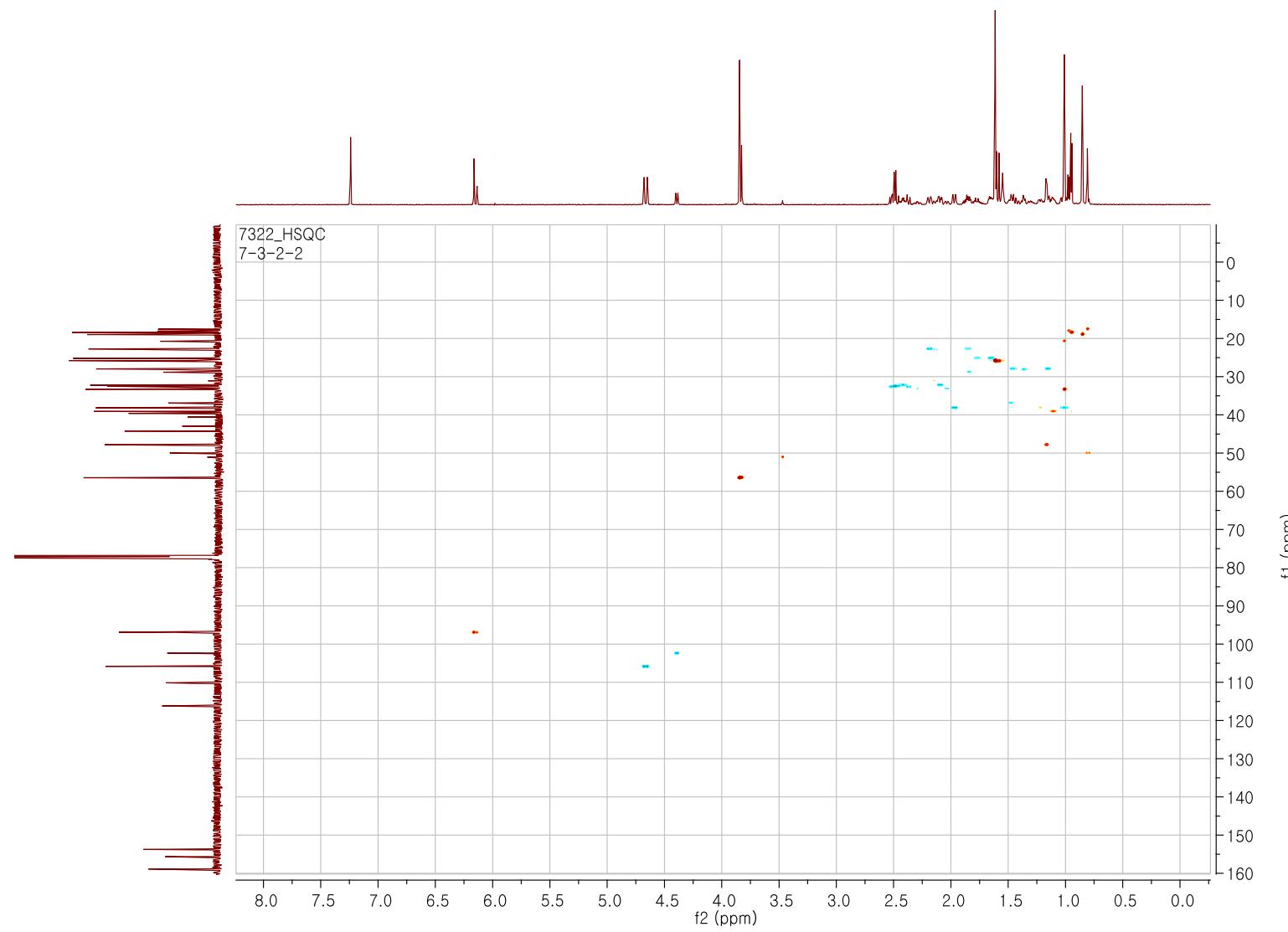
Figure S22. HMBC spectrum of a mixture of compounds 3 and 4 in CDCl₃ and its inspection
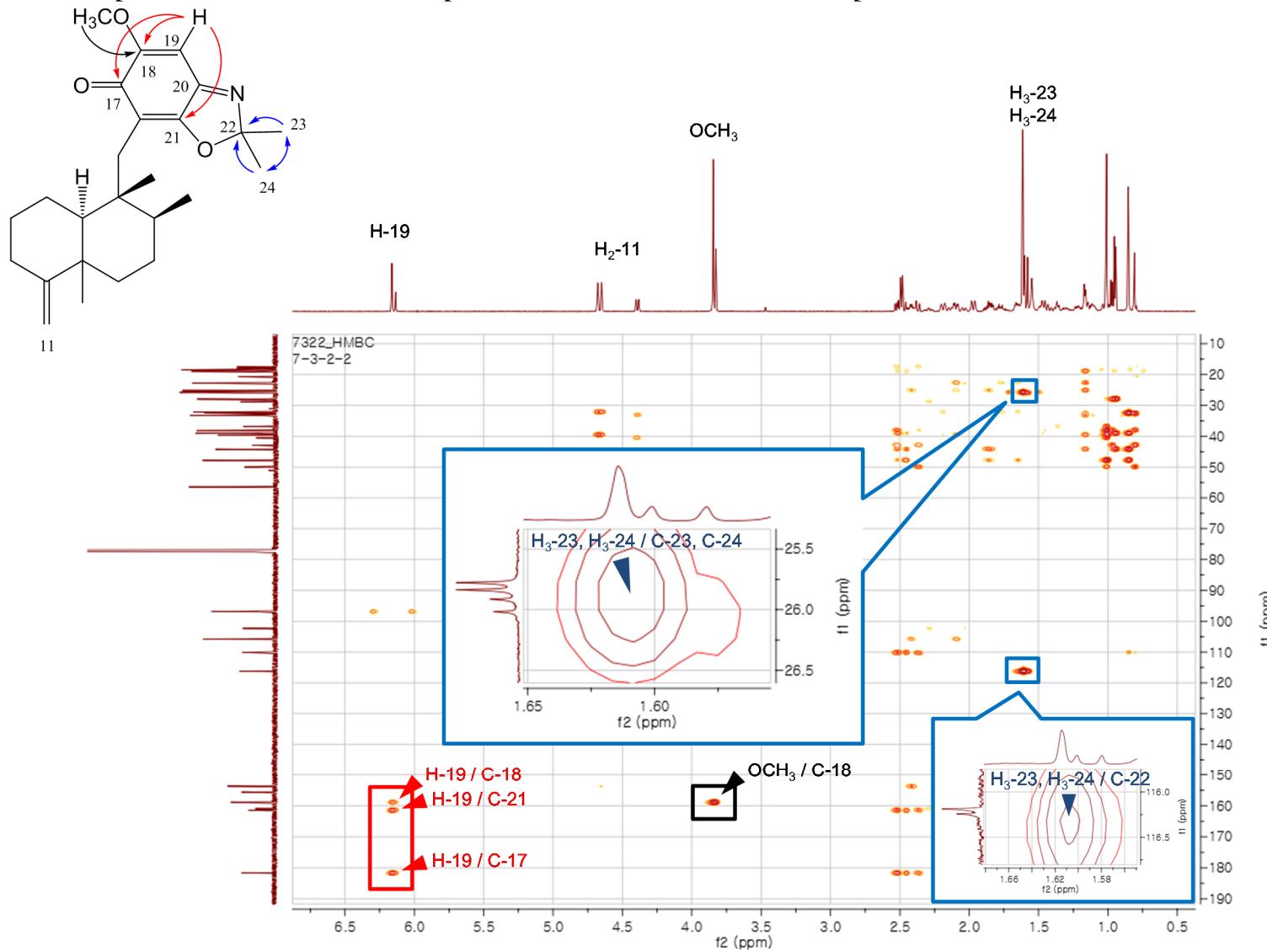
Figure S23. COSY spectrum of a mixture of compounds 3 and 4 in CDCl₃
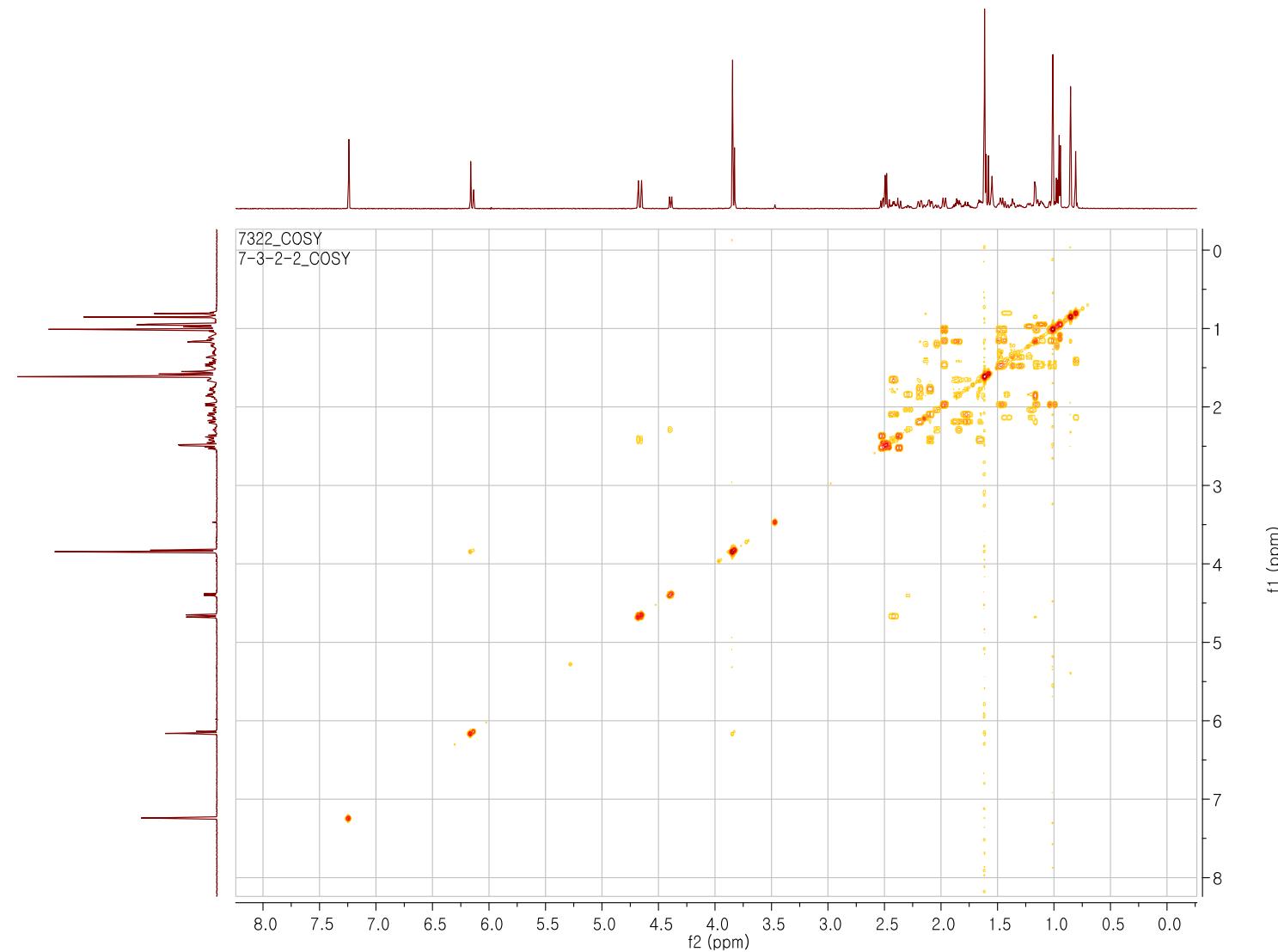
Figure S24. HRFABMS analysis of a mixture of compounds 3 and 4

[Mass Spectrum]
Data : Fr-7-3-2-2-C25H35NO3   Date : 25-Mar-2011 14:02
Sample: -
Note : -
Inlet : Direct   Ion Mode : FAB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.23 min   Scan# : (5,6)
BP : m/z 398.2696   Int. : 90.01
Output m/z range : 383.9911 to 412.2997   Cut Level : 0.00 %

```
[ Elemental Composition ]                                          Page: 1
Data   : Fr-7-3-2-3-4-C24H33NO3        Date : 25-Mar-2011 14:06
Sample: -
Note : -
Inlet : Direct                         Ion Mode : FAB+
RT : 0.43 min                          Scan#: (9,10)
Elements : C 24/0, H 34/1, O 3/1, N 1/1
Mass Tolerance     : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z Int%   Err[ppm / mmu]   U.S.  Composition
  383.2462   13.6     +0.4 /  +0.1    9.0  C 24 H 33 O 3 N

  384.2542   100.0    +0.7 /  +0.3    8.5  C 24 H 34 O 3 N

  385.2605   28.0

  398.2696   10.4
```

Figure S25. ^{1}H NMR spectrum of compound 5 in CDCl$_3$ (600 MHz)
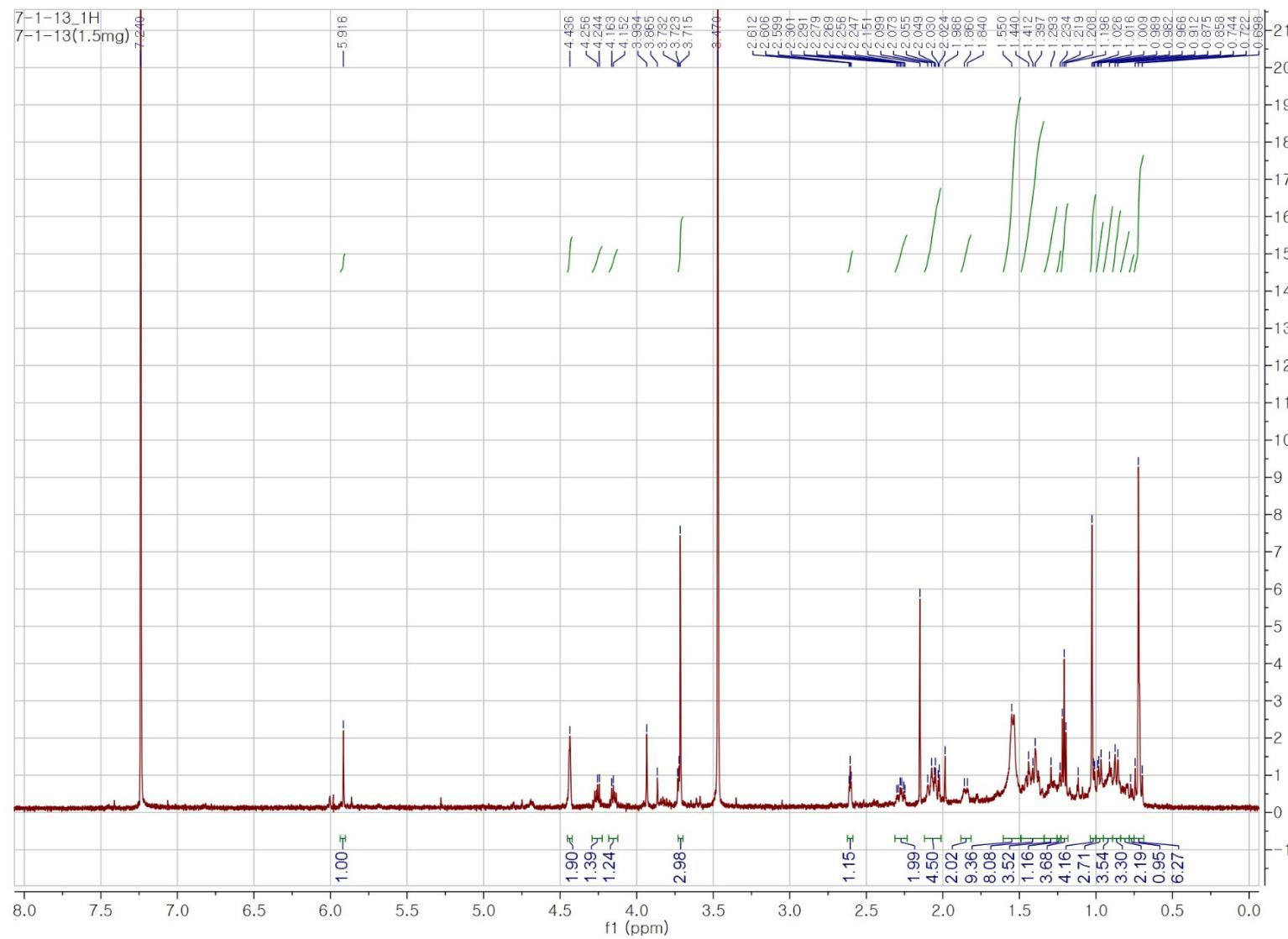
Figure S26. ¹³C NMR spectrum of compound 5 in CDCl₃ (150 MHz)
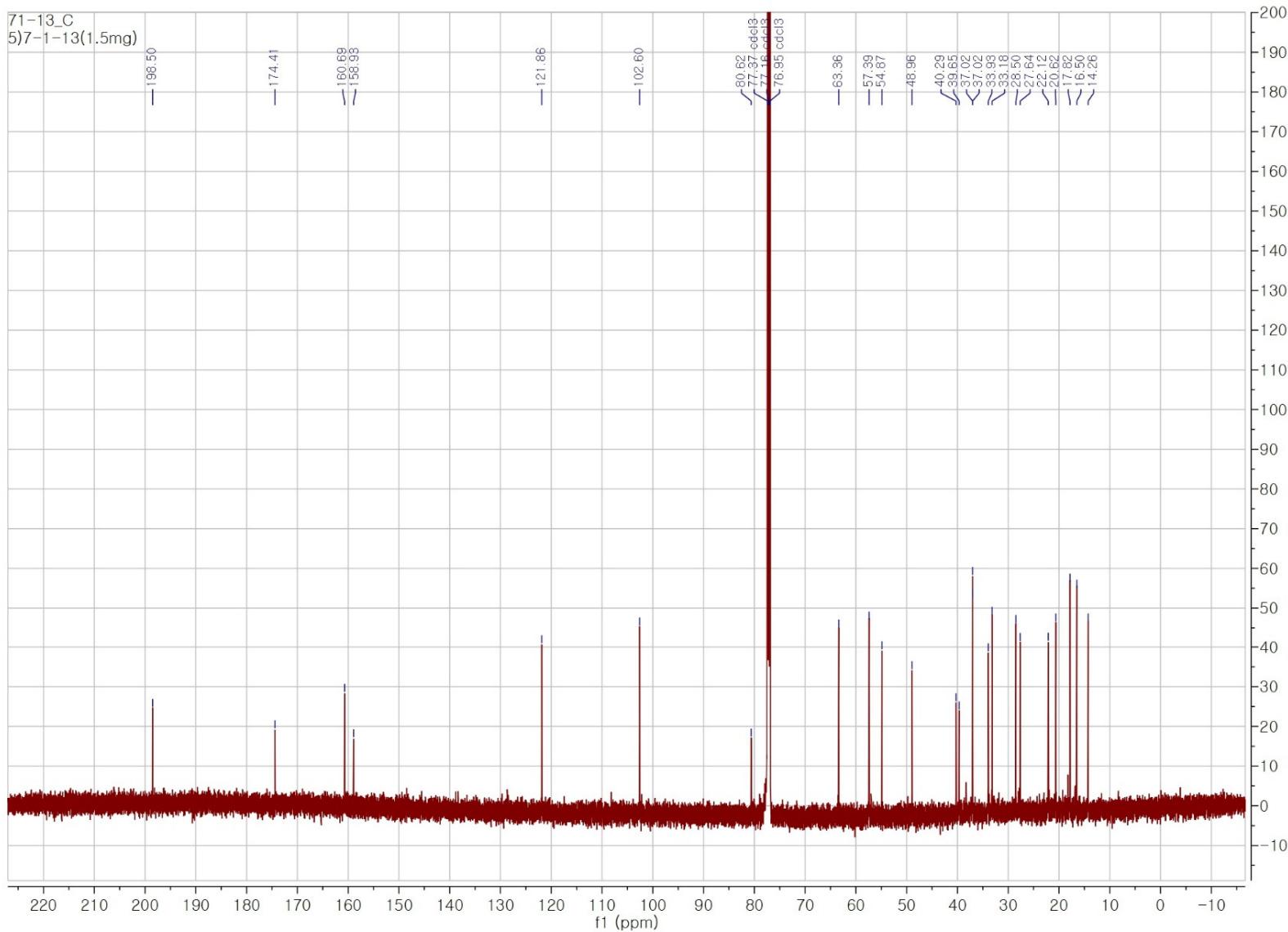
Figure S27. HSQC spectrum of compound 5 in CDCl₃
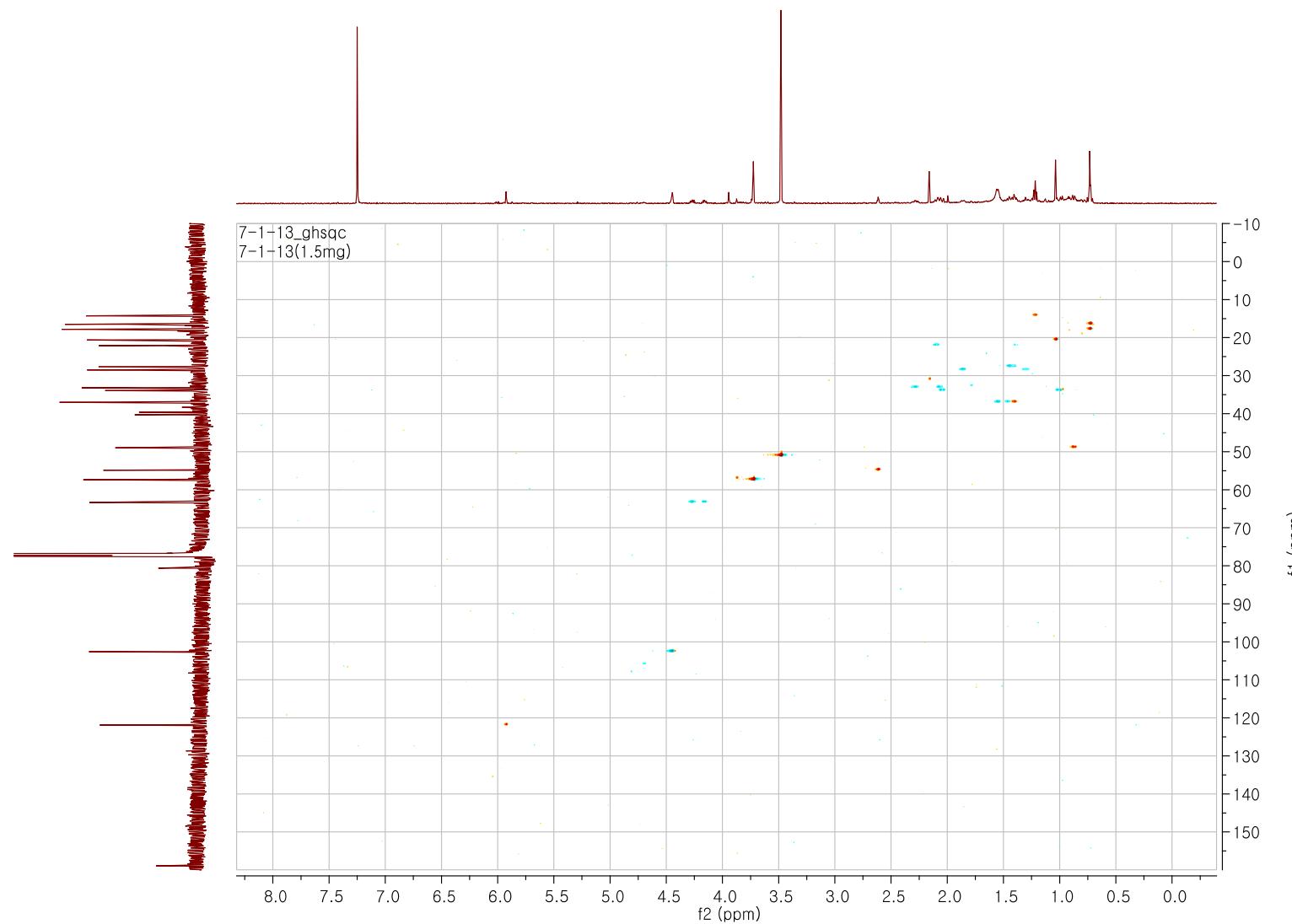
Figure S28. HMBC spectrum of compound 5 in CDCl₃
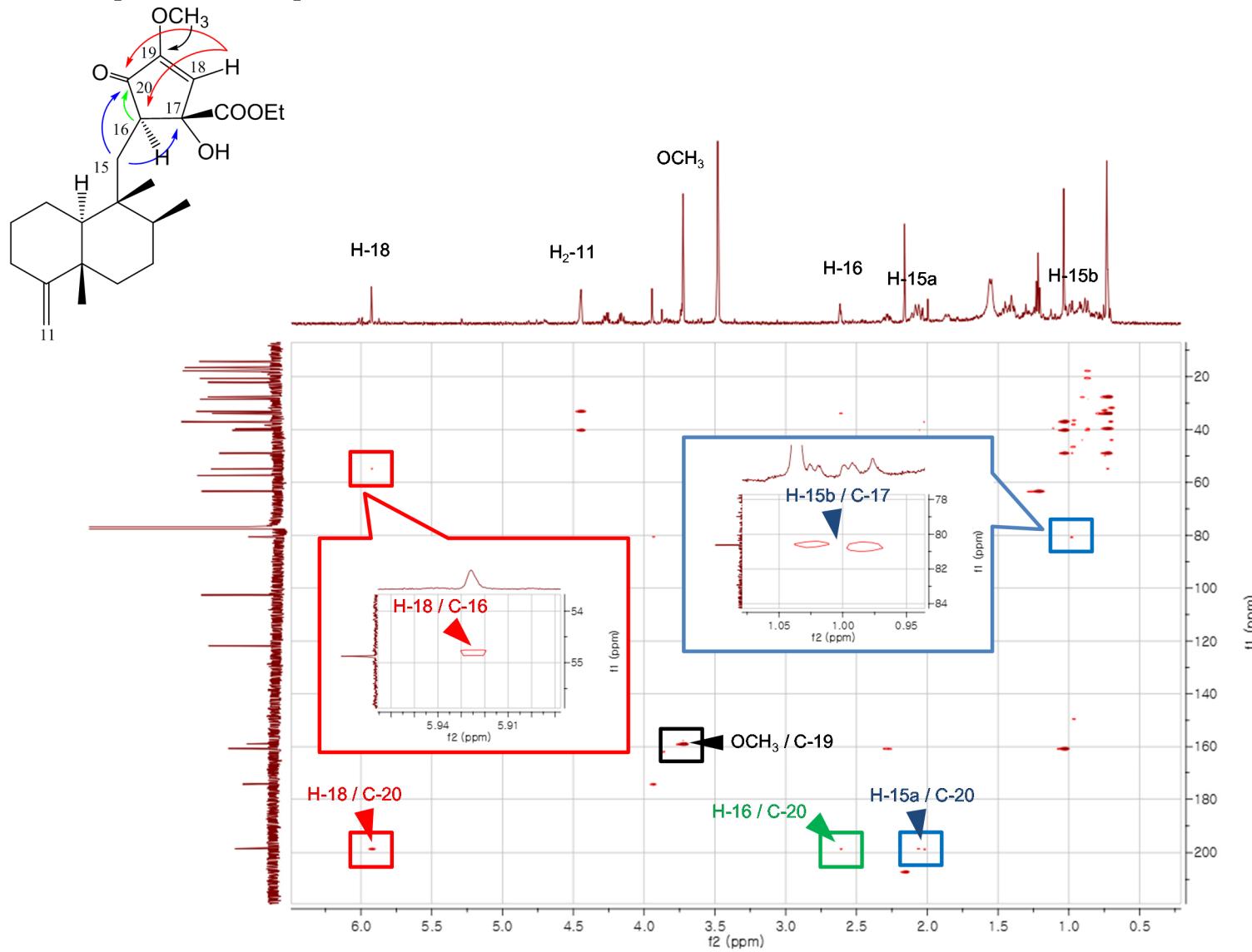
Figure S29. COSY spectrum of compound 5 in CDCl₃
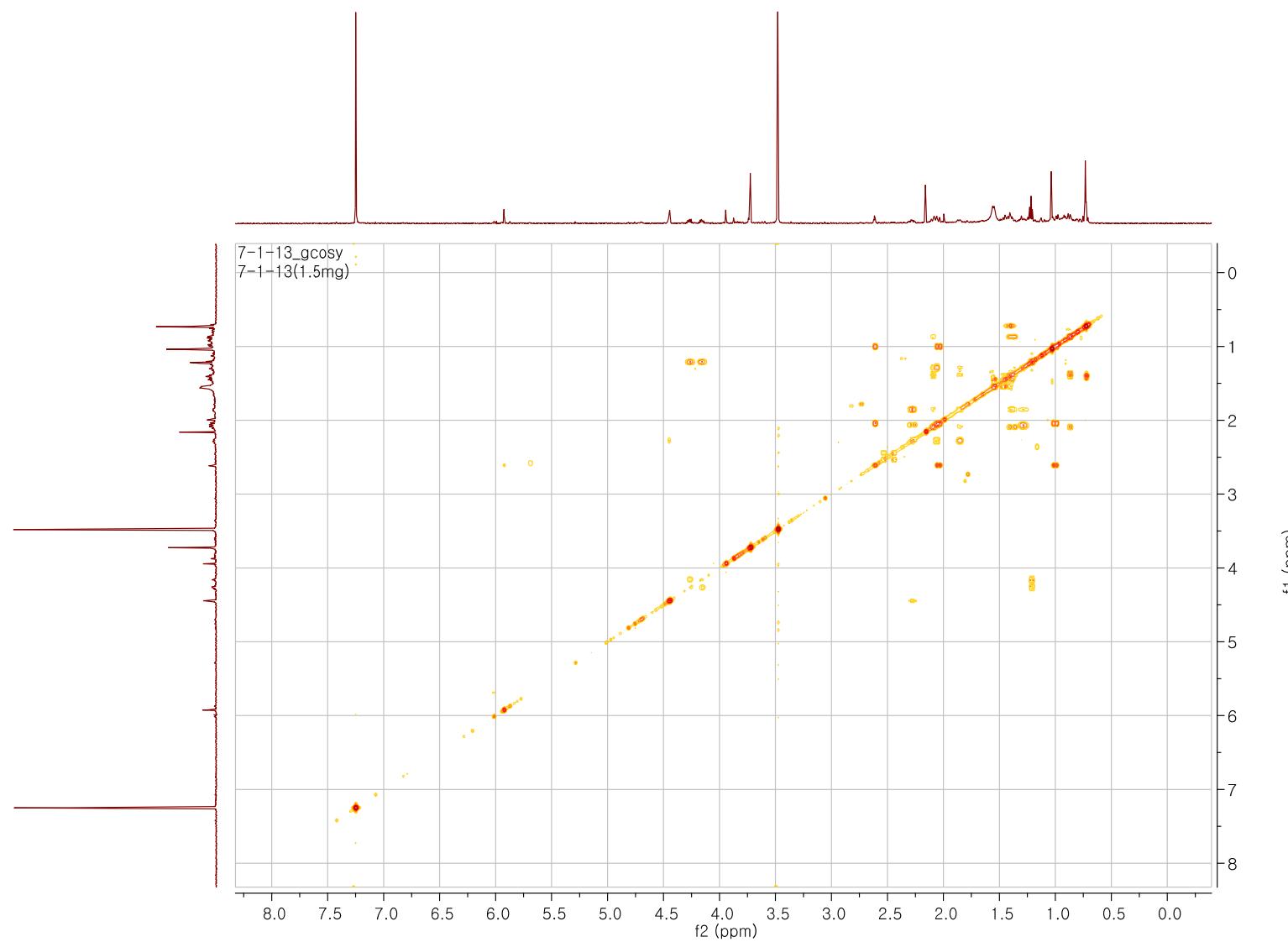
Figure S30. NOESY spectrum of compound 5 in CDCl₃
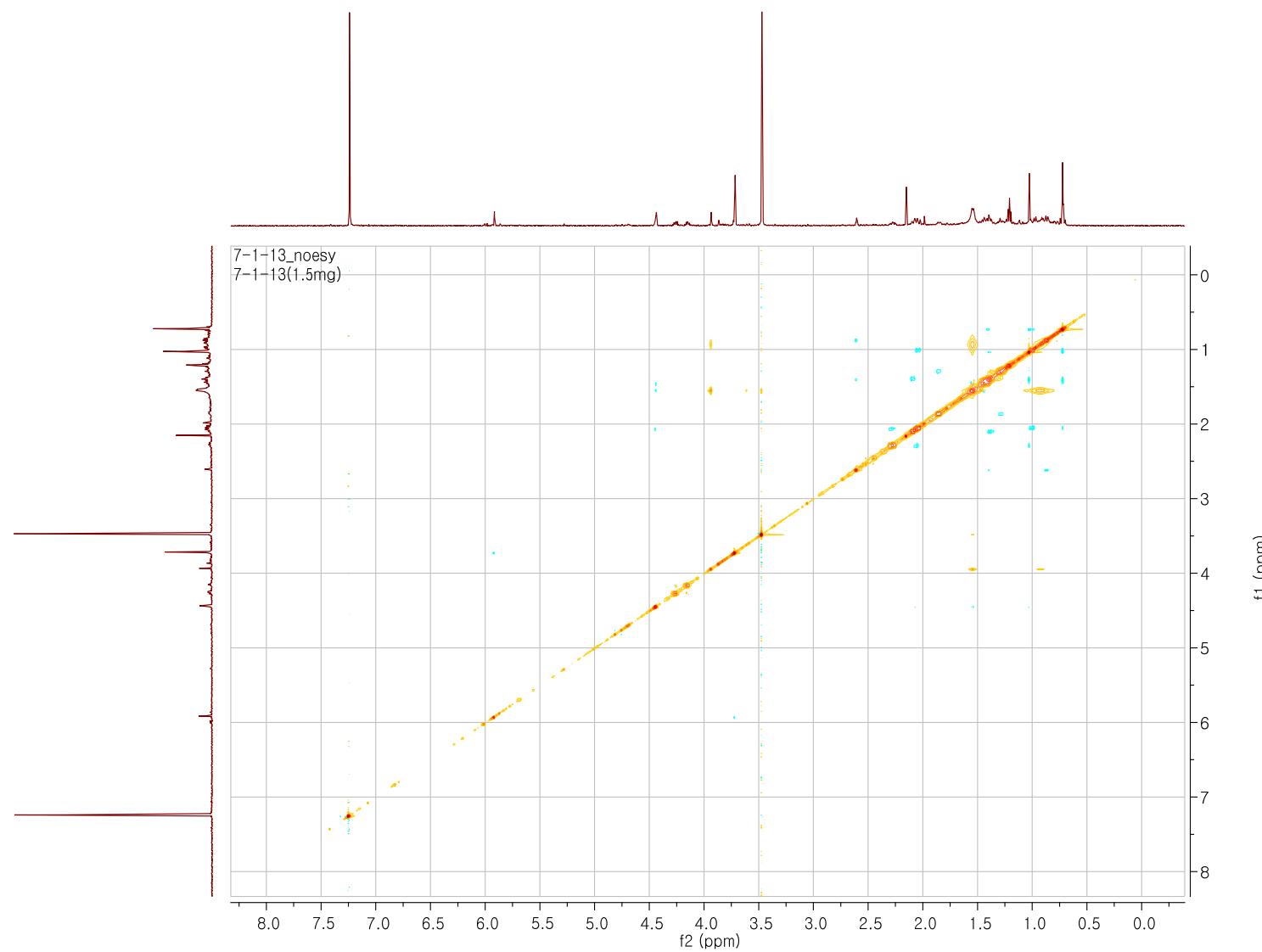
Figure S31. HRFABMS analysis of compound 5

[Mass Spectrum]
Data : Fr-7-1-13-C24H36O5   Date : 17-Mar-2011 13:56
Sample: -
Note : -
Inlet : Direct   Ion Mode : FAB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.53 min   Scan# : (11,12)
BP : m/z 427.2464   Int. : 80.61
Output m/z range : 401.6469 to 437.0772   Cut Level : 0.00 %
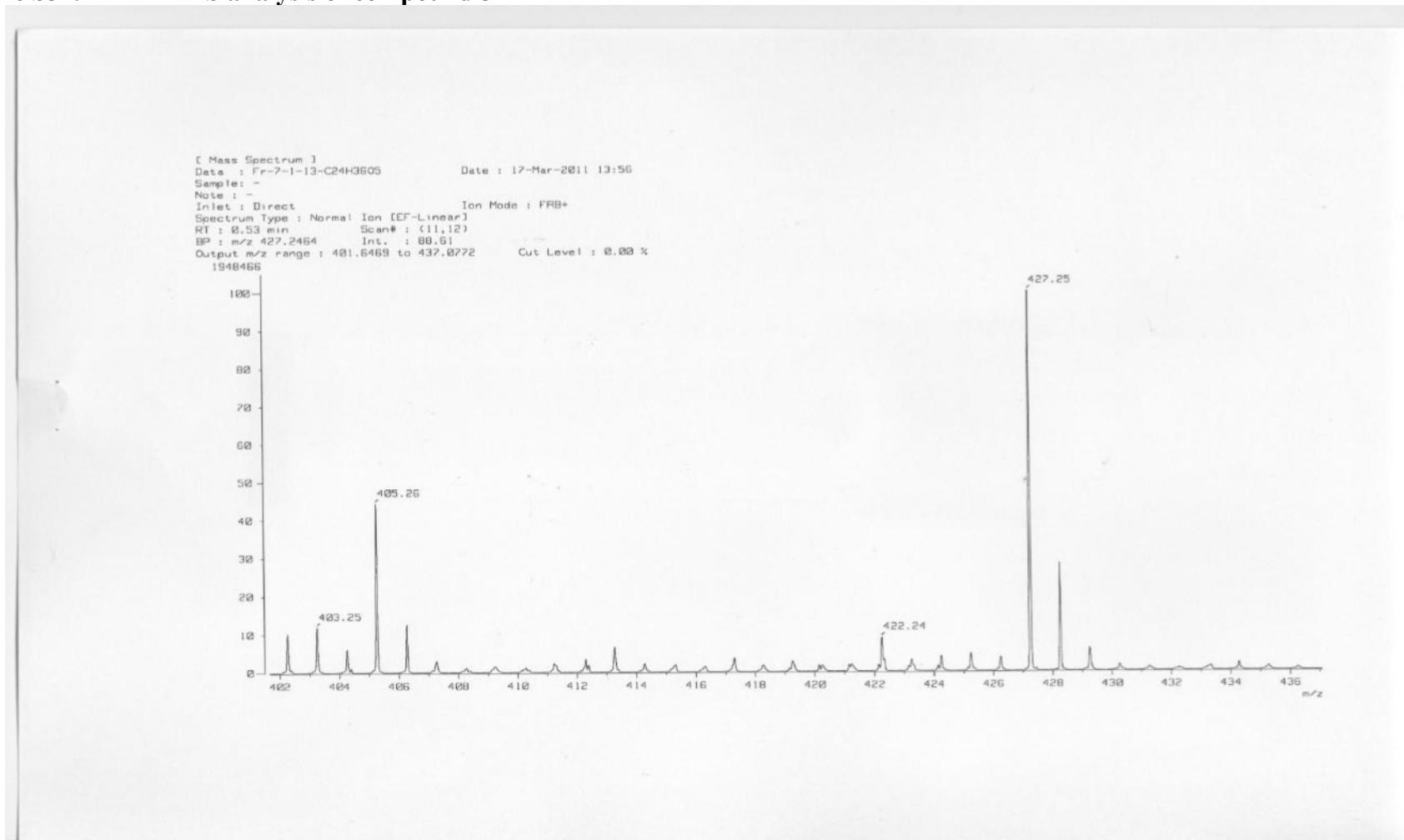
```
[ Elemental Composition ]
Data  : Fr-7-1-13-C24H36O5          Date : 17-Mar-2011 13:56
Sample: -
Note : -
Inlet : Direct                     Ion Mode : FAB+
RT : 0.53 min                      Scan#: (11,12)
Elements : C 24/0, H 36/1, O 5/1, Na 1/1
Mass Tolerance    : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0
```

