Supporting Information

Radical-scavenging Activity and Mechanism of Resveratrol-oriented Analogues: Influence of the Solvent, Radical and Substitution

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1 General parallel procedure for preparation of *trans*-stilbenes

Witting-Horner reaction: The corresponding methoxybenzylhalide (5.0 mmol) was heated in a flame-dried three necked flask with an excess of triethyl phosphate (9.5 mL, 5.5 mmol). After 4-6 h the mixture was cooled to room temperature and purified by distillation under high vacuum to yield pale oils.

To a solution of diethyl benzylphosphonate (10 mmol) in anhydrous DMF (10 mL) at 0 ^{0}C, sodium hydride (2.80 g, 50 mmol) was added, and the resulting solution was stirred under nitrogen for 2-3 h. A solution of the corresponding methoxy-protected benzaldehyde (10 mmol) in anhydrous DMF was added, and the mixture was stirred under nitrogen overnight at room temperature. The solution was poured into ice-water, the precipitate was filtered off and was further purified by silica gel chromatography (ethyl acetate/petroleum ether) to yield solid. This procedure gave exclusively the *trans*-isomer.

Perkin reaction: Under nitrogen, 4-trifluoromethylbenzaldehyde (2 mmol), 4-hydroxyphenyl-acetic acid (1 equiv.), 1.62 mL of acetic anhydride (1.8 equiv.) and triethylamine (0.7 equiv.) were refluxed at 150 ^{0}C for 10 h, cooled at room temperature. Excess triethylamine was distilled off under high vacuum; the residue diluted in 10% NaOH during 30min, extracted with ethyl acetate (3×30 mL), washed with brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel chromatograph and eluted with ethyl acetate-petroleum ether to give acid.

To a quinoline solution (4 mL) of acid (1 mmol) and copper power (6 mmol) were added, and the resulting solution was stirred under nitrogen for 2-3 h at 230-240 ^{0}C. Excess quinoline was distilled off under high vacuum. The residue was diluted in 0.5 N HCl in ethyl acetate, extracted with ethyl acetate (3×30mL), washed with brine, and dried over Na_2SO_4. The residue was purified by silica gel chromatograph and eluted with ethyl acetate-petroleum ether to give white solid (4-hydroxy-4'-trifluoromethyl-*trans*-stilbene).

Methoxy deprotection: A mixture of methoxy protection *trans*-stilbenes (5 mmol) and pyridine·HCl was heated under nitrogen (180-200 ^{0}C, 3-6 h). Excess pyridine·HCl was distilled off under high vacuum; the residue was mixed with 1 N HCl, extracted

with ether, washed with brine, and dried over Na_2SO_4. The residue was purified by silica gel chromatograph and eluted with ethyl acetate-petroleum ether to yield white crystals.

Resveratrol: ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ 6.26 (t, *J* = 1.8 Hz, 1H), 6.54 (d, *J* = 1.8 Hz, 2H), 6.83 (d, *J* = 9.0 Hz, 2H), 6.89, 6.99 (d, *J* = 16.5 Hz, each 1H), 7.40 (d, *J* = 9.0 Hz, 2H); MS-EI (*m/z*): 228 [M^+].

3,5-DHS: ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ 6.33 (t, *J* = 2.4 Hz, 1H), 6.61 (d, *J* = 1.5 Hz, 2H), 7.10 (s, 2H), 7.24 (t, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 7.8 Hz, 2H); MS-EI (*m/z*): 212 [M^+].

4-HS: ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ 6.84 (d, *J* = 8.7 Hz, 2H), 7.08, 7.15 (d, *J* = 16.5 Hz, each 1H), 7.23 (dd, *J* = 7.8, 2 Hz, 1H), 7.34 (t, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 8.7 Hz, each 1H), 7.53 (d, *J* = 7.5 Hz, 2H); MS-EI (*m/z*): 196 [M^+].

3,4-DHS: ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ 6.81 (d, *J* = 8.1 Hz, 1H), 6.91 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.00 (s, 1H), 7.07, 7.12 (d, *J* = 16.2 Hz, each 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.32 (t, *J* = 7.8 Hz, 2H), 7.51 (d, *J* = 7.8 Hz, 2H); MS-EI (*m/z*): 212 [M^+].

4,4'-DHS: ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ 6.82 (d, *J* = 8.7 Hz, 4H), 6.96 (s, 2H), 7.39 (d, *J* = 8.7 Hz, 4H), 8.50 (s, OH); MS-EI (*m/z*): 212 [M^+].

3-MeO-4-HS: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, *J* = 6.4 Hz, 2H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 6.8 Hz, 2H), 6.88, 7.26 (d, *J* = 16.4 Hz, each 1H), 6.92 (d, *J* = 8.4 Hz, 2H), 3.85 (s, OCH_3); MS-EI (*m/z*): 226 [M^+].

4'-MeO-4-HS: ^{1}H NMR (400 MHz, $(CD_3)_2CO$) : δ 8.40 (s, OH), 7.46 (dd, *J* = 8.8, 2.0 Hz, 2H), 7.40 (d, *J* = 8.8 Hz, 2H), 7.55 (d, *J* = 8.8Hz, 2H), 7.00 (s, 2H), 6.90 (*J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.80 (s, OCH_3); MS-EI (*m/z*): 226 [M^+].

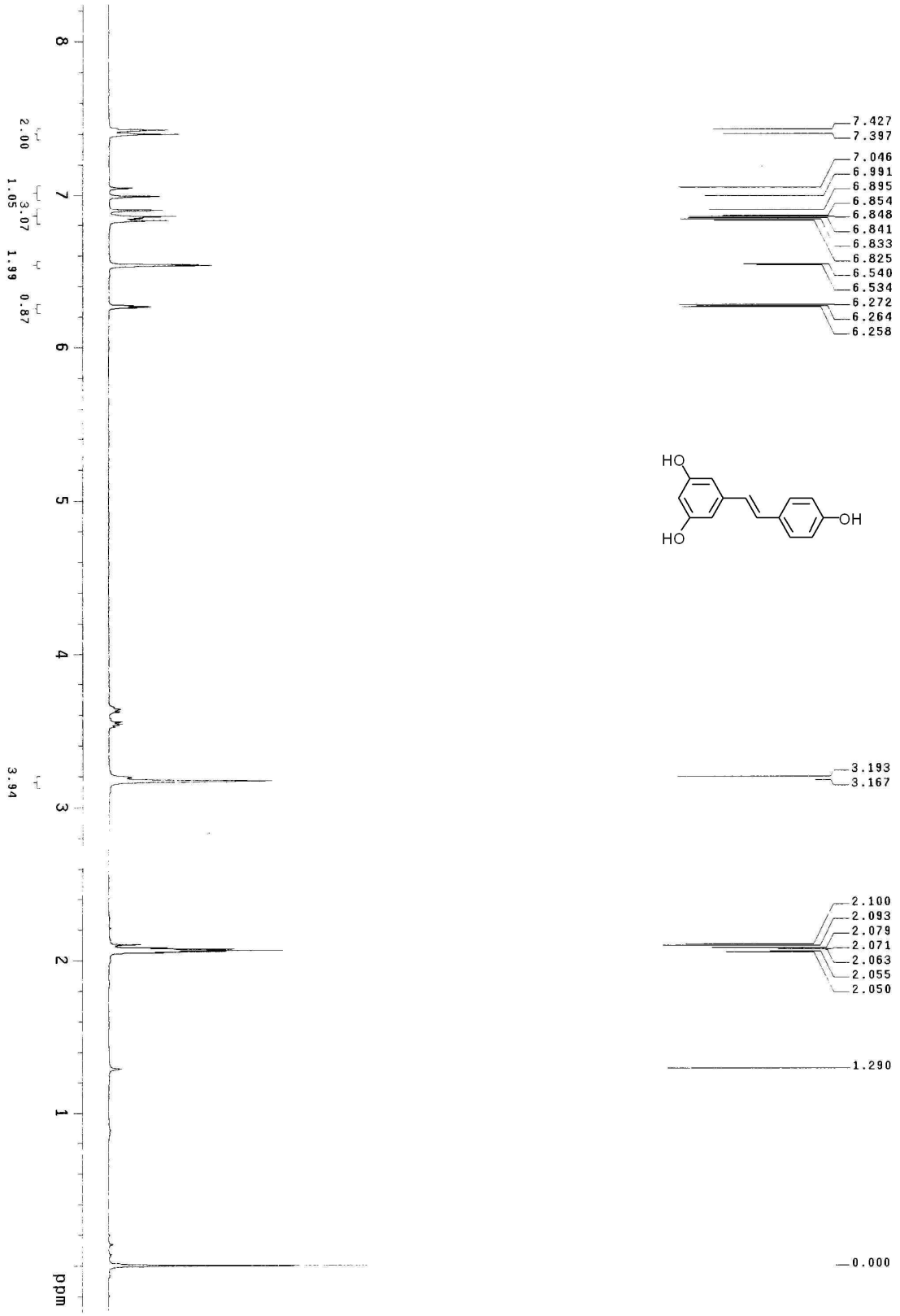
4'-Me-4-HS: ^{1}H NMR (400 MHz, $(CD_3)_2CO$): δ 8.44 (s, OH), 7.43 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.00, 7.10 (d, *J* = 16.7 Hz, each 1H), 6.84 (d, *J* = 8.8 Hz, 2H), 2.31 (s, CH_3); MS-EI (m/z): 210 [M^+].

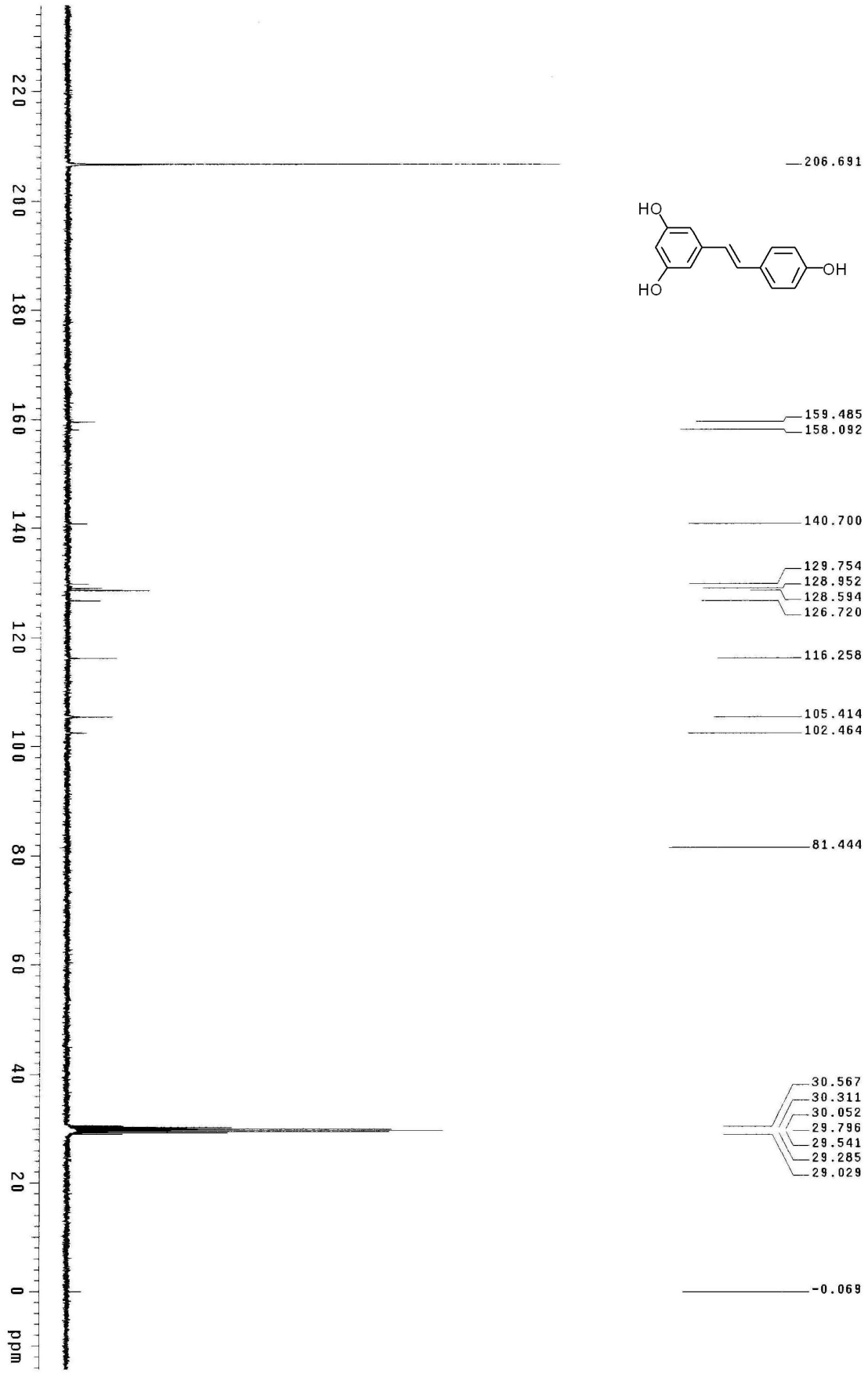
4'-NO_2-4-HS: ^{1}H NMR (400 MHz, $(CD_3)_2CO$): δ 8.67 (s, OH), 8.21 (dd, *J* = 7.2, 1.6 Hz, 2H), 7.81 (d, *J* = 8.8 Hz, 2H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.20, 7.46 (d, *J* = 16.7 Hz, each 1H), 6.89 (dd, *J* = 6.8, 2.0 Hz, 2H); MS-EI (*m/z*): 241 [M^+].

4'-CF_3-4-HS: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 - 7.57 (m, 4H), 7.43 (d, *J* = 8.4 Hz, 2H), 6.97, 7.13 (d, *J* = 16.4 Hz, each 1H), 6.85 (d, *J* = 8.4 Hz, 2H), 4.92 (s, OH); MS-EI (*m/z*): 264 [M^+].

2 ^{1}H, ^{13}C NMR spectrum of resveratrol analogues

Resveratrol

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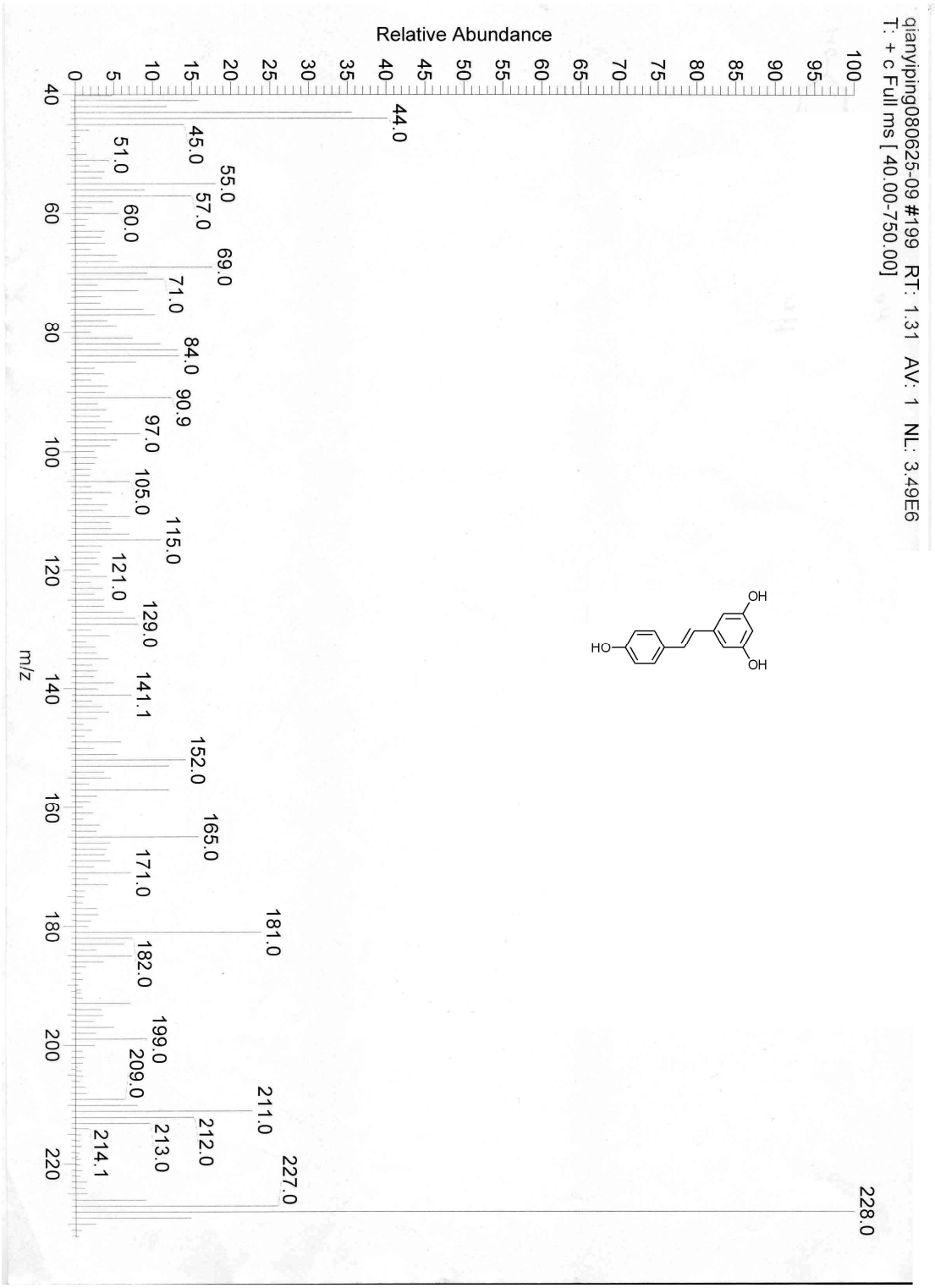
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71.0
84.0
90.9
97.0
105.0
115.0
121.0
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152.0
165.0
171.0
181.0
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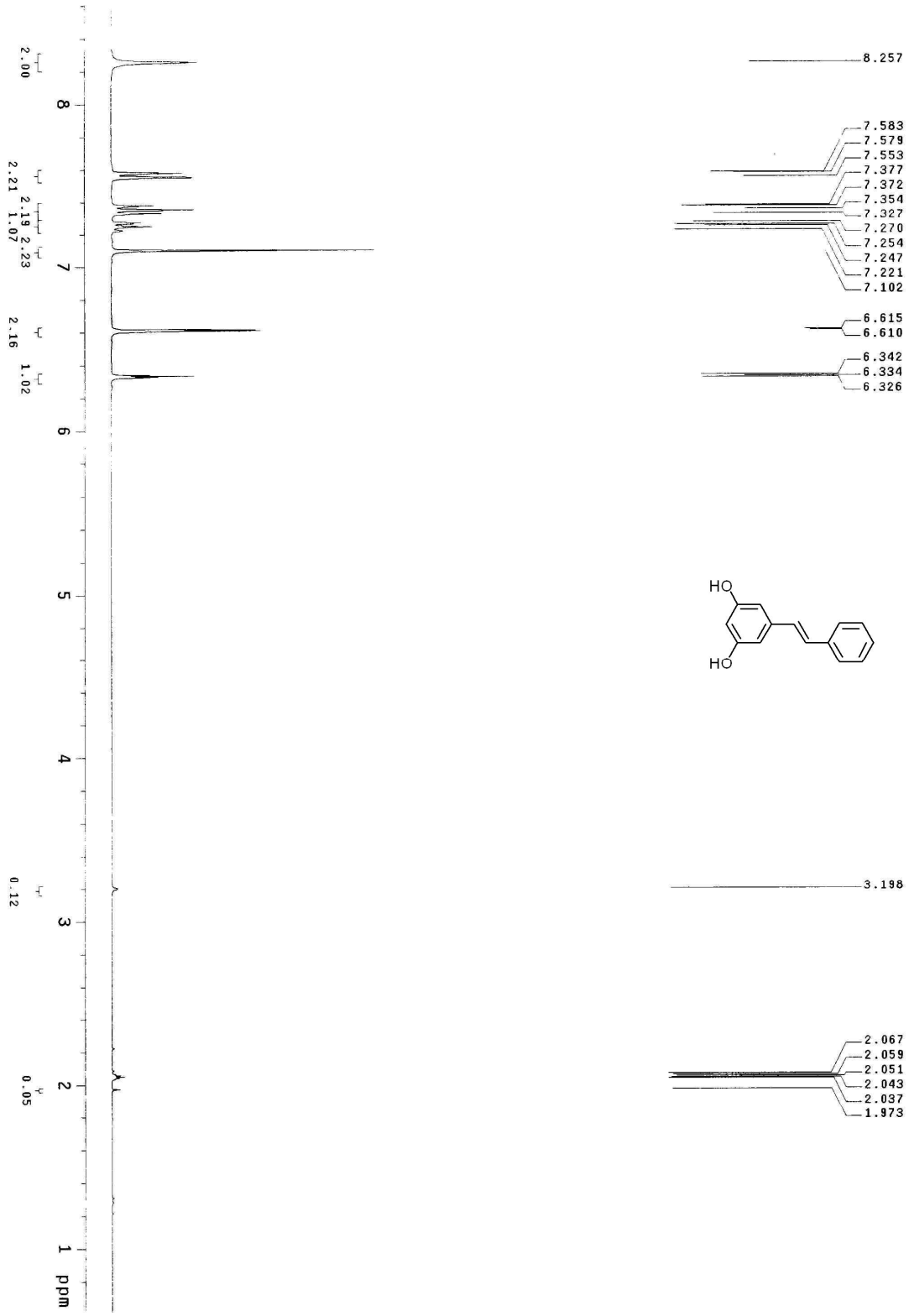
HO
OH

