Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis of new fluorescent amino acids with triazolopyridine core: Diacids sensors ESI

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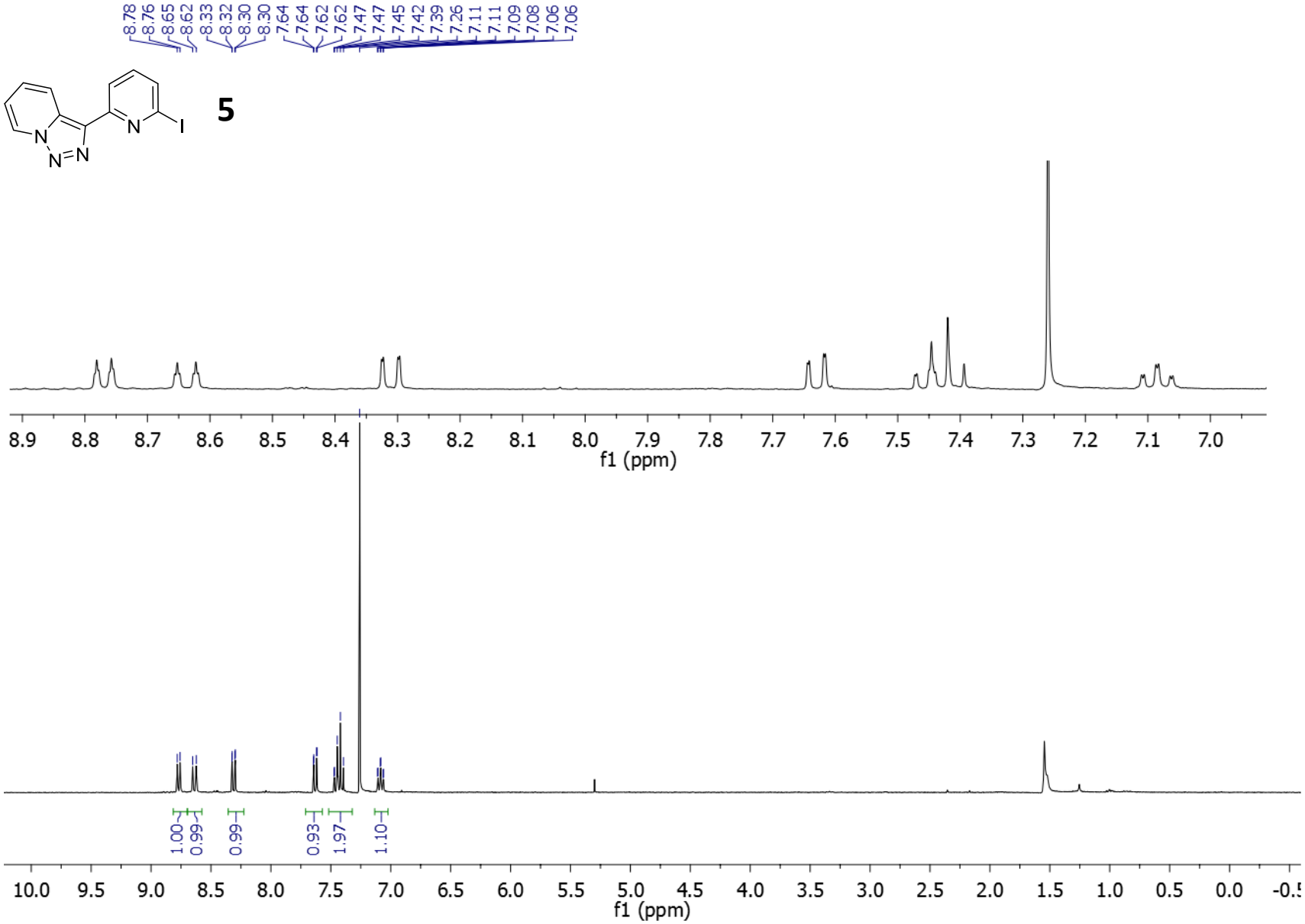
S1: Materials and Methods
S2: ^{1}H NMR Spectra of starting material
S3: NMR Spectra of new compounds

S1: Materials and Methods

Starting materials, if commercially available, were purchased and used as such. The solvents used were of spectroscopic or equivalent grade. When known compounds had to be prepared by literature procedures, pertinent references are given. Melting points or ranges (m.p.) given were determined on a Büchi B-545 heated stage. ^{1}H and (^{1}H decoupled) ^{13}C nuclear magnetic resonance (NMR) spectra were recorded at 300 and 75 MHz. Chemical shifts are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual deuterated Chlorophorm or deuterated methanol. Coupling constants (J) are given in Hz. Coupling patterns are abbreviated as, for example, s (singlet), d (doublet), t (triplet), q (quartet), td (triplet of doublets), m (multiplet), app. s (apparent singlet) and br. (broad). COSY and DEPT/ed-HSQC experiments were performed for all compounds. IR spectra were recorded using FT-IR ATR. HRMS were recorded using TOF electro-spray ionization (ESI-positive). UV-Visible spectra were measured on an Agilent 8453 spectrometer equipped with a Peltier temperature controller system (±0.1 °C). The emission spectra were recorded with a PTI MO- 5020 spectrofluorimeter in the 300–700 nm range.

S2: ^{1}H NMR Spectra of starting material



S3: NMR Spectra of new compounds

(2S*)-2-{[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl-amino} propanoic acid **4a**.*

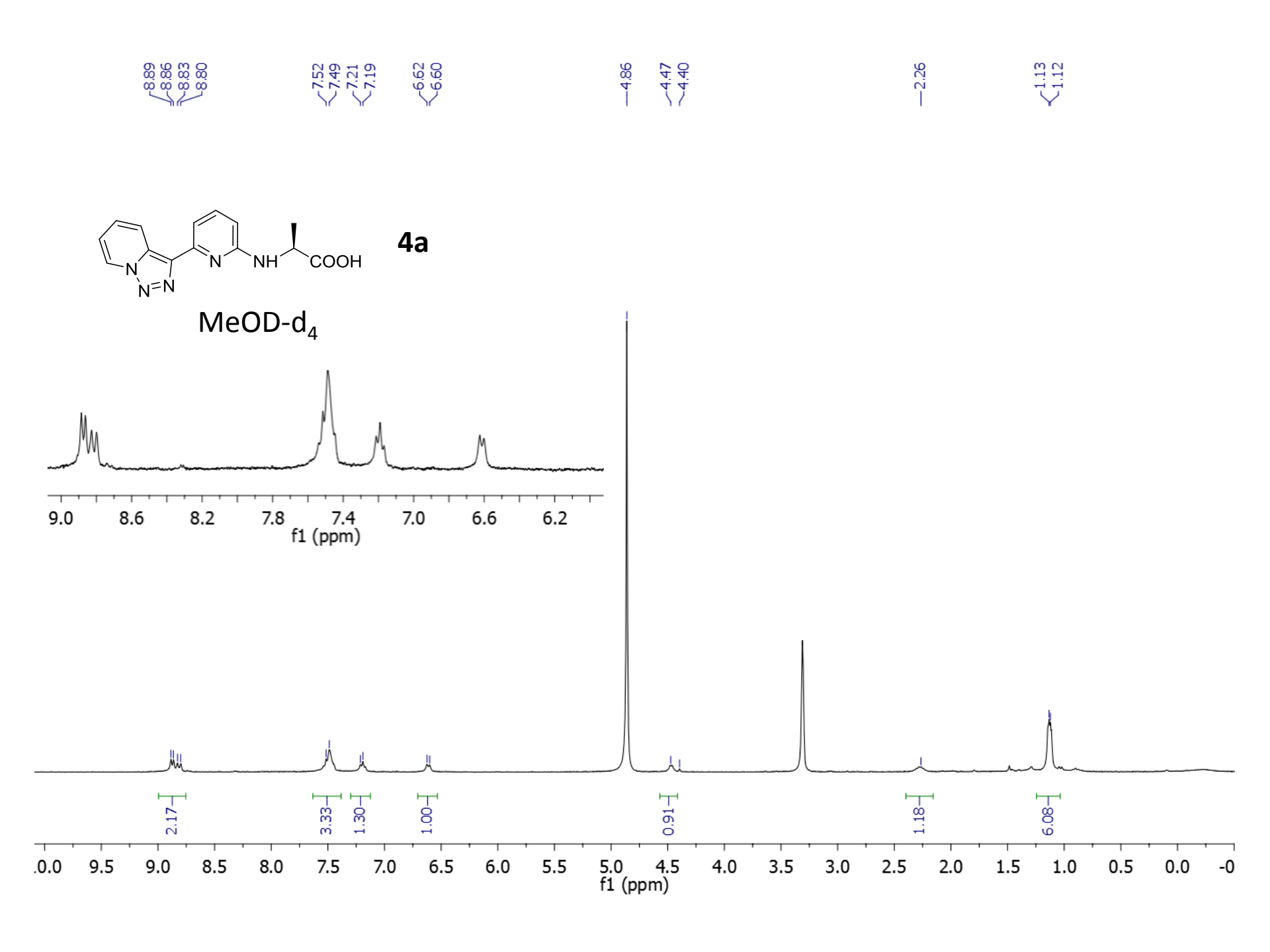
(2S)-3-Methyl-2-{[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl]amino}butanoic acid **4b**

(2S)-1-[6-([1,2,3]Triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl] pyrrolidine-2-carboxylic acid. **4c**

(2S)-3-(1H-Indol-3-yl)-2-{[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl]amino} propanoic acid. **4d**

(2S)-3-(4-Hydroxyphenyl)-2-{[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl]amino} propanoic acid **4e**

