

Supporting information

II

Copies of NMR spectra

The Effect of Deoxyfluorination and O-Acylation on the Cytotoxicity of N-Acetyl-D-Gluco- and D-Galactosamine Hemiacetals

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Roman Hrstka,^d Petr Voňka,^d Jindřich Karban^{a,*}

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*Email: karban@icpf.cas.cz.

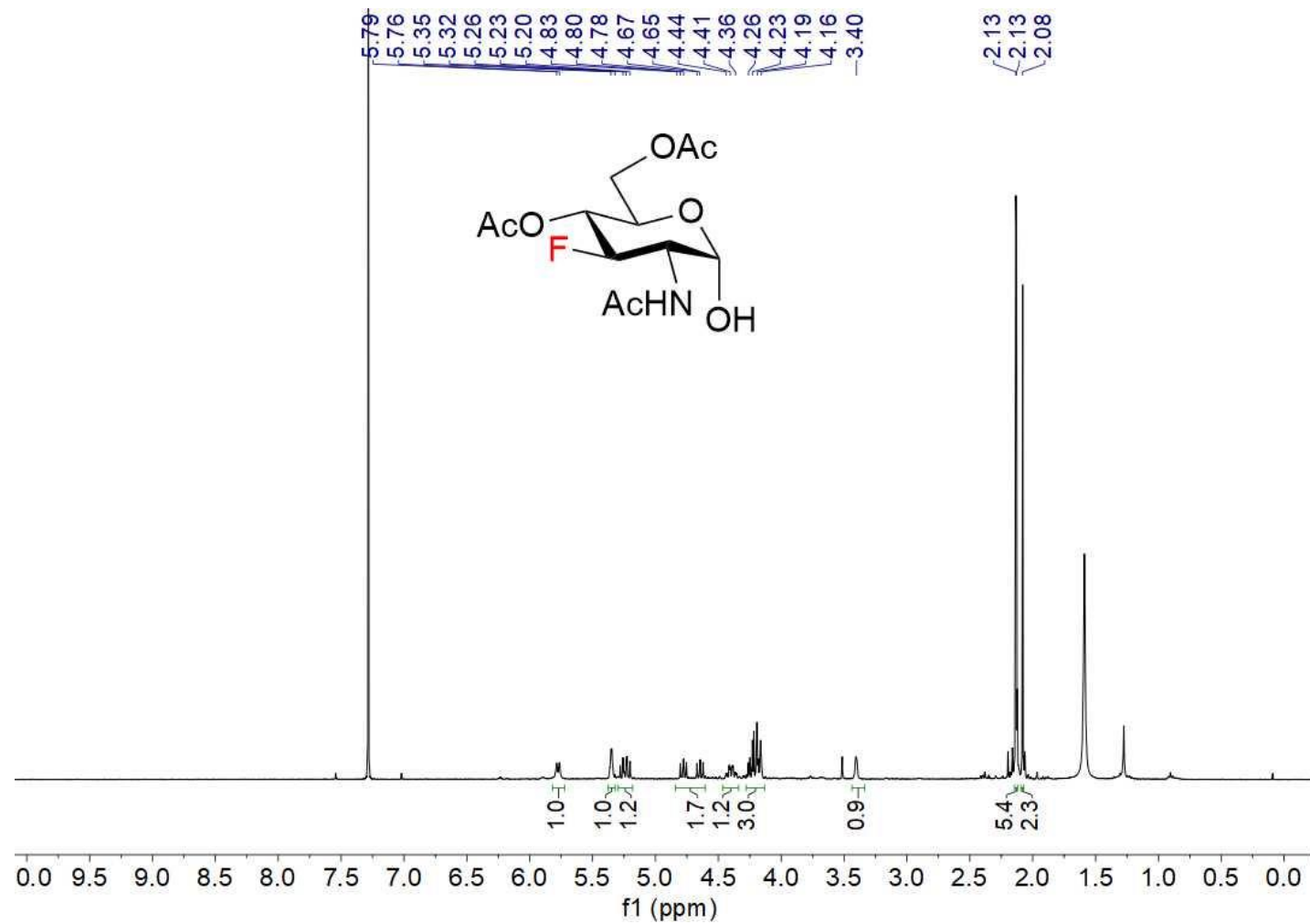
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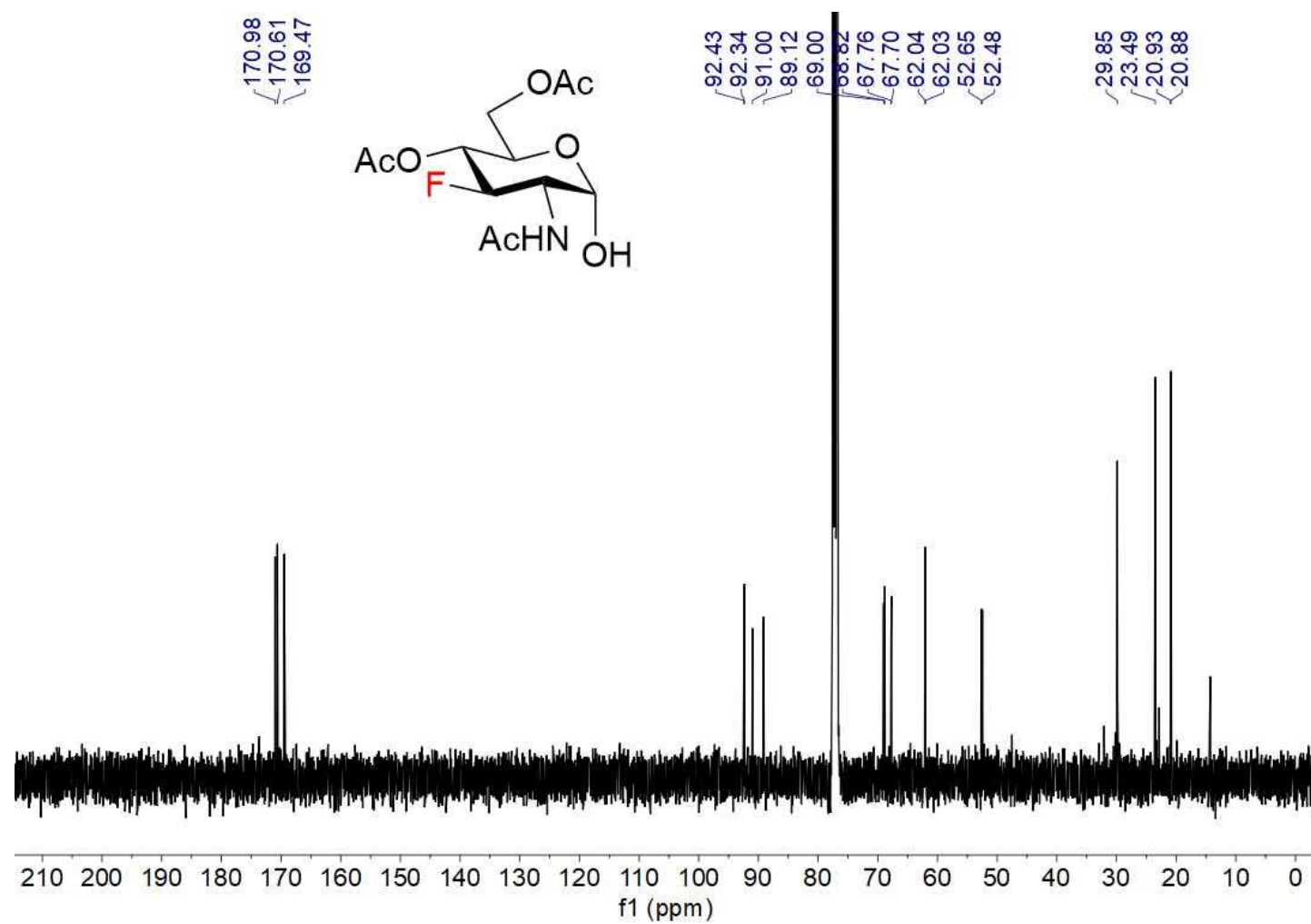
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NMR COMPOUND 11

