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

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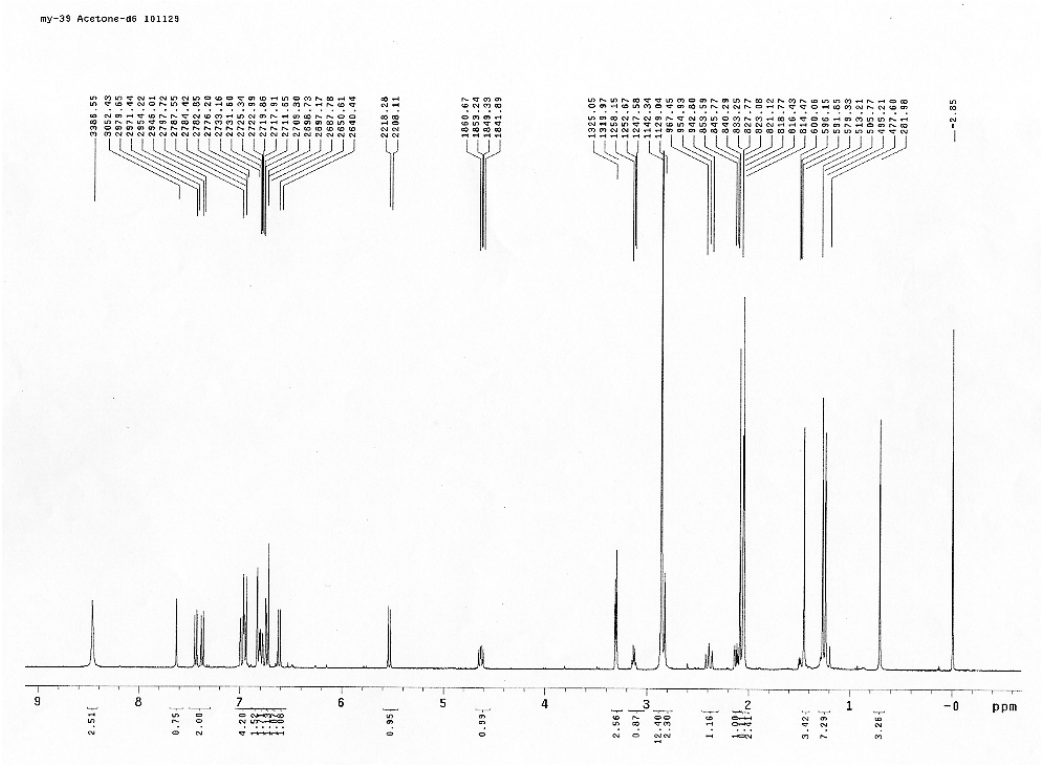
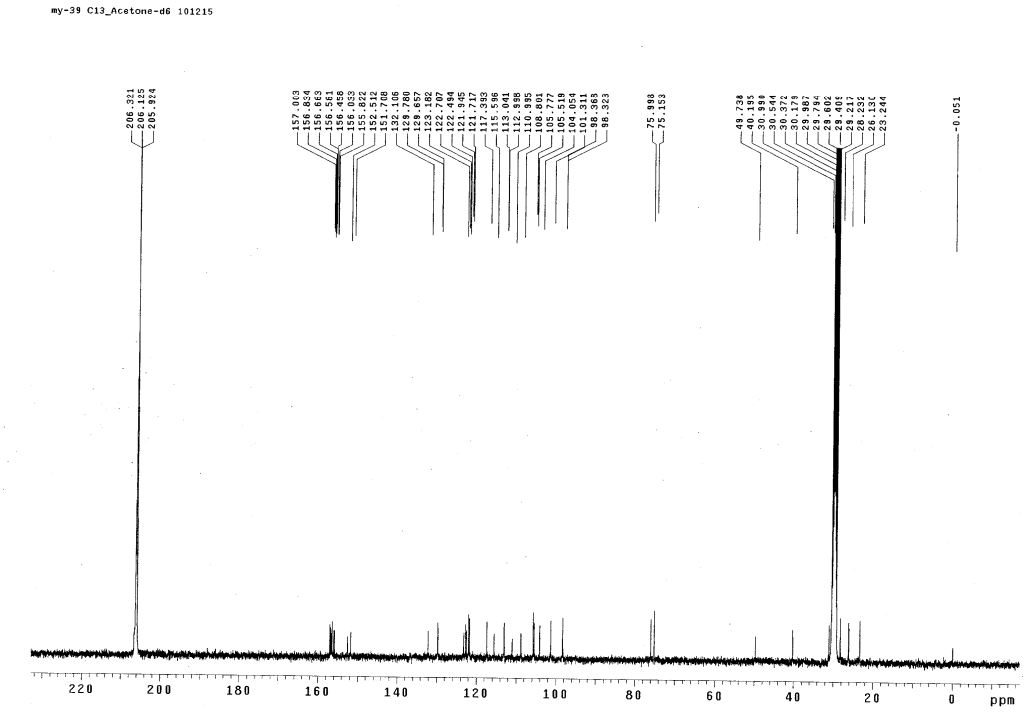
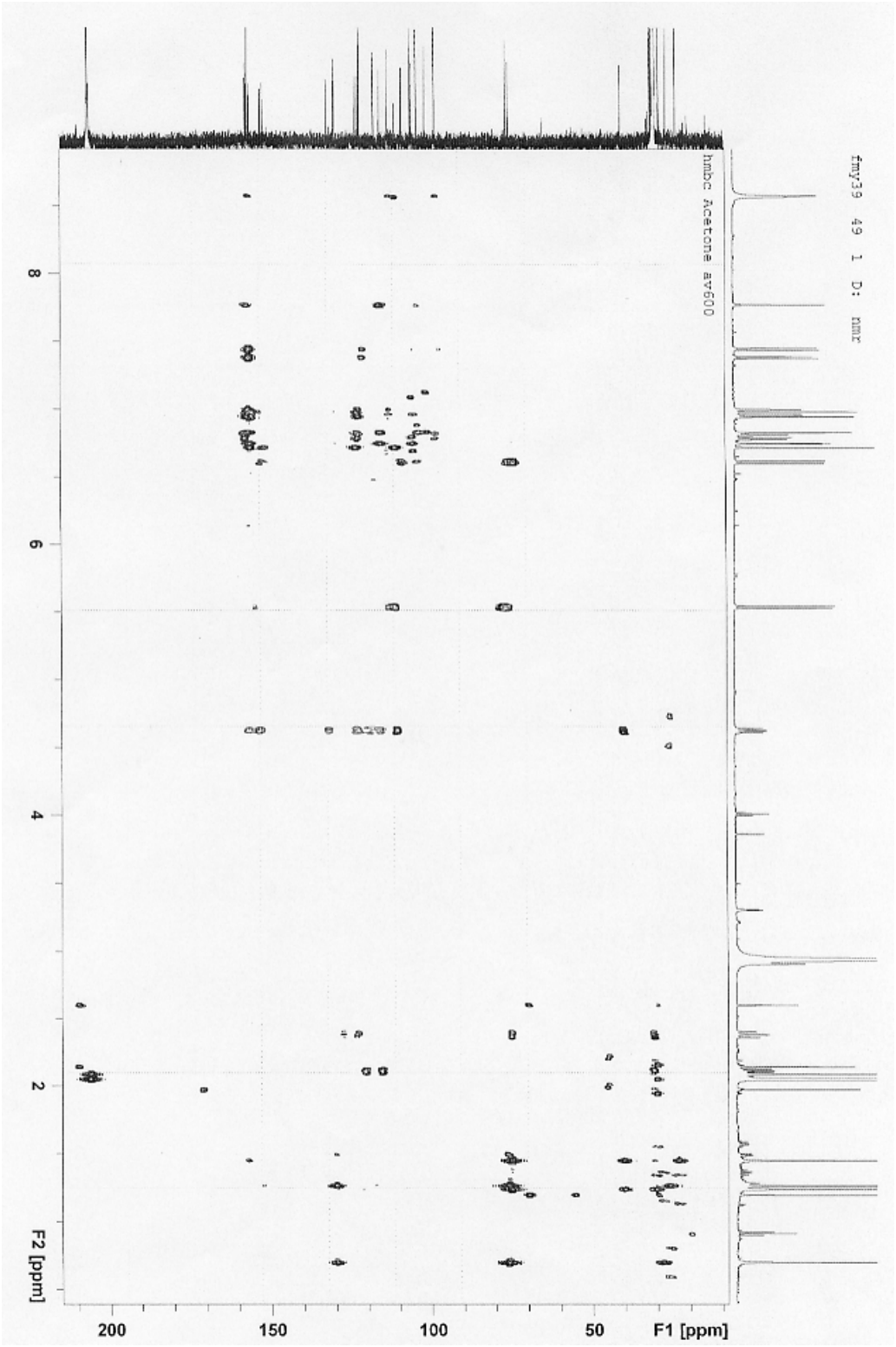
The list of supporting information

S 1.1 ^{1}H NMR and ^{13}C NMR Spectra of **1**

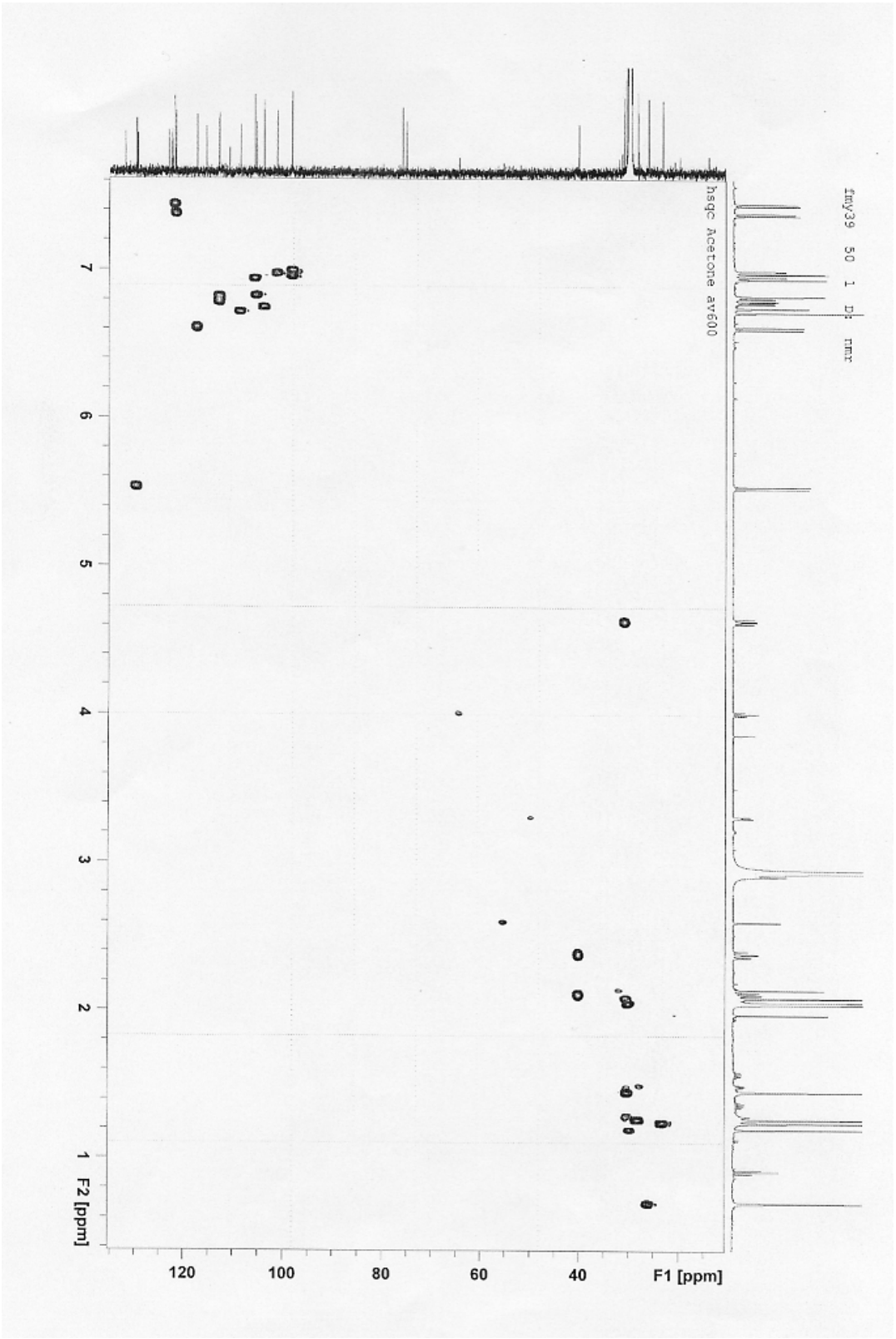




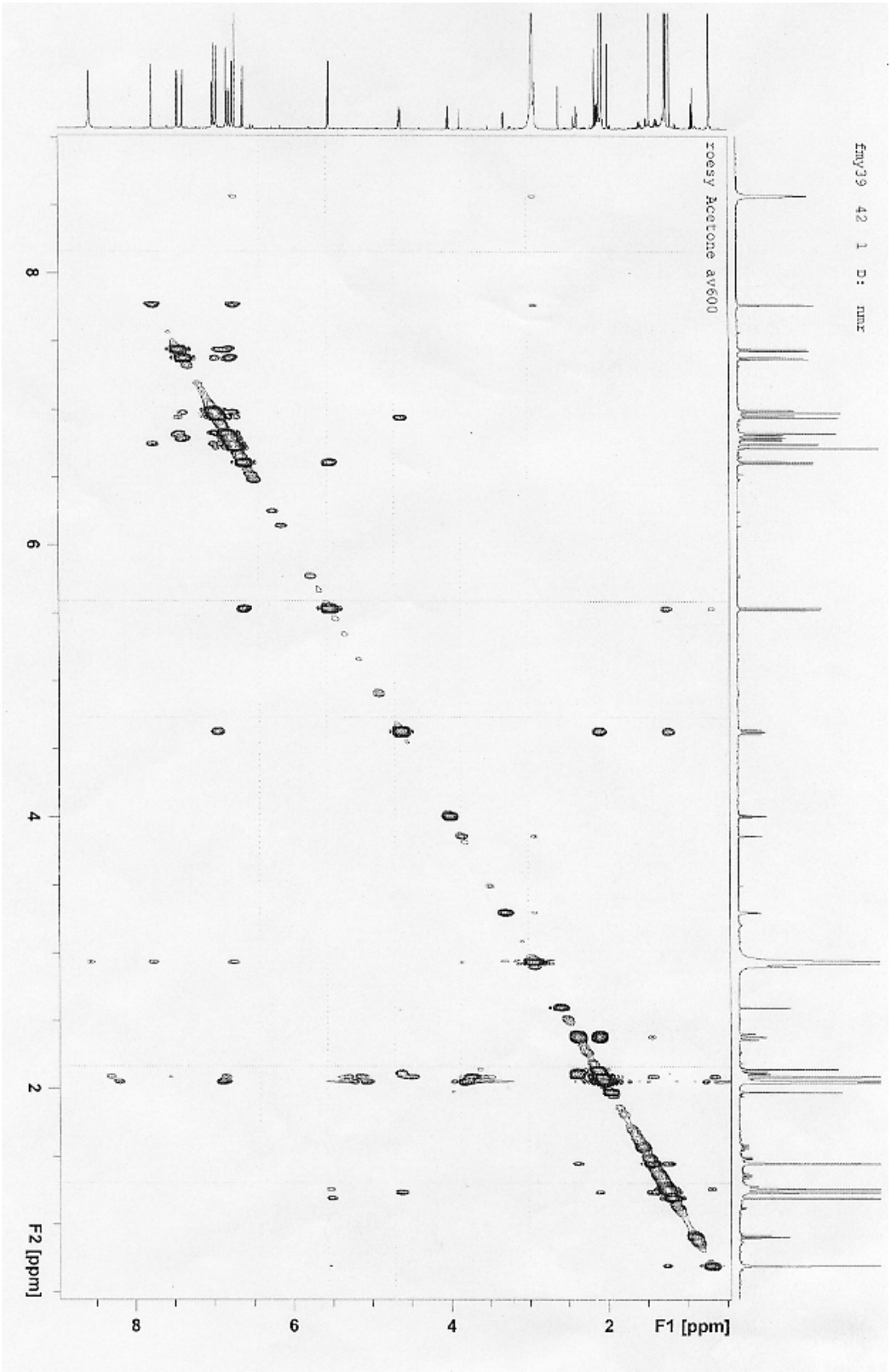
S 1.2 HMBC Spectrum of **1**



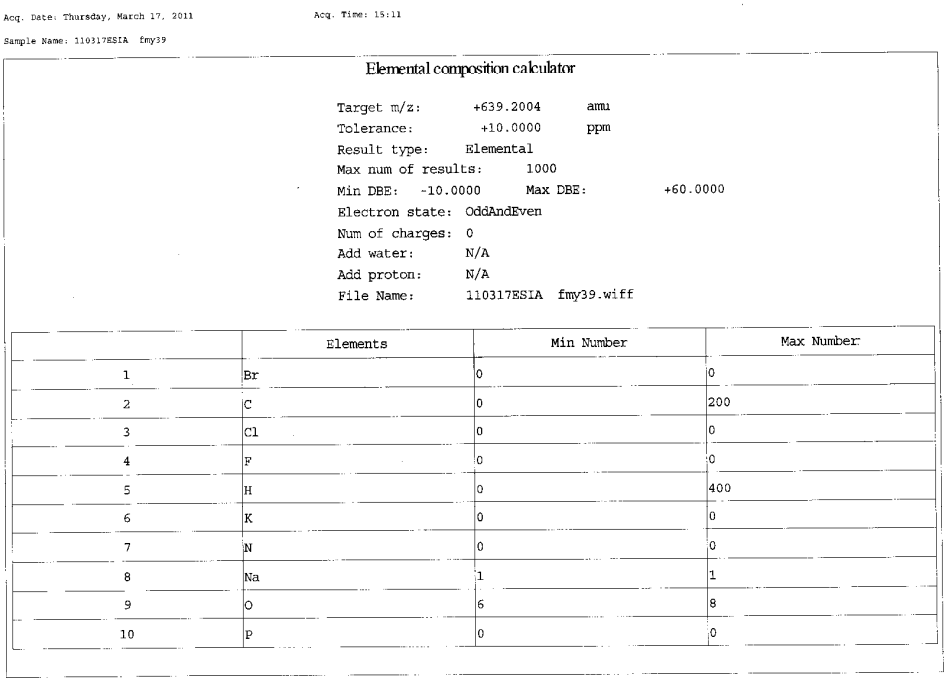
S 1.3 HSQC Spectrum of **1**



S 1.4 ROESY Spectrum of **1**



S 1.5 HRESIMS Spectrum of **1**



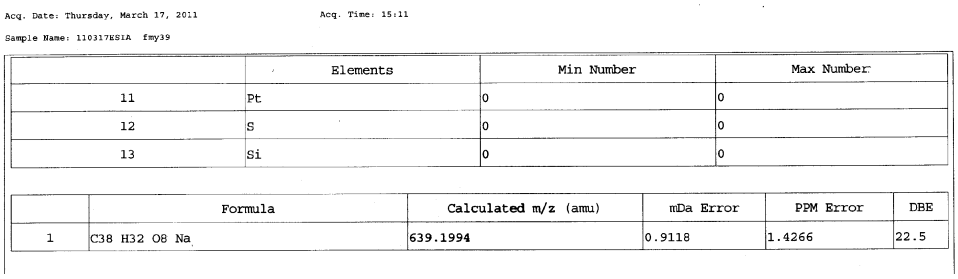
Acq. Date: Thursday, March 17, 2011 Acq. Time: 15:11

