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

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Supporting Information

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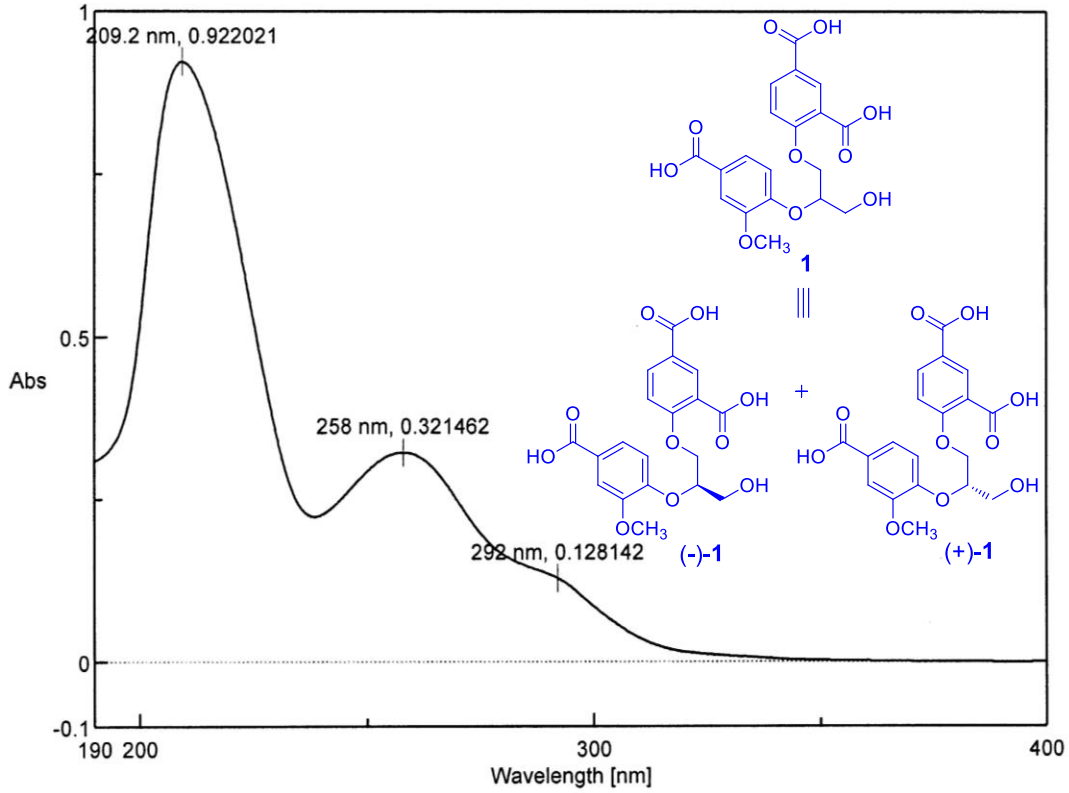
List of Contents



BLG-L-118

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Comment 0.02
User
Division UV
Company 324

[Measurement Information]
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Model Name V-650
Serial No. A034461150

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Accessory S/N A001761114
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Cell Length 10 mm
Temperature 19.94 C
Control Sonsor 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

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Horizontal Wavelength [nm]
Vertical Abs
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End 190 nm
Data pitch 0.2 nm
Data points 1051

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

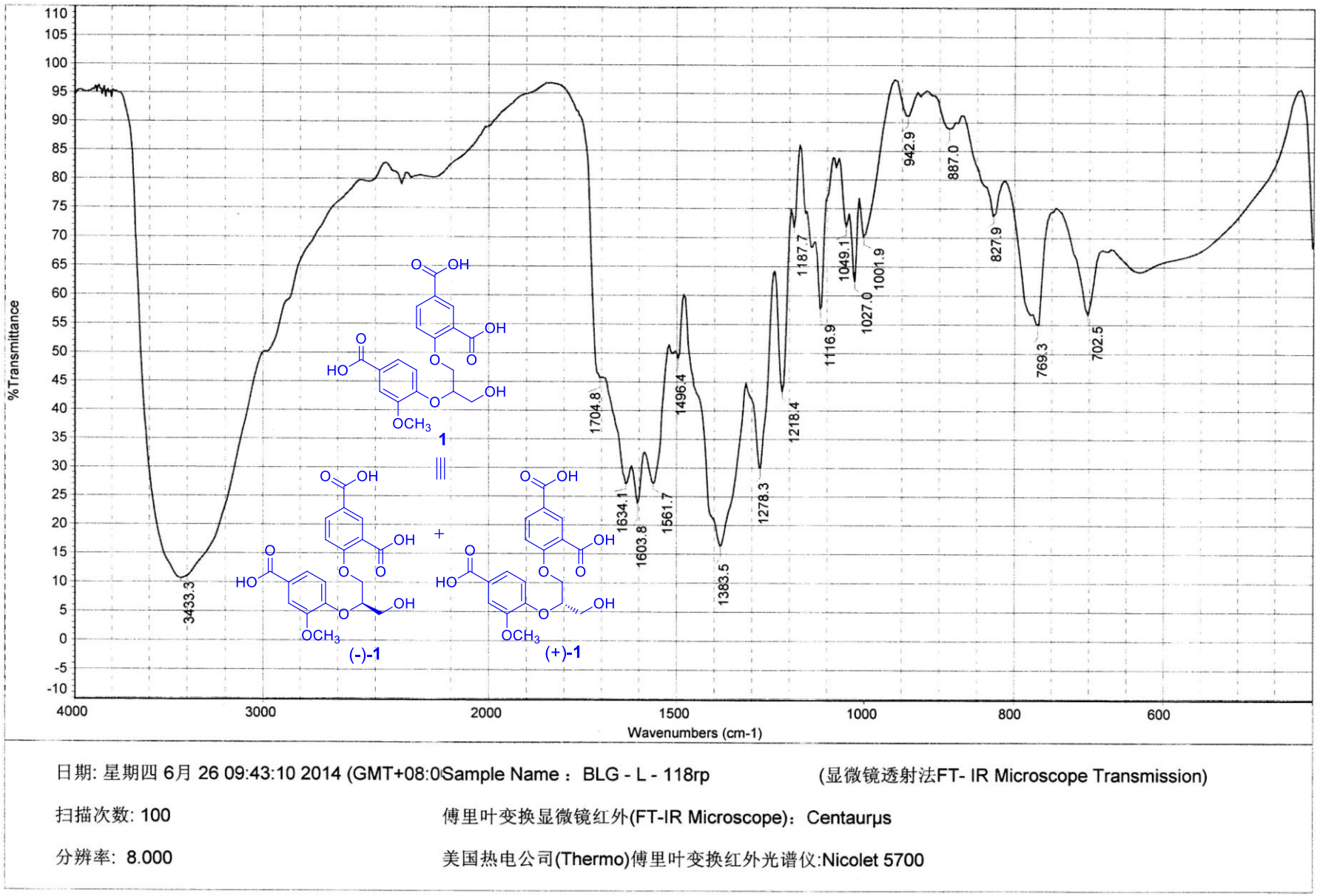

Figure S2. The IR spectrum of **1**.

Single Mass Spectrum Deconvolution Report

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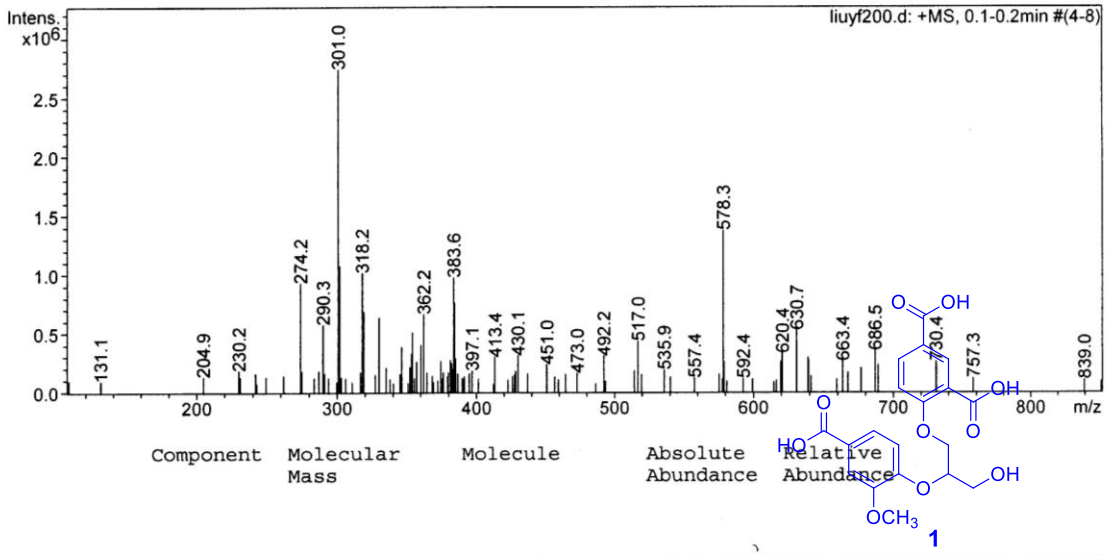
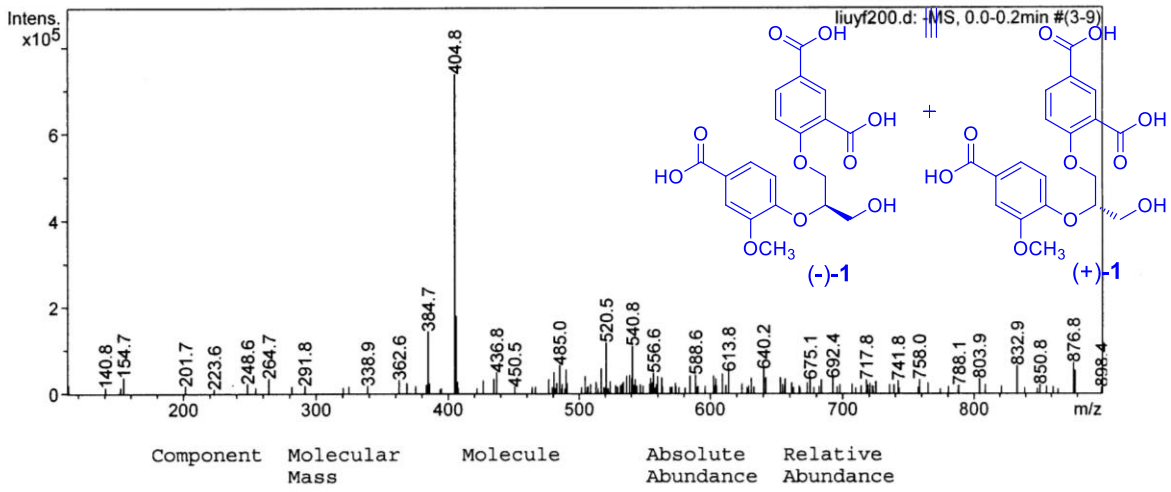
Method: TEST.MS **Operator:** Operator **Acq. Date:** 8/22/2013 11:54:01 AM
Sample Name: BLG-L-118RP
Analysis Info:

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





MSD Trap Report v 4 (A4-Opt2) Page 1 of 1 Agilent Technologies

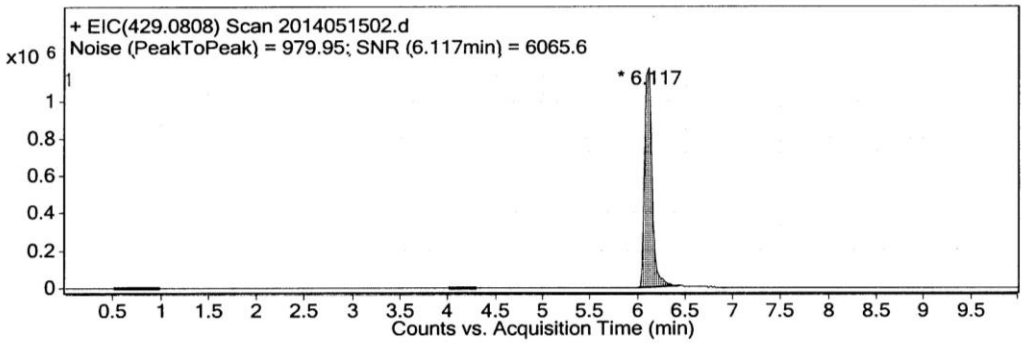
Figure S3. The ESI mass spectrum of **1**

Qualitative Analysis Report

Data Filename	2014051502.d	**Sample Name**	BLG-L-118rp
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	TEST LCMS.m	**IRM Calibration Status**	[redacted]
DA Method	TEST LCMS.m	**Comment**	

User Chromatograms

Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** ESI



Integration Peak List

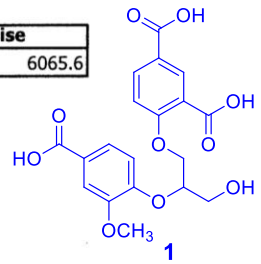
Peak	Start	RT	End	Height	Area	Area %	Signal To Noise
1	6.004	6.117	6.455	1171470	5943982	100	6065.6

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



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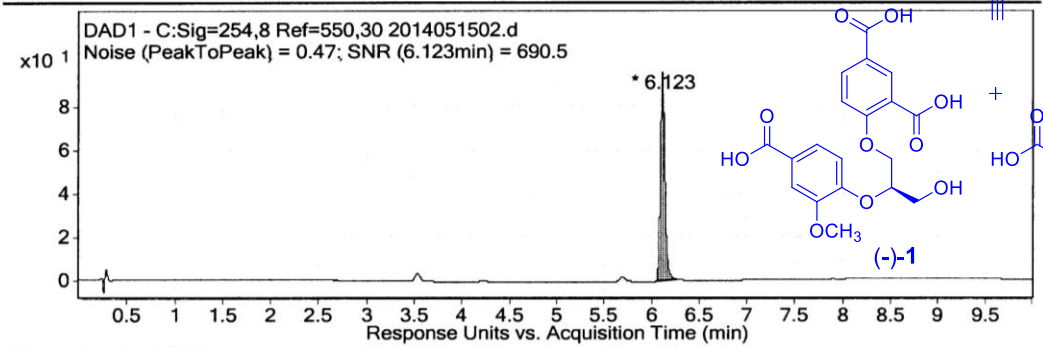

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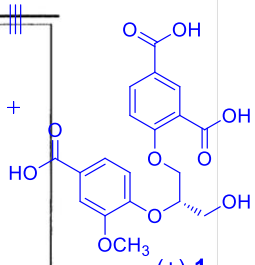