3,5-DHS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6.610
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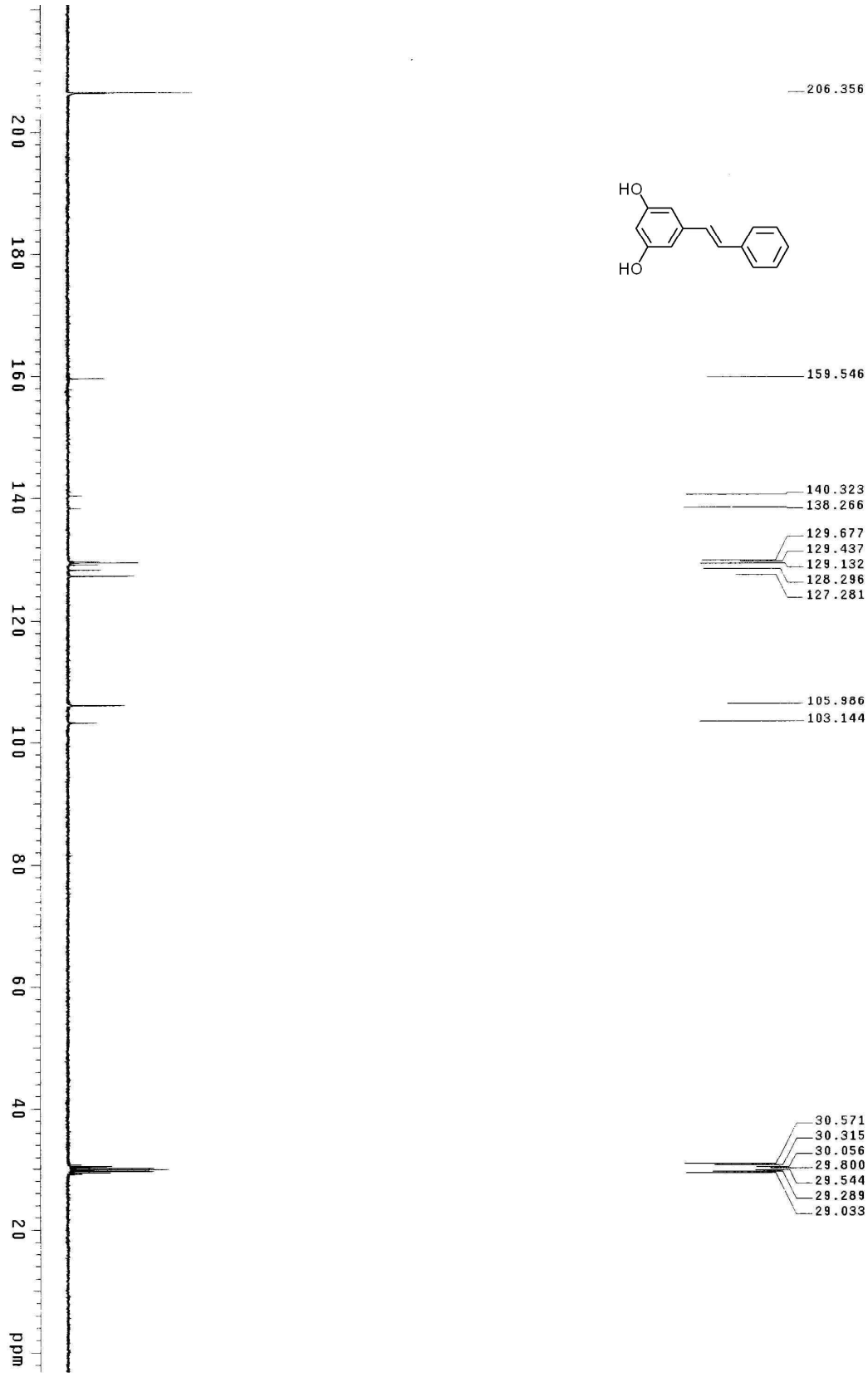
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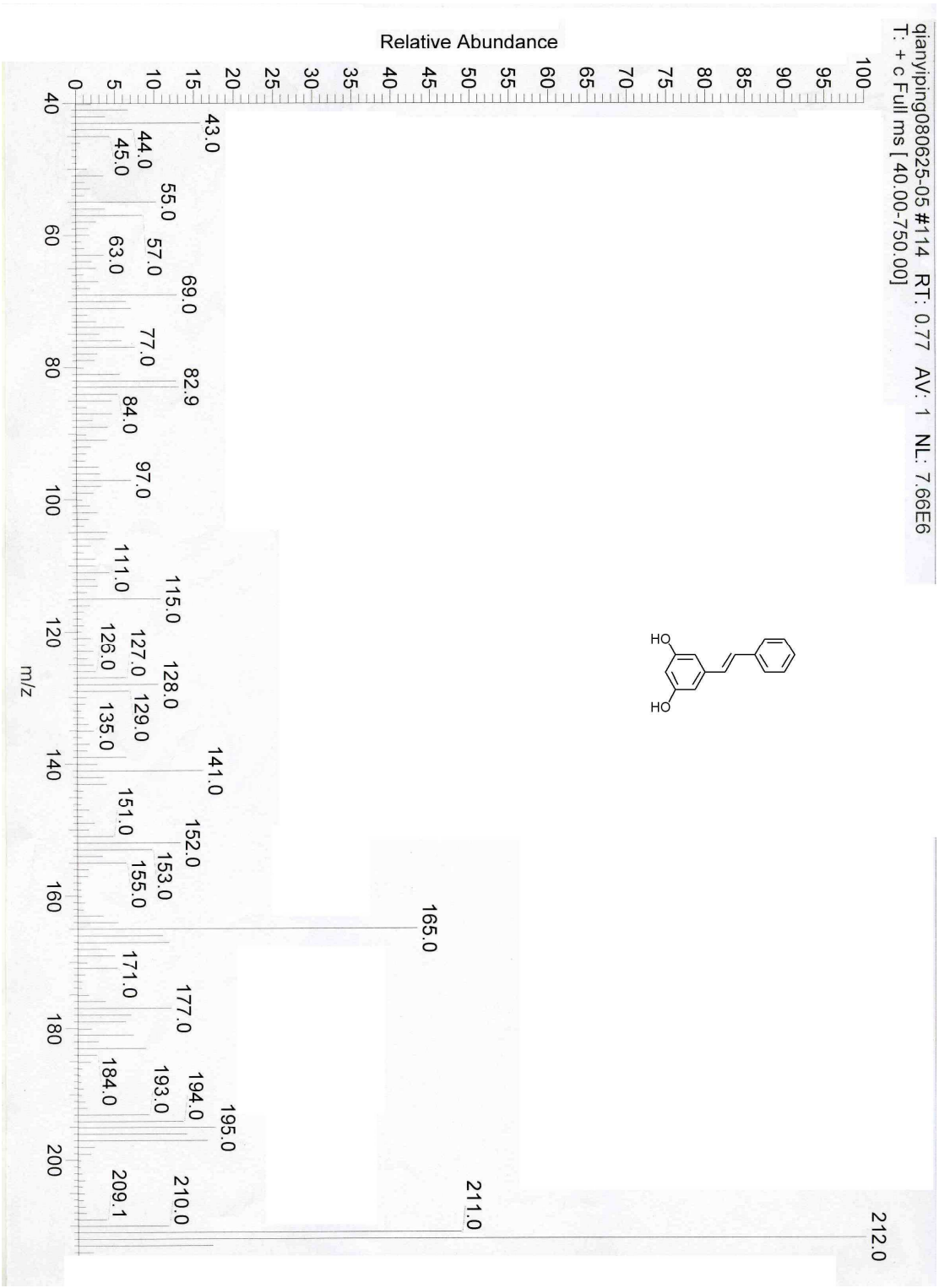
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63.0
69.0
77.0
82.9
84.0
97.0
111.0
115.0
126.0
127.0
128.0
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152.0
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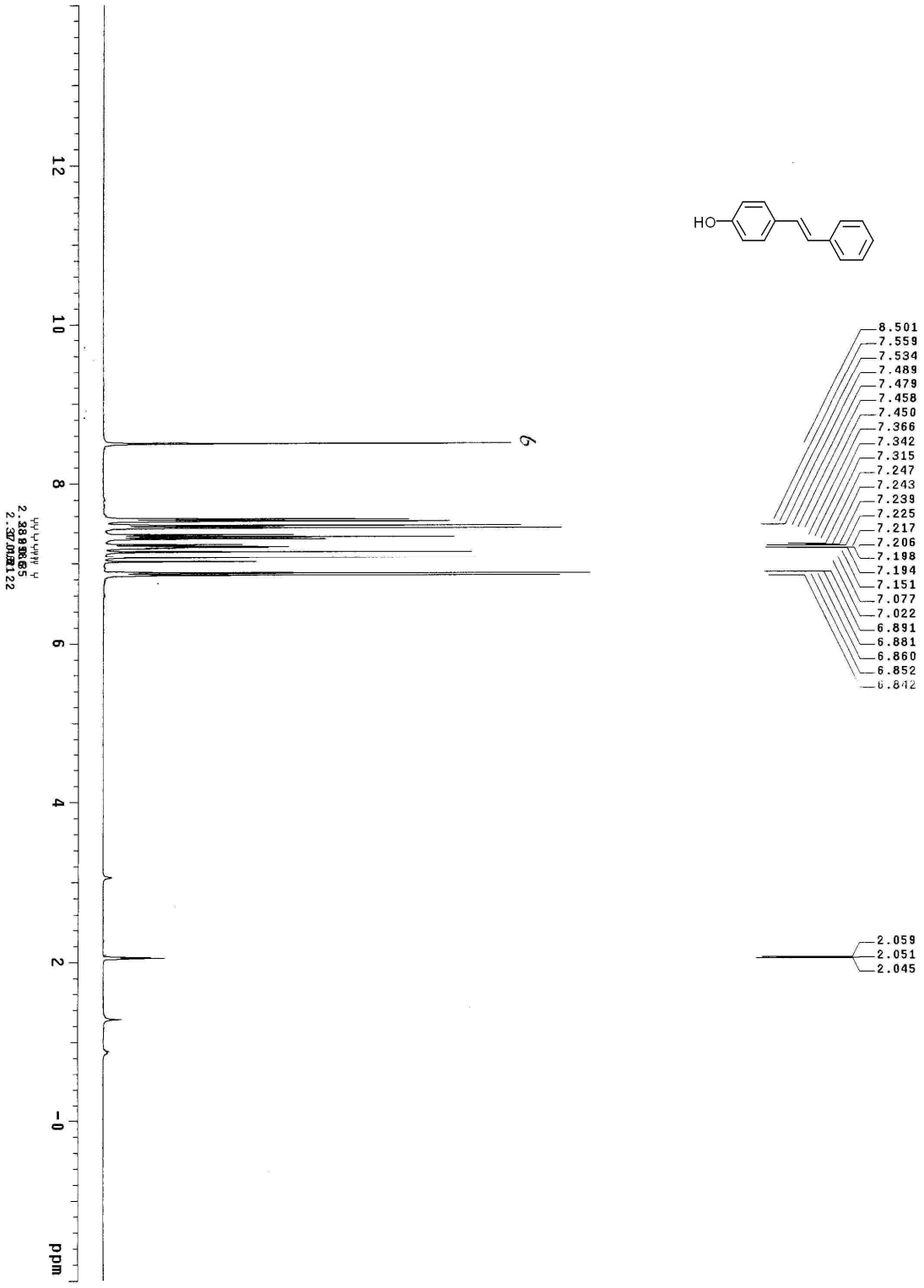
4-HS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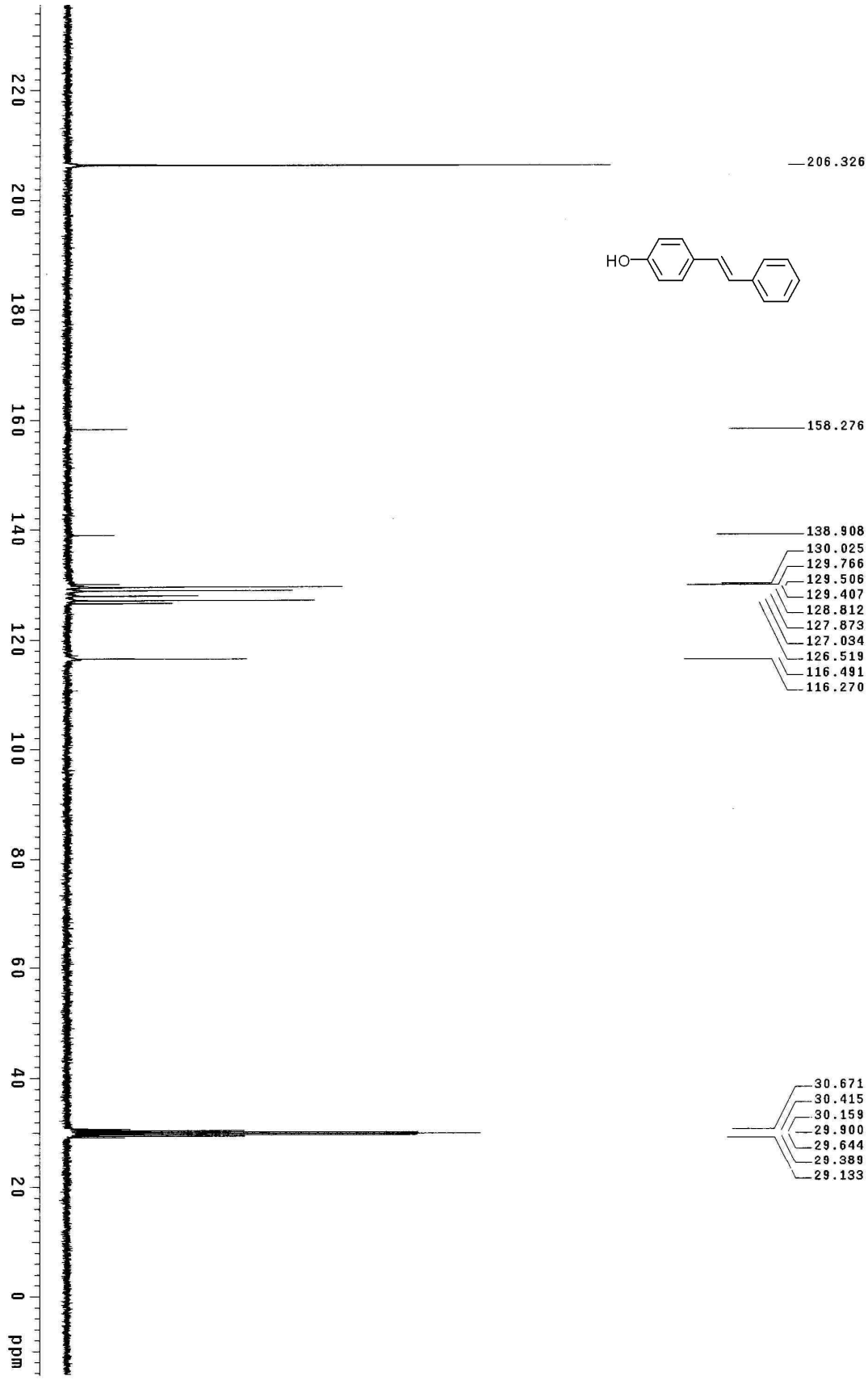
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30.159
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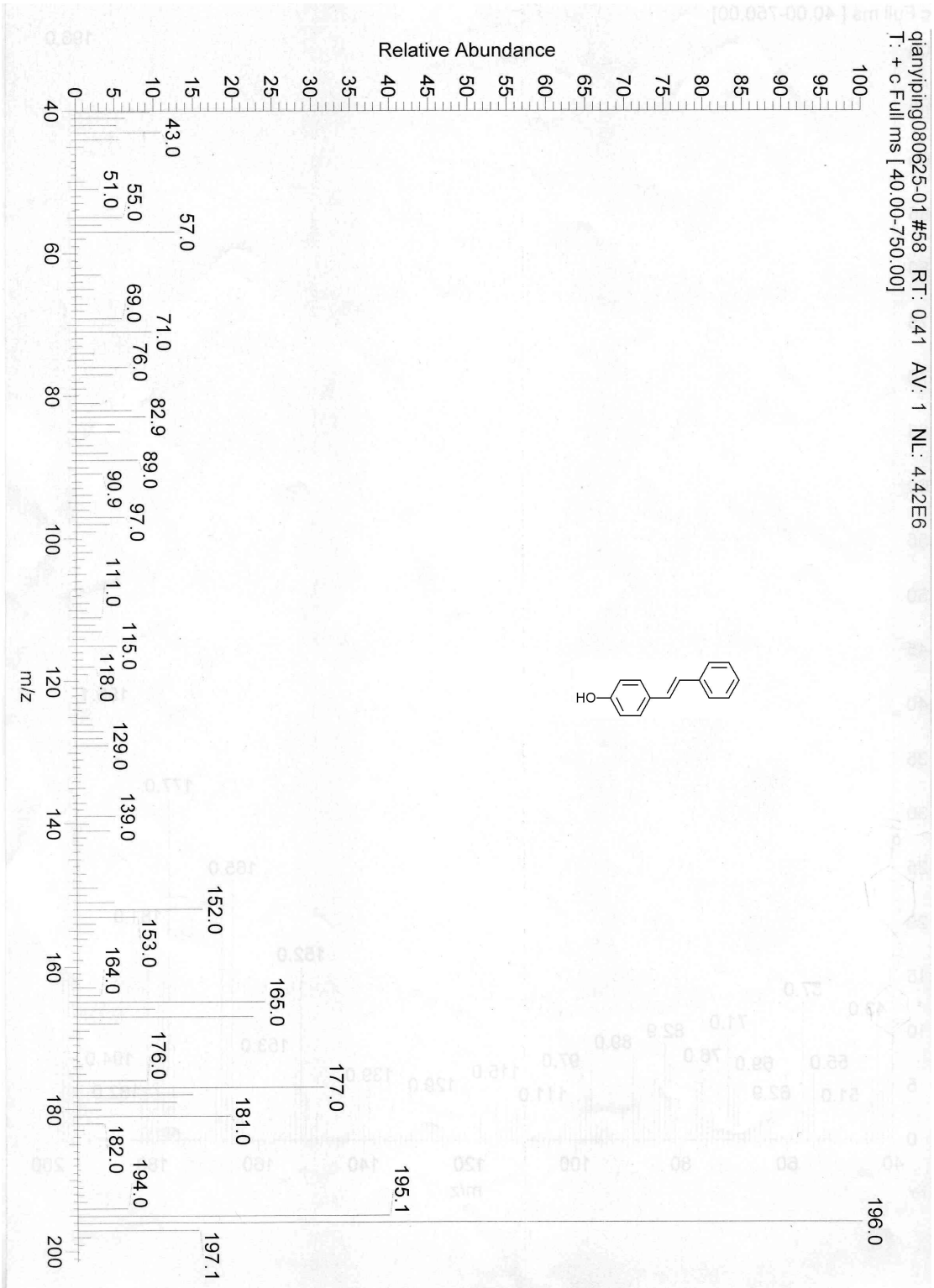
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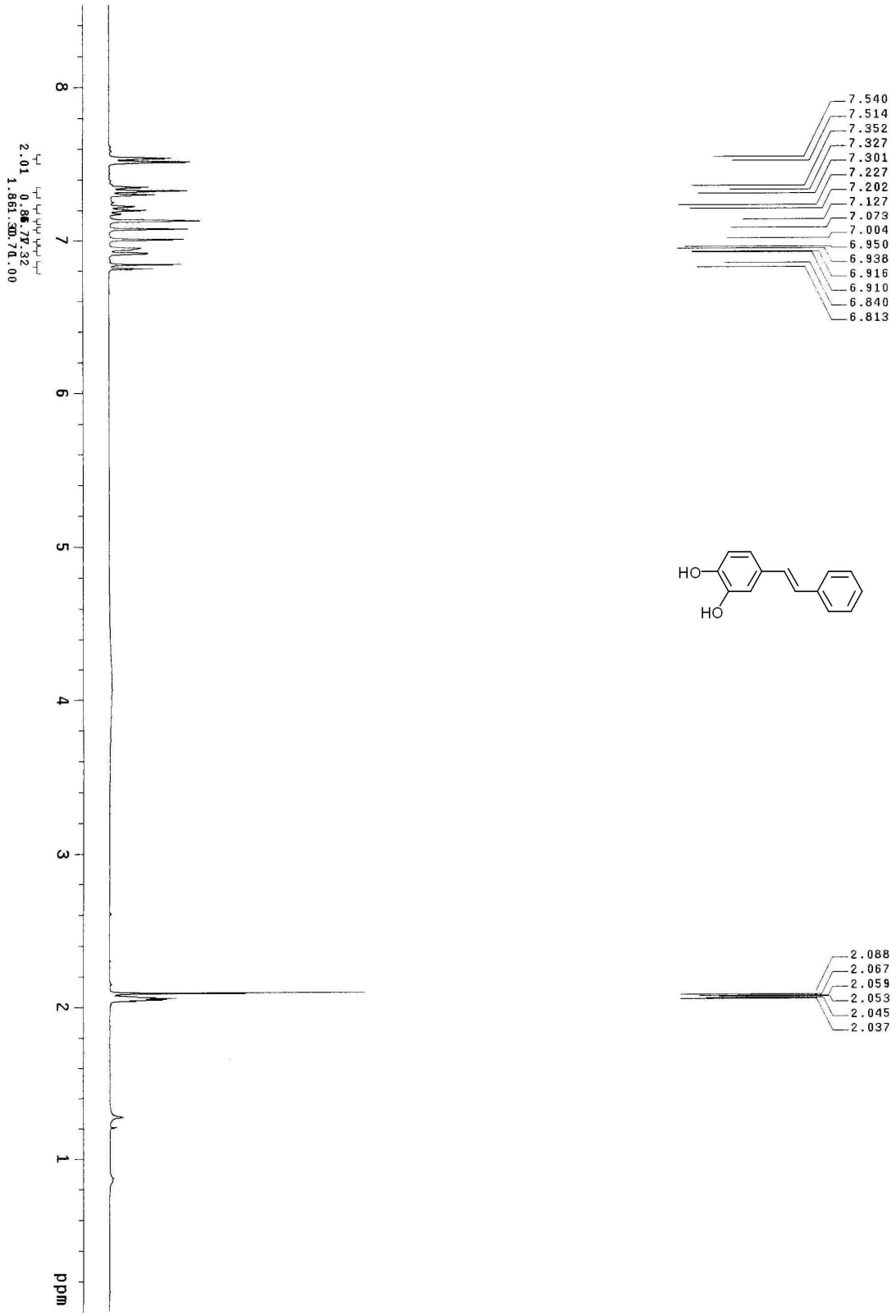
197.1

3,4-DHS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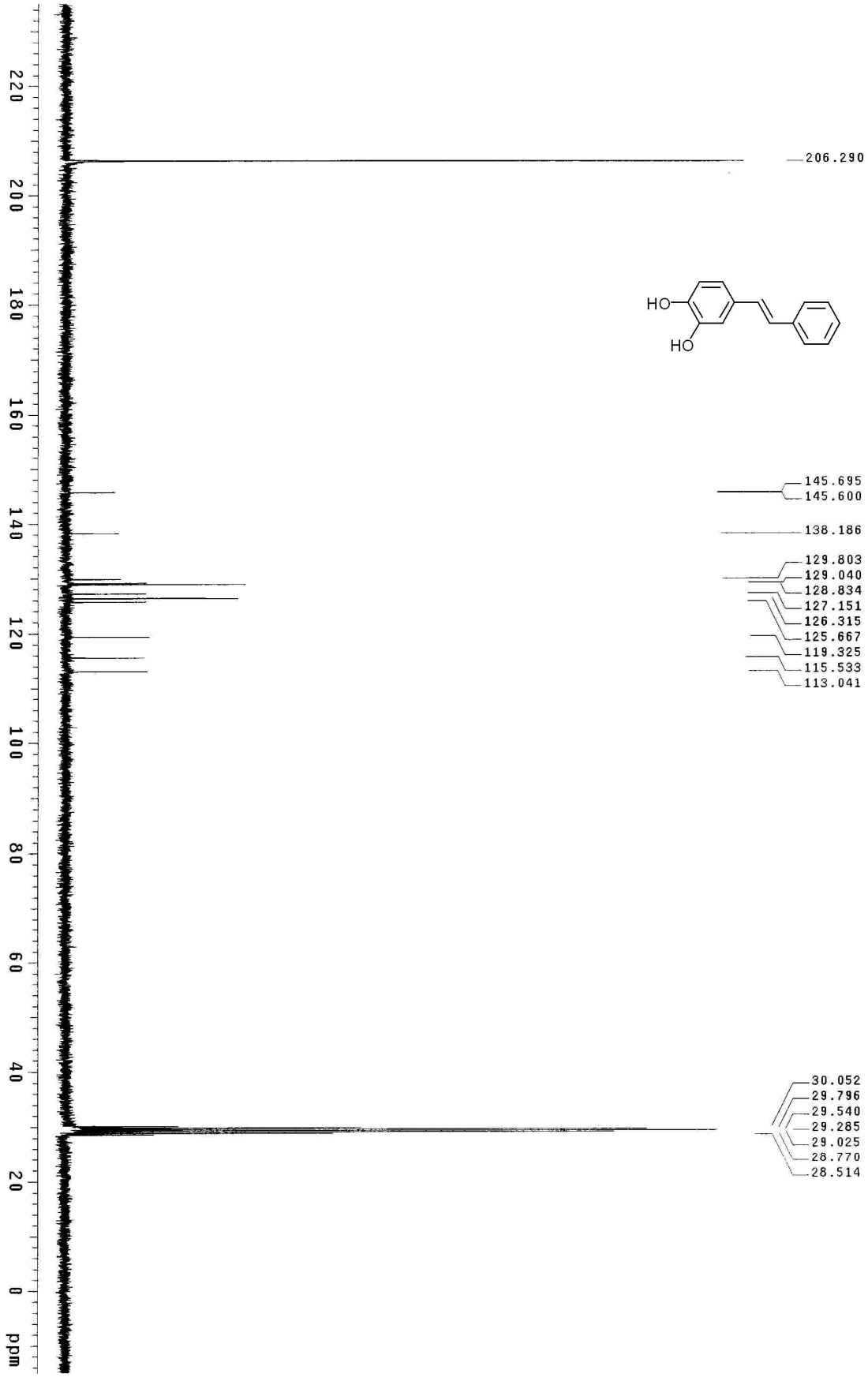
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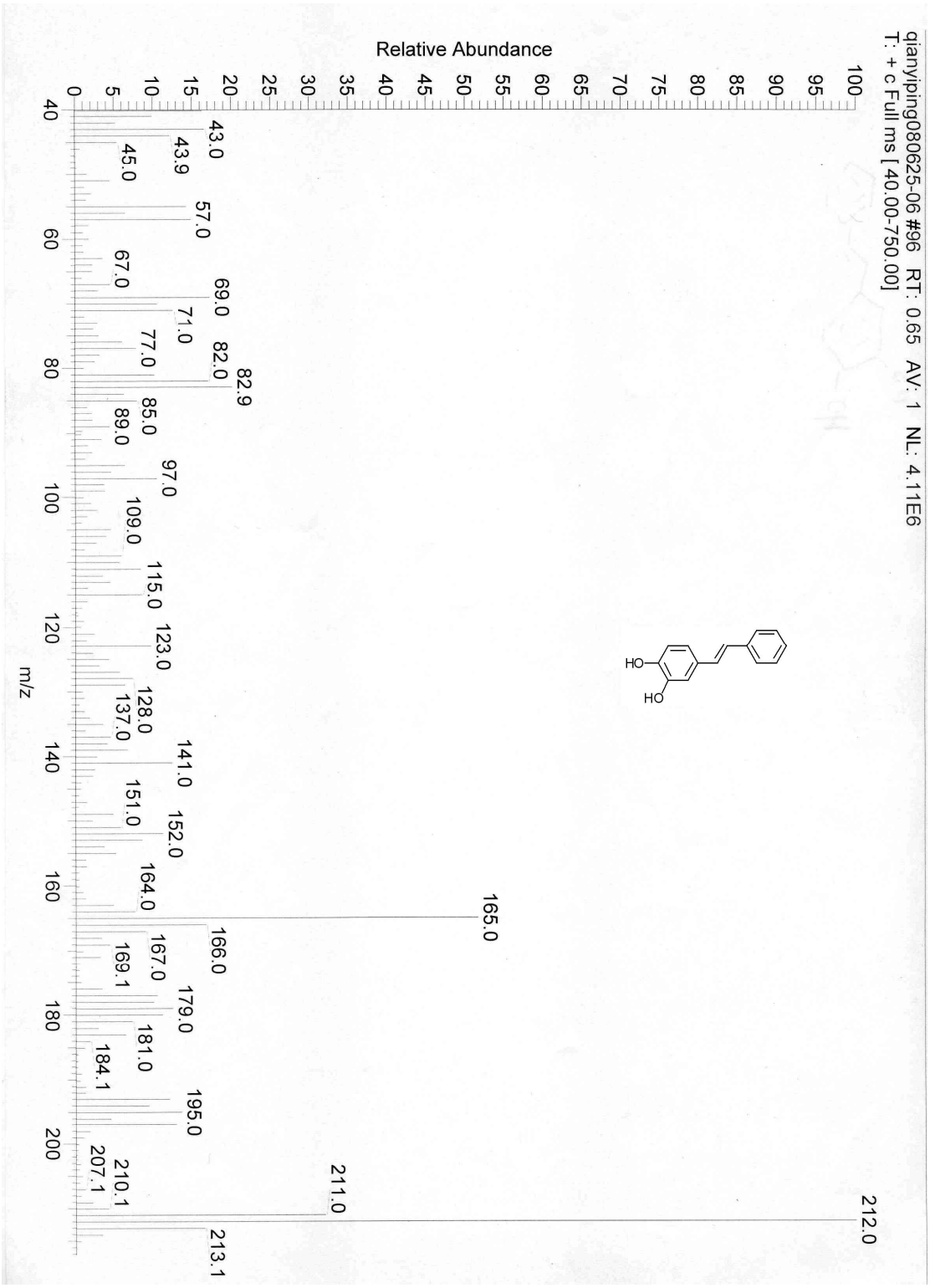
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77.0
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82.9
85.0
89.0
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109.0
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123.0
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165.0
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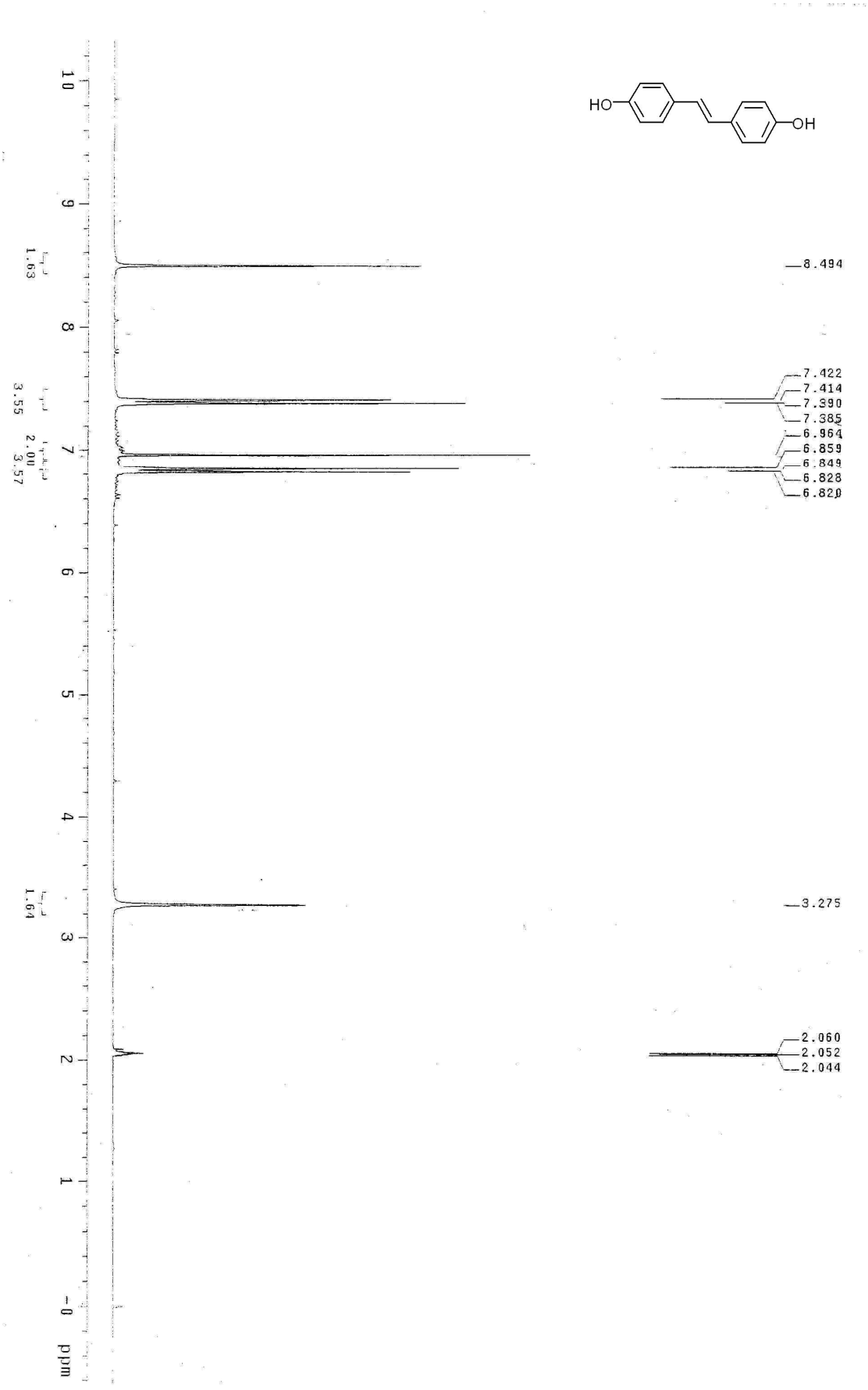
213.1

