

Ferrocene- and ruthenium arene-containing glycomimetics as selective inhibitors of human galectin-1 and -3

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*E-mail: hrstka@mou.cz, karban@icpf.cas.cz

SUPPORTING INFORMATION II

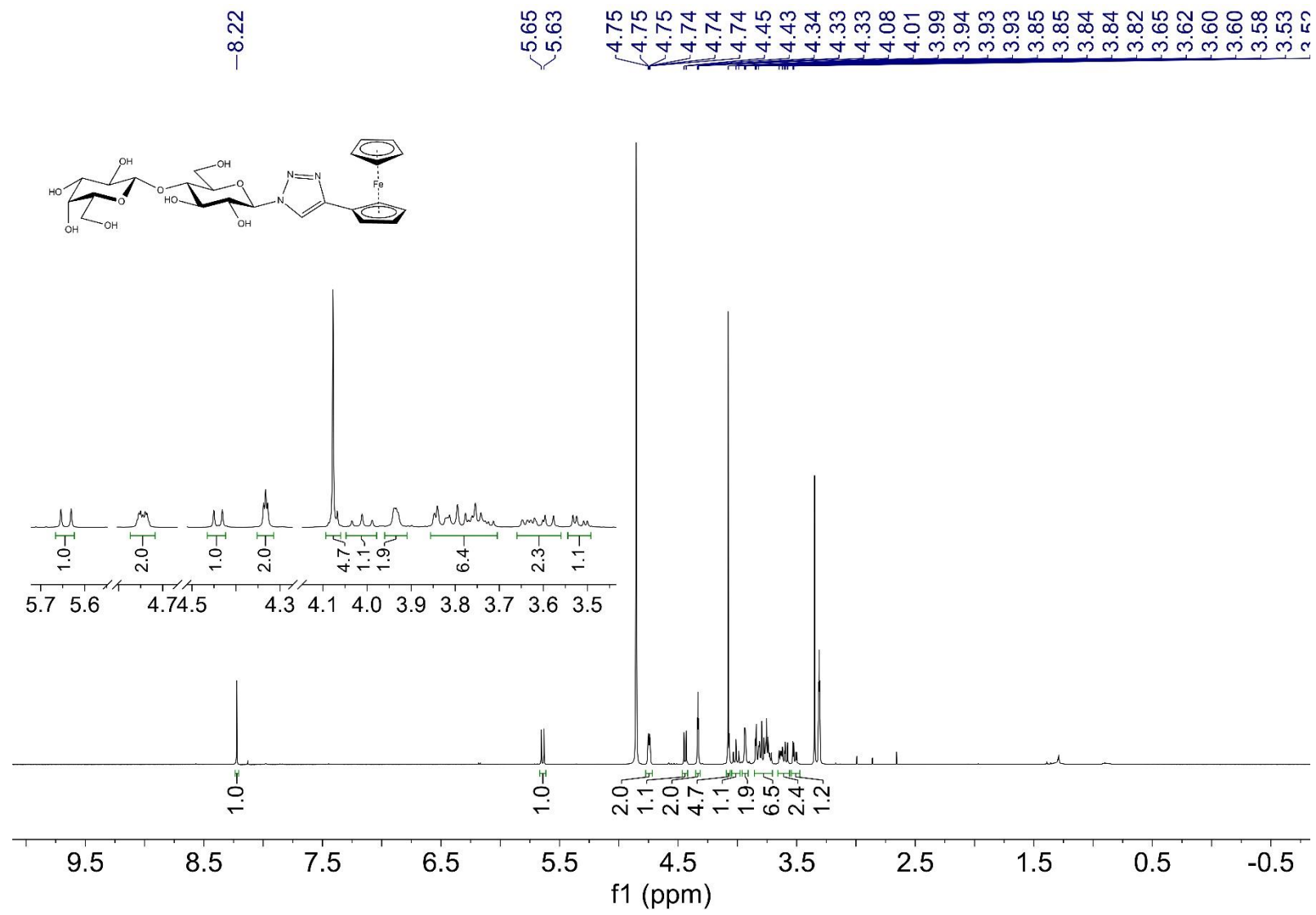
Copies of NMR Spectra

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NMR COMPOUND 16	41
NMR COMPOUND 18	47

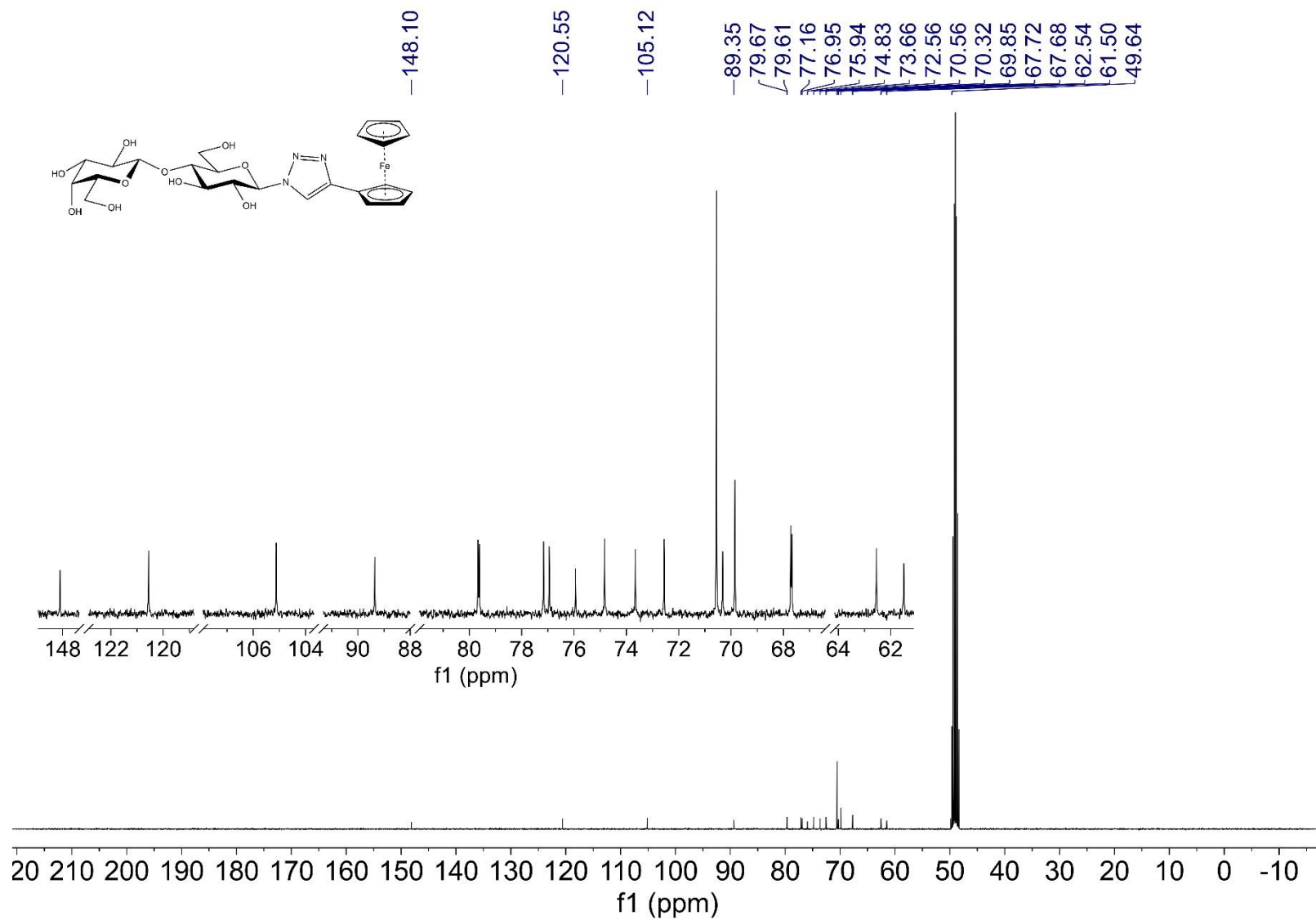
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NMR COMPOUND 29	92
NMR COMPOUND 30	97
NMR COMPOUND 33	103
NMR COMPOUND 34	105
NMR COMPOUND 36	111
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NMR COMPOUND 37	121
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NMR COMPOUND 41	128
NMR COMPOUND 42	135
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NMR COMPOUND 6

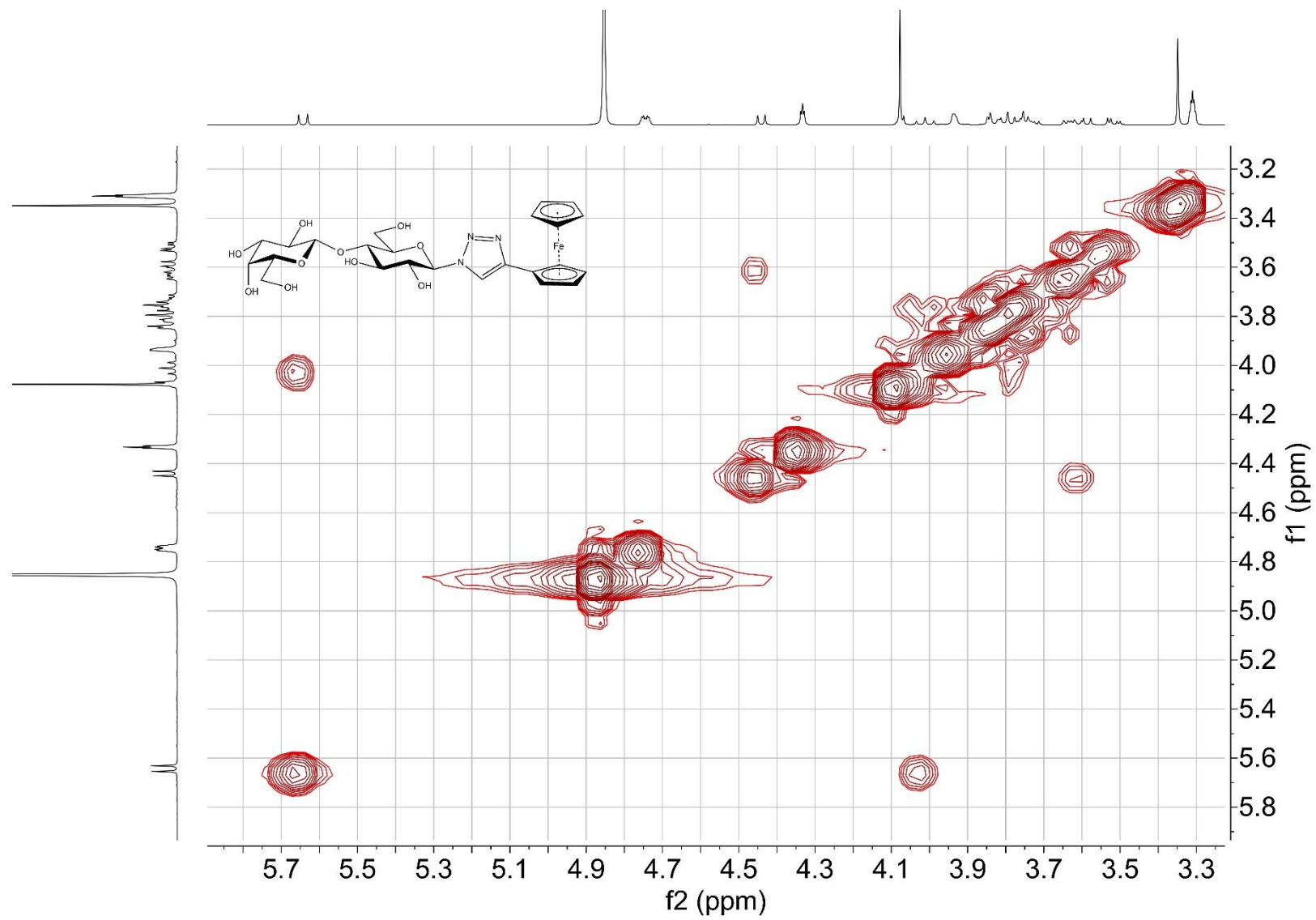
¹H NMR (400 MHz, MeOD) 6



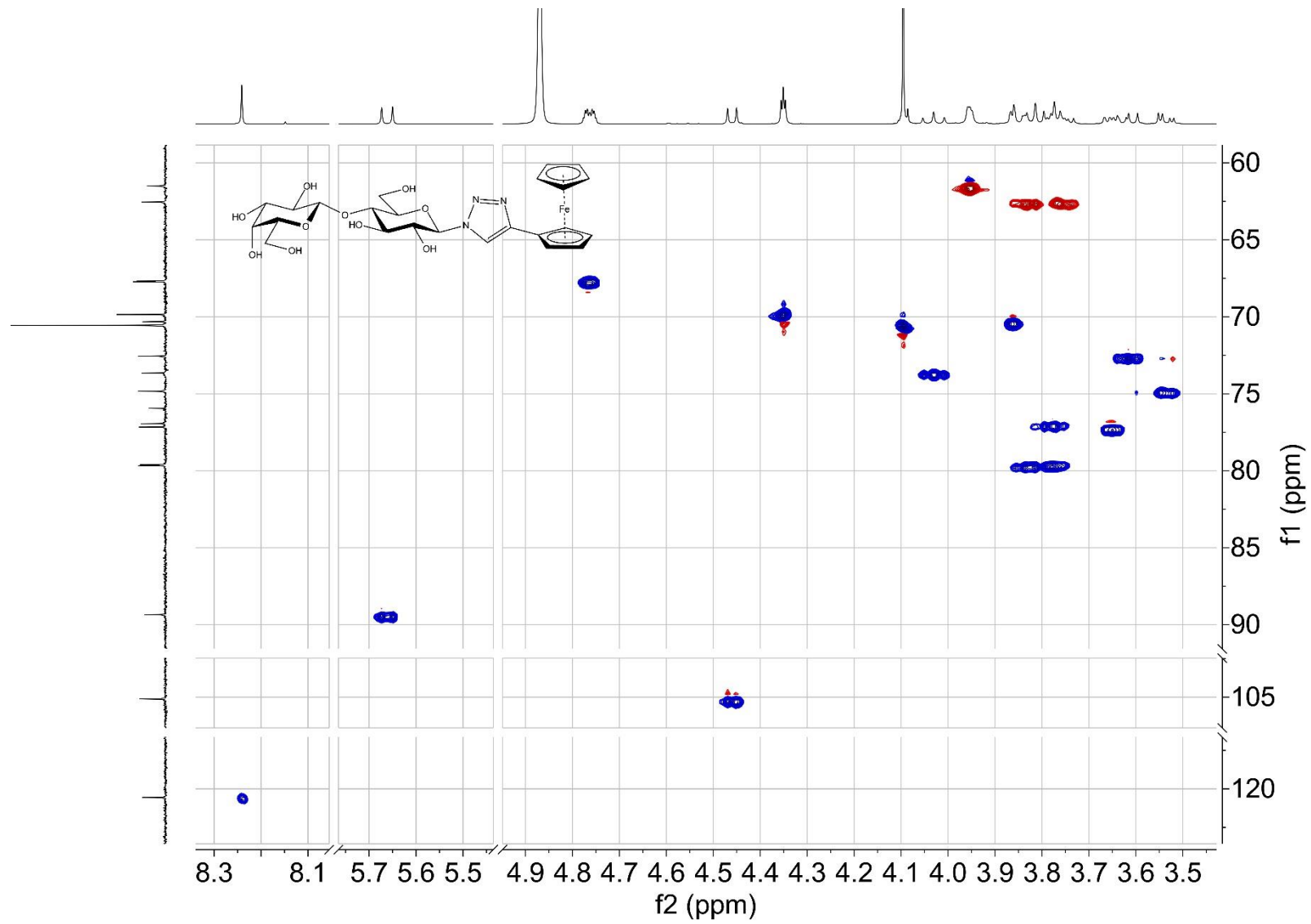
¹³C NMR (101 MHz, MeOD) 6



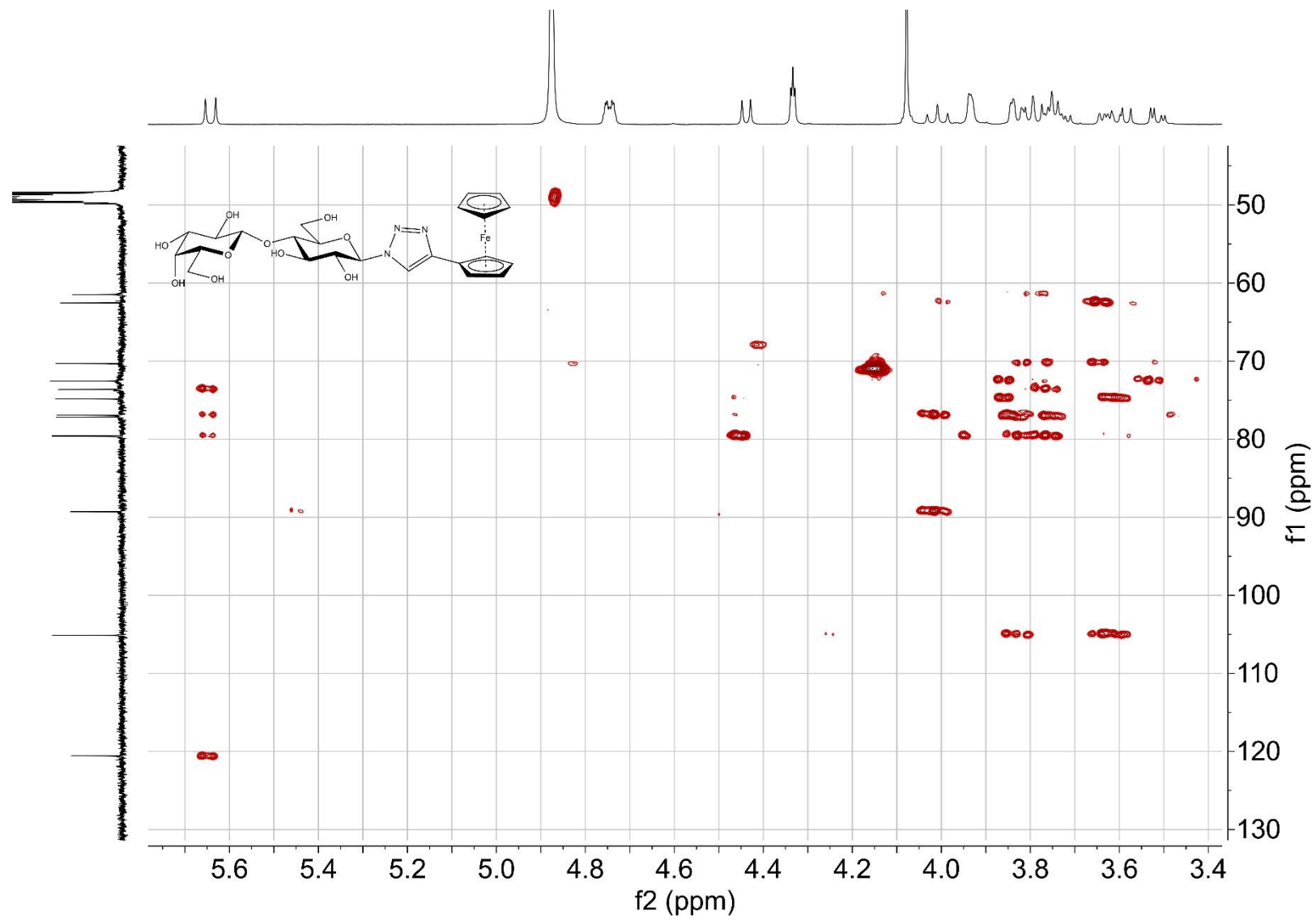
¹H-¹H COSY 6



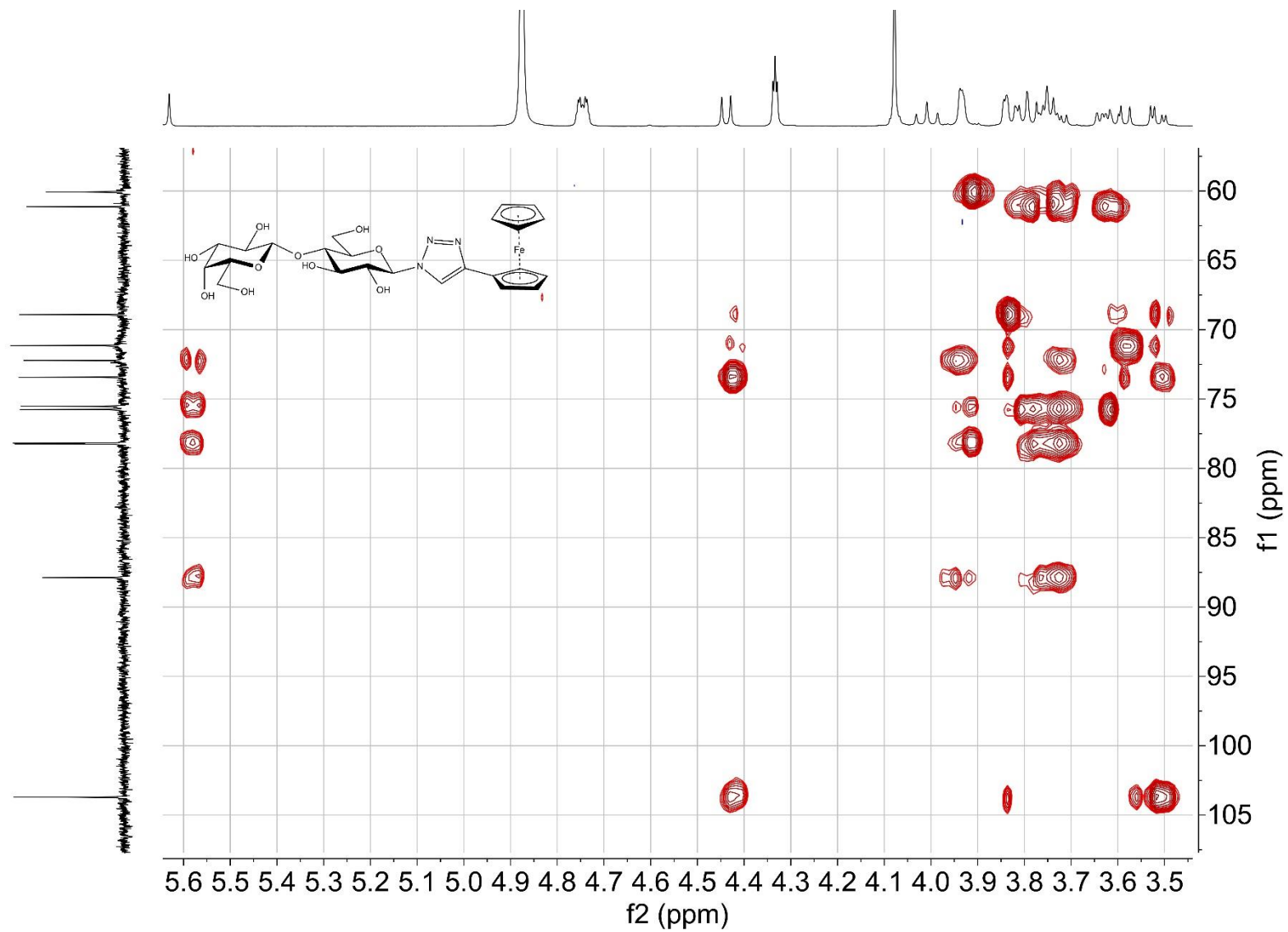
^1H - ^{13}C HSQC 6



^1H - ^{13}C HMBC 6

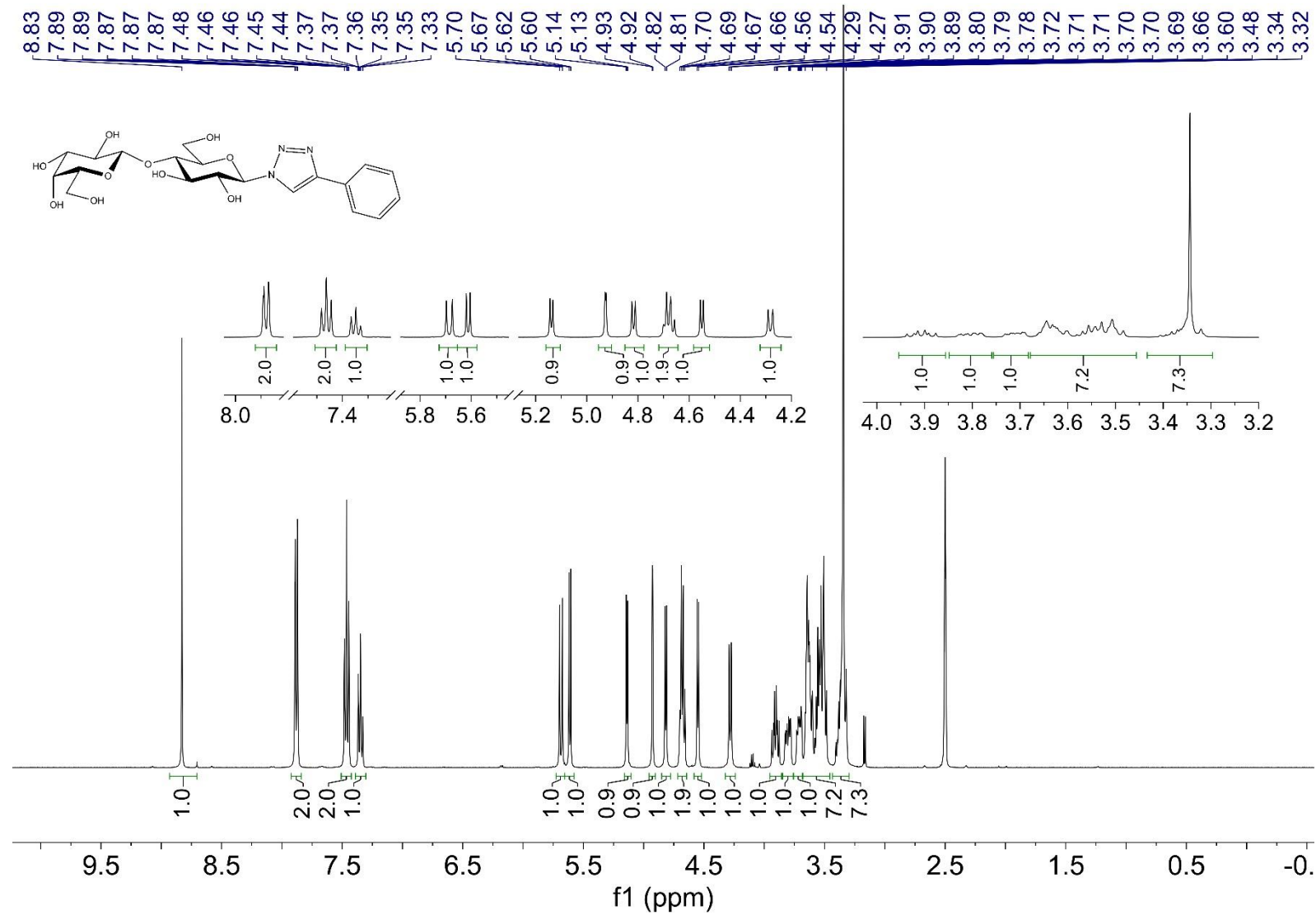


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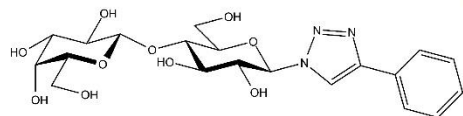


NMR COMPOUND 7

¹H NMR (400 MHz, DMSO-d₆) 7



¹³C NMR (101 MHz, CDCl₃) 7

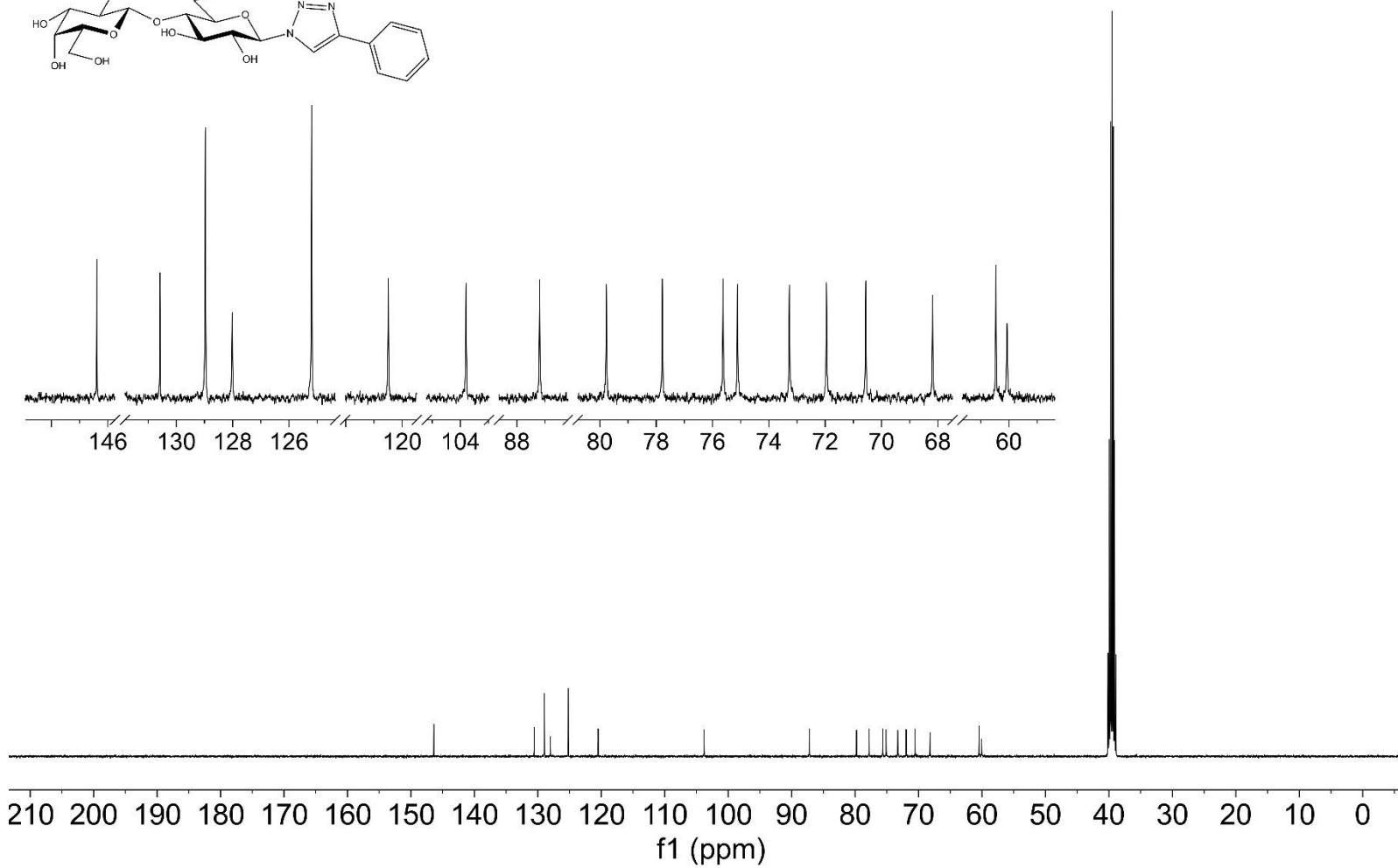


—146.39

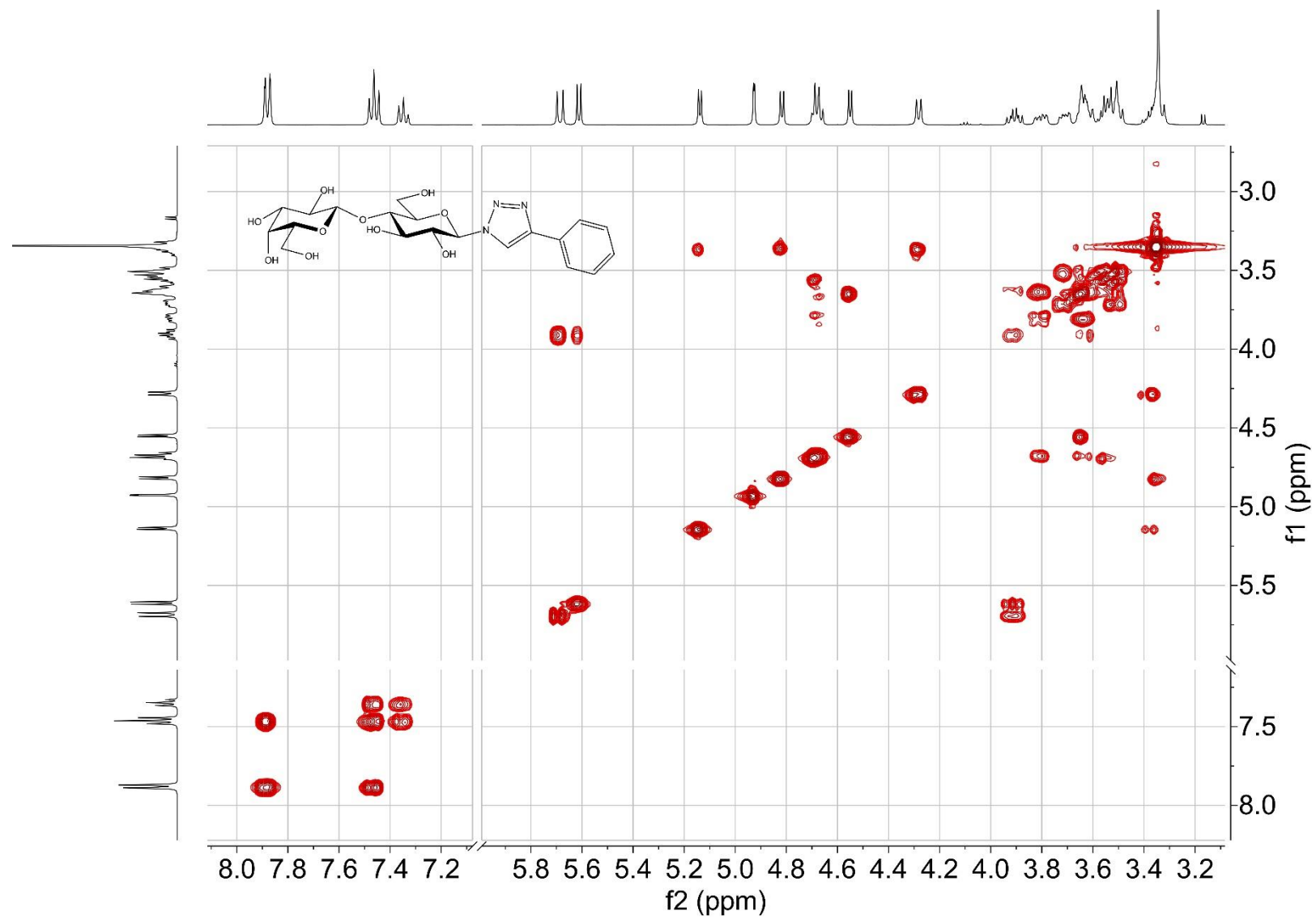
130.58
128.97
128.02
125.20
120.49

—103.80

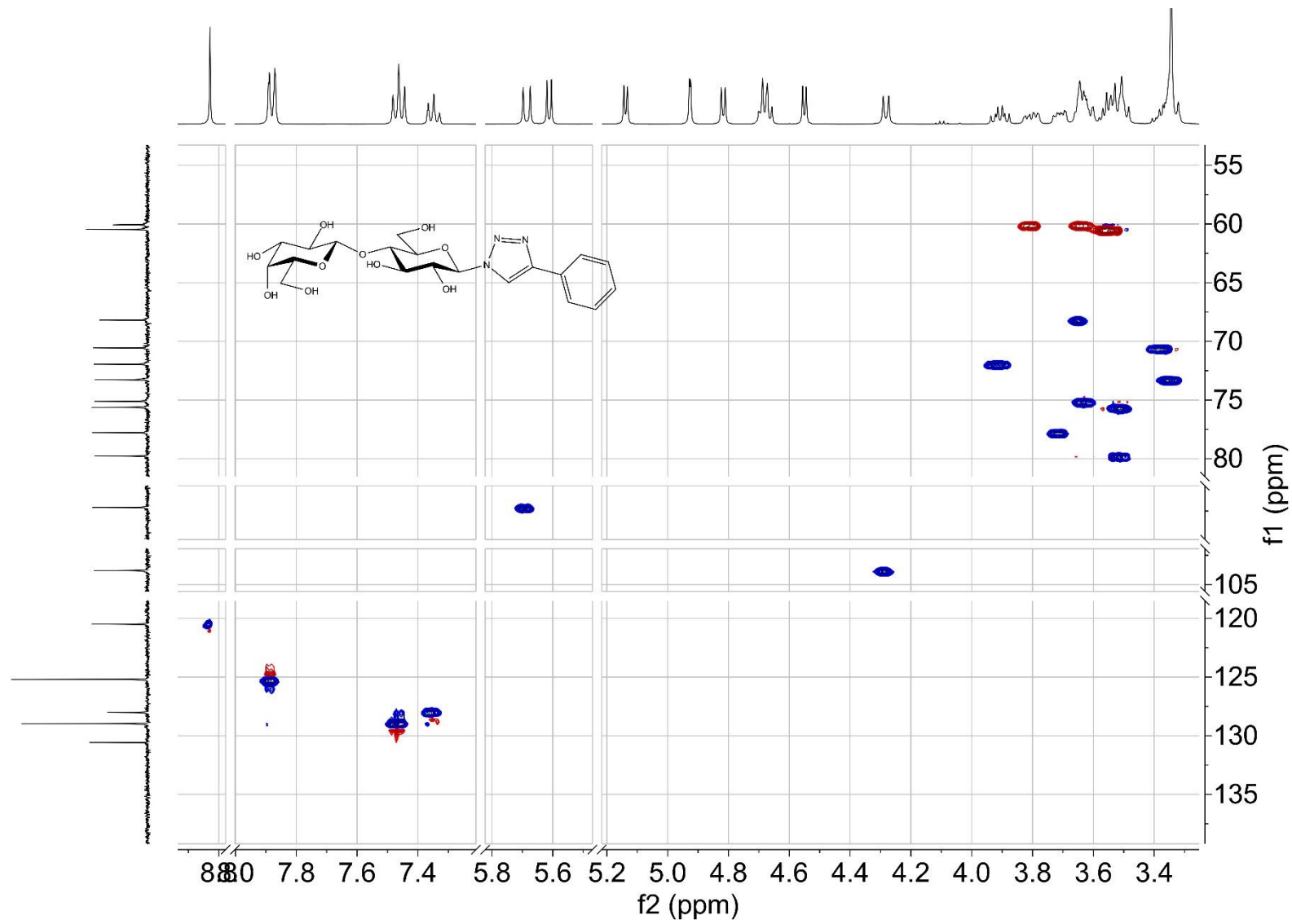
87.19
79.77
77.78
75.63
75.11
73.27
71.96
70.56
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60.46
60.07



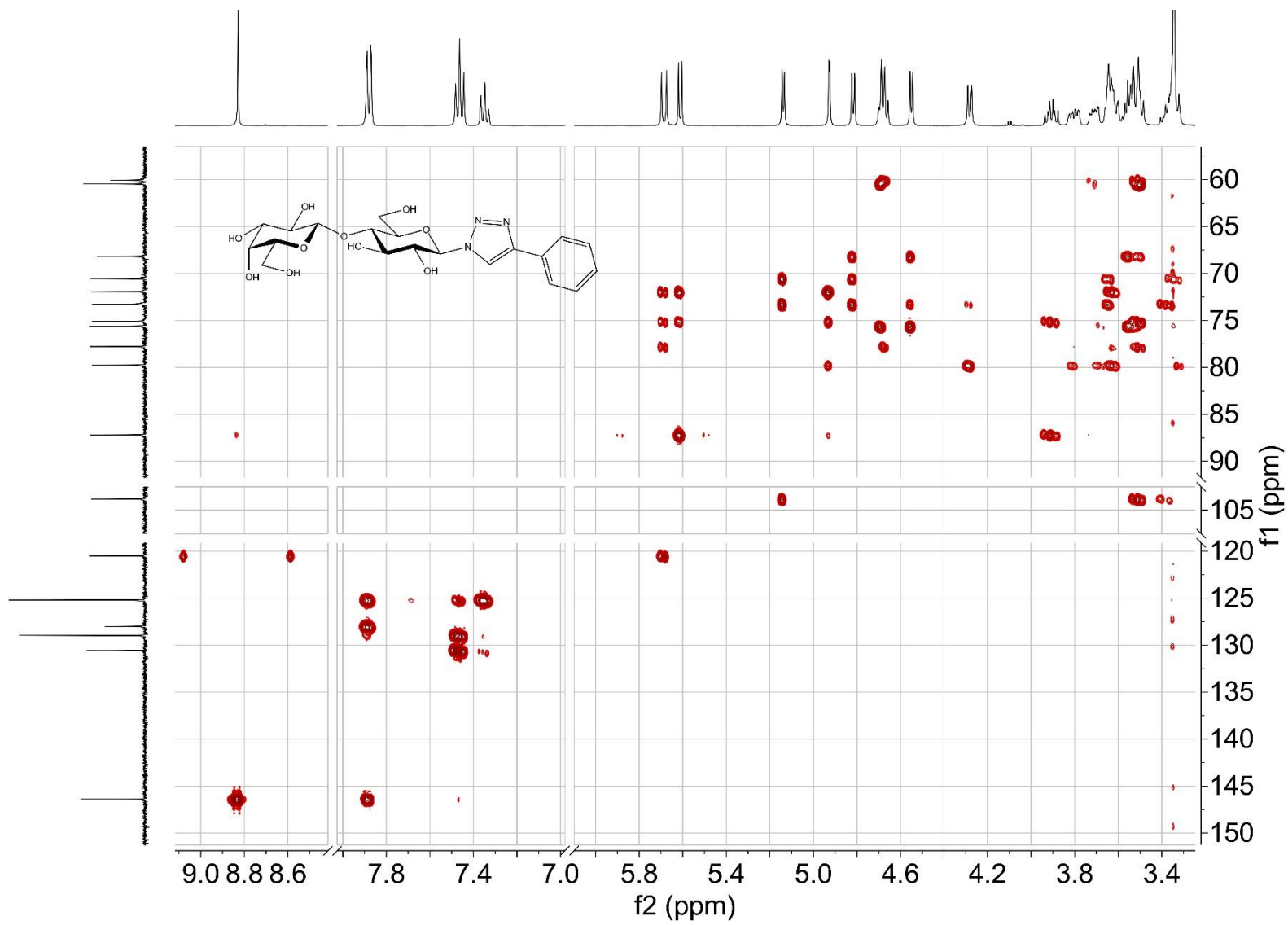
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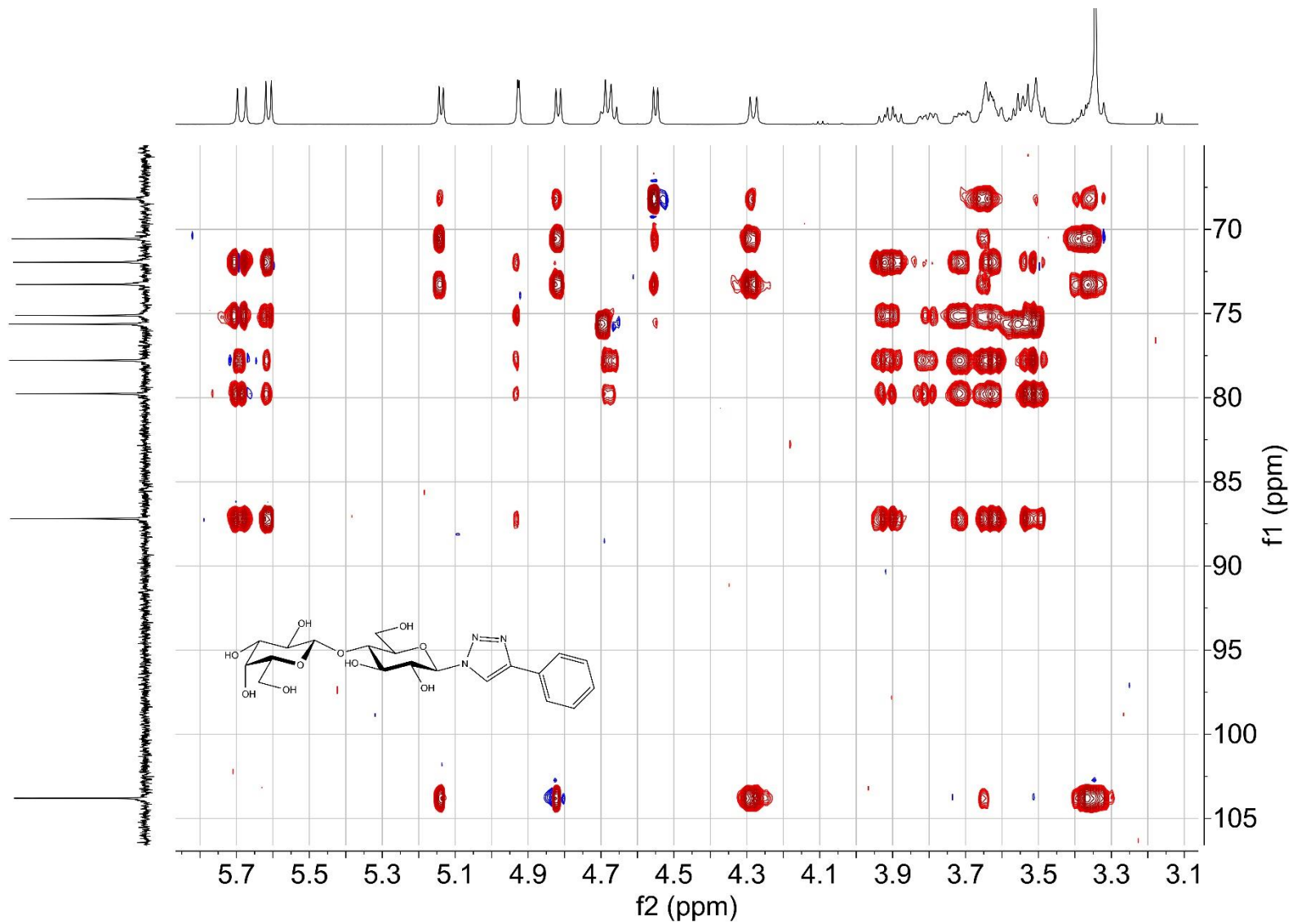
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^1H - ^{13}C HMBC 7

