

# Isoprenylated Flavonoid and Adipogenesis-promoting Constituents of *Dodonaea viscosa*

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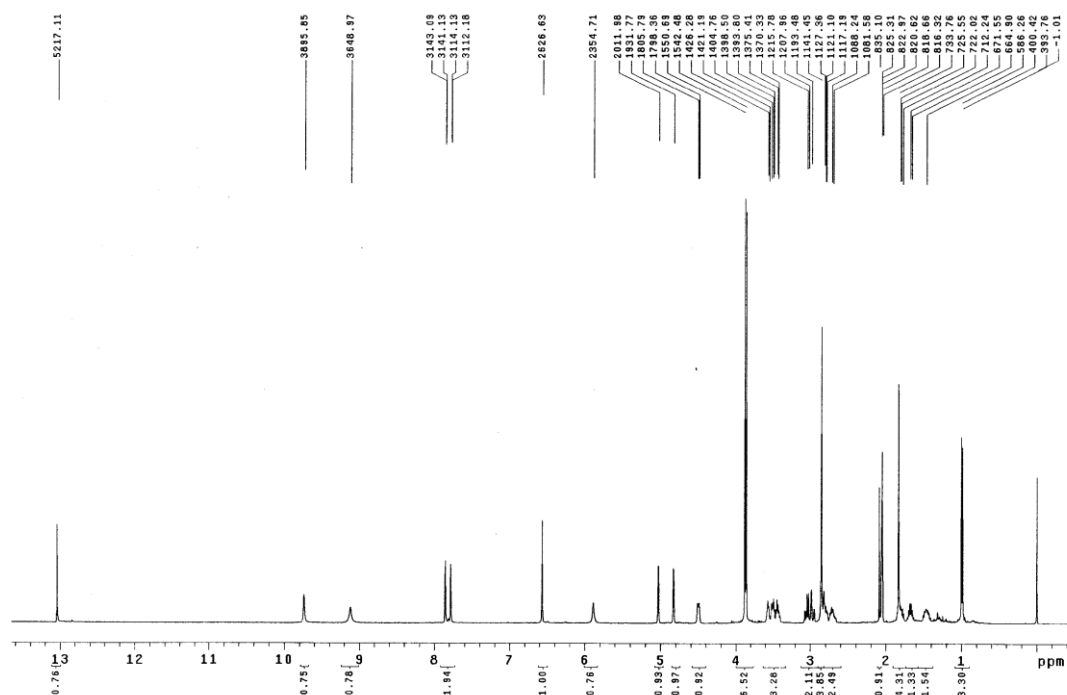
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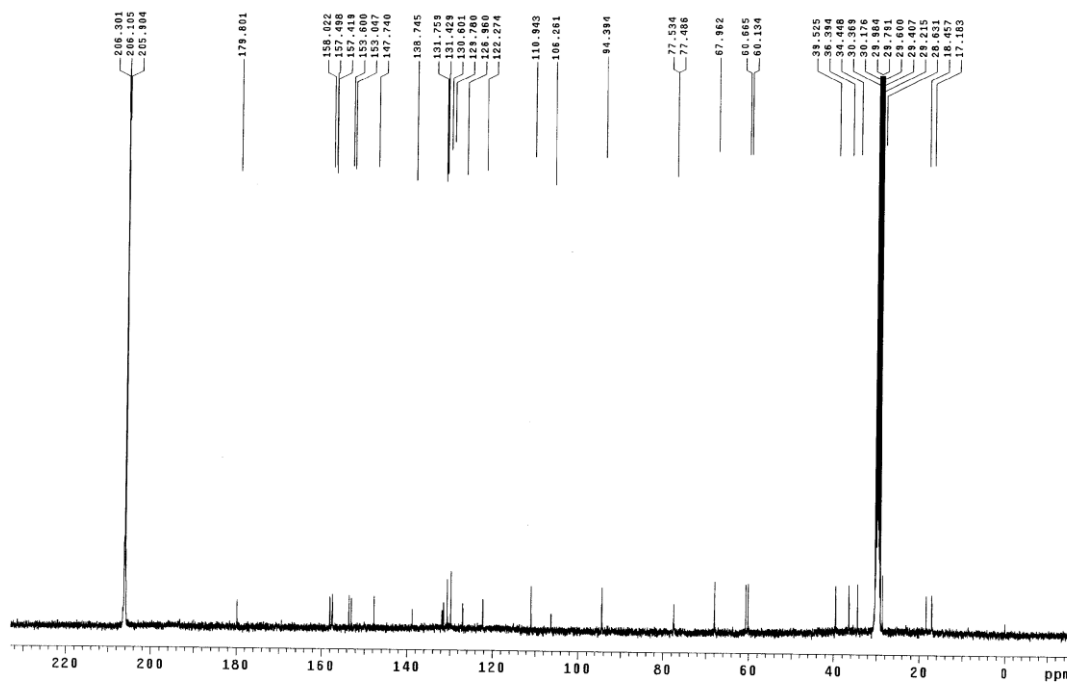
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# S 1.1 $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of 1

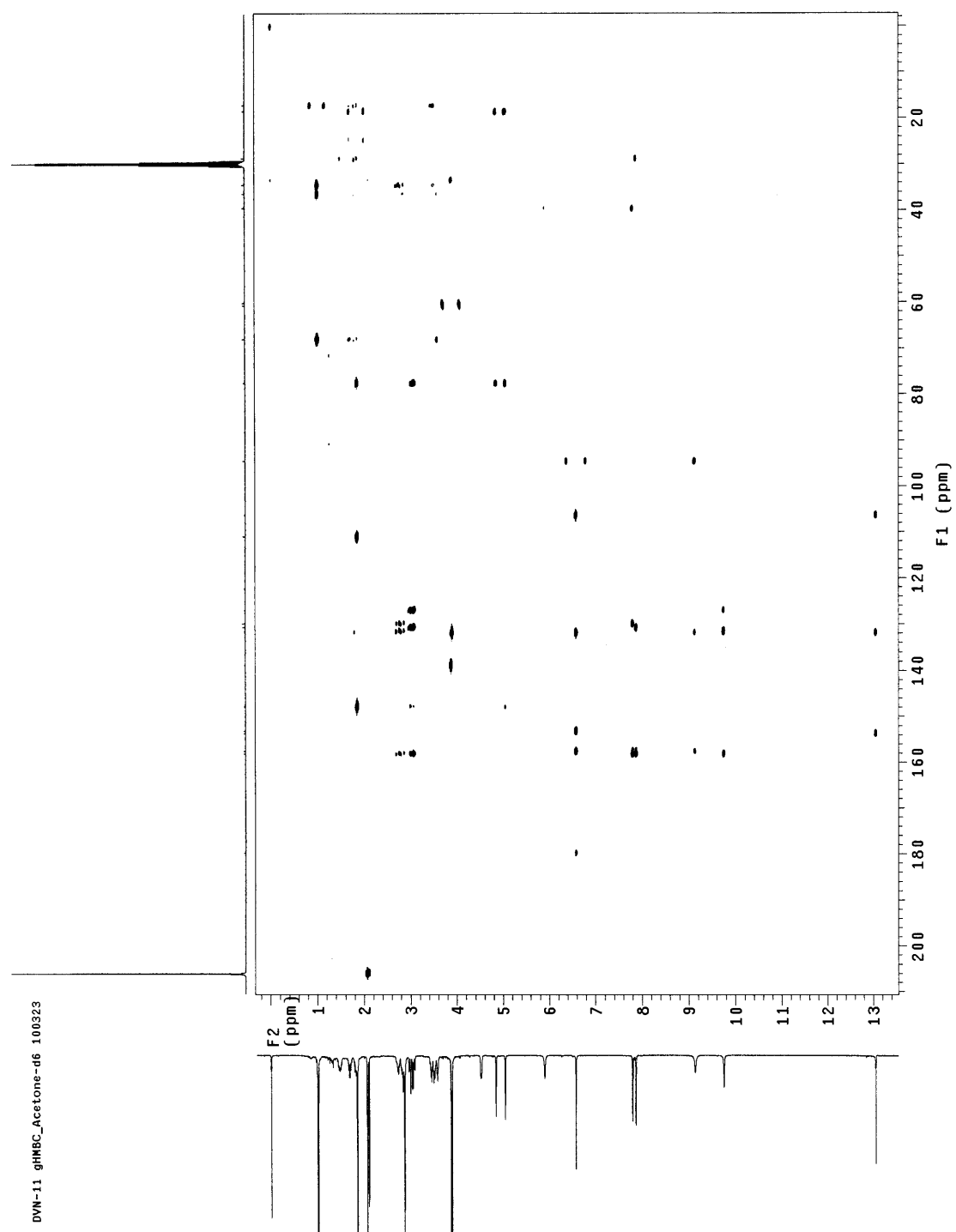
DVN-11 Acetone 100316



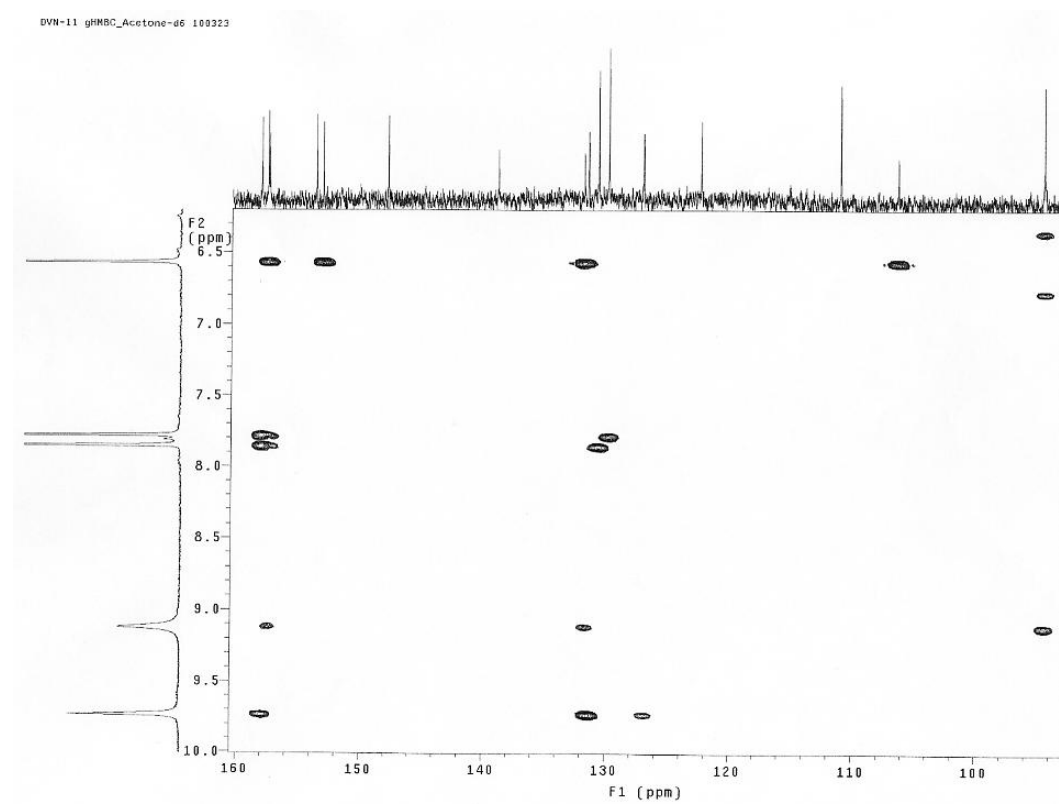
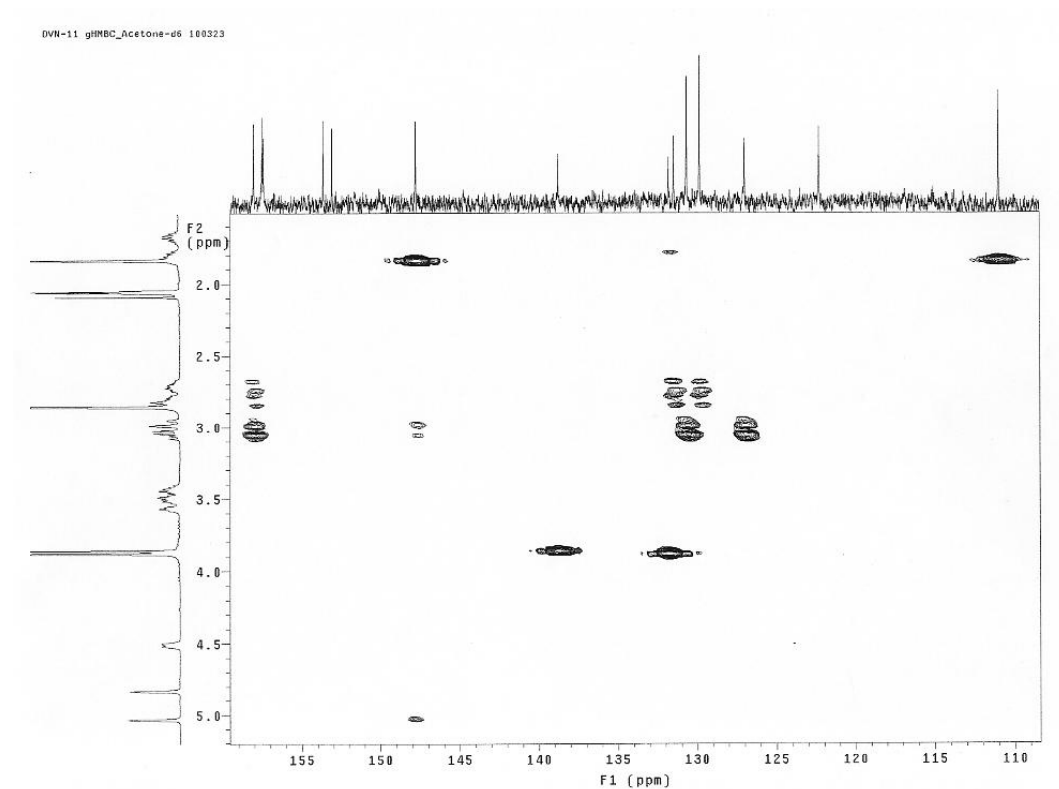
DVN-11  $\text{CDCl}_3$ -d6 100323



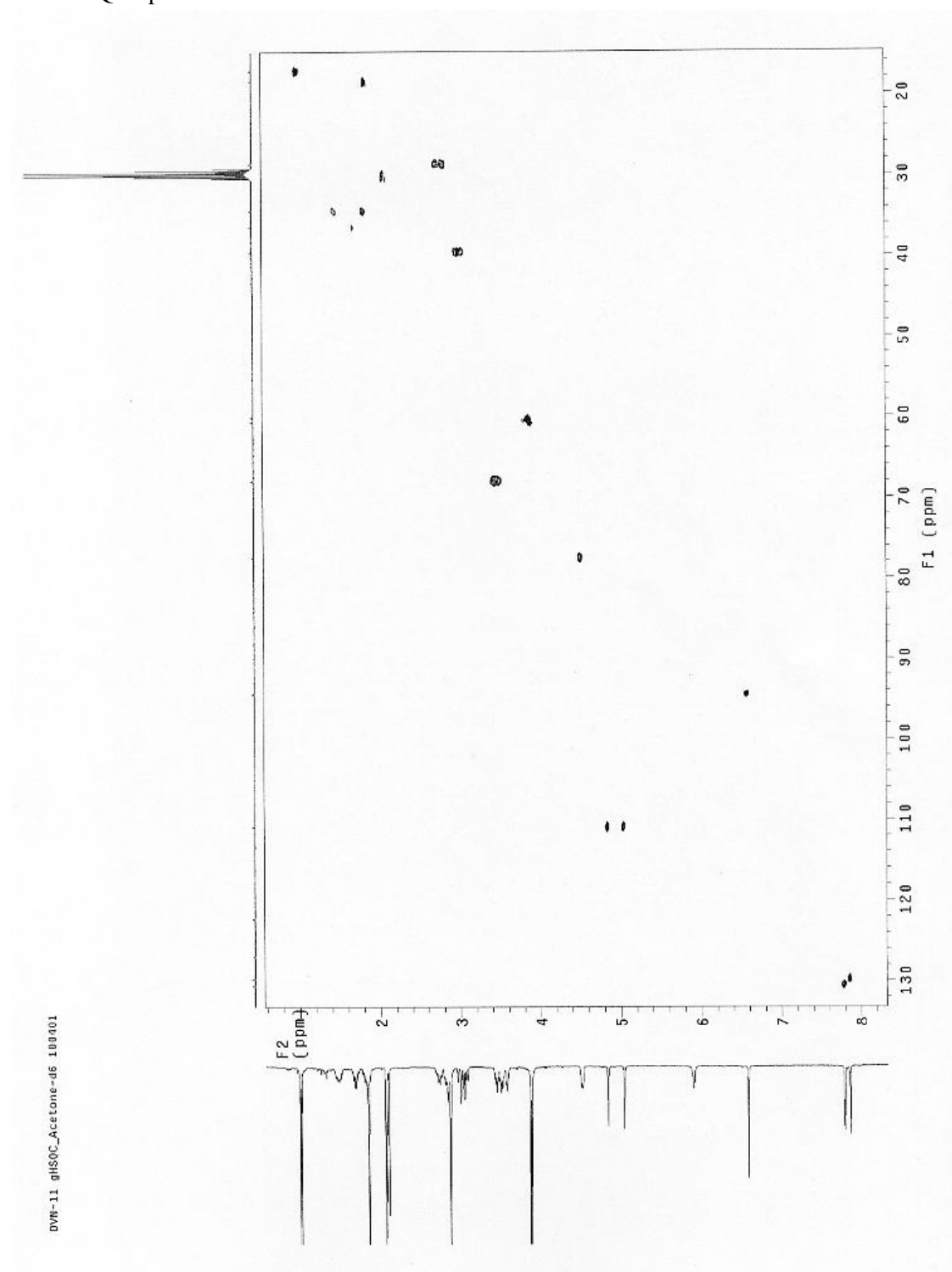
S 1.2 HMBC Spectrum of **1**



### S 1.3 HMBC Spectrum magnified of 1



S 1.4 HSQC Spectrum of **1**

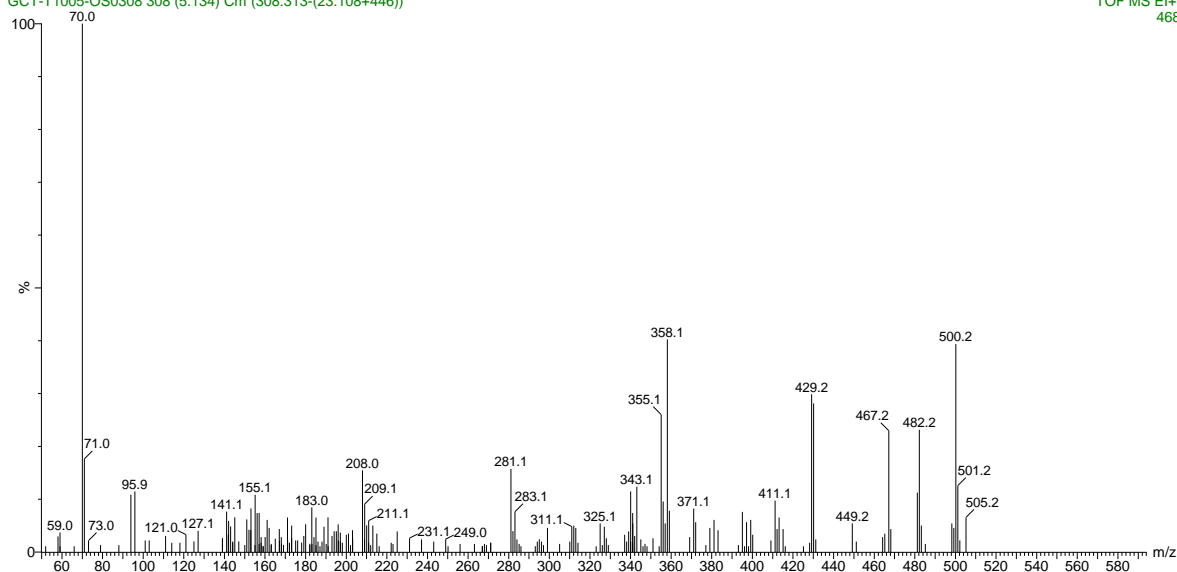


### DefaultInstrument

CA176-Cal

TOF MS EI+  
468

GCT-T1005-OS0308 308 (5.134) Cm (308:313-(23:108+446))



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Chinese Academic of Sciences  
High Resolution MS Data Report



Instrument: Waters Micromass GCT

Card Serial Number: GCT-T1005-OS0308

Sample Serial Number: DVK-11

Operator: Li

Date: 2010/05/21

## Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Single Mass Analysis (displaying only valid results)  
Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0    Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

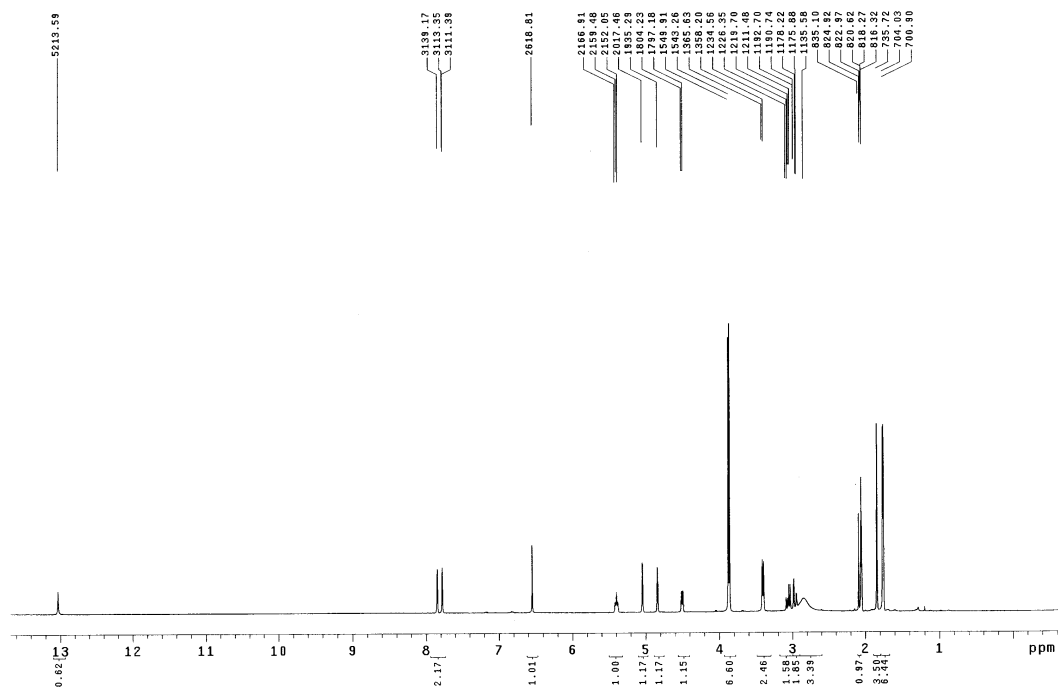
614 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

Minimum:		1.5	5.0	-1.5					
Maximum:				50.0					
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula			
500.2050	500.2051	-0.1	-0.2	7.5	4	C24 H35 N O8	C1		
	500.2046	0.4	0.7	12.0	1	C27 H32 O9			
	500.2060	-1.0	-1.9	17.0	2	C28 H28 N4 O5			
	500.2038	1.2	2.4	8.0	3	C22 H33 N4 O7	C1		