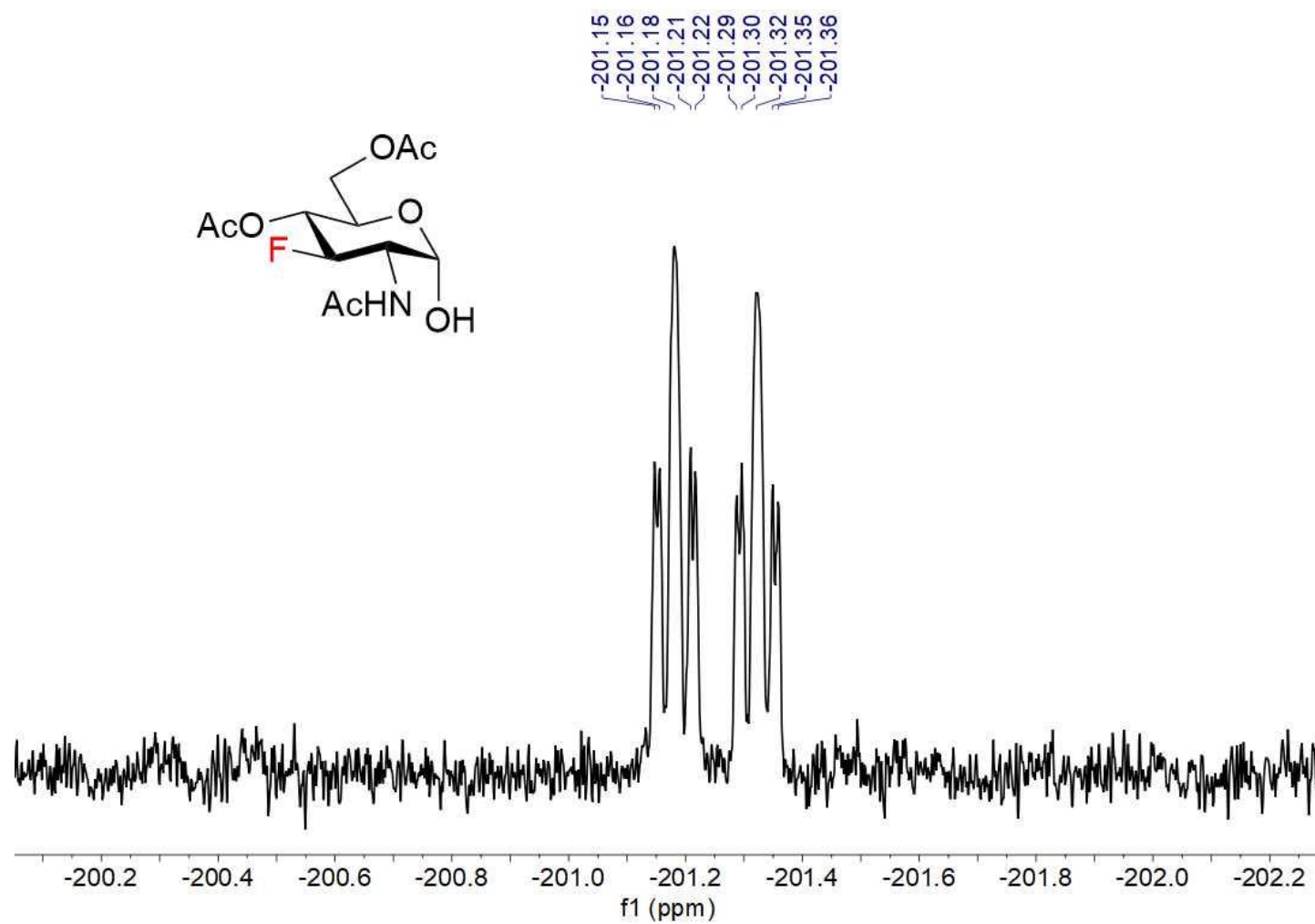
^1H NMR (400 MHz, CDCl_3) 11



^{13}C NMR (100 MHz, CDCl_3) 11

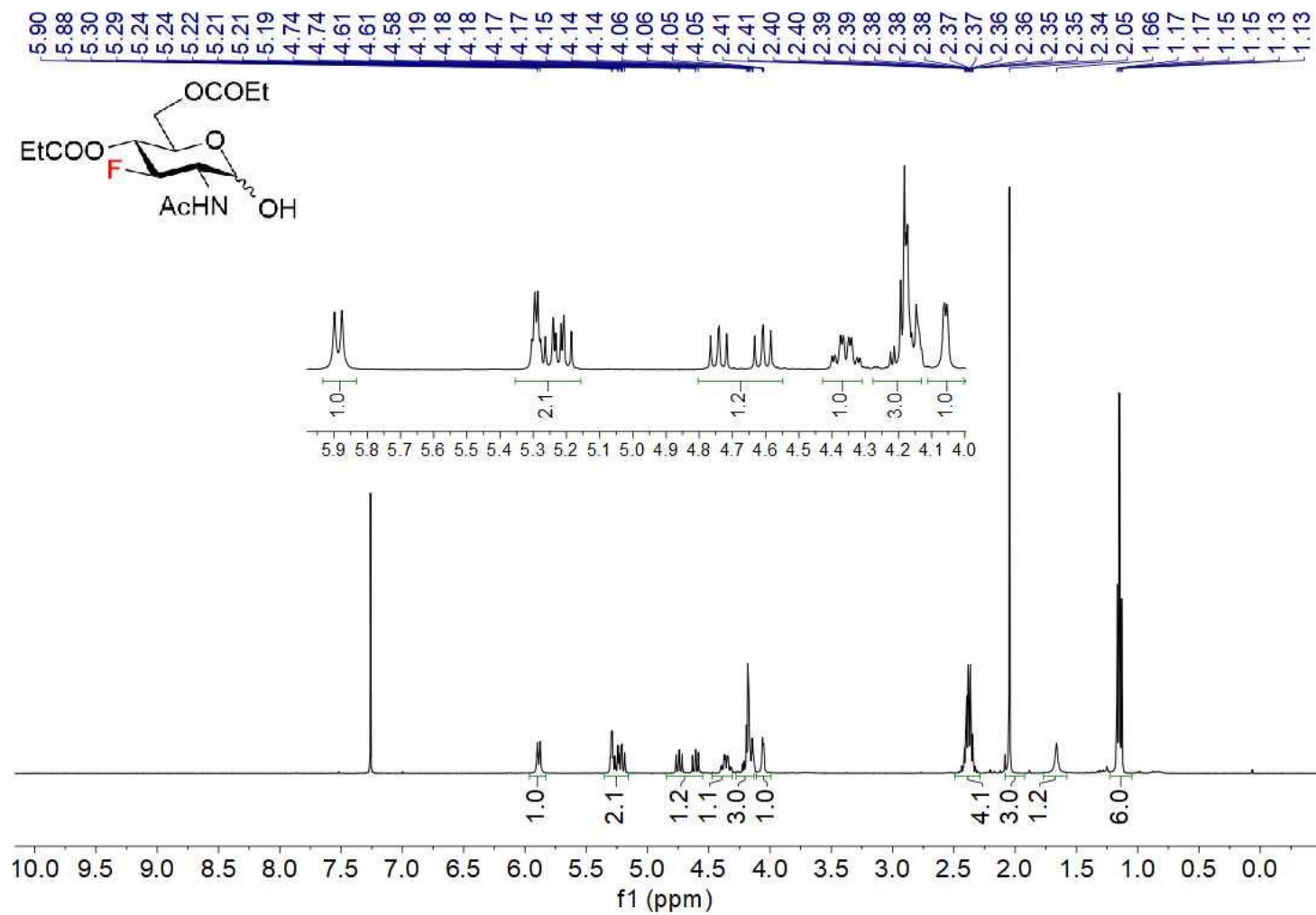


^{19}F NMR (376 MHz, CDCl_3) 11

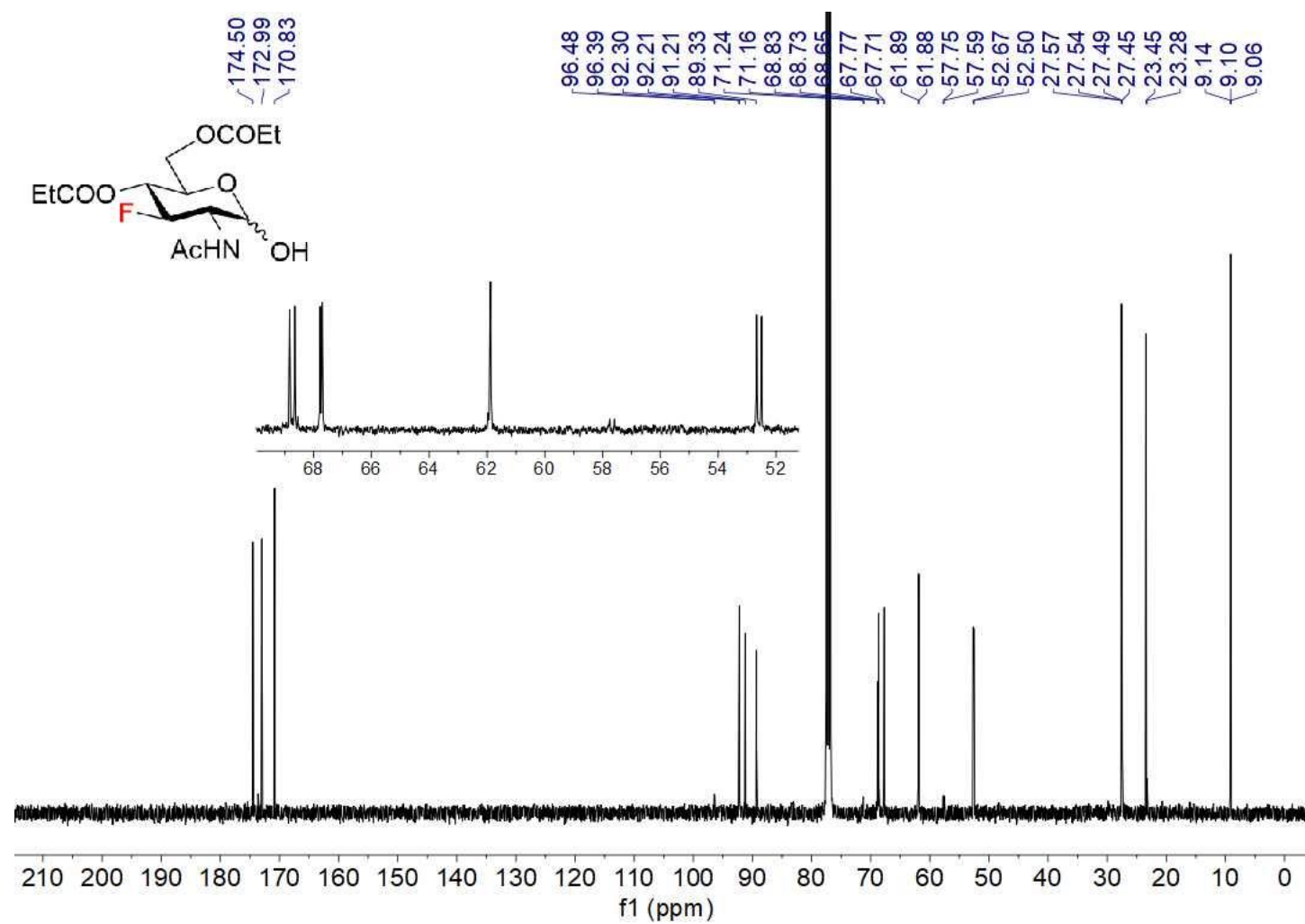


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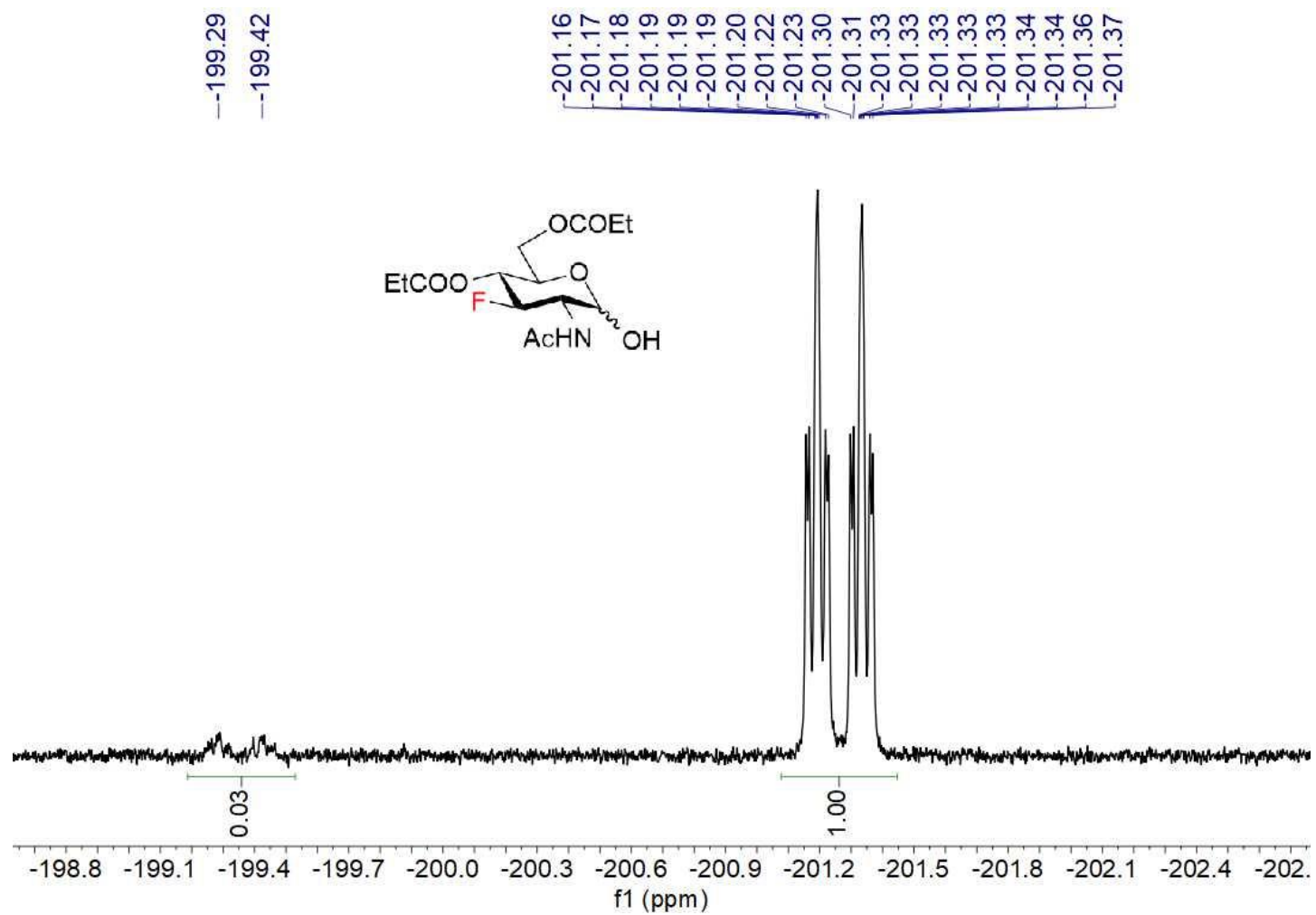