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
355.2250	10.0	+0.3 / +0.1	5.5	C 21 H 32 O 3 Na
357.2041	12.1	-0.1 / +0.0	5.5	C 20 H 30 O 4 Na
369.2438	59.4			
370.2435	16.5			
385.2377	15.2	+5.8 / +2.3	5.5	C 22 H 34 O 4 Na
387.2525	88.9	+3.5 / +1.4	4.5	C 22 H 36 O 4 Na
388.2535	24.8			
388.3937	80.1			
389.3974	23.8			
391.2845	10.3			
396.3853	90.1			
397.3874	24.2			
400.2617	25.3			
402.2593	10.2			
403.2501	12.0			
405.2638	44.4			
406.2693	12.6			
427.2464	100.0	+0.8 / +0.4	6.5	C 24 H 36 O 5 Na
428.2478	28.2			

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Figure S32. ^{1}H NMR spectrum of a mixture of compounds 6 and 7 in CDCl$_3$ (600 MHz)
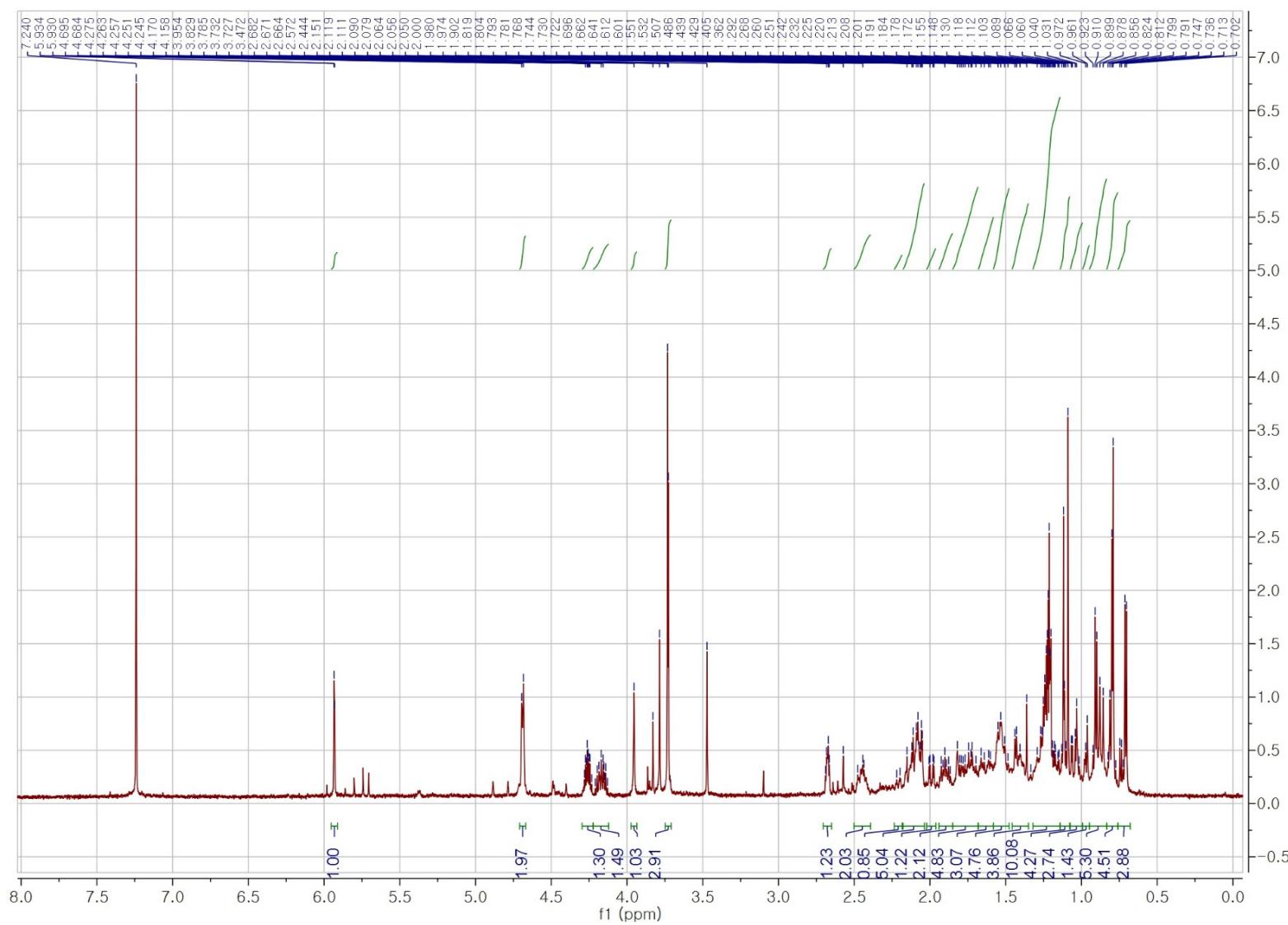
Figure S33. ^{13}C NMR spectrum of a mixture of compounds 6 and 7 CDCl$_3$ (150 MHz)
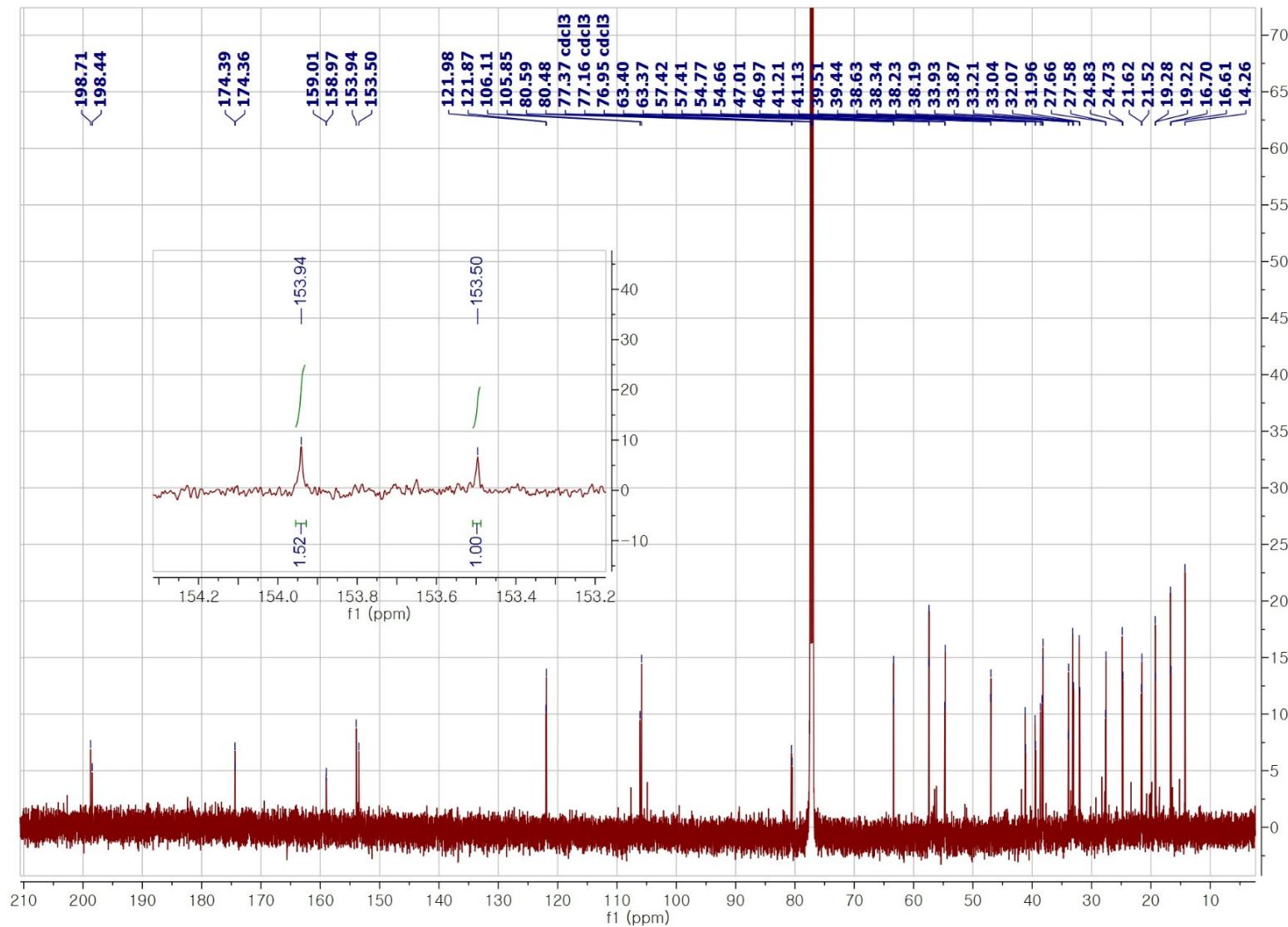
Figure S34. HSQC spectrum of a mixture of compounds 6 and 7 in CDCl₃
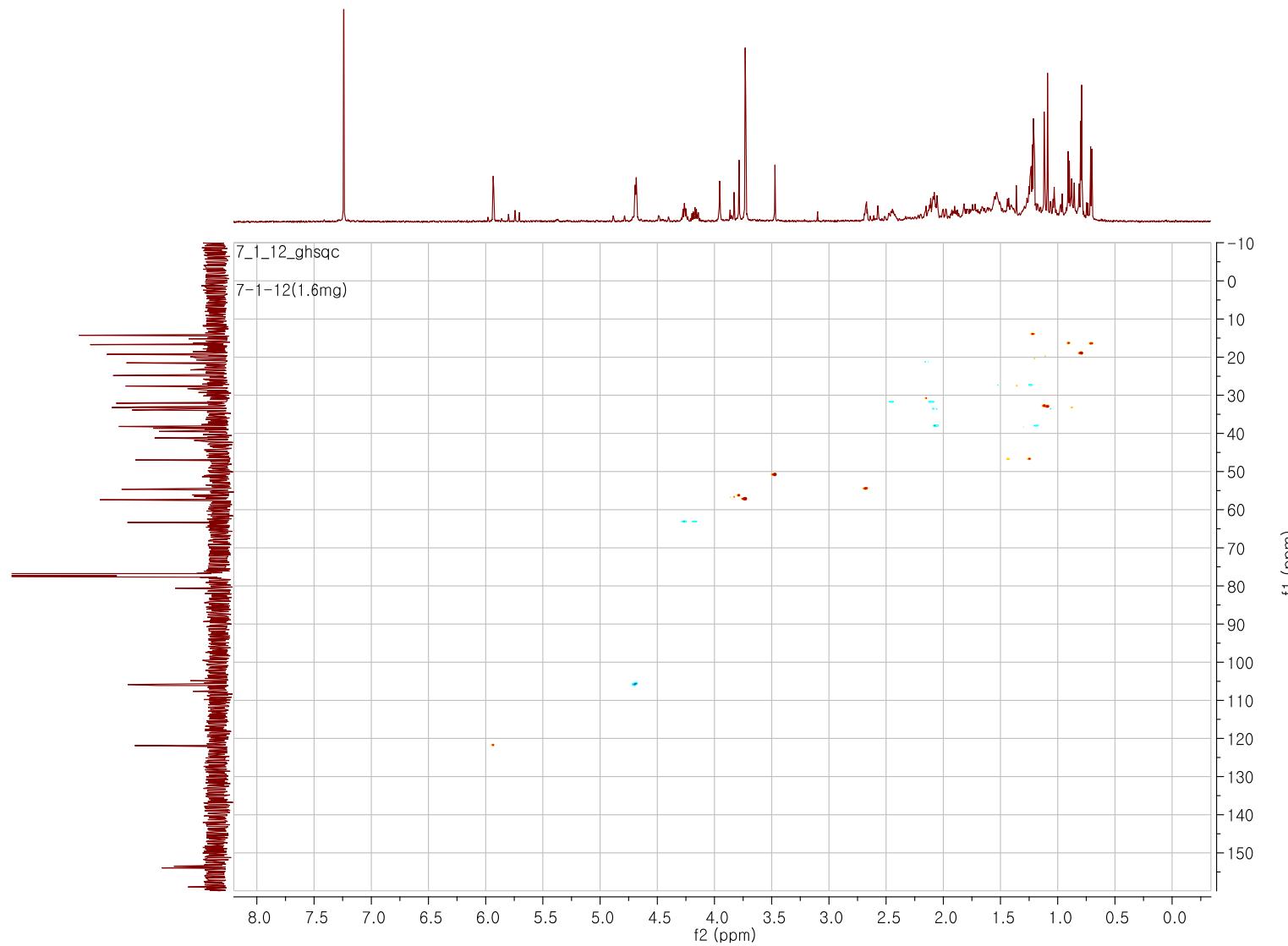
Figure S35. HMBC spectrum of a mixture of compounds 6 and 7 in CDCl₃ and its interpretation
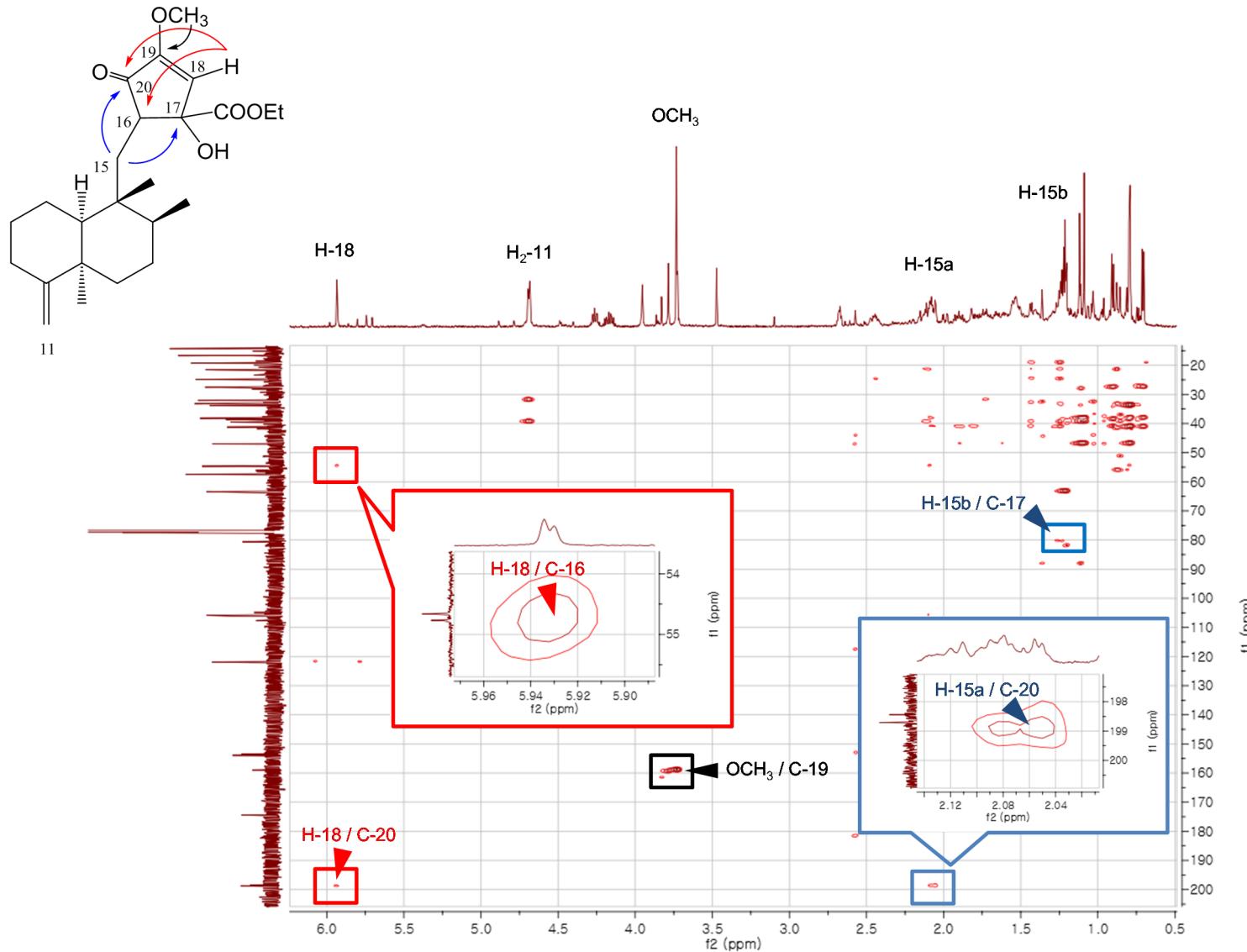
Figure S36. COSY spectrum of a mixture of compounds 6 and 7 in CDCl₃

7_1_12_gcosy

7-1-12(1.6mg)
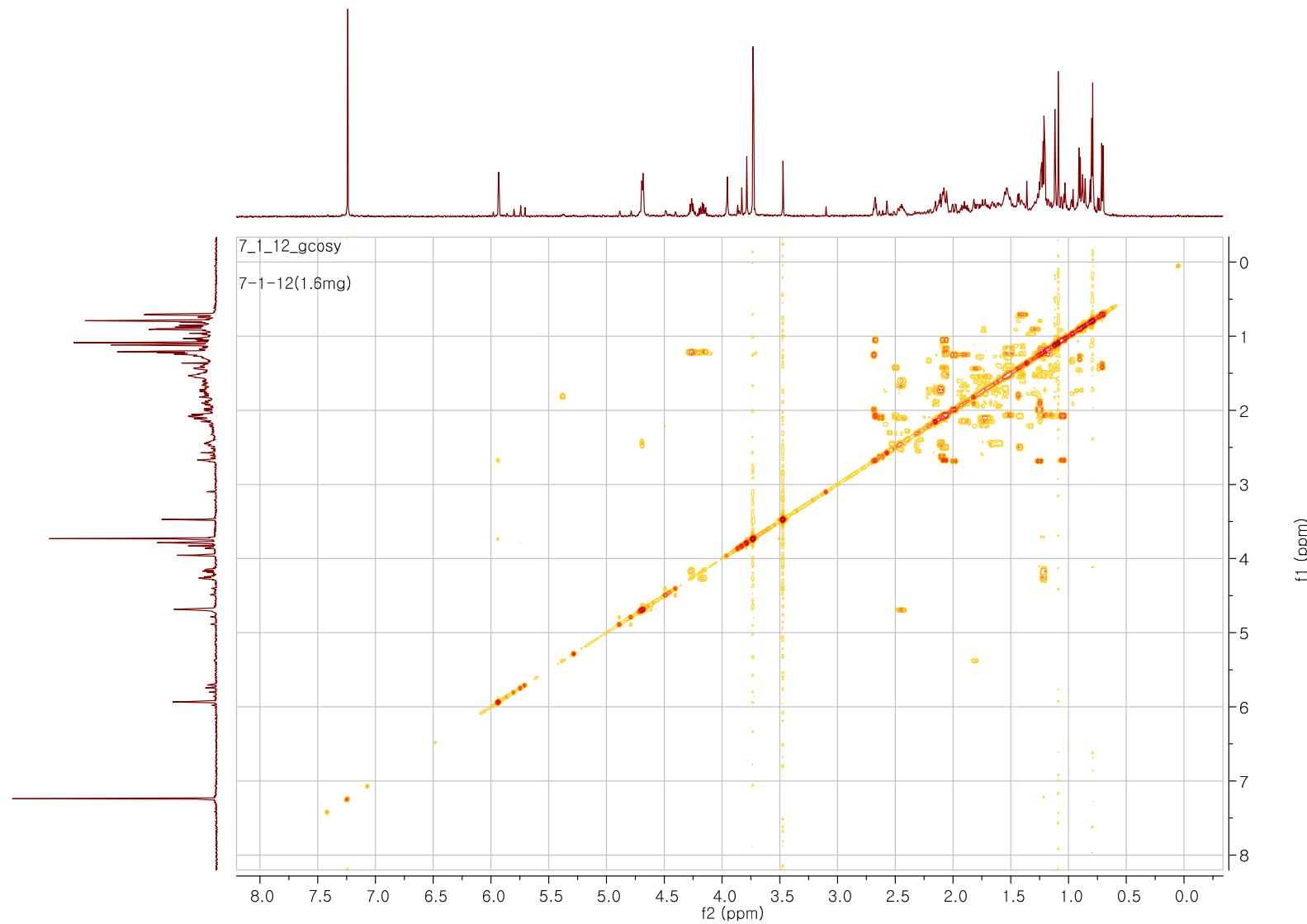
Figure S37. NOESY spectrum of a mixture of compounds 6 and 7 in CDCl₃

7_1_12_noesy

7-1-12(1.6mg)
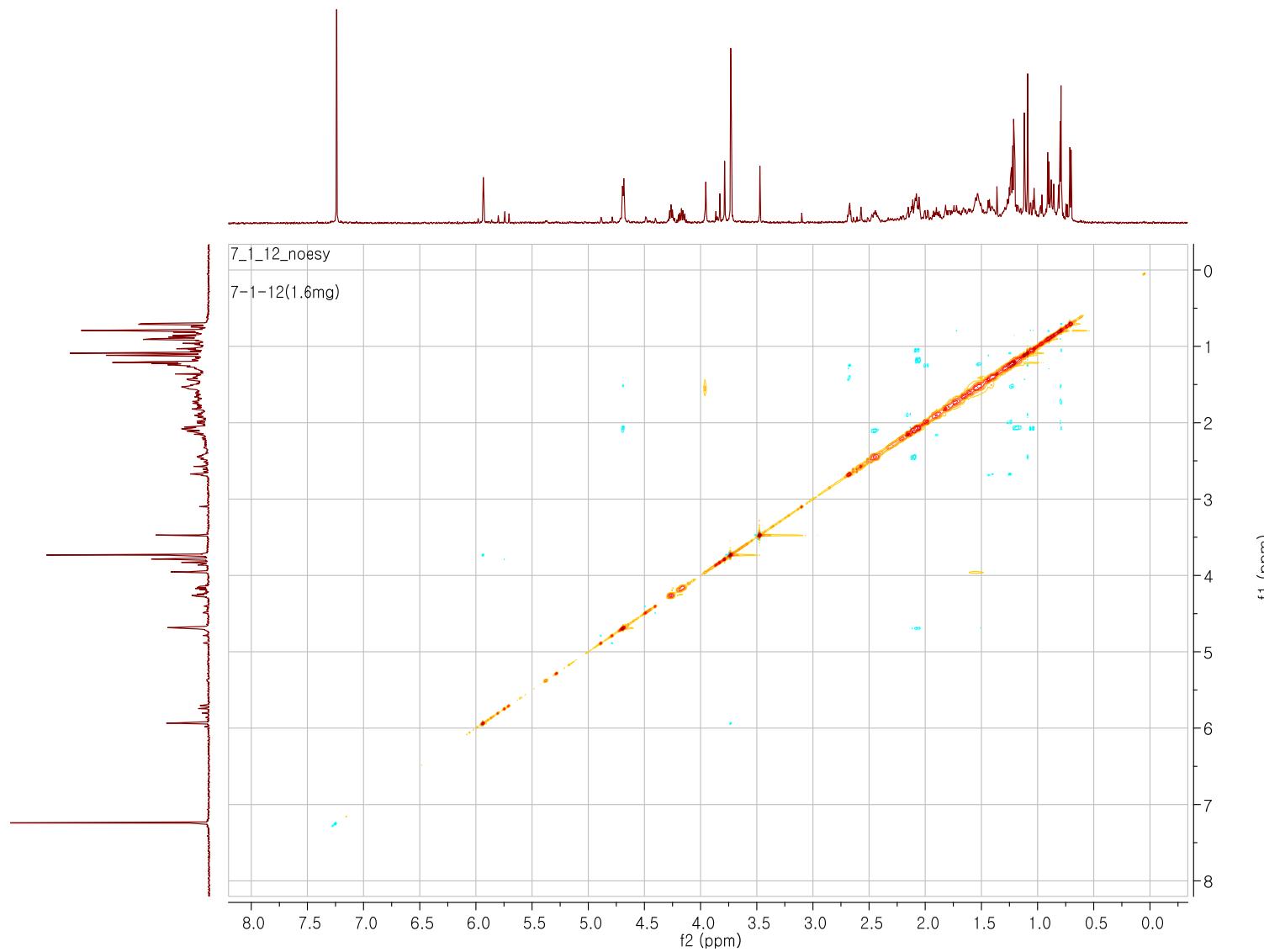
Figure S38. HRFABMS analysis of mixture of compounds 6 and 7
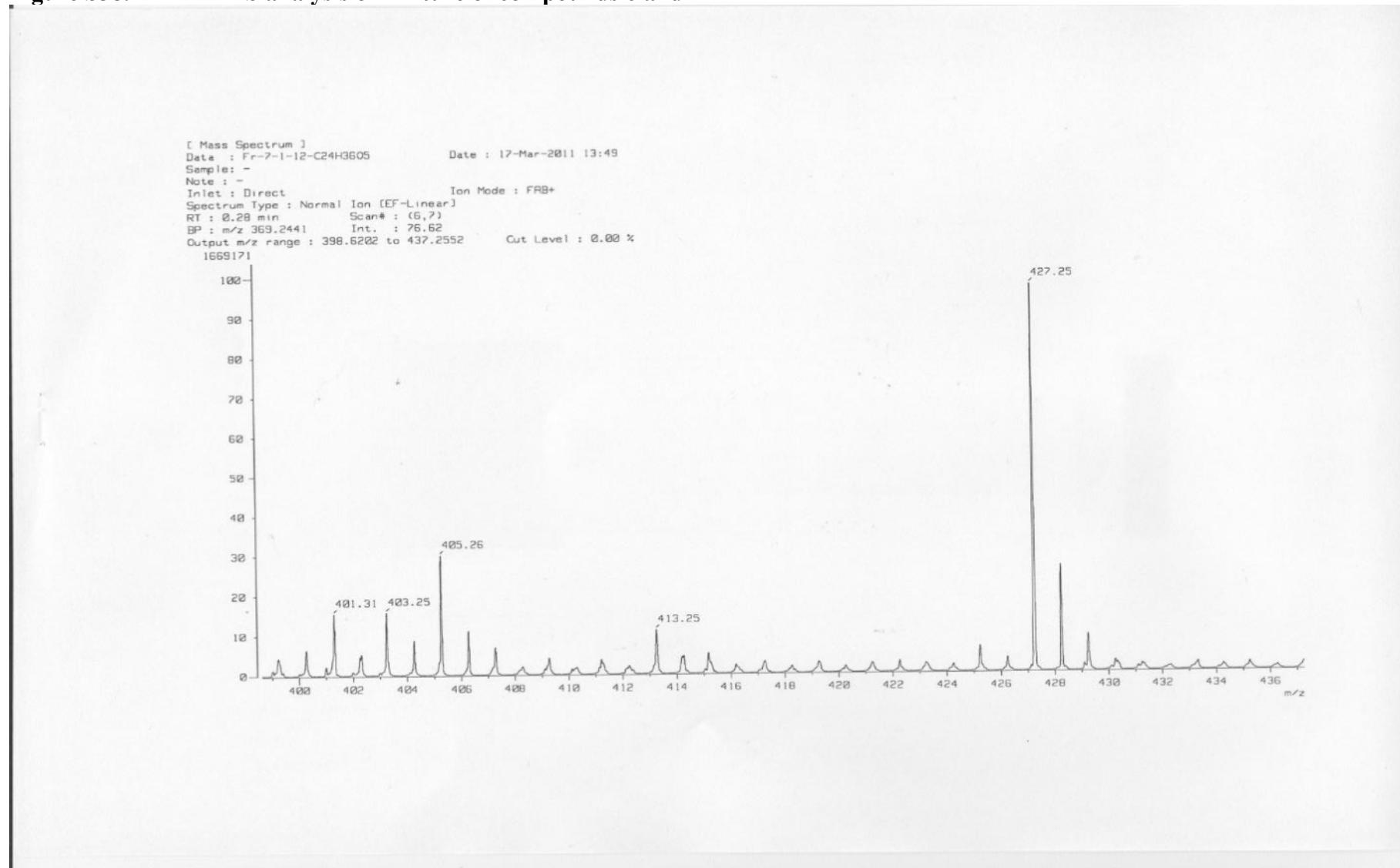
[Elemental Composition]
Data : Fr-7-1-12-C24H36O5   Date : 17-Mar-2011 13:49
Sample: -
Note : -
Inlet : Direct   Ion Mode : FAB+
RT : 0.28 min   Scan#: (6,7)
Elements : C 24/0, H 37/1, O 5/1
Mass Tolerance   : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
369.2441	100.0	+3.1 / +1.1	8.5	C 24 H 33 O 3
370.2496	29.0	-3.2 / -1.2	8.0	C 24 H 34 O 3
371.2286	13.0			
373.2374	10.1	-1.2 / -0.5	7.5	C 23 H 33 O 4
375.2265	10.2			
379.1929	12.3	+5.1 / +1.9	11.5	C 24 H 27 O 4
387.2527	94.3	-2.2 / -0.8	7.5	C 24 H 35 O 4
388.2569	25.9			
389.2470	10.0			
391.2847	18.5			
396.3853	66.3			
397.3874	18.8			
401.3073	15.5			
403.2500	15.7	+3.9 / +1.6	7.5	C 24 H 35 O 5
405.2637	30.0	-1.0 / -0.4	6.5	C 24 H 37 O 5
406.2727	11.1			
413.2549	11.0			
427.2463	97.5			
428.2516	26.6			
447.3391	10.7			