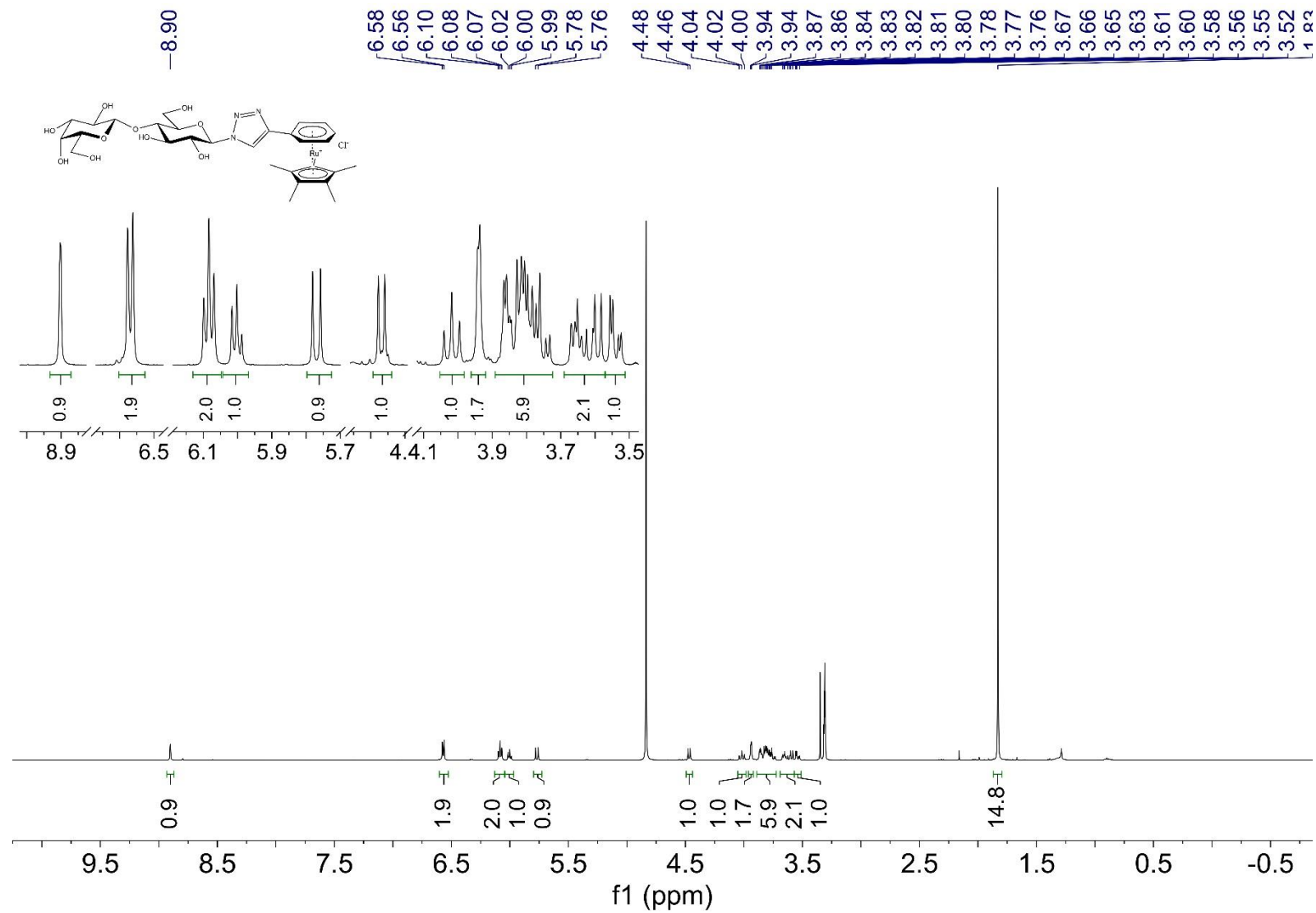


^1H - ^{13}C HSQCTOCSY 7

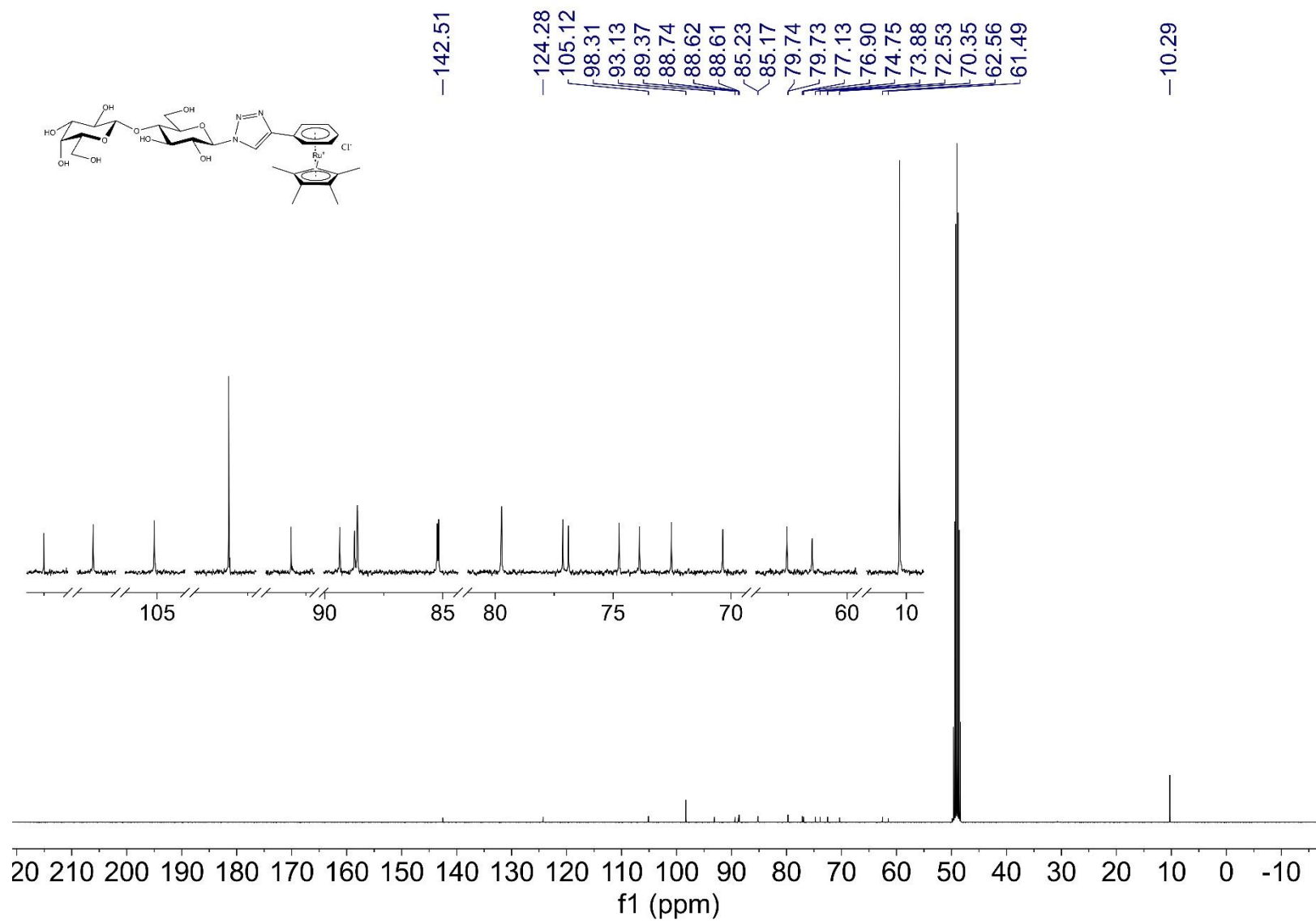


NMR COMPOUND 8

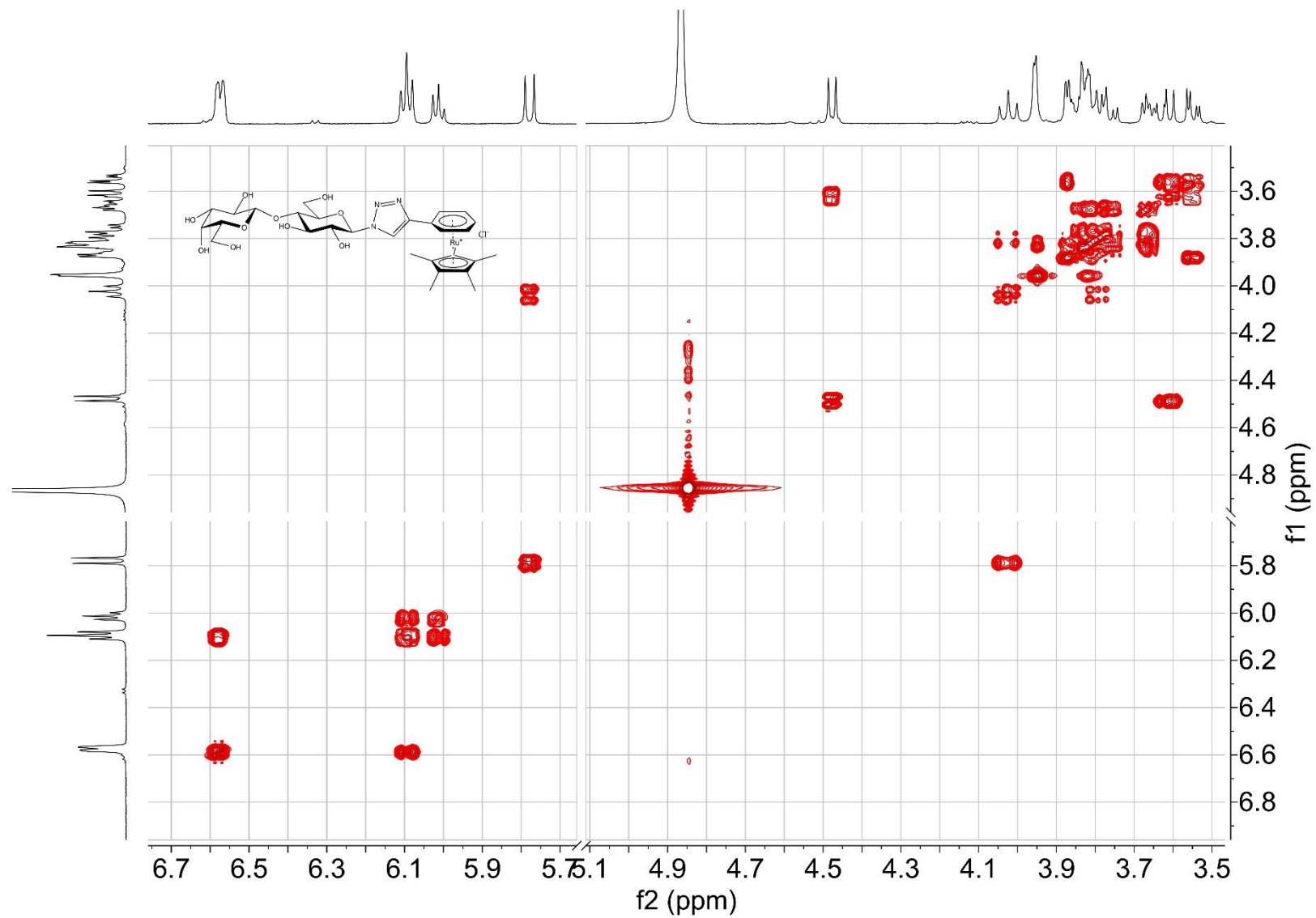
¹H NMR (400 MHz, MeOD) 8



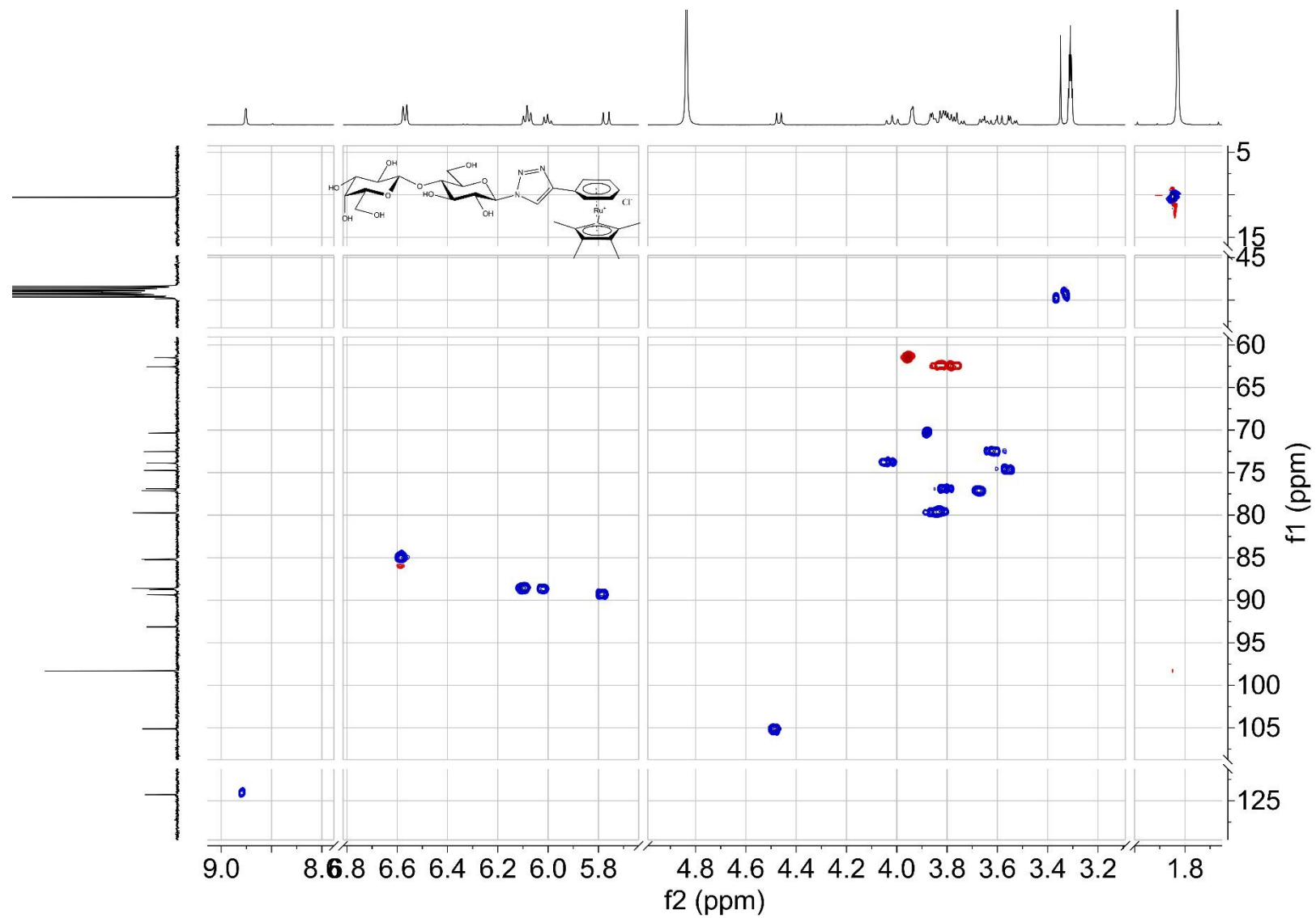
¹³C NMR (101 MHz, MeOD) 8



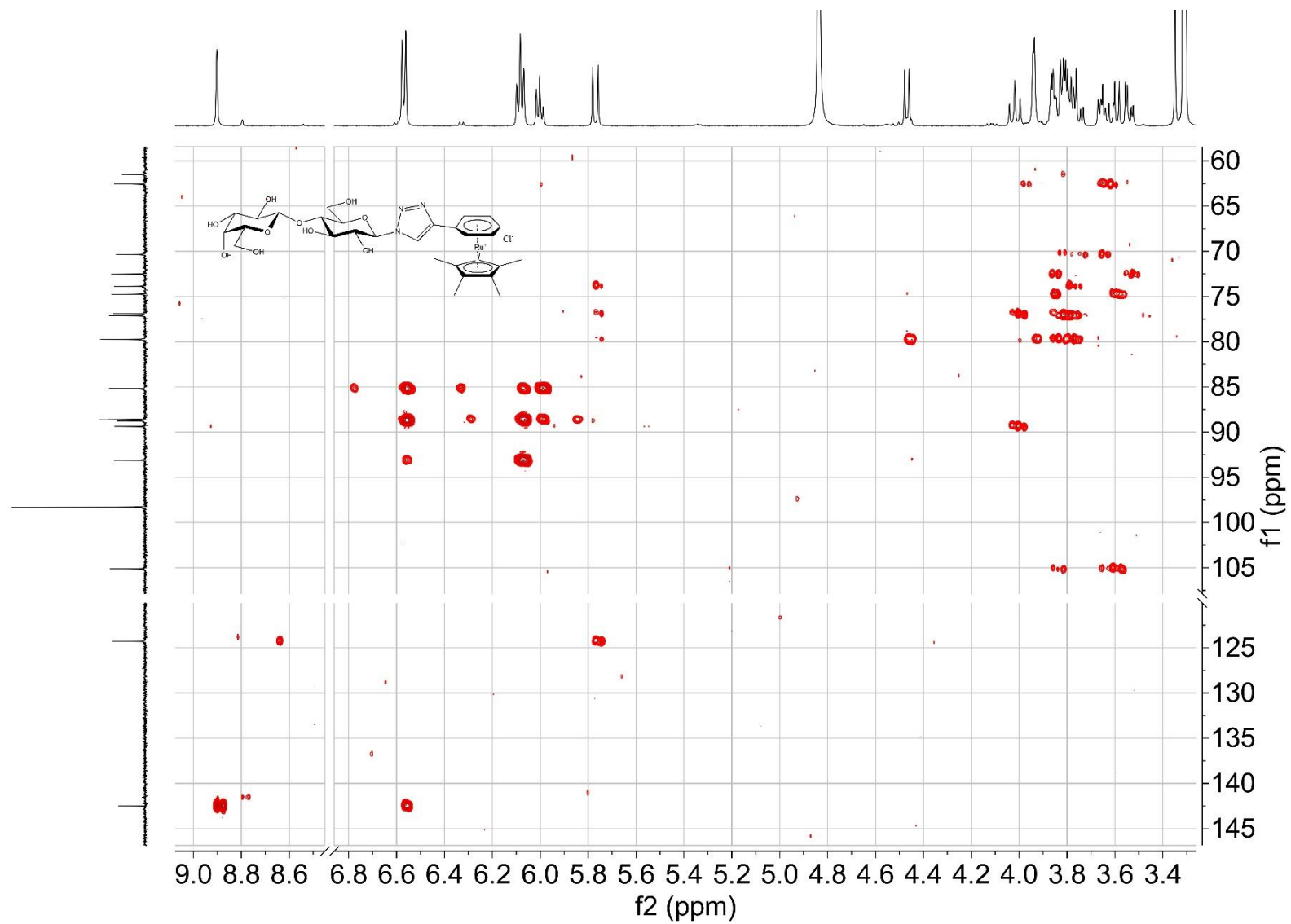
¹H-¹H COSY 8



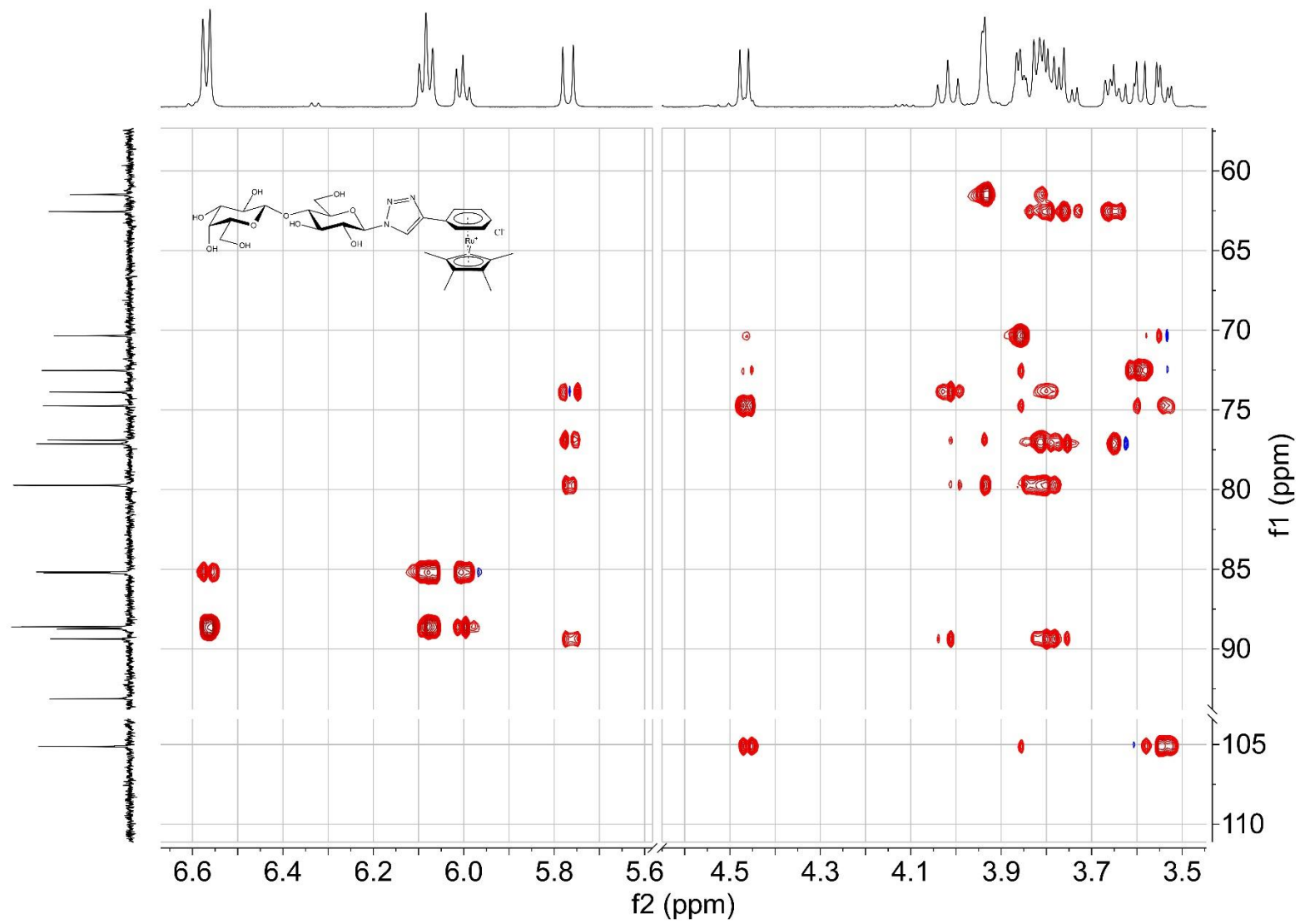
^1H - ^{13}C HSQC 8



¹H-¹³C HMBC 8

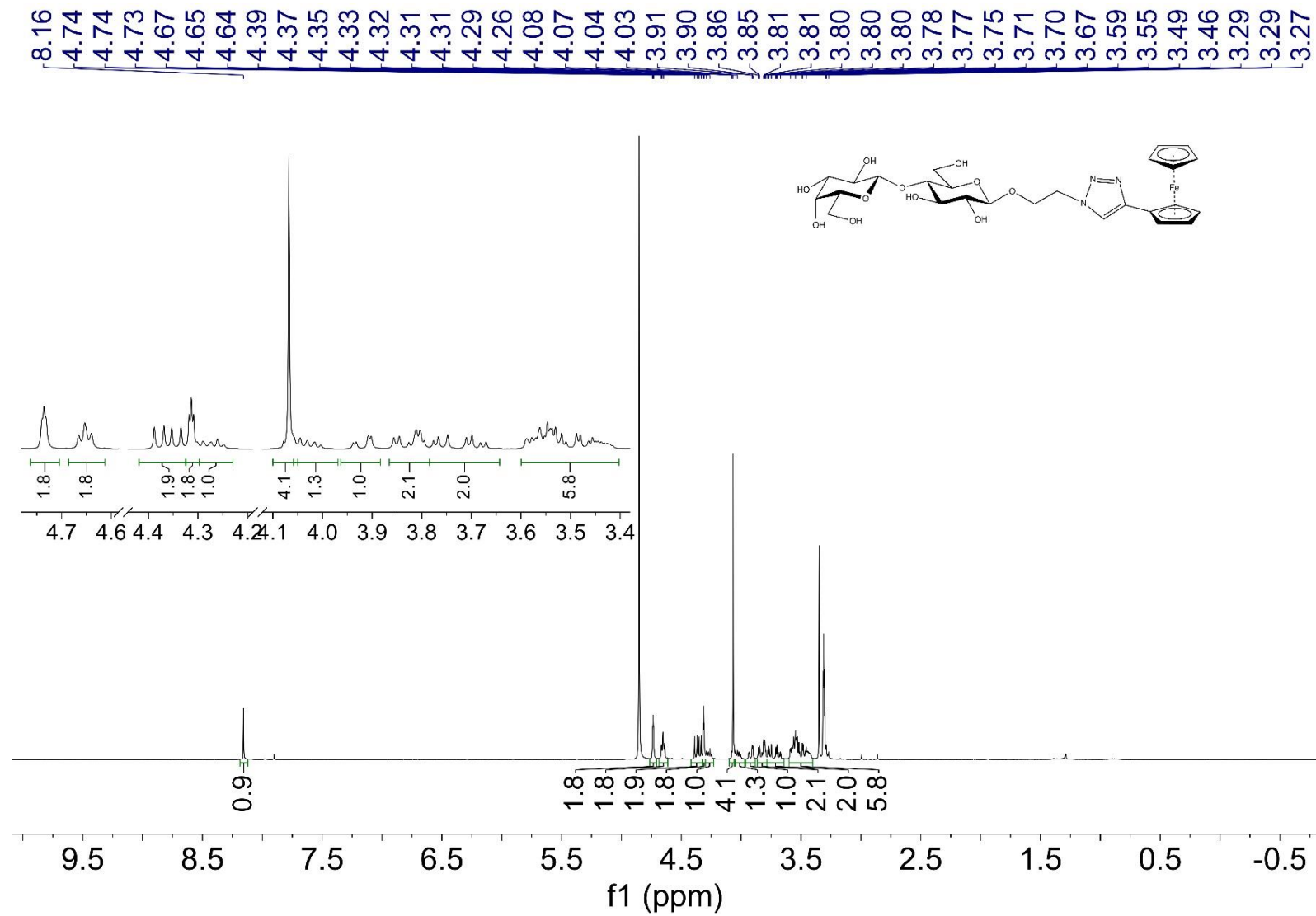


^1H - ^{13}C HSQCTOCSY 8

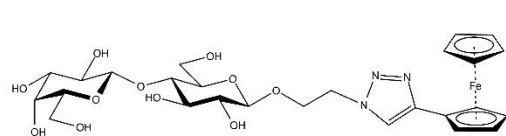


NMR COMPOUND 10

¹H NMR (400 MHz, MeOD) 10

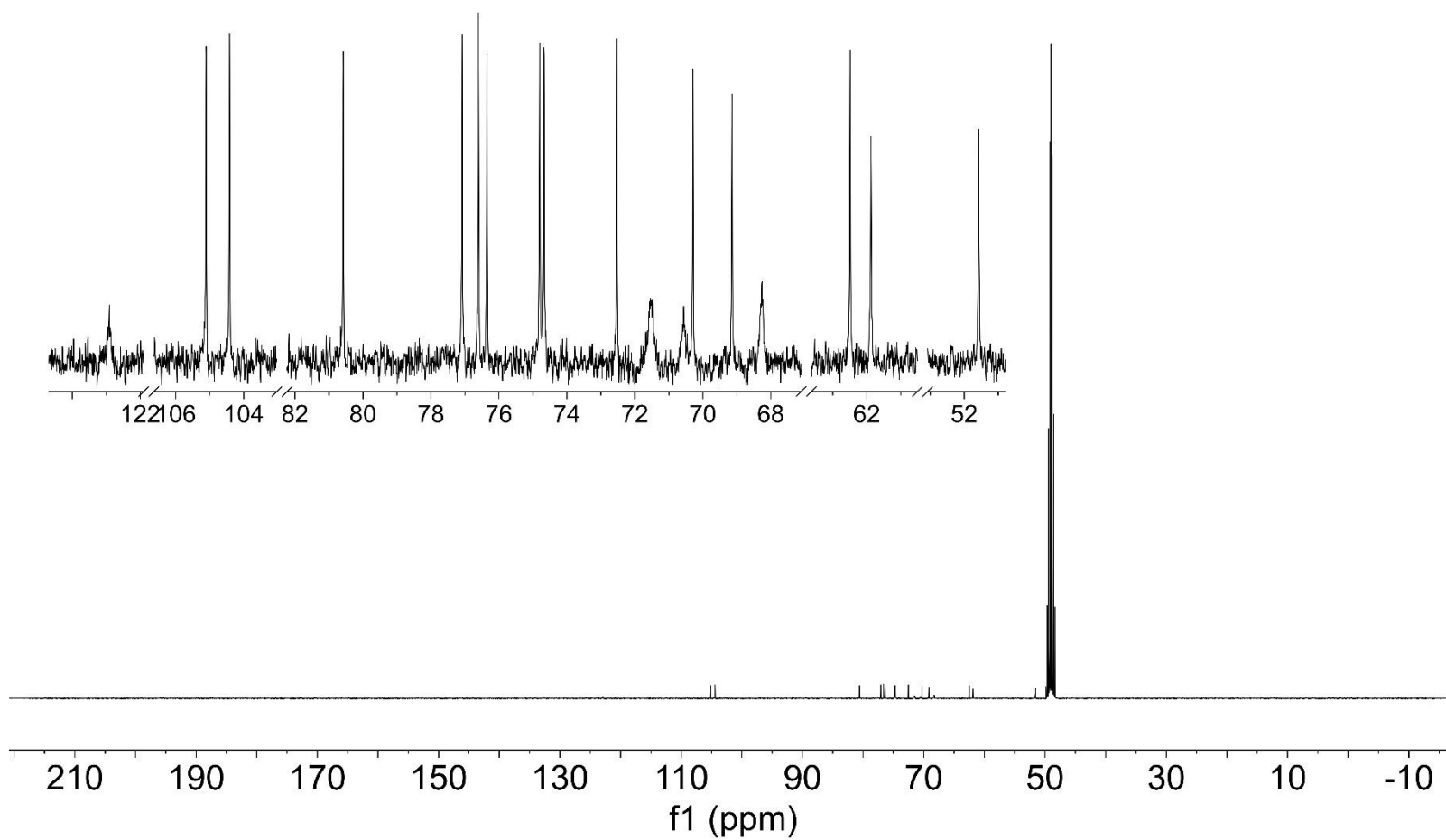


¹³C NMR (101 MHz, MeOD) 10

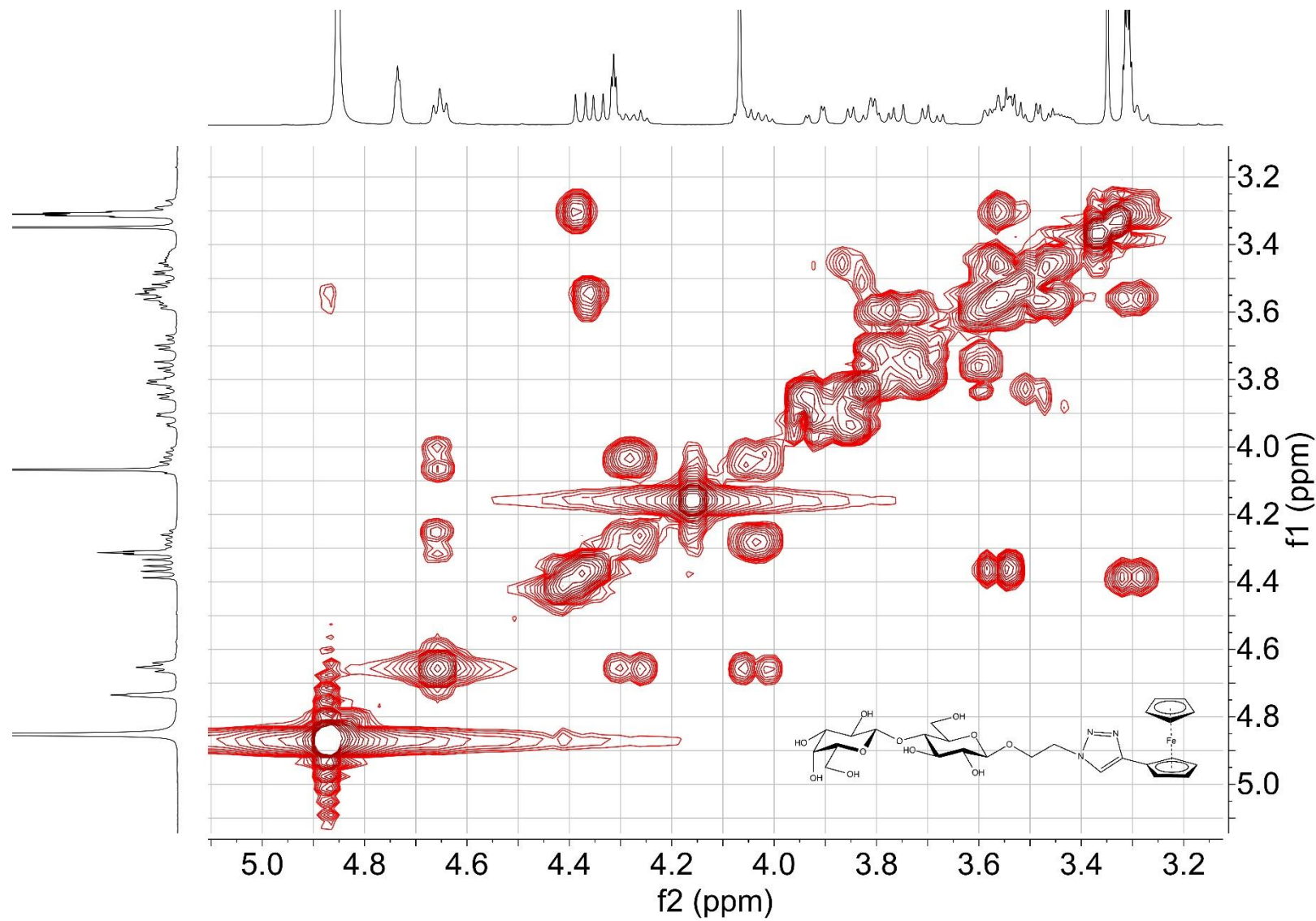


-122.91

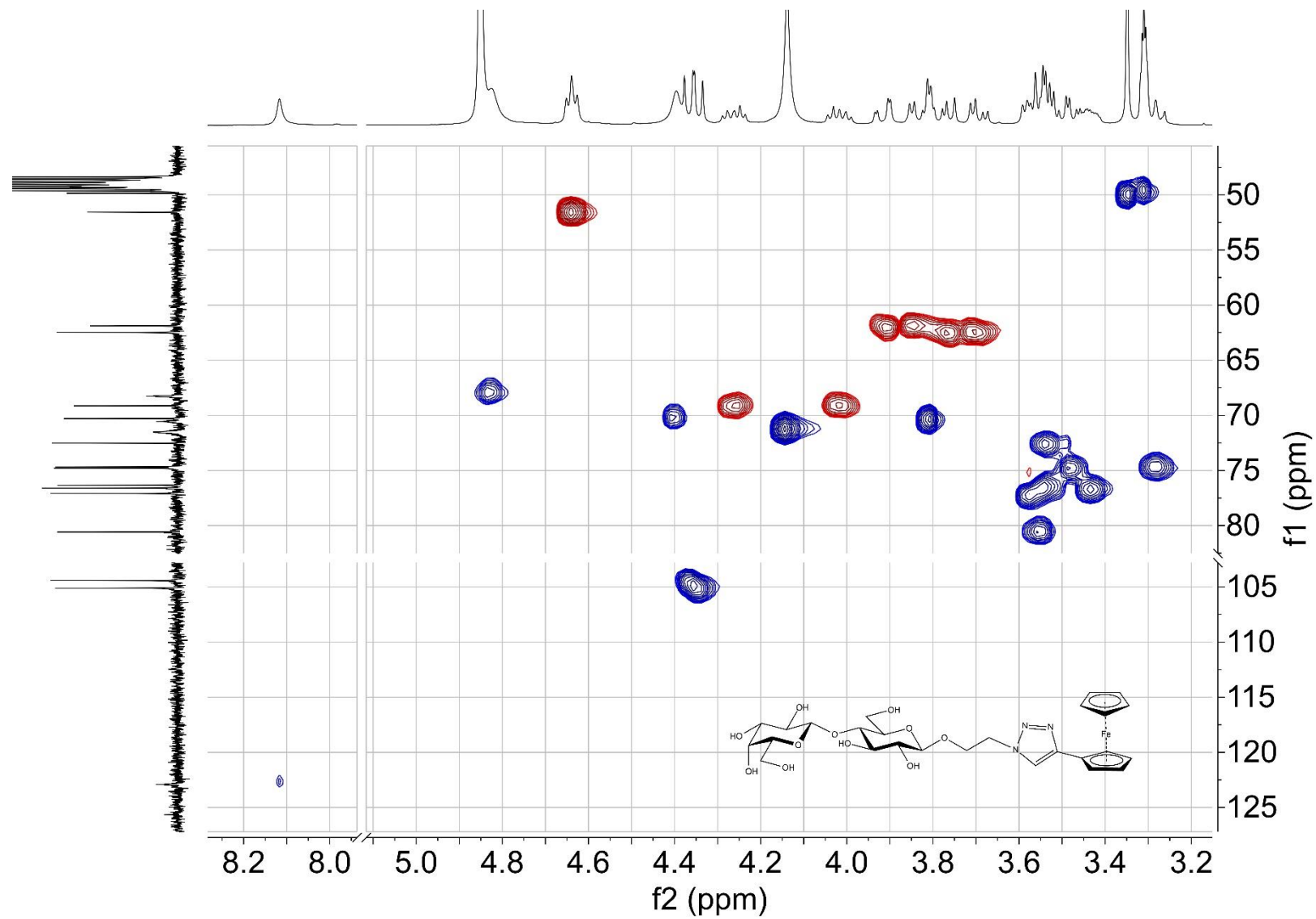
105.11
104.41
80.58
77.08
76.60
76.35
74.80
74.67
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70.60
70.29
69.14
68.26
62.49
61.88
51.58
49.85



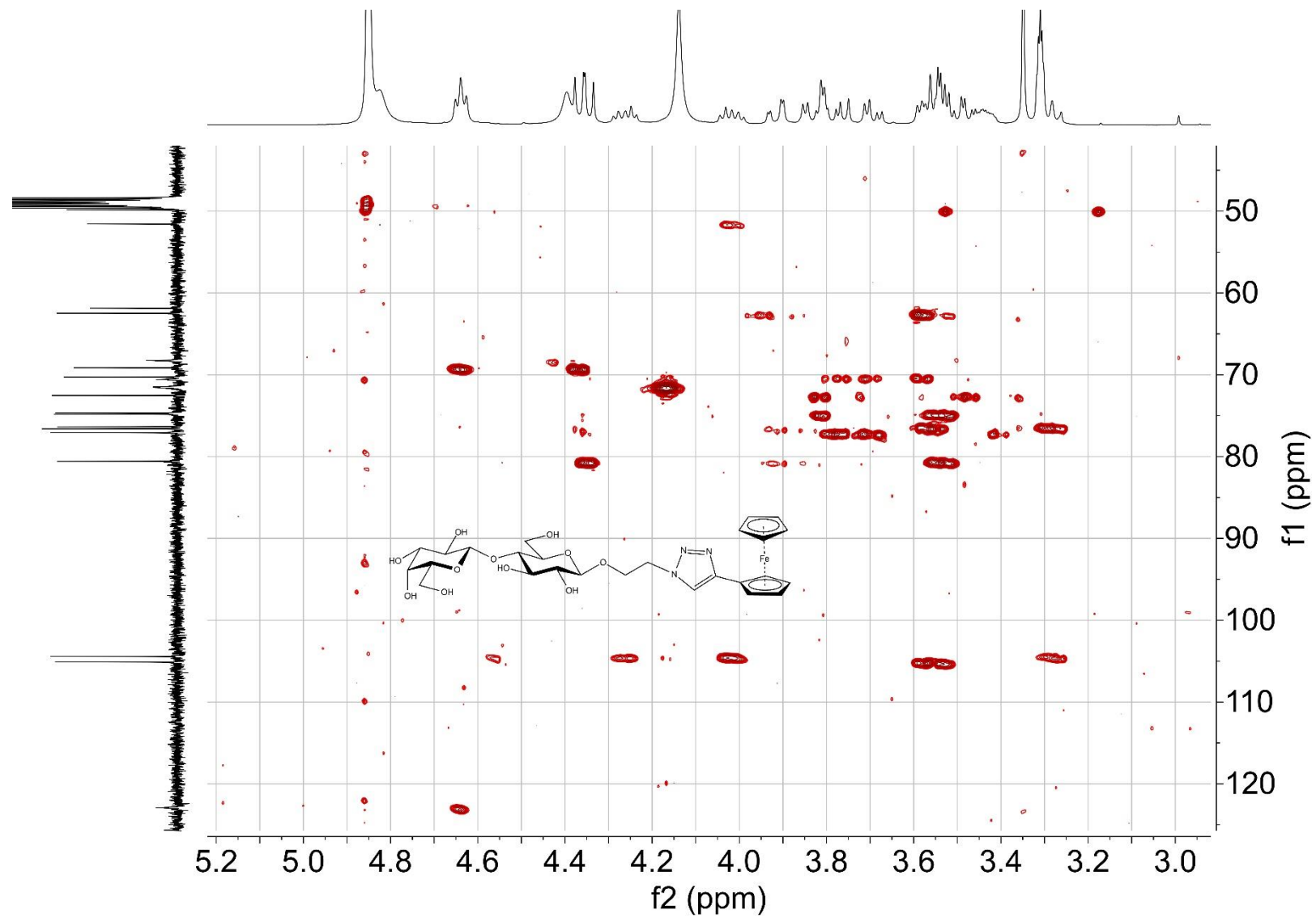
^1H - ^1H COSY 10



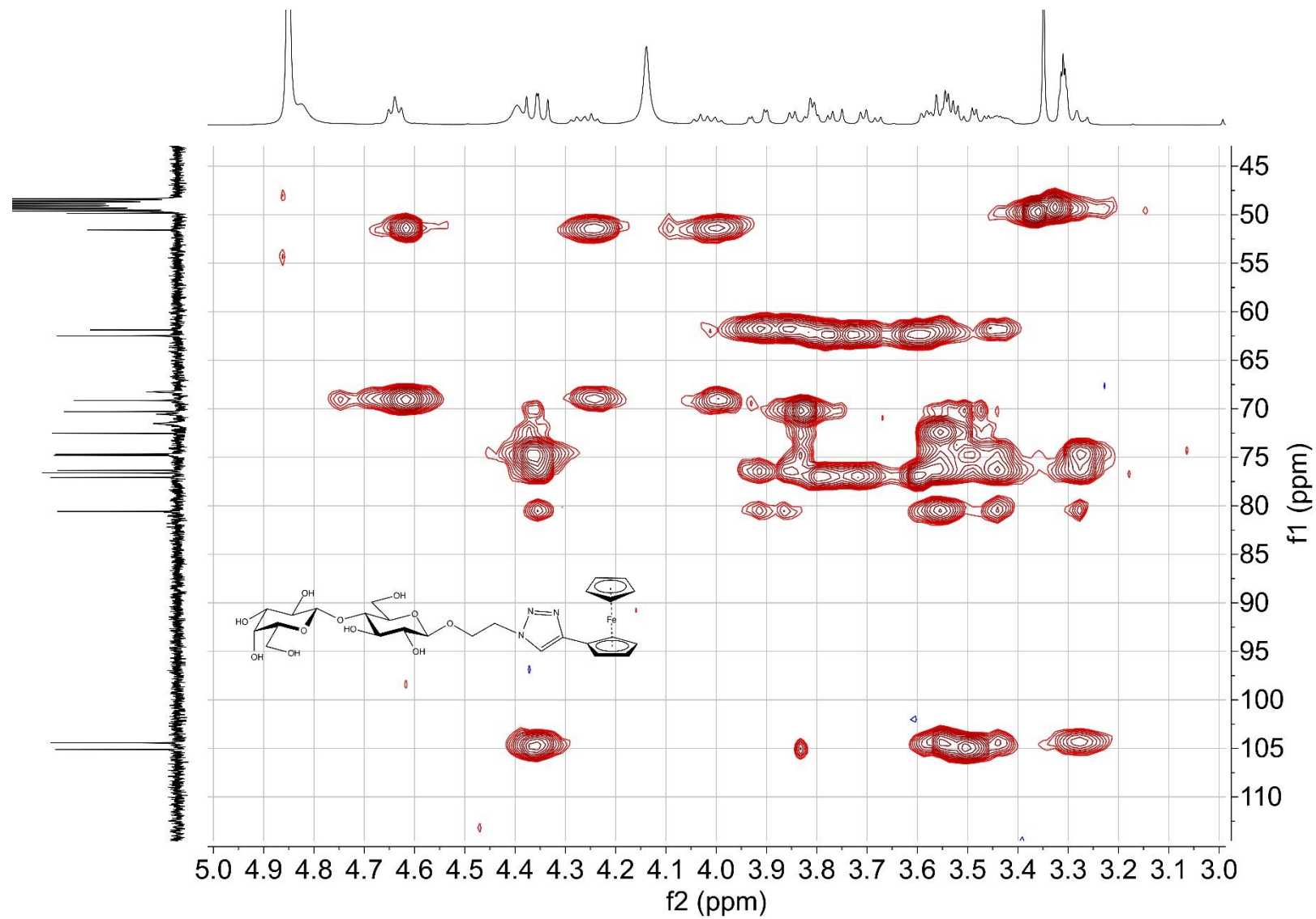
^1H - ^{13}C HSQC 10



^1H - ^{13}C HMBC 10

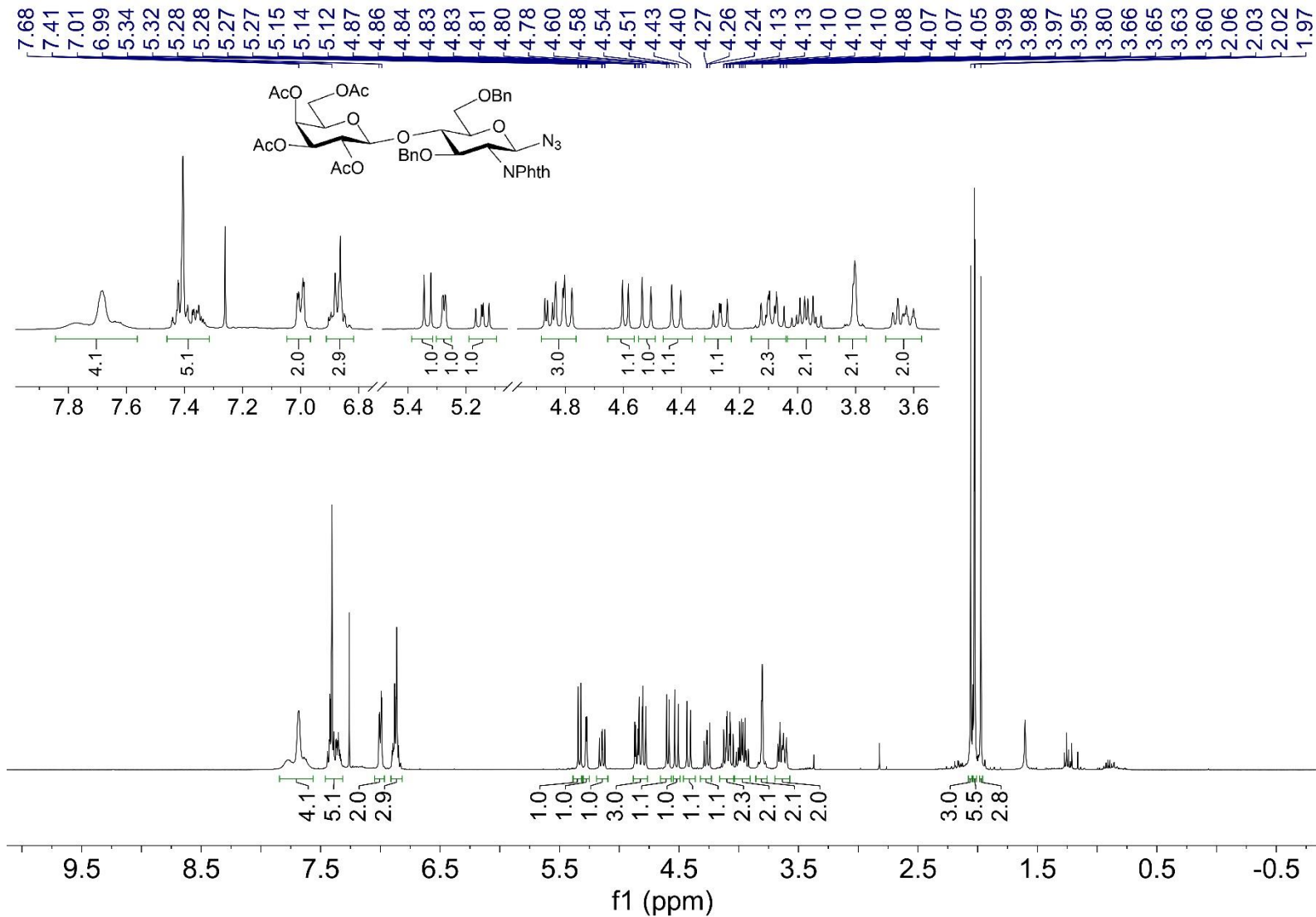


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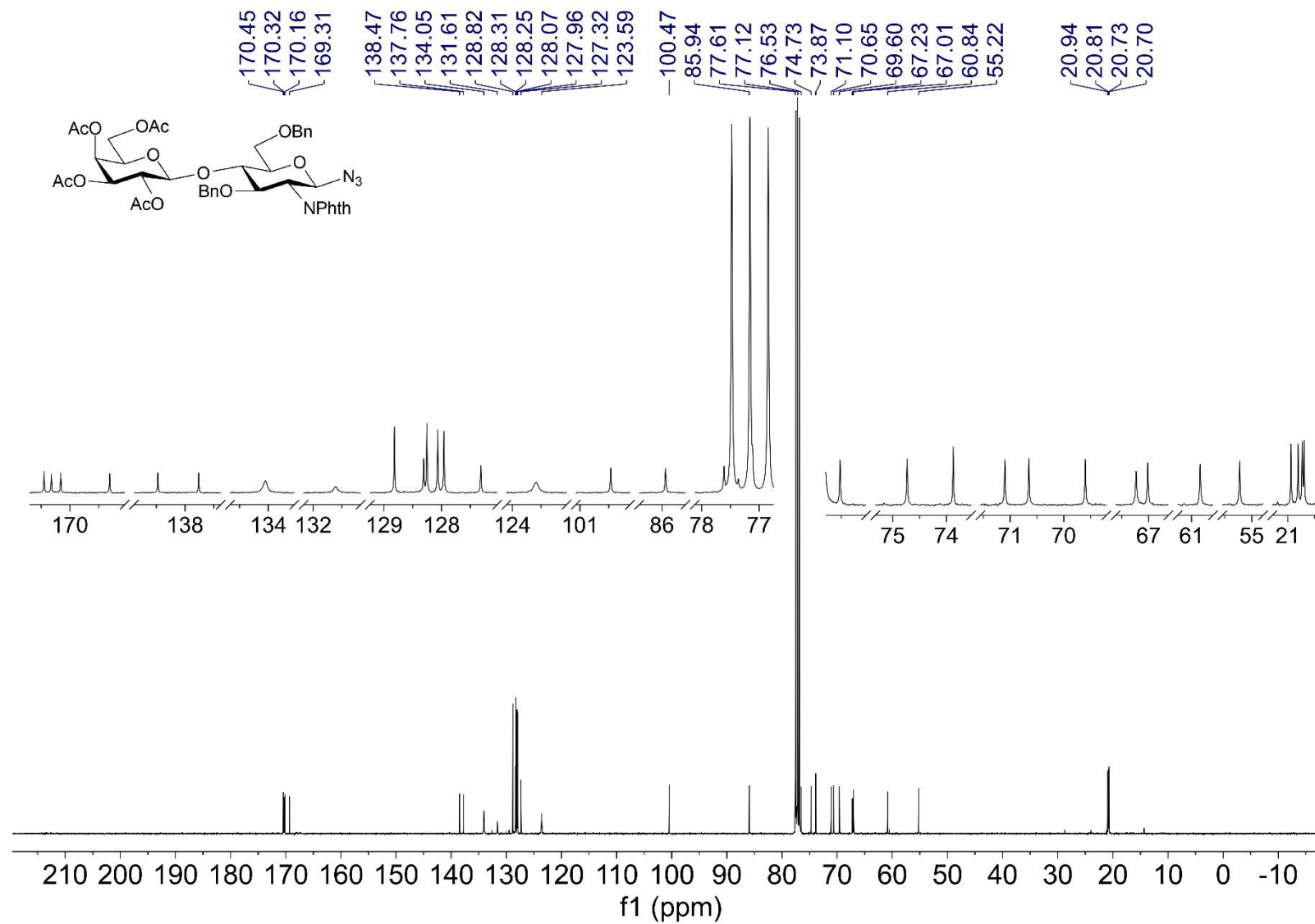


NMR COMPOUND 13

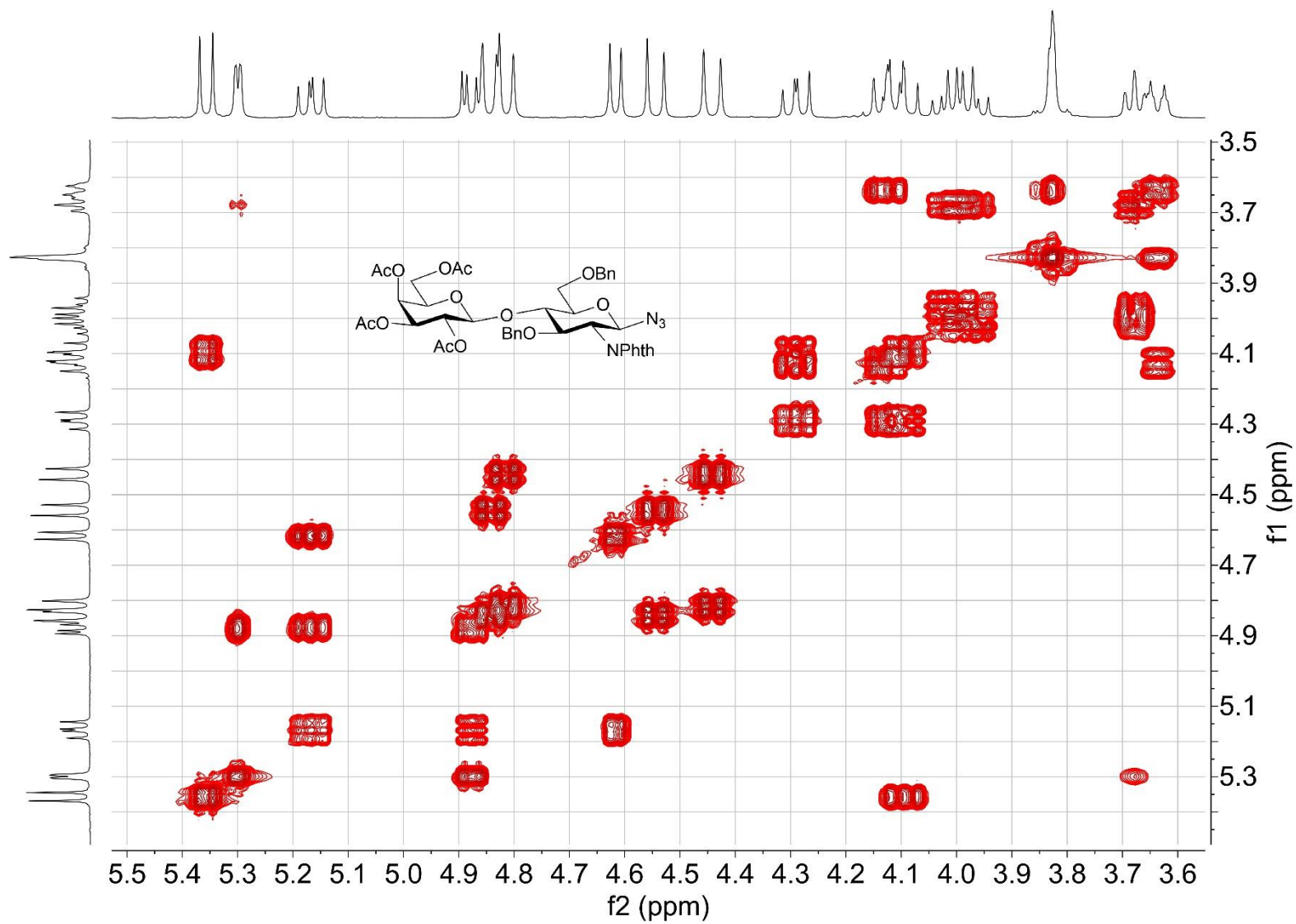
¹H NMR (400 MHz, CDCl₃) 13



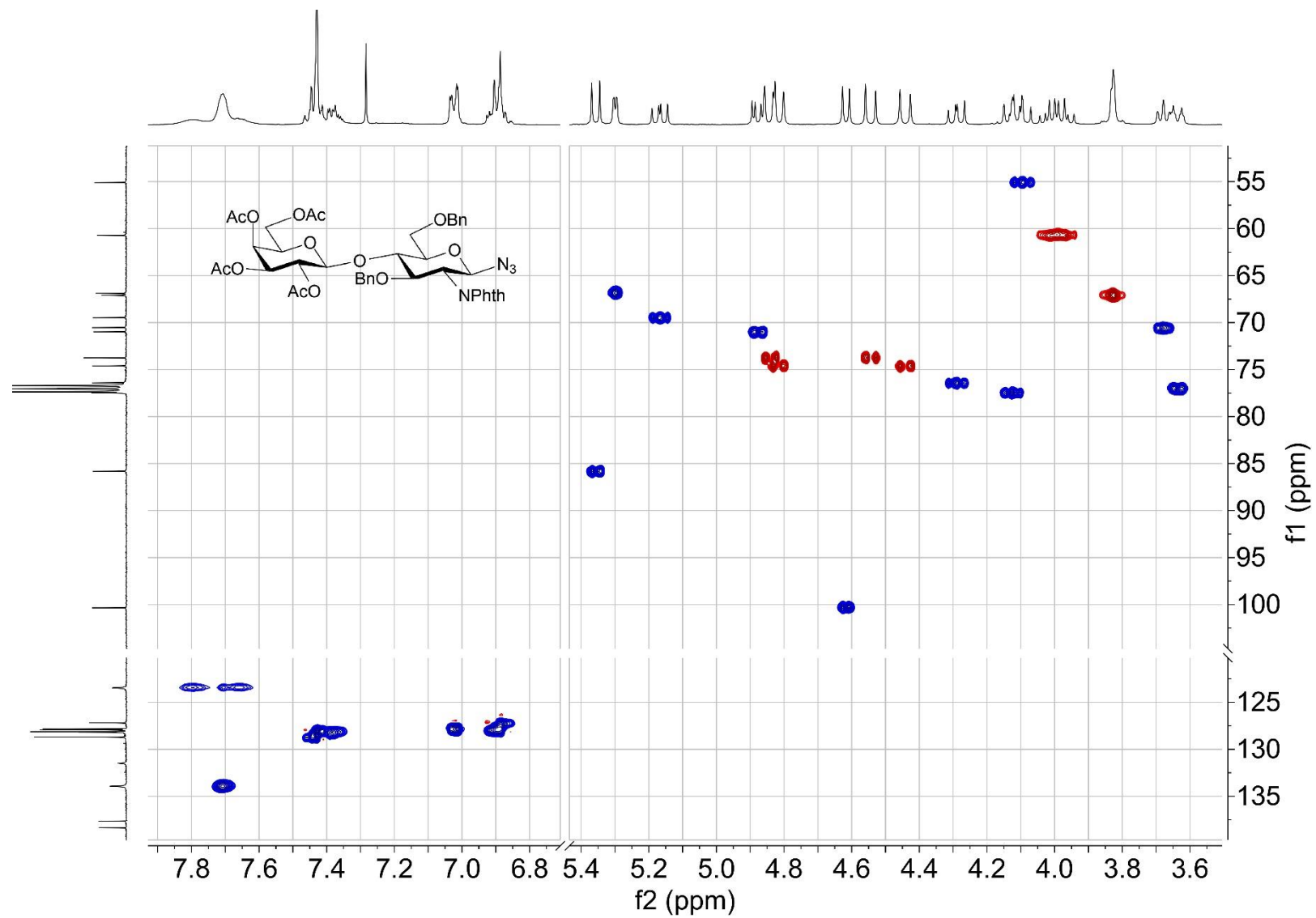
¹³C NMR (101 MHz, CDCl₃) 13



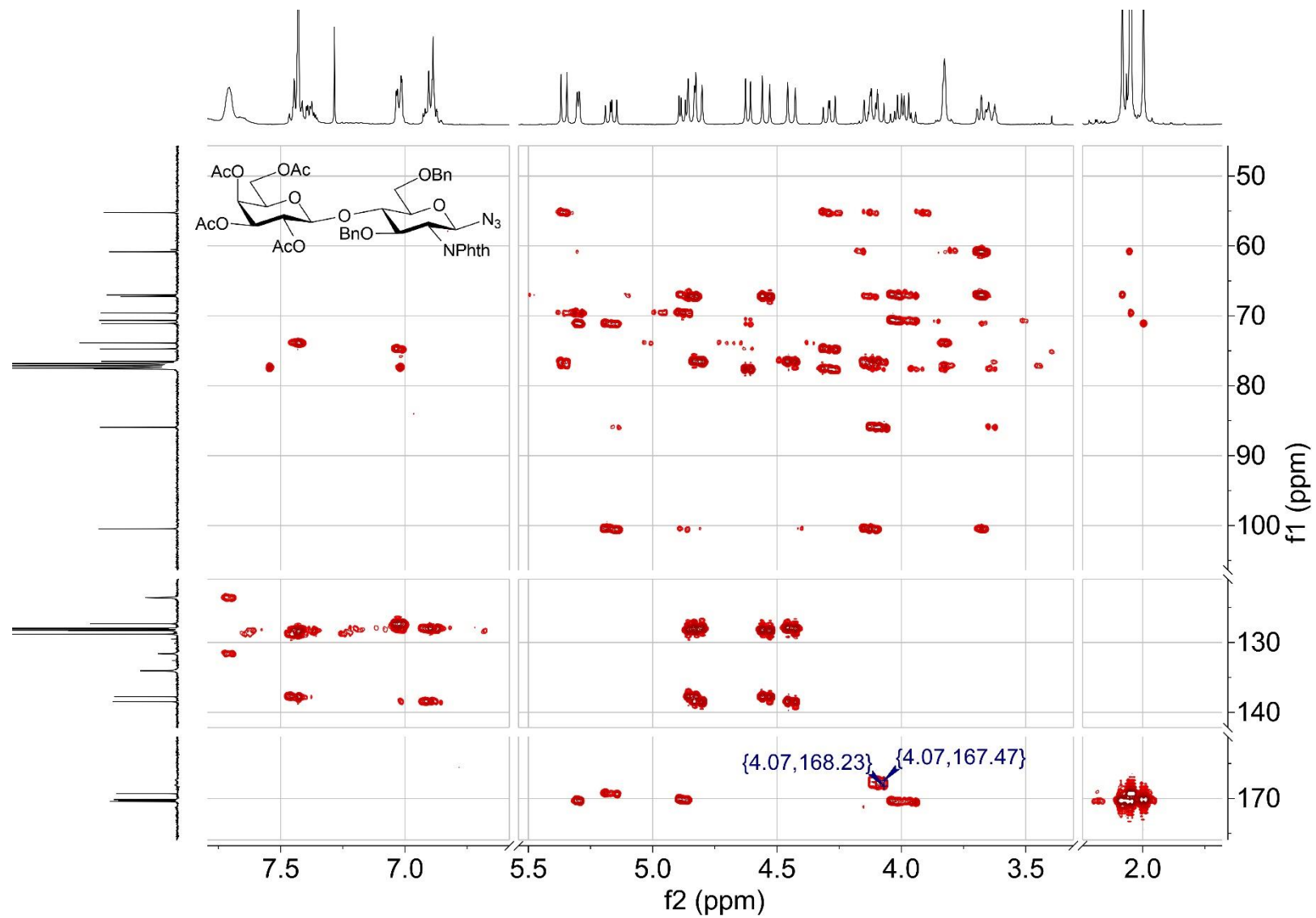
¹H-¹H COSY 13



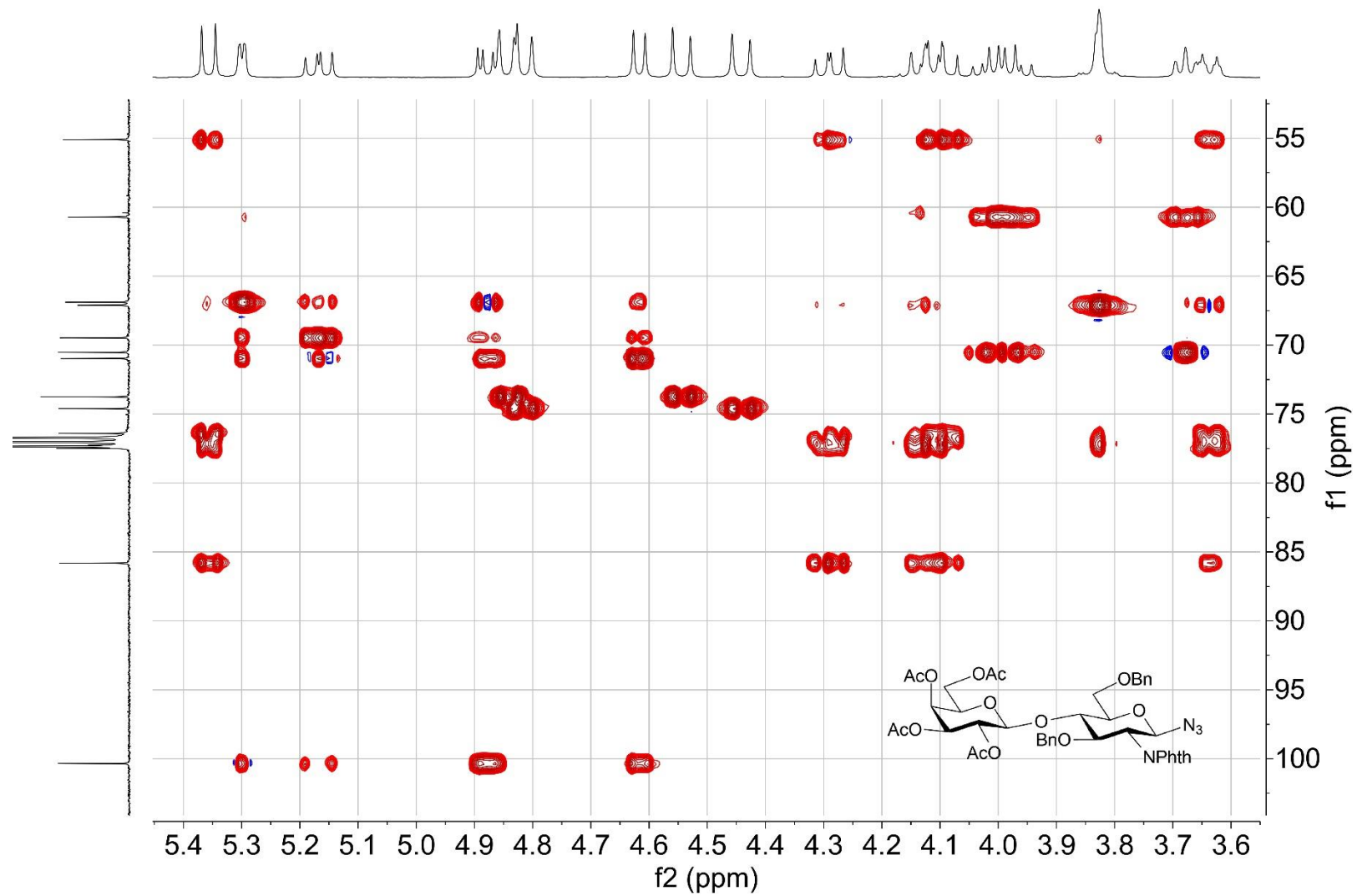
^1H - ^{13}C HSQC 13



¹H-¹³C HMBC 13

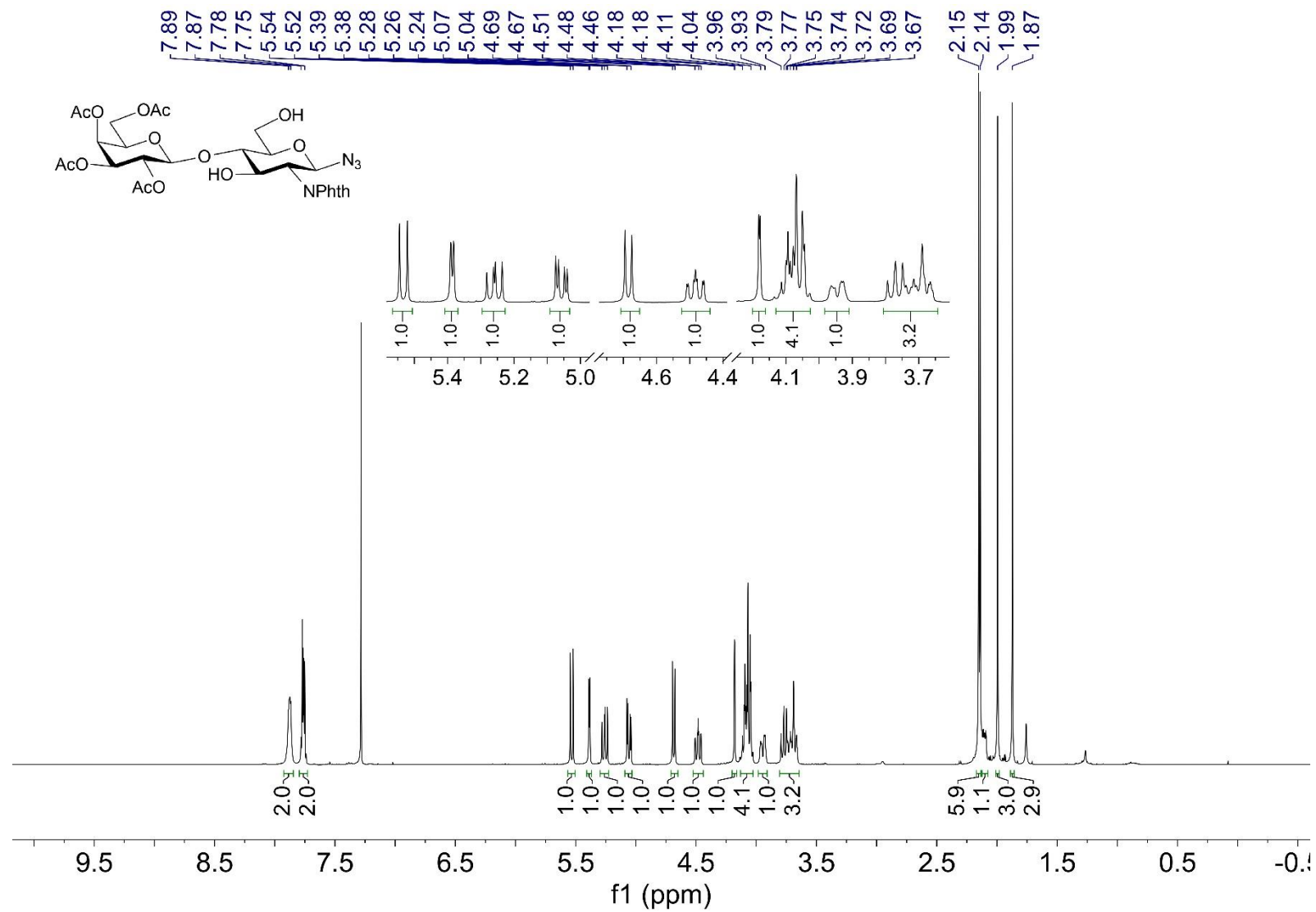


^1H - ^{13}C HSQCTOCSY 13

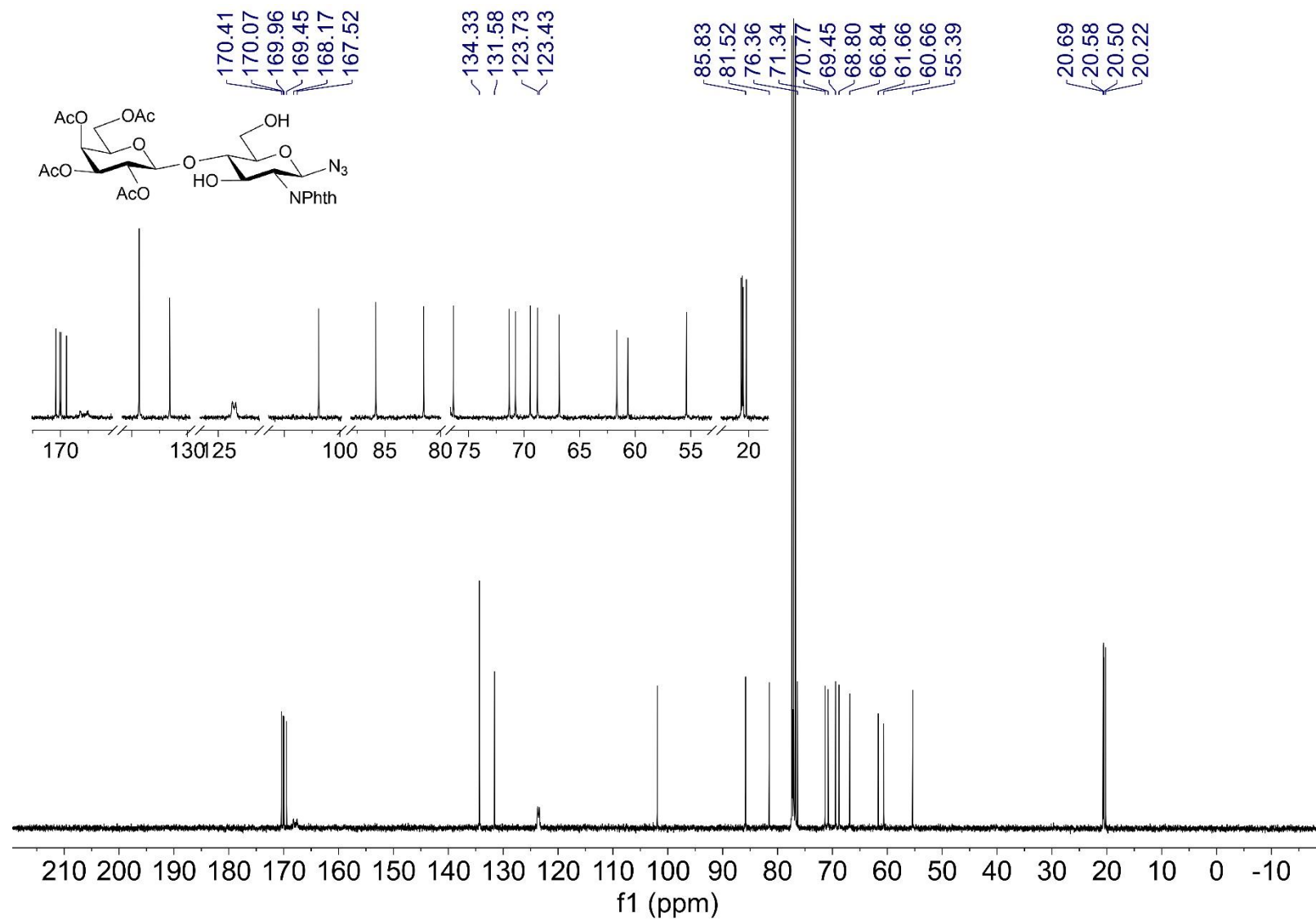


NMR COMPOUND 14

¹H NMR (400 MHz, CDCl₃) 14

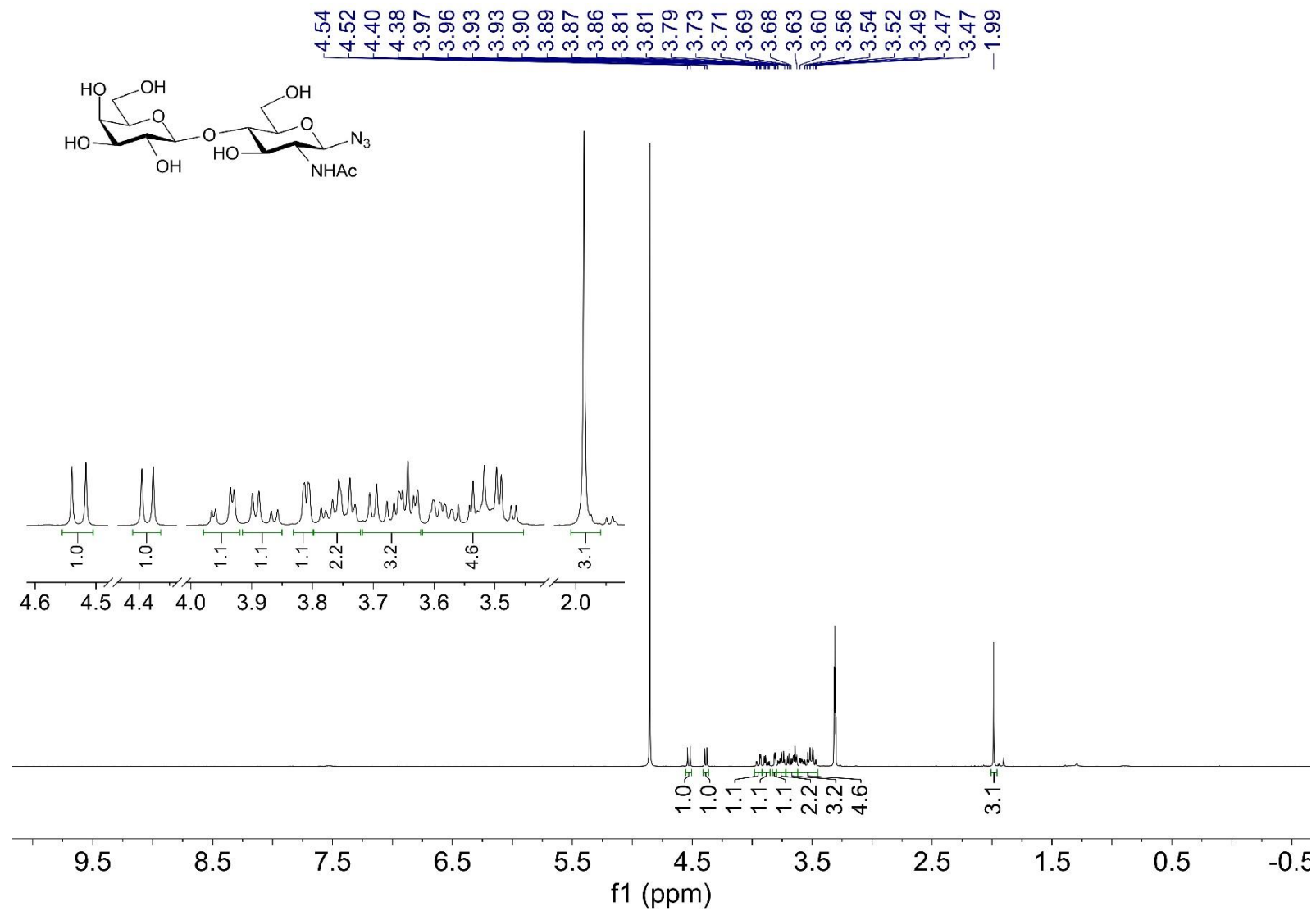


¹³C NMR (101 MHz, CDCl₃) 14

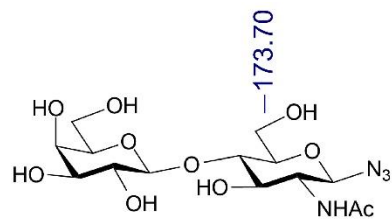


NMR COMPOUND 15

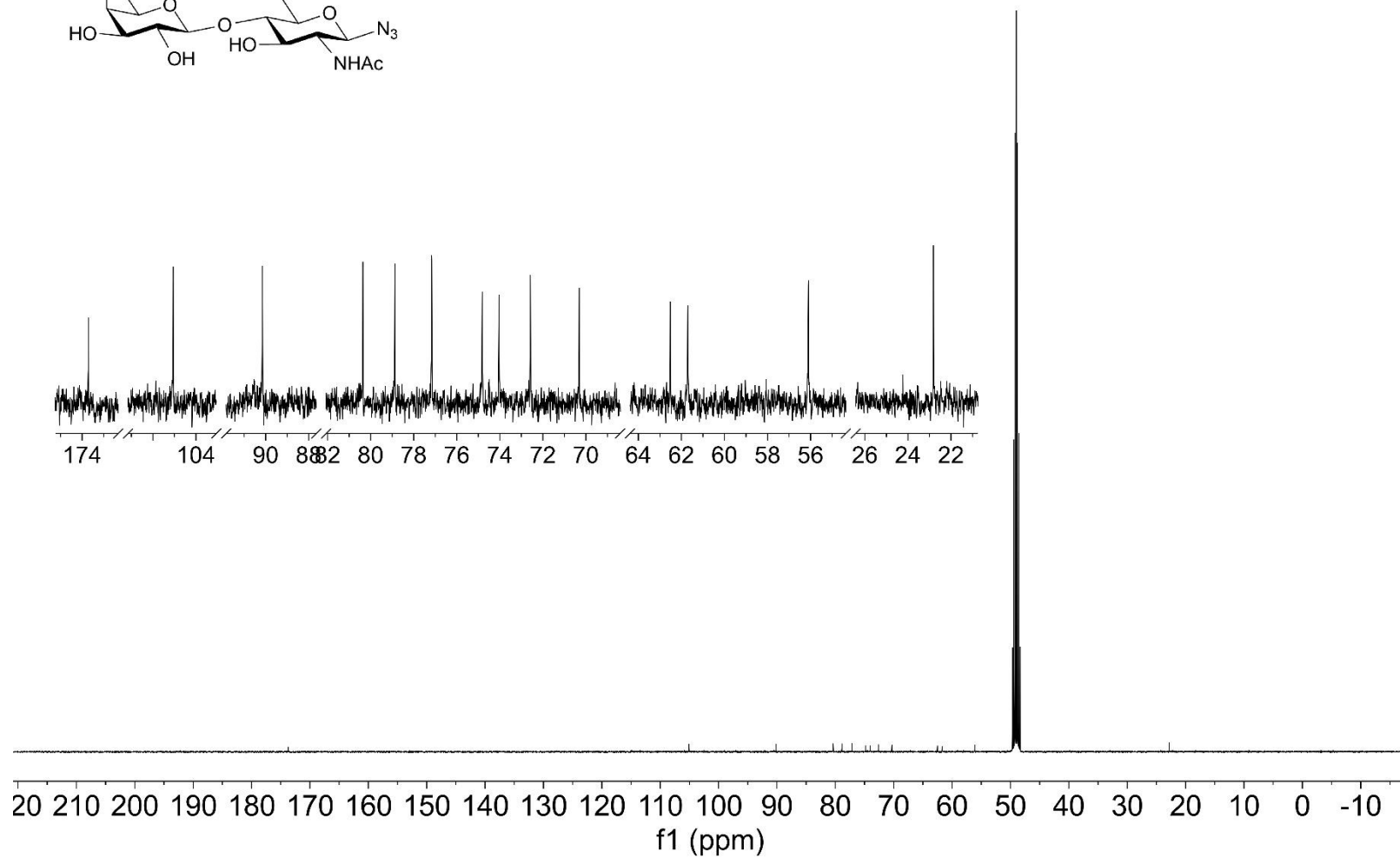
¹H NMR (400 MHz, MeOD) 15



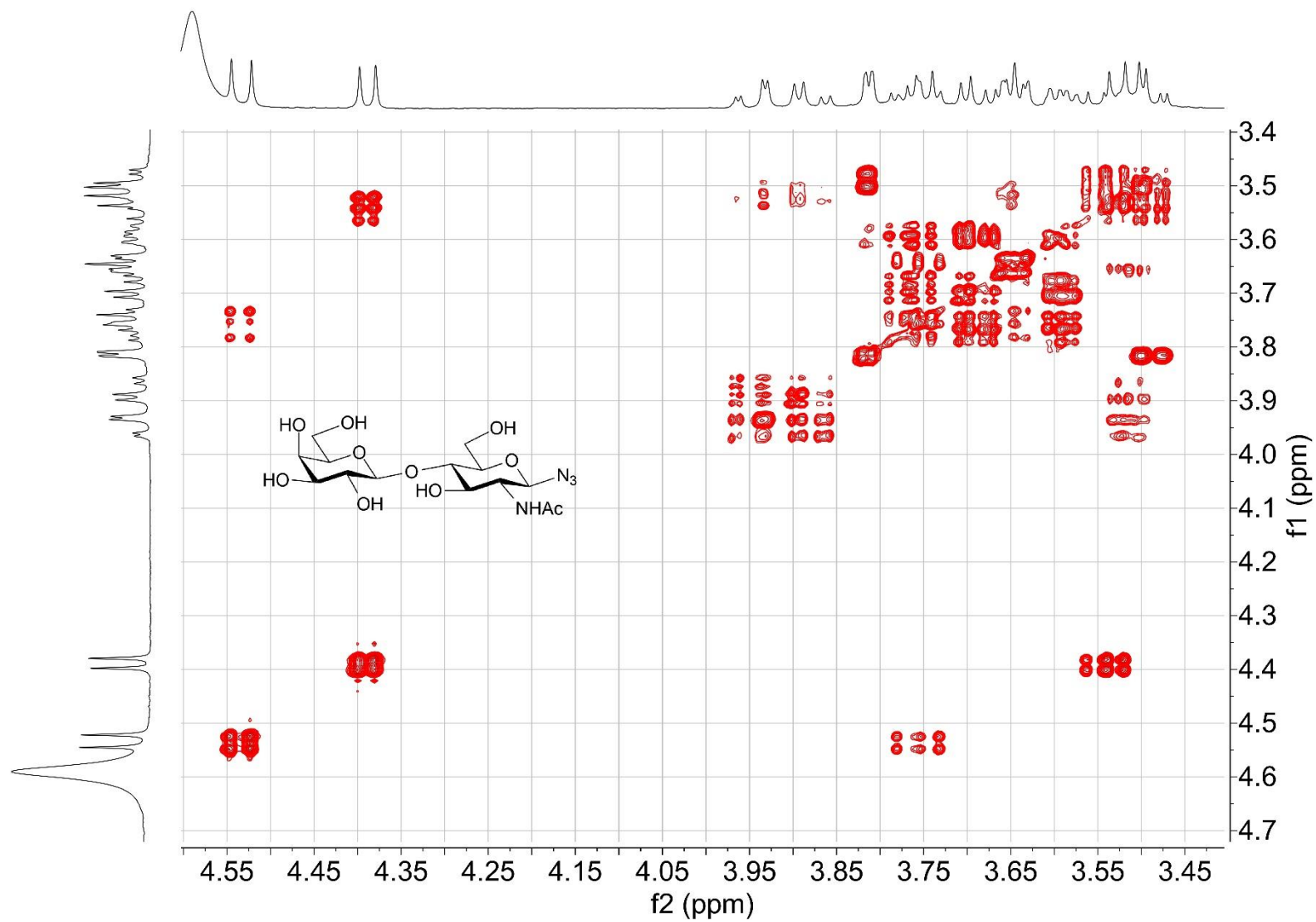
¹³C NMR (101 MHz, MeOD) 15



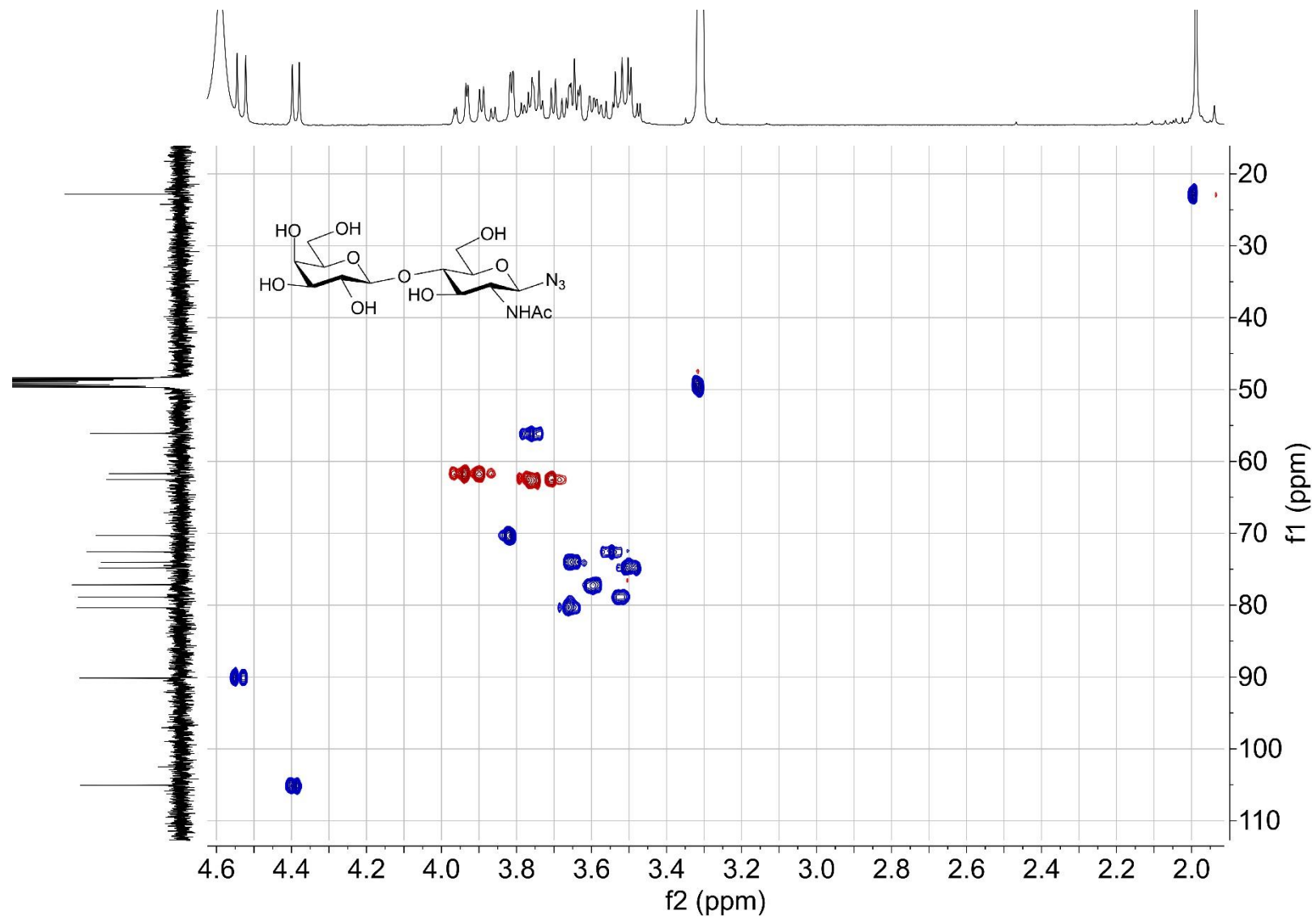
- 105.06
- 90.15
- 80.36
- 78.87
- 77.16
- 74.82
- 74.04
- 72.58
- 70.31
- 62.51
- 61.70
- 56.10
- 22.82



