

## **2-Arylbenzofuran, Flavonoid, and Tyrosinase Inhibitory Constituents of *Morus yunnanensis***

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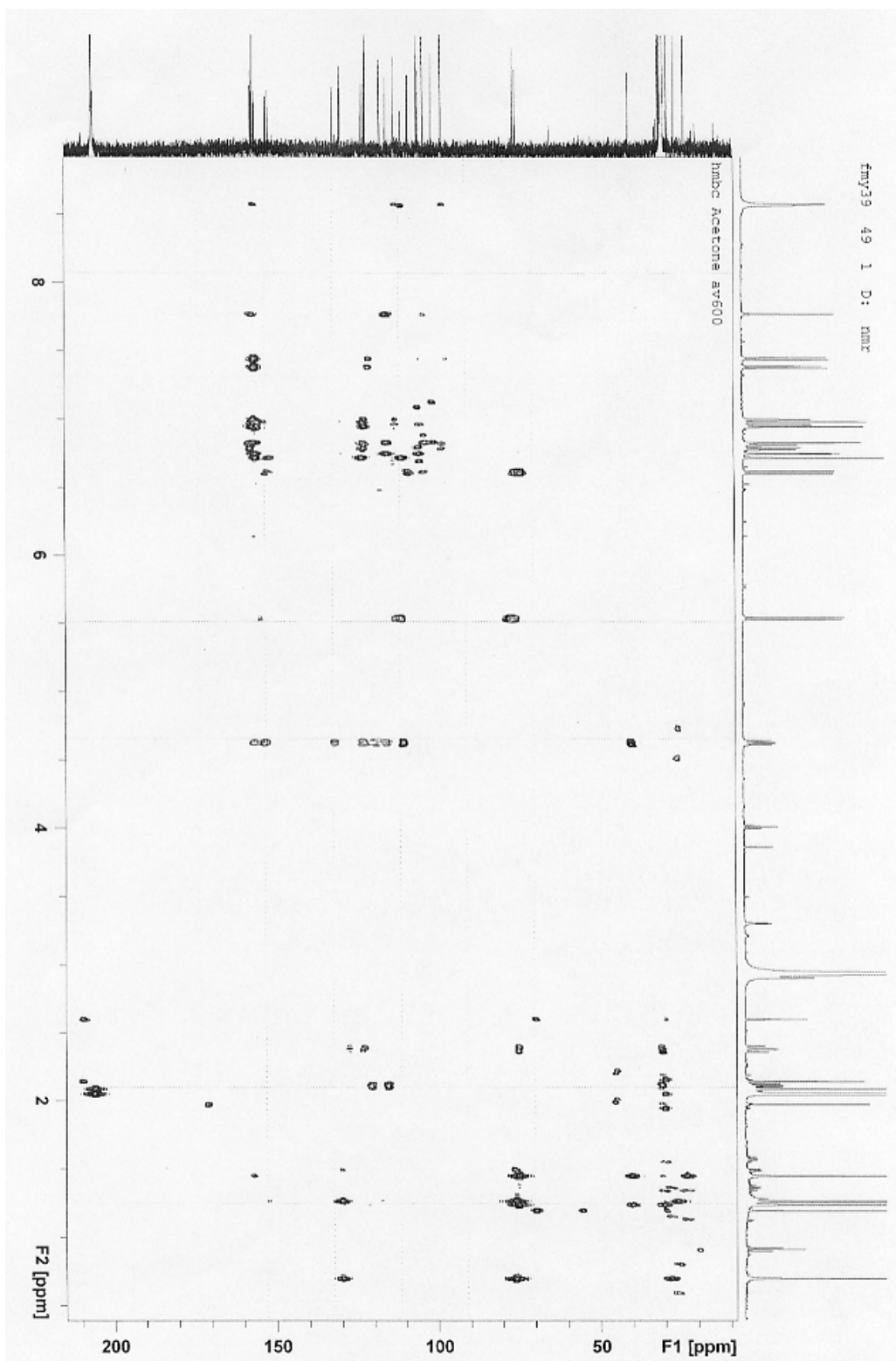
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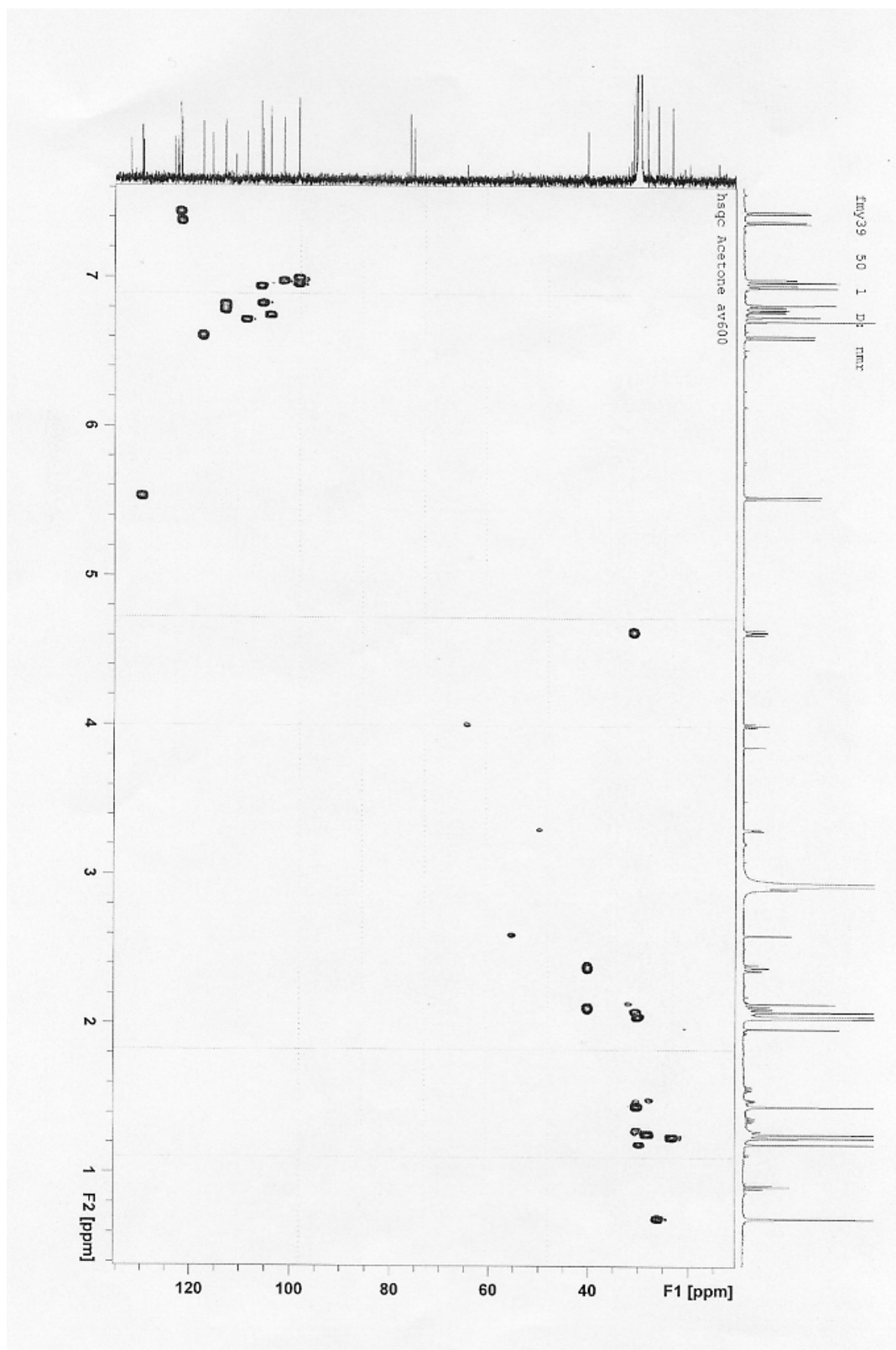
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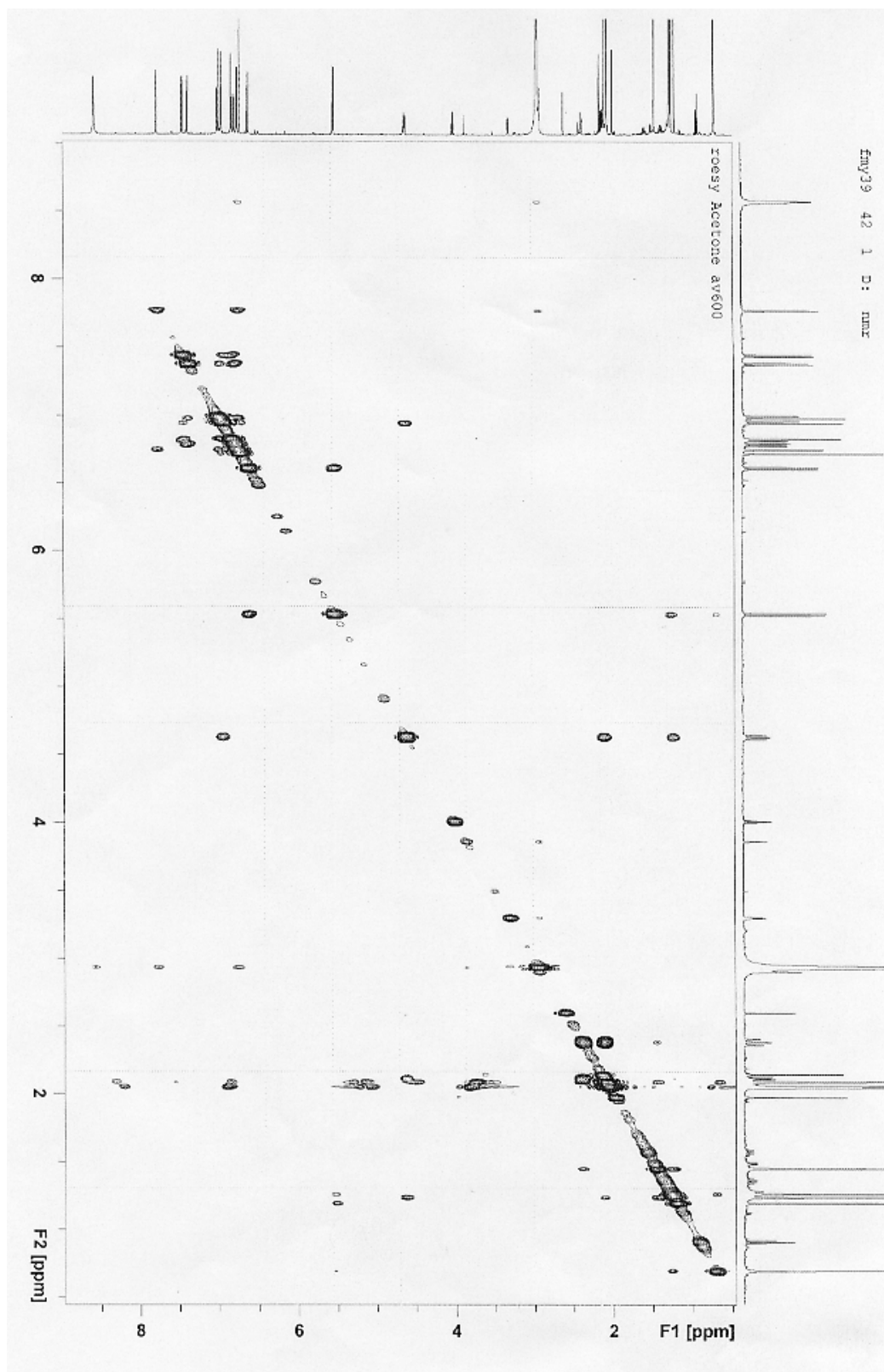
S 1.2 HMBC Spectrum of 1



S 1.3 HSQC Spectrum of 1



S 1.4 ROESY Spectrum of 1



# S 1.5 HRESIMS Spectrum of 1

Acq. Date: Thursday, March 17, 2011  
 Sample Name: 110317ESIA fmy39

Acq. Time: 15:11

**Elemental composition calculator**

Target m/z: +639.2004 amu  
 Tolerance: +10.0000 ppm  
 Result type: Elemental  
 Max num of results: 1000  
 Min DBE: -10.0000 Max DBE: +60.0000  
 Electron state: OddAndEven  
 Num of charges: 0  
 Add water: N/A  
 Add proton: N/A  
 File Name: 110317ESIA fmy39.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	200
3	Cl	0	0
4	F	0	0
5	H	0	400
6	K	0	0
7	N	0	0
8	Na	1	1
9	O	6	8
10	P	0	0

Acq. Date: Thursday, March 17, 2011  
 Sample Name: 110317ESIA fmy39

Acq. Time: 15:11

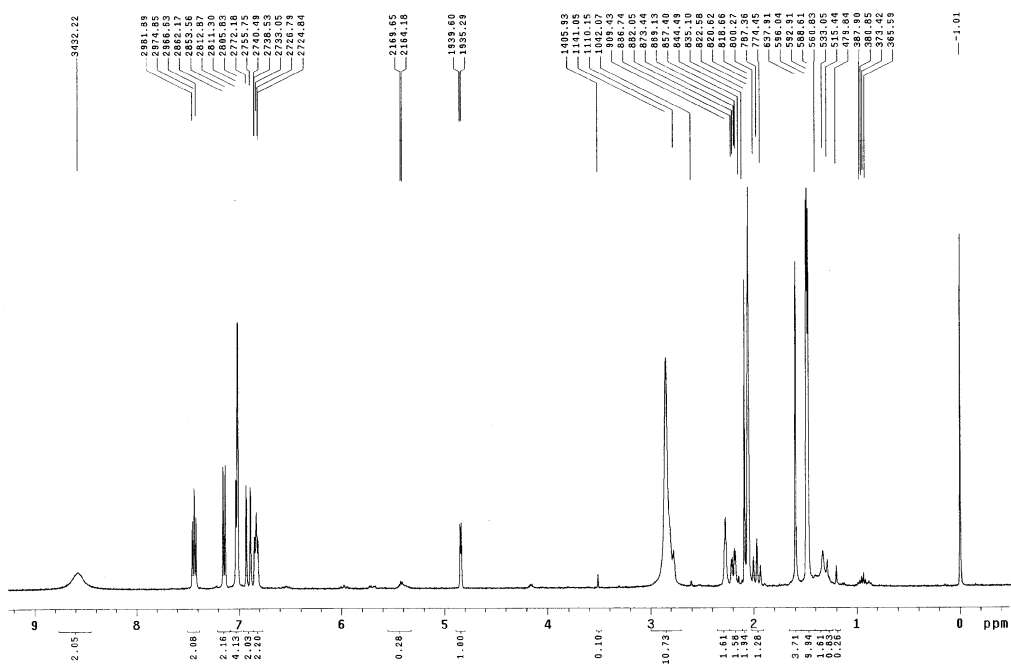
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12	S	0	0
13	Si	0	0

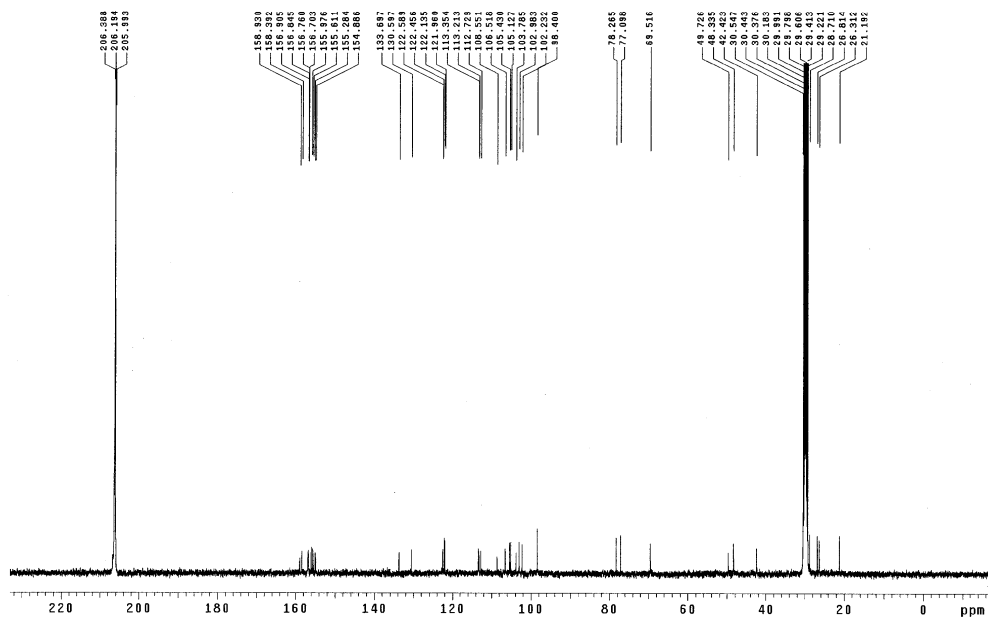
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C38 H32 O8 Na	639.1994	0.9118	1.4266	22.5