Sample Name: 110317ESIA fmy39

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



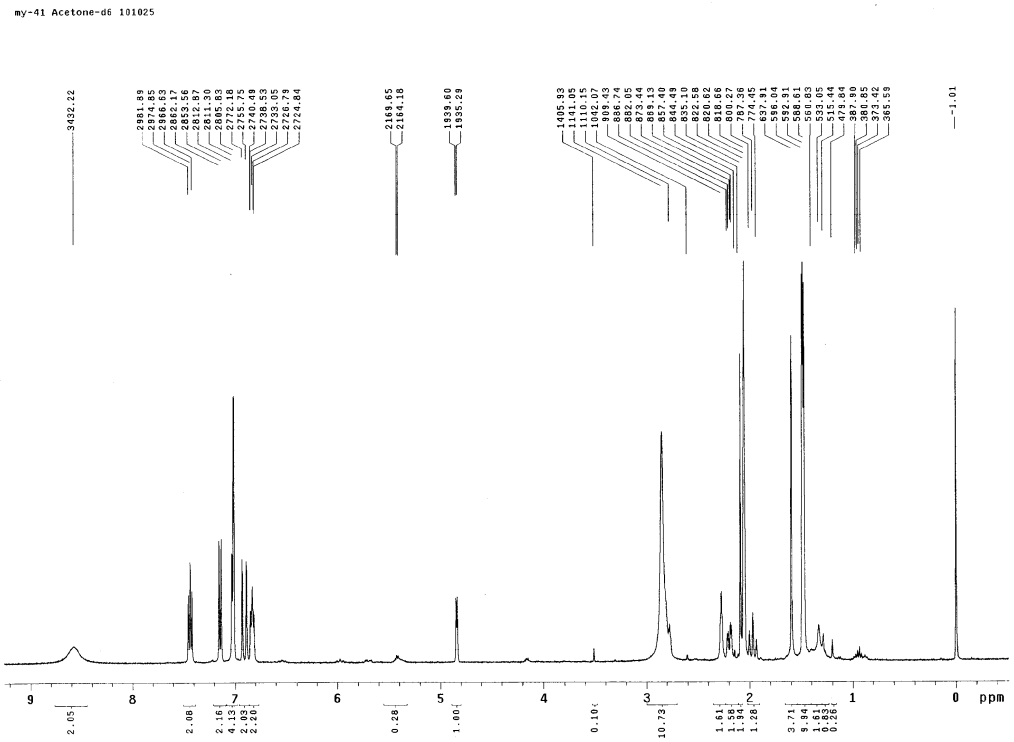
Acq. Date: Thursday, March 17, 2011 Acq. Time: 15:11

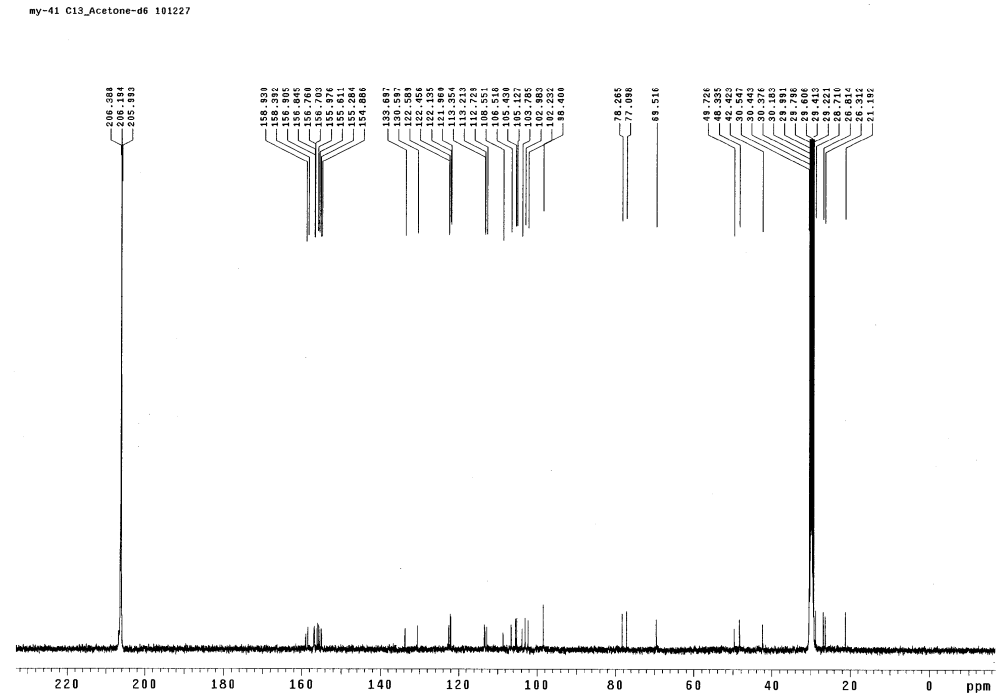
Sample Name: 110317ESIA fmy39

	Elements	Min Number	Max Number
11	Pt	0	0
12	S	0	0
13	Si	0	0

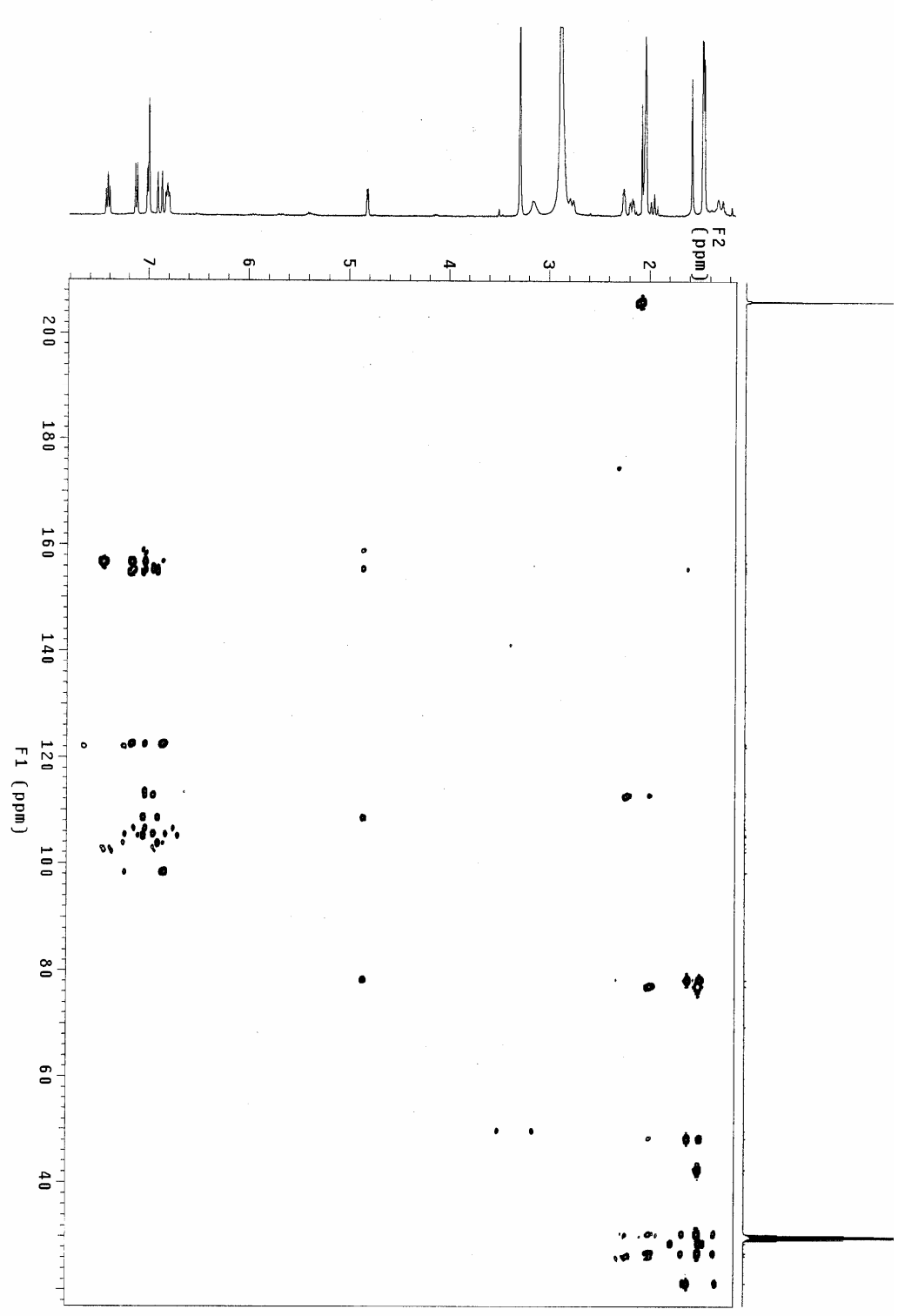
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C38 H32 O8 Na	639.1994	0.9118	1.4266	22.5

S 2.1 ^{1}H NMR and ^{13}C NMR Spectra of **2**

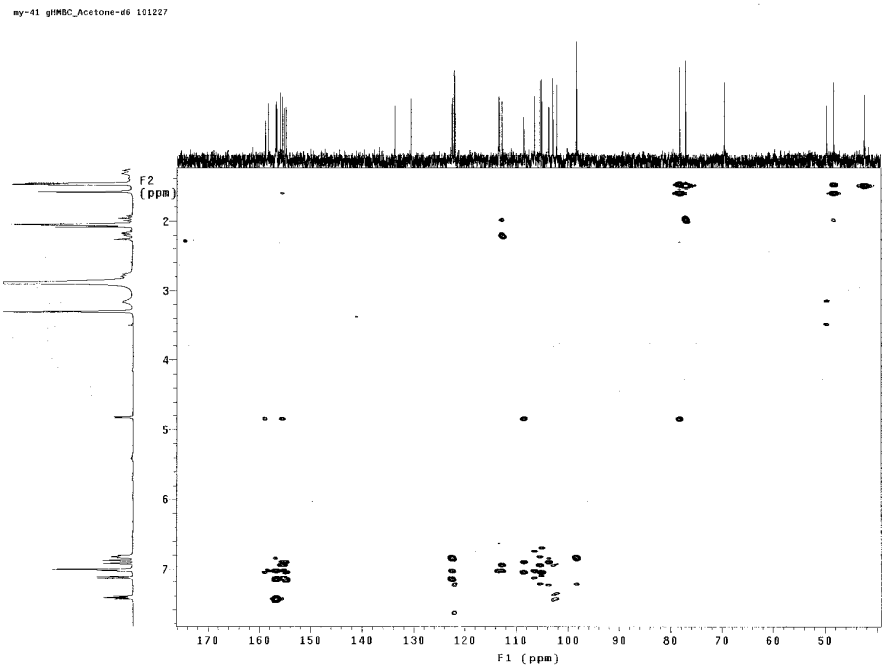




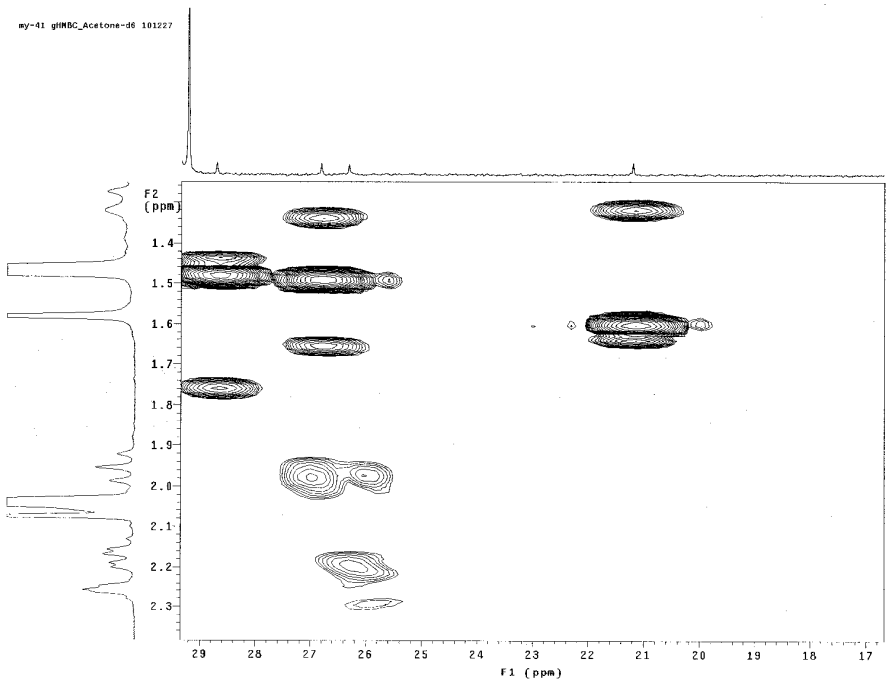
S 2.2 HMBC Spectrum of **2**



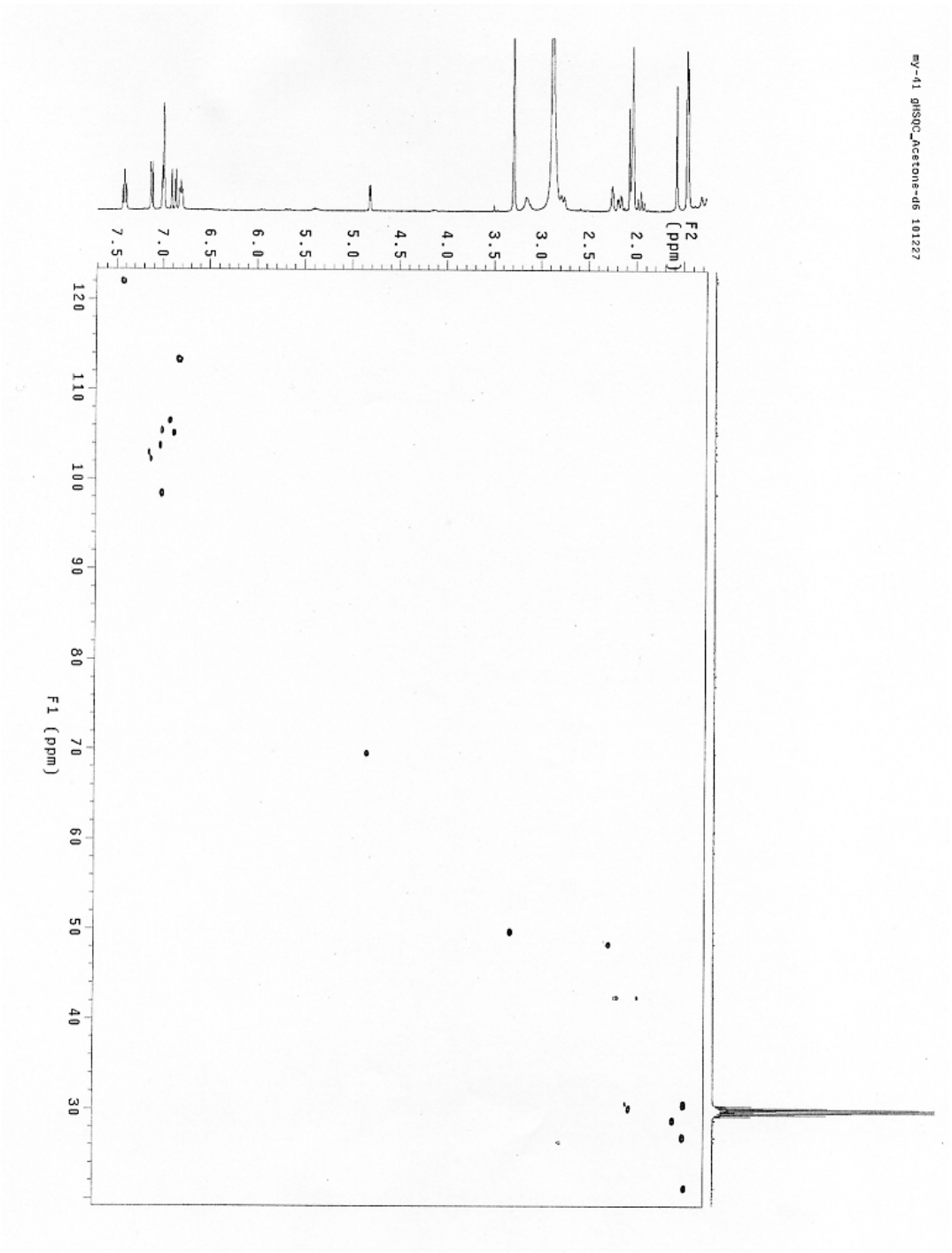
S 2.2.1 The magnified HMBC Spectrum of **2**



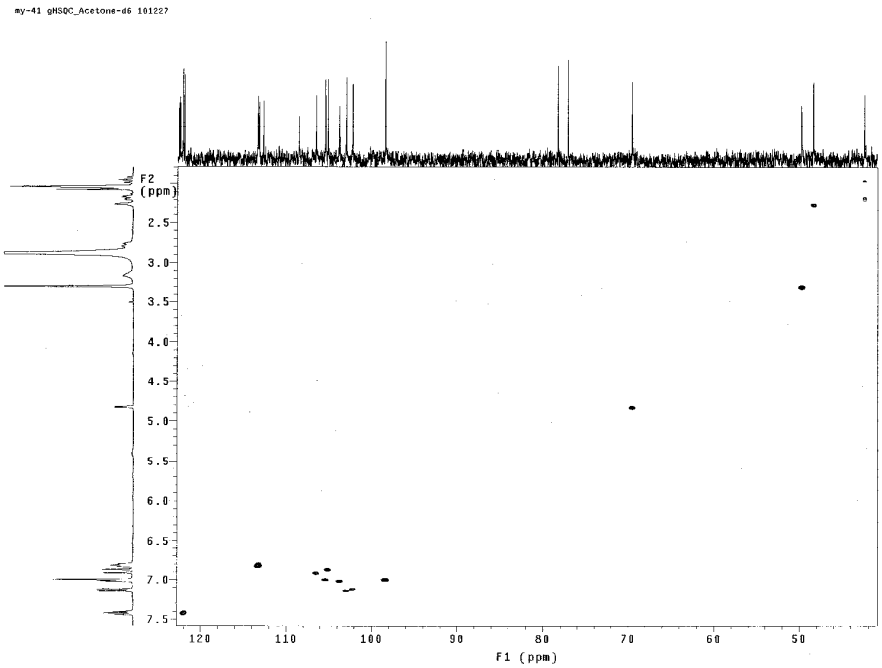
S 2.2.2 The magnified HMBC Spectrum of **2**