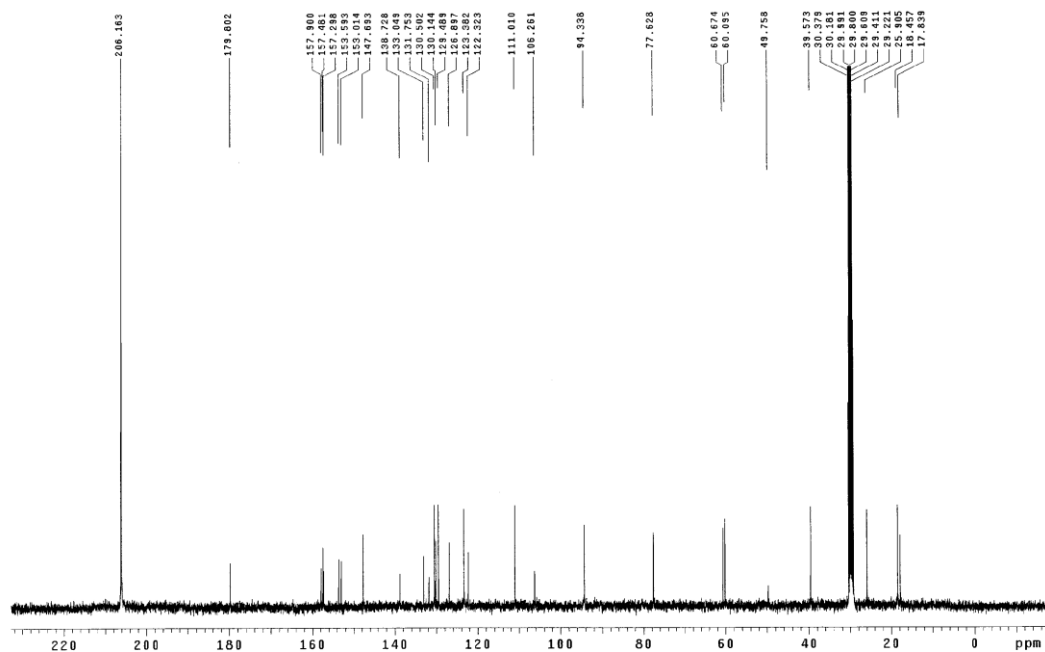


### S 2.1 $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of **2**

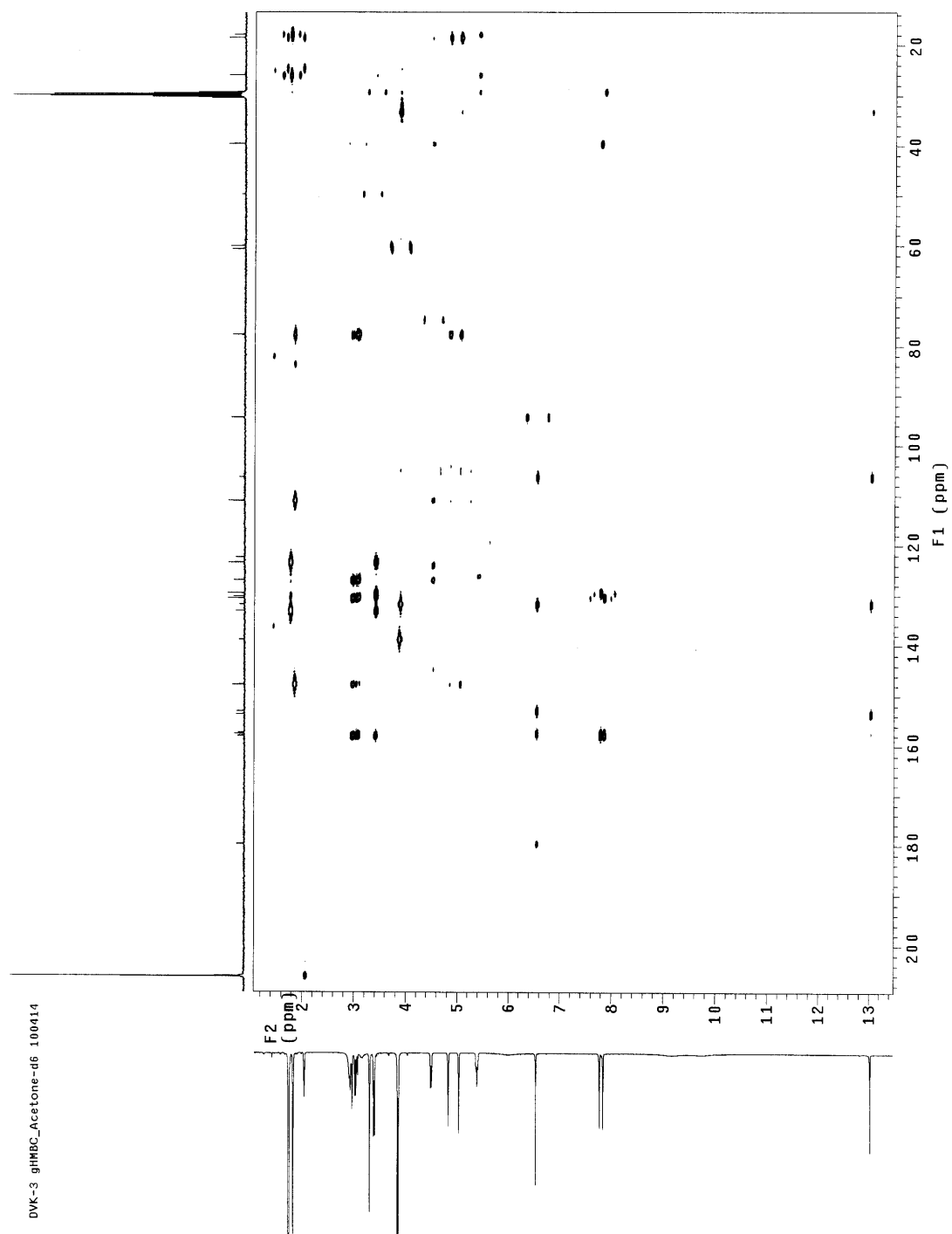
DVK-3 Acetone-d6 120320



DVK-3 C13\_Acetone-d6 100414



# S 2.2 HMBC Spectrum of 2



### S 2.3 HSQC Spectrum of 2



## S 2.4 EIMS and HREIMS Spectra of 2

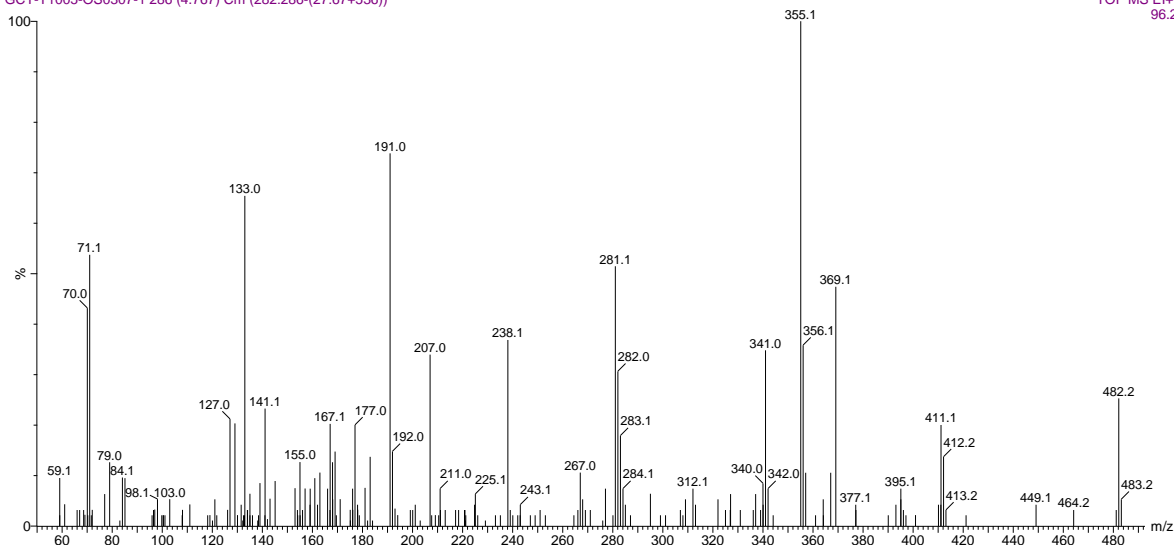
DefaultInstrument

14:26:57  
DVK-3

CA176-Cal

GCT-T1005-OS0307-1 286 (4.767) Cm (282:286-(27:67+536))

TOF MS EI+  
96.2



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High Resolution MS Data Report



Instrument: Waters Micromass GCT

Card Serial Number: GCT-T1005-OS0307

Sample Serial Number: DVK-3

Operator: Li

Date: 2010/05/21

### Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0

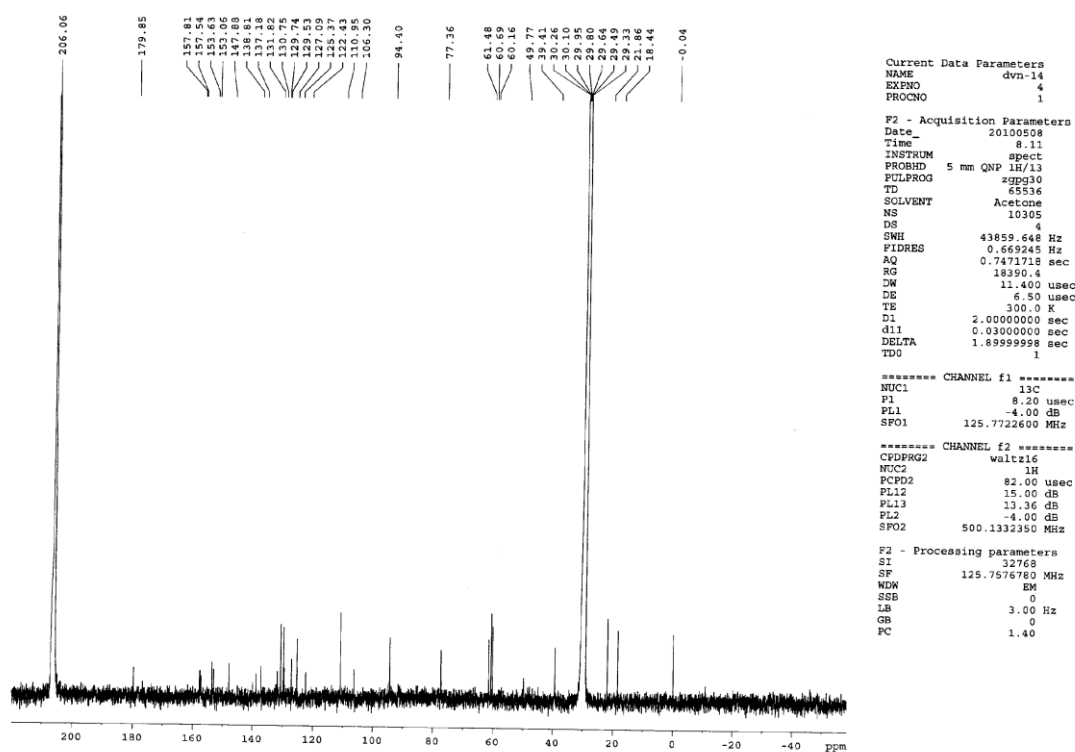
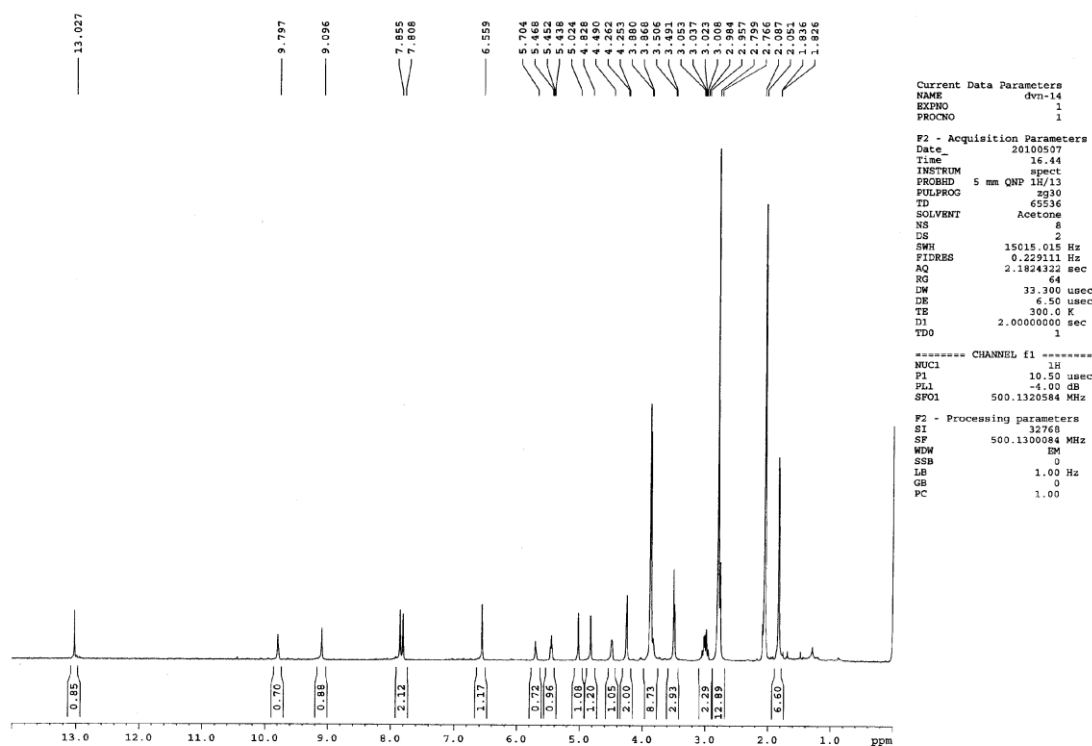
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

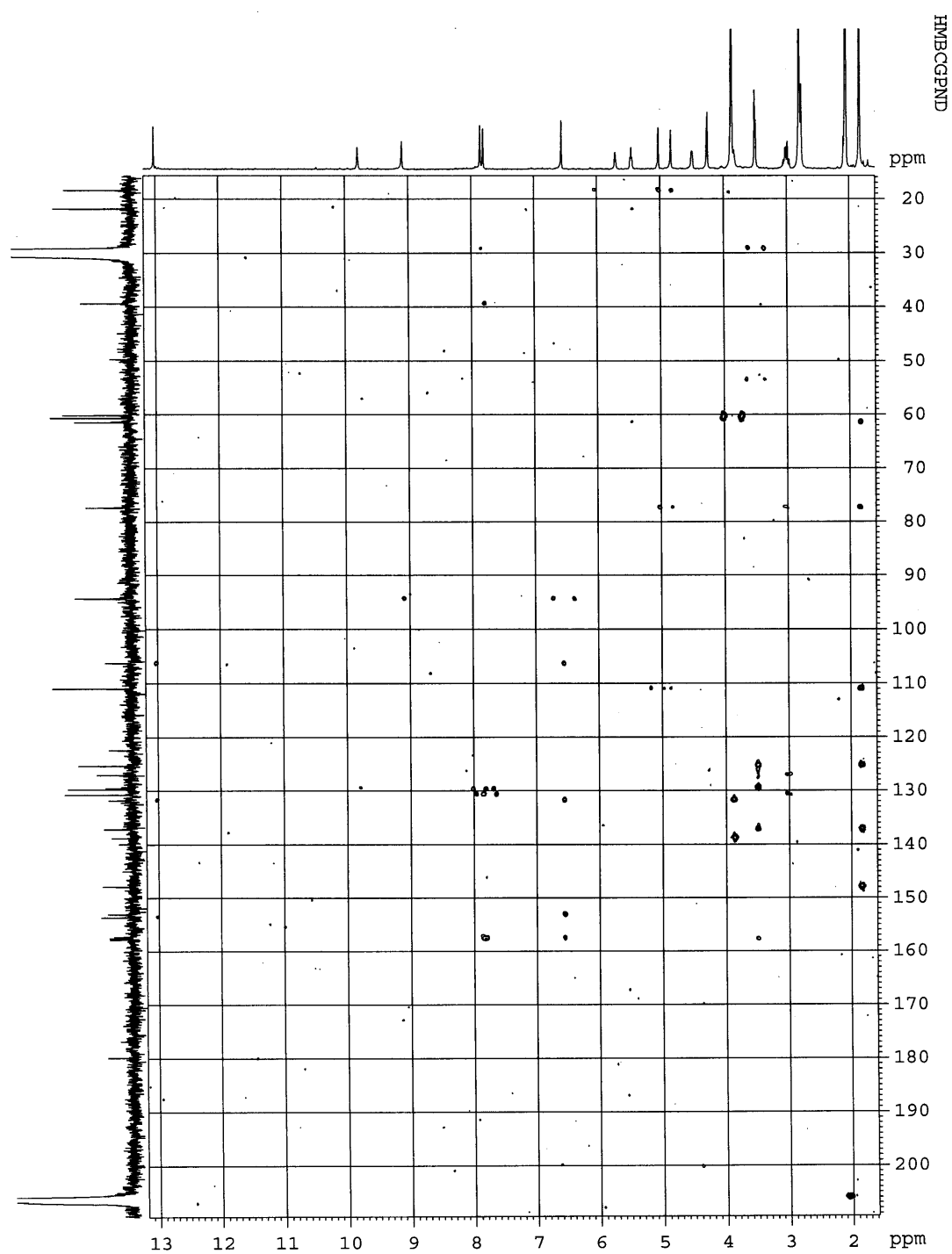
501 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
482.1943	482.1941	0.2	0.5	13.0	1	C27 H30 O8
	482.1946	-0.3	-0.5	8.5	4	C24 H33 N O7 Cl
	482.1932	1.1	2.3	9.0	3	C22 H31 N4 O6 Cl
	482.1954	-1.1	-2.3	18.0	2	C28 H26 N4 O4

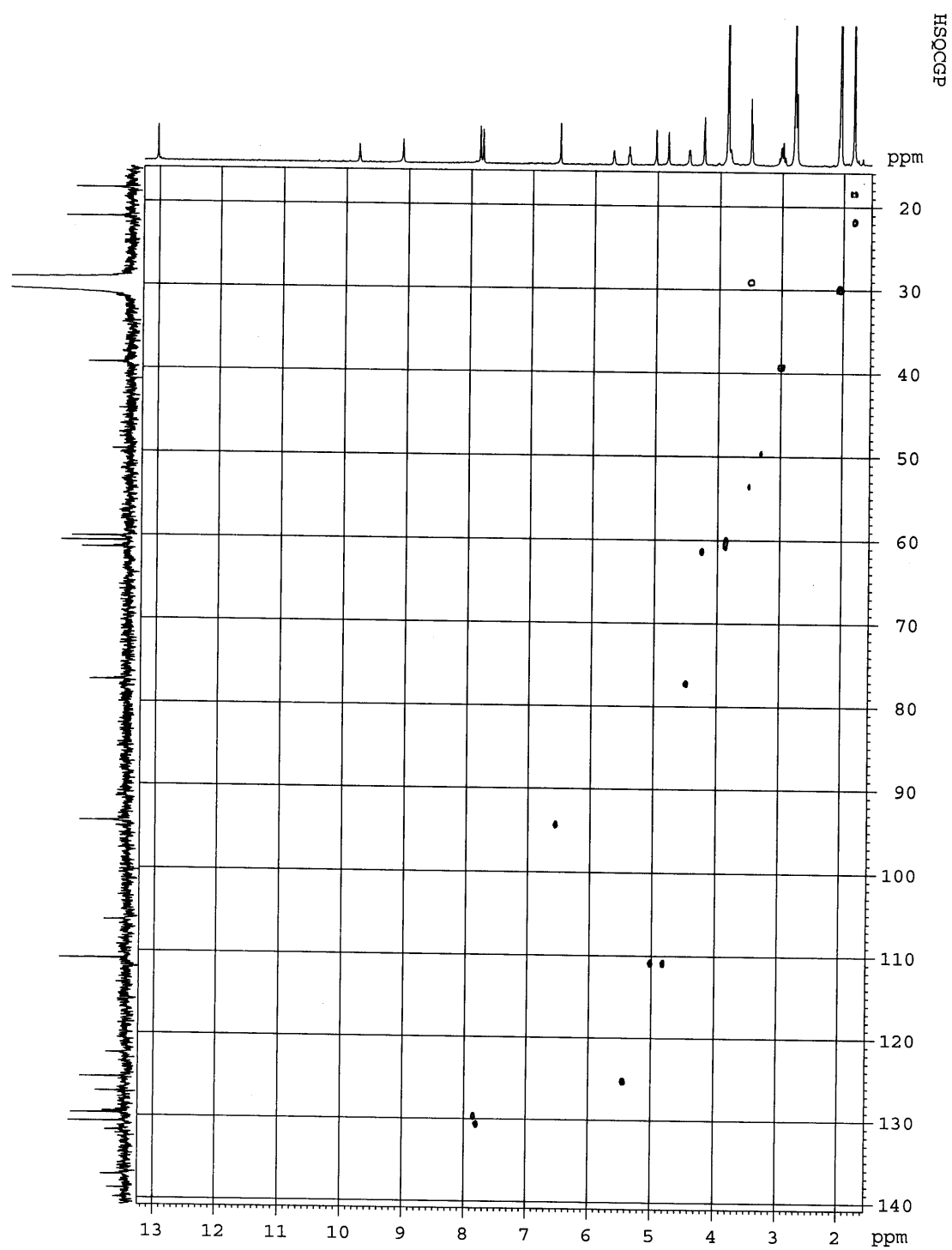
# S 3.1 $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of 3