# S 2.1 <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 2

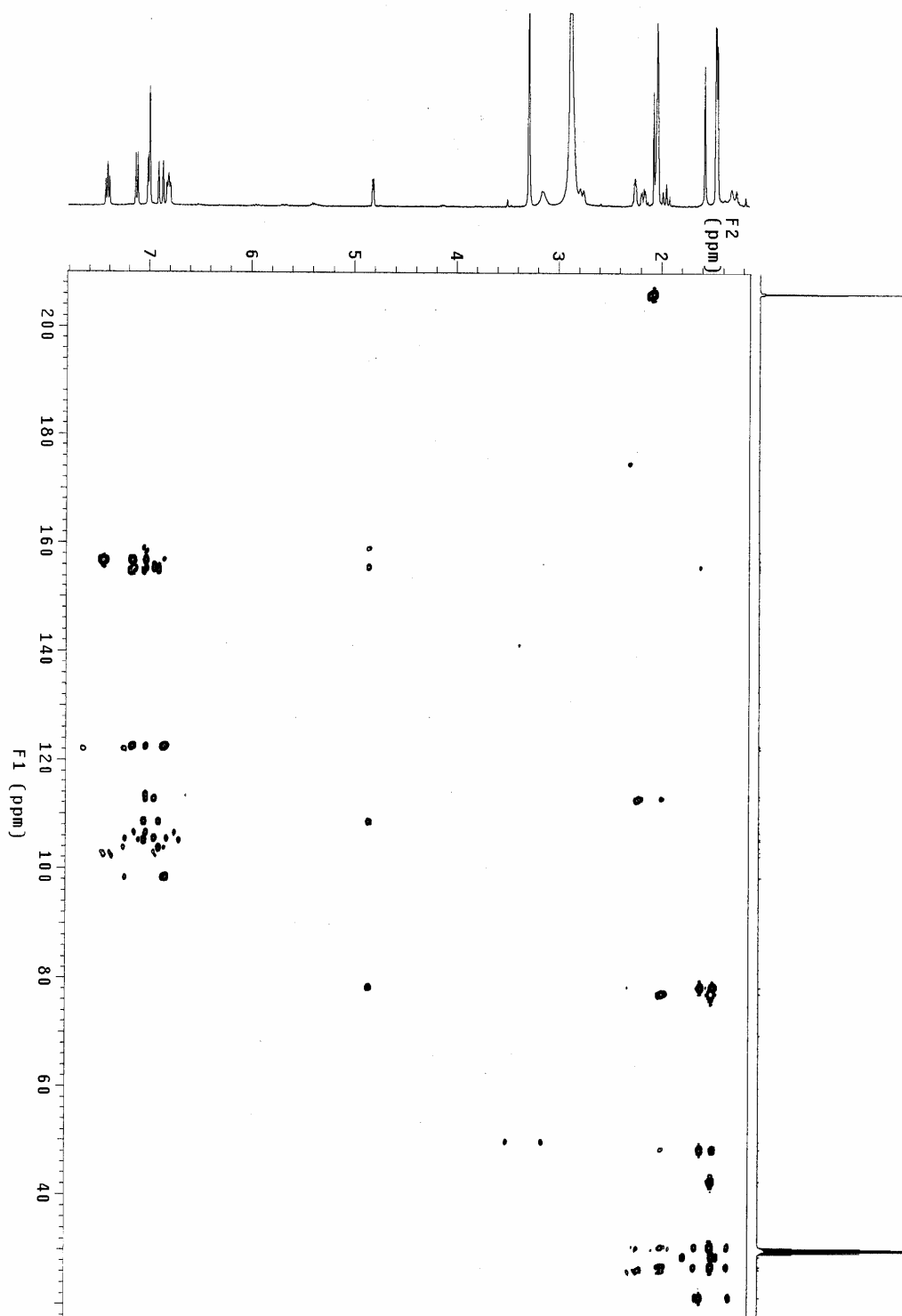
my-41 Acetone-d6 101025



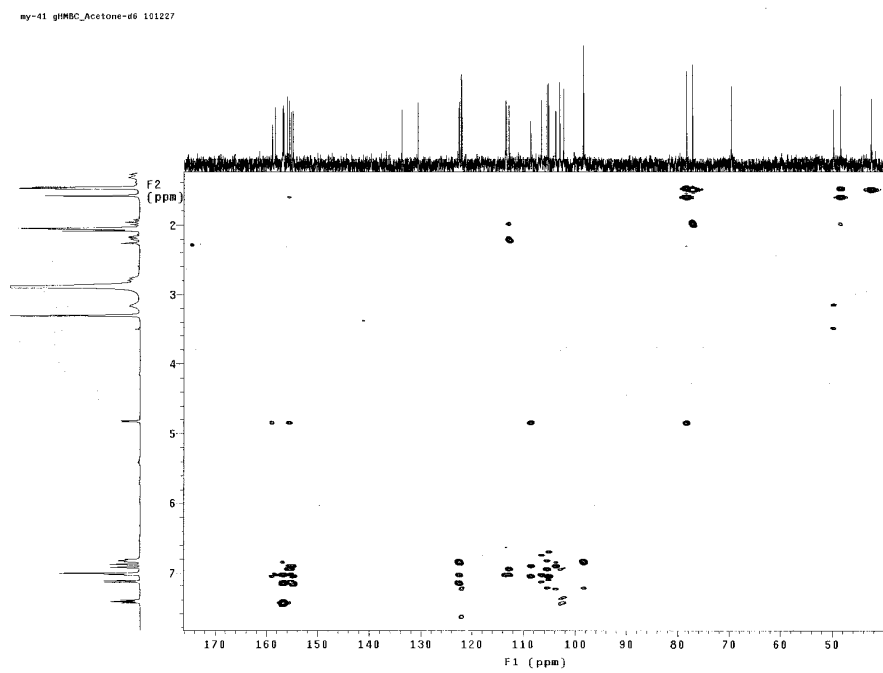
my-41 C13\_Acetone-d6 101227



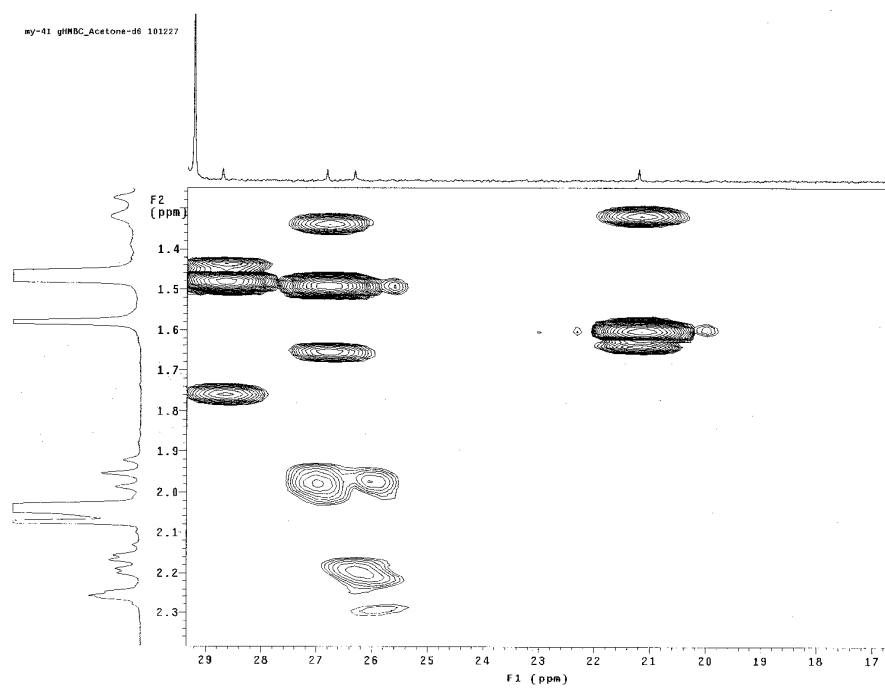
S 2.2 HMBC Spectrum of 2



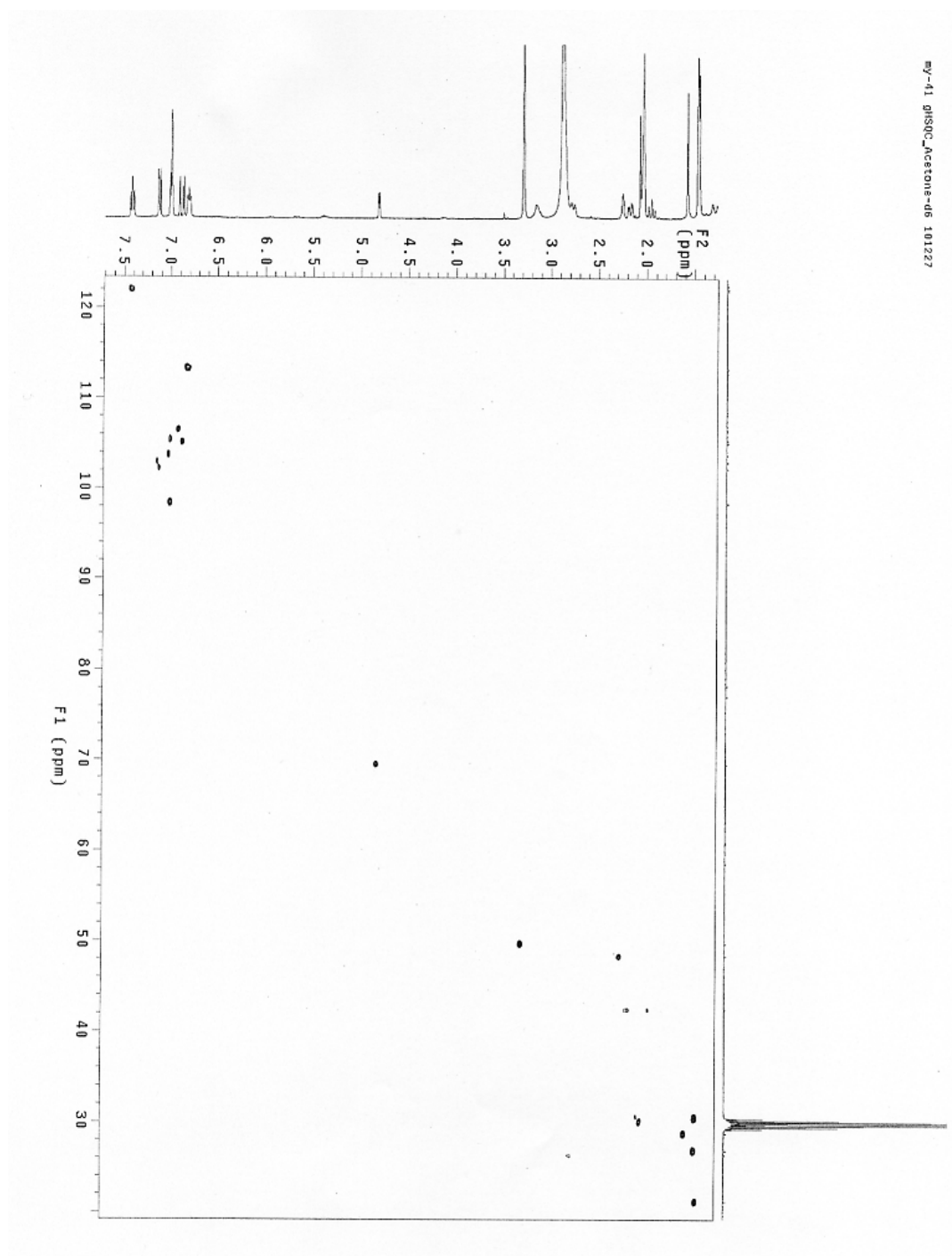
### S 2.2.1 The magnified HMBC Spectrum of 2



### S 2.2.2 The magnified HMBC Spectrum of 2

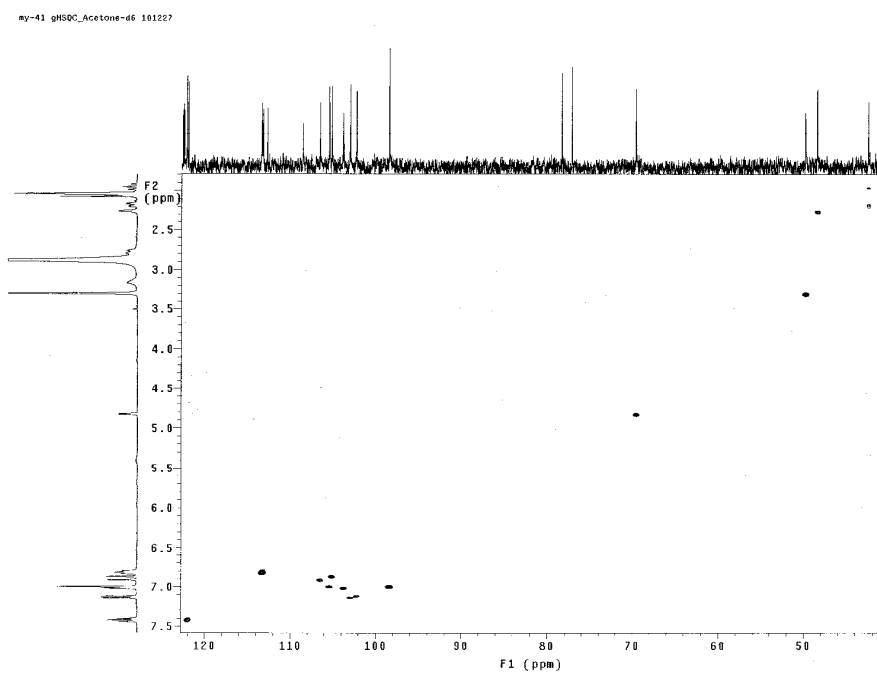


S 2.3 HSQC Spectrum of 2

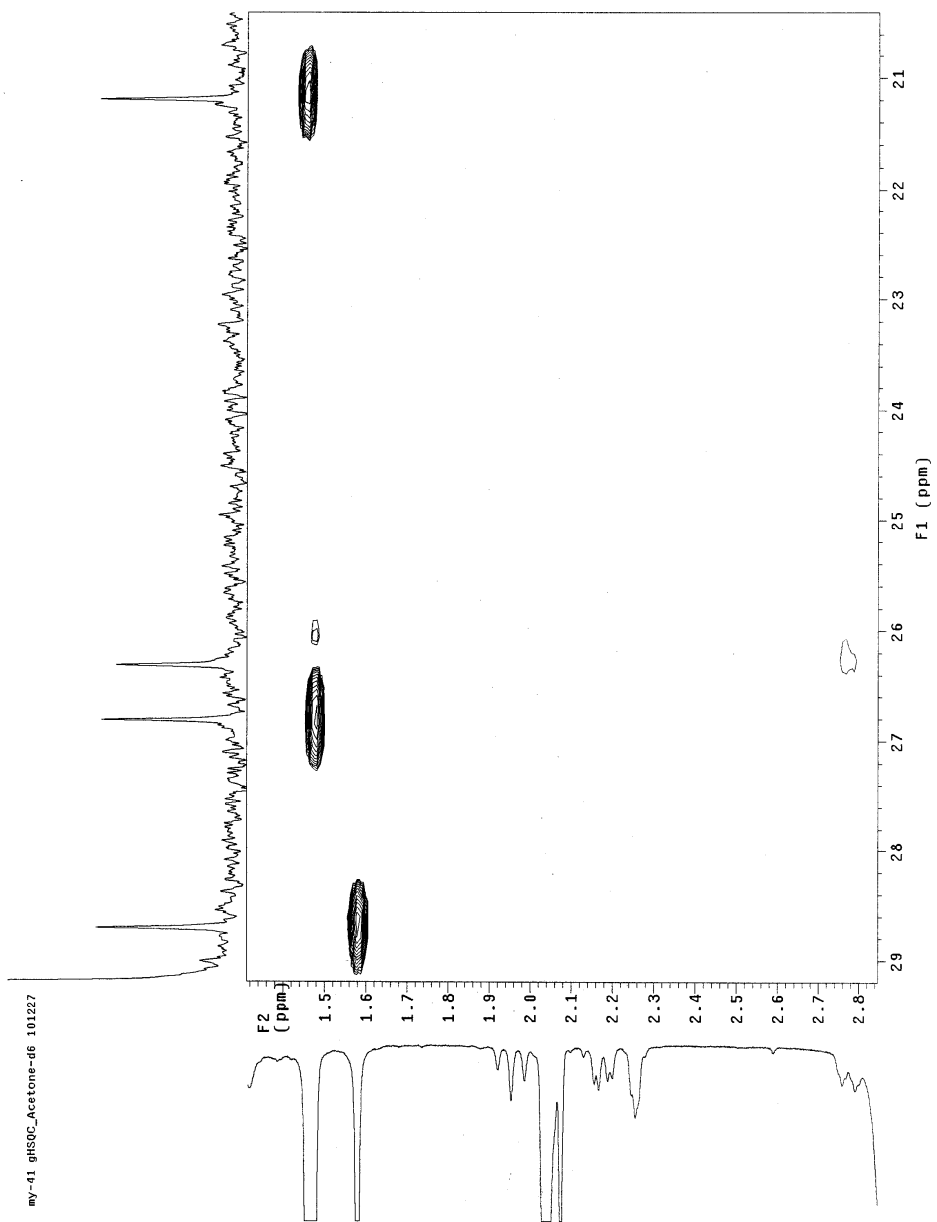


ny-41 gHSQC\_Acetone-d6 181227

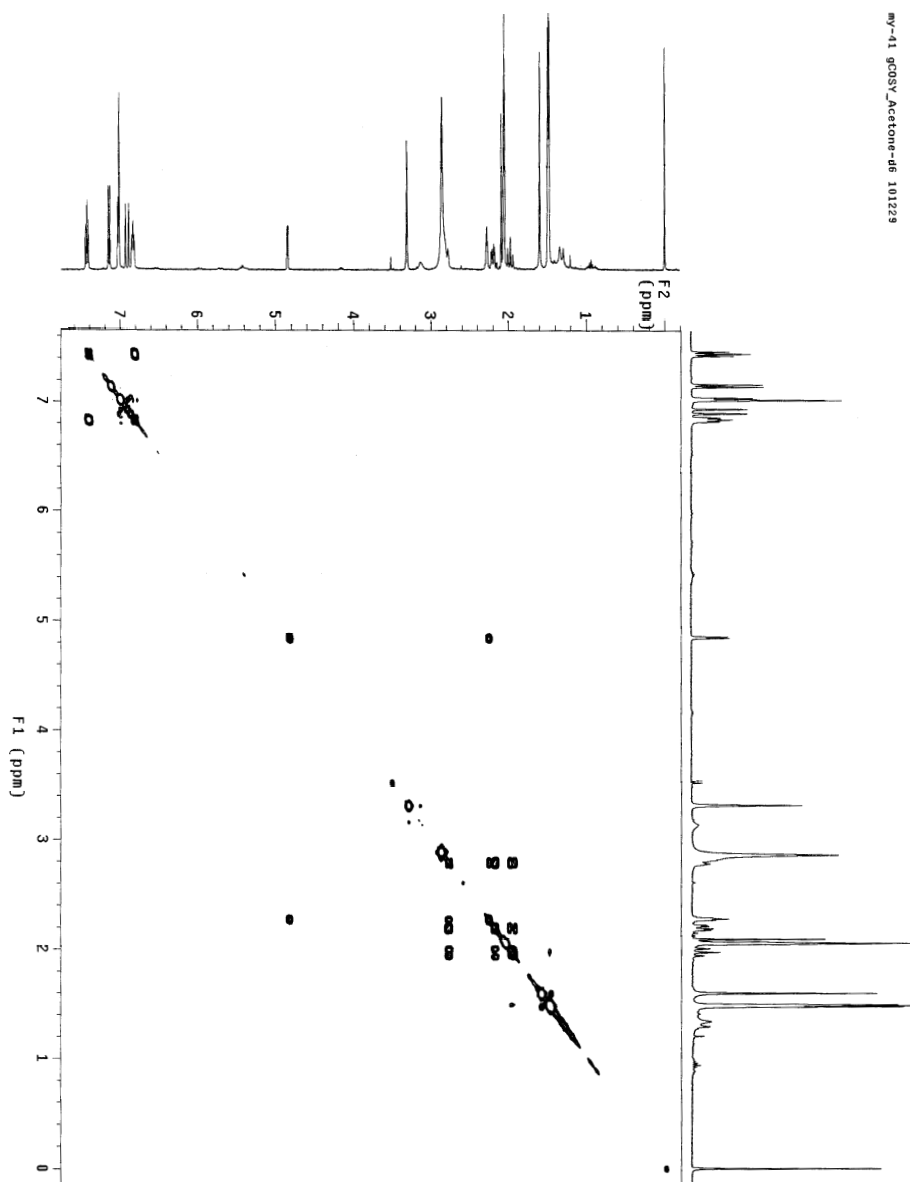
### S 2.3.1 The Magnified HSQC Spectrum of 2