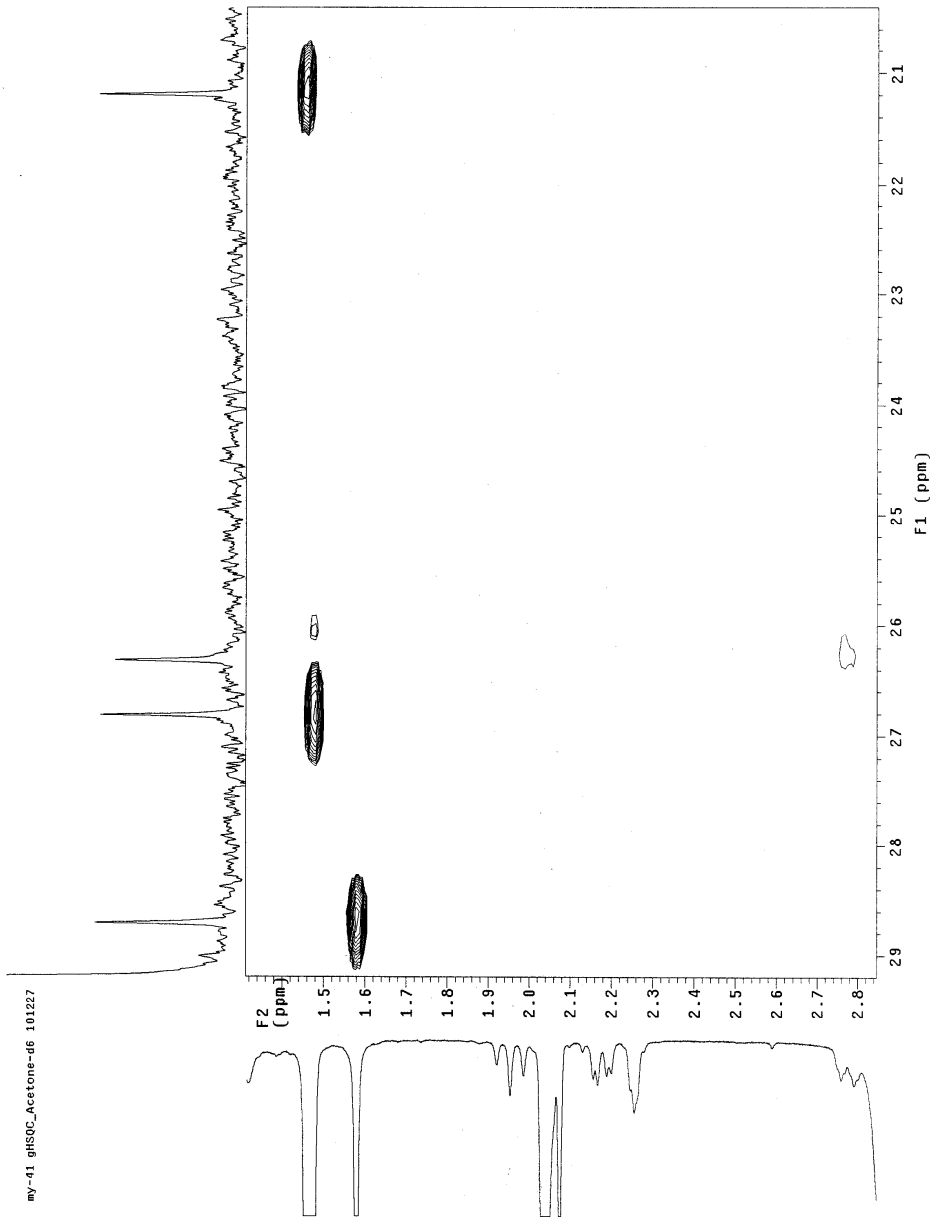
S 2.3 HSQC Spectrum of **2**



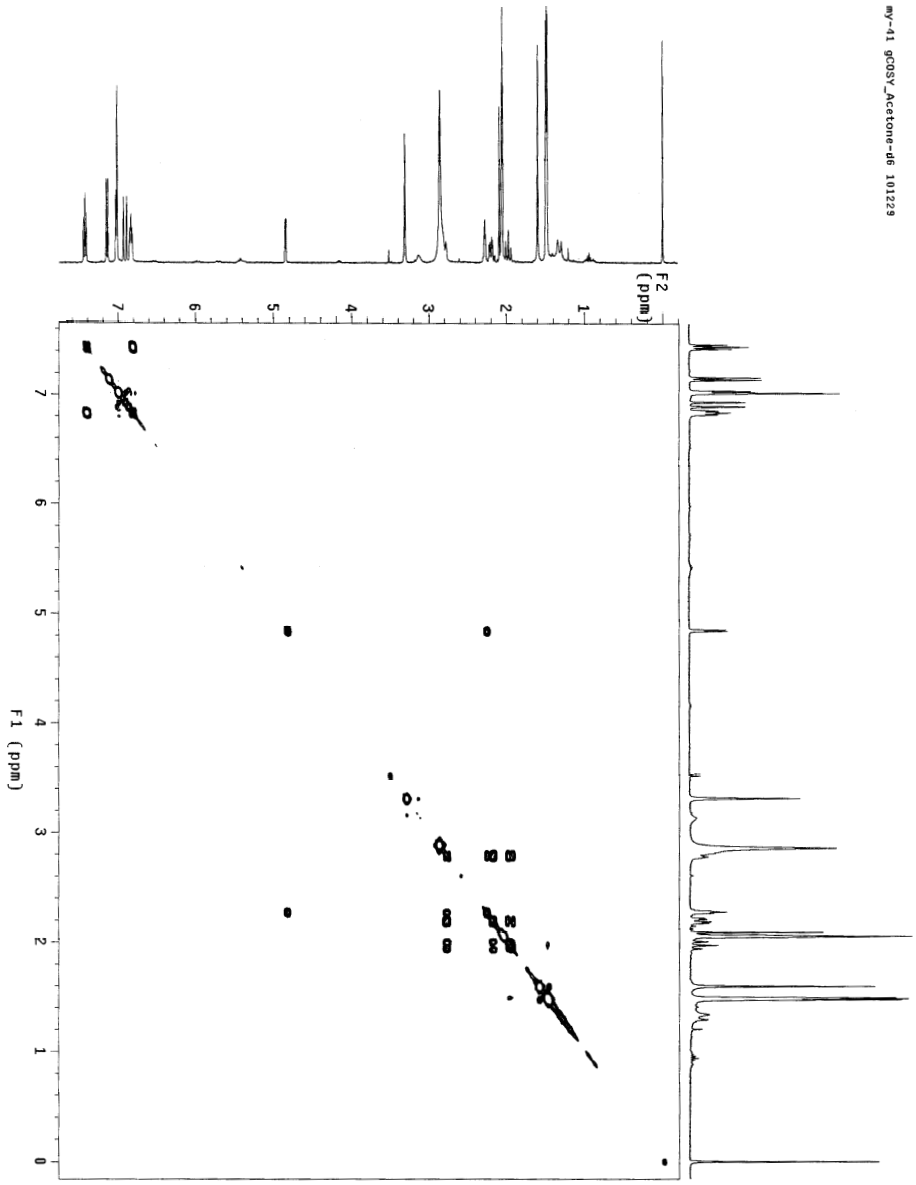
S 2.3.1 The Magnified HSQC Spectrum of **2**



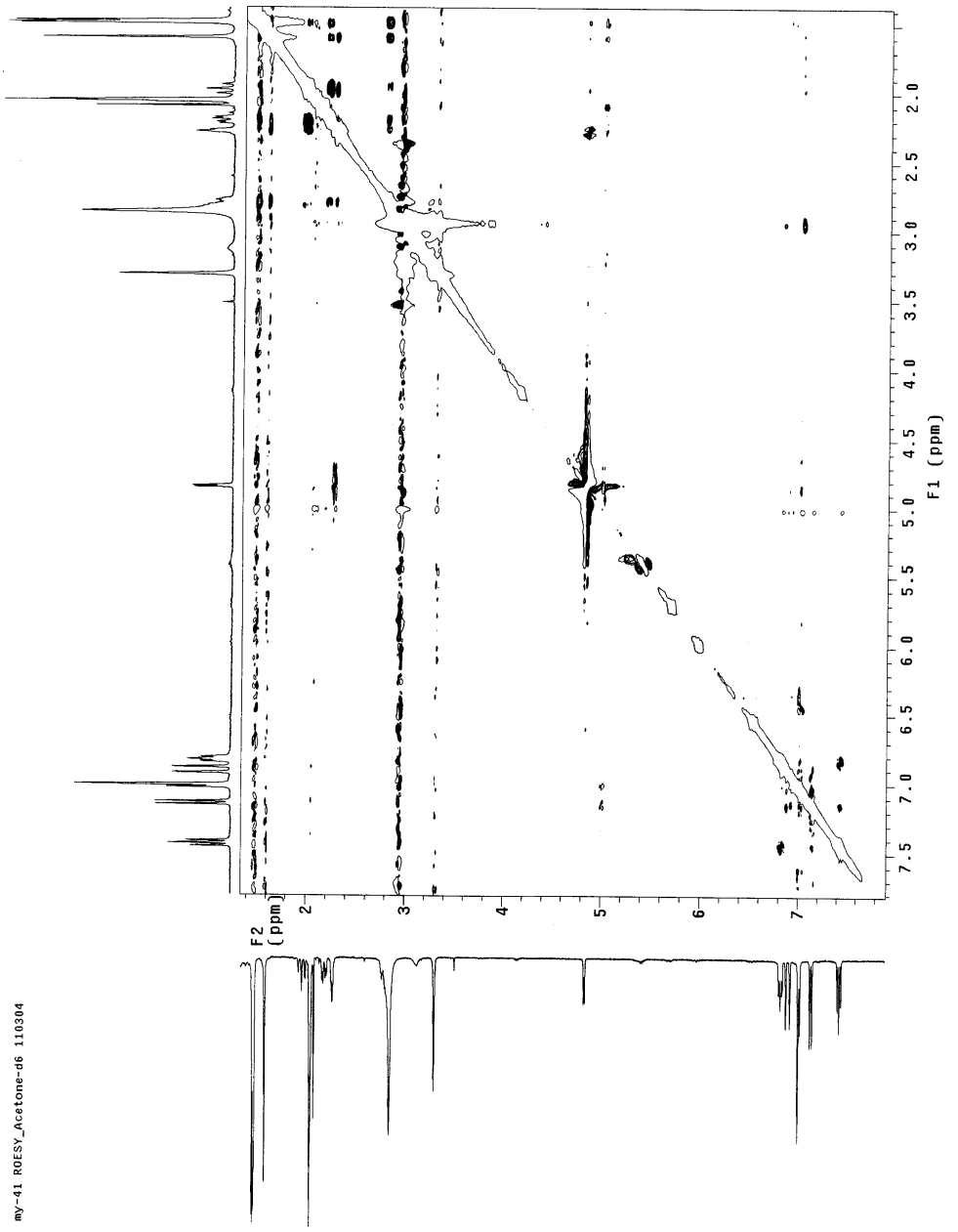
S 2.3.1 The Magnified HSQC Spectrum of **2**



S 2.4 ^{1}H-^{1}HCOSY Spectrum of **2**



S 2.5 ROESY Spectrum of **2**



S 2.6 HRESIMS Spectrum of **2**

Shanghai Mass Spectrometry Center

Shanghai Institute of Organic Chemistry

Chinese Academy of Sciences

High Resolution MS Data Report

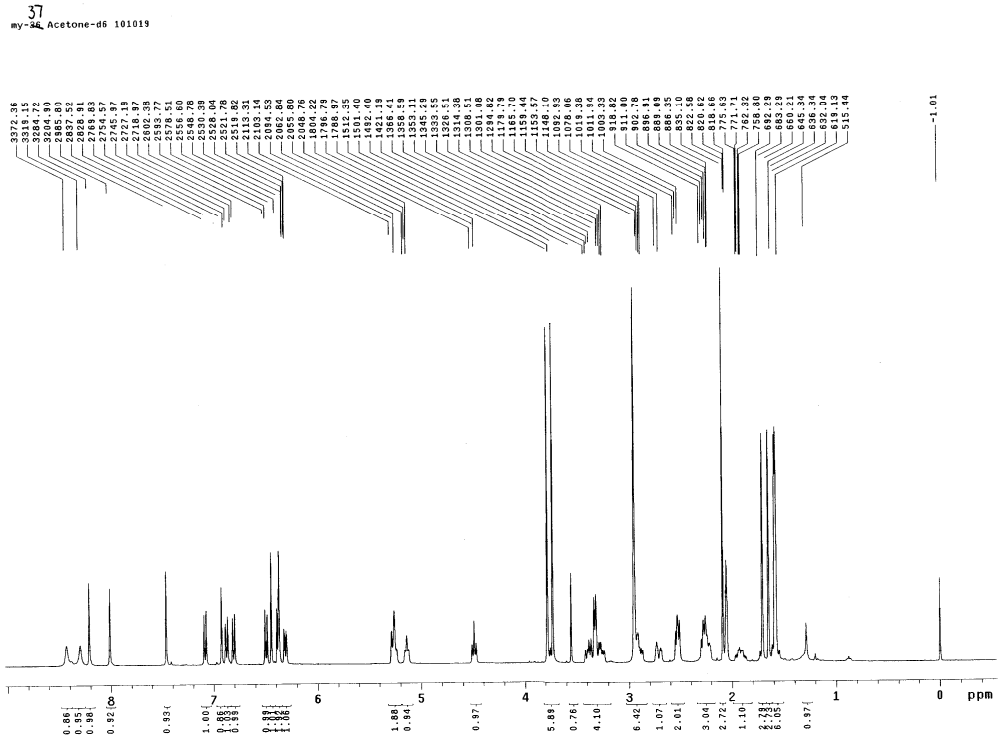
Instrument

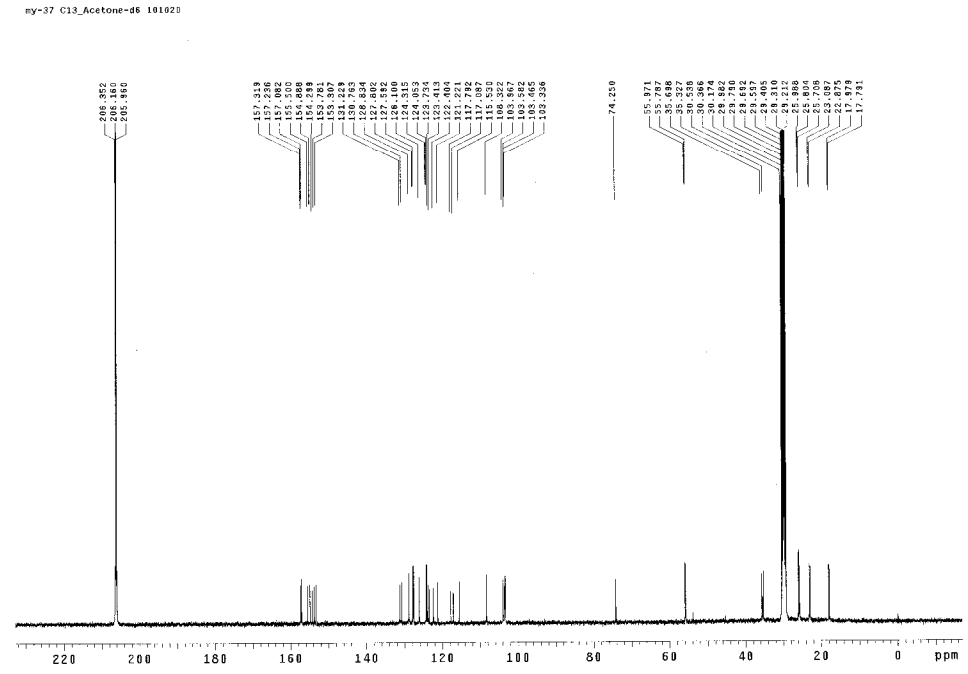
Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	F110055
Analysis Name	D:\Data\zfj2011\20110321neg_000004.d
Sample Name	A3
Acquisition Date	3/21/2011 10:45:41 AM
Operator:	zfj
Ion Mass (Measured)	615.20503

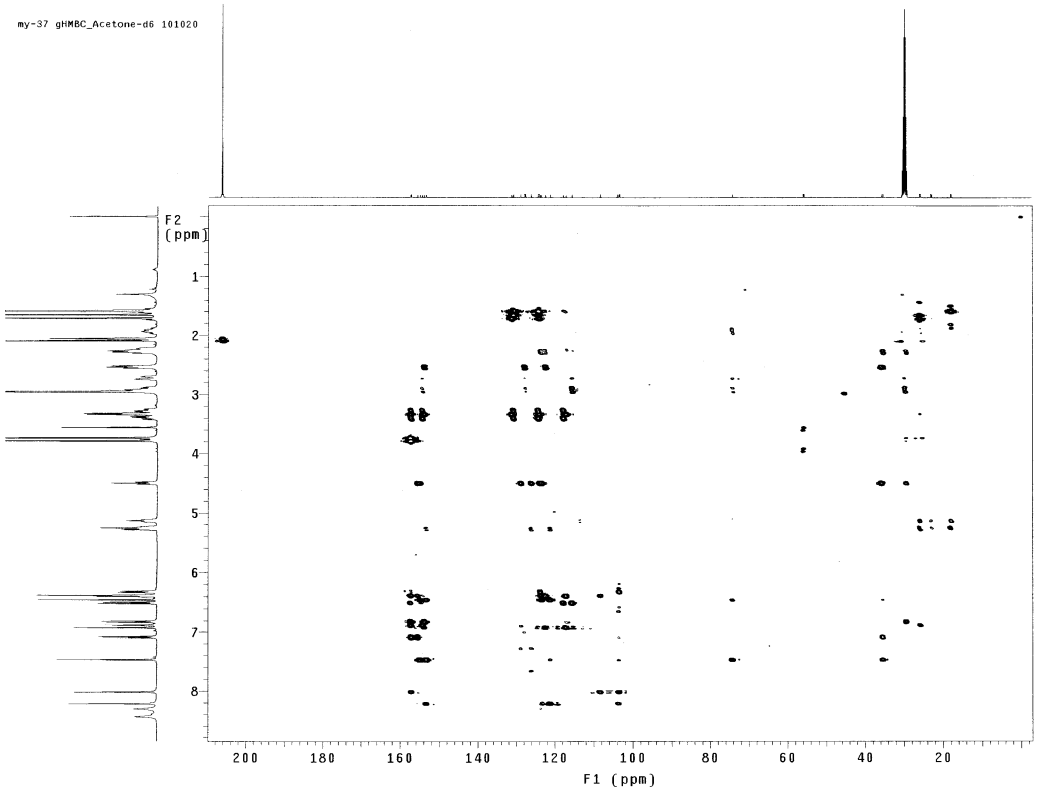
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e^-
C 38 H 31 O 8	0.008	615.20244	-4.21	-4.53	-2.59	23.50	ok	even
C 41 H 29 N 1 O 5	0.018	615.20512	0.15	-0.20	0.09	28.00	ok	odd

S 3.1 ^{1}H NMR and ^{13}C NMR Spectra of **3**

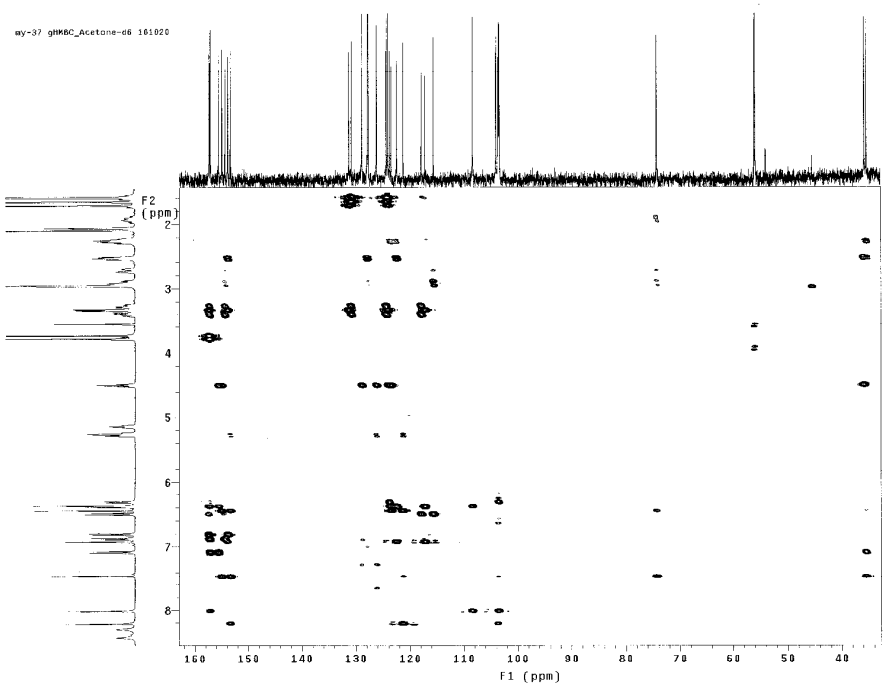




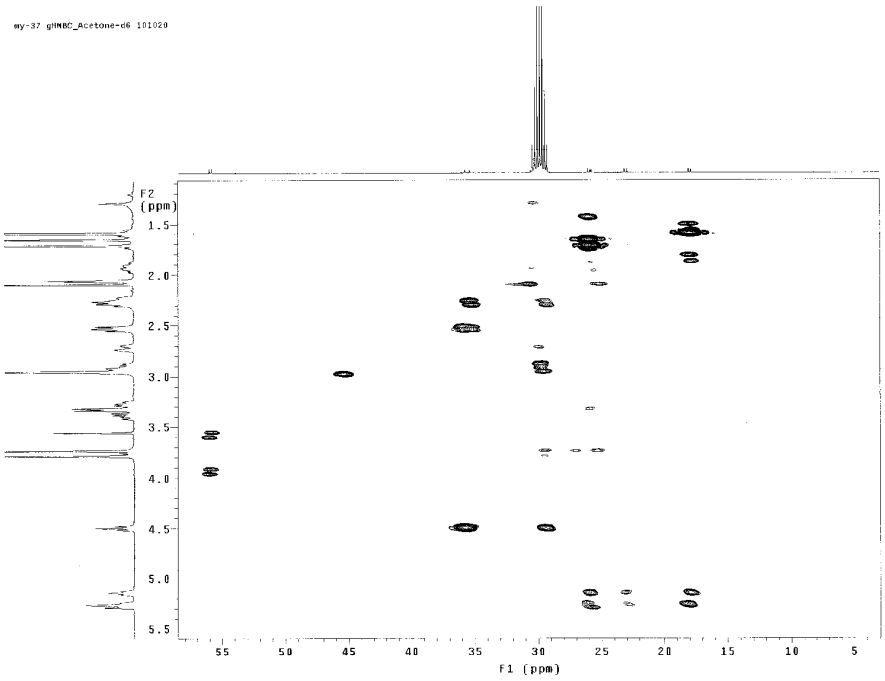
S 3.2 HMBC Spectrum of **3**



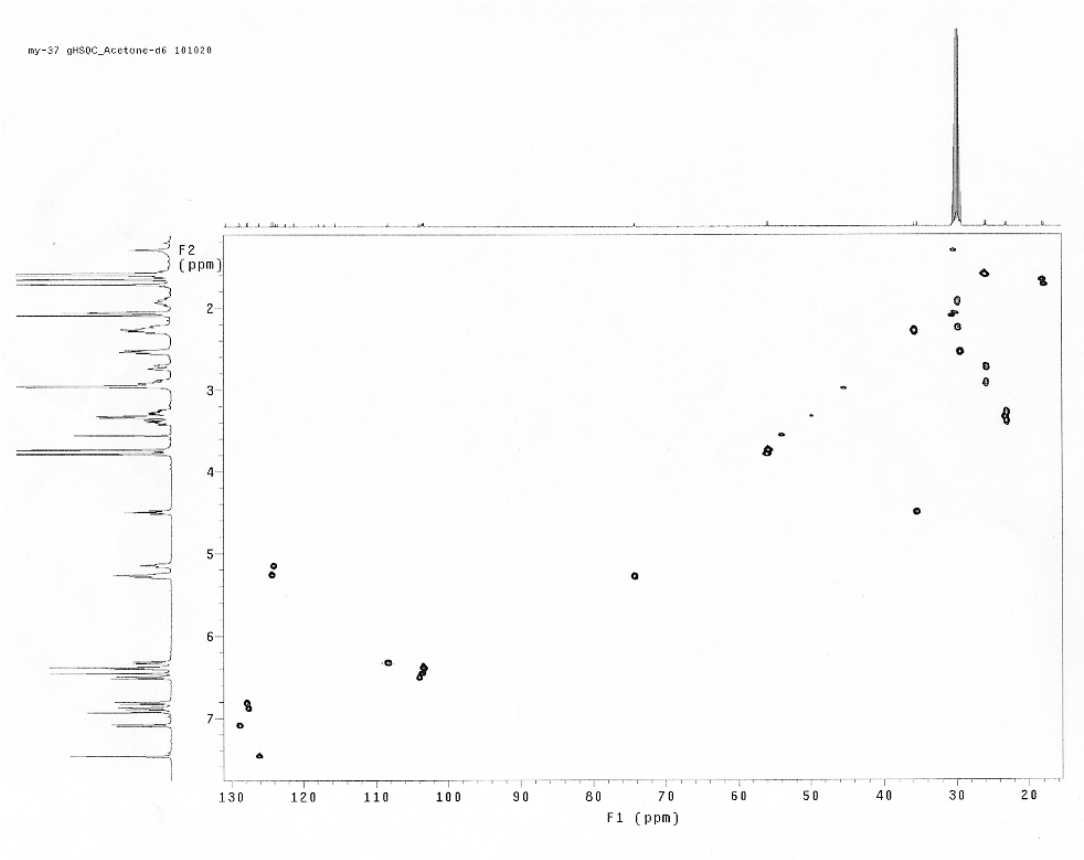
S 3.2.1 The magnified HMBC Spectrum of **3**



