Supporting Information for

Silver-catalyzed intramolecular hydroamination of alkynes in aqueous media: efficient and regioselective synthesis for fused benzimidazoles

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Contents

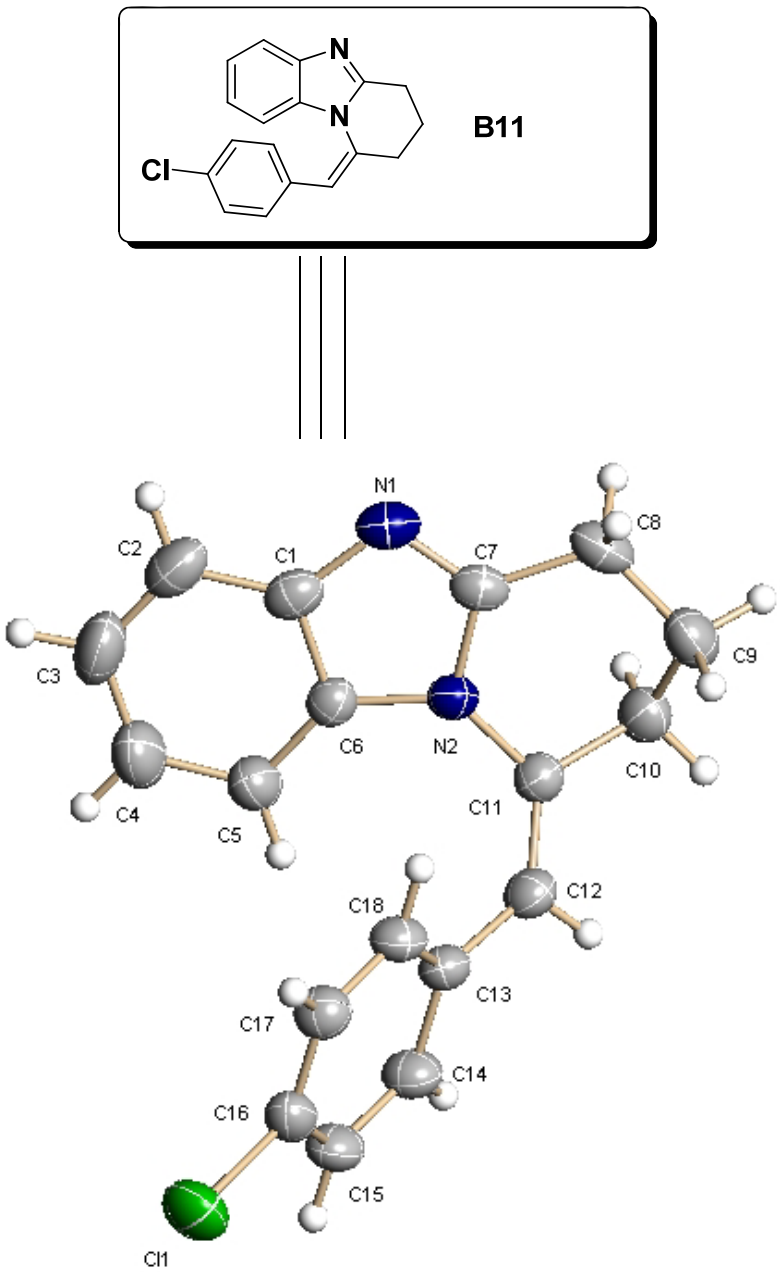


Figure S1. X-ray crystallographic structure of **B11**

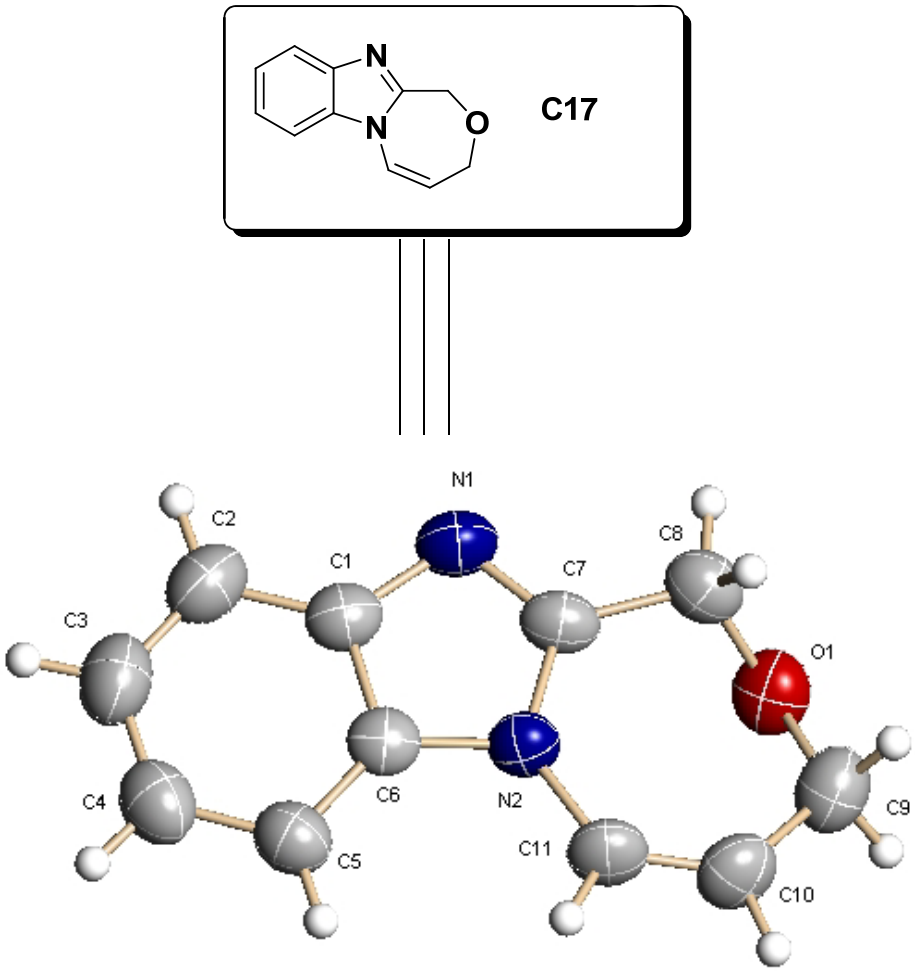


Figure S2. X-ray crystallographic structure of **C17**

The Details of X-ray Crystallographic Structure of B11

Bond precision: C-C = 0.0022 A Wavelength=0.71073

Cell: a=7.0977(9) b=9.8929(12) c=10.5583(13)

alpha=81.903(2) beta=84.345(2) gamma=84.315(2)

Temperature: 293 K

	Calculated	Reported
Volume	727.67(16)	727.67(16)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C18 H15 Cl N2	?
Sum formula	C18 H15 Cl N2	C18 H15 Cl N2
Mr	294.77	294.77
Dx,g cm-3	1.345	1.345
Z	2	2
Mu (mm-1)	0.257	0.257
F000	308.0	308.0
F000'	308.39	
h,k,lmax	8,12,13	8,12,13
Nref	2854	2802
Tmin,Tmax	0.923,0.949	0.800,1.000
Tmin'	0.923	

Correction method= EMPIRICAL

Data completeness= 0.982 Theta(max)= 26.000

R(reflections)= 0.0450(2315) wR2(reflections)= 0.1316(2802)

S = 1.075 Npar= 190

CCDC 781700 contains the supplementary crystallographic data for this paper. These data can be also obtained free of charge from The Cambridge Crystallographic Data Centre via

www.ccdc.cam.ac.uk/data_request/cif.

The Details of X-ray Crystallographic Structure of C17

Bond precision: C-C = 0.0041 A Wavelength=0.71073

Cell: a=8.3263(15) b=5.9839(11) c=9.1599(16)

alpha=90 beta=94.155(3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	455.18(14)	455.18(14)
Space group	P 21	P2(1)
Hall group	P 2yb	?
Moiety formula	C11 H10 N2 O	?
Sum formula	C11 H10 N2 O	C11 H10 N2 O
Mr	186.21	186.21
Dx,g cm-3	1.359	1.359
Z	2	2
Mu (mm-1)	0.090	0.090
F000	196.0	196.0
F000'	196.08	
h,k,lmax	10,7,11	10,7,11
Nref	1090[1985]	1080
Tmin,Tmax	0.964,0.987	0.822,1.000
Tmin'	0.964	

Correction method= EMPIRICAL

Data completeness= 0.99/0.54 Theta(max)= 27.000

R(reflections)= 0.0421(844) wR2(reflections)= 0.0942(1080)

S = 0.925 Npar= 127

CCDC 781699 contains the supplementary crystallographic data for this paper. These data can be also obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

General Information

Commercially available reagents and solvents were used without further purification. Column chromatography was carried out on silica gel. ^{1}H and ^{13}C NMR spectra were obtained on Varian Mercury-300 and/or Varian Mercury-400 spectrometers (TMS as IS). Chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), quartet (q), multipet (m) and broad (br). Low- and high-resolution mass spectra (LRMS and HRMS) were measured on Finnigan MAT 95 spectrometer.

General Procedure for Synthesis of B1-B27 (C27)

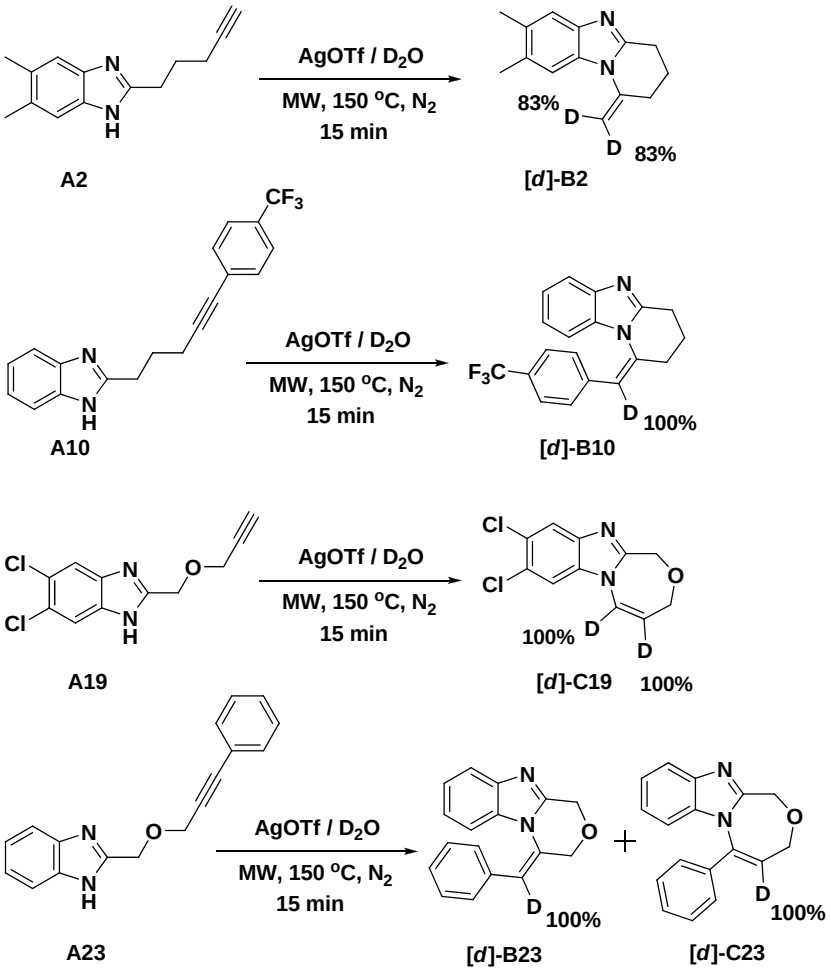
Classical method using a thermostate oil bath (Method A)

A mixture of **A** (0.40 mmol), AgOTf (0.02 mmol) was stirred in water (3-5 mL) under N_2. The vial was sealed and the mixture was then stirred at 80 °C with oil heating for 8-60 h. After the reaction was cooled to ambient temperature, the crude reaction mixture was extracted three times with EA (15 mL × 3). The combined organic phase was wash with saturated $NaHCO_3$ solution, brine, dried with Na_2SO_4 and concentrated. The residue was purified by column chromatography on combiflash to provide the desired product **B**.

Microwave method (Method B)

A mixture of **A** (0.40 mmol), AgOTf (0.02 mmol) was stirred in water (3-5 mL) under N_2. The vial was sealed and the mixture was then irradiated for 15 min at 150 °C. After the reaction was cooled to ambient temperature, the crude reaction mixture was extracted three times with EA (15 mL × 3). The combined organic phase was wash with saturated $NaHCO_3$ solution, brine, dried with Na_2SO_4 and concentrated. The residue was purified by column chromatography on combiflash to provide the desired product **B(C)**.

Labeling studies with deuterated solvents.



A mixture of substituted benzimidazoles **A2**, **A10**, **A19**, or **A23** (0.1 mmol), AgOTf (0.005 mmol) was stirred in D_2O (2 mL) under N_2 atmosphere, respectively. The vial was sealed and the mixture was then irradiated for 15 min at 150 °C. After the reaction was cooled to ambient temperature, the crude reaction mixture was extracted three times with EA (15 mL × 3). The combined organic phase was wash with saturated $NaHCO_3$ solution, brine, dried with Na_2SO_4 and concentrated. The residue was purified by column chromatography on combiflash to provide the desired products **[*d*]-B2**, **[*d*]-B10**, **[*d*]-C19**, **[*d*]-B23** and **[*d*]-C23** which were analyzed using ^{1}H NMR spectroscopy to determine the content of the deuterium incorporation.

[*d*]-B2: ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.00-2.08 (m, 2H, CH_2), 2.35 (s, 3H, CH_3), 2.37 (s, 3H, CH_3), 2.61-2.65 (m, 2H, CH_2), 3.11 (t, 2H, CH_2), 7.44-7.45 (m, 2H, ArH);

LC-MS: m/z 215 $[M + H]^+$.

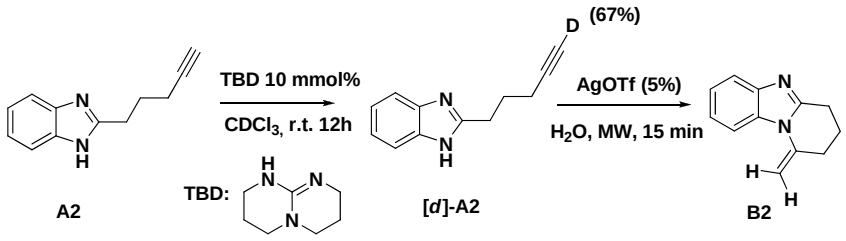
[*d*]-B10: ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.24-2.28 (m, 2H, CH_2), 2.69 (t, 2H, CH_2), 3.31 (t, 2H, CH_2), 6.27-6.30 (d, *J* = 8.4 Hz, 1H, ArH), 6.80-6.86 (m, 1H, ArH), 7.04-7.07 (d, 2H, ArH), 7.11-7.16 (m, 1H, ArH), 7.35-7.38 (d, 2H, ArH), 7.64-7.66 (d, *J* = 7.5 Hz, 1H, ArH); LC-MS: m/z 330 $[M + H]^+$.

[*d*]-C19: ^{1}H NMR (300 MHz, $CDCl_3$): δ 4.61 (s, 2H, CH_2), 4.94 (s, 2H, CH_2), 7.48 (s, 1H, ArH), 7.79 (s, 1H, ArH); LC-MS: m/z 257 $[M + H]^+$.

[*d*]-B23: ^{1}H NMR (300 MHz, $CDCl_3$): δ 4.46 (s, 2H, CH_2), 5.24 (s, 2H, CH_2), 6.22-6.25 (d, *J* = 8.4 Hz, 1H, ArH), 6.81-6.86 (m, 1H, ArH), 7.01-7.16 (m, 2H, ArH), 7.19-7.23 (m, 4H, ArH), 7.67-7.70 (d, *J* = 8.1 Hz, 1H, ArH); LC-MS: m/z 264 $[M + H]^+$.

[*d*]-C23: ^{1}H NMR (300 MHz, $CDCl_3$): δ 4.18 (s, 2H, CH_2), 4.94 (s, 2H, CH_2), 6.50-6.53 (d, *J* = 8.4 Hz, 1H, ArH), 7.01-7.07 (m, 1H, ArH), 7.23-7.28 (m, 1H, ArH), 7.34-7.49 (m, 5H, ArH), 7.80-7.83 (d, *J* = 7.8 Hz, 1H, ArH); LC-MS: m/z 264 $[M + H]^+$.

Labeling studies with deuterated starting materials.



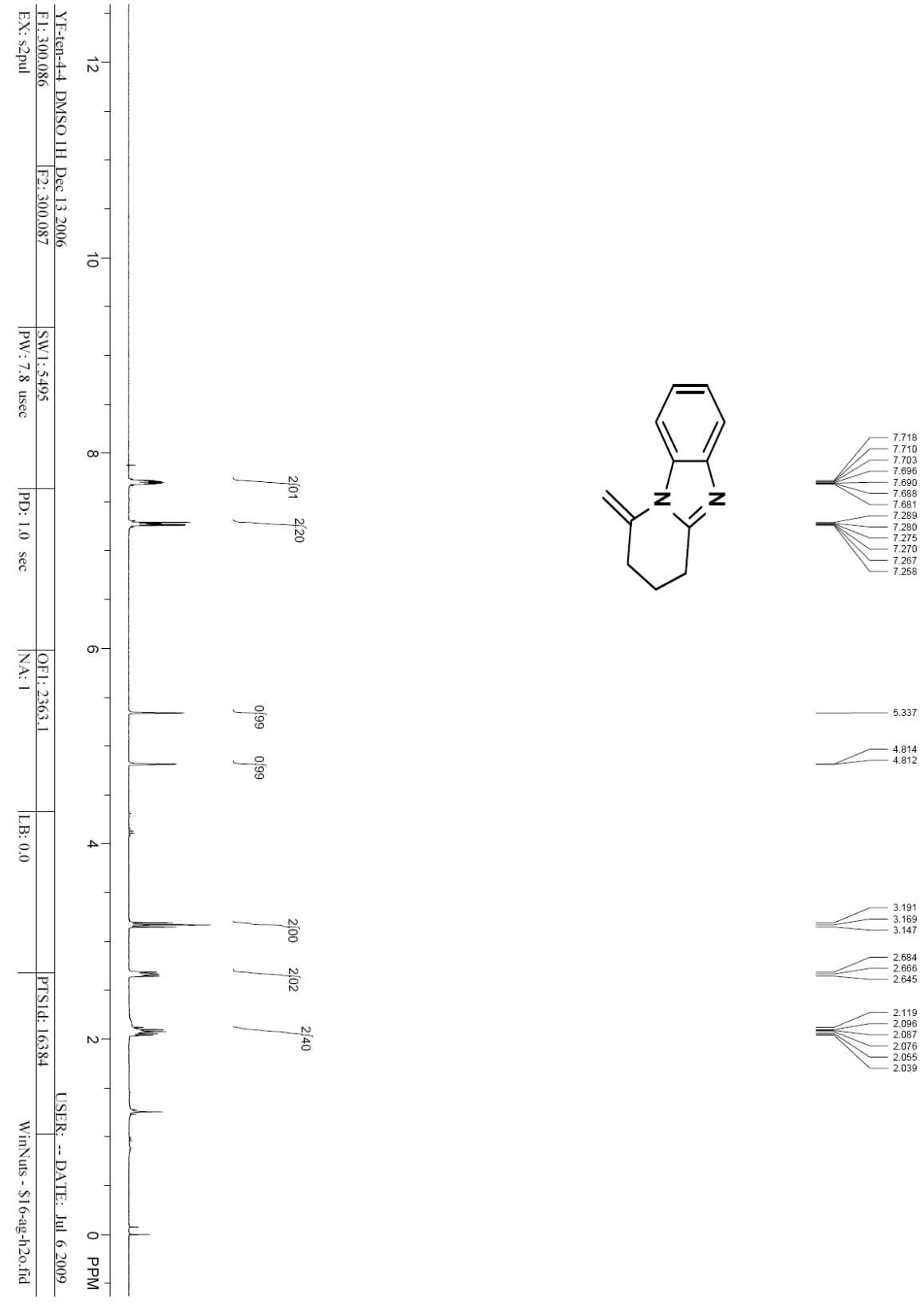
Deuterated 5,6-Dimethyl-2-(pent-4-ynyl)-1*H*-benzo[*d*]imidazole **[*d*]-A2** was prepared in 85% yield with 67% deuterium incorporation at the terminal alkynyl site according to the method reported in ref S(1). A mixture of **[*d*]-A2** (0.1 mmol), AgOTf (0.005 mmol) was stirred in H_2O (2 mL) under N_2 atmosphere. The vial was sealed and the mixture was then irradiated for 15 min at 150 °C. After the reaction was cooled to ambient temperature, the crude reaction mixture was extracted three times with EA (15 mL × 3). The combined organic phase was wash with saturated $NaHCO_3$ solution, brine, dried with Na_2SO_4 and concentrated. The residue was purified by column chromatography on combiflash to provide the desired product **B2**, which was analyzed using ^{1}H NMR spectroscopy to determine the content of the deuterium incorporation.

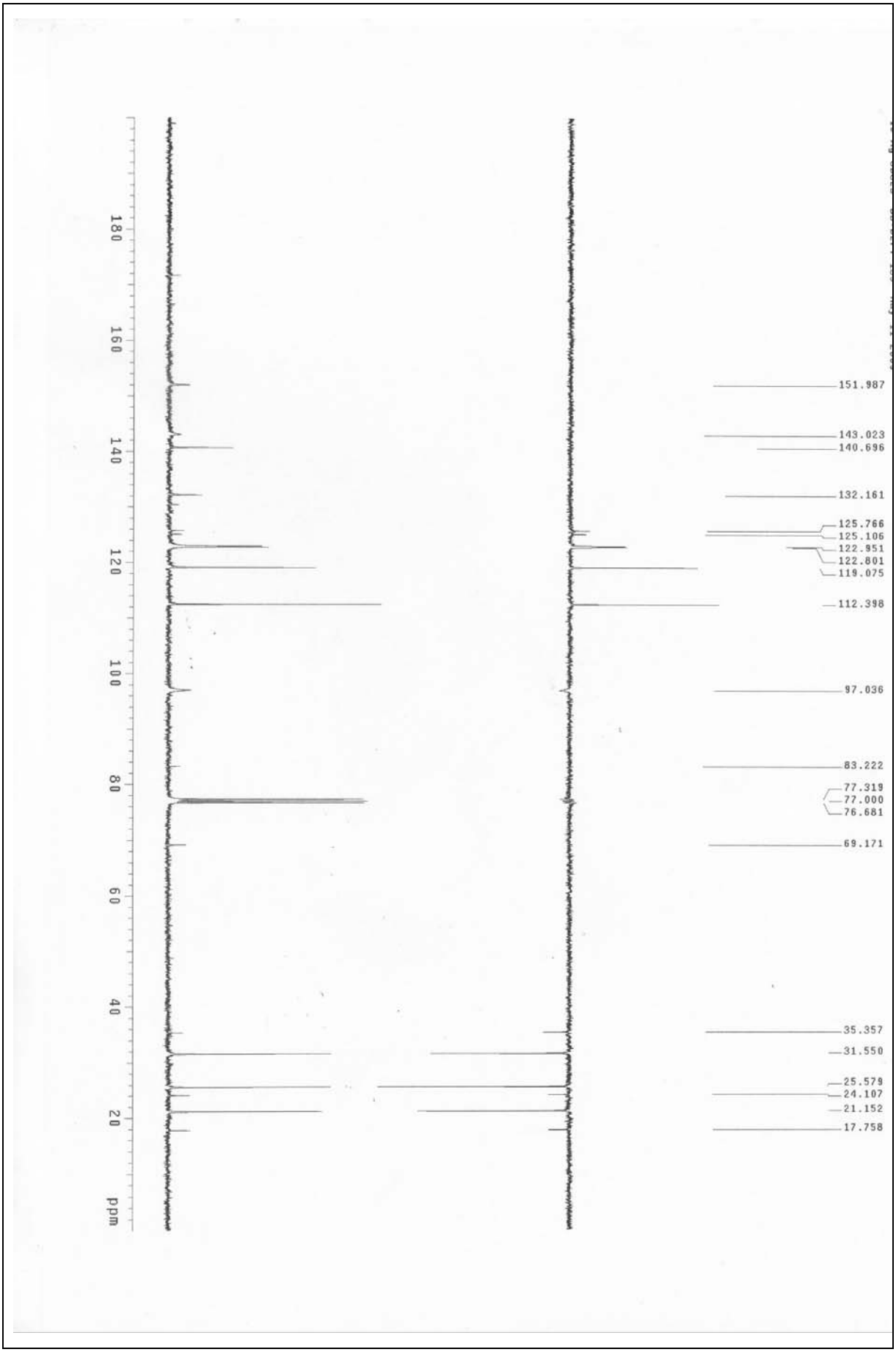
[*d*]-A2: ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.93-1.96 (m, 0.33H, CH), 2.03-2.11 (m, 2H, CH_2), 2.24-2.83 (m, 2H, CH_2), 2.34 (s, 6H, CH_3), 3.02-3.07 (m, 2H, CH_2), 7.32(s, 2H, ArH); LC-MS: m/z 214 $[M + H]^+$.

Ref S(1). Sabot, C.; Kumar, K. A.; Antherume, C.; Mioskowski, C. *J. Org. Chem.* **2007**, *72*, 5001-5007.

Copies of ^{1}H NMR and ^{13}C NMR of B1-[*d*]C24

1-Methylene-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B1)

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140
120
100
80
60
40
20
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132.161
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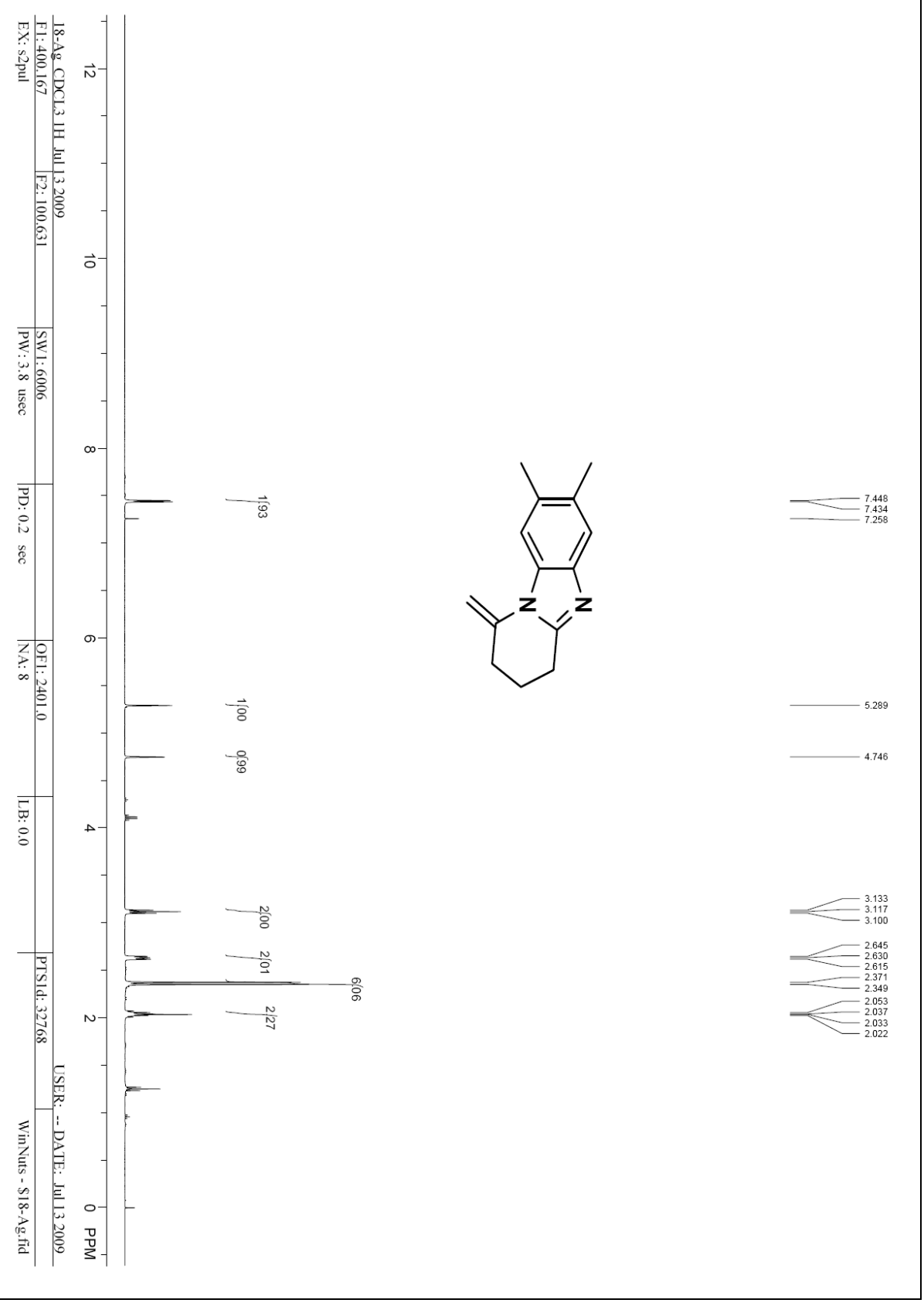
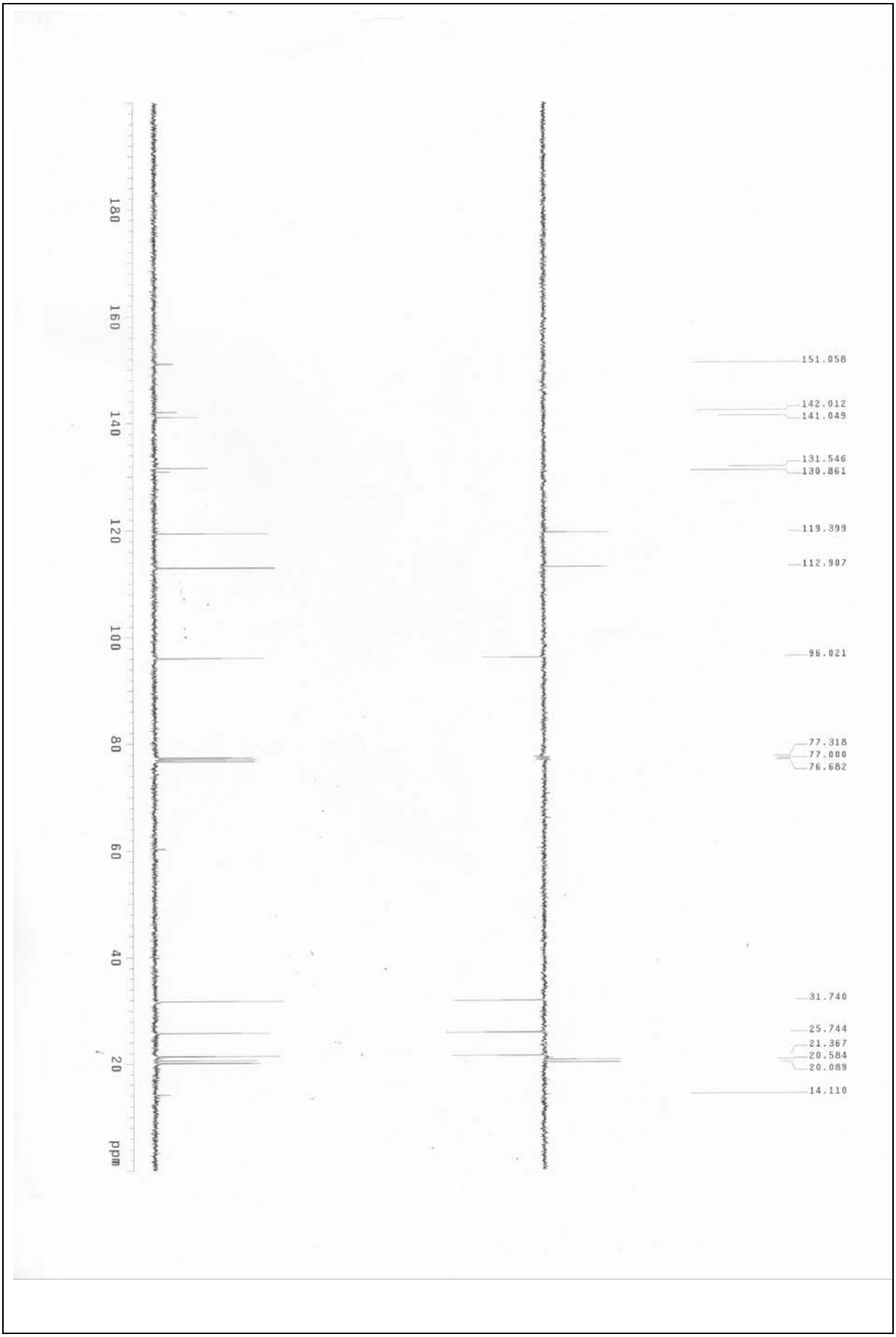
122.851
122.801
119.075
112.398
97.036
83.222
77.319
77.000
76.681
69.171
35.357
31.550
25.579
24.107
21.152
17.758

7,8-Dimethyl-1-methylene-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B2)