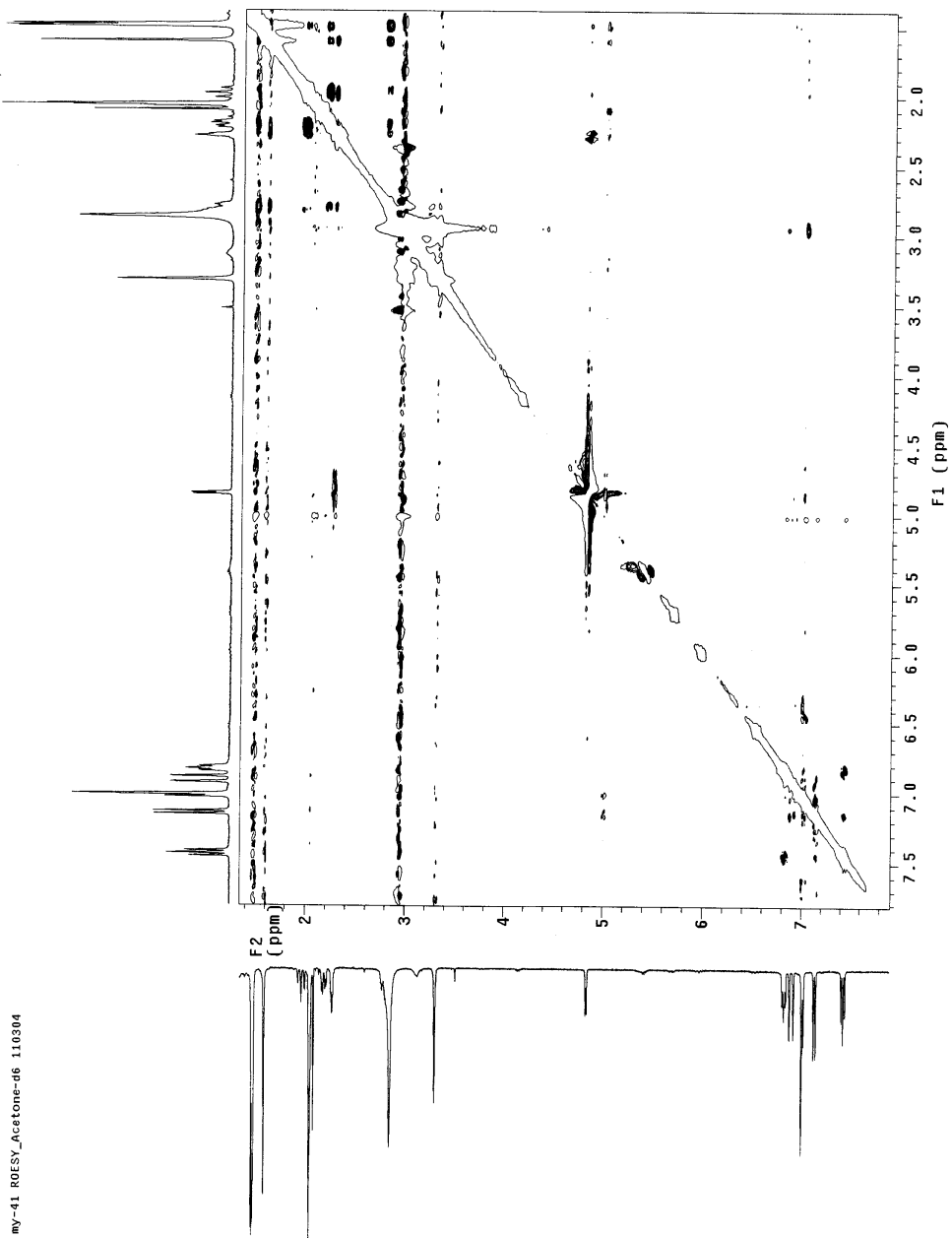
### S 2.3.1 The Magnified HSQC Spectrum of 2



S 2.4  $^1\text{H}$ - $^1\text{H}$  COSY Spectrum of 2



S 2.5 ROESY Spectrum of 2



Shanghai Mass Spectrometry Center  
Shanghai Institute of Organic Chemistry  
Chinese Academy of Sciences  
High Resolution MS Data Report



Instrument



Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

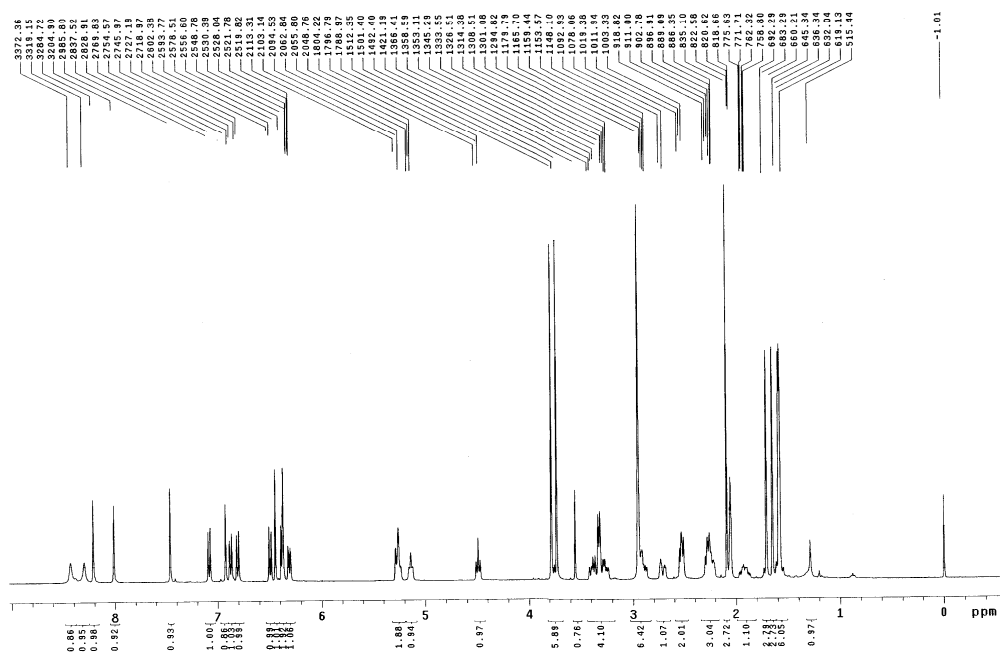
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Analysis Name            D:\Data\zj\2011\20110321neg\_000004.d  
Sample Name              A3  
Acquisition Date        3/21/2011 10:45:41 AM  
Operator:                 zj  
  
Ion Mass (Measured)    615.20503

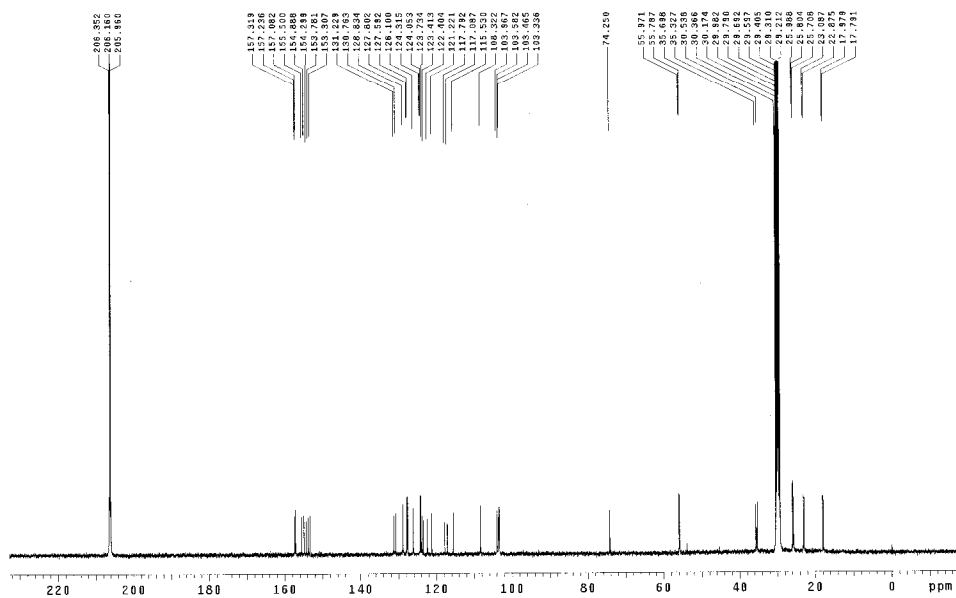
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e <sup>-</sup>
C <sub>38</sub> H <sub>31</sub> O <sub>8</sub>	0.008	615.20244	-4.21	-4.53	-2.59	23.50	ok	even
C <sub>41</sub> H <sub>29</sub> N <sub>1</sub> O <sub>5</sub>	0.018	615.20512	0.15	-0.20	0.09	28.00	ok	odd

# S 3.1 <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 3

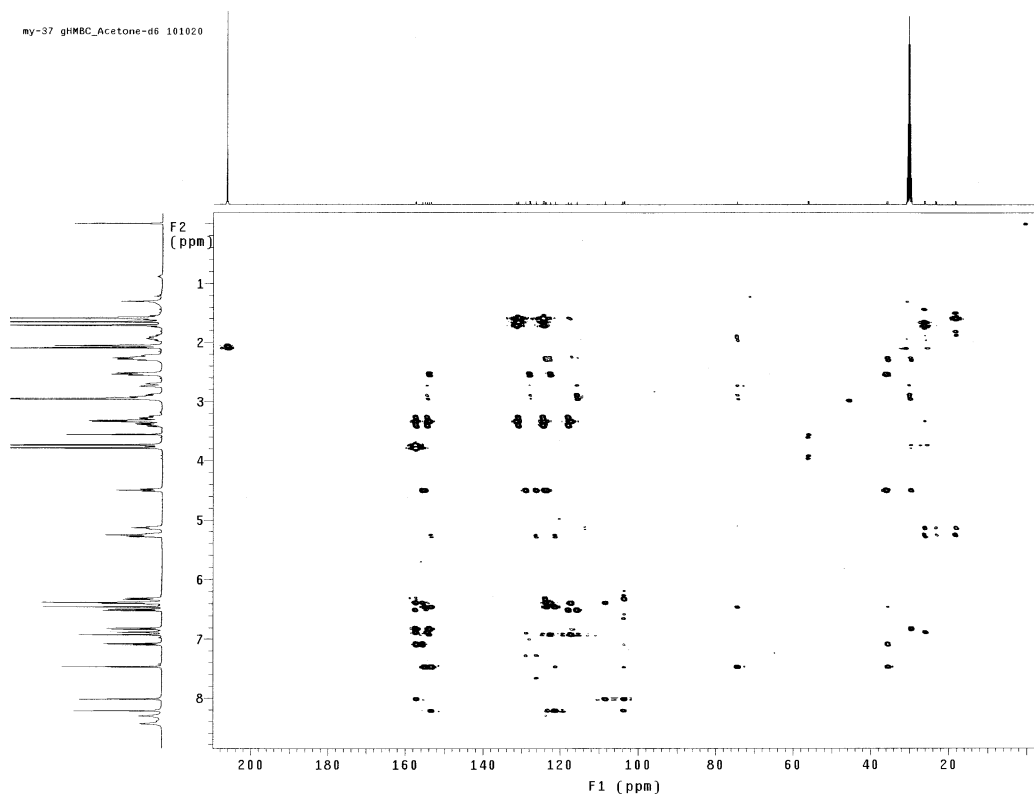
57  
my-34\_Acetone-d6 101019



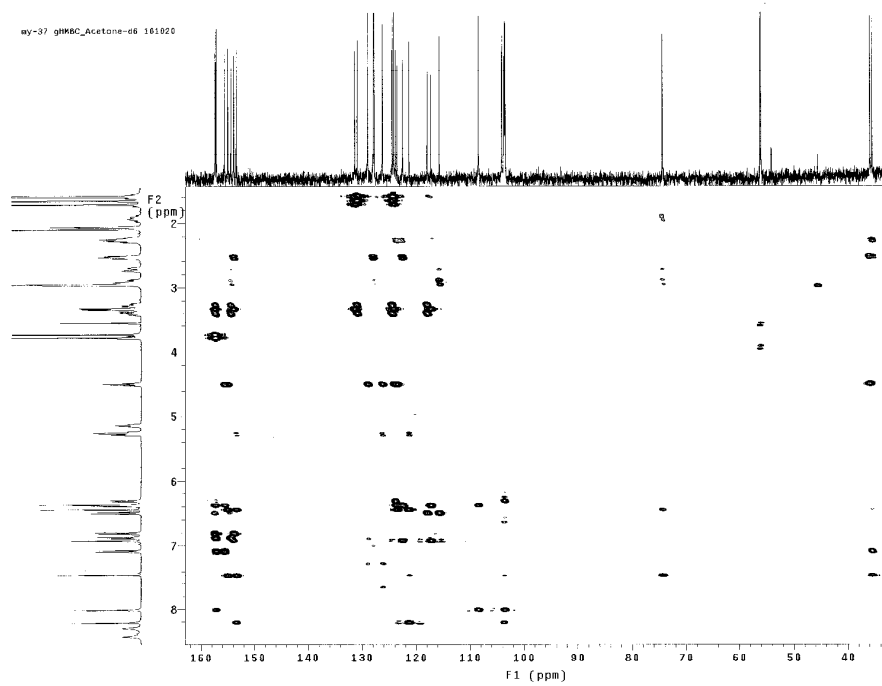
my-37\_C13\_Acetone-d6 101020



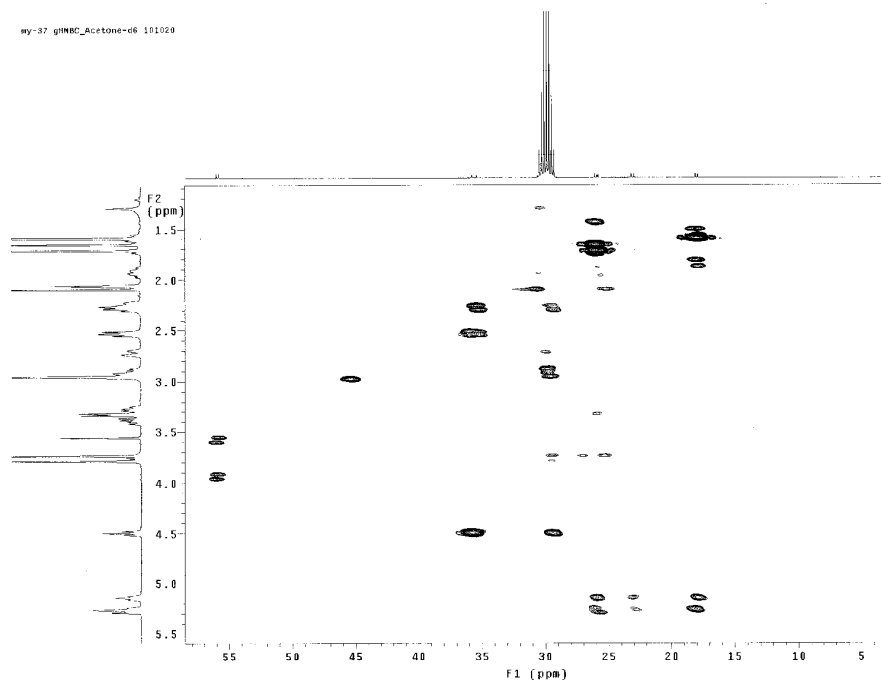
### S 3.2 HMBC Spectrum of 3



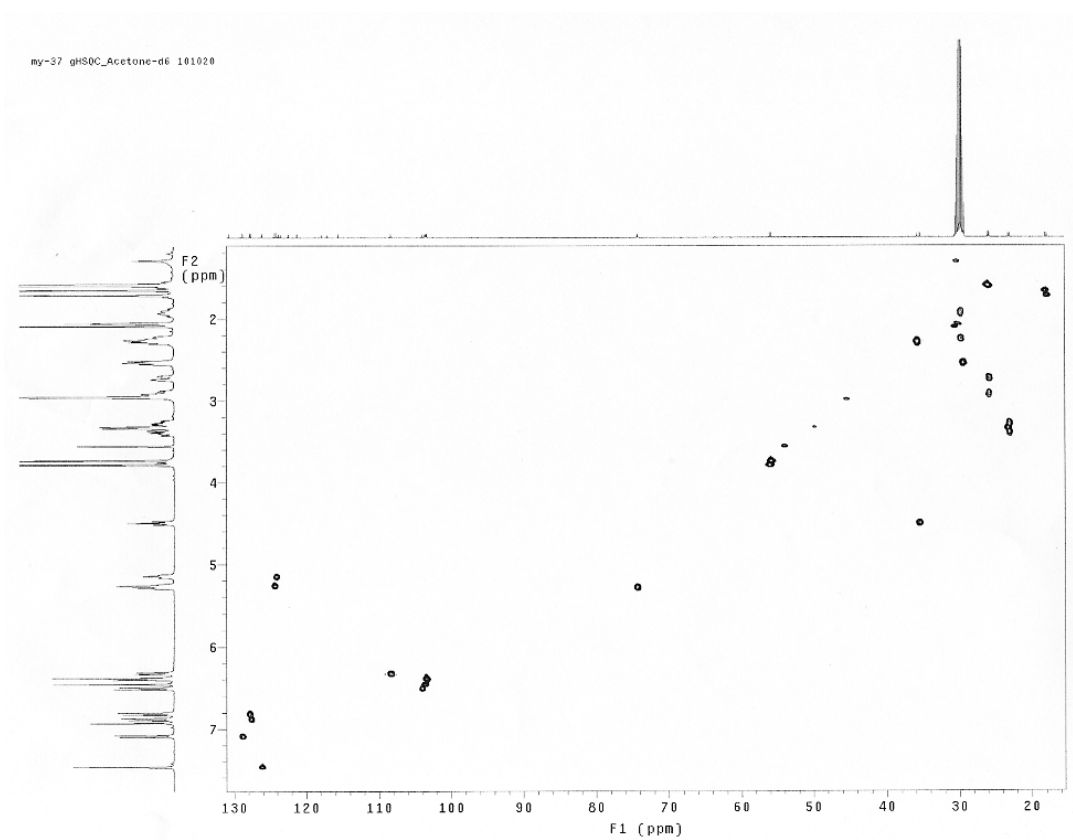
### S 3.2.1 The magnified HMBC Spectrum of 3



