

Supplementary File

**Substituted thiophenes and one sulf-polyacetylene ester compounds from *Echinops ritro* L.
and their antimicrobial activities**

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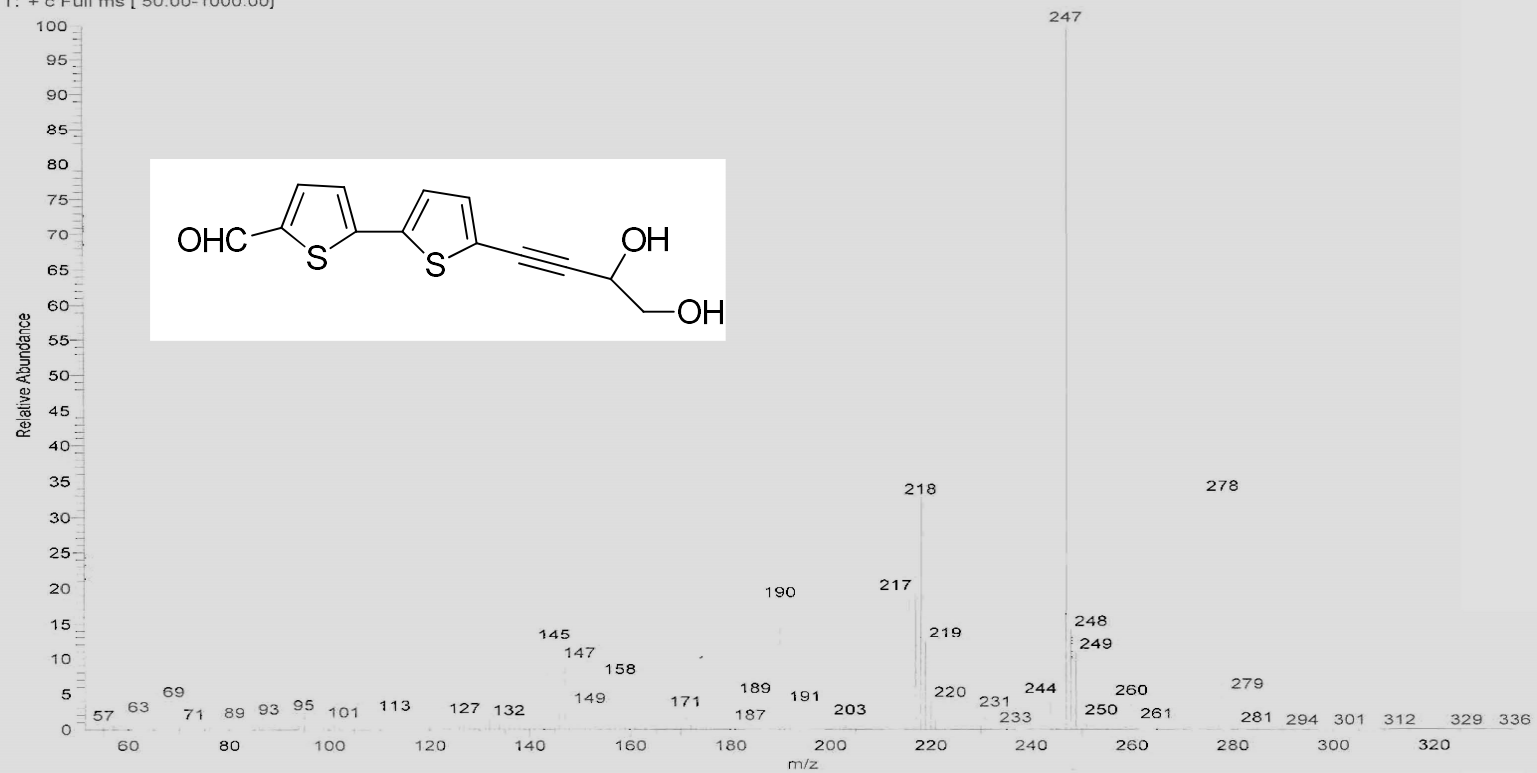
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C:\Xcalibur\data\070430e-10

04/30/2007 04:24:32 PM

Br-7

070430e-10 #33-37 RT: 1.53-1.66 AV: 5 SB: 2 2.20, 2.20 NL: 1.26E6
T: + c Full ms [50.00-1000.00]



Acq. Date: Tuesday, June 03, 2008

Acq. Time: 08:47

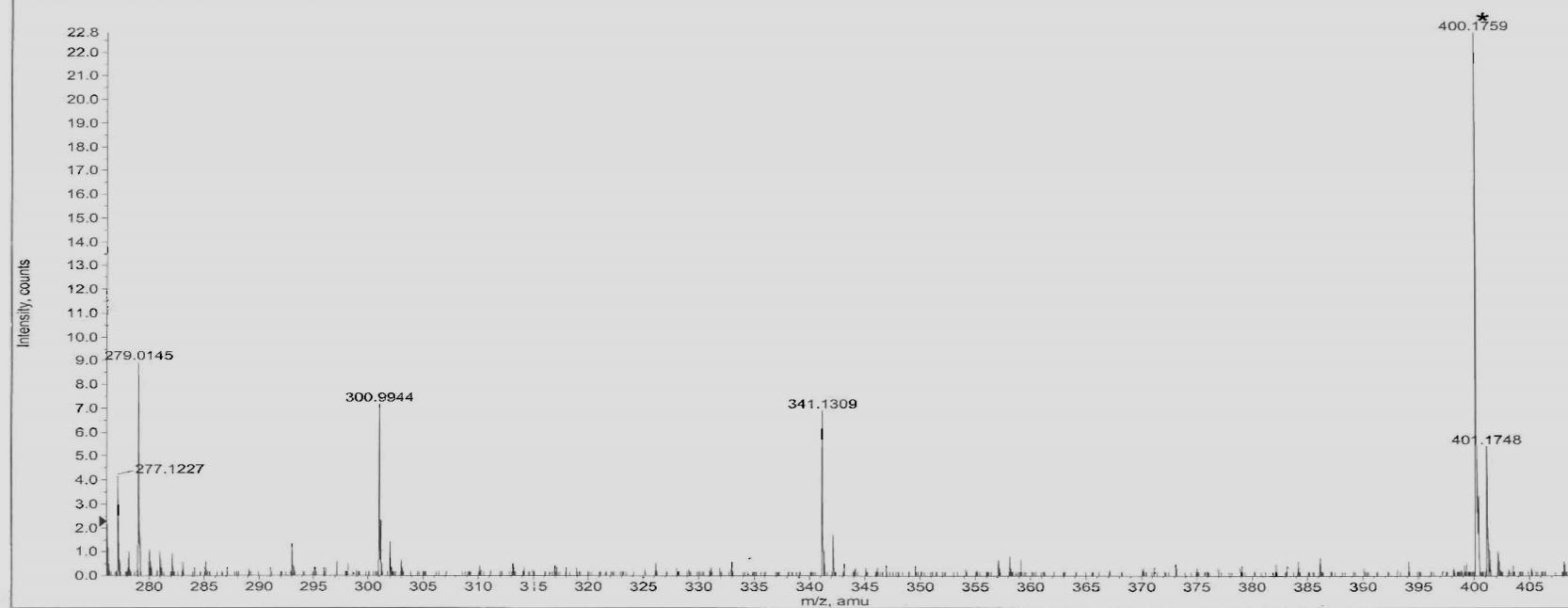
Scan Mode: Zero Width

Sample Name: 080603ESIA Br7

Sample Comment:

+TOF MS: 3.284 to 3.467 min from 080603ESIA Br7.wiff
a=3.55806450296741750e-004, t0=8.01690510042244570e+001

Max. 22.8 counts.



Acq. Date: Tuesday, June 03, 2008

Acq. Time: 08:47

Scan Mode: Zero Width

Sample Name: 080603ESIA Br7

Sample Comment:

Elemental composition calculator

Target m/z: +279.0145 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -5.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 080603ESIA Br7.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	100
3	Cl	0	0
4	F	0	0
5	H	0	400
6	I	0	0
7	N	0	0
8	Na	0	0
9	O	0	4
10	S	2	2

Acq. Date: Tuesday, June 03, 2008

Acq. Time: 08:47

Scan Mode: Zero Width

Sample Name: 080603ESIA Br7

Sample Comment:

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C13 H11 O3 S2	279.0149	-0.4629	-1.6592	8.5