(2S)-3-Phenyl-2-{[6-([1,2,3]triazolo[1,5-a]pyridin-3-yl)pyridin-2-yl]amino}propanoic acid. **4f**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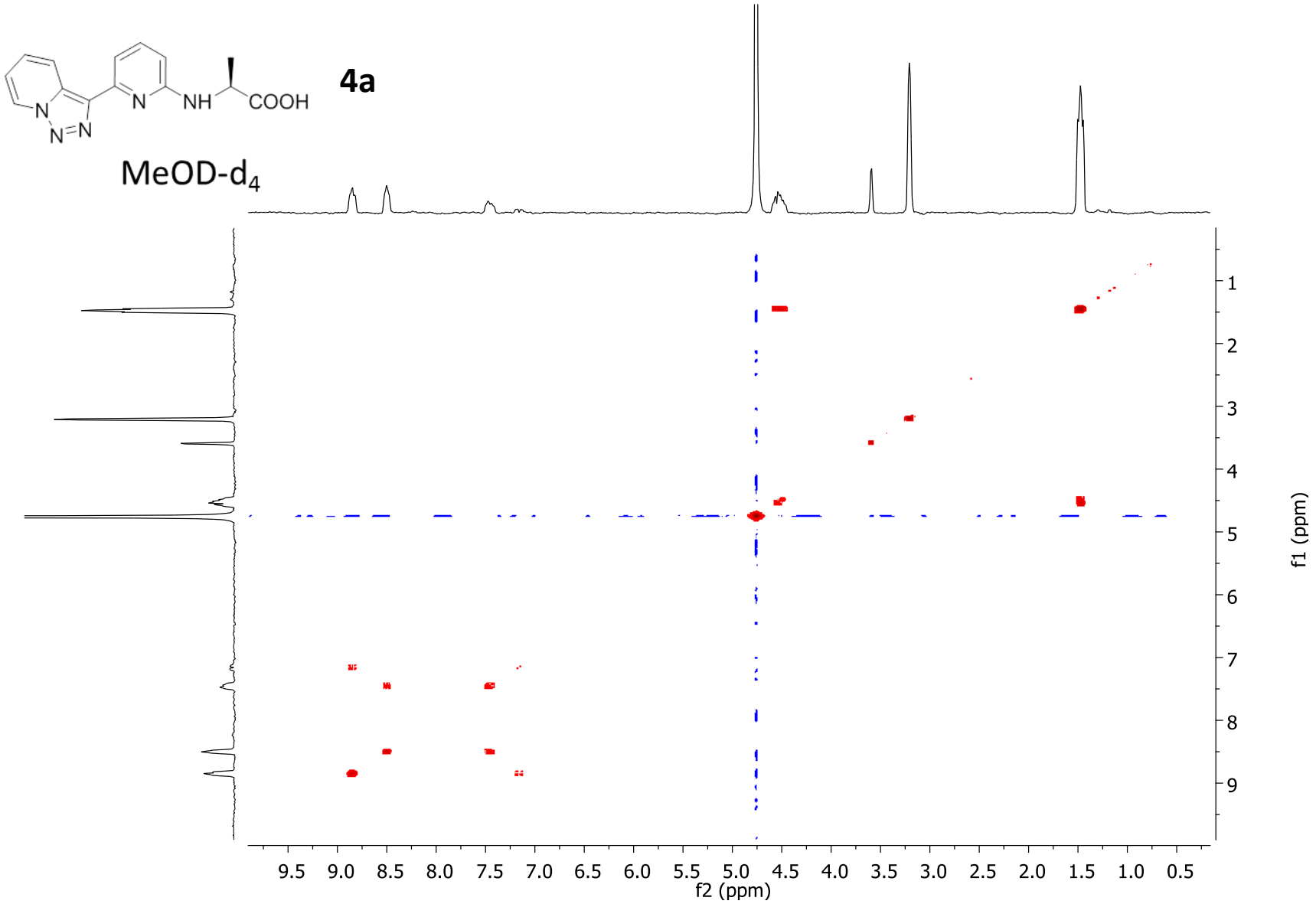
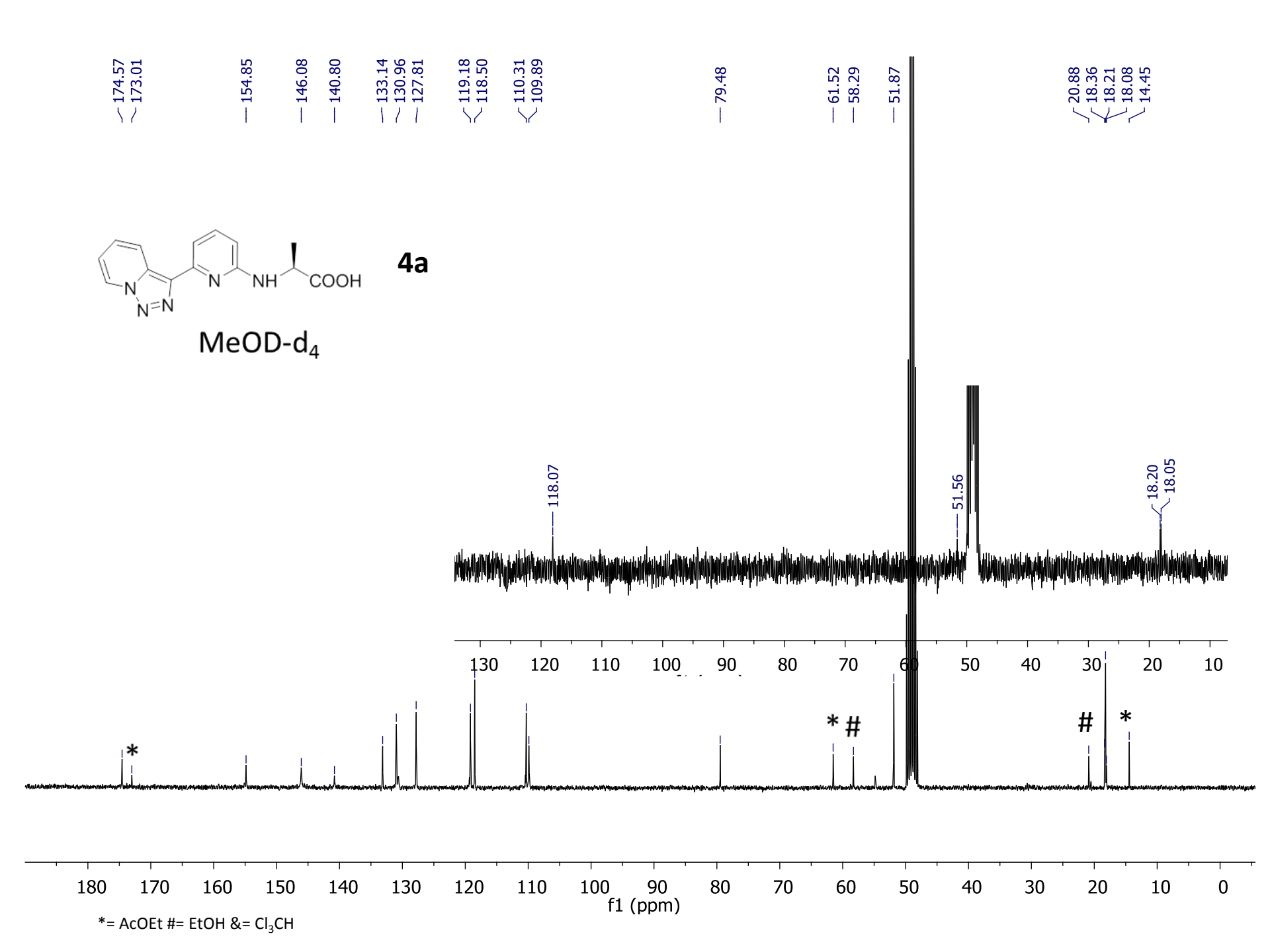
8.86
8.83
8.80
7.52
7.49
7.21
7.19
6.62
6.60
4.86
4.47
4.40
2.26
1.13
1.12
4a
N
N=N
N
NH
COOH
MeOD-d4
9.0
8.6
8.2
7.8
7.4
7.0
6.6
6.2
f1 (ppm)
2.17
3.33
1.30
1.00
0.91
1.18
6.08
f1 (ppm)