(+)-1

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

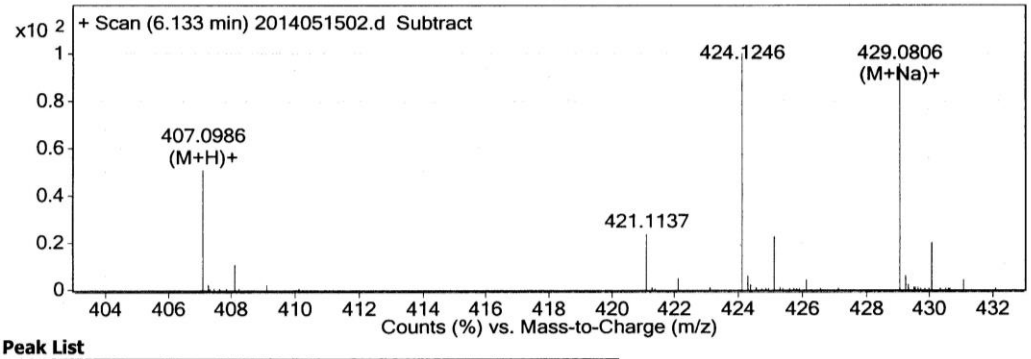
Start	End
0.5	1
4	4.3
9.99	11

User Spectra

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

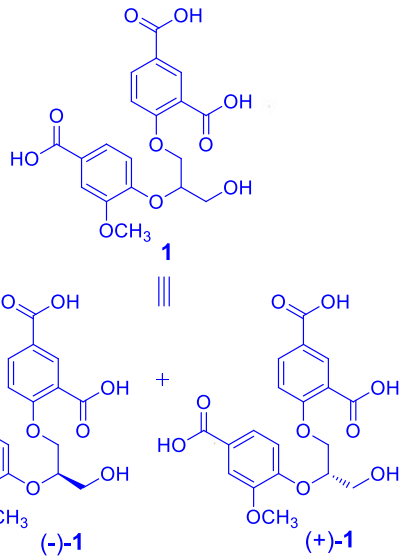
Qualitative Analysis Report

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi



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)+	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)+	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

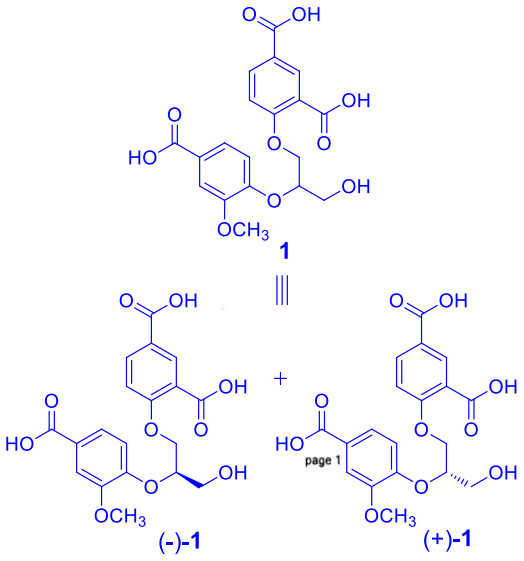


Figure S6. The (+)-HRESIMS report of **1**, page 3.

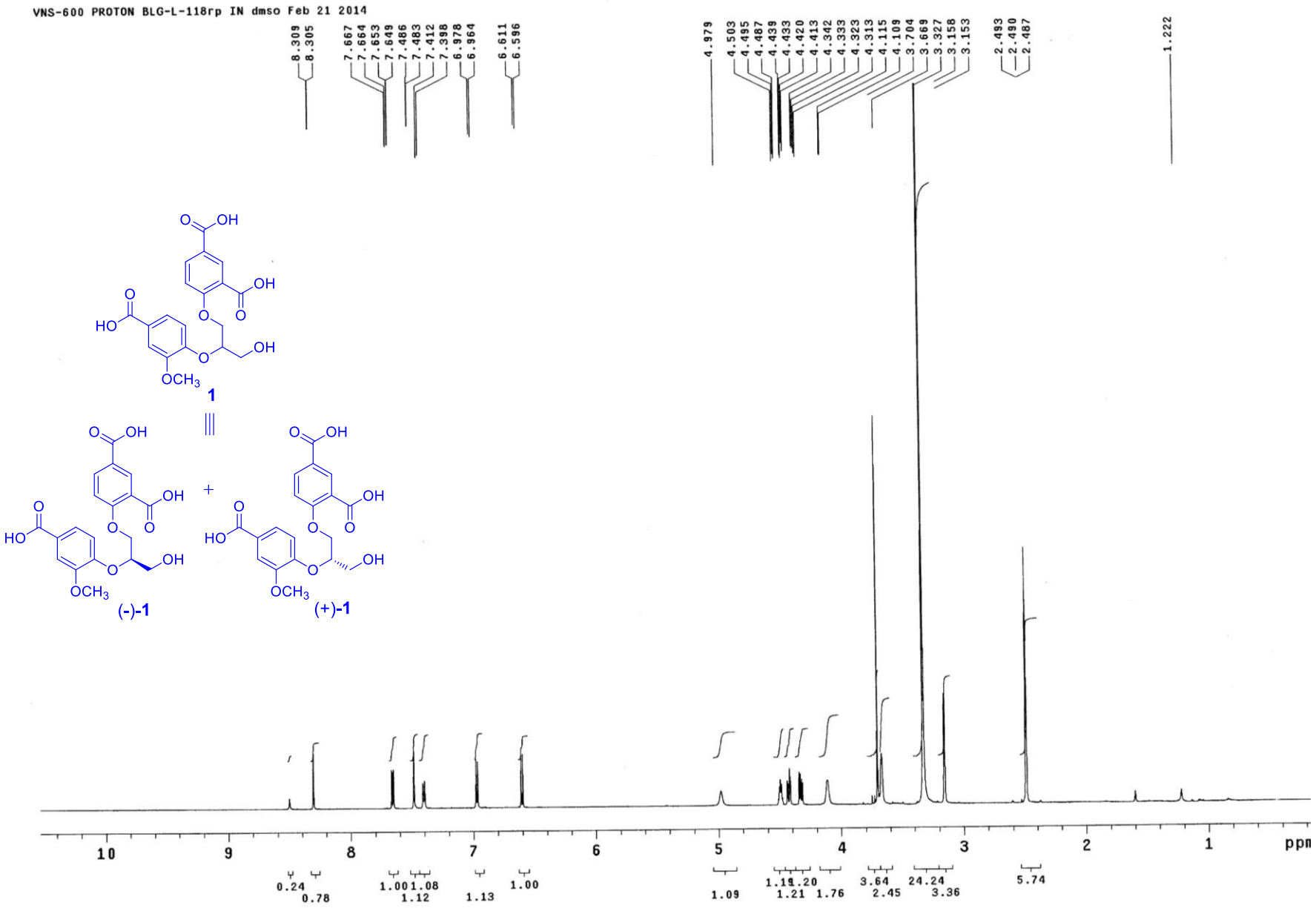


Figure S7.The ^{1}H NMR spectrum of **1** in DMSO-d_6 (600 MHz).

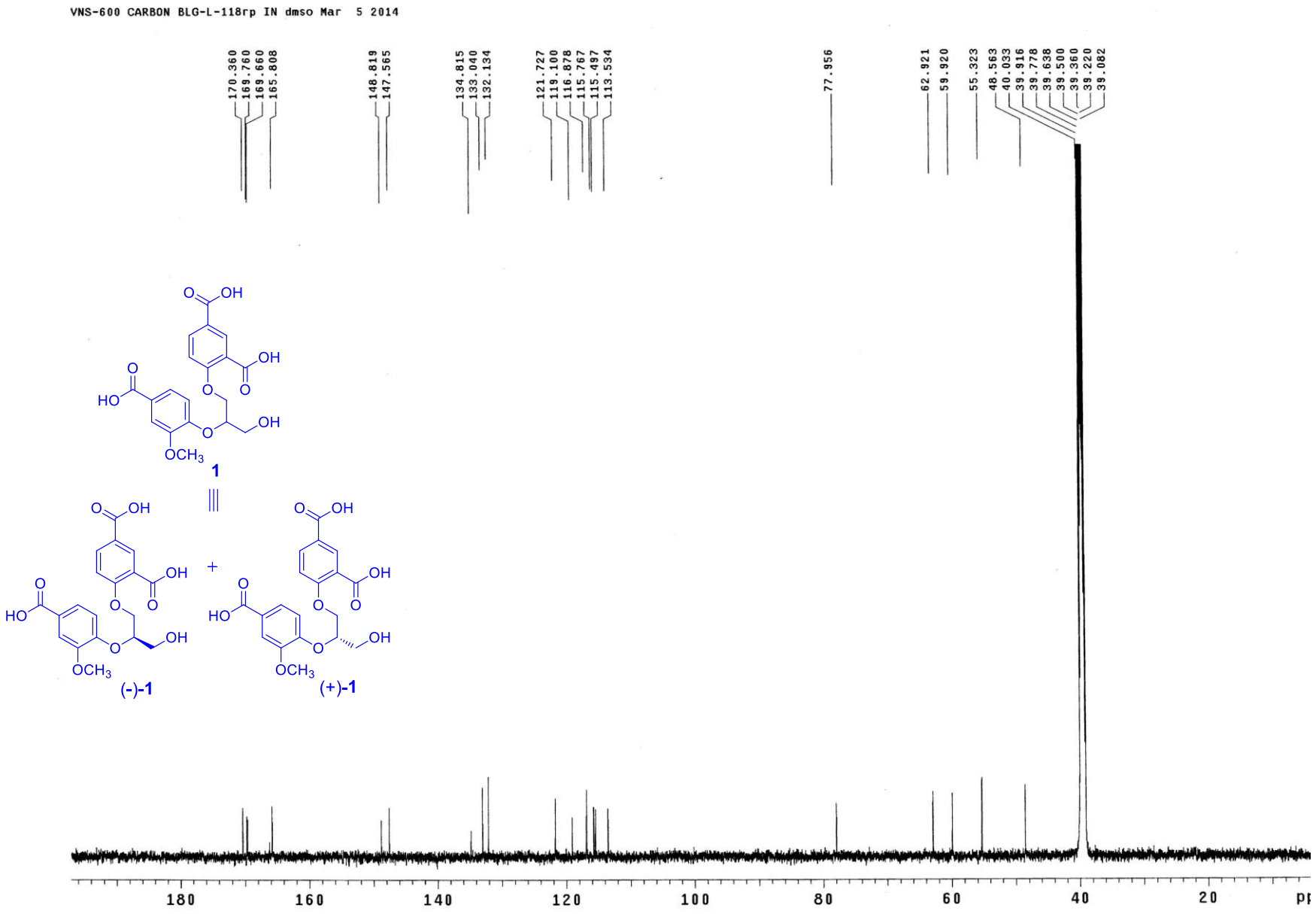


Figure S8. The ^{13}C NMR spectrum of **1** in DMSO-d_6 (150 MHz).

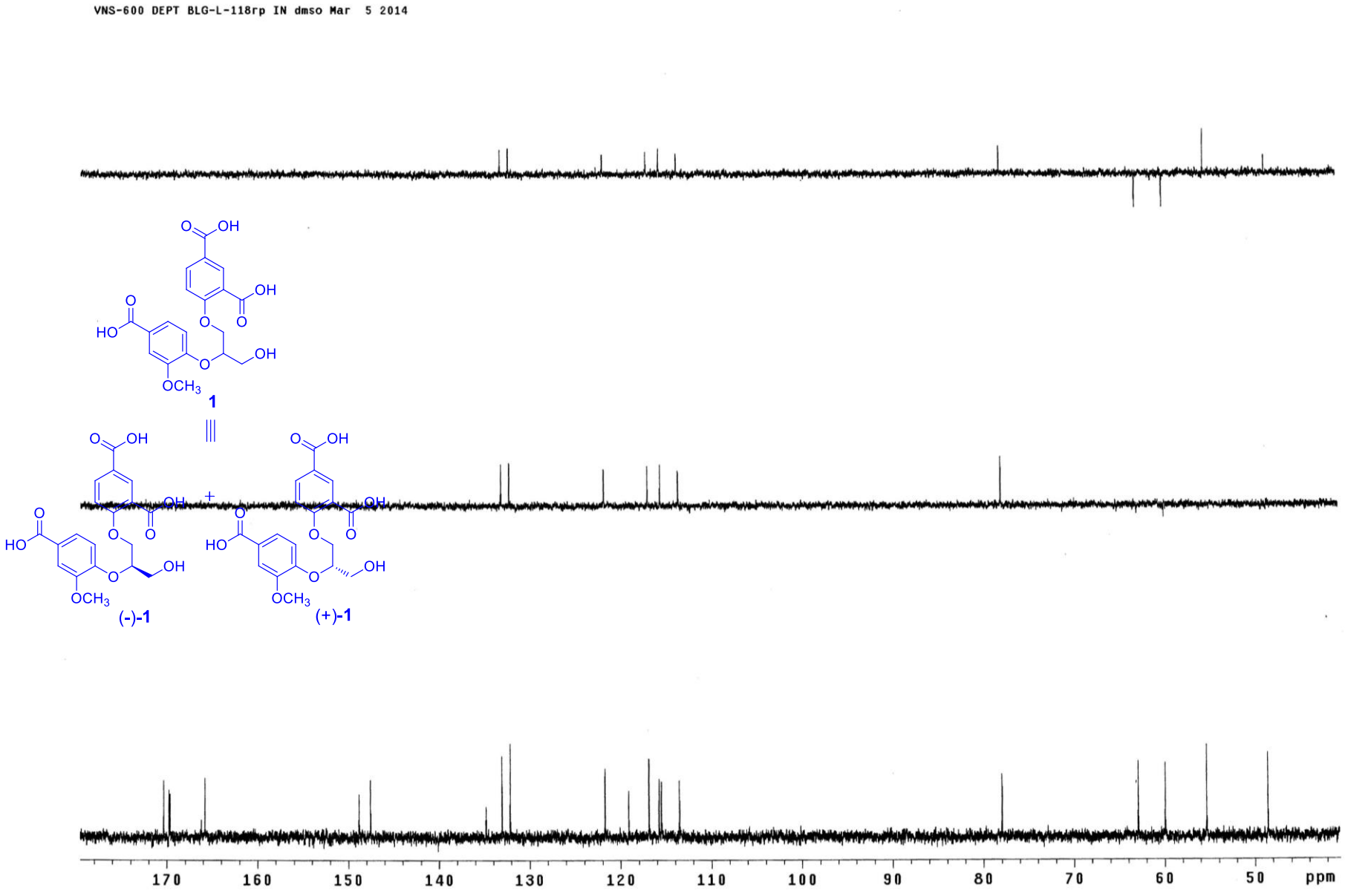


Figure S9. The DEPT spectrum of **1** in DMSO-d_6 (150 MHz).