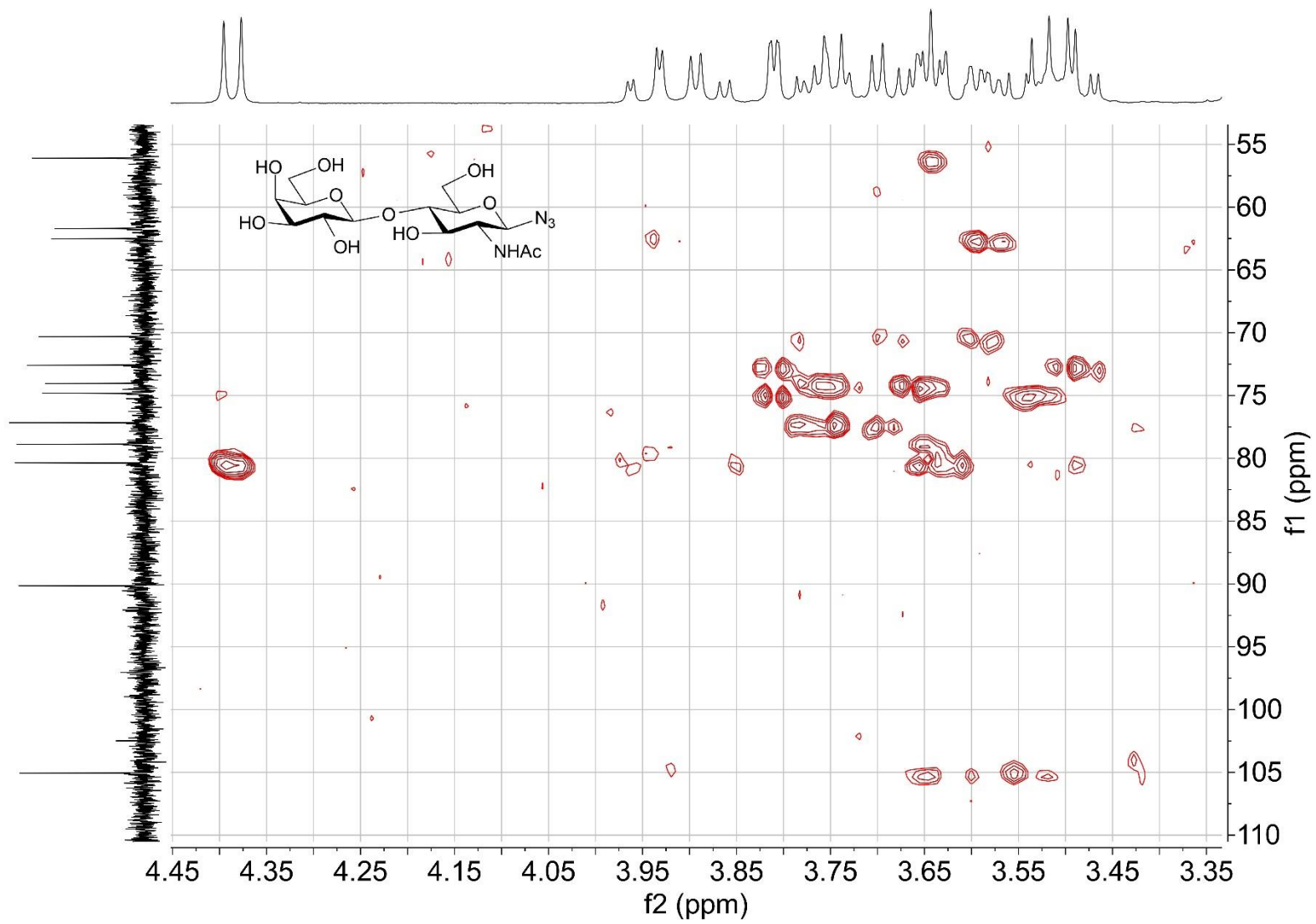
¹H-¹H COSY 15



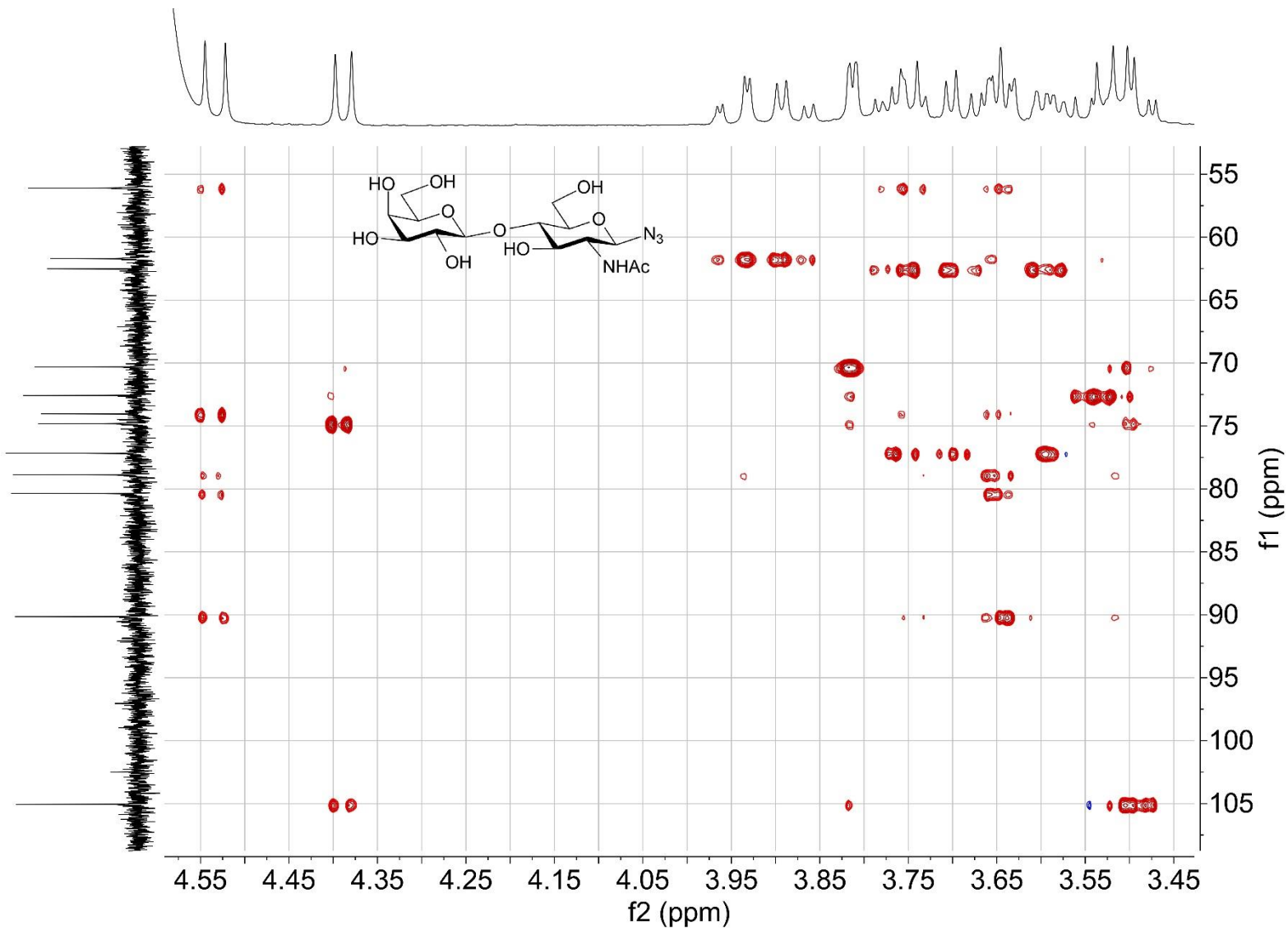
^1H - ^{13}C HSQC 15



^1H - ^{13}C HMBC 15

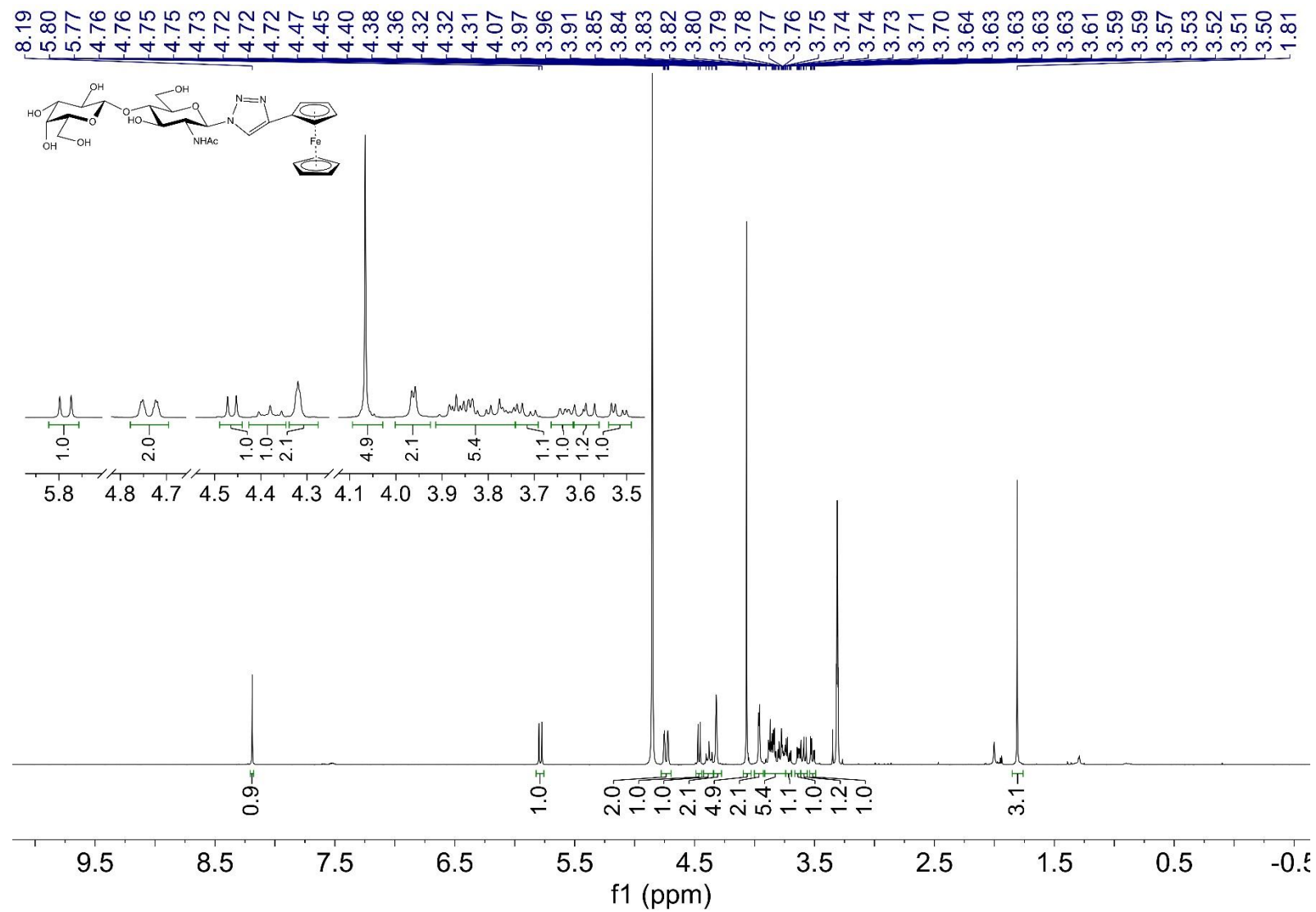


^1H - ^{13}C HSQCTOCSY 15

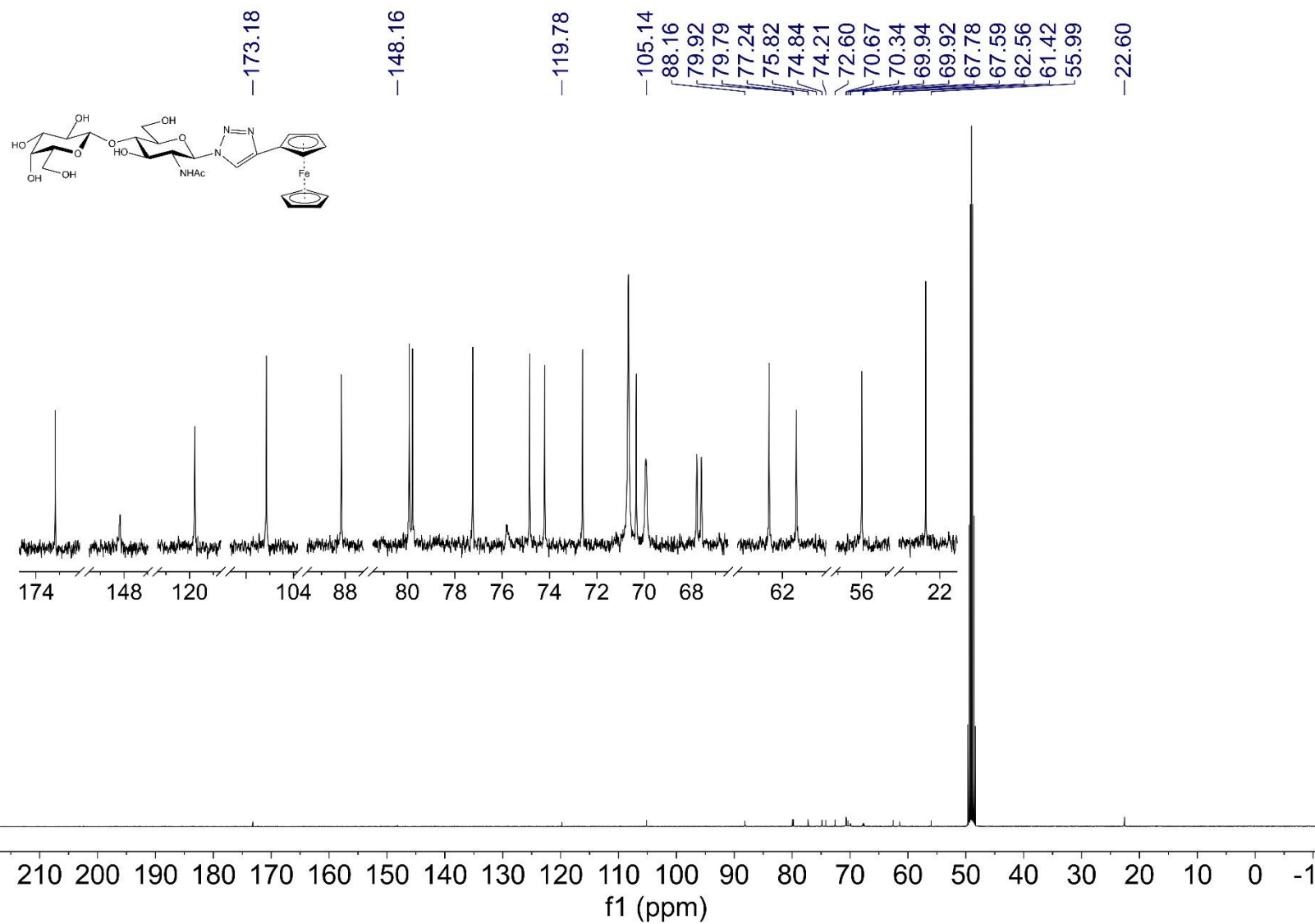


NMR COMPOUND 16

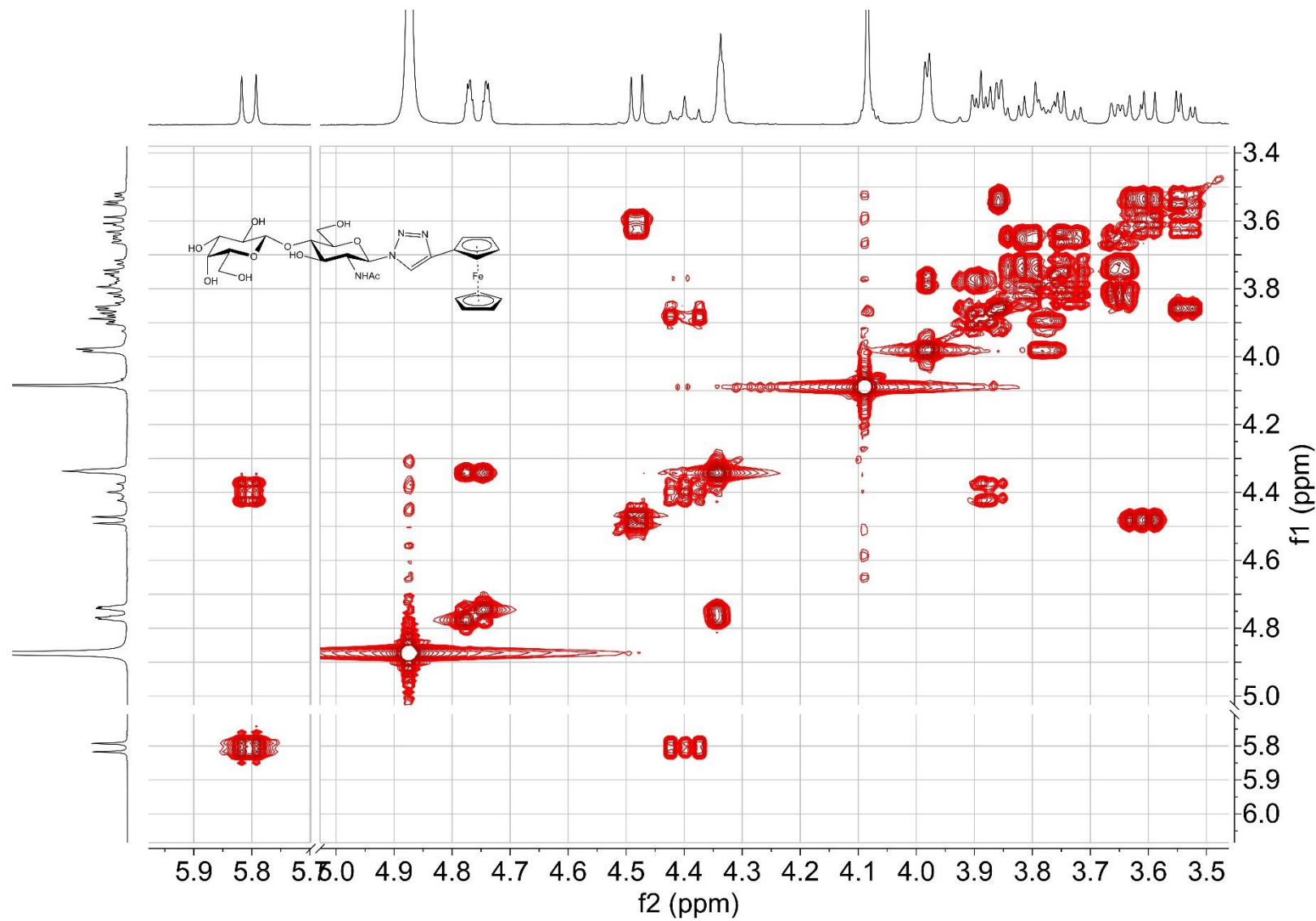
¹H NMR (400 MHz, MeOD) 16



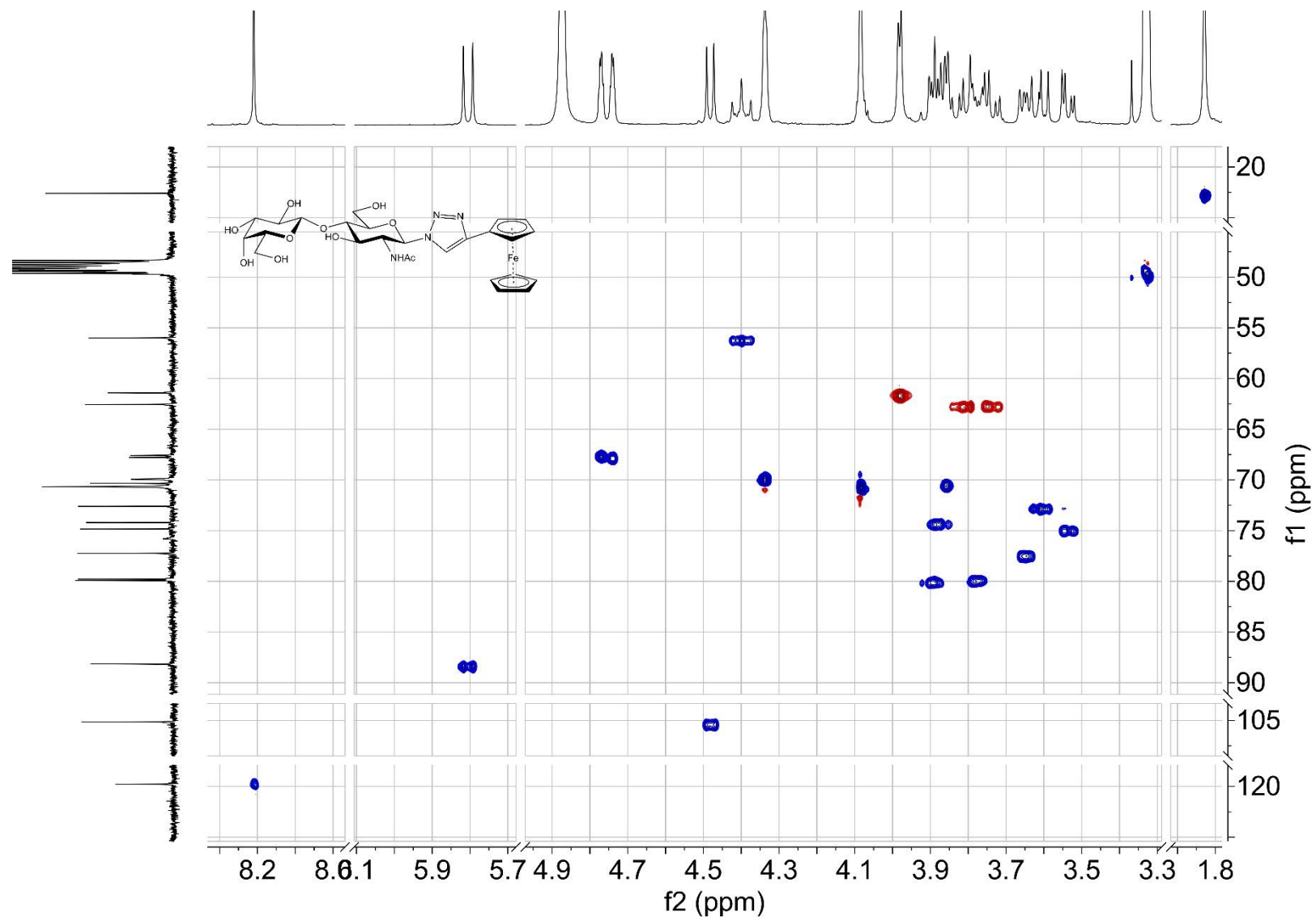
¹³C NMR (101 MHz, MeOD) 16



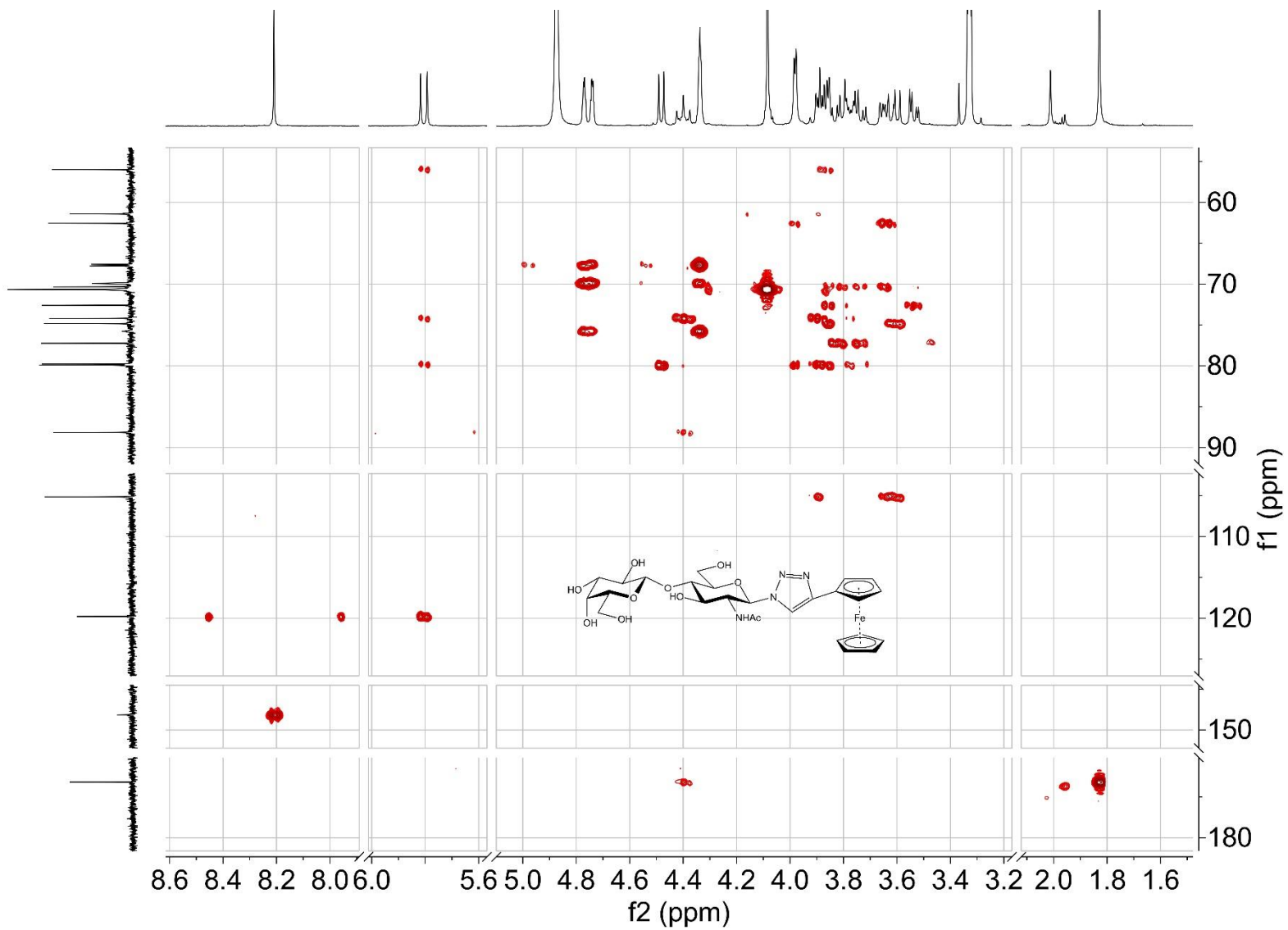
¹H-¹H COSY 16



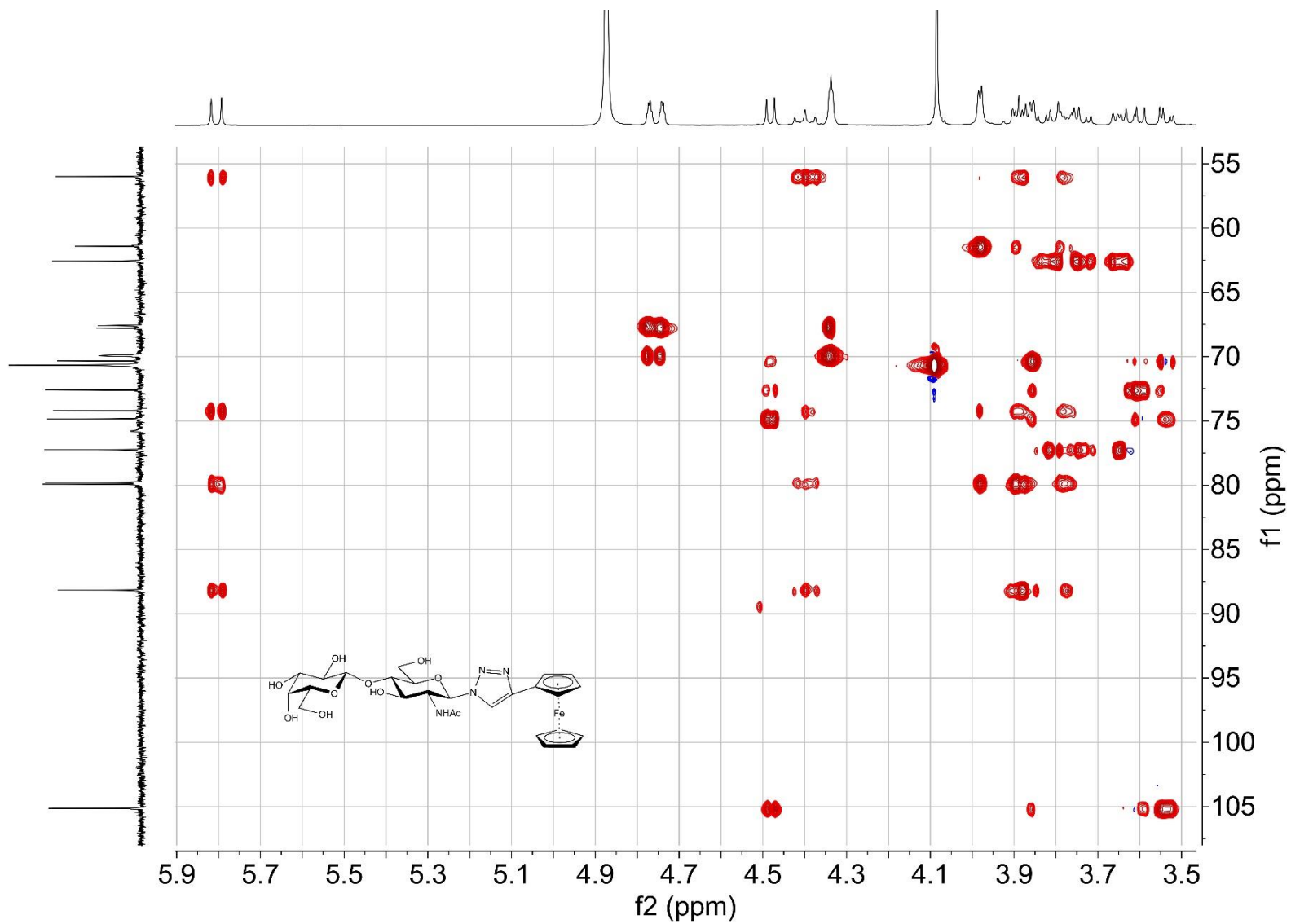
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^1H - ^{13}C HMBC 16

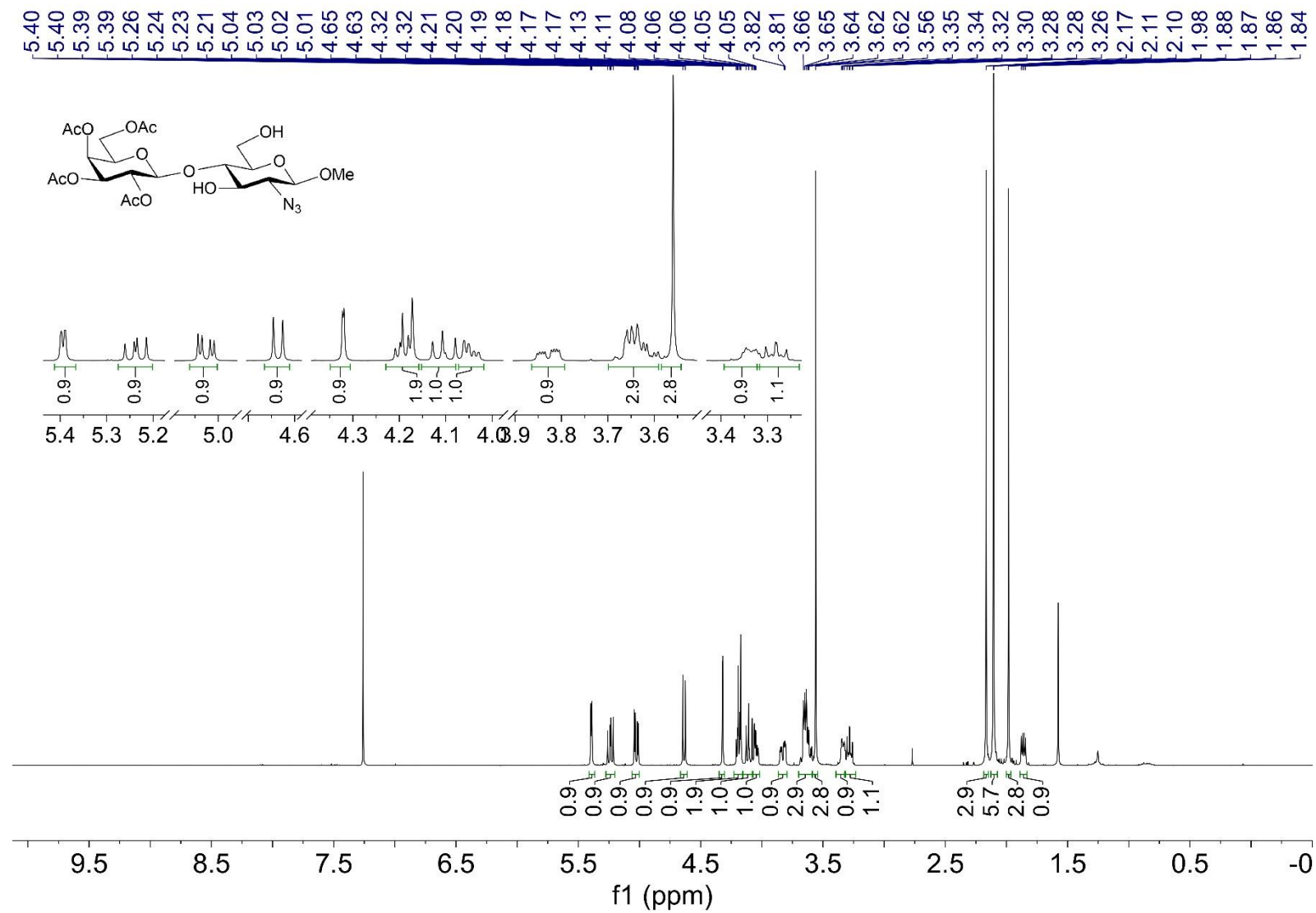


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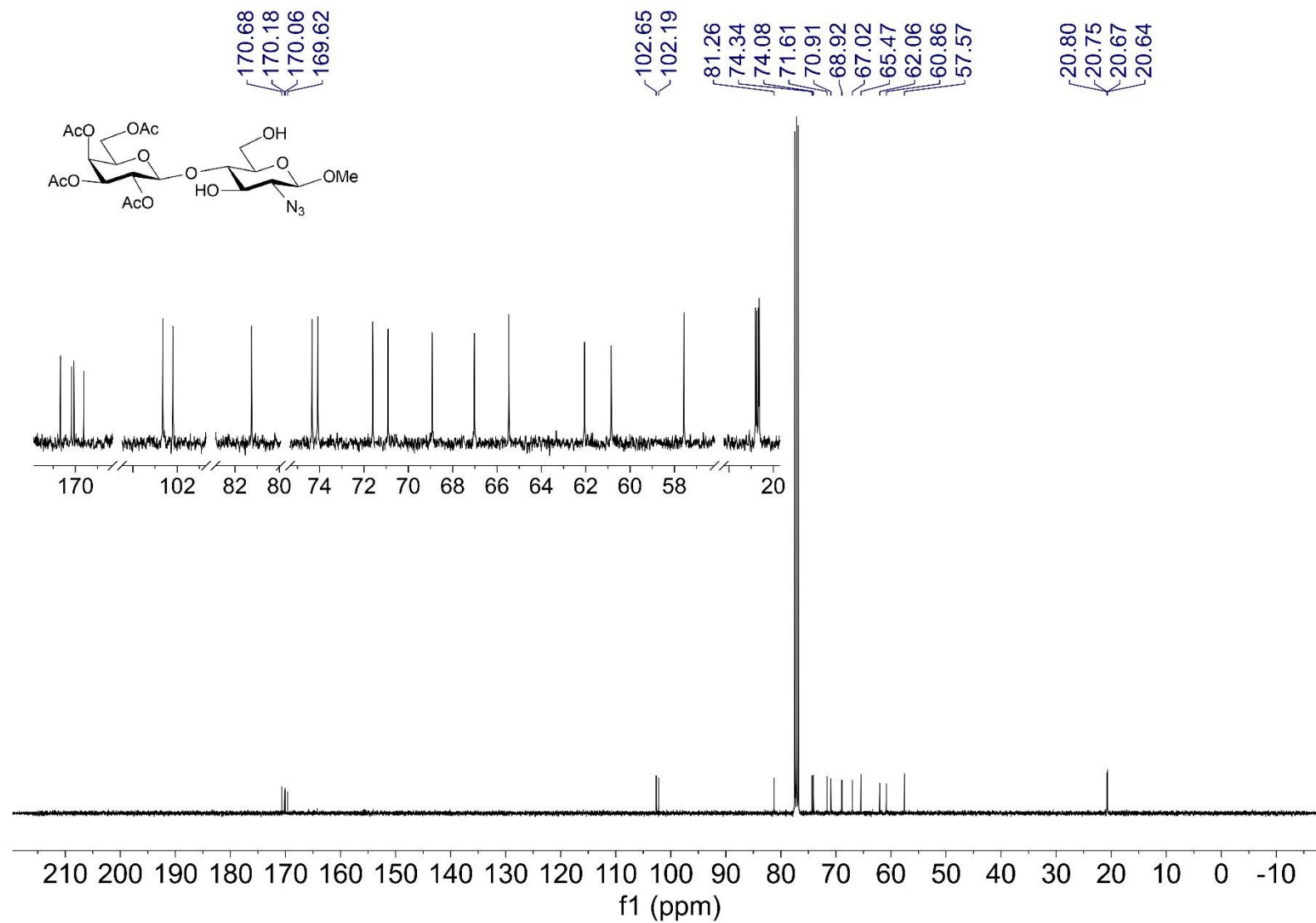


NMR COMPOUND 18

¹H NMR (400 MHz, CDCl₃) 18

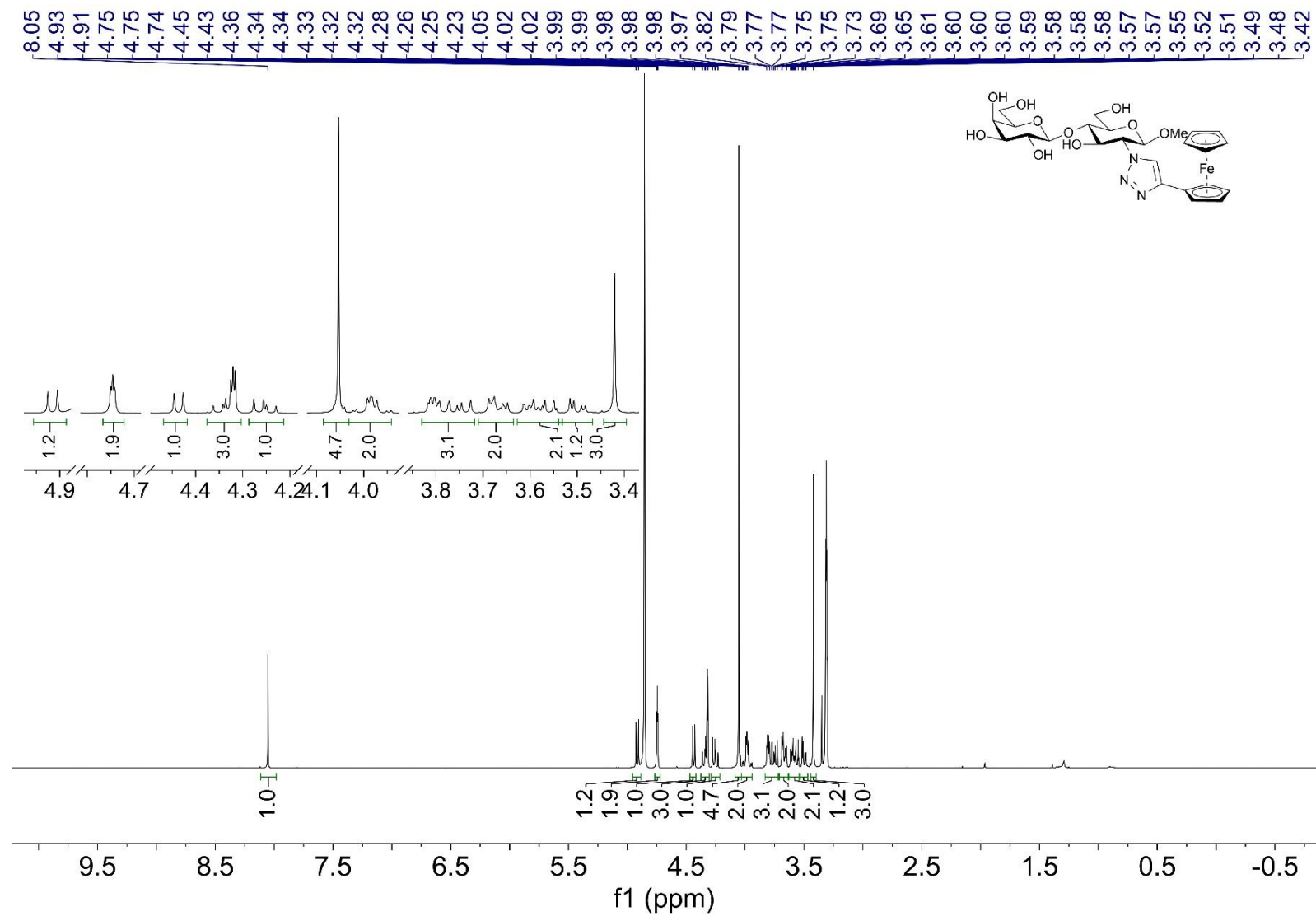


¹³C NMR (101 MHz, CDCl₃) 18

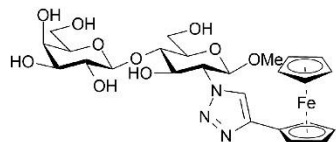


NMR COMPOUND 19

¹H NMR (400 MHz, MeOD) 19



¹³C NMR (101 MHz, MeOD) 19



— 147.36

— 122.79

~ 105.29

~ 102.82

81.00

77.14

76.74

76.04

74.85

74.00

72.64

70.59

70.30

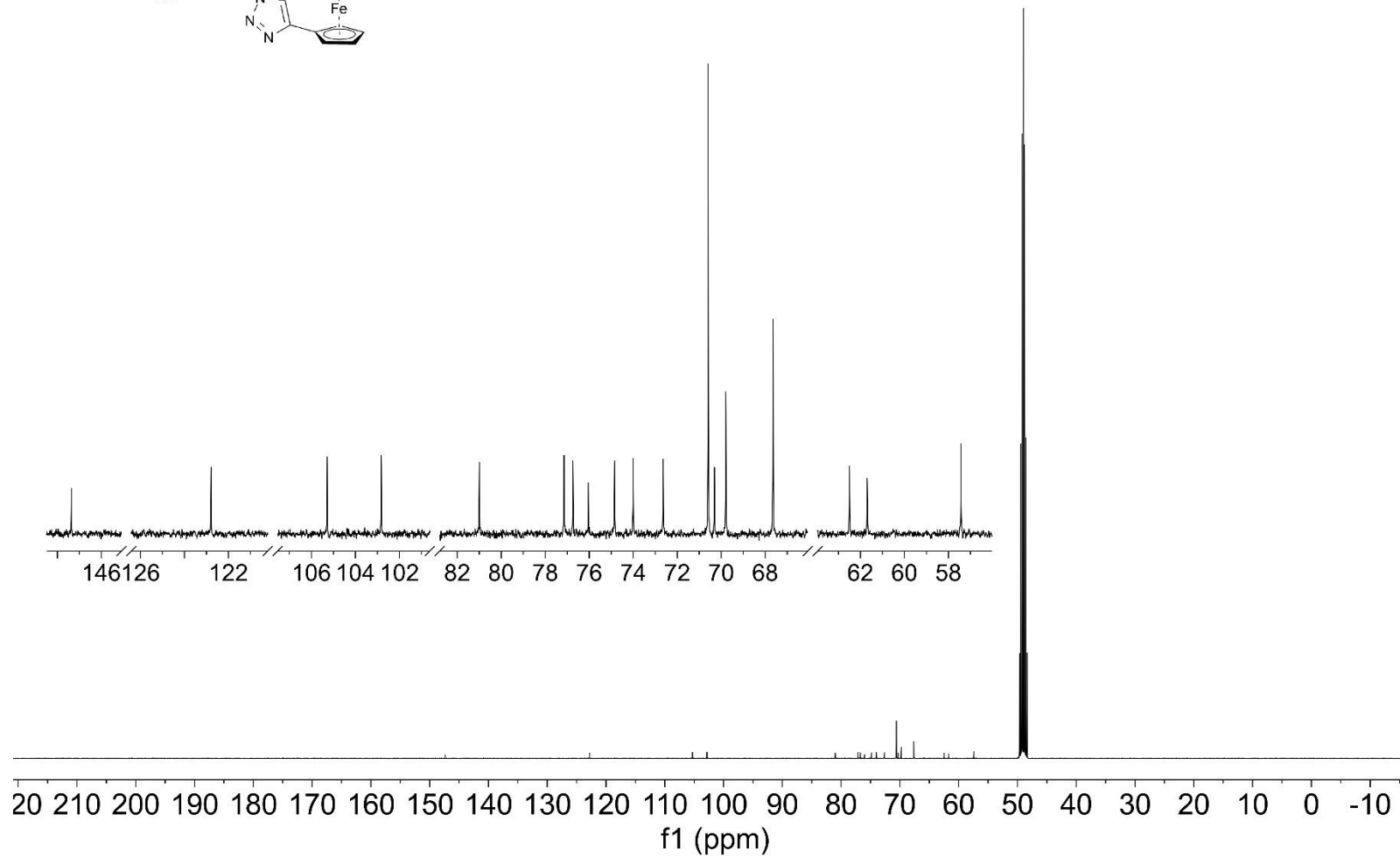
69.79

67.64

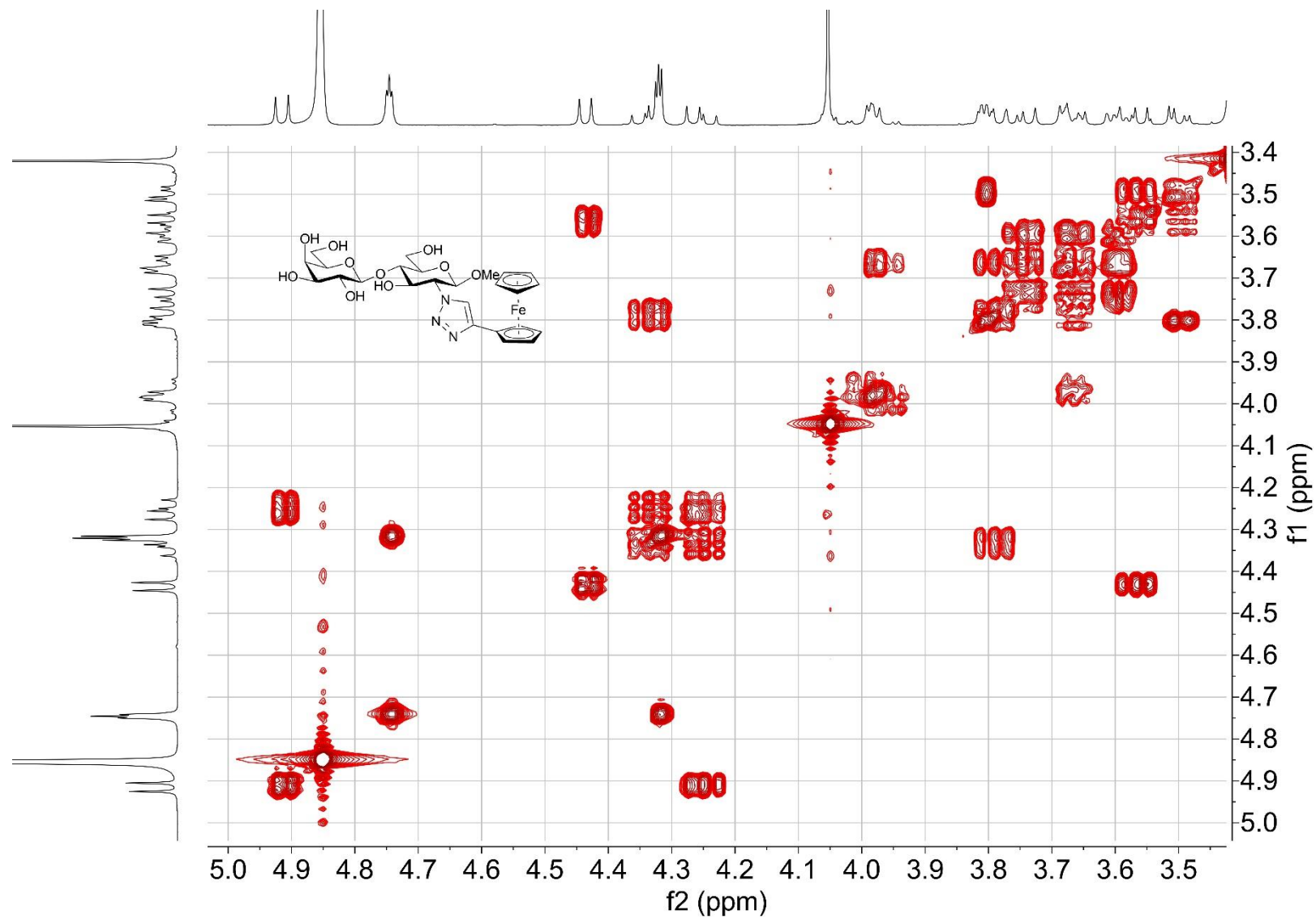
62.50

61.69

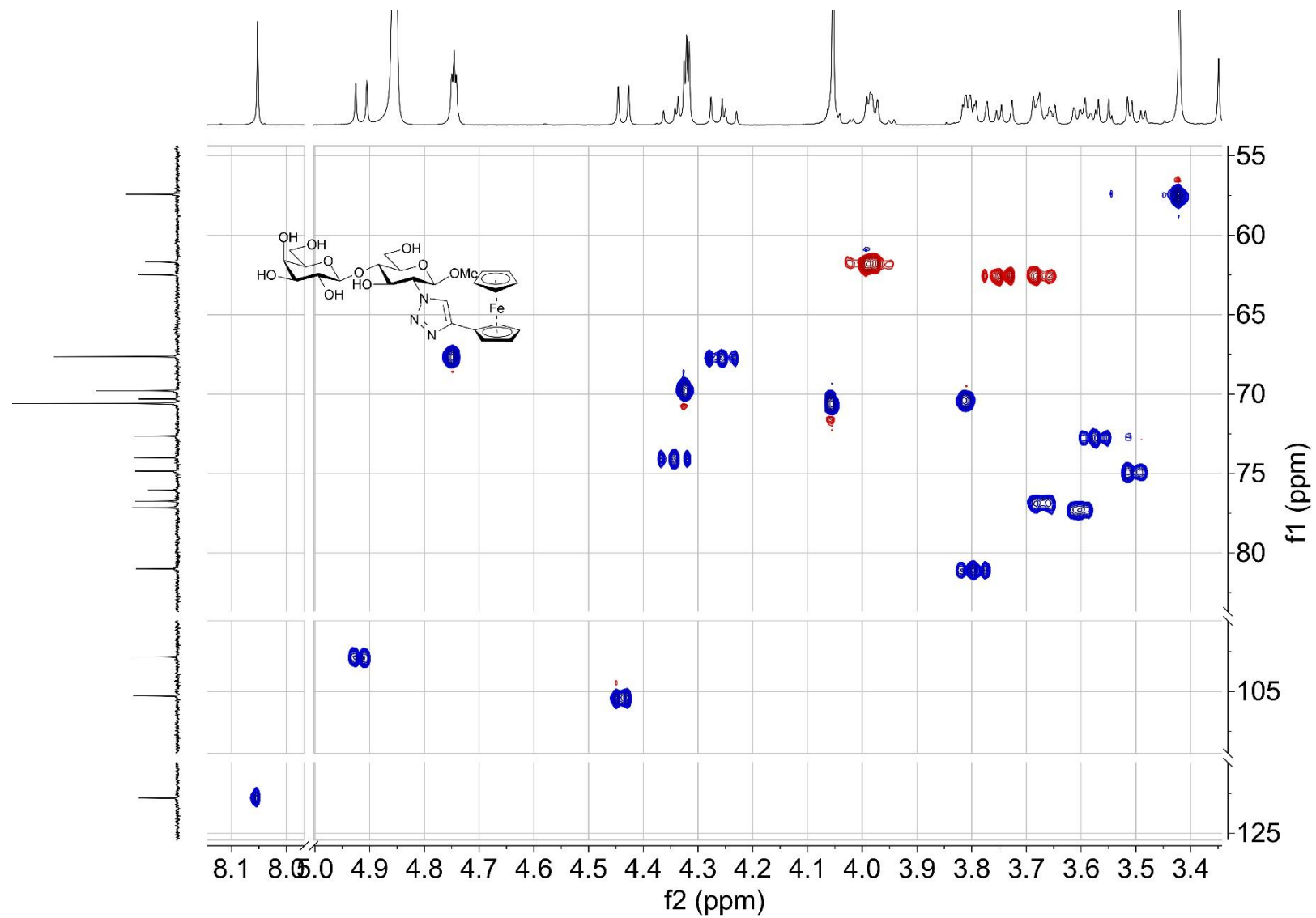
57.43



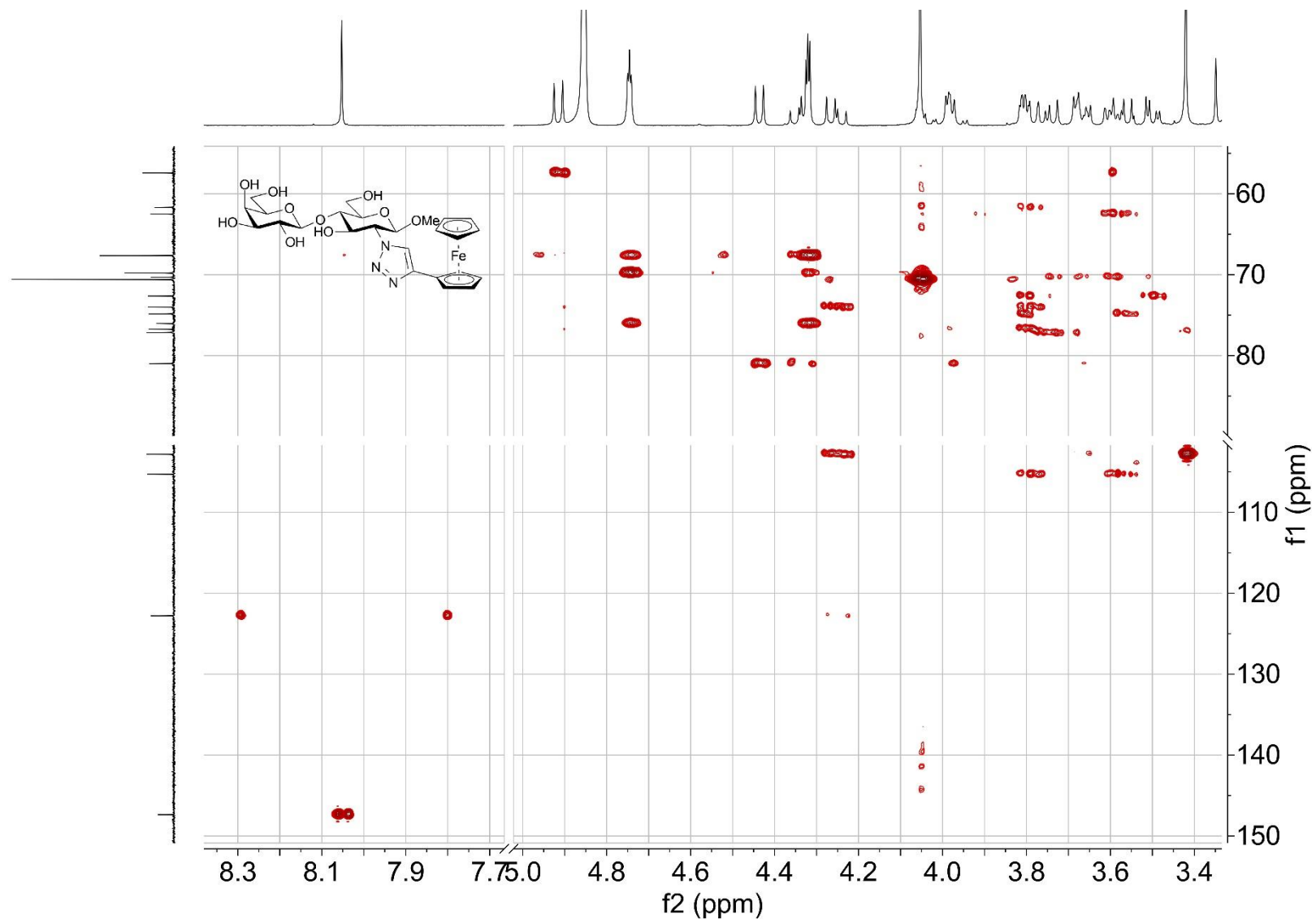
¹H-¹H COSY 19



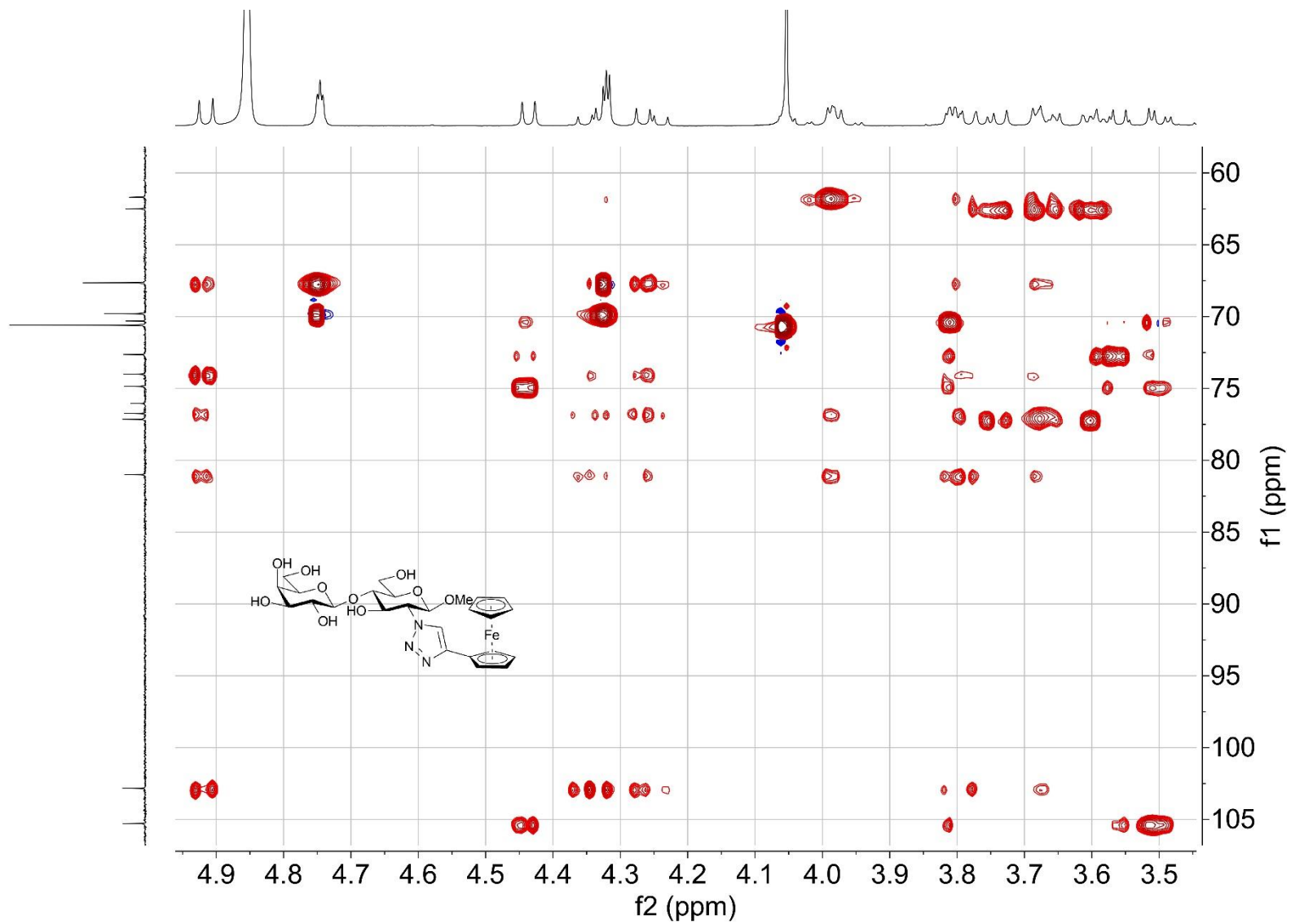
^1H - ^{13}C HSQC 19



¹H-¹³C HMBC 19

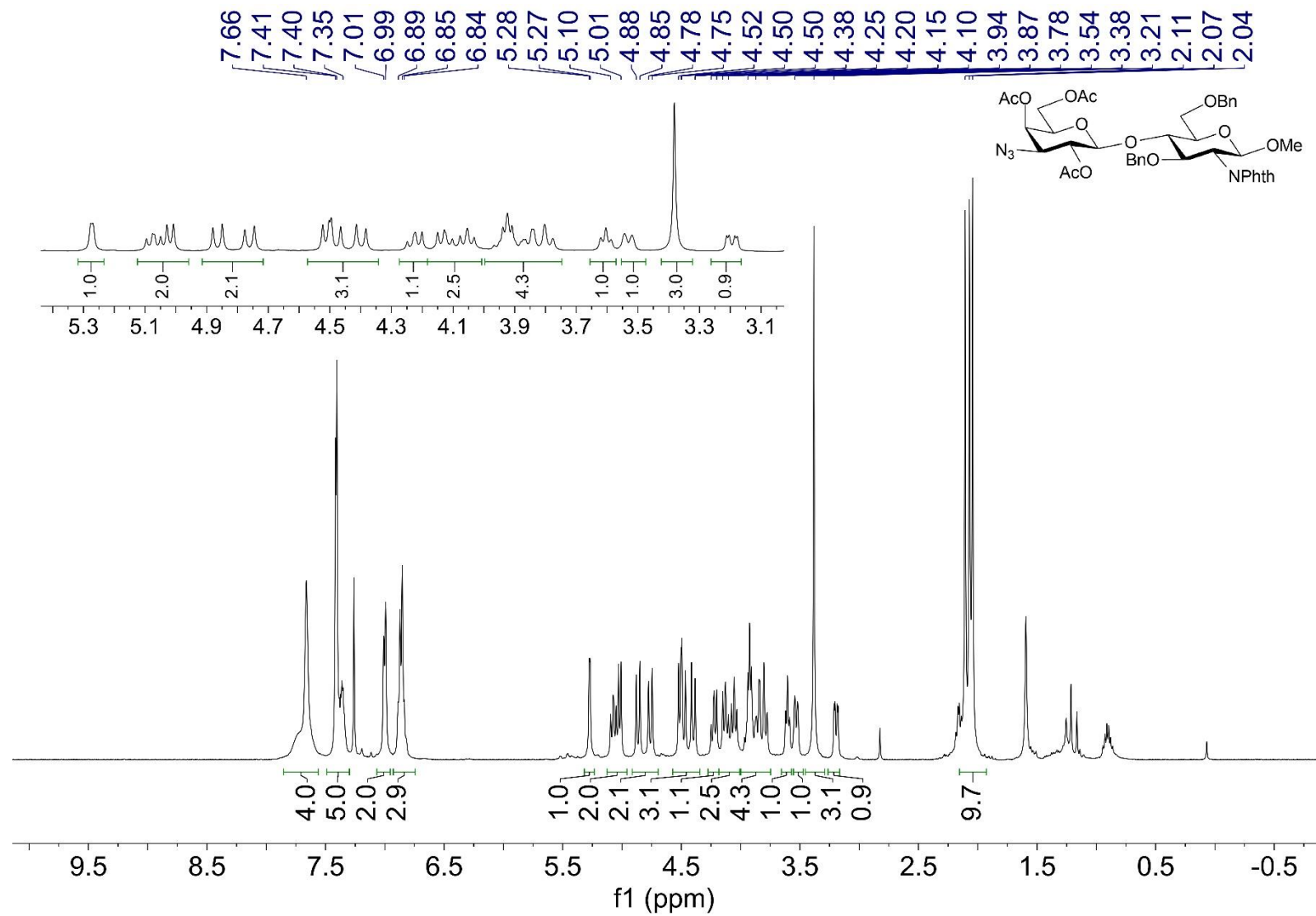


^1H - ^{13}C HSQTOCSY 19



NMR COMPOUND 22

¹H NMR (400 MHz, CDCl₃) 22

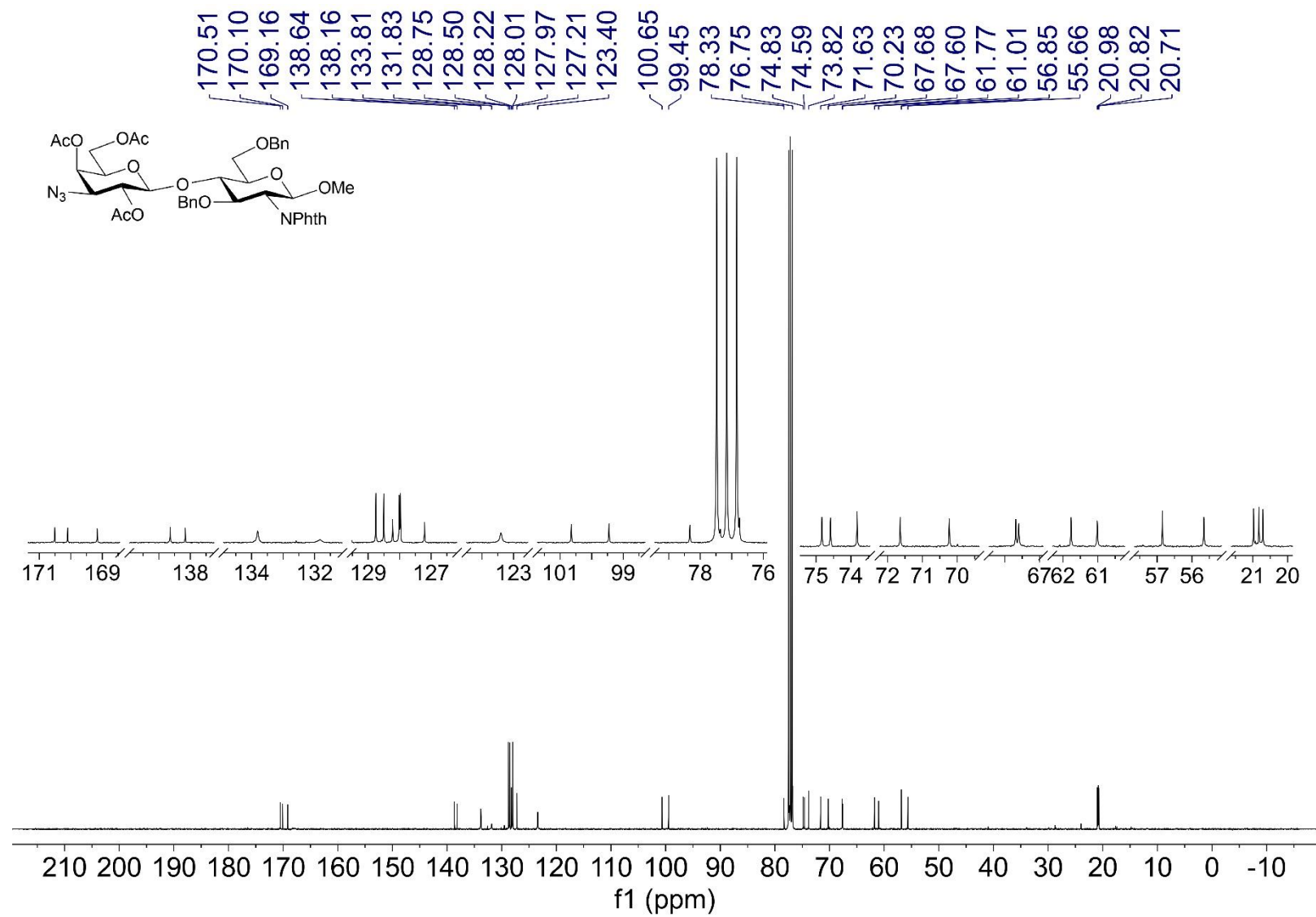


7.66
7.41
7.40
7.35
7.01
6.99
6.89
6.85
6.84
5.28
5.27
5.10
5.01
4.88
4.85
4.78
4.75
4.52
4.50
4.50
4.38
4.25
4.20
4.15
4.10
3.94
3.87
3.78
3.54
3.38
3.21
2.11
2.07
2.04

