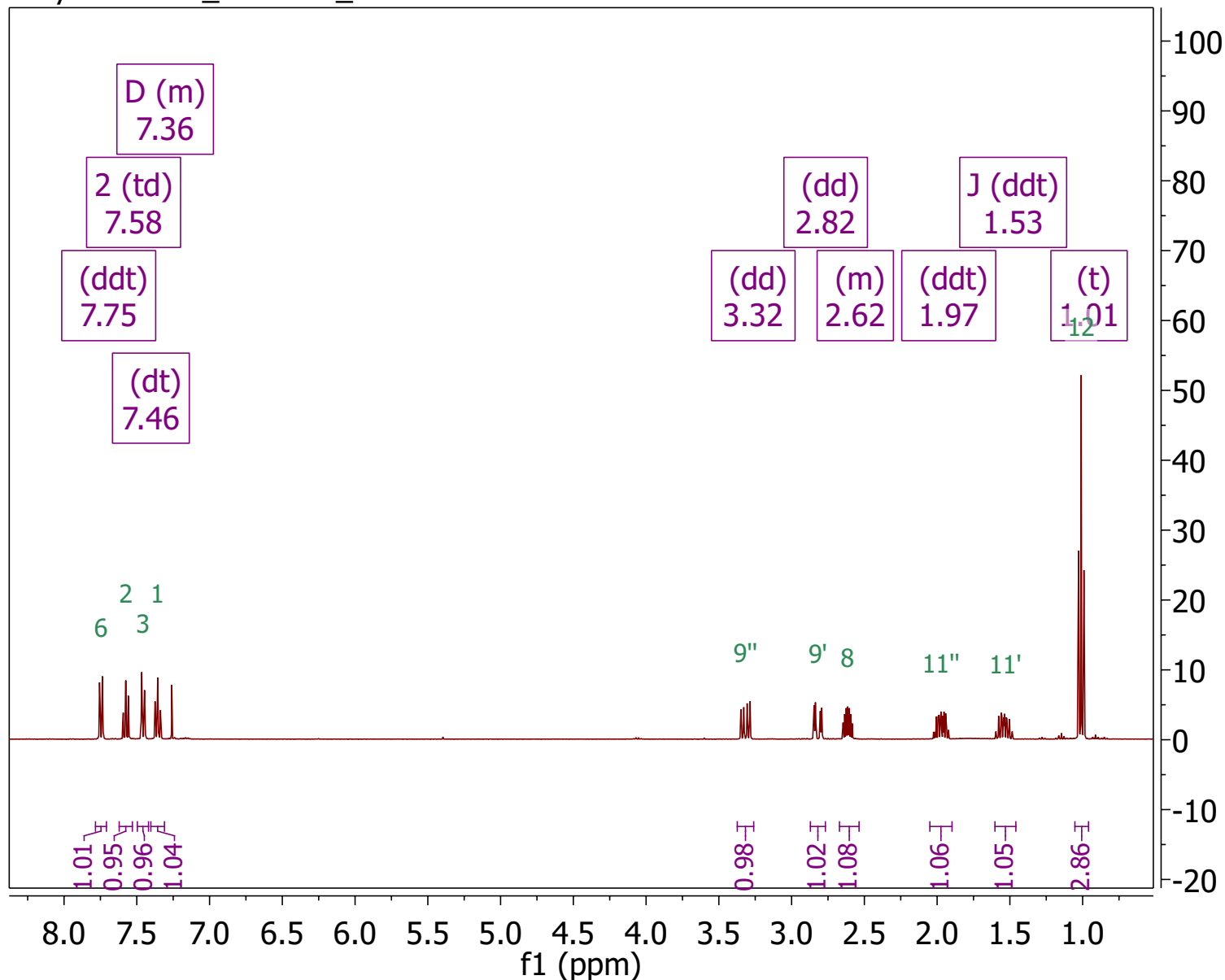
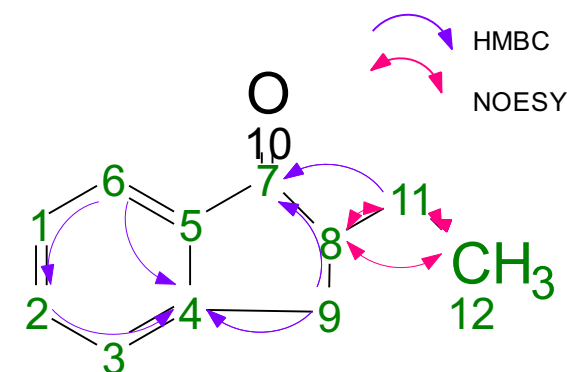