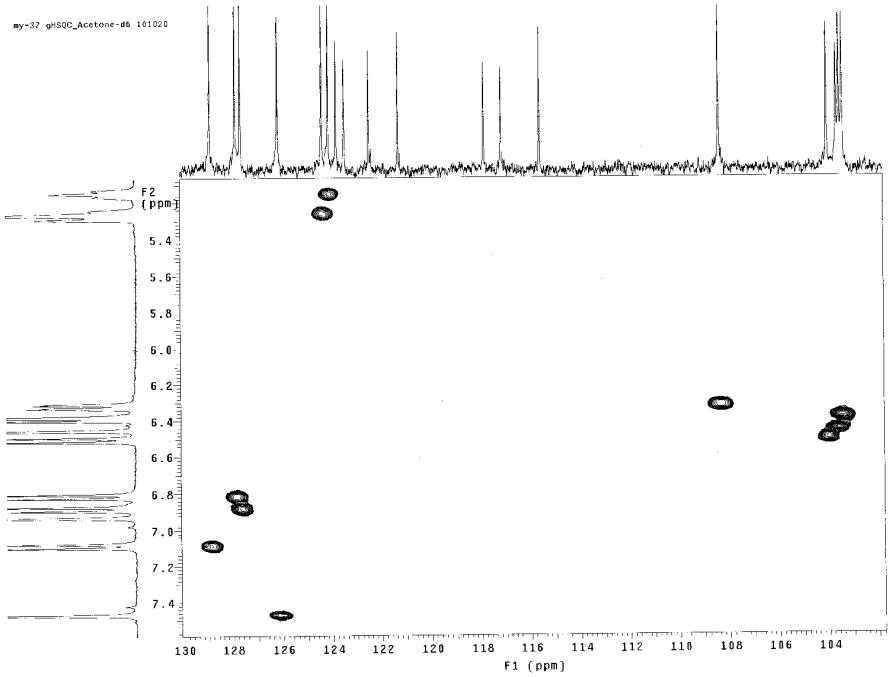
S 3.2.2 The magnified HMBC Spectrum of **3**



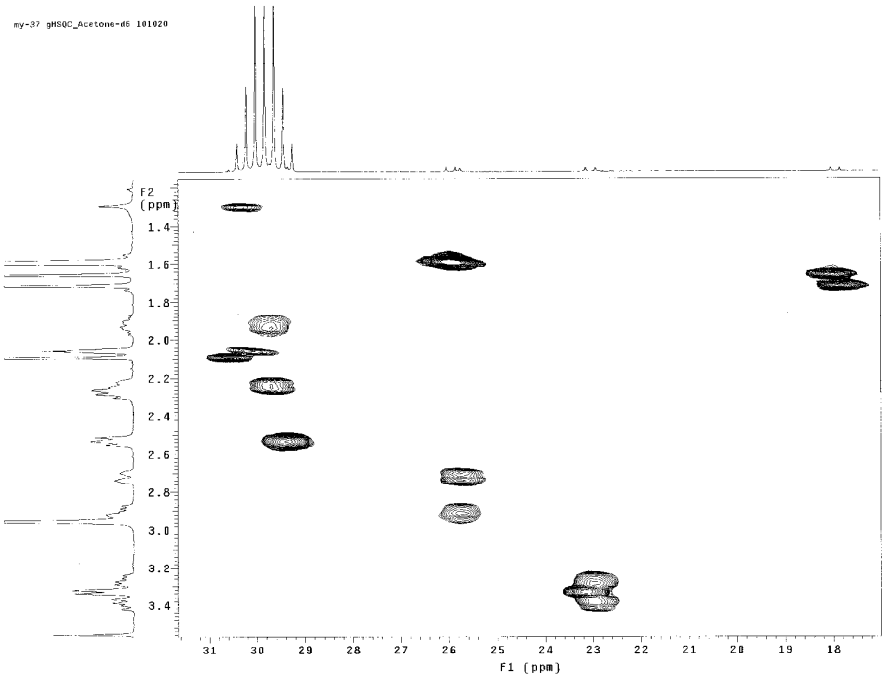
S 3.3 HSQC Spectrum of **3**



S 3.3.1 The magnified HSQC Spectrum of **3**



S 3.3.2 The magnified HSQC Spectrum of **3**



S 3.4 HRMALDIMS Spectrum of **3**

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

SIOC

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:

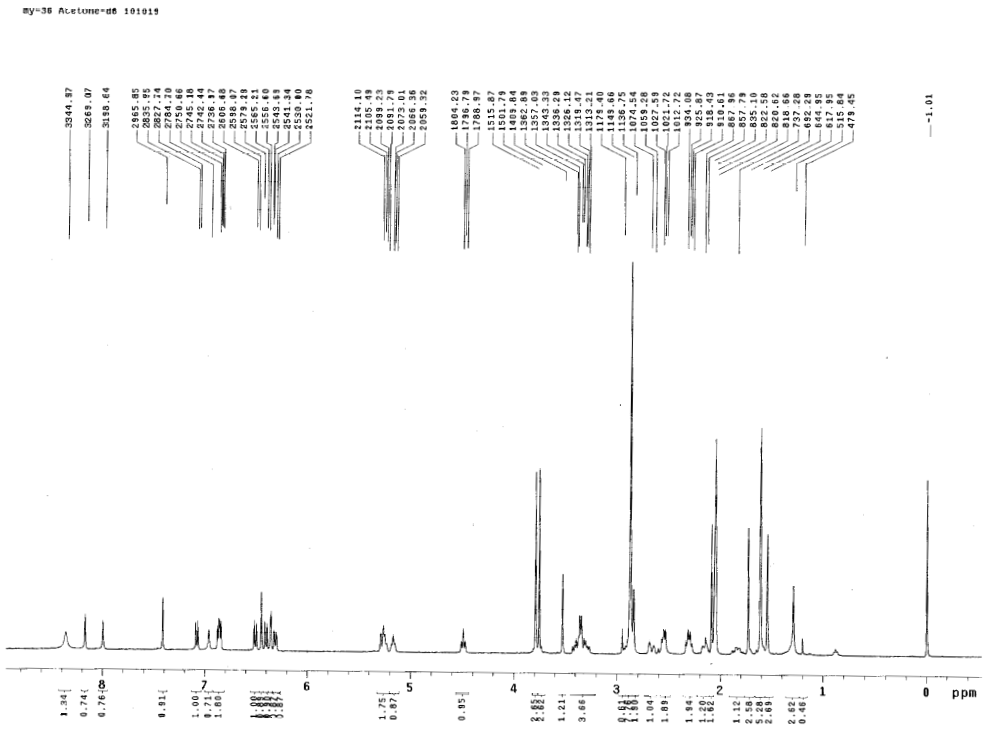
DBE Limit Mode = Both Integer and Half-Integer
Minimum DBE = 0

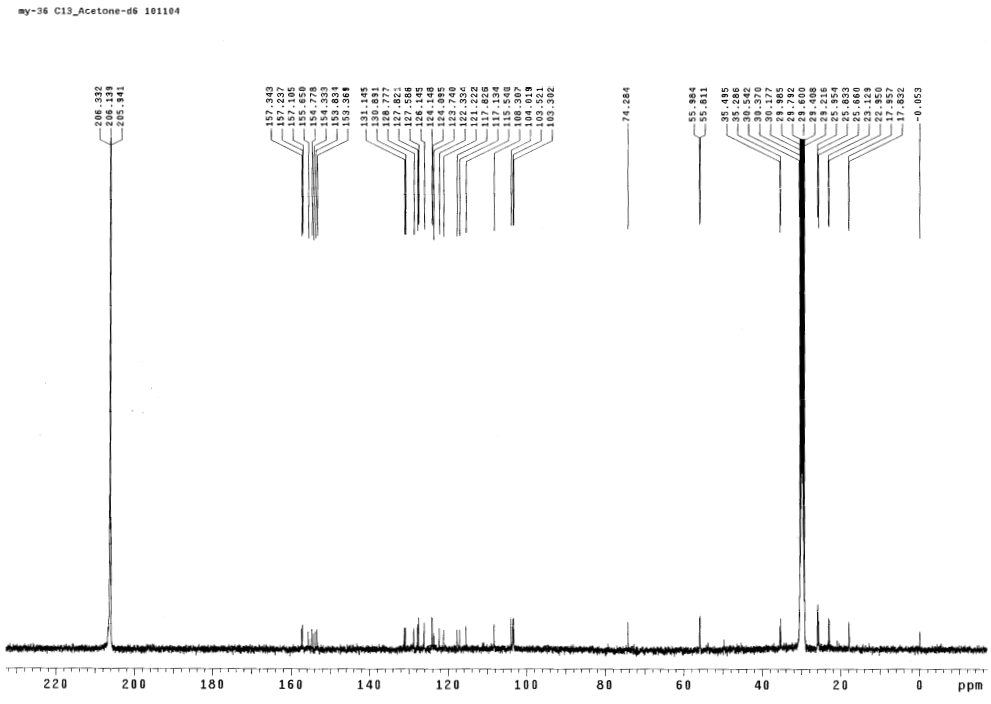
Search Results:

Number of Hits = 2

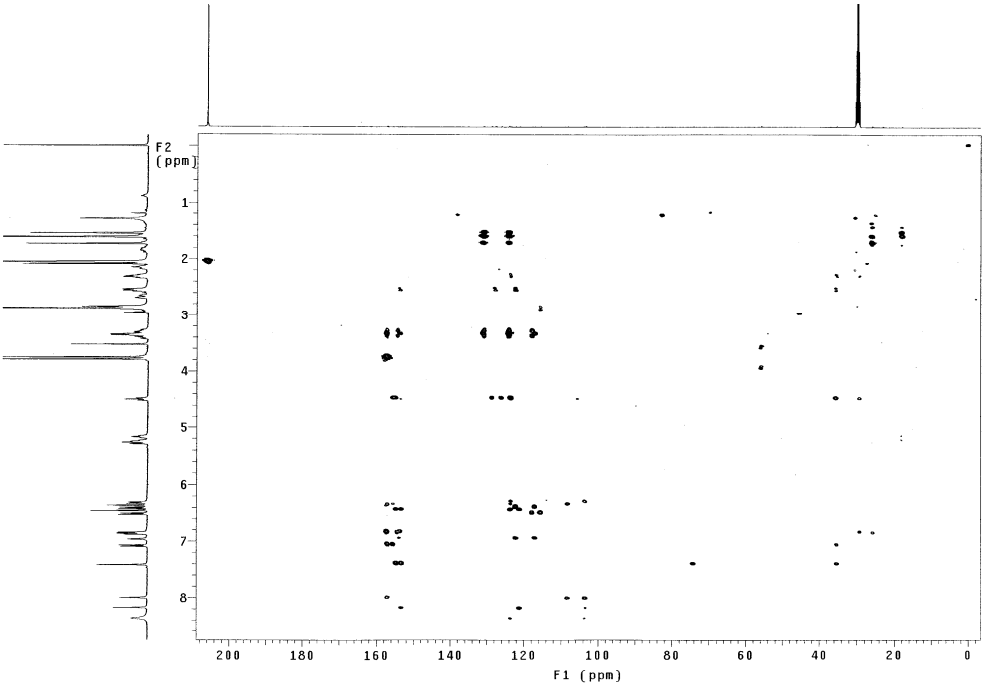
m/z	Delta m/z	DBE	Formula
703.32655	-0.00015	21.5	$C_{44}H_{47}O_8^{+1}$
703.32414	0.00226	19.0	$C_{42}H_{48}O_8Na^{+1}$

S 4.1 ^{1}H NMR and ^{13}C NMR Spectra of **4**

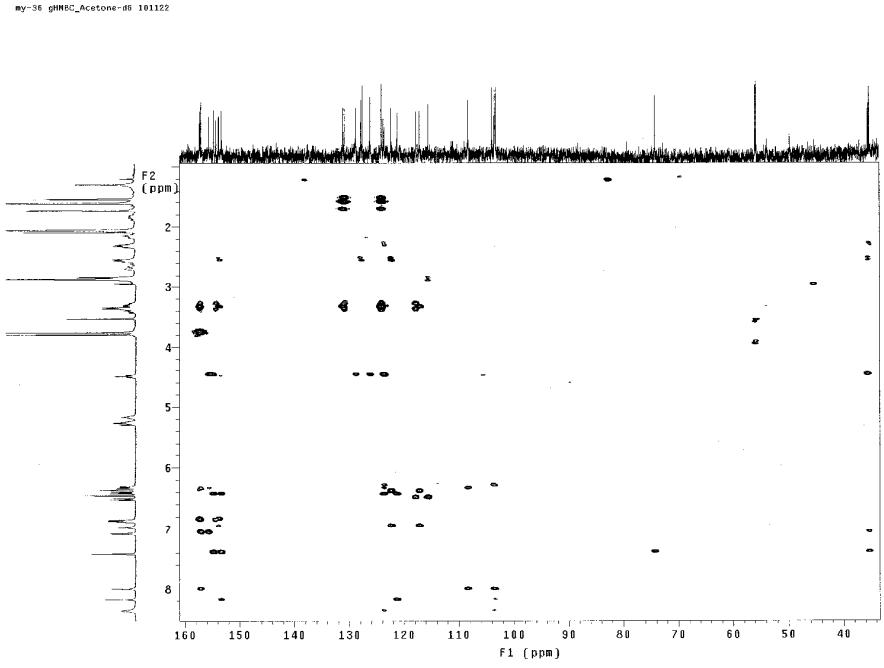




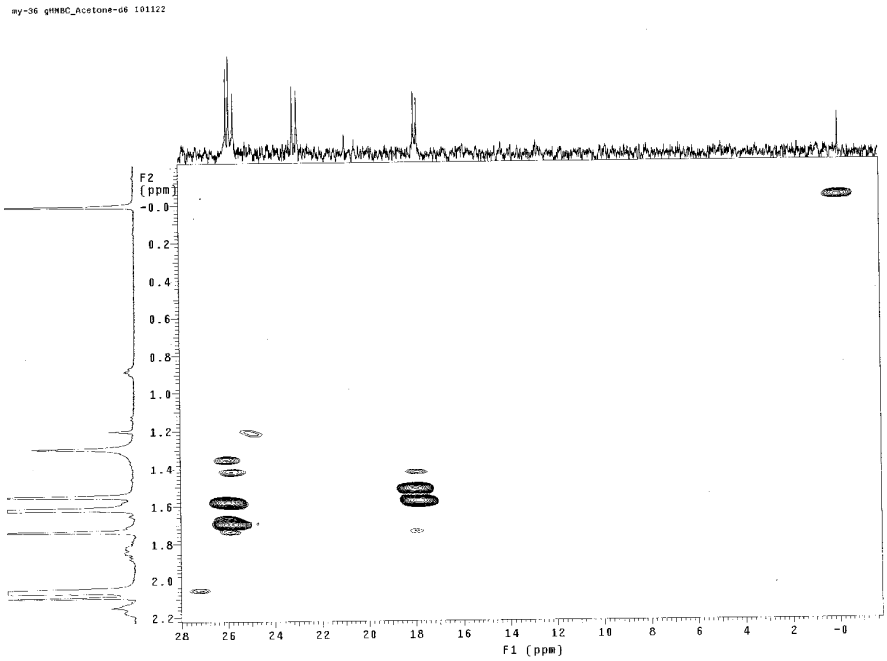
S 4.2 HMBC Spectrum of **4**



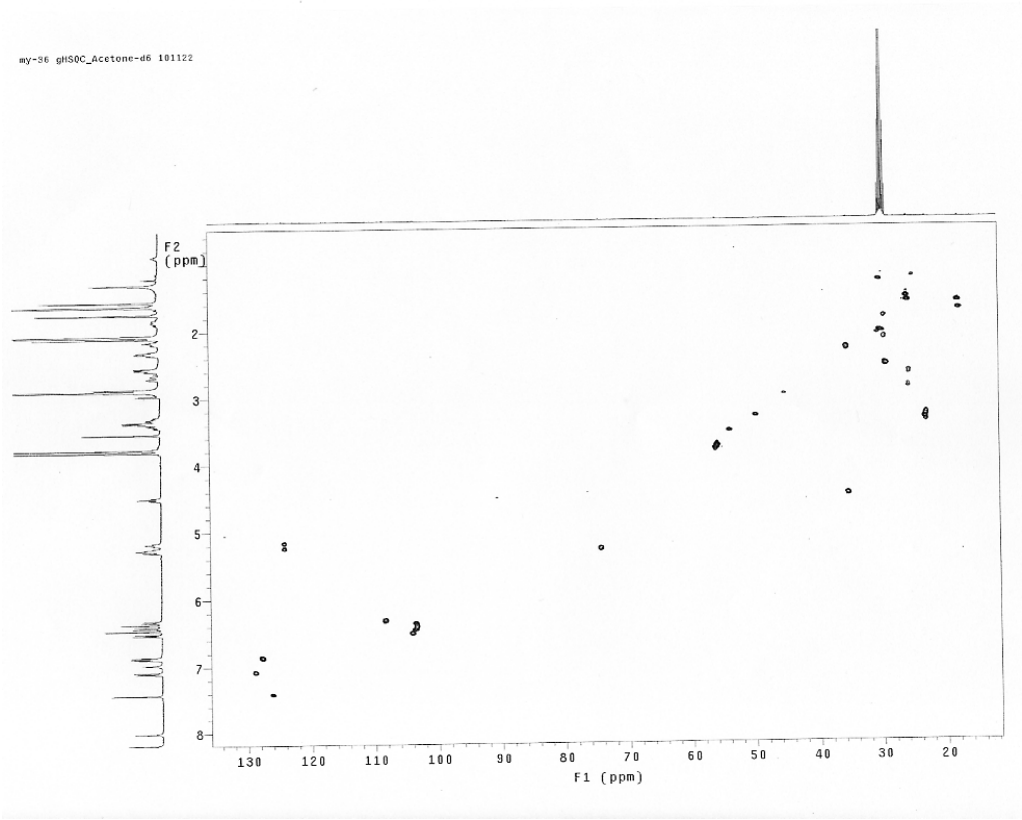
S 4.2.1 The magnified HMBC Spectrum of **4**