180
160
140
120
100
80
60
40
20
ppm
151.058
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131.546
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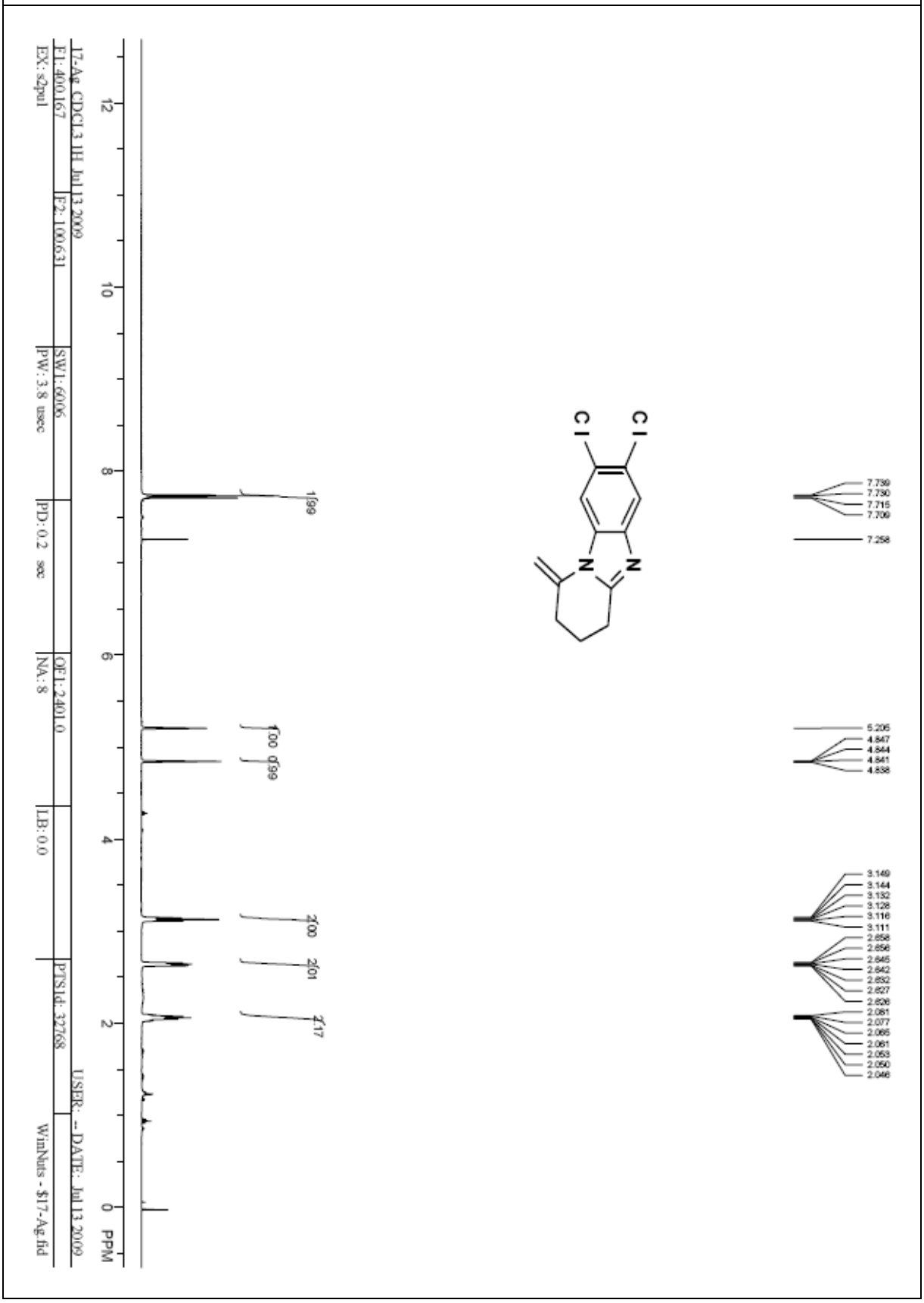
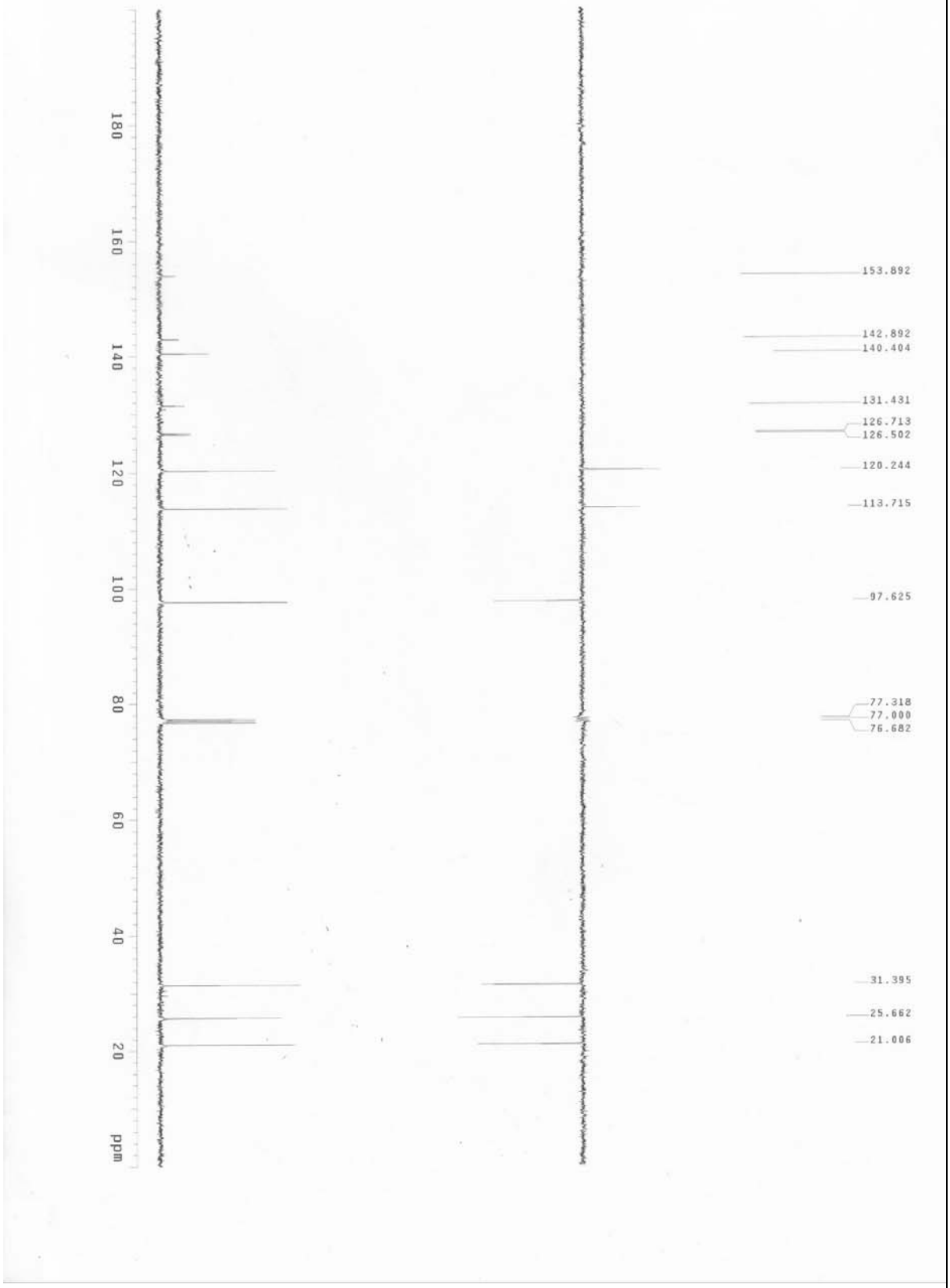
119.399
112.907
96.021
77.318
77.000
76.682
31.740
25.744
21.367
20.584
20.089
14.110

7,8-Dichloro-1-methylene-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B3)

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140
120
100
80
60
40
20
ppm
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140.404
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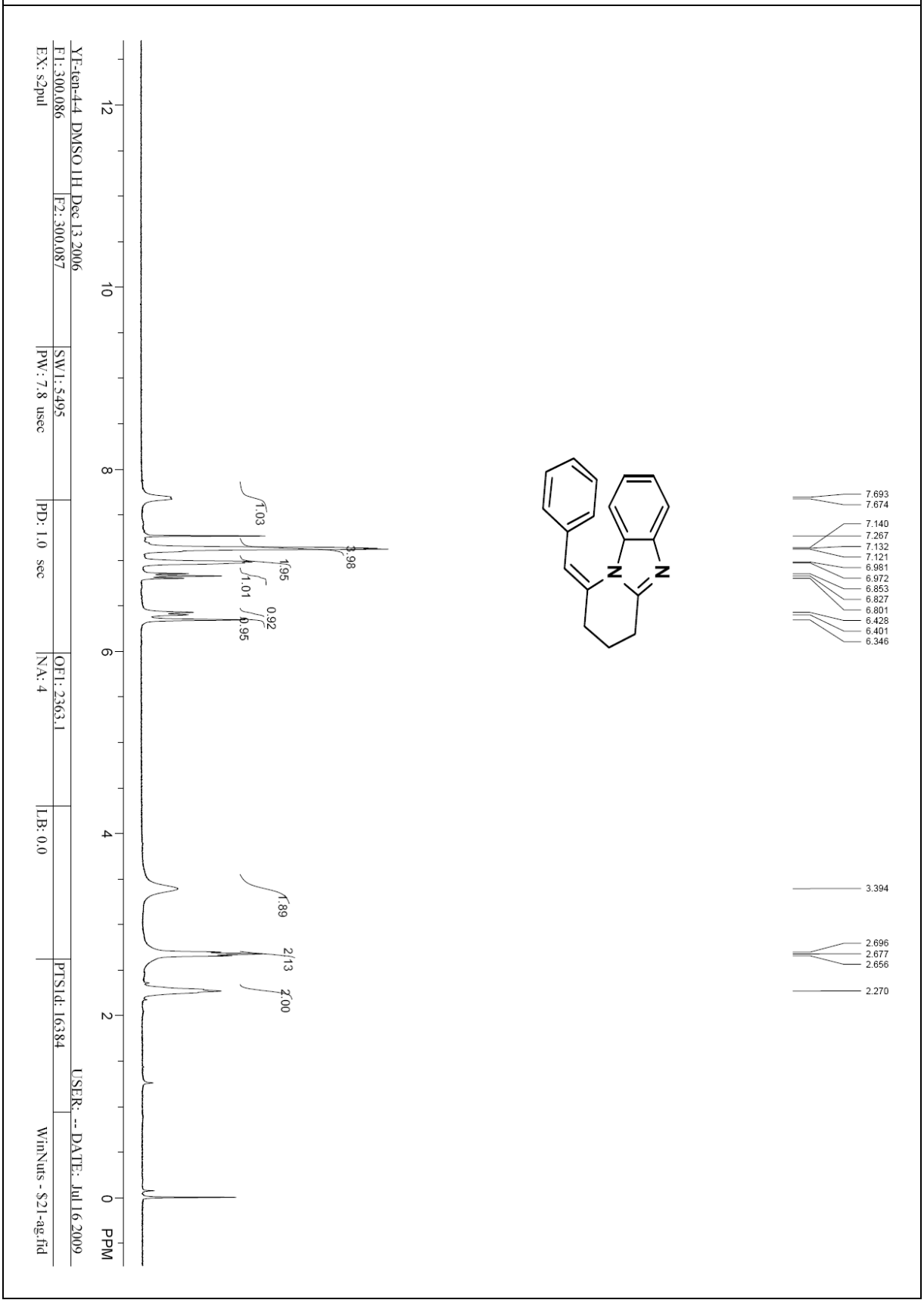
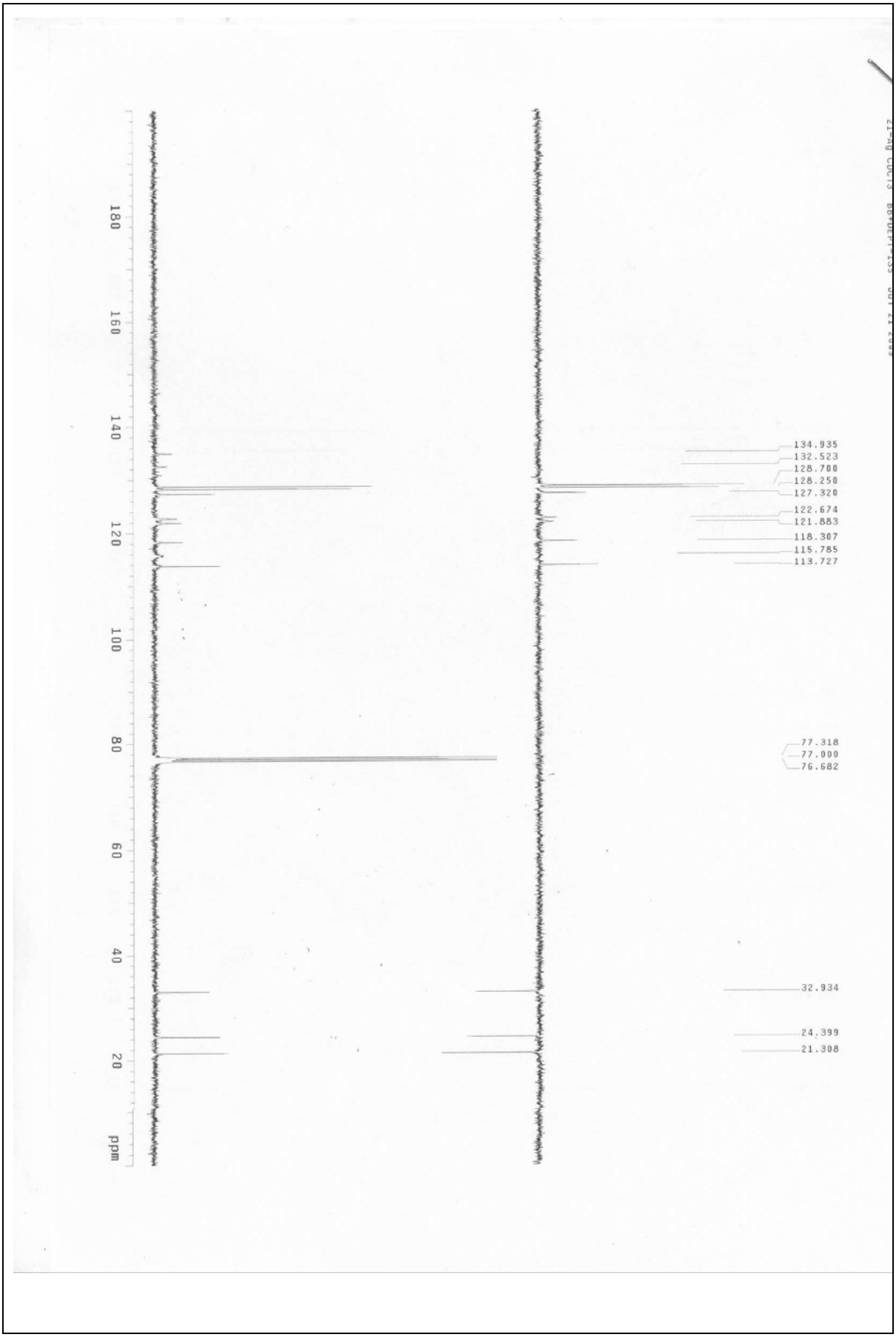
126.502
120.244
113.715
97.625
77.318
77.000
76.682
31.395
25.662
21.006

1-[1-Phenyl-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B4)

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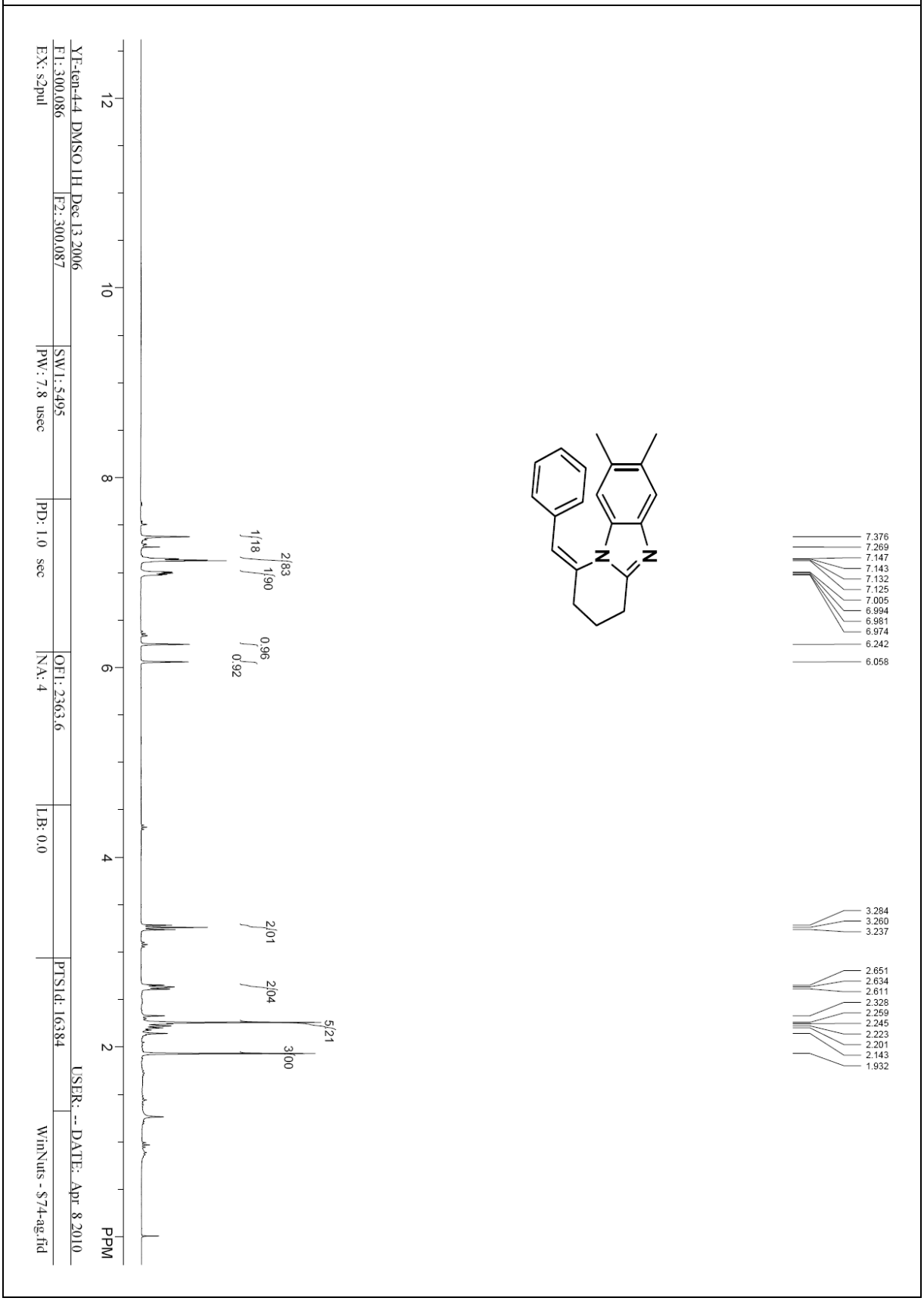
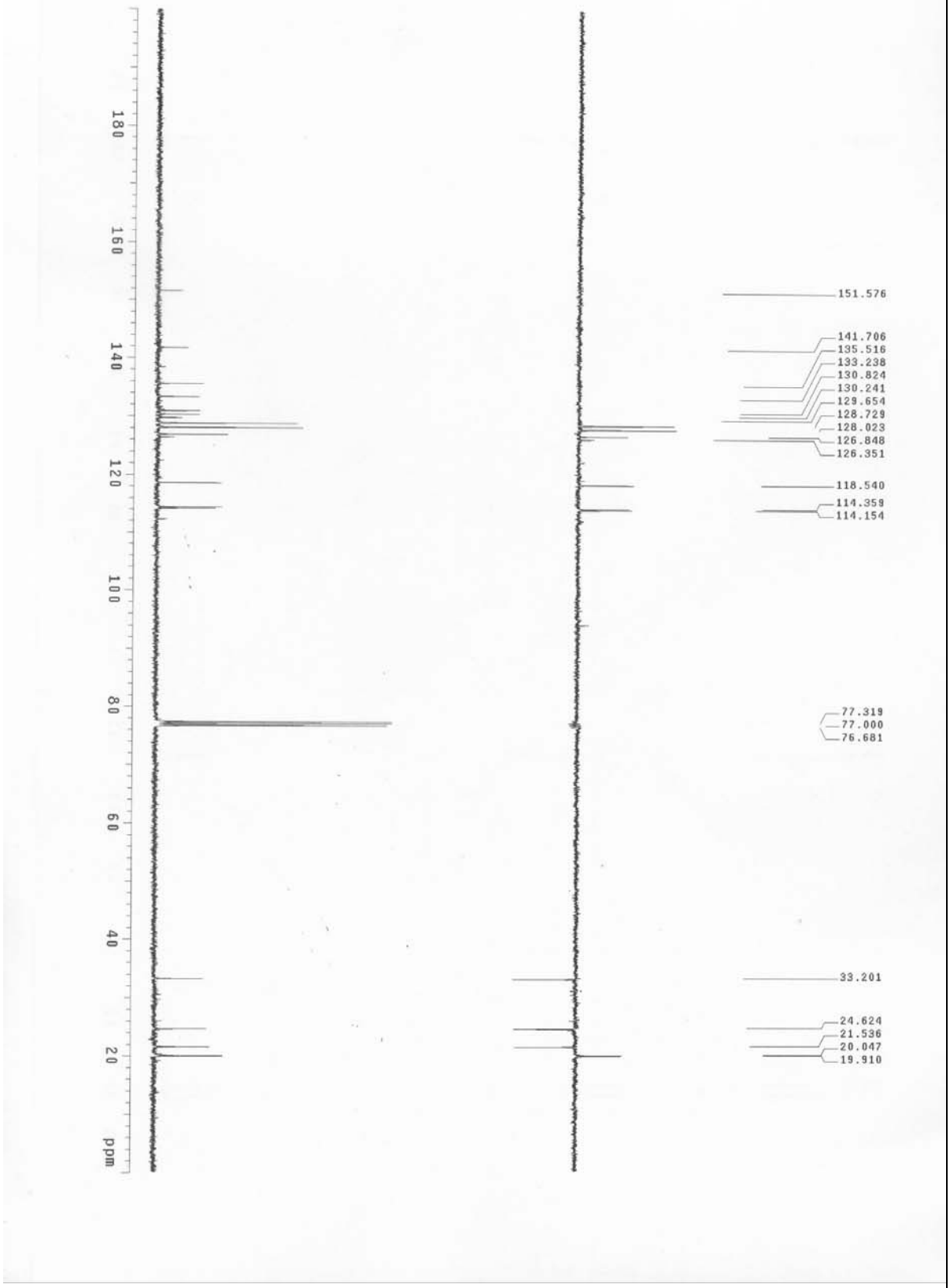
128.250
127.320
122.674
121.883
118.307
115.785
113.727
77.318
77.000
76.682
32.934
24.399
21.308
180
160
140
120
100
80
60
40
20
ppm

7,8-Dimethyl-1-[1-phenyl-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B5)

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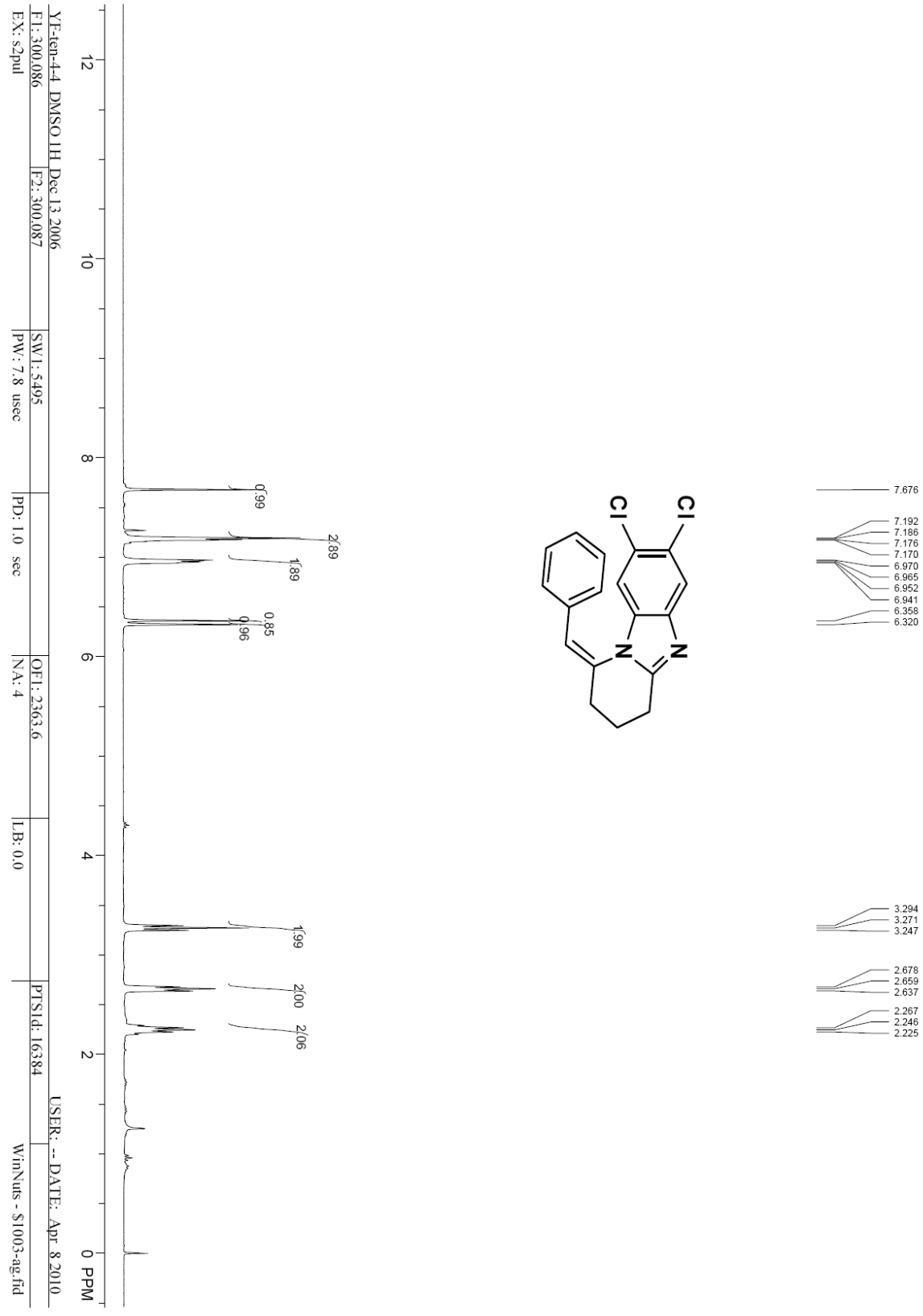
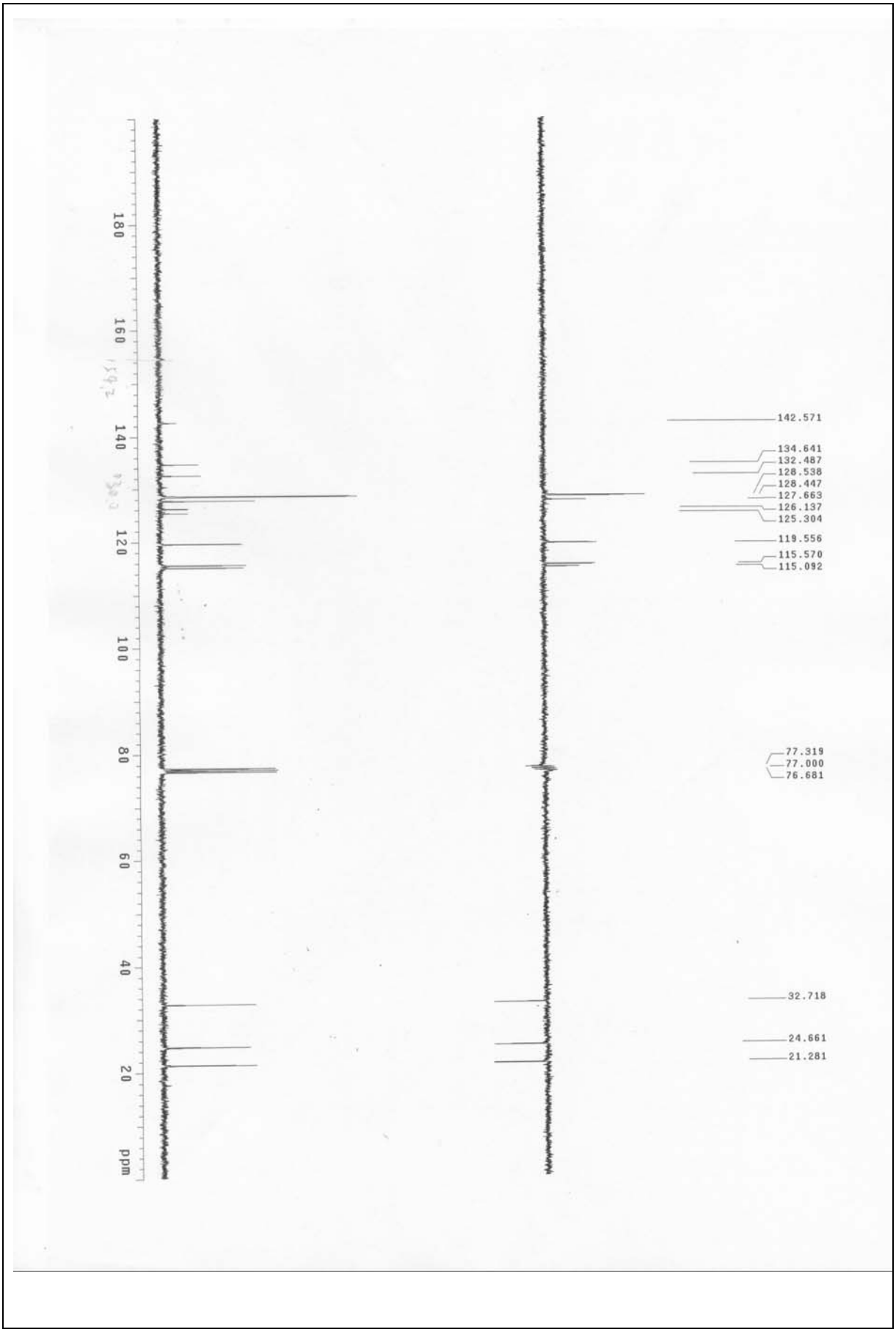
128.023
126.848
126.351
118.540
114.359
114.154
77.319
77.000
76.681
33.201
24.624
21.536
20.047
19.910

7,8-Dichloro-1-[1-phenyl-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B6)