### Ethylindanone\_PROTON\_01

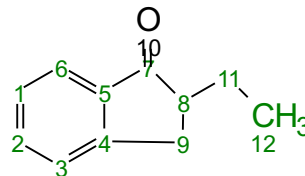


Parameter	Value
1 Title	Ethylindanone_PROTON_01
2 Spectrometer	nmrs
3 Solvent	cdcl3
4 Pulse Sequence	s2pul
5 Number of Scans	1
6 Acquisition Date	2010-05-03T23:09:04
7 Spectrometer Frequency	399.51
8 Spectral Width	6410.3
9 Acquired Size	16384

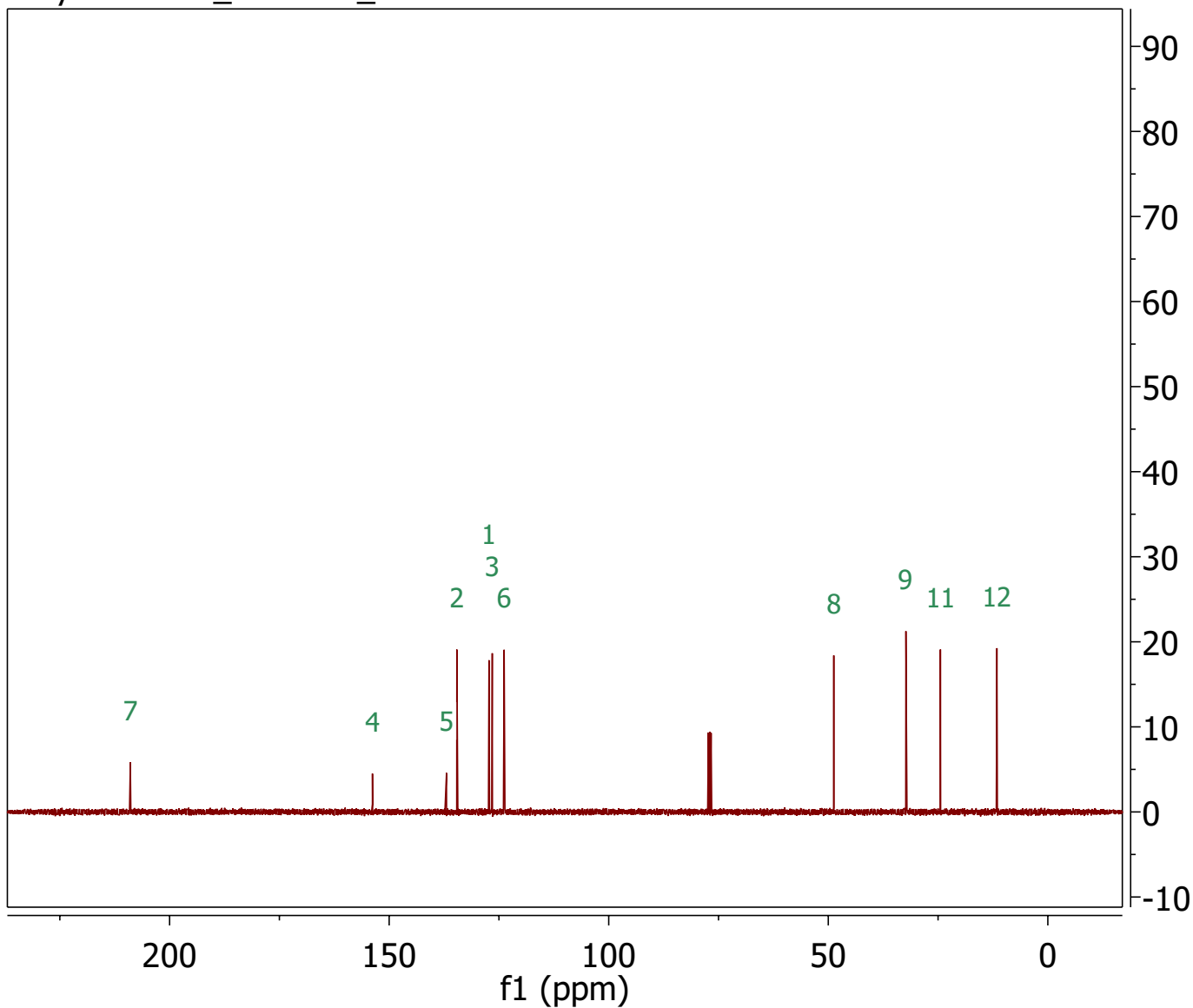
$^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  1.01 (t,  $J$  = 7.4 Hz, 3H), 1.53 (ddt,  $J$  = 14.4, 9.1, 7.3 Hz, 1H), 1.97 (ddt,  $J$  = 13.6, 7.5, 4.6 Hz, 1H), 2.54 – 2.67 (m, 1H), 2.82 (dd,  $J$  = 17.2, 3.9 Hz, 1H), 3.32 (dd,  $J$  = 17.2, 7.9 Hz, 1H), 7.31 – 7.40 (m, 1H), 7.46 (dt,  $J$  = 7.7, 1.0 Hz, 1H), 7.58 (td,  $J$  = 7.5, 1.3 Hz, 1H, 2), 7.75 (ddt,  $J$  = 7.6, 1.2, 0.6 Hz, 1H).



