# Selective Deuteration of Aromatic Compounds *via* Deutero-decarboxylation of (Hetero)aromatic Carboxylic Acids

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## General Information

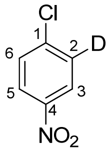
All reactions were carried out under nitrogen atmosphere. Anhydrous DMSO and all other reagents were purchased from commercial suppliers and used without further purification, $D_2O$ (99.9 % D) was purchased from Cambridge Isotope Laboratories Inc. and used without further treatment. Melting points were obtained using a hot-stage apparatus and are uncorrected. IR spectra were recorded using a Bruker Tensor 37 FTIR machine and quoted in $cm^{-1}$. Unless otherwise noted, $^1H$ NMR spectra, recorded at 400 MHz are referenced to the residual solvent peak at 7.26 ppm ($CDCl_3$). $^2H$ NMR spectra, recorded at 61 MHz, are referenced using $CDCl_3$ as an internal reference (7.26 ppm in $CDCl_3$ or 8.32 ppm in $d_6$-DMSO). $^{13}C$ NMR spectra, recorded at 101 MHz, are referenced to the residual solvent peak at 77.02 ppm ($CDCl_3$). Chemical shifts ($\delta$) are quoted in ppm. Impurity peaks observed at 1.43, 1.25 and 0.88 ppm in the $^1H$ NMR and 29.8 ppm in the $^{13}C$ NMR are likely due to high order alkanes such as icosane. A superfluous peak observed at 4.73 ppm in the $^2H$ NMR is an artefact due to the spectrometer and not a deuterium resonance signal. Mass spectra were recorded on an Agilent GC-MS, comprising a 6890 GC and 5973 MS.

## General procedure for the Ag-catalysed deutero-decarboxylation of *ortho*-substituted benzoic acids.

A mixture of benzoic acid (0.5 mmol), $Ag_2CO_3$ (14 mg, 0.05 mmol) and $D_2O$ (452 μL, 25.0 mmol) in dry DMSO (2.5 mL) was stirred for 16 hours at 120 °C in a sealed vessel. After this time the reaction was partitioned with $Et_2O$ (10 mL) and saturated aqueous $NaHCO_3$ (10 mL). The two layers were separated and the aqueous layer was re-extracted with $Et_2O$ (2 × 10 mL). The organic extracts were combined and washed with saturated aqueous $NaHCO_3$ (2 × 30 mL) and brine (2 × 30 mL). The ethereal layer was dried over anhydrous $MgSO_4$, filtered and evaporated to dryness under reduced pressure. No further purification was necessary.

Exemplar spectra to indicate how the extent of deuteration was calculated are included on pages SI-8 and SI-17.

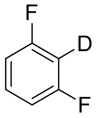
### 1-Chloro-4-nitro-6-deuterobenzene (2a)



**2a**

The reaction was carried out following the general procedure with 2-chloro-5-nitrobenzoic acid (0.102 g, 0.5 mmol) to afford **2a** as a pale yellow solid (0.072 g, 91%, (93% deuteration)). m.p.: 81-83 °C; IR: 2928, 2860, 1573, 1519, 1342, 748; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.17-8.20 (2H, m), 7.52 (1.067H, app d, *J* = 9.2 Hz); $^2$H NMR (61 MHz, $CDCl_3$) δ 7.55 (1D, s); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 146.7 (C4), 141.4 (C1), 129.7 (C6), 129.4 (1:1:1 t, *J* = 27.2 Hz) (C2), 125.1 (C5/3), 125.0 (C3/5); MS (EI) *m/z* 158 ($M^+$, 100).

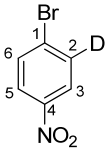
### 1,5-Difluoro-6-deuterobenzene (2b)



**2b**

The reaction was carried out following the general procedure in a sealed vessel with 2,6-difluorobenzoic acid (0.016 g, 0.1 mmol)) and $d_6$-DMSO (0.5 mL) to afford **2b** (96%, (95% deuteration)) as calculated by $^1$H NMR using mesitylene as the internal standard. $^1$H NMR (400 MHz, $d_6$-DMSO) δ 7.44 (1H, app quin, (*J* = 7.6 Hz); 7.11-7.17 (0.047H, m); 7.05 (2H, t, *J* = 6.8 Hz). $^2$H NMR (61 MHz, $d_6$-DMSO) δ 7.23 (1D, s); MS (EI) *m/z* 115 ($M^+$, 100).

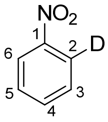
### 1-Bromo-4-nitro-6-deuterobenzene (2c)



**2c**

The reaction was carried out following the general procedure with 2-bromo-5-nitrobenzoic acid (0.123 g, 0.5 mmol) to afford **2c** as a white solid (0.096 g, 94%, (90% deuteration)). m.p.: 124- 126 °C; IR: 3097, 2919, 2850, 1571, 1510, 1336, 739. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.09-8.12 (2H, m), 7.69 (1.104H, app d, $J$ = 9.2 Hz); $^{2}$H NMR (61 MHz, $CDCl_3$) δ 7.56 (1D, s); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 147.2 (C4), 132.8 (C6), 132.5 (1:1:1 t, $J$ = 17.4 Hz) (C2), 130.0 (C1), 125.2 (C5/3), 125.1 (C3/5); MS (EI) *m/z* 204 ($M^+$, 100), 202 ($M^+$, 100).

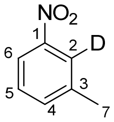
### 1-Nitro-2-deuterobenzene (2d)



**2d**

The reaction was carried out following the general procedure with 2-nitrobenzoic acid (0.084 g, 0.5 mmol) to afford **2d** as a yellow oil (0.58 g, 93%, (98% deuteration)). IR: 3019, 2923, 2855, 1697, 1547, 1215, 750; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.23 (1.025H, dd, $J$ = 8.4, 0.8 Hz), 7.70 (1H, td, $J$ = 7.6, 1.2 Hz), 7.56 (1H, m); $^{2}$H NMR (61 MHz, $CDCl_3$) δ 8.16 (1D, s); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 148.3 (C1), 134.7 (C4), 129.4 (C5/3), 129.3 (C3/5), 123.6 (C6), 123.4 (1:1:1 t, $J$ = 17.2 Hz) (C2); MS (EI) *m/z* 124 ($M^+$, 100).

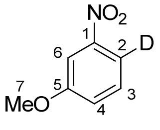
### 3-Nitro-2-deuterotoluene (2e)



**2e**

The reaction was carried out following the general procedure with 2-methyl-6-nitrobenzoic acid (0.091g, 0.5 mmol) to afford **2e** as a pale yellow oil (0.057g, 82%, (97% deuteration)). IR: 2924, 2864, 1521, 1346, 1091, 930, 801; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.01 (1.035H, app d, *J* = 8.4 Hz ), 7.49 (1H, d, *J* = 7.2 Hz), 7.41 (1H, t, *J* = 8.0 Hz); 2.47 (3H, s); $^2$H NMR (61 MHz, $CDCl_3$) δ 8.07 (1D, s); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 148.4 (C1), 139.8 (C3), 135.4 (C4), 129.2 (C5), 123.7 (1:1:1 t, *J* = 25.6 Hz) (C2), 120.8 (C6), 21.3 (C7); MS (EI) *m/z* 138 ($M^+$, 100).

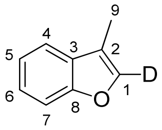
### 1-Methoxy-3-nitro-4-deuterobenzene (2f)



**2f**

The reaction was carried out following the general procedure with 4-methoxy-2-nitrobenzoic acid (0.099g, 0.5 mmol) to afford **2f** as a pale yellow solid (0.075 g, 97%, (95% deuteration)). m.p.: 35-37 °C; IR: 2936, 2845, 1523, 1347, 1235, 1036; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.81 (0.050H, ddd, *J* = 8.0, 2.0, 0.8 Hz), 7.71 (1H, d, *J* = 2.4 Hz), 7.42 (0.048H, t, *J* = 8.2 Hz), 7.41 (0.952H, d, 8.4 Hz), 7.21 (1H, dd, 8.4, 2.8 Hz), 3.88 (3H, s); $^2$H NMR (61 MHz, $CDCl_3$) δ 7.87 (1D, s); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 160.3 (C5), 149.4 (C1), 129.9 (C3), 121.3 (C4), 115.6 (1:1:1 t, *J* = 26.2 Hz) (C2), 108.3 (C6), 55.9 (C7); MS (EI) *m/z* 154 ($M^+$, 100).

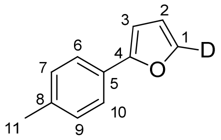
### 2-Deutero-3-methylbenzofuran (2g)



**2g**

The reaction was carried out following the general procedure with 3-methylbenzofuran-2-carboxylic acid (0.088g, 0.5 mmol) to afford **2g** as an orange-red oil (0.54 g, 81%, (93% deuteration)). IR: 2923, 2855, 1722, 1461, 1218, 1122, 1070; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.55 (1H, d, *J* = 7.6 Hz); 7.48 (1H, d, *J* = 7.6 Hz); 7.42 (0.075H, s); 7.31 (1H, t, *J* = 7.6 Hz); 7.26 (1H, t, *J* = 7.6 Hz); 2.27 (3H, s); $^2$H NMR (61 MHz, $CDCl_3$) δ 7.45 (1D, s); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 155.3 (C8), 141.2 (1:1:1 t, *J* = 30.5 Hz) (C1), 129.2 (C3), 124.2 (C6), 122.3 (C5), 119.5 (C4), 115.5 (C2), 111.4 (C7), 7.9 (C9). MS (EI) *m/z* 133 ($M^+$, 100).

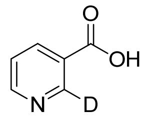
## 2-Deutero-5-(*p*-tolyl)furan (2h)



**2h**

The reaction was carried out following the general procedure with 5-(*p*-tolyl)furan-2-carboxylic acid (0.088g, 0.5 mmol) to afford **2h** as an yellow oil (0.64 g, 81%, (95% deuteration)). IR: 2919, 2852, 1458, 1208, 1017, 817; $^1$H NMR (400 MHz, $CDCl_3$) δ 7.59 (2H, d, 8.4 Hz); 7.46 (0.054H, dd, 2.0, 0.8 Hz); 7.21 (2H, d, 8.0 Hz), 6.61 (1H, d, 3.2 Hz); 6.47 (1H, d, 3.2 Hz); $^2$H NMR (61 MHz, $CDCl_3$) δ 7.49; $^{13}$C NMR (101 MHz, $CDCl_3$) δ 154.3 (C4), 141.6 (1:1:1 t, $J$ = 31.1 Hz) (C1), 137.3 (C8), 129.5 (C7 & 9), 128.5 (C5), 123.9 (C6 & 10), 111.5 (C3), 104.3 (C2), 21.4 (C11); MS (EI) *m/z* 159 ($M^+$, 100).

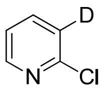
## 2-deutero-3-pyridinecarboxylic acid (2i)



**2i**

The reaction was carried out following the general procedure in a sealed vessel with pyridine-2,3-dicarboxylic acid (0.017 g, 0.1 mmol)) and $d_6$-DMSO (0.2 mL) to afford **2i** (91%, (95% deuteration)) as calculated by $^1$H NMR using mesitylene as the internal standard. $^1$H NMR (400 MHz, $d_6$-DMSO) δ 9.05 (0.054H, s): 8.77 (1H, d, $J$ = 1.6 Hz); 8.27 (1H, d, $J$ = 7.6 Hz); 7.54 (1H, t, 6.2 Hz); $^2$H NMR (61 MHz, $CDCl_3$) δ 10.19 (1D, s).

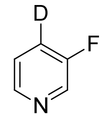
## 2-Chloro-3-deuteropyridine (2j)



**2j**

The reaction was carried out following the general procedure in a sealed vessel with 2-chloronicotinic acid (0.016 g, 0.1 mmol)) and $d_6$-DMSO (0.5 mL) to afford **2j** (100%, (95% deuteration)) as calculated by $^1$H NMR using mesitylene as the internal standard. $^1$H NMR (400 MHz, $d_6$-DMSO) δ 8.39 (1H, dd, $J$ = 4.8, 2.0 Hz); 7.84 (1H, d, $J$ = 7.2 Hz); 7.48 (0.048H, d, $J$ = 8.0 Hz); 7.40 (1H, dd, J = 7.6, 4.8 Hz). $^2$H NMR (61 MHz, $CDCl_3$) δ 7.77 (1D, s); MS (EI) *m/z* 114 ($M^+$, 100).

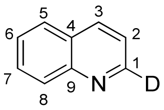
### 3-Fluoro-4-deuteropyridine (2k)



**2k**

The reaction was carried out following the general procedure in a sealed vessel with 3-fluoroisonicotinic acid (0.014 g, 0.1 mmol)) and $d_6$-DMSO (0.5 mL) to afford **2k** (81%, (95% deuteration)) as calculated by $^1$H NMR using mesitylene as the internal standard. $^1$H NMR (400 MHz, $d_6$-DMSO) δ 8.46 (1H, s); 8.39 (1H, dd, *J* = 4.8, 2.0 Hz); 7.60 (0.053H, dddd, *J* = 8.8, 8.8, 2.8, 1.2 Hz), 7.43 (1H, t, *J* = 4.8 Hz). $^2$H NMR (61 MHz, $CDCl_3$) δ 7.98 (1D, s); MS (EI) *m/z* 98 (M$^+$, 100).

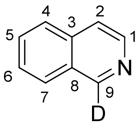
### 2-Deuteroquinoline (2l)



**2l**

The reaction was carried out following the general procedure with 2-quinolinecarboxylic acid (0.087 g, 0.5 mmol)) to afford **2l** as a colourless oil (0.60 g, 93%, (97% deuteration)). IR: 2928, 2856, 1625, 1584, 1327, 1217, 898; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.90 (0.029H, dd, 4.0, 1.6 Hz); 8.11 (2H, t, 7.2 Hz); 7.79 (1H, d, 8.0 Hz); 7.70 (1H, t, 7.6 Hz); 7.52 (1H, t, 7.4 Hz); 7.36 (1H, d, 8.0 Hz); $^2$H NMR (61 MHz, $CDCl_3$) δ 8.95 (1D, s); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 150.1 (1:1:1 t, *J* = 27.3 Hz) (C1), 148.4 (C9), 136.1 (C3), 129.6 (C7), 129.5 (C8), 128.4 (C4), 127.9 (C5), 126.6 (C6), 121.0 (C2); MS (EI) *m/z* 130 (M$^+$, 100).

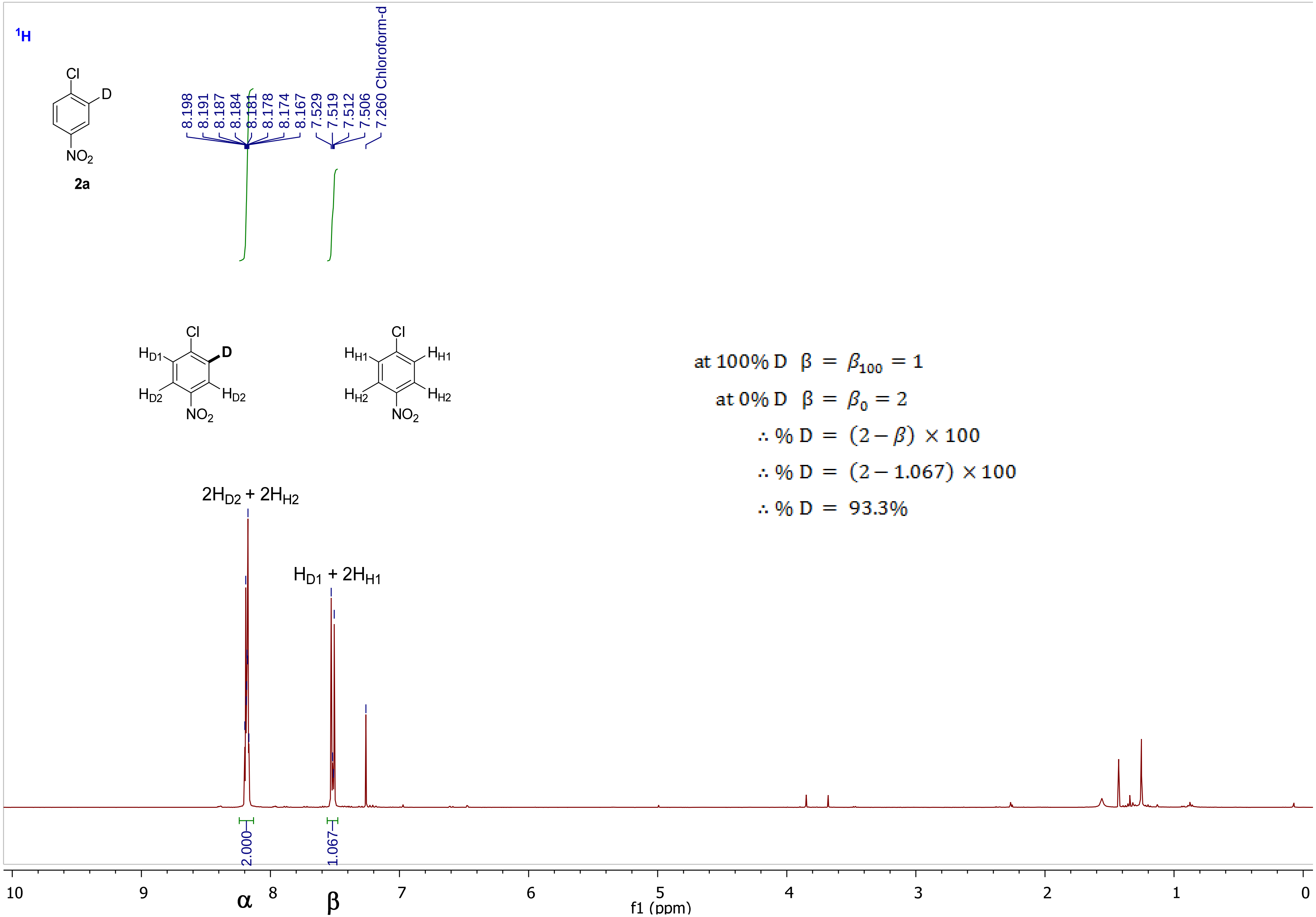
### 1-Deuteroisoquinoline (2m)



**2m**

The reaction was carried out following the general procedure with 1-isoquinolinecarboxylic acid (0.087 g, 0.5 mmol)) to afford **2l** as a colourless oil (0.59 g, 91%, (98% deuteration)). IR: 2916, 2849, 1626, 1463, 1330, 1255, 890; $^1$H NMR (400 MHz, $CDCl_3$) δ 9.25 (0.023H, s); 8.52 (1H, d, 6.0 Hz); 7.95 (1H, d, 8.0 Hz); 7.79 (1H, t, 7.6 Hz); 7.67 (1H, t, 7.6 Hz); 7.63 (1H, d, 5.6 Hz); 7.58 (1H, t, 7.4 Hz); $^2$H NMR (61 MHz, $CDCl_3$) δ 9.29 (1D, s); $^{13}$C NMR

(101 MHz, $CDCl_3$) δ 152.3 (1:1:1 t, *J* = 31.1 Hz) (C9), 143.1 (C1), 135.9 (C3), 130.4 (C5), 128.7 (C5), 127.7 (C7), 127.3 (C6), 126.5 (C4), 120.5 (C2); MS (EI) *m/z* 130 ($M^+$, 100).