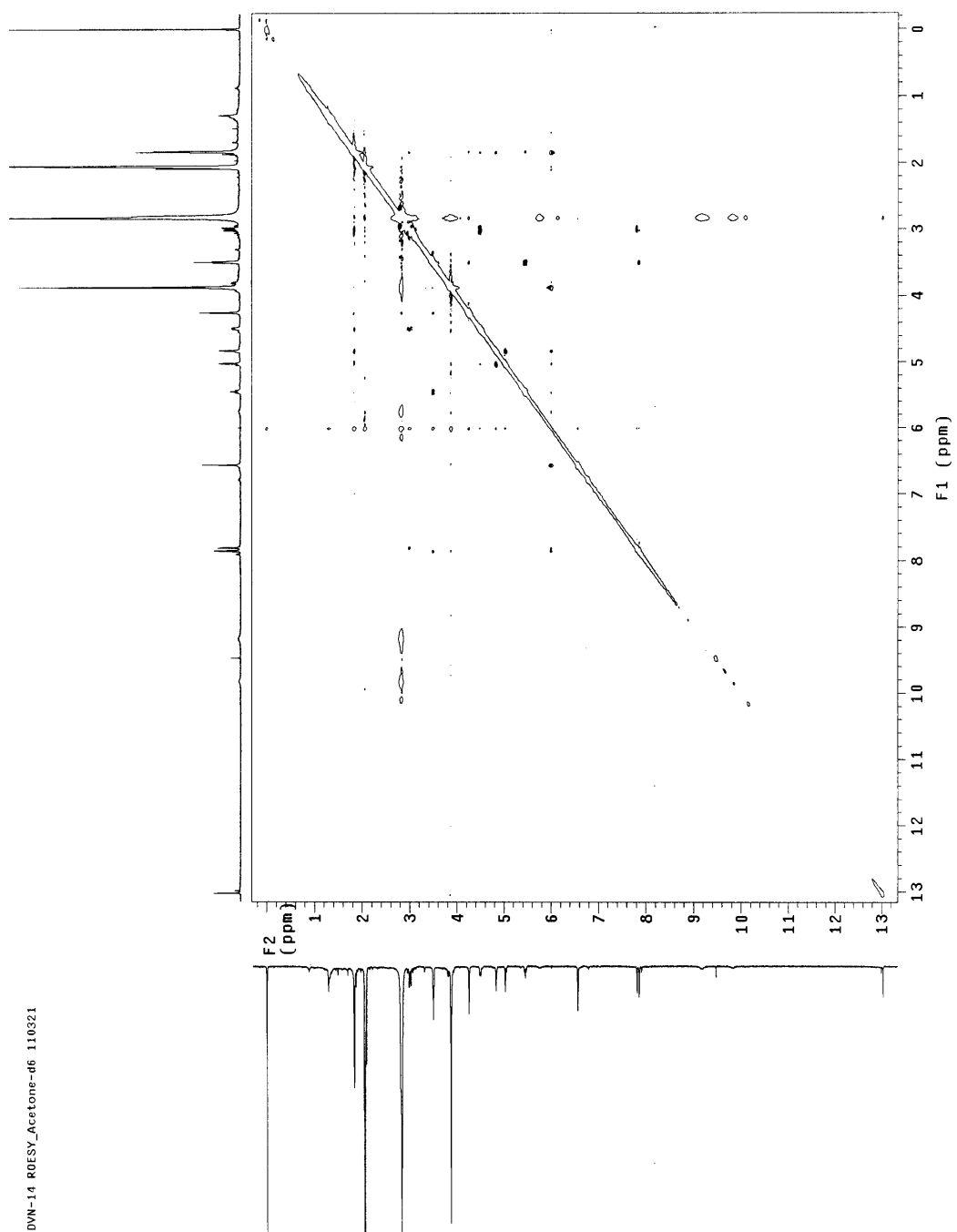
### S 3.2 HMBC Spectrum of **3**



S 3.3 HSQC Spectrum of **3**



### S 3.4 ROESY Spectrum of **3**





### S 3.5 EIMS and HREIMS Spectra of **3**

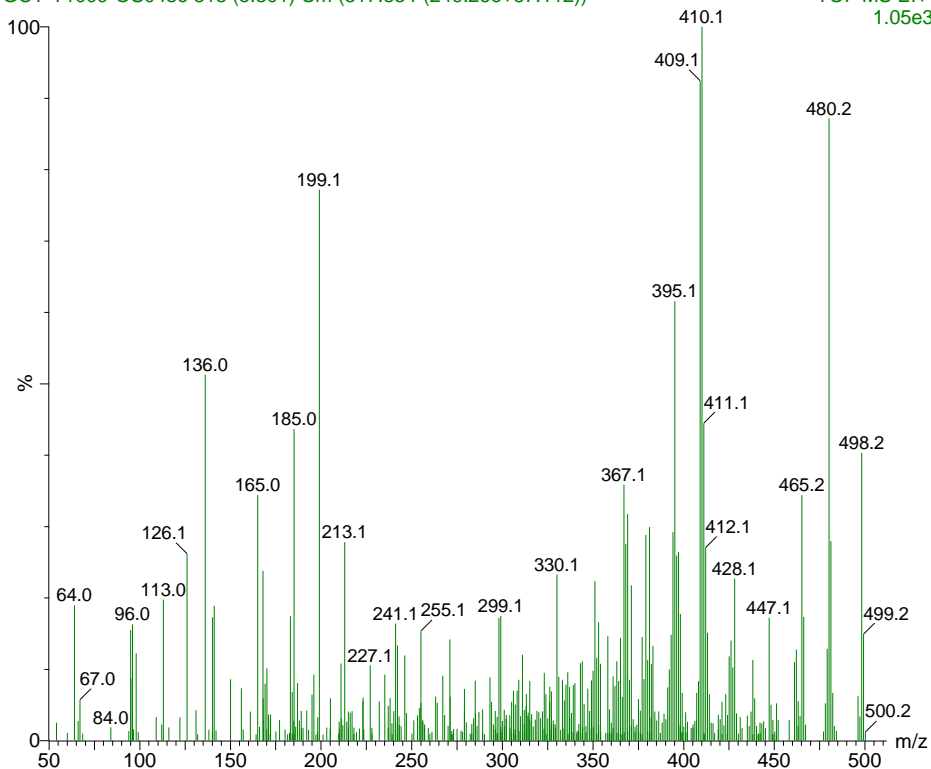
DefaultInstrument

10:15:25  
DVN-14

CA176-Cal

GCT-T1009-OS0486 318 (5.301) Cm (317:334-(249:266+87:112))

TOF MS EI+  
1.05e3



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High Resolution MS Data Report



Instrument: Waters Micromass GCT    Ionisation Mode: EI+    Electron Energy: 70eV

Card Serial Number: GCT-T1009-OS0486

Sample Serial Number: DVN-14

Operator: Li

Date: 2010/09/27

#### Elemental Composition Report

##### Single Mass Analysis

Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0    Abundance = 1.0%

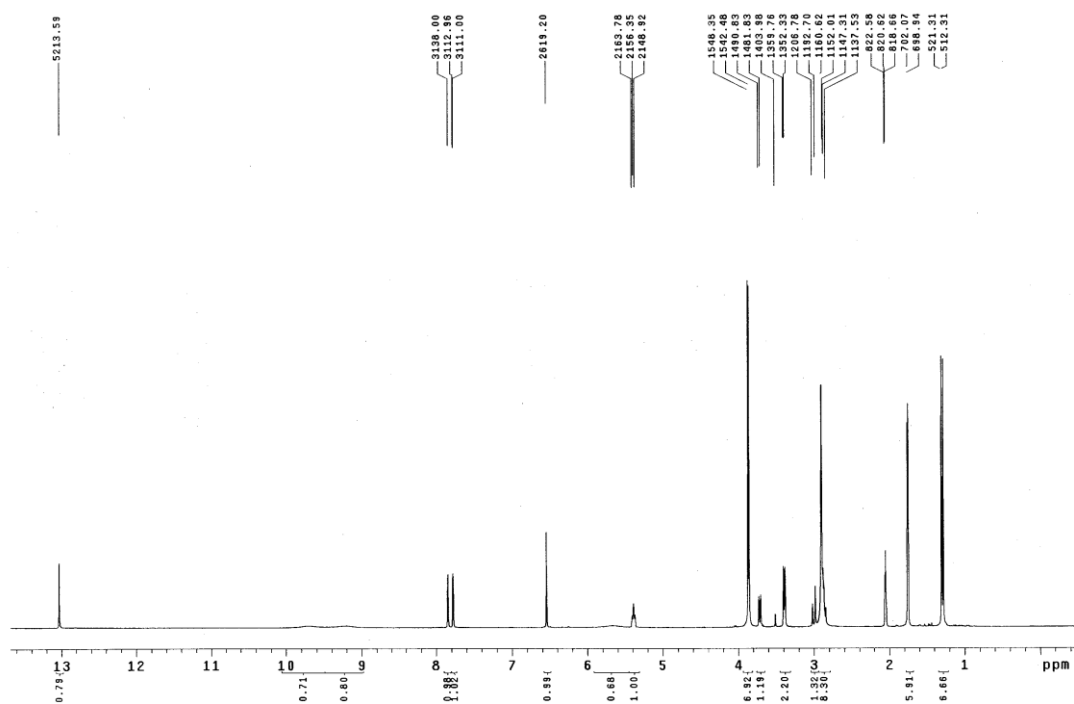
##### Monoisotopic Mass, Odd and Even Electron Ions

595 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

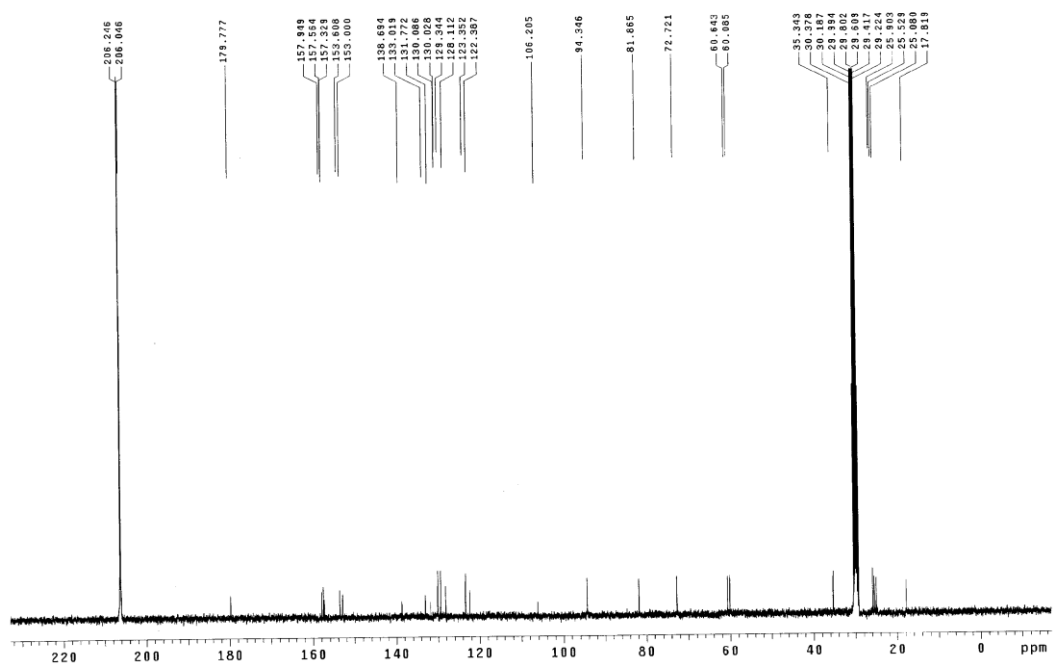
Minimum:				-1.5			
Maximum:		1.5	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula	
498.1893	498.1895	-0.2	-0.3	8.5	4	C24	H33 N 08 C1
	498.1890	0.3	0.6	13.0	1	C27	H30 O9
	498.1903	-1.0	-2.0	18.0	2	C28	H26 N4 O5
	498.1881	1.2	2.4	9.0	3	C22	H31 N4 O7 C1

#### S 4.1 <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of **4**

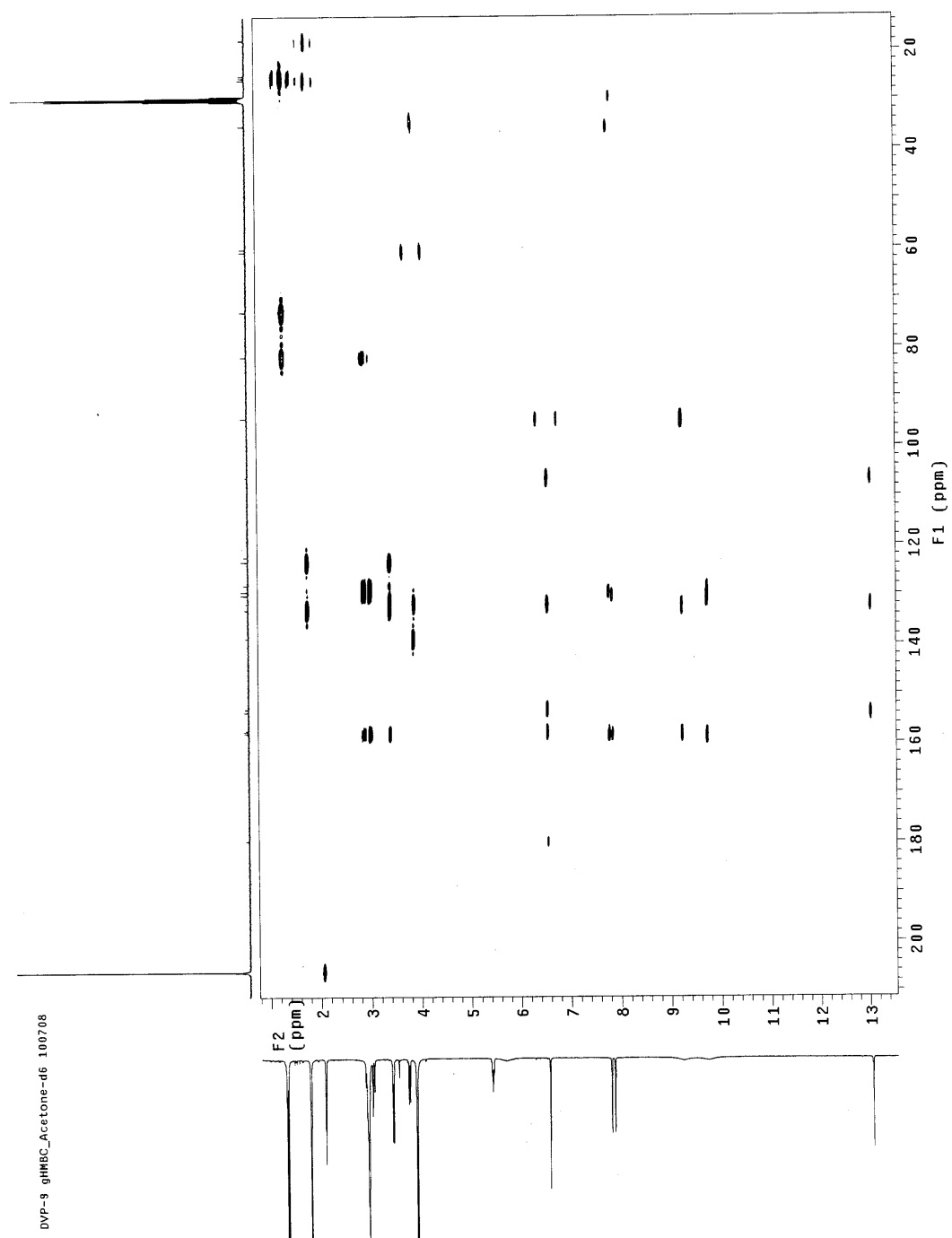
DVP-9 Acetone-d6 100622



DVP-9 C13-Acetone 100708

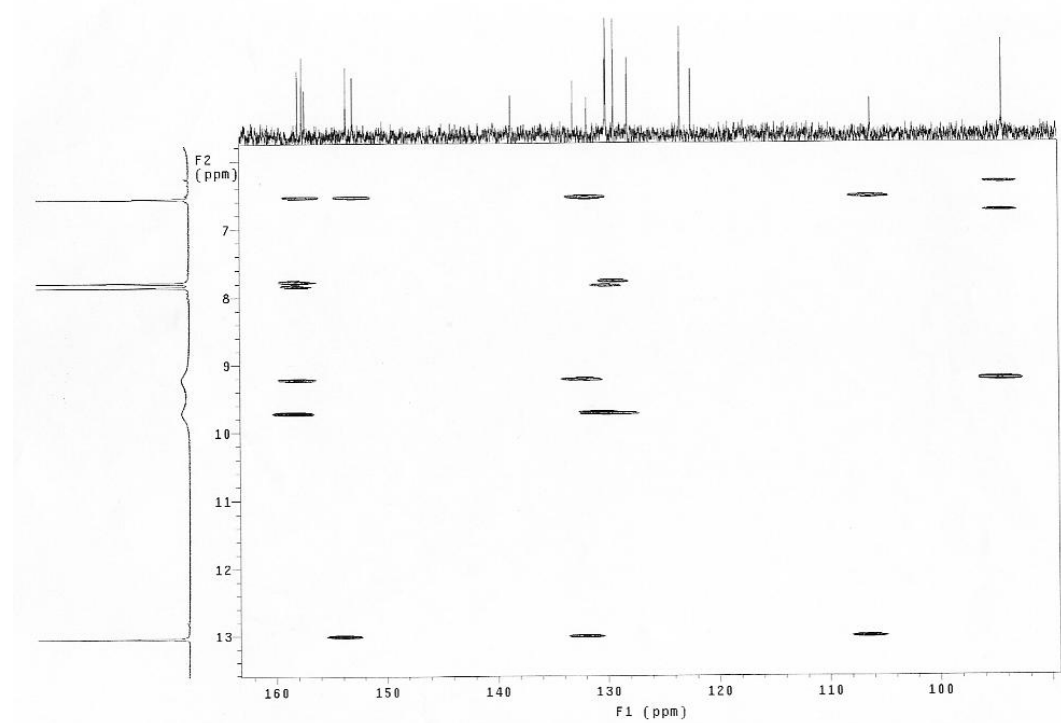


# S 4.2 HMBC Spectrum of **4**

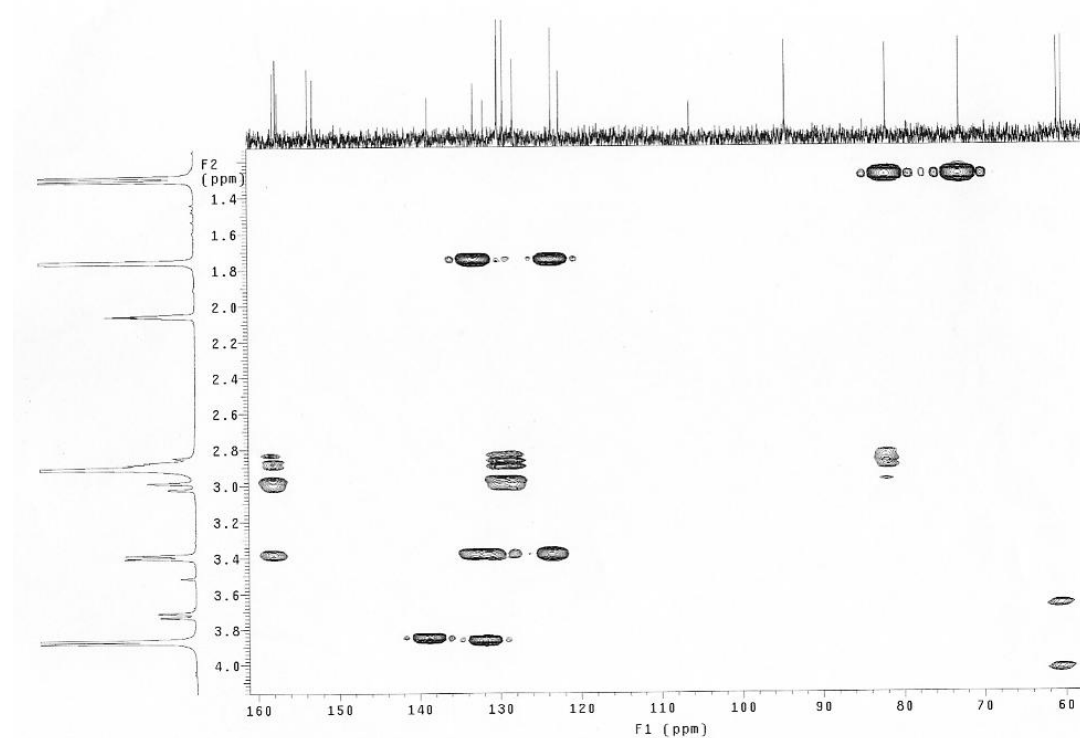


### S 4.3 HMBC Spectrum magnified of 4

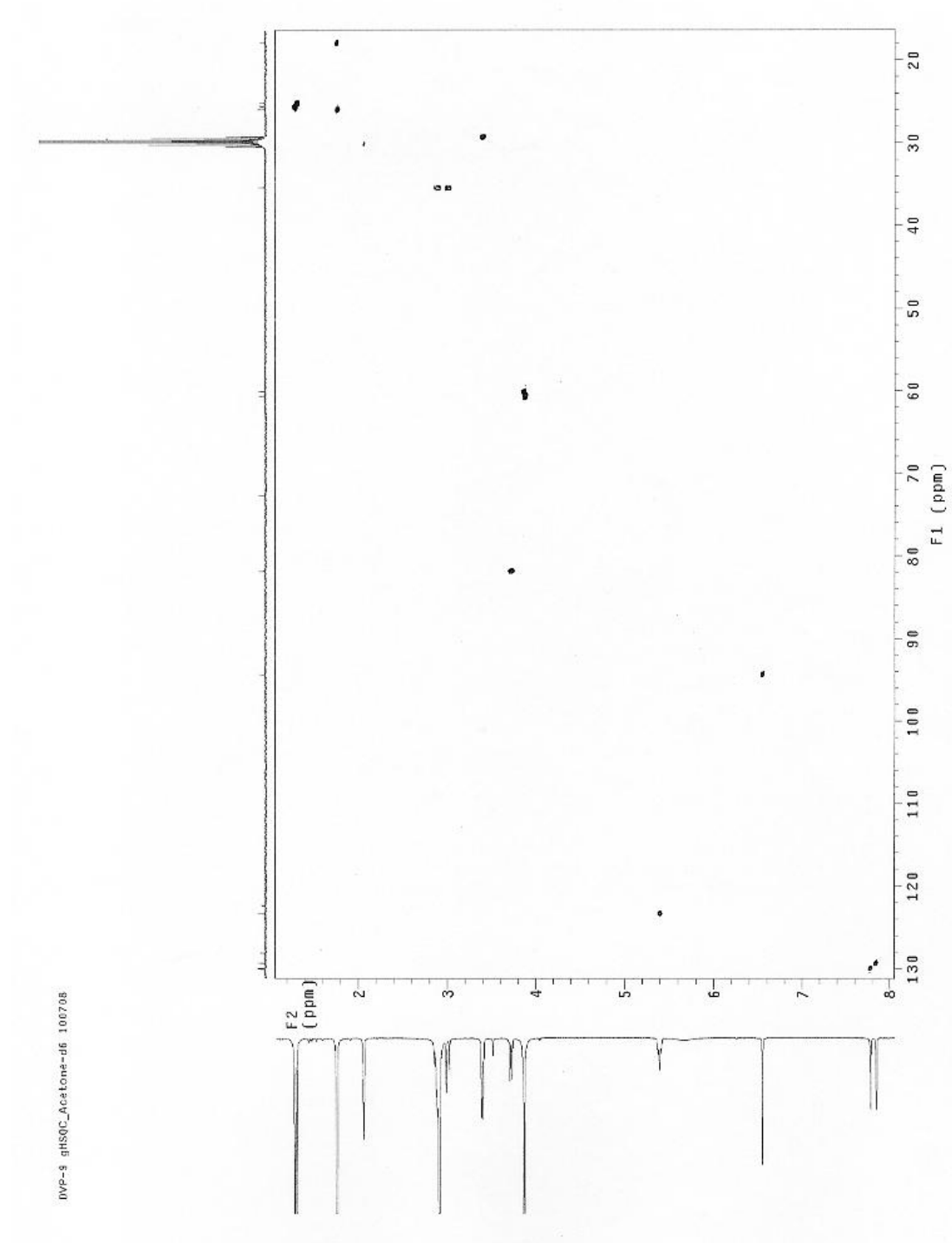
DVP-9 gHMBC\_Acetone-d6 100708



DVP-9 gHMBC\_Acetone-d6 100708



#### S 4.4 HSQC Spectrum of **4**



# S 4.5 EIMS and HREIMS Spectra of 4

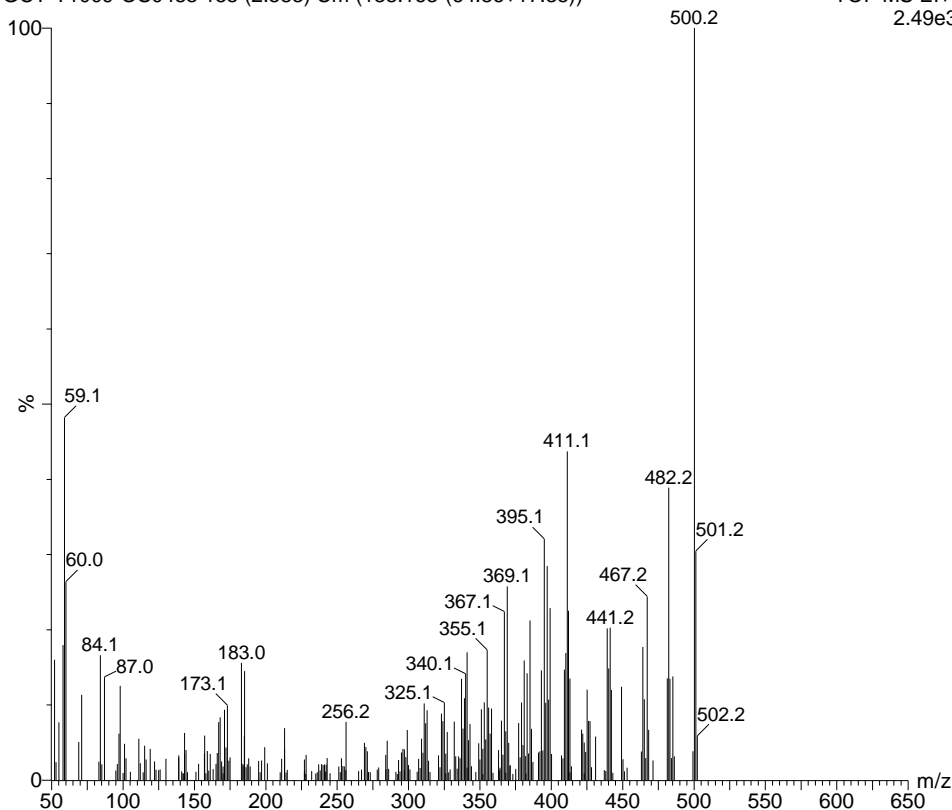
DefaultInstrument

10:38:08  
DVP-9

CA176-Cal

GCT-T1009-OS0488 155 (2.583) Cm (138:163-(64:86+17:35))