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Figure S39. ¹H NMR spectrum of compound **8** in CDCl₃ (600 MHz)
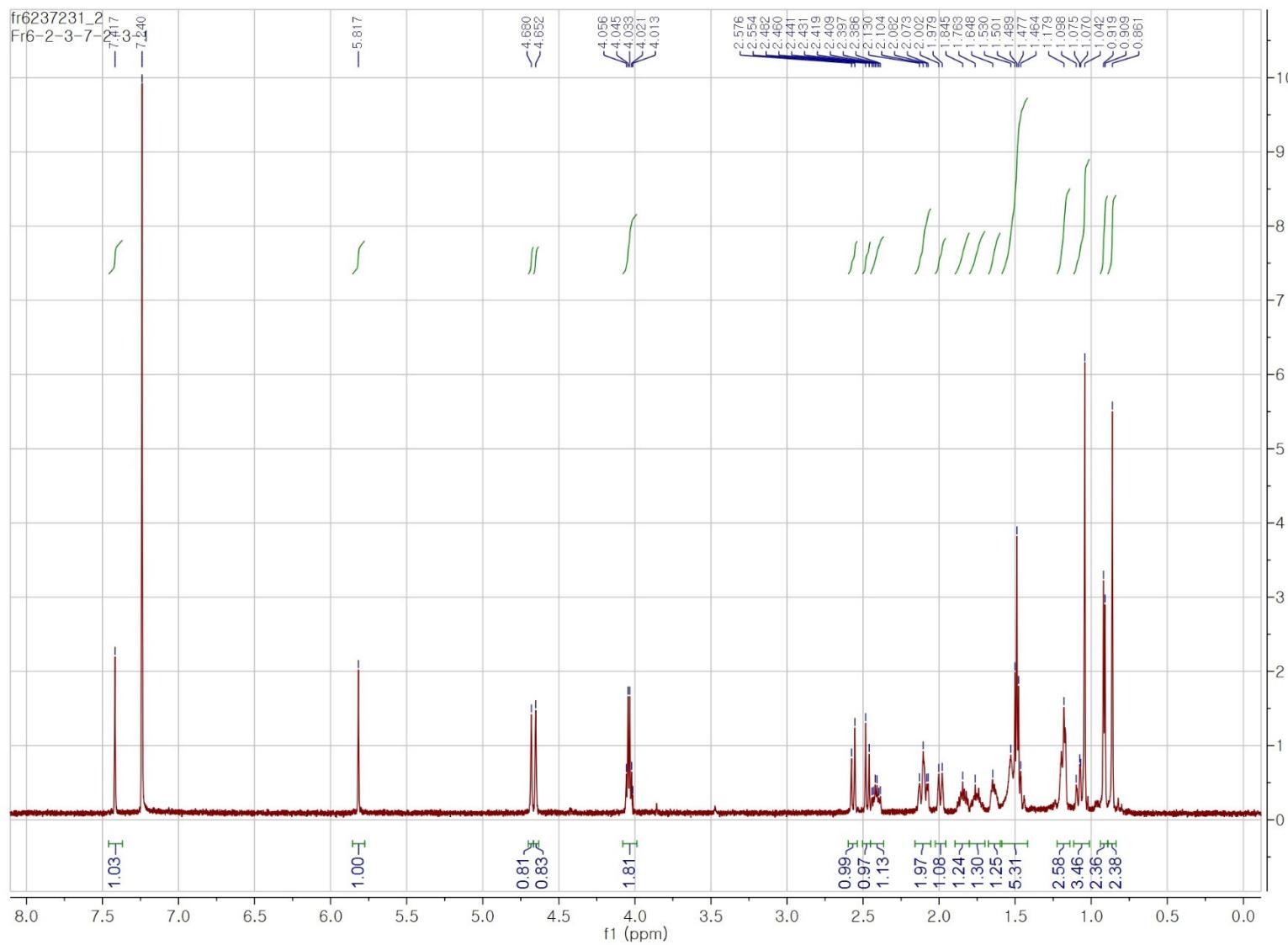
Figure S40. ^{13}C NMR spectrum of compound 8 in CDCl$_3$ (150 MHz)
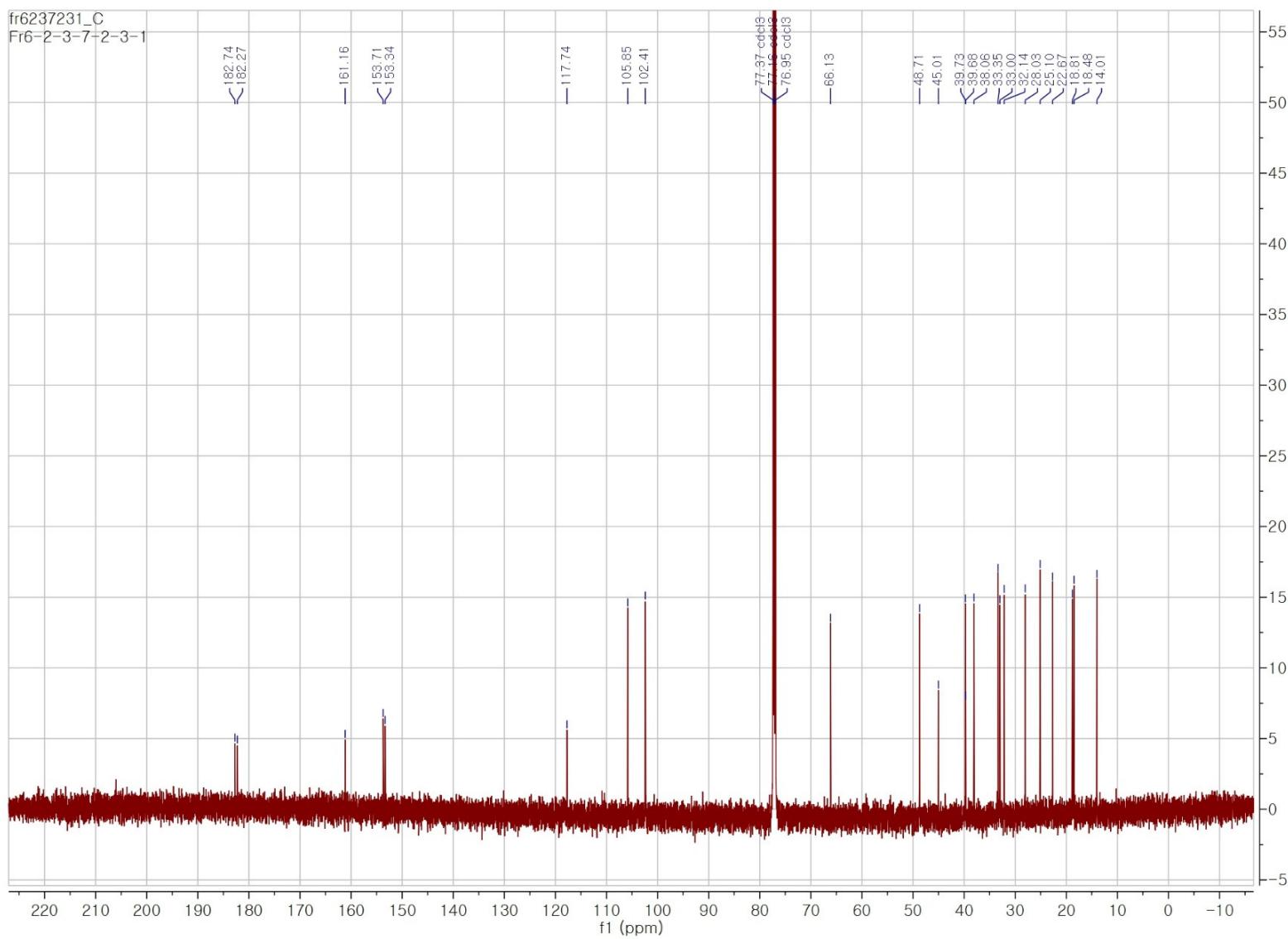
Figure S41. HSQC spectrum of compound 8 in CDCl₃
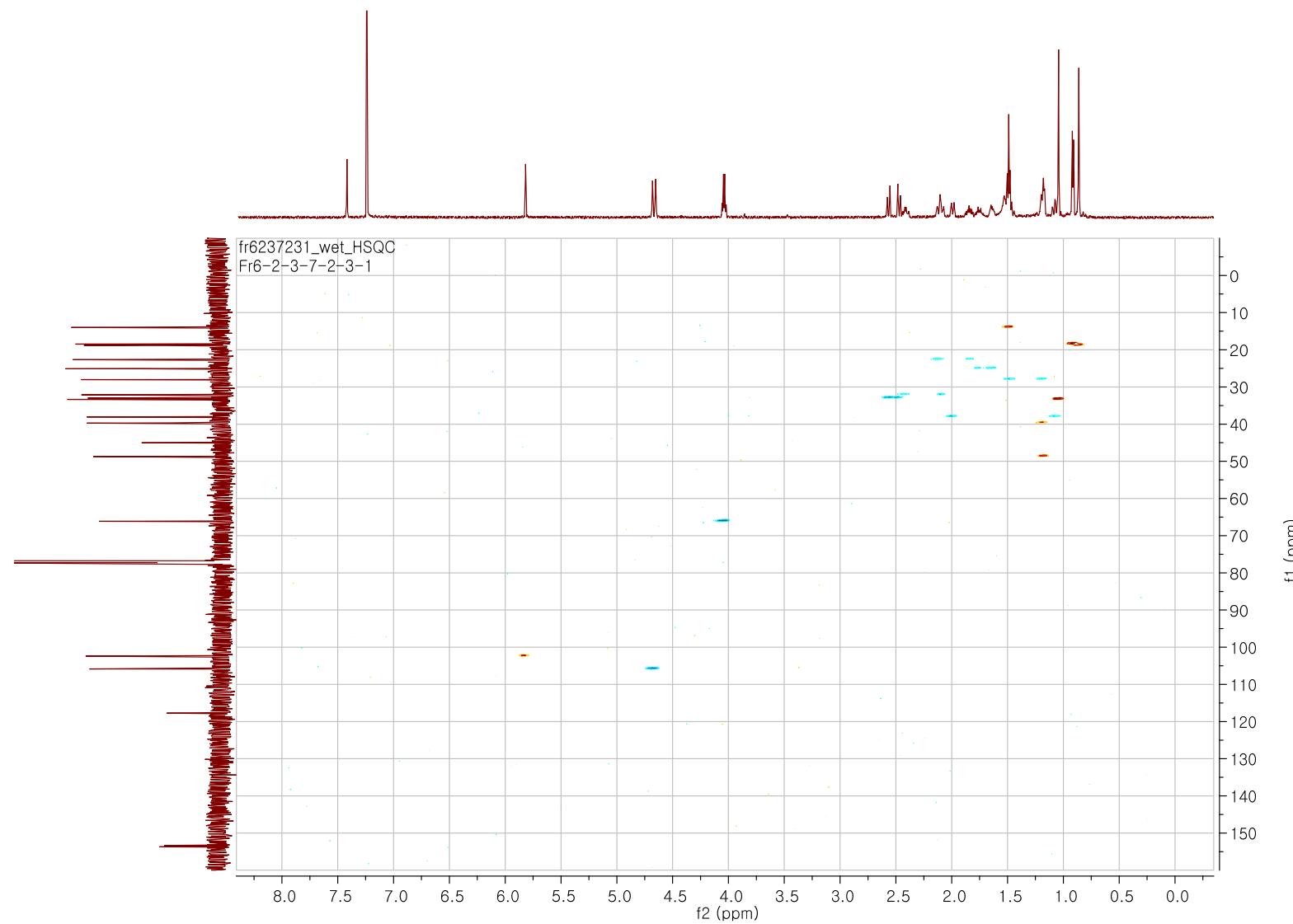
Figure S42. HMBC spectrum of compound 8 in CDCl₃
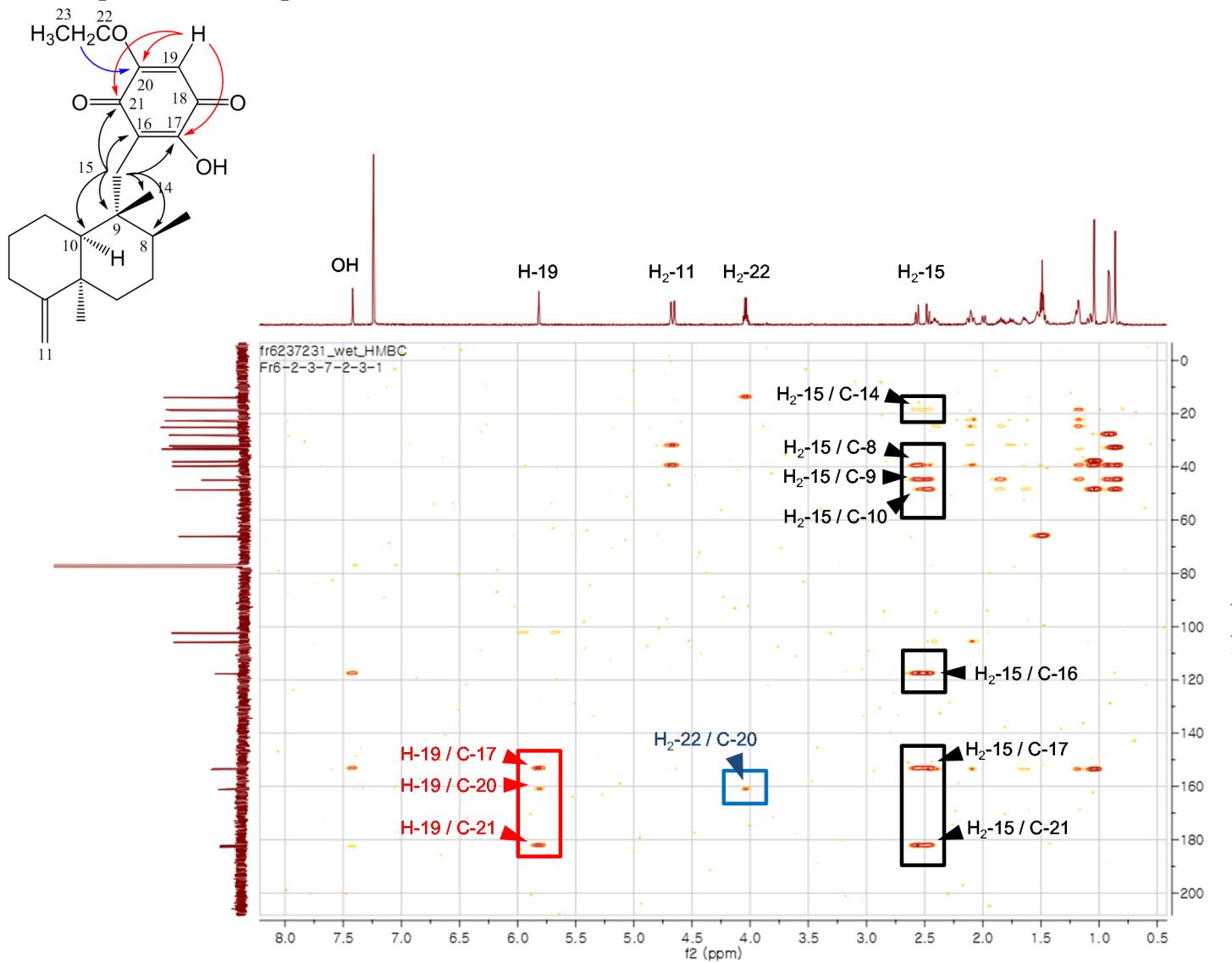
Figure S43. COSY spectrum of compound 8 in CDCl₃
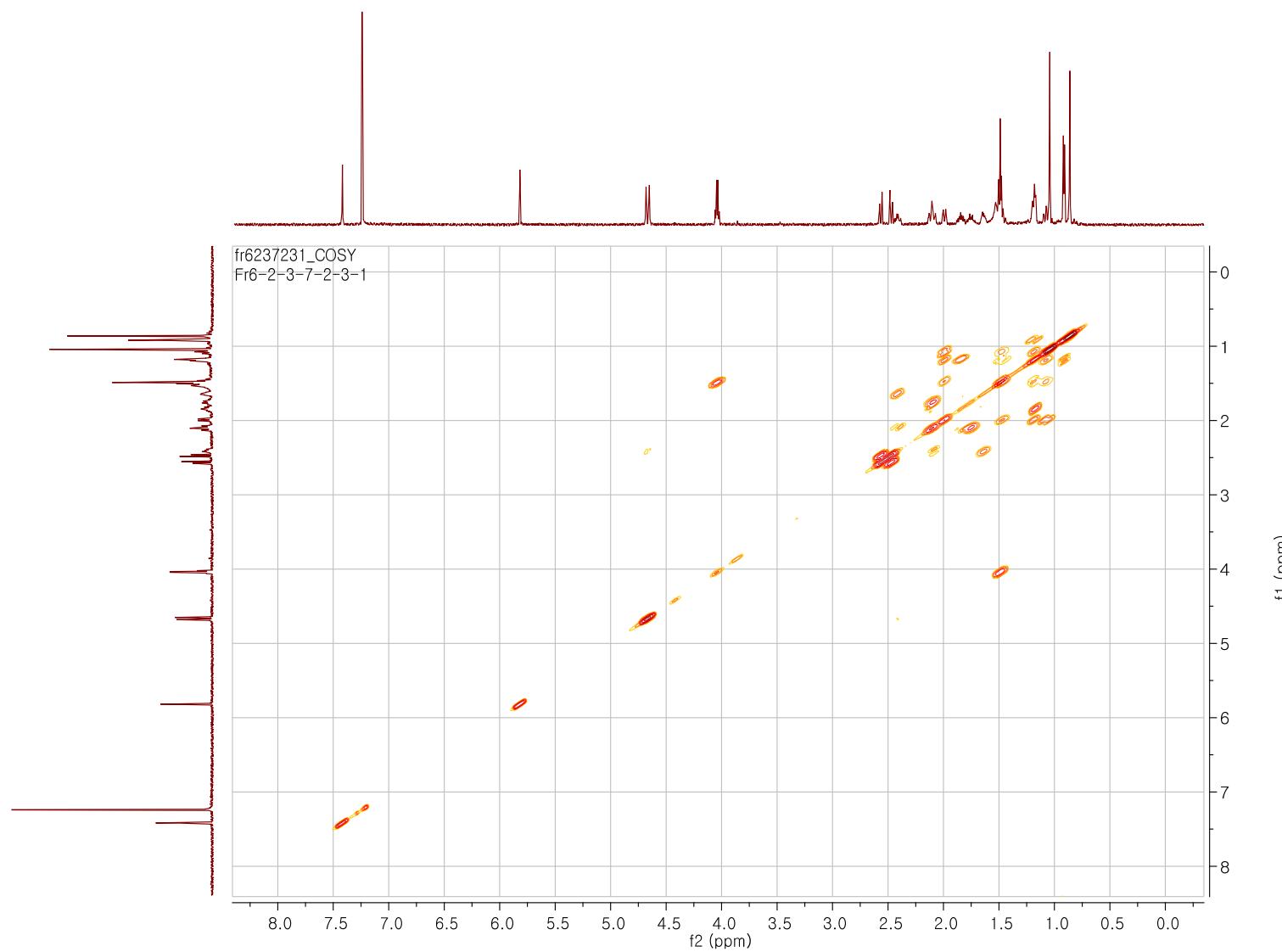
Figure S44. HRFABMS analysis of of compound 8

[Mass Spectrum]
Data : Fr-G-2-3-7-2-3-1-C23H32O4   Date : 11-Apr-2011 10:36
Sample: —
Note : —
Inlet : Direct   Ion Mode : FAB+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.43 min   Scan# : (9,10)
BP : m/z 373.2381   Int. : 72.18
Output m/z range : 356.2315 to 391.6068   Cut Level : 0.00 %
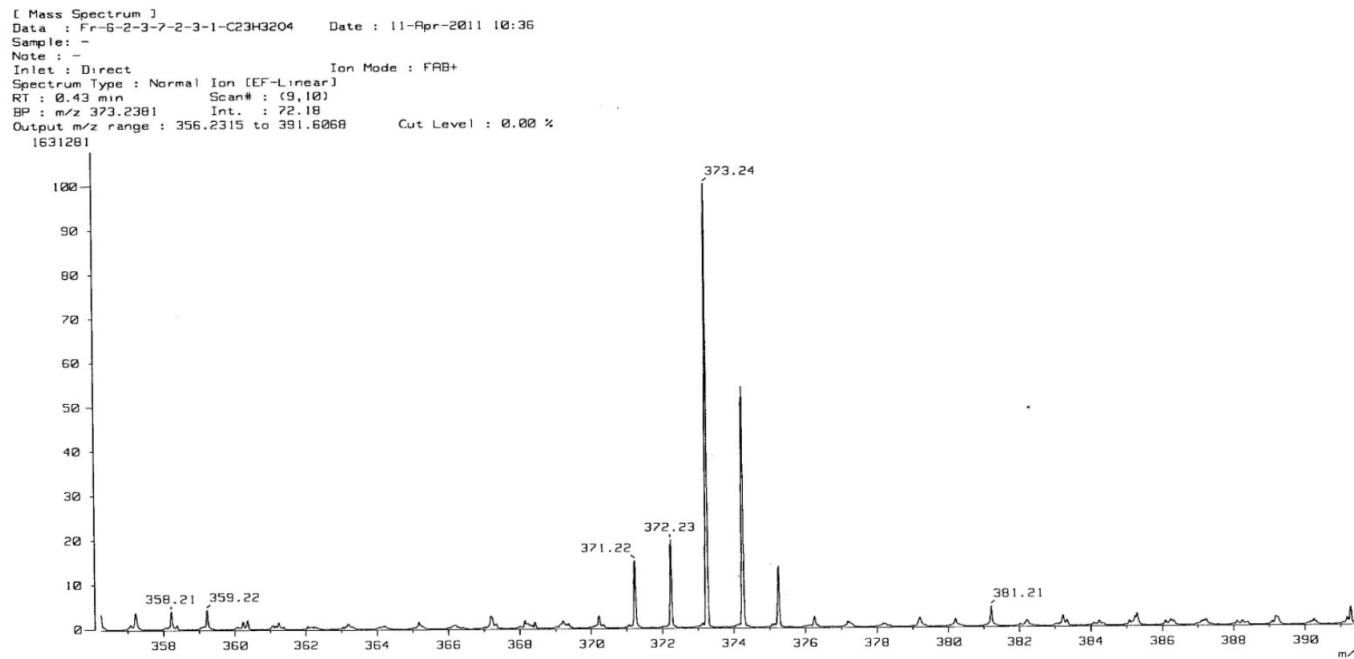
[Elemental Composition]
Data : Fr-6-2-3-7-2-3-1-C23H32O4   Date : 11-Apr-2011 10:36
Sample: -
Note : -
Inlet : Direct   Ion Mode : FAB+
RT : 0.43 min   Scan#: (9,10)
Elements : C 23/0, H 33/1, O 4/1
Mass Tolerance   : 1000ppm, 1mmu if m/z < 1, 3mmu if m/z > 3
Unsaturation (U.S.) : -0.5 - 100.0

Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
329.0721	35.6			
371.2231	15.1	+2.4 / +0.9	8.5	C 23 H 31 O 4
372.2298	19.7	-0.7 / -0.3	8.0	C 23 H 32 O 4
373.2381	100.0	+0.6 / +0.2	7.5	C 23 H 33 O 4
374.2428	54.1			
375.2463	13.7			
393.2009	12.4			
394.2131	11.2			
395.2203	85.9			
396.2327	29.3			
417.3130	10.1			

Cartesian coordinates of conformers shown in Table S1

Compound **1**_1
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-9.9878	-1.4549	7.903
C	-11.2274	-1.0361	7.1114
C	-11.9816	-2.2305	6.5424
C	-11.0567	-3.1538	5.7739
C	-9.0392	-2.3305	7.0427
C	-7.5913	-2.5287	7.6694
C	-6.7484	-3.5298	6.7917
C	-7.5183	-4.783	6.3551
C	-8.8269	-4.4393	5.6589
C	-11.3686	-3.4921	4.5094
C	-6.828	-1.1339	7.7774
C	-6.578	-0.3202	6.5272
C	-5.4214	-0.4477	5.7305
C	-5.1748	0.3056	4.5612
C	-6.0915	1.2706	4.1433
C	-7.2293	1.4691	4.9349
C	-7.4257	0.694	6.0688
O	-8.5855	1.1264	6.6504
C	-9.0279	2.1251	5.8283
N	-8.2584	2.366	4.7867
C	-10.2914	2.7819	6.2161
C	-7.6798	-3.0463	9.13
C	-5.4344	-4.	7.4406
O	-4.4508	-1.342	6.1191
O	-3.9911	0.0046	3.9283
C	-3.7061	0.7256	2.7338
H	-9.4899	-0.5491	8.2542
H	-10.3043	-1.9869	8.8058
H	-11.8949	-0.4533	7.7566
H	-10.9277	-0.3758	6.289
H	-12.4644	-2.7874	7.3537
H	-12.7948	-1.8603	5.9059
H	-8.8596	-1.7564	6.1208
H	-6.4848	-3.0128	5.8616
H	-6.9	-5.3561	5.6513
H	-7.689	-5.4508	7.2054
H	-8.586	-3.8749	4.7477
H	-9.3006	-5.3745	5.3327
H	-7.3683	-0.4888	8.4824
H	-5.8611	-1.2848	8.2745
H	-5.9586	1.8841	3.2633
H	-10.3477	2.9099	7.3012
H	-10.3689	3.7696	5.752
H	-11.1463	2.1818	5.8919
H	-6.6974	-3.0339	9.6166
H	-8.0422	-4.0716	9.1942
H	-8.3266	-2.4182	9.7496
H	-5.619	-4.6992	8.2634
H	-4.8158	-4.5247	6.7035
H	-4.8385	-3.1748	7.8346
H	-3.6034	1.7968	2.9355
H	-2.7472	0.3659	2.3484
H	-4.4653	0.5363	1.9678
H	-10.7533	-4.1484	3.9047
H	-12.2699	-3.1189	4.031
H	-3.7501	-1.2756	5.4408
C	-9.7953	-3.6248	6.5482
C	-10.3143	-4.5553	7.674
H	-10.9656	-5.3347	7.2569
H	-9.5209	-5.0837	8.2014
H	-10.8998	-4.0292	8.4326

Compound **1**_2
Charge =   0 Multiplicity = 1
  S-ymbolic Z-Matrix:

C	-10.7562	-1.6373	6.5079
C	-11.3837	-1.9195	5.1424
C	-11.5019	-3.4118	4.8584
C	-10.1878	-4.1336	5.0889
C	-9.371	-2.323	6.6392
C	-8.5014	-1.8015	7.863
C	-7.1808	-2.6515	7.9968
C	-7.3959	-4.1645	7.8681
C	-8.1232	-4.5271	6.5812
C	-9.687	-4.9132	4.1132
C	-8.1346	-0.2622	7.6733
C	-7.2918	0.1579	6.4899
C	-7.8278	0.6345	5.2769
C	-7.0494	1.0222	4.1633
C	-5.6562	0.9727	4.2296
C	-5.0796	0.5509	5.4338
C	-5.8928	0.1771	6.4935
O	-5.0671	-0.1589	7.531
C	-3.8064	0.0122	7.0322
N	-3.7569	0.4345	5.7853
C	-2.6948	-0.2978	7.9518
C	-9.309	-1.859	9.1869
C	-6.3861	-2.4017	9.2903
O	-9.1925	0.7582	5.165
O	-7.7804	1.4397	3.0753
C	-7.0416	1.8165	1.9179
H	-10.685	-0.5551	6.6308
H	-11.4398	-1.9759	7.2931
H	-12.3767	-1.4578	5.0934
H	-10.7783	-1.4467	4.3588
H	-12.2756	-3.8509	5.4989
H	-11.8539	-3.5446	3.8278
H	-8.7989	-2.0136	5.7511
H	-6.5267	-2.3829	7.1595
H	-6.4191	-4.6663	7.8587
H	-7.9206	-4.5599	8.7435
H	-7.4956	-4.2086	5.7377
H	-8.1964	-5.621	6.5218
H	-9.0523	0.3385	7.6782
H	-7.6075	0.0873	8.5714
H	-5.0058	1.259	3.4151
H	-1.7308	-0.1574	7.4541
H	-2.7282	0.358	8.8268
H	-2.7574	-1.3358	8.2917
H	-8.771	-1.363	10.0032
H	-9.503	-2.878	9.5196
H	-10.2687	-1.3402	9.1045
H	-6.8921	-2.8282	10.163
H	-5.3998	-2.8751	9.2251
H	-6.2222	-1.3402	9.4852
H	-6.4562	0.9755	1.532
H	-7.7592	2.1057	1.1441
H	-6.4047	2.6834	2.1223
H	-8.7553	-5.4581	4.2124
H	-10.2068	-5.0367	3.1672
H	-9.3497	1.0862	4.2577
C	-9.5261	-3.8849	6.4723
C	-10.4486	-4.5709	7.5123
H	-10.6171	-5.6212	7.24
H	-10.0309	-4.5877	8.5184
H	-11.4347	-4.1056	7.5894

Compound **2**_1
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-13.7193	1.5212	9.549
C	-12.8144	0.3078	9.3329
C	-13.4882	-0.8193	8.5714
C	-14.1614	-0.3197	7.312
C	-15.1549	0.8423	7.5124
C	-14.4846	2.0403	8.2949
C	-13.6787	3.1242	7.4355
C	-14.4549	3.4644	6.1082
C	-14.9038	2.2119	5.3513
C	-15.8174	1.3622	6.2131
C	-13.8844	-0.9302	6.1454
C	-13.4512	4.4502	8.2847
C	-14.6543	5.2223	8.7774
C	-15.2137	5.0573	10.0609
C	-16.3373	5.7707	10.534
C	-16.9543	6.7248	9.7233
C	-16.4061	6.9502	8.4545
C	-15.303	6.2183	8.0403
O	-14.9764	6.6624	6.7888
C	-15.9106	7.6209	6.5127
N	-16.7874	7.832	7.473
C	-15.8036	8.2733	5.1935
C	-12.2577	2.6178	7.0815
C	-13.6961	4.3571	5.1098
O	-14.6267	4.1601	10.9227
O	-16.7246	5.4412	11.8121
C	-17.8583	6.1285	12.3317
H	-14.4618	1.2501	10.311
H	-13.1195	2.3108	10.0079
H	-11.8981	0.5933	8.8097
H	-12.486	-0.0671	10.3104
H	-12.7359	-1.5858	8.346
H	-14.2266	-1.313	9.2132
H	-15.3377	2.6064	8.6937
H	-15.3707	4.0008	6.384
H	-15.4605	2.5078	4.4526
H	-14.0394	1.6416	4.998
H	-16.6935	1.9752	6.4697
H	-16.2173	0.5319	5.6174
H	-12.808	4.2317	9.1458
H	-12.8421	5.149	7.6963
H	-17.8143	7.305	10.0271
H	-16.6075	9.0027	5.0567
H	-14.8469	8.7956	5.1017
H	-15.8738	7.5312	4.3927
H	-11.7144	3.3327	6.4549
H	-12.2759	1.665	6.5481
H	-11.639	2.5046	7.9762
H	-14.3818	4.7184	4.3344
H	-13.2499	5.2355	5.5788
H	-12.8984	3.8075	4.5988
H	-17.6679	7.2044	12.4038
H	-18.7525	5.9223	11.7344
H	-18.04	5.754	13.3436
H	-14.3453	-0.6519	5.2054
H	-13.1785	-1.7547	6.0936
H	-15.1583	4.2011	11.7419
C	-16.3406	0.2792	8.356
H	-17.1091	1.0447	8.5181
H	-16.8211	-0.564	7.8445
H	-16.0385	-0.0703	9.3473

Compound **2**_2
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-14.2338	3.0897	5.7052
C	-14.0306	1.9598	4.6954
C	-12.8378	1.0747	5.0108
C	-12.8386	0.6236	6.4551
C	-12.9451	1.7528	7.4988
C	-14.1883	2.6822	7.2081
C	-15.6029	2.2354	7.8123
C	-15.4303	1.6954	9.2811
C	-14.2942	0.676	9.4041
C	-12.9728	1.2812	8.9733
C	-12.7109	-0.6888	6.7229
C	-16.6252	3.4548	7.8035
C	-16.2625	4.7242	8.54
C	-16.6214	4.9842	9.8776
C	-16.2847	6.1669	10.5732
C	-15.5694	7.1791	9.9311
C	-15.227	6.9795	8.5881
C	-15.5819	5.7975	7.9553
O	-15.1447	5.8891	6.6627
C	-14.5356	7.1107	6.5953
N	-14.5563	7.8021	7.7165
C	-13.9478	7.474	5.2915
C	-16.2673	1.1406	6.9399
C	-16.6853	1.0527	9.8995
O	-17.3635	4.0441	10.5534
O	-16.724	6.206	11.8762
C	-16.4033	7.3757	12.6222
H	-13.4454	3.834	5.5317
H	-15.1655	3.6041	5.4573
H	-14.926	1.3374	4.6212
H	-13.8976	2.3968	3.6978
H	-12.8483	0.2186	4.3244
H	-11.9081	1.6129	4.7941
H	-13.9534	3.608	7.75
H	-15.1574	2.545	9.9193
H	-14.1995	0.3599	10.4512
H	-14.524	-0.2297	8.8346
H	-12.7708	2.1363	9.6342
H	-12.1608	0.5703	9.1723
H	-16.8336	3.7379	6.7636
H	-17.6043	3.117	8.1656
H	-15.2834	8.1067	10.4069
H	-13.4736	8.4585	5.3422
H	-13.1895	6.7426	4.9968
H	-14.7212	7.5048	4.5184
H	-17.2142	0.7964	7.3686
H	-15.6287	0.2636	6.8142
H	-16.5325	1.5237	5.9507
H	-16.545	0.9203	10.9786
H	-17.5846	1.6548	9.7626
H	-16.8813	0.0602	9.4796
H	-16.8131	7.2514	13.6292
H	-15.3194	7.4986	12.7164
H	-16.8672	8.264	12.181
H	-12.6737	-1.0882	7.7293
H	-12.6272	-1.4224	5.9257
H	-17.5007	4.4145	11.4475
C	-11.6362	2.5949	7.3846
H	-11.5046	3.0597	6.4034
H	-11.6256	3.4106	8.1177
H	-10.752	1.9737	7.573

Compound **3**_1
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-16.0098	-9.6293	4.7207
C	-14.9995	-8.5896	4.2345
C	-13.8743	-9.213	3.4182
C	-13.2457	-10.392	4.1372
C	-15.3118	-10.7562	5.5268
C	-16.3108	-11.6727	6.3563
C	-15.5283	-12.8684	7.0248
C	-14.5307	-13.5621	6.0893
C	-13.5506	-12.5753	5.4716
C	-11.9114	-10.4202	4.3092
C	-17.039	-10.8189	7.4909
C	-16.1926	-10.1897	8.5815
C	-15.7014	-8.7877	8.4017
C	-14.7378	-8.2219	9.4163
C	-14.5065	-8.8709	10.562
C	-15.1313	-10.1624	10.8085
C	-15.9547	-10.7644	9.7669
O	-16.4198	-11.992	10.1753
C	-15.8386	-12.0729	11.4996
N	-15.0146	-10.885	11.8788
C	-14.9399	-13.3101	11.5388
C	-17.4537	-12.213	5.4583
C	-16.4249	-13.9571	7.6395
O	-16.0999	-8.1065	7.4626
O	-14.1192	-6.9913	9.233
C	-13.6712	-6.7409	7.9029
H	-16.7645	-9.1138	5.3178
H	-16.5469	-10.0369	3.8583
H	-15.5142	-7.8332	3.6309
H	-14.5736	-8.0649	5.0985
H	-14.2596	-9.5424	2.4463
H	-13.1302	-8.4372	3.1991
H	-14.711	-10.2465	6.2951
H	-14.9219	-12.4558	7.84
H	-13.9537	-14.2994	6.6631
H	-15.054	-14.1349	5.3172
H	-12.9763	-12.1152	6.2874
H	-12.832	-13.1375	4.8608
H	-17.6531	-10.0388	7.0248
H	-17.7887	-11.4576	7.9778
H	-13.8525	-8.474	11.3278
H	-14.1297	-13.2227	10.8054
H	-14.4878	-13.4493	12.5264
H	-15.5038	-14.2126	11.278
H	-18.2201	-12.7237	6.0528
H	-17.1045	-12.9332	4.7192
H	-17.9741	-11.4089	4.9295
H	-15.8231	-14.6444	8.2452
H	-17.1992	-13.5472	8.2903
H	-16.9194	-14.5554	6.8668
H	-12.8654	-6.0024	7.9578
H	-13.2681	-7.6422	7.4281
H	-14.4746	-6.3053	7.3028
H	-11.3963	-11.2335	4.8073
H	-11.2781	-9.6183	3.9395
C	-14.2405	-11.4811	4.6236
C	-14.8021	-12.1497	3.3431
H	-15.4198	-13.0239	3.5461
H	-15.4058	-11.4741	2.7316
H	-13.9815	-12.5029	2.7049
C	-16.9797	-12.2066	12.5086
H	-16.6035	-12.3057	13.5322
H	-17.6326	-11.3268	12.4728
H	-17.6076	-13.0743	12.2778

Compound **3_2**
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-17.1114	-11.276	5.7315
C	-17.6316	-9.9273	5.235
C	-16.9939	-9.5072	3.9178
C	-15.4812	-9.5837	3.988
C	-15.5652	-11.273	5.8561
C	-14.9777	-12.5097	6.6646
C	-13.4027	-12.4797	6.6333
C	-12.8089	-12.1858	5.2495
C	-13.3726	-10.9089	4.6439
C	-14.753	-8.5023	3.6551
C	-15.4897	-12.4762	8.1751
C	-15.1802	-11.2689	9.0417
C	-13.884	-11.2373	9.7933
C	-13.5092	-9.9826	10.5428
C	-14.4228	-9.0297	10.7516
C	-15.7627	-9.1714	10.2019
C	-16.0558	-10.2933	9.3165
O	-17.3486	-10.2088	8.8549
C	-17.8139	-9.0376	9.5723
N	-16.7639	-8.3722	10.4009
C	-18.9506	-9.4752	10.4987
C	-15.4976	-13.8556	6.0945
C	-12.7282	-13.7583	7.1613
O	-13.1569	-12.2253	9.8174
O	-12.2503	-9.8033	11.1029
C	-11.1654	-10.3273	10.3417
H	-17.5902	-11.487	6.6893
H	-17.4506	-12.0624	5.0499
H	-18.7205	-9.9736	5.1187
H	-17.4268	-9.1625	5.9922
H	-17.3566	-10.1485	3.1064
H	-17.3311	-8.4923	3.6733
H	-15.3211	-10.3992	6.4805
H	-13.0743	-11.6509	7.2708
H	-11.7215	-12.065	5.3446
H	-12.9511	-13.0368	4.5759
H	-13.0923	-10.073	5.2994
H	-12.8744	-10.7335	3.6814
H	-16.577	-12.6295	8.1758
H	-15.1216	-13.3682	8.6985
H	-14.2062	-8.1386	11.3268
H	-18.5944	-10.2119	11.2281
H	-19.3686	-8.628	11.0526
H	-19.7545	-9.9571	9.9314
H	-15.2254	-14.6944	6.746
H	-15.0891	-14.0842	5.1108
H	-16.589	-13.8766	6.0221
H	-11.6536	-13.5901	7.2963
H	-13.1287	-14.0811	8.124
H	-12.8391	-14.5916	6.459
H	-10.2607	-9.7882	10.6392
H	-11.0083	-11.384	10.5748
H	-11.3069	-10.1759	9.266
H	-13.6693	-8.4891	3.677
H	-15.228	-7.5789	3.3349
C	-14.9076	-10.9475	4.4586
C	-15.2318	-11.9566	3.3278
H	-14.7459	-12.9233	3.4558
H	-16.3015	-12.1545	3.2201
H	-14.8824	-11.5729	2.3601
C	-18.323	-8.02	8.5515
H	-18.7403	-7.1332	9.0402
H	-17.5081	-7.6883	7.8982
H	-19.0907	-8.4608	7.9062

Compound **3**_3
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-15.9082	-9.6319	4.7
C	-14.836	-8.6516	4.223
C	-13.7473	-9.3391	3.4081
C	-13.192	-10.5566	4.1236
C	-15.2792	-10.7949	5.5111
C	-16.3312	-11.6485	6.3412
C	-15.6215	-12.8873	7.0119
C	-14.6665	-13.6409	6.0783
C	-13.6283	-12.7153	5.4611
C	-11.8618	-10.6668	4.294
C	-17.0098	-10.7503	7.4729
C	-16.1325	-10.1509	8.5578
C	-15.6061	-8.759	8.379
C	-14.6599	-8.199	9.4177
C	-14.4072	-8.8869	10.5362
C	-15.0424	-10.1749	10.7692
C	-15.8944	-10.744	9.7337
O	-16.3836	-11.9645	10.1352
C	-15.7716	-12.0831	11.4424
N	-14.9205	-10.9161	11.8261
C	-14.8924	-13.3348	11.4344
C	-17.5032	-12.1228	5.4431
C	-16.5813	-13.9201	7.6278
O	-15.9643	-8.0897	7.4156
O	-14.0032	-6.9835	9.2621
C	-14.7064	-5.9651	8.5589
H	-16.6387	-9.0756	5.29
H	-16.4604	-10.0092	3.8333
H	-15.3023	-7.8638	3.6199
H	-14.3832	-8.1564	5.0912
H	-14.1491	-9.6419	2.4342
H	-12.9576	-8.6085	3.1934
H	-14.6516	-10.319	6.2799
H	-14.9915	-12.5097	7.8259
H	-14.1354	-14.411	6.6536
H	-15.2223	-14.1821	5.3061
H	-13.0287	-12.2891	6.277
H	-12.9438	-13.3204	4.8523
H	-17.5883	-9.9463	7.0016
H	-17.7877	-11.347	7.9687
H	-13.735	-8.5158	11.2995
H	-14.0987	-13.2451	10.6836
H	-14.4192	-13.5018	12.4077
H	-15.4769	-14.2227	11.1689
H	-18.3003	-12.5828	6.0385
H	-17.1971	-12.8667	4.7083
H	-17.9726	-11.2912	4.9089
H	-16.0214	-14.6417	8.2337
H	-17.3296	-13.4645	8.2787
H	-17.111	-14.4885	6.8558
H	-14.2417	-5.0071	8.8119
H	-14.6027	-6.1019	7.4788
H	-15.758	-5.9138	8.8602
H	-11.3968	-11.51	4.7915
H	-11.1814	-9.9032	3.9269
C	-14.2507	-11.5832	4.6107
C	-14.8483	-12.2194	3.3299
H	-15.5226	-13.0507	3.5331
H	-15.4035	-11.5087	2.7121
H	-14.0492	-12.6279	2.6973
C	-16.8903	-12.22	12.4757
H	-16.4915	-12.3465	13.4877
H	-17.5295	-11.3295	12.4738
H	-17.5375	-13.0727	12.2424

Compound **3**_4
Charge = 0 Multiplicity = 1
Symbolic Z-Matrix:

C	-17.1098	-11.3288	5.7118
C	-17.647	-10.0034	5.1722
C	-17.0214	-9.6212	3.8379
C	-15.5079	-9.6796	3.9026
C	-15.5629	-11.3069	5.8264
C	-14.9584	-12.5115	6.6702
C	-13.3841	-12.4733	6.6236
C	-12.8027	-12.2148	5.2275
C	-13.3823	-10.9621	4.5877
C	-14.7927	-8.6018	3.5318
C	-15.4567	-12.4322	8.1842
C	-15.1443	-11.2012	9.0179
C	-13.8485	-11.1553	9.7736
C	-13.4957	-9.9019	10.5404
C	-14.398	-8.9265	10.6837
C	-15.7278	-9.0697	10.1125
C	-16.0177	-10.2142	9.2566
O	-17.3057	-10.1361	8.7803
C	-17.7697	-8.9388	9.4543
N	-16.7253	-8.2581	10.2769
C	-18.9226	-9.3379	10.3782
C	-15.4746	-13.879	6.1495
C	-12.6976	-13.7335	7.1803
O	-13.106	-12.1319	9.7789
O	-12.2427	-9.6982	11.1065
C	-11.6244	-10.8436	11.6842
H	-17.5806	-11.5116	6.6795
H	-17.4454	-12.1413	5.0596
H	-18.736	-10.0647	5.0644
H	-17.4455	-9.2112	5.9012
H	-17.3818	-10.293	3.0505
H	-17.3707	-8.6186	3.5615
H	-15.3231	-10.4112	6.4208
H	-13.0558	-11.6249	7.2351
H	-11.7158	-12.0814	5.3113
H	-12.9413	-13.0868	4.5806
H	-13.1058	-10.1041	5.2156
H	-12.8922	-10.8114	3.6169
H	-16.5436	-12.5876	8.1988
H	-15.0831	-13.3087	8.7297
H	-14.1832	-8.0193	11.234
H	-18.5827	-10.0549	11.1345
H	-19.3402	-8.4705	10.9001
H	-19.7232	-9.8301	9.815
H	-15.1887	-14.6947	6.8239
H	-15.0759	-14.1357	5.1687
H	-16.5666	-13.9106	6.0909
H	-11.6236	-13.5544	7.3051
H	-13.0912	-14.0353	8.1526
H	-12.8061	-14.585	6.4997
H	-10.8744	-10.49	12.3985
H	-12.3418	-11.4624	12.2337
H	-11.0989	-11.4225	10.9196
H	-13.709	-8.5766	3.5492
H	-15.2786	-7.6939	3.1848
C	-14.9178	-11.0213	4.4143
C	-15.2396	-12.0702	3.3194
H	-14.7439	-13.0277	3.4757
H	-16.3081	-12.2816	3.2255
H	-14.9001	-11.7154	2.3373
C	-18.2562	-7.9477	8.3971
H	-18.6658	-7.0404	8.8536
H	-17.4314	-7.6479	7.7407
H	-19.0247	-8.3985	7.7598

Compound **3**_5
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-16.0009	-9.7057	4.6502
C	-14.9653	-8.6944	4.158
C	-13.8544	-9.3536	3.3498
C	-13.254	-10.5412	4.0795
C	-15.329	-10.8336	5.4759
C	-16.348	-11.7124	6.3205
C	-15.5909	-12.9123	7.0098
C	-14.6125	-13.6462	6.0847
C	-13.6099	-12.6939	5.4495
C	-11.92	-10.6027	4.2453
C	-17.0591	-10.8222	7.438
C	-16.2031	-10.1649	8.5047
C	-15.7508	-8.7534	8.3035
C	-14.8166	-8.1236	9.3103
C	-14.5257	-8.772	10.4483
C	-15.095	-10.0893	10.704
C	-15.9237	-10.7229	9.6881
O	-16.3441	-11.9594	10.1171
C	-15.7172	-12.0195	11.421
N	-14.924	-10.8022	11.774
C	-14.7746	-13.2241	11.4308
C	-17.5019	-12.2454	5.4321
C	-16.5096	-13.9685	7.6481
O	-16.1525	-8.1	7.3449
O	-14.3425	-6.8712	8.9632
C	-13.4695	-6.2029	9.8635
H	-16.7498	-9.1679	5.2343
H	-16.5407	-10.1146	3.7901
H	-15.4604	-7.9318	3.5456
H	-14.529	-8.172	5.0187
H	-14.2473	-9.6836	2.3811
H	-13.0918	-8.5982	3.1233
H	-14.7177	-10.324	6.2365
H	-14.9719	-12.4975	7.814
H	-14.0525	-14.3877	6.67
H	-15.151	-14.2189	5.323
H	-13.0231	-12.2344	6.2566
H	-12.9063	-13.2837	4.8474
H	-17.6734	-10.0531	6.9538
H	-17.8084	-11.4411	7.9501
H	-13.8812	-8.3812	11.2231
H	-13.9921	-13.1089	10.6717
H	-14.2862	-13.3465	12.4032
H	-15.3144	-14.1462	11.188
H	-18.2816	-12.7231	6.0368
H	-17.1693	-12.9914	4.7111
H	-18.0012	-11.4415	4.883
H	-15.9206	-14.6603	8.2612
H	-17.269	-13.5293	8.2977
H	-17.0239	-14.5671	6.8888
H	-13.2011	-5.2394	9.4203
H	-13.967	-6.0074	10.8189
H	-12.5474	-6.7743	10.0117
H	-11.424	-11.4226	4.7514
H	-11.2687	-9.8206	3.8646
C	-14.2745	-11.5974	4.5844
C	-14.8514	-12.2733	3.3146
H	-15.494	-13.1259	3.5316
H	-15.4339	-11.5922	2.6885
H	-14.0394	-12.661	2.6853
C	-16.8195	-12.1924	12.4666
H	-16.4069	-12.2773	13.4774
H	-17.5037	-11.3361	12.4522
H	-17.4236	-13.0818	12.2561