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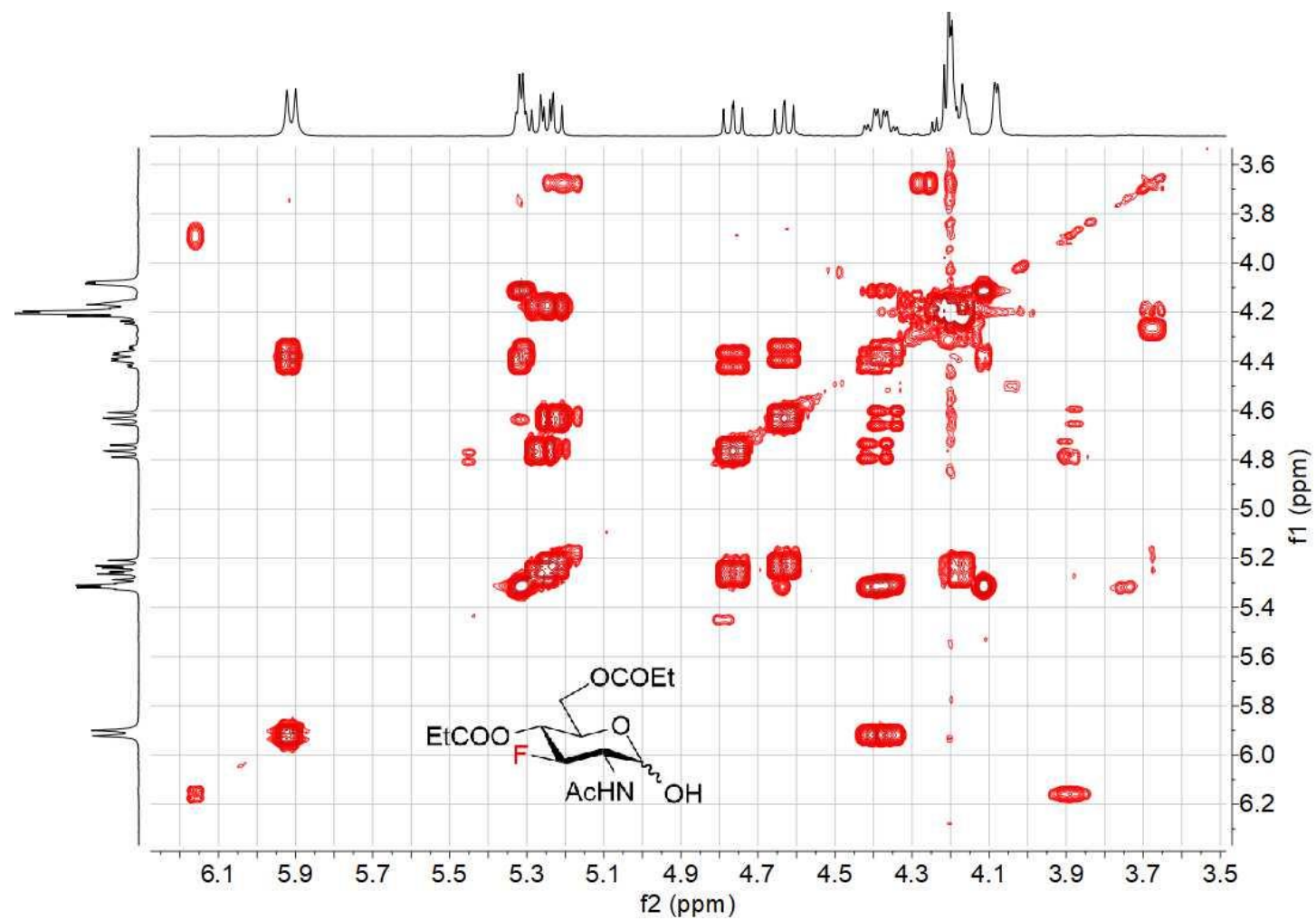
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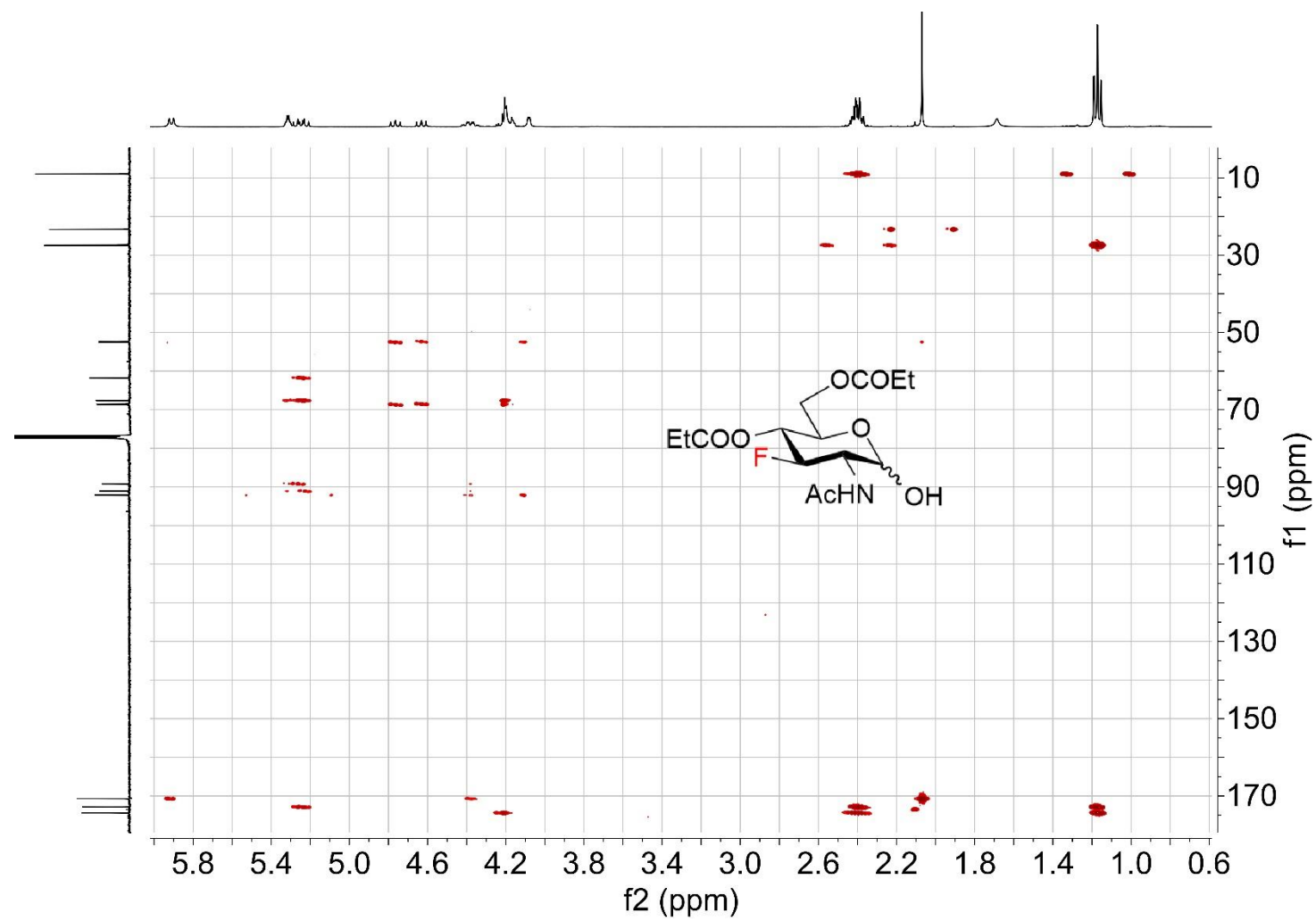
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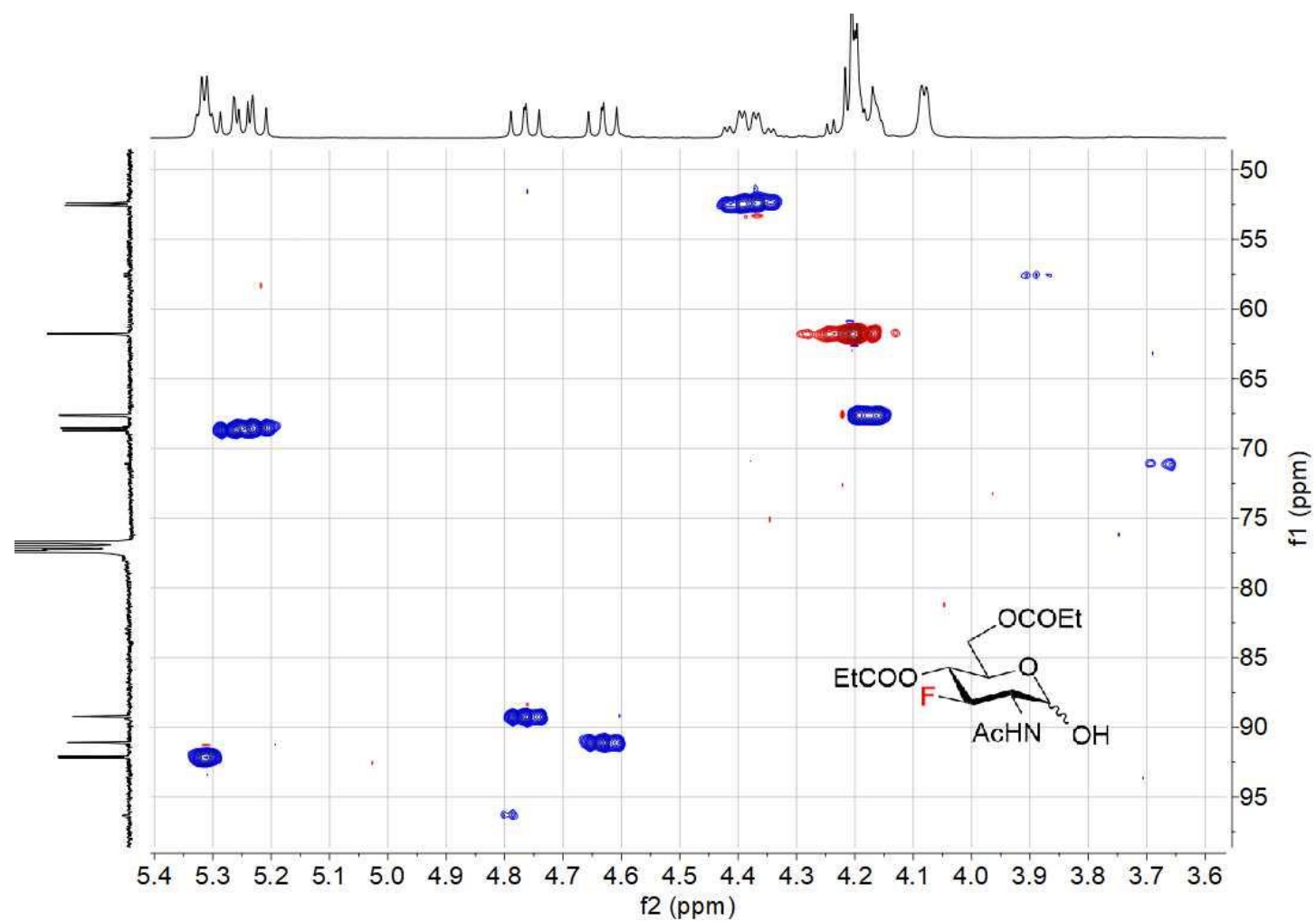
^1H - ^1H COSY 14