1.0
2.0
2.1
3.1
1.1
2.5
4.3
1.0
1.0
3.0
0.9

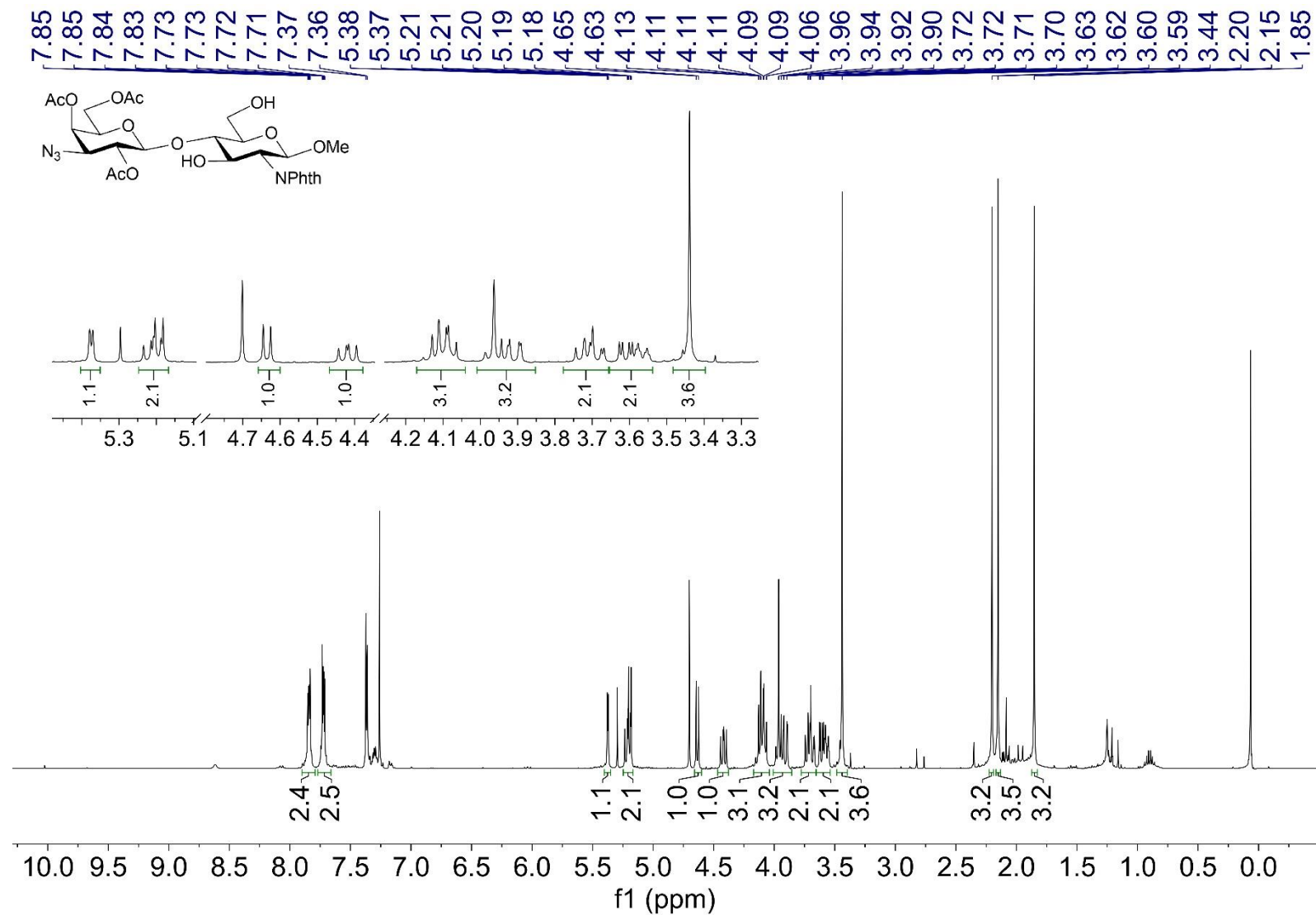
4.0
5.0
2.0
2.9
1.0
2.0
2.1
3.1
1.1
2.5
4.3
1.0
1.0
3.1
0.9
9.7