4a
MeOD-d4
N
NH
COOH
N
N=N
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f2 (ppm)
1 2 3 4 5 6 7 8 9
f1 (ppm)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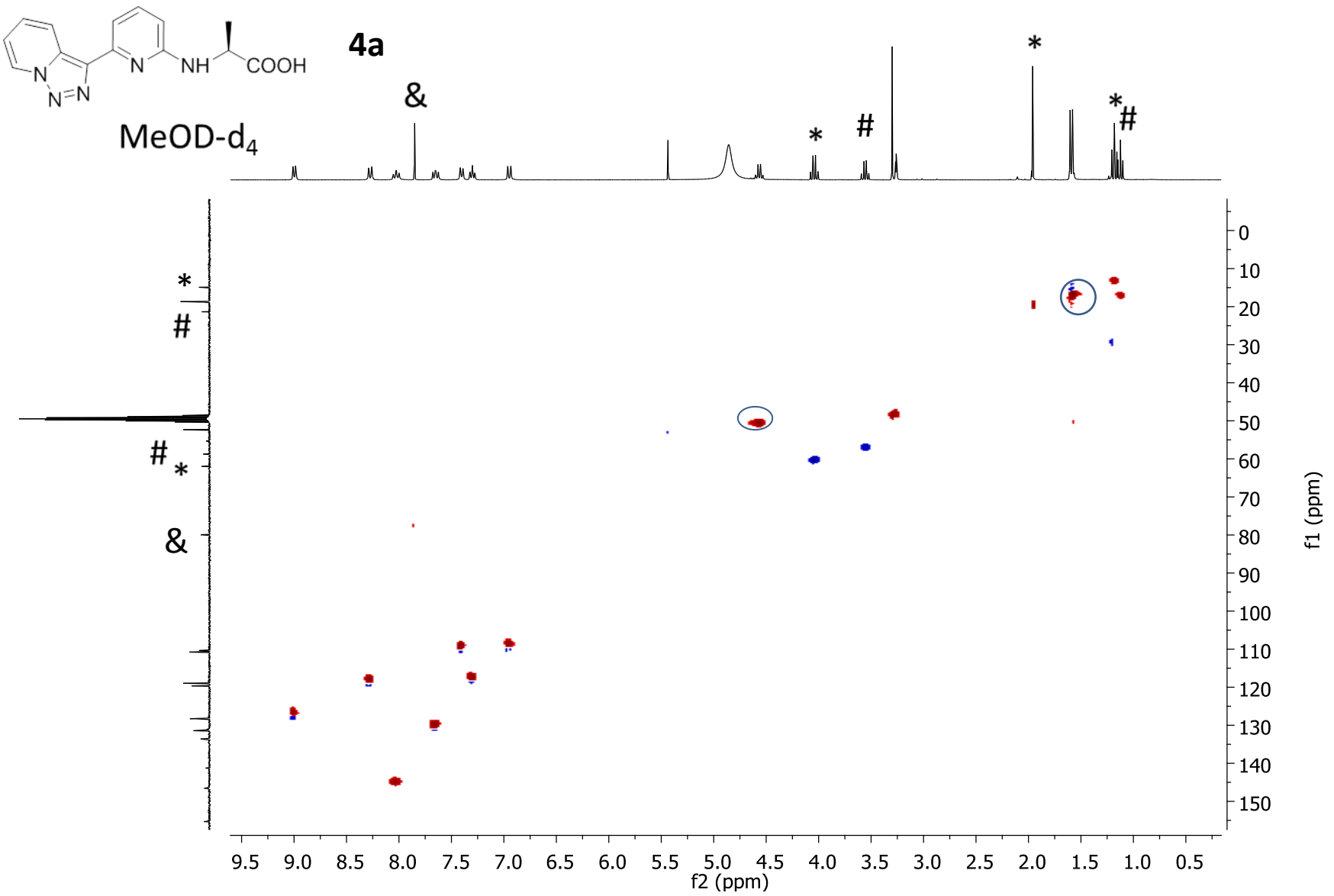
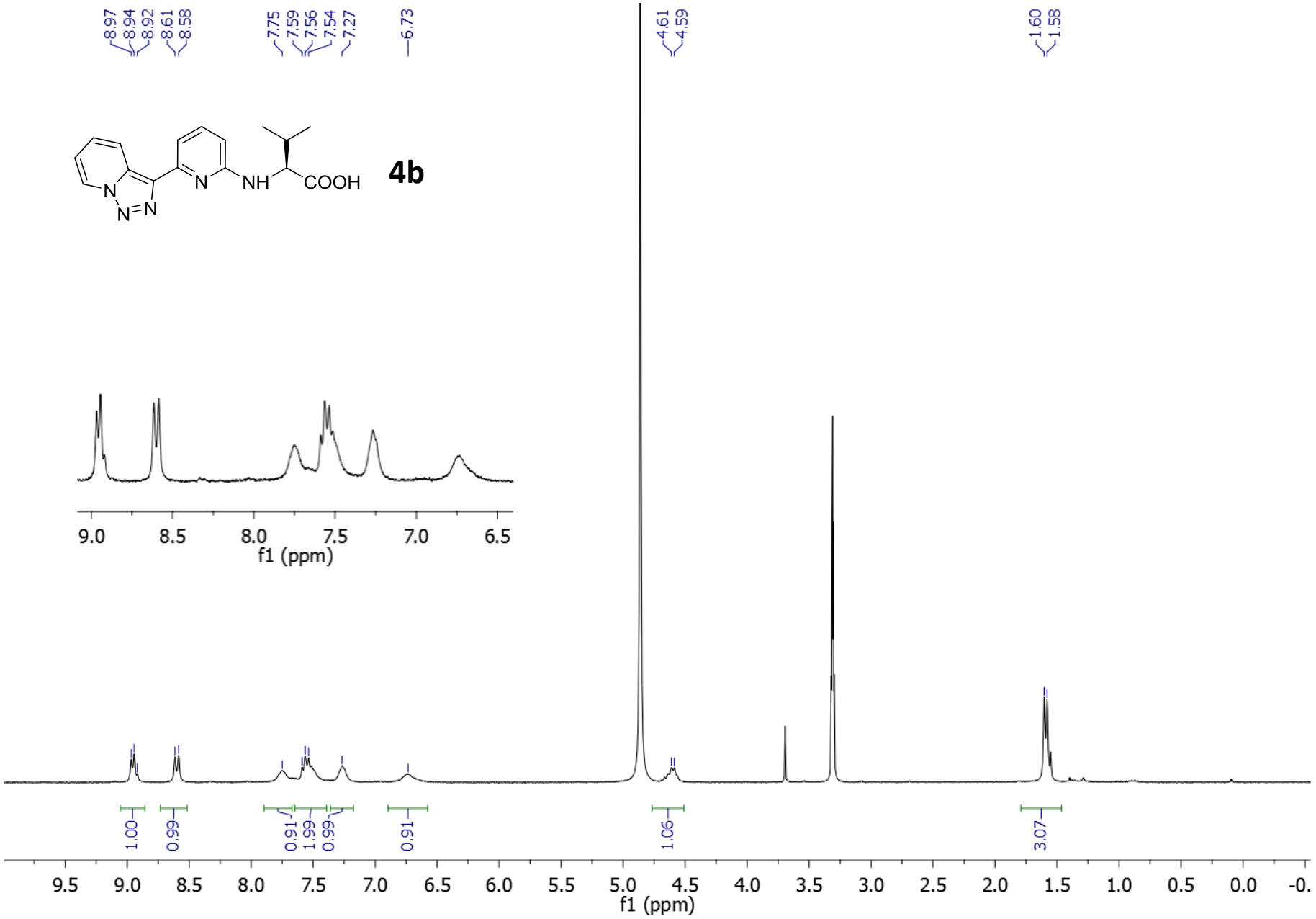
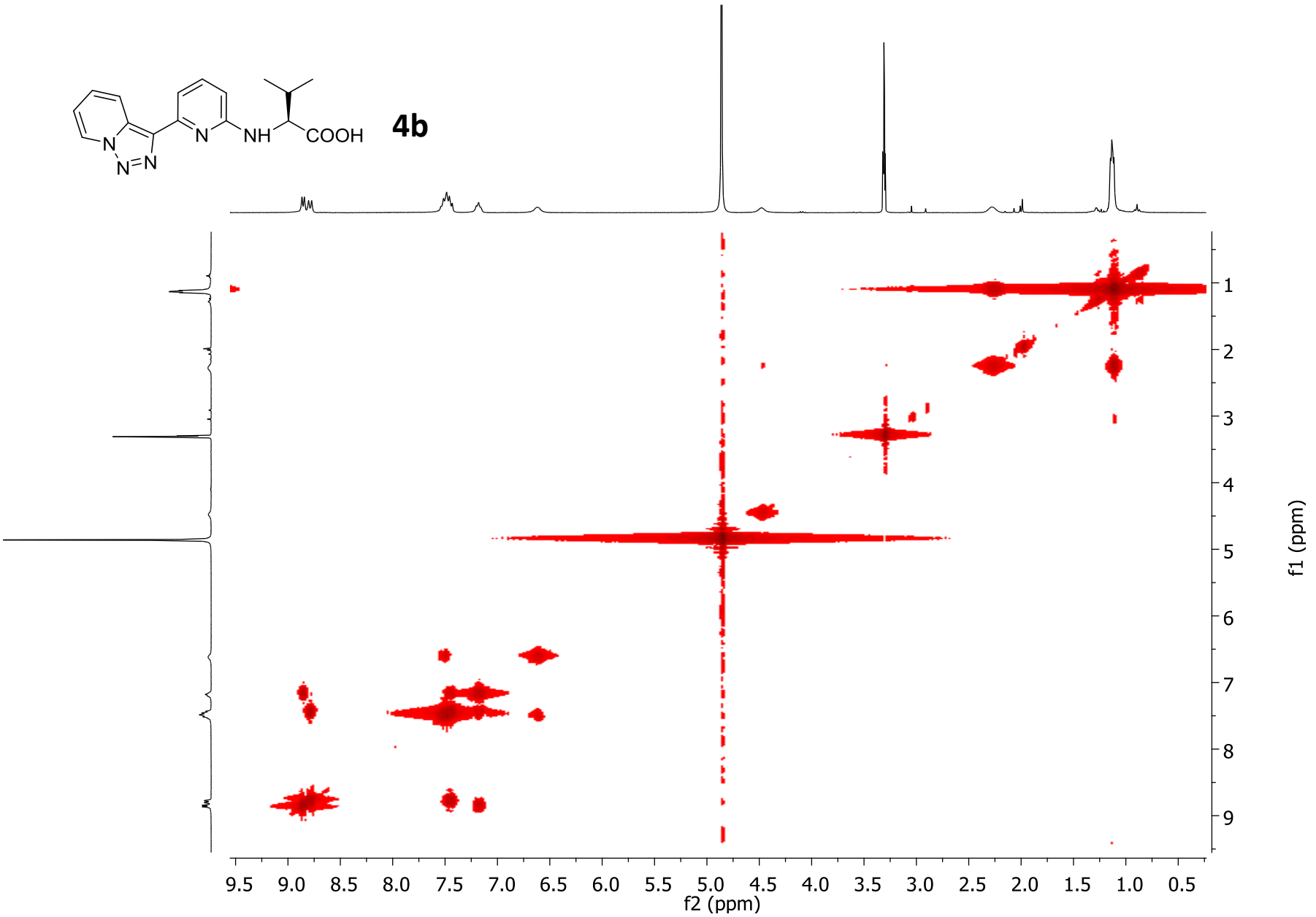
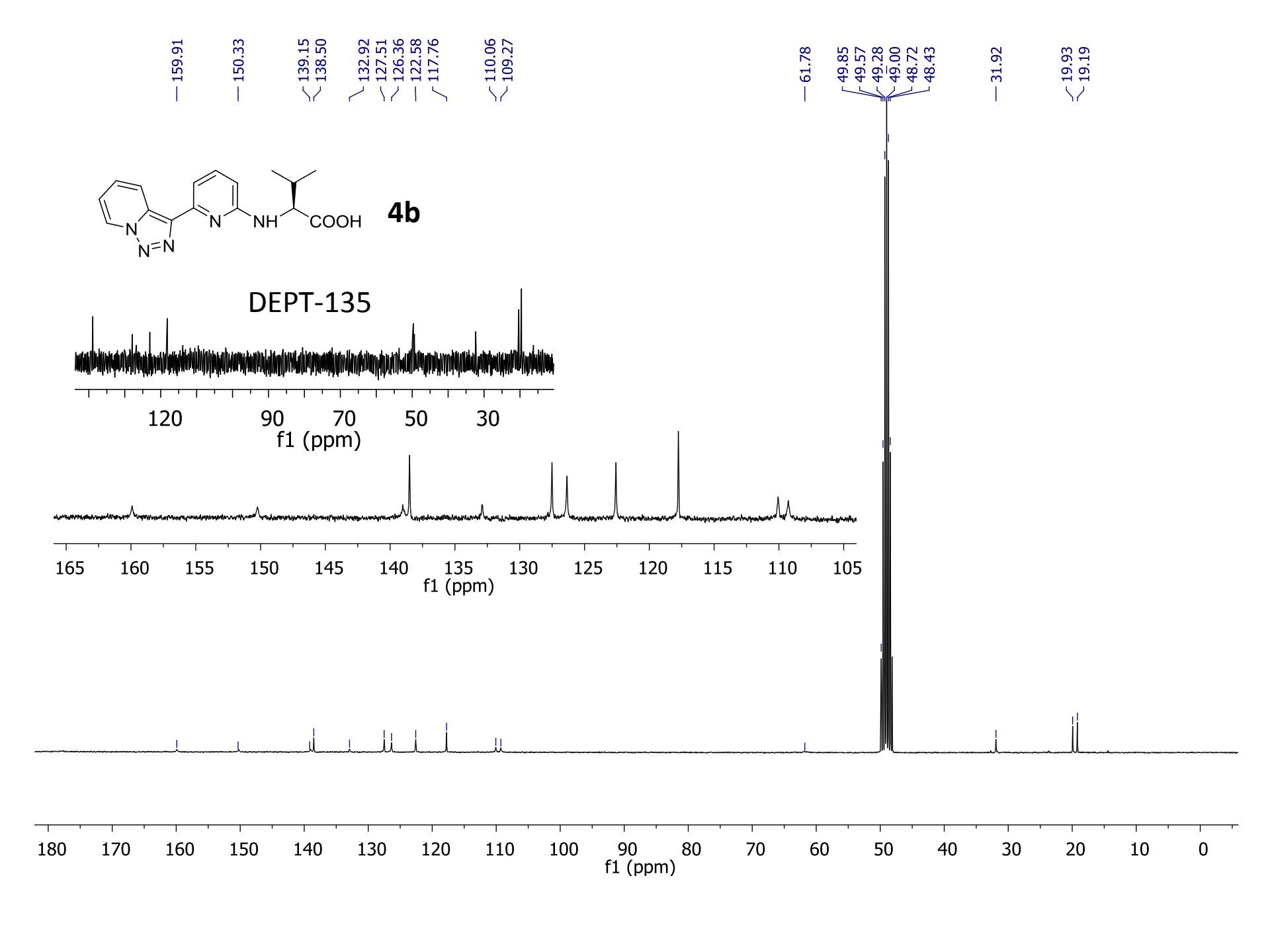
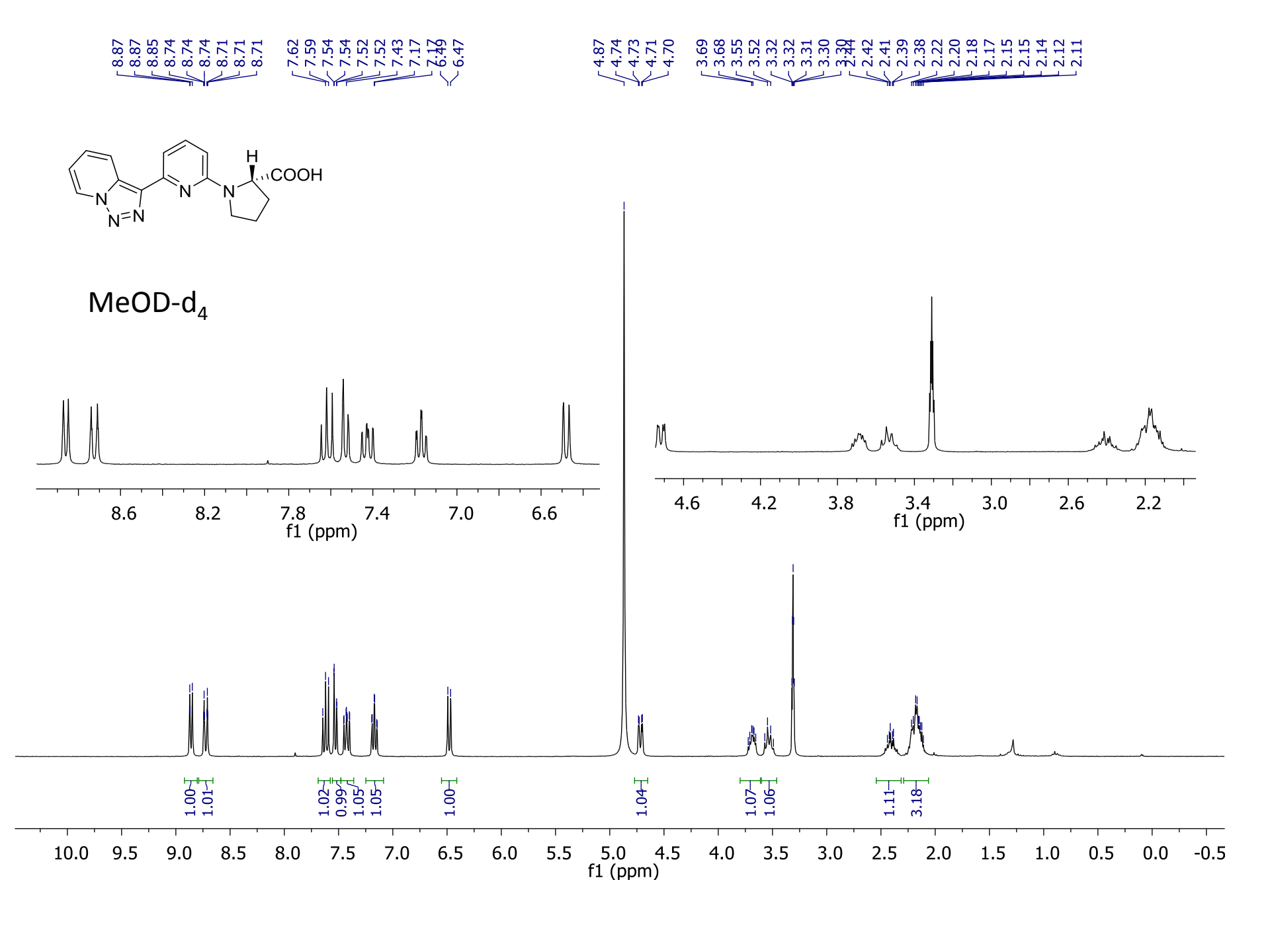
173.01
154.85
146.08
140.80
133.14
130.96
127.81
119.18
118.50
110.31
109.89
79.48
61.52
58.29
51.87
20.88
18.36
18.21
18.08
14.45
118.07
51.56
18.20
18.05
4a
MeOD-d4
NH
COOH
*
*
#
#
*
130
120
110
100
90
80
70
60
50
40
30
20
10
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
*= AcOEt #= EtOH &= Cl3CH