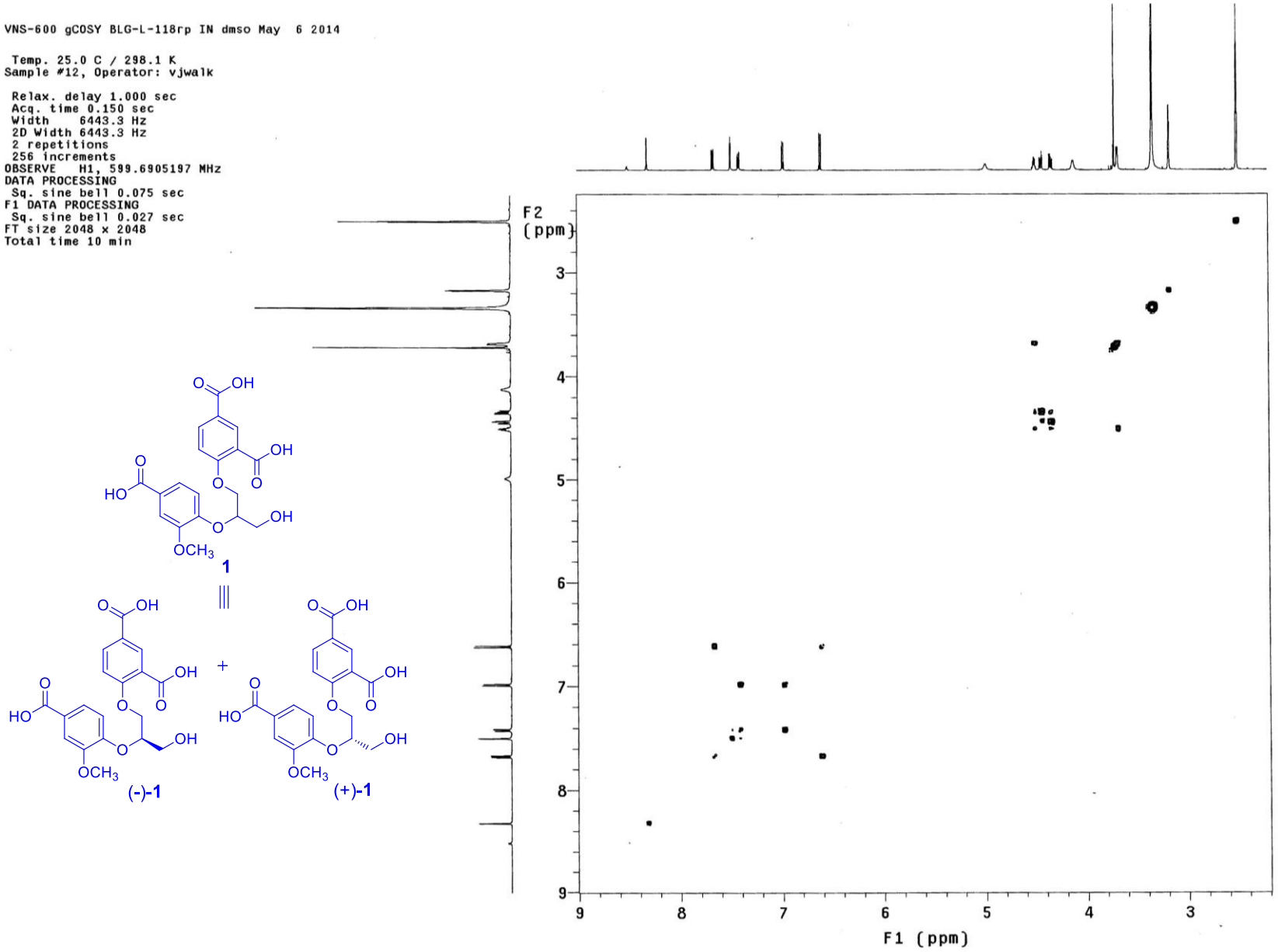


Figure S10. The ^{1}H-^{1}H COSY spectrum of **1** in DMSO-d_6 (600 MHz).

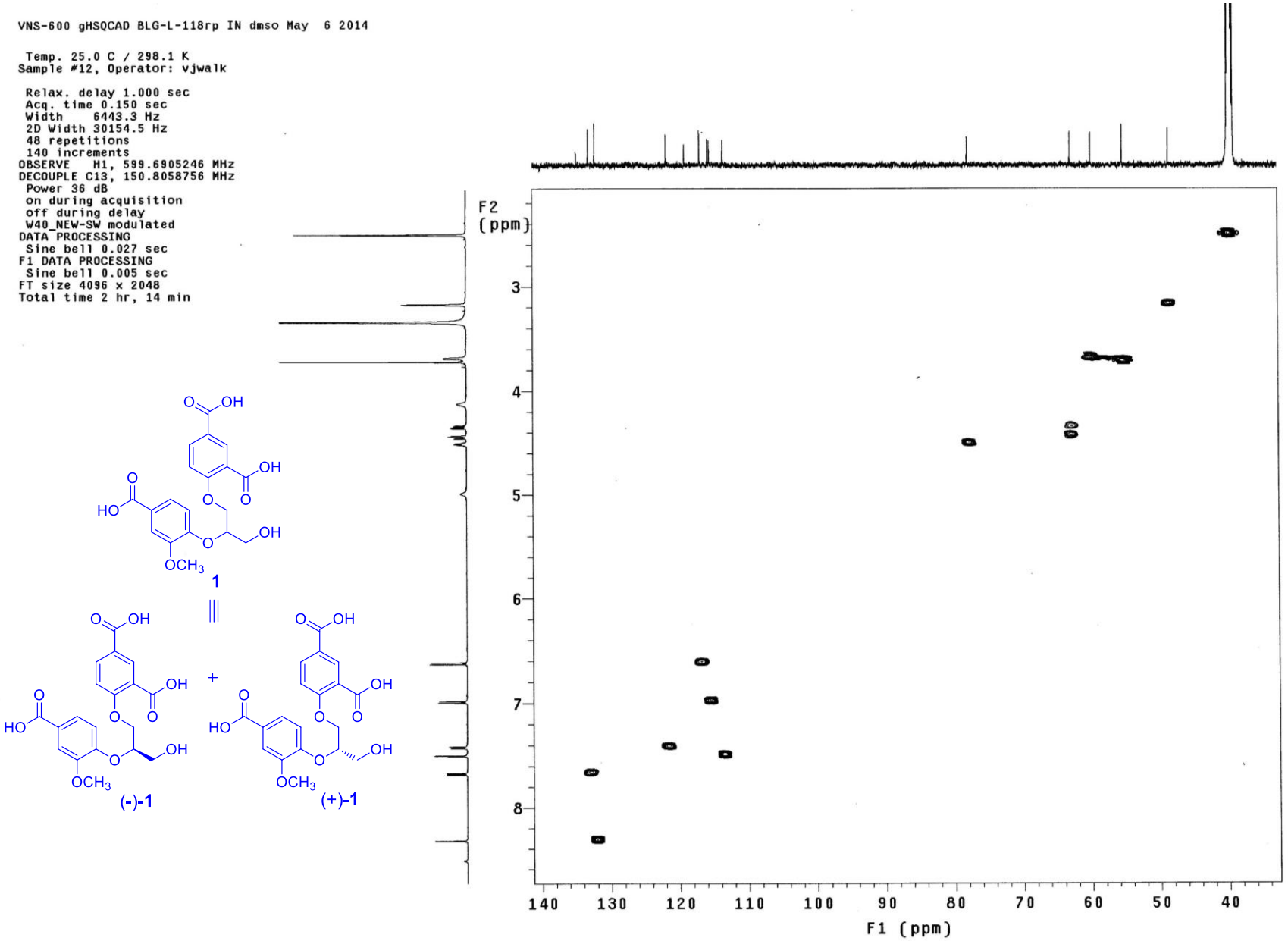


Figure S11. The HSQC spectrum of **1** in DMSO-d_6 (600 MHz for ^{1}H).

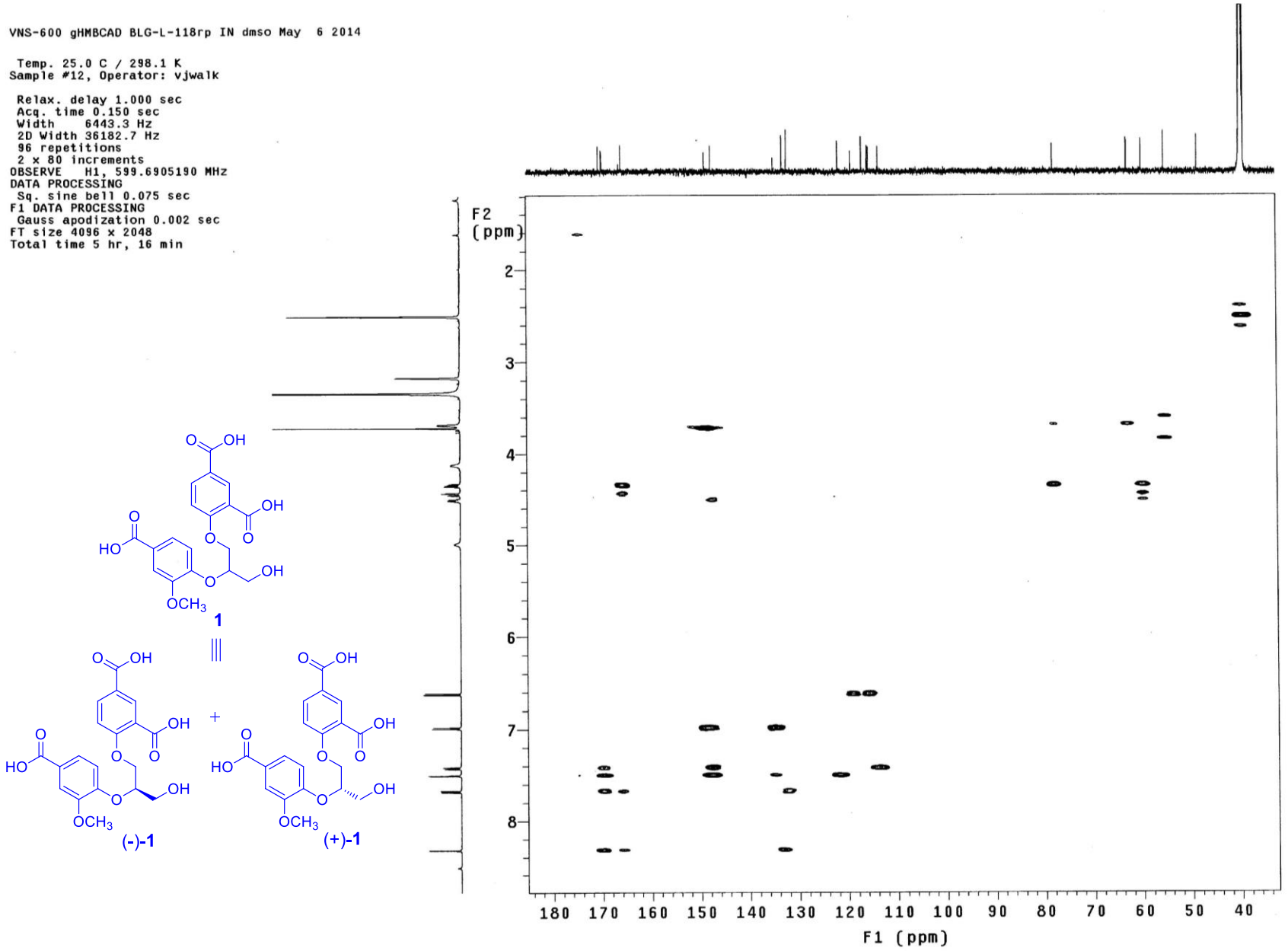


Figure S12. The HMBC spectrum of **1** in DMSO-d_6 (600 MHz for ^{1}H).

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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
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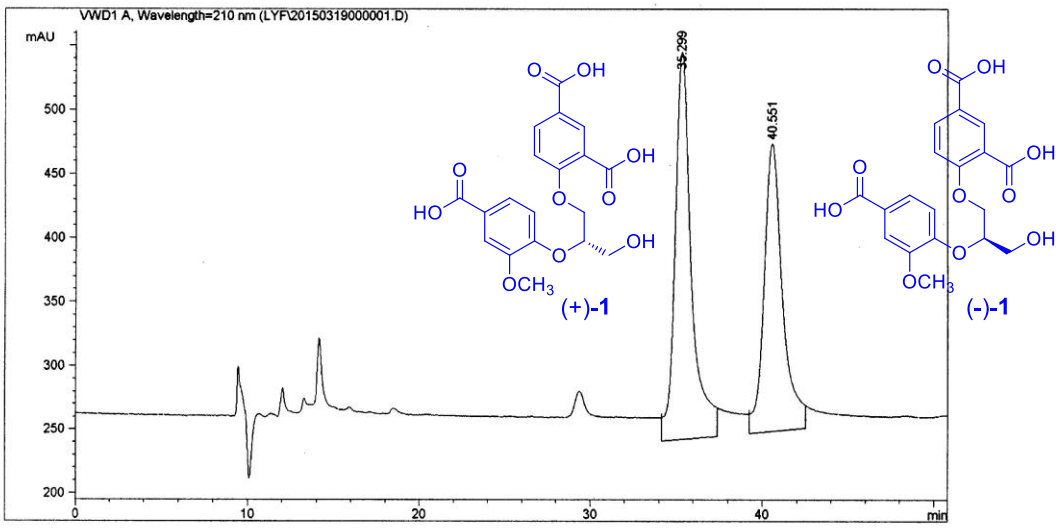


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                          Area Percent Report

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


Signal 1: VWD1 A, Wavelength=210 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s    [mAU   ]     %
----|-------|----|-------|----------|----------|--------|
   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 ***
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Instrument 1 2015-3-21 9:51:12 Page 1 of 1

Figure S13. The HPLC chromatogram of **1** on Chiralpak AD-H column [5 μm, 250 × 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℃].

