

Supporting Information II

for

Synthesis of multiply fluorinated *N*-acetyl-D-glucosamine and D-galactosamine analogs via the corresponding deoxyfluorinated glucosazide and galactosazide thiodonors

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*E-mail: karban@icpf.cas.cz

Copies of NMR spectra

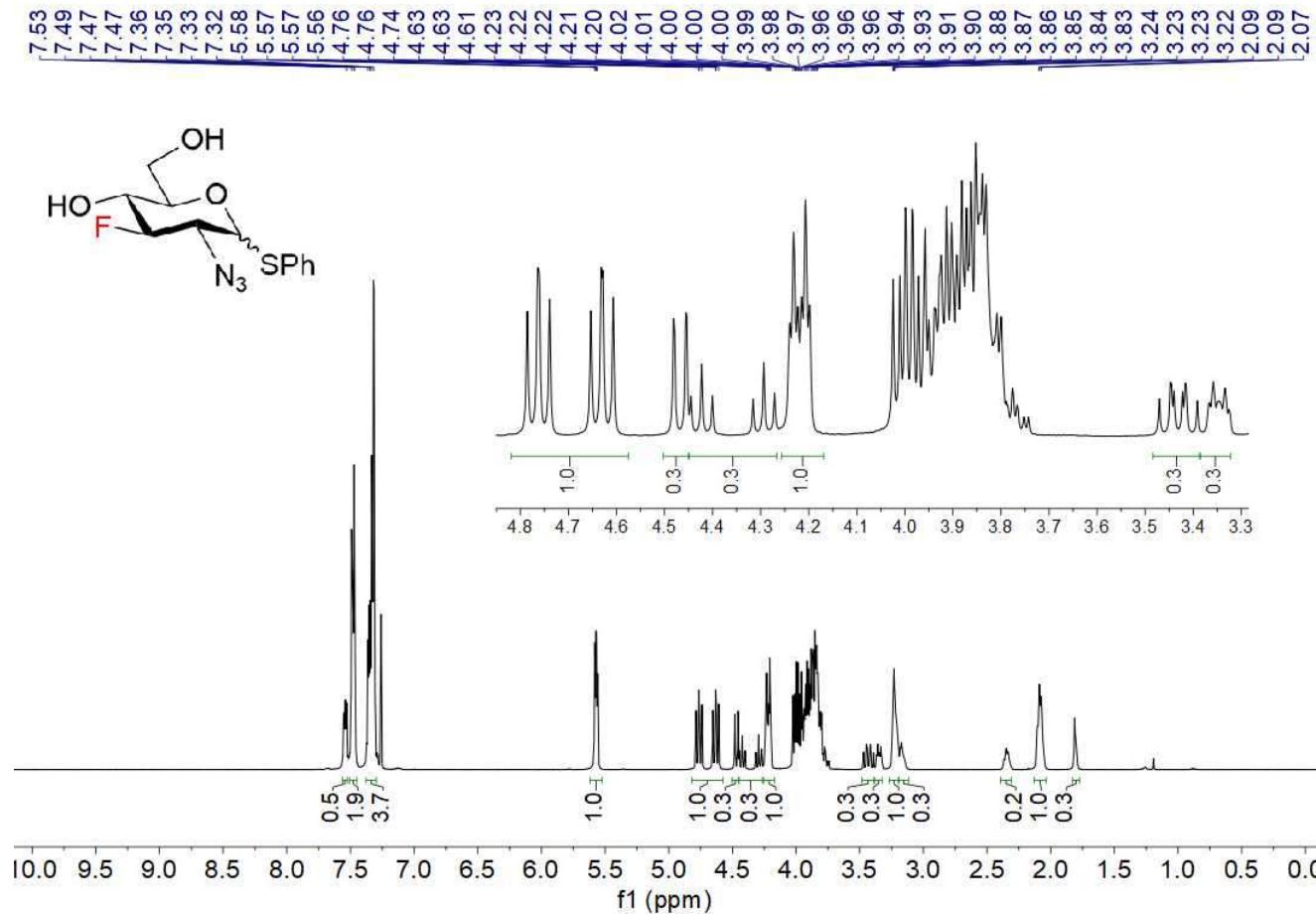
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NMR COMPOUND 36	95
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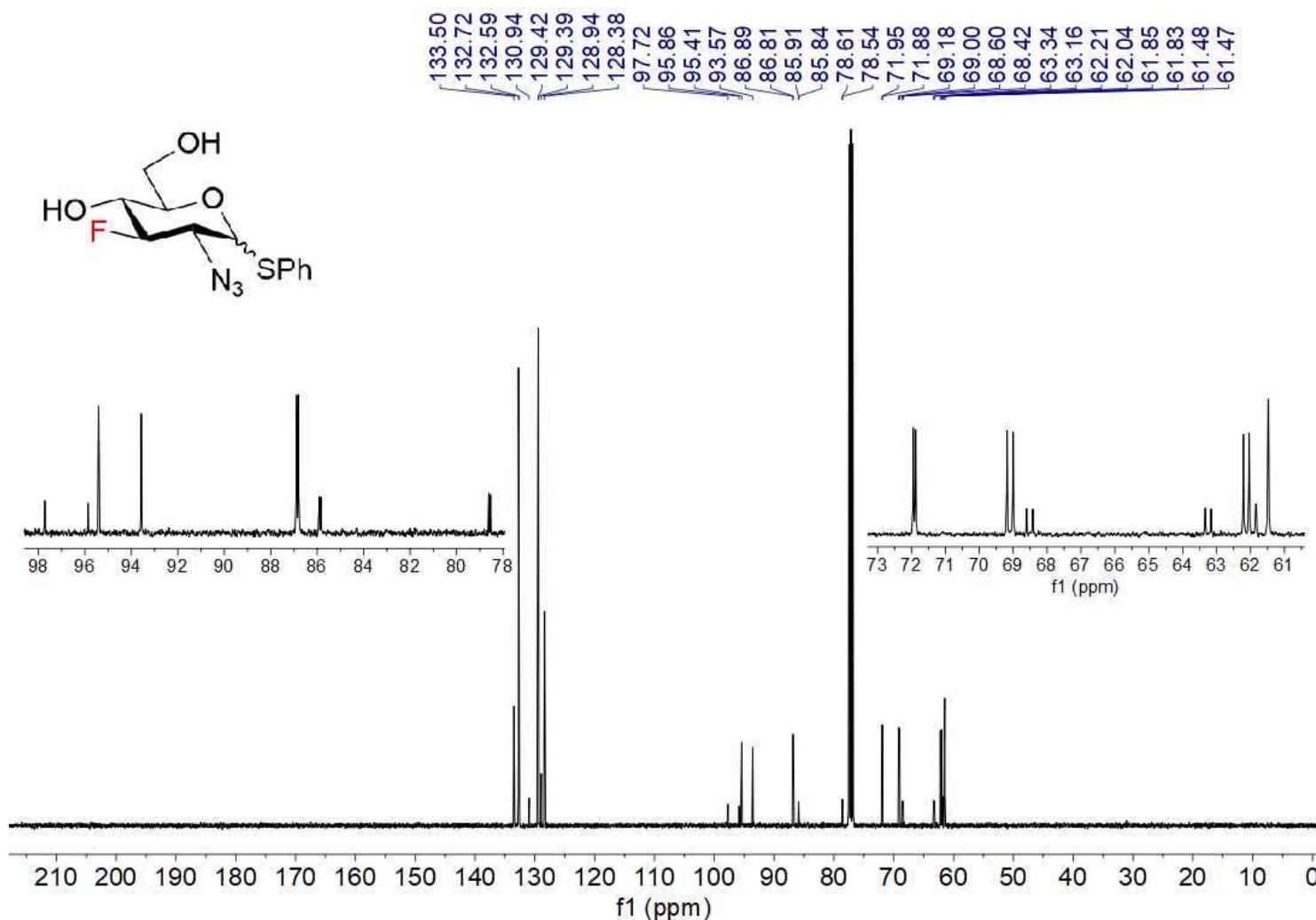
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NMR COMPOUND 18

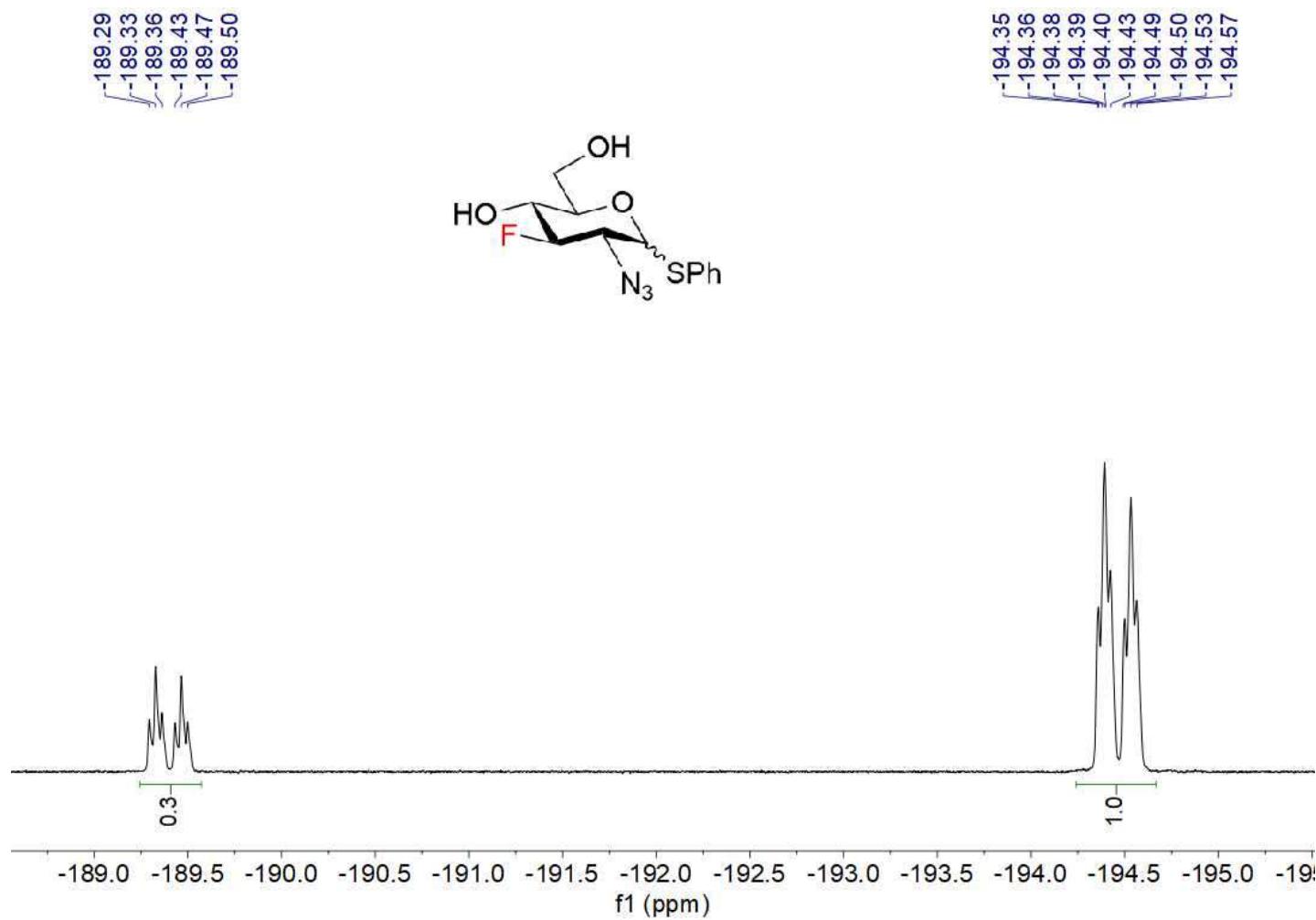
^1H NMR (400 MHz, CDCl_3) 18 (α/β ca. 10/3)



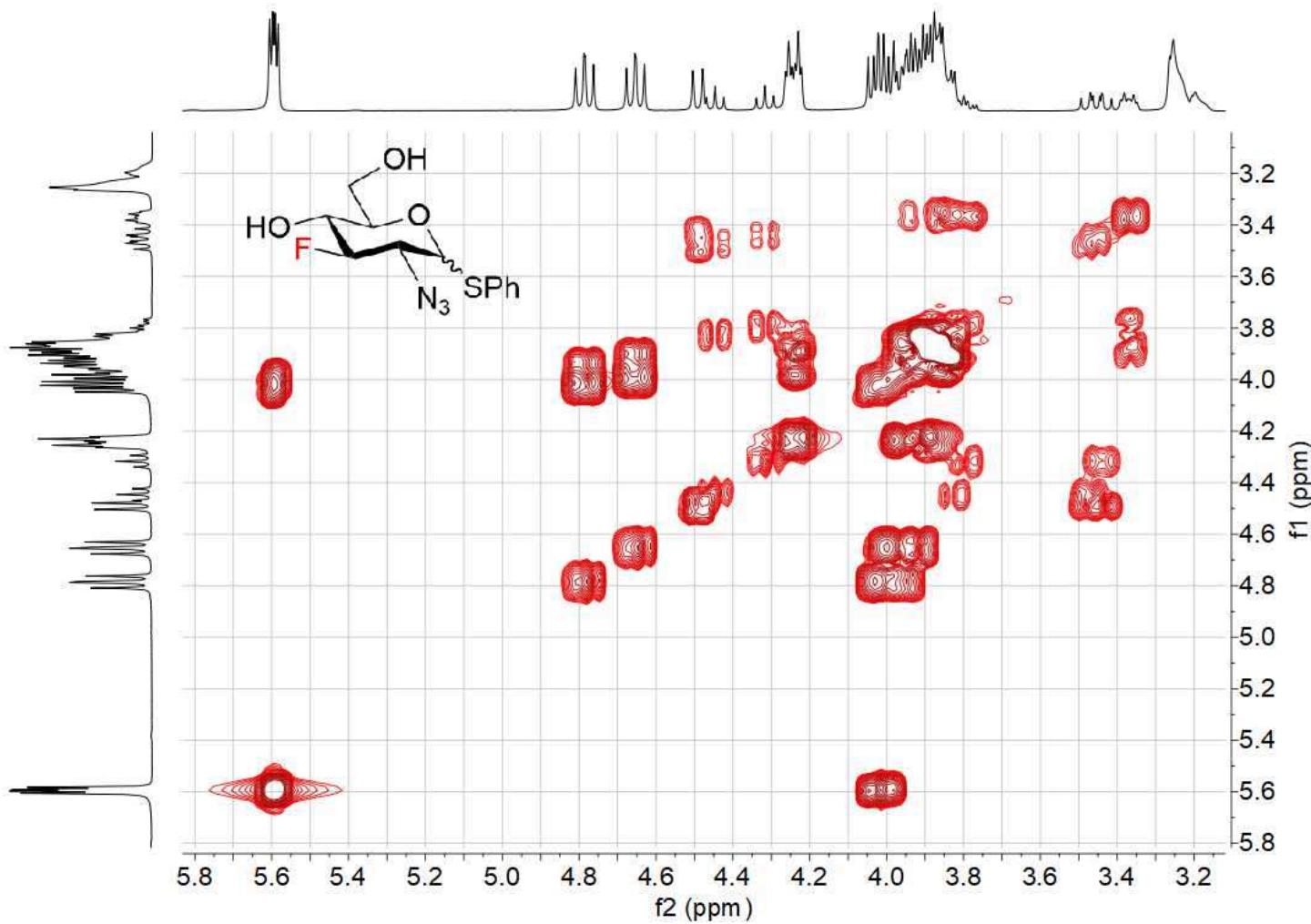
¹³C NMR (100 MHz, CDCl₃) 18



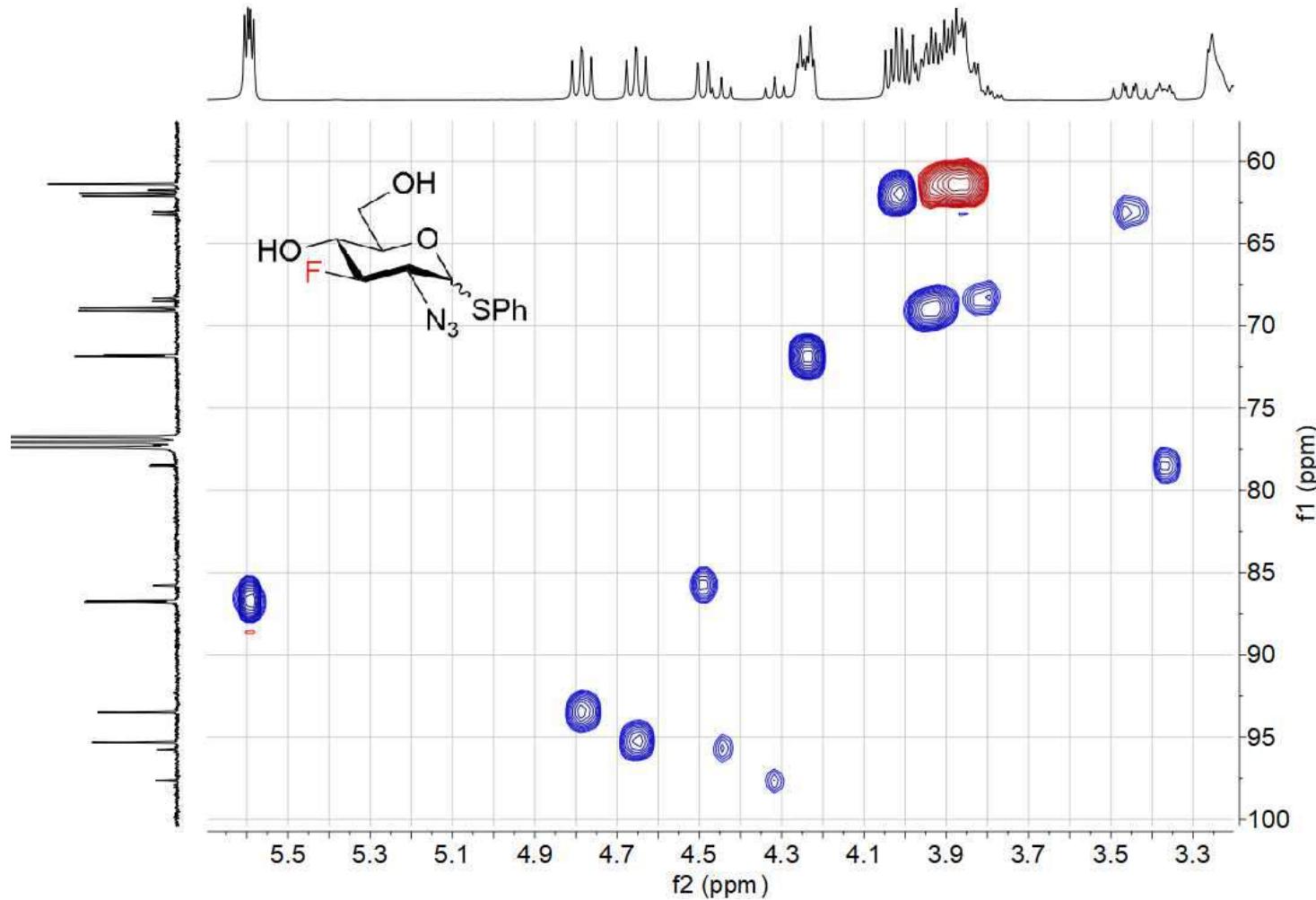
¹⁹F NMR (376 MHz, CDCl₃) 18 (α/β ca. 10/3)



¹H-¹H COSY 18

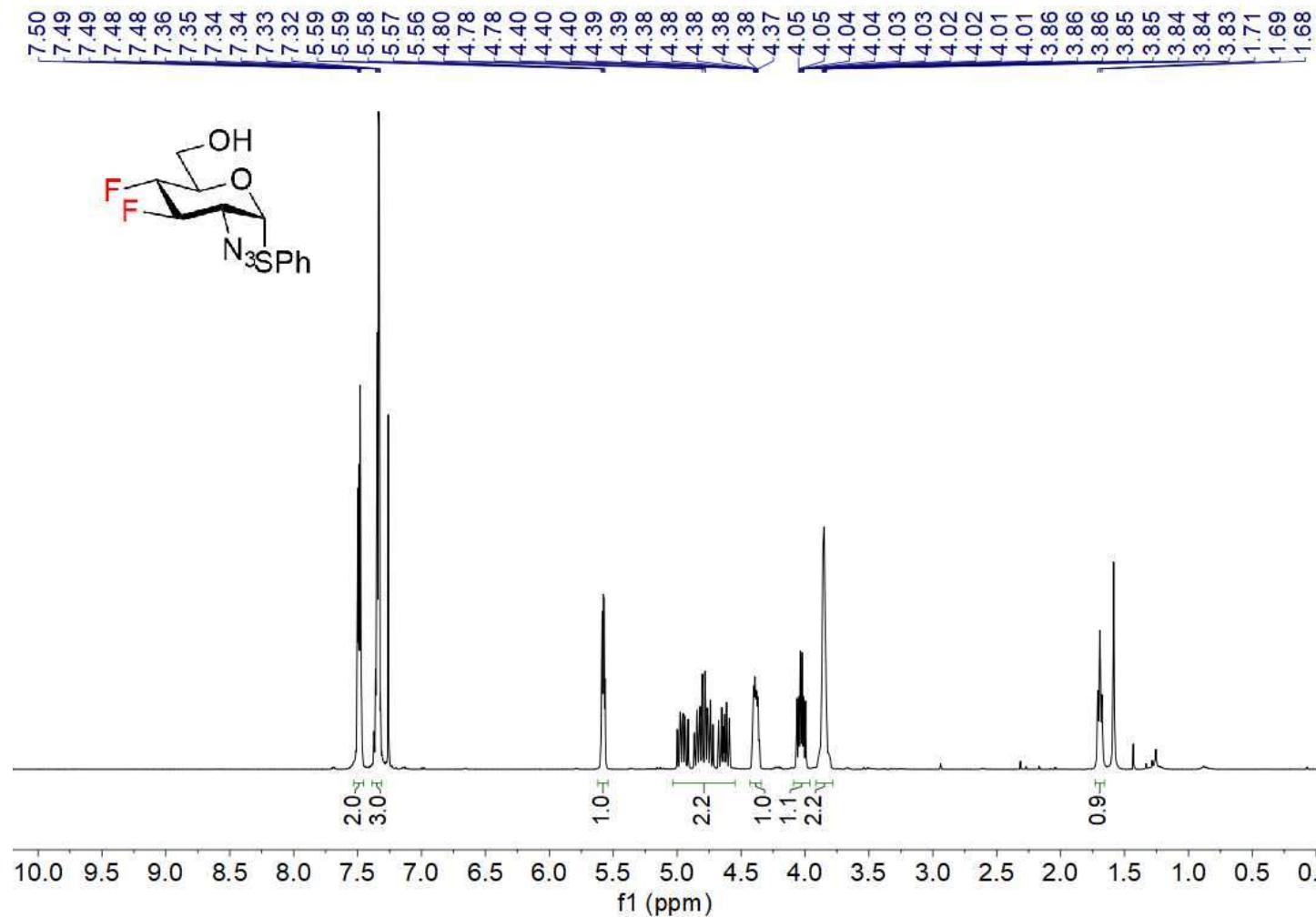


¹H-¹³C HSQC 18

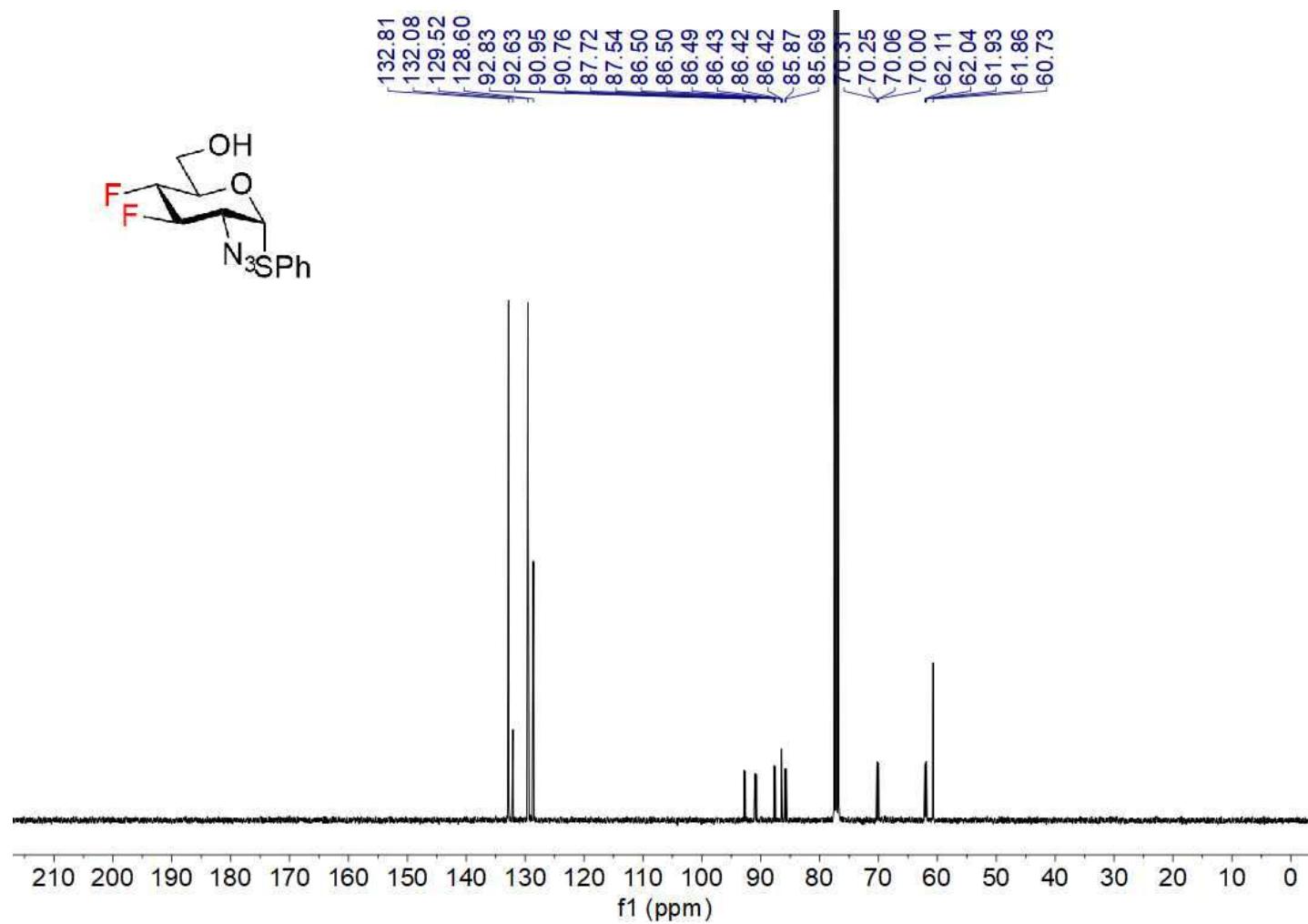


NMR COMPOUND α -19

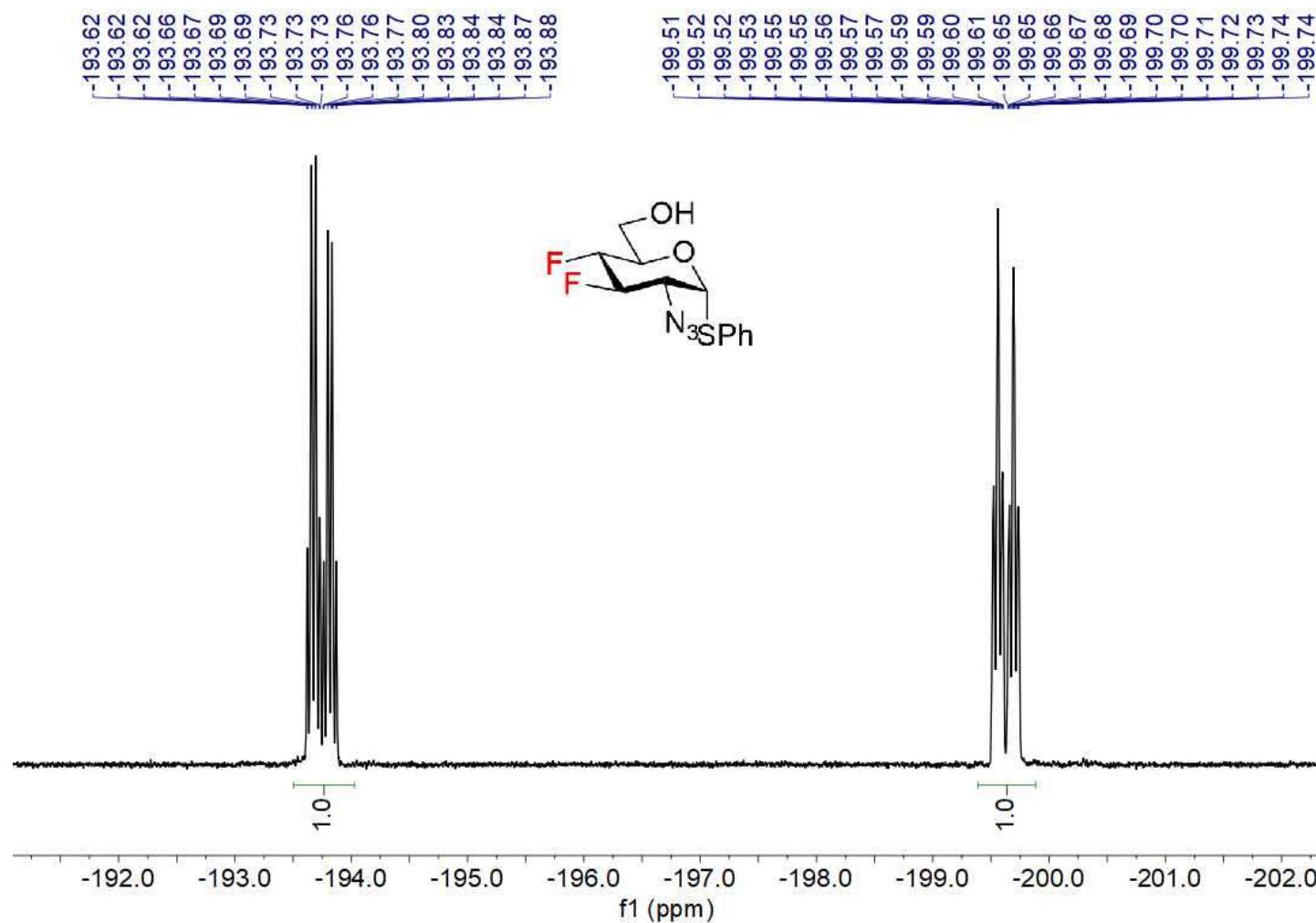
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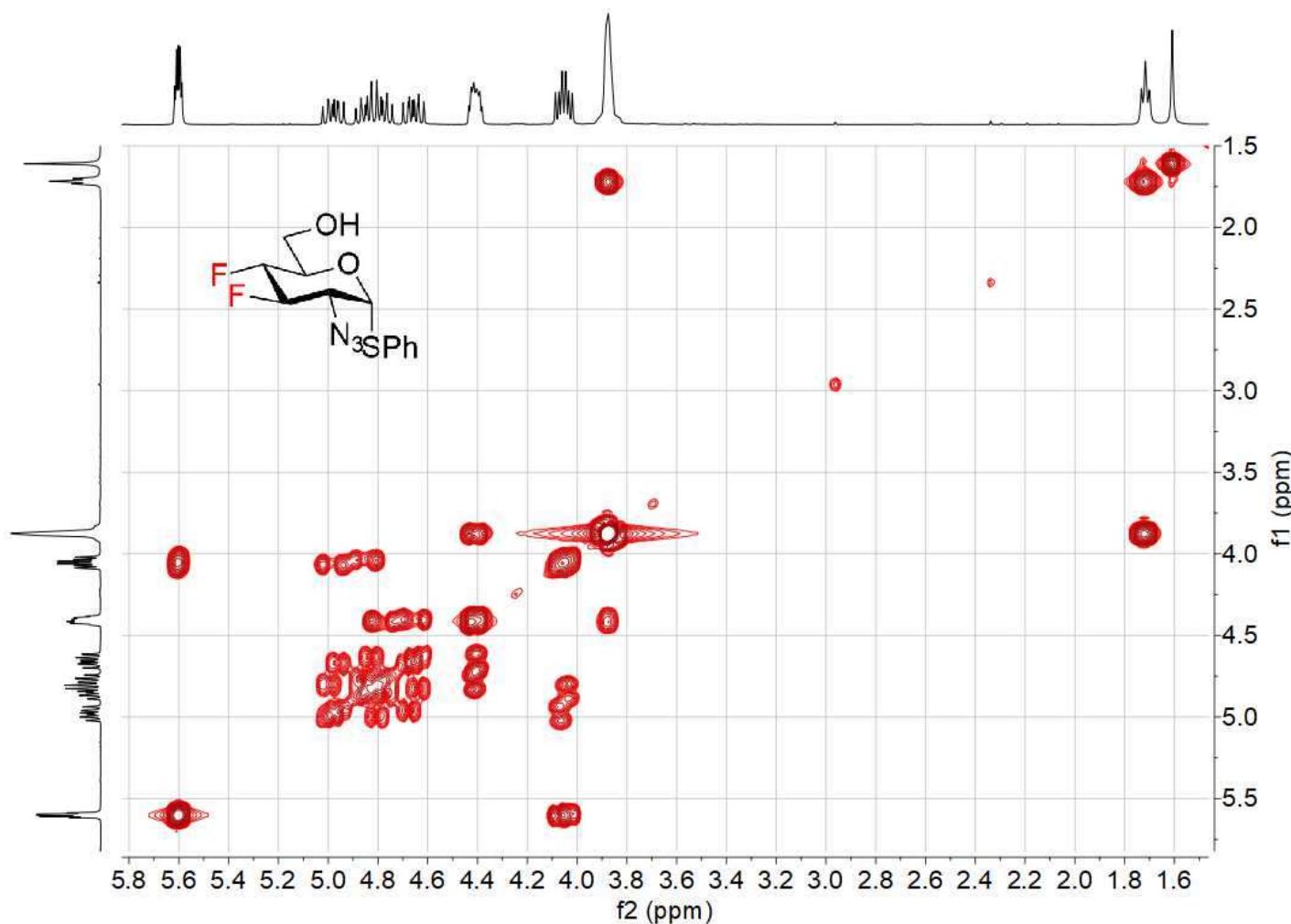
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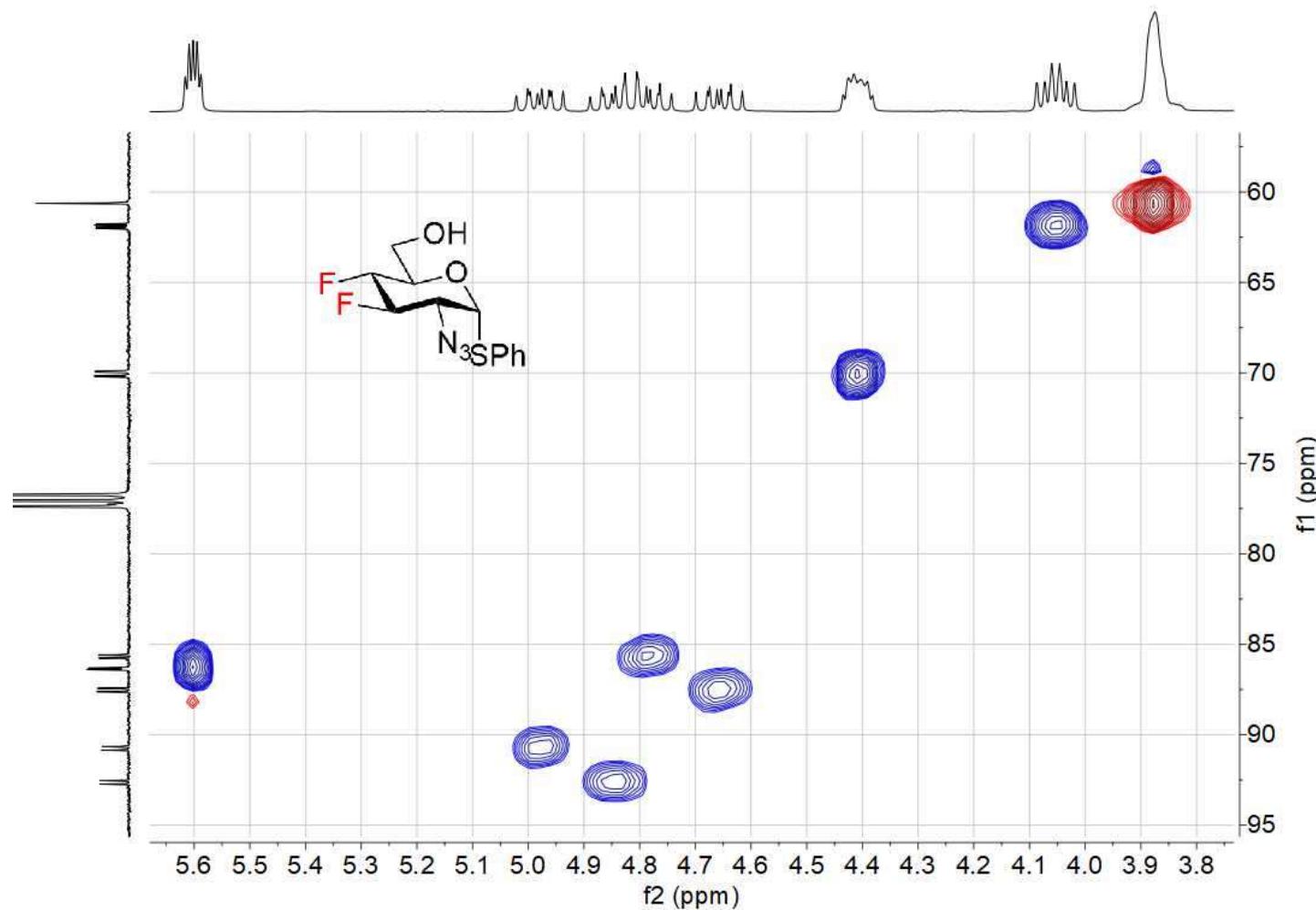
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¹H-¹H COSY *a*-19



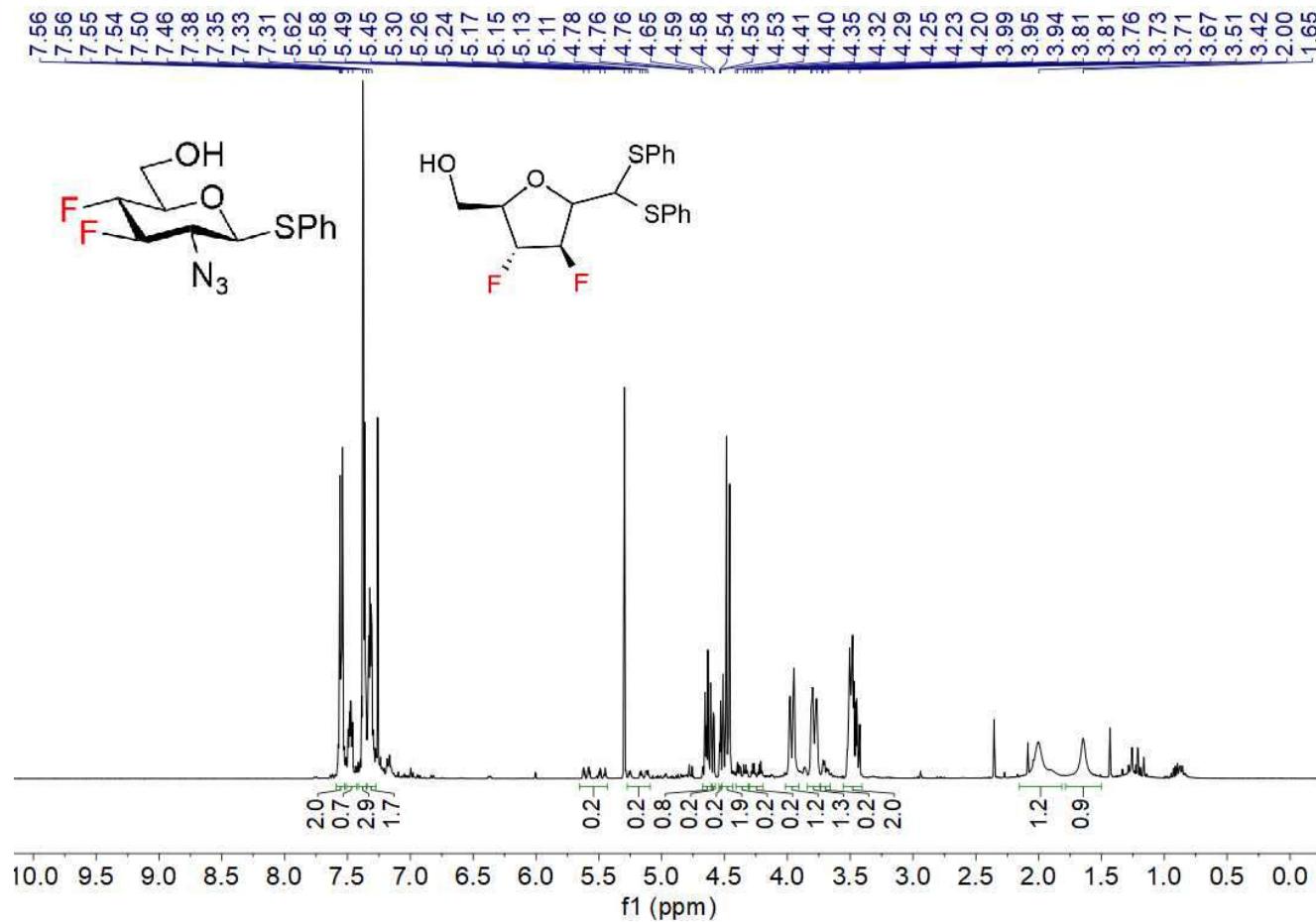
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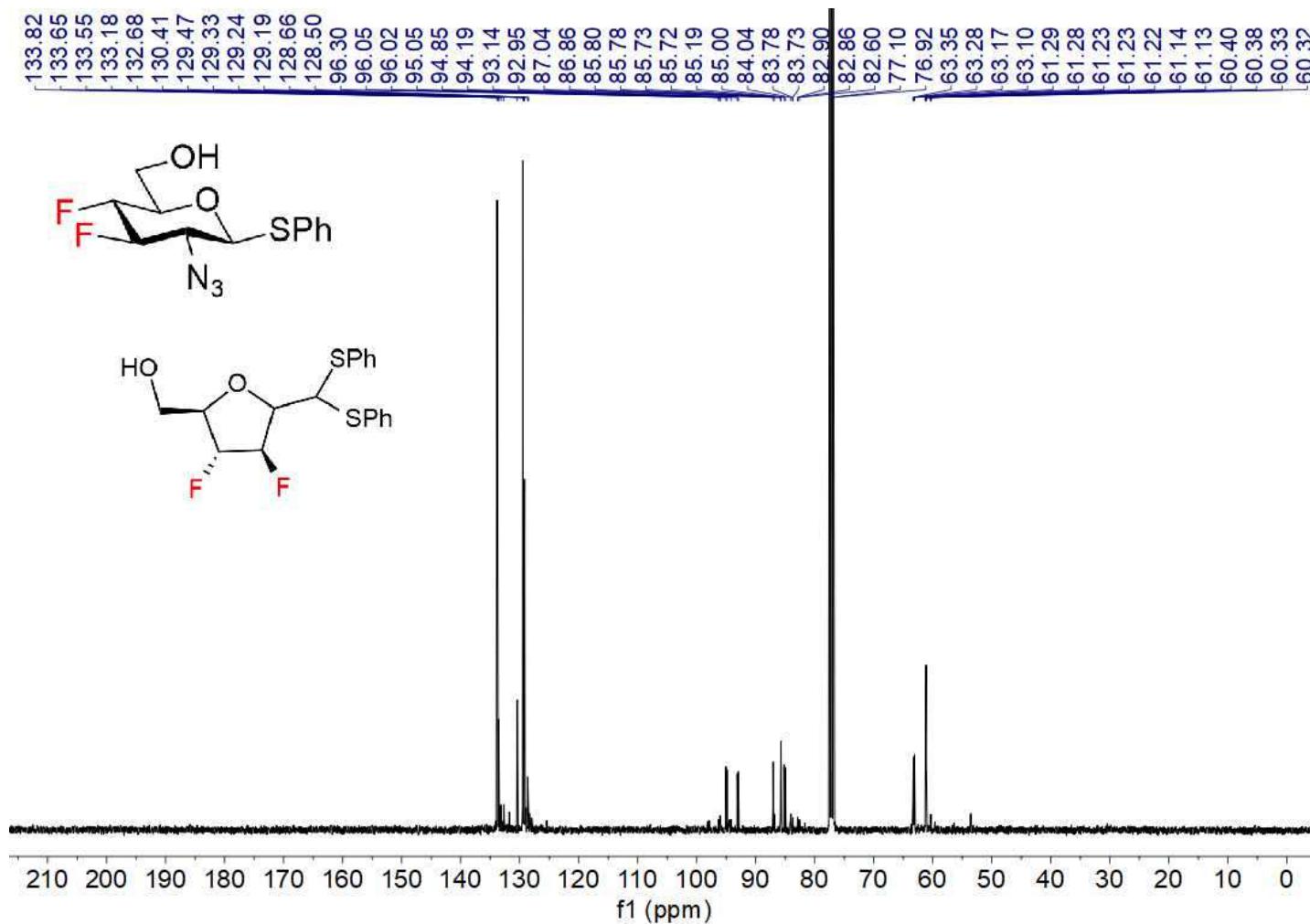
NMR COMPOUND β -19

(ca 16% of 2,3-dideoxy-2,3-difluoro- C - α - or β -D-arabinofuranosyl-formaldehyde diphenyl dithioacetal S1)

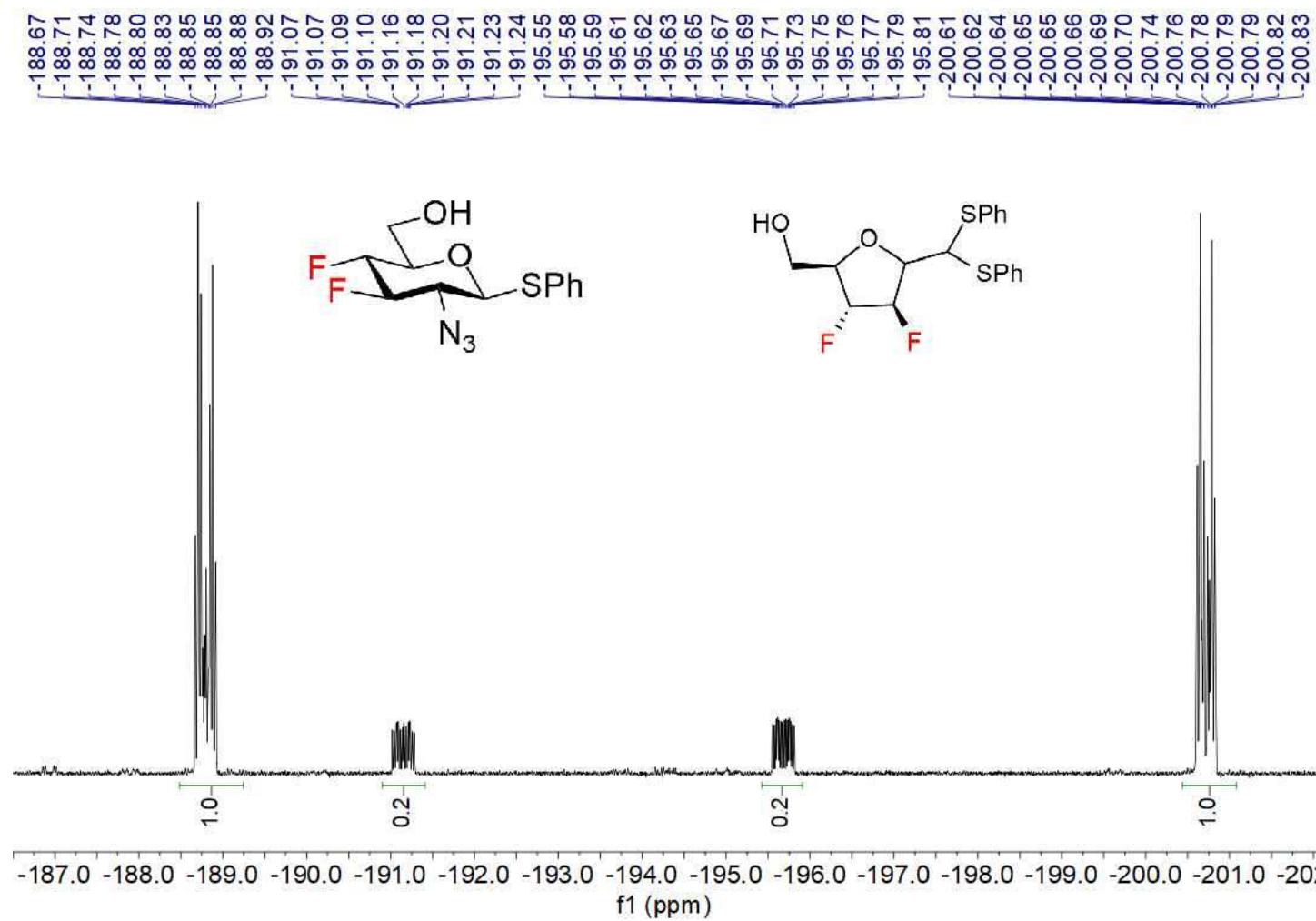
^1H NMR (400 MHz, CDCl_3) β -19 (and ca 16% S1)



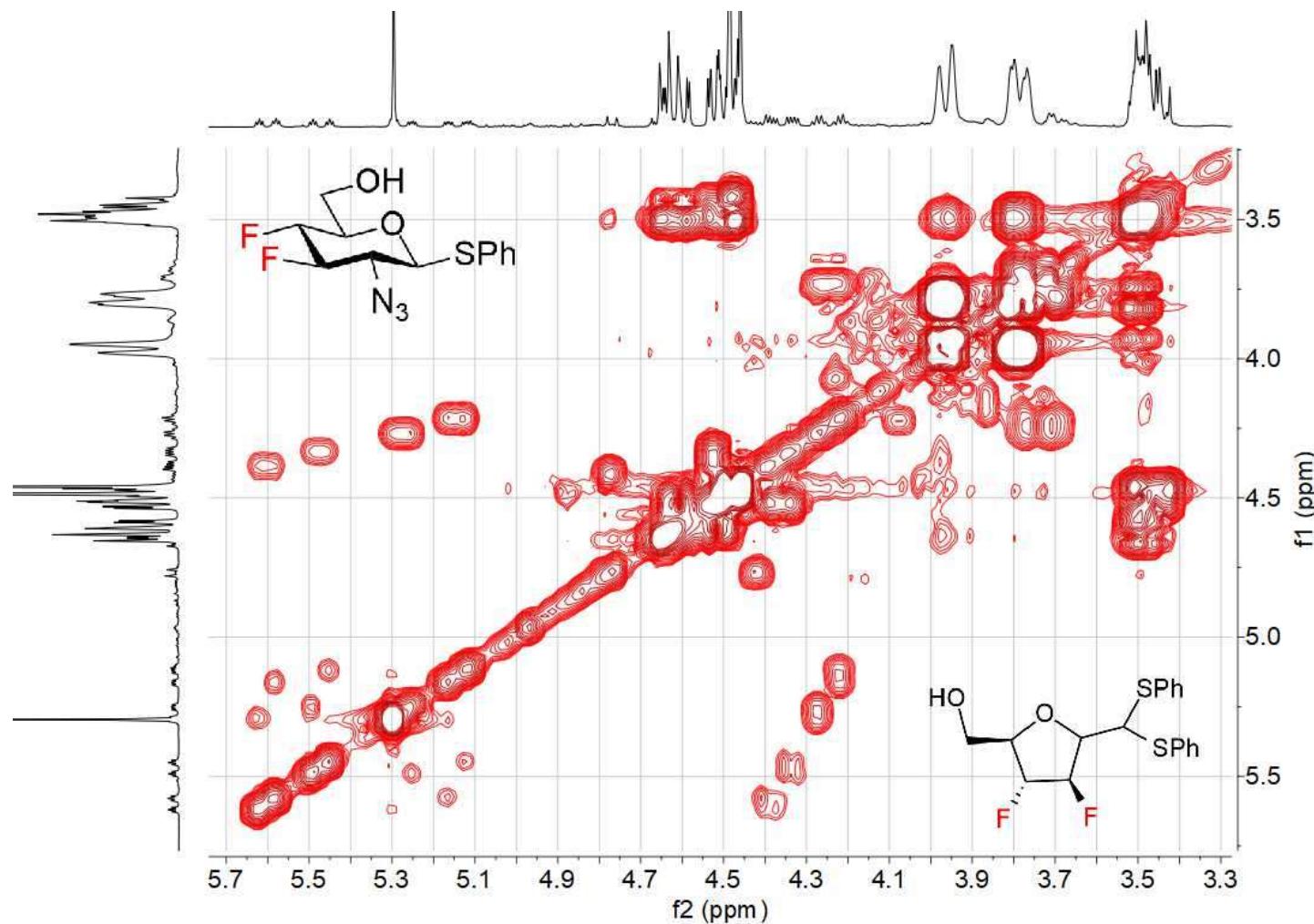
¹³C NMR (100 MHz, CDCl₃) β -19 (and ca 16% S1)



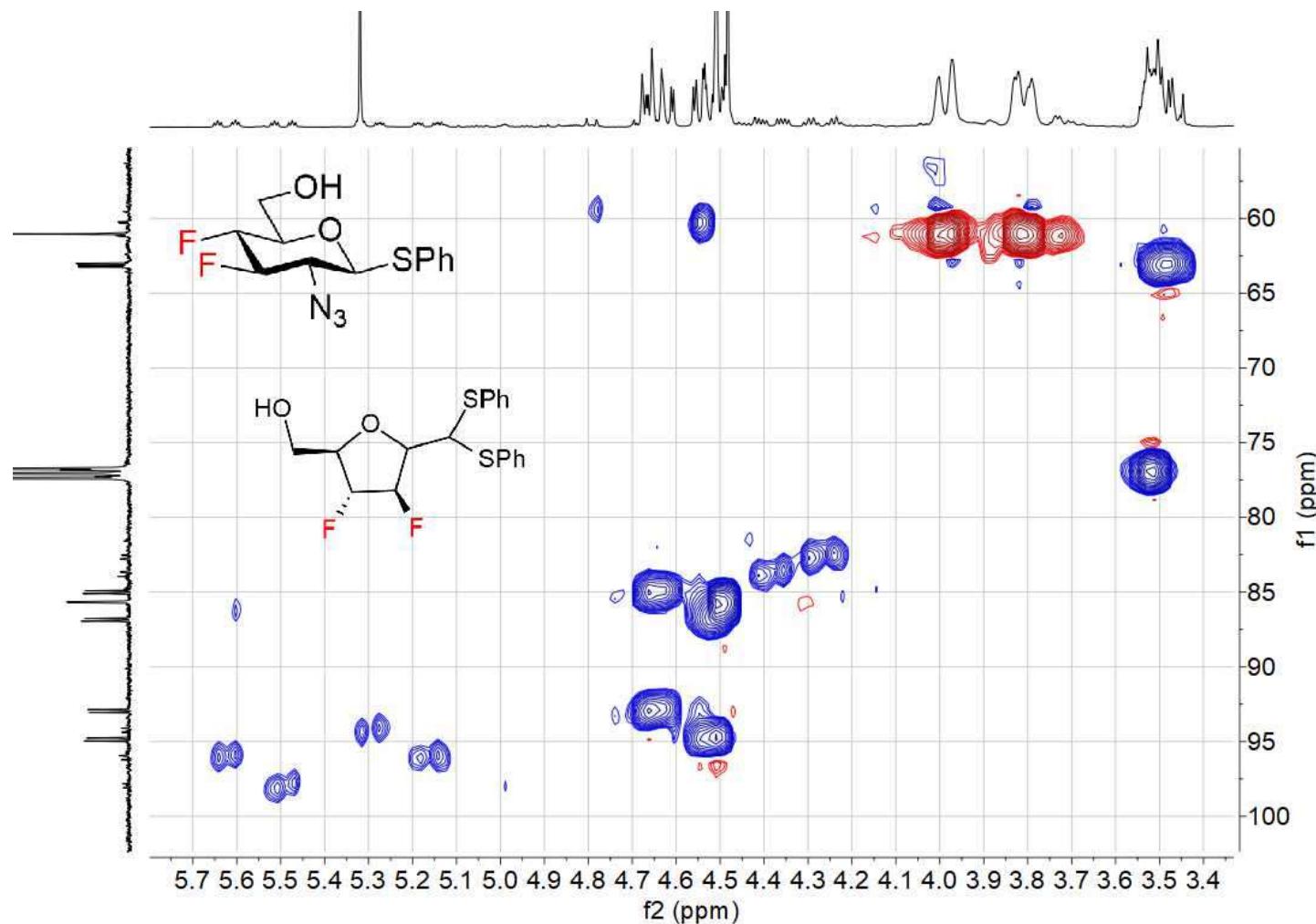
¹⁹F NMR (376 MHz, CDCl₃) β -19 (and ca 16% S1)



^1H - ^1H COSY β -19

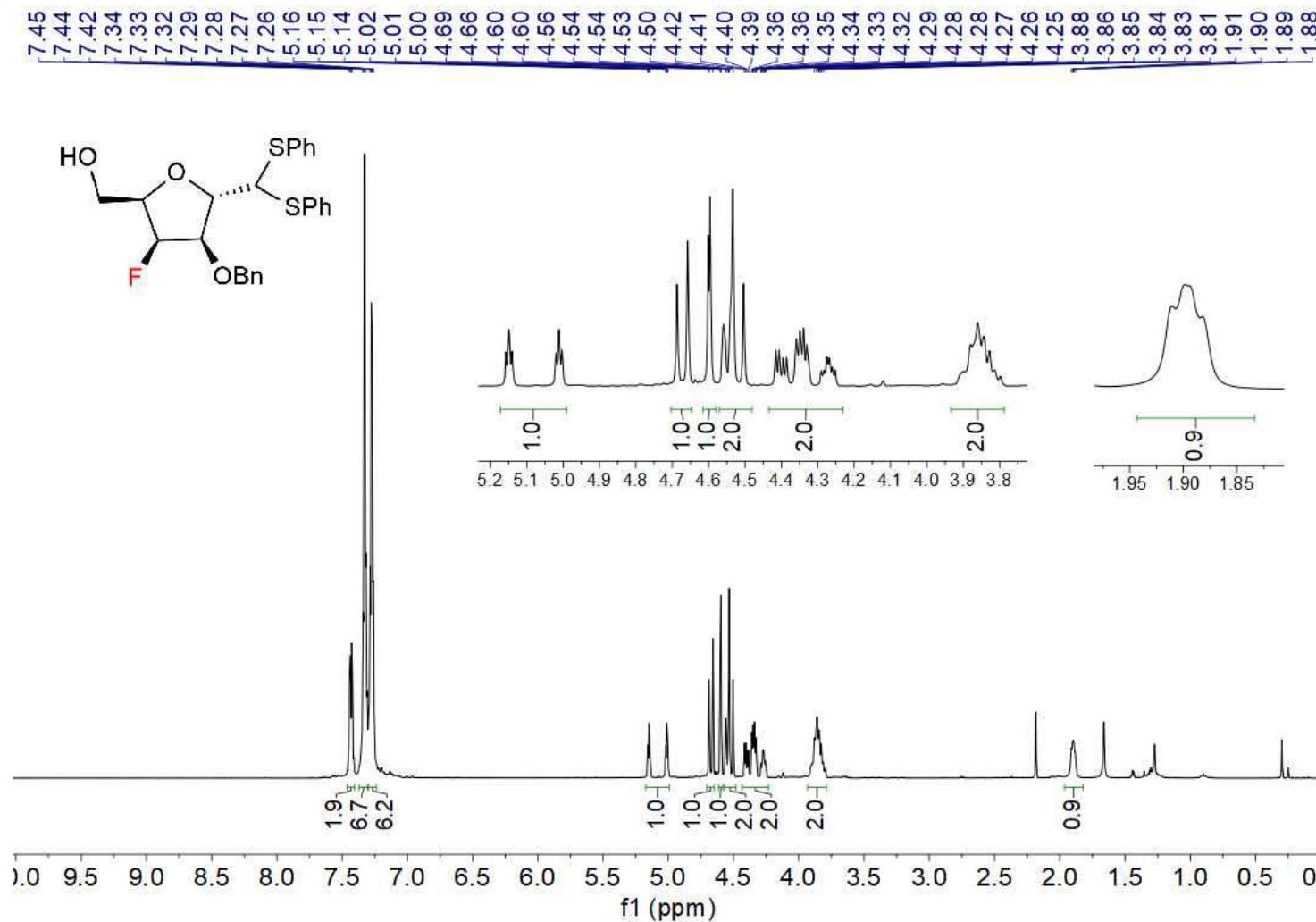


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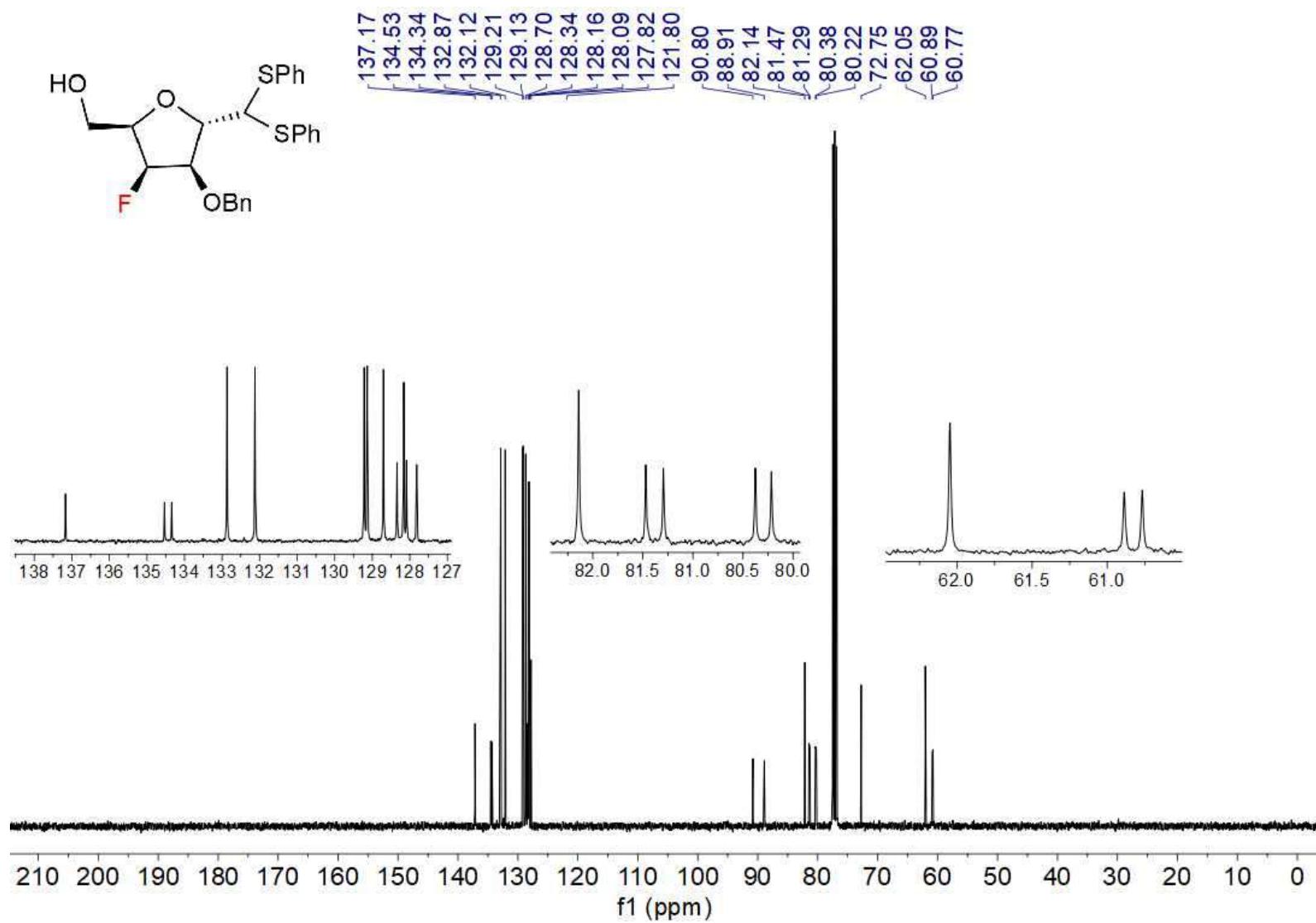


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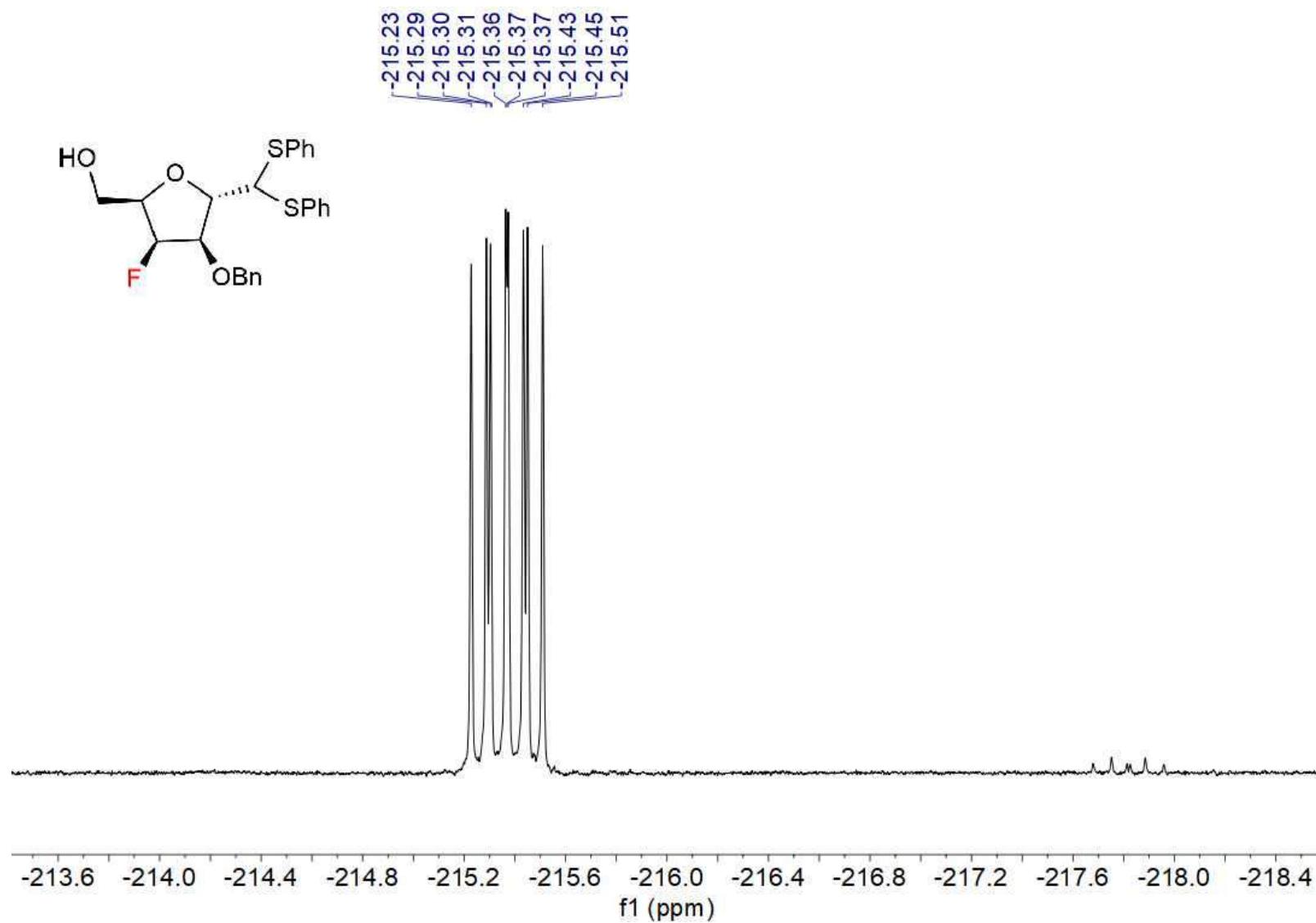
^1H NMR (400 MHz, CDCl_3) 20



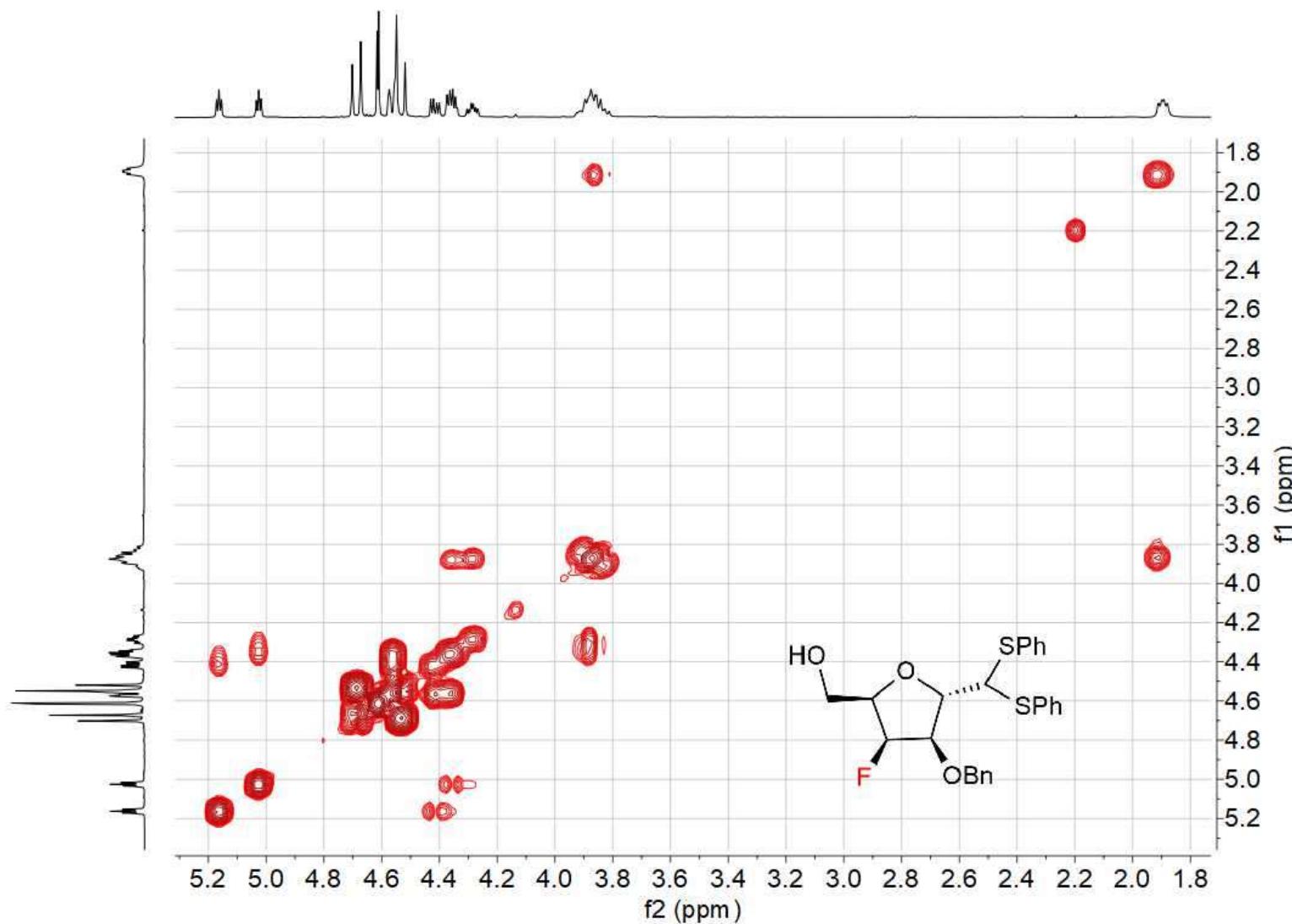
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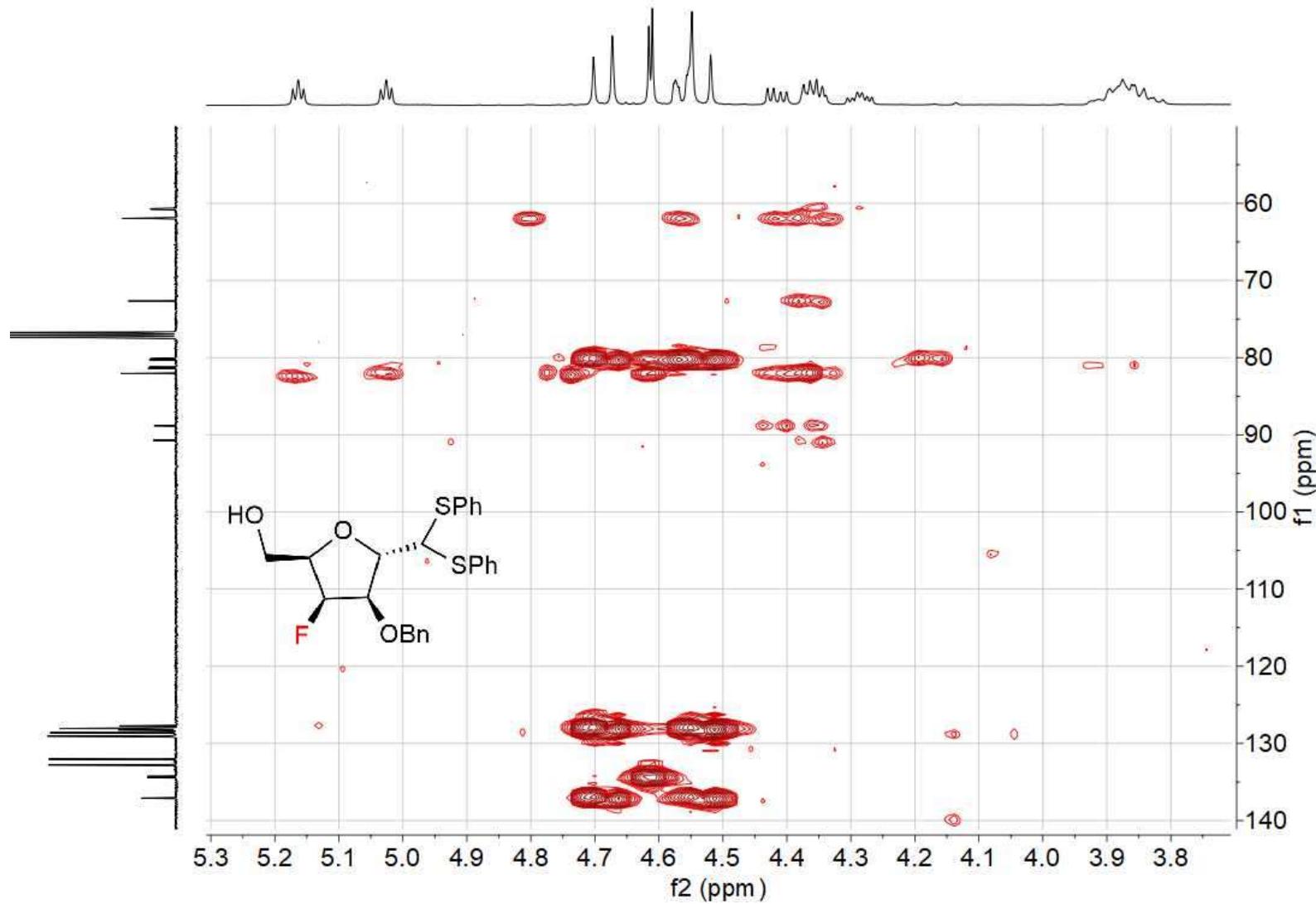
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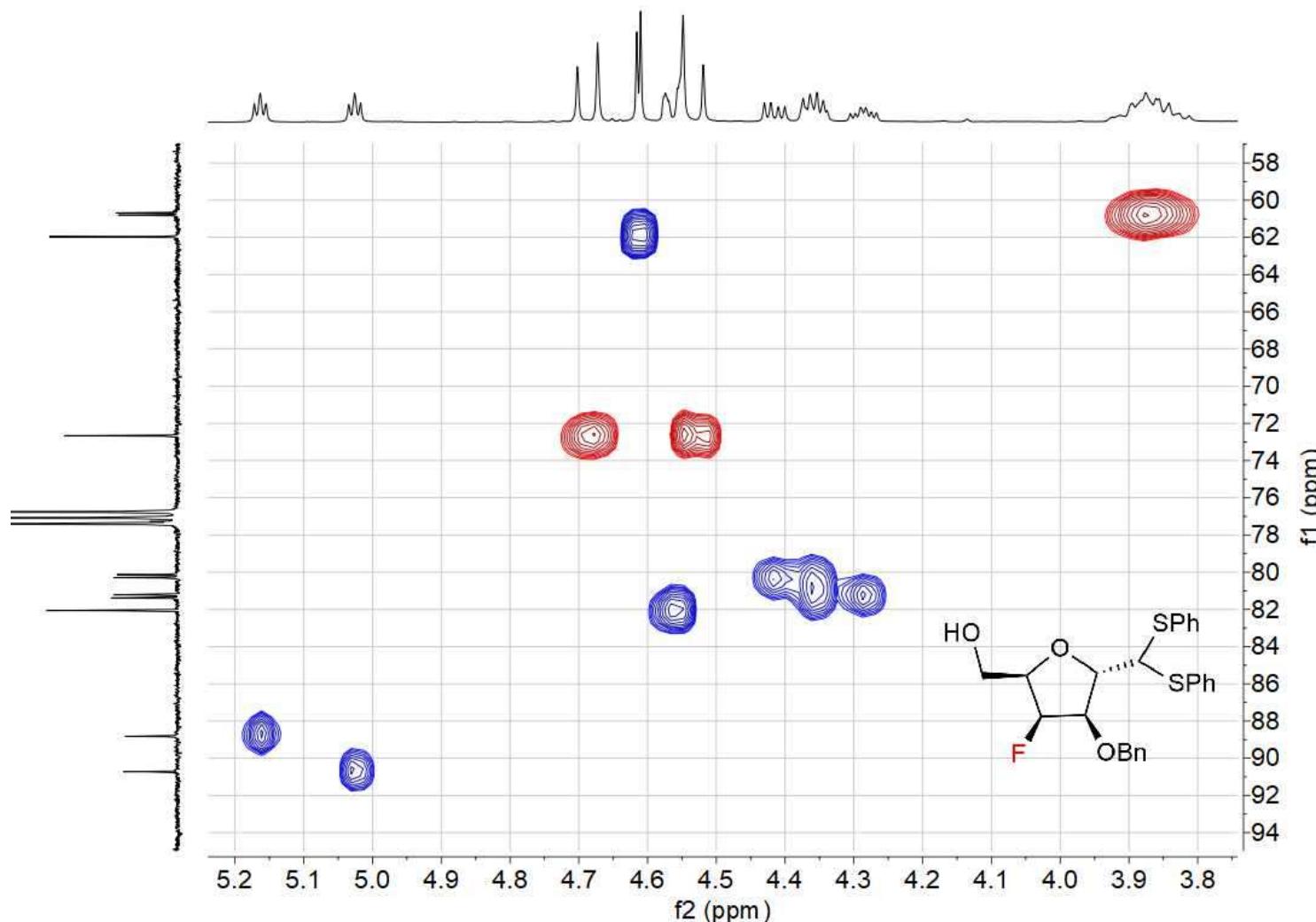
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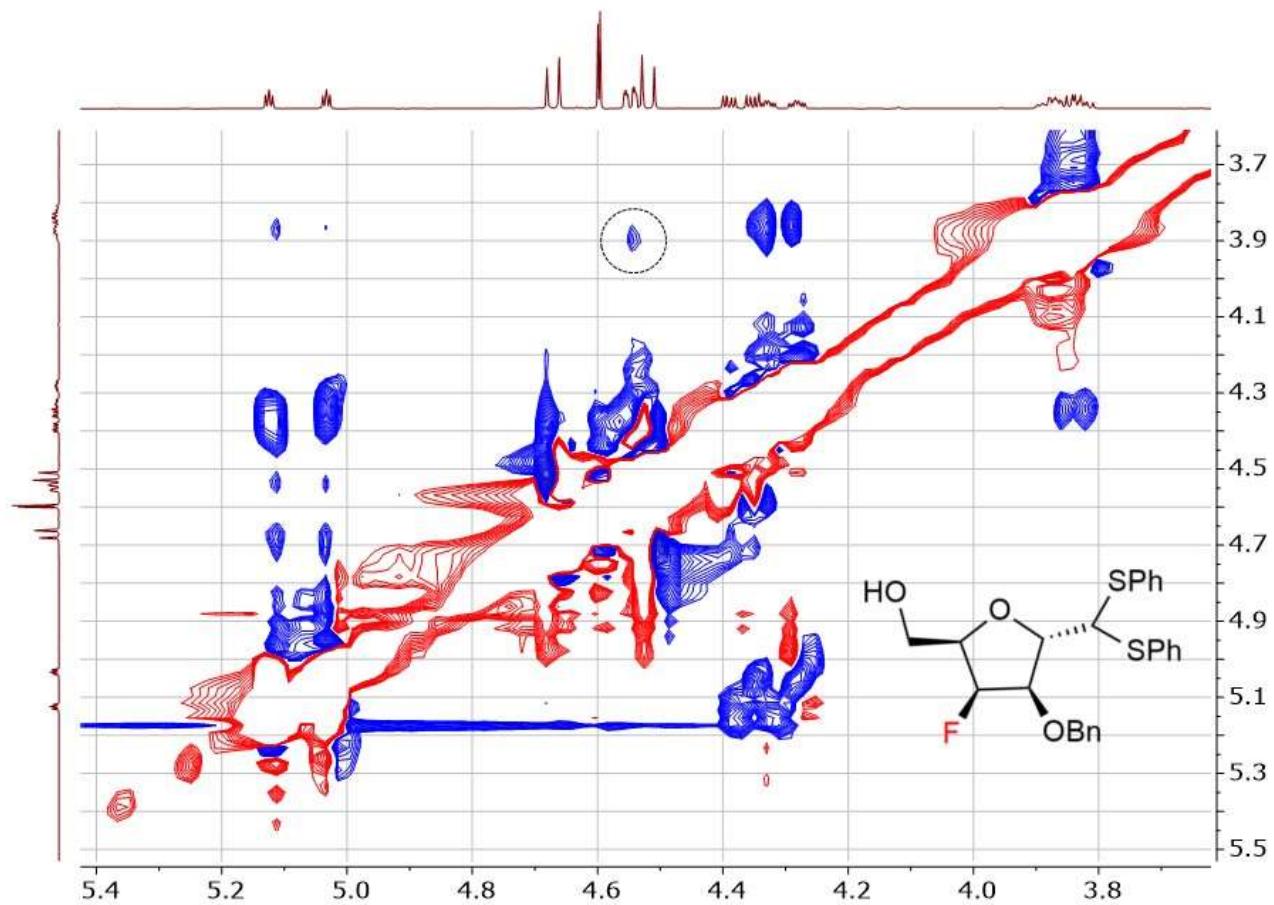
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^1H - ^{13}C HSQC 20

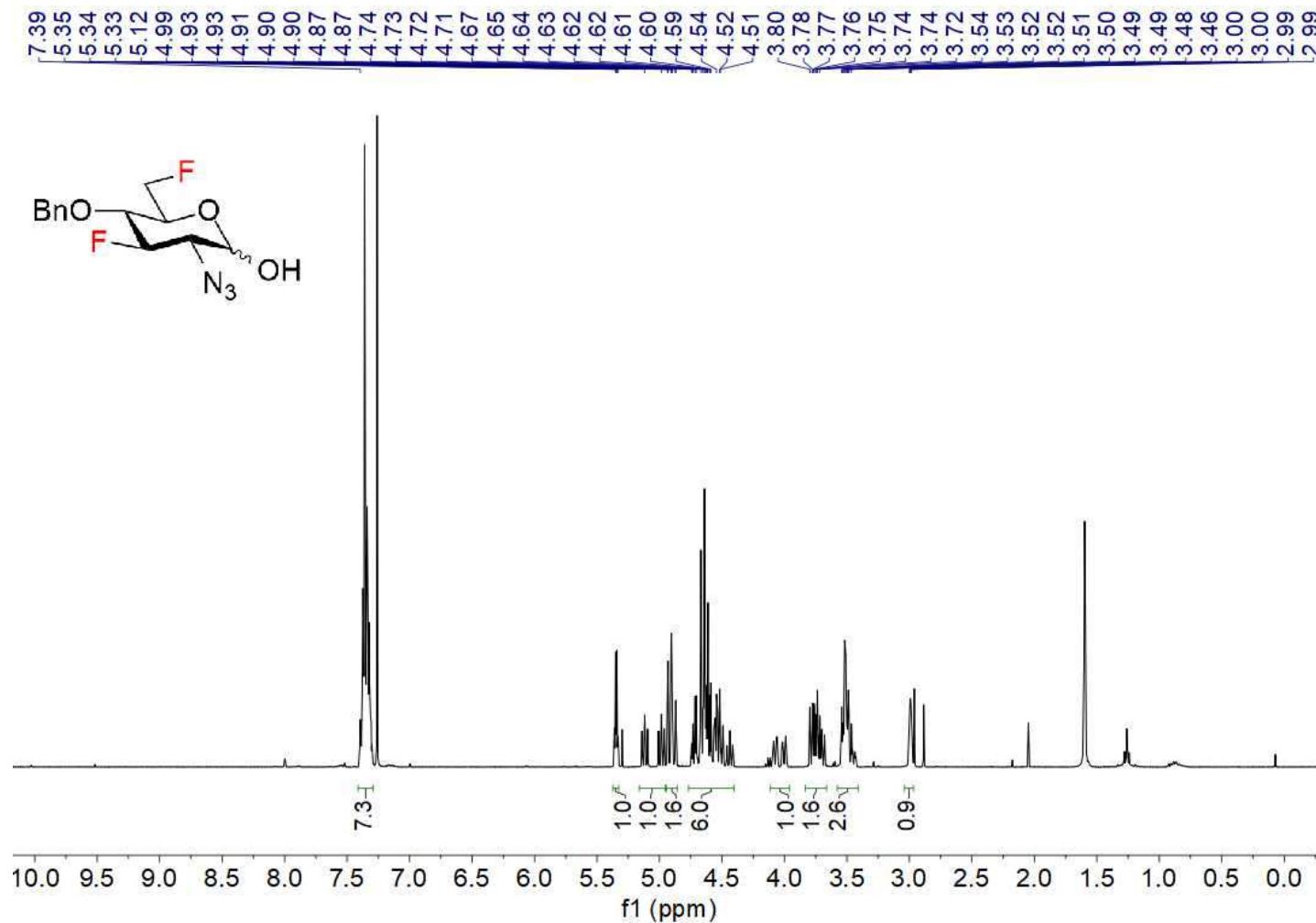


¹H-³H ROESY 20

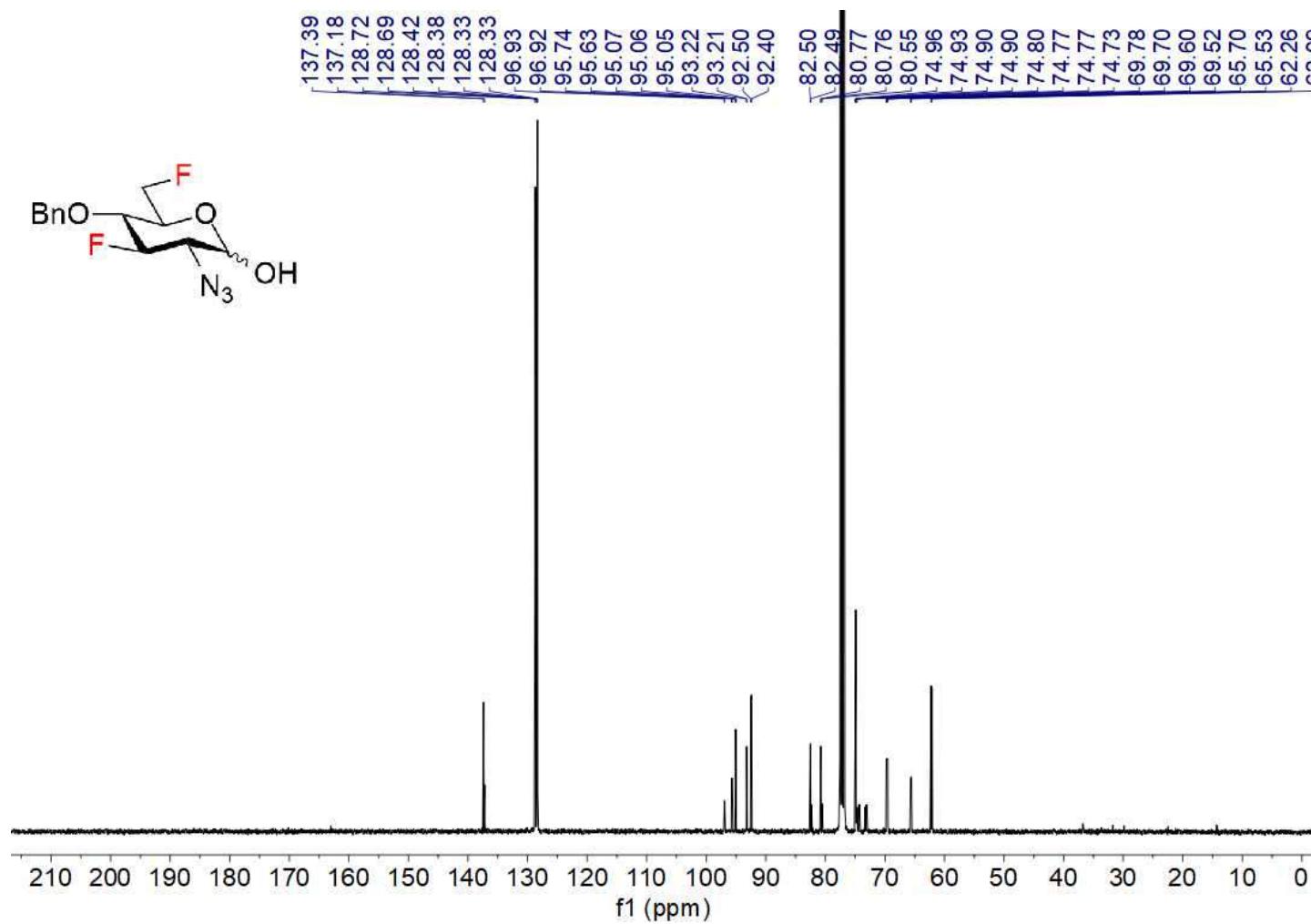


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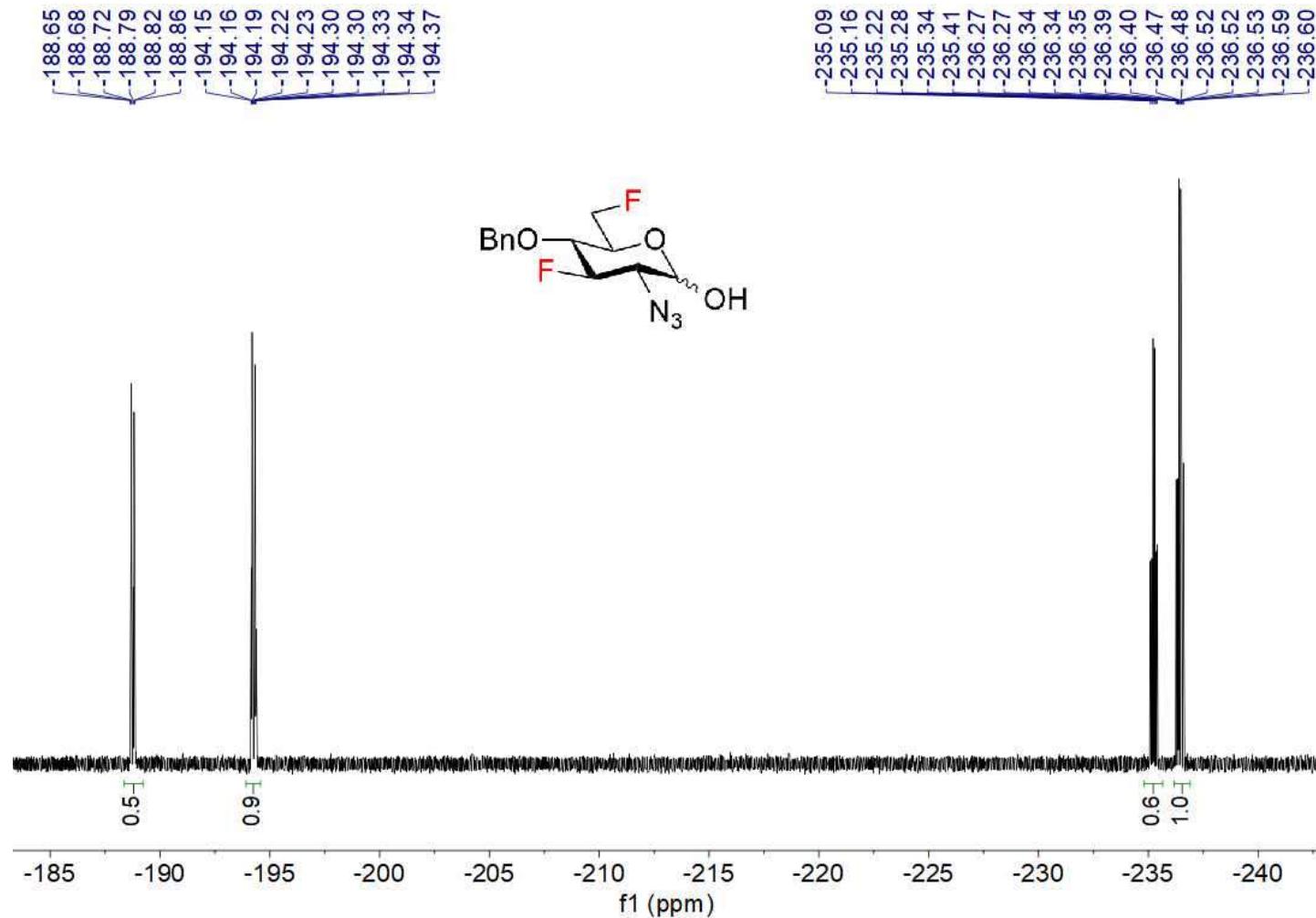
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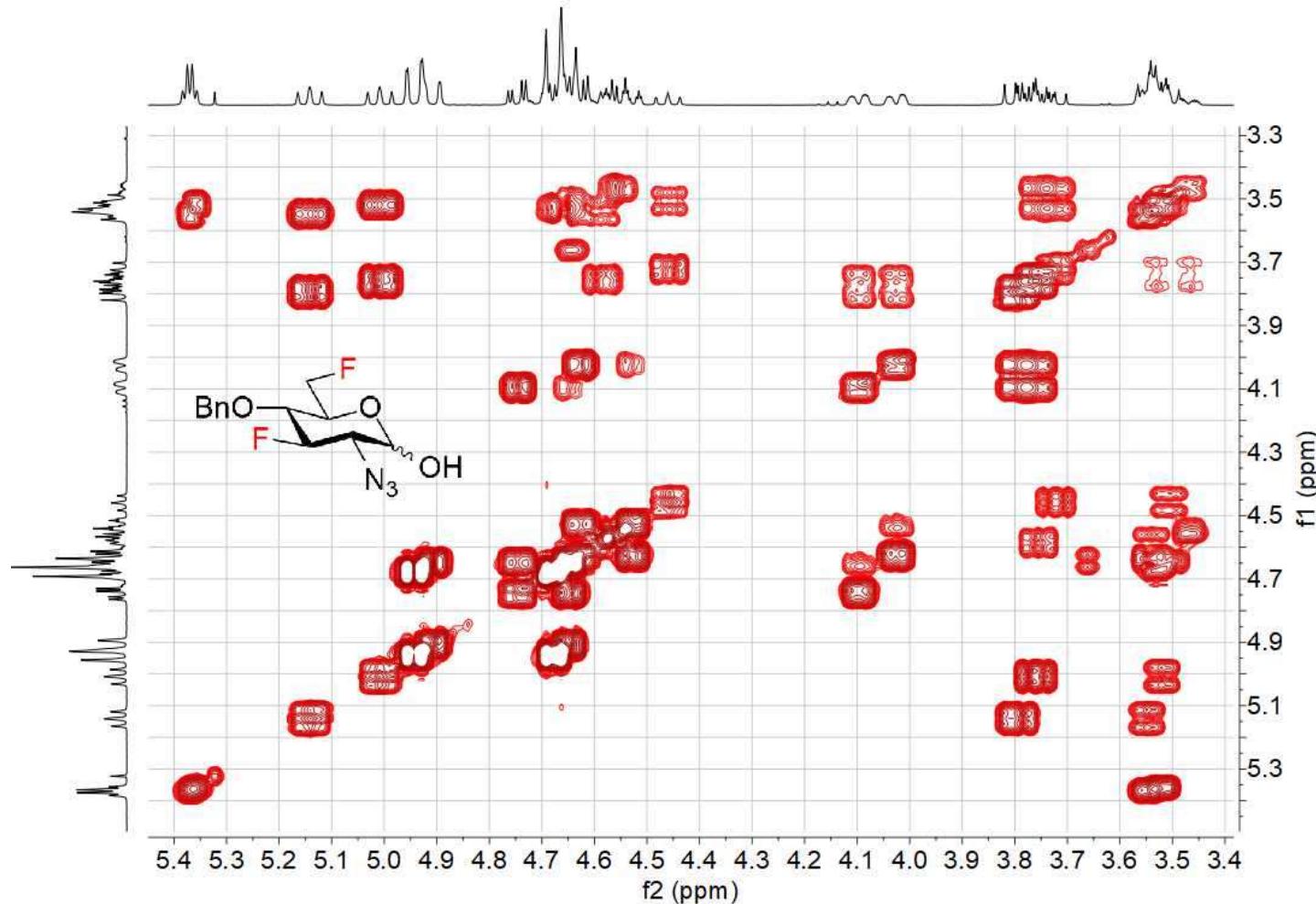
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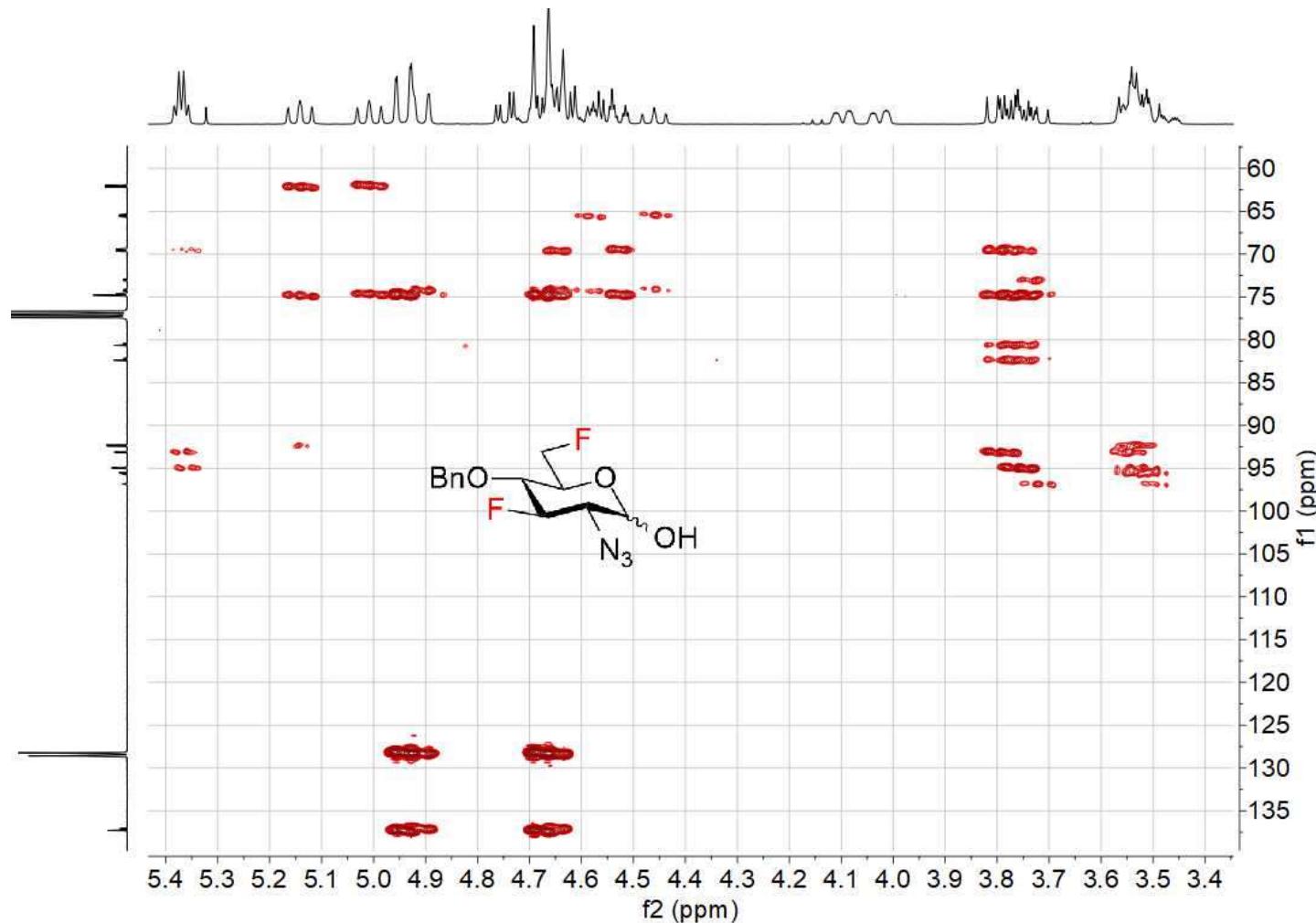
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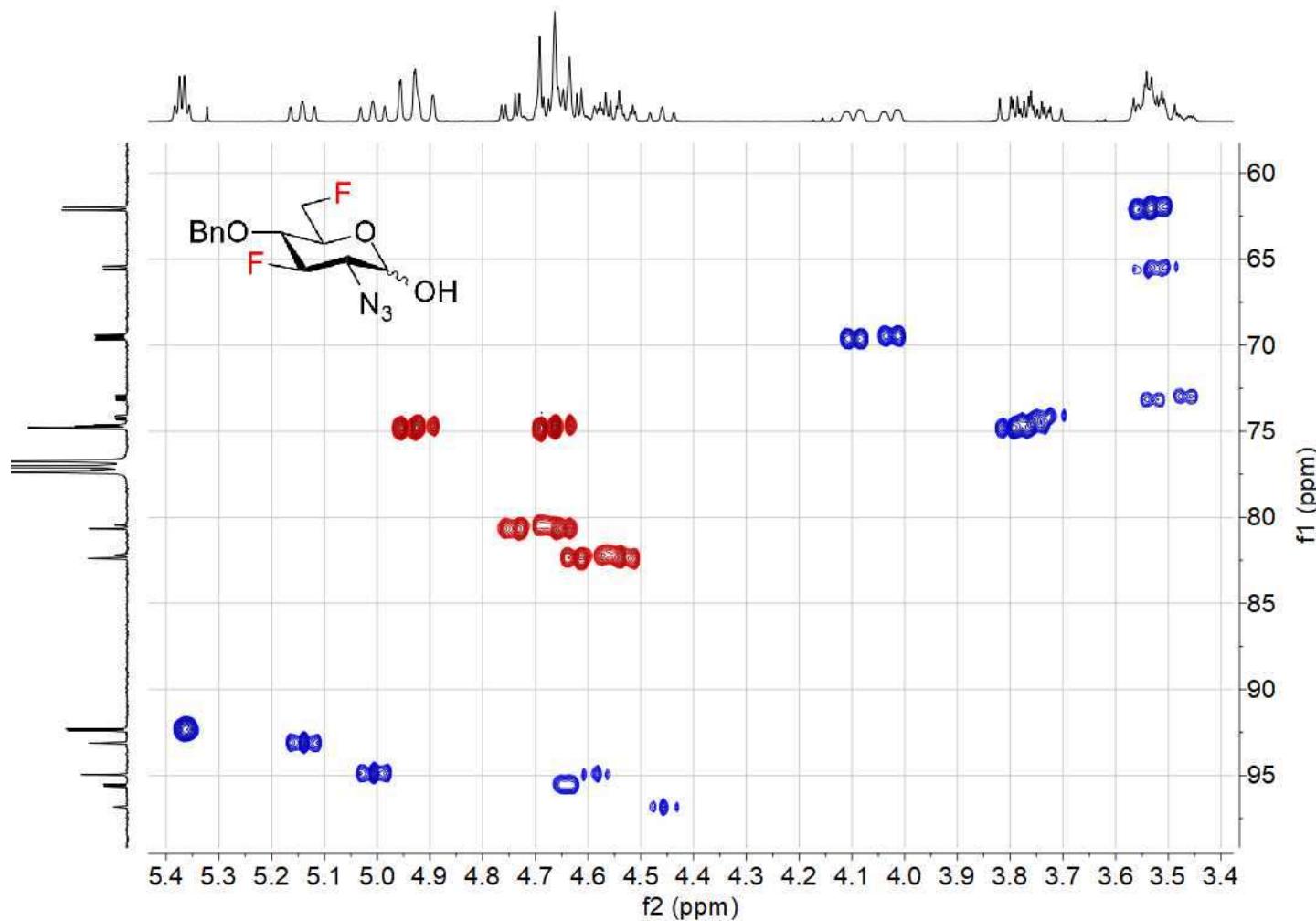
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^1H - ^{13}C HMBC 22