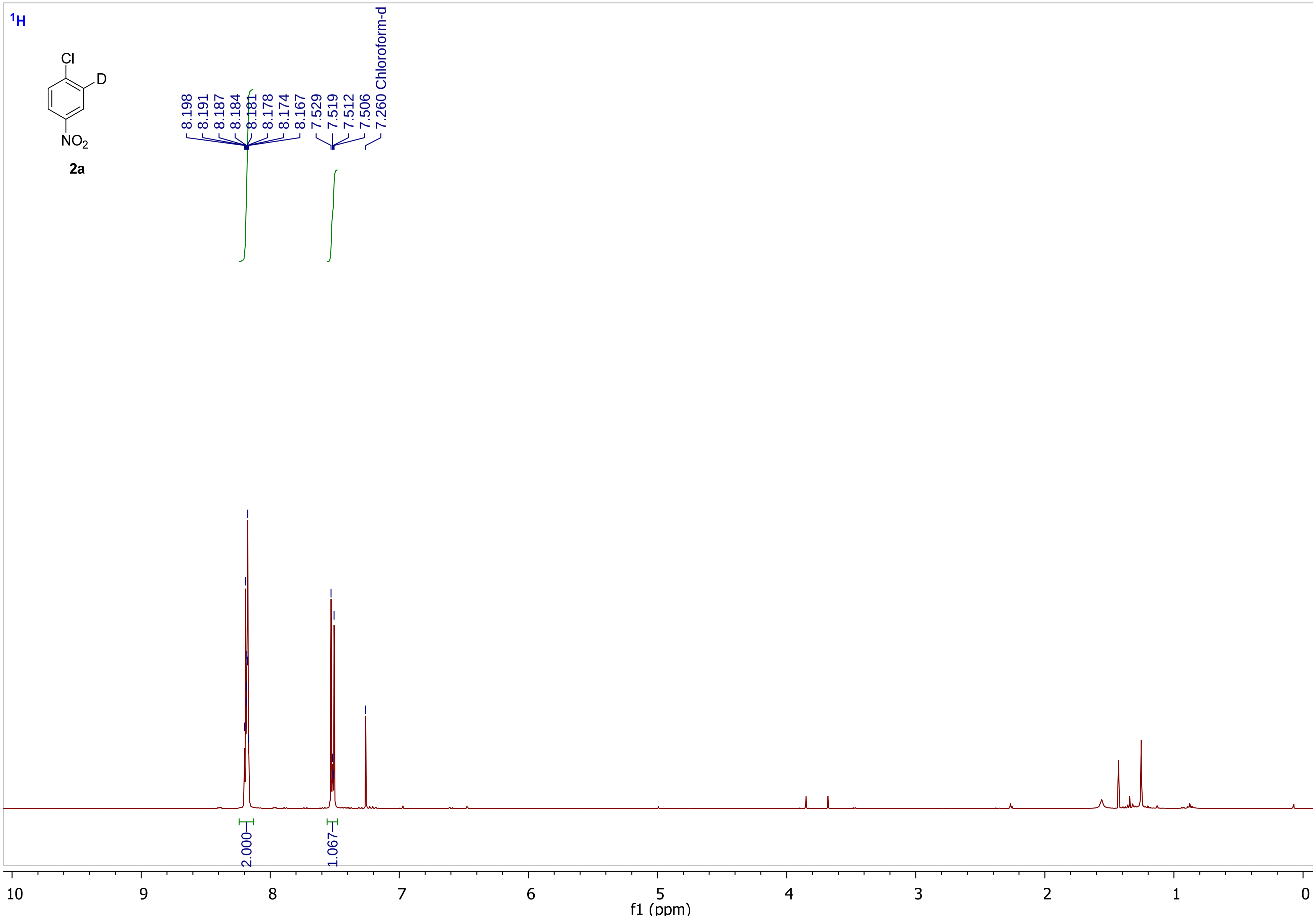
$$\text{at 100\% D} \quad \beta = \beta_{100} = 1$$

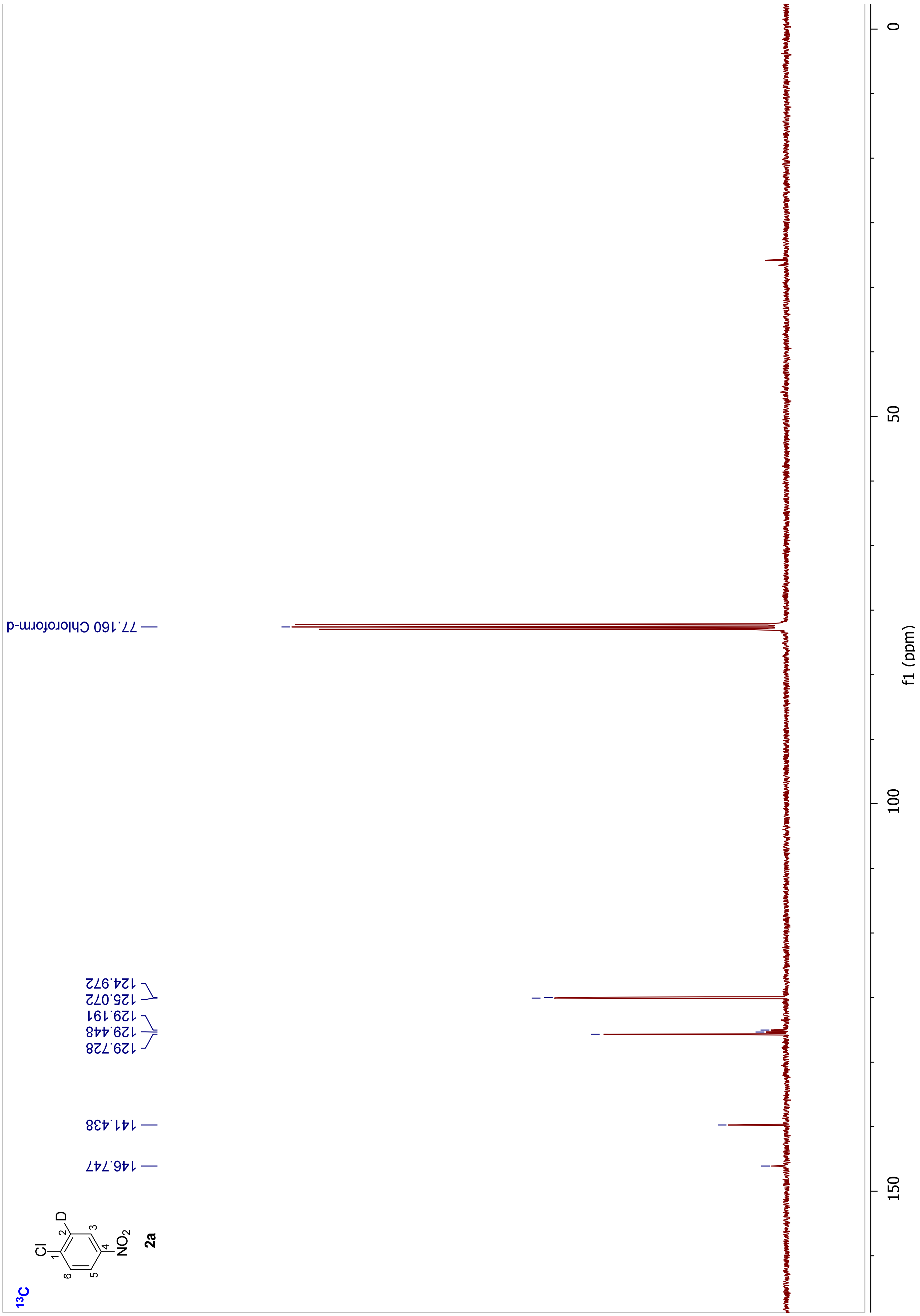
$$\text{at 0\% D} \quad \beta = \beta_0 = 2$$

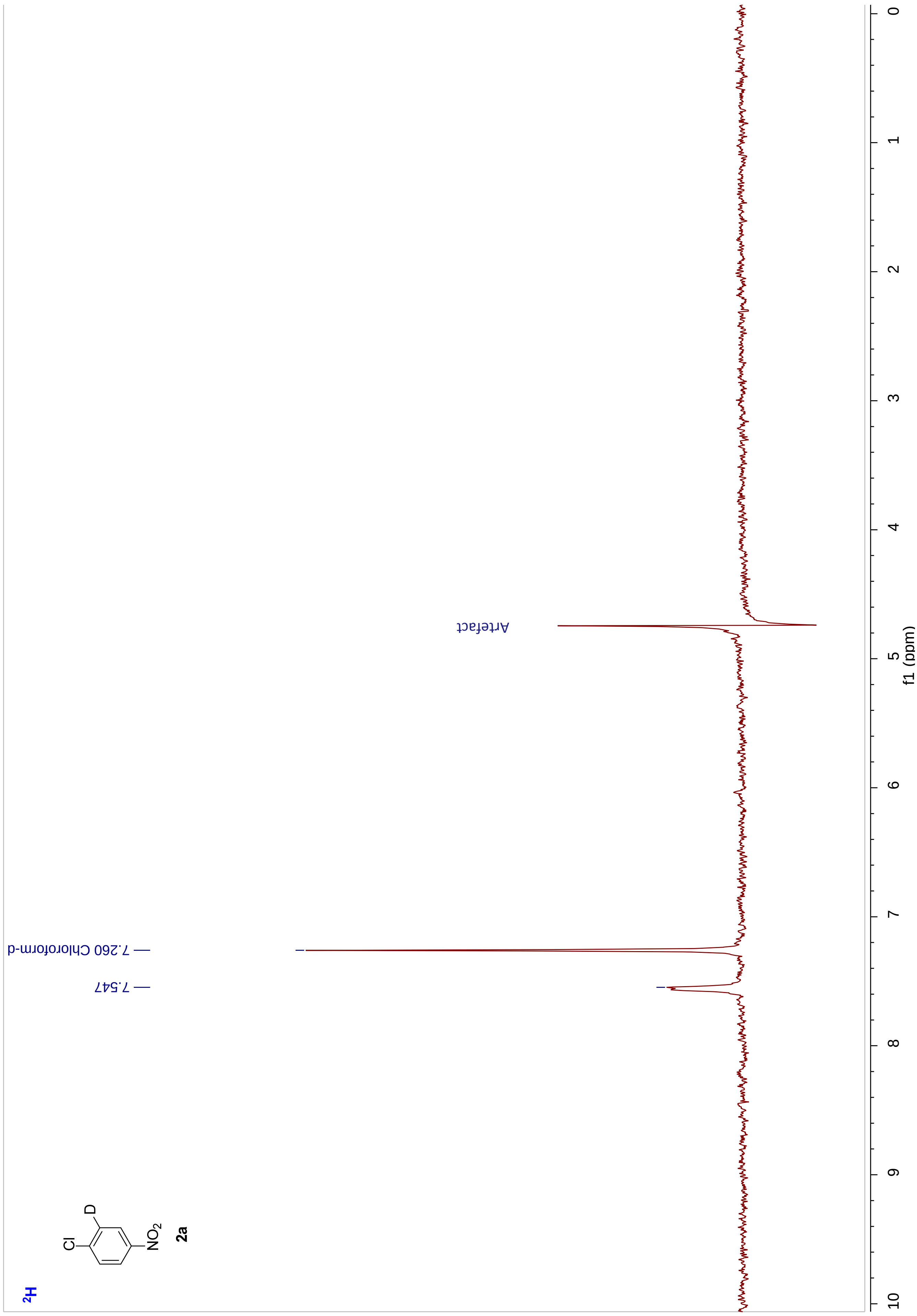
$$\therefore \% \text{ D} = (2 - \beta) \times 100$$

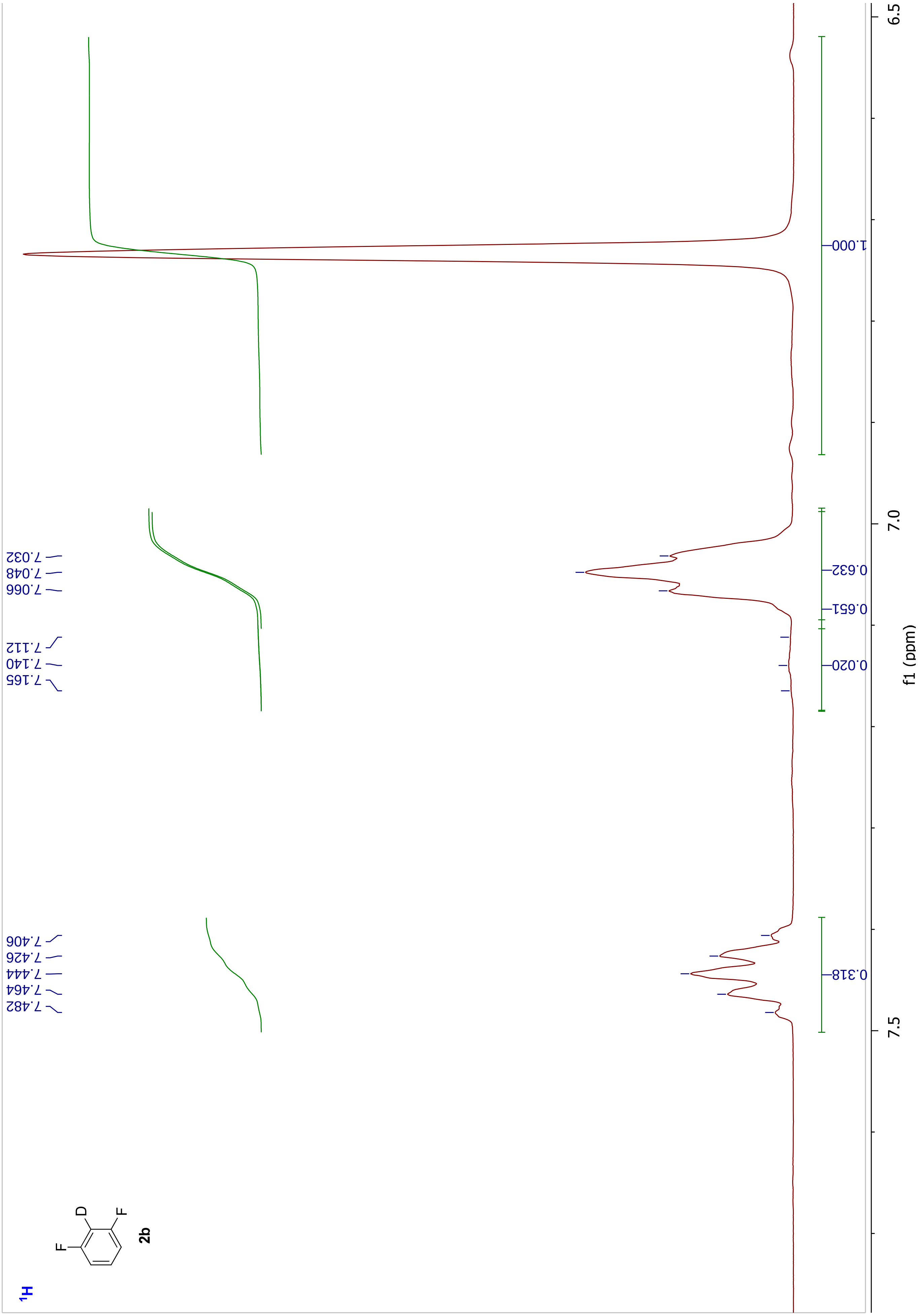
$$\therefore \% \text{ D} = (2 - 1.067) \times 100$$

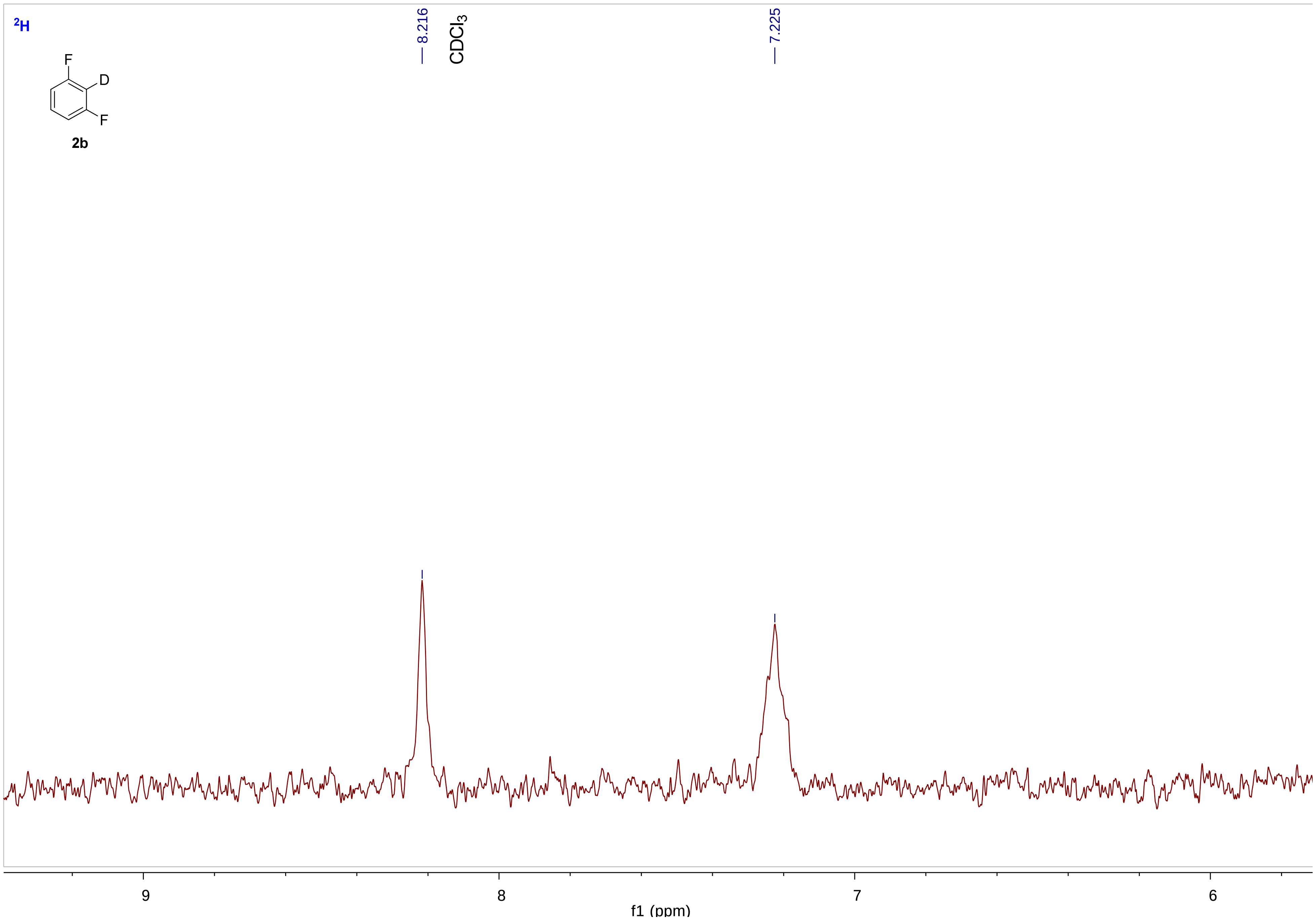
$$\therefore \% \text{ D} = 93.3\%$$

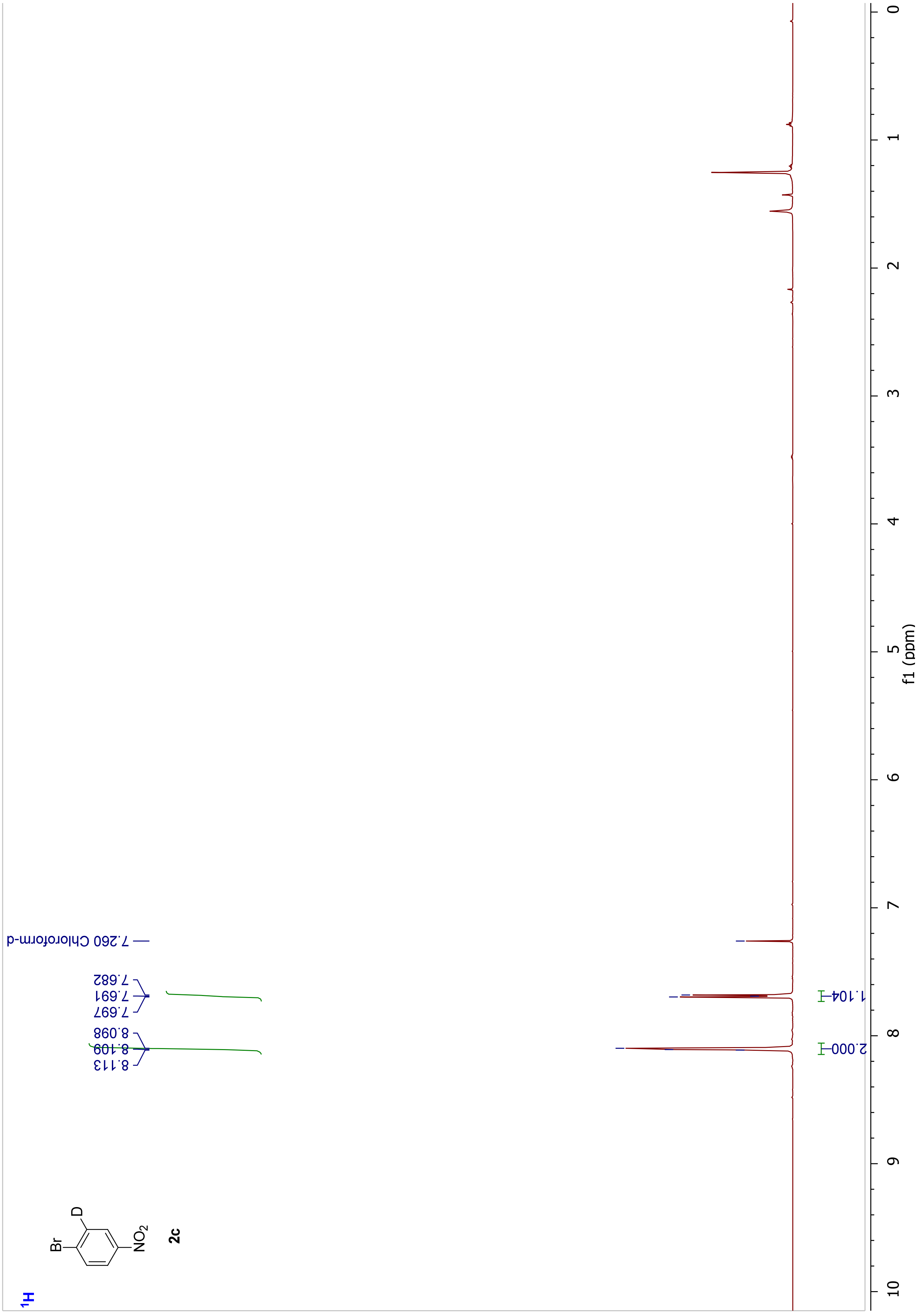

$^1$H
Cl
D
NO$_2$
2a
8.198
8.191
8.187
8.184
8.181
8.178
8.174
8.167
7.529
7.519
7.512
7.506
7.260 Chloroform-d
2.000
1.067
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