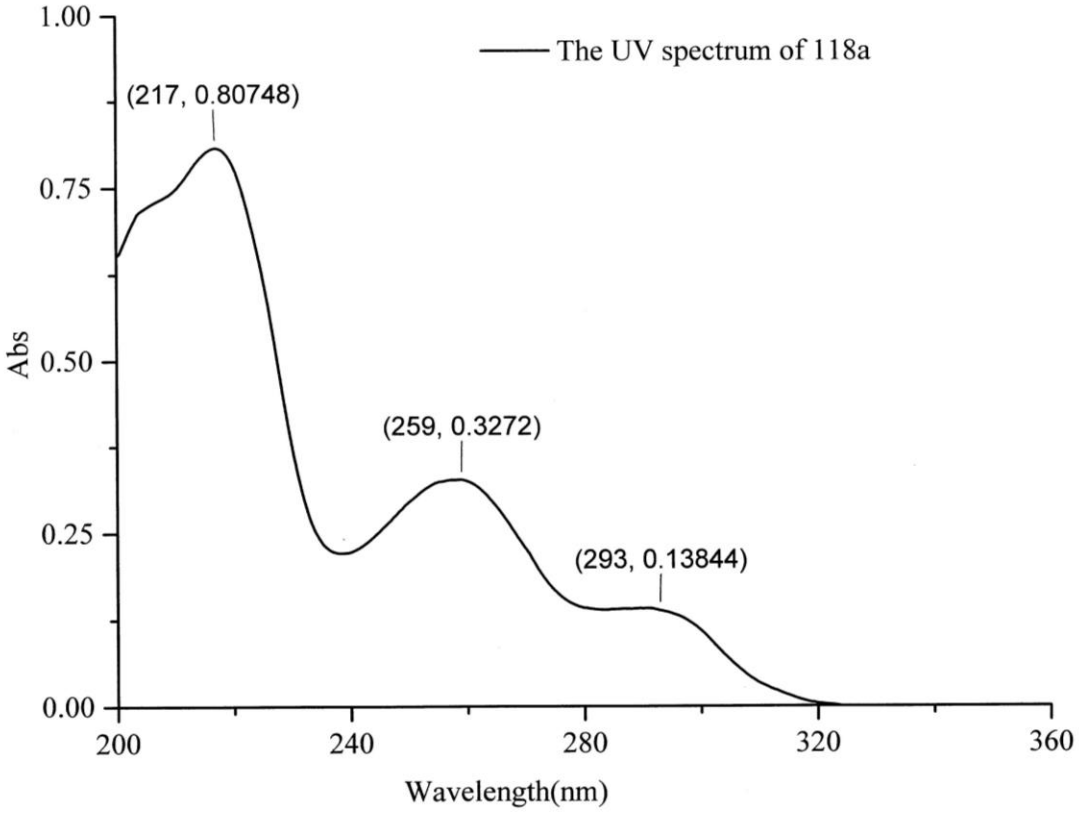
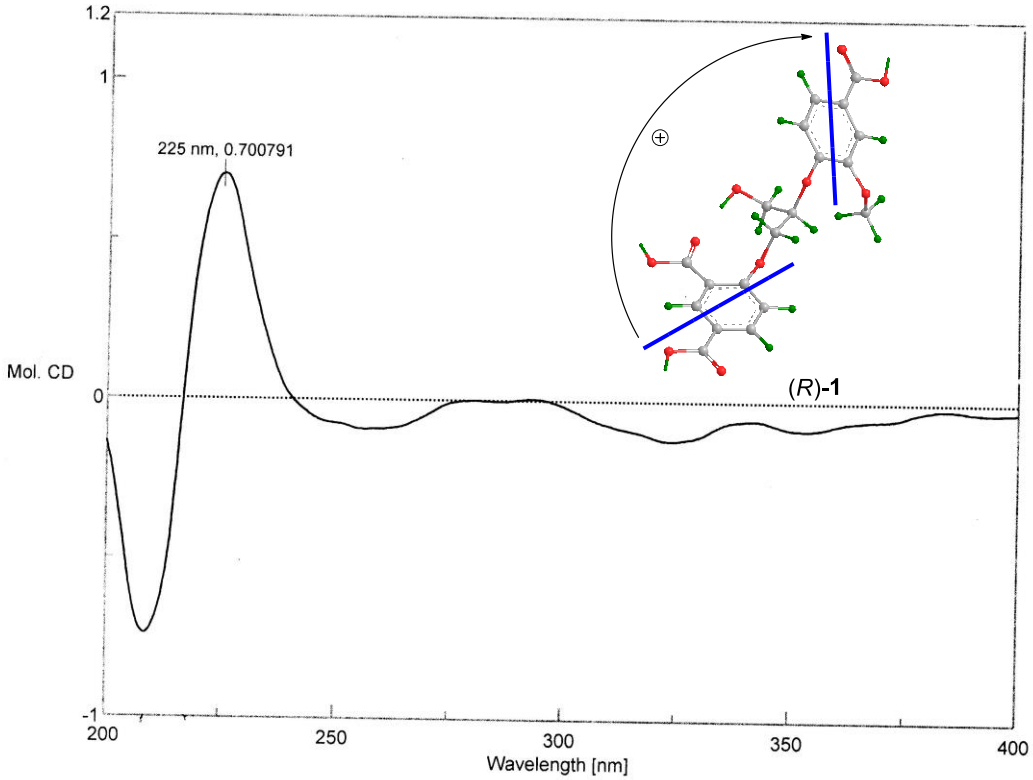


Figure S14. The UV spectrum of compound (**–**)-**1** in MeOH



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Comment	
User	
Division	
Company	dell

[Measurement Information]

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Accessory	Standard
Accessory S/N	A024461168
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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]

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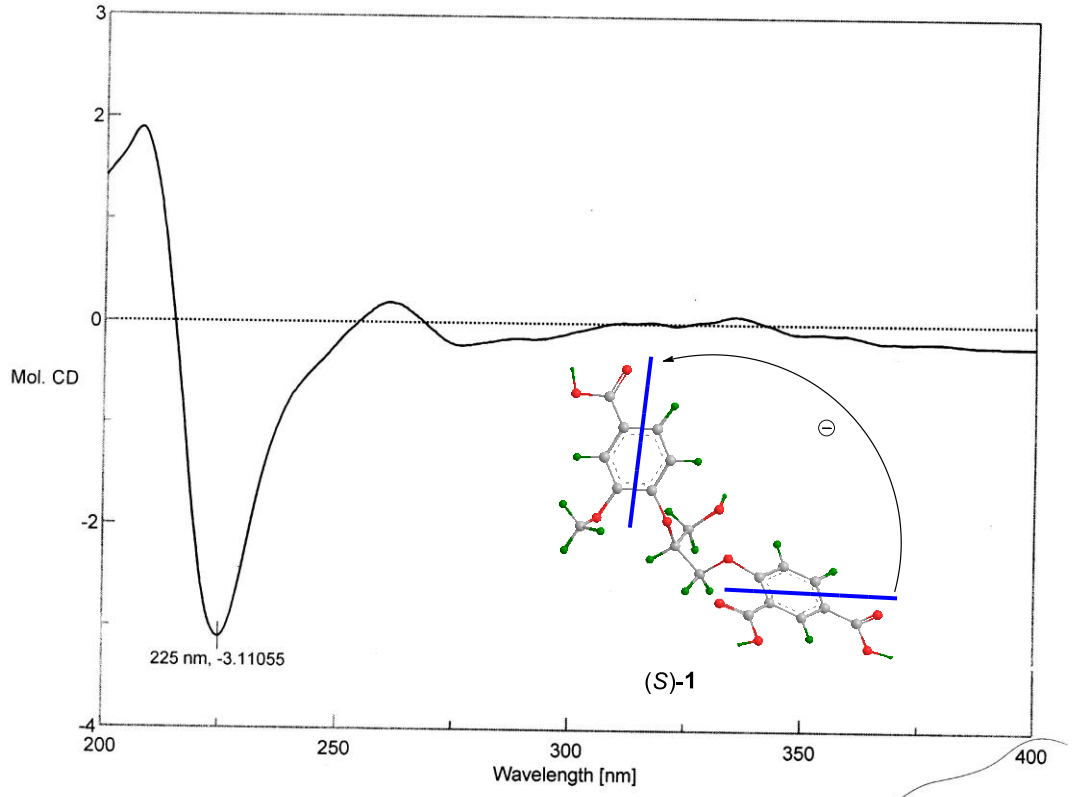
Vertical axis(1)	Mol. CD
Vertical axis(2)	HT [V]
Vertical axis(3)	Abs
Start	400 nm
End	200 nm
Data interval	0.5 nm
Data points	401

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



[Comments]

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Comment	
User	
Division	
Company	dell

[Measurement Information]

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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.

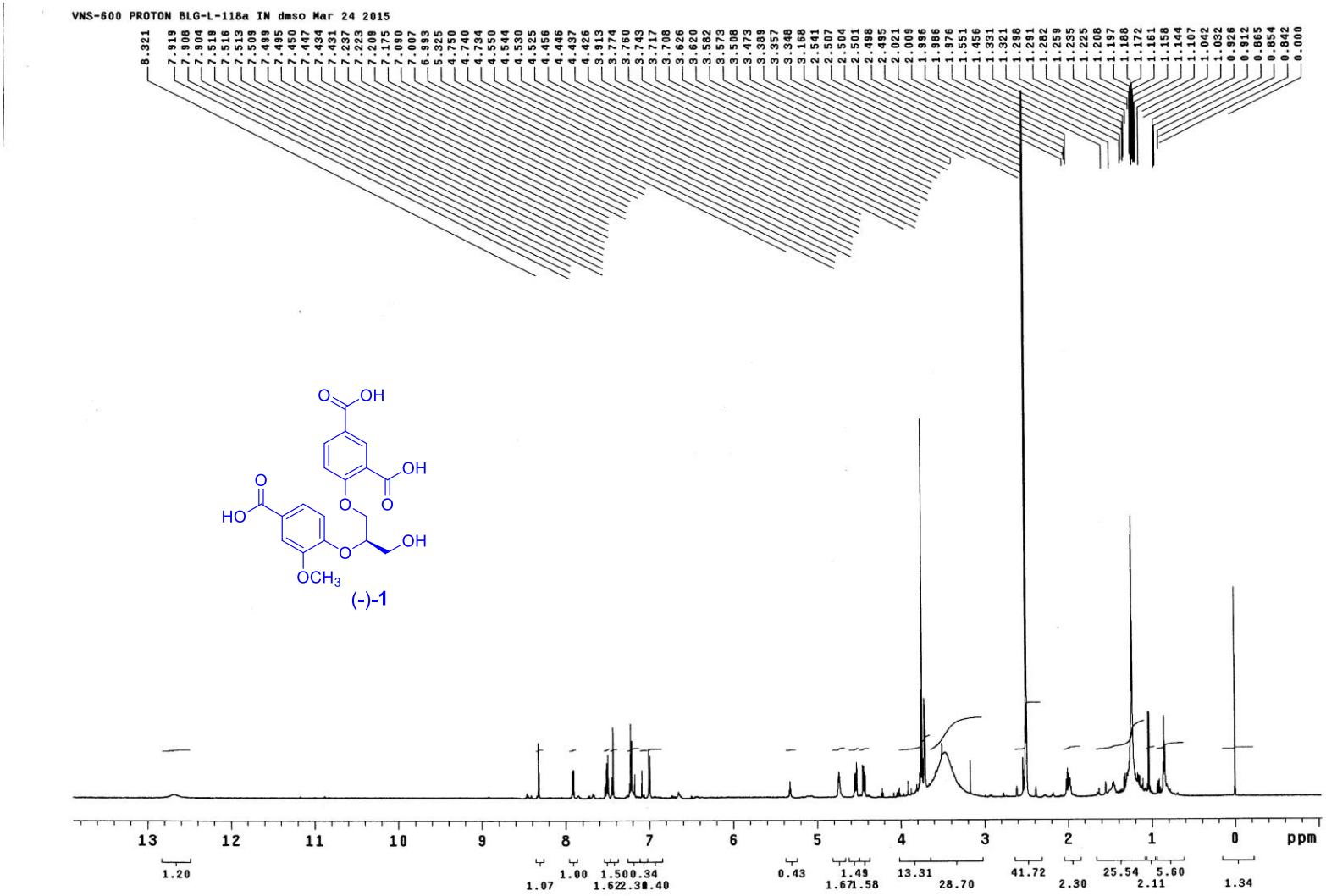


Figure S17. The ^{1}H NMR spectrum of compound (−)-**1** in DMSO-d_6 (600 MHz).

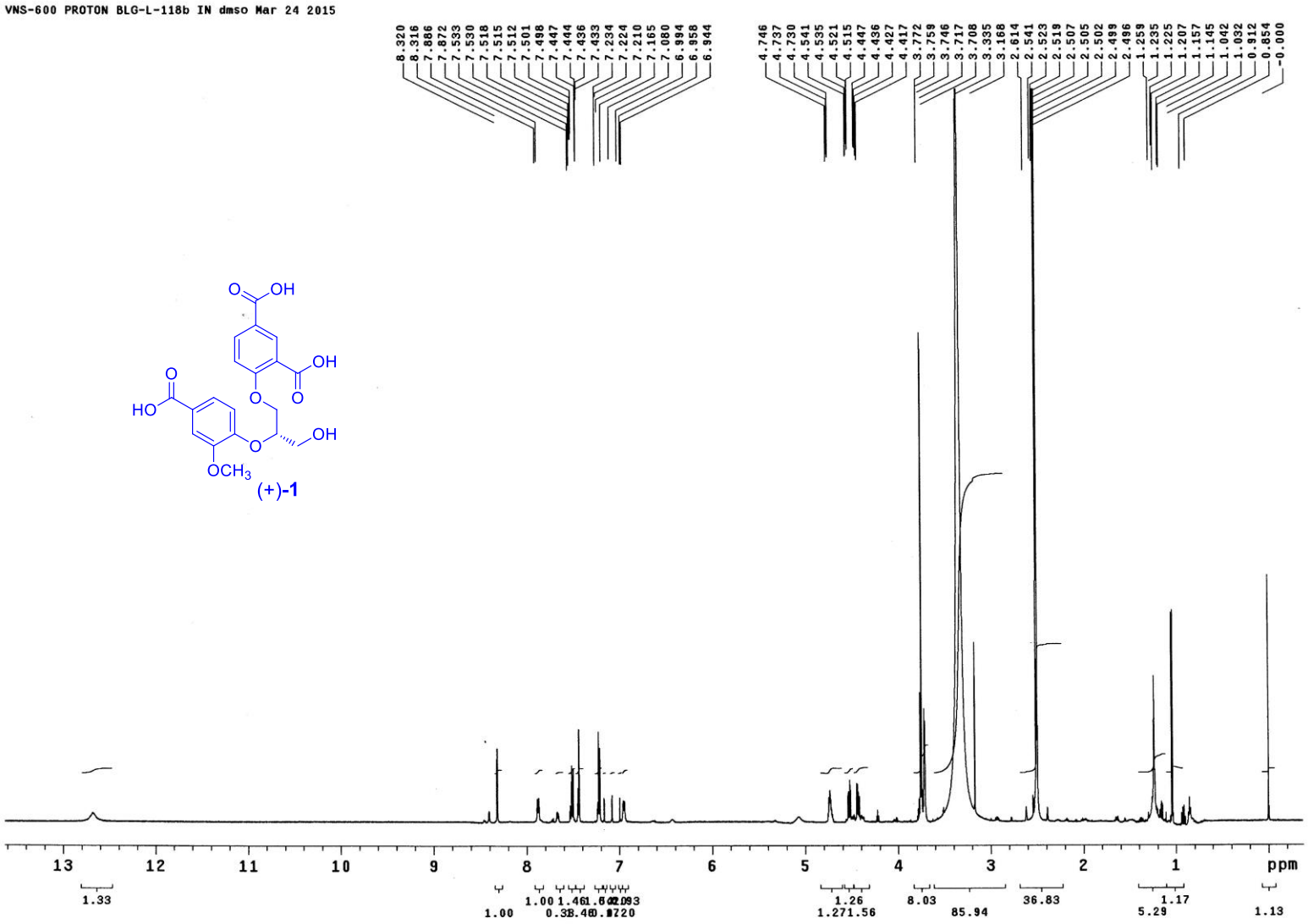
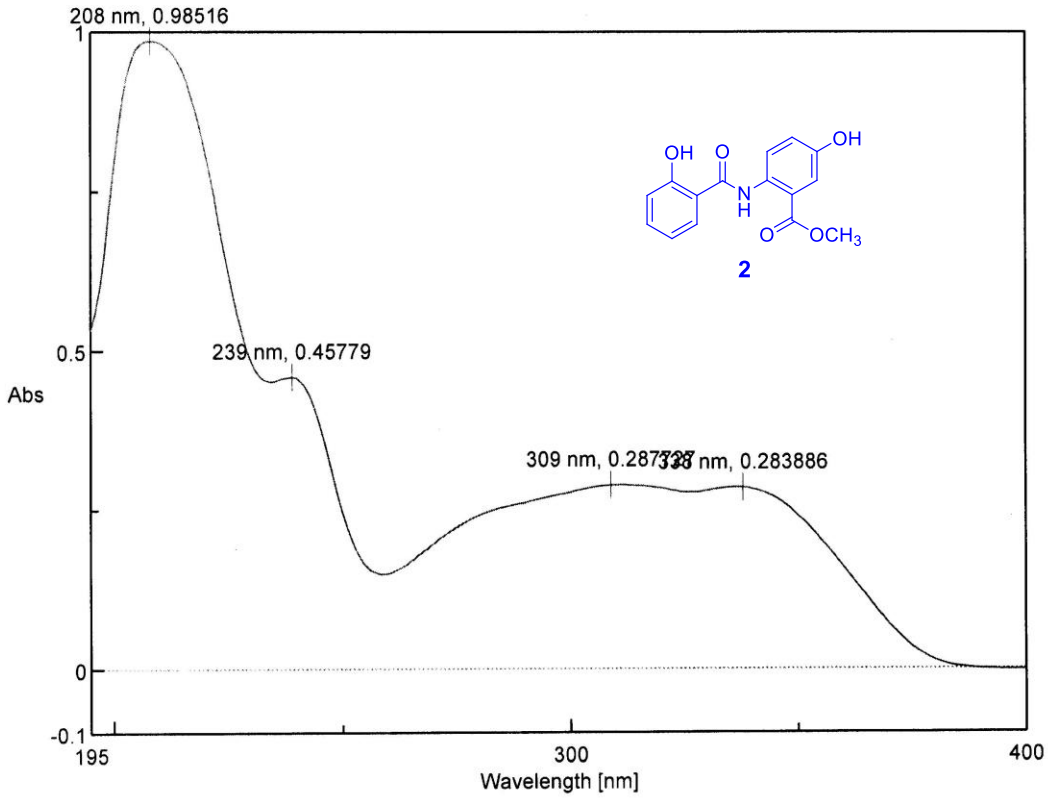


Figure S18. The ^{1}H NMR spectrum of compound (+)-**1** in DMSO-d_6 (600 MHz).