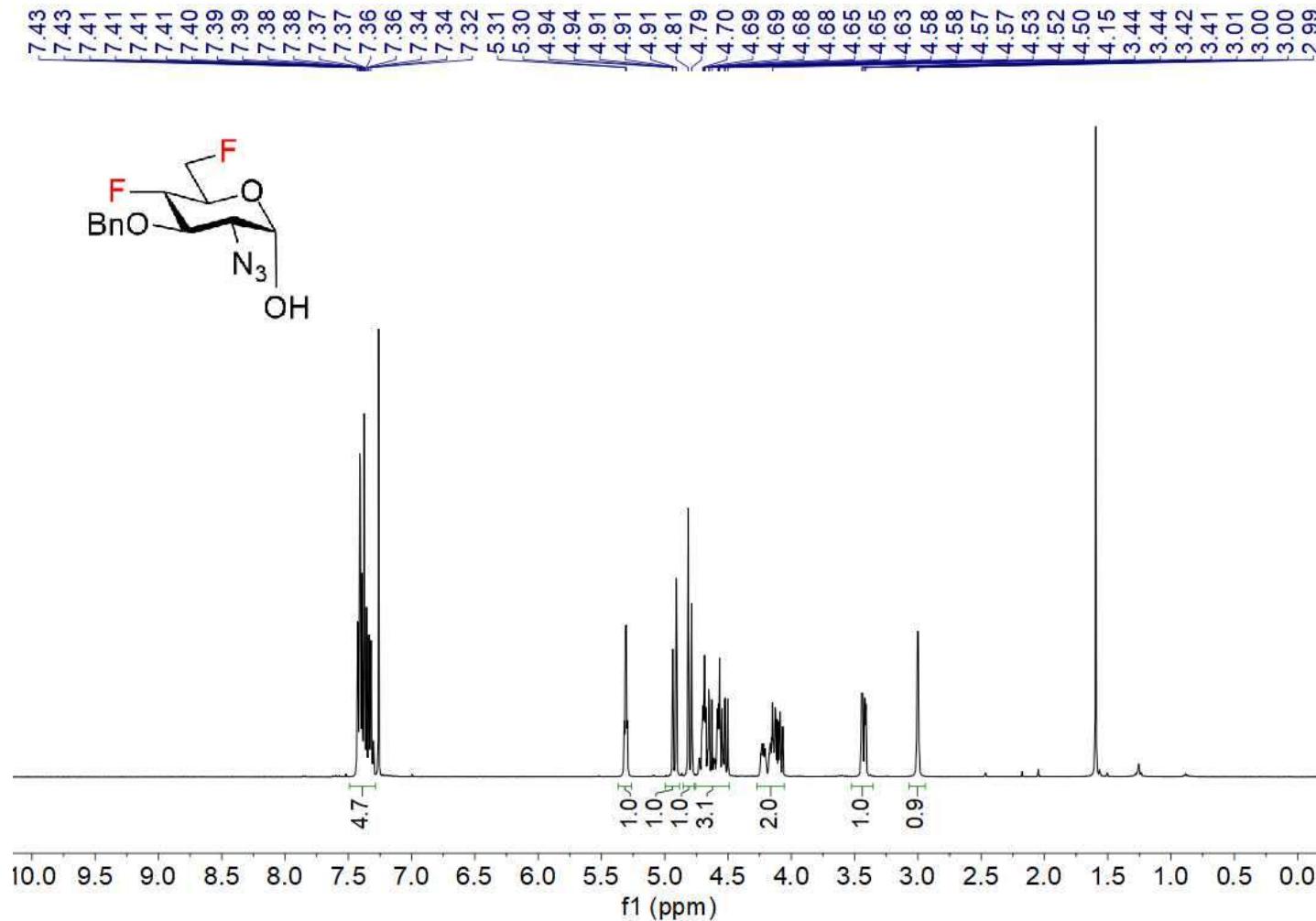


^1H - ^{13}C HSQC 22

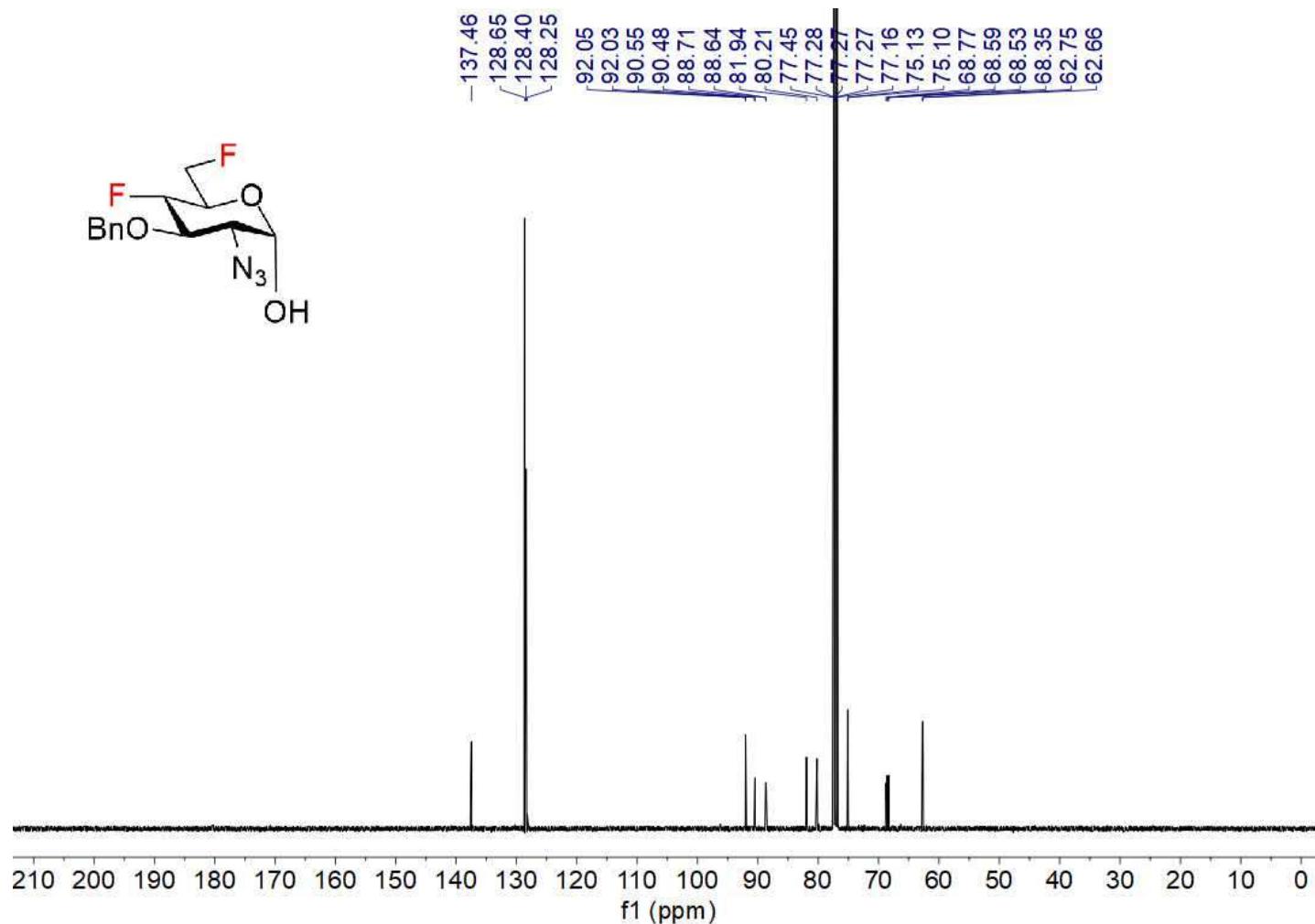


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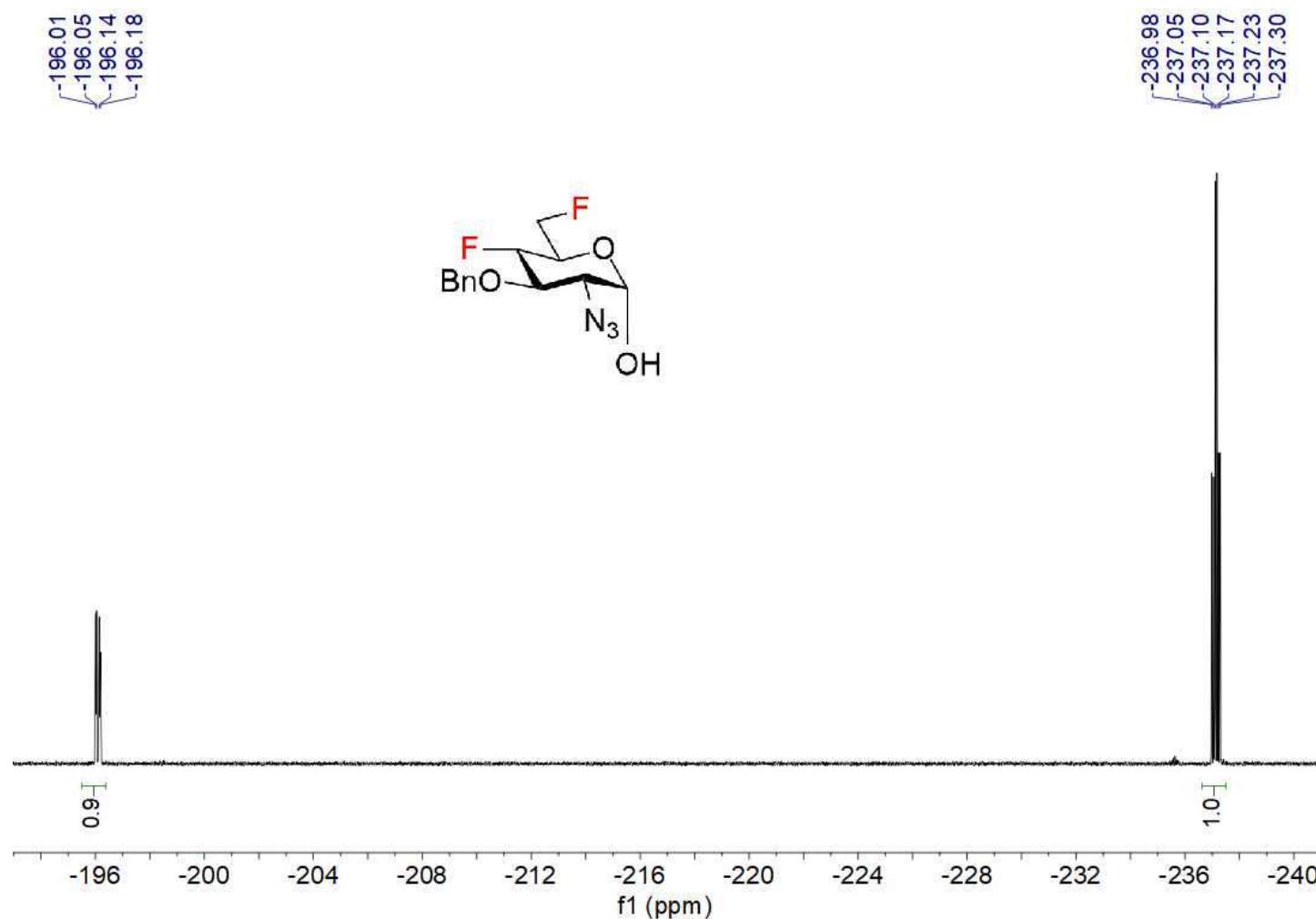
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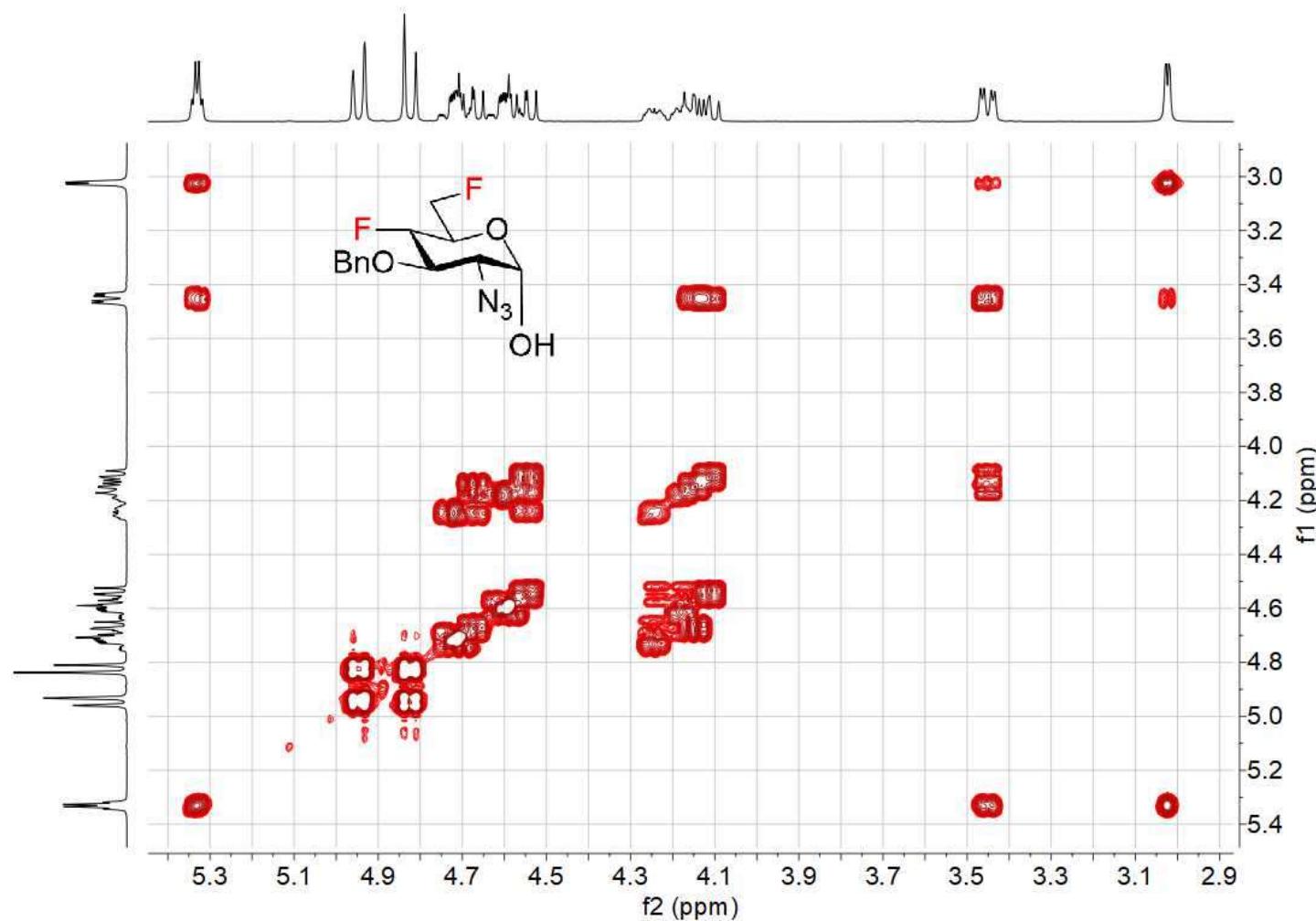
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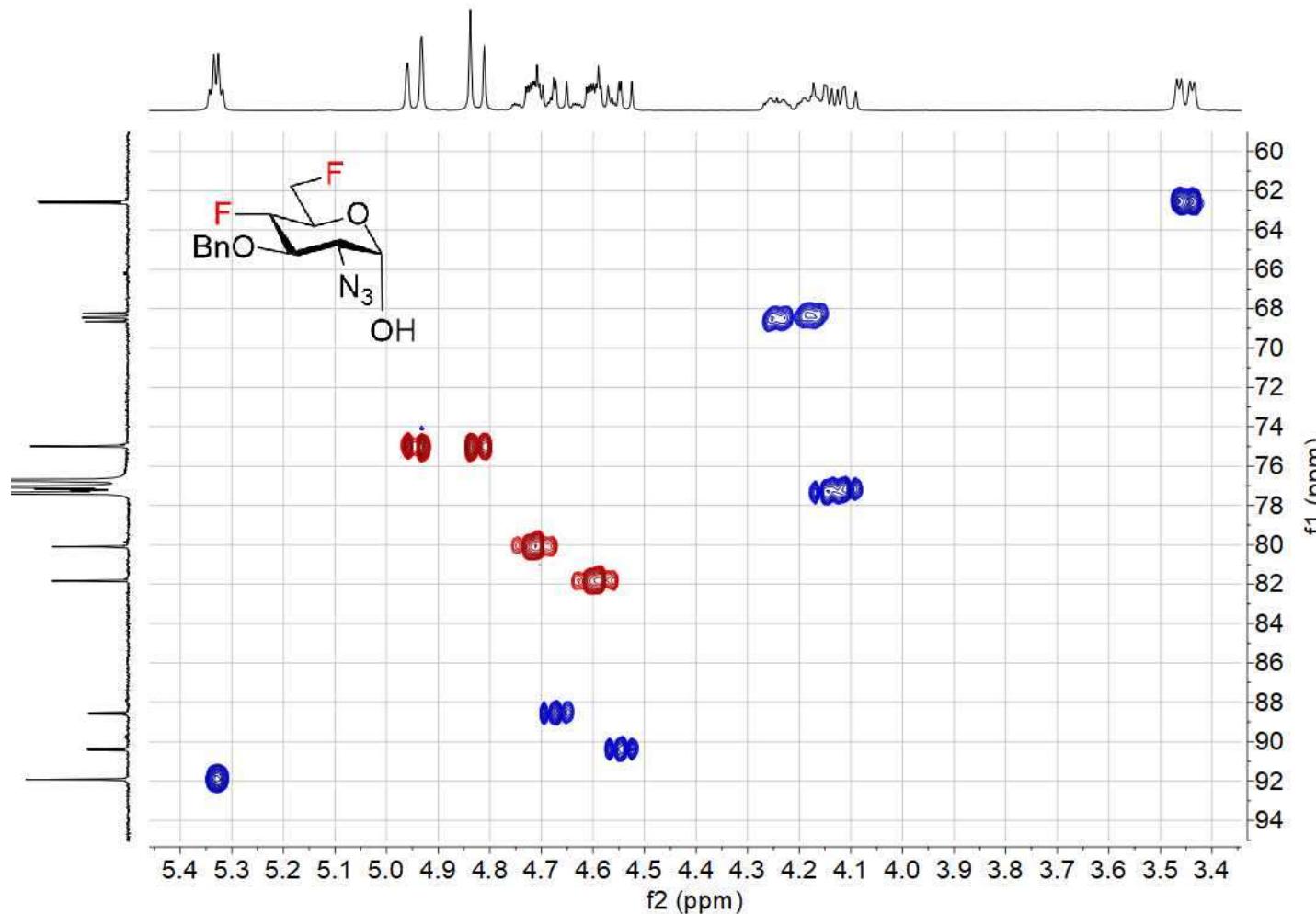
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¹H-¹H COSY 23

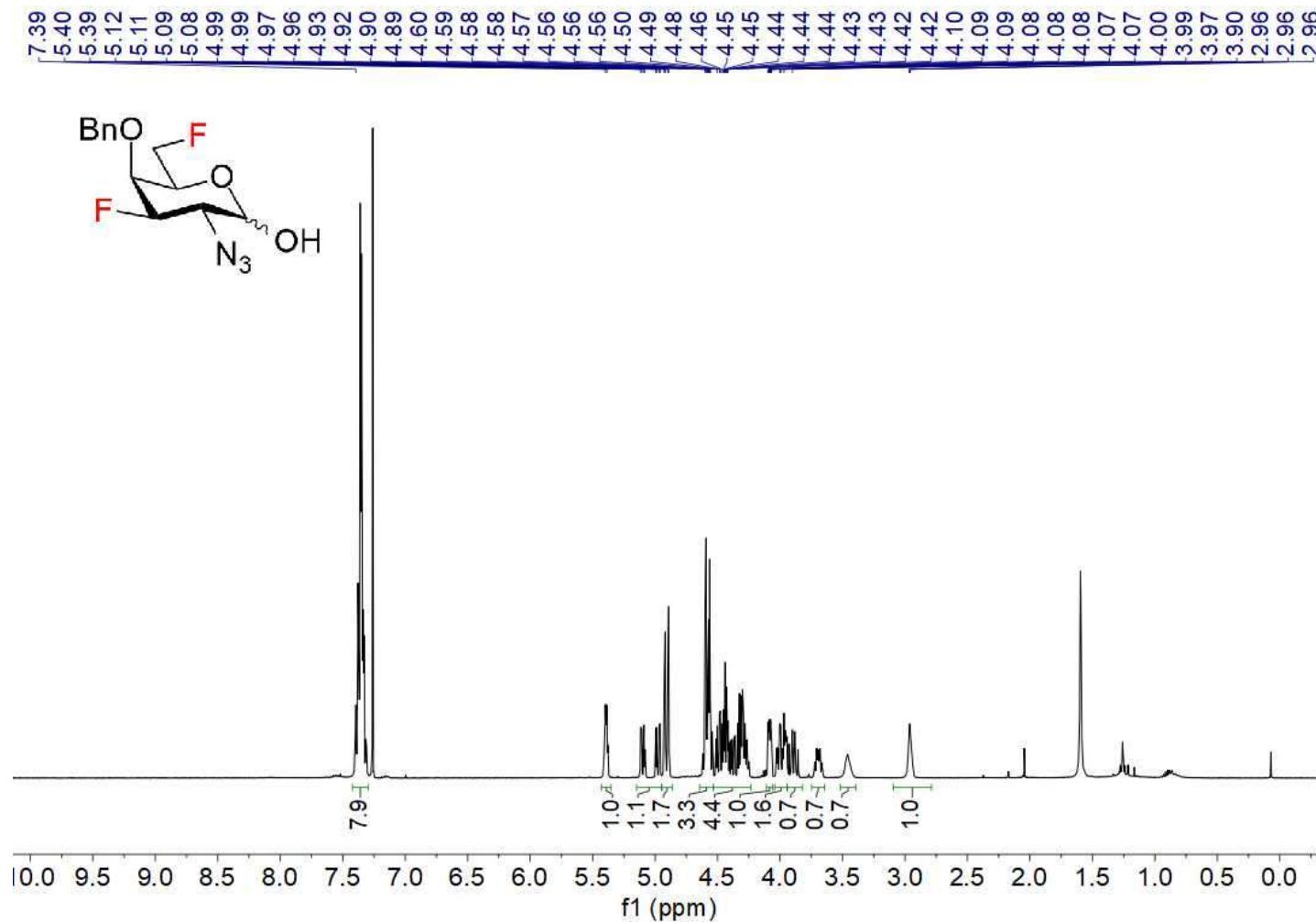


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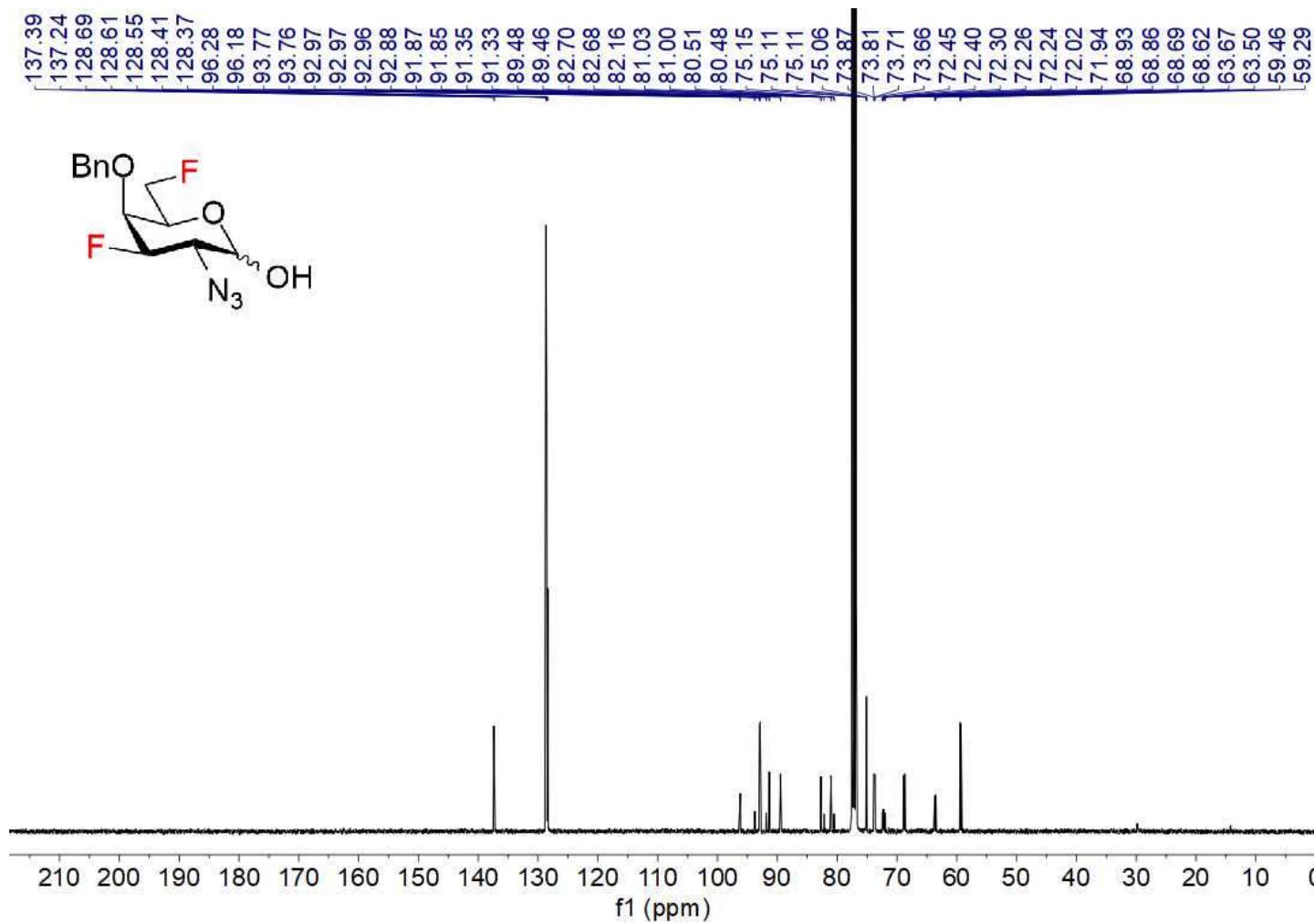


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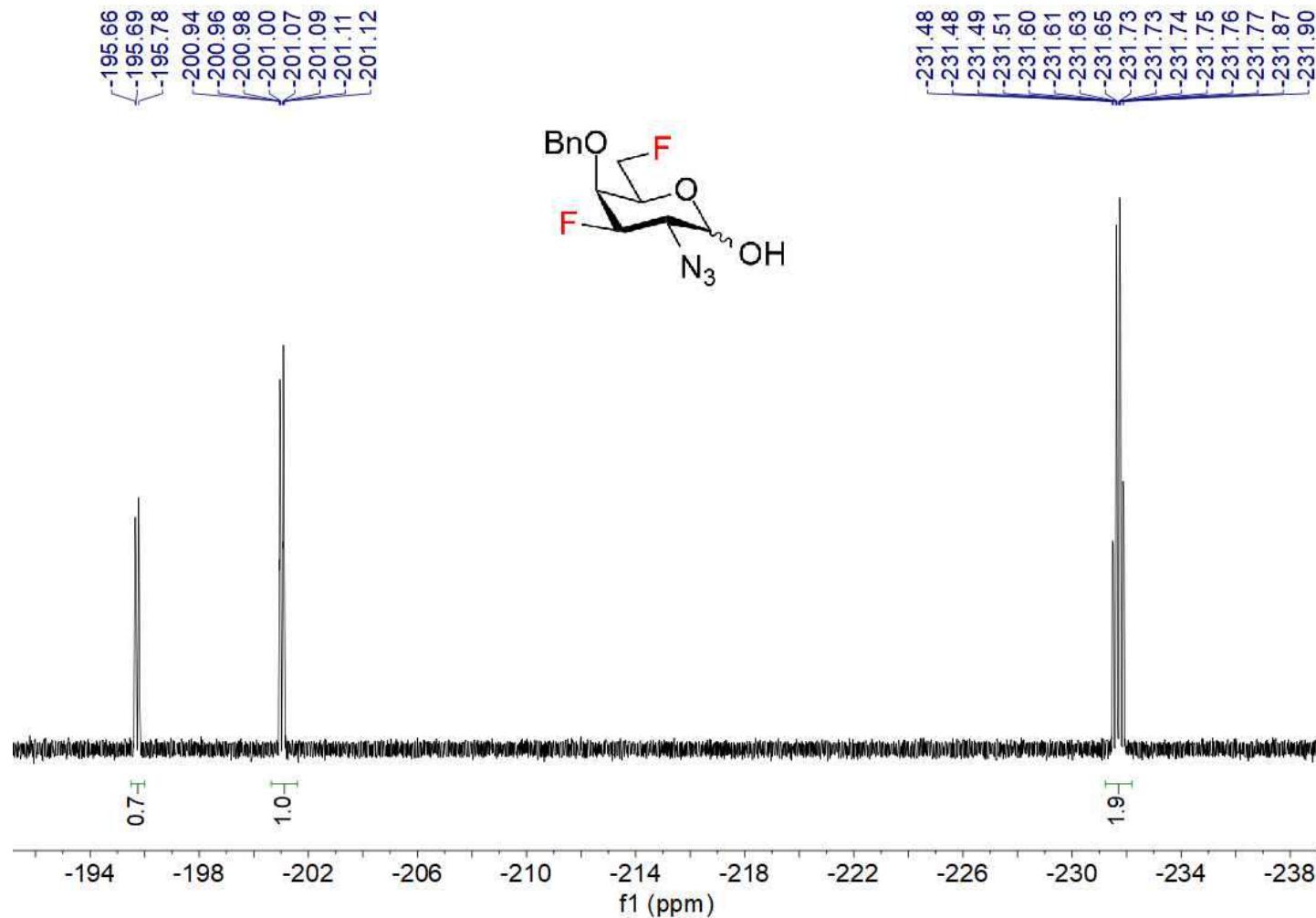
¹H NMR (400 MHz, CDCl₃) 24 (ca. 40% β -anomer)



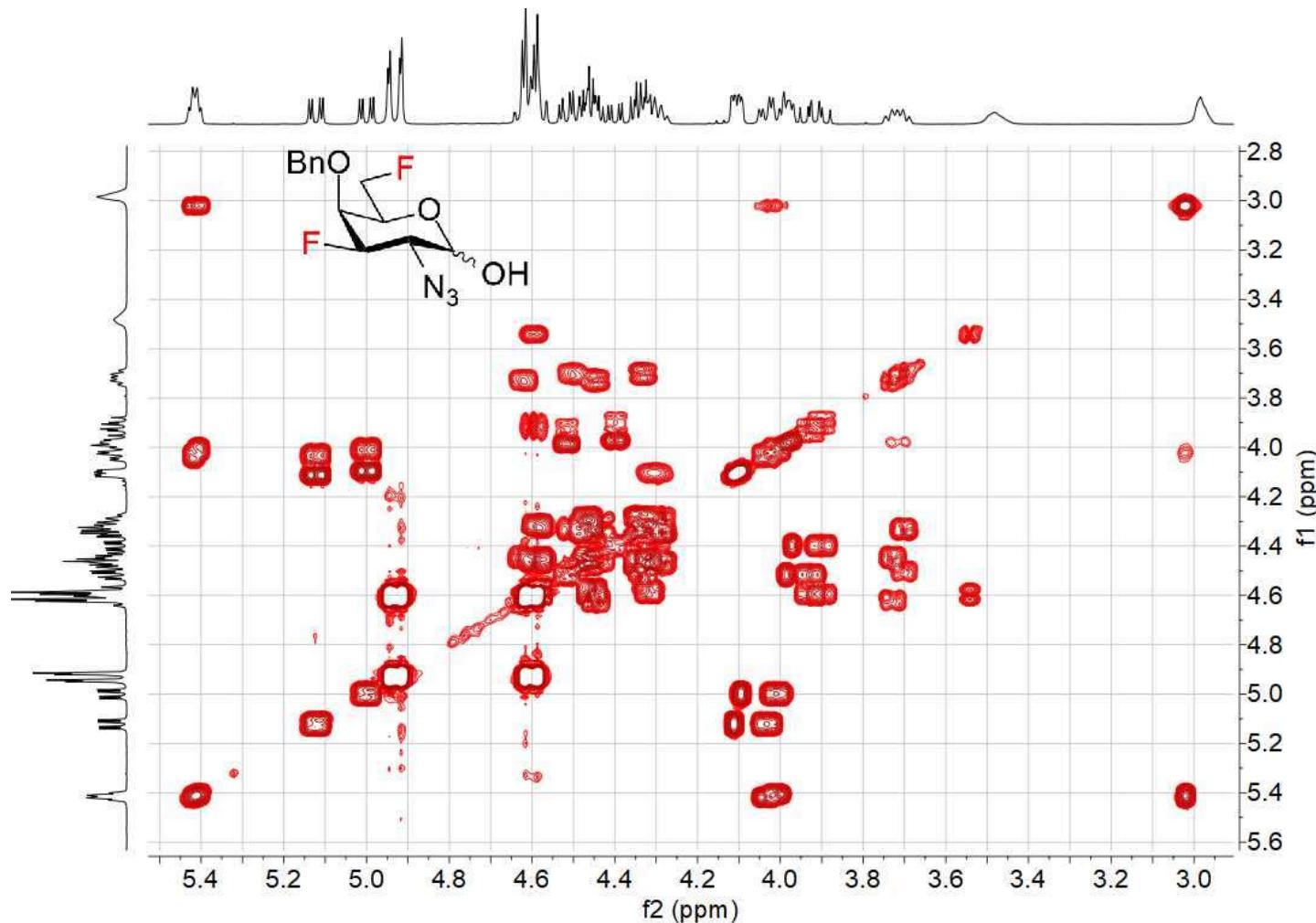
¹³C NMR (100 MHz, CDCl₃) 24



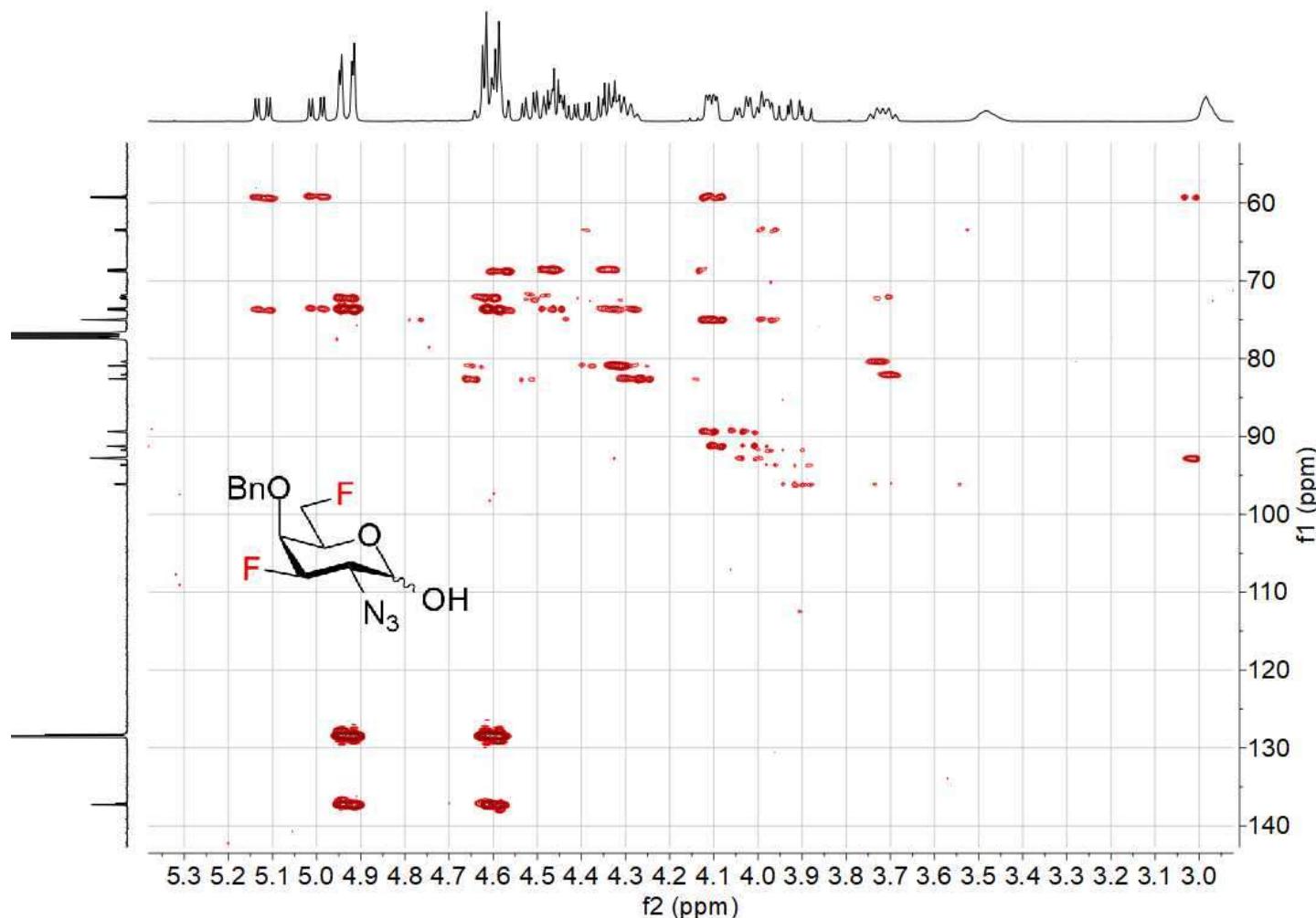
¹⁹F NMR (376 MHz, CDCl₃) 24 (ca. 40% β -anomer)



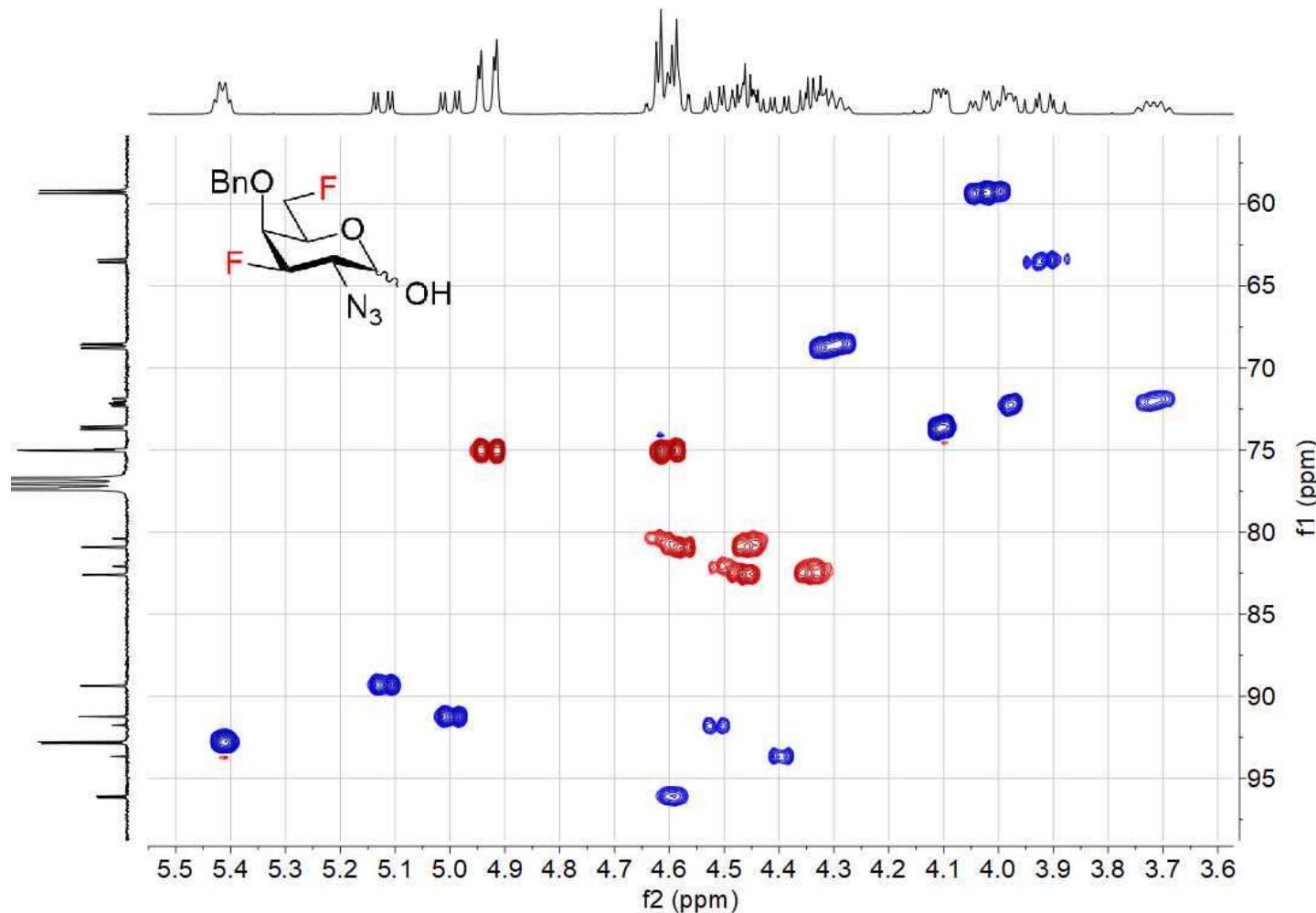
¹H-¹H COSY 24



^1H - ^{13}C HMBC 24

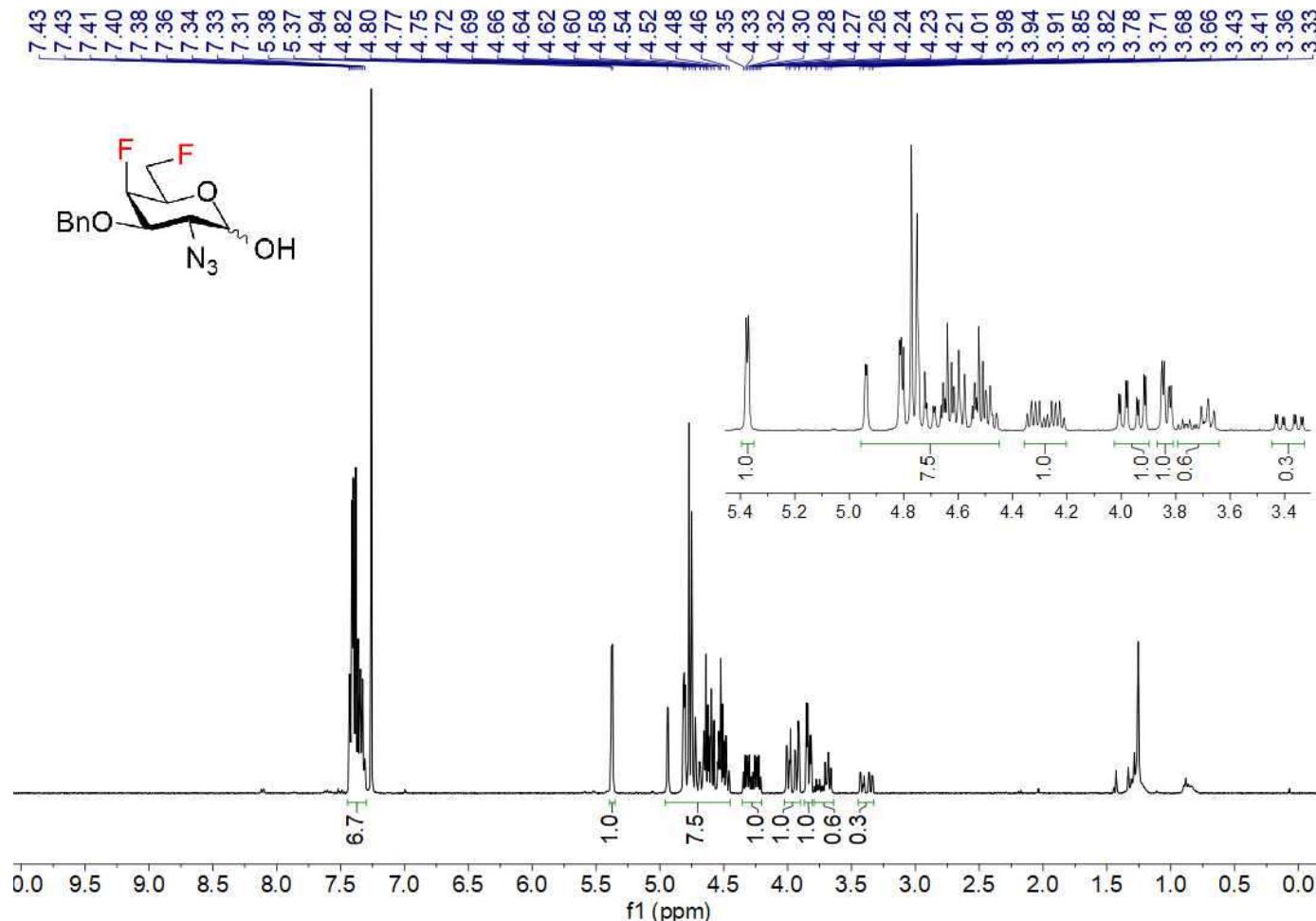


^1H - ^{13}C HSQC 24

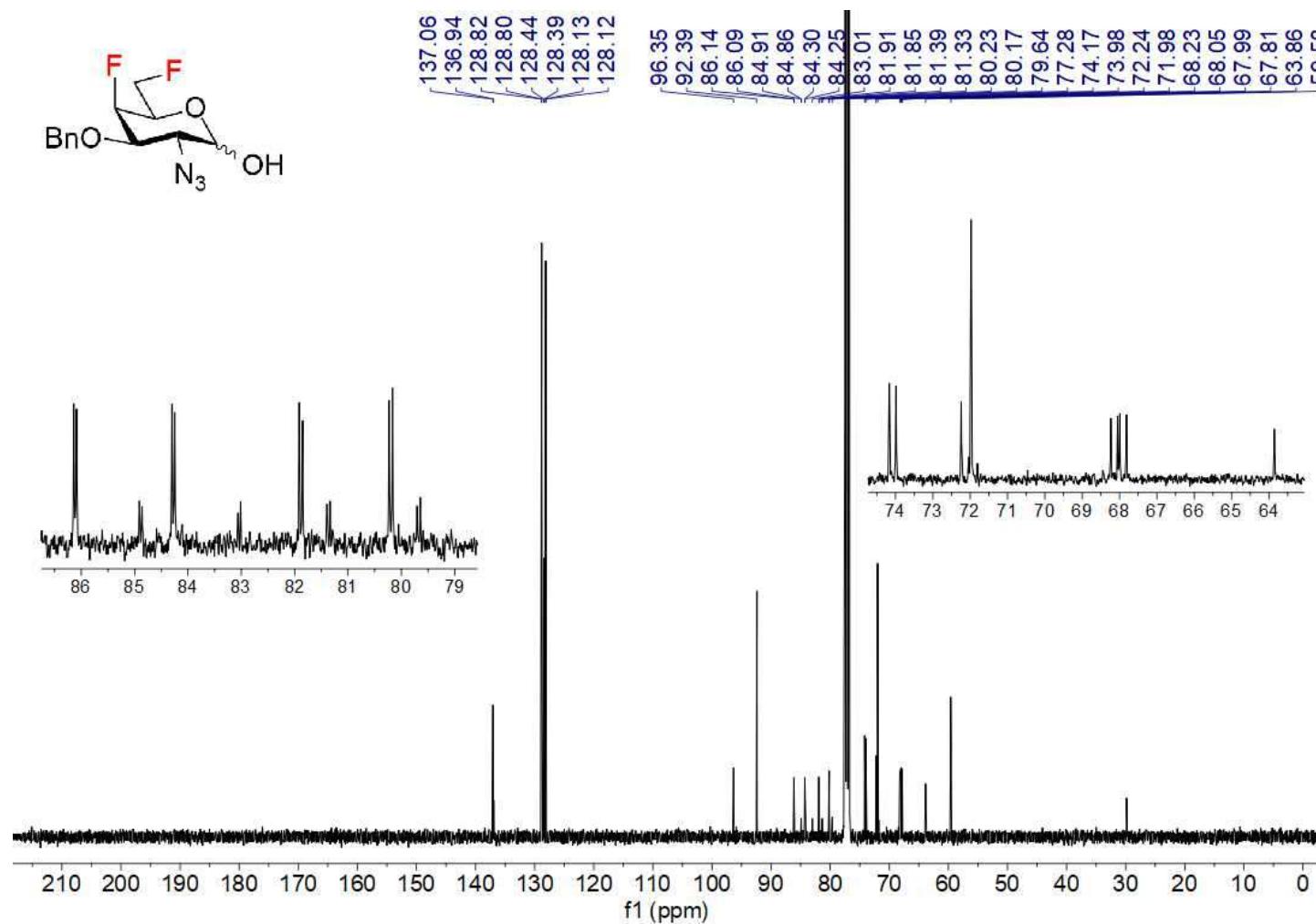


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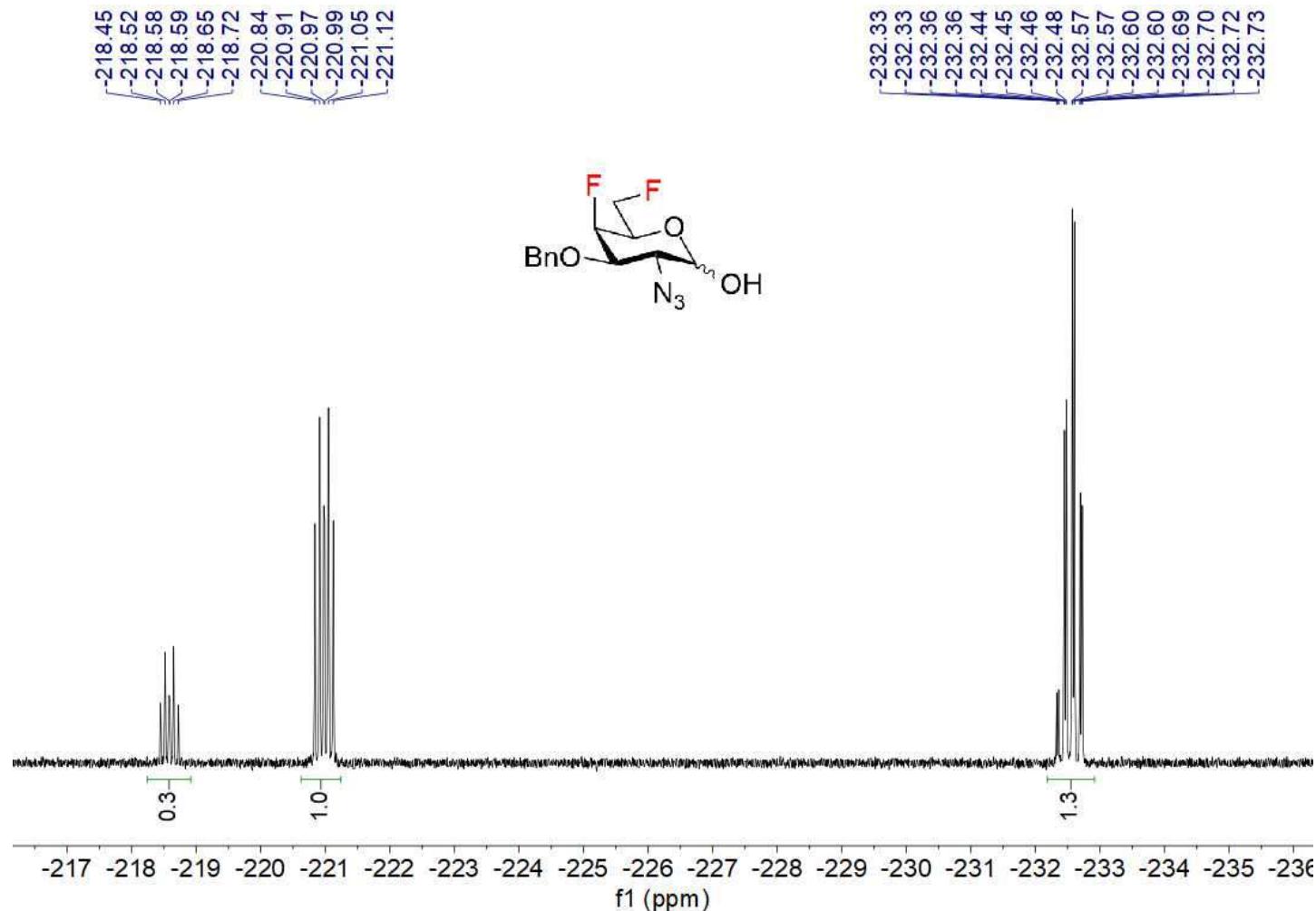
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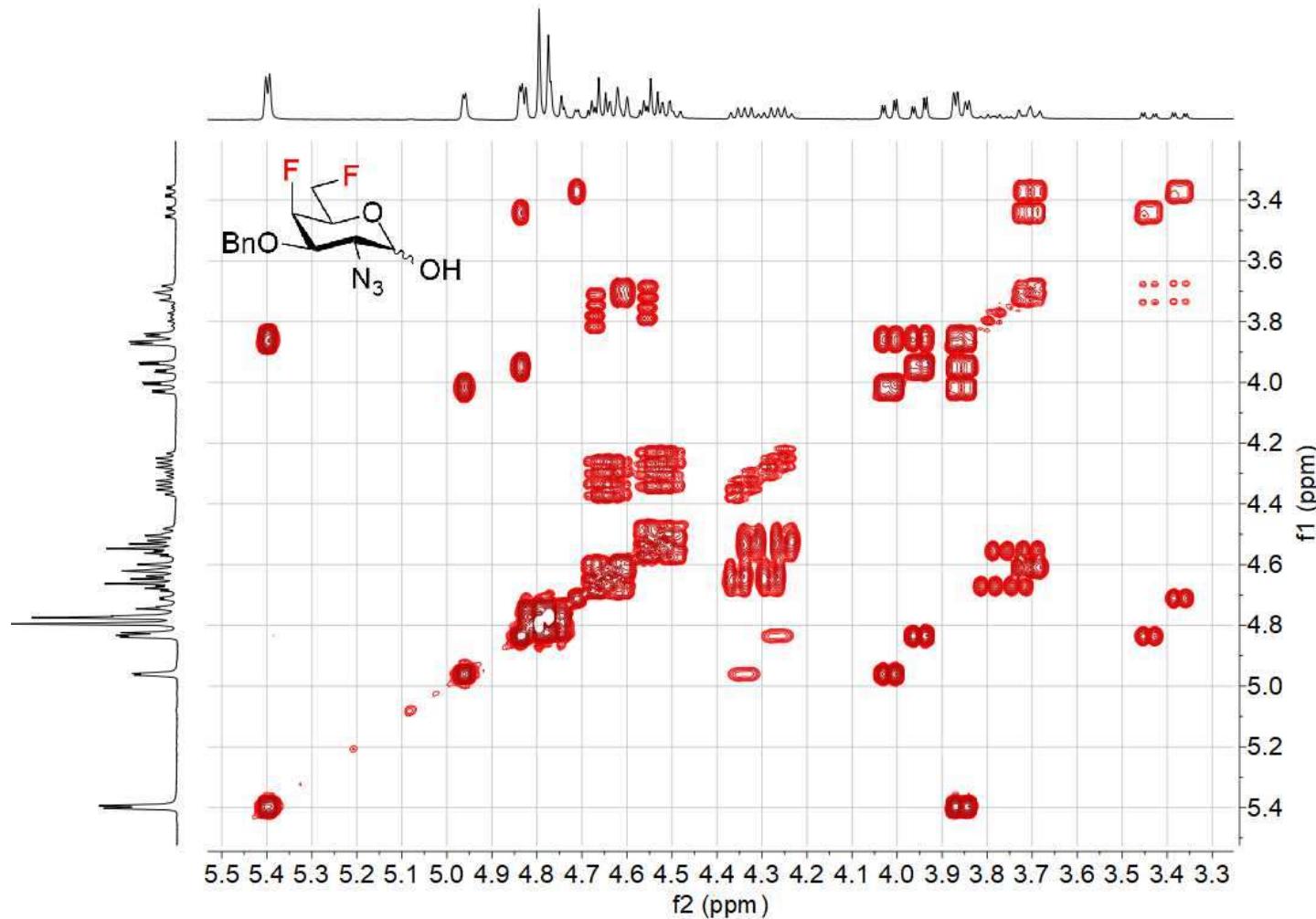
¹³C NMR (100 MHz, CDCl₃) 25



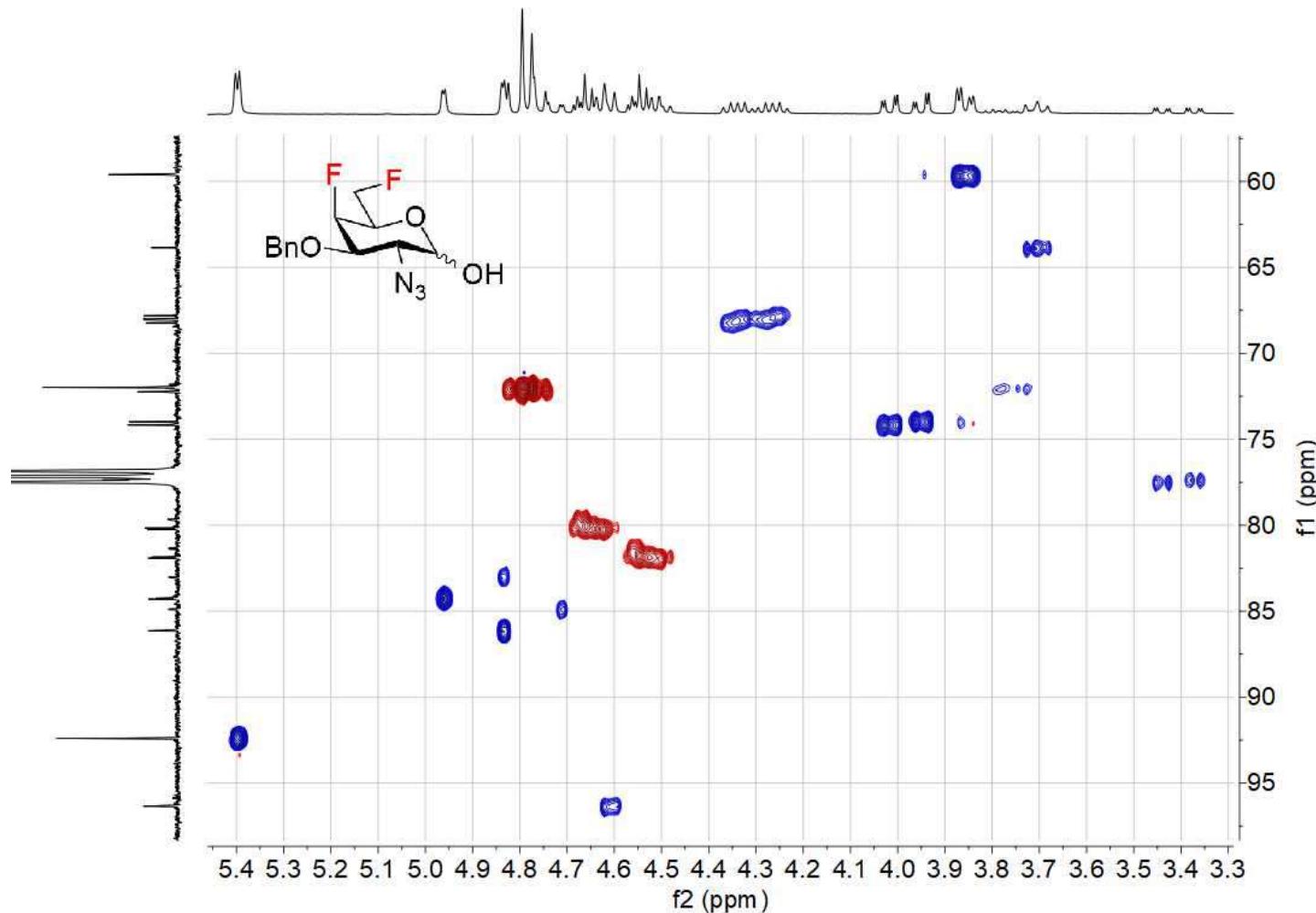
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¹H-¹H COSY 25

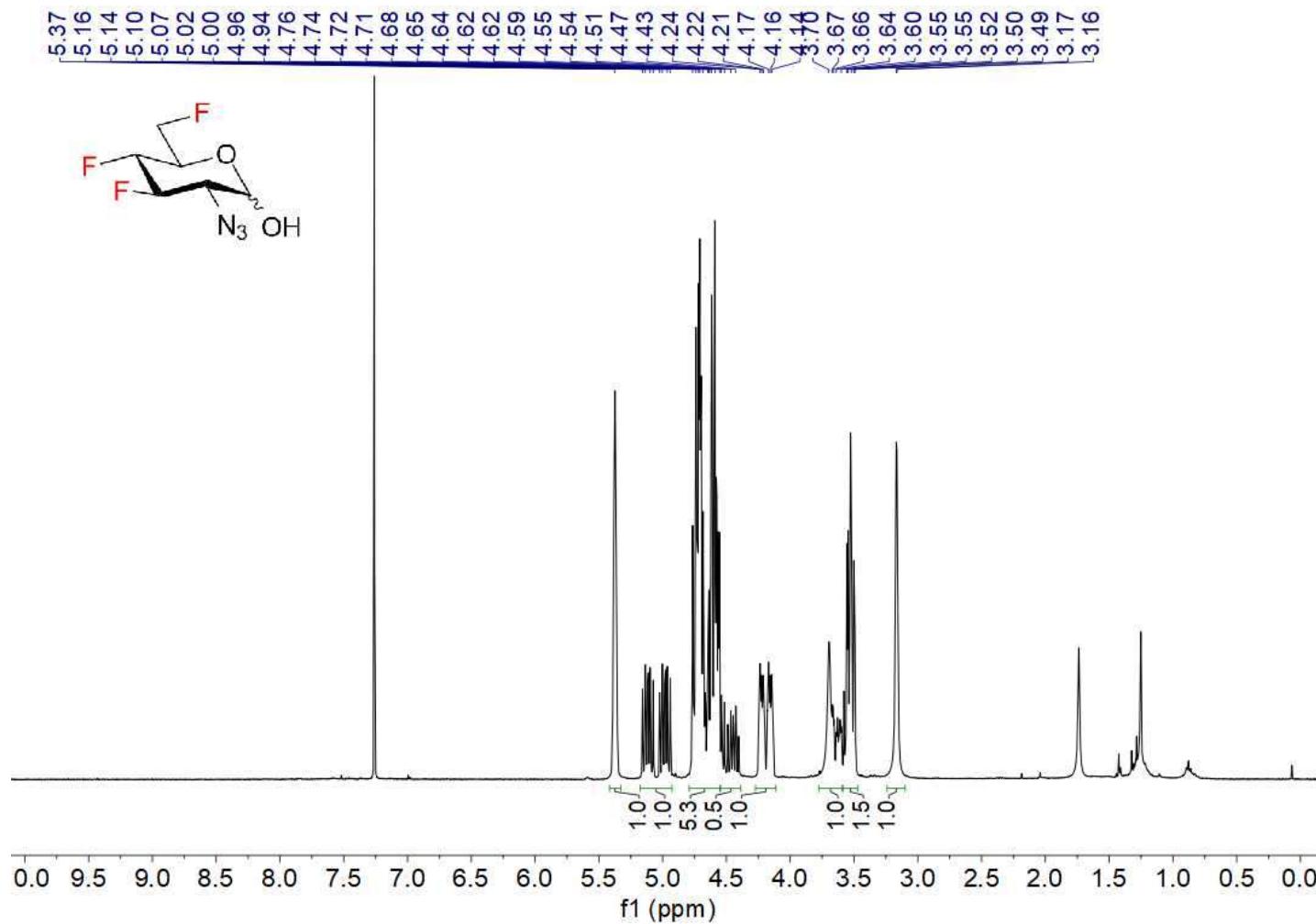


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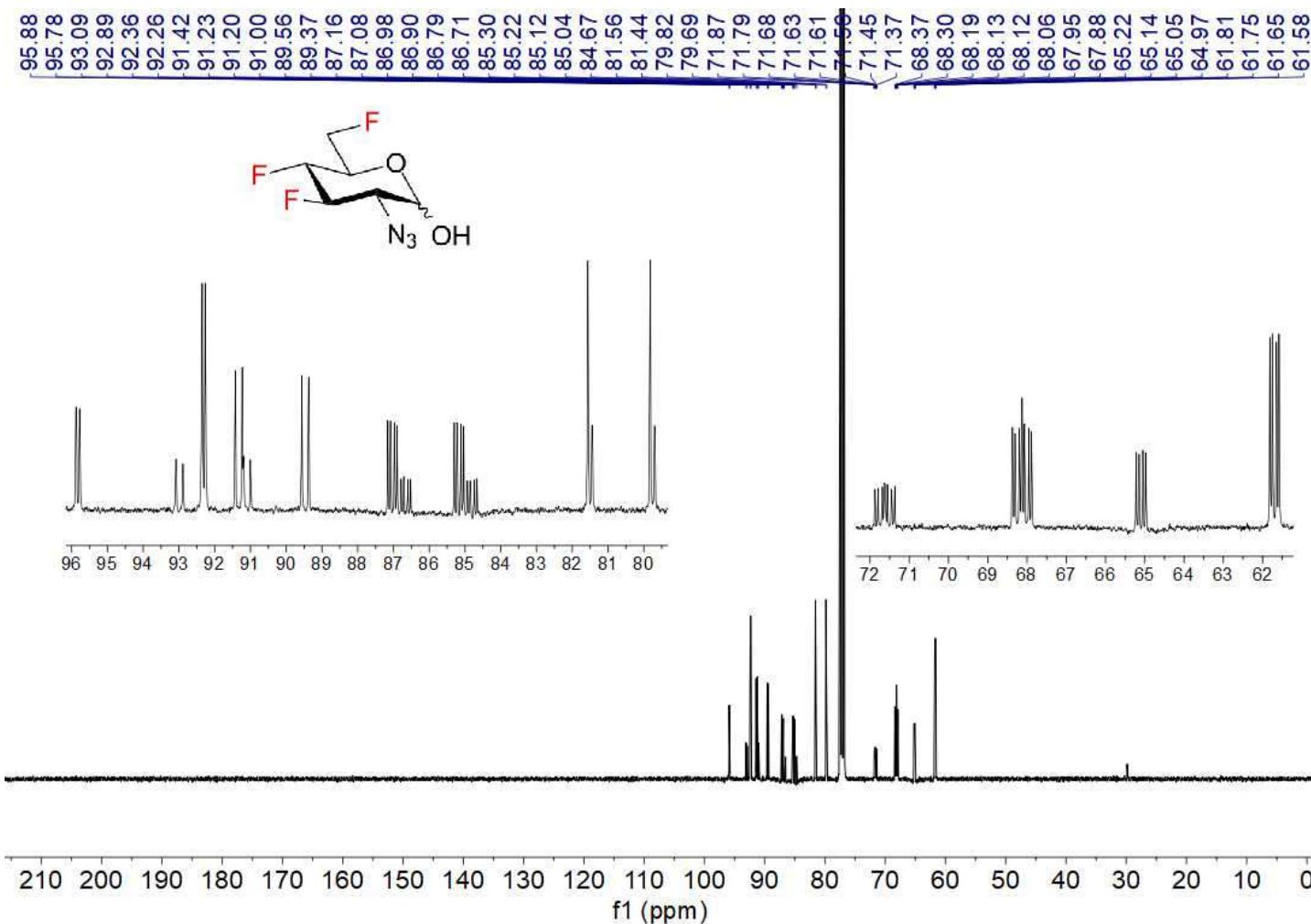


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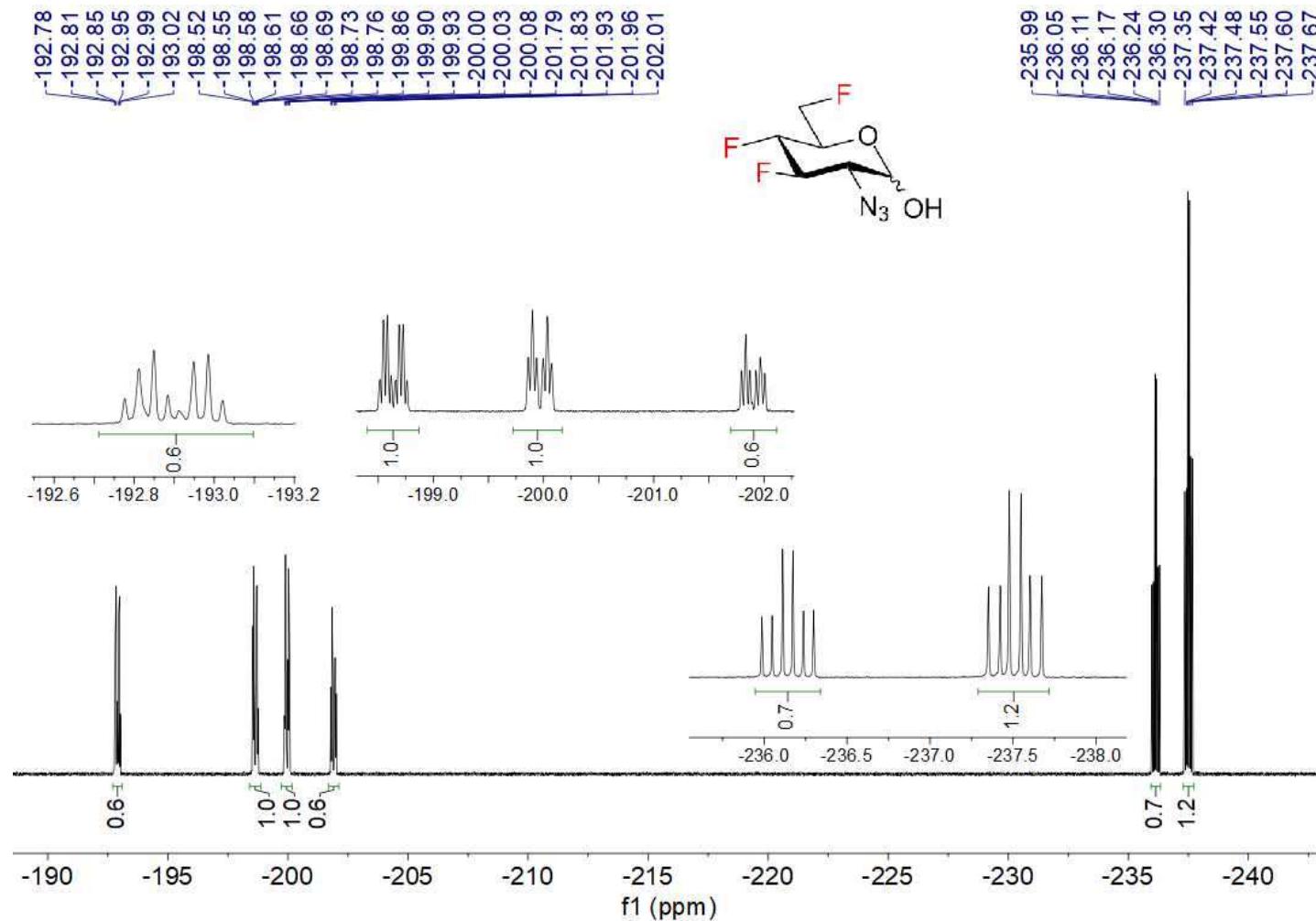
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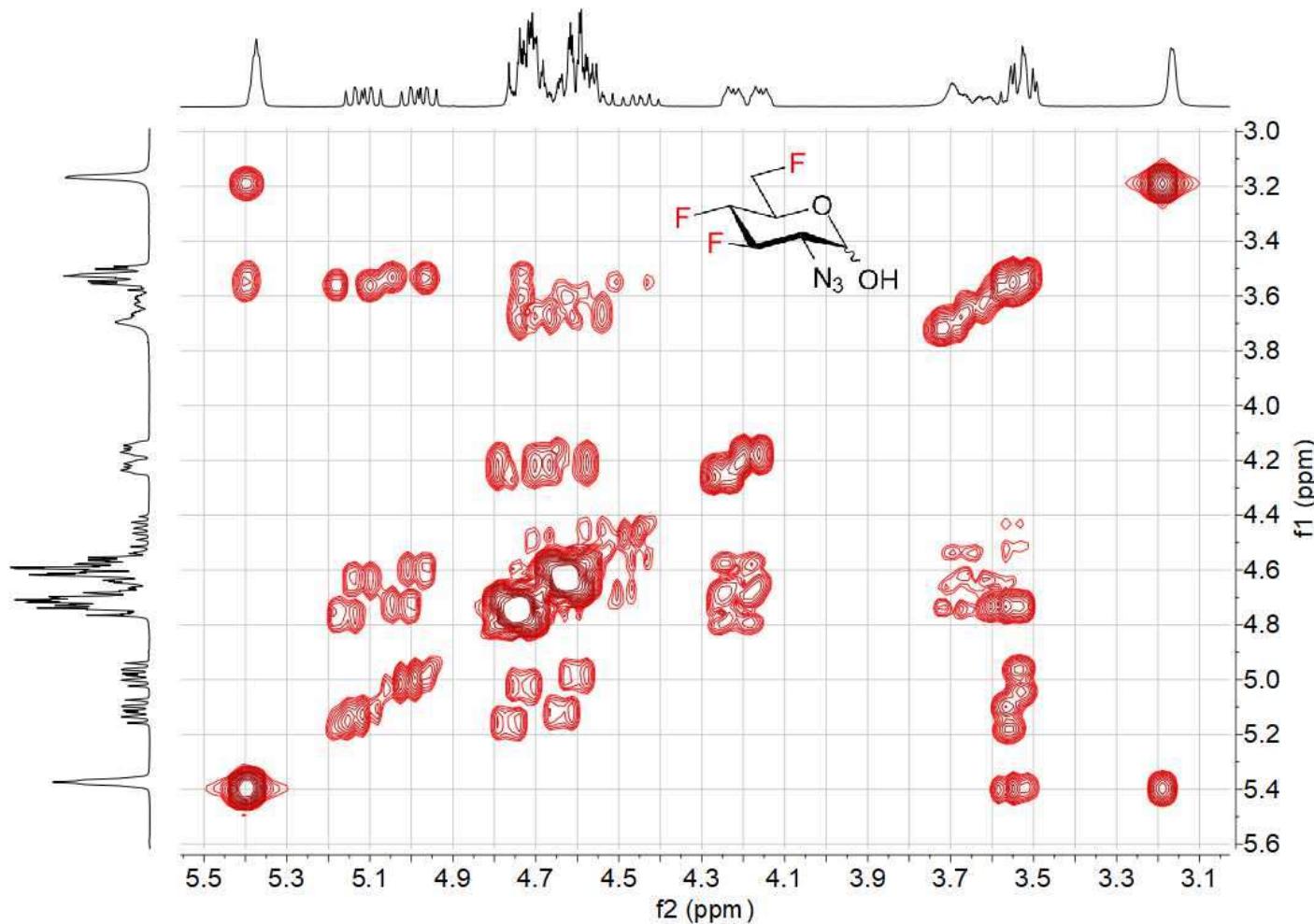
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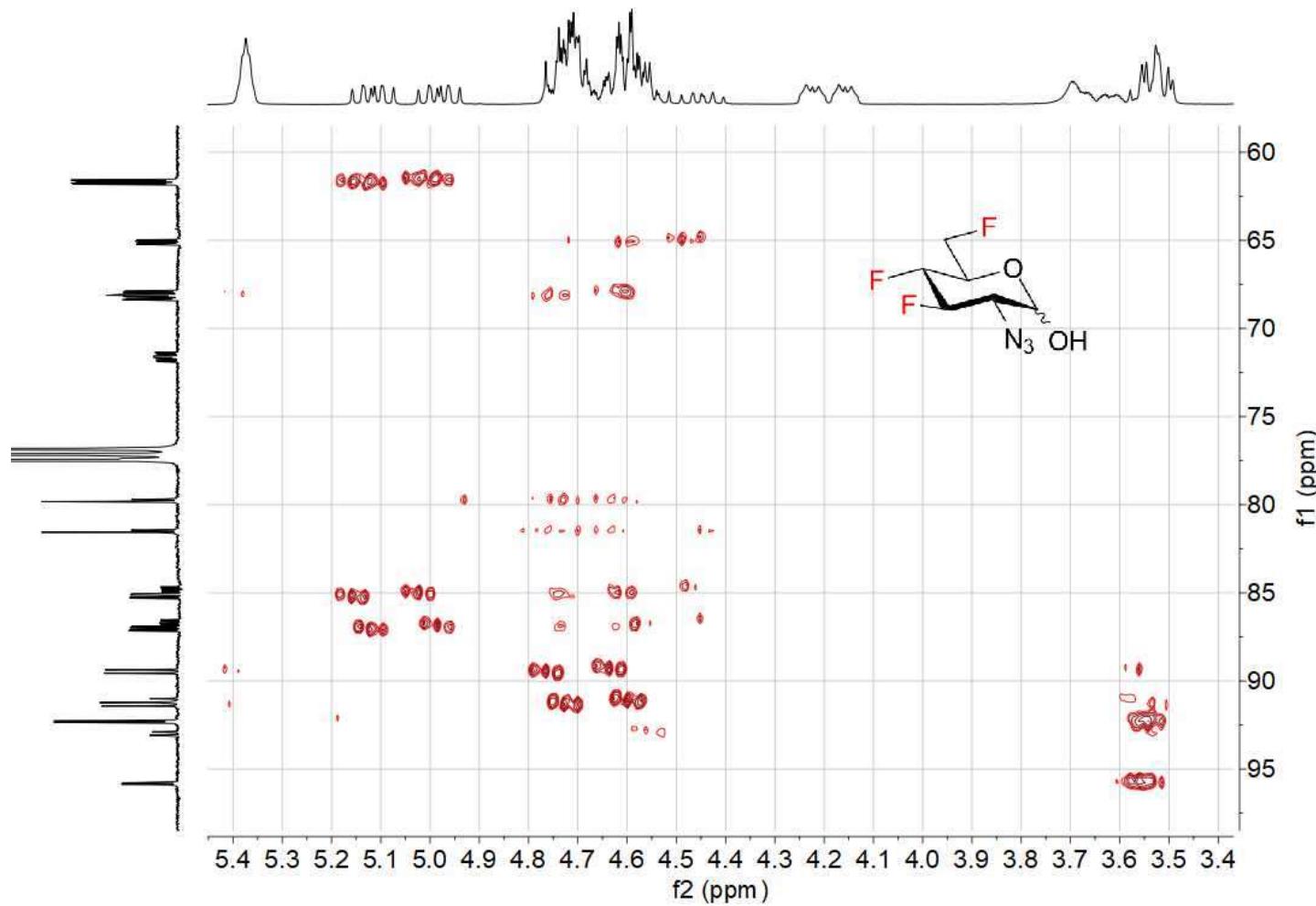
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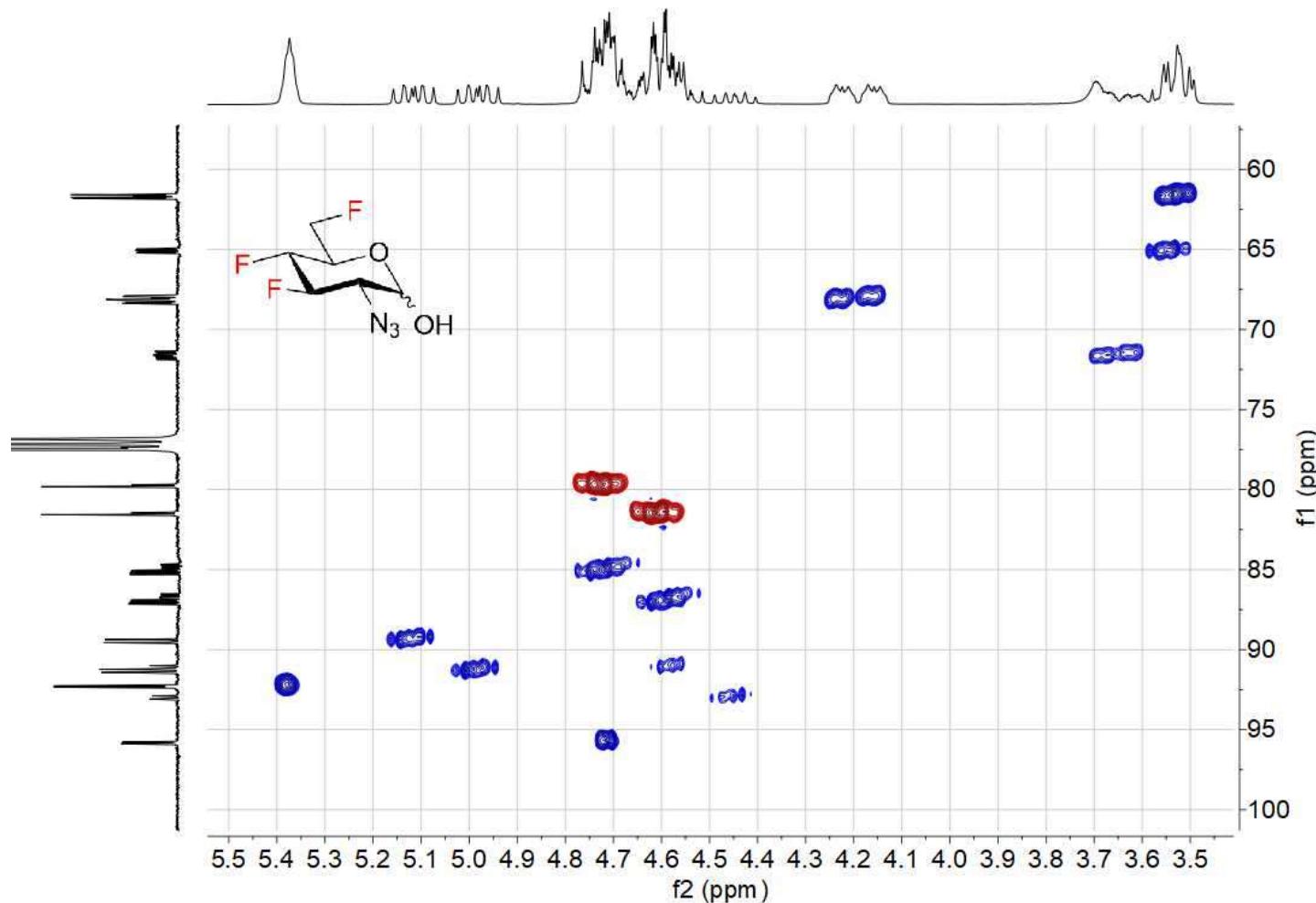
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^1H - ^{13}C HMBC 26

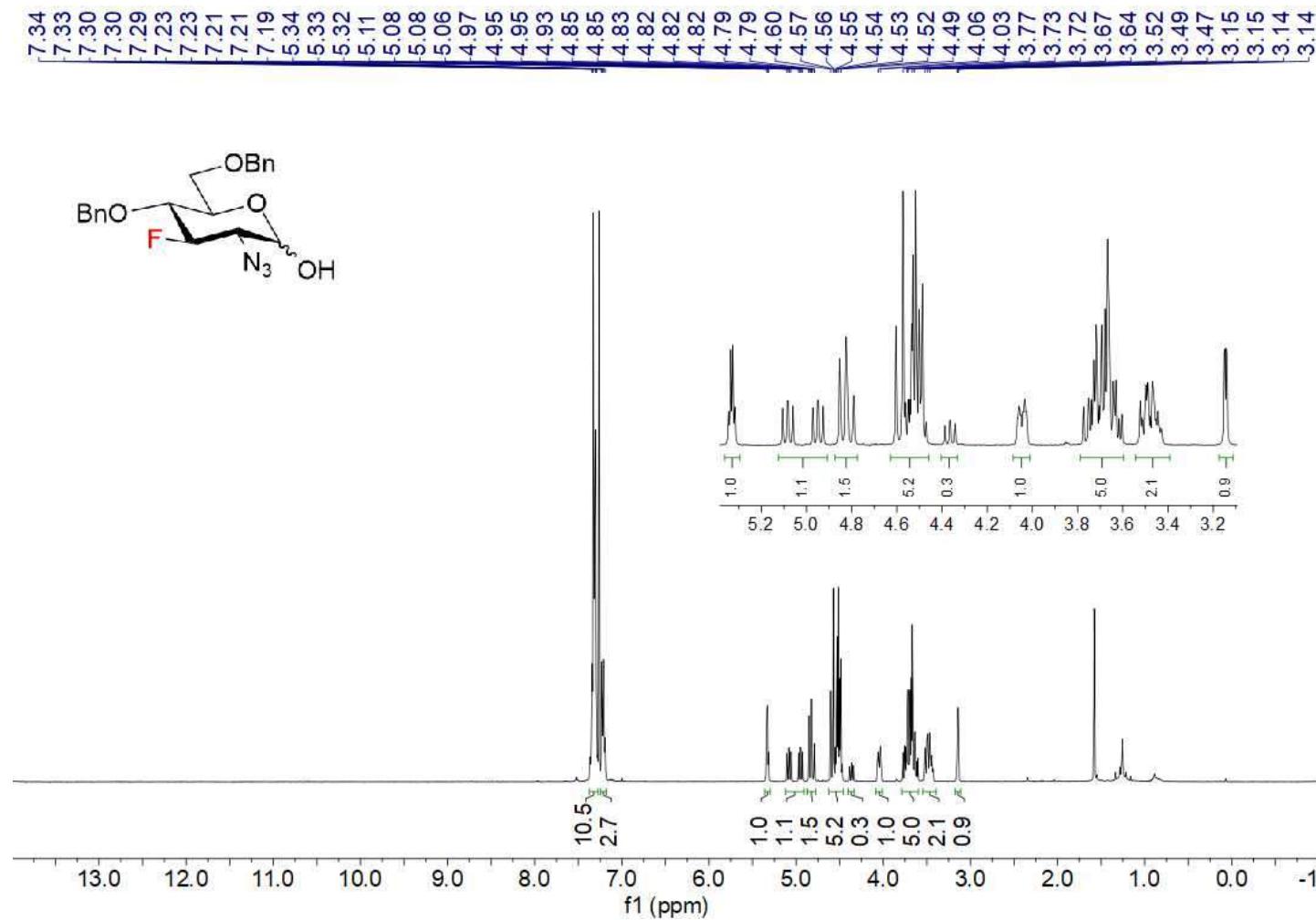


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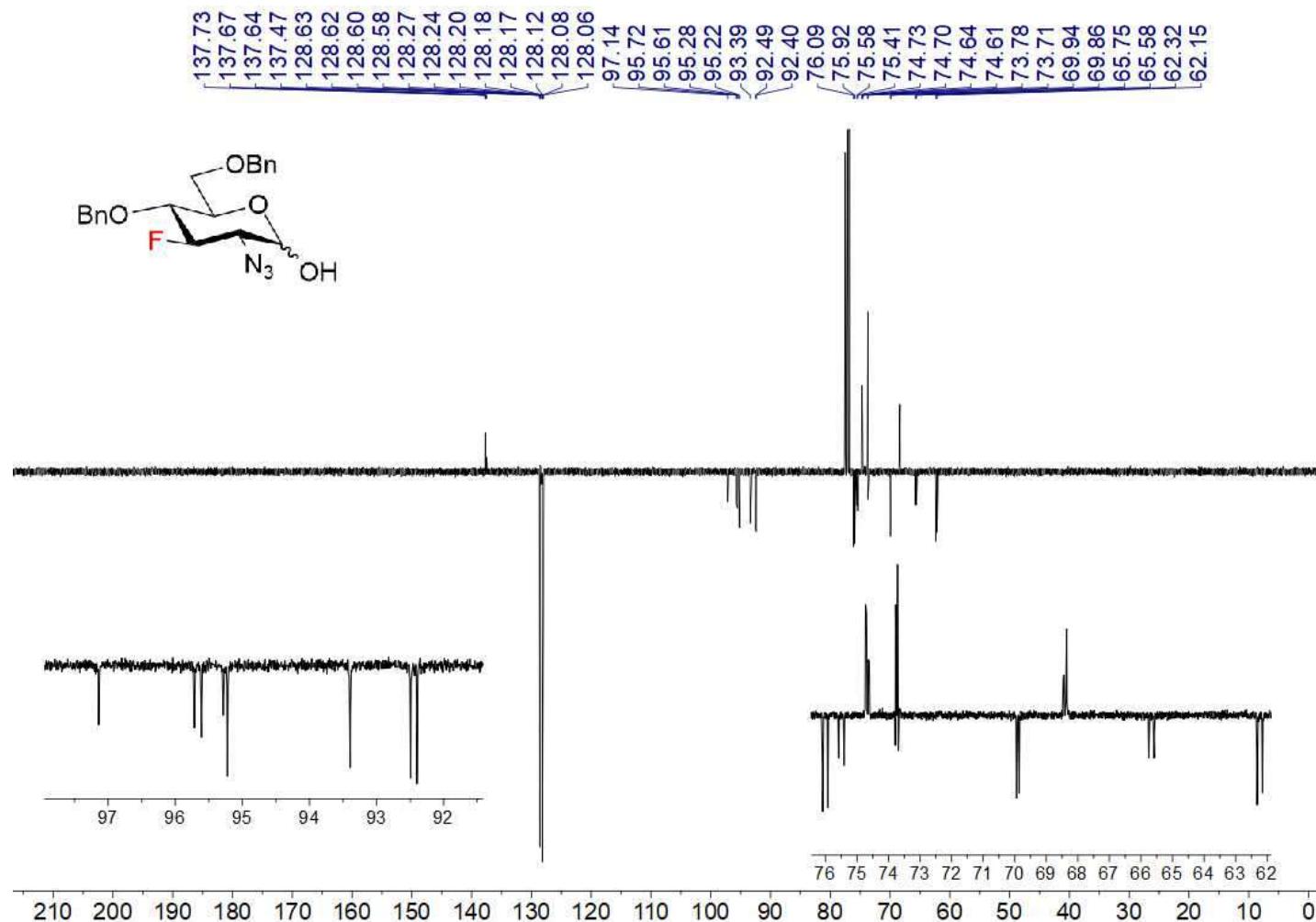


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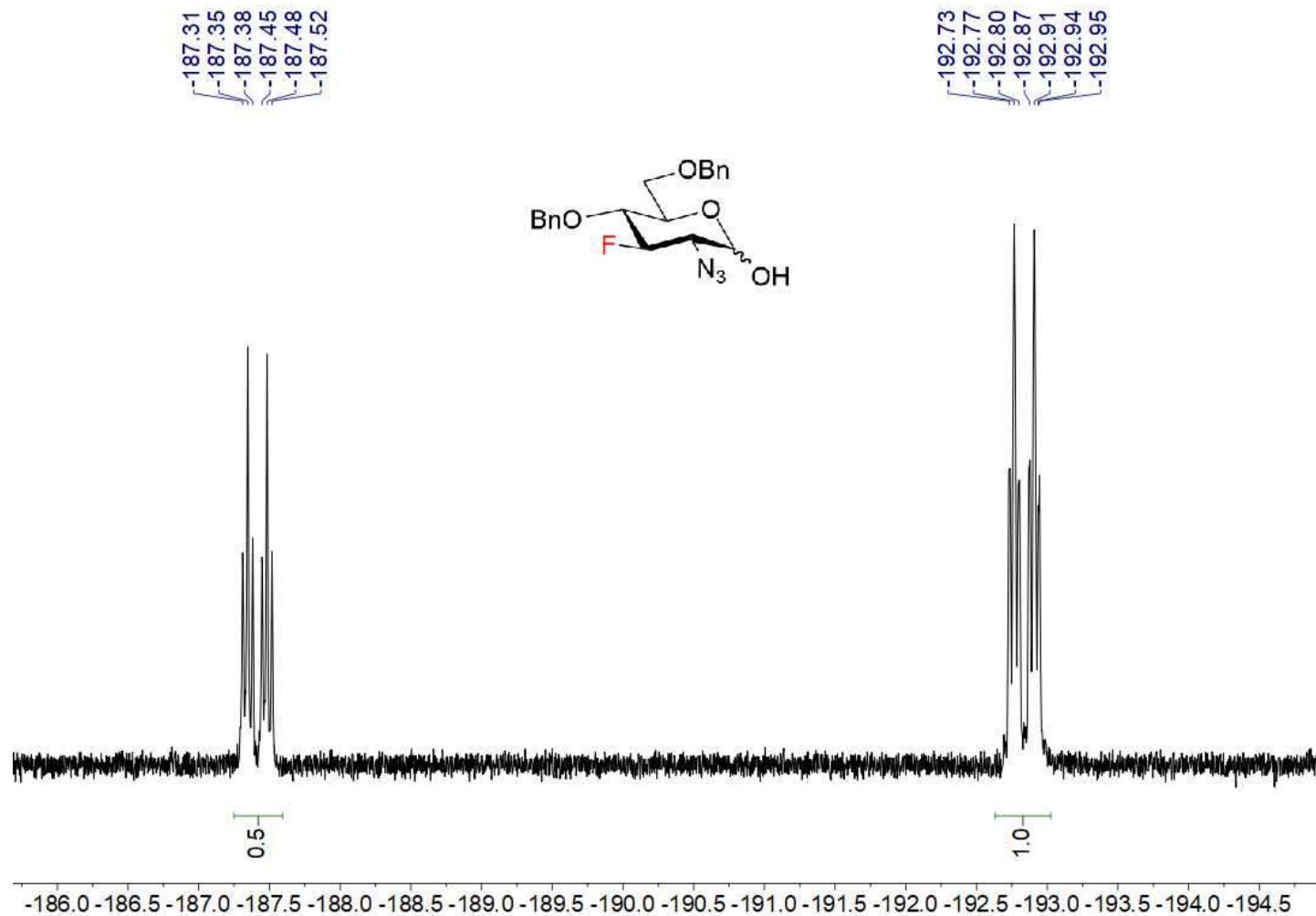
¹H NMR (400 MHz, CDCl₃) 27 (α/β ca. 2/1)



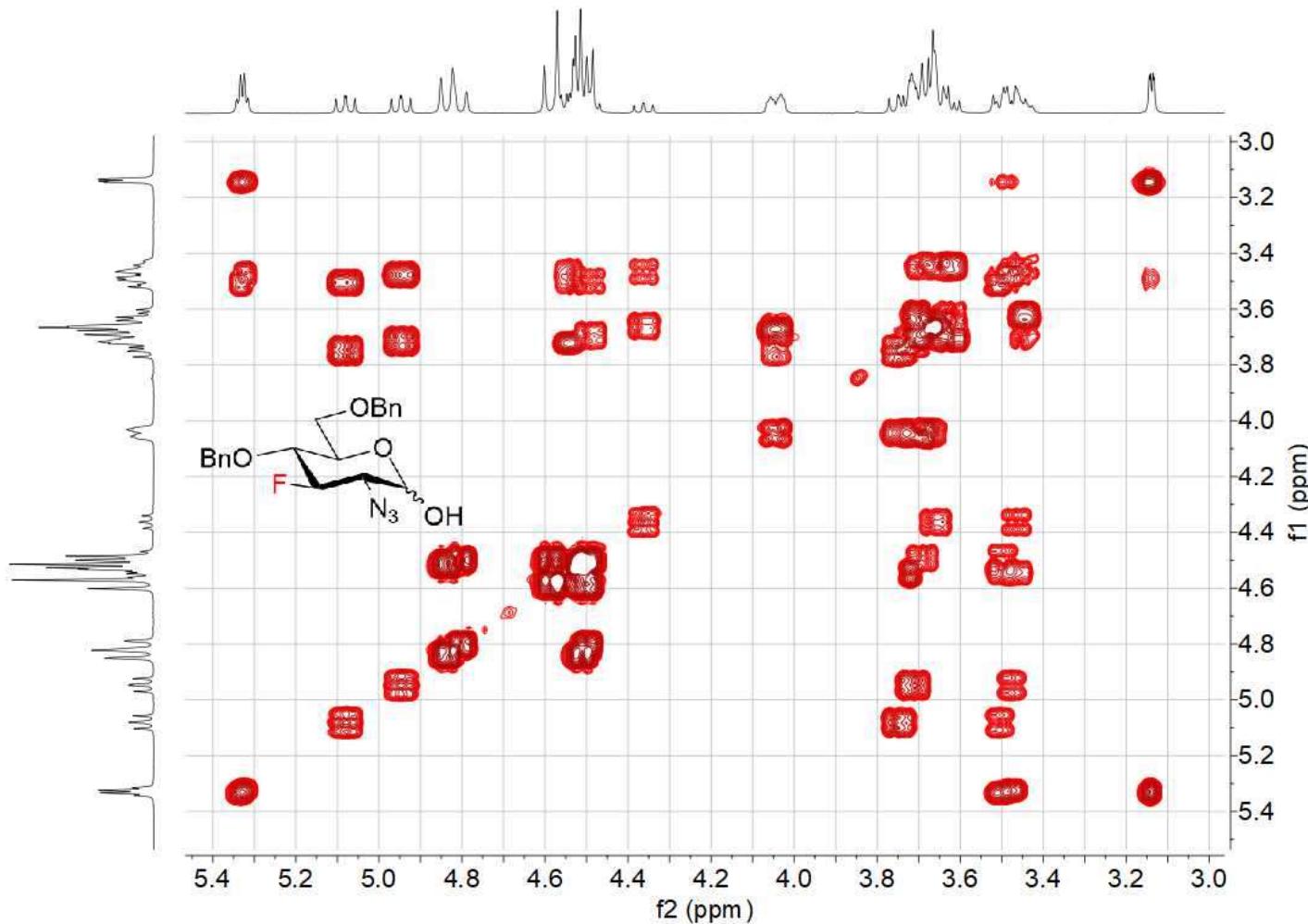
¹³C APT NMR (100 MHz, CDCl₃) 27



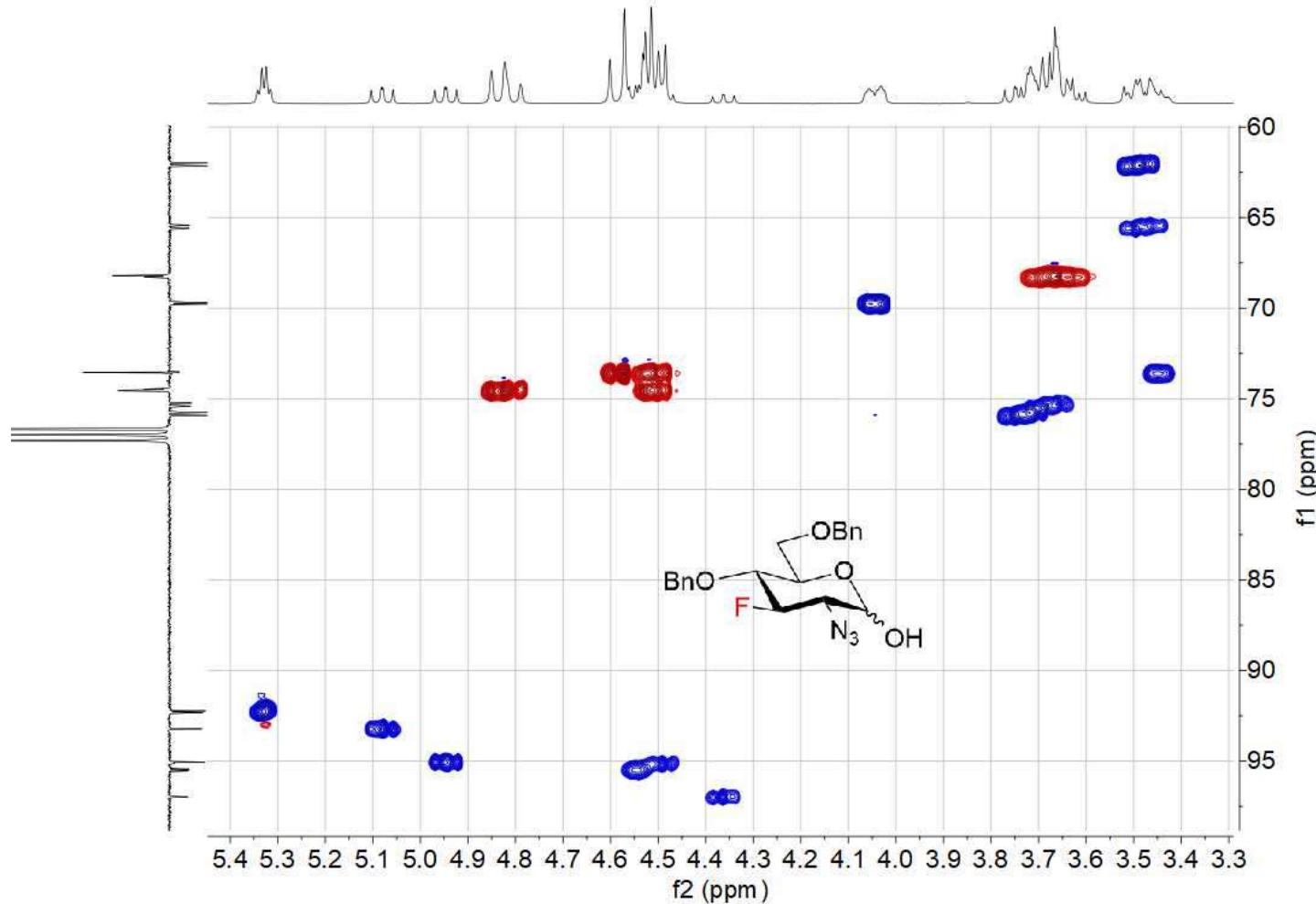
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¹H-¹H COSY 27

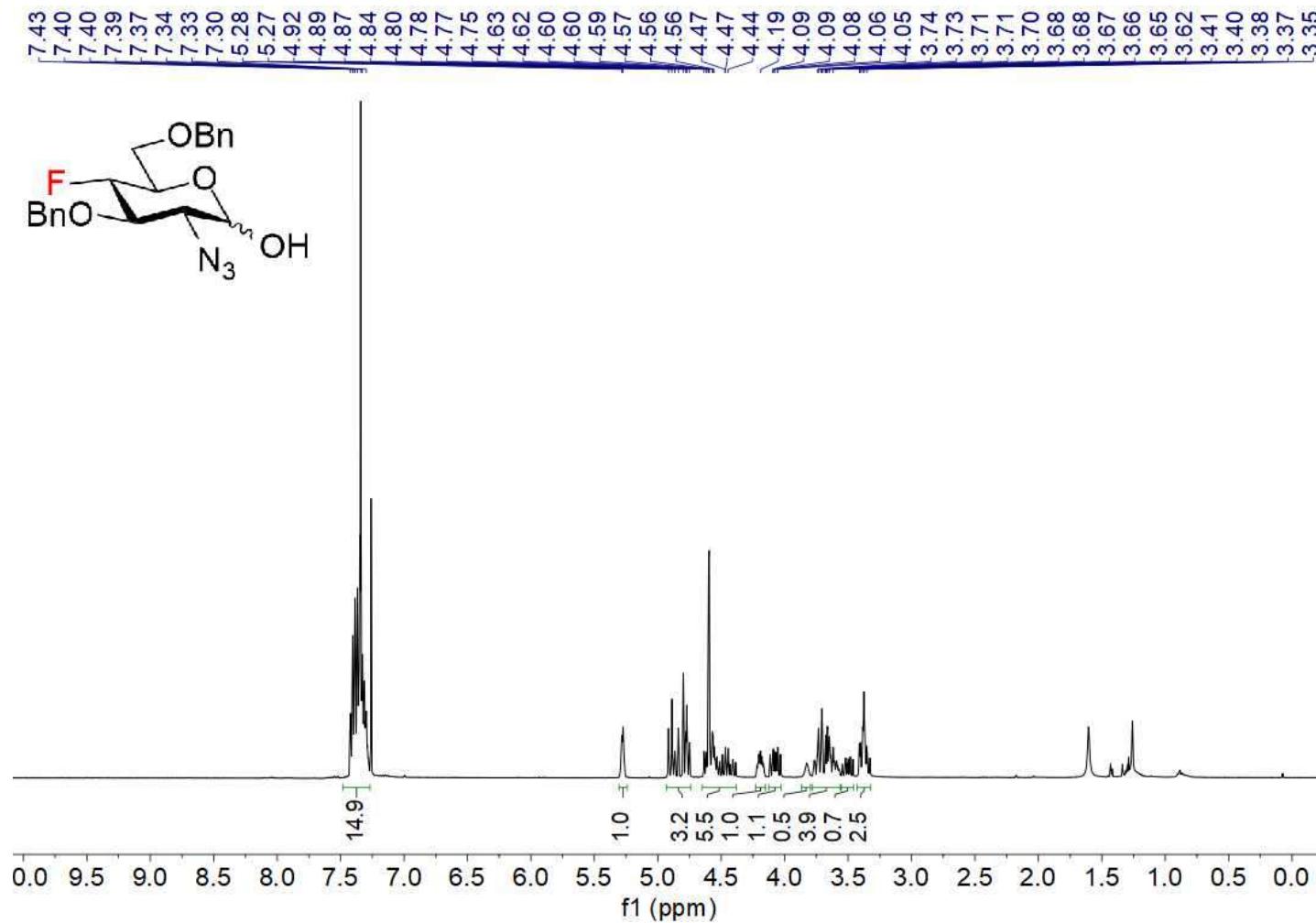


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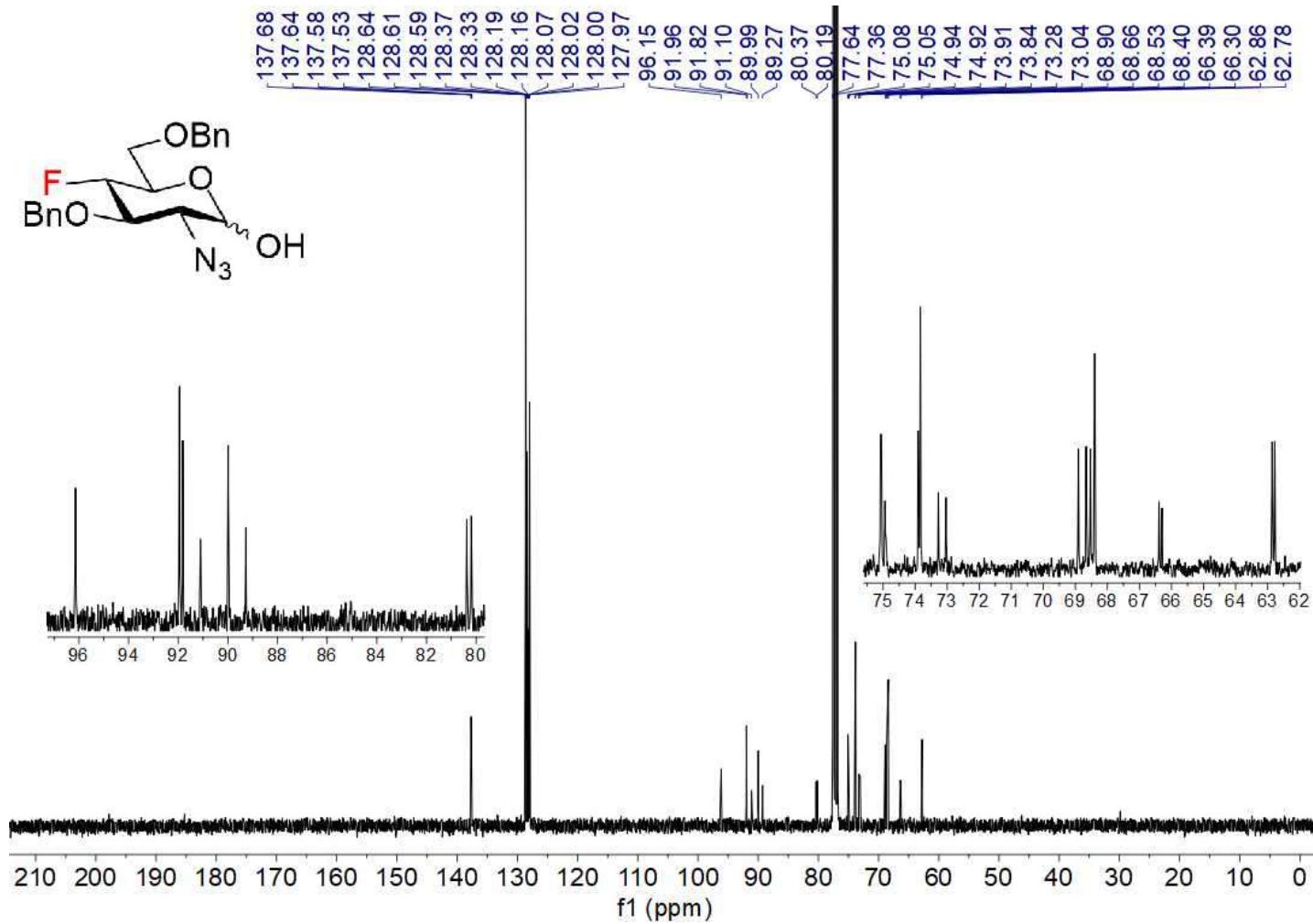


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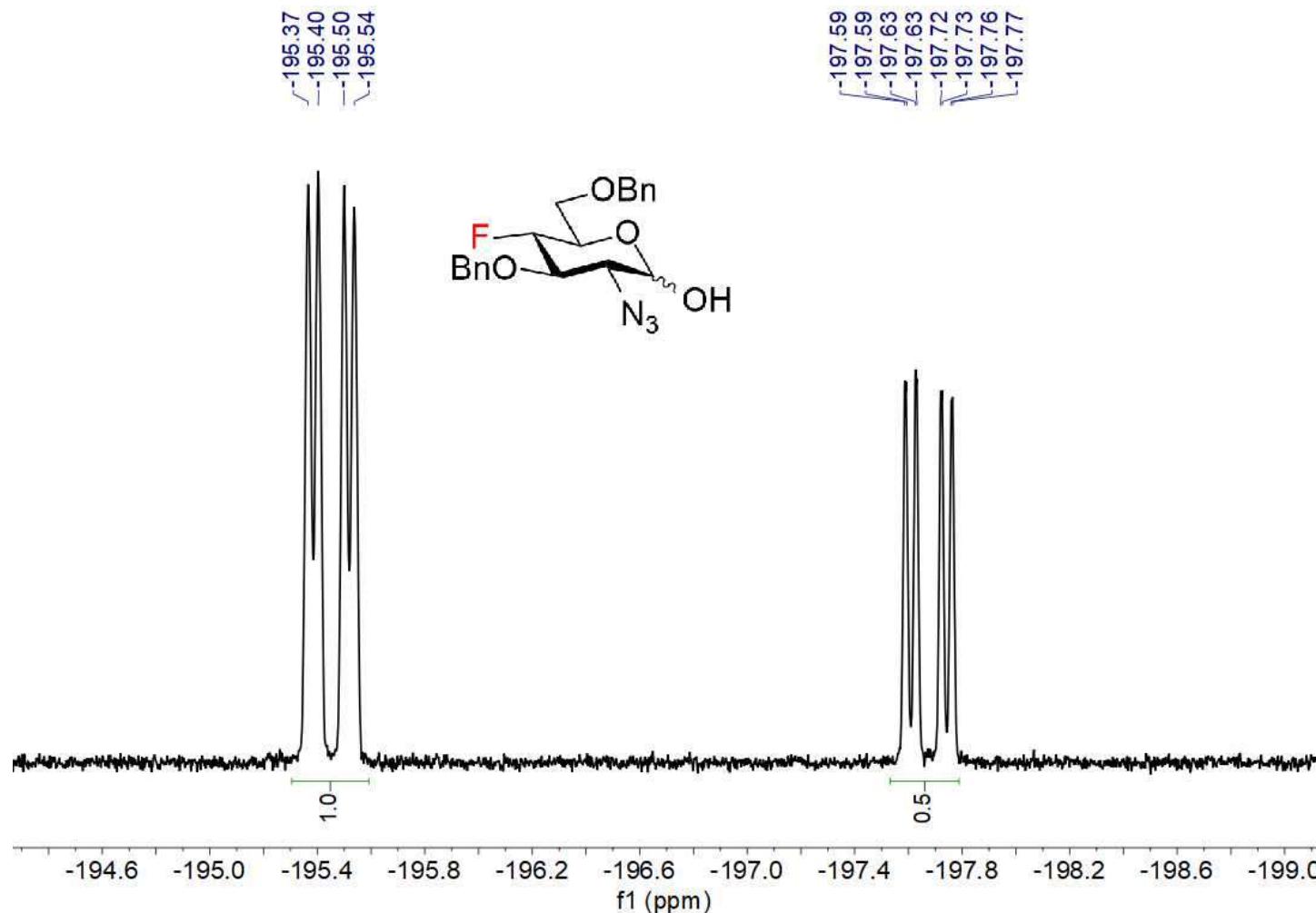
¹H NMR (400 MHz, CDCl₃) 28 (α/β ca. 2/1)



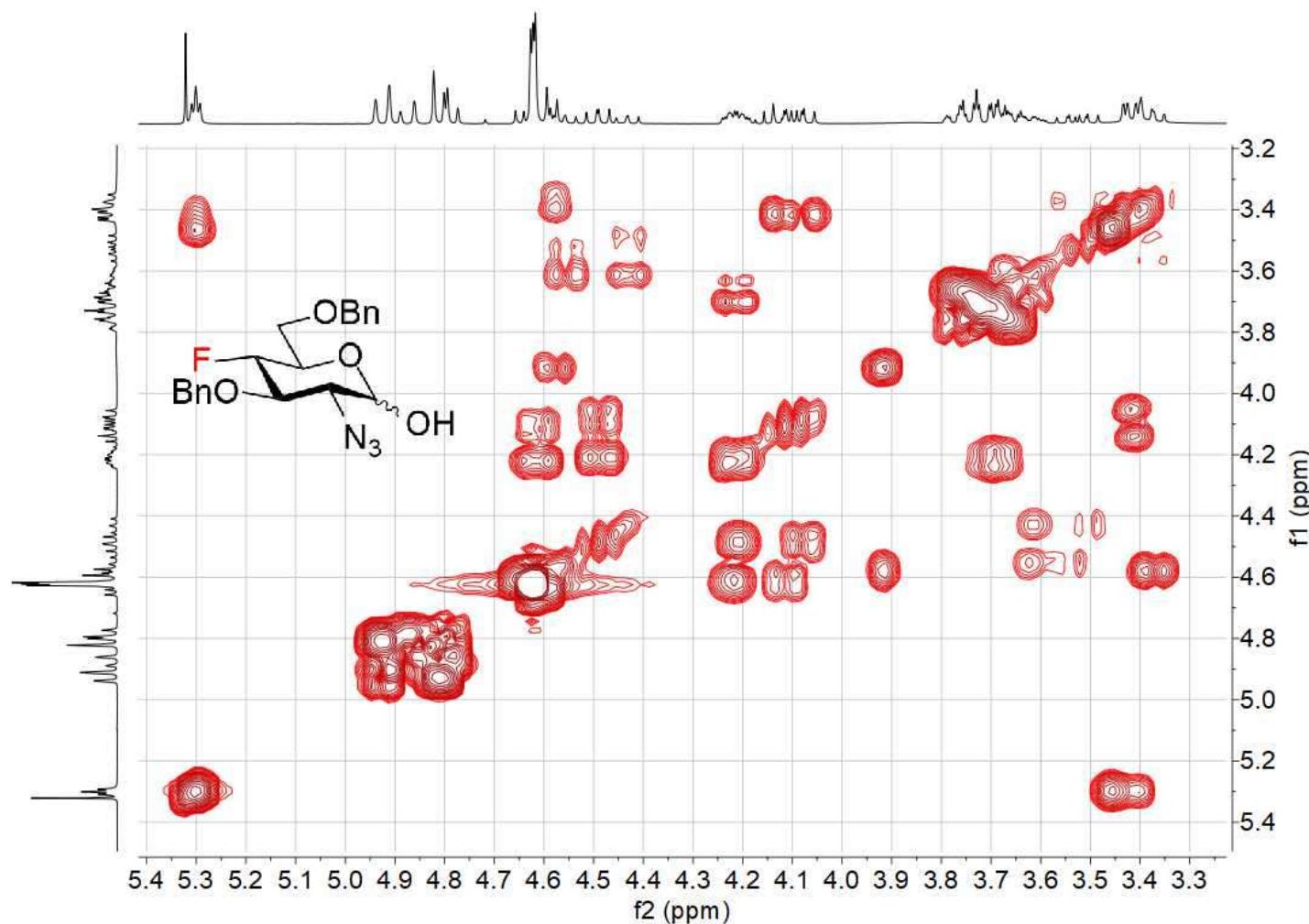
¹³C NMR (100 MHz, CDCl₃) 28



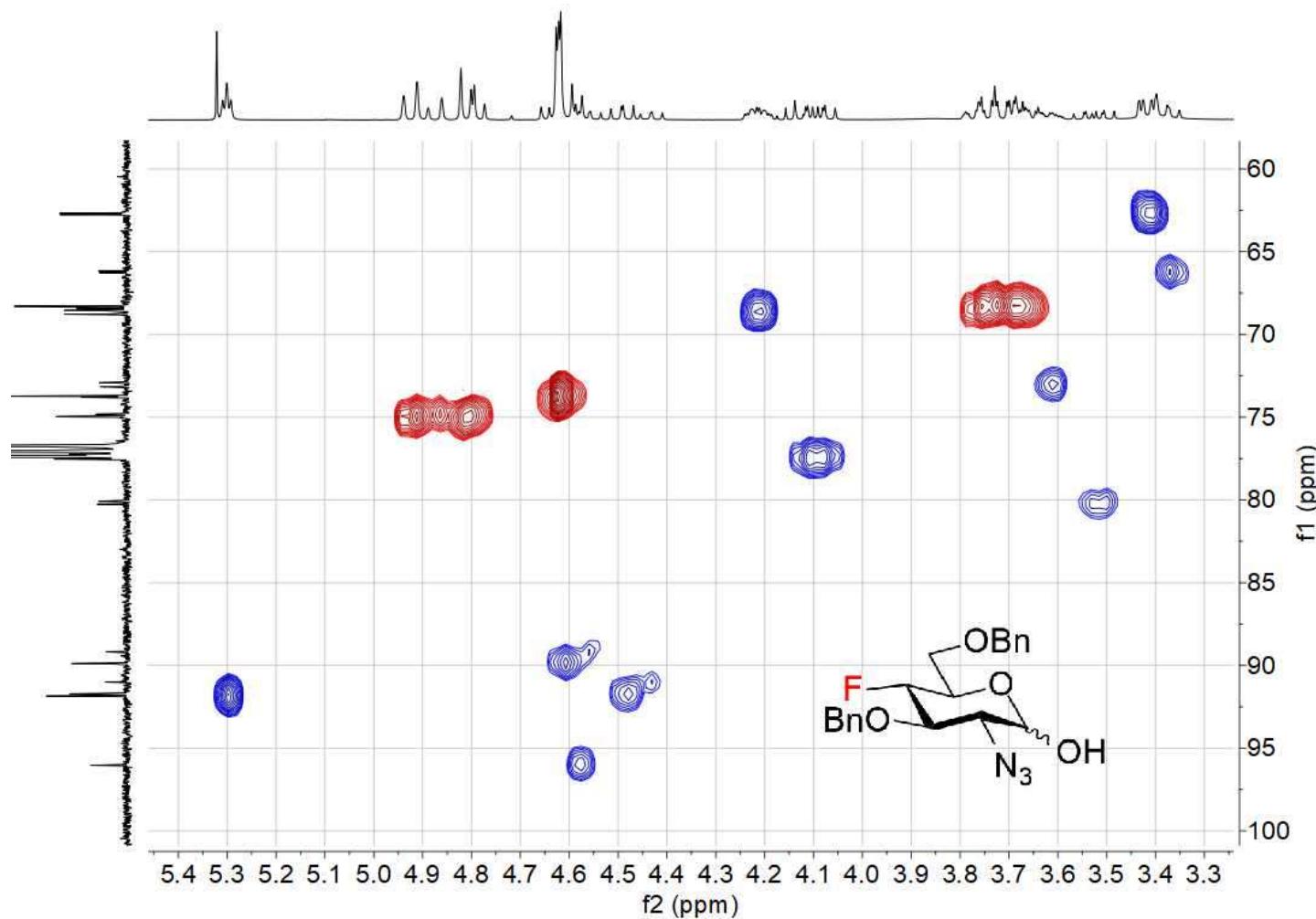
¹⁹F NMR (376 MHz, CDCl₃) 28 (α/β ca. 2/1)