4,4'-DHS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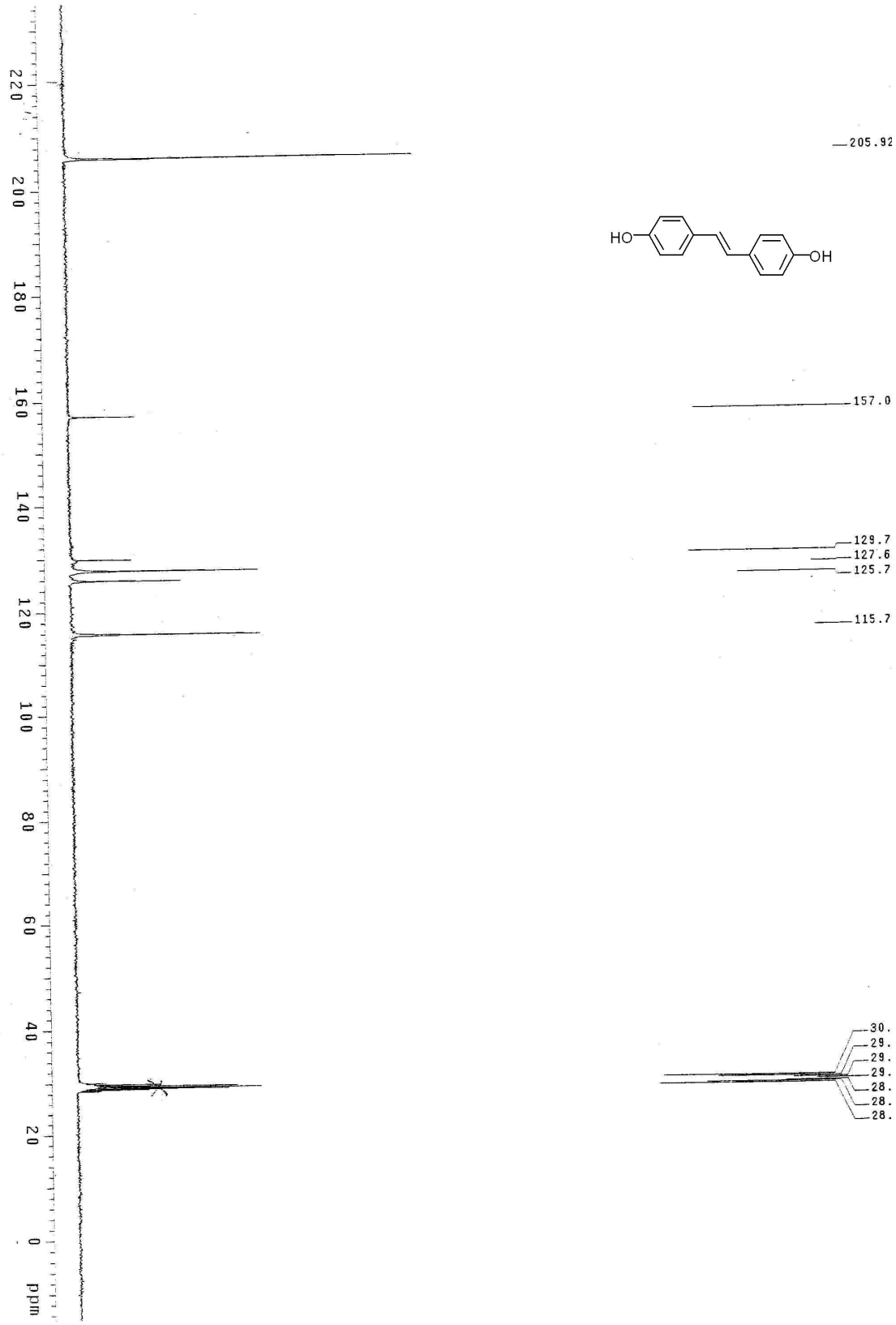
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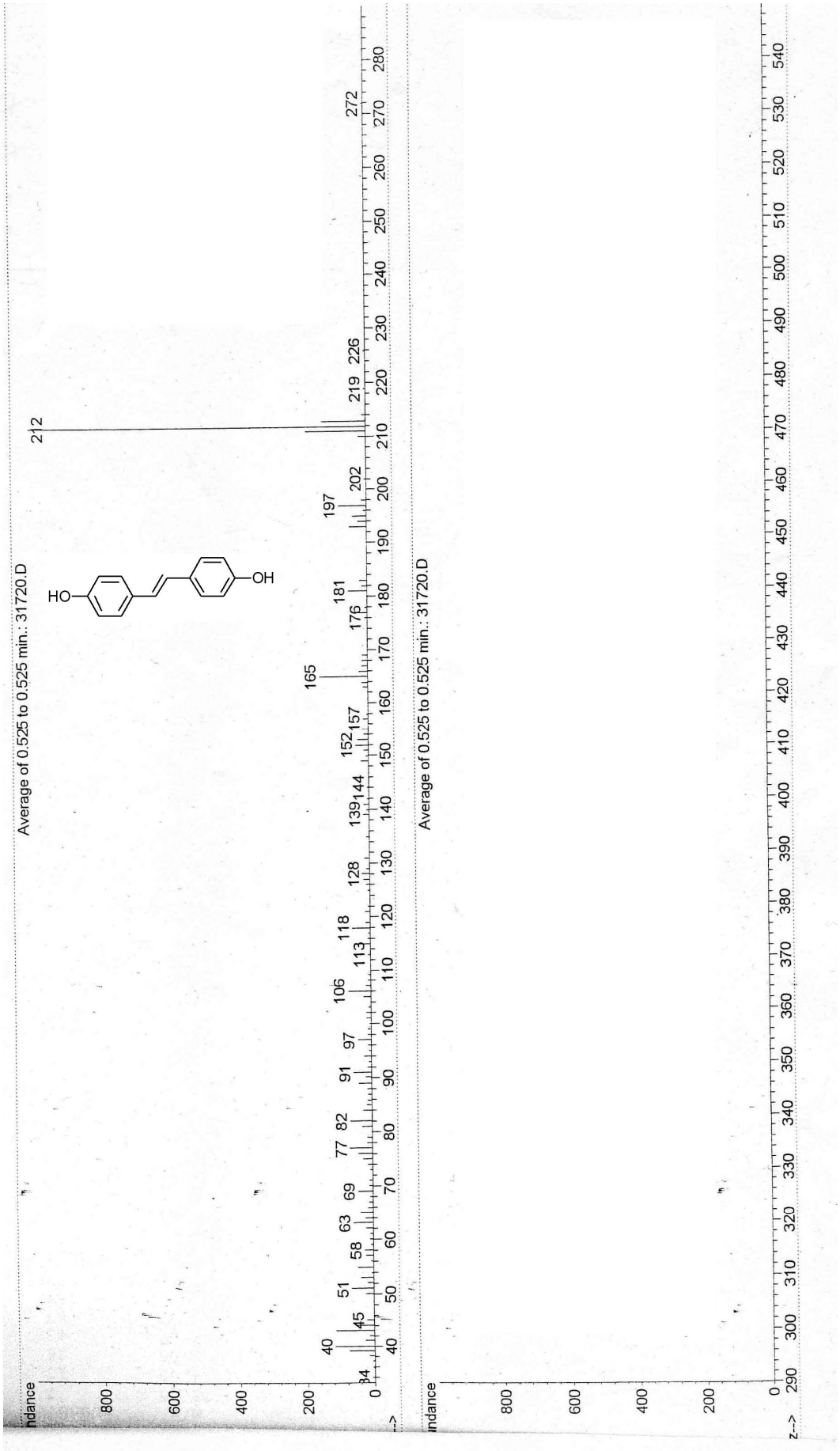
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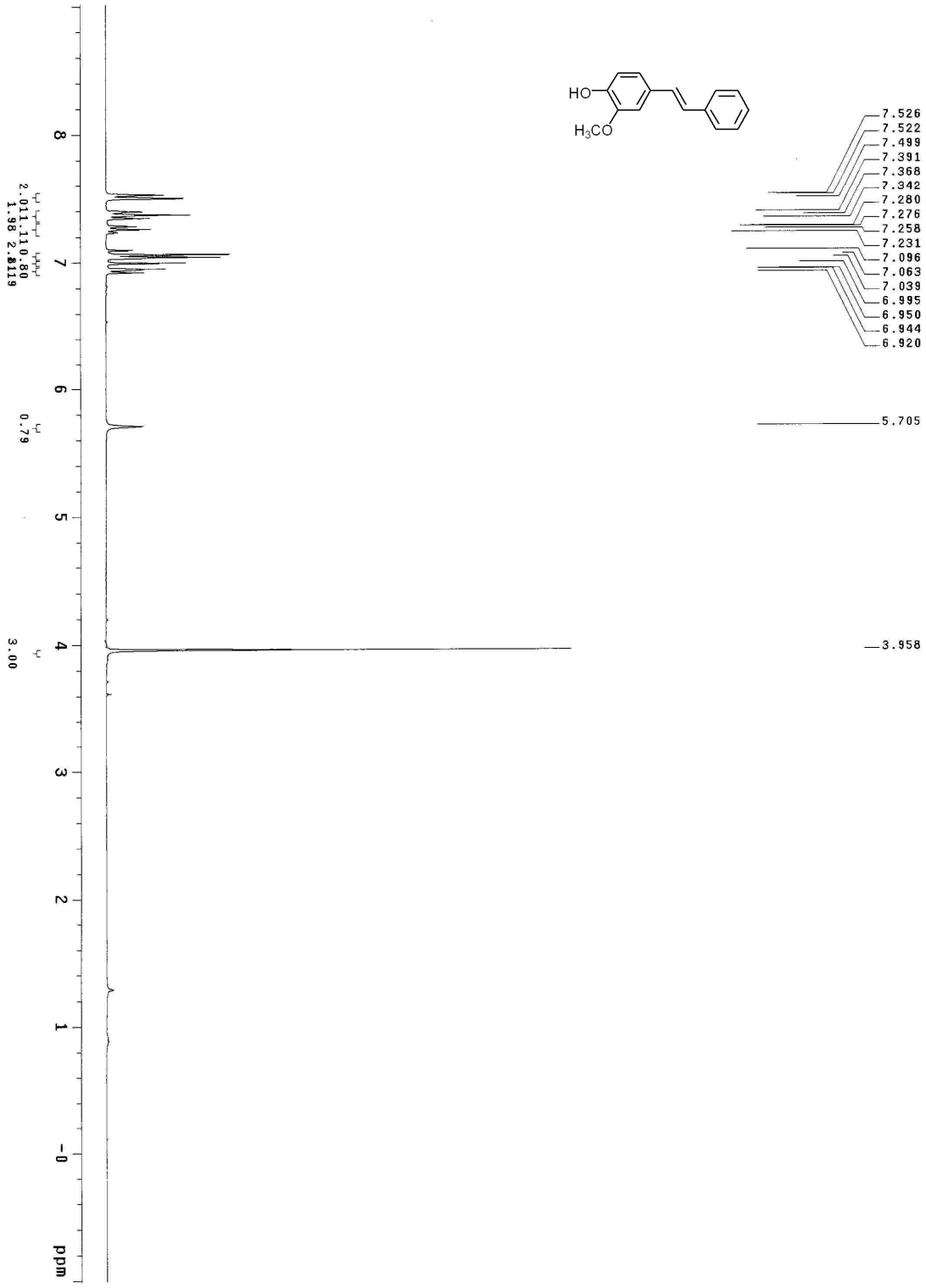
3-MeO-4-HS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7.039
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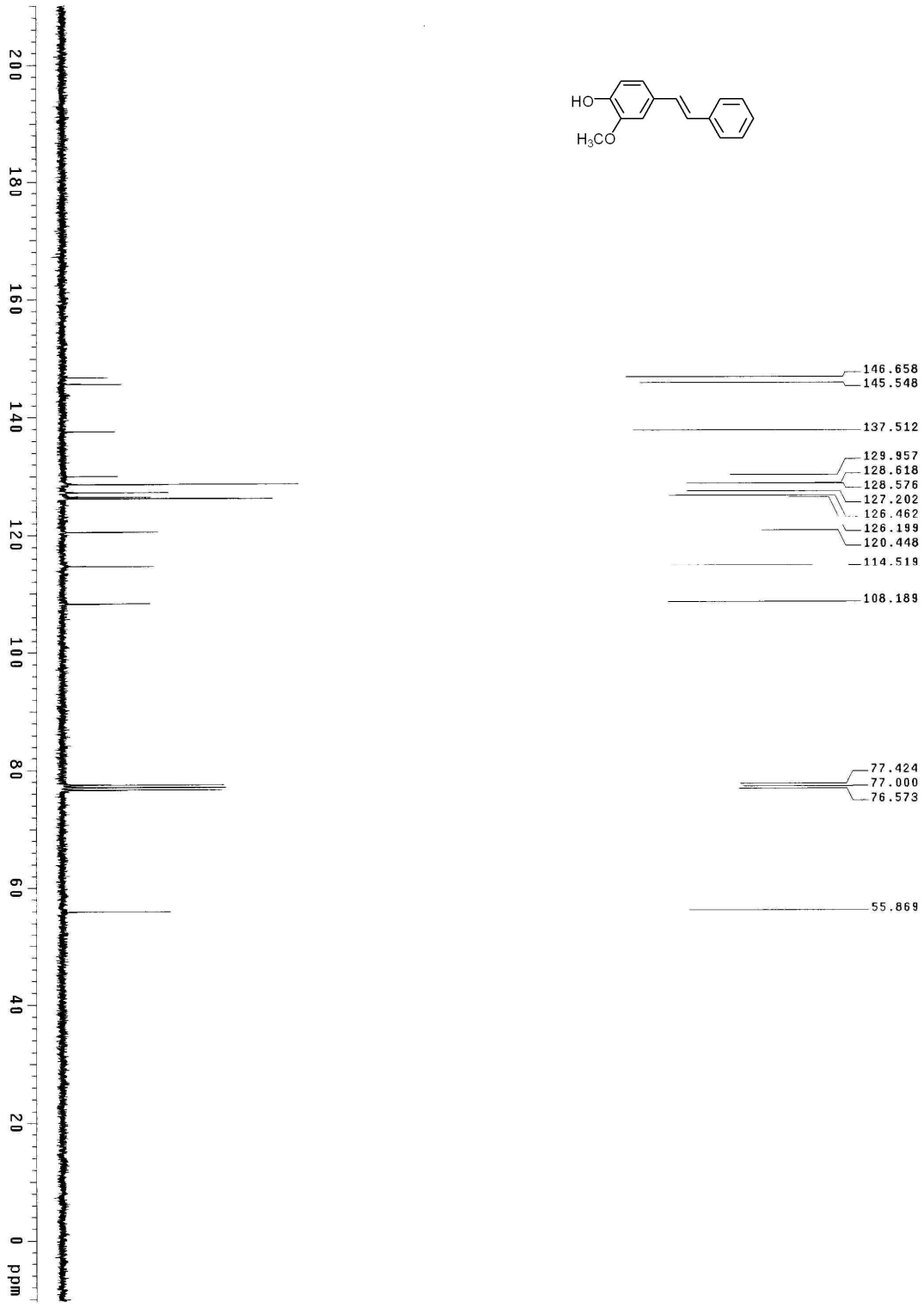
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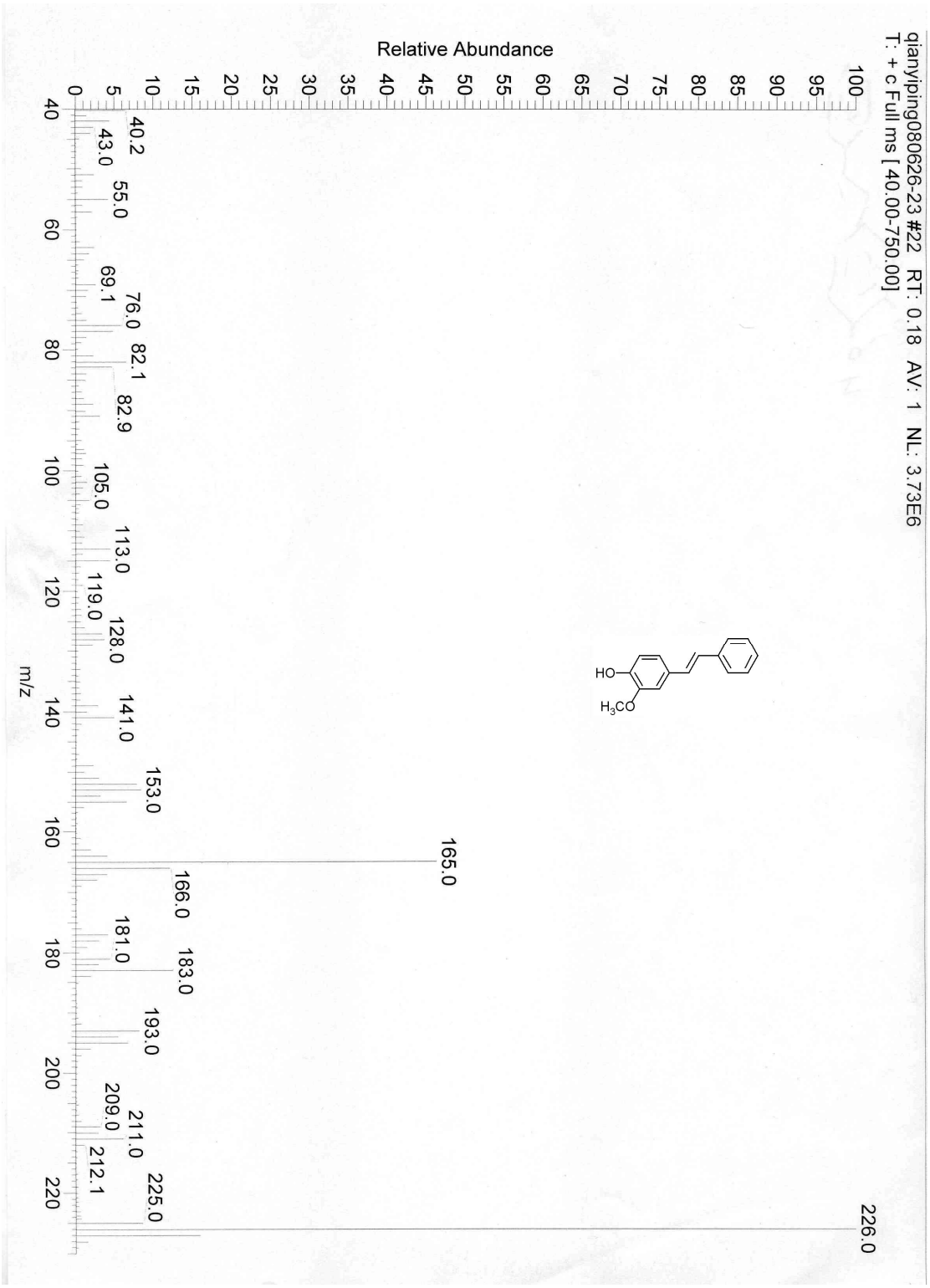
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82.1
82.9
105.0
113.0
119.0
128.0
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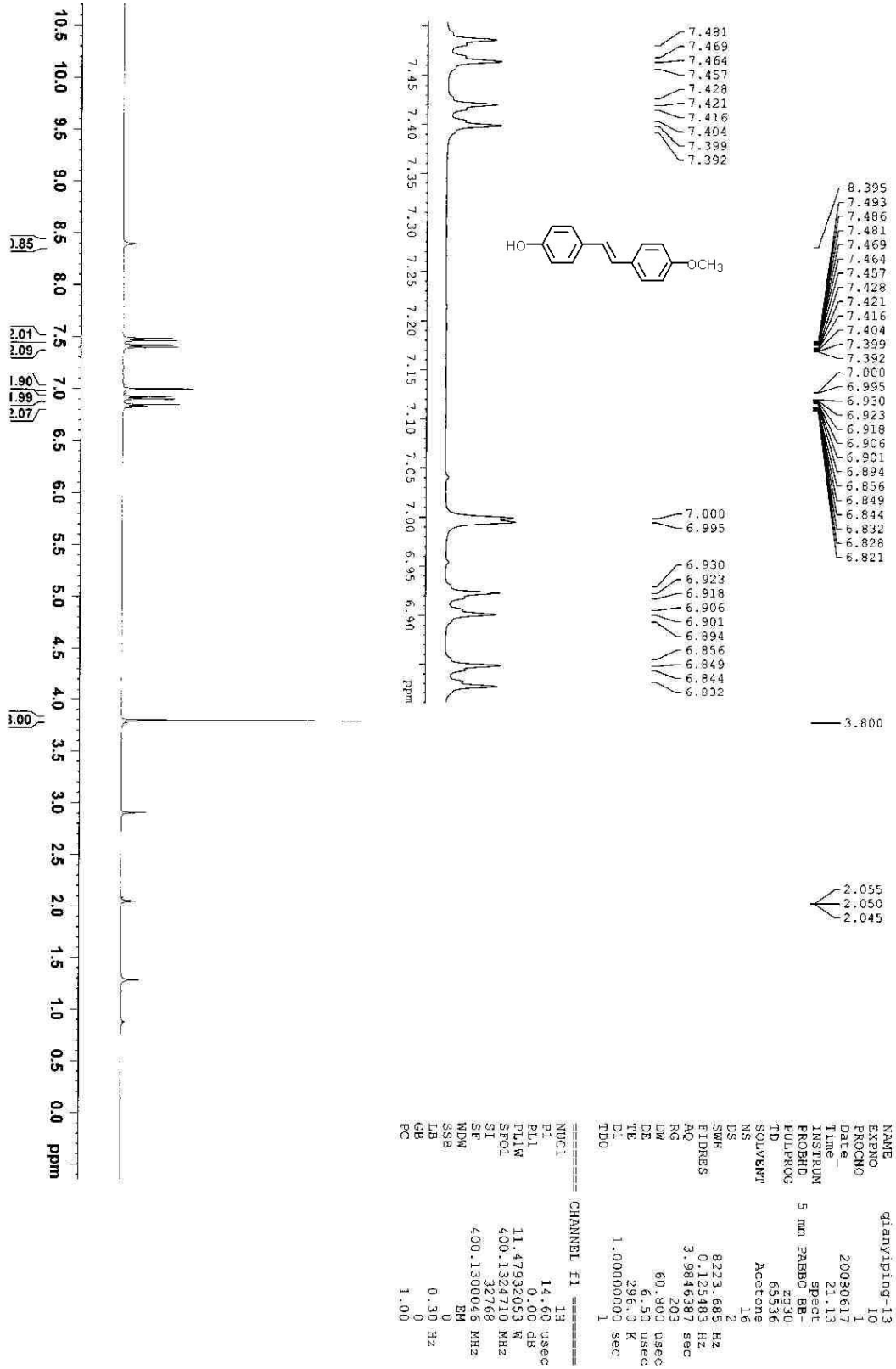
226.0

