

# **Aromatic compounds from an aqueous extract of “ban lan gen” and their antiviral activities**

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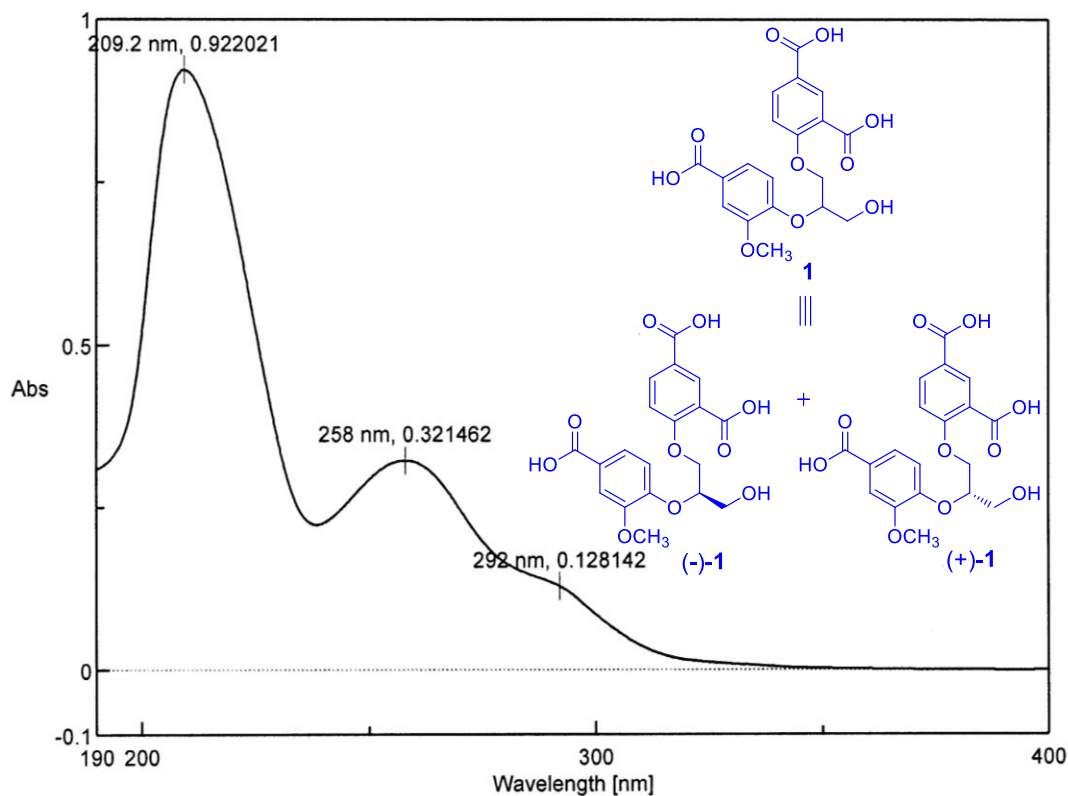
## **Supporting Information**

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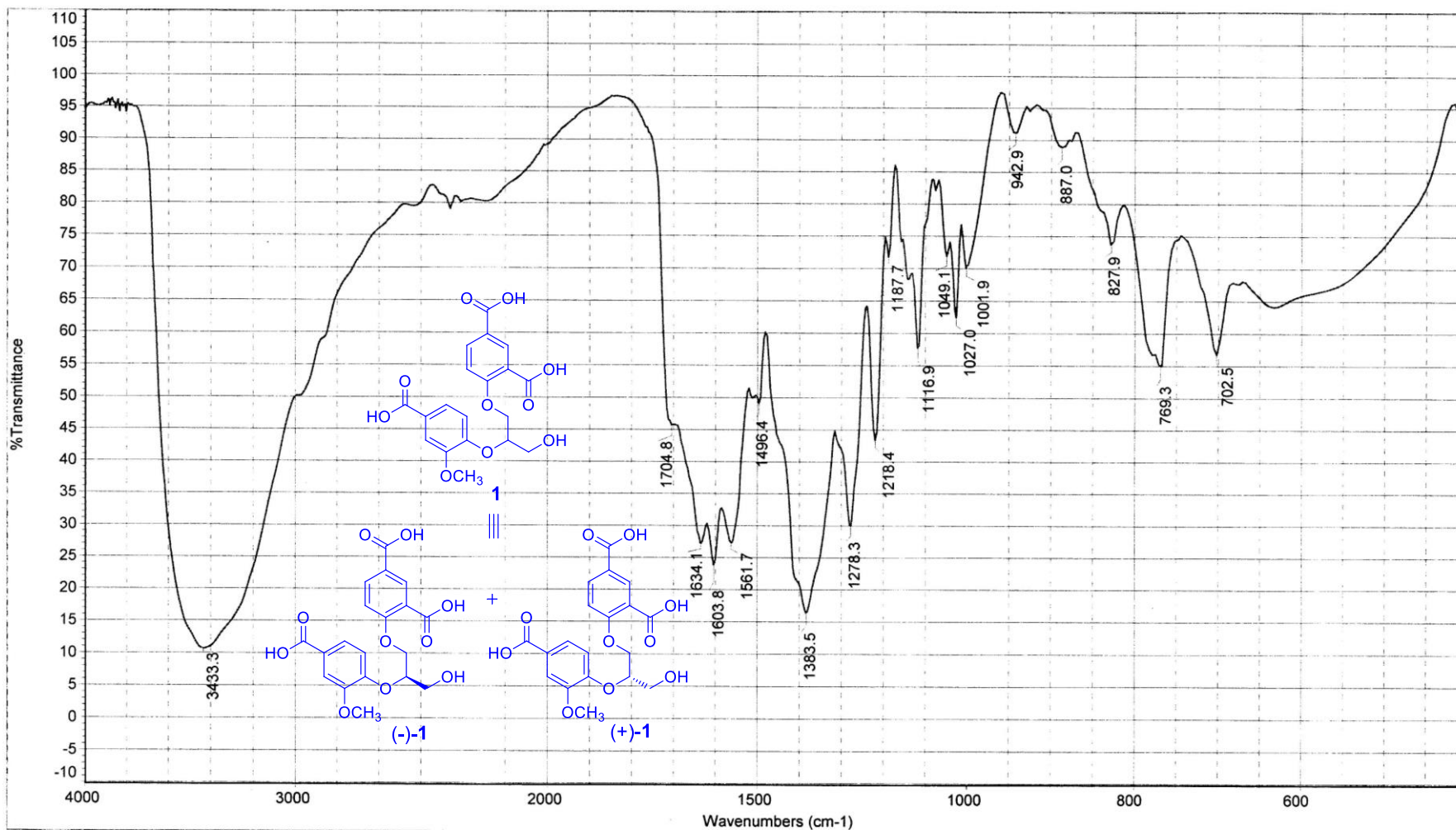
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 Comment 0.02  
 User  
 Division UV  
 Company 324  
 [Measurement Information]  
 Instrument Name V-650  
 Model Name V-650  
 Serial No. A034461150

Accessory PSC-718  
 Accessory S/N A001761114  
 Position 1  
 Cell Length 10 mm  
 Temperature 19.94 C  
 Control Sensor Holder  
 Monitor Sensor Holder  
 Start Mode Start immediately

Photometric Mode Abs  
 Measurement range 400 - 190 nm  
 Data pitch 0.2 nm  
 Band width(UV/Vis) 2.0 nm  
 Response Medium  
 Scanning speed 200 nm/min  
 Source Change 340 nm  
 Light Source D2/WI  
 Filter Exchange Step  
 Correction Baseline

[Data Information]  
 Creation Date 2014-6-10 10:32  
 Data array type Linear data array  
 Horizontal Wavelength [nm]  
 Vertical Abs  
 Start 400 nm  
 End 190 nm  
 Data pitch 0.2 nm  
 Data points 1051

**Figure S1.** The UV spectrum of **1** in MeOH



日期: 星期四 6月 26 09:43:10 2014 (GMT+08:00) Sample Name : BLG - L - 118rp

(显微镜透射法FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换显微镜红外(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S2. The IR spectrum of 1.

# Single Mass Spectrum Deconvolution Report

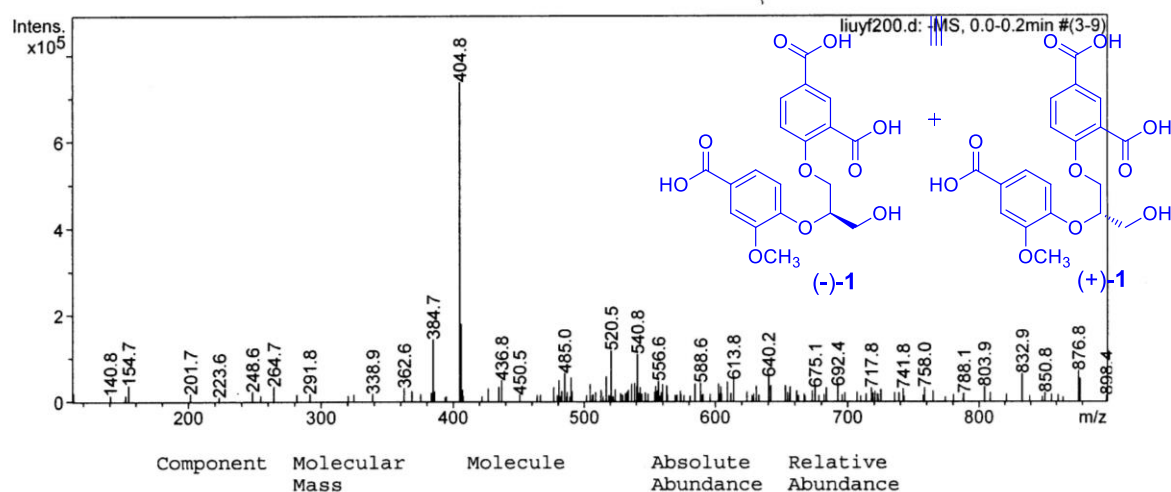
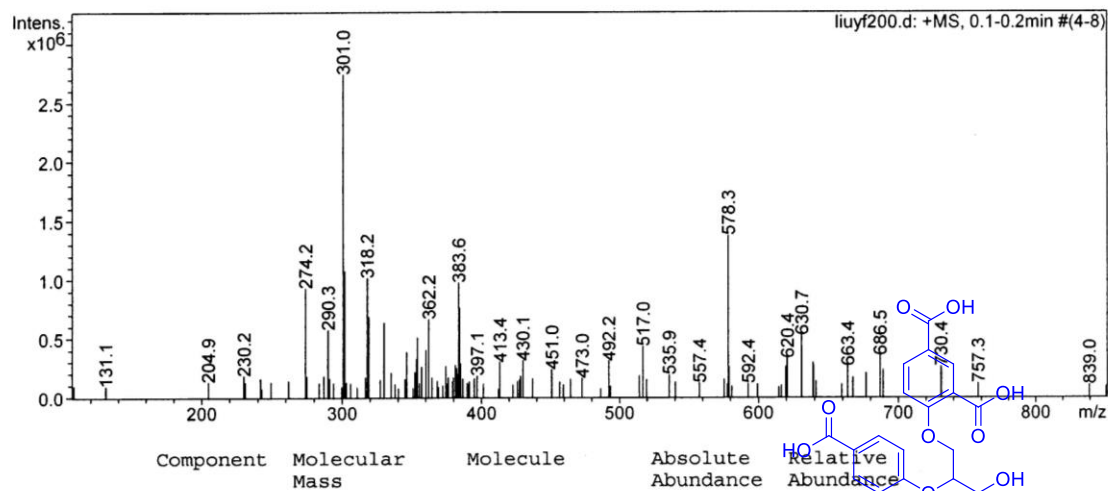
**Analysis Name:** liuyf200.d  
**Method:** TEST.MS  
**Sample Name:** BLG-L-118RP  
**Analysis Info:**

**Instrument:** LC-MSD-Trap-SL  
**Operator:** Operator

**Print Date:** 8/22/2013 11:56:16 AM  
**Acq. Date:** 8/22/2013 11:54:01 AM

## Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	53.0	Scan Begin	100 m/z
Ion Polarity	Positive	Octopole RF Amplitude	171.0 Vpp	Scan End	900 m/z
Ion Source Type	ESI	Capillary Exit	-121.0 Volt	Averages	5 Spectra
Dry Temp (Set)	330 °C	Skimmer	-40.0 Volt	Max. Accu Time	200000 µs
Nebulizer (Set)	15.00 psi	Oct 1 DC	-12.00 Volt	ICC Target	467
Dry Gas (Set)	6.00 l/min	Oct 2 DC	-1.70 Volt	Charge Control	on



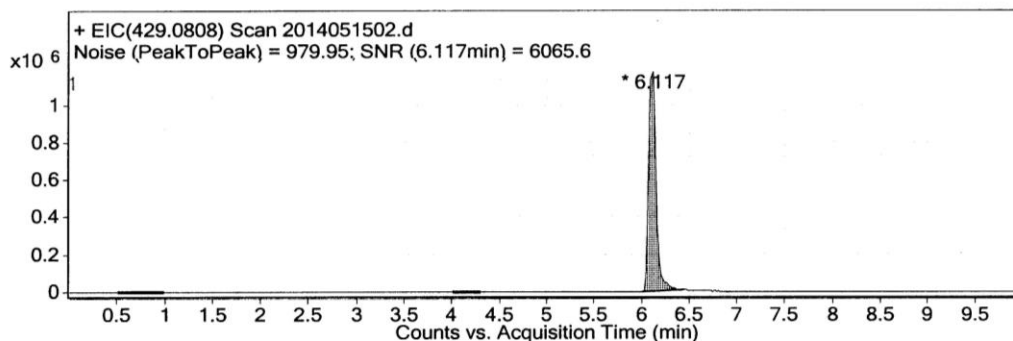
**Figure S3.** The ESI mass spectrum of **1**

# Qualitative Analysis Report

<b>Data Filename</b>	2014051502.d	<b>Sample Name</b>	BLG-L-118rp
<b>Sample Type</b>	Sample	<b>Position</b>	P1-C2
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	TEST LCMS.m	<b>IRM Calibration Status</b>	XXXXXXXXXX
<b>DA Method</b>	TEST LCMS.m	<b>Comment</b>	

## User Chromatograms

Fragmentor Voltage 135    Collision Energy 0    Ionization Mode ESI



### Integration Peak List

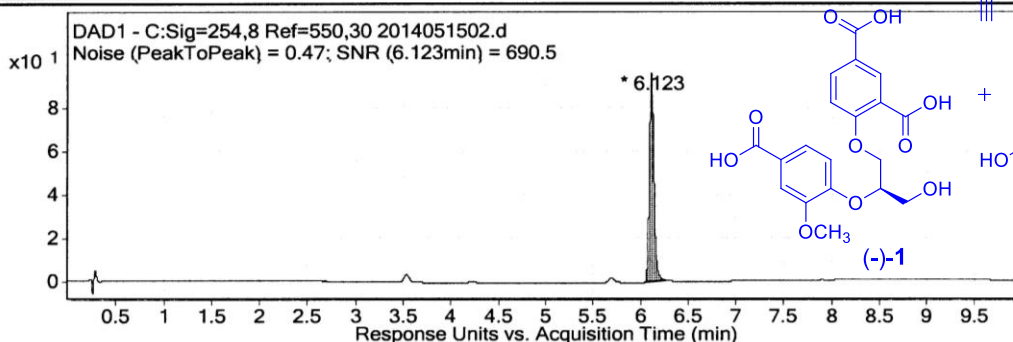
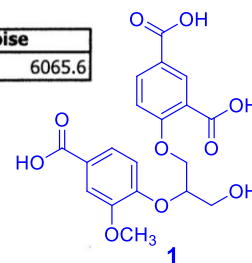
Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	6.004	6.117	6.455	1171470	5943982	100	6065.6

### Noise Measurements

Noise Type	Signal Definition	Noise Multiplier	Noise Value
Peak-to-Peak	Area	1	979.9468994

### Noise Regions

Start	End
0.5	1
4	4.3
9.99	11



### Integration Peak List

Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	6.038	6.123	6.27	96.3	322.99	100	690.5

### Noise Measurements

Noise Type	Signal Definition	Noise Multiplier	Noise Value
Peak-to-Peak	Area	1	0.467777252

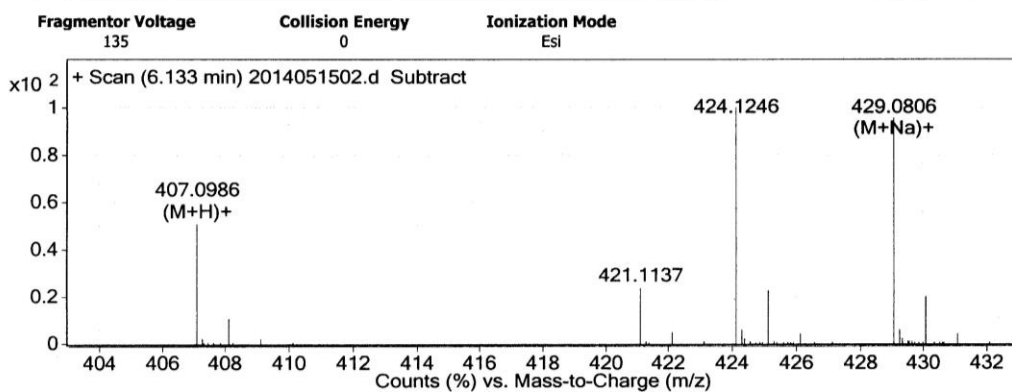
### Noise Regions

Start	End
0.5	1
4	4.3
9.99	11

## User Spectra

Figure S4. The (+)-HRESIMS report of 1, page 1.