CI-12-2-W

[Comment]
Sample Name CI-12
Comment
User
Division
Company 324

[Measurement Information]
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Model Name V-650
Serial No. A034461150

Accessory PSC-718
Accessory S/N A001761114
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Control Sonsor Holder
Monitor Sensor Holder
Start Mode Start immediately

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

[Data Information]
Creation Date 2011-9-14 16:13

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Vertical Abs
Start 400 nm
End 195 nm
Data pitch 1 nm
Data points 206

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

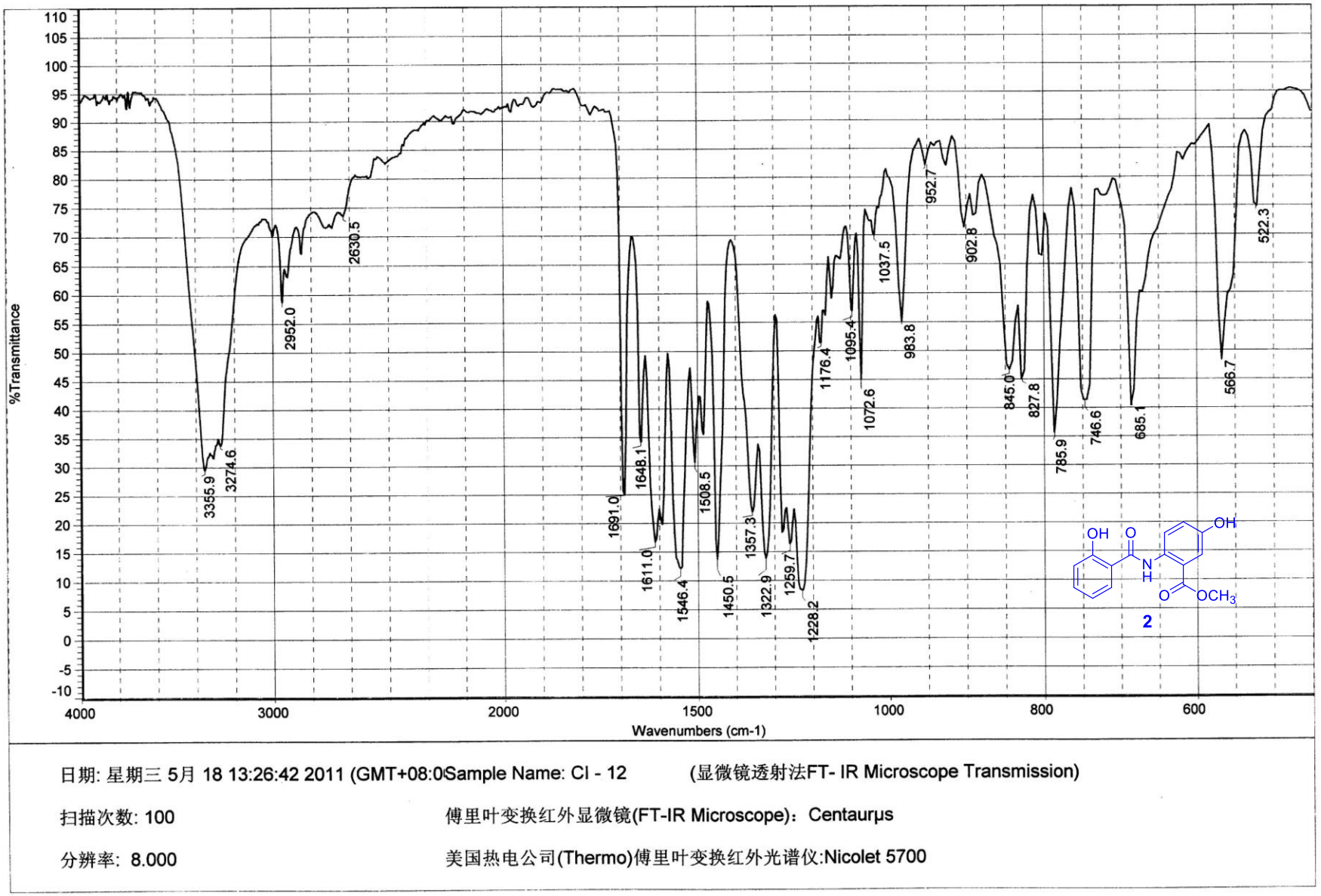


Figure S20. The IR spectrum of compound **2**.

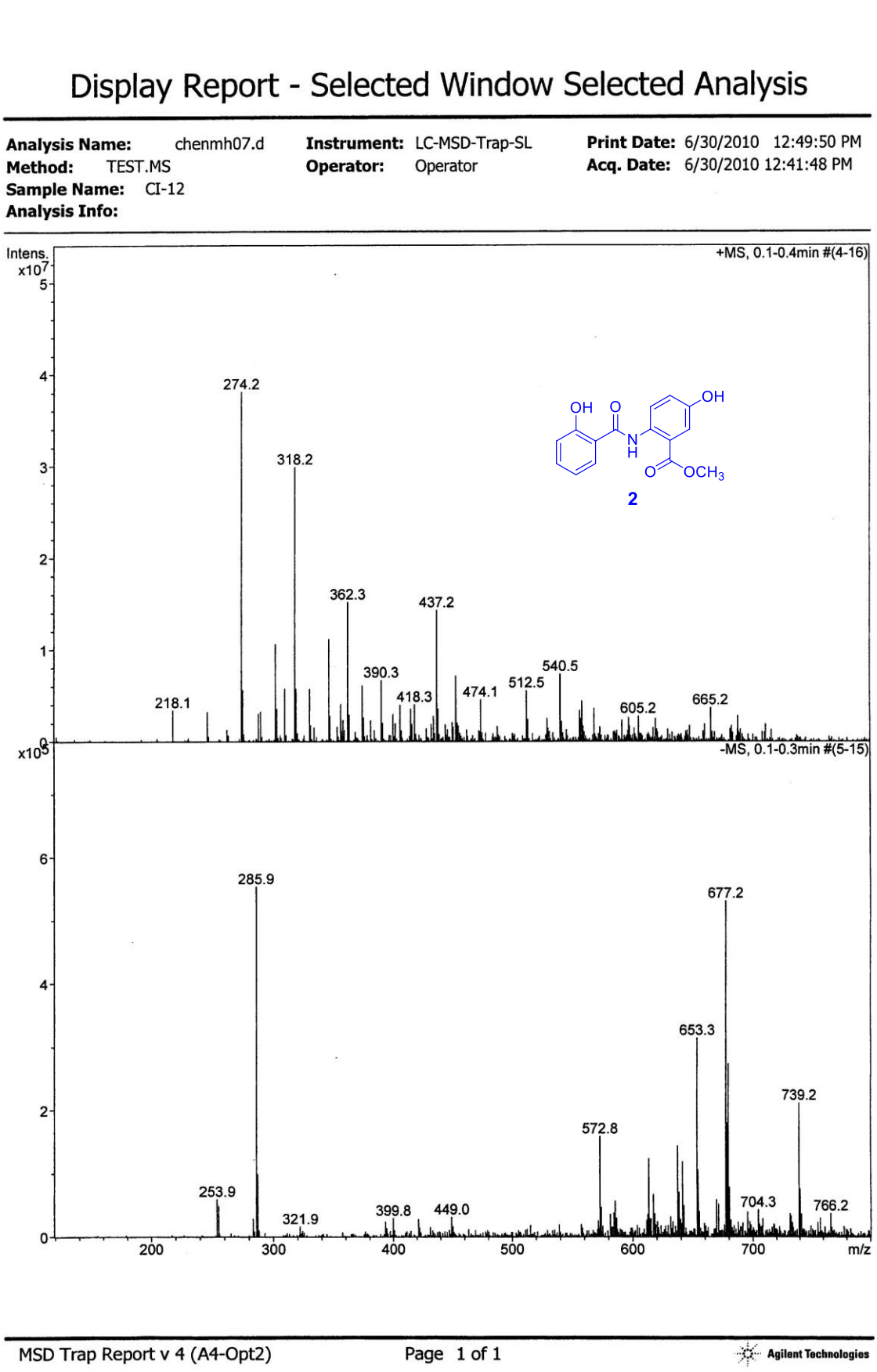


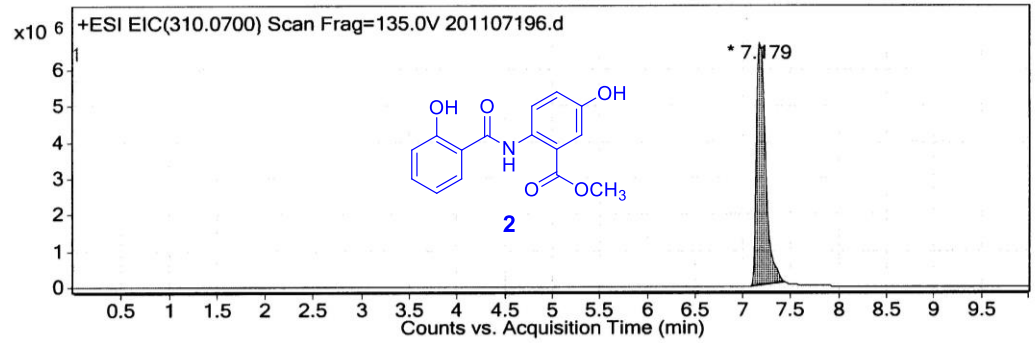
Figure S21. The ESIMS report of compound **2**.

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**	[redacted]
DA Method	TEST LCMS.m	**Comment**	

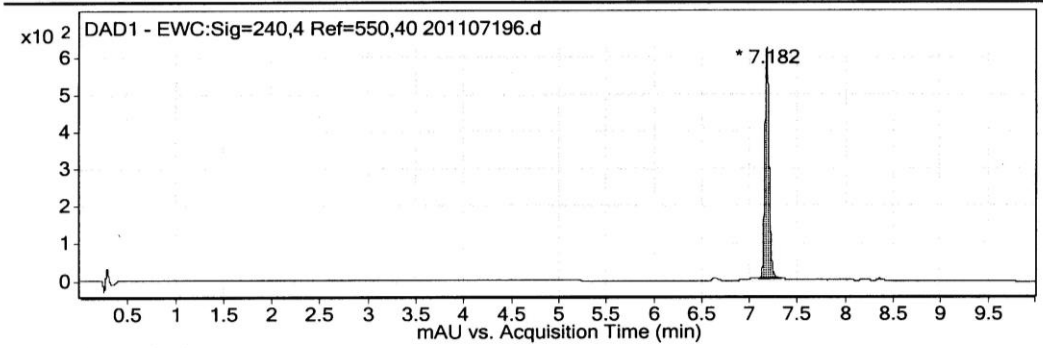
User Chromatograms

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

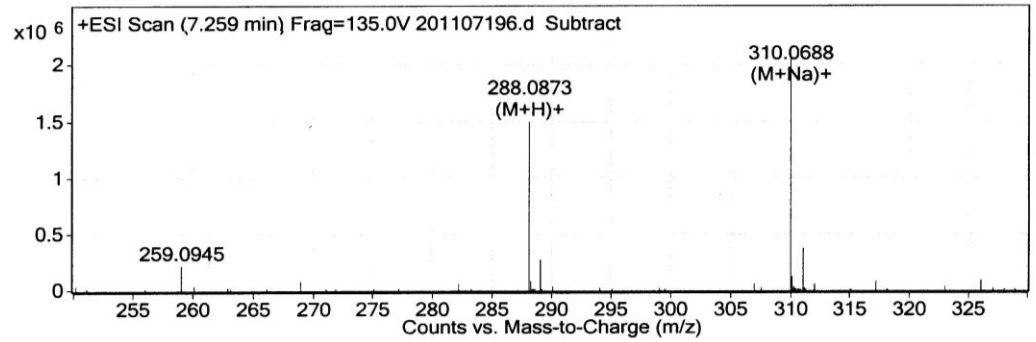


Figure S22. The (+)-HRESIMS report of compound **2**, page 1.