^1H - ^{13}C HMBC 14

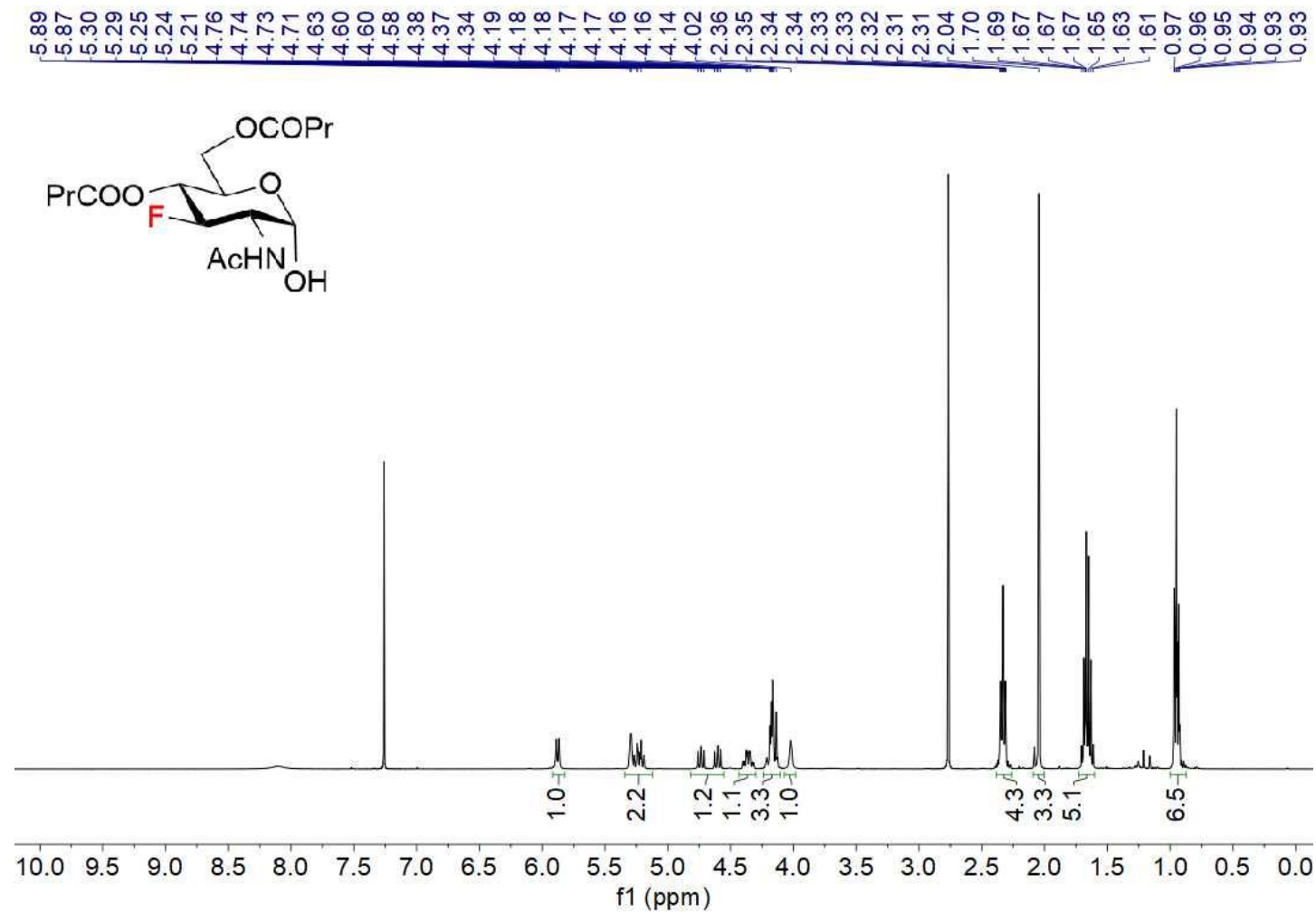


^1H - ^{13}C HSQC 14

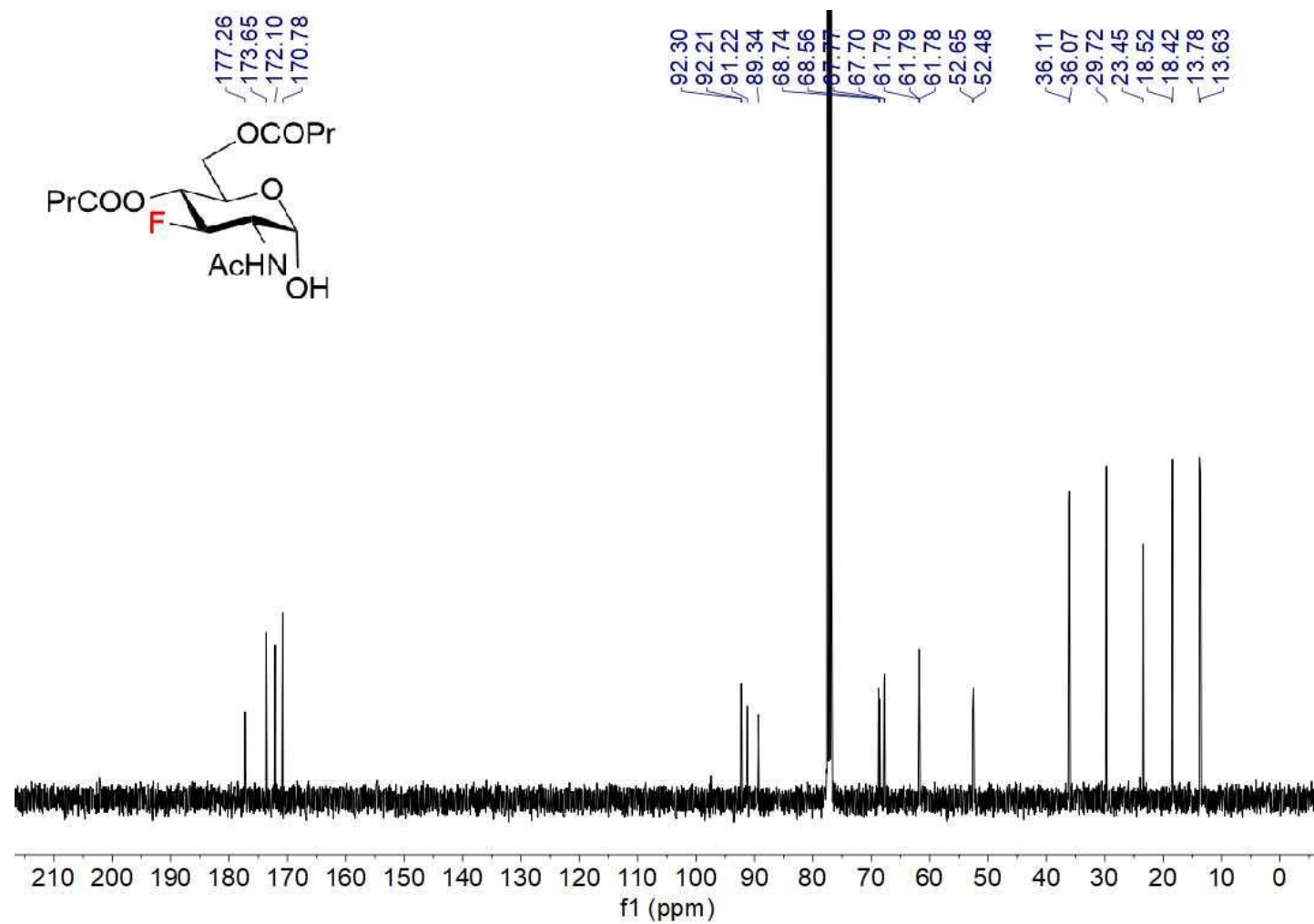


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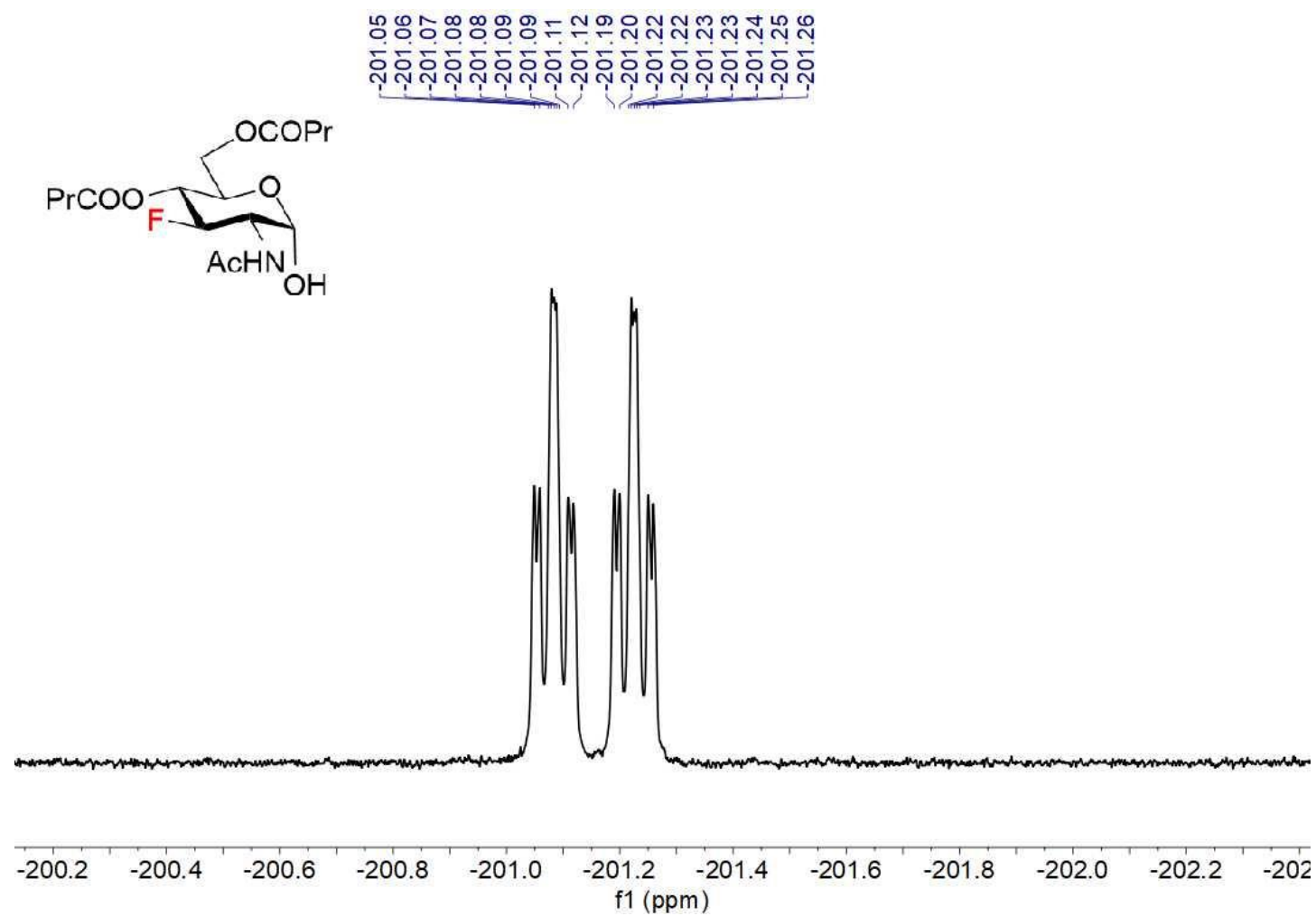
¹H NMR (400 MHz, CDCl₃) 15