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115.570
115.092
77.319
77.000
76.681
32.718
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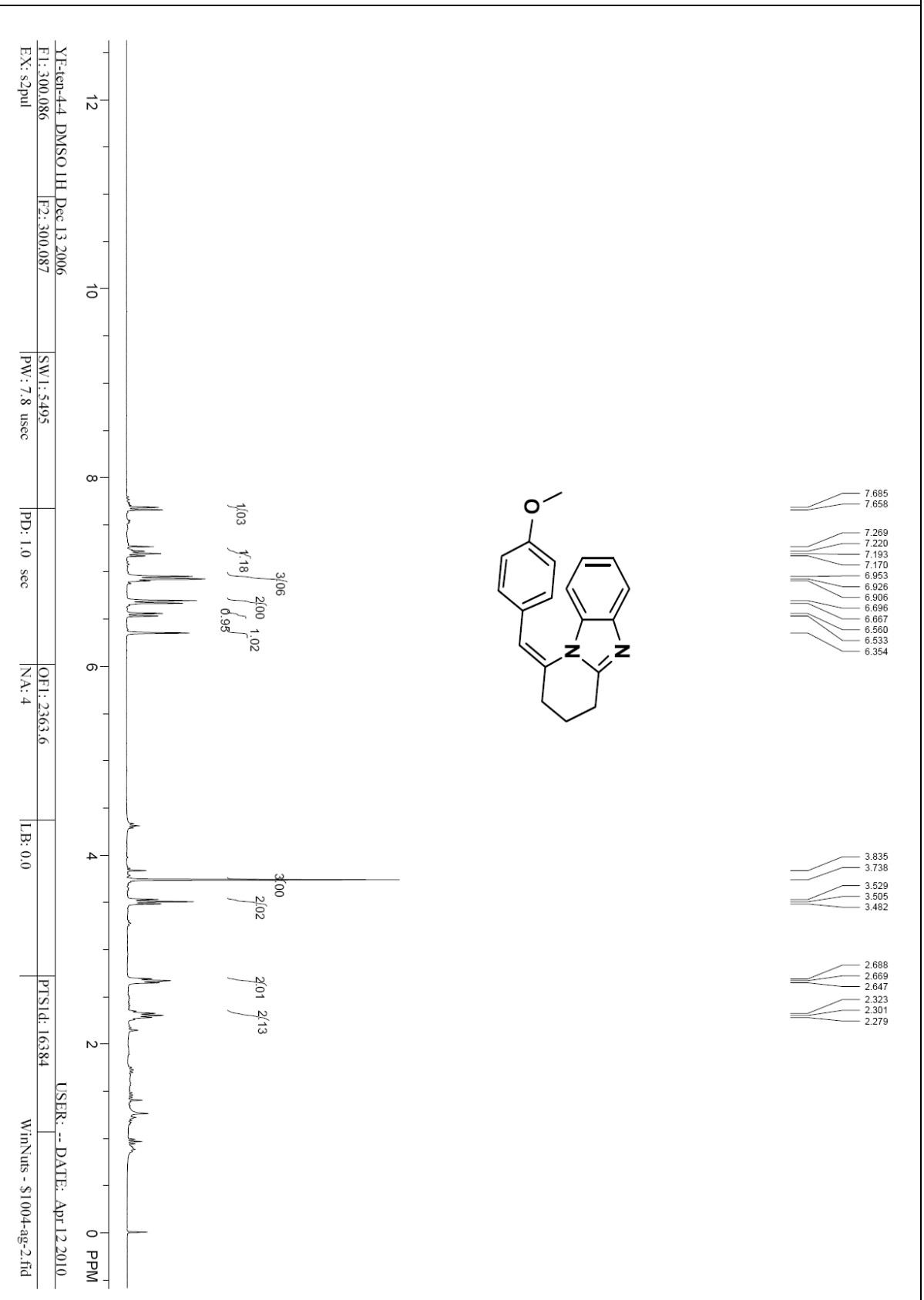
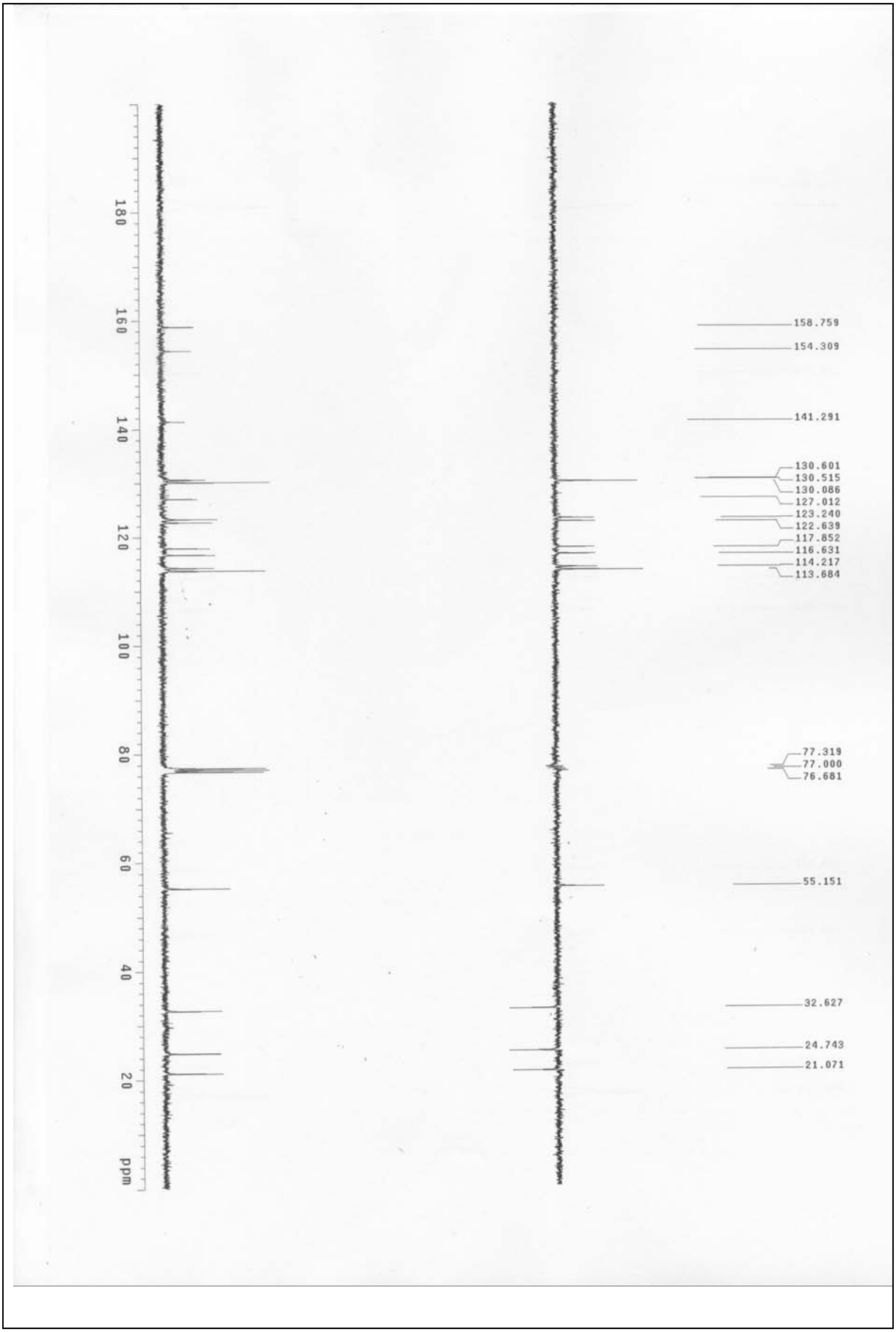
21.281

1-[1-(4-Methoxy-phenyl)-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B7)

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77.319
77.000
76.681
55.151
32.627
24.743
21.071
180
160
140
120
100
80
60
40
20
ppm

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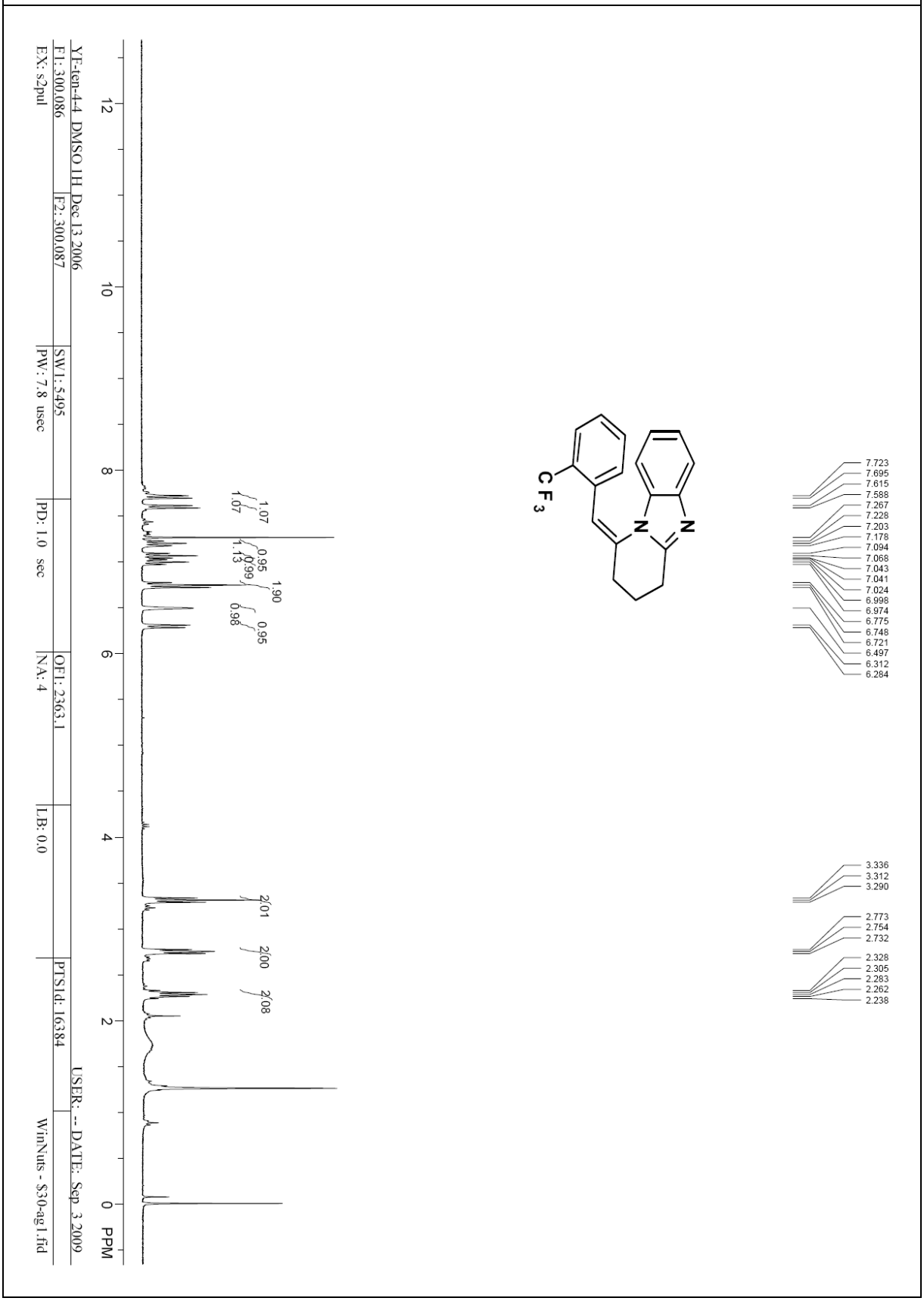

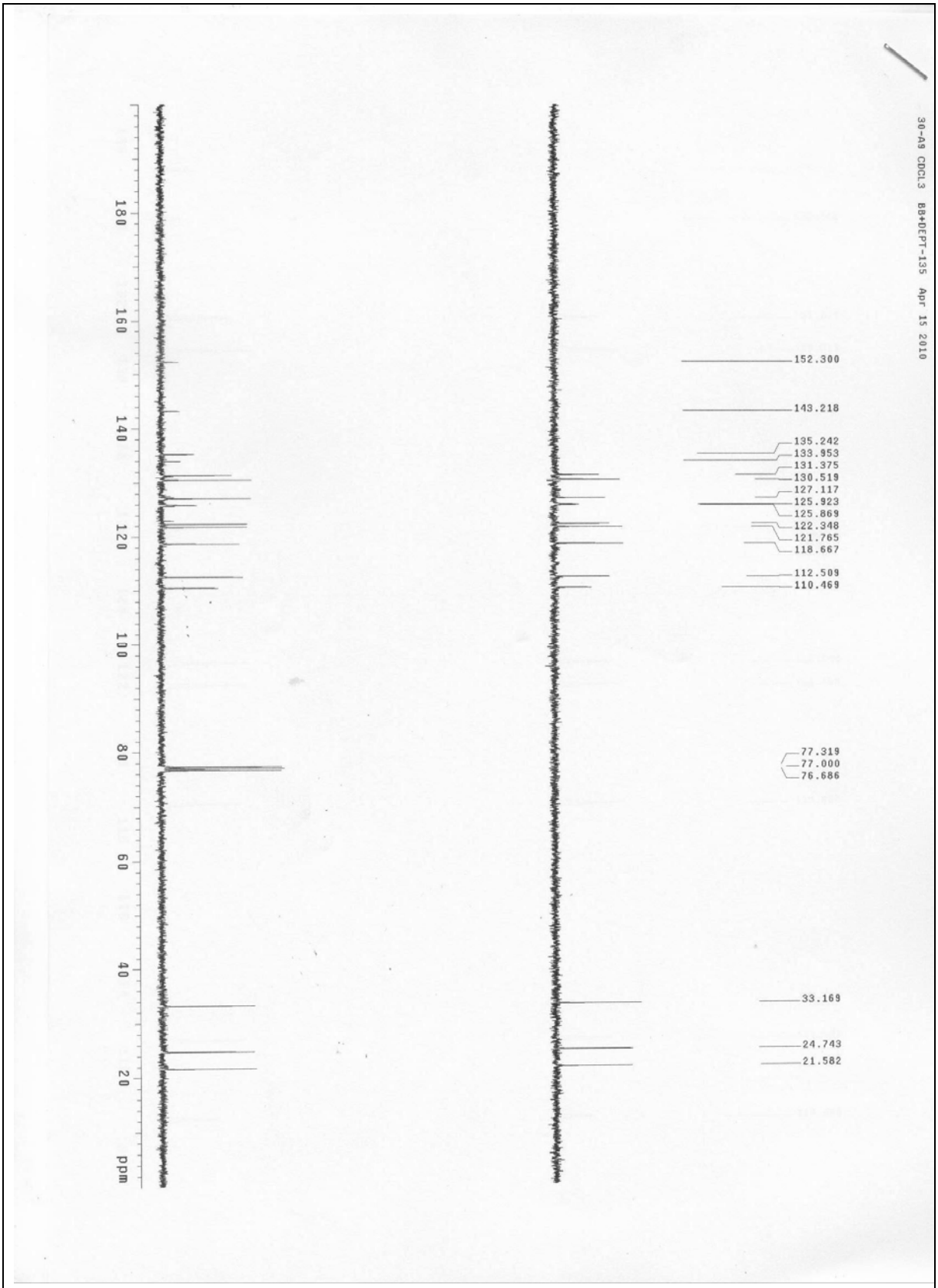
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77.000
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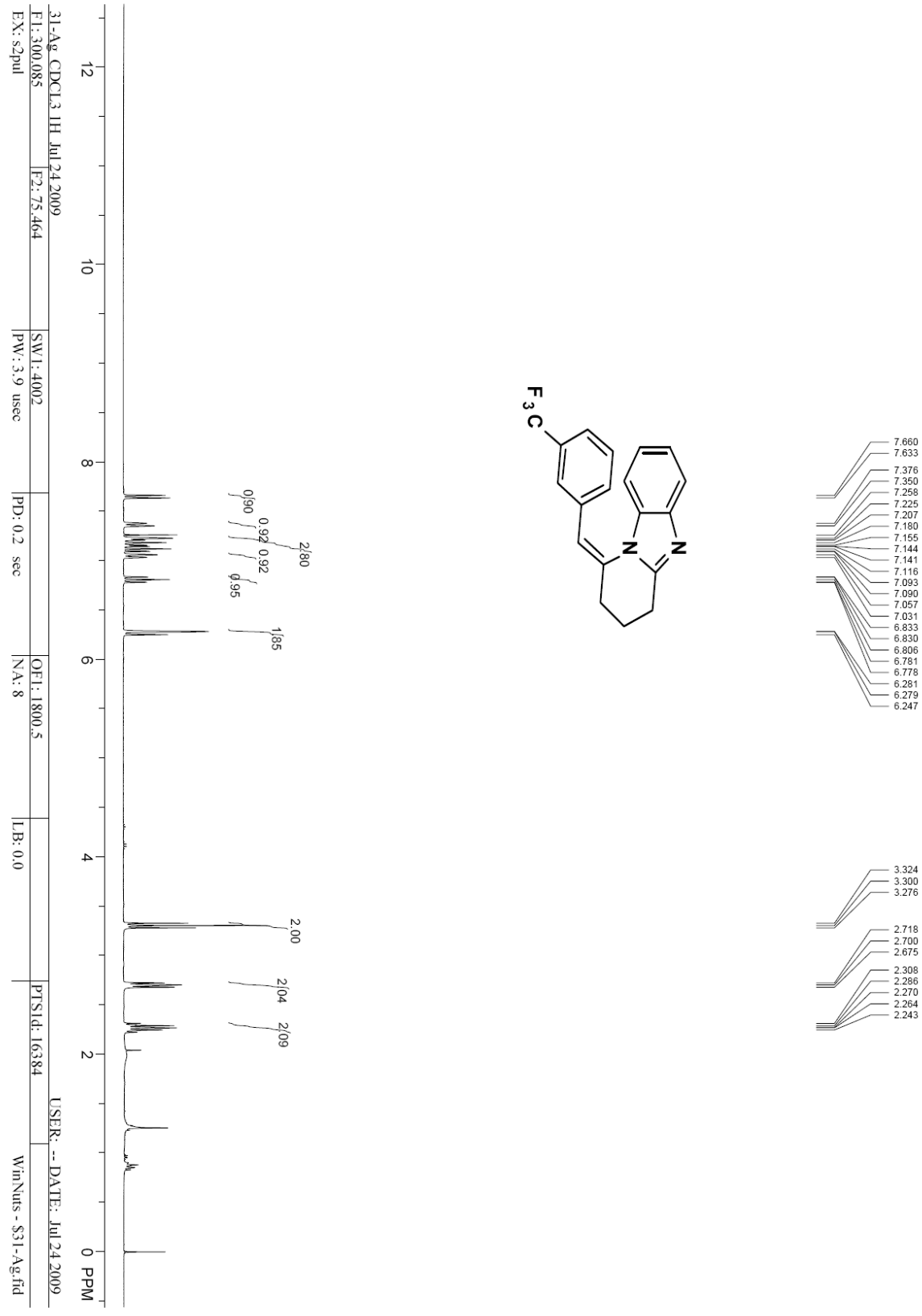
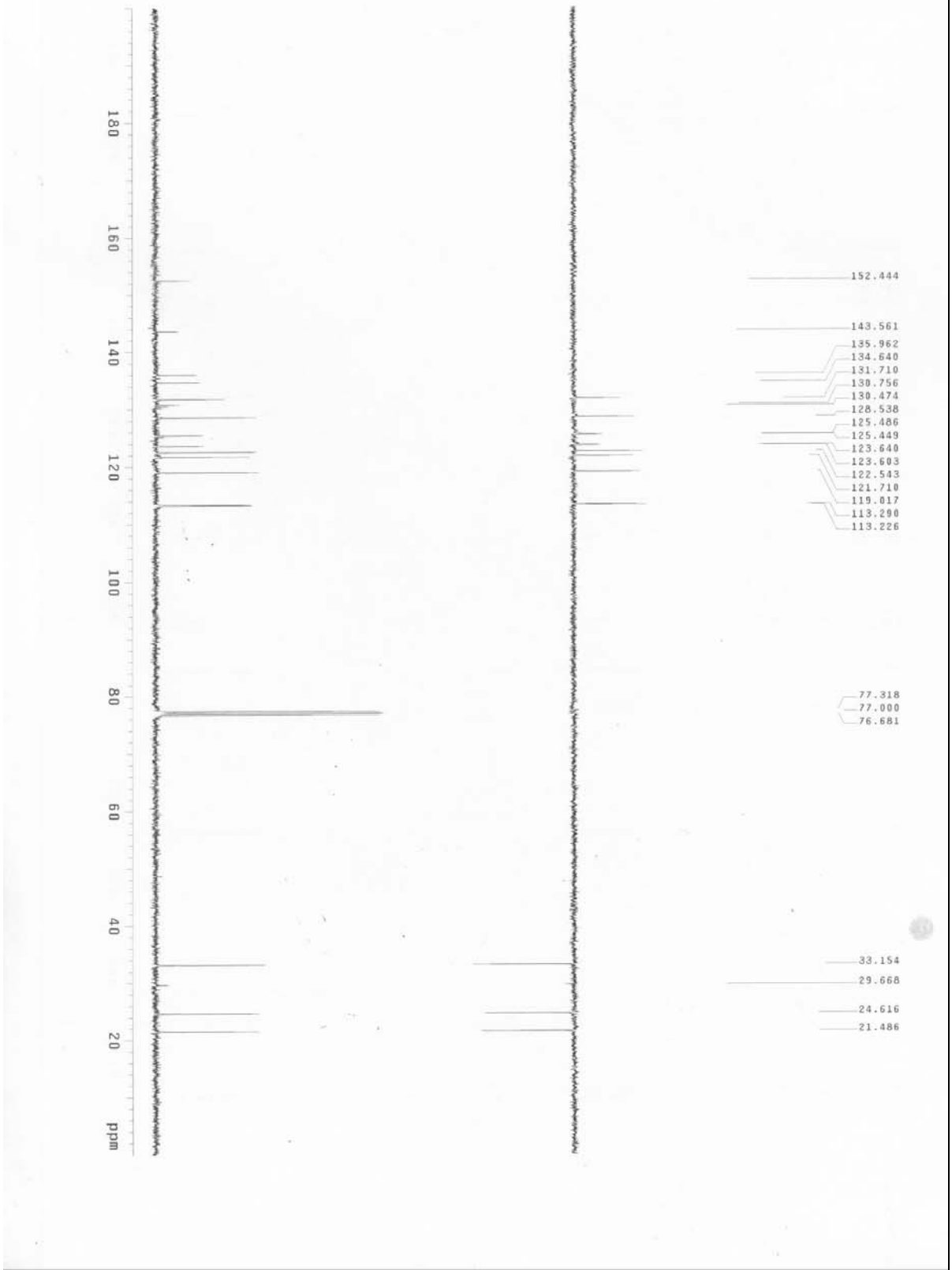
180
160
140
120
100
80
60
40
20
ppm

1-[1-(3-Trifluoromethyl-phenyl)-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B9)

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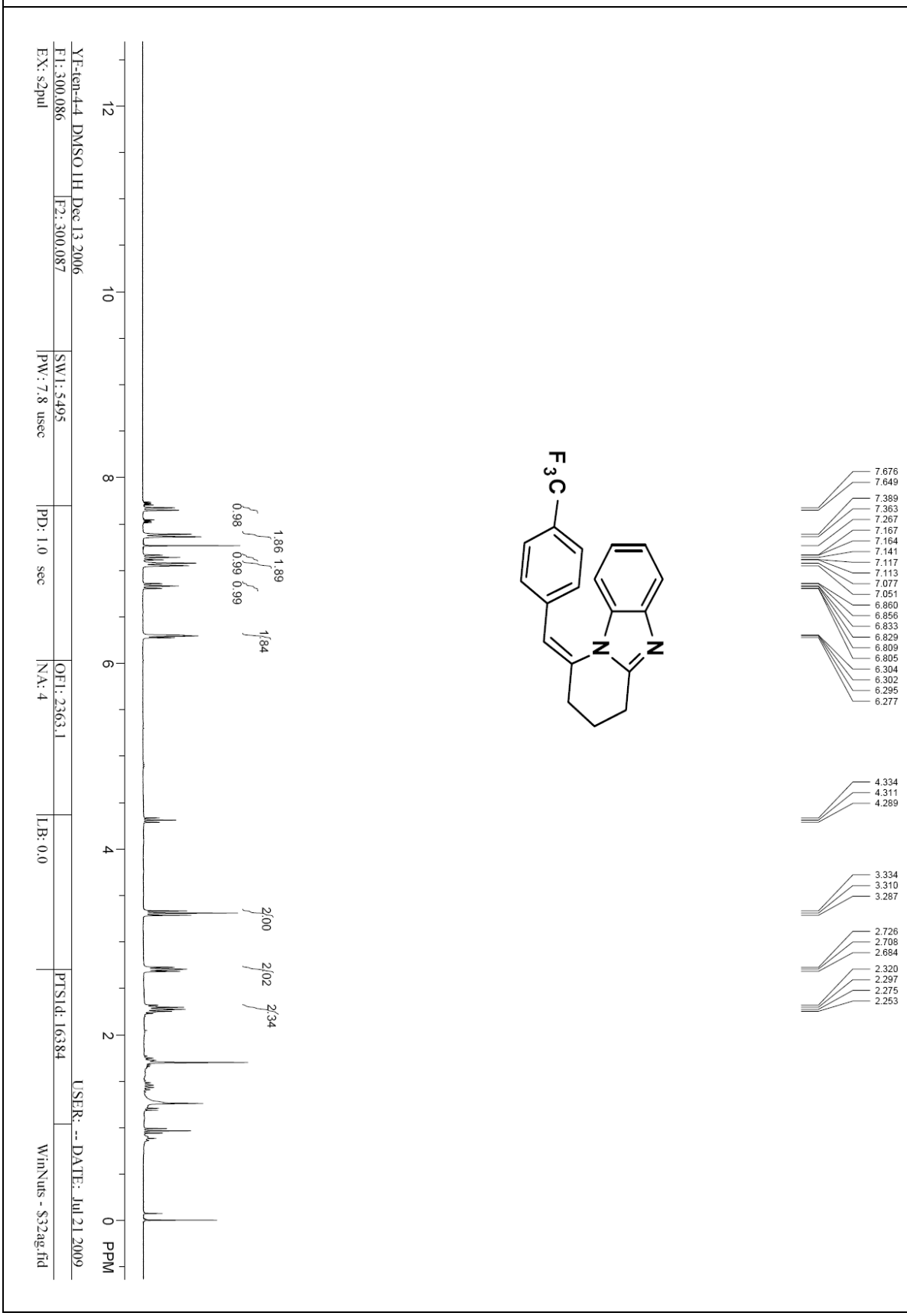
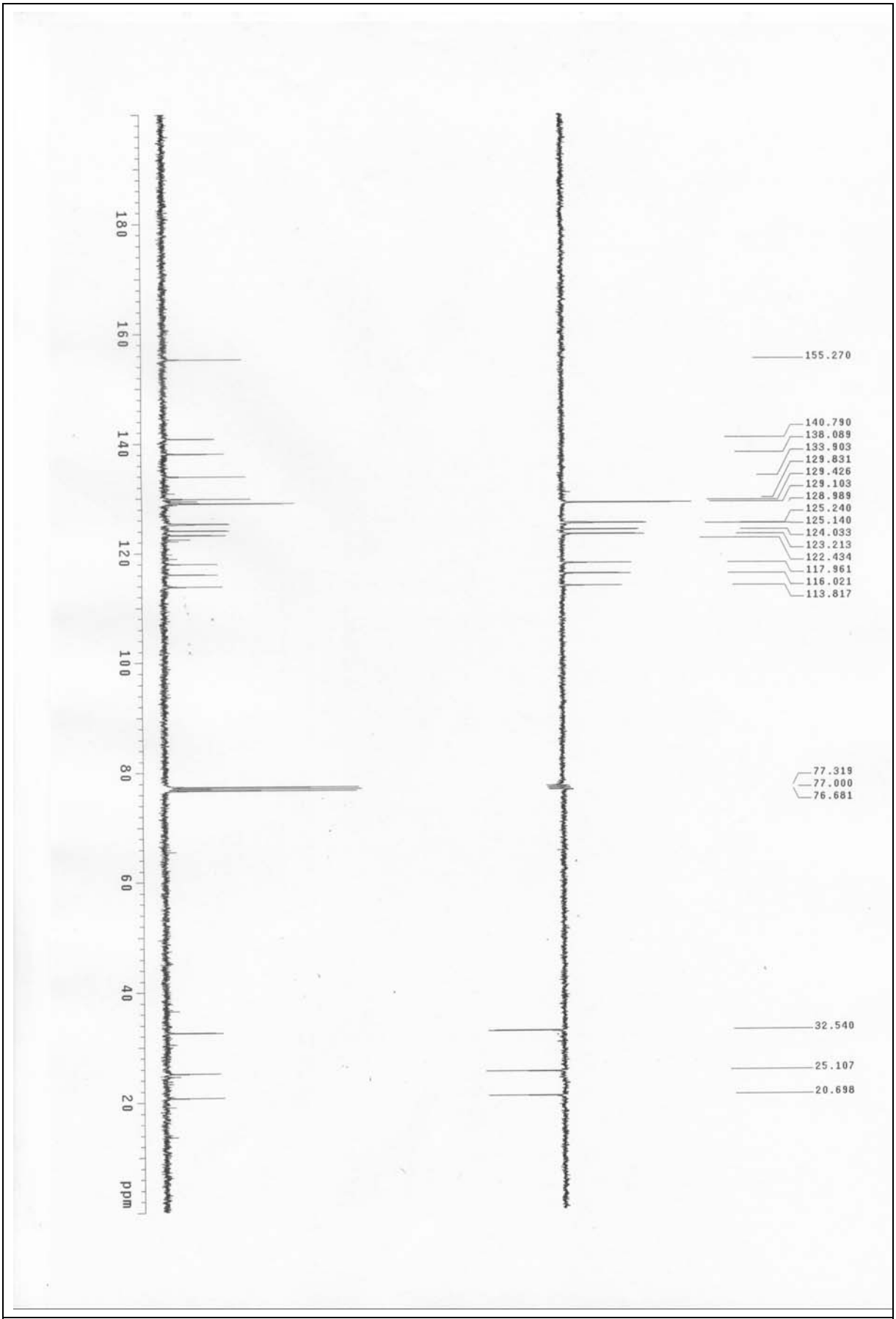
123.640
123.603
122.543
121.710
119.017
113.290
113.226
77.318
77.000
76.681
33.154
29.668
24.616
21.486

1-[1-(4-Trifluoromethyl-phenyl)-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B10)

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116.021
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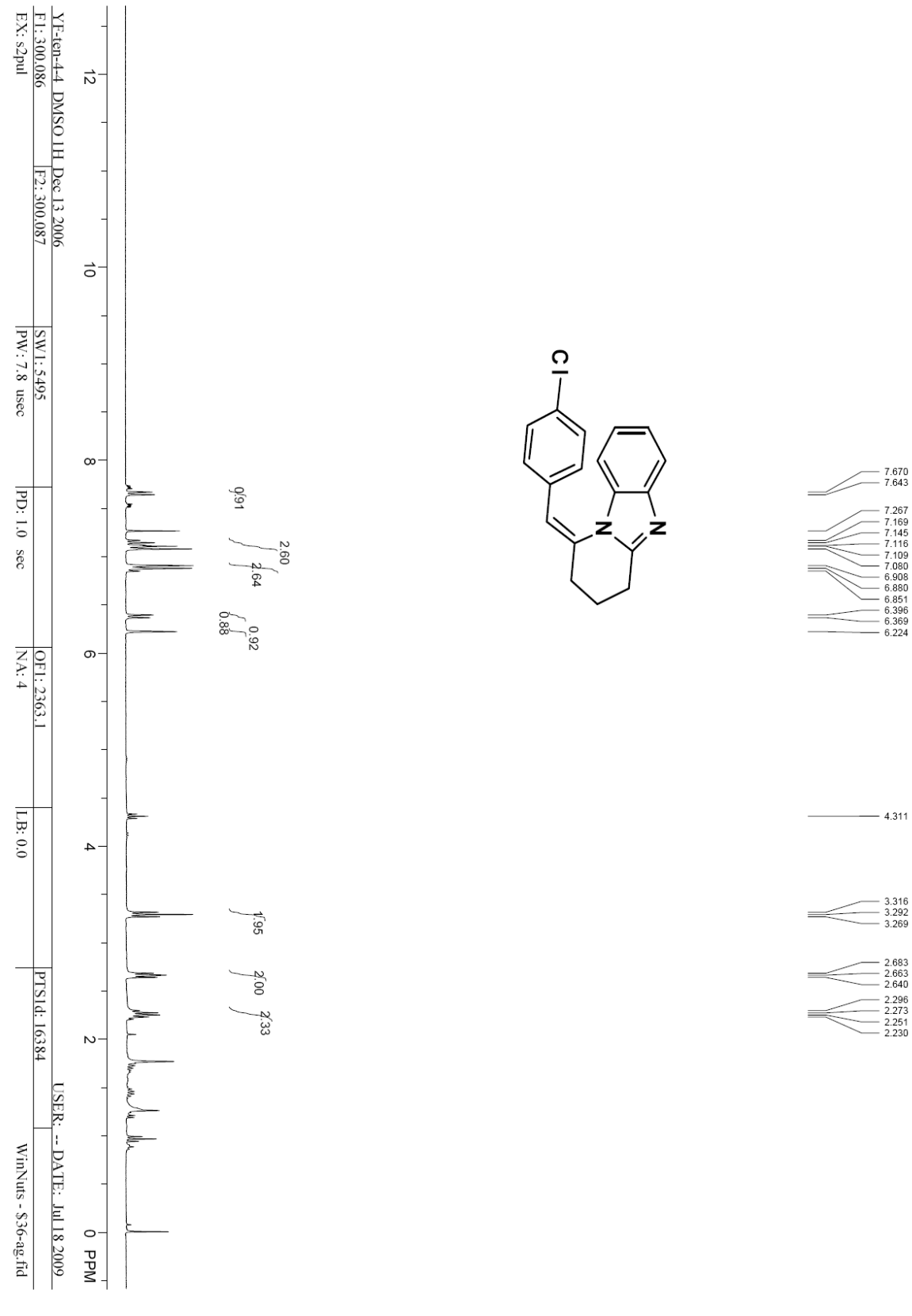
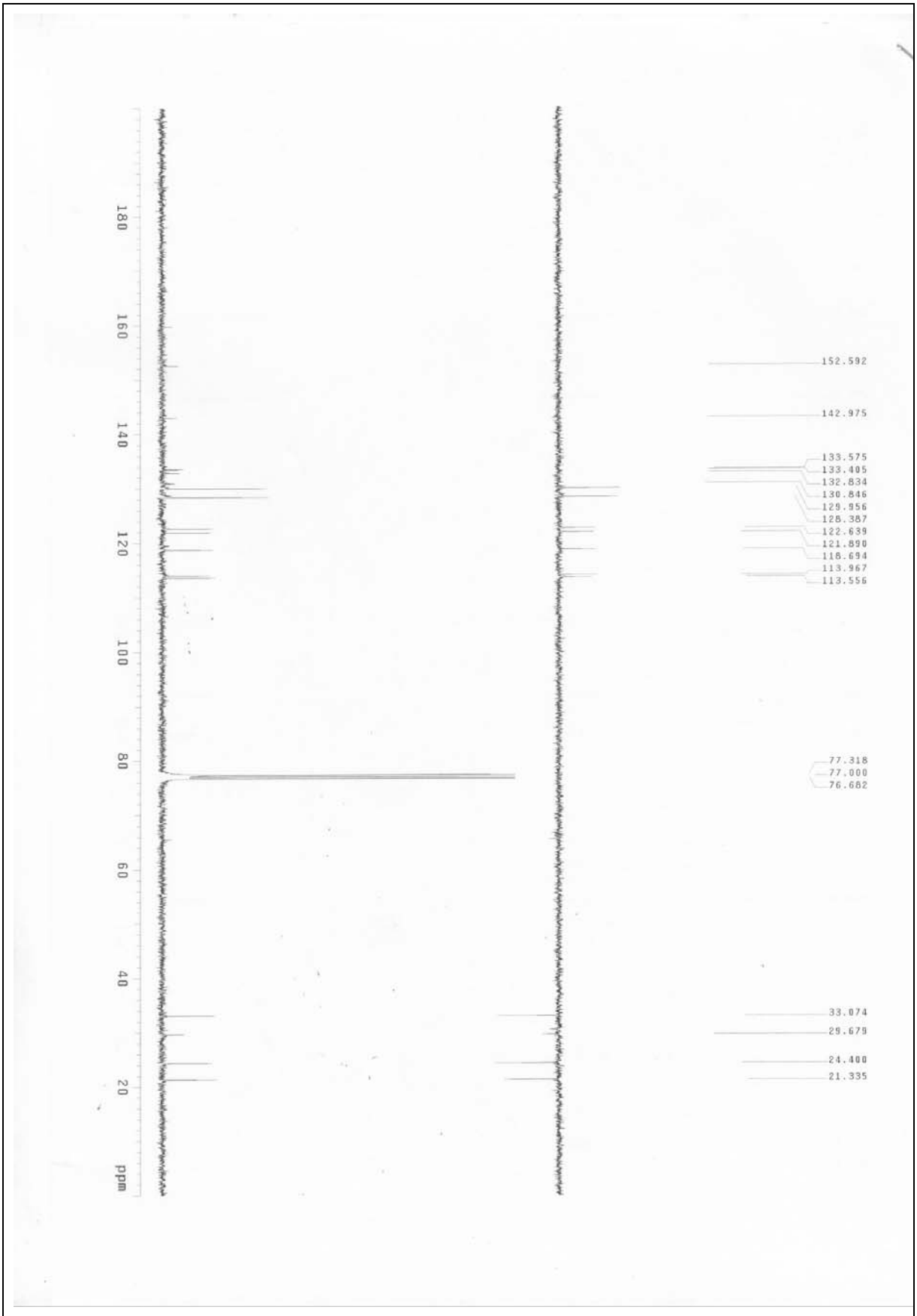
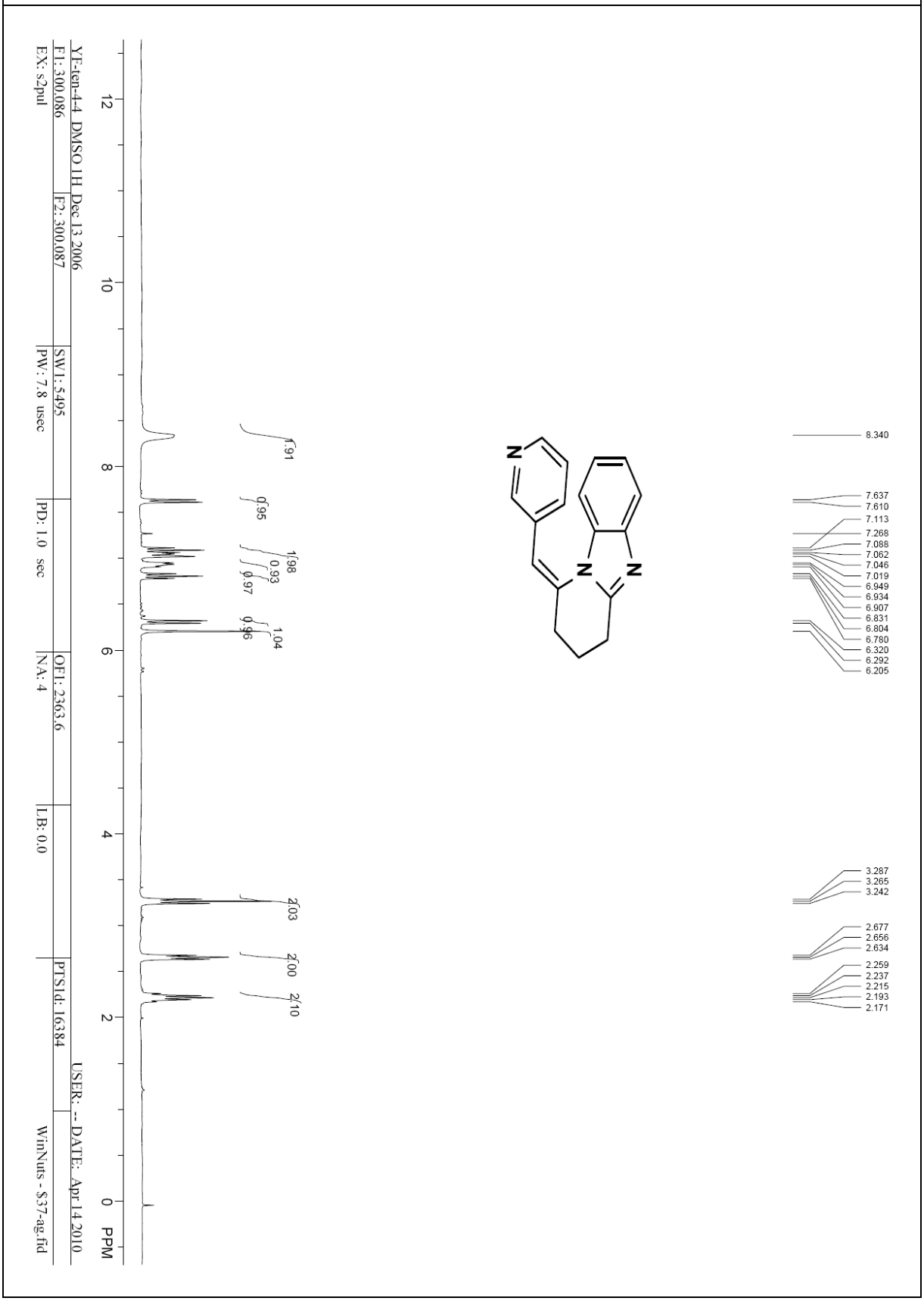
77.319
77.000
76.681
32.540
25.107
20.698
180
160
140
120
100
80
60
40
20
ppm