Compound **3**_6
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-17.1157	-11.1506	5.6444
C	-17.4829	-9.7656	5.112
C	-16.7777	-9.4395	3.8026
C	-15.283	-9.67	3.9095
C	-15.5804	-11.3057	5.8038
C	-15.142	-12.5818	6.6451
C	-13.5725	-12.7193	6.6467
C	-12.9228	-12.5117	5.2724
C	-13.3377	-11.1939	4.6352
C	-14.4396	-8.676	3.5761
C	-15.6759	-12.467	8.144
C	-15.2554	-11.2882	9.0036
C	-13.9887	-11.3924	9.7957
C	-13.5032	-10.1969	10.5801
C	-14.3034	-9.1313	10.7308
C	-15.6261	-9.1231	10.1194
C	-16.0191	-10.2135	9.2359
O	-17.2762	-9.9835	8.7277
C	-17.6214	-8.7523	9.4111
N	-16.5294	-8.2052	10.2722
C	-18.8363	-9.0328	10.2984
C	-15.7907	-13.8757	6.0863
C	-13.0486	-14.0543	7.2056
O	-13.3569	-12.4448	9.8285
O	-12.237	-10.3267	11.1214
C	-11.7204	-9.2567	11.9012
H	-17.6335	-11.2916	6.5948
H	-17.5209	-11.911	4.9693
H	-18.568	-9.7015	4.9718
H	-17.2155	-9.0111	5.8597
H	-17.1876	-10.0558	2.9943
H	-17.0028	-8.4003	3.5328
H	-15.2595	-10.4507	6.4193
H	-13.171	-11.9201	7.2804
H	-11.8309	-12.503	5.39
H	-13.1387	-13.3548	4.6084
H	-12.9856	-10.3803	5.284
H	-12.8041	-11.088	3.6815
H	-16.7732	-12.501	8.124
H	-15.4181	-13.3857	8.6871
H	-14.043	-8.25	11.2998
H	-18.5996	-9.7945	11.0503
H	-19.1681	-8.1317	10.8249
H	-19.6716	-9.4234	9.7066
H	-15.6202	-14.7269	6.756
H	-15.3913	-14.1634	5.1145
H	-16.8768	-13.7834	5.9931
H	-11.9653	-13.999	7.3621
H	-13.5012	-14.3186	8.163
H	-13.2329	-14.8815	6.5116
H	-10.7186	-9.5385	12.2385
H	-11.6304	-8.3442	11.3031
H	-12.3387	-9.0846	12.7881
H	-13.3612	-8.7748	3.624
H	-14.8091	-7.7147	3.2294
C	-14.864	-11.0766	4.4161
C	-15.2681	-12.068	3.2952
H	-14.888	-13.0772	3.4499
H	-16.3502	-12.1563	3.1673
H	-14.8613	-11.7408	2.3293
C	-17.9647	-7.6974	8.3595
H	-18.2829	-6.7567	8.8213
H	-17.0938	-7.4824	7.73
H	-18.7607	-8.0498	7.6945

Compound **4**_1
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-17.1985	1.8211	6.8506
C	-17.8059	0.9219	7.9277
C	-17.6237	1.459	9.3362
C	-18.0297	2.9132	9.4395
C	-17.3573	3.8595	8.4265
C	-17.5447	3.3368	6.9483
C	-18.8872	3.7565	6.1794
C	-19.2349	5.2654	6.4639
C	-19.1778	5.6122	7.9542
C	-17.7986	5.3405	8.5218
C	-18.8937	3.2758	10.4051
C	-18.7168	3.5297	4.6114
C	-17.5936	4.2513	3.8909
C	-17.862	5.5986	3.2954
C	-16.7141	6.3607	2.6768
C	-15.5284	5.7685	2.5008
C	-15.3172	4.4017	2.9541
C	-16.3963	3.7063	3.6439
O	-15.9943	2.4435	4.0097
C	-14.6358	2.4376	3.5072
N	-14.2289	3.7074	2.8322
C	-14.5116	1.2967	2.4967
C	-20.0823	2.8651	6.5983
C	-20.6045	5.7353	5.9406
O	-18.9994	6.0583	3.2935
O	-16.8555	7.6638	2.2145
C	-17.694	8.504	3.0031
H	-16.1071	1.718	6.91
H	-17.4666	1.41	5.8745
H	-18.8709	0.7585	7.7439
H	-17.3441	-0.0712	7.8612
H	-18.2029	0.8319	10.0257
H	-16.5783	1.3461	9.6448
H	-16.7504	3.8481	6.3874
H	-18.4741	5.8831	5.9709
H	-19.3983	6.6791	8.0893
H	-19.9518	5.0711	8.5069
H	-17.0854	5.9705	7.971
H	-17.7511	5.6973	9.5585
H	-18.604	2.4542	4.422
H	-19.6618	3.7638	4.1052
H	-14.6958	6.2753	2.0298
H	-13.4935	1.2172	2.1013
H	-14.7898	0.339	2.9504
H	-15.1908	1.4538	1.6508
H	-21.012	3.1735	6.109
H	-20.2587	2.8852	7.6759
H	-19.935	1.8269	6.2883
H	-21.4261	5.3552	6.5575
H	-20.6618	6.8295	5.9716
H	-20.7949	5.4309	4.9105
H	-17.4023	9.5405	2.8079
H	-18.739	8.3957	2.6999
H	-17.5709	8.318	4.0756
H	-19.2114	4.2992	10.5648
H	-19.3132	2.5448	11.0911
C	-15.836	3.8836	8.7736
H	-15.2886	4.5591	8.1051
H	-15.673	4.2352	9.7998
H	-15.3559	2.905	8.6845
C	-13.6999	2.2068	4.695
H	-12.6517	2.1662	4.381
H	-13.8018	3.0137	5.4302
H	-13.9489	1.275	5.2149

Compound **4_2**
Charge = 0 Multiplicity = 1
Symbolic Z-Matrix:

C	-17.1706	5.3832	8.2543
C	-17.3622	5.0926	9.7432
C	-18.8139	4.8865	10.1363
C	-19.5083	3.903	9.2196
C	-19.4148	4.2249	7.7155
C	-17.9141	4.4332	7.2681
C	-17.0778	3.1315	6.8559
C	-17.966	2.158	5.9914
C	-19.3387	1.9013	6.6184
C	-20.1061	3.1982	6.7853
C	-20.1724	2.8683	9.7663
C	-15.78	3.5431	6.0283
C	-15.9624	4.2792	4.7144
C	-15.958	5.7768	4.7209
C	-16.2603	6.5088	3.4354
C	-16.3357	5.8398	2.2804
C	-16.1851	4.3921	2.2609
C	-16.0072	3.6784	3.5194
O	-15.9119	2.3262	3.2922
C	-16.0411	2.2854	1.8501
N	-16.2157	3.6269	1.2146
C	-17.2676	1.4347	1.5159
C	-16.5516	2.3788	8.1027
C	-17.3379	0.7859	5.6878
O	-15.6936	6.39	5.7501
O	-16.4075	7.89	3.3898
C	-17.0826	8.467	4.5046
H	-17.5206	6.407	8.0676
H	-16.0973	5.4107	8.0518
H	-16.7832	4.2165	10.0465
H	-16.9498	5.9281	10.3225
H	-18.8477	4.5523	11.181
H	-19.3443	5.8452	10.1177
H	-17.9955	4.9991	6.3301
H	-18.1523	2.6428	5.025
H	-19.9221	1.2415	5.963
H	-19.2365	1.37	7.5694
H	-20.2324	3.638	5.7855
H	-21.1249	2.9807	7.1303
H	-15.109	4.1306	6.6666
H	-15.1903	2.6379	5.8305
H	-16.5158	6.3383	1.3364
H	-17.4087	1.3374	0.4344
H	-17.1809	0.4334	1.9524
H	-18.1754	1.8832	1.9363
H	-16.0191	1.4615	7.8307
H	-17.3539	2.0983	8.7886
H	-15.8173	2.9765	8.6499
H	-17.3413	0.1347	6.5685
H	-17.9156	0.2736	4.9096
H	-16.3099	0.8577	5.3302
H	-17.91	7.8399	4.8545
H	-16.3769	8.6773	5.3129
H	-17.5024	9.4237	4.179
H	-20.7194	2.1378	9.1827
H	-20.2005	2.7214	10.8427
C	-20.2057	5.5507	7.4886
H	-20.2071	5.8339	6.429
H	-21.252	5.4421	7.8
H	-19.7897	6.4017	8.0352
C	-14.7739	1.6466	1.2807
H	-14.8226	1.5563	0.1905
H	-13.892	2.2479	1.5304
H	-14.6089	0.6523	1.7102

Compound **4**_3

Charge = 0 Multiplicity = 1

Symbolic Z-Matrix:

C	-17.2474	1.7837	6.8148
C	-17.8781	0.8617	7.8588
C	-17.6756	1.3386	9.2861
C	-18.0394	2.7985	9.4468
C	-17.3431	3.7639	8.4682
C	-17.5487	3.3043	6.9714
C	-18.8794	3.792	6.2227
C	-19.1869	5.2964	6.569
C	-19.1152	5.5826	8.0714
C	-17.742	5.2517	8.6219
C	-18.8897	3.1481	10.4291
C	-18.7171	3.6247	4.6459
C	-17.5774	4.3419	3.9448
C	-17.8156	5.7135	3.3901
C	-16.6664	6.441	2.7298
C	-15.4838	5.8374	2.5739
C	-15.2958	4.4644	3.0167
C	-16.3918	3.7769	3.6868
O	-16.0172	2.4979	4.0247
C	-14.6515	2.4807	3.5425
N	-14.2187	3.7538	2.8905
C	-14.5284	1.3525	2.5179
C	-20.0978	2.9166	6.6077
C	-20.5467	5.8212	6.0724
O	-18.9299	6.2213	3.4624
O	-16.7727	7.7567	2.2937
C	-18.0103	8.1064	1.6812
H	-16.1595	1.6466	6.8668
H	-17.5299	1.4184	5.8246
H	-18.948	0.7369	7.6734
H	-17.4459	-0.1411	7.7522
H	-18.2702	0.7021	9.9536
H	-16.6328	1.184	9.5853
H	-16.741	3.8136	6.4284
H	-18.4122	5.9133	6.0969
H	-19.3063	6.649	8.2493
H	-19.9017	5.0412	8.6058
H	-17.0134	5.8822	8.0923
H	-17.681	5.5671	9.6712
H	-18.6342	2.5548	4.4137
H	-19.657	3.9035	4.1528
H	-14.6399	6.3352	2.1132
H	-13.506	1.2646	2.1356
H	-14.8258	0.3924	2.9541
H	-15.1936	1.5306	1.665
H	-21.0193	3.2687	6.1327
H	-20.2727	2.8986	7.6856
H	-19.9785	1.8881	6.2562
H	-21.3746	5.4391	6.6795
H	-20.5755	6.9145	6.1454
H	-20.7505	5.5611	5.0326
H	-17.8296	8.9766	1.0426
H	-18.3964	7.3013	1.0468
H	-18.7417	8.4034	2.438
H	-19.1771	4.1734	10.6293
H	-19.328	2.4037	11.0884
C	-15.8208	3.7315	8.8103
H	-15.2562	4.4169	8.1666
H	-15.6453	4.0381	9.8489
H	-15.3689	2.744	8.6815
C	-13.7353	2.2208	4.7397
H	-12.6834	2.1721	4.4396
H	-13.8379	3.0176	5.4856
H	-14.0025	1.2843	5.2417

Compound **4**_4
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-17.1851	1.7947	6.8525
C	-17.7608	0.8598	7.9166
C	-17.5744	1.3711	9.3341
C	-18.0115	2.8131	9.4727
C	-17.3719	3.7957	8.4728
C	-17.5634	3.3002	6.9857
C	-18.9225	3.7059	6.239
C	-19.3024	5.1994	6.5603
C	-19.2367	5.5154	8.057
C	-17.8455	5.2638	8.6041
C	-18.8727	3.1358	10.4547
C	-18.7633	3.5178	4.6647
C	-17.6654	4.278	3.9445
C	-17.9724	5.6243	3.3693
C	-16.8692	6.4168	2.7067
C	-15.6601	5.8627	2.5308
C	-15.4058	4.5027	2.9892
C	-16.456	3.77	3.6821
O	-16.0127	2.5171	4.0334
C	-14.6554	2.5608	3.5305
N	-14.2948	3.8464	2.8576
C	-14.4918	1.4279	2.5167
C	-20.0924	2.7778	6.6497
C	-20.6888	5.6473	6.0625
O	-19.1123	6.078	3.4167
O	-17.2255	7.6929	2.3087
C	-16.252	8.4977	1.6575
H	-16.0912	1.7147	6.8987
H	-17.4547	1.3983	5.8707
H	-18.824	0.6769	7.741
H	-17.2782	-0.1212	7.824
H	-18.1314	0.7167	10.0165
H	-16.5231	1.2753	9.6287
H	-16.7866	3.8407	6.4279
H	-18.5619	5.8452	6.0723
H	-19.4803	6.5738	8.2175
H	-19.9919	4.9447	8.606
H	-17.1529	5.9214	8.0592
H	-17.7946	5.5998	9.6475
H	-18.6286	2.4494	4.4509
H	-19.719	3.741	4.1738
H	-14.8265	6.3605	2.0555
H	-13.472	1.3858	2.12
H	-14.7352	0.4596	2.968
H	-15.1772	1.563	1.672
H	-21.0339	3.0746	6.176
H	-20.2585	2.7706	7.7291
H	-19.9242	1.7503	6.3158
H	-21.494	5.2336	6.6794
H	-20.7723	6.7389	6.1191
H	-20.8832	5.3616	5.0278
H	-16.7143	9.4604	1.4202
H	-15.3974	8.6872	2.315
H	-15.9291	8.0382	0.7178
H	-19.2117	4.1483	10.6388
H	-19.2685	2.3815	11.1295
C	-15.8479	3.8471	8.8043
H	-15.3232	4.549	8.1447
H	-15.6816	4.1806	9.8361
H	-15.3468	2.8819	8.6892
C	-13.7102	2.3605	4.7165
H	-12.6616	2.3591	4.401
H	-13.8405	3.1608	5.4544
H	-13.9243	1.4186	5.2336

Compound **4_5**
Charge = 0 Multiplicity = 1
Symbolic Z-Matrix:

C	-17.1704	5.2848	8.3632
C	-17.337	4.9431	9.8442
C	-18.7803	4.706	10.2504
C	-19.4757	3.7439	9.3119
C	-19.4076	4.1165	7.8179
C	-17.9161	4.3586	7.3563
C	-17.0702	3.0819	6.8902
C	-17.9585	2.1243	6.0085
C	-19.319	1.8307	6.6455
C	-20.0995	3.1119	6.8643
C	-20.1194	2.6837	9.8336
C	-15.7897	3.5368	6.0581
C	-15.9931	4.3113	4.7693
C	-15.9861	5.8069	4.8182
C	-16.2523	6.5915	3.5545
C	-16.3687	5.9508	2.3814
C	-16.2516	4.499	2.3267
C	-16.0609	3.7465	3.5587
O	-15.9816	2.4013	3.2892
C	-16.1496	2.4038	1.851
N	-16.3153	3.7664	1.2582
C	-17.3998	1.5848	1.525
C	-16.516	2.2966	8.1046
C	-17.318	0.7699	5.6546
O	-15.7514	6.3954	5.8701
O	-16.3398	7.9614	3.7257
C	-16.5674	8.7751	2.5829
H	-17.5358	6.3096	8.2158
H	-16.1005	5.3329	8.1467
H	-16.7432	4.0649	10.1107
H	-16.9266	5.7643	10.4451
H	-18.7952	4.3377	11.284
H	-19.3226	5.658	10.2704
H	-18.017	4.9537	6.4383
H	-18.1645	2.6363	5.0603
H	-19.9035	1.1849	5.9774
H	-19.197	1.2707	7.5776
H	-20.2449	3.582	5.881
H	-21.1107	2.8708	7.2159
H	-15.1173	4.1118	6.7064
H	-15.1915	2.6457	5.8244
H	-16.5461	6.4424	1.4352
H	-17.5704	1.5214	0.4453
H	-17.3202	0.57	1.9303
H	-18.288	2.0368	1.9816
H	-15.9758	1.3957	7.7958
H	-17.3044	1.9837	8.7925
H	-15.7813	2.8861	8.6602
H	-17.3032	0.0915	6.5144
H	-17.899	0.2752	4.8675
H	-16.2951	0.8652	5.2877
H	-15.7477	8.6782	1.8637
H	-17.5283	8.5351	2.1165
H	-16.6043	9.8174	2.9131
H	-20.6661	1.9661	9.234
H	-20.1302	2.5017	10.9049
C	-20.2186	5.4384	7.6462
H	-20.2398	5.7556	6.5966
H	-21.2585	5.3059	7.9694
H	-19.8051	6.2765	8.2141
C	-14.9094	1.7596	1.2304
H	-14.988	1.7016	0.1398
H	-14.0106	2.3379	1.4739
H	-14.7516	0.7505	1.627

Compound **6**_1
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-13.9046	6.0838	10.1889
C	-14.0664	7.5487	9.7837
C	-14.0188	8.5124	10.9595
C	-12.8492	8.2369	11.8816
C	-12.7278	6.784	12.3778
C	-12.7293	5.779	11.1614
C	-11.3187	5.5055	10.4479
C	-10.2004	5.2794	11.531
C	-10.1822	6.3971	12.5793
C	-11.5146	6.4943	13.299
C	-12.0395	9.2547	12.2257
C	-11.4212	4.2352	9.5056
C	-11.8395	2.9064	10.169
C	-10.7901	1.8133	10.122
C	-11.4274	0.4775	9.9718
C	-10.9083	6.6714	9.514
C	-8.7699	5.1309	10.9856
O	-9.5879	1.9931	10.2461
O	-10.8784	-0.7683	10.0769
C	-9.4989	-0.8068	10.4235
H	-14.8375	5.7708	10.6764
H	-13.8522	5.4698	9.2865
H	-13.3059	7.8376	9.0545
H	-15.0252	7.6681	9.2637
H	-13.9845	9.5368	10.5675
H	-14.954	8.4475	11.5274
H	-12.9984	4.8167	11.6148
H	-10.4264	4.3463	12.0626
H	-9.4063	6.1841	13.3261
H	-9.9068	7.353	12.1233
H	-11.6738	5.5375	13.8171
H	-11.4446	7.2419	14.0993
H	-12.1189	4.4901	8.704
H	-10.4661	4.0972	8.9846
H	-9.9229	6.5045	9.0666
H	-10.8704	7.632	10.0301
H	-11.5885	6.7614	8.6632
H	-8.0975	4.7965	11.7843
H	-8.6988	4.3975	10.1813
H	-8.3741	6.0818	10.614
H	-9.3195	-0.3215	11.3883
H	-9.2089	-1.8575	10.5209
H	-8.8844	-0.3655	9.6325
H	-11.1994	9.1419	12.9005
H	-12.2004	10.2587	11.8425
C	-13.9712	6.5117	13.2806
H	-13.9535	5.4904	13.68
H	-13.9919	7.198	14.1362
H	-14.9233	6.6214	12.7541
C	-12.7121	0.7145	9.6982
C	-13.047	2.1676	9.5562
C	-13.3351	2.4621	8.065
O	-14.4352	2.8348	7.668
O	-12.2472	2.2433	7.2783
C	-12.4592	2.5006	5.885
C	-11.1543	2.2469	5.1564
O	-14.195	2.4138	10.3673
H	-12.0235	3.0565	11.2391
H	-13.4378	-0.071	9.5361
H	-13.2363	1.8305	5.501
H	-12.766	3.543	5.7436
H	-10.3628	2.8949	5.5474
H	-10.8232	1.214	5.3071
H	-11.2639	2.4303	4.084
H	-14.9233	2.6498	9.7571

Compound **6_2**

Charge = 0 Multiplicity = 1

Symbolic Z-Matrix:

C	-13.8569	6.0325	10.0822
C	-13.9979	7.4882	9.6378
C	-13.9773	8.4794	10.7913
C	-12.8356	8.2194	11.7522
C	-12.7372	6.7783	12.286
C	-12.711	5.7445	11.0943
C	-11.2829	5.4464	10.4275
C	-10.1967	5.2399	11.5464
C	-10.2006	6.3822	12.5678
C	-11.5519	6.504	13.2474
C	-12.0296	9.2407	12.0946
C	-11.3672	4.1551	9.5132
C	-11.8123	2.8441	10.1944
C	-10.7692	1.7439	10.1957
C	-11.4102	0.4092	10.0521
C	-10.8394	6.5871	9.4776
C	-8.7525	5.07	11.0448
O	-9.5697	1.919	10.3488
O	-10.8713	-0.8375	10.1929
C	-9.5038	-0.8774	10.5837
H	-14.805	5.7365	10.5506
H	-13.7833	5.3971	9.1963
H	-13.2155	7.7552	8.9236
H	-14.941	7.6005	9.0884
H	-13.9256	9.4939	10.3762
H	-14.9284	8.4333	11.3341
H	-12.9985	4.7946	11.5625
H	-10.4432	4.3211	12.0935
H	-9.4471	6.1829	13.341
H	-9.9067	7.3253	12.0971
H	-11.7315	5.5608	13.7835
H	-11.4996	7.2701	14.0314
H	-12.0417	4.3961	8.6885
H	-10.3996	3.9999	9.0209
H	-9.8429	6.4041	9.0622
H	-10.8103	7.5597	9.9712
H	-11.495	6.6599	8.6059
H	-8.1047	4.7512	11.8697
H	-8.664	4.317	10.2607
H	-8.3406	6.0093	10.6616
H	-9.3519	-0.3757	11.5449
H	-9.2235	-1.9278	10.7091
H	-8.8619	-0.454	9.8048
H	-11.2093	9.1394	12.7952
H	-12.1734	10.2362	11.6833
C	-14.007	6.5345	13.1598
H	-14.0068	5.523	13.5836
H	-14.0472	7.2411	13.998
H	-14.9433	6.6369	12.6044
C	-12.6861	0.6482	9.7416
C	-13.0098	2.1002	9.5679
C	-13.267	2.3743	8.0669
O	-14.3522	2.7674	7.6491
O	-12.1698	2.1216	7.3032
C	-12.3151	2.3538	5.8942
C	-12.022	3.8074	5.5731
O	-14.1735	2.3646	10.3511
H	-12.0209	3.0185	11.2563
H	-13.4121	-0.136	9.5748
H	-11.5884	1.7104	5.3876
H	-13.3098	2.0571	5.5426
H	-12.74	4.4709	6.0654
H	-11.0282	4.0887	5.9368
H	-12.0669	3.9832	4.4947
H	-14.8769	2.6327	9.7249

Compound **6_3**
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-13.8422	6.1123	10.1277
C	-13.9854	7.5847	9.7429
C	-14.0073	8.525	10.9382
C	-12.8906	8.2336	11.9191
C	-12.7929	6.7715	12.3928
C	-12.7228	5.7906	11.1589
C	-11.2736	5.5339	10.5209
C	-10.2178	5.288	11.6612
C	-10.2615	6.3853	12.73
C	-11.6326	6.4662	13.3752
C	-12.1047	9.246	12.328
C	-11.3188	4.2826	9.5492
C	-11.7712	2.9406	10.1616
C	-10.7217	1.8466	10.143
C	-11.3521	0.5156	9.9323
C	-10.8142	6.719	9.6353
C	-8.7584	5.1509	11.1951
O	-9.527	2.0213	10.3302
O	-10.81	-0.7332	10.037
C	-9.451	-0.7822	10.4556
H	-14.8002	5.7877	10.5553
H	-13.7368	5.5166	9.2177
H	-13.1858	7.8894	9.0636
H	-14.9137	7.7124	9.172
H	-13.9543	9.557	10.5689
H	-14.9728	8.4469	11.451
H	-13.014	4.819	11.5774
H	-10.4714	4.3447	12.1613
H	-9.5284	6.1592	13.5152
H	-9.9635	7.3503	12.3088
H	-11.8181	5.4993	13.865
H	-11.61	7.1982	14.1924
H	-11.9695	4.552	8.7135
H	-10.3349	4.1563	9.0817
H	-9.8046	6.5627	9.2412
H	-10.8083	7.6691	10.1717
H	-11.4454	6.825	8.7492
H	-8.1314	4.8041	12.0249
H	-8.6403	4.431	10.3842
H	-8.3446	6.1085	10.8624
H	-9.3226	-0.3179	11.4388
H	-9.1678	-1.8353	10.5459
H	-8.7948	-0.3255	9.708
H	-11.3034	9.1216	13.0467
H	-12.2467	10.2571	11.9561
C	-14.0844	6.4789	13.2185
H	-14.086	5.45	13.5983
H	-14.1555	7.1482	14.0848
H	-15.0057	6.597	12.6414
C	-12.6215	0.7611	9.6011
C	-12.9478	2.2177	9.4749
C	-13.1651	2.5445	7.9783
O	-14.2462	2.9278	7.5413
O	-12.0428	2.3338	7.2387
C	-12.1557	2.5974	5.8324
C	-12.669	1.3652	5.1119
O	-14.1335	2.4477	10.2353
H	-12.0071	3.0679	11.2245
H	-13.3391	-0.0191	9.3861
H	-12.7915	3.4693	5.6409
H	-11.152	2.8448	5.4718
H	-12.0228	0.5047	5.3142
H	-13.6725	1.0977	5.4574
H	-12.7047	1.534	4.0319
H	-14.8306	2.701	9.5961

Compound **6**_4
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-13.0928	6.1622	9.1612
C	-12.9385	7.6383	8.7961
C	-13.5042	8.5788	9.8456
C	-13.0105	8.2307	11.2328
C	-13.2357	6.7685	11.668
C	-12.6485	5.759	10.5982
C	-11.1061	5.3731	10.7336
C	-10.7616	5.0962	12.2433
C	-11.1969	6.2435	13.1577
C	-12.7026	6.4265	13.0834
C	-12.4533	9.1998	11.9819
C	-10.7434	4.1034	9.8506
C	-11.1608	2.6955	10.3226
C	-10.386	1.5851	9.6351
C	-11.2067	0.3478	9.5583
C	-10.2007	6.5091	10.1897
C	-9.288	4.7706	12.5333
O	-9.2308	1.6745	9.2457
O	-10.8428	-0.923	9.2178
C	-9.4621	-1.1107	8.9292
H	-14.1547	5.9074	9.0506
H	-12.5816	5.5685	8.4012
H	-11.8896	7.8885	8.6181
H	-13.4469	7.8214	7.8412
H	-13.2369	9.6073	9.5718
H	-14.5994	8.5448	9.8248
H	-13.1667	4.8161	10.8035
H	-11.342	4.2224	12.565
H	-10.9334	6.0063	14.1966
H	-10.6639	7.1668	12.913
H	-13.1635	5.4891	13.4274
H	-13.0191	7.1794	13.8161
H	-11.0545	4.2571	8.8143
H	-9.6466	4.0882	9.7703
H	-9.1392	6.3022	10.3602
H	-10.4147	7.4765	10.6467
H	-10.2991	6.6082	9.1047
H	-9.1731	4.4468	13.5744
H	-8.9114	3.959	11.906
H	-8.6409	5.6425	12.3976
H	-8.838	-0.841	9.7873
H	-9.3058	-2.1745	8.7256
H	-9.1712	-0.5553	8.032
H	-12.0949	9.039	12.9916
H	-12.3417	10.2124	11.6035
C	-14.7785	6.5613	11.7722
H	-15.0187	5.542	12.098
H	-15.219	7.2515	12.5022
H	-15.3012	6.7137	10.8237
C	-12.4441	0.7154	9.8985
C	-12.6005	2.1899	10.1402
C	-13.4031	2.7582	8.9478
O	-14.5615	3.149	9.0625
O	-12.7101	2.6974	7.7799
C	-13.4429	3.1255	6.625
C	-12.5031	3.0965	5.4361
O	-13.3031	2.3275	11.3733
H	-10.8748	2.5842	11.3759
H	-13.2765	0.0253	9.9348
H	-14.2823	2.4428	6.4535
H	-13.8204	4.143	6.773
H	-11.6471	3.7579	5.6064
H	-12.1017	2.0887	5.2862
H	-13.0175	3.4116	4.524
H	-14.2338	2.5238	11.1429

Compound **6_5**
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-13.5898	6.0067	9.715
C	-13.6255	7.4672	9.2656
C	-13.8089	8.4495	10.4115
C	-12.866	8.1666	11.562
C	-12.8877	6.7216	12.0946
C	-12.66	5.6907	10.9217
C	-11.1394	5.3618	10.5286
C	-10.2725	5.1524	11.8247
C	-10.4518	6.2946	12.8298
C	-11.9023	6.4267	13.2542
C	-12.1217	9.174	12.0529
C	-11.0795	4.0577	9.6261
C	-11.6545	2.7597	10.2354
C	-10.6195	1.6743	10.4663
C	-11.1827	0.3305	10.1781
C	-10.5158	6.486	9.6643
C	-8.7622	4.9773	11.5889
O	-9.4917	1.8711	10.8942
O	-10.6557	-0.907	10.4143
C	-9.3452	-0.925	10.9675
H	-14.6133	5.7195	9.9905
H	-13.3539	5.3811	8.8521
H	-12.7185	7.7275	8.7146
H	-14.4463	7.5969	8.5491
H	-13.6706	9.4664	10.0228
H	-14.8442	8.4108	10.7691
H	-13.05	4.746	11.3207
H	-10.6174	4.2356	12.3192
H	-9.8517	6.0894	13.7259
H	-10.0701	7.2349	12.4203
H	-12.1867	5.4825	13.7406
H	-11.9859	7.1876	14.0406
H	-11.5904	4.2948	8.6905
H	-10.0416	3.8845	9.3167
H	-9.4646	6.2846	9.433
H	-10.5596	7.4624	10.1499
H	-11.0058	6.5602	8.6899
H	-8.2752	4.644	12.5128
H	-8.5368	4.2346	10.8225
H	-8.2835	5.9185	11.2987
H	-9.3285	-0.4536	11.9554
H	-9.0513	-1.9714	11.0946
H	-8.6248	-0.4582	10.2881
H	-11.445	9.0578	12.8912
H	-12.1733	10.1735	11.6296
C	-14.2994	6.4939	12.7193
H	-14.3897	5.4825	13.1338
H	-14.4848	7.201	13.5372
H	-15.1158	6.6074	12.0007
C	-12.3751	0.5471	9.6208
C	-12.7044	1.9913	9.4024
C	-12.6376	2.2666	7.8763
O	-11.7474	1.8987	7.1222
O	-13.7078	3.0374	7.5074
C	-13.724	3.3914	6.1185
C	-14.925	4.2841	5.8753
O	-13.9953	2.2004	9.9668
H	-12.0701	2.9542	11.2307
H	-13.0299	-0.2523	9.3007
H	-12.8054	3.9311	5.8622
H	-13.804	2.4845	5.5091
H	-15.8509	3.7678	6.1492
H	-14.8675	5.1847	6.4957
H	-14.9836	4.582	4.8247
H	-14.4045	2.9263	9.4579

Compound **6_6**
Charge = 0 Multiplicity = 1
Symbolic Z-Matrix:

C	-13.927	6.0312	10.2051
C	-14.1592	7.4847	9.7928
C	-14.1445	8.4569	10.9624
C	-12.9543	8.2408	11.8737
C	-12.7617	6.7985	12.3778
C	-12.73	5.7859	11.168
C	-11.3158	5.5708	10.442
C	-10.1774	5.4041	11.5151
C	-10.1993	6.5295	12.5549
C	-11.5272	6.5709	13.2881
C	-12.1882	9.2967	12.2025
C	-11.3699	4.2894	9.5106
C	-11.7213	2.949	10.1899
C	-10.6247	1.9064	10.1304
C	-11.1923	0.5411	9.9867
C	-10.9681	6.7466	9.4952
C	-8.7471	5.3159	10.9559
O	-9.429	2.1316	10.2425
O	-10.4332	-0.579	10.1197
C	-11.1165	-1.8172	9.9767
H	-14.8401	5.6789	10.7032
H	-13.8546	5.4151	9.3057
H	-13.4194	7.8032	9.0547
H	-15.1272	7.557	9.2814
H	-14.1613	9.4793	10.5641
H	-15.0701	8.3527	11.5402
H	-12.9513	4.8156	11.63
H	-10.3553	4.466	12.056
H	-9.4068	6.358	13.295
H	-9.9727	7.4934	12.0891
H	-11.6373	5.6115	13.8142
H	-11.4833	7.3265	14.0827
H	-12.0845	4.5059	8.7128
H	-10.4142	4.1902	8.9819
H	-9.9809	6.6208	9.0385
H	-10.9686	7.7119	10.0039
H	-11.6606	6.7991	8.6511
H	-8.052	5.0202	11.7505
H	-8.6508	4.5787	10.1578
H	-8.3991	6.2803	10.5716
H	-11.5481	-1.913	8.9747
H	-10.3884	-2.6228	10.1099
H	-11.8898	-1.9291	10.744
H	-11.3366	9.2266	12.8688
H	-12.3982	10.2898	11.8148
C	-13.9822	6.4759	13.2951
H	-13.9136	5.4595	13.7013
H	-14.0259	7.1667	14.1462
H	-14.9435	6.538	12.7777
C	-12.4951	0.7101	9.7307
C	-12.9004	2.1492	9.5996
C	-13.2346	2.4422	8.1177
O	-14.3368	2.8454	7.7582
O	-12.1776	2.2043	7.2959
C	-12.425	2.4796	5.9118
C	-11.1502	2.1984	5.1413
O	-14.0462	2.3269	10.4325
H	-11.8962	3.0974	11.2616
H	-13.2045	-0.0904	9.5772
H	-13.2309	1.8337	5.5464
H	-12.7083	3.5309	5.7886
H	-10.3302	2.8218	5.5129
H	-10.8422	1.1559	5.2732
H	-11.2877	2.3942	4.0742
H	-14.718	2.7877	9.8896

Compound **6**_7
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-13.7268	5.9897	9.8771
C	-13.8001	7.4403	9.4013
C	-13.8659	8.4488	10.538
C	-12.8228	8.1827	11.6033
C	-12.8002	6.7484	12.1631
C	-12.6839	5.6966	10.9929
C	-11.2061	5.362	10.4627
C	-10.2274	5.1608	11.6769
C	-10.3089	6.3155	12.681
C	-11.714	6.4665	13.2326
C	-12.0333	9.1949	12.0058
C	-11.2286	4.054	9.5653
C	-11.7569	2.7595	10.2196
C	-10.7042	1.687	10.4277
C	-11.2717	0.3335	10.1971
C	-10.6609	6.4787	9.5373
C	-8.7449	4.9768	11.3076
O	-9.5597	1.8994	10.7998
O	-10.73	-0.8953	10.4453
C	-9.397	-0.8934	10.9422
H	-14.7192	5.7164	10.2597
H	-13.5825	5.34	9.0117
H	-12.9514	7.6828	8.7575
H	-14.6871	7.5599	8.7665
H	-13.7567	9.4557	10.1154
H	-14.8636	8.4283	10.9915
H	-13.0322	4.7603	11.4458
H	-10.5327	4.2506	12.2089
H	-9.6323	6.1155	13.5221
H	-9.9588	7.2483	12.2283
H	-11.9581	5.5328	13.7597
H	-11.7209	7.2414	14.0096
H	-11.8217	4.2929	8.68
H	-10.2234	3.8735	9.1654
H	-9.6347	6.2733	9.215
H	-10.6593	7.4592	10.0161
H	-11.2353	6.546	8.6097
H	-8.1789	4.6453	12.186
H	-8.5917	4.2302	10.5272
H	-8.2899	5.9143	10.971
H	-9.3405	-0.3951	11.9152
H	-9.093	-1.9349	11.085
H	-8.7084	-0.4428	10.2202
H	-11.2834	9.0899	12.7809
H	-12.1197	10.1868	11.5704
C	-14.1492	6.5401	12.9195
H	-14.2071	5.5351	13.3549
H	-14.2528	7.2596	13.7411
H	-15.0286	6.6508	12.2791
C	-12.4856	0.531	9.6803
C	-12.8268	1.9683	9.4346
C	-12.7956	2.2037	7.8993
O	-11.9101	1.8327	7.1413
O	-13.8903	2.9398	7.5301
C	-13.9895	3.2459	6.1302
C	-13.2295	4.5213	5.8176
O	-14.1022	2.1893	10.0275
H	-12.1378	2.9645	11.2262
H	-13.1487	-0.2784	9.4061
H	-13.6413	2.4092	5.5139
H	-15.0525	3.3875	5.9092
H	-13.595	5.3484	6.4348
H	-12.1632	4.4079	6.0366
H	-13.3428	4.7915	4.764
H	-14.5303	2.8947	9.5058

Compound **6_8**
Charge = 0 Multiplicity = 1
Symbolic Z-Matrix:

C	-13.8873	5.9874	10.1105
C	-14.0982	7.4328	9.6601
C	-14.1017	8.4314	10.8073
C	-12.934	8.2271	11.75
C	-12.7644	6.7952	12.2908
C	-12.7139	5.7551	11.1053
C	-11.2855	5.513	10.4164
C	-10.1724	5.3627	11.5177
C	-10.2088	6.5112	12.5314
C	-11.5524	6.5789	13.2335
C	-12.167	9.2843	12.0722
C	-11.3295	4.2114	9.5137
C	-11.7051	2.8885	10.2134
C	-10.6119	1.8407	10.2068
C	-11.1806	0.4747	10.0749
C	-10.9081	6.6638	9.4503
C	-8.731	5.2527	10.9921
O	-9.4188	2.0637	10.3481
O	-10.4301	-0.6451	10.2522
C	-11.1145	-1.8836	10.1177
H	-14.8141	5.6539	10.5961
H	-13.8005	5.3503	9.2272
H	-13.3396	7.7286	8.9317
H	-15.054	7.5008	9.1255
H	-14.101	9.4445	10.3855
H	-15.0407	8.3476	11.3663
H	-12.9532	4.7972	11.5839
H	-10.3691	4.4381	12.0751
H	-9.4343	6.3507	13.2926
H	-9.9645	7.4628	12.0493
H	-11.6818	5.6324	13.7782
H	-11.5202	7.3518	14.0118
H	-12.0275	4.4159	8.699
H	-10.3647	4.094	9.0058
H	-9.9119	6.5205	9.0189
H	-10.9126	7.6408	9.9362
H	-11.5811	6.7012	8.5898
H	-8.0558	4.9679	11.8075
H	-8.6229	4.4991	10.2109
H	-8.3672	6.2066	10.5963
H	-11.5192	-1.9997	9.1068
H	-10.3938	-2.6888	10.2882
H	-11.9088	-1.9758	10.866
H	-11.3312	9.2231	12.7591
H	-12.3603	10.27	11.6575
C	-14.0076	6.503	13.1876
H	-13.9564	5.4955	13.6179
H	-14.0645	7.2132	14.0217
H	-14.9566	6.5607	12.6475
C	-12.475	0.6428	9.779
C	-12.8712	2.0801	9.6086
C	-13.1683	2.3465	8.1133
O	-14.2579	2.7559	7.7239
O	-12.0939	2.0832	7.3218
C	-12.2696	2.3229	5.9175
C	-11.9682	3.7743	5.5945
O	-14.0372	2.2779	10.4087
H	-11.9085	3.0617	11.2764
H	-13.1831	-0.1583	9.6221
H	-11.5622	1.6735	5.3915
H	-13.2755	2.0385	5.5885
H	-12.6692	4.4437	6.1032
H	-10.9642	4.0444	5.9383
H	-12.0337	3.9539	4.5177
H	-14.6887	2.7409	9.8433

Compound **6_9**

Charge =   0 Multiplicity = 1

Symbolic Z-Matrix:

C	-12.9844	6.2179	9.1448
C	-12.8104	7.7024	8.8252
C	-13.436	8.6175	9.8634
C	-13.0235	8.2351	11.2681
C	-13.2716	6.7626	11.6532
C	-12.6216	5.78	10.5947
C	-11.0886	5.3924	10.8096
C	-10.8323	5.0768	12.3292
C	-11.3222	6.2001	13.2458
C	-12.8213	6.3852	13.0883
C	-12.5124	9.1853	12.0722
C	-10.6712	4.1466	9.9172
C	-11.1124	2.7262	10.3259
C	-10.297	1.636	9.653
C	-11.1104	0.4023	9.4891
C	-10.1558	6.5431	10.3492
C	-9.3776	4.7443	12.6965
O	-9.1206	1.736	9.3366
O	-10.7256	-0.8573	9.1305
C	-9.3297	-1.0379	8.9218
H	-14.0386	5.9677	8.9688
H	-12.4324	5.6416	8.3998
H	-11.7532	7.9562	8.7135
H	-13.2636	7.9091	7.8476
H	-13.1538	9.652	9.6308
H	-14.5281	8.5851	9.7784
H	-13.1485	4.832	10.7475
H	-11.4288	4.1947	12.5938
H	-11.1196	5.9363	14.2918
H	-10.7772	7.1295	13.0565
H	-13.3001	5.4396	13.3814
H	-13.1808	7.1197	13.8199
H	-10.9203	4.3278	8.8686
H	-9.5715	4.1344	9.9019
H	-9.1057	6.3329	10.5764
H	-10.3986	7.4982	10.8174
H	-10.1907	6.6699	9.2632
H	-9.323	4.3944	13.734
H	-8.9635	3.9489	12.0721
H	-8.7252	5.6196	12.6207
H	-8.7598	-0.7958	9.8247
H	-9.1606	-2.0951	8.6953
H	-8.9843	-0.4554	8.062
H	-12.2133	8.9995	13.0967
H	-12.3803	10.2069	11.726
C	-14.8176	6.5531	11.6626
H	-15.0749	5.5257	11.9475
H	-15.3004	7.2243	12.3837
H	-15.2849	6.7303	10.69
C	-12.3661	0.7595	9.7674
C	-12.5382	2.2254	10.0469
C	-13.2747	2.8323	8.8315
O	-14.4377	3.2205	8.8987
O	-12.5181	2.8071	7.702
C	-13.1517	3.2819	6.5046
C	-13.8903	2.145	5.8246
O	-13.3088	2.3232	11.2429
H	-10.8871	2.586	11.3905
H	-13.1983	0.0692	9.7327
H	-13.8196	4.1253	6.7128
H	-12.3581	3.653	5.8481
H	-13.2101	1.3109	5.6229
H	-14.6882	1.7569	6.4656
H	-14.3309	2.4779	4.8806
H	-14.2247	2.5309	10.9672

Compound **6**_10

Charge = 0 Multiplicity = 1

Symbolic Z-Matrix:

C	-13.6426	6.0762	9.8279
C	-13.6973	7.5483	9.4196
C	-13.8627	8.4979	10.5955
C	-12.8951	8.1904	11.7189
C	-12.896	6.7311	12.2112
C	-12.6846	5.7353	11.0055
C	-11.1696	5.4309	10.5722
C	-10.2755	5.1905	11.8439
C	-10.4428	6.3014	12.8856
C	-11.8854	6.4109	13.3421
C	-12.1483	9.1893	12.2232
C	-11.1177	4.1552	9.6298
C	-11.6705	2.8345	10.2094
C	-10.6222	1.7558	10.4081
C	-11.1743	0.4128	10.0949
C	-10.572	6.5854	9.7296
C	-8.7688	5.0354	11.573
O	-9.4932	1.9545	10.8319
O	-10.6345	-0.8243	10.3026
C	-9.3199	-0.8411	10.8458
H	-14.6579	5.7753	10.1187
H	-13.4235	5.4741	8.9435
H	-12.8042	7.83	8.8567
H	-14.5342	7.6918	8.7246
H	-13.7385	9.5258	10.232
H	-14.8902	8.4428	10.9729
H	-13.0587	4.7768	11.3863
H	-10.604	4.2567	12.3175
H	-9.8237	6.0744	13.7633
H	-10.0757	7.256	12.4967
H	-12.1535	5.4512	13.8071
H	-11.9583	7.1486	14.1513
H	-11.6514	4.4165	8.7132
H	-10.0854	3.9995	9.2936
H	-9.524	6.3997	9.472
H	-10.6136	7.5467	10.2446
H	-11.0816	6.6842	8.7676
H	-8.2611	4.6764	12.4759
H	-8.5529	4.3198	10.7785
H	-8.3031	5.9893	11.304
H	-9.3004	-0.39	11.843
H	-9.0153	-1.8871	10.9492
H	-8.6089	-0.3537	10.171
H	-11.4543	9.0549	13.0444
H	-12.2154	10.1998	11.8291
C	-14.2931	6.4756	12.8577
H	-14.3684	5.4521	13.2444
H	-14.466	7.1575	13.6995
H	-15.1249	6.6045	12.1597
C	-12.3715	0.6298	9.5479
C	-12.7139	2.0755	9.3603
C	-12.6454	2.382	7.8397
O	-11.7392	2.0512	7.0876
O	-13.7381	3.1242	7.4774
C	-13.7971	3.5095	6.0952
C	-14.4461	2.4118	5.2738
O	-14.0062	2.2615	9.9289
H	-12.0844	2.9981	11.211
H	-13.0206	-0.1686	9.214
H	-14.4063	4.4178	6.0436
H	-12.8034	3.7666	5.711
H	-13.8547	1.4915	5.3102
H	-15.4371	2.1692	5.6714
H	-14.5502	2.7189	4.2294
H	-14.4286	2.9823	9.4236

Compound **6**_11
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-13.627	5.9897	9.7425
C	-13.718	7.4432	9.2784
C	-13.9152	8.4315	10.4167
C	-12.9452	8.1923	11.5543
C	-12.9103	6.7534	12.1023
C	-12.6679	5.7175	10.9368
C	-11.1437	5.4333	10.5219
C	-10.2485	5.2694	11.8048
C	-10.4503	6.4156	12.801
C	-11.8971	6.5035	13.2483
C	-12.2267	9.2289	12.0225
C	-11.0554	4.1203	9.6338
C	-11.5748	2.8103	10.2669
C	-10.4918	1.7823	10.5248
C	-10.9717	0.4075	10.2442
C	-10.5727	6.5667	9.6334
C	-8.7369	5.1463	11.5443
O	-9.38	2.0291	10.9683
O	-10.2439	-0.6956	10.5646
C	-10.8236	-1.9471	10.2211
H	-14.6359	5.6722	10.0379
H	-13.3845	5.3626	8.8827
H	-12.8291	7.727	8.7099
H	-14.5541	7.5379	8.5742
H	-13.8169	9.4481	10.0152
H	-14.9428	8.3628	10.7918
H	-13.0207	4.7654	11.3522
H	-10.5529	4.3465	12.3144
H	-9.8288	6.2406	13.6889
H	-10.1076	7.3637	12.3754
H	-12.1417	5.5555	13.7488
H	-11.9933	7.2694	14.0284
H	-11.5915	4.3293	8.7058
H	-10.018	3.9781	9.3071
H	-9.5195	6.3975	9.3861
H	-10.6408	7.5471	10.1083
H	-11.0816	6.6125	8.667
H	-8.223	4.8356	12.4615
H	-8.4979	4.4084	10.7773
H	-8.2969	6.1023	11.2413
H	-10.9702	-2.0275	9.1388
H	-10.1312	-2.7364	10.5283
H	-11.7688	-2.1002	10.7527
H	-11.533	9.1441	12.8506
H	-12.3181	10.2216	11.5898
C	-14.3034	6.4864	12.7529
H	-14.3535	5.4773	13.1796
H	-14.4987	7.1962	13.5663
H	-15.1347	6.5652	12.0468
C	-12.1723	0.5473	9.6714
C	-12.5776	1.9735	9.4415
C	-12.5365	2.2376	7.9126
O	-11.6643	1.8563	7.1445
O	-13.6114	3.0077	7.5559
C	-13.6518	3.3491	6.1642
C	-14.8597	4.2355	5.9324
O	-13.8809	2.1096	10.0017
H	-12.0081	3.0042	11.2545
H	-12.7972	-0.2716	9.3445
H	-12.7392	3.8892	5.8883
H	-13.7388	2.4366	5.5642
H	-15.7792	3.7191	6.2272
H	-14.7948	5.1427	6.5423
H	-14.9371	4.5224	4.88
H	-14.2942	2.8726	9.5543

Compound **6**_12
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-13.1639	6.139	9.1921
C	-13.0938	7.6208	8.8241
C	-13.6692	8.5327	9.8934
C	-13.1126	8.2092	11.2627
C	-13.2511	6.7379	11.7031
C	-12.652	5.7578	10.6125
C	-11.0891	5.4476	10.6949
C	-10.6806	5.1883	12.1917
C	-11.1396	6.3135	13.1219
C	-12.6541	6.4228	13.0991
C	-12.5782	9.2045	11.9939
C	-10.6955	4.1966	9.7984
C	-11.0279	2.7707	10.2828
C	-10.2184	1.7025	9.5733
C	-10.9711	0.4239	9.5117
C	-10.2589	6.6261	10.1222
C	-9.1842	4.934	12.4312
O	-9.0789	1.8394	9.1529
O	-10.3897	-0.7472	9.1405
C	-11.2311	-1.8927	9.1492
H	-14.2154	5.8332	9.1171
H	-12.6507	5.5706	8.4142
H	-12.0649	7.9217	8.6115
H	-13.6423	7.7788	7.887
H	-13.4619	9.573	9.6123
H	-14.7614	8.4451	9.9094
H	-13.1161	4.7906	10.8337
H	-11.2072	4.2878	12.532
H	-10.8295	6.0899	14.1508
H	-10.6607	7.2616	12.8601
H	-13.0567	5.4643	13.4575
H	-12.9817	7.1597	13.8432
H	-11.0494	4.3344	8.7735
H	-9.6027	4.2349	9.6805
H	-9.1835	6.4711	10.2566
H	-10.5042	7.582	10.5873
H	-10.3986	6.7198	9.0413
H	-9.0184	4.6168	13.4674
H	-8.7907	4.1409	11.7906
H	-8.5847	5.8358	12.2743
H	-12.0577	-1.7768	8.4402
H	-10.6339	-2.7538	8.8349
H	-11.6103	-2.0928	10.1569
H	-12.178	9.0617	12.9905
H	-12.5289	10.2213	11.6133
C	-14.7774	6.4556	11.8593
H	-14.9563	5.4257	12.1915
H	-15.226	7.1234	12.605
H	-15.3389	6.5822	10.9295
C	-12.2214	0.7222	9.8858
C	-12.4428	2.1903	10.1361
C	-13.3063	2.7219	8.97
O	-14.4739	3.069	9.1253
O	-12.6531	2.6827	7.7793
C	-13.4368	3.0875	6.6498
C	-12.5357	3.092	5.4309
O	-13.1216	2.2823	11.3876
H	-10.7091	2.6742	11.328
H	-13.0315	0.0101	9.9539
H	-14.2578	2.3771	6.5039
H	-13.8436	4.0914	6.8125
H	-11.6973	3.7817	5.5751
H	-12.1057	2.0986	5.2656
H	-13.0897	3.3909	4.5368
H	-14.0437	2.5428	11.1868

Compound **6**_13
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-13.7614	5.9665	9.9084
C	-13.8934	7.4083	9.4187
C	-13.9749	8.4264	10.5458
C	-12.9048	8.2084	11.5951
C	-12.8221	6.782	12.1693
C	-12.6896	5.7218	11.0084
C	-11.2104	5.432	10.4555
C	-10.204	5.2801	11.6537
C	-10.3089	6.4423	12.6471
C	-11.7084	6.5498	13.2221
C	-12.1442	9.2518	11.9728
C	-11.2025	4.1131	9.5729
C	-11.673	2.8072	10.2484
C	-10.5712	1.7922	10.4758
C	-11.0557	0.4089	10.2488
C	-10.7214	6.556	9.5077
C	-8.7224	5.1467	11.2592
O	-9.4414	2.0541	10.8608
O	-10.3103	-0.6834	10.5659
C	-10.8971	-1.9449	10.2756
H	-14.7368	5.6632	10.3113
H	-13.6096	5.3128	9.0473
H	-13.0649	7.673	8.7576
H	-14.7948	7.49	8.7984
H	-13.9082	9.4317	10.1109
H	-14.9631	8.3761	11.0171
H	-12.9975	4.7794	11.4775
H	-10.4671	4.3656	12.2005
H	-9.6109	6.2756	13.4779
H	-10.0001	7.3818	12.1784
H	-11.9102	5.6139	13.763
H	-11.729	7.3324	13.9912
H	-11.8197	4.3218	8.6971
H	-10.199	3.9634	9.1564
H	-9.6946	6.3829	9.1689
H	-10.7458	7.5416	9.9755
H	-11.3144	6.5922	8.5901
H	-8.1293	4.8427	12.1296
H	-8.5559	4.4005	10.4811
H	-8.3077	6.0974	10.9078
H	-11.0867	-2.0515	9.2022
H	-10.189	-2.724	10.5731
H	-11.8194	-2.0891	10.8482
H	-11.3775	9.1812	12.7354
H	-12.2726	10.2353	11.5289
C	-14.1497	6.5354	12.9518
H	-14.1648	5.534	13.3988
H	-14.264	7.2601	13.7674
H	-15.0435	6.6083	12.326
C	-12.2793	0.5304	9.7224
C	-12.6978	1.9496	9.4726
C	-12.6988	2.1782	7.936
O	-11.8379	1.7901	7.1586
O	-13.795	2.9222	7.5875
C	-13.924	3.222	6.1887
C	-13.1559	4.4858	5.8497
O	-13.9836	2.0954	10.0685
H	-12.0686	3.0098	11.2495
H	-12.9134	-0.2981	9.4406
H	-13.6014	2.3774	5.5692
H	-14.9901	3.3758	5.9926
H	-13.4948	5.3209	6.4715
H	-12.0859	4.3596	6.042
H	-13.2926	4.752	4.7978
H	-14.4135	2.8454	9.6149

Compound **7**_1
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-11.8826	8.1376	10.5321
C	-11.789	7.219	11.7503
C	-13.1289	6.6463	12.1781
C	-13.8826	6.0487	11.0097
C	-14.0791	6.9873	9.8021
C	-12.6981	7.5926	9.3225
C	-11.8472	6.7175	8.2932
C	-12.7946	6.1383	7.1727
C	-13.9975	5.4012	7.7663
C	-14.8339	6.3523	8.605
C	-14.3443	4.7891	11.1139
C	-10.7017	7.5842	7.622
C	-11.1343	8.7927	6.7666
C	-10.8787	10.1503	7.3932
C	-10.4993	11.1479	6.357
C	-11.1089	5.5556	9.0045
C	-12.1228	5.2252	6.135
O	-11.013	10.4109	8.5792
O	-10.3747	12.5041	6.455
C	-10.6992	13.0634	7.7224
H	-12.3504	9.0752	10.8602
H	-10.8685	8.4191	10.2387
H	-11.0915	6.3979	11.5661
H	-11.3583	7.7835	12.5868
H	-12.9538	5.901	12.9642
H	-13.736	7.4293	12.6465
H	-12.975	8.4852	8.7436
H	-13.2067	6.9787	6.6021
H	-14.6302	5.0165	6.9559
H	-13.6785	4.5274	8.3418
H	-15.1892	7.1502	7.9369
H	-15.745	5.8417	8.9414
H	-9.9974	7.9201	8.3919
H	-10.1164	6.8943	7.005
H	-10.5811	4.9126	8.2929
H	-11.7814	4.9167	9.579
H	-10.3306	5.9304	9.6752
H	-12.8387	4.9613	5.3476
H	-11.2807	5.7134	5.639
H	-11.7747	4.2864	6.5754
H	-11.7332	12.8369	8.0021
H	-9.994	12.7287	8.4896
H	-10.6077	14.1507	7.6402
H	-14.9123	4.2978	10.3331
H	-14.1723	4.1975	12.009
C	-15.0082	8.1463	10.2784
H	-15.2142	8.8484	9.4614
H	-15.9728	7.7579	10.628
H	-14.5805	8.7373	11.0931
C	-10.2823	10.45	5.2405
C	-10.4072	8.9684	5.416
C	-8.9962	8.3394	5.3245
O	-8.6779	7.5633	4.4283
O	-8.1793	8.7619	6.3265
C	-6.8582	8.2089	6.2905
C	-6.0933	8.7417	7.4859
O	-11.2586	8.4949	4.3733
H	-12.2141	8.7656	6.5842
H	-9.988	10.9054	4.3046
H	-6.9127	7.1157	6.3429
H	-6.358	8.5108	5.3637
H	-5.0735	8.3473	7.5044
H	-6.0494	9.8356	7.459
H	-6.5965	8.4664	8.4188
H	-10.706	7.9299	3.7955

Compound **7_2**
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-11.9122	8.216	10.5301
C	-11.7983	7.3188	11.7625
C	-13.1185	6.6929	12.1767
C	-13.8254	6.0468	11.0049
C	-14.0431	6.9595	9.7813
C	-12.6825	7.6191	9.3154
C	-11.7768	6.7691	8.3126
C	-12.6785	6.1334	7.1852
C	-13.8574	5.3515	7.7695
C	-14.7489	6.2754	8.5813
C	-14.2325	4.7693	11.1194
C	-10.6595	7.6761	7.6479
C	-11.1282	8.8525	6.7671
C	-10.9458	10.2279	7.3802
C	-10.5839	11.2277	6.3399
C	-10.9993	5.6508	9.0519
C	-11.9497	5.2375	6.1713
O	-11.1194	10.4978	8.5591
O	-10.5185	12.5891	6.4228
C	-10.9034	13.1503	7.6724
H	-12.4266	9.1362	10.8374
H	-10.9068	8.5384	10.2491
H	-11.0622	6.5273	11.601
H	-11.407	7.9131	12.5977
H	-12.9236	5.9667	12.976
H	-13.7673	7.4542	12.6242
H	-12.9889	8.4906	8.7193
H	-13.1179	6.947	6.5964
H	-14.4587	4.9282	6.9546
H	-13.5096	4.5005	8.3624
H	-15.1281	7.0477	7.8963
H	-15.642	5.7293	8.9101
H	-9.9833	8.053	8.424
H	-10.0355	7.0032	7.051
H	-10.4317	5.0226	8.3579
H	-11.6522	4.9902	9.6245
H	-10.2496	6.0689	9.7295
H	-12.64	4.9311	5.3765
H	-11.1222	5.7562	5.6817
H	-11.5672	4.3212	6.6304
H	-11.9339	12.8817	7.9266
H	-10.2061	12.8577	8.4637
H	-10.8577	14.2394	7.5768
H	-14.765	4.2428	10.3366
H	-14.0494	4.198	12.0254
C	-15.0305	8.0822	10.2261
H	-15.2537	8.7634	9.3961
H	-15.9826	7.656	10.5656
H	-14.643	8.7025	11.0392
C	-10.3116	10.526	5.2382
C	-10.3807	9.0431	5.4294
C	-8.9458	8.465	5.375
O	-8.5931	7.6659	4.5126
O	-8.159	8.9499	6.3732
C	-6.8115	8.4571	6.4105
C	-6.7537	7.1631	7.2005
O	-11.1913	8.5248	4.3751
H	-12.2016	8.7746	6.5631
H	-10.0148	10.9816	4.3032
H	-6.4057	8.3299	5.4005
H	-6.2051	9.2207	6.9084
H	-5.7232	6.8081	7.2891
H	-7.1663	7.3069	8.2046
H	-7.3523	6.3827	6.72
H	-10.6187	7.9304	3.8484

Compound **7**_3

Charge =   0 Multiplicity = 1

Symbolic Z-Matrix:

C	-12.0005	8.1373	10.5796
C	-11.9541	7.2246	11.8048
C	-13.3089	6.6505	12.1808
C	-14.0134	6.0458	10.9857
C	-14.163	6.9784	9.7669
C	-12.7652	7.5847	9.3406
C	-11.8714	6.707	8.3505
C	-12.7714	6.1202	7.1954
C	-13.9958	5.3832	7.7433
C	-14.8674	6.3361	8.5432
C	-14.4761	4.7855	11.077
C	-10.7019	7.5737	7.7219
C	-11.1037	8.7773	6.845
C	-10.8716	10.1382	7.4733
C	-10.4551	11.1306	6.4463
C	-11.1597	5.5503	9.0964
C	-12.0562	5.2037	6.1903
O	-11.0492	10.4049	8.6522
O	-10.3342	12.4874	6.5418
C	-10.7095	13.0535	7.7919
H	-12.4833	9.0754	10.884
H	-10.976	8.42	10.326
H	-11.2479	6.4044	11.6528
H	-11.5589	7.794	12.6554
H	-13.1639	5.9092	12.9768
H	-13.9361	7.4341	12.6207
H	-13.0205	8.4742	8.7471
H	-13.1618	6.9569	6.6044
H	-14.5943	4.9932	6.91
H	-13.6984	4.5128	8.3354
H	-15.1971	7.13	7.8575
H	-15.7903	5.8248	8.8448
H	-10.0299	7.9148	8.5179
H	-10.0904	6.8829	7.132
H	-10.602	4.9054	8.4098
H	-11.8534	4.9122	9.6462
H	-10.4101	5.9301	9.7964
H	-12.739	4.9346	5.3757
H	-11.1956	5.6914	5.7265
H	-11.7244	4.2677	6.649
H	-11.7534	12.8267	8.0321
H	-10.0346	12.7248	8.5884
H	-10.6167	14.1406	7.7068
H	-15.0109	4.2893	10.2762
H	-14.3391	4.1984	11.9811
C	-15.1133	8.1372	10.1998
H	-15.2877	8.835	9.3719
H	-16.0903	7.7481	10.512
H	-14.7201	8.733	11.0284
C	-10.198	10.427	5.342
C	-10.3293	8.9463	5.5205
C	-8.9159	8.3167	5.4797
O	-8.571	7.5362	4.5974
O	-8.1315	8.75	6.5032
C	-6.7947	8.2288	6.5375
C	-5.8797	9.0877	5.6854
O	-11.144	8.4682	4.4507
H	-12.1763	8.7487	6.6244
H	-9.8699	10.8775	4.415
H	-6.4654	8.2612	7.5811
H	-6.7686	7.1792	6.2233
H	-4.8464	8.7354	5.7491
H	-6.1907	9.0715	4.6361
H	-5.9182	10.1319	6.0126
H	-10.5721	7.8979	3.8971

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Compound **7_4**

Charge =   0 Multiplicity = 1

Symbolic Z-Matrix:

C	-11.8933	8.0187	10.5944
C	-11.7973	7.0505	11.7733
C	-13.137	6.4638	12.1823
C	-13.8966	5.9163	10.9932
C	-14.0953	6.9047	9.8264
C	-12.7146	7.5258	9.3665
C	-11.8699	6.6917	8.2991
C	-12.8229	6.1615	7.1593
C	-14.0257	5.4036	7.7266
C	-14.8563	6.3213	8.6071
C	-14.3612	4.6546	11.0474
C	-10.7241	7.5821	7.6596
C	-11.1562	8.8254	6.8552
C	-10.8974	10.1515	7.5406
C	-10.5036	11.1952	6.5595
C	-11.1322	5.4996	8.9592
C	-12.1576	5.2903	6.0823
O	-11.0388	10.3721	8.734
O	-10.4248	12.5115	6.8908
C	-10.0541	13.398	5.8434
H	-12.3577	8.943	10.9626
H	-10.8796	8.3098	10.3088
H	-11.1025	6.2362	11.5528
H	-11.3621	7.5791	12.6306
H	-12.9607	5.6863	12.9365
H	-13.7403	7.2281	12.6849
H	-12.9916	8.4419	8.8256
H	-13.235	7.0257	6.6255
H	-14.6623	5.0542	6.9035
H	-13.7068	4.506	8.2644
H	-15.2122	7.1469	7.9738
H	-15.7675	5.7994	8.9257
H	-10.0159	7.8847	8.4397
H	-10.143	6.9155	7.014
H	-10.6091	4.8847	8.2198
H	-11.8044	4.8394	9.5097
H	-10.3503	5.8443	9.6416
H	-12.877	5.0612	5.2873
H	-11.3158	5.7962	5.6039
H	-11.8106	4.3331	6.4822
H	-9.0521	13.1641	5.4685
H	-10.7876	13.3729	5.0306
H	-10.0346	14.4133	6.2505
H	-14.9336	4.1974	10.2495
H	-14.1872	4.0265	11.9169
C	-15.0197	8.0451	10.3537
H	-15.2271	8.7808	9.5672
H	-15.9839	7.6449	10.6908
H	-14.5874	8.6011	11.1904
C	-10.2832	10.5513	5.4074
C	-10.4247	9.062	5.5166
C	-9.0244	8.413	5.3999
O	-8.7435	7.6058	4.519
O	-8.1776	8.8403	6.3743
C	-6.8715	8.2534	6.3286
C	-6.0698	8.7997	7.4934
O	-11.2752	8.6555	4.4446
H	-12.2354	8.8076	6.669
H	-9.9827	11.0222	4.4824
H	-6.952	7.1639	6.4129
H	-6.3826	8.5167	5.3842
H	-5.0599	8.3803	7.5033
H	-5.9994	9.891	7.4348
H	-6.5608	8.5632	8.4433
H	-10.829	7.9046	4.0025

Compound **7**_5
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-12.2871	8.4013	10.5914
C	-12.2473	7.5727	11.8754
C	-13.5278	6.7981	12.1331
C	-13.971	6.0235	10.9108
C	-14.1158	6.8548	9.6204
C	-12.7923	7.6658	9.3149
C	-11.6513	6.904	8.4976
C	-12.2908	6.1078	7.2951
C	-13.4417	5.2077	7.7514
C	-14.5483	6.0423	8.3722
C	-14.2336	4.7098	11.0378
C	-10.5726	7.9262	7.9411
C	-11.0581	8.9936	6.9363
C	-11.1244	10.4002	7.5036
C	-10.7033	11.4046	6.4936
C	-10.8554	5.9297	9.4023
C	-11.3164	5.2646	6.4575
O	-11.527	10.6805	8.6228
O	-10.7789	12.7676	6.5317
C	-11.2848	13.325	7.7387
H	-12.949	9.2587	10.7717
H	-11.2979	8.839	10.4375
H	-11.4047	6.8768	11.8639
H	-12.0585	8.2431	12.7232
H	-13.3656	6.1331	12.9909
H	-14.3232	7.4859	12.4418
H	-13.113	8.4675	8.6348
H	-12.7297	6.8312	6.5981
H	-13.86	4.6781	6.8858
H	-13.0858	4.4331	8.437
H	-14.9102	6.7336	7.5974
H	-15.4087	5.4006	8.6002
H	-10.0693	8.4221	8.7793
H	-9.7872	7.3187	7.4822
H	-10.1169	5.3563	8.8326
H	-11.4968	5.2107	9.9146
H	-10.2722	6.4704	10.153
H	-11.8347	4.8457	5.5869
H	-10.485	5.8566	6.0699
H	-10.9112	4.42	7.0226
H	-11.2838	14.4139	7.6292
H	-12.3184	13.0105	7.9148
H	-10.6398	13.0765	8.5876
H	-14.5792	4.0907	10.2188
H	-14.118	4.2013	11.9912
C	-15.2873	7.857	9.8585
H	-15.4676	8.4722	8.9687
H	-16.2197	7.3248	10.0837
H	-15.1018	8.552	10.6823
C	-10.2106	10.7066	5.4695
C	-10.1713	9.2269	5.6915
C	-8.6871	8.8129	5.8832
O	-7.8706	9.388	6.5896
O	-8.4423	7.664	5.1789
C	-7.1048	7.1671	5.3165
C	-6.9976	5.8807	4.5216
O	-10.7918	8.6337	4.5552
H	-12.0785	8.7742	6.604
H	-9.8204	11.17	4.5733
H	-6.3959	7.9059	4.9269
H	-6.8903	6.9676	6.3724
H	-5.9912	5.4592	4.5949
H	-7.7185	5.1415	4.8864
H	-7.2308	6.0588	3.4666
H	-10.3864	7.7521	4.4479

Compound **7_6**

Charge =   0 Multiplicity = 1

Symbolic Z-Matrix:

C	-12.1547	8.3788	10.5647
C	-12.0699	7.5366	11.8376
C	-13.3523	6.7858	12.1503
C	-13.8704	6.0328	10.944
C	-14.0602	6.8799	9.6698
C	-12.7363	7.6667	9.3076
C	-11.6528	6.8898	8.4295
C	-12.3672	6.1214	7.2513
C	-13.5124	5.2392	7.7543
C	-14.57	6.0889	8.437
C	-14.1537	4.7235	11.0716
C	-10.5787	7.8933	7.8327
C	-11.082	8.9809	6.8596
C	-11.1029	10.382	7.4439
C	-10.7008	11.3902	6.4299
C	-10.8362	5.8881	9.2847
C	-11.453	5.2702	6.3562
O	-11.4598	10.657	8.5798
O	-10.7516	12.7539	6.4849
C	-11.2023	13.3064	7.7158
H	-12.7891	9.2475	10.7849
H	-11.1652	8.798	10.3669
H	-11.2435	6.8238	11.7786
H	-11.8262	8.1943	12.6813
H	-13.1626	6.109	12.993
H	-14.1172	7.4865	12.5037
H	-13.0723	8.4813	8.6504
H	-12.8255	6.862	6.5856
H	-13.9834	4.7277	6.9049
H	-13.1395	4.45	8.4137
H	-14.9555	6.7952	7.6875
H	-15.4311	5.4621	8.7011
H	-10.0245	8.3688	8.6503
H	-9.8319	7.2717	7.3312
H	-10.1388	5.3053	8.6742
H	-11.4679	5.1775	9.8201
H	-10.2057	6.4075	10.0118
H	-10.6335	5.8525	5.9304
H	-11.0329	4.4135	6.8914
H	-12.0234	4.8686	5.5103
H	-12.2342	13.008	7.9268
H	-10.5308	13.0371	8.5373
H	-11.1859	14.3962	7.6178
H	-14.5511	4.1199	10.2647
H	-14.0025	4.2031	12.0135
C	-15.1974	7.9035	9.9739
H	-15.4076	8.5315	9.0996
H	-16.1289	7.3884	10.2392
H	-14.9577	8.5861	10.794
C	-10.2569	10.6955	5.3817
C	-10.2348	9.213	5.5869
C	-8.751	8.7742	5.7245
O	-7.9093	9.3217	6.4231
O	-8.5436	7.6404	4.9842
C	-7.2158	7.0959	5.0393
C	-7.0864	6.1573	6.2243
O	-10.9044	8.6425	4.4671
H	-12.1172	8.7825	6.5614
H	-9.8911	11.1621	4.4769
H	-7.0609	6.5387	4.1096
H	-6.4602	7.8891	5.0694
H	-6.1003	5.6846	6.2388
H	-7.2303	6.6932	7.1677
H	-7.8528	5.3764	6.1821
H	-10.5107	7.7596	4.3305

Compound **7**_7
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.0157	8.023	10.6416
C	-11.9645	7.0625	11.8296
C	-13.3175	6.472	12.1862
C	-14.0246	5.9138	10.9701
C	-14.179	6.8941	9.7898
C	-12.7831	7.5188	9.3839
C	-11.8911	6.6821	8.3576
C	-12.7936	6.1404	7.1826
C	-14.0156	5.3806	7.7042
C	-14.8861	6.2999	8.5436
C	-14.4855	4.6503	11.0128
C	-10.7239	7.5742	7.7605
C	-11.129	8.8106	6.9321
C	-10.8996	10.1422	7.6174
C	-10.4728	11.1803	6.6441
C	-11.1761	5.4975	9.0552
C	-12.0802	5.2654	6.1399
O	-11.0857	10.3702	8.8032
O	-10.4093	12.4991	6.969
C	-10.0016	13.3792	5.93
H	-12.499	8.9474	10.9844
H	-10.9924	8.3171	10.3965
H	-11.2576	6.2501	11.6432
H	-11.5677	7.5984	12.7009
H	-13.1692	5.7	12.9519
H	-13.9446	7.2366	12.6586
H	-13.0413	8.4304	8.8264
H	-13.1867	6.9994	6.6264
H	-14.616	5.0234	6.8576
H	-13.7155	4.4878	8.2604
H	-15.2188	7.12	7.8909
H	-15.8075	5.7759	8.8273
H	-10.0499	7.8848	8.5674
H	-10.1134	6.907	7.1434
H	-10.6199	4.8808	8.342
H	-11.8676	4.8375	9.5813
H	-10.4249	5.8501	9.7674
H	-12.7648	5.0283	5.317
H	-11.2212	5.772	5.6938
H	-11.7463	4.3122	6.5601
H	-9.9992	14.3973	6.3304
H	-8.9859	13.1449	5.5942
H	-10.7044	13.3469	5.0907
H	-15.0223	4.1856	10.1946
H	-14.3452	4.0283	11.8927
C	-15.1295	8.0335	10.2712
H	-16.1051	7.6309	10.5704
H	-14.7347	8.5965	11.1216
H	-15.3072	8.7634	9.4721
C	-10.2087	10.5292	5.5054
C	-10.3499	9.0403	5.6198
C	-8.9439	8.3955	5.5565
O	-8.6316	7.5867	4.6878
O	-8.1328	8.8353	6.5557
C	-6.8071	8.286	6.5814
C	-5.8881	9.1043	5.6945
O	-11.1601	8.6241	4.5205
H	-12.2006	8.7886	6.7066
H	-9.8755	10.9945	4.5888
H	-6.4602	8.3359	7.6186
H	-6.8088	7.229	6.292
H	-4.8616	8.7313	5.7502
H	-6.2166	9.07	4.6509
H	-5.899	10.1566	5.9969
H	-10.6914	7.8776	4.0943

Compound **7**_8
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
 C   -12.2725   8.3246   10.6118
 C   -12.2583   7.4713   11.88
 C   -13.5726   6.7565   12.1406
 C   -14.0688   6.0277   10.9105
 C   -14.1877   6.8891   9.6372
 C   -12.8291   7.639   9.329
 C   -11.7376   6.8368   8.4835
 C   -12.4315   6.0976   7.2747
 C   -13.6194   5.2463   7.7295
 C   -14.6756   6.1222   8.3806
 C   -14.3948   4.7265   11.0172
 C   -10.6143   7.8131   7.9328
 C   -11.0542   8.9221   6.9528
 C   -11.0555   10.3194   7.5463
 C   -10.5978   11.3228   6.5512
 C   -10.982   5.8059   9.3596
 C   -11.5109   5.2255   6.4066
 O   -11.4385   10.5967   8.6732
 O   -10.6162   12.6869   6.6131
 C   -11.0903   13.2438   7.8332
 H   -12.8887   9.2101   10.8163
 H   -11.2647   8.7157   10.4529
 H   -11.4516   6.7347   11.8448
 H   -12.0258   8.1155   12.7372
 H   -13.4332   6.0685   12.984
 H   -14.3288   7.4771   12.4721
 H   -13.1175   8.4679   8.6671
 H   -12.8436   6.8557   6.5985
 H   -14.0743   4.7547   6.8598
 H   -13.2938   4.442   8.3956
 H   -15.0128   6.8449   7.6234
 H   -15.5637   5.5194   8.6085
 H   -10.0771   8.2672   8.7737
 H   -9.8664   7.1752   7.4527
 H   -10.281   5.2064   8.7699
 H   -11.6531   5.1111   9.8671
 H   -10.3628   6.3018   10.1124
 H   -10.6577   5.7849   6.0175
 H   -11.1387   4.3516   6.9493
 H   -12.0612   4.849   5.5362
 H   -12.1351   12.9699   8.0112
 H   -10.4508   12.9535   8.6729
 H   -11.0441   14.3334   7.7424
 H   -14.7805   4.1406   10.1918
 H   -14.293   4.1953   11.9597
 C   -15.3046   7.9436   9.9087
 H   -15.4648   8.5836   9.0326
 H   -16.2597   7.4544   10.1363
 H   -15.0747   8.613   10.7424
 C   -10.1393   10.6226   5.5129
 C   -10.1599   9.1389   5.7106
 C   -8.6923   8.6652   5.8957
 O   -7.8635   9.1877   6.6281
 O   -8.4818   7.5386   5.1456
 C   -7.1668   6.9685   5.2368
 C   -6.237   7.637   4.242
 O   -10.8052   8.5899   4.5661
 H   -12.0841   8.7553   6.6192
 H   -9.7342   11.0844   4.6226
 H   -6.776   7.0309   6.2588
 H   -7.2631   5.9051   4.9941
 H   -5.2482   7.1702   4.2611
 H   -6.6429   7.5641   3.2277
 H   -6.1245   8.7029   4.4639
 H   -10.4198   7.7033   4.4305