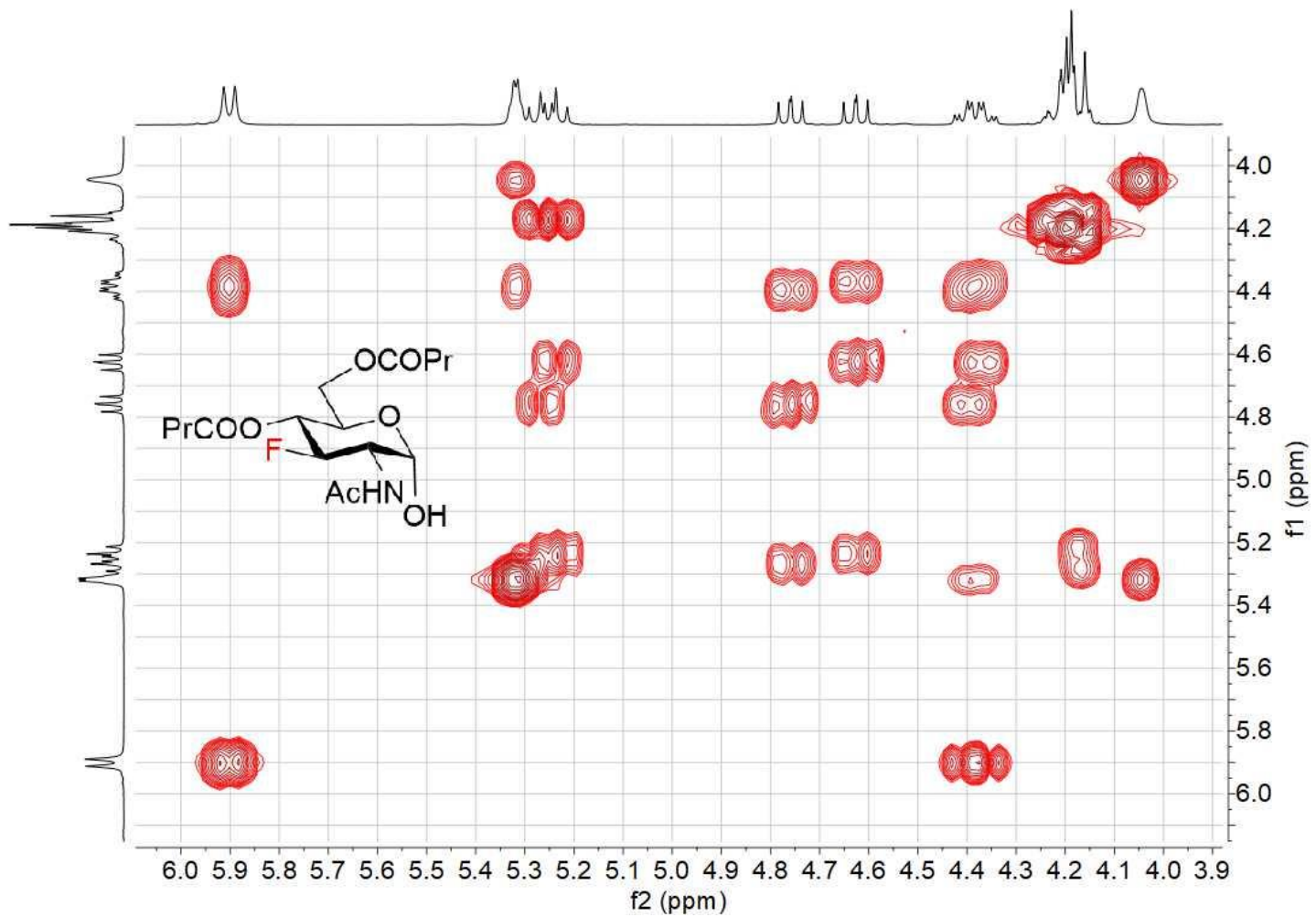


^{13}C NMR (100 MHz, CDCl_3) 15

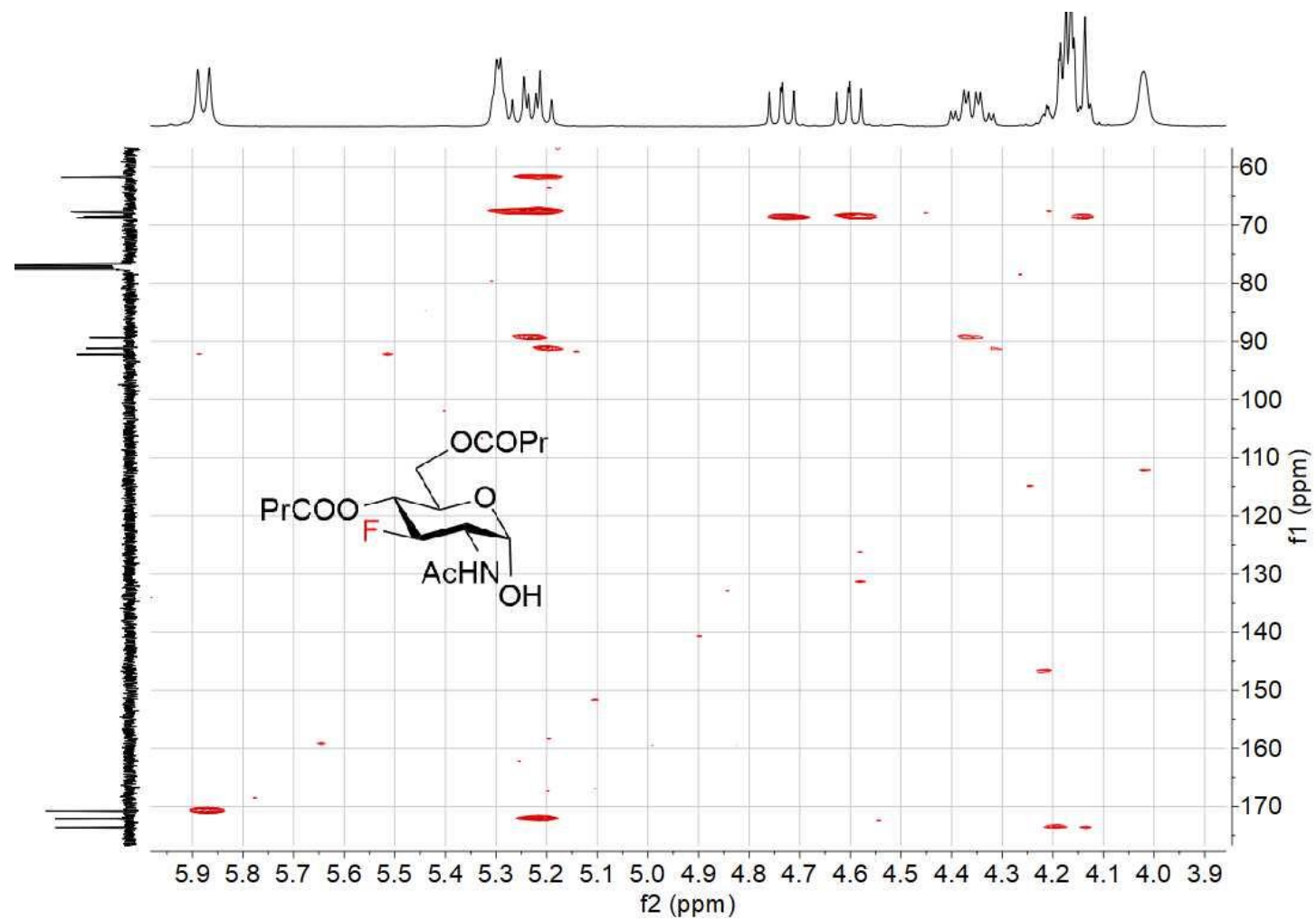


^{19}F NMR (376 MHz, CDCl_3) 15

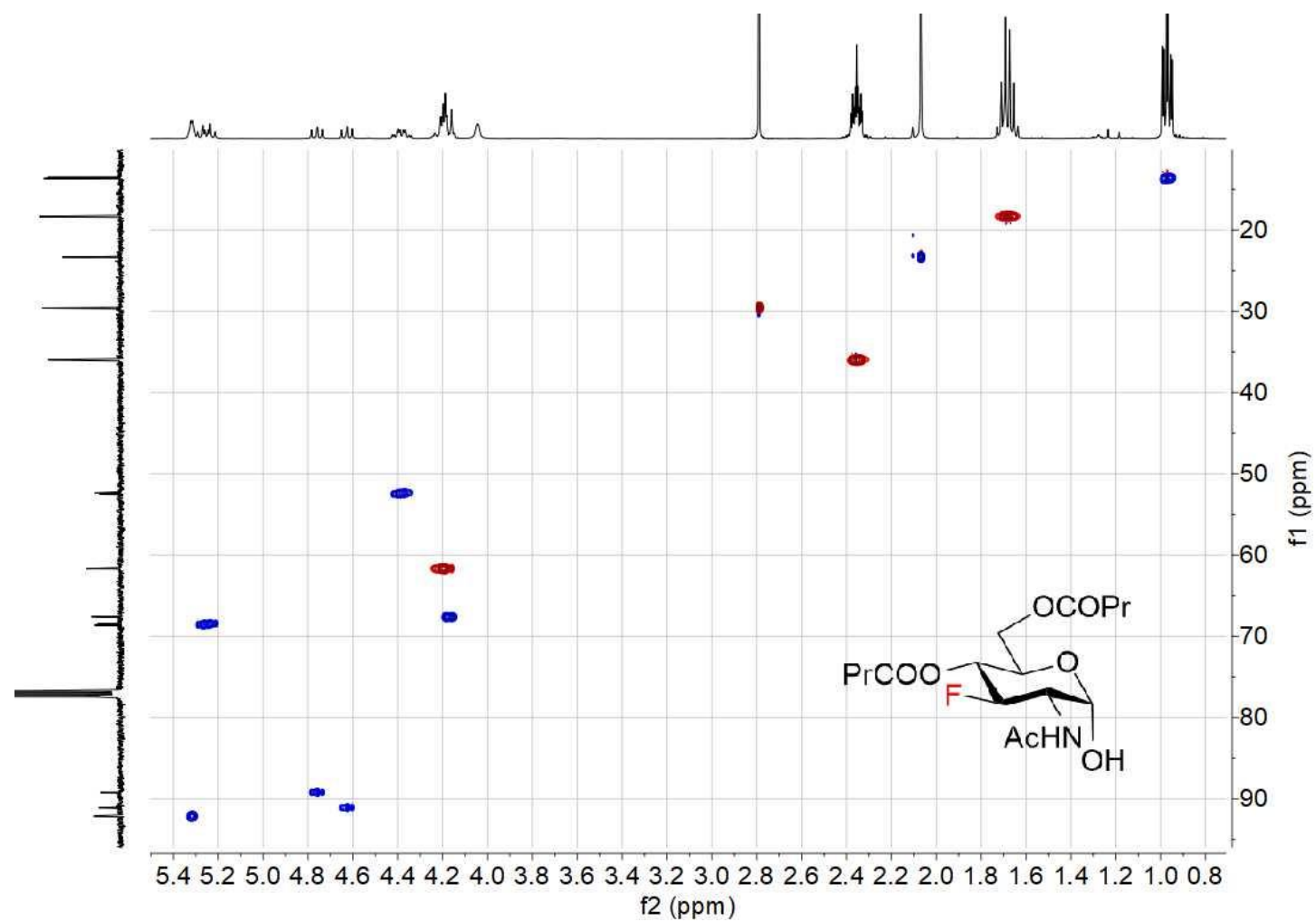