¹H-¹H COSY 28

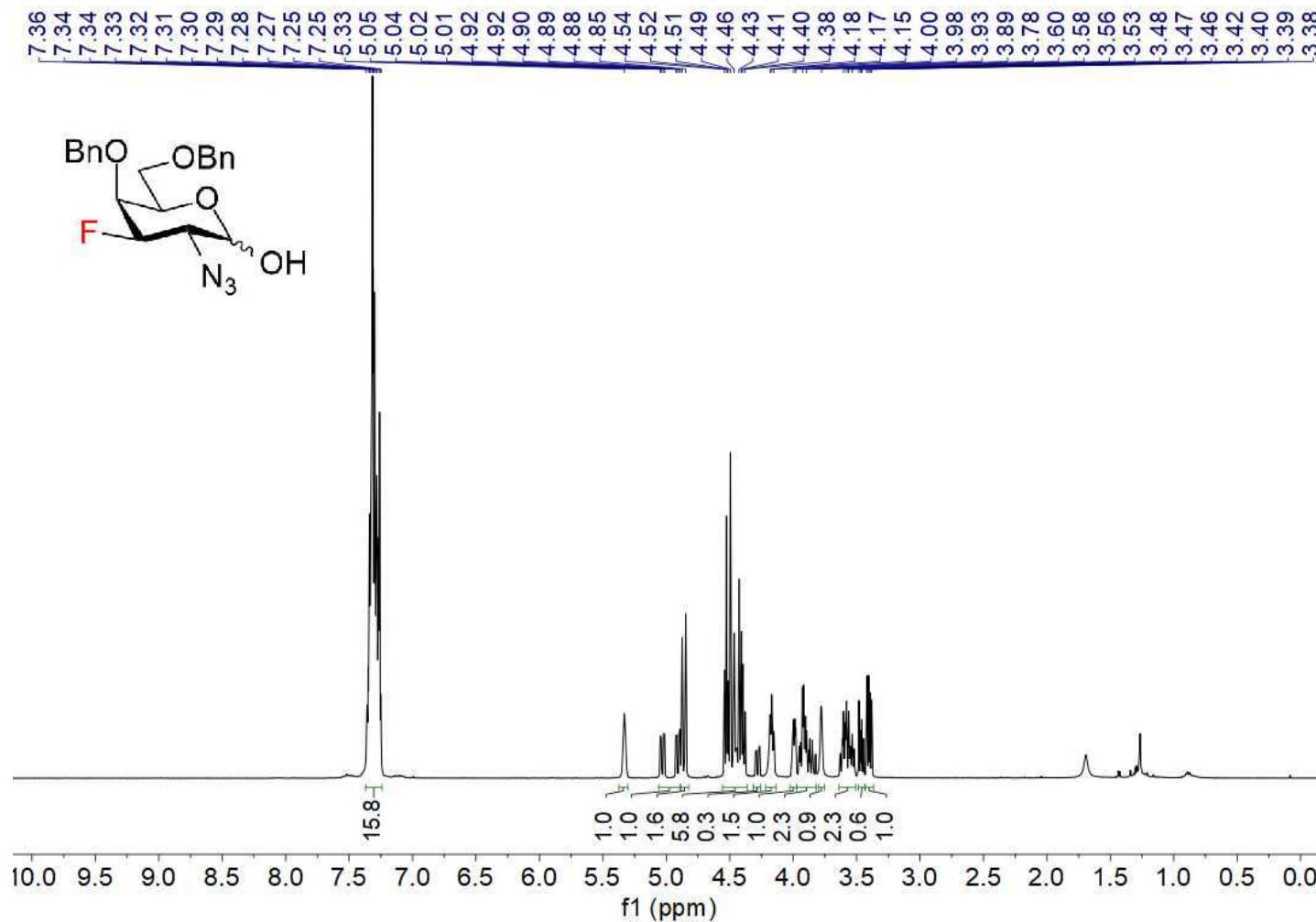


^1H - ^{13}C HSQC 28

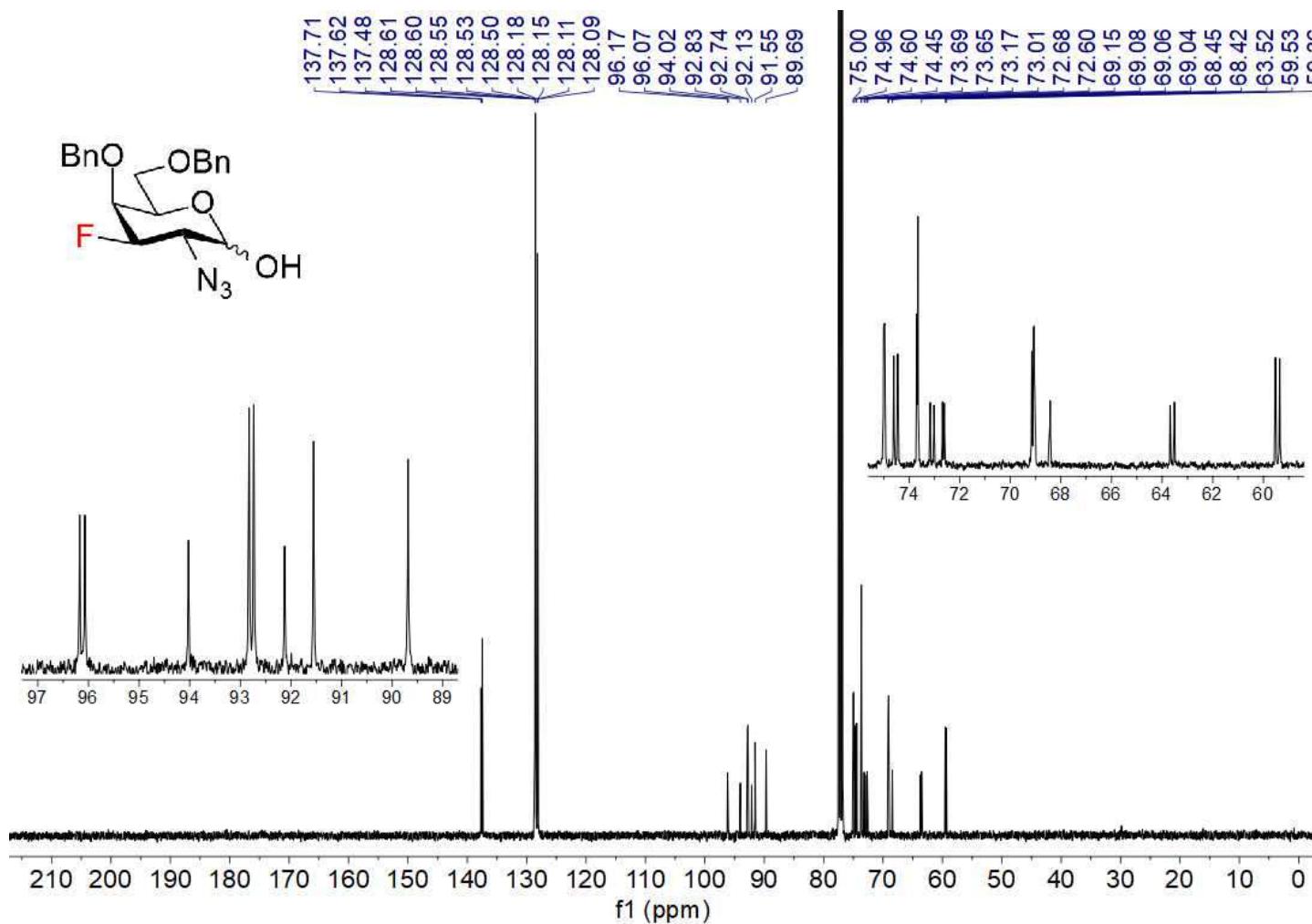


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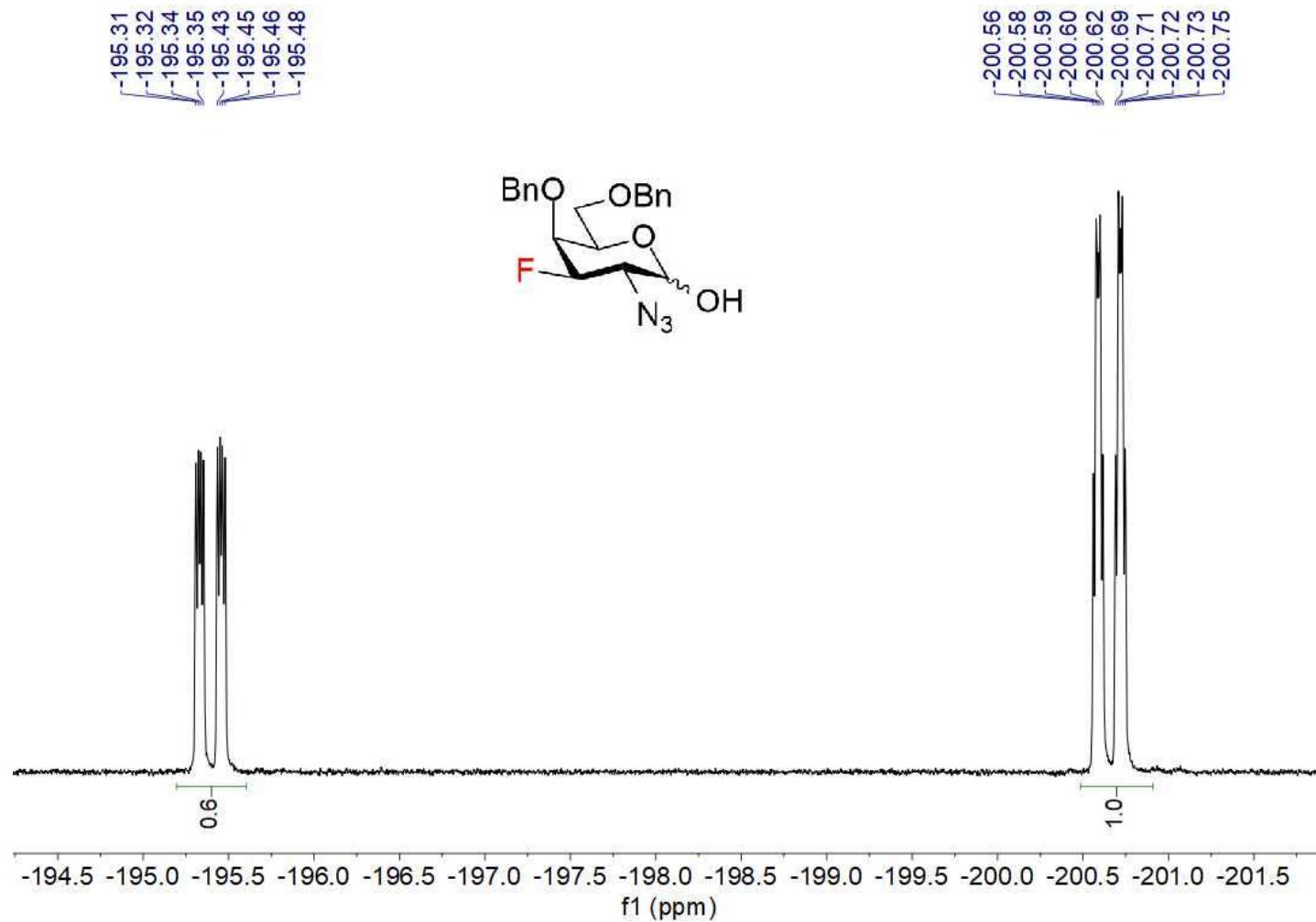
¹H NMR (400 MHz, CDCl₃) 29 (α/β ca. 5/3)



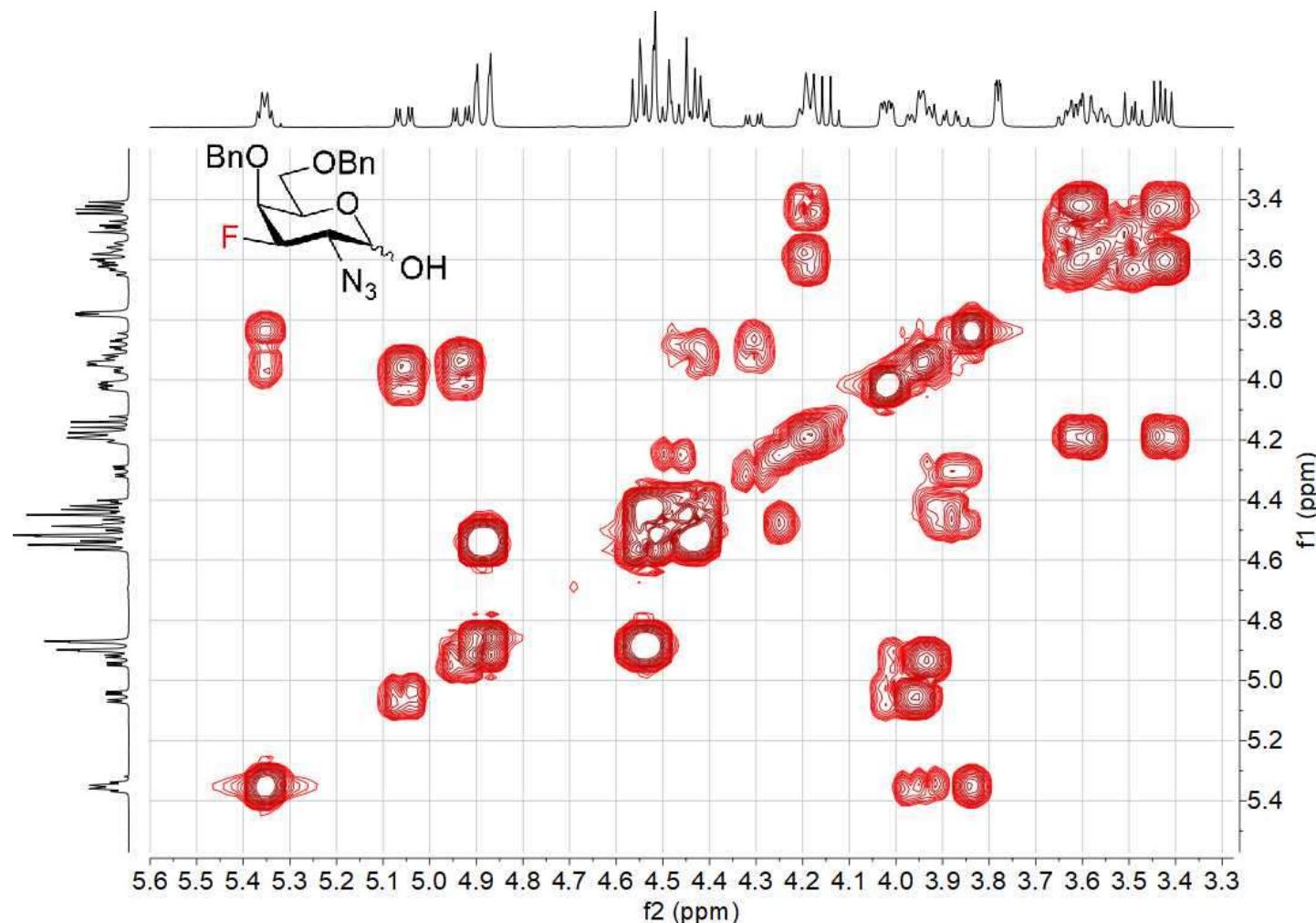
¹³C NMR (100 MHz, CDCl₃) 29



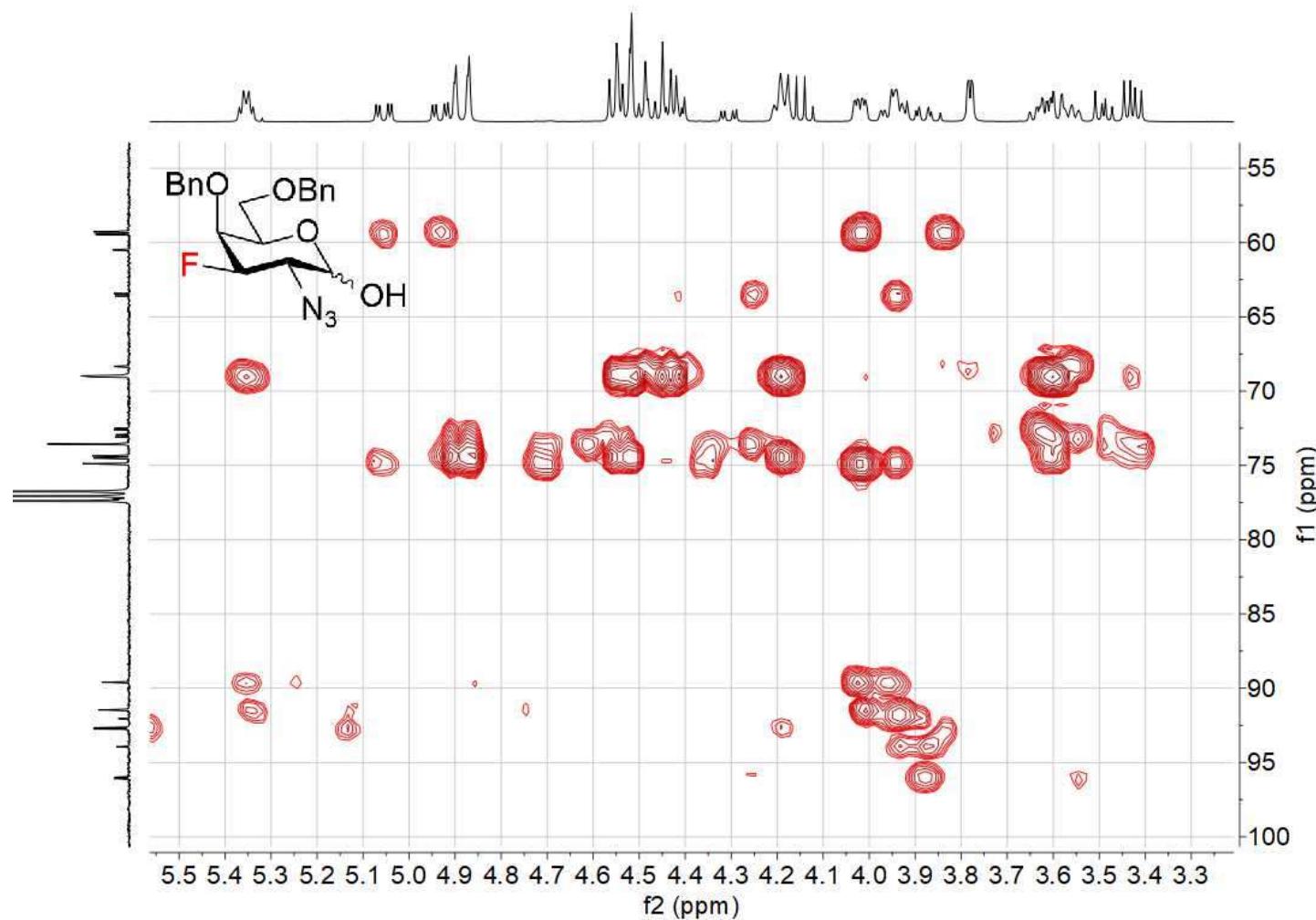
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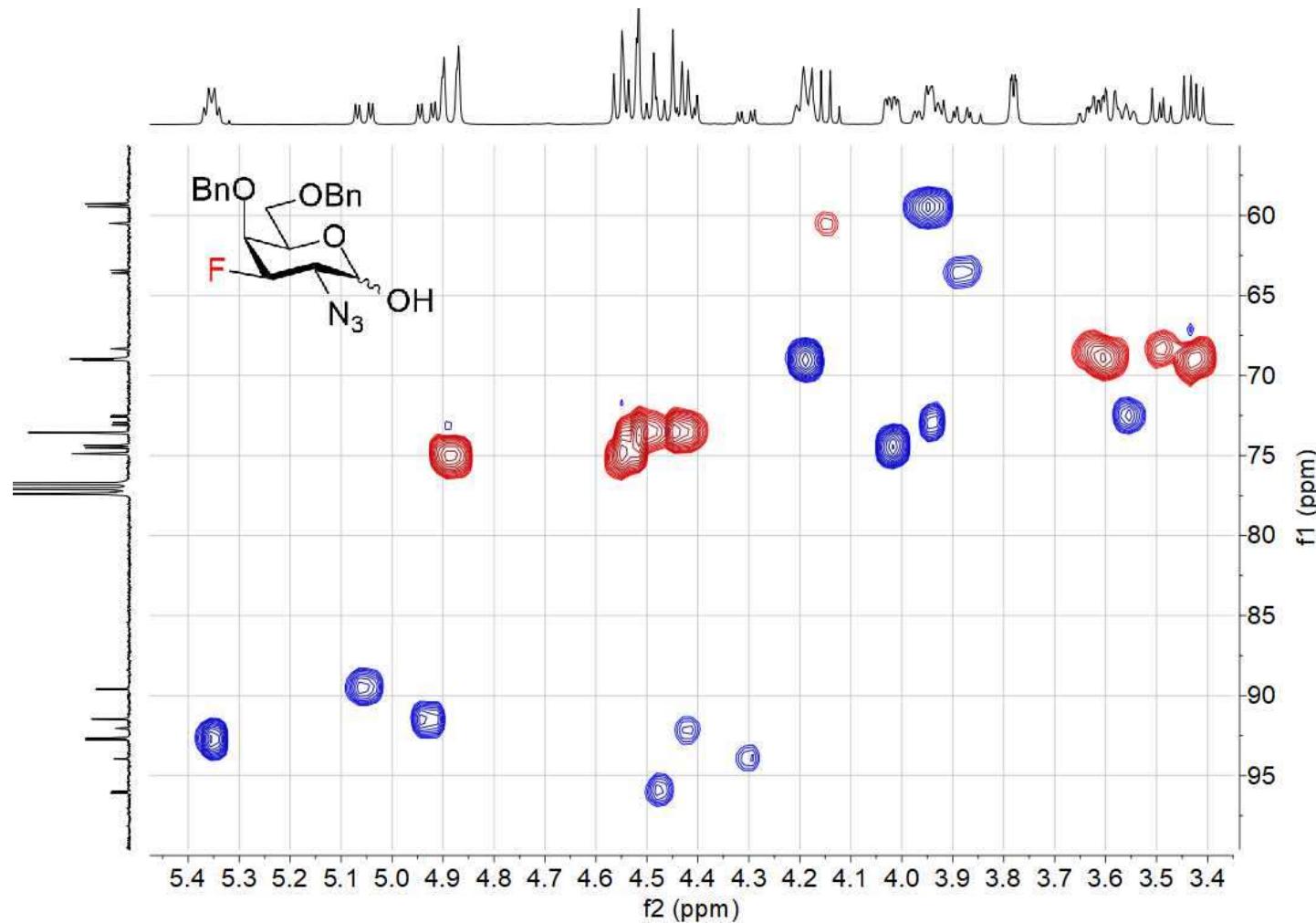
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^1H - ^{13}C HMBC 29

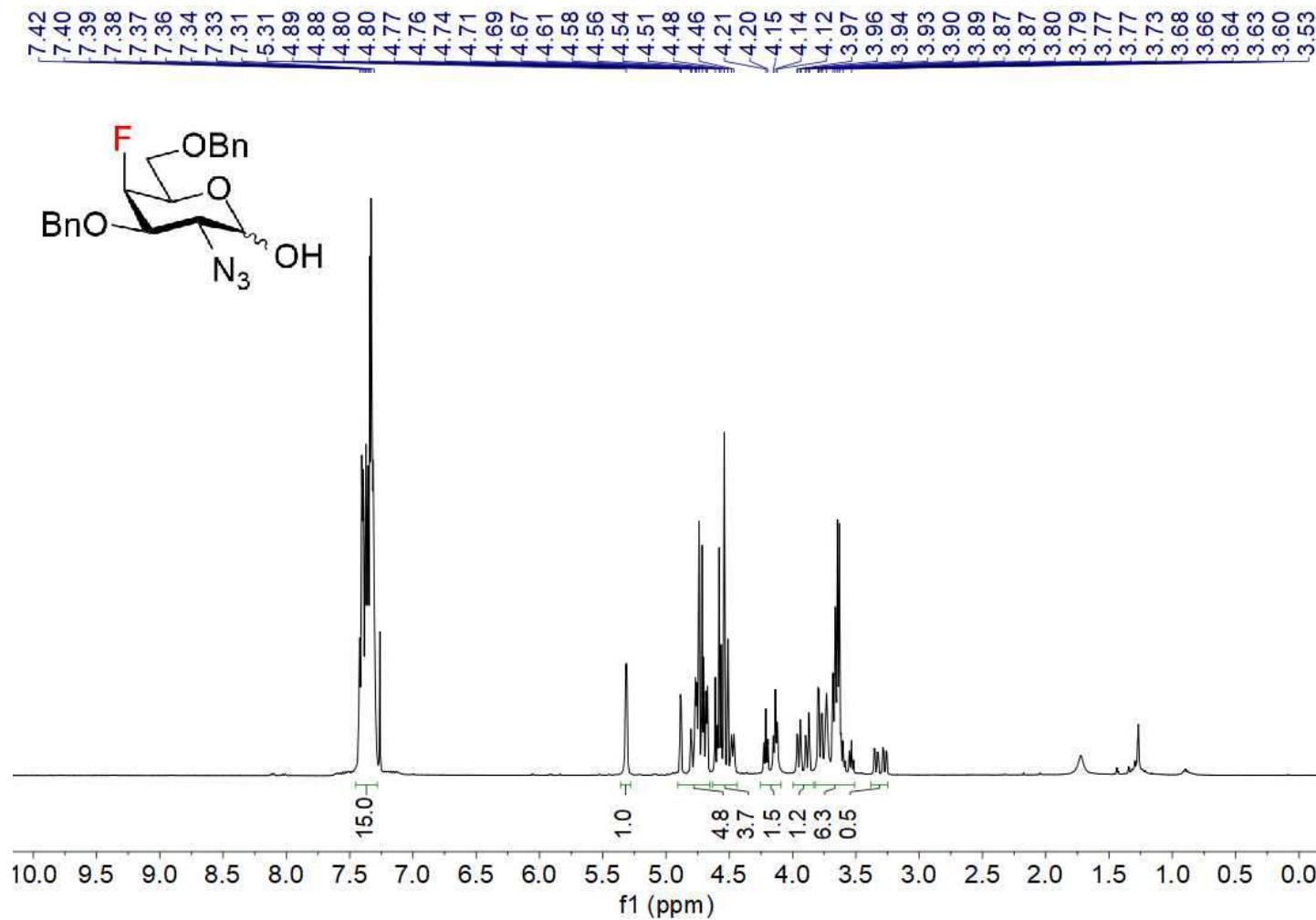


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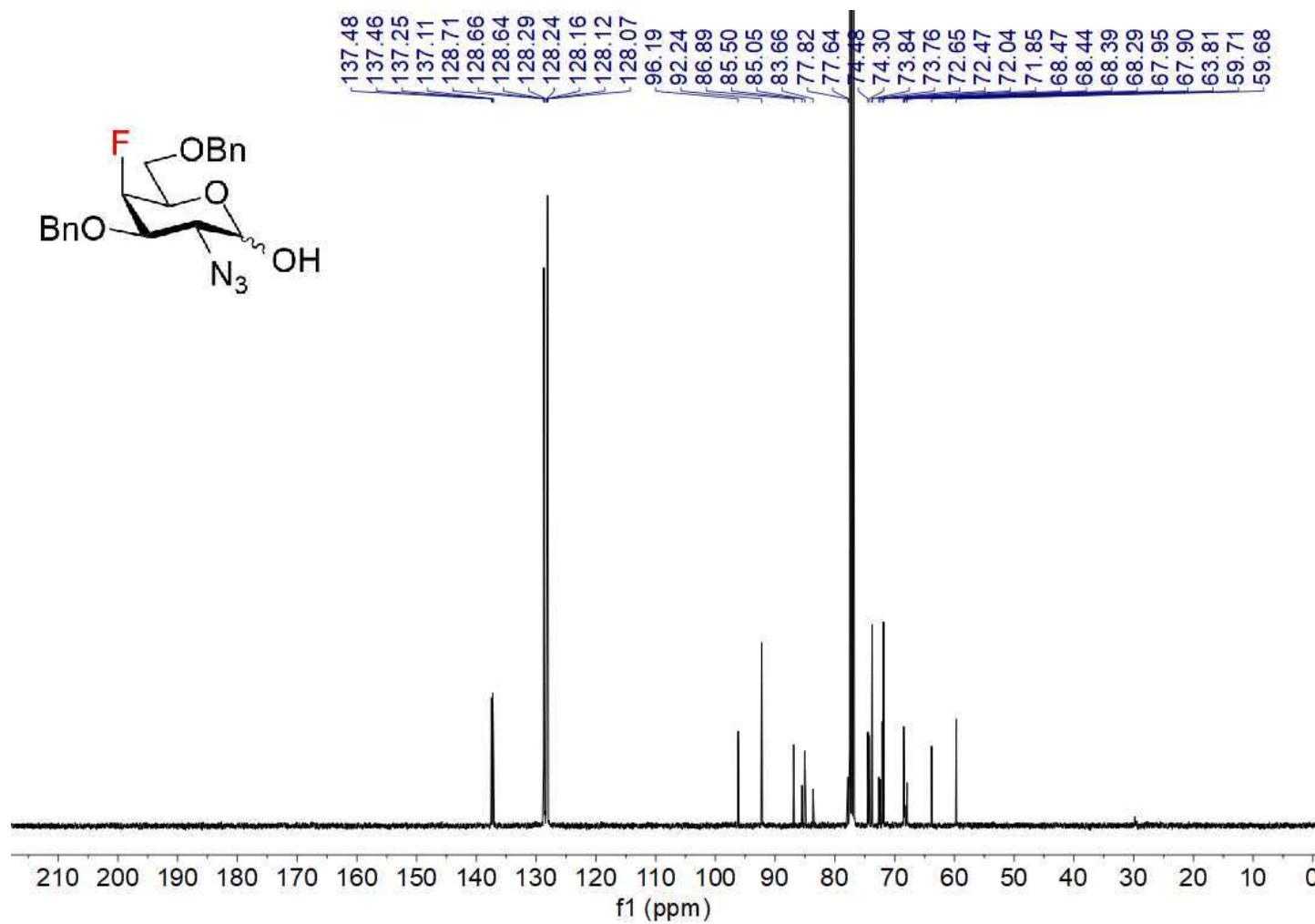


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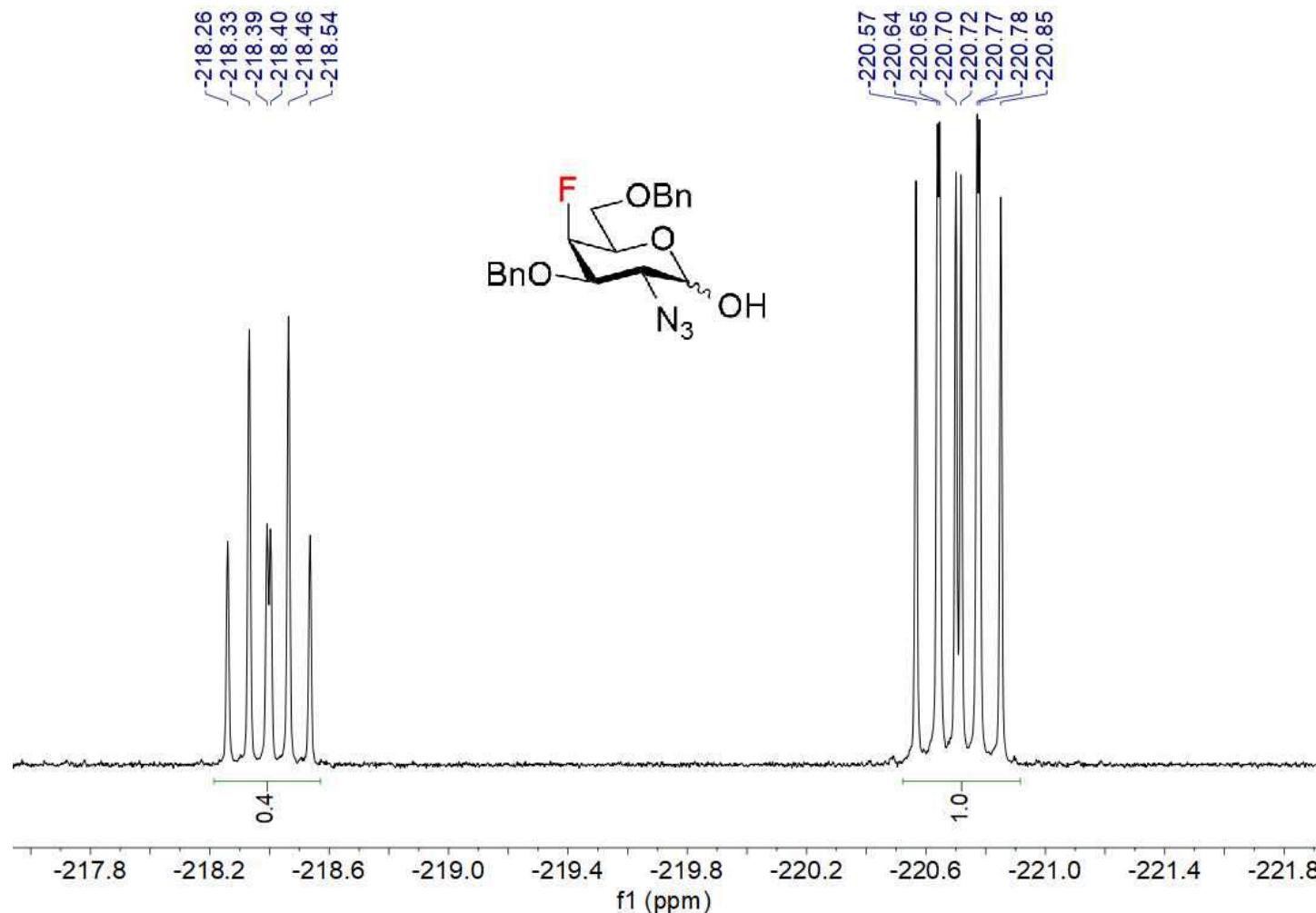
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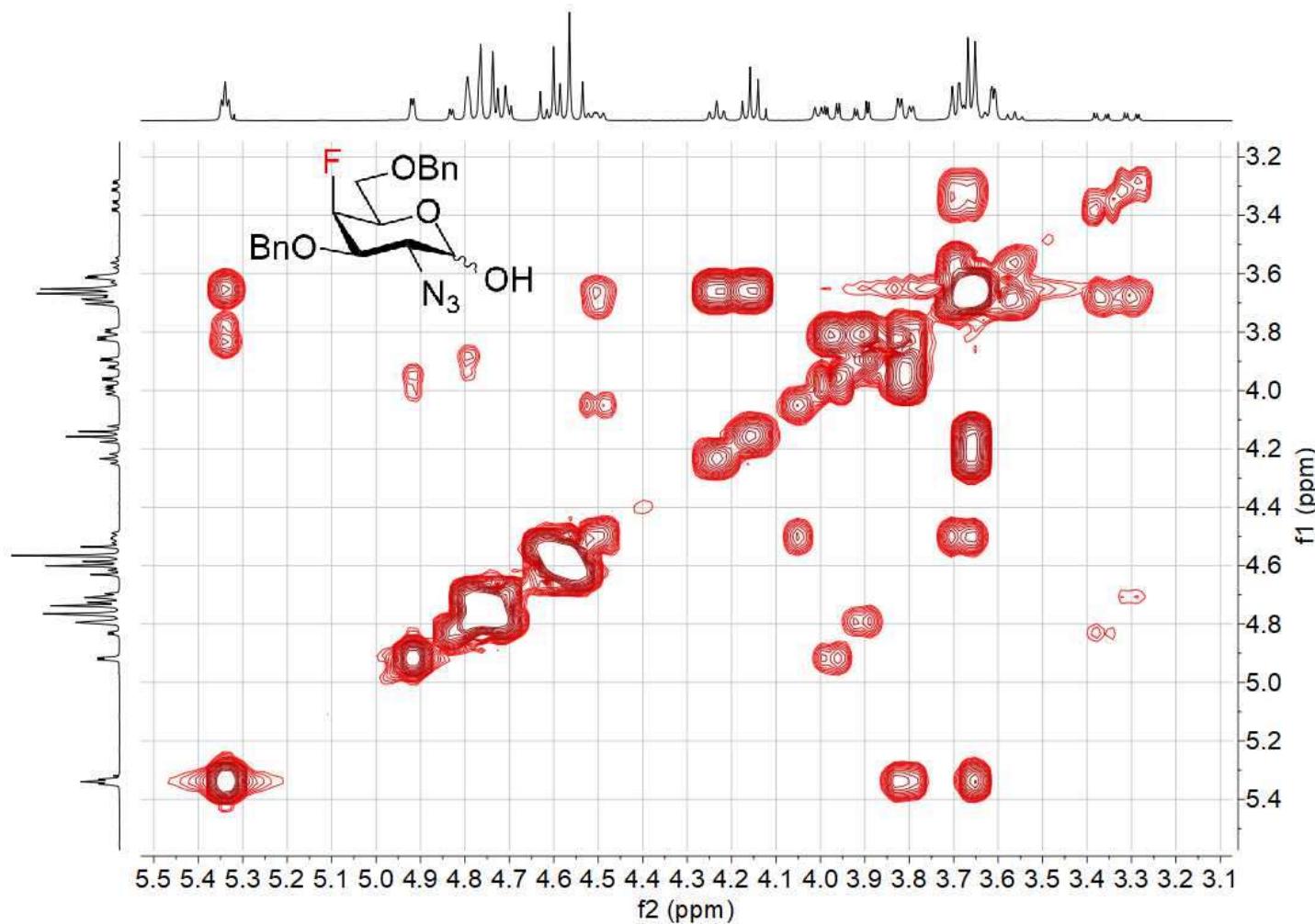
¹³C NMR (100 MHz, CDCl₃) 30



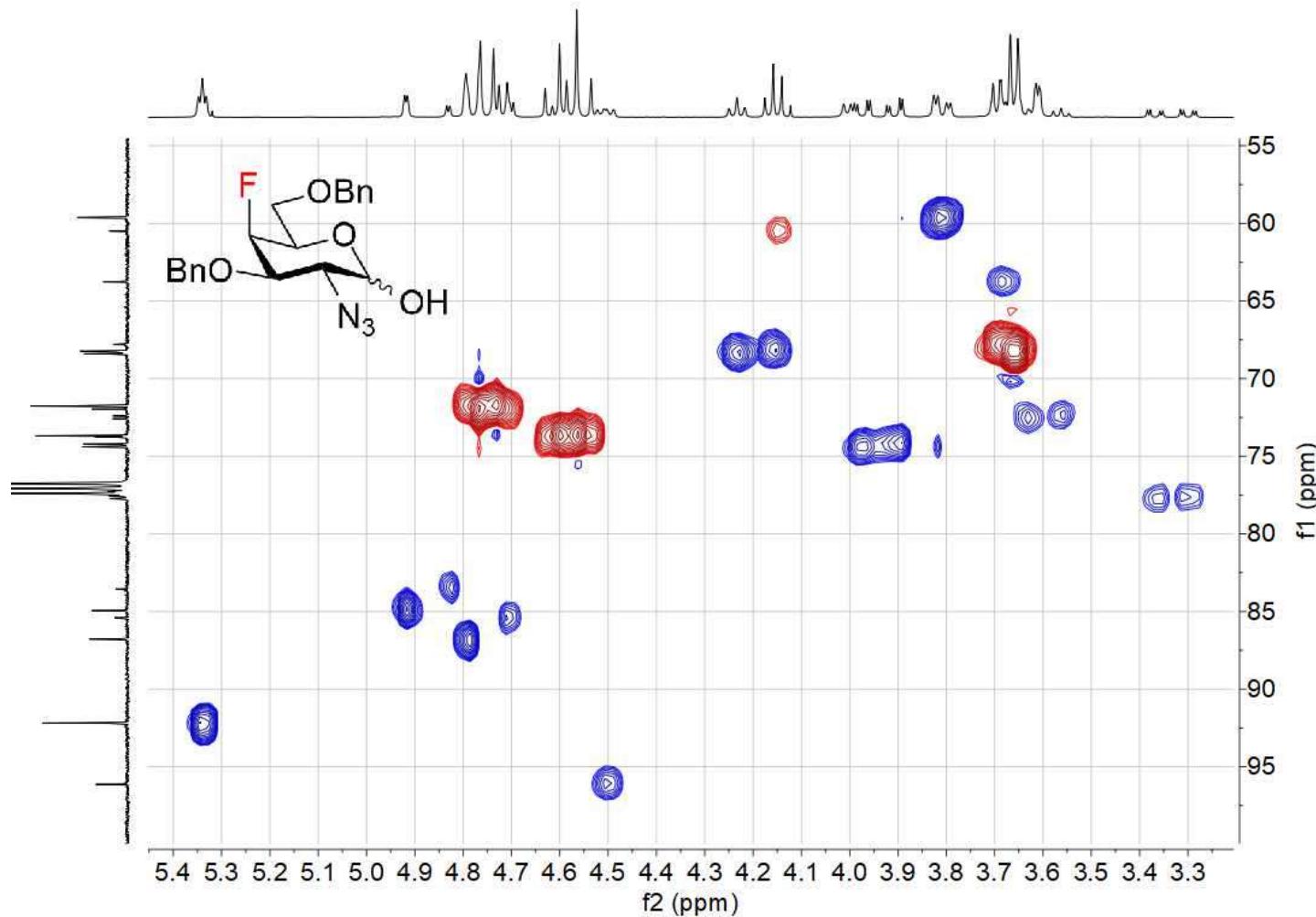
¹⁹F NMR (376 MHz, CDCl₃) 30 (α/β ca. 5/2)



^1H - ^1H COSY 30

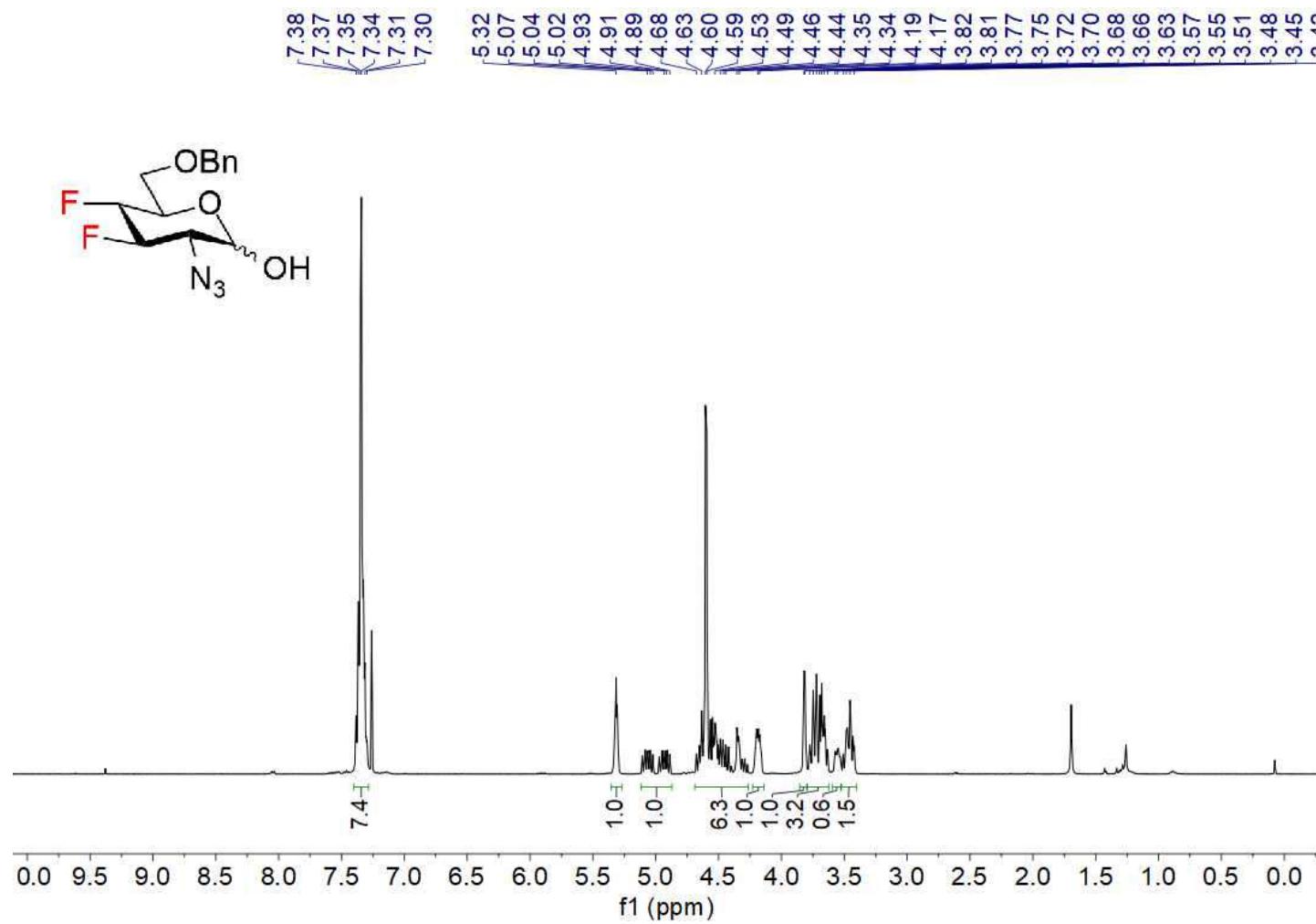


^1H - ^{13}C HSQC 30

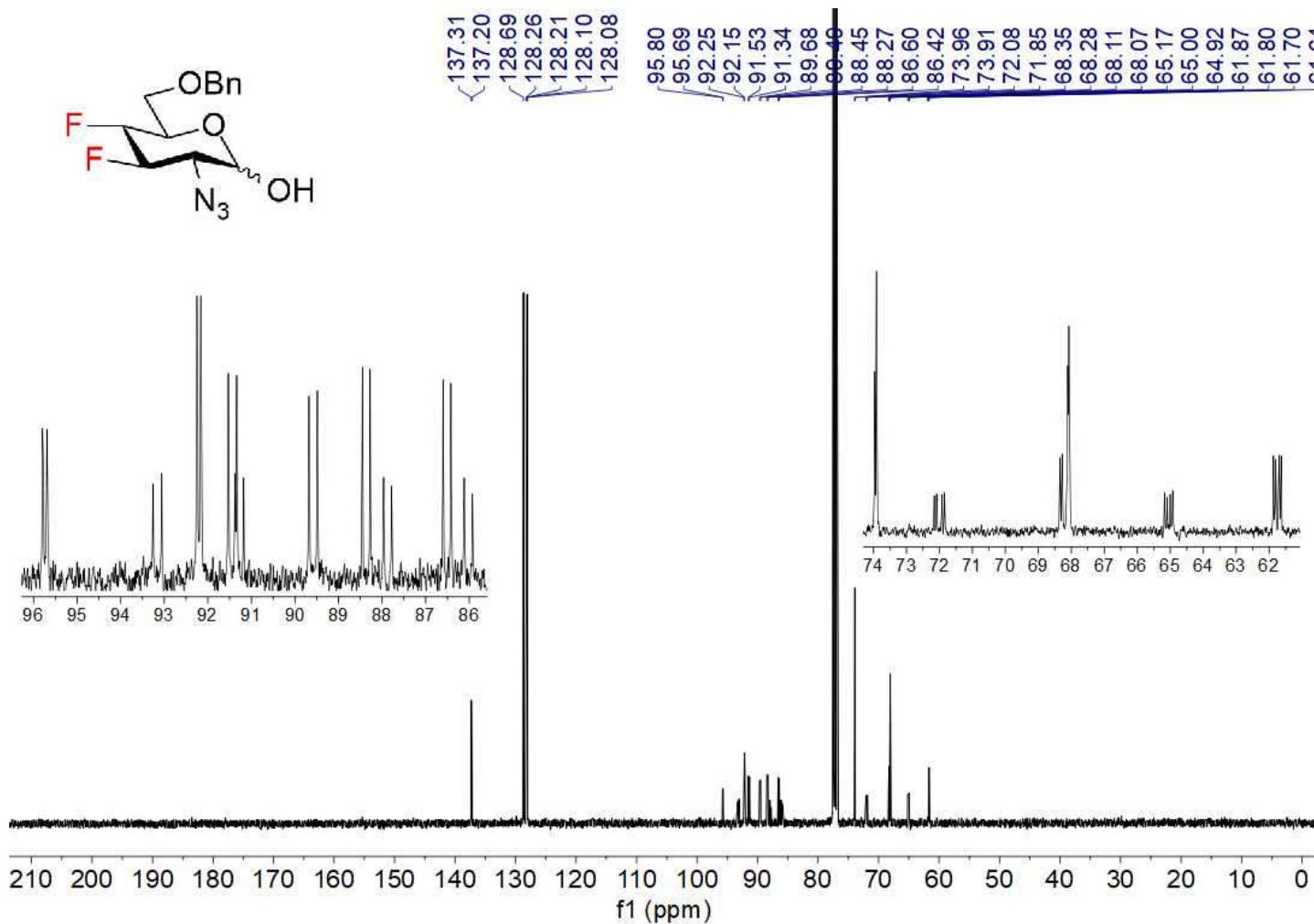


NMR COMPOUND 31

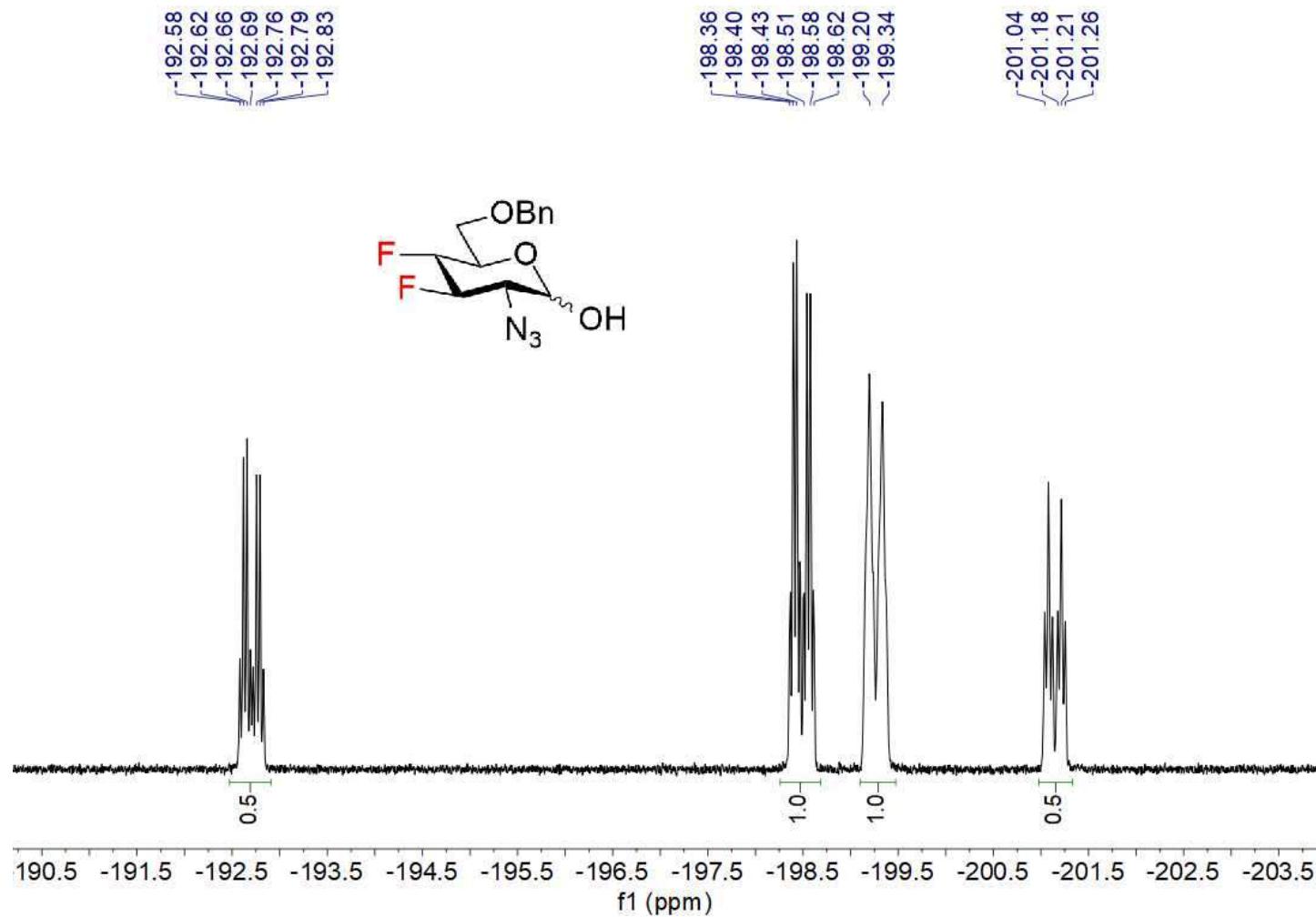
¹H NMR (400 MHz, CDCl₃) 31 (α/β ca. 2/1)



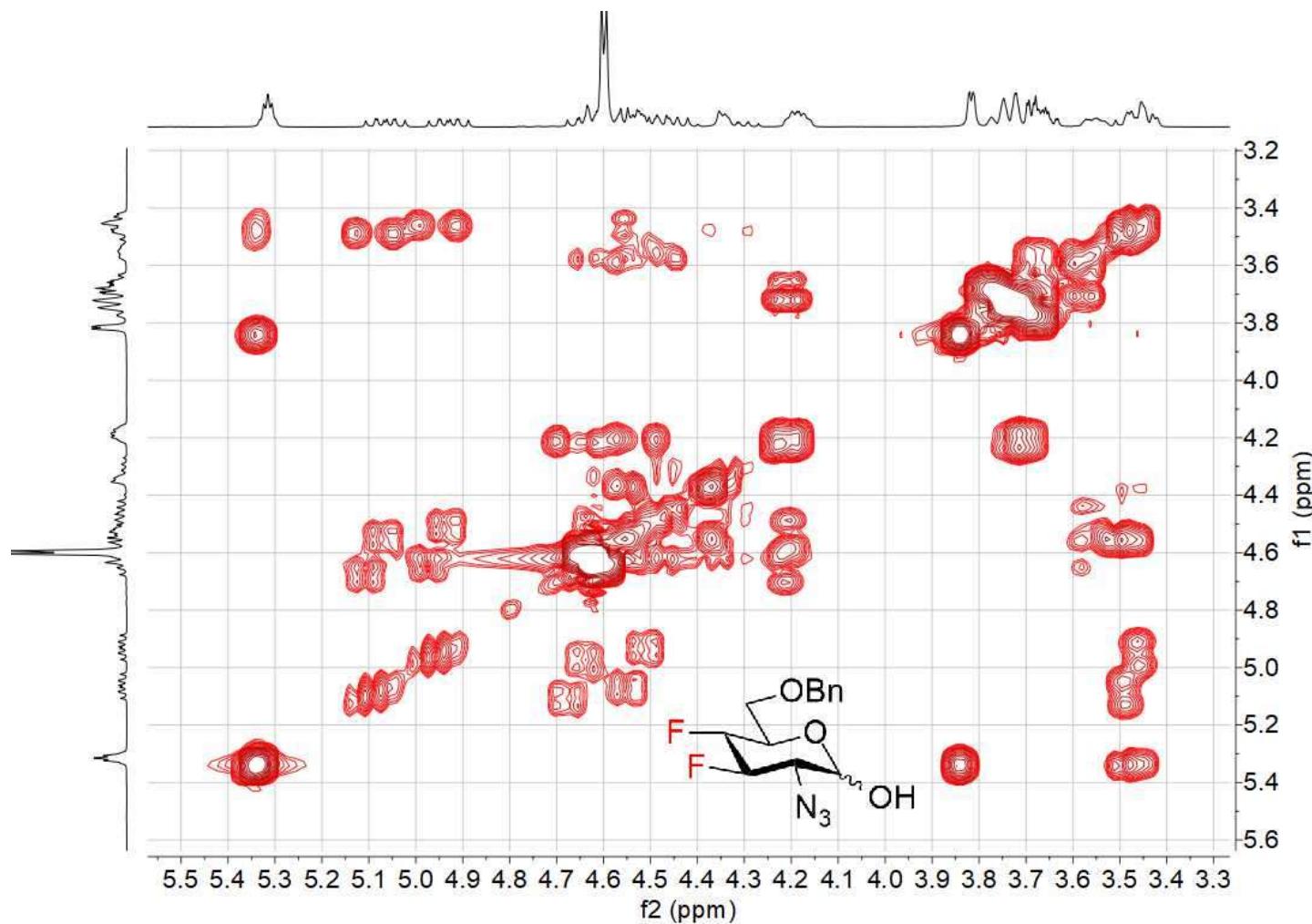
¹³C NMR (100 MHz, CDCl₃) 31



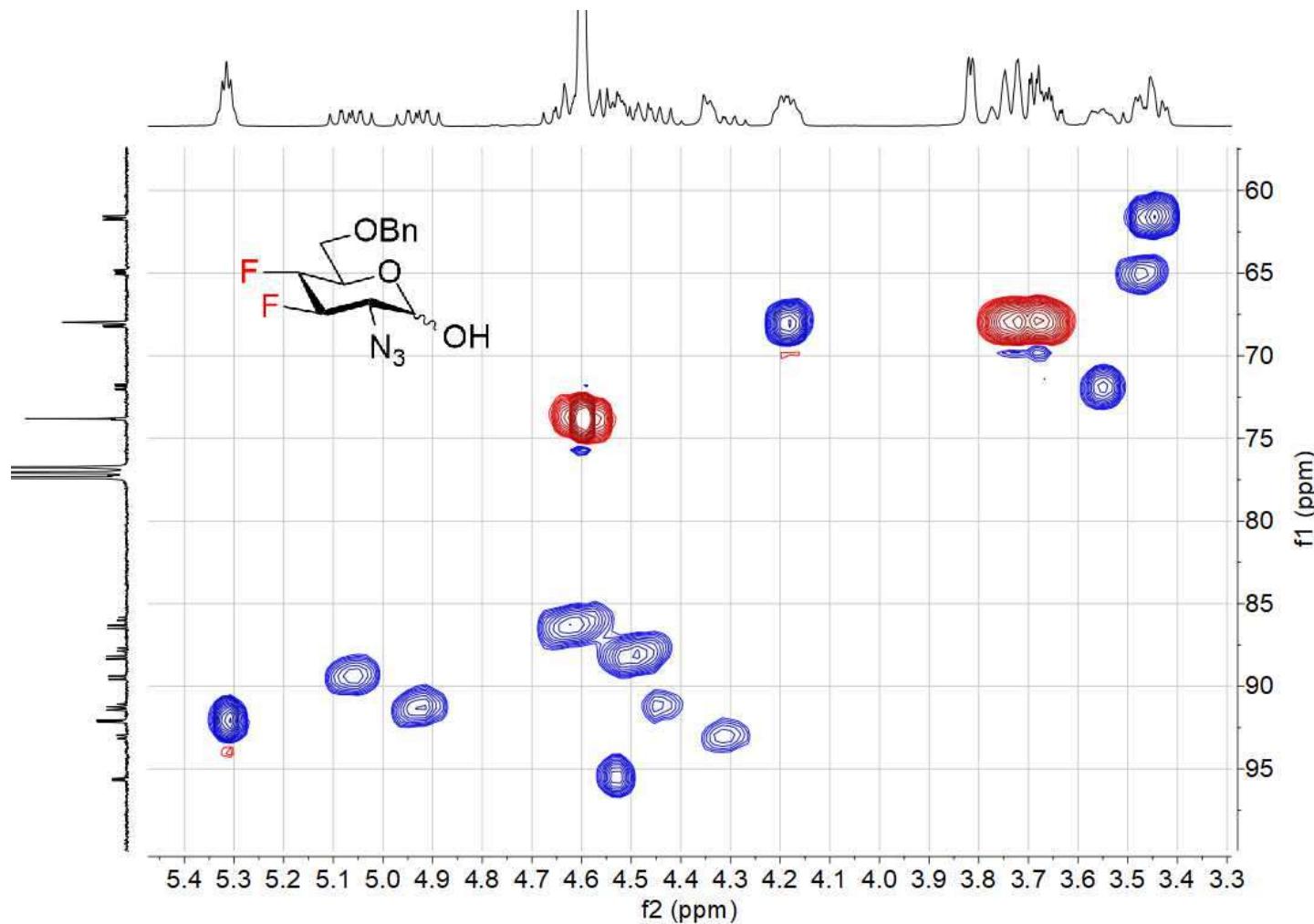
¹⁹F NMR (376 MHz, CDCl₃) 31 (α/β ca. 2/1)



¹H-¹H COSY 31

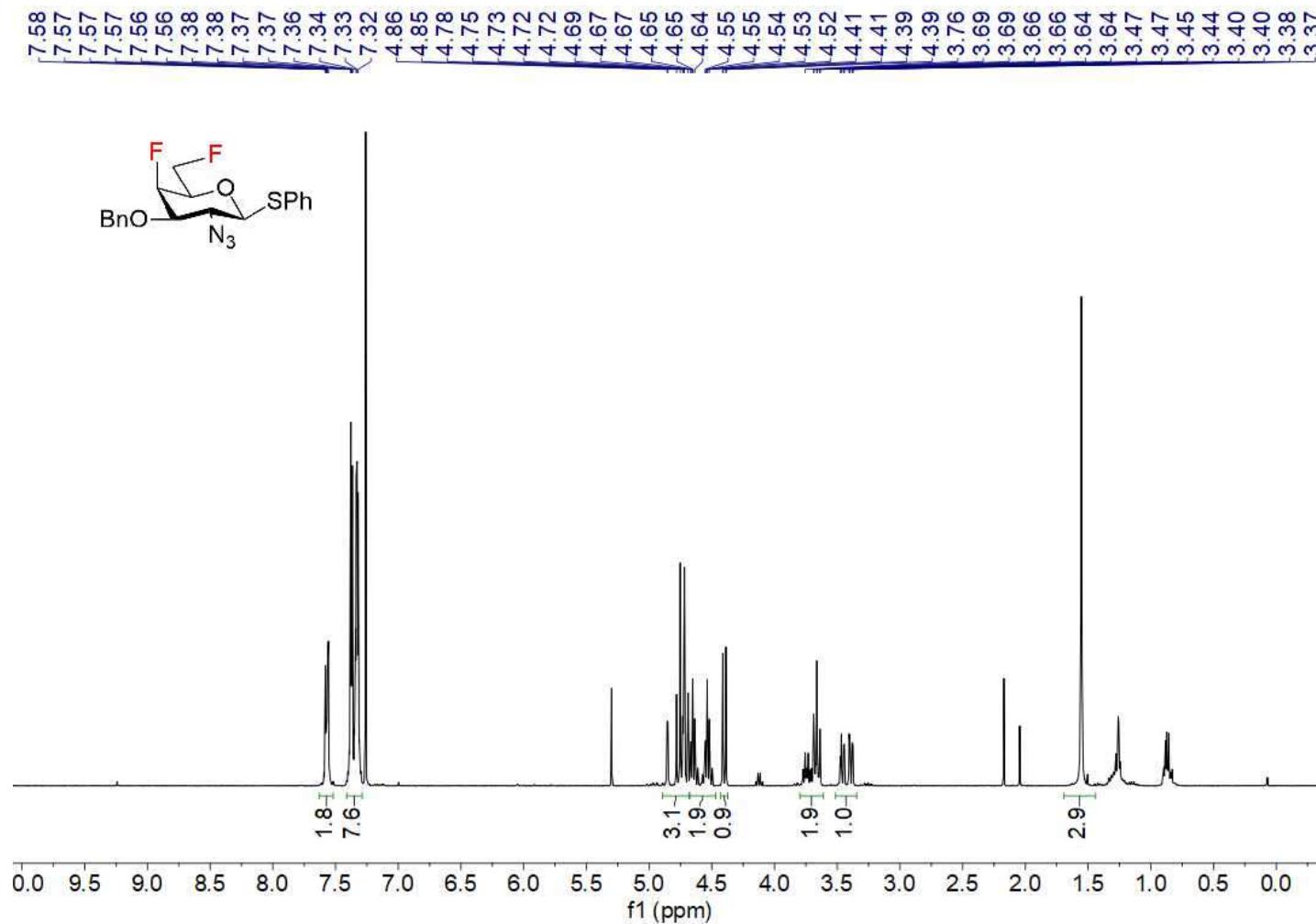


^1H - ^{13}C HSQC 31

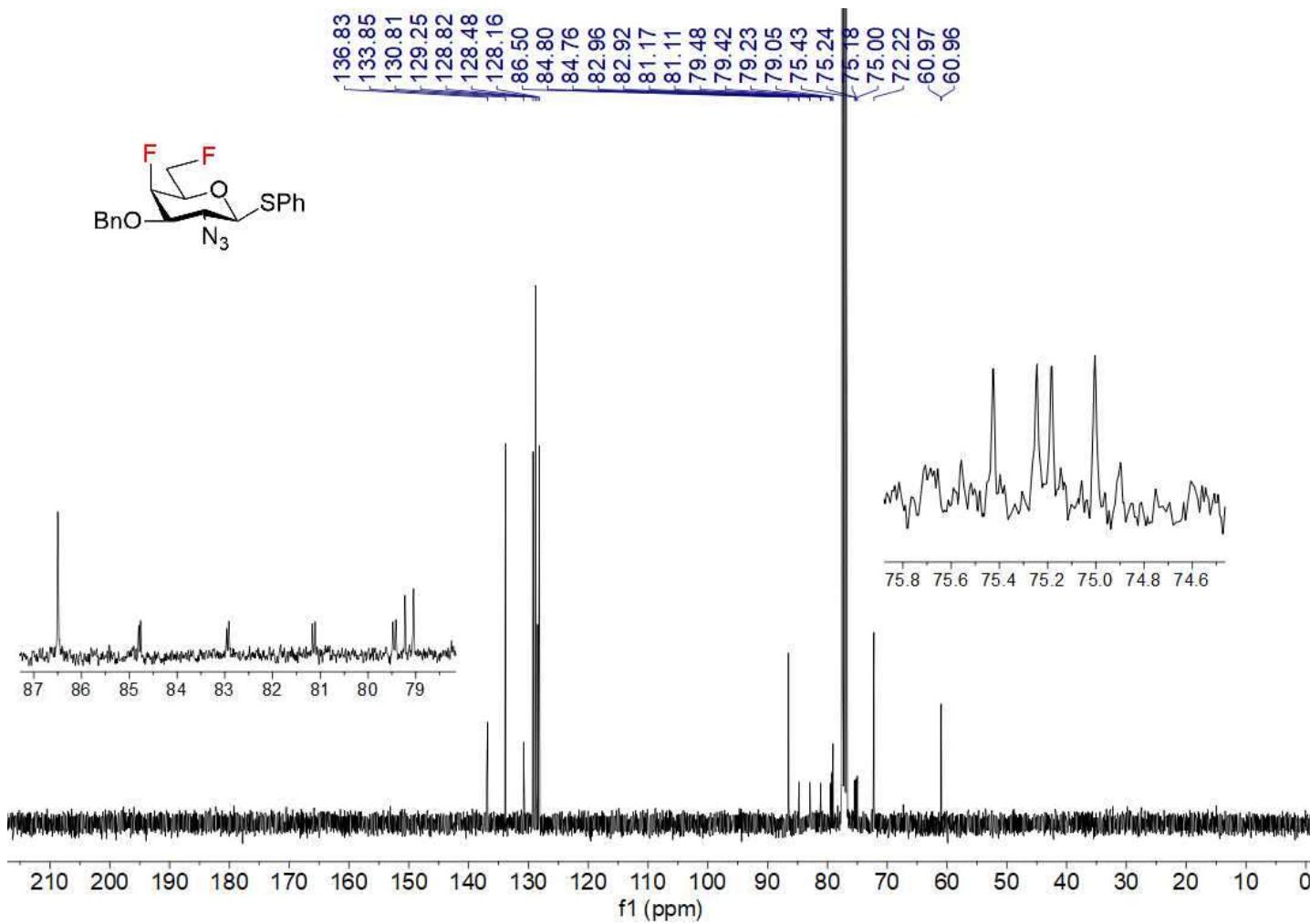


NMR COMPOUND 32

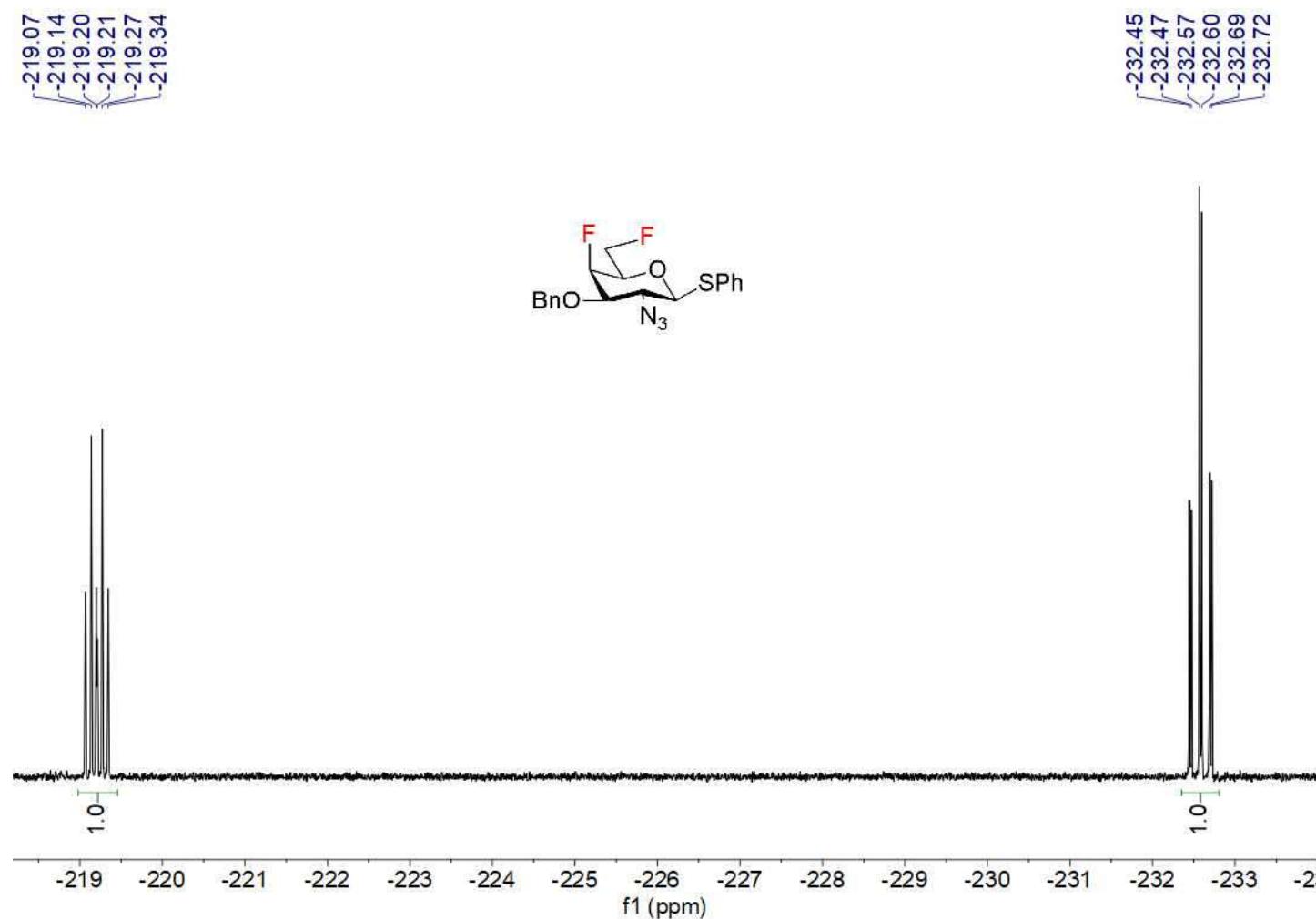
^1H NMR (400 MHz, CDCl_3) 32



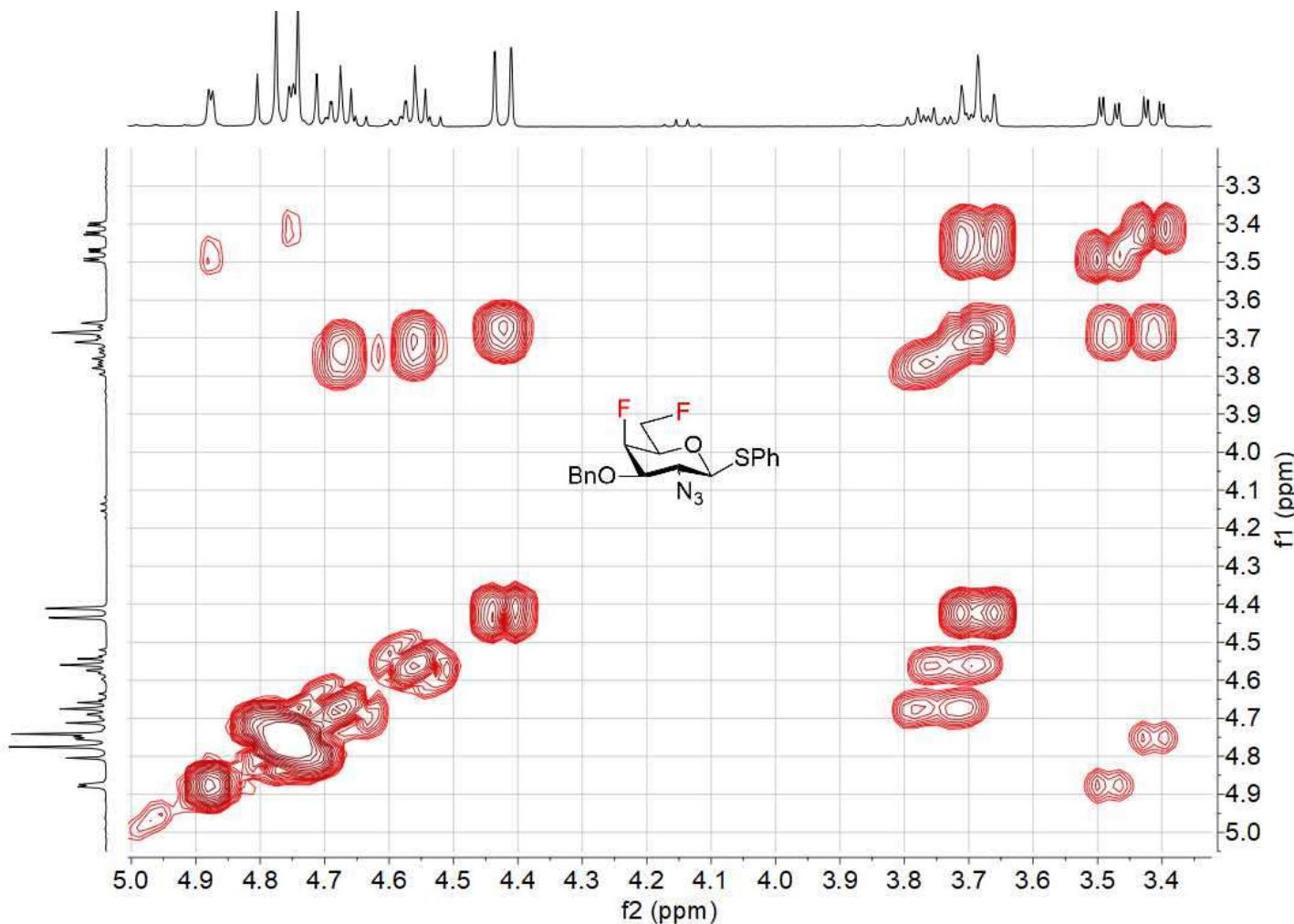
¹³C NMR (100 MHz, CDCl₃) 32



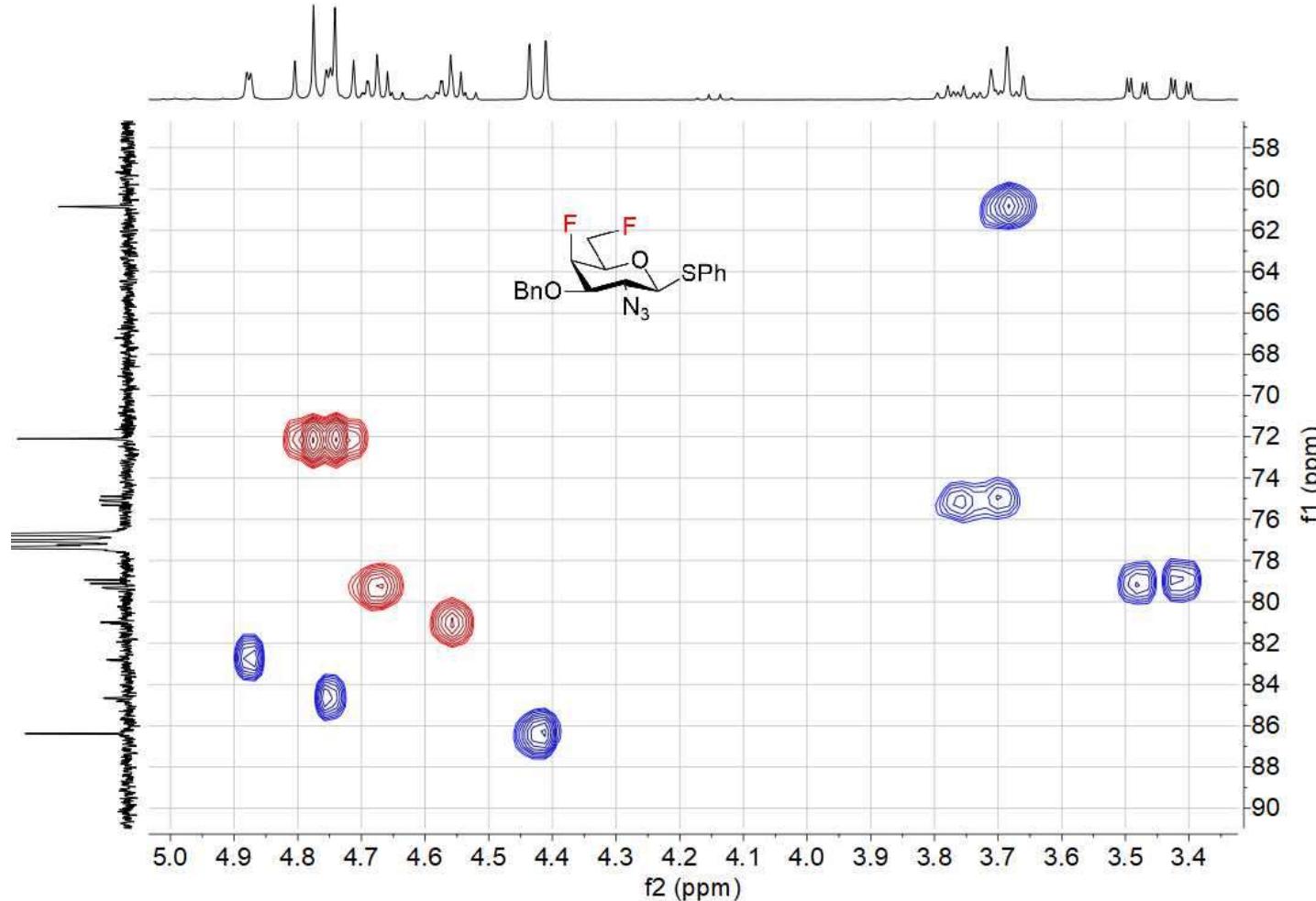
¹⁹F NMR (376 MHz, CDCl₃) 32



¹H-¹H COSY 32

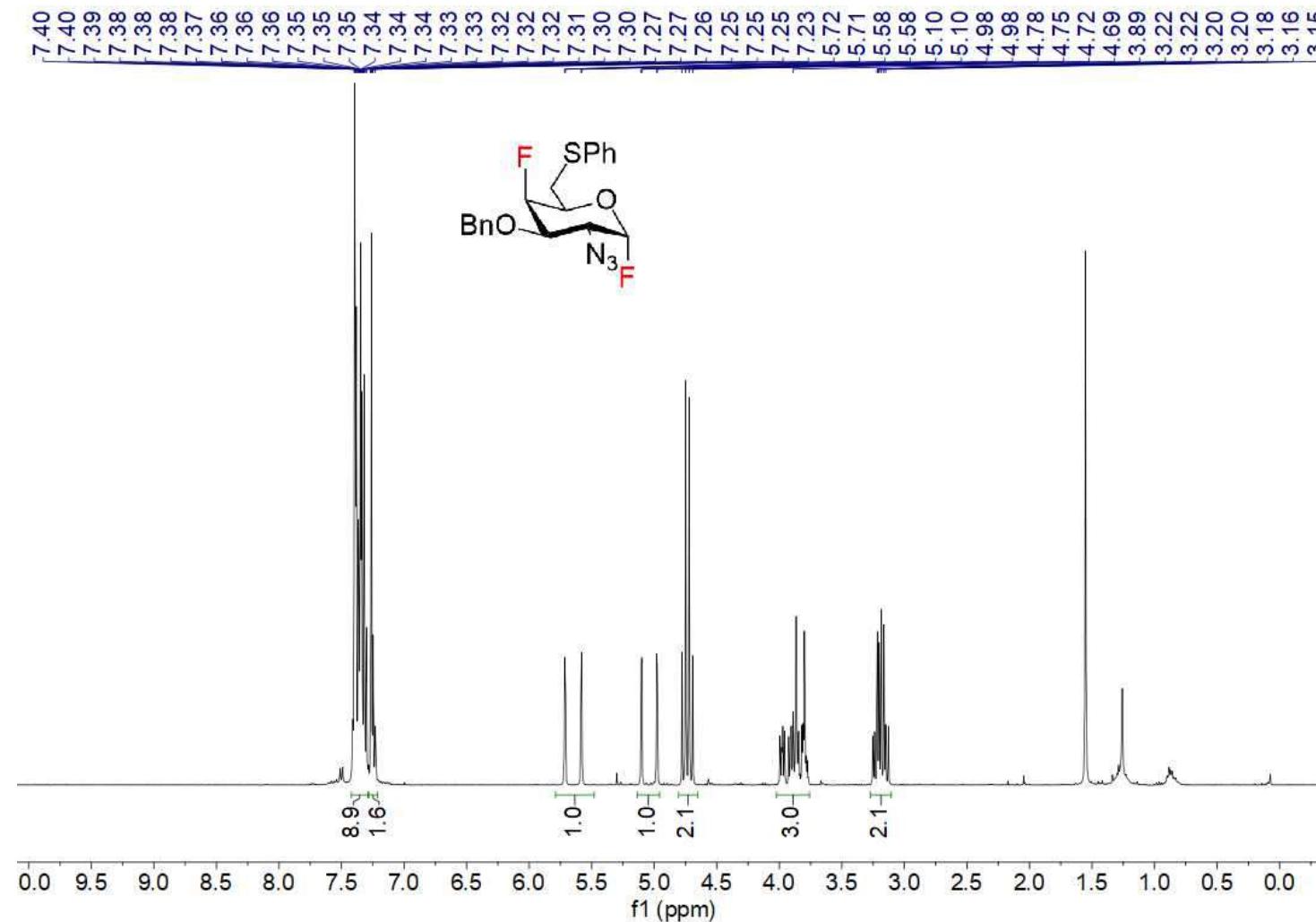


¹H-¹³C HSQC 32

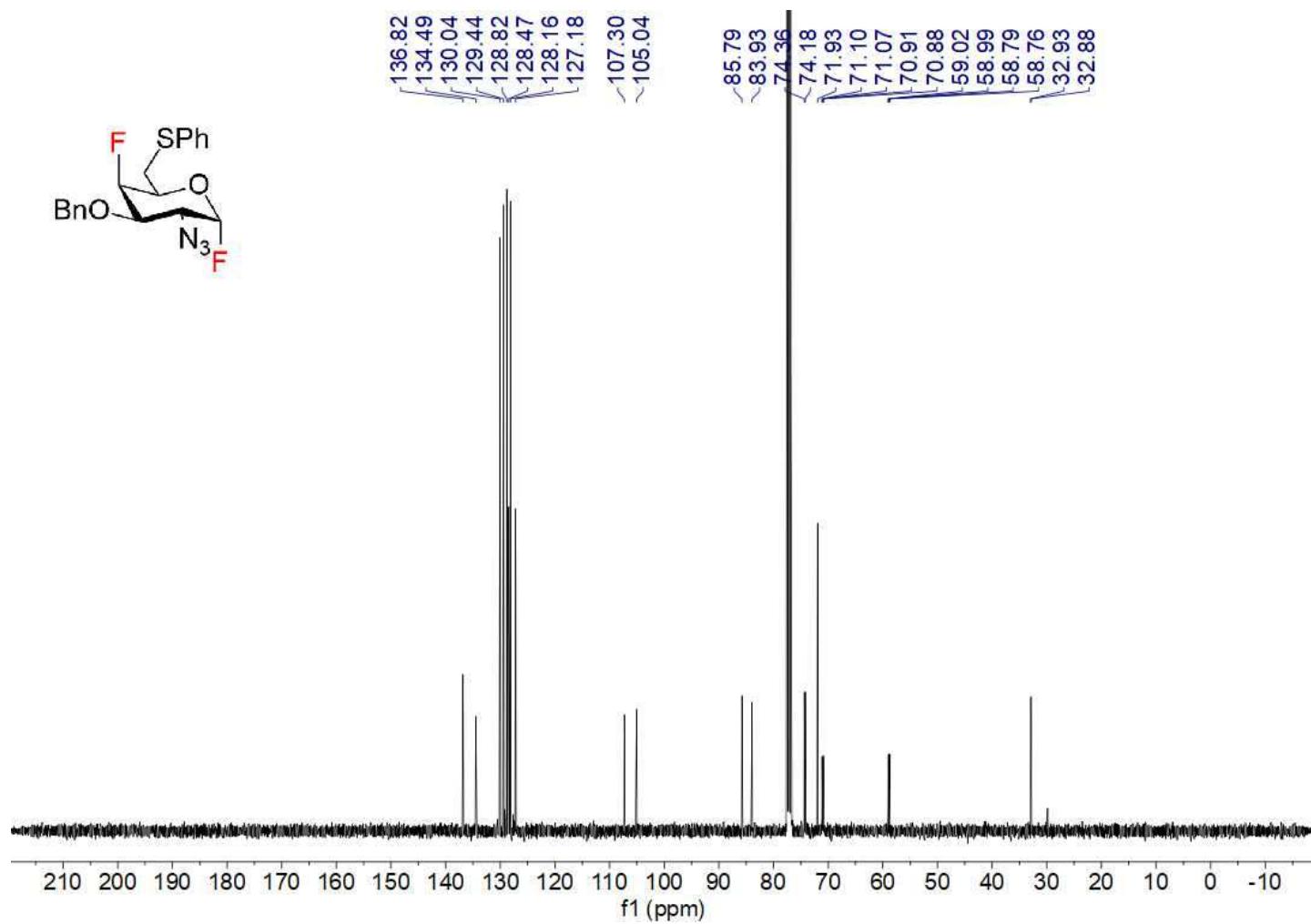


NMR COMPOUND 33

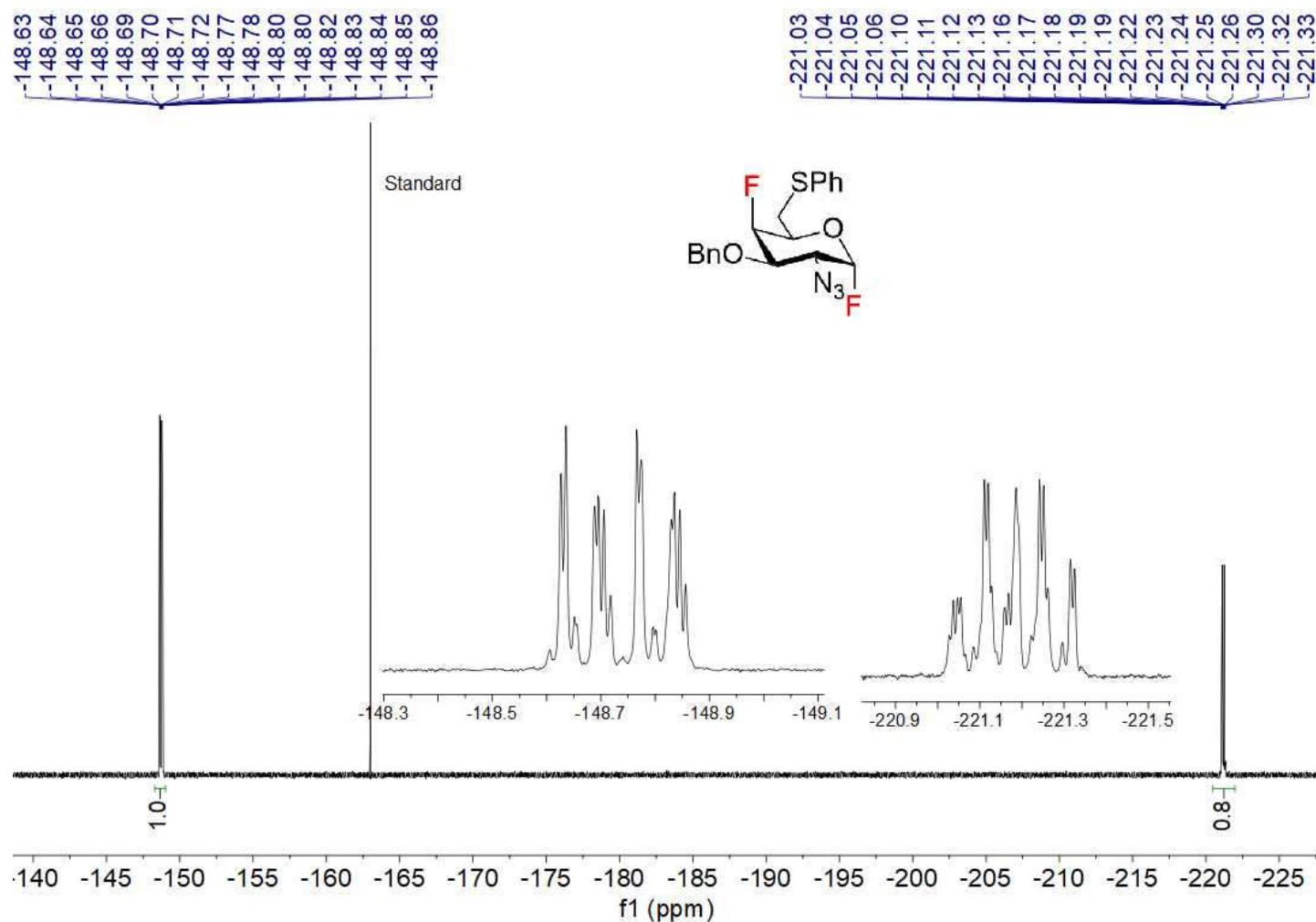
^1H NMR (400 MHz, CDCl_3) 33



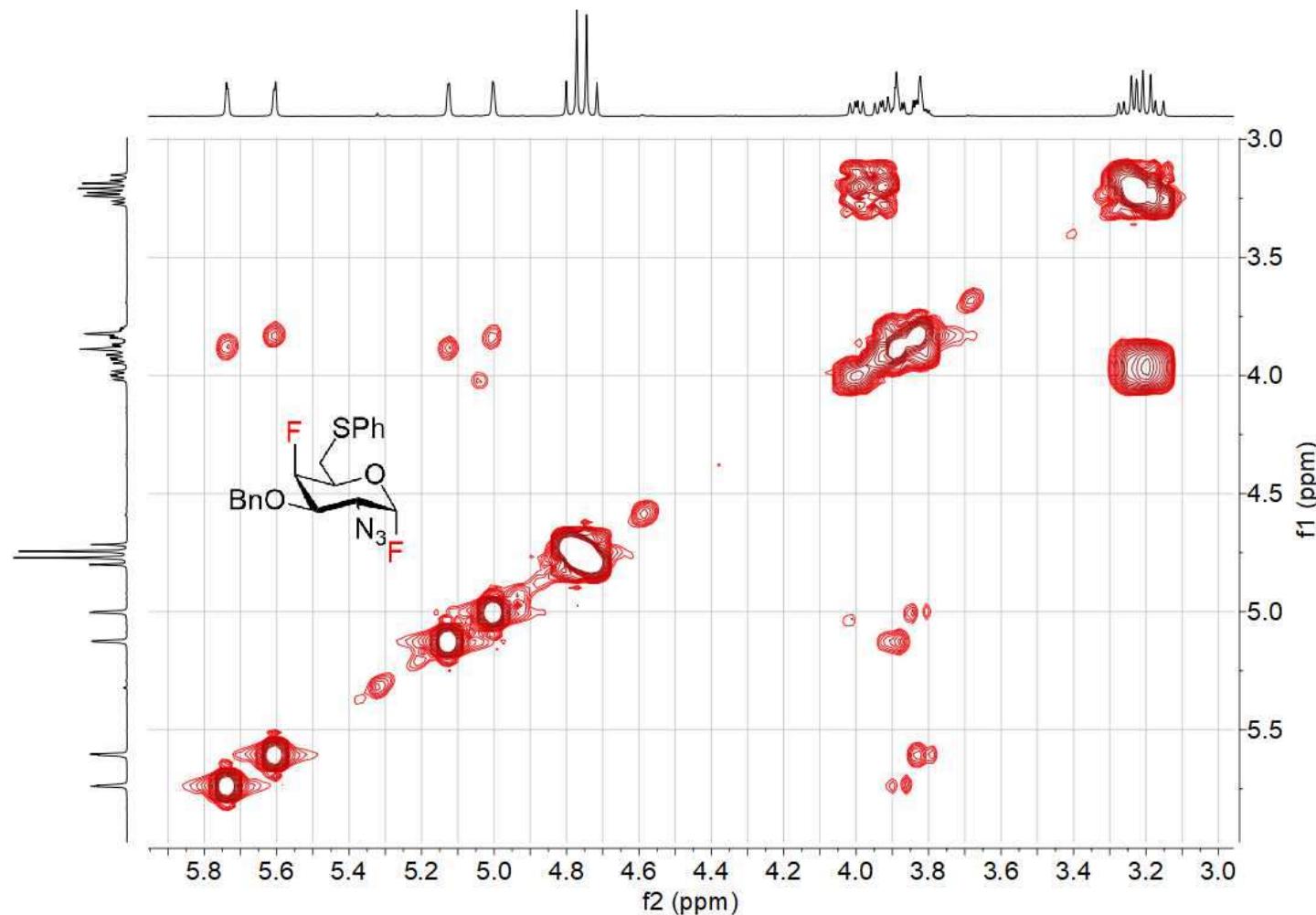
¹³C NMR (100 MHz, CDCl₃) 33



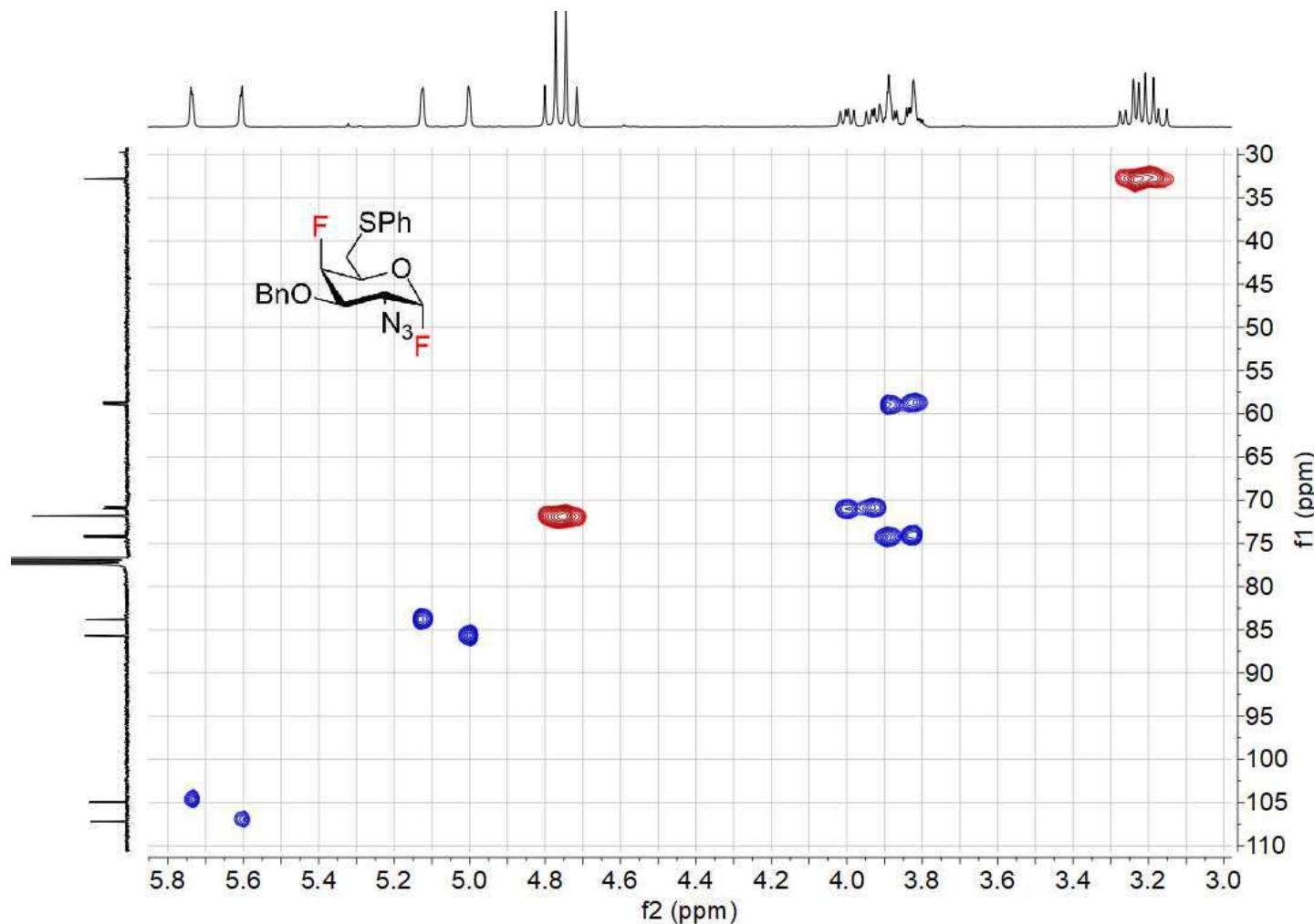
¹⁹F NMR (376 MHz, CDCl₃) 33



¹H-¹H COSY 33

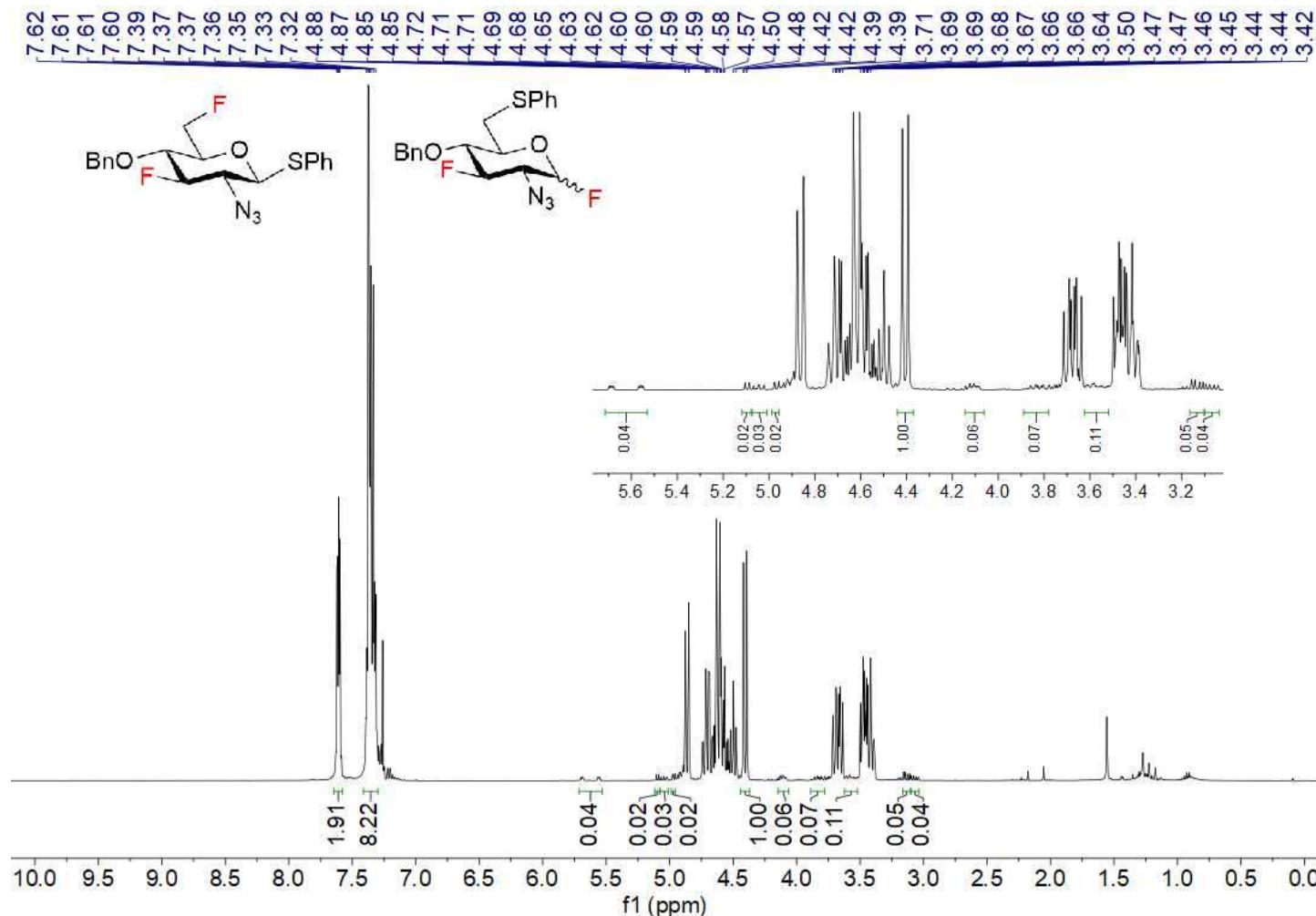


^1H - ^{13}C HSQC 33

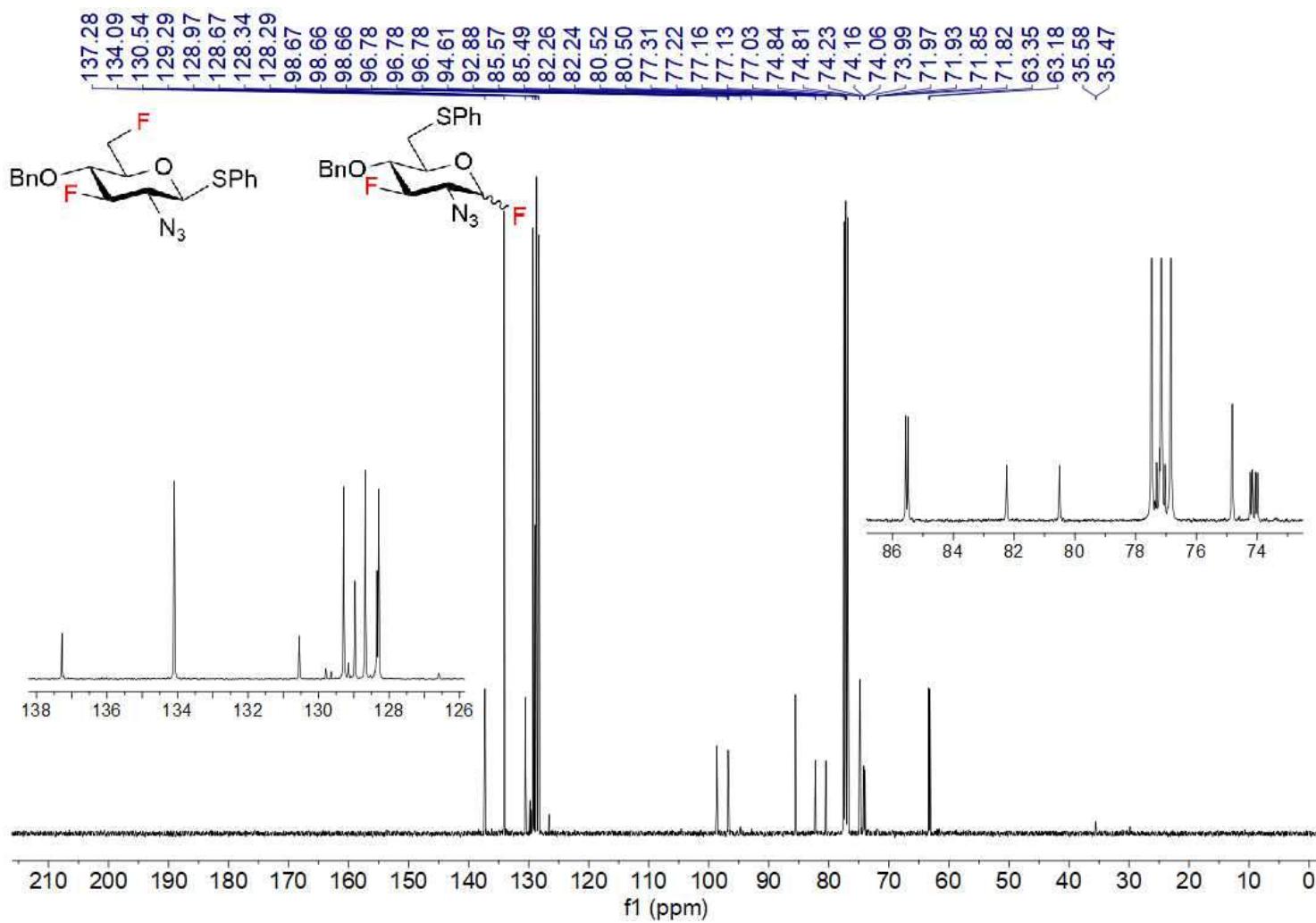


NMR COMPOUNDS 34 and 35

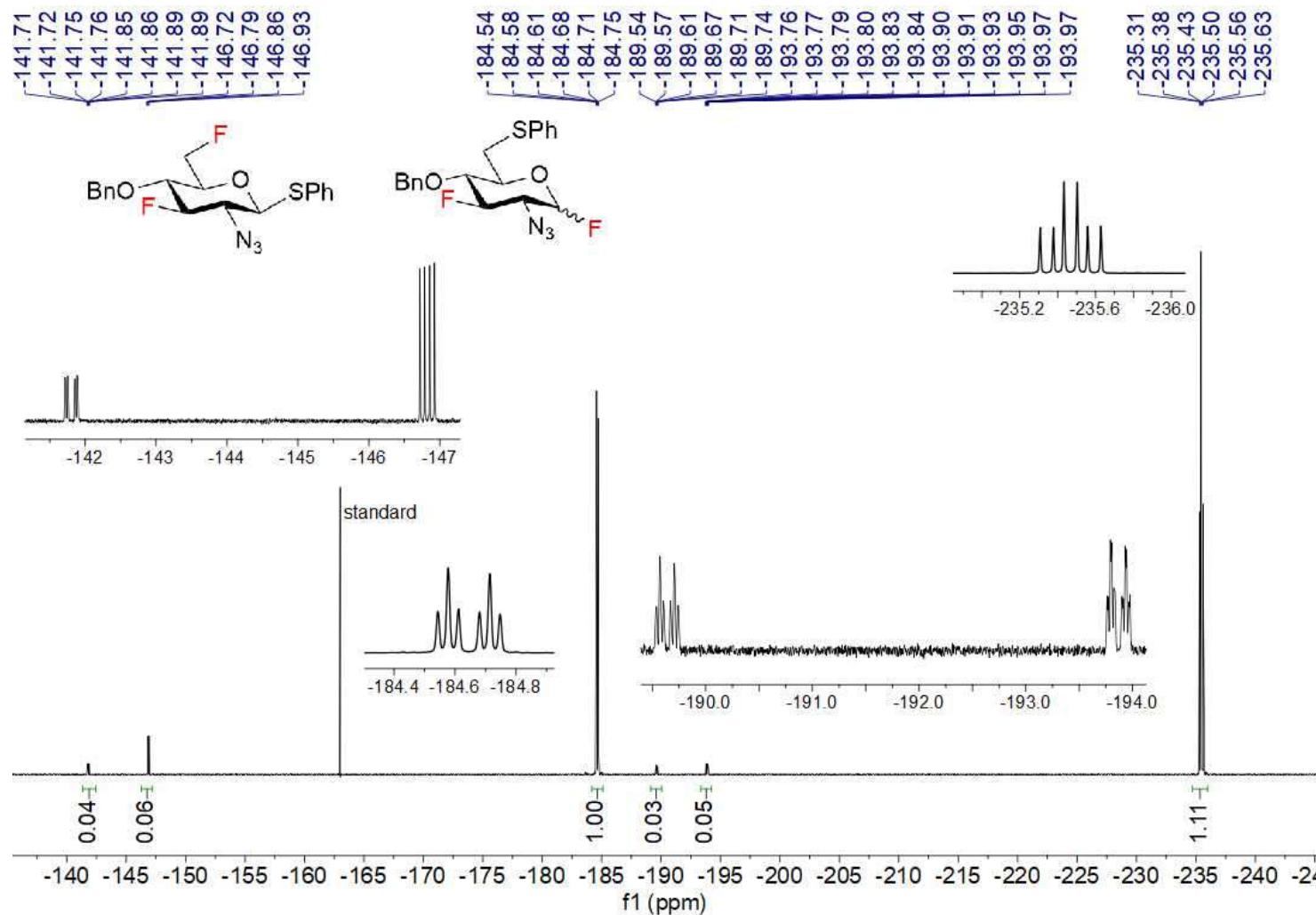
¹H NMR (400 MHz, CDCl₃) 34 (ca. 9% of 35)



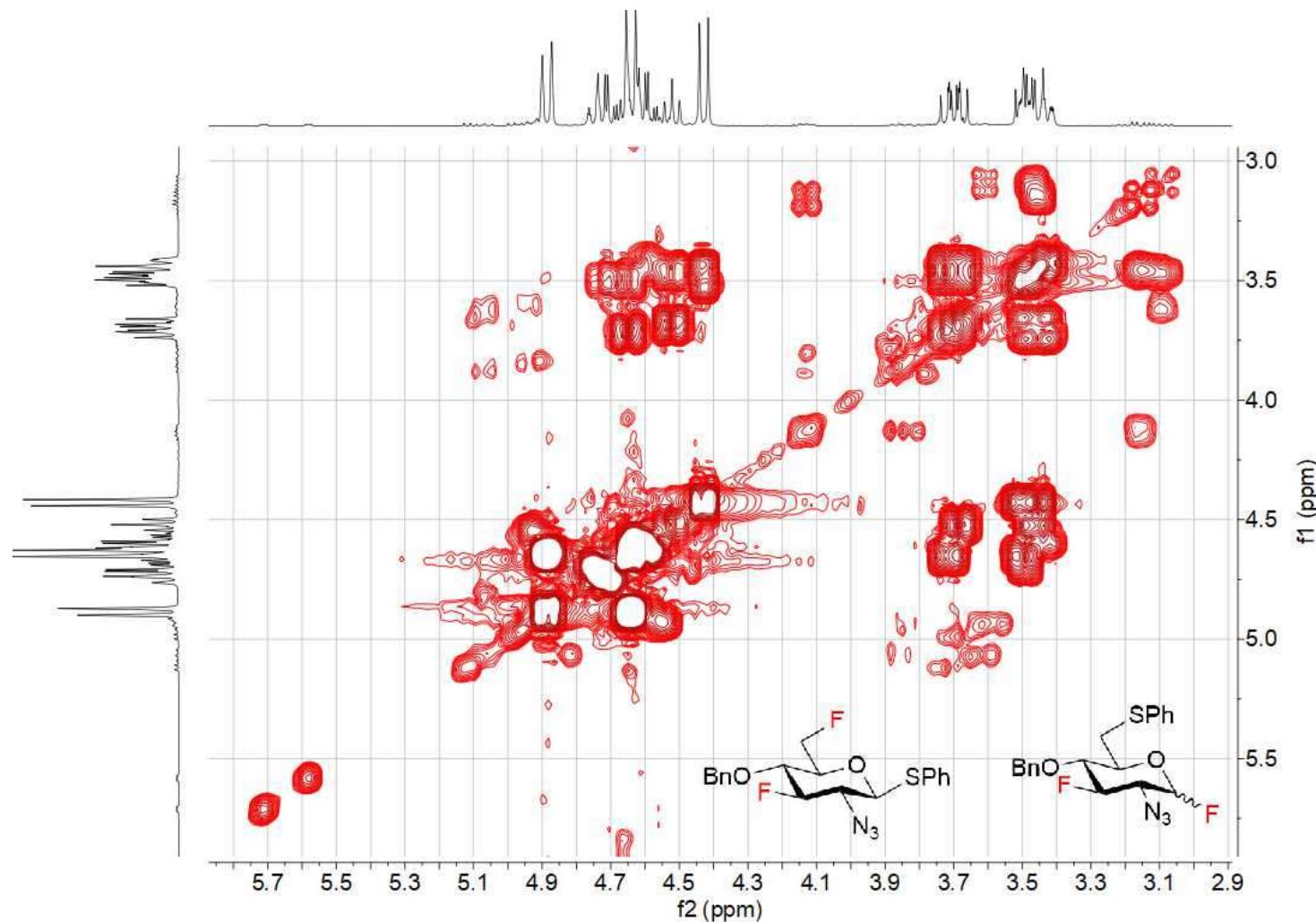
¹³C NMR (100 MHz, CDCl₃) 34



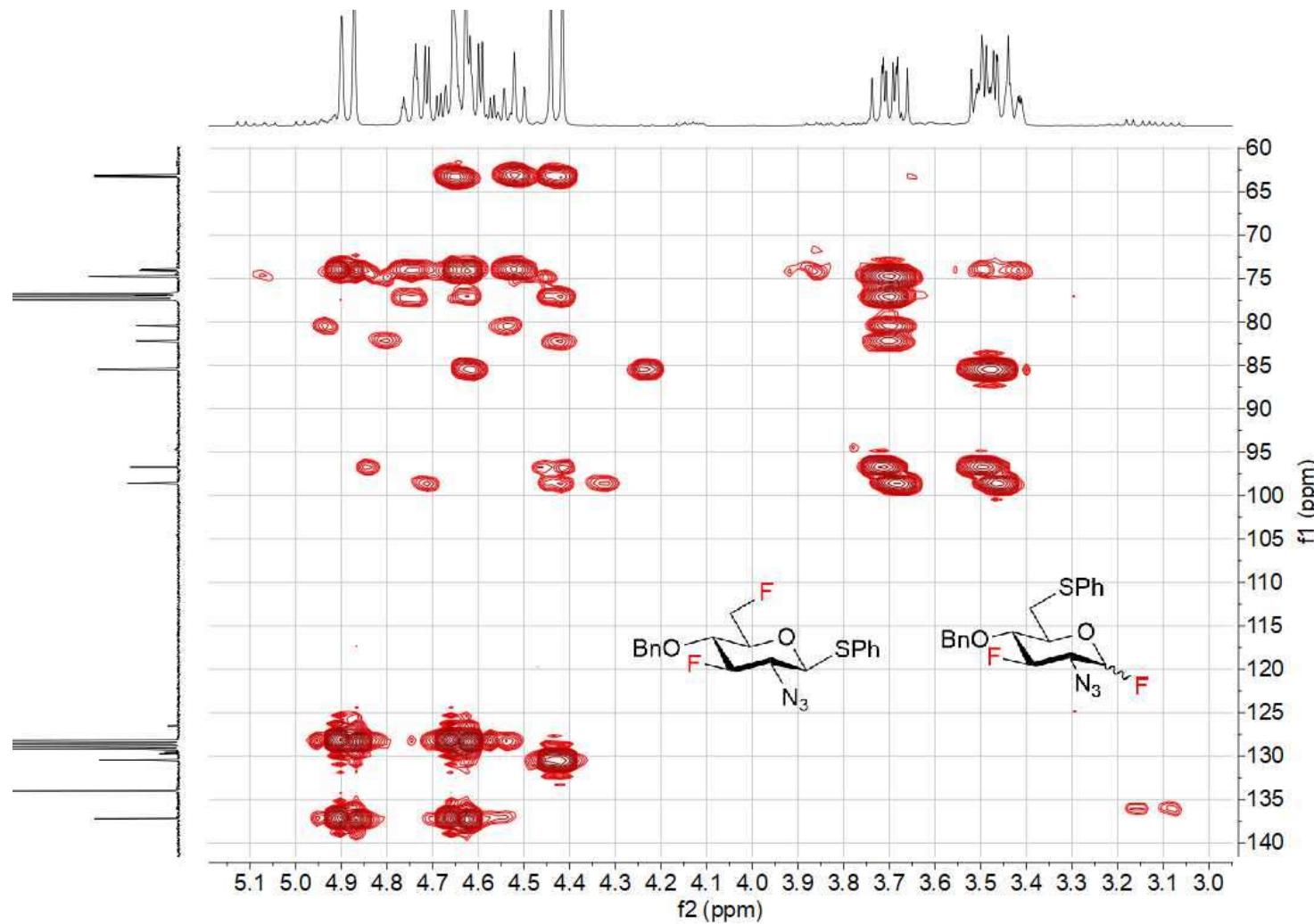
¹⁹F NMR (376 MHz, CDCl₃) 34 (ca. 5% of α -35 and 4% of β -35)