TOF MS EI+  
2.49e3



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High Resolution MS Data Report



Instrument: Waters Micromass GCT Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-T1009-OS0488

Sample Serial Number: DVP-9

Operator: Li

Date: 2010/09/27

## Elemental Composition Report

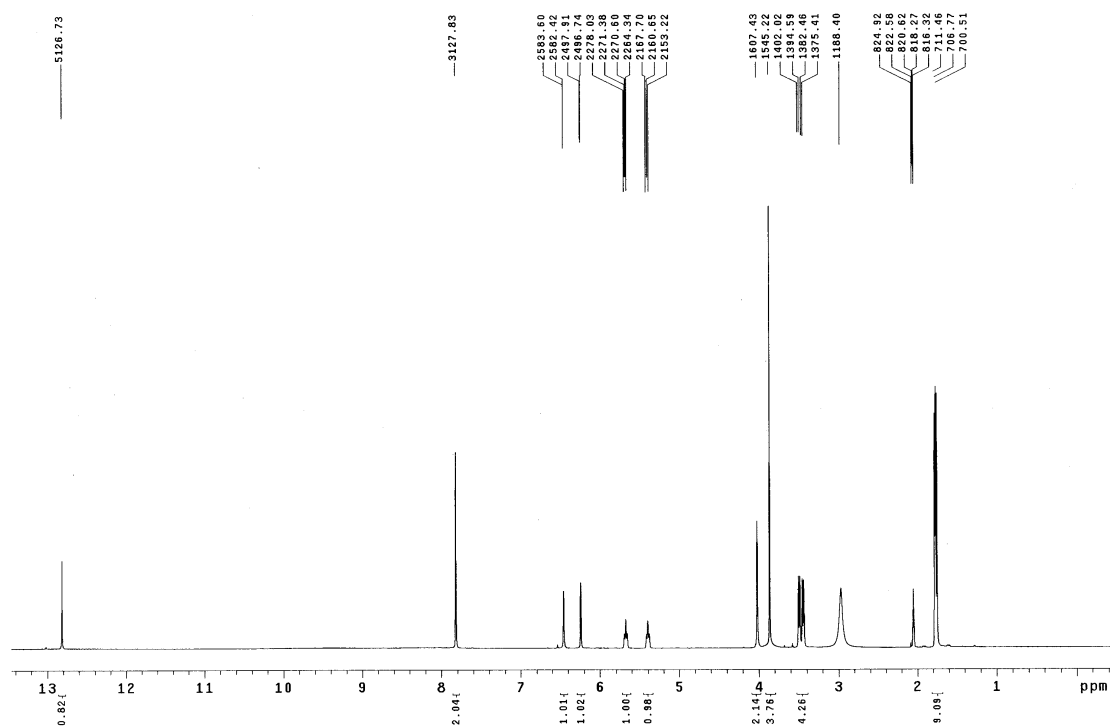
Single Mass Analysis  
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0  
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
91 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

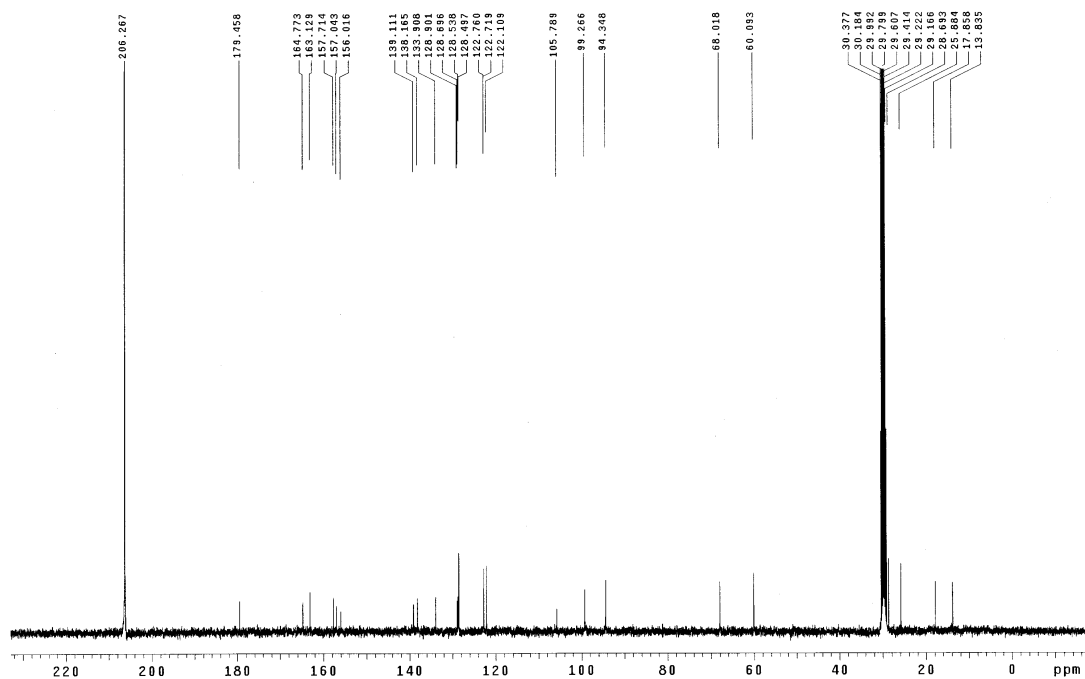
Minimum:				-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
500.2045	500.2046	-0.1	-0.3	12.0	2	C27 H32 O9
	500.1988	5.7	11.5	21.0	3	C34 H28 O4
	500.2105	-6.0	-12.0	3.0	1	C20 H36 O14
	500.2140	-9.5	-19.0	25.0	4	C38 H28 O

### S 5.1 <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of **5**

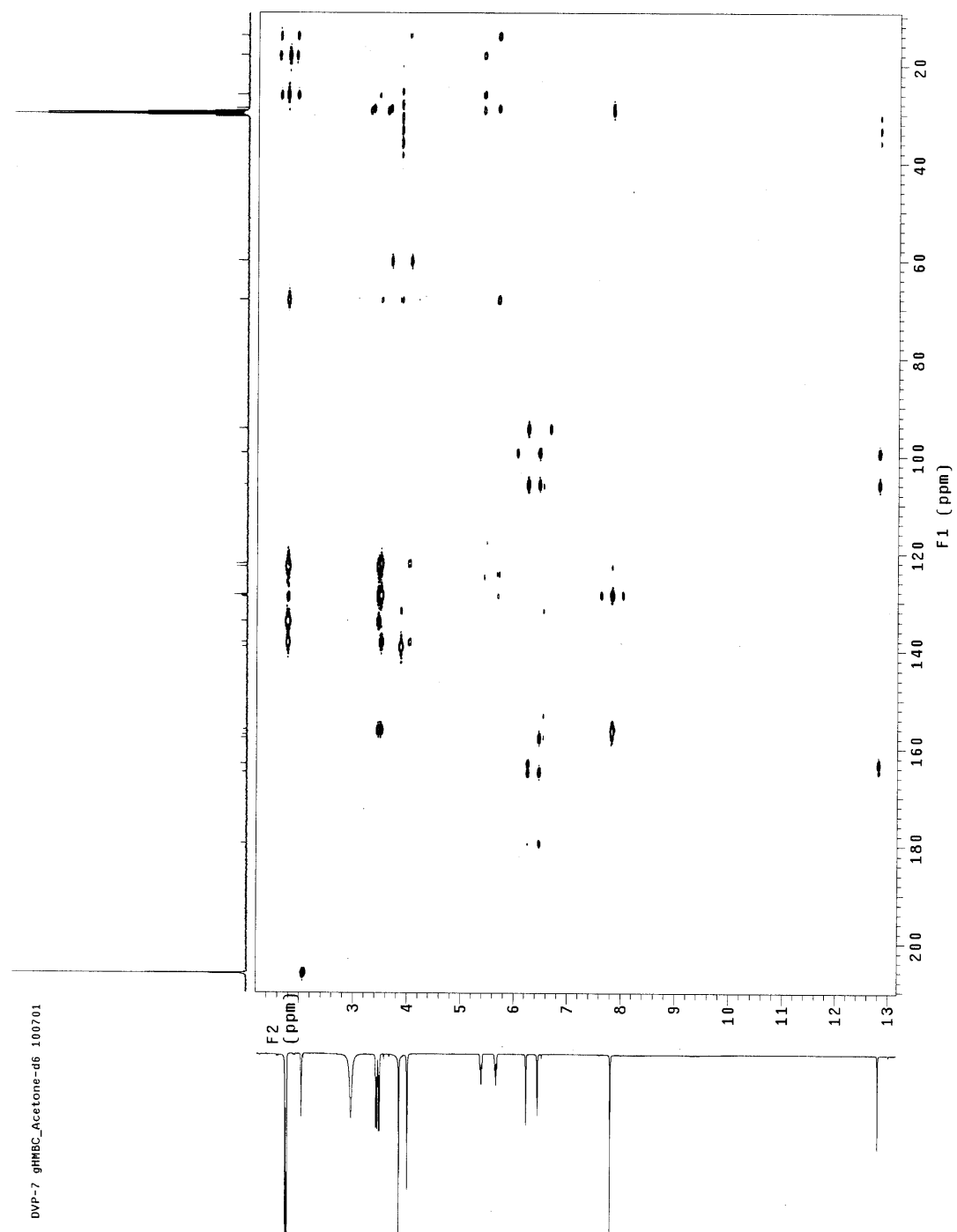
DVP-7 Acetone-d6 100622



DVP-7 C13\_Acetone-d6 100701



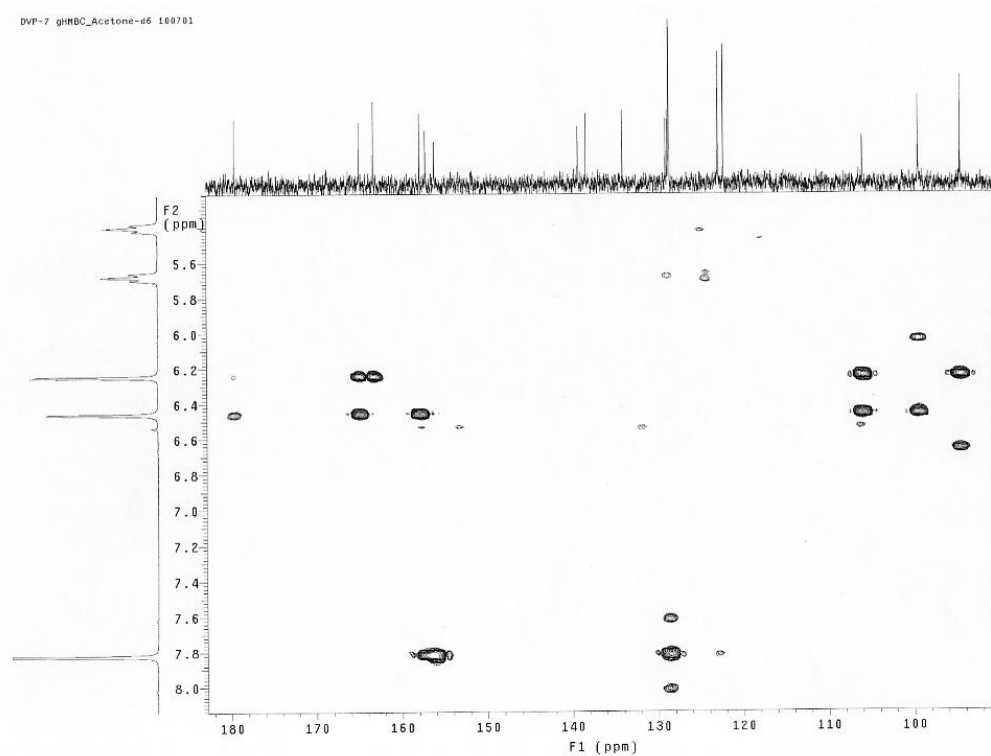
S 5.2 HMBC Spectrum of **5**



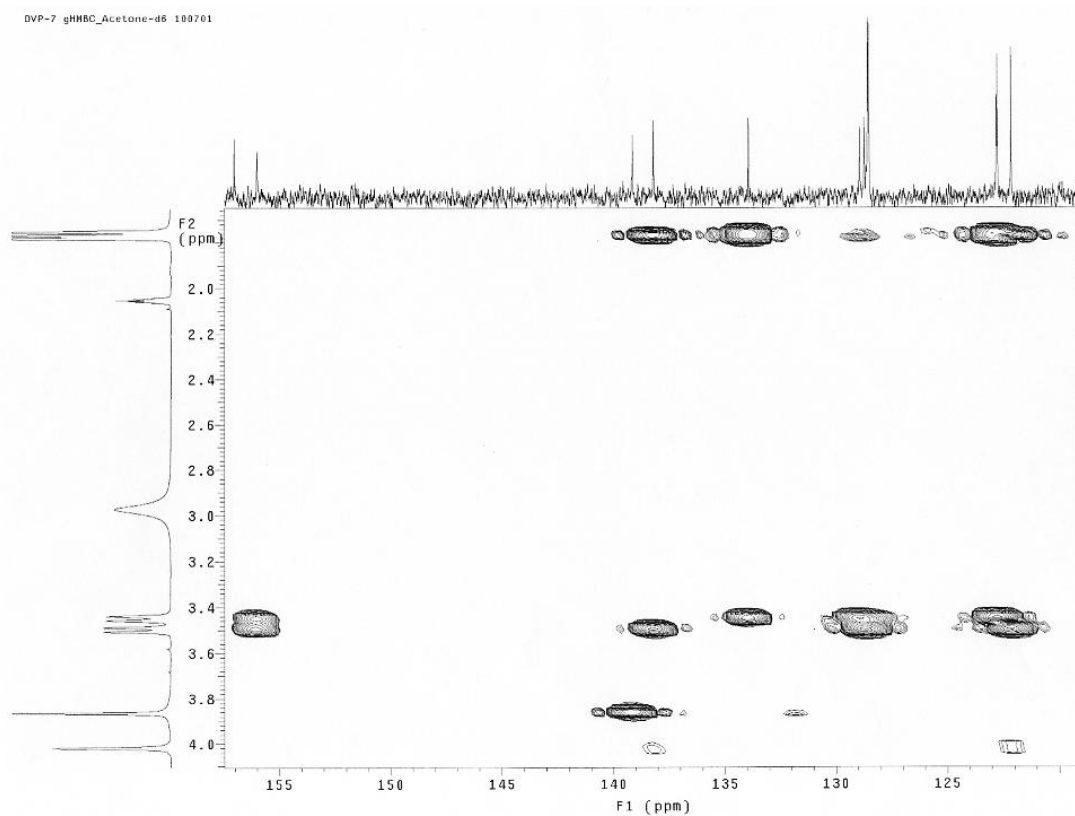


### S 5.3 HMBC Spectrum magnified of 5

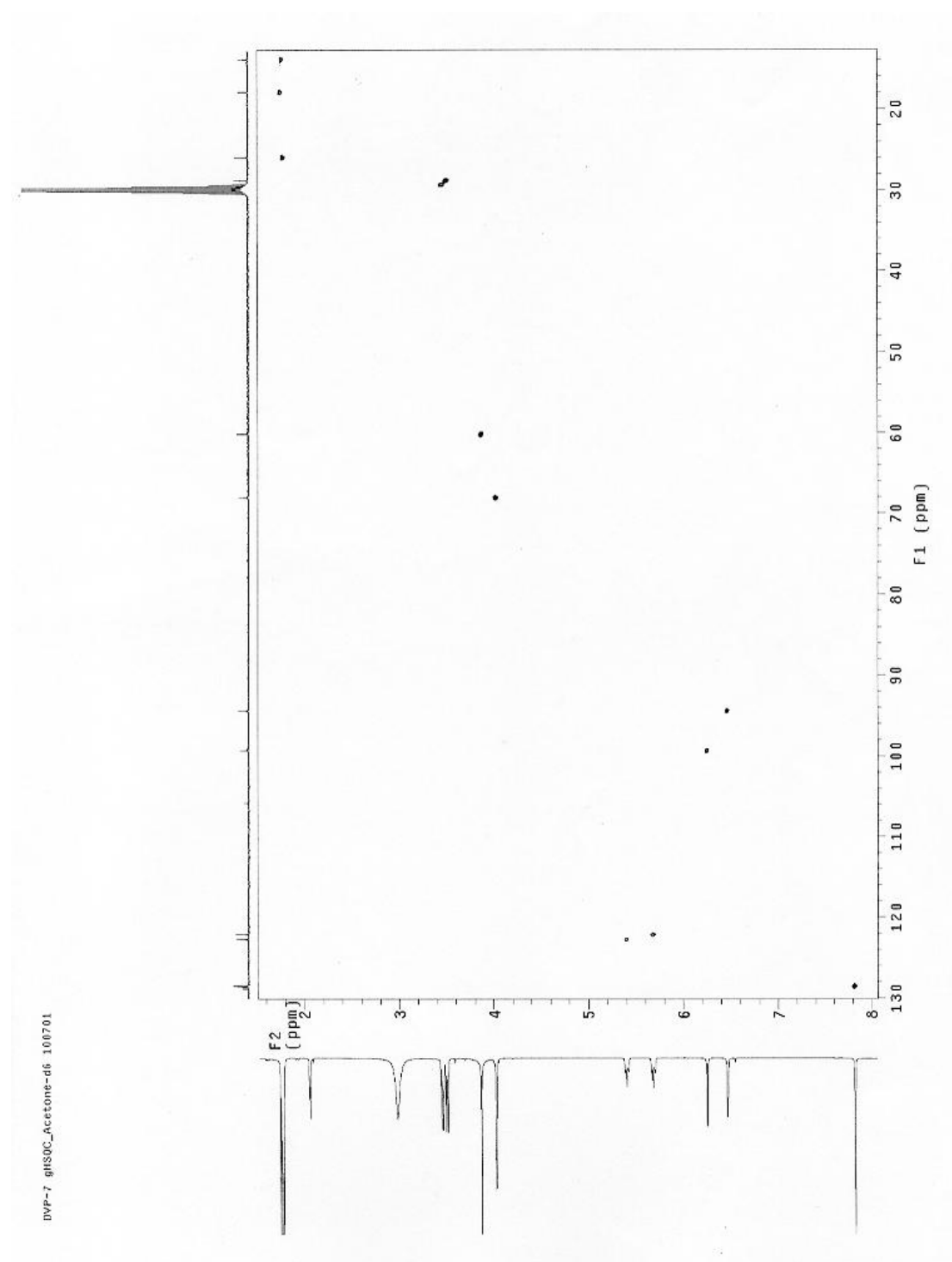
DVP-7 gHMBC\_Acetone-d6 100701



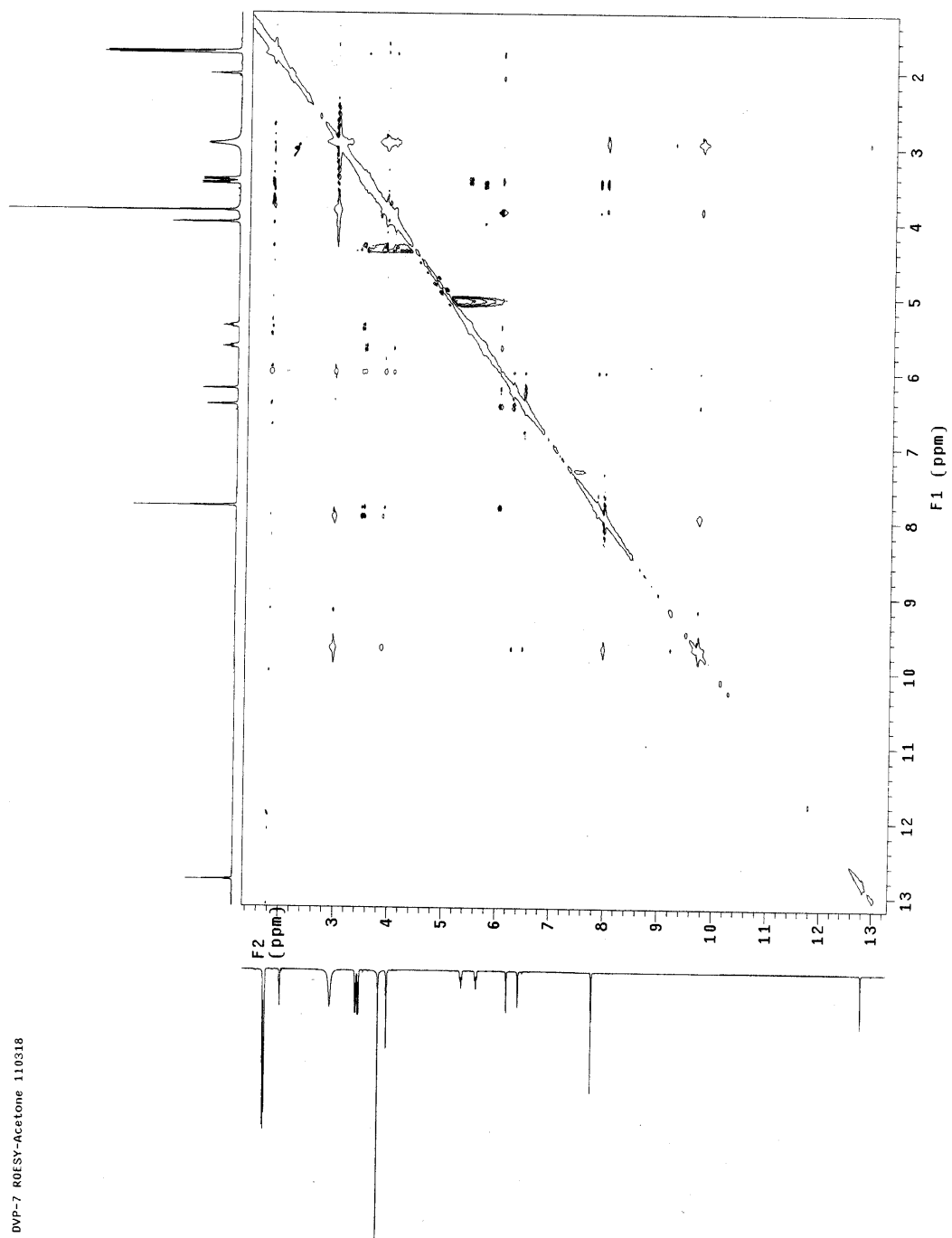
DVP-7 gHMBC\_Acetone-d6 100701



# S 5.4 HSQC Spectrum of **5**

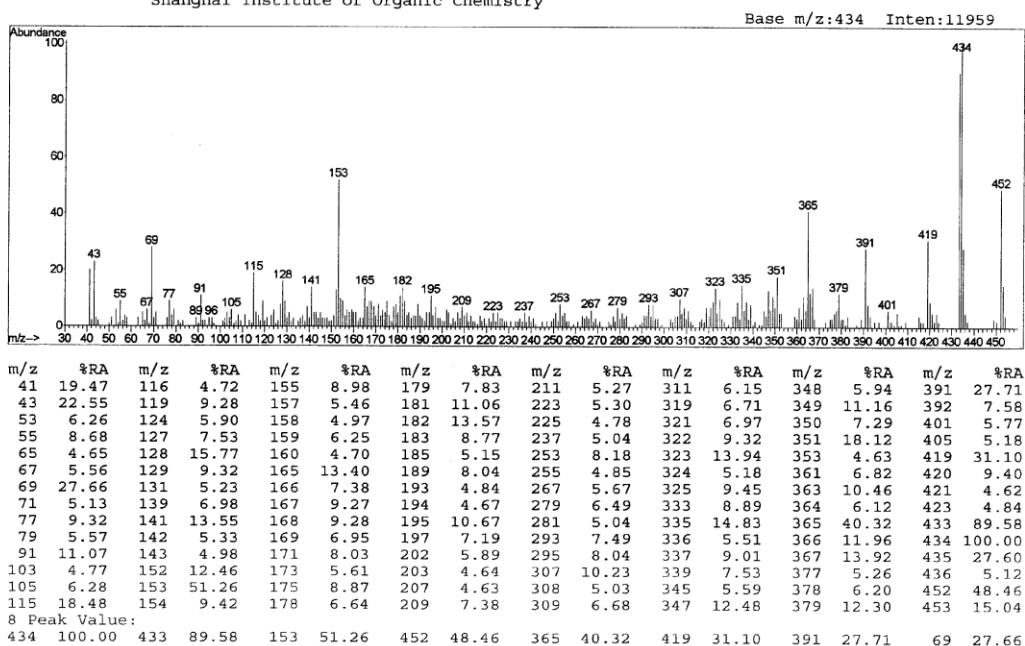


S 5.5 ROESY Spectrum of **5**



## S 5.6 EIMS and HREIMS Spectra of 5

File : C:\MSDCHEM\1\DATA\SNAPSHOT\10091403.D #242 (2.132 min)  
 Acquired : 14 Sep 2010 9:17 am  
 Sample Name : DVP-7 M.W.452  
 Misc Info : Agilent 5973N MSD EI 70eV  
 Shanghai Institute of Organic Chemistry