# Qualitative Analysis Report



**Peak List**

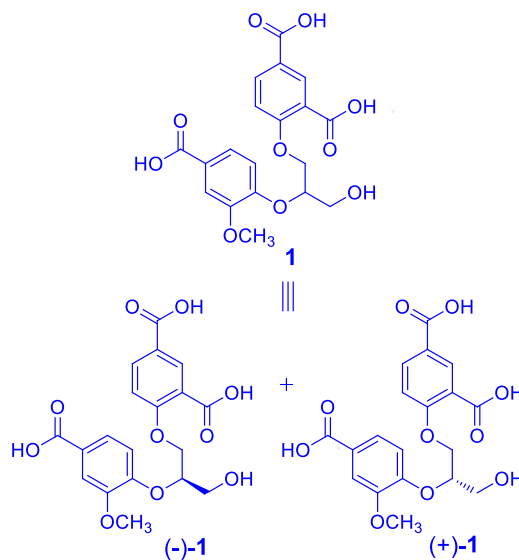
m/z	z	Abund	Formula	Ion
389.0878	1	453643		
390.0905	1	100196		
407.0986	1	505708	C19 H19 O10	(M+H)+
408.1012	1	107887	C19 H19 O10	(M+H)+
421.1137	1	235482		
424.1246	1	998151		
424.2951		58730		
425.1278	1	225058		
429.0806	1	958115	C19 H18 Na O10	(M+Na)+
430.0838	1	199649	C19 H18 Na O10	(M+Na)+

**Formula Calculator Element Limits**

Element	Min	Max
C	3	100
H	0	500
O	0	90
N	0	5
S	0	2
Cl	0	0
Br	0	0
Si	0	0
F	0	0
P	0	0

**Formula Calculator Results**

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C19 H18 O10	TRUE	406.0913	406.09	-3.18	C19 H19 O10	99.81
C20 H14 N4 O6		406.0913	406.0913	0.1	C20 H15 N4 O6	99.81
C16 H22 O10 S		406.0913	406.0934	5.12	C16 H23 O10 S	98.57
C21 H18 N4 O S2		406.0913	406.0922	2.24	C21 H19 N4 O S2	97.65
C20 H22 O5 S2		406.0913	406.0909	-1.05	C20 H23 O5 S2	97.64
C11 H22 N2 O12 S		406.0913	406.0893	-4.8	C11 H23 N2 O12 S	97.03
C19 H18 O10	TRUE	406.0914	406.09	-3.42	C19 H18 Na O10	99.82
C20 H14 N4 O6		406.0914	406.0913	-0.14	C20 H14 N4 Na O6	99.75
C16 H22 O10 S		406.0914	406.0934	4.87	C16 H22 Na O10 S	98.71
C20 H22 O5 S2		406.0914	406.0909	-1.29	C20 H22 Na O5 S2	97.58
C21 H18 N4 O S2		406.0914	406.0922	1.99	C21 H18 N4 Na O S2	97.55
C11 H22 N2 O12 S		406.0914	406.0893	-5.04	C11 H22 N2 Na O12 S	97.19



--- End Of Report ---

**Figure S5.** The (+)-HRESIMS report of **1**, page 2.

MS Formula Results: + Scan (6.133 min) Sub (2014051502.d)

m/z	Ion	Formula	Abundance
407.0986	(M+H) <sup>+</sup>	C19 H19 O10	505708.2

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
✓	C19 H18 O10	C19 H19 O10	407.0973	99.81		406.0913	406.09	-3.18	3.18	99.99	99.88	99.67	407.0986	11
☐	C20 H14 N4 O6	C20 H15 N4 O6	407.0986	99.81		406.0913	406.0913	0.1	0.1	99.35	99.96	100	407.0986	16
☐	C16 H22 O10 S	C16 H23 O10 S	407.1006	98.57		406.0913	406.0934	5.12	5.12	96.69	99.7	99.14	407.0986	6
☐	C21 H18 N4 O S2	C21 H19 N4 O S2	407.0995	97.65		406.0913	406.0922	2.24	2.24	92.43	99.54	99.84	407.0986	15
☐	C20 H22 O5 S2	C20 H23 O5 S2	407.0981	97.64		406.0913	406.0909	-1.05	1.05	92.2	99.53	99.96	407.0986	10
☐	C11 H22 N2 O12 S	C11 H23 N2 O12 S	407.0966	97.03		406.0913	406.0893	-4.8	4.8	91.12	99.69	99.24	407.0986	2

m/z	Ion	Formula	Abundance
429.0806	(M+Na) <sup>+</sup>	C19 H18 Na O10	958114.7

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
✓	C19 H18 O10	C19 H18 Na O10	429.0792	99.82		406.0914	406.09	-3.42	3.42	99.98	99.98	99.65	429.0806	11
☐	C20 H14 N4 O6	C20 H14 N4 Na O6	429.0806	99.75		406.0914	406.0913	-0.14	0.14	99.15	99.98	100	429.0806	16
☐	C16 H22 O10 S	C16 H22 Na O10 S	429.0826	98.71		406.0914	406.0934	4.87	4.87	96.87	99.75	99.29	429.0806	6
☐	C20 H22 O5 S2	C20 H22 Na O5 S2	429.0801	97.58		406.0914	406.0909	-1.29	1.29	91.96	99.57	99.95	429.0806	10
☐	C21 H18 N4 O S2	C21 H18 N4 Na O S2	429.0814	97.55		406.0914	406.0922	1.99	1.99	92.02	99.51	99.88	429.0806	15
☐	C11 H22 N2 O12 S	C11 H22 N2 Na O12 S	429.0786	97.19		406.0914	406.0893	-5.04	5.04	91.69	99.68	99.24	429.0806	2

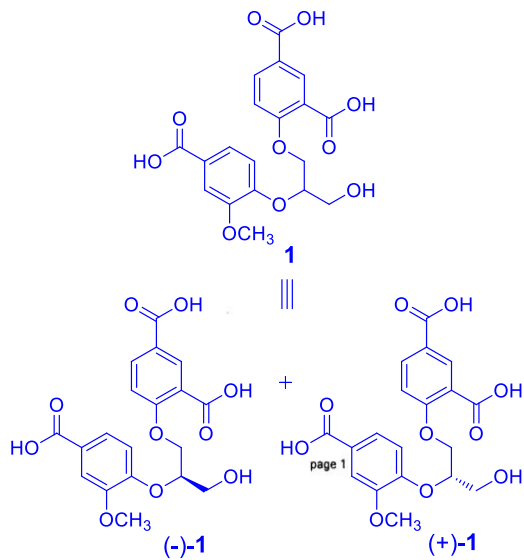


Figure S6. The (+)-HRESIMS report of 1, page 3.



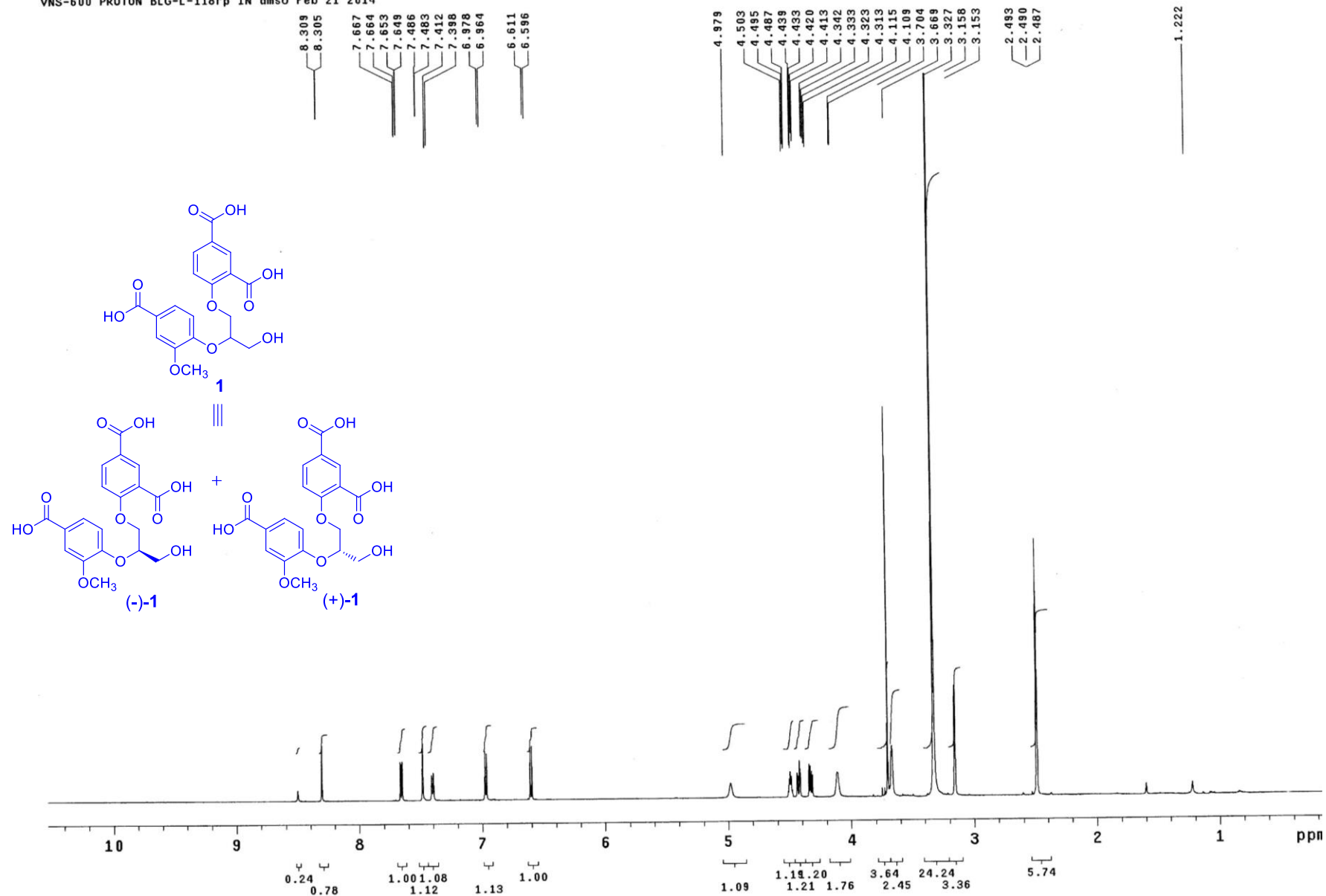


Figure S7. The <sup>1</sup>H NMR spectrum of **1** in DMSO-*d*<sub>6</sub> (600 MHz).

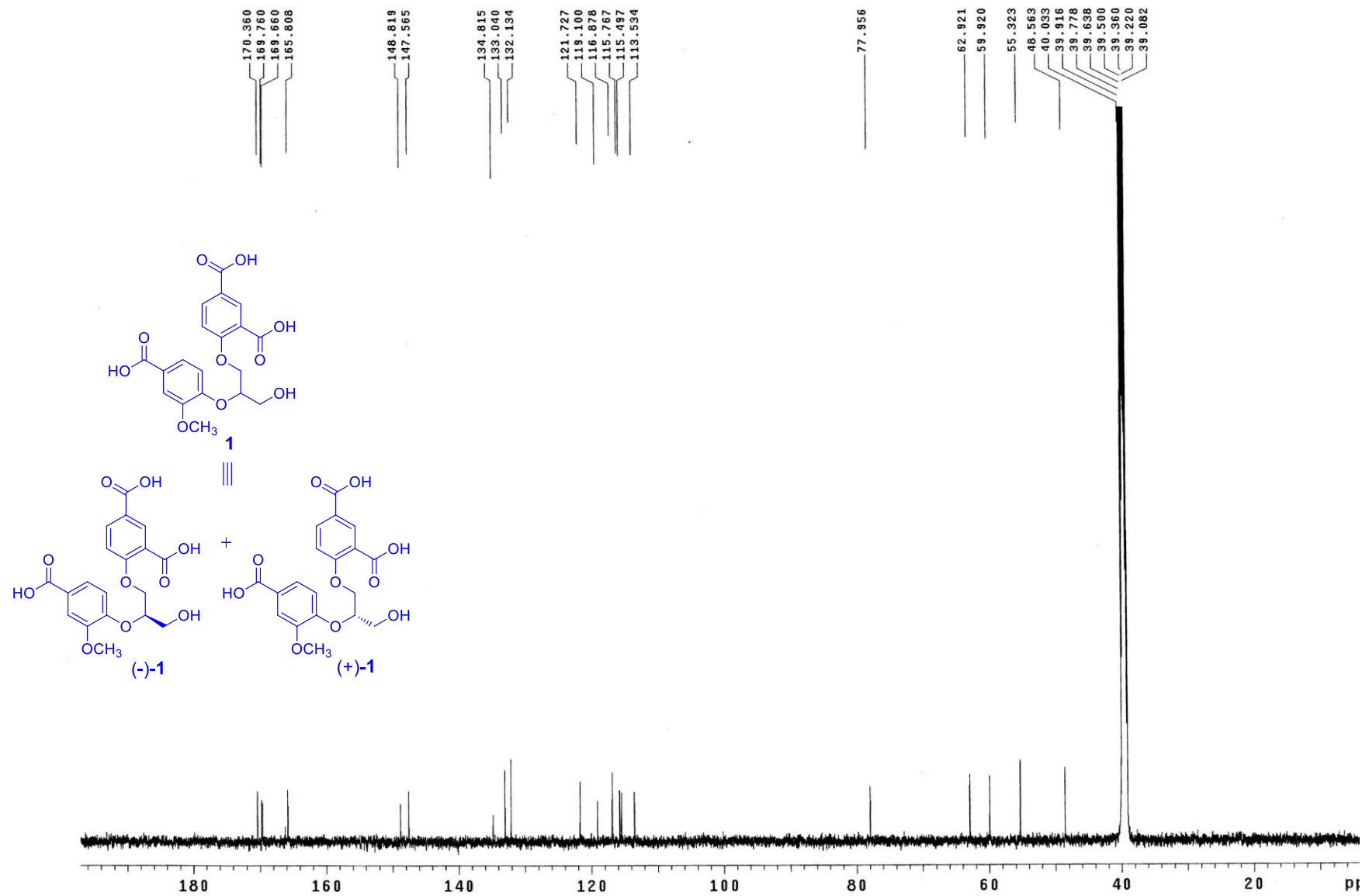


Figure S8. The <sup>13</sup>C NMR spectrum of **1** in DMSO-*d*<sub>6</sub> (150 MHz).

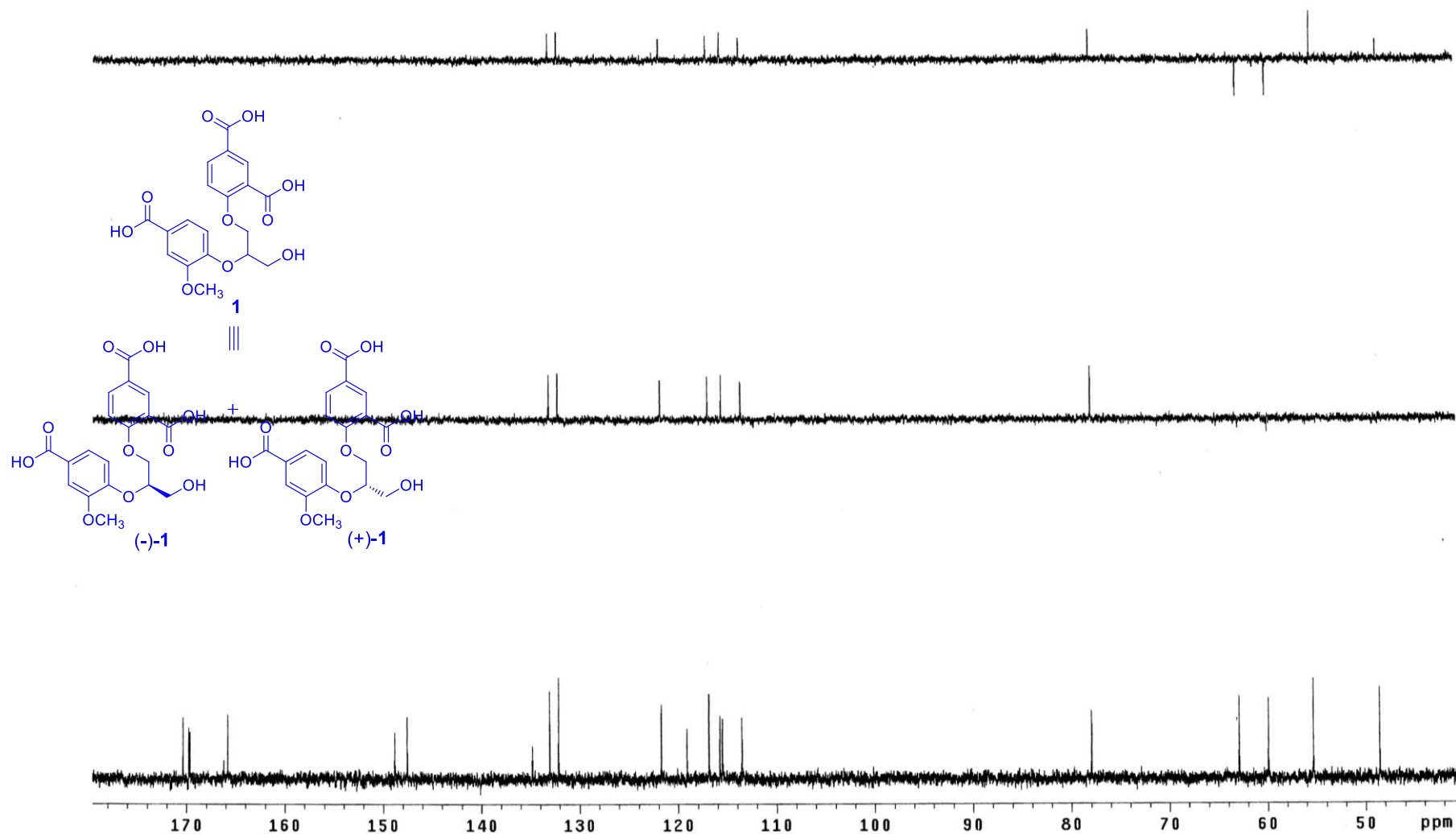


Figure S9. The DEPT spectrum of **1** in DMSO-*d*<sub>6</sub> (150 MHz).