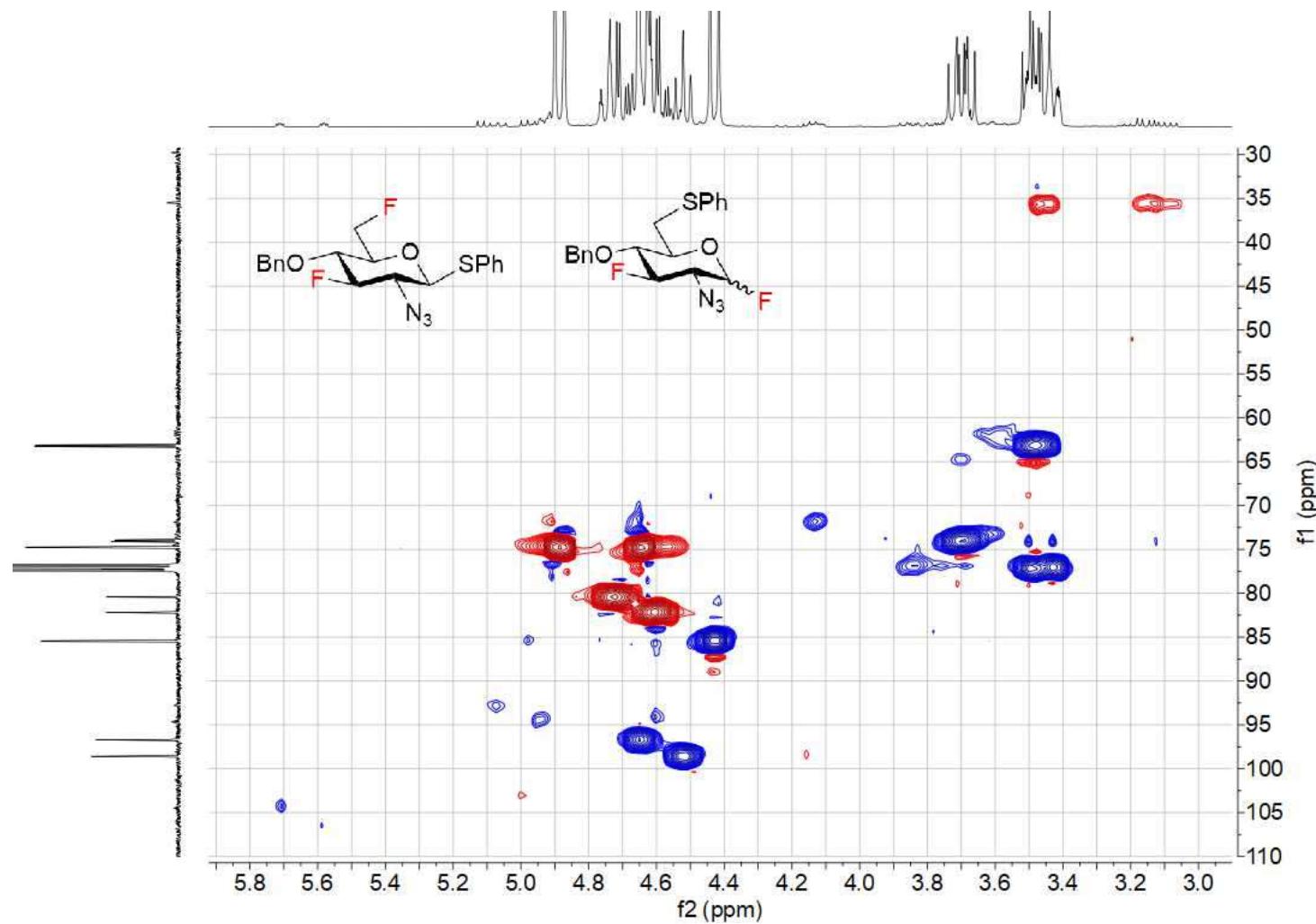
^1H - ^1H COSY 34 (ca. 9% of 35)



¹H-¹³C HMBC 34 (ca. 9% of 35)

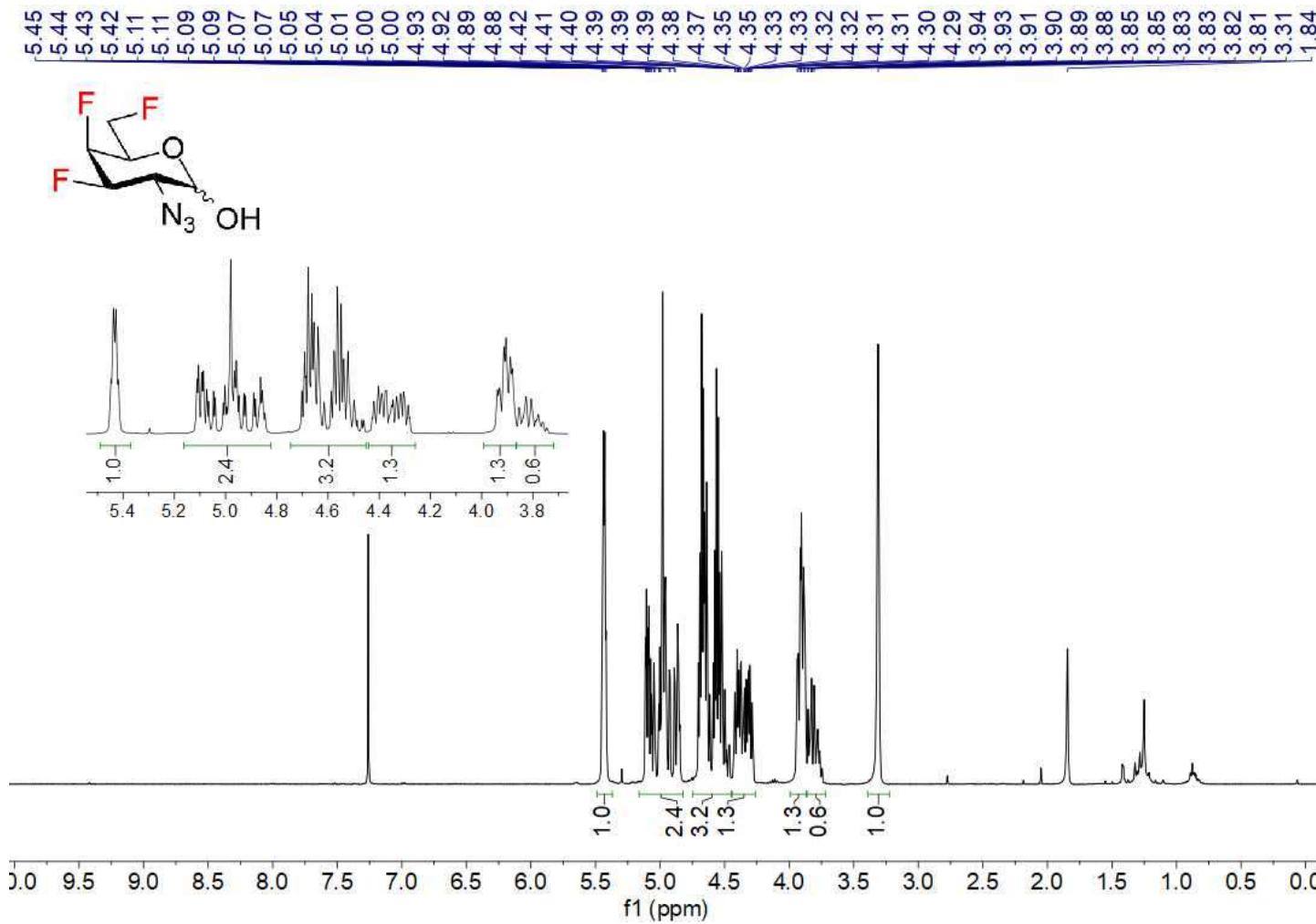


¹H-¹³C HSQC 34 (ca. 9% of 35)

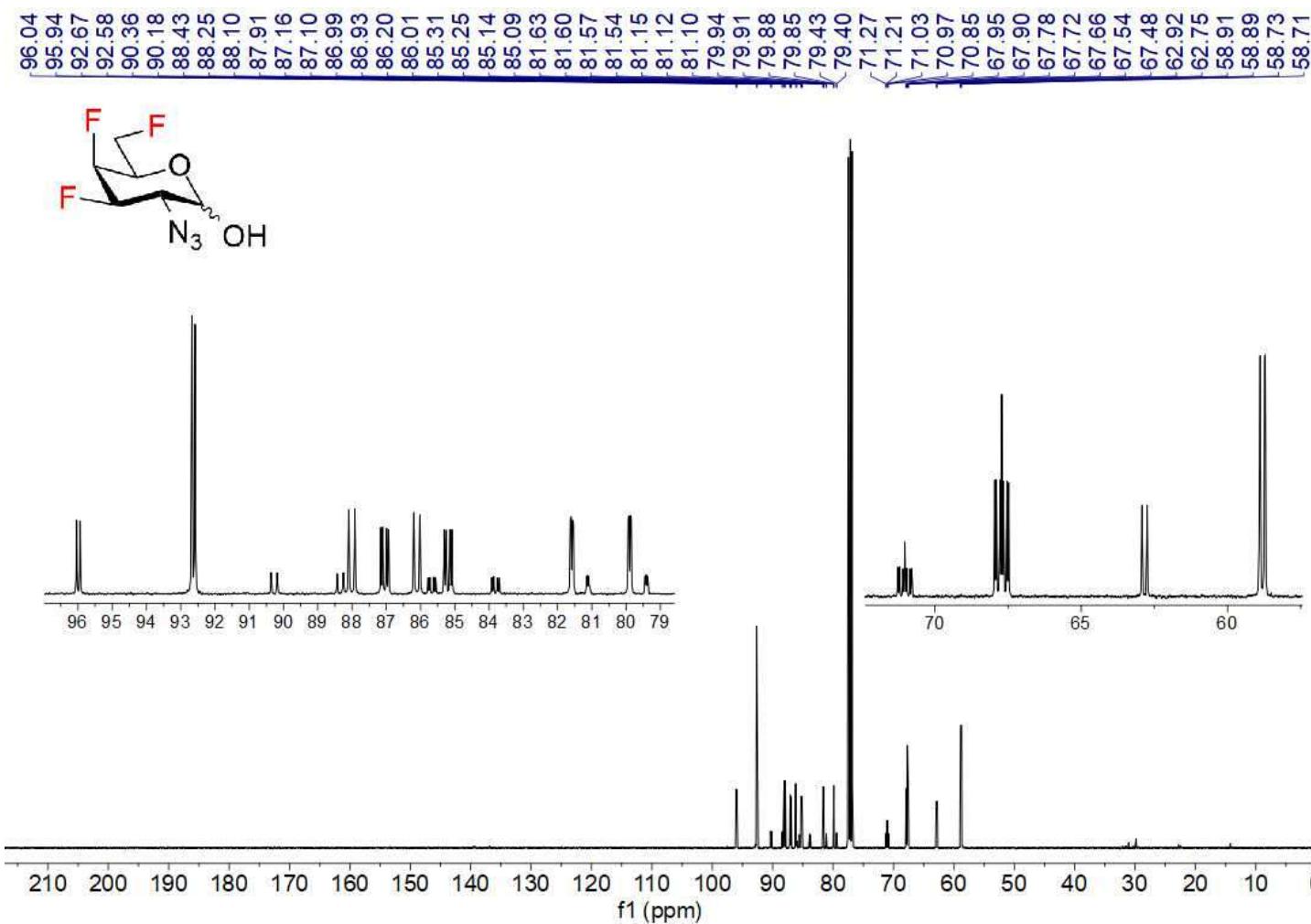


NMR COMPOUND 36

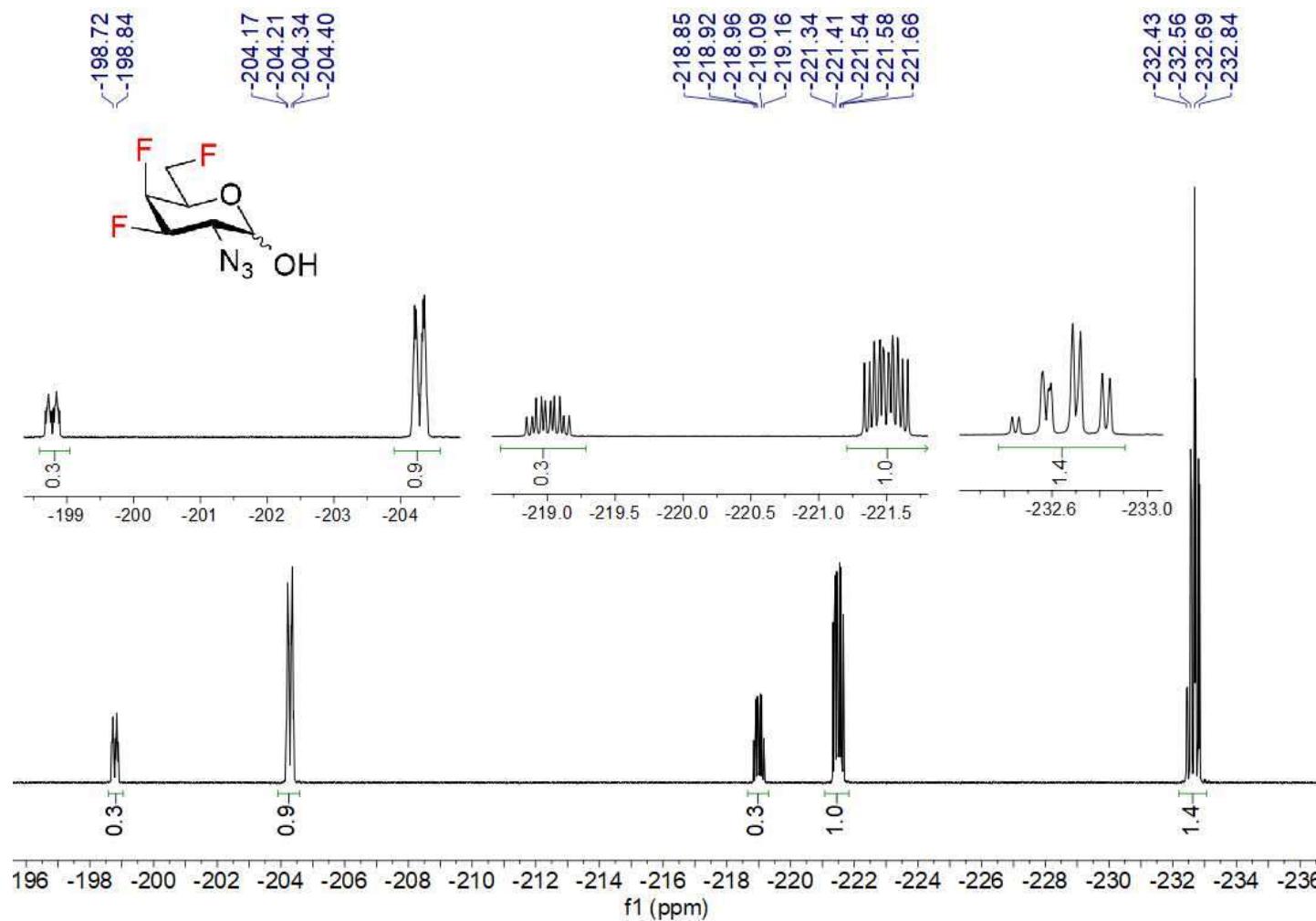
¹H NMR (400 MHz, CDCl₃) 36 (α/β ca. 10/3)



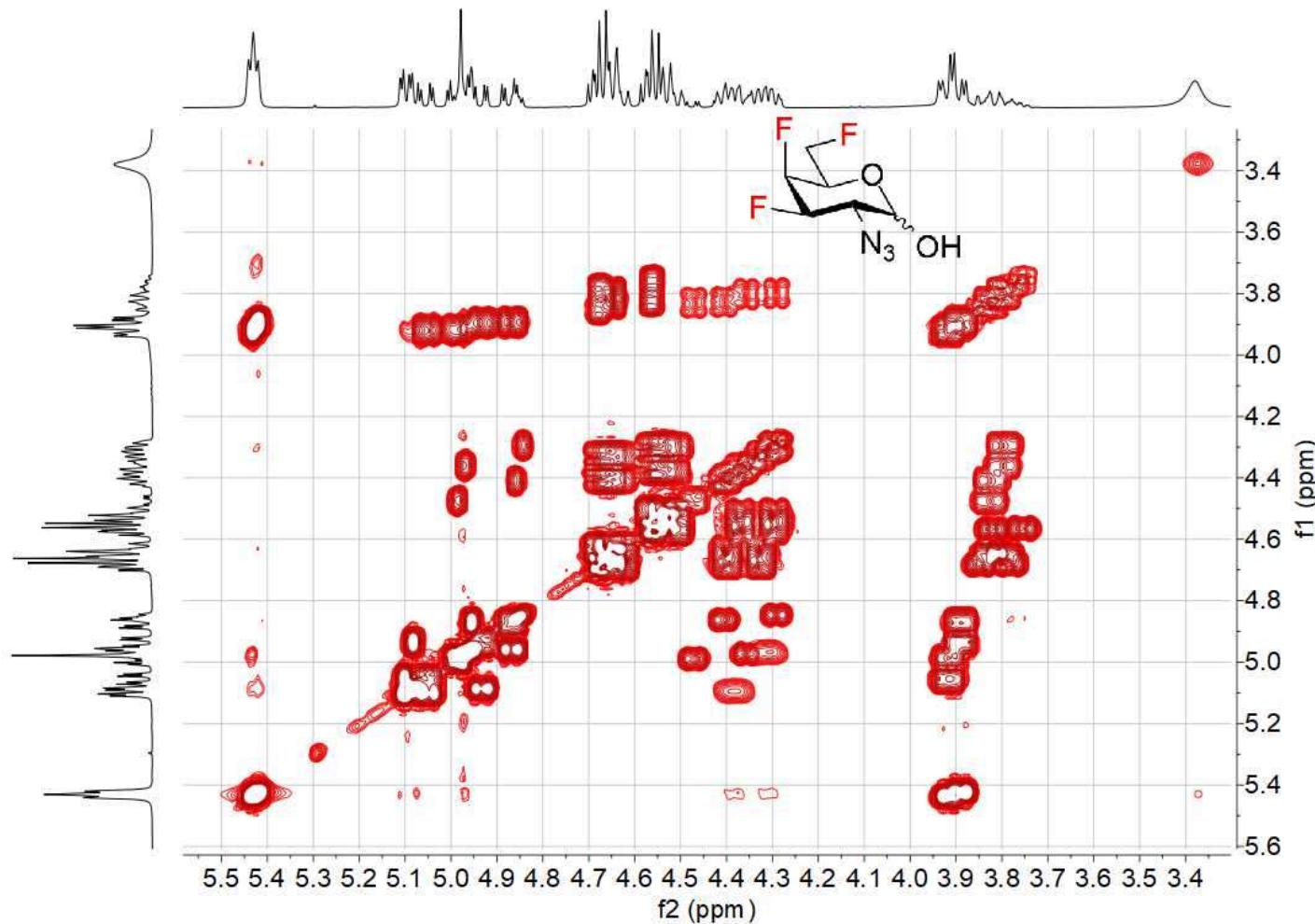
¹³C NMR (100 MHz, CDCl₃) 36



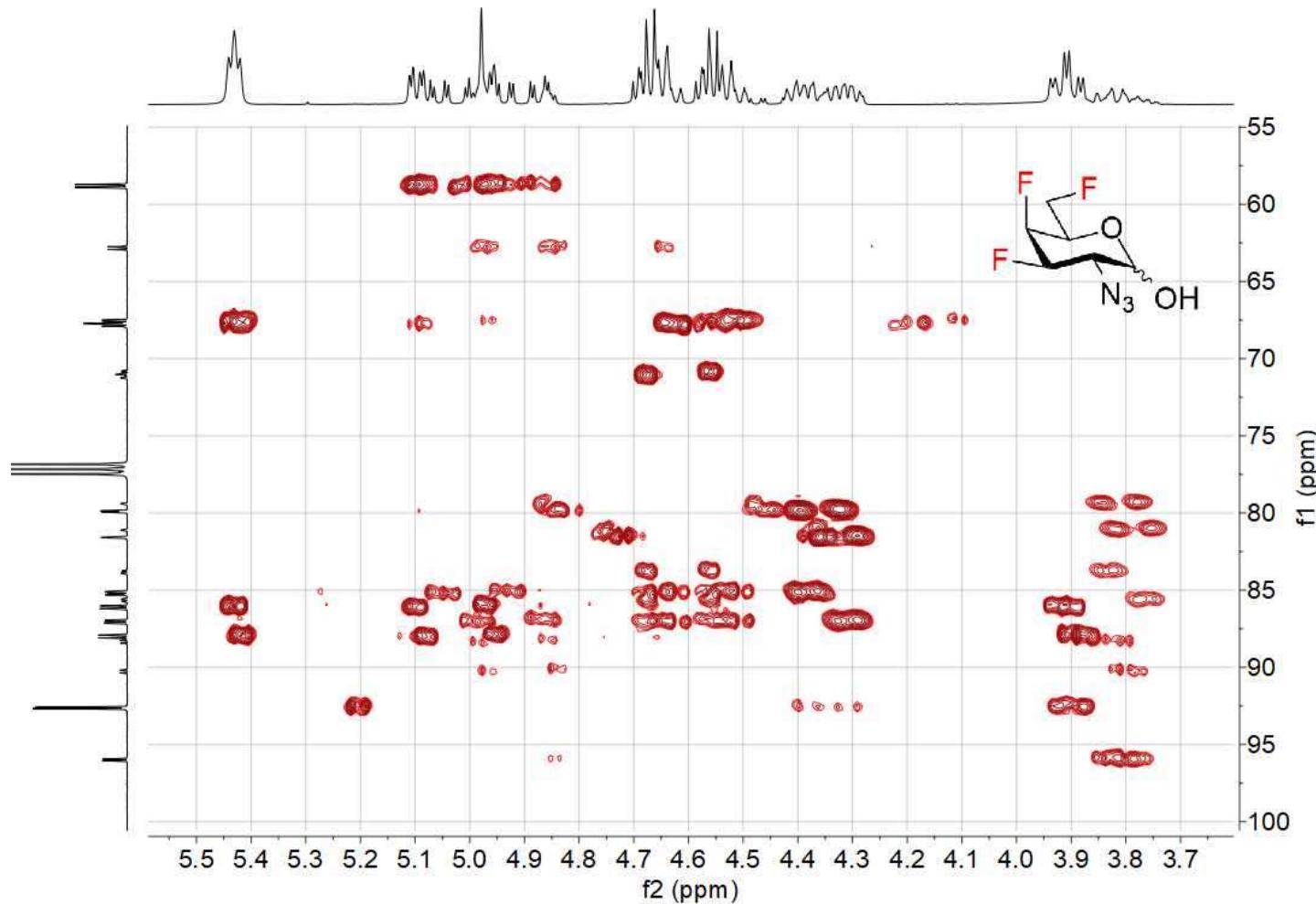
¹⁹F NMR (376 MHz, CDCl₃) 36 (α/β ca. 10/3)



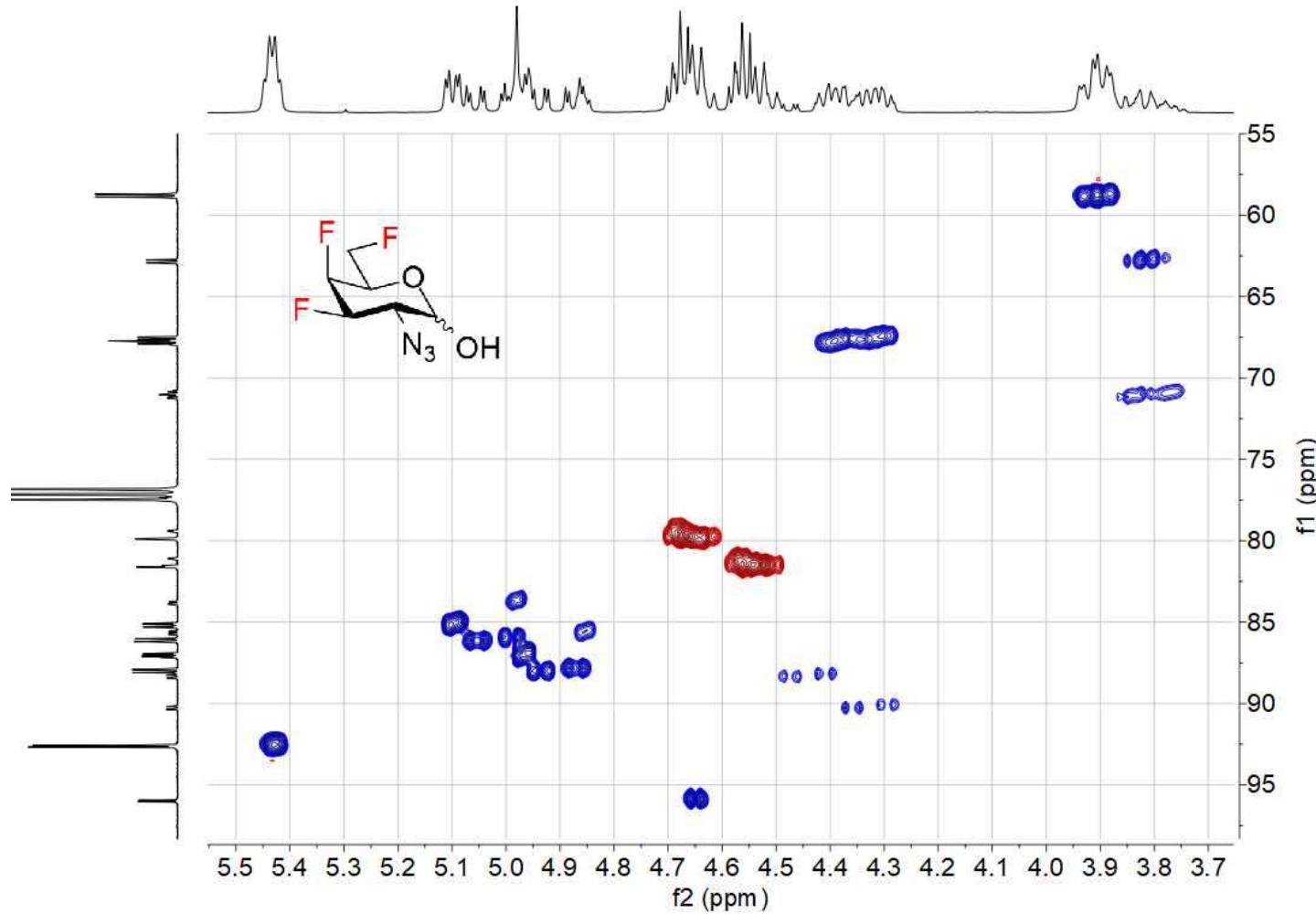
¹H-¹H COSY 36



^1H - ^{13}C HMBC 36

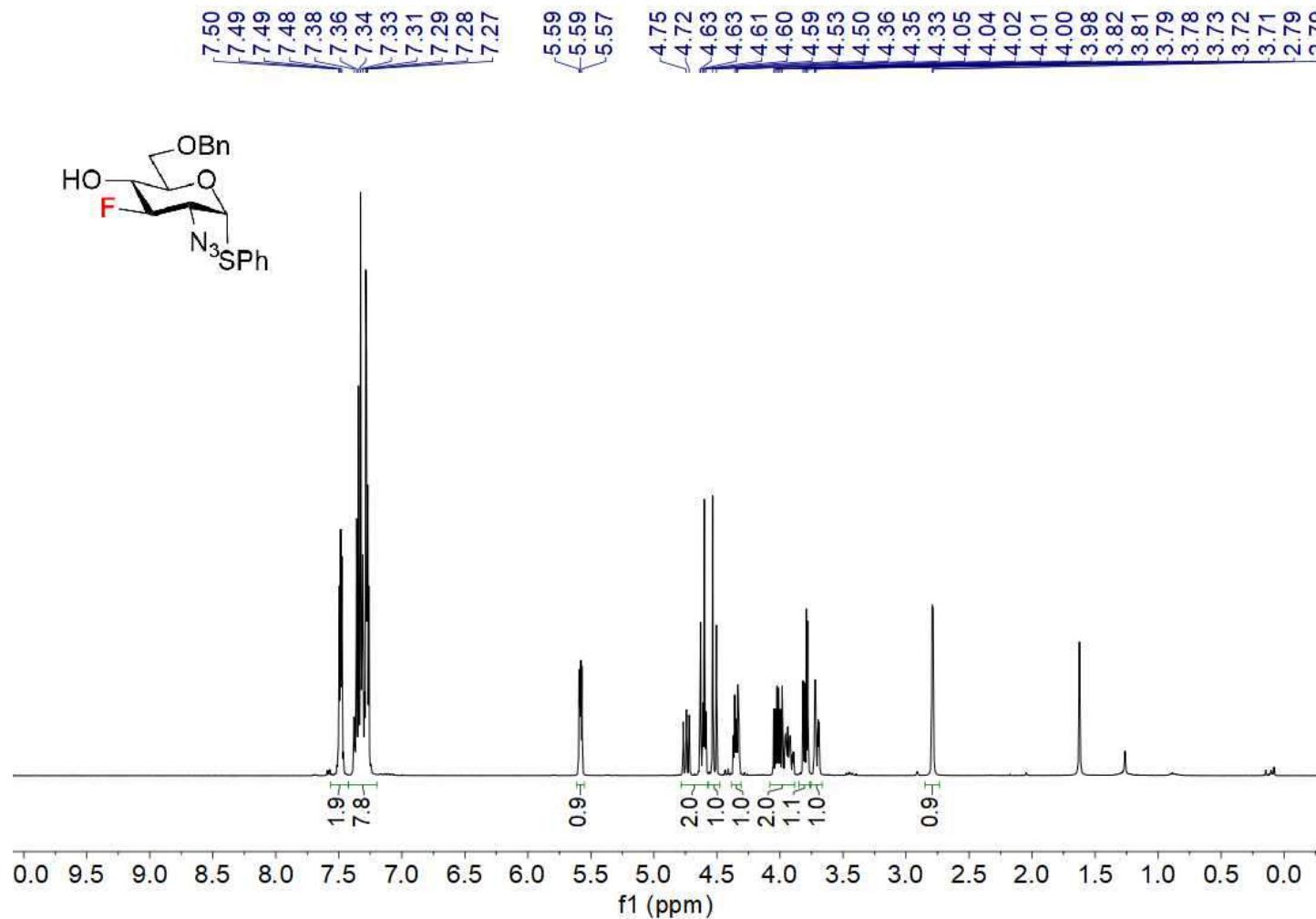


¹H-¹³C HSQC 36

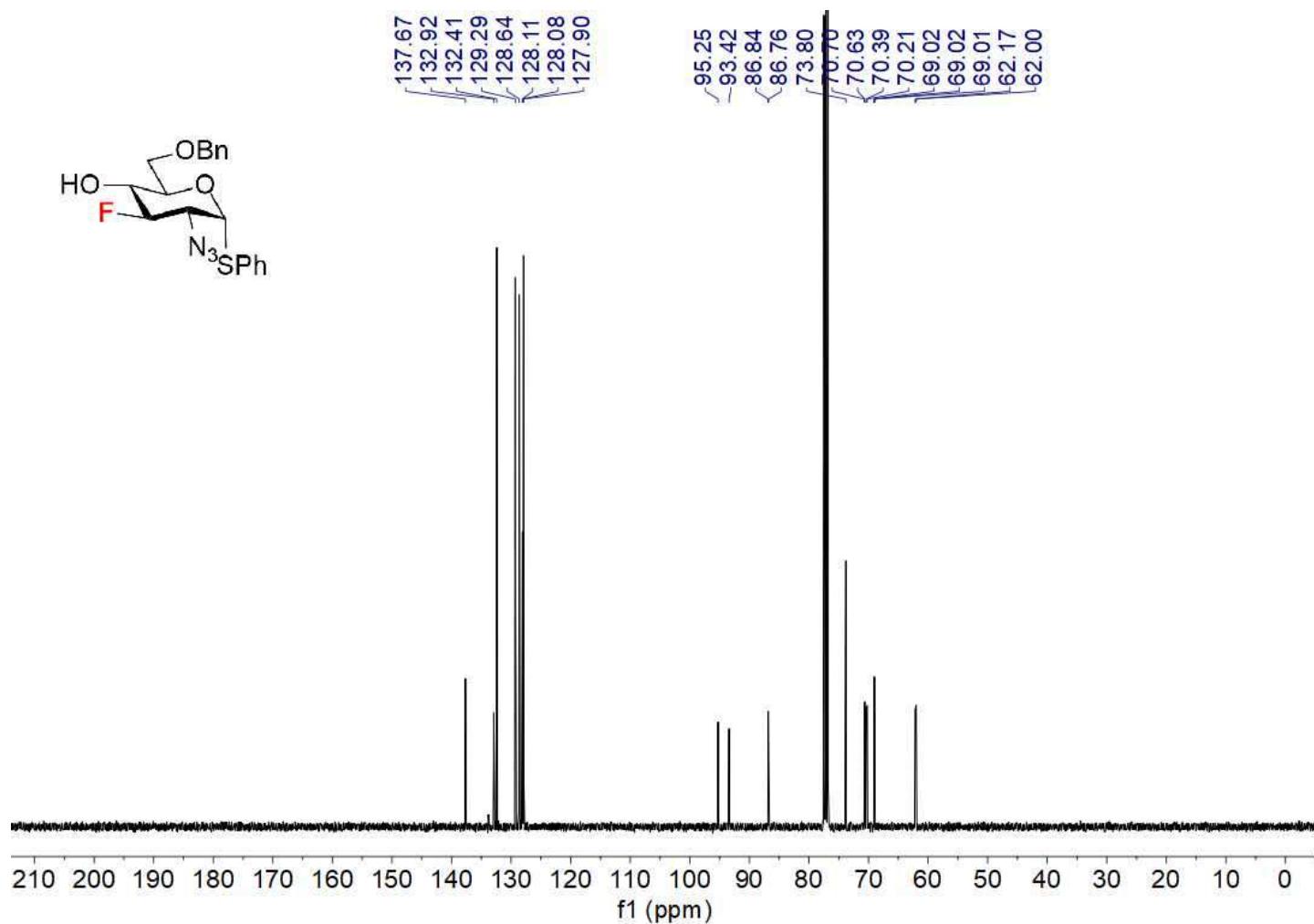


NMR COMPOUND α -37

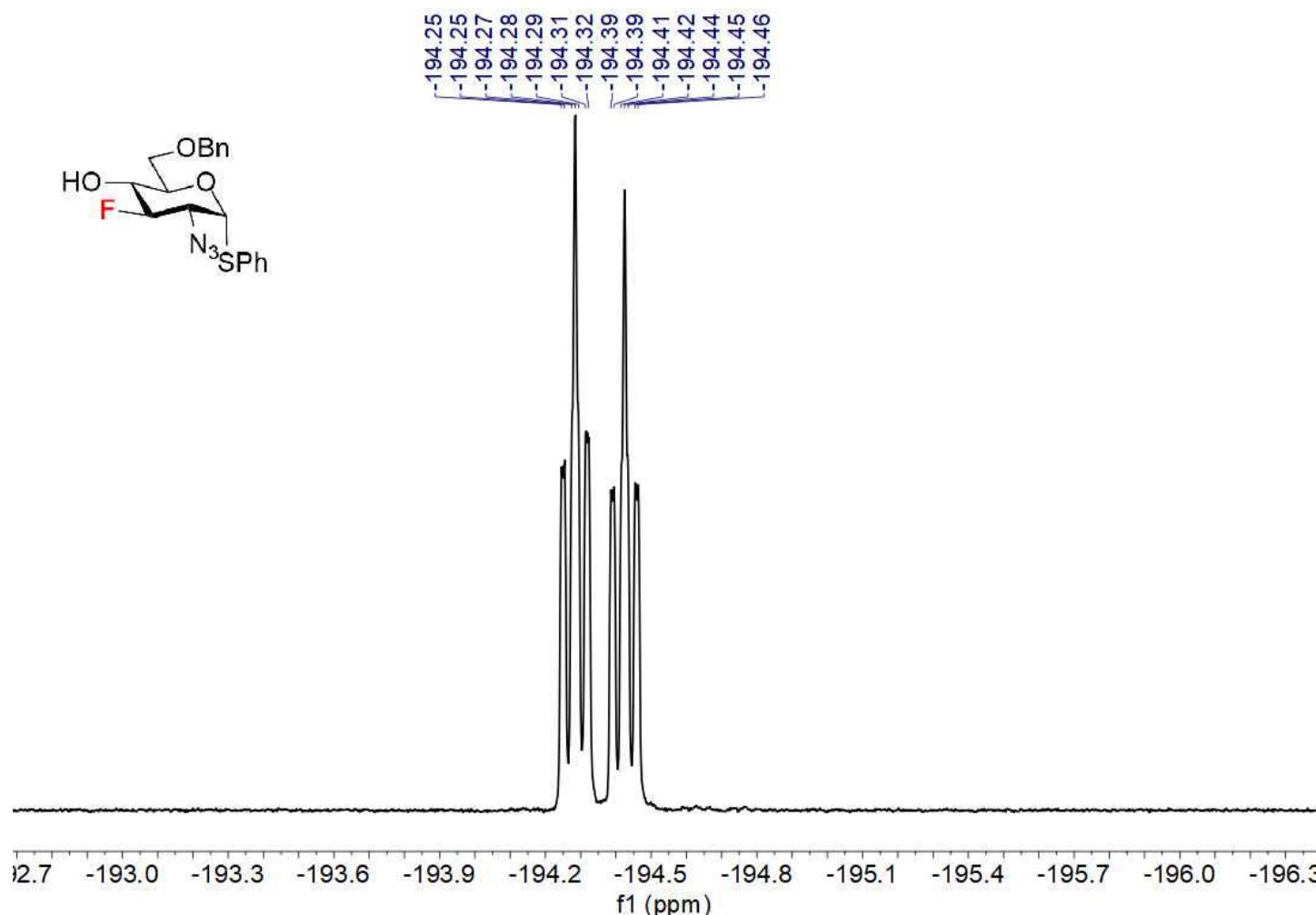
^1H NMR (400 MHz, CDCl_3) α -37



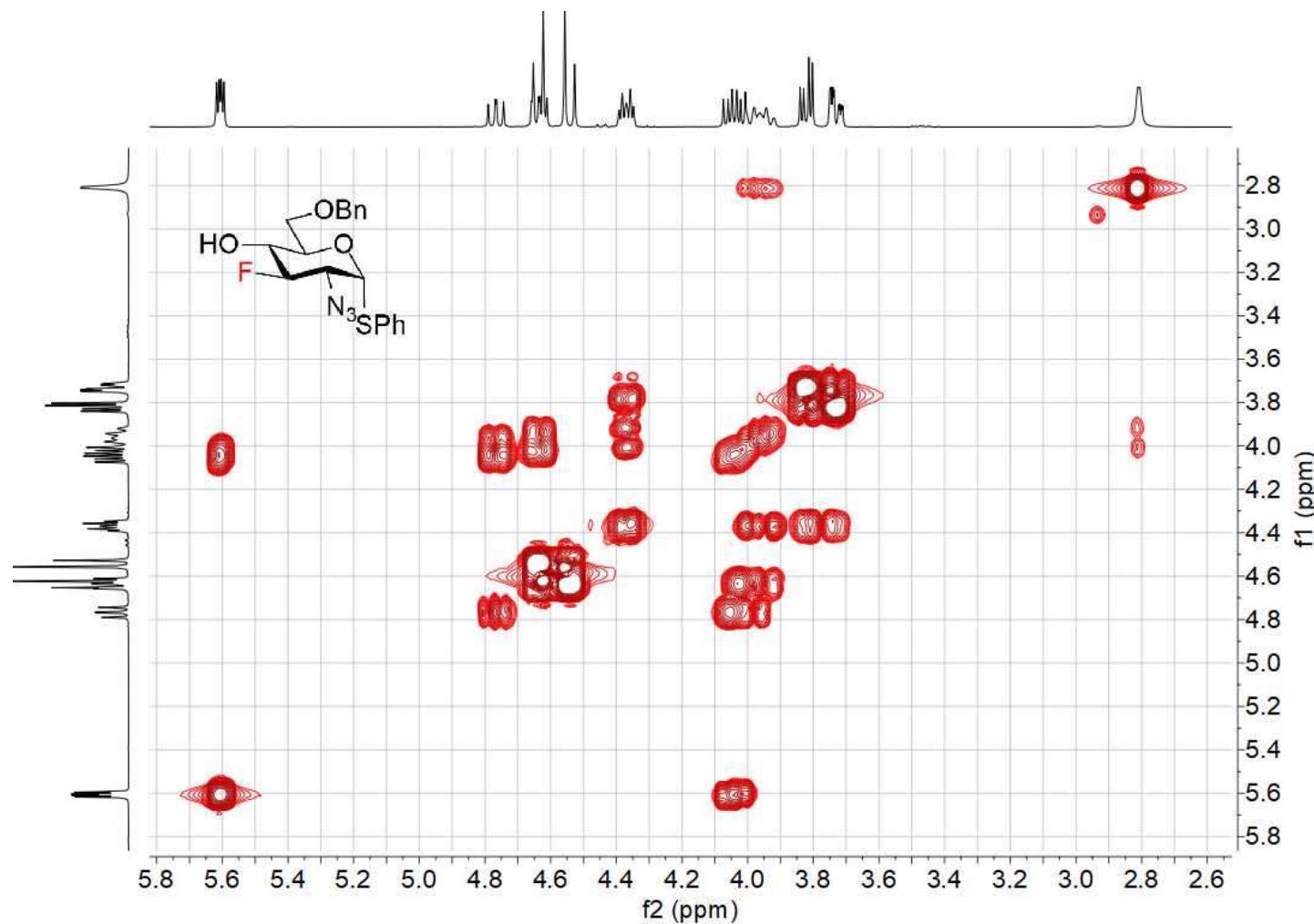
¹³C NMR (100 MHz, CDCl₃) *a*-37



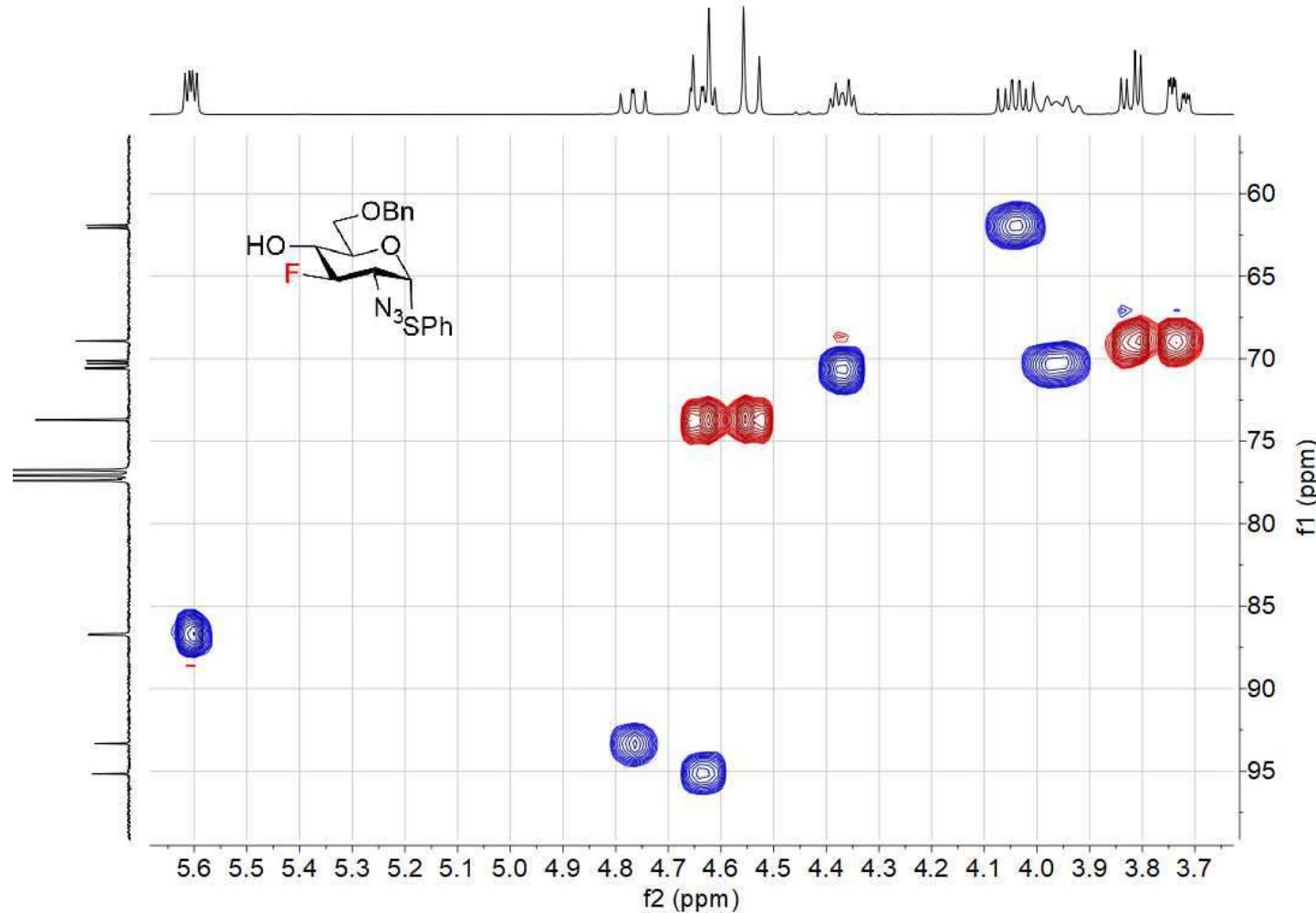
¹⁹F NMR (376 MHz, CDCl₃) α -37



¹H-¹H COSY *a*-37

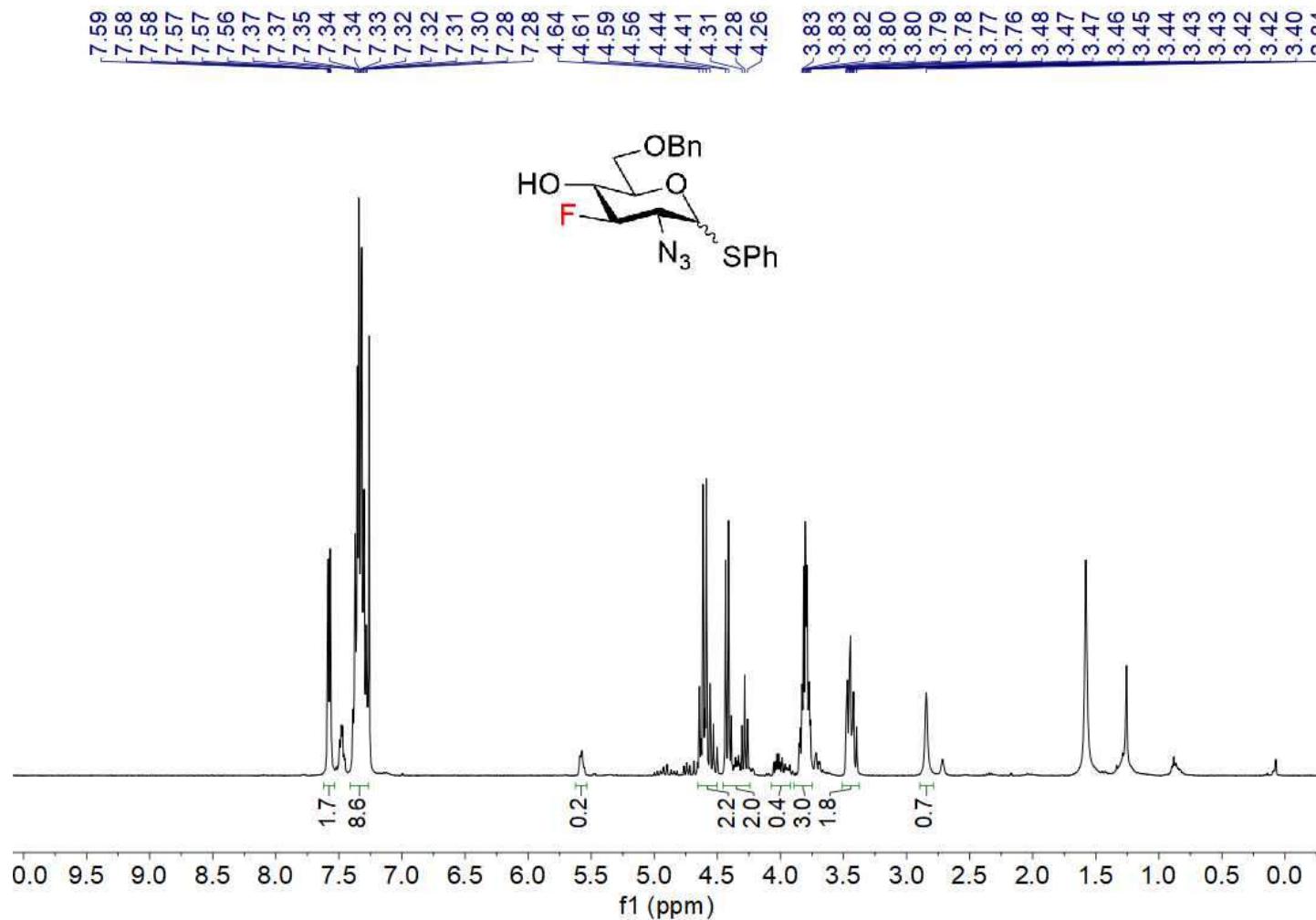


^1H - ^{13}C HSQC *a*-37

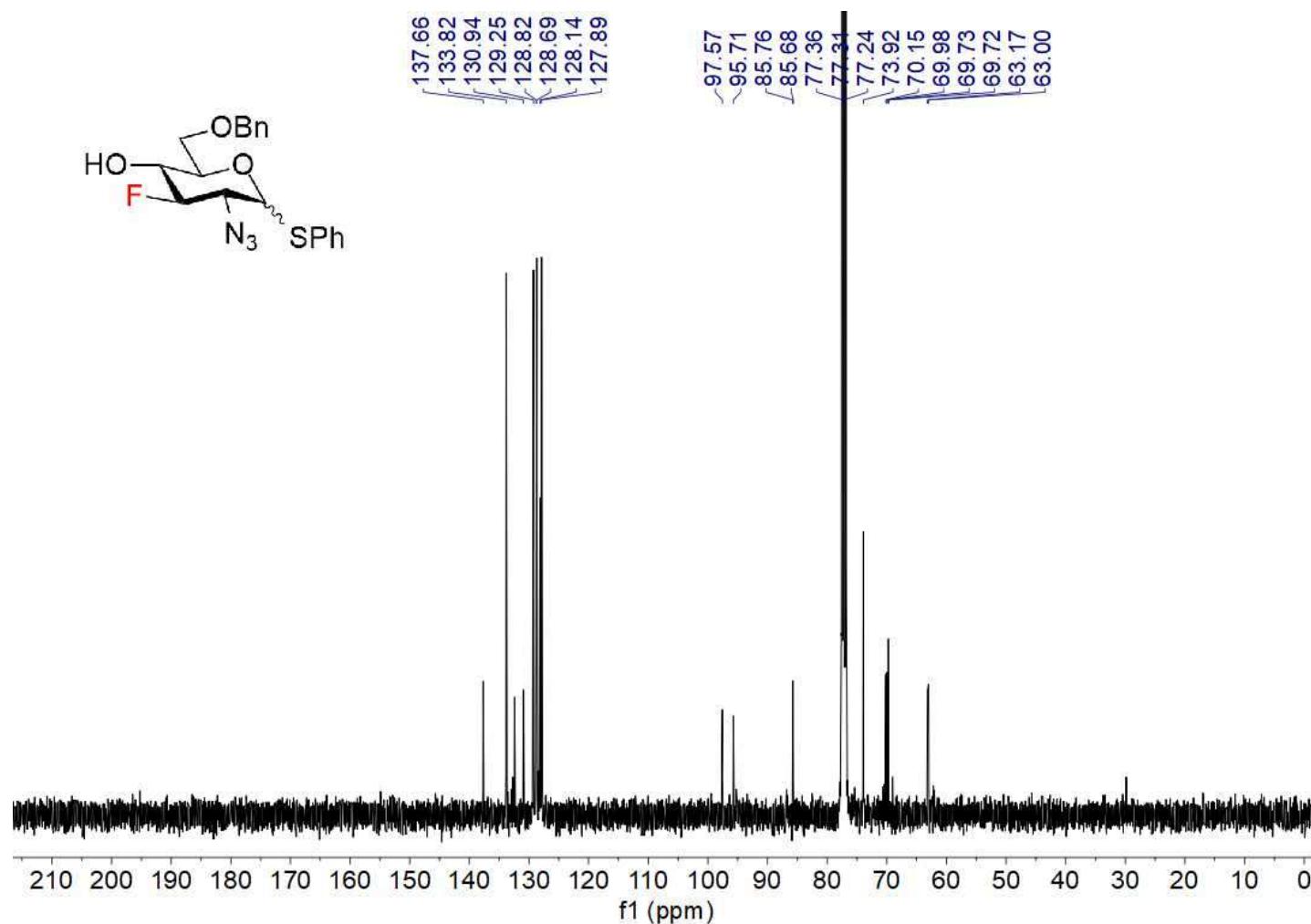


NMR COMPOUND 37 (α/β ca. 1/5)

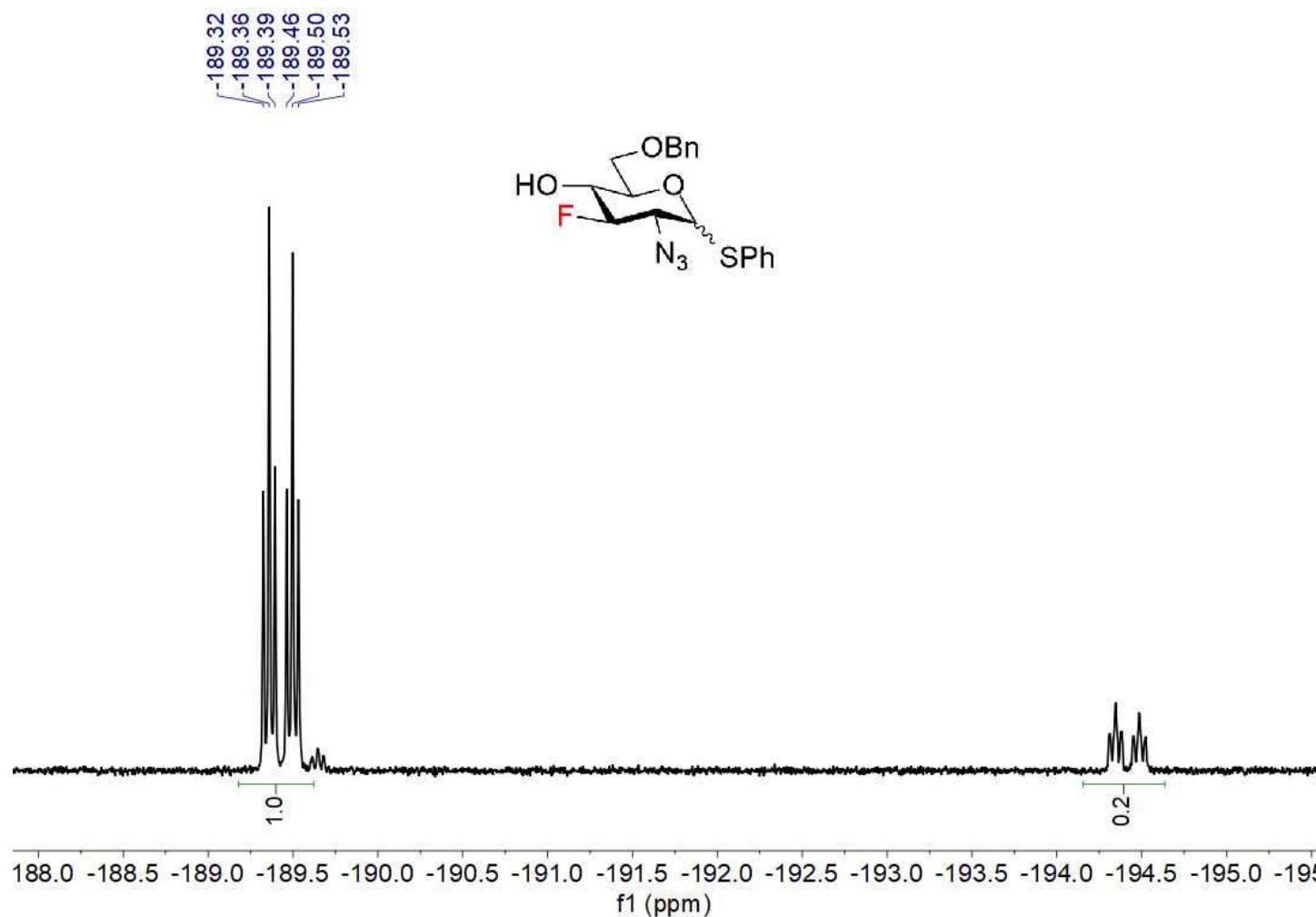
^1H NMR (400 MHz, CDCl_3) 37 (α/β ca. 1/5)



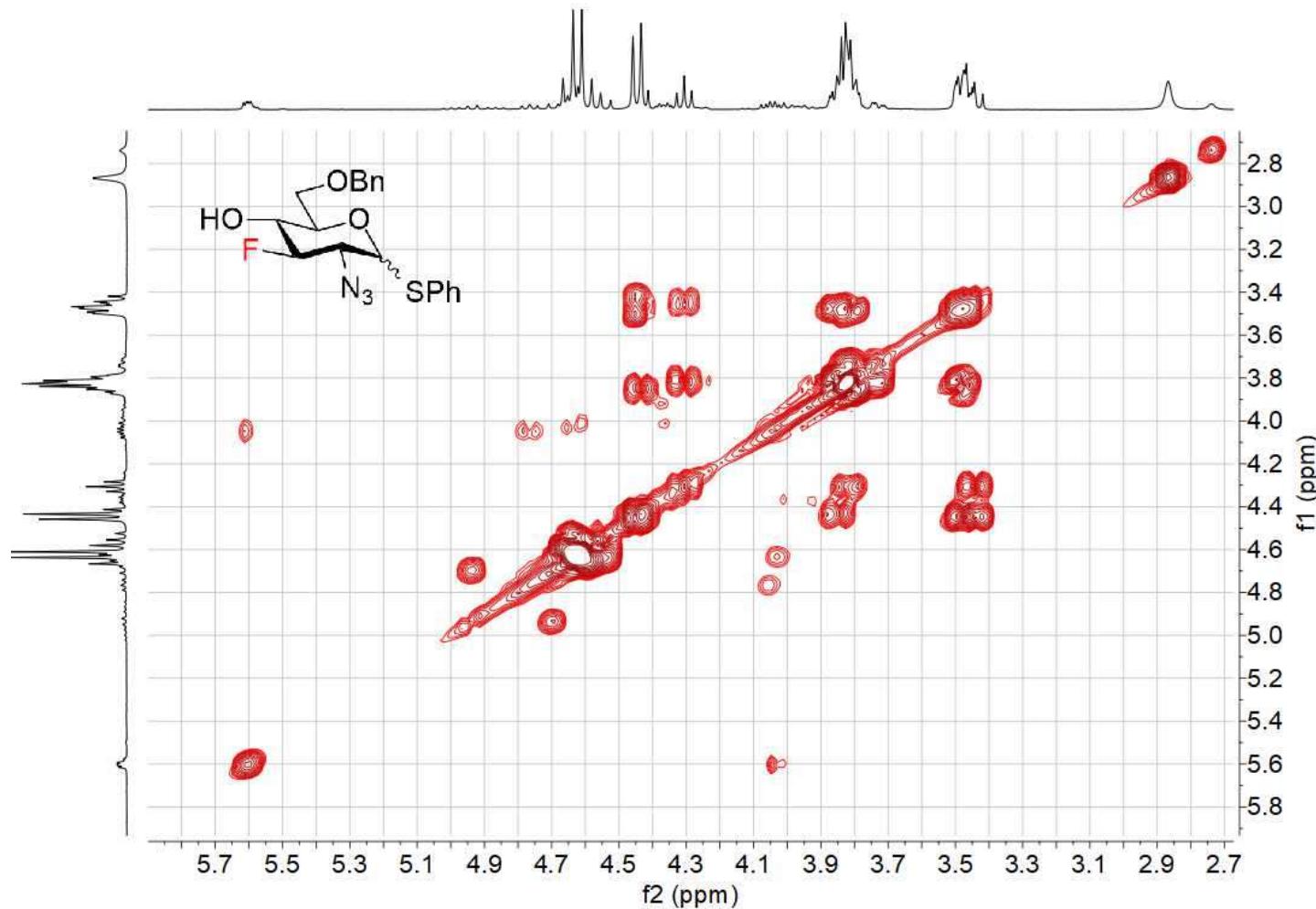
¹³C NMR (100 MHz, CDCl₃) 37 (α/β ca. 1/5)



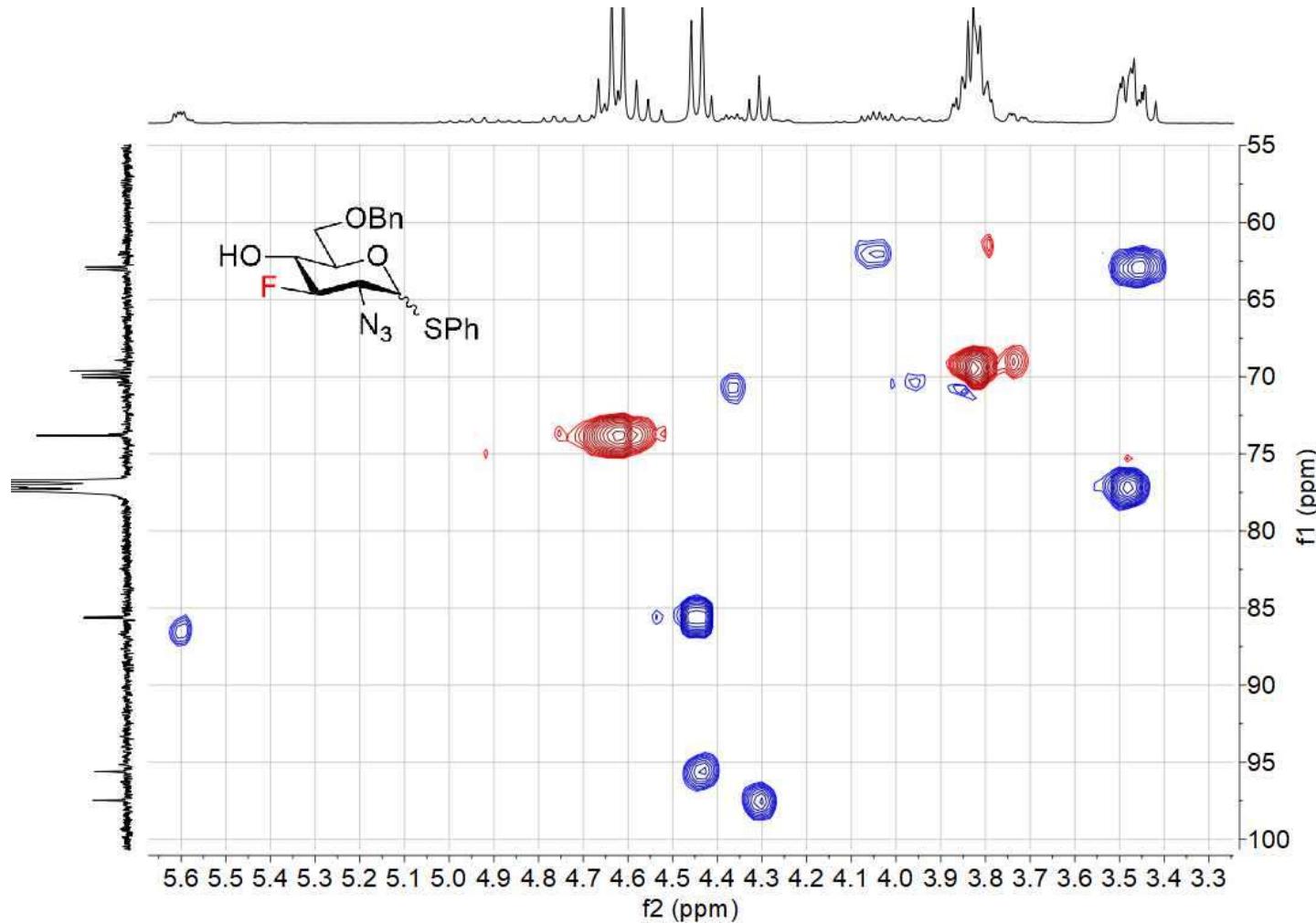
¹⁹F NMR (376 MHz, CDCl₃) 37 (α/β ca. 1/5)



^1H - ^1H COSY 37 (α/β ca. 1/5)

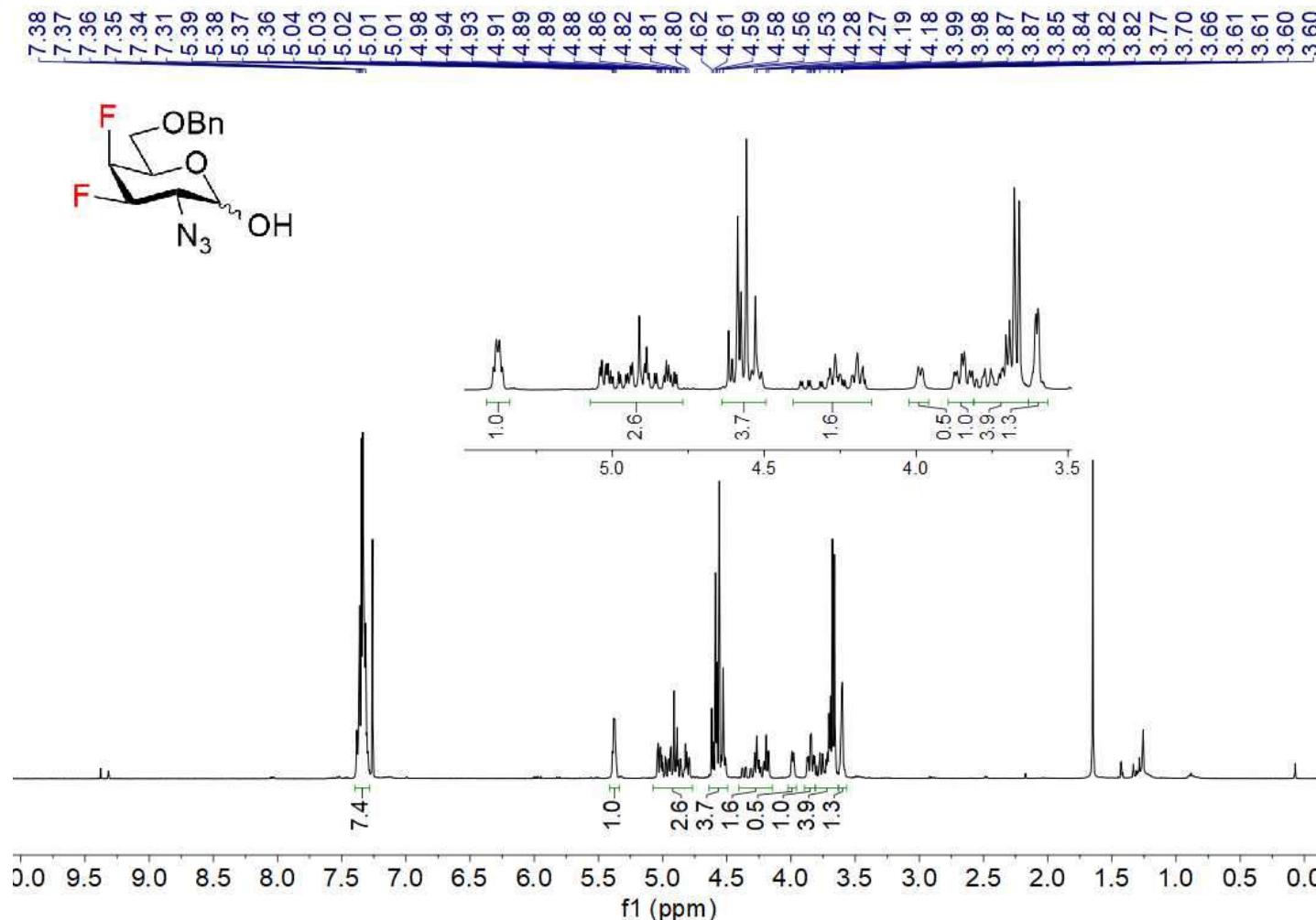


^1H - ^{13}C HSQC 37 (α/β ca. 1/5)

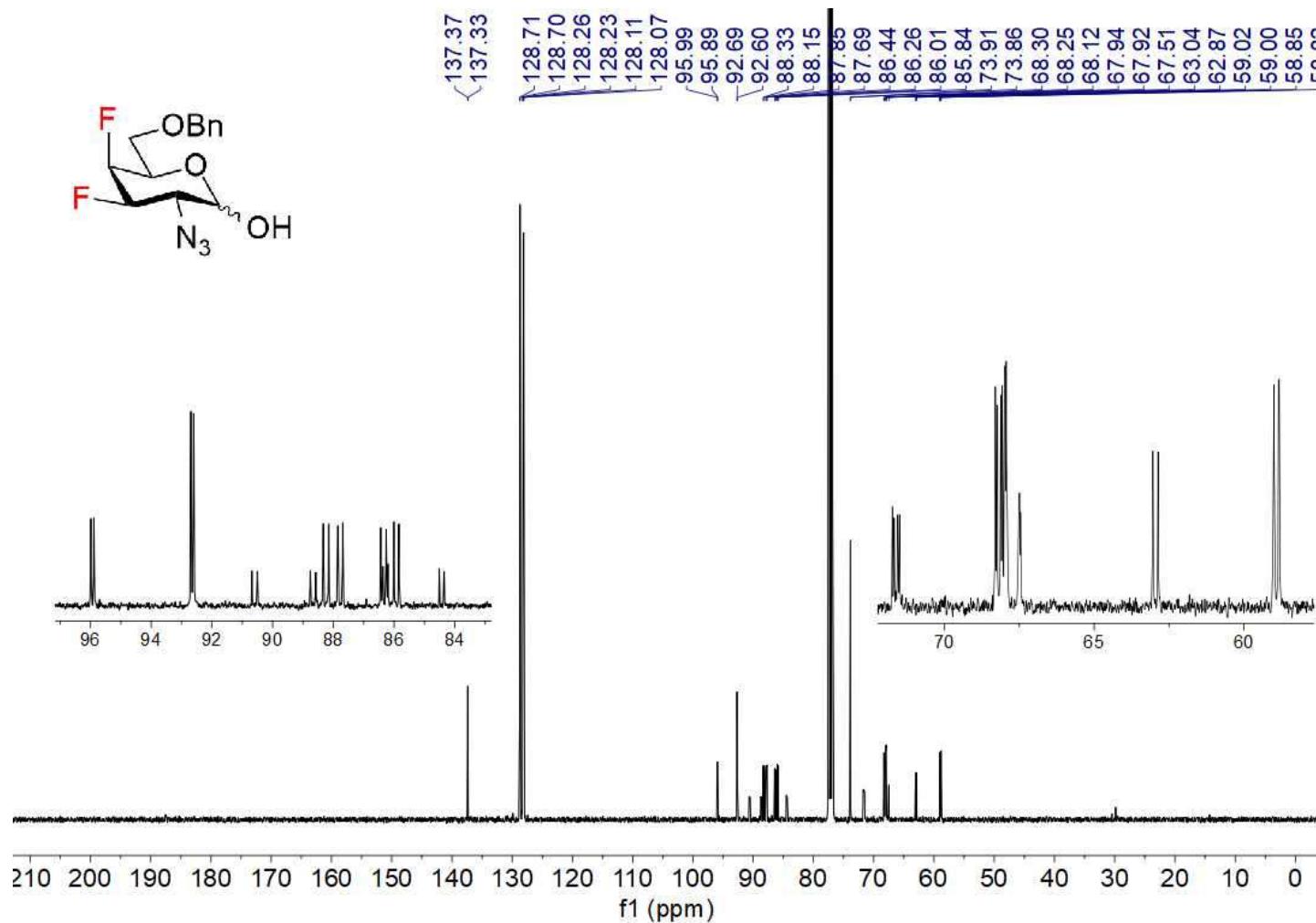


NMR COMPOUND 38

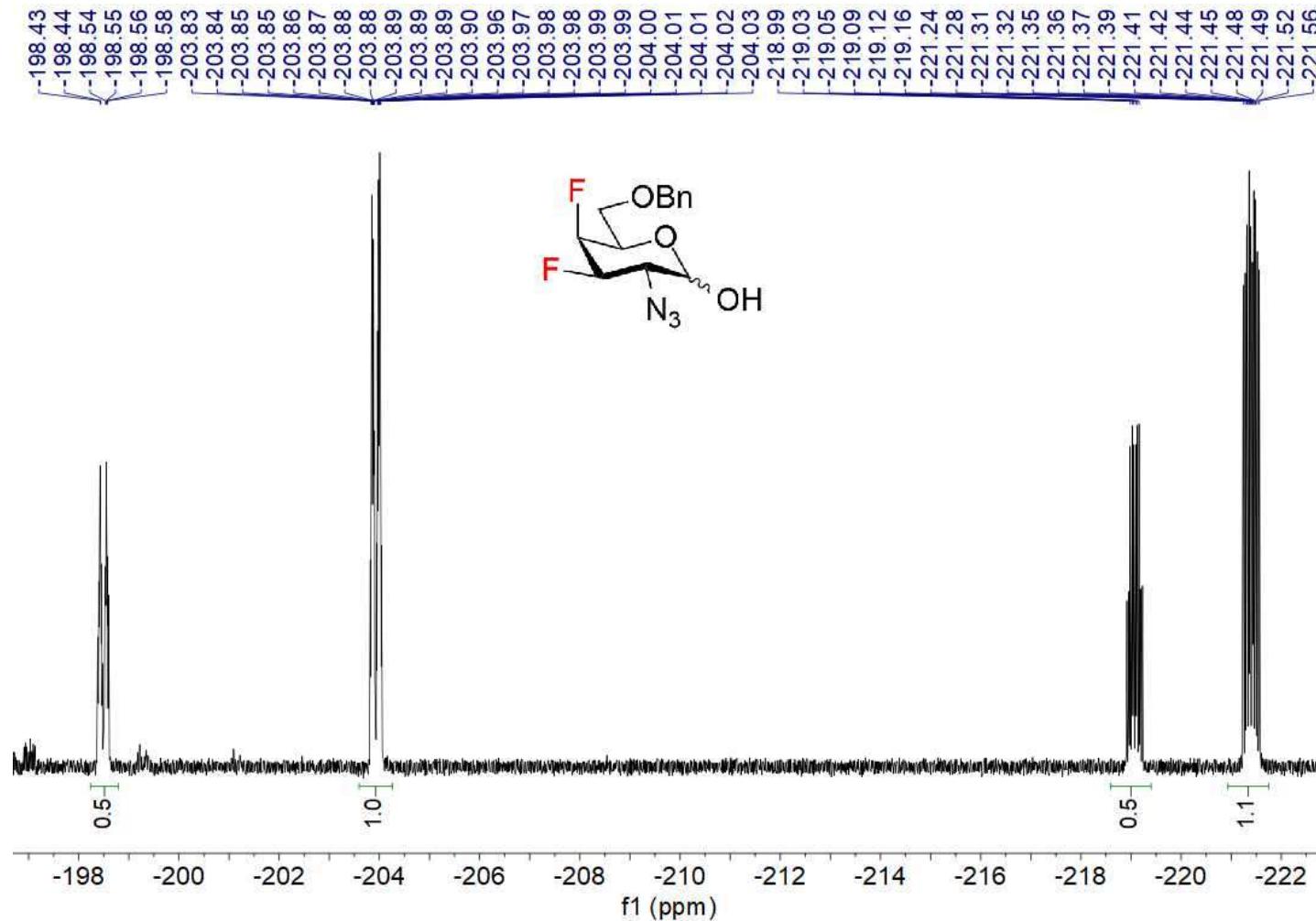
¹H NMR (400 MHz, CDCl₃) 38 (α/β ca. 2/1)



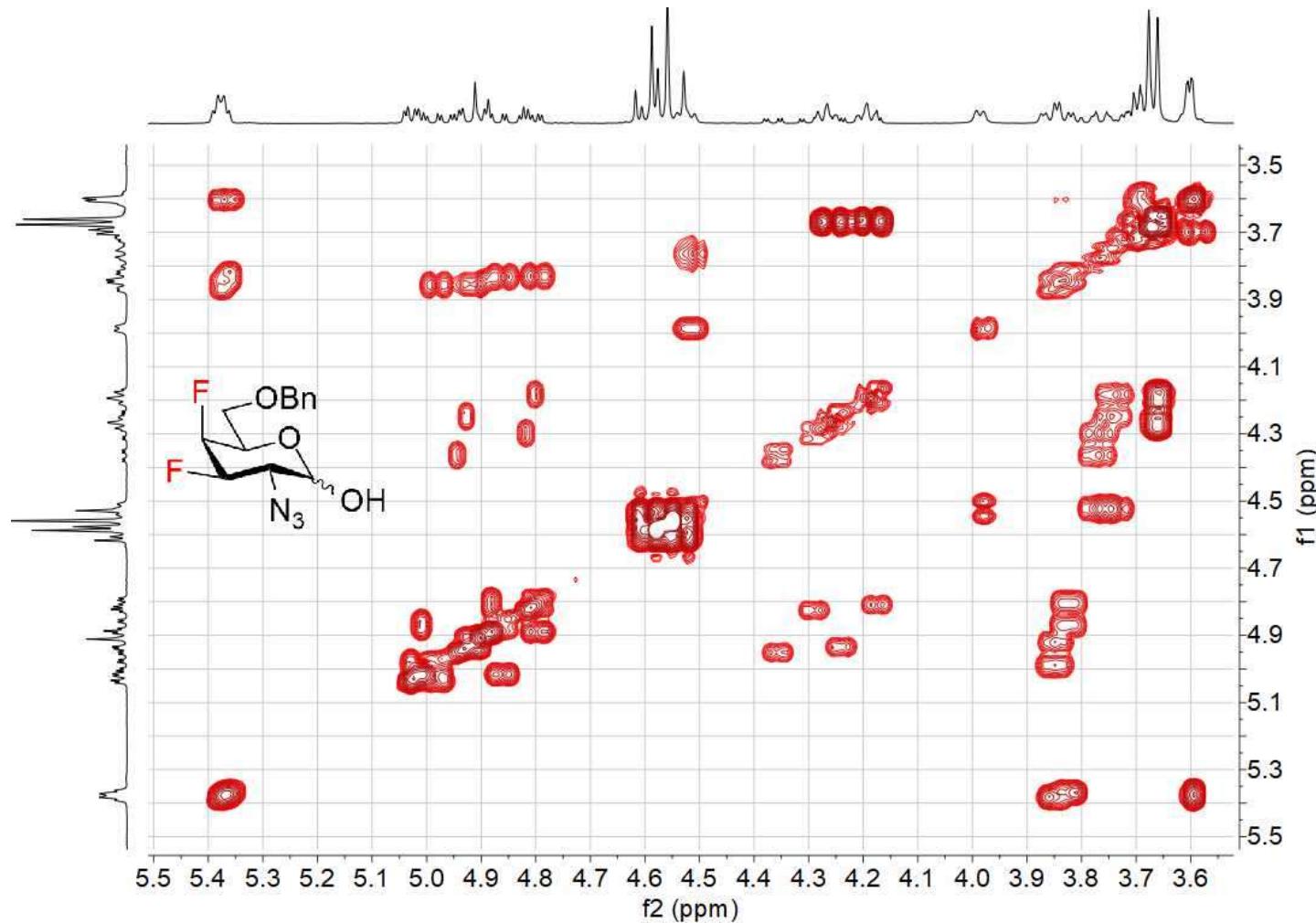
¹³C NMR (100 MHz, CDCl₃) 38



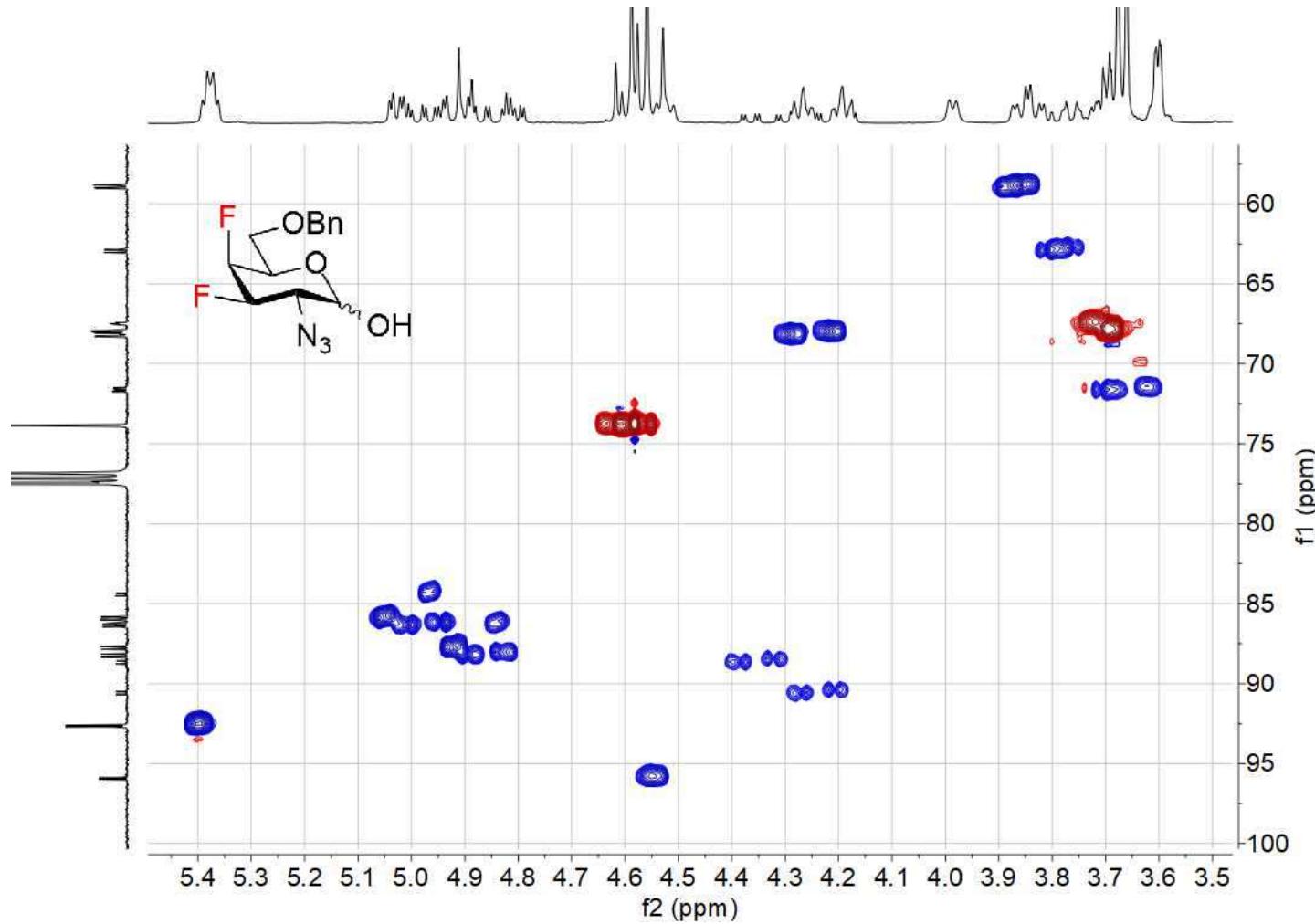
¹⁹F NMR (376 MHz, CDCl₃) 38 (α/β ca. 2/1)



¹H-¹H COSY 38

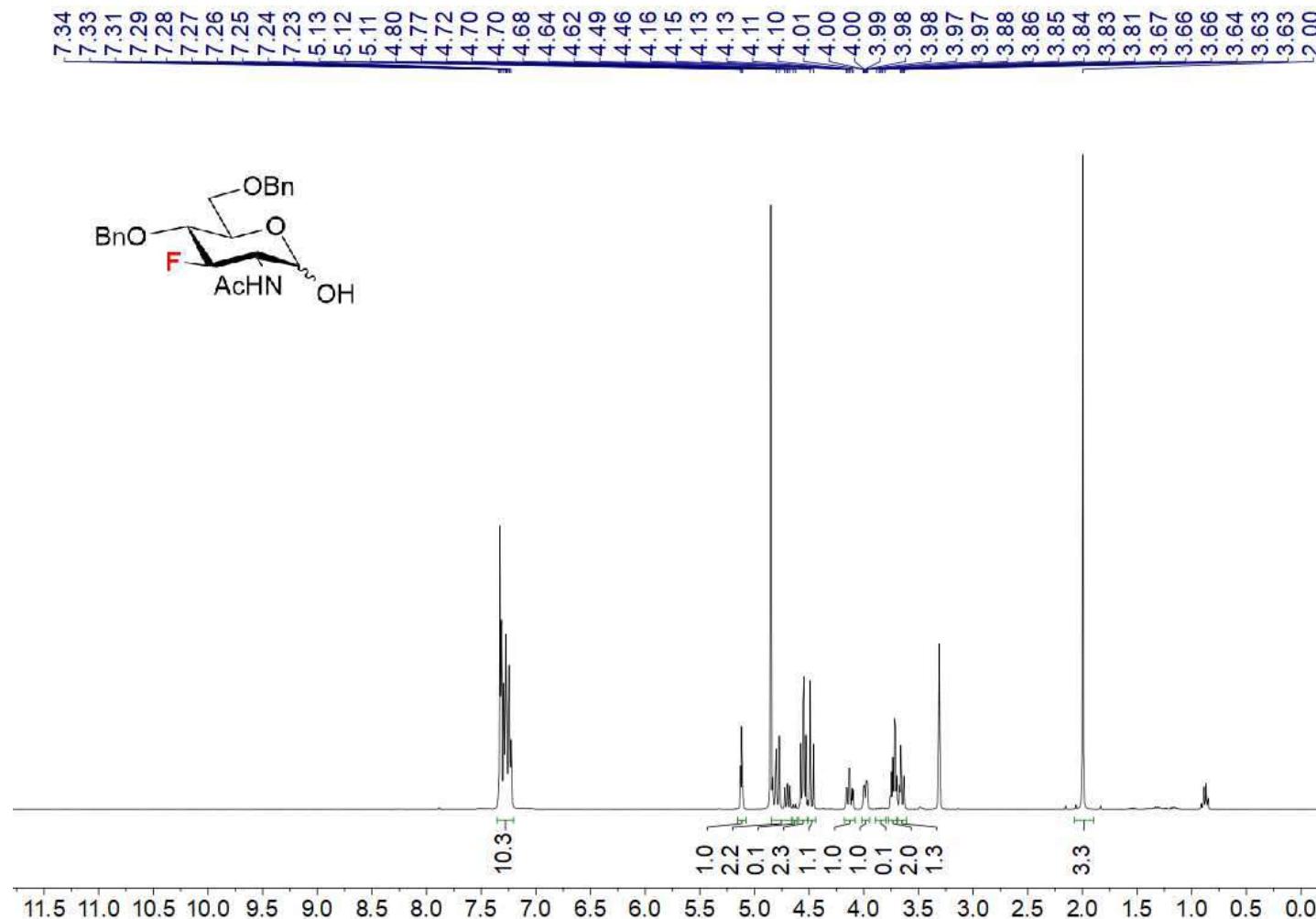


^1H - ^{13}C HSQC 38

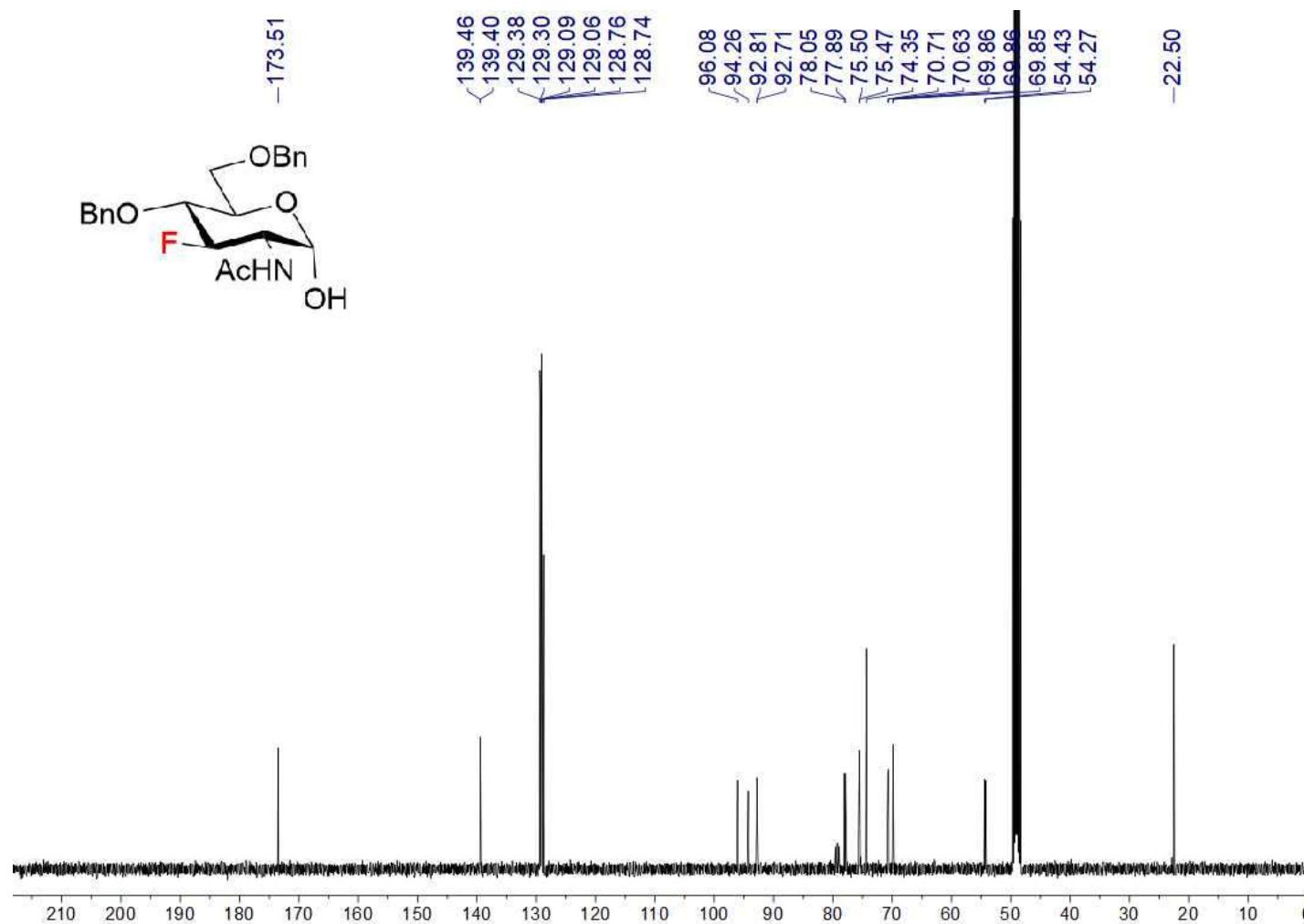


NMR COMPOUND 39

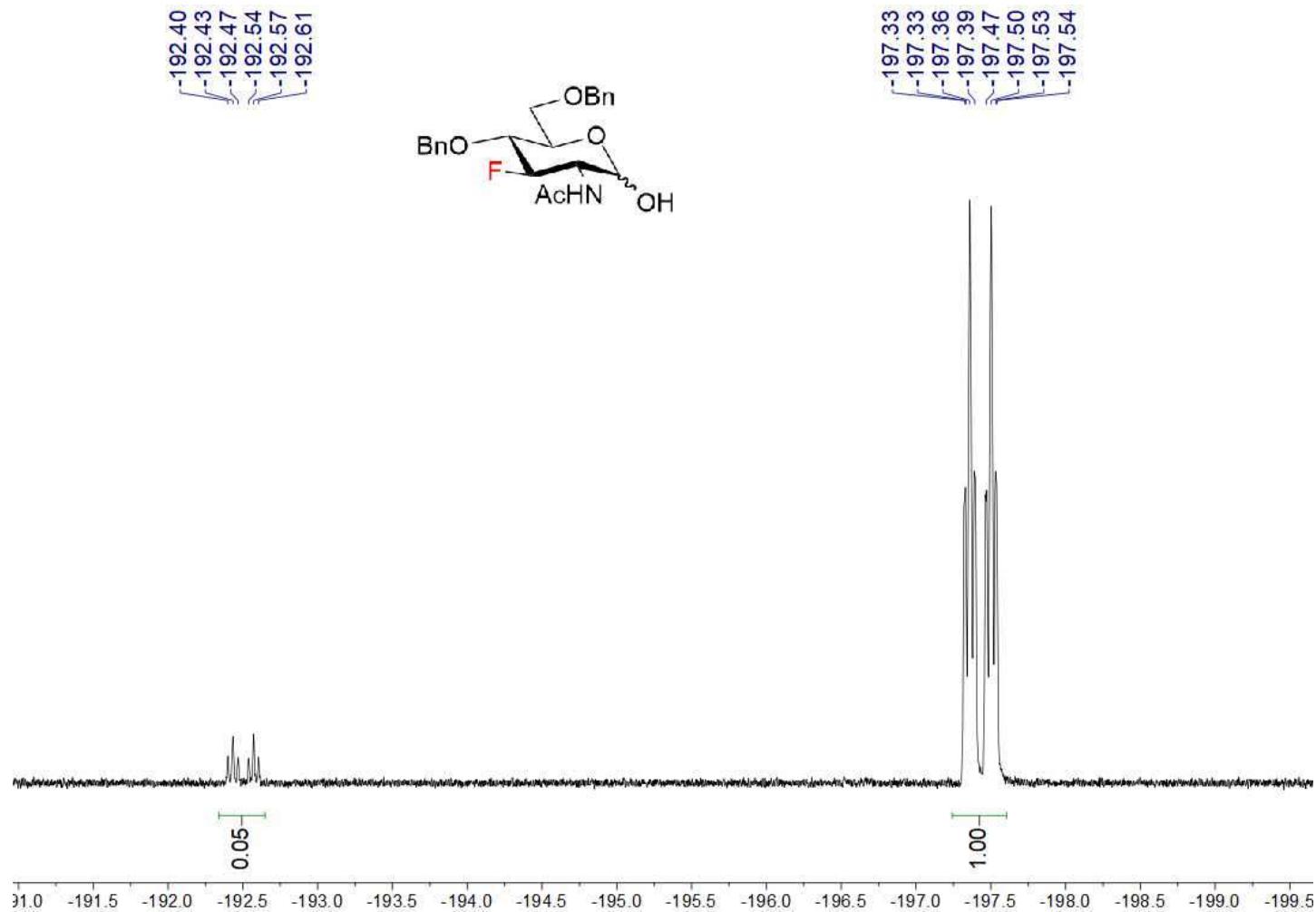
¹H NMR (400 MHz, CD₃OD) 39 (ca. 5% β -anomer)



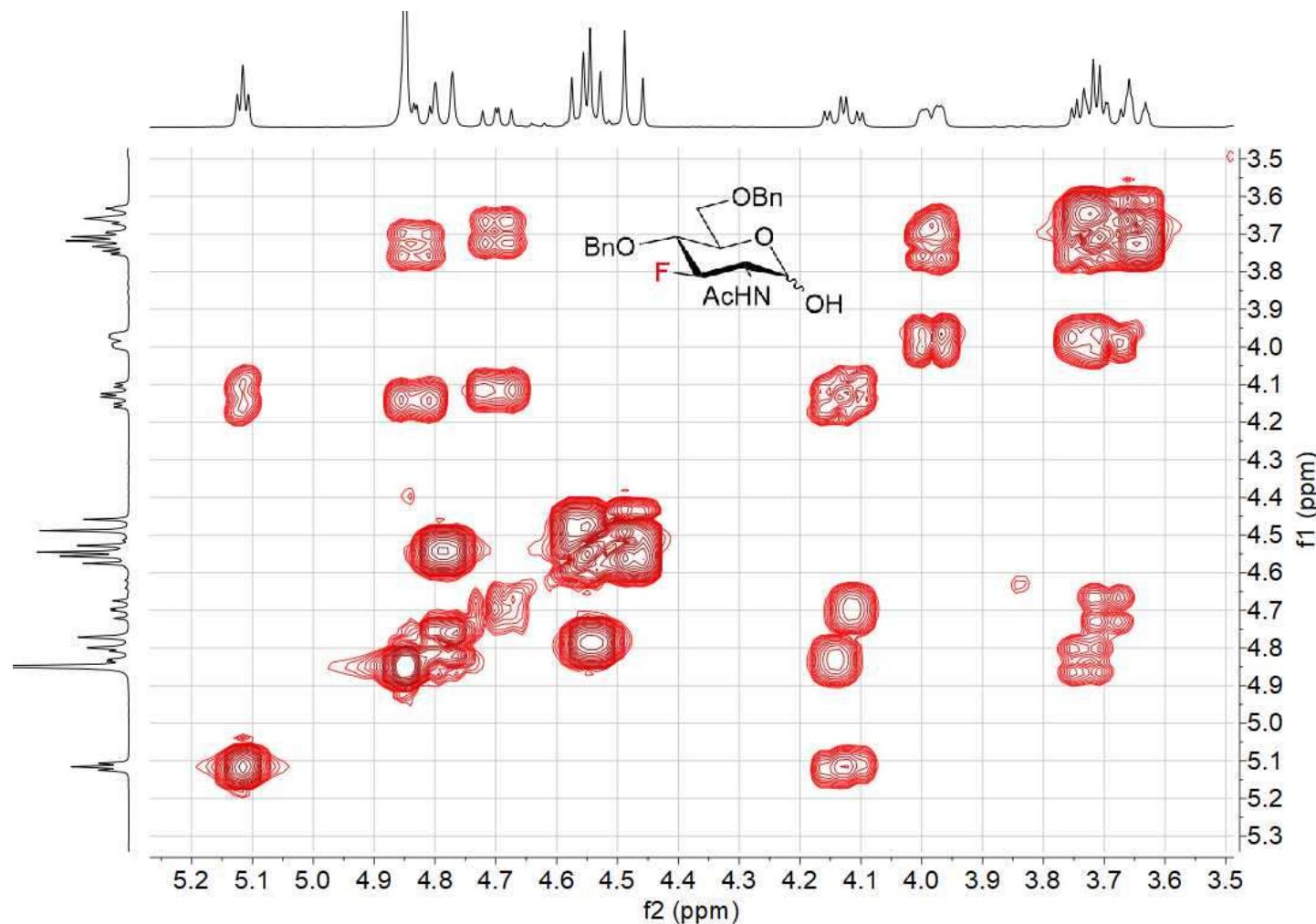
¹³C NMR (100 MHz, CD₃OD) 39



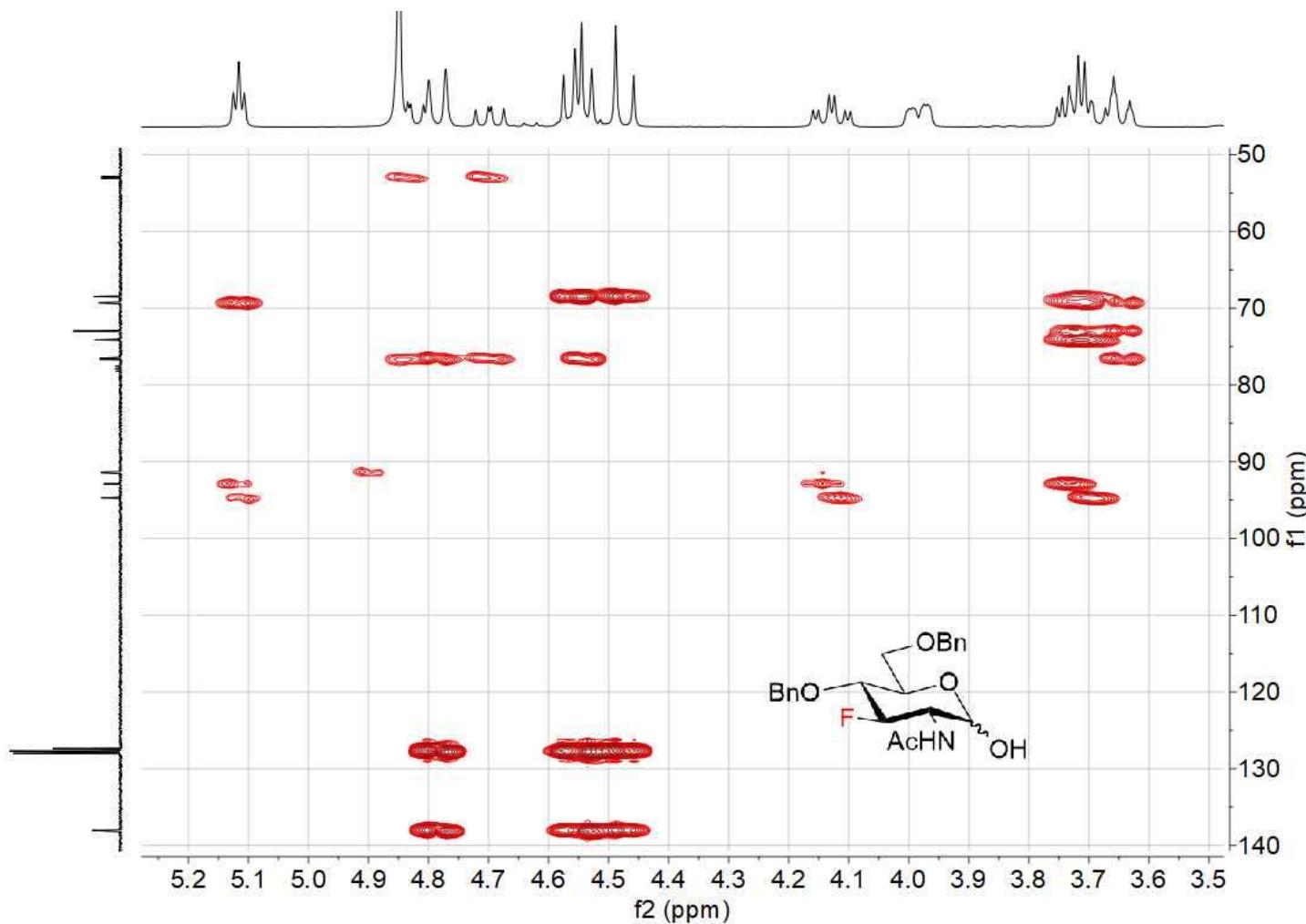
¹⁹F NMR (376 MHz, CD₃OD) 39 (ca. 5% β -anomer)



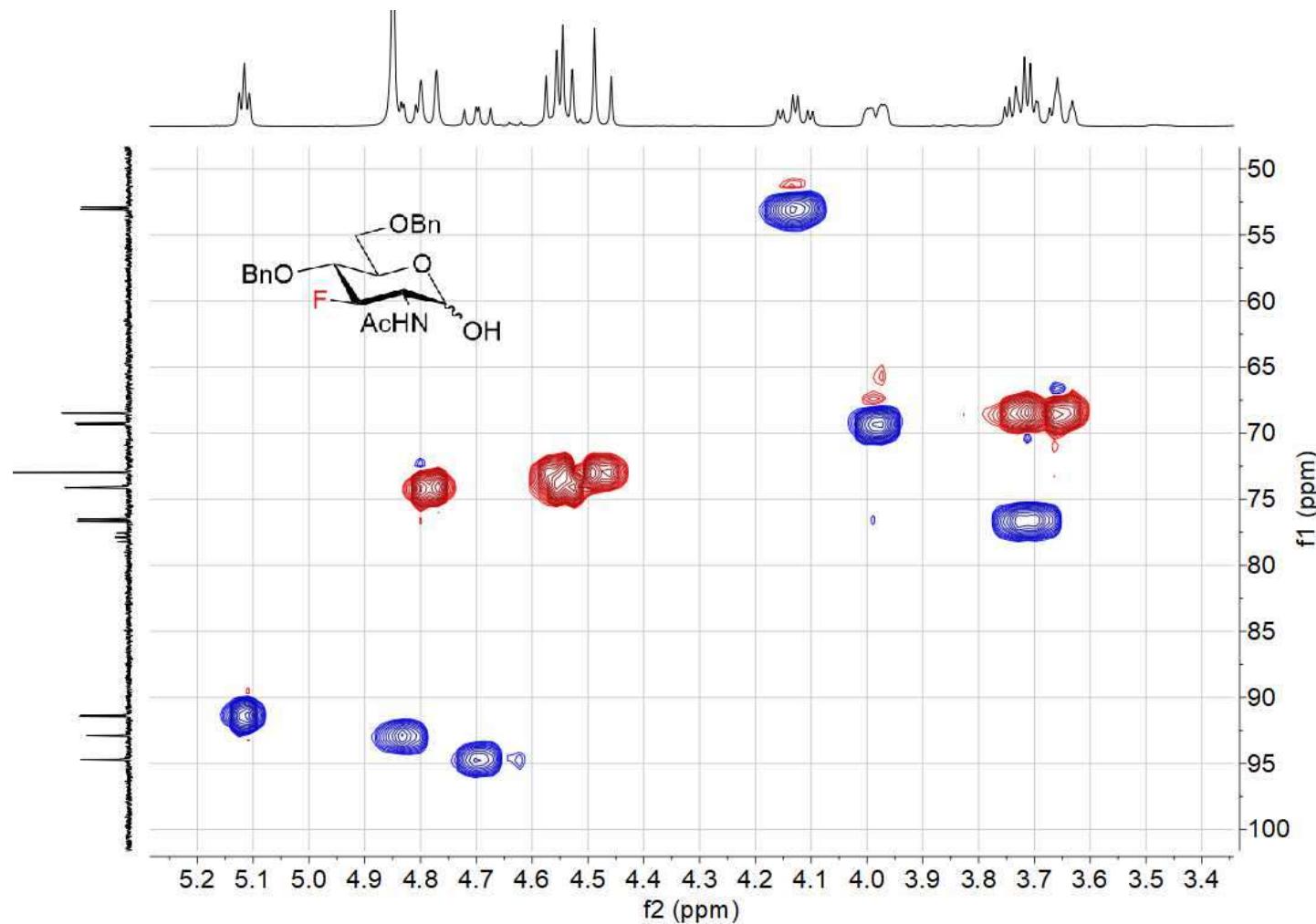
¹H-¹H COSY 39



¹H-¹³C HMBC 39

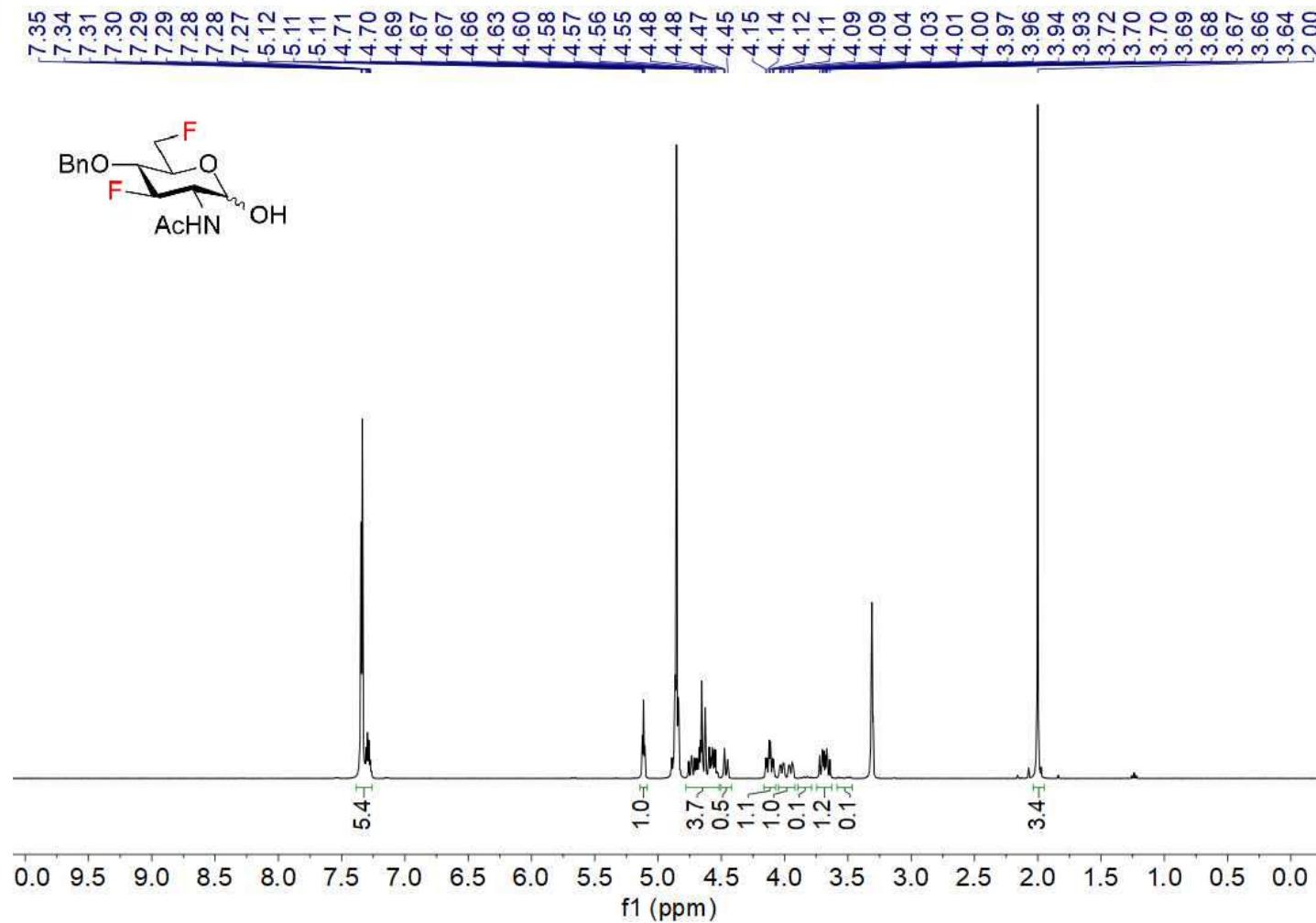


^1H - ^{13}C HSQC 39

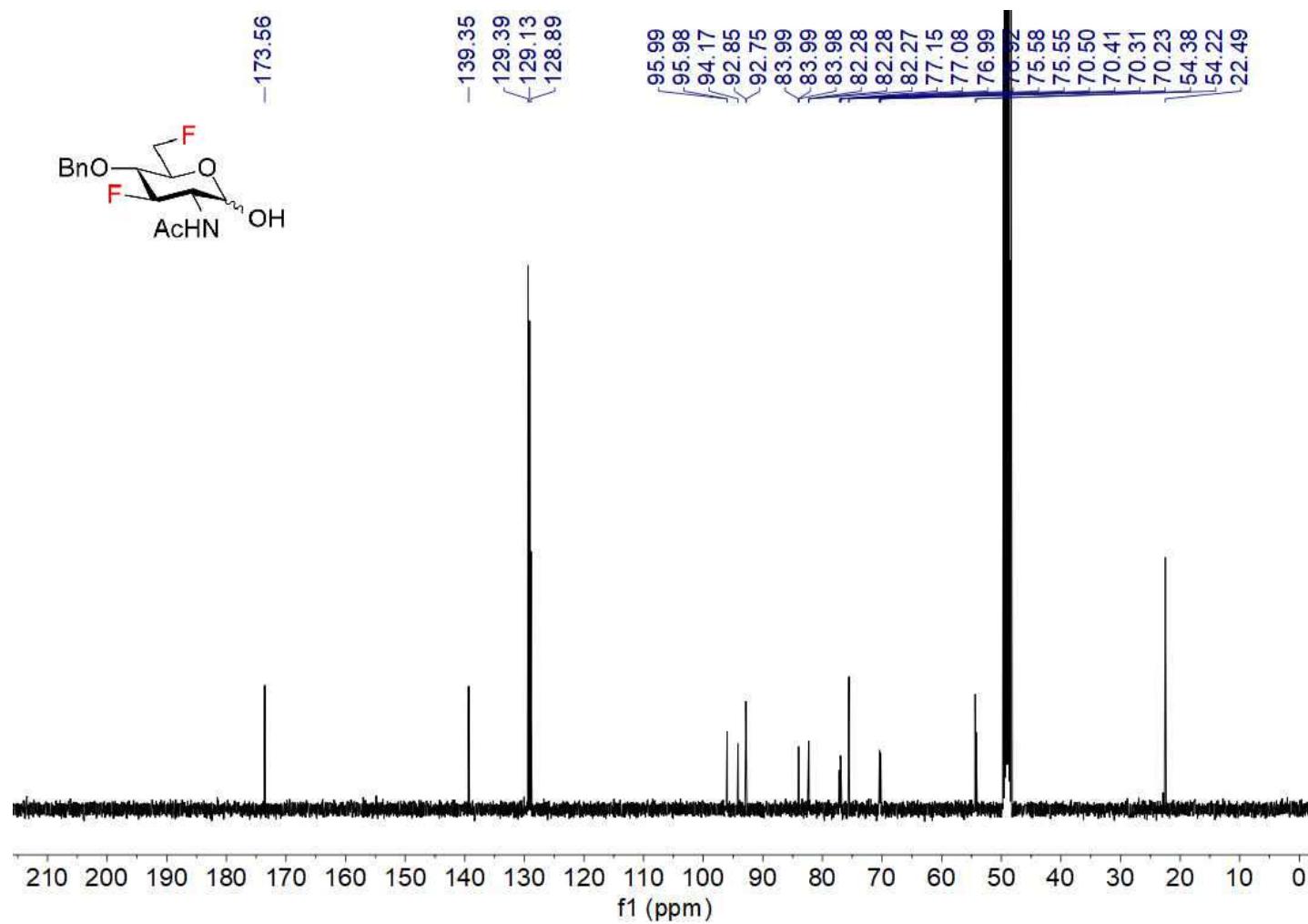


NMR COMPOUND 40

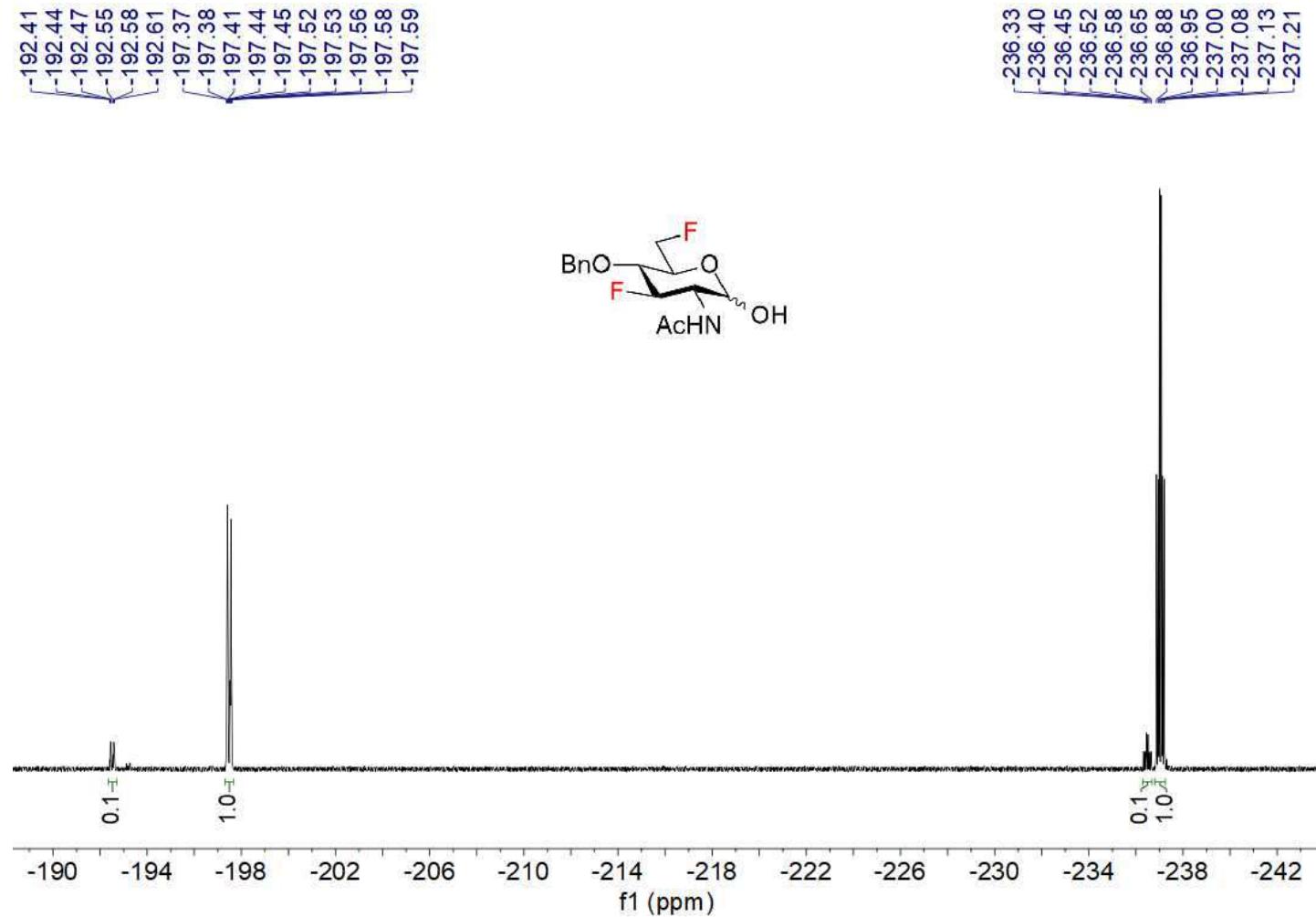
¹H NMR (400 MHz, CD₃OD) 40 (α/β ca. 10/1)