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		

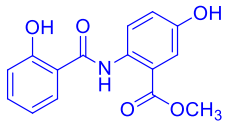
Formula Calculator Element Limits

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 ---



2

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

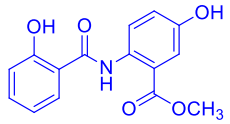
MS Formula Results: + Scan (7.259 min) Sub (201107196.d)

m/z	Ion	Formula	Abundance
288.0873	(M+H)+	C15 H14 N O5	1499512.5

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
☑	C15 H13 N O5	C15 H14 N O5	288.0866	99.86		287.0801	287.0794	-2.37	2.37	99.8	100	99.83	288.0873	10
☐	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
☐	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
☐	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
☐	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
☐	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)+	C15 H13 N Na O5	2091715.9

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
☑	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
☐	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
☐	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
☐	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
☐	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
☐	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



2

page 1

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

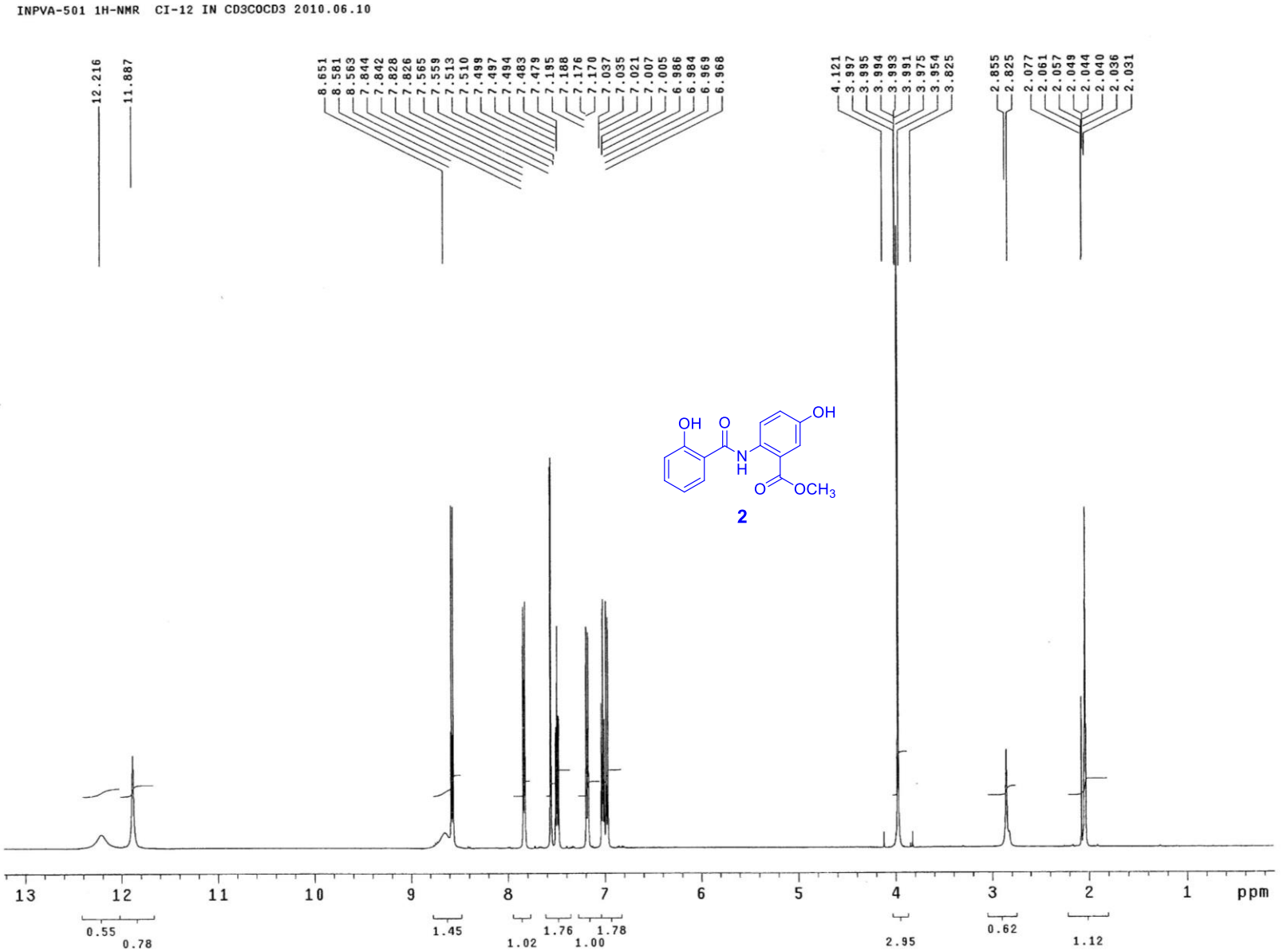


Figure S25.The ^{1}H NMR spectrum of compound **2** in acetone-d_6 (500 MHz).

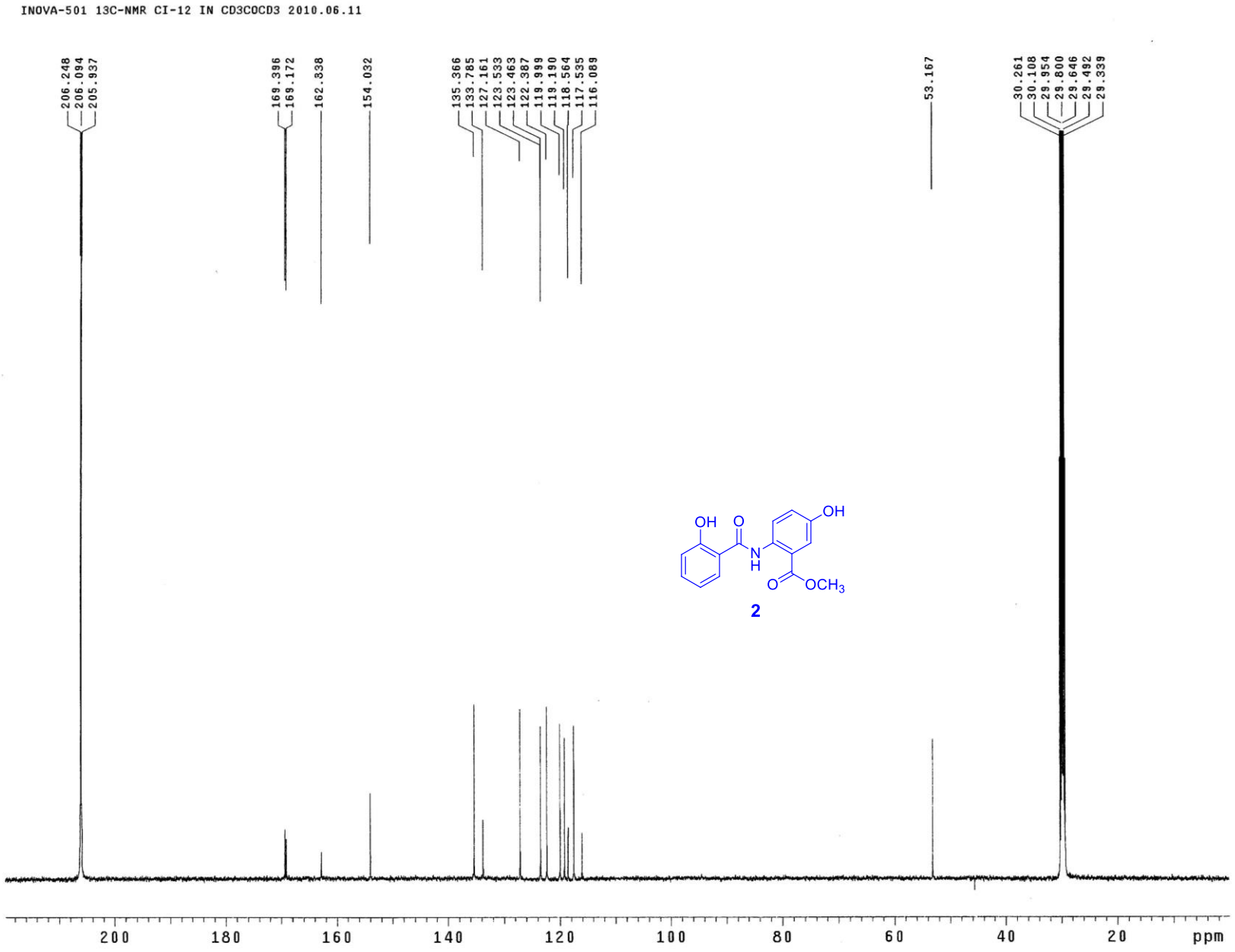


Figure S26. The ^{13}C NMR spectrum of compound **2** in acetone-d_6 (125 MHz).

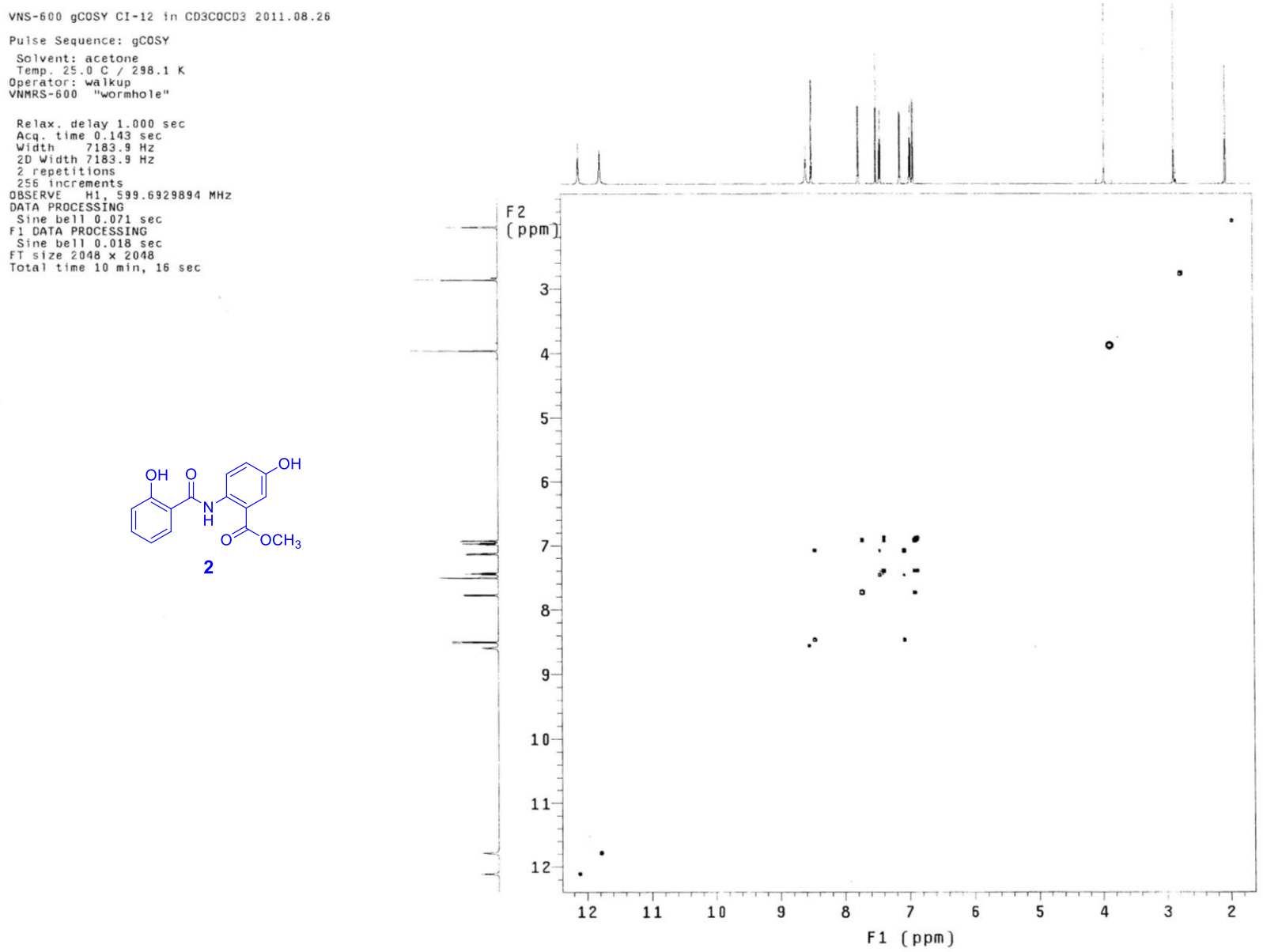


Figure S27. The ^{1}H-^{1}H COSY spectrum of compound **2** in acetone-d_6 (500 MHz).

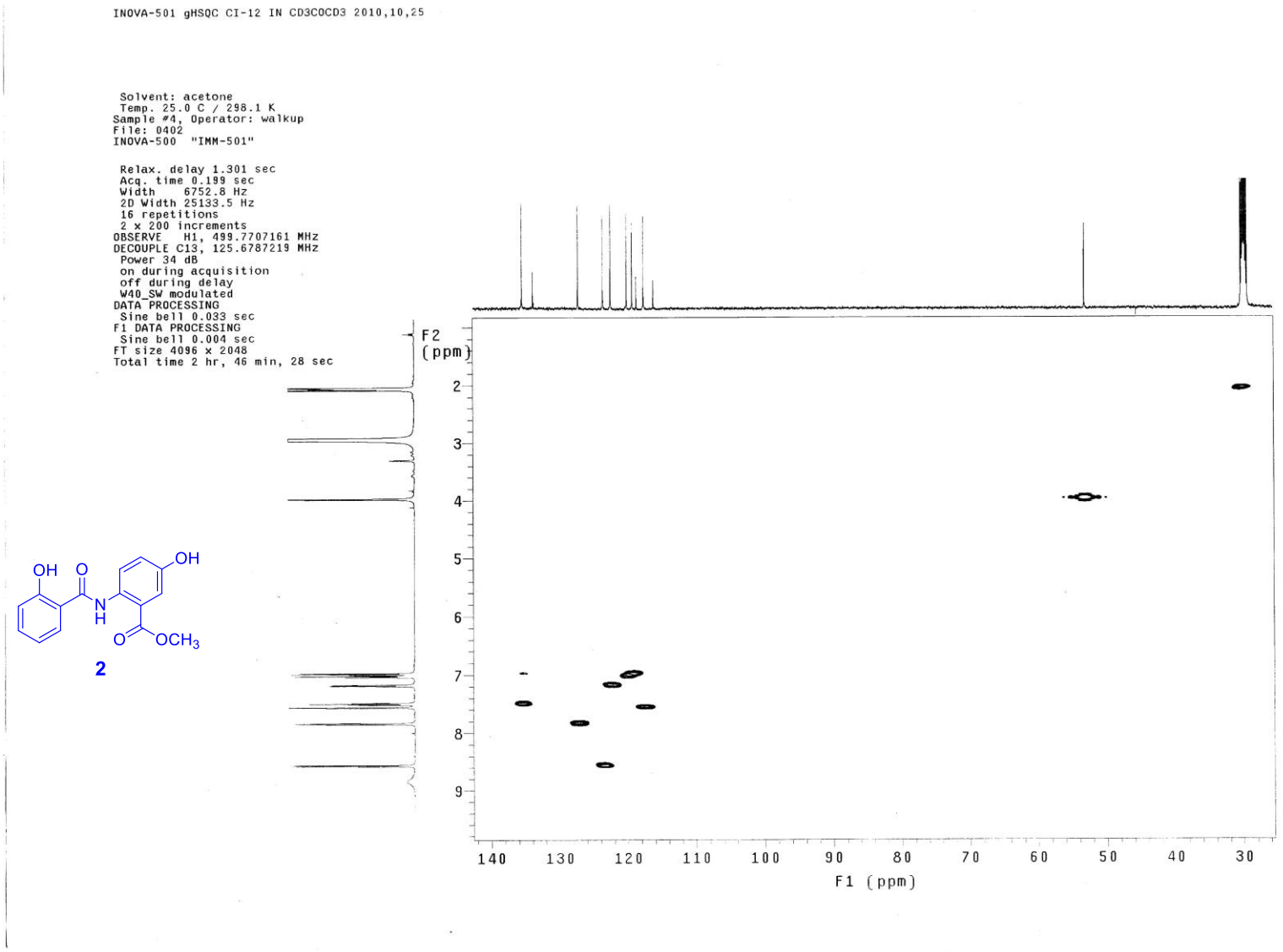


Figure S28. The HSQC spectrum of compound **2** in acetone-d_6 (500 MHz for ^{1}H).