Shanghai Institute of Organic Chemistry  
 Chinese Academic of Sciences  
 High Resolution MS Data Report

Instrument: Waters Micromass GCT Ionisation Mode: EI+ Electron Energy: 70eV



Card Serial Number: GCT-T1009-OS0441

Sample Serial Number: DVP-7

Operator: Li

Date: 2010/09/17

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

#### Monoisotopic Mass, Odd and Even Electron Ions

242 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

Minimum:							-1.5
Maximum:							50.0
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula	
452.1837	452.1835	0.2	0.4	13.0	2	C26 H28 O7	
	452.1848	-1.1	-2.5	18.0	3	C27 H24 N4 O3	
	452.1822	1.5	3.4	13.5	1	C24 H26 N3 O6	

**Top Spectrum: <sup>1</sup>H NMR (CDCl<sub>3</sub>)**

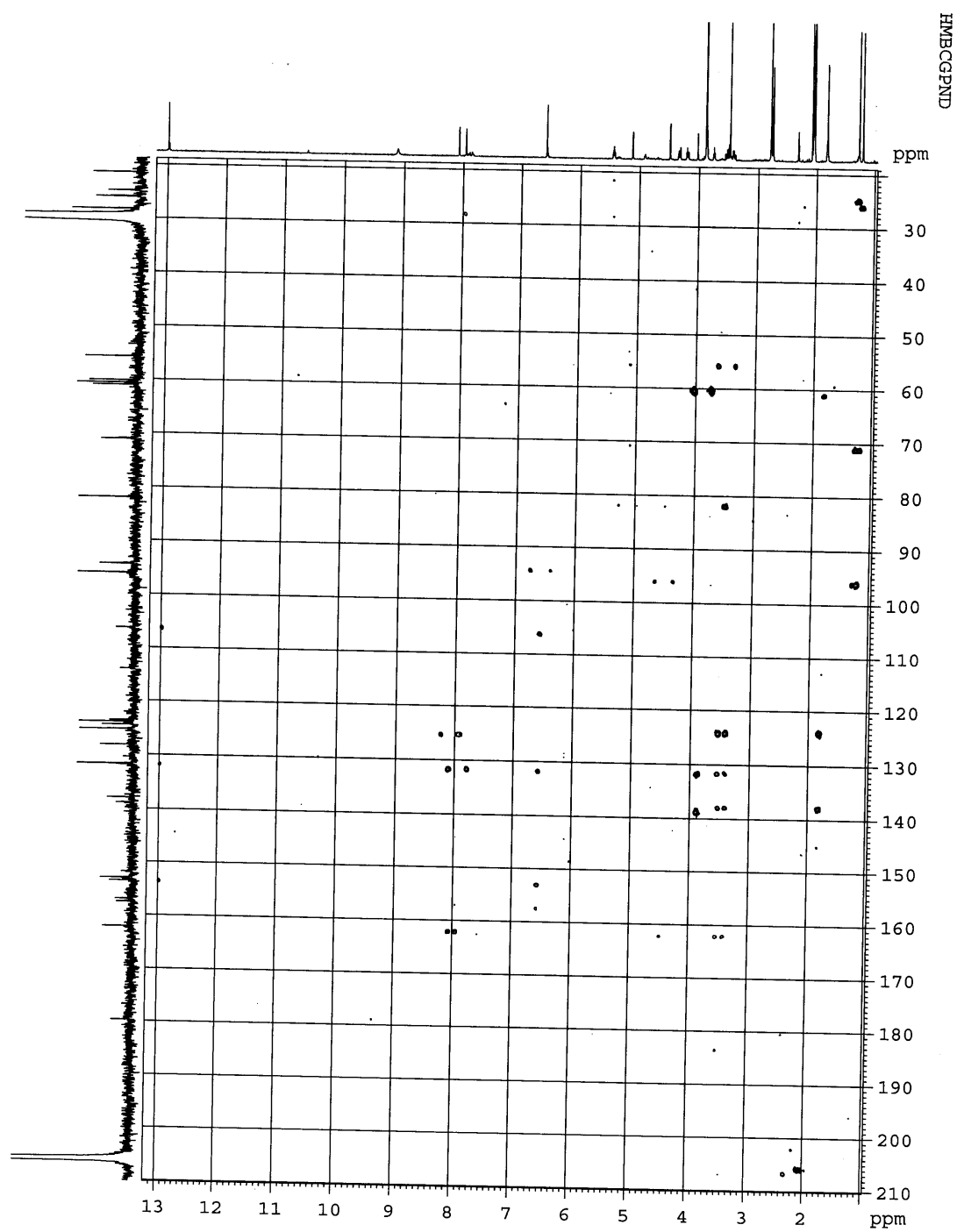
Chemical Shifts (ppm): 9.112, 8.076, 8.073, 8.070, 7.582, 6.579, 6.579, 5.437, 5.437, 5.436, 5.126, 4.422, 4.422, 4.421, 4.421, 4.356, 4.356, 4.352, 4.352, 4.320, 4.320, 4.218, 4.218, 3.883, 3.883, 3.875, 3.875, 3.871, 3.871, 3.860, 3.860, 3.764, 3.764, 3.743, 3.743, 3.564, 3.564, 3.547, 3.547, 3.517, 3.517, 3.504, 3.504, 3.483, 3.483, 3.421, 3.421, 3.405, 3.405, 2.320, 2.320, 2.280, 2.280, 2.756, 2.756, 2.328, 2.328, 2.314, 2.314, 2.124, 2.124, 2.087, 2.087, 2.071, 2.071.

Integration values: 0.97, 0.80, 0.93, 0.93, 0.64, 0.64, 1.23, 0.53, 0.53, 0.32, 0.32, 0.96, 0.96, 0.56, 0.56, 0.50, 0.50, 8.58, 8.58, 0.74, 0.74, 5.70, 8.13, 8.13, 3.97, 3.97, 0.73, 0.73, 4.93, 4.93, 3.70, 3.70, 3.64, 3.64.

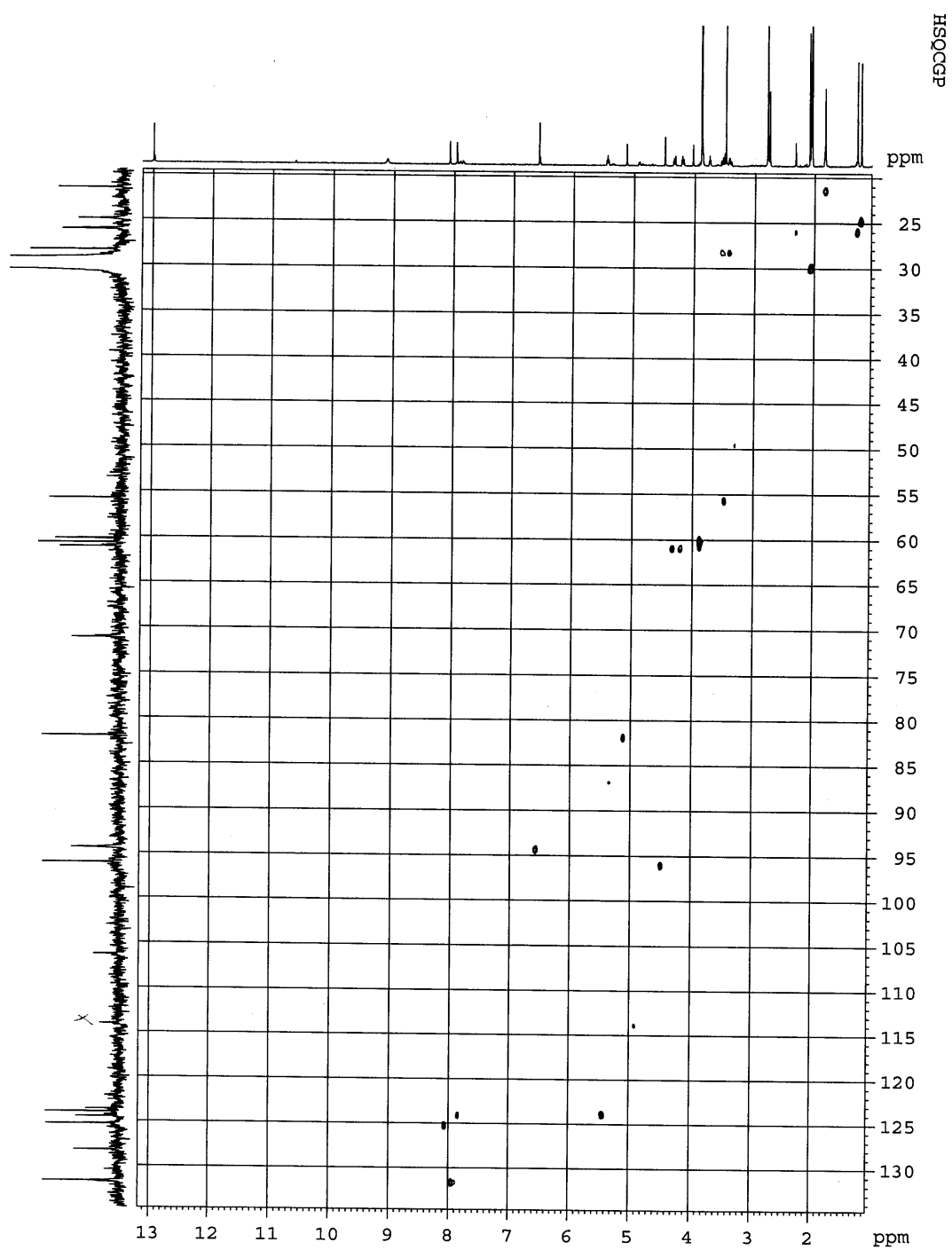
**Bottom Spectrum: <sup>13</sup>C NMR (CDCl<sub>3</sub>)**

Chemical Shifts (ppm): 206.06, 179.87, 162.21, 157.62, 157.05, 153.63, 153.09, 151.97, 138.90, 137.97, 137.74, 131.74, 128.72, 125.36, 124.53, 124.02, 123.69, 114.11, 106.35, 96.13, 94.45, 82.05, 71.20, 61.33, 60.70, 60.25, 55.62, 30.26, 29.95, 29.95, 29.80, 29.80, 29.64, 29.49, 29.49, 28.43, 28.43, 26.11, 25.00, 21.56.

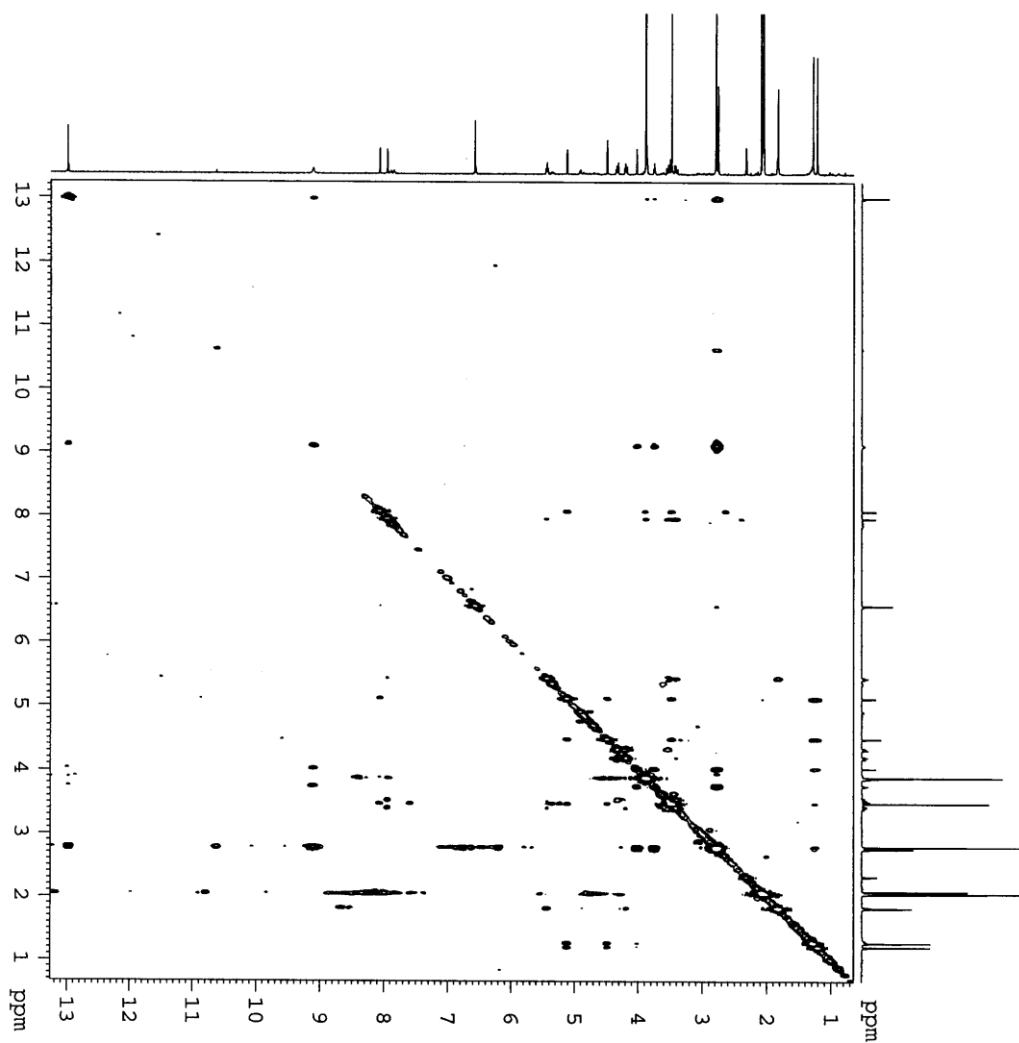
S 6.2 HMBC Spectrum of **6**



# S 6.3 HSQC Spectrum of **6**



# S 6.4 NOESY Spectrum of 6



```

Current Data Parameters
NAME          dwg-12
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20100519
Time          17:52:11
INSTRUM       spect
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            1024
SOLVENT       Acetone
NS            16
DS            4
SWH           7062.147 Hz
FIDRES       0.0726200 sec
AQ           0.0726200 sec
RG           70.800 usec
DE           6.50 usec
TE           300.0 K
D0           0.0005743 sec
D1           2.0000000 sec
D2           0.0000000 sec
D8           1.0000000 sec
RG           0.0001460 sec
STCNT        128
TAU          0.4988001 sec

===== CHANNEL f1 =====
NUC1          1H
P1           10.50 usec
P2           21.00 usec
PL1          -4.00 dB
PL2          -4.00 dB
SFO1         500.132630 MHz

===== GRADIENT CHANNEL =====
GPNAM1       SINE.100
GPNAM2       SINE.100
GPD1         10.00 usec
GPD2         -40.00 usec
P16          1000.00 usec

F1 - Acquisition parameters
WDW          1
SSB          0
GB           0
PC           1.40

F2 - Processing parameters
SI           1024
SF           500.130008 MHz
WDW          COSINE
SSB          2
GB           0
PC           1.40

F1 - Processing parameters
SI           1024
SF           500.130008 MHz
WDW          COSINE
SSB          2
GB           0
PC           1.40
  
```



# S 6.5 EIMS and HREIMS Spectra of 6

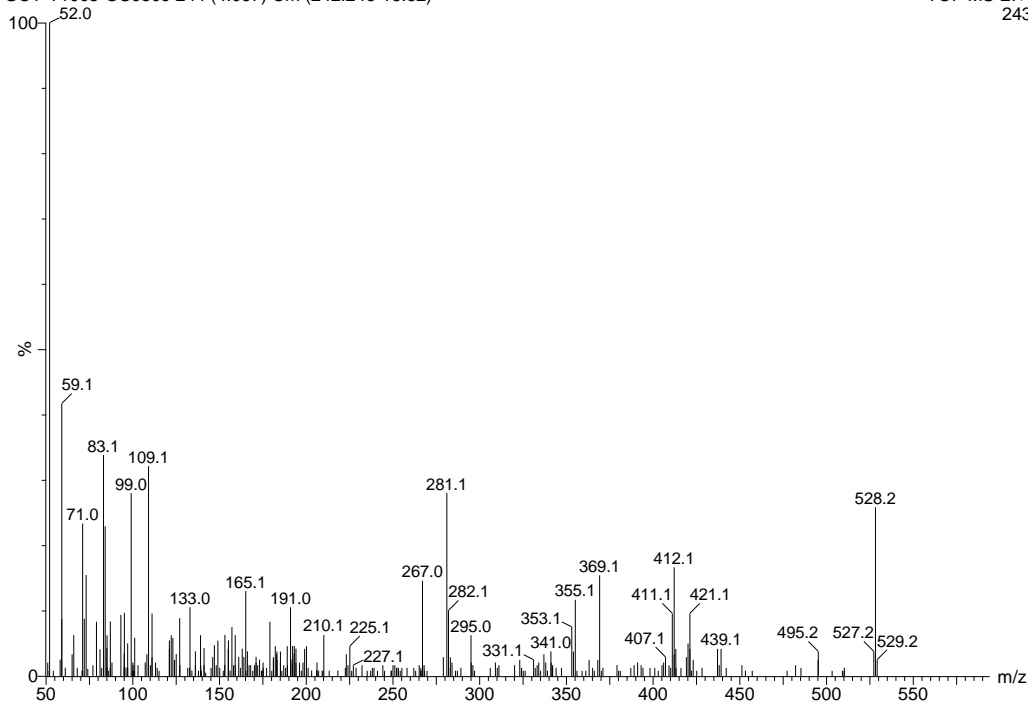
DefaultInstrument

14:52:38  
DVK-12

CA176-Cal

GCT-T1005-OS0309 244 (4.067) Cm (242:246-16:62)

TOF MS EI+  
243



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Chinese Academic of Sciences  
High Resolution MS Data Report



Instrument: Waters Micromass GCT

Card Serial Number: GCT-T1005-OS0309

Sample Serial Number: DVK-12

Operator: Li

Date: 2010/05/21

## Elemental Composition Report

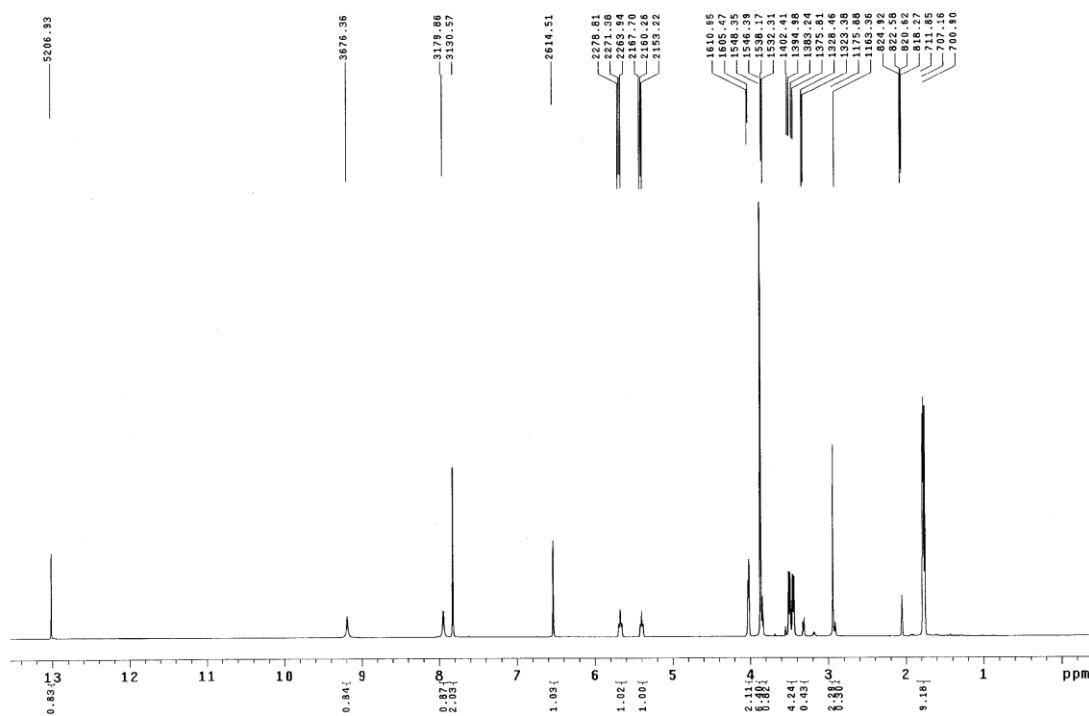
Single Mass Analysis (displaying only valid results)  
Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0  
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
648 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