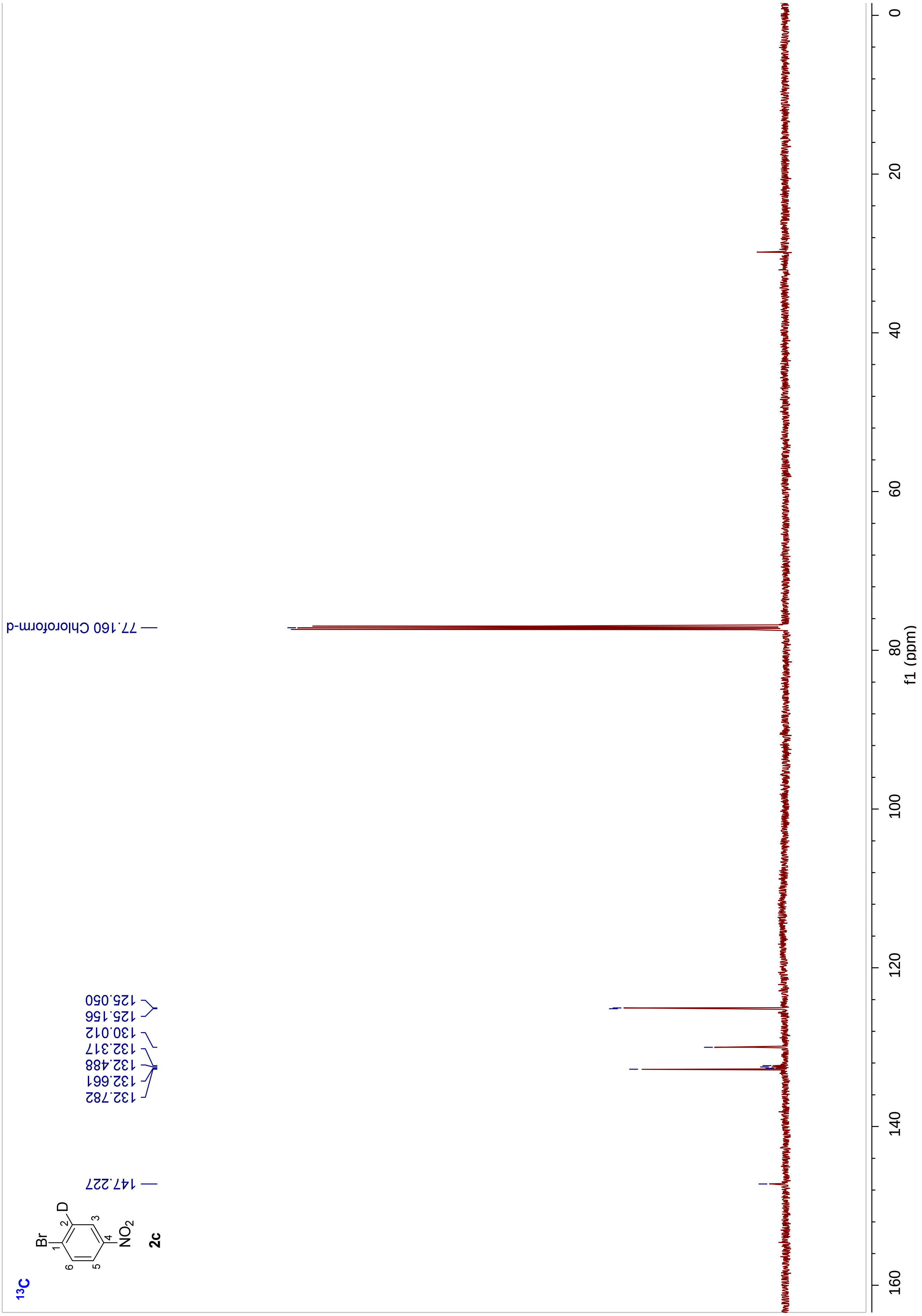

13C
Cl
D
NO2
1
2
3
4
5
6
2a
146.747
141.438
129.728
129.448
129.191
125.072
124.972
77.160 Chloroform-d
0
50
100
150
f1 (ppm)

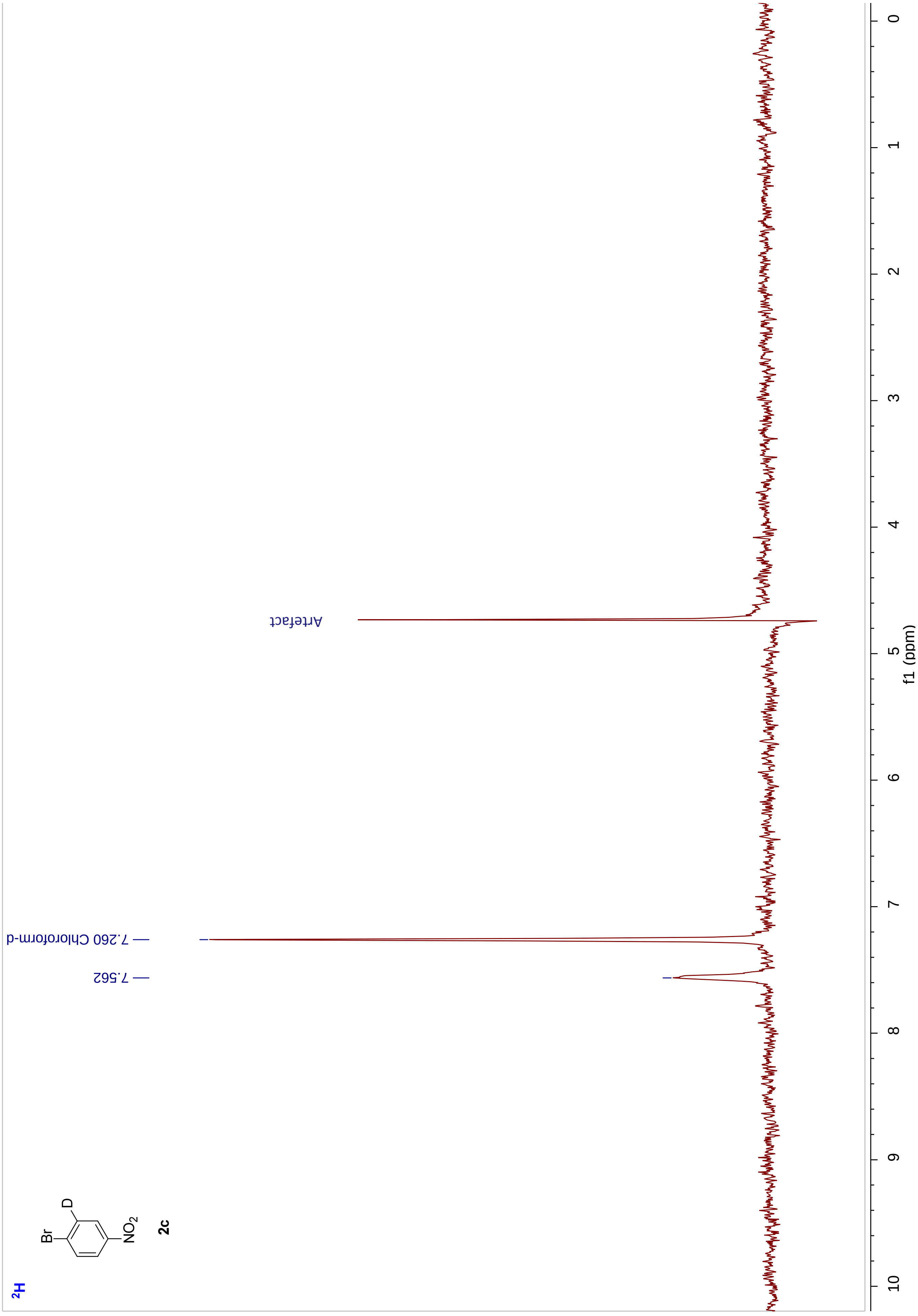

²H
Cl
D
NO2
2a
7.547
7.260 Chloroform-d
Artefact
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)

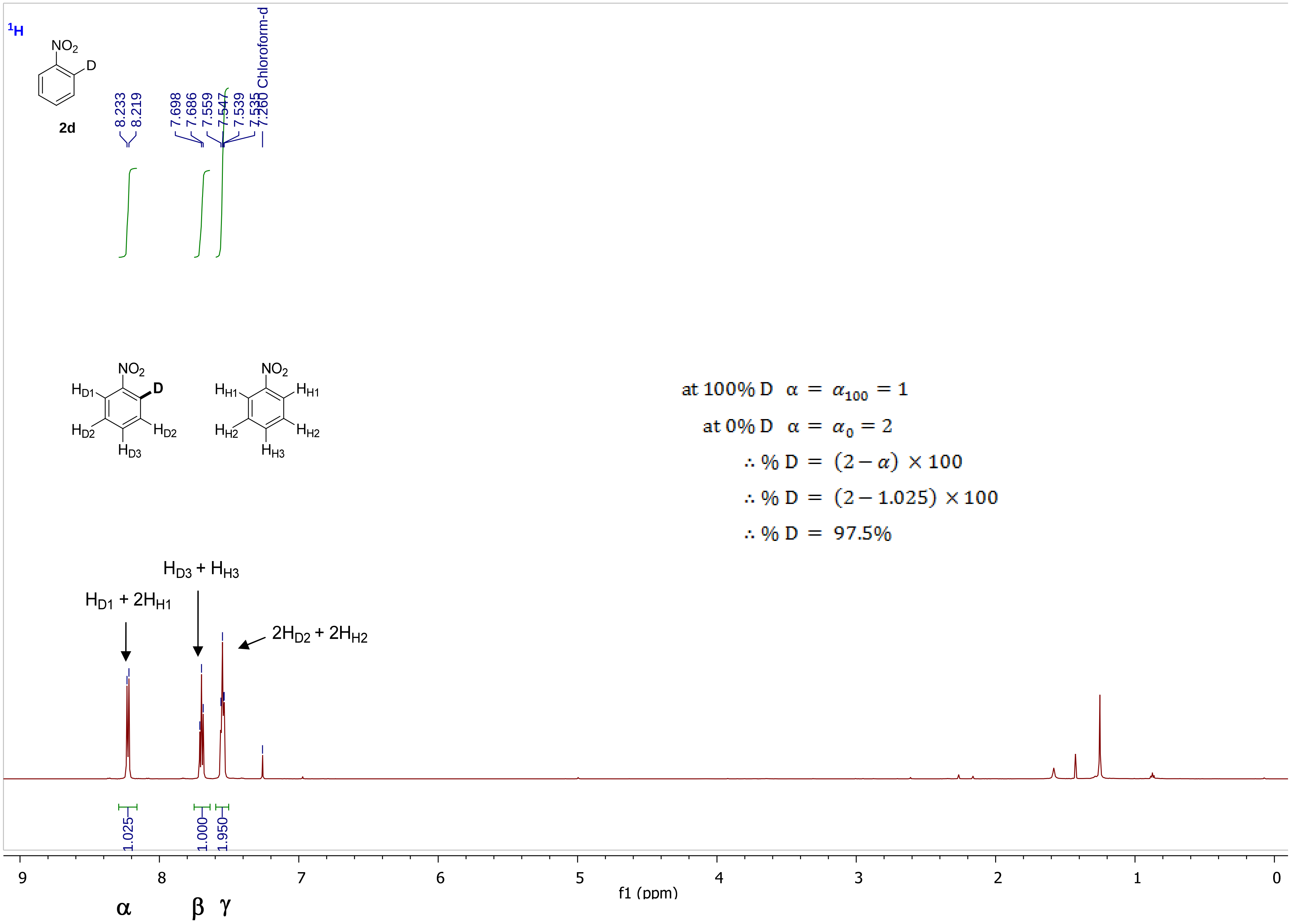

¹H
2b
F
D
F
7.032
7.048
7.066
7.112
7.140
7.165
7.406
7.426
7.444
7.464
7.482
1.000
0.632
0.651
0.020
0.318
6.5
7.0
7.5
f1 (ppm)


$^2H$
F
D
F
2b
8.216
$CDCl_3$
7.225
9
8
7
6
f1 (ppm)


1H
Br
D
NO2
2c
7.260 Chloroform-d
7.682
7.691
7.697
8.098
8.109
8.113
1.104
2.000
f1 (ppm)
0
1
2
3
4
5
6
7
8
9
10


$^{13}C$
Br
D
NO$_2$
1
2
3
4
5
6
2c
147.227
132.782
132.661
132.488
132.317
130.012
125.156
125.050
77.160 Chloroform-d
0
20
40
60
80
100
120
140
160
f1 (ppm)


²H
Br
D
NO2
2c
7.562
7.260 Chloroform-d
Artefact
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)



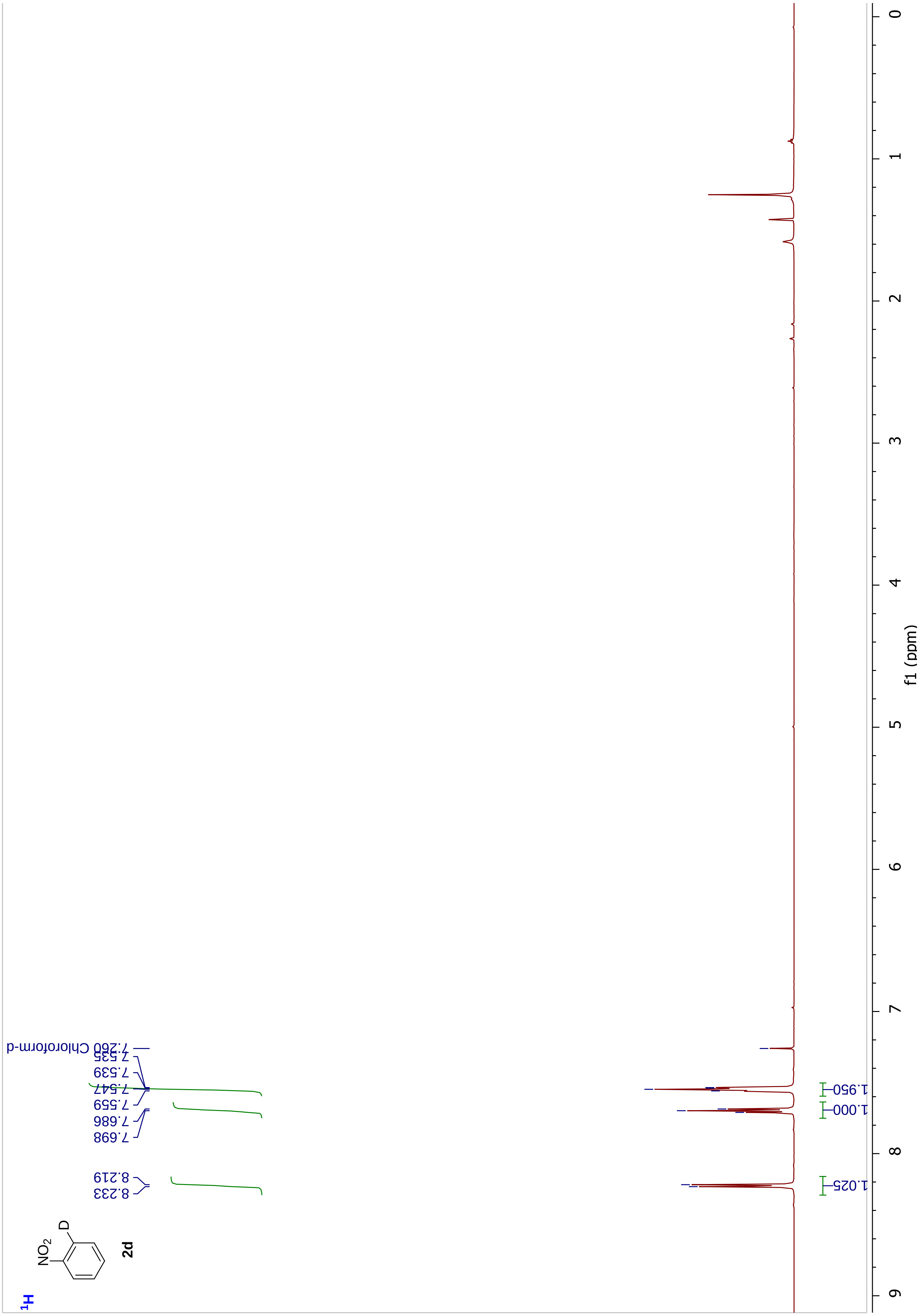
$$\text{at } 100\%\text{ D} \quad \alpha = \alpha_{100} = 1$$

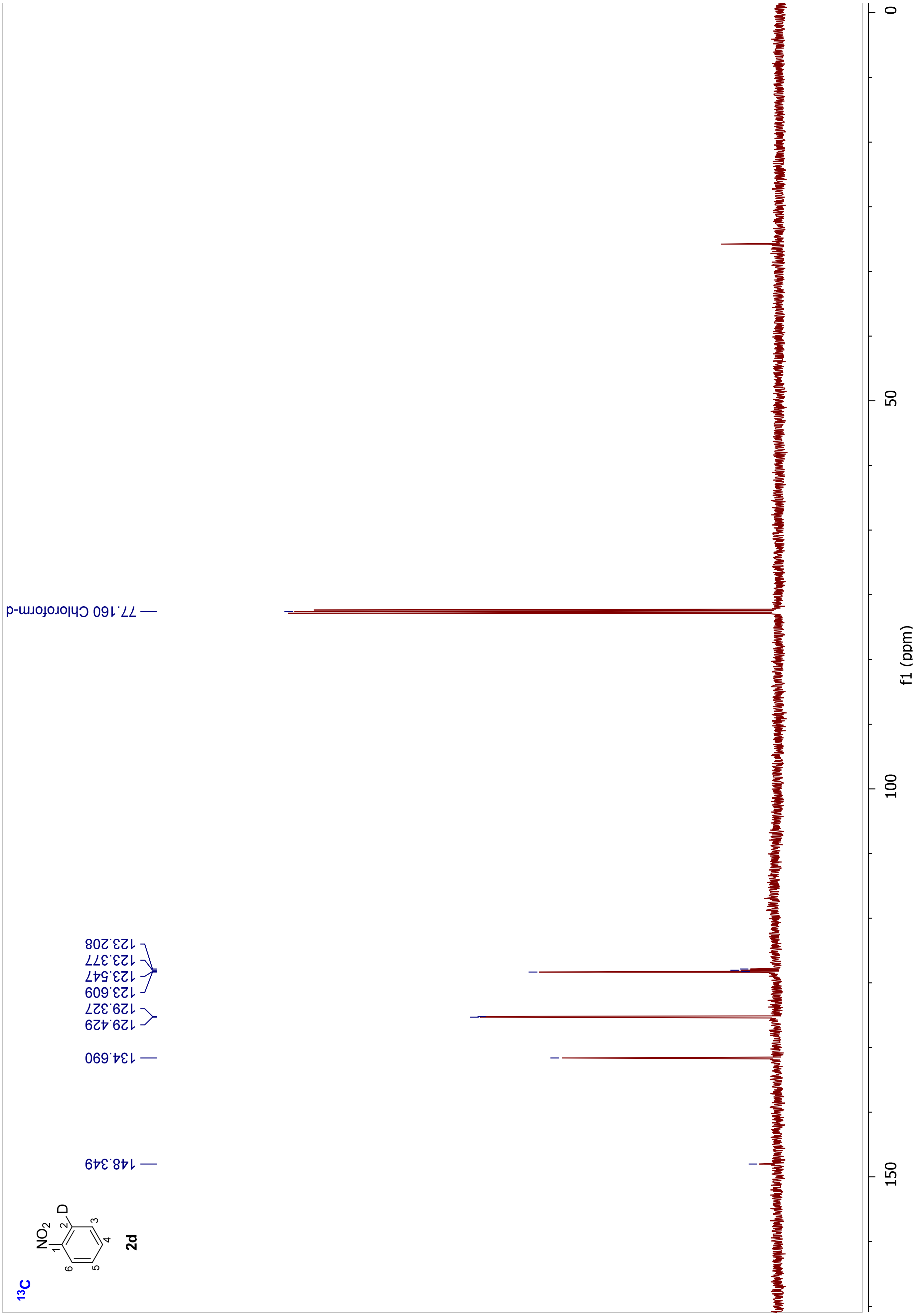
$$\text{at } 0\%\text{ D} \quad \alpha = \alpha_0 = 2$$