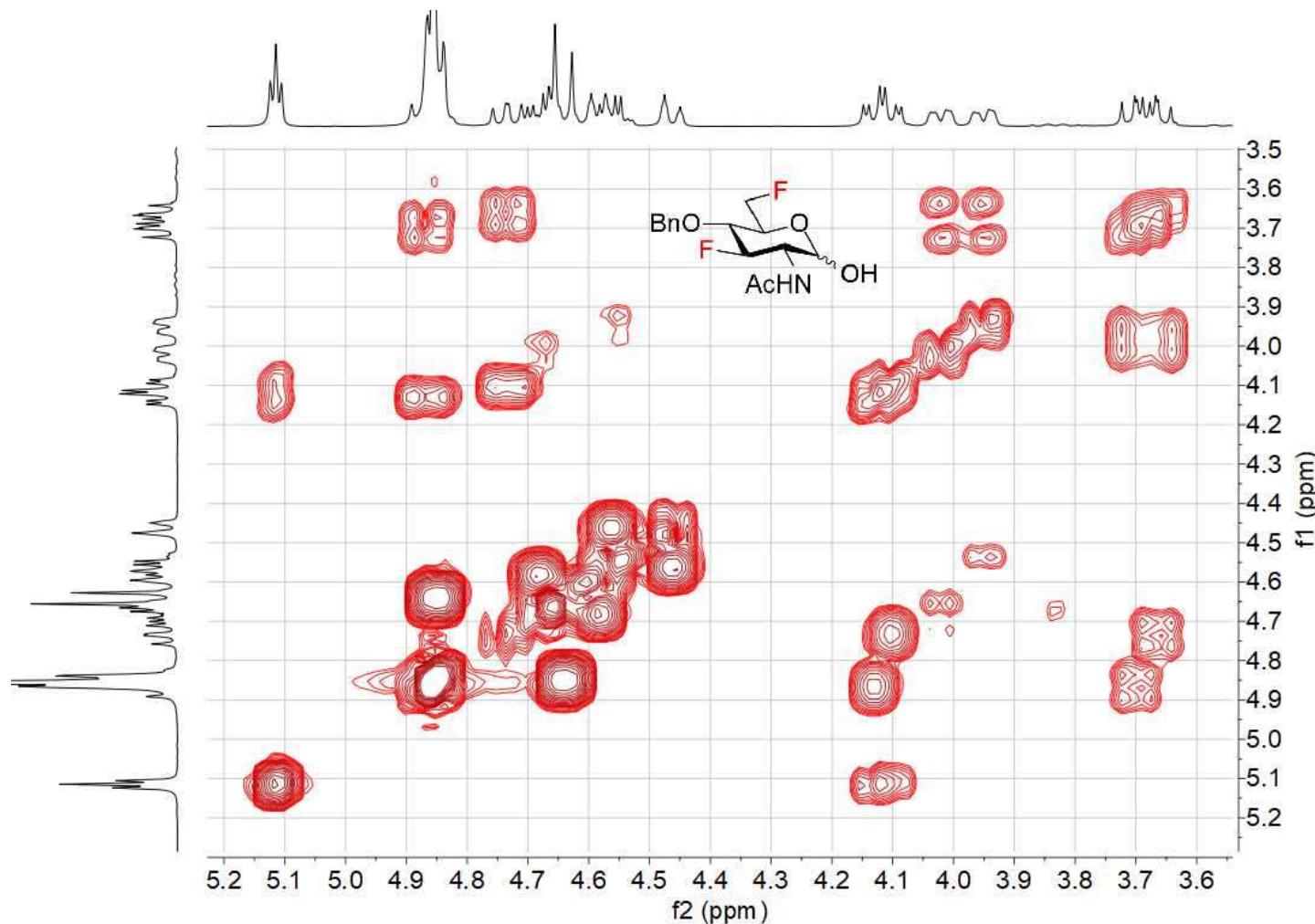
¹³C NMR (100 MHz, CD₃OD) 40



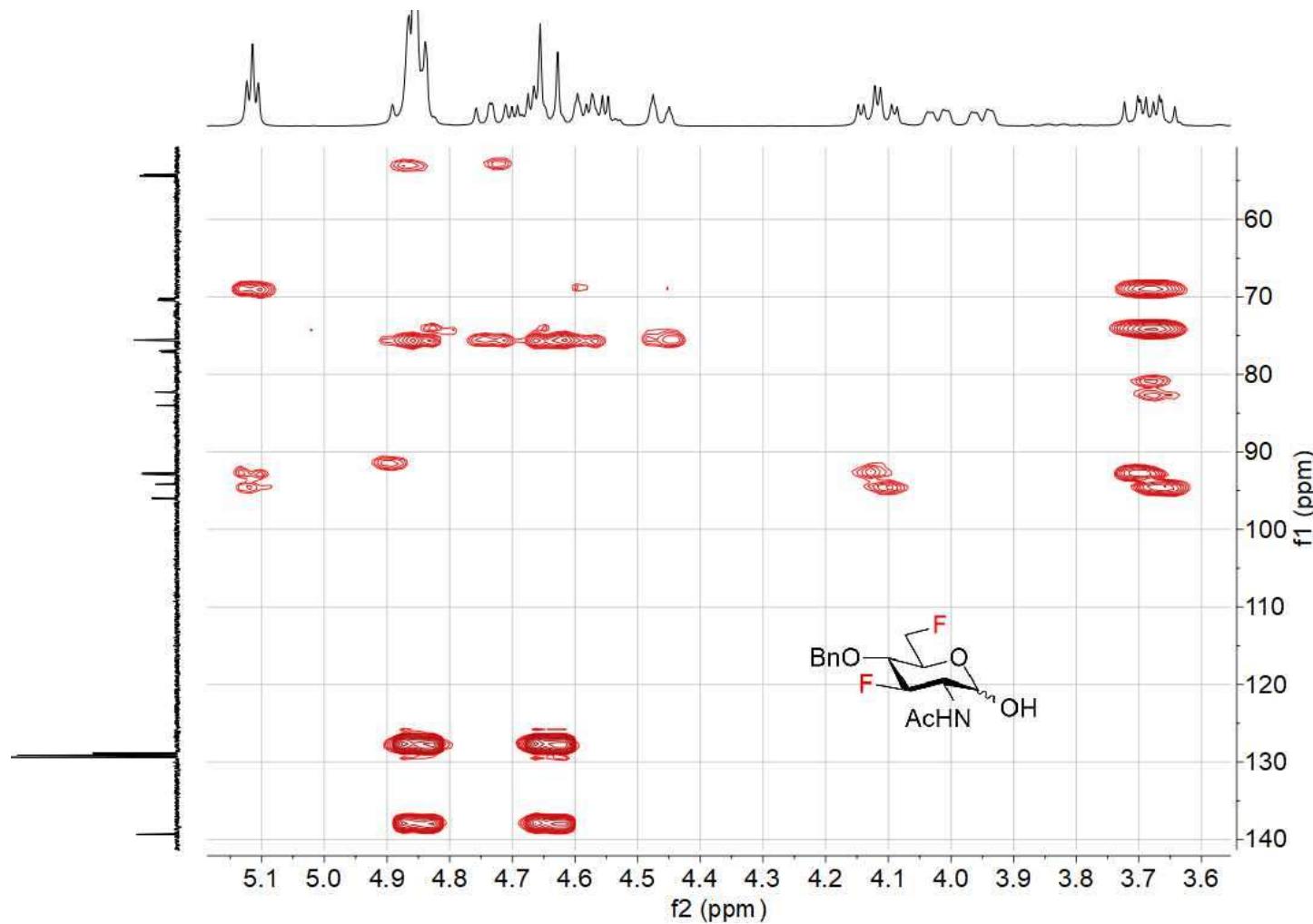
¹⁹F NMR (376 MHz, CD₃OD) 40 (α/β ca. 10/1)



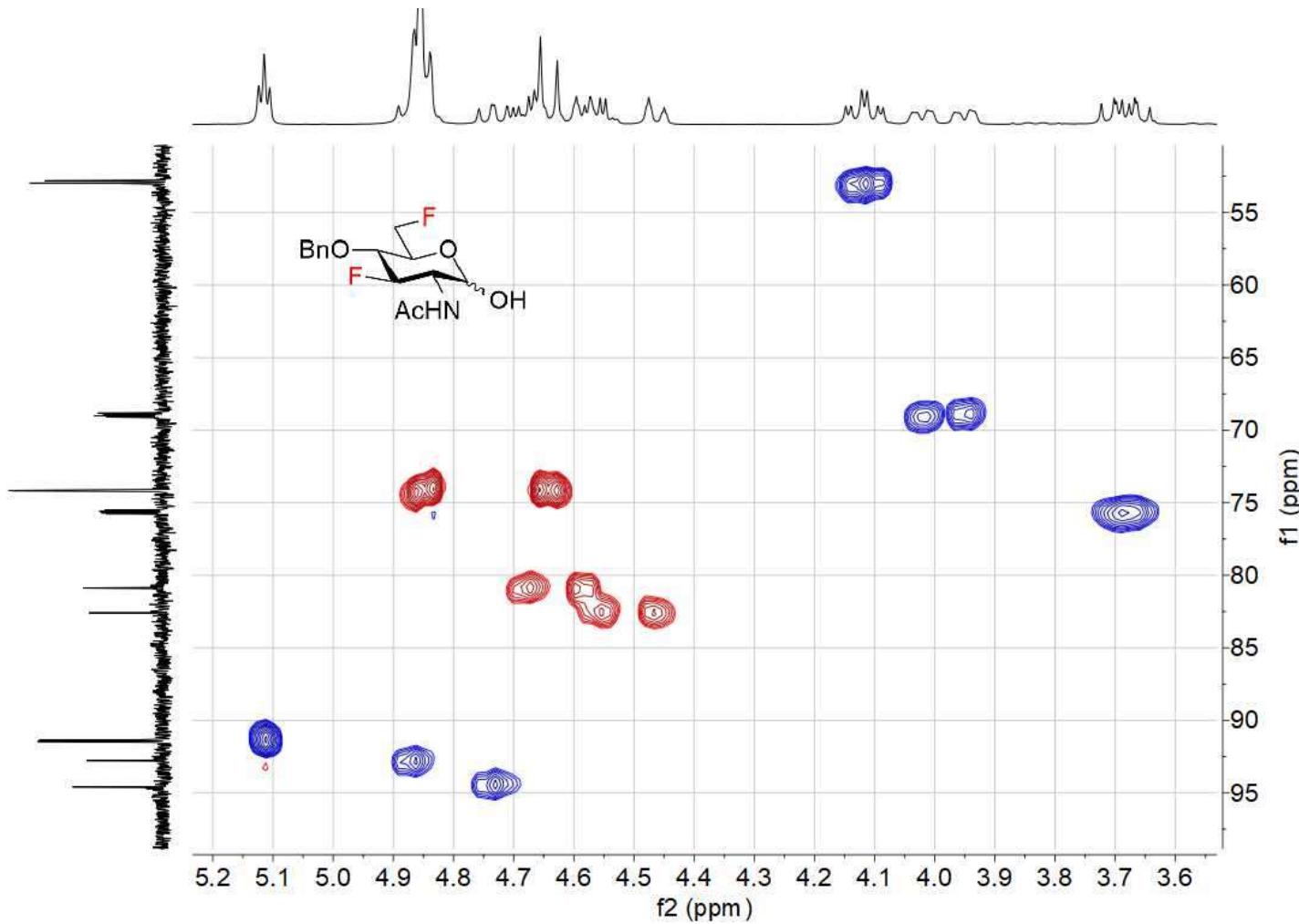
¹H-¹H COSY 40



¹H-¹³C HMBC 40

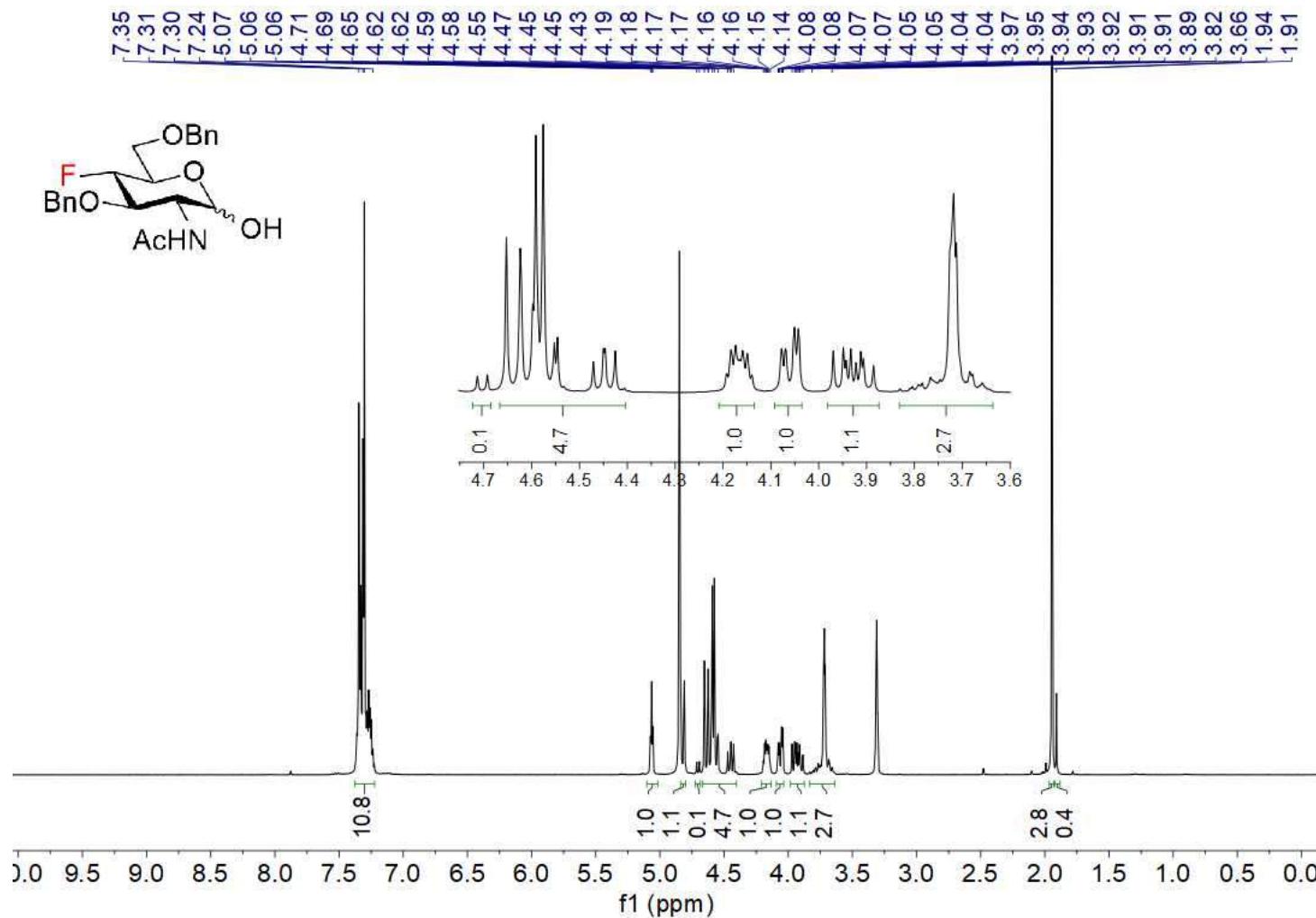


^1H - ^{13}C HSQC 40

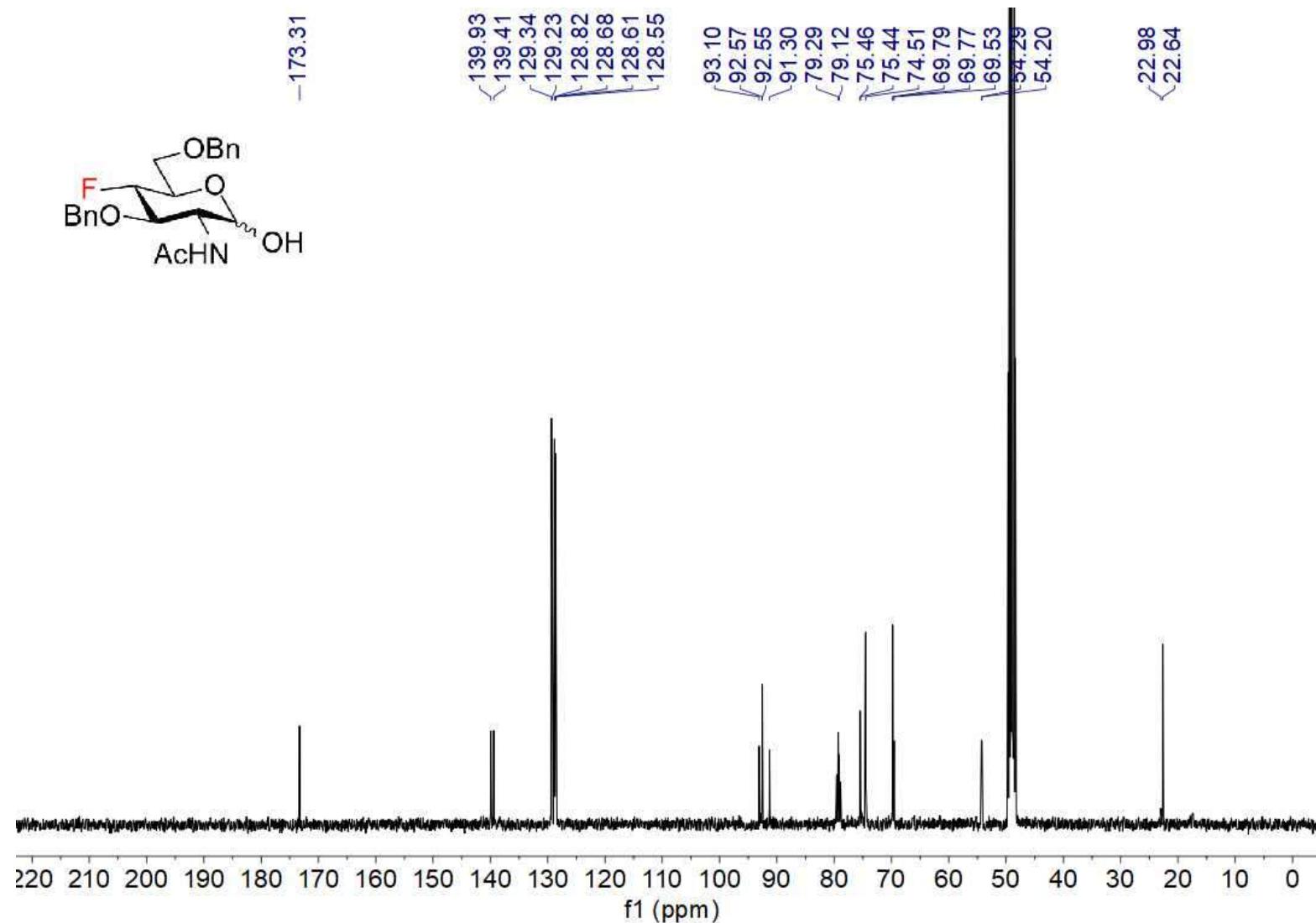


NMR COMPOUND 41

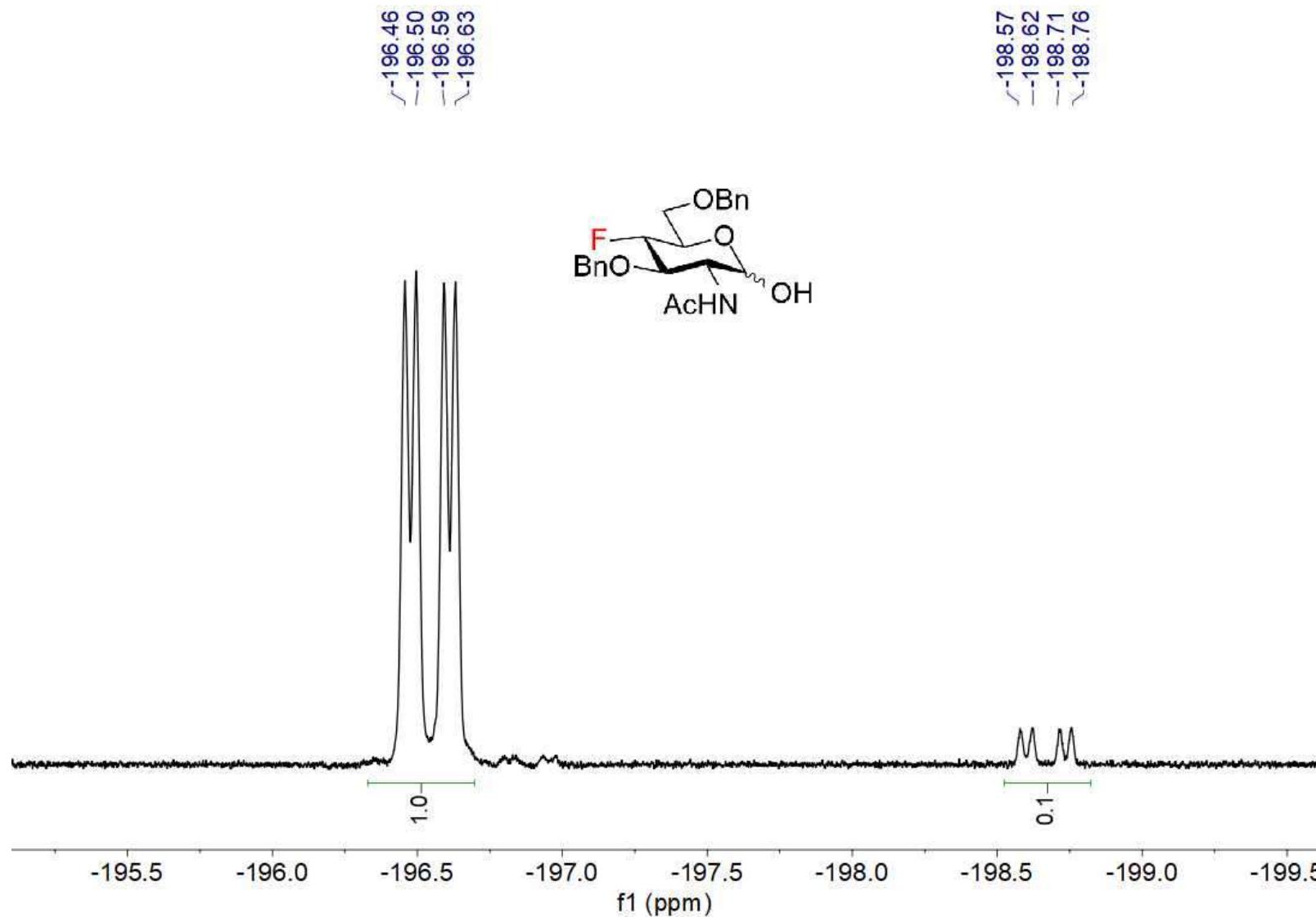
¹H NMR (400 MHz, CD₃OD) 41 (α/β ca. 10/1)



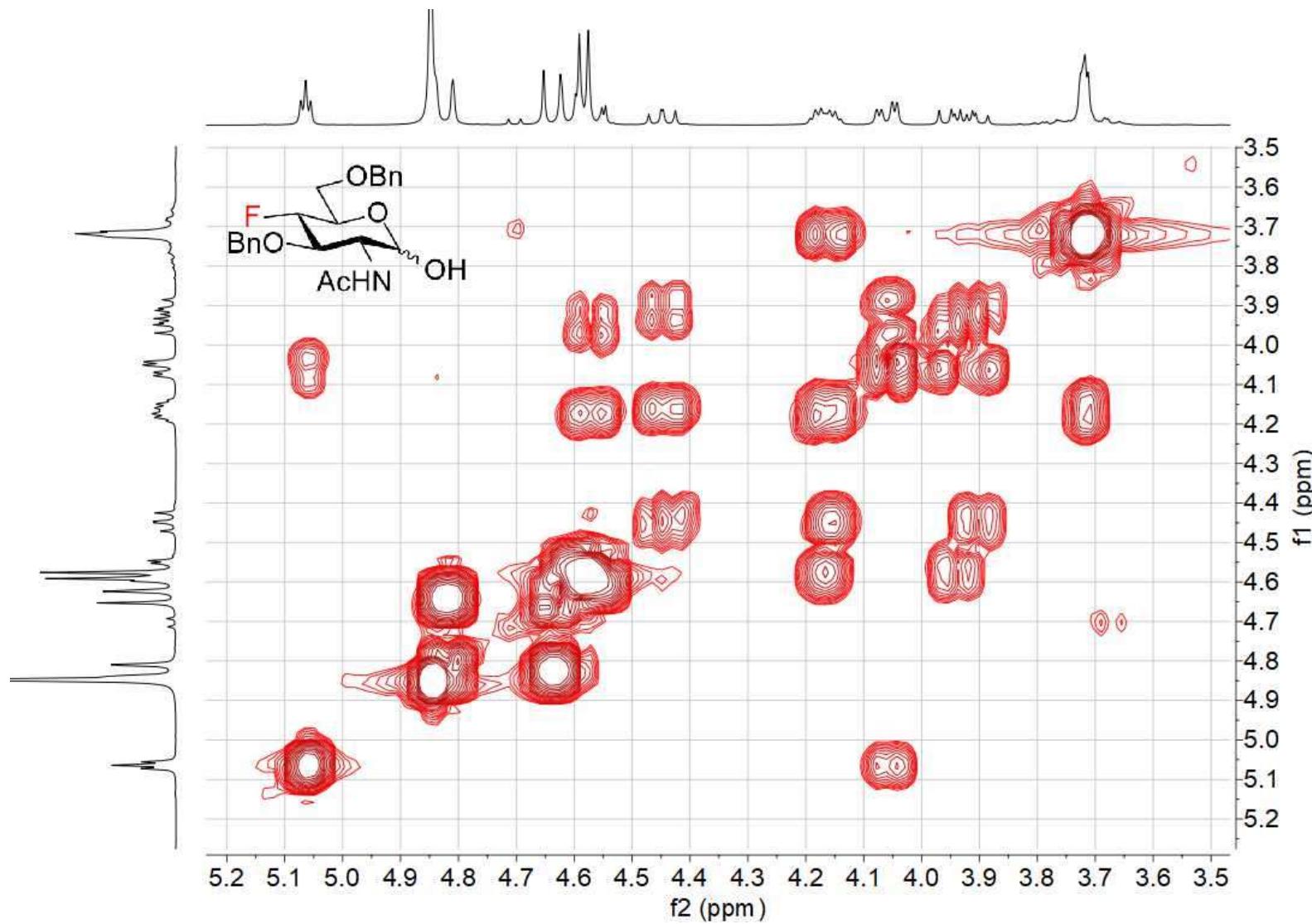
¹³C NMR (100 MHz, CD₃OD) 41



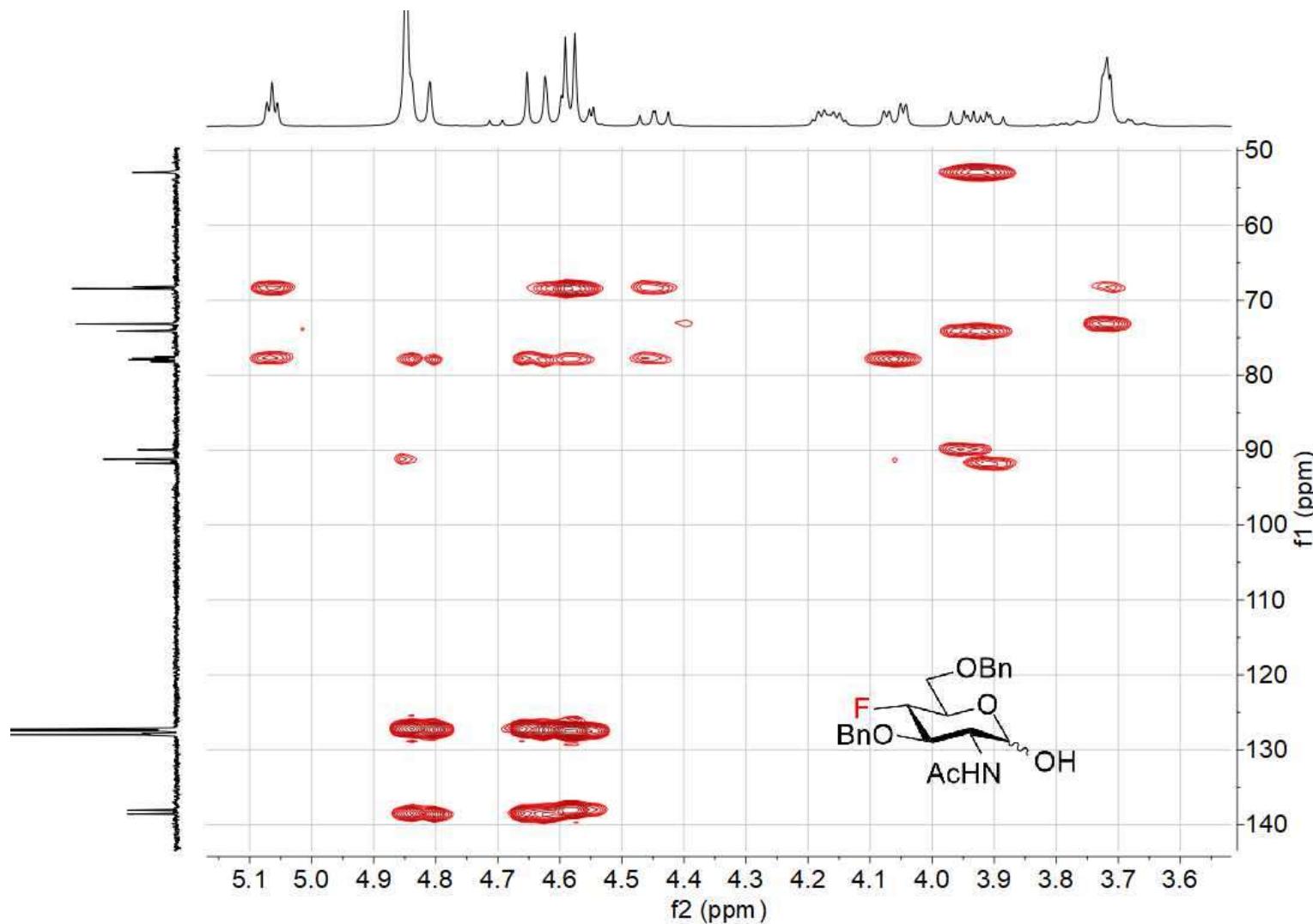
¹⁹F NMR (376 MHz, CD₃OD) 41 (α/β ca. 10/1)



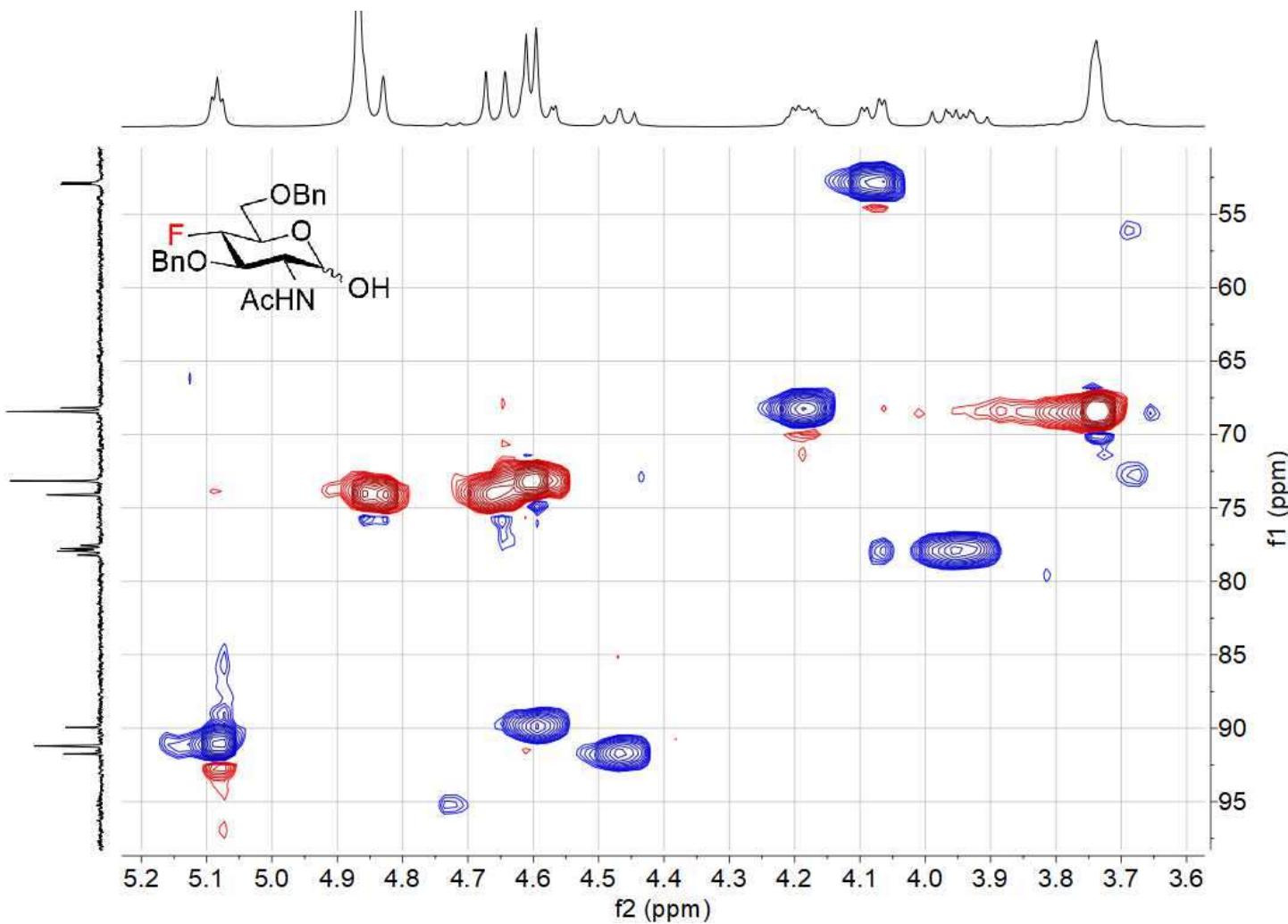
¹H-¹H COSY 41



^1H - ^{13}C HMBC 41

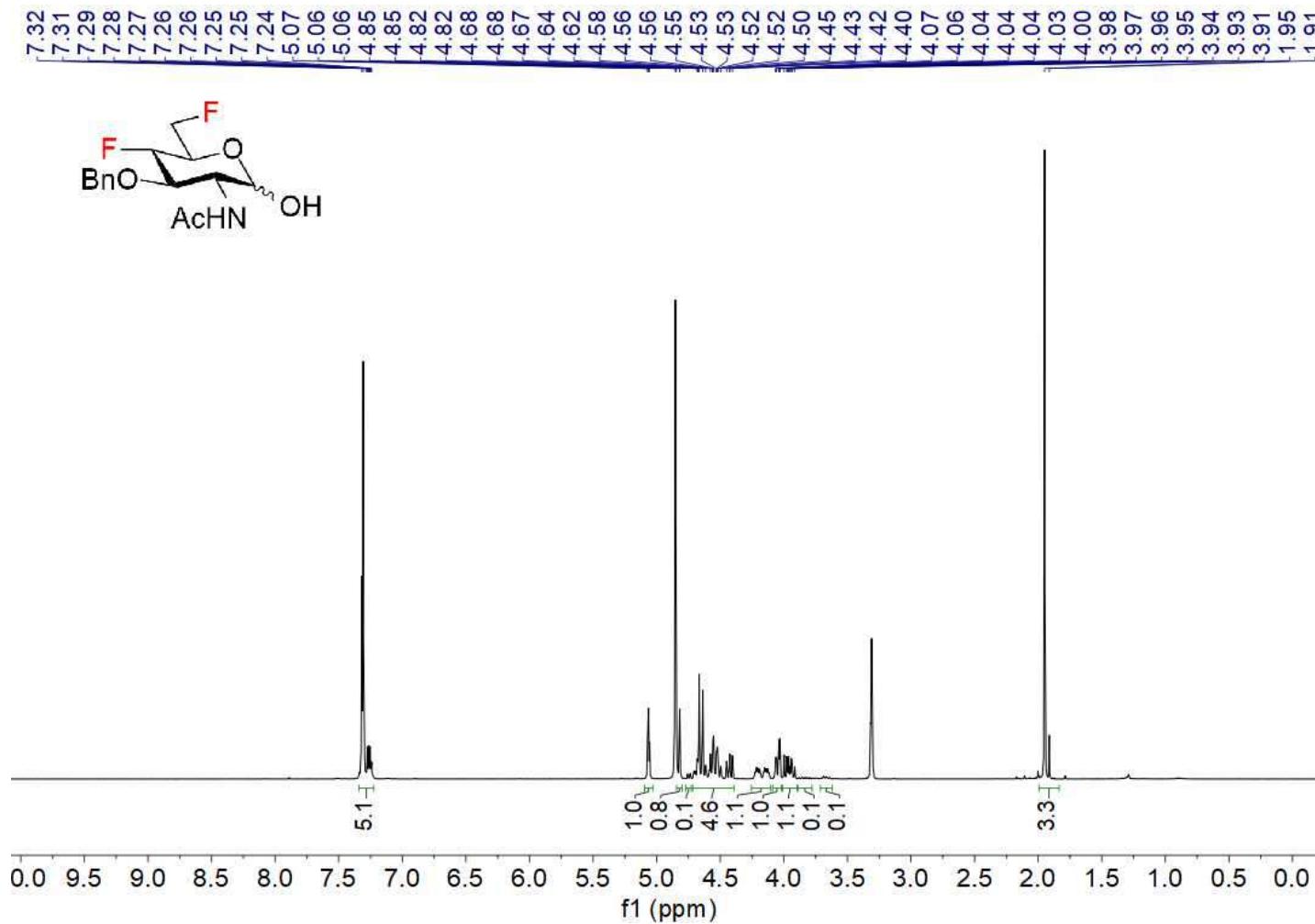


^1H - ^{13}C HSQC 41

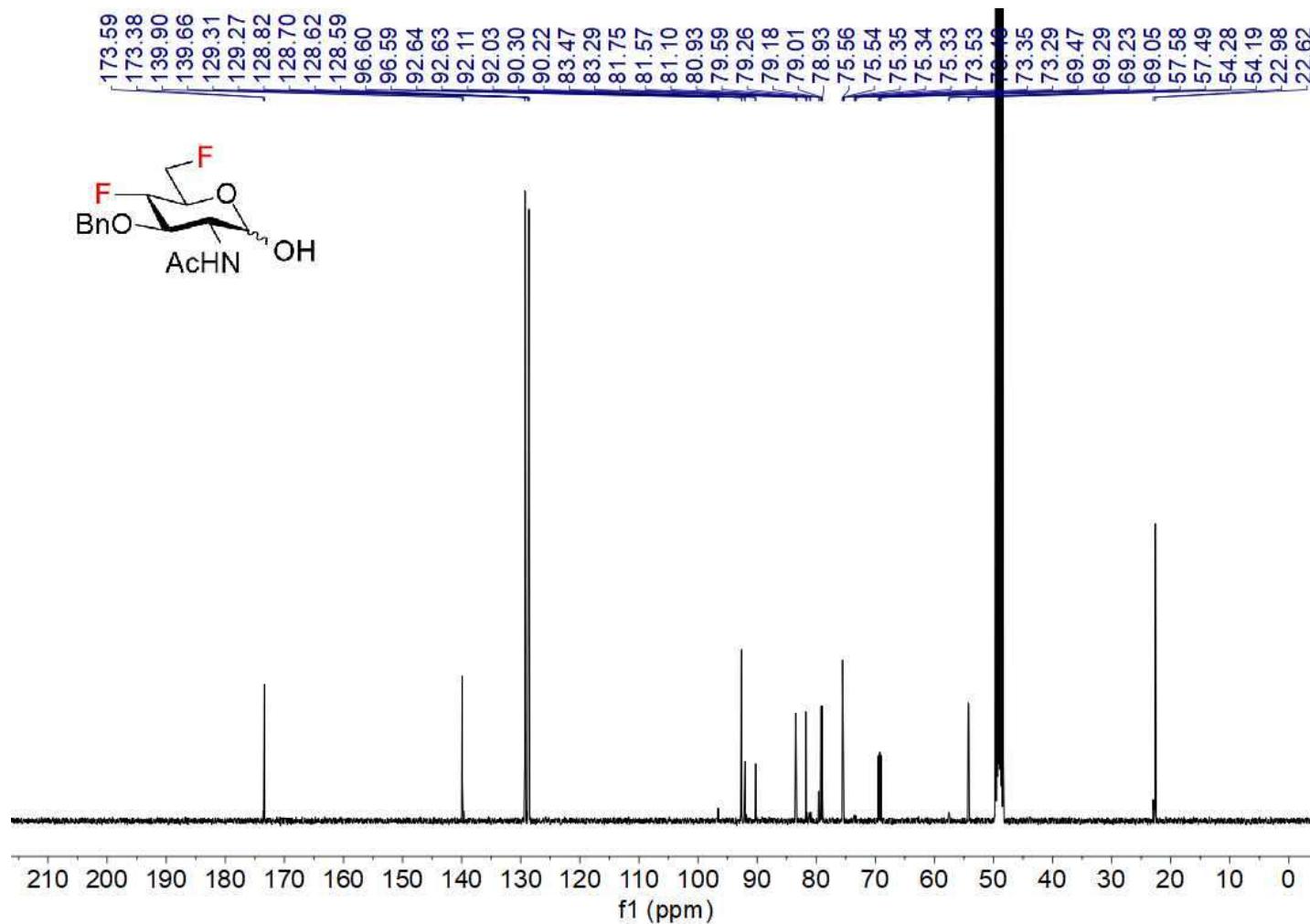


NMR COMPOUND 42

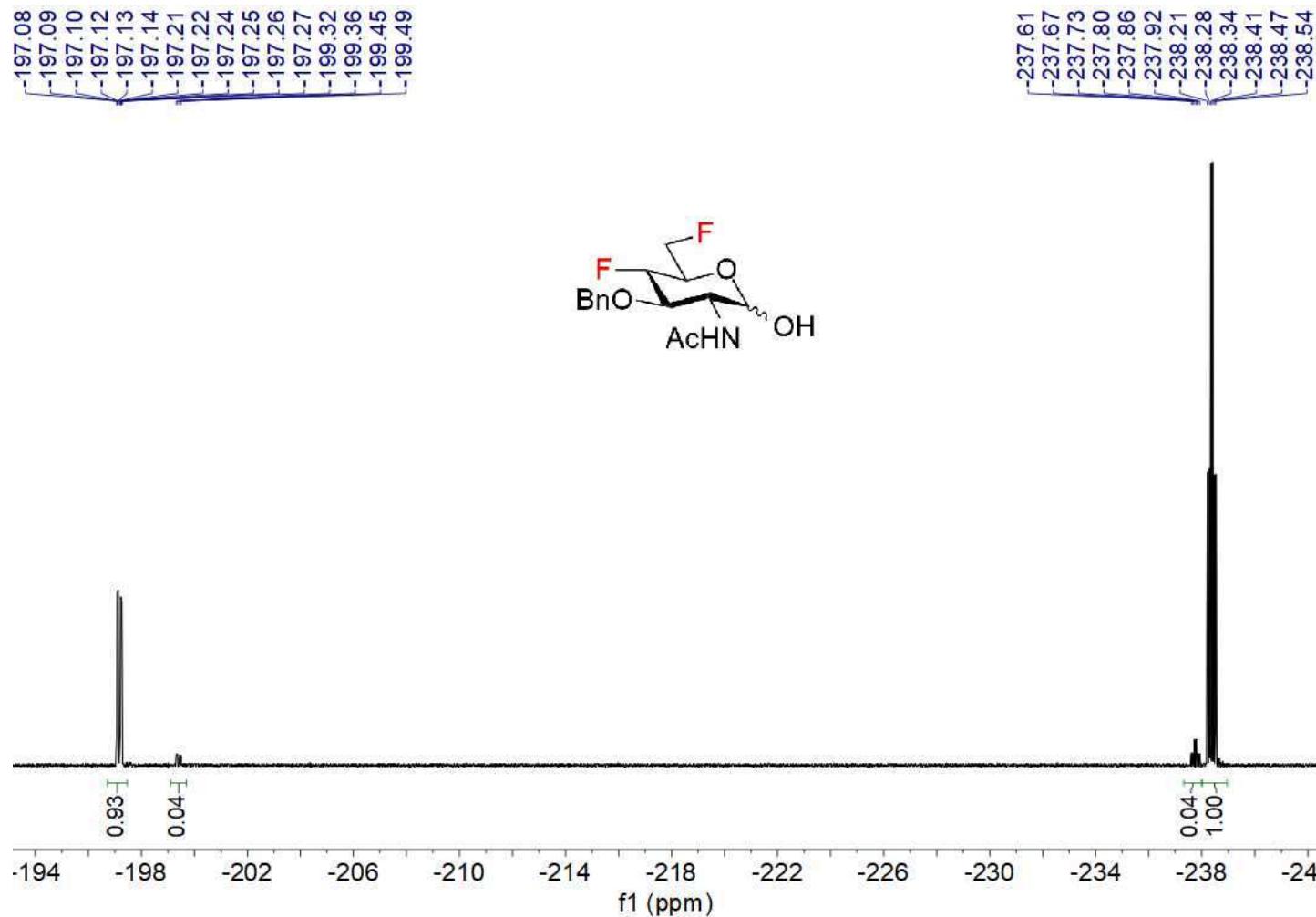
¹H NMR (400 MHz, CD₃OD) 42 (ca. 4% β -anomer)



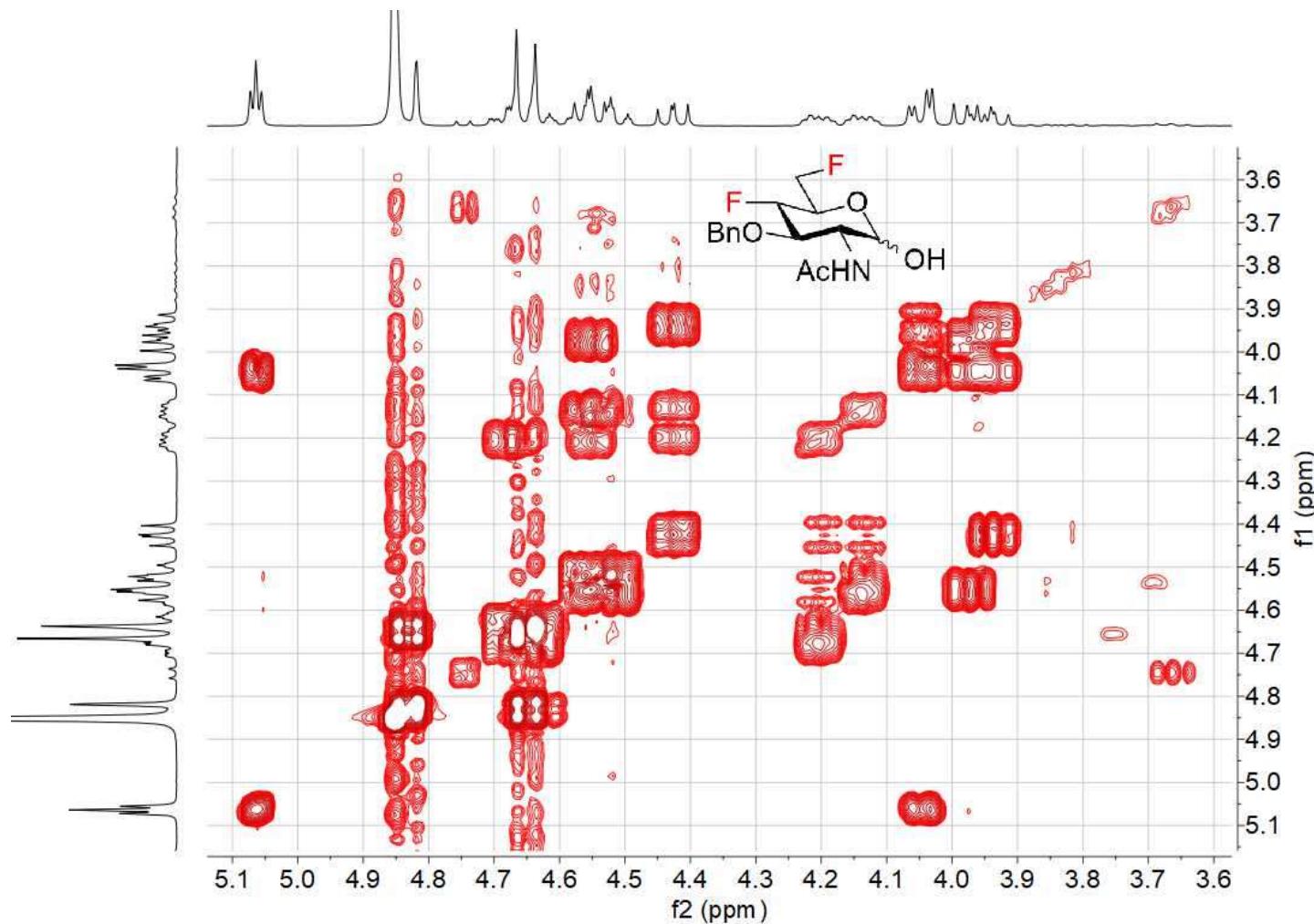
¹³C NMR (100 MHz, CD₃OD) 42



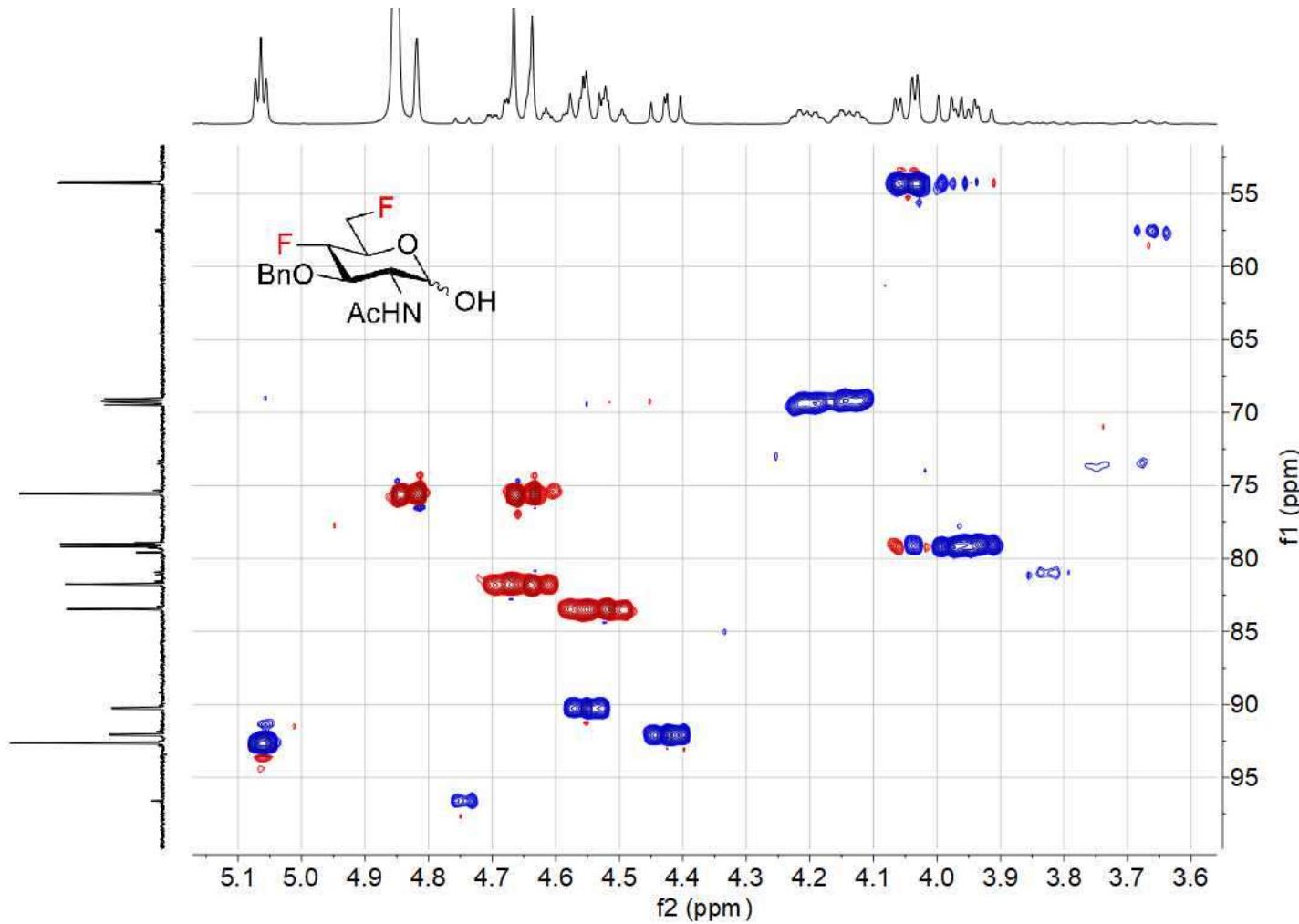
¹⁹F NMR (376 MHz, CD₃OD) 42 (ca. 4% β -anomer)



¹H-¹H COSY 42

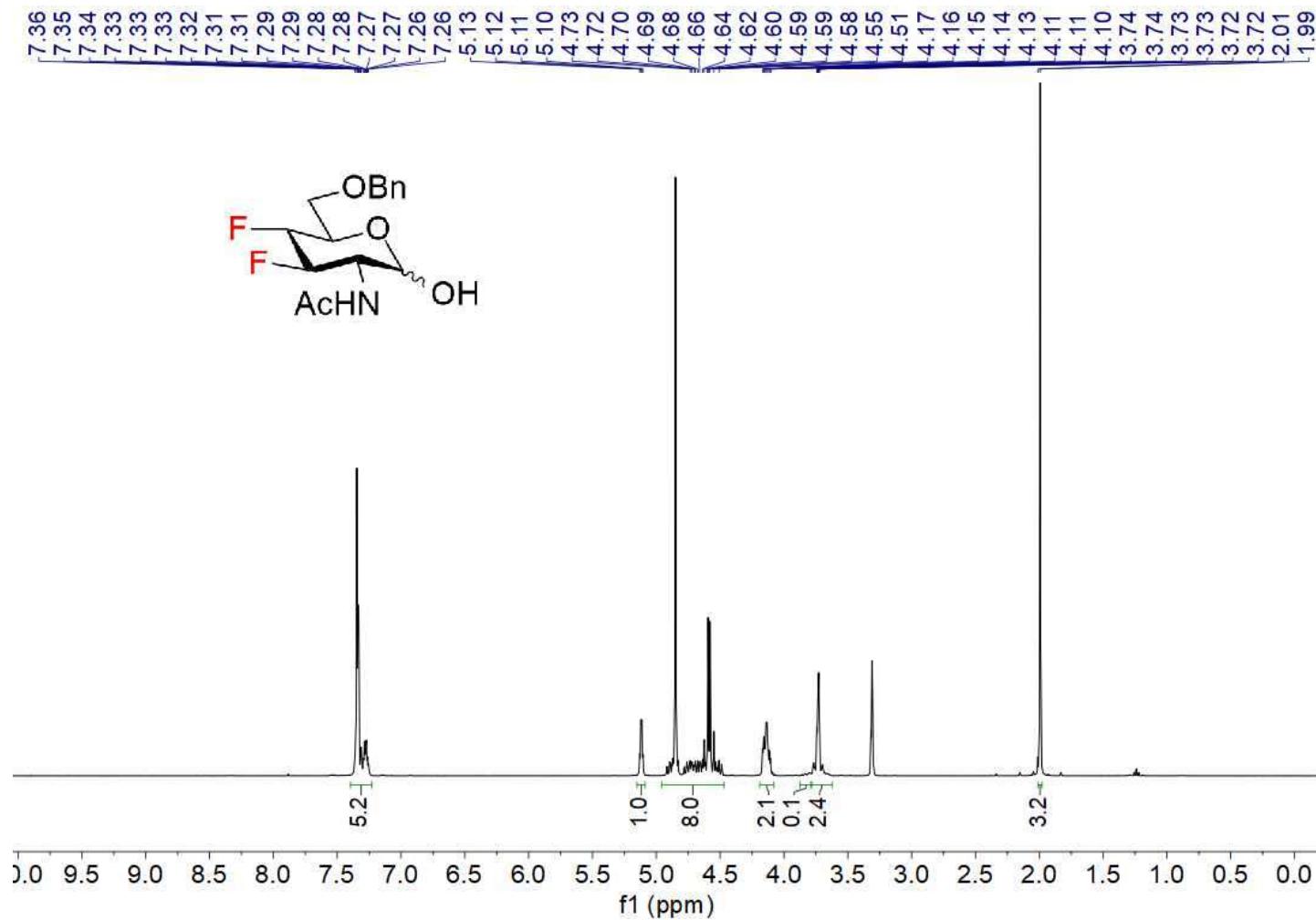


^1H - ^{13}C HSQC 42

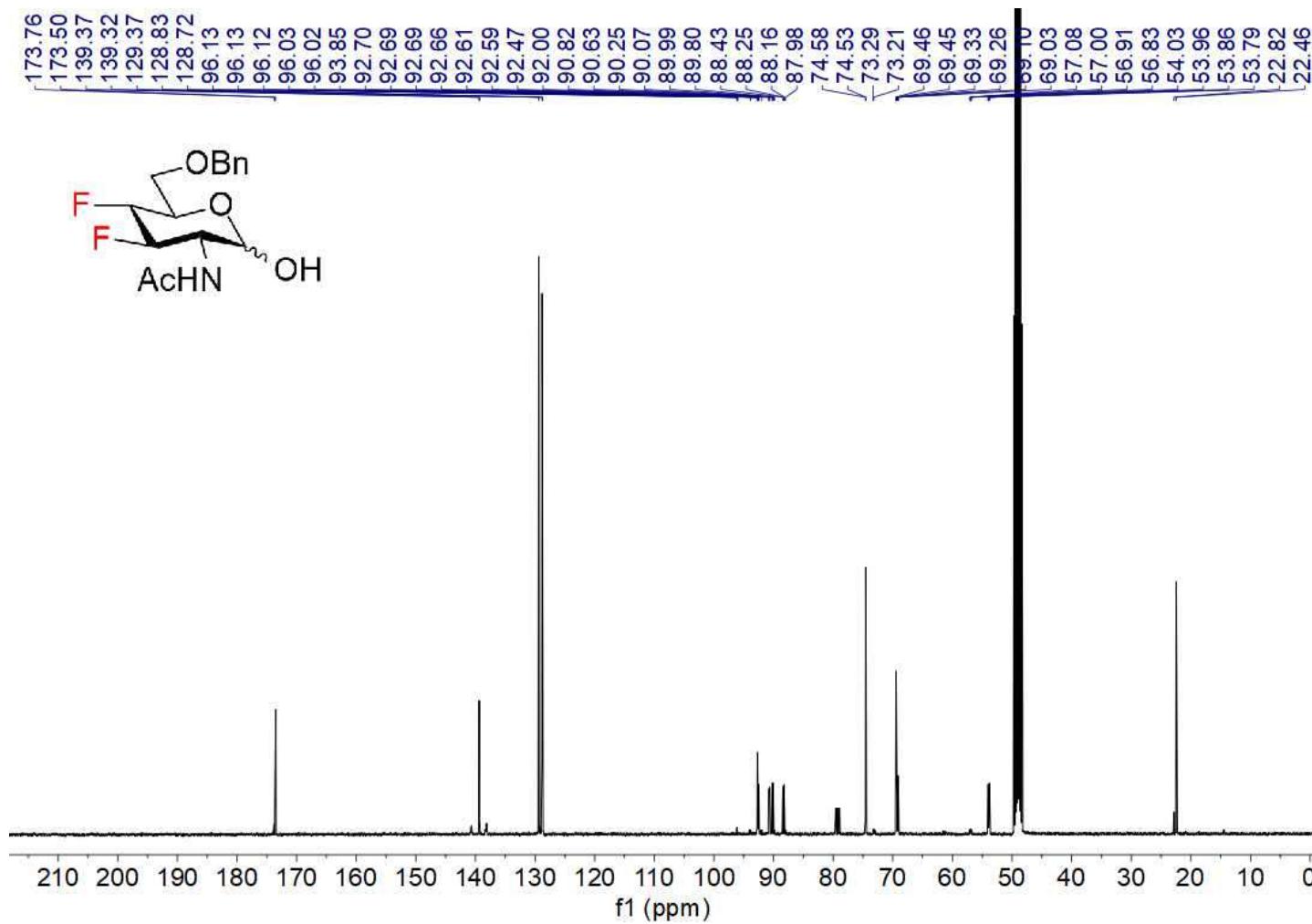


NMR COMPOUND 43

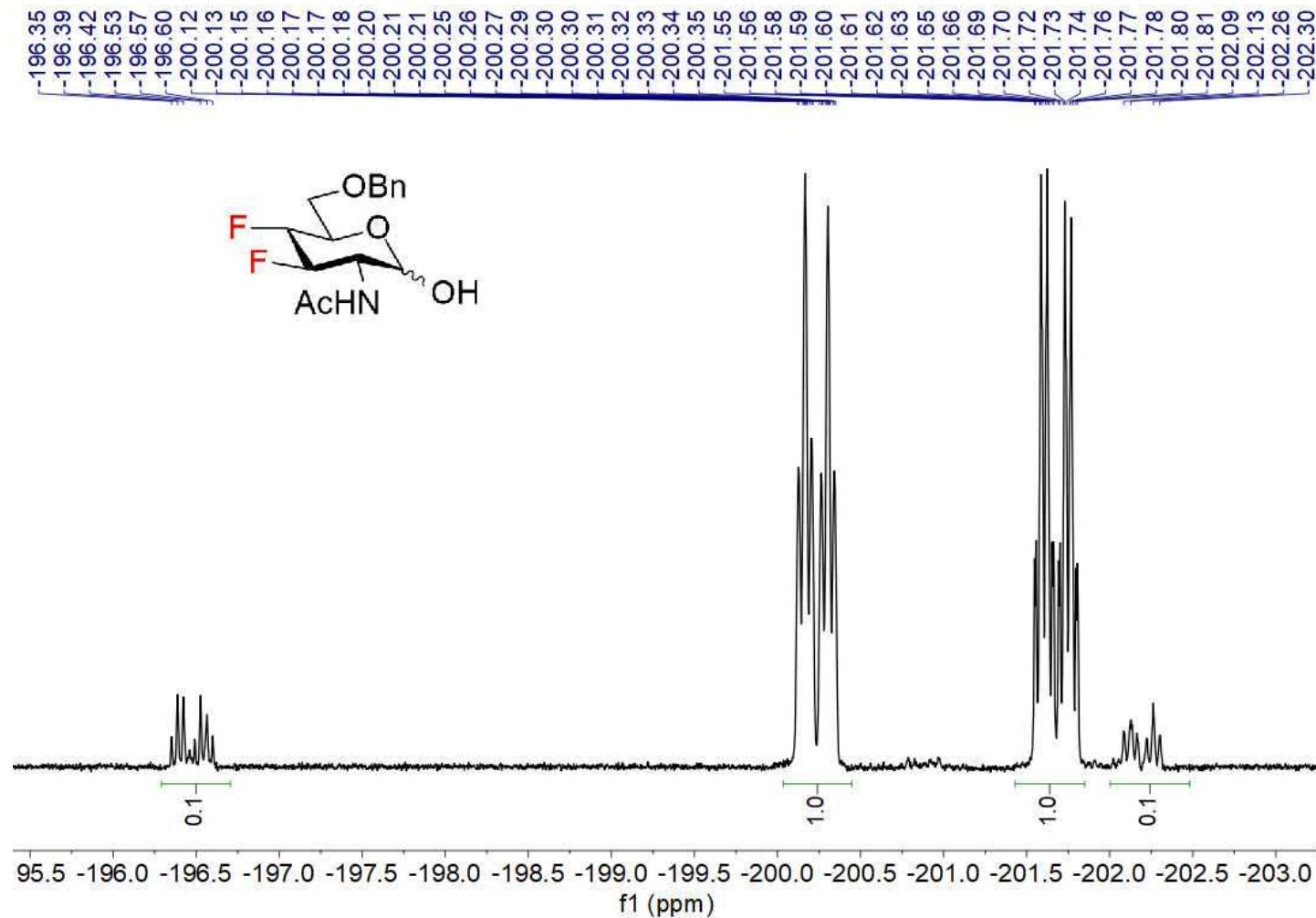
¹H NMR (400 MHz, CD₃OD) 43 (α/β ca. 10/1)



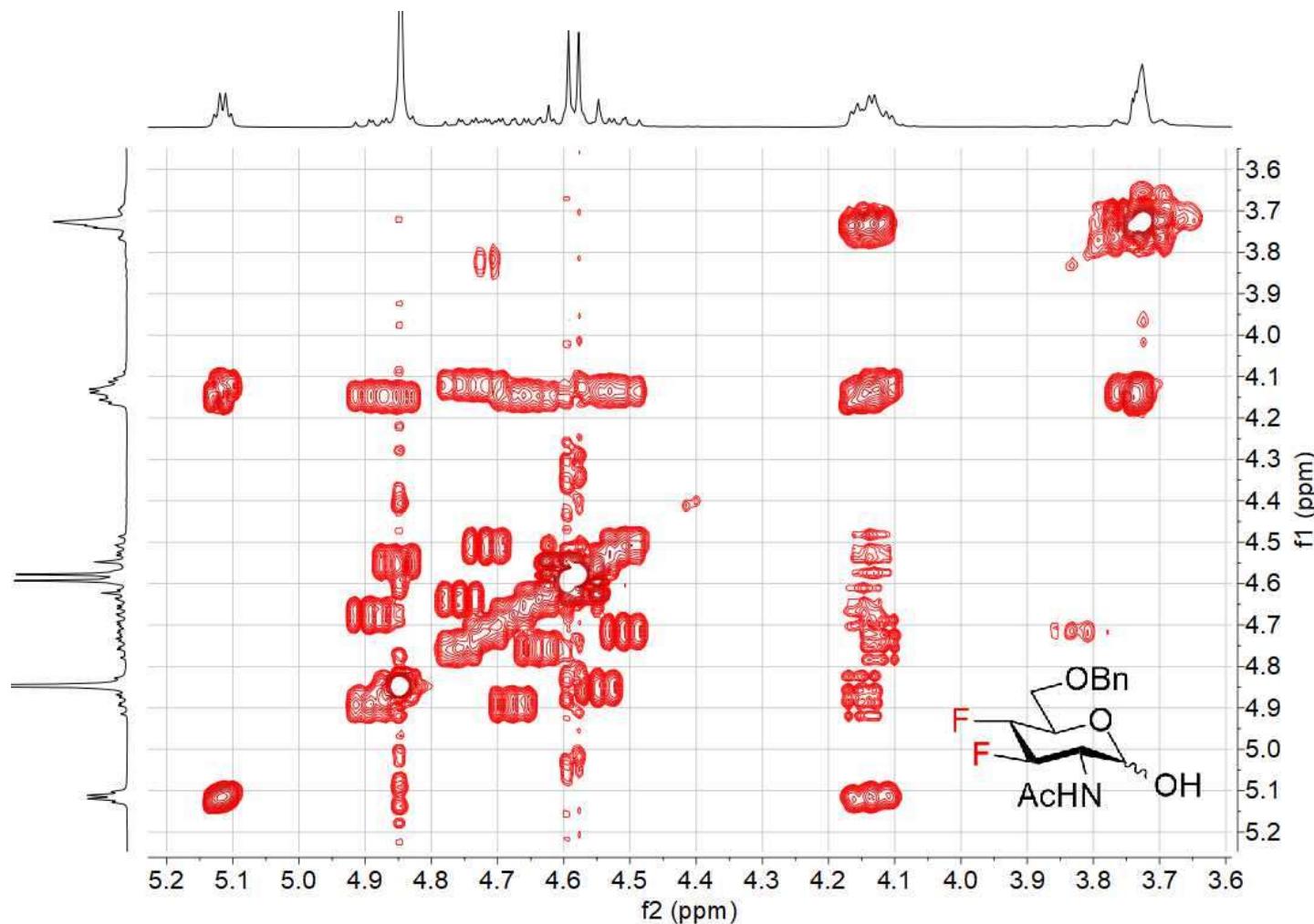
¹³C NMR (100 MHz, CD₃OD) 43



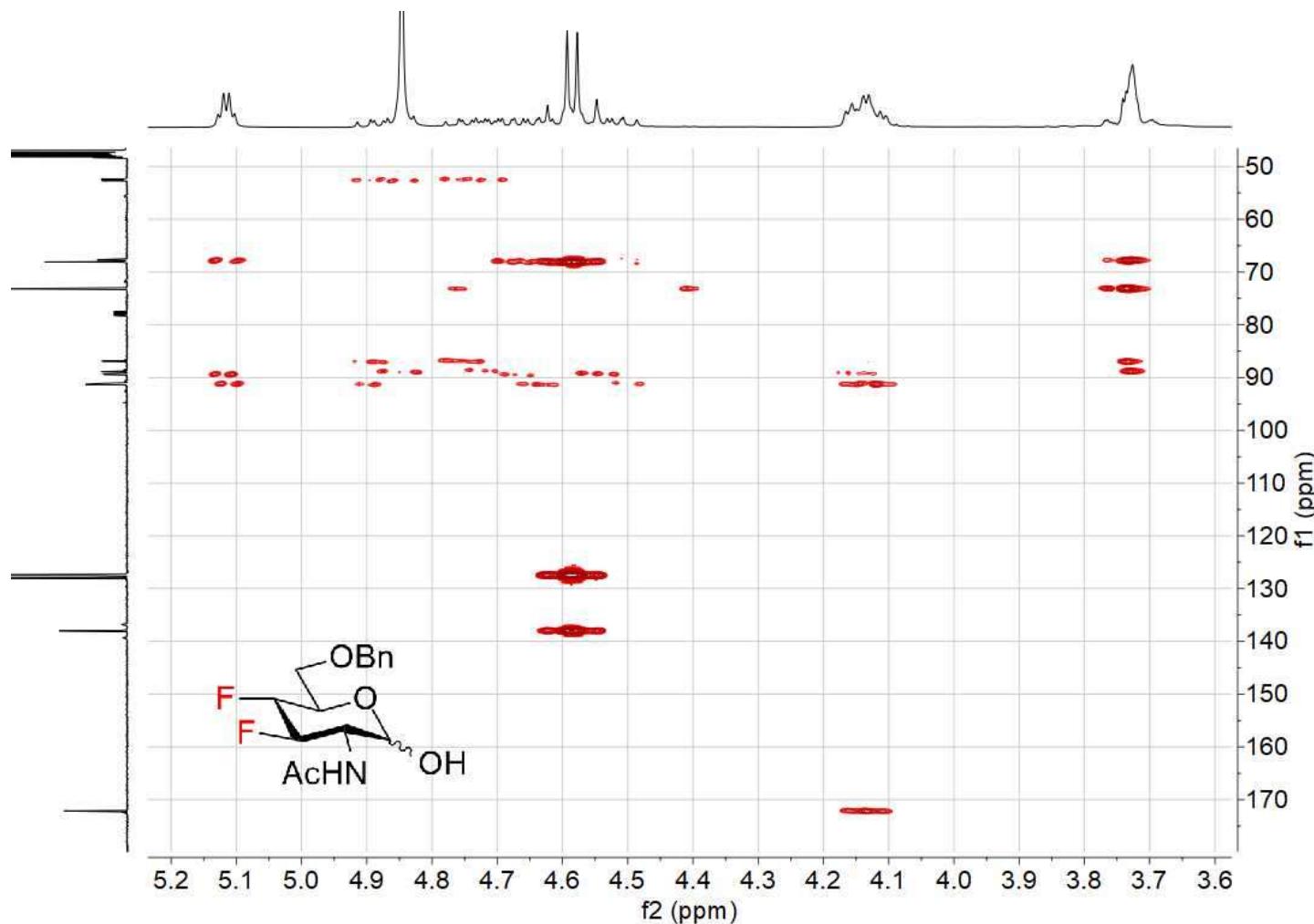
¹⁹F NMR (376 MHz, CD₃OD) 43 (α/β ca. 10/1)



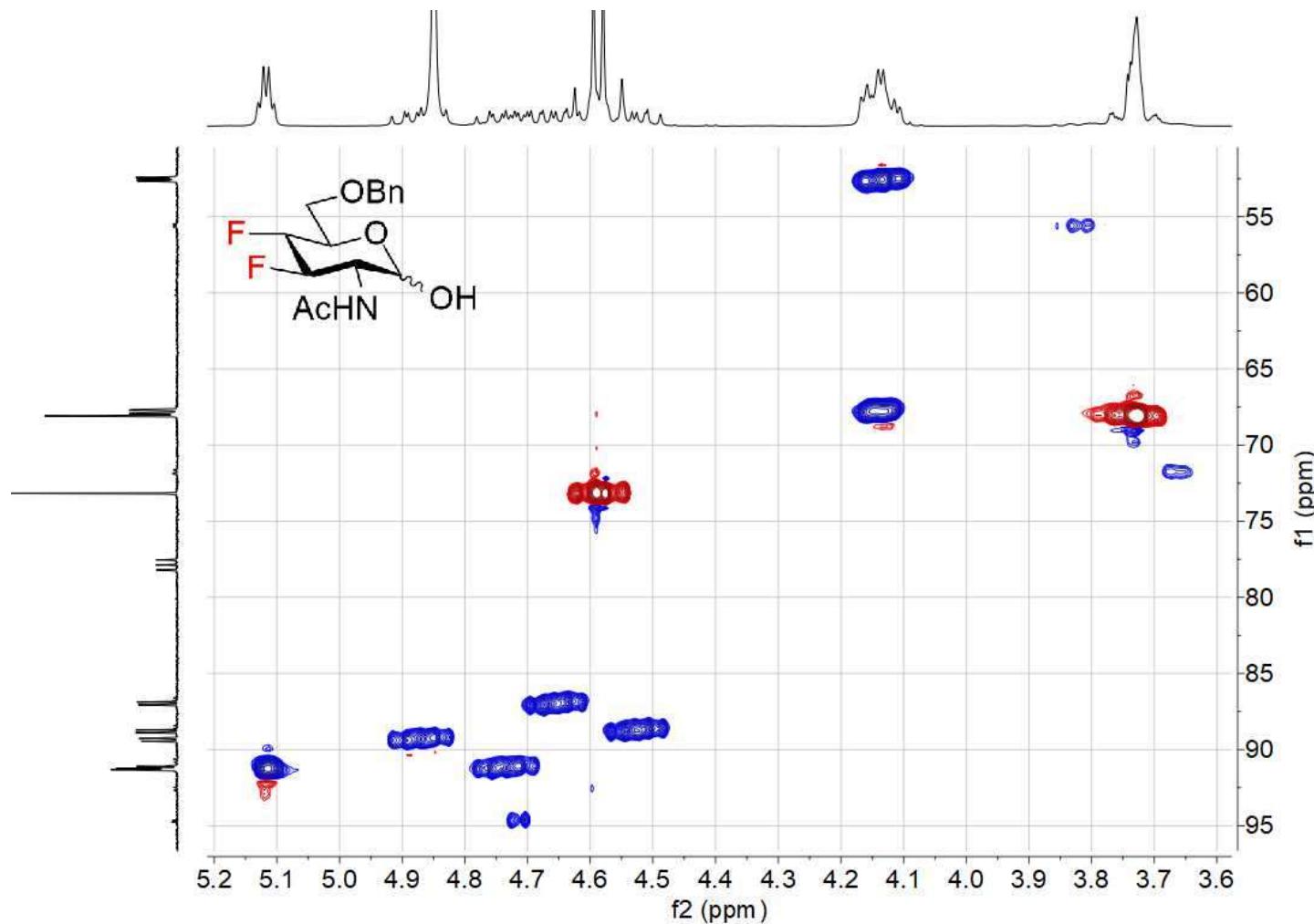
¹H-¹H COSY 43



¹H-¹³C HMBC 43

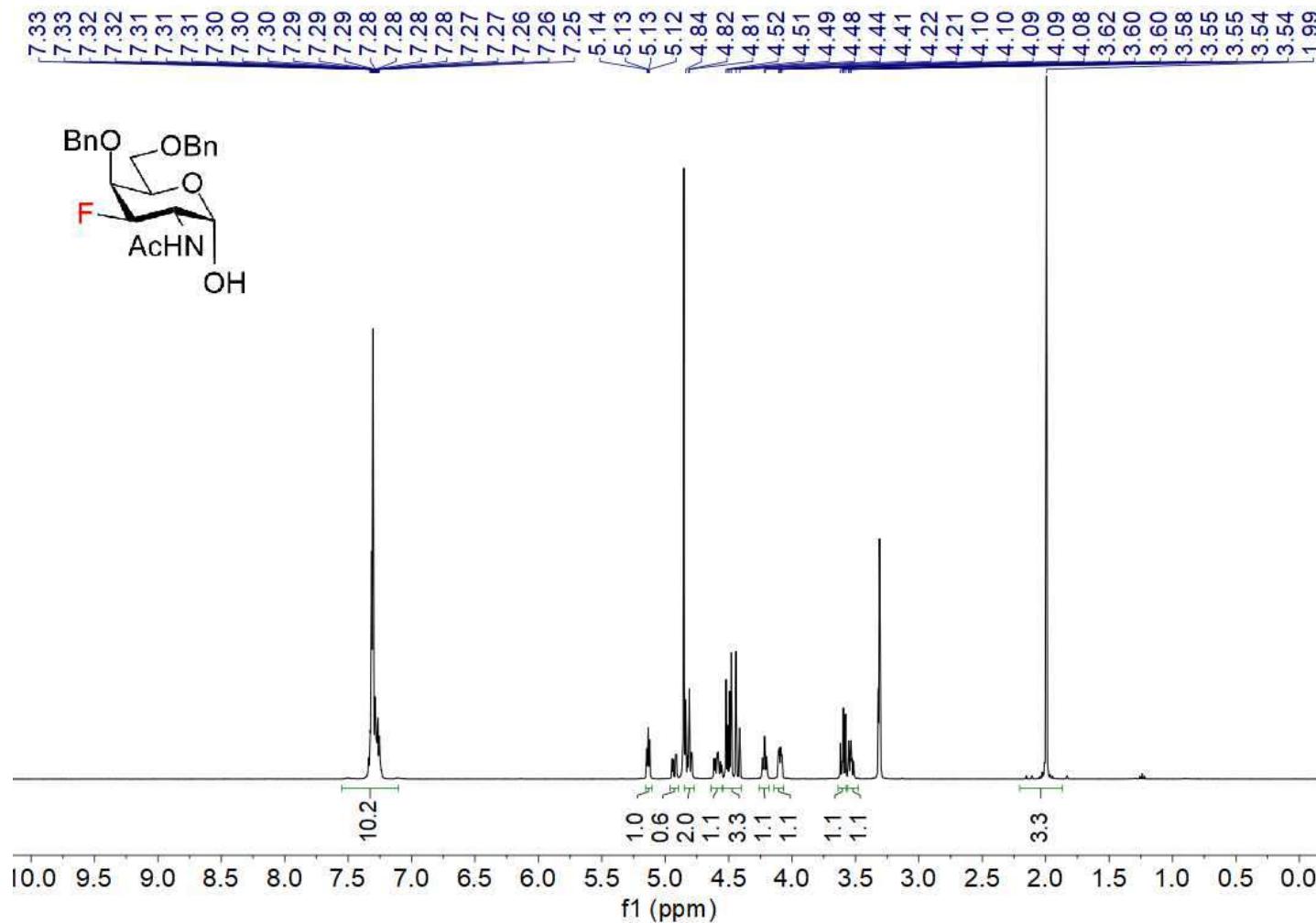


^1H - ^{13}C HSQC 43

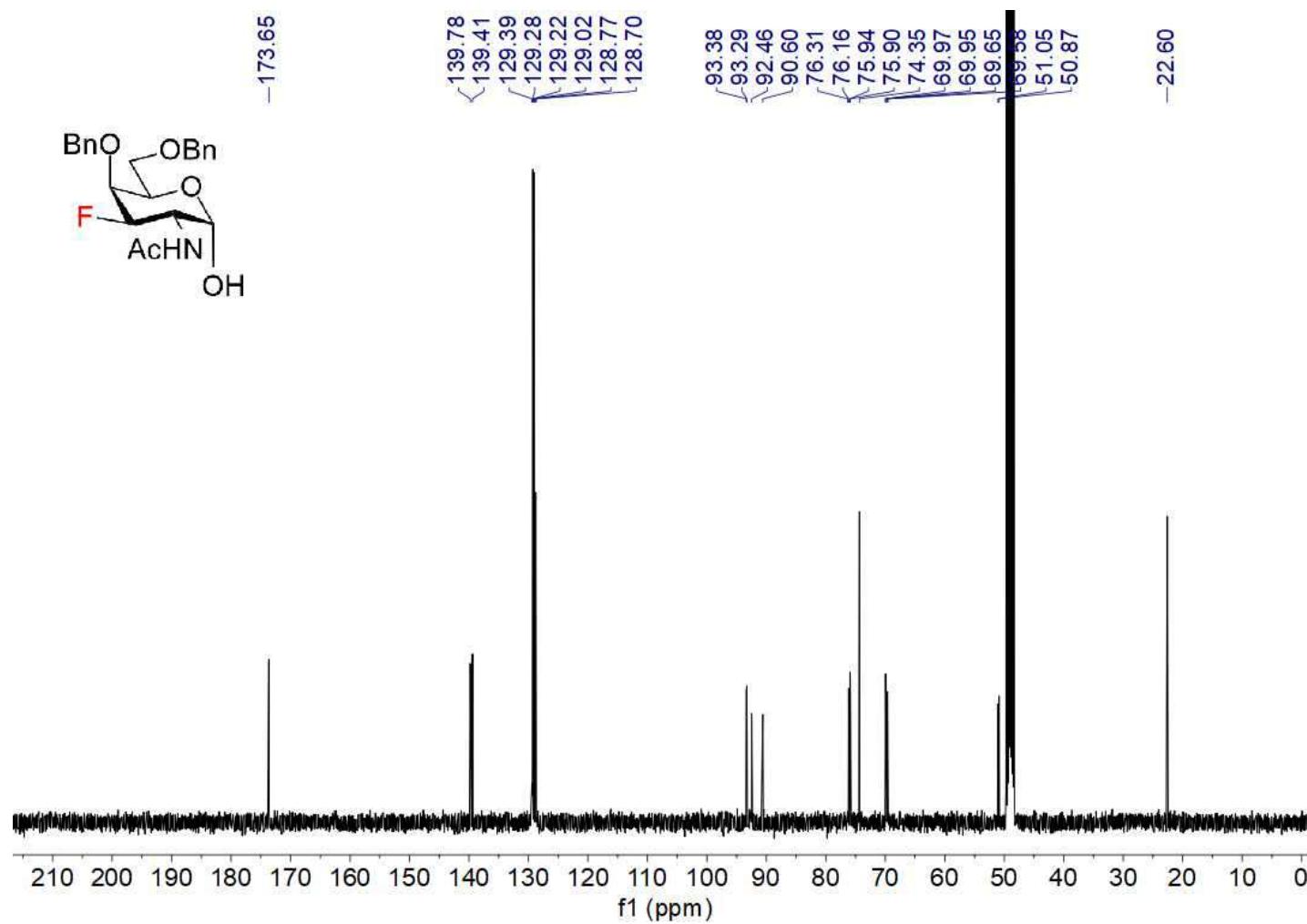


NMR COMPOUND 44

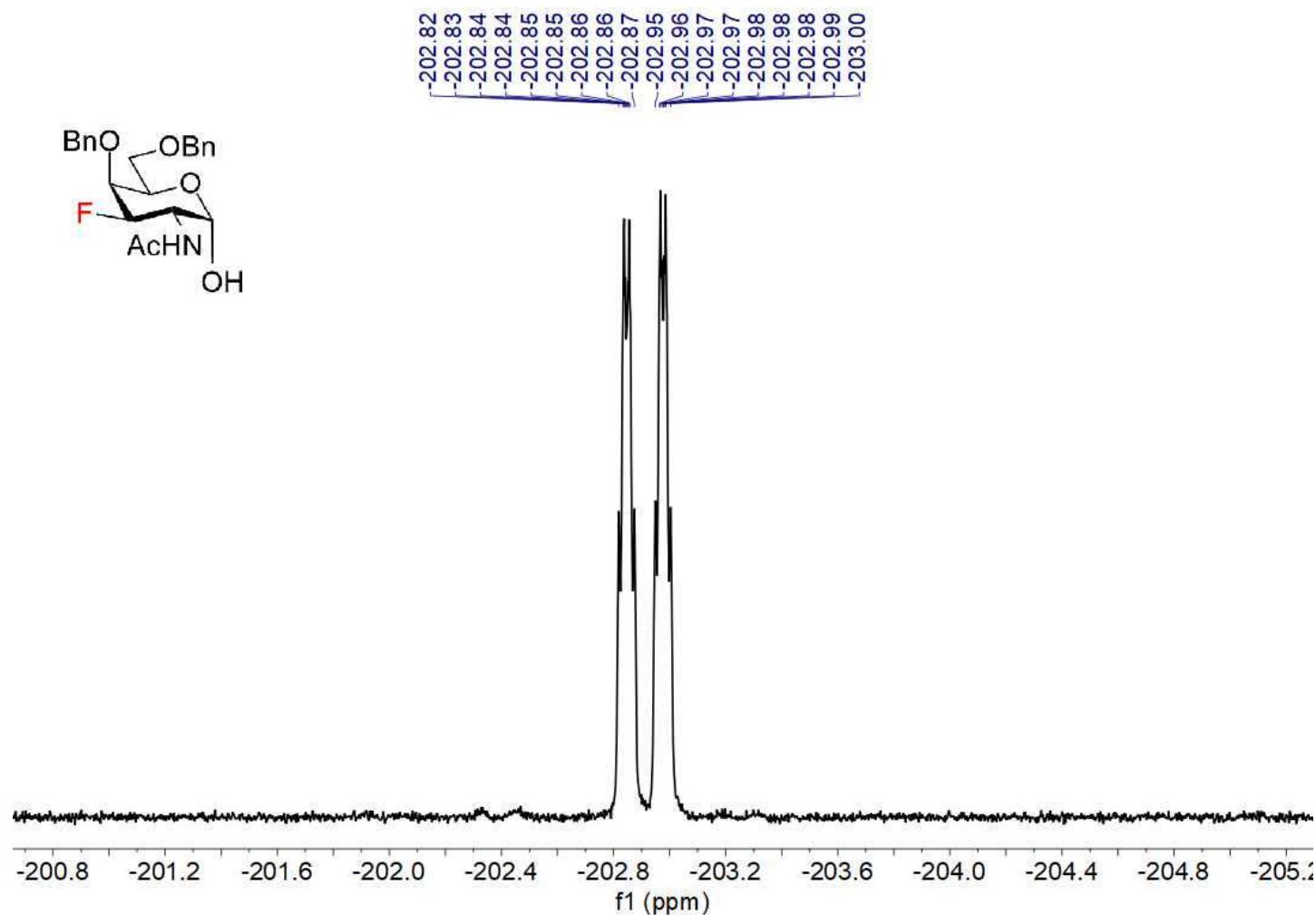
^1H NMR (400 MHz, CD_3OD) 44



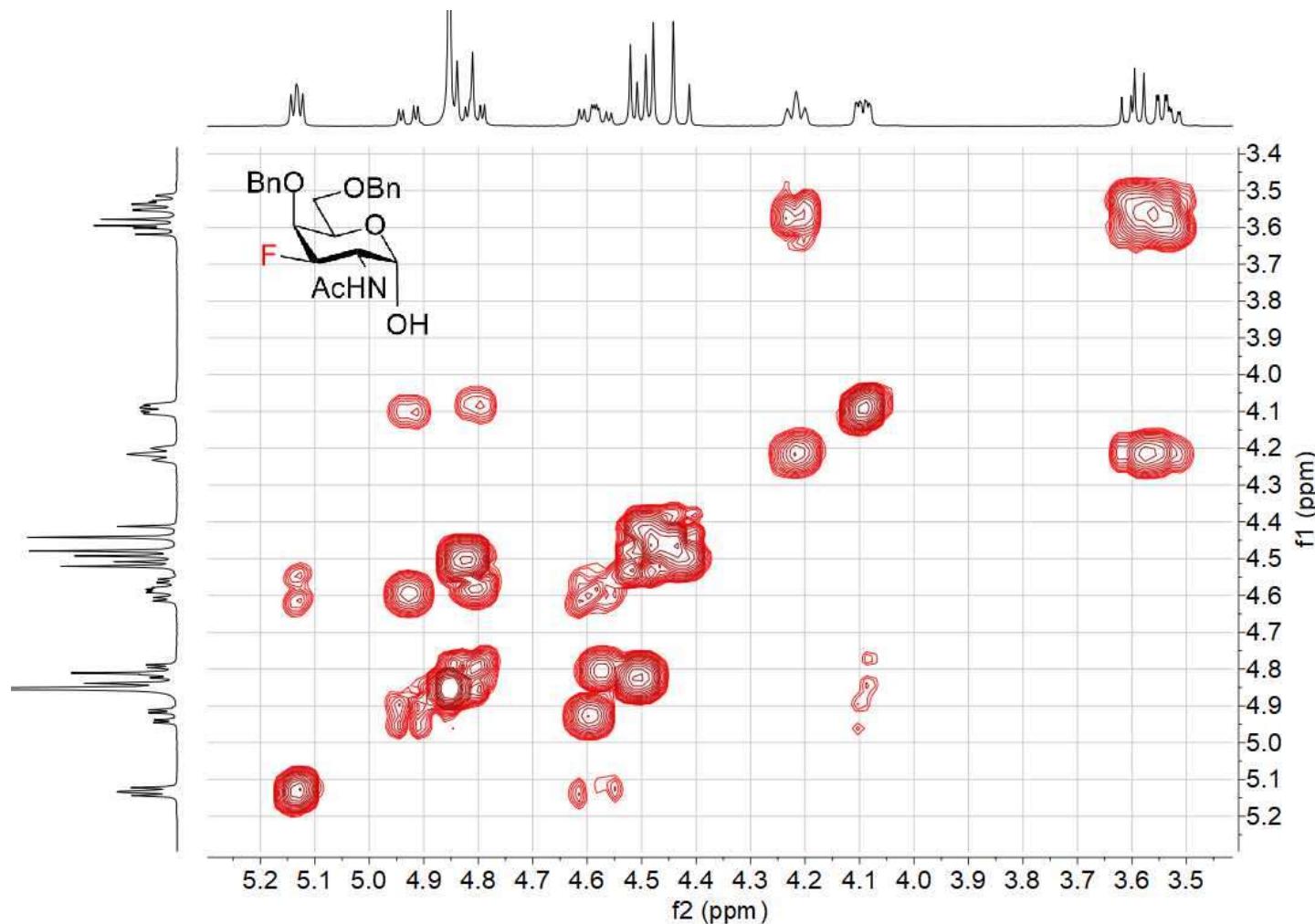
¹³C NMR (100 MHz, CD₃OD) 44



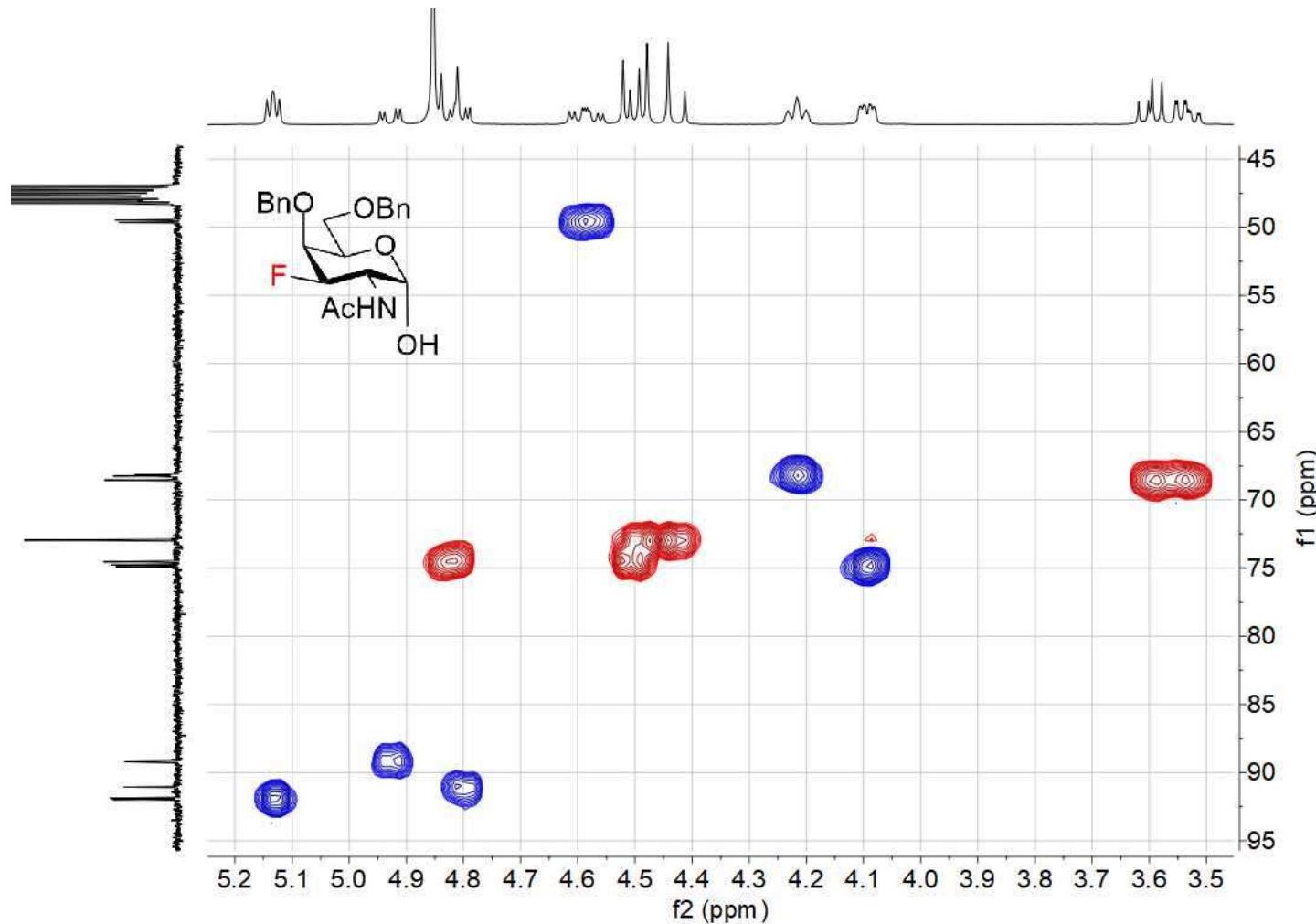
¹⁹F NMR (376 MHz, CD₃OD) 44



¹H-¹H COSY 44

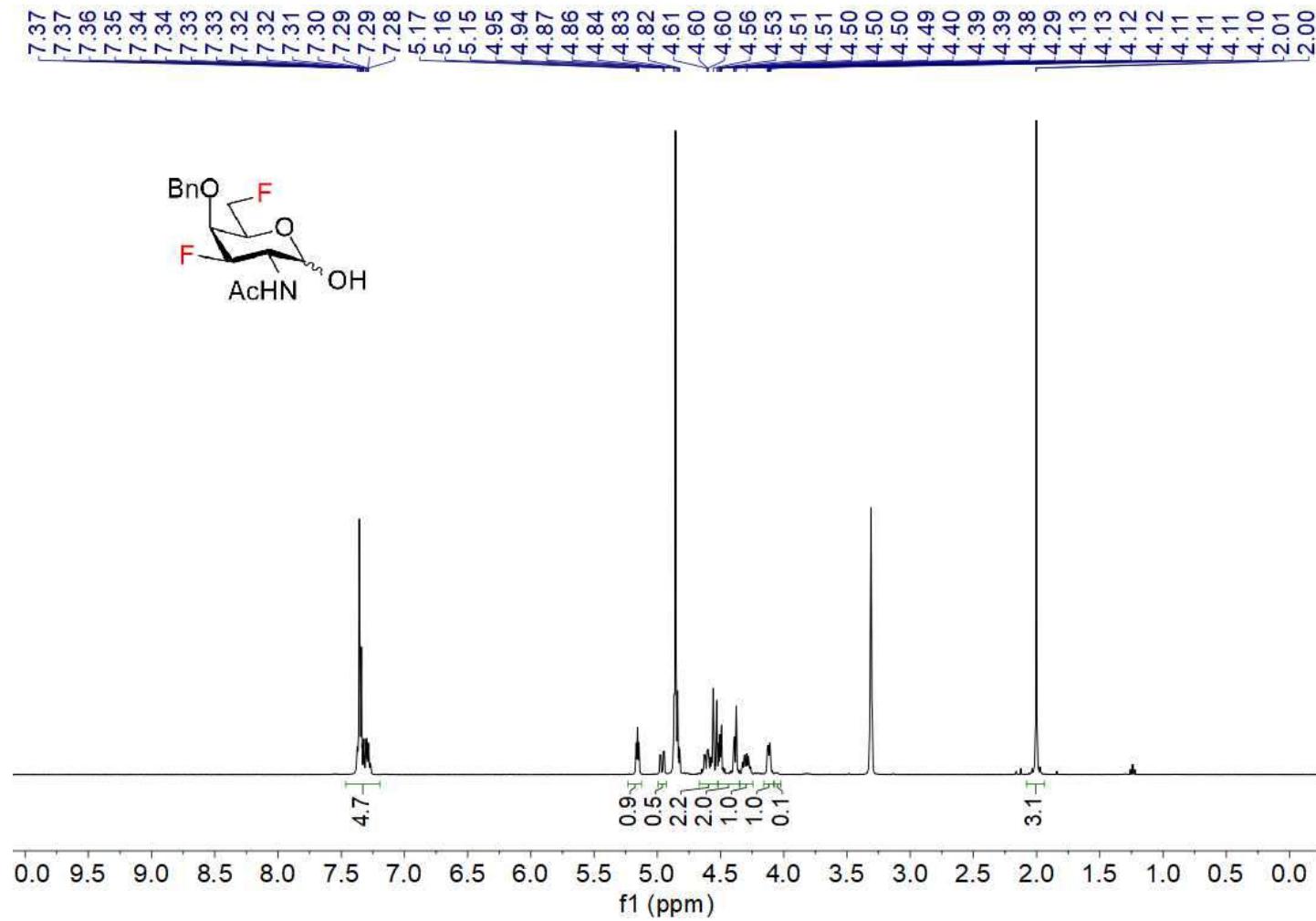


^1H - ^{13}C HSQC 44

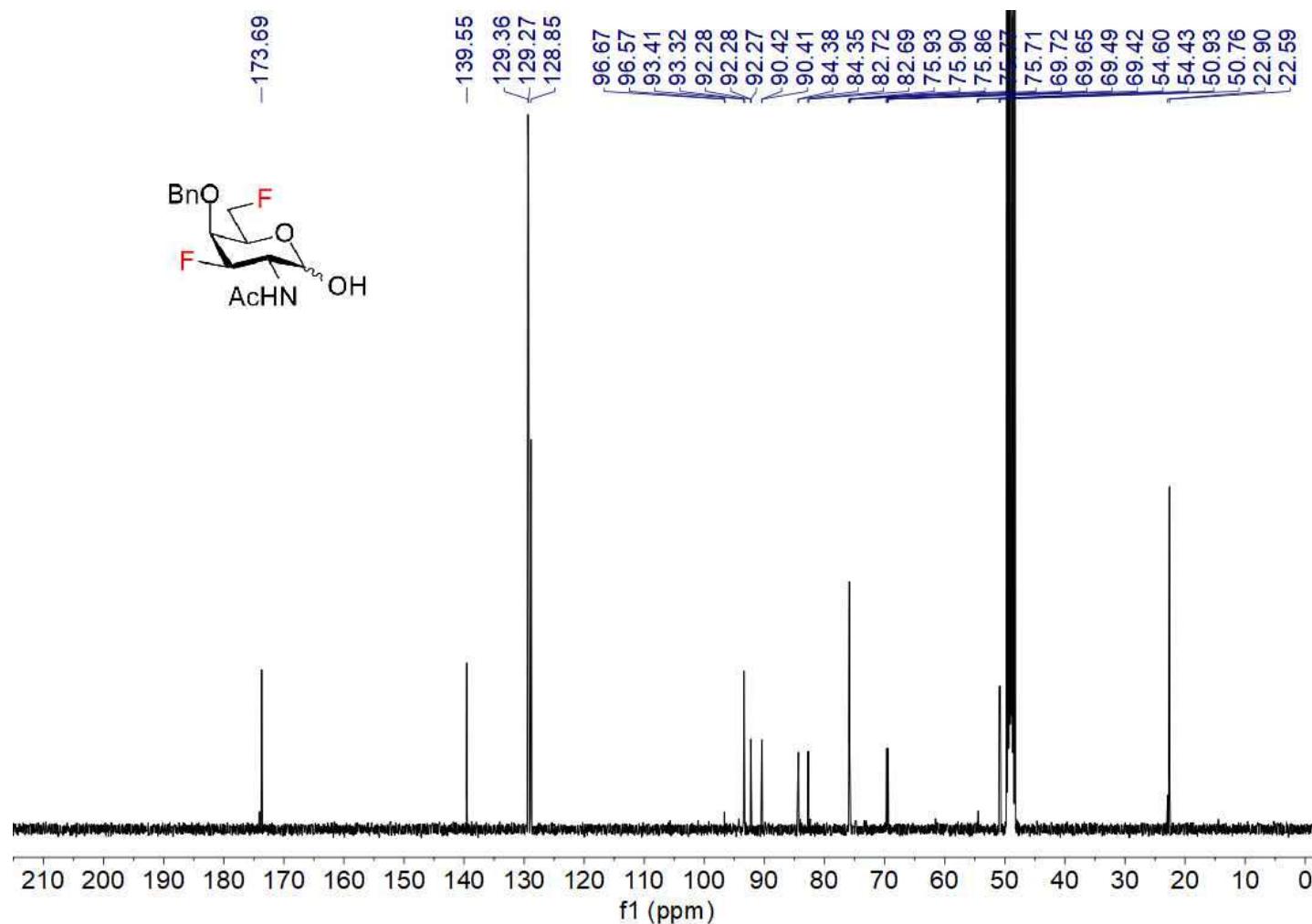


NMR COMPOUND 45

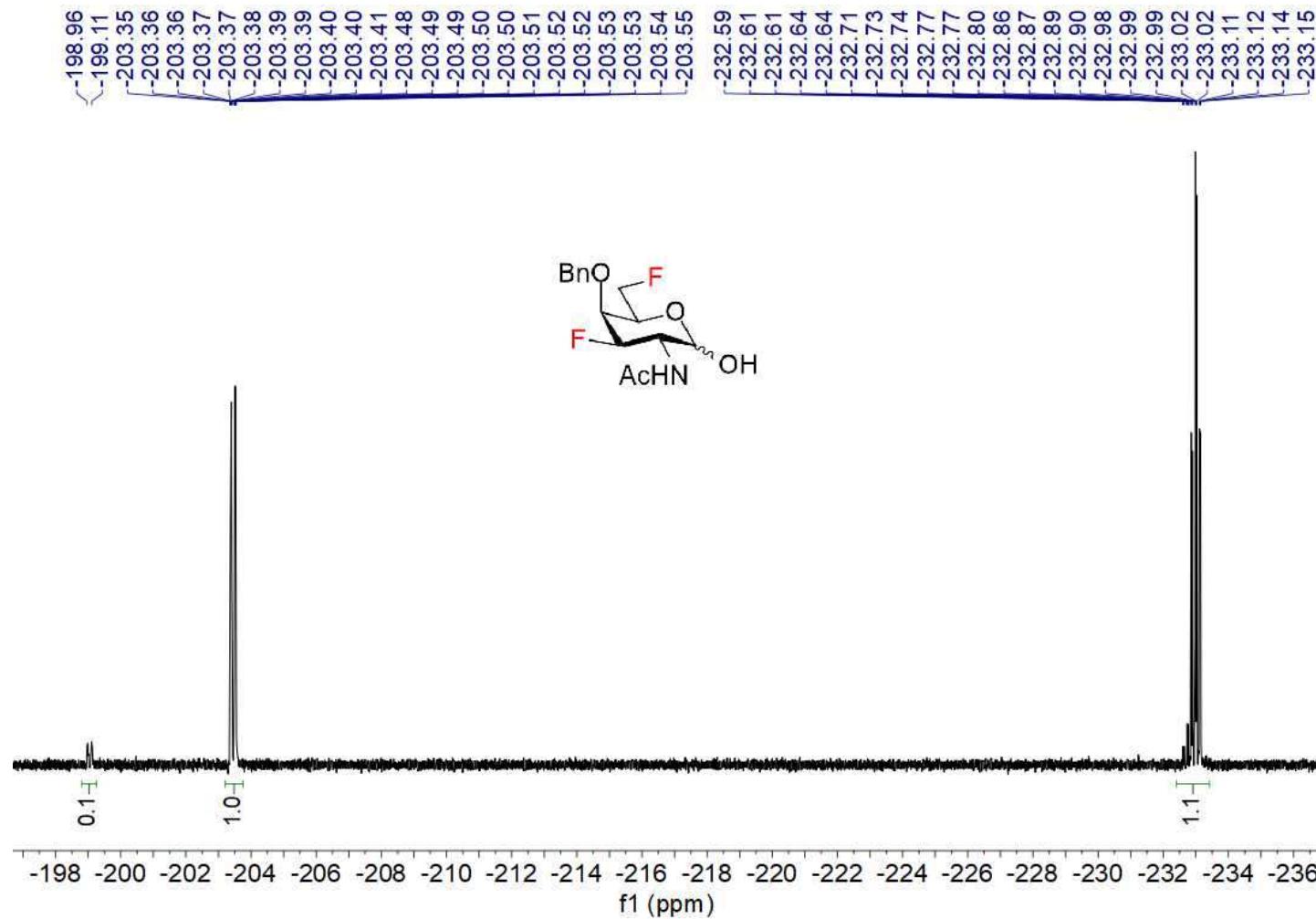
¹H NMR (400 MHz, CD₃OD) 45 (α/β ca. 10/1)