VNS-600 gCOSY BLG-L-118rp IN dms0 May 6 2014

Temp. 25.0 C / 298.1 K  
Sample #12, Operator: vjwalk

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 6443.3 Hz  
2D Width 6443.3 Hz  
2 repetitions  
256 increments  
OBSERVE H1, 599.6905197 MHz  
DATA PROCESSING  
Sq. sine bell 0.075 sec  
F1 DATA PROCESSING  
Sq. sine bell 0.027 sec  
FT size 2048 x 2048  
Total time 10 min

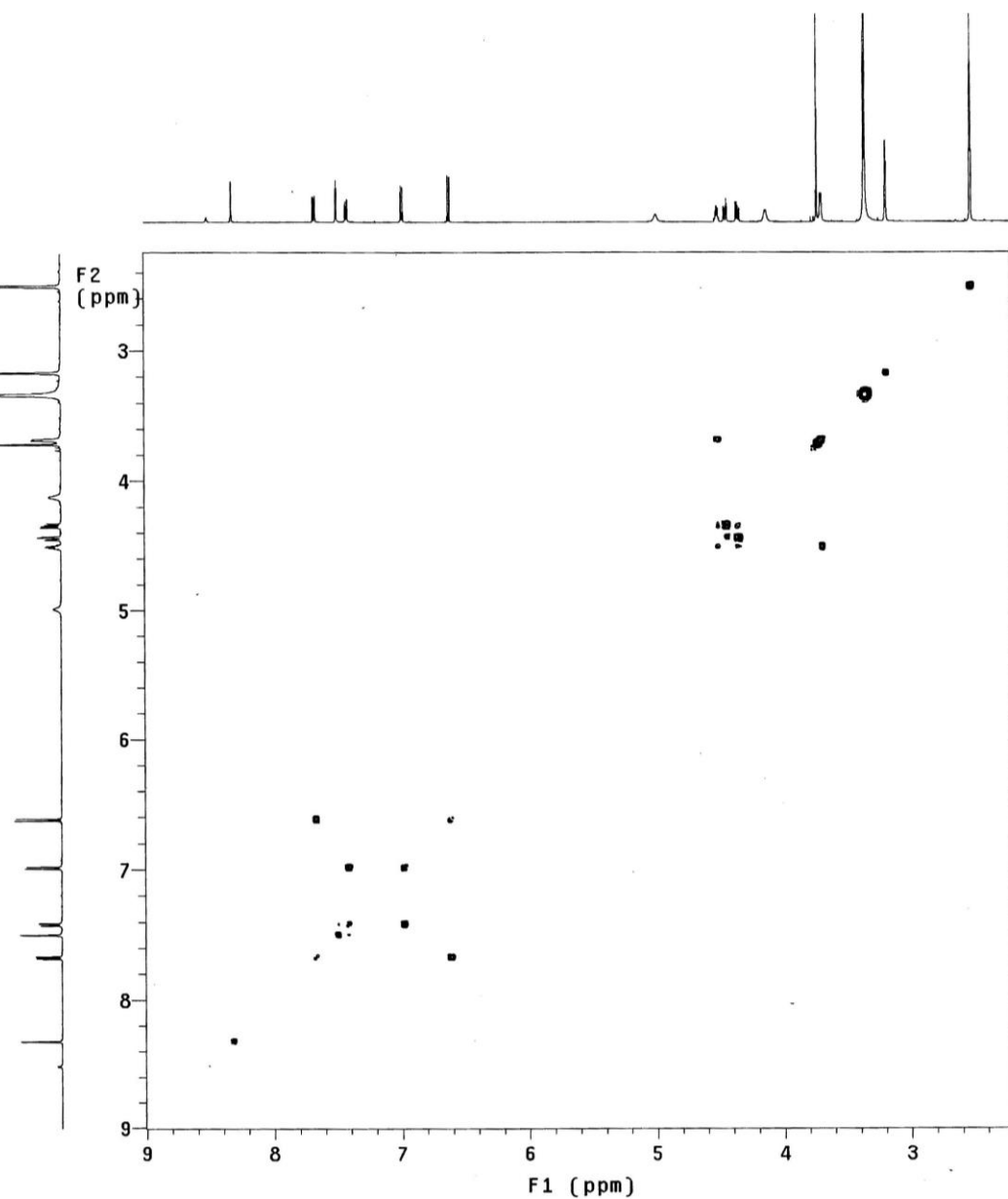
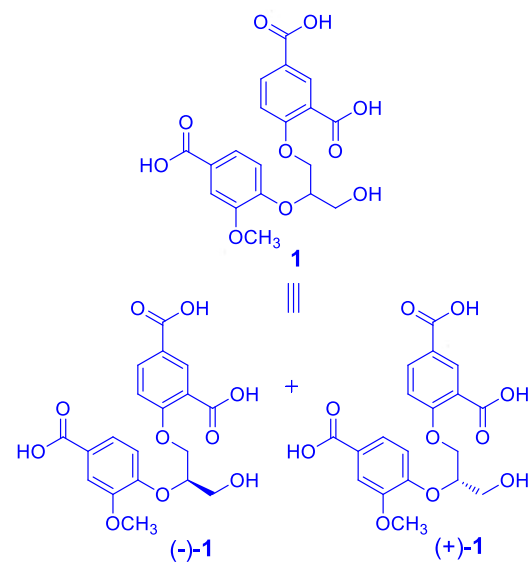


Figure S10. The <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 1 in DMSO-*d*<sub>6</sub> (600 MHz).

Temp. 25.0 C / 298.1 K  
 Sample #12, Operator: vjwalk

Relax. delay 1.000 sec  
 Acq. time 0.150 sec  
 Width 6443.3 Hz  
 2D Width 30154.5 Hz  
 48 repetitions  
 140 increments  
 OBSERVE H1, 599.6905246 MHz  
 DECOUPLE C13, 150.8058756 MHz  
 Power 36 dB  
 on during acquisition  
 off during delay  
 W40\_NEW-SW modulated  
 DATA PROCESSING  
 Sine bell 0.027 sec  
 F1 DATA PROCESSING  
 Sine bell 0.005 sec  
 FT size 4096 x 2048  
 Total time 2 hr, 14 min

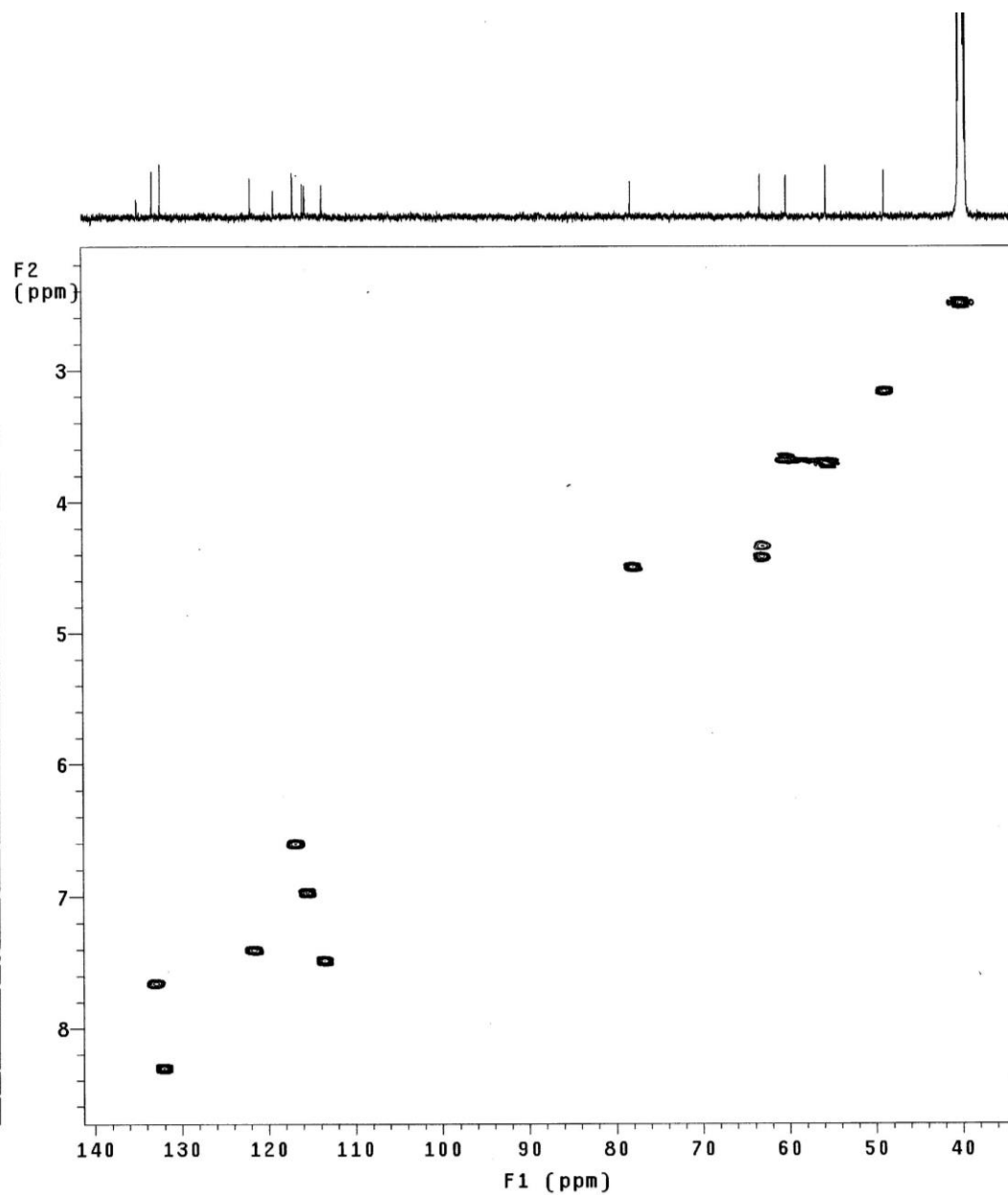
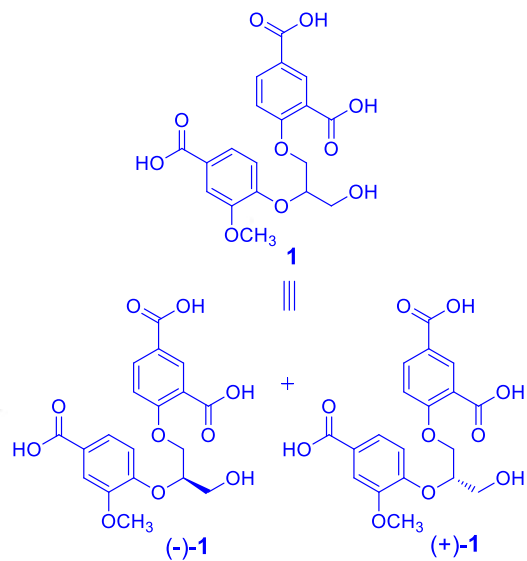
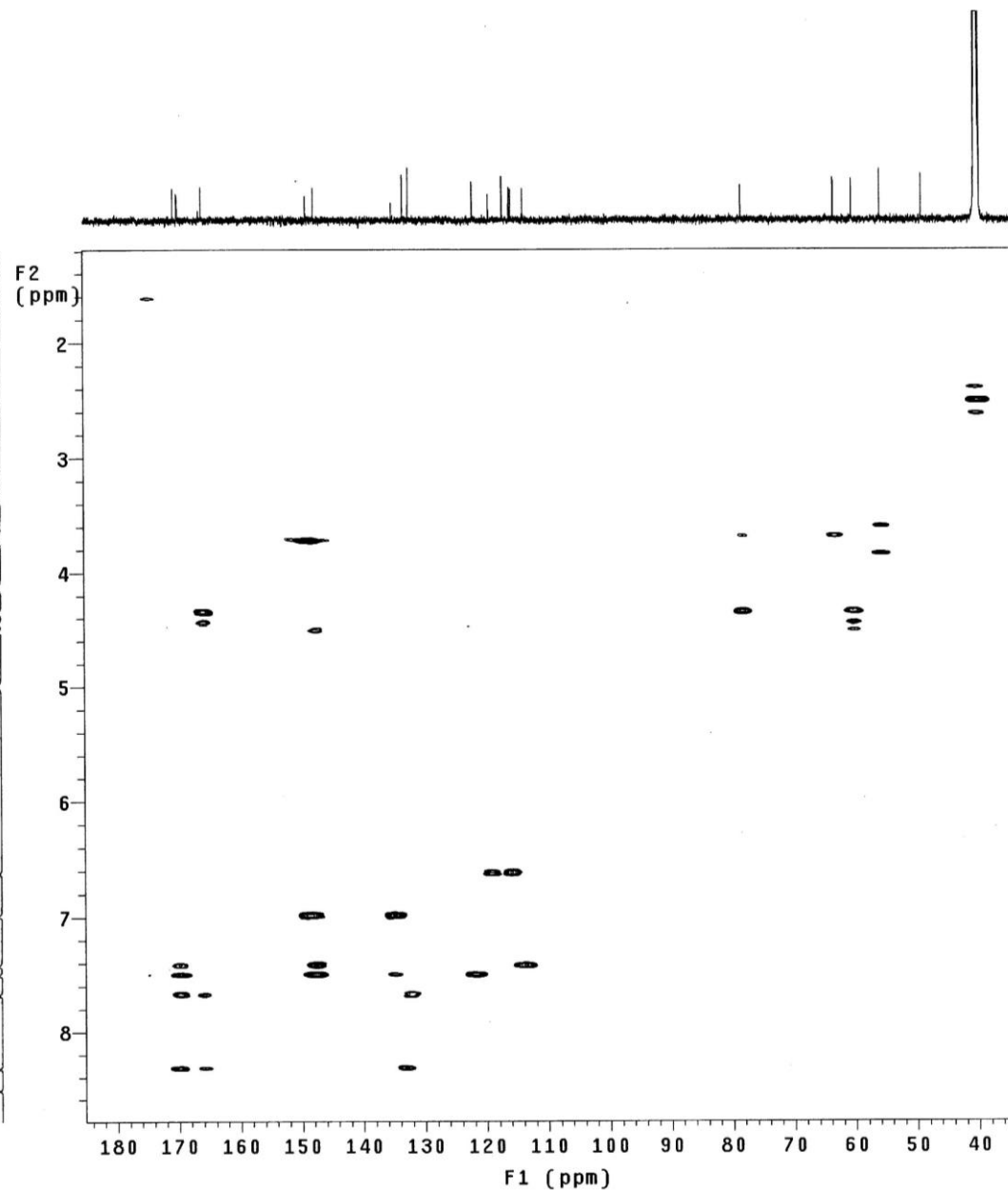
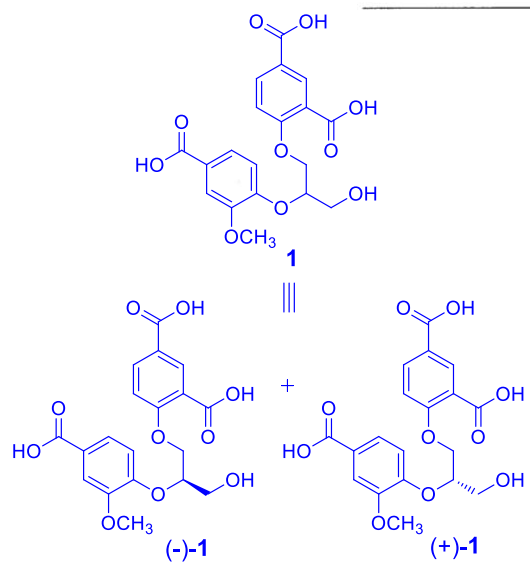


Figure S11. The HSQC spectrum of 1 in DMSO- $d_6$  (600 MHz for  $^1\text{H}$ ).

Temp. 25.0 C / 298.1 K  
Sample #12, Operator: vjwalk

Relax. delay 1.000 sec  
Acq. time 0.150 sec  
Width 6443.3 Hz  
2D Width 36182.7 Hz  
96 repetitions  
2 x 80 increments  
OBSERVE H1, 599.6905190 MHz  
DATA PROCESSING  
Sq. sine bell 0.075 sec  
F1 DATA PROCESSING  
Gauss apodization 0.002 sec  
FT size 4096 x 2048  
Total time 5 hr, 16 min

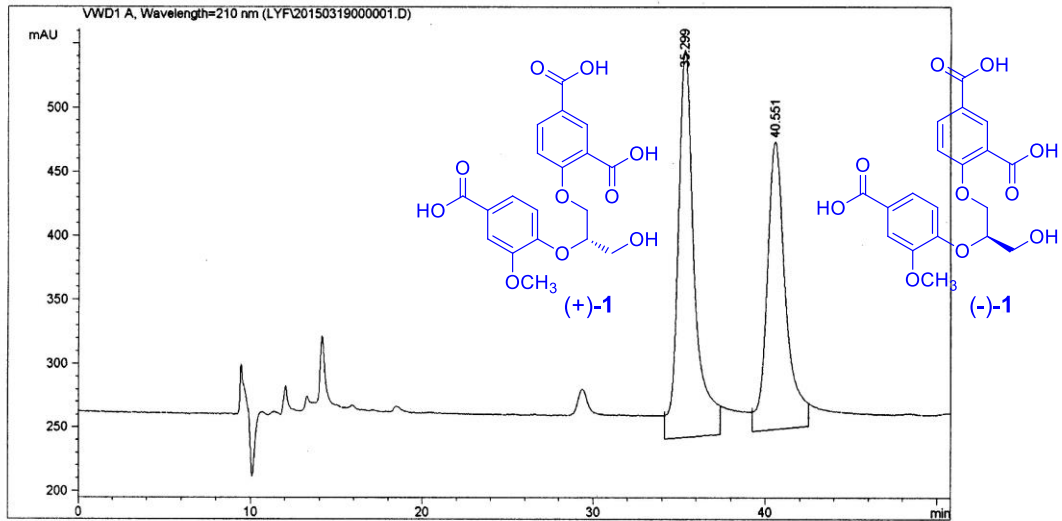


**Figure S12.** The HMBC spectrum of **1** in DMSO-*d*<sub>6</sub> (600 MHz for <sup>1</sup>H).

Data File C:\CHEM32\1\DATA\LYF\20150319000001.D  
 Sample Name: blg-1-118rp

```

-----
Acq. Operator   :
Acq. Instrument : Instrument 1           Location : Vial 1
Injection Date  : 2015-3-19 17:34:03
Acq. Method     : D:\DEF_LC.M
Last changed    : 2015-3-19 17:05:33
                  (modified after loading)
Analysis Method : D:\DEF_LC.M
Last changed    : 2015-3-21 9:47:20
                  (modified after loading)
Sample Info     : ZHENG:YI 4:1 0.1%tfa 1.5ml 210nm
  