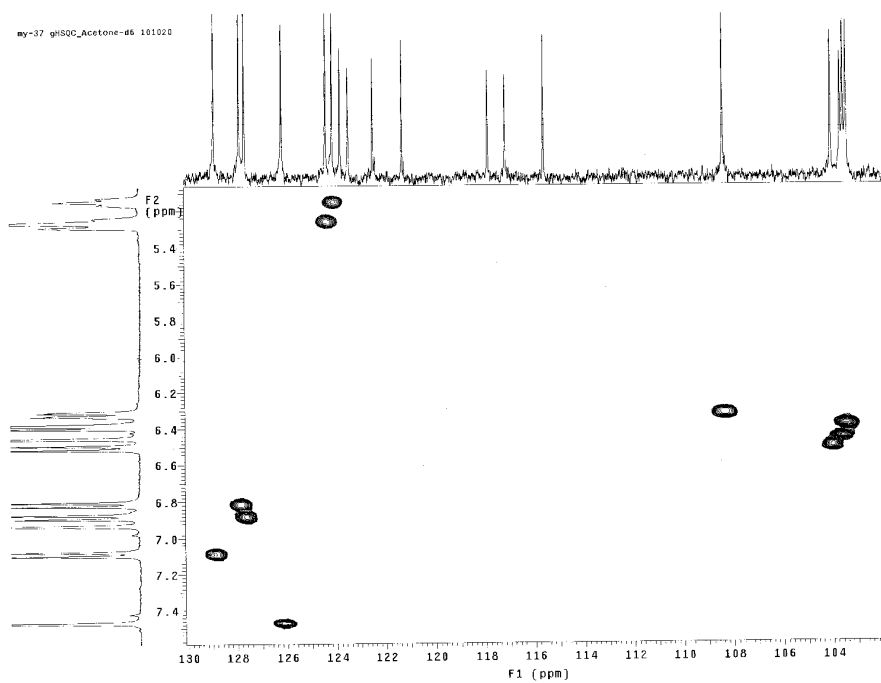
### S 3.2.2 The magnified HMBC Spectrum of 3



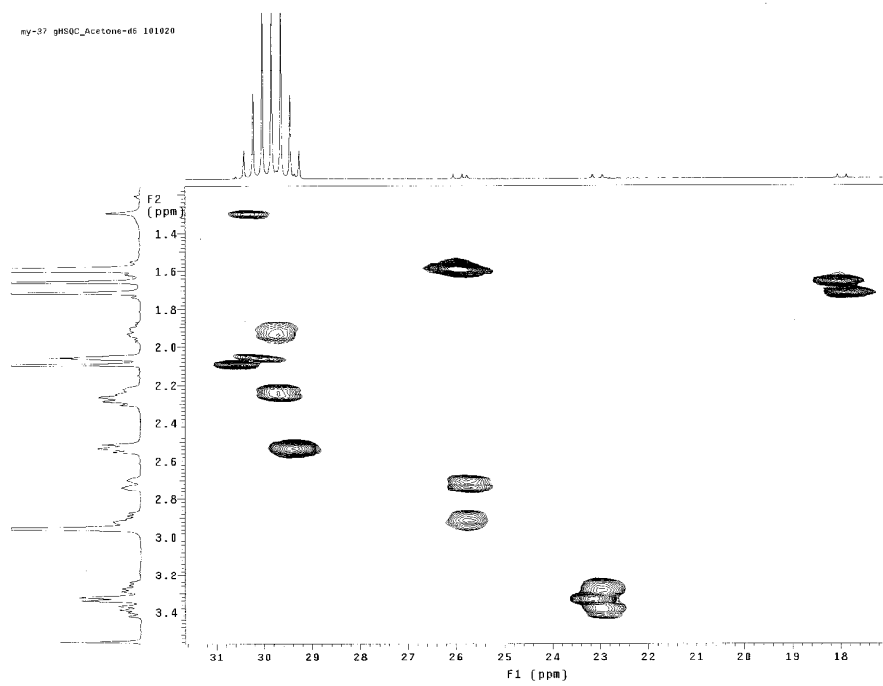
### S 3.3 HSQC Spectrum of **3**



### S 3.3.1 The magnified HSQC Spectrum of 3



### S 3.3.2 The magnified HSQC Spectrum of 3



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 High Resolution MS DATA REPORT



Instrument:



IonSpec 4.7 Tesla FTMS

Card Serial Number: I110028

Sample Serial Number: mg-37

Operator : HuaQin Date: 2010/12/17

Operation Mode: MALDI/DHB

**Elemental Composition Search Report:****Target Mass:**

Target m/z = 703.3264 ± 0.003

Charge = +1

**Possible Elements:**

Element:	Exact Mass:	Min:	Max:
C	12.000000	0	100
H	1.007825	0	100
O	15.994915	0	100
Na	22.989770	0	1

**Additional Search Restrictions:**

DBE Limit Mode = Both Integer and Half-Integer

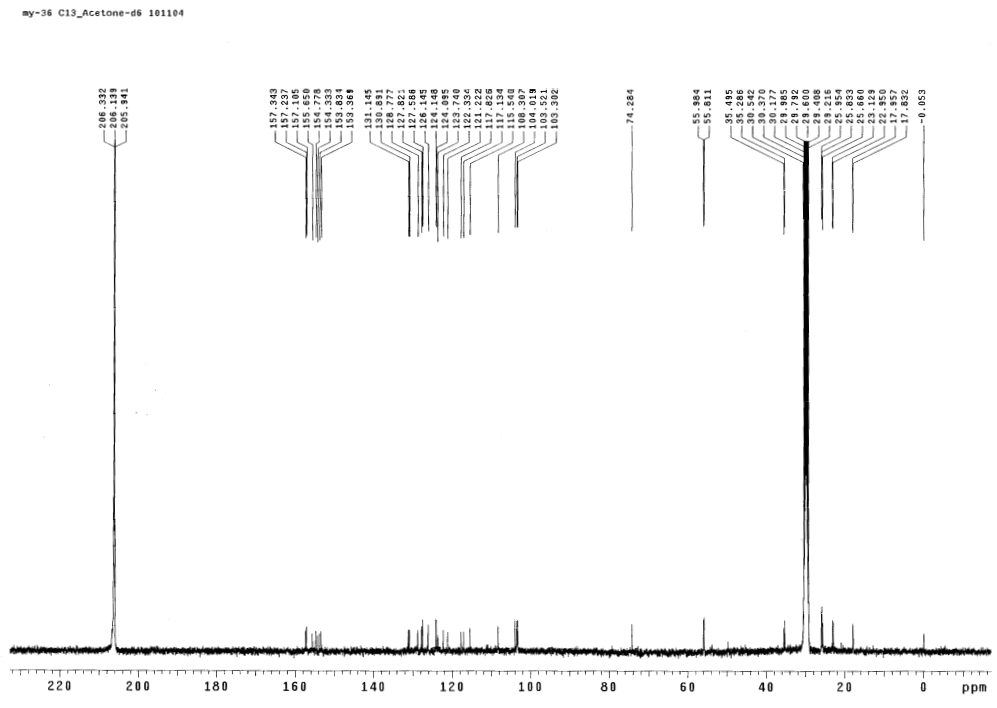
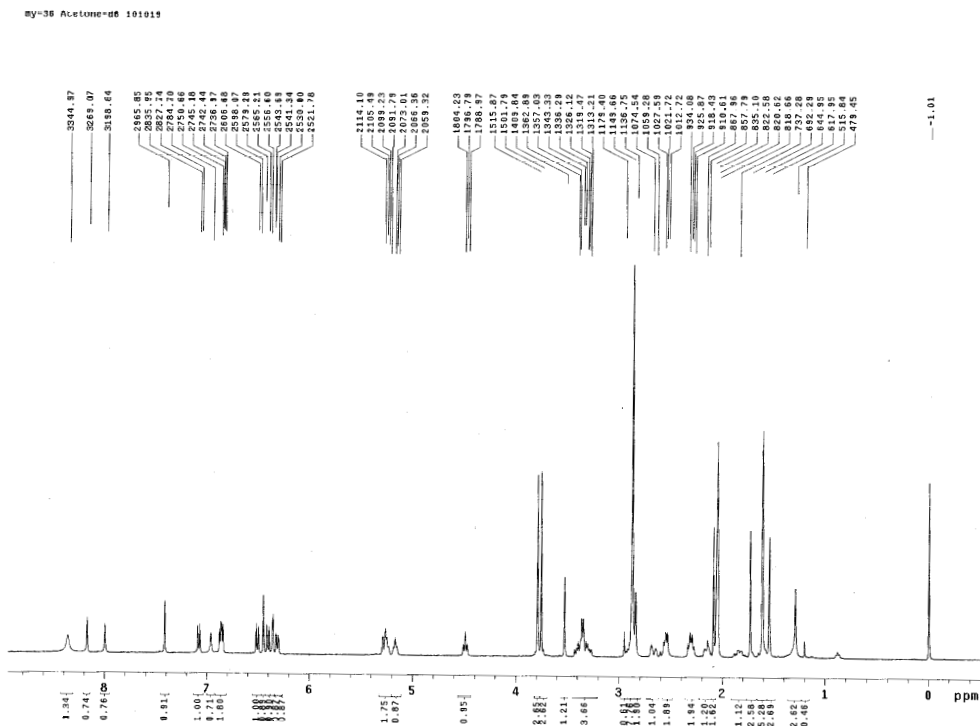
Minimum DBE = 0

**Search Results:**

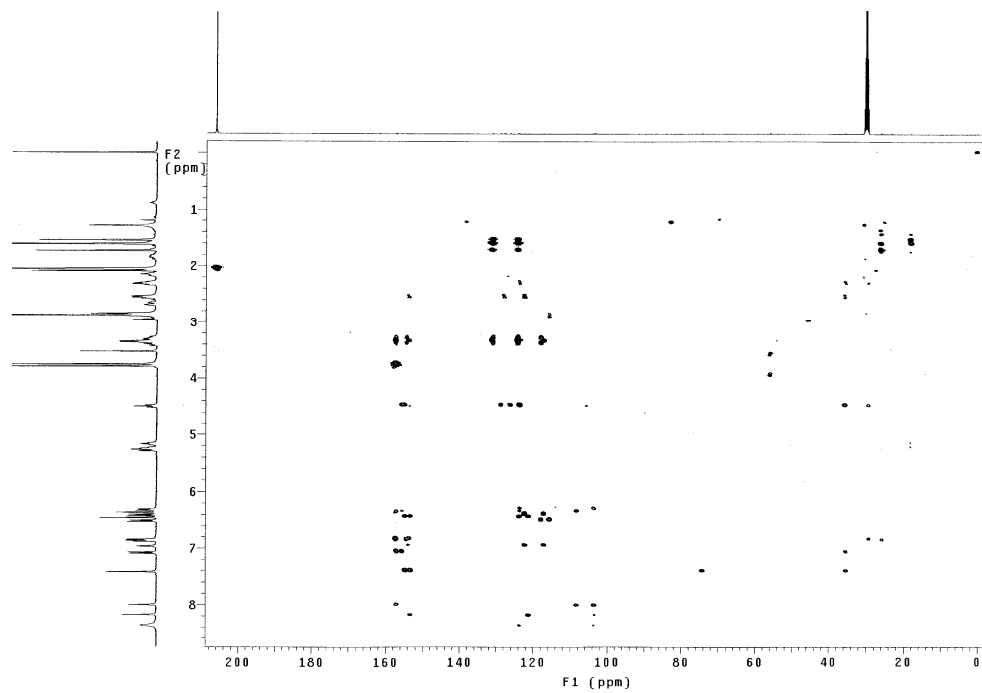
Number of Hits = 2

m/z	Delta m/z	DBE	Formula
703.32655	-0.00015	21.5	C <sub>44</sub> H <sub>47</sub> O <sub>8</sub> <sup>+1</sup>
703.32414	0.00226	19.0	C <sub>42</sub> H <sub>48</sub> O <sub>8</sub> Na <sup>+1</sup>

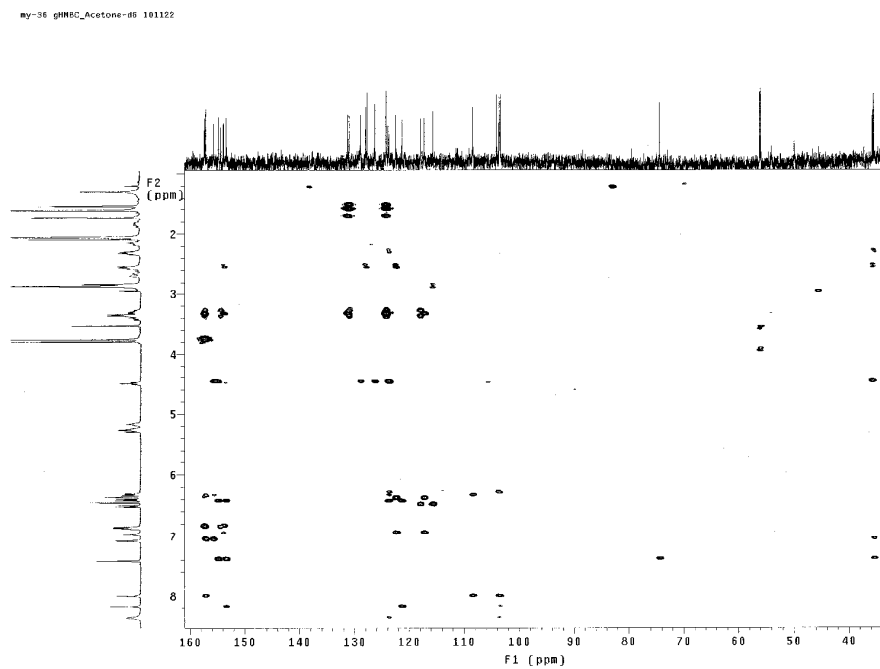
# S 4.1 <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 4



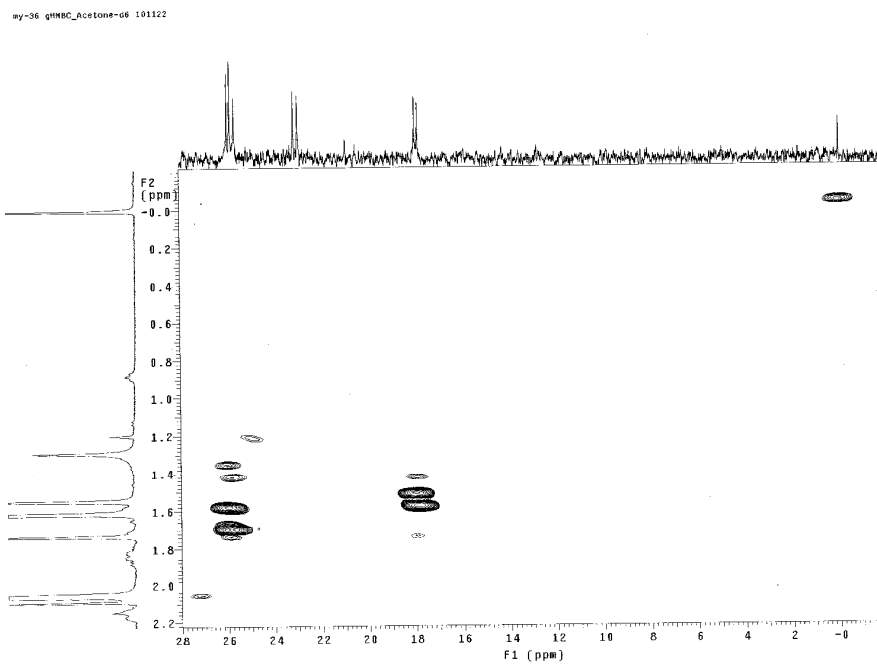
### S 4.2 HMBC Spectrum of 4



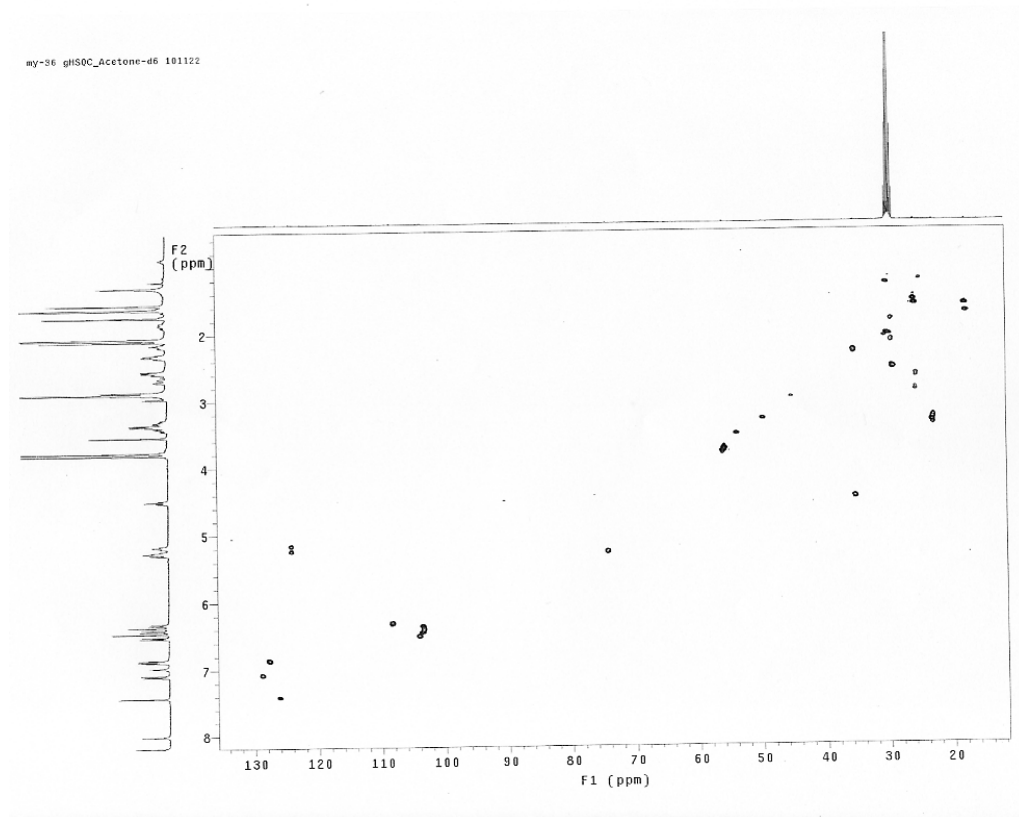
### S 4.2.1 The magnified HMBC Spectrum of 4