¹H-¹H COSY 15

^1H - ^{13}C HMBC 15

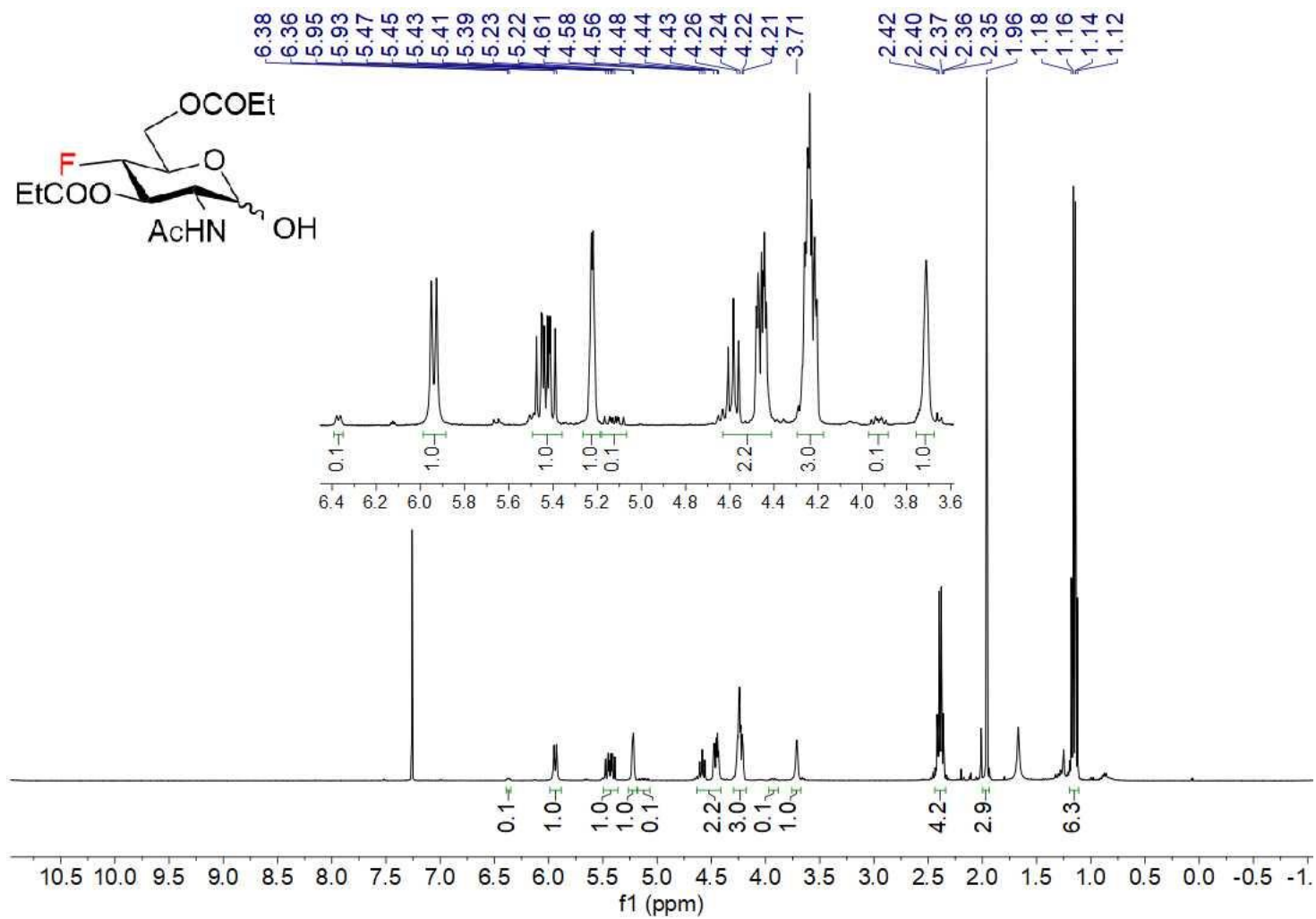


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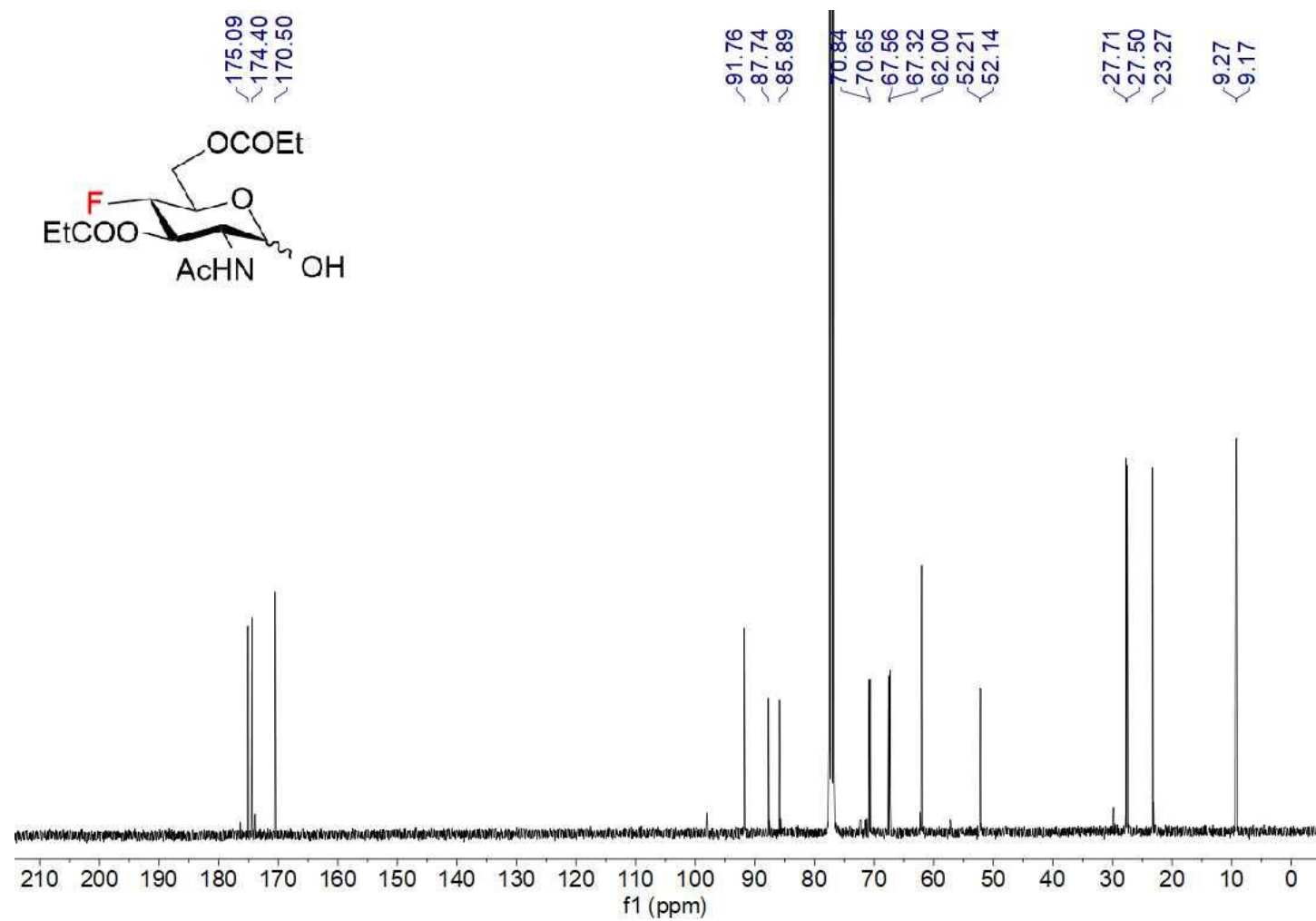