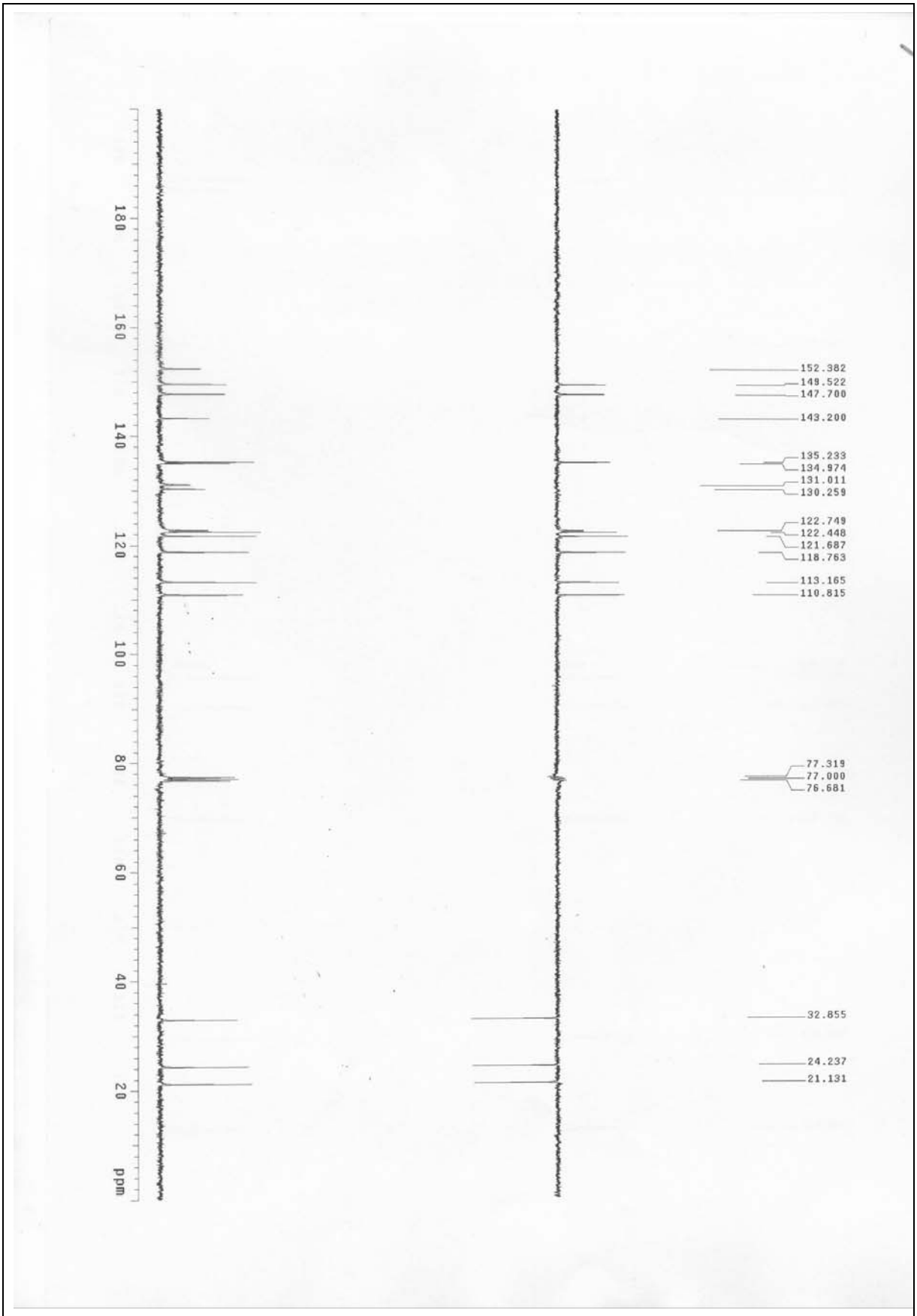
1-[1-(4-Chloro-phenyl)-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B11)



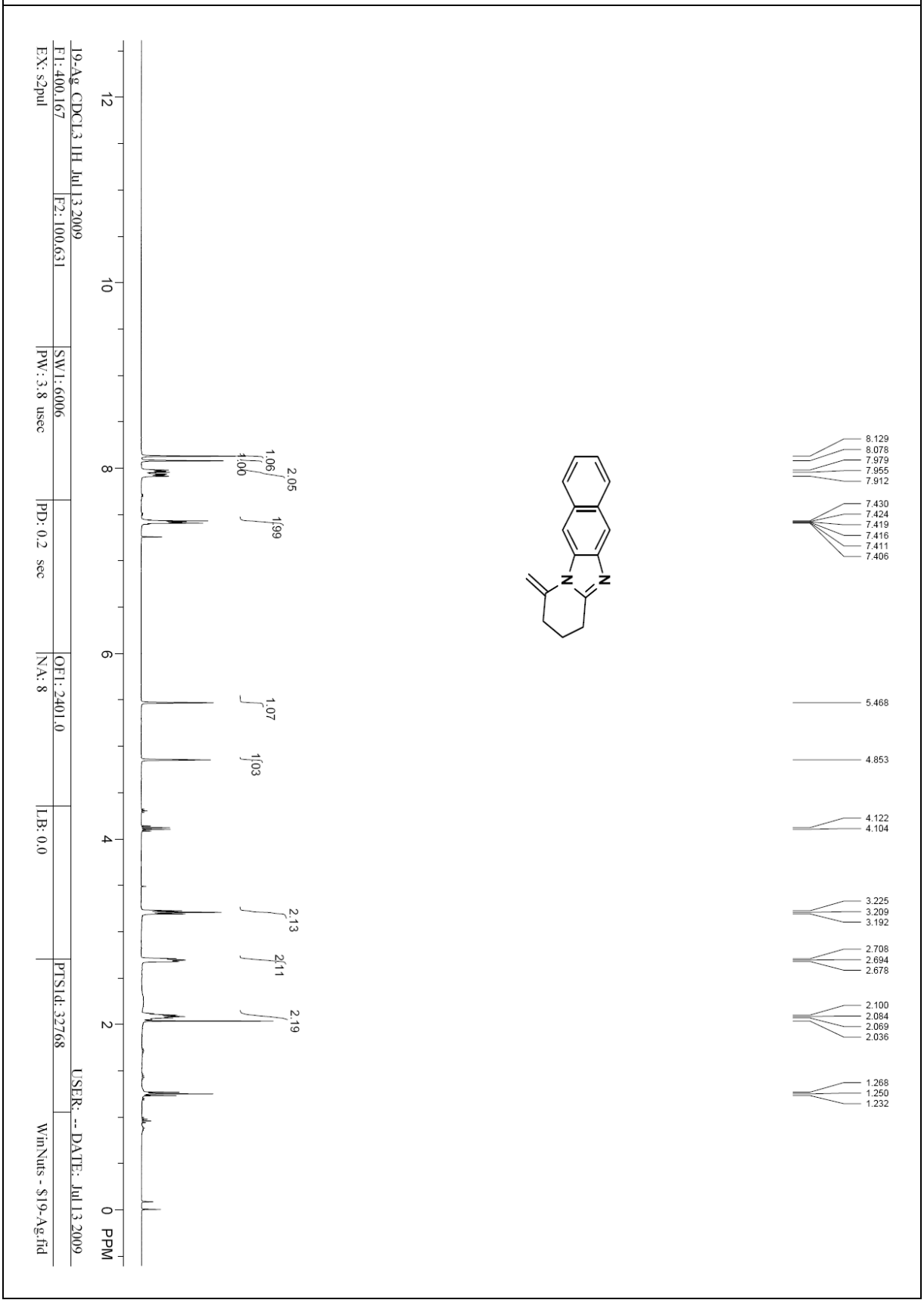

152.592
142.975
133.575
133.405
132.834
130.846
129.956
128.387
122.639
121.890
118.694
113.967
113.556
77.318
77.000
76.682
33.074
29.679
24.400
21.335
180
160
140
120
100
80
60
40
20
ppm

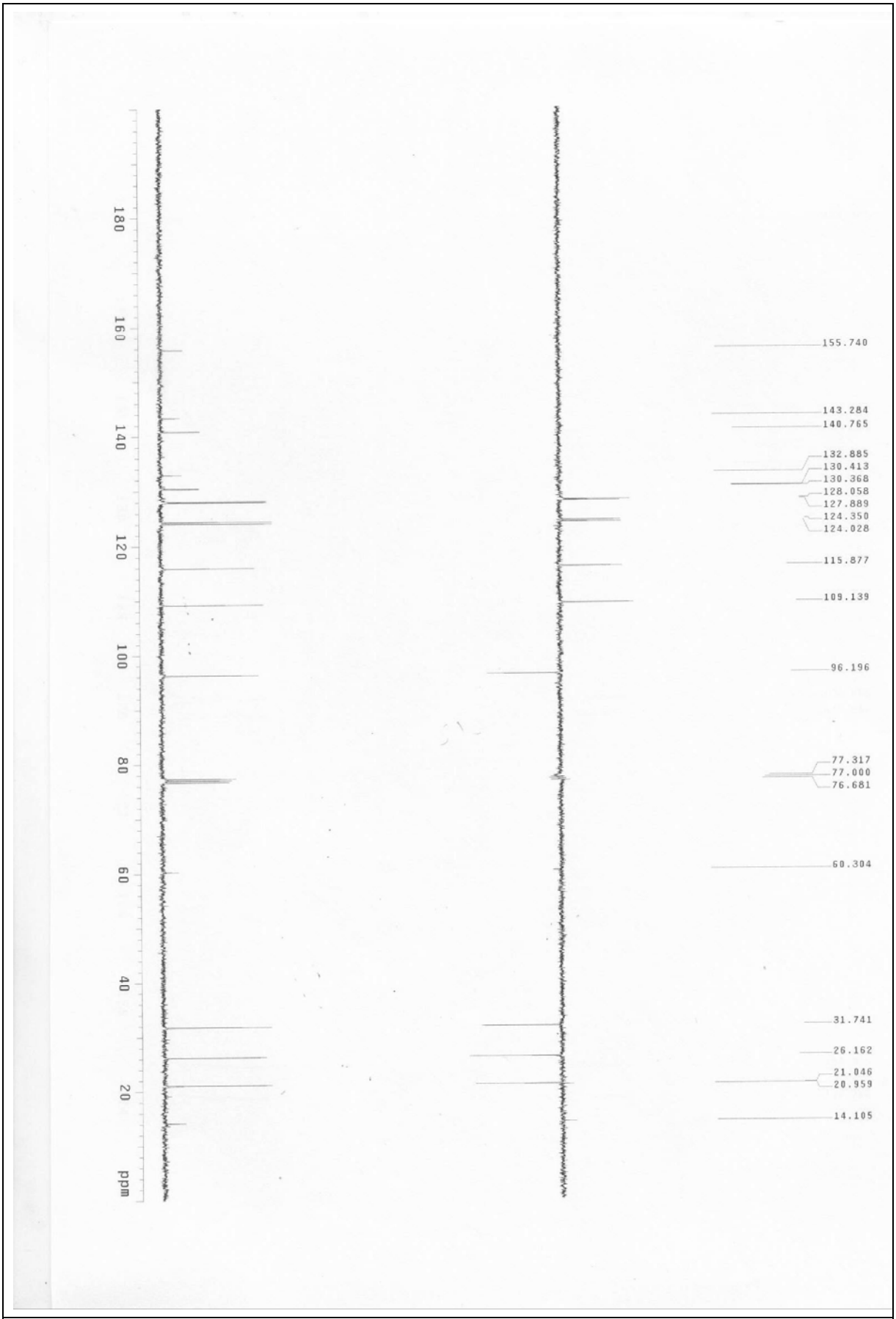
1-[1-Pyridin-3-yl-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-pyrido[1,2-*a*]benzimidazole (B12)



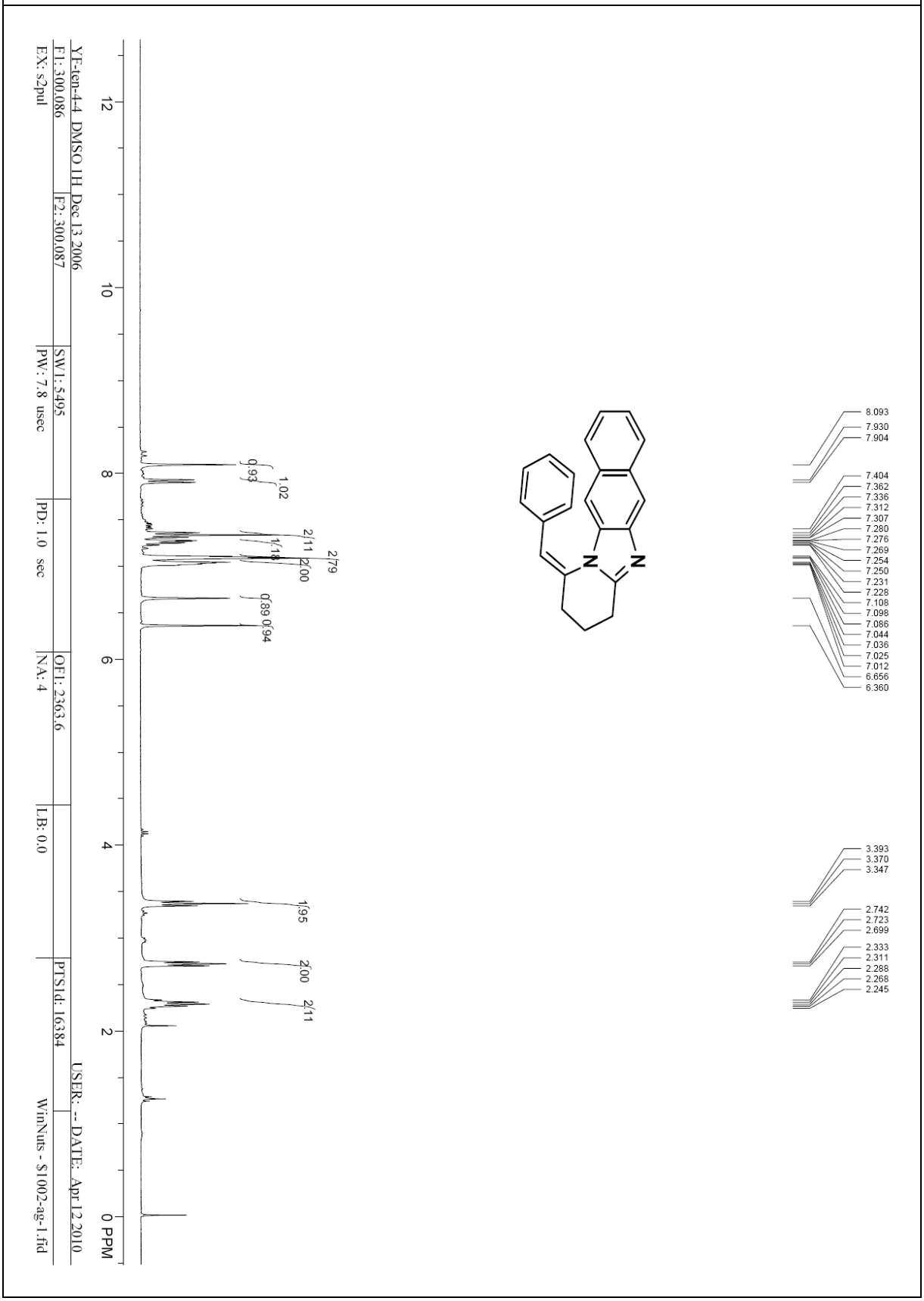

180
160
140
120
100
80
60
40
20
ppm
152.382
149.522
147.700
143.200
135.233
134.974
131.011
130.259
122.749
122.448
121.687
118.763
113.165
110.815
77.319
77.000
76.681
32.855
24.237
21.131

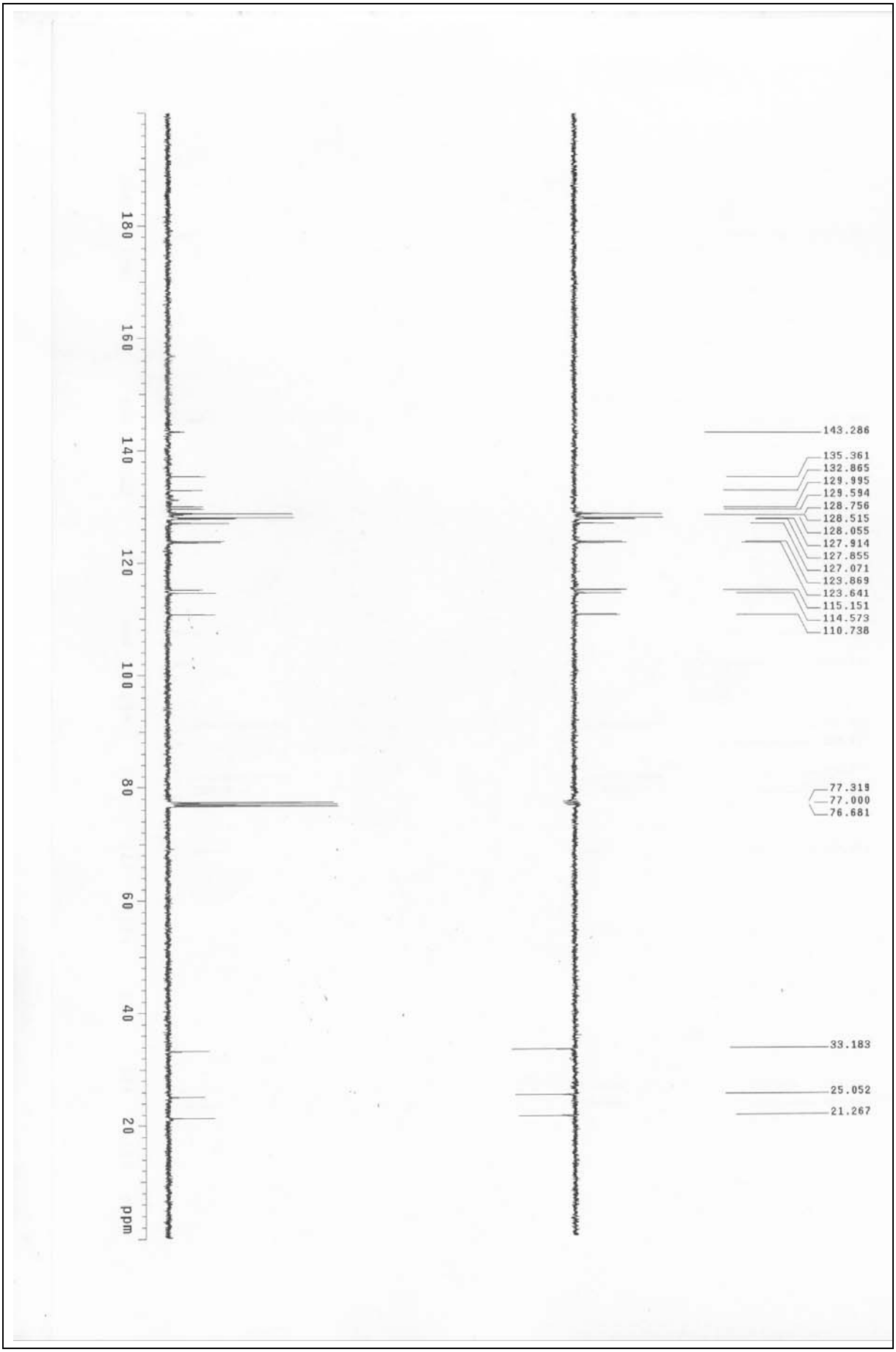
1-Methylene-1,2,3,4-tetrahydro-naphth[2',3':4,5]imidazo[1,2-*a*]pyridine (B13)



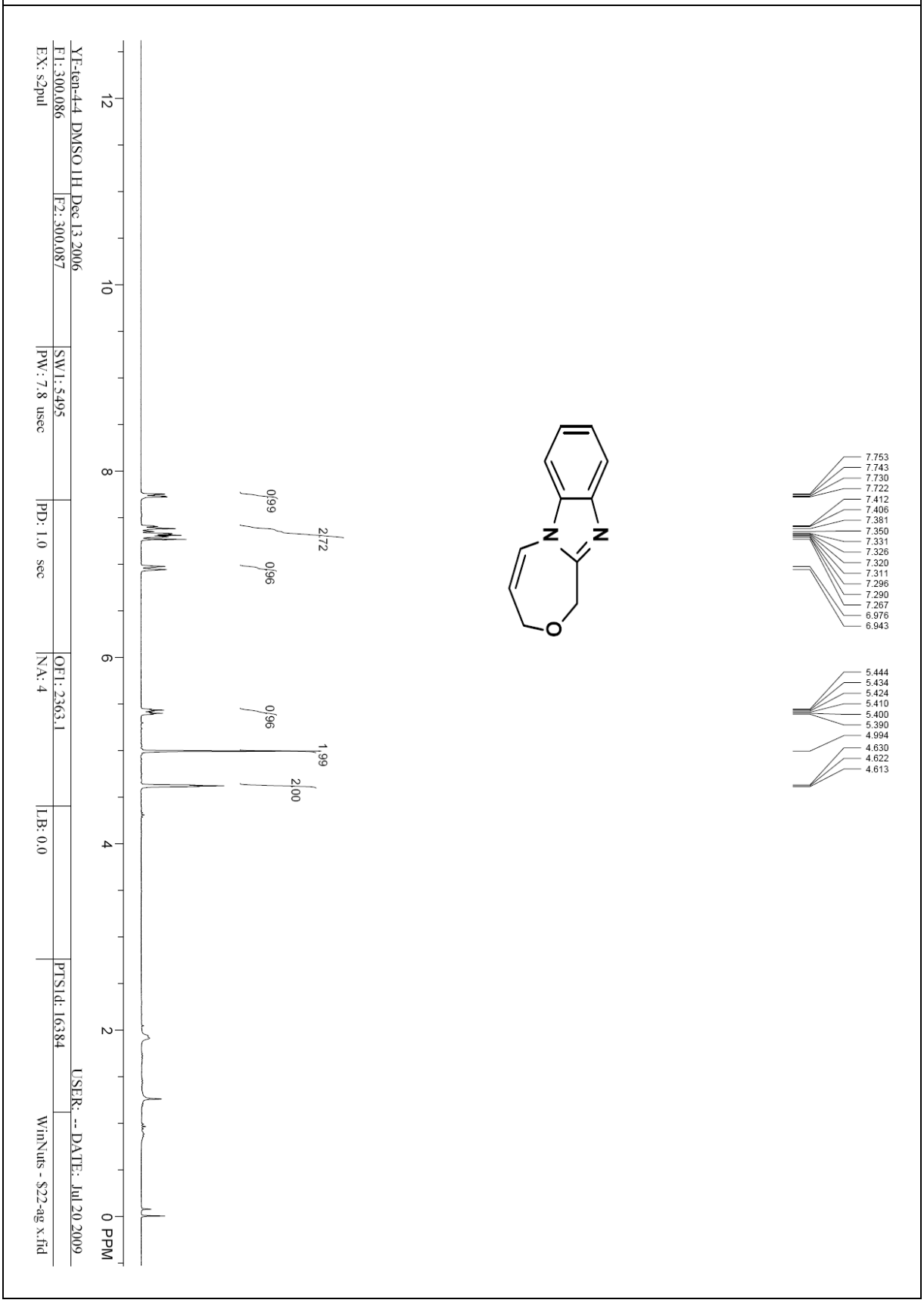

180
160
140
120
100
80
60
40
20
ppm
155.740
143.284
140.765
132.885
130.413
130.368
128.058
127.889
124.350
124.028
115.877
109.139
96.196
77.317
77.000
76.681
60.304
31.741
26.162
21.046
20.959
14.105

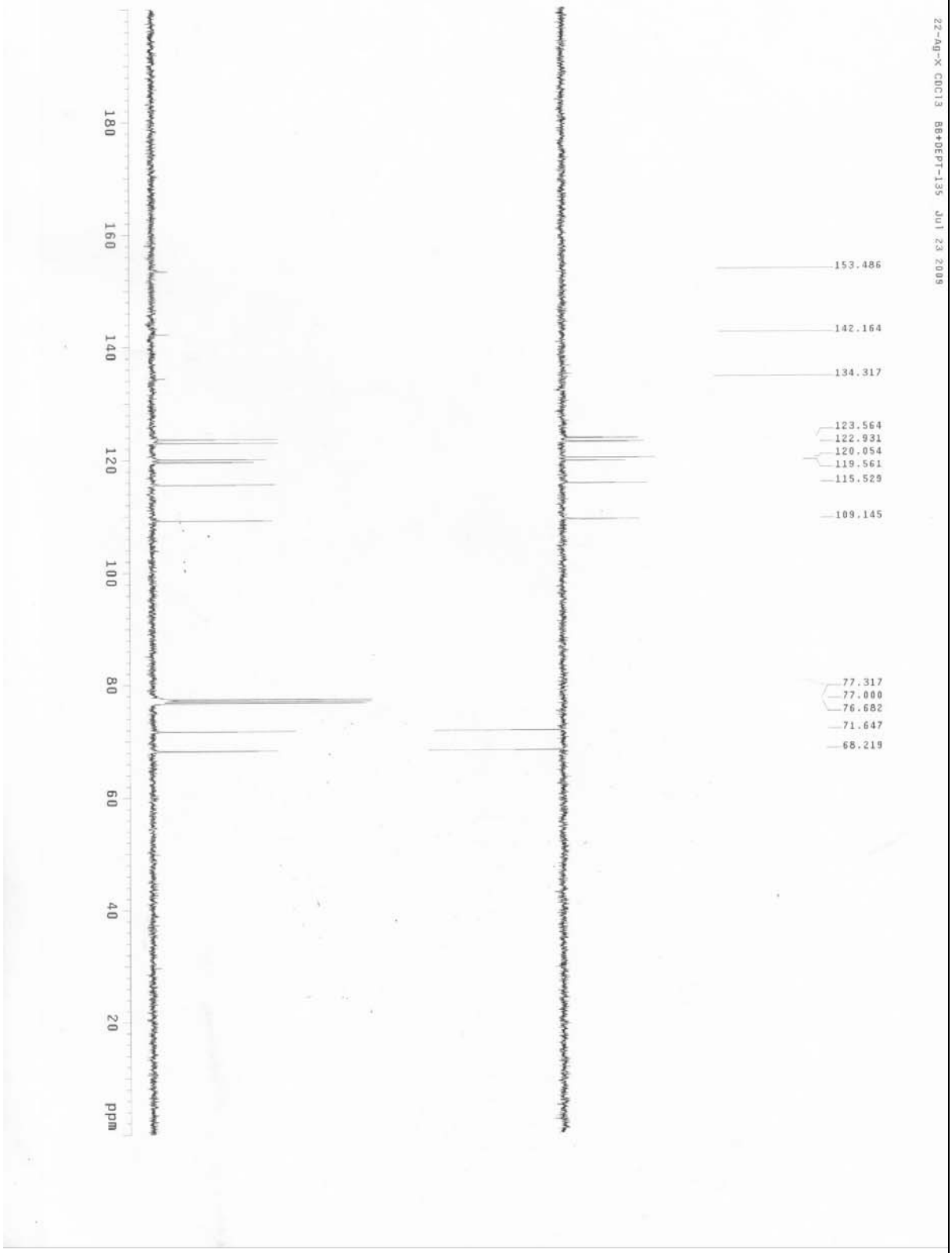
1-[1-Phenyl-meth-(*Z*)-ylidene]-1,2,3,4-tetrahydro-naphth[2',3':4,5]imidazo[1,2-*a*]pyridine (B14)