Compound **7_9**
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-13.0441	8.4704	10.2867
C	-13.2473	7.8042	11.6479
C	-14.3254	6.7306	11.6499
C	-14.1901	5.7727	10.4841
C	-14.0933	6.4335	9.0979
C	-12.9363	7.5042	9.0734
C	-11.4548	6.9766	8.7806
C	-11.4866	5.9795	7.5665
C	-12.5401	4.8779	7.7448
C	-13.9311	5.4621	7.9009
C	-14.2003	4.449	10.7239
C	-10.4685	8.1892	8.491
C	-10.9162	9.3434	7.5734
C	-10.0541	10.5856	7.7051
C	-10.0635	11.3586	6.4347
C	-10.8408	6.2496	10.0065
C	-10.1542	5.2827	7.242
O	-9.4778	10.9339	8.725
O	-9.615	12.6216	6.1765
C	-9.0836	13.3251	7.2933
H	-13.8974	9.1393	10.1135
H	-12.1796	9.1381	10.3452
H	-12.3127	7.3706	12.0114
H	-13.5111	8.5752	12.3828
H	-14.2835	6.1988	12.609
H	-15.3143	7.2023	11.6205
H	-13.1781	8.1162	8.1944
H	-11.7745	6.549	6.6778
H	-12.5417	4.2295	6.8588
H	-12.2876	4.2297	8.5895
H	-14.1634	5.9954	6.9676
H	-14.6666	4.6494	7.9539
H	-10.2379	8.6454	9.4642
H	-9.493	7.8148	8.1677
H	-9.8433	5.8564	9.7829
H	-11.449	5.4126	10.3522
H	-10.6886	6.9314	10.8464
H	-10.2236	4.7729	6.274
H	-9.3172	5.9776	7.1779
H	-9.9013	4.5197	7.9857
H	-9.8314	13.4326	8.0857
H	-8.1743	12.8412	7.6637
H	-8.8104	14.3295	6.9554
H	-14.1342	3.7043	9.9398
H	-14.2864	4.0592	11.7346
C	-15.4622	7.1374	8.8386
H	-15.4735	7.632	7.8597
H	-16.284	6.4108	8.8482
H	-15.7021	7.908	9.5764
C	-10.6195	10.5514	5.5278
C	-10.9399	9.1776	6.0466
C	-9.9029	8.2117	5.4275
O	-10.2063	7.3756	4.5811
O	-8.6401	8.4559	5.8686
C	-7.6214	7.6683	5.2393
C	-6.2996	7.9907	5.9077
O	-12.2698	8.882	5.6285
H	-11.9003	9.6912	7.9126
H	-10.765	10.8346	4.4939
H	-7.843	6.6018	5.3528
H	-7.572	7.9221	4.1747
H	-5.4845	7.4169	5.4581
H	-6.0726	9.0582	5.8184
H	-6.3444	7.7633	6.978
H	-12.1928	8.2677	4.8704

Compound **7**_10
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.3038	8.2973	10.655
C	-12.2533	7.4287	11.9118
C	-13.5278	6.6383	12.1501
C	-13.9716	5.8999	10.9056
C	-14.1269	6.7711	9.643
C	-12.8097	7.5995	9.3577
C	-11.6673	6.8714	8.5123
C	-12.3072	6.1092	7.288
C	-13.4509	5.1883	7.7203
C	-14.5599	5.9961	8.3715
C	-14.2259	4.5813	10.992
C	-10.5963	7.9174	7.9843
C	-11.0896	9.0129	7.0141
C	-11.1754	10.3941	7.6333
C	-10.7437	11.4449	6.6802
C	-10.8618	5.8738	9.3826
C	-11.3316	5.2978	6.4211
O	-11.5992	10.6393	8.7531
O	-10.8992	12.7706	6.9407
C	-10.4222	13.6627	5.9423
H	-12.9704	9.1441	10.8652
H	-11.3181	8.7463	10.511
H	-11.4064	6.7388	11.8748
H	-12.0649	8.073	12.7797
H	-13.3578	5.9475	12.9856
H	-14.3261	7.311	12.4837
H	-13.1382	8.4197	8.7039
H	-12.7531	6.8513	6.6157
H	-13.8697	4.6837	6.8401
H	-13.0877	4.3946	8.3797
H	-14.9291	6.7094	7.6204
H	-15.4156	5.3423	8.5824
H	-10.0933	8.39	8.8361
H	-9.8092	7.3285	7.5053
H	-10.1224	5.3232	8.7923
H	-11.4969	5.1351	9.8745
H	-10.2788	6.3941	10.1477
H	-11.851	4.9037	5.5395
H	-10.505	5.9061	6.0495
H	-10.9198	4.4381	6.9579
H	-10.6053	14.6848	6.2866
H	-9.3438	13.5437	5.793
H	-10.9619	13.5211	5.
H	-14.5715	3.9865	10.1554
H	-14.1032	4.0438	11.9285
C	-15.3034	7.7579	9.9177
H	-16.2317	7.2131	10.1296
H	-15.1187	8.4275	10.7624
H	-15.4914	8.4	9.0487
C	-10.2326	10.7981	5.6274
C	-10.1975	9.307	5.7858
C	-8.7143	8.8797	5.9528
O	-7.876	9.4573	6.6309
O	-8.4946	7.7213	5.2559
C	-7.1604	7.2106	5.3739
C	-7.0843	5.9114	4.5963
O	-10.811	8.7725	4.616
H	-12.1046	8.793	6.6662
H	-9.8265	11.2773	4.748
H	-6.4513	7.9353	4.9588
H	-6.9264	7.0242	6.428
H	-6.0814	5.4794	4.655
H	-7.8057	5.1861	4.9871
H	-7.3376	6.0766	3.5438
H	-10.4802	7.8586	4.5245

Compound **7**_11
Charge = 0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.1693	8.2718	10.6293
C	-12.0753	7.3883	11.8731
C	-13.3535	6.6228	12.167
C	-13.8751	5.9082	10.9389
C	-14.074	6.7968	9.6946
C	-12.7545	7.5997	9.352
C	-11.6725	6.8563	8.4437
C	-12.3903	6.1247	7.2443
C	-13.5303	5.2225	7.7233
C	-14.5873	6.0455	8.4387
C	-14.1535	4.5944	11.0244
C	-10.6034	7.8824	7.8758
C	-11.1116	8.9998	6.9395
C	-11.1479	10.3745	7.5776
C	-10.7311	11.4287	6.6215
C	-10.8488	5.8294	9.2616
C	-11.478	5.3058	6.3177
O	-11.5259	10.6142	8.7148
O	-10.8524	12.7537	6.9025
C	-10.3949	13.649	5.8978
H	-12.806	9.1302	10.8814
H	-11.1825	8.7014	10.4407
H	-11.2467	6.6808	11.7866
H	-11.8297	8.0185	12.737
H	-13.1572	5.9191	12.9858
H	-14.119	7.3086	12.5471
H	-13.0966	8.4337	8.723
H	-12.8541	6.8853	6.6056
H	-14.0038	4.7379	6.8596
H	-13.1517	4.4131	8.3543
H	-14.9788	6.775	7.7149
H	-15.4451	5.4074	8.686
H	-10.0476	8.3329	8.7065
H	-9.8572	7.279	7.3526
H	-10.1527	5.2692	8.629
H	-11.4758	5.0995	9.7763
H	-10.2163	6.3265	10.0025
H	-12.0512	4.9308	5.4616
H	-10.662	5.904	5.9079
H	-11.0533	4.4332	6.8225
H	-10.5464	14.6701	6.2601
H	-9.325	13.5121	5.7083
H	-10.9706	13.5286	4.9741
H	-14.5533	4.0167	10.1999
H	-13.996	4.0439	11.9479
C	-15.2131	7.8058	10.0381
H	-16.1415	7.2788	10.2905
H	-14.9716	8.4614	10.8794
H	-15.4297	8.4617	9.1863
C	-10.2703	10.7854	5.5436
C	-10.2574	9.2921	5.6838
C	-8.7762	8.8376	5.7954
O	-7.9124	9.3853	6.4662
O	-8.5956	7.6957	5.0607
C	-7.2722	7.1386	5.0907
C	-7.1242	6.2094	6.281
O	-10.9215	8.7831	4.5305
H	-12.1422	8.8031	6.6257
H	-9.8873	11.2677	4.6556
H	-7.144	6.5715	4.163
H	-6.5086	7.9246	5.0962
H	-7.242	6.7551	7.2225
H	-7.8982	5.4351	6.2633
H	-6.1423	5.728	6.2775
H	-10.6052	7.8672	4.4123

Diastereomer **III**_1
Charge = 0 Multiplicity = 1
Symbolic Z-Matrix:

C	-11.4721	9.77	11.2141
C	-11.3428	9.8605	9.6938
C	-11.7308	11.2188	9.135
C	-11.0582	12.35	9.8831
C	-11.2541	12.3377	11.4118
C	-10.8406	10.9398	12.0245
C	-9.2958	10.739	12.3837
C	-8.7418	12.0231	13.1119
C	-9.04	13.3016	12.3254
C	-10.5391	13.4876	12.1685
C	-10.3841	13.2793	9.1813
C	-9.0958	9.4757	13.3211
C	-9.7731	9.5292	14.7077
C	-10.8828	8.5063	14.8651
C	-10.7822	7.7833	16.158
C	-8.4479	10.4471	11.1209
C	-7.2442	12.0015	13.4555
O	-11.7837	8.3404	14.0544
O	-11.6265	6.8621	16.7106
C	-12.715	6.4508	15.8921
H	-12.5431	9.7323	11.4535
H	-11.0817	8.8015	11.5356
H	-10.3257	9.6199	9.3744
H	-11.9795	9.0918	9.2382
H	-11.4788	11.2404	8.0671
H	-12.8187	11.3428	9.1818
H	-11.3479	10.9082	12.9986
H	-9.2644	12.126	14.0699
H	-8.6447	14.1687	12.8702
H	-8.5305	13.2941	11.3574
H	-10.9642	13.5757	13.1789
H	-10.7413	14.4555	11.6928
H	-9.4199	8.5725	12.7913
H	-8.0164	9.3357	13.4356
H	-7.3807	10.3761	11.3547
H	-8.5591	11.2134	10.352
H	-8.7049	9.4778	10.6846
H	-6.6162	12.0433	12.5606
H	-6.9868	12.8745	14.0668
H	-6.9649	11.1198	14.0361
H	-13.2729	5.6851	16.4397
H	-13.398	7.2844	15.7004
H	-12.3602	6.	14.9596
H	-9.8963	14.1316	9.6386
H	-10.3039	13.2203	8.0992
C	-12.7721	12.5845	11.6737
H	-12.9883	12.61	12.7486
H	-13.0921	13.5453	11.2521
H	-13.4167	11.811	11.247
C	-9.6521	8.1994	16.7294
C	-8.8779	9.1917	15.9243
C	-8.5853	10.4625	16.7547
O	-7.4437	10.8707	16.9469
O	-9.721	11.0518	17.2171
C	-9.5409	12.2585	17.9734
C	-9.4612	13.4512	17.0386
O	-7.673	8.5248	15.5618
H	-10.2736	10.4897	14.8646
H	-9.3022	7.8247	17.6821
H	-10.4139	12.3597	18.6264
H	-8.6588	12.1946	18.6205
H	-9.3951	14.3843	17.605
H	-8.5877	13.3788	16.383
H	-10.3427	13.4918	16.3901
H	-6.9363	9.1241	15.7997

Diastereomer **III**_2
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-11.5144	9.7801	11.2252
C	-11.4206	9.8209	9.7001
C	-11.778	11.174	9.1094
C	-11.0499	12.3037	9.806
C	-11.2076	12.3437	11.3388
C	-10.8247	10.9516	11.9842
C	-9.2791	10.7101	12.3117
C	-8.6664	11.9959	12.9888
C	-8.9408	13.2594	12.1698
C	-10.4363	13.4912	12.0418
C	-10.3632	13.1883	9.0599
C	-9.0952	9.4673	13.2791
C	-9.7328	9.5788	14.6813
C	-10.8799	8.6067	14.8875
C	-10.7675	7.8915	16.1836
C	-8.4729	10.3554	11.0375
C	-7.1627	11.9339	13.2995
O	-11.8135	8.4715	14.1089
O	-11.629	7.0085	16.7708
C	-12.7592	6.6351	15.9915
H	-12.5797	9.7854	11.4913
H	-11.1479	8.809	11.5663
H	-10.4203	9.5369	9.3637
H	-12.0933	9.0606	9.2838
H	-11.5525	11.1553	8.0356
H	-12.8597	11.3357	9.1789
H	-11.3074	10.9662	12.9713
H	-9.1623	12.1451	13.9553
H	-8.5039	14.1289	12.6778
H	-8.4553	13.2054	11.1909
H	-10.8338	13.6248	13.0585
H	-10.6178	14.4505	11.5408
H	-9.4611	8.5607	12.7835
H	-8.0179	9.2966	13.3695
H	-7.4029	10.257	11.2471
H	-8.5794	11.1025	10.2493
H	-8.7711	9.3829	10.6361
H	-6.862	12.8164	13.8764
H	-6.8997	11.0619	13.9021
H	-6.5545	11.9259	12.39
H	-13.3289	5.8964	16.5635
H	-13.4144	7.4939	15.8149
H	-12.4533	6.1636	15.052
H	-9.836	14.0367	9.4789
H	-10.3123	13.0943	7.9785
C	-12.7095	12.6489	11.6296
H	-12.8977	12.7137	12.7081
H	-13.0084	13.6069	11.1865
H	-13.3897	11.885	11.2425
C	-9.6056	8.2689	16.7166
C	-8.8199	9.2258	15.8805
C	-8.4672	10.495	16.6894
O	-7.31	10.8723	16.849
O	-9.5705	11.1202	17.1818
C	-9.2929	12.3093	17.9315
C	-10.6139	12.9017	18.3814
O	-7.6458	8.5161	15.4988
H	-10.1868	10.5632	14.8314
H	-9.2417	7.8897	17.6623
H	-8.6807	12.0595	18.8051
H	-8.7606	13.0292	17.2997
H	-10.4548	13.8155	18.9606
H	-11.2452	13.1354	17.5177
H	-11.1683	12.1849	18.9961
H	-6.8852	9.0972	15.7043

Diastereomer **III**_3
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-11.2487	9.5955	11.0774
C	-10.9706	9.7127	9.5788
C	-11.4931	11.0008	8.967
C	-11.0794	12.2147	9.7711
C	-11.4368	12.1653	11.2697
C	-10.8912	10.8417	11.9403
C	-9.3838	10.8665	12.471
C	-9.0954	12.2196	13.2278
C	-9.5001	13.4406	12.3984
C	-10.9853	13.4031	12.0868
C	-10.4791	13.2377	9.1357
C	-9.1118	9.6482	13.4516
C	-9.9499	9.5903	14.7491
C	-10.948	8.4453	14.7506
C	-10.9025	7.6767	16.0183
C	-8.3693	10.692	11.3133
C	-7.6471	12.4219	13.7016
O	-11.7288	8.2133	13.8381
O	-11.6827	6.6368	16.4387
C	-12.6857	6.2058	15.5269
H	-12.3216	9.396	11.1997
H	-10.7534	8.6949	11.4485
H	-9.9006	9.6281	9.3732
H	-11.4328	8.8602	9.0656
H	-11.1336	11.0654	7.9322
H	-12.586	10.9619	8.8956
H	-11.4923	10.7329	12.8535
H	-9.7123	12.2449	14.1338
H	-9.2947	14.356	12.9684
H	-8.8986	13.5103	11.4872
H	-11.5216	13.4197	13.0467
H	-11.2787	14.3332	11.5838
H	-9.229	8.7063	12.9027
H	-8.046	9.6756	13.6972
H	-7.3347	10.7684	11.663
H	-8.4997	11.4353	10.5247
H	-8.4411	9.696	10.8676
H	-7.5813	13.3153	14.3335
H	-7.2842	11.5846	14.3004
H	-6.9586	12.5738	12.8647
H	-13.2252	5.3756	15.9931
H	-13.4096	7.0035	15.332
H	-12.2402	5.8323	14.5994
H	-10.1773	14.1514	9.6331
H	-10.2753	13.1971	8.069
C	-12.994	12.1839	11.3627
H	-13.3275	12.1739	12.4074
H	-13.4044	13.0881	10.8963
H	-13.467	11.3247	10.8789
C	-9.9	8.194	16.7274
C	-9.1685	9.3119	16.0578
C	-9.2277	10.5739	16.9568
O	-10.2158	10.9818	17.5518
O	-8.0093	11.1978	16.9432
C	-7.9575	12.3974	17.7266
C	-6.5422	12.938	17.6693
O	-7.853	8.8215	15.8448
H	-10.5643	10.489	14.8696
H	-9.6184	7.8207	17.7031
H	-8.6536	13.1351	17.3124
H	-8.2266	12.1756	18.7654
H	-6.4524	13.8588	18.2524
H	-5.8326	12.2012	18.06
H	-6.2486	13.1443	16.635
H	-7.2569	9.594	15.8855

Diastereomer **III**_4
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-11.4883	9.7231	11.1706
C	-11.3636	9.7374	9.6472
C	-11.747	11.0681	9.0228
C	-11.0663	12.2315	9.7119
C	-11.2575	12.2962	11.24
C	-10.8487	10.9284	11.9205
C	-9.3041	10.7383	12.2843
C	-8.7434	12.0538	12.949
C	-9.0361	13.2931	12.0998
C	-10.5346	13.4789	11.936
C	-10.3896	13.1212	8.9629
C	-9.1045	9.5196	13.2788
C	-9.7737	9.6371	14.6659
C	-10.8978	8.6365	14.8637
C	-10.7868	7.9348	16.1671
C	-8.4613	10.3838	11.0339
C	-7.2456	12.0415	13.2926
O	-11.8151	8.4697	14.0717
O	-11.6314	7.0302	16.746
C	-12.7337	6.6141	15.9487
H	-12.5588	9.7026	11.4146
H	-11.1016	8.7697	11.5382
H	-10.3487	9.4762	9.3372
H	-12.0053	8.9502	9.2323
H	-11.4983	11.0354	7.9545
H	-12.8341	11.1997	9.0668
H	-11.352	10.9478	12.8972
H	-9.2643	12.2066	13.9017
H	-8.6353	14.1844	12.5997
H	-8.5284	13.2347	11.1325
H	-10.9574	13.6206	12.9412
H	-10.7326	14.4227	11.4123
H	-9.4335	8.5936	12.793
H	-8.0248	9.3823	13.3936
H	-7.3935	10.3209	11.2672
H	-8.5729	11.1125	10.2294
H	-8.7226	9.3956	10.6453
H	-6.9827	12.9436	13.8575
H	-6.9712	11.1897	13.9186
H	-6.6178	12.033	12.3966
H	-13.2895	5.861	16.5158
H	-13.4133	7.4495	15.7533
H	-12.3948	6.1462	15.0187
H	-9.8957	13.9924	9.3758
H	-10.3131	13.0081	7.8847
C	-12.7735	12.563	11.4937
H	-12.9862	12.6429	12.5666
H	-13.0902	13.5033	11.0258
H	-13.4231	11.7725	11.1077
C	-9.6471	8.3521	16.7179
C	-8.8769	9.3277	15.889
C	-8.5866	10.6166	16.6919
O	-7.4468	11.0396	16.862
O	-9.7216	11.1966	17.1678
C	-9.5417	12.4003	17.9291
C	-9.2848	12.0627	19.3855
O	-7.6701	8.656	15.542
H	-10.2565	10.6112	14.791
H	-9.2892	7.9922	17.6733
H	-8.7388	13.0186	17.5117
H	-10.4693	12.9753	17.8417
H	-9.2042	12.973	19.9863
H	-10.0958	11.4455	19.7857
H	-8.3611	11.4864	19.4982
H	-6.9362	9.2711	15.7458

Diastereomer **III**_5
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-11.9688	10.7696	11.9802
C	-12.3425	10.9235	10.5057
C	-12.0937	12.3194	9.9539
C	-10.7241	12.8512	10.3235
C	-10.3793	12.7977	11.8217
C	-10.5802	11.339	12.3851
C	-9.3678	10.311	12.2065
C	-8.0249	11.0192	12.6137
C	-7.8349	12.3605	11.8926
C	-8.9699	13.3179	12.2047
C	-9.9364	13.3511	9.3544
C	-9.6068	9.0017	13.0735
C	-10.121	9.13	14.5227
C	-10.6541	7.8046	15.0397
C	-10.2479	7.5682	16.4475
C	-9.2412	9.8023	10.7462
C	-6.7418	10.1972	12.4007
O	-11.3815	7.0583	14.3983
O	-10.611	6.57	17.3063
C	-11.4251	5.5435	16.7514
H	-12.7343	11.2872	12.5732
H	-12.0686	9.7175	12.2624
H	-11.8056	10.1968	9.8915
H	-13.4043	10.6757	10.3823
H	-12.2295	12.2914	8.8653
H	-12.8631	13.005	10.3269
H	-10.638	11.4933	13.4704
H	-8.0812	11.2469	13.682
H	-6.8982	12.8249	12.2278
H	-7.7265	12.213	10.8138
H	-8.9382	13.5132	13.2866
H	-8.7701	14.2896	11.7356
H	-10.3455	8.3937	12.5325
H	-8.7148	8.3656	13.06
H	-8.3822	9.1334	10.627
H	-9.1257	10.6105	10.0228
H	-10.1048	9.2018	10.4509
H	-5.8906	10.7055	12.8689
H	-6.7958	9.2009	12.842
H	-6.5002	10.0858	11.3387
H	-11.6031	4.7998	17.5341
H	-12.398	5.9386	16.4424
H	-10.9155	5.0393	15.924
H	-8.9552	13.7694	9.5445
H	-10.2579	13.3644	8.3164
C	-11.3591	13.775	12.5443
H	-11.1717	13.7961	13.6246
H	-11.237	14.7991	12.1705
H	-12.4119	13.5074	12.4191
C	-9.4005	8.5503	16.7552
C	-9.1269	9.5088	15.6381
C	-9.3249	10.9528	16.1548
O	-8.3817	11.71	16.3666
O	-10.6316	11.255	16.3773
C	-10.8625	12.5905	16.8427
C	-12.3602	12.8211	16.8835
O	-7.7776	9.2623	15.264
H	-11.0092	9.7693	14.5432
H	-8.9167	8.6252	17.7203
H	-10.4388	12.7041	17.8464
H	-10.398	13.3118	16.1608
H	-12.5905	13.83	17.2368
H	-12.7971	12.6863	15.8882
H	-12.8445	12.095	17.5448
H	-7.2363	9.9612	15.6834

Diastereomer **III_6**

Charge =   0 Multiplicity = 1

Symbolic Z-Matrix:

C	-11.4517	9.7259	11.2152
C	-11.2913	9.8112	9.6973
C	-11.6931	11.1584	9.1222
C	-11.0601	12.3065	9.8791
C	-11.2916	12.2981	11.4027
C	-10.8642	10.9136	12.0334
C	-9.3252	10.7431	12.4337
C	-8.7979	12.0451	13.1487
C	-9.1182	13.3113	12.3512
C	-10.6175	13.4638	12.1709
C	-10.3908	13.2467	9.1873
C	-9.1317	9.5015	13.4026
C	-9.8737	9.5514	14.7602
C	-10.9459	8.4775	14.839
C	-10.7675	7.5984	16.0188
C	-8.4463	10.4368	11.1953
C	-7.2965	12.0595	13.4804
O	-11.8626	8.3699	14.0359
O	-11.5094	6.5279	16.4311
C	-12.6233	6.1926	15.6126
H	-12.5267	9.6656	11.431
H	-11.0462	8.7682	11.5508
H	-10.2631	9.5891	9.4007
H	-11.9027	9.0276	9.2325
H	-11.4173	11.1795	8.0603
H	-12.784	11.261	9.1437
H	-11.3958	10.8794	12.9939
H	-9.3199	12.1424	14.108
H	-8.7496	14.1905	12.8956
H	-8.5951	13.3091	11.3903
H	-11.0614	13.5426	13.1739
H	-10.8333	14.4263	11.69
H	-9.4121	8.5847	12.8701
H	-8.056	9.3844	13.5614
H	-7.3848	10.3706	11.4547
H	-8.5426	11.1938	10.4149
H	-8.6894	9.4609	10.7659
H	-7.0519	12.9401	14.0853
H	-6.99	11.1862	14.0582
H	-6.6775	12.1145	12.5797
H	-13.3542	7.0072	15.5903
H	-12.3015	5.9144	14.6039
H	-13.1127	5.3204	16.0567
H	-9.9338	14.1128	9.6504
H	-10.2857	13.1842	8.1075
C	-12.8199	12.5159	11.6277
H	-13.0616	12.5449	12.6971
H	-13.1494	13.4669	11.1914
H	-13.4386	11.7262	11.1923
C	-9.6903	8.0526	16.6573
C	-9.0378	9.24	16.0279
C	-9.1238	10.4516	16.9933
O	-10.0431	10.6867	17.7651
O	-8.0308	11.2556	16.8053
C	-7.9752	12.4257	17.6369
C	-8.7659	13.5603	17.0124
O	-7.7025	8.84	15.7599
H	-10.4087	10.4975	14.8957
H	-9.3127	7.6009	17.5652
H	-8.3242	12.2047	18.6522
H	-6.9212	12.7116	17.715
H	-9.8212	13.2929	16.9002
H	-8.6972	14.4631	17.6259
H	-8.388	13.7881	16.011
H	-7.1664	9.6552	15.7347

Diastereomer **III_7**
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-11.3136	9.6054	11.082
C	-11.0703	9.6806	9.5747
C	-11.5549	10.977	8.9491
C	-11.0709	12.1886	9.7166
C	-11.3907	12.1842	11.2244
C	-10.8824	10.8529	11.9086
C	-9.3616	10.8256	12.4004
C	-8.996	12.1807	13.1194
C	-9.3741	13.4004	12.2757
C	-10.8675	13.4179	12.0041
C	-10.4463	13.173	9.0447
C	-9.1164	9.6184	13.4013
C	-9.9257	9.6252	14.7187
C	-10.9521	8.5068	14.7739
C	-10.8864	7.7607	16.0539
C	-8.3861	10.5832	11.2216
C	-7.5269	12.3322	13.5462
O	-11.7651	8.2778	13.8892
O	-11.6734	6.7429	16.5137
C	-12.7092	6.3153	15.6377
H	-12.3902	9.4533	11.2358
H	-10.8464	8.6926	11.4598
H	-10.0104	9.5471	9.3437
H	-11.5807	8.8381	9.0915
H	-11.22	11.0056	7.9044
H	-12.6499	10.9823	8.9059
H	-11.464	10.7871	12.8383
H	-9.5845	12.2494	14.042
H	-9.1162	14.3177	12.8207
H	-8.7954	13.4272	11.3476
H	-11.3765	13.475	12.9771
H	-11.1363	14.3493	11.4899
H	-9.2874	8.6713	12.876
H	-8.0446	9.6032	13.62
H	-7.3404	10.6222	11.5434
H	-8.5054	11.3149	10.4205
H	-8.5118	9.5821	10.8001
H	-7.4063	13.2307	14.1628
H	-7.1781	11.4894	14.1456
H	-6.8594	12.4452	12.6863
H	-13.2502	5.503	16.1328
H	-13.4238	7.1229	15.4493
H	-12.2968	5.9184	14.7046
H	-10.0947	14.0833	9.5149
H	-10.2723	13.1026	7.9743
C	-12.9428	12.2695	11.3563
H	-13.249	12.2942	12.4091
H	-13.3277	13.1804	10.8816
H	-13.4632	11.4212	10.9029
C	-9.8576	8.2736	16.7275
C	-9.126	9.3682	16.0206
C	-9.157	10.6527	16.8892
O	-10.1196	11.062	17.5232
O	-7.9487	11.2894	16.7947
C	-7.8357	12.5215	17.524
C	-7.4208	12.2449	18.9565
O	-7.8182	8.8611	15.8001
H	-10.5146	10.543	14.8228
H	-9.5582	7.9146	17.7033
H	-7.064	13.1172	17.0255
H	-8.7666	13.0979	17.4777
H	-7.2738	13.1796	19.505
H	-8.1774	11.6496	19.4772
H	-6.4896	11.6695	18.9826
H	-7.2182	9.6313	15.7901

Diastereomer **III**_8
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-11.4649	9.8474	11.1244
C	-11.3052	9.9518	9.6078
C	-11.6559	11.3235	9.0572
C	-10.9754	12.4331	9.8303
C	-11.2005	12.4078	11.3549
C	-10.8258	10.9955	11.9594
C	-9.2923	10.76	12.3446
C	-8.7271	12.0251	13.0974
C	-8.9856	13.3178	12.3202
C	-10.4776	13.5349	12.1378
C	-10.2704	13.3567	9.1517
C	-9.1344	9.4823	13.2708
C	-9.8373	9.5321	14.6444
C	-10.9767	8.5405	14.7619
C	-10.918	7.7741	16.0298
C	-8.4267	10.4656	11.0945
C	-7.2367	11.9705	13.4679
O	-11.8779	8.4156	13.9442
O	-11.8872	6.8883	16.3858
C	-11.6769	6.1859	17.6034
H	-12.5407	9.8285	11.3433
H	-11.0998	8.8678	11.4422
H	-10.2873	9.6945	9.3046
H	-11.9482	9.2009	9.1318
H	-11.3835	11.3517	7.9946
H	-12.7419	11.4685	9.0852
H	-11.3512	10.9636	12.9239
H	-9.2649	12.1277	14.047
H	-8.5838	14.1709	12.882
H	-8.4584	13.3109	11.3617
H	-10.9198	13.6202	13.1411
H	-10.652	14.5119	11.6695
H	-9.4651	8.5916	12.7242
H	-8.0603	9.3209	13.4046
H	-7.3657	10.3711	11.3472
H	-8.5086	11.2425	10.3325
H	-8.6942	9.5066	10.6423
H	-6.9742	12.8309	14.0948
H	-6.9848	11.0766	14.0421
H	-6.5917	12.0113	12.585
H	-12.5237	5.51	17.7547
H	-10.7652	5.5811	17.5549
H	-11.6391	6.8765	18.4525
H	-9.775	14.1942	9.6276
H	-10.1713	13.3078	8.0706
C	-12.718	12.6816	11.5913
H	-12.9539	12.6995	12.6622
H	-13.0112	13.6531	11.1747
H	-13.3695	11.9257	11.1439
C	-9.7861	8.1428	16.6379
C	-8.9785	9.1438	15.8719
C	-8.6826	10.3925	16.7345
O	-7.5424	10.8071	16.9198
O	-9.8169	10.9603	17.2265
C	-9.6377	12.1574	17.9984
C	-9.5802	13.3646	17.0807
O	-7.7755	8.4641	15.5277
H	-10.3112	10.5044	14.8109
H	-9.4382	7.7475	17.5817
H	-10.503	12.241	18.6639
H	-8.7467	12.0913	18.6333
H	-9.5156	14.2897	17.6603
H	-8.7142	13.3102	16.4135
H	-10.4699	13.4066	16.4437
H	-7.0439	9.1004	15.661

Diastereomer **III_9**

Charge =   0 Multiplicity = 1

Symbolic Z-Matrix:

C	-11.5203	9.8635	11.1402
C	-11.402	9.9105	9.617
C	-11.7139	11.2761	9.0294
C	-10.9667	12.382	9.7438
C	-11.1472	12.4171	11.2743
C	-10.8113	11.0117	11.9168
C	-9.2779	10.7269	12.2661
C	-8.6418	11.9919	12.9605
C	-8.8701	13.2673	12.1456
C	-10.3568	13.5396	11.9963
C	-10.2454	13.2524	9.0138
C	-9.1416	9.4735	13.2279
C	-9.799	9.5911	14.6202
C	-10.9794	8.6563	14.7925
C	-10.9046	7.891	16.0599
C	-8.462	10.3587	11.0019
C	-7.145	11.8884	13.2928
O	-11.9185	8.5708	14.0133
O	-11.894	7.0444	16.4539
C	-11.669	6.34	17.6676
H	-12.5891	9.896	11.39
H	-11.1854	8.8809	11.4811
H	-10.4046	9.6016	9.2941
H	-12.0883	9.171	9.1859
H	-11.4724	11.2575	7.959
H	-12.7918	11.4663	9.0832
H	-11.3079	11.0338	12.8968
H	-9.148	12.1482	13.9205
H	-8.4182	14.1217	12.6658
H	-8.3713	13.2063	11.1739
H	-10.7662	13.6776	13.0075
H	-10.505	14.5062	11.4986
H	-9.5225	8.5799	12.7199
H	-8.0708	9.2746	13.3342
H	-7.3983	10.2304	11.227
H	-8.5364	11.1132	10.217
H	-8.7797	9.397	10.5896
H	-6.8297	12.7594	13.8795
H	-6.9142	11.0065	13.8939
H	-6.5238	11.8696	12.3924
H	-12.5355	5.6981	17.852
H	-10.7835	5.7	17.5913
H	-11.5752	7.0325	18.5108
H	-9.7026	14.0841	9.4461
H	-10.1805	13.1632	7.9327
C	-12.6449	12.7605	11.5439
H	-12.848	12.8239	12.6198
H	-12.9112	13.7287	11.1023
H	-13.339	12.0174	11.1416
C	-9.7386	8.2172	16.6259
C	-8.9225	9.1882	15.8309
C	-8.5723	10.435	16.6757
O	-7.4194	10.8306	16.8201
O	-9.6759	11.0237	17.211
C	-9.4047	12.1987	17.9851
C	-10.7258	12.7481	18.4861
O	-7.7467	8.4728	15.4664
H	-10.2199	10.589	14.7778
H	-9.3732	7.8118	17.5588
H	-8.7635	11.9401	18.835
H	-8.906	12.9471	17.359
H	-10.5716	13.6497	19.0855
H	-11.3856	12.99	17.6463
H	-11.247	12.0026	19.0958
H	-6.9972	9.0954	15.5594

Diastereomer **III**_10
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-11.9861	10.6894	11.899
C	-12.2975	10.759	10.4036
C	-12.0757	12.1352	9.7917
C	-10.756	12.7541	10.2065
C	-10.4901	12.7822	11.721
C	-10.6439	11.3387	12.3359
C	-9.3748	10.3673	12.2399
C	-8.0905	11.1519	12.6914
C	-7.9336	12.4857	11.947
C	-9.1328	13.3898	12.1596
C	-9.9449	13.2576	9.2588
C	-9.5899	9.0675	13.1263
C	-10.1187	9.2046	14.5715
C	-10.739	7.8957	15.0348
C	-10.2522	7.4983	16.378
C	-9.1512	9.8289	10.8016
C	-6.7586	10.3944	12.5427
O	-11.5777	7.2734	14.396
O	-10.6044	6.4314	17.155
C	-11.4995	5.5004	16.5581
H	-12.7997	11.1987	12.432
H	-12.0549	9.6489	12.2286
H	-11.7087	10.0241	9.8503
H	-13.3428	10.4645	10.2465
H	-12.1467	12.0447	8.7003
H	-12.8957	12.8019	10.0832
H	-10.7523	11.531	13.4118
H	-8.2079	11.3931	13.7532
H	-7.044	13.0084	12.3224
H	-7.7534	12.3177	10.8807
H	-9.172	13.6241	13.2334
H	-8.9576	14.3534	11.6647
H	-10.3028	8.4318	12.583
H	-8.6807	8.4555	13.1295
H	-8.2555	9.2011	10.743
H	-9.037	10.6221	10.0622
H	-9.9676	9.1776	10.4817
H	-5.9607	10.9366	13.0636
H	-6.7877	9.3885	12.9633
H	-6.4537	10.3099	11.4943
H	-11.6511	4.6817	17.2683
H	-12.4748	5.9603	16.3701
H	-11.0744	5.0729	15.6443
H	-8.9992	13.7369	9.4822
H	-10.2105	13.2119	8.2061
C	-11.5565	13.7384	12.3404
H	-11.4304	13.8218	13.4253
H	-11.4657	14.7488	11.9227
H	-12.5863	13.4107	12.1736
C	-9.3462	8.4111	16.7265
C	-9.1138	9.483	15.7089
C	-9.3503	10.8649	16.3613
O	-8.4514	11.6905	16.4928
O	-10.6328	11.0234	16.7869
C	-10.9277	12.2626	17.4487
C	-11.2829	13.3268	16.4287
O	-7.7634	9.3169	15.3018
H	-10.9591	9.9042	14.6068
H	-8.8021	8.3696	17.661
H	-11.7855	12.0788	18.1039
H	-10.0956	12.5795	18.0877
H	-11.5712	14.2585	16.9234
H	-10.4369	13.5312	15.7651
H	-12.1111	12.9908	15.7962
H	-7.272	10.0998	15.6236

Diastereomer **III**_11
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-11.2394	9.6697	10.9911
C	-10.9338	9.7993	9.4989
C	-11.4246	11.1029	8.8935
C	-11.0047	12.3006	9.7186
C	-11.3888	12.2396	11.2103
C	-10.8763	10.8997	11.8746
C	-9.3782	10.8928	12.431
C	-9.0802	12.2325	13.2078
C	-9.4511	13.4694	12.3861
C	-10.9313	13.4602	12.0495
C	-10.3771	13.3208	9.1055
C	-9.1423	9.6589	13.4019
C	-10.0041	9.5961	14.6837
C	-11.0298	8.4793	14.6395
C	-11.0133	7.6559	15.8702
C	-8.3472	10.7145	11.2884
C	-7.6367	12.4059	13.7066
O	-11.8181	8.293	13.7229
O	-11.8991	6.6445	16.0777
C	-11.7609	5.9334	17.3006
H	-12.3174	9.4868	11.0926
H	-10.7654	8.7567	11.36
H	-9.862	9.6993	9.3102
H	-11.4012	8.9606	8.9679
H	-11.0465	11.1733	7.8657
H	-12.5166	11.083	8.8032
H	-11.4942	10.7913	12.7766
H	-9.7113	12.2576	14.104
H	-9.2405	14.3747	12.9702
H	-8.8333	13.5397	11.486
H	-11.4834	13.4744	13.0004
H	-11.2008	14.4007	11.5527
H	-9.2633	8.7255	12.8392
H	-8.081	9.668	13.6667
H	-7.3175	10.7689	11.6563
H	-8.4515	11.4691	10.5067
H	-8.4282	9.7251	10.8297
H	-7.5664	13.2928	14.3471
H	-7.2979	11.5575	14.3039
H	-6.9321	12.5534	12.8824
H	-10.7843	5.4415	17.3598
H	-11.9138	6.5962	18.1589
H	-12.5323	5.1582	17.3302
H	-10.0692	14.2236	9.6186
H	-10.1559	13.2889	8.042
C	-12.9468	12.2829	11.2769
H	-13.2983	12.2664	12.3157
H	-13.3342	13.199	10.8143
H	-13.4254	11.4372	10.7752
C	-10.0089	8.1234	16.6168
C	-9.2558	9.2606	15.9985
C	-9.3204	10.4884	16.9432
O	-10.2971	10.8421	17.5894
O	-8.1216	11.1482	16.9118
C	-8.0751	12.3177	17.74
C	-6.6677	12.8788	17.6877
O	-7.9379	8.7678	15.8052
H	-10.5941	10.509	14.8172
H	-9.7251	7.7254	17.5809
H	-8.7861	13.0602	17.3614
H	-8.3284	12.0546	18.7731
H	-6.3883	13.1286	16.6592
H	-6.583	13.7777	18.3047
H	-5.9442	12.1371	18.0421
H	-7.3459	9.5444	15.8104