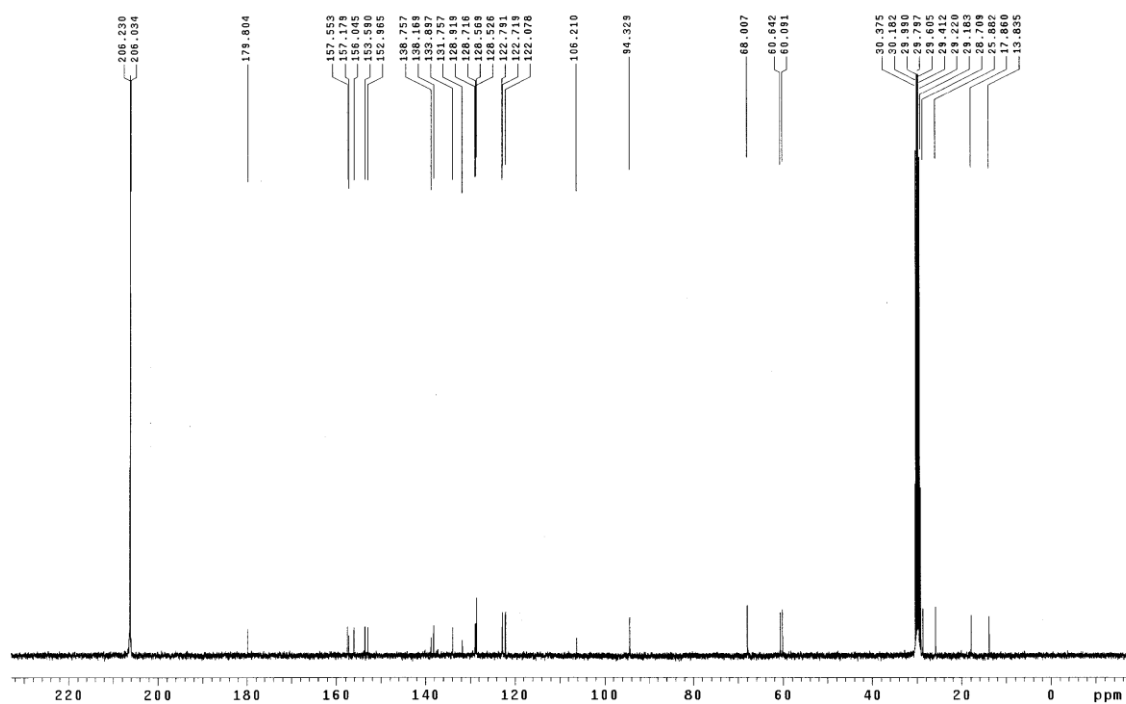
Minimum:									-1.5
Maximum:									50.0
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula			
528.1996	528.1995	0.1	0.1	13.0	2	C28 H32 O10			
	528.2000	-0.4	-0.8	8.5	5	C25 H35 N O9 Cl			
	528.1987	0.9	1.7	9.0	4	C23 H33 N4 O8 Cl			
	528.2009	-1.3	-2.4	18.0	3	C29 H28 N4 O6			
	528.1982	1.4	2.6	13.5	1	C26 H30 N3 O9			

# S 7.1 $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of 7

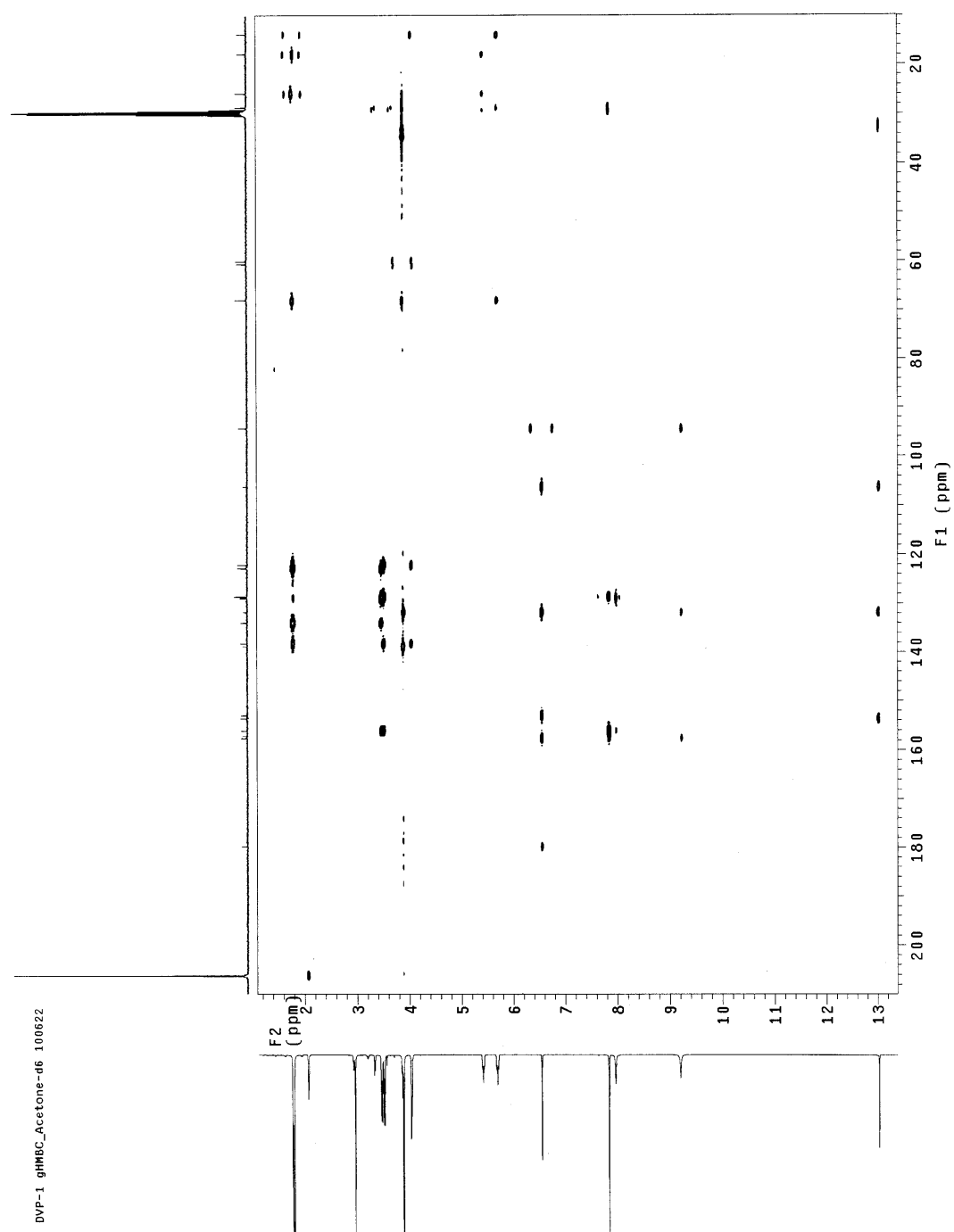
DVP-1 Acetone-d<sub>6</sub> 100609



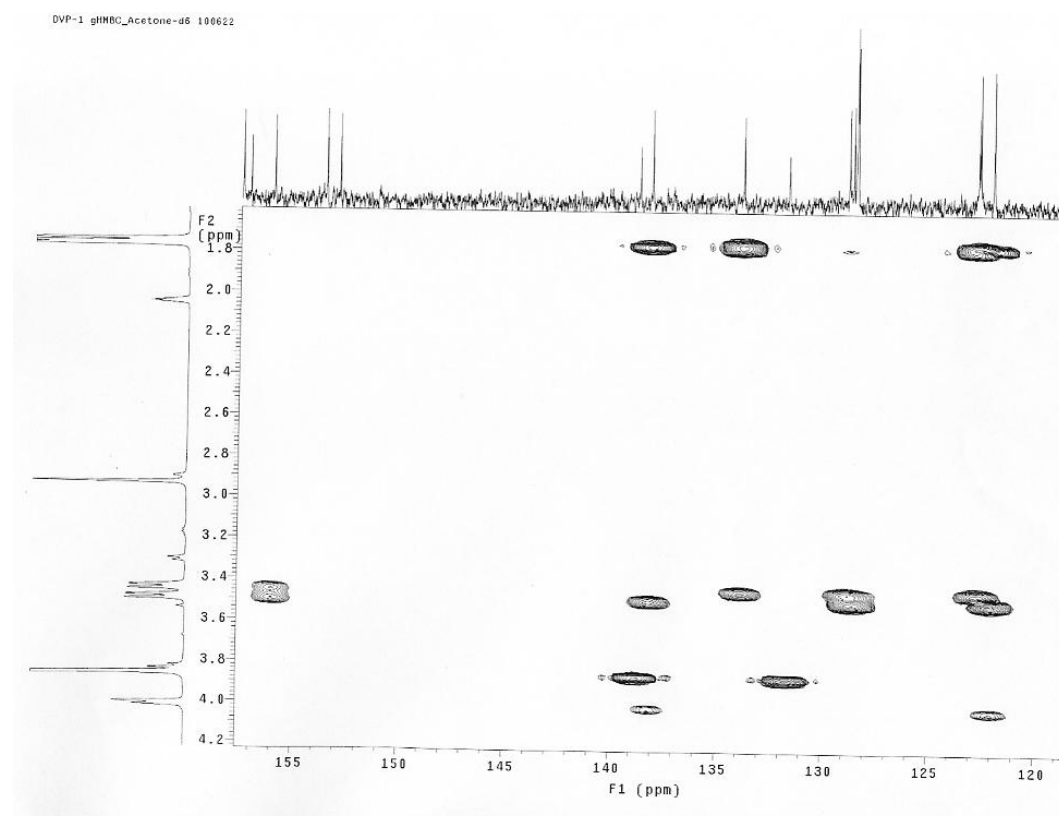
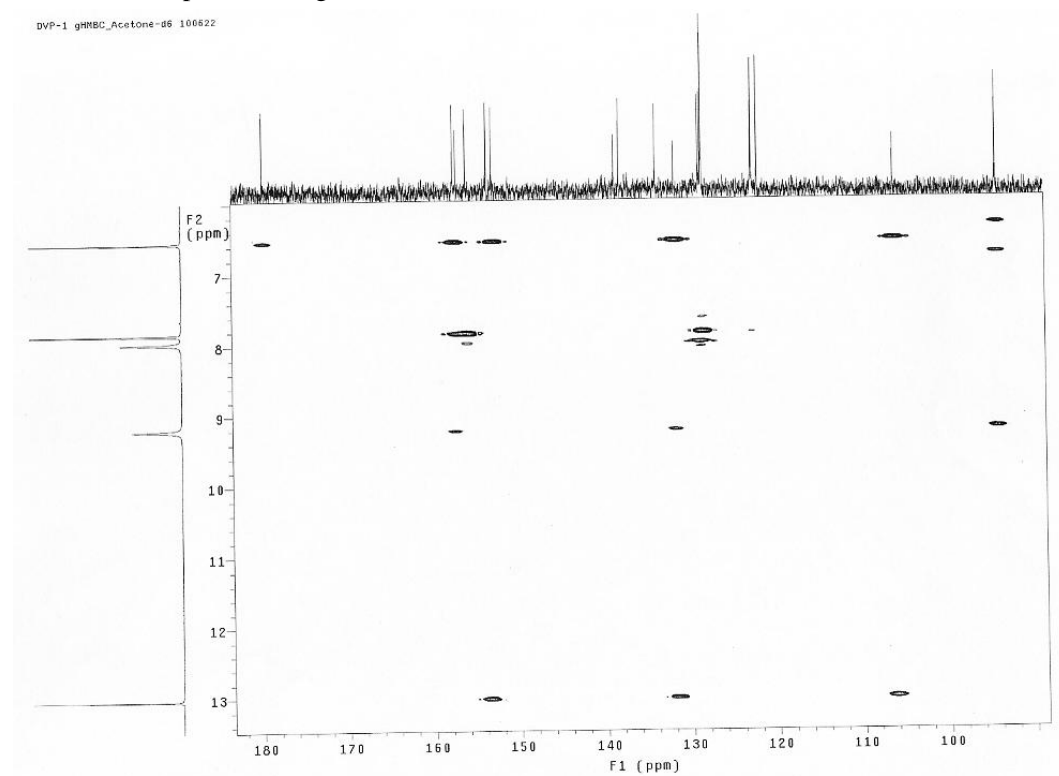
DVP-1 C13\_Acetone-d6 100622



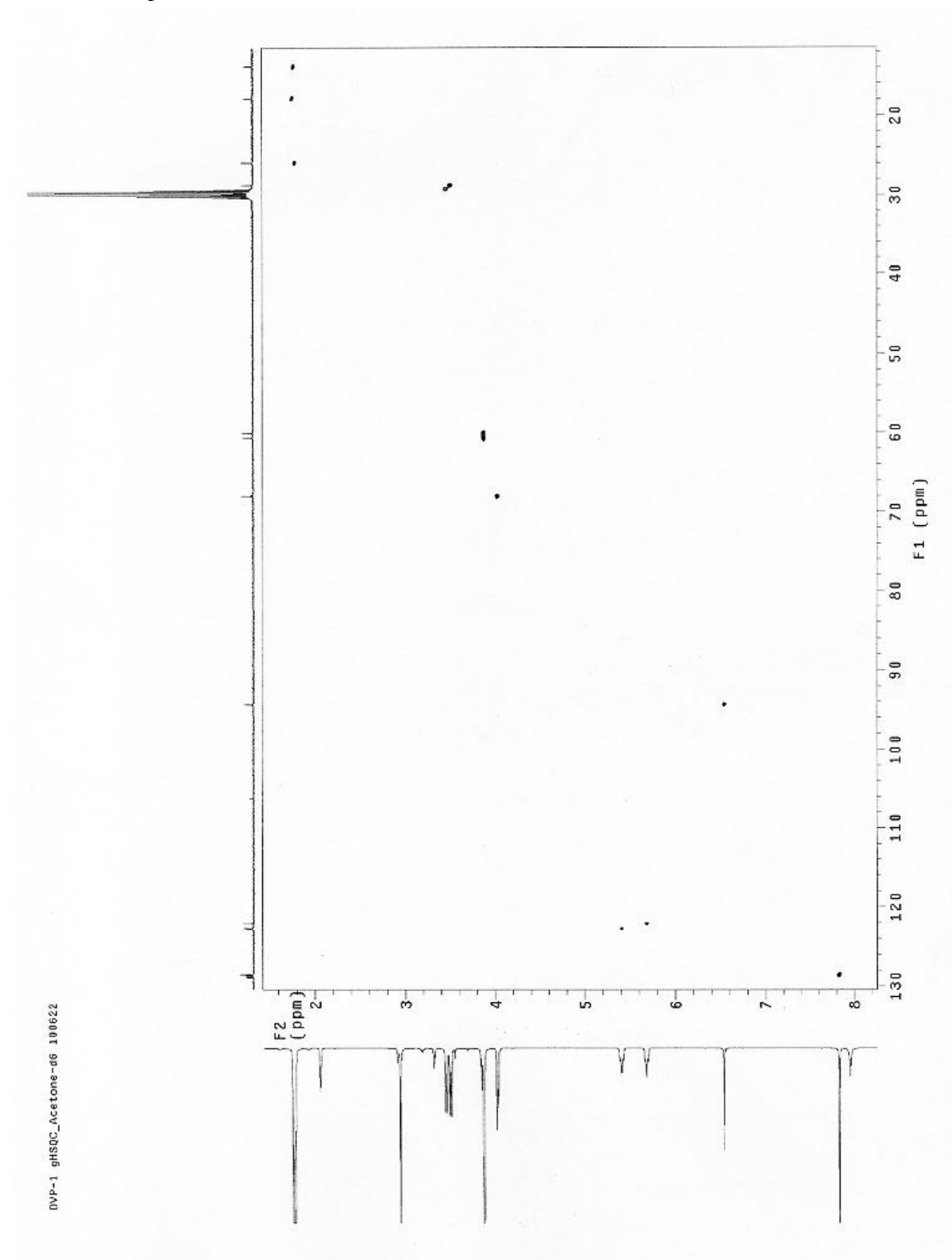
S 7.2 HMBC Spectrum of 7



### S 7.3 HMBC Spectrum magnified of 7

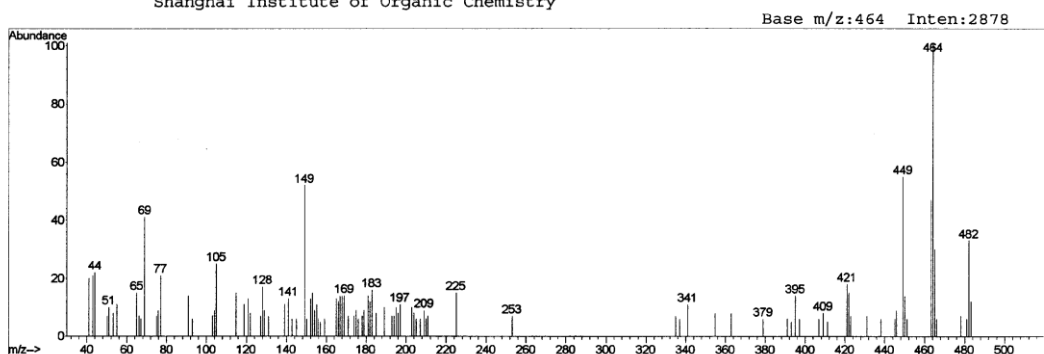


S 7.4 HSQC Spectrum of **7**



### S 7.5 EIMS and HREIMS Spectra of 7

File : C:\MSDCHEM\1\DATA\SNAPSHOT\10091402.D #267(2.344 min)  
Acquired : 14 Sep 2010 9:09 am  
Sample Name : DVP-1 M.W.482  
Misc Info : Agilent 5973N MSD EI 70eV  
Shanghai Institute of Organic Chemistry



m/z	%RA	m/z	%RA	m/z	%RA	m/z	%RA	m/z	%RA	m/z	%RA	m/z	%RA	m/z	%RA
41	19.67	91	13.72	141	12.72	167	13.69	193	7.33	335	6.95	422	15.08	481	5.84
43	21.23	93	6.39	143	6.15	168	13.90	194	6.60	337	5.87	423	7.33	482	32.24
44	21.40	103	6.88	145	5.46	169	13.93	195	10.39	341	10.49	431	7.40	483	11.47
50	7.02	104	9.31	149	51.63	171	6.81	196	8.20	355	7.64	438	5.52		
51	9.59	105	24.39	150	6.32	174	7.09	197	11.12	363	8.27	445	5.77		
53	8.10	115	15.29	152	12.93	175	9.14	203	9.69	379	5.66	446	8.86		
55	10.95	119	10.88	153	14.42	176	5.84	204	7.96	391	5.73	449	54.69		
65	14.42	121	12.65	154	8.76	178	7.16	205	5.73	393	5.25	450	14.11		
66	6.46	122	7.92	155	10.56	179	8.62	207	5.63	395	14.07	451	6.05		
67	5.63	127	7.19	156	6.15	181	14.00	209	8.48	397	5.46	463	46.49		
69	40.76	128	16.92	157	5.25	182	12.13	210	5.56	407	6.18	464	100.00		
75	7.09	129	8.51	159	5.49	183	15.36	211	6.53	409	7.68	465	30.19		
76	8.48	131	6.50	165	12.72	185	7.44	225	15.11	411	5.21	466	6.22		
77	20.67	139	11.29	166	11.47	189	9.66	253	7.02	421	17.62	478	6.88		
8 Peak Value:															
464	100.00	449	54.69	149	51.63	463	46.49	69	40.76	482	32.24	465	30.19	105	24.39

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Chinese Academic of Sciences  
High Resolution MS Data Report



Instrument: Waters Micromass GCT      Ionisation Mode: EI+      Electron Energy: 70eV

Card Serial Number: GCT-T1009-OS0440

Sample Serial Number: DVP-1

Operator: Li

Date: 2010/09/17

## Elemental Composition Report

### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0  
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

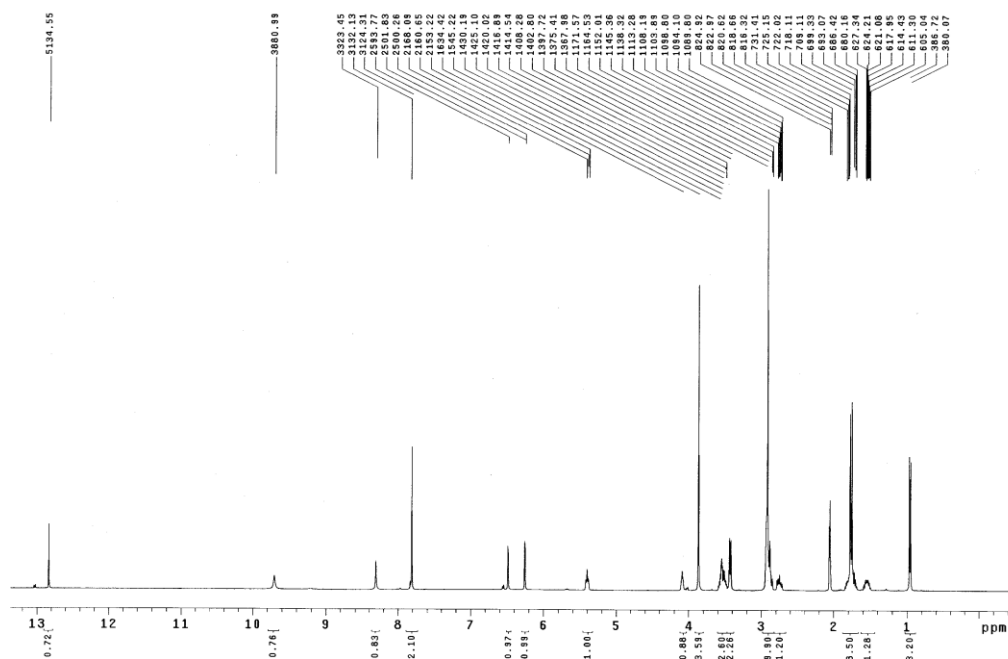
Monoisotopic Mass, Odd and Even Electron Ions

250 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

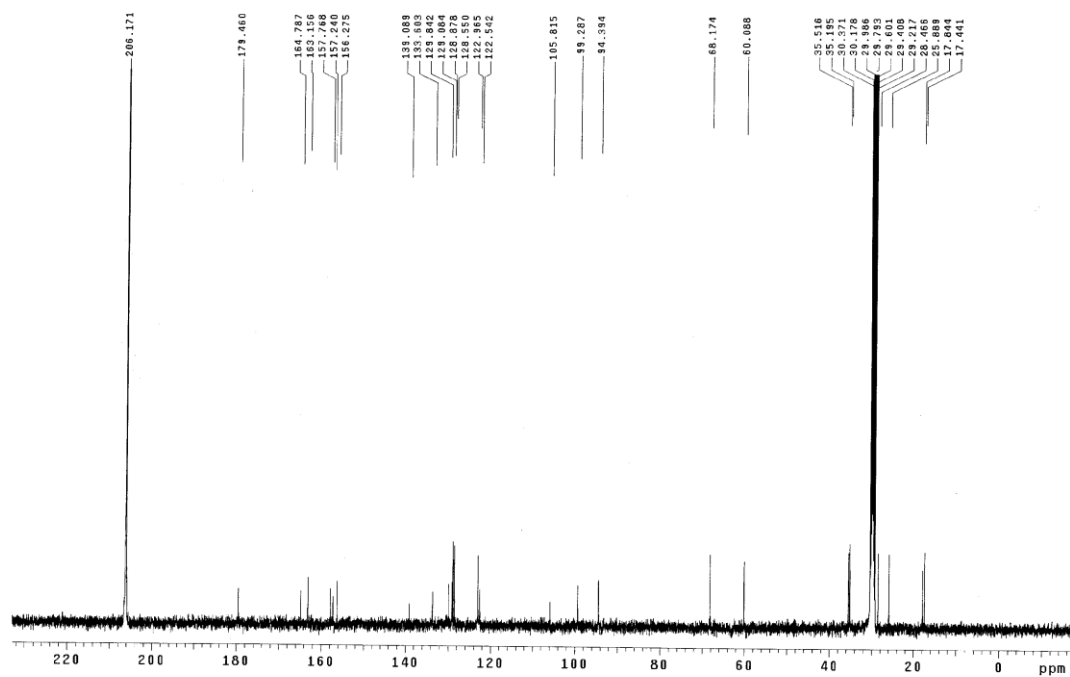
Minimum:				-1.5				
Maximum:		1.5	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula		
482.1940	482.1941	-0.1	-0.1	13.0	2	C27 H30 O8		
	482.1927	1.3	2.6	13.5	1	C25 H28 N3 O7		
	482.1954	-1.4	-2.9	18.0	3	C28 H26 N4 O4		