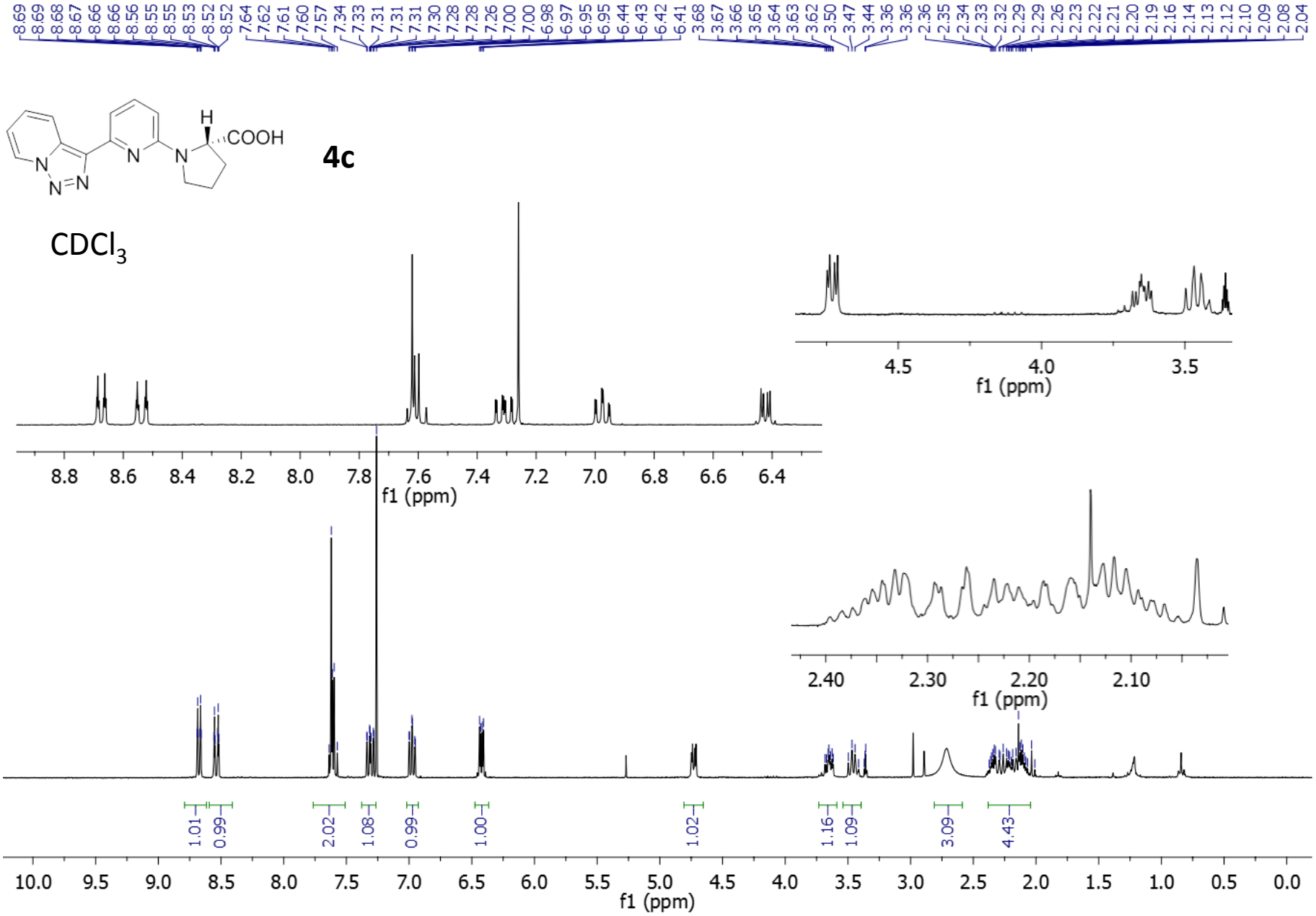

4a
MeOD-d4
NH
COOH
N
N=N
&
*
#
f2 (ppm)
f1 (ppm)
*= AcOEt #= EtOH &= Cl3CH


8.97
8.94
8.92
8.61
8.58
7.75
7.59
7.56
7.54
7.27
6.73
4.61
4.59
1.60
1.58
N
N=N
NH
COOH
4b
9.0
8.5
8.0
7.5
7.0
6.5
f1 (ppm)
1.00
0.99
0.91
1.99
0.99
0.91
1.06
3.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


4b
N
N=N
N
NH
COOH
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f2 (ppm)
1 2 3 4 5 6 7 8 9
f1 (ppm)


159.91
150.33
139.15
138.50
132.92
127.51
126.36
122.58
117.76
110.06
109.27
61.78
49.85
49.57
49.28
49.00
48.72
48.43
31.92
19.93
19.19
4b
N
N=N
NH
COOH
DEPT-135
120
90
70
50
30
f1 (ppm)
165
160
155
150
145
140
135
130
125
120
115
110
105
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.87
8.87
8.85
8.74
8.74
8.74
8.71
8.71
8.71
7.62
7.59
7.54
7.54
7.52
7.52
7.43
7.17
6.49
6.47
4.87
4.74
4.73
4.71
4.70
3.69
3.68
3.55
3.52
3.32
3.32
3.31
3.30
3.30
2.44
2.42
2.41
2.39
2.38
2.22
2.20
2.18
2.17
2.15
2.15
2.14
2.12
2.11
H
COOH
N
N
N
N=N
MeOD-d4
8.6
8.2
7.8
7.4
7.0
6.6
f1 (ppm)
4.6
4.2
3.8
3.4
3.0
2.6
2.2
f1 (ppm)
1.00
1.01
1.02
0.99
1.05
1.05
1.00
1.04
1.07
1.06
1.11
3.18
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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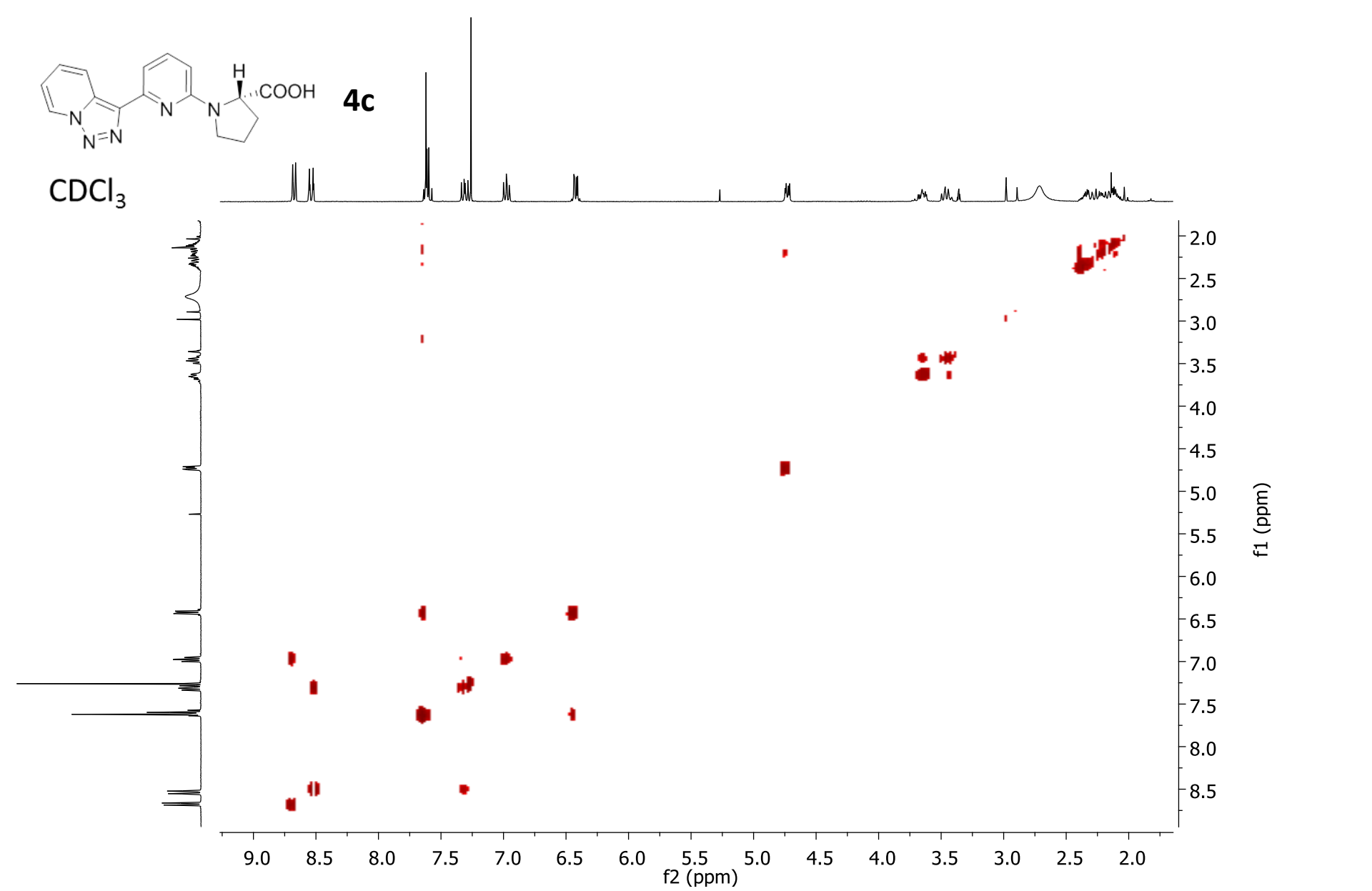
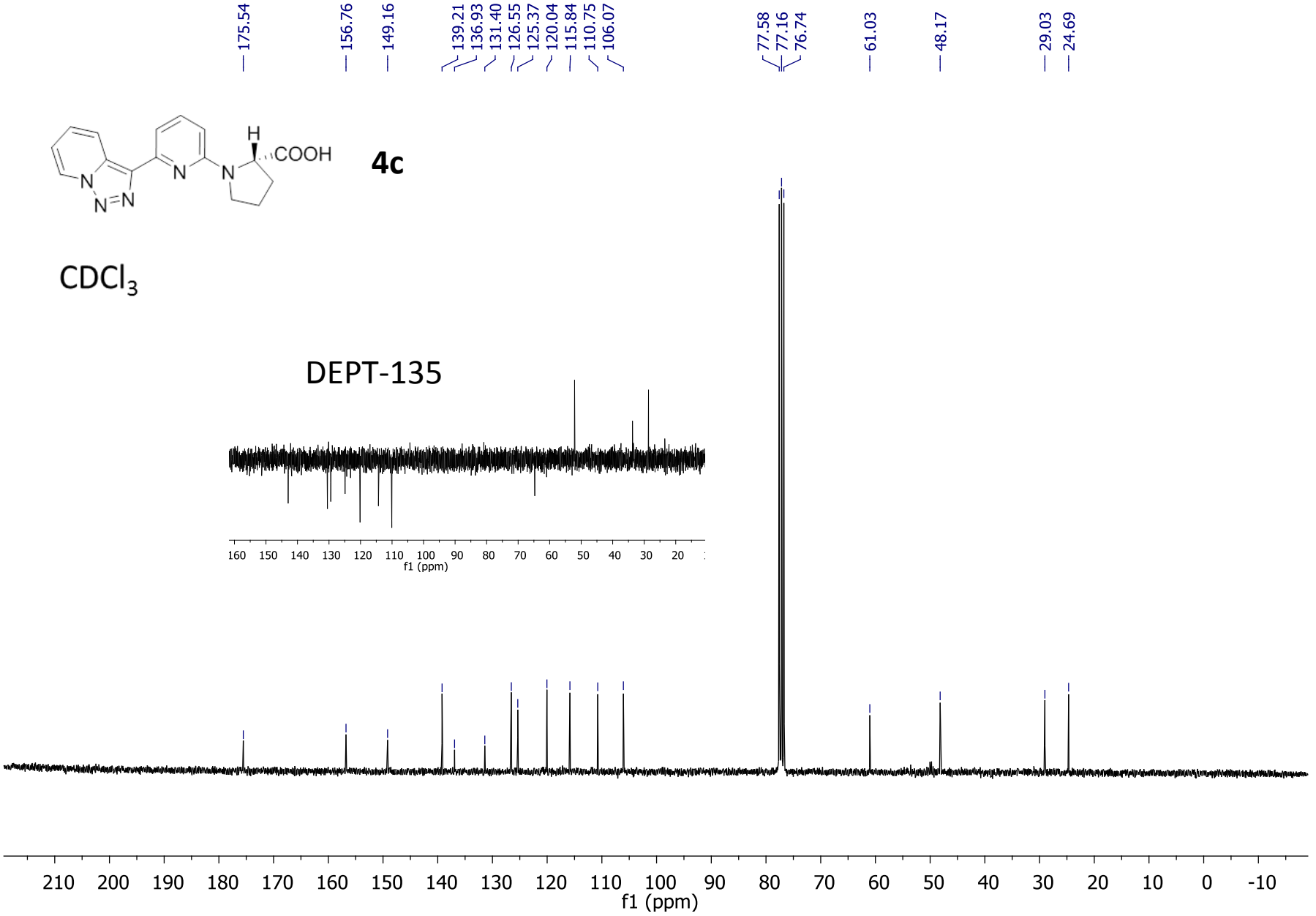
7.64 7.62 7.61 7.60 7.57 7.34 7.33 7.31 7.31 7.31 7.30 7.28 7.28 7.26 7.00 7.00 6.98 6.97 6.95 6.95 6.44 6.43 6.42 6.41
3.68 3.67 3.66 3.65 3.64 3.63 3.62 3.50 3.47 3.44 3.36 3.36
2.36 2.35 2.34 2.33 2.32 2.29 2.29 2.26 2.23 2.22 2.21 2.20 2.19 2.16 2.14 2.13 2.12 2.10 2.09 2.08 2.04
H
COOH
N
N
N
N
4c
CDCl3
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4
f1 (ppm)
4.5 4.0 3.5
f1 (ppm)
2.40 2.30 2.20 2.10
f1 (ppm)
1.01 0.99 2.02 1.08 0.99 1.00 1.02 1.16 1.09 3.09 4.43
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


4c
CDCl3
COOH
H
N
N
N
N
f2 (ppm)
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0