Figure 1 HR-ESI-MS of Compound 1

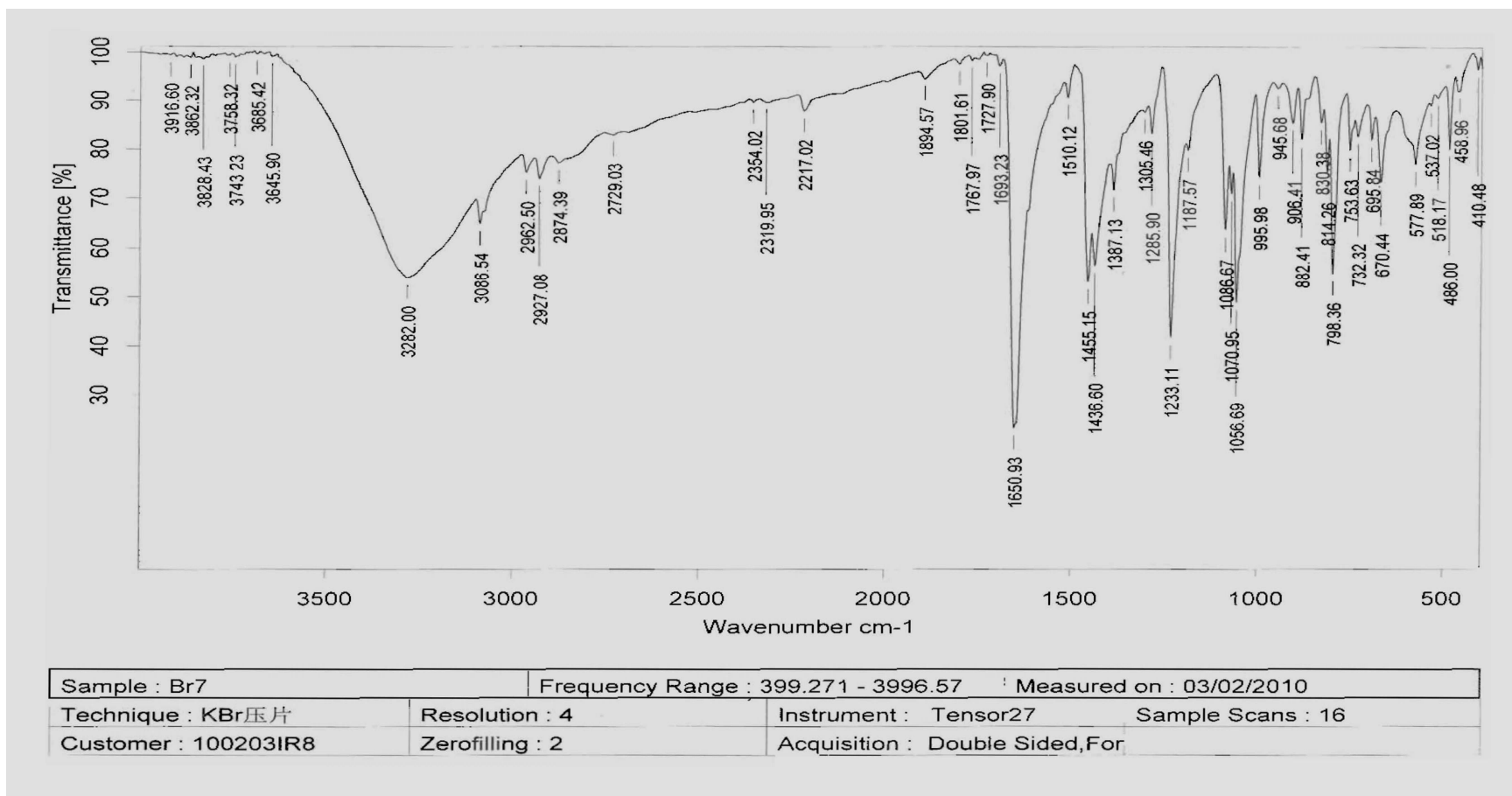


Figure 2 IR of Compound 1

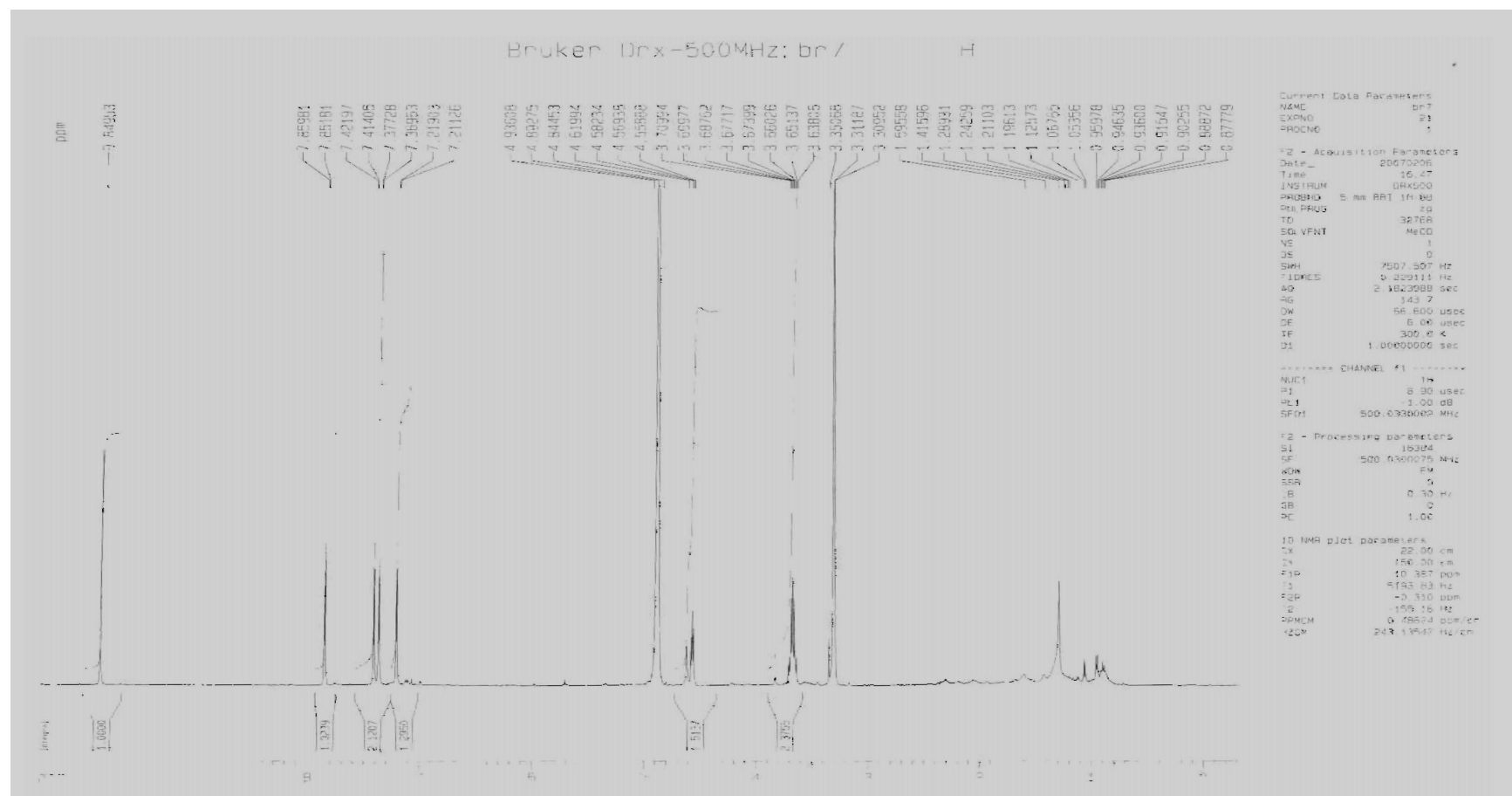


Figure 3 ^1H NMR (500 MHz, CD_3OD) of Compound 1

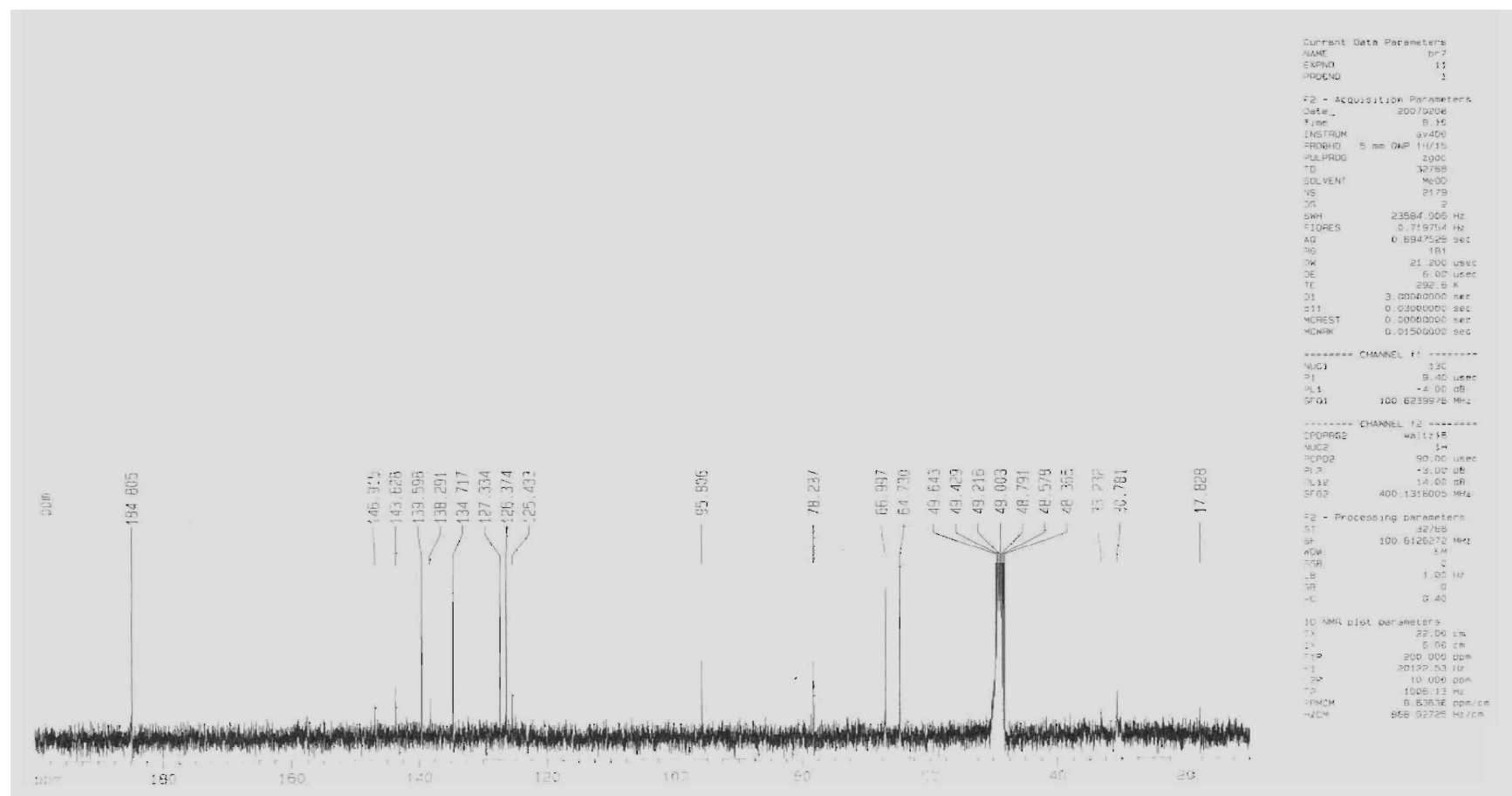


Figure 4 ^{13}C NMR (125 MHz, CD_3OD) of Compound 1

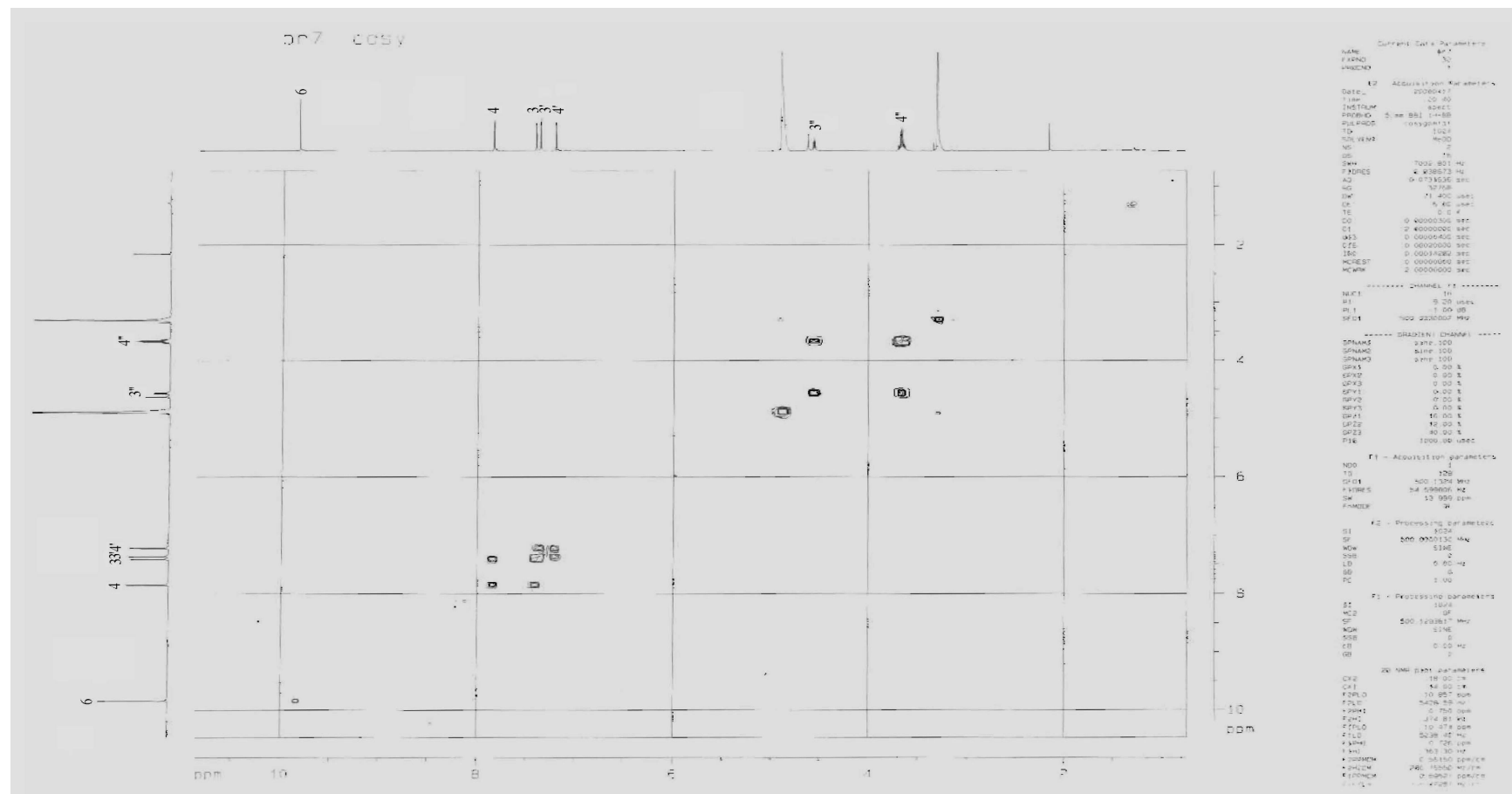
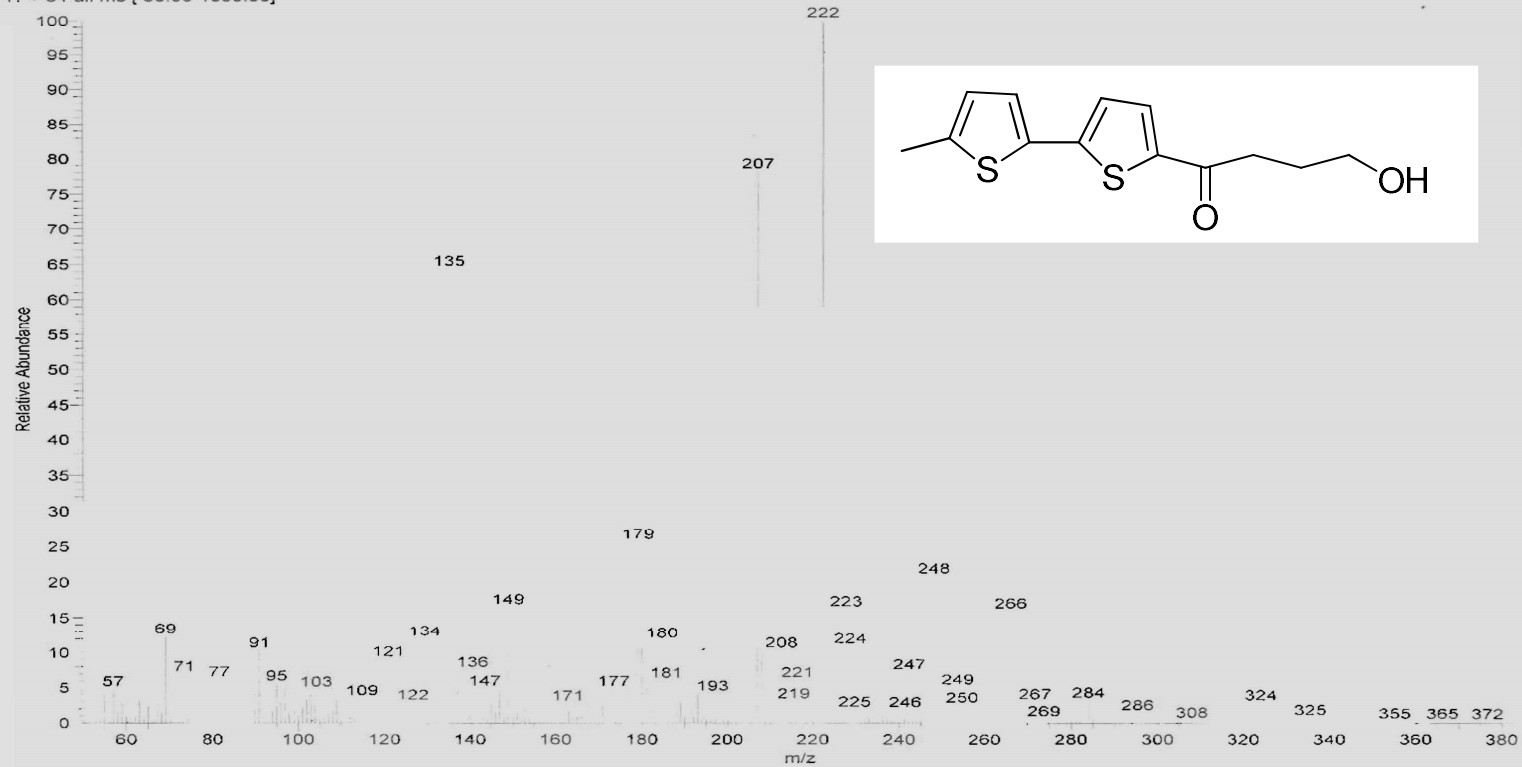


Figure 7 2D NMR (^1H - ^1H COSY) of Compound 1

080310e-06 #22-25 RT: 1.18-1.27 AV: 4 SB: 2 2.36, 2.36 NL: 1.48E6
T: + c Full ms [50.00-1000.00]



Acq. Date: Tuesday, June 03, 2008

Acq. Time: 08:57

Scan Mode: Zero Width

Sample Name: 080603ESIA Br53

Sample Comment:

+TOF MS: 0.867 to 1.050 min from 080603ESIA Br53.wiff