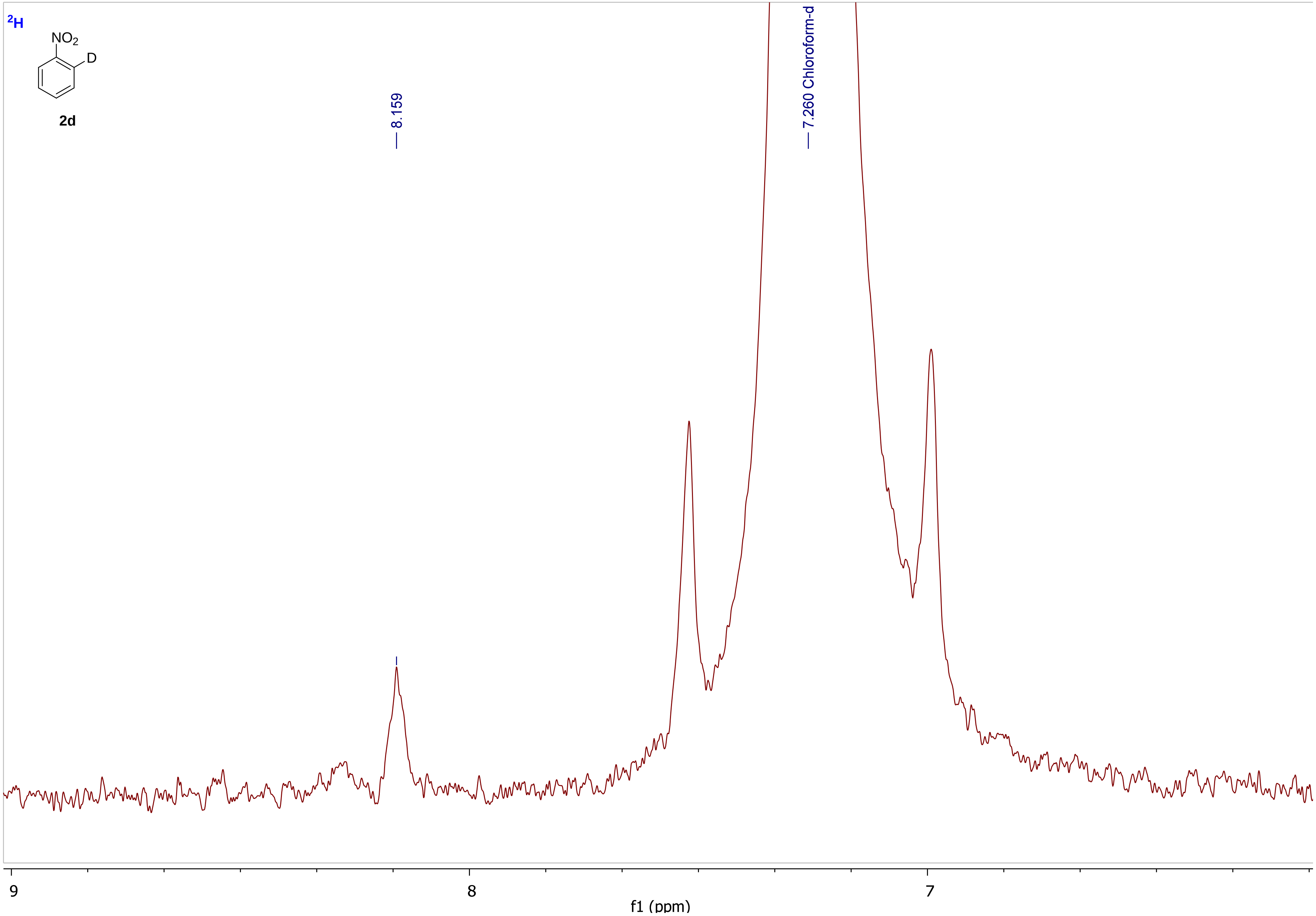
$$\therefore \%\text{ D} = (2 - \alpha) \times 100$$

$$\therefore \%\text{ D} = (2 - 1.025) \times 100$$

$$\therefore \%\text{ D} = 97.5\%$$


1H
NO2
D
2d
8.233
8.219
7.698
7.686
7.559
7.547
7.539
7.535
7.260 Chloroform-d
1.025
1.000
1.950
0
1
2
3
4
5
6
7
8
9
f1 (ppm)


13C
NO2
D
1
2
3
4
5
6
2d
148.349
134.690
129.429
129.327
123.609
123.547
123.377
123.208
77.160 Chloroform-d
0
50
100
150
f1 (ppm)


$^2$H
NO$_2$
D
2d
8.159
7.260 Chloroform-d
9
8
7
f1 (ppm)

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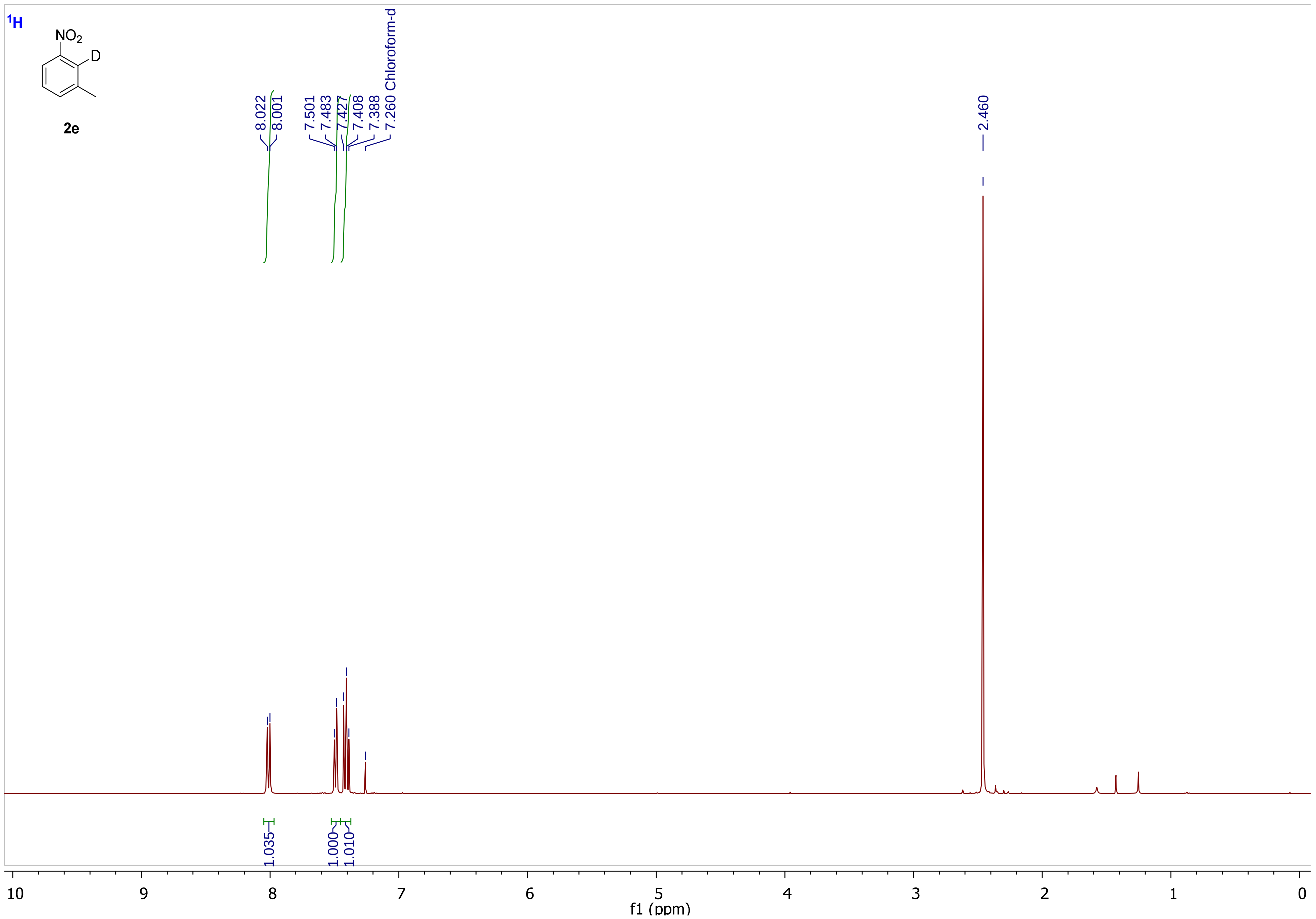
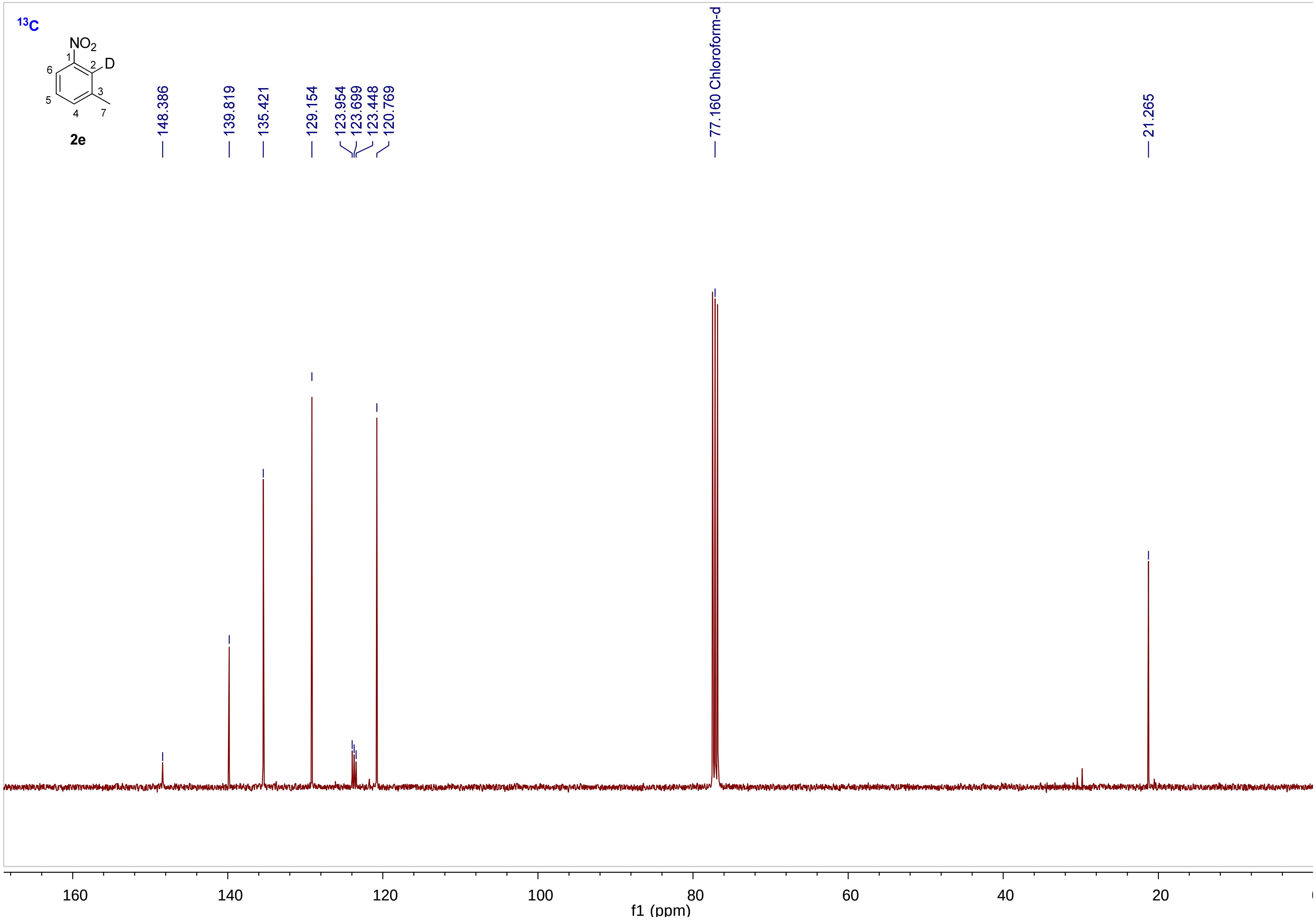
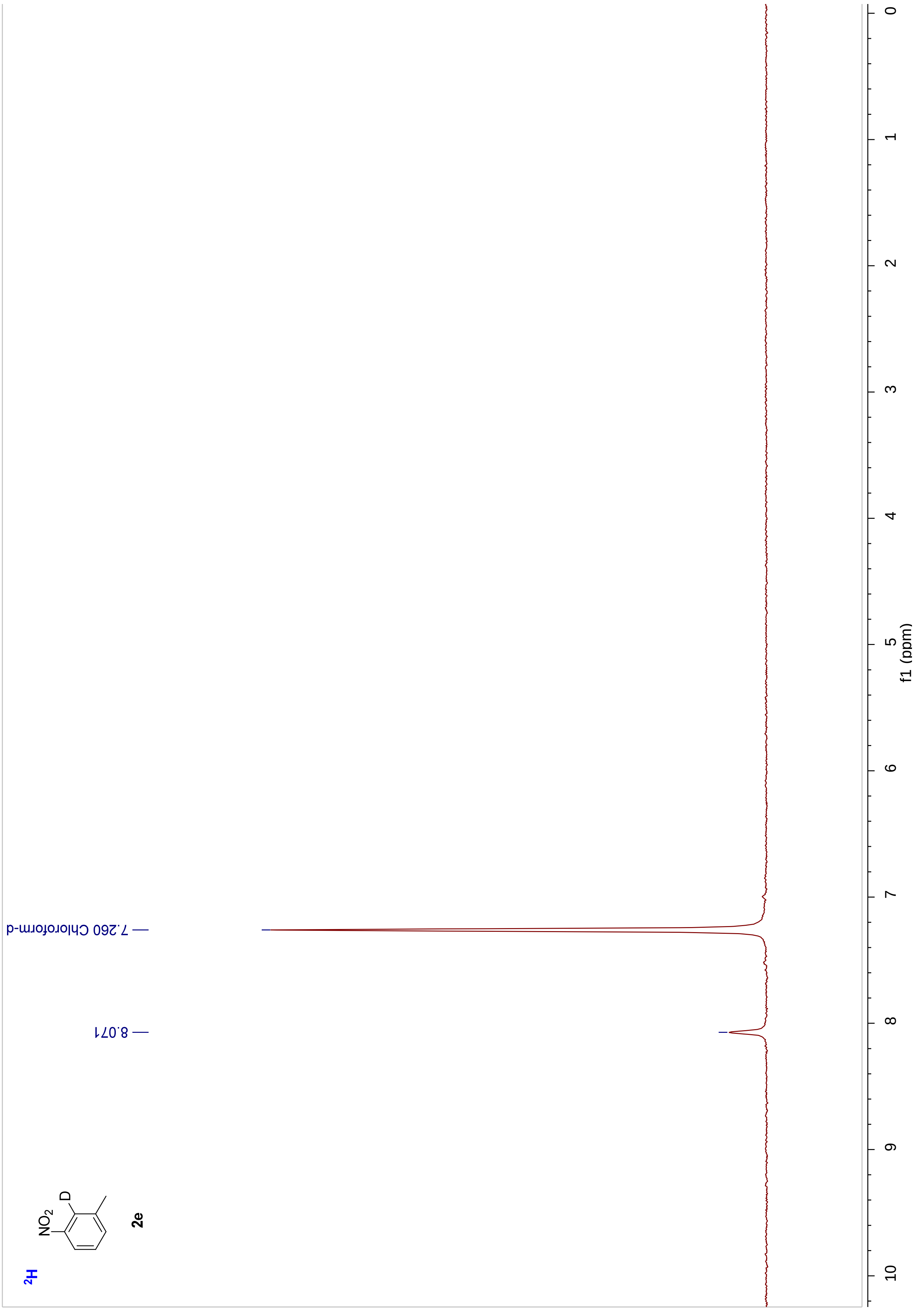
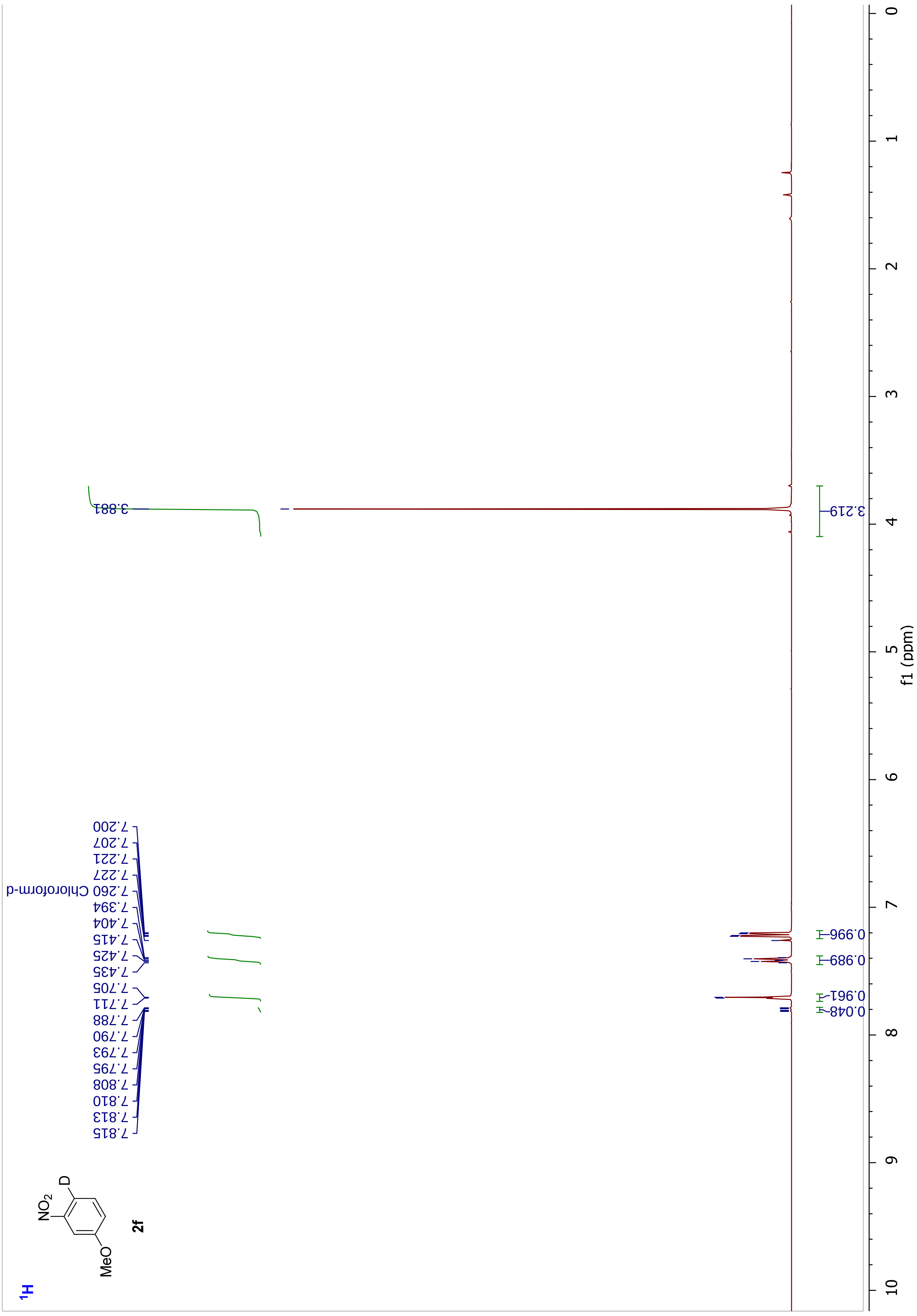
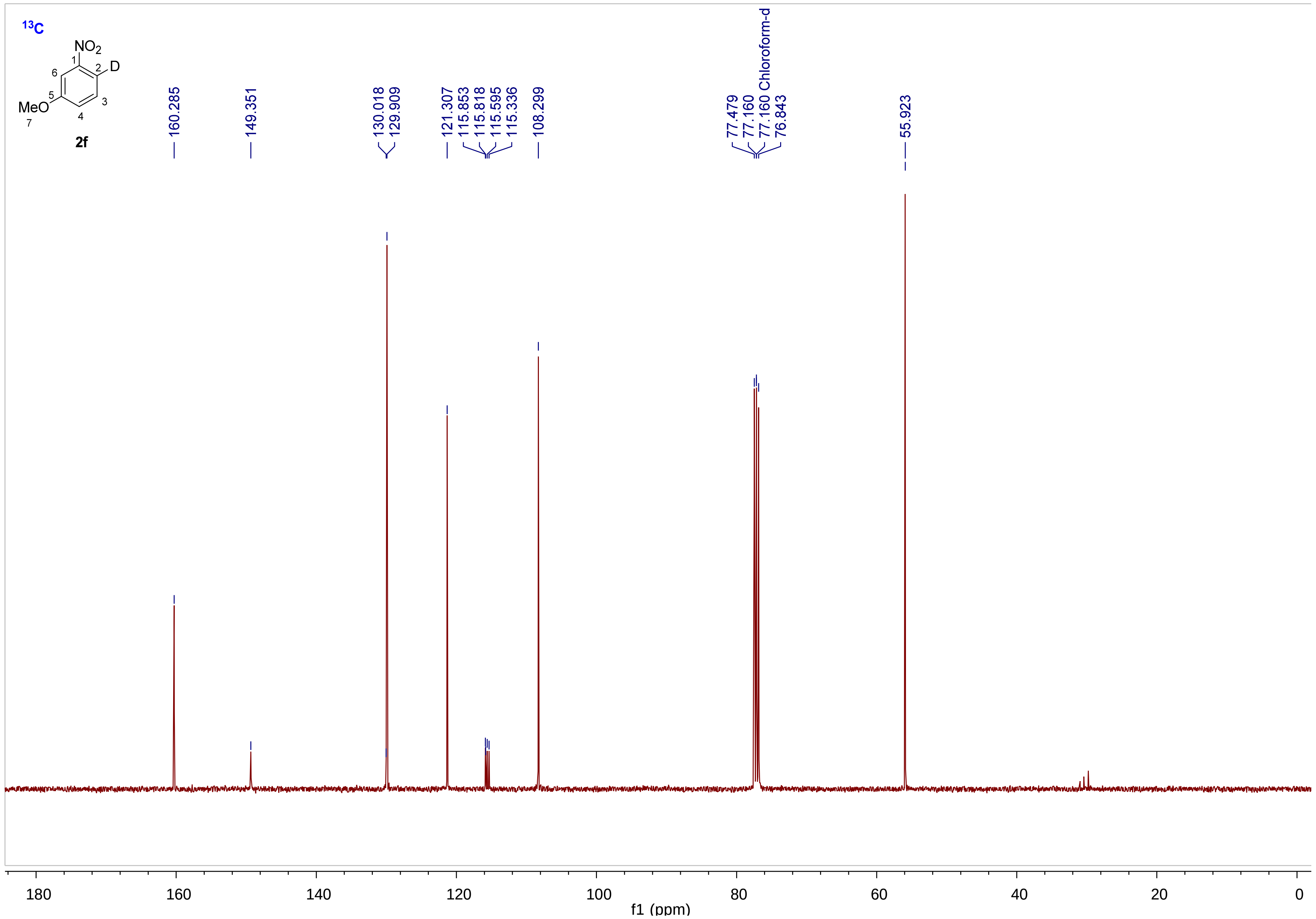
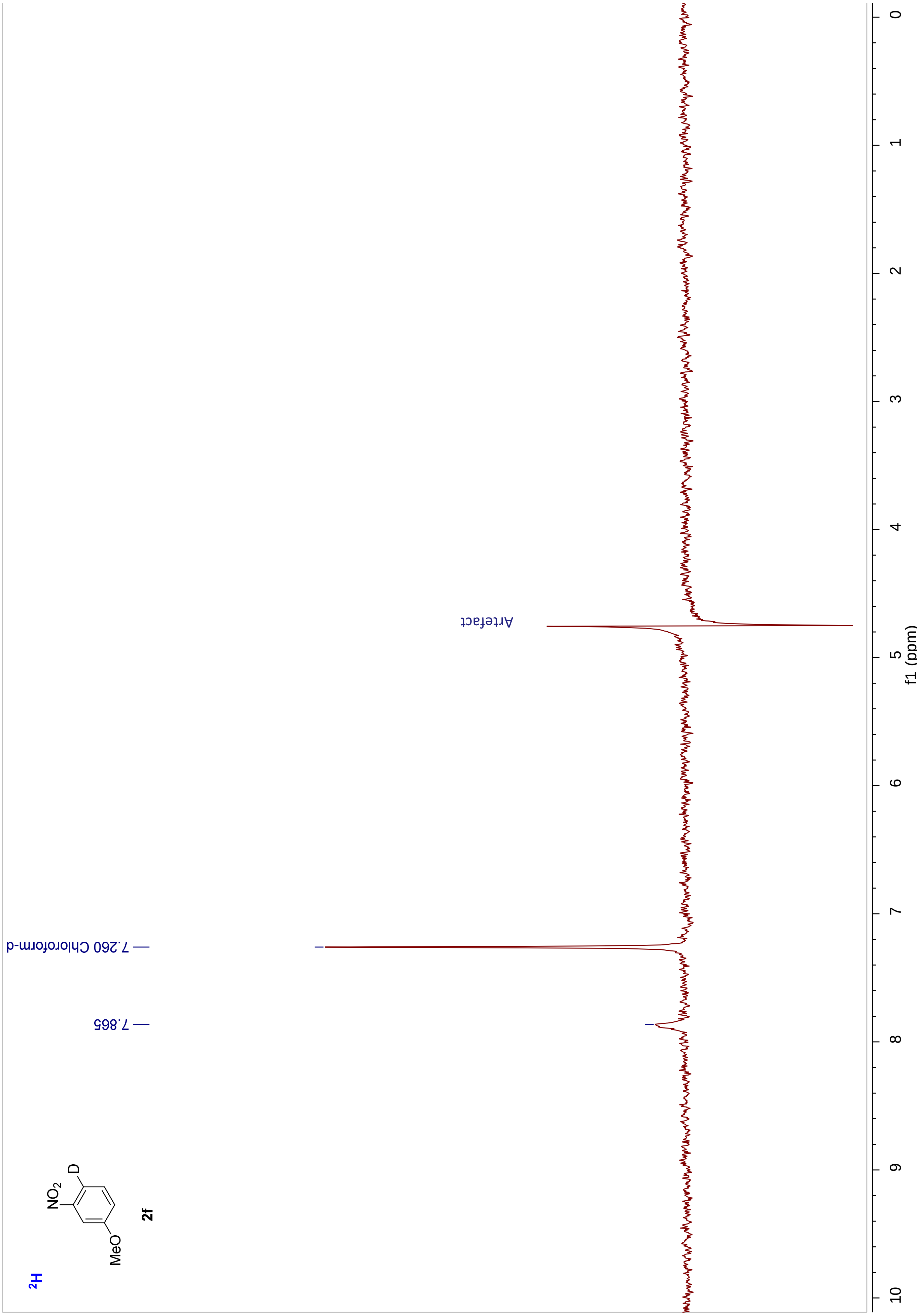