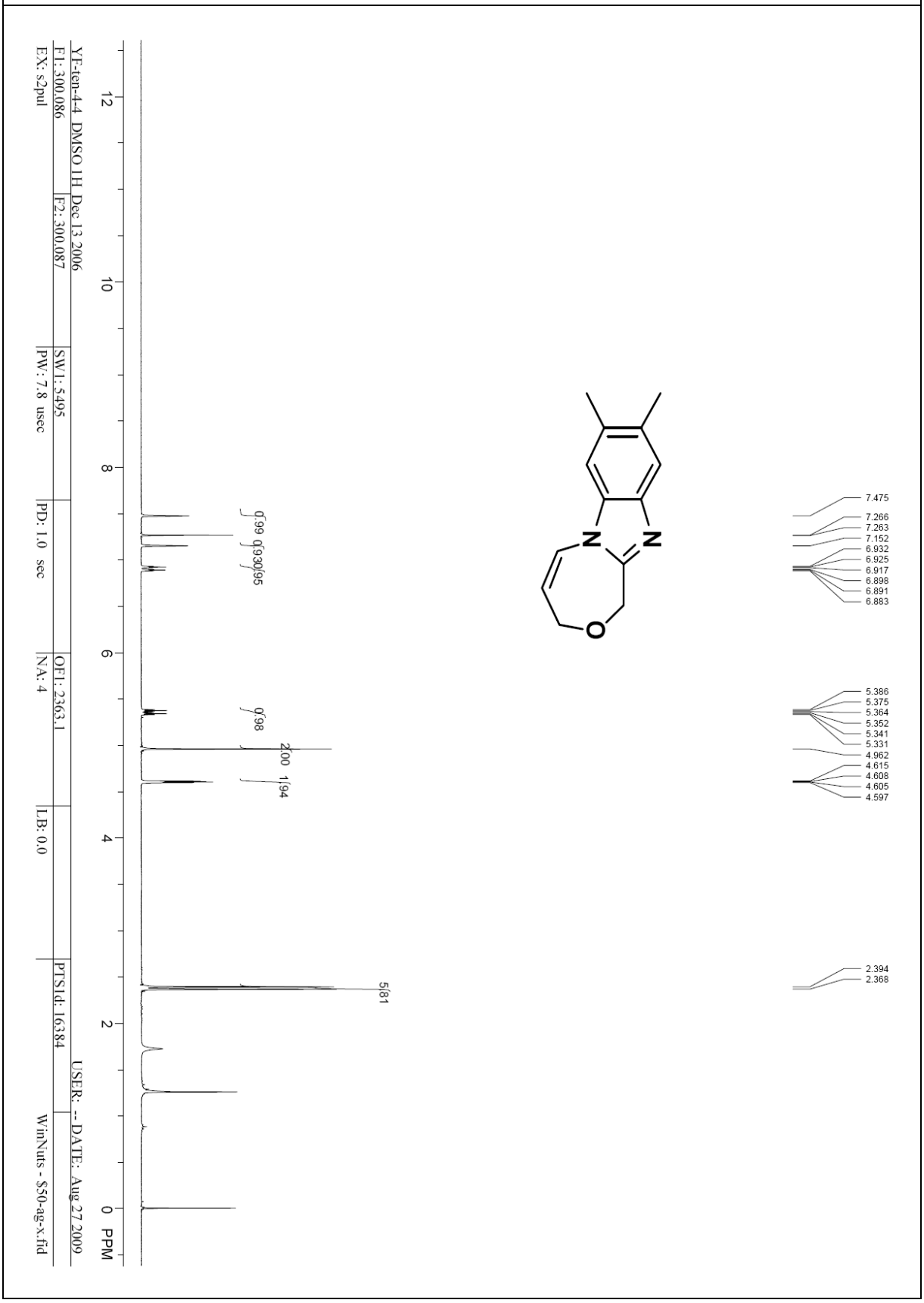

180
160
140
120
100
80
60
40
20
ppm
143.286
135.361
132.865
129.995
129.594
128.756
128.515
128.055
127.914
127.855
127.071
123.869
123.641
115.151
114.573
110.738
77.319
77.000
76.681
33.183
25.052
21.267

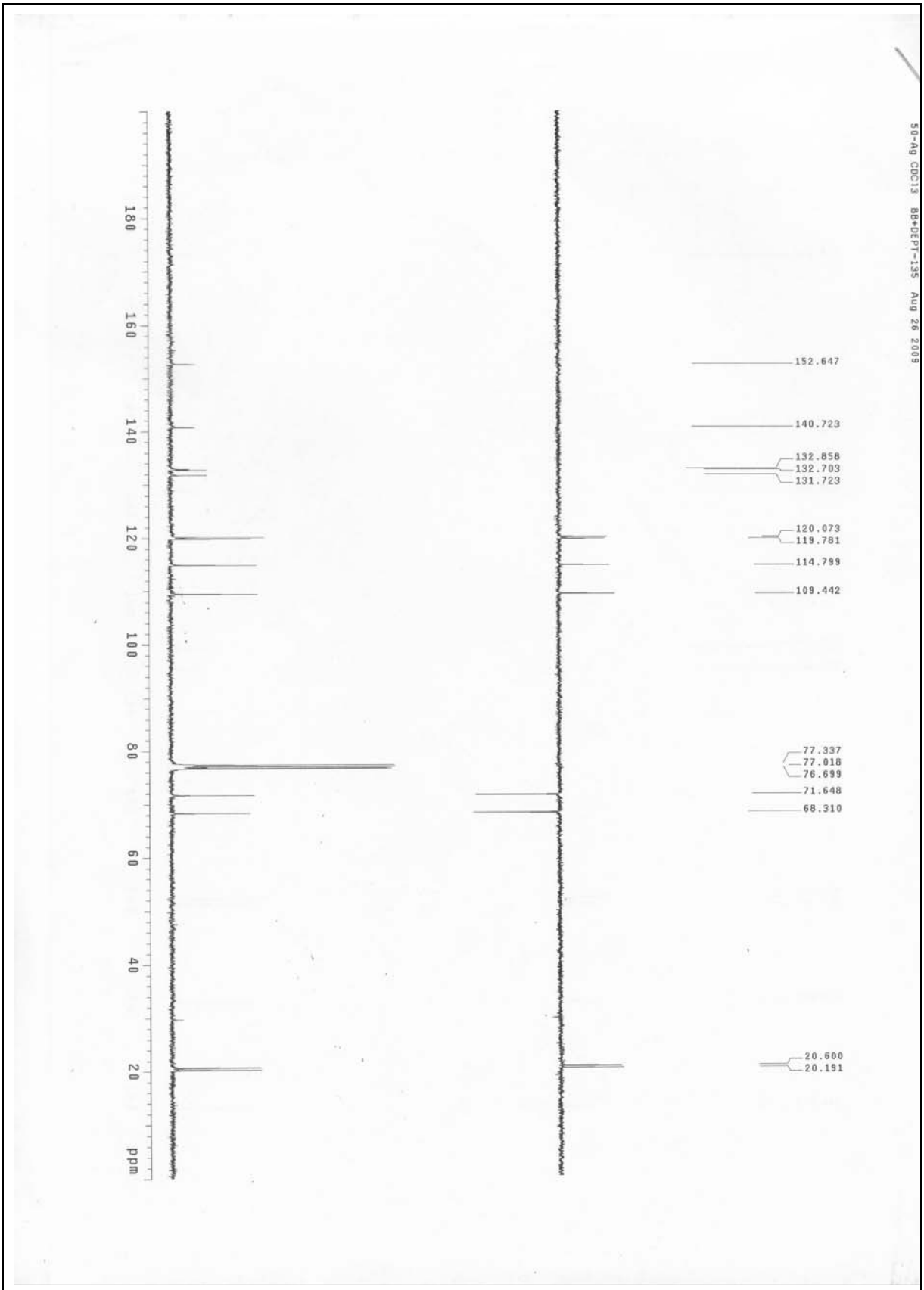
7*H*,9*H*-8-Oxa-4*b*,10-diaza-benz[*a*]azulene (C17)



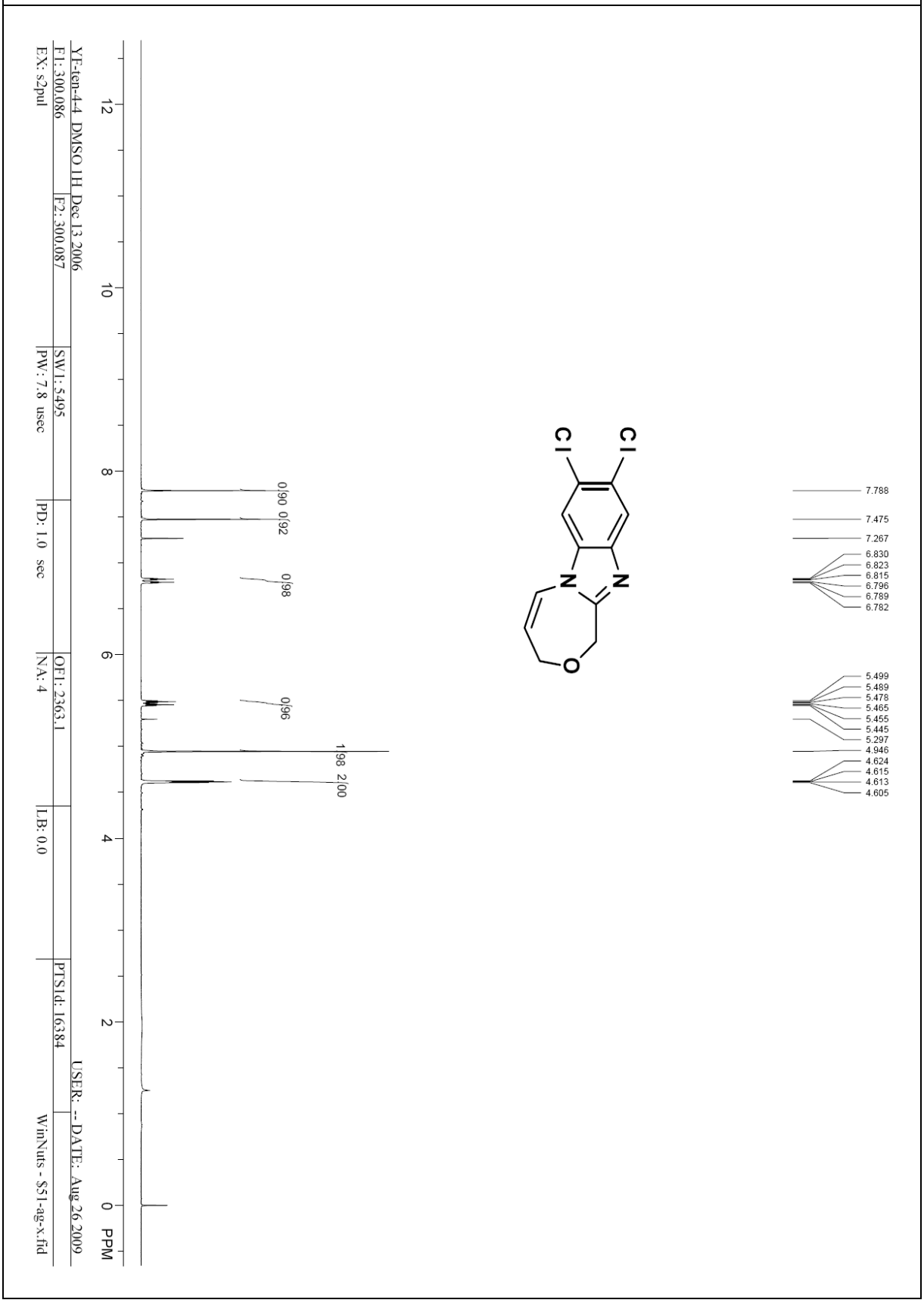

22-Ag-X CDCl3 BB+DEPT-135 Jul 23 2009
153.486
142.164
134.317
123.564
122.931
120.054
119.561
115.529
109.145
77.317
77.000
76.682
71.647
68.219
180
160
140
120
100
80
60
40
20
ppm

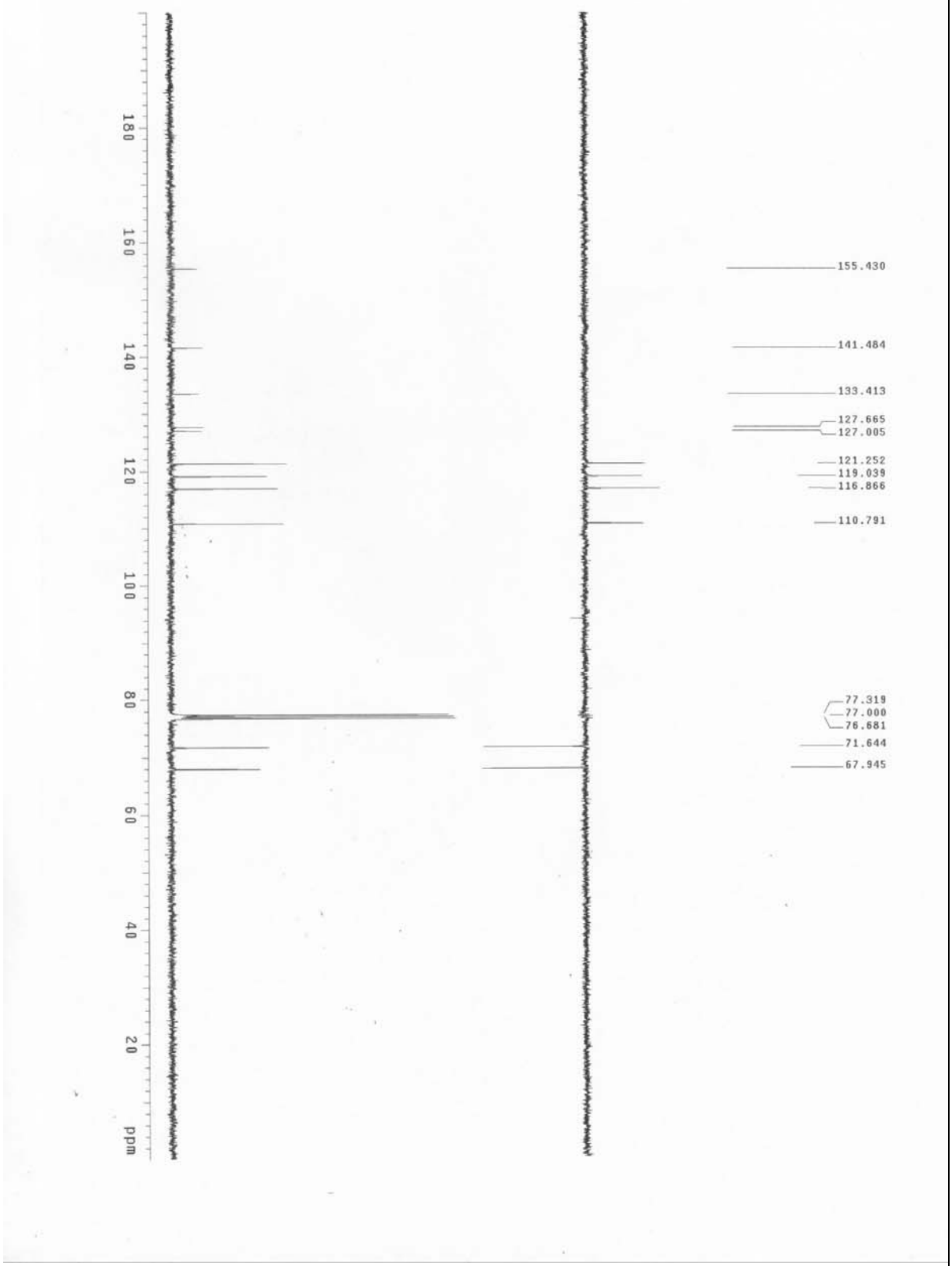
2,3-Dimethyl-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C18)



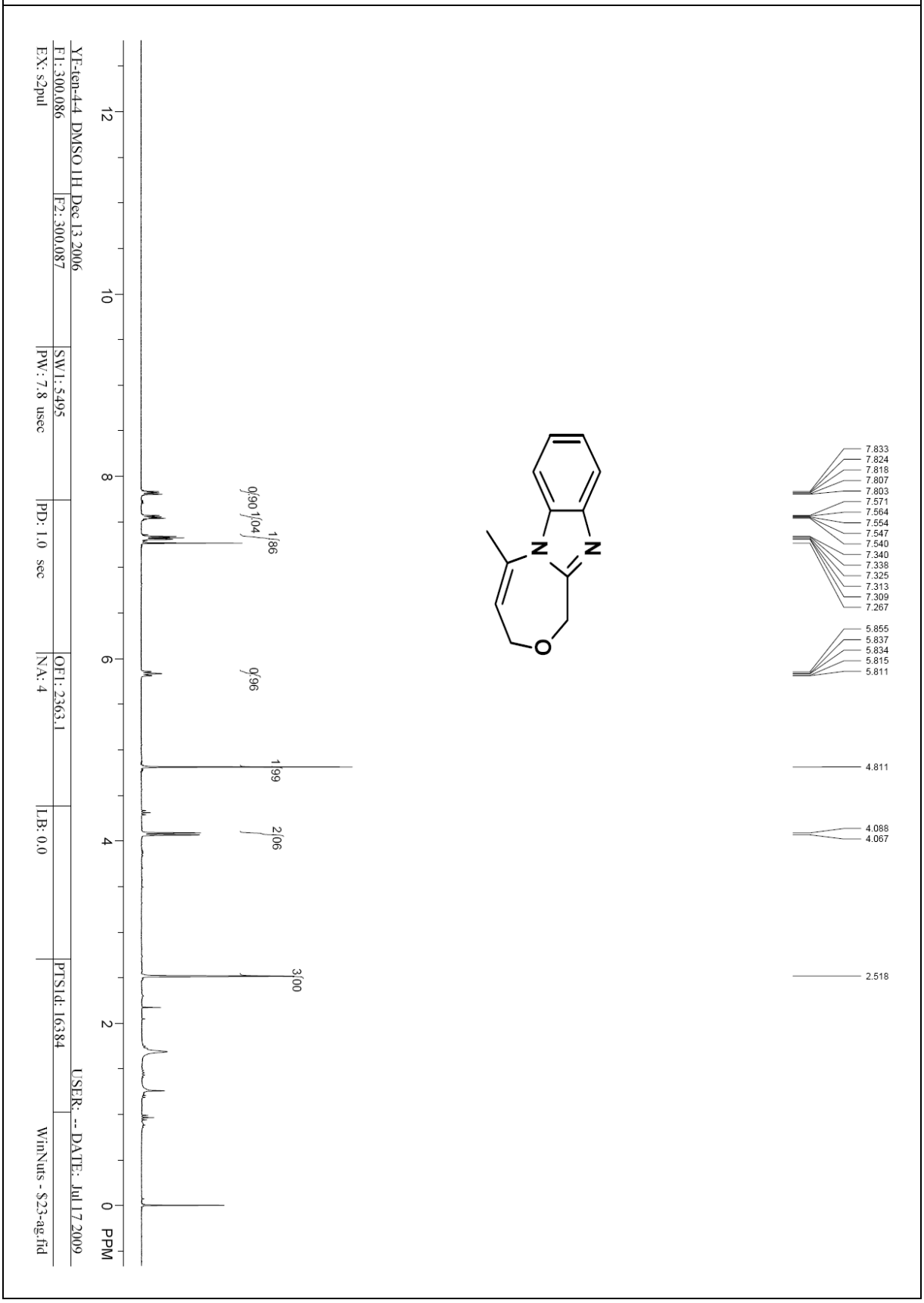

50-Ag CDCl3 BB+DEPT-135 Aug 26 2009
152.647
140.723
132.858
132.703
131.723
120.073
119.781
114.799
109.442
77.337
77.018
76.699
71.648
68.310
20.600
20.191
180
160
140
120
100
80
60
40
20
ppm

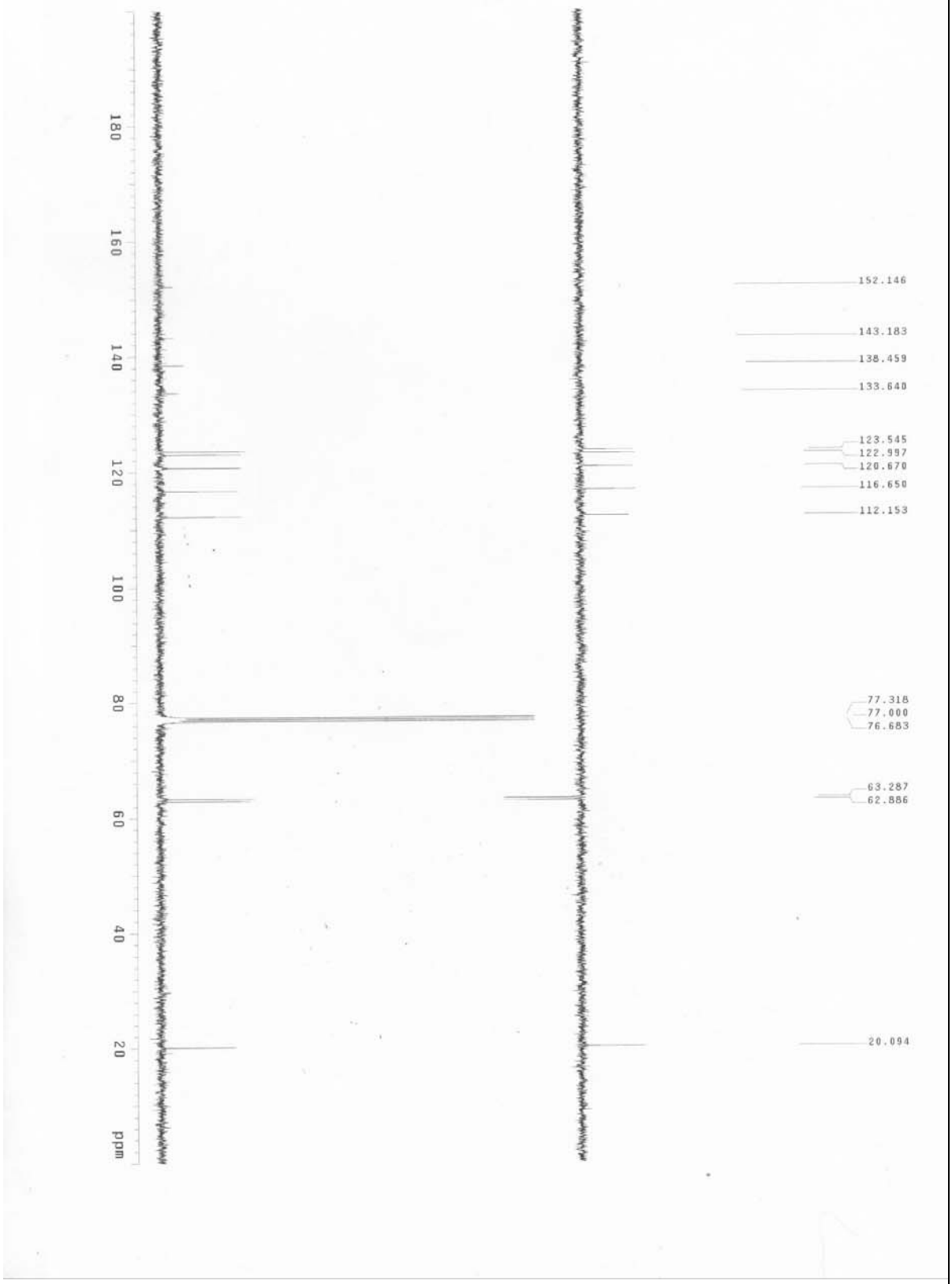
2,3-Dichloro-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C19)



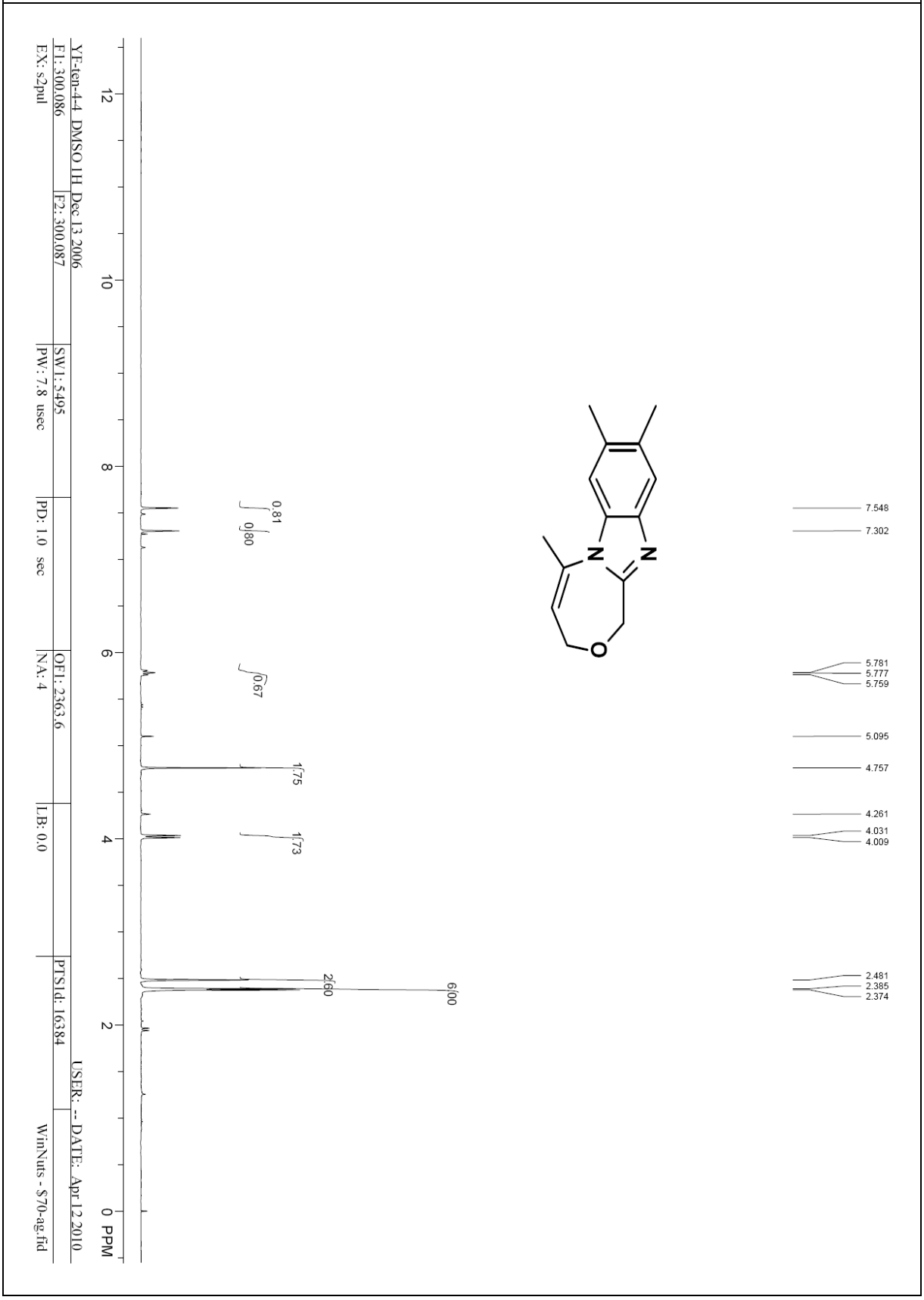

155.430
141.484
133.413
127.665
127.005
121.252
119.039
116.866
110.791
77.319
77.000
76.681
71.644
67.945
180
160
140
120
100
80
60
40
20
ppm

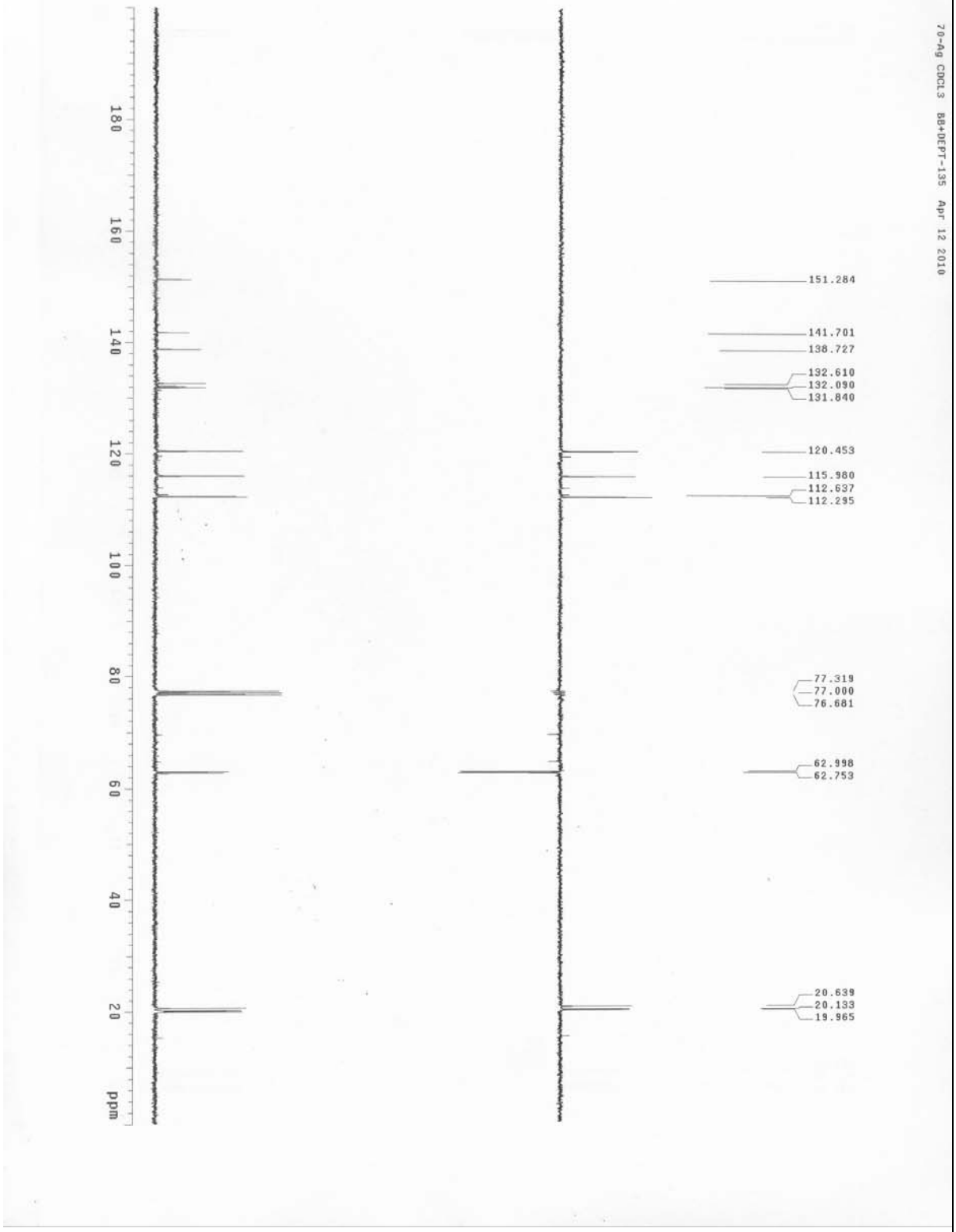
5-Methyl-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C20)



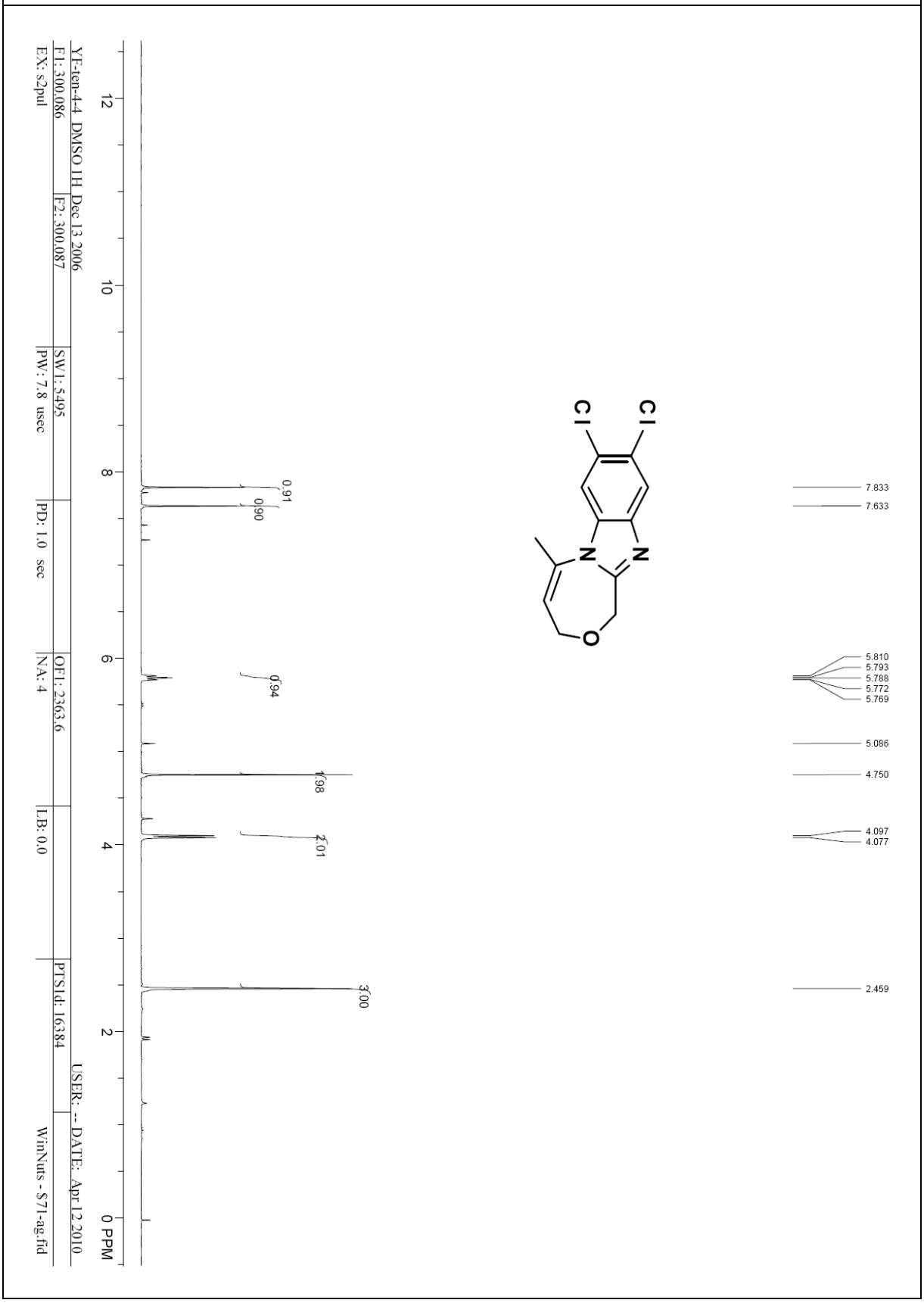

180
160
140
120
100
80
60
40
20
ppm
152.146
143.183
138.459
133.640
123.545
122.997
120.670
116.650
112.153
77.318
77.000
76.683
63.287
62.886
20.094