--0.55794391862438430e-004, t0=7.96575916585934460e+001

Max. 4111.0 counts.



Acq. Date: Tuesday, June 03, 2008

Acq. Time: 08:57

Scan Mode: Zero Width

Sample Name: 080603ESIA Br53

Sample Comment:

Elemental composition calculator

Target m/z: +267.0506 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -5.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 080603ESIA Br53.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	100
3	Cl	0	0
4	F	0	0
5	H	0	400
6	I	0	0
7	N	0	0
8	Na	0	0
9	O	0	3
10	S	2	2

Acq. Date: Tuesday, June 03, 2008

Acq. Time: 08:57

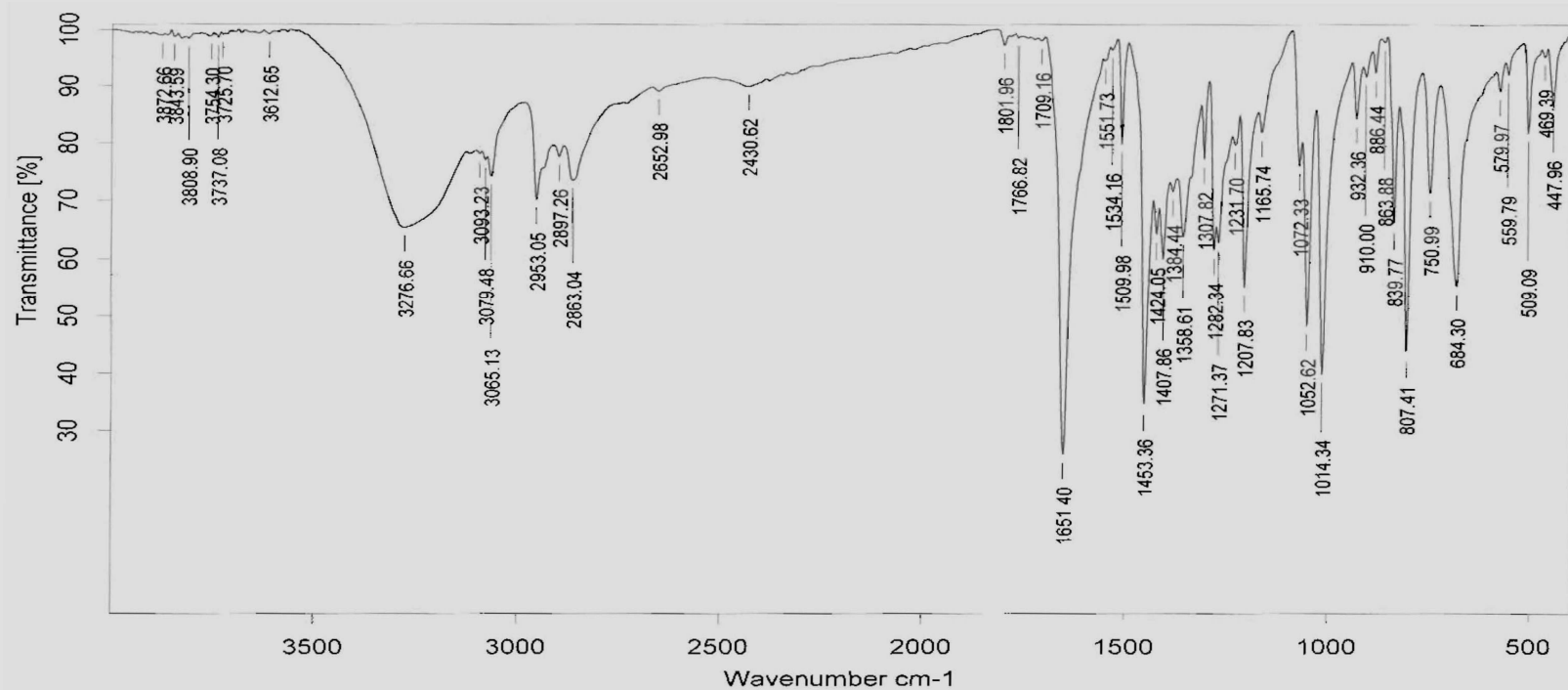
Scan Mode: Zero Width

Sample Name: 080603ESIA Br53

Sample Comment:

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C13 H15 O2 S2	267.0513	-0.7484	-2.8027	6.5

Figure 8 HR-ESI-MS of Compound 2



Sample : Br53		Frequency Range : 399.271 - 3996.57		Measured on : 03/02/2010	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27		Sample Scans : 16	
Customer : 100203IR9	Zerofilling : 2	Acquisition : Double Sided, For			

Figure 9 IR of Compound 2

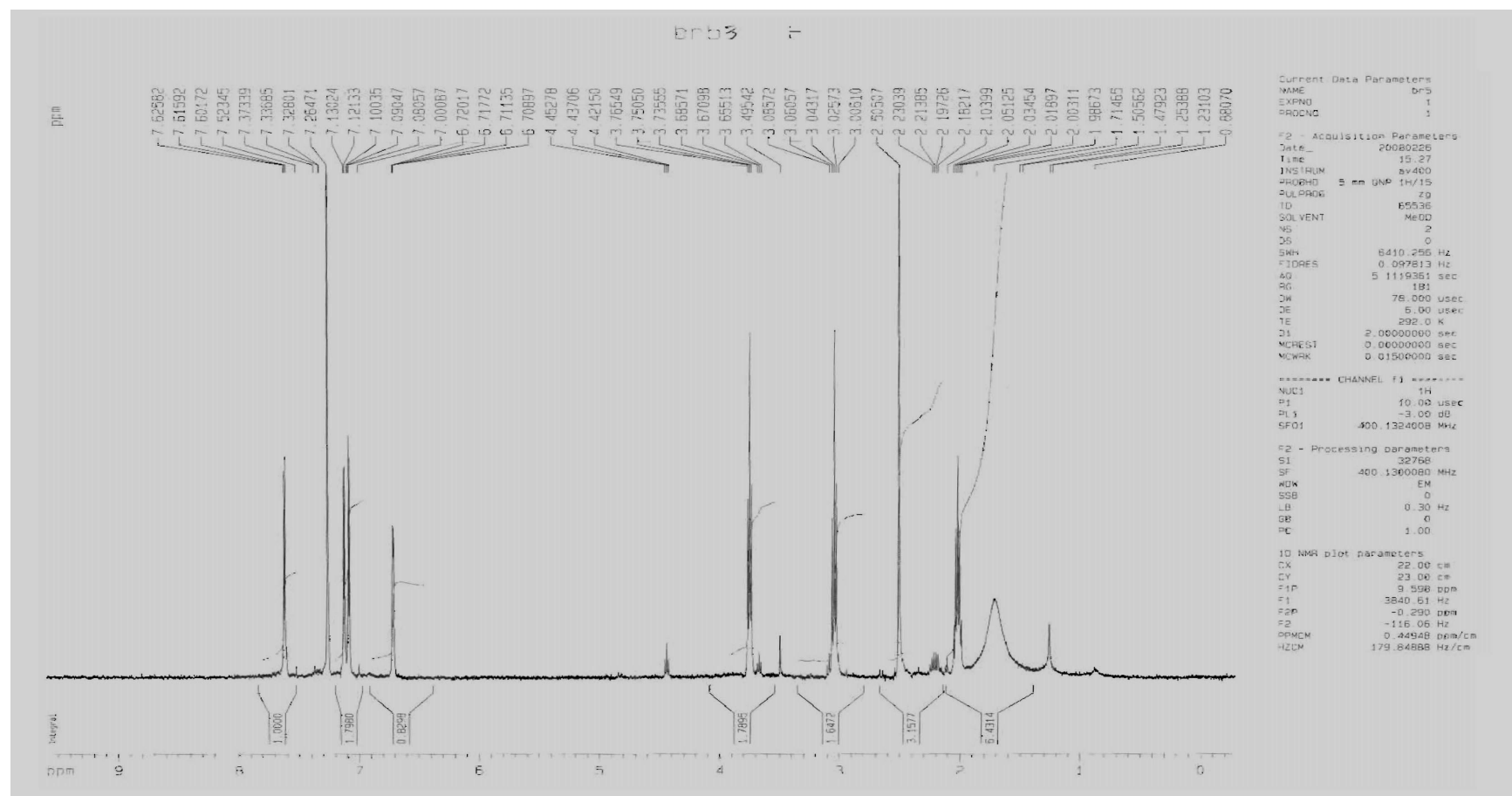


Figure 10 ^1H NMR (500 MHz, CDCl_3) of Compound 2

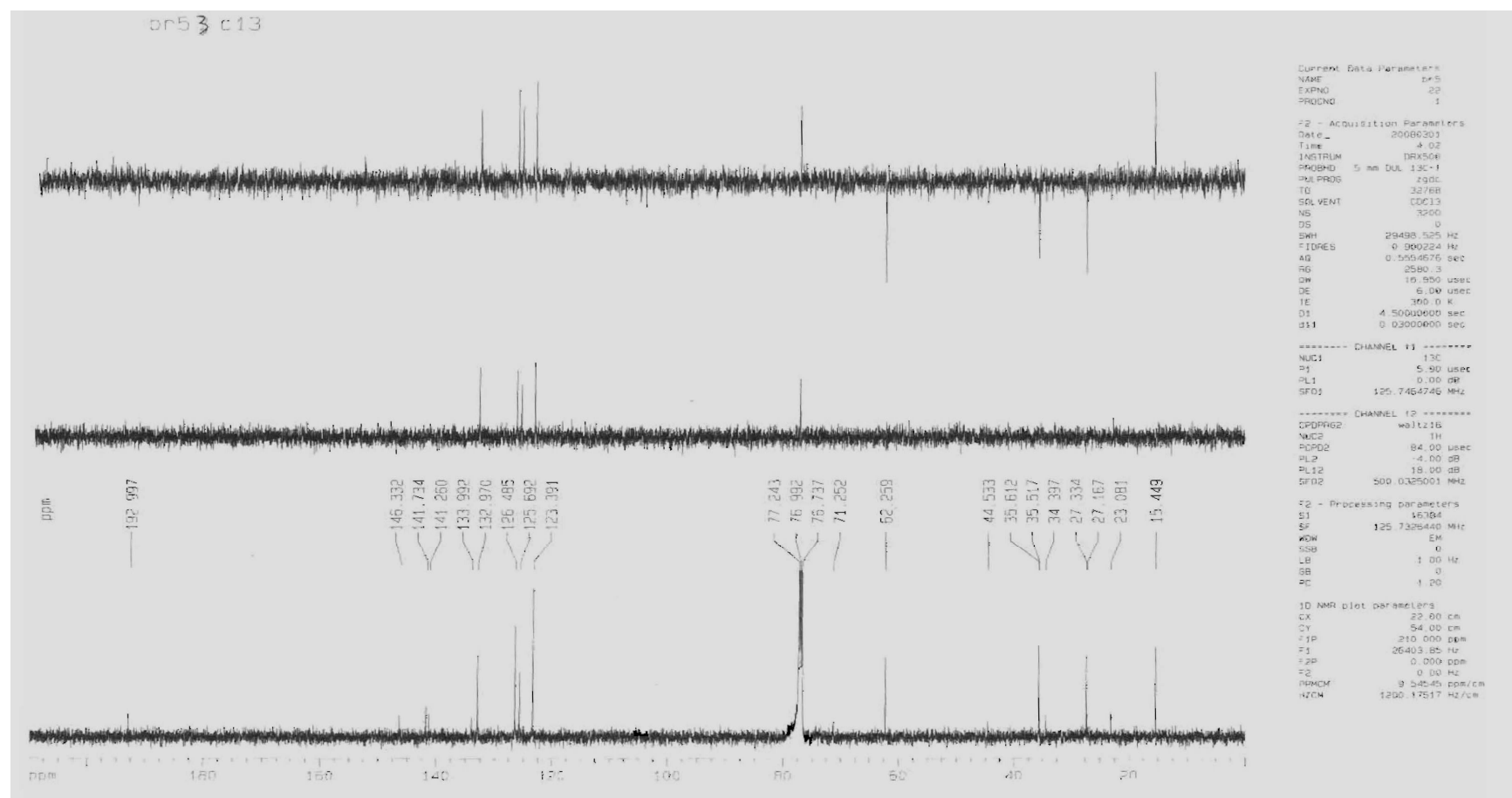


Figure 11 ^{13}C NMR (125 MHz, CDCl_3) of Compound **2**

Acq. Date: Friday, April 18, 2008

Acq. Time: 10:37

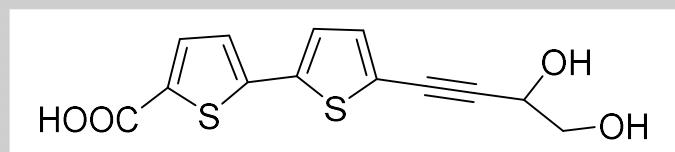
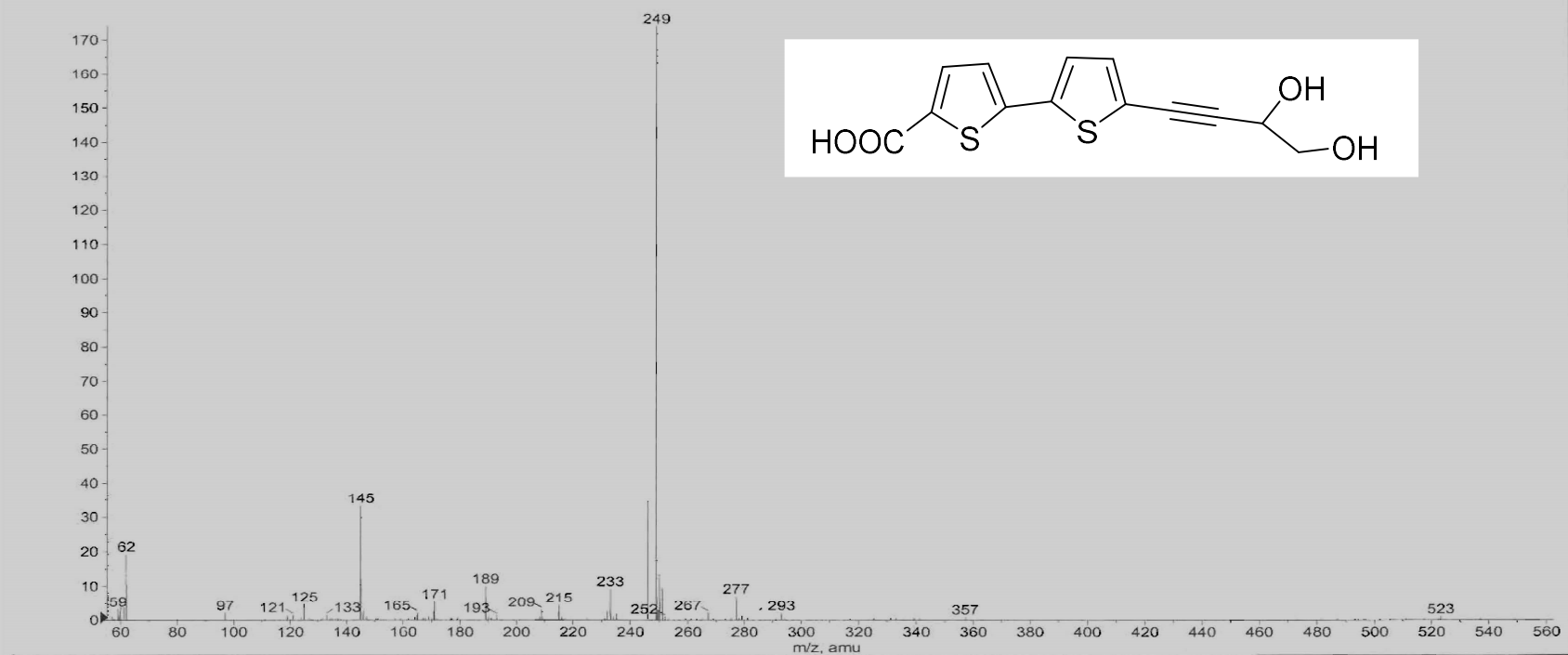
Scan Mode: Zero Width

Sample Name: 080418ESIN Br61

Sample Comment:

-TOF MS: 1.617 to 2.017 min from 080418ESIN Br61.wiff
a=3.5592659999999990e-004, t0=9.23179534642000020e+001, subtracted (0.967 to 1.300 min)