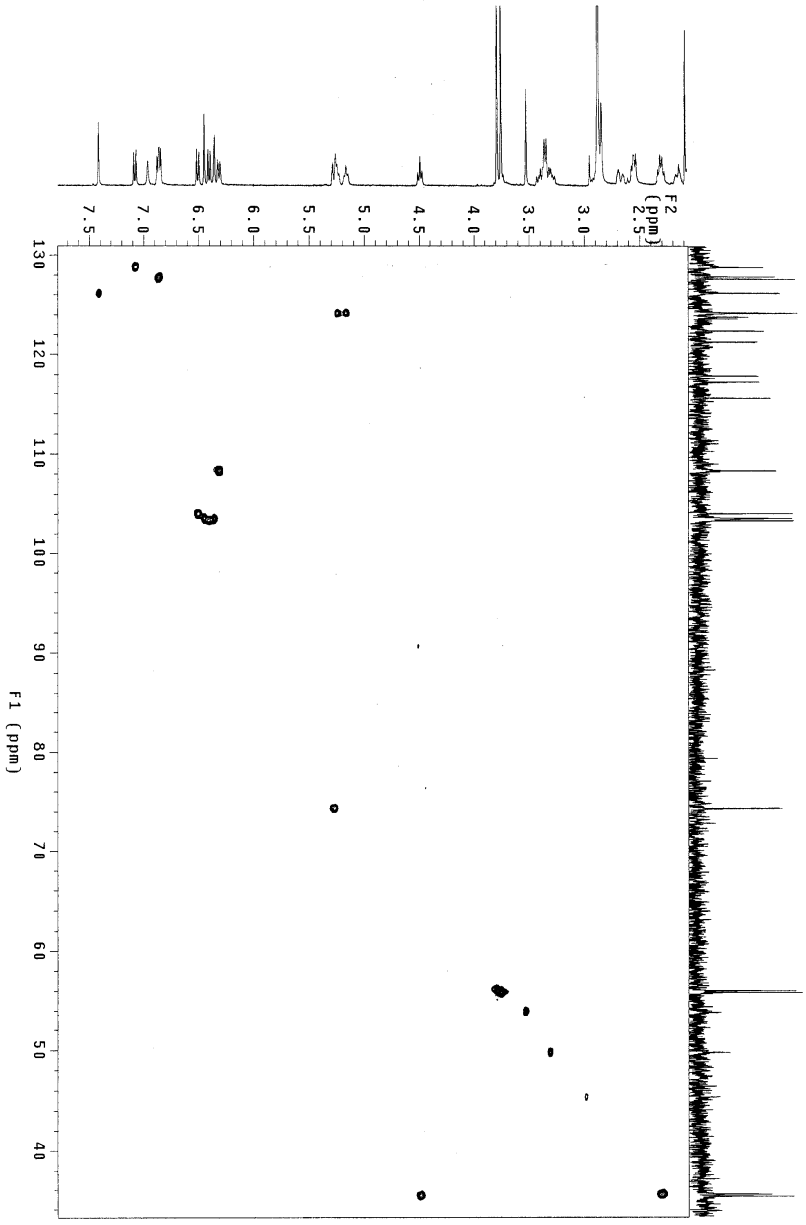
S 4.2.2 The magnified HMBC Spectrum of **4**



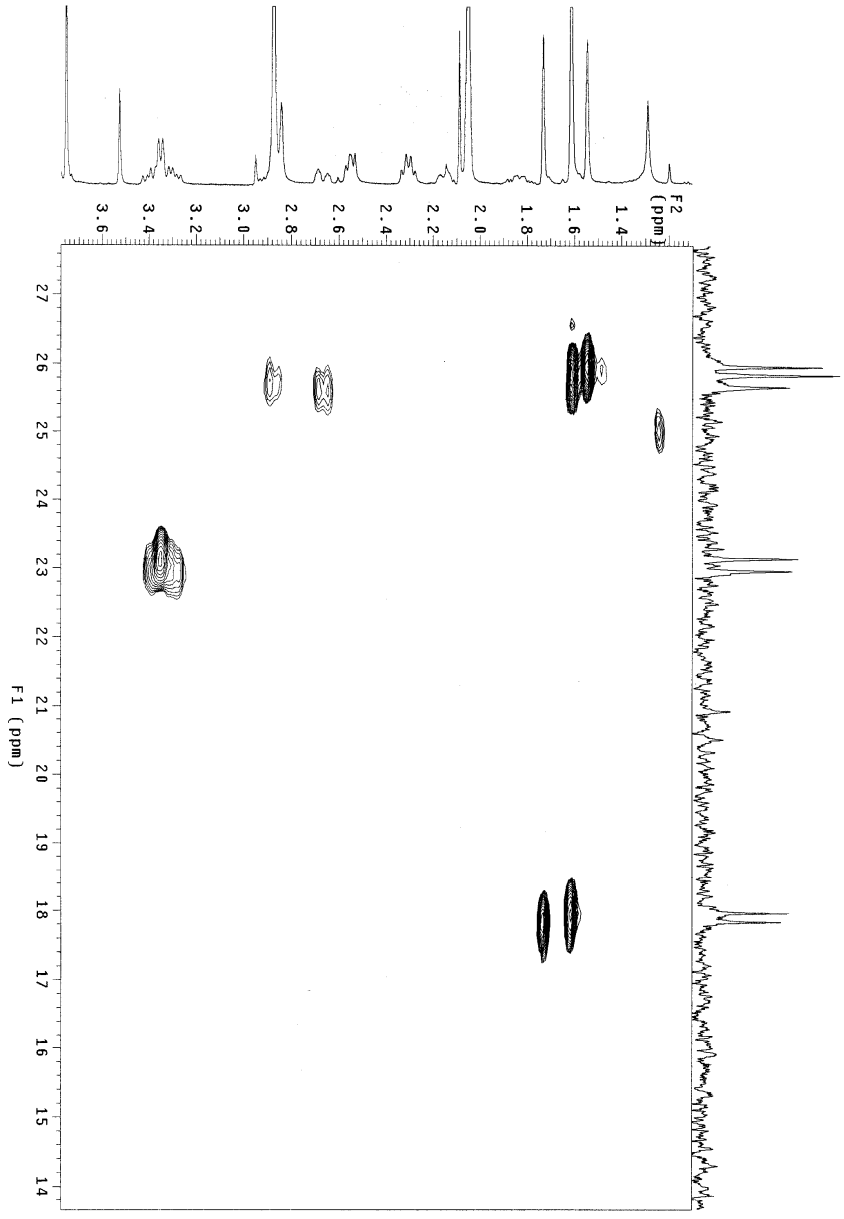
S 4.3 HSQC Spectrum of **4**



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**

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

SIOC

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:

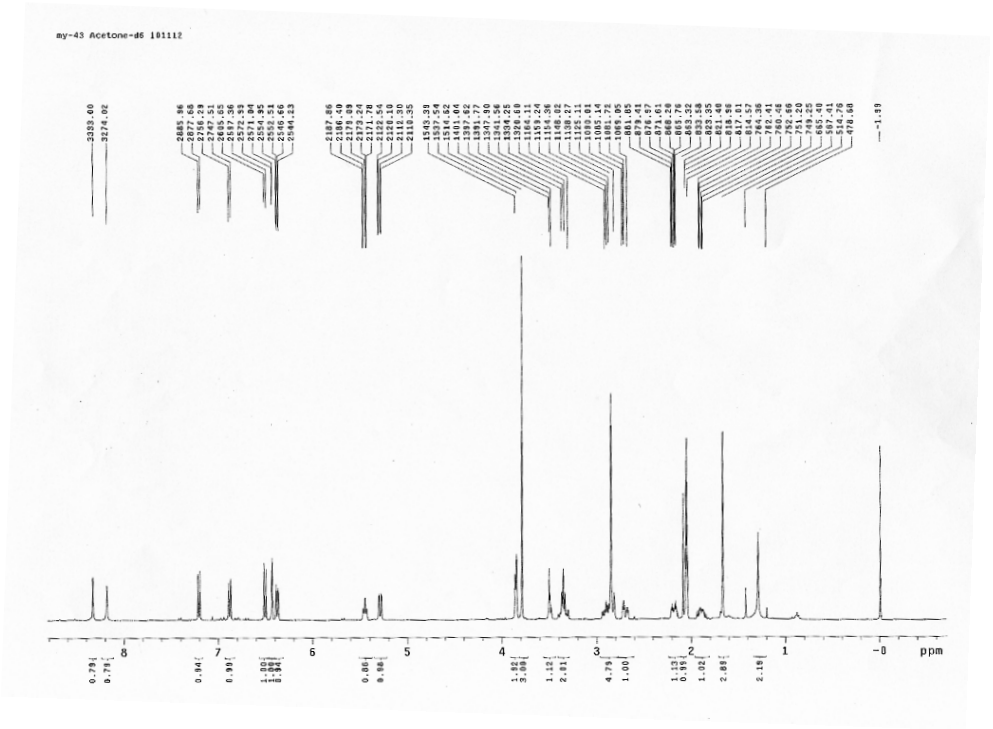
DBE Limit Mode = Both Integer and Half-Integer
Minimum DBE = 0

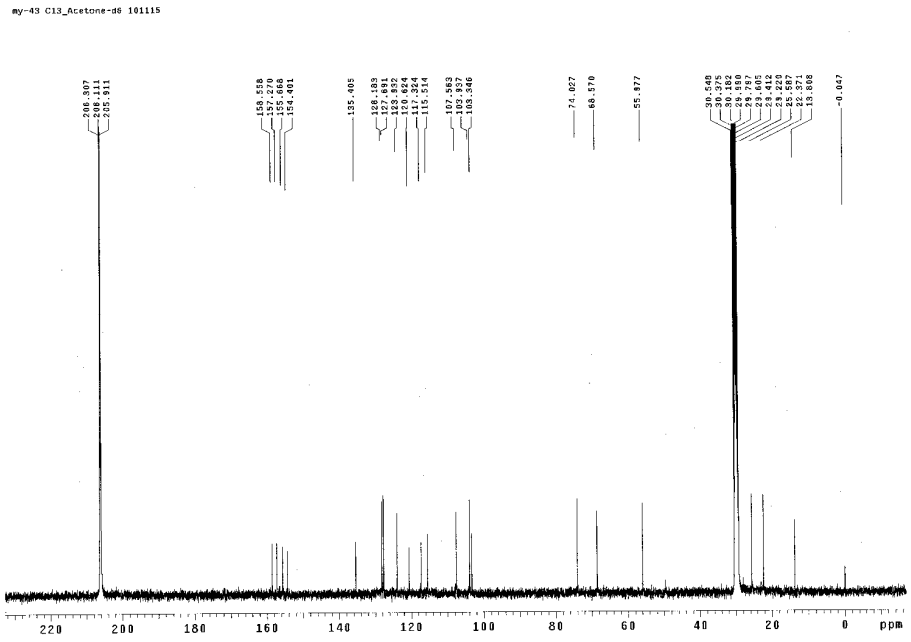
Search Results:

Number of Hits = 2

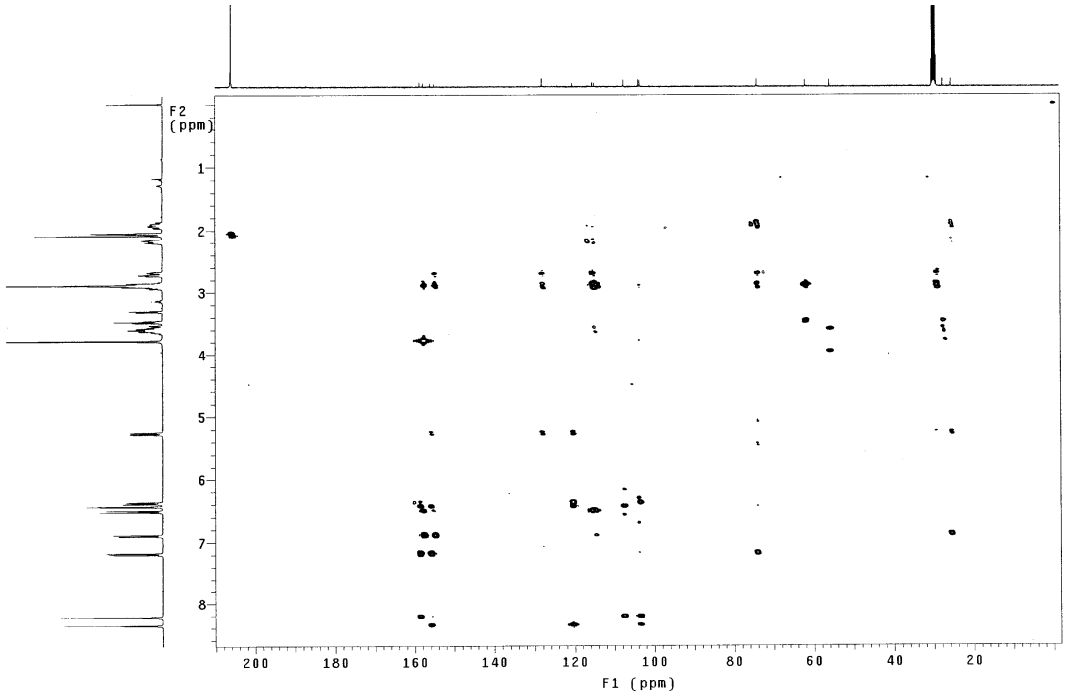
m/z	Delta m/z	DBE	Formula
703.32655	-0.00065	21.5	$C_{44}H_{47}O_8^{+1}$
703.32414	0.00176	19.0	$C_{42}H_{48}O_8Na^{+1}$