Submitted by: Yongbo Zhang  
 Sample Name: EI  
 Concentration: 10mg/ml  
 Analysis Date:



### Ethylindanone\_CARBON\_01



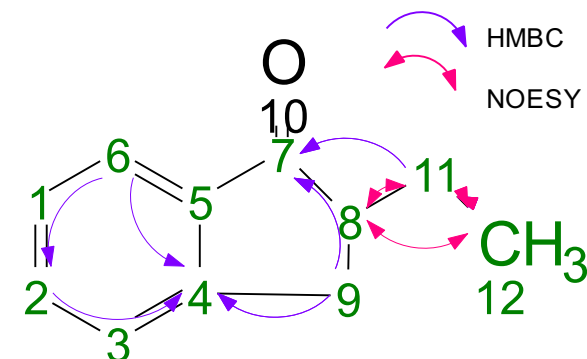
Parameter	Value
Title	Ethylindanone_CARBON_01
Spectrometer	nmrs
Solvent	cdcl3
Pulse Sequence	s2pul
Number of Scans	256
Acquisition Date	2010-03-08T01:29:44
Spectrometer Frequency	100.47
Spectral Width	25510.2
Acquired Size	32768

Atom	Chemical Shift	Predicted Shift	HSQC	HMBC	NOESY
1 C	127.31	126.19			
H	7.36	7.34			
2 C	134.60	131.22	2	6	
H	7.58	7.50	2	4	
3 C	126.55	125.14	3		
H	7.46	7.36	3		
4 C	153.80	152.26		2, 6, 9', 9''	
5 C	136.94	136.96			
6 C	123.85	123.58			
H	7.75	7.83		4, 2	
7 C	208.94	207.16		9', 9'', 11', 11''	
8 C	48.71	50.25	8		
H	2.62	3.16	8		11', 11'', 12
9 C	32.47	34.16			
H'	2.82	2.60, 2.99		4, 7	
H''	3.32	2.60, 2.99		4, 7	
10 O					
11 C	24.45	22.26			
H'	1.53	1.58, 1.71		7	8, 12
H''	1.97	1.58, 1.71		7	8, 12
12 C	11.61	11.78	12		
H3	1.01	0.96	12		11', 11'', 8