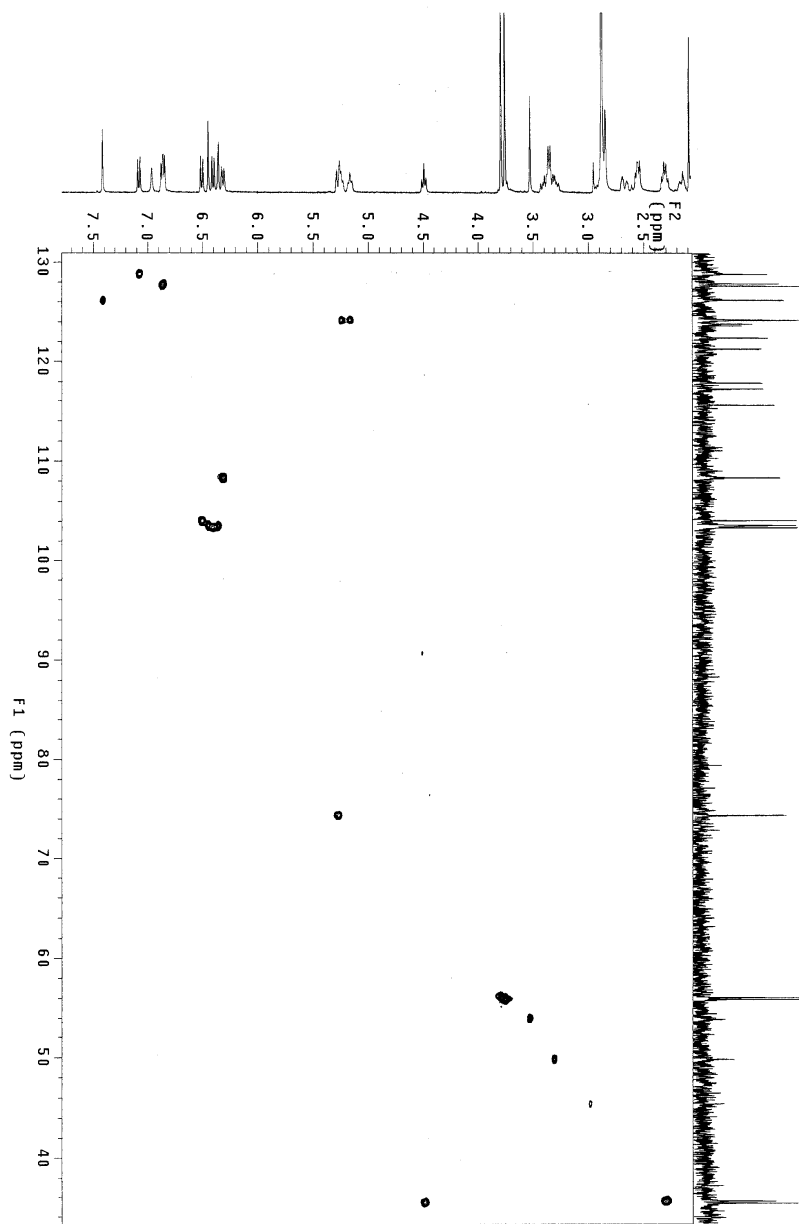
### S 4.2.2 The magnified HMBC Spectrum of 4



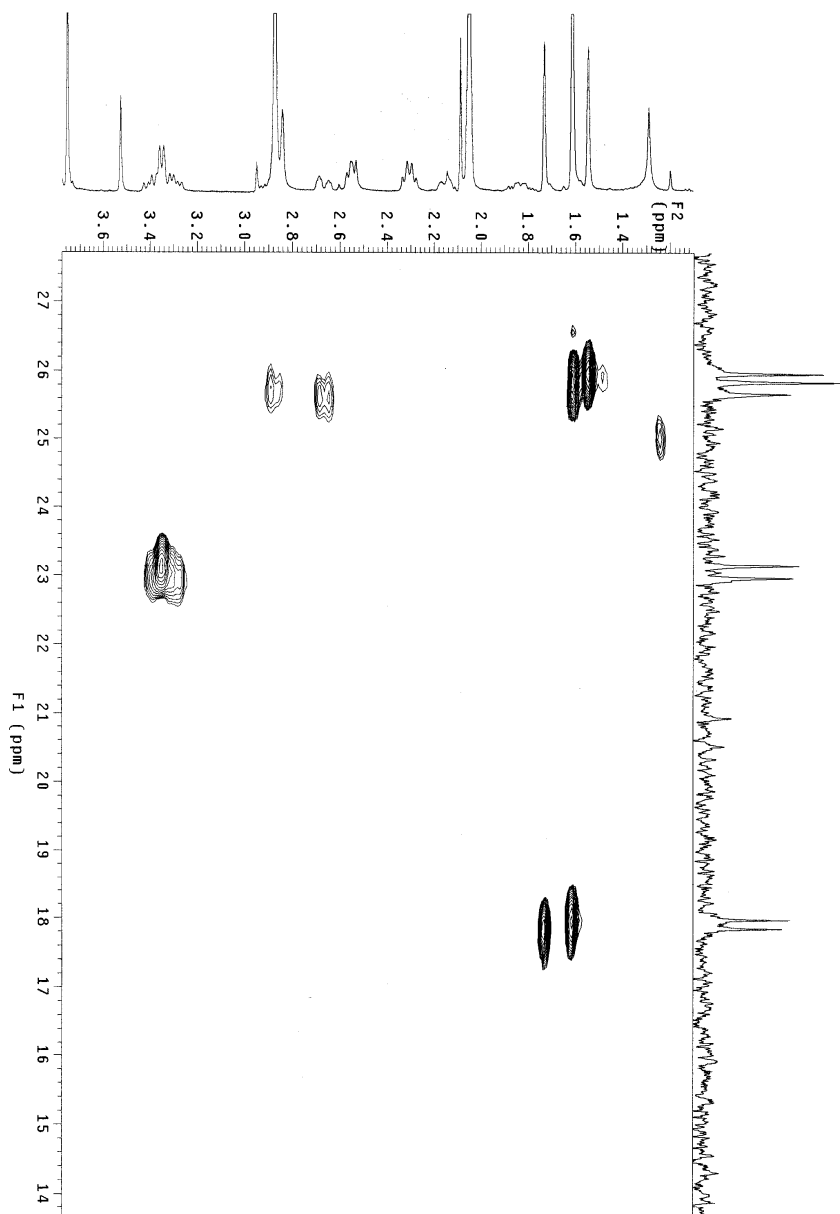
### S 4.3 HSQC Spectrum of 4



S 4.3.1 The magnified HSQC Spectrum of 4



### S 4.3.2 The magnified HSQC Spectrum of 4



#### S 4.4 HRMALDIMS Spectrum of 4

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High Resolution MS DATA REPORT



Instrument:



IonSpec 4.7 Tesla FTMS

Card Serial Number: I110027

Sample Serial Number: mg-36

Operator : HuaQin Date: 2010/12/17

Operation Mode: MALDI/DHB

#### **Elemental Composition Search Report:**

##### **Target Mass:**

Target m/z = 703.3259 ± 0.002  
Charge = +1

##### **Possible Elements:**

Element:	Exact Mass:	Min:	Max:
C	12.000000	0	100
H	1.007825	0	100
O	15.994915	0	100
Na	22.989770	0	1

##### **Additional Search Restrictions:**

DBE Limit Mode = Both Integer and Half-Integer  
Minimum DBE = 0

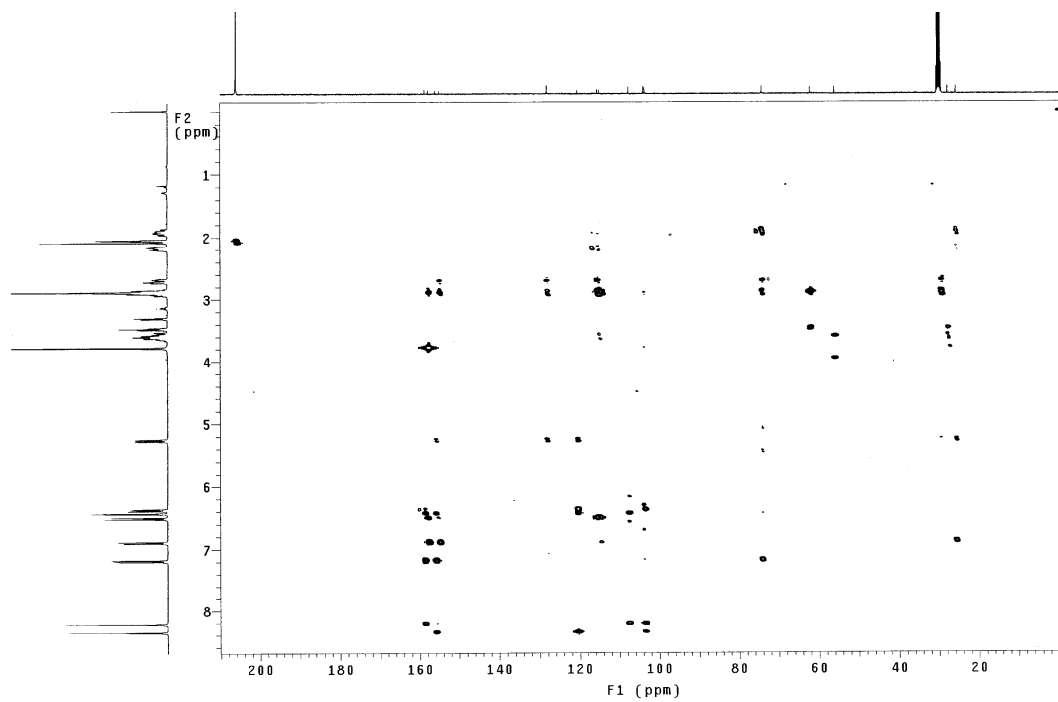
##### **Search Results:**

Number of Hits = 2

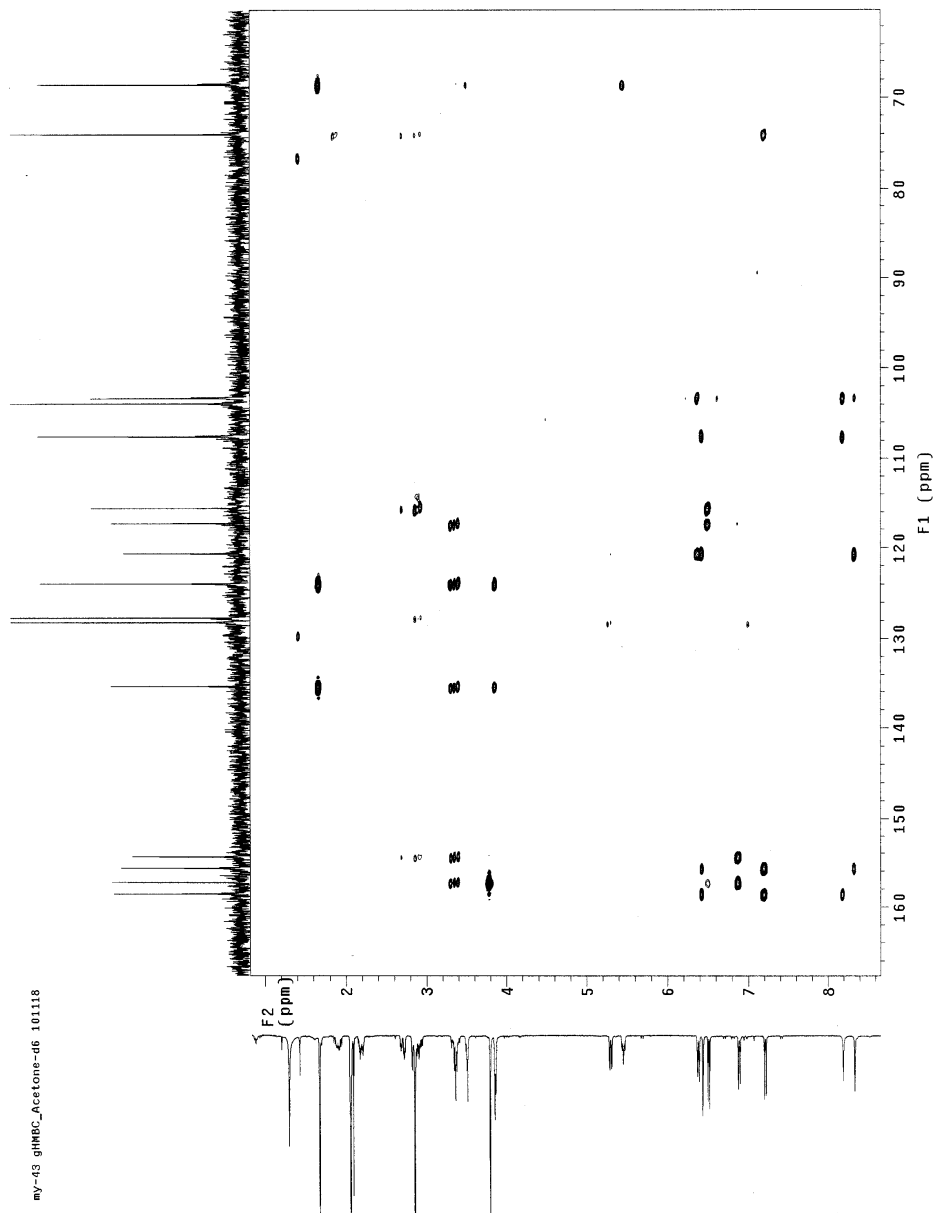
m/z	Delta m/z	DBE	Formula
703.32655	-0.00065	21.5	C <sub>44</sub> H <sub>47</sub> O <sub>8</sub> <sup>+1</sup>
703.32414	0.00176	19.0	C <sub>42</sub> H <sub>48</sub> O <sub>8</sub> Na <sup>+1</sup>



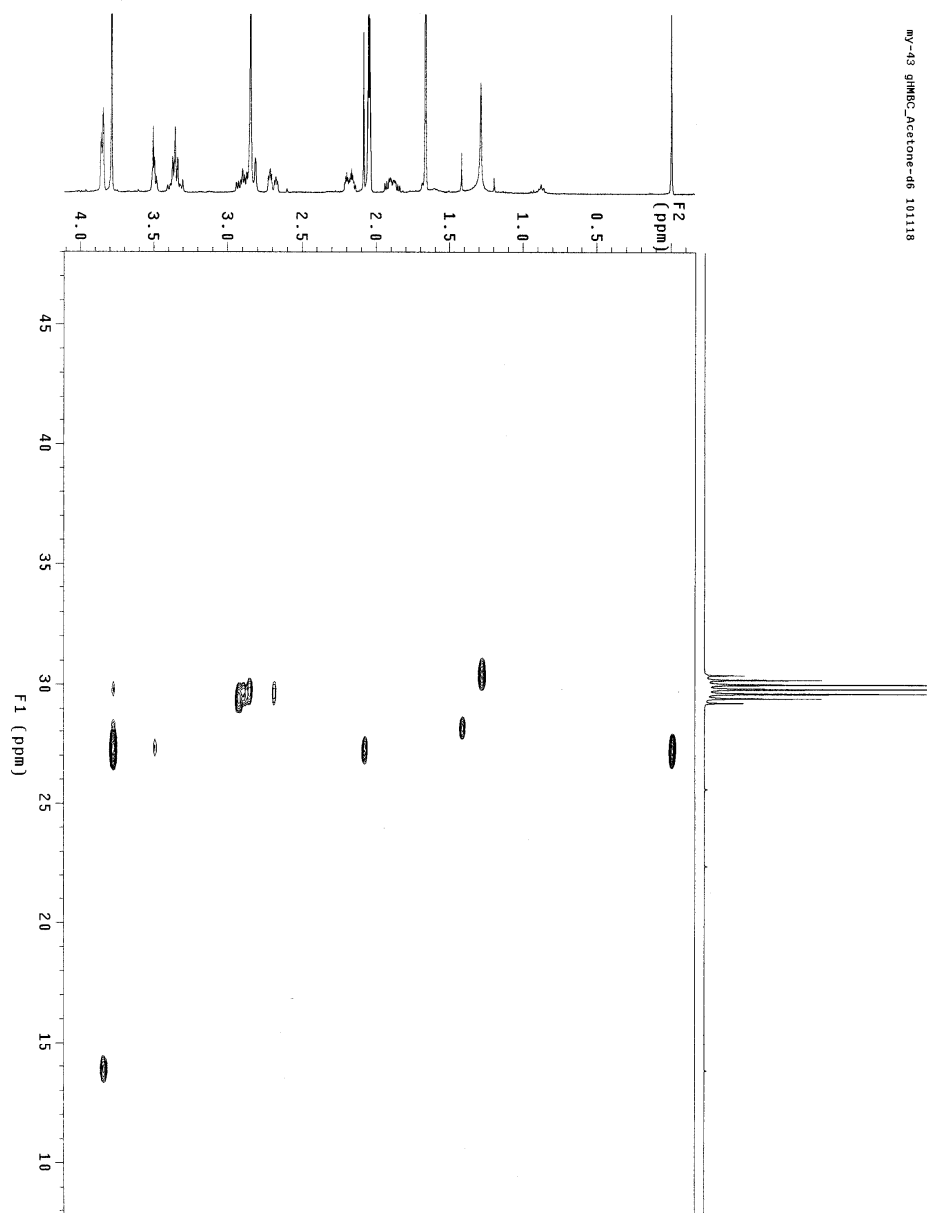
S 5.2 HMBC Spectrum of 5



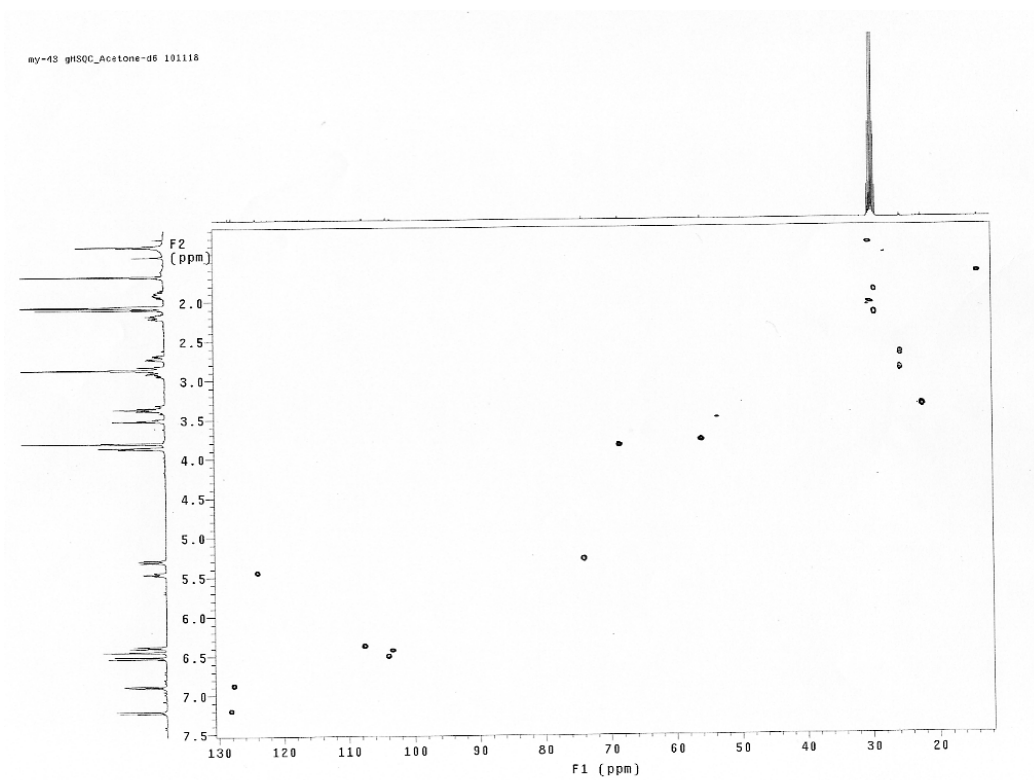
### S 5.2.1 The magnified HMBC Spectrum of 5