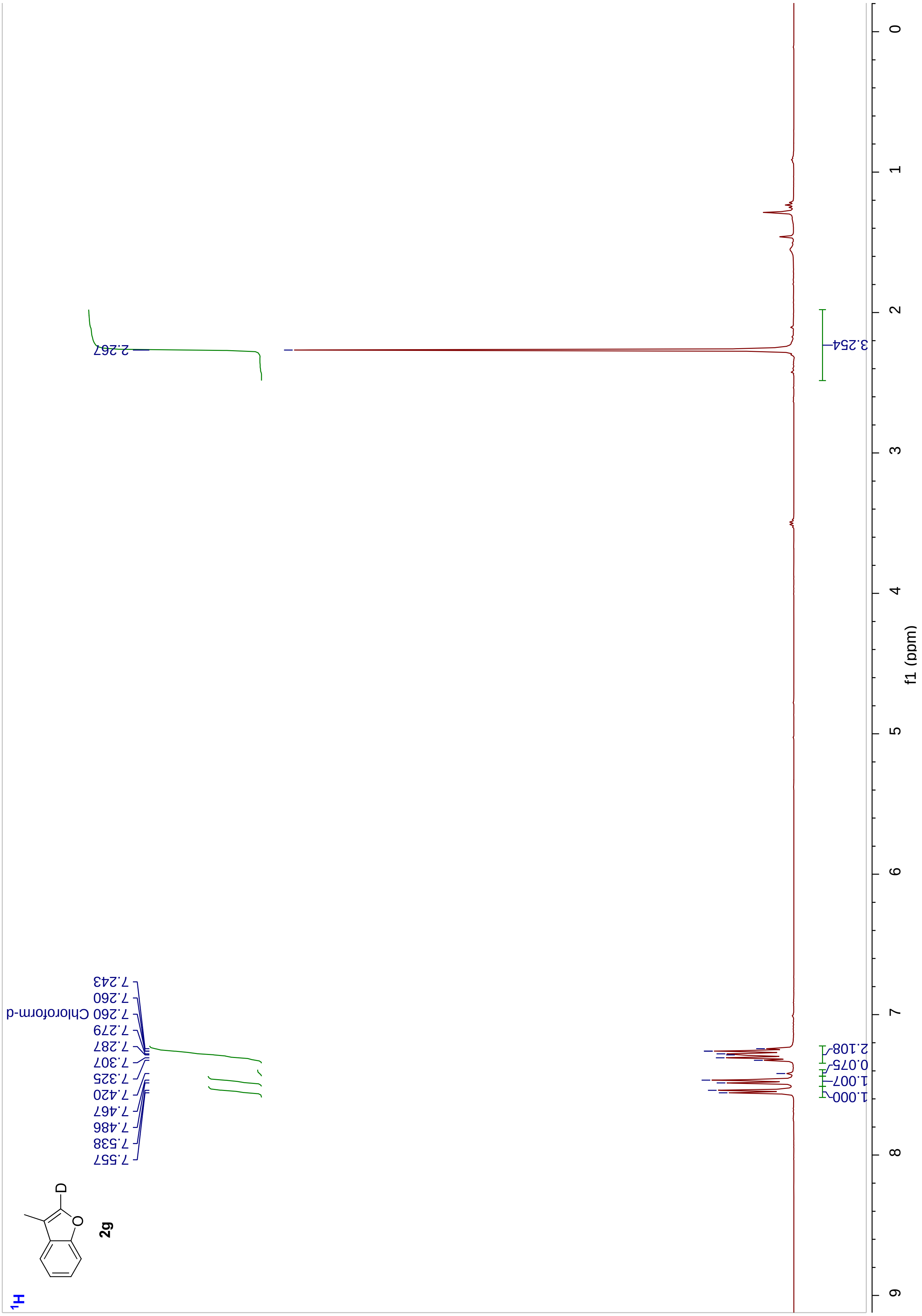

$^{13}C$
NO2
D
1
2
3
4
5
6
7
2e
148.386
139.819
135.421
129.154
123.954
123.699
123.448
120.769
77.160 Chloroform-d
21.265
160
140
120
100
80
60
40
20
f1 (ppm)


$^2H$
$NO_2$
D
2e
7.260 Chloroform-d
8.071
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)


¹H
MeO
NO2
D
2f
7.815
7.813
7.810
7.808
7.795
7.793
7.790
7.788
7.711
7.705
7.435
7.425
7.415
7.404
7.394
7.260 Chloroform-d
7.227
7.221
7.207
7.200
3.881
0.048
0.961
0.989
0.996
3.219
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

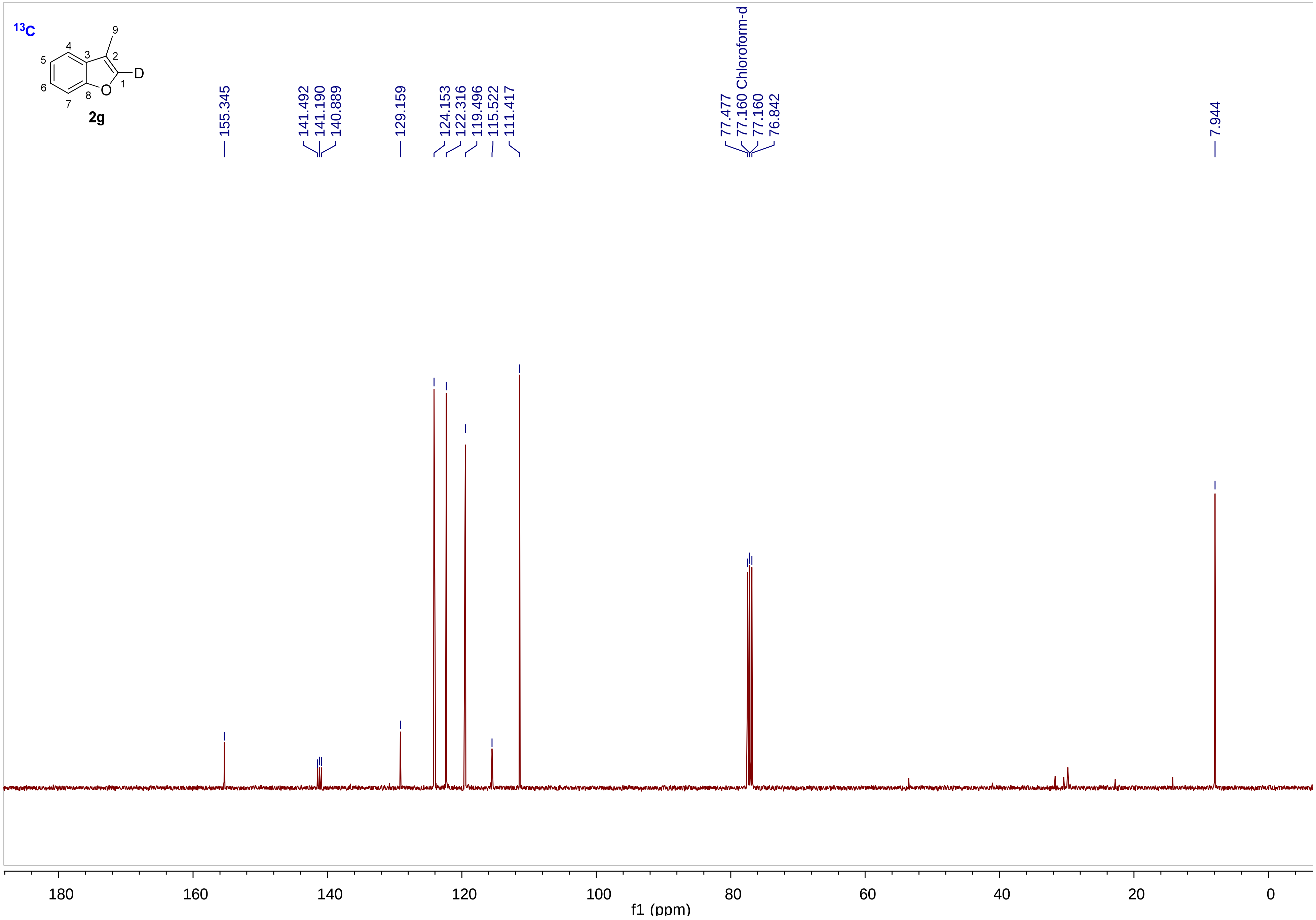

$^{13}$C
NO$_2$
D
MeO
1
2
3
4
5
6
7
2f
160.285
149.351
130.018
129.909
121.307
115.853
115.818
115.595
115.336
108.299
77.479
77.160
77.160 Chloroform-d
76.843
55.923
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

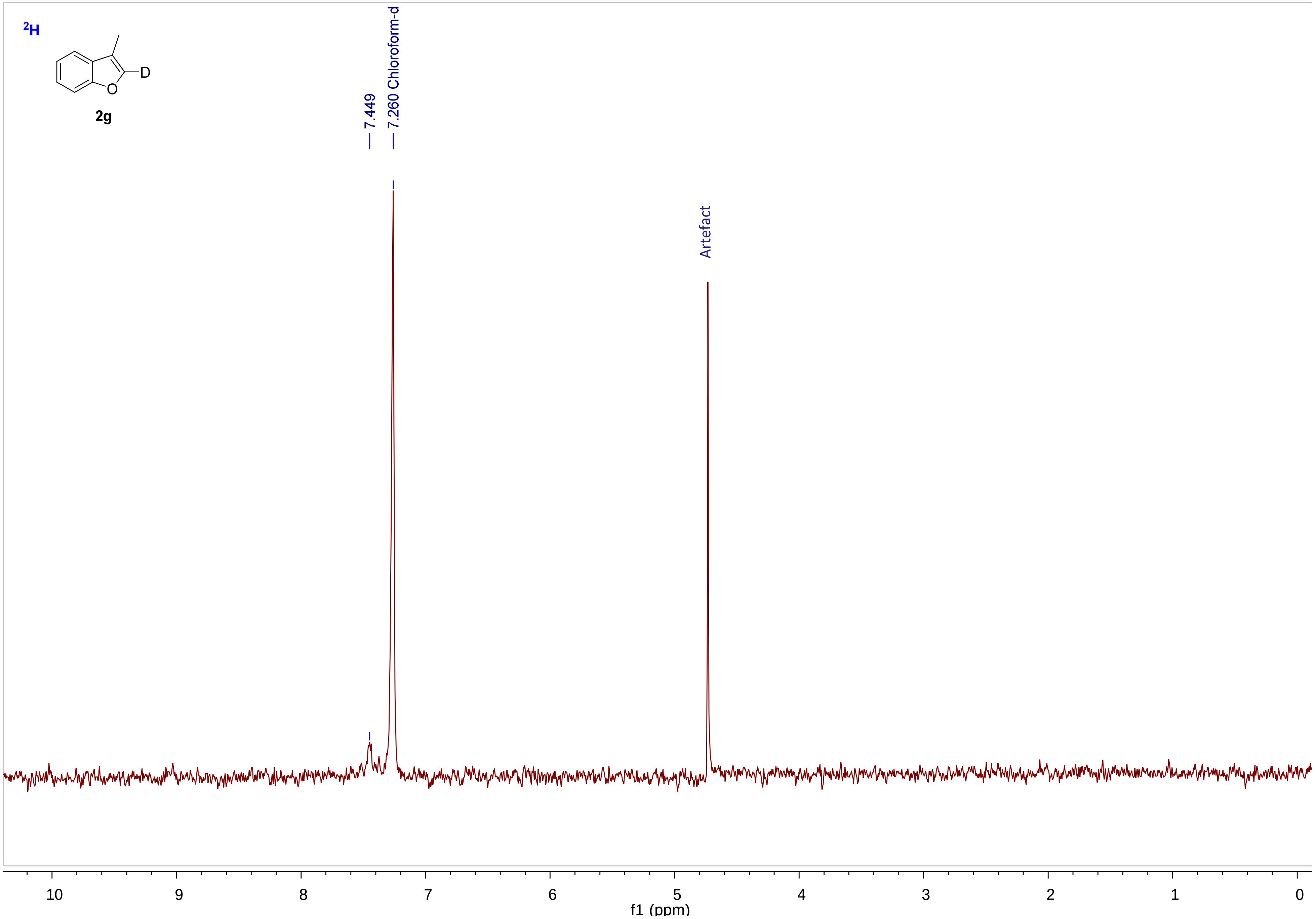

$^2H$
MeO
$NO_2$
D
2f
7.865
7.260 Chloroform-d
Artefact
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)