```



Area Percent Report

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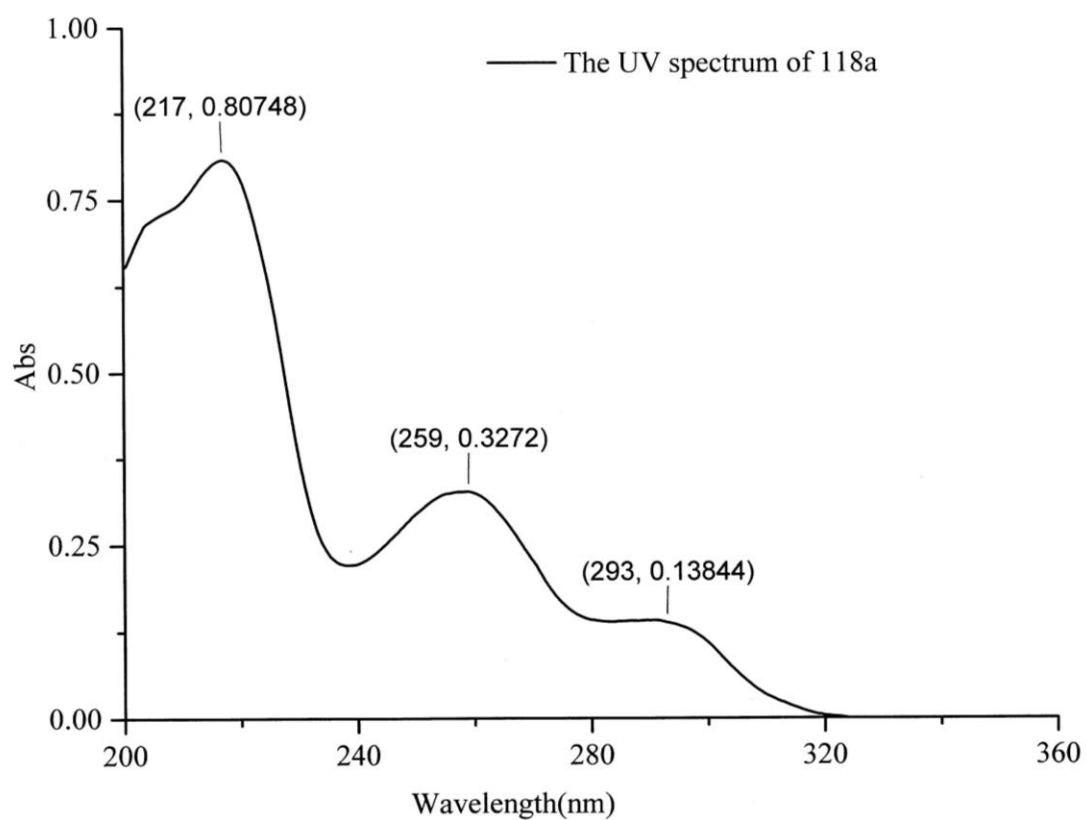
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Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	35.299	VV	0.9215	2.00012e4	303.01370	54.2378
2	40.551	VV	0.9077	1.68756e4	224.83284	45.7622
Totals :				3.68768e4	527.84654	

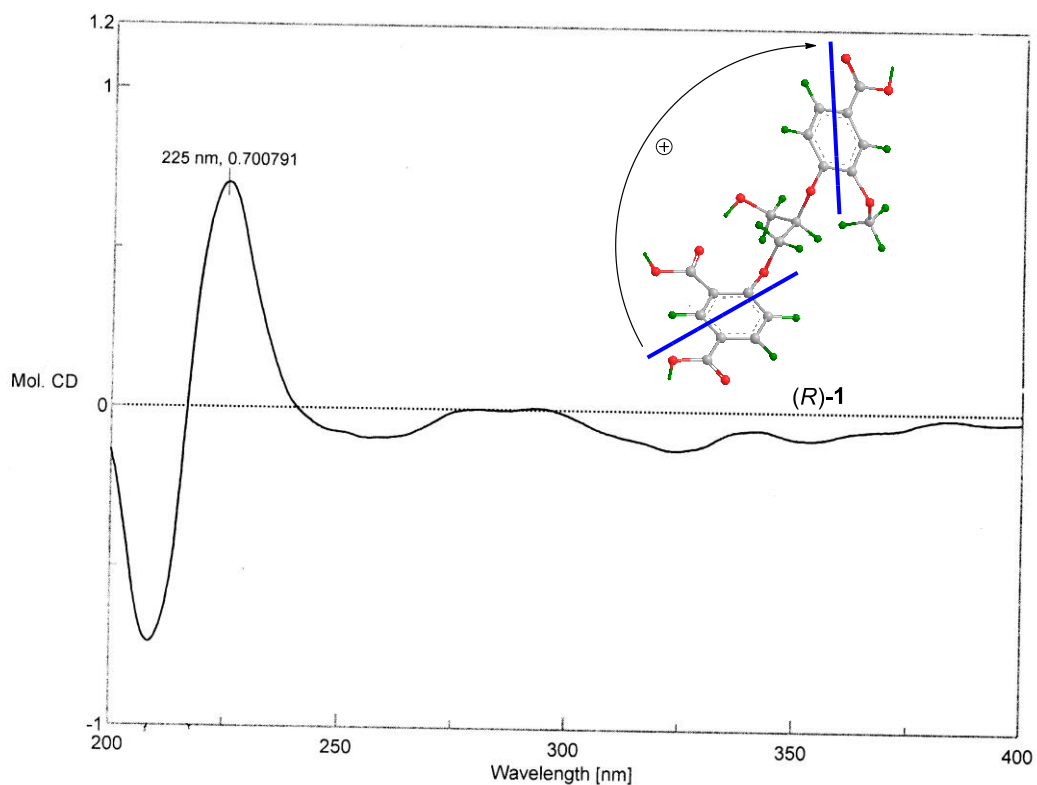
\*\*\* End of Report \*\*\*

**Figure S13.** The HPLC chromatogram of **1** on Chiralpak AD-H column [5  $\mu$ m, 250  $\times$  10 mm; Flow rate: 1.5 mL/min; mobile phase: iPrOH:n-hexane mixture (4:1, containing 0.1% TFA, v/v/v); temperature 23°C].



**Figure S14.** The UV spectrum of compound (–)-**1** in MeOH





[Comments]  
 Sample name BLG-118a  
 Comment  
 User  
 Division  
 Company dell

[Measurement Information]  
 Instrument Name J-815  
 Model Name J-815  
 Serial No. A024461168

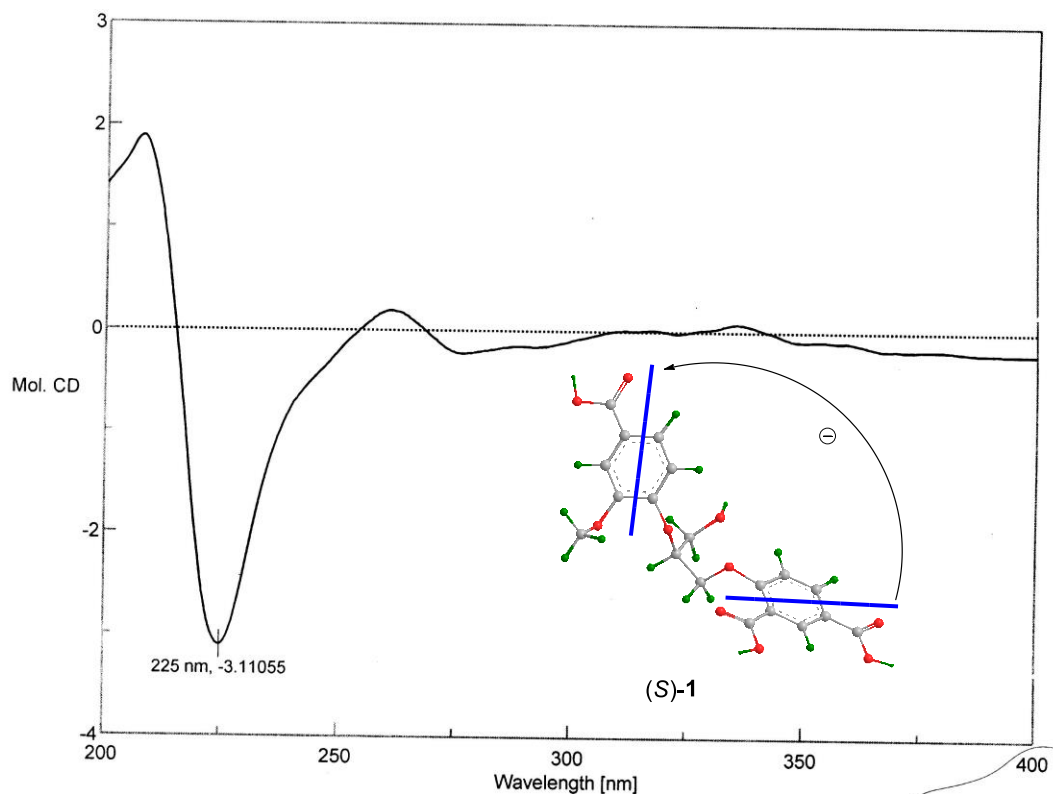
Accessory Standard  
 Accessory S/N A024461168  
 Cell Length 1 mm

Photometric Mode CD, HT, Abs  
 Measure Range 400 - 200 nm  
 Data pitch 0.5 nm  
 Sensitivity Standard  
 D.I.T. 1 sec  
 Band width 2.00 nm  
 Start Mode Immediately  
 Scanning Speed 200 nm/min  
 Baseline Correction Baseline  
 Shutter Control Auto  
 PMT Voltage Auto  
 Accumulations 2  
 Solvent MEOH  
 Concentration 0.3 (w/v)%

[Detailed Information]  
 Creation date 2015-4-1 17:27

Data array type Linear data array \* 3  
 Horizontal axis Wavelength [nm]  
 Vertical axis(1) Mol. CD  
 Vertical axis(2) HT [V]  
 Vertical axis(3) Abs  
 Start 400 nm  
 End 200 nm  
 Data interval 0.5 nm  
 Data points 401

**Figure S15.** The CD spectrum of (–)-1 in MeOH.



[Comments]  
 Sample name BLG-L-118b  
 Comment  
 User  
 Division  
 Company dell

[Measurement Information]  
 Instrument Name J-815  
 Model Name J-815  
 Serial No. A024461168

Accessory Standard  
 Accessory S/N A024461168  
 Cell Length 1 mm

Photometric Mode CD, HT, Abs  
 Measure Range 400 - 200 nm  
 Data pitch 0.5 nm  
 Sensitivity Standard  
 D.I.T. 1 sec  
 Band width 2.00 nm  
 Start Mode Immediately  
 Scanning Speed 200 nm/min  
 Baseline Correction Baseline  
 Shutter Control Auto  
 PMT Voltage Auto  
 Accumulations 2  
 Solvent MEOH  
 Concentration 0.123 (w/v)%

[Detailed Information]  
 Creation date 2015-4-1 17:25  
 Data array type Linear data array \* 3  
 Horizontal axis Wavelength [nm]  
 Vertical axis(1) Mol. CD  
 Vertical axis(2) HT [V]  
 Vertical axis(3) Abs  
 Start 400 nm  
 End 200 nm  
 Data interval 0.5 nm  
 Data points 401

Figure S16. The CD spectrum of compound (+)-1 in MeOH.

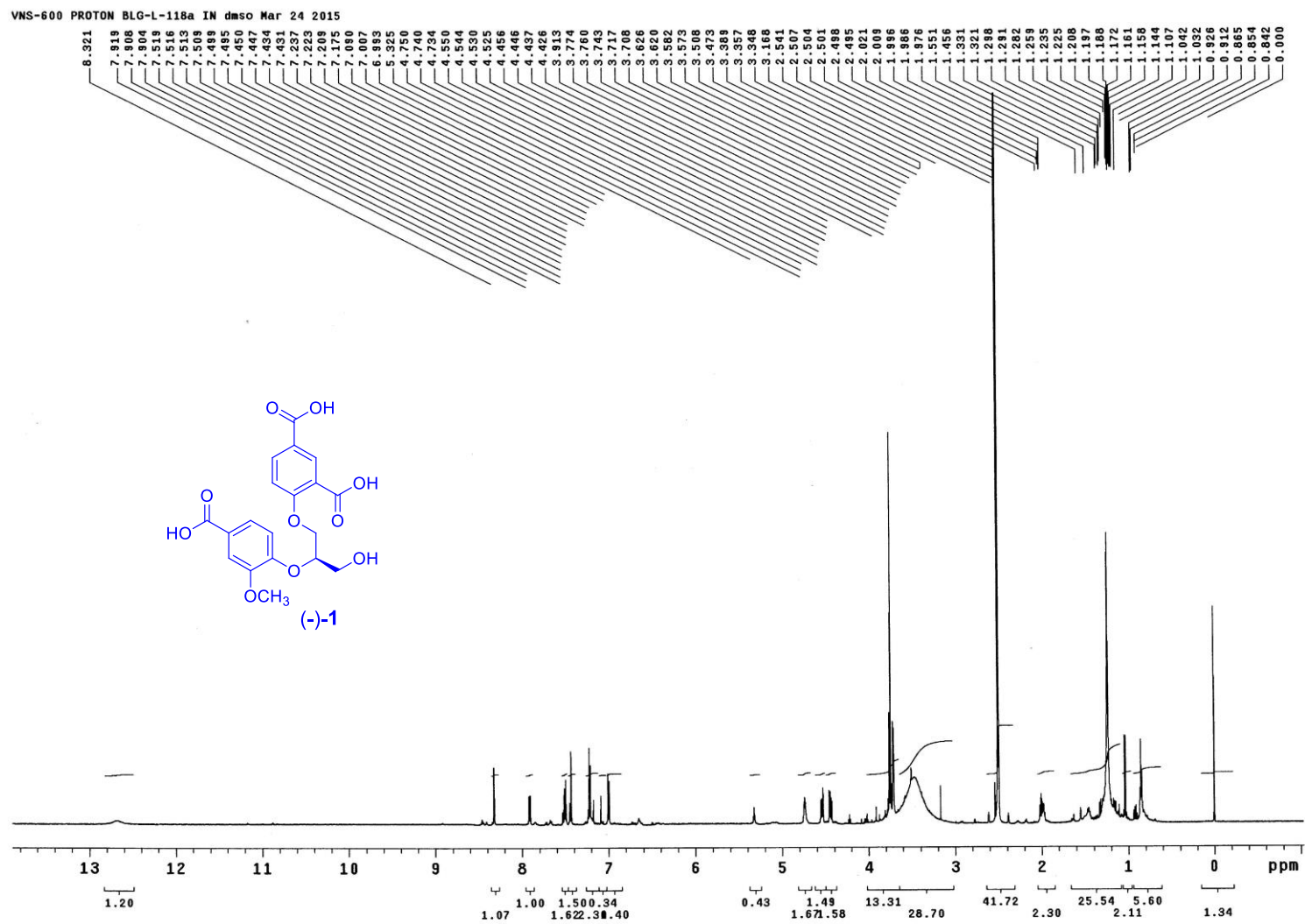
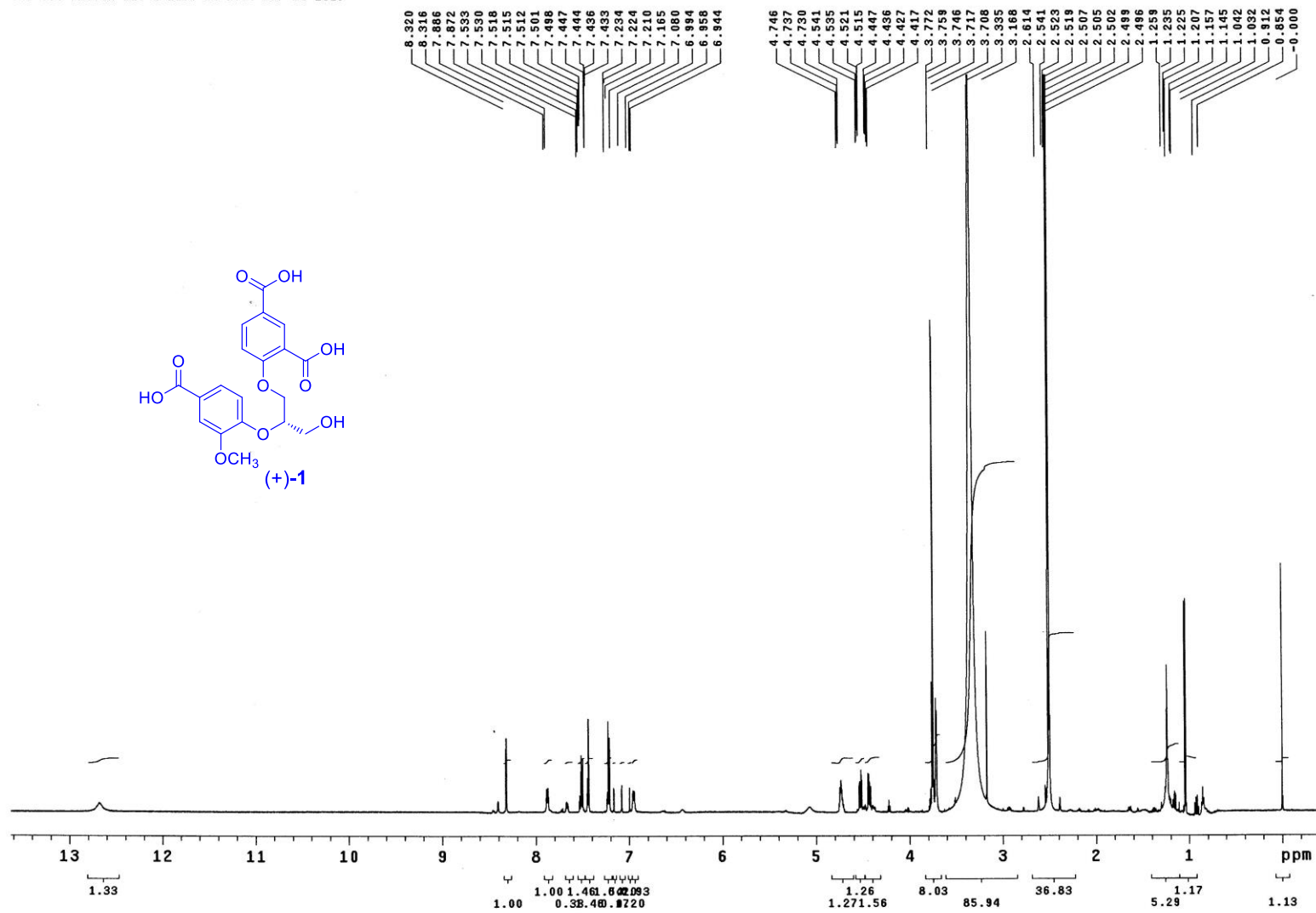
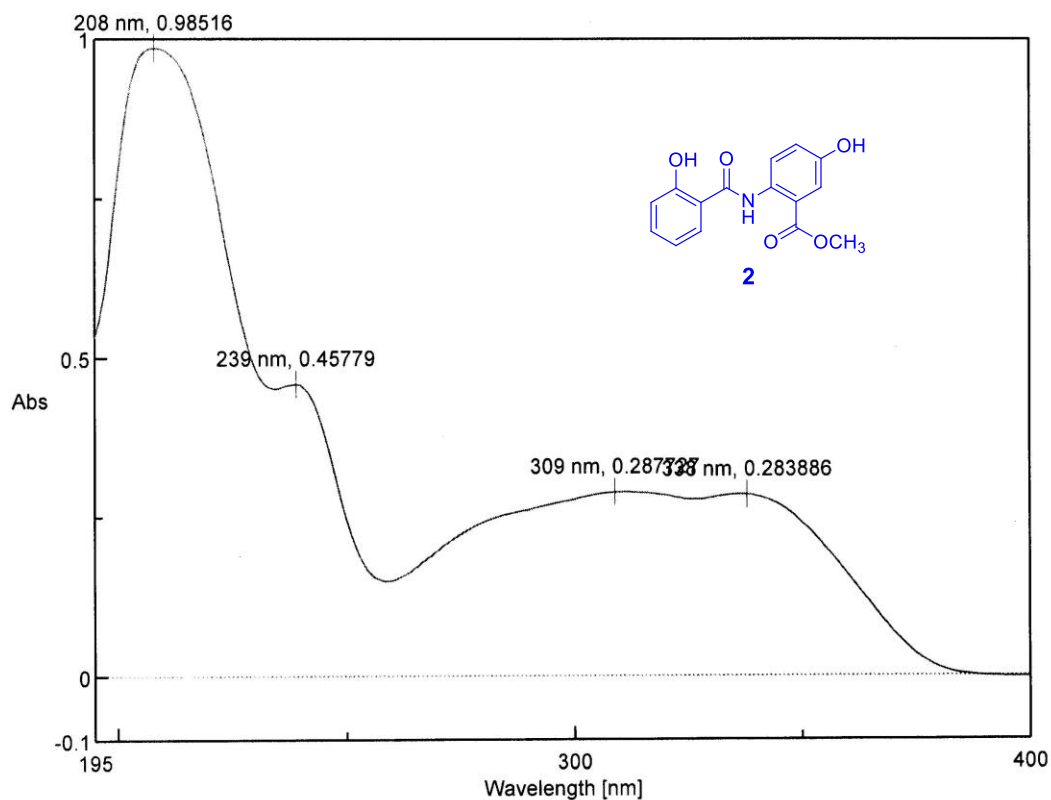