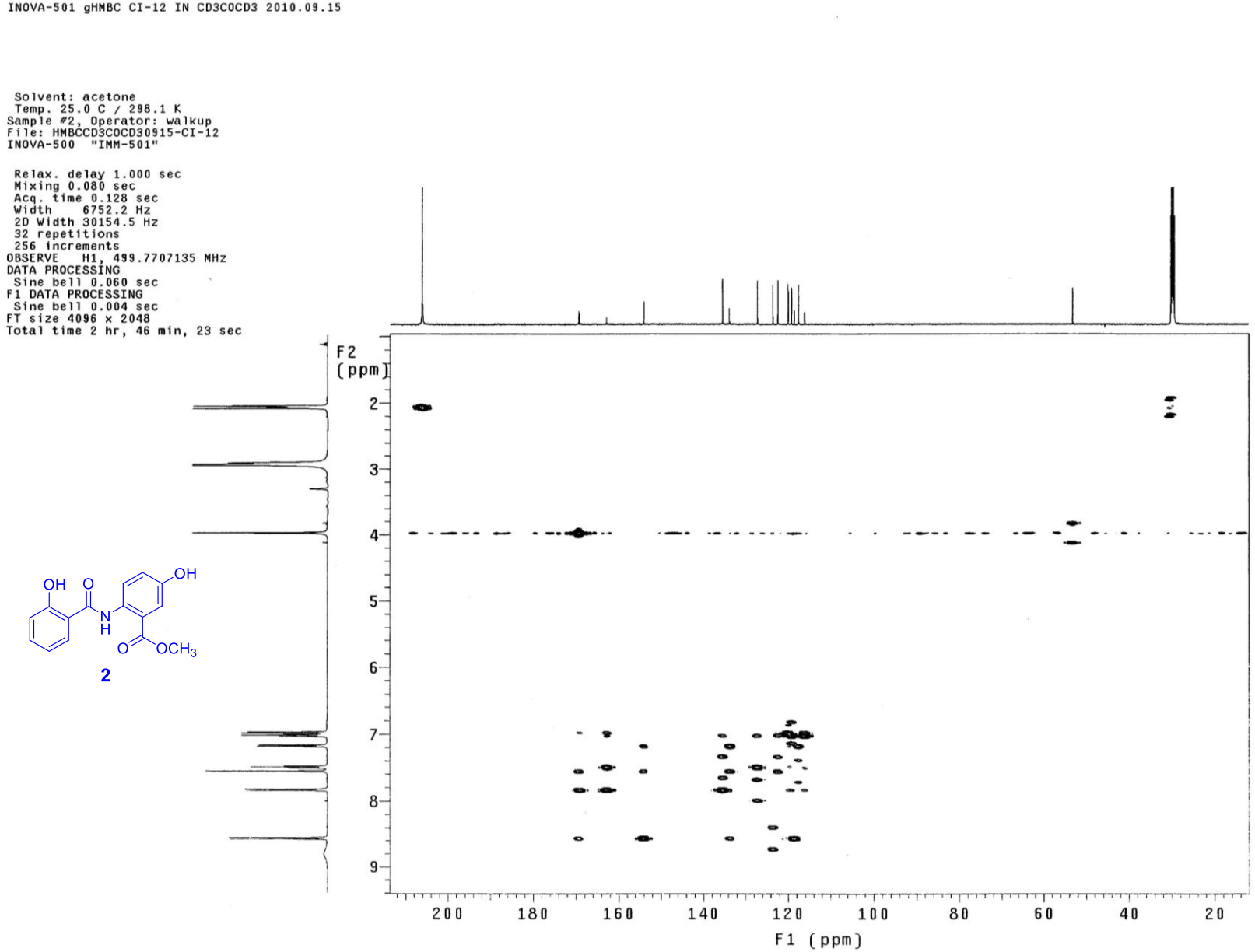
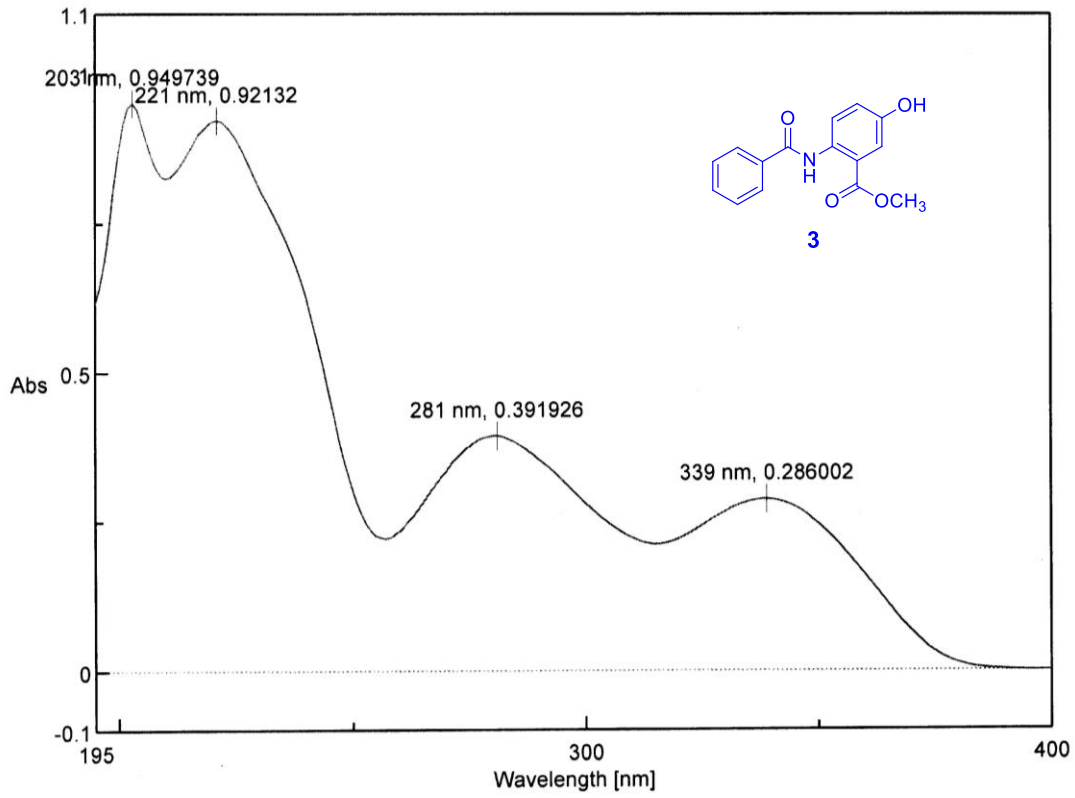


Figure S29. The HMBC spectrum of compound **2** in acetone-d_6 (500 MHz for ^{1}H).



Memory-10

[Comment]
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 Sonsor Holder
Monitor Sensor Holder
Start Mode Start immediately

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

[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

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

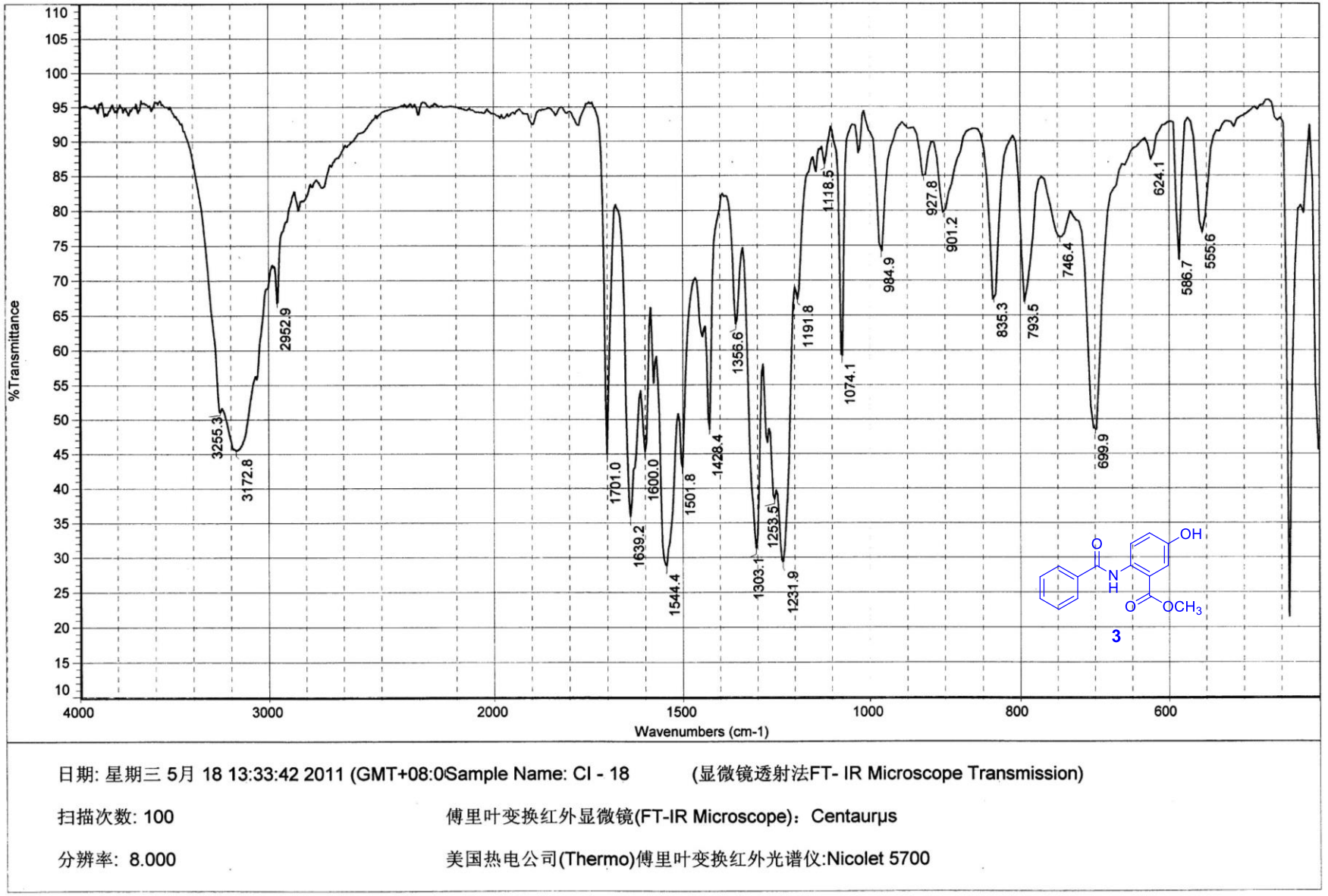


Figure S31. The IR spectrum of compound **3**.

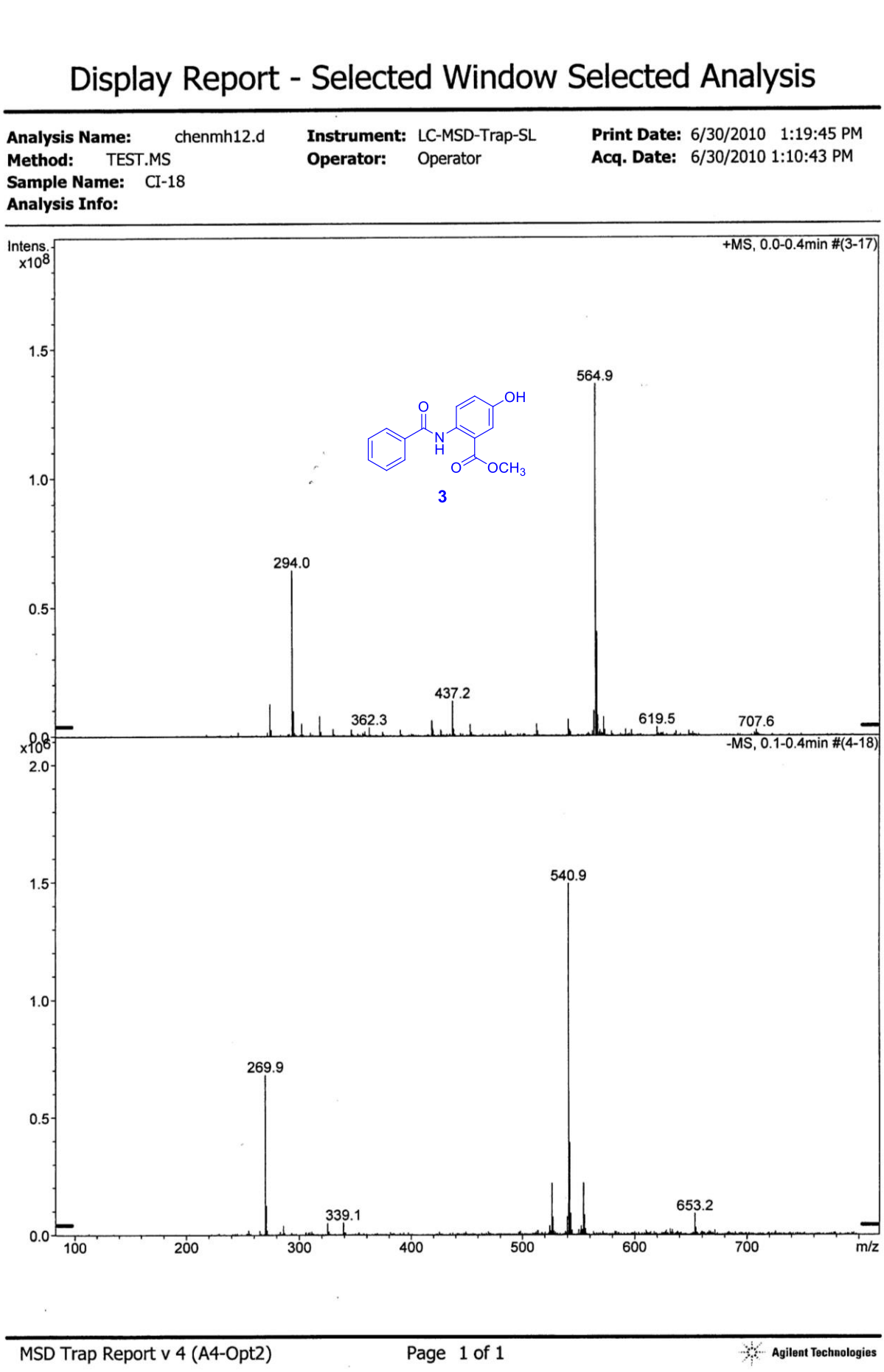


Figure S32. The ESI mass spectrum of compound **3**.