175.54
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149.16
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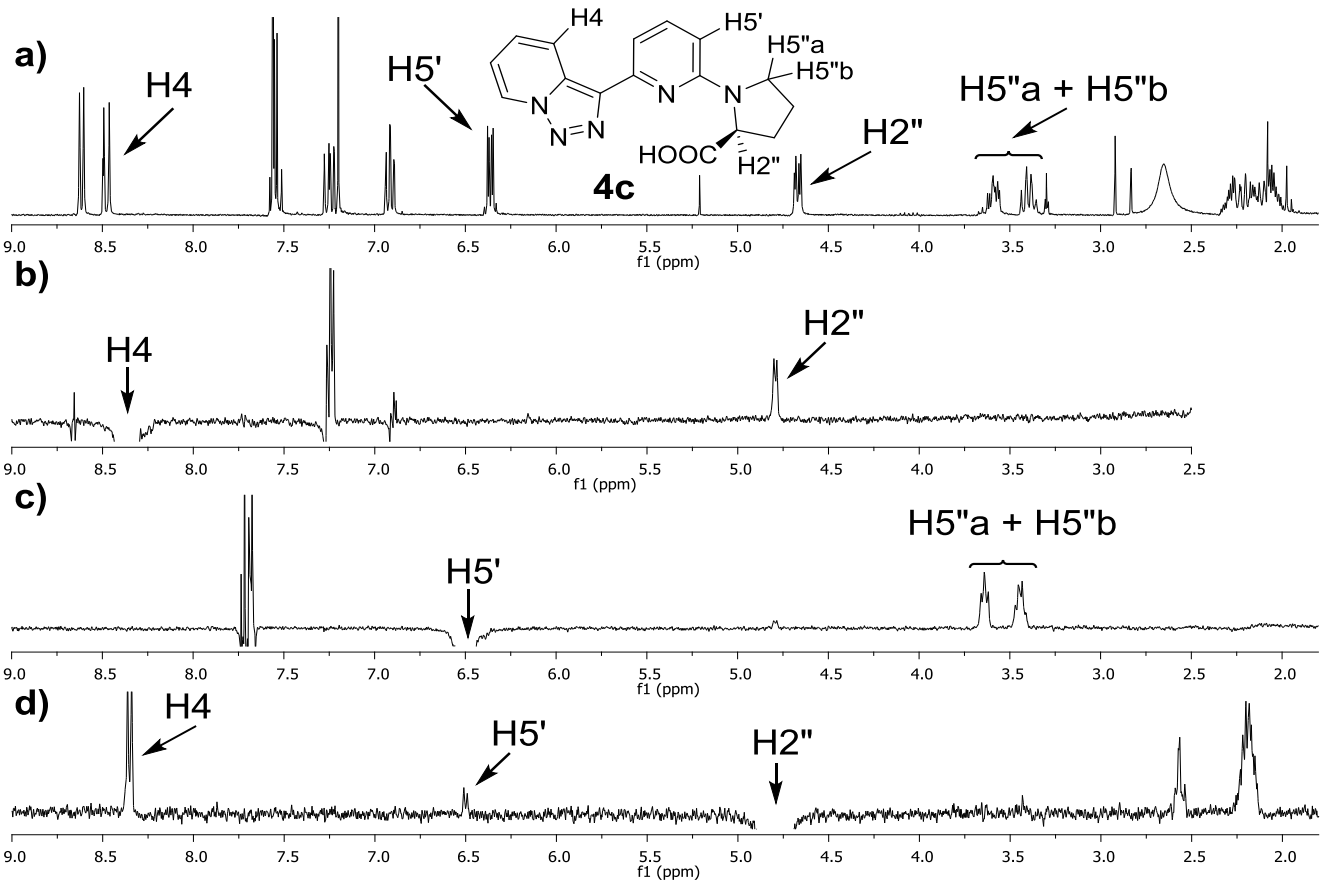
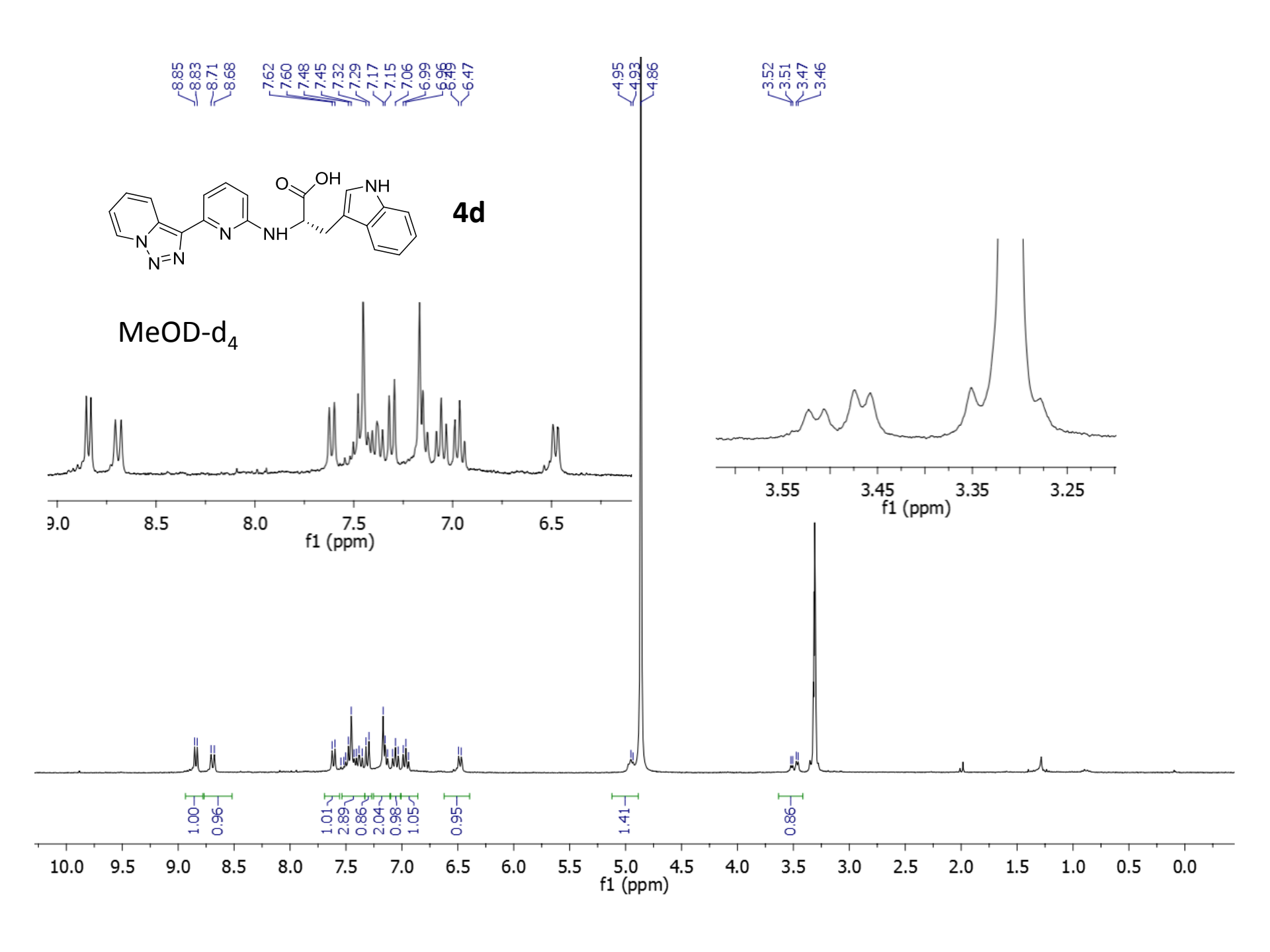
136.93
131.40
126.55
125.37
120.04
115.84
110.75
106.07
77.58
77.16
76.74
61.03
48.17
29.03
24.69
4c
CDCl3
DEPT-135
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



1D-NOE experiences with compound 4c


8.85
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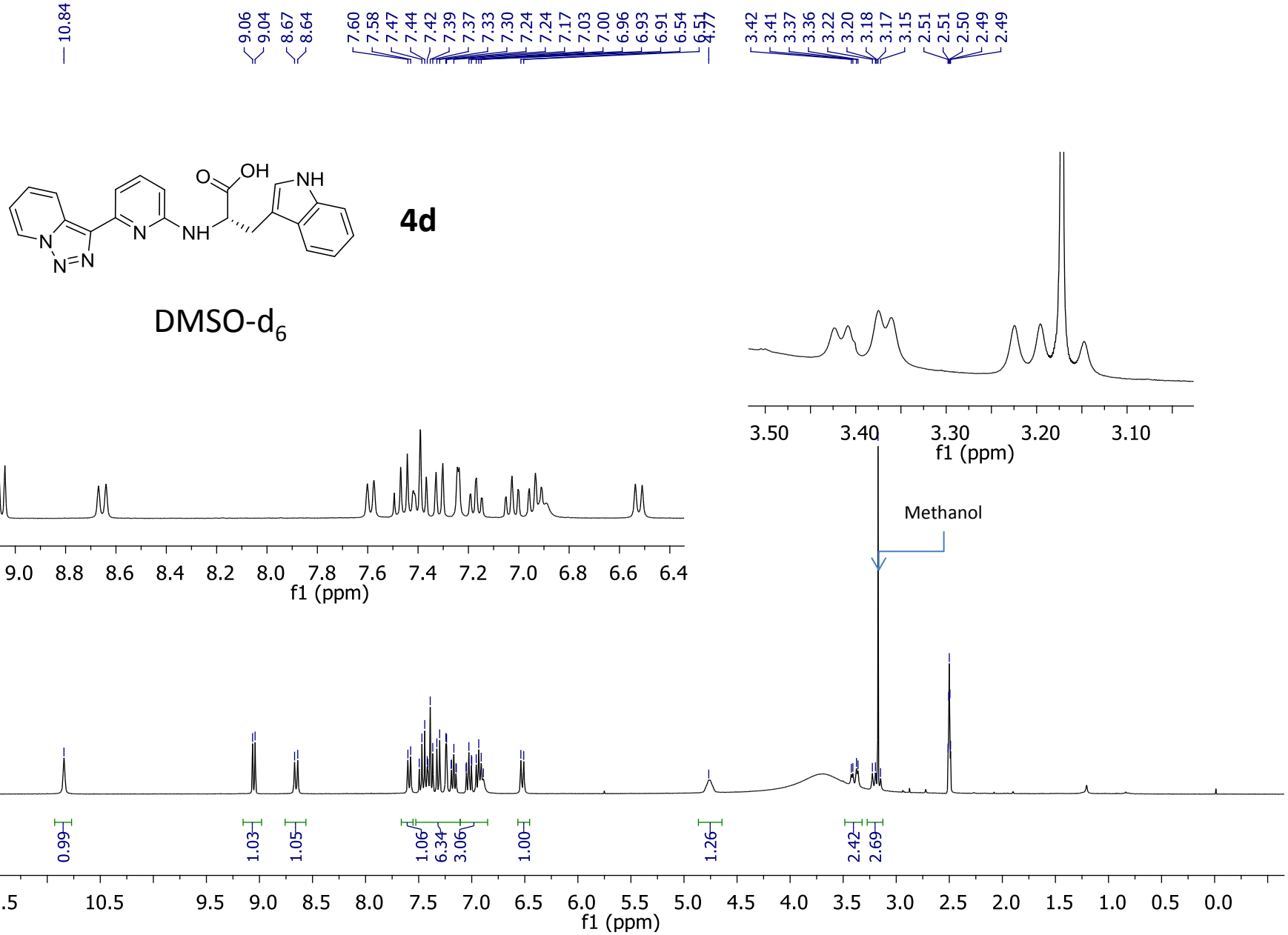
8.71
8.68
7.62
7.60
7.48
7.45
7.32
7.29
7.17
7.15
7.06
6.99
6.96
6.49
6.47
4.95
4.93
4.86
3.52
3.51
3.47
3.46
O
OH
NH
N
N
NH
N=N
4d
MeOD-d4
9.0
8.5
8.0
7.5
7.0
6.5
f1 (ppm)
3.55
3.45
3.35
3.25
f1 (ppm)
1.00
0.96
1.01
2.89
0.86
2.04
0.98
1.05
0.95
1.41
0.86
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