Diastereomer **III**_12
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-11.9757	10.6836	11.8735
C	-12.3197	10.7994	10.3883
C	-12.1013	12.1925	9.817
C	-10.7568	12.7717	10.2063
C	-10.444	12.756	11.7124
C	-10.6146	11.3024	12.2992
C	-9.3687	10.3084	12.1683
C	-8.0572	11.0648	12.5909
C	-7.8901	12.3964	11.8466
C	-9.0593	13.3254	12.1151
C	-9.9628	13.277	9.245
C	-9.5886	9.0094	13.0558
C	-10.1455	9.1474	14.4886
C	-10.6458	7.8129	15.0154
C	-10.2558	7.6067	16.4324
C	-9.1935	9.7758	10.7216
C	-6.7456	10.2777	12.4249
O	-11.3382	7.0358	14.3718
O	-10.5968	6.6048	17.296
C	-11.361	5.5421	16.7383
H	-12.7701	11.1882	12.4391
H	-12.0501	9.6342	12.1728
H	-11.7465	10.0792	9.7999
H	-13.3702	10.5165	10.2456
H	-12.2123	12.1415	8.7264
H	-12.8991	12.8607	10.161
H	-10.7023	11.4747	13.38
H	-8.1459	11.3128	13.6524
H	-6.9751	12.8949	12.1923
H	-7.7537	12.2309	10.7736
H	-9.0571	13.5424	13.1933
H	-8.8778	14.2934	11.6313
H	-10.2927	8.3672	12.5081
H	-8.6766	8.4024	13.0785
H	-8.3123	9.1313	10.6349
H	-9.0859	10.5731	9.985
H	-10.0317	9.1438	10.419
H	-5.9209	10.8216	12.9005
H	-6.7798	9.29	12.8872
H	-6.4764	10.1508	11.3713
H	-11.5237	4.7998	17.5258
H	-12.3431	5.8962	16.4092
H	-10.8184	5.0498	15.9249
H	-8.9987	13.7278	9.4484
H	-10.2613	13.2616	8.2002
C	-11.4676	13.7163	12.3957
H	-11.3053	13.7611	13.4795
H	-11.3668	14.737	12.0065
H	-12.5091	13.4158	12.2518
C	-9.4516	8.6231	16.7439
C	-9.1958	9.5811	15.6223
C	-9.4779	11.0209	16.112
O	-8.5819	11.843	16.2813
O	-10.7971	11.236	16.3643
C	-11.1435	12.5499	16.8273
C	-11.0129	12.6219	18.3367
O	-7.8285	9.3925	15.2834
H	-11.0546	9.7572	14.4744
H	-8.9886	8.7269	17.7164
H	-10.5376	13.3182	16.3334
H	-12.1846	12.7263	16.5378
H	-11.3296	13.6009	18.7073
H	-11.6249	11.8487	18.8127
H	-9.9789	12.447	18.6504
H	-7.3367	10.1482	15.6638

Diastereomer **III**_13
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-11.4389	9.8002	11.1262
C	-11.2453	9.8999	9.613
C	-11.6176	11.2584	9.0449
C	-10.9854	12.3898	9.8274
C	-11.249	12.3677	11.3457
C	-10.8532	10.9707	11.9699
C	-9.3256	10.7748	12.4
C	-8.7964	12.0619	13.14
C	-9.0828	13.341	12.35
C	-10.5759	13.5159	12.1405
C	-10.2896	13.3285	9.1601
C	-9.1685	9.5195	13.3587
C	-9.9373	9.5618	14.7015
C	-11.0419	8.5222	14.7352
C	-10.9218	7.6098	15.8942
C	-8.4248	10.4706	11.177
C	-7.3025	12.0532	13.5041
O	-11.9504	8.4513	13.9189
O	-11.8062	6.6006	16.1174
C	-11.5722	5.8093	17.2748
H	-12.519	9.7522	11.3185
H	-11.0533	8.8335	11.4593
H	-10.2141	9.6676	9.3356
H	-11.8568	9.1295	9.1267
H	-11.3196	11.2875	7.9891
H	-12.7073	11.3753	9.045
H	-11.4044	10.9339	12.9193
H	-9.3378	12.1561	14.0887
H	-8.7139	14.2091	12.9116
H	-8.5399	13.342	11.4002
H	-11.0395	13.5898	13.1349
H	-10.7688	14.4863	11.666
H	-9.4485	8.6121	12.8101
H	-8.0979	9.3889	13.5388
H	-7.3699	10.3885	11.4578
H	-8.4953	11.237	10.403
H	-8.6709	9.5026	10.7319
H	-7.0611	12.9222	14.127
H	-7.0187	11.1681	14.0756
H	-6.6636	12.1133	12.6177
H	-12.3549	5.0467	17.327
H	-10.6056	5.2985	17.2115
H	-11.6308	6.4173	18.1838
H	-9.8313	14.1833	9.6422
H	-10.1631	13.2762	8.0821
C	-12.7787	12.6034	11.5414
H	-13.0423	12.624	12.6058
H	-13.0864	13.5635	11.109
H	-13.3985	11.8269	11.0844
C	-9.8408	8.0083	16.5702
C	-9.1388	9.1901	15.9771
C	-9.1954	10.3793	16.9715
O	-10.0762	10.5818	17.7956
O	-8.1208	11.1995	16.7516
C	-8.0405	12.3548	17.6016
C	-8.8677	13.4919	17.0316
O	-7.8108	8.7521	15.7304
H	-10.4437	10.5214	14.8507
H	-9.4772	7.5426	17.4754
H	-8.3439	12.1123	18.6266
H	-6.9868	12.6499	17.64
H	-8.7822	14.3843	17.658
H	-8.5345	13.7414	16.0195
H	-9.924	13.2151	16.9589
H	-7.2591	9.5547	15.6677

Diastereomer **III**_14
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-11.4896	9.8031	11.0826
C	-11.3379	9.8276	9.5618
C	-11.6798	11.1721	8.9429
C	-10.9849	12.3137	9.6539
C	-11.2015	12.3693	11.1791
C	-10.8357	10.9868	11.8542
C	-9.3024	10.7579	12.2425
C	-8.7236	12.0545	12.9288
C	-8.9736	13.3077	12.0862
C	-10.4643	13.5291	11.8983
C	-10.2752	13.1942	8.9248
C	-9.1476	9.5258	13.2287
C	-9.8394	9.6442	14.6044
C	-10.9938	8.6753	14.7642
C	-10.9197	7.9236	16.0397
C	-8.4462	10.3956	11.0034
C	-7.2326	12.0053	13.2974
O	-11.9149	8.5537	13.9683
O	-11.8882	7.0478	16.4214
C	-11.665	6.3621	17.6462
H	-12.5644	9.8053	11.3078
H	-11.1314	8.8378	11.4484
H	-10.3241	9.5456	9.2669
H	-11.9903	9.0589	9.1288
H	-11.4133	11.1428	7.8788
H	-12.7642	11.3282	8.9691
H	-11.3549	11.0097	12.8224
H	-9.2572	12.2106	13.8739
H	-8.5615	14.1851	12.6012
H	-8.4505	13.2464	11.1273
H	-10.9013	13.6715	12.8973
H	-10.6317	14.4817	11.3799
H	-9.4878	8.612	12.7279
H	-8.0735	9.3641	13.3616
H	-7.3844	10.3061	11.2544
H	-8.5272	11.1339	10.204
H	-8.7231	9.4172	10.6011
H	-6.9591	12.8964	13.8747
H	-6.9883	11.1423	13.9202
H	-6.5899	11.9902	12.4121
H	-12.5133	5.6932	17.8189
H	-10.7573	5.7516	17.594
H	-11.6118	7.0648	18.4844
H	-9.7693	14.0504	9.3542
H	-10.1827	13.0886	7.8472
C	-12.7152	12.6686	11.4088
H	-12.945	12.7438	12.4786
H	-13.0023	13.6199	10.9441
H	-13.3759	11.8966	11.0044
C	-9.7773	8.2938	16.6264
C	-8.9785	9.2858	15.8399
C	-8.6934	10.5528	16.6796
O	-7.5585	10.9906	16.8428
O	-9.8301	11.1	17.1896
C	-9.6588	12.2889	17.9757
C	-9.3721	11.9223	19.4194
O	-7.7689	8.61	15.5116
H	-10.2936	10.631	14.7376
H	-9.4182	7.9094	17.5705
H	-8.8737	12.9309	17.5601
H	-10.5977	12.8491	17.9167
H	-9.2975	12.8196	20.0401
H	-10.1655	11.2815	19.818
H	-8.4367	11.3601	19.5037
H	-7.0452	9.2607	15.6157