S 5.1 ^{1}H NMR and ^{13}C NMR Spectra of **5**

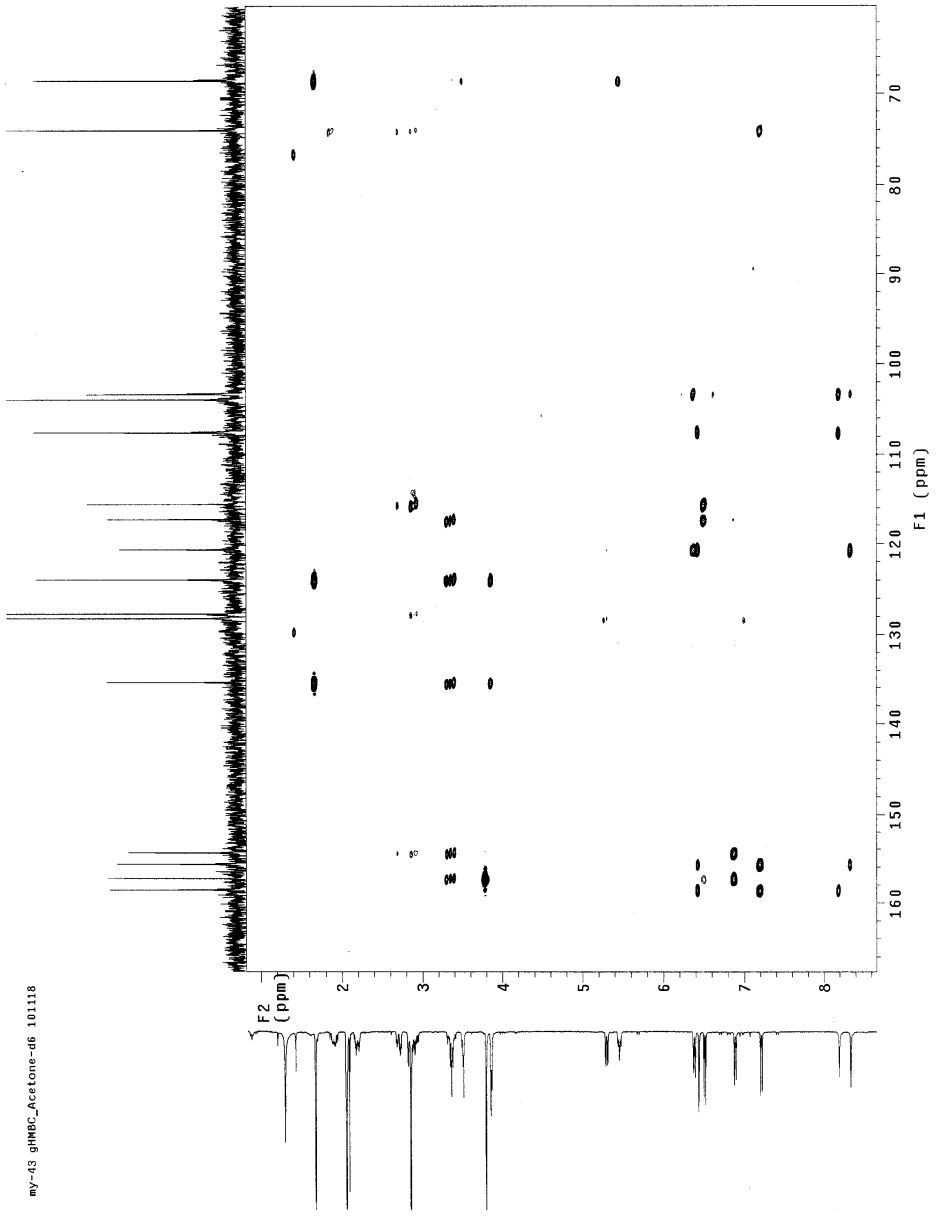




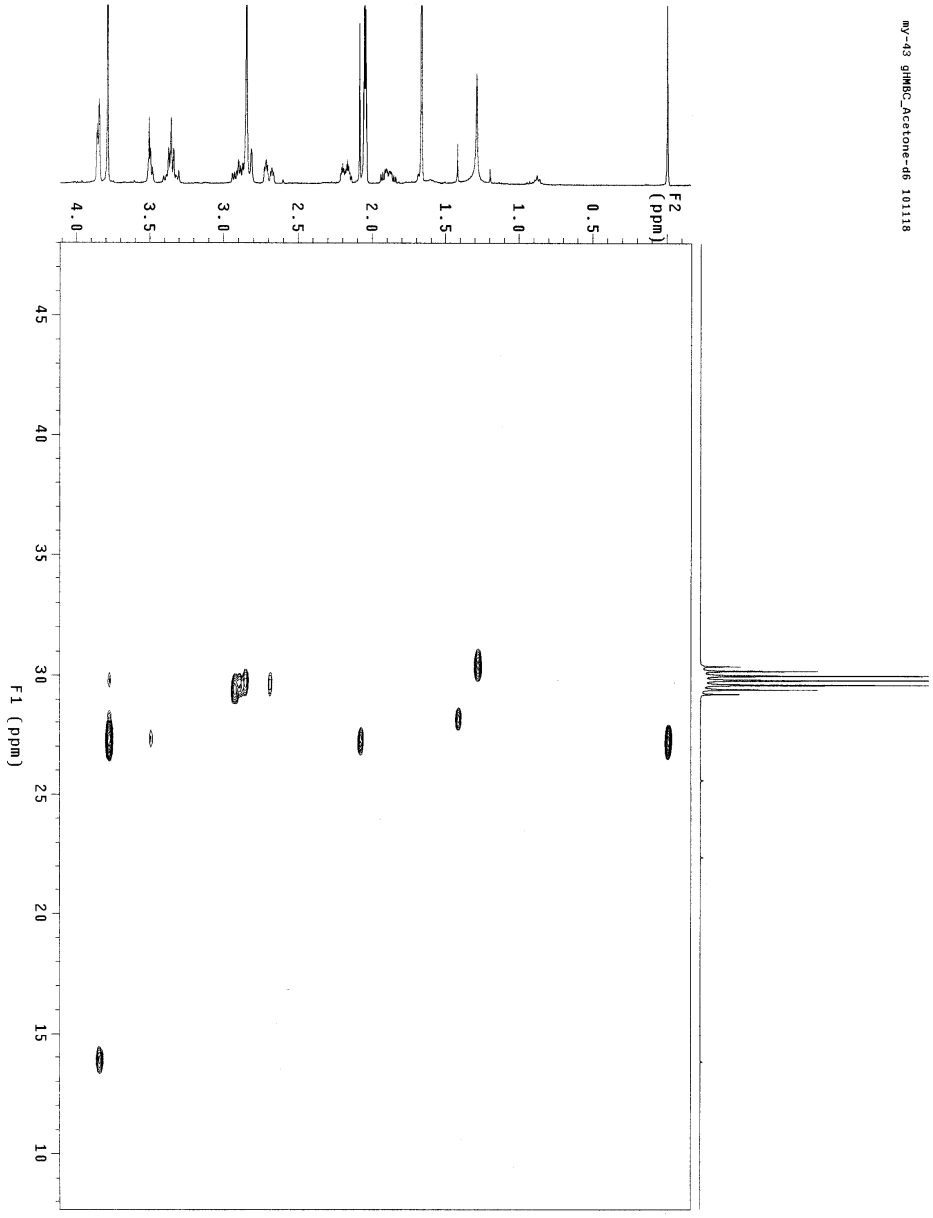
S 5.2 HMBC Spectrum of **5**



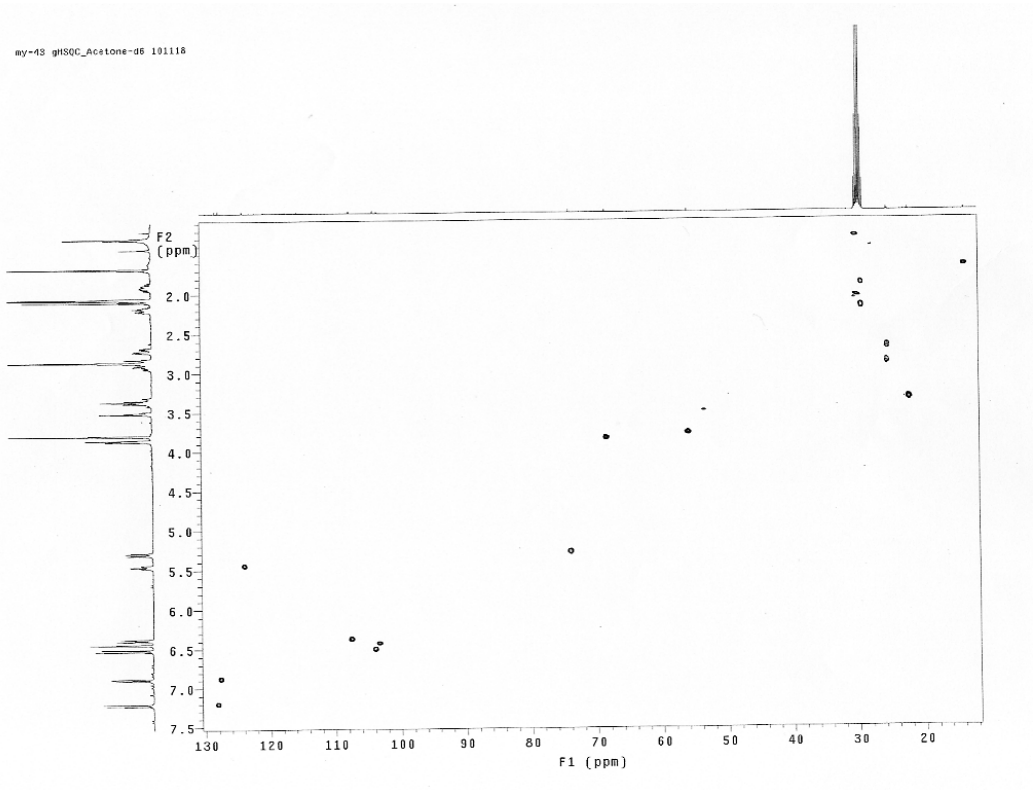
S 5.2.1 The magnified HMBC Spectrum of **5**



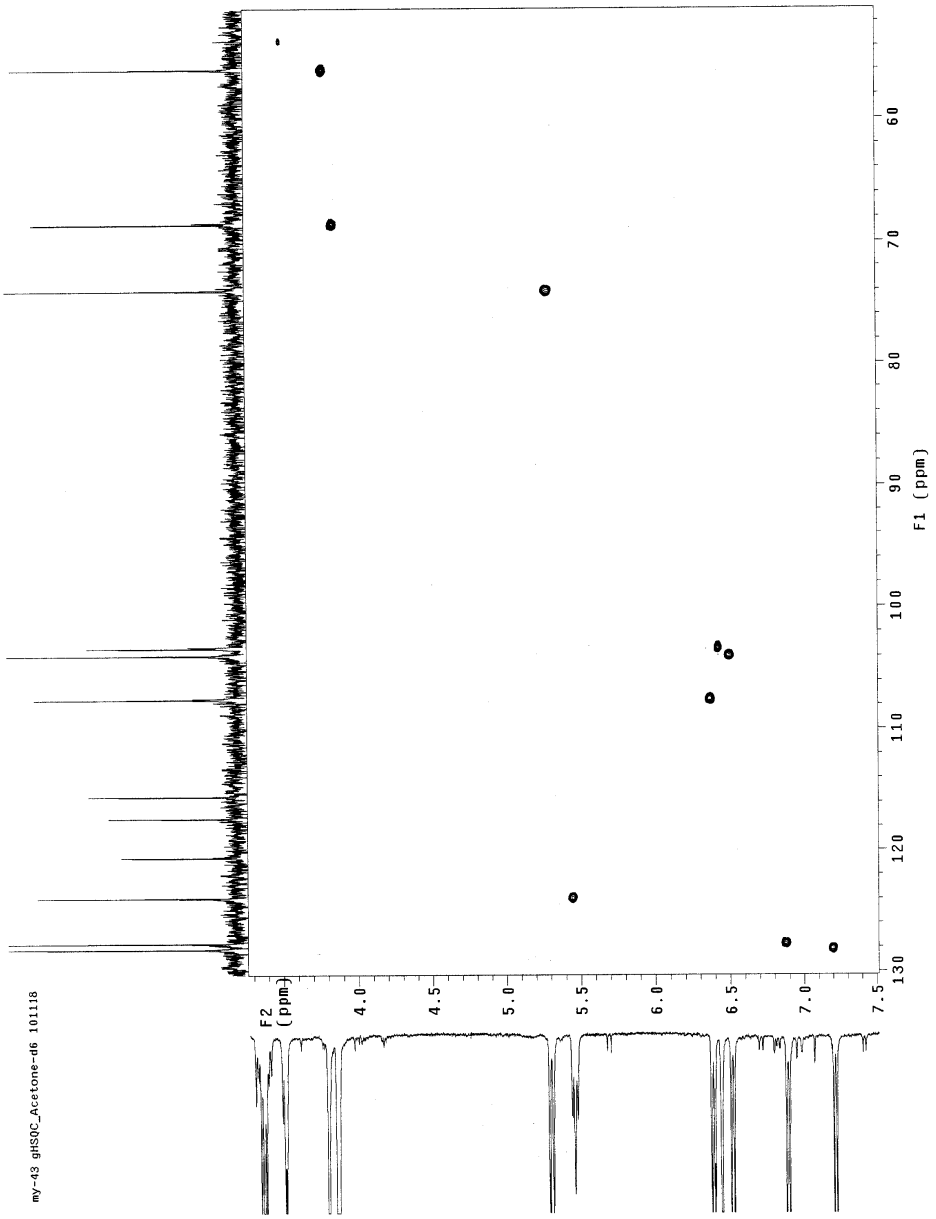
S 5.2.2 The magnified HMBC Spectrum of **5**



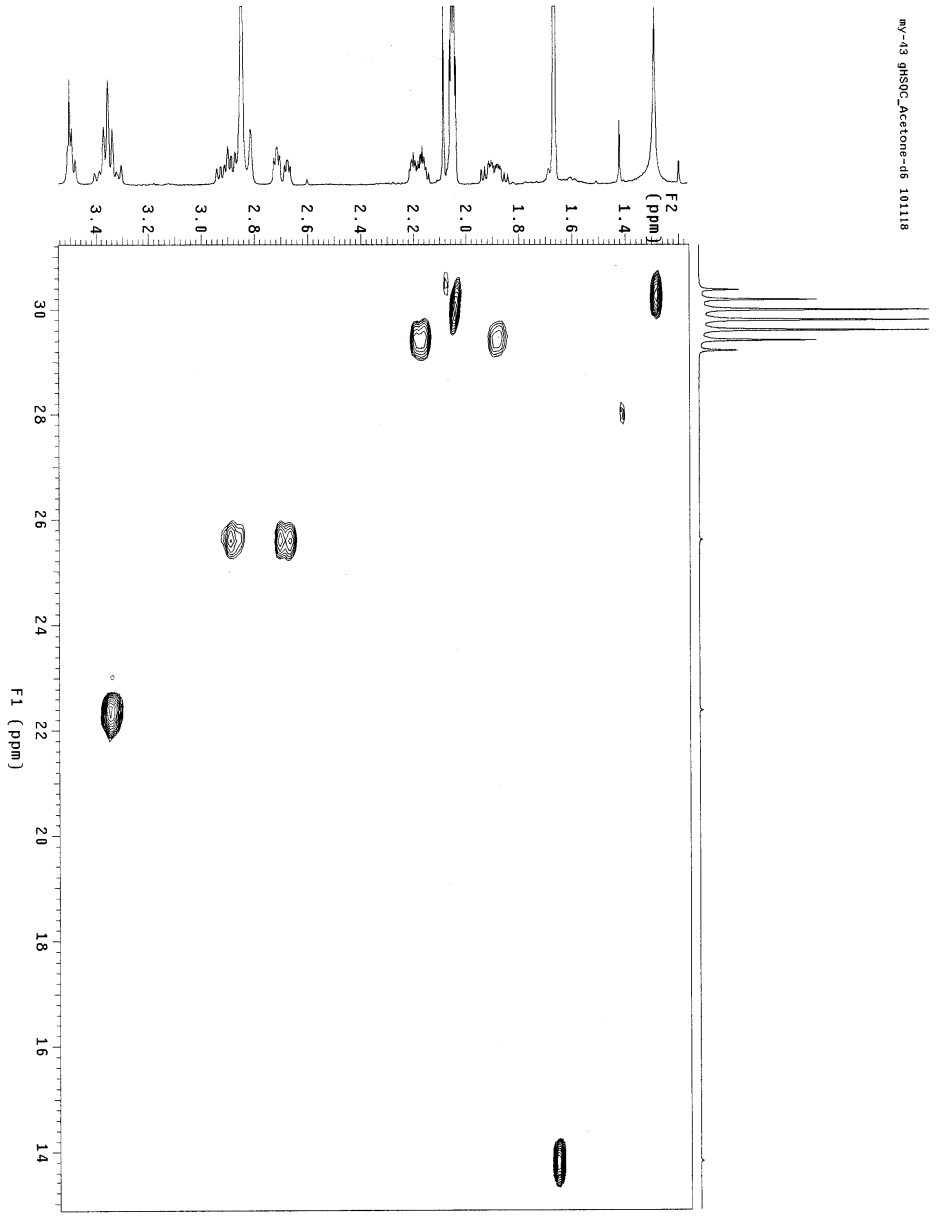
S 5.3 HSQC Spectrum of **5**



S 5.3.1 The magnified HSQC Spectrum of **5**



S 5.3.2 The magnified HSQC Spectrum of **5**



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

SIOC

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

Card Serial Number: **GCT-T*1011*-OS0610**

Sample Serial Number: **My-43**

Operator: **Li**

Date: **2010/11/26**

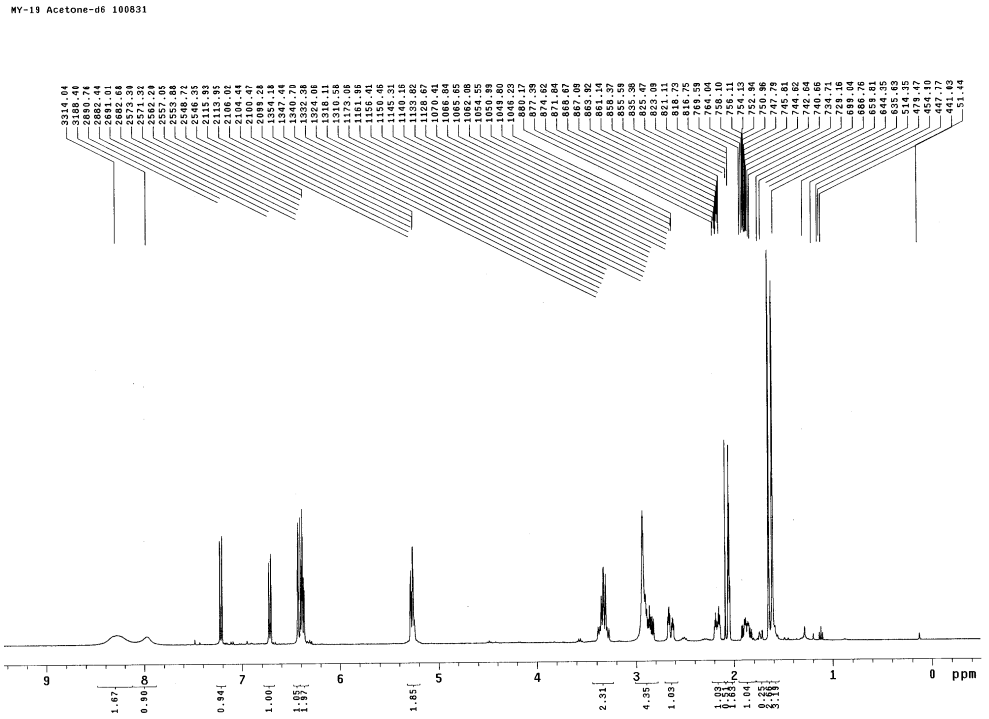
Elemental Composition Report

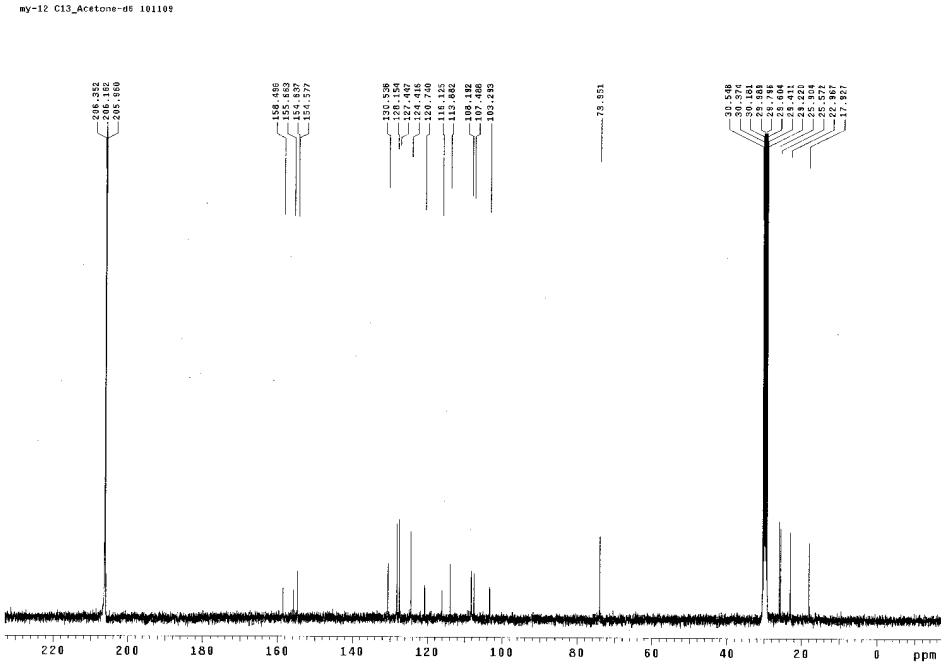
Single Mass Analysis
Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

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

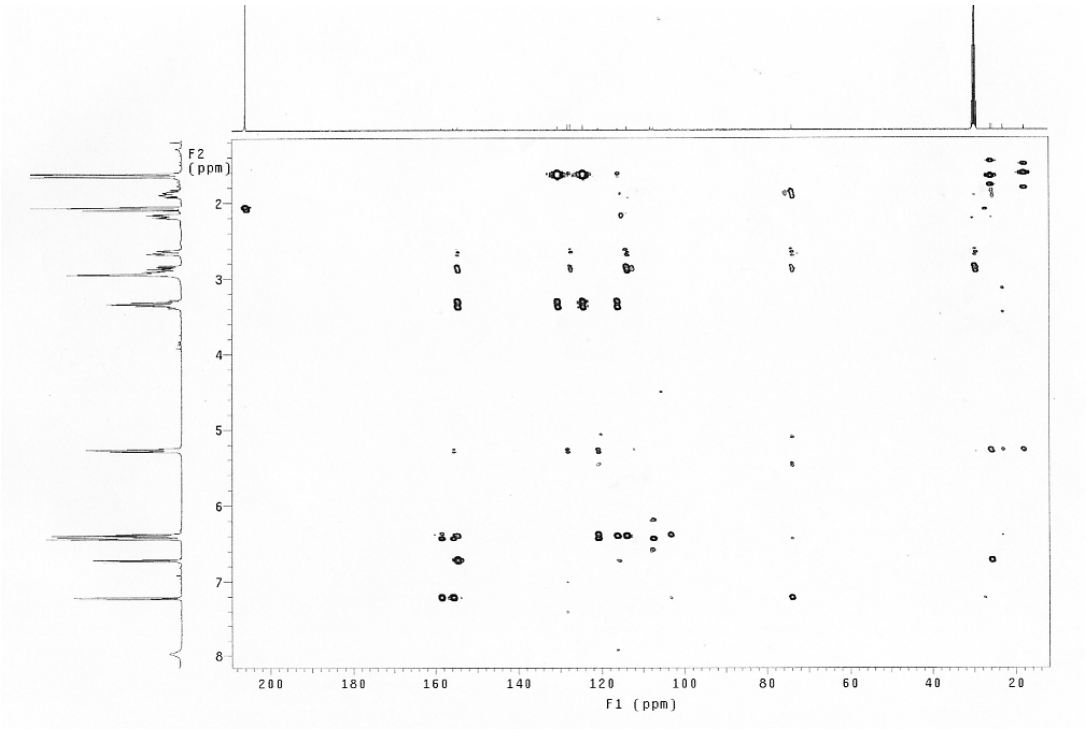
Minimum:				-1.5		
Maximum:		1.5	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
356.1628	356.1624	0.4	1.2	10.0	1	C21 H24 O5
	356.1637	-0.9	-2.6	15.0	2	C22 H20 N4 O