NMR COMPOUND 16

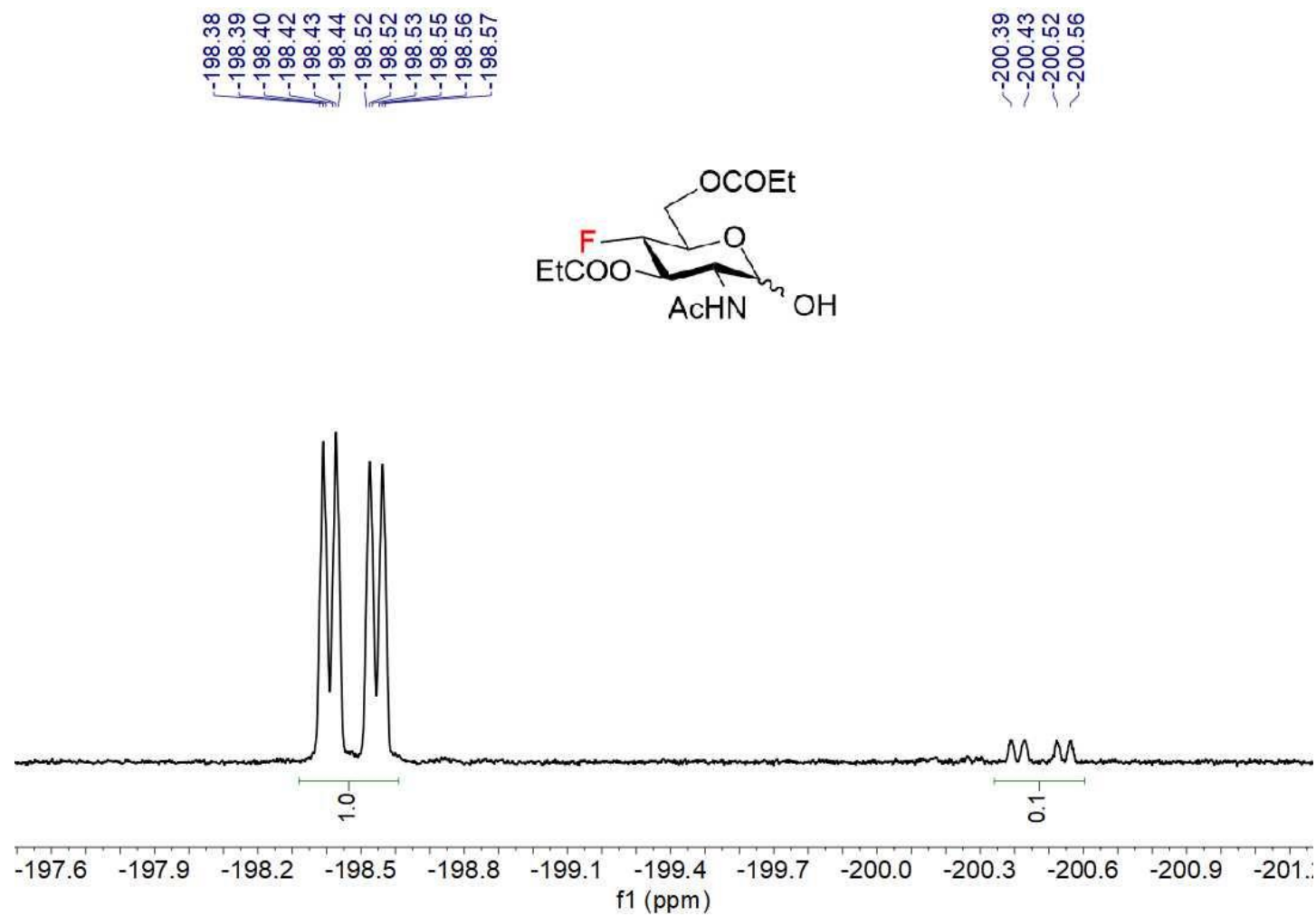
^1H NMR (400 MHz, CDCl_3) 16



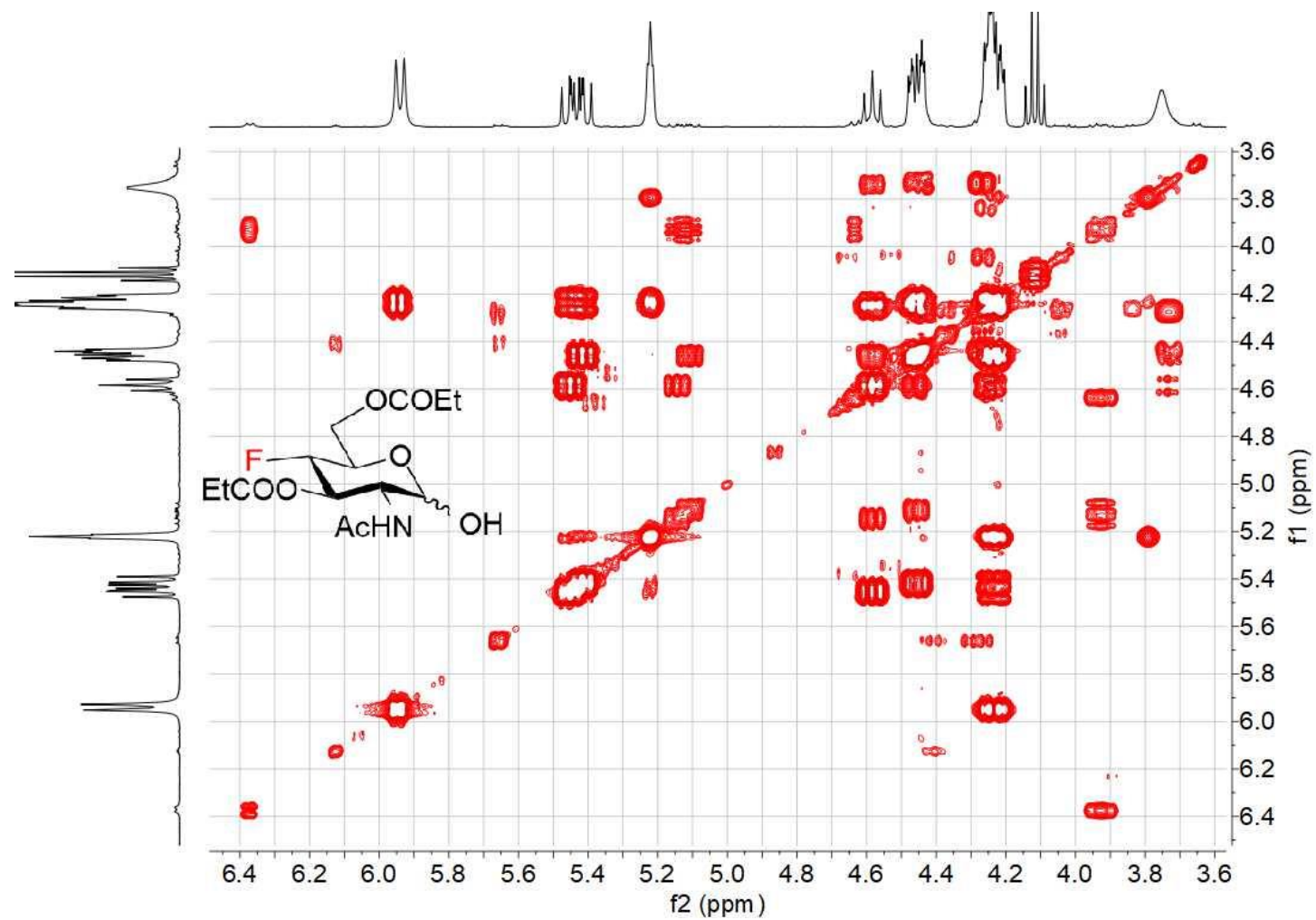
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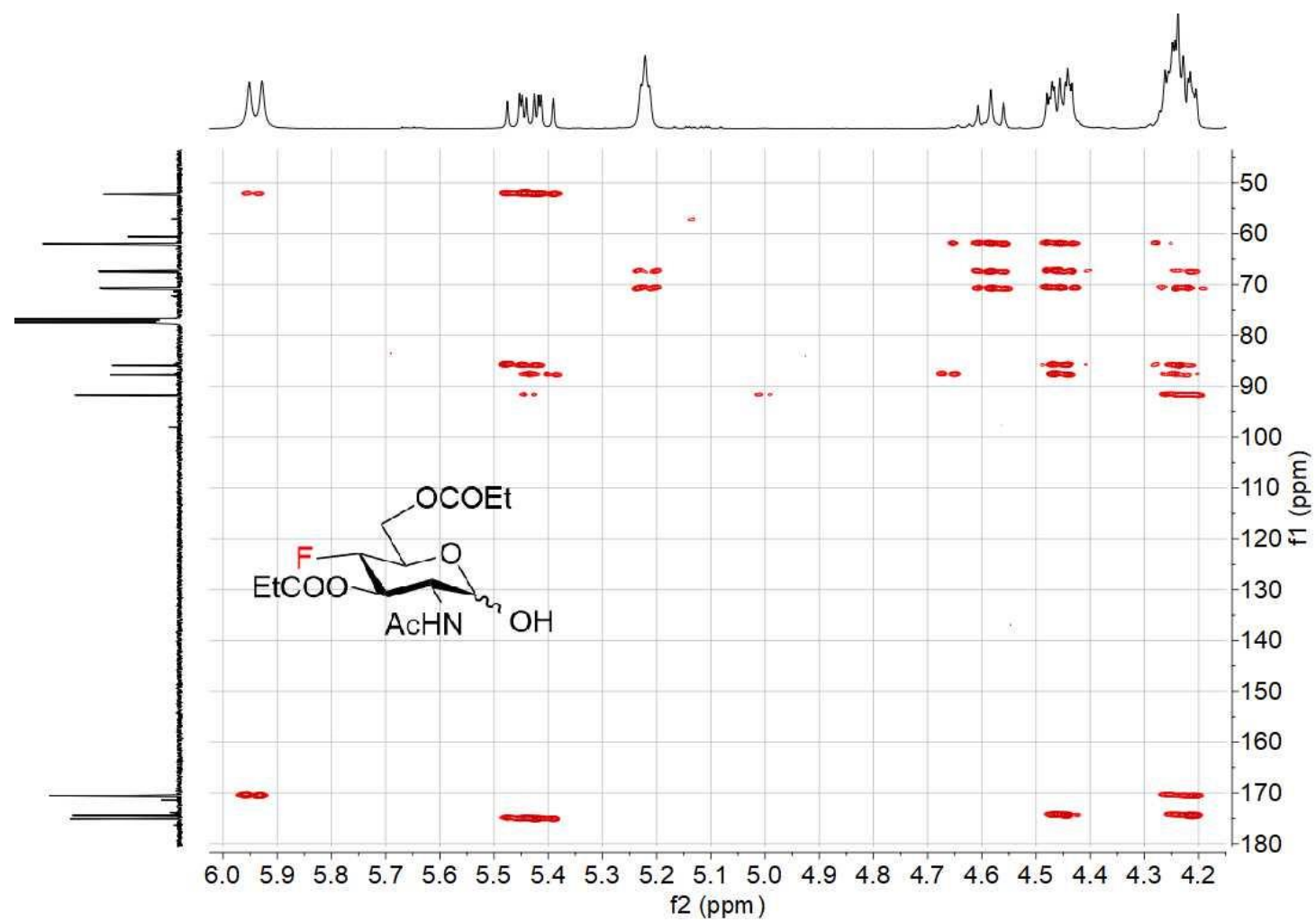
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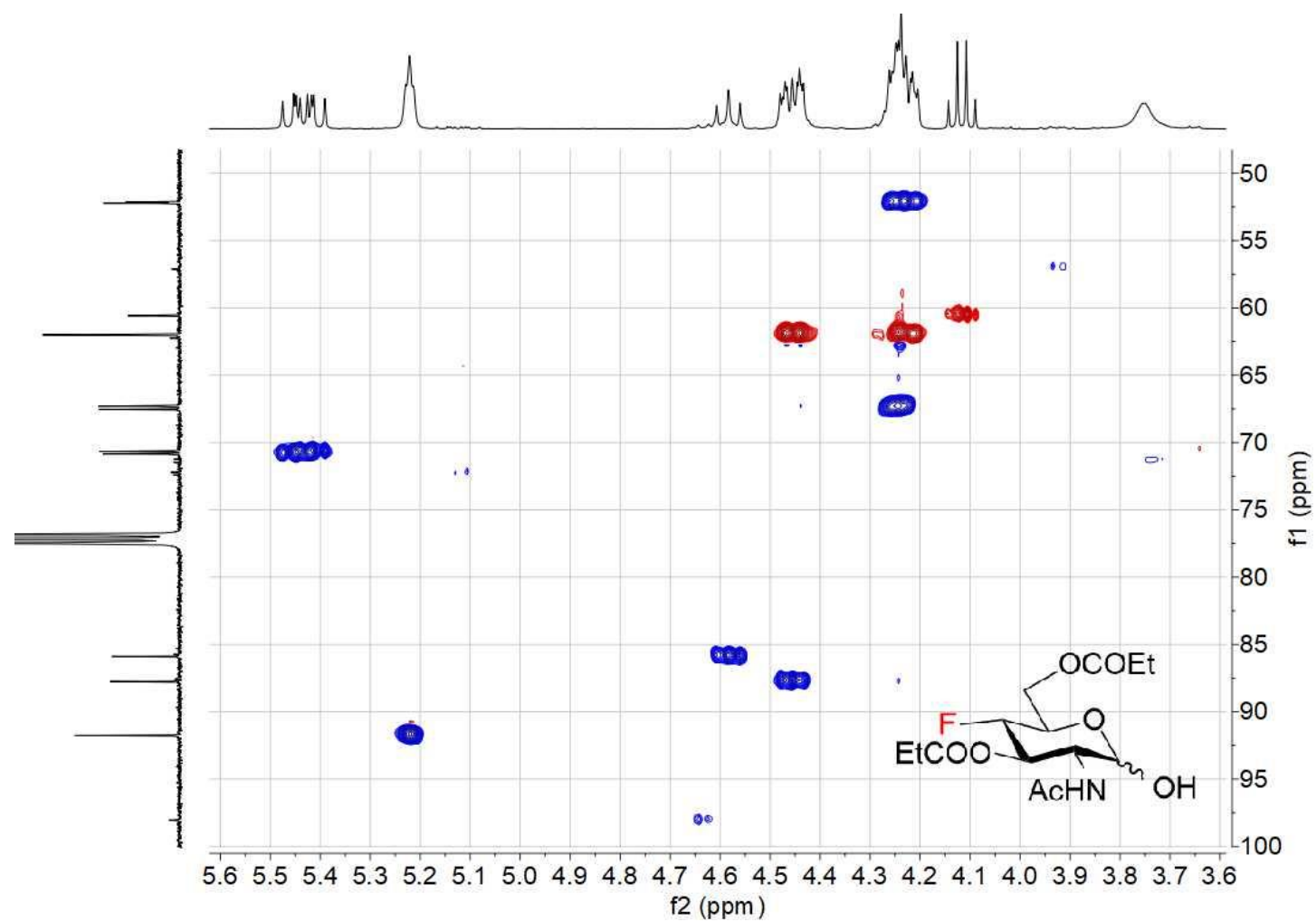
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^1H - ^{13}C HMBC 16