Figure S17. The  $^1\text{H}$  NMR spectrum of compound (-)-1 in  $\text{DMSO-}d_6$  (600 MHz).

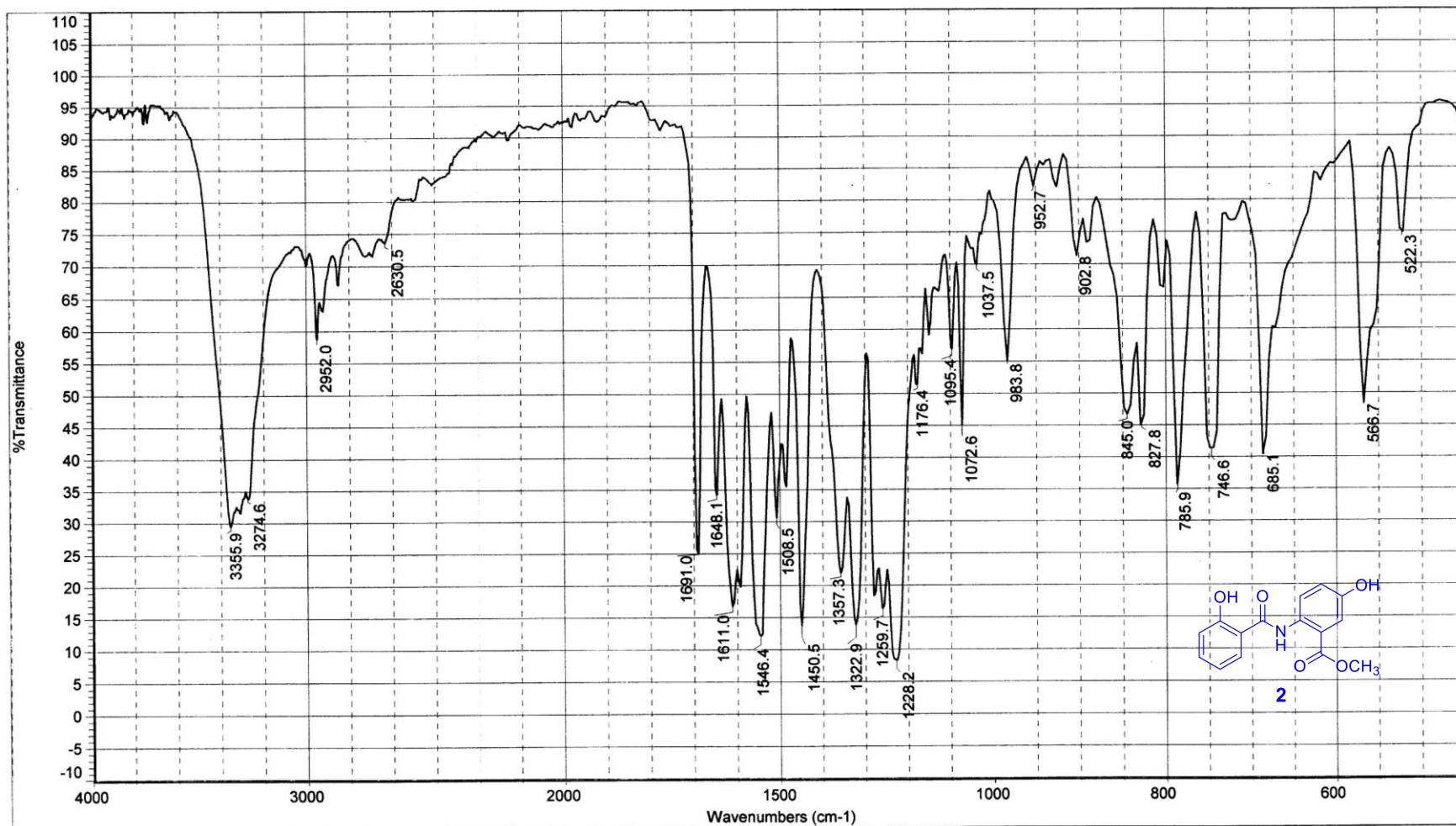


**Figure S18.** The <sup>1</sup>H NMR spectrum of compound (+)-1 in DMSO-d<sub>6</sub> (600 MHz).



[Comment]		CI-12-2-W
Sample Name	CI-12	
Comment		
User		
Division		
Company	324	
[Measurement Information]		
Instrument Name	V-650	
Model Name	V-650	
Serial No.	A034461150	
Accessory	PSC-718	[Data Information]
Accessory S/N	A001761114	Creation Date
Position	1	2011-9-14 16:13
Cell Length	10 mm	Data array type
Temperature	19.94 C	Linear data array
Control Sensor	Holder	Horizontal
Monitor Sensor	Holder	Wavelength [nm]
Start Mode	Start immediately	Vertical
		Abs
		Start
		400 nm
		End
		195 nm
		Data pitch
		1 nm
		Data points
		206
Photometric Mode	Abs	
Measurement range	400 - 195 nm	
Data pitch	1 nm	
Band width(UV/Vis)	1.0 nm	
Response	Medium	
Scanning speed	200 nm/min	
Source Change	340 nm	
Light Source	D2/MI	
Filter Exchange	Step	
Correction	Baseline	

**Figure S19.** The UV spectrum of compound **2** in MeOH.



日期: 星期三 5月 18 13:26:42 2011 (GMT+08:00) Sample Name: CI - 12 (显微镜透射法FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换红外显微镜(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S20. The IR spectrum of compound 2.

# Display Report - Selected Window Selected Analysis

**Analysis Name:** chenmh07.d  
**Method:** TEST.MS  
**Sample Name:** CI-12  
**Analysis Info:**

**Instrument:** LC-MSD-Trap-SL  
**Operator:** Operator

**Print Date:** 6/30/2010 12:49:50 PM  
**Acq. Date:** 6/30/2010 12:41:48 PM

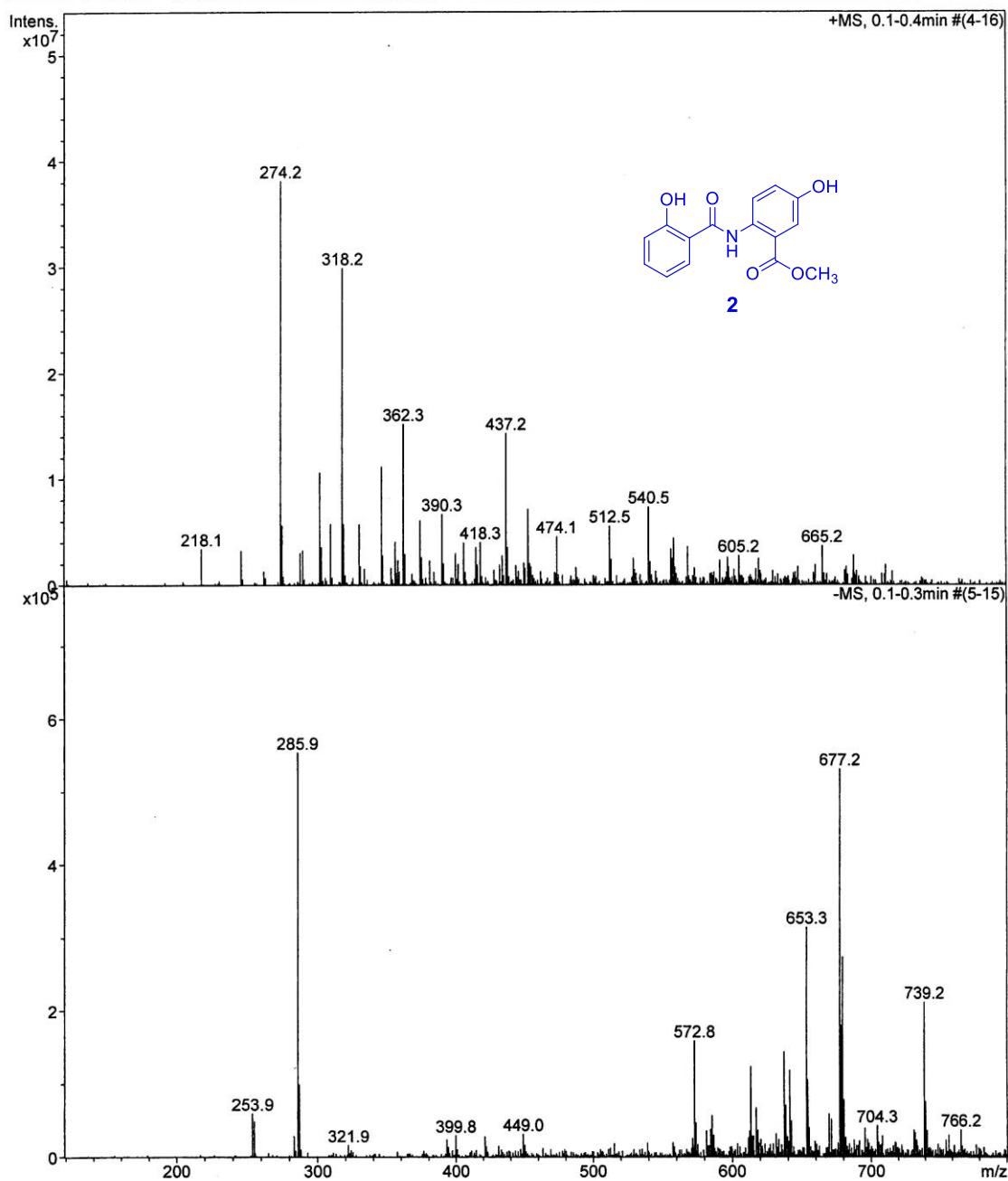


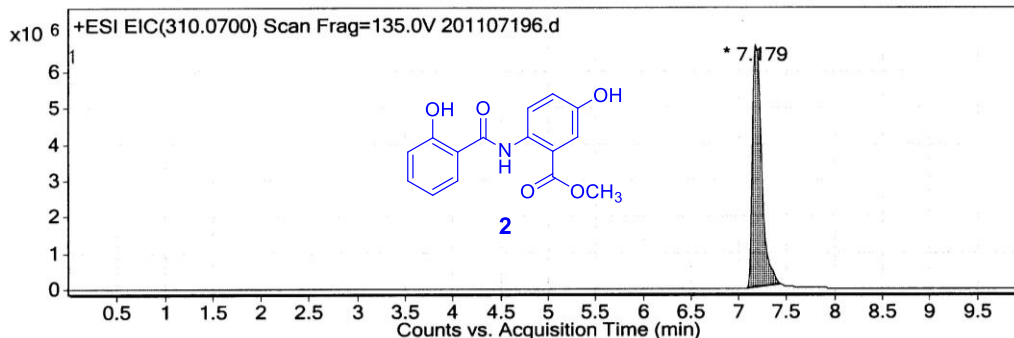
Figure S21. The ESIMS report of compound 2.

# Qualitative Analysis Report

Data Filename	201107196.d	Sample Name	CI-12
Sample Type	Sample	Position	P1-C7
Instrument Name	Instrument 1	User Name	
Acq Method		IRM Calibration Status	XXXXXXXXXX
DA Method	TEST LCMS.m	Comment	

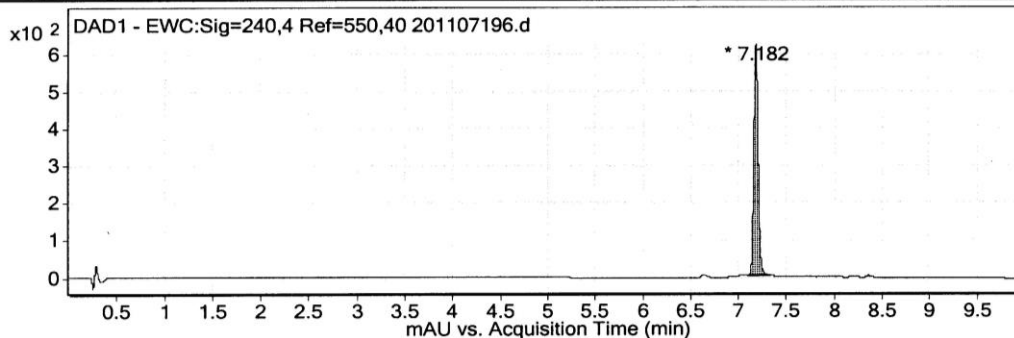
## User Chromatograms

Fragmentor Voltage 135    Collision Energy 0    Ionization Mode ESI



### Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	7.083	7.179	7.436	6688542	43970364	100



### Integration Peak List

Peak	Start	RT	End	Height	Area	Area %
1	7.089	7.182	7.337	621.4	1971.465	100

## User Spectra

Fragmentor Voltage 135    Collision Energy 0    Ionization Mode ESI

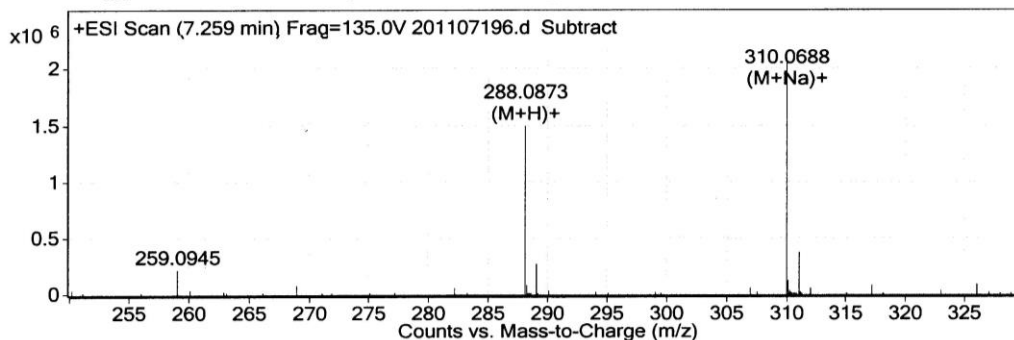


Figure S22. The (+)-HRESIMS report of compound 2, page 1.