10.84
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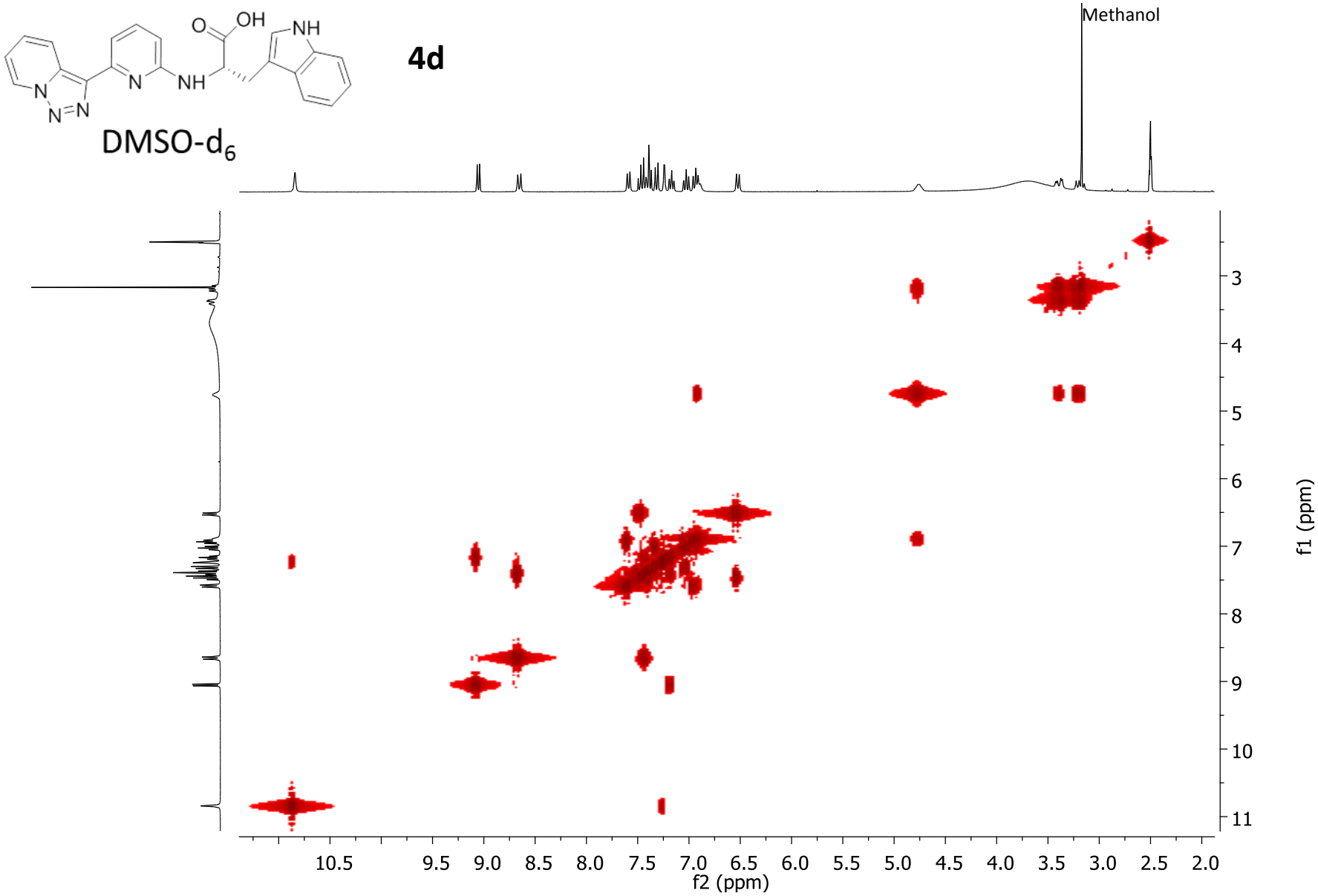
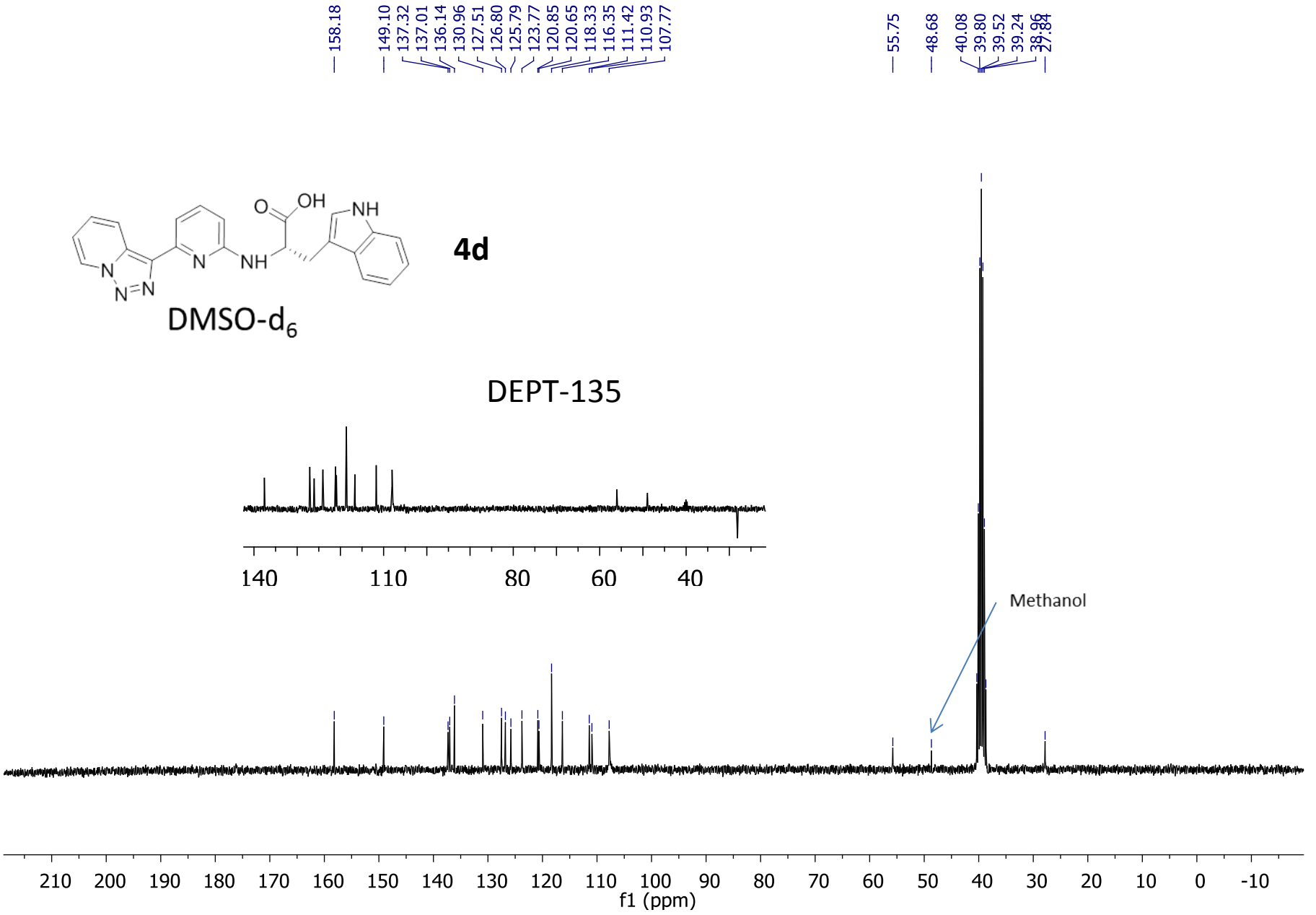
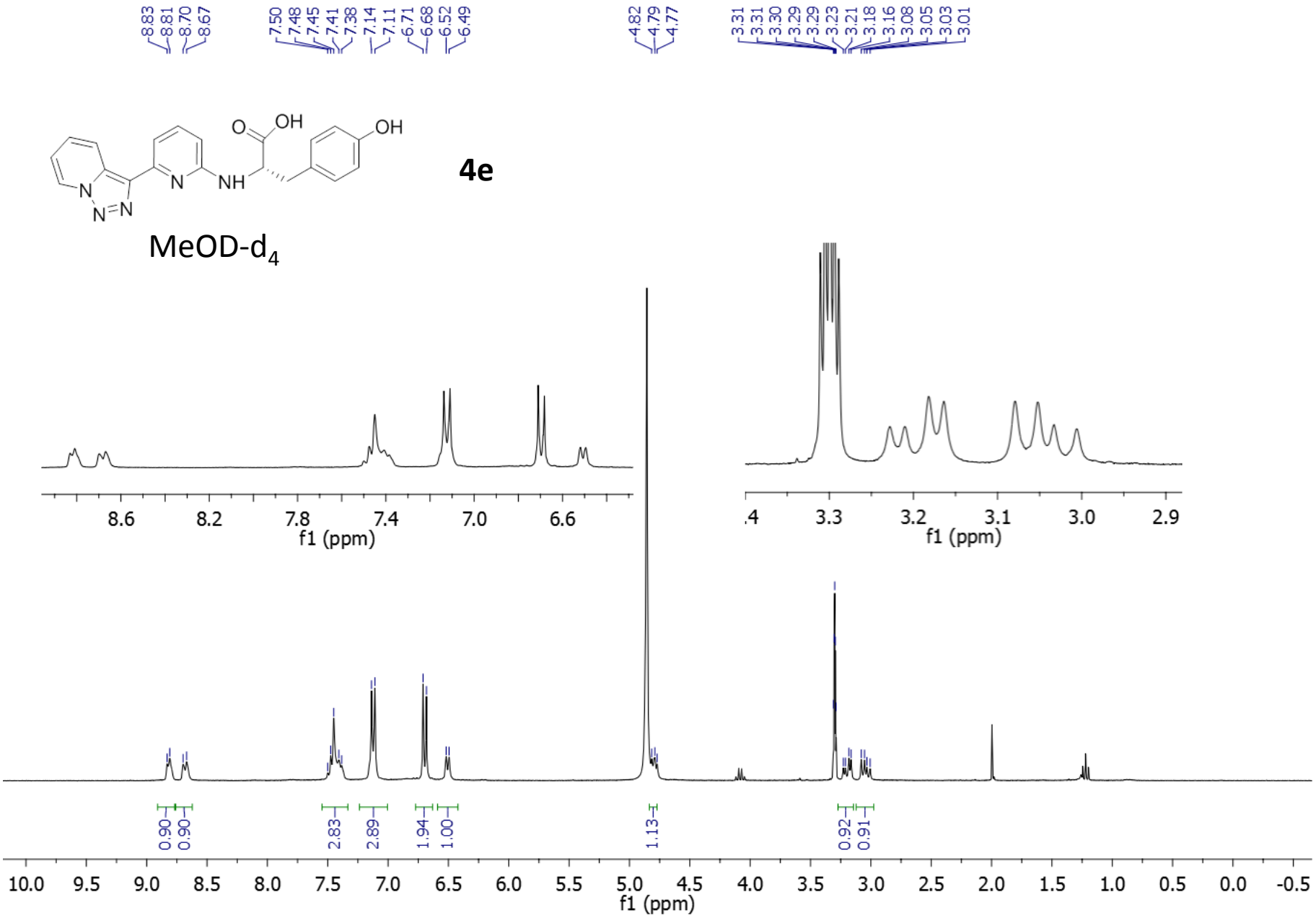
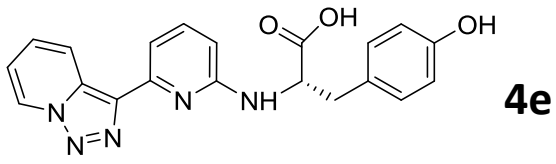
9.04
8.67
8.64
7.60
7.58
7.47
7.44
7.42
7.39
7.37
7.33
7.30
7.24
7.24
7.17
7.03
7.00
6.96
6.93
6.91
6.54
6.51
4.77
3.42
3.41
3.37
3.36
3.22
3.20
3.18
3.17
3.15
2.51
2.51
2.50
2.49
2.49
O
OH
NH
N
N
NH
N=N
4d
DMSO-d6
3.50
3.40
3.30
3.20
3.10
f1 (ppm)
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
f1 (ppm)
Methanol
0.99
1.03
1.05
1.06
6.34
3.06
1.00
1.26
2.42
2.69
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


4d
DMSO-d6
Methanol
f2 (ppm)
f1 (ppm)


158.18
149.10
137.32
137.01
136.14
130.96
127.51
126.80
125.79
123.77
120.85
120.65
118.33
116.35
111.42
110.93
107.77
55.75
48.68
40.08
39.80
39.52
39.24
38.96
27.84
O
OH
NH
N
NH
N
N=N
4d
DMSO-d6
DEPT-135
140
110
80
60
40
Methanol
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

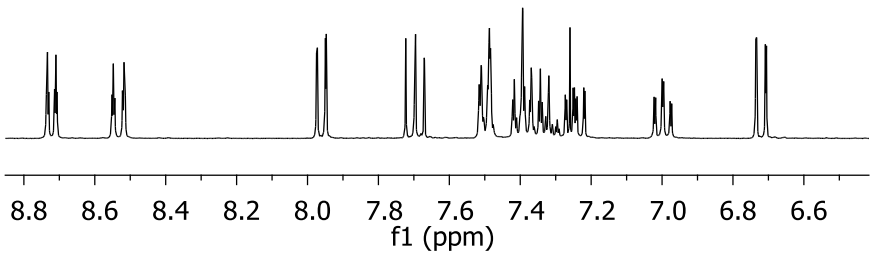

8.83
8.81
8.70
8.67
7.50
7.48
7.45
7.41
7.38
7.14
7.11
6.71
6.68
6.52
6.49
4.82
4.79
4.77
3.31
3.31
3.30
3.29
3.29
3.23
3.21
3.18
3.16
3.08
3.05
3.03
3.01
O
OH
OH
N
NH
N
N=N
4e
MeOD-d4
8.6
8.2
7.8
7.4
7.0
6.6
f1 (ppm)
3.4
3.3
3.2
3.1
3.0
2.9
f1 (ppm)
0.90
0.90
2.83
2.89
1.94
1.00
1.13
0.92
0.91
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

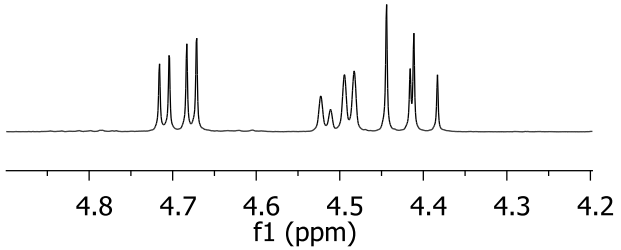

8.74 8.73 8.73 8.71 8.71 8.71 8.55 8.55 8.54 8.52 8.52 8.51 7.97 7.97 7.95 7.95 7.72 7.70 7.70 7.67 7.52 7.51 7.50 7.49 7.49 7.49 7.48 7.42 7.42 7.41 7.39 7.39 7.37 7.37 7.35 7.34 7.34 7.33 7.32 7.27 7.27 7.26 7.25 7.25 7.24 7.24 7.22 7.02 7.02 7.00 7.00 6.98 6.97 6.74 6.73 6.71 6.71 4.72 4.70 4.68 4.67 4.52 4.49 4.48 4.44 4.42 4.41 4.38