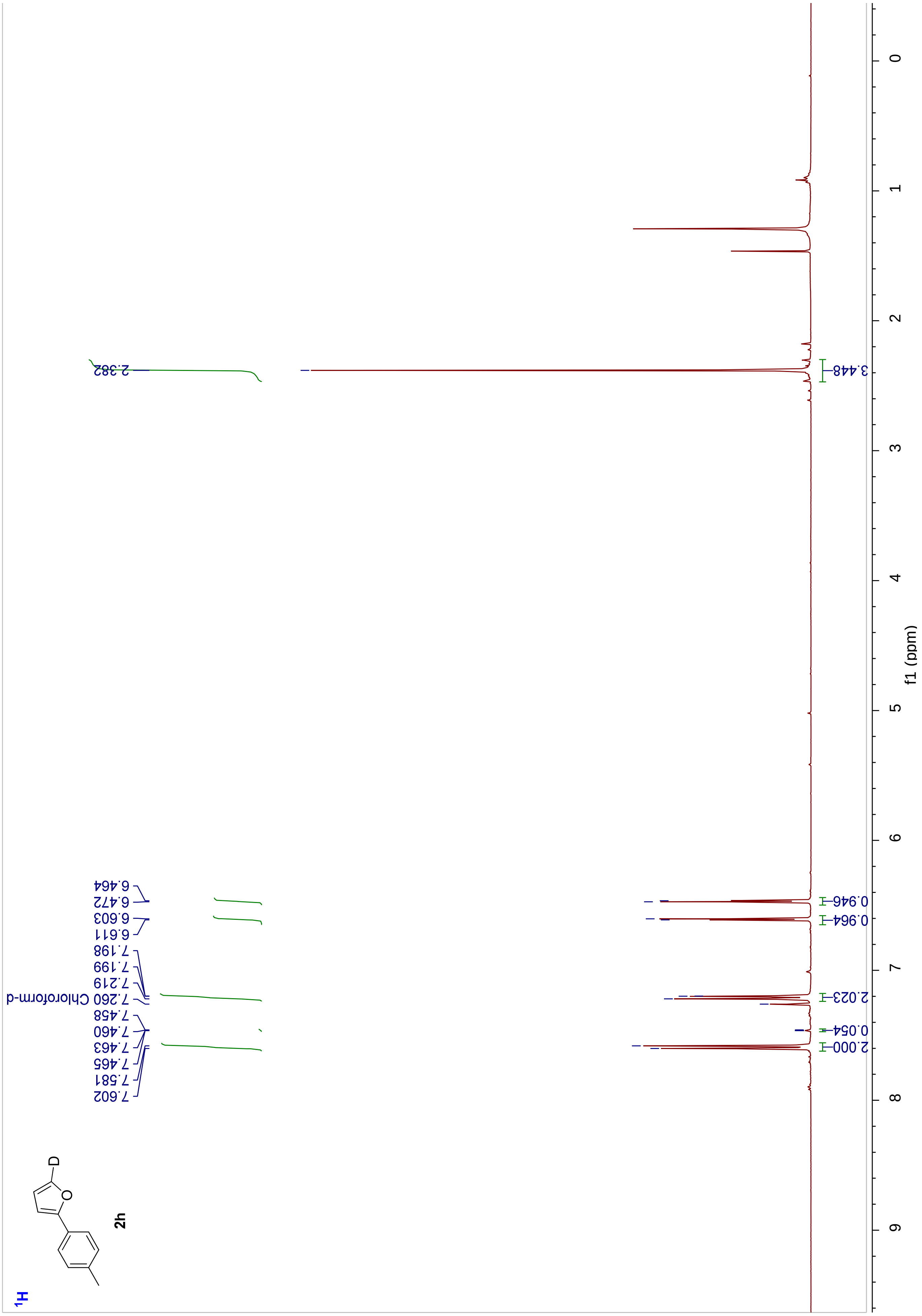


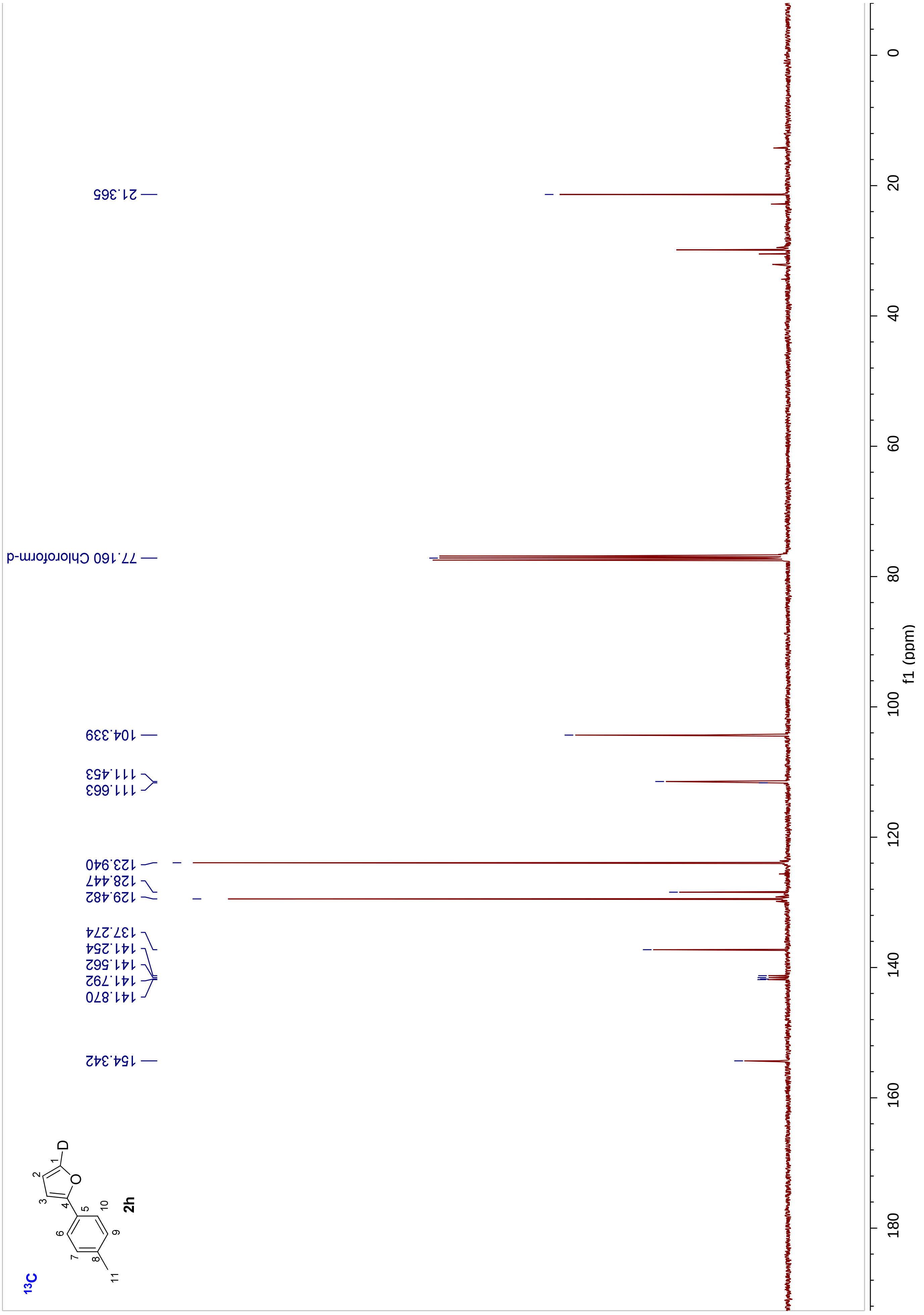
2g

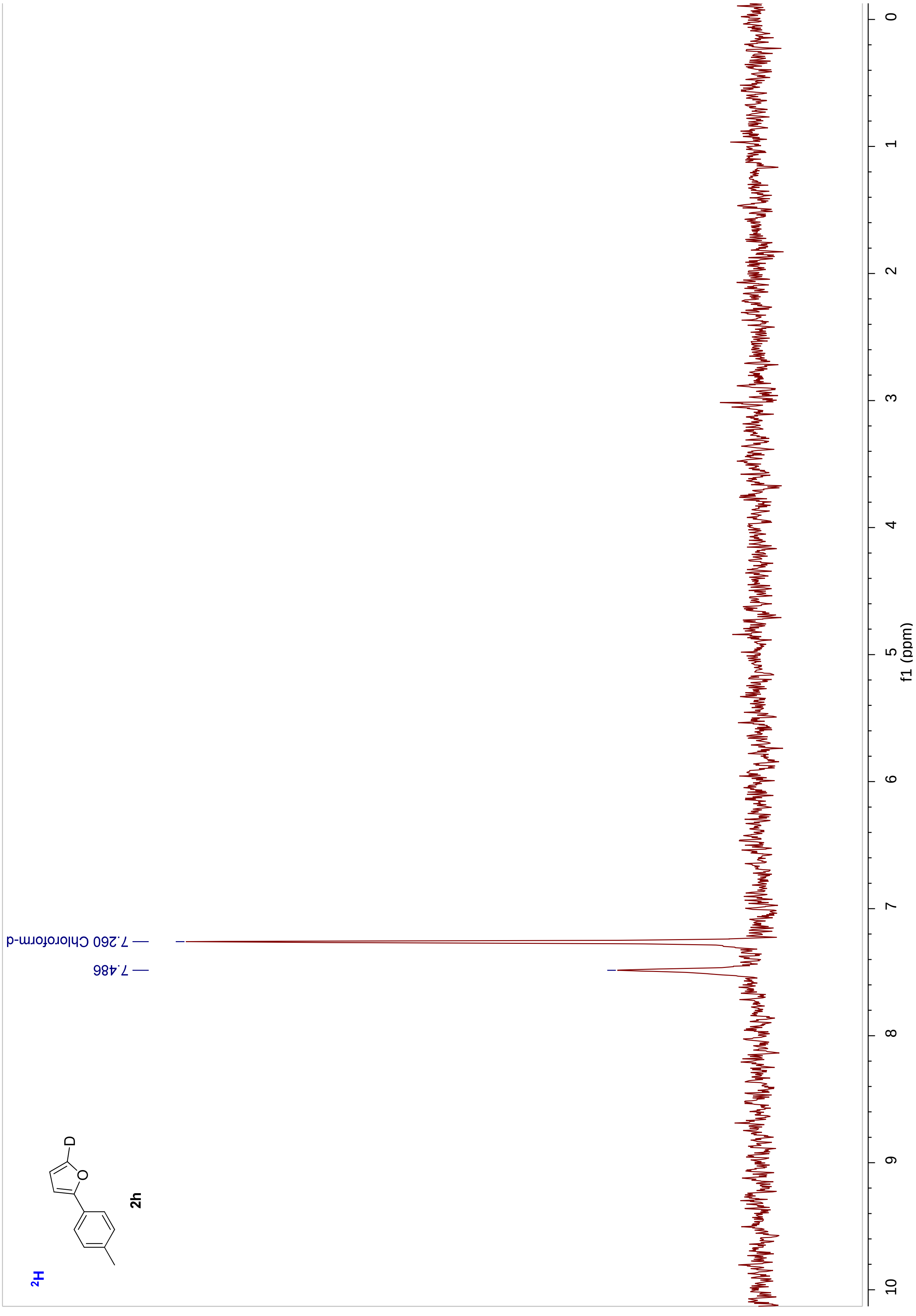
¹H
7.557
7.538
7.486
7.467
7.420
7.325
7.307
7.287
7.279
7.260 Chloroform-d
7.260
7.243
2.267
1.000
1.007
0.075
2.108
3.254
0
1
2
3
4
5
6
7
8
9
f1 (ppm)
D
O

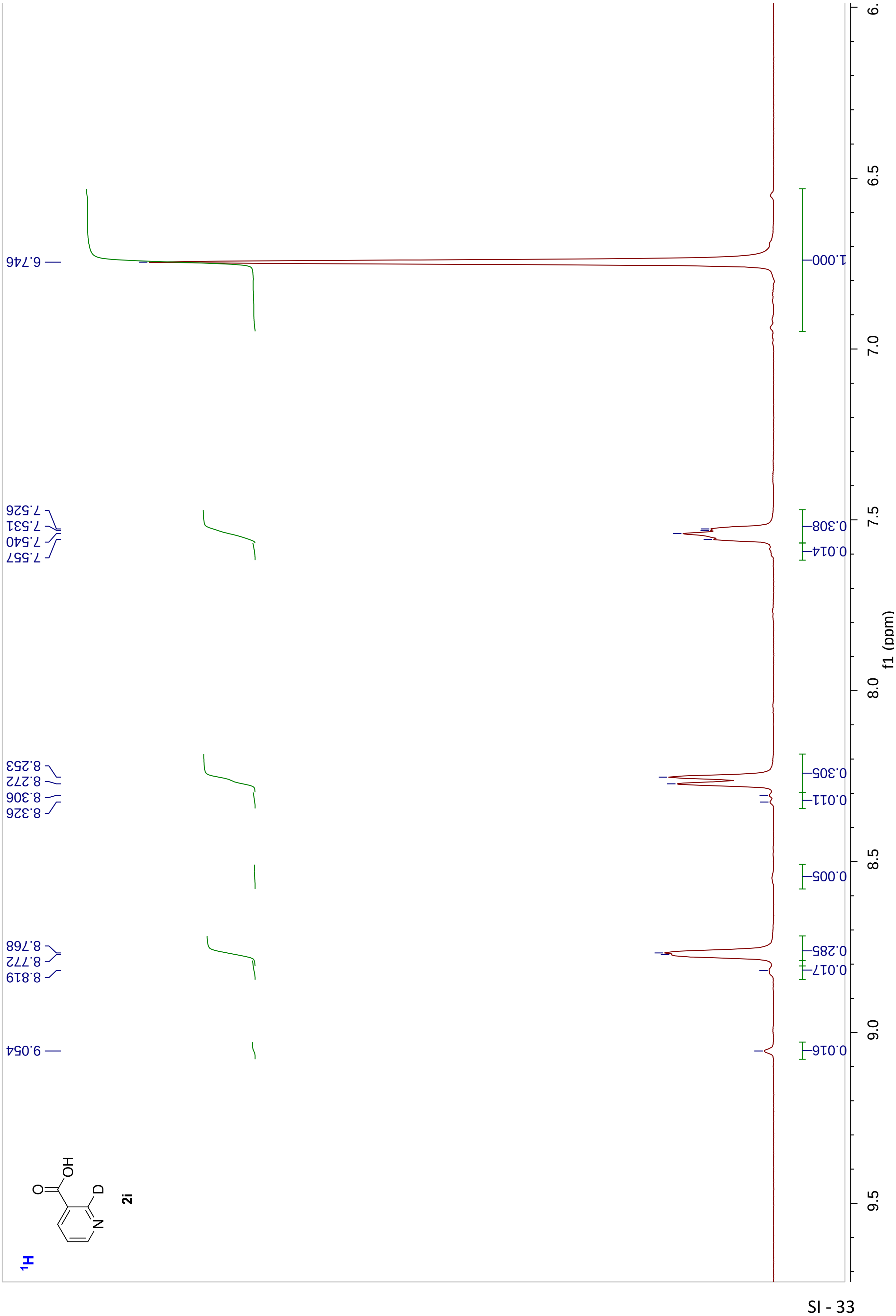

$^{13}$C
9
4
3
2
5
D
1
6
8
O
7
2g
155.345
141.492
141.190
140.889
129.159
124.153
122.316
119.496
115.522
111.417
77.477
77.160 Chloroform-d
77.160
76.842
7.944
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


²H
D
O
2g
7.449
7.260 Chloroform-d
Artefact
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

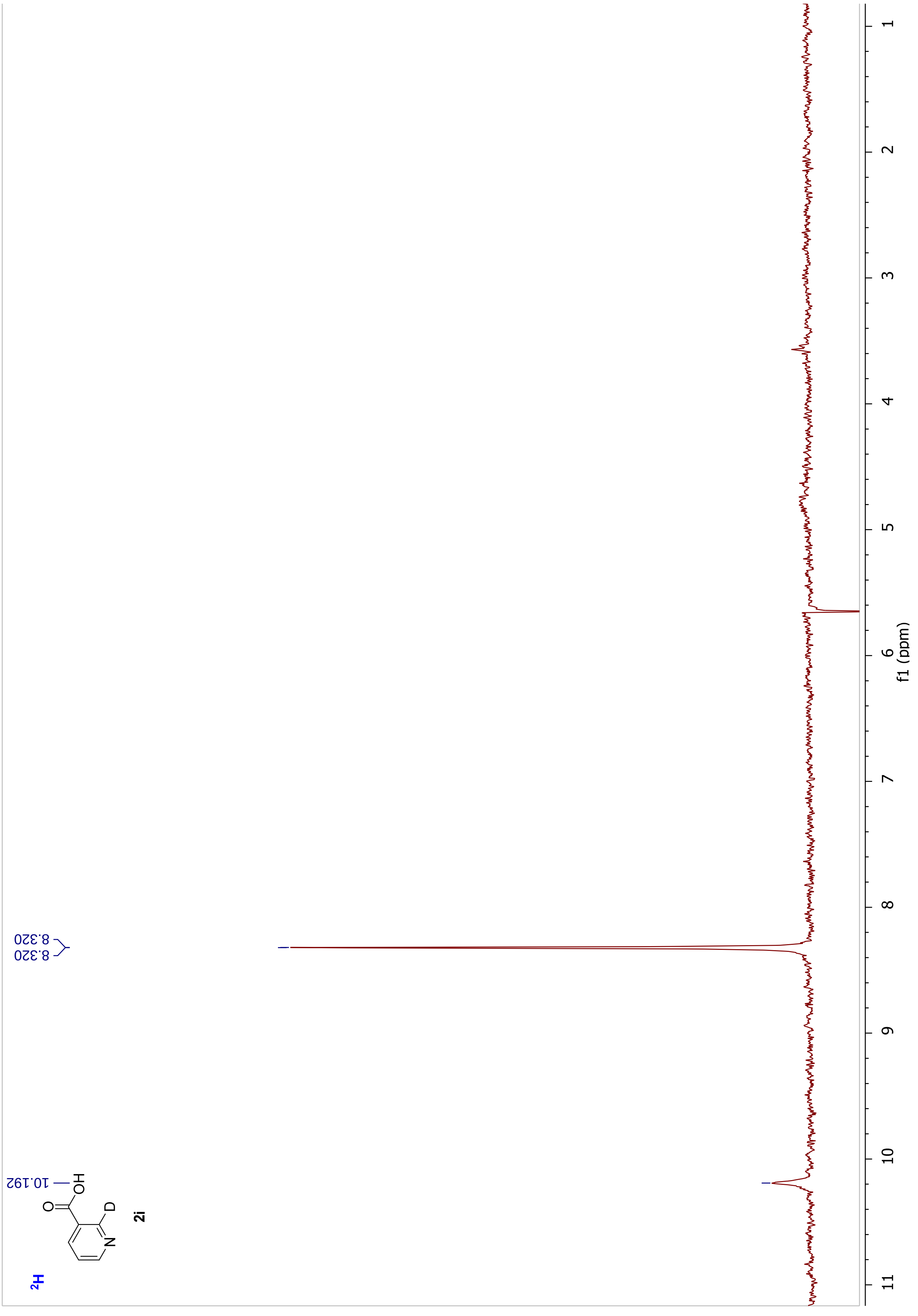

1H
2h
D
O
7.602
7.581
7.465
7.463
7.460
7.458
7.260 Chloroform-d
7.219
7.199
7.198
6.611
6.603
6.472
6.464
2.382
2.000
0.054
2.023
0.964
0.946
3.448
f1 (ppm)
0
1
2
3
4
5
6
7
8
9