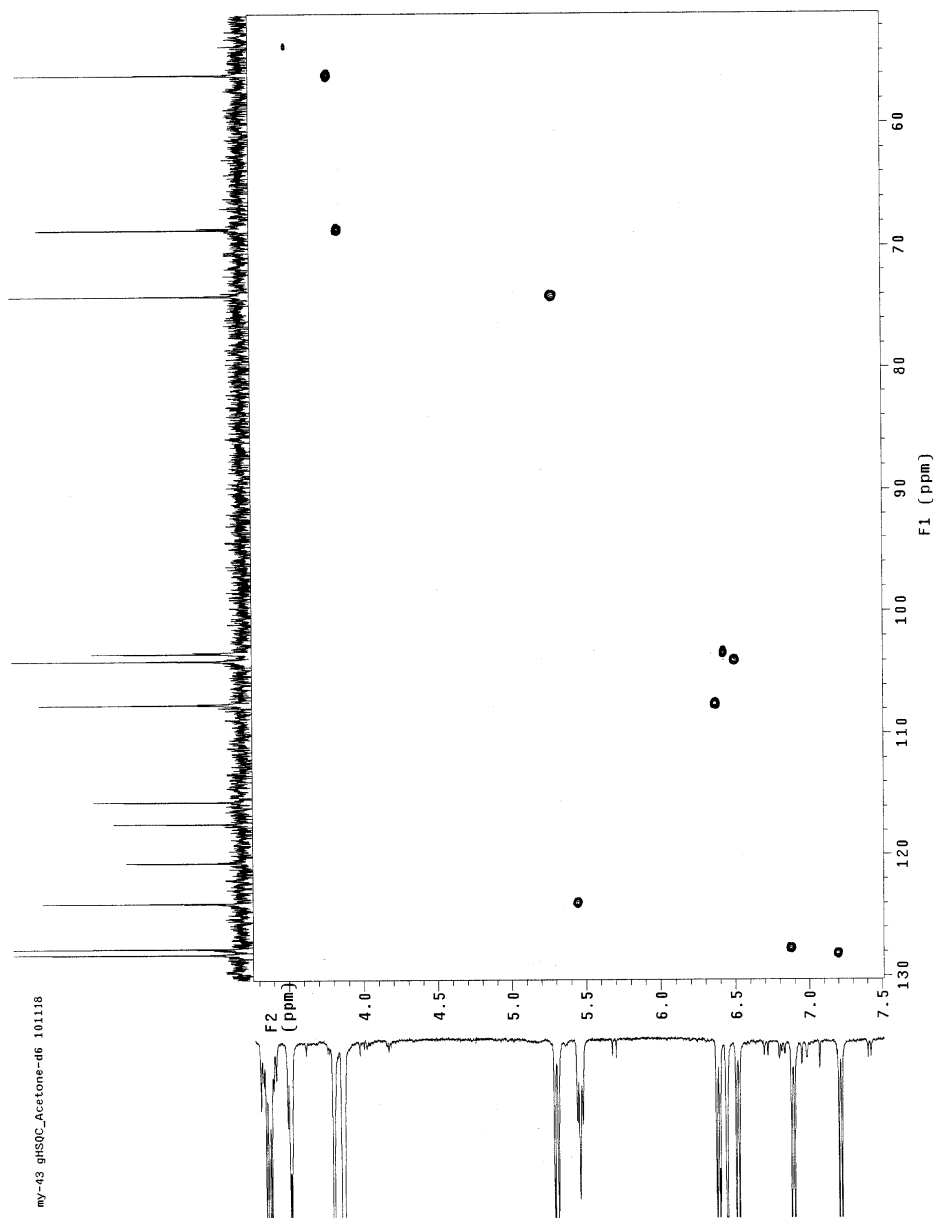
S 5.2.2 The magnified HMBC Spectrum of 5



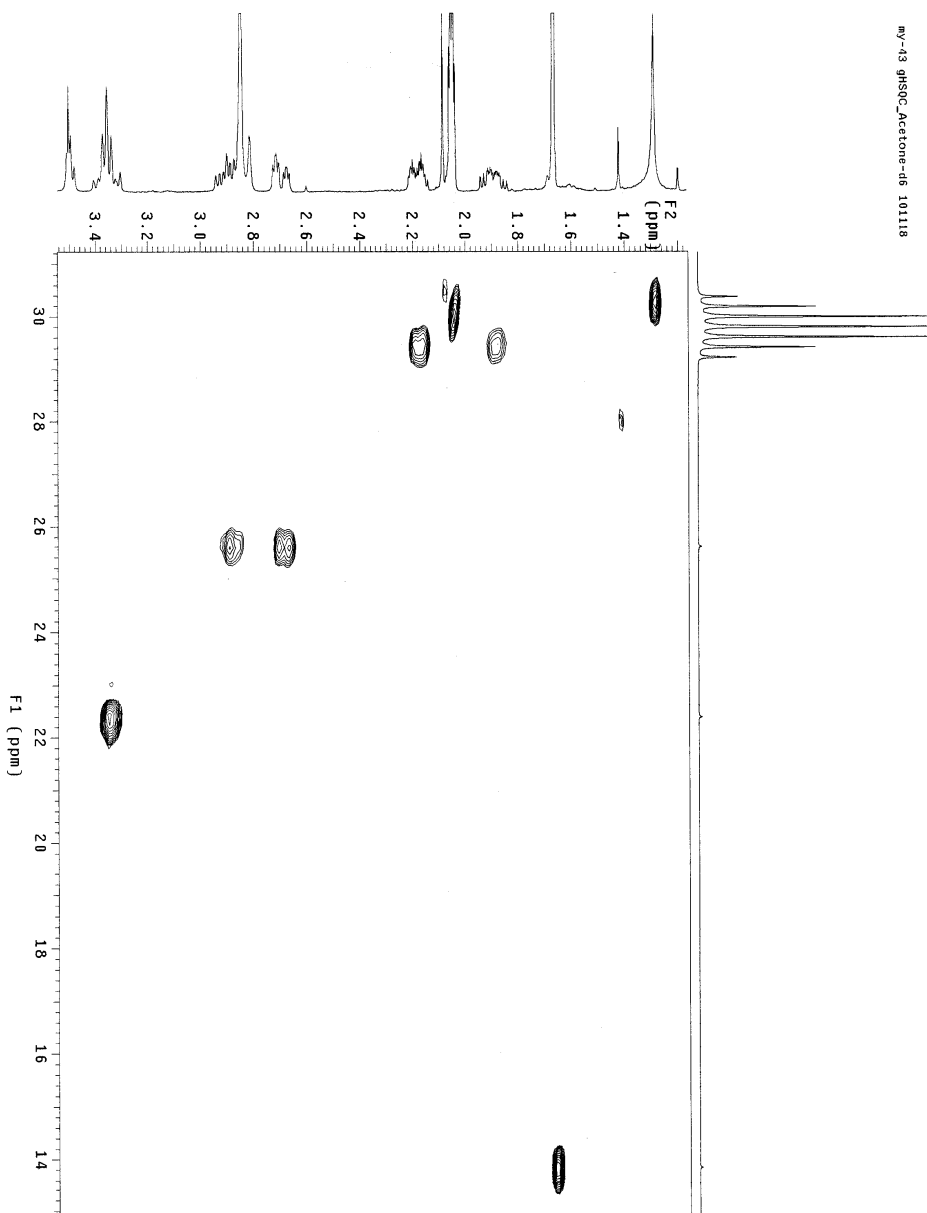
S 5.3 HSQC Spectrum of **5**



### S 5.3.1 The magnified HSQC Spectrum of 5



S 5.3.2 The magnified HSQC Spectrum of 5



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 High Resolution MS Data Report



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

Card Serial Number: GCT-T1011-OS0610

Sample Serial Number: My-43

Operator: Li

Date: 2010/11/26

Elemental Composition Report

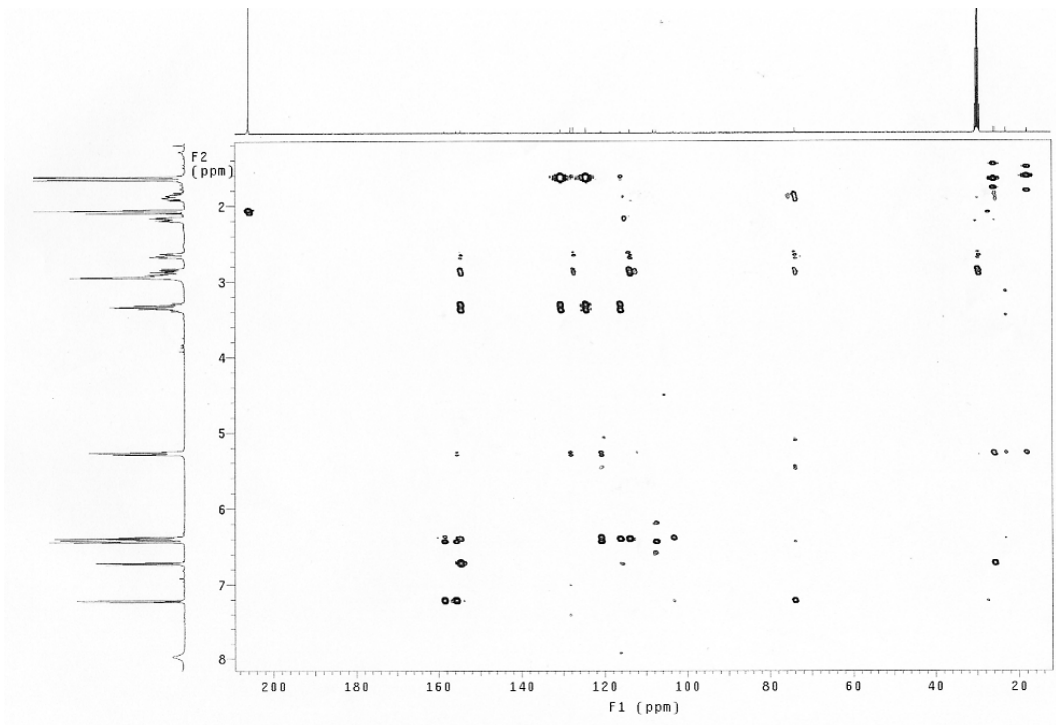
Single Mass Analysis  
 Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0    Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
 223 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

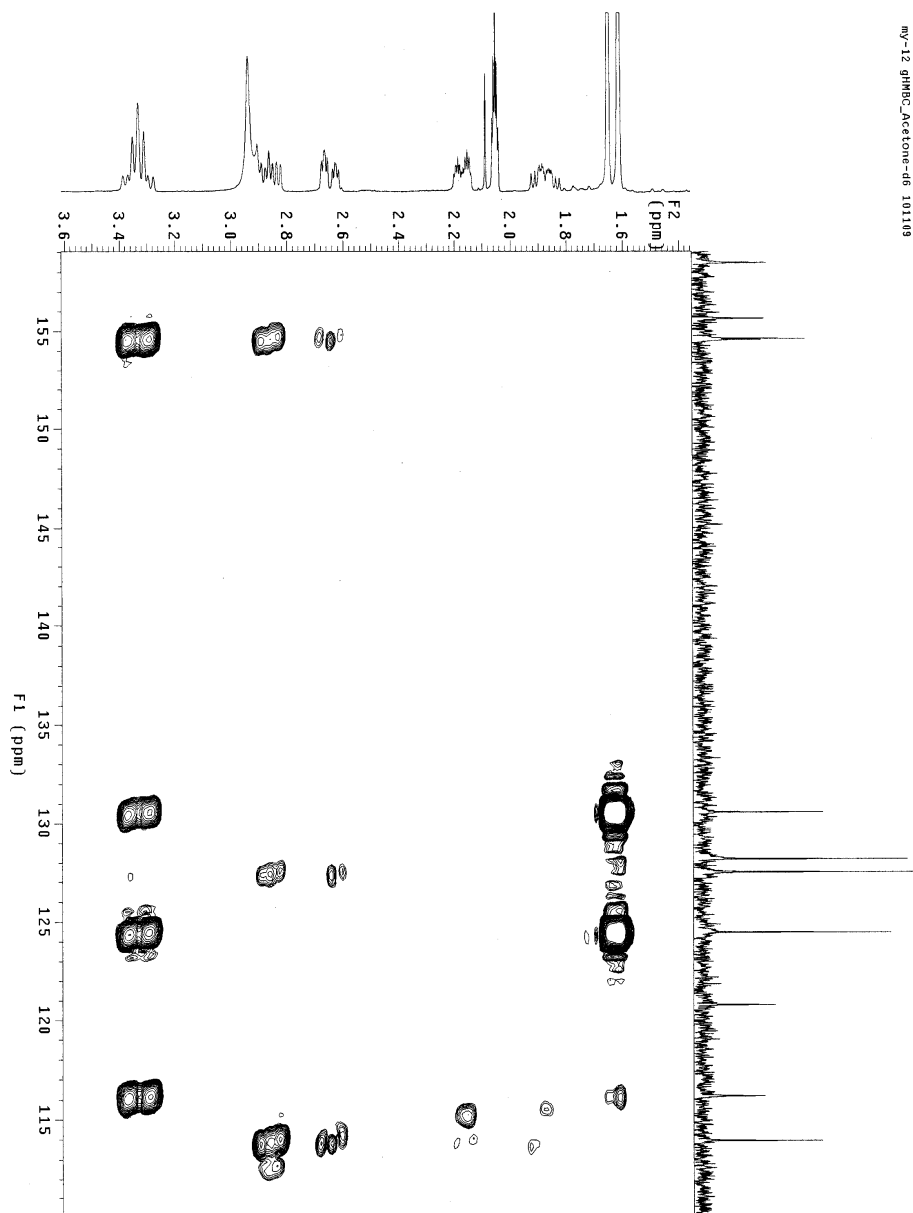
Minimum:						
Maximum:	1.5	5.0				
Mass	Calc. Mass	PPM	DBE	Score	Formula	
356.1628	356.1624	0.4	10.0	1	C21 H24 O5	
	356.1637	-0.9	15.0	2	C22 H20 N4 O	