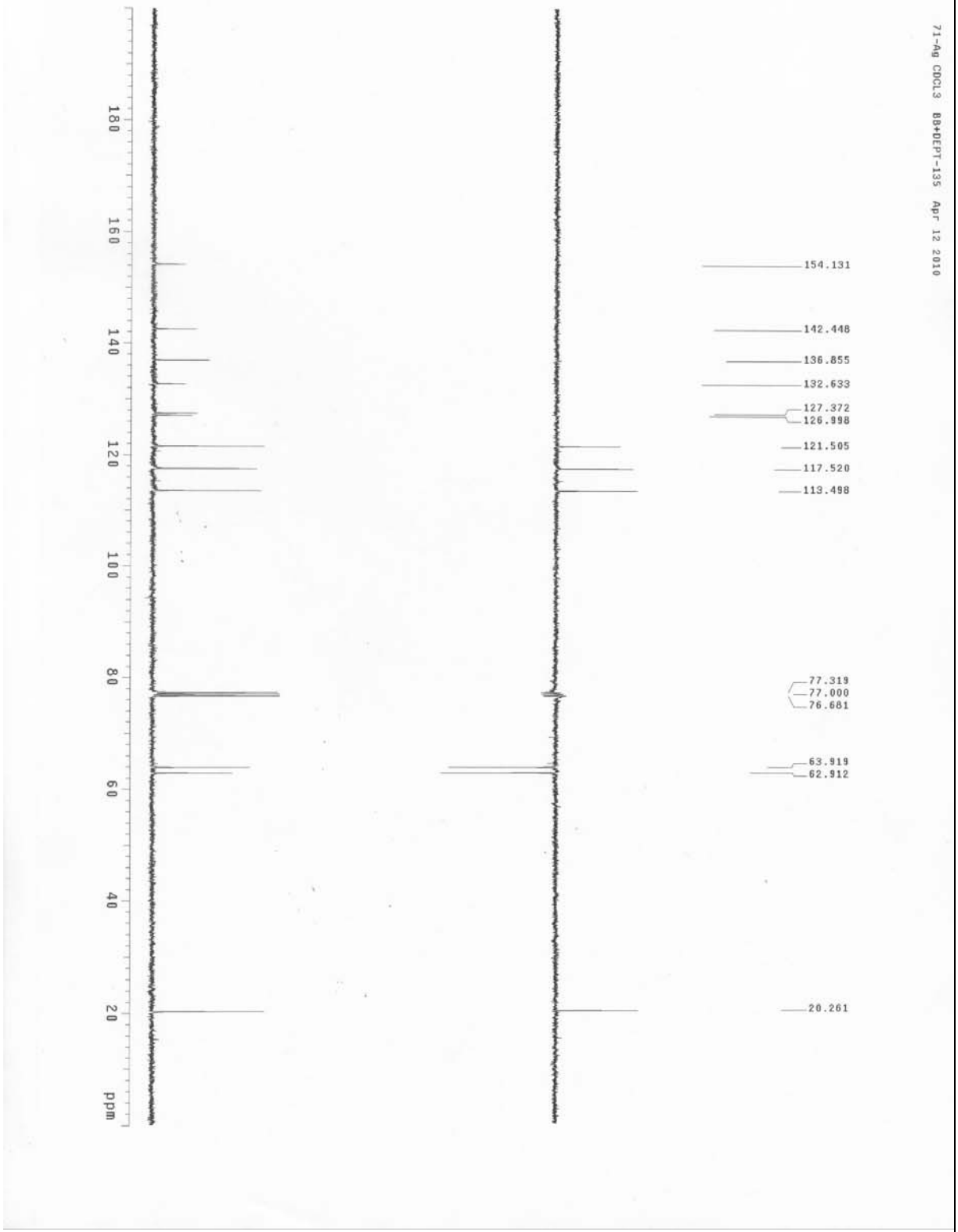
2,3,5-Trimethyl-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C21)



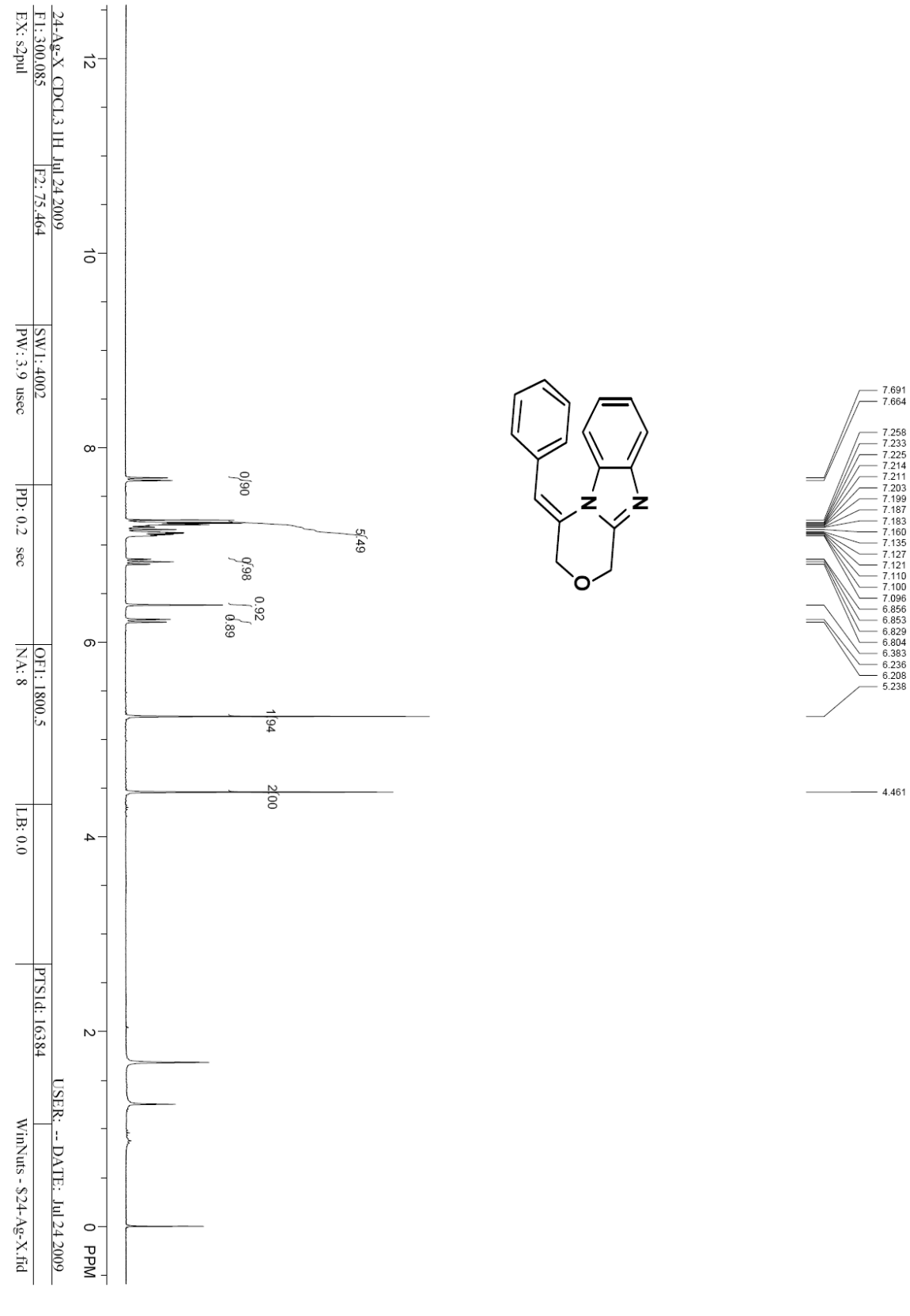

70-Ag CDCl3 BB+DEPT-135 Apr 12 2010
151.284
141.701
138.727
132.610
132.090
131.840
120.453
115.980
112.637
112.295
77.319
77.000
76.681
62.998
62.753
20.639
20.133
19.965
180
160
140
120
100
80
60
40
20
ppm

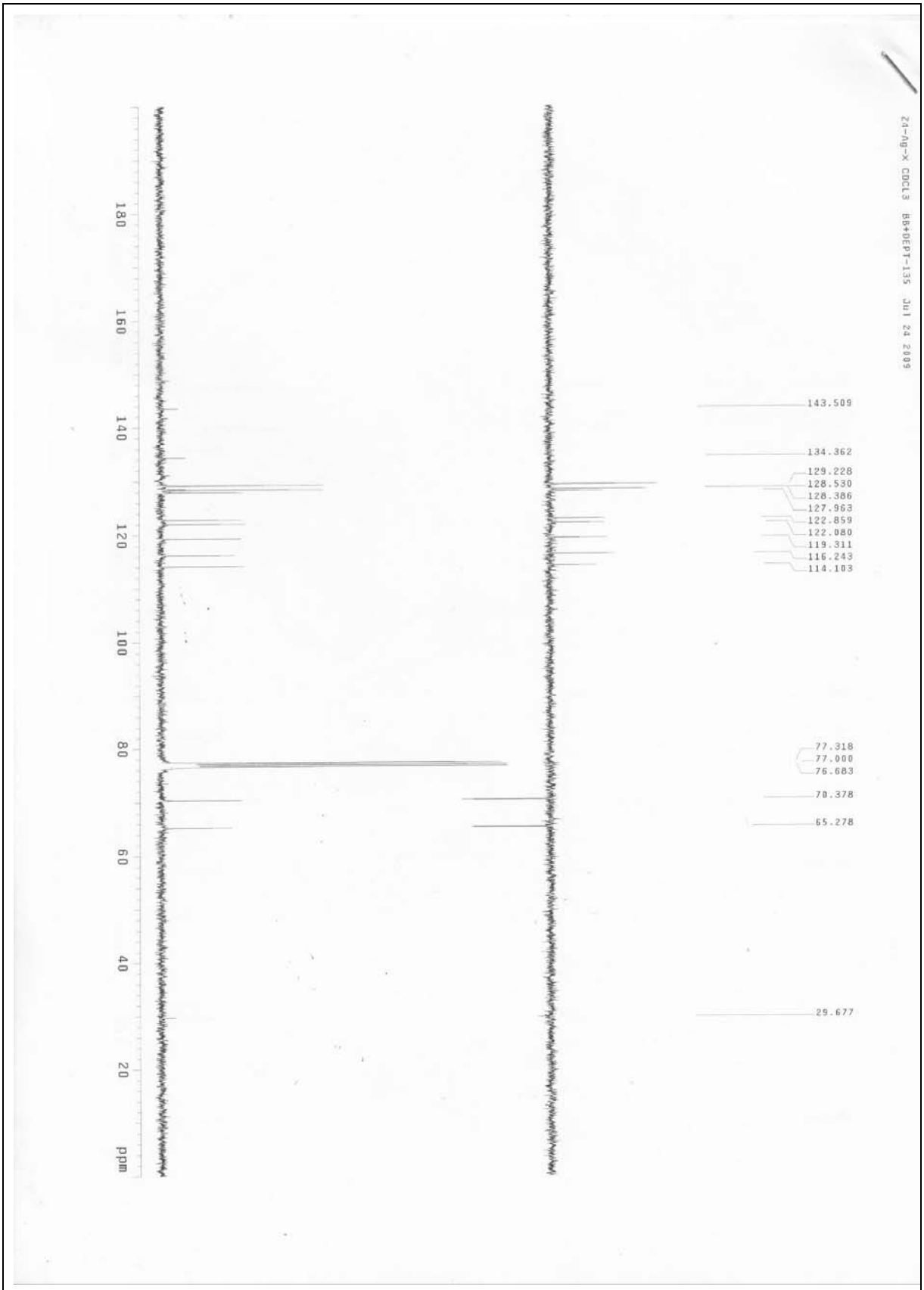
2,3-Dichloro-5-methyl-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C22)



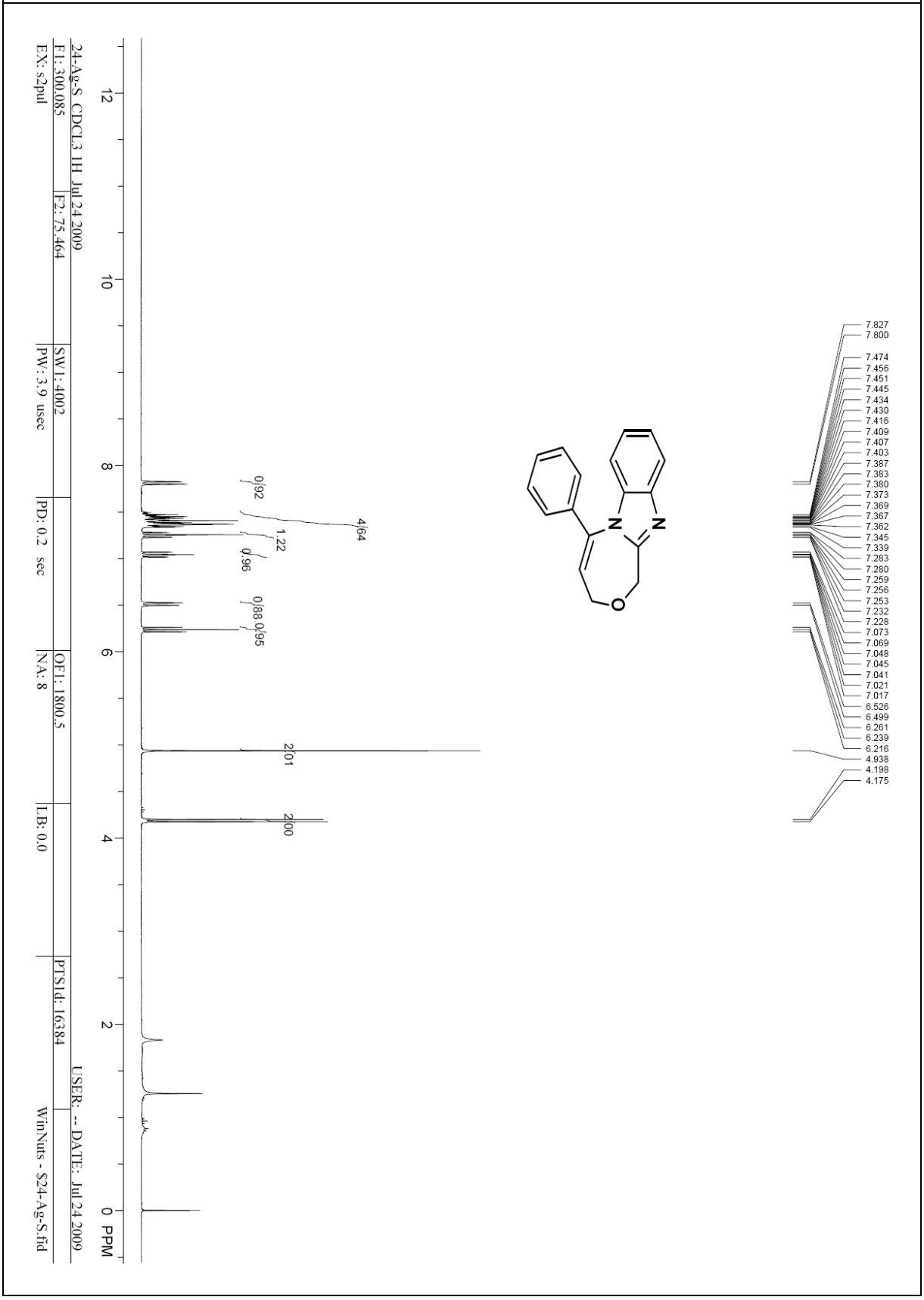

71-Ag CDCL3 BB+DEPT-135 Apr 12 2010
154.131
142.448
136.855
132.633
127.372
126.998
121.505
117.520
113.498
77.319
77.000
76.681
63.919
62.912
20.261
180
160
140
120
100
80
60
40
20
ppm

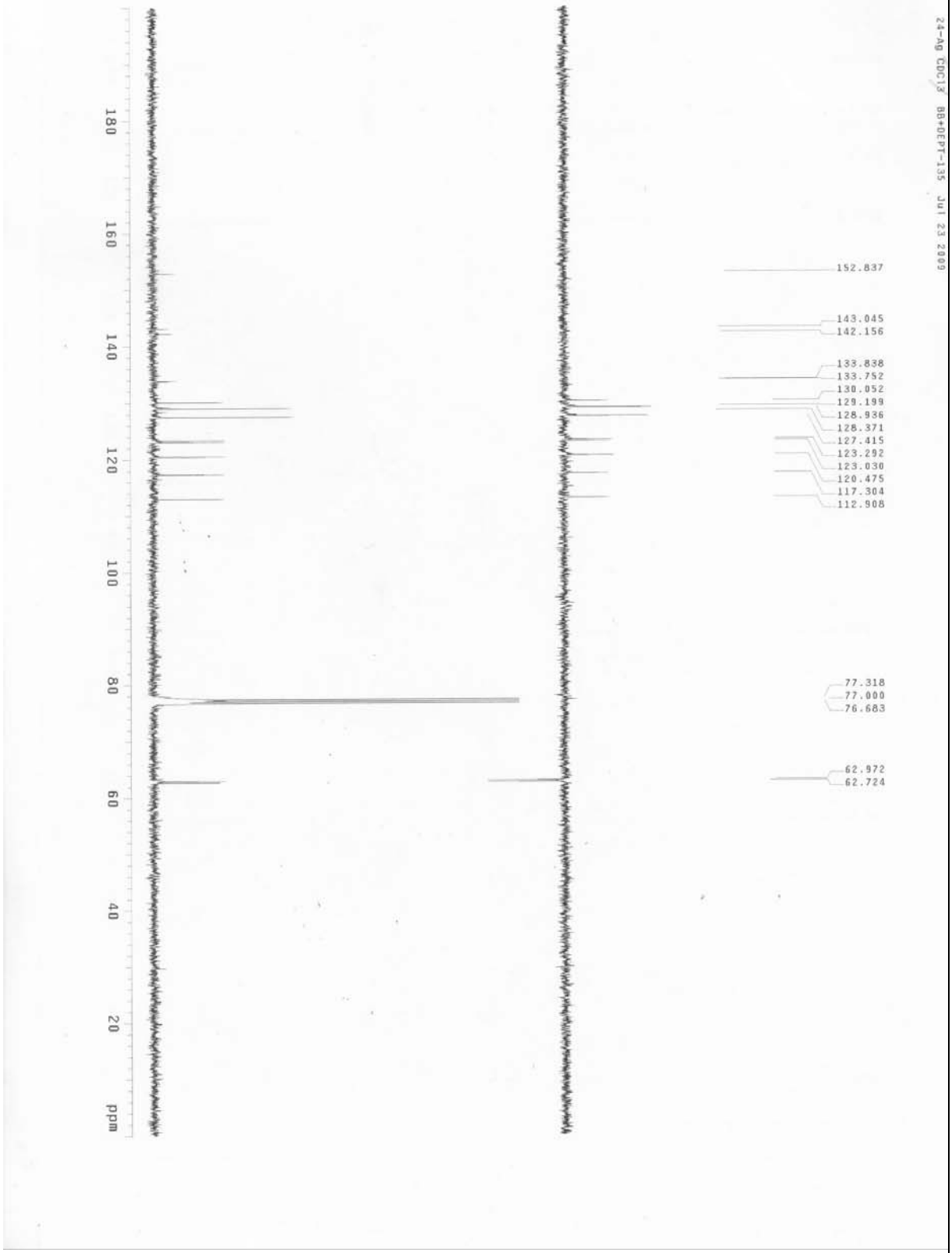
4-[1-Phenyl-meth-(*Z*)-ylidene]-3,4-dihydro-1*H*-2-oxa-4*a*,9-diaza-fluorene (B23)



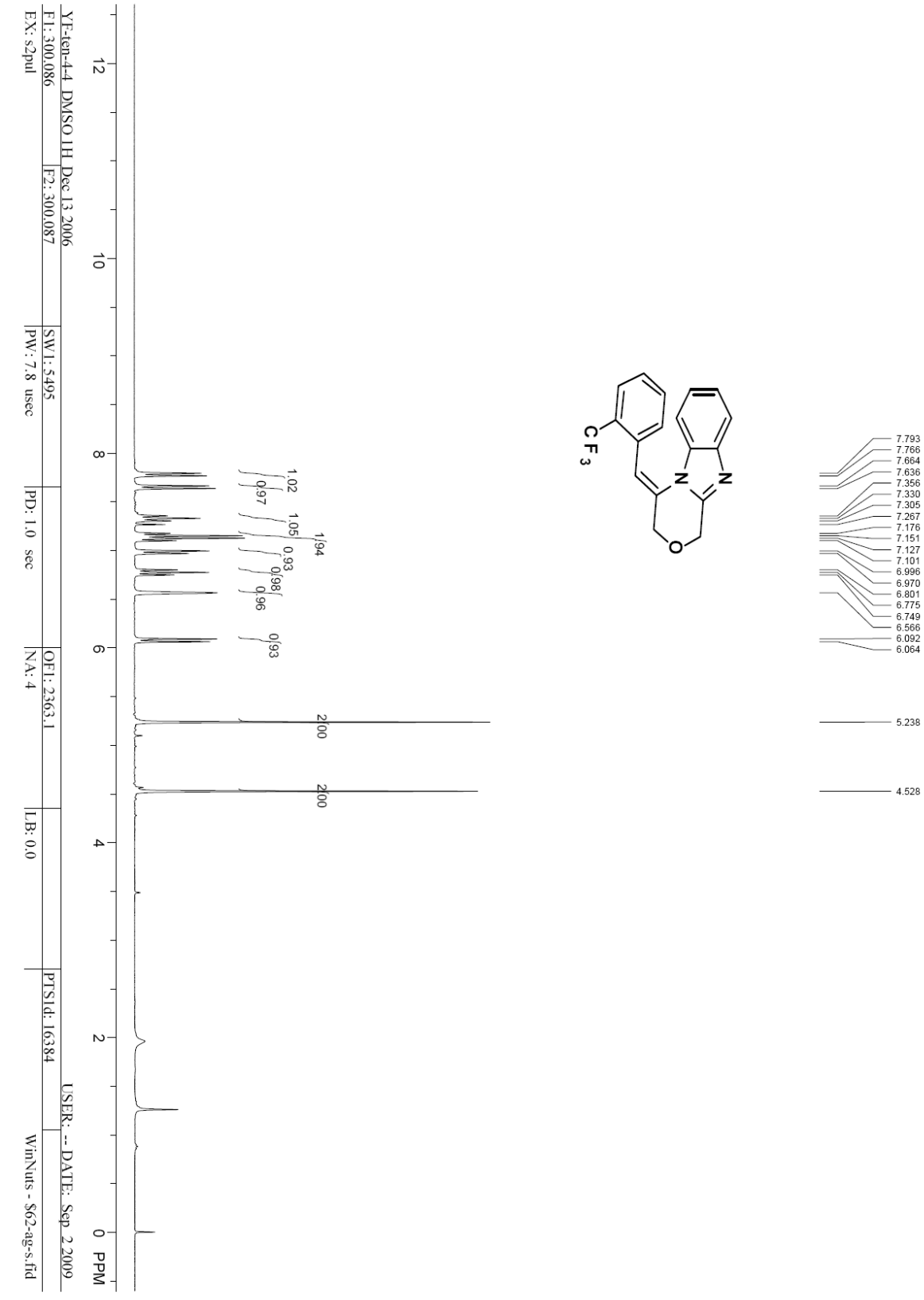

24-Ag-X CDCl3 BB+DEPT-135 Jul 24 2009
143.509
134.362
129.228
128.530
128.386
127.963
122.859
122.080
119.311
116.243
114.103
77.318
77.000
76.683
70.378
65.278
29.677
180
160
140
120
100
80
60
40
20
ppm

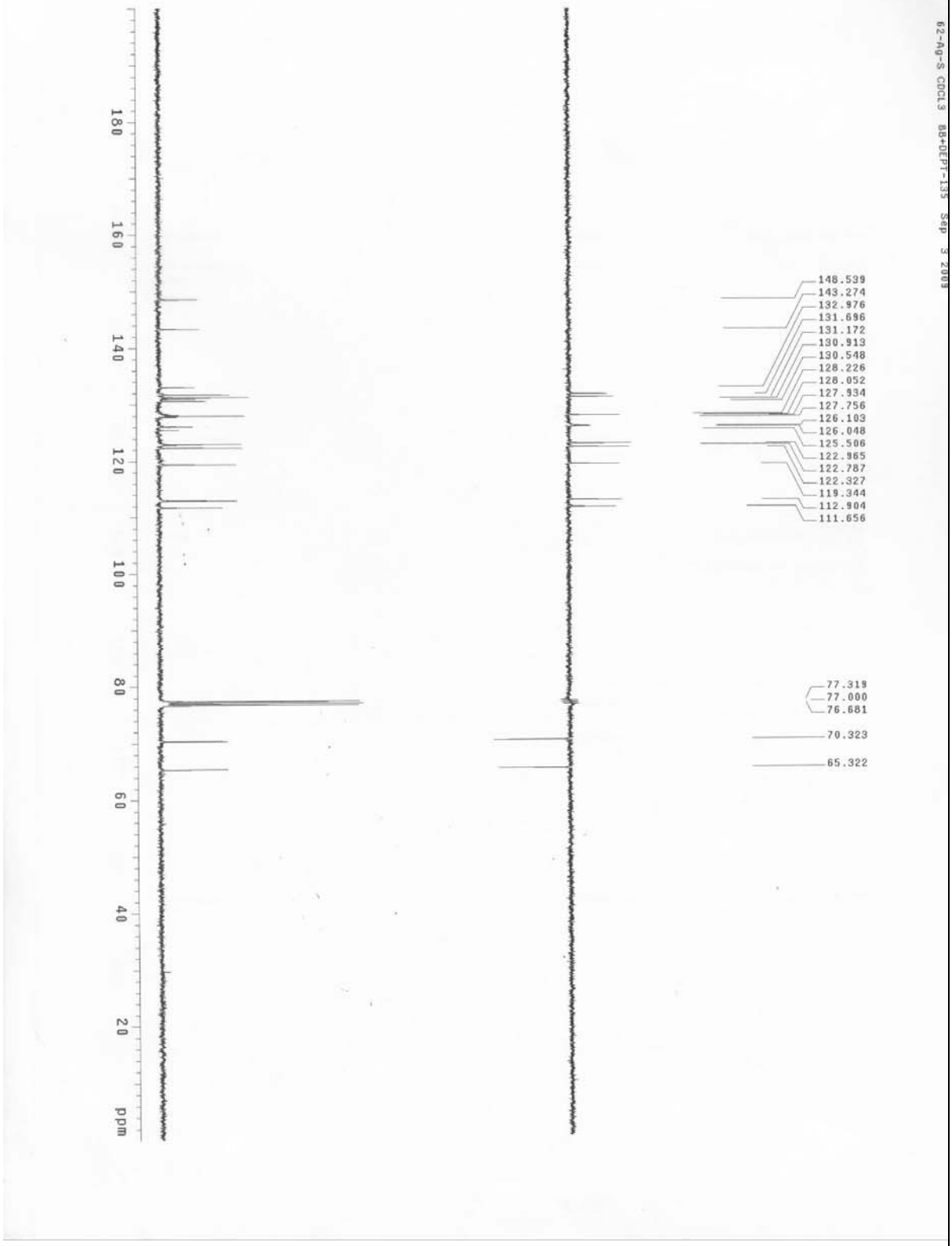
5-Phenyl-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C23)



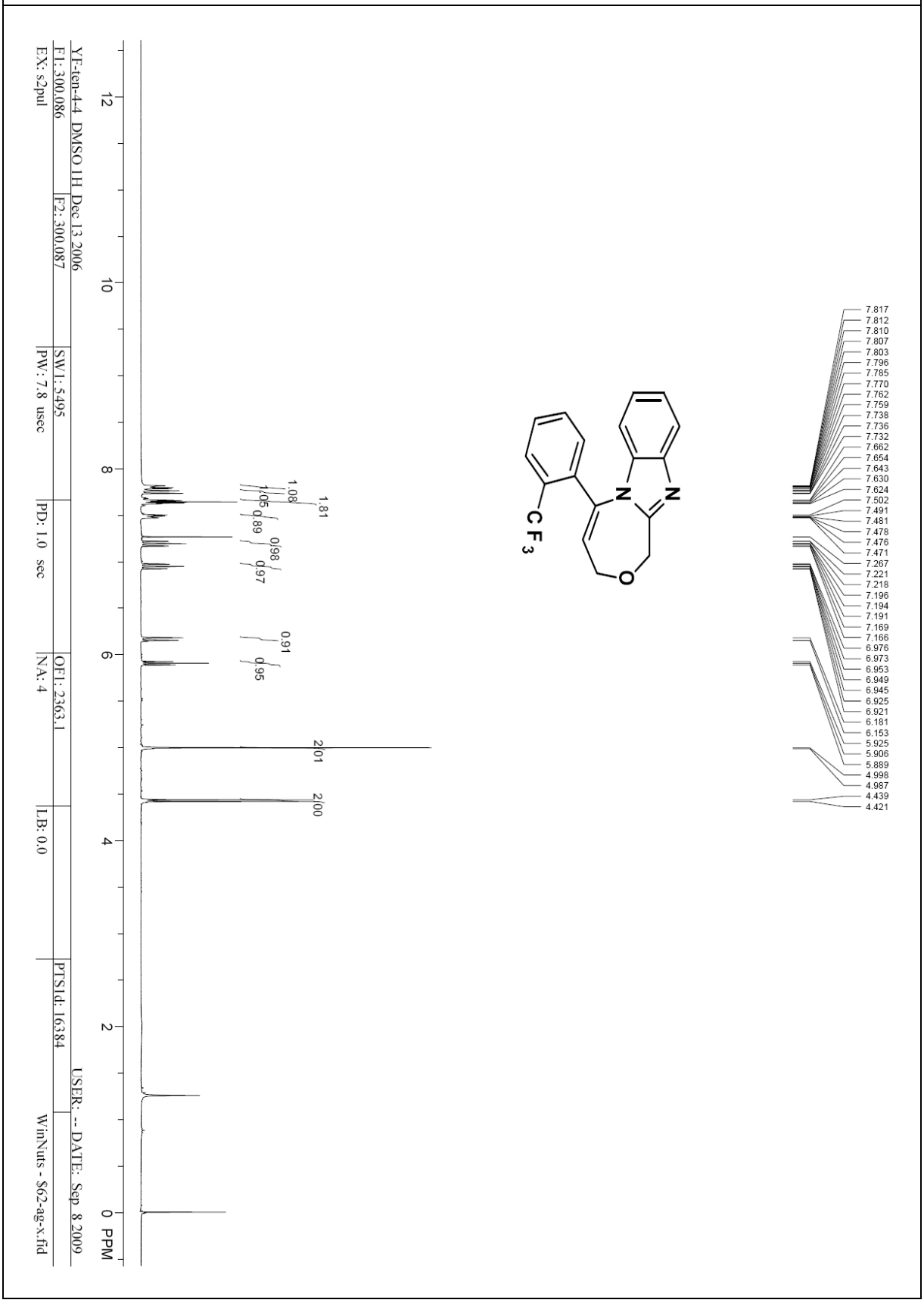

24-Ag CDCl3 BB+DEPT-135 Jul 23 2009
152.837
143.045
142.156
133.838
133.752
130.052
129.199
128.936
128.371
127.415
123.292
123.030
120.475
117.304
112.908
77.318
77.000
76.683
62.972
62.724
180
160
140
120
100
80
60
40
20
ppm

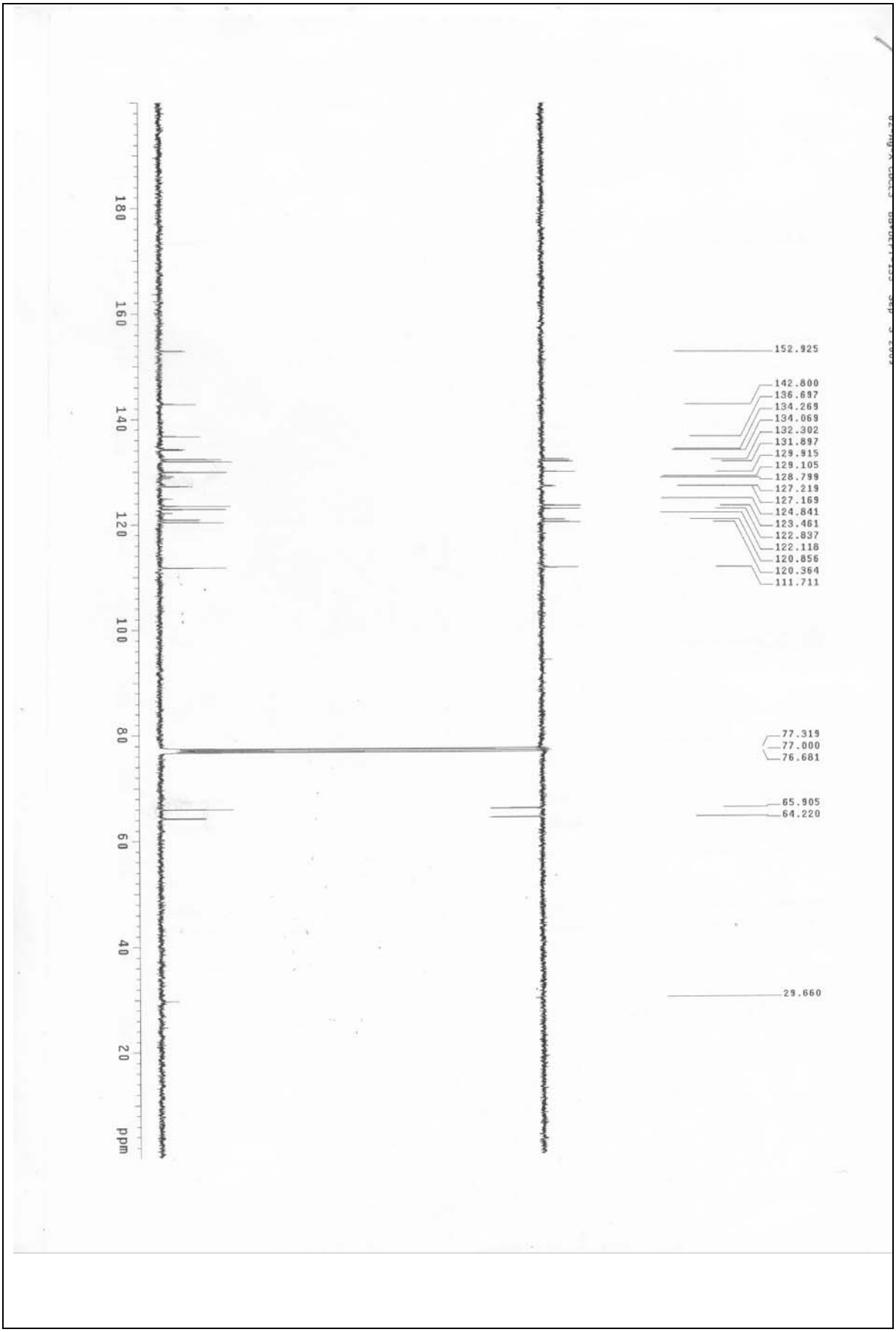
4-[1-(2-Trifluoromethyl-phenyl)-meth-(*Z*)-ylidene]-3,4-dihydro-1*H*-2-oxa-4*a*,9-diaza-fluorene (B24)