## Qualitative Analysis Report

### Peak List

m/z	z	Abund	Formula	Ion
104.9927		223506		
186.9955		128728		
259.0945		218619		
288.0873	1	1499513	C15 H14 N O5	(M+H)+
289.0907	1	272132	C15 H14 N O5	(M+H)+
310.0688	1	2091716	C15 H13 N Na O5	(M+Na)+
310.2213		126911		
311.0727	1	377445	C15 H13 N Na O5	(M+Na)+
450.6009		110671		

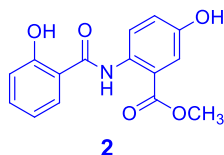
### Formula Calculator Element Limits

Element	Min	Max
C	3	100
H	0	120
O	0	30
N	0	5
S	0	5
Cl	0	0

### Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C15 H13 N O5	TRUE	287.0796	287.0794	-0.84	C15 H13 N Na O5	99.92
C16 H9 N5 O		287.0796	287.0807	3.81	C16 H9 N5 Na O	99.65
C19 H13 N S		287.0796	287.0769	-9.56	C19 H13 N Na S	97.78
C16 H17 N S2		287.0796	287.0802	2.18	C16 H17 N Na S2	97.22
C7 H17 N3 O7 S		287.0796	287.0787	-3.13	C7 H17 N3 Na O7 S	96.12
C8 H21 N3 O2 S3		287.0796	287.0796	-0.11	C8 H21 N3 Na O2 S3	92.63
C15 H13 N O5	TRUE	287.0801	287.0794	-2.37	C15 H14 N O5	99.86
C16 H9 N5 O		287.0801	287.0807	2.28	C16 H10 N5 O	99.83
C16 H17 N S2		287.0801	287.0802	0.65	C16 H18 N S2	97.22
C12 H17 N O5 S		287.0801	287.0827	9.36	C12 H18 N O5 S	97.2
C7 H17 N3 O7 S		287.0801	287.0787	-4.66	C7 H18 N3 O7 S	95.89
C8 H21 N3 O2 S3		287.0801	287.0796	-1.64	C8 H22 N3 O2 S3	92.51

--- End Of Report ---



**Figure S23.** The (+)-HRESIMS report of compound **2**, page 2.

MS Formula Results: + Scan (7.259 min) Sub (201107196.d)

m/z	Ion	Formula	Abundance											
288.0873	(M+H) <sup>+</sup>	C15 H14 N O5	1499512.5											
<b>Best</b>	<b>Formula (M)</b>	<b>Ion Formula</b>	<b>Calc m/z</b>	<b>Score</b>	<b>Cross S</b>	<b>Mass</b>	<b>Calc Mass</b>	<b>Diff (ppm)</b>	<b>Abs Diff (ppm)</b>	<b>Abund Match</b>	<b>Spacing Mat</b>	<b>Mass Match</b>	<b>m/z</b>	<b>DBE</b>
<input checked="" type="checkbox"/>	C15 H13 N O5	C15 H14 N O5	288.0866	99.96		287.0801	287.0794	-2.37	2.37	99.8	100	99.83	288.0873	10
<input type="checkbox"/>	C16 H9 N5 O	C16 H10 N5 O	288.088	99.83		287.0801	287.0807	2.28	2.28	99.77	99.9	99.84	288.0873	15
<input type="checkbox"/>	C16 H17 N S2	C16 H18 N S2	288.0875	97.22		287.0801	287.0802	0.65	0.65	90.78	99.43	99.99	288.0873	9
<input type="checkbox"/>	C12 H17 N O5 S	C12 H18 N O5 S	288.09	97.2		287.0801	287.0827	9.36	9.36	94.96	99.59	97.35	288.0873	5
<input type="checkbox"/>	C7 H17 N3 O7 S	C7 H18 N3 O7 S	288.086	95.89		287.0801	287.0787	-4.66	4.66	87.28	99.33	99.34	288.0873	1
<input type="checkbox"/>	C8 H21 N3 O2 S3	C8 H22 N3 O2 S3	288.0869	92.51		287.0801	287.0796	-1.64	1.64	74.87	98.87	99.92	288.0873	0
m/z	Ion	Formula	Abundance											
310.0688	(M+Na) <sup>+</sup>	C15 H13 N Na O5	2091715.9											
<b>Best</b>	<b>Formula (M)</b>	<b>Ion Formula</b>	<b>Calc m/z</b>	<b>Score</b>	<b>Cross S</b>	<b>Mass</b>	<b>Calc Mass</b>	<b>Diff (ppm)</b>	<b>Abs Diff (ppm)</b>	<b>Abund Match</b>	<b>Spacing Mat</b>	<b>Mass Match</b>	<b>m/z</b>	<b>DBE</b>
<input checked="" type="checkbox"/>	C15 H13 N O5	C15 H13 N Na O5	310.0686	99.92		287.0796	287.0794	-0.84	0.84	99.85	99.89	99.98	310.0688	10
<input type="checkbox"/>	C16 H9 N5 O	C16 H9 N5 Na O	310.0699	99.65		287.0796	287.0807	3.81	3.81	99.7	99.66	99.61	310.0688	15
<input type="checkbox"/>	C19 H13 N S	C19 H13 N Na S	310.0661	97.78		287.0796	287.0769	-9.56	9.56	96.73	99.48	97.57	310.0688	14
<input type="checkbox"/>	C16 H17 N S2	C16 H17 N Na S2	310.0695	97.22		287.0796	287.0802	2.18	2.18	91.19	99.17	99.87	310.0688	9
<input type="checkbox"/>	C7 H17 N3 O7 S	C7 H17 N3 Na O7 S	310.0679	96.12		287.0796	287.0787	-3.13	3.13	87.74	98.94	99.74	310.0688	1
<input type="checkbox"/>	C8 H21 N3 O2 S3	C8 H21 N3 Na O2 S3	310.0688	92.63		287.0796	287.0796	-0.11	0.11	75.53	98.41	100	310.0688	0

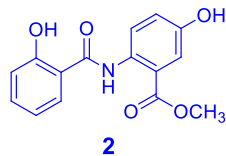
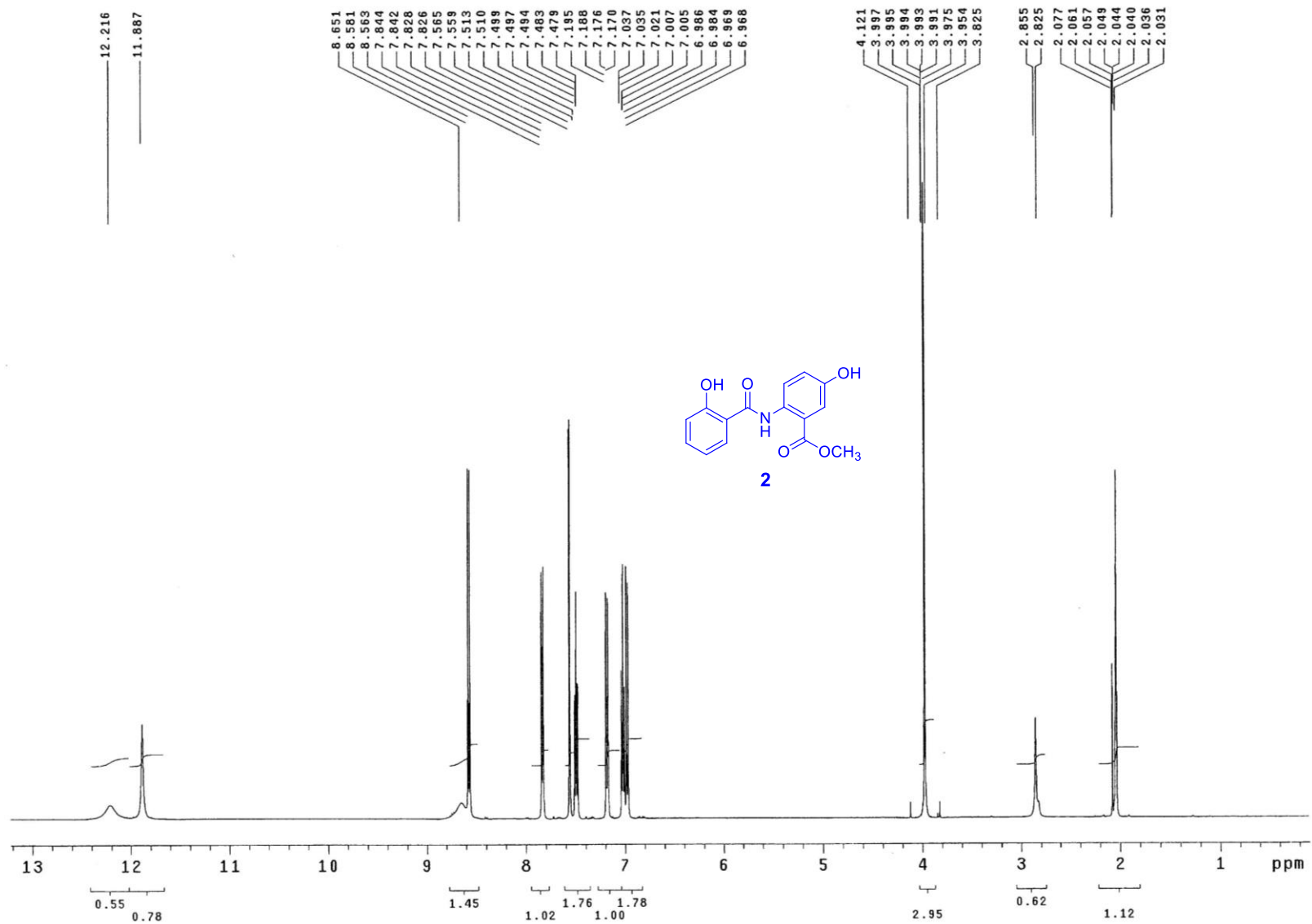


Figure S24. The (+)-HRESIMS report of compound 2, page 3.



**Figure S25.** The <sup>1</sup>H NMR spectrum of compound **2** in acetone-*d*<sub>6</sub> (500 MHz).

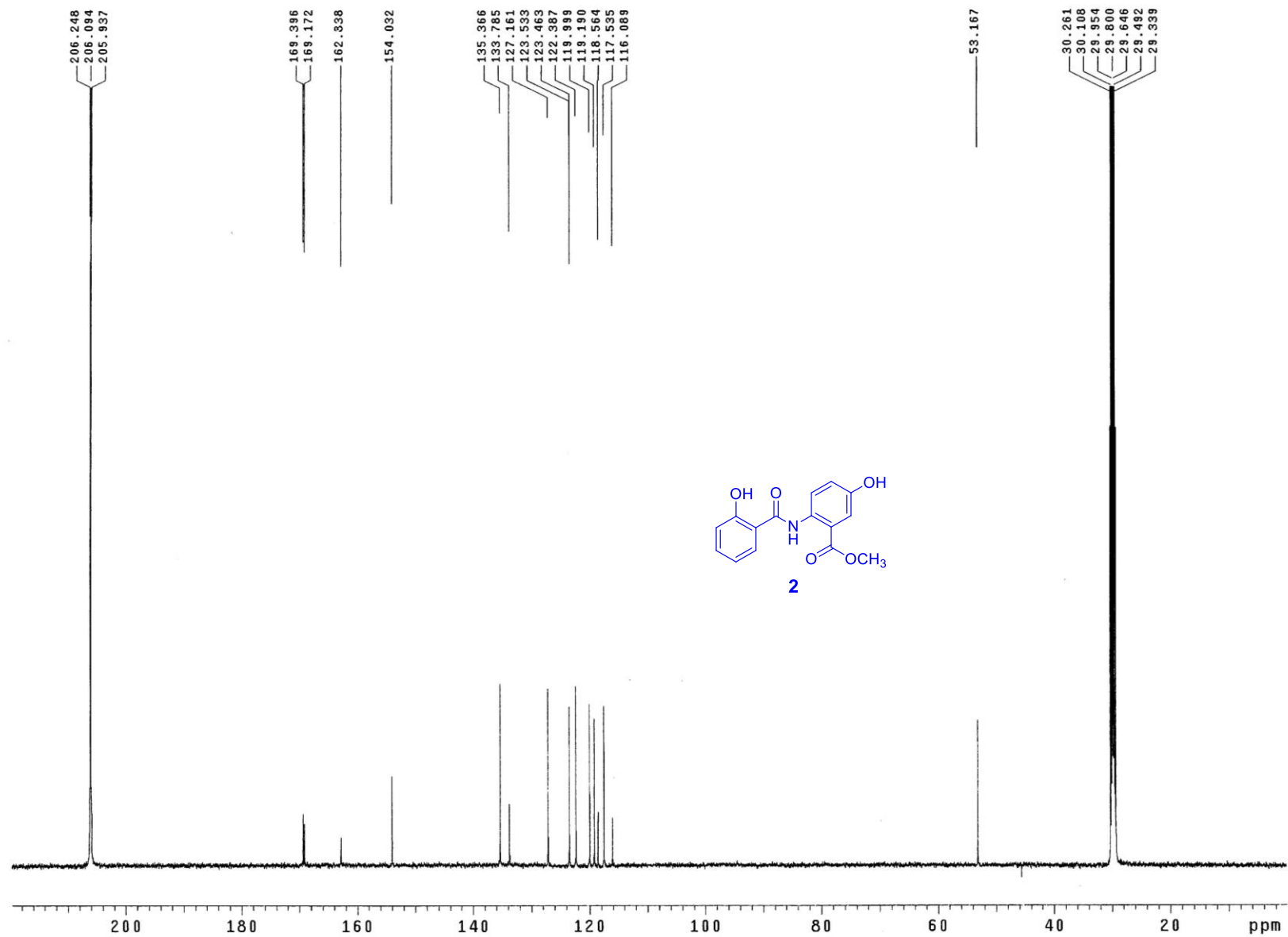
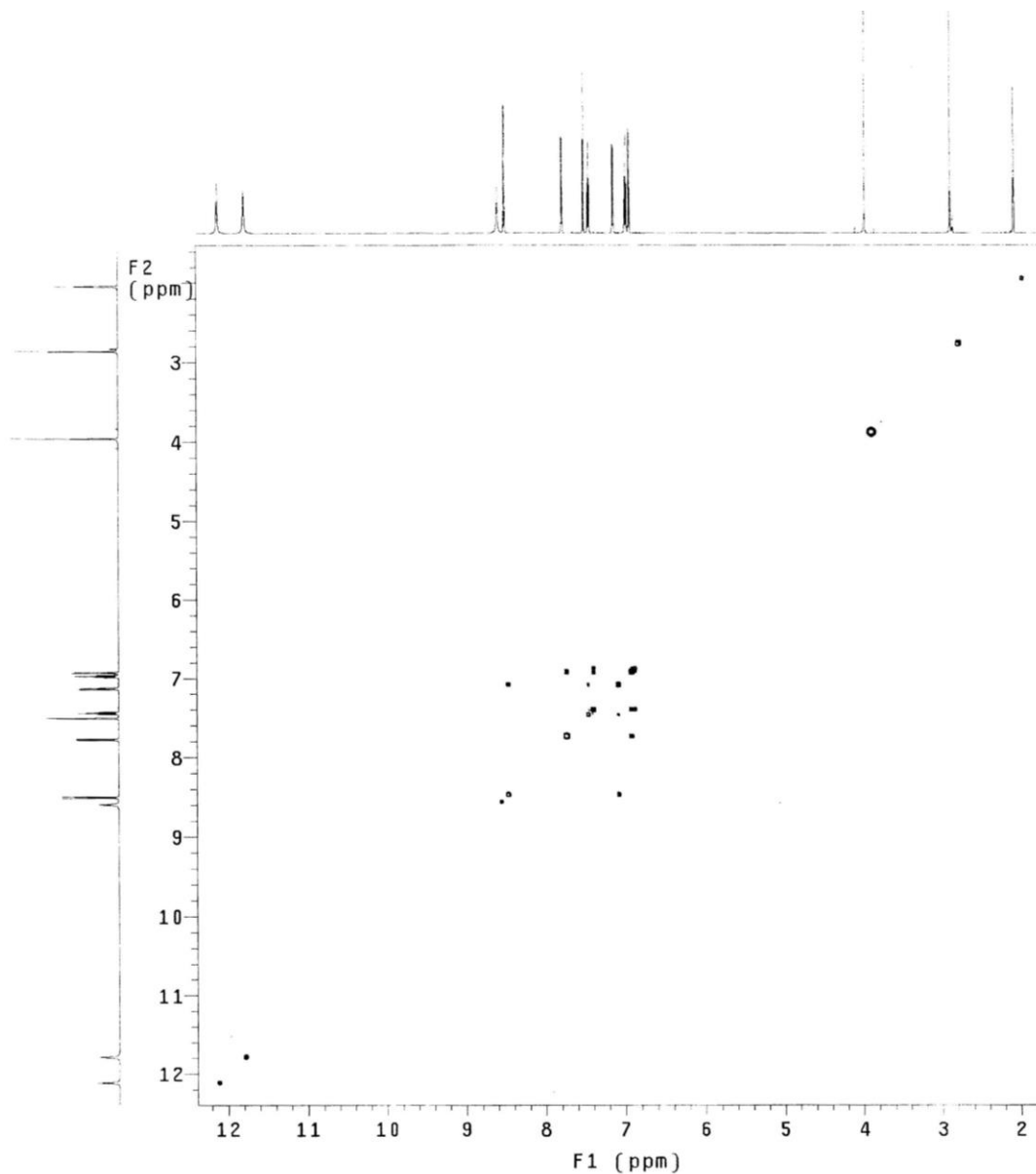
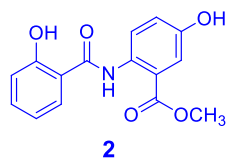


Figure S26. The  $^{13}\text{C}$  NMR spectrum of compound 2 in acetone- $d_6$  (125 MHz).