¹³C NMR (101 MHz, CDCl₃) 22

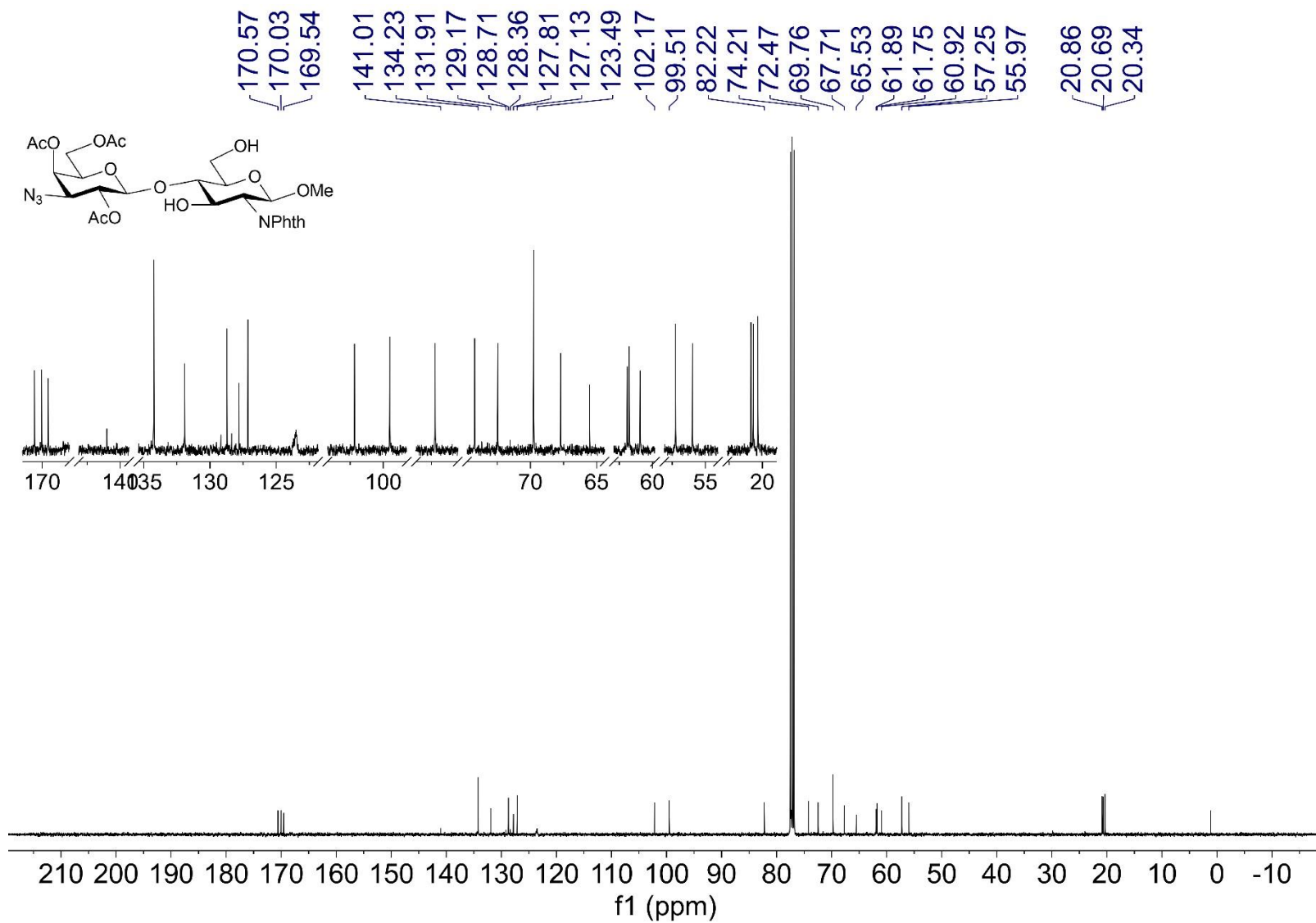


NMR COMPOUND 23

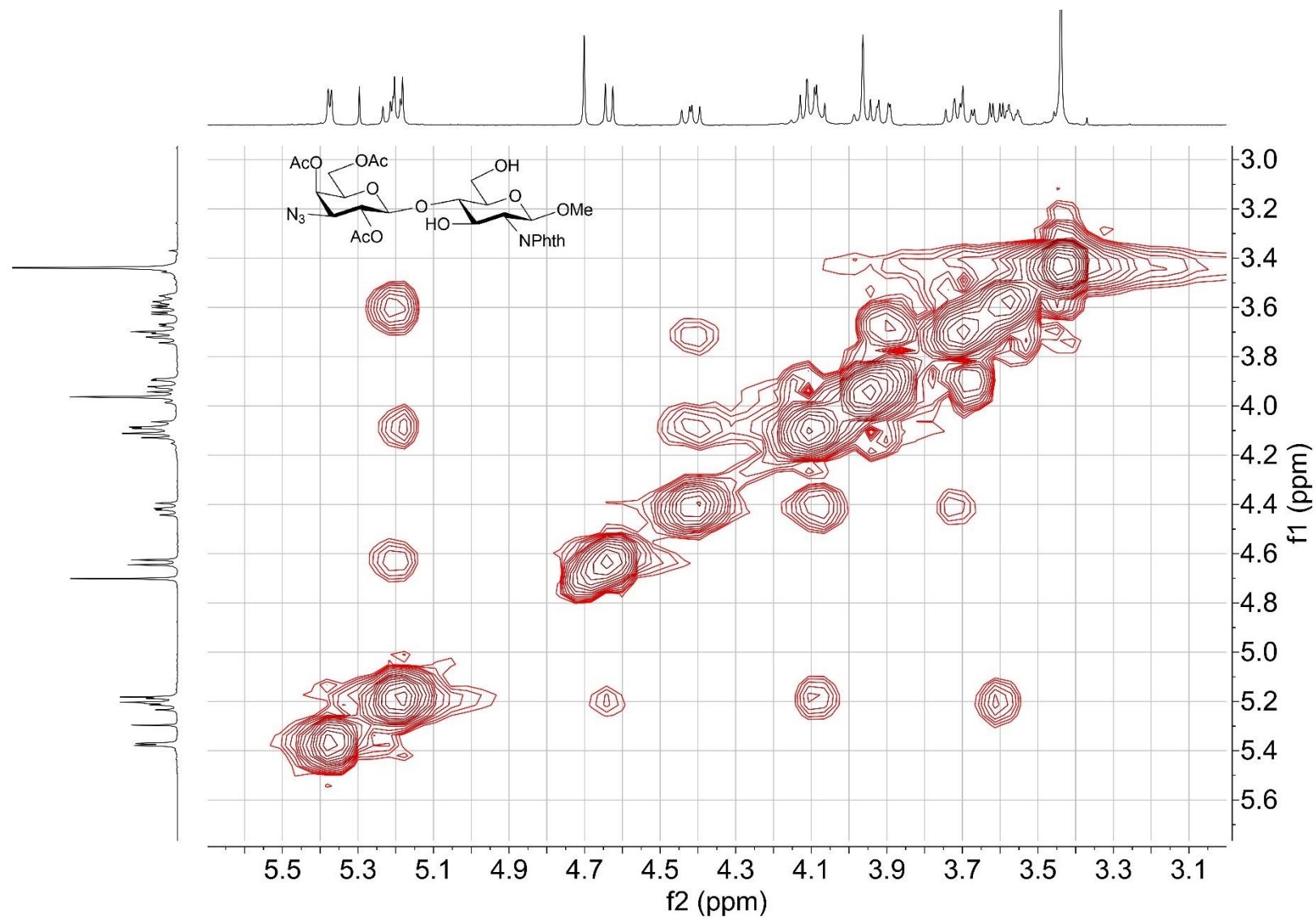
¹H NMR (400 MHz, CDCl₃) 23



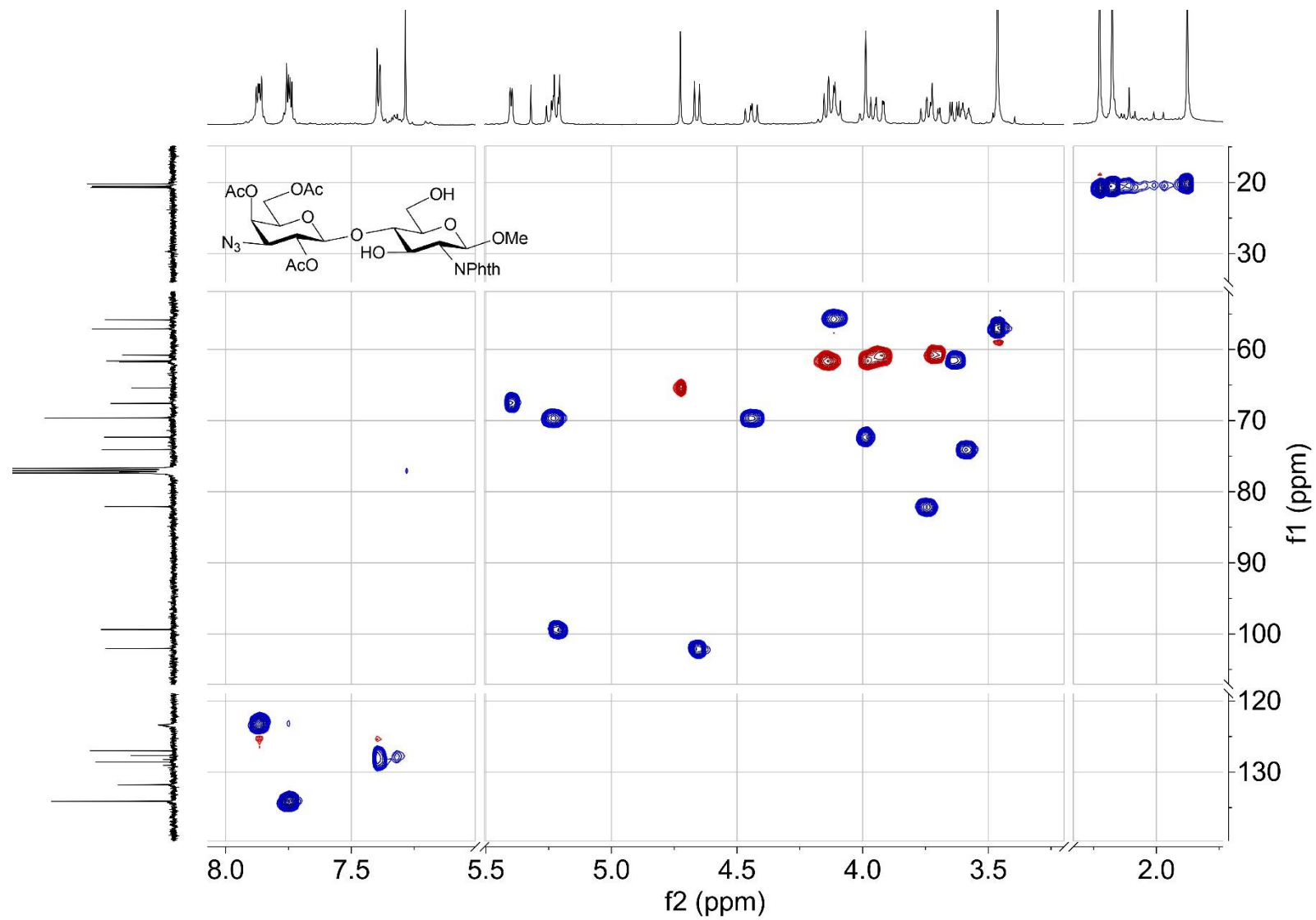
¹³C NMR (101 MHz, CDCl₃) 23



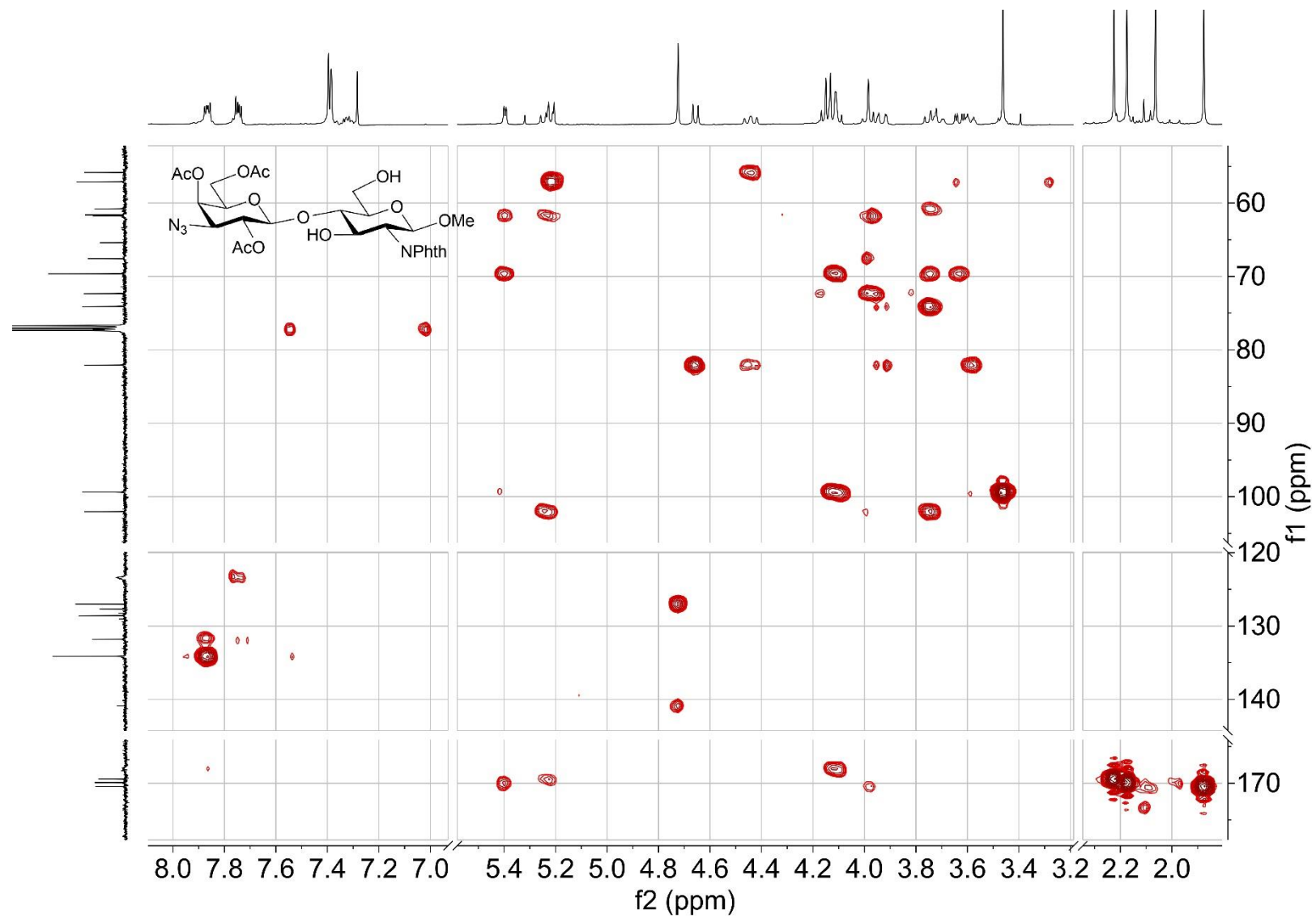
¹H-¹H COSY 23



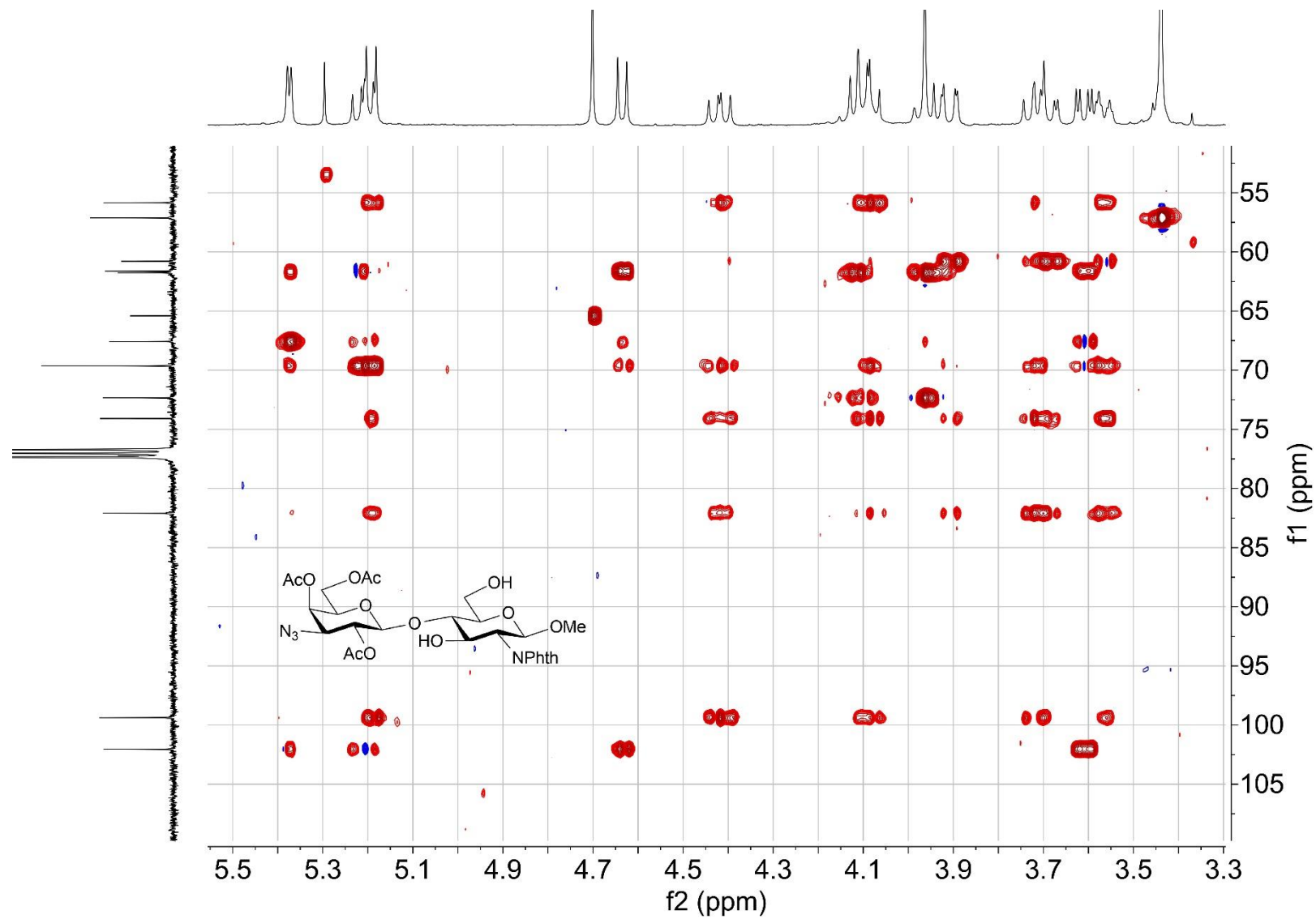
^1H - ^{13}C HSQC 23



^1H - ^{13}C HMBC 23

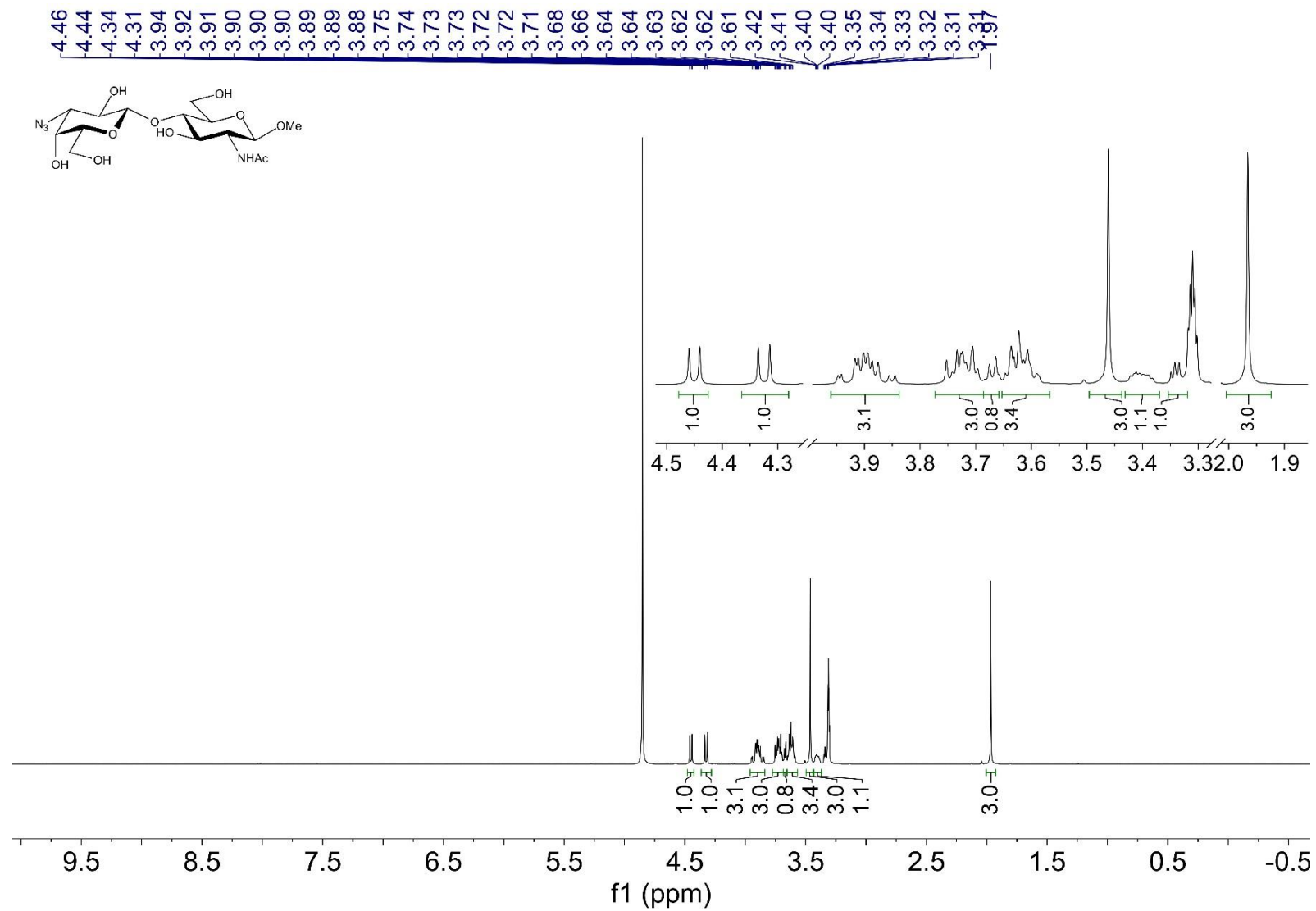


^1H - ^{13}C HSQCTOCSY 23



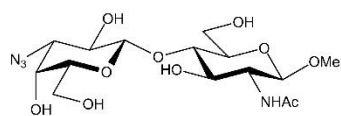
NMR COMPOUND 24

¹H NMR (400 MHz, MeOD) 24



¹³C NMR (101 MHz, MeOD) 24

173.58

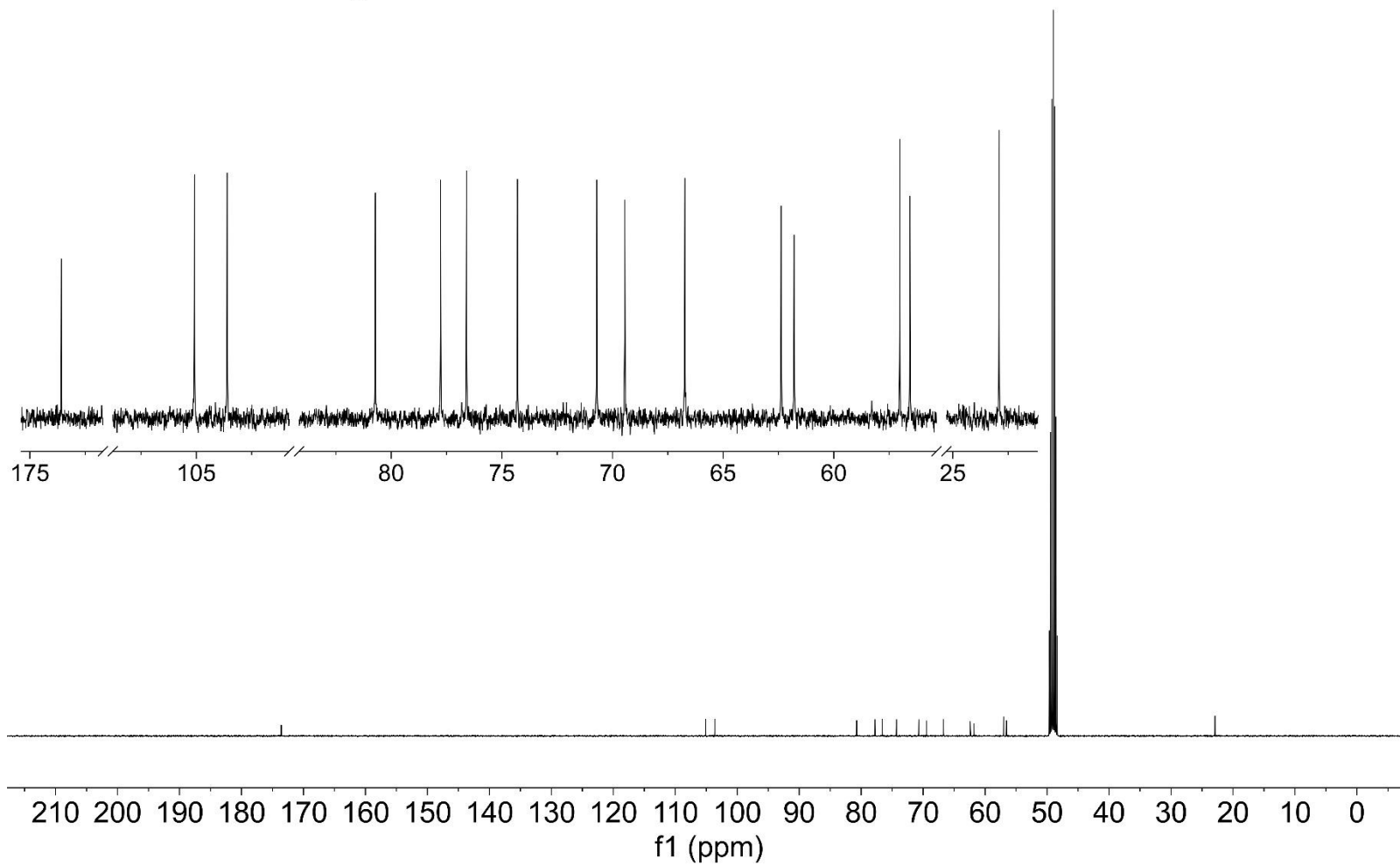


105.08

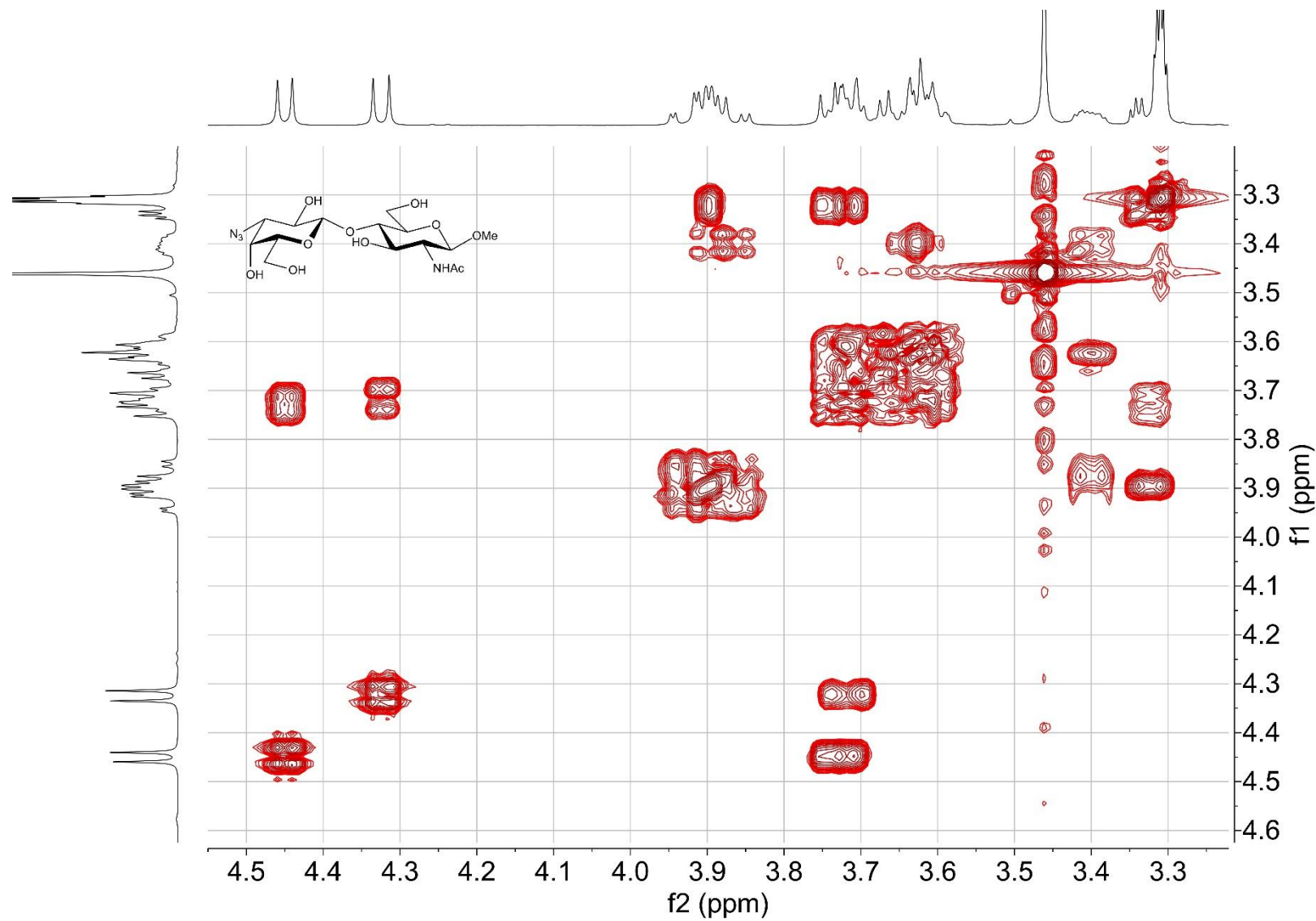
103.61

80.72
77.77
76.60
74.29
70.71
69.44
66.73
62.38
61.79
57.02
56.56

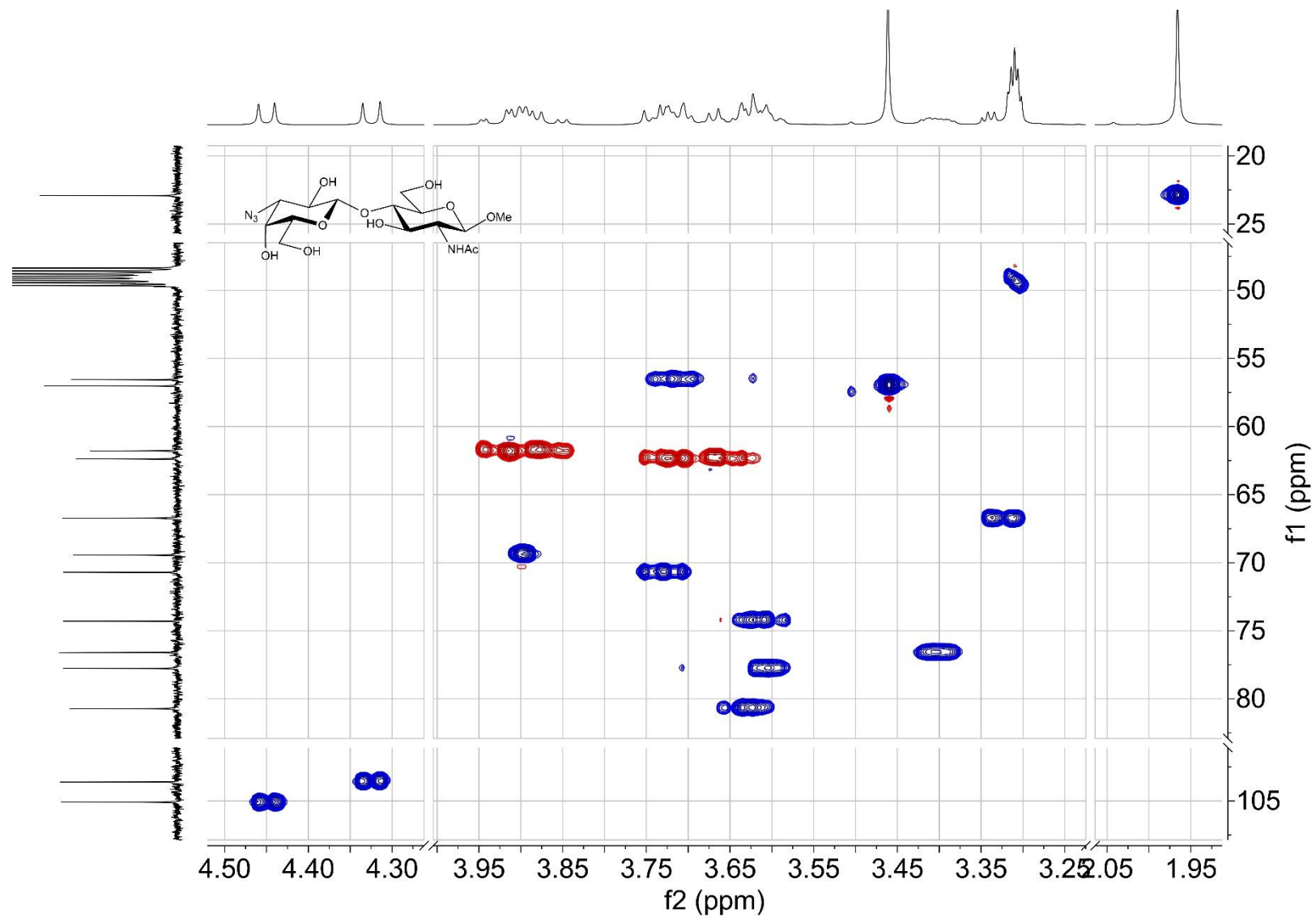
22.91



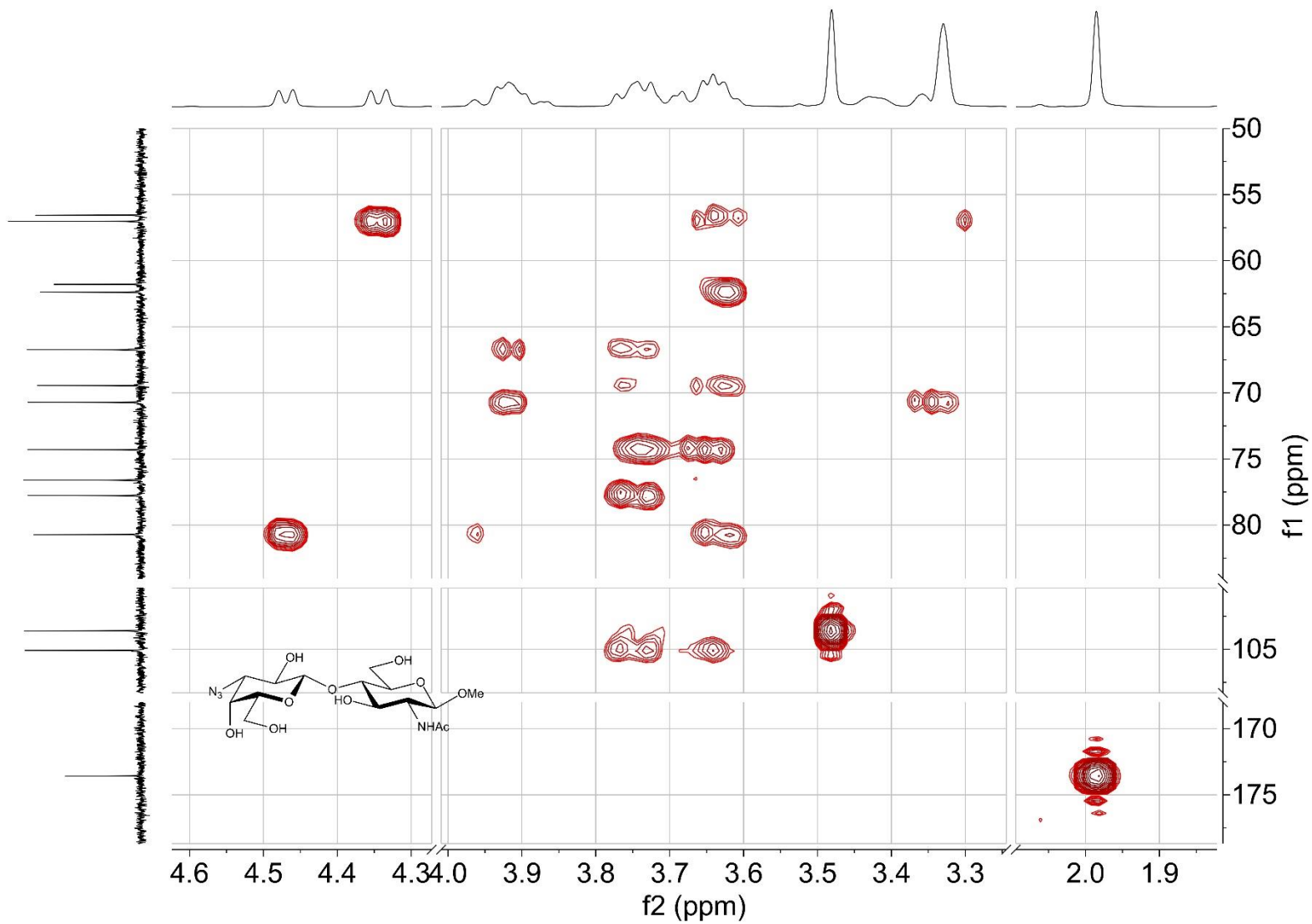
¹H-¹H COSY 24



^1H - ^{13}C HSQC 24

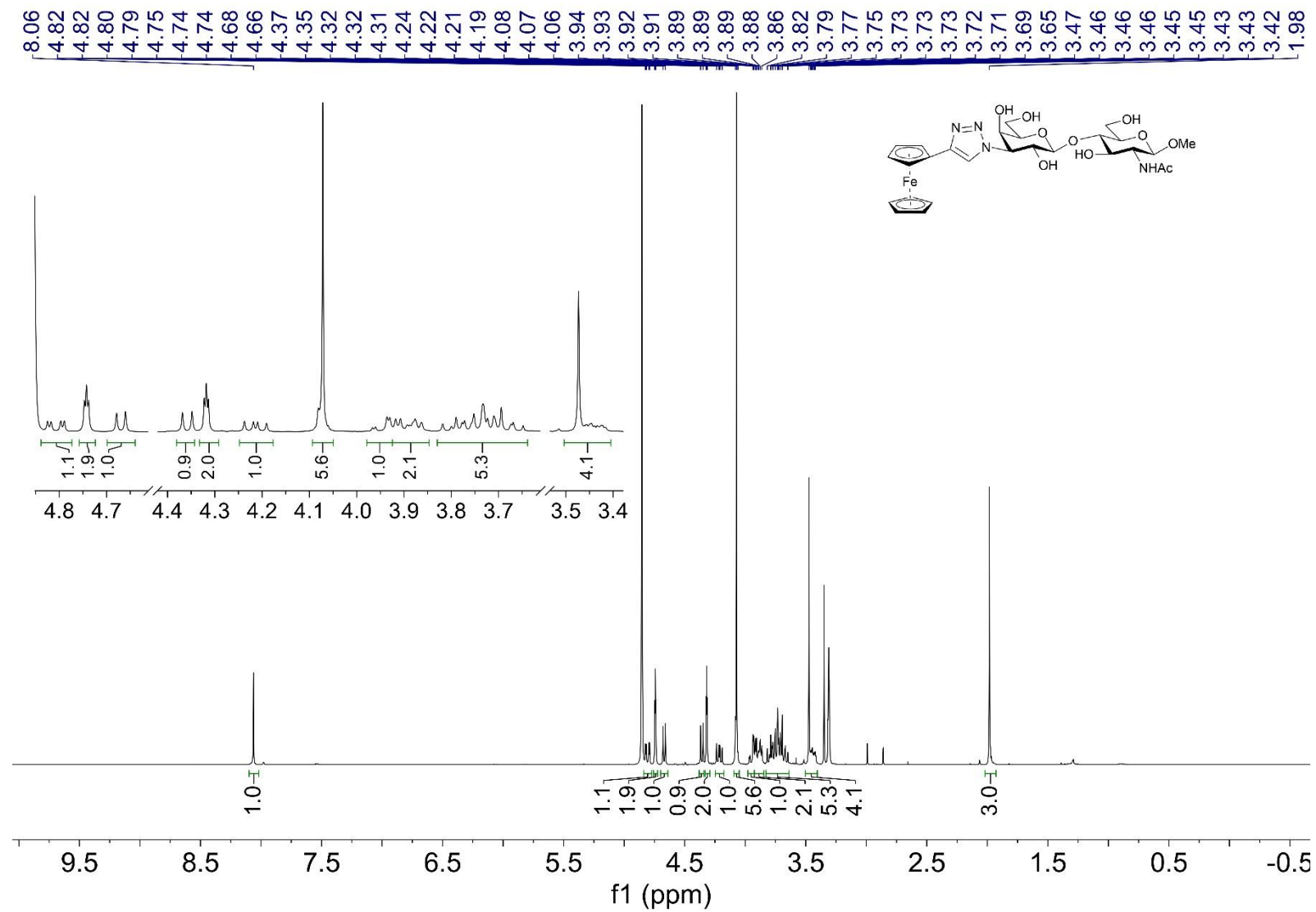


^1H - ^{13}C HMBC 24

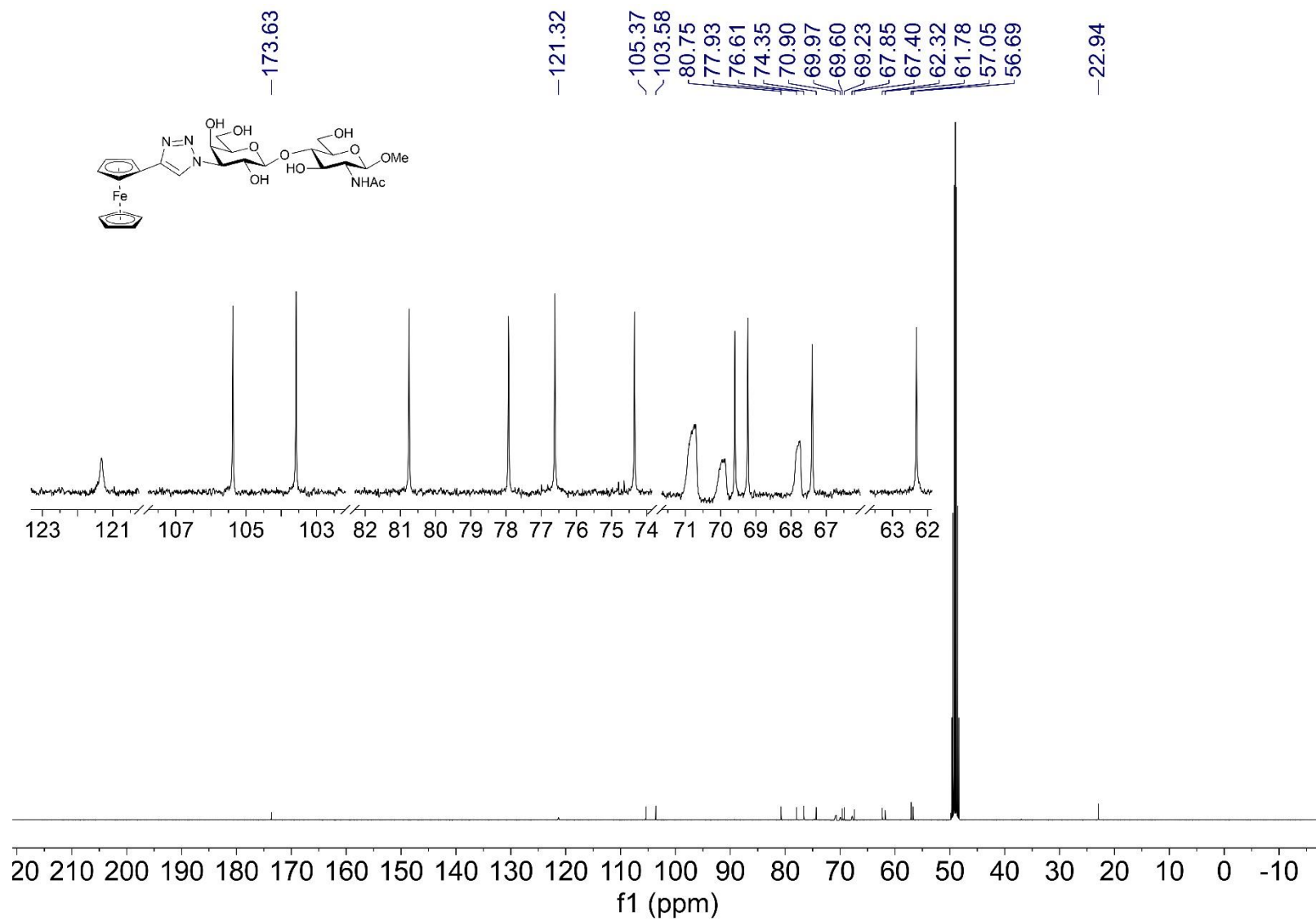


NMR COMPOUND 25

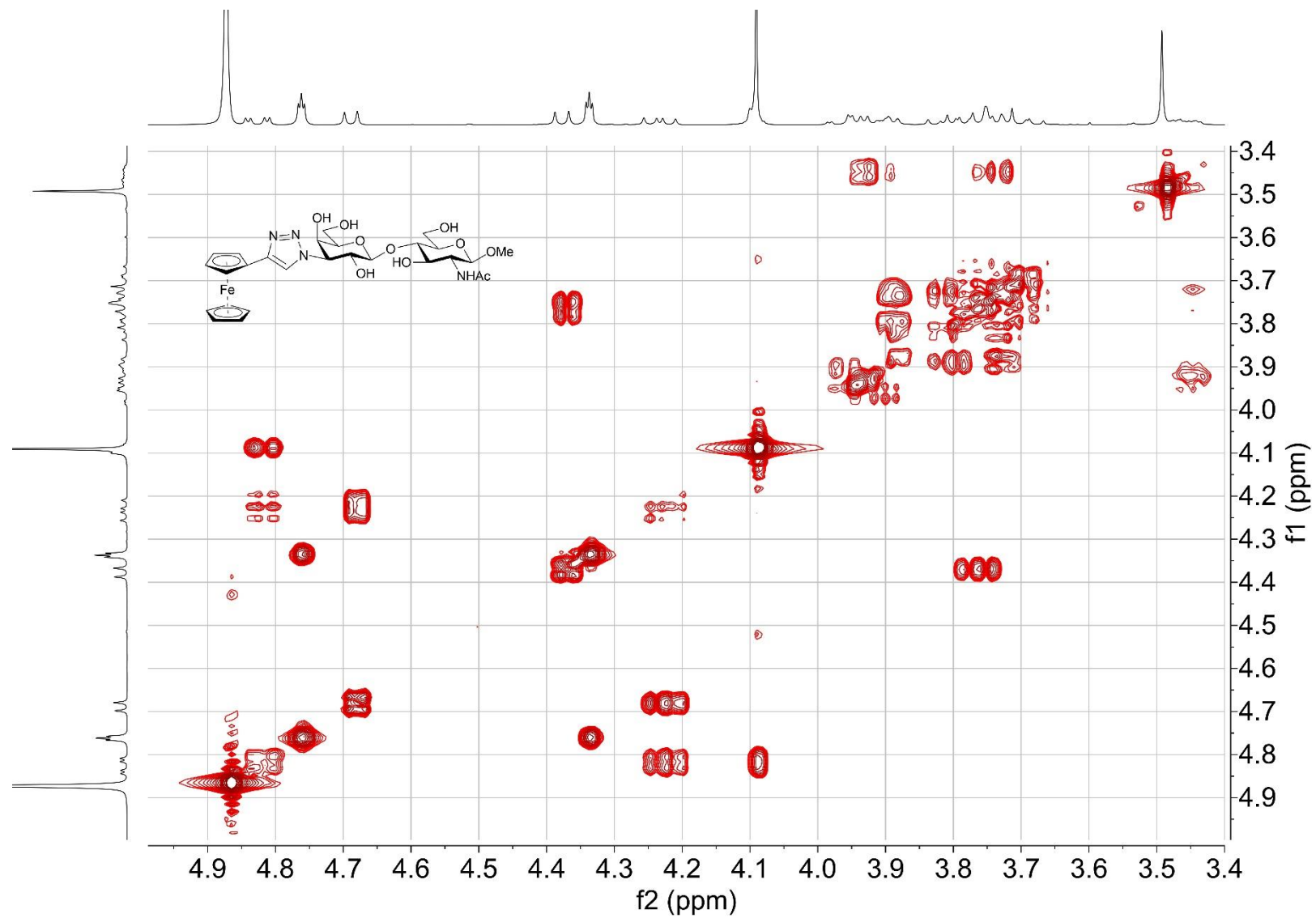
¹H NMR (400 MHz, MeOD) 25



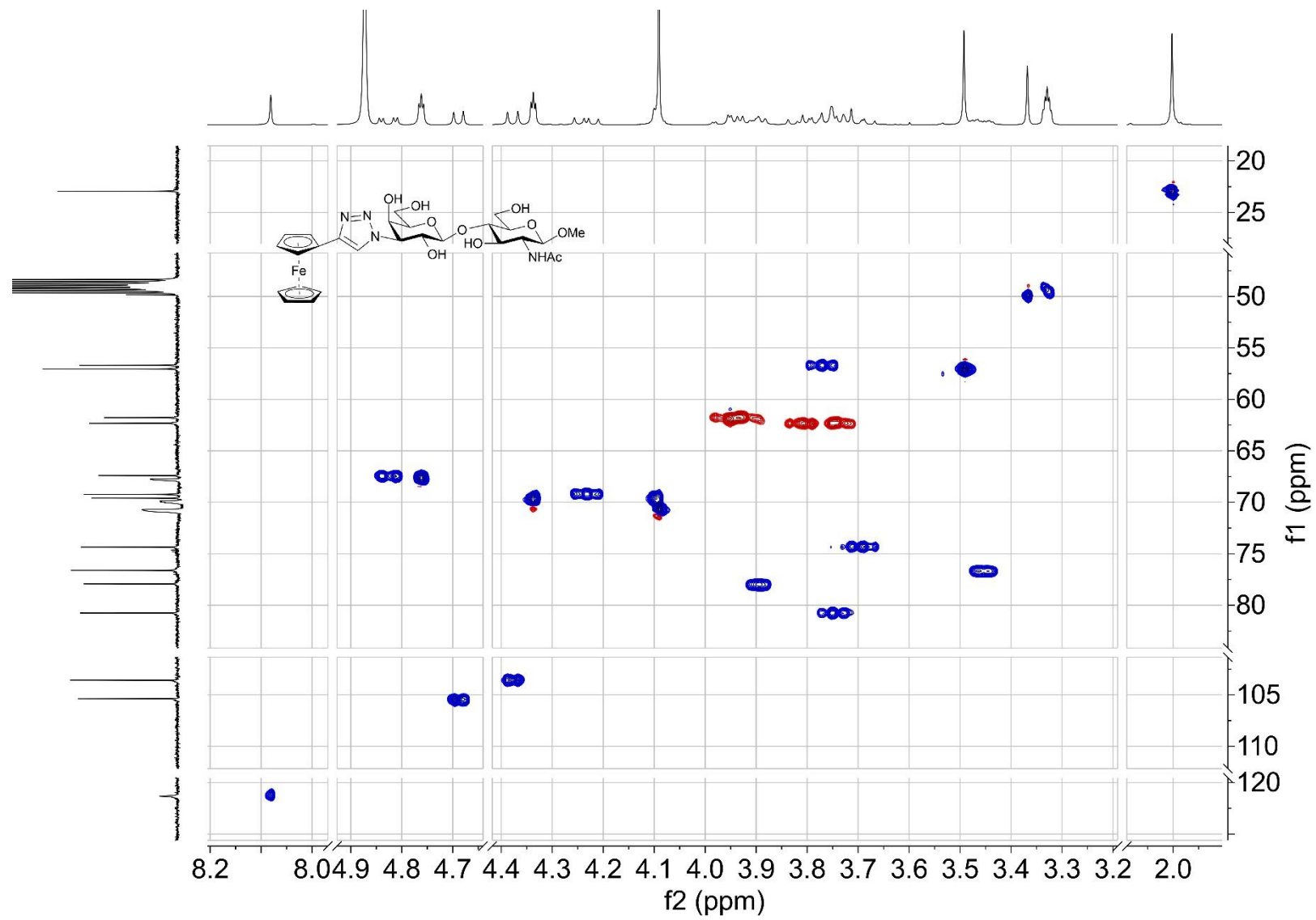
¹³C NMR (101 MHz, MeOD) 25



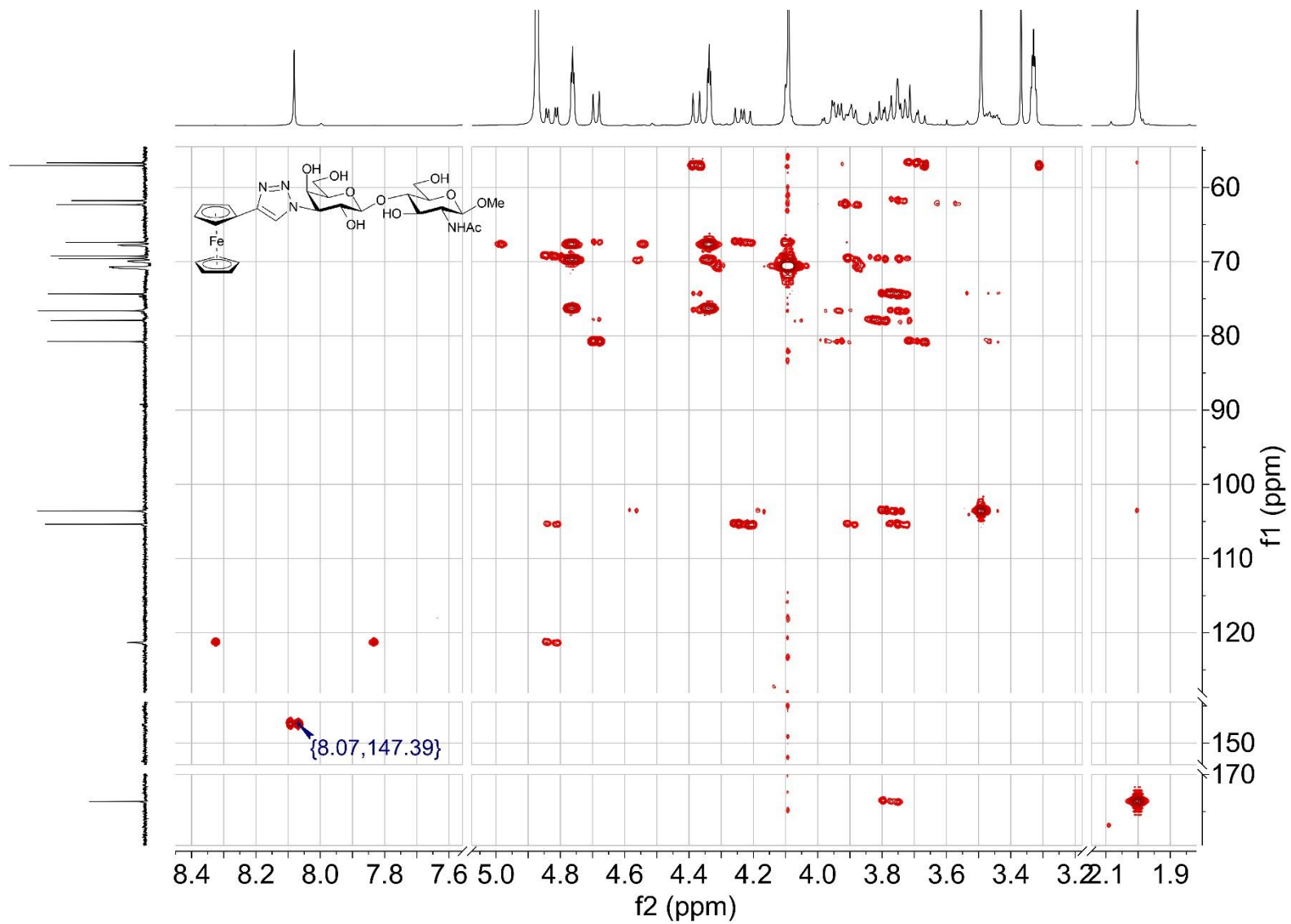
¹H-¹H COSY 25



^1H - ^{13}C HSQC 25

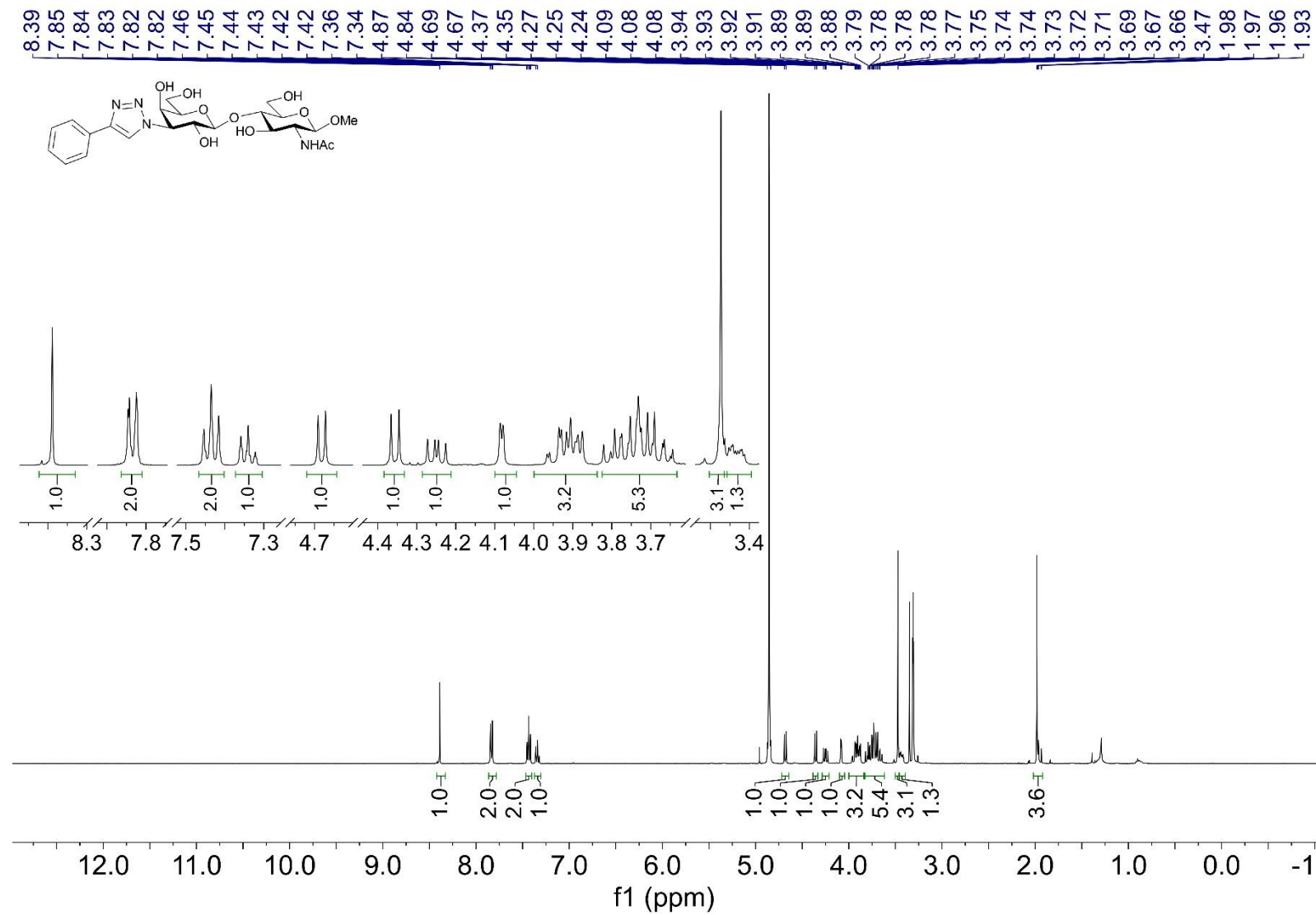


¹H-¹³C HMBC 25

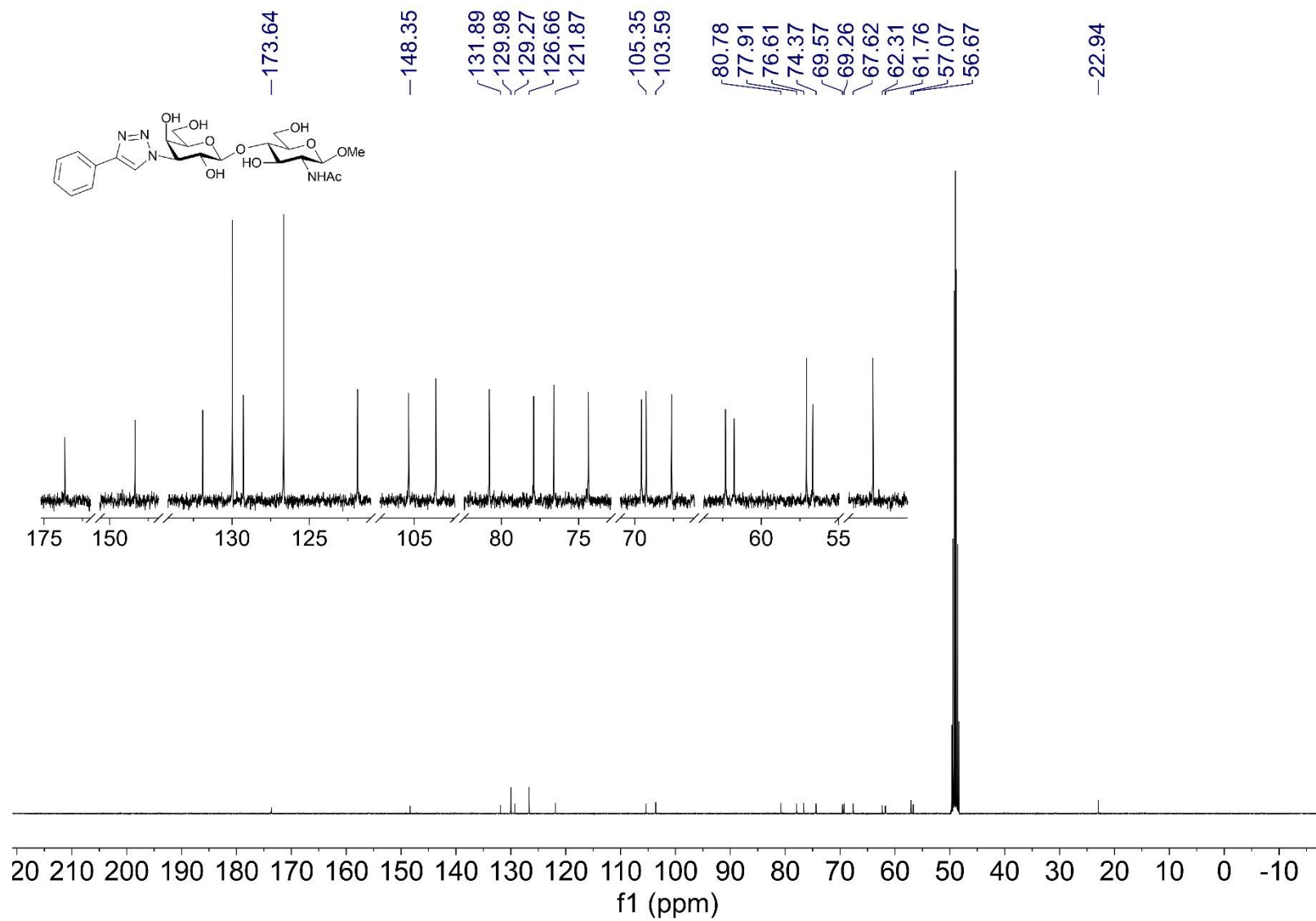


NMR COMPOUND 26

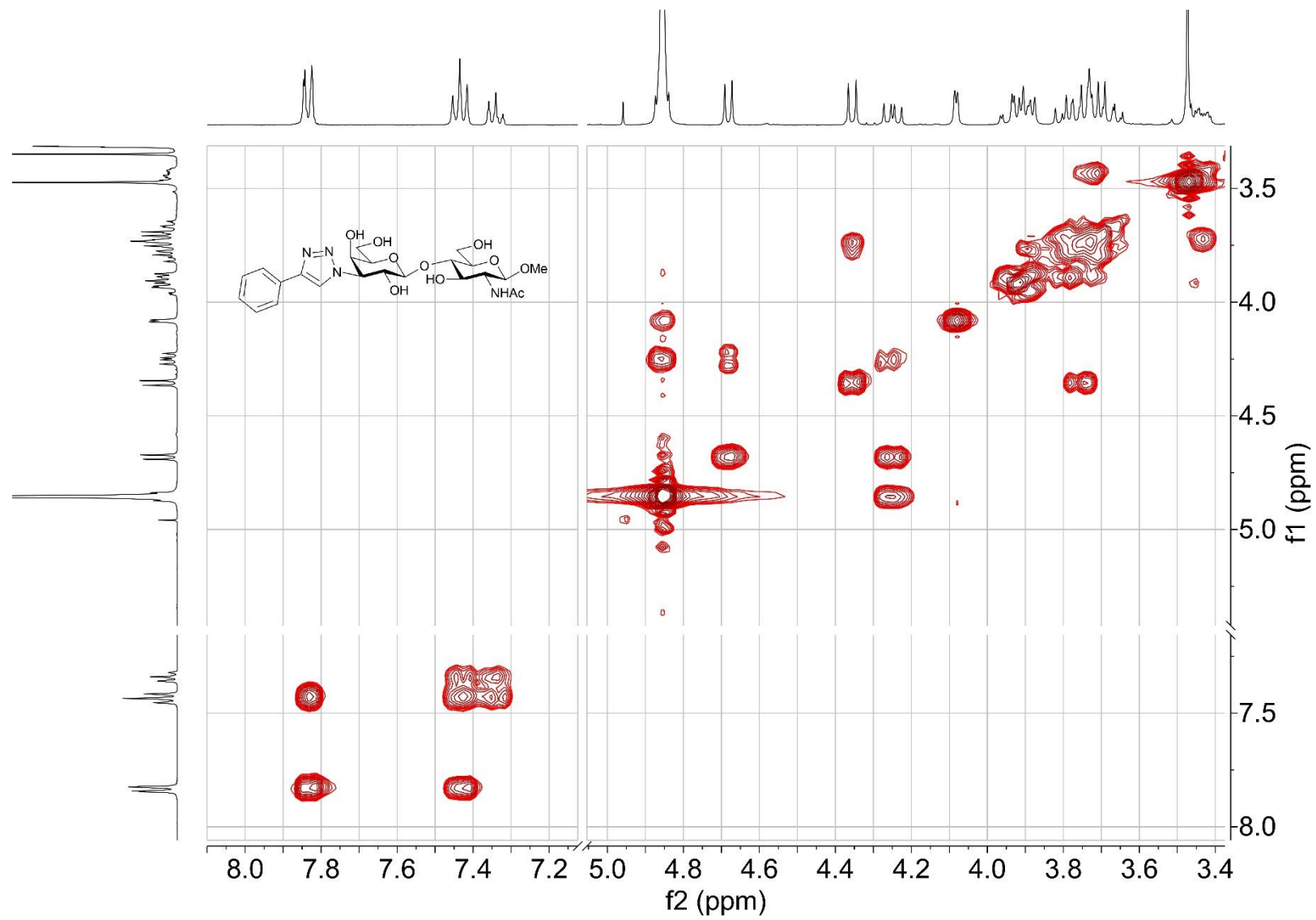
¹H NMR (400 MHz, MeOD) 26



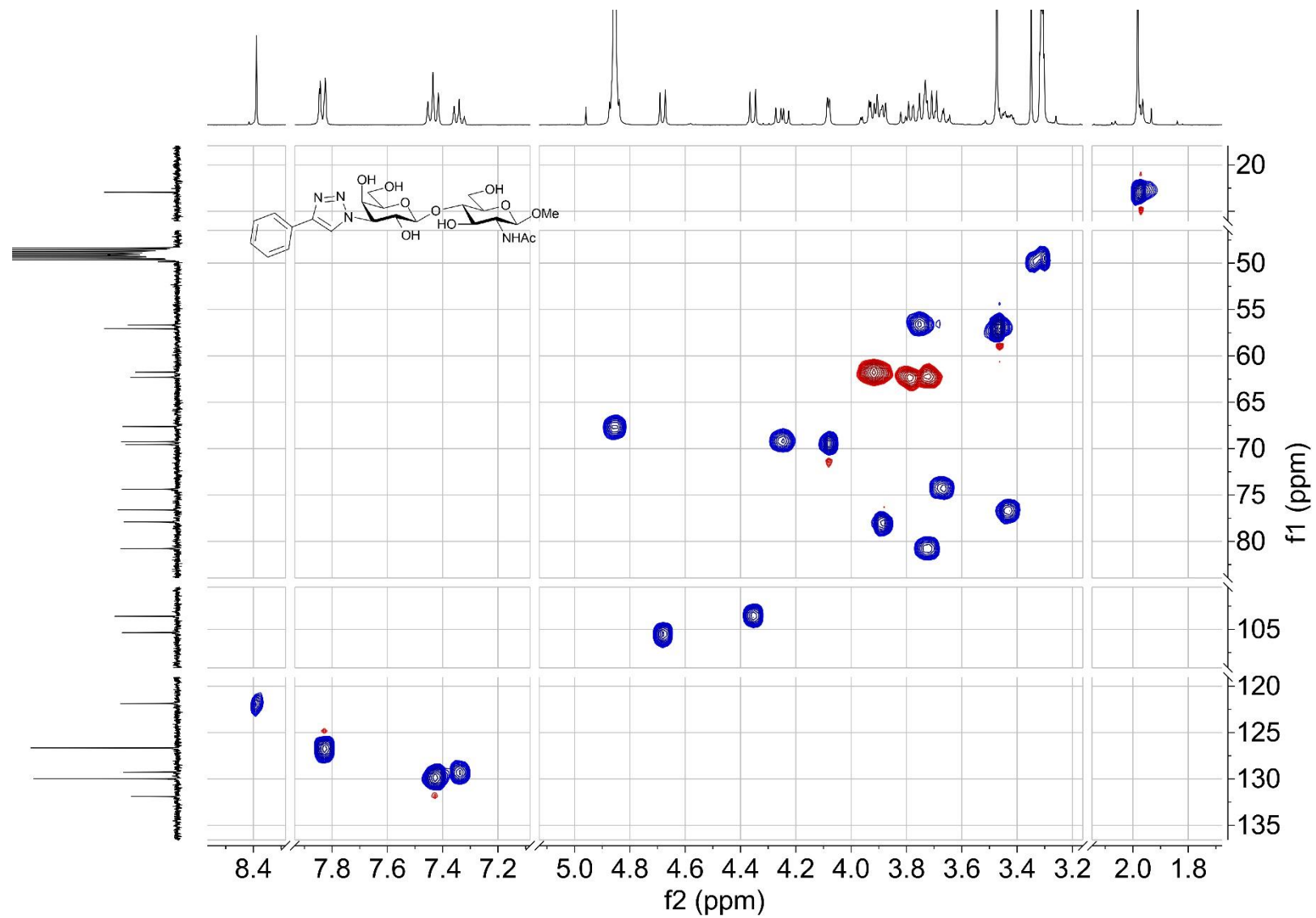
¹³C NMR (101 MHz, MeOD) 26



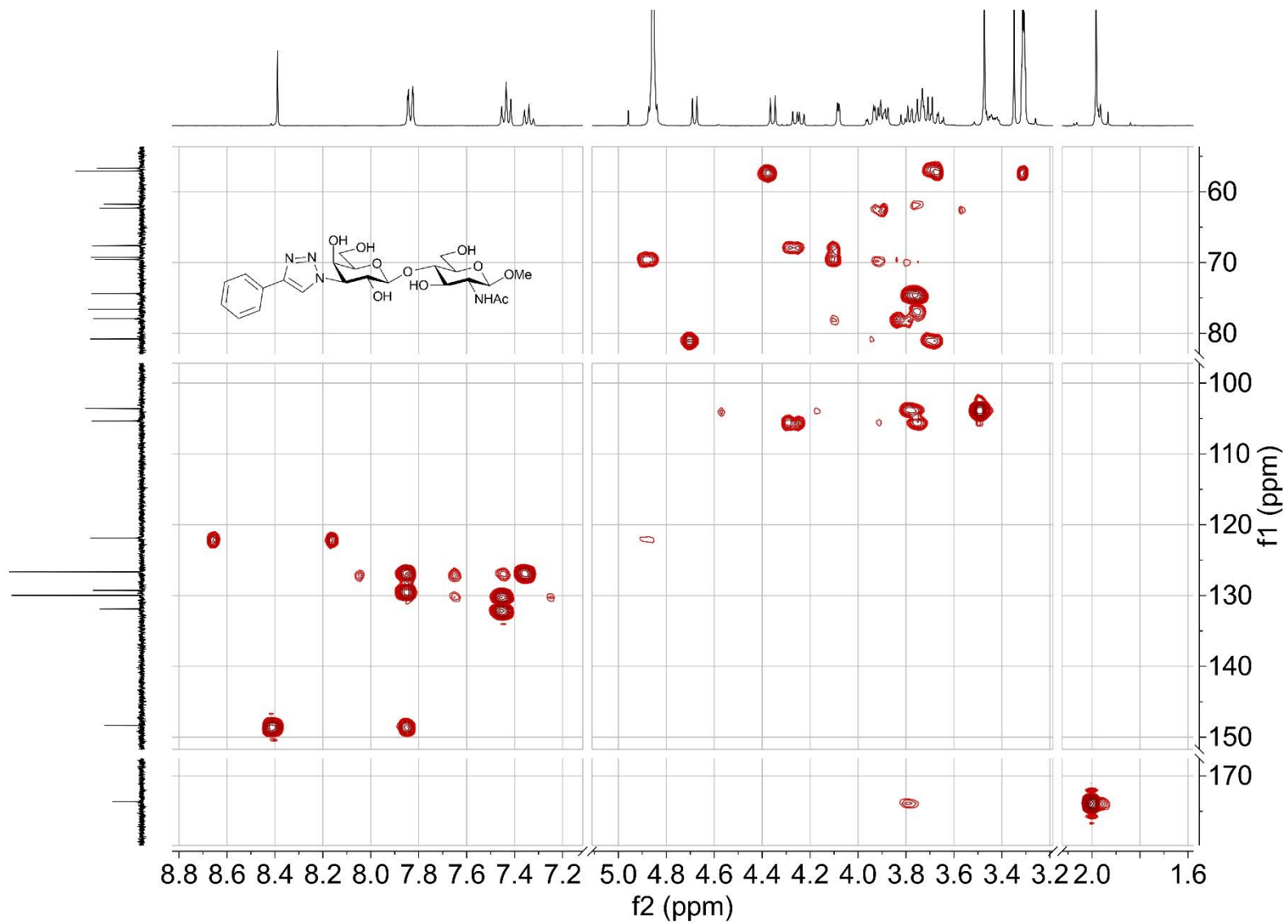
¹H-¹H COSY 26



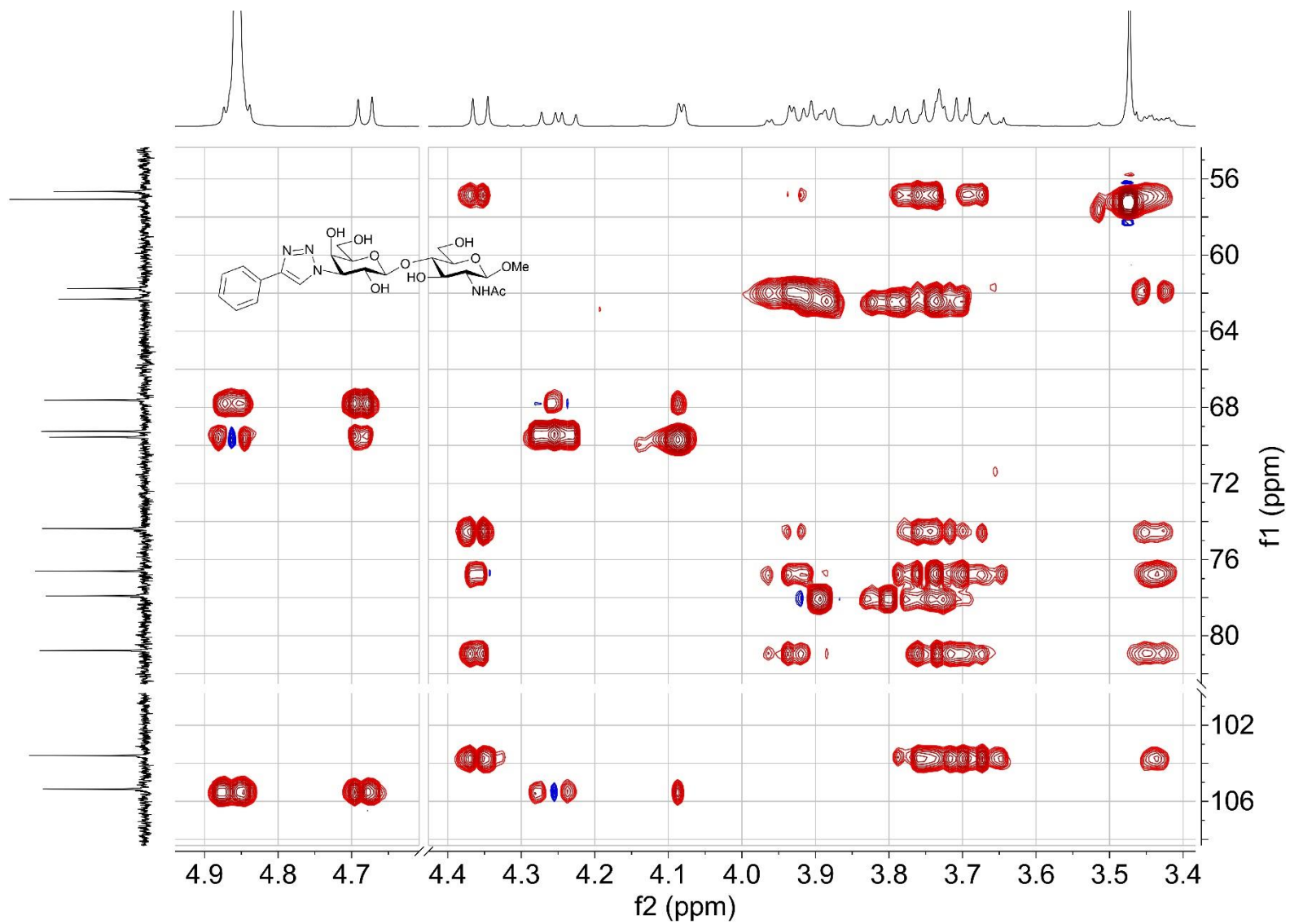
^1H - ^{13}C HSQC 26



^1H - ^{13}C HMBC 26

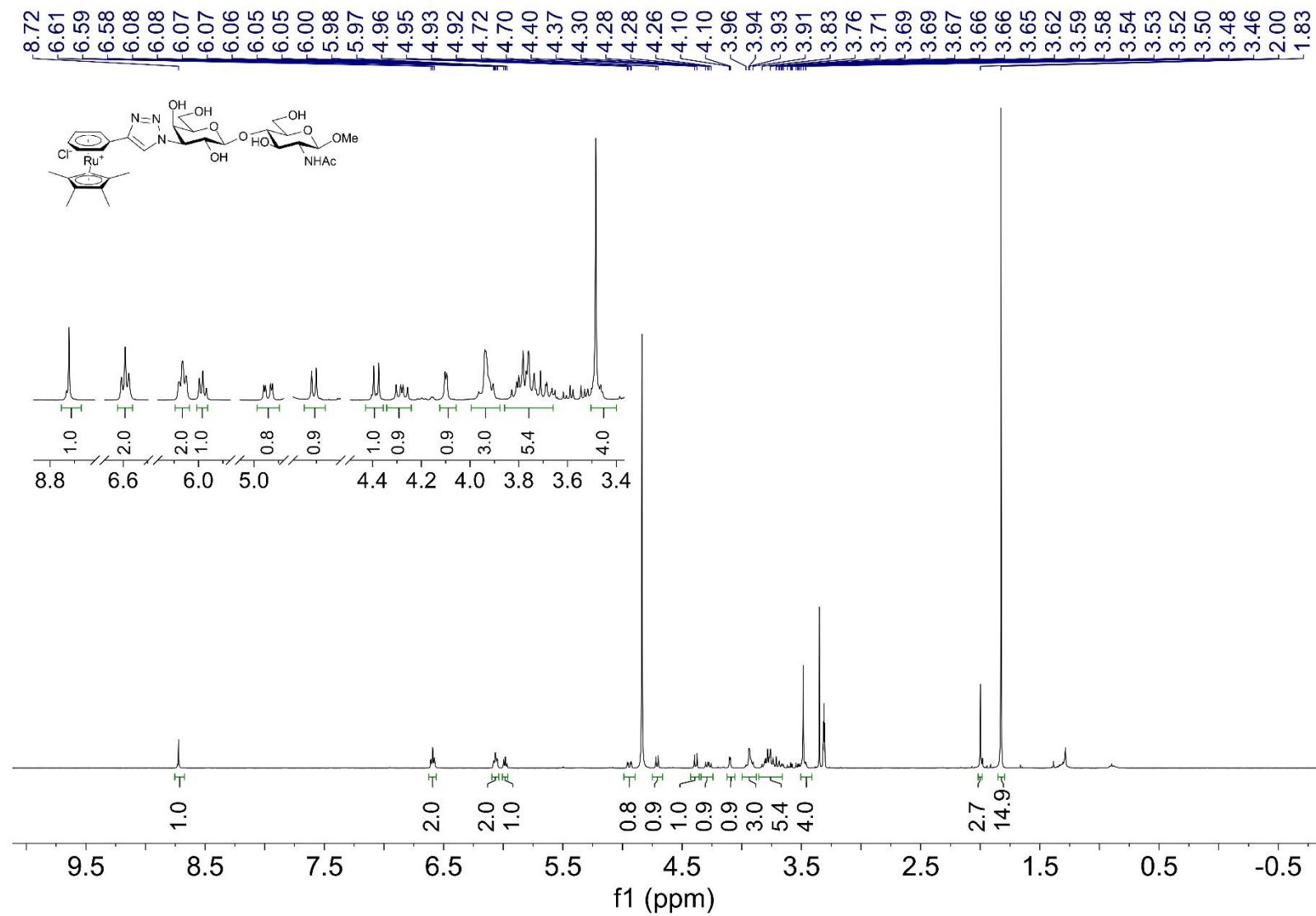


^1H - ^{13}C HSQCTOCSY 26

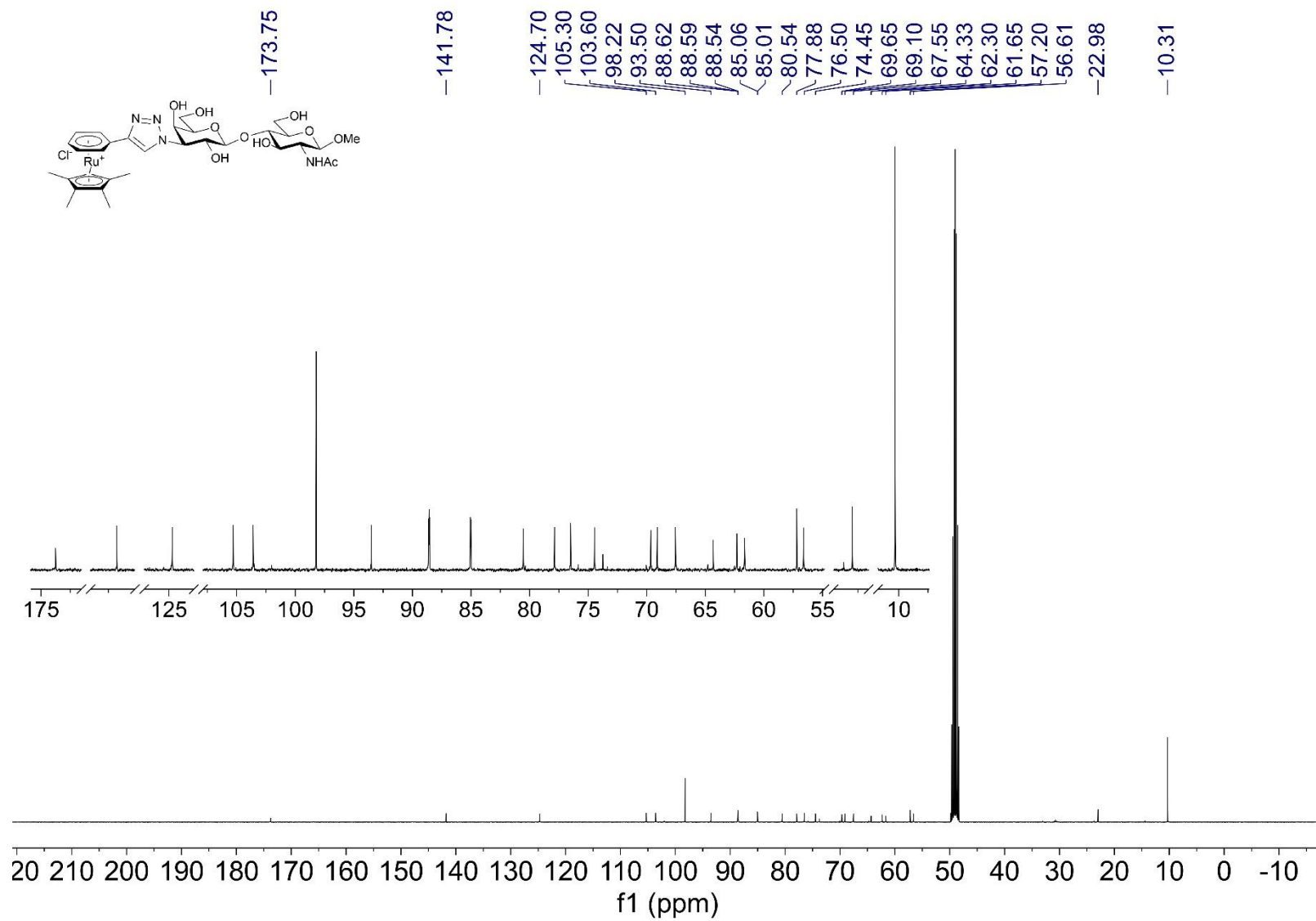


NMR COMPOUND 27

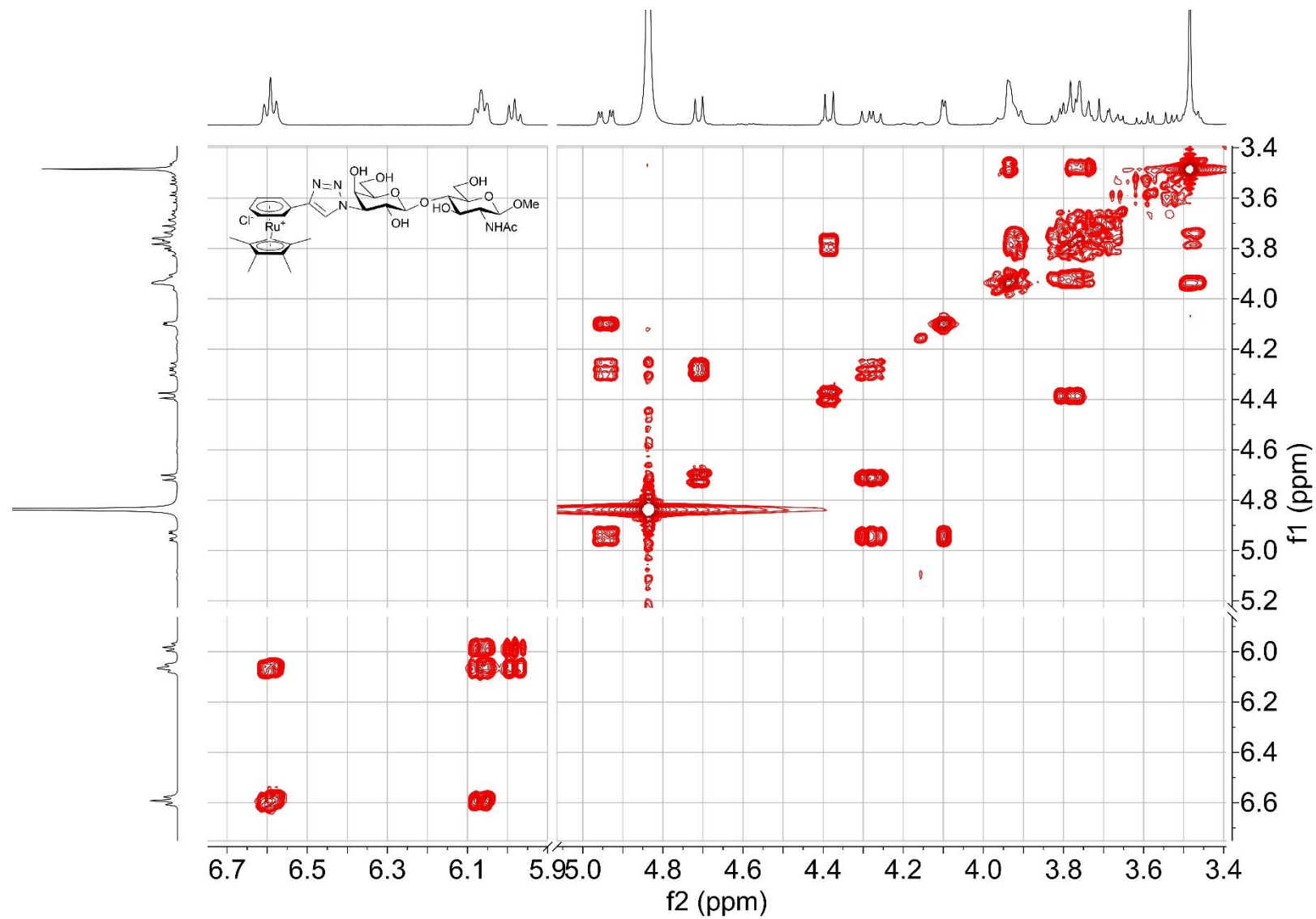
¹H NMR (400 MHz, MeOD) 27



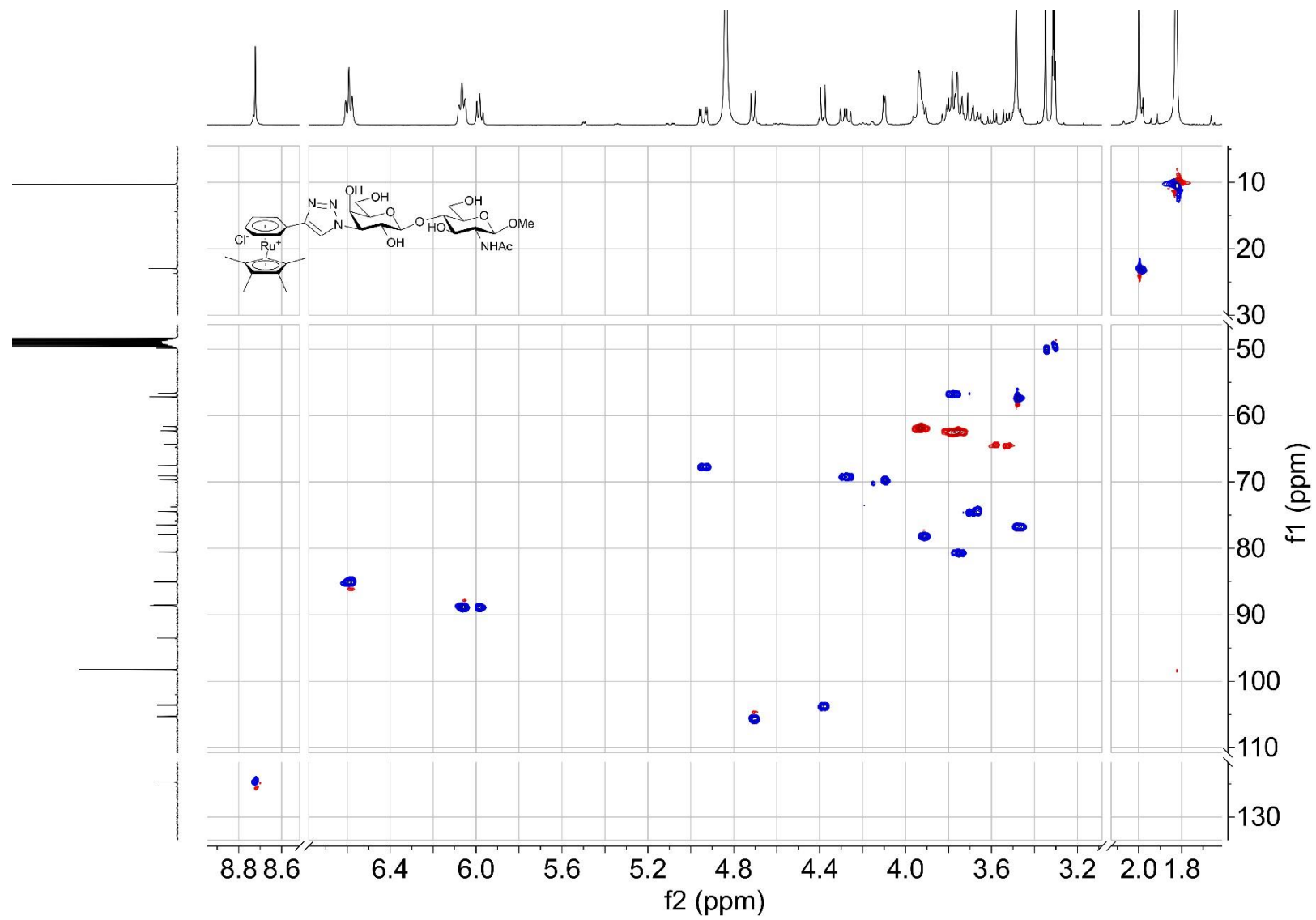
¹³C NMR (101 MHz, MeOD) 27



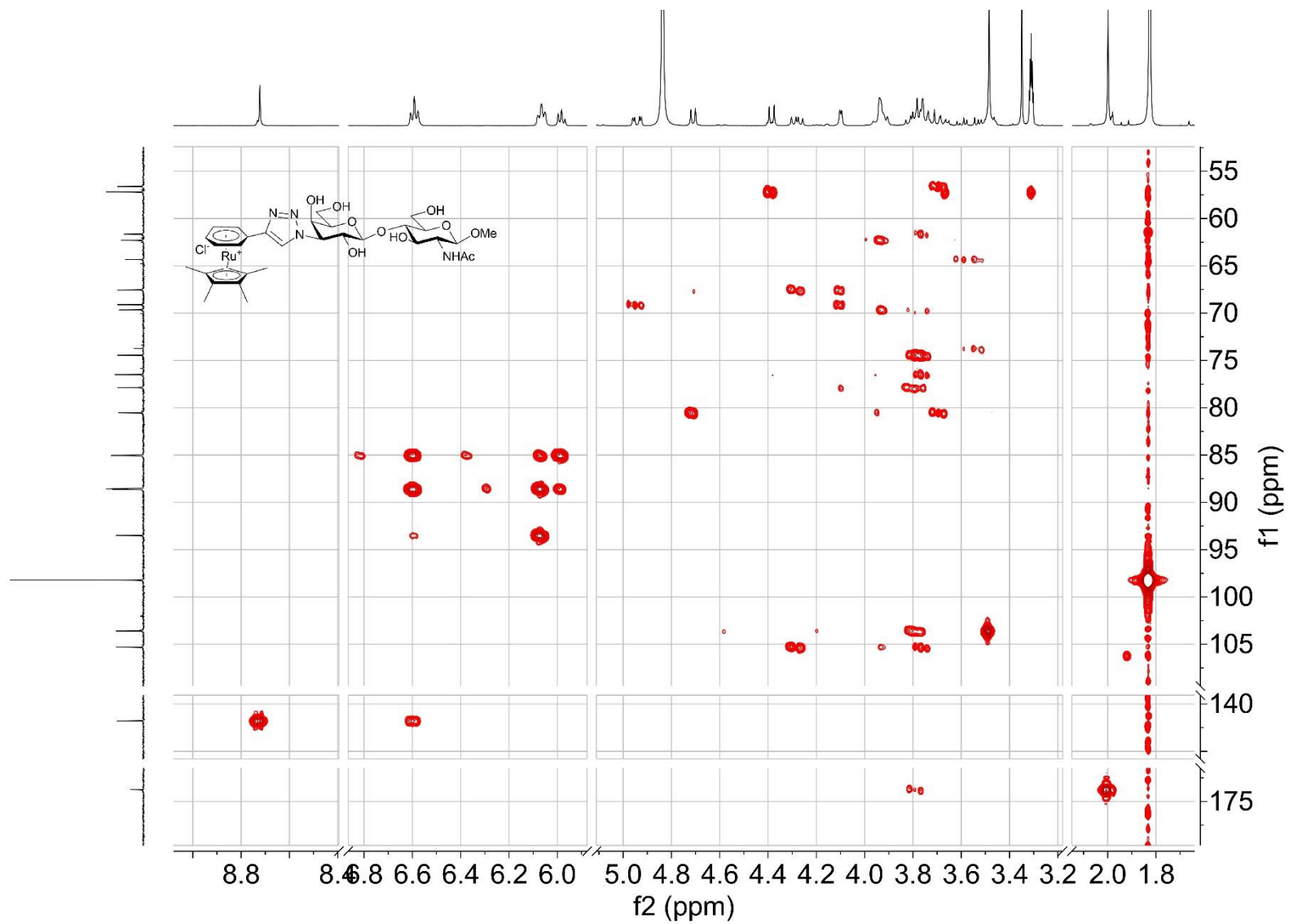
¹H-¹H COSY 27



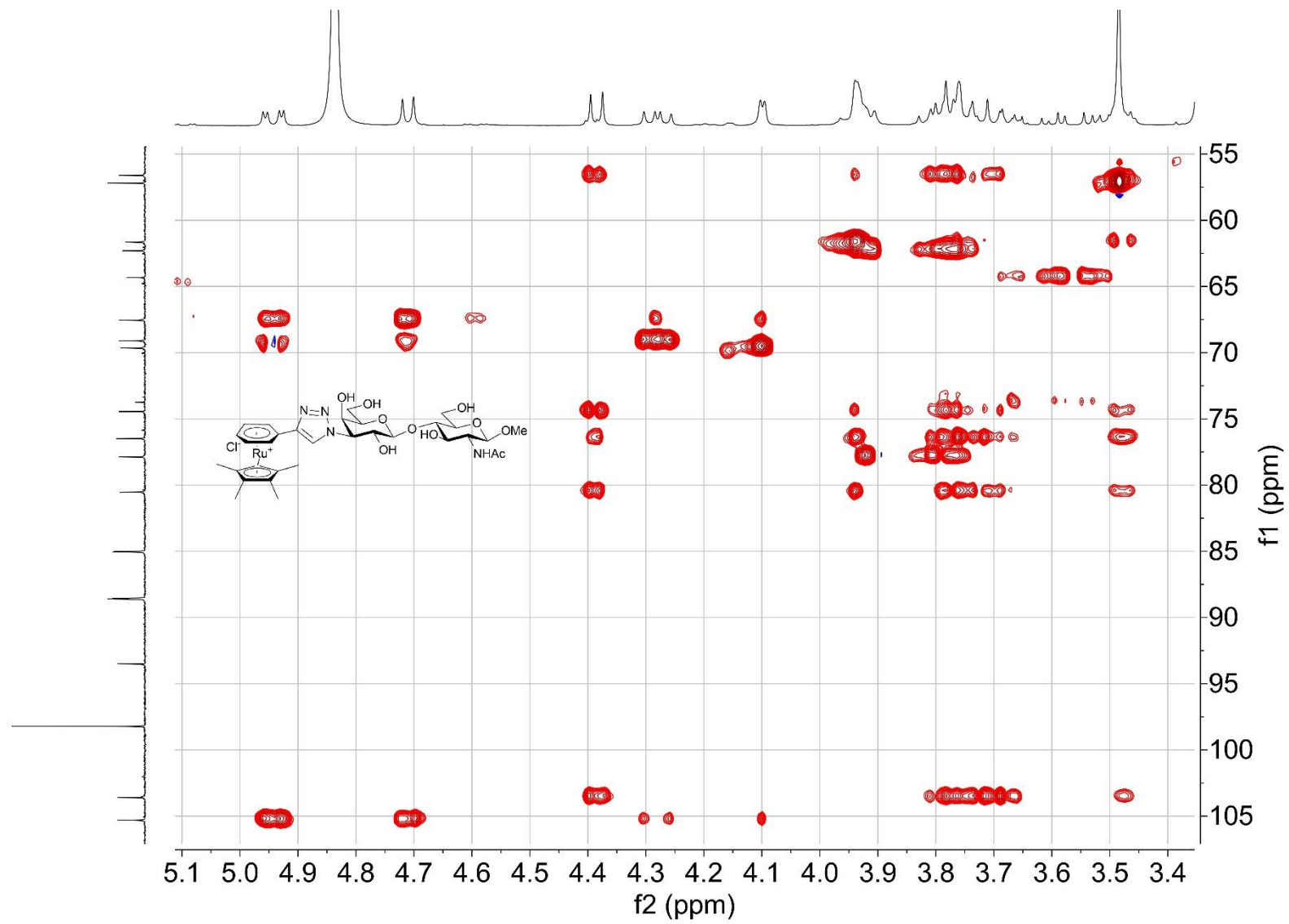
^1H - ^{13}C HSQC 27



^1H - ^{13}C HMBC 27

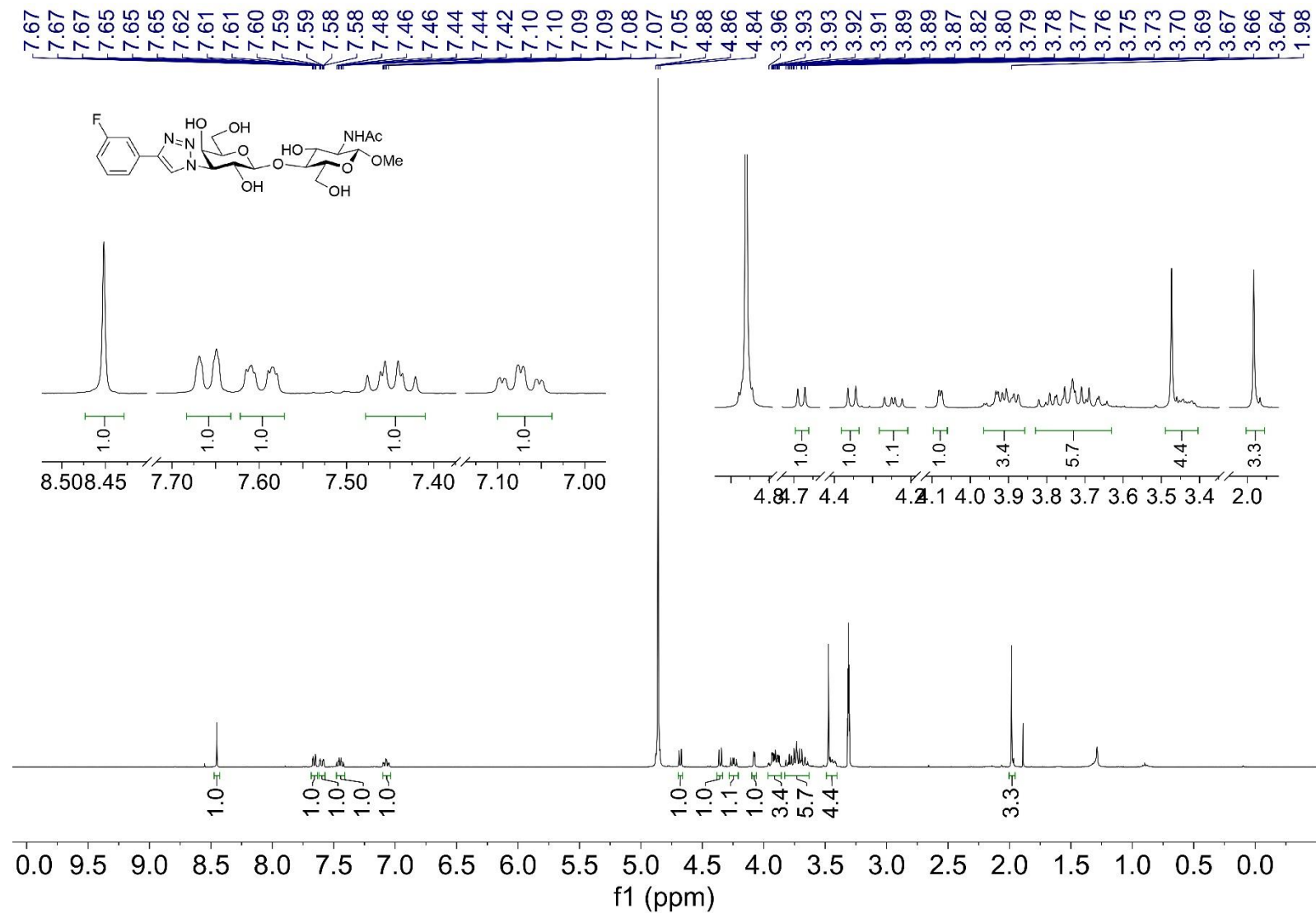


^1H - ^{13}C HSQCTOCSY 27

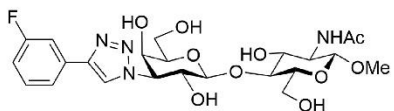


NMR COMPOUND 28

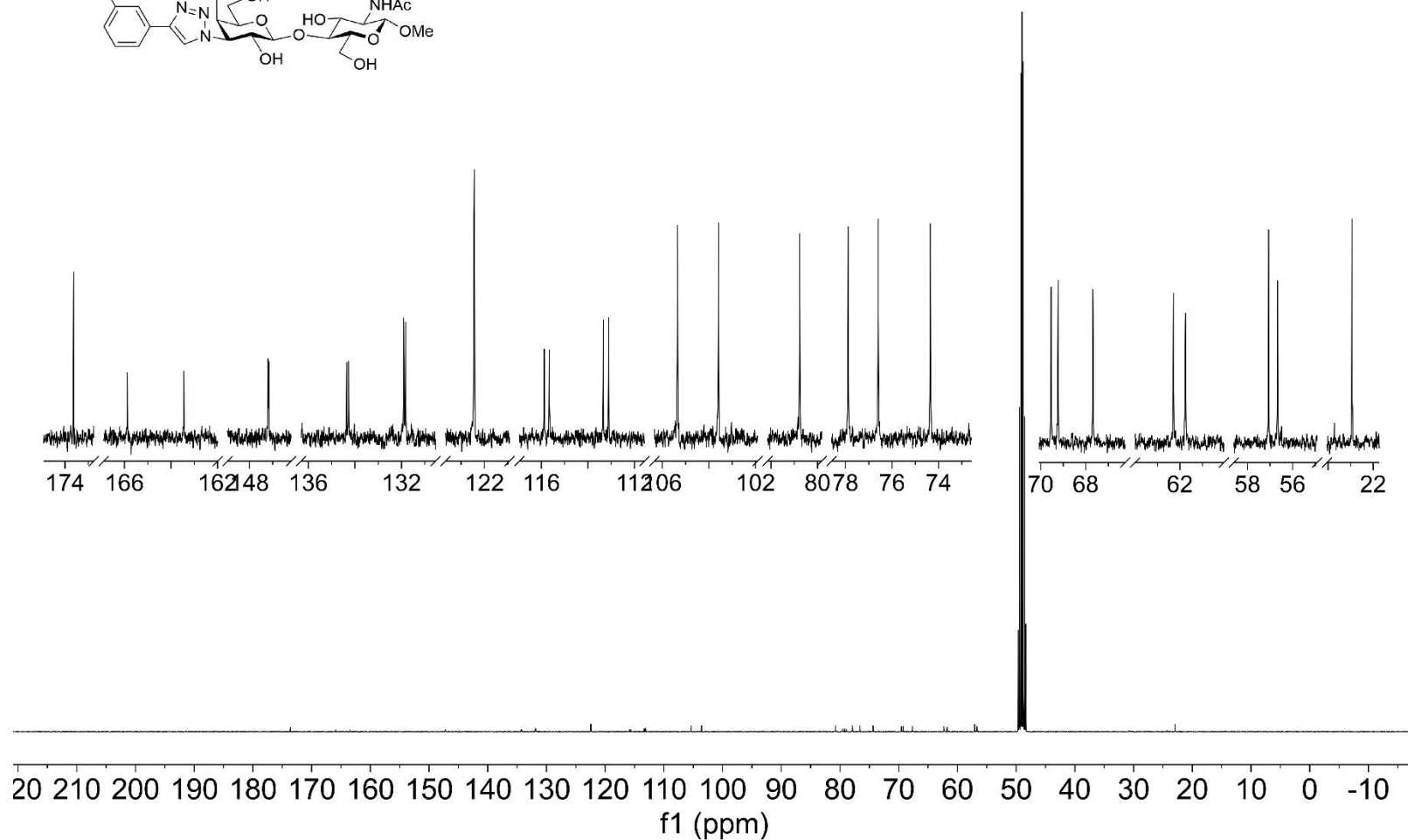
¹H NMR (400 MHz, MeOD) 28



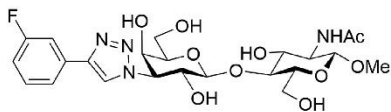
¹³C NMR (101 MHz, MeOD) 28



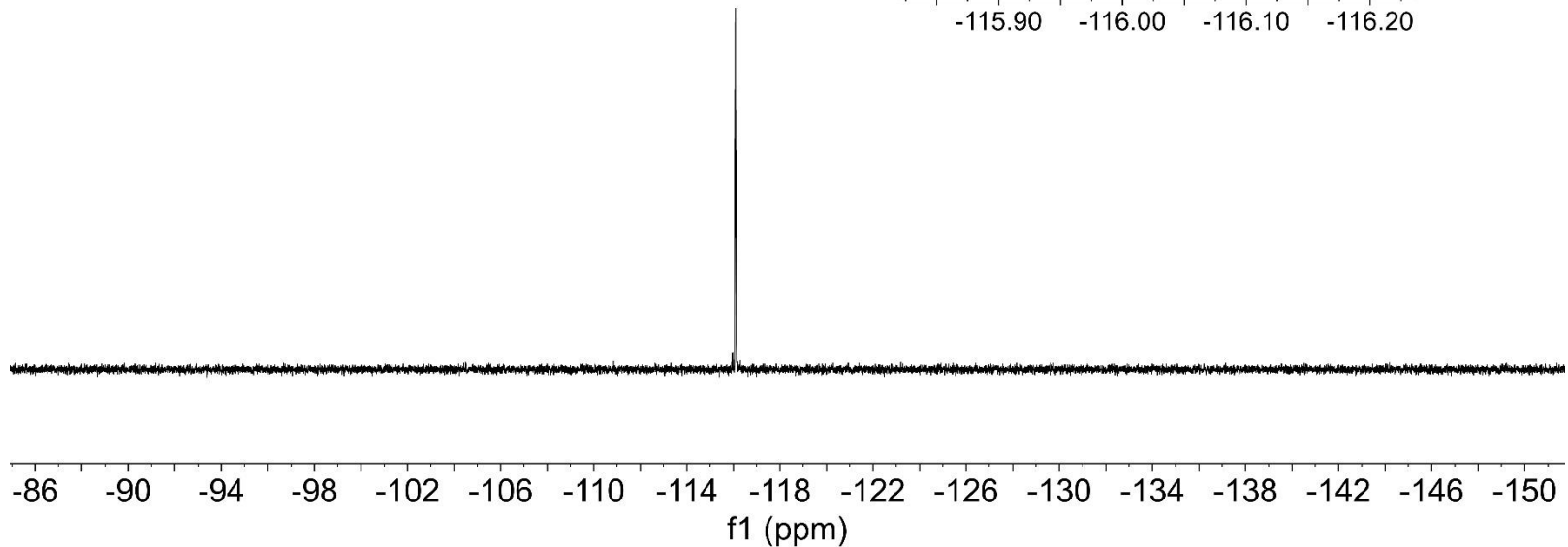
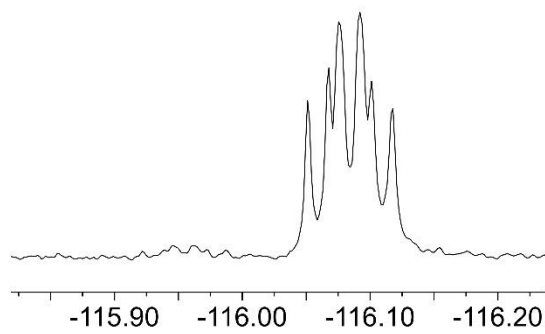
- 173.63
- 165.87
- 163.45
- 147.20
- 147.17
- 134.35
- 134.27
- 131.90
- 131.82
- 122.44
- 115.87
- 115.66
- 113.34
- 113.11
- 105.35
- 103.58
- 80.77
- 77.88
- 76.59
- 74.36
- 69.54
- 69.23
- 67.68
- 62.29
- 61.75
- 57.06
- 56.67
- 22.94



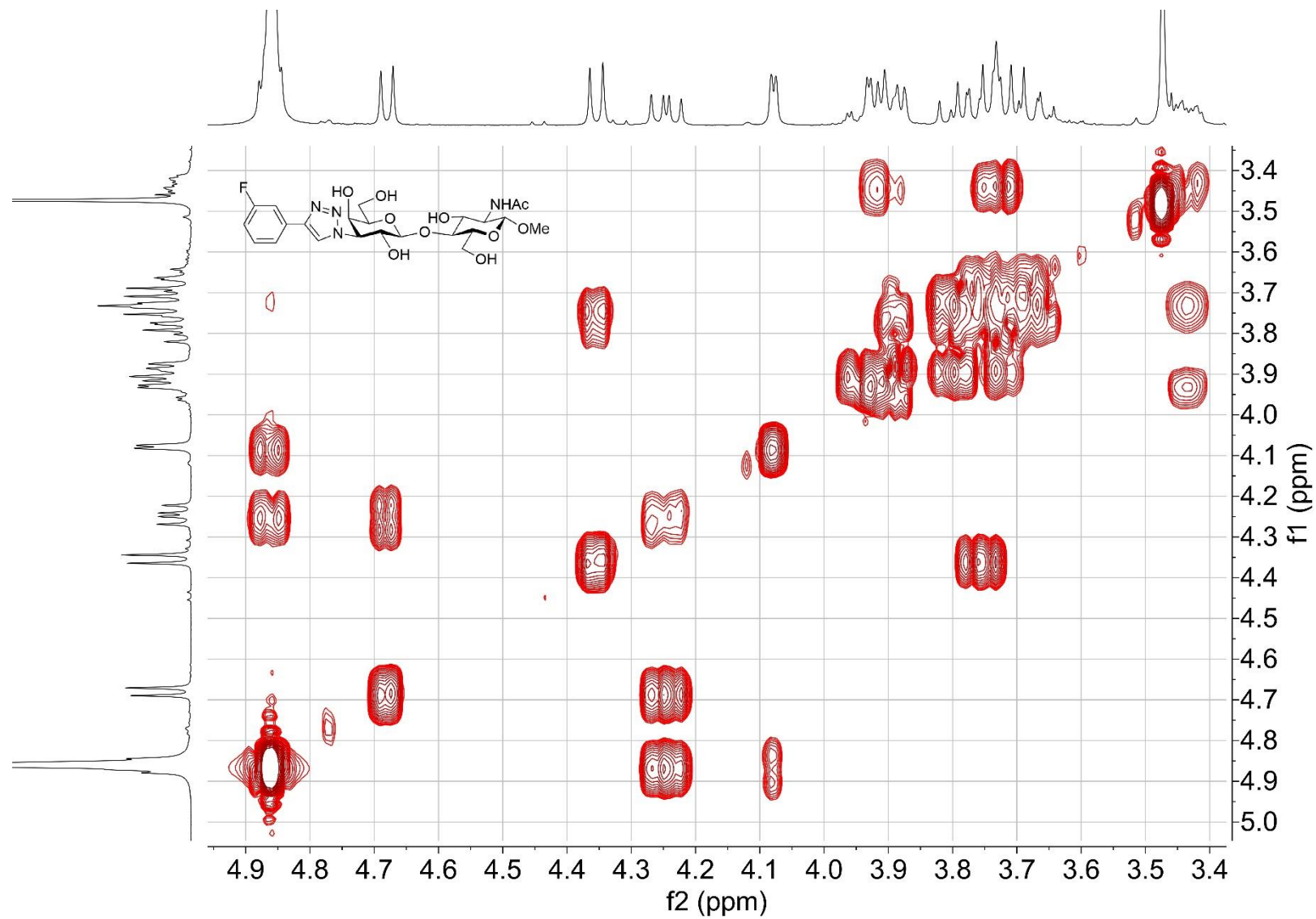
¹⁹F NMR (376 MHz, MeOD) 28



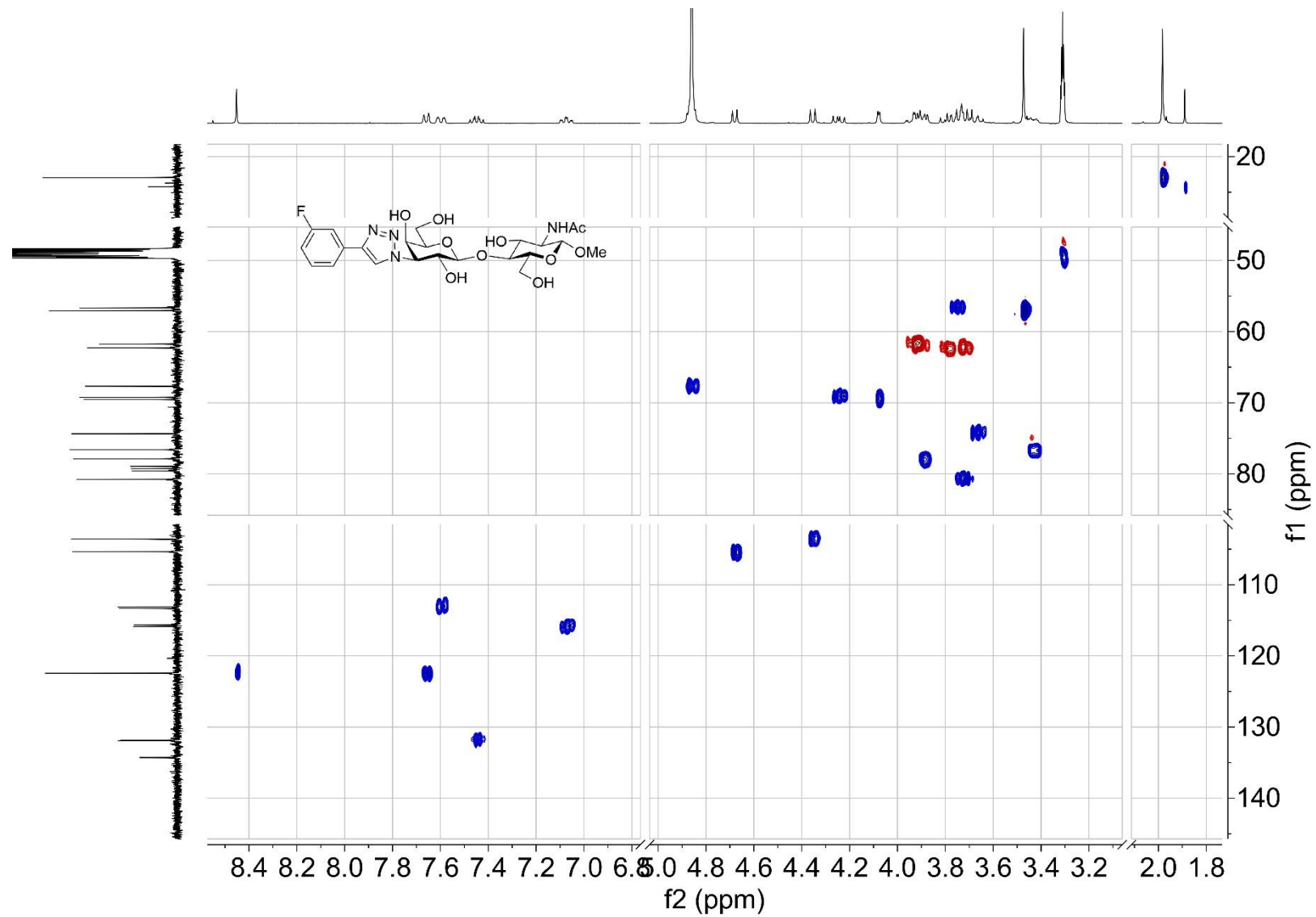
-116.05
-116.07
-116.08
-116.09
-116.10
-116.12