Parameter	Value
1 Title	Ethylindanone_PROTON_01
2 Spectrometer	vnmsr
3 Solvent	cdcl3
4 Pulse Sequence	s2pul
5 Number of Scans	1
6 Acquisition Date	2010-05-03T23:09:04
7 Spectrometer Frequency	399.51
8 Spectral Width	6410.3
9 Acquired Size	16384

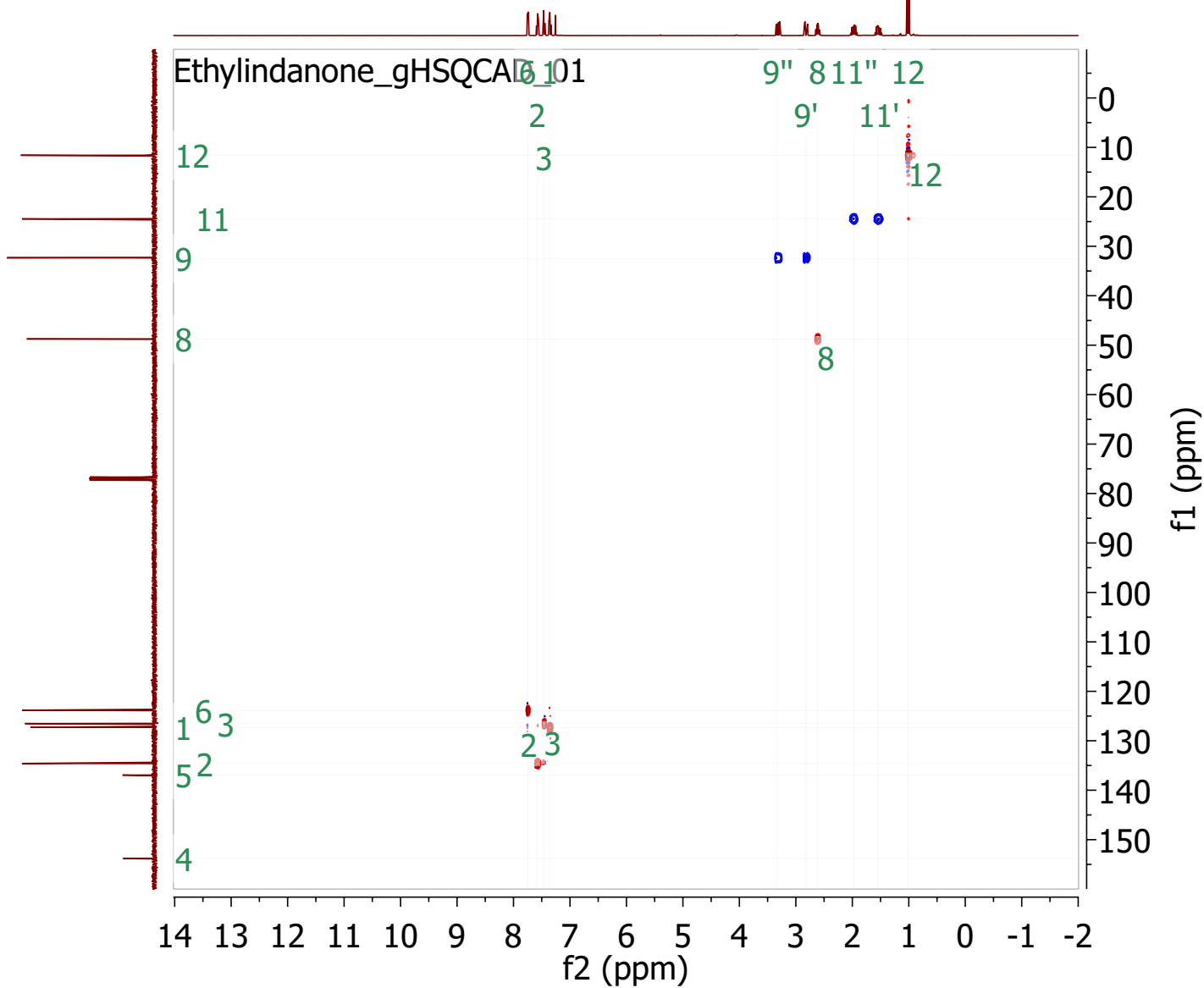
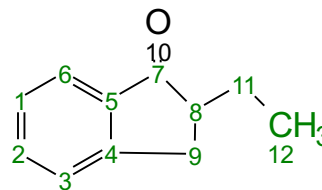
$^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  1.01 (t,  $J = 7.4$  Hz, 3H), 1.53 (ddt,  $J = 14.4, 9.1, 7.3$  Hz, 1H), 1.97 (ddt,  $J = 13.6, 7.5, 4.6$  Hz, 1H), 2.54 – 2.67 (m, 1H), 2.82 (dd,  $J = 17.2, 3.9$  Hz, 1H), 3.32 (dd,  $J = 17.2, 7.9$  Hz, 1H), 7.31 – 7.40 (m, 1H), 7.46 (dt,  $J = 7.7, 1.0$  Hz, 1H), 7.58 (td,  $J = 7.5, 1.3$  Hz, 1H, 2), 7.75 (ddt,  $J = 7.6, 1.2, 0.6$  Hz, 1H).