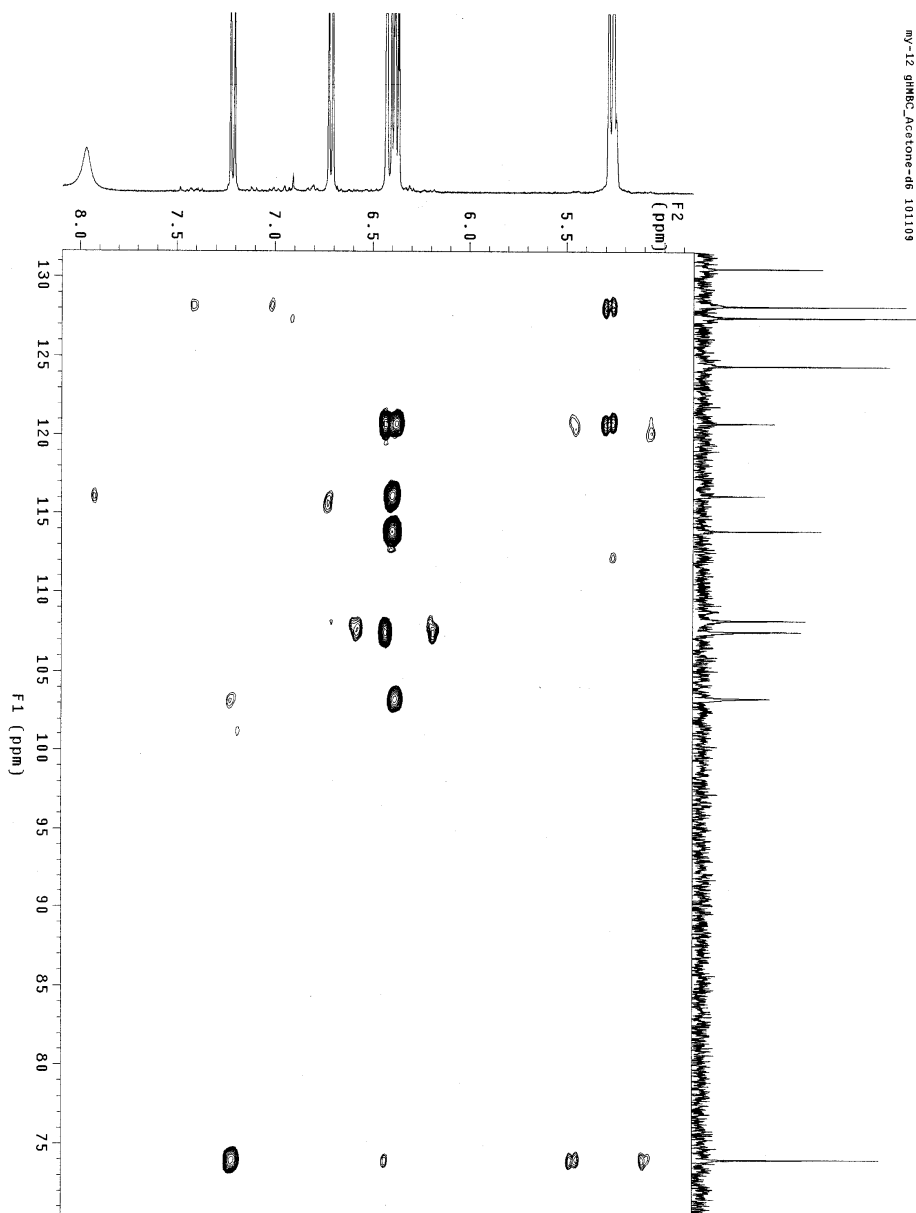
S 6.2 HMBC Spectrum of **6**



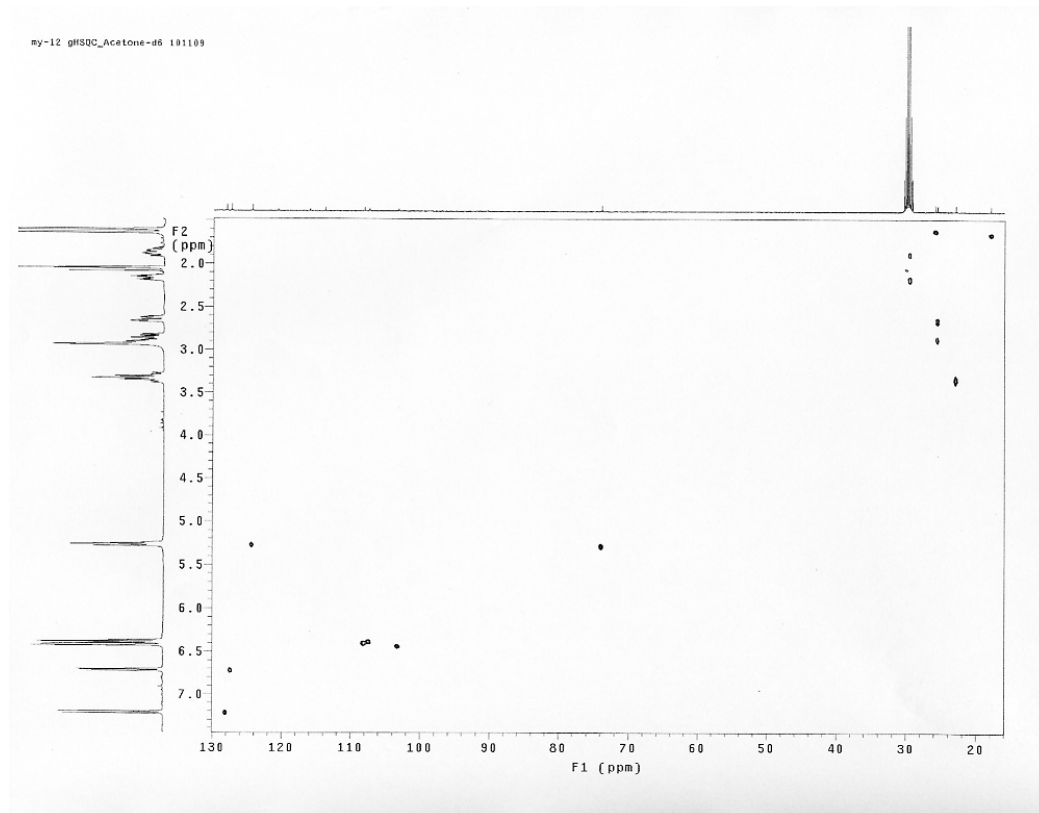
S 6.2.1 The magnified HMBC Spectrum of 6



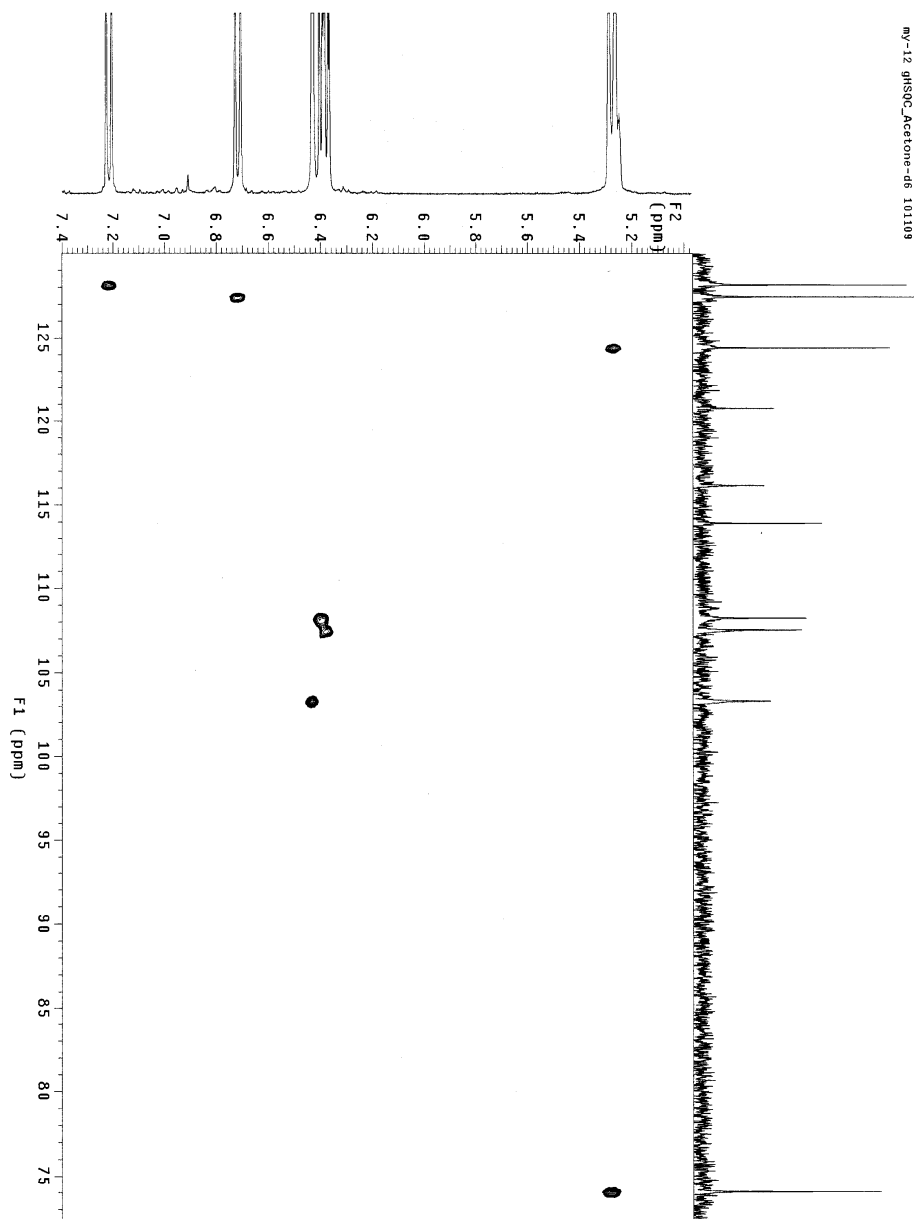
S 6.2.2 The magnified HMBC Spectrum of 6



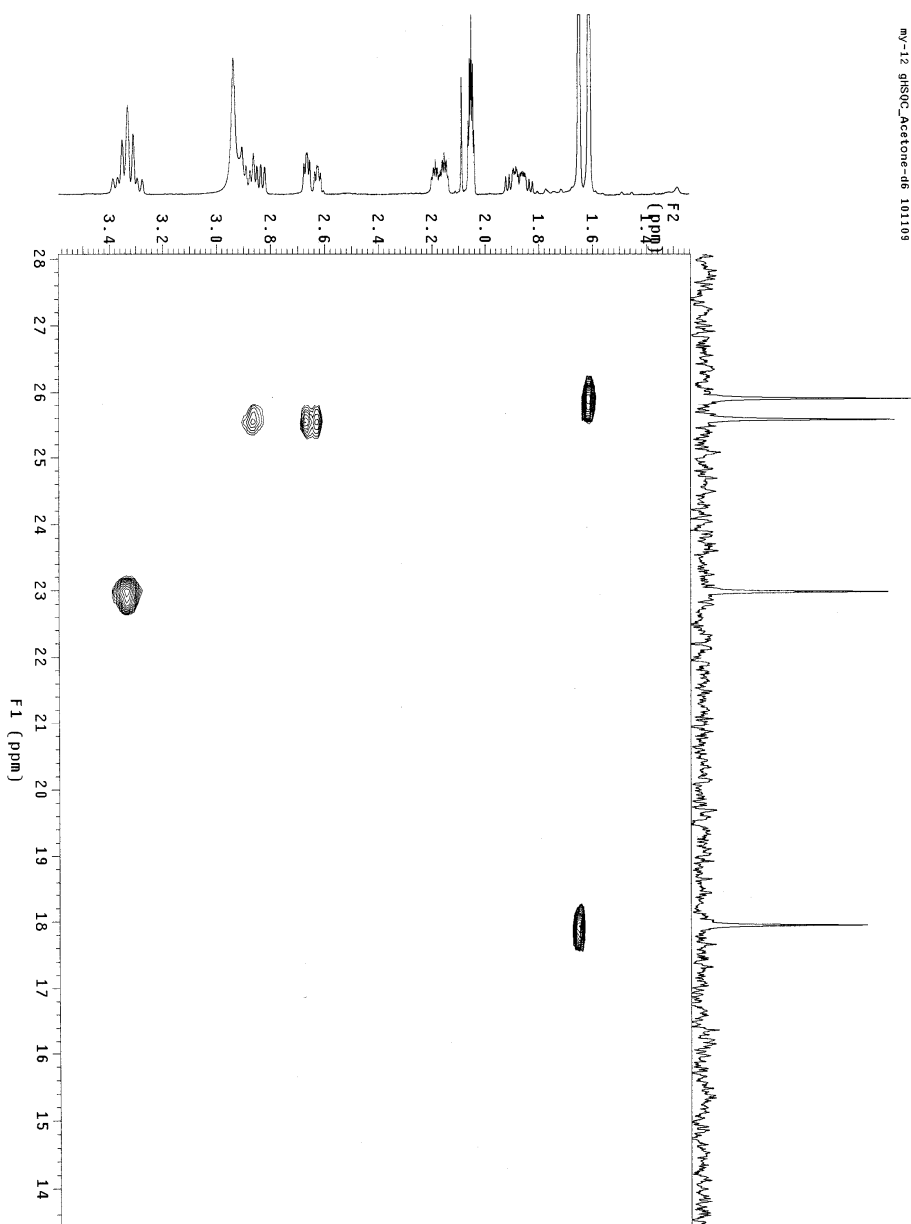
### S 6.3 HSQC Spectrum of **6**



### S 6.3.1 The magnified HSQC Spectrum of 6



### S 6.3.2 The magnified HSQC Spectrum of 6



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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-T1011-OS0606

Sample Serial Number: My-12

Operator: Li

Date: 2010/11/25

Elemental Composition Report

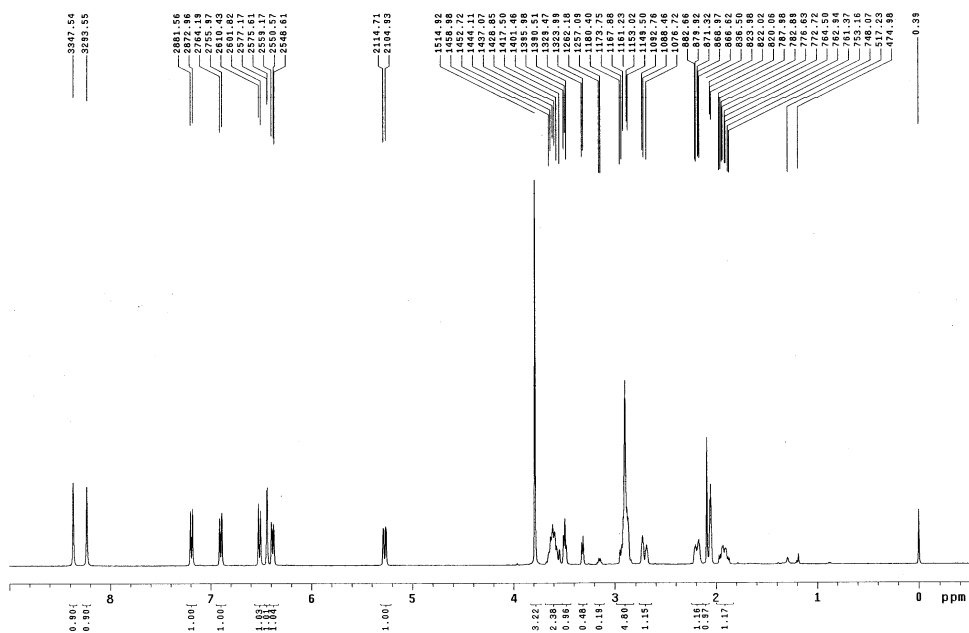
Single Mass Analysis  
 Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
 173 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

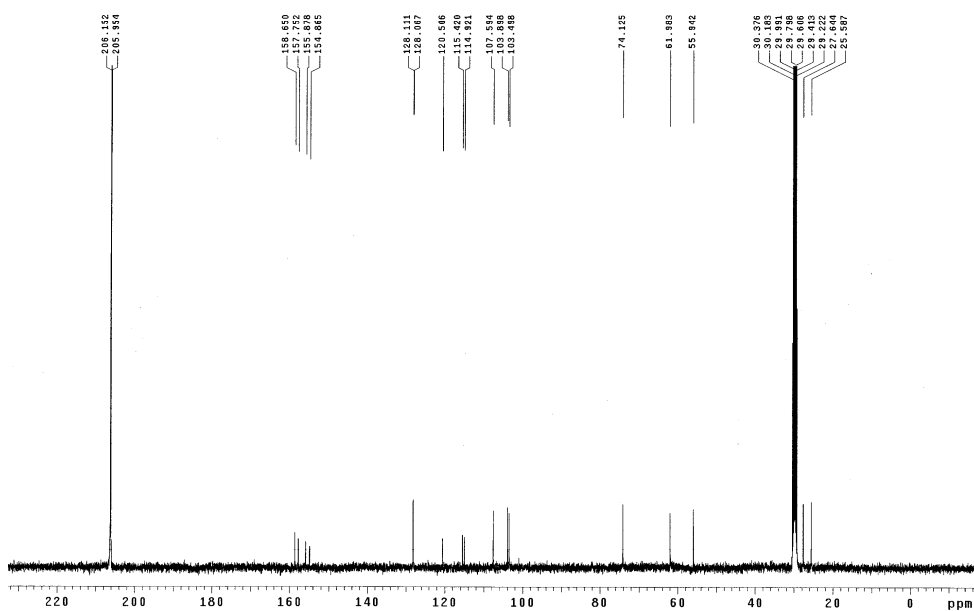
Minimum:	1.5	5.0	-1.5
Maximum:	326.1518	326.1531	50.0
Mass	Calc. Mass	mDa	DBE
326.1522	326.1518	0.4	10.0
	326.1531	-0.9	15.0
		PPM	Score
		1.2	1
		-2.9	2
			Formula
			C20 H22 O4
			C21 H18 N4