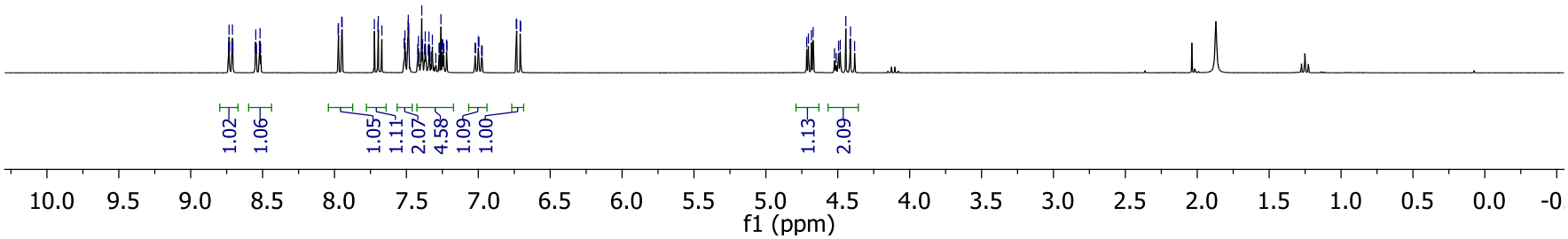

O
OH
OH
N
NH
N
N=N

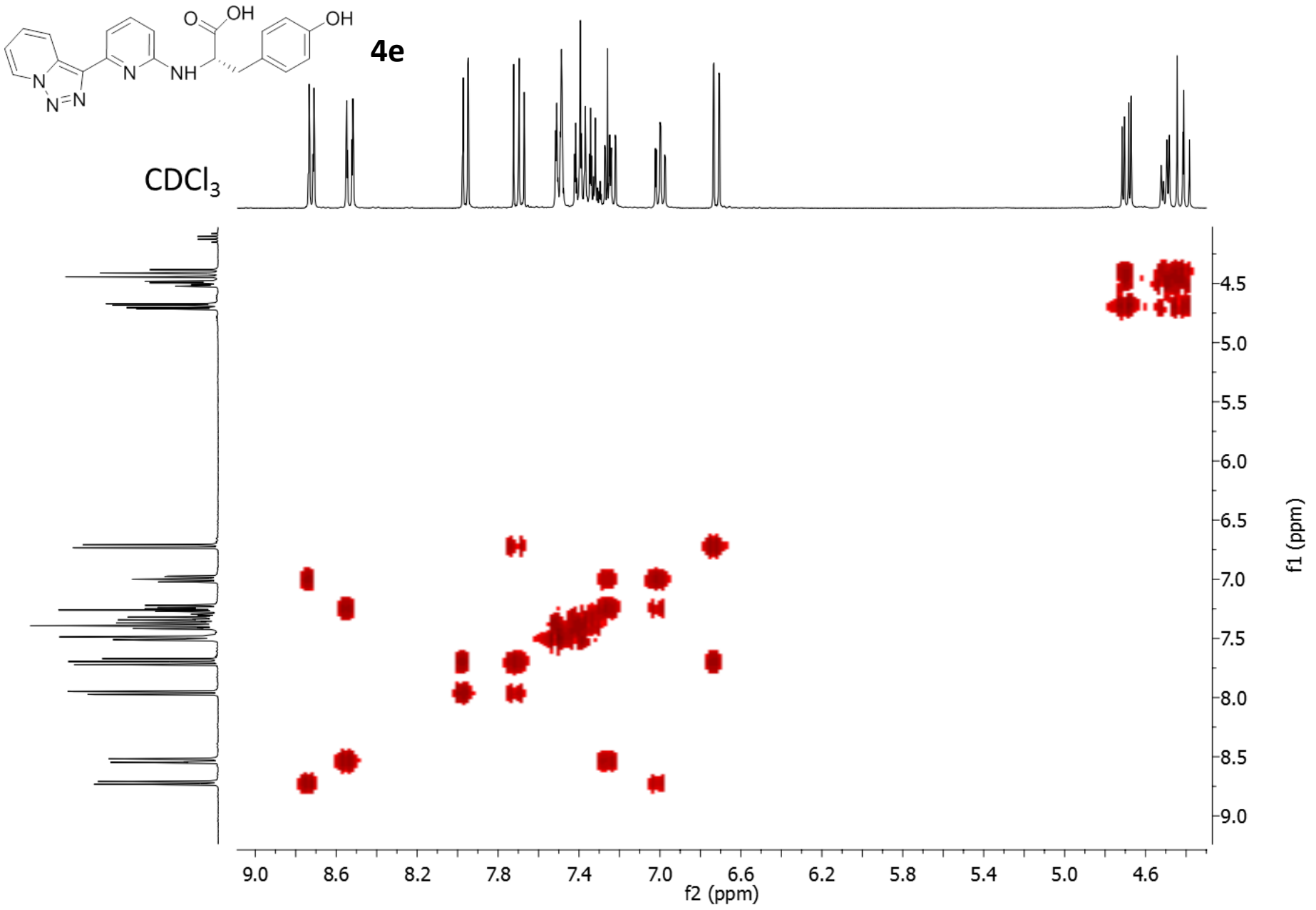
4e

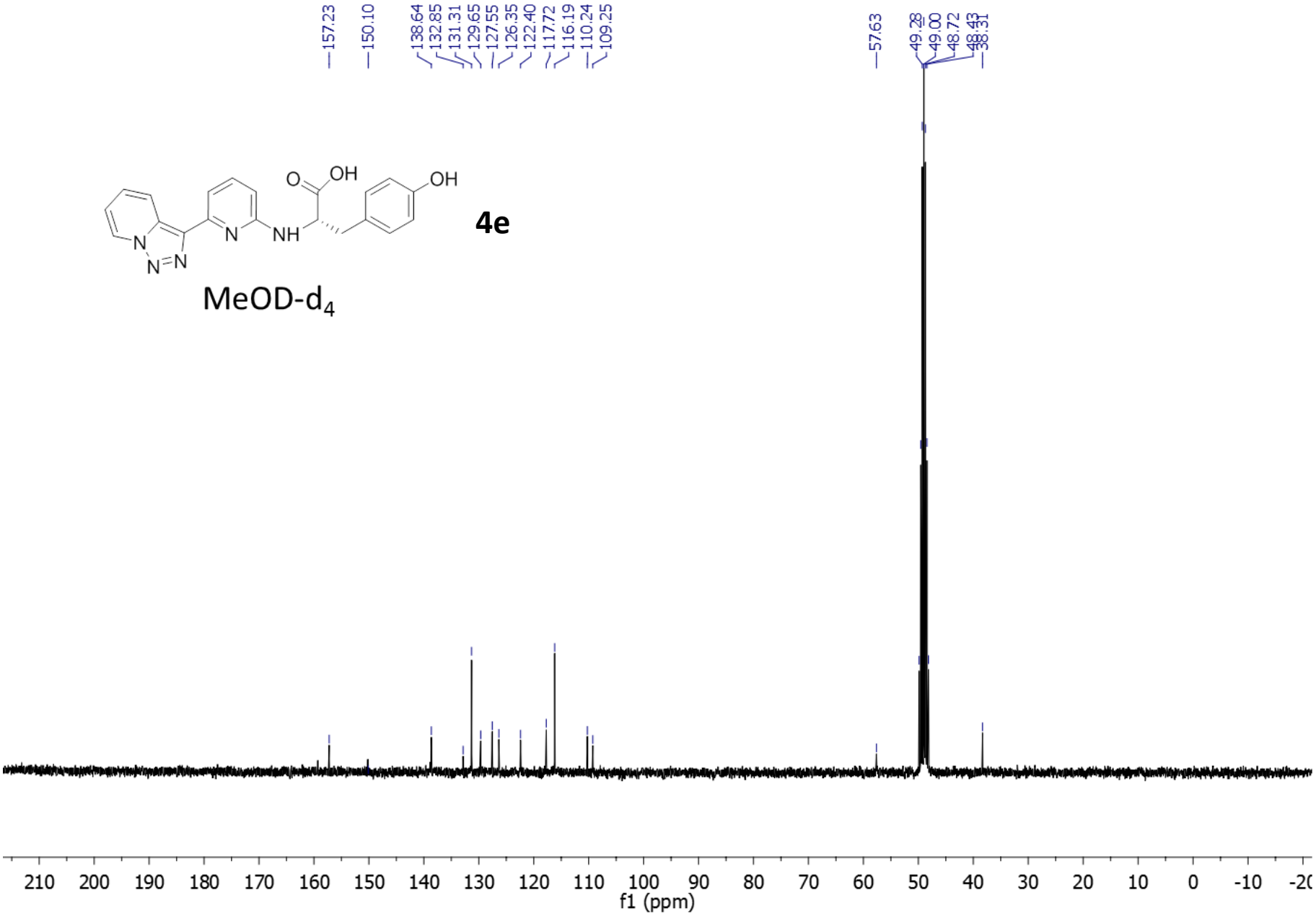
$CDCl_3$

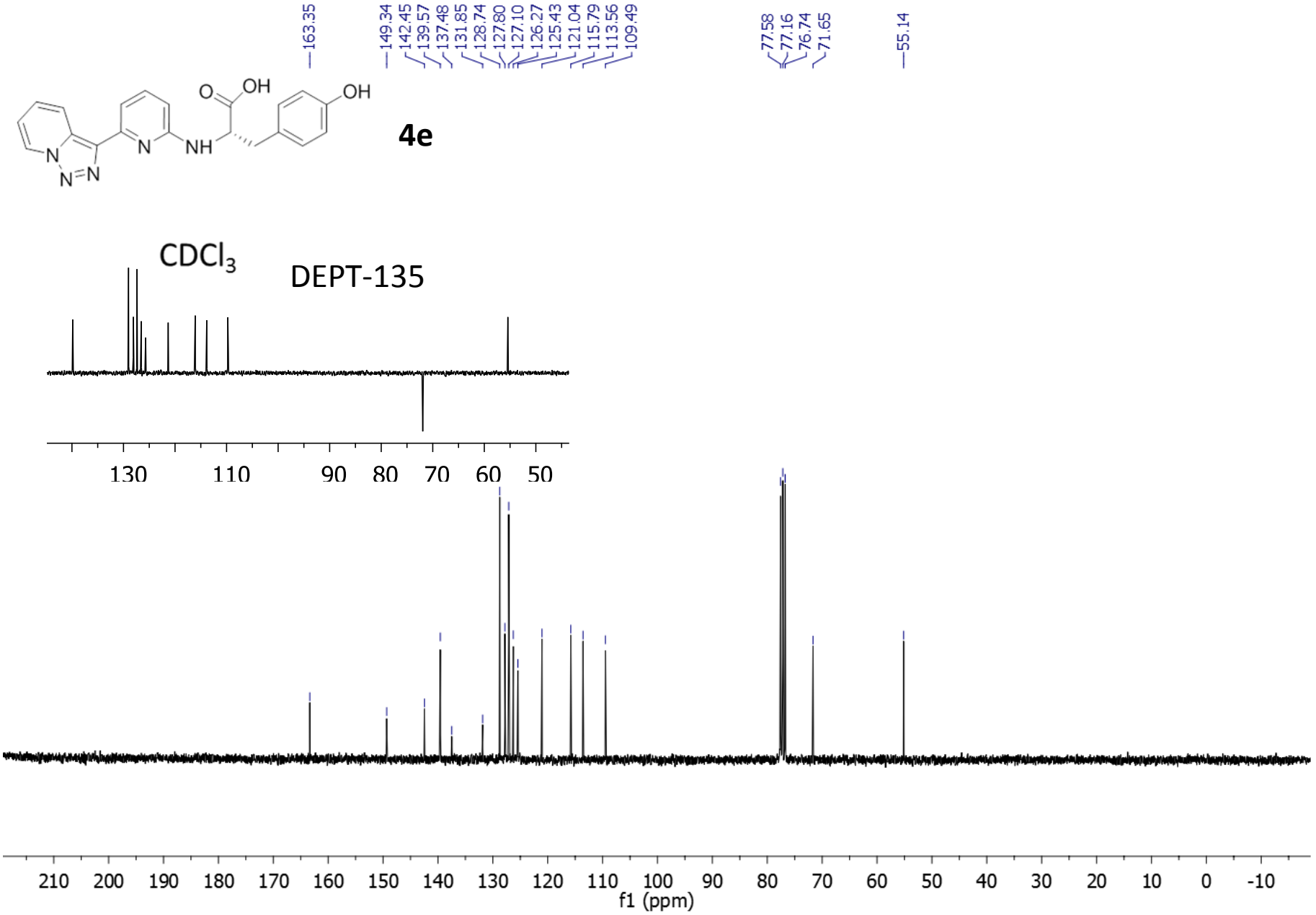

8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6
f1 (ppm)