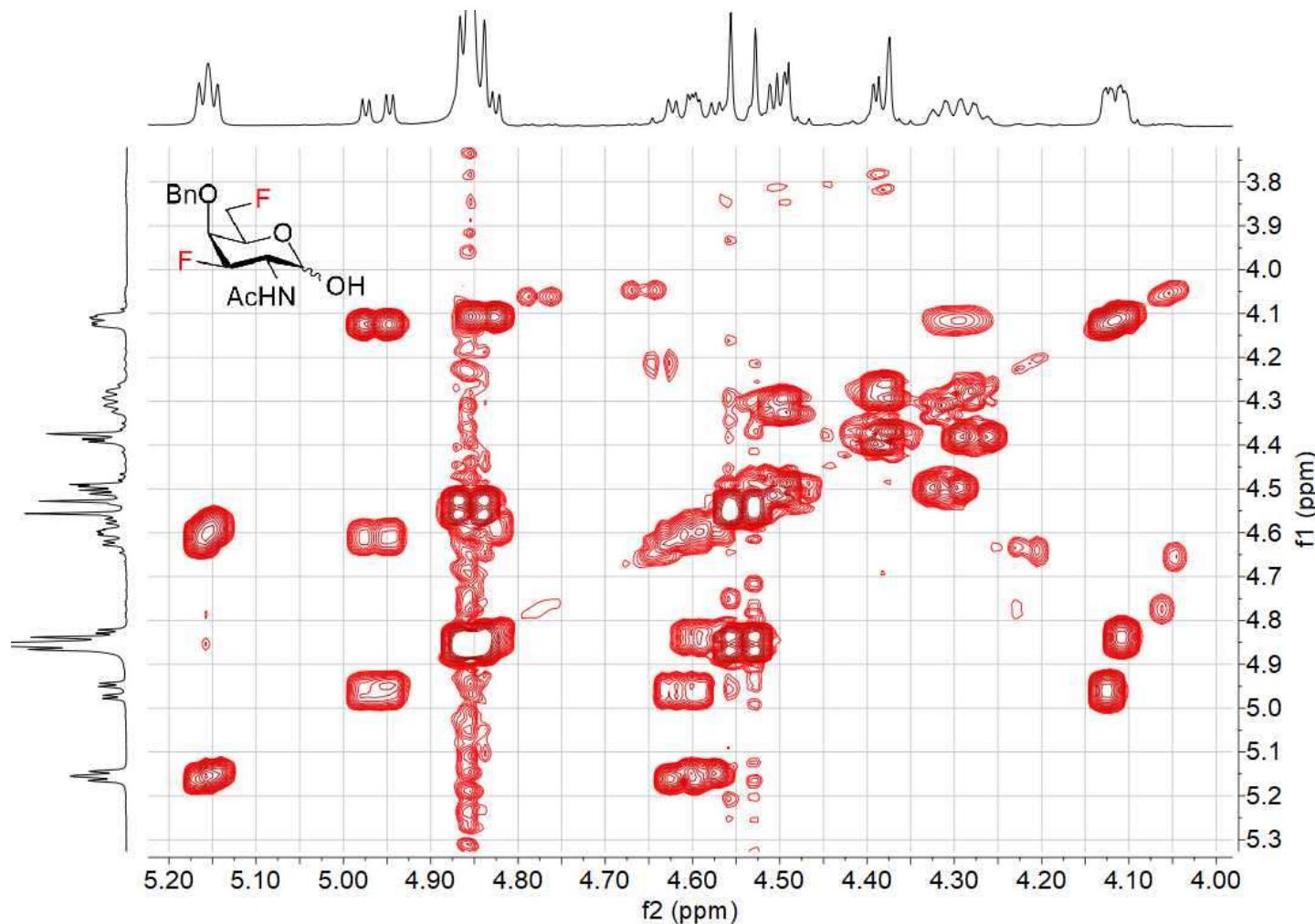
¹³C NMR (100 MHz, CD₃OD) 45



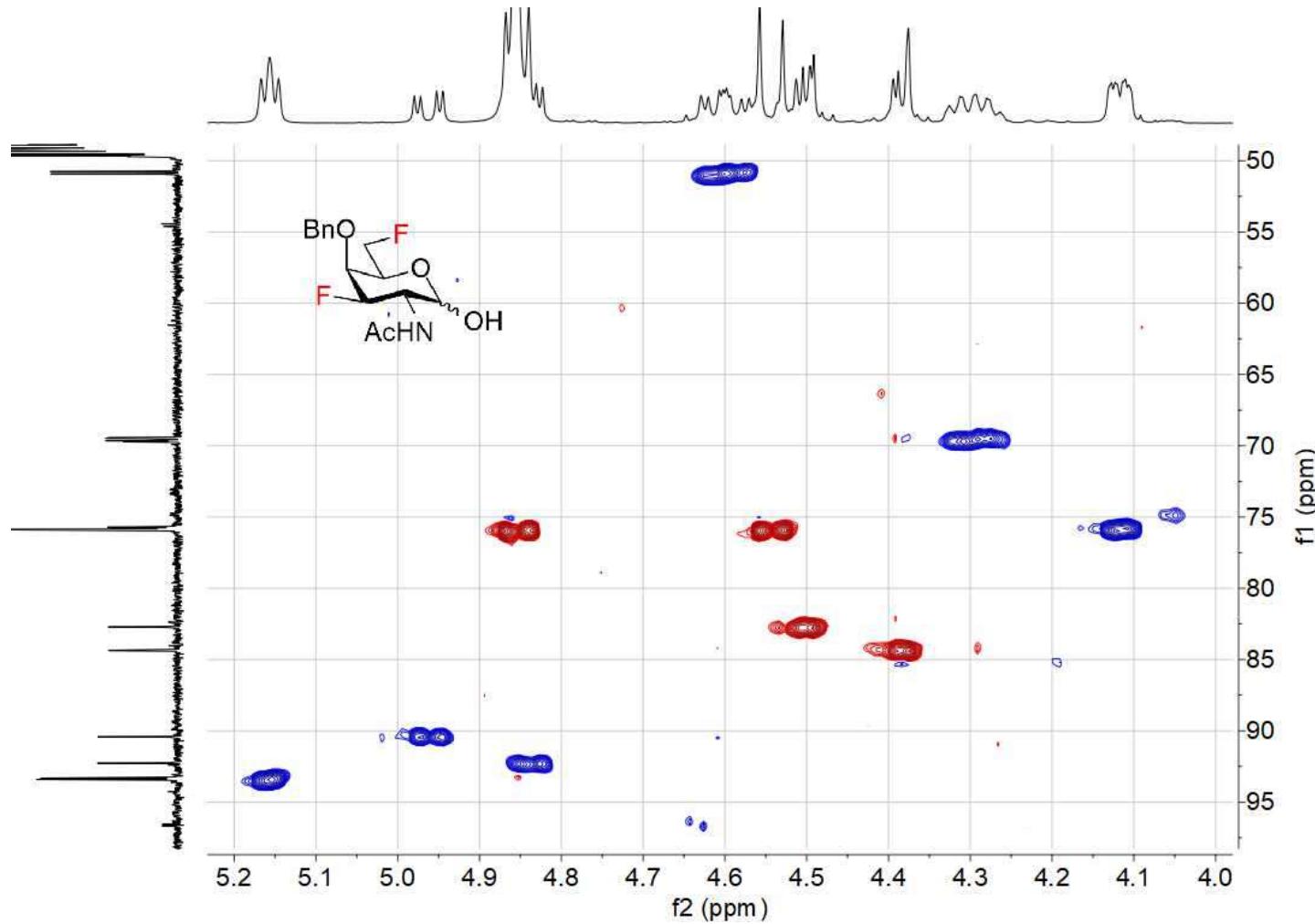
¹⁹F NMR (376 MHz, CD₃OD) 45 (α/β ca. 10/1)



¹H-¹H COSY 45

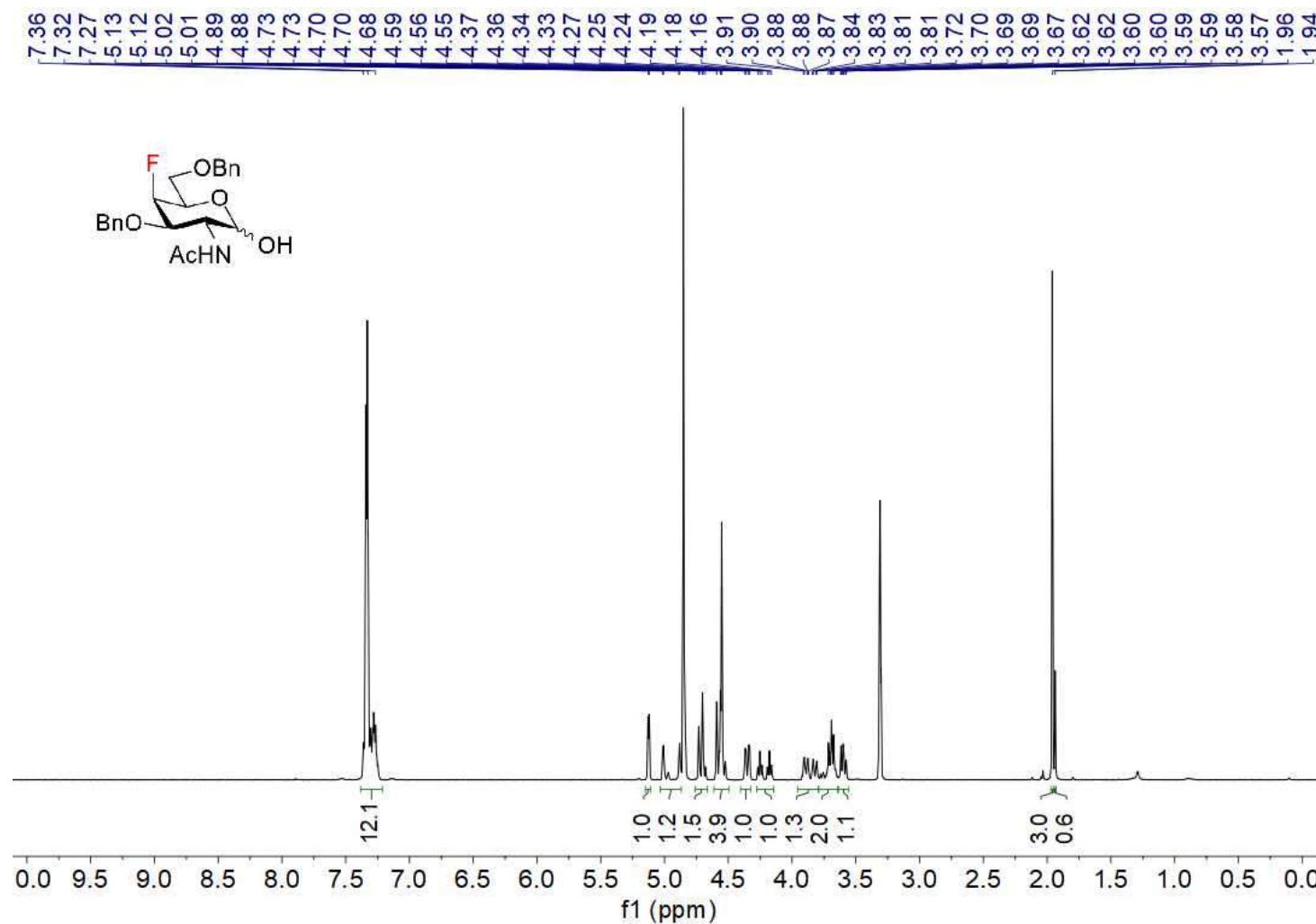


¹H-¹³C HSQC 45

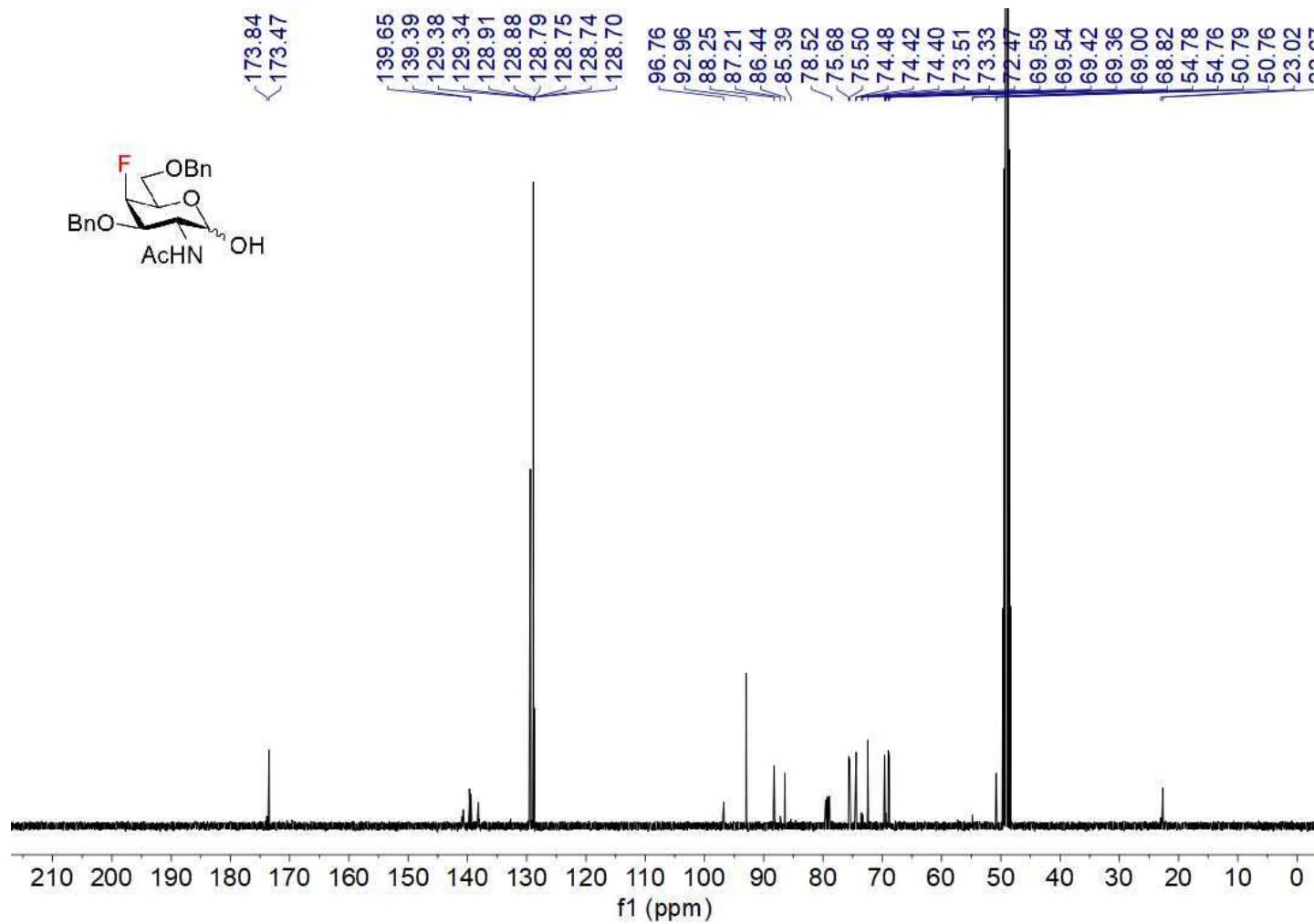


NMR COMPOUND 46

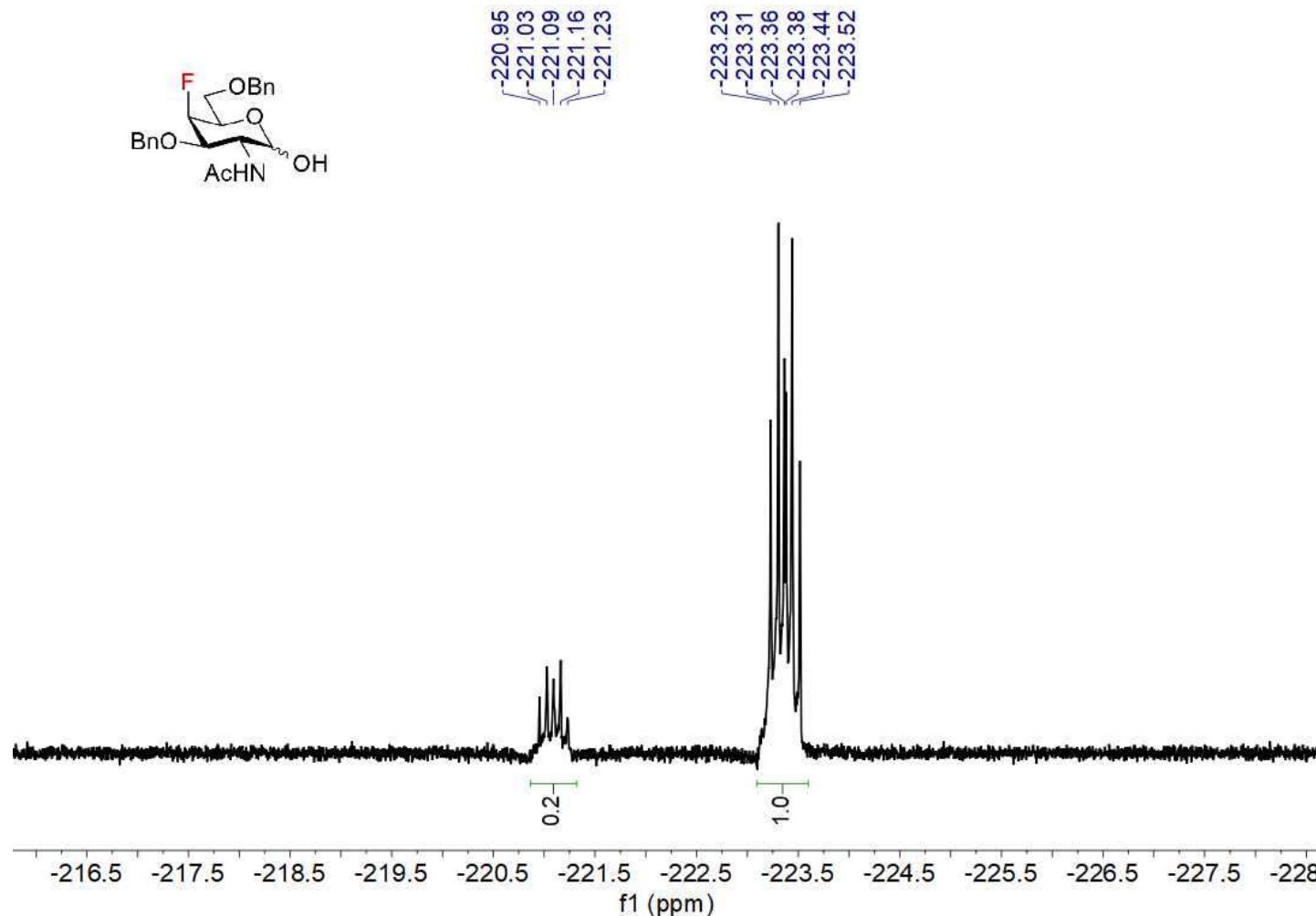
¹H NMR (400 MHz, CD₃OD) 46 (α/β ca. 5/1)



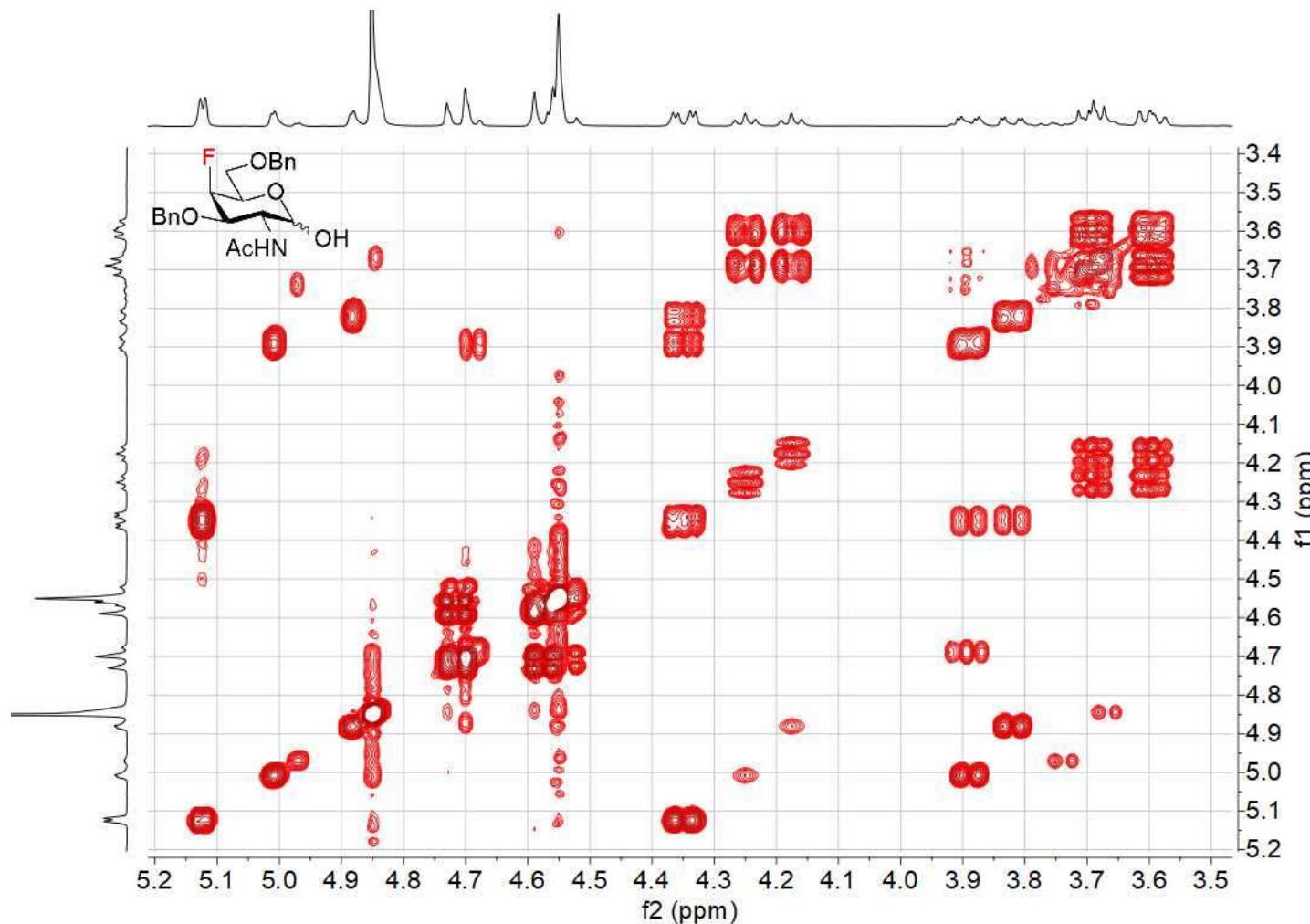
¹³C NMR (100 MHz, CD₃OD) 46



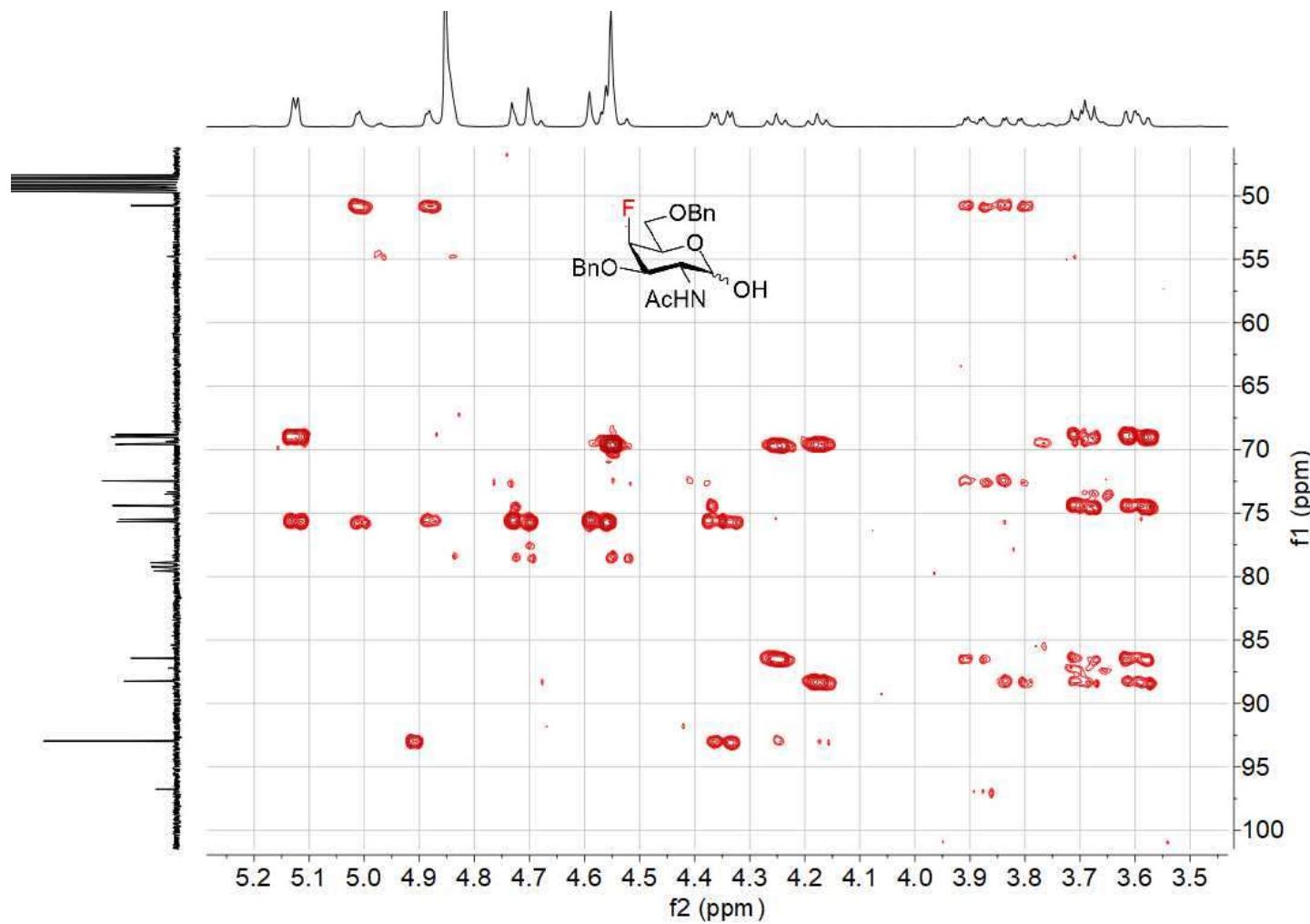
¹⁹F NMR (376 MHz, CD₃OD) 46 (α/β ca. 5/1)



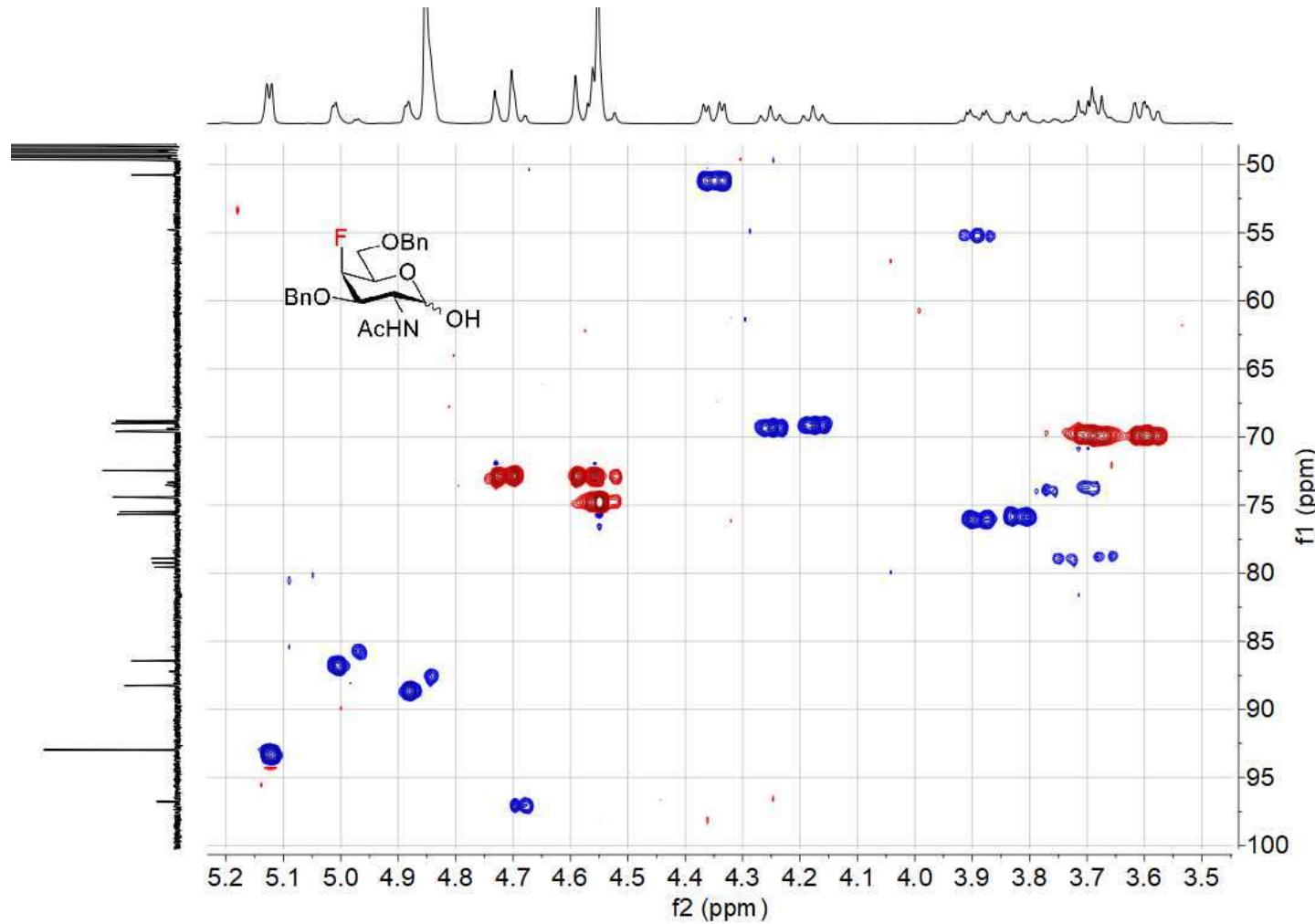
¹H-¹H COSY 46



^1H - ^{13}C HMBC 46

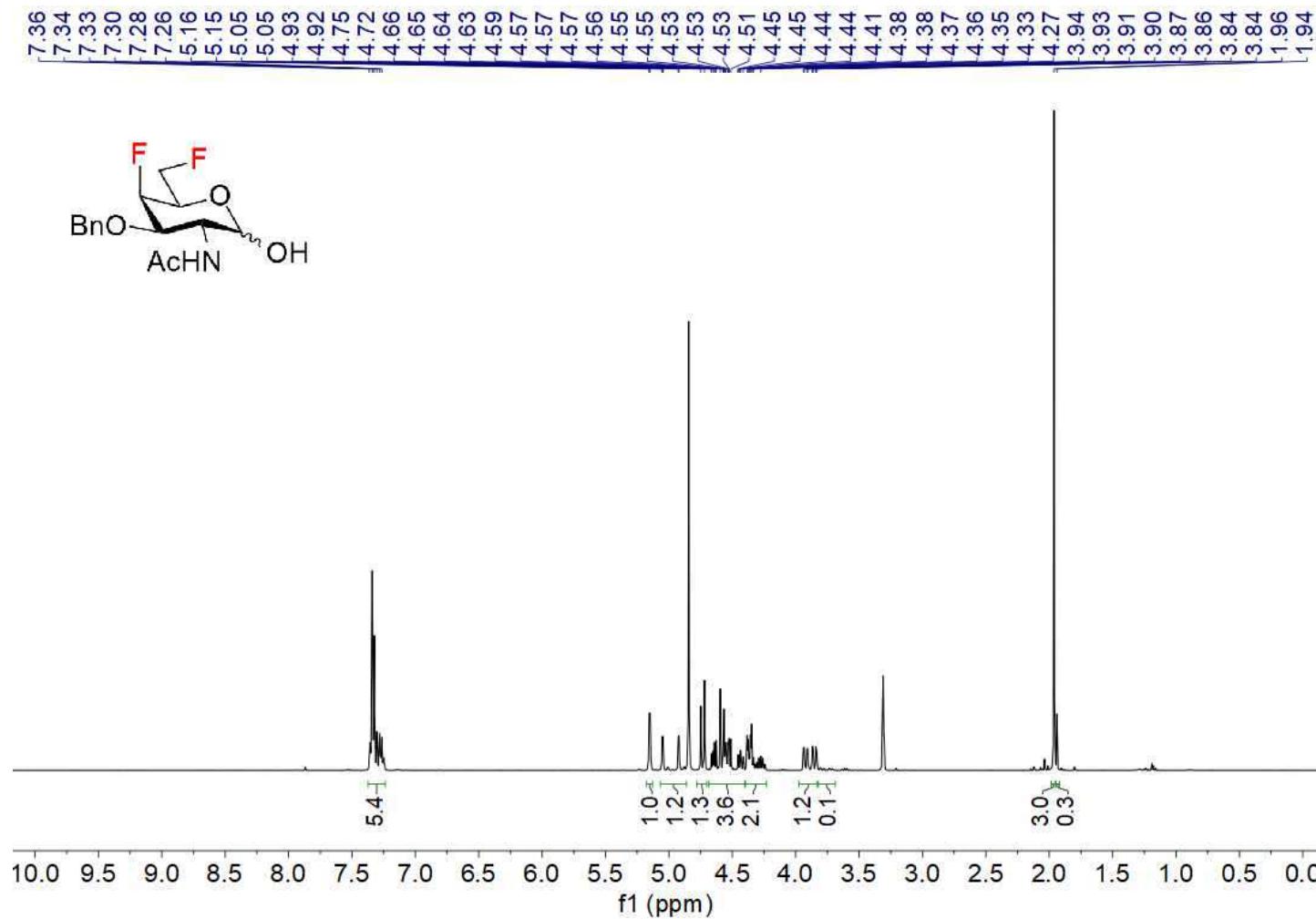


¹H-¹³C HSQC 46

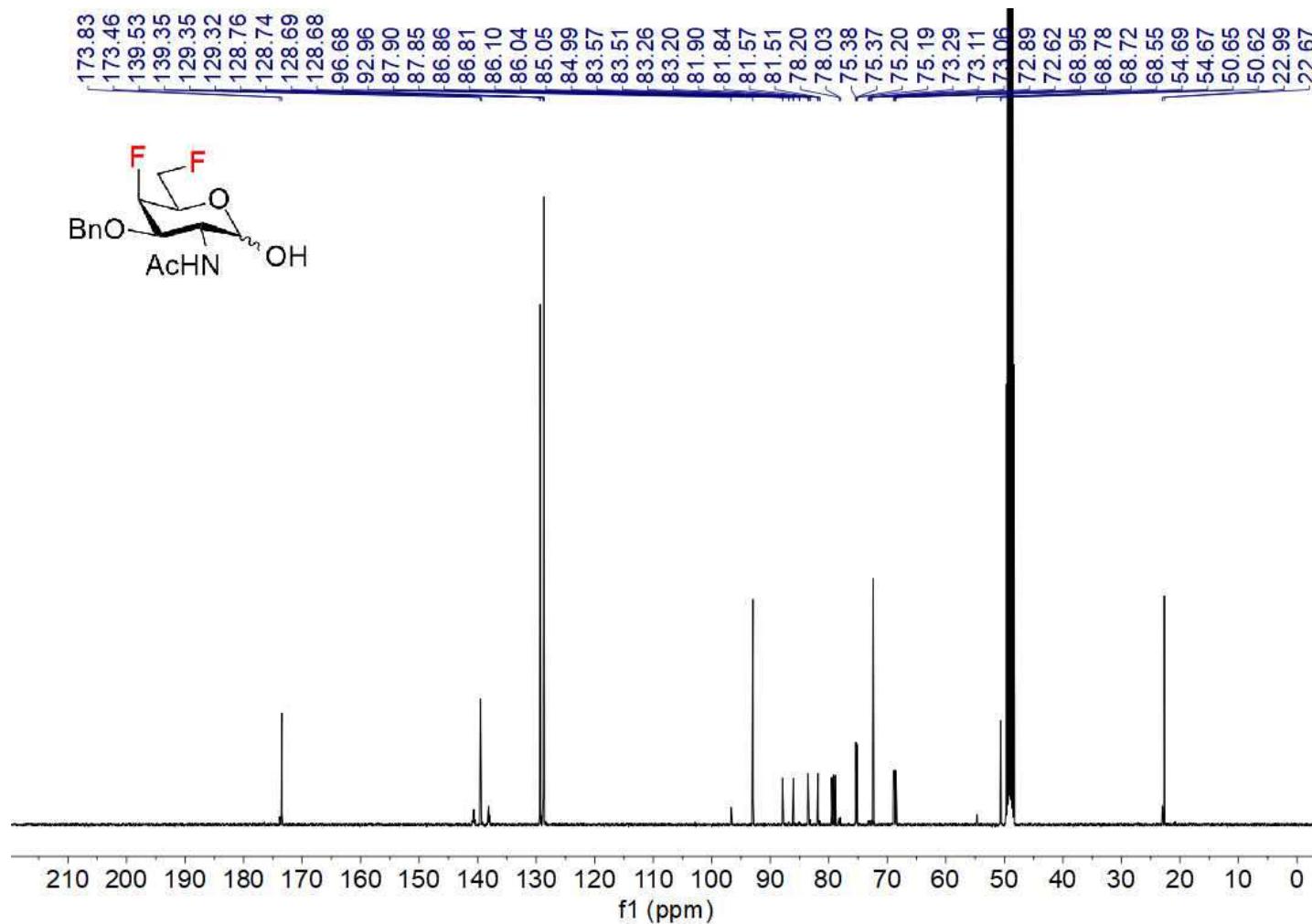


NMR COMPOUND 47

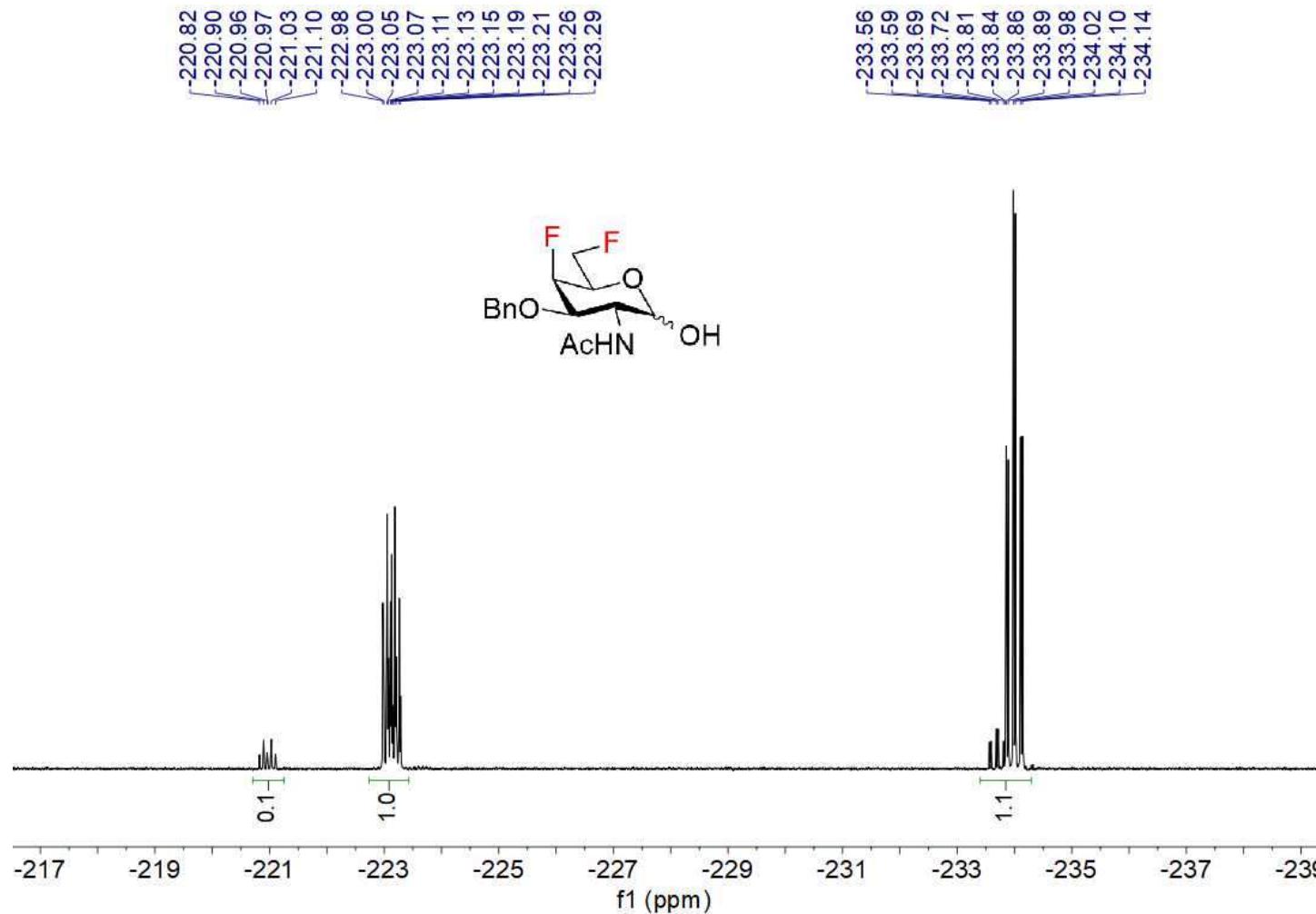
¹H NMR (400 MHz, CD₃OD) 47 (α/β ca. 10/1)



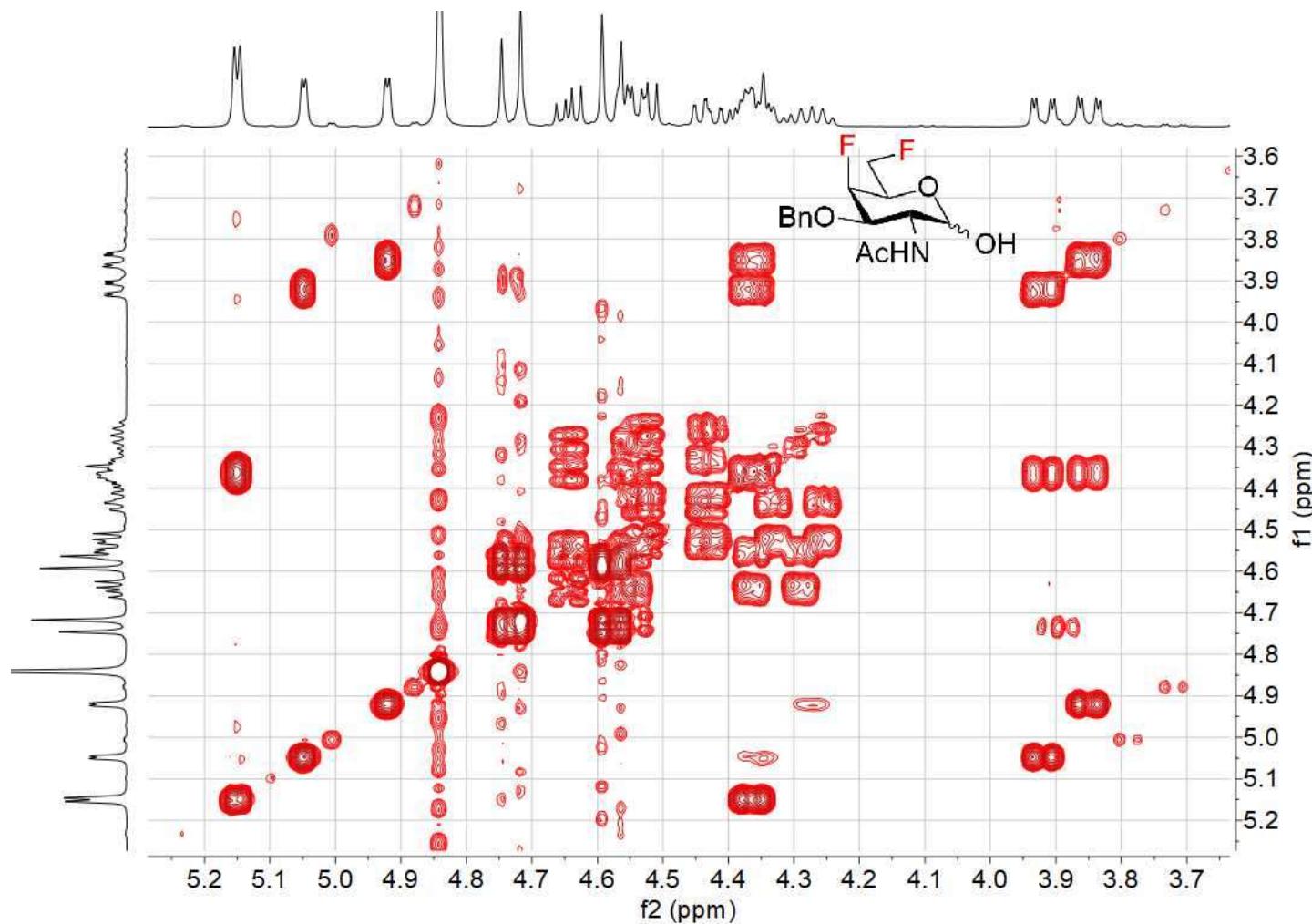
¹³C NMR (100 MHz, CD₃OD) 47



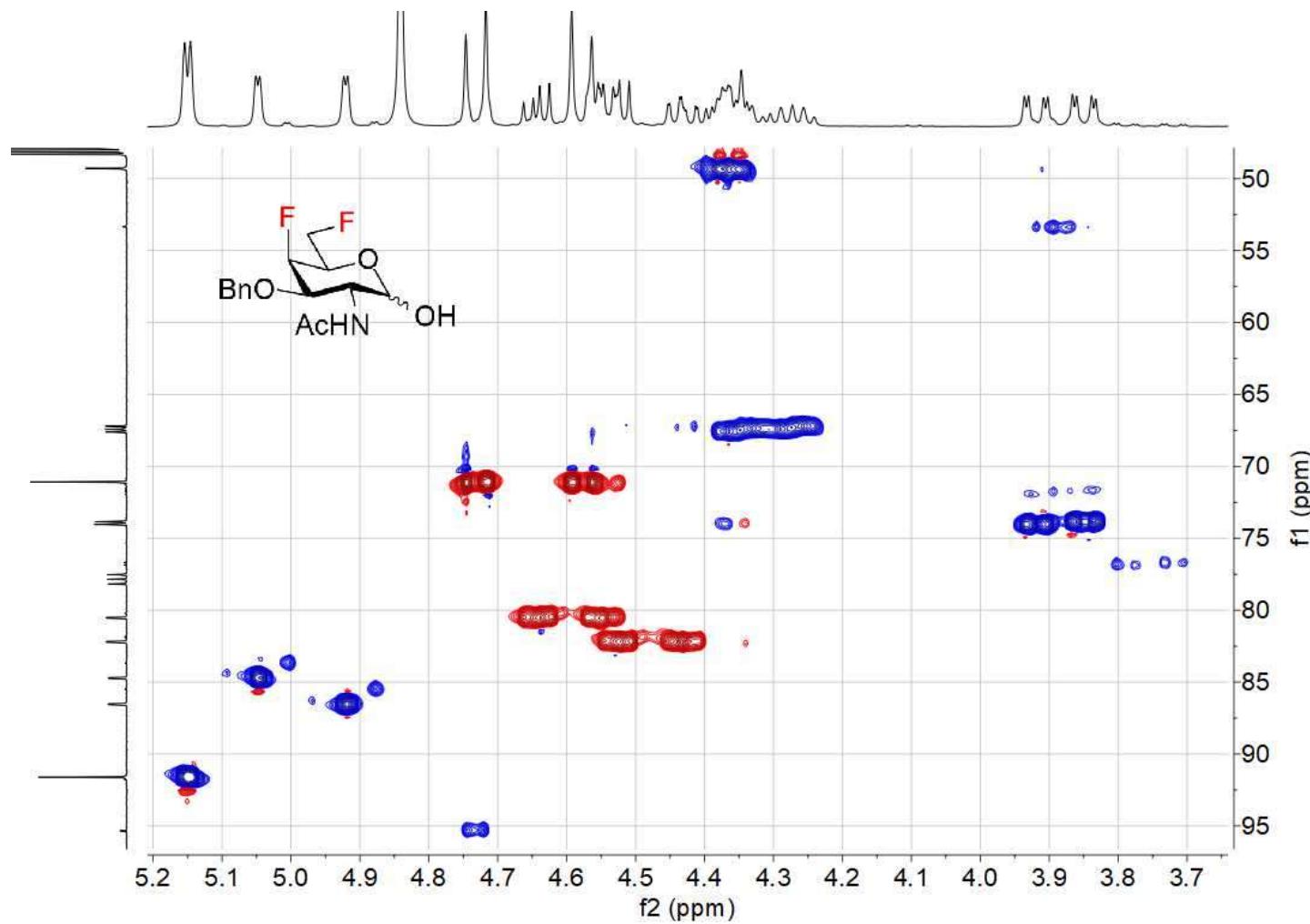
¹⁹F NMR (376 MHz, CD₃OD) 47 (α/β ca. 10/1)



¹H-¹H COSY NMR 47

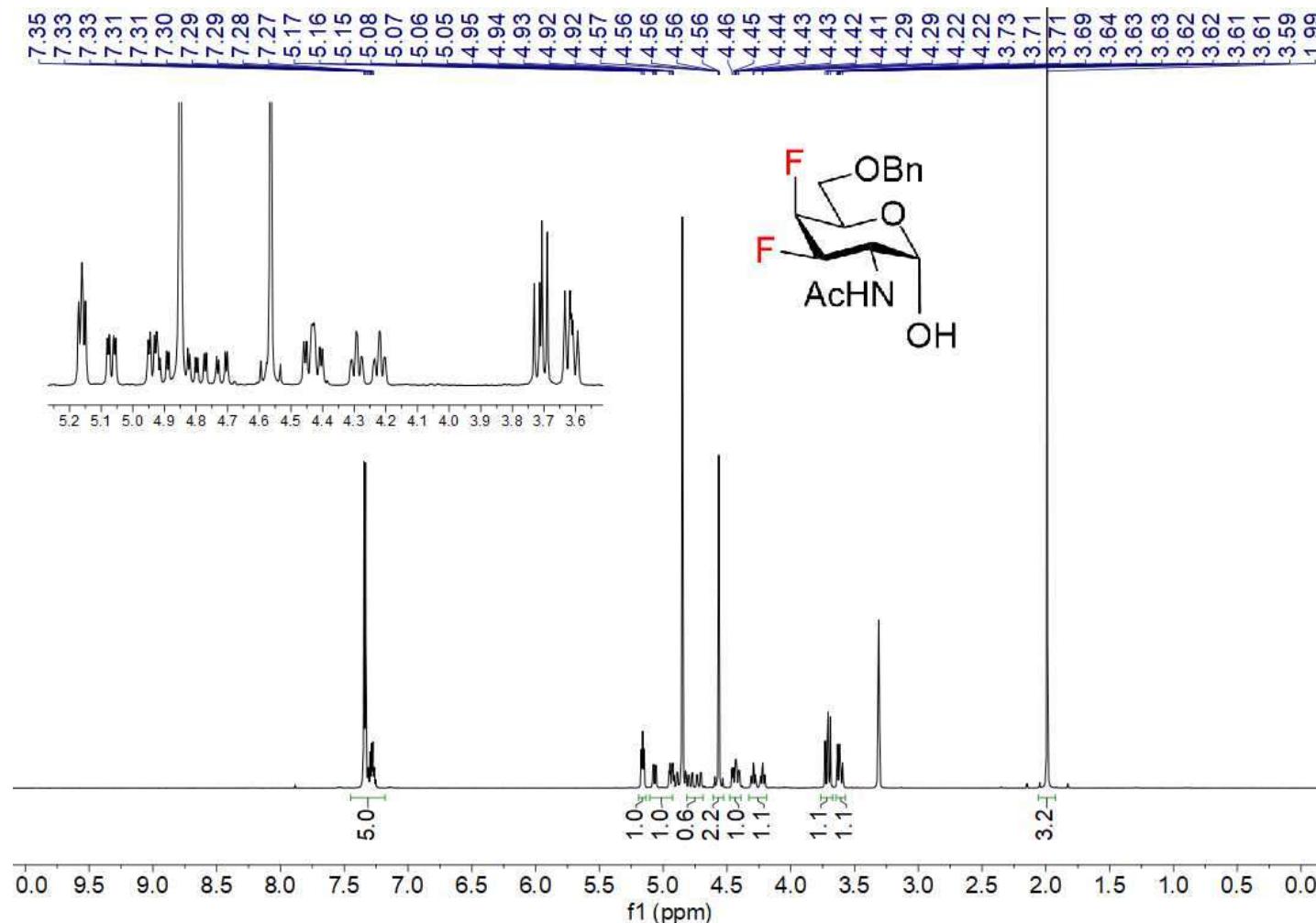


^1H - ^{13}C HSQC NMR 47

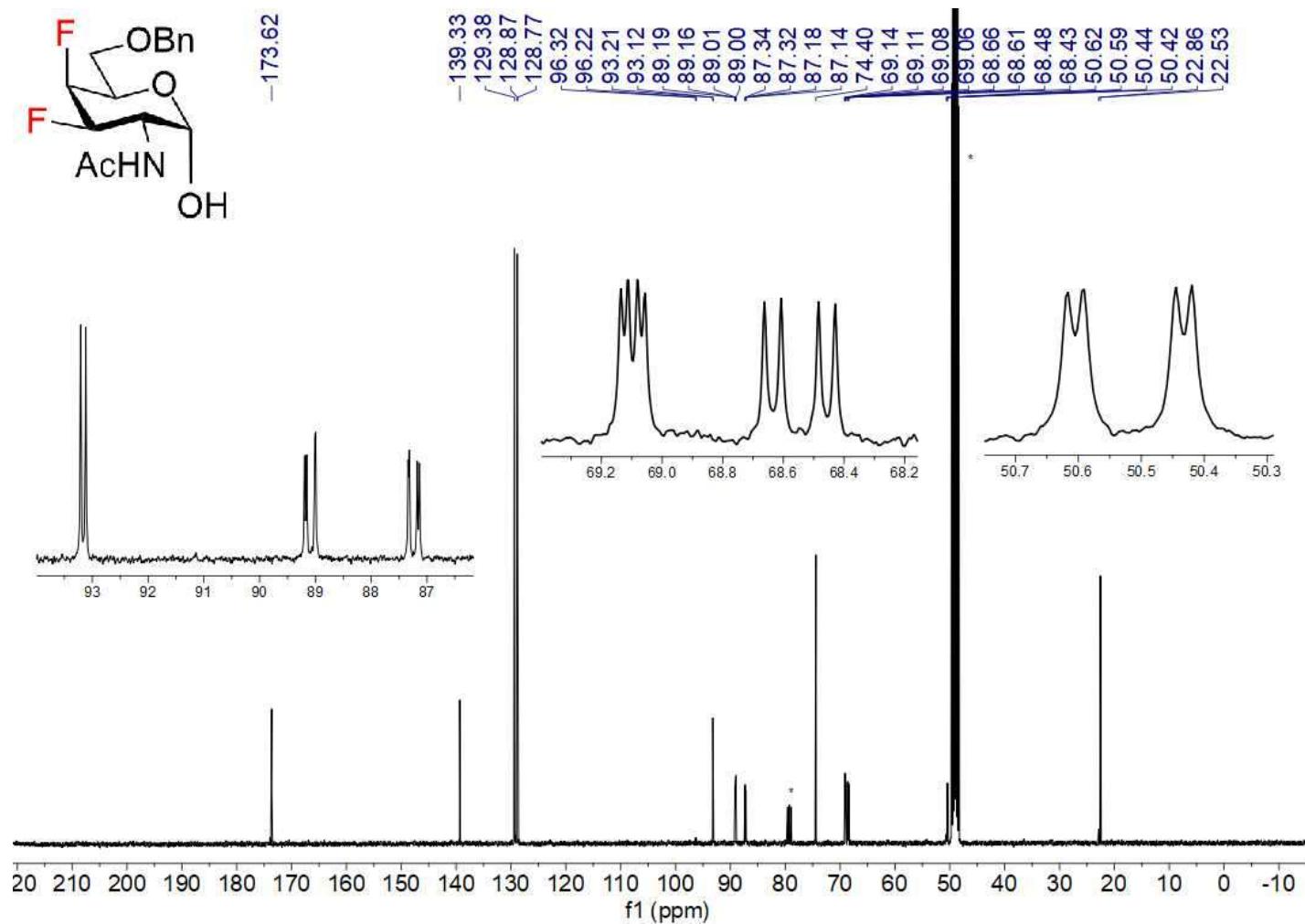


NMR COMPOUND 48

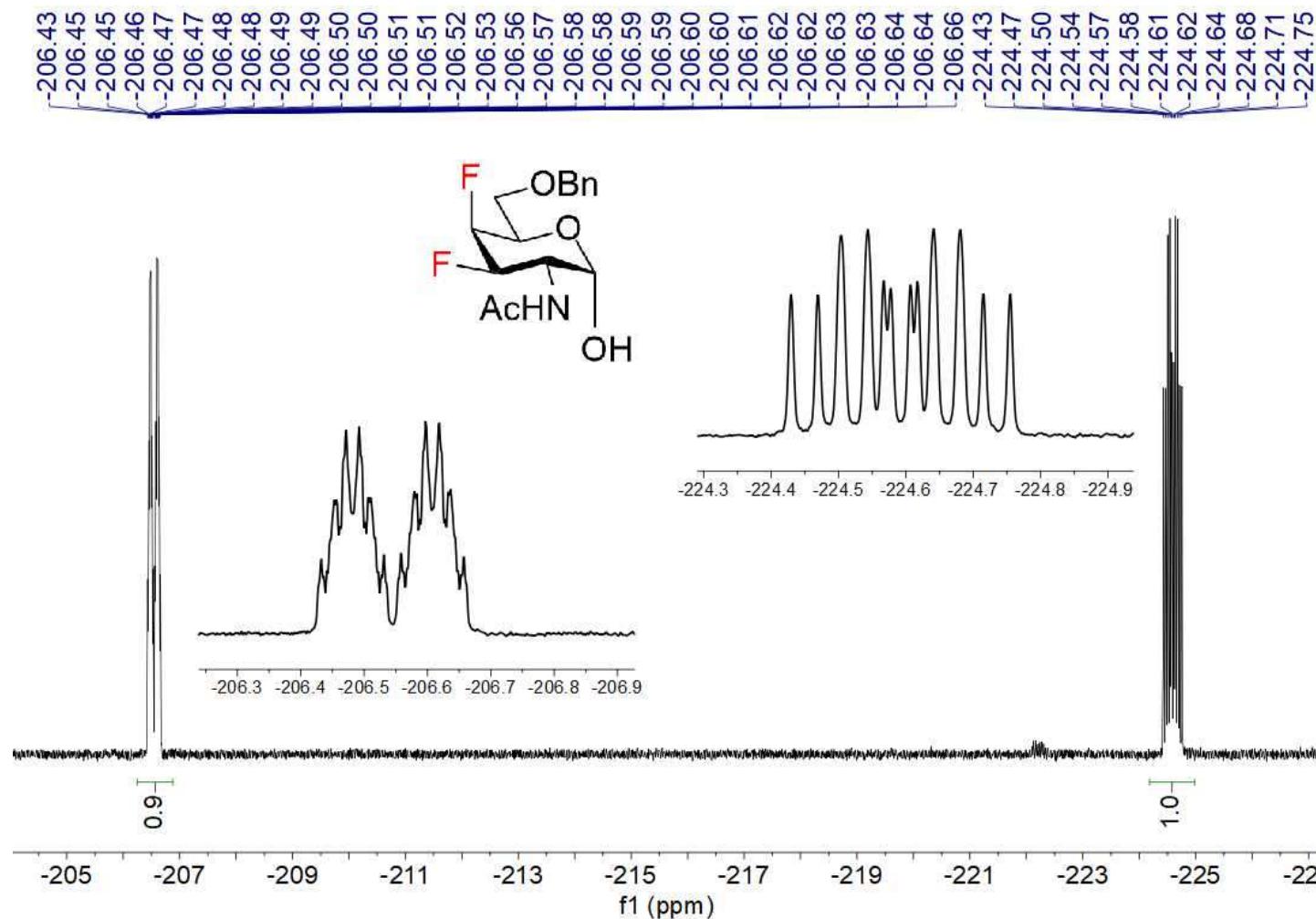
^1H NMR (400 MHz, CD_3OD) 48



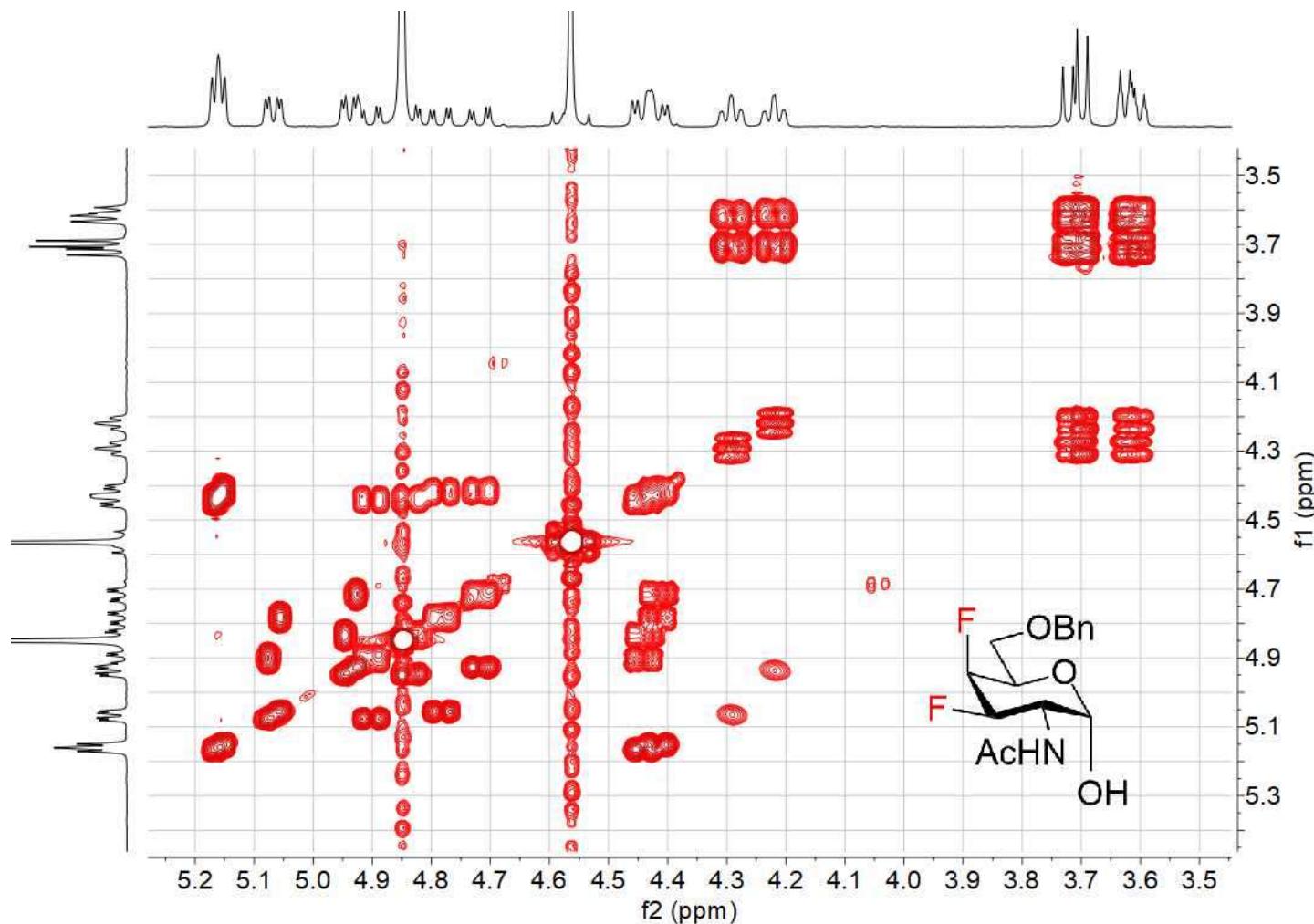
¹³C NMR (100 MHz, CD₃OD) 48



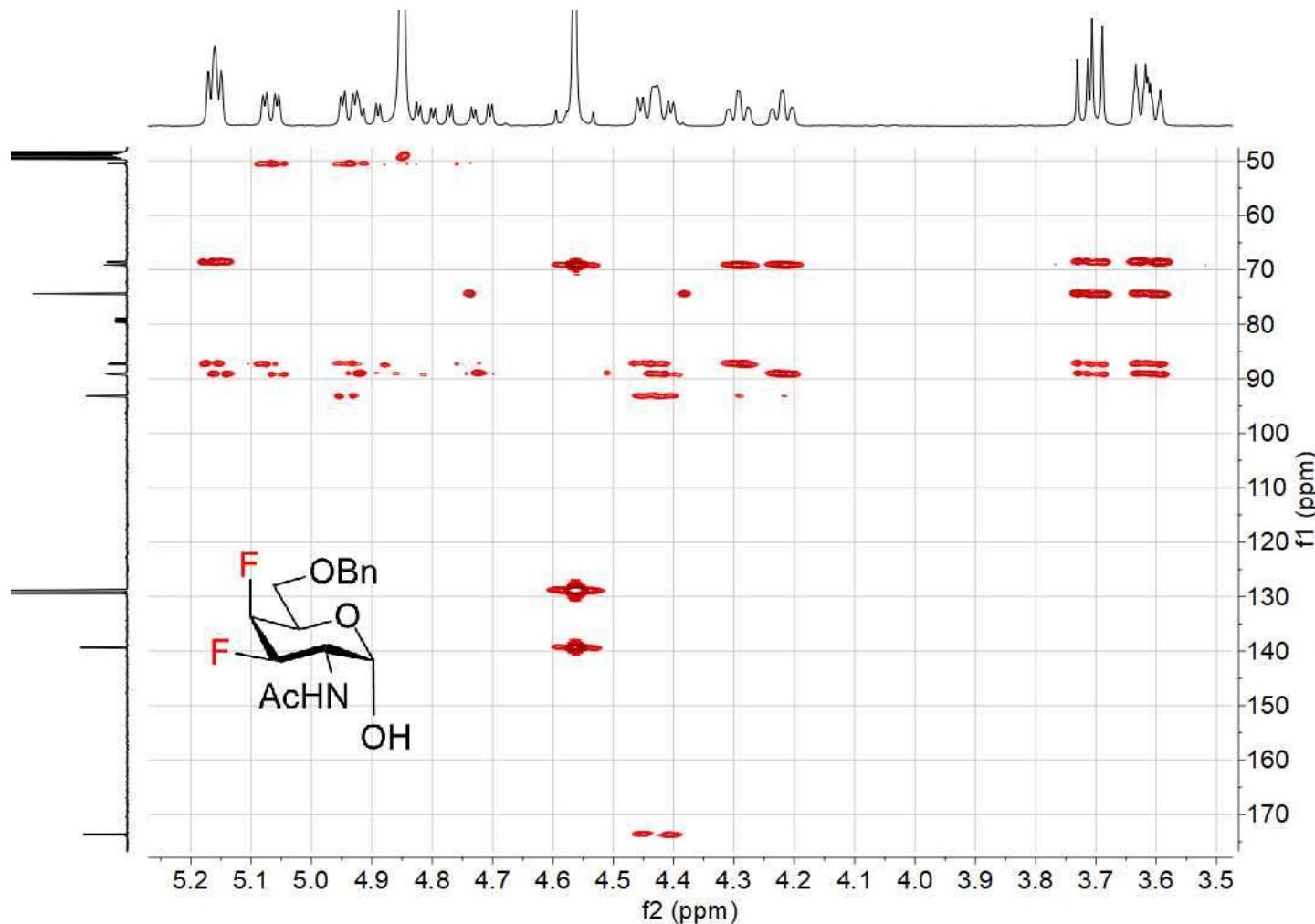
¹⁹F NMR (376 MHz, CD₃OD) 48



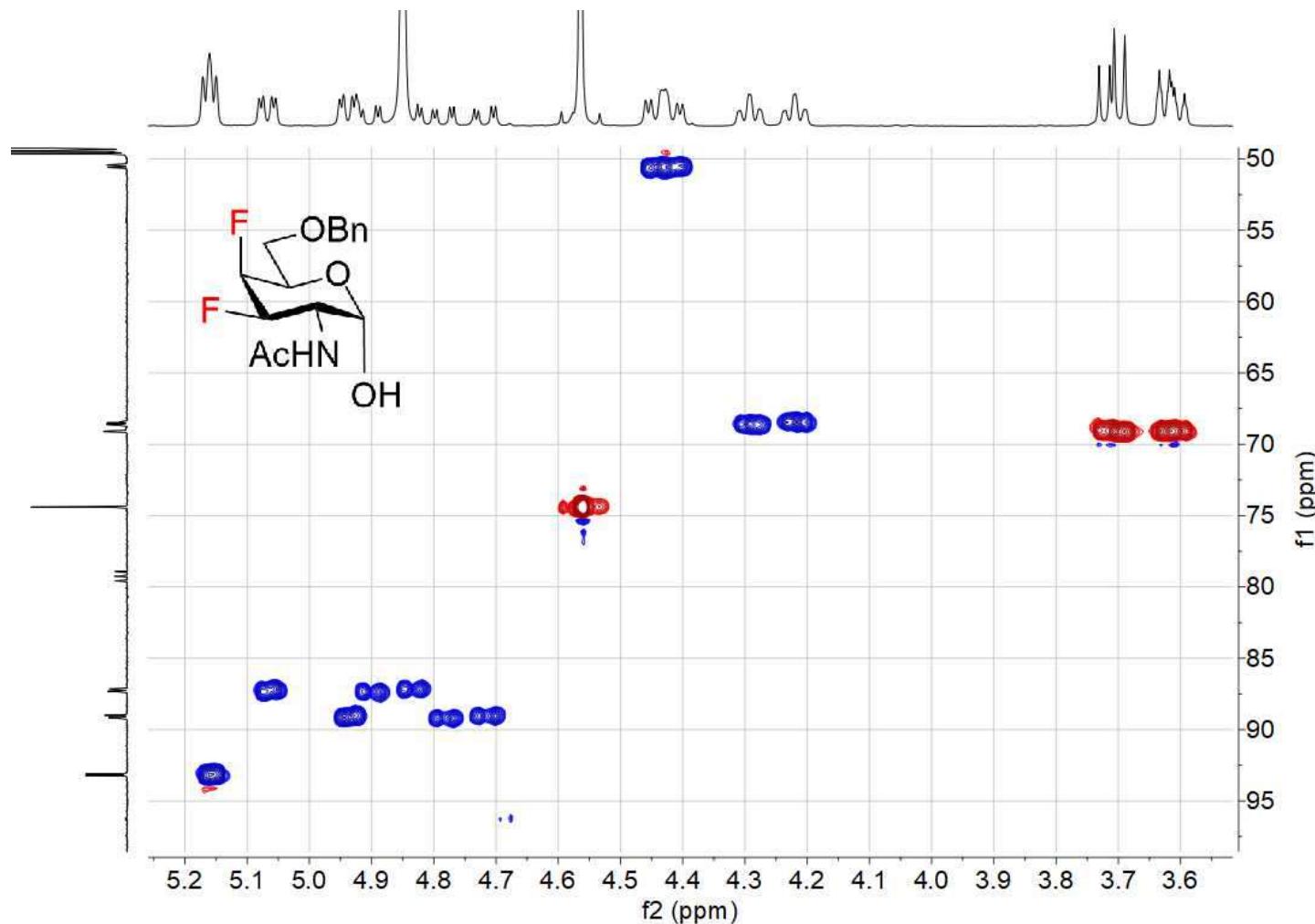
¹H-¹H COSY NMR 48



¹H-¹³C HMBC 48

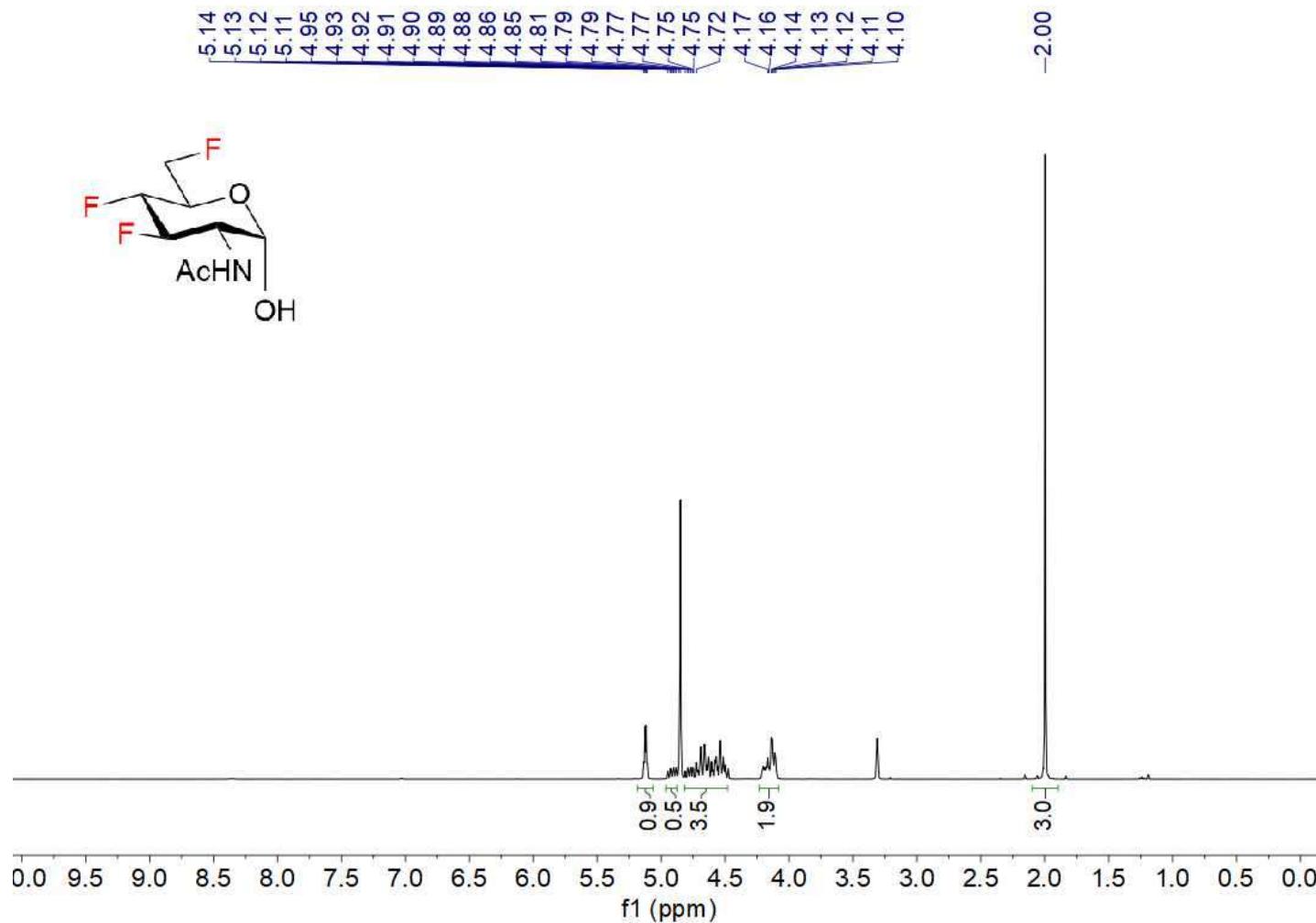


^1H - ^{13}C HSQC 48

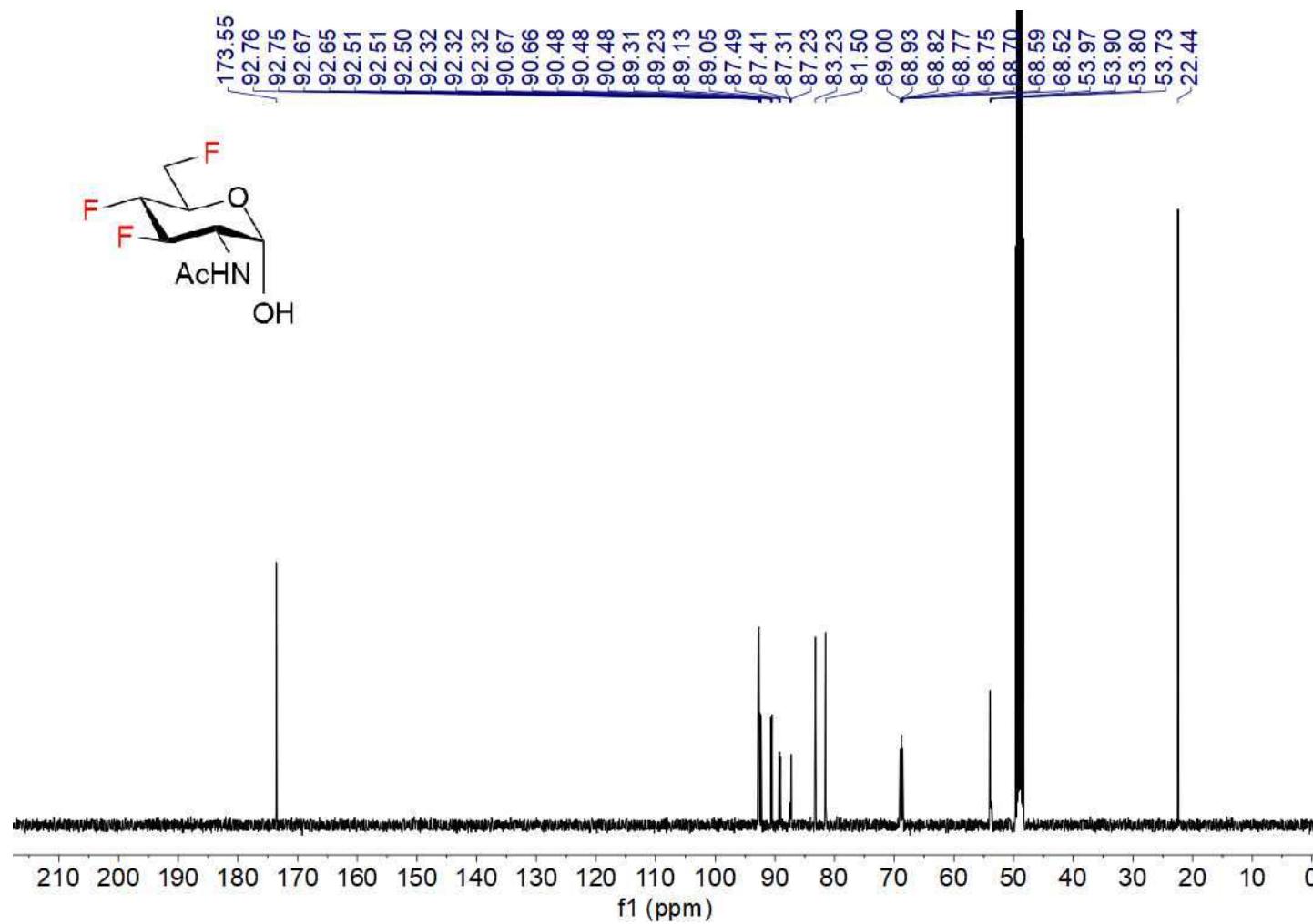


NMR COMPOUND 49

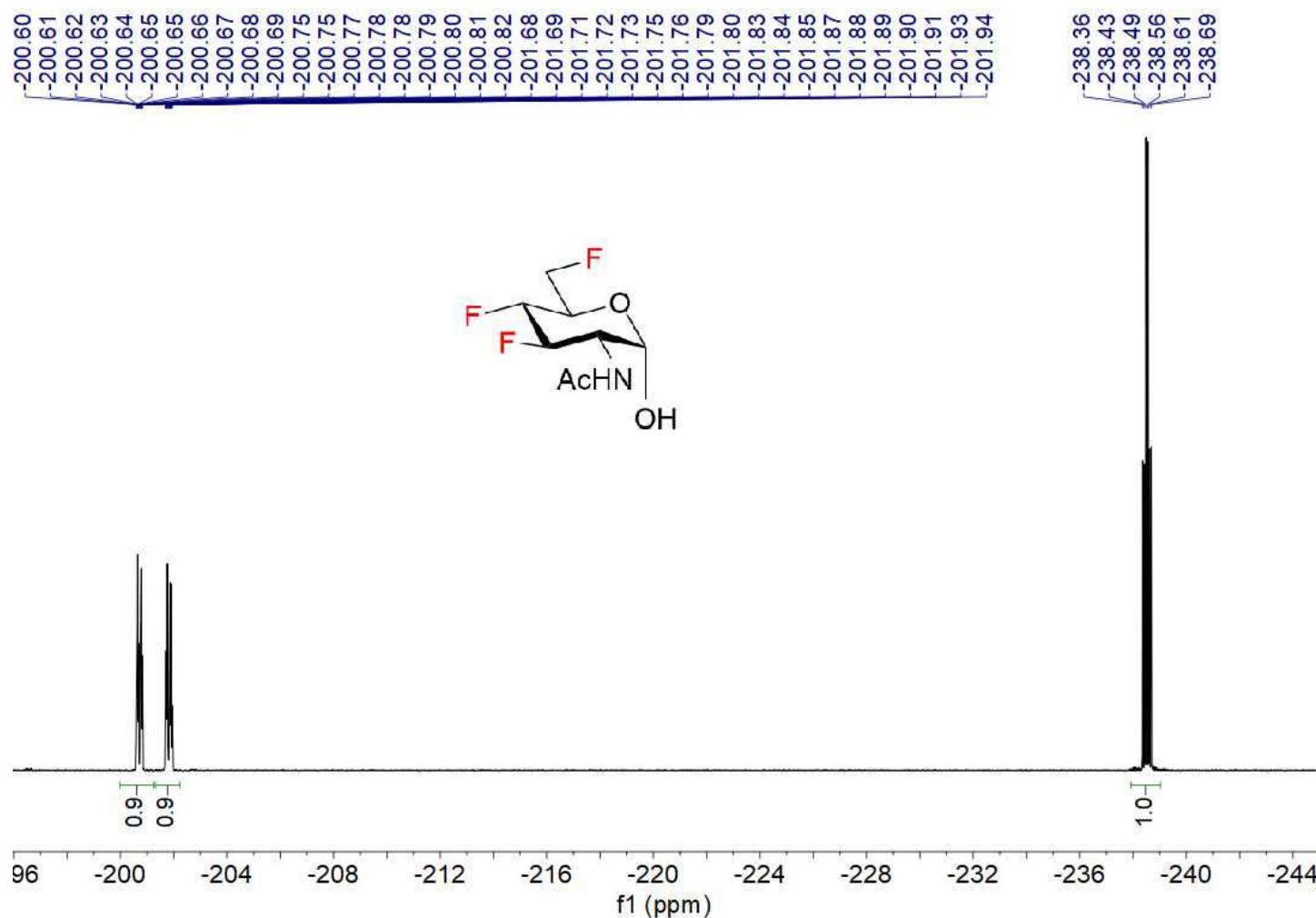
^1H NMR (400 MHz, CD_3OD) 49



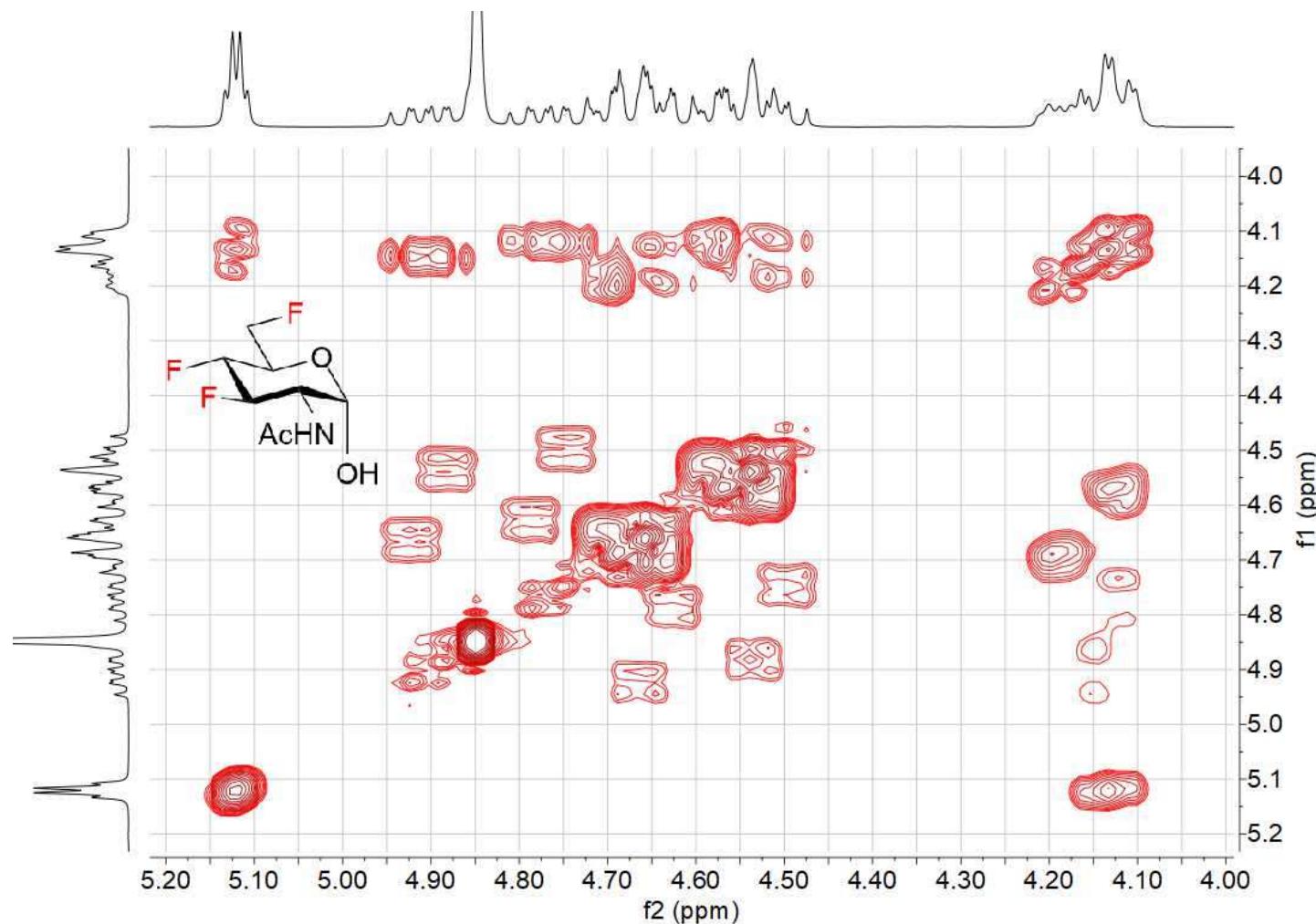
¹³C NMR (100 MHz, CD₃OD) 49



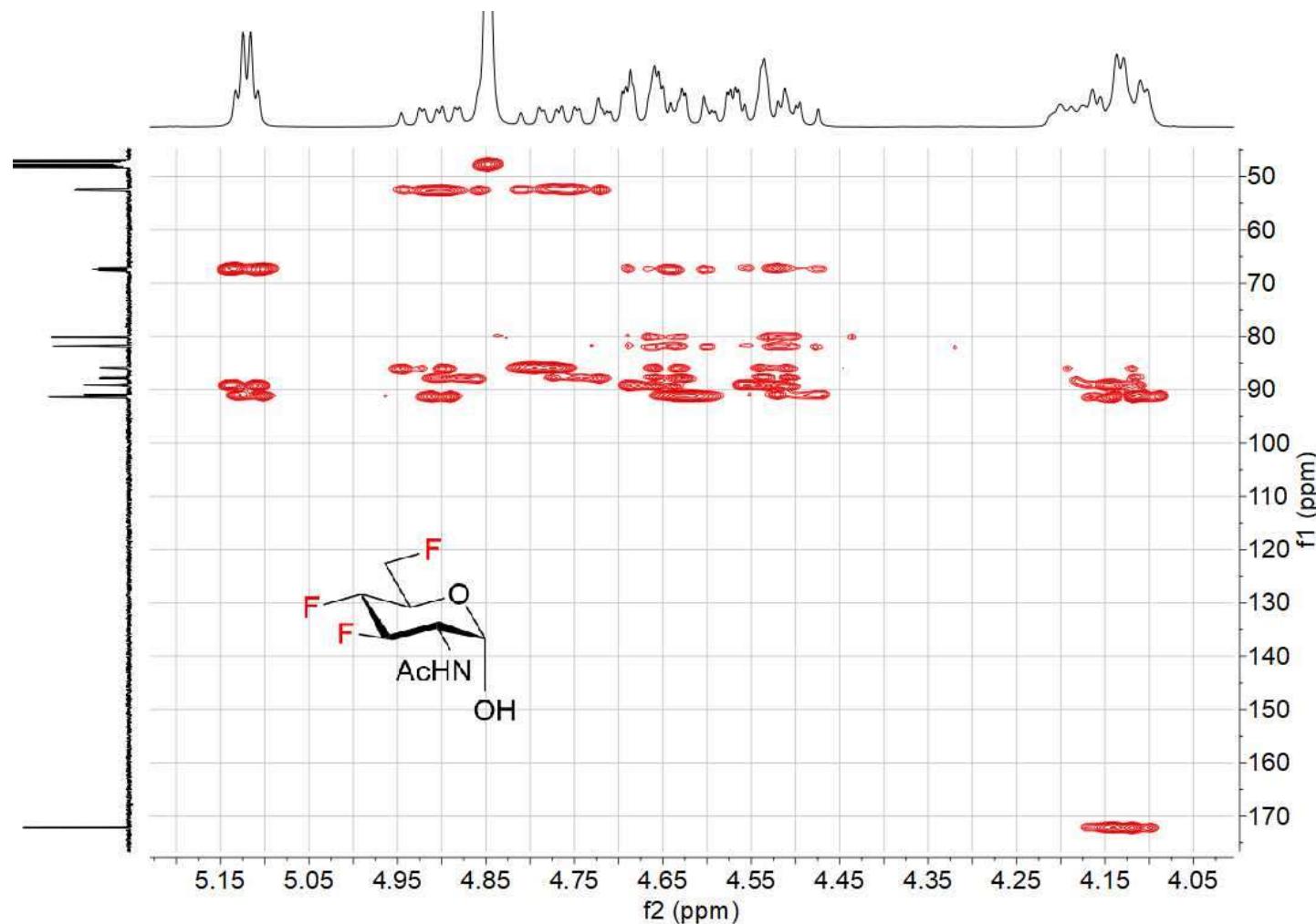
¹⁹F NMR (376 MHz, CD₃OD) 49



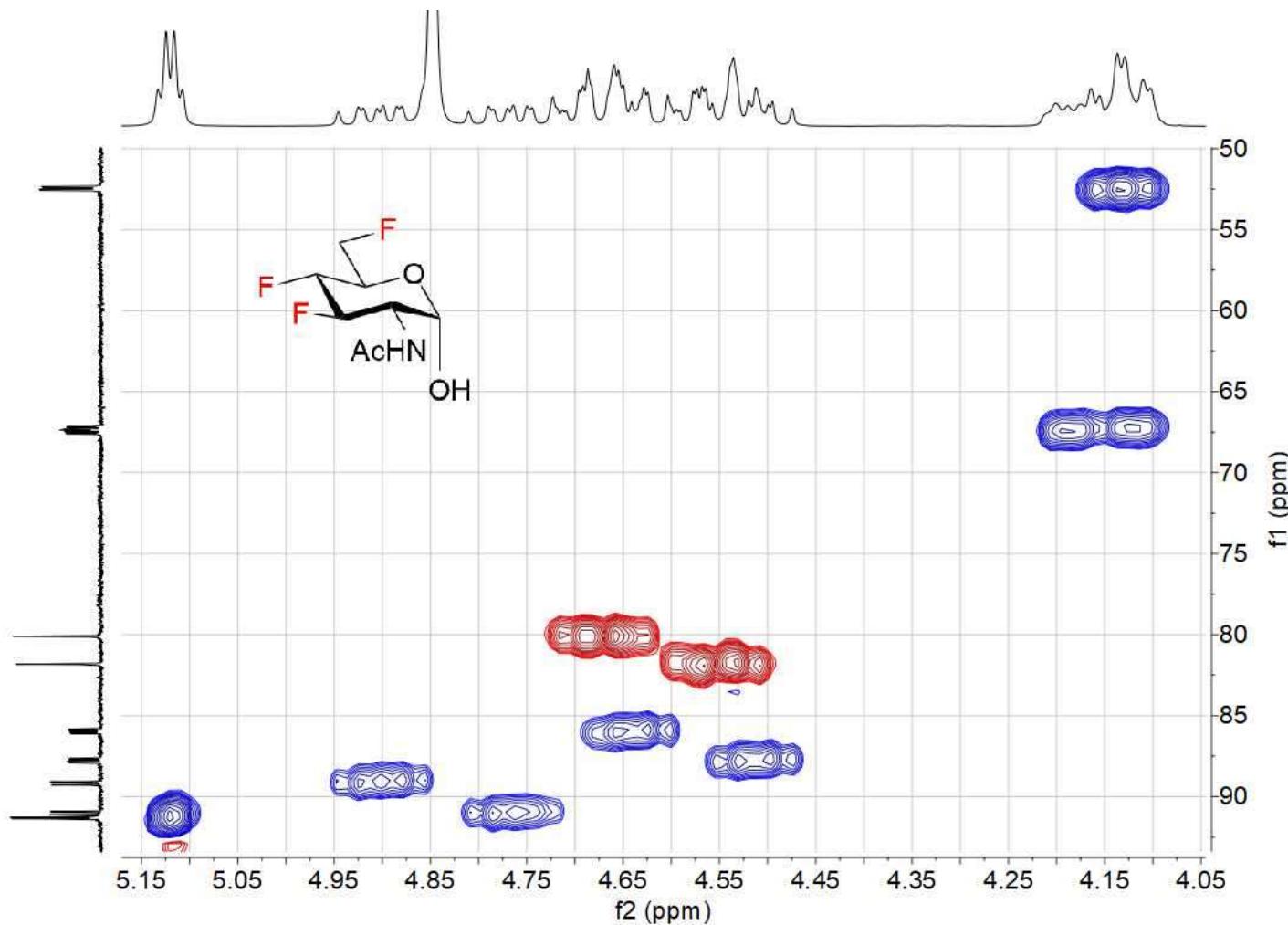
¹H-¹H COSY 49



^1H - ^{13}C HMBC 49

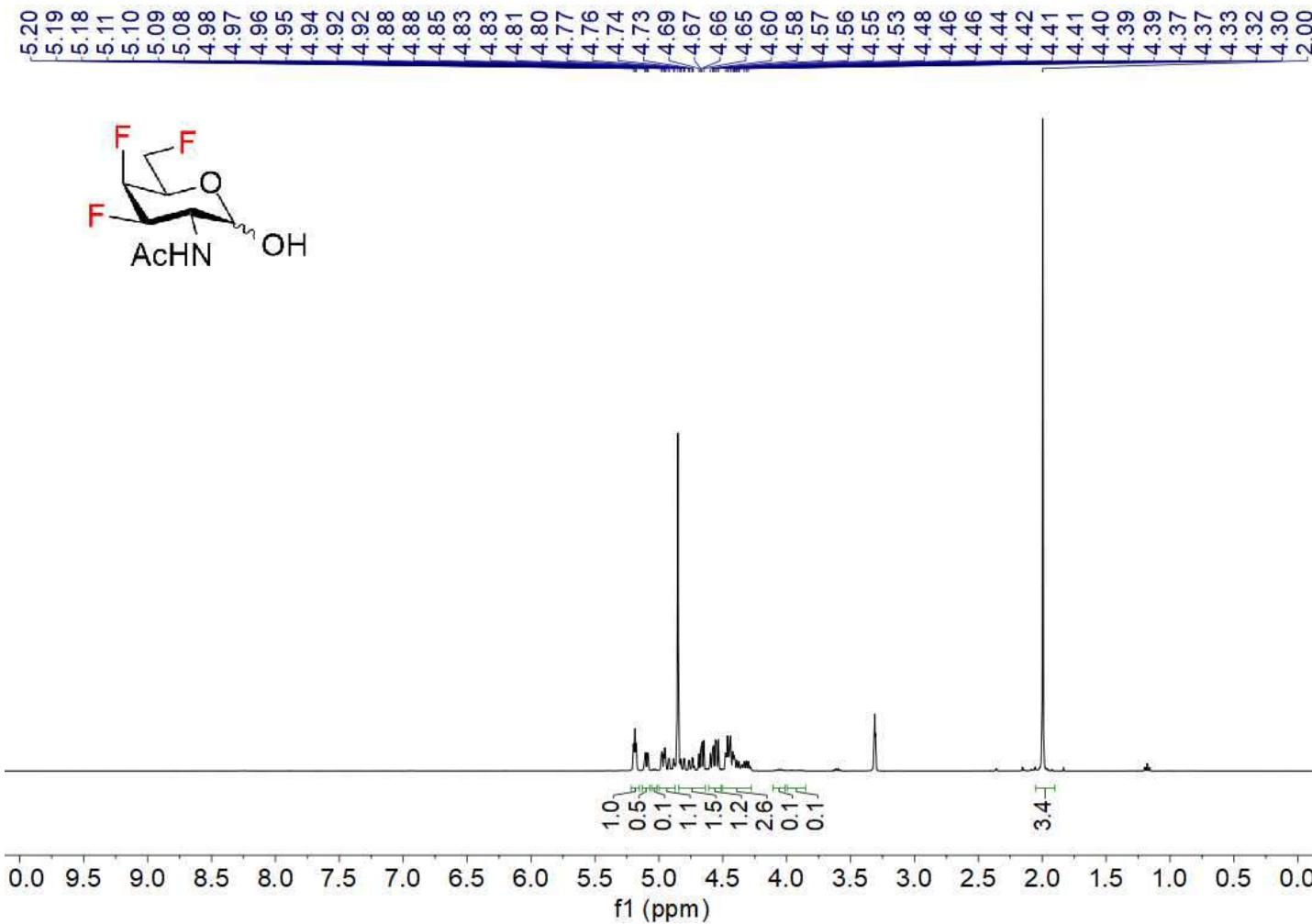


^1H - ^{13}C HSQC 49

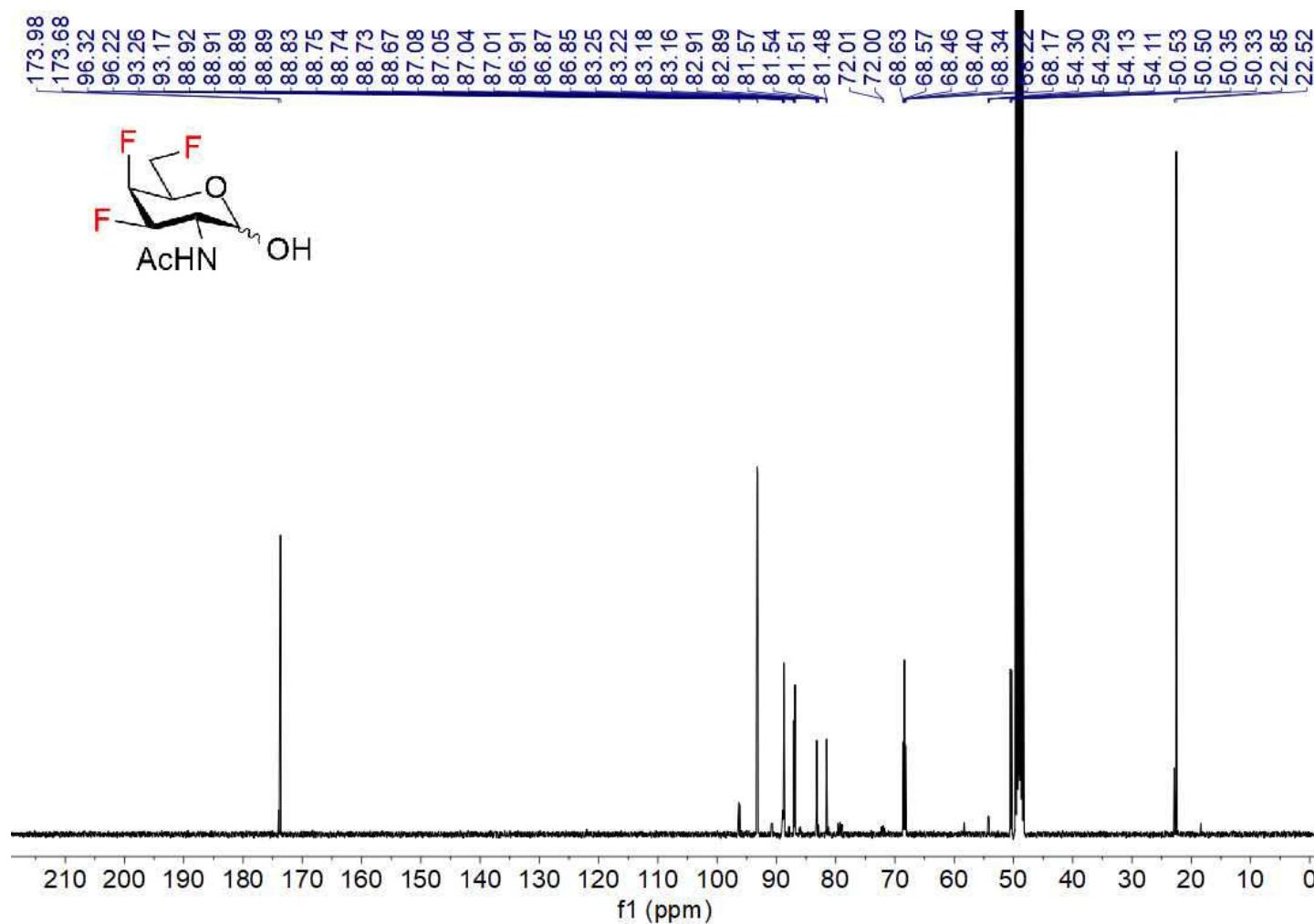


NMR COMPOUND 50

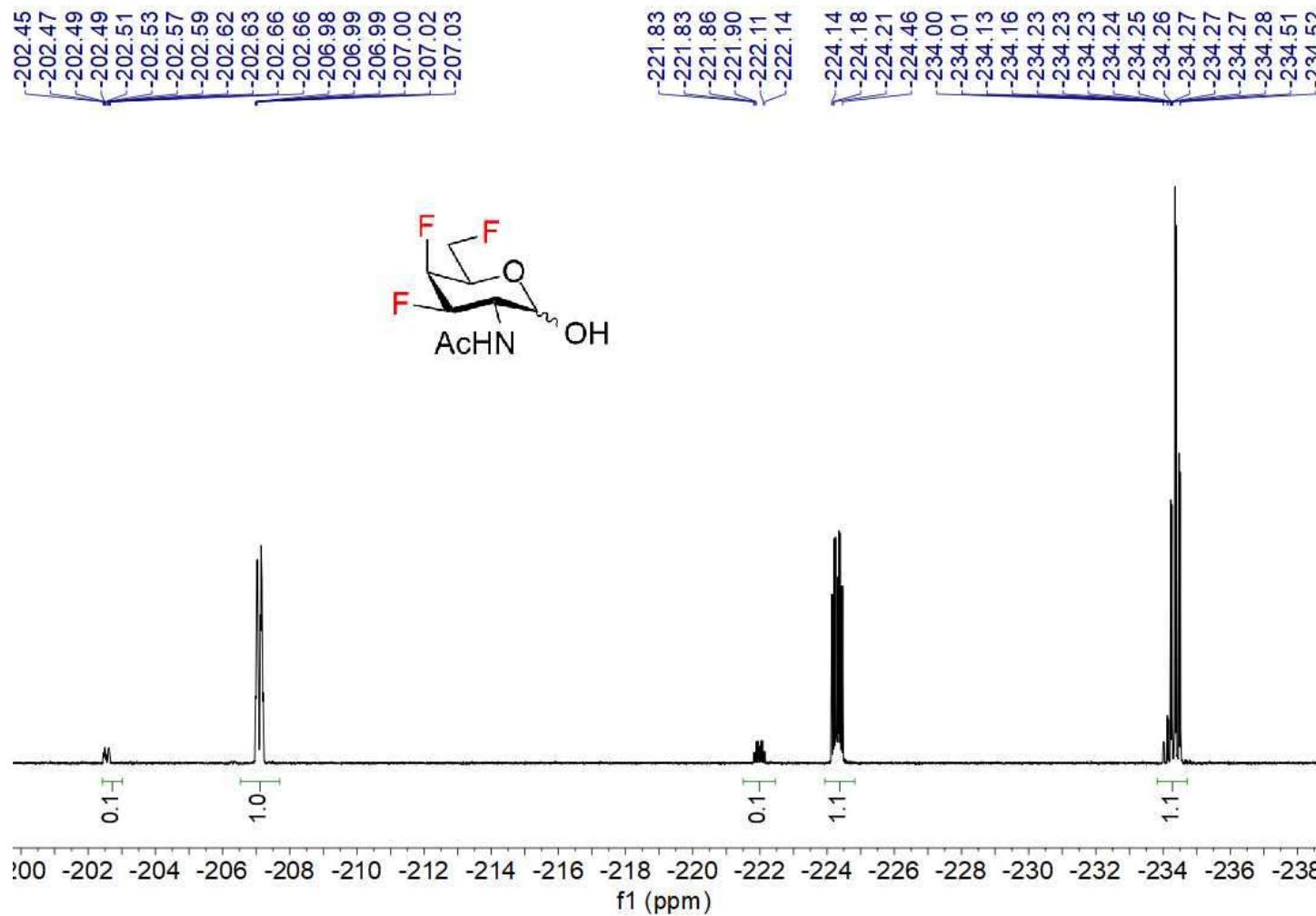
¹H NMR (400 MHz, CD₃OD) 50 (α/β ca. 10/1)



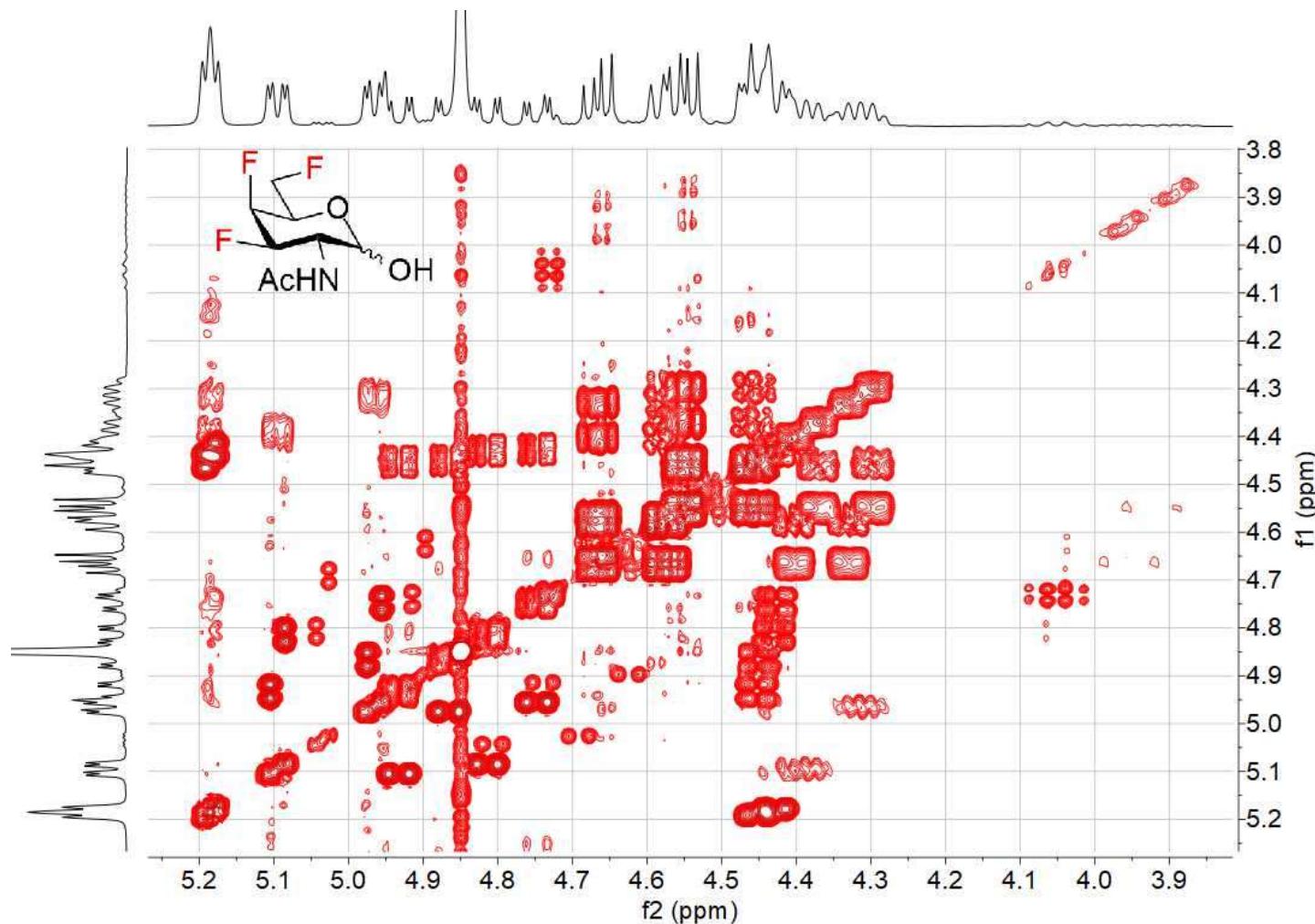
¹³C NMR (100 MHz, CD₃OD) 50



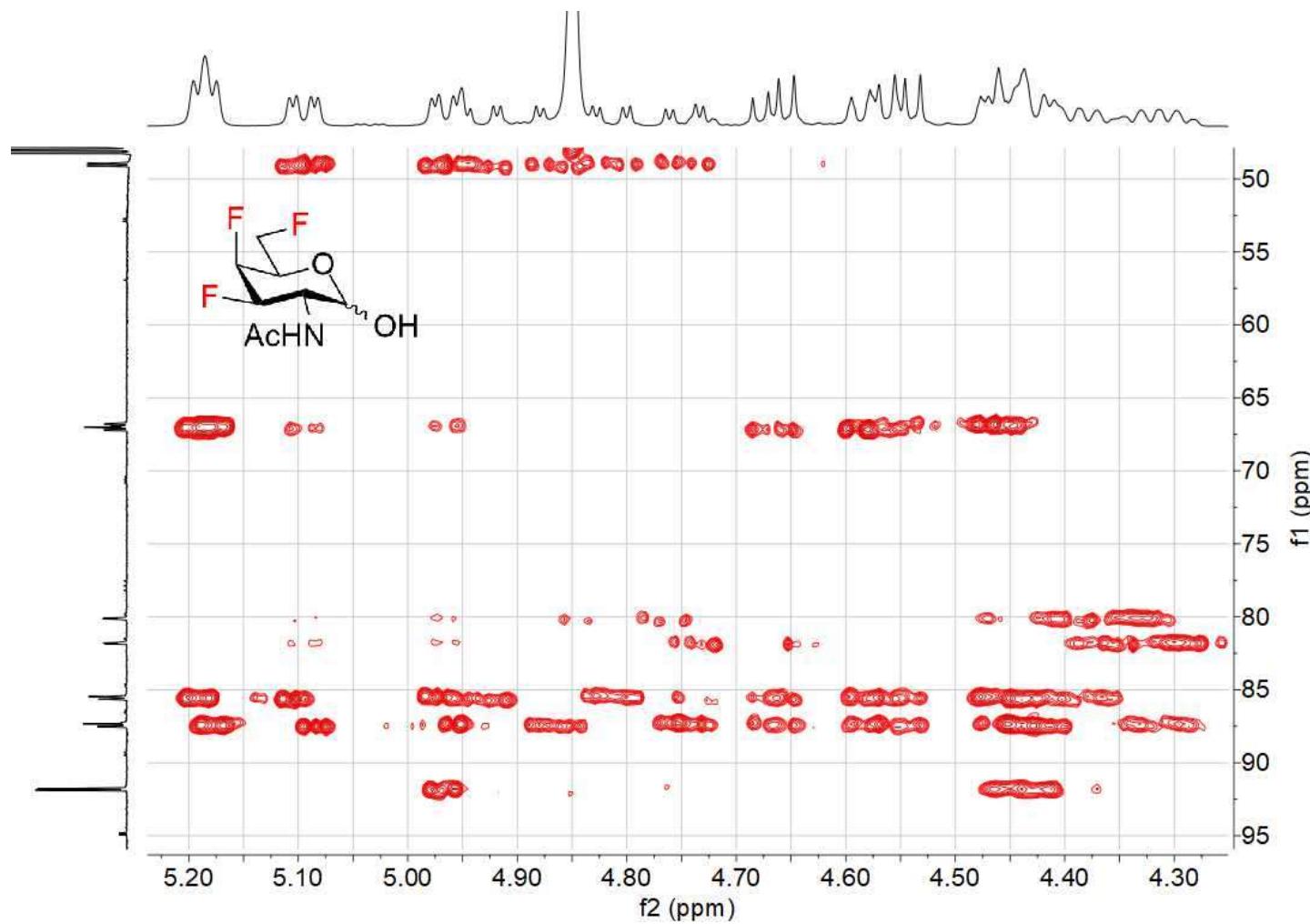
¹⁹F NMR (376 MHz, CD₃OD) 50 (α/β ca. 10/1)