4'-MeO-4-HS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3.00
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EXPNO 10
PROCNO 1
Date_ 20080617
Time_ 21.13
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.60 usec
PL1 0.00 dB
PL1W 11.47932053 W
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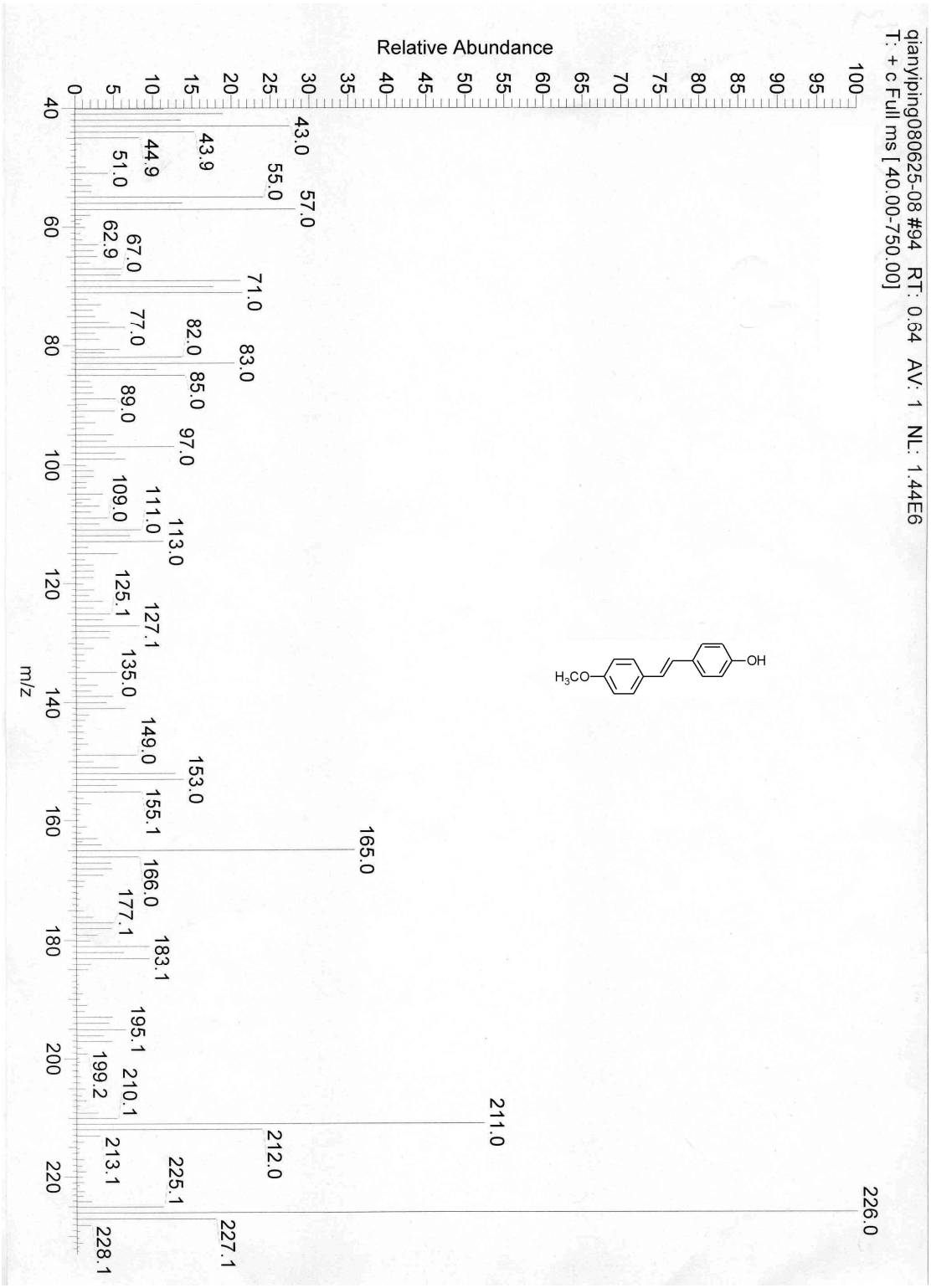
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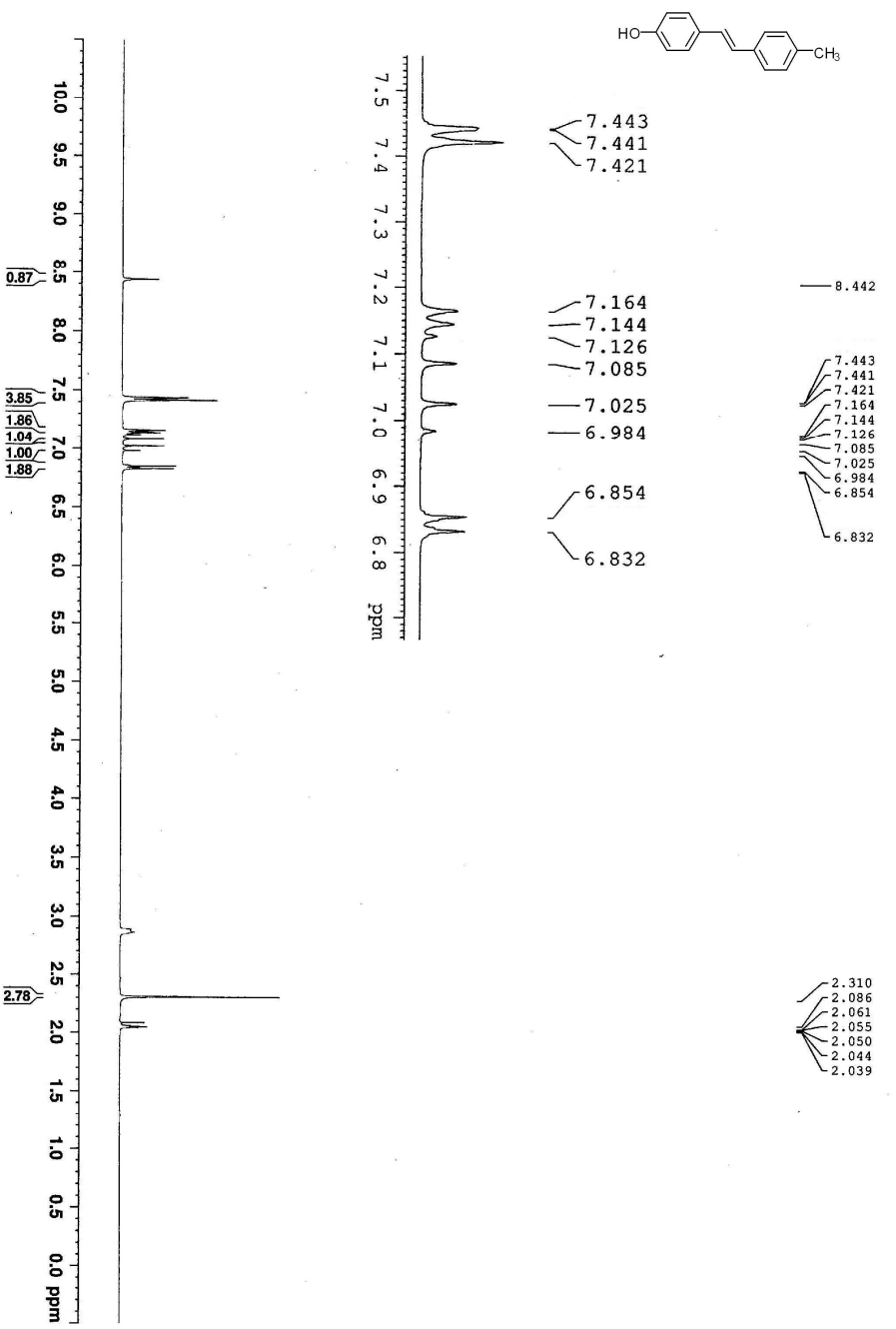
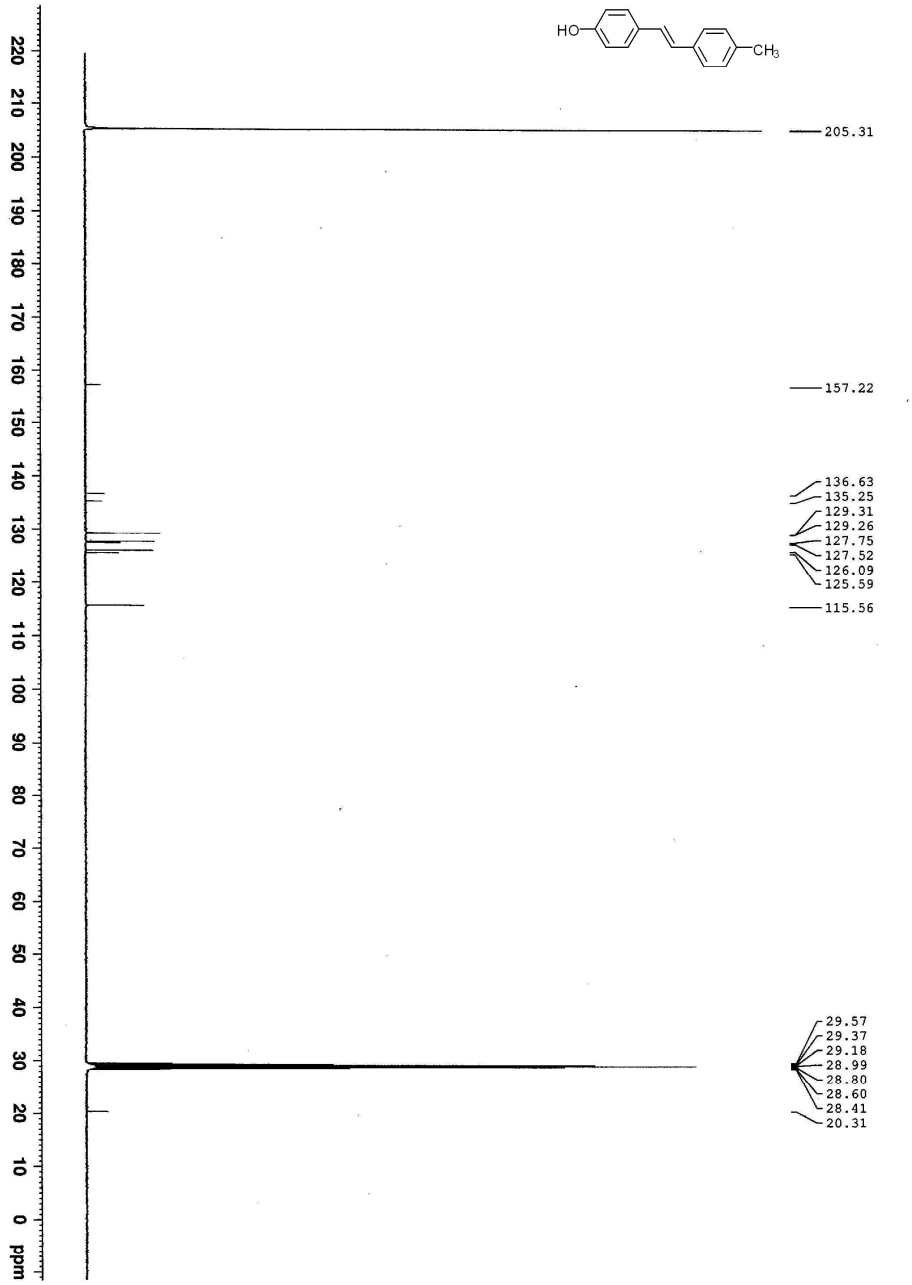
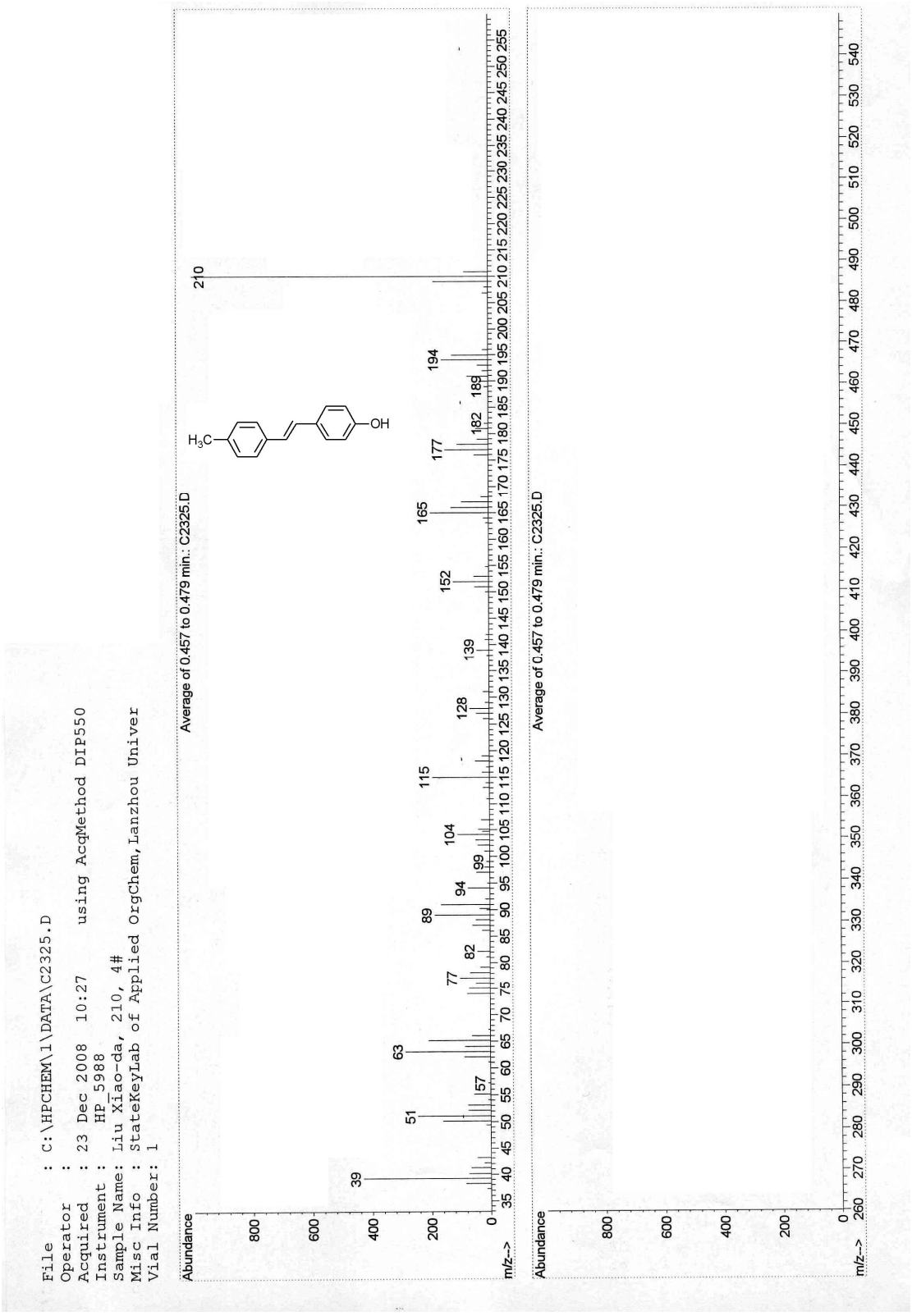
43.0
43.9
44.9
51.0
55.0
57.0
62.9
67.0
71.0
77.0
82.0
83.0
85.0
89.0
97.0
109.0
111.0
113.0
125.1
127.1
135.0
149.0
153.0
155.1
165.0
166.0
177.1
183.1
195.1
199.2
210.1
211.0
212.0
213.1
225.1
226.0
227.1
228.1

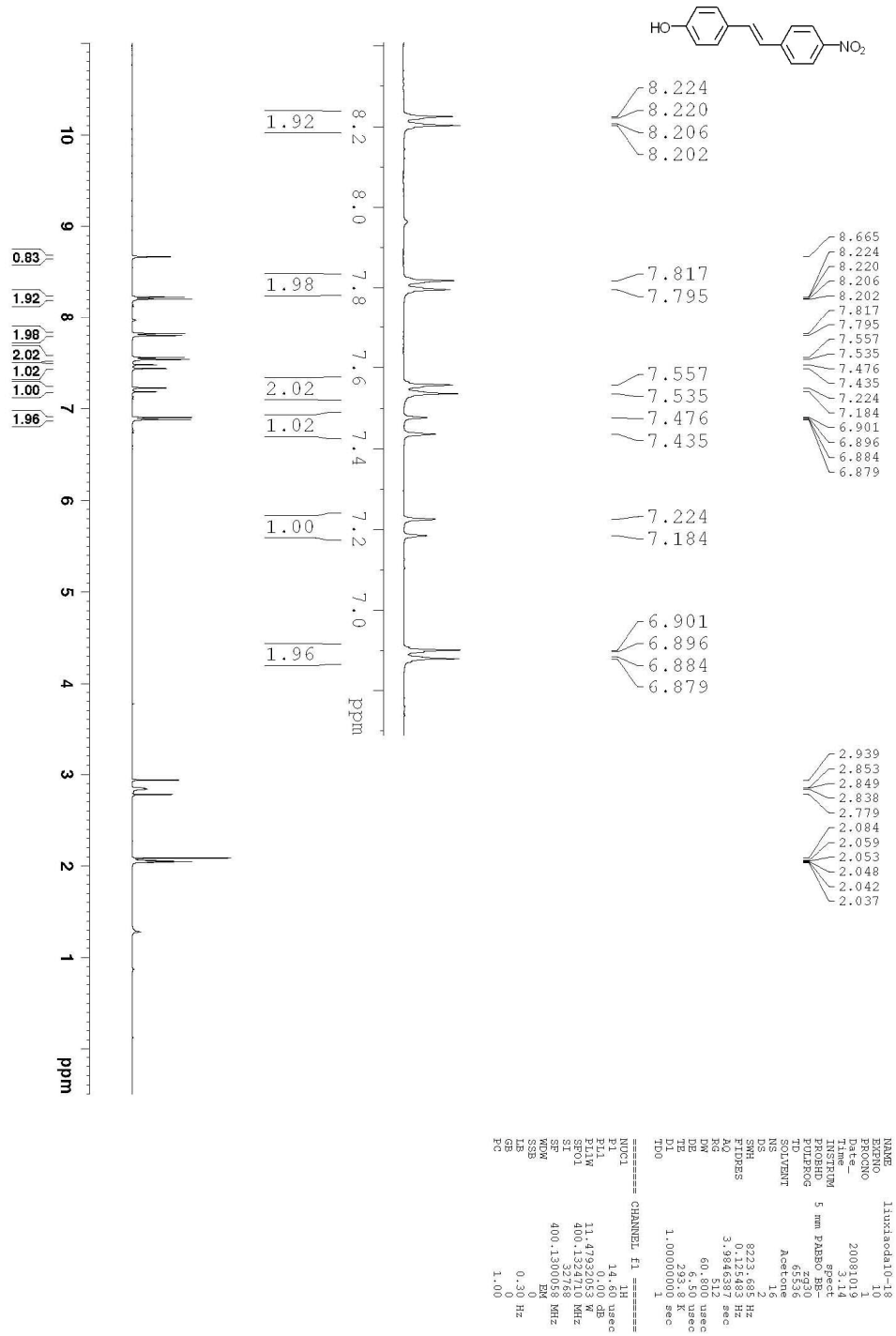
4’-Me-4-HS

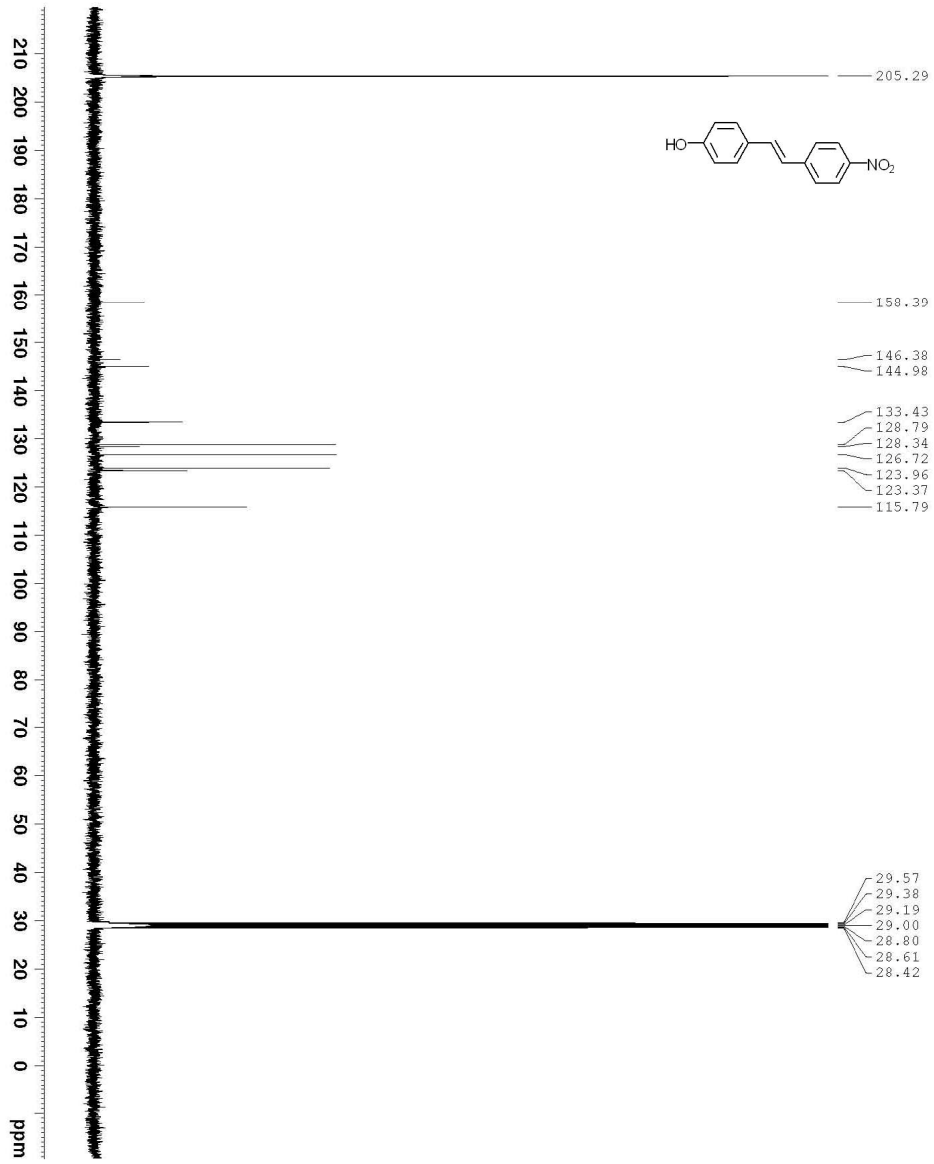

HO
CH3
7.443
7.441
7.421
7.164
7.144
7.126
7.085
7.025
6.984
6.854
6.832
8.442
2.310
2.086
2.061
2.055
2.050
2.044
2.039
0.87
3.85
1.86
1.04
1.00
1.88
2.78
ppm


HO
CH3
205.31
157.22
136.63
135.25
129.31
129.26
127.75
127.52
126.09
125.59
115.56
29.57
29.37
29.18
28.99
28.80
28.60
28.41
20.31
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


File : C:\HPCHEM\1\DATA\C2325.D
Operator :
Acquired : 23 Dec 2008 10:27 using AcqMethod DIP550
Instrument : HP 5988
Sample Name: Liu Xiao-da, 210, 4#
Misc Info : StateKeyLab of Applied OrgChem,Lanzhou Univer
Vial Number: 1
Abundance
Average of 0.457 to 0.479 min.: C2325.D
m/z-->
H3C
OH
Abundance
Average of 0.457 to 0.479 min.: C2325.D
m/z-->

4'-NO_2-4-HS


HO
NO2
8.224
8.220
8.206
8.202
7.817
7.795
7.557
7.535
7.476
7.435
7.224
7.184
6.901
6.896
6.884
6.879
8.665
8.224
8.220
8.206
8.202
7.817
7.795
7.557
7.535
7.476
7.435
7.224
7.184
6.901
6.896
6.884
6.879
2.939
2.853
2.849
2.838
2.779
2.084
2.059
2.053
2.048
2.042
2.037
0.83
1.92
1.98
2.02
1.02
1.00
1.96
1.92
1.98
2.02
1.02
1.00
1.96
ppm
ppm
NAME liuxiaodali0-10
EXPNO 10
PROCNO 1
Date_ 20081019
Time_ 3.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.98463872 sec
RG 512
DW 60.800 usec
DE 6.50 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
PL1W 111.47932053 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME liuxiaoda10-18
EXPNO 11
PROCNO 1
Date_ 20081019
Time 3.44
INSTRUM spect
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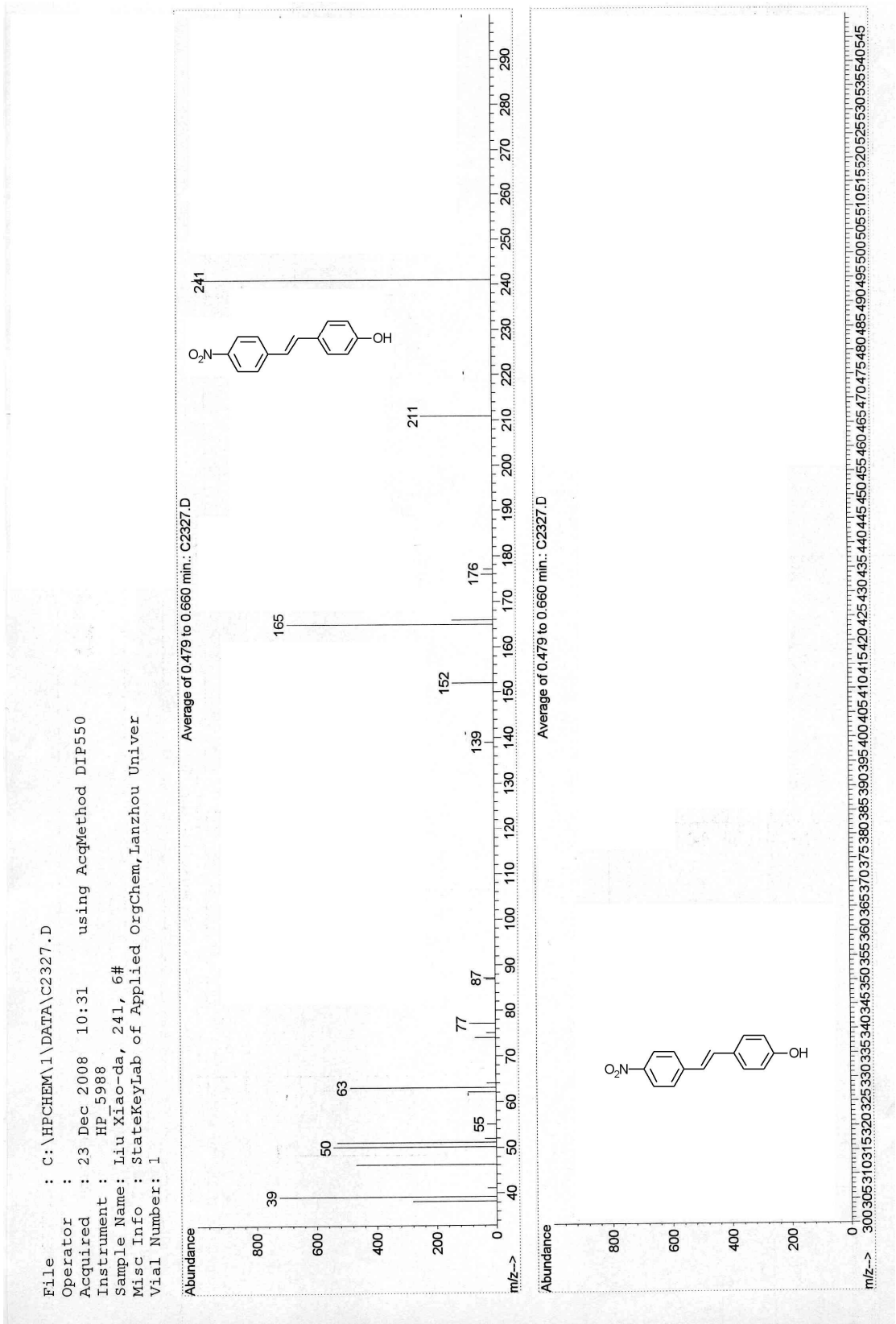
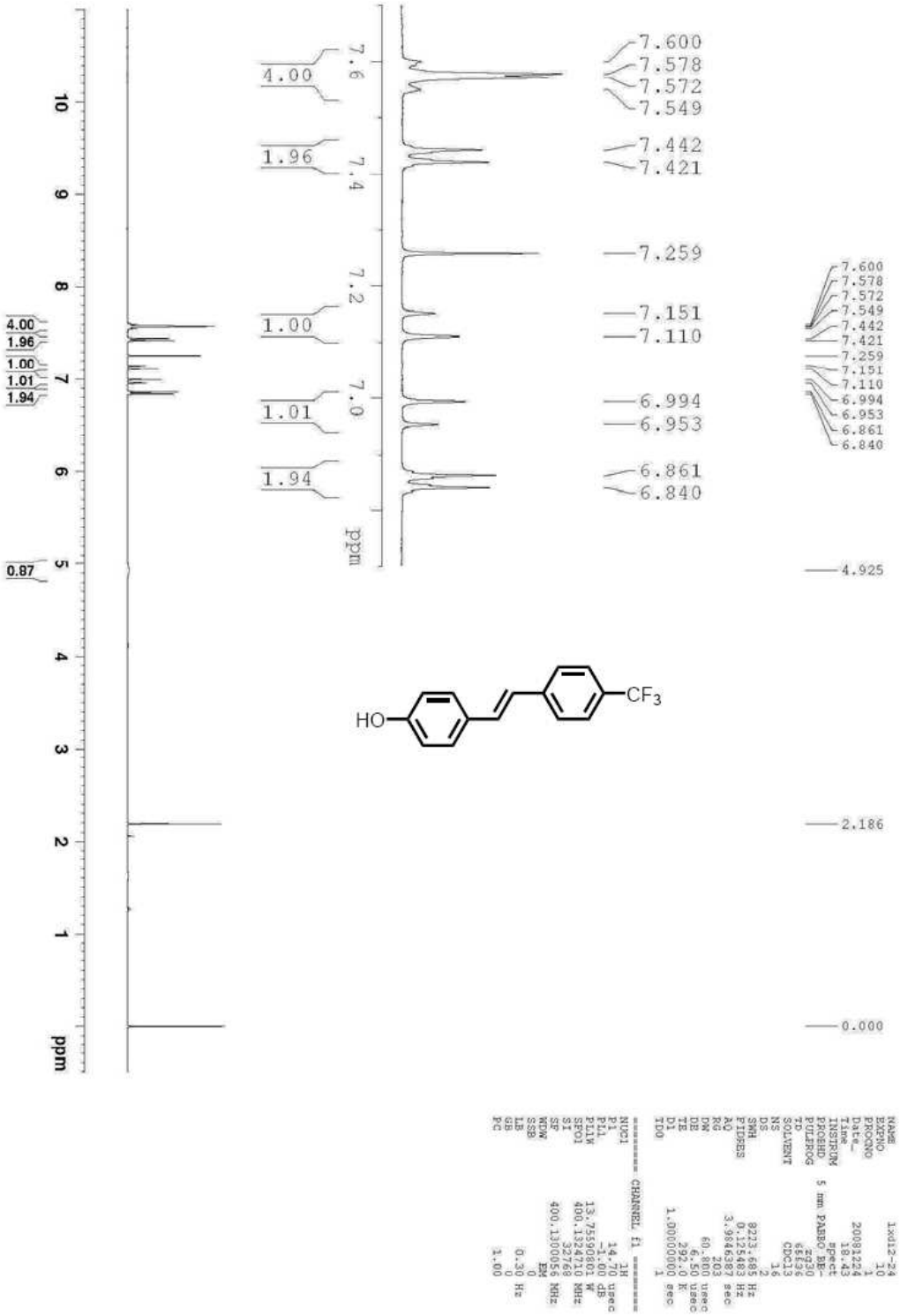
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