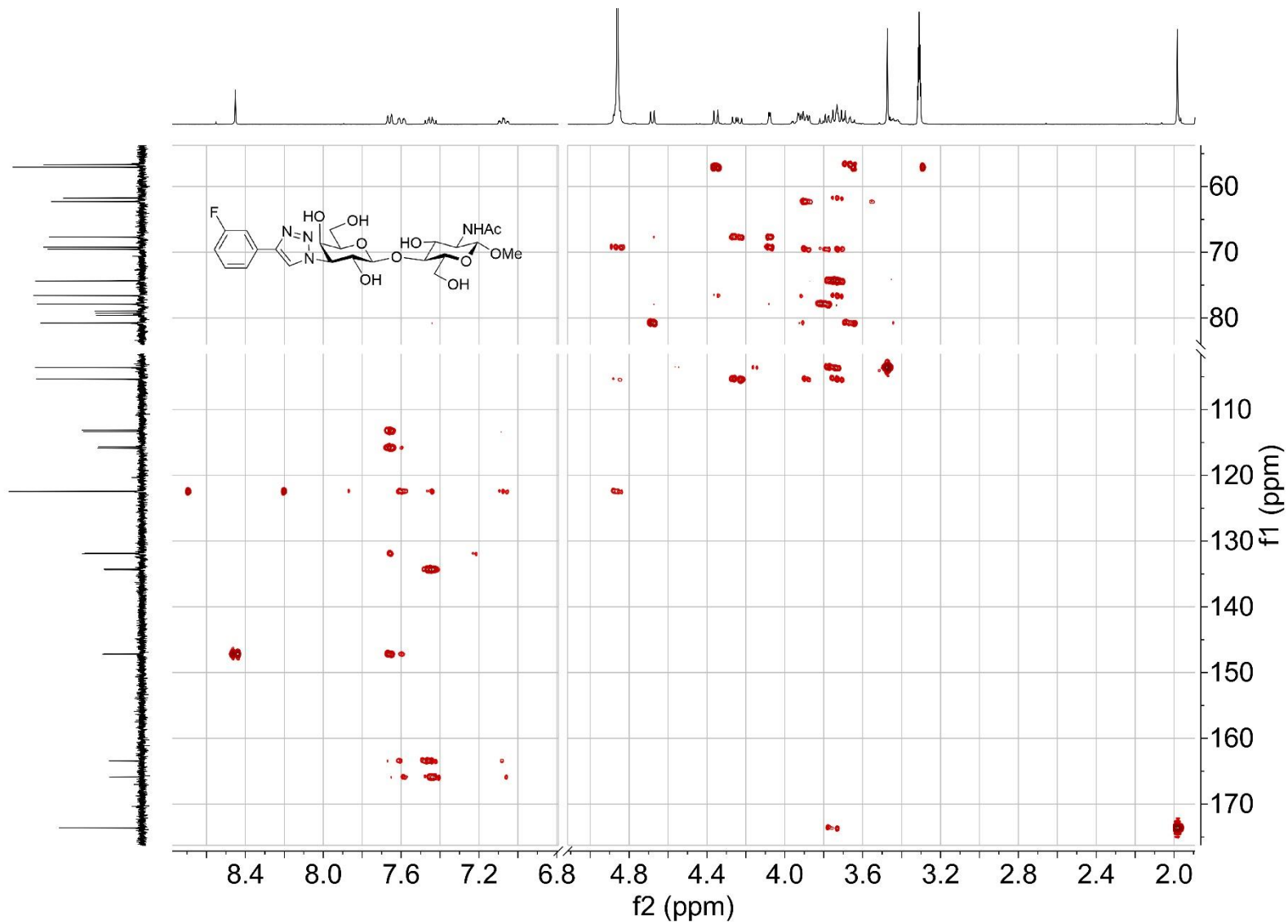
¹H-¹H COSY 28



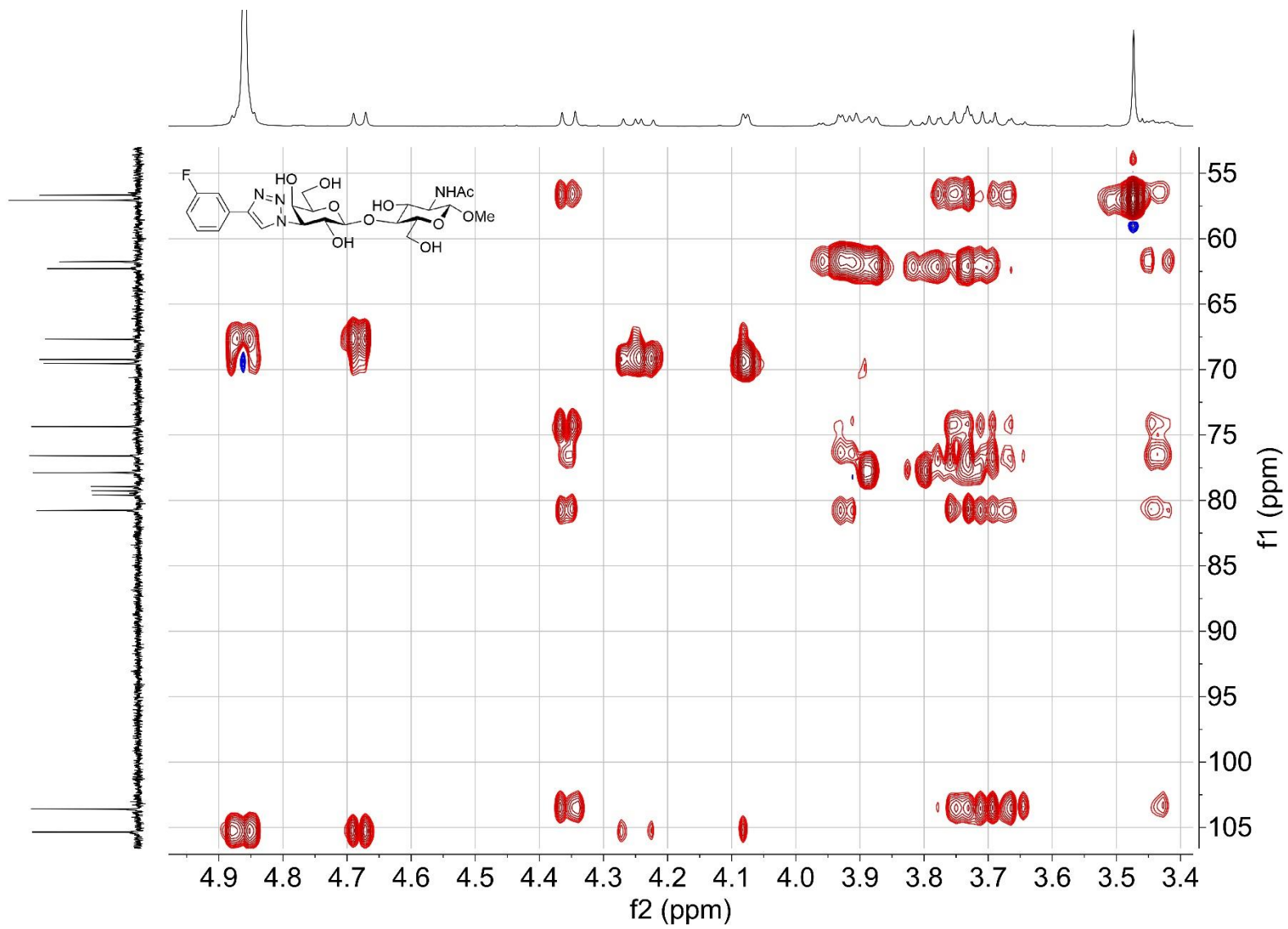
^1H - ^{13}C HSQC 28



^1H - ^{13}C HMBC 28

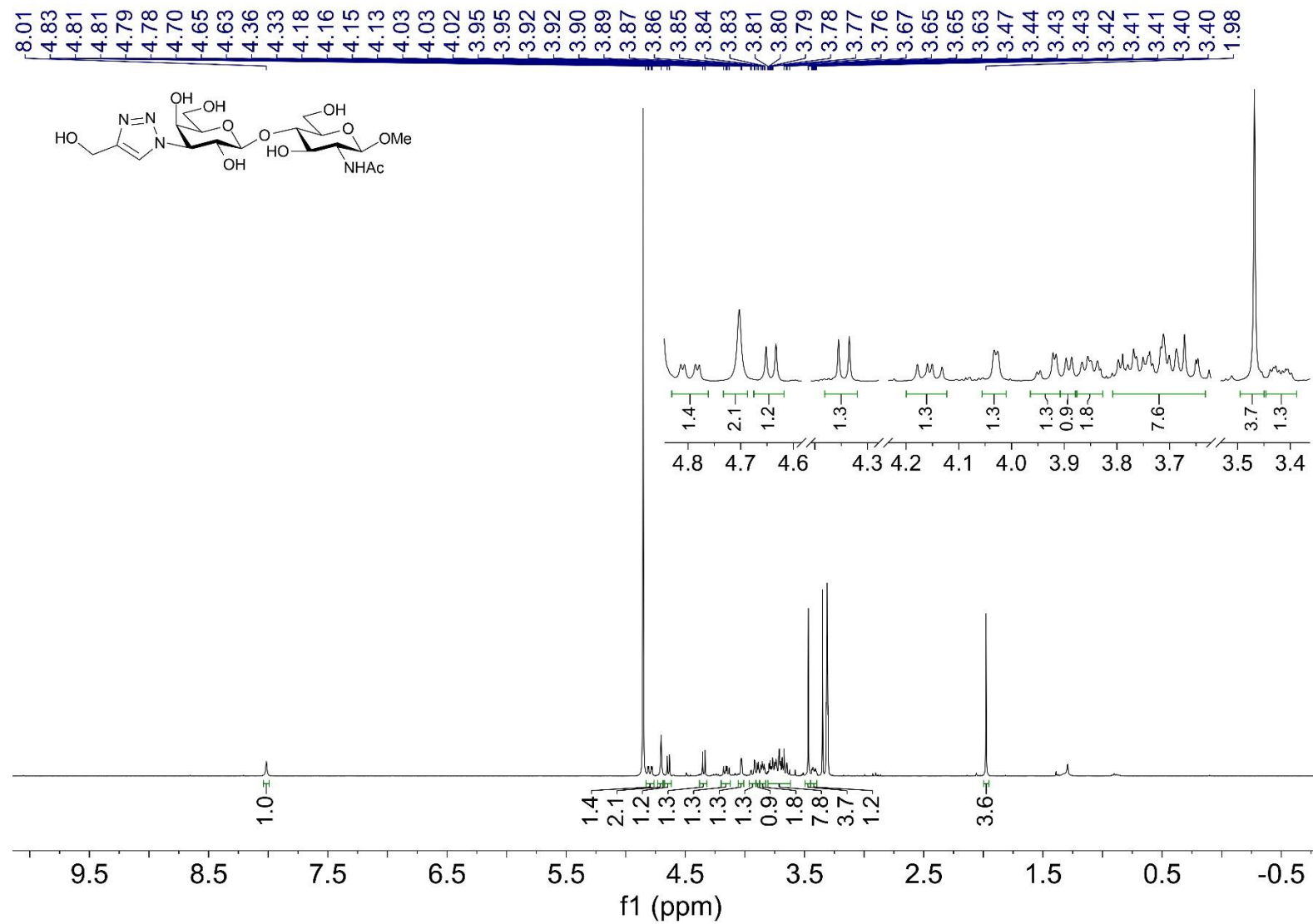


^1H - ^{13}C HSQCTOCSY 28

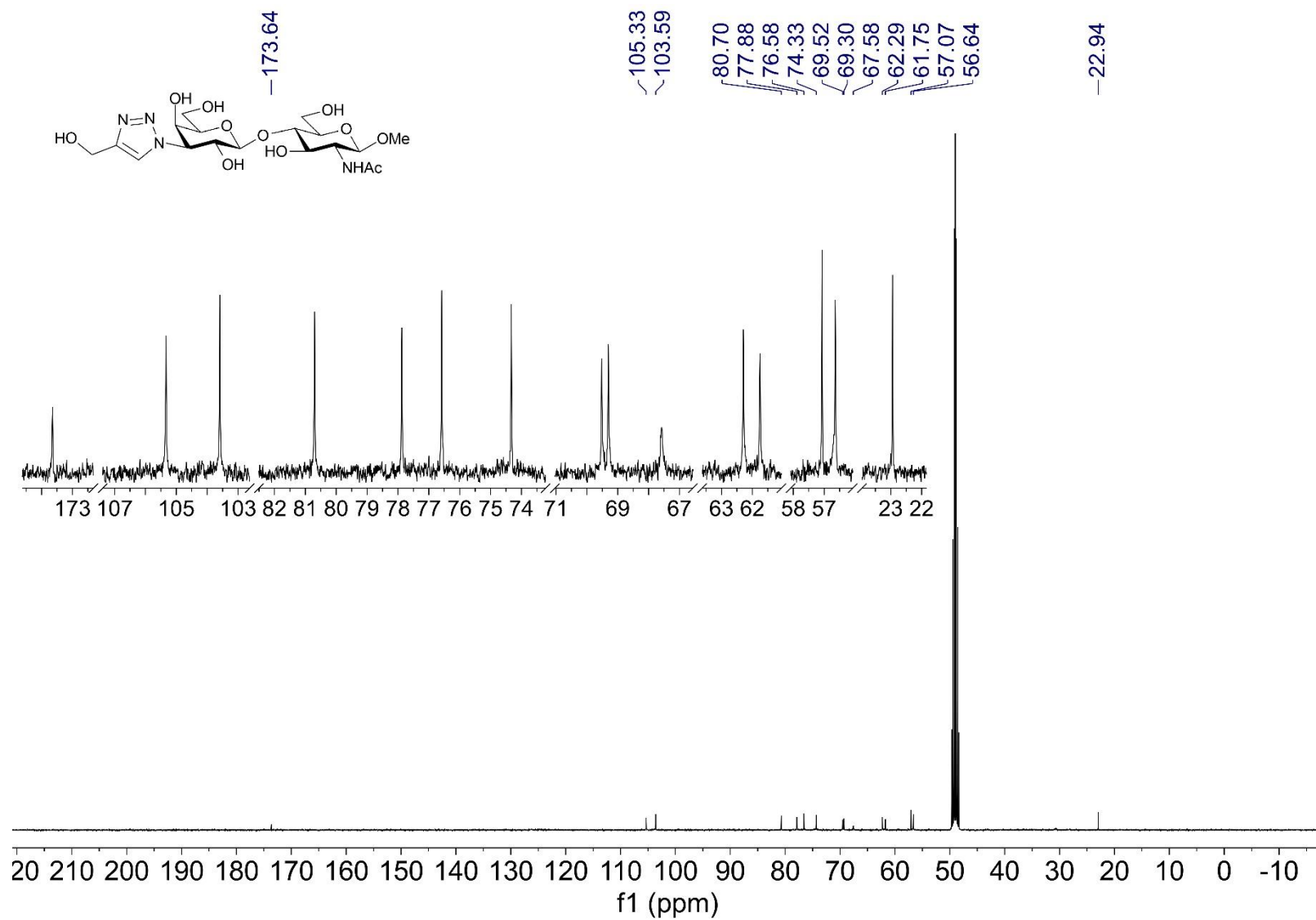


NMR COMPOUND 29

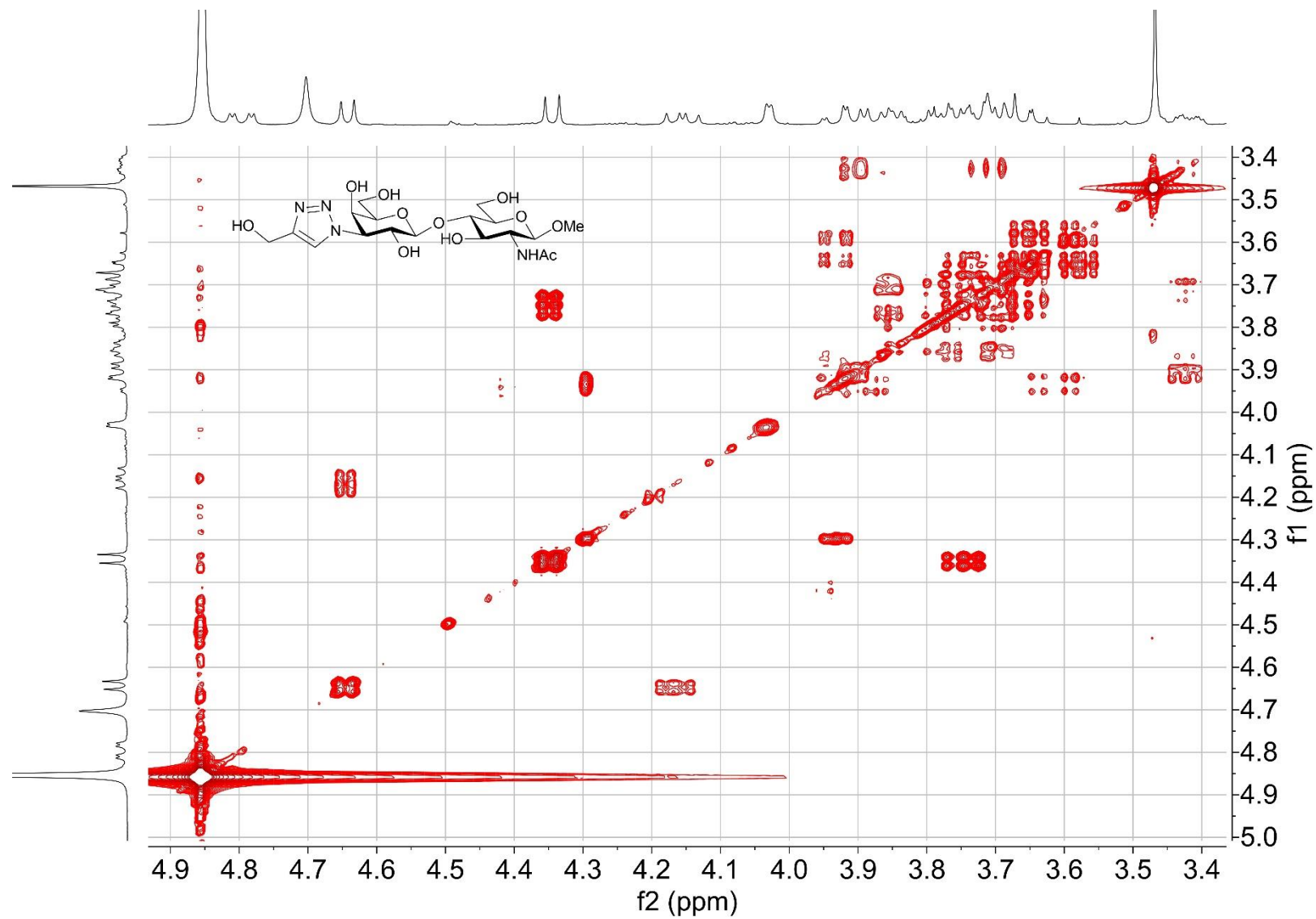
¹H NMR (400 MHz, MeOD) 29



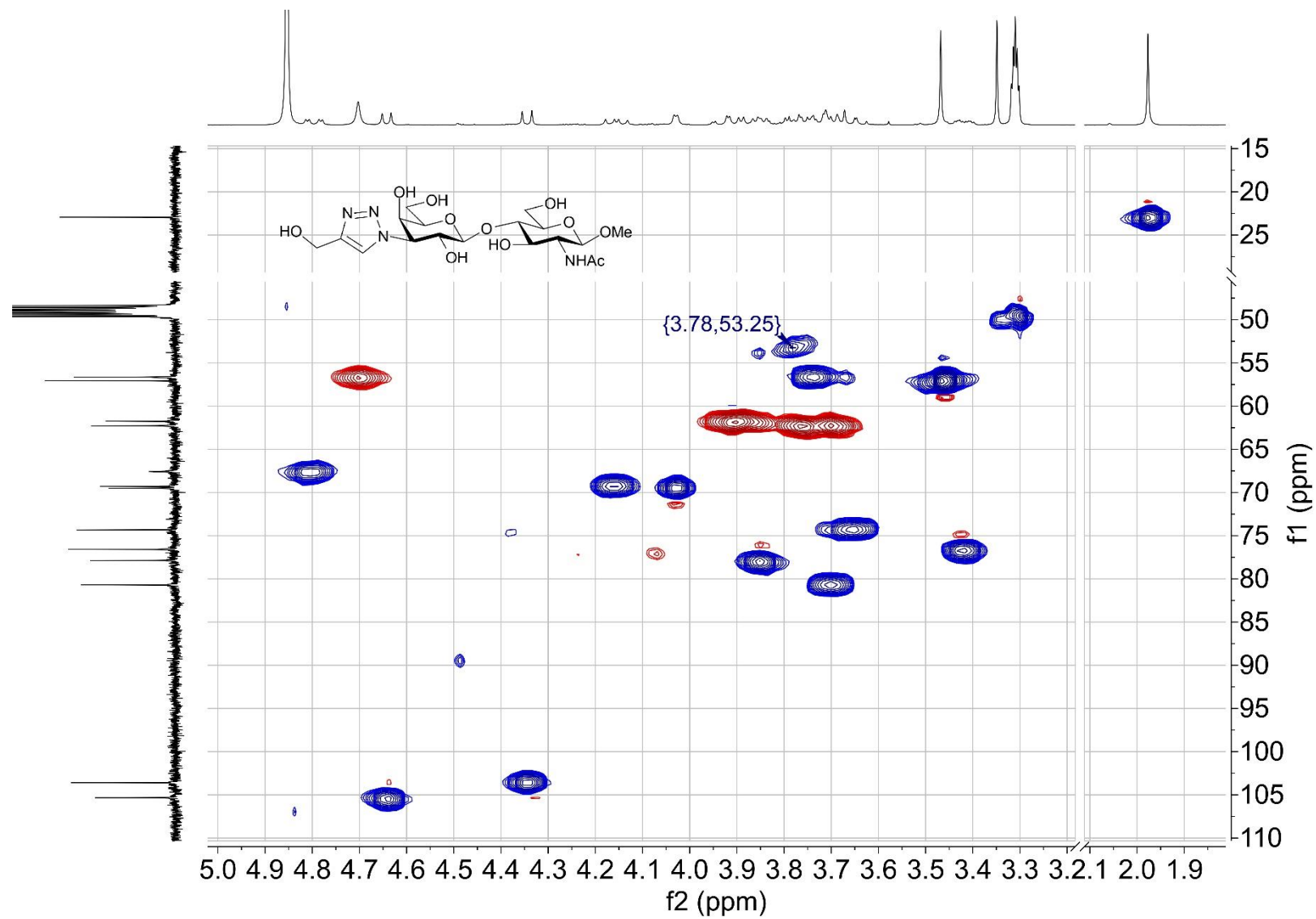
¹³C NMR (101 MHz, MeOD) 29



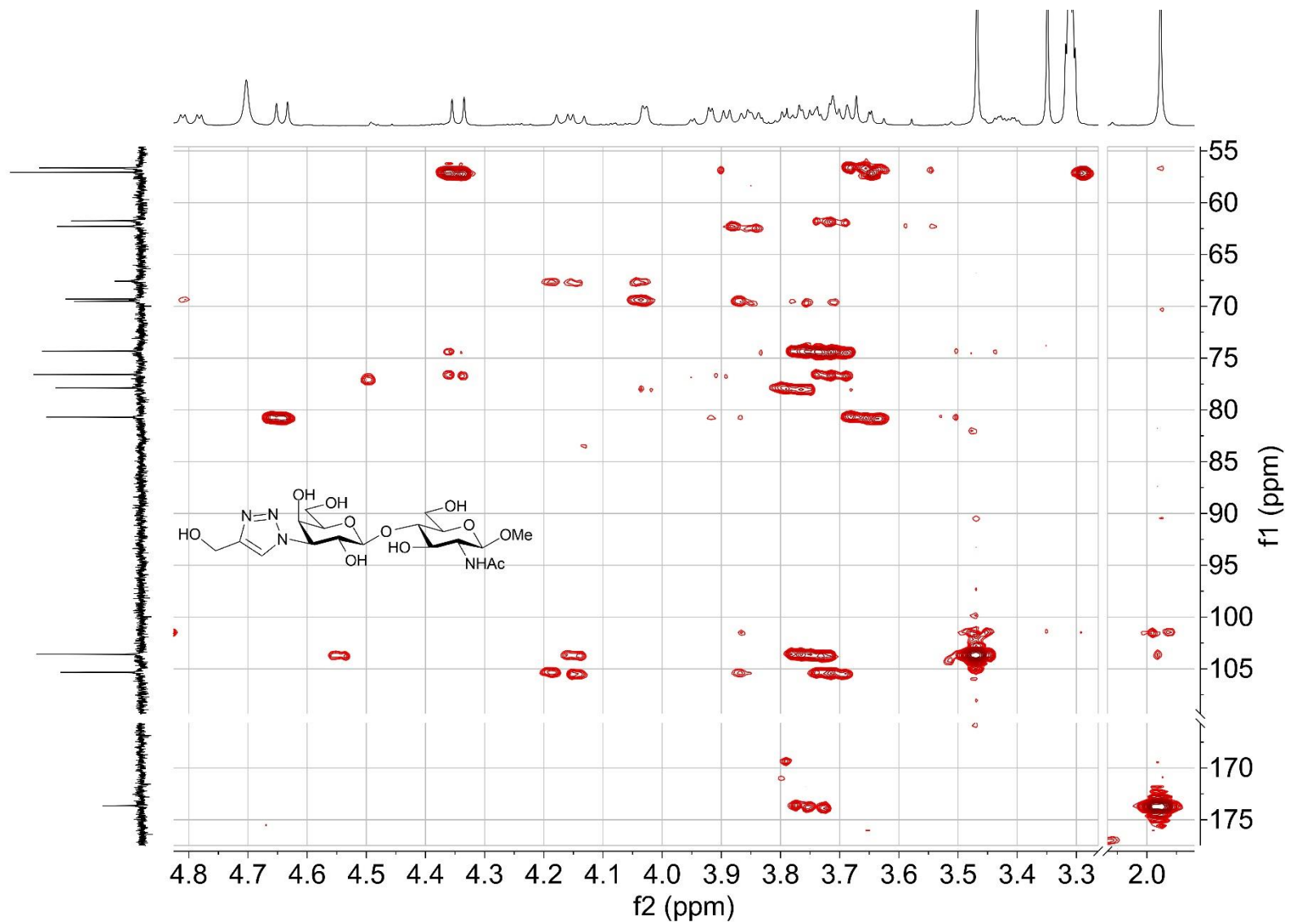
¹H-¹H COSY 29



^1H - ^{13}C HSQC 29

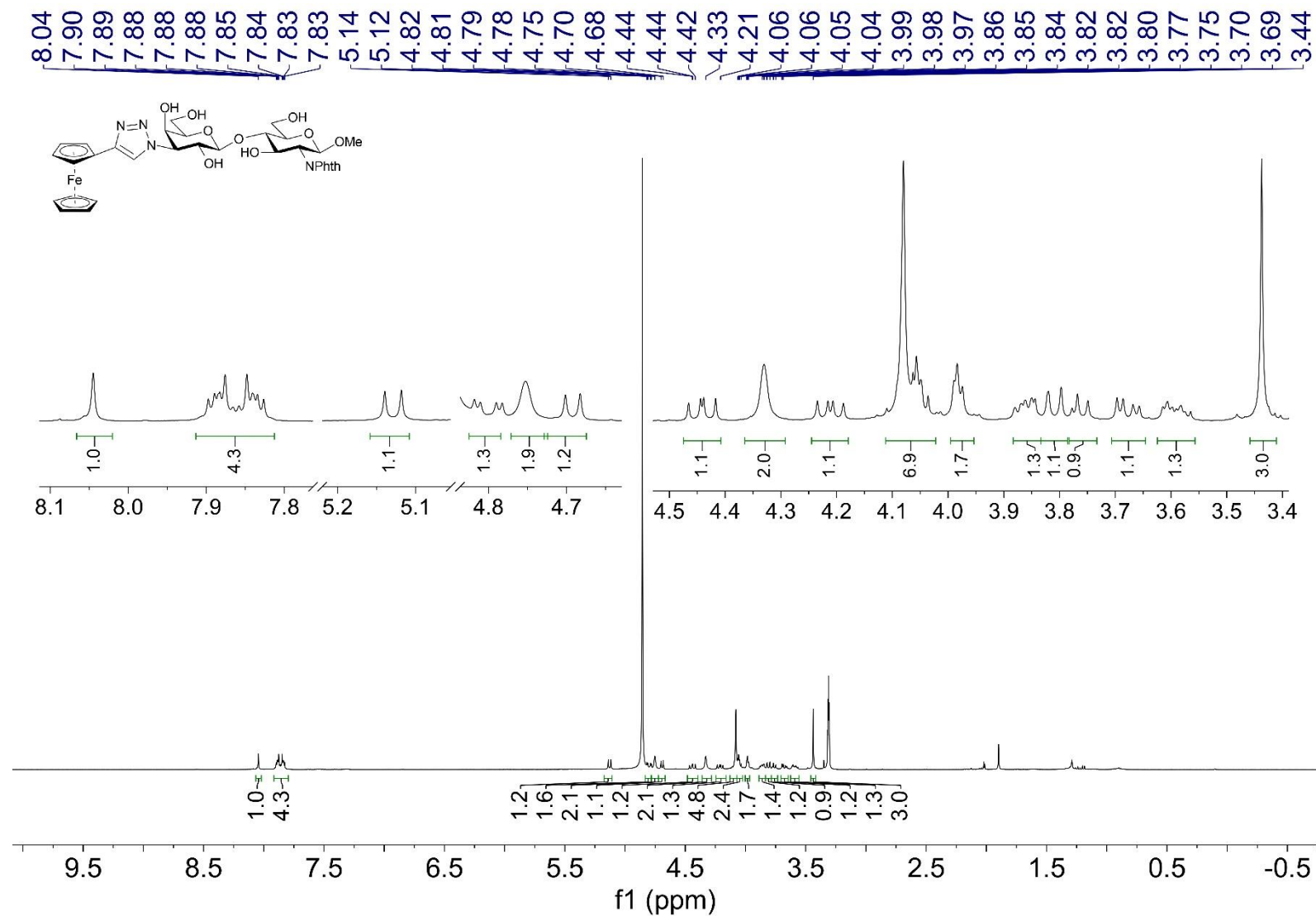


^1H - ^{13}C HMBC 29

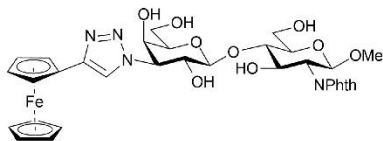


NMR COMPOUND 30

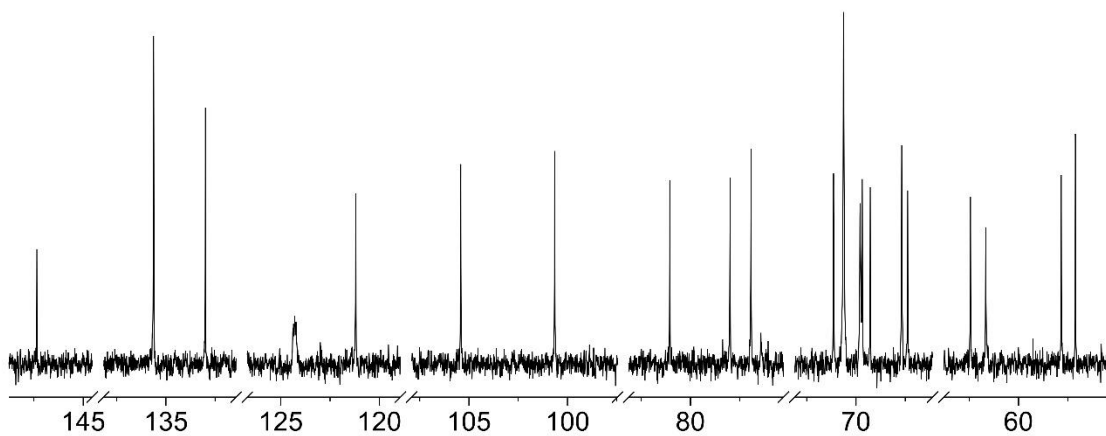
¹H NMR (400 MHz, MeOD) 30



¹³C NMR (101 MHz, MeOD) 30

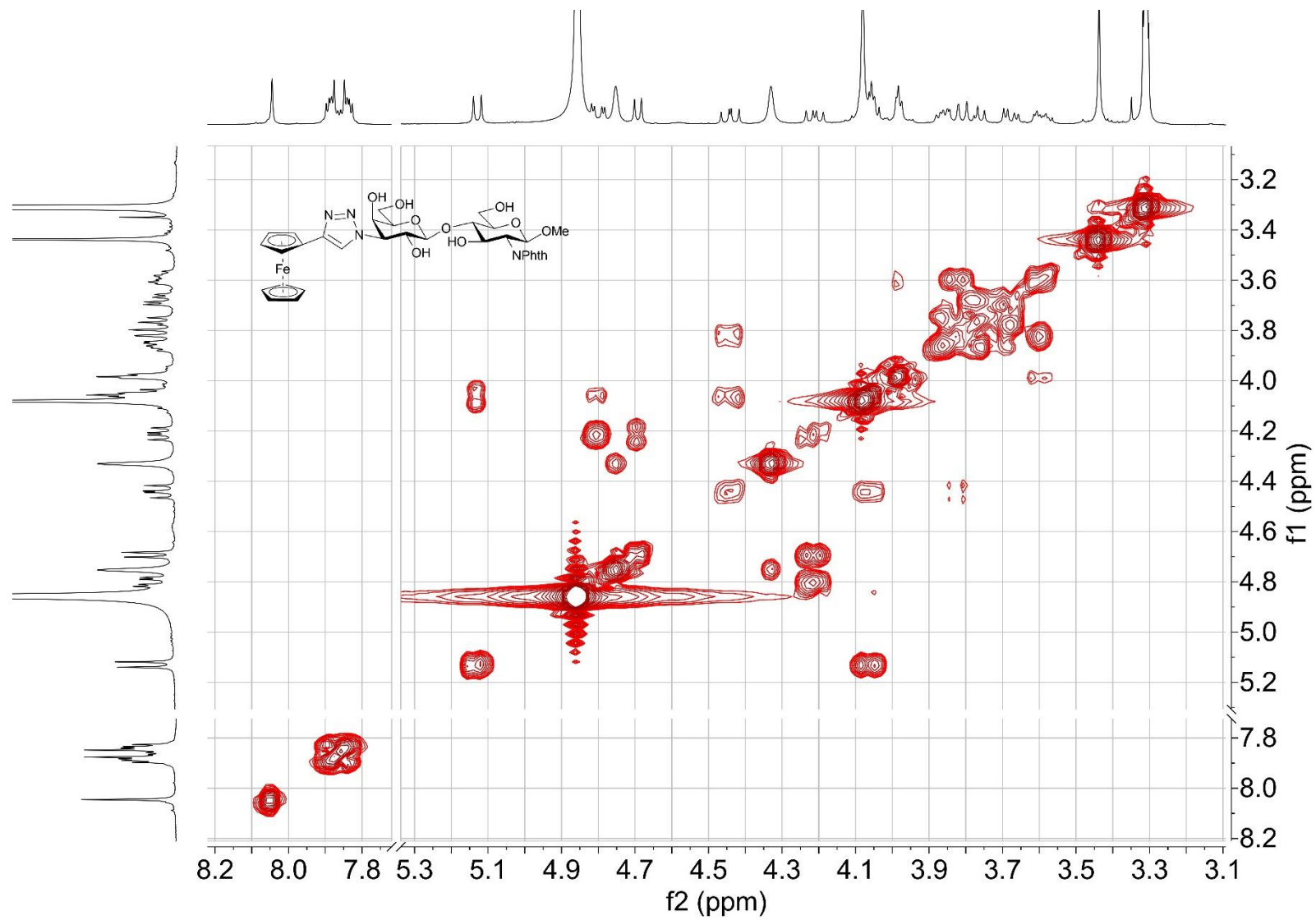


- ~147.35
- ~135.62
- ~132.99
- ~124.20
- ~121.19
- ~105.42
- ~100.65
- 81.05
- 77.99
- 76.93
- 71.14
- 70.63
- 69.79
- 69.68
- 69.28
- 67.68
- 67.38
- 62.44
- 61.66
- 57.83
- 57.11

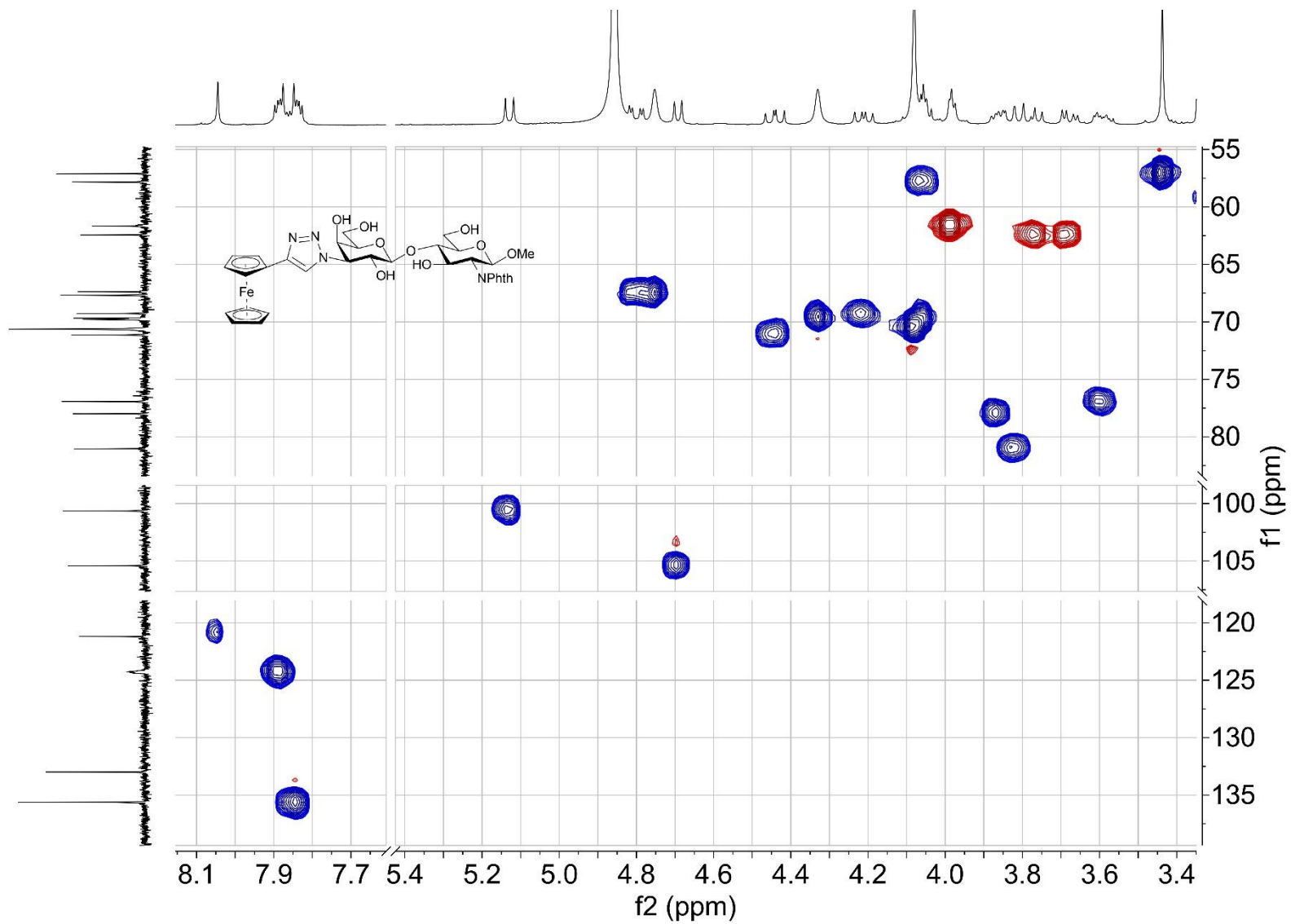


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

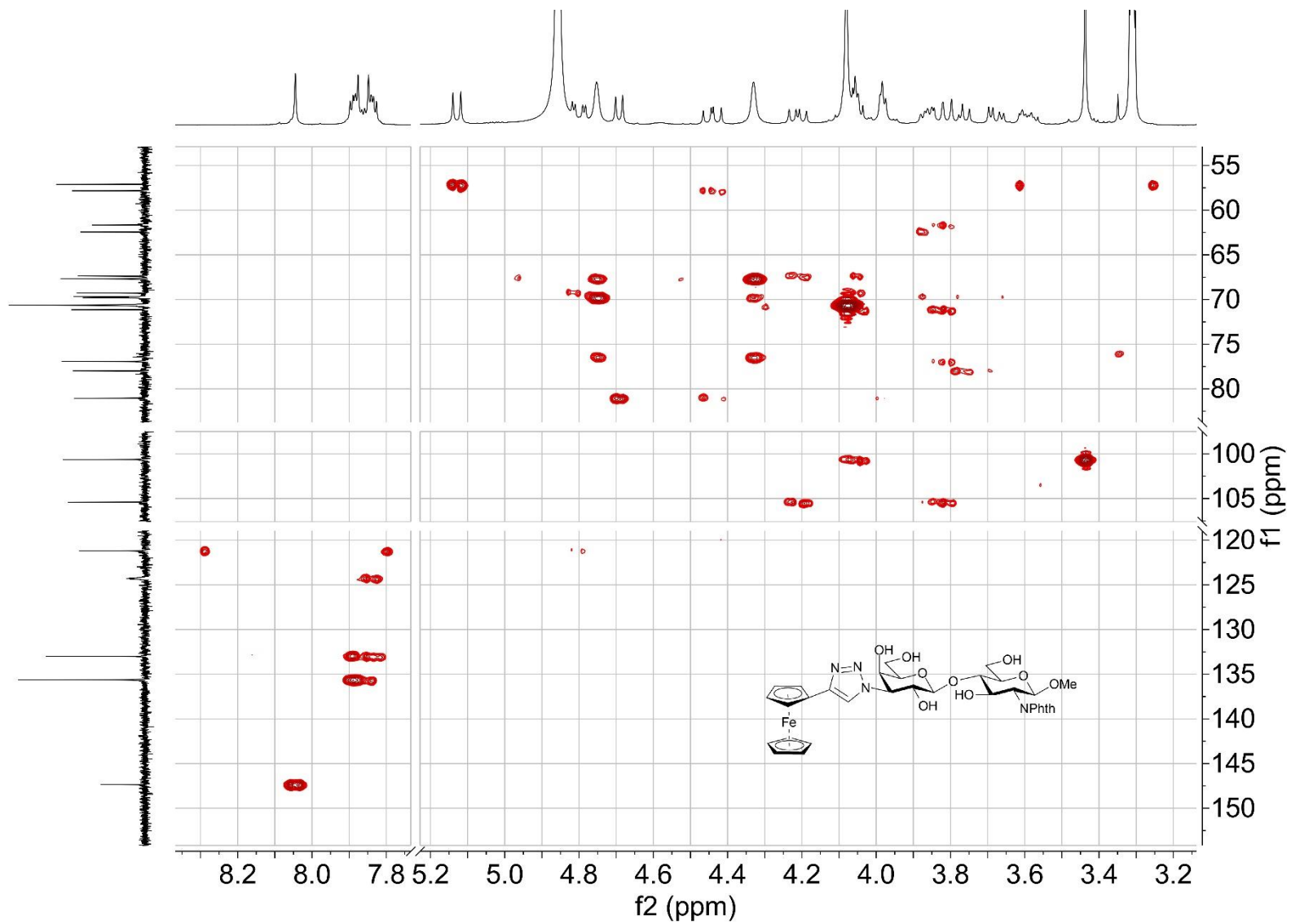
¹H-¹H COSY 30



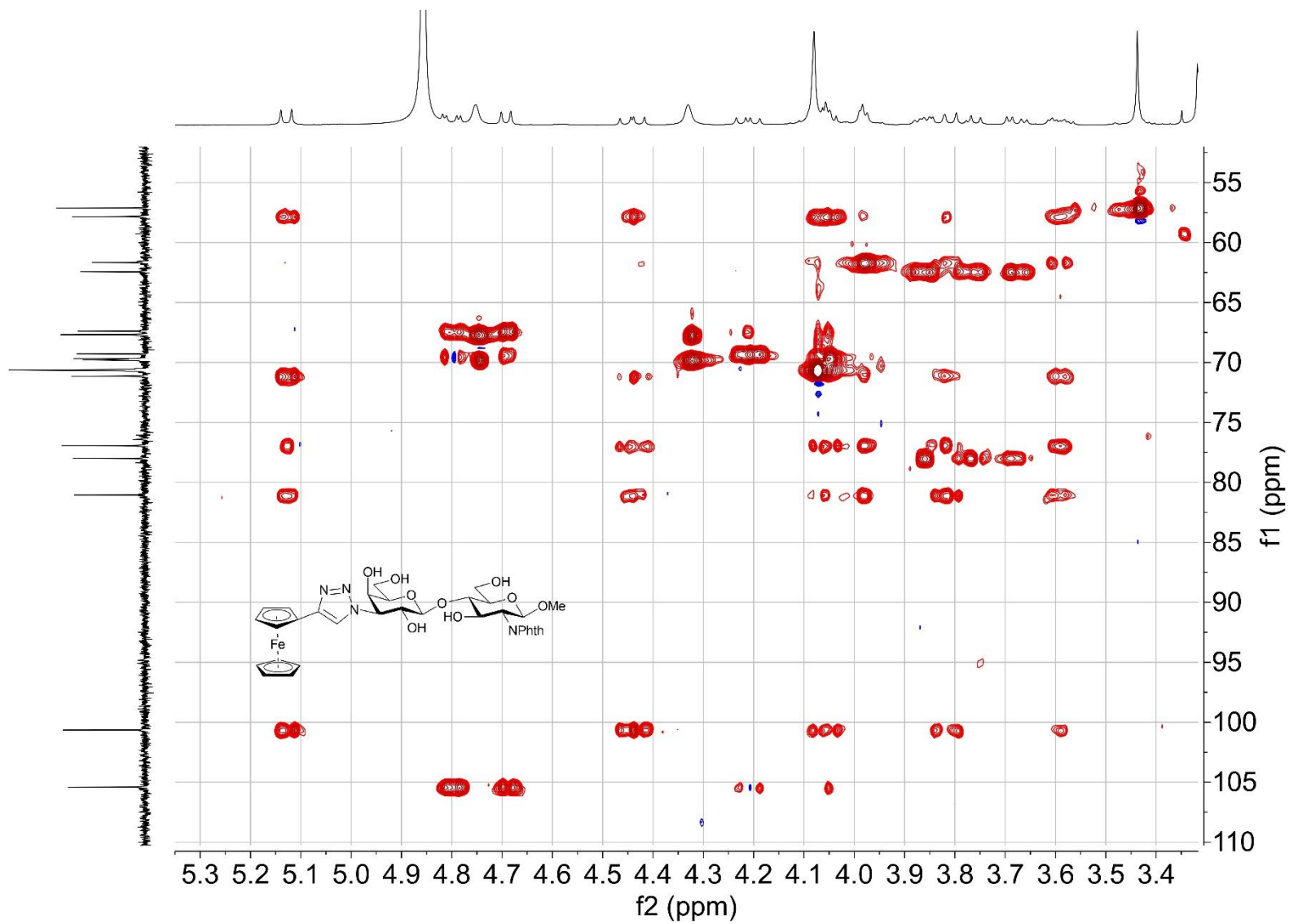
^1H - ^{13}C HSQC 30



^1H - ^{13}C HMBC 30

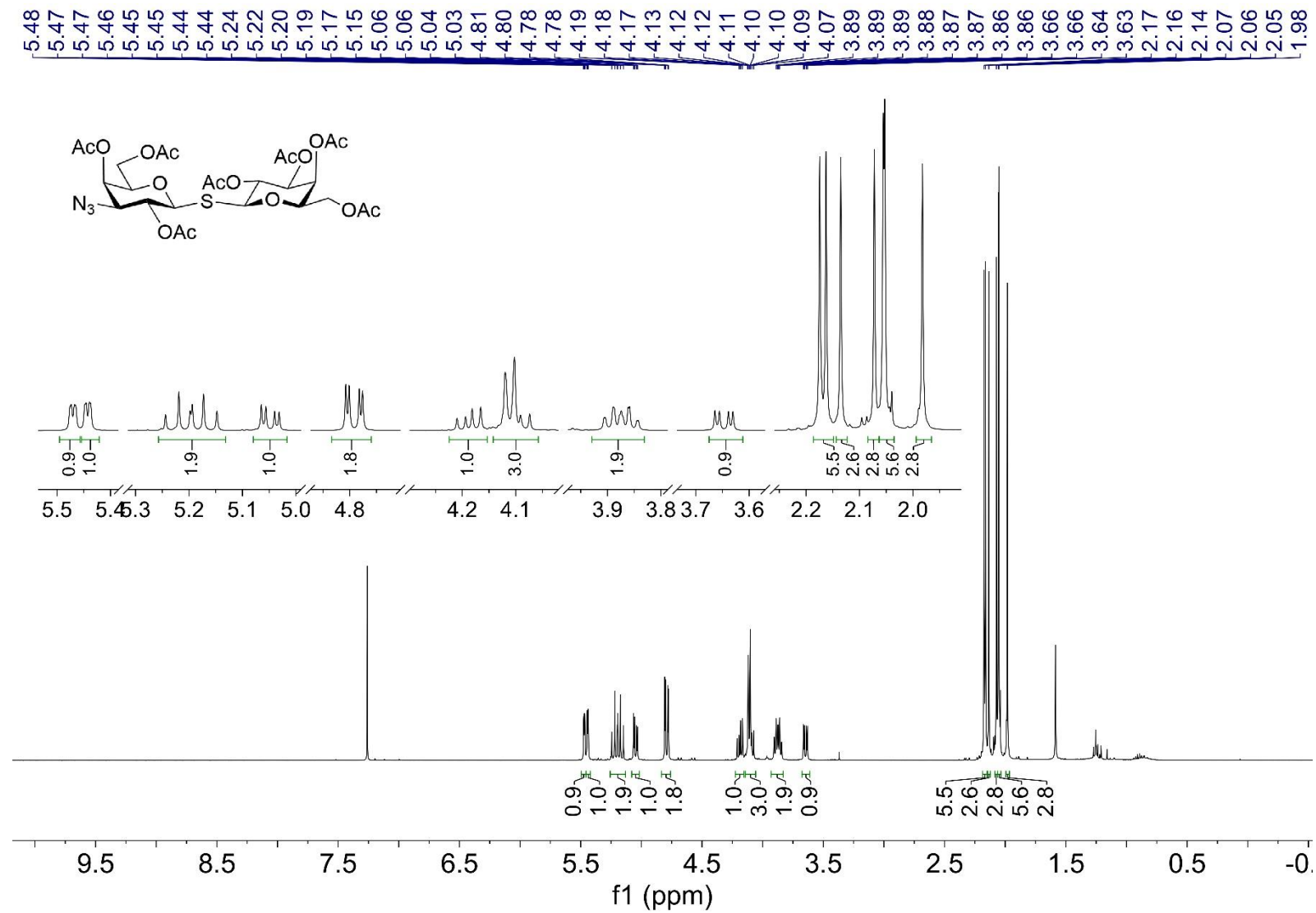


^1H - ^{13}C HSQCTOCSY 30



NMR COMPOUND 33

¹H NMR (400 MHz, CDCl₃) 33

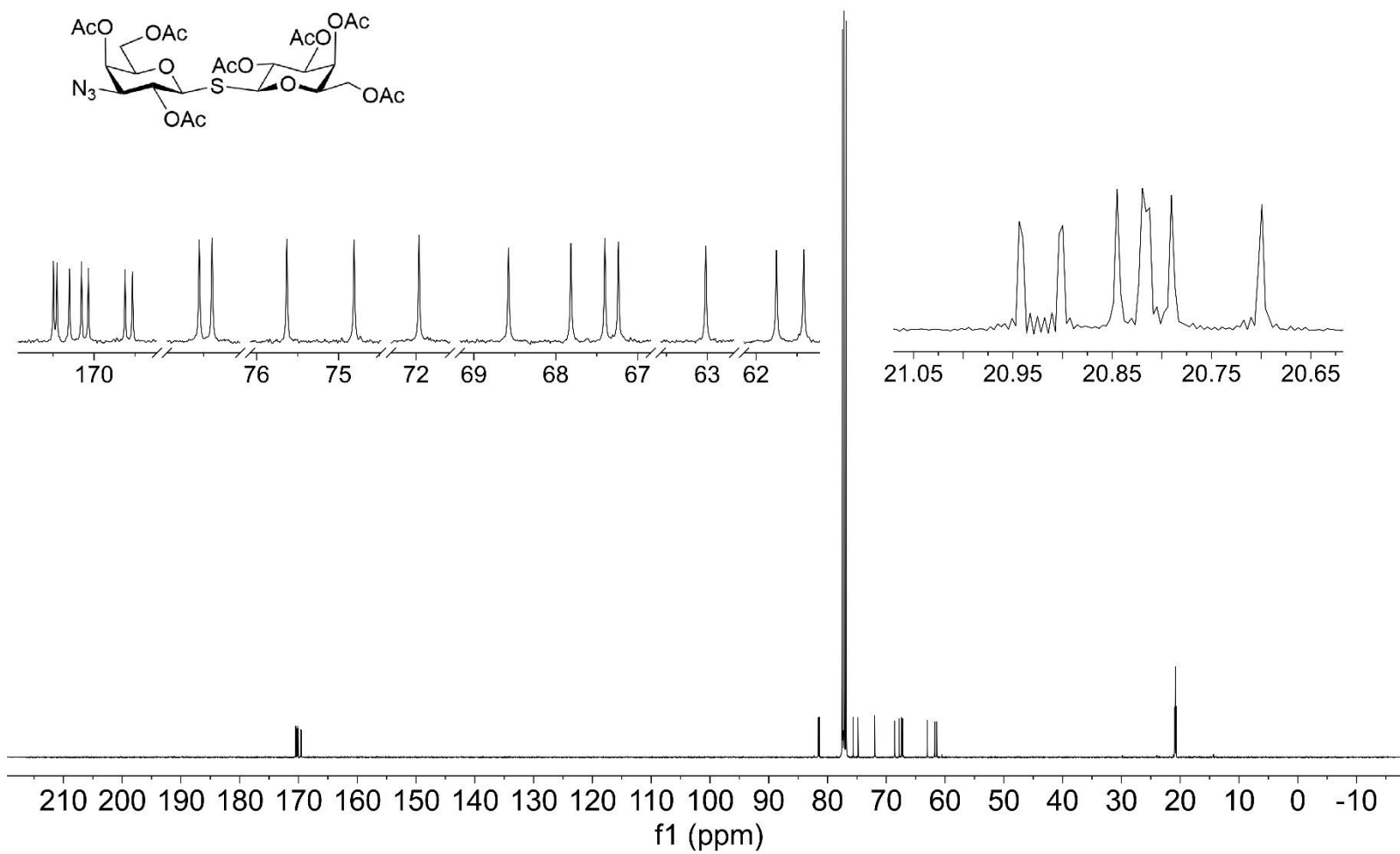
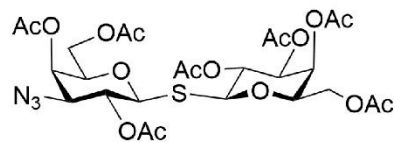


¹³C NMR (101 MHz, CDCl₃) 33

170.50
170.45
170.30
170.15
170.07
169.62
169.53

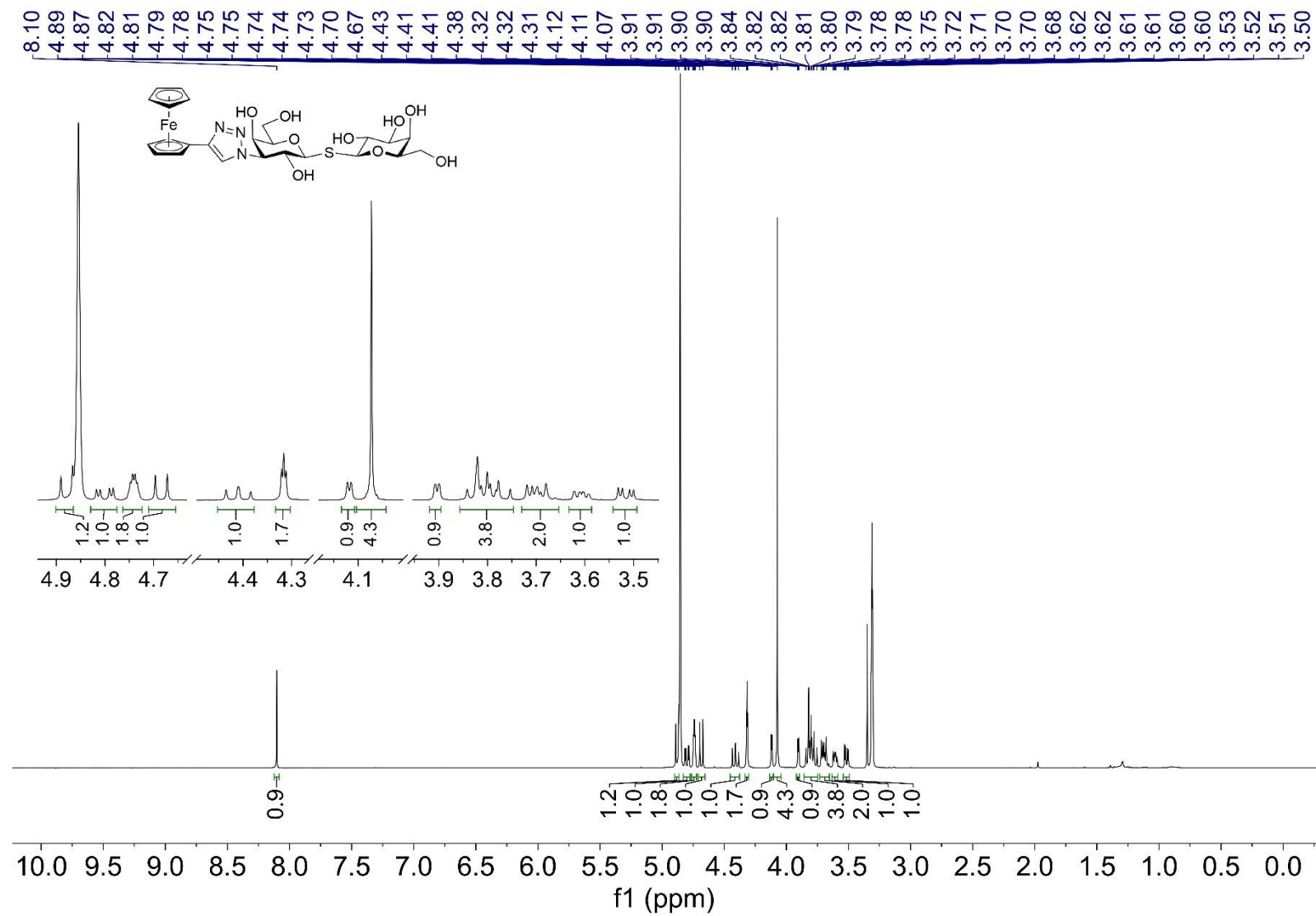
81.55
81.40
75.63
74.81
71.96
68.58
67.82
67.40
67.24
63.02
61.75
61.42

20.94
20.90
20.84
20.82
20.81
20.79
20.70

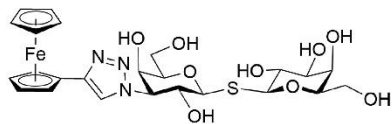


NMR COMPOUND 34

¹H NMR (400 MHz, MeOD) 34



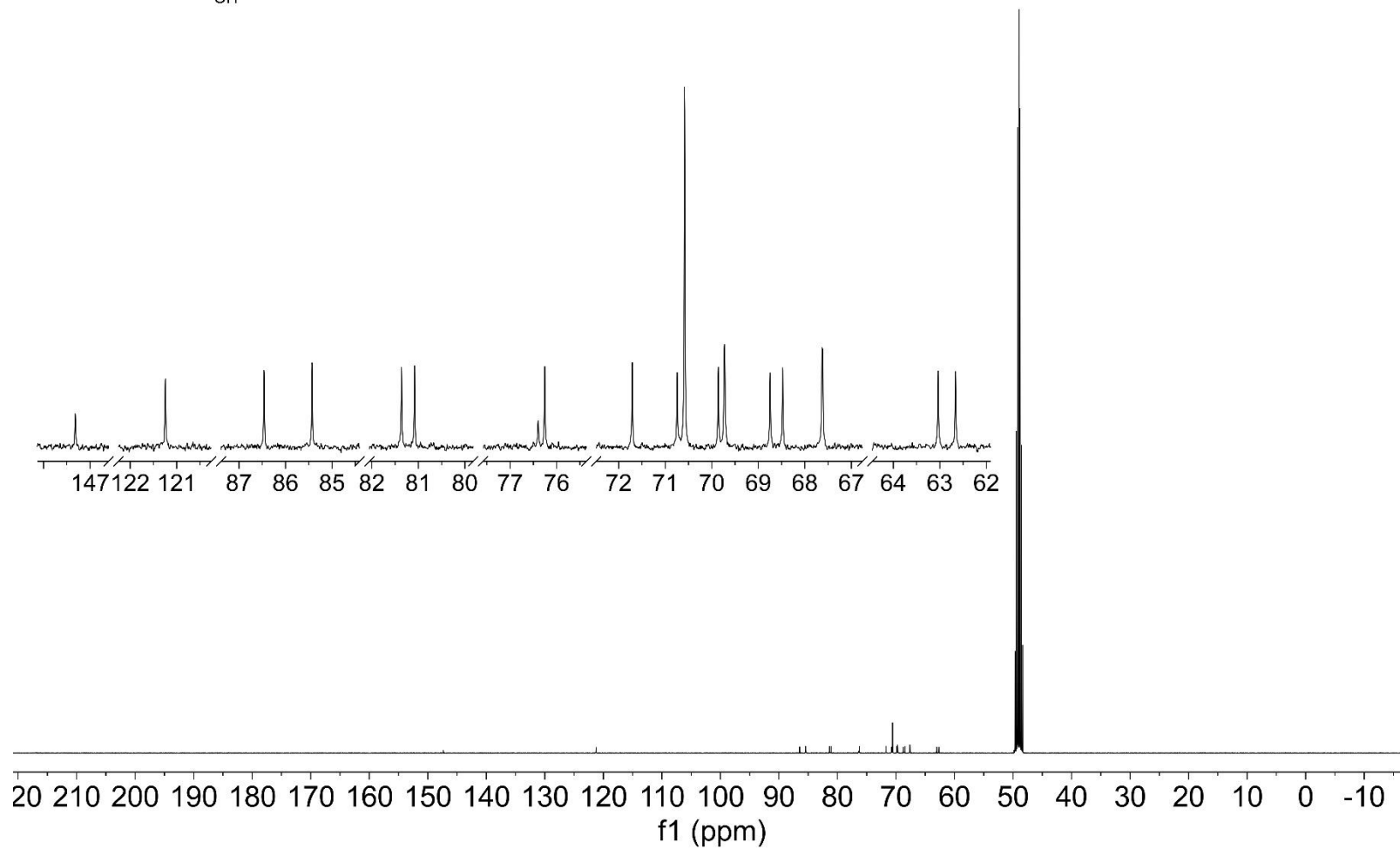
¹³C NMR (101 MHz, MeOD) 34



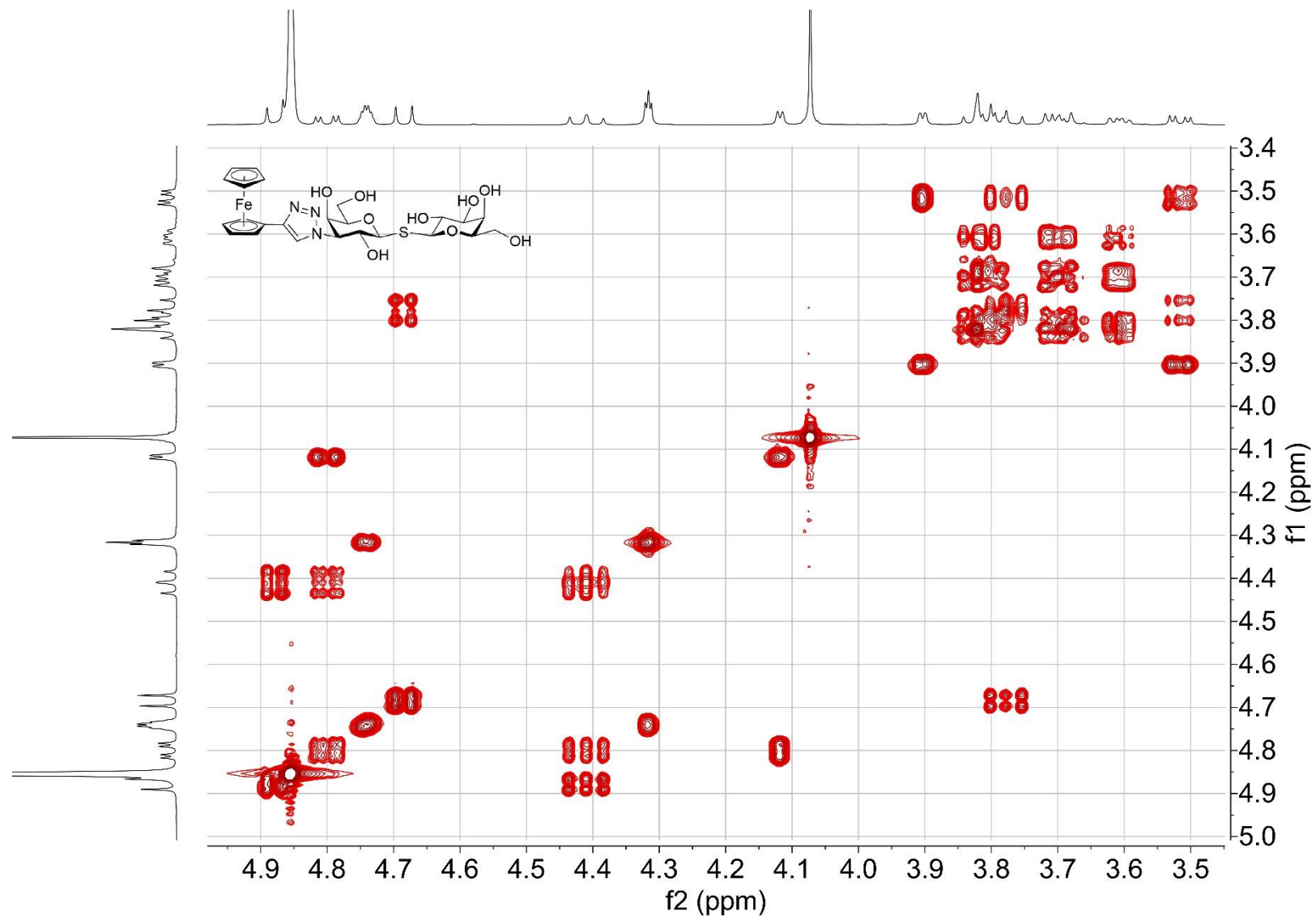
-147.32

-121.24

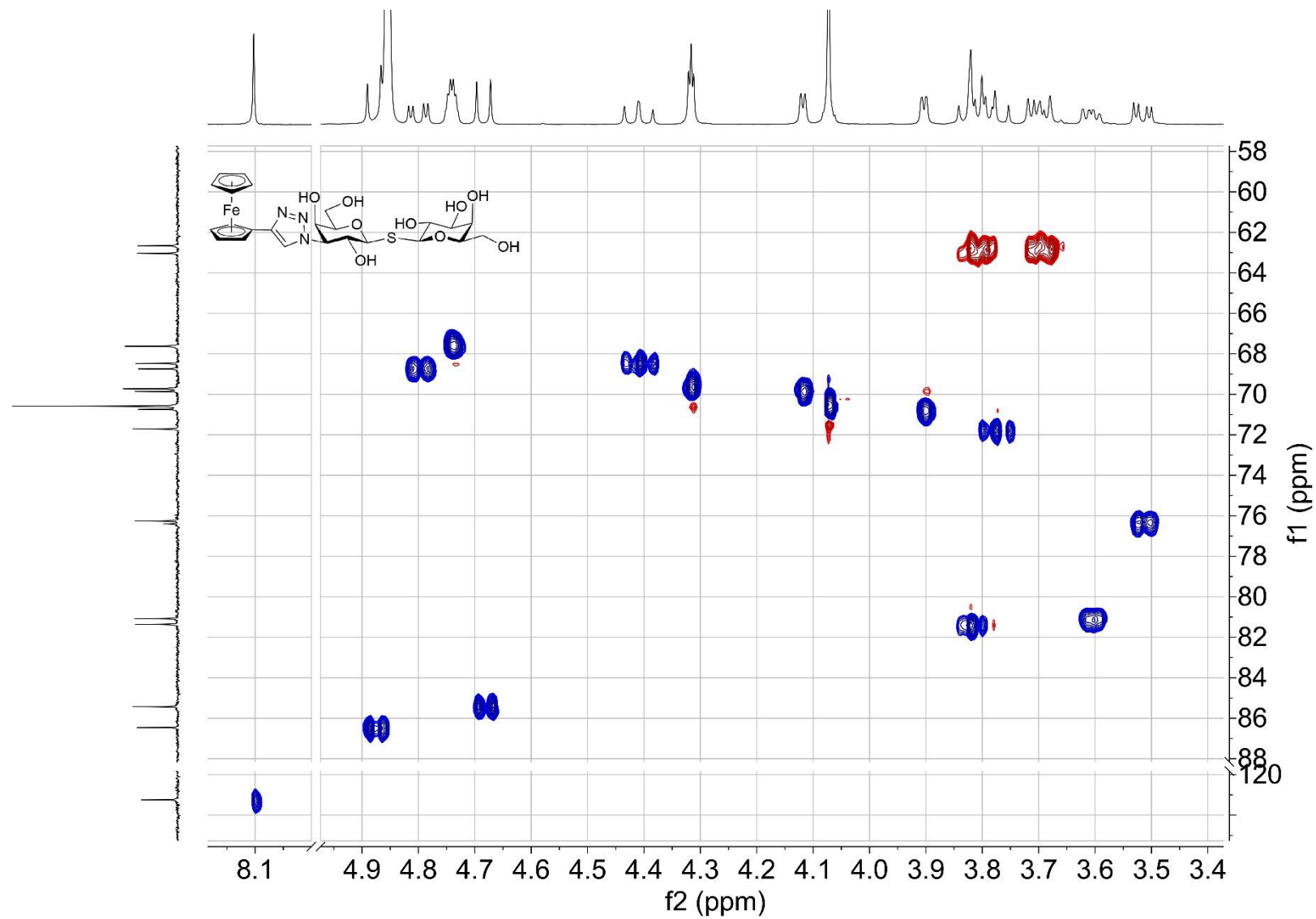
86.46
85.43
81.36
81.08
76.40
76.26
71.71
70.74
70.58
69.86
69.73
68.75
68.48
67.63
67.62
63.04
62.66