Diastereomer **III**_15
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
```
C                 -11.9129    10.4125    11.6806
C                 -12.0837    10.5724    10.1698
C                 -12.0091    12.0161    9.6957
C                 -10.8246    12.7556    10.2833
C                 -10.7023    12.6896    11.8155
C                 -10.7244    11.1923    12.3102
C                 -9.337      10.398     12.3018
C                 -8.2164     11.3069    12.9246
C                 -8.1594     12.6923    12.2677
C                 -9.4789     13.4256    12.4203
C                 -10.0026    13.4282    9.4577
C                 -9.4672     9.0281     13.0952
C                 -10.22      8.9855     14.4427
C                 -10.5513    7.556      14.8371
C                 -10.328     7.3274     16.2856
C                 -8.9055     9.9877     10.8688
C                 -6.7914     10.7275    12.9032
O                 -10.9989    6.7156     14.0683
O                 -10.608     6.2319     17.0521
C                 -11.1831    5.1273     16.3642
H                 -12.8383    10.7602    12.1583
H                 -11.8642    9.3462     11.9197
H                 -11.3398    9.9815     9.6303
H                 -13.0535    10.1509    9.877
H                 -11.9766    12.0198    8.5988
H                 -12.9344    12.5396    9.9624
H                 -10.9711    11.2804    13.3765
H                 -8.4734     11.474     13.9732
H                 -7.3798     13.2941    12.7531
H                 -7.8675     12.6156    11.216
H                 -9.6422     13.5739    13.4975
H                 -9.3865     14.4378    12.0067
H                 -9.9865     8.3257     12.4279
H                 -8.4831     8.5619     13.2168
H                 -7.9339     9.4824     10.8714
H                 -8.8278     10.8368    10.1886
H                 -9.5954     9.2627     10.4306
H                 -6.1233     11.3569    13.503
H                 -6.7346     9.7212     13.321
H                 -6.3771     10.6998    11.8902
H                 -11.3535    4.3314     17.0957
H                 -12.1532    5.3939     15.9326
H                 -10.4987    4.7378     15.6039
H                 -9.1493     13.9984    9.8048
H                 -10.1649    13.4356    8.3831
C                 -11.9345    13.4487    12.4
H                 -11.9148    13.4492    13.4967
H                 -11.9414    14.4955    12.0717
H                 -12.8933    13.0111    12.1087
C                 -9.7547     8.4386     16.7478
C                 -9.5116     9.4955     15.7154
C                 -10.182     10.8091    16.1986
O                 -11.3826    10.9767    16.3647
O                 -9.2223     11.7574    16.4255
C                 -9.7394     13.0323    16.8281
C                 -8.5819     14.0091    16.8907
O                 -8.1043     9.5498     15.5609
H                 -11.2089    9.445      14.333
H                 -9.4563     8.5536     17.7814
H                 -10.4787    13.3844    16.0997
H                 -10.2058    12.9408    17.8151
H                 -8.9246     15.0015    17.1965
H                 -7.8226     13.6626    17.5995
H                 -8.0929     14.0888    15.914
H                 -7.7961     10.3292    16.0619
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Diastereomer **III**_16
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-11.3169	9.6871	11.0009
C	-11.0517	9.7772	9.498
C	-11.4985	11.0925	8.8841
C	-10.998	12.2826	9.6747
C	-11.3385	12.2646	11.1779
C	-10.8693	10.9133	11.8503
C	-9.3563	10.8445	12.362
C	-8.9685	12.1816	13.1027
C	-9.3097	13.4207	12.2715
C	-10.7987	13.4751	11.9818
C	-10.3429	13.2619	9.0248
C	-9.1527	9.6195	13.3511
C	-9.9837	9.6248	14.6554
C	-11.0362	8.5324	14.6667
C	-10.992	7.7247	15.9068
C	-8.3709	10.5938	11.1933
C	-7.5006	12.2952	13.5455
O	-11.8607	8.3525	13.7812
O	-11.8825	6.7264	16.154
C	-11.7186	6.0331	17.3839
H	-12.3986	9.5573	11.1381
H	-10.8754	8.759	11.3723
H	-9.9921	9.6229	9.2791
H	-11.5743	8.9531	8.9966
H	-11.1489	11.1278	7.8445
H	-12.5925	11.1231	8.8265
H	-11.4647	10.8487	12.7712
H	-9.565	12.2511	14.0201
H	-9.0385	14.3246	12.8323
H	-8.719	13.4473	11.3509
H	-11.3188	13.5297	12.9491
H	-11.0404	14.4194	11.4777
H	-9.3352	8.6835	12.8099
H	-8.0854	9.5782	13.5861
H	-7.329	10.6029	11.5294
H	-8.4617	11.3387	10.4006
H	-8.5149	9.6016	10.7567
H	-6.8224	12.405	12.6935
H	-7.3664	13.1828	14.1749
H	-7.1758	11.4372	14.1366
H	-12.4974	5.2673	17.4469
H	-10.7462	5.531	17.4243
H	-11.8407	6.7109	18.2354
H	-9.9781	14.1578	9.5121
H	-10.1563	13.2021	7.9559
C	-12.89	12.383	11.2902
H	-13.2099	12.4003	12.3391
H	-13.248	13.3087	10.823
H	-13.423	11.5528	10.8182
C	-9.9617	8.1913	16.6179
C	-9.2178	9.3156	15.9664
C	-9.2666	10.5653	16.8832
O	-10.2057	10.8927	17.5952
O	-8.1046	11.2742	16.7375
C	-8.0143	12.4859	17.5032
C	-7.4902	12.1867	18.8948
O	-7.9007	8.8225	15.7685
H	-10.5484	10.5563	14.77
H	-9.6555	7.8048	17.5798
H	-7.3127	13.1428	16.9787
H	-8.9778	13.007	17.5384
H	-7.3609	13.1096	19.4672
H	-8.1752	11.5301	19.4403
H	-6.5278	11.6673	18.8395
H	-7.3158	9.6025	15.7149

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Diastereomer **III**_17
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C		-11.9522	10.7924	11.8773
C		-12.2855	10.9768	10.3966
C		-12.0214	12.3835	9.8805
C		-10.6623	12.9068	10.2982
C		-10.3584	12.822	11.8036
C		-10.5748	11.3521	12.3311
C		-9.3585	10.3268	12.164
C		-8.0274	11.0253	12.6228
C		-7.8169	12.381	11.9349
C		-8.9596	13.3329	12.2354
C		-9.8485	13.4261	9.3613
C		-9.6213	8.9997	12.9966
C		-10.1747	9.099	14.4331
C		-10.7324	7.769	14.9027
C		-10.3567	7.4792	16.3068
C		-9.192	9.8487	10.6974
C		-6.739	10.2069	12.429
O		-11.4591	7.0438	14.2366
O		-10.8397	6.4003	16.9795
C		-10.3504	6.2145	18.3008
H		-12.7333	11.2986	12.4597
H		-12.0599	9.7349	12.1351
H		-11.7324	10.2624	9.7825
H		-13.3436	10.7325	10.2394
H		-12.1274	12.3779	8.7883
H		-12.8006	13.0619	10.2464
H		-10.6616	11.4844	13.4175
H		-8.1141	11.231	13.6934
H		-6.8896	12.8374	12.3053
H		-7.679	12.2556	10.8567
H		-8.9574	13.5062	13.3215
H		-8.7468	14.3138	11.7918
H		-10.345	8.4035	12.423
H		-8.7293	8.3634	12.9944
H		-8.3299	9.1821	10.5877
H		-9.0568	10.6718	9.9945
H		-10.0471	9.255	10.366
H		-5.9011	10.7049	12.931
H		-6.8054	9.2018	12.8482
H		-6.4679	10.1169	11.3721
H		-10.8148	5.3124	18.71
H		-9.2653	6.0665	18.2998
H		-10.6257	7.0581	18.9426
H		-8.8727	13.8395	9.5865
H		-10.1418	13.461	8.3154
C		-11.3571	13.7847	12.5198
H		-11.1998	13.7821	13.6051
H		-11.2239	14.8165	12.1717
H		-12.4062	13.5214	12.3596
C		-9.507	8.4456	16.6695
C		-9.2101	9.4396	15.5856
C		-9.4262	10.8681	16.1368
O		-8.492	11.6325	16.362
O		-10.7359	11.1473	16.3696
C		-10.985	12.4723	16.8556
C		-12.4858	12.679	16.9078
O		-7.8493	9.2065	15.2452
H		-11.0573	9.7463	14.4457
H		-9.0277	8.5081	17.6364
H		-10.5575	12.578	17.8585
H		-10.5353	13.2103	16.1817
H		-12.7296	13.6788	17.2775
H		-12.926	12.5525	15.913
H		-12.9553	11.9357	17.5606
H		-7.3351	9.9608	15.5982

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Diastereomer **III**_18
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-11.9316	10.4392	11.6794
C	-12.0968	10.5423	10.163
C	-12.0037	11.9654	9.6318
C	-10.8193	12.7206	10.2001
C	-10.7072	12.7093	11.7343
C	-10.7367	11.2307	12.2807
C	-9.3517	10.4311	12.2944
C	-8.2358	11.3492	12.9121
C	-8.1677	12.7192	12.2215
C	-9.4863	13.4617	12.3227
C	-9.9879	13.359	9.3569
C	-9.4918	9.0752	13.1074
C	-10.2065	9.0714	14.4767
C	-10.641	7.6632	14.8497
C	-10.3385	7.3558	16.2682
C	-8.9097	9.9934	10.8727
C	-6.8108	10.7675	12.9029
O	-11.2152	6.896	14.0881
O	-10.6464	6.2503	17.0095
C	-11.3476	5.2207	16.3221
H	-12.8545	10.8151	12.1404
H	-11.8968	9.3831	11.9613
H	-11.3596	9.9209	9.6496
H	-13.0711	10.1215	9.8842
H	-11.9606	11.9243	8.536
H	-12.927	12.5069	9.8676
H	-10.9803	11.3564	13.3444
H	-8.5005	11.534	13.9588
H	-7.3959	13.3319	12.7056
H	-7.8556	12.6157	11.1777
H	-9.663	13.6541	13.3891
H	-9.3832	14.4562	11.8707
H	-10.0414	8.3769	12.4608
H	-8.5149	8.5884	13.2069
H	-7.9389	9.4864	10.893
H	-8.8227	10.8284	10.1768
H	-9.597	9.2616	10.4423
H	-6.1495	11.3905	13.5166
H	-6.7582	9.7555	13.3063
H	-6.3849	10.7495	11.8942
H	-11.5235	4.4064	17.0317
H	-12.3236	5.5737	15.9741
H	-10.7487	4.8189	15.4985
H	-9.1338	13.9361	9.6901
H	-10.1426	13.3288	8.2817
C	-11.9408	13.4937	12.2821
H	-11.9326	13.528	13.3784
H	-11.9373	14.5298	11.9215
H	-12.8997	13.0541	11.9943
C	-9.6563	8.4019	16.7333
C	-9.4117	9.4895	15.7329
C	-9.9769	10.8078	16.3246
O	-11.1622	11.0943	16.4213
O	-8.9419	11.584	16.7753
C	-9.3182	12.8091	17.4235
C	-9.534	13.9056	16.3988
O	-8.0128	9.4912	15.5087
H	-11.1564	9.6118	14.4118
H	-9.284	8.4485	17.7482
H	-10.2034	12.6674	18.0541
H	-8.4918	13.0839	18.0871
H	-9.7422	14.8602	16.8901
H	-8.649	14.0192	15.7643
H	-10.3733	13.6646	15.7393
H	-7.6273	10.125	16.1435

Diastereomer **IV**_1
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
 C   -12.7258   2.3064   8.8605
 C   -13.7994   2.6089   7.8153
 C   -14.9397   1.6035   7.8104
 C   -15.4747   1.342   9.2028
 C   -14.4204   0.9407   10.2507
 C   -13.2449   1.9934   10.2927
 C   -13.4569   3.2804   11.2208
 C   -14.0539   2.8453   12.6126
 C   -15.2979   1.9657   12.4521
 C   -14.9686   0.7004   11.6811
 C   -16.7991   1.4419   9.4178
 C   -12.0787   4.0323   11.4404
 C   -10.9299   3.1983   12.0508
 C   -10.3306   3.8555   13.2797
 C   -8.8472   3.8649   13.2284
 C   -14.3903   4.3241   10.5593
 C   -14.4069   3.9916   13.5748
 O   -10.9891   4.2728   14.2227
 O   -7.9446   4.2926   14.1606
 C   -8.4958   4.9109   15.3173
 H   -12.1575   1.4358   8.5076
 H   -12.0013   3.1239   8.8656
 H   -14.2087   3.6121   7.9562
 H   -13.3324   2.6236   6.8225
 H   -15.7277   1.975   7.1432
 H   -14.5999   0.6609   7.3662
 H   -12.4203   1.4497   10.7711
 H   -13.3035   2.2361   13.1313
 H   -15.6699   1.6733   13.4427
 H   -16.1111   2.523   11.9773
 H   -14.22   0.1482   12.2677
 H   -15.8487   0.0454   11.658
 H   -11.7717   4.4663   10.4847
 H   -12.26   4.9161   12.0639
 H   -14.5736   5.1791   11.2183
 H   -15.3625   3.9089   10.2888
 H   -13.937   4.755   9.6627
 H   -14.6741   3.5867   14.558
 H   -13.5733   4.6776   13.7331
 H   -15.2679   4.5698   13.2249
 H   -9.0872   4.1968   15.899
 H   -7.6639   5.2417   15.9466
 H   -9.083   5.7957   15.0509
 H   -17.261   1.248   10.3785
 H   -17.4814   1.7203   8.6191
 C   -13.8555   -0.4472   9.8146
 H   -13.1002   -0.807   10.5238
 H   -14.6527   -1.1998   9.7747
 H   -13.3745   -0.4313   8.8327
 C   -8.5128   3.36   12.0408
 C   -9.6715   2.9782   11.1767
 C   -9.5371   1.5031   10.7344
 O   -9.3986   1.181   9.5576
 O   -9.5759   0.6382   11.783
 C   -9.4716   -0.7431   11.4162
 C   -9.6132   -1.5764   12.6746
 O   -9.6108   3.8542   10.0558
 H   -11.3034   2.2406   12.4263
 H   -7.4863   3.2615   11.7134
 H   -10.2692   -1.0019   10.7106
 H   -8.4951   -0.9272   10.9551
 H   -10.5774   -1.384   13.157
 H   -9.5387   -2.6433   12.4468
 H   -8.8363   -1.314   13.4003
 H   -9.4504   3.2957   9.2678

Diastereomer **IV**_2
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
 C   -12.724   1.9986   8.9173
 C   -13.7677   2.2739   7.835
 C   -14.9898   1.3726   7.9252
 C   -15.5426   1.2914   9.3333
 C   -14.5212   0.9152   10.4216
 C   -13.272   1.8781   10.3675
 C   -13.4002   3.2702   11.1546
 C   -14.015   3.0231   12.5813
 C   -15.3111   2.2074   12.5145
 C   -15.0768   0.8551   11.8681
 C   -16.8553   1.5099   9.5302
 C   -11.9792   3.96   11.2899
 C   -10.8676   3.1428   11.9856
 C   -10.4005   3.7799   13.2819
 C   -8.9214   3.8845   13.3446
 C   -14.2735   4.2934   10.3855
 C   -14.3087   4.2886   13.4058
 O   -11.15   4.1145   14.189
 O   -8.1207   4.3393   14.354
 C   -8.7952   4.8919   15.4782
 H   -12.2261   1.0533   8.6635
 H   -11.9328   2.749   8.8464
 H   -14.0908   3.3171   7.8622
 H   -13.3   2.1424   6.8512
 H   -15.7461   1.7416   7.2209
 H   -14.7315   0.366   7.5768
 H   -12.4907   1.3277   10.9069
 H   -13.294   2.4336   13.162
 H   -15.6881   2.0379   13.5315
 H   -16.0949   2.765   11.9926
 H   -14.3656   0.3111   12.5065
 H   -16.0015   0.2655   11.9071
 H   -11.6647   4.2458   10.2826
 H   -12.0964   4.9228   11.802
 H   -14.3985   5.2235   10.9499
 H   -15.2719   3.9145   10.1629
 H   -13.802   4.5982   9.4479
 H   -14.5572   4.0135   14.4376
 H   -13.4579   4.9697   13.4541
 H   -15.1652   4.8438   13.0096
 H   -9.4182   5.7436   15.1865
 H   -9.3795   4.1269   15.9991
 H   -8.0356   5.2595   16.1749
 H   -17.3279   1.4448   10.503
 H   -17.5164   1.759   8.7045
 C   -14.0705   -0.5483   10.1228
 H   -13.3588   -0.9037   10.8767
 H   -14.9278   -1.2328   10.1362
 H   -13.5786   -0.6632   9.153
 C   -8.467   3.4363   12.1748
 C   -9.5299   3.0065   11.2172
 C   -9.3063   1.5442   10.7696
 O   -9.2271   1.2264   9.5865
 O   -9.2207   0.6879   11.8232
 C   -8.9953   -0.6913   11.4953
 C   -10.314   -1.3823   11.2062
 O   -9.4219   3.8978   10.1117
 H   -11.2309   2.157   12.2927
 H   -7.4149   3.4097   11.9238
 H   -8.2968   -0.7903   10.6565
 H   -8.5203   -1.1533   12.3668
 H   -10.1615   -2.4496   11.0233
 H   -11.0036   -1.2619   12.0481
 H   -10.8016   -0.9448   10.3294
 H   -9.4472   3.3479   9.3022

Diastereomer **IV**_3

Charge =   0 Multiplicity = 1

Symbolic Z-Matrix:

C	-12.9627	3.2489	8.7893
C	-14.2071	3.707	8.0291
C	-15.1497	2.5699	7.6751
C	-15.4448	1.6923	8.8722
C	-14.2075	1.1364	9.6045
C	-13.2102	2.3015	10.0002
C	-13.4775	3.0462	11.3856
C	-13.8031	1.9799	12.4963
C	-14.9339	1.0369	12.0789
C	-14.5289	0.2561	10.8406
C	-16.7283	1.4402	9.1881
C	-12.2319	3.9257	11.8282
C	-10.9602	3.2228	12.3525
C	-10.1188	4.1743	13.1874
C	-8.679	4.0803	12.842
C	-14.6511	4.0519	11.2613
C	-14.1248	2.5513	13.8855
O	-10.5674	4.8873	14.0753
O	-7.6012	4.6962	13.4124
C	-7.898	5.6411	14.4339
H	-12.3136	2.7236	8.0762
H	-12.3956	4.1363	9.0792
H	-14.7545	4.4622	8.5989
H	-13.8927	4.2104	7.1063
H	-16.0694	2.9978	7.2564
H	-14.7162	1.9635	6.8718
H	-12.2546	1.7926	10.1653
H	-12.9178	1.344	12.6218
H	-15.1308	0.3184	12.885
H	-15.8686	1.5841	11.9255
H	-13.6403	-0.3358	11.1044
H	-15.3006	-0.4875	10.605
H	-11.9581	4.6328	11.0379
H	-12.588	4.5877	12.6305
H	-14.9081	4.4998	12.2267
H	-15.561	3.5955	10.8689
H	-14.3826	4.8958	10.6192
H	-14.2056	1.7384	14.6166
H	-13.3428	3.2235	14.2469
H	-15.0783	3.0876	13.8984
H	-8.5249	6.4529	14.0512
H	-8.3578	5.1522	15.2985
H	-6.9524	6.0804	14.7662
H	-17.0241	0.8069	10.0157
H	-17.5453	1.8649	8.6108
C	-13.4938	0.1667	8.6123
H	-12.6085	-0.2882	9.0729
H	-14.1625	-0.6491	8.3113
H	-13.1486	0.6584	7.6986
C	-8.6022	3.2471	11.8047
C	-9.9184	2.712	11.3353
C	-9.846	1.1677	11.2883
O	-9.8365	0.5424	10.2314
O	-9.7569	0.6108	12.5255
C	-9.6892	-0.8206	12.5284
C	-9.6544	-1.2873	13.9702
O	-10.1052	3.2695	10.0411
H	-11.2312	2.4412	13.0682
H	-7.6668	3.0011	11.3194
H	-10.5713	-1.2345	12.0269
H	-8.781	-1.1466	12.0096
H	-9.6019	-2.3781	14.0263
H	-8.7896	-0.8638	14.4917
H	-10.5469	-0.9478	14.5064
H	-9.9029	2.5611	9.3969

Diastereomer **IV**_4
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
 C   -12.7376   2.2756   8.8704
 C   -13.7781   2.5901   7.7956
 C   -14.9515   1.624   7.7882
 C   -15.5249   1.4153   9.174
 C   -14.5078   1.0021   10.2539
 C   -13.2959   2.0129   10.2982
 C   -13.4794   3.327   11.1932
 C   -14.1249   2.947   12.5797
 C   -15.3969   2.1106   12.4093
 C   -15.096   0.8158   11.6765
 C   -16.8491   1.5671   9.3571
 C   -12.0787   4.0305   11.4298
 C   -10.9781   3.1695   12.0908
 C   -10.3734   3.852   13.3035
 C   -8.8901   3.8312   13.2644
 C   -14.3564   4.39   10.4866
 C   -14.4559   4.1277   13.5075
 O   -11.031   4.3145   14.226
 O   -7.9865   4.2839   14.1838
 C   -8.5344   4.9659   15.3058
 H   -12.1914   1.379   8.5491
 H   -11.9875   3.0693   8.8726
 H   -14.1559   3.6095   7.9058
 H   -13.2901   2.5666   6.8132
 H   -15.7117   2.0057   7.0948
 H   -14.6348   0.66   7.3739
 H   -12.5008   1.4518   10.8058
 H   -13.4109   2.3223   13.1301
 H   -15.8028   1.8559   13.397
 H   -16.1771   2.6858   11.9019
 H   -14.381   0.2518   12.2929
 H   -15.9983   0.1919   11.6483
 H   -11.7302   4.4311   10.4737
 H   -12.2425   4.9352   12.0278
 H   -14.522   5.2662   11.1219
 H   -15.3372   4.0056   10.202
 H   -13.866   4.7826   9.5919
 H   -14.7627   3.7559   14.4923
 H   -13.5997   4.7839   13.672
 H   -15.2846   4.7309   13.1236
 H   -9.1421   4.2905   15.9162
 H   -7.701   5.3118   15.9249
 H   -9.1043   5.847   14.9935
 H   -17.3384   1.4128   10.3113
 H   -17.5037   1.8501   8.537
 C   -13.9836   -0.4147   9.8626
 H   -13.2567   -0.7837   10.5965
 H   -14.8059   -1.1396   9.8223
 H   -13.4814   -0.4388   8.8916
 C   -8.5565   3.2649   12.1047
 C   -9.715   2.8608   11.2509
 C   -9.6212   1.356   10.9077
 O   -9.521   0.9539   9.7521
 O   -9.6486   0.5679   12.016
 C   -9.5688   -0.8465   11.7842
 C   -8.1178   -1.2806   11.7014
 O   -9.6147   3.659   10.0765
 H   -11.3988   2.2431   12.4943
 H   -7.5296   3.1299   11.7915
 H   -10.053   -1.3375   12.6347
 H   -10.1271   -1.1342   10.8859
 H   -8.0435   -2.3653   11.5832
 H   -7.6118   -0.8015   10.8574
 H   -7.5762   -0.9856   12.6062
 H   -9.5181   3.0422   9.3222

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Diastereomer **IV**_5
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-12.6279	2.0369	8.9809
C	-13.6539	2.2406	7.8661
C	-14.8268	1.2785	7.9437
C	-15.4214	1.2276	9.3345
C	-14.4244	0.9287	10.4703
C	-13.2	1.925	10.4241
C	-13.3718	3.3264	11.1768
C	-14.0721	3.1201	12.5733
C	-15.3482	2.2819	12.4602
C	-15.0394	0.9085	11.8927
C	-16.7472	1.4066	9.4772
C	-11.9537	4.0049	11.3865
C	-10.9188	3.2058	12.2157
C	-10.3938	4.0395	13.3709
C	-8.9145	4.1302	13.3616
C	-14.1907	4.3328	10.3312
C	-14.4194	4.4079	13.3388
O	-11.1104	4.5516	14.2205
O	-8.0737	4.7839	14.2173
C	-8.6992	5.487	15.284
H	-12.0831	1.1111	8.7599
H	-11.8765	2.8257	8.9068
H	-14.0326	3.2658	7.8665
H	-13.1534	2.1164	6.8976
H	-15.5746	1.5804	7.1995
H	-14.5041	0.2747	7.645
H	-12.4142	1.4114	10.9935
H	-13.3887	2.559	13.2214
H	-15.7877	2.1478	13.4572
H	-16.1038	2.8023	11.8642
H	-14.3393	0.4178	12.5843
H	-15.9444	0.2884	11.9191
H	-11.5435	4.2613	10.406
H	-12.11	4.9872	11.8499
H	-14.3482	5.2771	10.8624
H	-15.174	3.9458	10.0567
H	-13.6598	4.6125	9.4172
H	-14.7433	4.1627	14.3571
H	-13.5675	5.0835	13.4314
H	-15.242	4.9549	12.867
H	-9.3512	6.2801	14.9041
H	-9.2427	4.8013	15.9418
H	-7.9117	5.9612	15.8777
H	-17.2539	1.3599	10.4338
H	-17.3867	1.6019	8.6204
C	-13.9092	-0.5272	10.2471
H	-13.2025	-0.8211	11.0326
H	-14.7389	-1.2445	10.2672
H	-13.3867	-0.6606	9.2957
C	-8.5082	3.423	12.3079
C	-9.6032	2.7884	11.5121
C	-9.4541	1.2454	11.5939
O	-9.2199	0.605	12.6098
O	-9.6749	0.6976	10.3581
C	-9.5729	-0.7327	10.3312
C	-9.7573	-1.1984	8.9004
O	-9.4633	3.3035	10.1979
H	-11.3749	2.3312	12.6916
H	-7.4647	3.3136	12.0435
H	-8.5859	-1.0416	10.6937
H	-10.3532	-1.1669	10.9661
H	-9.6693	-2.2862	8.8306
H	-10.7392	-0.9008	8.5197
H	-9.009	-0.7396	8.2458
H	-9.7218	2.5865	9.5879

Diastereomer **IV**_6
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
 C   -12.6432   1.7178   9.0852
 C   -13.626   1.876   7.9254
 C   -14.8826   1.0344   8.081
 C   -15.5012   1.1817   9.4551
 C   -14.5486   0.936   10.6403
 C   -13.2532   1.8285   10.5119
 C   -13.3387   3.3217   11.089
 C   -14.0622   3.3283   12.4866
 C   -15.3901   2.5654   12.4535
 C   -15.1779   1.1198   12.0446
 C   -16.8115   1.4725   9.5473
 C   -11.8812   3.9308   11.2367
 C   -10.899   3.1697   12.1571
 C   -10.4751   3.9958   13.3584
 C   -9.0044   3.9773   13.5479
 C   -14.0831   4.2707   10.1171
 C   -14.3421   4.7199   13.0803
 O   -11.2562   4.5667   14.107
 O   -8.2436   4.5334   14.5371
 C   -8.9556   5.2534   15.5362
 H   -12.1864   0.7248   8.9917
 H   -11.8145   2.416   8.9453
 H   -13.9109   2.9224   7.7936
 H   -13.121   1.5936   6.9931
 H   -15.5904   1.3176   7.2917
 H   -14.6459   -0.02   7.898
 H   -12.5211   1.3281   11.1583
 H   -13.4166   2.8094   13.2061
 H   -15.8411   2.5741   13.4544
 H   -16.1076   3.0645   11.7951
 H   -14.5231   0.6599   12.7988
 H   -16.1269   0.5742   12.122
 H   -11.4632   4.0241   10.2311
 H   -11.9645   4.9708   11.5755
 H   -14.1831   5.2794   10.531
 H   -15.0872   3.9187   9.8738
 H   -13.5267   4.4064   9.1859
 H   -14.6623   4.624   14.1244
 H   -13.4638   5.367   13.0734
 H   -15.1473   5.236   12.5469
 H   -9.4821   6.1102   15.1039
 H   -9.6392   4.5961   16.0829
 H   -8.2245   5.6406   16.2525
 H   -17.3334   1.5678   10.4921
 H   -17.4219   1.6189   8.6603
 C   -14.1463   -0.571   10.59
 H   -13.4691   -0.8268   11.4139
 H   -15.0295   -1.2155   10.6791
 H   -13.631   -0.8527   9.6675
 C   -8.5086   3.2884   12.5206
 C   -9.527   2.7893   11.5468
 C   -9.4258   1.2446   11.4529
 O   -9.3443   0.4761   12.4013
 O   -9.4893   0.8625   10.1396
 C   -9.4122   -0.5553   9.9391
 C   -9.3508   -0.8205   8.4475
 O   -9.2365   3.458   10.3286
 H   -11.3683   2.2831   12.5973
 H   -7.4484   3.1199   12.3857
 H   -8.5121   -0.9543   10.4203
 H   -10.3024   -1.0306   10.3657
 H   -8.4766   -0.331   8.0055
 H   -9.295   -1.8936   8.2443
 H   -10.2321   -0.4112   7.9435
 H   -9.4759   2.8437   9.6084

Diastereomer **IV**_7
Charge = 0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.913	3.15	8.766
C	-14.1138	3.6184	7.9444
C	-15.0973	2.5057	7.6263
C	-15.4654	1.7127	8.8615
C	-14.2756	1.1452	9.6608
C	-13.2363	2.2852	10.0202
C	-13.5063	3.1193	11.353
C	-13.9117	2.1343	12.5114
C	-15.0738	1.2212	12.1138
C	-14.6718	0.3529	10.9341
C	-16.7674	1.5371	9.1525
C	-12.2335	3.9654	11.7828
C	-11.0081	3.2364	12.3781
C	-10.1547	4.193	13.1949
C	-8.7115	4.043	12.8858
C	-14.6277	4.1683	11.1376
C	-14.2435	2.798	13.8564
O	-10.6	4.9539	14.0441
O	-7.6283	4.6537	13.4514
C	-7.9185	5.6538	14.4209
H	-12.2693	2.5568	8.1031
H	-12.3146	4.027	9.0227
H	-14.6416	4.4284	8.4544
H	-13.7514	4.054	7.0048
H	-15.9843	2.949	7.1564
H	-14.6699	1.8354	6.872
H	-12.3097	1.7445	10.242
H	-13.0611	1.467	12.6986
H	-15.3264	0.5598	12.9526
H	-15.9771	1.8005	11.9017
H	-13.8195	-0.2624	11.2574
H	-15.4705	-0.3675	10.7175
H	-11.9082	4.616	10.964
H	-12.5794	4.6851	12.5385
H	-14.8895	4.6821	12.0682
H	-15.5469	3.7317	10.7445
H	-14.3027	4.9609	10.4574
H	-14.3839	2.0327	14.6286
H	-13.4399	3.452	14.2035
H	-15.1698	3.3786	13.8107
H	-8.409	5.2192	15.2976
H	-6.9677	6.0825	14.7522
H	-8.5146	6.4633	13.9874
H	-17.1148	0.9665	10.0053
H	-17.5476	1.964	8.5279
C	-13.5805	0.0891	8.7466
H	-12.7304	-0.3779	9.2586
H	-14.2779	-0.7119	8.4718
H	-13.1877	0.5116	7.8177
C	-8.6374	3.1606	11.8899
C	-9.9581	2.6393	11.4179
C	-9.9344	1.0931	11.4607
O	-9.9462	0.4098	10.4407
O	-9.8562	0.6091	12.7293
C	-9.8131	-0.8202	12.8563
C	-8.3812	-1.3097	12.7522
O	-10.0958	3.1272	10.09
H	-11.3311	2.4985	13.1182
H	-7.6996	2.8654	11.4377
H	-10.2162	-1.0656	13.8442
H	-10.4591	-1.3049	12.1152
H	-8.3288	-2.3912	12.9054
H	-7.9557	-1.0744	11.7716
H	-7.751	-0.8158	13.4992
H	-9.9309	2.3696	9.4928

Diastereomer **IV**_8
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
 C   -12.7172   1.8953   8.9622
 C   -13.7524   2.1488   7.8663
 C   -14.9937   1.28   7.9929
 C   -15.5522   1.2823   9.4003
 C   -14.5454   0.9342   10.5125
 C   -13.266   1.8548   10.4176
 C   -13.3486   3.2839   11.1409
 C   -14.0028   3.1385   12.5641
 C   -15.3211   2.3597   12.5176
 C   -15.1122   0.9667   11.9547
 C   -16.8601   1.5432   9.5779
 C   -11.8982   3.9112   11.277
 C   -10.8506   3.0958   12.0739
 C   -10.442   3.8254   13.3429
 C   -8.9846   4.0902   13.389
 C   -14.1574   4.306   10.3031
 C   -14.2738   4.4593   13.3061
 O   -11.2238   4.1361   14.2313
 O   -8.2436   4.7402   14.3349
 C   -8.9673   5.2439   15.4511
 H   -12.2461   0.9273   8.75
 H   -11.9076   2.6211   8.8571
 H   -14.0525   3.1991   7.8477
 H   -13.2863   1.9643   6.8903
 H   -15.7385   1.6307   7.2672
 H   -14.7566   0.2521   7.6956
 H   -12.4993   1.3073   10.981
 H   -13.3151   2.5615   13.195
 H   -15.7221   2.2599   13.5346
 H   -16.0767   2.9096   11.9483
 H   -14.4188   0.4433   12.6289
 H   -16.0509   0.4017   12.0185
 H   -11.5358   4.1128   10.2661
 H   -11.987   4.9126   11.717
 H   -14.2549   5.2671   10.8186
 H   -15.1661   3.9578   10.0742
 H   -13.6505   4.5446   9.3645
 H   -14.5387   4.2546   14.35
 H   -13.4078   5.1229   13.32
 H   -15.1132   5.0084   12.8668
 H   -9.7064   5.9884   15.1383
 H   -9.4317   4.4307   16.0179
 H   -8.2534   5.7435   16.1132
 H   -17.3399   1.537   10.5494
 H   -17.511   1.7677   8.7372
 C   -14.1349   -0.5546   10.2939
 H   -13.4208   -0.8837   11.0583
 H   -15.0083   -1.2155   10.3561
 H   -13.6602   -0.7361   9.3258
 C   -8.4774   3.5515   12.2813
 C   -9.4743   2.8792   11.3942
 C   -9.1658   1.3594   11.3432
 O   -8.8175   0.6719   12.2932
 O   -9.3867   0.8921   10.0746
 C   -9.0782   -0.4957   9.8683
 C   -10.2735   -1.3617   10.2155
 O   -9.3447   3.5147   10.1312
 H   -11.2532   2.1372   12.4175
 H   -7.4233   3.5897   12.0402
 H   -8.8331   -0.6145   8.8078
 H   -8.1897   -0.7927   10.4374
 H   -10.0479   -2.4187   10.0482
 H   -10.5716   -1.2265   11.2597
 H   -11.1344   -1.0874   9.5993
 H   -9.6258   2.863   9.461

Diastereomer **IV**_9
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-12.6925	2.7326	8.8362
C	-13.8111	3.08	7.8541
C	-14.8255	1.964	7.6753
C	-15.3134	1.4316	9.0052
C	-14.2091	0.982	9.9819
C	-13.1401	2.1307	10.2009
C	-13.4603	3.2098	11.3317
C	-13.9845	2.4735	12.62
C	-15.1608	1.543	12.3148
C	-14.7265	0.4564	11.3466
C	-16.6388	1.3616	9.2265
C	-12.1841	4.0824	11.6894
C	-11.0264	3.4392	12.4858
C	-10.194	4.5042	13.1809
C	-8.7412	4.2497	13.0265
C	-14.5176	4.2341	10.8442
C	-14.37	3.3876	13.7928
O	-10.6637	5.4295	13.8301
O	-7.6745	4.9106	13.5667
C	-7.9913	6.0237	14.3943
H	-12.0341	2.0039	8.345
H	-12.0724	3.6216	8.9703
H	-14.3308	3.9904	8.1636
H	-13.3656	3.3168	6.8798
H	-15.6563	2.3427	7.0667
H	-14.3827	1.1484	7.0924
H	-12.257	1.6093	10.5877
H	-13.1795	1.8248	12.9873
H	-15.4974	1.059	13.2407
H	-16.0204	2.1034	11.9361
H	-13.9286	-0.1186	11.8389
H	-15.5441	-0.2621	11.2079
H	-11.7846	4.5661	10.7916
H	-12.5476	4.9361	12.279
H	-14.8169	4.9217	11.6419
H	-15.4276	3.7609	10.473
H	-14.1138	4.8741	10.0543
H	-14.5999	2.7849	14.6793
H	-13.5583	4.0632	14.0738
H	-15.2602	3.9846	13.5735
H	-8.5114	6.8013	13.8257
H	-8.5696	5.7115	15.2697
H	-7.0498	6.45	14.7539
H	-17.0694	0.9759	10.1428
H	-17.3543	1.6917	8.4781
C	-13.5107	-0.2514	9.3308
H	-12.7296	-0.6527	9.9865
H	-14.2301	-1.059	9.1475
H	-13.027	-0.023	8.3771
C	-8.6357	3.2052	12.2055
C	-9.9395	2.6567	11.7152
C	-9.9911	1.1508	12.0857
O	-10.1431	0.6971	13.2116
O	-9.7974	0.3966	10.9589
C	-9.8072	-1.0178	11.1926
C	-9.5797	-1.7158	9.8661
O	-9.9684	2.9259	10.3238
H	-11.4189	2.8478	13.3189
H	-7.6801	2.8024	11.8966
H	-9.0065	-1.2824	11.8921
H	-10.7758	-1.3164	11.6085
H	-9.5851	-2.8022	9.9908
H	-10.3555	-1.4382	9.145
H	-8.6206	-1.4143	9.4321
H	-9.5937	2.142	9.8785

Diastereomer **IV**_10
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-12.7264	2.3205	8.8422
C	-13.7758	2.6202	7.7719
C	-14.9078	1.6063	7.734
C	-15.4758	1.3359	9.1113
C	-14.4456	0.9373	10.1841
C	-13.278	1.9968	10.2601
C	-13.5203	3.2784	11.1894
C	-14.1562	2.8374	12.5617
C	-15.3884	1.9491	12.3636
C	-15.0284	0.6883	11.5991
C	-16.8059	1.4258	9.293
C	-12.1497	4.031	11.4521
C	-11.022	3.1979	12.1015
C	-10.4982	3.8342	13.3723
C	-9.0179	3.9057	13.3905
C	-14.4361	4.3231	10.5052
C	-14.5481	3.9811	13.5121
O	-11.201	4.2011	14.3044
O	-8.3294	4.3859	14.461
C	-6.9159	4.4406	14.3237
H	-12.1431	1.4558	8.4994
H	-12.0086	3.1433	8.8689
H	-14.1962	3.6196	7.9073
H	-13.2843	2.6432	6.7912
H	-15.6814	1.9746	7.0483
H	-14.5498	0.6681	7.295
H	-12.4611	1.4557	10.7544
H	-13.4172	2.2338	13.1028
H	-15.7861	1.6516	13.3426
H	-16.1916	2.5021	11.8672
H	-14.2907	0.1409	12.2036
H	-15.9022	0.0263	11.5514
H	-11.8122	4.4603	10.5049
H	-12.3501	4.9166	12.0674
H	-14.6402	5.1752	11.1618
H	-15.3992	3.9065	10.2054
H	-13.9577	4.7583	9.6238
H	-14.8329	3.5747	14.4898
H	-13.729	4.6803	13.6876
H	-15.4087	4.5459	13.14
H	-6.4972	3.4389	14.1803
H	-6.6272	5.1028	13.5005
H	-6.5016	4.851	15.2493
H	-17.2907	1.2247	10.2408
H	-17.4698	1.7027	8.4783
C	-13.8611	-0.4453	9.7573
H	-13.1215	-0.8031	10.484
H	-14.6521	-1.2028	9.6944
H	-13.3556	-0.4224	8.7879
C	-8.6059	3.4354	12.2089
C	-9.7152	3.0213	11.2917
C	-9.5347	1.549	10.8561
O	-9.4509	1.2179	9.677
O	-9.4874	0.6962	11.9145
C	-9.3536	-0.6852	11.5575
C	-9.3699	-1.505	12.8325
O	-9.6175	3.8965	10.1731
H	-11.3952	2.2231	12.4316
H	-7.572	3.372	11.9001
H	-10.1893	-0.9844	10.9147
H	-8.4064	-0.8381	11.0287
H	-9.2694	-2.5714	12.6122
H	-8.5533	-1.202	13.4961
H	-10.3033	-1.3436	13.382
H	-9.6691	3.338	9.3709

Diastereomer **IV**_11
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.6911	1.9404	8.9698
C	-13.7032	2.1628	7.846
C	-14.9281	1.2699	7.9538
C	-15.5241	1.2914	9.345
C	-14.5431	0.9801	10.4912
C	-13.2722	1.9134	10.4136
C	-13.3797	3.3498	11.115
C	-14.087	3.2278	12.5167
C	-15.3979	2.4405	12.4359
C	-15.1544	1.0365	11.9142
C	-16.8398	1.5379	9.4808
C	-11.9318	3.9715	11.3
C	-10.9319	3.1579	12.1565
C	-10.4526	3.9523	13.3586
C	-8.9733	3.9804	13.4494
C	-14.1527	4.3609	10.2324
C	-14.3851	4.5595	13.2268
O	-11.2017	4.4739	14.1734
O	-8.1663	4.5597	14.3874
C	-8.8328	5.2476	15.439
H	-12.2034	0.9753	8.7826
H	-11.8912	2.6777	8.8722
H	-14.0242	3.2066	7.8091
H	-13.2097	1.9771	6.8838
H	-15.6591	1.5898	7.2004
H	-14.6613	0.2413	7.6854
H	-12.514	1.3821	11.0033
H	-13.4246	2.6661	13.1865
H	-15.8385	2.3603	13.4382
H	-16.133	2.9727	11.8245
H	-14.4759	0.5375	12.6211
H	-16.0873	0.4606	11.9621
H	-11.5187	4.1607	10.306
H	-12.0365	4.9785	11.7226
H	-14.267	5.3301	10.7288
H	-15.1527	4.0096	9.9712
H	-13.6097	4.5834	9.3099
H	-14.7004	4.3709	14.2597
H	-13.5149	5.2159	13.274
H	-15.1992	5.1075	12.741
H	-9.421	6.0853	15.051
H	-9.4506	4.5621	16.028
H	-8.0683	5.6597	16.1048
H	-17.3474	1.5446	10.4381
H	-17.4697	1.7367	8.6179
C	-14.1018	-0.5064	10.3159
H	-13.4065	-0.8083	11.1086
H	-14.966	-1.1803	10.3636
H	-13.5918	-0.6986	9.3678
C	-8.5256	3.305	12.3917
C	-9.5891	2.7624	11.4927
C	-9.4853	1.2148	11.4537
O	-9.2652	0.4903	12.4143
O	-9.7338	0.7779	10.18
C	-9.7095	-0.6465	9.9961
C	-8.2912	-1.1161	9.7343
O	-9.3649	3.3754	10.2326
H	-11.4047	2.2696	12.5895
H	-7.472	3.1649	12.1892
H	-10.1554	-1.1655	10.8522
H	-10.3365	-0.8666	9.1259
H	-8.2695	-2.191	9.5336
H	-7.8638	-0.5875	8.8759
H	-7.6432	-0.9075	10.5914
H	-9.6765	2.7445	9.5559

Diastereomer **IV**_12
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-12.705	2.002	8.9132
C	-13.72	2.2652	7.801
C	-14.9301	1.345	7.852
C	-15.5237	1.2521	9.2425
C	-14.5303	0.8882	10.3606
C	-13.294	1.8691	10.3462
C	-13.4646	3.2567	11.1335
C	-14.1206	2.9974	12.5394
C	-15.4024	2.164	12.4303
C	-15.1287	0.8166	11.7893
C	-16.8448	1.4512	9.4002
C	-12.0571	3.9639	11.3157
C	-10.9593	3.1599	12.0466
C	-10.5559	3.787	13.366
C	-9.0857	3.9262	13.4929
C	-14.3262	4.271	10.3399
C	-14.4576	4.2568	13.3566
O	-11.3369	4.0966	14.2552
O	-8.4991	4.412	14.6202
C	-7.0835	4.5349	14.5867
H	-12.1858	1.065	8.6718
H	-11.9234	2.7643	8.8678
H	-14.0599	3.3033	7.8218
H	-13.2212	2.1444	6.8312
H	-15.6704	1.7041	7.1258
H	-14.6459	0.3433	7.5096
H	-12.5214	1.3278	10.9066
H	-13.4101	2.4163	13.1411
H	-15.8088	1.987	13.4347
H	-16.1771	2.7119	11.885
H	-14.4294	0.2816	12.4482
H	-16.0454	0.2135	11.799
H	-11.7131	4.2531	10.3191
H	-12.2024	4.9248	11.8243
H	-14.4812	5.1976	10.9024
H	-15.312	3.8797	10.0846
H	-13.8291	4.5846	9.4185
H	-14.7336	3.976	14.3798
H	-13.6187	4.95	13.4319
H	-15.3096	4.8004	12.9353
H	-6.6086	3.5571	14.4539
H	-6.7687	5.2288	13.8001
H	-6.7564	4.942	15.548
H	-17.3454	1.3771	10.3583
H	-17.4845	1.6927	8.5555
C	-14.049	-0.5678	10.0729
H	-13.3541	-0.914	10.8467
H	-14.8958	-1.2651	10.0599
H	-13.5271	-0.6732	9.1177
C	-8.5682	3.5029	12.3357
C	-9.5885	3.0617	11.3333
C	-9.3244	1.6086	10.8772
O	-9.2324	1.2991	9.693
O	-9.2258	0.7481	11.9263
C	-8.9852	-0.6269	11.5914
C	-10.2954	-1.329	11.2896
O	-9.4486	3.9655	10.2416
H	-11.3132	2.1625	12.3257
H	-7.5132	3.4932	12.101
H	-8.2805	-0.7135	10.7564
H	-8.5113	-1.0897	12.4631
H	-10.1316	-2.3942	11.1042
H	-10.993	-1.2179	12.1262
H	-10.7801	-0.8932	10.4104
H	-9.5491	3.4375	9.4236

Diastereomer **IV**_13
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.647	1.6548	9.0962
C	-13.5955	1.7897	7.9053
C	-14.8588	0.9551	8.0431
C	-15.5158	1.133	9.3955
C	-14.598	0.9112	10.6124
C	-13.2973	1.7985	10.5018
C	-13.3957	3.3046	11.0439
C	-14.1594	3.3433	12.4186
C	-15.4866	2.5803	12.3654
C	-15.2658	1.1261	11.9943
C	-16.8276	1.4279	9.4444
C	-11.9412	3.9154	11.2194
C	-10.9848	3.1799	12.1861
C	-10.6525	4.0051	13.414
C	-9.1968	4.0432	13.6833
C	-14.1097	4.2326	10.0297
C	-14.4574	4.749	12.9694
O	-11.4808	4.5411	14.137
O	-8.6777	4.6645	14.7765
C	-7.2625	4.6293	14.9029
H	-12.1914	0.6584	9.0383
H	-11.8117	2.3469	8.9647
H	-13.873	2.8336	7.7422
H	-13.0648	1.4854	6.9945
H	-15.5431	1.2233	7.2281
H	-14.6205	-0.1036	7.8893
H	-12.5853	1.3104	11.1791
H	-13.5343	2.8408	13.1674
H	-15.9651	2.6115	13.353
H	-16.185	3.0652	11.6765
H	-14.6331	0.6819	12.7763
H	-16.2176	0.5835	12.0569
H	-11.4957	3.9769	10.2234
H	-12.0303	4.9647	11.5273
H	-14.2196	5.2507	10.4176
H	-15.1072	3.8768	9.7656
H	-13.5264	4.3466	9.1122
H	-14.8002	4.6791	14.0083
H	-13.5821	5.4004	12.9636
H	-15.2526	5.2473	12.4048
H	-6.9023	3.599	14.9917
H	-6.781	5.1371	14.0604
H	-6.9913	5.1626	15.8188
H	-17.3755	1.5445	10.3719
H	-17.4125	1.5563	8.5375
C	-14.1986	-0.5974	10.6058
H	-13.5454	-0.8369	11.4537
H	-15.0857	-1.238	10.6842
H	-13.6587	-0.9002	9.7043
C	-8.6151	3.3852	12.6762
C	-9.5683	2.8608	11.6466
C	-9.403	1.3232	11.5359
O	-9.259	0.5516	12.4743
O	-9.4839	0.9502	10.2211
C	-9.3467	-0.4605	10.0031
C	-9.2743	-0.7049	8.5083
O	-9.2343	3.5512	10.4512
H	-11.4416	2.2702	12.5906
H	-7.5486	3.2434	12.5722
H	-8.4307	-0.8286	10.4789
H	-10.2162	-0.977	10.4242
H	-9.1747	-1.7722	8.2923
H	-10.1711	-0.3257	8.0083
H	-8.4206	-0.1749	8.0732
H	-9.4979	2.9715	9.7109

Diastereomer **IV**_14
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.868	3.1067	8.8079
C	-14.0704	3.5173	7.9584
C	-14.9919	2.3589	7.6201
C	-15.3528	1.5558	8.8505
C	-14.1579	1.0438	9.6797
C	-13.1766	2.2293	10.0573
C	-13.5118	3.0528	11.3812
C	-13.8971	2.0513	12.533
C	-15.0136	1.0919	12.1144
C	-14.5522	0.2388	10.9456
C	-16.6525	1.3266	9.1133
C	-12.2865	3.9549	11.8343
C	-11.0302	3.2741	12.4221
C	-10.2748	4.2325	13.3245
C	-8.8241	4.2556	13.0258
C	-14.6739	4.0507	11.1411
C	-14.2778	2.6992	13.8725
O	-10.7845	4.8792	14.2303
O	-7.9467	5.0022	13.7489
C	-6.592	4.9682	13.3202
H	-12.1822	2.544	8.1608
H	-12.3195	4.0123	9.0757
H	-14.6476	4.3015	8.4553
H	-13.7077	3.9691	7.0266
H	-15.8865	2.7584	7.1259
H	-14.5147	1.7064	6.8803
H	-12.2299	1.7327	10.3002
H	-13.0247	1.418	12.7357
H	-15.2565	0.4221	12.9493
H	-15.9351	1.6338	11.8825
H	-13.6852	-0.3429	11.2893
H	-15.3169	-0.5129	10.713
H	-11.9911	4.6347	11.028
H	-12.6736	4.6441	12.5981
H	-14.9762	4.5539	12.0652
H	-15.5648	3.5733	10.7307
H	-14.3711	4.8557	10.465
H	-14.4093	1.9271	14.6397
H	-13.5018	3.3762	14.238
H	-15.2207	3.2503	13.8097
H	-6.4939	5.3533	12.2998
H	-6.0108	5.6155	13.9836
H	-6.1836	3.9547	13.3929
H	-16.9952	0.7466	9.9617
H	-17.4359	1.7172	8.4692
C	-13.3955	0.0162	8.787
H	-12.5386	-0.4116	9.3215
H	-14.0503	-0.8151	8.4983
H	-12.9985	0.453	7.8664
C	-8.648	3.4495	11.9745
C	-9.9095	2.8232	11.4611
C	-9.7458	1.2853	11.447
O	-9.7325	0.6389	10.4032
O	-9.598	0.7671	12.6953
C	-9.4556	-0.6593	12.7729
C	-10.8207	-1.3214	12.7714
O	-10.0657	3.3418	10.1469
H	-11.3155	2.4643	13.0991
H	-7.696	3.2648	11.4969
H	-8.8228	-1.0387	11.9625
H	-8.9409	-0.878	13.7141
H	-10.7278	-2.4025	12.9068
H	-11.4469	-0.9158	13.5729
H	-11.3465	-1.1325	11.8305
H	-9.9855	2.5843	9.5321

Diastereomer **IV**_15
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
 C   -12.7303   2.2668   8.8625
 C   -13.7445   2.5691   7.7595
 C   -14.91   1.594   7.7254
 C   -15.5181   1.3872   9.0966
 C   -14.5269   0.9862   10.2049
 C   -13.3237   2.0056   10.2765
 C   -13.5396   3.3224   11.1616
 C   -14.2231   2.9468   12.5306
 C   -15.4824   2.0982   12.3292
 C   -15.1507   0.8021   11.6124
 C   -16.8477   1.5298   9.244
 C   -12.1485   4.0321   11.4354
 C   -11.068   3.1796   12.1384
 C   -10.5417   3.8501   13.3908
 C   -9.0605   3.8872   13.4239
 C   -14.3999   4.3783   10.4247
 C   -14.5935   4.1322   13.4374
 O   -11.2457   4.2707   14.2989
 O   -8.3726   4.4014   14.4788
 C   -6.9565   4.4139   14.3572
 H   -12.1692   1.373   8.5595
 H   -11.9863   3.0661   8.8811
 H   -14.1327   3.586   7.8553
 H   -13.2307   2.5453   6.7903
 H   -15.6544   1.9669   7.0106
 H   -14.5753   0.6307   7.3241
 H   -12.5375   1.4516   10.8055
 H   -13.5201   2.3332   13.1071
 H   -15.9137   1.8457   13.3066
 H   -16.2526   2.6642   11.7967
 H   -14.4474   0.2479   12.2507
 H   -16.0466   0.1703   11.5637
 H   -11.7722   4.4213   10.4855
 H   -12.3317   4.9425   12.019
 H   -14.5874   5.257   11.0504
 H   -15.3706   3.9879   10.1141
 H   -13.8855   4.7686   9.5426
 H   -14.9178   3.7662   14.4187
 H   -13.7522   4.8043   13.614
 H   -15.4221   4.7182   13.0274
 H   -6.6414   5.0281   13.5071
 H   -6.5427   4.858   15.2674
 H   -6.5621   3.3962   14.2675
 H   -17.3608   1.3758   10.1858
 H   -17.4827   1.8043   8.4058
 C   -13.983   -0.4287   9.834
 H   -13.2735   -0.7896   10.5887
 H   -14.799   -1.1594   9.7749
 H   -13.4547   -0.4534   8.8768
 C   -8.6468   3.3504   12.2717
 C   -9.7551   2.9157   11.3629
 C   -9.6144   1.4145   11.0196
 O   -9.5365   1.0117   9.8627
 O   -9.5887   0.6298   12.1305
 C   -9.4781   -0.783   11.9009
 C   -8.0189   -1.1786   11.7787
 O   -9.6134   3.7173   10.1951
 H   -11.4868   2.2352   12.5007
 H   -7.6114   3.2462   11.9796
 H   -9.9249   -1.2833   12.7662
 H   -10.0534   -1.0886   11.0194
 H   -7.9189   -2.2613   11.6618
 H   -7.5498   -0.6894   10.9192
 H   -7.4602   -0.8657   12.6669
 H   -9.6732   3.1125   9.4277

Diastereomer **IV**_16
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.7571	2.8503	8.8007
C	-13.8901	3.24	7.8514
C	-14.9047	2.1307	7.6354
C	-15.3725	1.5349	8.9454
C	-14.2536	1.0444	9.8851
C	-13.1853	2.1853	10.1422
C	-13.4914	3.2103	11.326
C	-13.9974	2.4148	12.5859
C	-15.1747	1.4948	12.2538
C	-14.7502	0.455	11.2313
C	-16.6945	1.4495	9.1814
C	-12.2111	4.0675	11.7065
C	-11.0466	3.3937	12.4662
C	-10.1921	4.4311	13.1759
C	-8.7449	4.1565	13.0036
C	-14.5563	4.2539	10.9001
C	-14.3714	3.2741	13.8032
O	-10.6415	5.3496	13.8486
O	-7.6633	4.785	13.5529
C	-7.9555	5.8804	14.4126
H	-12.105	2.146	8.2673
H	-12.1356	3.7329	8.967
H	-14.4072	4.1337	8.2099
H	-13.4588	3.5228	6.883
H	-15.745	2.5353	7.0571
H	-14.4687	1.3446	7.0084
H	-12.2965	1.6489	10.4924
H	-13.1858	1.7532	12.9136
H	-15.4977	0.968	13.1609
H	-16.0408	2.069	11.9121
H	-13.9436	-0.1386	11.6859
H	-15.5673	-0.2595	11.0712
H	-11.8191	4.5865	10.8252
H	-12.5682	4.8967	12.3338
H	-14.8461	4.9035	11.7324
H	-15.4705	3.7964	10.5193
H	-14.1636	4.9304	10.1355
H	-14.5852	2.6315	14.6653
H	-13.5599	3.9421	14.1021
H	-15.2681	3.8743	13.6227
H	-8.4655	6.682	13.8688
H	-8.5336	5.5545	15.2831
H	-7.0044	6.2804	14.7772
H	-17.1112	1.0198	10.0844
H	-17.4213	1.8115	8.459
C	-13.56	-0.1554	9.1686
H	-12.7647	-0.5805	9.7918
H	-14.2785	-0.9583	8.9625
H	-13.095	0.1176	8.2173
C	-8.6631	3.1328	12.1543
C	-9.98	2.621	11.6586
C	-10.052	1.1043	11.9795
O	-10.2022	0.6185	13.092
O	-9.8765	0.3862	10.8261
C	-9.9073	-1.042	10.9725
C	-8.528	-1.5605	11.3323
O	-10.0181	2.9392	10.2778
H	-11.4323	2.7848	13.2901
H	-7.7169	2.7223	11.8273
H	-10.659	-1.3501	11.7082
H	-10.215	-1.455	10.0063
H	-8.5266	-2.6527	11.3881
H	-7.7918	-1.2437	10.5862
H	-8.1962	-1.161	12.2958
H	-9.6506	2.1697	9.8026

Diastereomer **IV**_17
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.7118	1.8556	8.9635
C	-13.7138	2.1063	7.8366
C	-14.9604	1.2409	7.9307
C	-15.5597	1.2497	9.3212
C	-14.5863	0.9048	10.4637
C	-13.3035	1.8239	10.4023
C	-13.4062	3.257	11.1162
C	-14.0991	3.1166	12.5207
C	-15.4162	2.3383	12.4412
C	-15.1941	0.9433	11.889
C	-16.8717	1.5133	9.4599
C	-11.9607	3.8887	11.2871
C	-10.928	3.0859	12.1152
C	-10.606	3.7885	13.4214
C	-9.167	4.1095	13.5503
C	-14.1937	4.2738	10.2517
C	-14.3912	4.4407	13.2489
O	-11.4284	4.0448	14.29
O	-8.6646	4.7685	14.6291
C	-7.2617	4.9966	14.6245
H	-12.2379	0.8849	8.7698
H	-11.8966	2.5778	8.8789
H	-14.0105	3.1573	7.8041
H	-13.2197	1.9161	6.8755
H	-15.6831	1.5903	7.1824
H	-14.7172	0.2112	7.6444
H	-12.5551	1.2781	10.991
H	-13.4283	2.5409	13.1708
H	-15.8446	2.2425	13.4474
H	-16.1559	2.8866	11.8499
H	-14.5212	0.4211	12.5845
H	-16.1352	0.3801	11.9278
H	-11.5749	4.0795	10.2829
H	-12.062	4.8939	11.7158
H	-14.3066	5.2372	10.7599
H	-15.1953	3.9233	9.9971
H	-13.6619	4.5089	9.3261
H	-14.6808	4.2407	14.2871
H	-13.5279	5.1072	13.2798
H	-15.2212	4.9852	12.7864
H	-6.7106	4.0502	14.6132
H	-6.9696	5.6254	13.7768
H	-7.0023	5.528	15.5449
H	-17.3791	1.5121	10.4173
H	-17.4979	1.7352	8.5999
C	-14.1722	-0.5855	10.2629
H	-13.4827	-0.9134	11.0501
H	-15.0484	-1.2446	10.3006
H	-13.6683	-0.7716	9.3105
C	-8.5794	3.6266	12.4524
C	-9.5114	2.9433	11.5008
C	-9.1421	1.4397	11.4104
O	-8.6803	0.7623	12.3181
O	-9.4475	0.9738	10.1589
C	-9.1068	-0.4002	9.914
C	-10.2309	-1.3137	10.3629
O	-9.3401	3.616	10.2614
H	-11.3096	2.1025	12.4079
H	-7.5218	3.6974	12.241
H	-8.9567	-0.5045	8.8345
H	-8.1587	-0.6645	10.3964
H	-9.9836	-2.3599	10.1622
H	-10.4328	-1.1991	11.4324
H	-11.1563	-1.0665	9.8355
H	-9.6572	3.0066	9.5678

Diastereomer **IV**_18
Charge =   0 Multiplicity = 1
Symbolic Z-Matrix:

C	-12.6887	1.9301	8.9594
C	-13.6771	2.1424	7.8128
C	-14.8949	1.2371	7.8929
C	-15.5228	1.2533	9.2701
C	-14.5653	0.9522	10.4388
C	-13.302	1.8977	10.3899
C	-13.4386	3.3333	11.0889
C	-14.1802	3.2069	12.472
C	-15.4801	2.4054	12.3607
C	-15.2095	1.0035	11.8472
C	-16.8437	1.4865	9.3755
C	-12.	3.9658	11.3104
C	-11.0176	3.1649	12.199
C	-10.6191	3.9535	13.4312
C	-9.1501	4.0641	13.5763
C	-14.1965	4.3378	10.186
C	-14.512	4.5379	13.1688
O	-11.4108	4.4211	14.2384
O	-8.5718	4.7184	14.6193
C	-7.1507	4.7408	14.6325
H	-12.1873	0.9699	8.7836
H	-11.8939	2.6752	8.8795
H	-14.0078	3.1829	7.7684
H	-13.16	1.9617	6.8621
H	-15.6117	1.5492	7.1228
H	-14.6116	0.2111	7.6315
H	-12.5524	1.3733	10.9963
H	-13.5285	2.6545	13.1598
H	-15.9439	2.322	13.3522
H	-16.2057	2.929	11.7309
H	-14.5421	0.5127	12.5703
H	-16.137	0.4177	11.8745
H	-11.5622	4.15	10.3263
H	-12.1223	4.9749	11.7237
H	-14.3308	5.3066	10.6782
H	-15.1869	3.9783	9.9001
H	-13.632	4.5637	9.2773
H	-14.8447	4.3499	14.1963
H	-13.6533	5.2083	13.2286
H	-15.3245	5.0708	12.664
H	-6.7432	3.7266	14.6996
H	-6.7587	5.2587	13.7508
H	-6.8294	5.2938	15.5201
H	-17.3731	1.4886	10.3209
H	-17.4558	1.6786	8.4982
C	-14.1058	-0.53	10.2748
H	-13.4262	-0.8248	11.0836
H	-14.9644	-1.2122	10.3028
H	-13.5721	-0.7177	9.3389
C	-8.6239	3.4225	12.5291
C	-9.6316	2.8272	11.595
C	-9.4581	1.286	11.5644
O	-9.1218	0.5859	12.5091
O	-9.7877	0.8219	10.3191
C	-9.7139	-0.6023	10.1473
C	-8.3031	-1.0103	9.7683
O	-9.3787	3.4335	10.3364
H	-11.48	2.2533	12.5932
H	-7.5642	3.324	12.34
H	-10.0597	-1.1297	11.0436
H	-10.4026	-0.8623	9.3368
H	-8.2485	-2.0857	9.577
H	-7.9762	-0.4746	8.8711
H	-7.5943	-0.7604	10.5641
H	-9.7358	2.8283	9.6589

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Diastereomer **IV**_19
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:

C	-12.8864	3.1288	8.7684
C	-14.0588	3.5792	7.8972
C	-15.0229	2.4563	7.5574
C	-15.4325	1.6786	8.7892
C	-14.2707	1.1284	9.6401
C	-13.25	2.2784	10.0216
C	-13.5723	3.1287	11.3321
C	-14.0168	2.1571	12.4878
C	-15.1607	1.2349	12.0599
C	-14.7114	0.3519	10.9085
C	-16.7437	1.5007	9.0342
C	-12.3185	3.9849	11.7966
C	-11.1083	3.2645	12.432
C	-10.3119	4.2203	13.3013
C	-8.8576	4.1413	13.0308
C	-14.6885	4.1704	11.0622
C	-14.3982	2.8364	13.8116
O	-10.7966	4.9404	14.1644
O	-7.948	4.8646	13.7376
C	-6.5908	4.727	13.3389
H	-12.2156	2.531	8.1372
H	-12.3035	4.013	9.0352
H	-14.6099	4.3921	8.377
H	-13.6645	4.0052	6.9661
H	-15.8941	2.8875	7.0482
H	-14.5635	1.7783	6.8293
H	-12.3288	1.7462	10.2848
H	-13.1724	1.4944	12.7144
H	-15.4427	0.5842	12.8977
H	-16.0571	1.8081	11.8061
H	-13.8695	-0.2553	11.272
H	-15.4986	-0.3749	10.6722
H	-11.9723	4.6327	10.9842
H	-12.6922	4.707	12.5365
H	-14.9855	4.6955	11.9757
H	-15.5914	3.7249	10.6418
H	-14.3418	4.9551	10.3835
H	-14.5677	2.0802	14.587
H	-13.6071	3.4937	14.1808
H	-15.3215	3.4167	13.7249
H	-6.4505	5.0584	12.3045
H	-5.9818	5.3664	13.9847
H	-6.2485	3.6944	13.4647
H	-17.1202	0.9408	9.8818
H	-17.5022	1.9149	8.3752
C	-13.5371	0.0633	8.7674
H	-12.7047	-0.3923	9.3173
H	-14.22	-0.7448	8.4777
H	-13.1115	0.4751	7.8481
C	-8.714	3.2793	12.0197
C	-10.0033	2.7091	11.5093
C	-9.9317	1.1646	11.5601
O	-9.9441	0.4758	10.5439
O	-9.8183	0.6915	12.8299
C	-9.739	-0.7354	12.9662
C	-8.2975	-1.1909	12.8411
O	-10.1078	3.1845	10.1738
H	-11.4465	2.5039	13.1413
H	-7.7673	3.0153	11.5695
H	-10.1193	-0.9831	13.9625
H	-10.3852	-1.2408	12.2394
H	-8.2163	-2.2697	13.0008
H	-7.8946	-0.9525	11.8518
H	-7.667	-0.6765	13.5738
H	-10.0545	2.4009	9.5894

Diastereomer **IV**_20
Charge =   0 Multiplicity = 1
 Symbolic Z-Matrix:
C	-13.177	1.2426	9.233
C	-14.1703	1.3725	8.0782
C	-15.5789	0.9214	8.4317
C	-16.0557	1.5092	9.7431
C	-15.1152	1.2923	10.9436
C	-13.6573	1.7937	10.606
C	-13.3564	3.3433	10.8345
C	-13.925	3.7874	12.2354
C	-15.4045	3.4153	12.3953
C	-15.5962	1.9126	12.2823
C	-17.2464	2.1343	9.7809
C	-11.8042	3.6427	10.728
C	-10.7558	2.6836	11.3356
C	-10.747	2.6251	12.8476
C	-9.5987	3.3703	13.4205
C	-14.0029	4.232	9.7365
C	-13.7587	5.2714	12.6004
O	-11.5498	1.9891	13.5159
O	-9.3352	3.6978	14.7195
C	-10.3819	3.423	15.6439
H	-12.9505	0.1754	9.3572
H	-12.227	1.6933	8.9311
H	-14.2066	2.4009	7.7112
H	-13.8073	0.777	7.2311
H	-16.2482	1.1942	7.6058
H	-15.6137	-0.1726	8.4869
H	-13.0249	1.2895	11.3499
H	-13.3916	3.2358	13.0104
H	-15.7553	3.7267	13.3879
H	-16.0277	3.9541	11.6757
H	-15.0389	1.4543	13.1123
H	-16.6465	1.6609	12.4761
H	-11.566	3.6941	9.6561
H	-11.6112	4.6557	11.097
H	-13.8234	5.2958	9.9238
H	-15.0817	4.0943	9.6554
H	-13.5642	4.0445	8.7536
H	-14.1187	5.4493	13.6209
H	-12.7139	5.5889	12.5844
H	-14.3361	5.927	11.9424
H	-10.5098	2.3444	15.7769
H	-10.0912	3.8436	16.6114
H	-11.3187	3.902	15.3398
H	-17.6633	2.5606	10.6855
H	-17.8595	2.2362	8.8896
C	-15.0833	-0.2435	11.2184
H	-14.438	-0.4786	12.0735
H	-16.0866	-0.6211	11.451
H	-14.7033	-0.8276	10.3756
C	-8.7938	3.6441	12.3937
C	-9.2915	3.1418	11.0773
C	-8.4207	1.968	10.5691
O	-7.7953	2.0206	9.5141
O	-8.4341	0.9097	11.4228
C	-7.6338	-0.2029	11.005
C	-7.7606	-1.2932	12.0507
O	-9.2151	4.2463	10.1778
H	-10.8925	1.6654	10.9578
H	-7.8548	4.1702	12.5006
H	-7.992	-0.573	10.0379
H	-6.5868	0.108	10.9176
H	-8.8062	-1.5979	12.1647
H	-7.1651	-2.1684	11.7763
H	-7.4266	-0.9301	13.0284
H	-8.6468	3.9648	9.4317