$^{13}\text{C}$  NMR (100 MHz,  $\text{cdCl}_3$ )  $\delta$  11.59, 24.46, 32.32, 48.75, 76.68, 77.00, 77.31, 123.81, 126.52, 126.59, 127.27, 134.59, 136.94, 143.70, 153.81, 208.94.



Atom	Chemical Shift	Predicted Shift	HSQC	HMBC	NOESY
1 C	127.31	126.19			
H	7.36	7.34			
2 C	134.60	131.22	2	6	
H	7.58	7.50	2	4	
3 C	126.55	125.14	3		
H	7.46	7.36	3		
4 C	153.80	152.26		2, 6, 9', 9''	
5 C	136.94	136.96			
6 C	123.85	123.58			
H	7.75	7.83		4, 2	
7 C	208.94	207.16		9', 9'', 11', 11''	
8 C	48.71	50.25	8		
H	2.62	3.16	8		11', 11'', 12
9 C	32.47	34.16			
H'	2.82	2.60, 2.99		4, 7	
H''	3.32	2.60, 2.99		4, 7	
10 O					
11 C	24.45	22.26			
H'	1.53	1.58, 1.71		7	8, 12
H''	1.97	1.58, 1.71		7	8, 12
12 C	11.61	11.78	12		
H3	1.01	0.96	12		11', 11'', 8

Submitted by: Yongbo Zhang  
 Sample Name: EI  
 Concentration: 10mg/ml  
 Analysis Date:



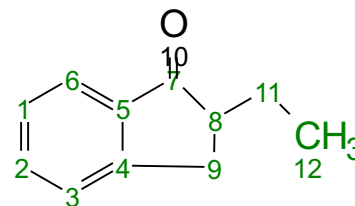
Parameter	Value
Title	Ethylindanone_gHSQCAD_01
Spectrometer	nmrs
Solvent	cdd3
Pulse Sequence	gHSQCAD
Number of Scans	2
Acquisition Date	2010-07-01T22:45:18
Spectrometer Frequency	(399.51, 100.46)
Spectral Width	(6410.3, 17075.8)
Nucleus	(1H, 13C)
Acquired Size	(962, 96)
Spectral Size	(1024, 1024)

	f1 (ppm)	f2 (ppm)	Type
1	134.59	7.57	Compound
2	127.31	7.35	Compound
3	126.55	7.45	Compound
4	123.85	7.75	Compound
5	48.72	2.61	Compound
6	32.33	3.31	Compound
7	32.33	2.81	Compound
8	24.46	1.54	Compound
9	24.44	1.98	Compound
10	11.59	1.01	Compound

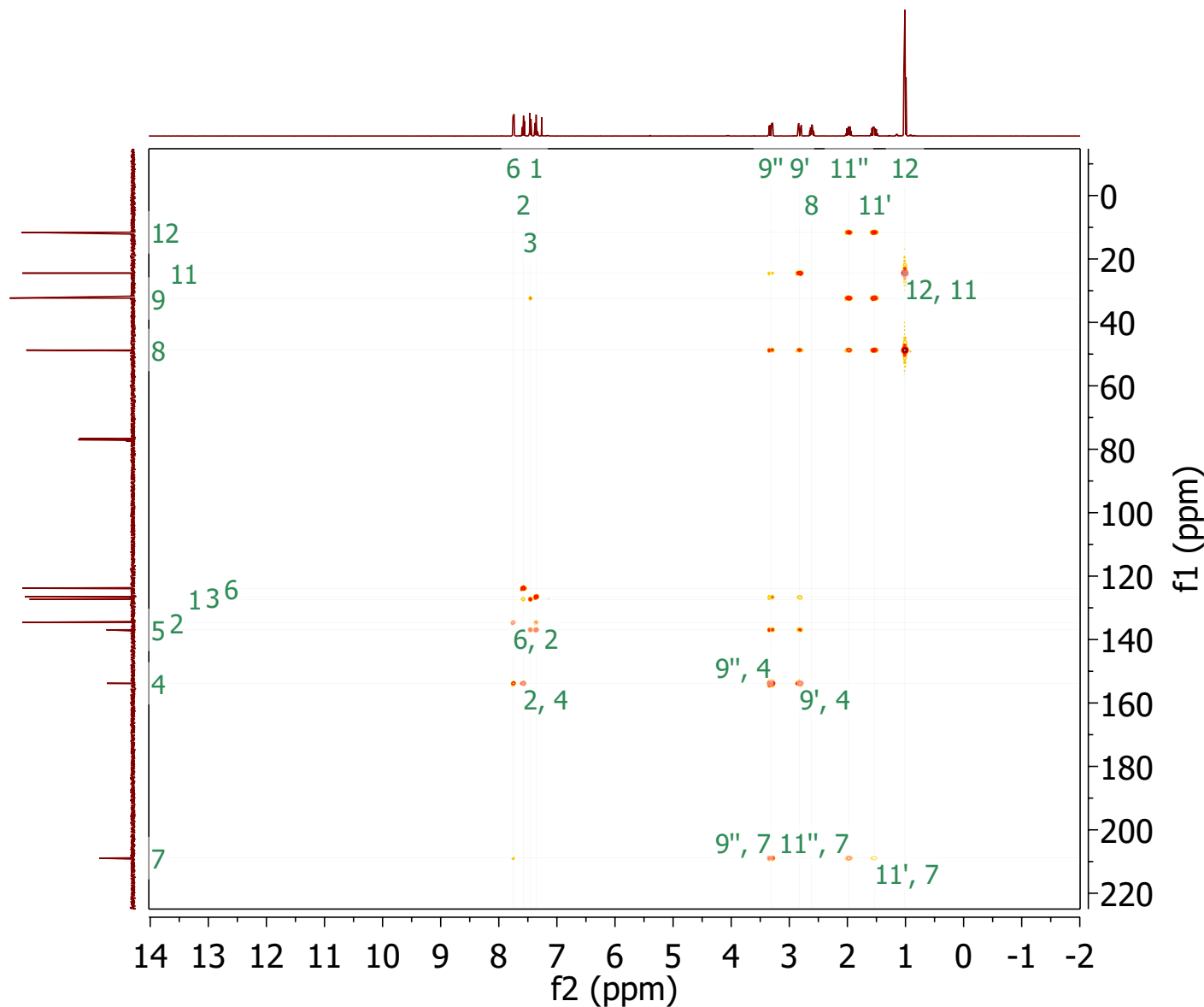


NORTHWESTERN  
UNIVERSITY

Submitted by: Yongbo Zhang  
Sample Name: EI  
Concentration: 10mg/ml  
Analysis Date:



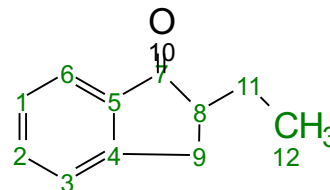
Ethylindanone\_gHMBCAD\_01



Parameter	Value
Title	Ethylindanone_gHMBCAD_01
Spectrometer	nmrs
Solvent	cdcl3
Pulse Sequence	gHMBCAD
Number of Scans	8
Acquisition Date	2010-03-08T11:28:22
Spectrometer Frequency	(399.51, 100.47)
Spectral Width	(6410.3, 24110.9)
Nucleus	(1H, 13C)
Acquired Size	(962, 200)
Spectral Size	(1024, 1024)