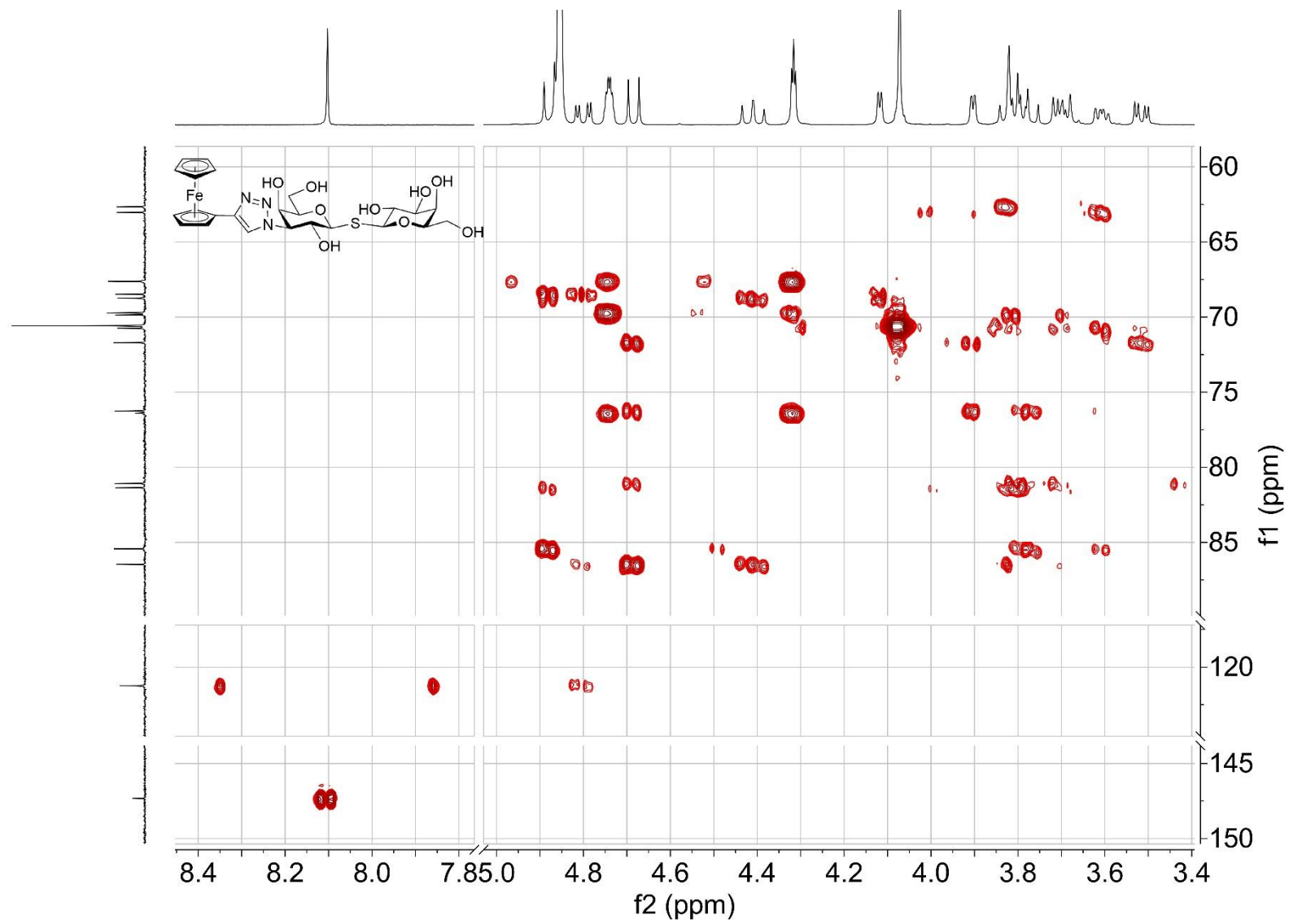
¹H-¹H COSY 34



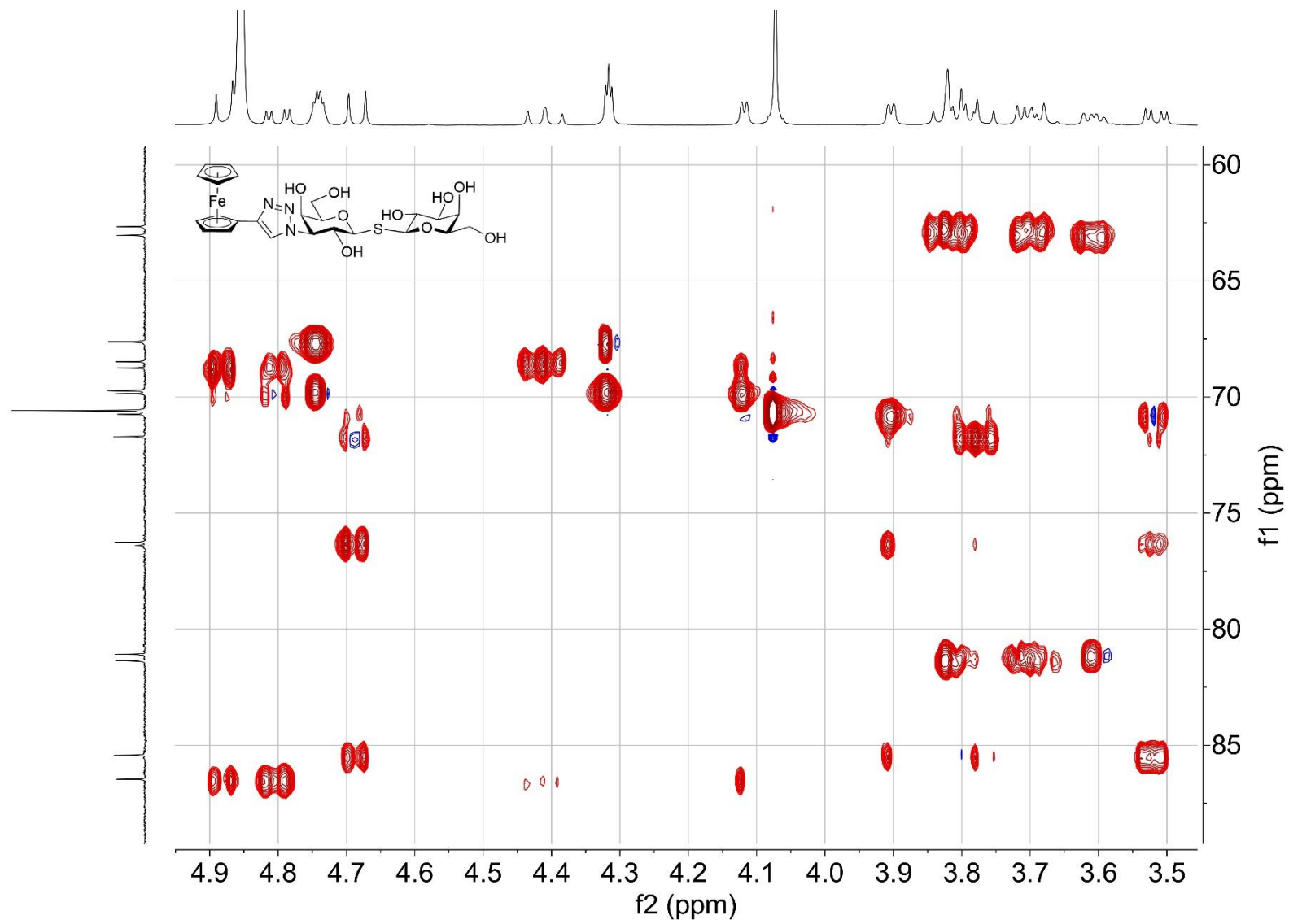
^1H - ^{13}C HSQC 34



^1H - ^{13}C HMBC 34

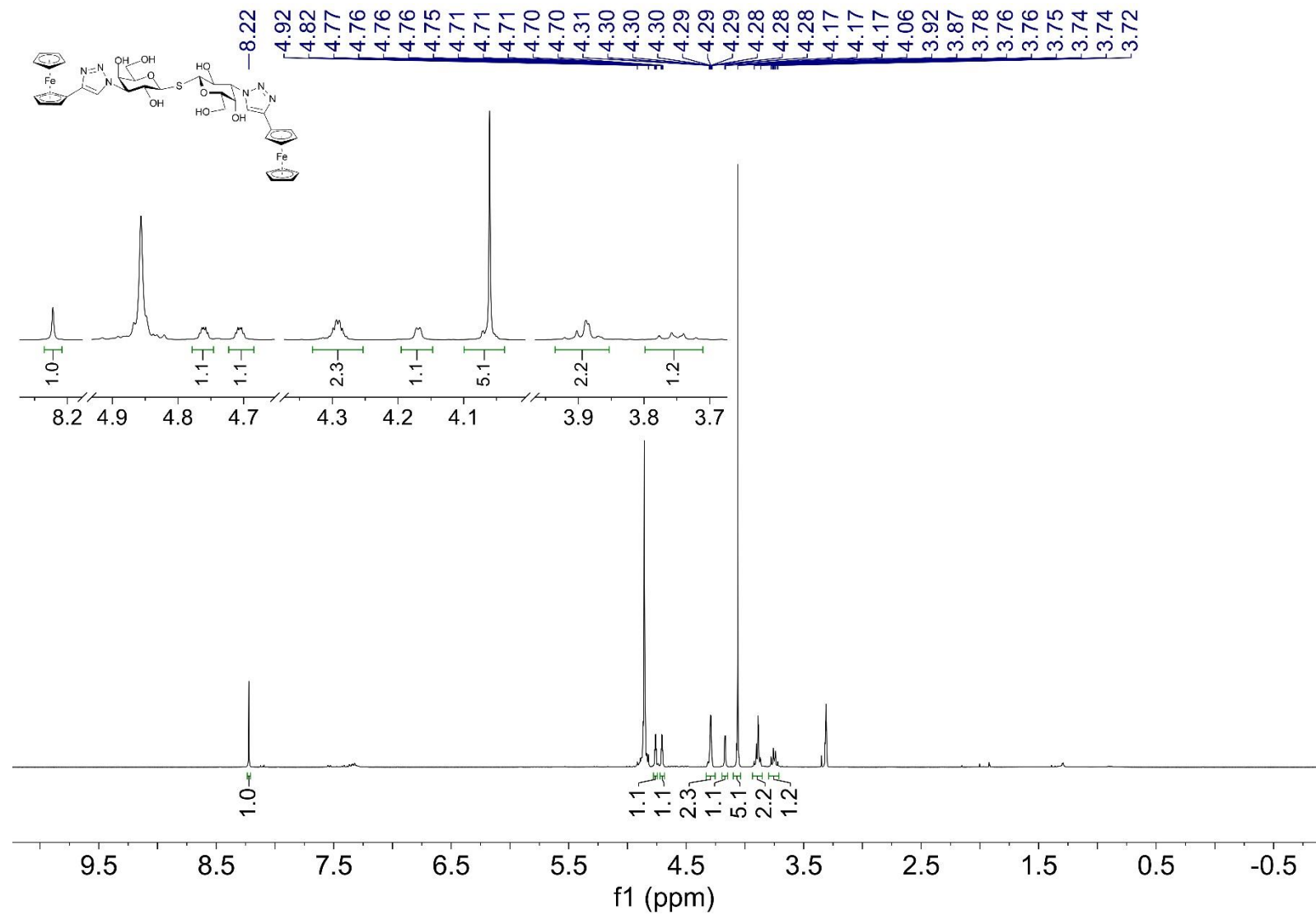


^1H - ^{13}C HSQCTOCSY 34

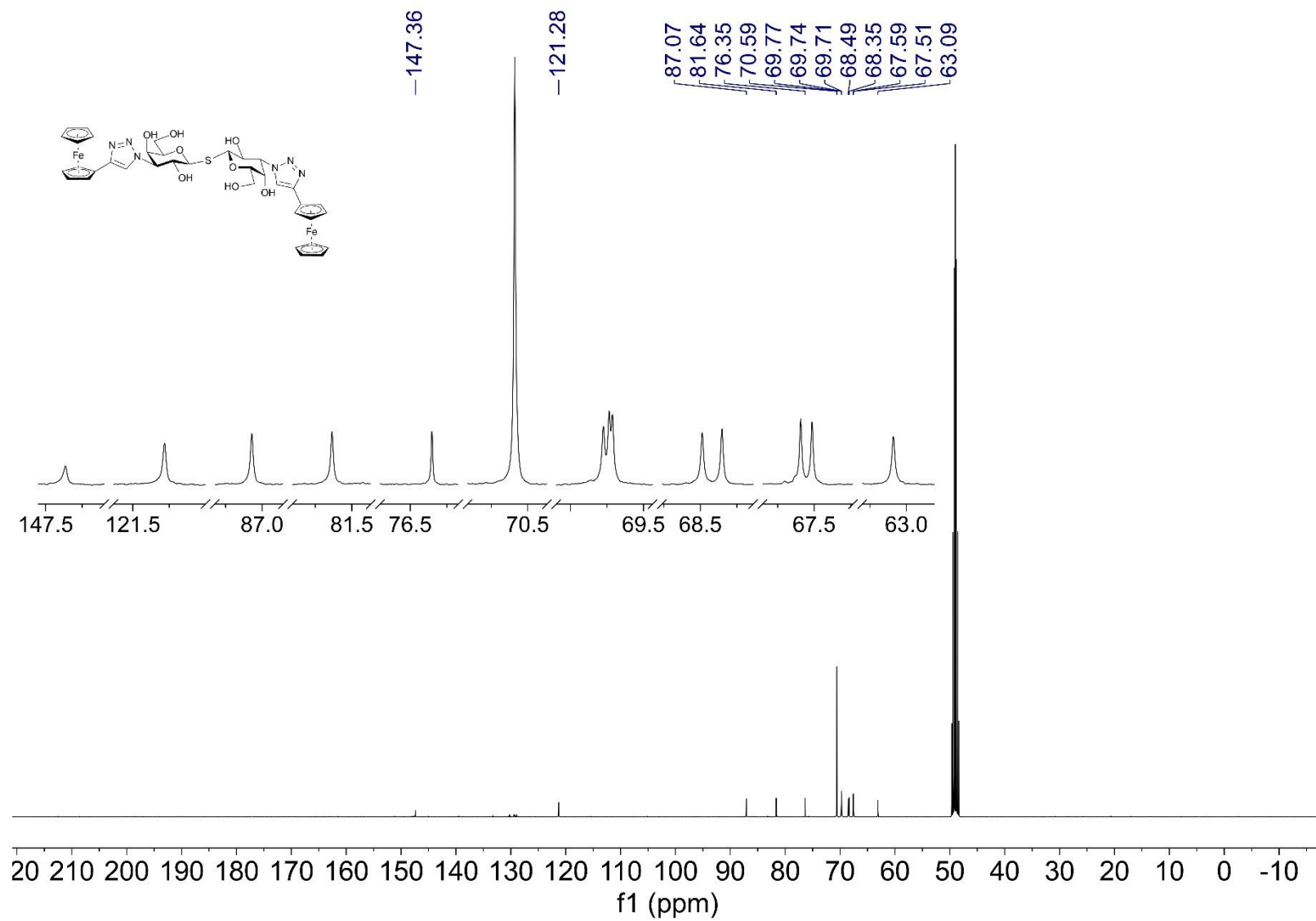


NMR COMPOUND 36

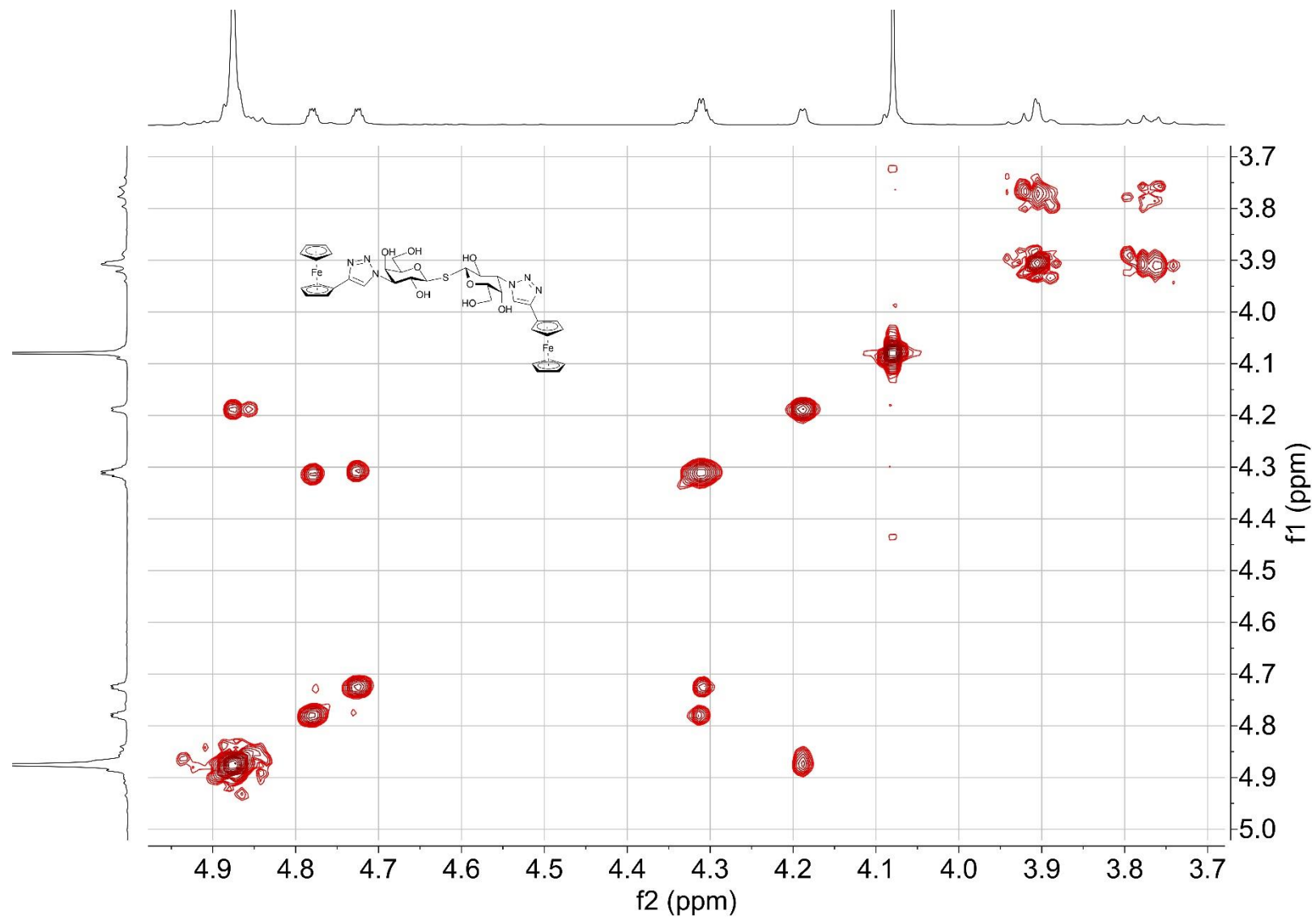
¹H NMR (400 MHz, MeOD) 36



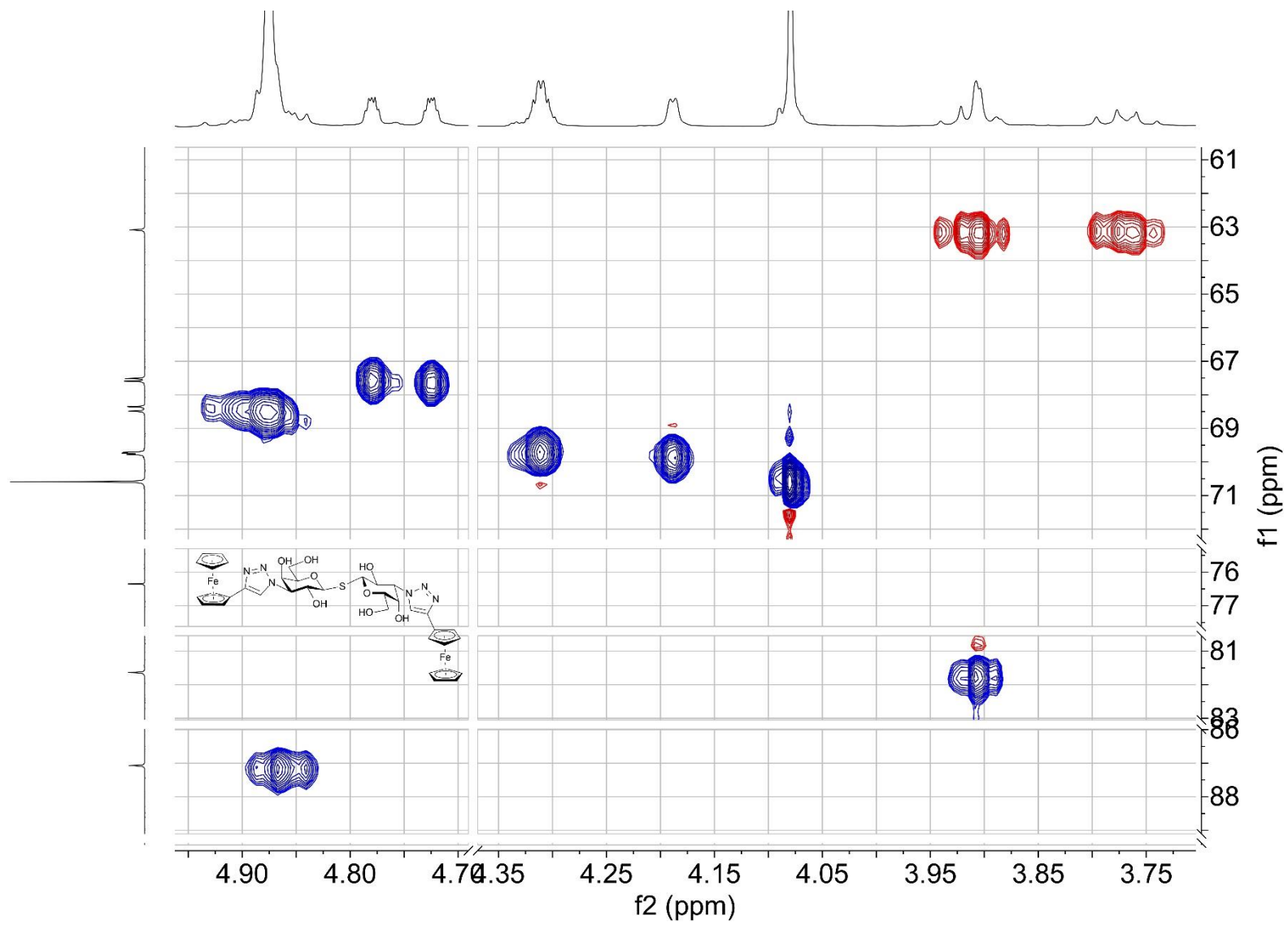
¹³C NMR (101 MHz, MeOD) 36



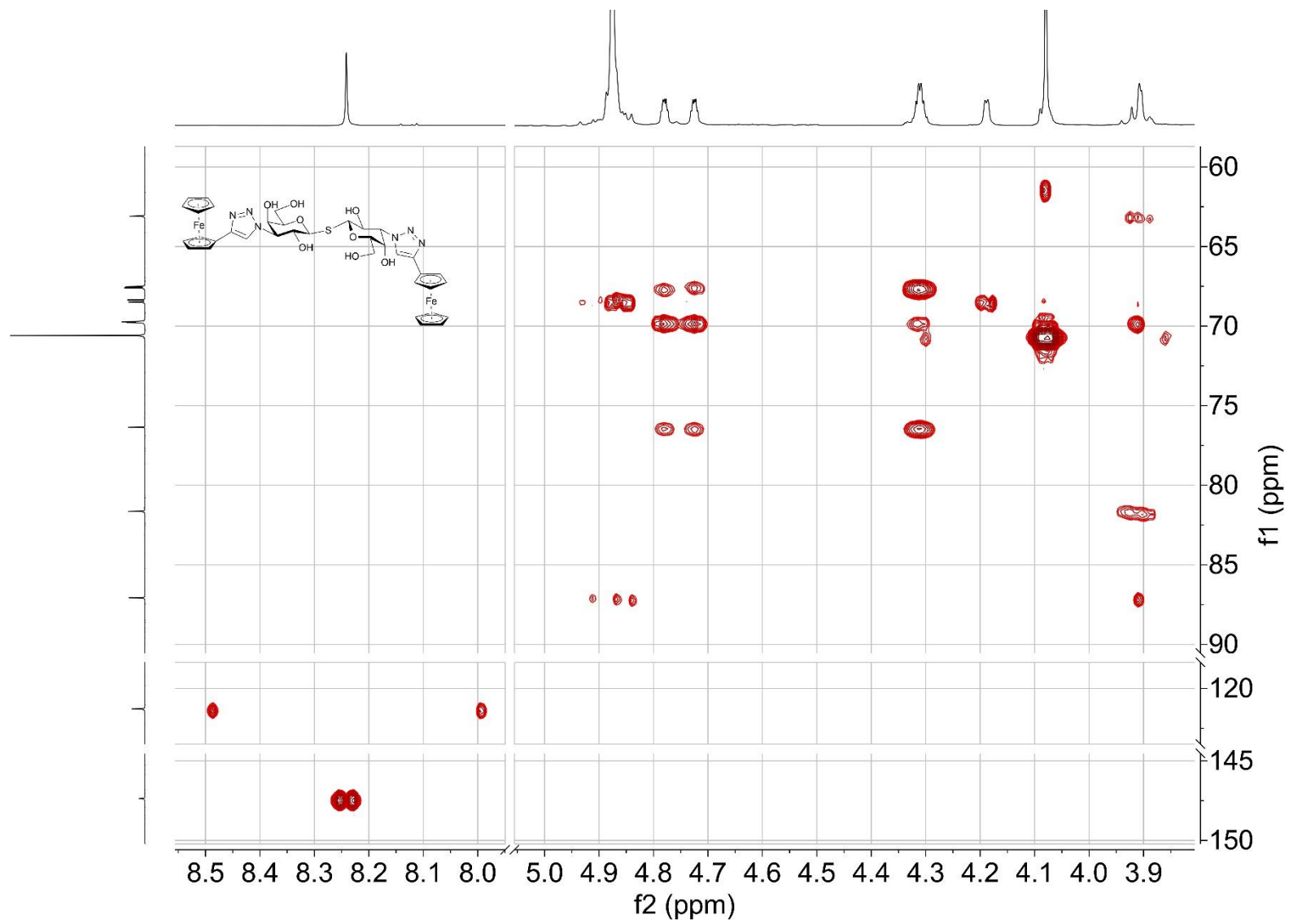
¹H-¹H COSY 36



^1H - ^{13}C HSQC 36

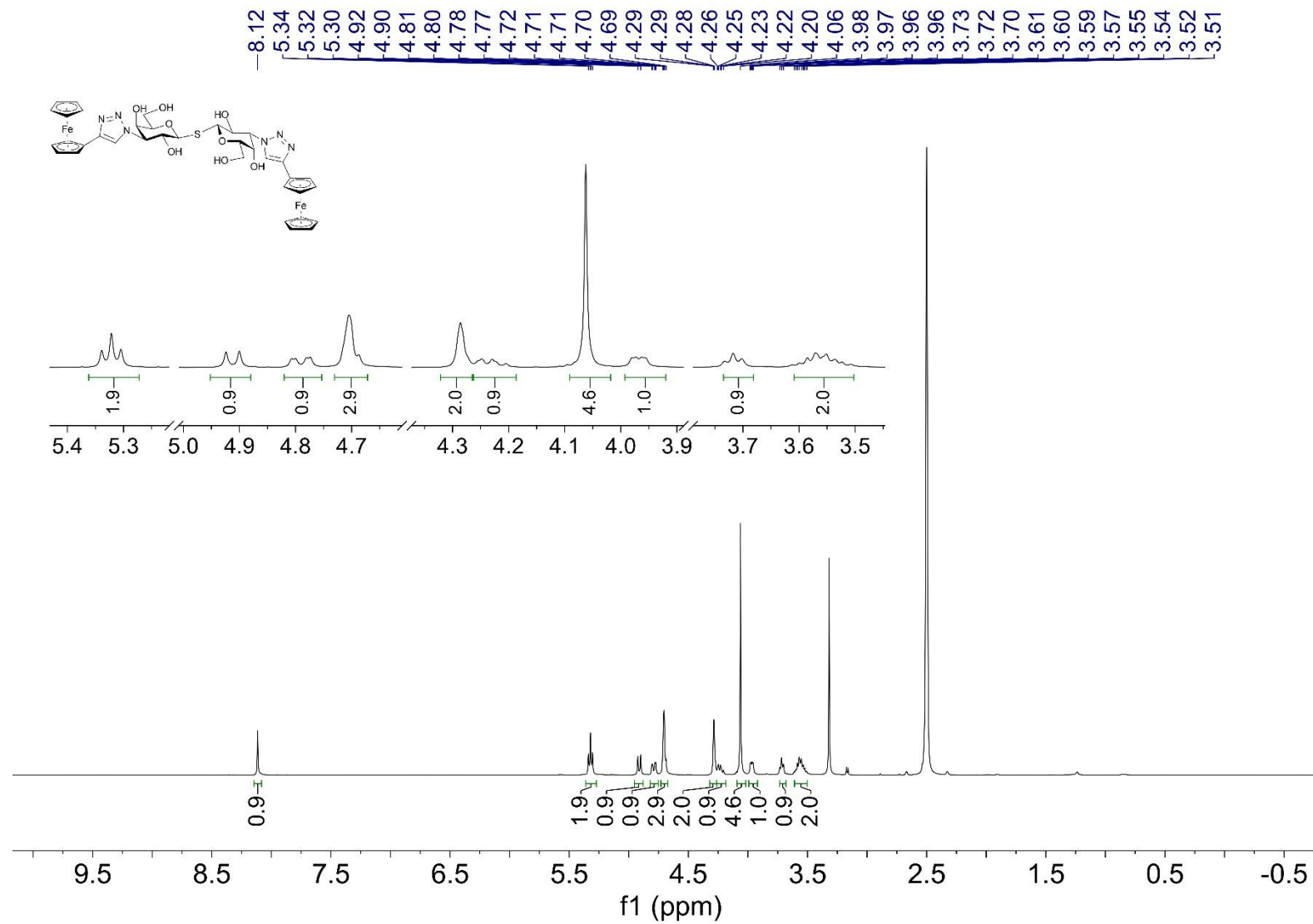


^1H - ^{13}C HMBC 36

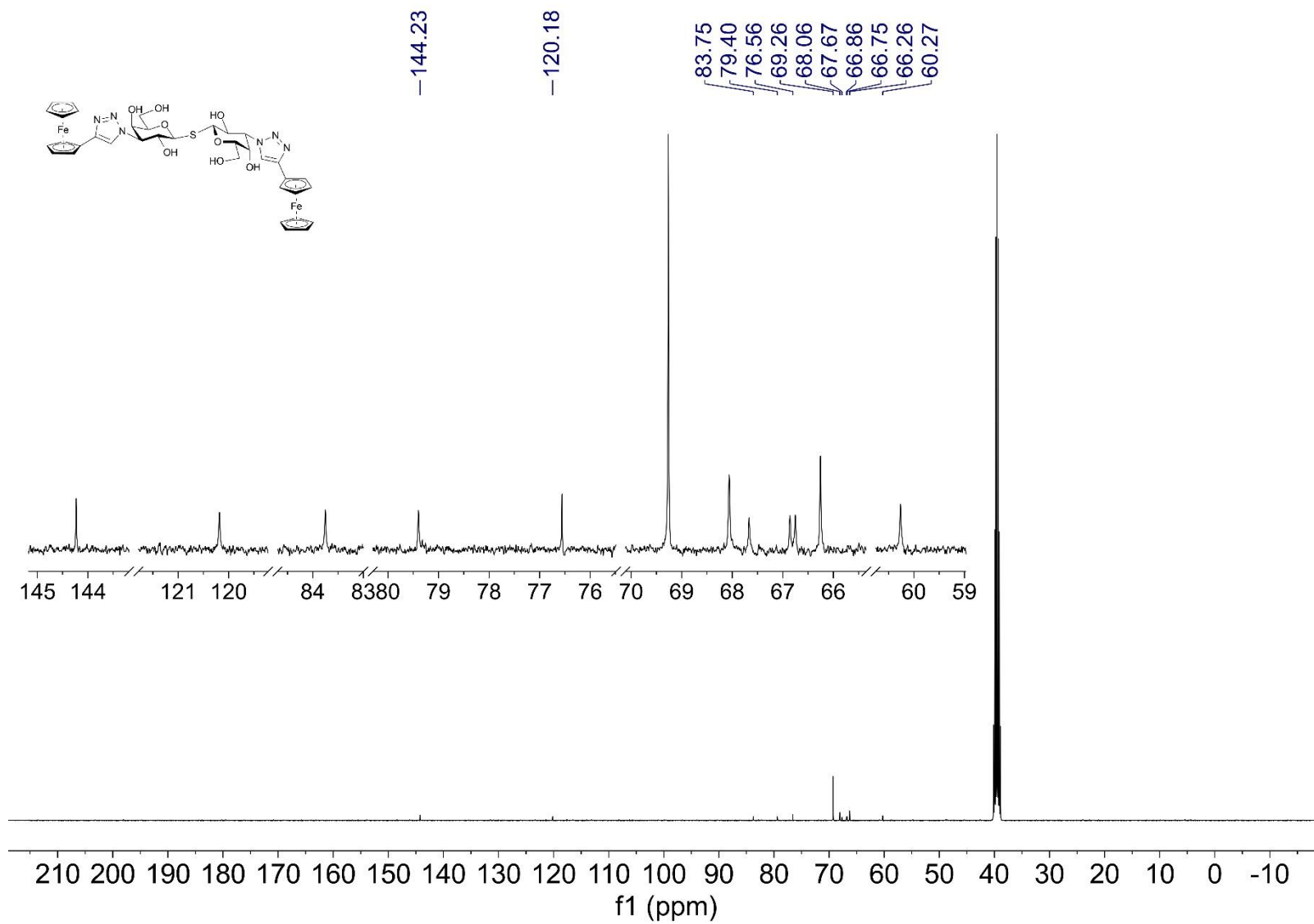


NMR COMPOUND 36

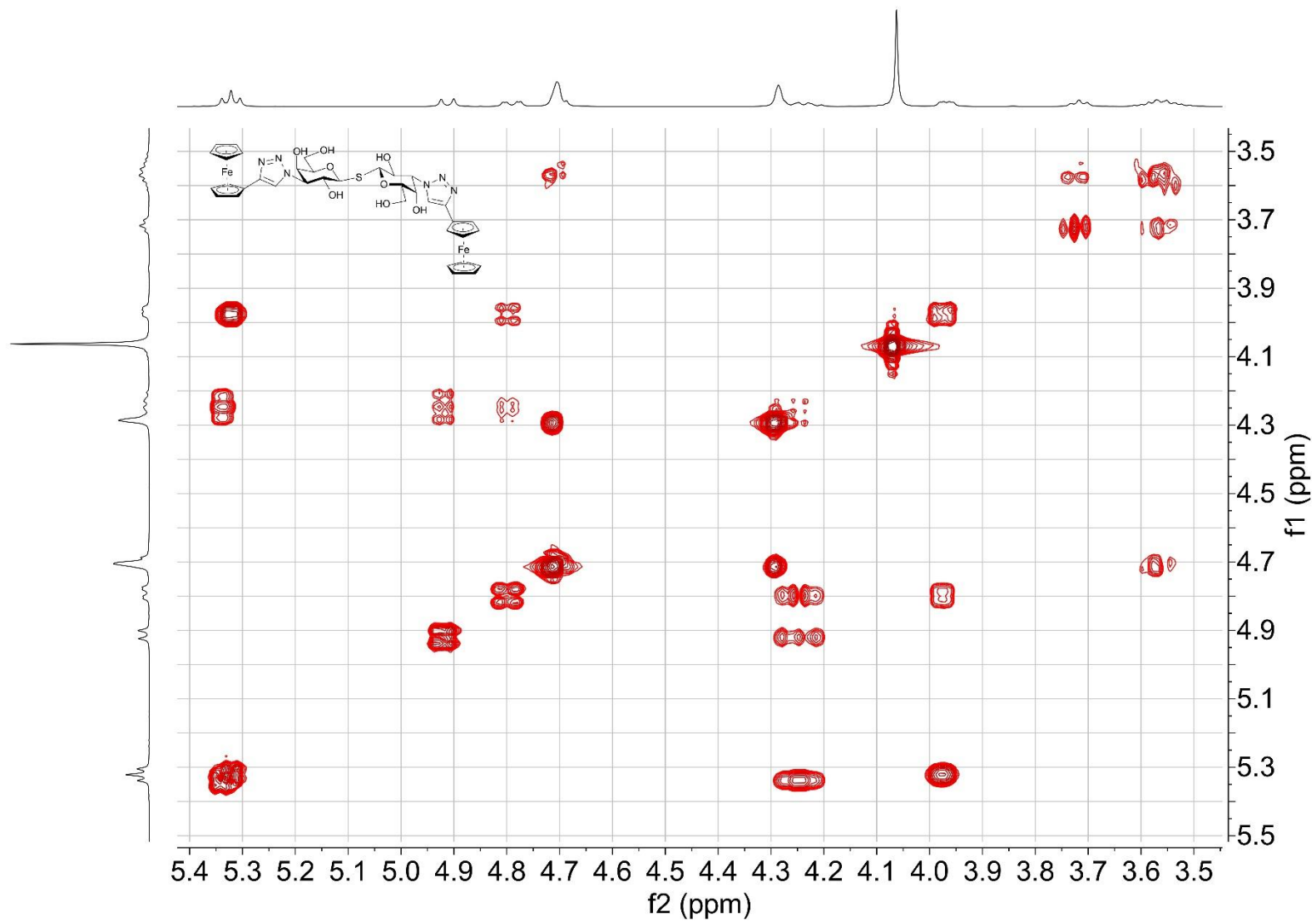
¹H NMR (400 MHz, DMSO-d₆) 36



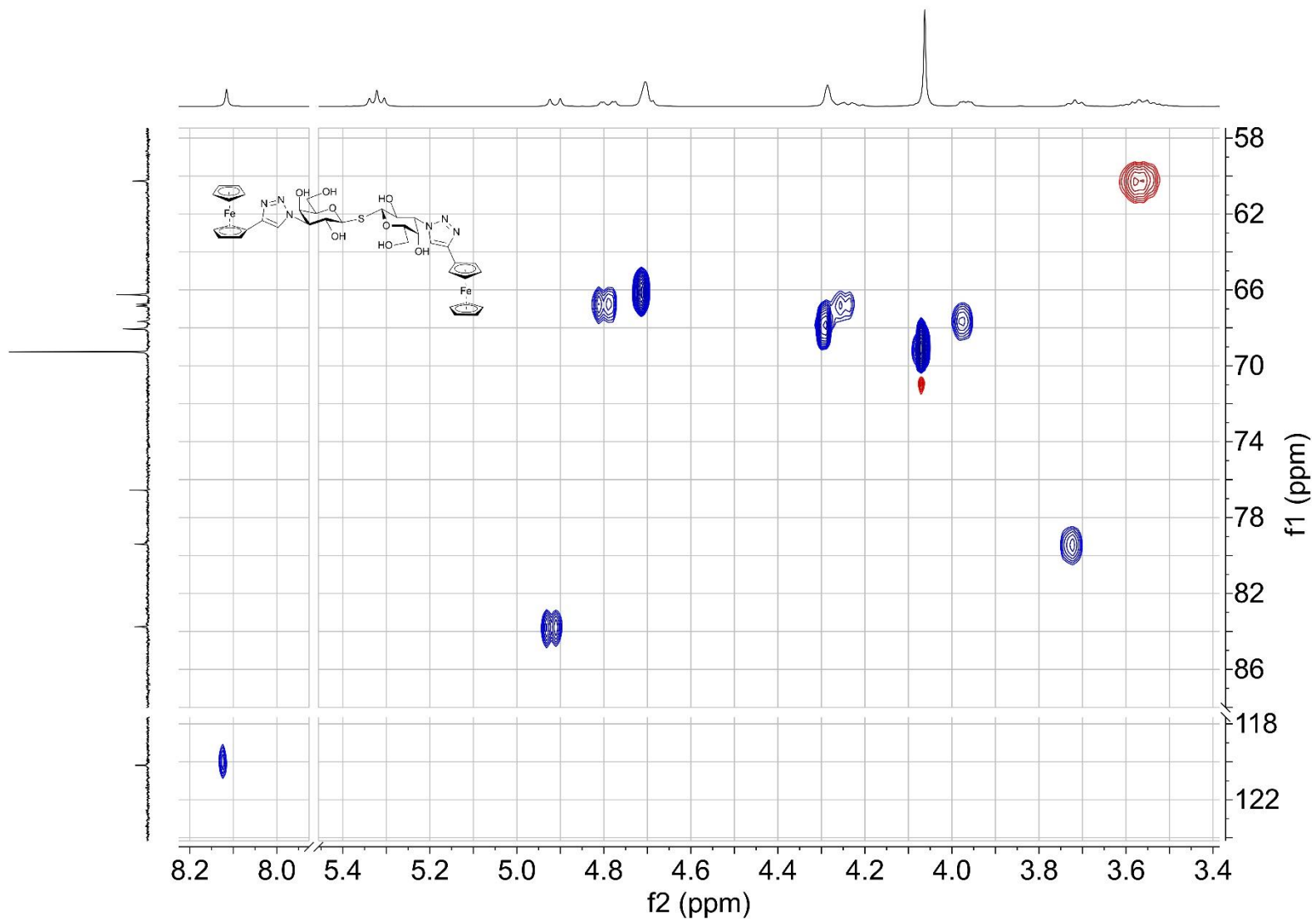
¹³C NMR (101 MHz, DMSO-d₆) 36



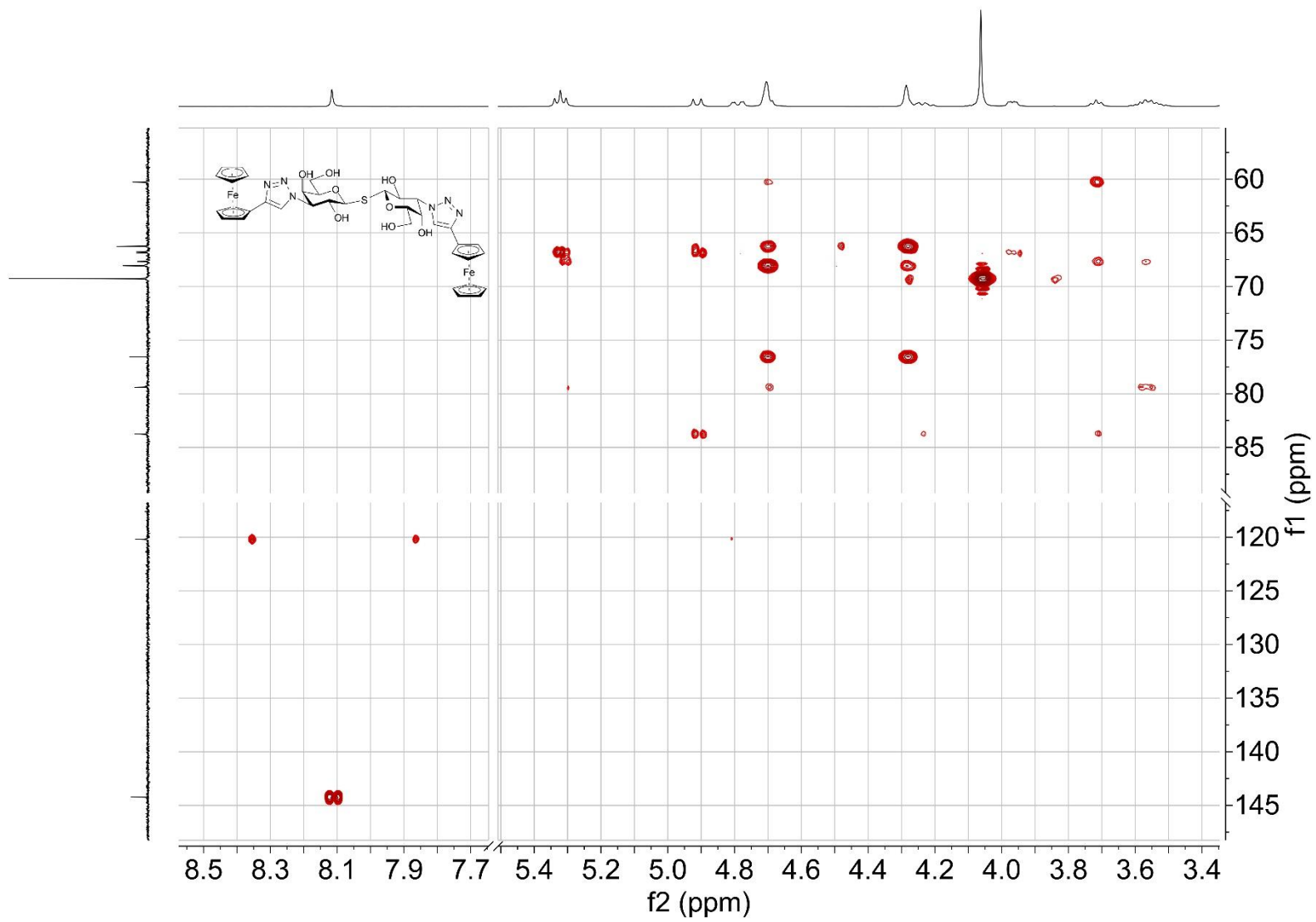
^1H - ^1H COSY 36



^1H - ^{13}C HSQC 36

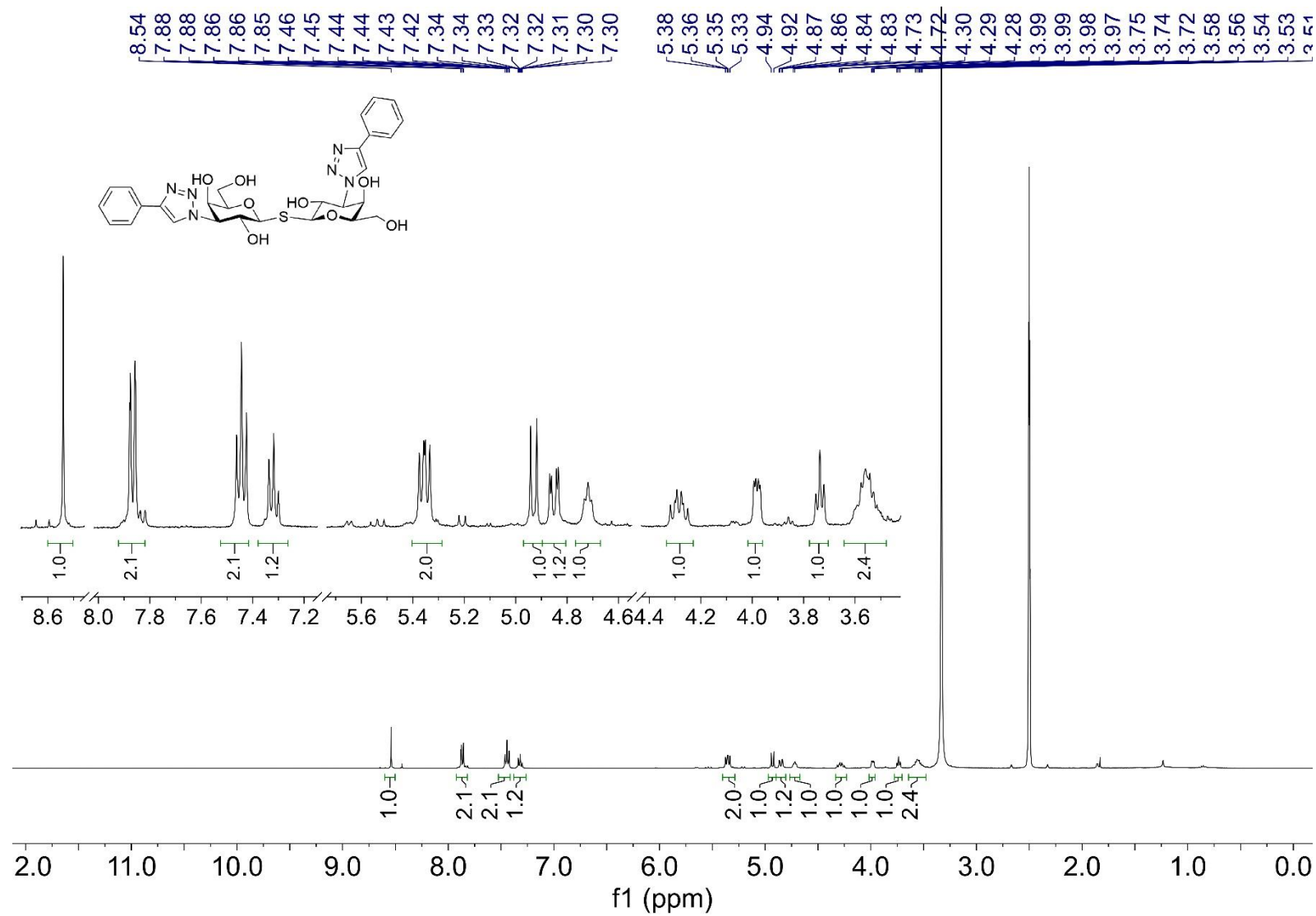


^1H - ^{13}C HMBC 36

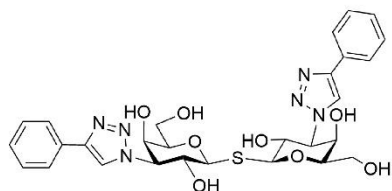


NMR COMPOUND 37

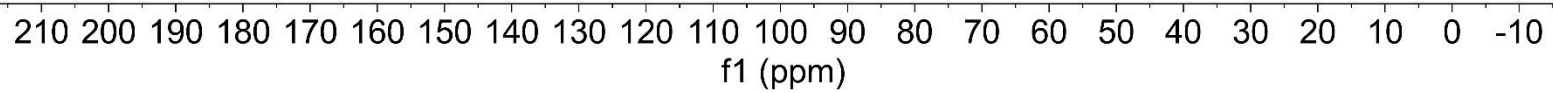
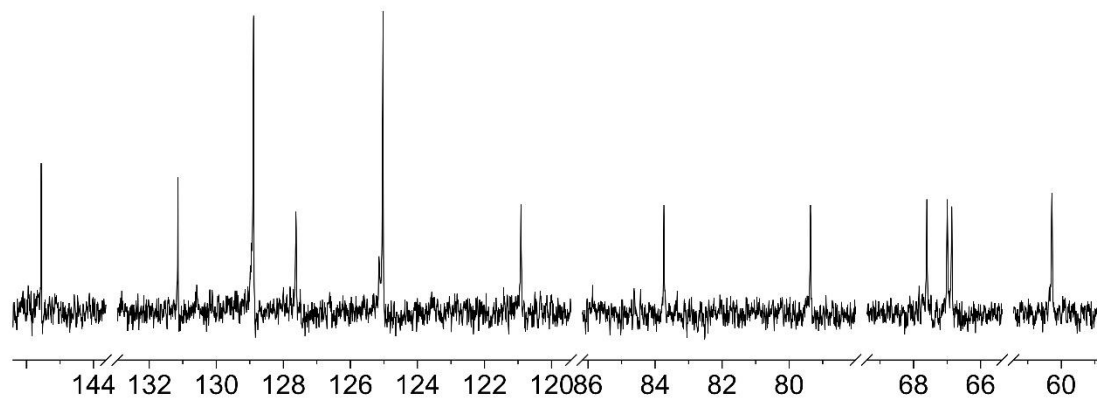
¹H NMR (400 MHz, DMSO-d₆) 37



¹³C NMR (101 MHz, DMSO-*d*₆) 37

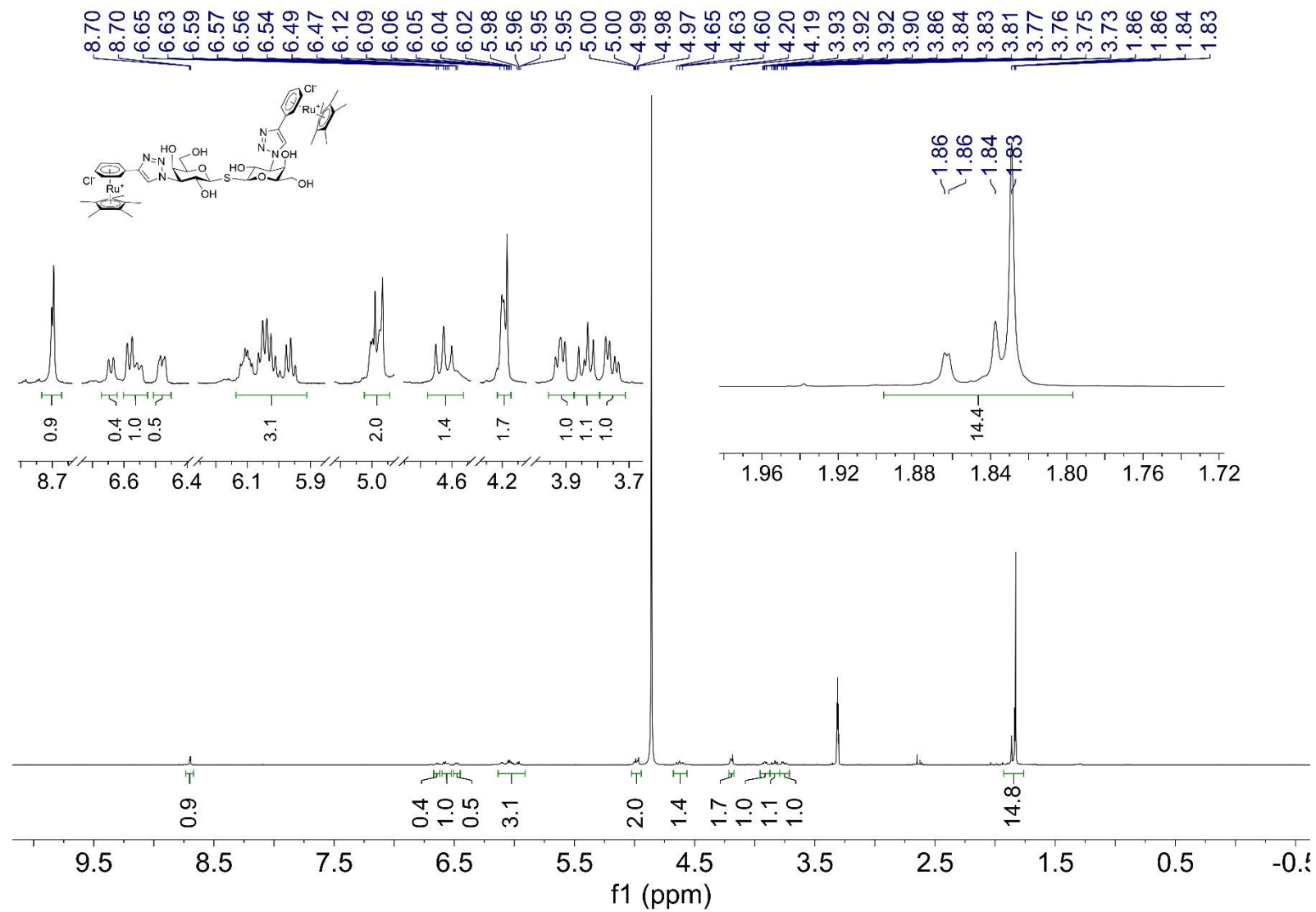


- 145.56
- 131.14
- 128.89
- 127.62
- 125.03
- 120.91
- 83.85
- 79.28
- 67.60
- 66.99
- 66.86
- 60.28