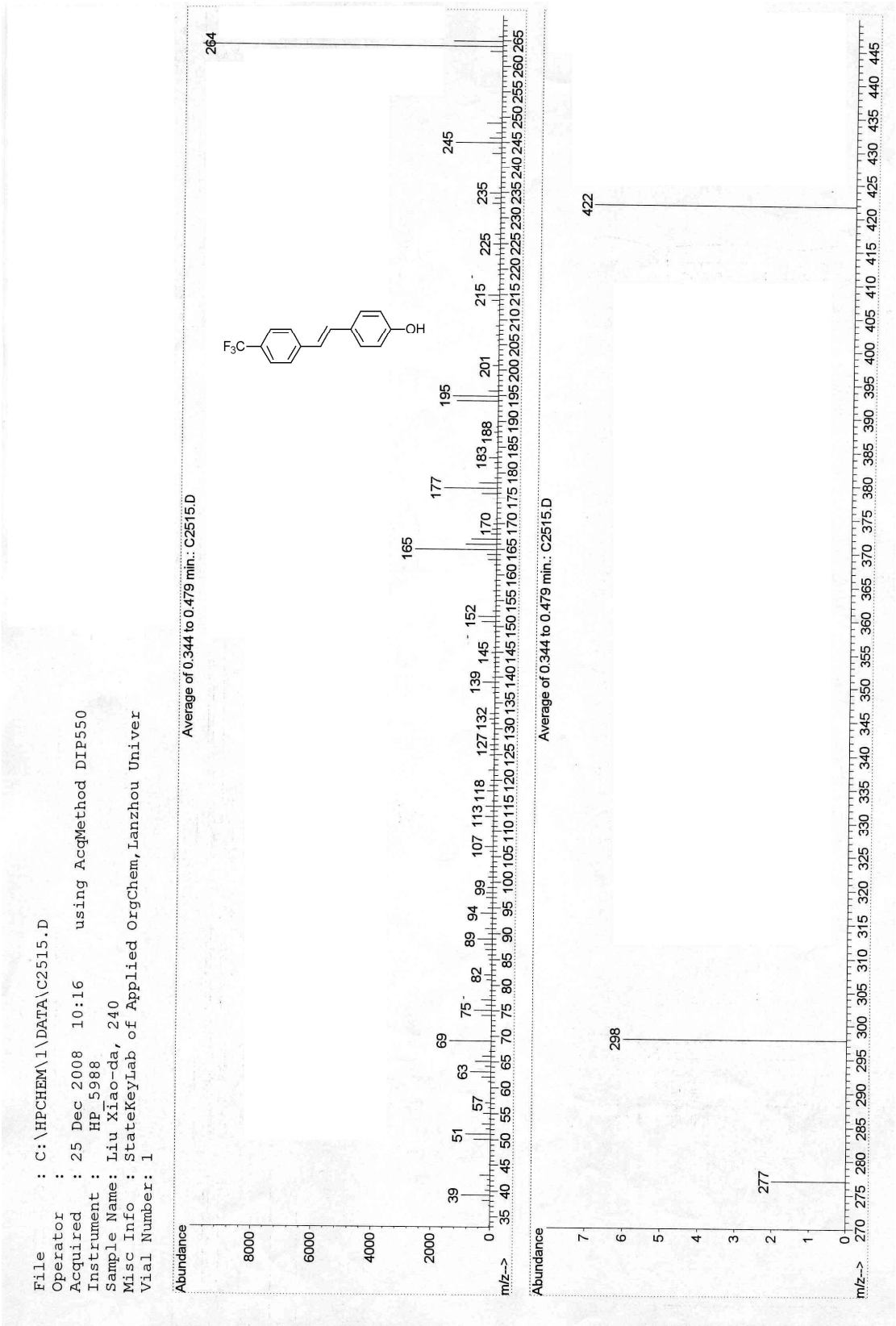
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 15.50 dB
PL13 15.50 dB
PL2W 18.19349861 W
PL12W 0.32353121 W
PL13W 0.32353121 W
SFO2 400.1316005 MHz
SI 32768
SP 100.6127621 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


File : C:\HPCHEM\1\DATA\C2327.D
Operator :
Acquired : 23 Dec 2008 10:31 using AcqMethod DIP550
Instrument : HP_5988
Sample Name: Liu Xiao-da, 241, 6#
Misc Info : StateKeyLab of Applied OrgChem,Lanzhou Univer
Vial Number: 1
Average of 0.479 to 0.660 min.: C2327.D
Abundance
m/z-->
241
211
176
165
152
139
87
77
63
55
50
39
O2N
OH
Average of 0.479 to 0.660 min.: C2327.D
Abundance
m/z-->

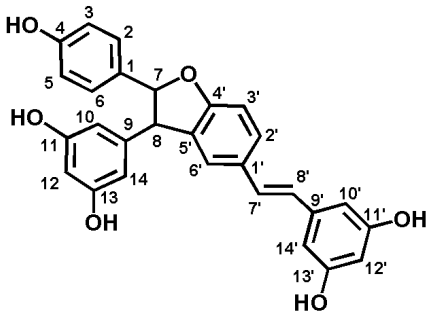
4'-CF_3-4-HS


7.600
7.578
7.572
7.549
7.442
7.421
7.259
7.151
7.110
6.994
6.953
6.861
6.840
4.925
2.186
0.000
4.00
1.96
1.00
1.01
1.94
0.87
ppm
HO
CF3


File : C:\HPCHEM\1\DATA\C2515.D
Operator :
Acquired : 25 Dec 2008 10:16 using AcqMethod DIP550
Instrument : HP_5988
Sample Name: Liu Xiao-da, 240
Misc Info : StateKeyLab of Applied OrgChem,Lanzhou Univer
Vial Number: 1
Average of 0.344 to 0.479 min.: C2515.D
Abundance
m/z-->
F3C
OH
Average of 0.344 to 0.479 min.: C2515.D
Abundance
m/z-->

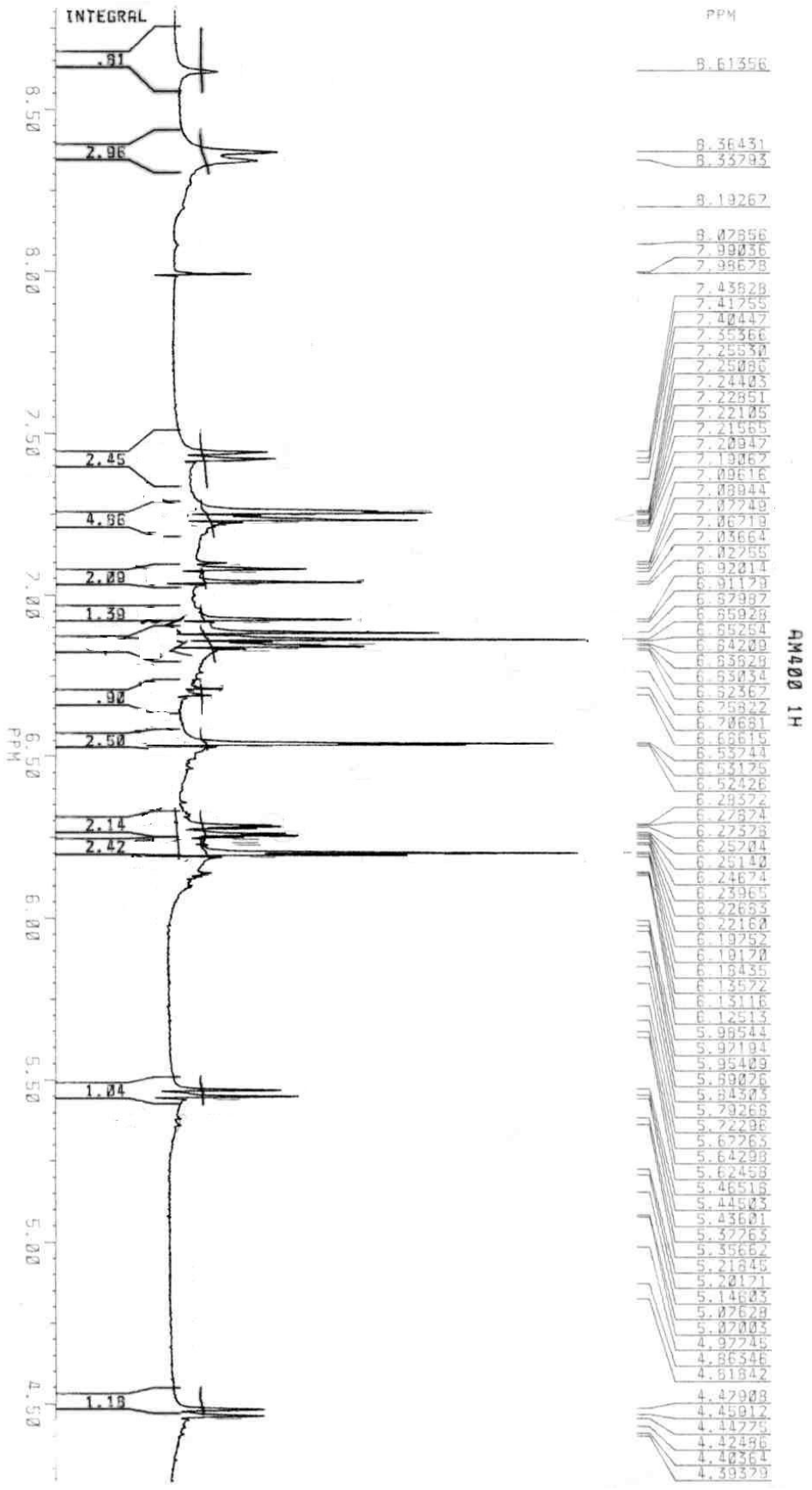
3 ^{1}H, ^{13}C, 2D NMR, HRMS (ESI) spectrum of dimer

NMR data for resveratrol dimer

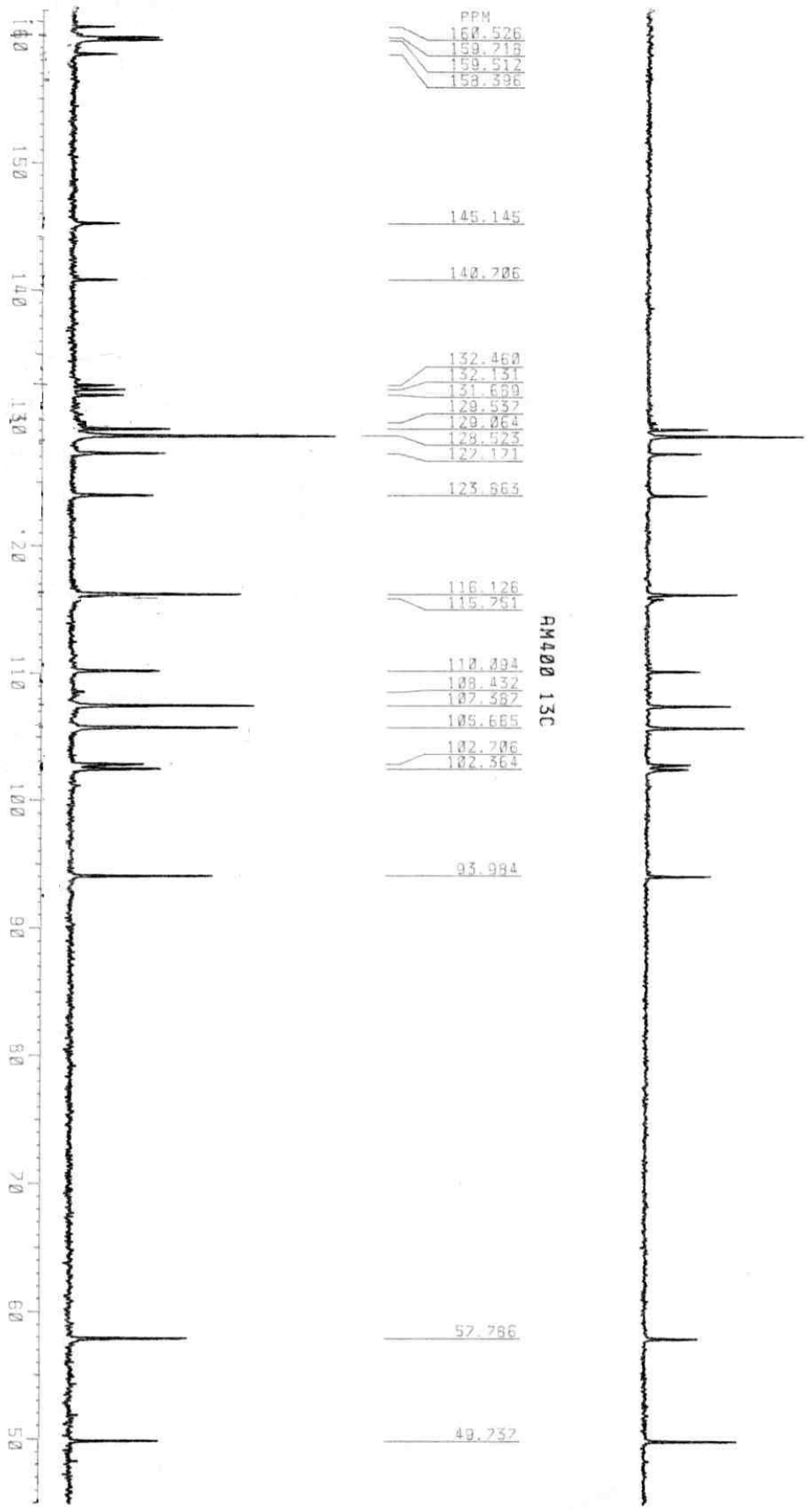


H	δ_H (mult., *J* Hz)	C	δ_C
		C-1	131.7
H-2, 6	7.24 (d, 8.0)	C-2, 6	128.5
H-3, 5	6.84 (d, 8.0)	C-3, 5	116.1
		C-4	158.4
H-7	5.48 (d, 8.0)	C-7	94.2
H-8	4.62 (d, 8.0)	C-8	57.7
		C-9	145.1
H-10, 14	6.19 (d, 2.0)	C-10, 14	107.4
		C-11, 13	159.7
H-12	6.25 (d, 2.0)	C-12	102.4
		C-1’	132.5
H-2’	7.25 (d, 8.0)	C-2’	123.9
H-3’	6.88 (d, 8.0)	C-3’	110.1
		C-4’	160.5
		C-5’	132.1
H-6’	7.45 (d, 2.0)	C-6’	128.5
H-7’	7.08 (d, 16.0)	C-7’	127.2
H-8’	6.92 (d, 16.0)	C-8’	129.1
		C-9’	140.7
H-10’, 14’	6.53 (d, 2.0)	C-10’, 14’	105.7
		C-11’,13’	159.5
H-12’	6.25 (d, 2.0)	C-12’	102.7

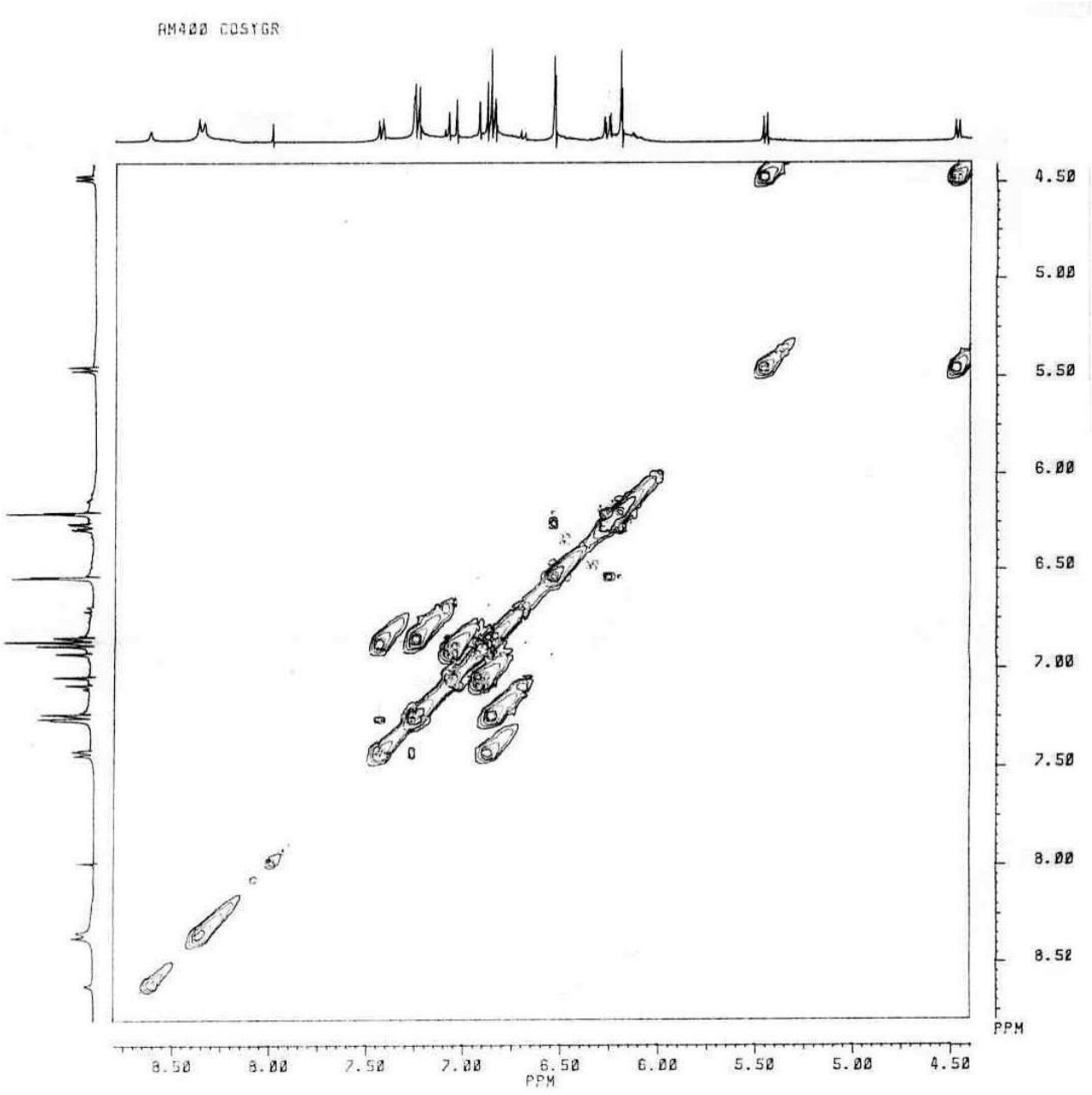
^{1}H-NMR spectrum of resveratrol dimer



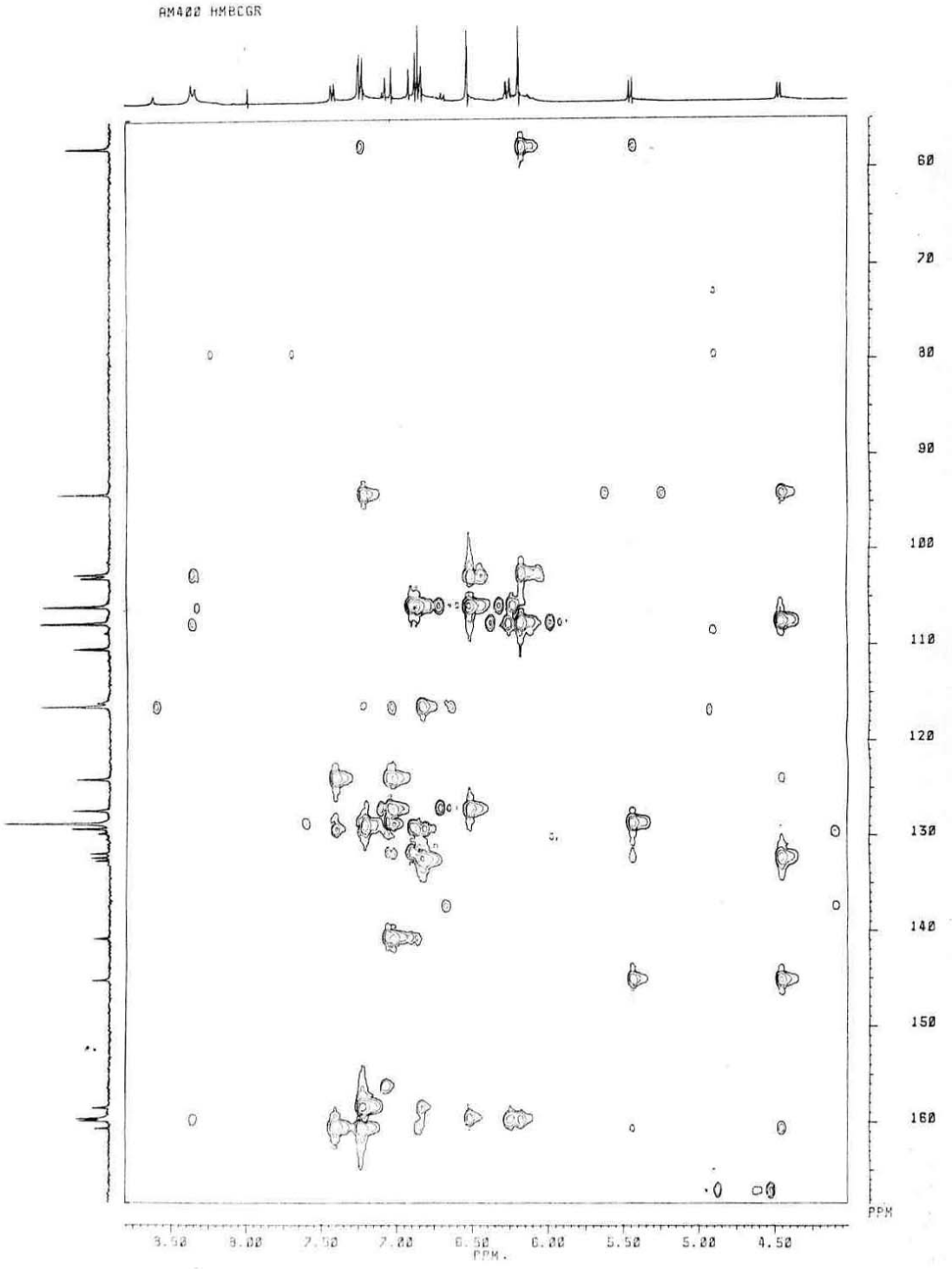
^{13}C-NMR spectrum of resveratrol dimer