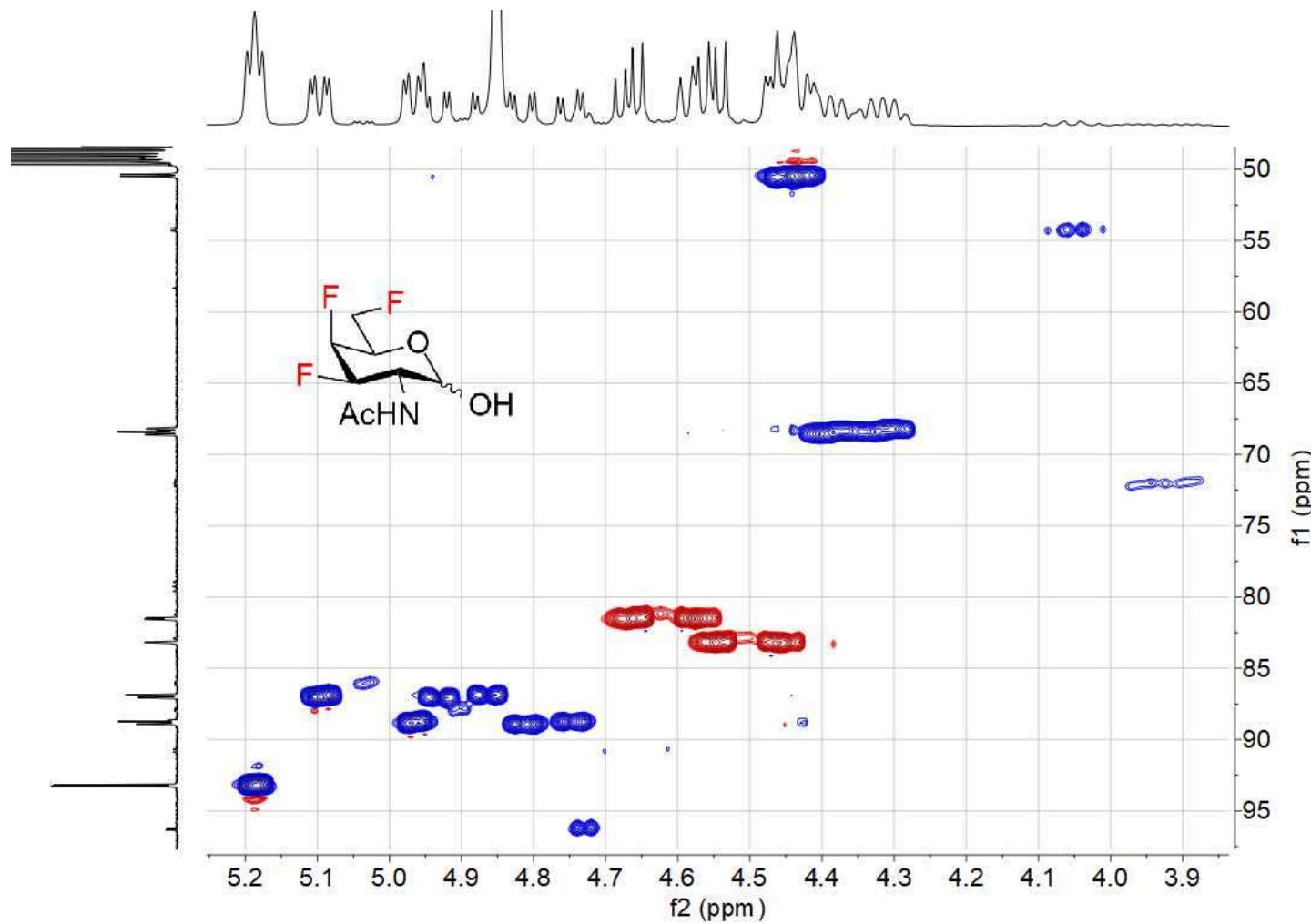
¹H-¹H COSY 50



^1H - ^{13}C HMBC 50

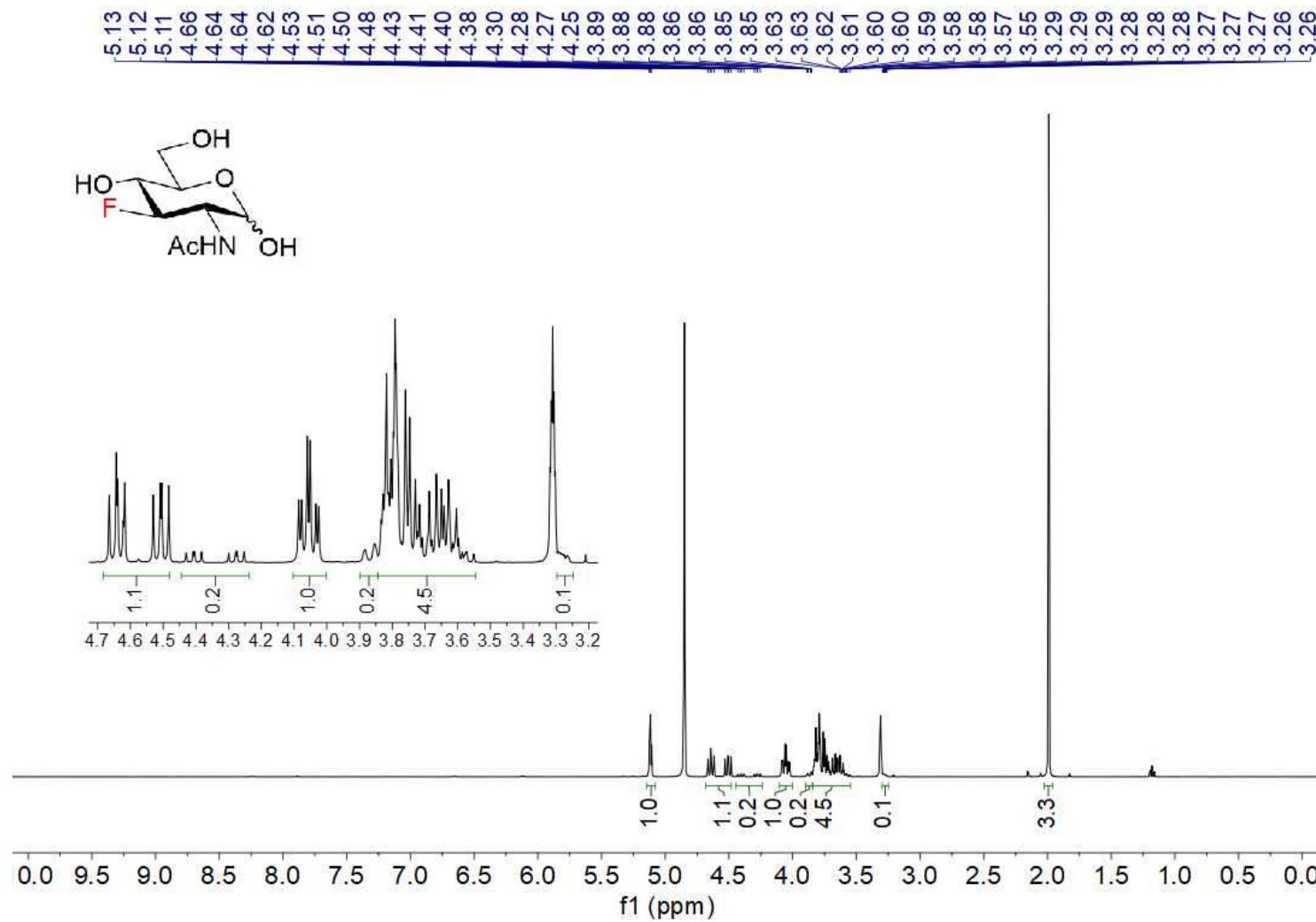


^1H - ^{13}C HSQC 50

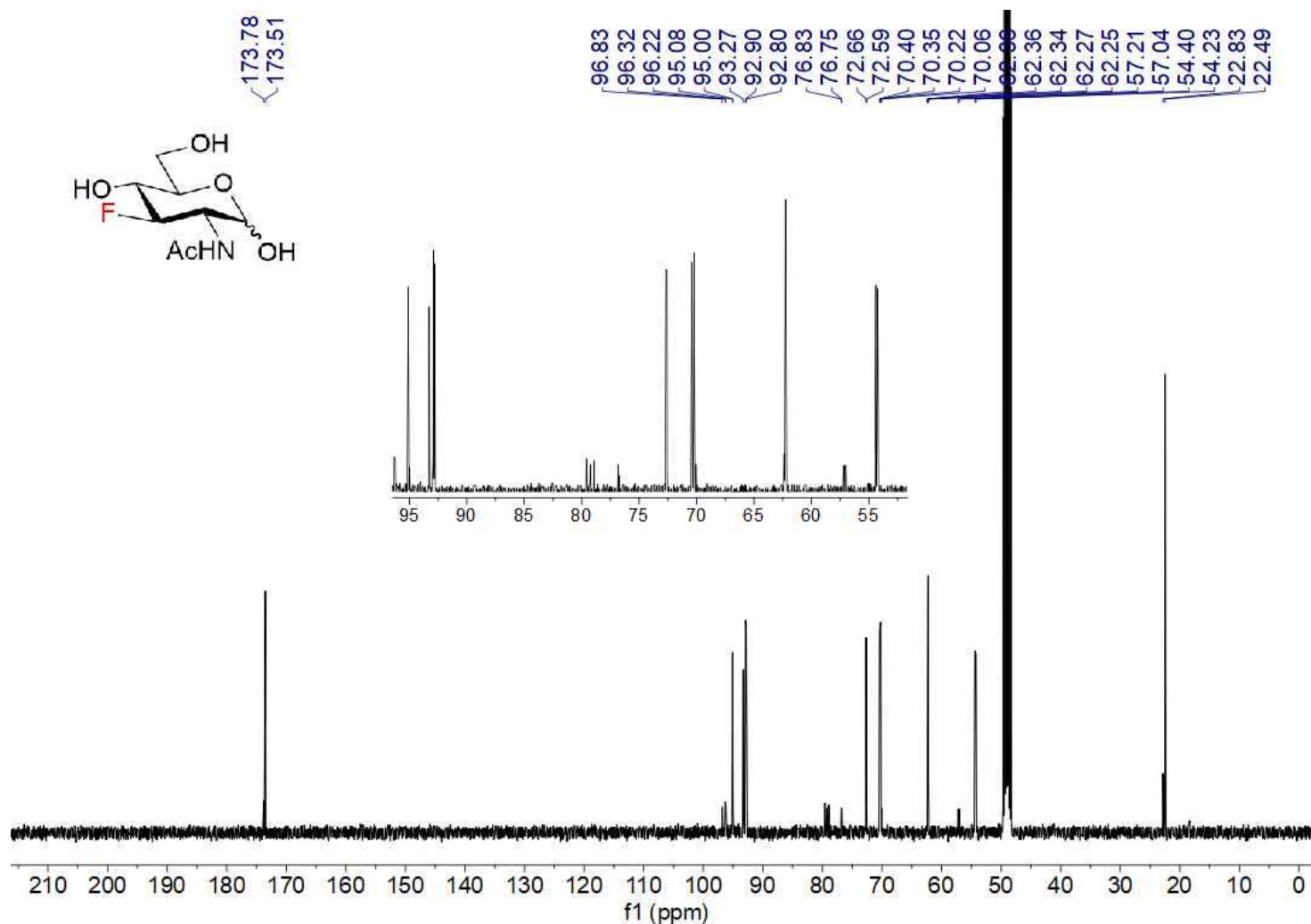


NMR COMPOUND 51

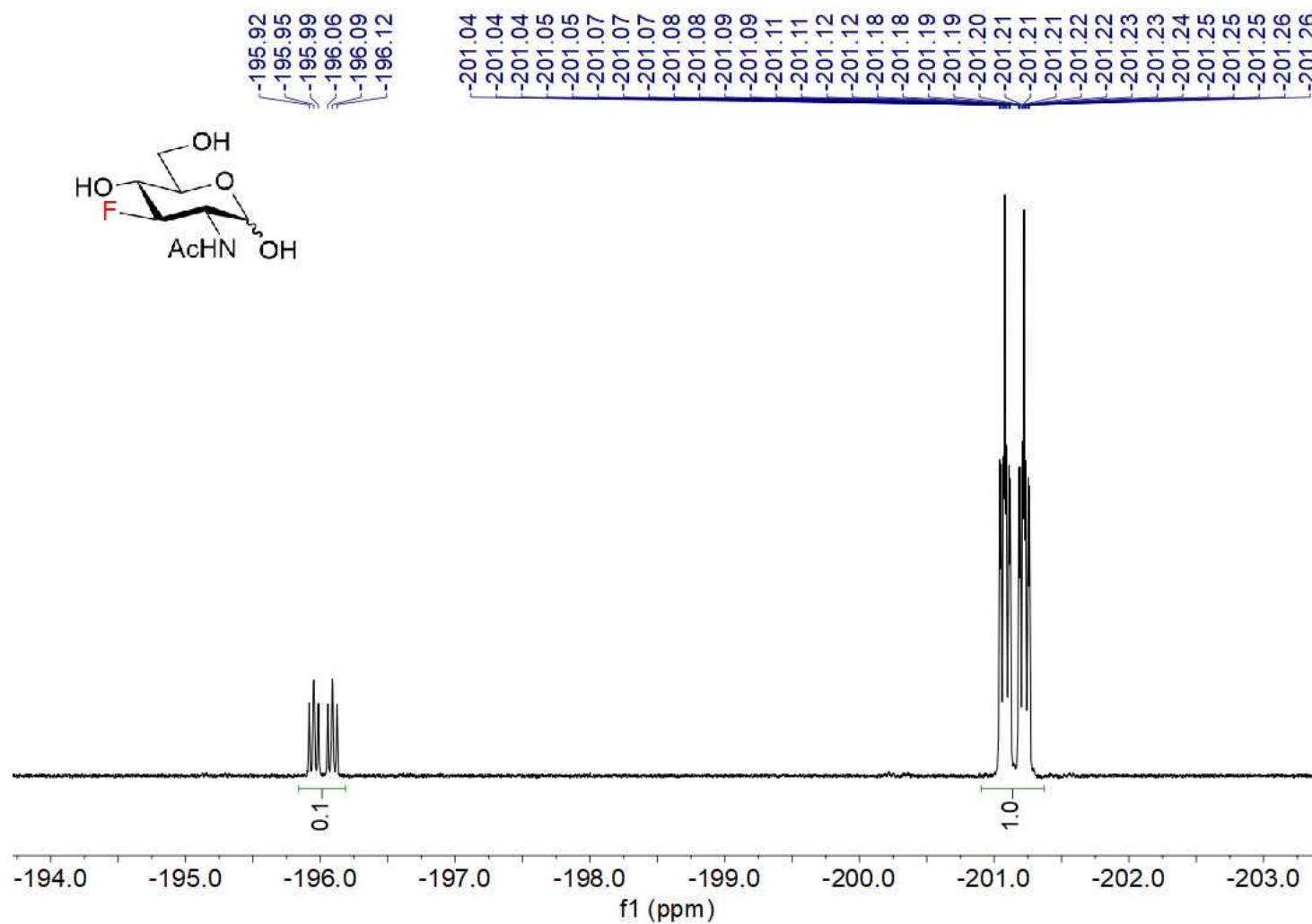
¹H NMR (400 MHz, CD₃OD) 51 (α/β ca. 10/1)



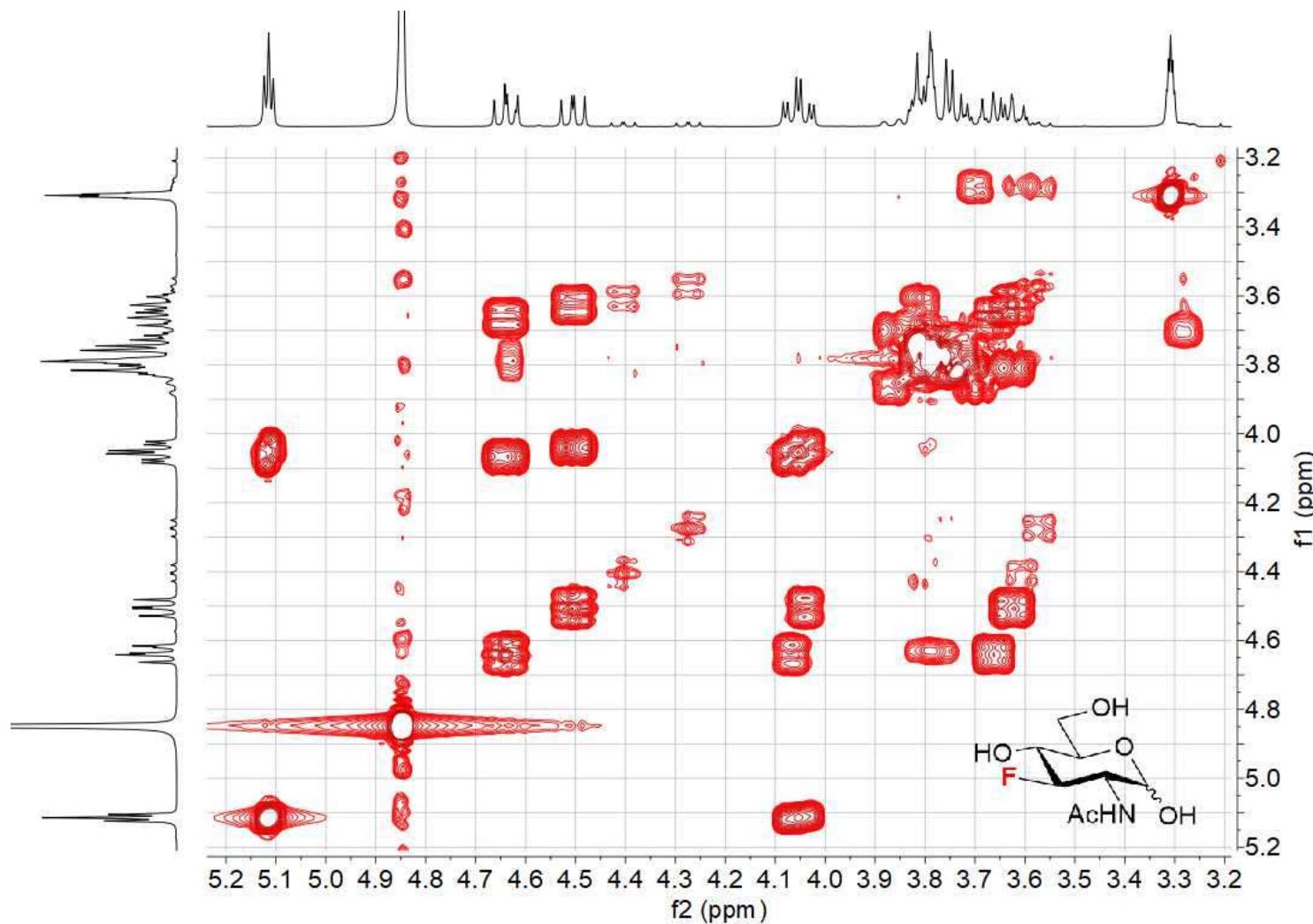
¹³C NMR (100 MHz, CD₃OD) 51



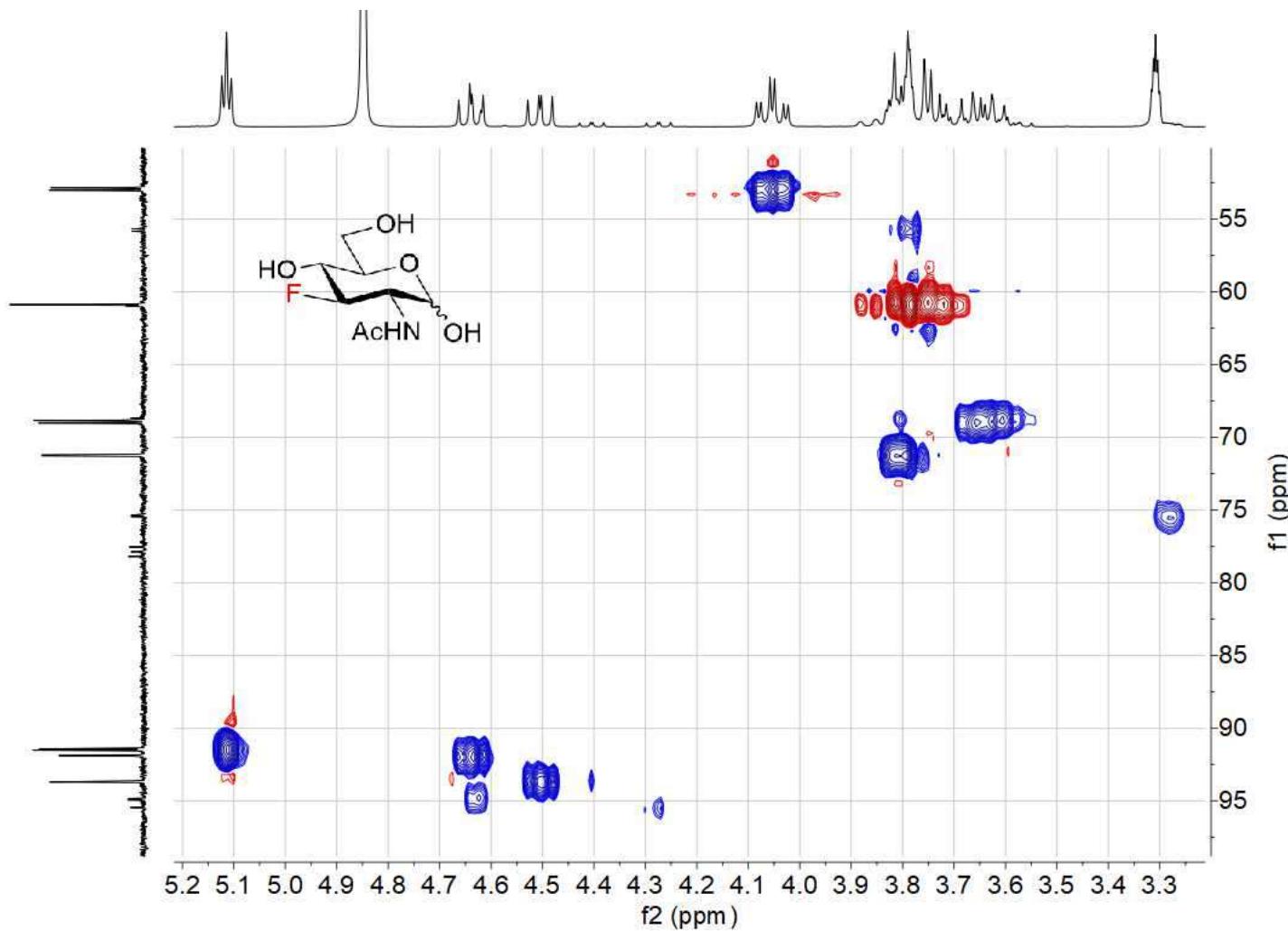
¹⁹F NMR (376 MHz, CD₃OD) 51 (α/β ca. 10/1)



¹H-¹H COSY 51

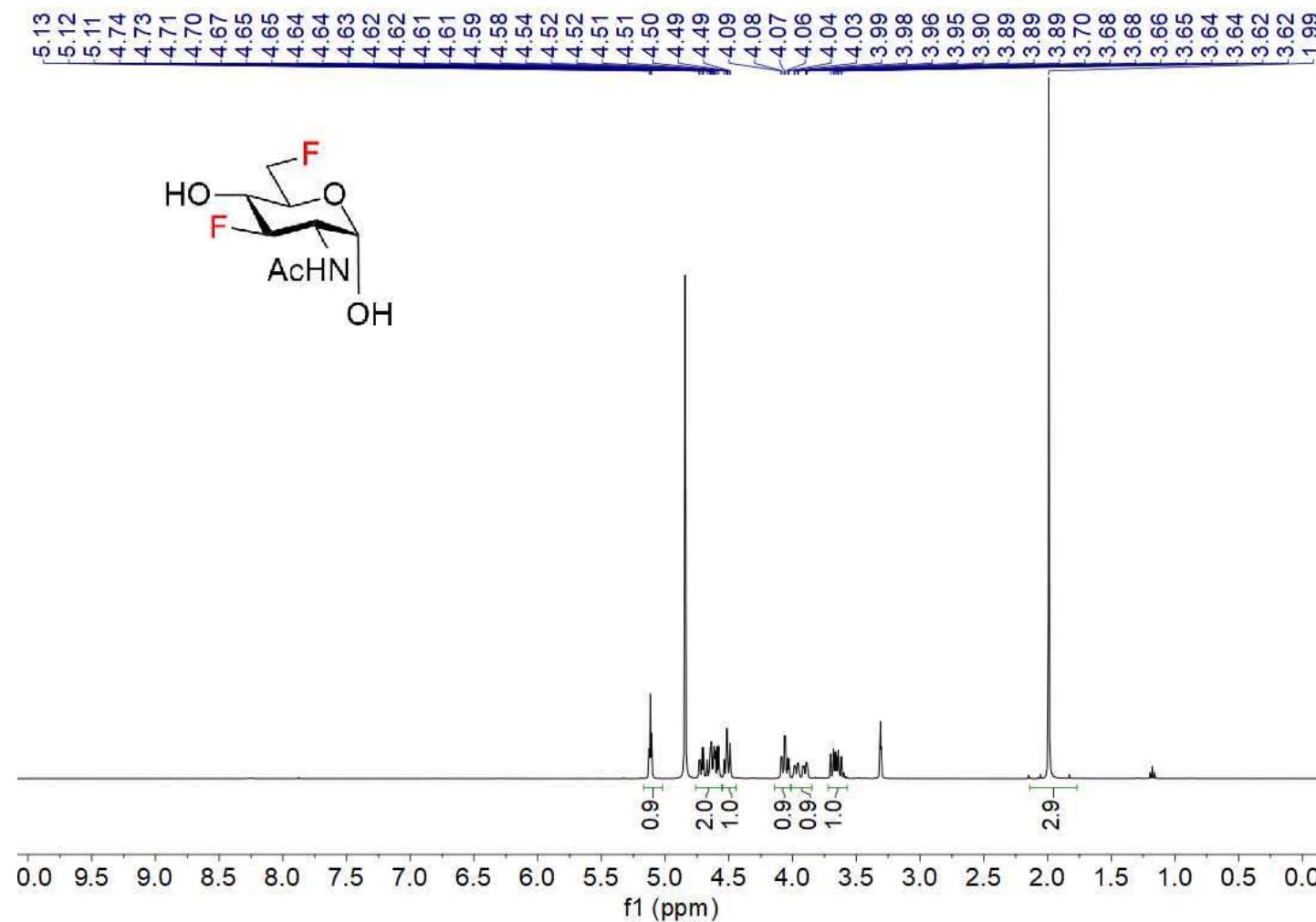


^1H - ^{13}C HSQC 51

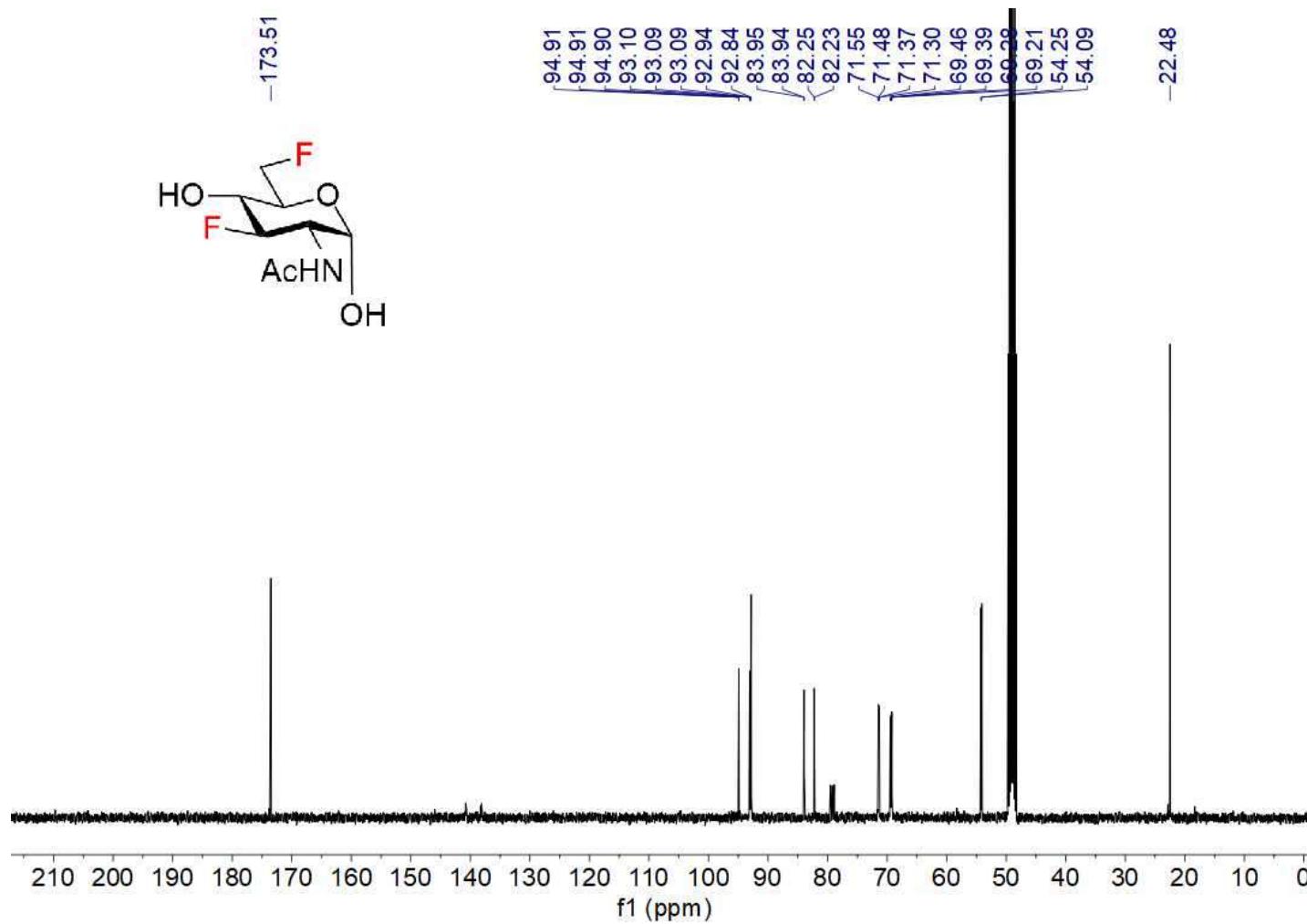


NMR COMPOUND 52

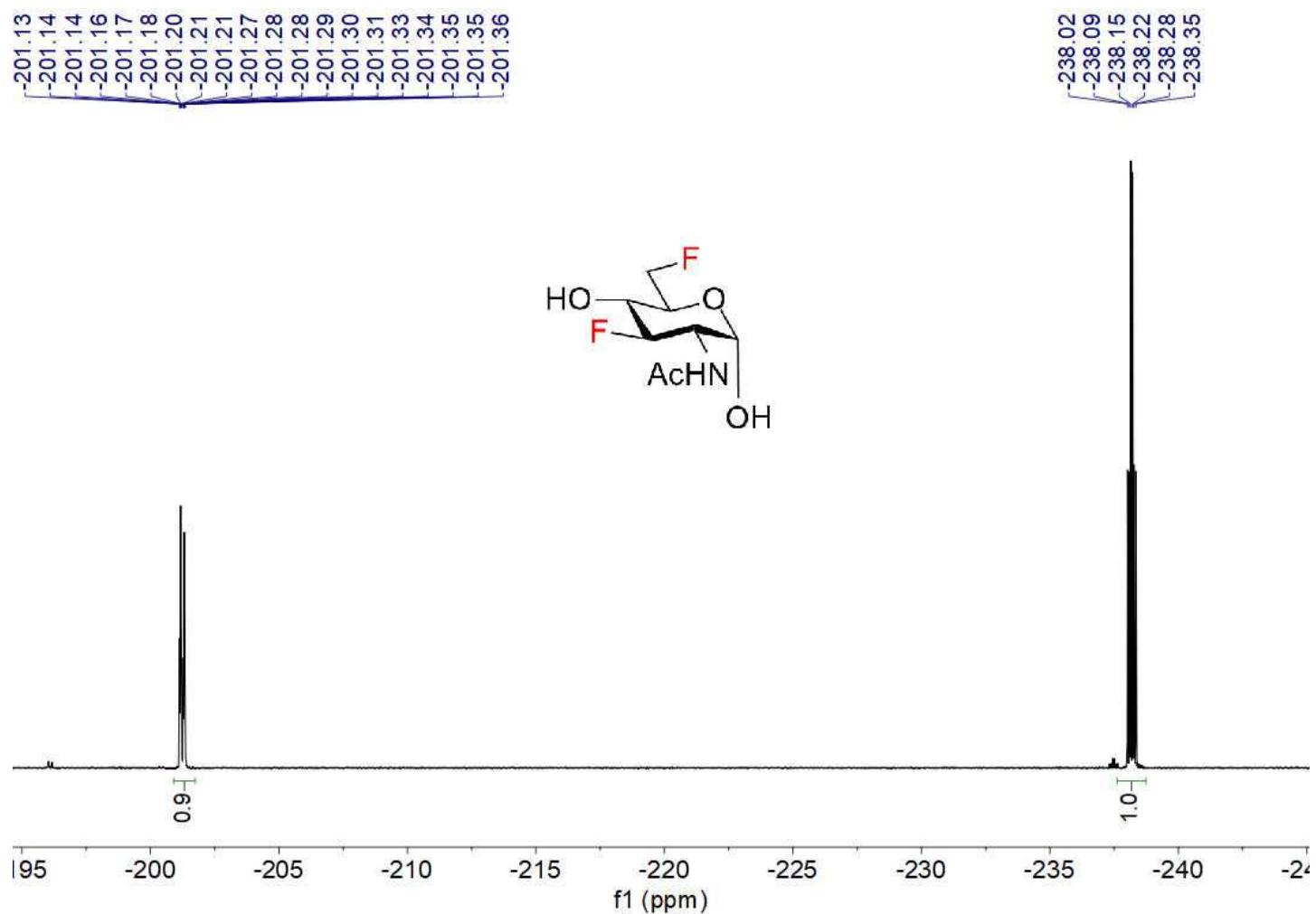
^1H NMR (400 MHz, CD_3OD) 52



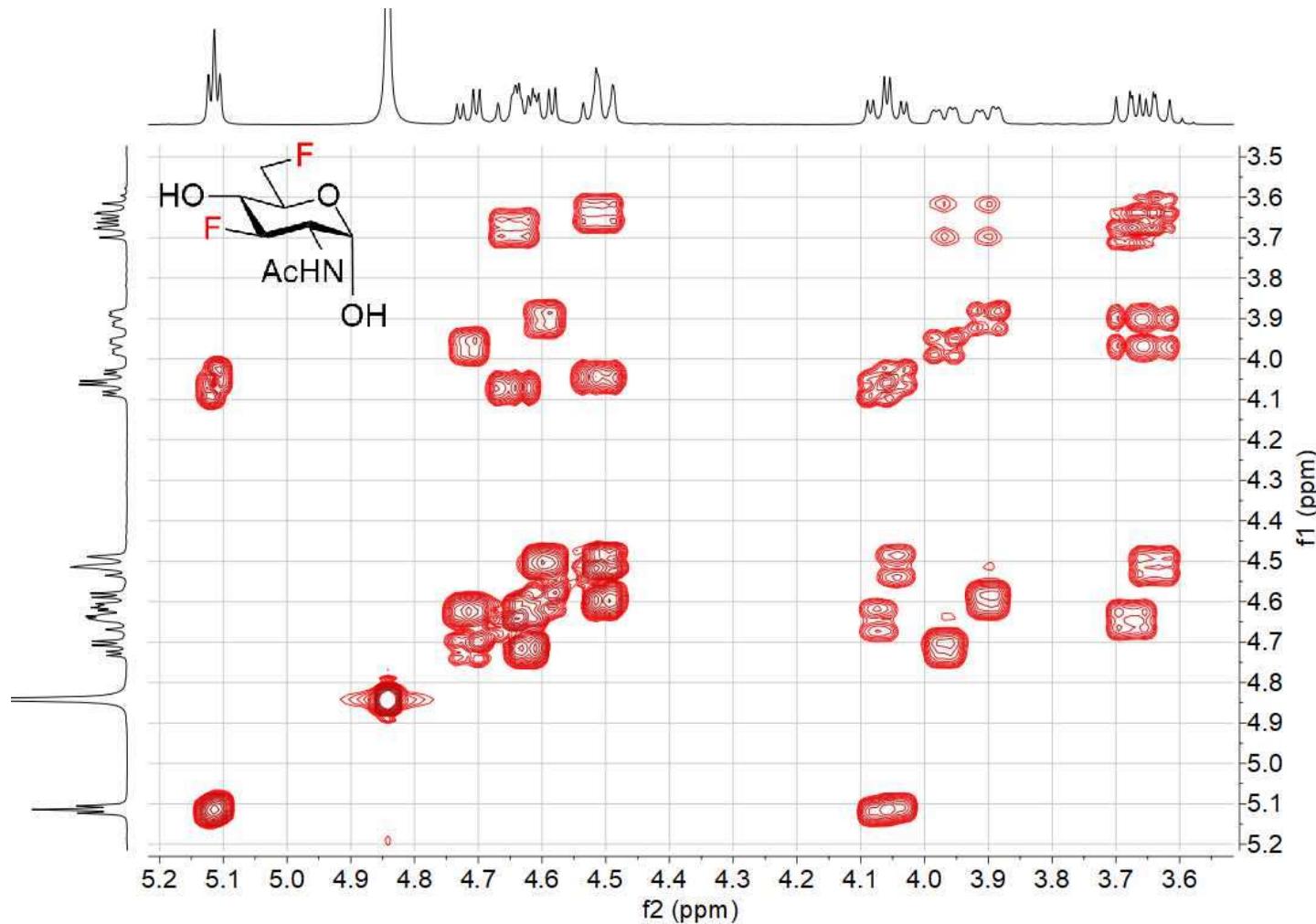
¹³C NMR (100 MHz, CD₃OD) 52



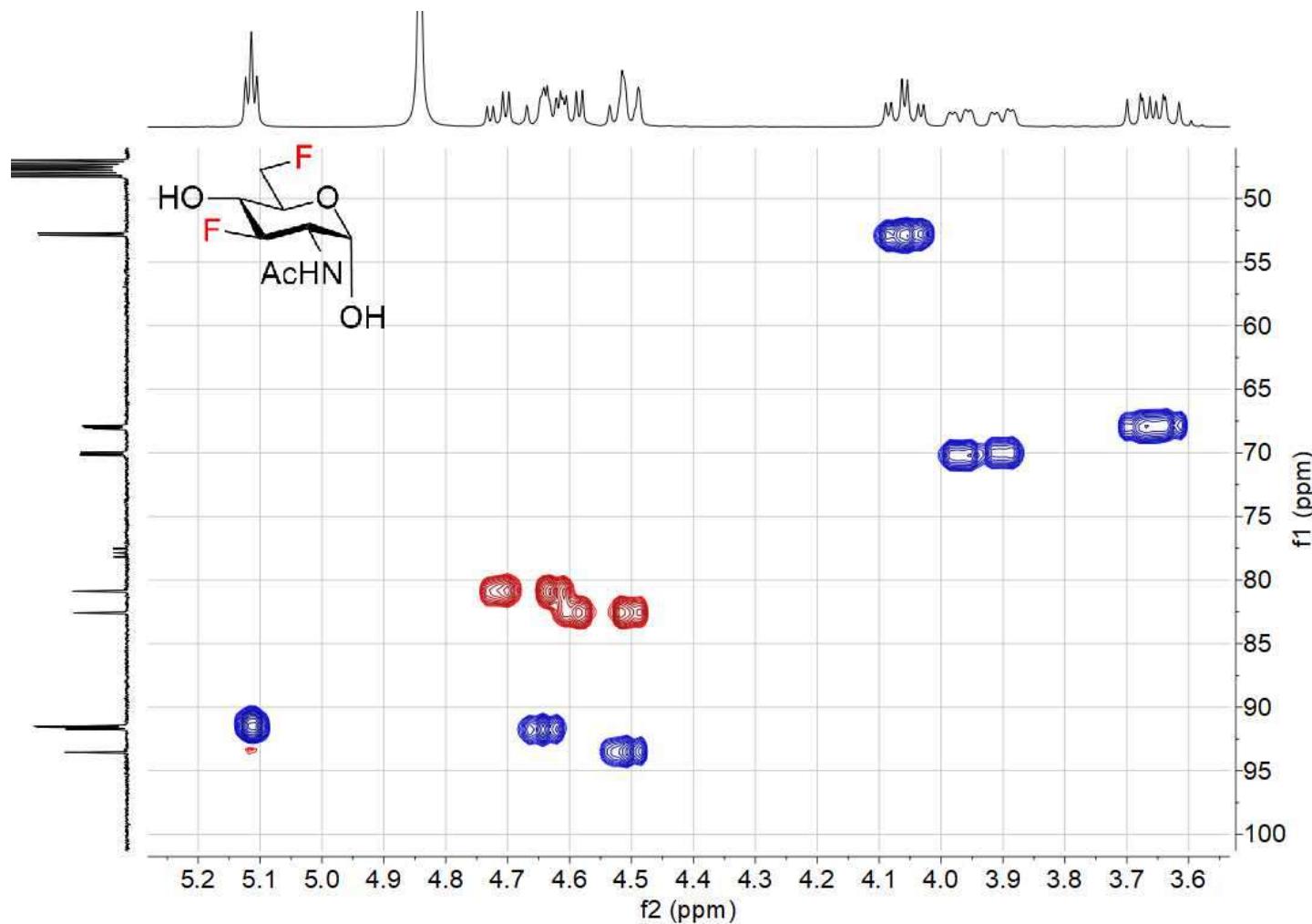
¹⁹F NMR (376 MHz, CD₃OD) 52



^1H - ^1H COSY 52

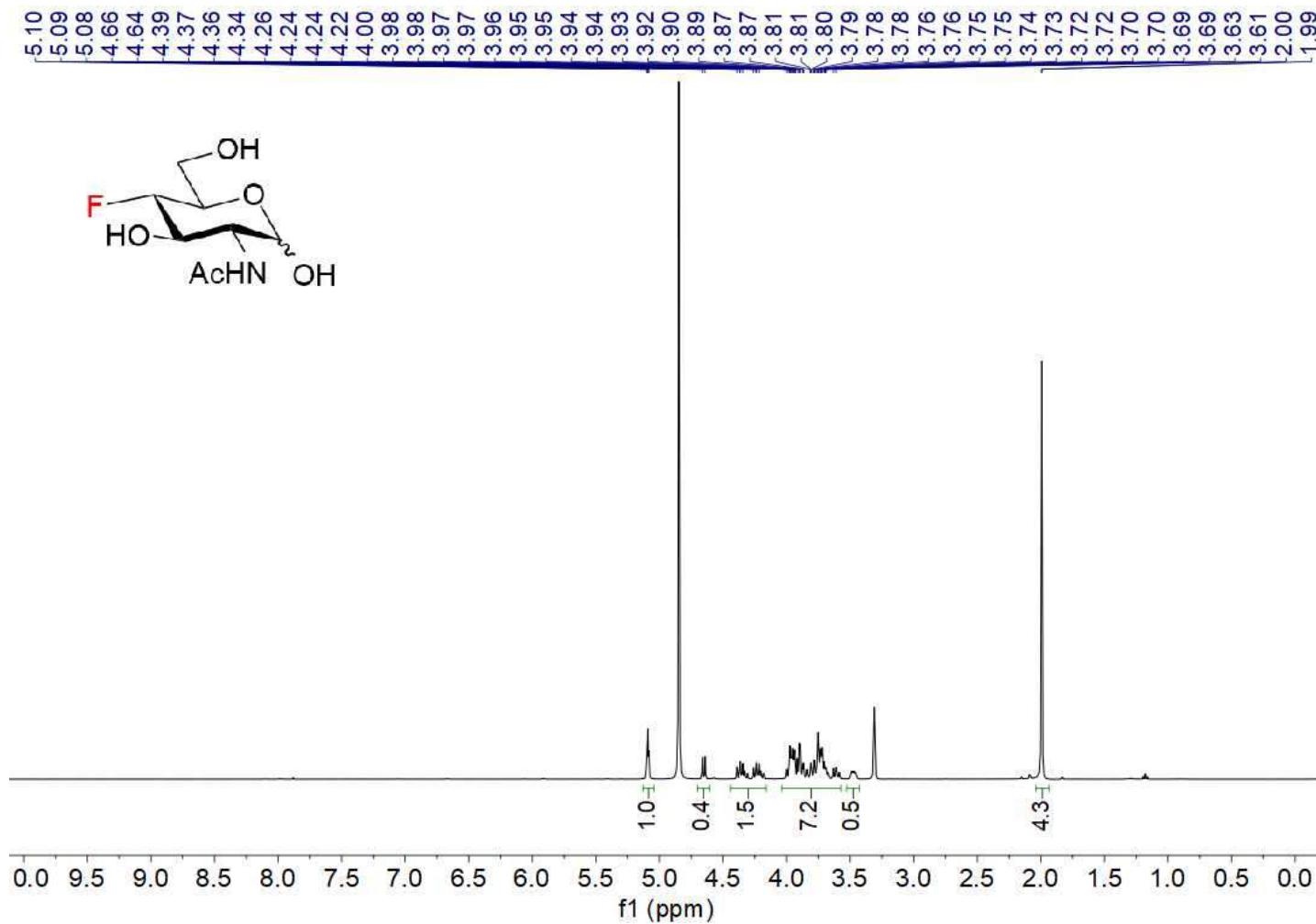


^1H - ^{13}C HSQC 52

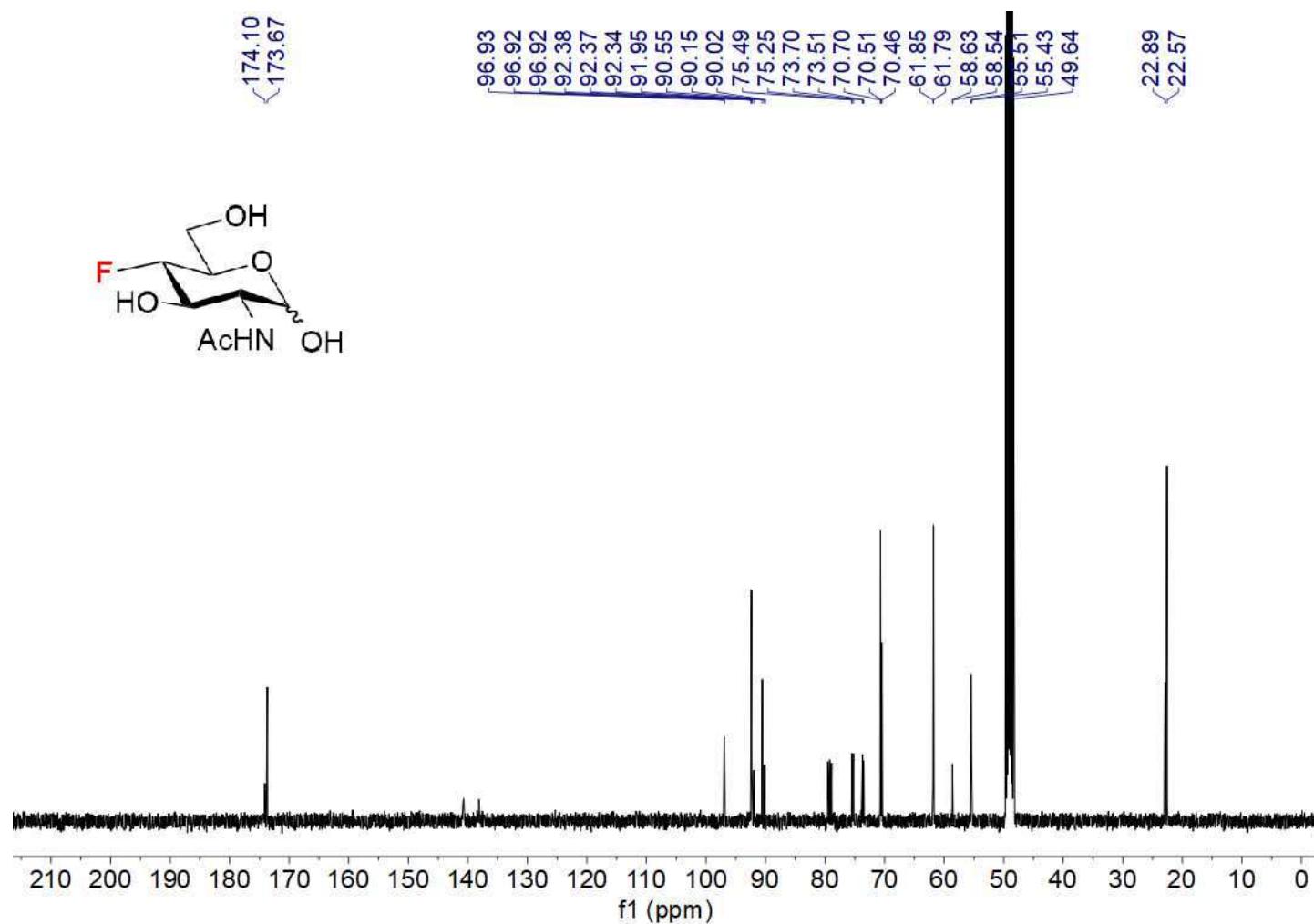


NMR COMPOUND 53

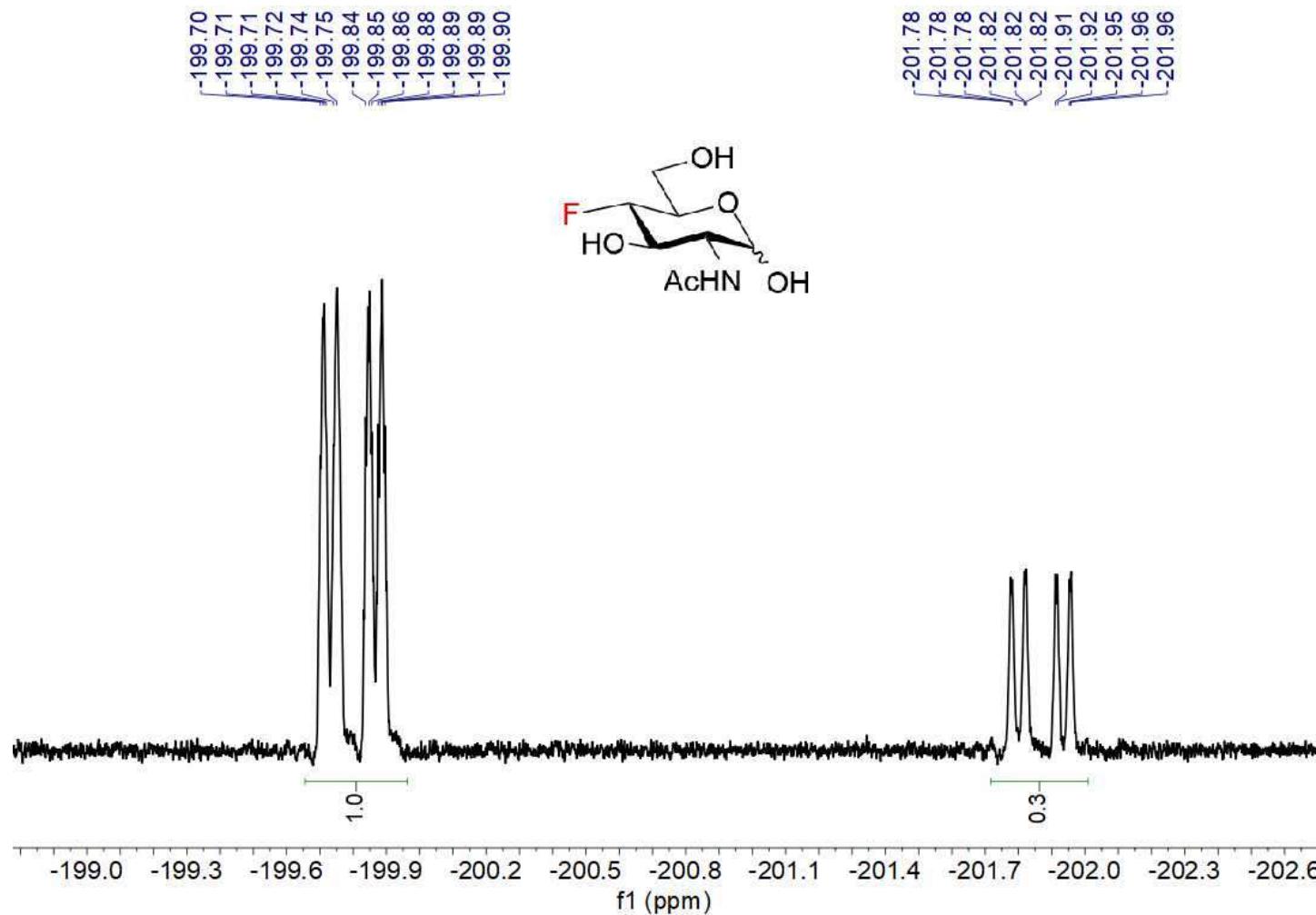
¹H NMR (400 MHz, CD₃OD) 53 (α/β ca. 10/3)



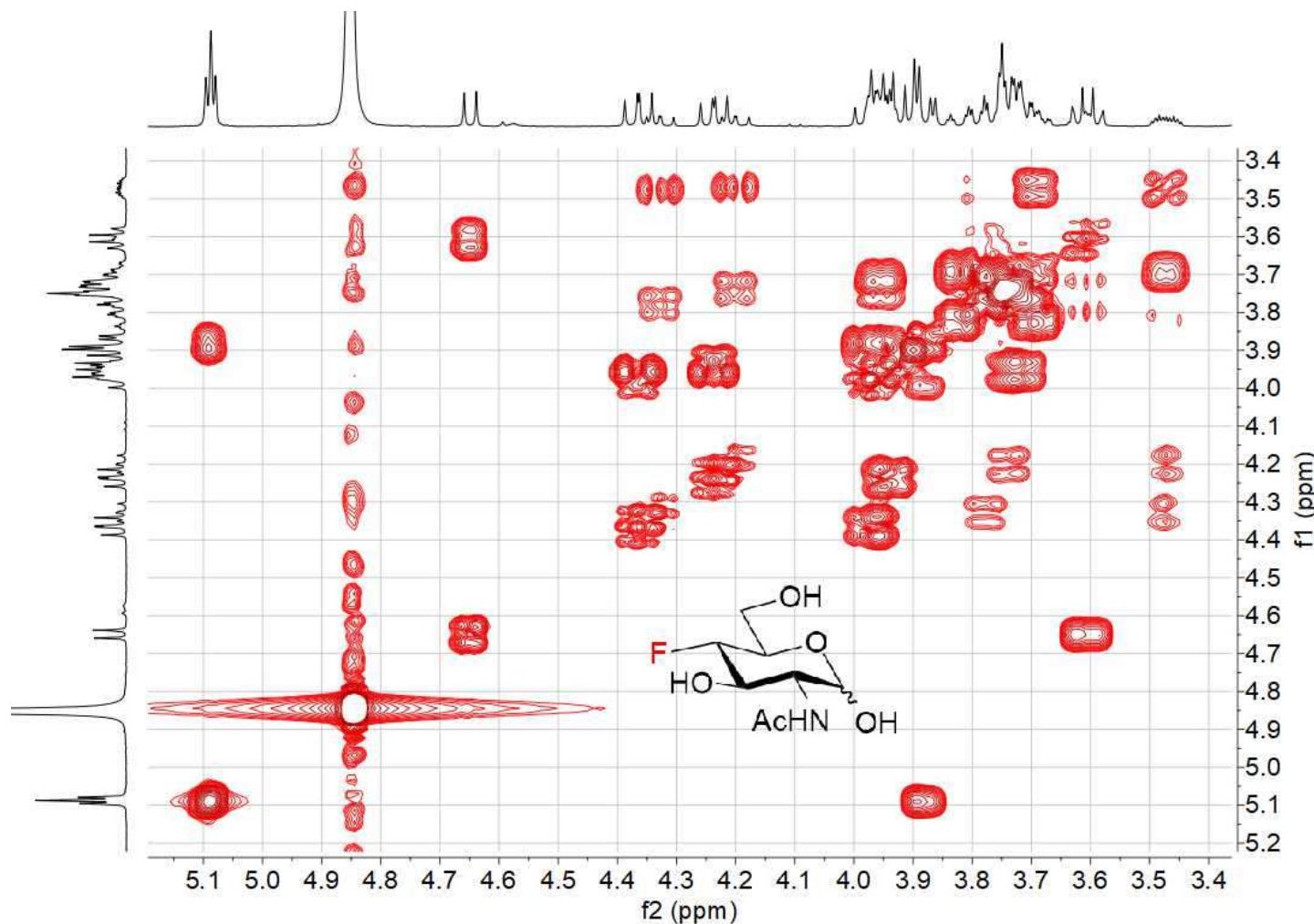
¹³C NMR (100 MHz, CD₃OD) 53



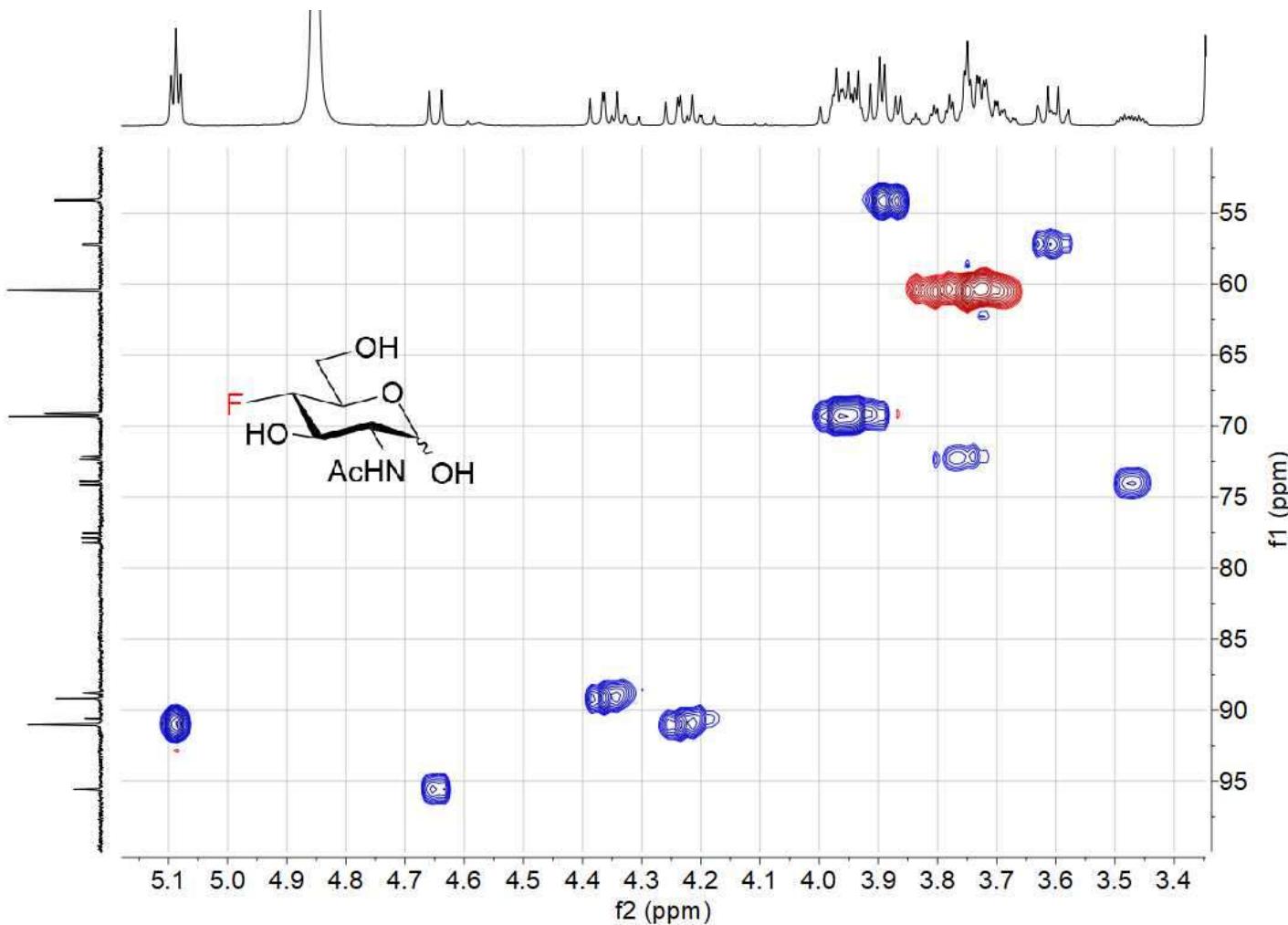
¹⁹F NMR (376 MHz, CD₃OD) 53 (α/β ca. 10/3)



¹H-¹H COSY 53

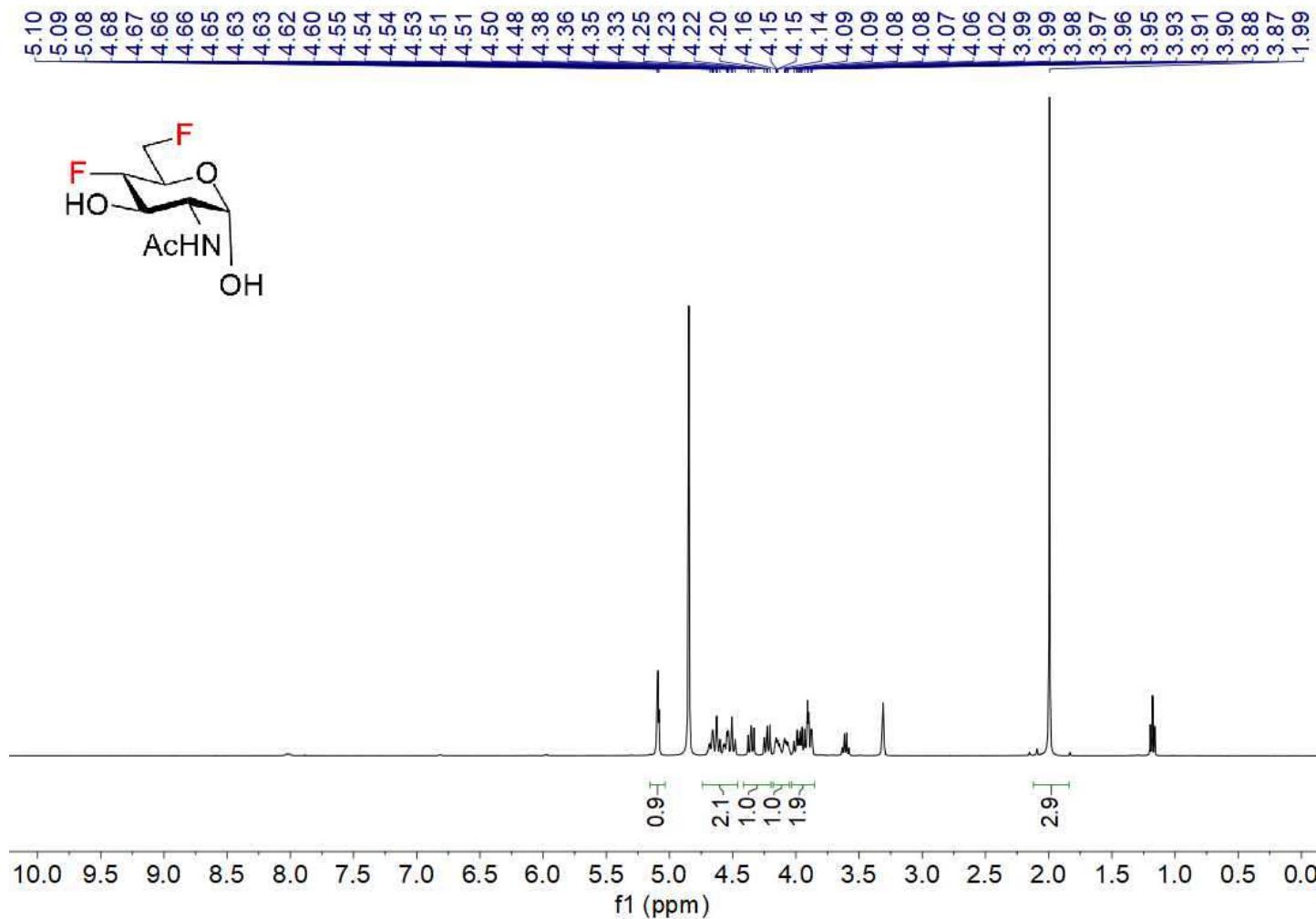


^1H - ^{13}C HSQC 53

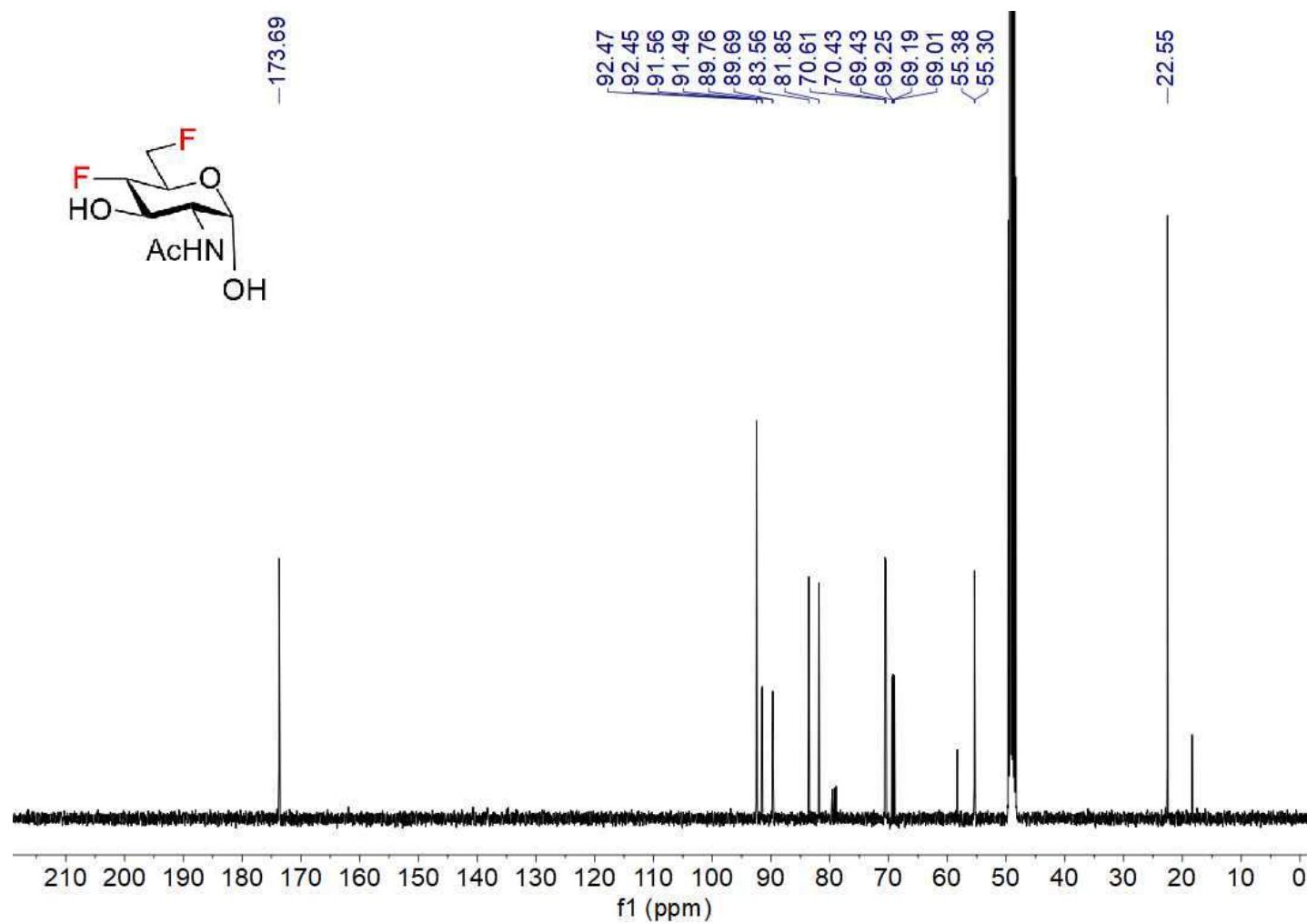


NMR COMPOUND 54

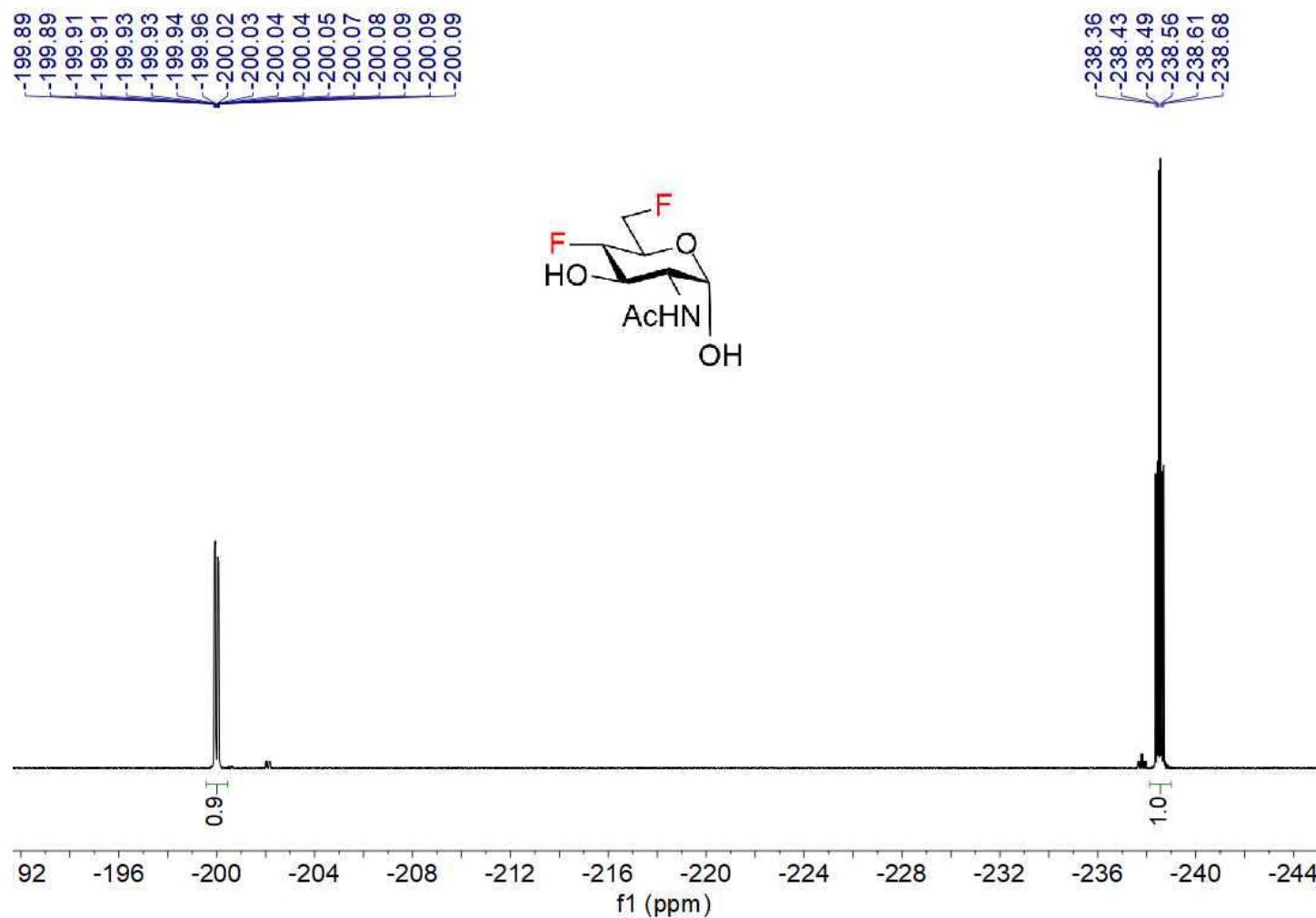
^1H NMR (400 MHz, CD_3OD) 54



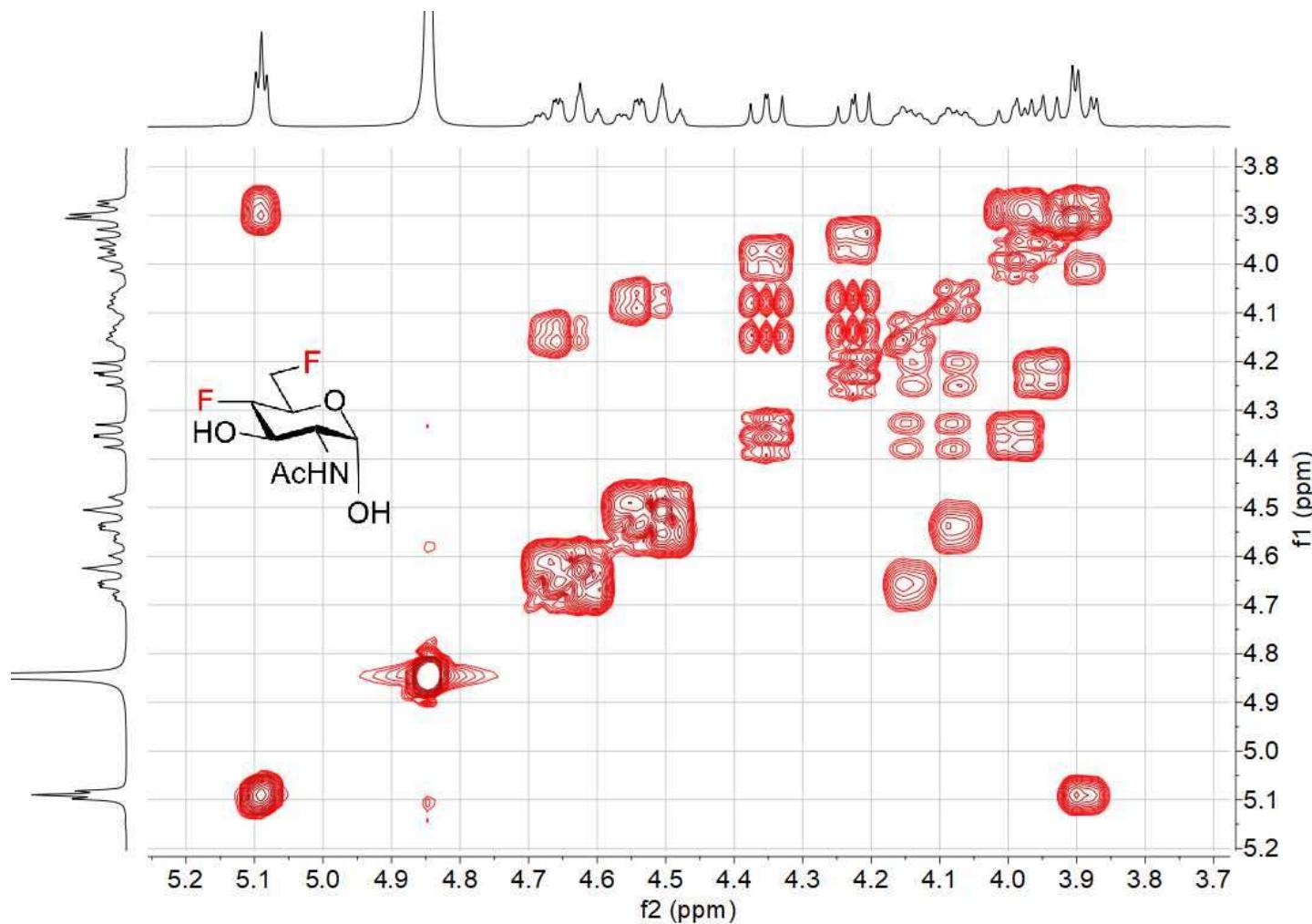
¹³C NMR (100 MHz, CD₃OD) 54



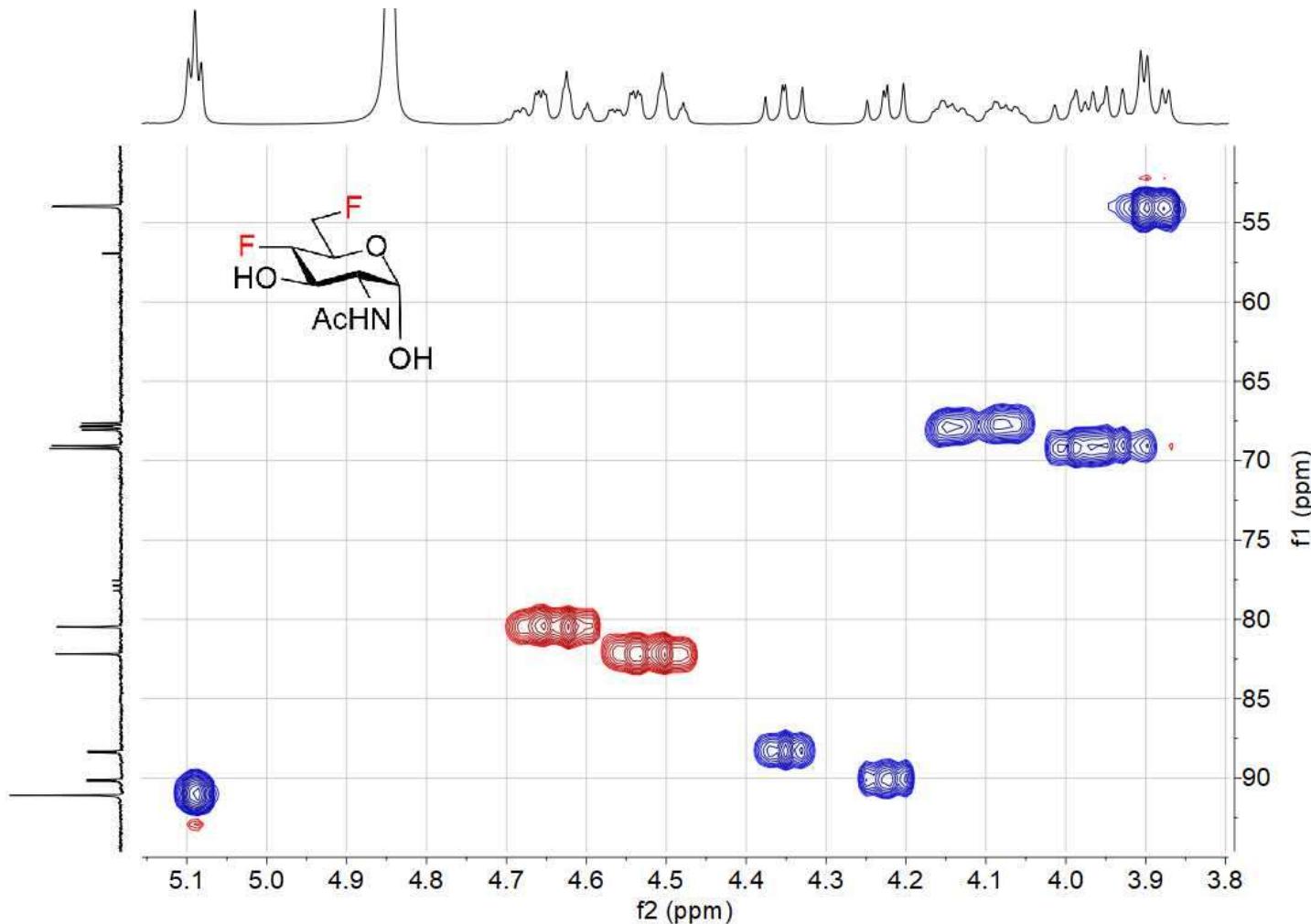
¹⁹F NMR (376 MHz, CD₃OD) 54



^1H - ^1H COSY 54

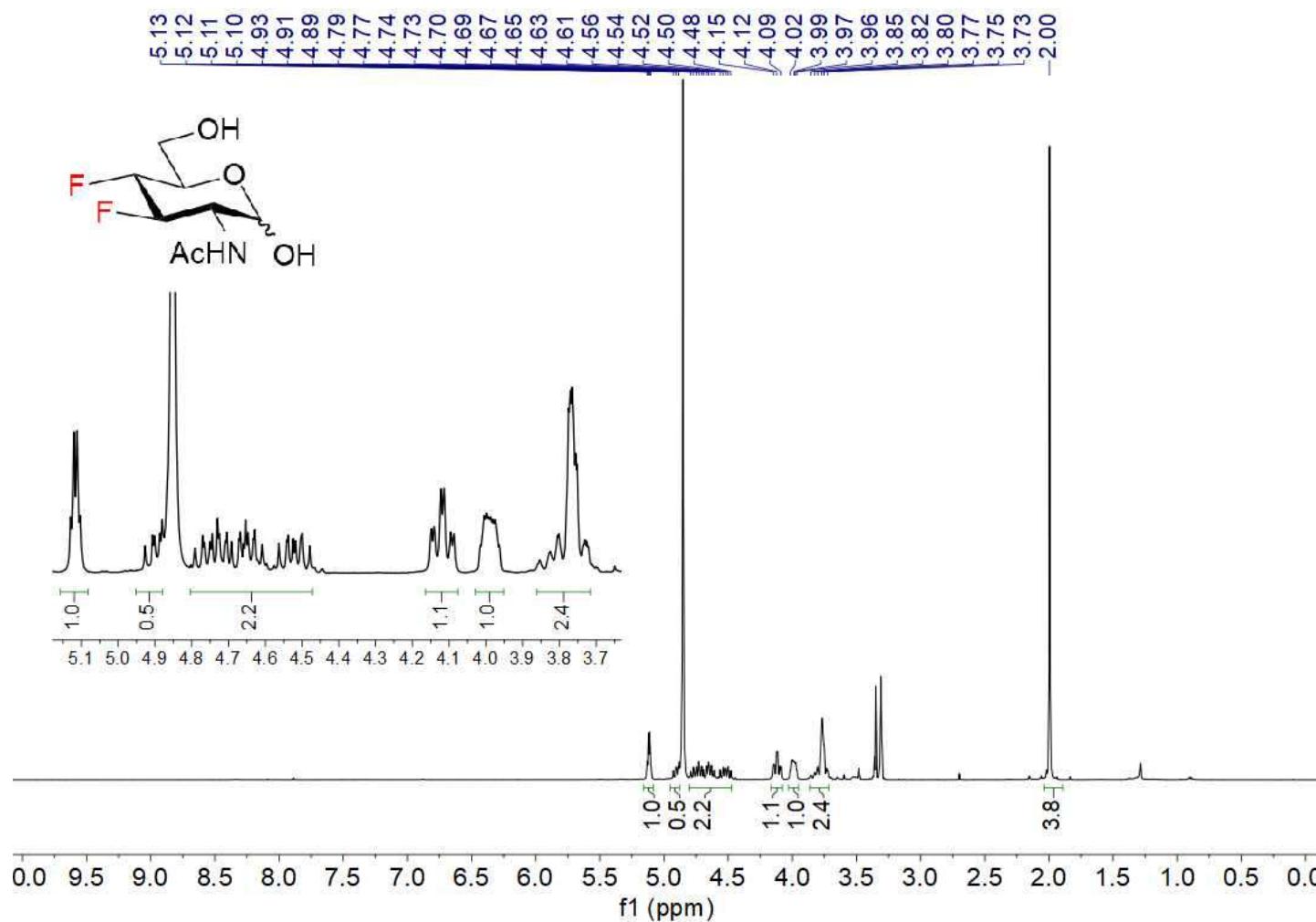


^1H - ^{13}C HSQC 54

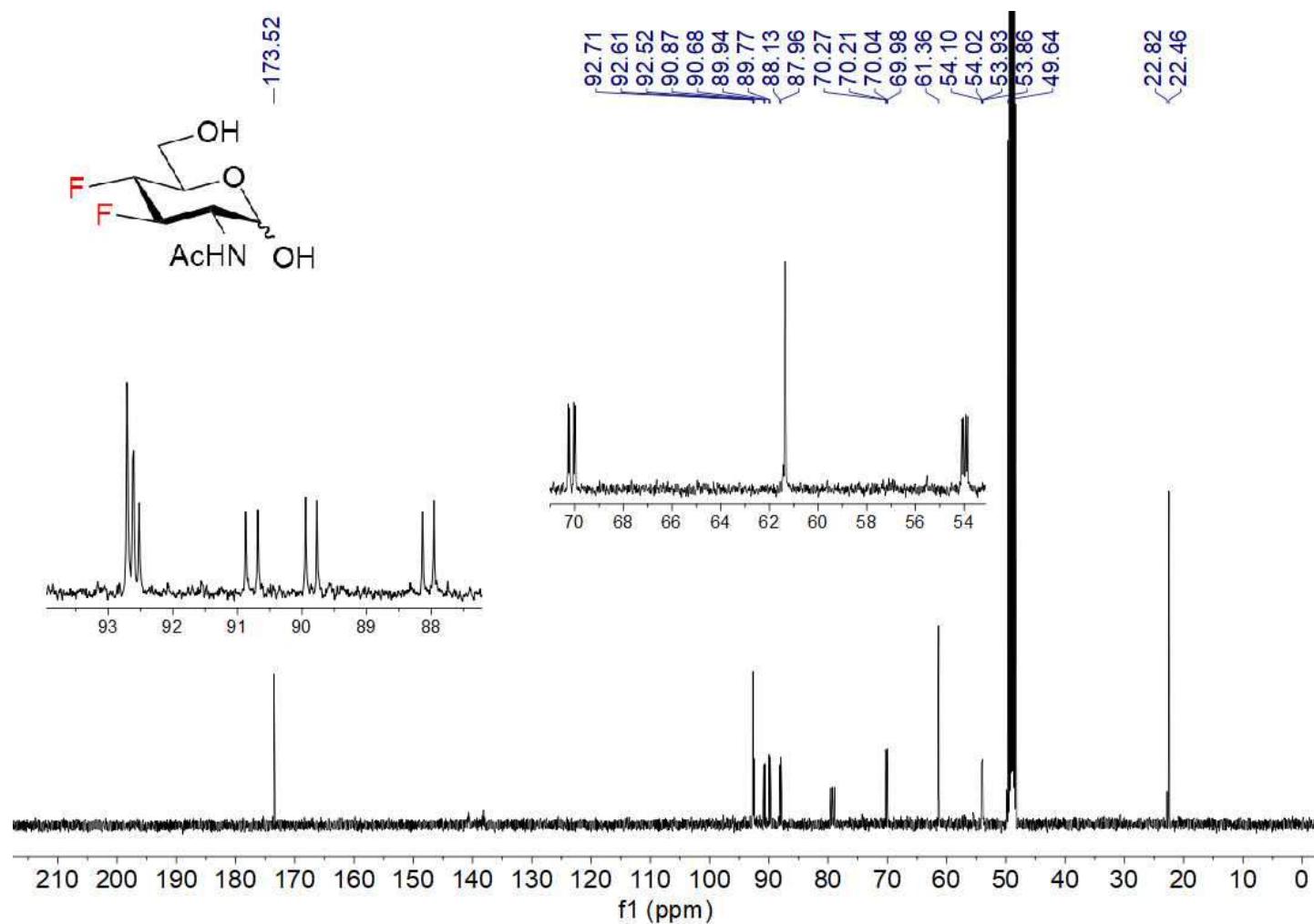


NMR COMPOUND 55

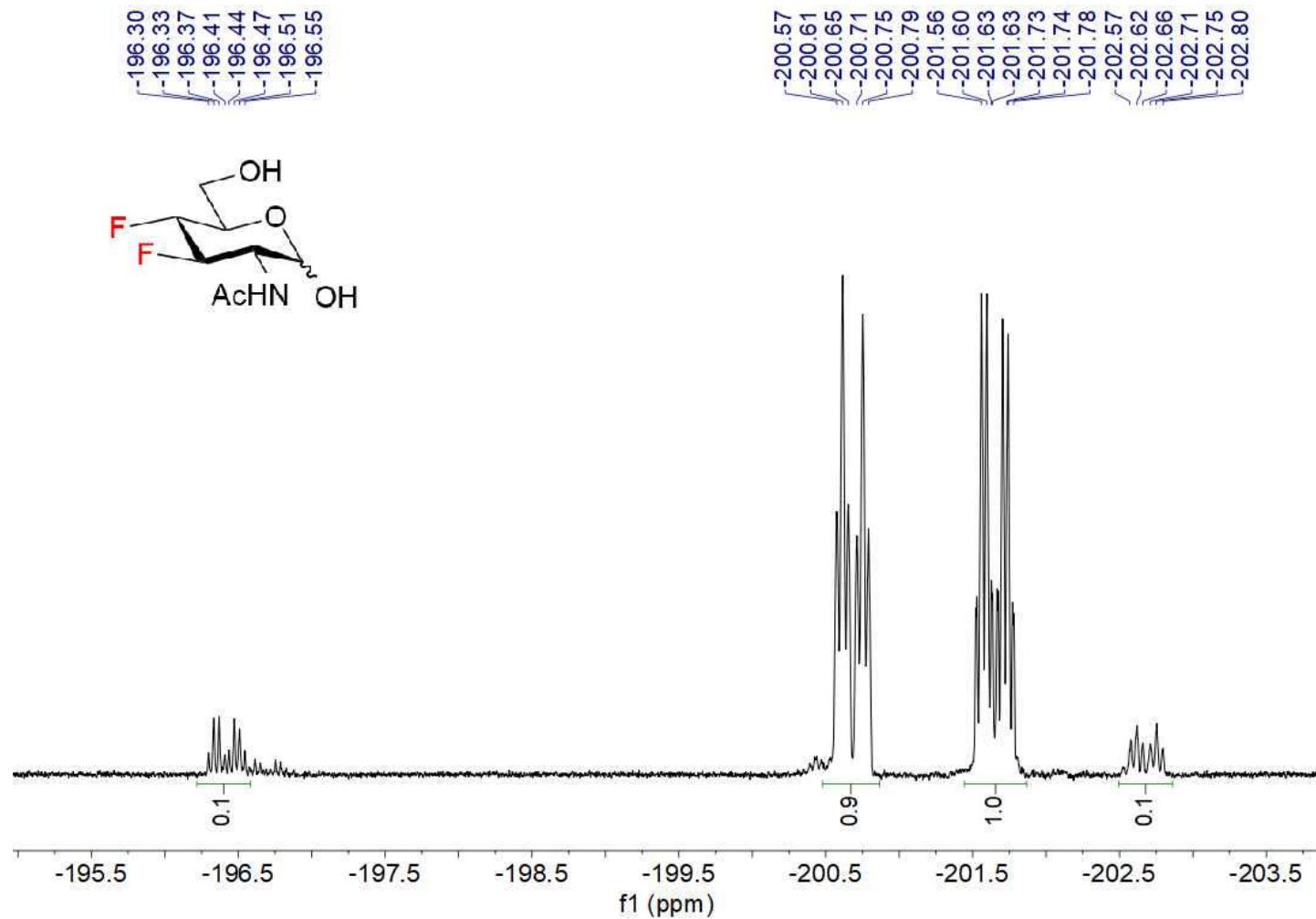
¹H NMR (400 MHz, CD₃OD) 55 (α/β ca. 10/1)



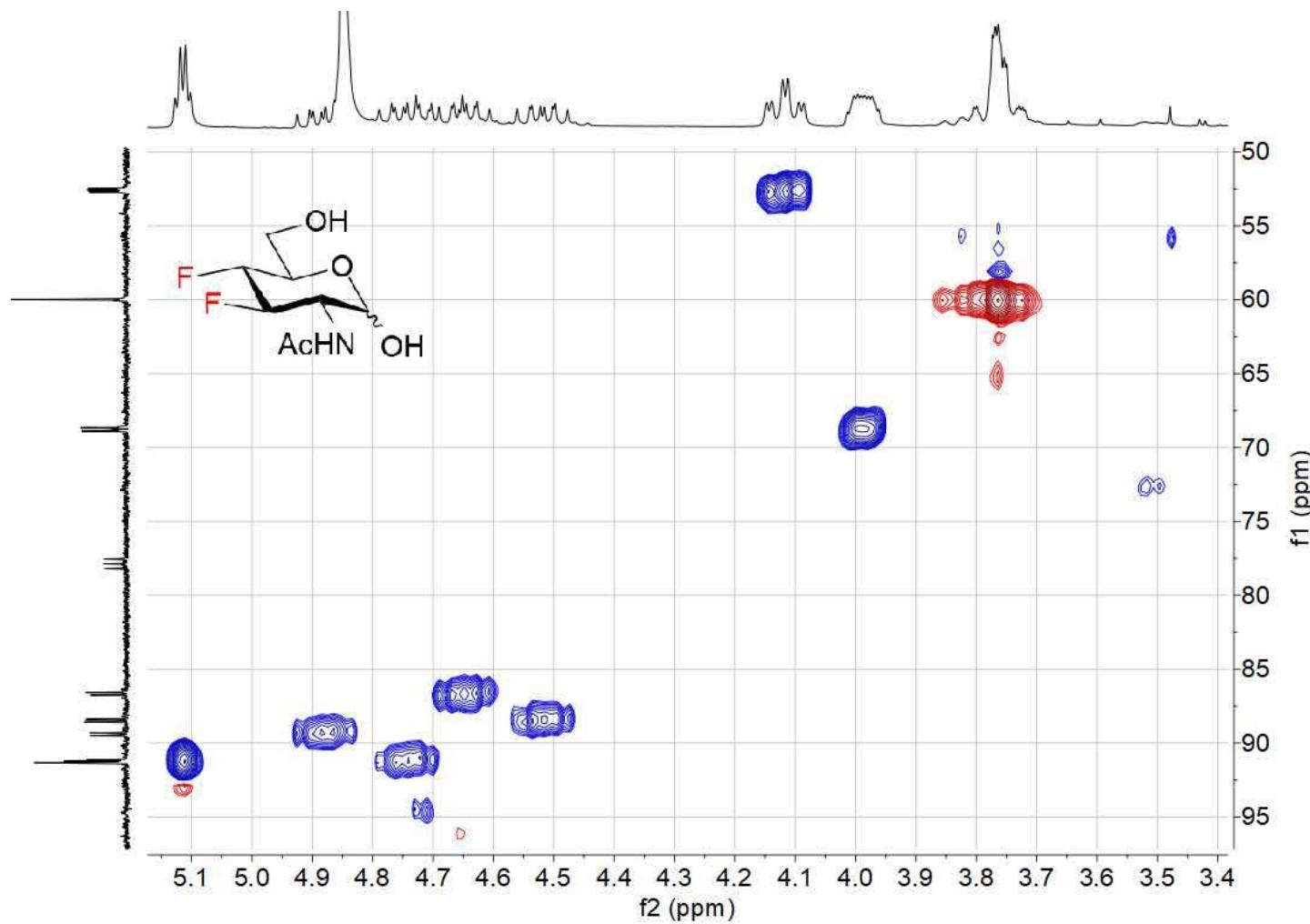
¹³C NMR (100 MHz, CD₃OD) 55



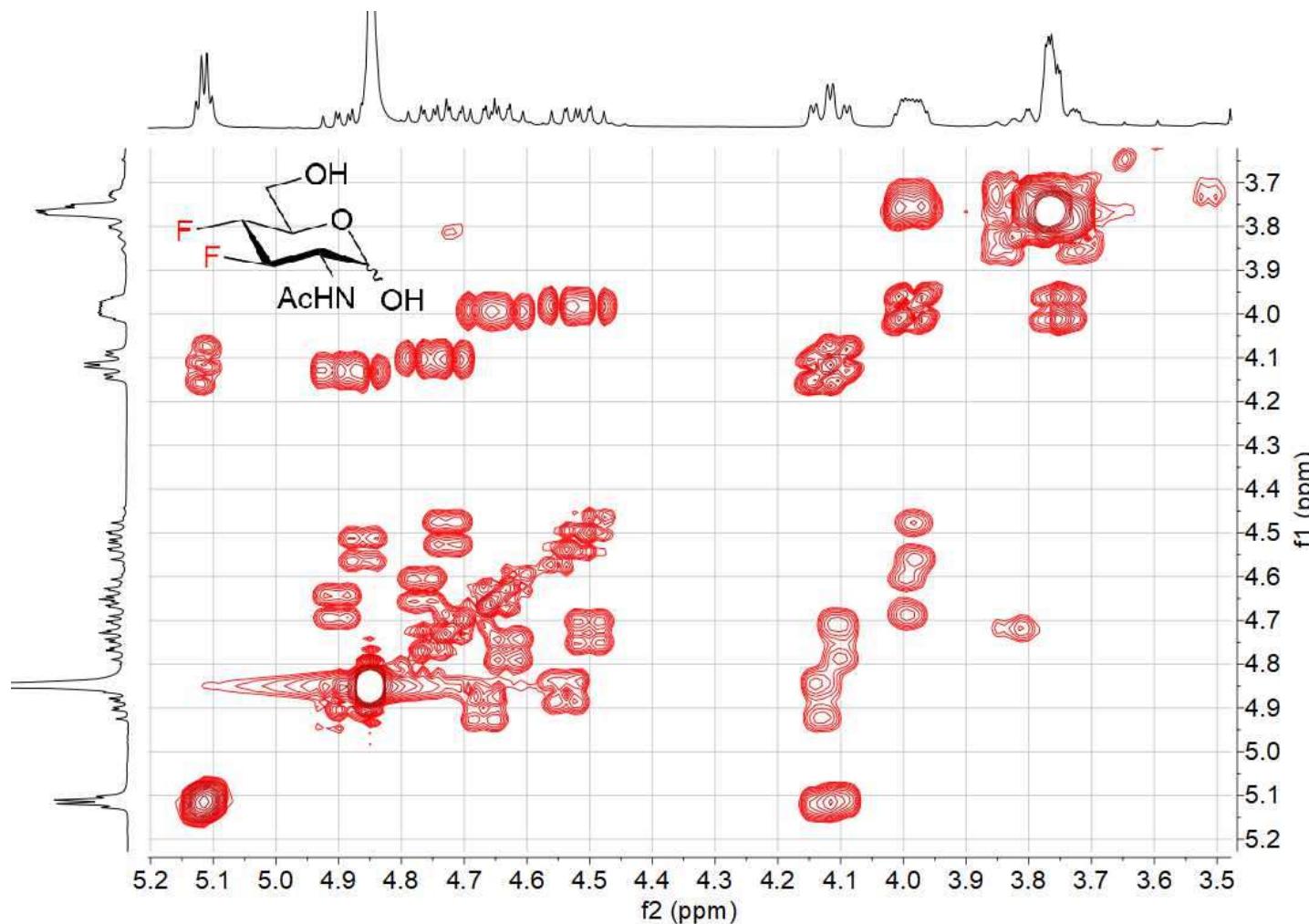
¹⁹F NMR (376 MHz, CD₃OD) 55 (α/β ca. 10/1)



^1H - ^1H COSY 55

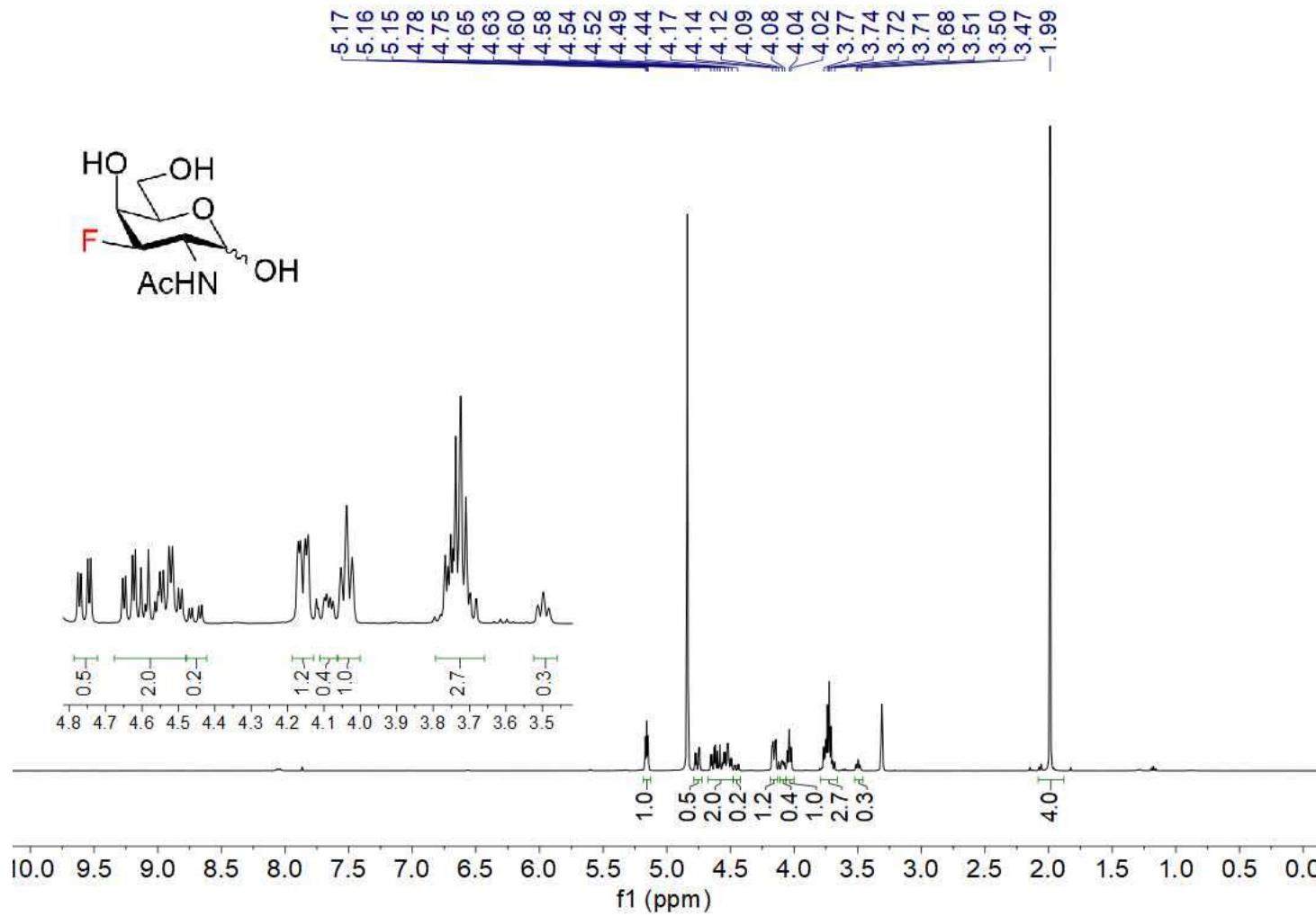


^1H - ^{13}C HSQC 55

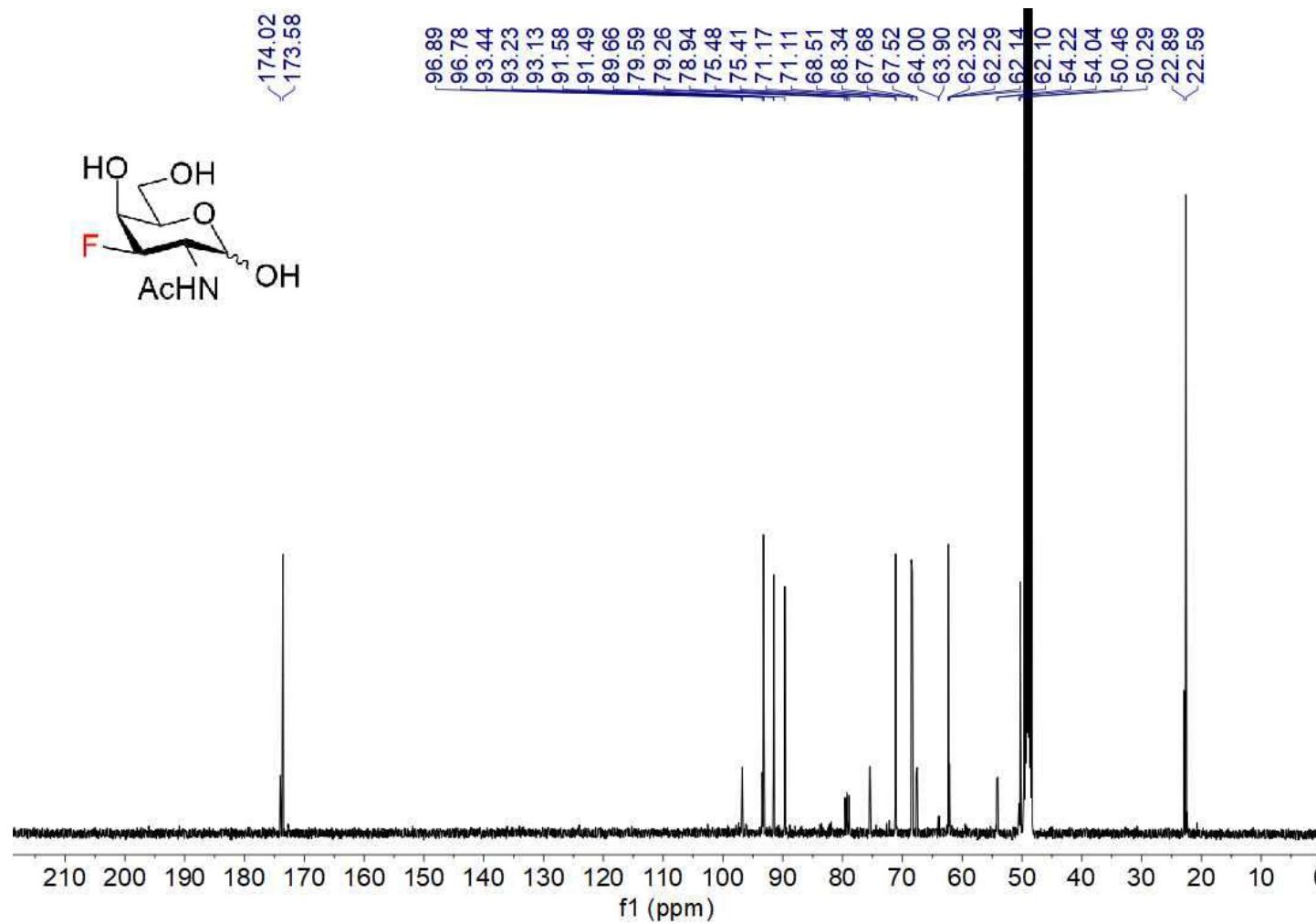


NMR COMPOUND 56

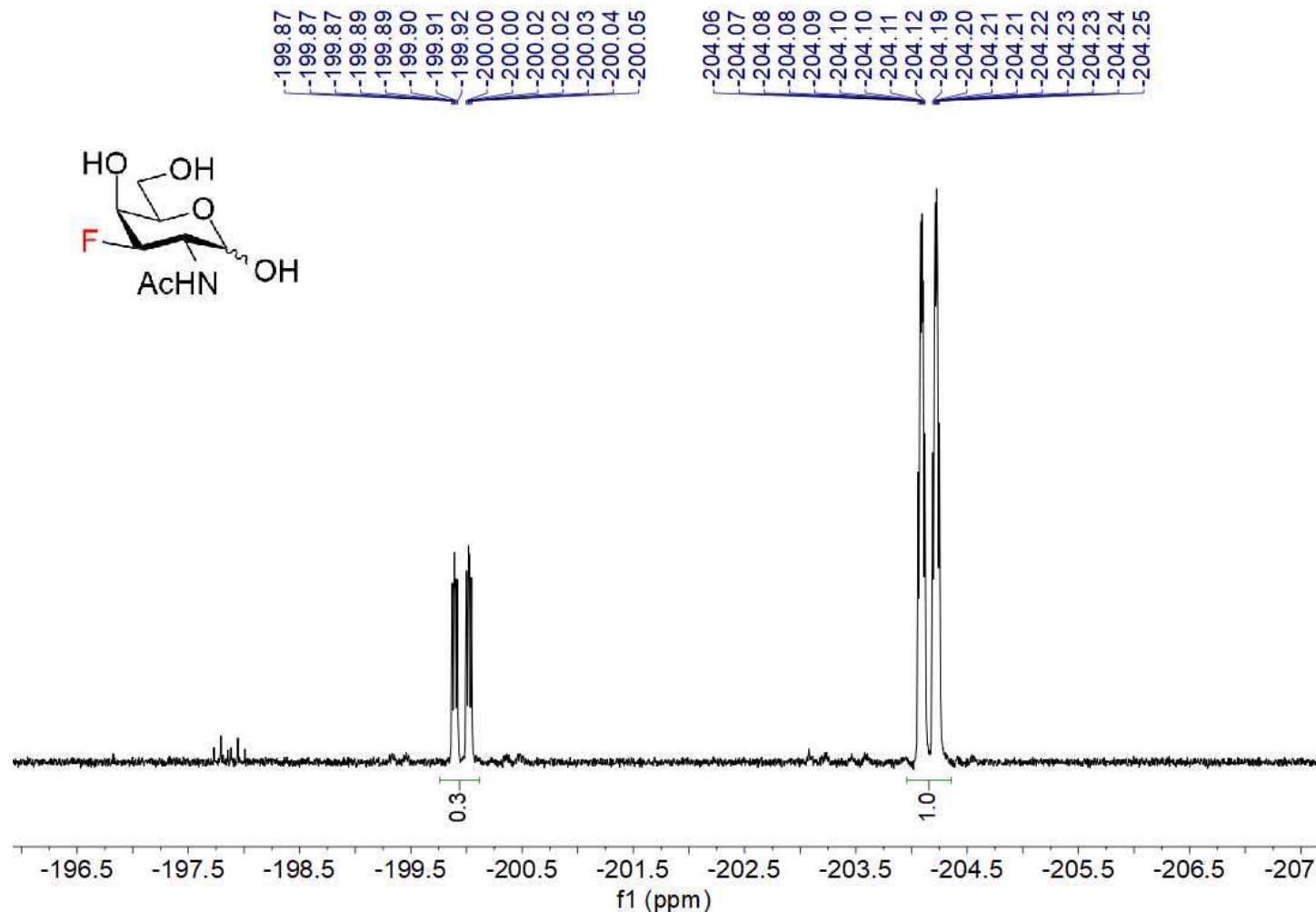
¹H NMR (400 MHz, CD₃OD) 56 (α/β ca. 10/3)



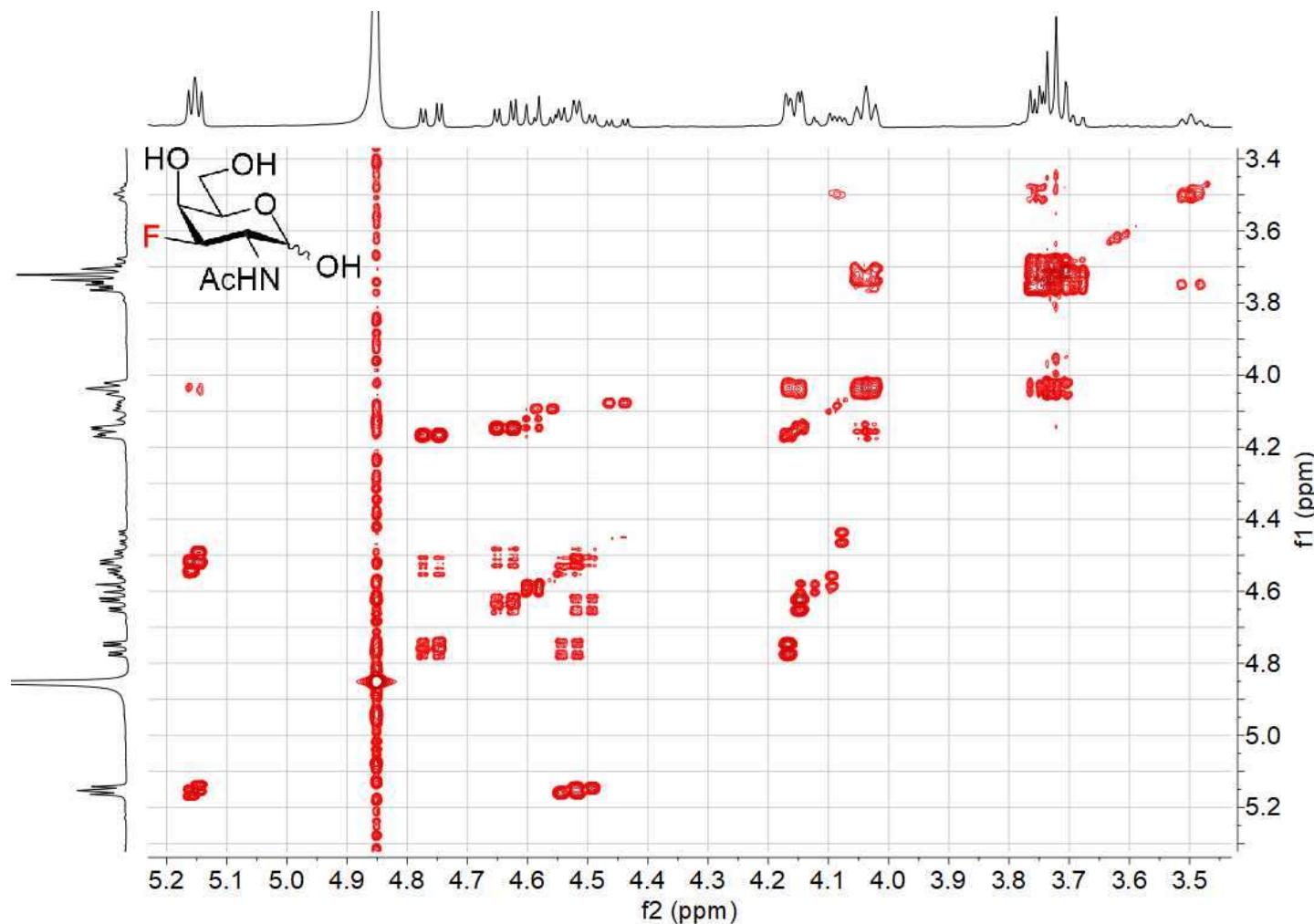
¹³C NMR (100 MHz, CD₃OD) 56



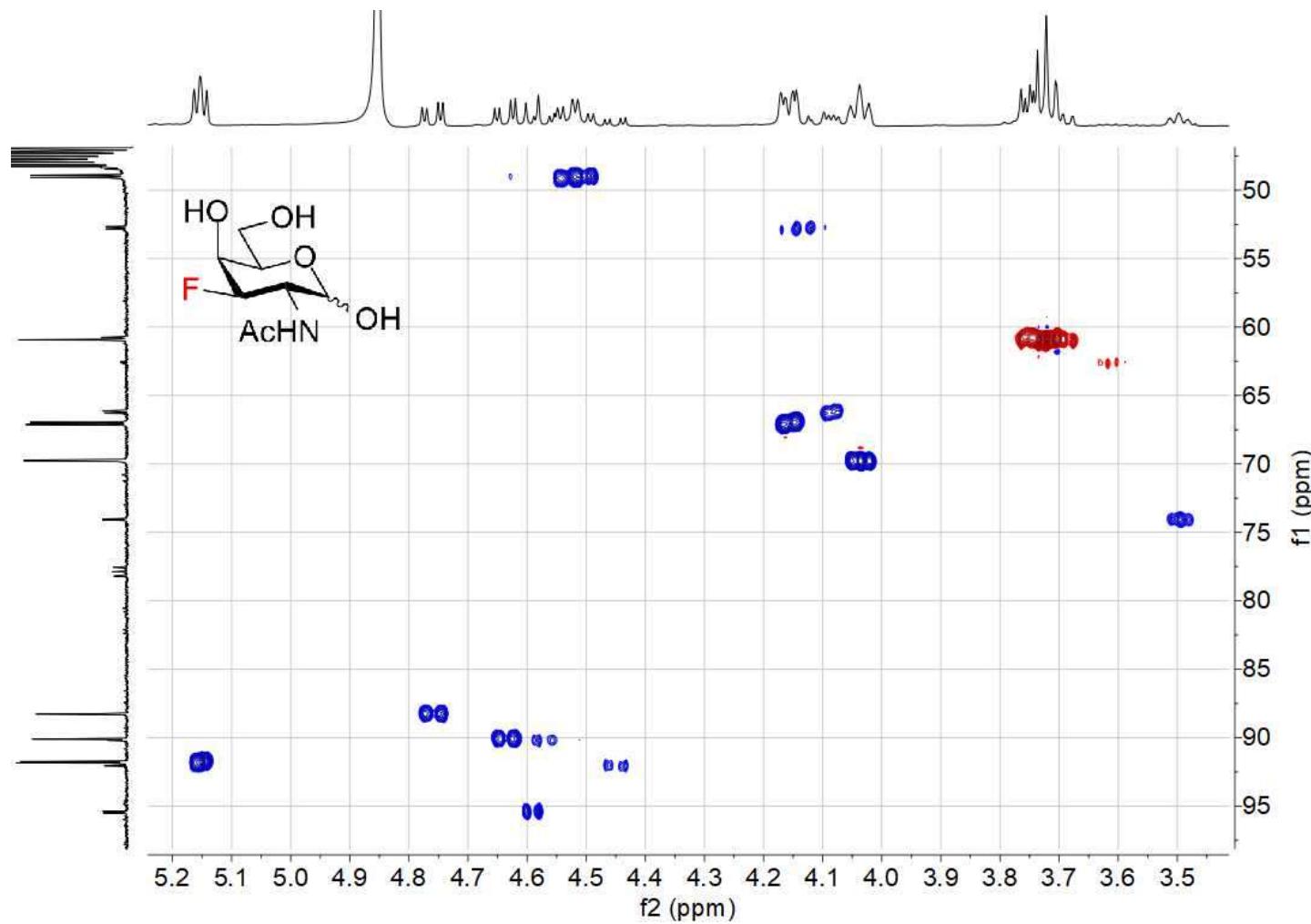
¹⁹F NMR (376 MHz, CD₃OD) 56 (α/β ca. 10/3)