S 6.1 ^{1}H NMR and ^{13}C NMR Spectra of **6**

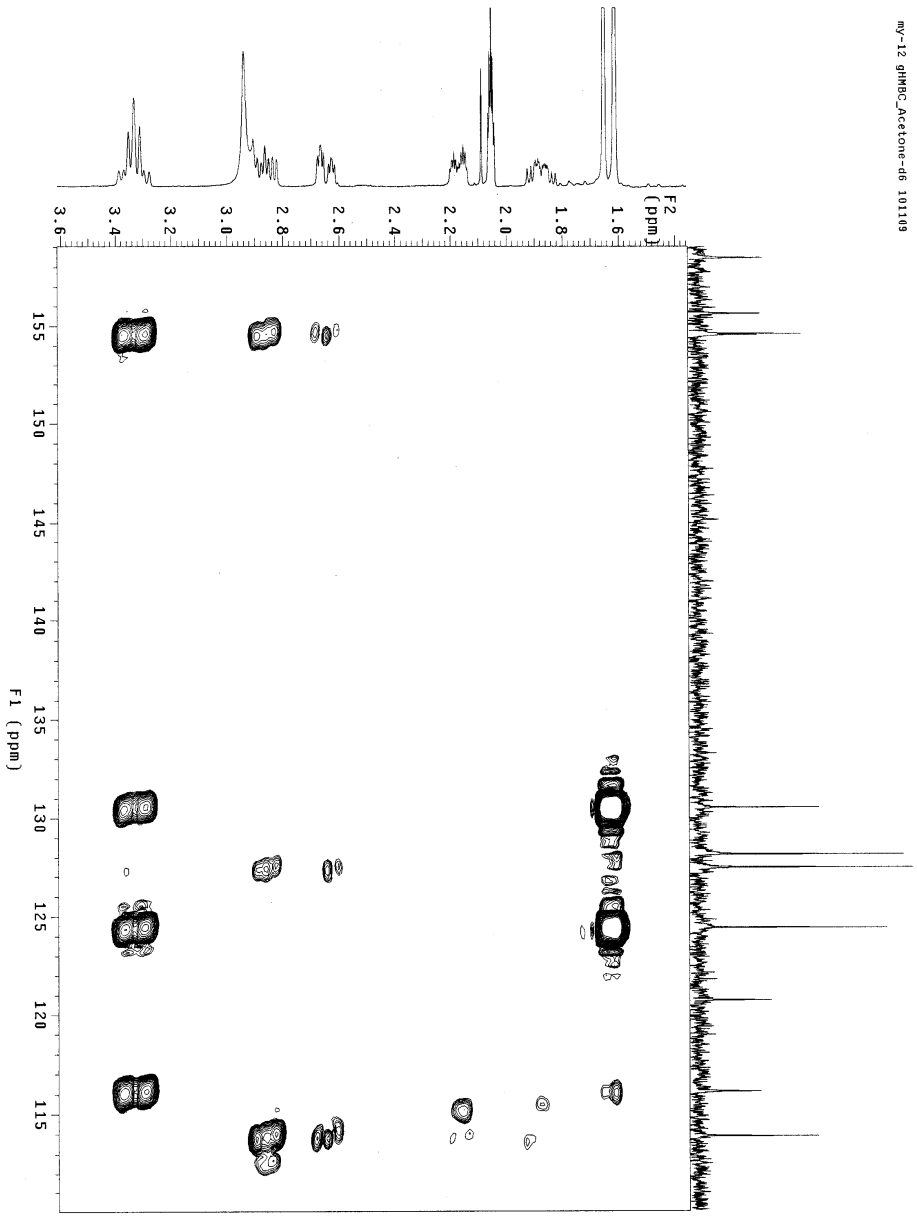




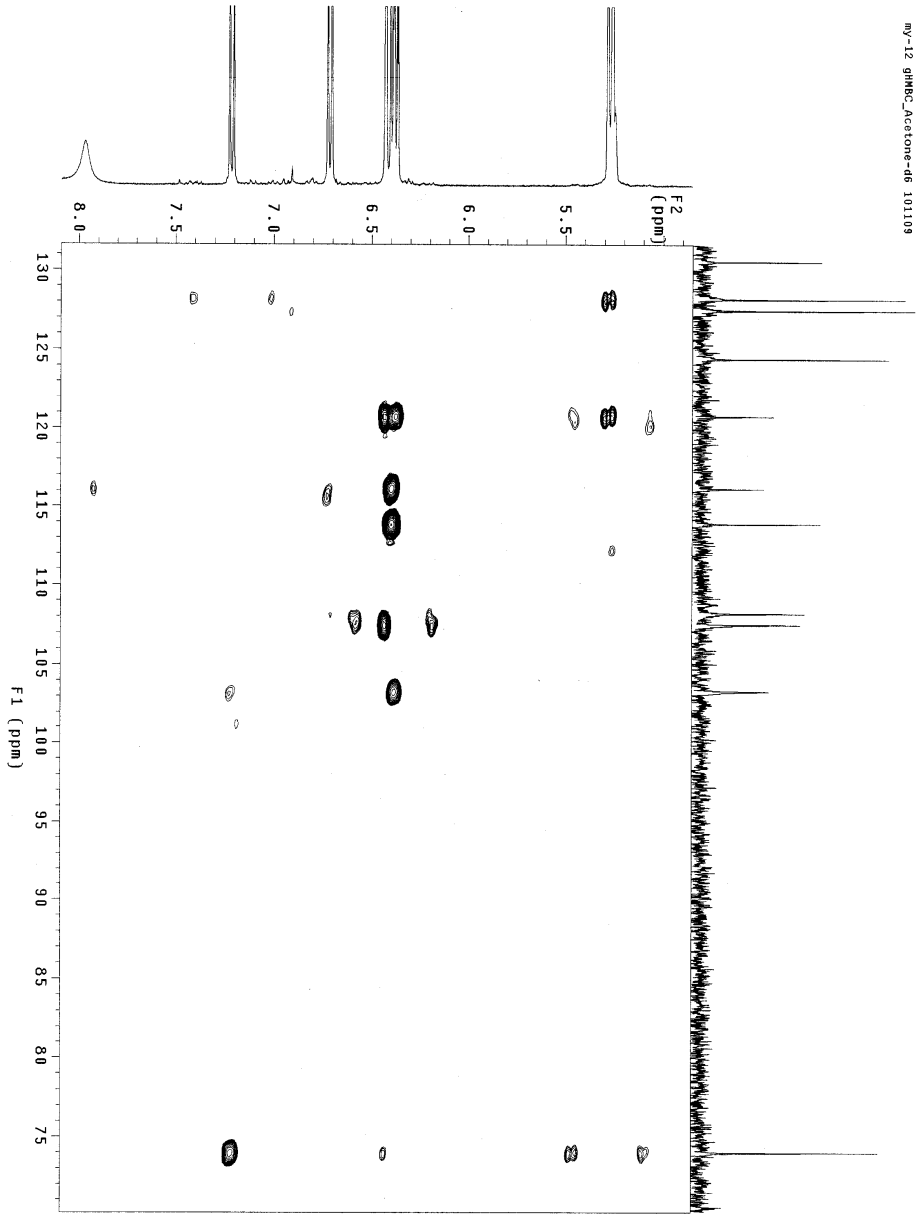
S 6.2 HMBC Spectrum of **6**



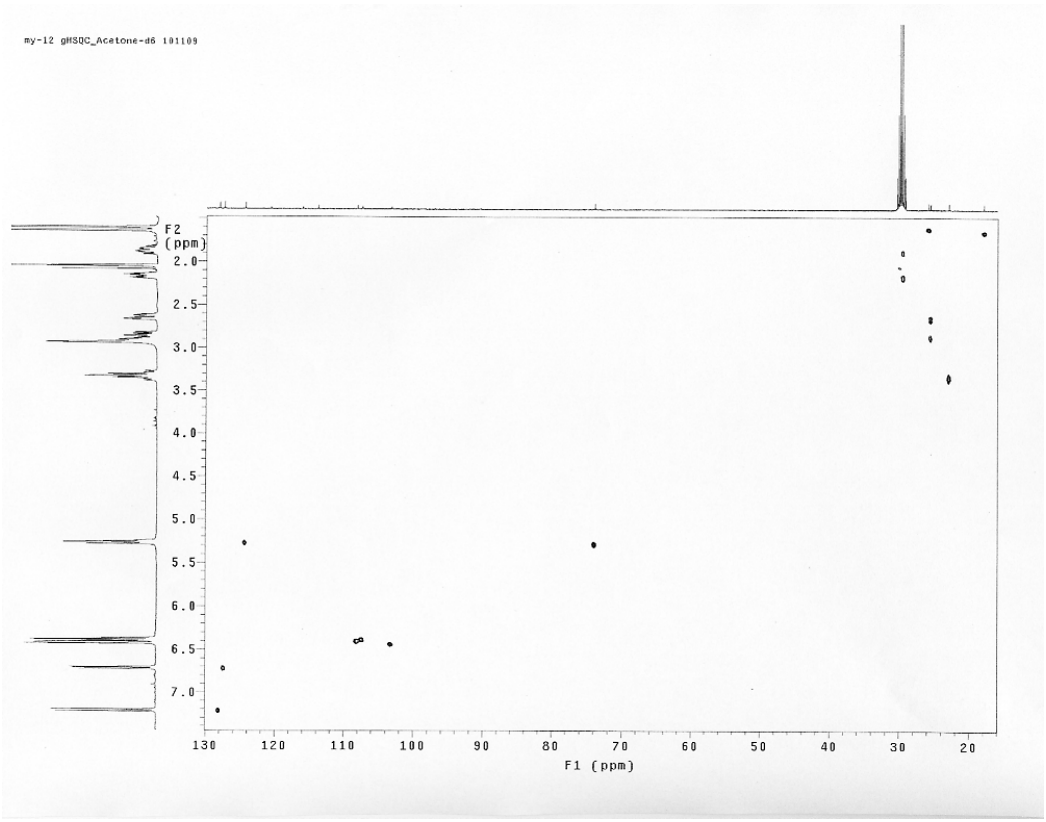
S 6.2.1 The magnified HMBC Spectrum of **6**



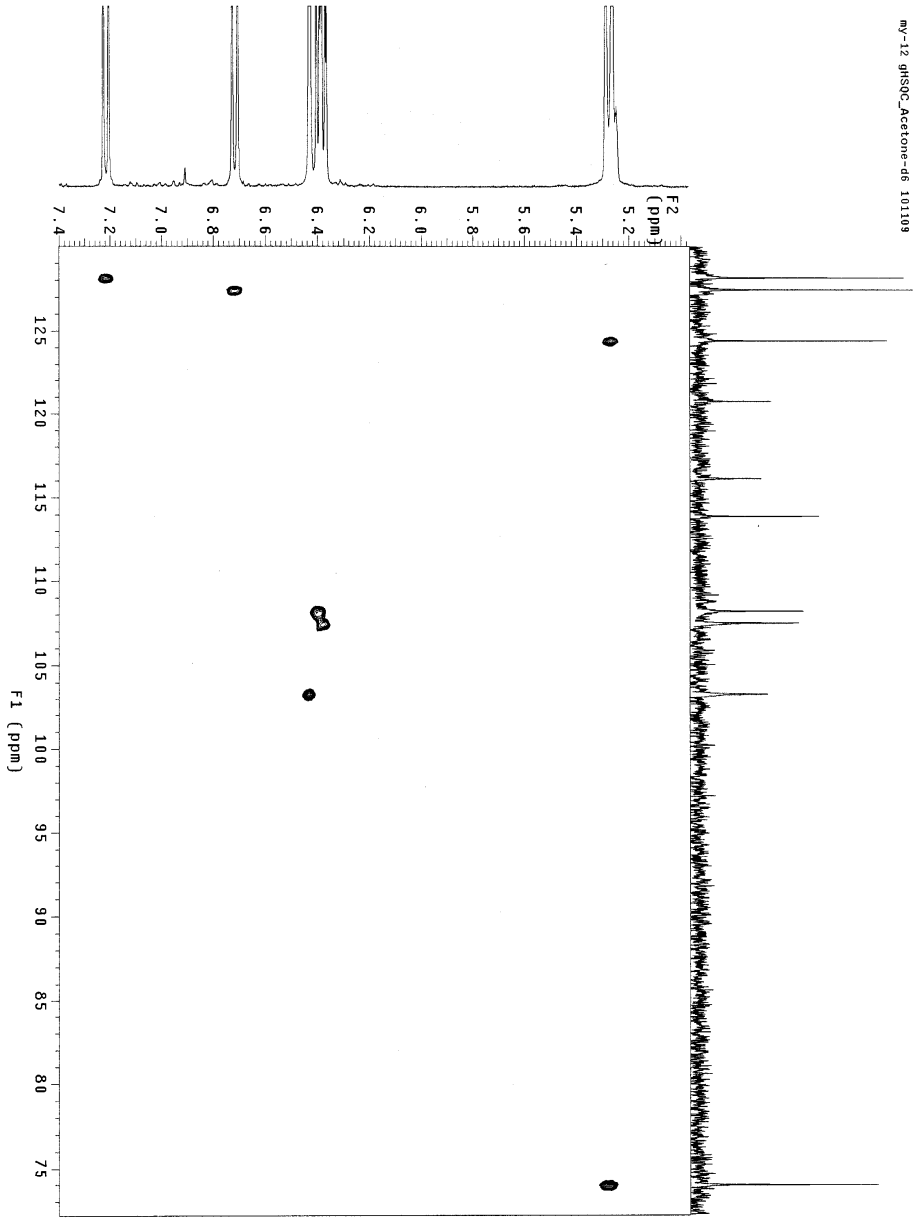
S 6.2.2 The magnified HMBC Spectrum of **6**



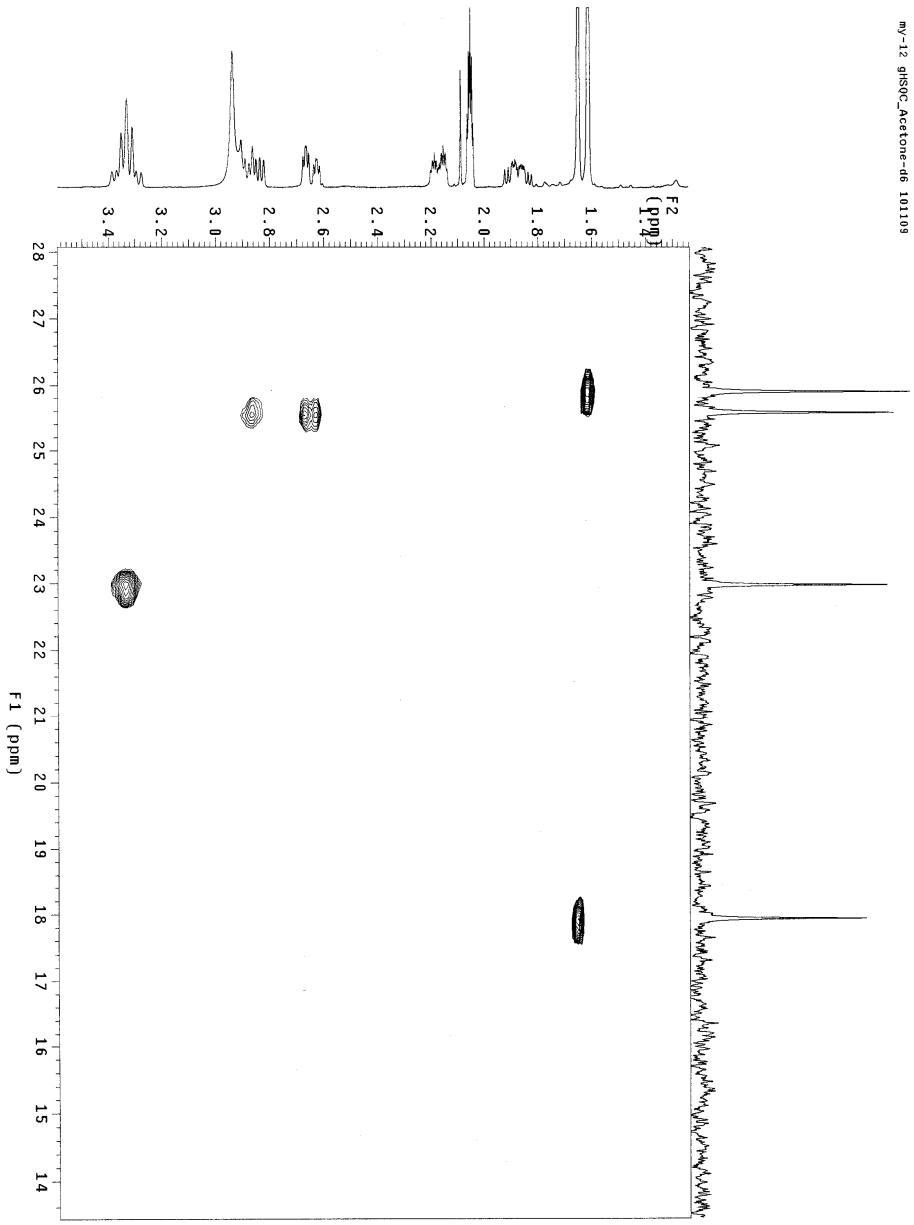
S 6.3 HSQC Spectrum of **6**



S 6.3.1 The magnified HSQC Spectrum of **6**



S 6.3.2 The magnified HSQC Spectrum of **6**



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

SIOC

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

Card Serial Number: **GCT-T*1011*-OS0606**

Sample Serial Number: **My-12**

Operator: **Li**

Date: **2010/11/25**

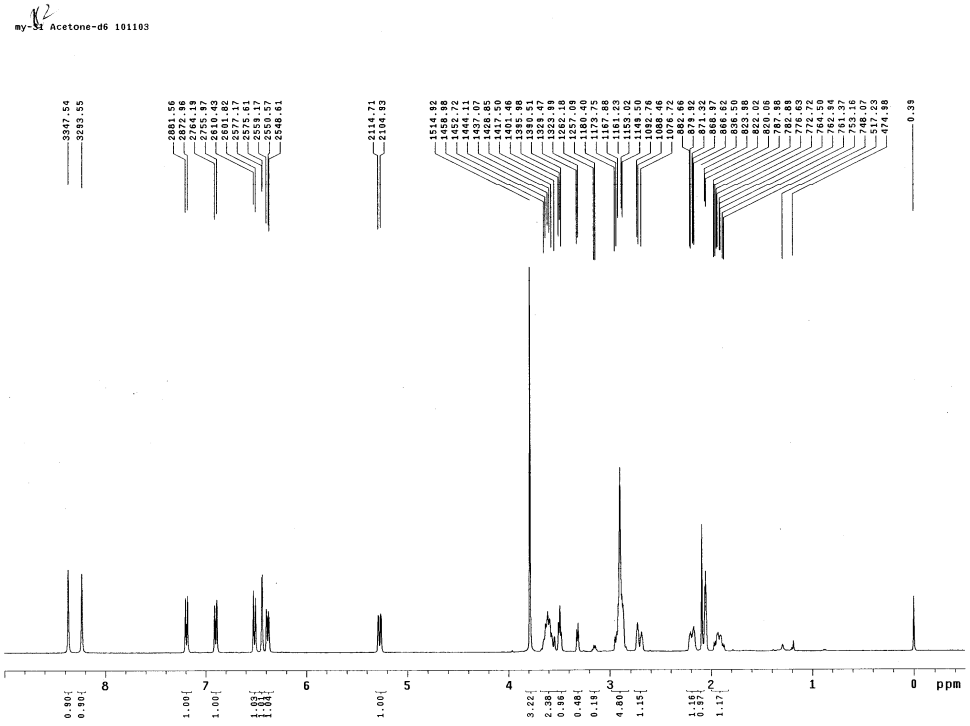
Elemental Composition Report

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

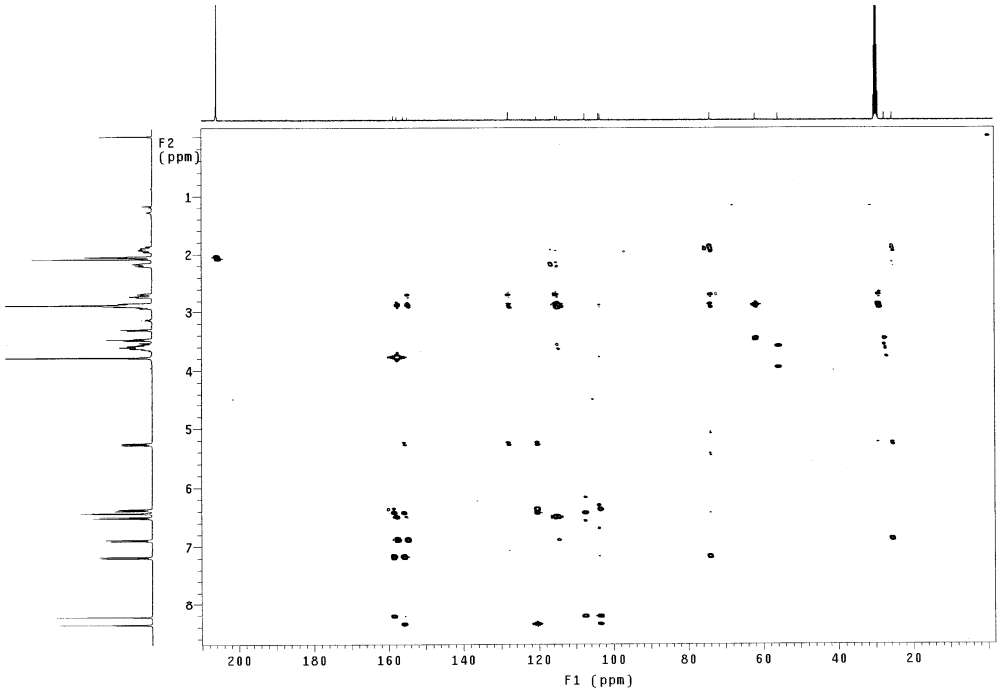
Monoisotopic Mass, Odd and Even Electron Ions
173 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