Max. 174.0 counts.



Acq. Date: Friday, April 18, 2008

Acq. Time: 17:16

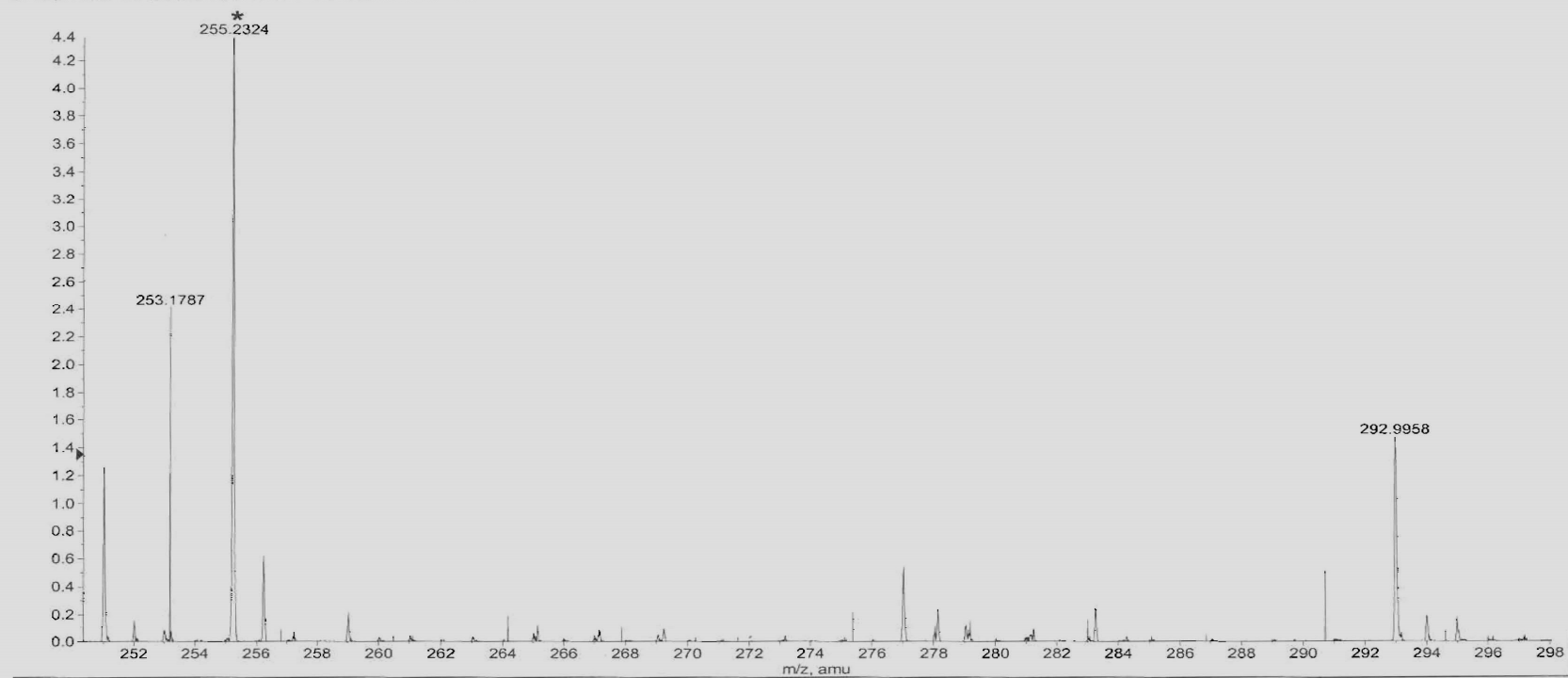
Scan Mode: Zero Width

Sample Name: 080418ESINA Br61

Sample Comment:

-TOF MS: 1.434 to 6.167 min from 080418ESINA Br61.wiff
a=3.55897876372389030e-004, t0=9.23179534642000020e+001

Max. 18.0 counts.



Acq. Date: Friday, April 18, 2008

Acq. Time: 17:16

Scan Mode: Zero Width

Sample Name: 080418ESINA Br61

Sample Comment:

Elemental composition calculator

Target m/z: +292.9958 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -5.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 080418ESINA Br61.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	I	0	0
7	N	0	0
8	Na	0	0
9	O	0	10
10	S	2	2

Acq. Date: Friday, April 18, 2008

Acq. Time: 17:16

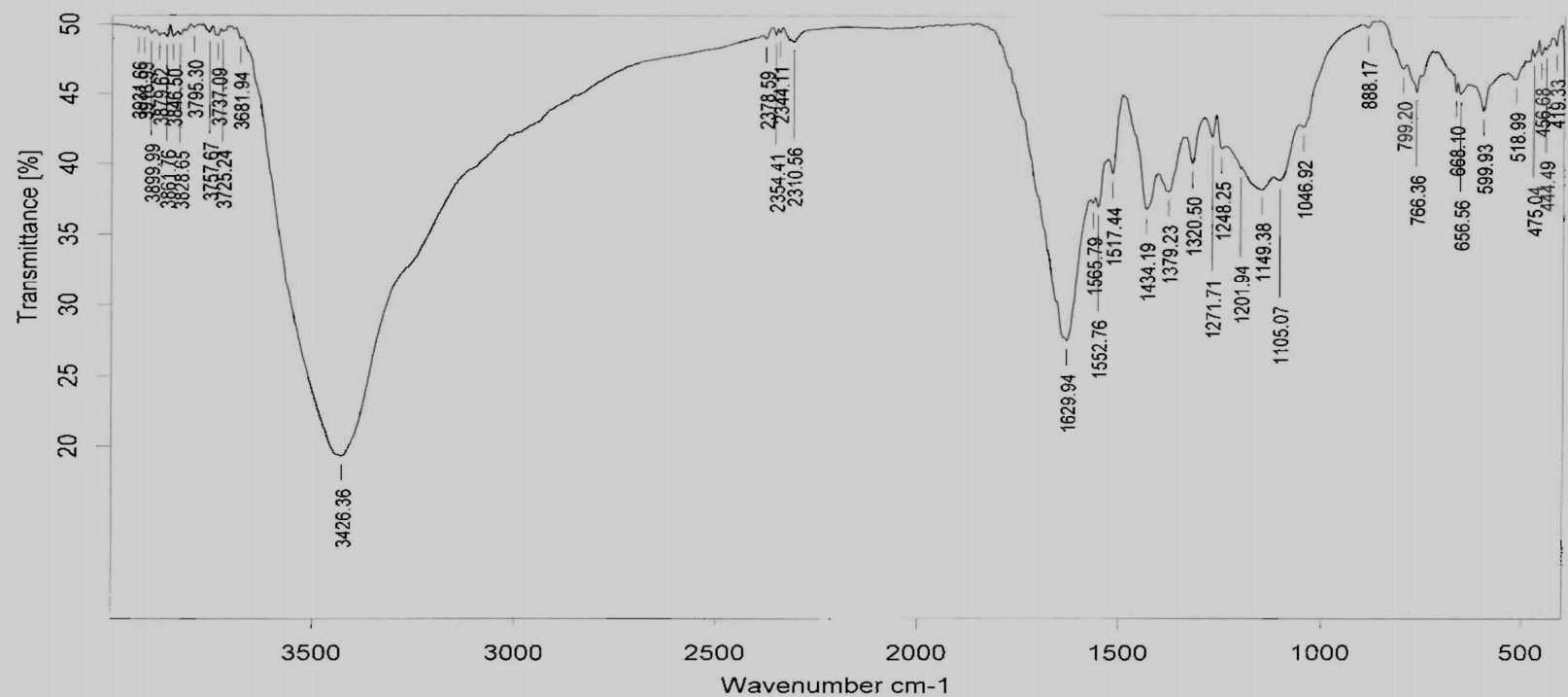
Scan Mode: Zero Width

Sample Name: 080418ESINA Br61

Sample Comment:

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C13 H9 O4 S2	292.9942	1.5724	5.3669	9.5

Figure 15 HR-ESI-MS of Compound 3



Sample : Br61		Frequency Range : 399.271 - 3996.57		Measured on : 03/02/2010
Technique : KBr压片	Resolution : 4	Instrument : Tensor27		Sample Scans : 16
Customer : 100203IR10	Zerofilling : 2	Acquisition : Double Sided,For		

Figure 16 IR of Compound 3

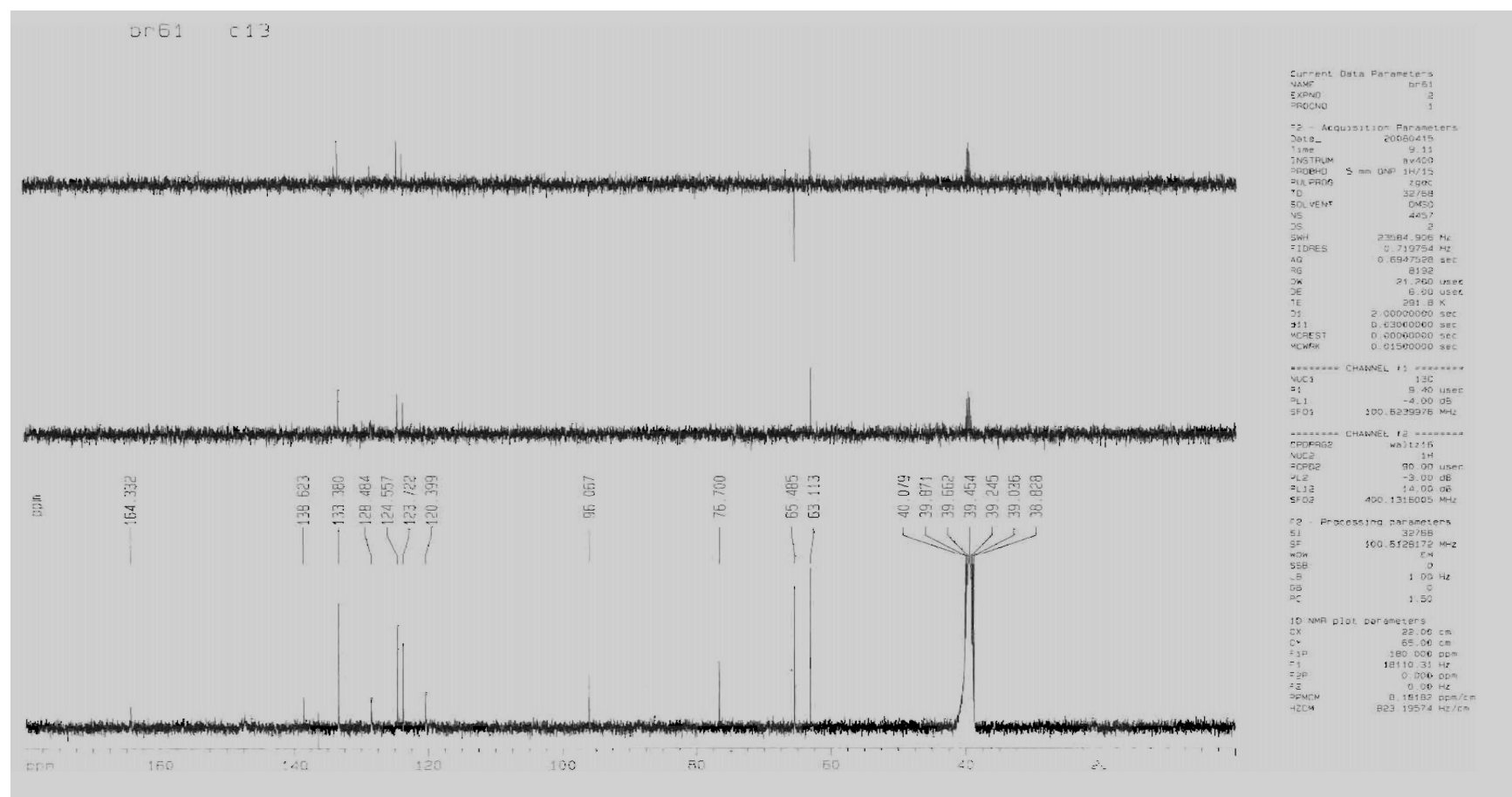
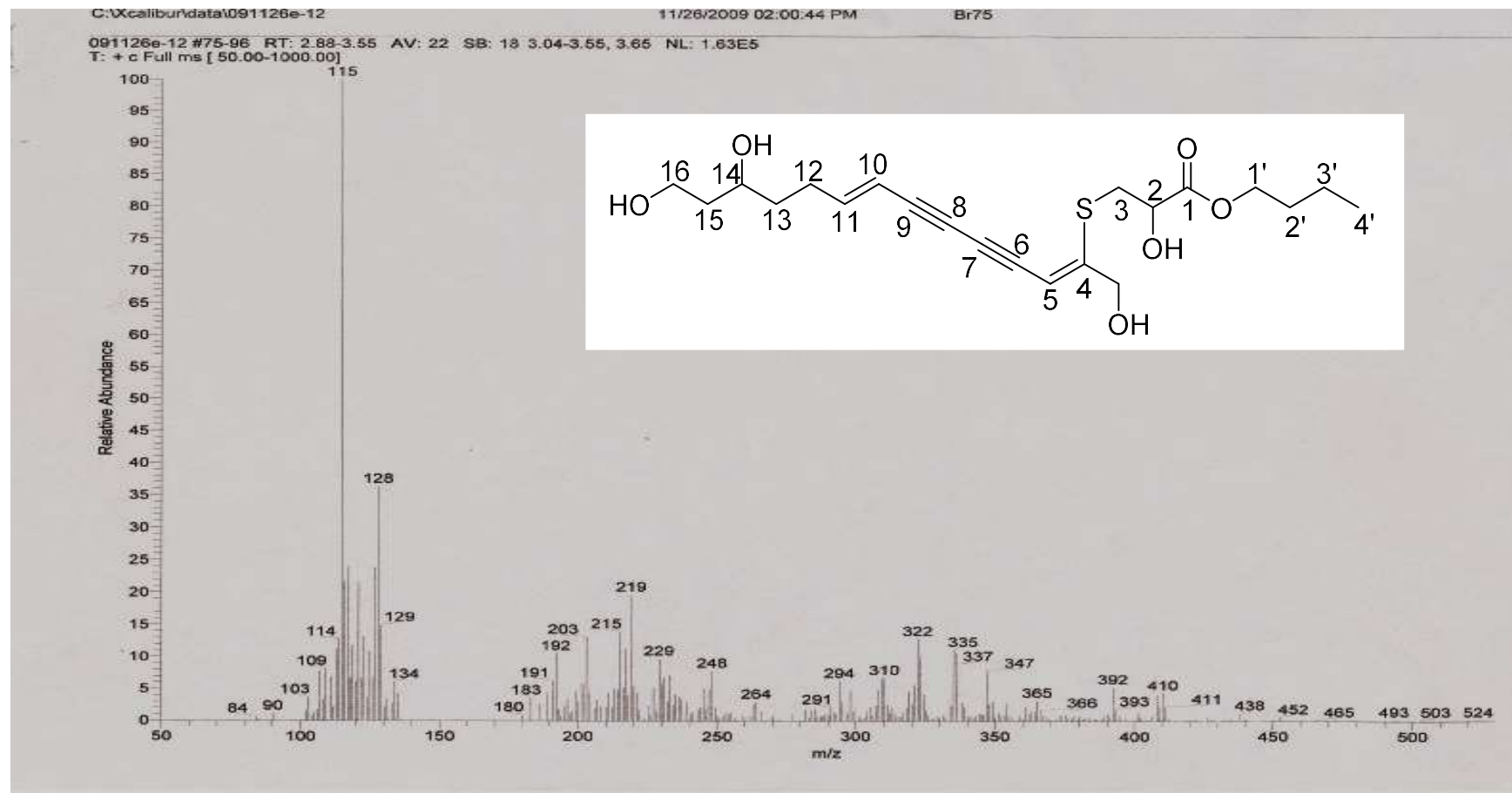


Figure 18 ^{13}C NMR (125 MHz, CD_3OD) of Compound **3**



Acq. Date: Monday, November 10, 2009

Acq. Time: 10:03

Sample Name: 091110ESI1 Br75

+TOF MS: 2.333 to 2.583 min from 091110ESI1 Br75.wiff
a=3.55957051457323440e-004, t0=7.96375916585934460e+001