^1H - ^1H COSY NMR 56

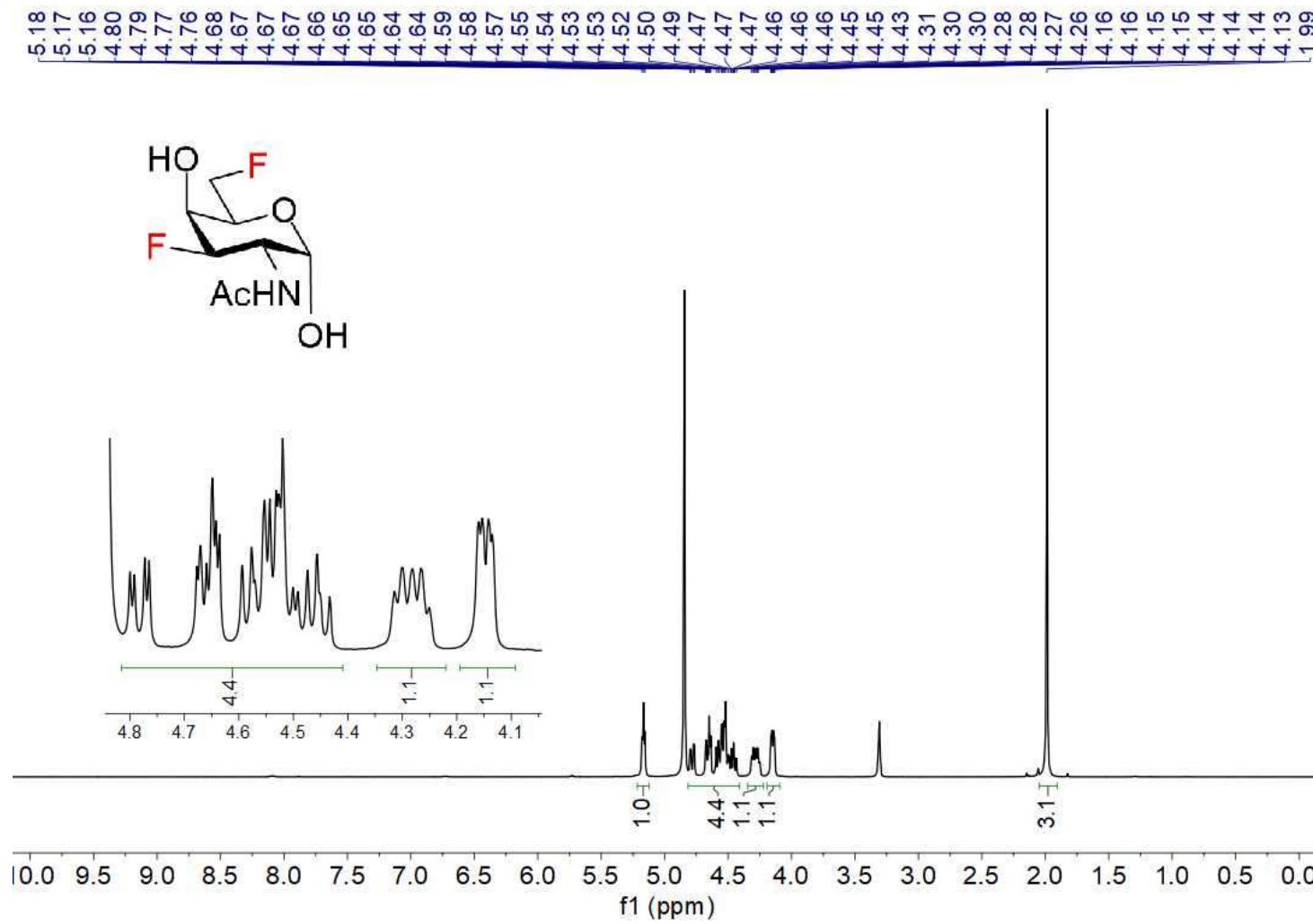


^1H - ^{13}C HSQC NMR 56

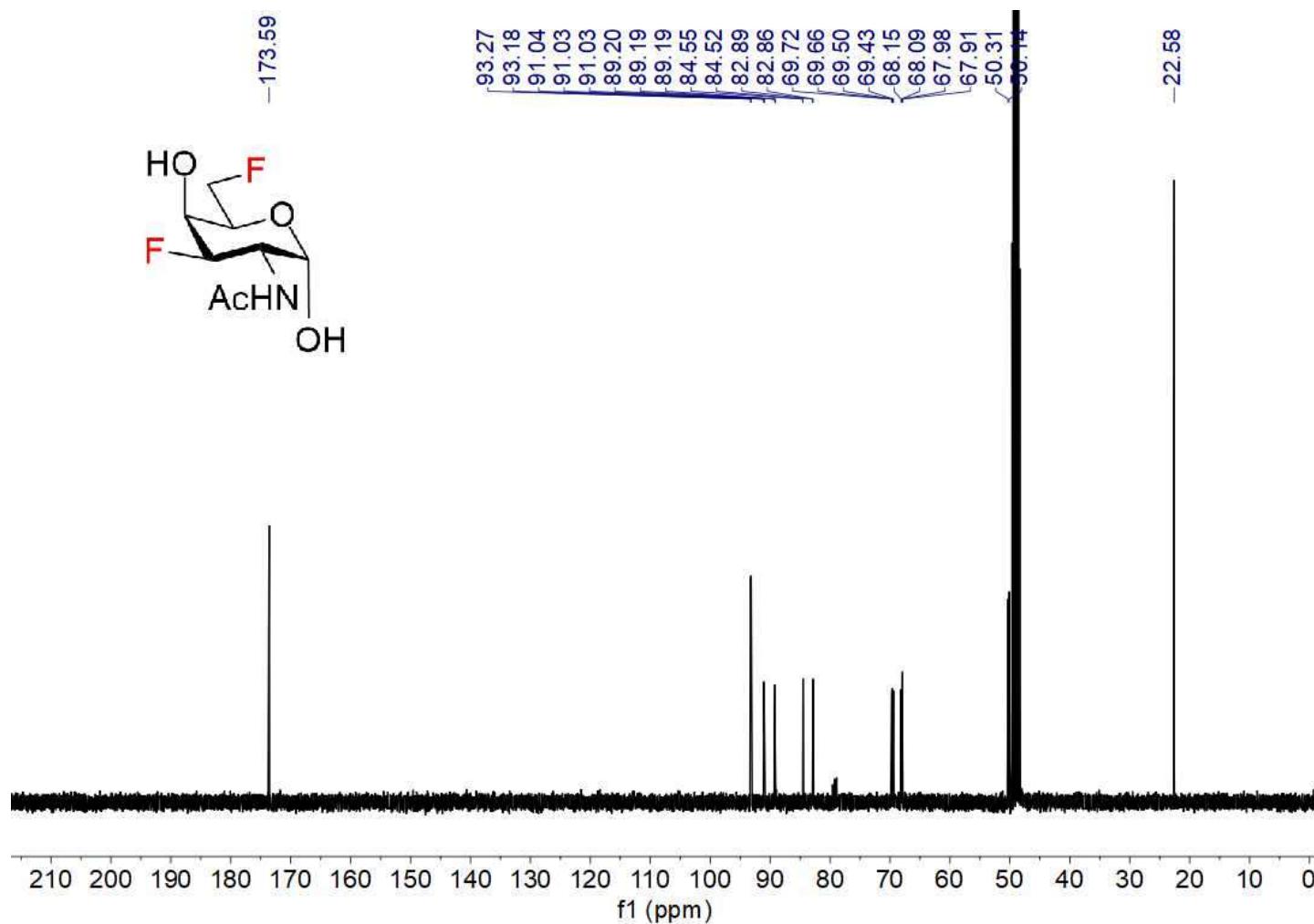


NMR COMPOUND 57

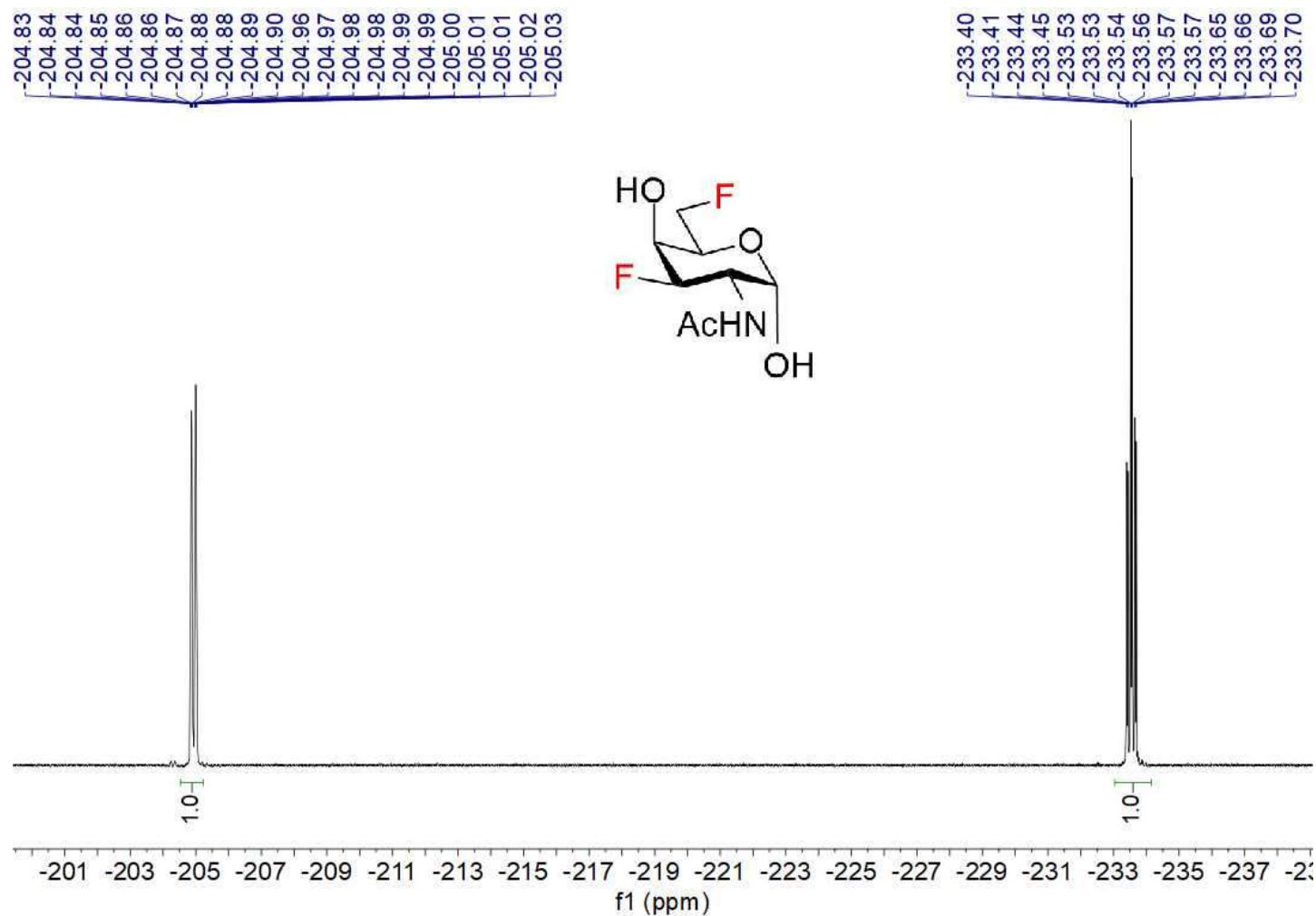
¹H NMR (400 MHz, CD₃OD) 57



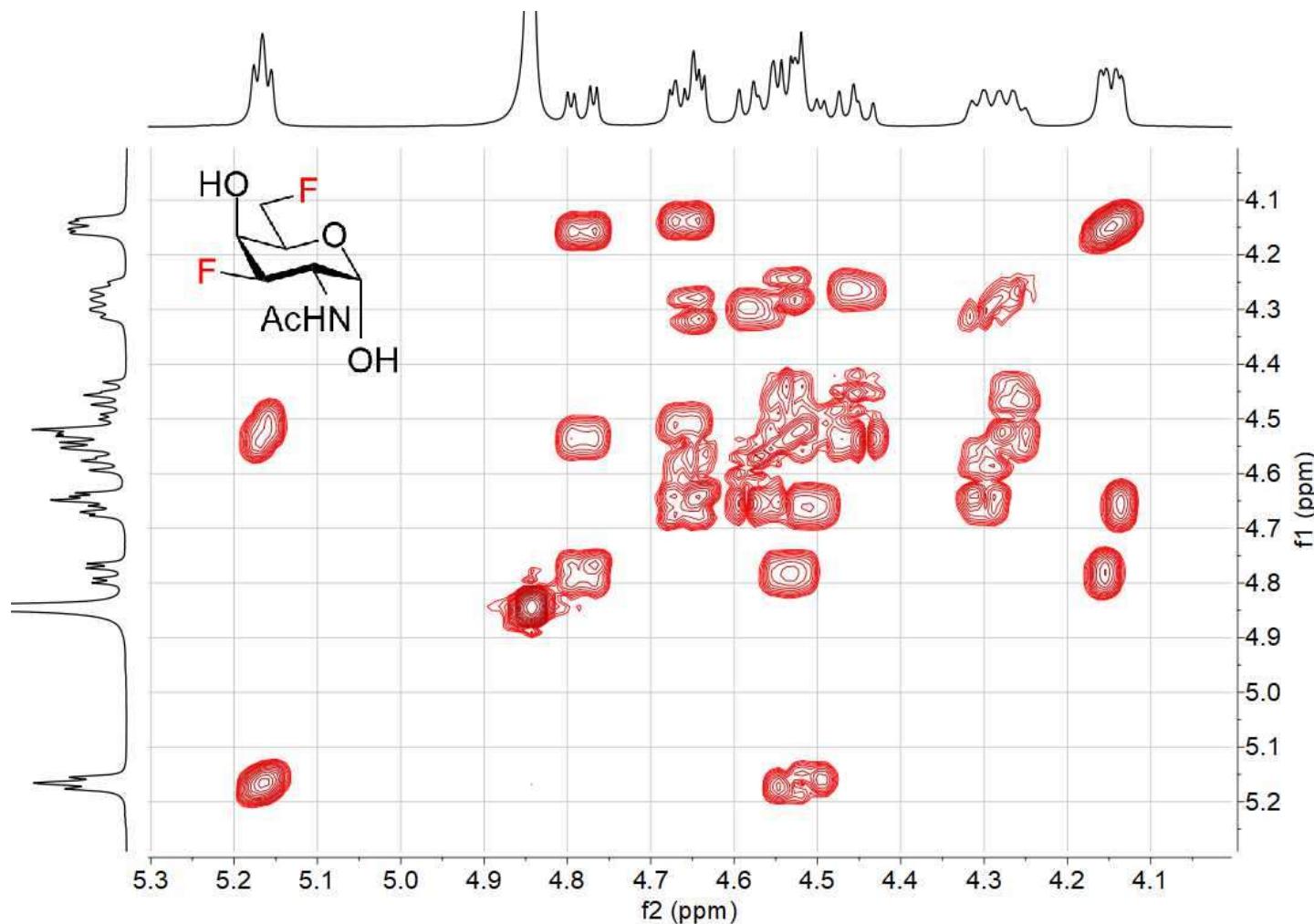
¹³C NMR (100 MHz, CD₃OD) 57



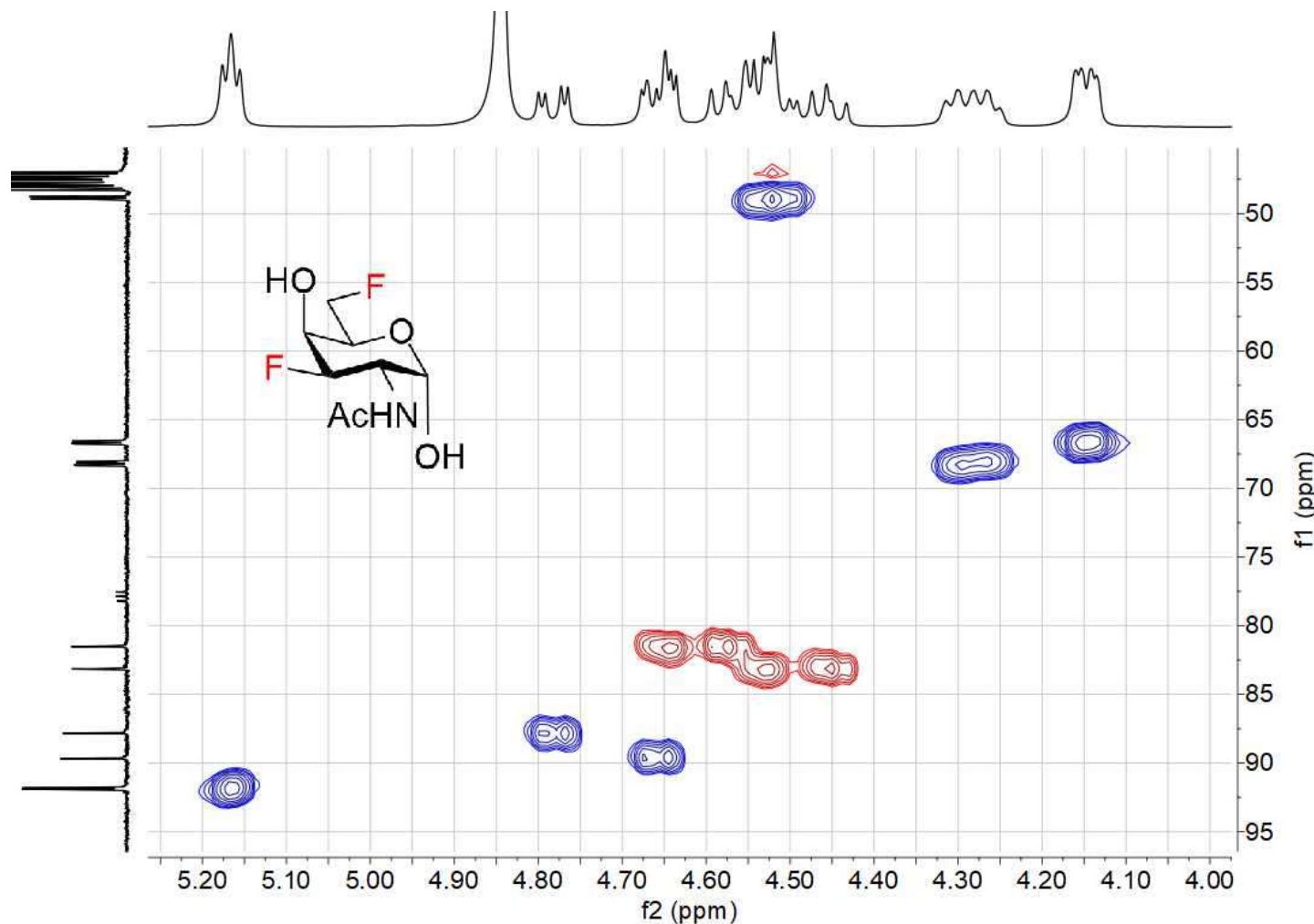
¹⁹F NMR (376 MHz, CD₃OD) 57



¹H-¹H COSY 57

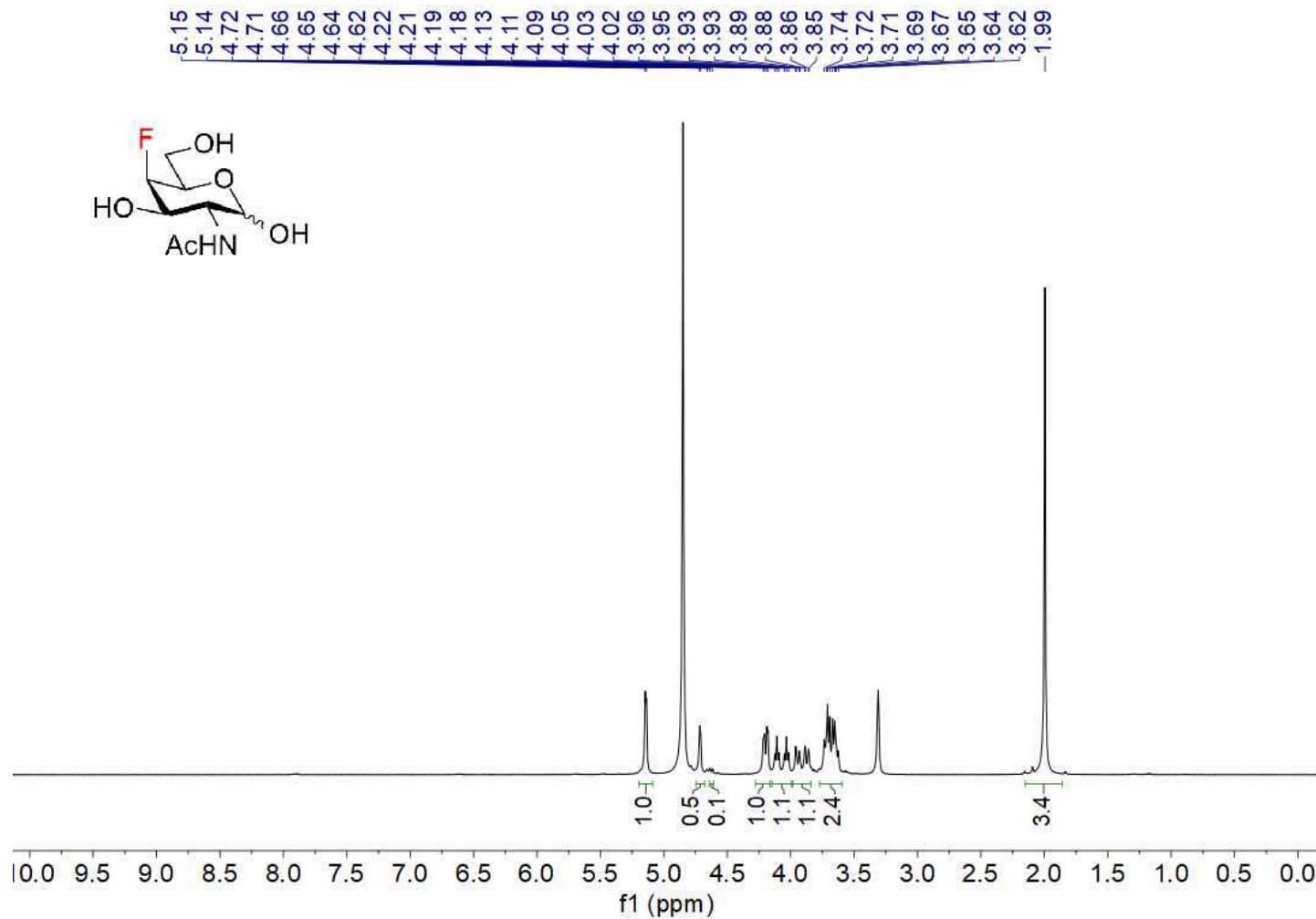


^1H - ^{13}C HSQC 57

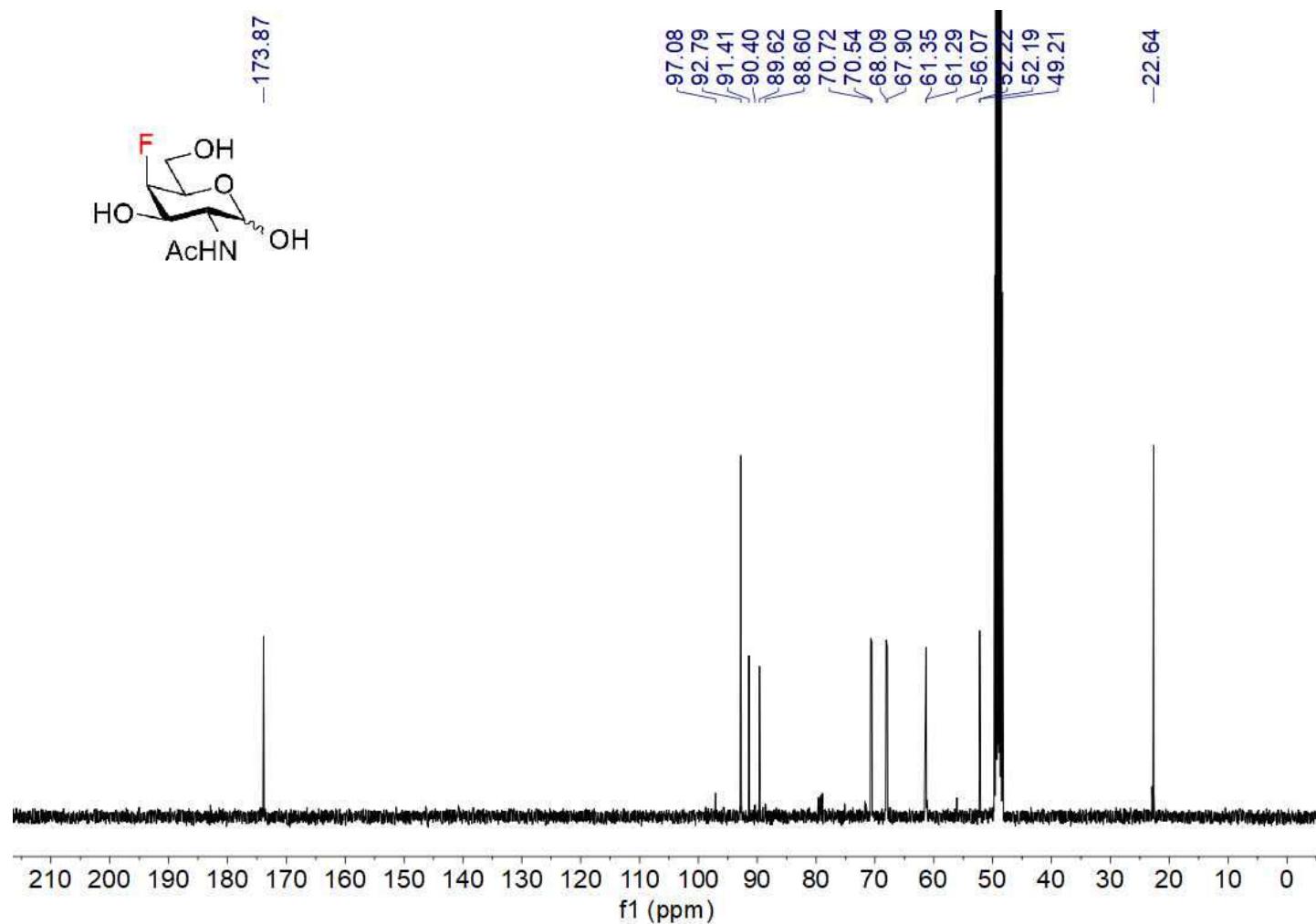


NMR COMPOUND 58

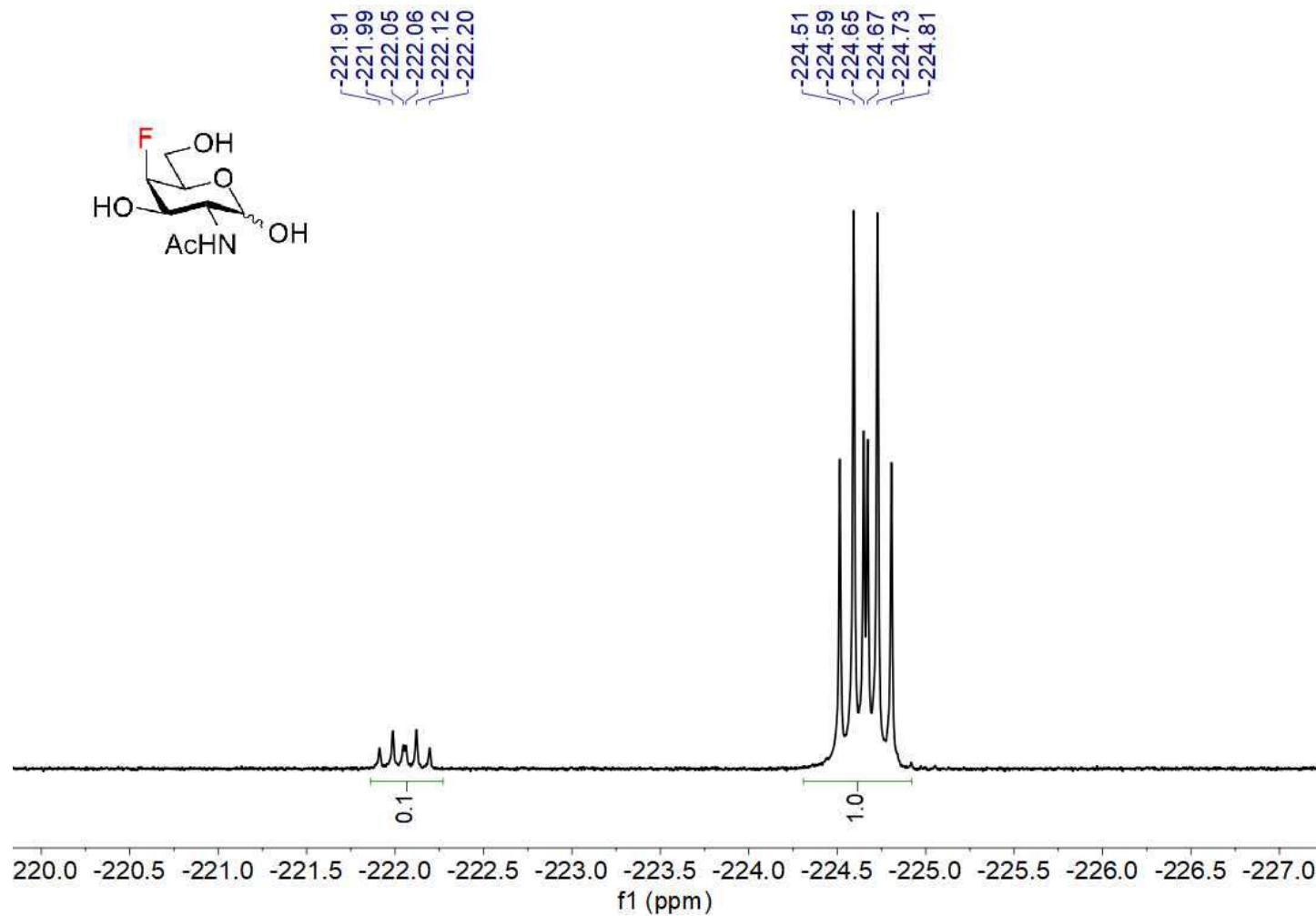
¹H NMR (400 MHz, CD₃OD) 58 (α/β ca. 10/1)



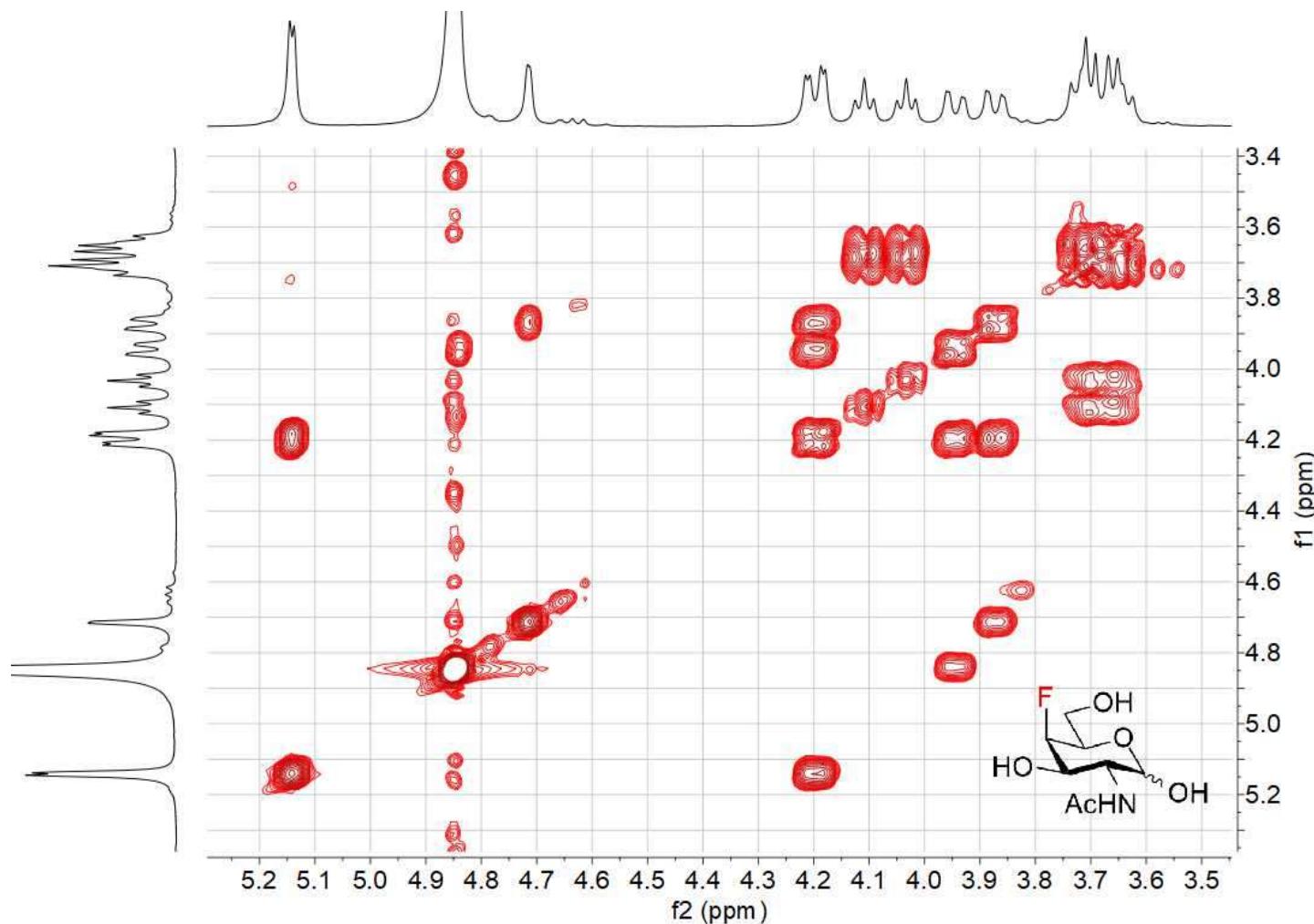
¹³C NMR (100 MHz, CD₃OD) 58



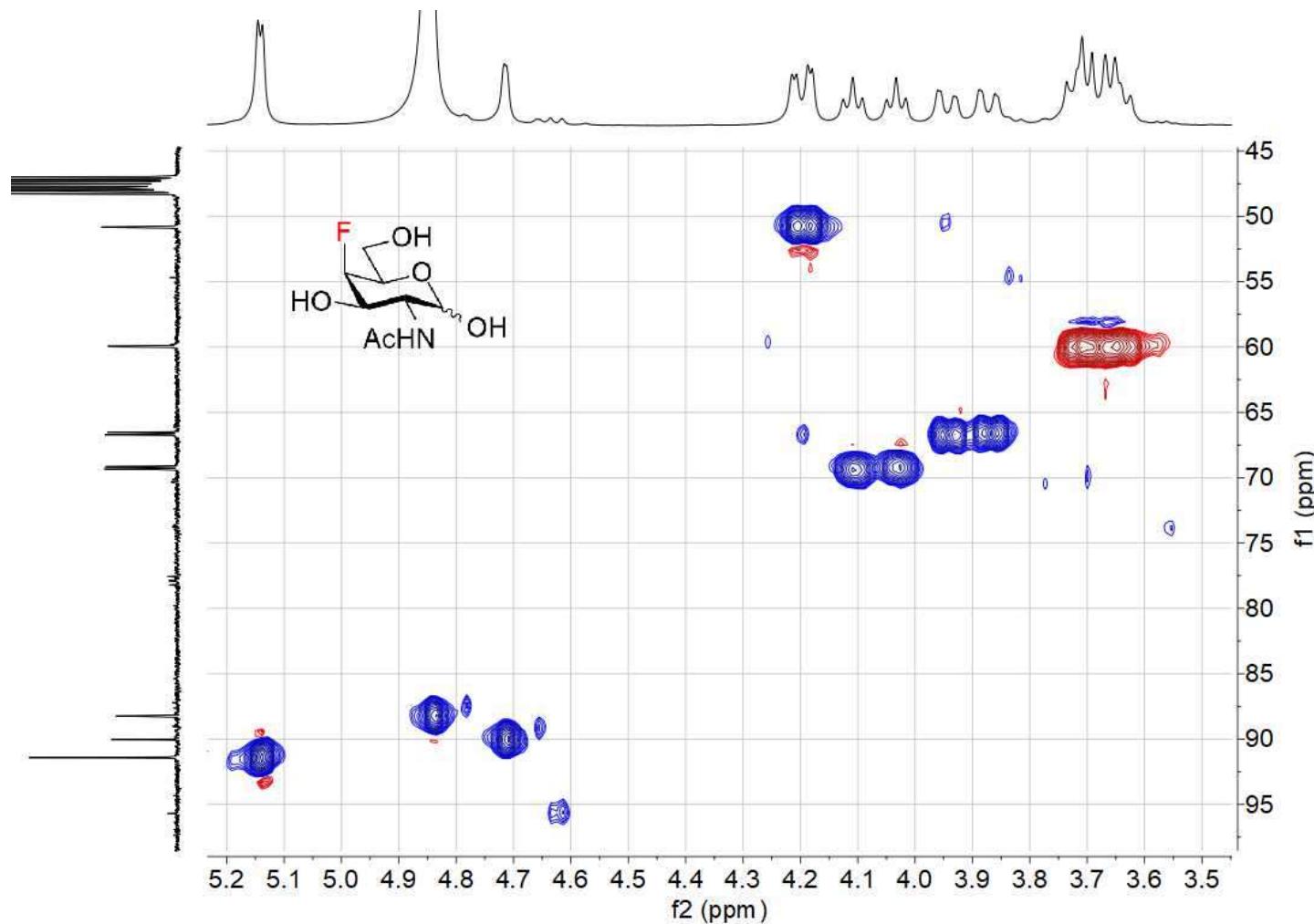
¹⁹F NMR (376 MHz, CD₃OD) 58 (α/β ca. 10/1)



¹H-¹H COSY 58

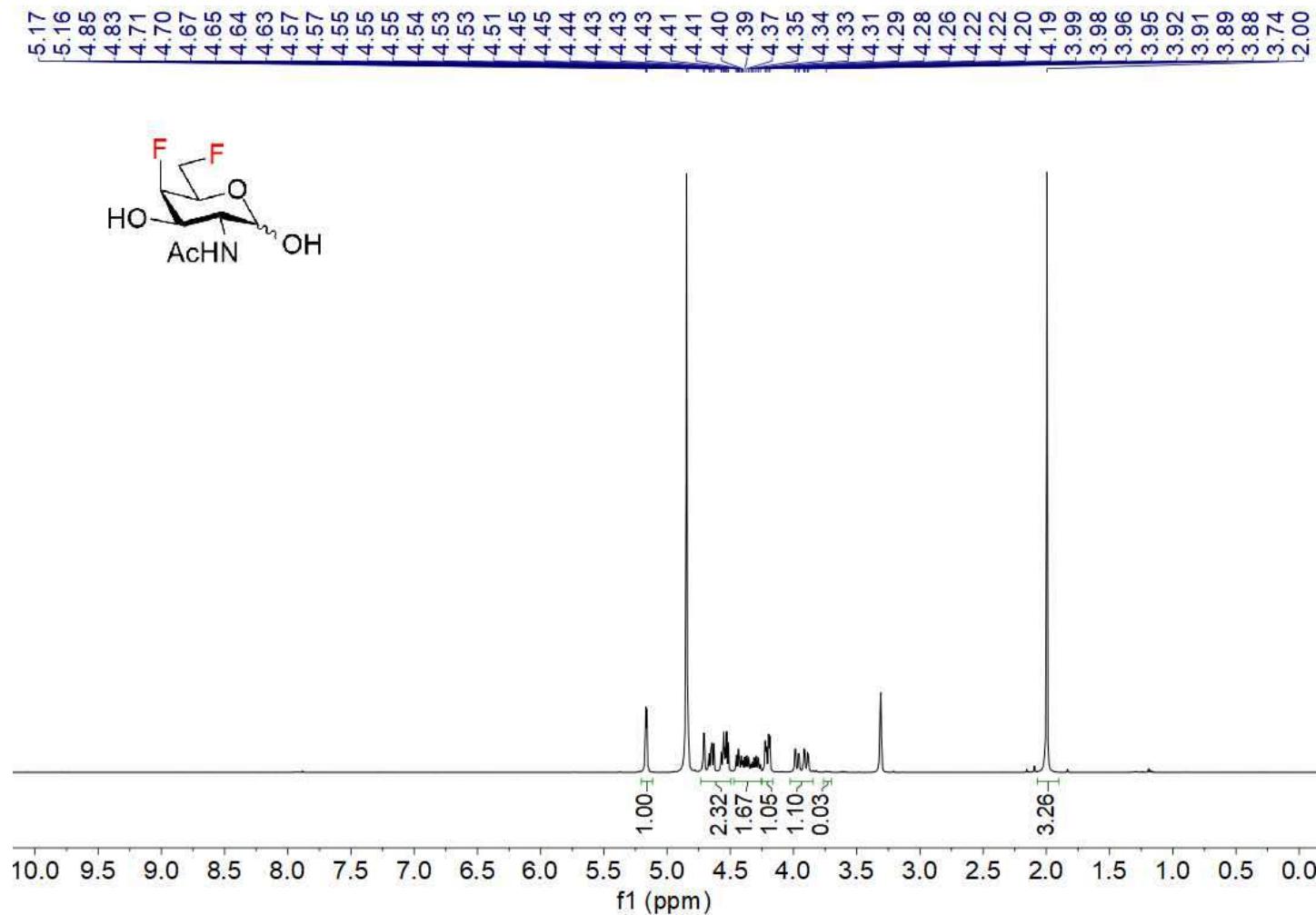


^1H - ^{13}C HSQC 58

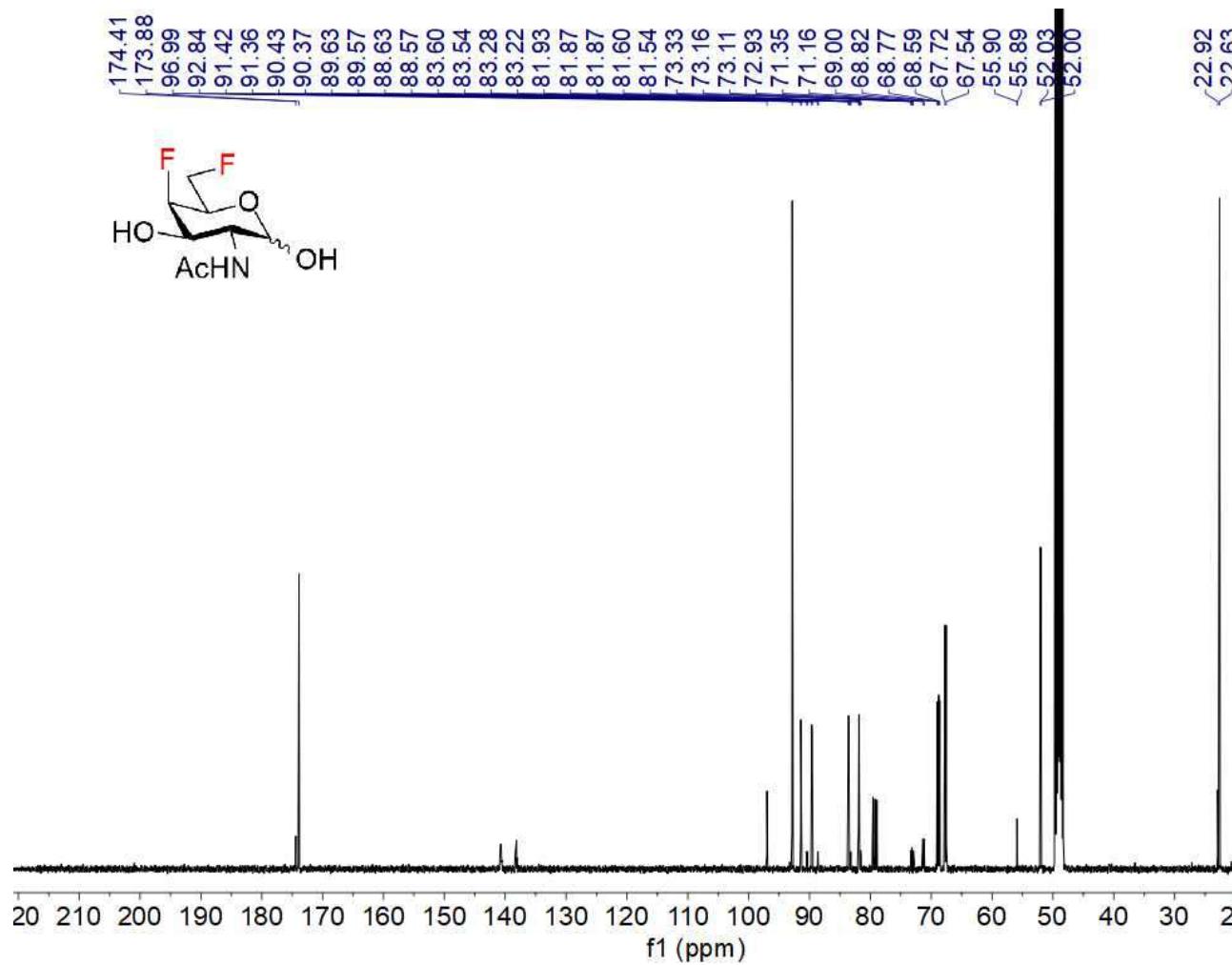


NMR COMPOUND 59

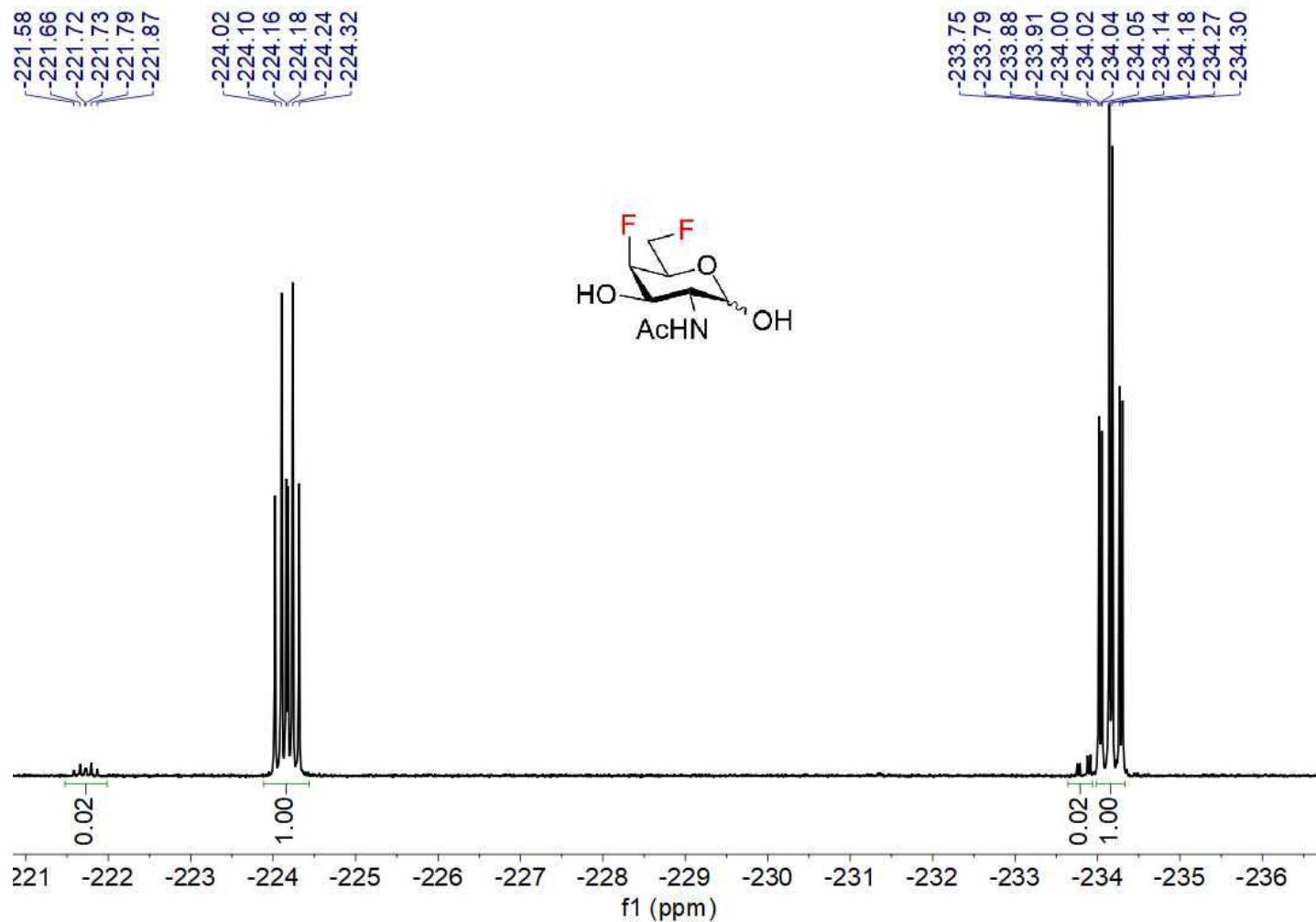
¹H NMR (400 MHz, CD₃OD) 59 (ca. 2-3% β -anomer)



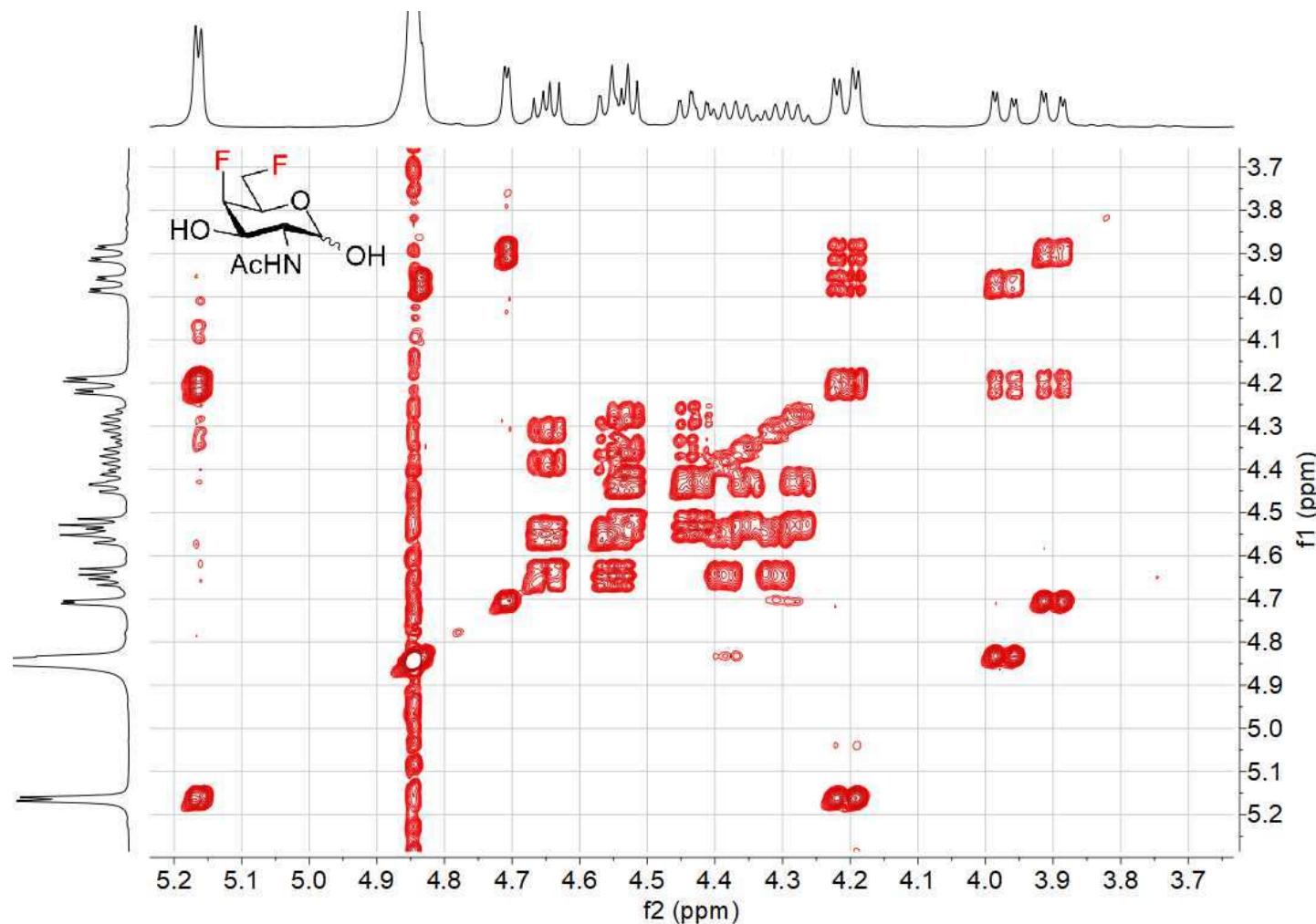
¹³C NMR (100 MHz, CD₃OD) 59



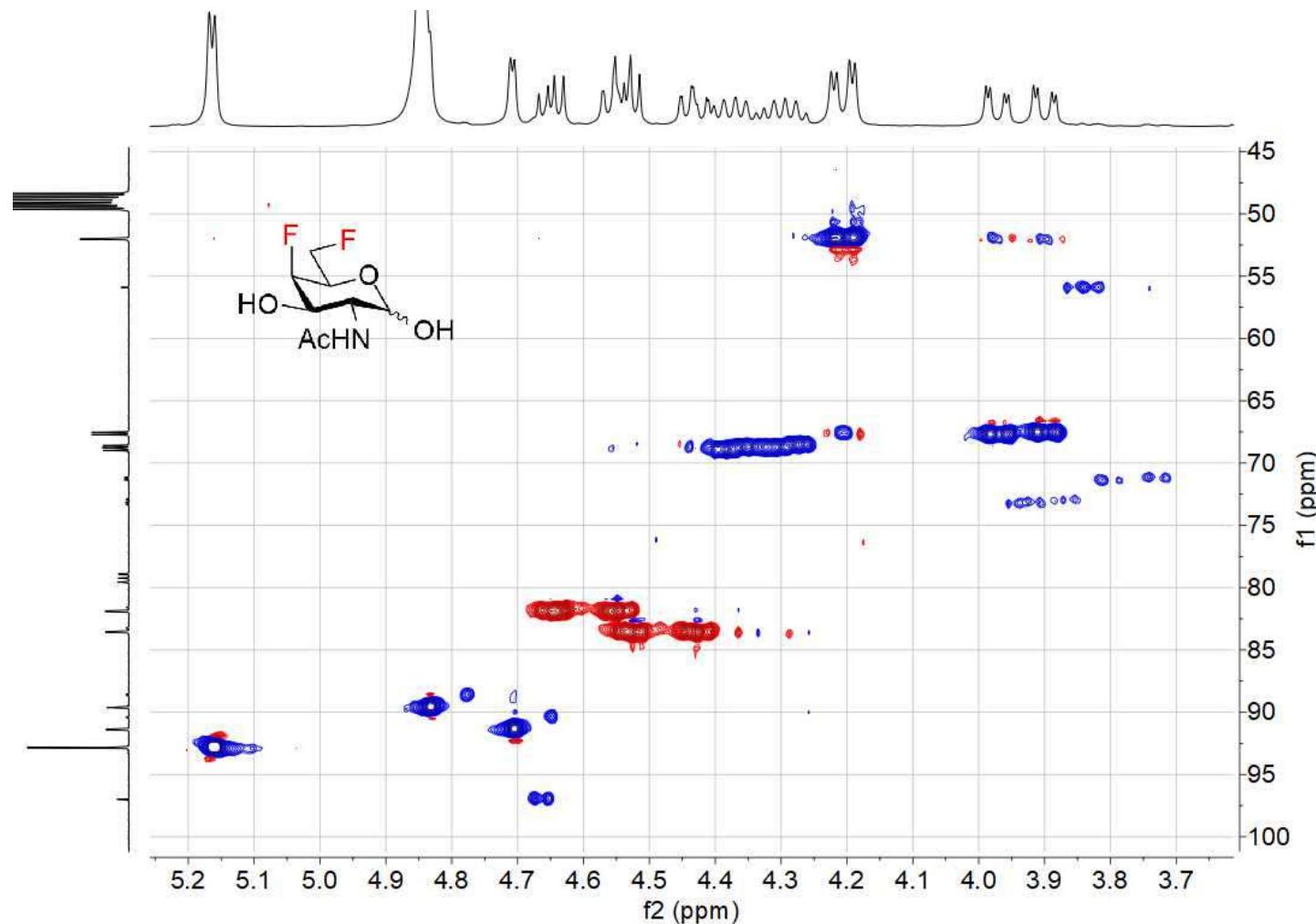
¹⁹F NMR (376 MHz, CD₃OD) 59 (ca. 2-3% β -anomer)



¹H-¹H COSY 59

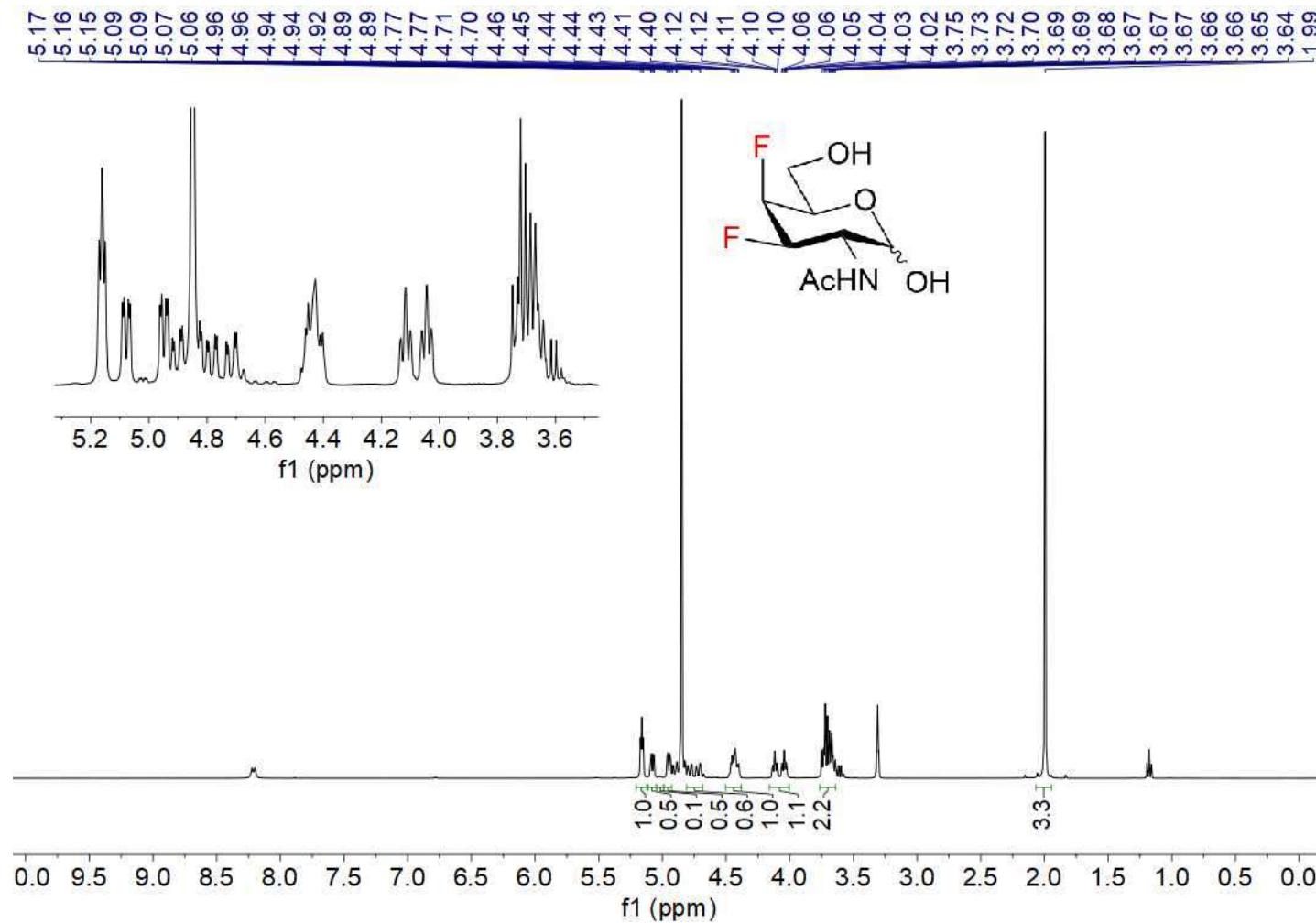


¹H-¹³C HSQC 59

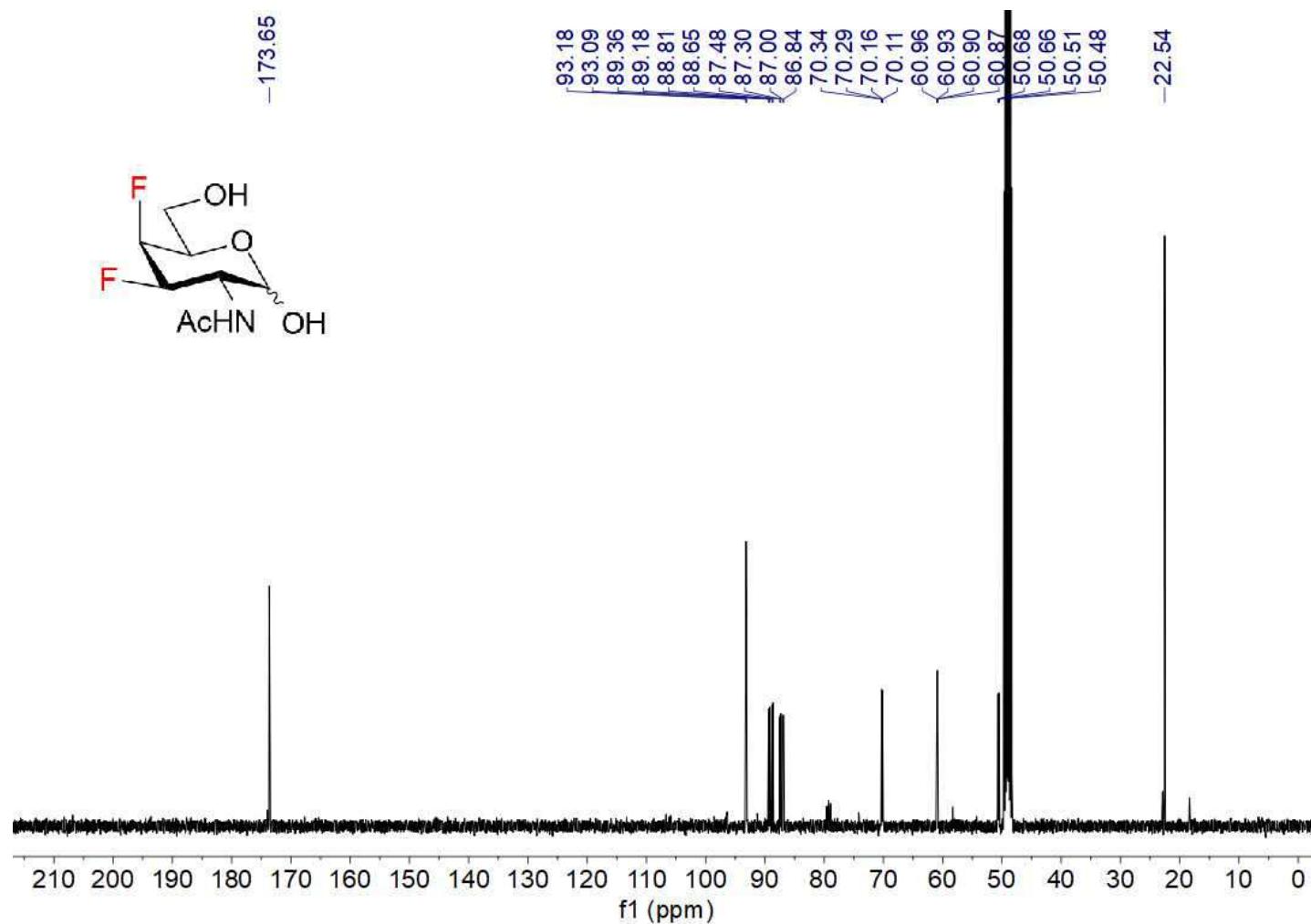


NMR COMPOUND 60

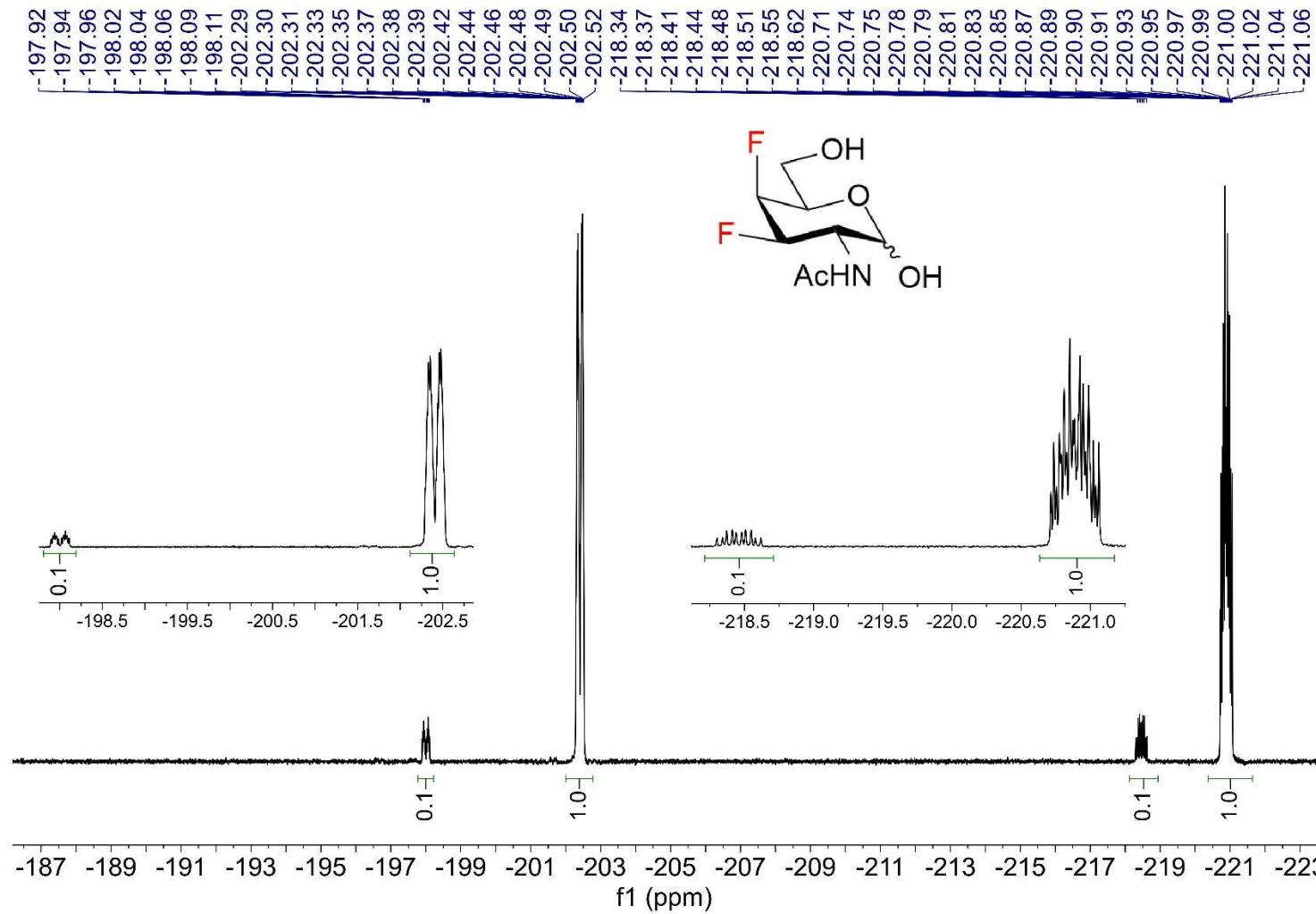
¹H NMR (400 MHz, CD₃OD) 60 (α/β ca. 10/1)



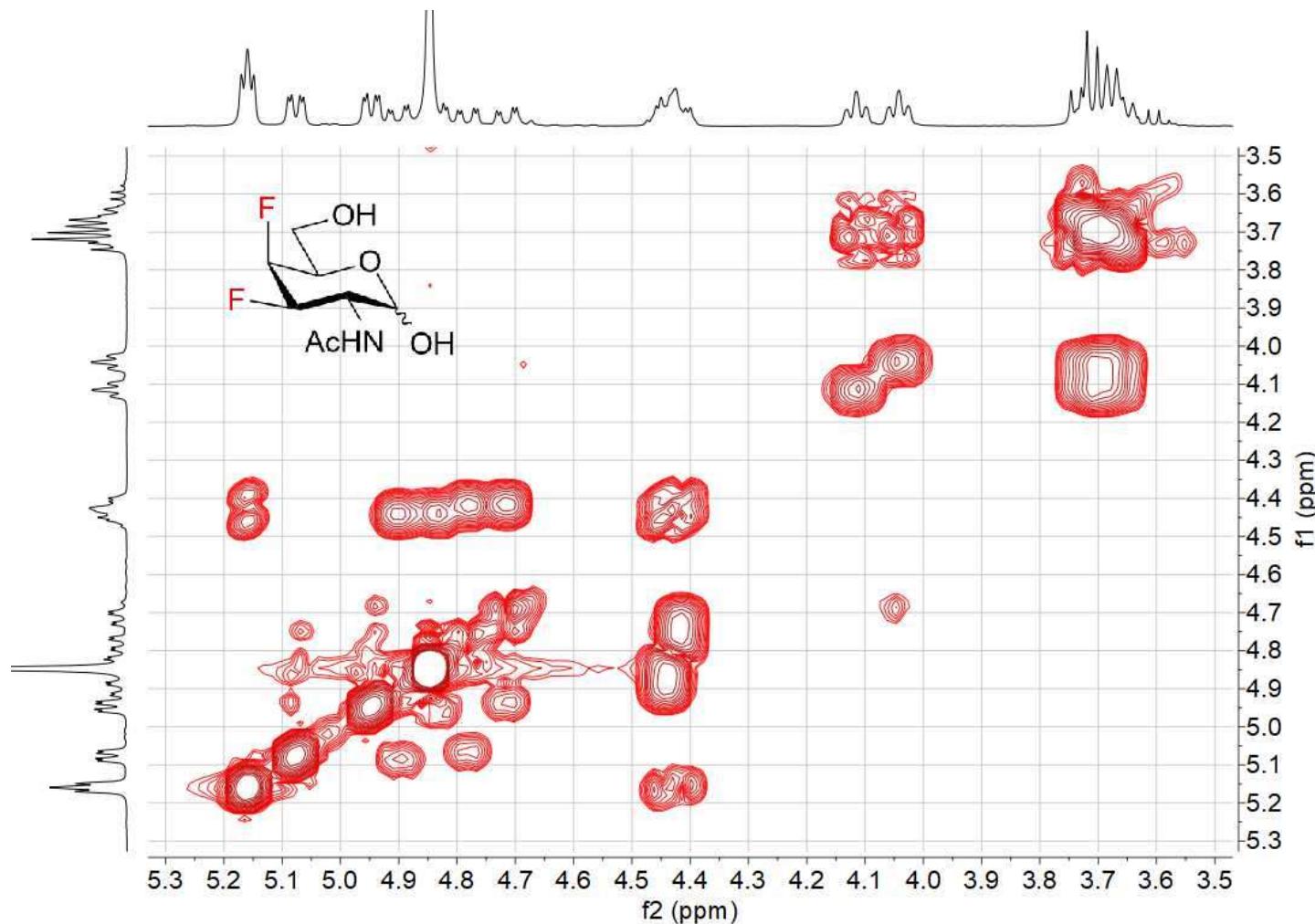
¹³C NMR (100 MHz, CD₃OD) 60



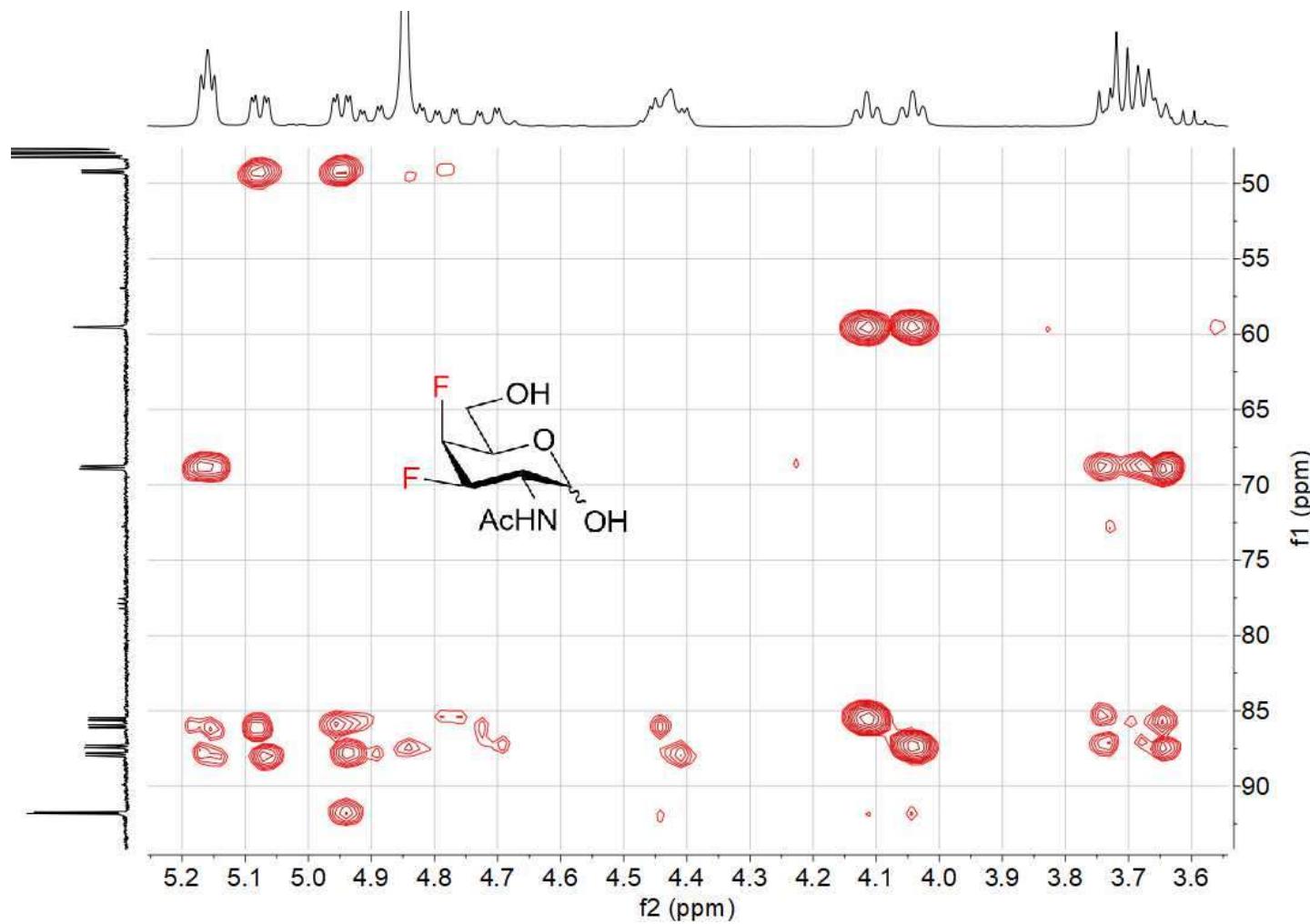
¹⁹F NMR (376 MHz, CD₃OD) 60 (α/β ca. 10/1)



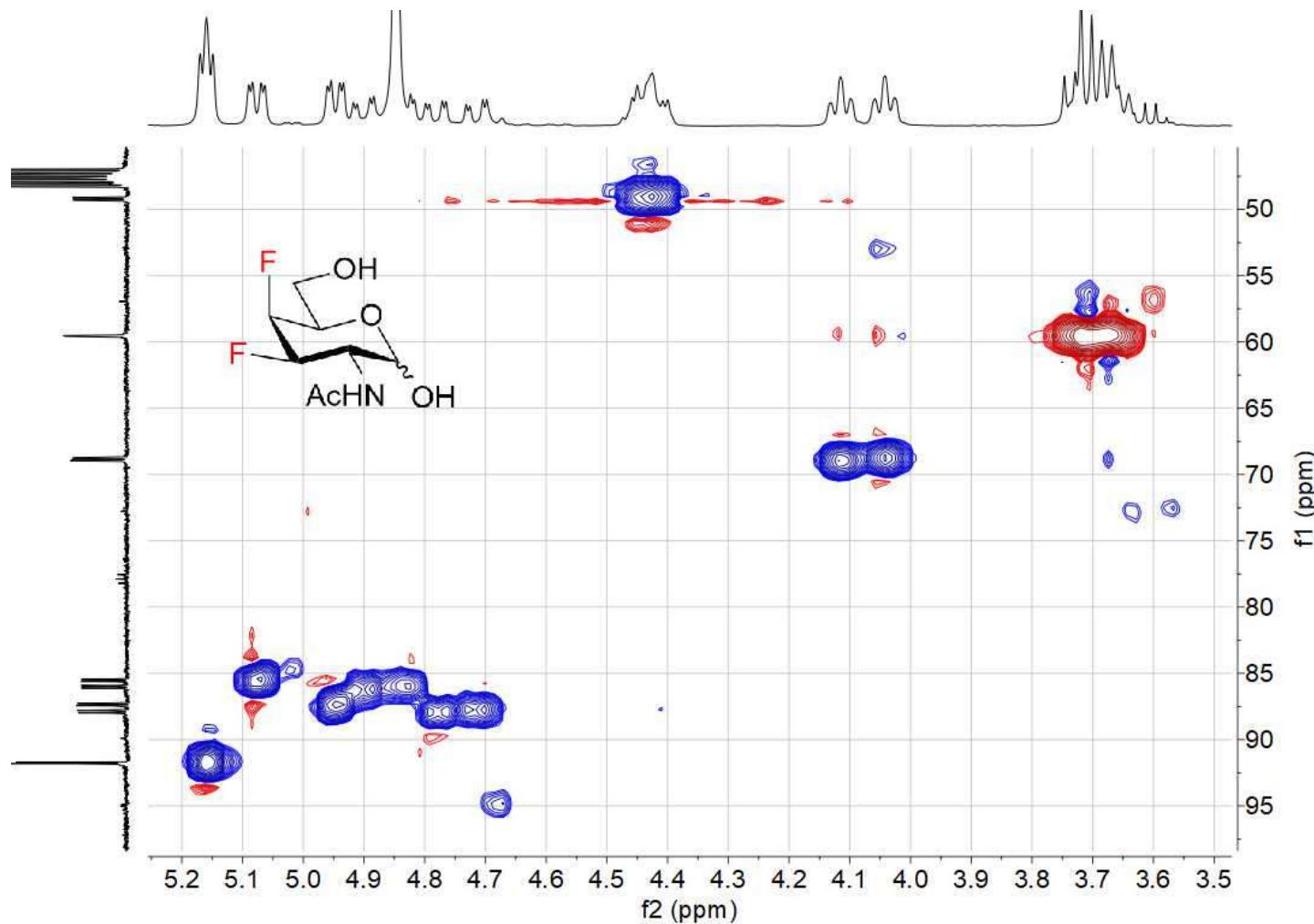
^1H - ^1H COSY 60



^1H - ^{13}C HMBC 60

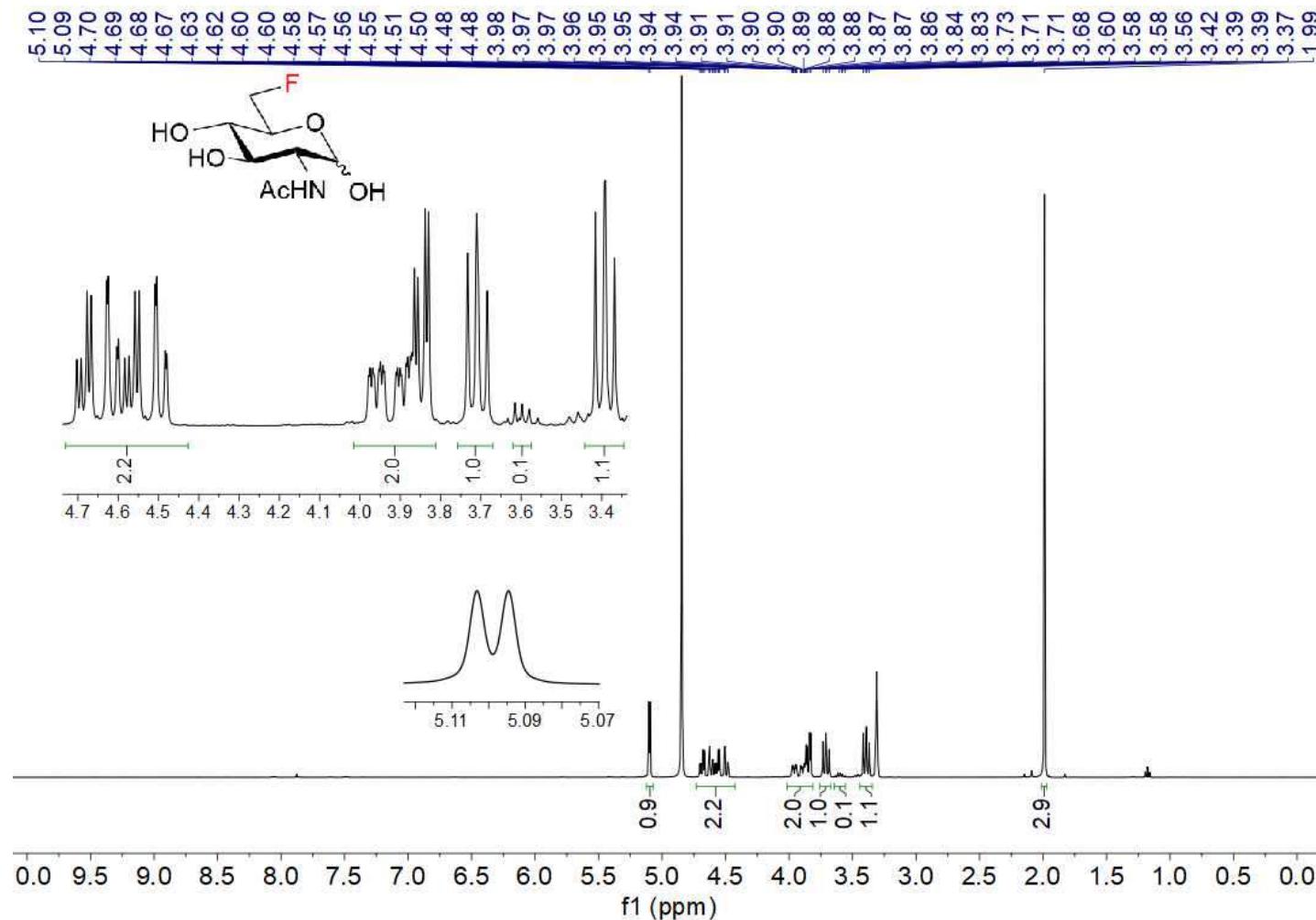


^1H - ^{13}C HSQC 60

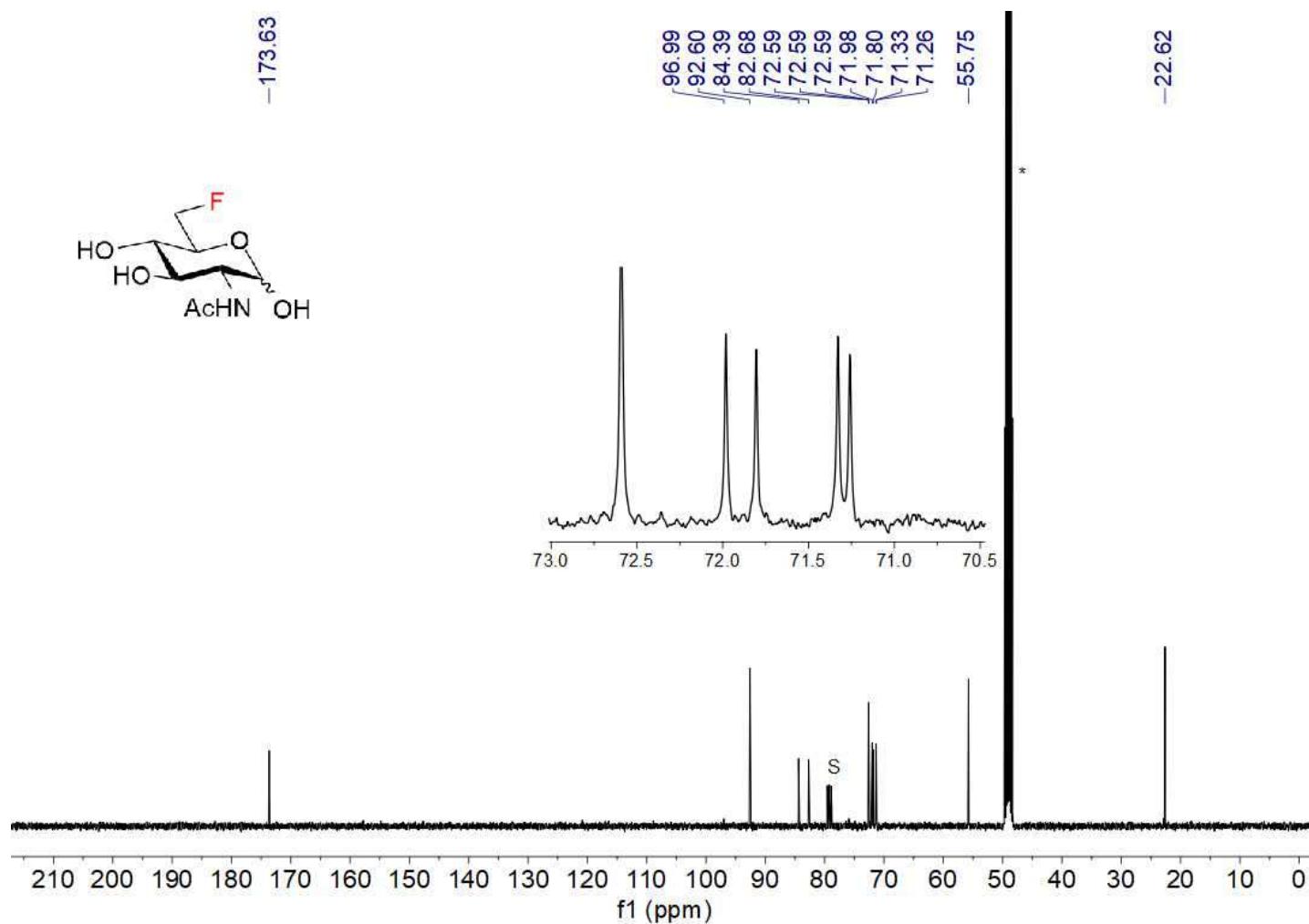


NMR COMPOUND 61

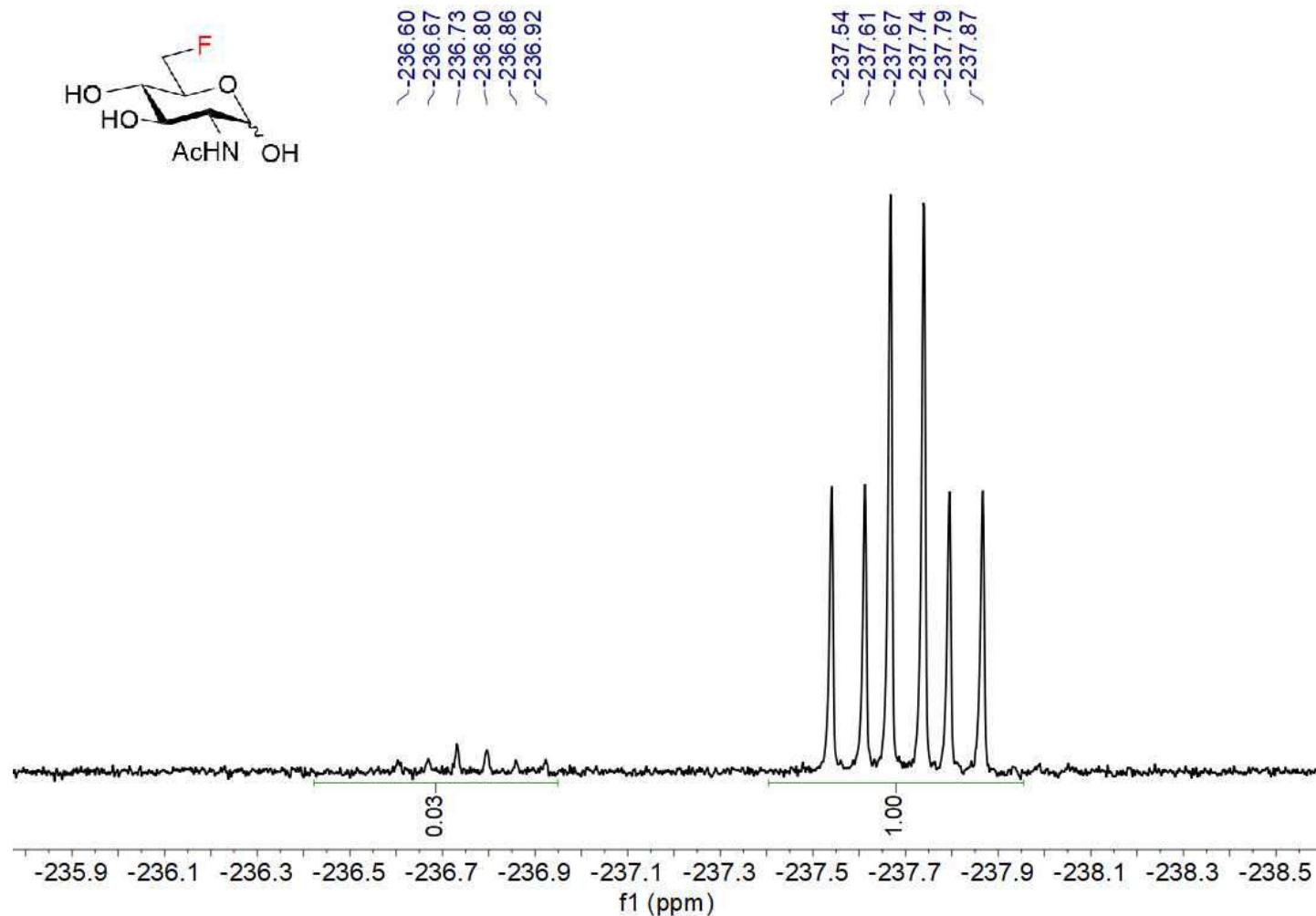
¹H NMR (400 MHz, CD₃OD) 61 (ca. 8% β -anomer)



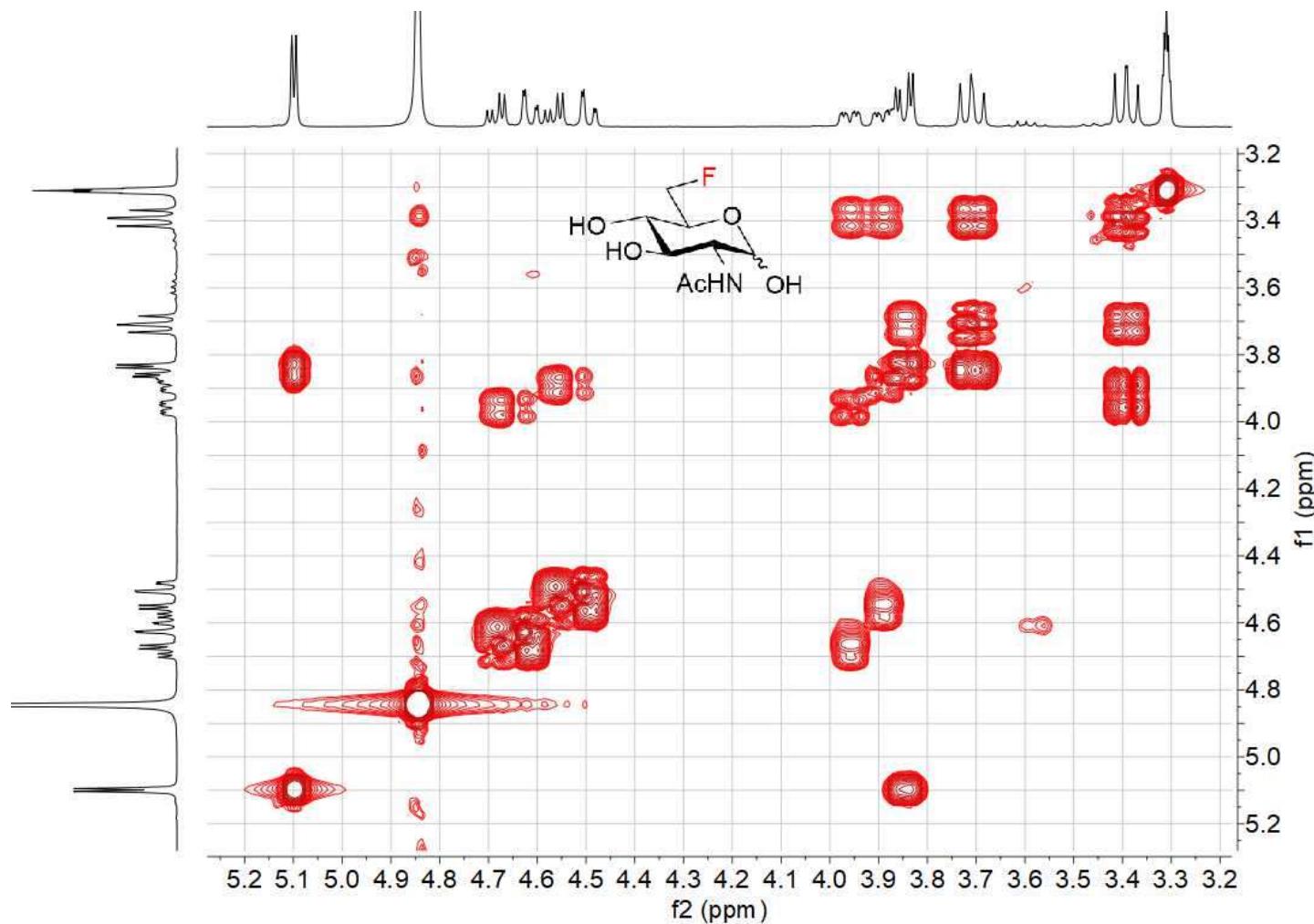
¹³C NMR (100 MHz, CD₃OD) 61



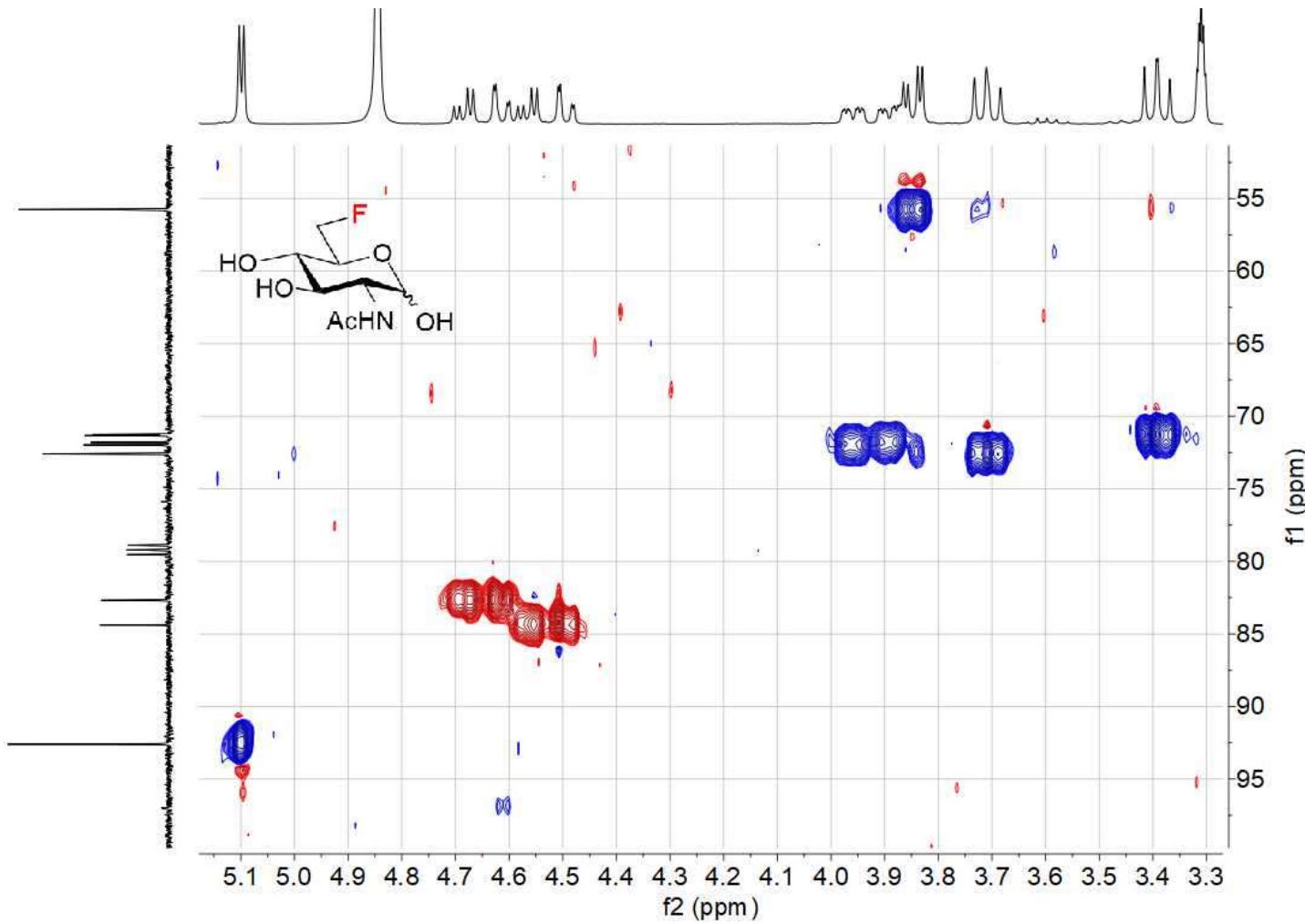
¹⁹F NMR (376 MHz, CD₃OD) 61 (ca. 3% β -anomer)



¹H-¹H COSY 61

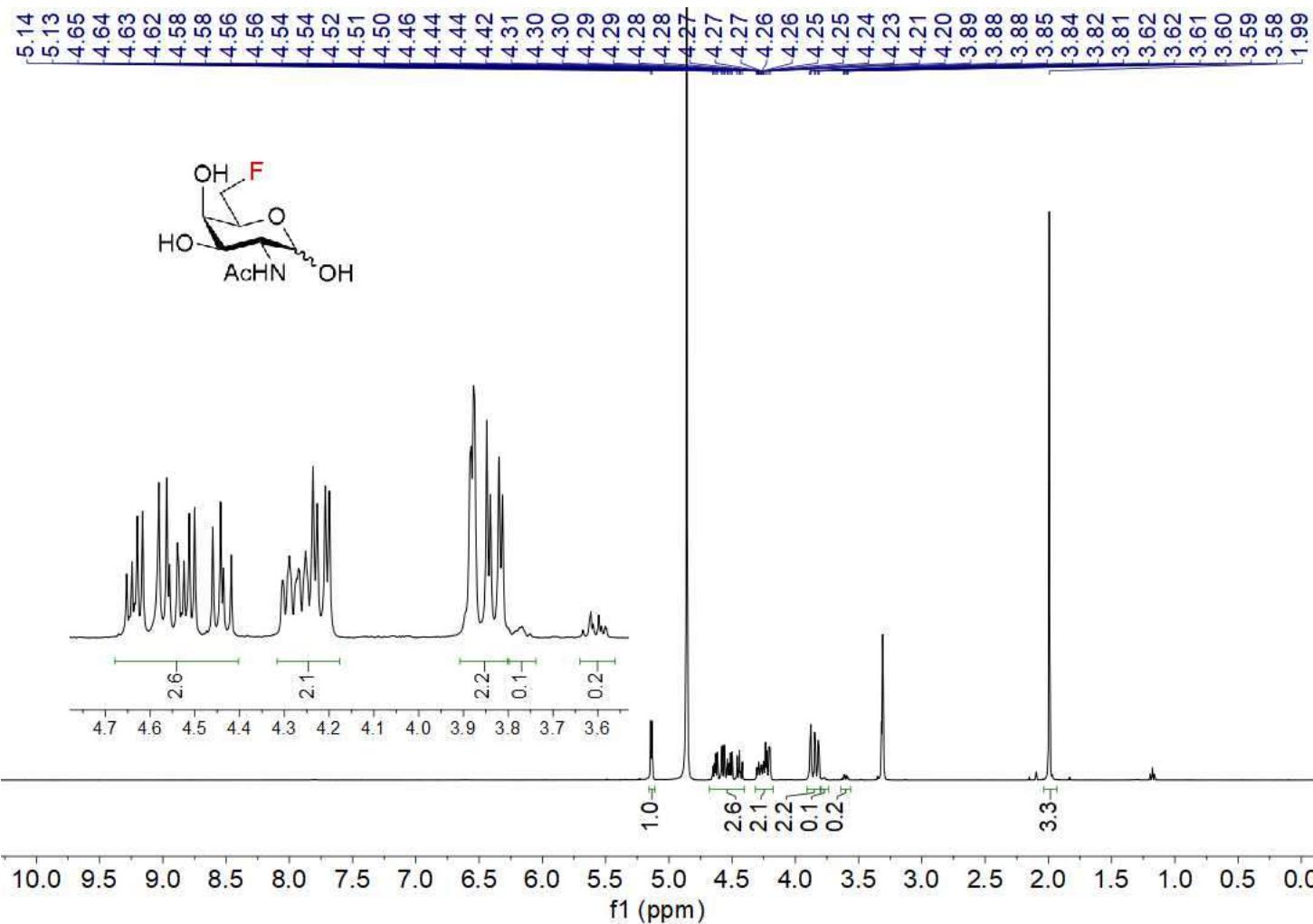


^1H - ^{13}C HSQC 61

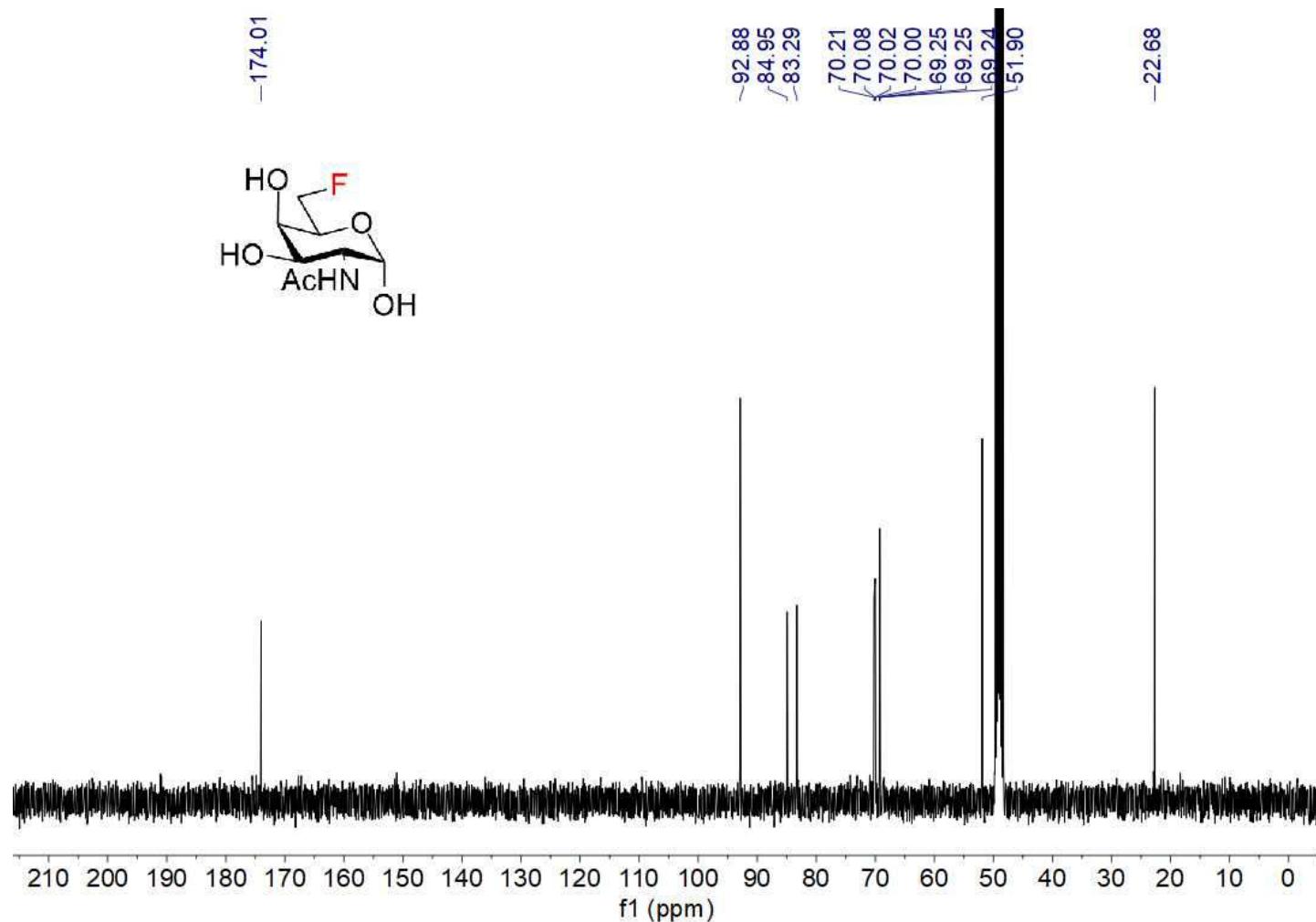


NMR COMPOUND 62

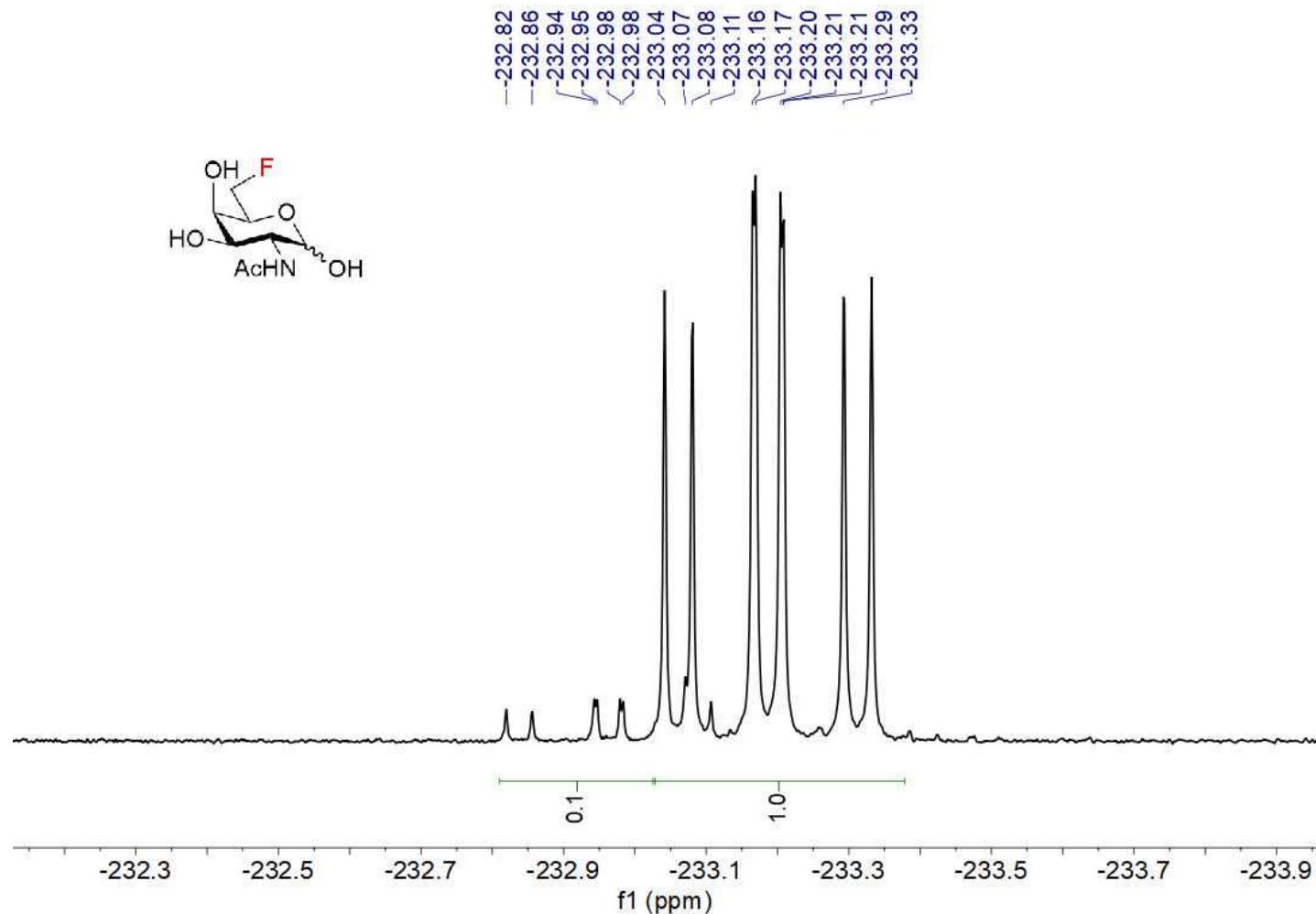
¹H NMR (400 MHz, CD₃OD) 62 (α/β ca. 10/1)



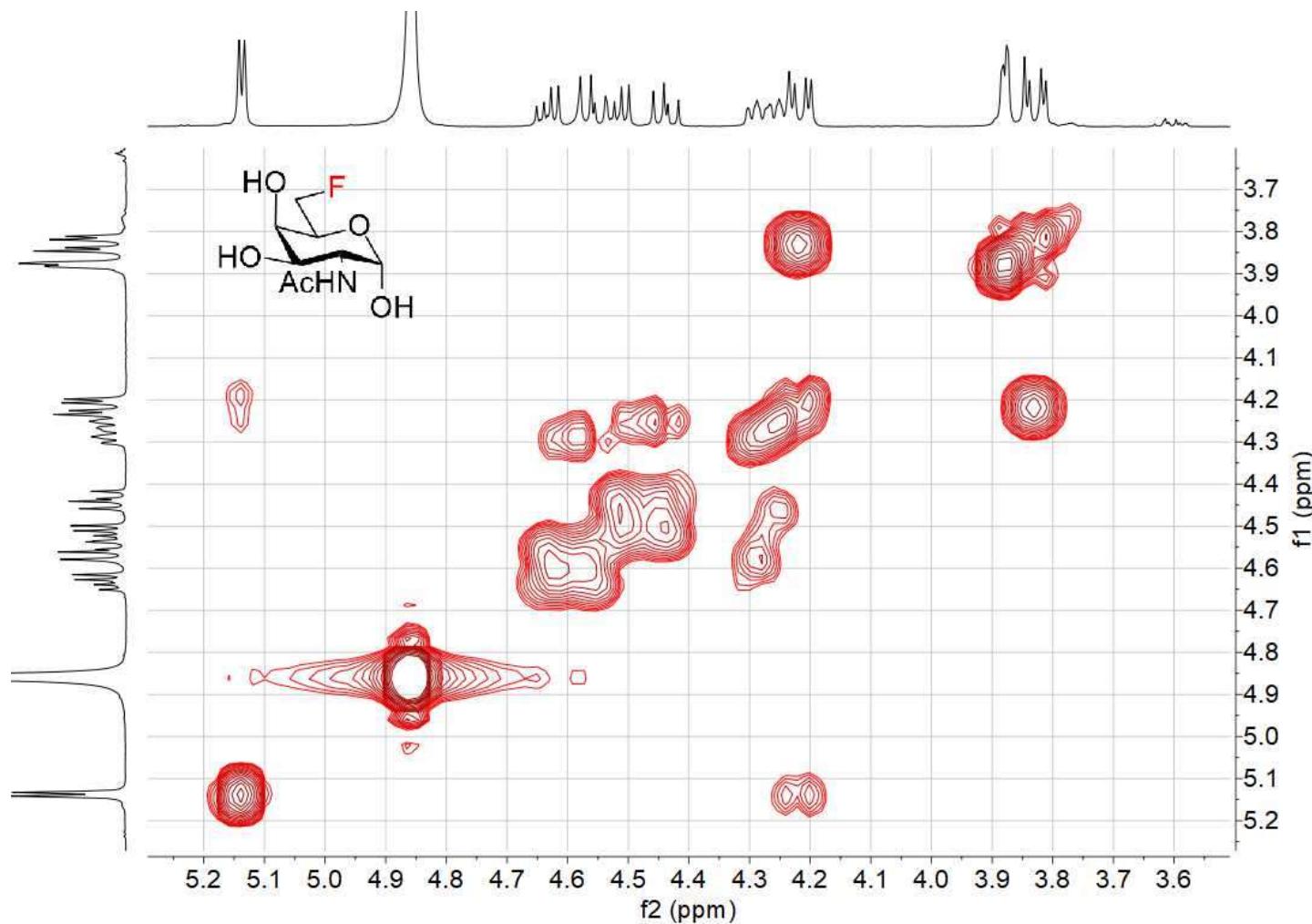
¹³C NMR (100 MHz, CD₃OD) 62



¹⁹F NMR (376 MHz, CD₃OD) 62 (α/β ca. 10/1)



¹H-¹H COSY 62



^1H - ^{13}C HSQC 62