# S 7.1 <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of 7

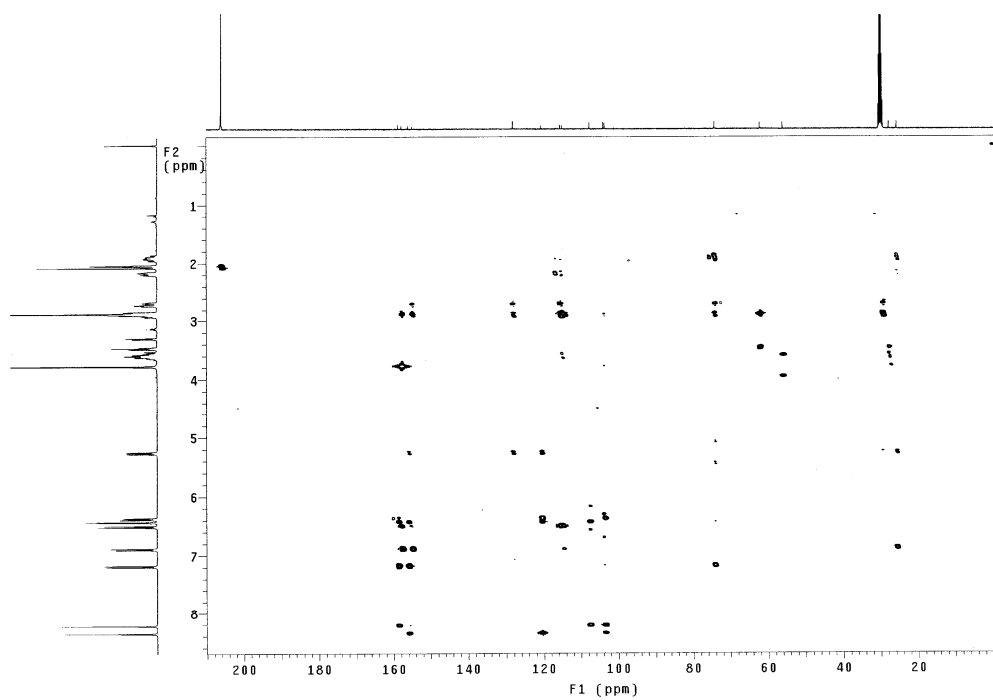
my-31 Acetone-d6 101103



my-42 Acetone-d6 101110

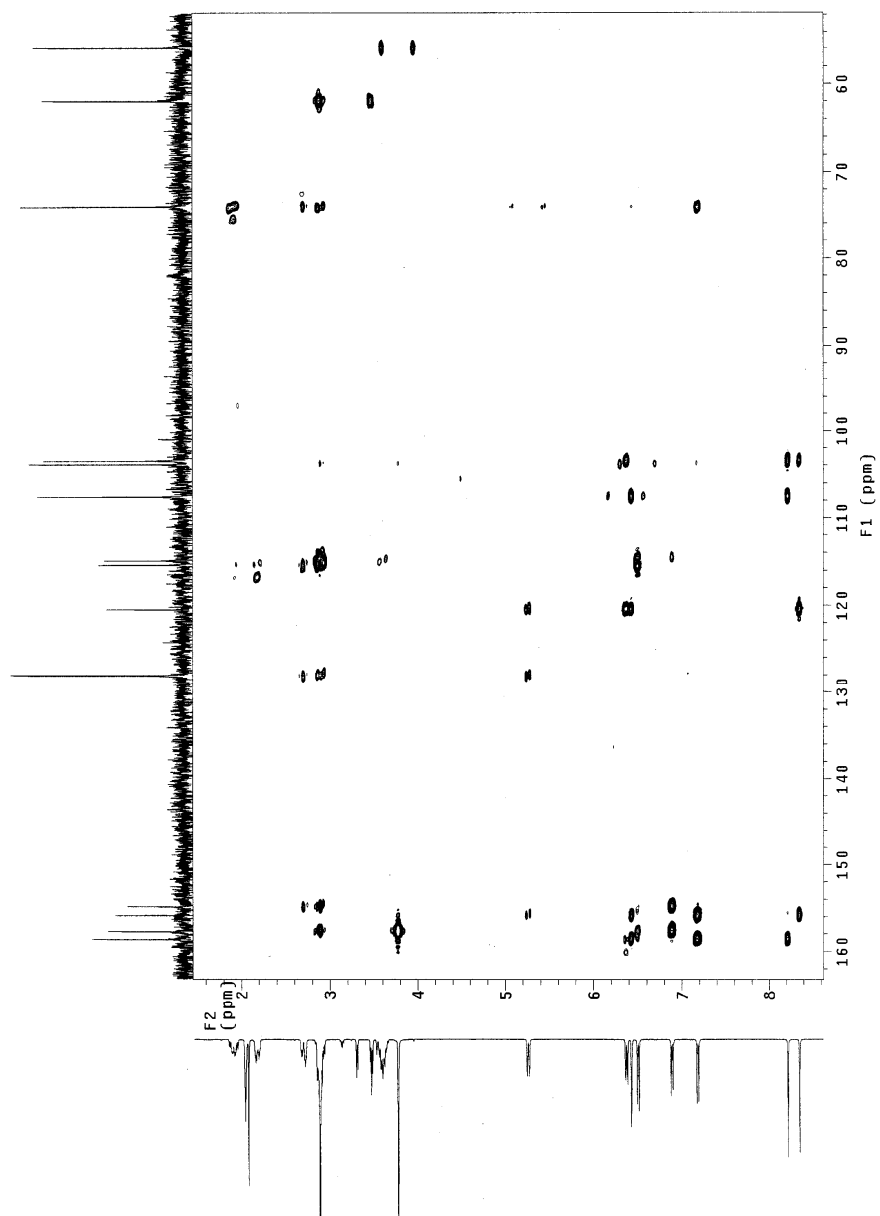


S 7.2 HMBC Spectrum of 7

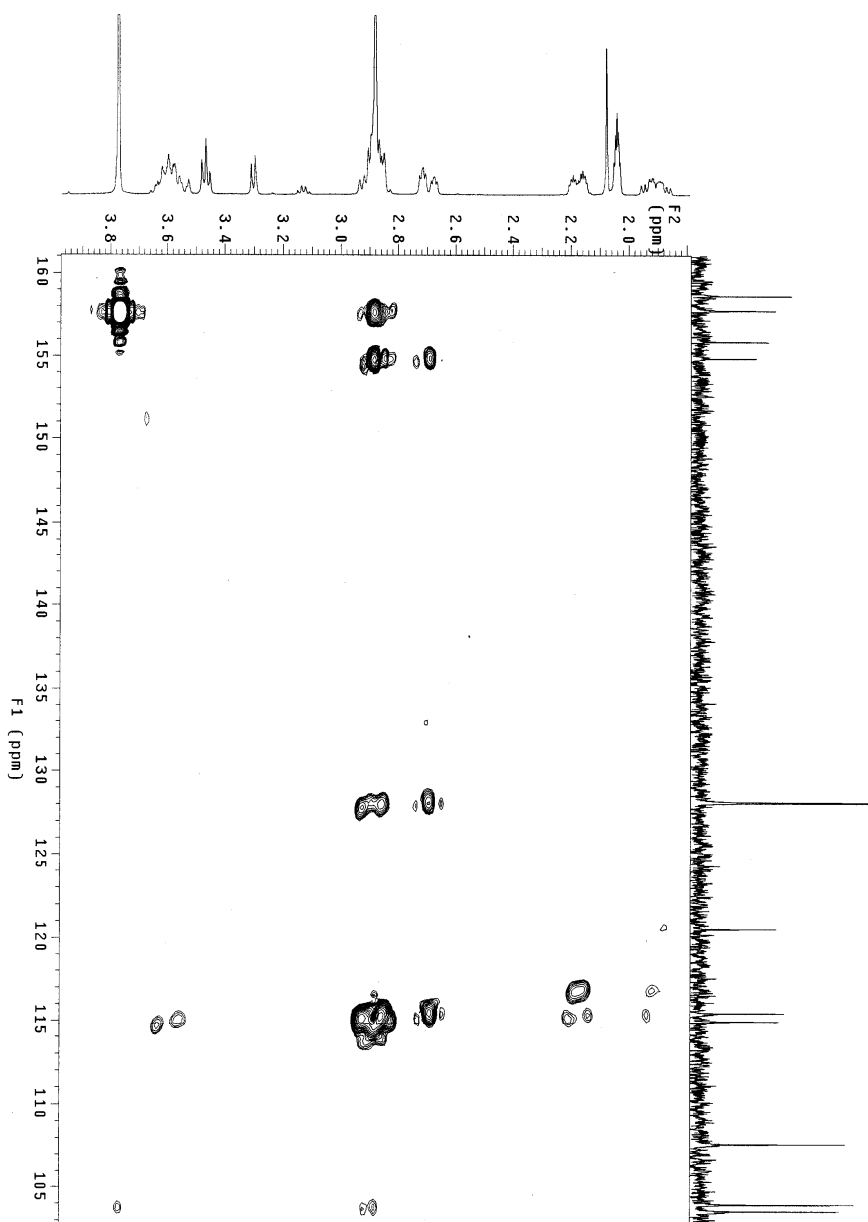


S 7.2.1 The magnified HMBC Spectrum of 7

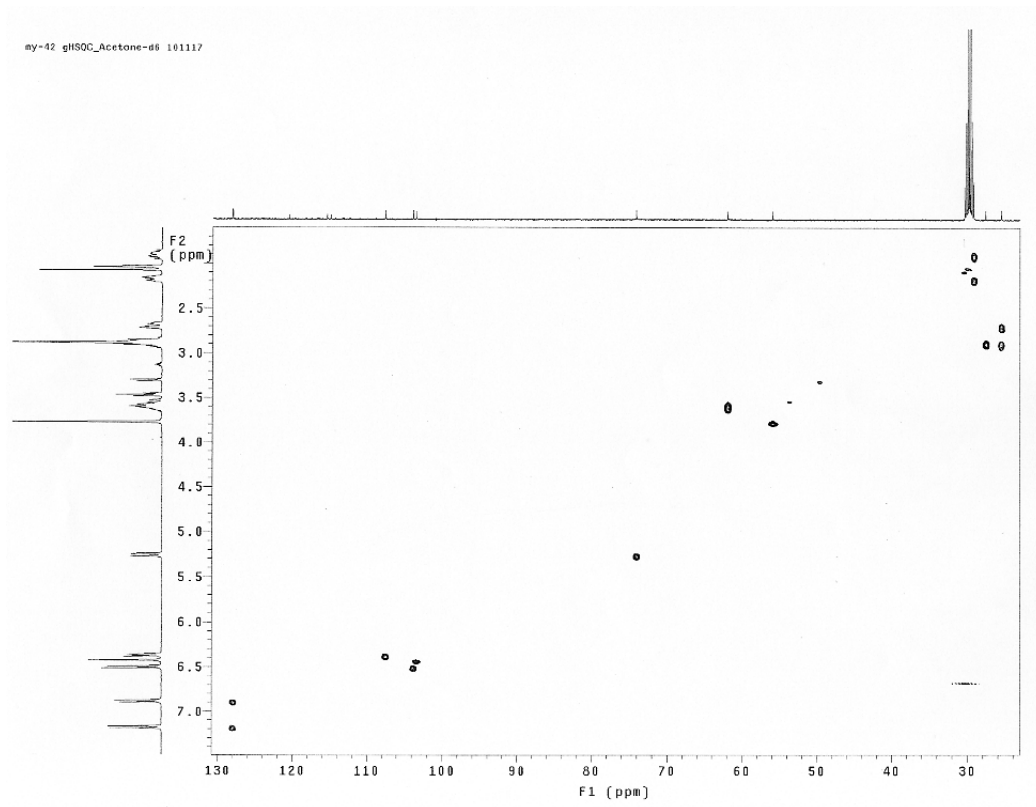
my-42 gHMBC\_Acetone-d6 10117



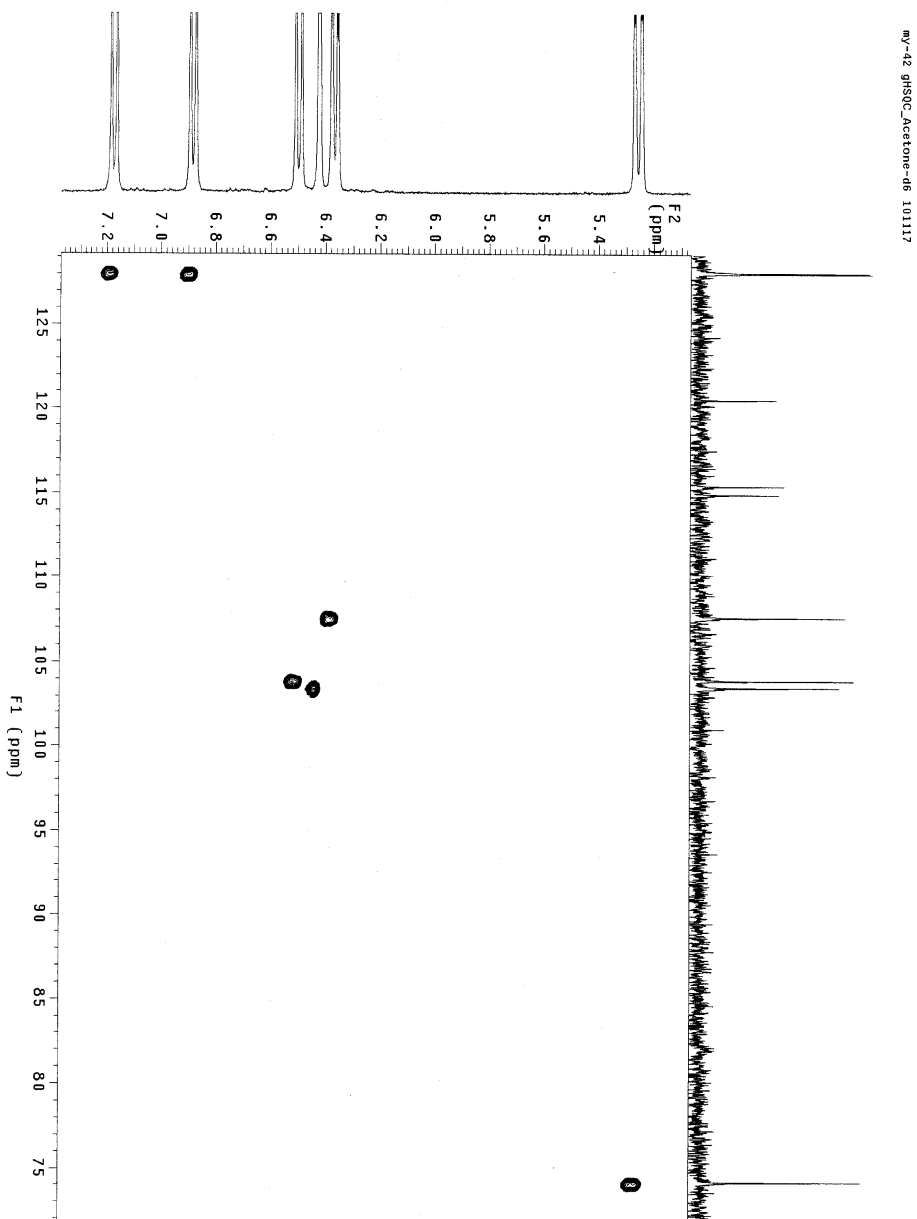
S 7.2.2 The magnified HMBC Spectrum of 7



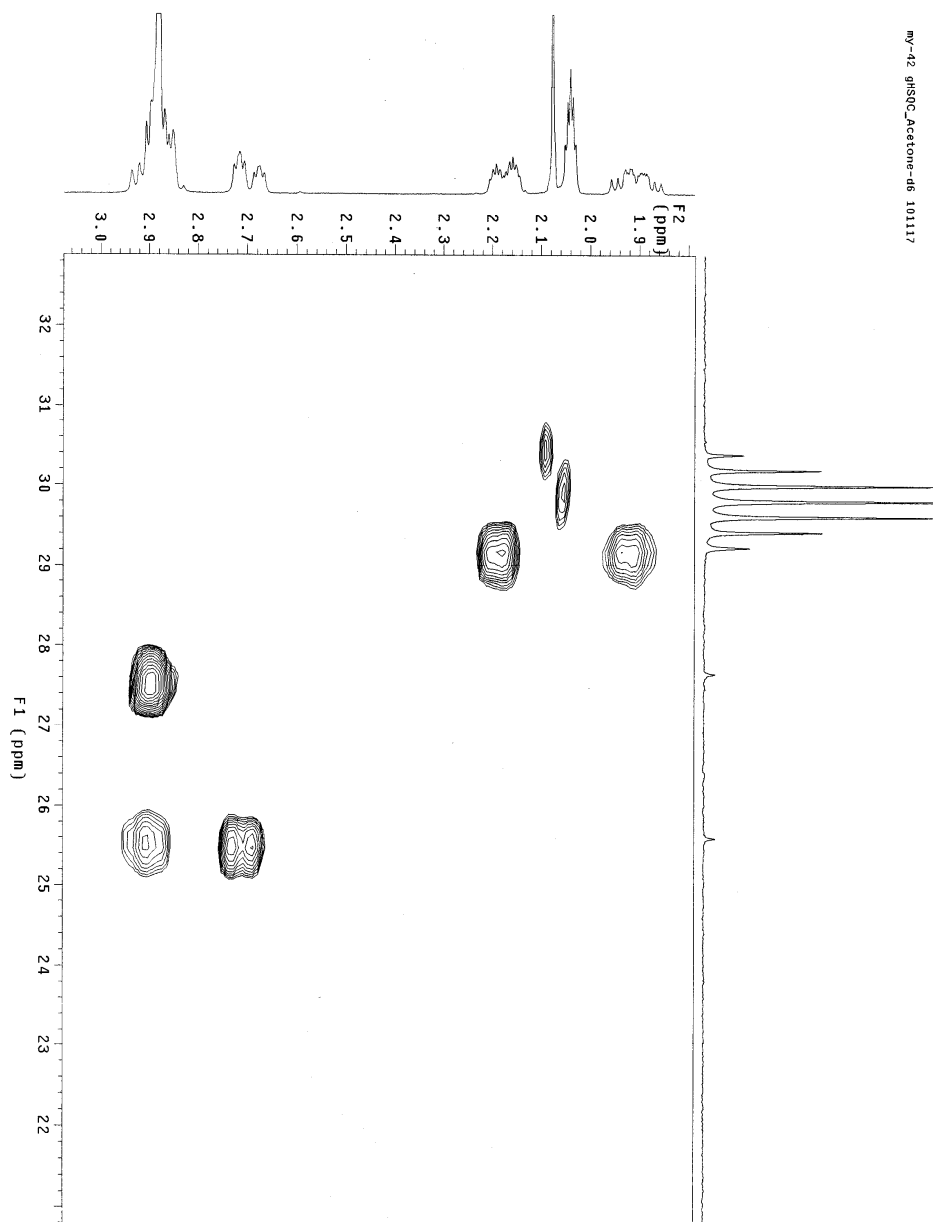
### S 7.3 HSQC Spectrum of 7



S 7.3.1 The magnified HSQC Spectrum of 7



S 7.3.2 The magnified HSQC Spectrum of 7



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-T1011-OS0612

Sample Serial Number: My-42

Operator: Li

Date: 2010/11/26

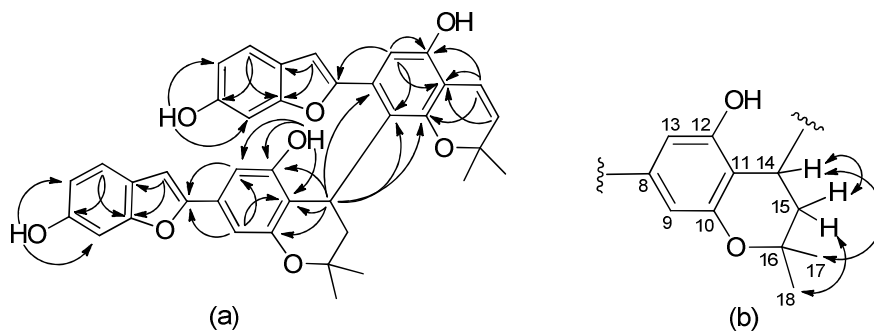
Elemental Composition Report

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  
 196 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

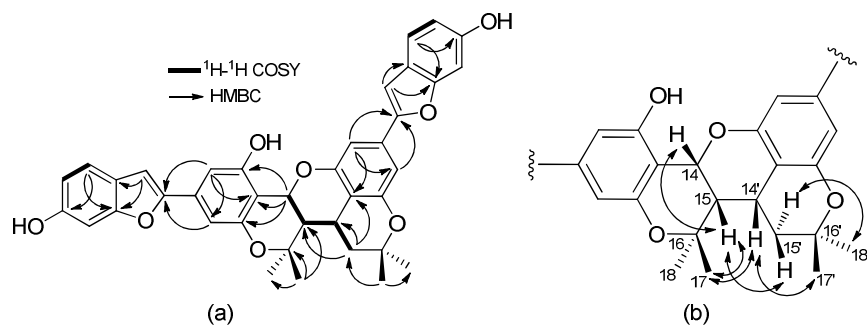
Minimum:							
Maximum:	1.5	5.0	-1.5	50.0			
Mass	Calc. Mass	PPM	DBE	Score	Formula		
316.1308	316.1311	-0.3	9.0	2	C18 H20 O5		
	316.1297	1.1	9.5	1	C16 H18 N3 O4		

**S 8.1 Figure 1.** Key HMBC and ROESY correlations of **1**.



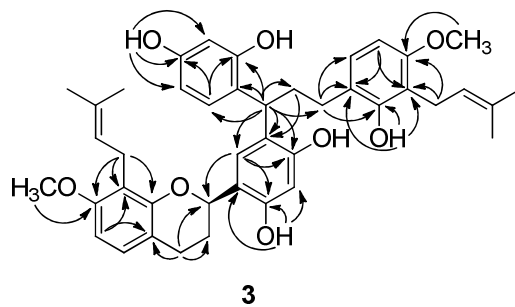
(a) Key HMBC correlations of **1**. (b) Key ROESY correlations of **1**

S 8.2 Figure 2. Key HMBC,  $^1\text{H}$ - $^1\text{H}$  COSY, and ROESY correlations of **2**



(a) Key HMBC and  $^1\text{H}$ - $^1\text{H}$  COSY correlations of **2**. (b) Key ROESY correlations of **2**.

**S 8.3 Figure 3.** Key HMBC correlations of **3**.



S 8.4 Figure 4. Key HMBC correlations of **5**.