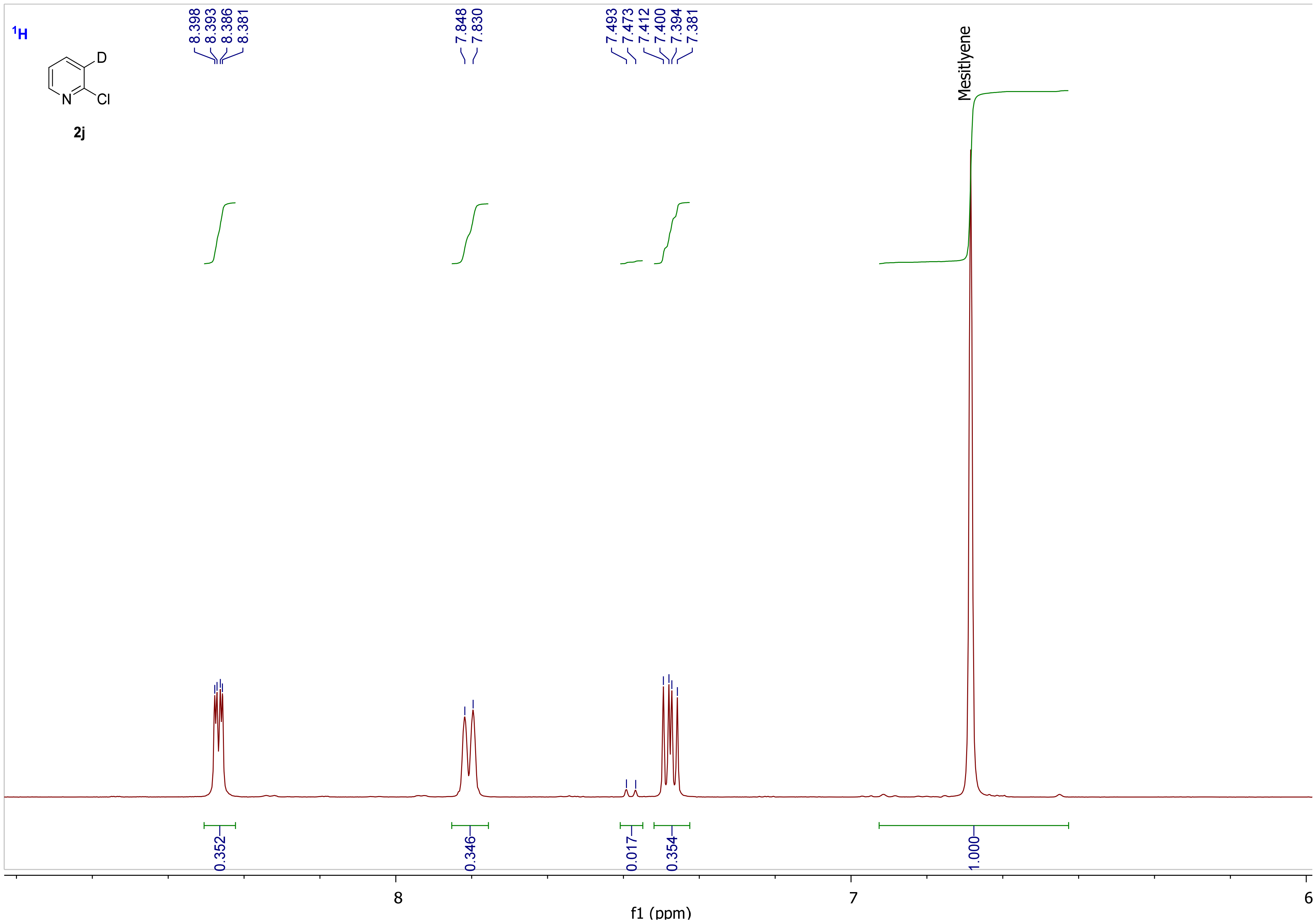

$^{13}C$
2h
1
2
3
4
5
6
7
8
9
10
11
D
O
21.365
77.160 Chloroform-d
104.339
111.453
111.663
123.940
128.447
129.482
137.274
141.254
141.562
141.792
141.870
154.342
0
20
40
60
80
100
120
140
160
180
f1 (ppm)

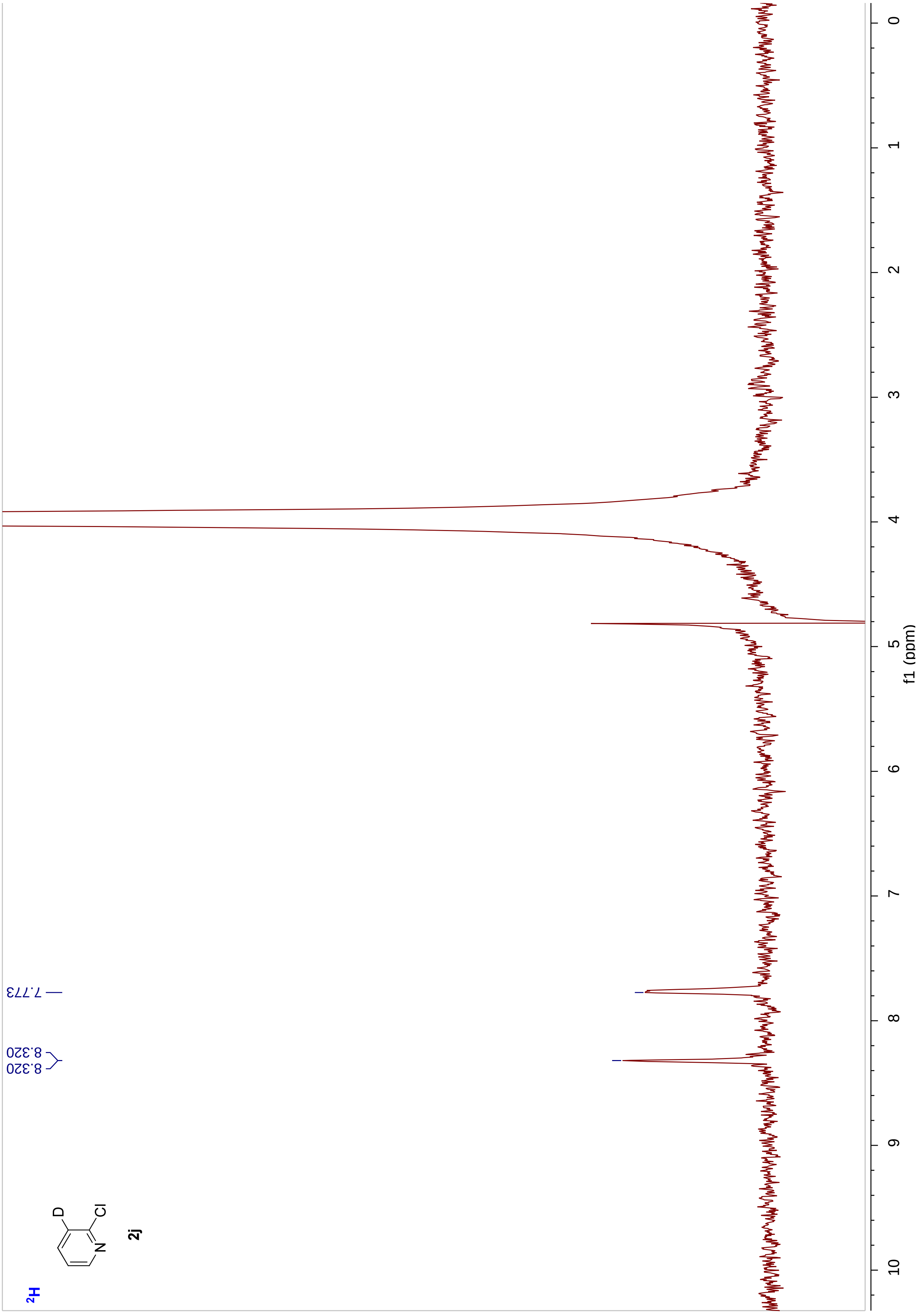

²H
D
O
2h
7.486
7.260 Chloroform-d
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)


1H
O
OH
D
N
9.054
8.819
8.772
8.768
8.326
8.306
8.272
8.253
7.557
7.540
7.531
7.526
6.746
0.016
0.017
0.285
0.005
0.011
0.305
0.014
0.308
1.000
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.
f1 (ppm)

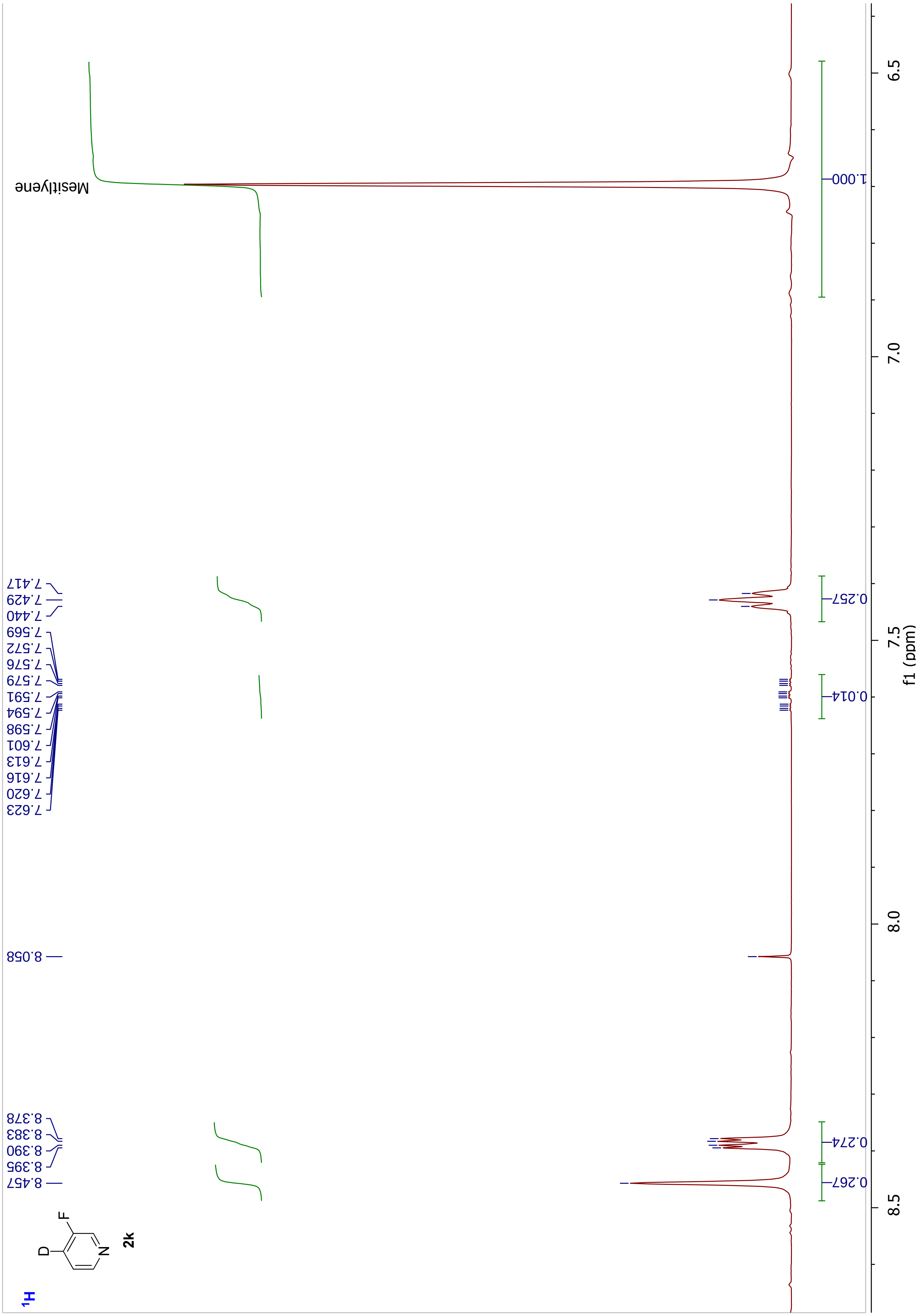
**2i**

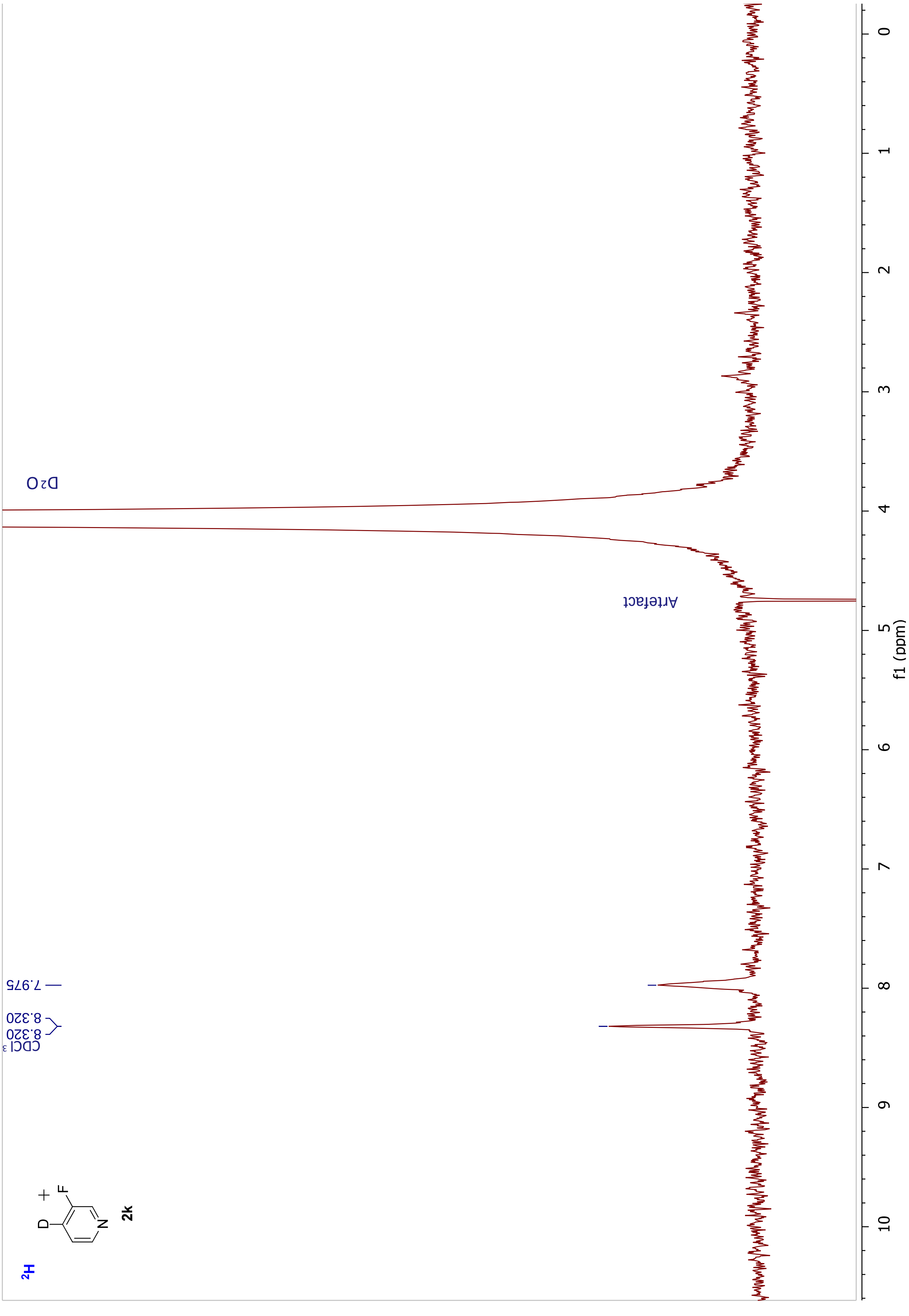

2H
2i
D
N
O
OH
10.192
8.320
8.320
f1 (ppm)
1
2
3
4
5
6
7
8
9
10
11


$^1H$
D
N
Cl
2j
8.398
8.393
8.386
8.381
7.848
7.830
7.493
7.473
7.412
7.400
7.394
7.381
Mesitlyene
0.352
0.346
0.017
0.354
1.000
8
7
6
f1 (ppm)