### S 8.1 $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of **8**

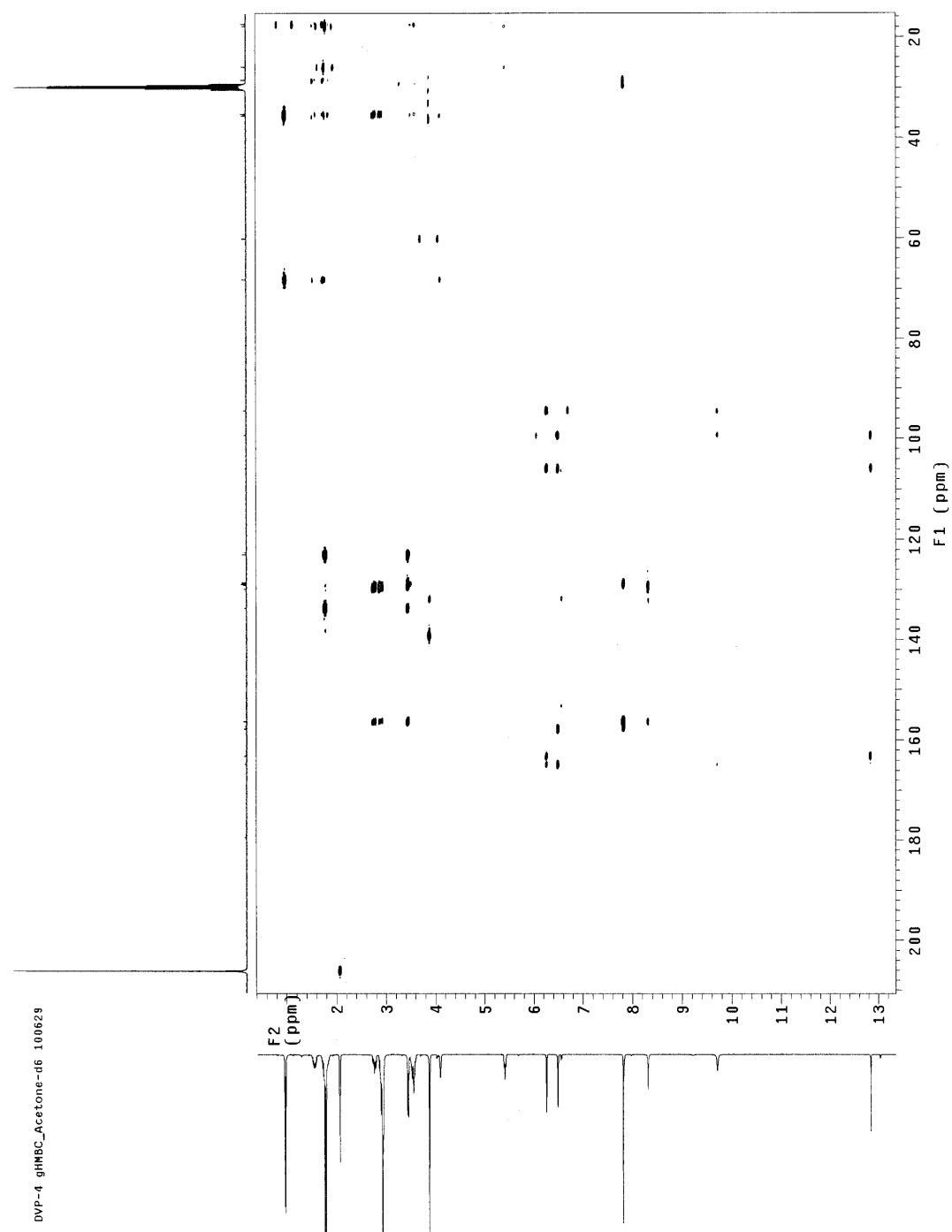
DVP-4 Acetone-d6 100617



DVP-4 C13\_Acetone-d6 100629

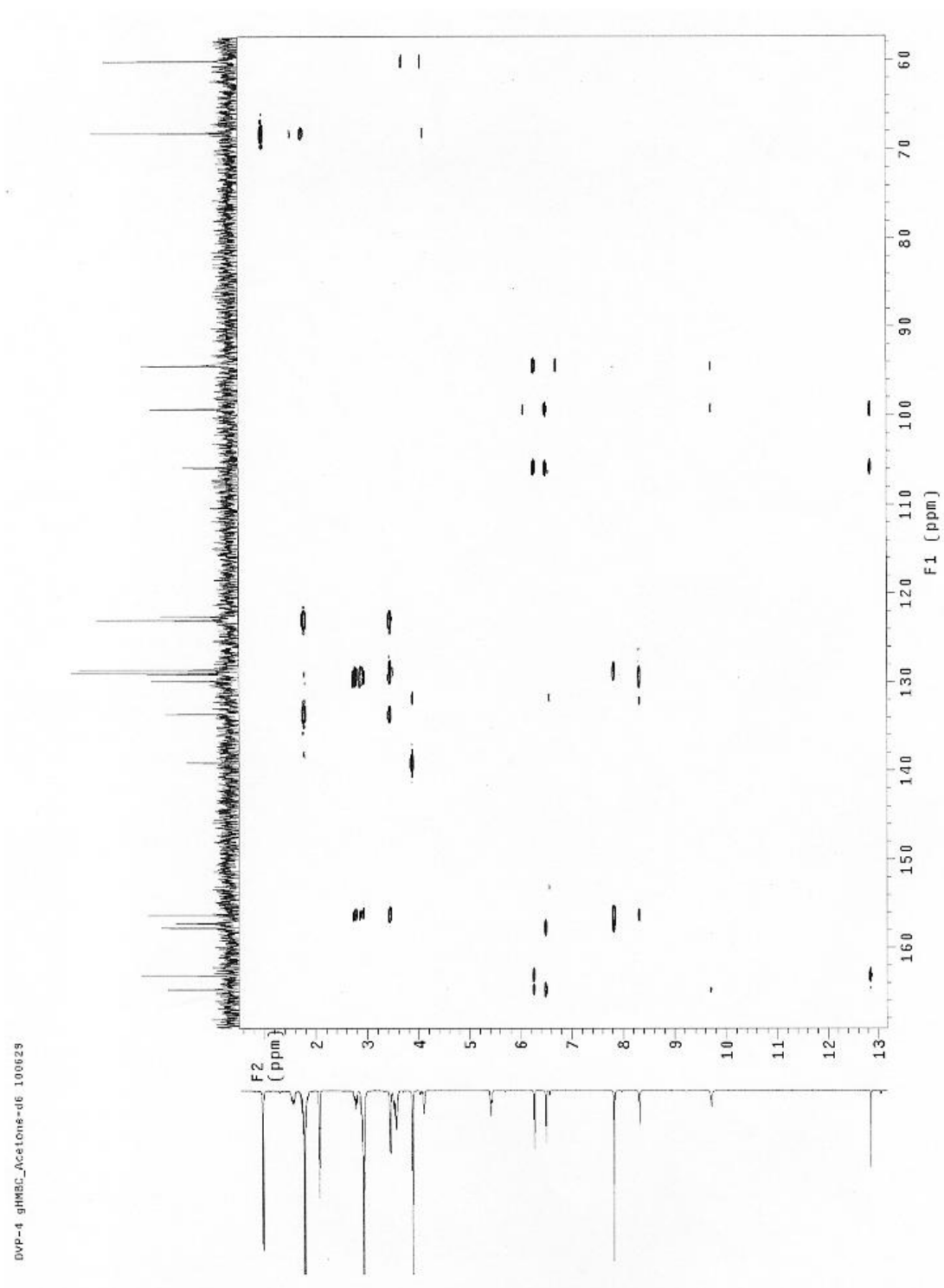


# S 8.2 HMBC Spectrum of **8**

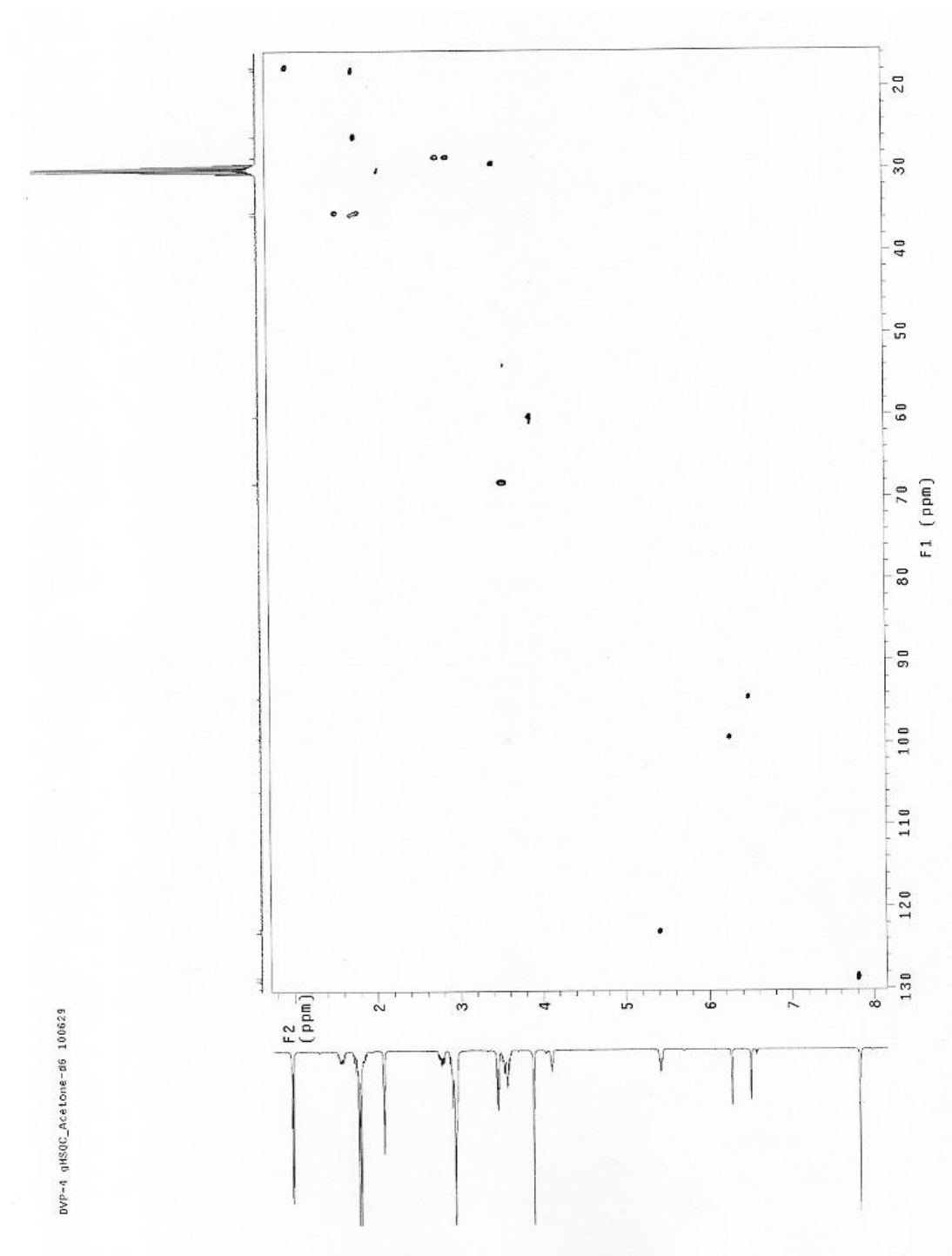




# S 8.3 HMBC Spectrum magnified of **8**

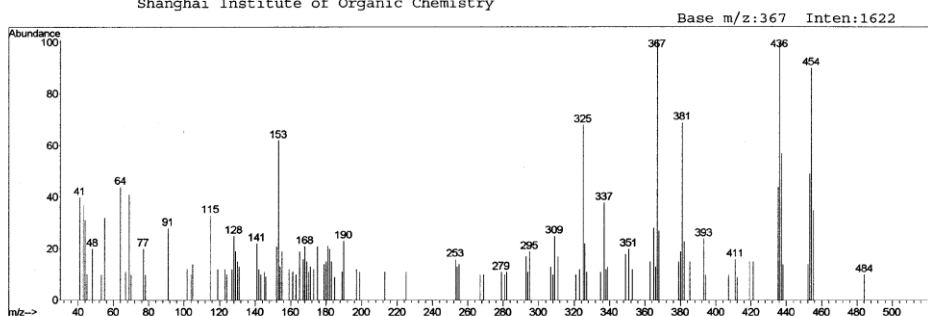


# S 8.4 HSQC Spectrum of **8**



### S 8.5 EIMS and HREIMS Spectra of **8**

File : C:\MSDCHEM\1\DATA\SnapShot\10092511.D #213 (1.886 min)  
Acquired : 25 Sep 2010 9:54 am  
Sample Name : DVP-4 M.W.454  
Misc Info : Agilent 5973N MSD EI 70eV  
Shanghai Institute of Organic Chemistry



m/z	$\delta R_A$	m/z	$\delta R_A$	m/z	$\delta R_A$	m/z	$\delta R_A$	m/z	$\delta R_A$	m/z	$\delta R_A$	m/z	$\delta R_A$	m/z	$\delta R_A$
41	39.70	102	11.90	143	9.68	170	10.42	213	10.85	308	10.05	353	11.84	411	15.97
43	36.19	104	9.49	145	10.42	171	12.70	225	10.91	309	24.66	363	15.23	412	9.25
44	31.07	105	13.87	146	9.25	173	11.53	253	16.21	311	16.40	365	27.44	419	14.98
45	9.56	115	32.80	152	21.09	175	21.15	254	12.89	321	10.36	366	12.76	421	14.43
48	20.10	119	12.21	153	61.47	179	13.75	255	13.75	323	11.78	367	100.00	435	43.59
53	9.99	123	12.21	154	13.13	180	14.36	267	9.99	325	67.51	368	27.07	436	98.58
55	31.63	124	9.56	155	18.80	181	21.15	269	9.74	326	21.39	379	14.98	437	55.98
64	43.46	127	12.08	159	11.84	182	19.67	279	10.97	327	11.28	380	18.56	438	13.75
67	10.60	128	24.54	161	10.60	183	14.67	281	9.49	335	10.73	381	68.62	452	13.87
69	40.38	129	19.11	163	9.99	185	9.22	282	10.85	337	37.24	382	23.00	453	48.34
70	10.11	130	14.98	165	18.37	185	11.25	293	17.26	338	11.71	385	15.23	454	89.15
71	16.1	131	15.58	166	20.81	190	22.79	297	17.79	339	19.73	387	24.37	455	34.16
78	9.62	141	22.26	168	20.41	197	12.02	295	19.05	349	17.57	394	9.62	484	9.74
91	27.93	142	11.84	169	14.36	199	10.54	307	12.76	351	19.73	407	10.23		
8 Peak Value:															
367	100.00	436	98.58	454	89.15	381	68.62	325	67.51	153	61.47	437	55.98	453	48.34

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High Resolution MS Data Report



Instrument: Waters Micromass GCT Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-T1009-OS0487

Sample Serial Number: DVP-4

Operator: Li

Date: 2010/09/27

## Elemental Composition Report

Single Mass Analysis  
Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0  
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

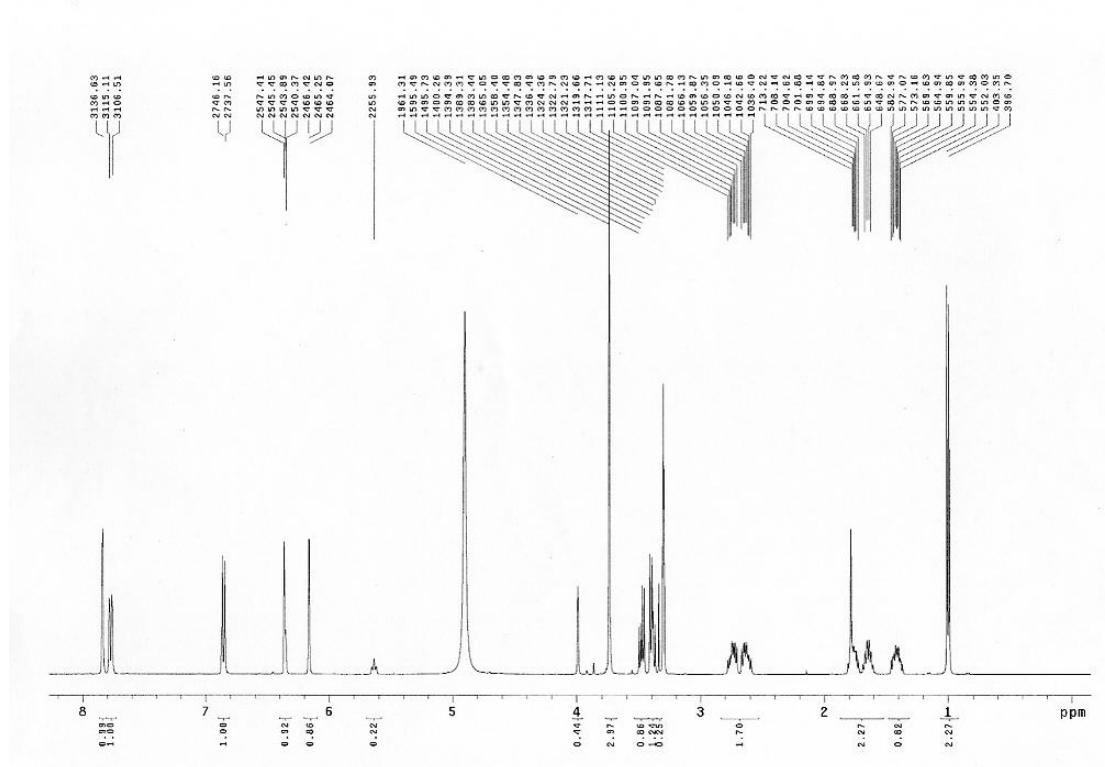
Monoisotopic Mass, Odd and Even Electron Ions

554 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

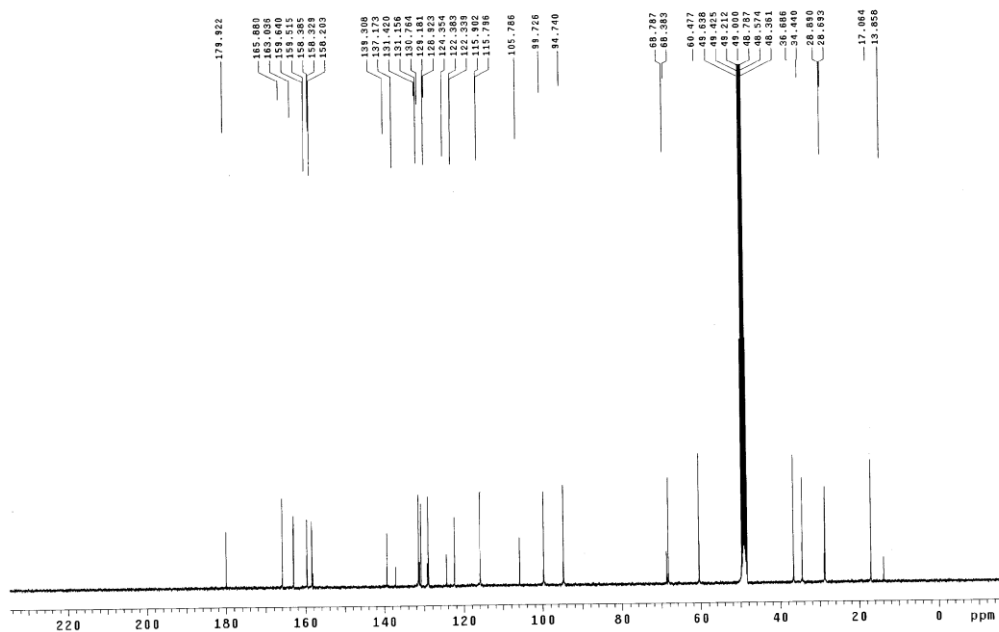
Minimum:	1.5	5.0	-1.5				
Maximum:			50.0				
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula	
454.1989	454.1992	-0.3	-0.6	12.0	2	C26 H30 O7	
	454.1983	0.6	1.3	8.0	3	C21 H31 N4 O5 Cl	
	454.1996	-0.7	-1.6	7.5	4	C23 H33 N O6 Cl	
	454.1978	1.1	2.4	12.5	1	C24 H28 N3 O6	