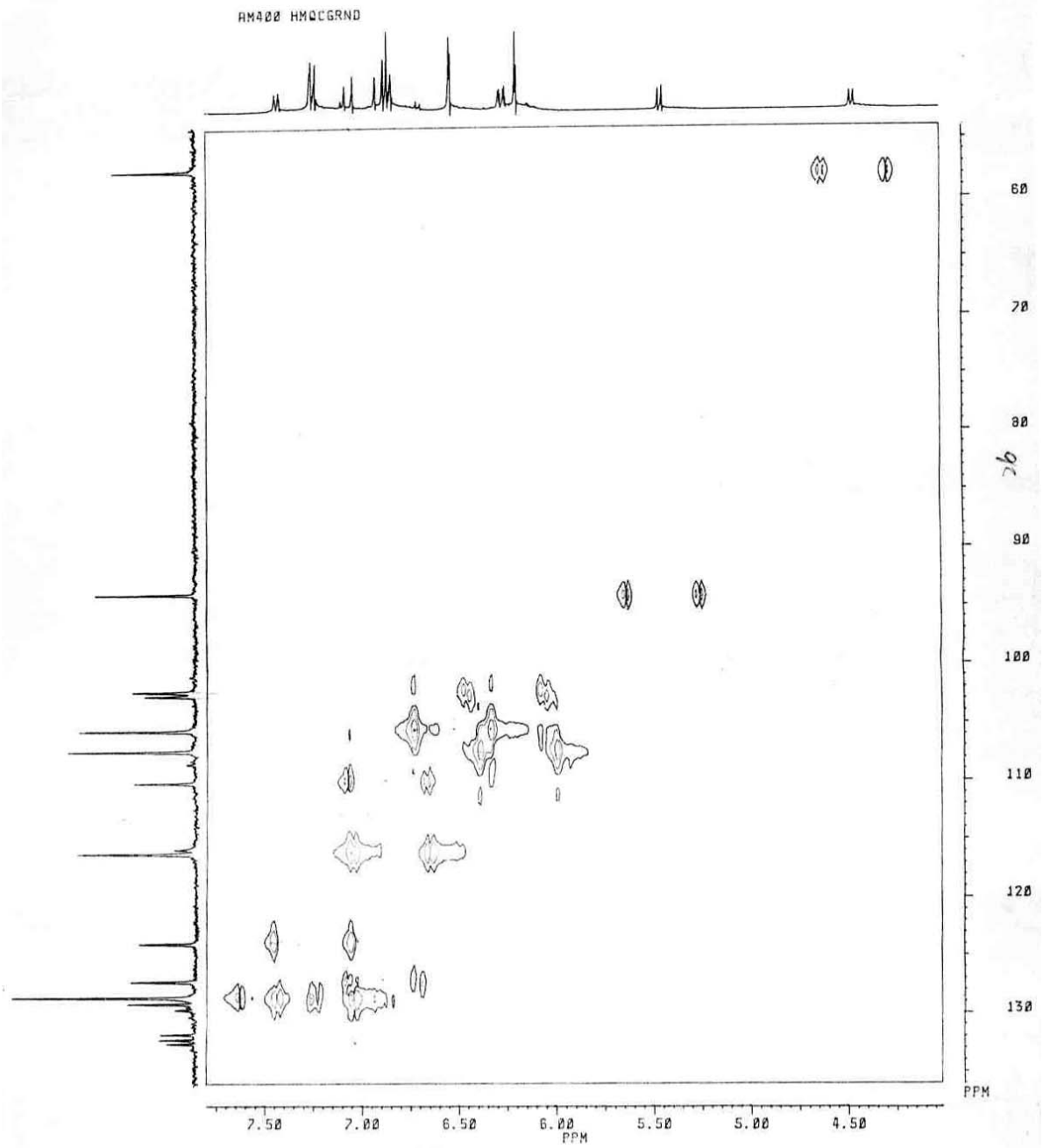
^{1}H, ^{1}H COSY spectrum of resveratrol dimer



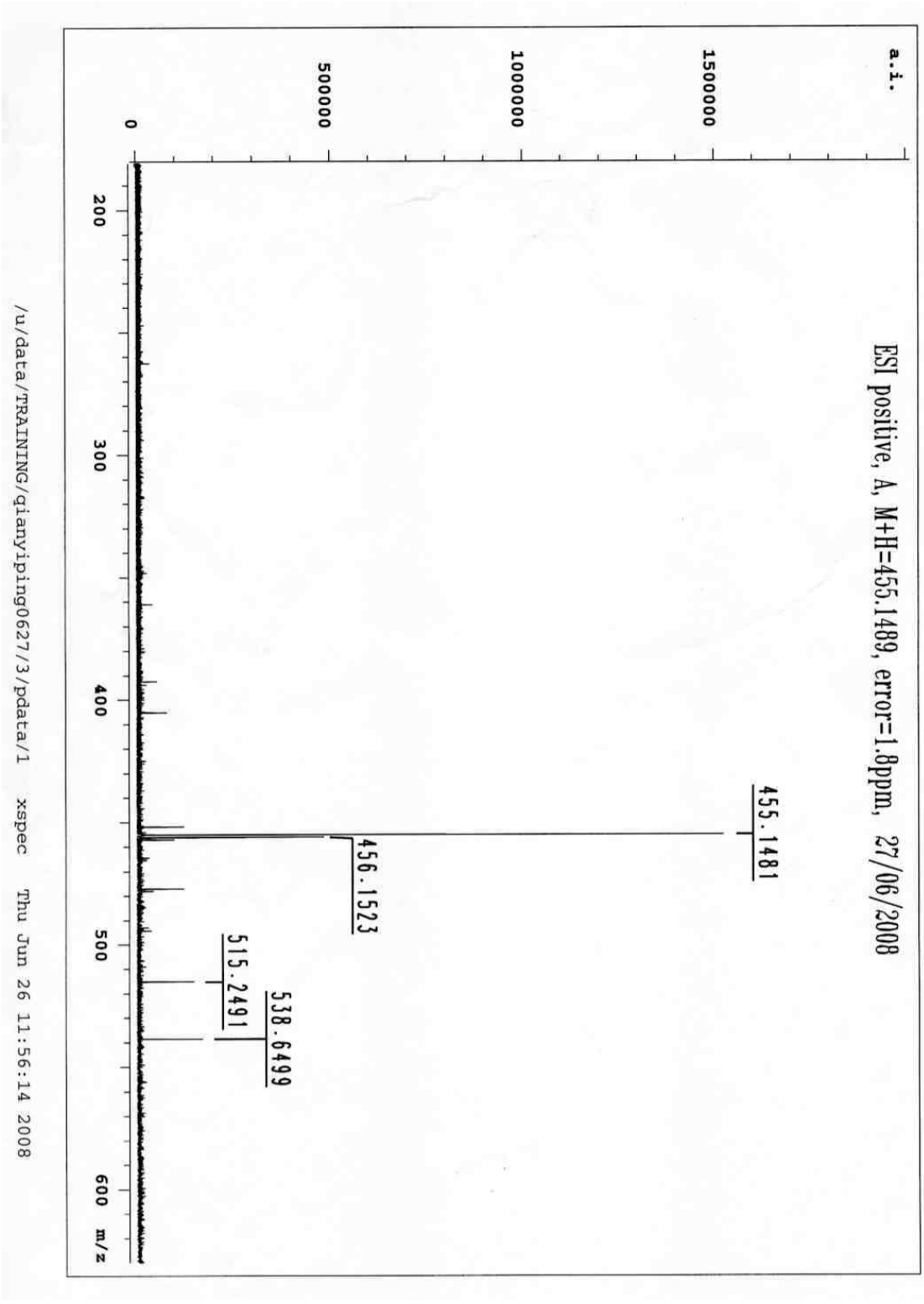
^{1}H, ^{13}C HMBC spectrum of resveratrol dimer



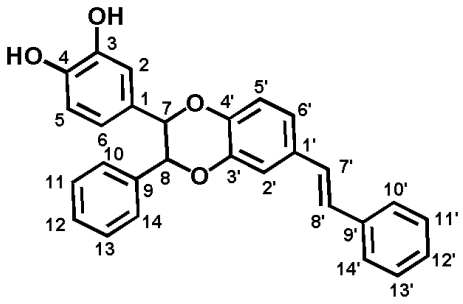
^{1}H, ^{13}C HMQC spectrum of resveratrol dimer



HRMS (ESI) spectrum of resveratrol dimer

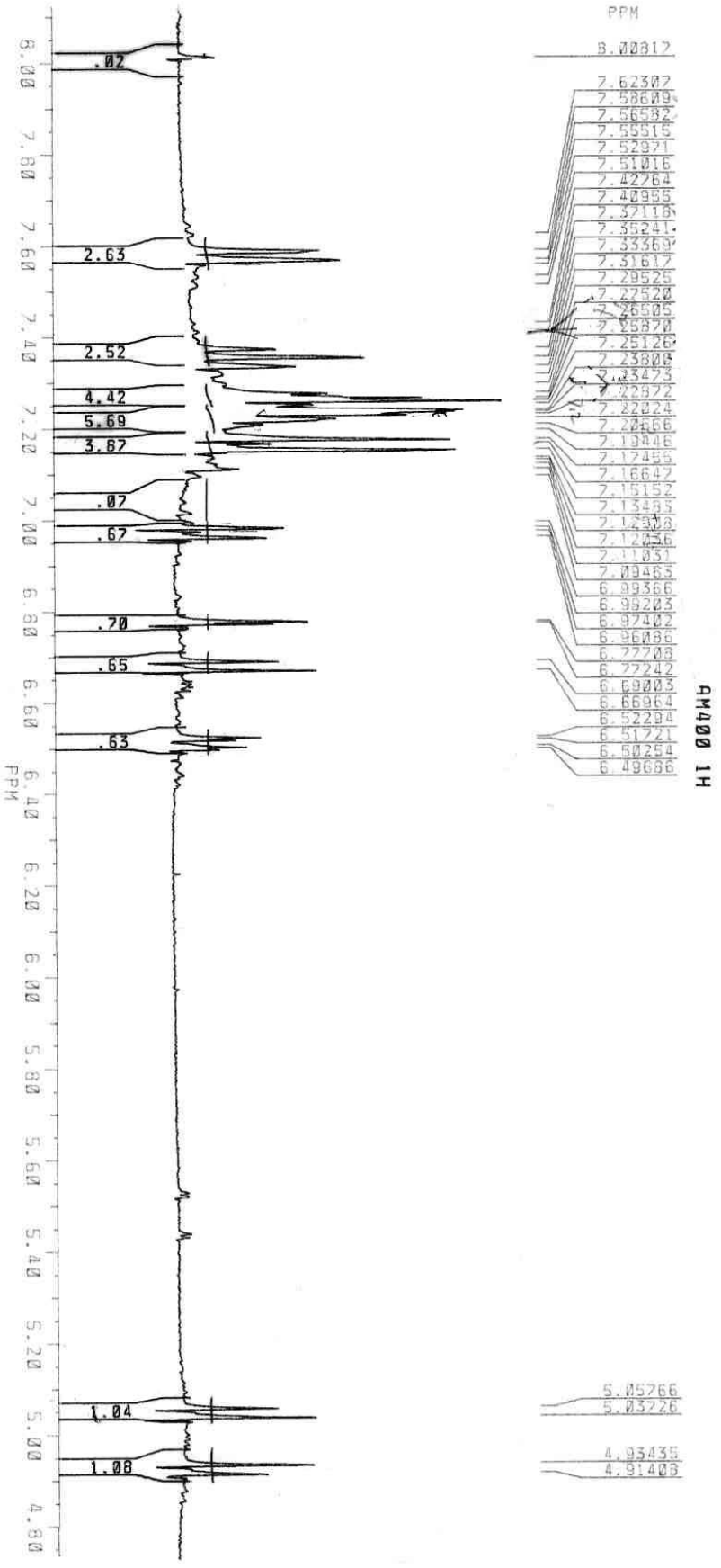


NMR data for 3,4-DHS dimer

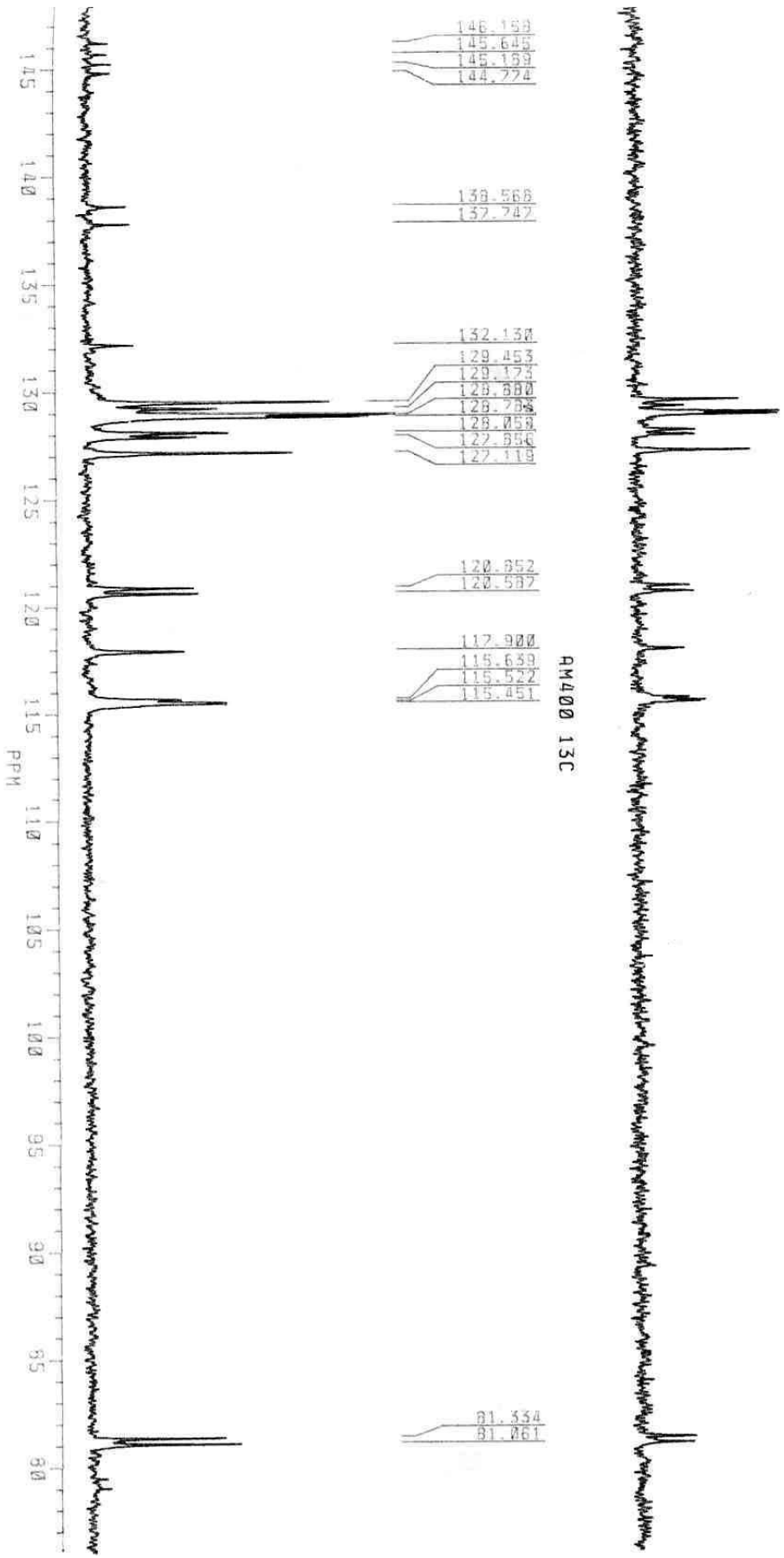


H	δ_H (mult., *J* Hz)	C	δ_C
		C-1	128.1
H-2	6.77 (d, 2.0)	C-2	115.4
		C-3	145.6
		C-4	146.2
H-5	6.68 (d, 8.0)	C-5	117.9
H-6	6.51 (d, 8.0)	C-6	120.6
H-7	4.92 (d, 8.0)	C-7	81.1
H-8	5.05 (d, 8.0)	C-8	81.3
		C-9	137.7
H-10, 14	7.26 (m)	C-10, 14	128.8
H-11, 13	7.23 (m)	C-11, 13	128.9
H-12	7.25 (m)	C-12	129.2
		C-1’	132.1
H-2’	7.27 (d, 2.4)	C-2’	115.6
		C-3’	145.2
		C-4’	144.8
H-5’	6.97 (d, 8.0)	C-5’	115.5
H-6’	7.17 (d, 8.0)	C-6’	120.9
H-7’	7.19 (d, 16.0)	C-7’	127.9
H-8’	7.13 (d, 16.0)	C-8’	128.1
		C-9’	138.6
H-10’, 14’	7.57 (d, 7.8)	C-10’, 14’	127.1
H-11’, 13’	7.35 (d, 7.8)	C-11’, 13’	129.5
H-12’	7.24 (d, 7.8)	C-12’	129.4

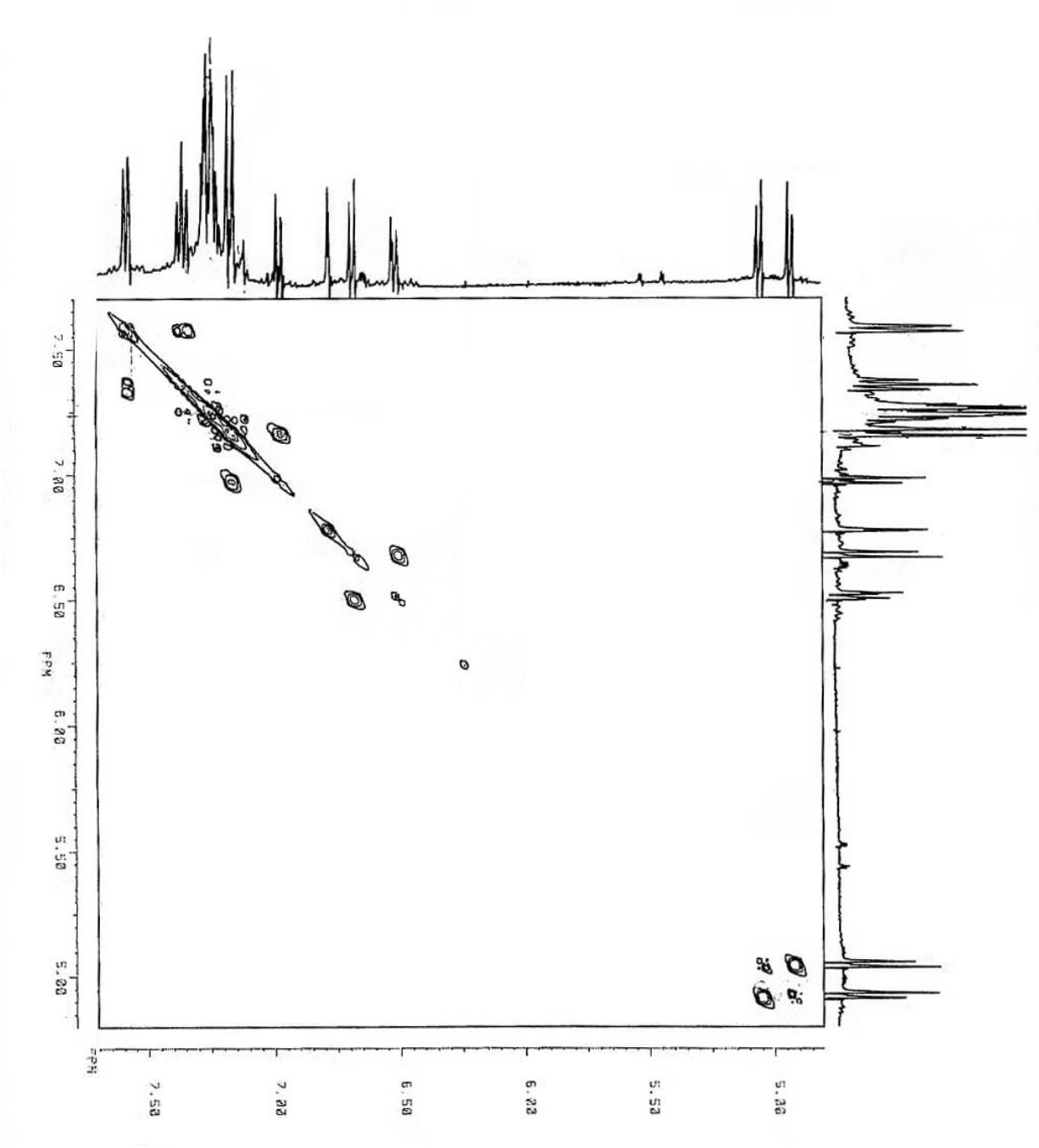
^{1}H-NMR spectrum of 3,4-DHS dimer



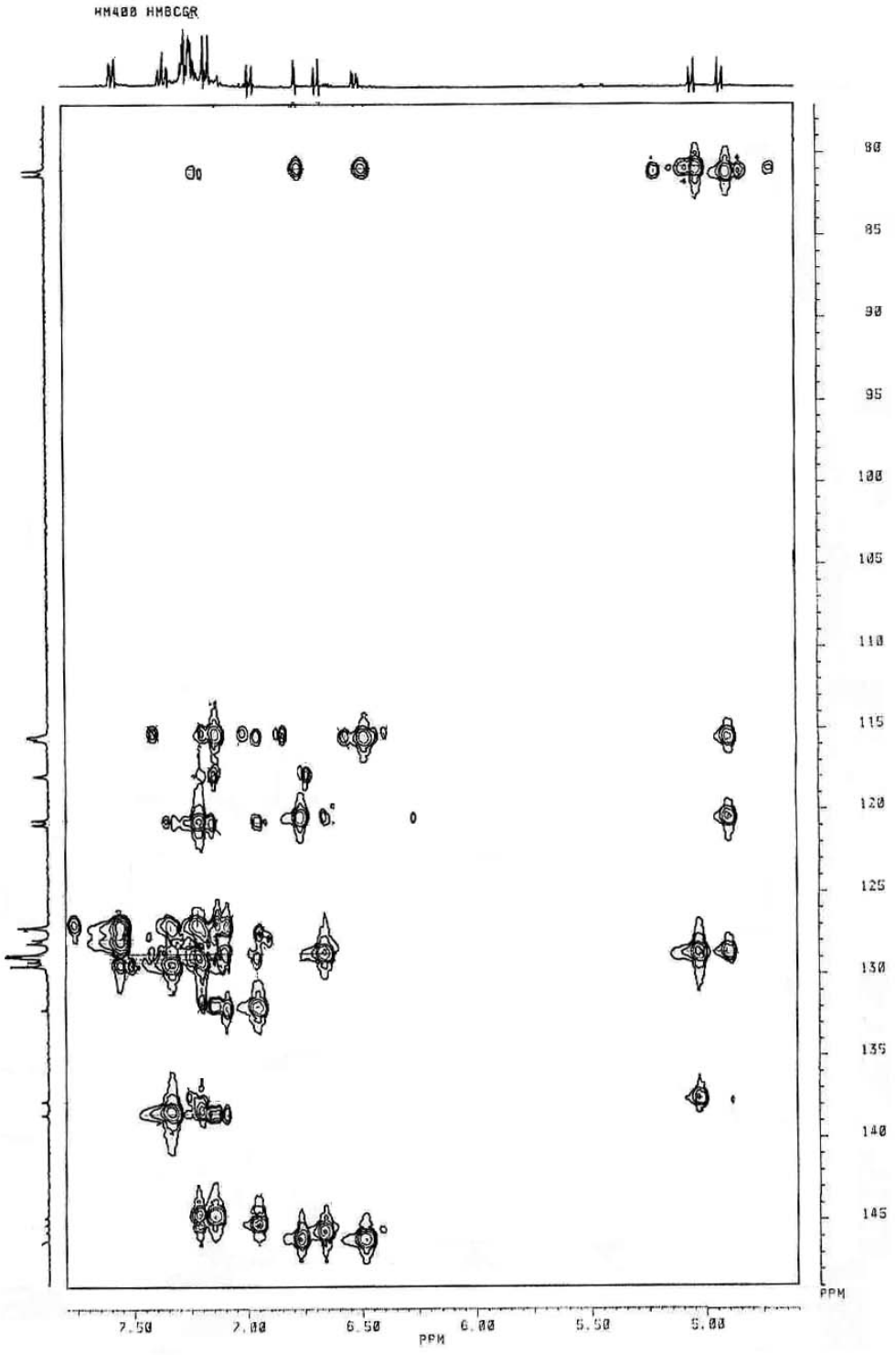
^{13}C-NMR spectrum of 3,4-DHS dimer



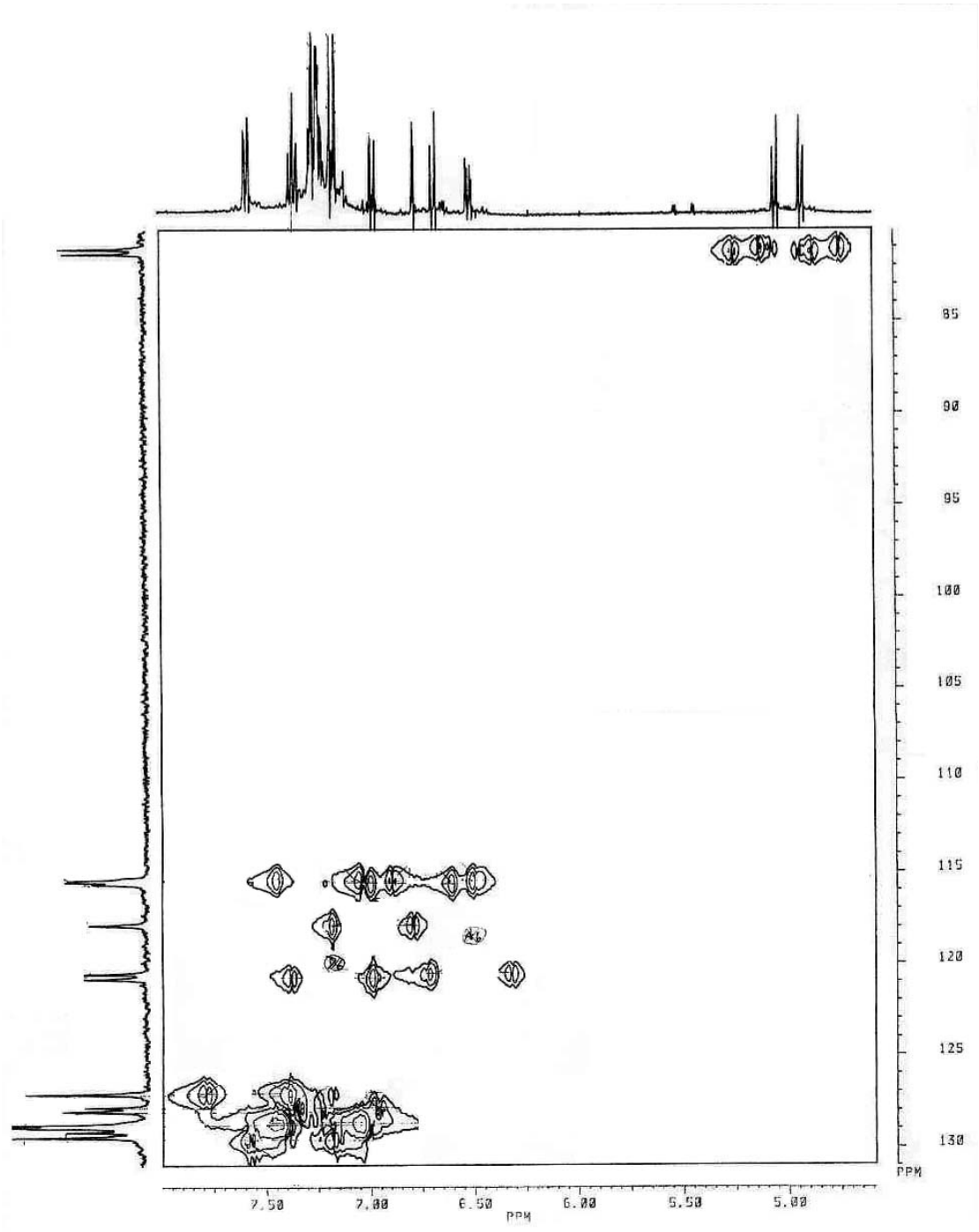
^{1}H, ^{1}H COSY spectrum of 3,4-DHS dimer