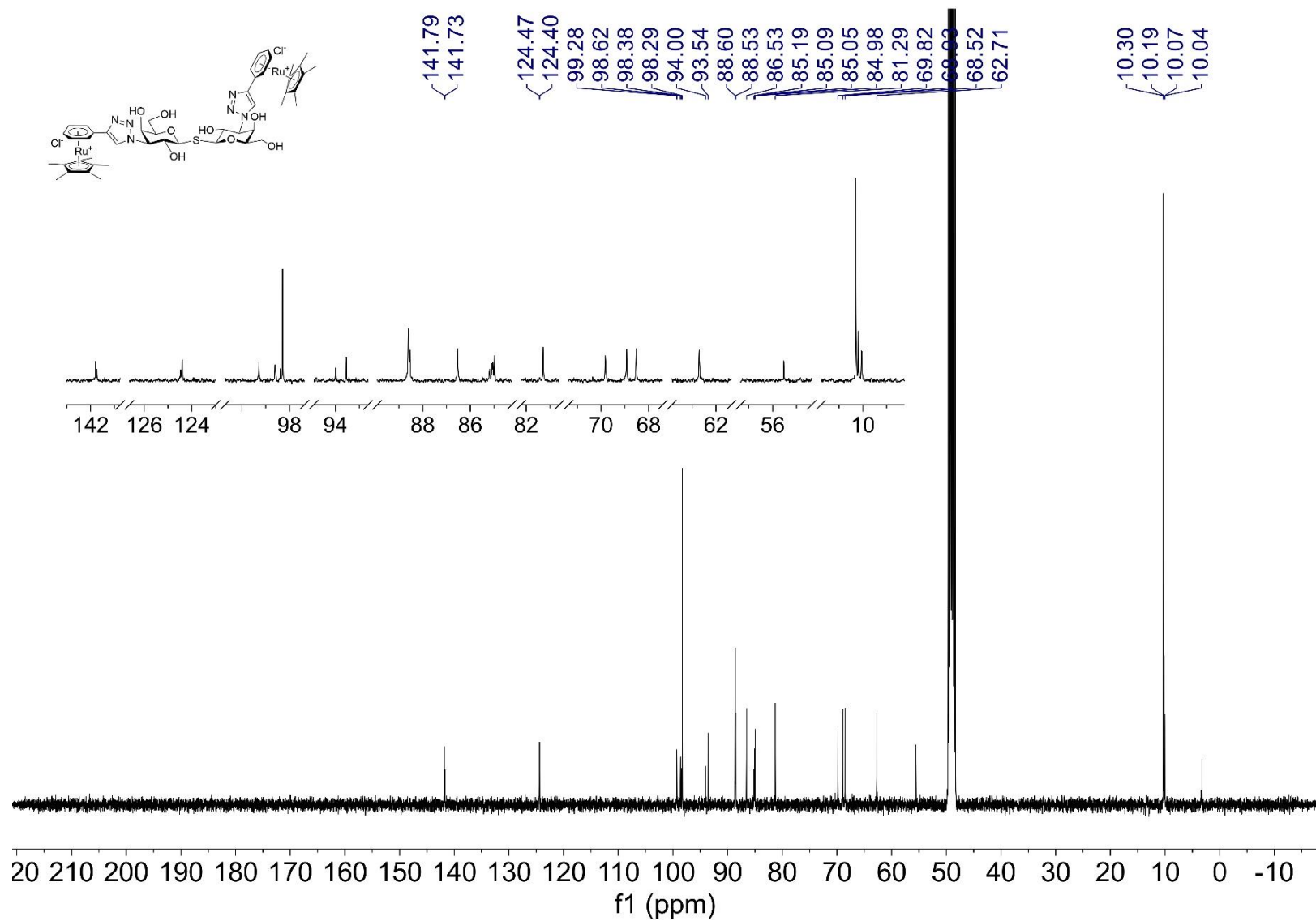


NMR COMPOUND 38

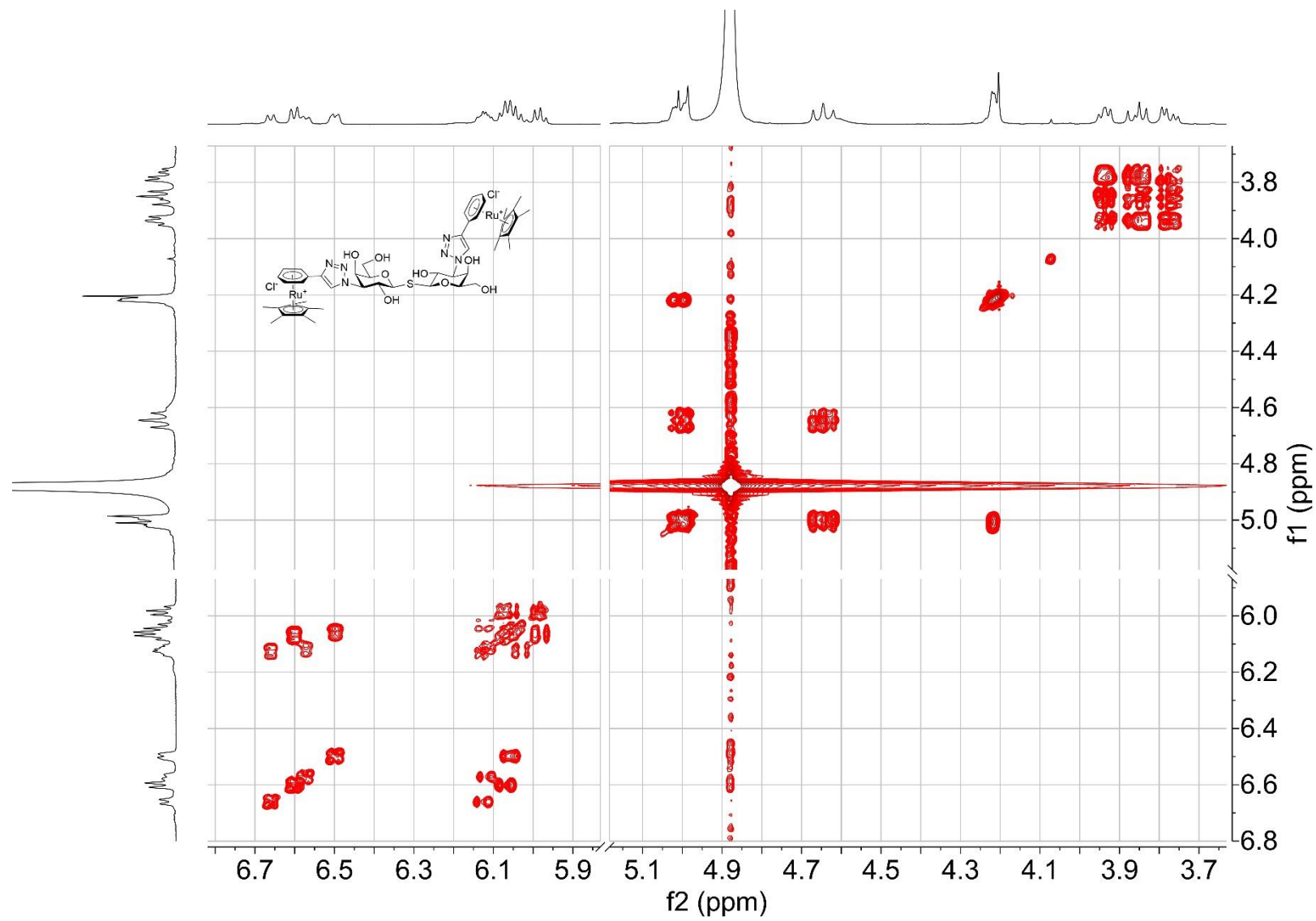
¹H NMR (400 MHz, MeOD) 38



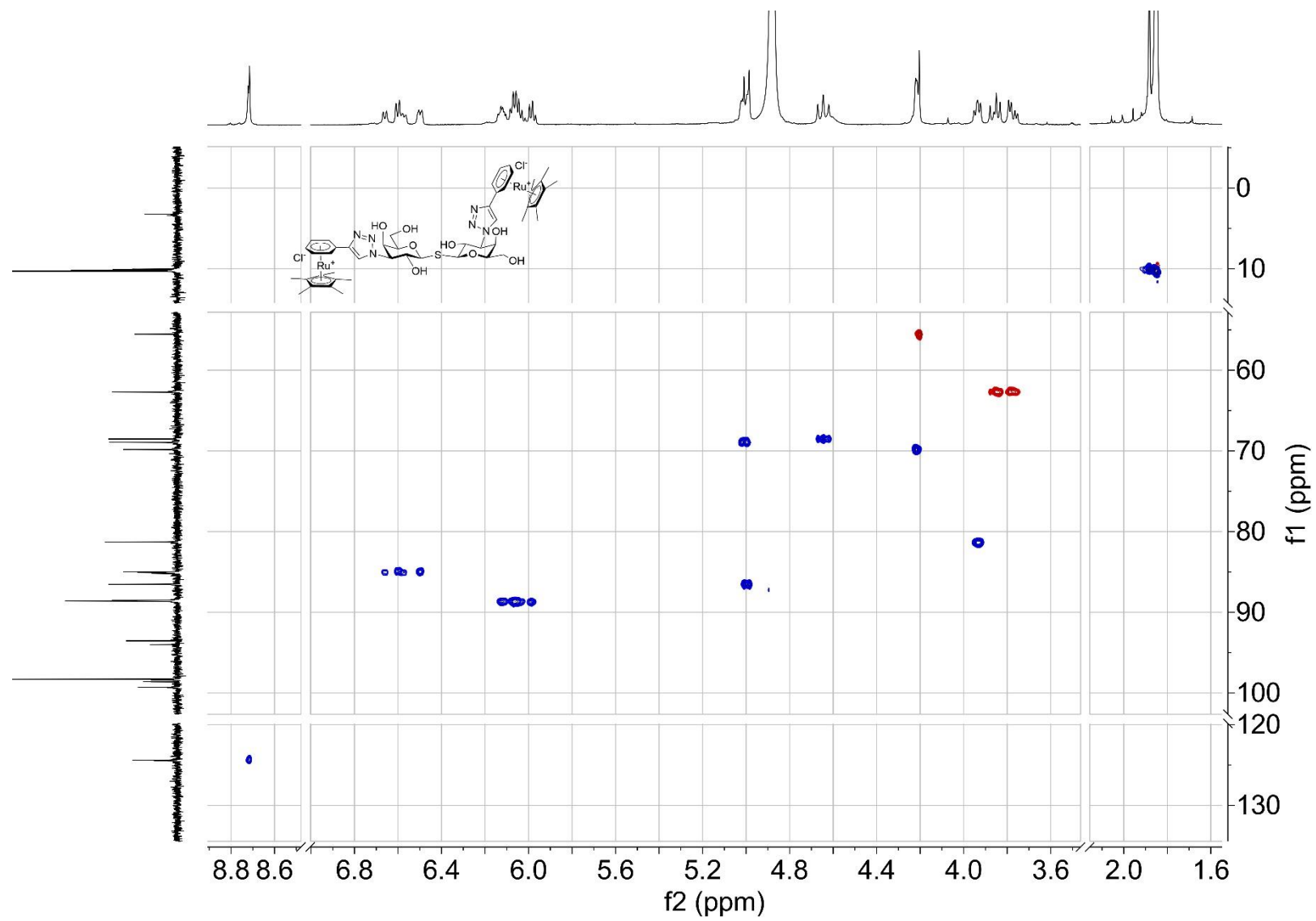
¹³C NMR (101 MHz, MeOD) 38



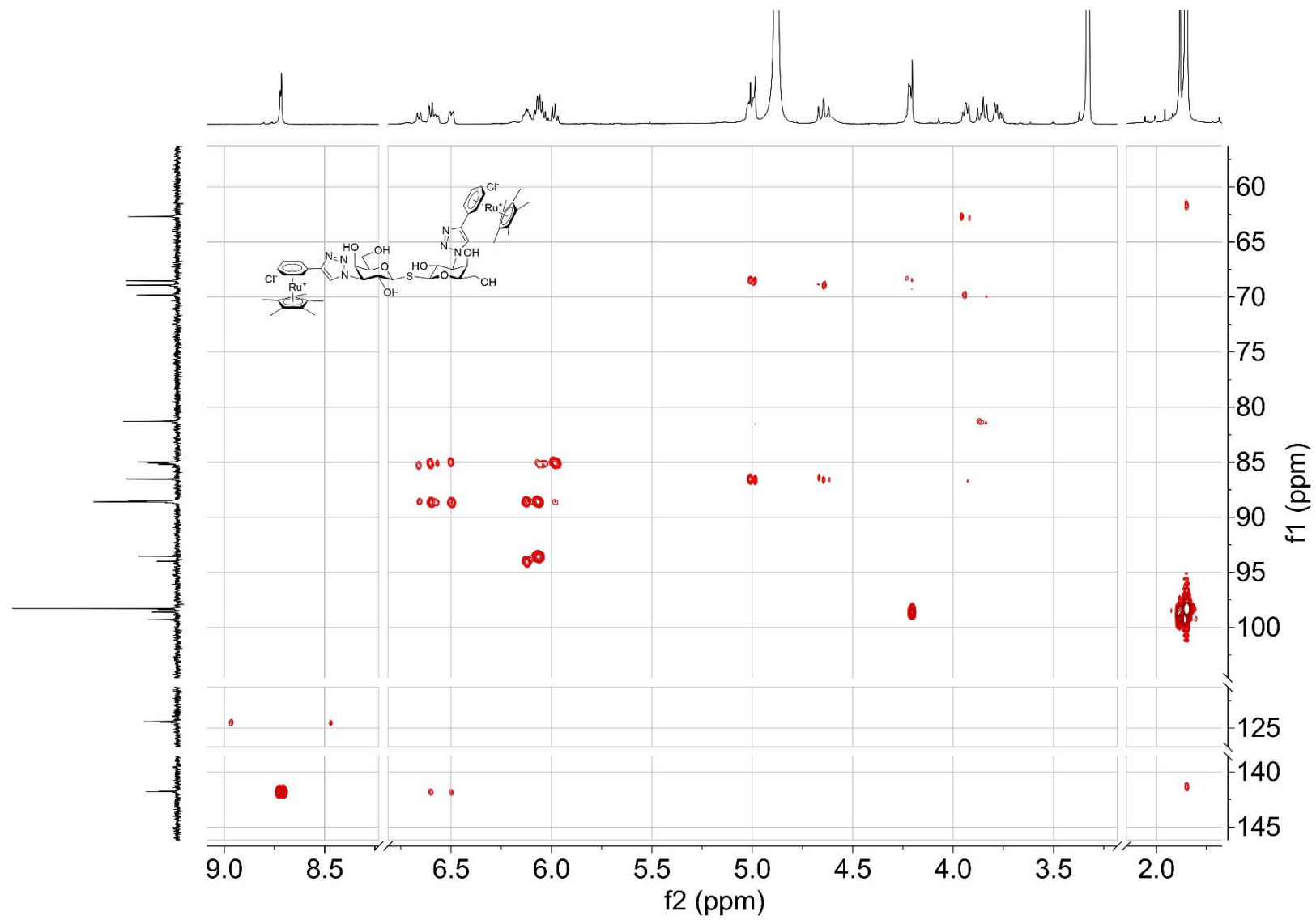
^1H - ^1H COSY 38



^1H - ^{13}C HSQC 38

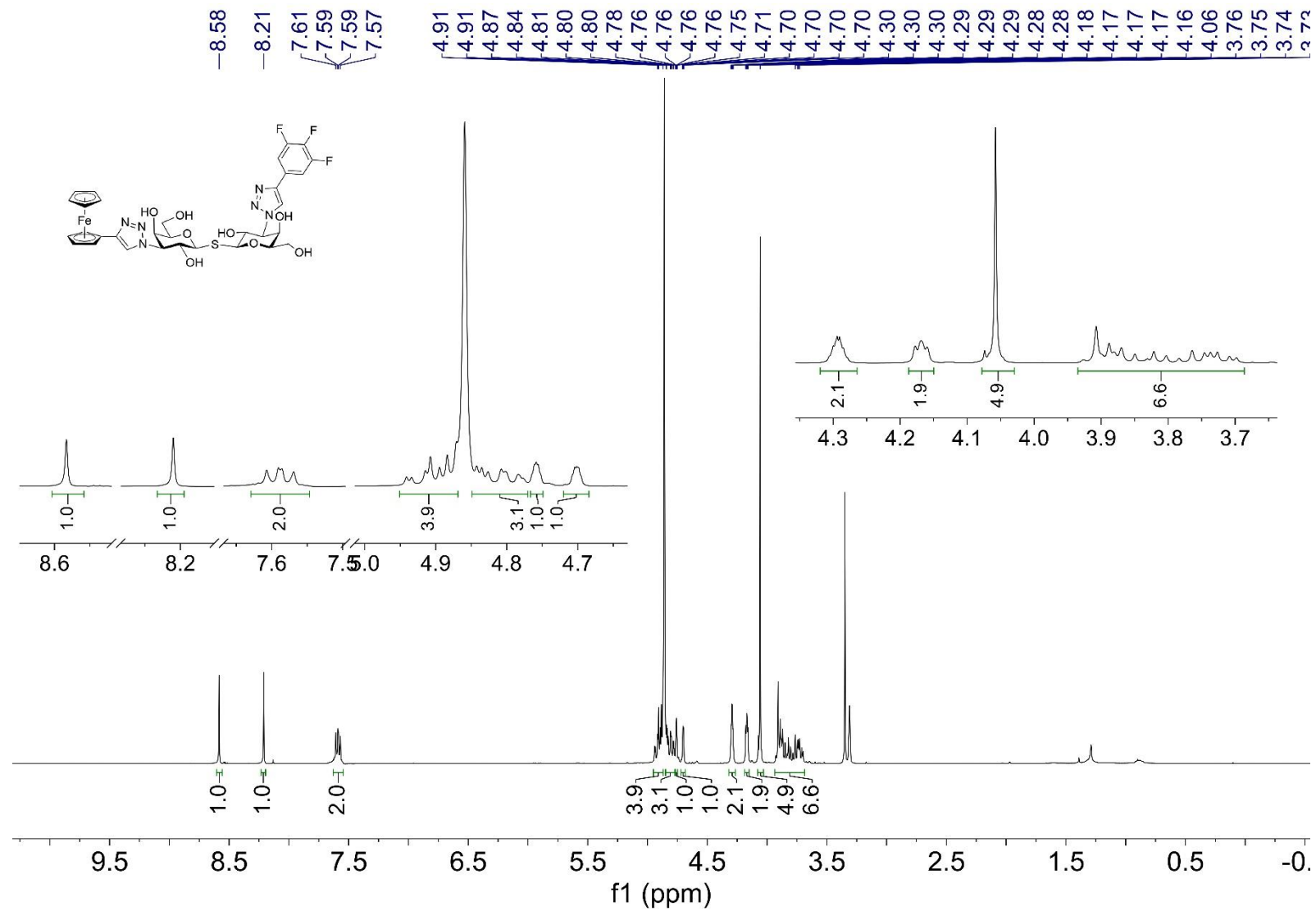


^1H - ^{13}C HMBC 38

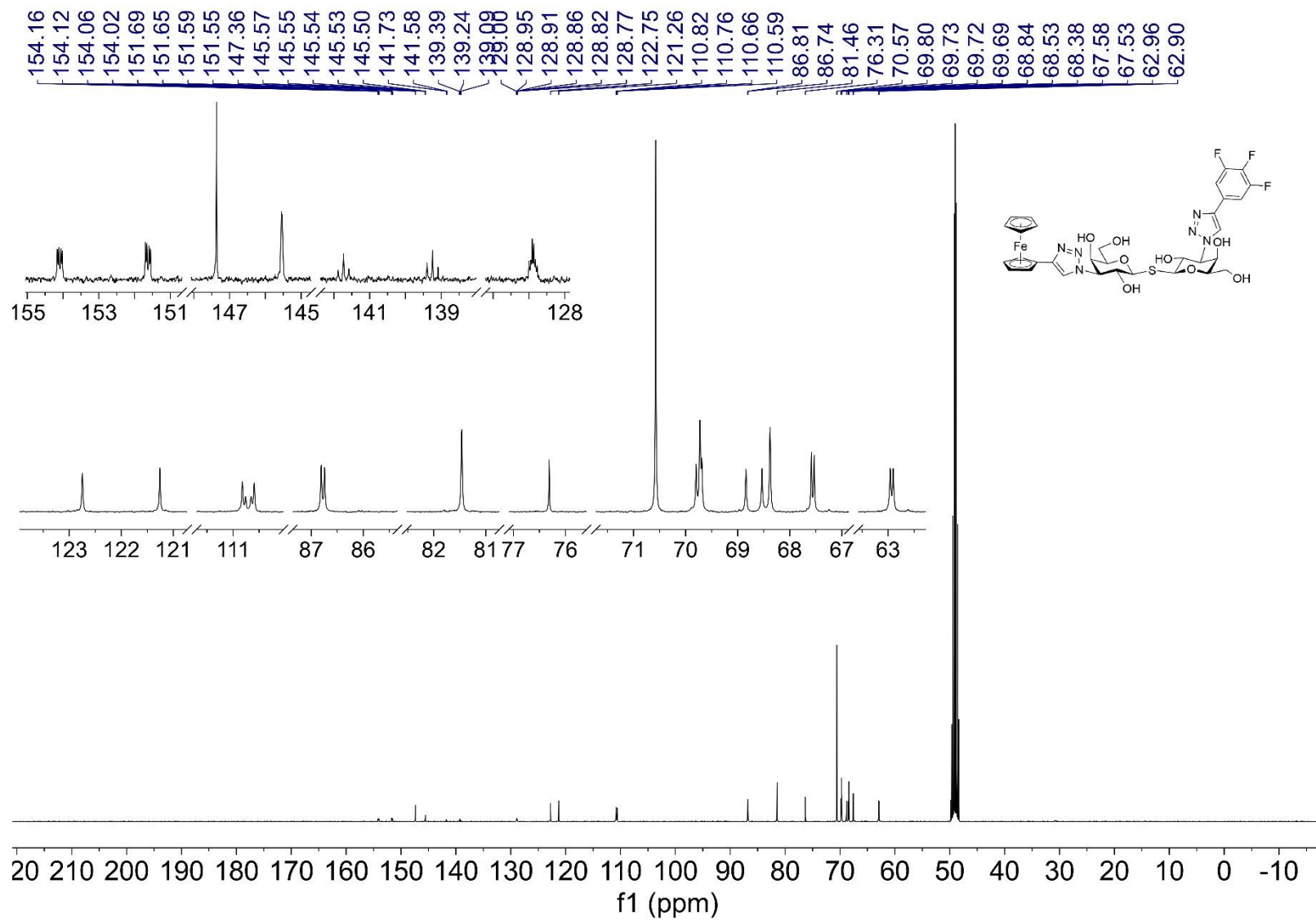


NMR COMPOUND 41

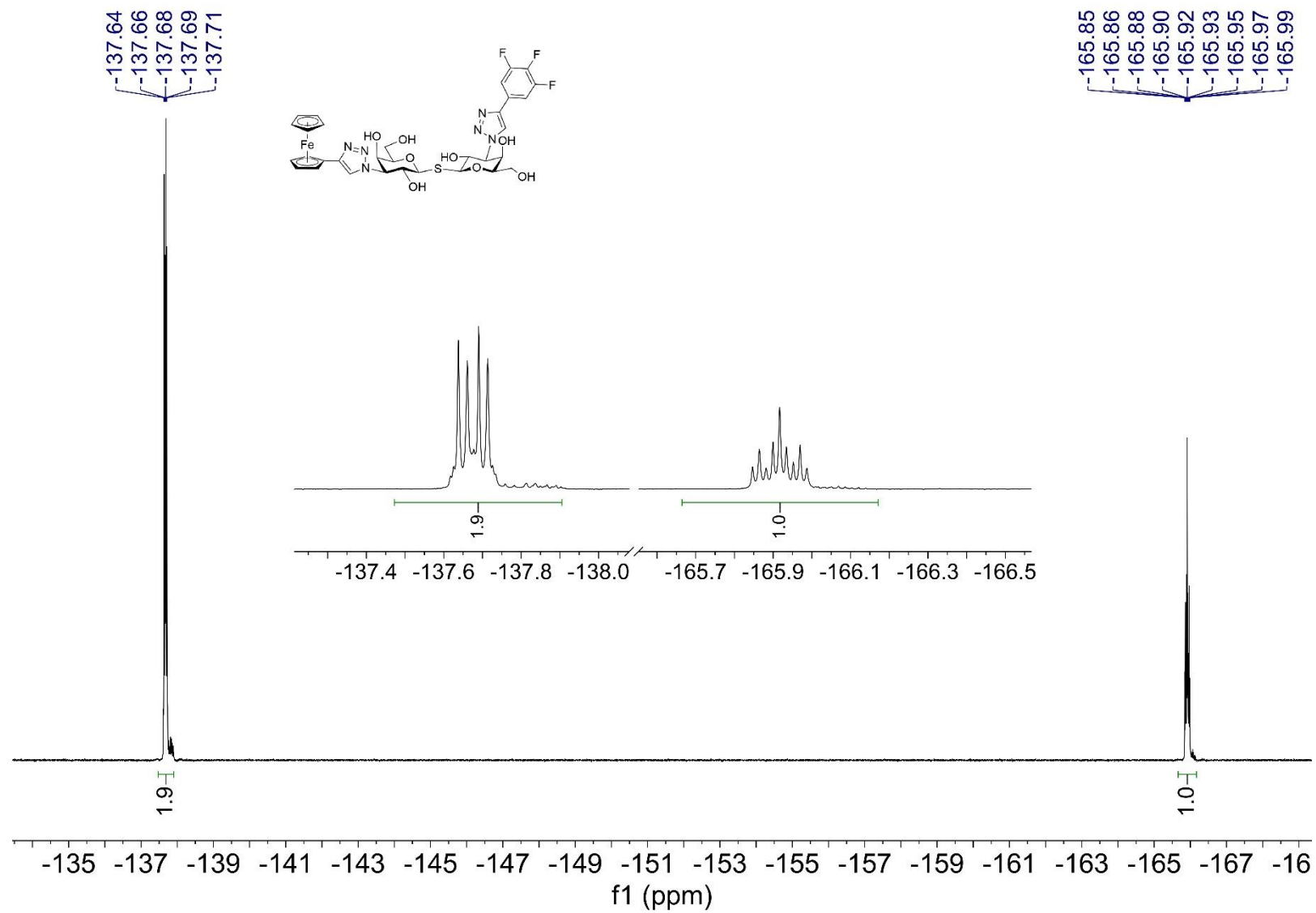
¹H NMR (400 MHz, MeOD) 41



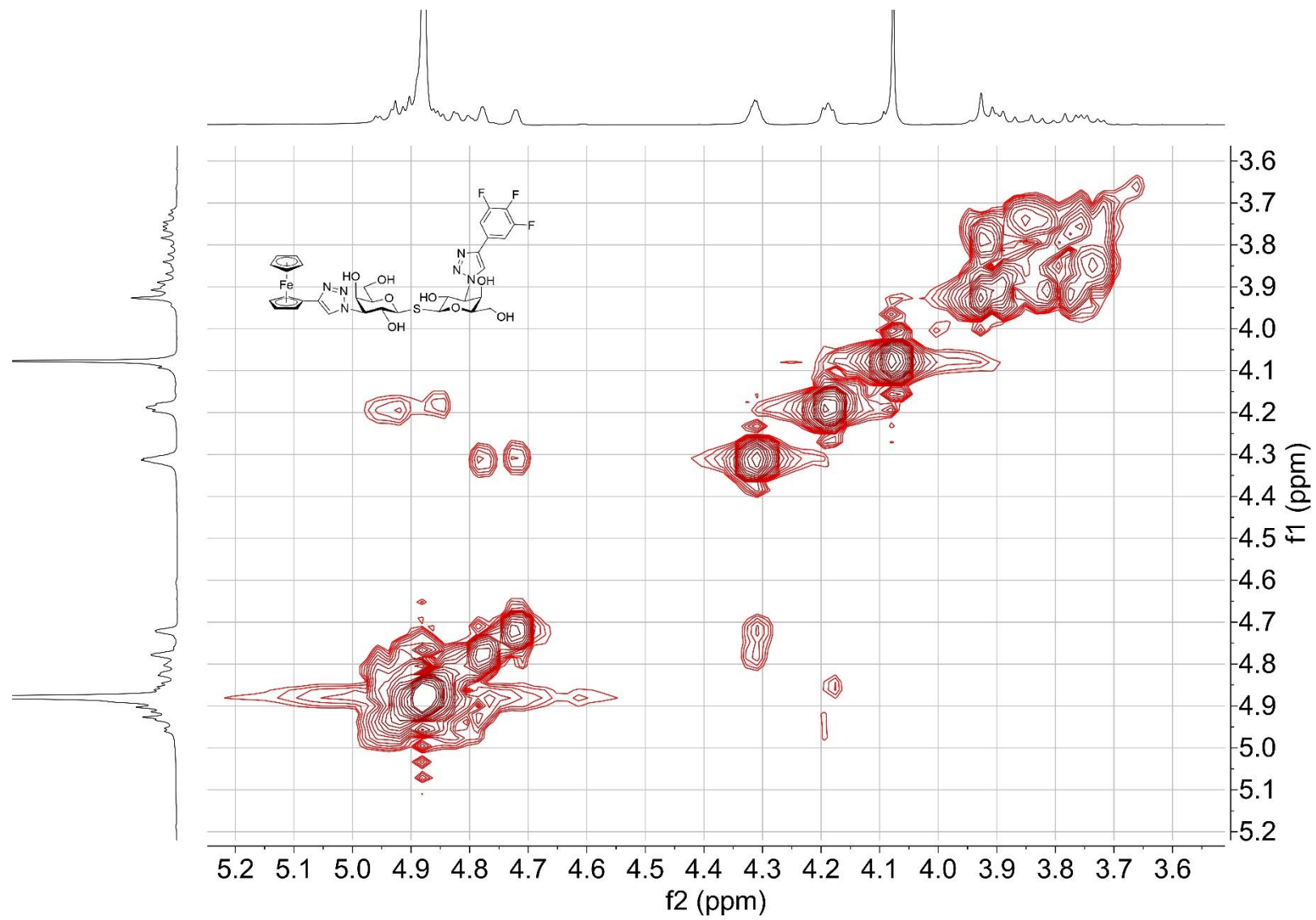
¹³C NMR (101 MHz, MeOD) 41



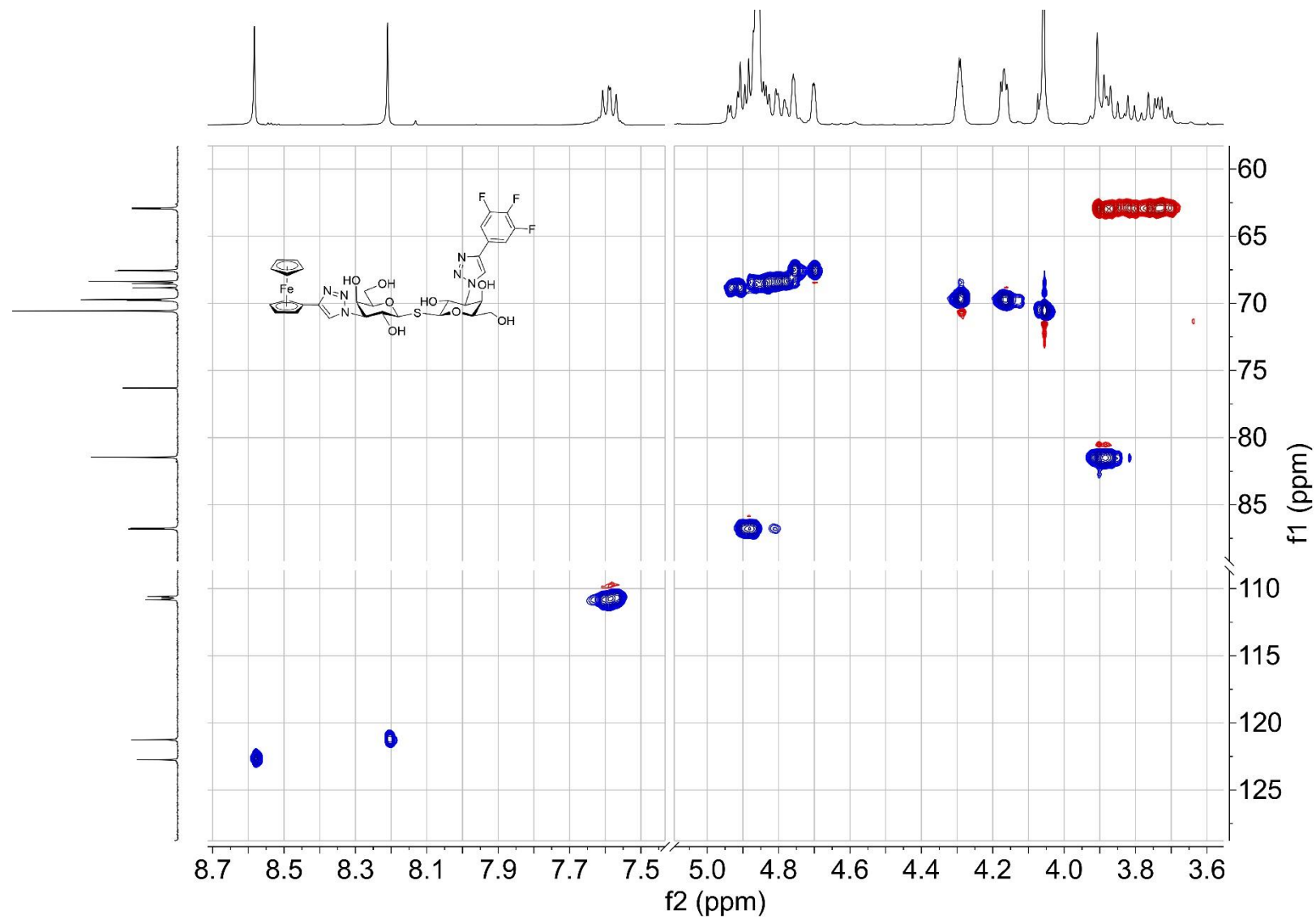
¹⁹F NMR (376 MHz, MeOD) 41



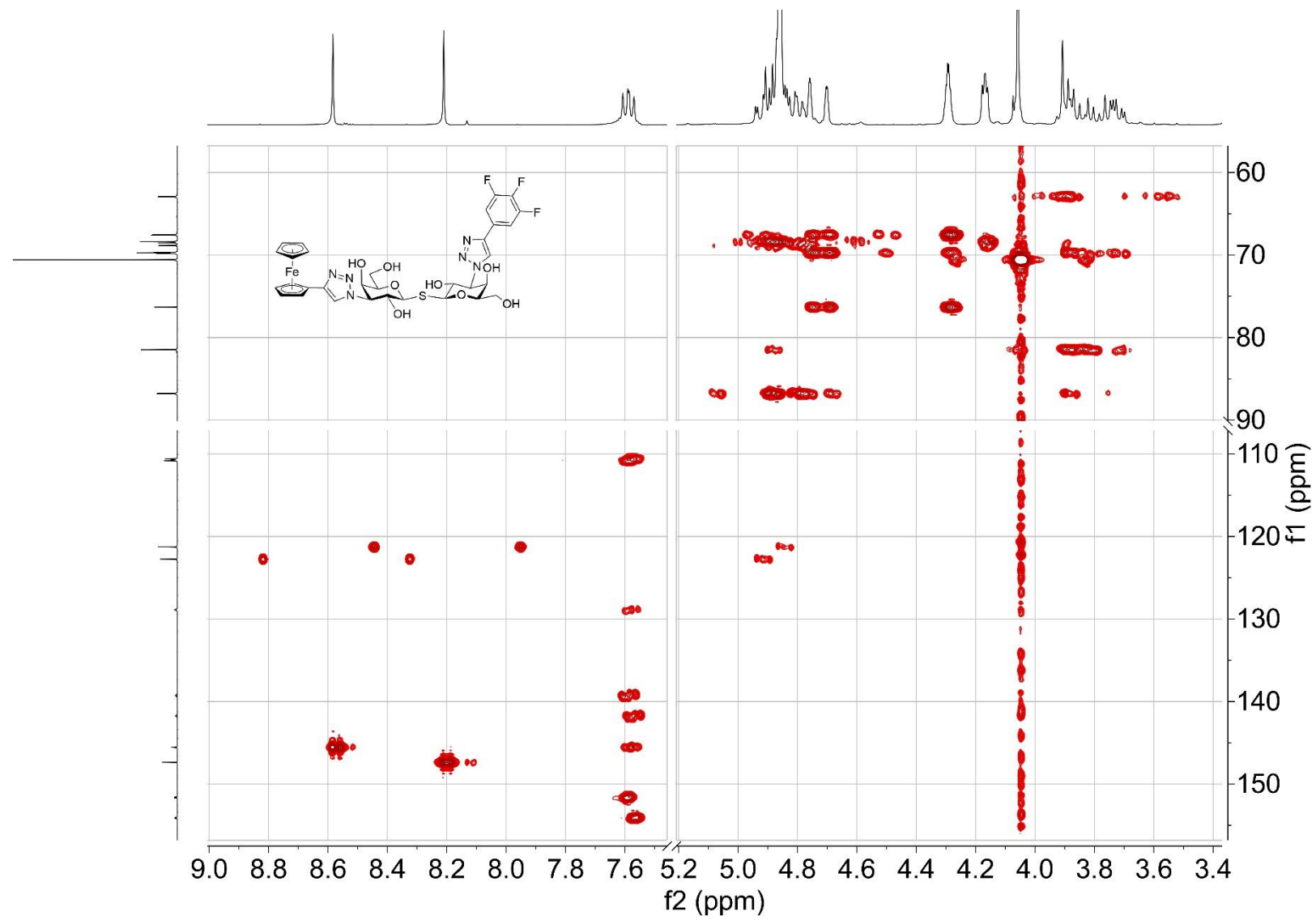
¹H-¹H COSY 41



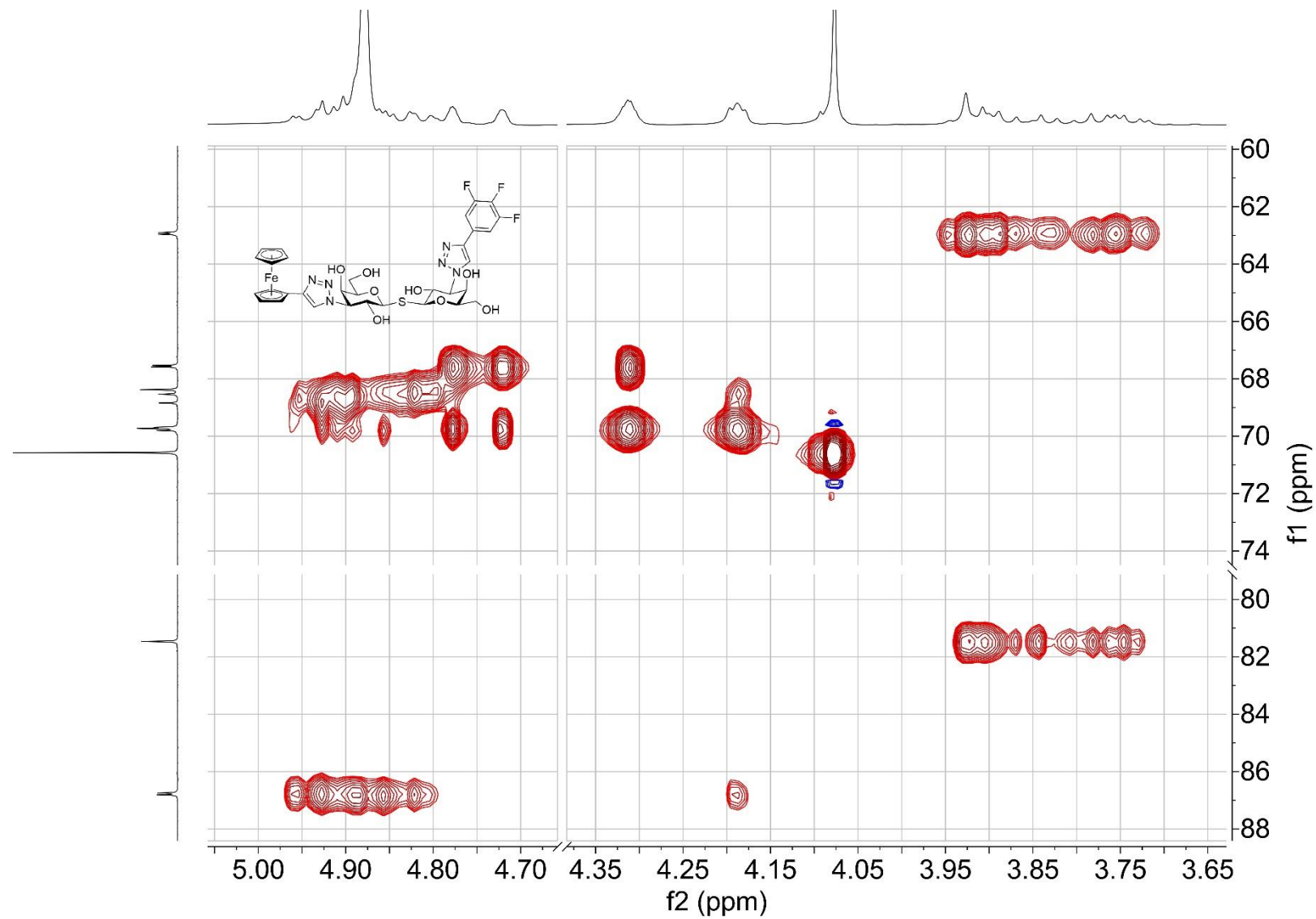
^1H - ^{13}C HSQC 41



^1H - ^{13}C HMBC 41

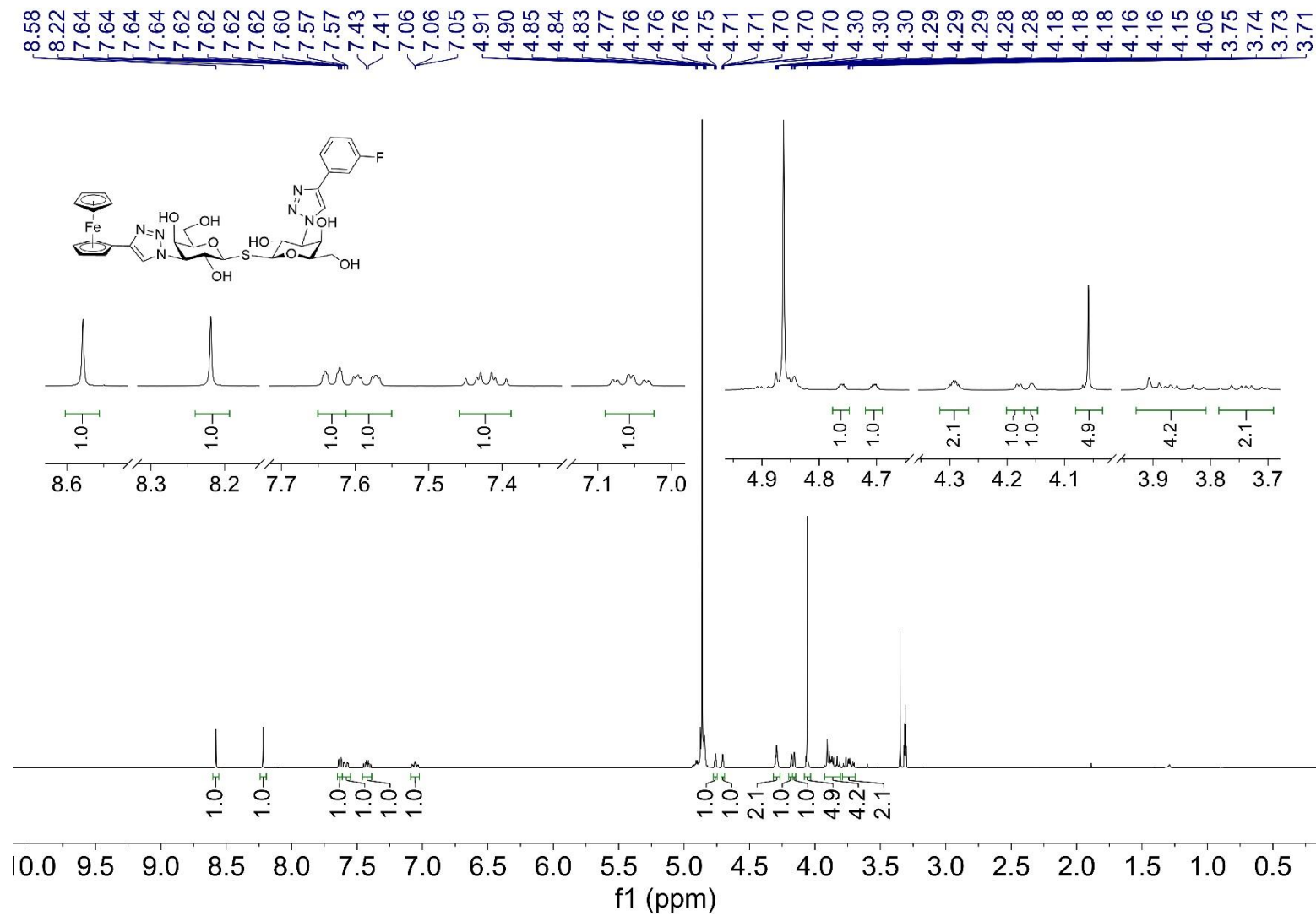


¹H-¹³C HSQCTOCSY 41

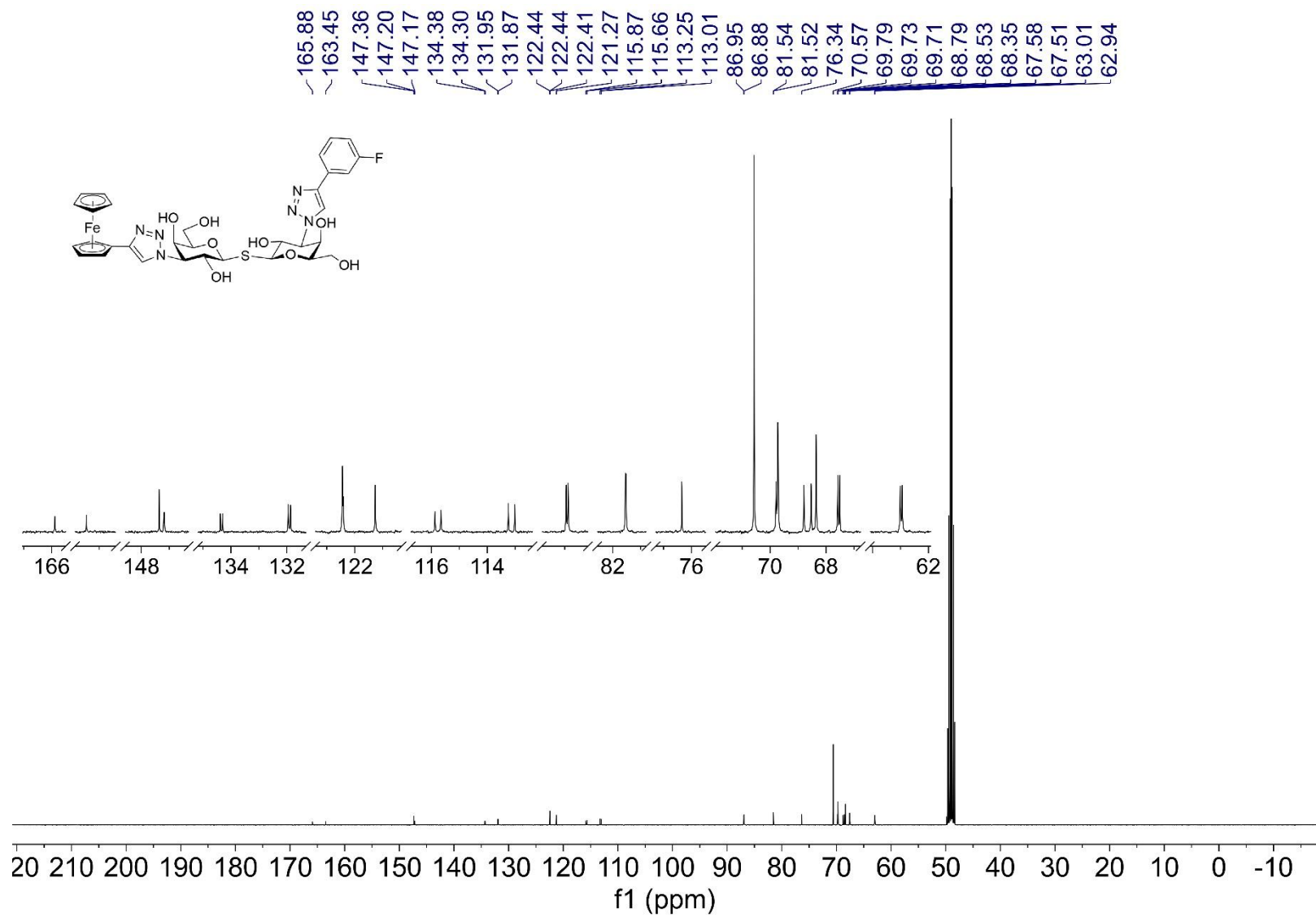


NMR COMPOUND 42

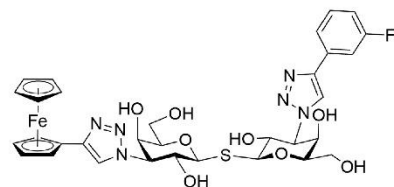
¹H NMR (400 MHz, MeOD) 42



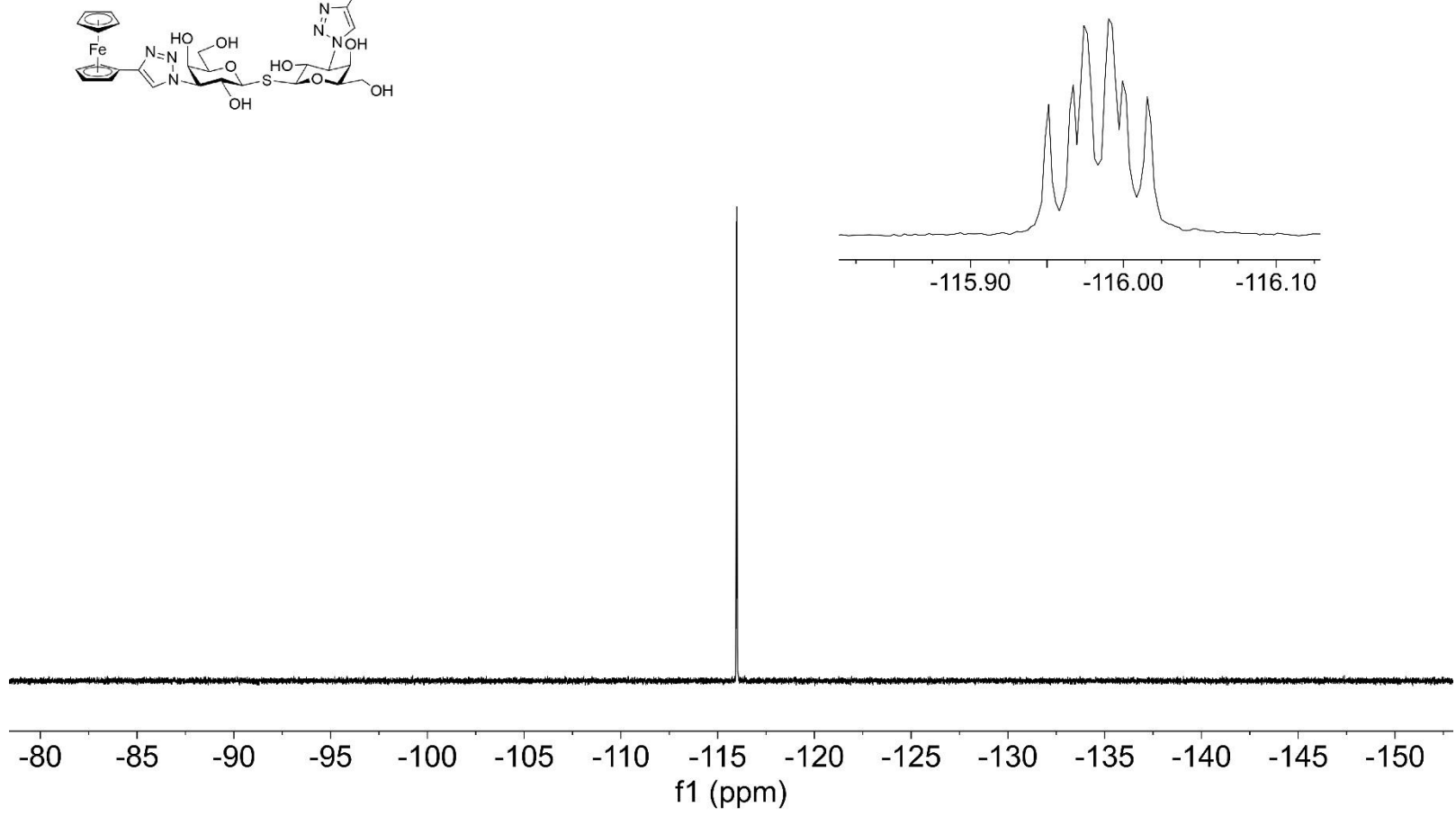
¹³C NMR (101 MHz, MeOD) 42



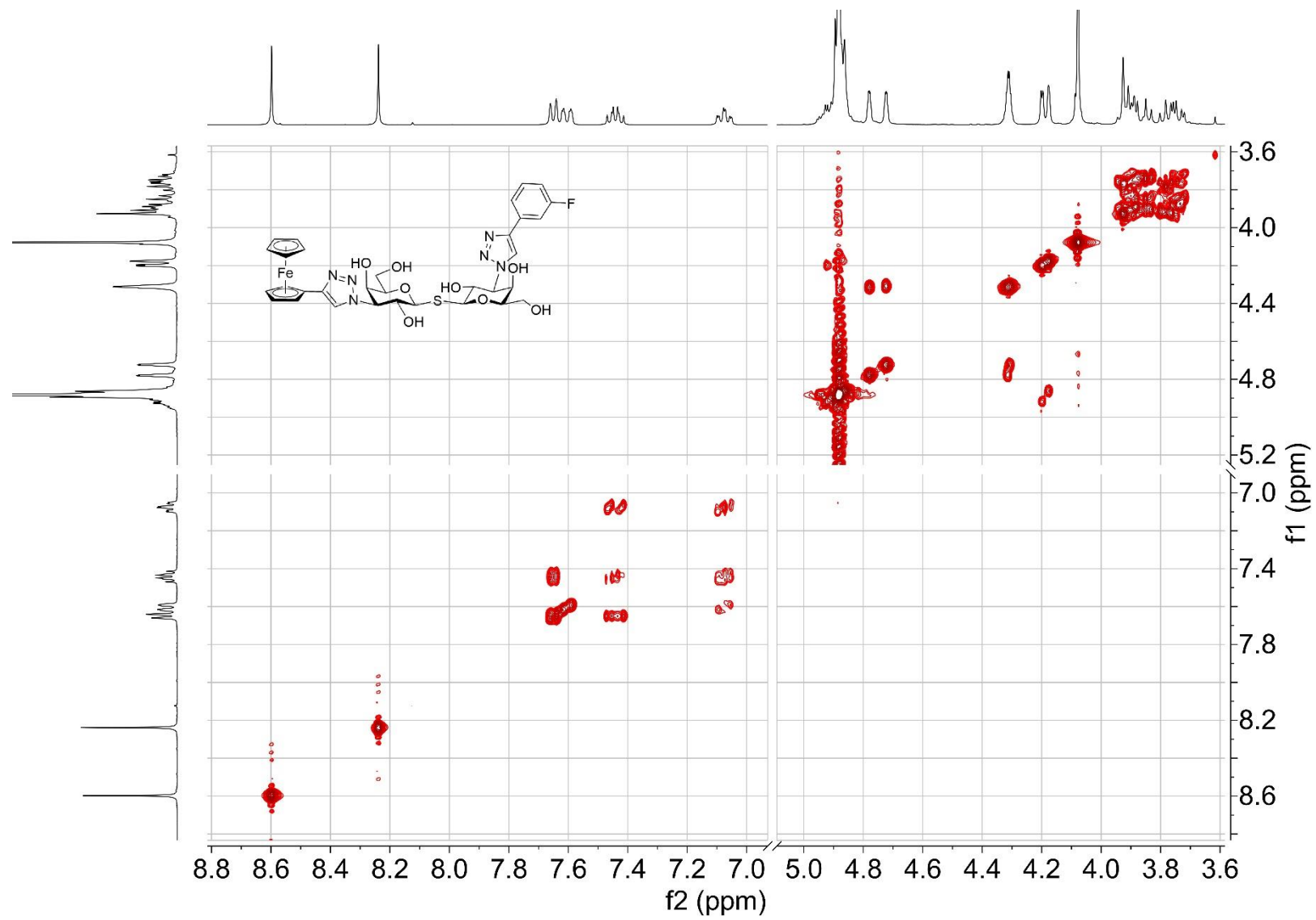
¹⁹F NMR (376 MHz, MeOD) 42



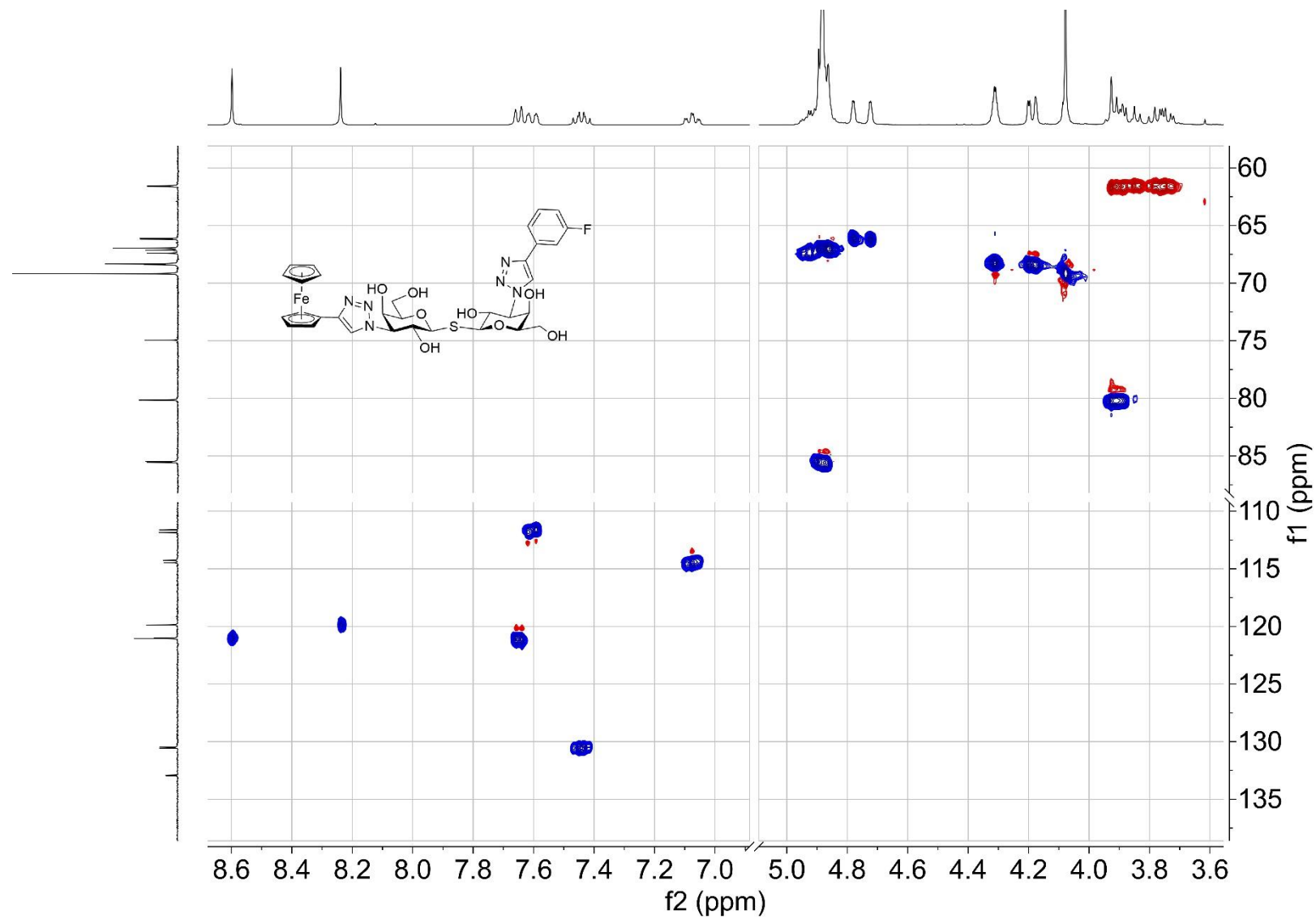
-115.95
-115.97
-115.98
-115.99
-116.00
-116.02



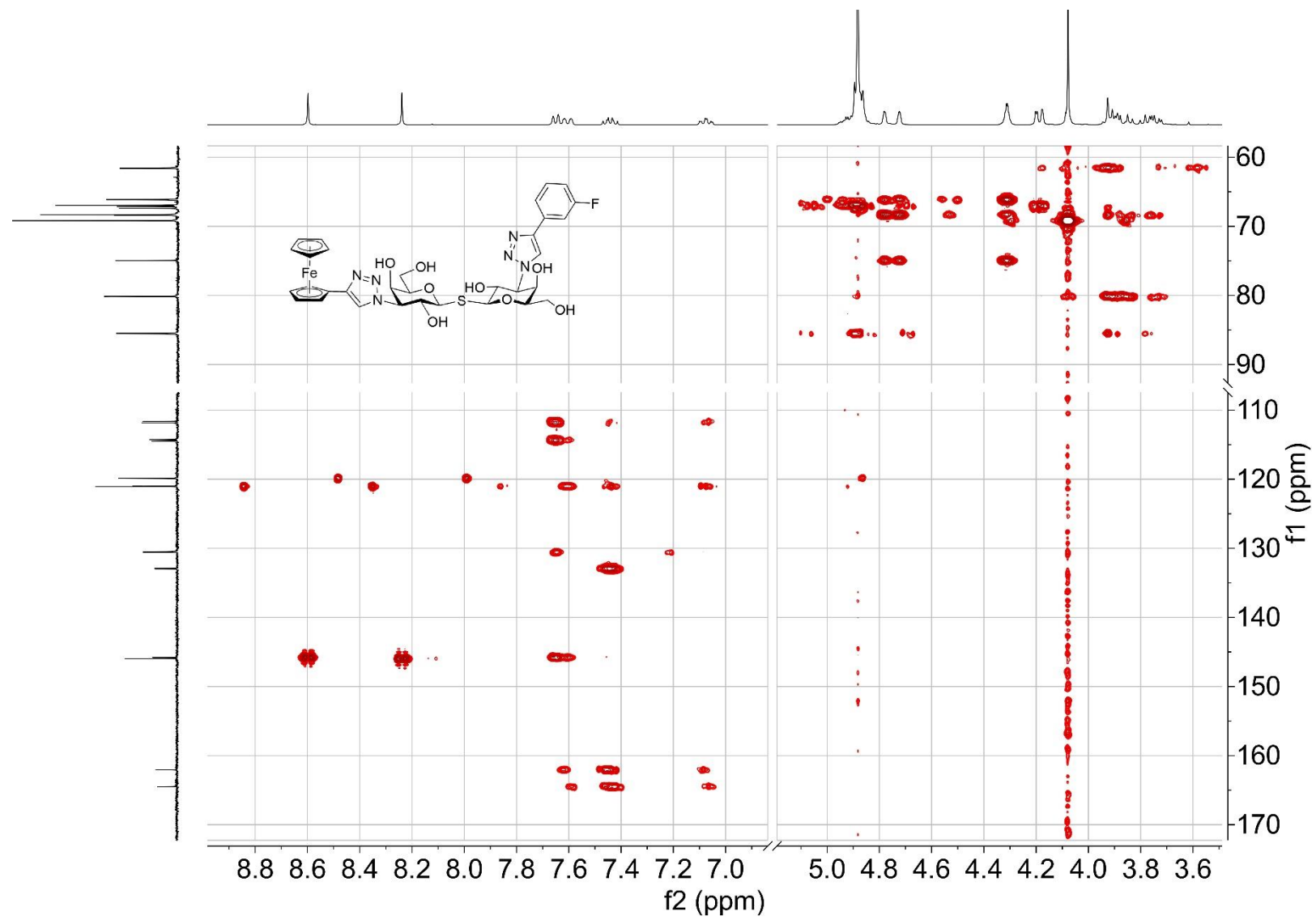
^1H - ^1H COSY 42



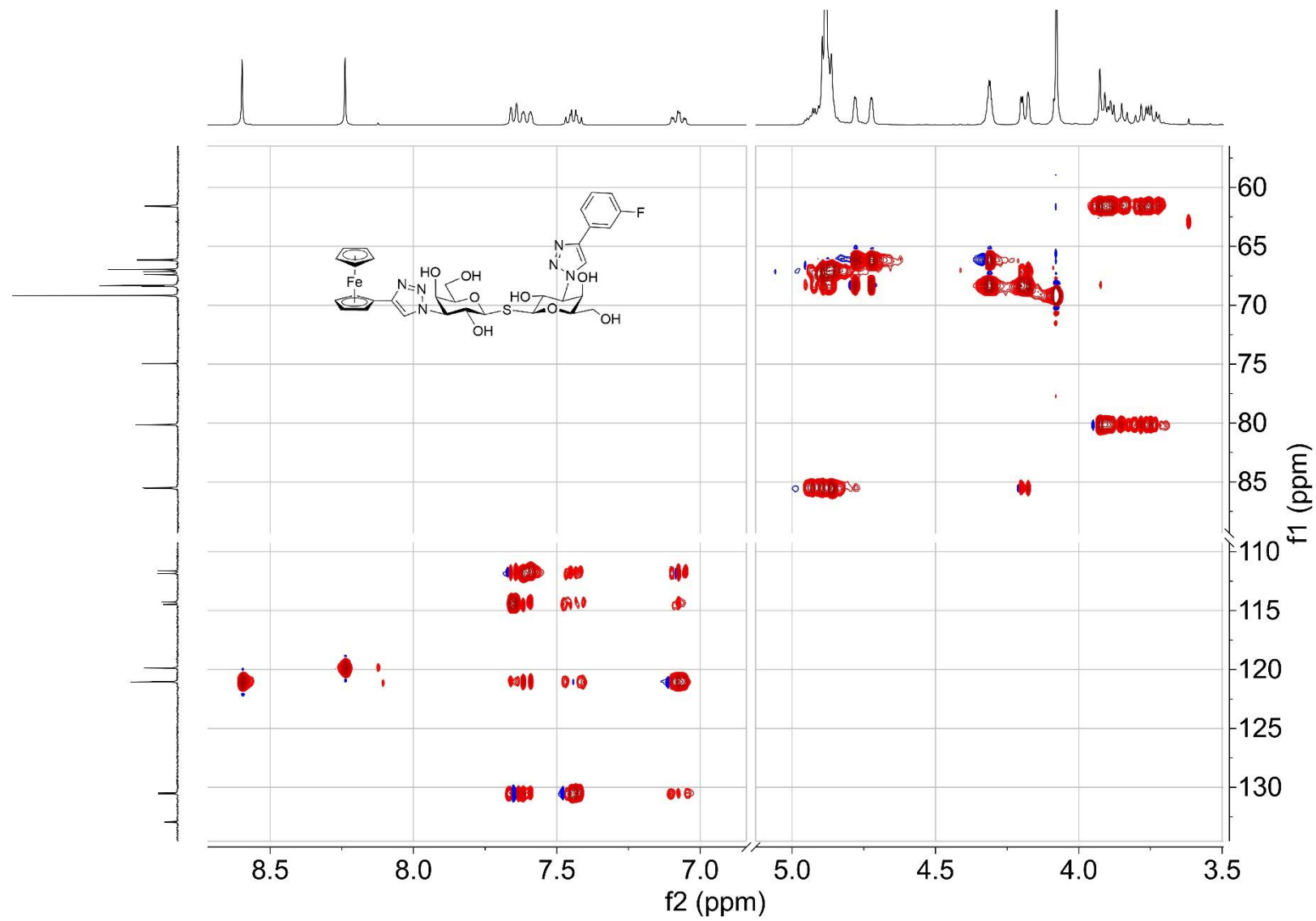
^1H - ^{13}C HSQC 42



^1H - ^{13}C HMBC 42

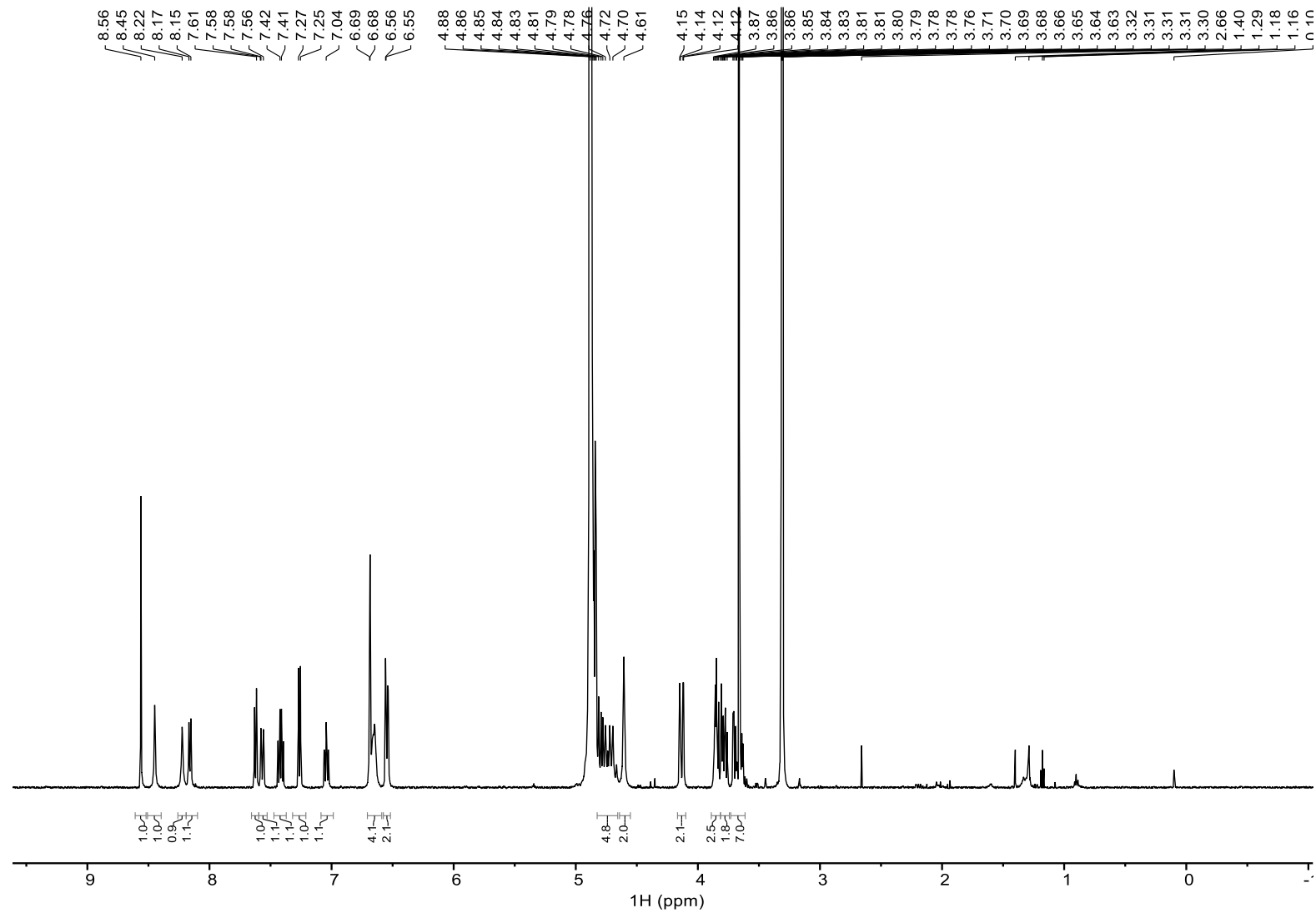


^1H - ^{13}C HSQCTOCSY 42

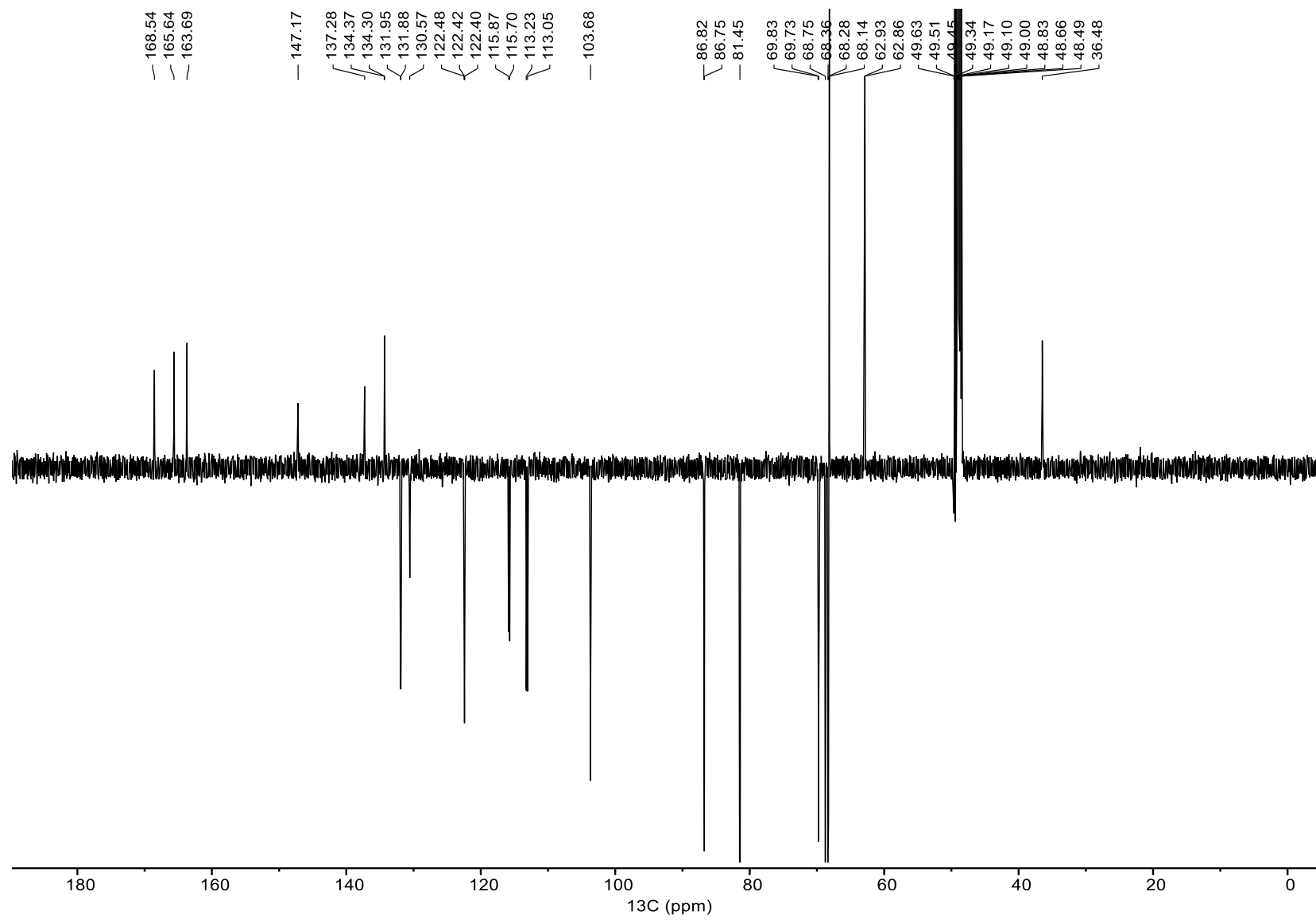


NMR COMPOUND S3

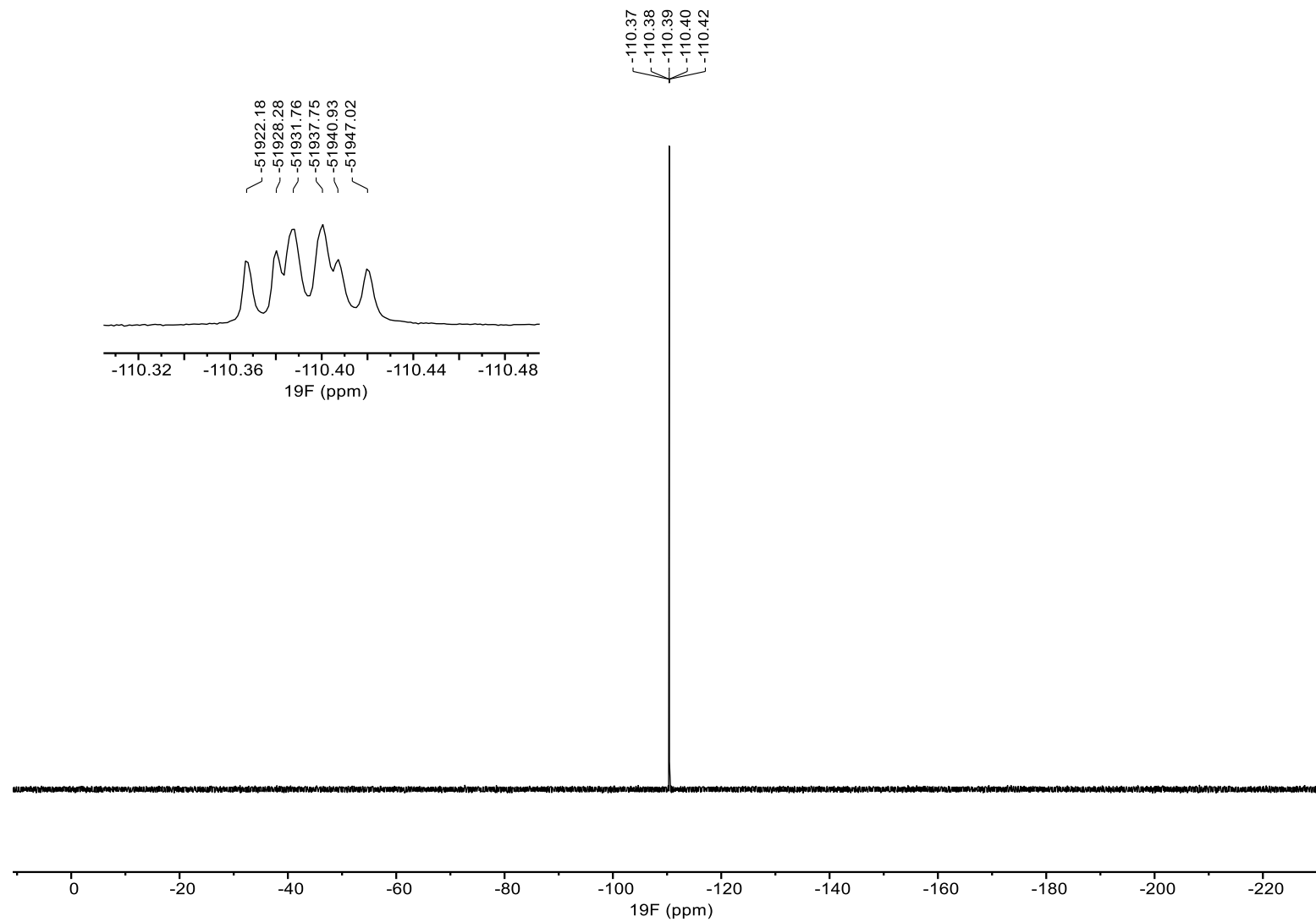
¹H NMR (500 MHz, MeOD) S3



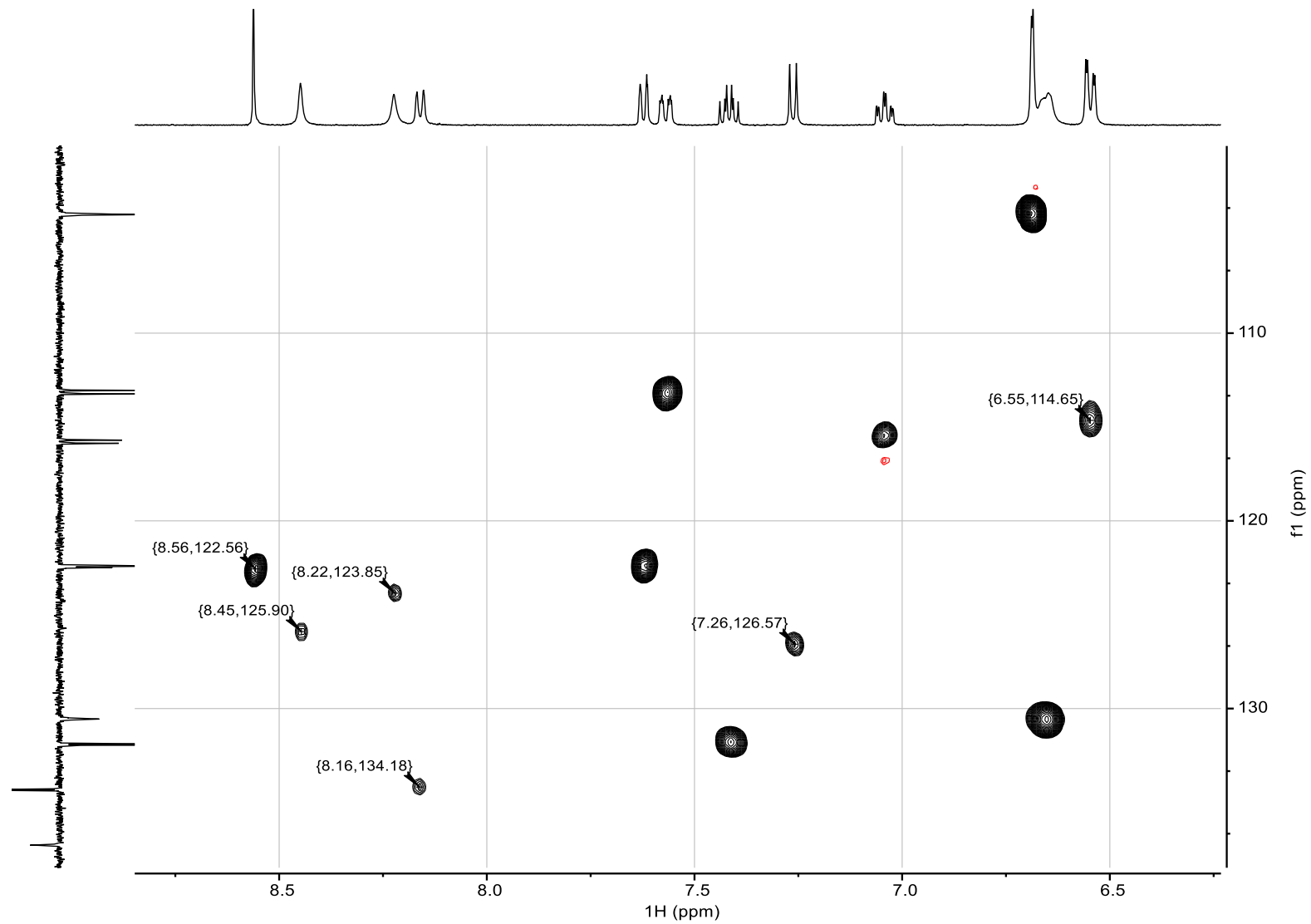
$^{13}\text{C}\{^1\text{H}\}$ APT NMR (126 MHz, MeOD) S3



¹⁹F NMR (470 MHz, MeOD) S3



^1H - ^{13}C HSQC S3



^1H - ^{13}C HMBC S3