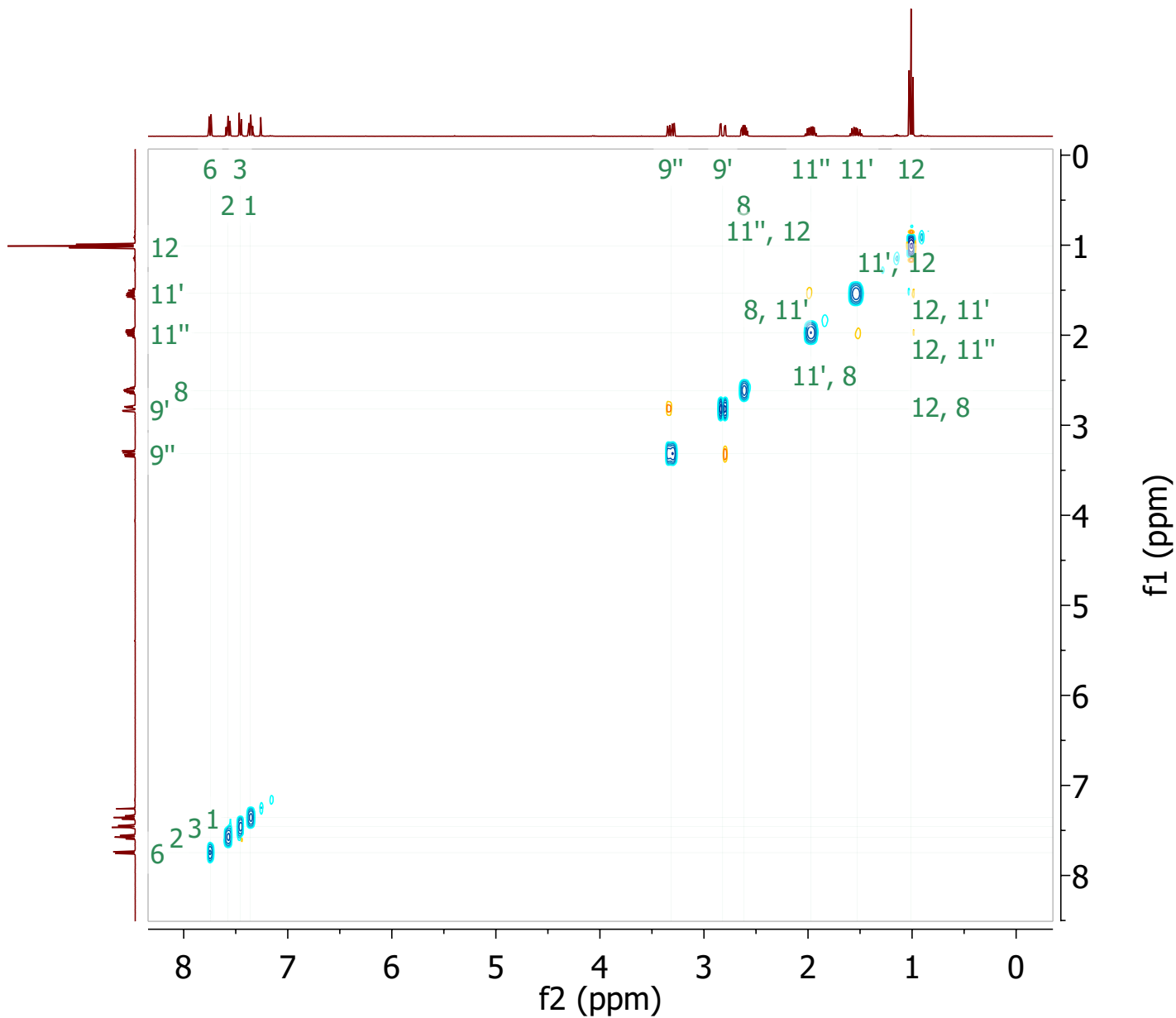
	f1 (ppm)	f2 (ppm)	Type	f1 (ppm)	f2 (ppm)	Type	
1	208.95	1.97	Compound	17	126.60	2.82	Compound
2	208.95	1.54	Compound	18	126.51	7.36	Compound
3	208.94	3.31	Compound	19	123.81	7.57	Compound
4	153.81	2.82	Compound	20	48.75	1.54	Compound
5	153.80	3.31	Compound	21	48.75	2.82	Compound
6	153.80	7.58	Compound	22	48.74	1.01	Compound
7	153.80	7.75	Compound	23	48.74	1.97	Compound
8	136.94	7.46	Compound	24	48.74	3.31	Compound
9	136.93	3.31	Compound	25	32.33	7.46	Compound
10	136.93	7.36	Compound	26	32.32	1.97	Compound
11	136.93	2.82	Compound	27	32.31	1.54	Compound
12	134.59	7.75	Compound	28	24.46	1.01	Compound
13	134.52	7.35	Compound	29	24.46	2.82	Compound
14	127.30	7.58	Compound	30	11.59	1.54	Compound
15	127.25	7.46	Compound	31	11.59	1.97	Compound
16	126.63	3.31	Compound				

Submitted by: Yongbo Zhang  
 Sample Name: EI  
 Concentration: 10mg/ml  
 Analysis Date:



Ethylindanone\_NOESY\_01 —

Parameter	Value
Title	Ethylindanone_NOESY_01
Spectrometer	vnmrs
Solvent	cdd3
Pulse Sequence	NOESY
Number of Scans	8
Acquisition Date	2011-07-08T22:39:58
Spectrometer Frequency	(399.47, 399.47)
Spectral Width	(6410.3, 6410.3)
Nucleus	(1H, 1H)
Acquired Size	(962, 128)
Spectral Size	(1024, 1024)



	f1 (ppm)	f2 (ppm)	Type
1	3.32	2.60	Compound
2	1.96	2.62	Compound
3	1.60	2.59	Compound
4	1.57	2.59	Compound
5	1.54	2.63	Compound
6	1.54	2.84	Compound
7	1.54	2.80	Compound
8	1.53	1.99	Compound
9	1.06	1.94	Compound
10	1.01	2.84	Compound
11	1.01	2.61	Compound
12	1.01	2.80	Compound
13	0.99	1.98	Compound
14	0.95	1.93	Compound