VNS-600 gCOSY CI-12 in CD3COCD3 2011.08.26

Pulse Sequence: gCOSY  
Solvent: acetone  
Temp. 25.0 C / 298.1 K  
Operator: walkup  
VNMR5-600 "wormhole"

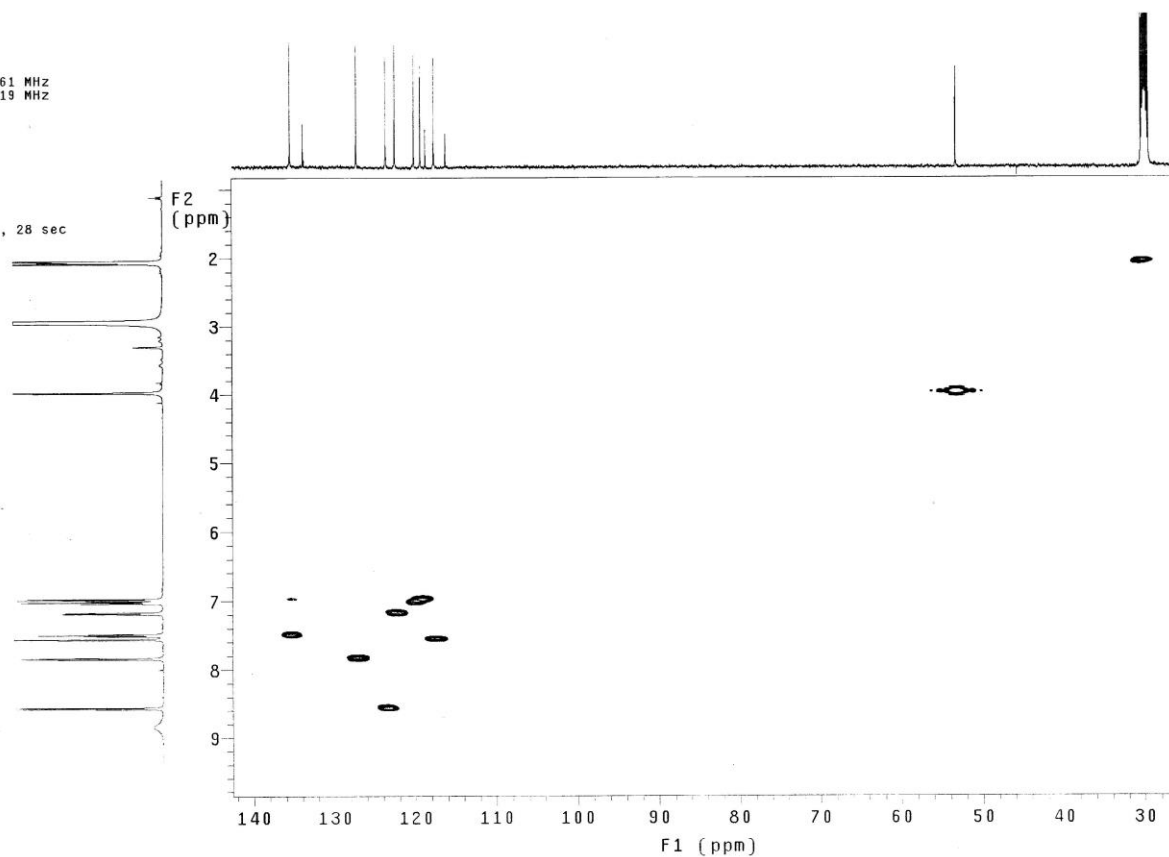
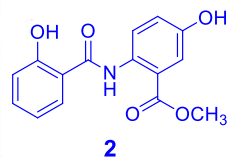
Relax. delay 1.000 sec  
Acq. time 0.143 sec  
Width 7183.9 Hz  
2D Width 7183.9 Hz  
2 repetitions  
256 increments  
OBSERVE H1, 599.6929894 MHz  
DATA PROCESSING  
Sine bell 0.071 sec  
F1 DATA PROCESSING  
Sine bell 0.018 sec  
FT size 2048 x 2048  
Total time 10 min, 16 sec



**Figure S27.** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2** in acetone- $d_6$  (500 MHz).

Solvent: acetone  
Temp. 25.0 C / 298.1 K  
Sample #4, Operator: walkup  
File: 0402  
INOVA-500 "IMM-501"

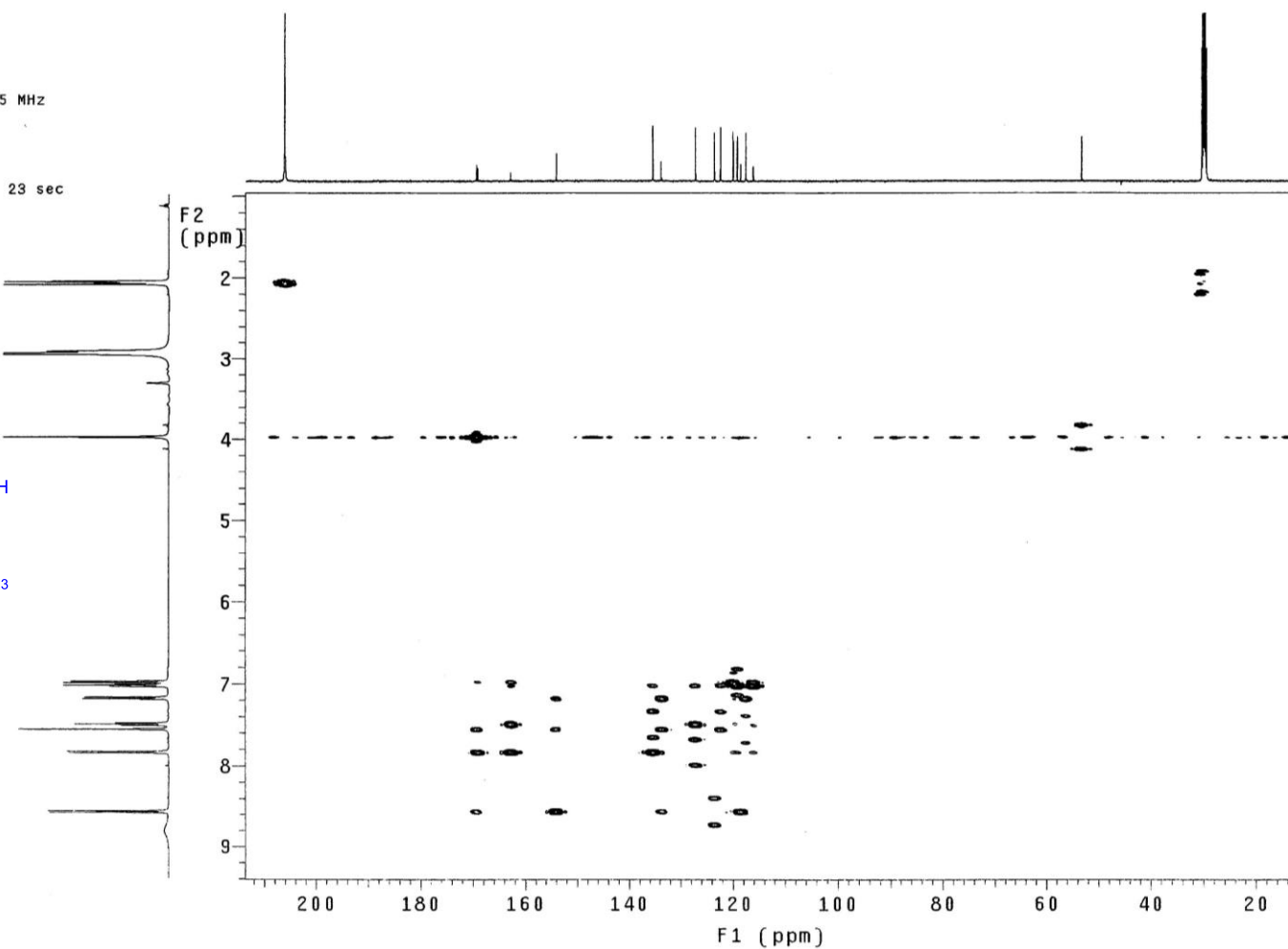
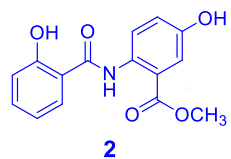
Relax. delay 1.301 sec  
Acq. time 0.199 sec  
Width 6752.6 Hz  
2D Width 25133.5 Hz  
16 repetitions  
2 x 200 increments  
OBSERVE H1, 499.7707161 MHz  
DECOUPLE C13, 125.6787219 MHz  
Power 34 dB  
on during acquisition  
off during delay  
W40\_SW modulated  
DATA PROCESSING  
Sine bell 0.033 sec  
F1 DATA PROCESSING  
Sine bell 0.004 sec  
FT size 4096 x 2048  
Total time 2 hr, 46 min, 28 sec



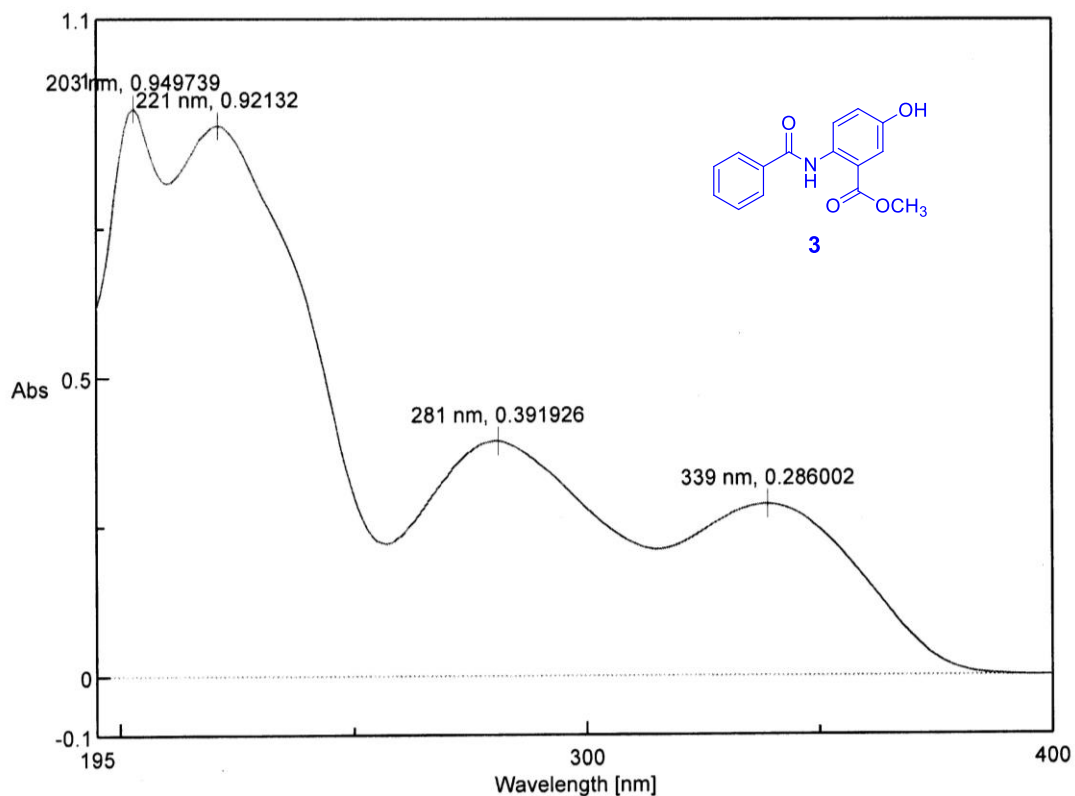
**Figure S28.** The HSQC spectrum of compound **2** in acetone- $d_6$  (500 MHz for  $^1\text{H}$ ).

Solvent: acetone  
 Temp. 25.0 C / 298.1 K  
 Sample #2, Operator: walkup  
 File: HMBCCD3COCD30915-CI-12  
 INOVA-500 "IMM-501"

Relax. delay 1.000 sec  
 Mixing 0.080 sec  
 Acq. time 0.128 sec  
 Width 6752.2 Hz  
 2D Width 30154.5 Hz  
 32 repetitions  
 256 increments  
 OBSERVE H1, 499.7707135 MHz  
 DATA PROCESSING  
 Sine bell 0.060 sec  
 F1 DATA PROCESSING  
 Sine bell 0.004 sec  
 FT size 4096 x 2048  
 Total time 2 hr, 46 min, 23 sec



**Figure S29.** The HMBC spectrum of compound **2** in acetone-*d*<sub>6</sub> (500 MHz for <sup>1</sup>H).



[Comment] Memory-10

Sample Name CI-18

Comment

User

Division

Company 324

[Measurement Information]

Instrument Name V-650

Model Name V-650

Serial No. A034461150

Accessory PSC-718

Accessory S/N A001761114

Position 1

Cell Length 10 mm

Temperature 20.00 C

Control Sensor Holder

Monitor Sensor Holder

Start Mode Start immediately

[Data Information]

Creation Date 2011-9-14 16:28

Data array type Linear data array

Horizontal Wavelength [nm]

Vertical Abs

Start 400 nm

End 195 nm

Data pitch 1 nm

Data points 206

Photometric Mode Abs

Measurement range 400 - 195 nm

Data pitch 1 nm

Band width(UV/Vis) 1.0 nm

Response Medium

Scanning speed 200 nm/min

Source Change 340 nm

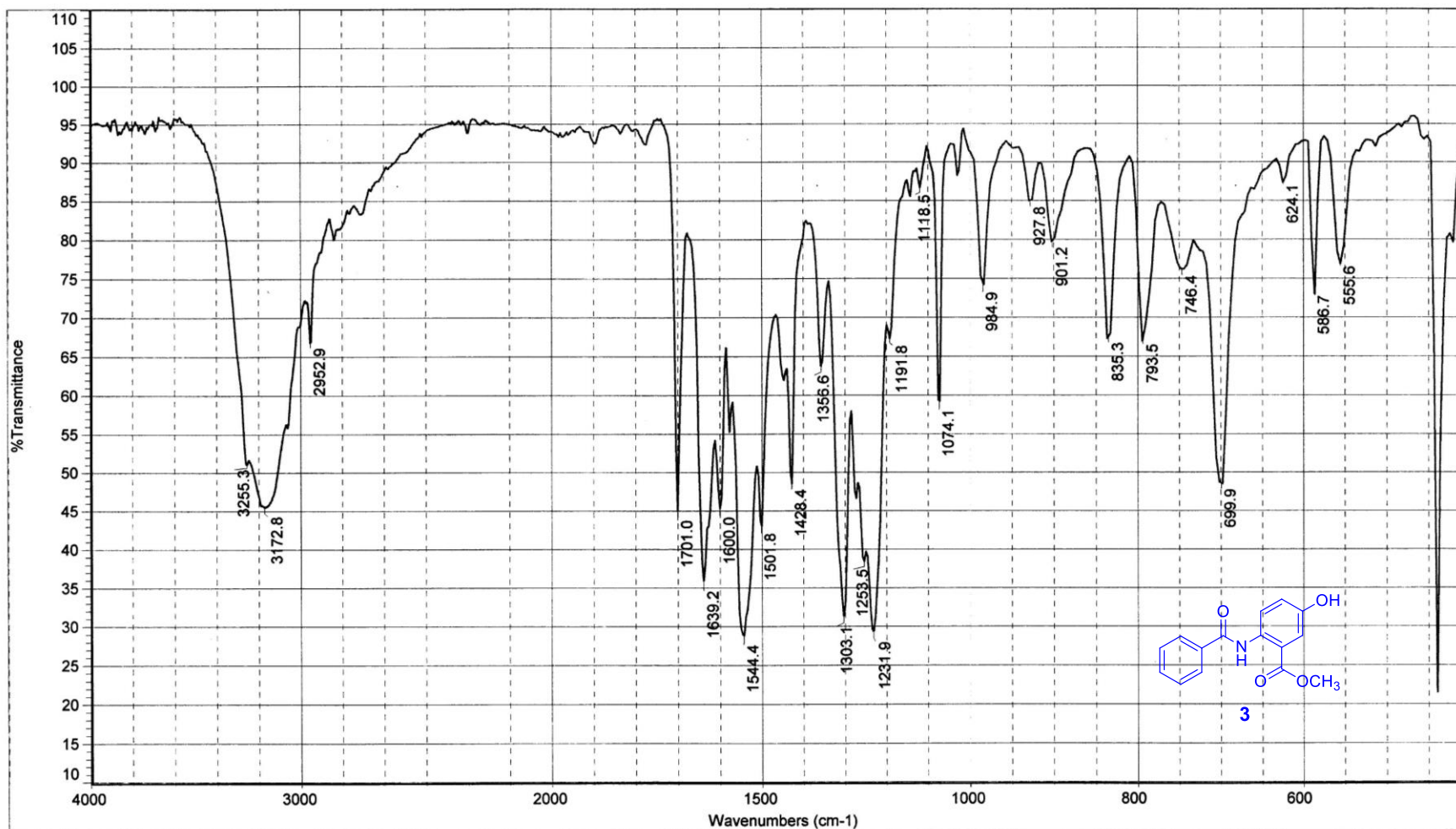
Light Source D2/WI

Filter Exchange Step

Correction Baseline

**Figure S30.** The UV spectrum of compound **3** in MeOH.





日期: 星期三 5月 18 13:33:42 2011 (GMT+08:00) Sample Name: Cl - 18

(显微镜透射法FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换红外显微镜 (FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司 (Thermo) 傅里叶变换红外光谱仪: Nicolet 5700

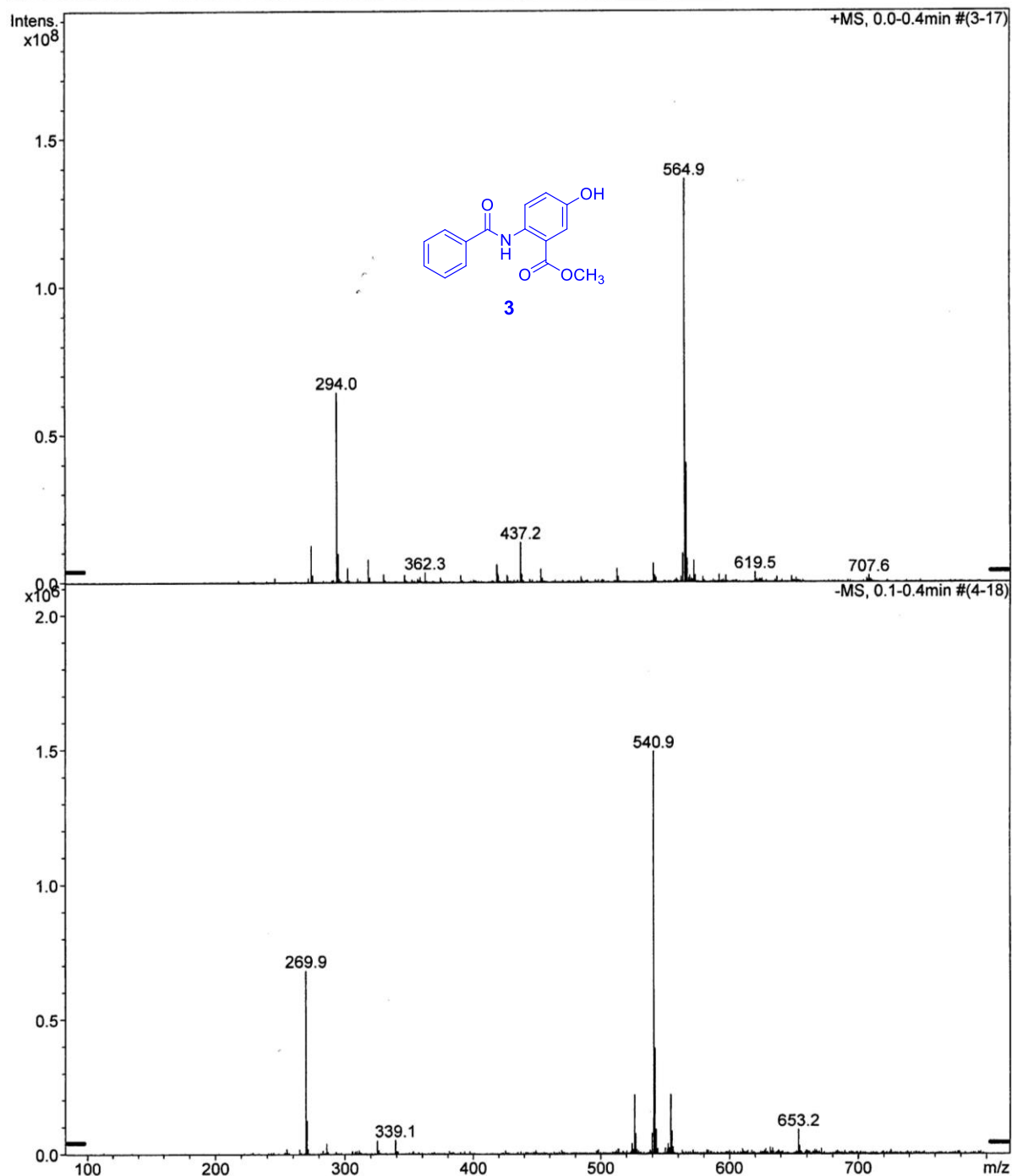
Figure S31. The IR spectrum of compound 3.