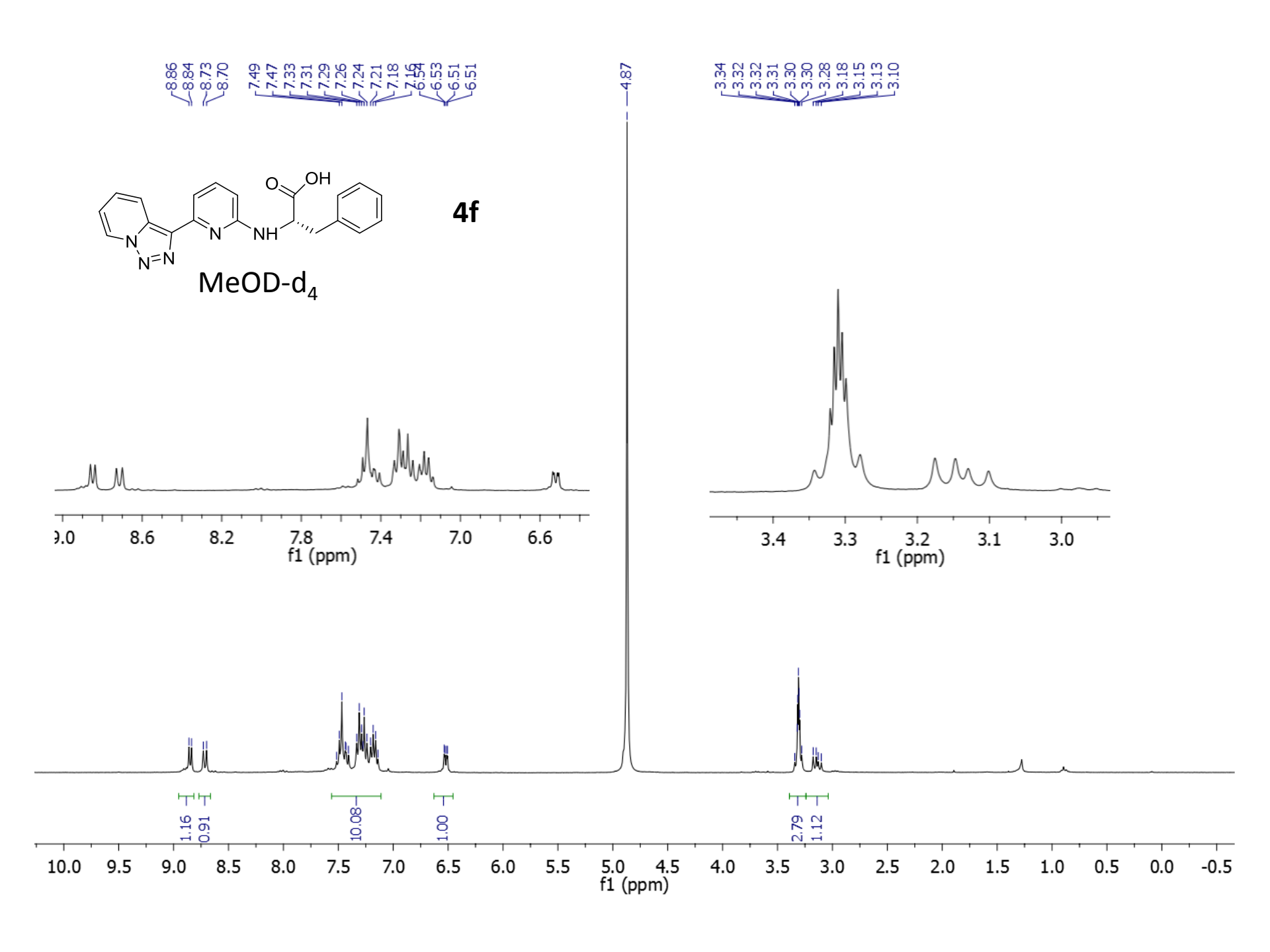

4.8 4.7 4.6 4.5 4.4 4.3 4.2
f1 (ppm)

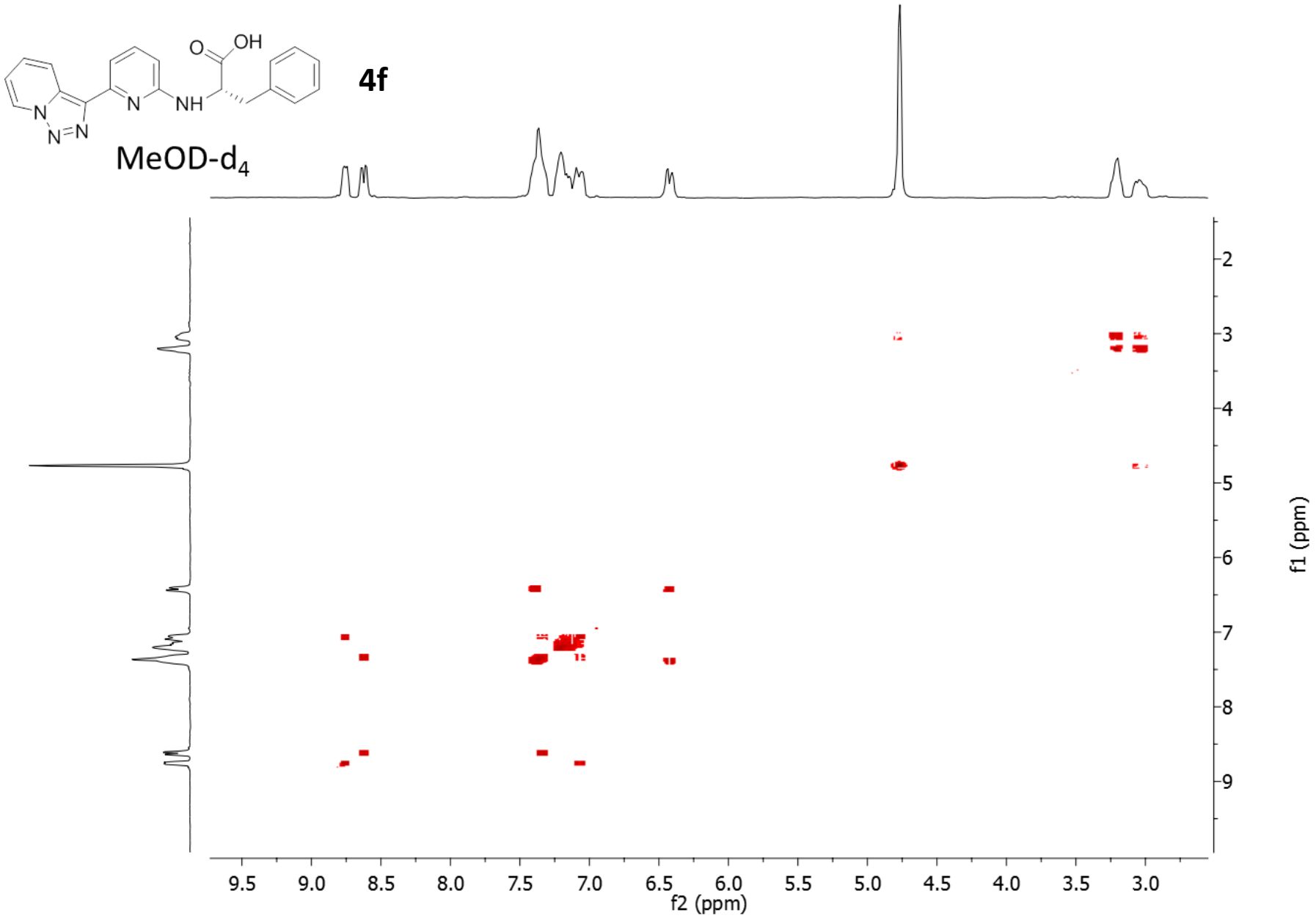

1.02 1.06 1.05 1.11 2.07 4.58 1.09 1.00 1.13 2.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

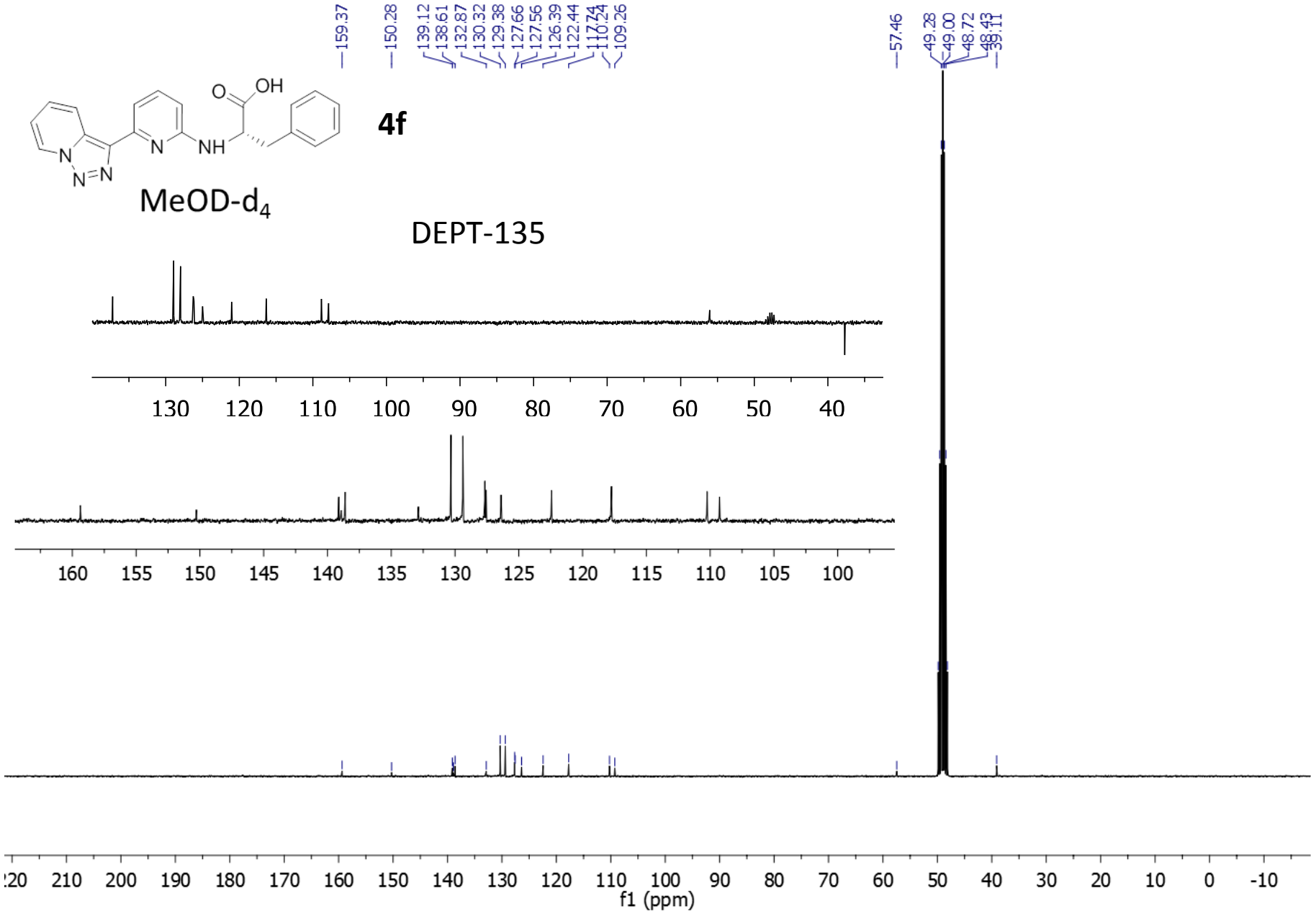

4e
CDCl3
f2 (ppm)
f1 (ppm)


157.23
150.10
138.64
132.85
131.31
129.65
127.55
126.35
122.40
117.72
116.19
110.24
109.25
57.63
49.28
49.00
48.72
48.43
38.31
OH
O
OH
N
NH
N
N=N
4e
MeOD-d4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


163.35
149.34
142.45
139.57
137.48
131.85
128.74
127.80
127.10
126.27
125.43
121.04
115.79
113.56
109.49
77.58
77.16
76.74
71.65
55.14
OH
O
OH
N
NH
N
N=N
4e
CDCl3
DEPT-135
130
110
90
80
70
60
50
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.86
8.84
8.73
8.70
7.49
7.47
7.33
7.31
7.29
7.26
7.24
7.21
7.18
6.53
6.51
6.51
4.87
3.34
3.32
3.32
3.31
3.30
3.30
3.28
3.18
3.15
3.13
3.10
O
OH
N
NH
N
N=N
4f
MeOD-d4
f1 (ppm)
f1 (ppm)
1.16
0.91
10.08
1.00
2.79
1.12
f1 (ppm)


4f
MeOD-d4
O
OH
N
NH
N
N=N
f2 (ppm)
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2
3
4
5
6
7
8
9


159.37
150.28
139.12
138.61
132.87
130.32
129.38
127.66
127.56
126.39
122.44
117.74
110.24
109.26
57.46
49.28
49.00
48.72
48.43
39.11
O
OH
N
NH
N
N=N
4f
MeOD-d4
DEPT-135
130 120 110 100 90 80 70 60 50 40
160 155 150 145 140 135 130 125 120 115 110 105 100
f1 (ppm)