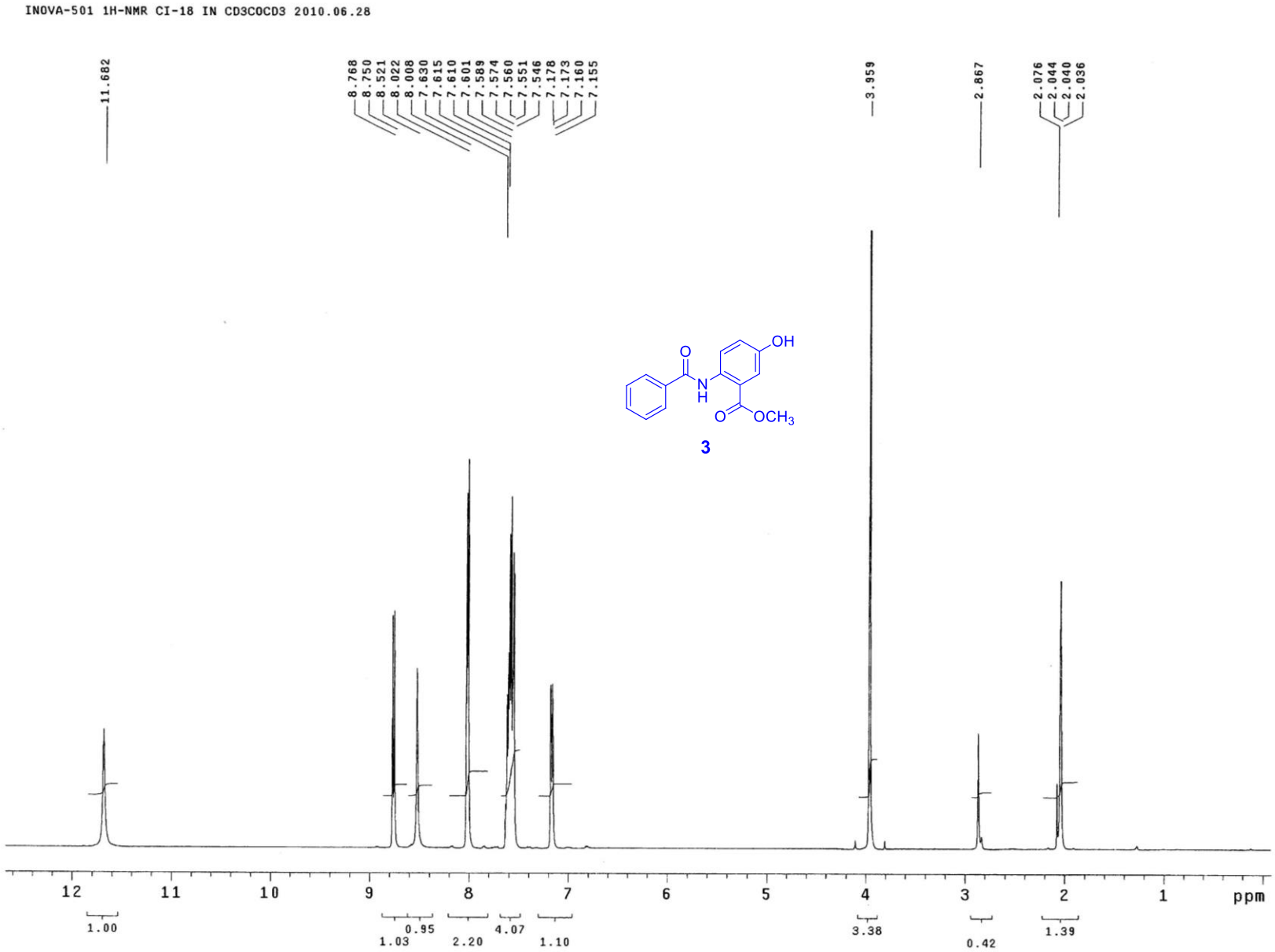


Figure S33. The ^{1}H NMR spectrum of compound **3** in acetone-d_6 (500 MHz).

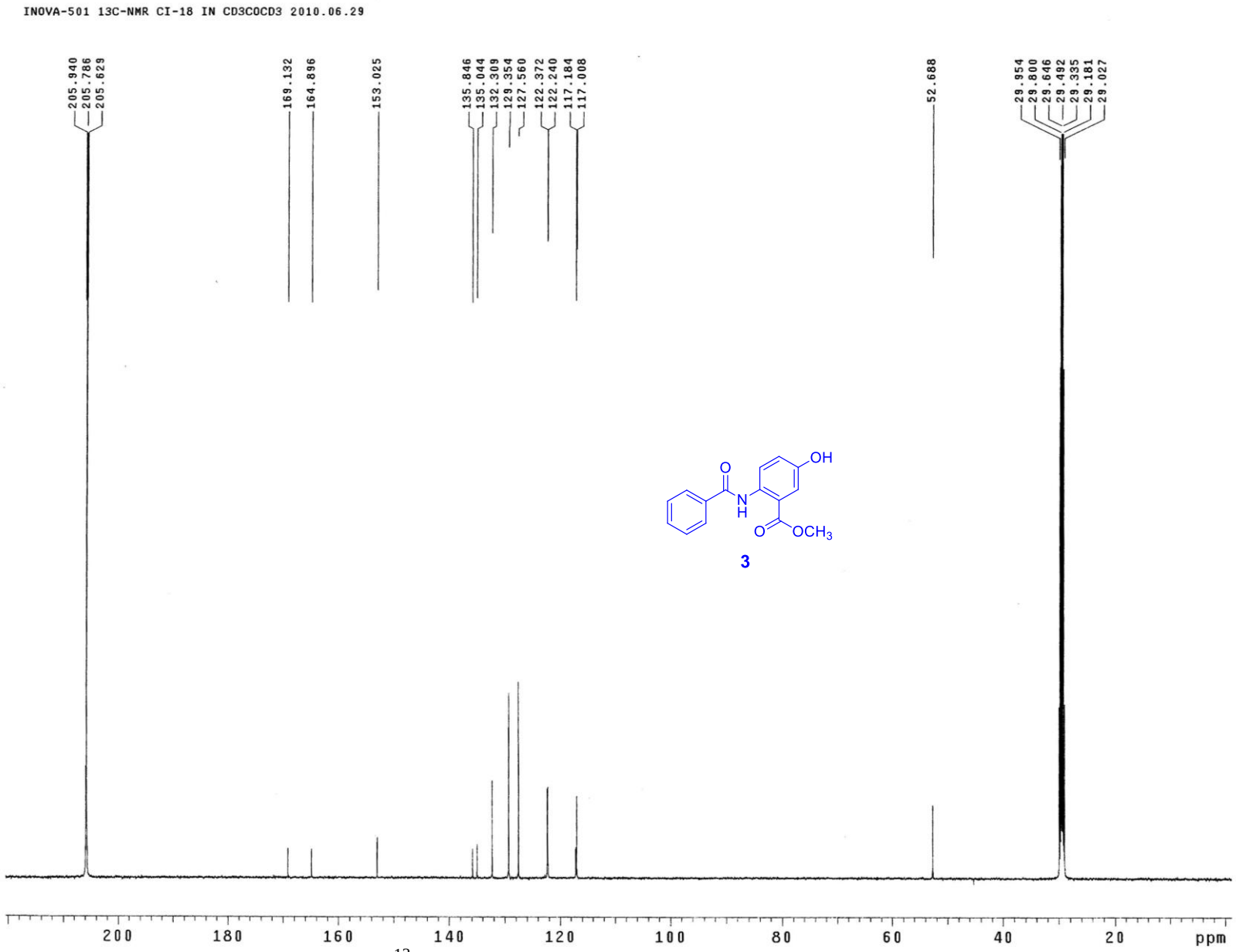


Figure S34. The ^{13}C NMR spectrum of compound **3** in acetone-d_6 (125 MHz).

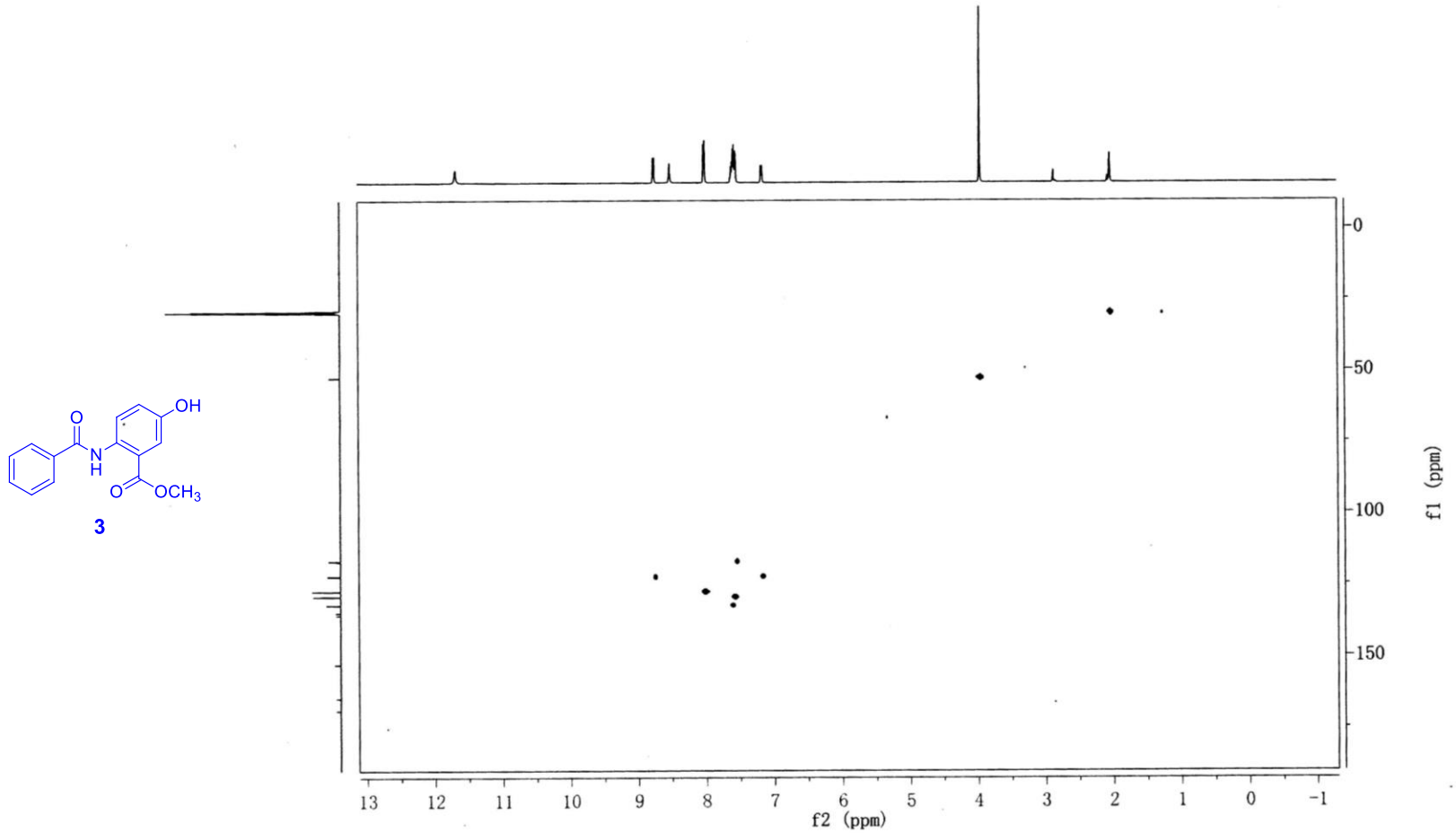


Figure S35. The HSQC spectrum of compound **3** in acetone-d_6 (500 MHz for ^{1}H).

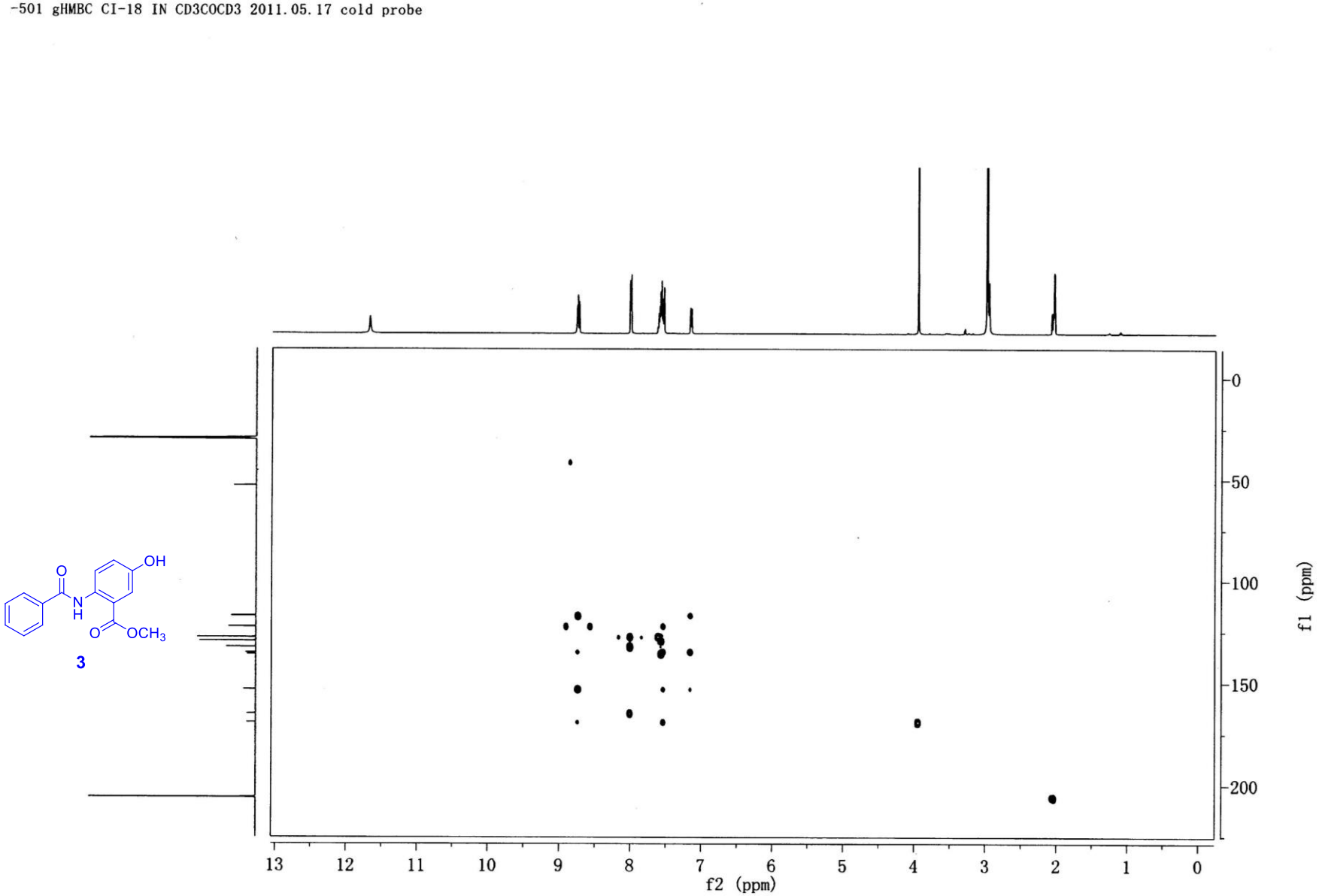


Figure S36. The HMBC spectrum of compound **3** in acetone-d_6 (500 MHz for ^{1}H).