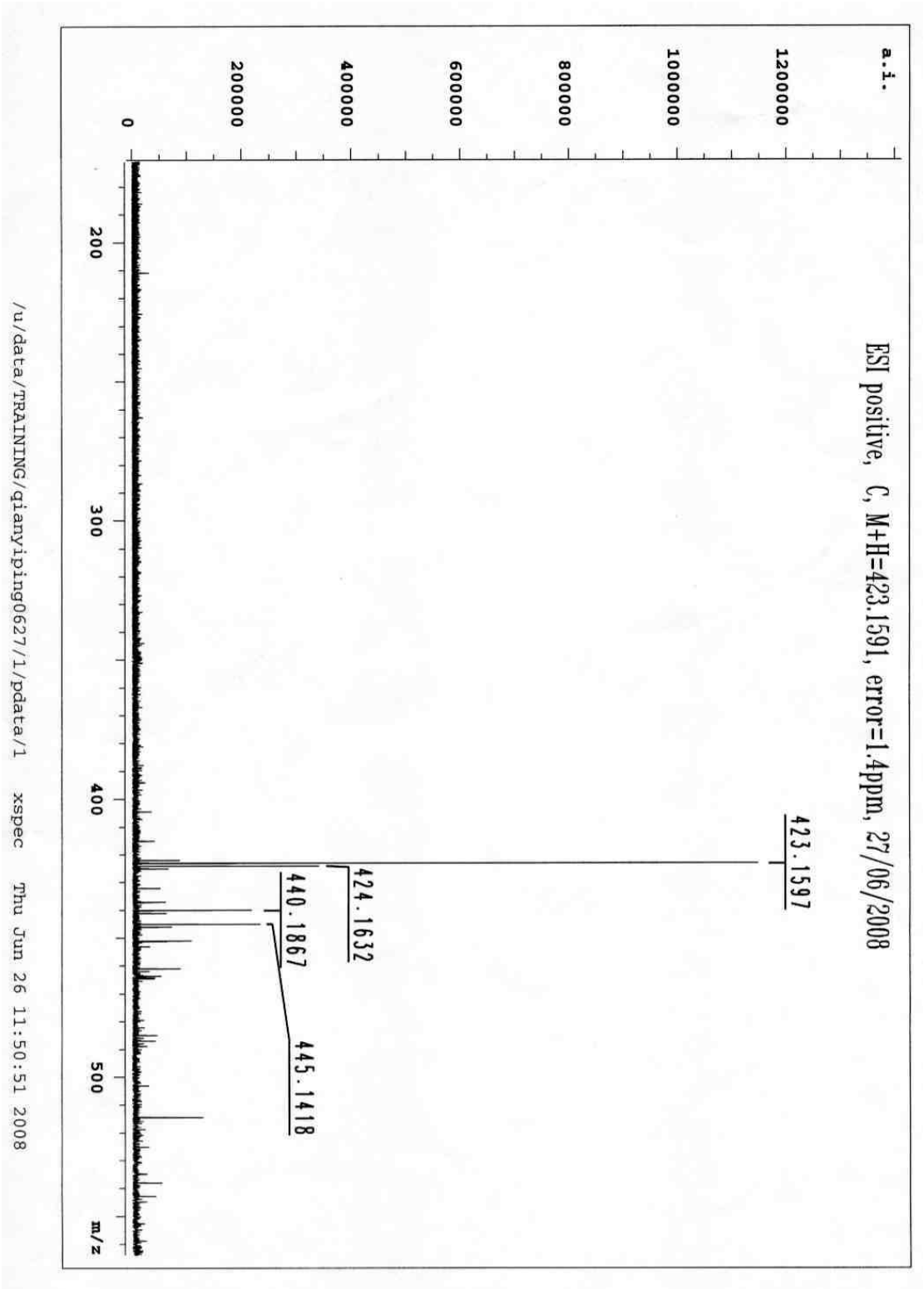
^{1}H, ^{13}C HMBC spectrum of 3,4-DHS dimer



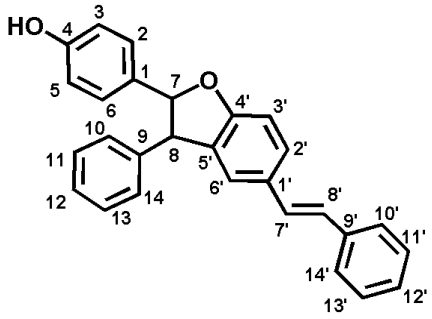
^{1}H, ^{13}C HMQC spectrum of 3,4-DHS dimer



HRMS (ESI) spectrum of 3,4-DHS dimer

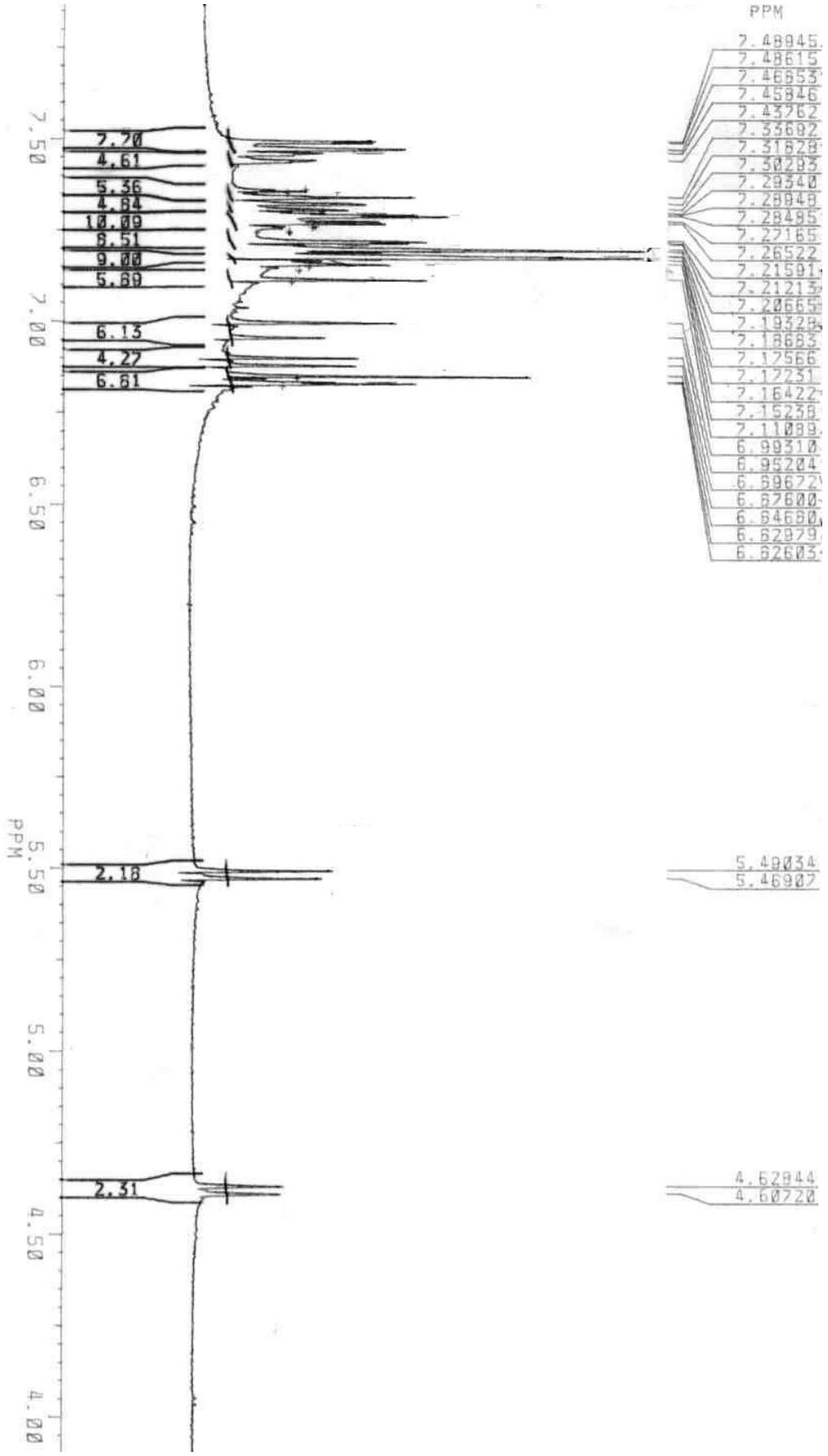


NMR data for 4-HS dimer

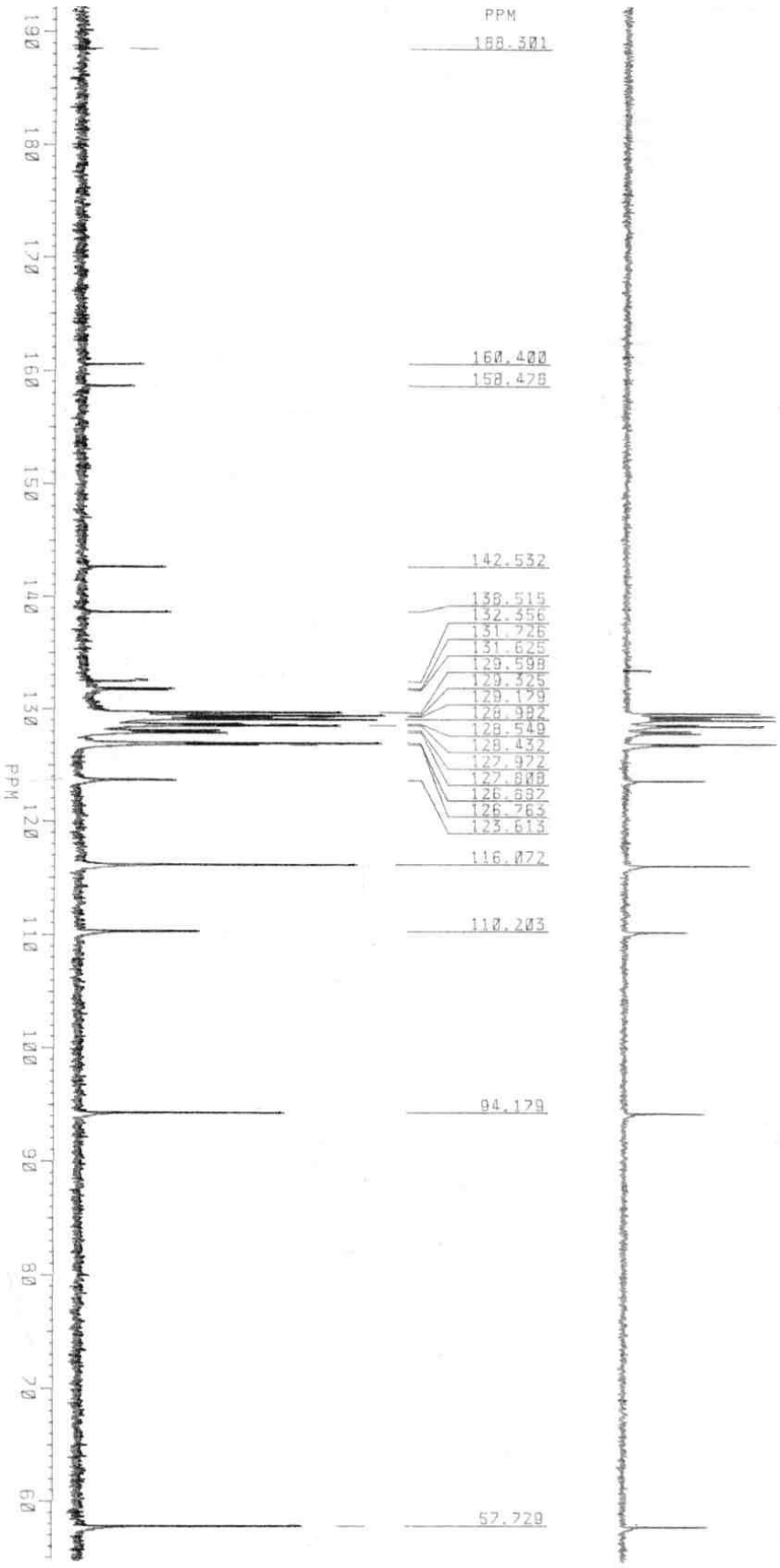


H	δ_H (mult., *J* Hz)	C	δ_C
		C-1	132.4
H-2, 6	7.19 (d, 8.0)	C-2, 6	128.4
H-3, 5	6.83 (d, 8.0)	C-3, 5	116.1
		C-4	158.5
H-7	5.49 (d, 8.5)	C-7	94.2
H-8	4.63 (d, 8.5)	C-8	57.9
		C-9	142.5
H-10, 14	7.19 (d, 8.3)	C-10, 14	129.0
H-11	7.34 (t, d, 8.0, 1.5)	C-11, 13	129.6
H-12	7.21 (t, d, 8.0, 1.5)	C-12	129.2
H-13	7.21 (t, 8.0)		
		C-1’	131.7
H-2’	7.46 (d, 8.4)	C-2’	128.5
H-3’	6.88 (d, 8.4)	C-3’	110.2
		C-4’	160.4
		C-5’	131.6
H-6’	7.16 (d, 2.0)	C-6’	123.6
H-7’	7.13 (d, 16.4)	C-7’	127.6
H-8’	6.98 (d, 16.4)	C-8’	126.8
		C-9’	138.5
H-10’, 14’	7.49 (t, d, 8.0, 2.0)	C-10’, 14’	126.9
H-11’, 13’	7.29 (t, d, 8.0, 2.0)	C-11’, 13’	129.3
H-12’	7.14 (t, d, 8.0, 2.0)	C-12’	128.0

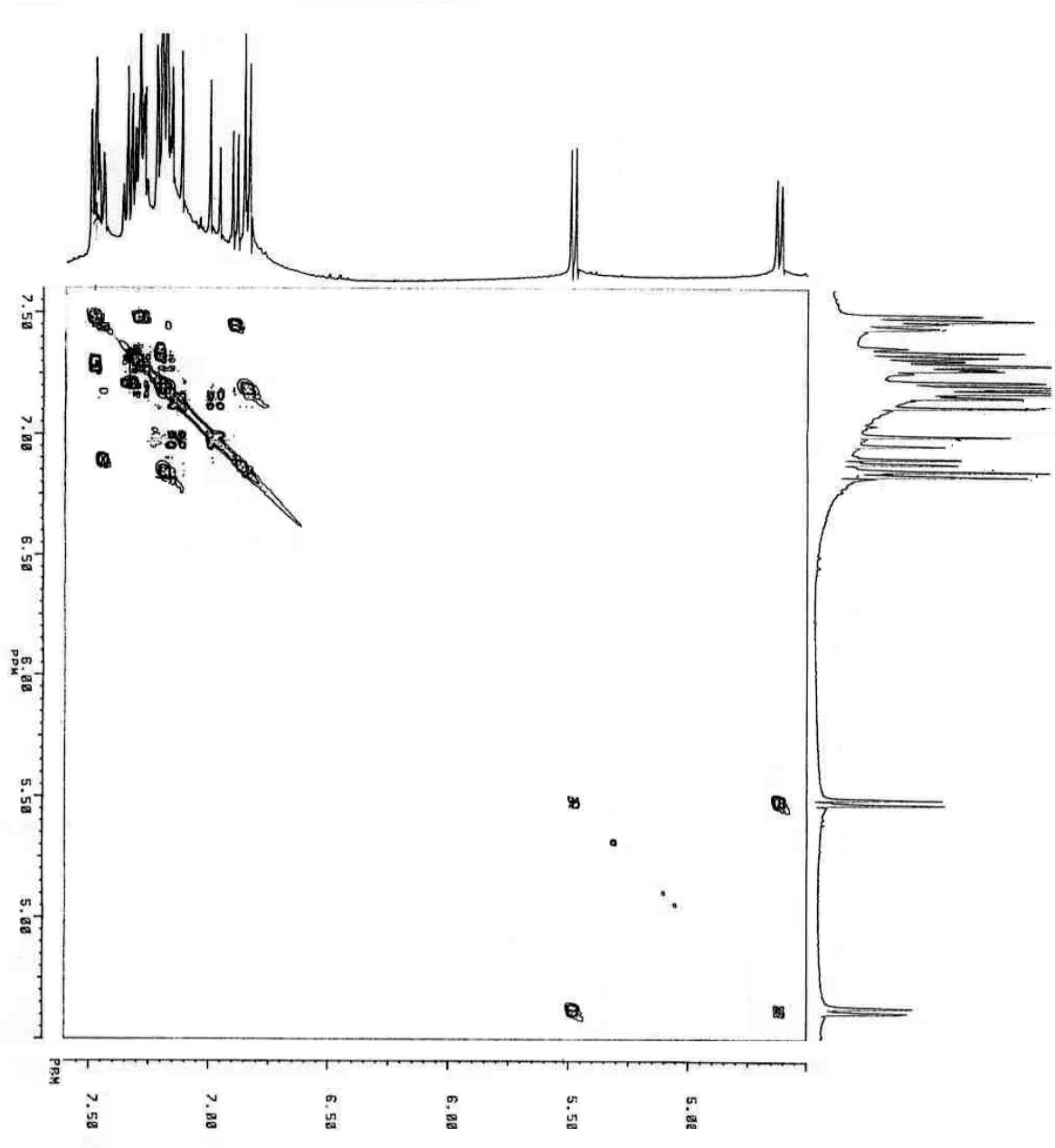
^{1}H-NMR spectrum of 4-HS dimer



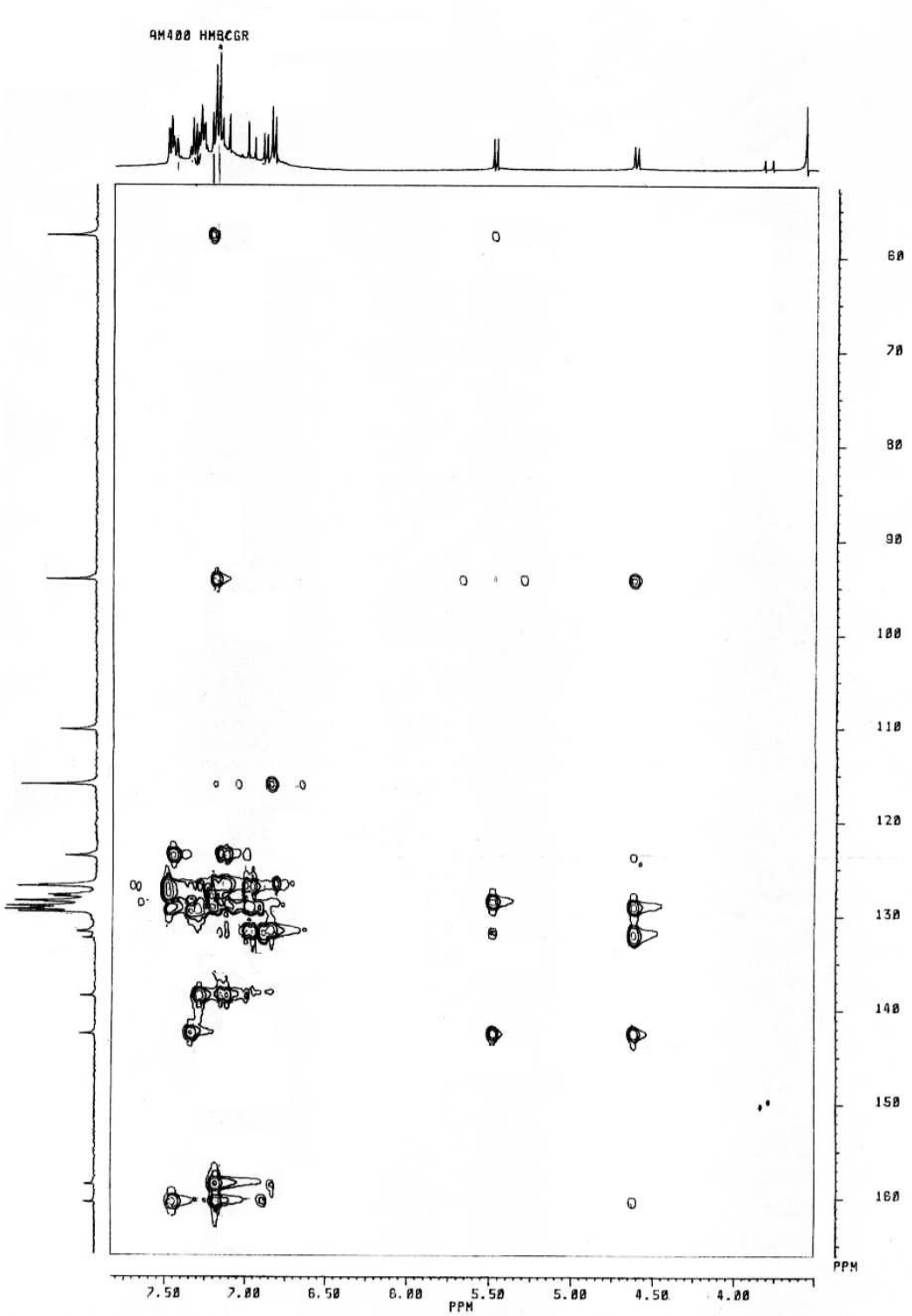
^{13}C-NMR spectrum of 4-HS dimer



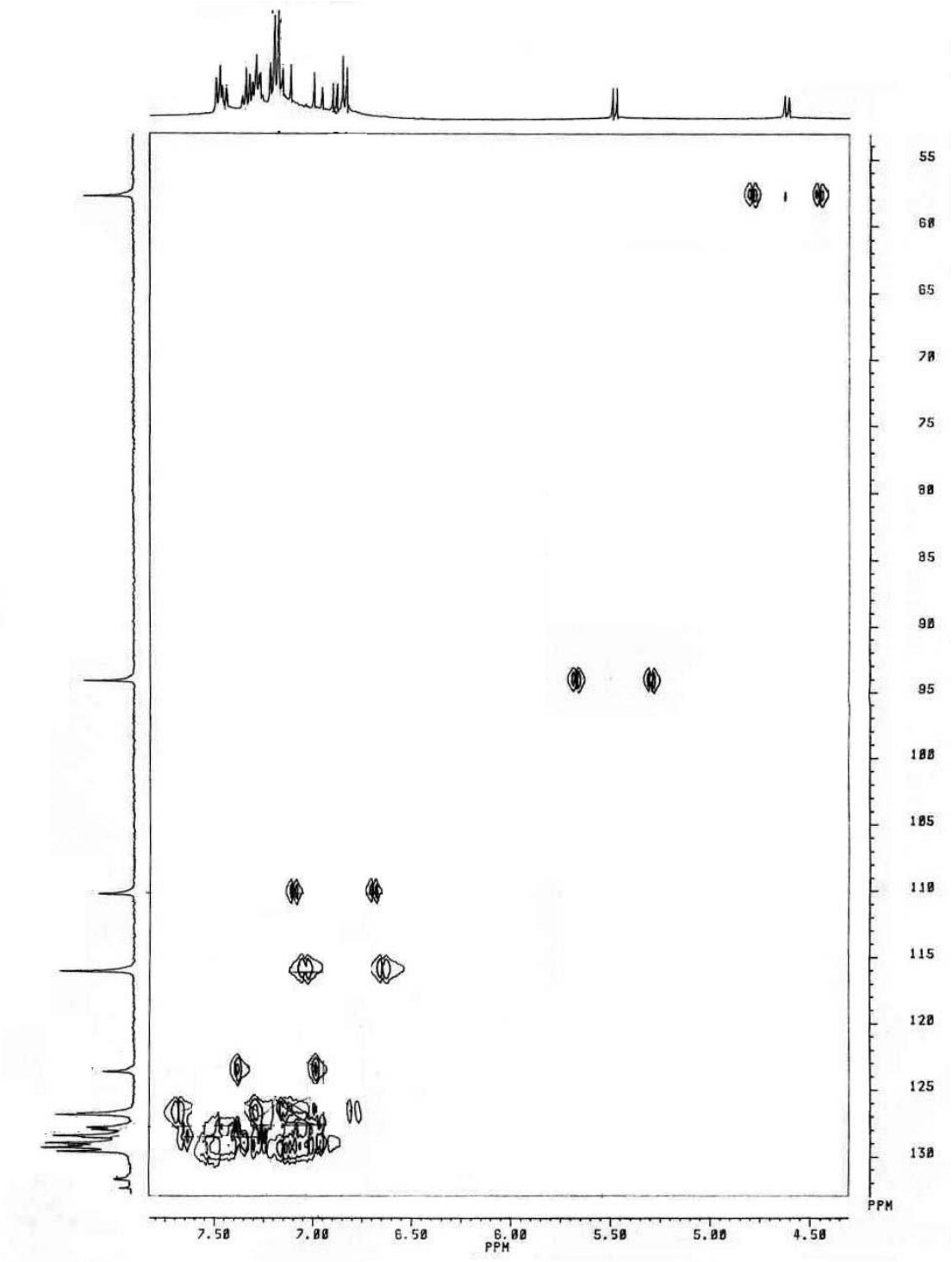
^{1}H, ^{1}H COSY spectrum of 4-HS dimer



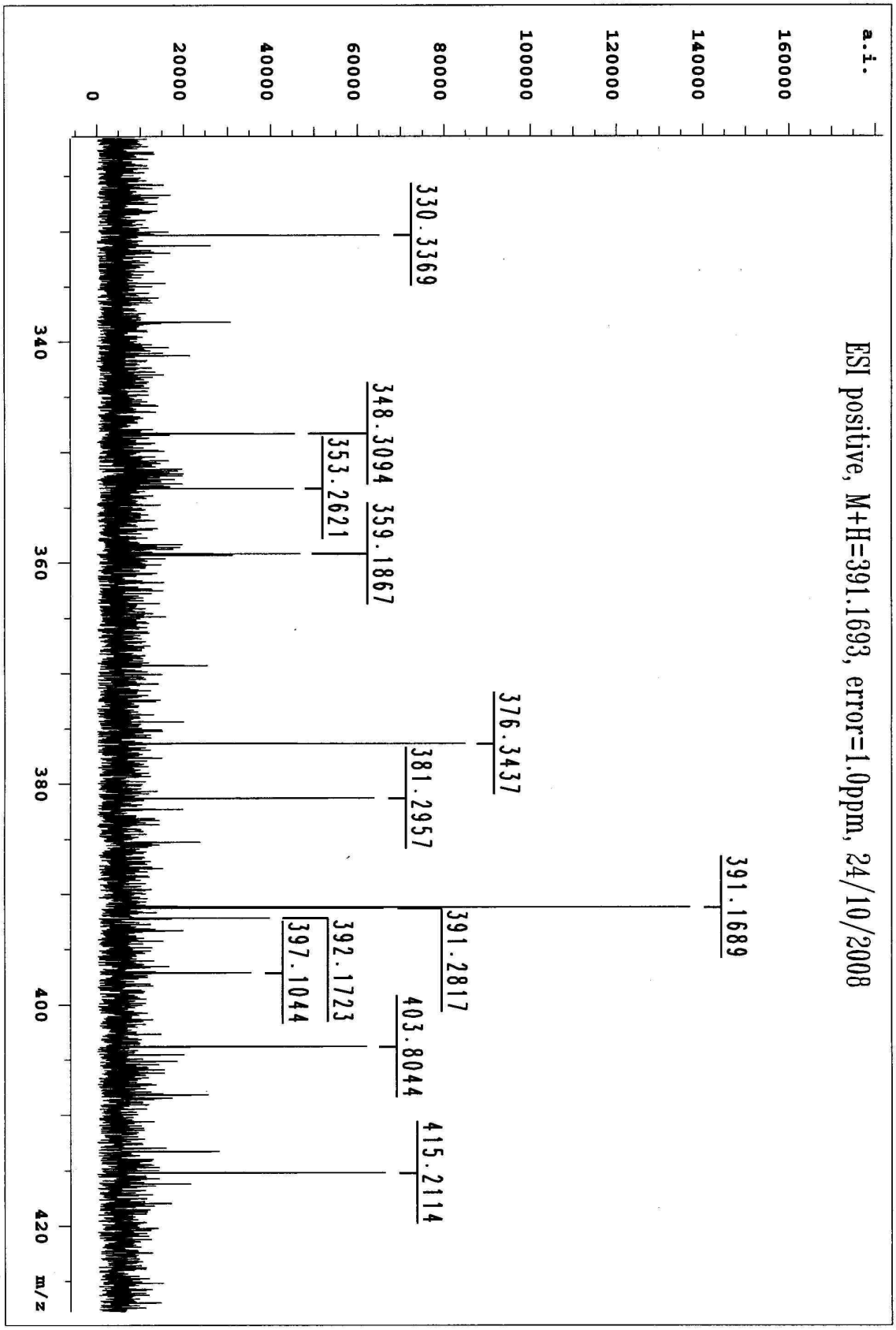
^{1}H, ^{13}C HMBC spectrum of 4-HS dimer