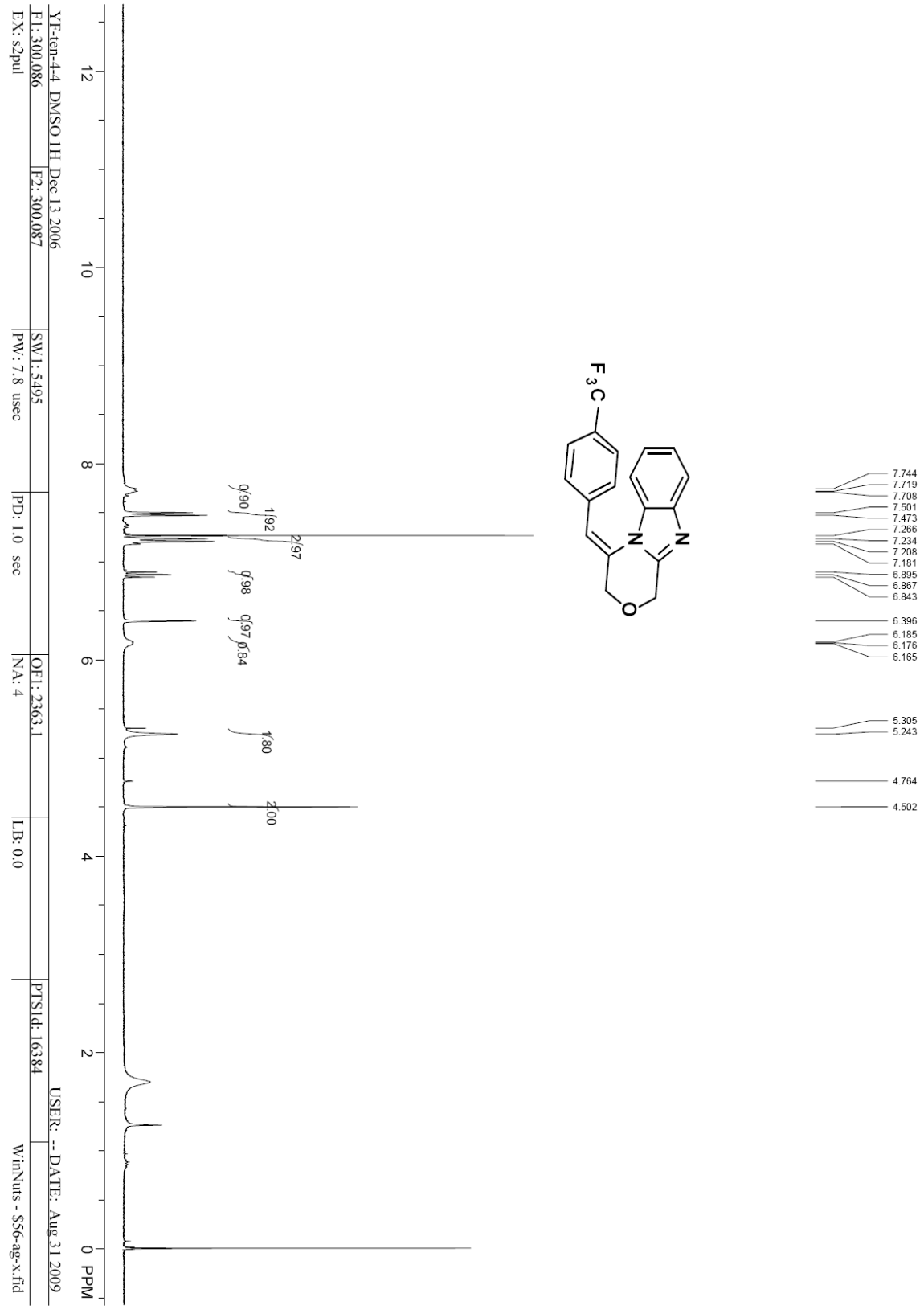

62-Ag-S CDCl3 BB+DEPT-135 Sep 3 2009
148.539
143.274
132.976
131.696
131.172
130.913
130.548
128.226
128.052
127.934
127.756
126.103
126.048
125.506
122.965
122.787
122.327
119.344
112.904
111.656
77.319
77.000
76.681
70.323
65.322
180
160
140
120
100
80
60
40
20
ppm

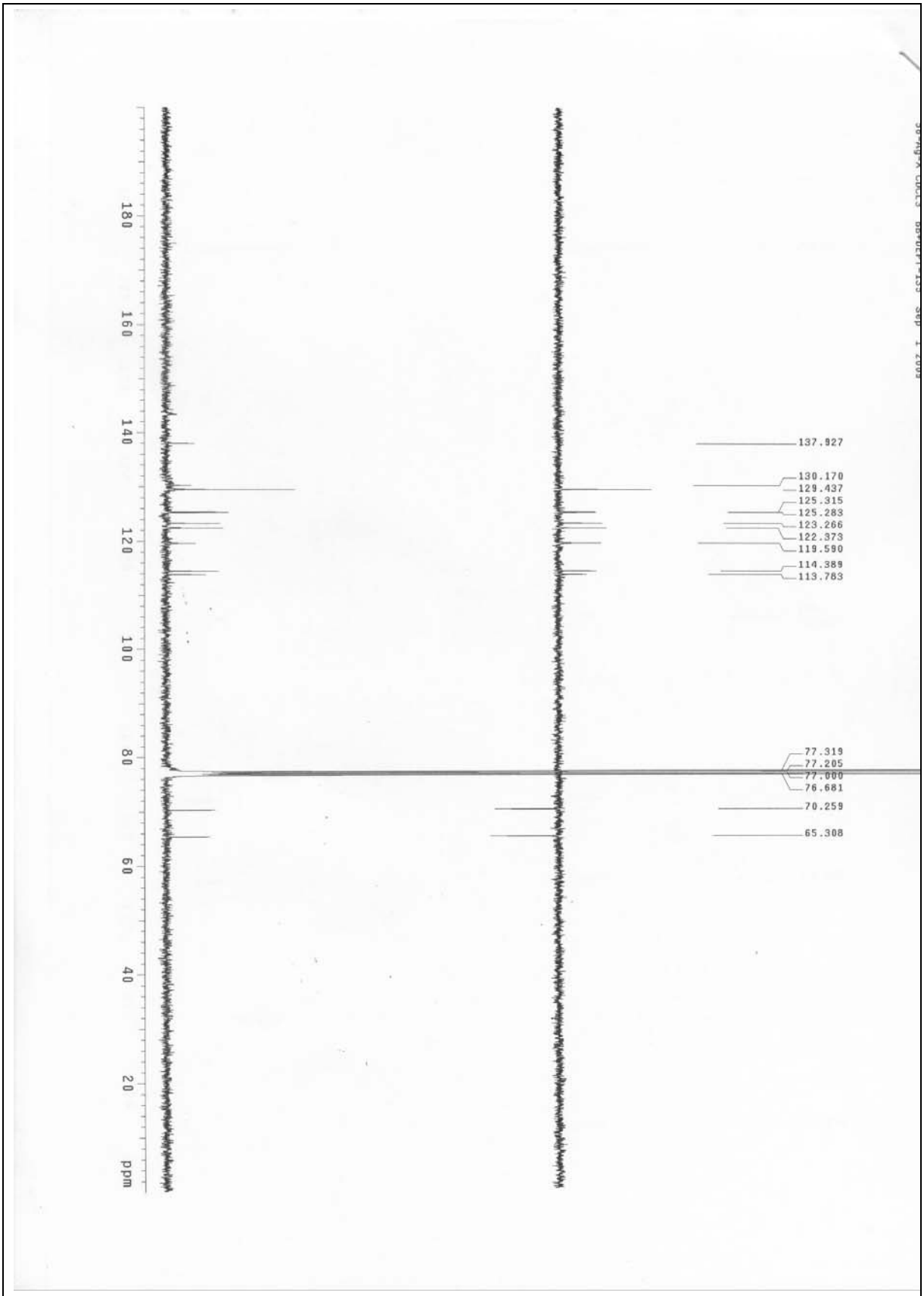
5-(2-tert-Butyl-phenyl)-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C24)



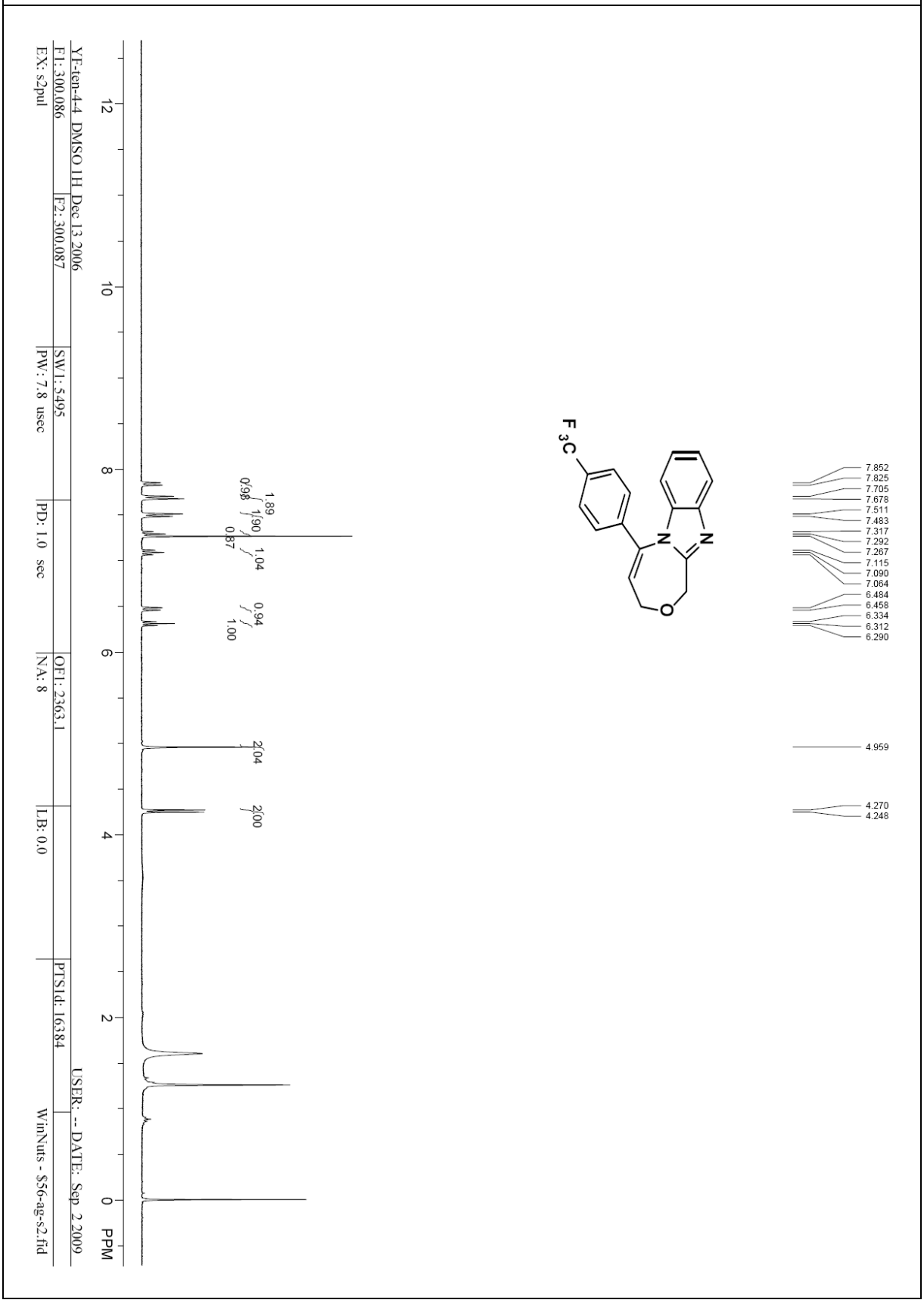

152.925
142.800
136.697
134.269
134.069
132.302
131.897
129.915
129.105
128.799
127.219
127.169
124.841
123.461
122.837
122.118
120.856
120.364
111.711
77.319
77.000
76.681
65.905
64.220
29.660
180
160
140
120
100
80
60
40
20
ppm

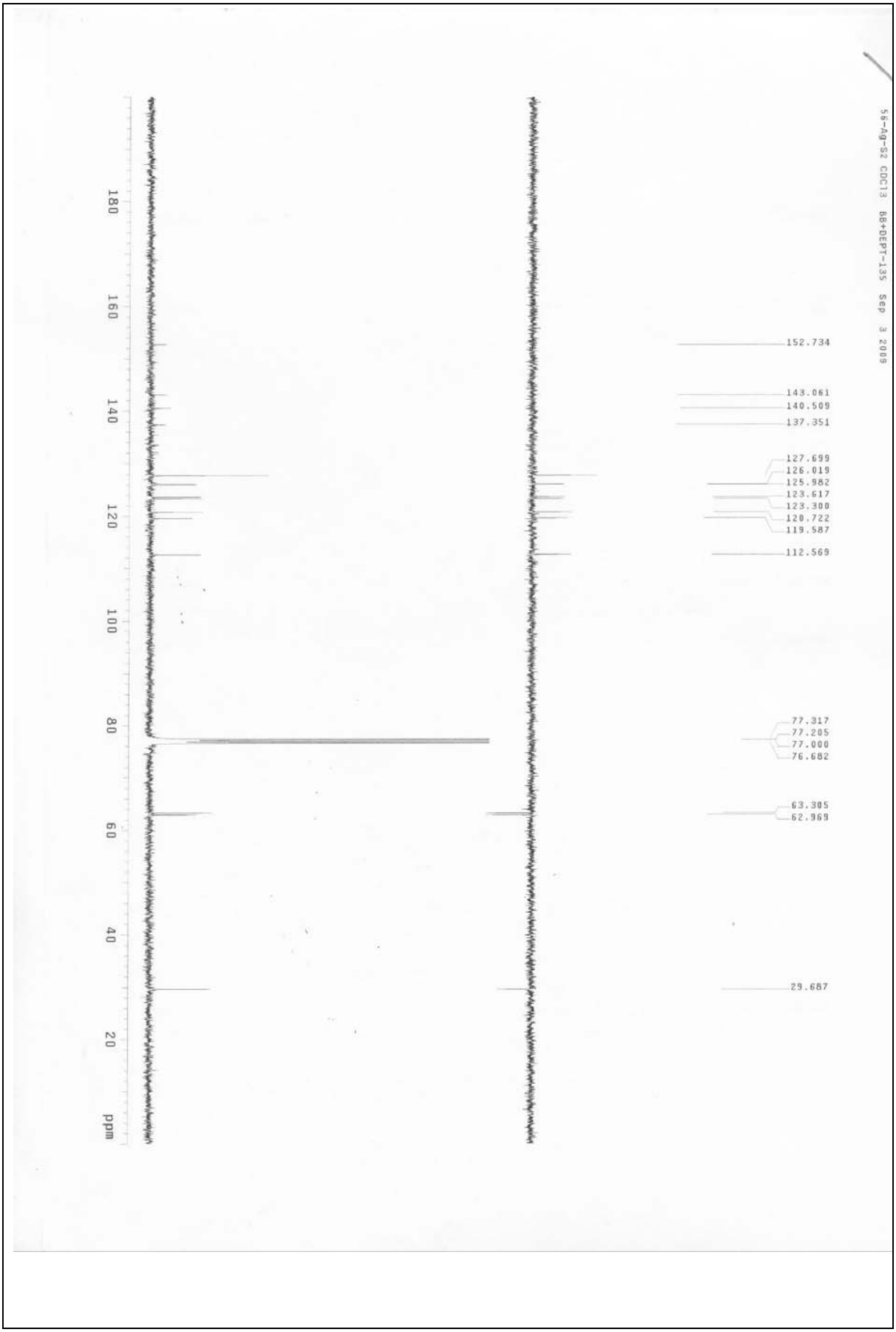
4-[1-(4-Trifluoromethyl-phenyl)-meth-(*Z*)-ylidene]-3,4-dihydro-1*H*-2-oxa-4*a*,9-diaza-fluorene (B25)



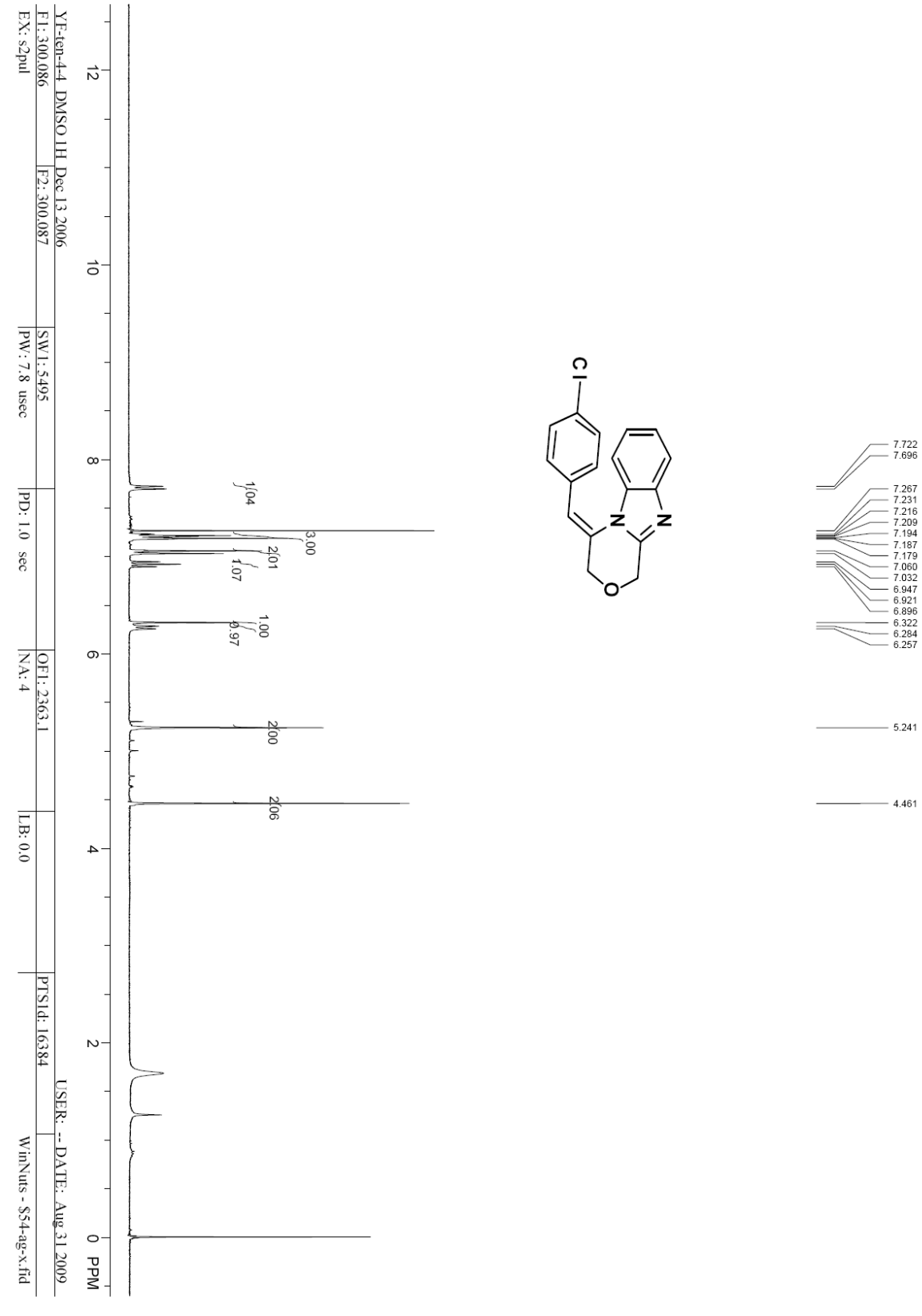

137.927
130.170
129.437
125.315
125.283
123.266
122.373
119.590
114.389
113.783
77.319
77.205
77.000
76.681
70.259
65.308
180
160
140
120
100
80
60
40
20
ppm

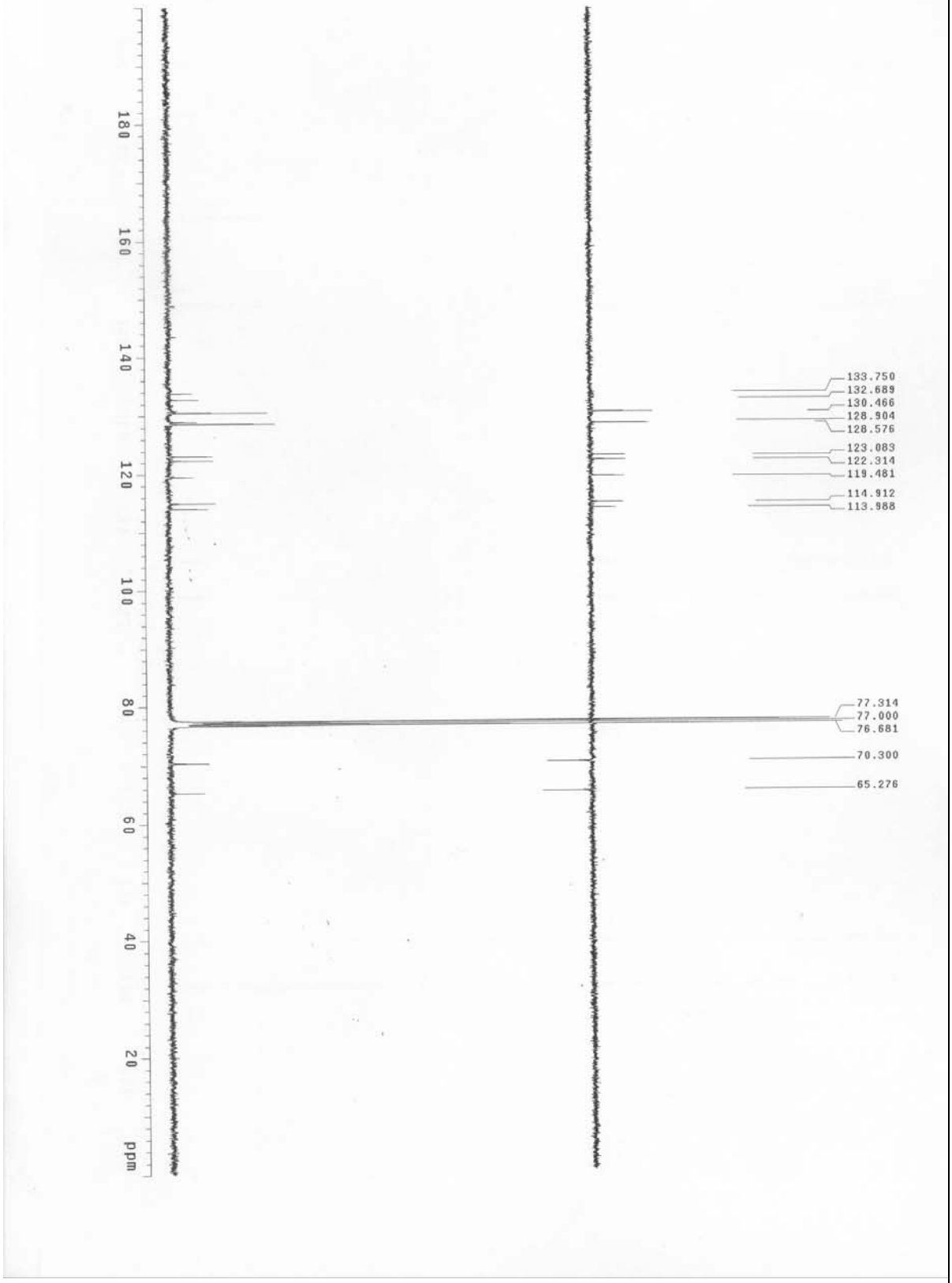
5-(4-Trifluoromethyl-phenyl)-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C25)



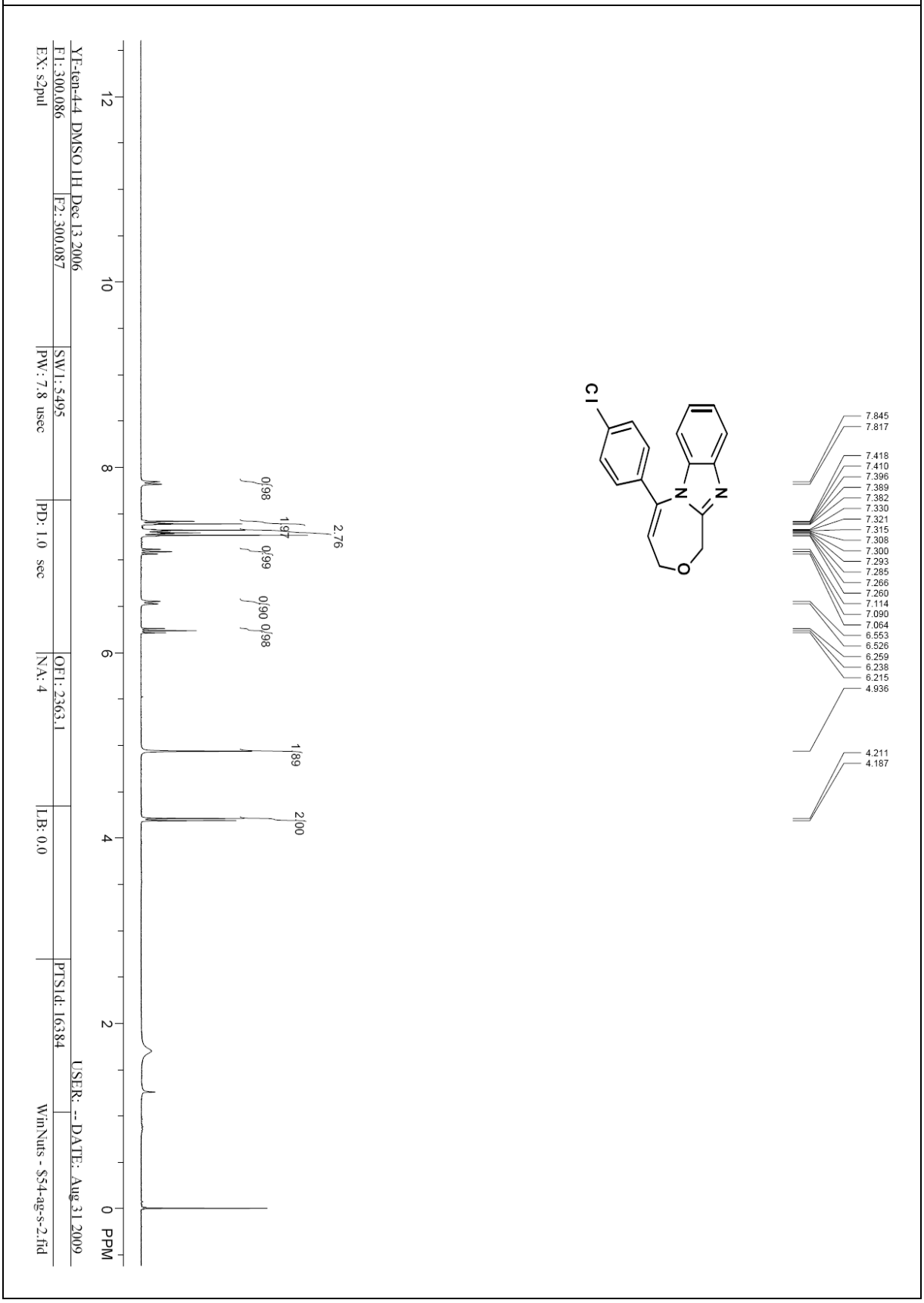

59-Ag-S2 CDCl3 BB+DEPT-135 Sep 3 2009
152.734
143.061
140.509
137.351
127.699
126.019
125.982
123.617
123.300
120.722
119.587
112.569
77.317
77.205
77.000
76.682
63.305
62.969
29.687
180
160
140
120
100
80
60
40
20
ppm

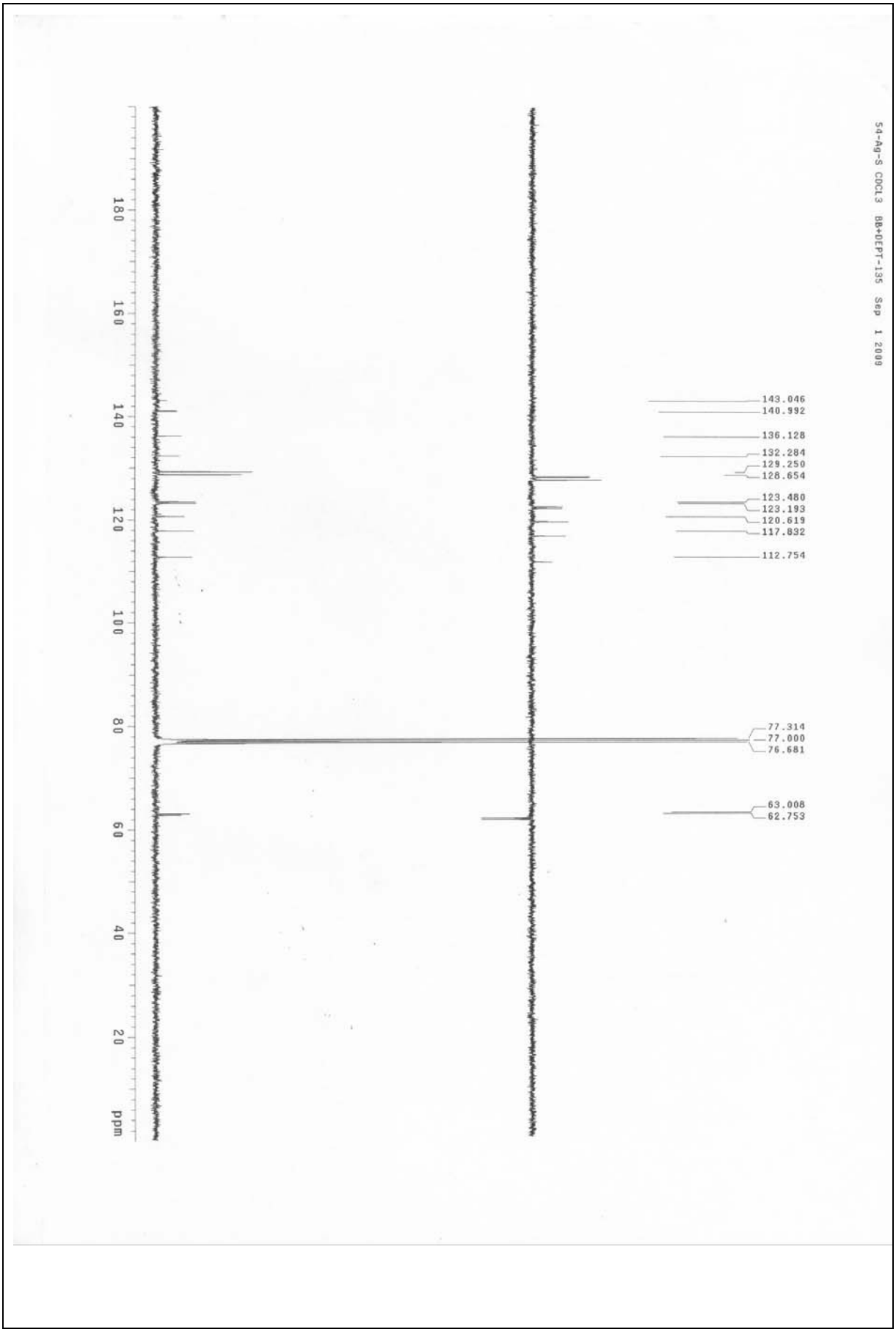
4-[1-(4-Chloro-phenyl)-meth-(*Z*)-ylidene]-3,4-dihydro-1*H*-2-oxa-4*a*,9-diaza-fluorene (B26)