### S 9.1 $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of **9**

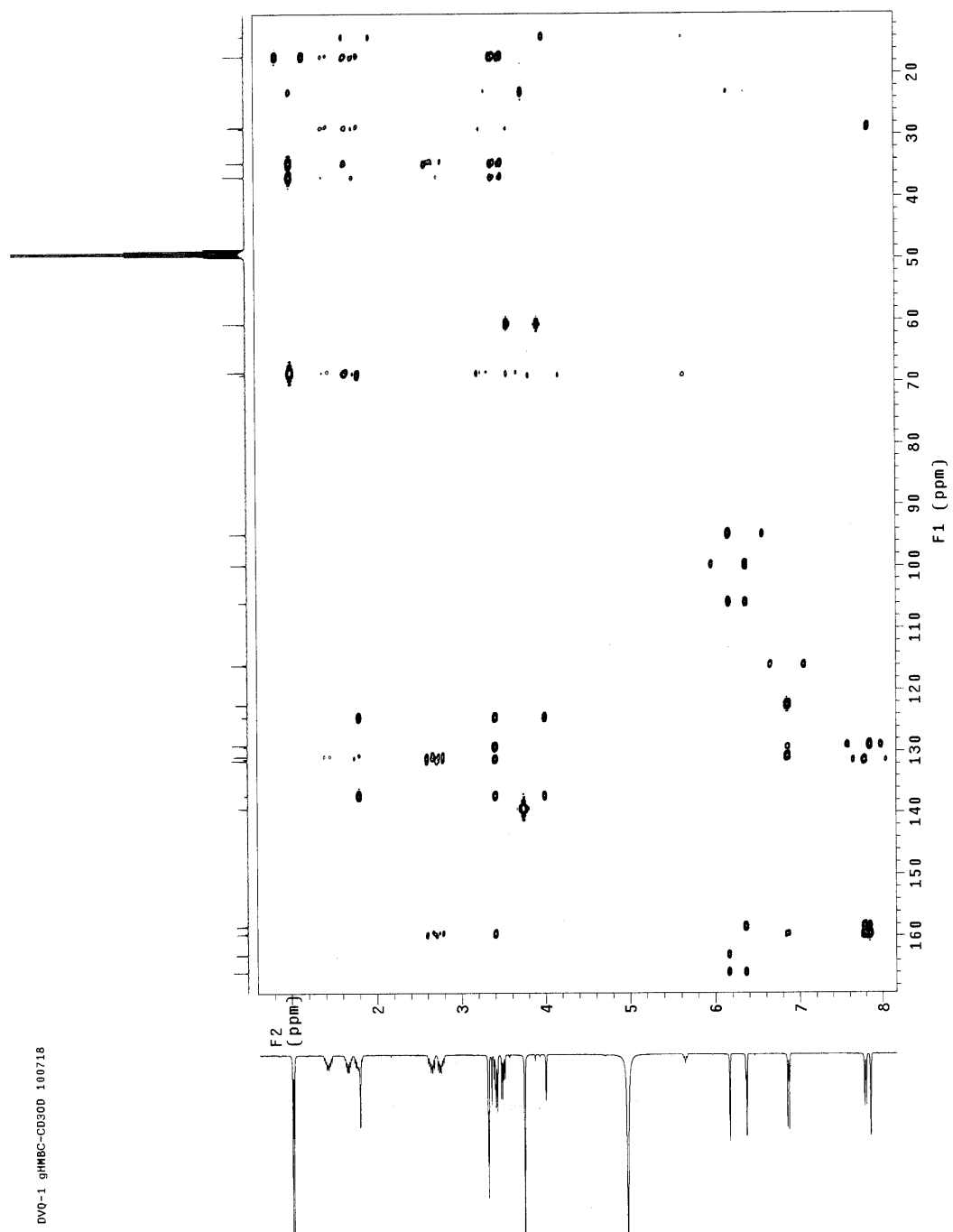
DVQ-1 CD30D 100707



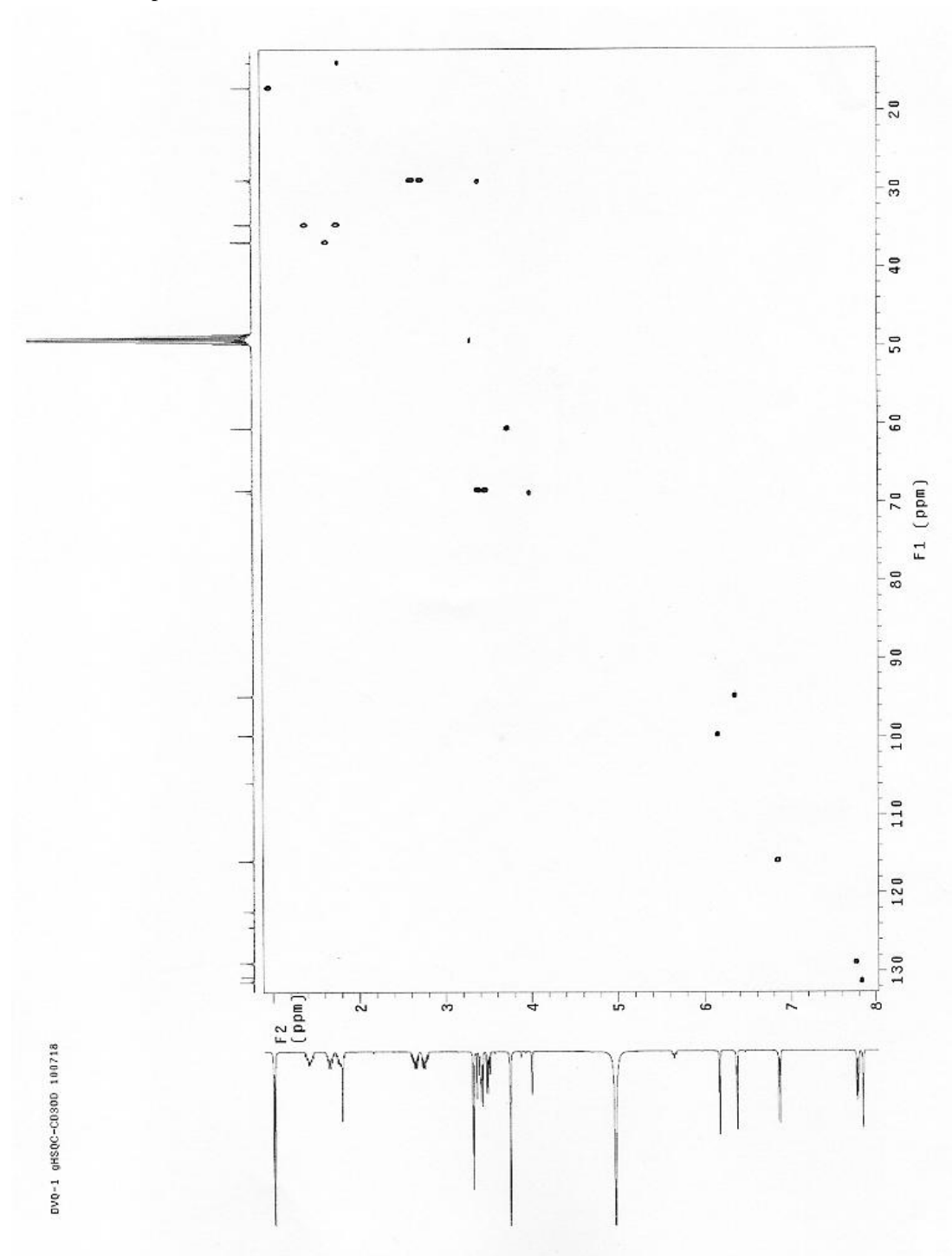
OVQ-1 C13-CD30D 100718



S 9.2 HMBC Spectrum of **9**

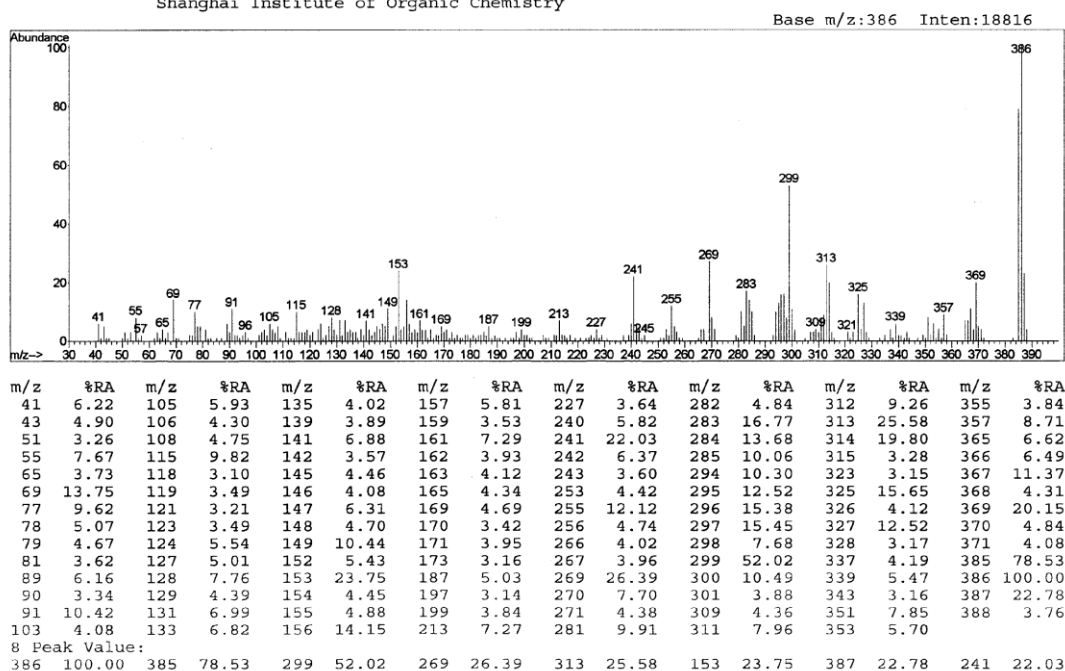


### S 9.3 HSQC Spectrum of **9**



## S 9.4 EIMS and HREIMS Spectra of 9

File : C:\MSDCHEM\1\DATA\SNAPSHOT\10091408.D #228(2.014 min)  
 Acquired : 14 Sep 2010 10:06 am  
 Sample Name : DVQ-1 M.W.388  
 Misc Info : Agilent 5973N MSD EI 70eV  
 Shanghai Institute of Organic Chemistry



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 Chinese Academic of Sciences  
 High Resolution MS Data Report



Instrument: Waters Micromass GCT Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-T1009-OS0445

Sample Serial Number: DVQ-1

Operator: Li

Date: 2010/09/17

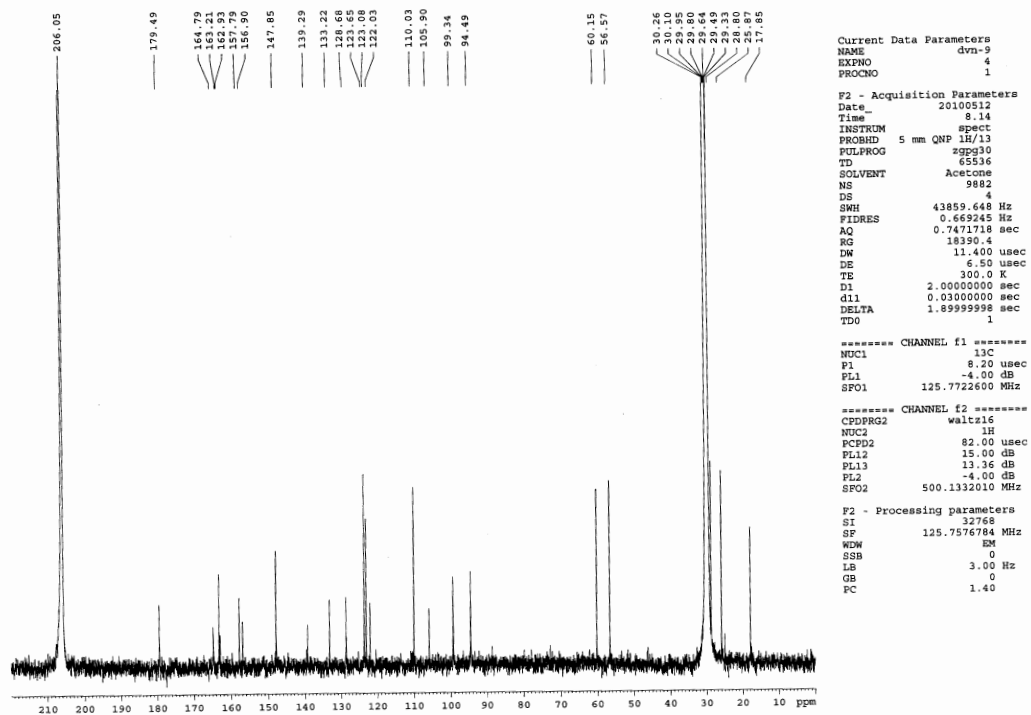
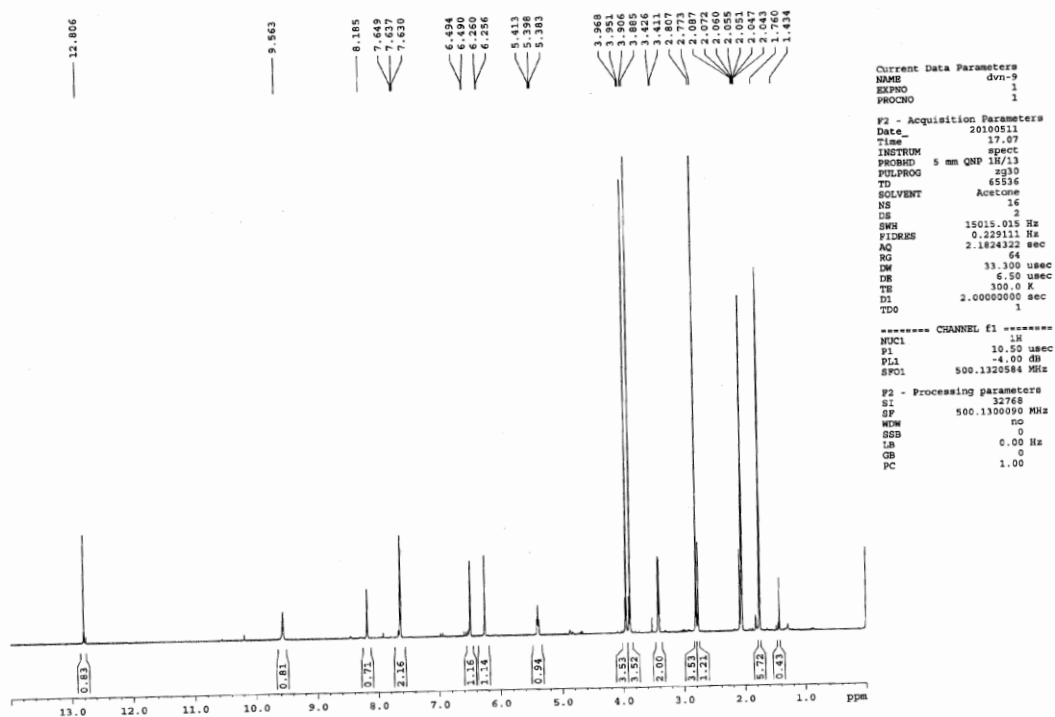
### Elemental Composition Report

Single Mass Analysis  
 Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
 207 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

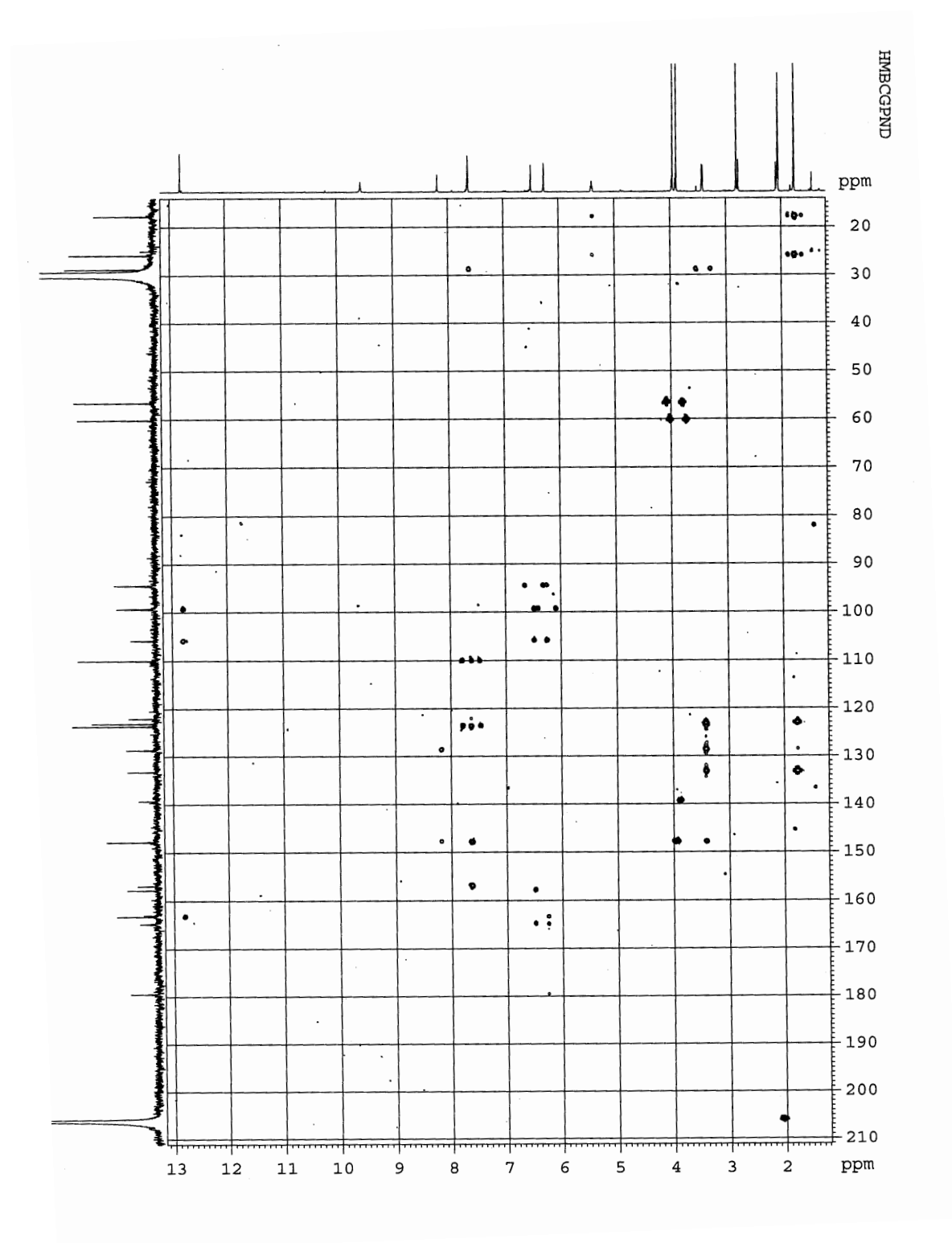
Minimum:				-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
386.1369	386.1366	0.3	0.9	11.0	2	C21 H22 O7
	386.1379	-1.0	-2.6	16.0	3	C22 H18 N4 O3
	386.1352	1.7	4.4	11.5	1	C19 H20 N3 O6

# S 10.1 $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra of **10**

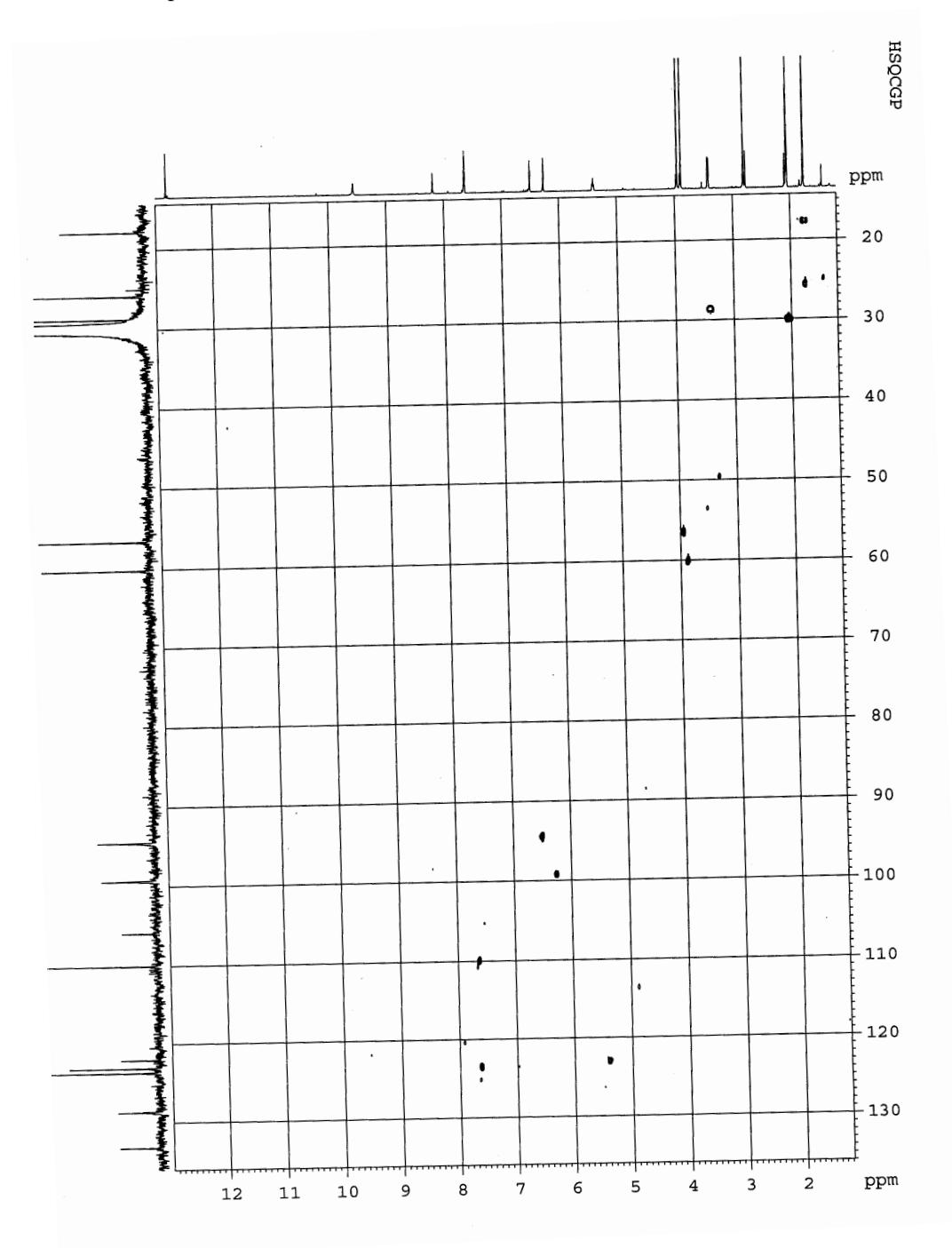




S 10.2 HMBC Spectrum of **10**

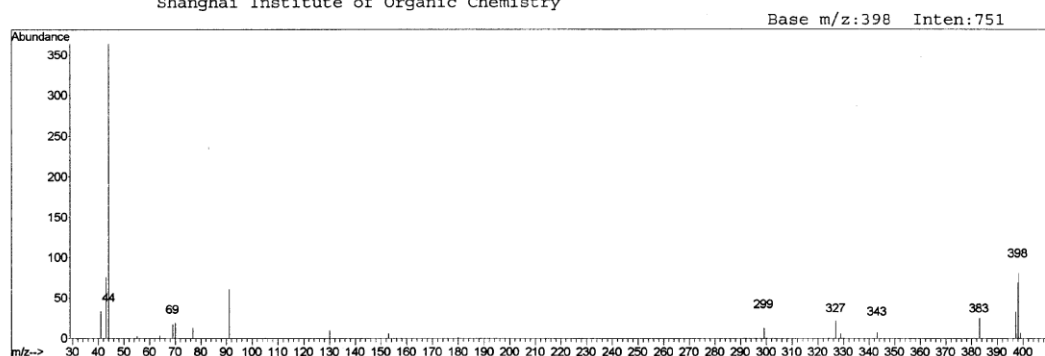


S 10.3 HSQC Spectrum of **10**



## S 10.4 EIMS and HREIMS Spectra of 10

File : C:\MSDCHEM\1\DATA\Snapshot\10092509.D #201(1.784 min)  
 Acquired : 25 Sep 2010 9:37 am  
 Sample Name : DVN-9 M.W.398  
 Misc Info : Agilent 5973N MSD EI 70eV  
 Shanghai Institute of Organic Chemistry



m/z %RA  
 41 21.44  
 43 26.76  
 44 41.94  
 69 26.63  
 299 33.95  
 327 28.76  
 329 28.23  
 343 24.37  
 383 28.50  
 397 49.00  
 398 100.00  
 399 31.69

8 Peak Value:  
 398 100.00 397 49.00 44 41.94 299 33.95 399 31.69 327 28.76 383 28.50 329 28.23

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 Chinese Academic of Sciences  
 High Resolution MS Data Report



Instrument: Waters Micromass GCT Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-T1009-OS0485

Sample Serial Number: DVN-9

Operator: Li

Date: 2010/09/27

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

#### Monoisotopic Mass, Odd and Even Electron Ions

481 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

Minimum:				-1.5			
Maximum:				50.0			
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula	
398.1364	398.1366	-0.2	-0.4	12.0	2	C22	H22 O7
	398.1370	-0.6	-1.6	7.5	5	C19	H25 N O6 Cl
	398.1357	0.7	1.8	8.0	4	C17	H23 N4 O5 Cl
	398.1352	1.2	3.0	12.5	1	C20	H20 N3 O6
	398.1379	-1.5	-3.7	17.0	3	C23	H18 N4 O3