# Display Report - Selected Window Selected Analysis

**Analysis Name:** chenmh12.d  
**Method:** TEST.MS  
**Sample Name:** CI-18  
**Analysis Info:**

**Instrument:** LC-MSD-Trap-SL  
**Operator:** Operator

**Print Date:** 6/30/2010 1:19:45 PM  
**Acq. Date:** 6/30/2010 1:10:43 PM



**Figure S32.** The ESI mass spectrum of compound 3.

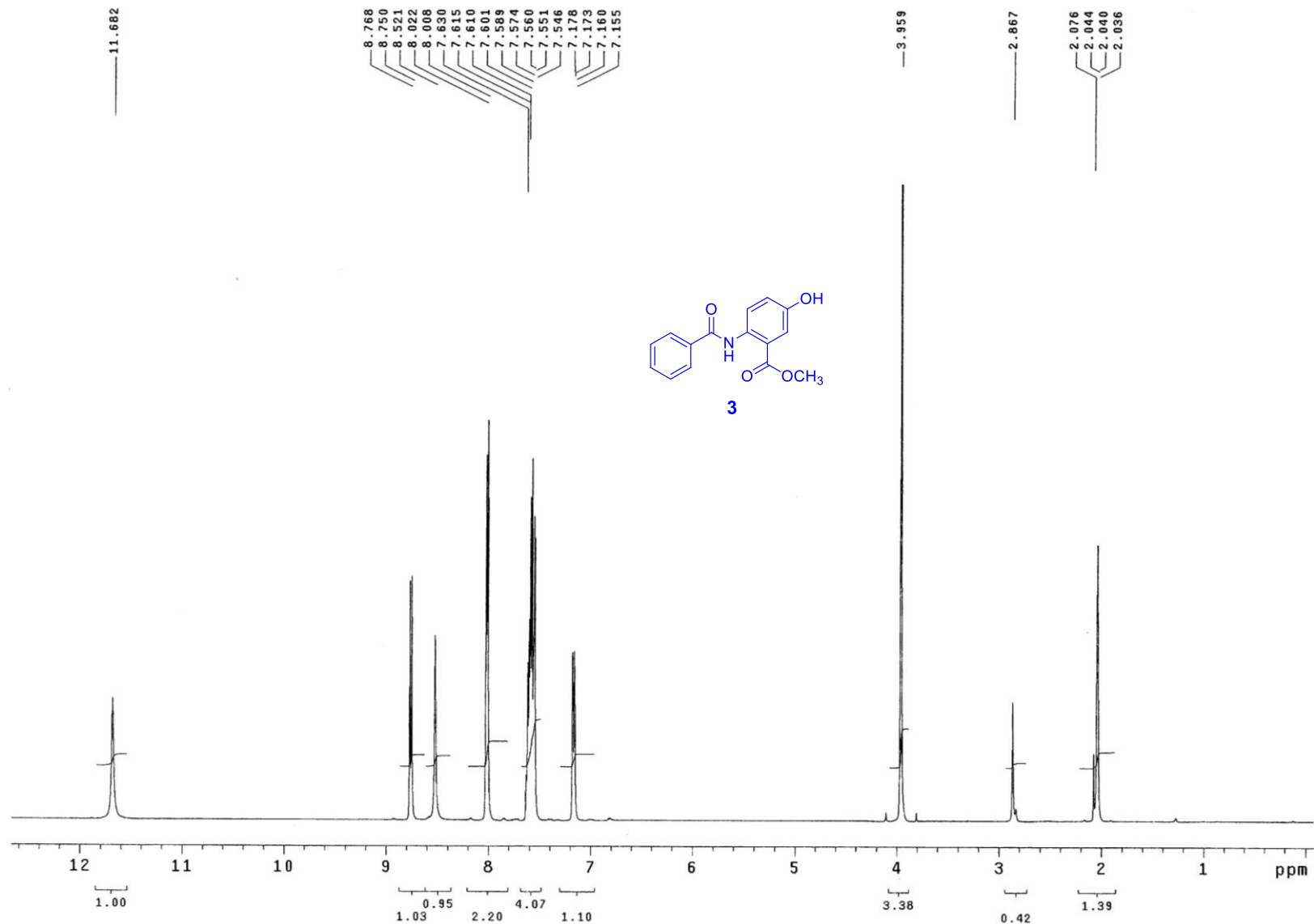


Figure S33. The  $^1\text{H}$  NMR spectrum of compound 3 in acetone- $d_6$  (500 MHz).

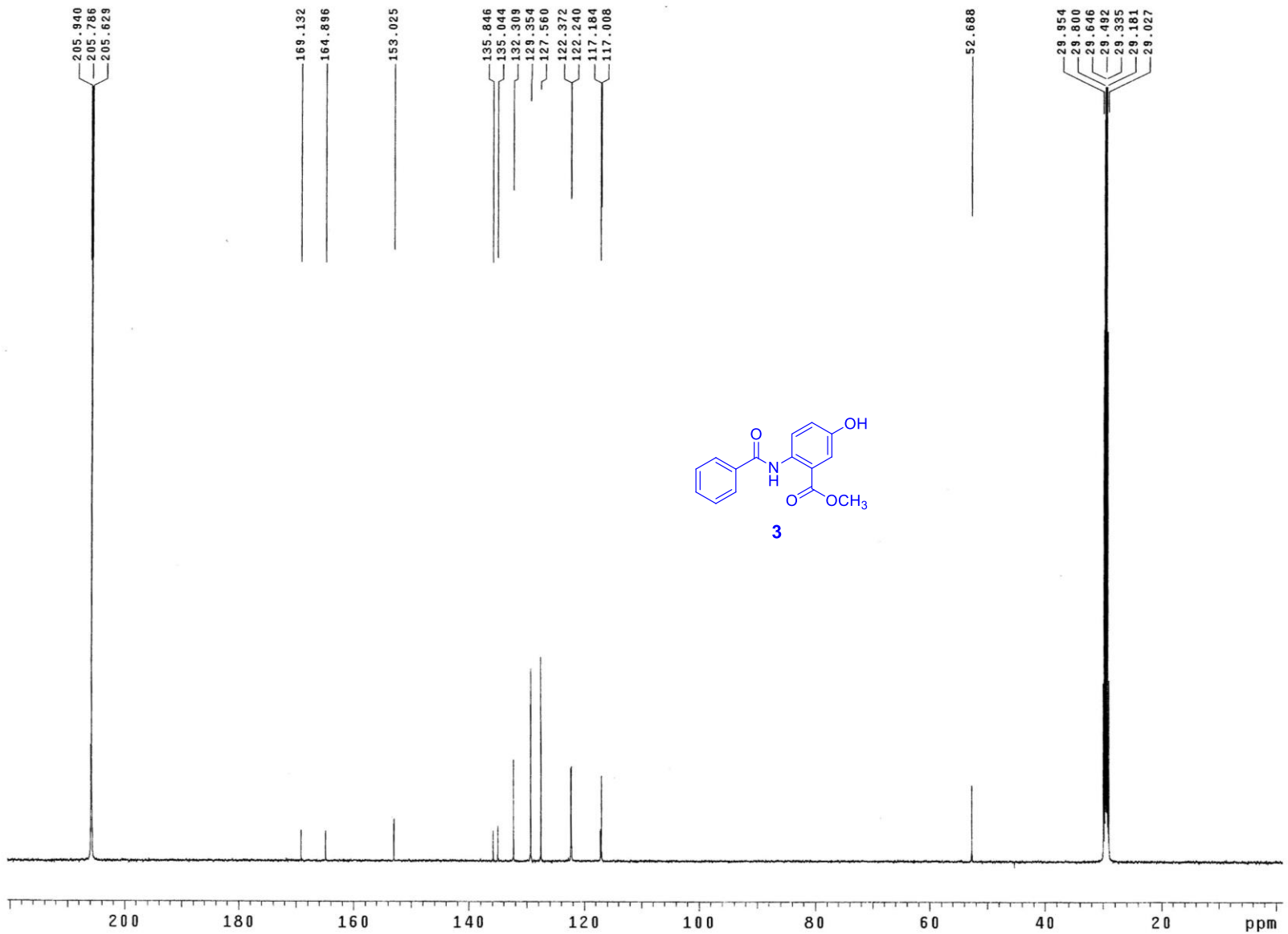
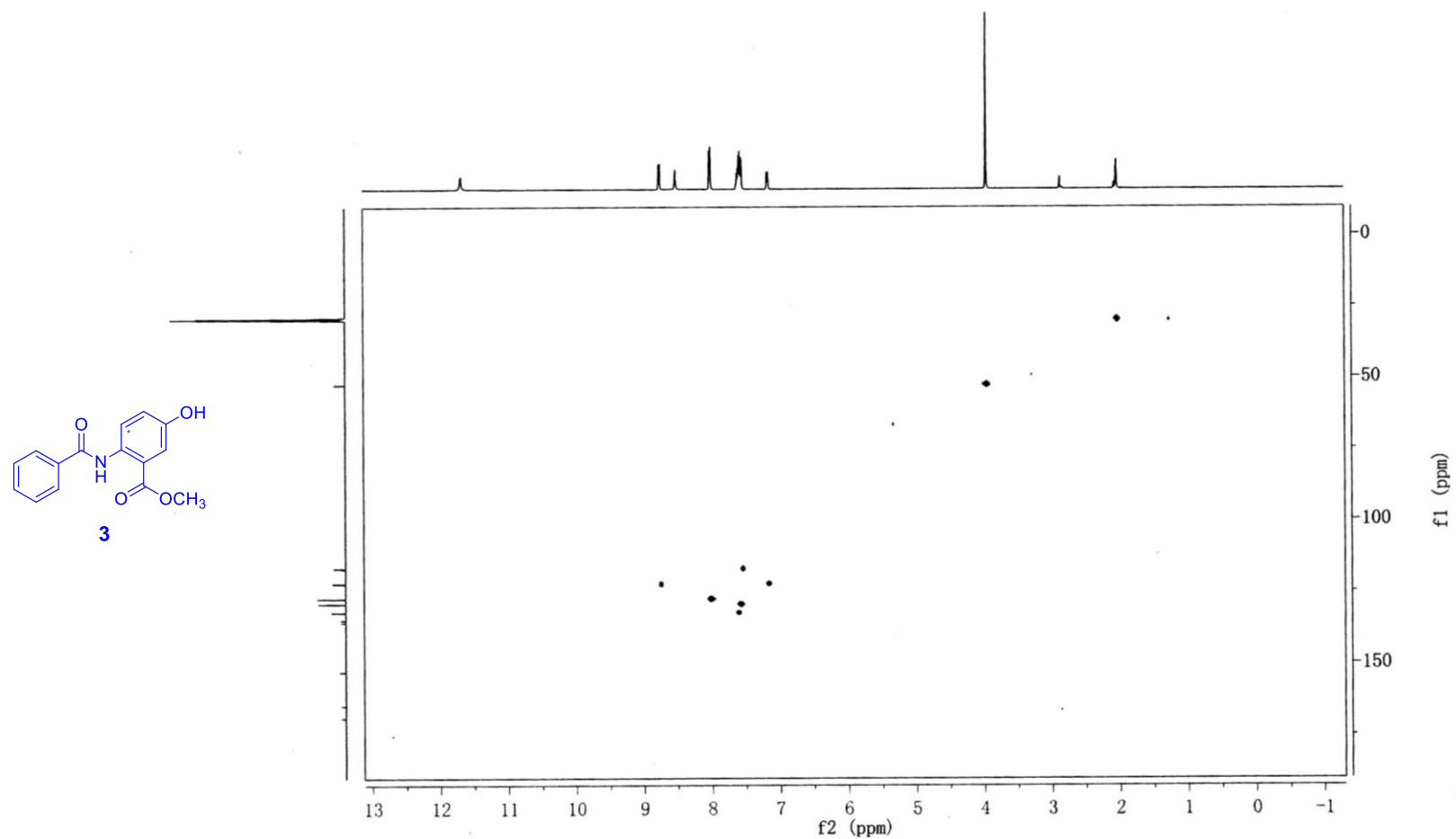
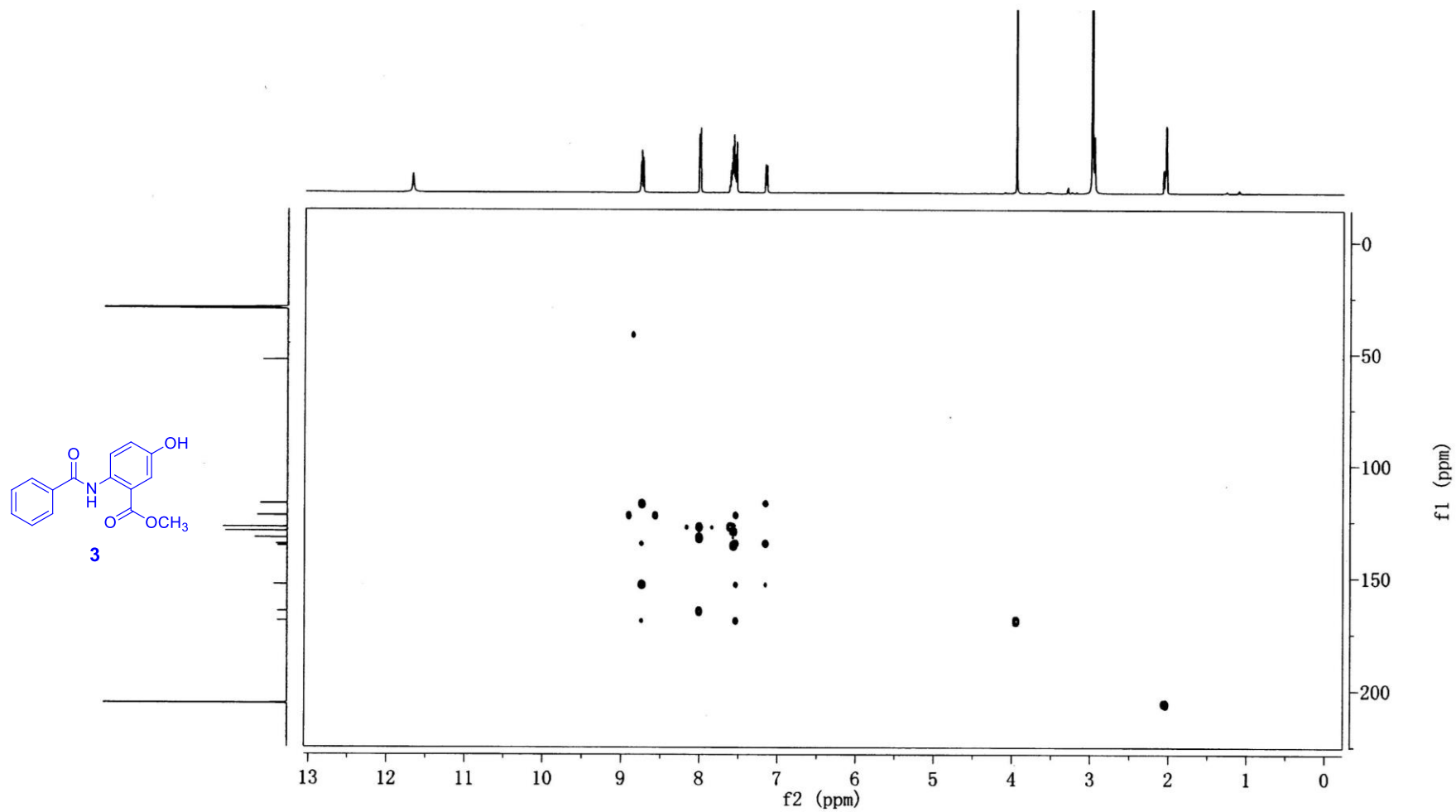


Figure S34. The  $^{13}\text{C}$  NMR spectrum of compound 3 in acetone- $d_6$  (125 MHz).



**Figure S35.** The HSQC spectrum of compound **3** in acetone-*d*<sub>6</sub> (500 MHz for <sup>1</sup>H).



**Figure S36.** The HMBC spectrum of compound **3** in acetone- $d_6$  (500 MHz for  $^1\text{H}$ ).