Max. 66.4 counts

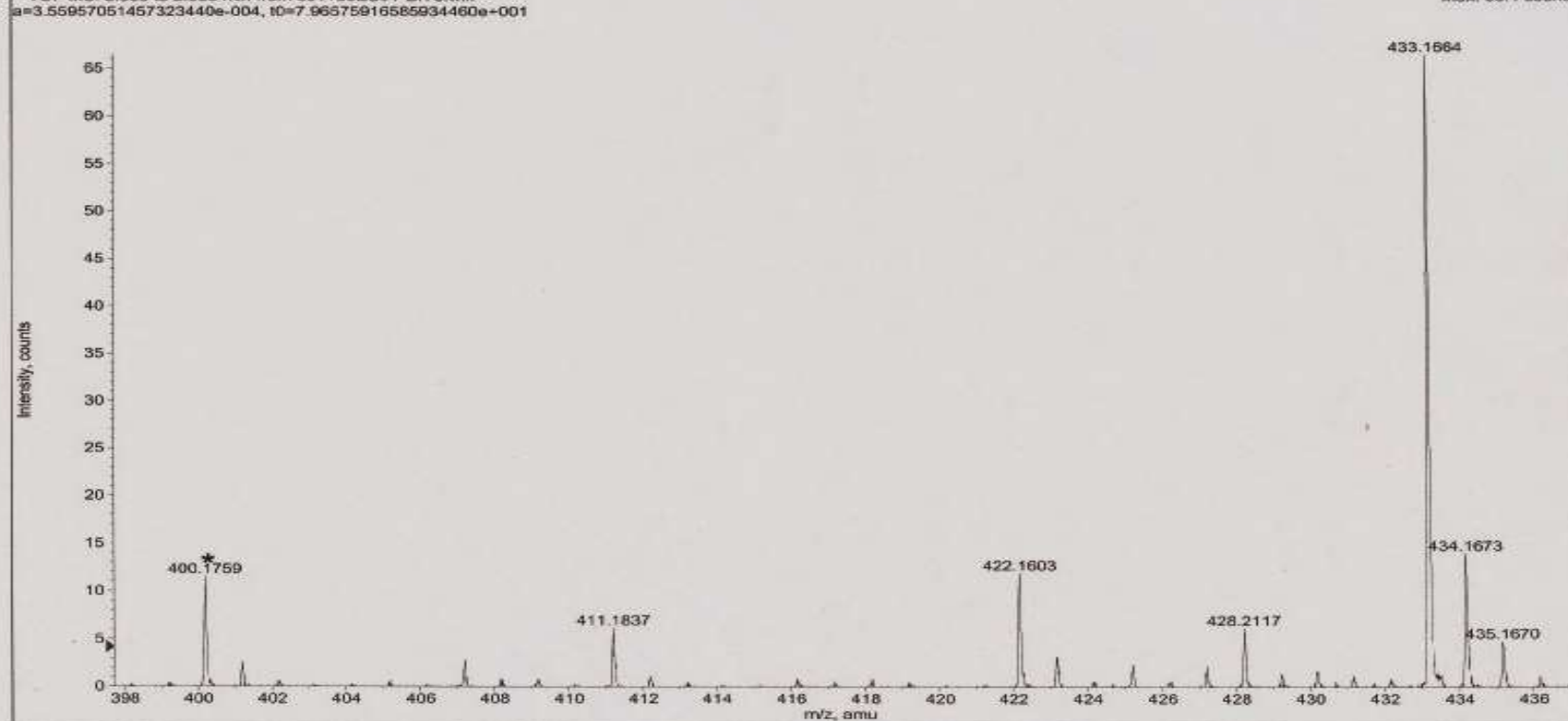


Figure 19 HR-ESI-MS of Compound 4

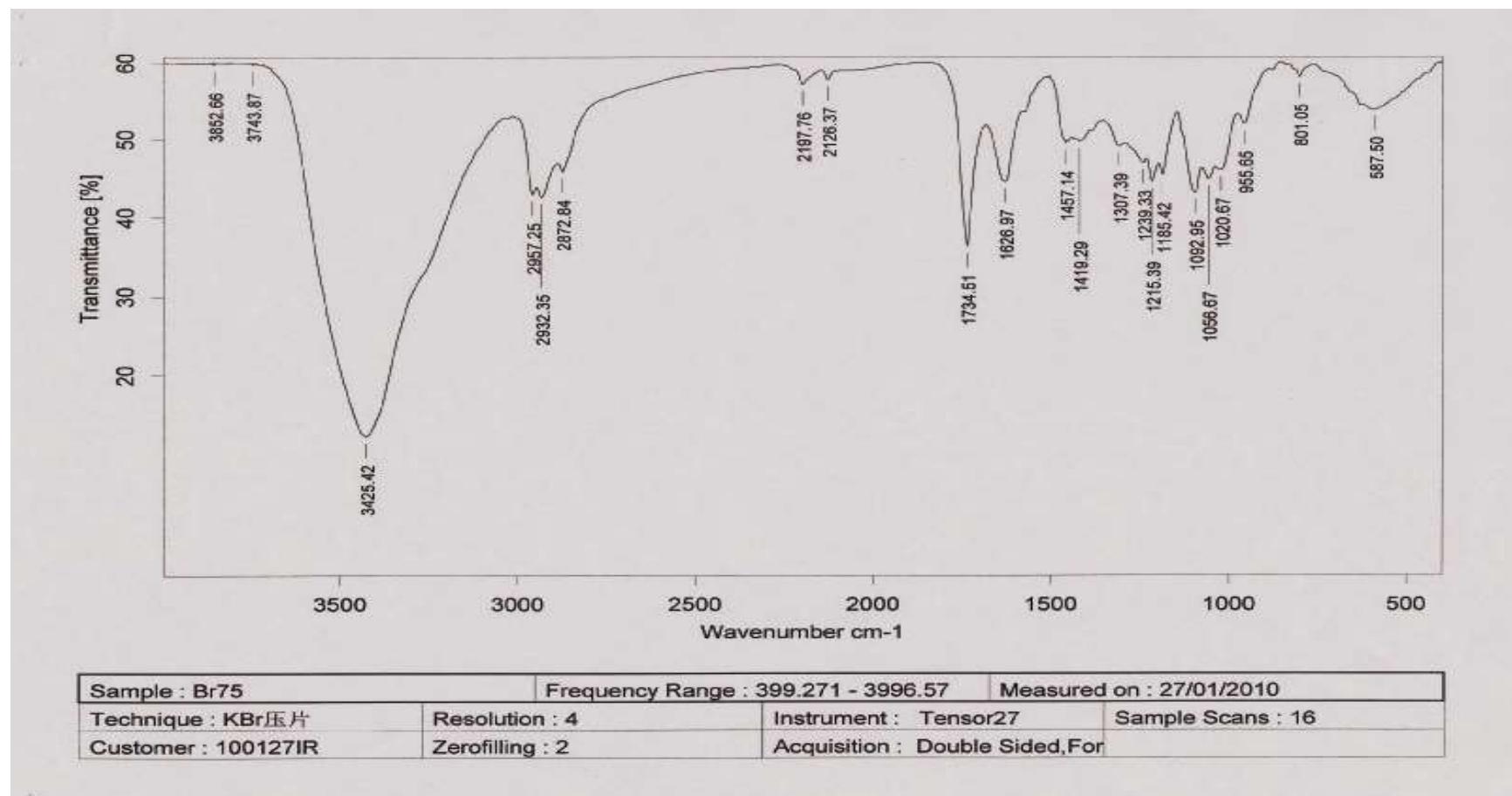


Figure 20 IR of Compound 4

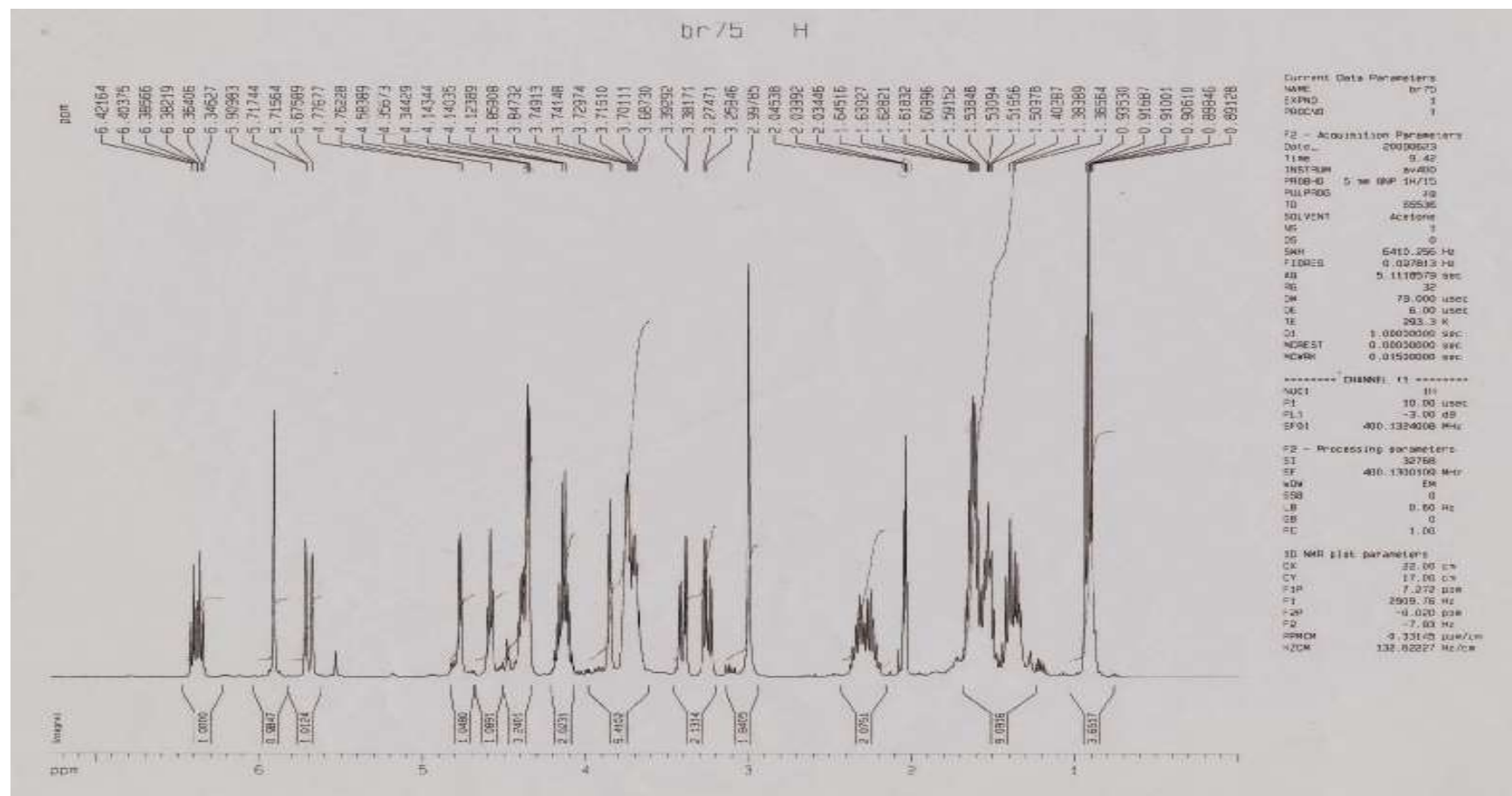


Figure 21 ^1H NMR (400 MHz, CD_3COCD_3) of Compound 4

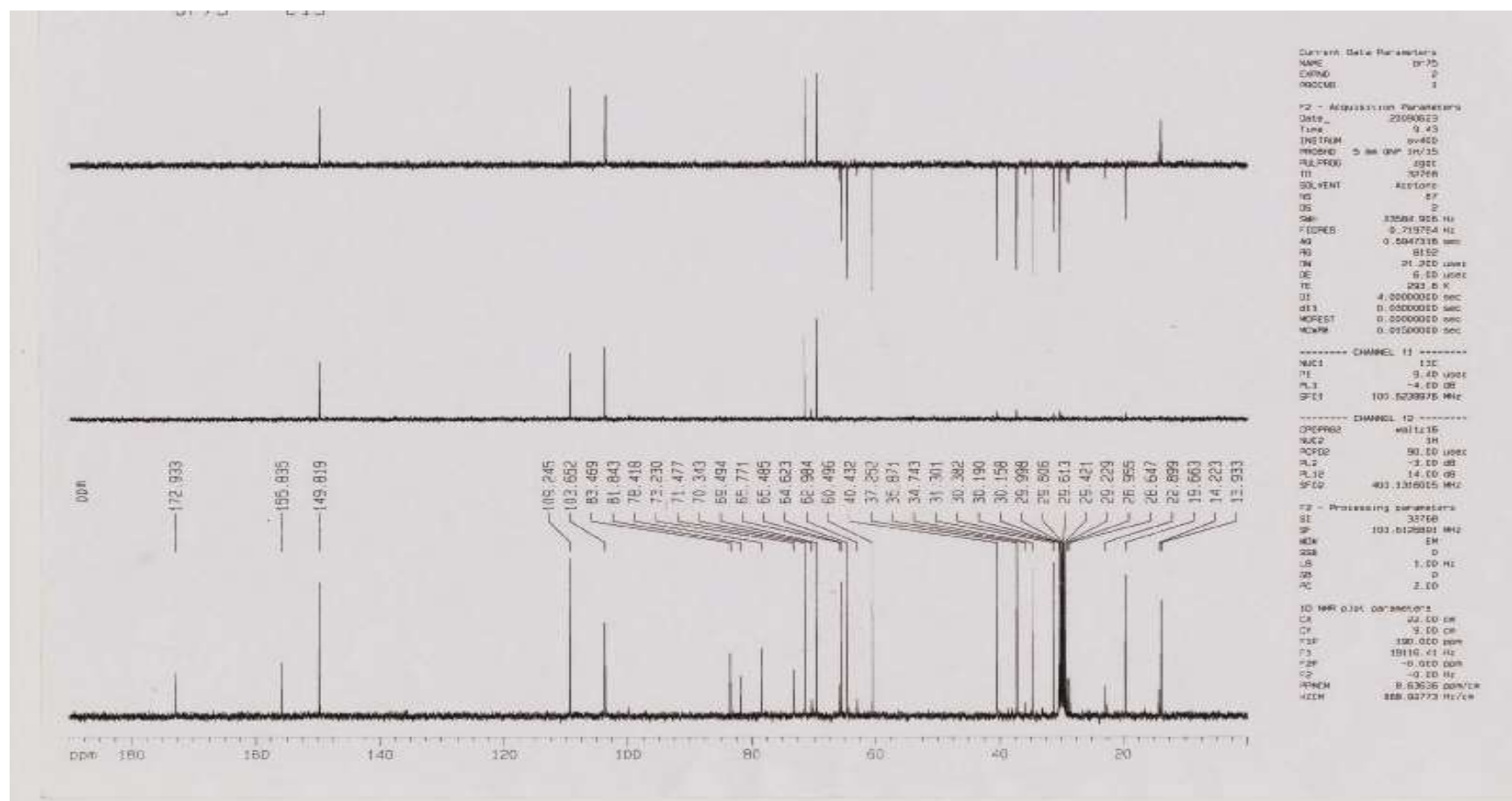