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

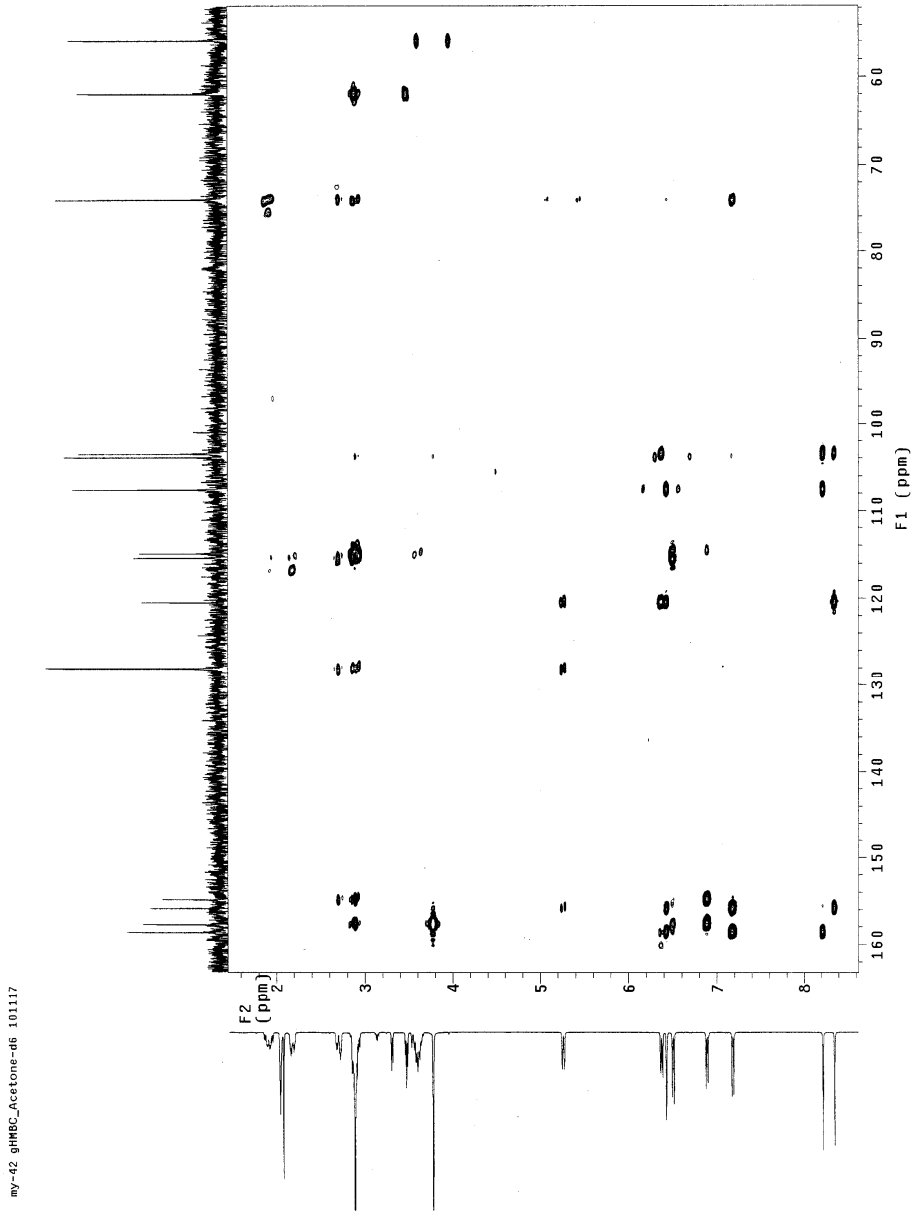
S 7.1 ^{1}H NMR and ^{13}C NMR Spectra of **7**



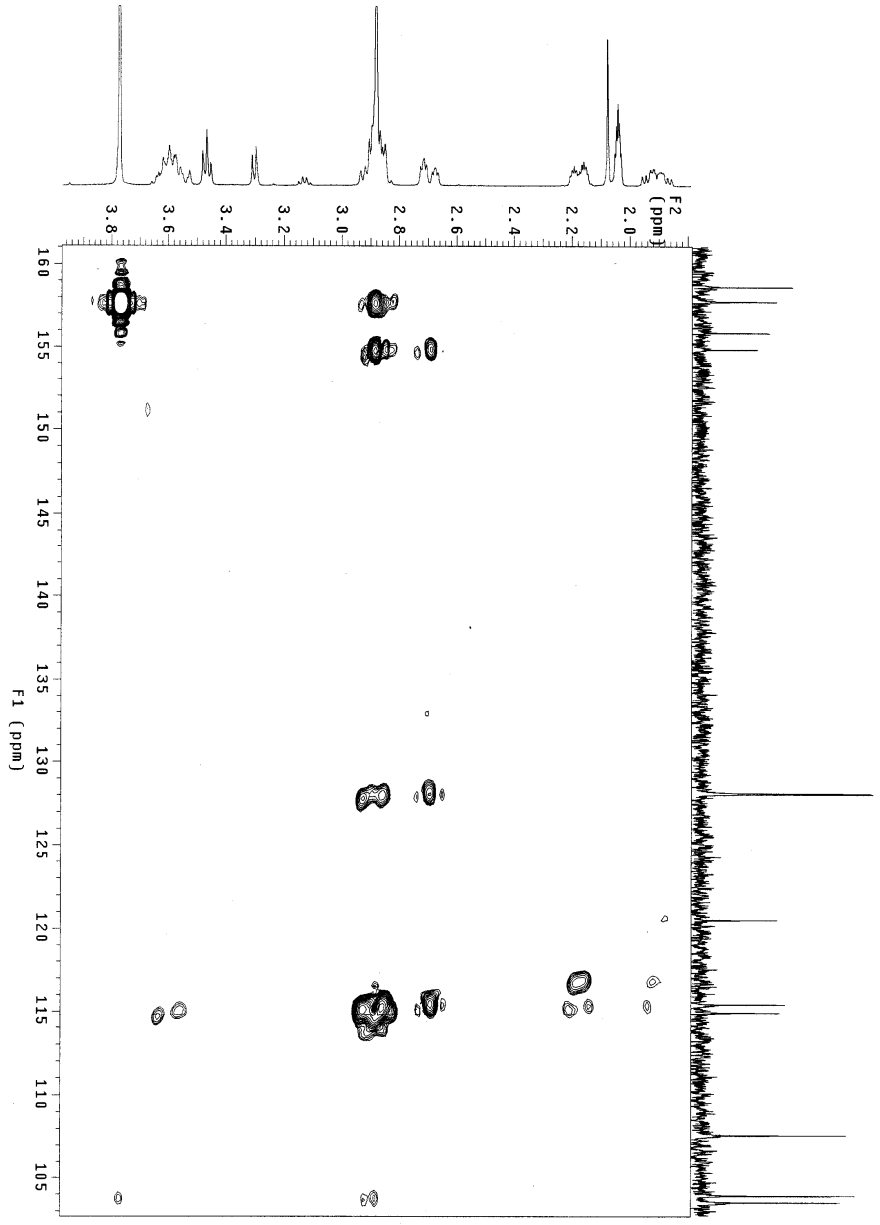
S 7.2 HMBC Spectrum of **7**



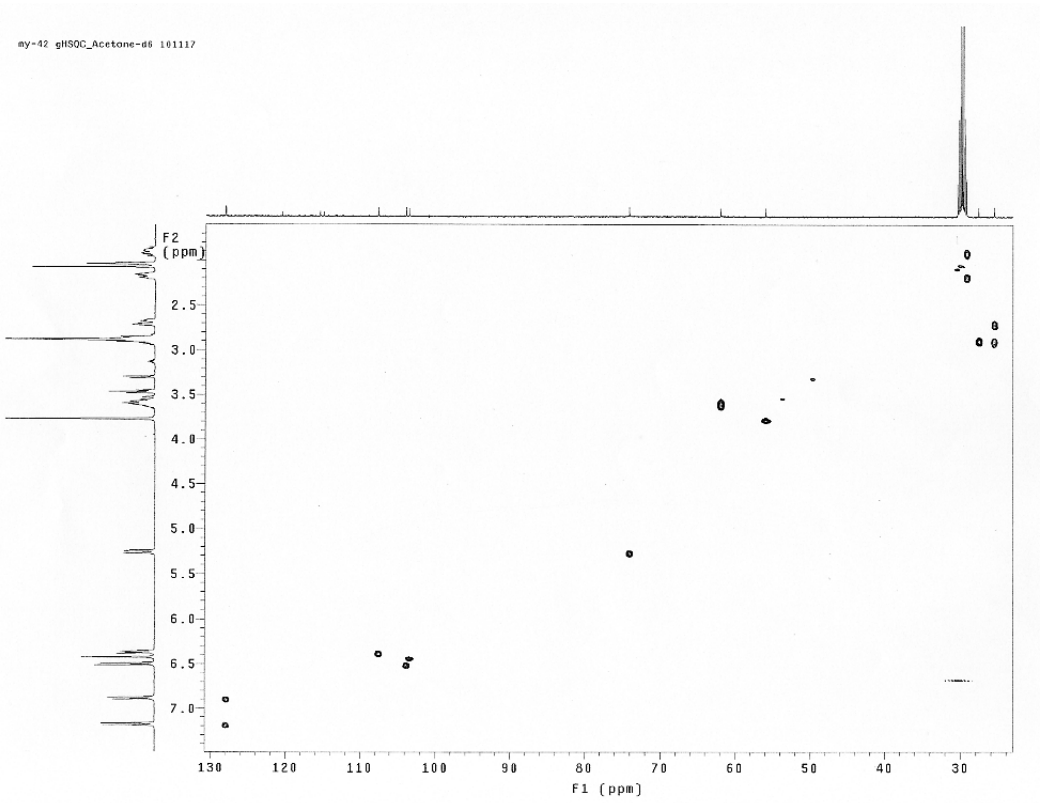
S 7.2.1 The magnified HMBC Spectrum of **7**



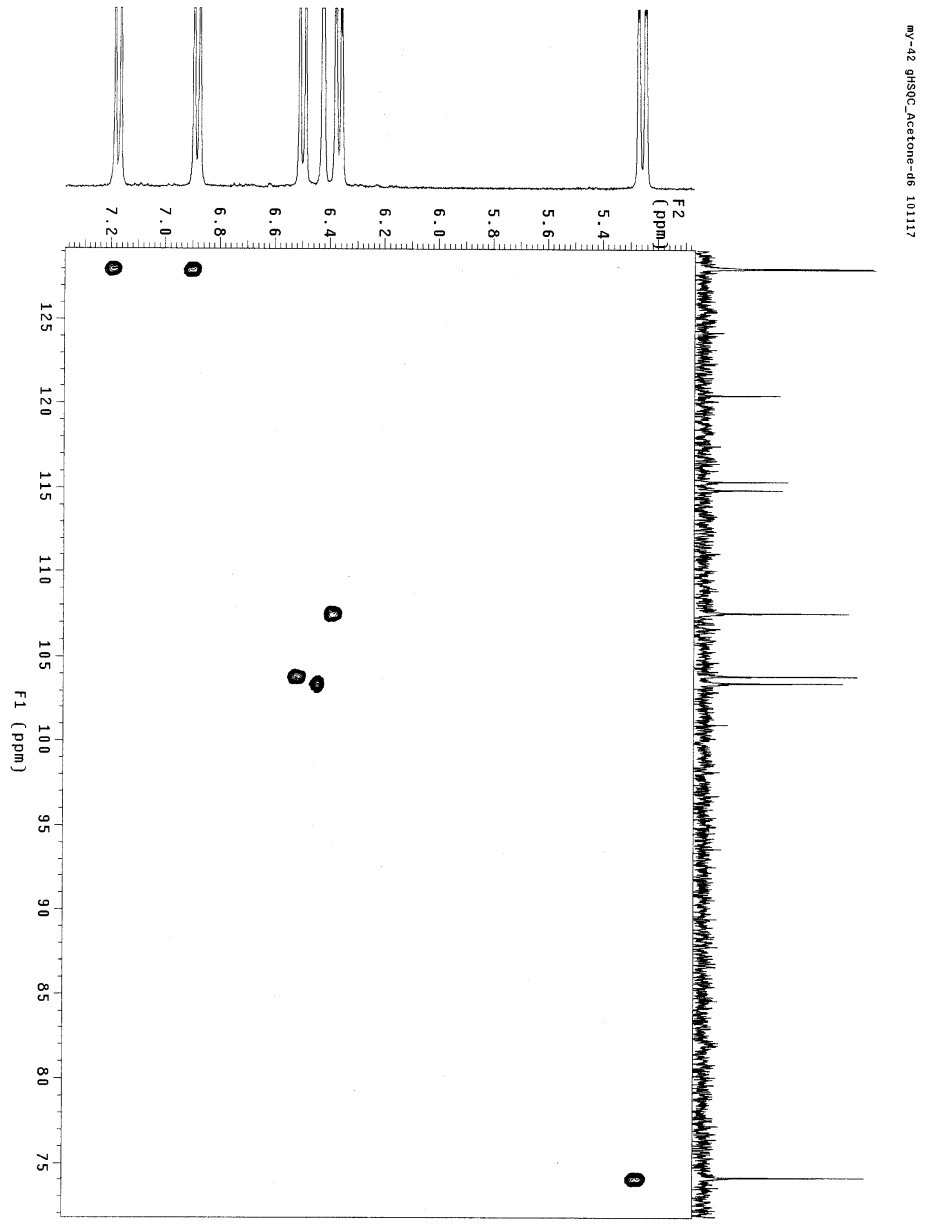
S 7.2.2 The magnified HMBC Spectrum of **7**



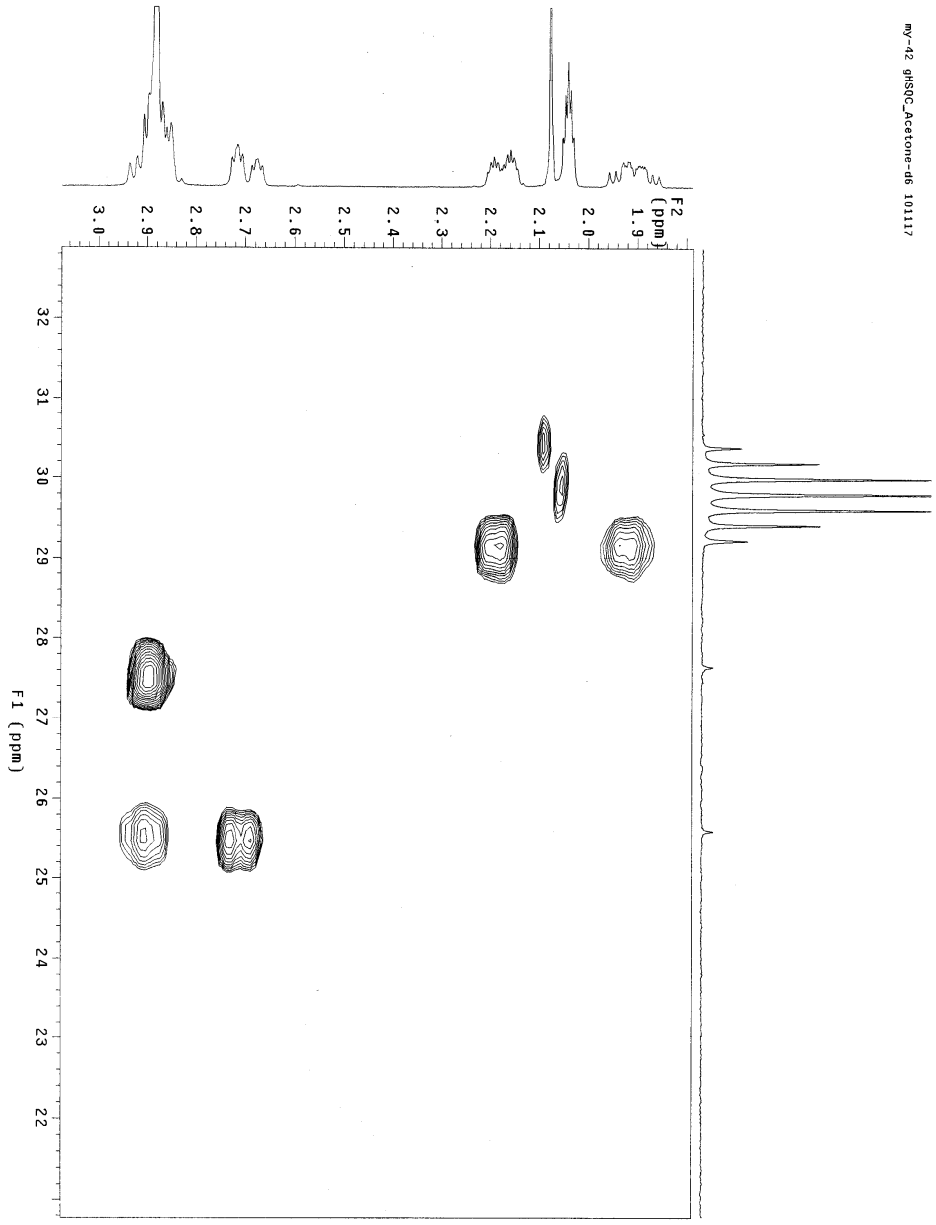
S 7.3 HSQC Spectrum of **7**



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

SIOC

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

Card Serial Number: **GCT-T*1011*-OS0612**

Sample Serial Number: **My-42**

Operator: **Li**

Date: **2010/11/26**

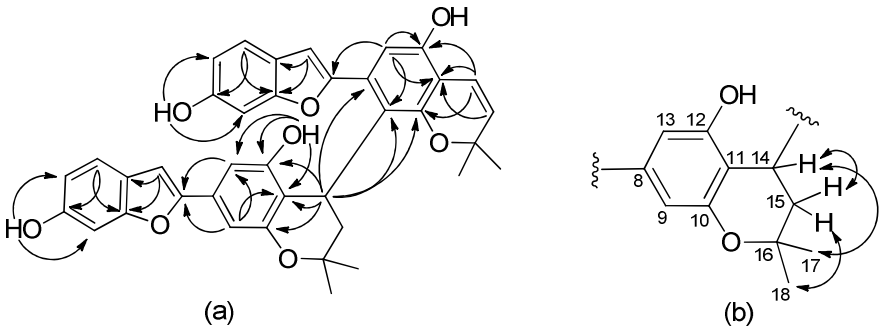
Elemental Composition Report

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)

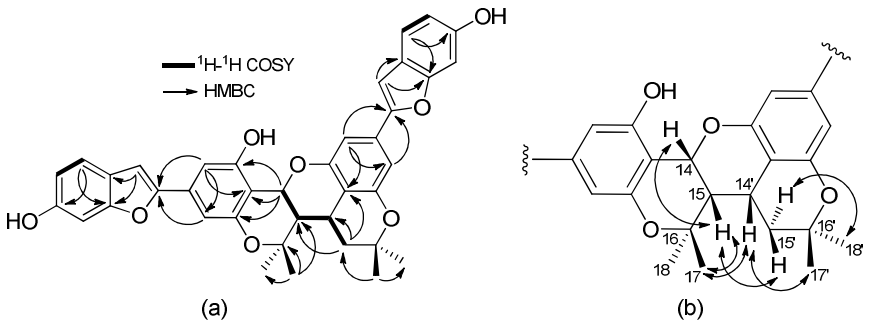
Minimum:				-1.5		
Maximum:		1.5	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
316.1308	316.1311	-0.3	-0.9	9.0	2	C18 H20 O5
	316.1297	1.1	3.4	9.5	1	C16 H18 N3 O4

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



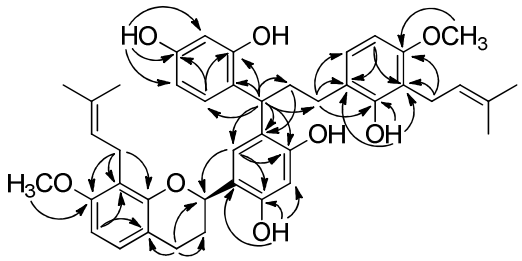
(a) Key HMBC correlations of **1**. (b) Key ROESY correlations of **1**

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



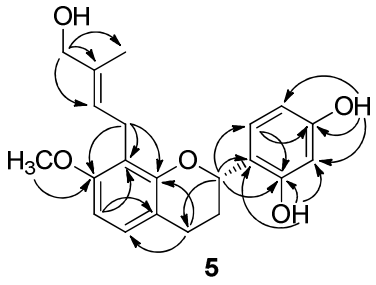
(a) Key HMBC and ^{1}H-^{1}H COSY correlations of **2**. (b) Key ROESY correlations of **2**.

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



3

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



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