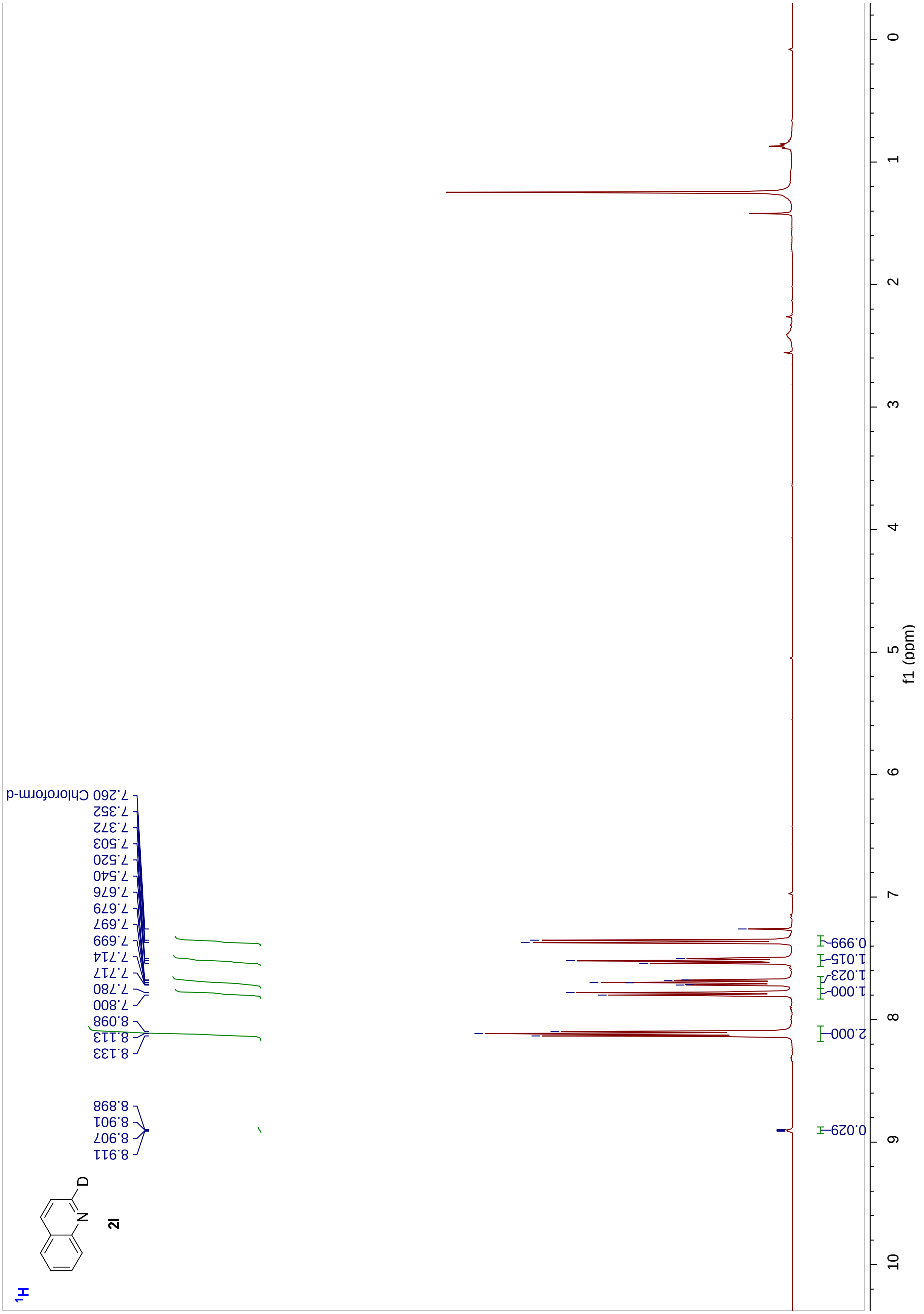


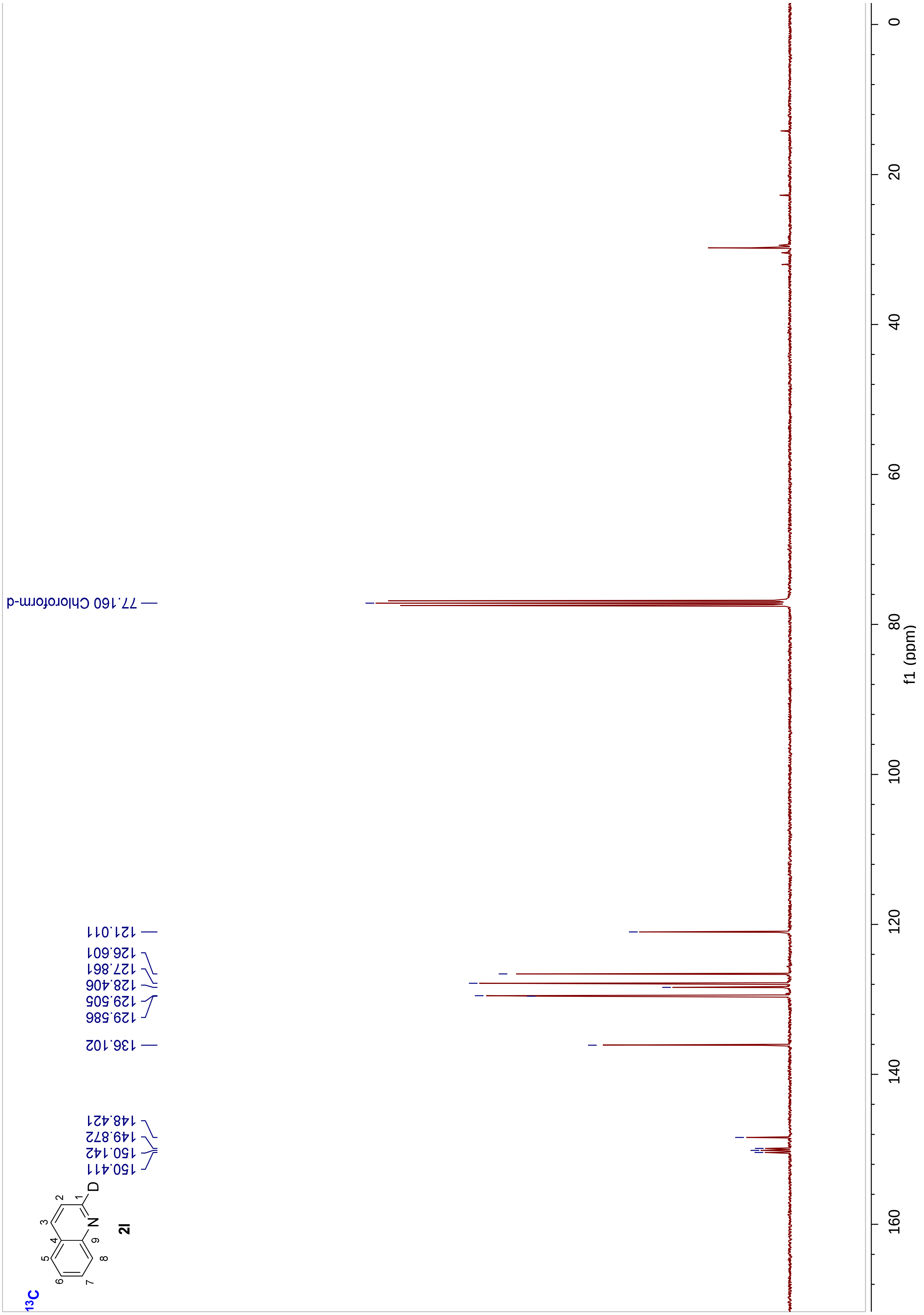
**2j**

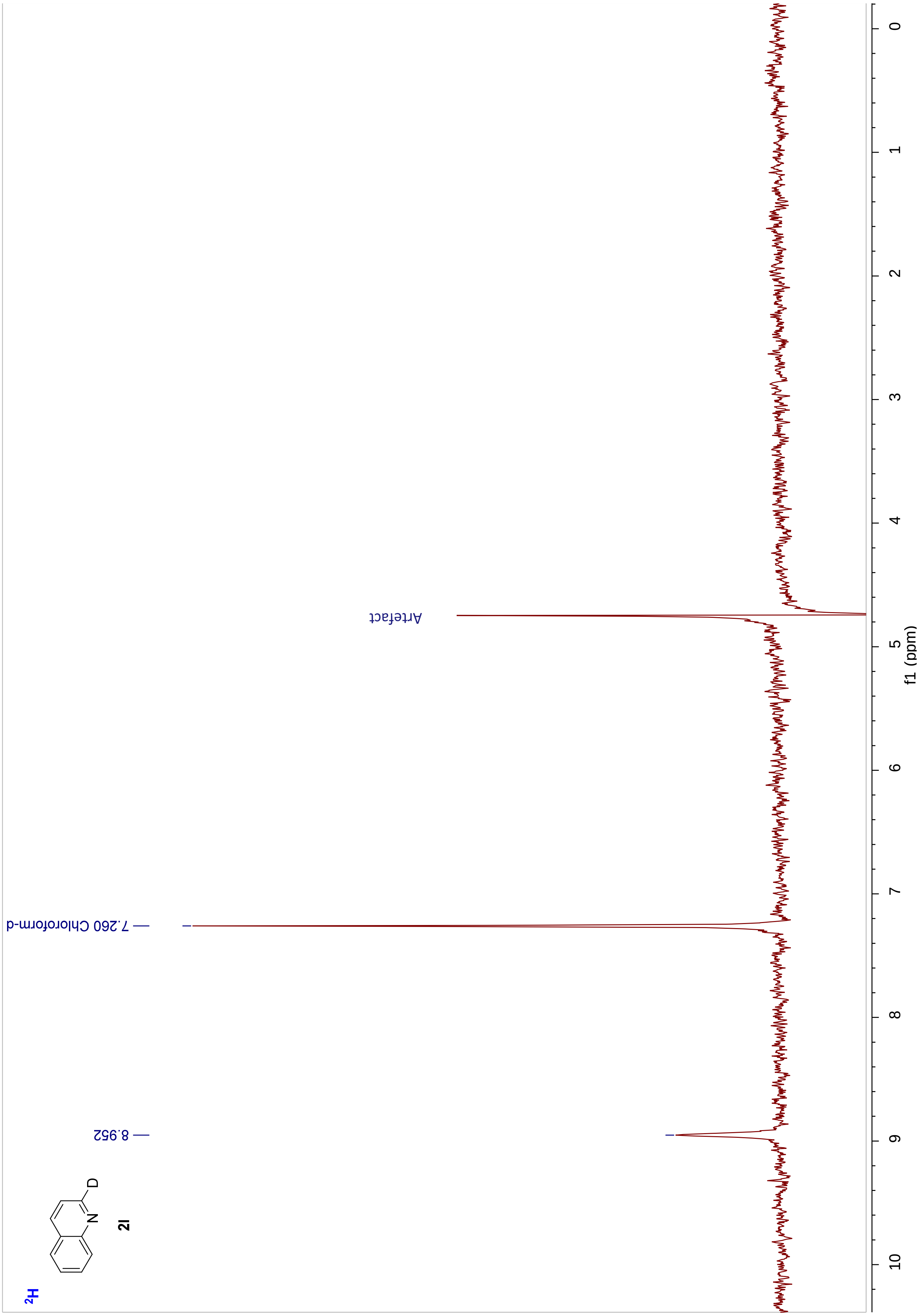

1H
D
F
N
2k
Mesitylene
7.417
7.429
7.440
7.569
7.572
7.576
7.579
7.591
7.594
7.598
7.601
7.613
7.616
7.620
7.623
8.058
8.378
8.383
8.390
8.395
8.457
1.000
0.257
0.014
0.274
0.267
6.5
7.0
7.5
8.0
8.5
f1 (ppm)

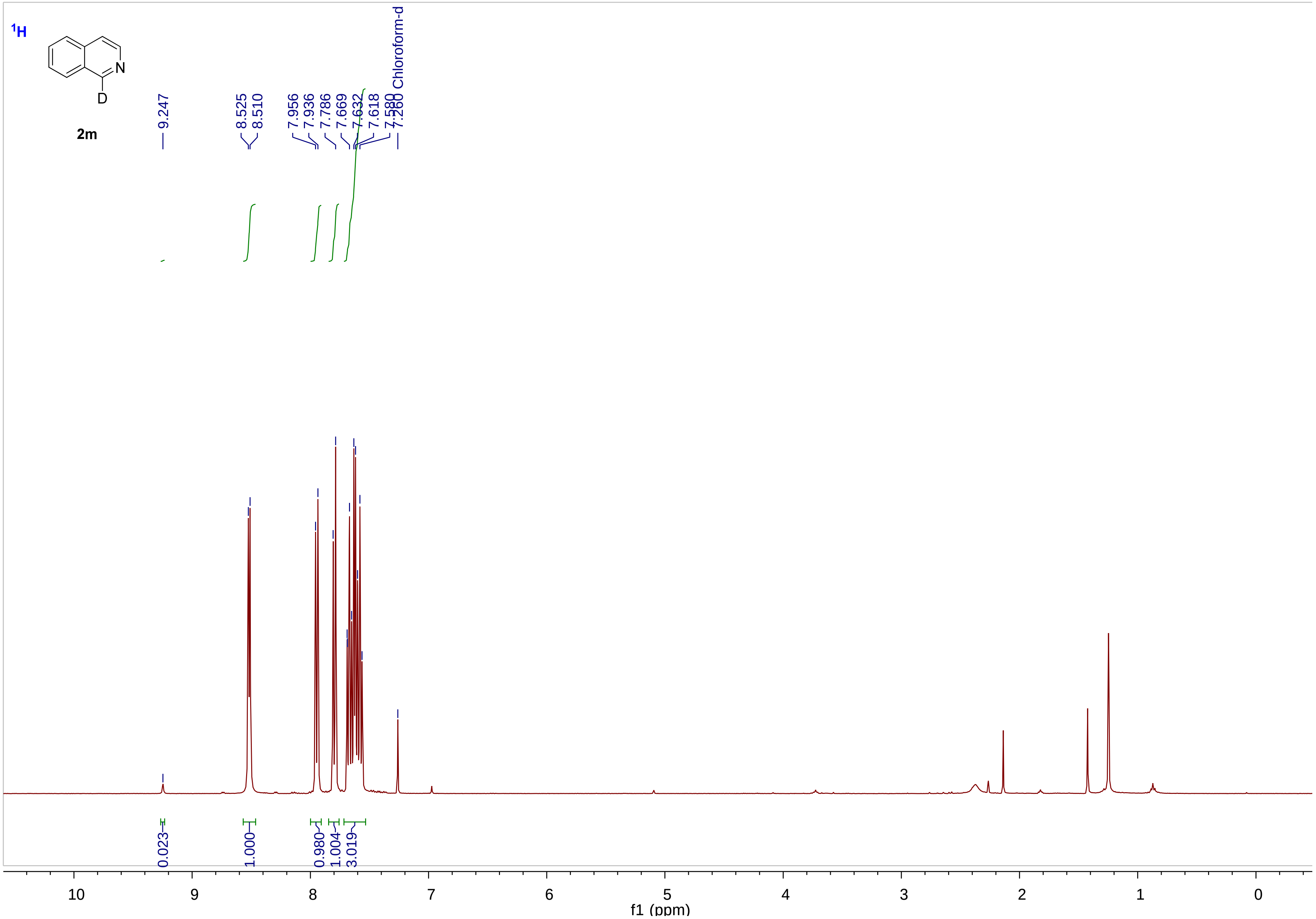

²H
D
F
N
D₂O
Artefact
7.975
8.320
8.320
CDCl₃
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)

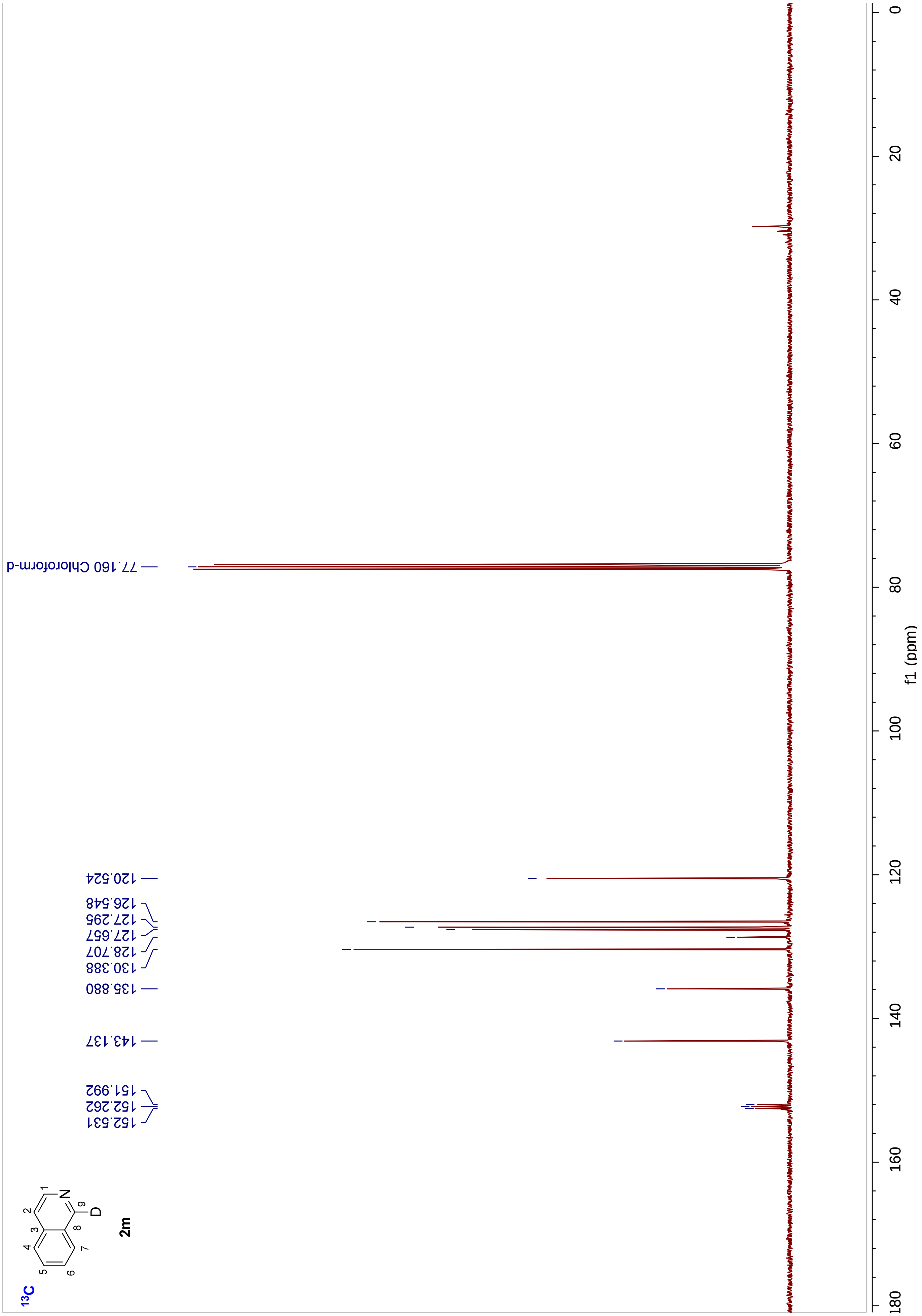
2k

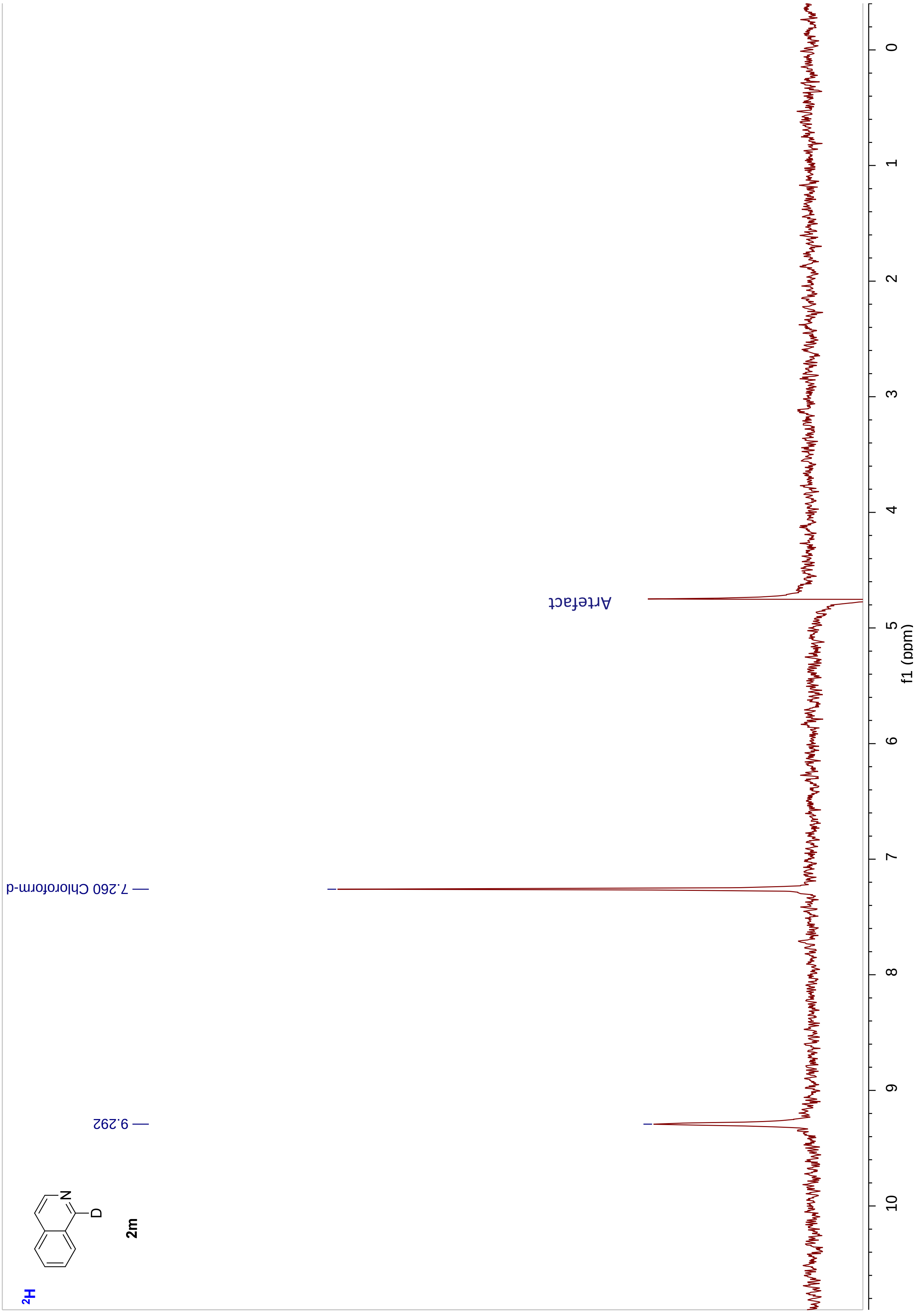

1H
N
D
2l
7.260 Chloroform-d
7.352
7.372
7.503
7.520
7.540
7.676
7.679
7.697
7.699
7.714
7.717
7.780
7.800
8.098
8.113
8.133
8.898
8.901
8.907
8.911
0.999
1.015
1.023
1.000
2.000
0.029
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)


13C
2l
N
D
1
2
3
4
5
6
7
8
9
150.411
150.142
149.872
148.421
136.102
129.586
129.505
128.406
127.861
126.601
121.011
77.160 Chloroform-d
f1 (ppm)
0
20
40
60
80
100
120
140
160


²H
D
N
2l
8.952
7.260 Chloroform-d
Artefact
f1 (ppm)
0
1
2
3
4
5
6
7
8
9
10


$^1$H
D
N
2m
9.247
8.525
8.510
7.956
7.936
7.786
7.669
7.632
7.618
7.580
7.260 Chloroform-d
0.023
1.000
0.980
1.004
3.019
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


13C
2m
1
2
3
4
5
6
7
8
9
N
D
77.160 Chloroform-d
120.524
126.548
127.295
127.657
128.707
130.388
135.880
143.137
151.992
152.262
152.531
0
20
40
60
80
100
120
140
160
180
f1 (ppm)


²H
D
N
2m
9.292
7.260 Chloroform-d
Artefact
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)