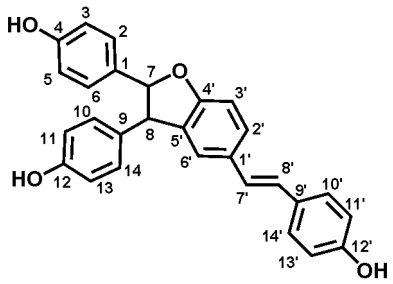
^{1}H, ^{13}C HMQC spectrum of 4-HS dimer



HRMS (ESI) spectrum of 4-HS dimer

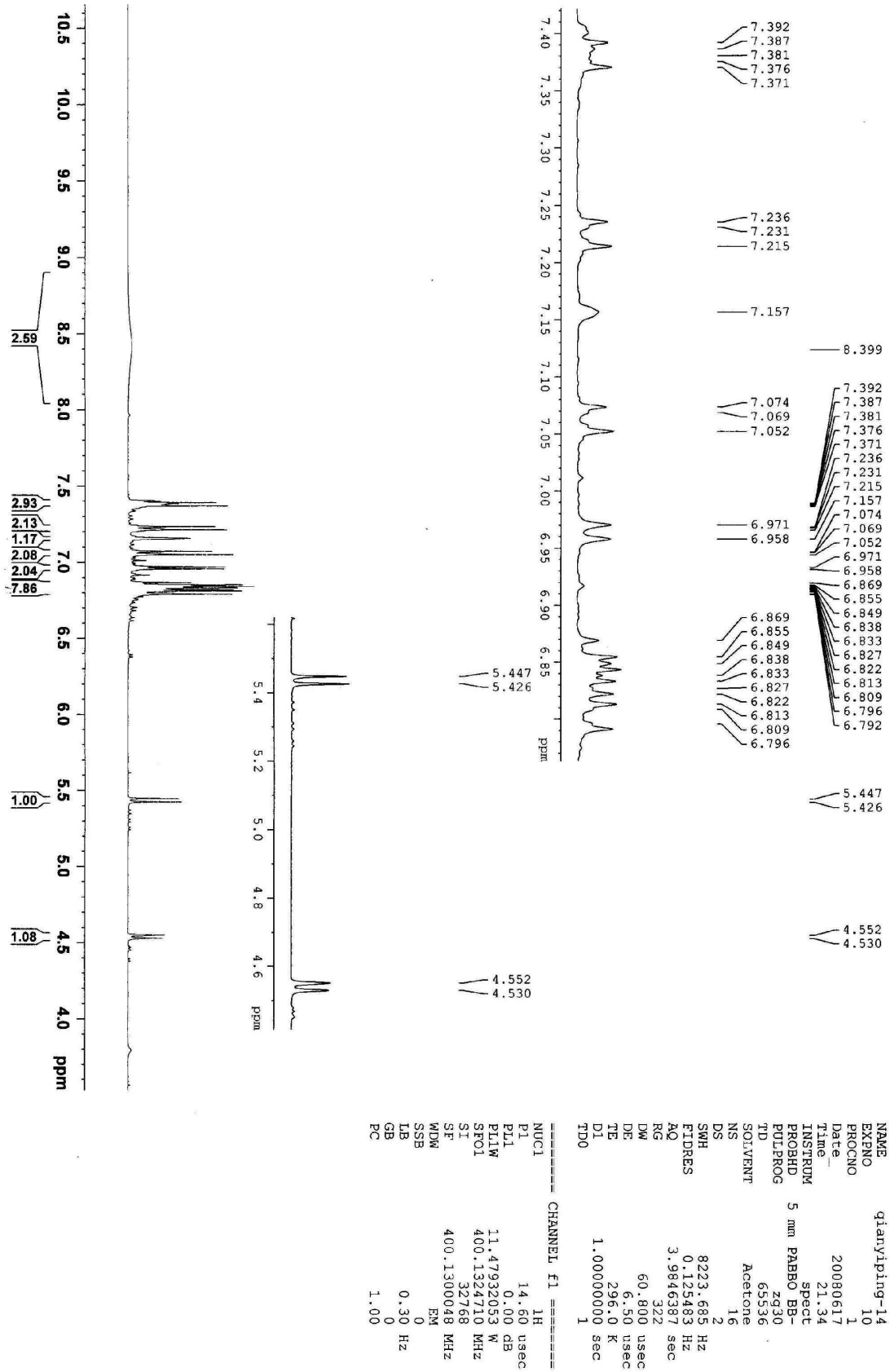


NMR data for 4,4'-DHS dimer

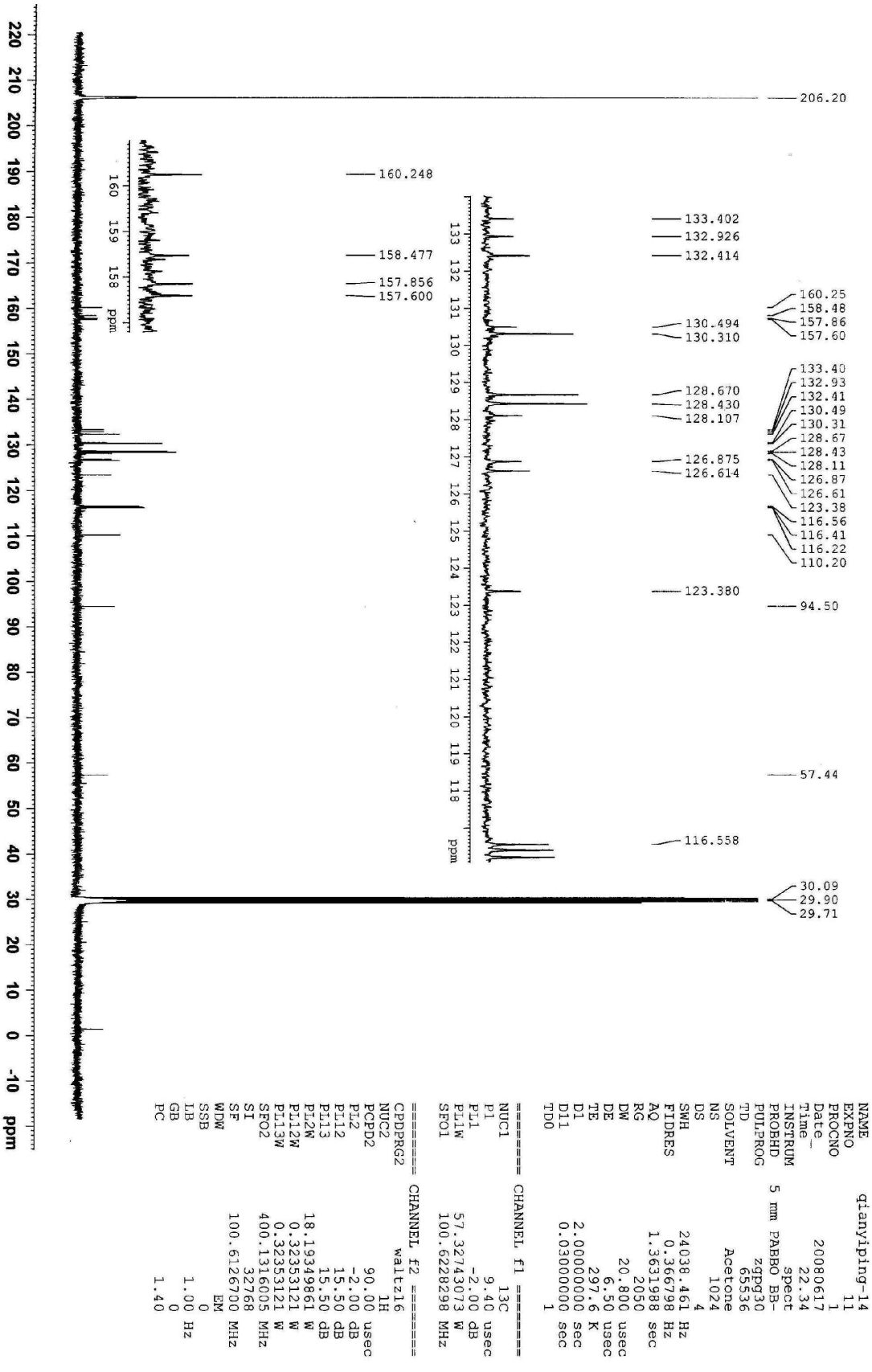


H	δ_H (mult., J Hz)	C	δ_C
		C-1	130.5
H-2, 6	7.24 (d, 8.4)	C-2, 6	128.4
H-3, 5	6.85 (d, 8.4)	C-3, 5	116.6
		C-4	157.9
H-7	5.43 (d, 8.8)	C-7	94.5
H-8	4.53 (d, 8.8)	C-8	57.5
		C-9	132.9
H-10, 14	7.05 (d, 8.8)	C-10, 14	130.3
H-11, 13	6.83 (d, 8.8)	C-11, 13	116.4
		C-12	157.6
		C-1’	132.4
H-2’	7.37 (d, 8.4)	C-2’	126.9
H-3’	6.87 (d, 8.4)	C-3’	110.2
		C-4’	158.5
		C-5’	133.4
H-6’	7.16 (bs)	C-6’	123.4
H-7’	6.97 (d, 18.4)	C-7’	126.6
H-8’	6.96 (d, 18.4)	C-8’	126.6
		C-9’	128.7
H-10’, 14’	7.39 (d, 8.4)	C-10’, 14’	128.1
H-11’, 13’	6.80 (d, 8.4)	C-11’, 13’	116.2
		C-12’	160.3

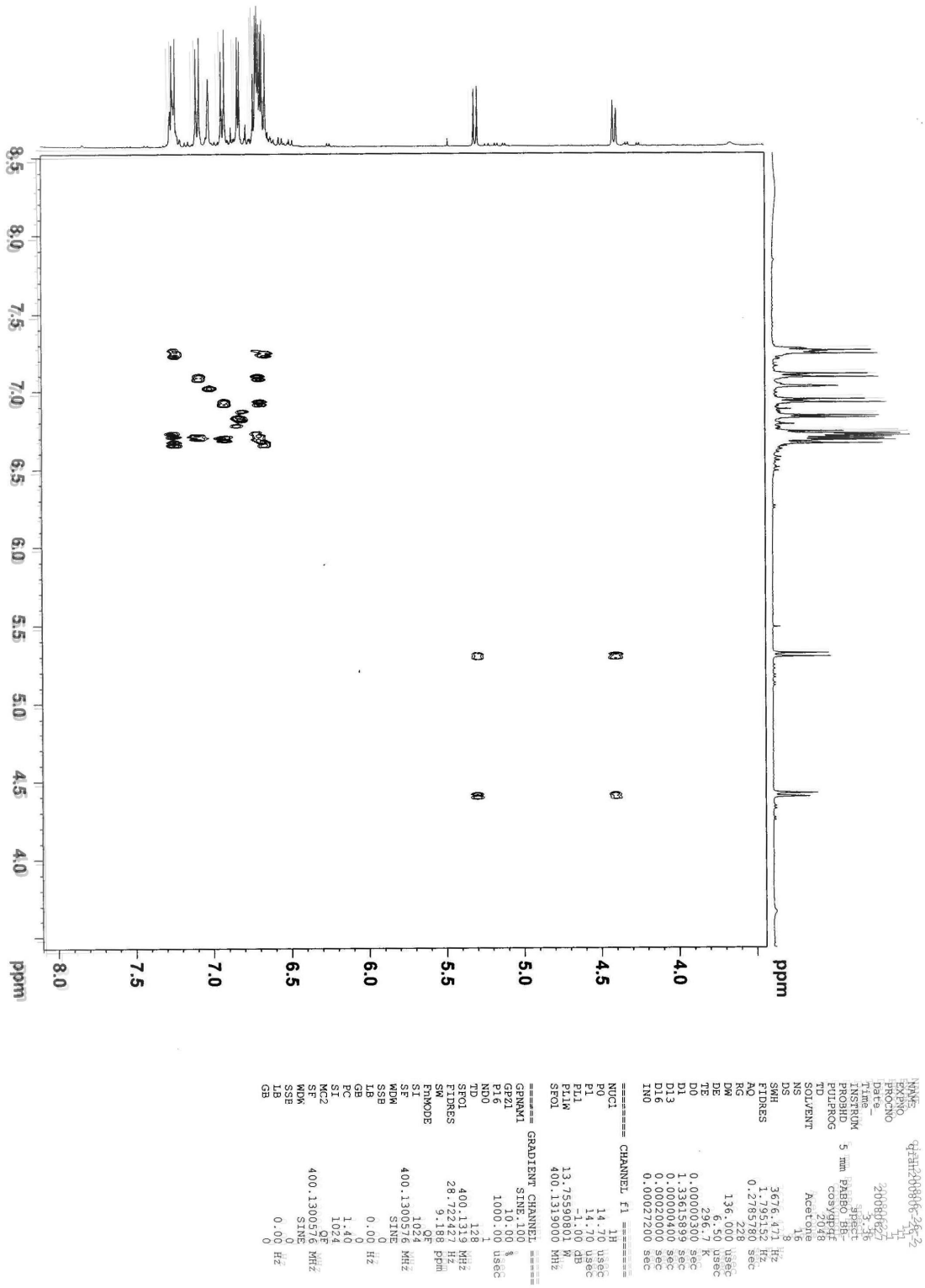
^{1}H-NMR spectrum of 4,4’-DHS dimer



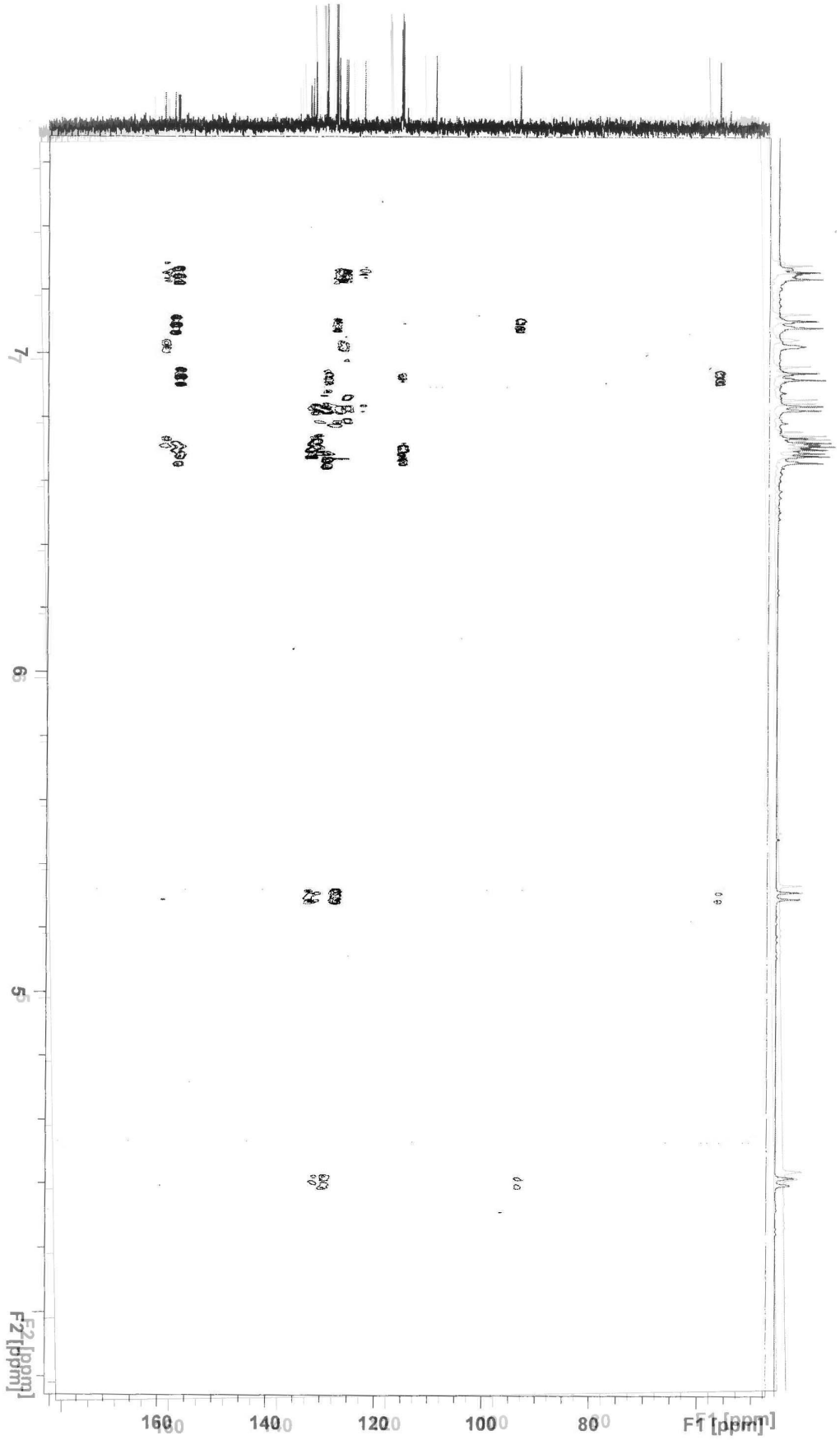
^{13}C-NMR spectrum of 4,4'-DHS dimer



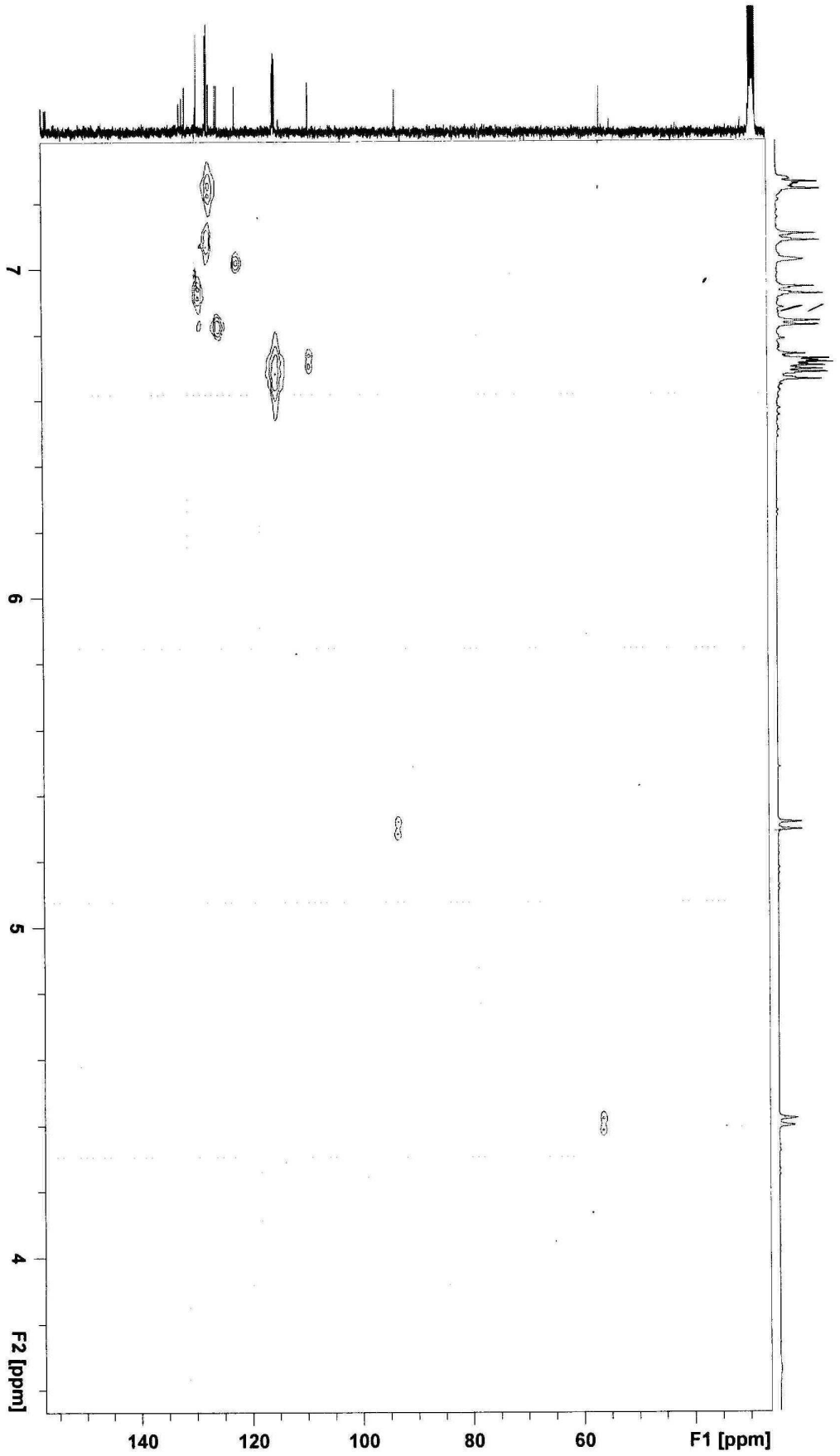
^{1}H, ^{1}H COSY spectrum of 4,4'-DHS dimer



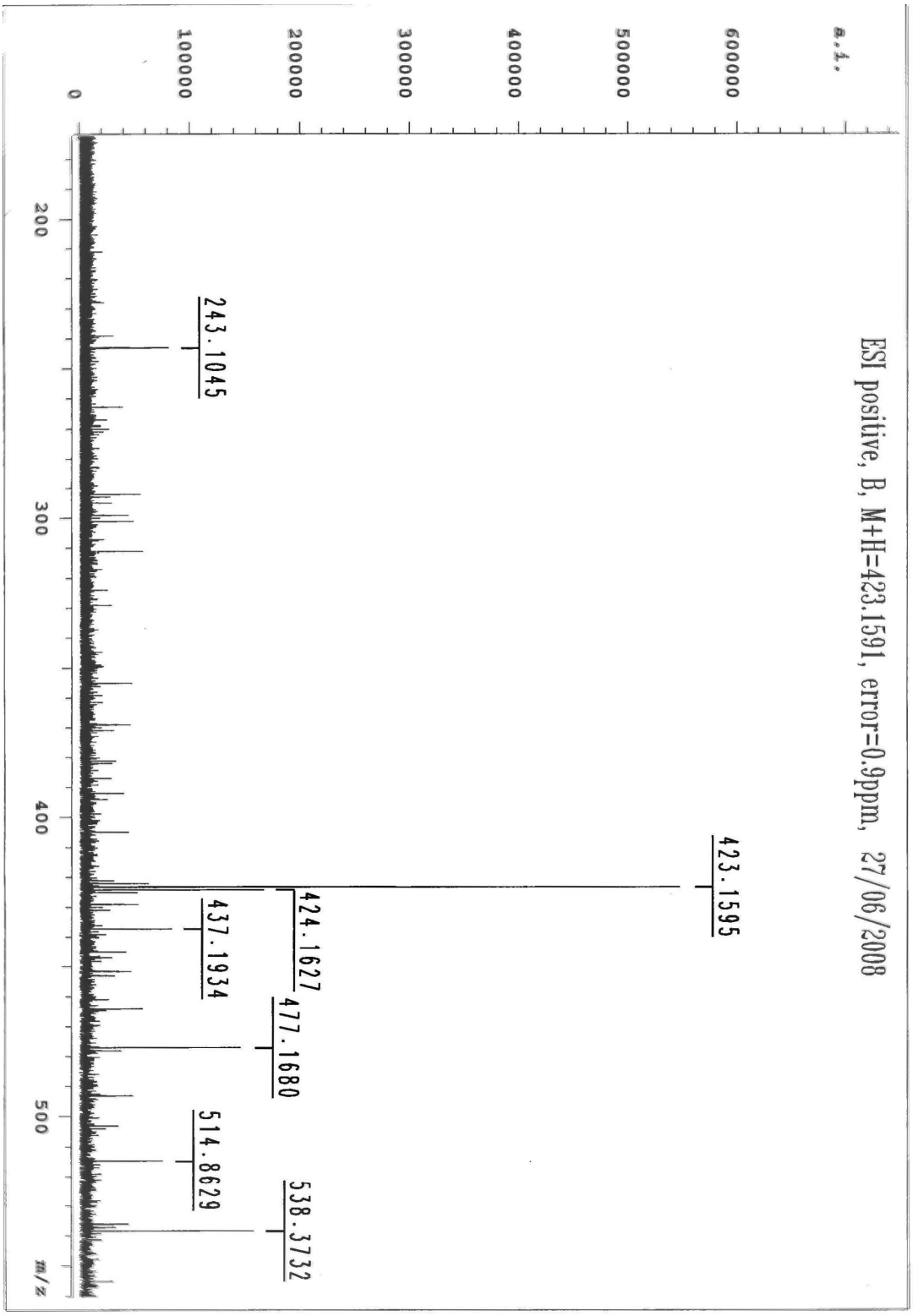
^{1}H, ^{13}C HMBC spectrum of 4,4'-DHS dimer



^{1}H, ^{13}C HMQC spectrum of 4,4'-DHS dimer



HRMS (ESI) spectrum of 4,4'-DHS dimer



4 HPLC analysis on a chiral OD column

Compound 4,4'-DHS dimer HPLC analysis on a chiral OD column (retention time for the two enantiomers, 17.379 and 21.119 min; eluent *n*-hexane:isopropanol, V:V= 80:20).