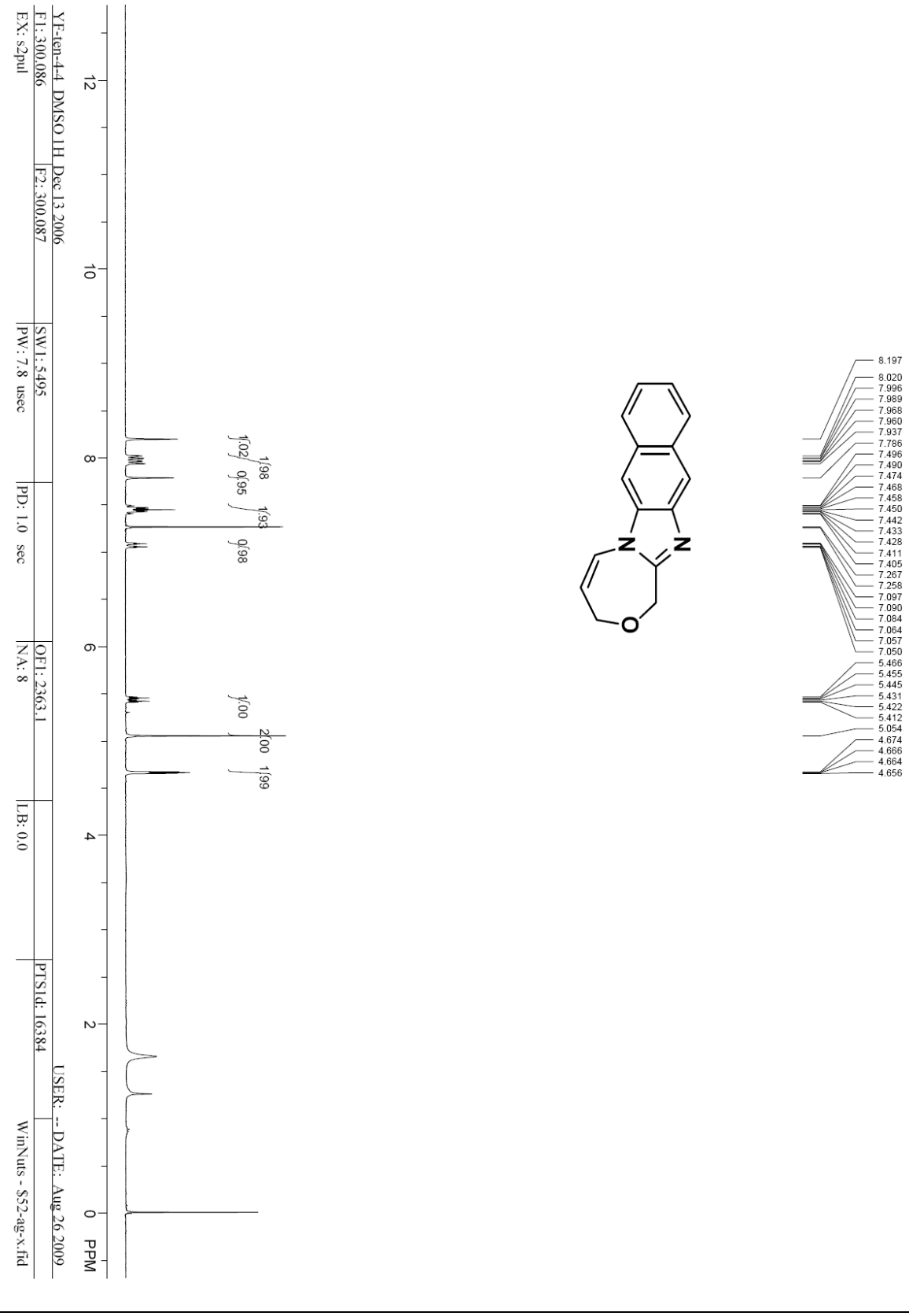

180
160
140
120
100
80
60
40
20
ppm
133.750
132.689
130.466
128.904
128.576
123.083
122.314
119.481
114.912
113.988
77.314
77.000
76.681
70.300
65.276

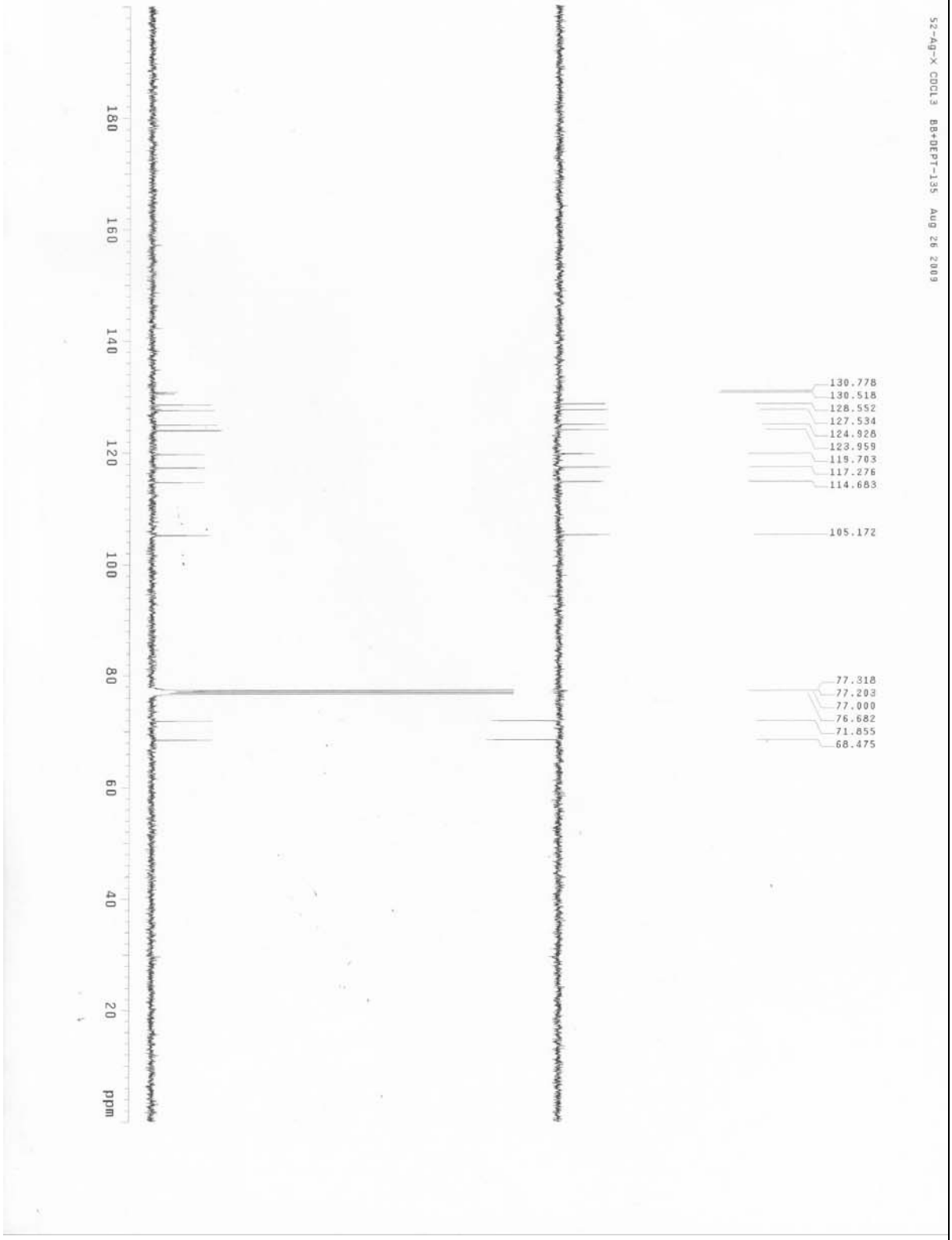
5-(4-Chloro-phenyl)-7*H*,9*H*-8-oxa-4*b*,10-diaza-benz[*a*]azulene (C26)



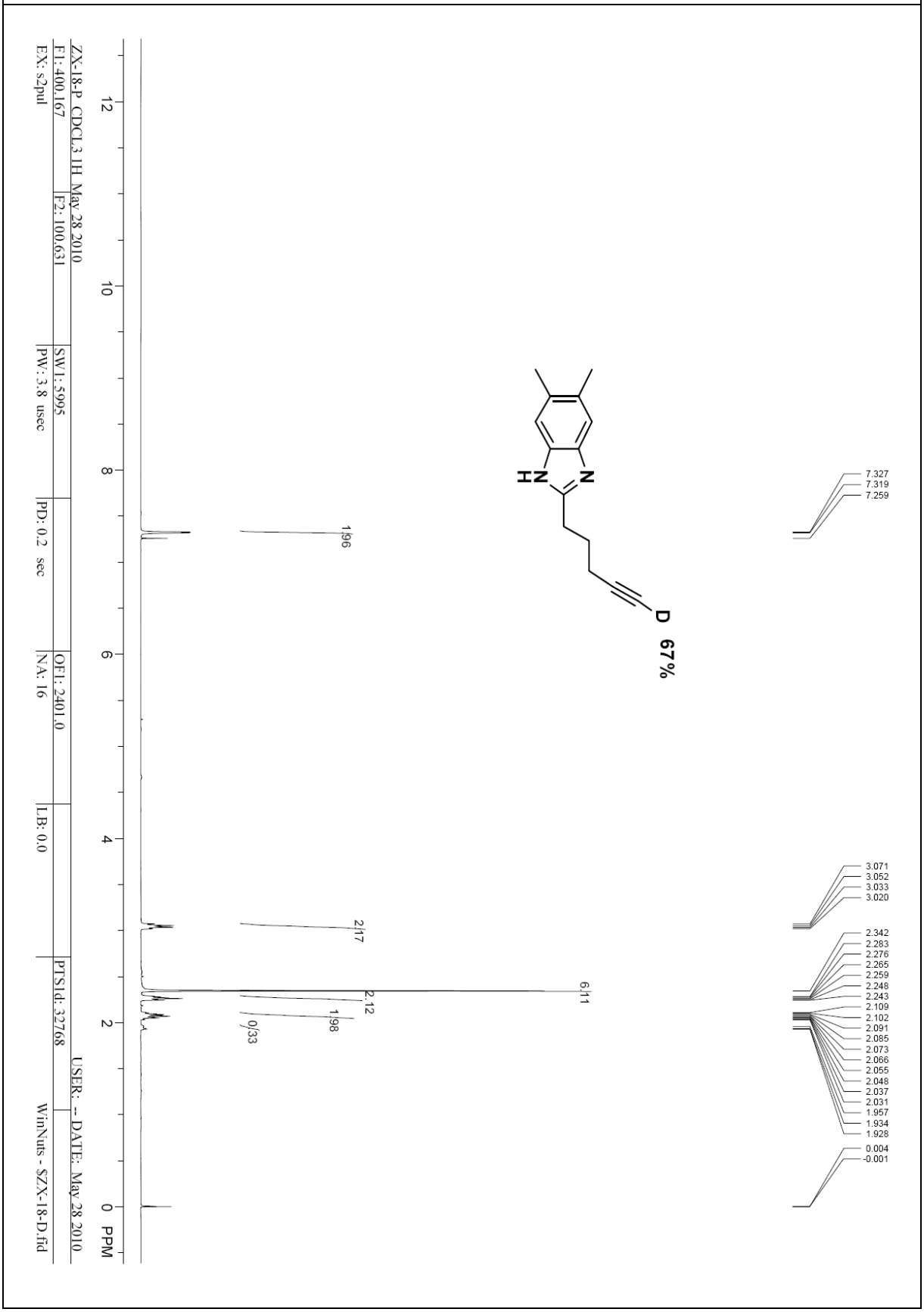

54-Ag-S CDCL3 BB+DEPT-135 Sep 1 2009
143.046
140.992
136.128
132.284
129.250
128.654
123.480
123.193
120.619
117.832
112.754
77.314
77.000
76.681
63.008
62.753
180
160
140
120
100
80
60
40
20
ppm

8*H*,10*H*-9-Oxa-5*b*,11-diaza-naphth[2,3-*a*]azulene (C27)

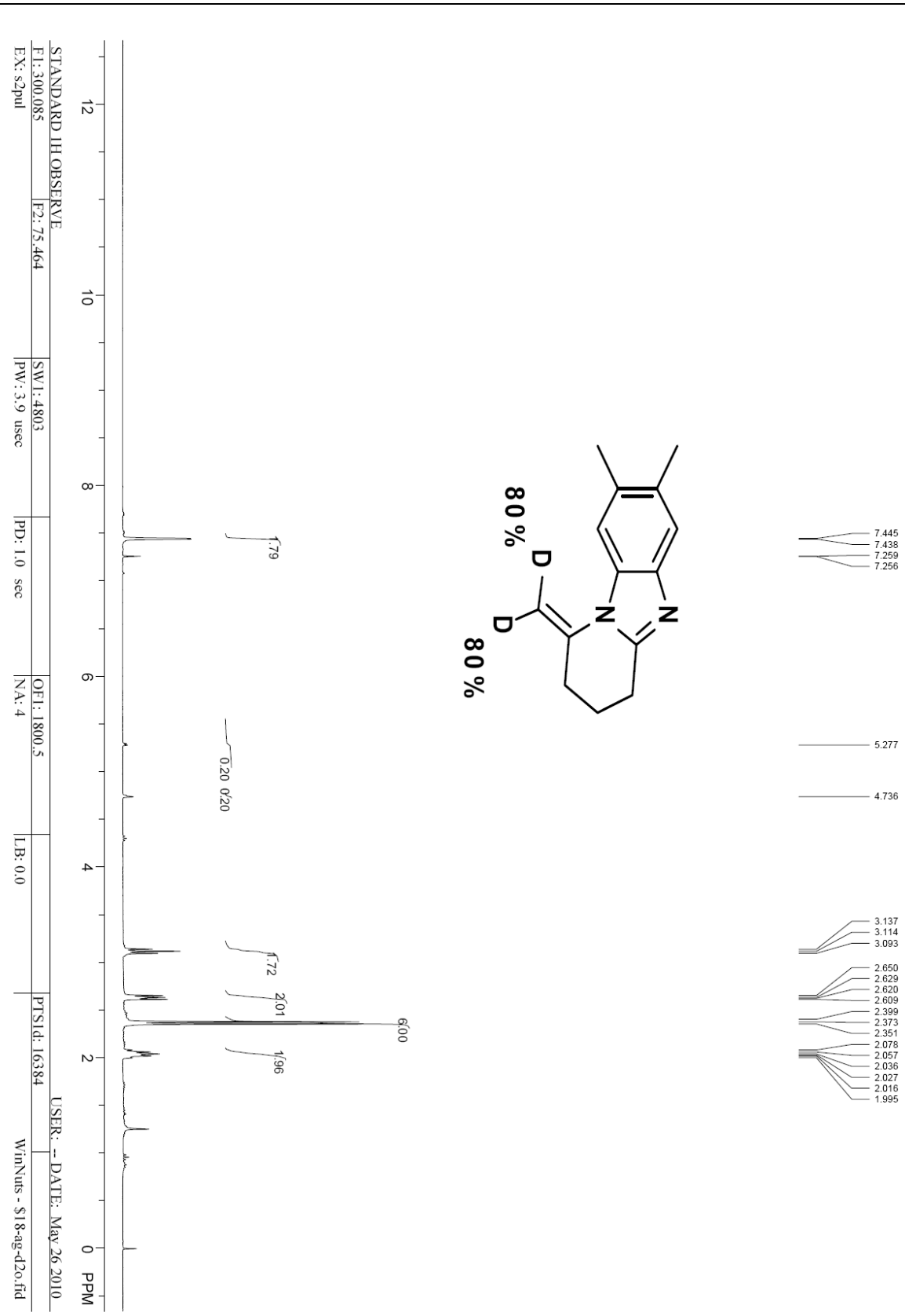



52-Ag-X CDCL3 BB+DEPT-135 Aug 26 2009
130.778
130.518
128.552
127.534
124.928
123.959
119.703
117.276
114.683
105.172
77.318
77.203
77.000
76.682
71.855
68.475
180
160
140
120
100
80
60
40
20
ppm

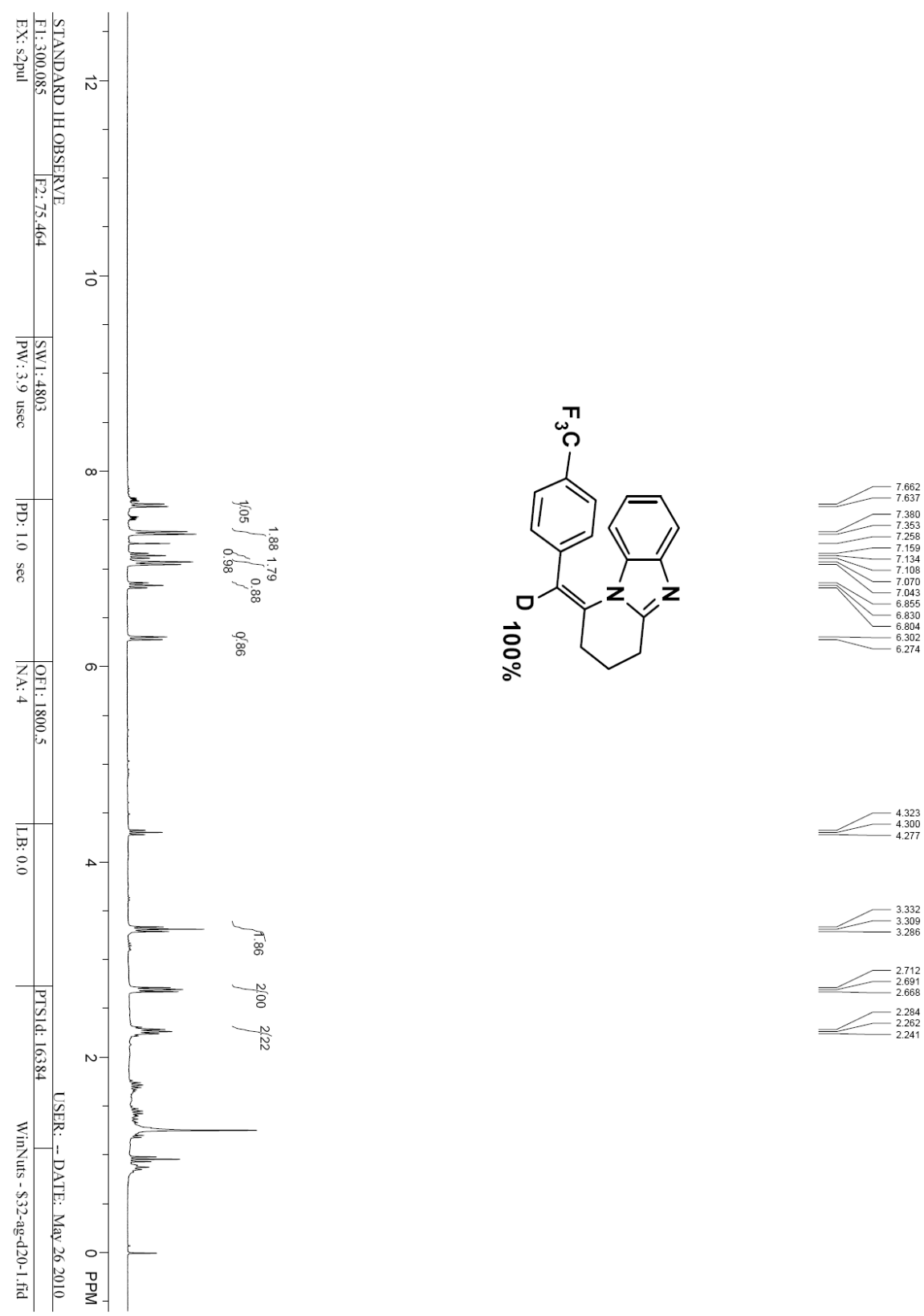
[*d*]-A2


ZX-18-P CDCL3 1H May 28 2010
F1: 400.167
F2: 100.631
SW1: 5995
PW: 3.8 usec
PD: 0.2 sec
OF1: 2401.0
NA: 16
LB: 0.0
PTS1d: 32768
USER: -- DATE: May 28 2010
EX: s2pul
WinNuts - SZX-18-D.fid
PPM
D 67%
7.327
7.319
7.259
3.071
3.052
3.033
3.020
2.342
2.283
2.276
2.265
2.259
2.248
2.243
2.109
2.102
2.091
2.085
2.073
2.066
2.055
2.048
2.037
2.031
1.957
1.934
1.928
0.004
-0.001
1.96
2.17
6.11
2.12
1.98
0.33

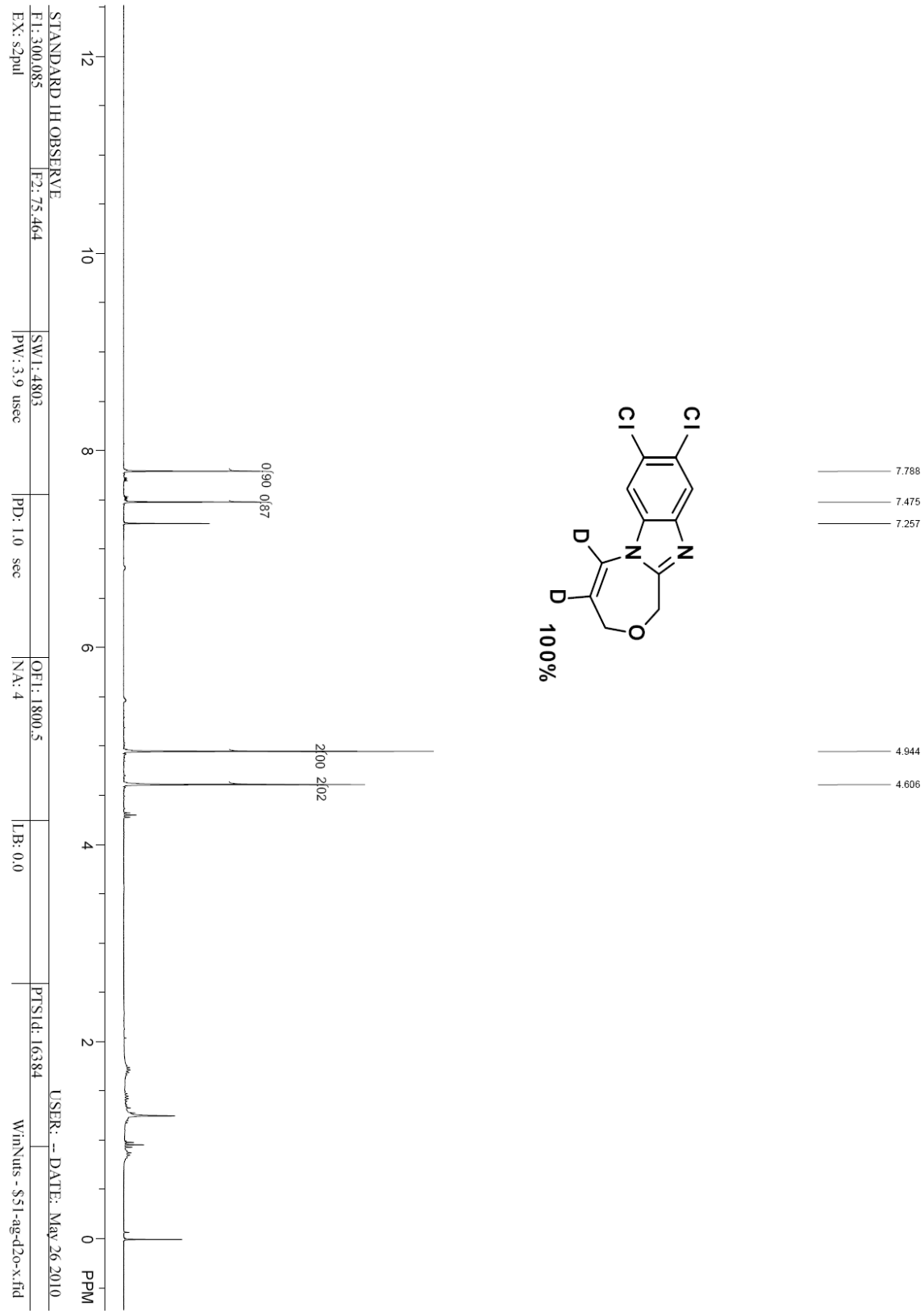
[*d*]-B2


STANDARD 1H OBSERVE
F1: 300.085
F2: 75.464
SW1: 4803
OF1: 1800.5
PTS1d: 16384
EX: s2pul
PW: 3.9 usec
PD: 1.0 sec
NA: 4
LB: 0.0
USER: -- DATE: May 26 2010
WinNuts - S18-ag-d2o.fid
PPM
0 2 4 6 8 10 12
1.79
0.20
0.20
1.72
2.01
6.00
1.96
80 %
D
D
80 %
N
N
7.445
7.438
7.259
7.256
5.277
4.736
3.137
3.114
3.093
2.650
2.629
2.620
2.609
2.399
2.373
2.351
2.078
2.057
2.036
2.027
2.016
1.995

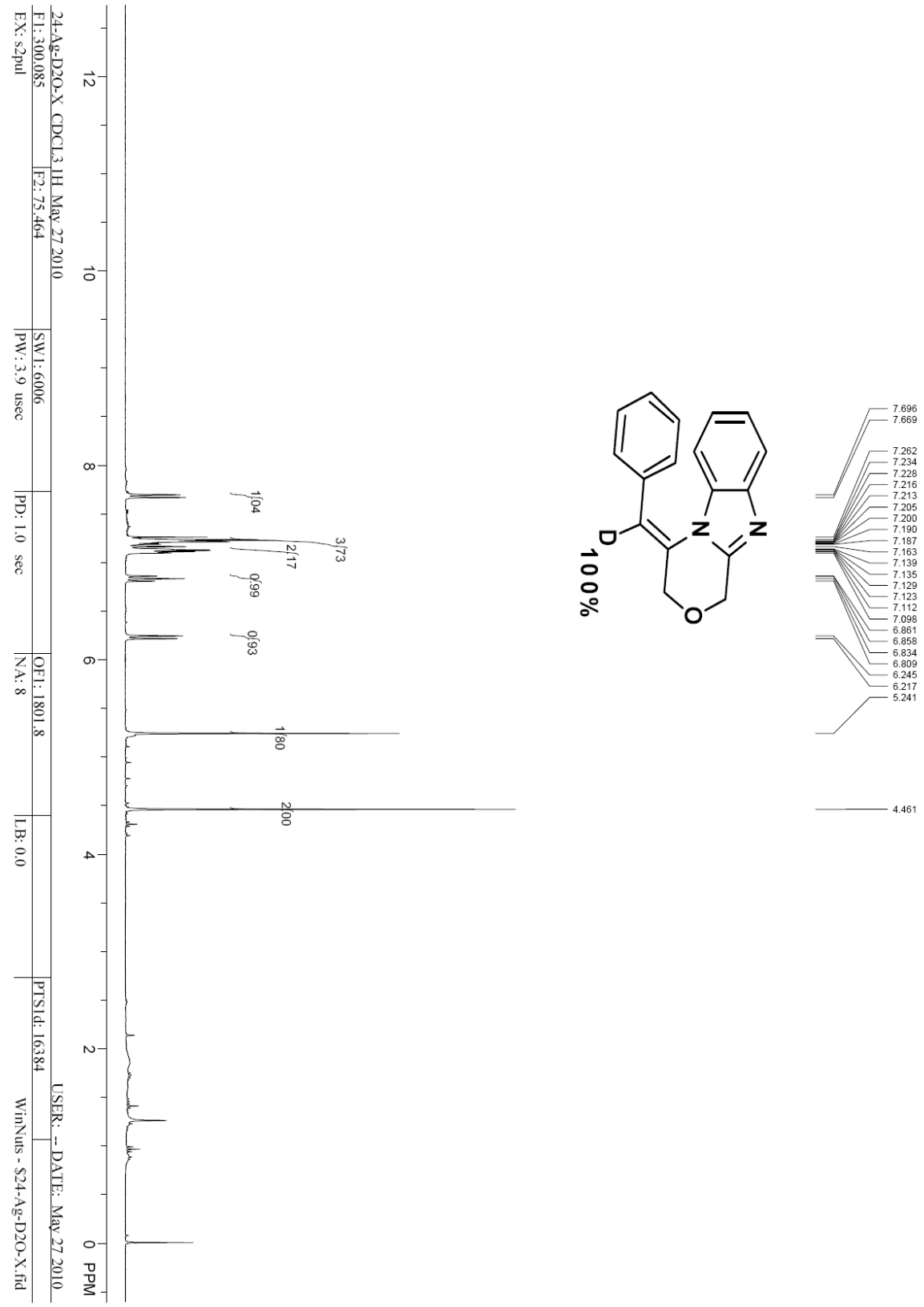
[*d*]-B10


F3C
D
100%
N
N
7.662
7.637
7.380
7.353
7.258
7.159
7.134
7.108
7.070
7.043
6.855
6.830
6.804
6.302
6.274
4.323
4.300
4.277
3.332
3.309
3.286
2.712
2.691
2.668
2.284
2.262
2.241
1.05
1.88
1.79
0.98
0.88
0.86
1.86
2.00
2.22
12
10
8
6
4
2
0 PPM
STANDARD 1H OBSERVE
F1: 300.085
F2: 75.464
SW1: 4803
OF1: 1800.5
PTS1d: 16384
USER: -- DATE: May 26 2010
EX: s2pul
PW: 3.9 usec
PD: 1.0 sec
NA: 4
LB: 0.0
WinNuts - S32-ag-d20-1.fid

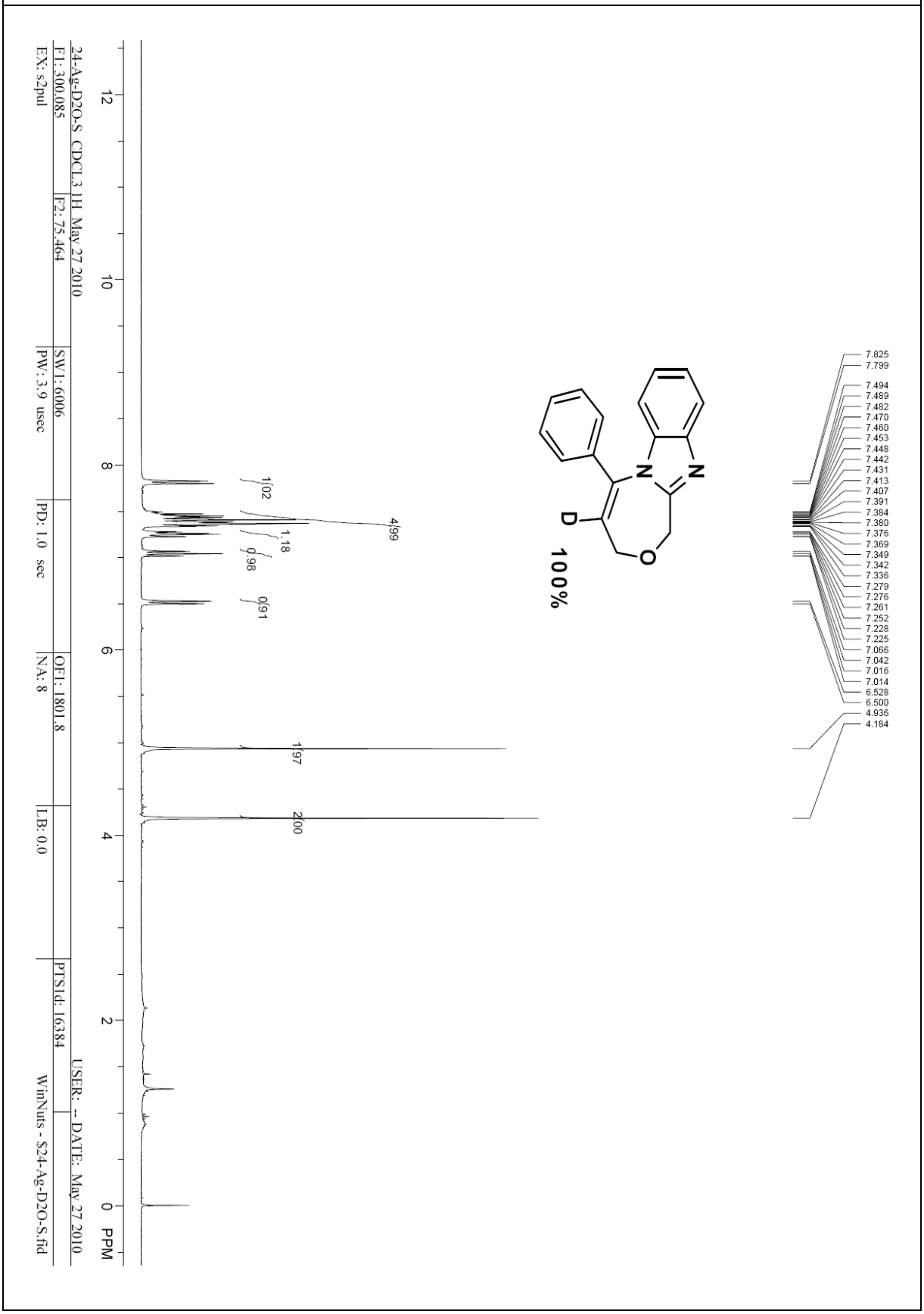
[*d*]-C19


STANDARD 1H OBSERVE
F1: 300.085
F2: 75.464
SW1: 4803
OF1: 1800.5
PTS1d: 16384
EX: s2pul
PW: 3.9 usec
PD: 1.0 sec
NA: 4
LB: 0.0
USER: -- DATE: May 26 2010
WinNuts - S51-ag-d2o-x.fid
PPM
0.90
0.87
2.00
2.02
7.788
7.475
7.257
4.944
4.606
100%

[*d*]-B23


24-Ag-D2O-X CDCL3 1H May 27 2010
F1: 300.085
F2: 75.464
SW1: 6006
OF1: 1801.8
PTS1d: 16384
USER: -- DATE: May 27 2010
EX: s2pul
PW: 3.9 usec
PD: 1.0 sec
NA: 8
LB: 0.0
WinNuts - \$24-Ag-D2O-X.fid
PPM
12
10
8
6
4
2
0
1.04
3.73
2.17
0.99
0.93
1.80
2.00
D
100%
N
N
O
7.696
7.669
7.262
7.234
7.228
7.216
7.213
7.205
7.200
7.190
7.187
7.163
7.139
7.135
7.129
7.123
7.112
7.098
6.861
6.858
6.834
6.809
6.245
6.217
5.241
4.461

[*d*]-C23


24-Ag-D2O-S CDCL3 1H May 27 2010
F1: 300.085
F2: 75.464
SW1: 6006
PW: 3.9 usec
PD: 1.0 sec
NA: 8
OF1: 1801.8
LB: 0.0
PTS1d: 16384
USER: -- DATE: May 27 2010
EX: s2pul
WinNuts - S24-Ag-D2O-S.fid
PPM
12
10
8
6
4
2
0
1.02
4.99
1.18
0.98
0.91
1.97
2.00
D
100%
7.825
7.799
7.494
7.489
7.482
7.470
7.460
7.453
7.448
7.442
7.431
7.413
7.407
7.391
7.384
7.380
7.376
7.369
7.349
7.342
7.336
7.279
7.276
7.261
7.252
7.228
7.225
7.066
7.042
7.016
7.014
6.528
6.500
4.936
4.184