Figure 22 ^{13}C NMR (100 MHz, CD_3COCD_3) of Compound 4



Figure 23 2D NMR (HSQC) of Compound 4

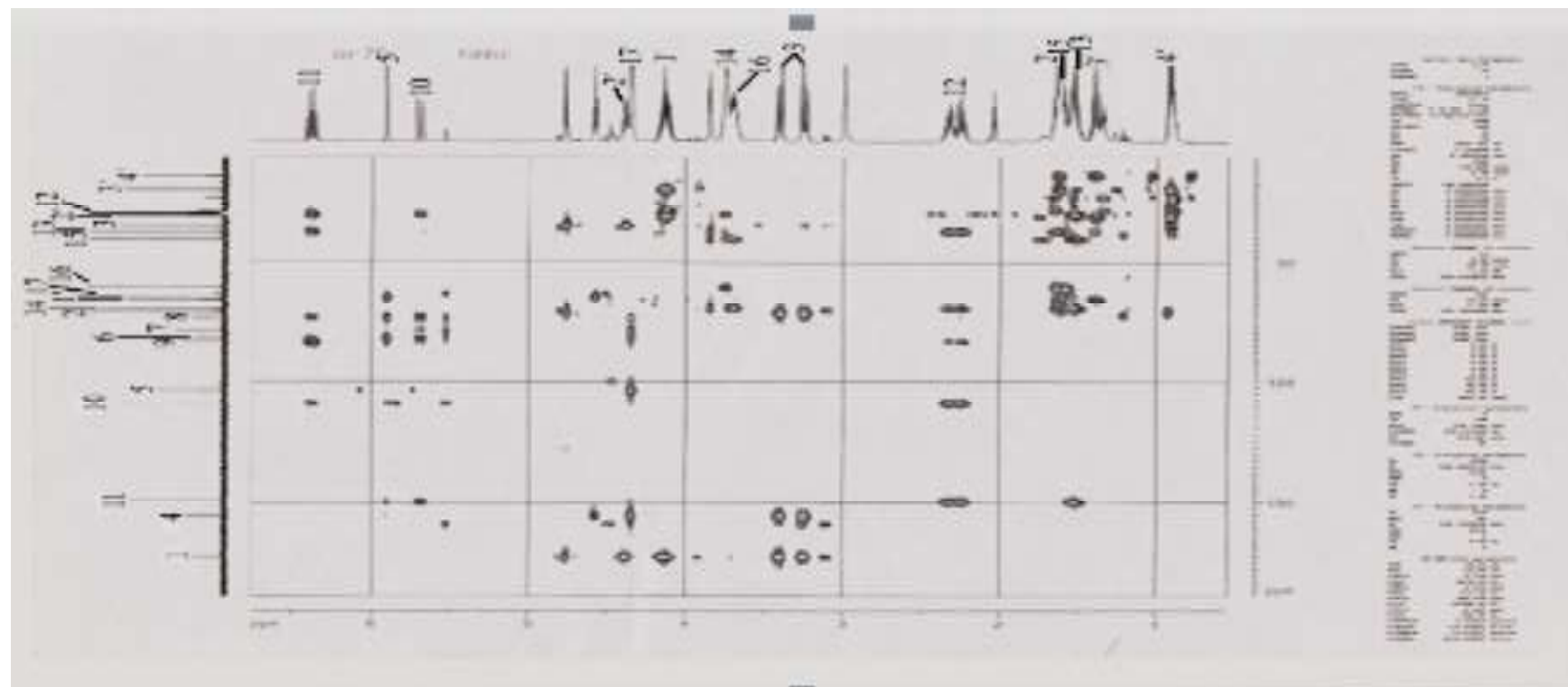


Figure 24 2D NMR (HMBC) of Compound 4

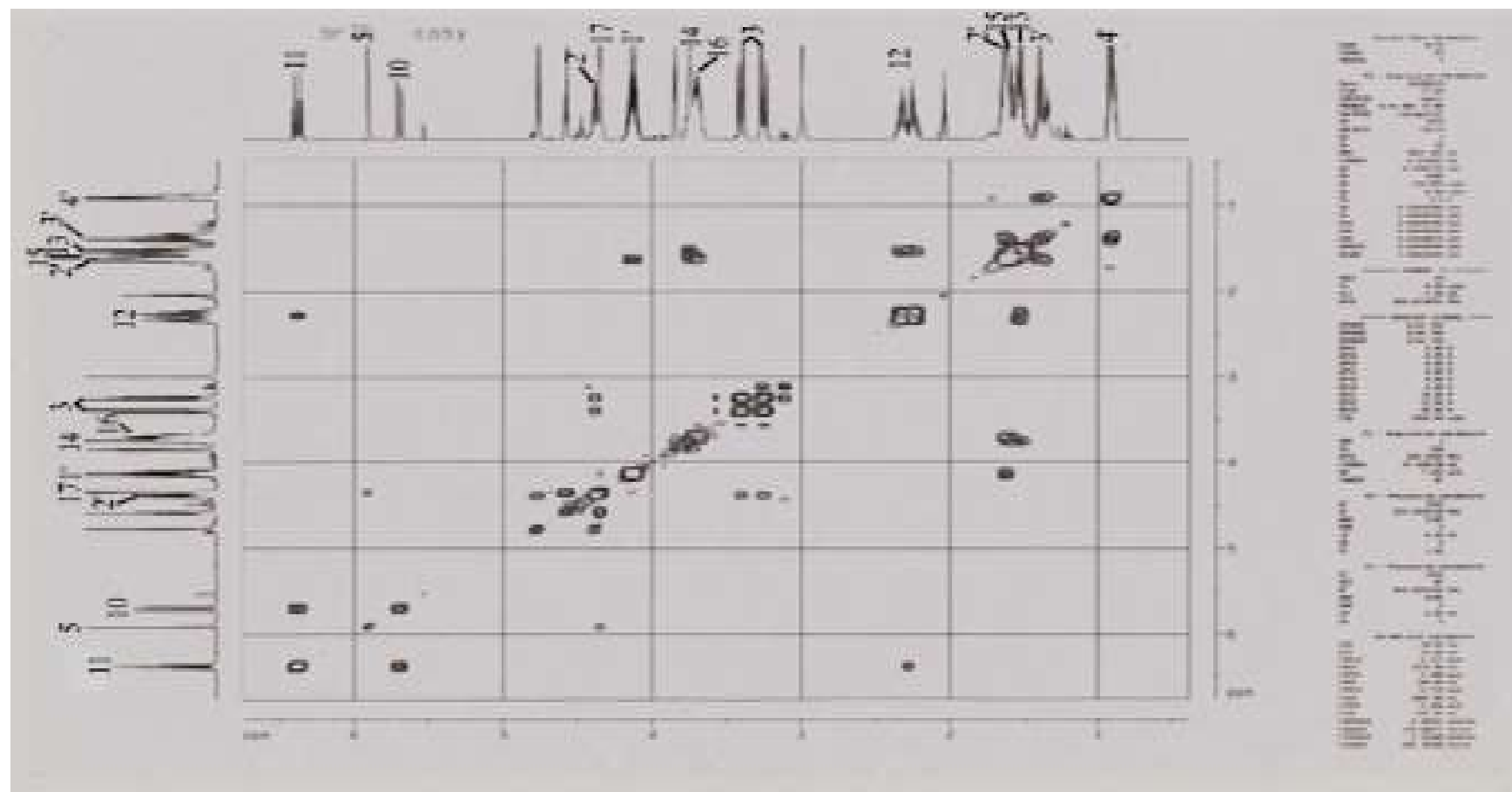


Figure 25 2D NMR (^1H - ^1H COSY) of Compound 4