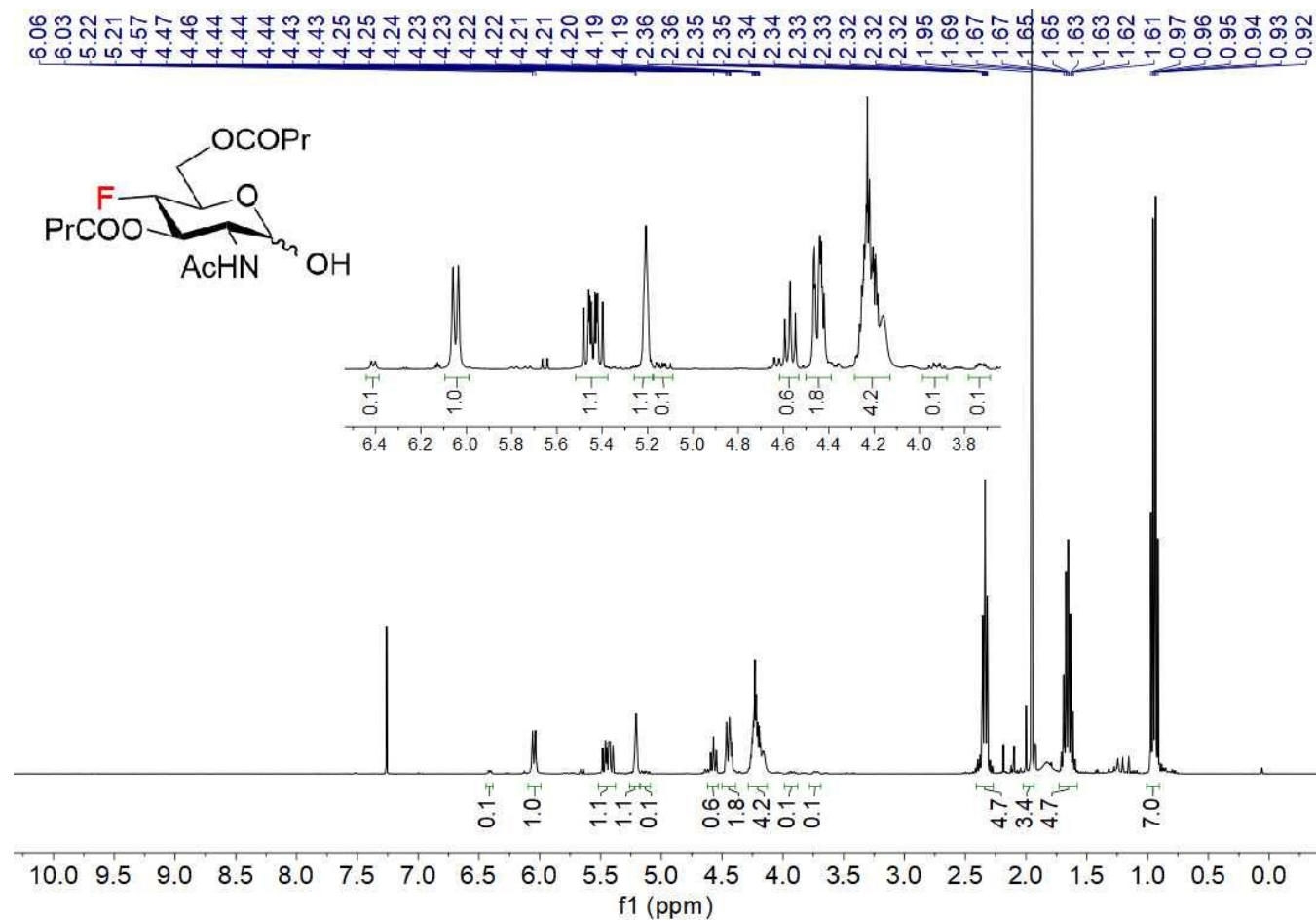


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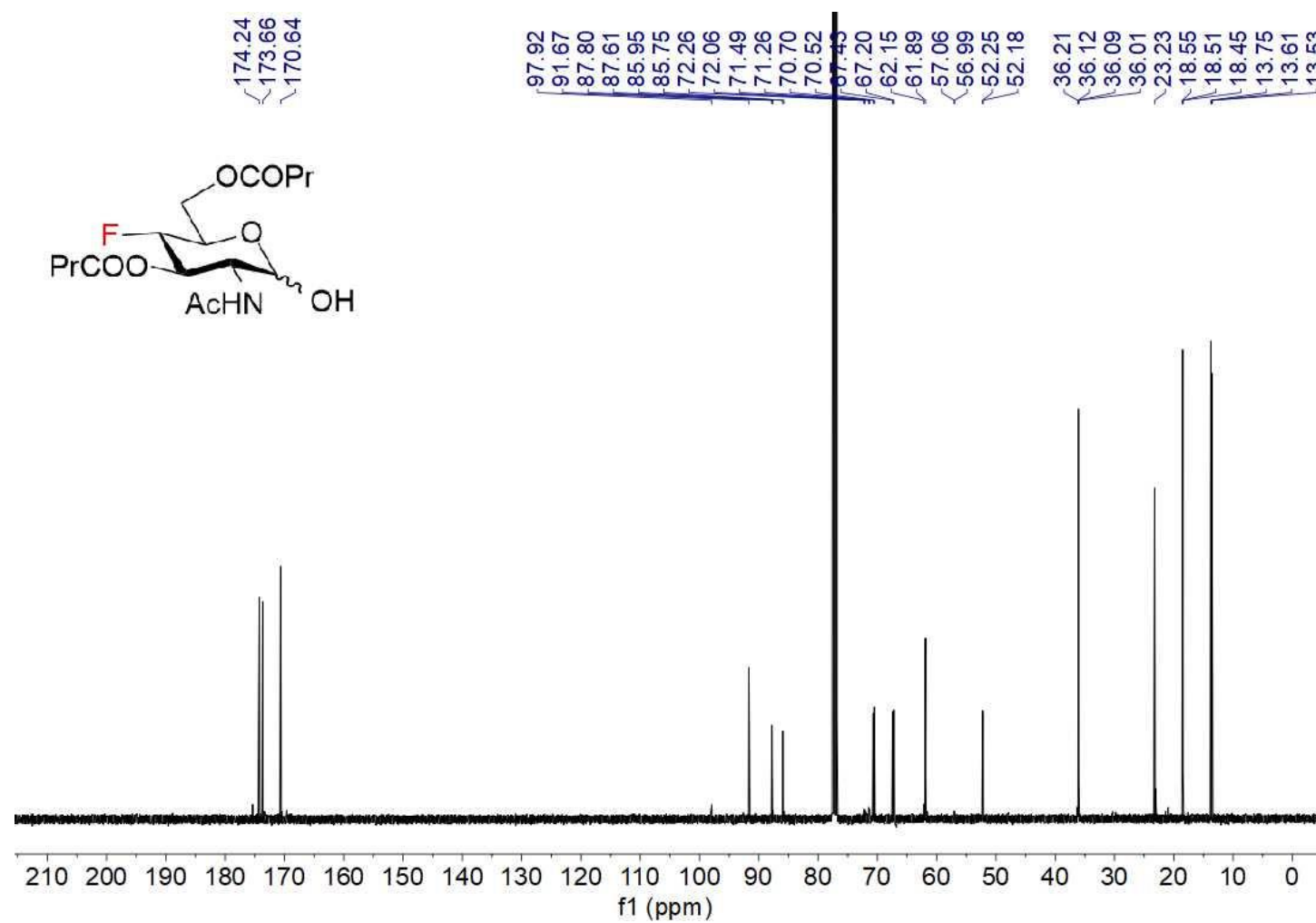


NMR COMPOUND 17

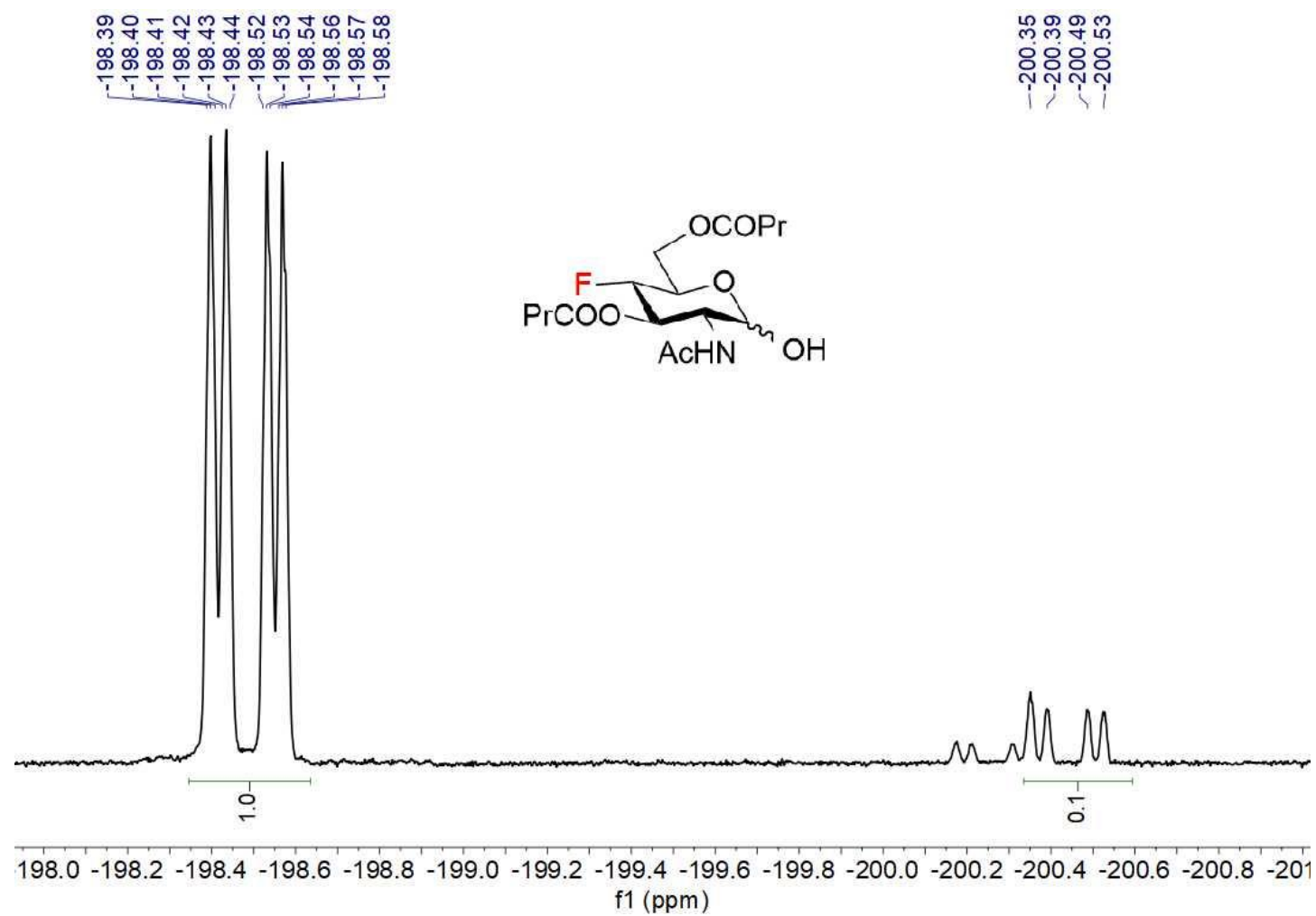
¹H NMR (400 MHz, CDCl₃) 17 ($\alpha/\beta \approx 10:1$, containing ca 5% of O1-Ac)



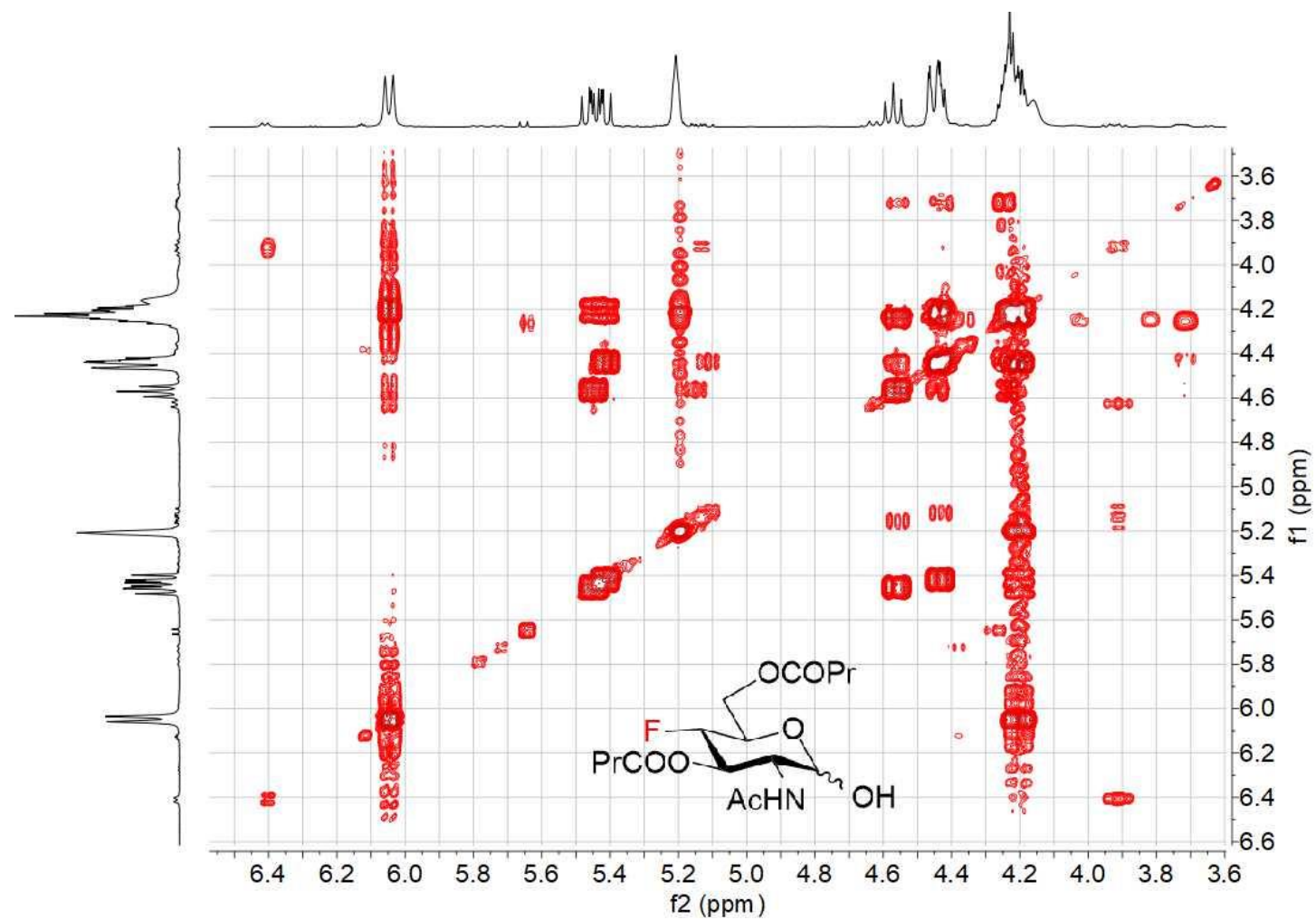
^{13}C NMR (100 MHz, CDCl_3) 17



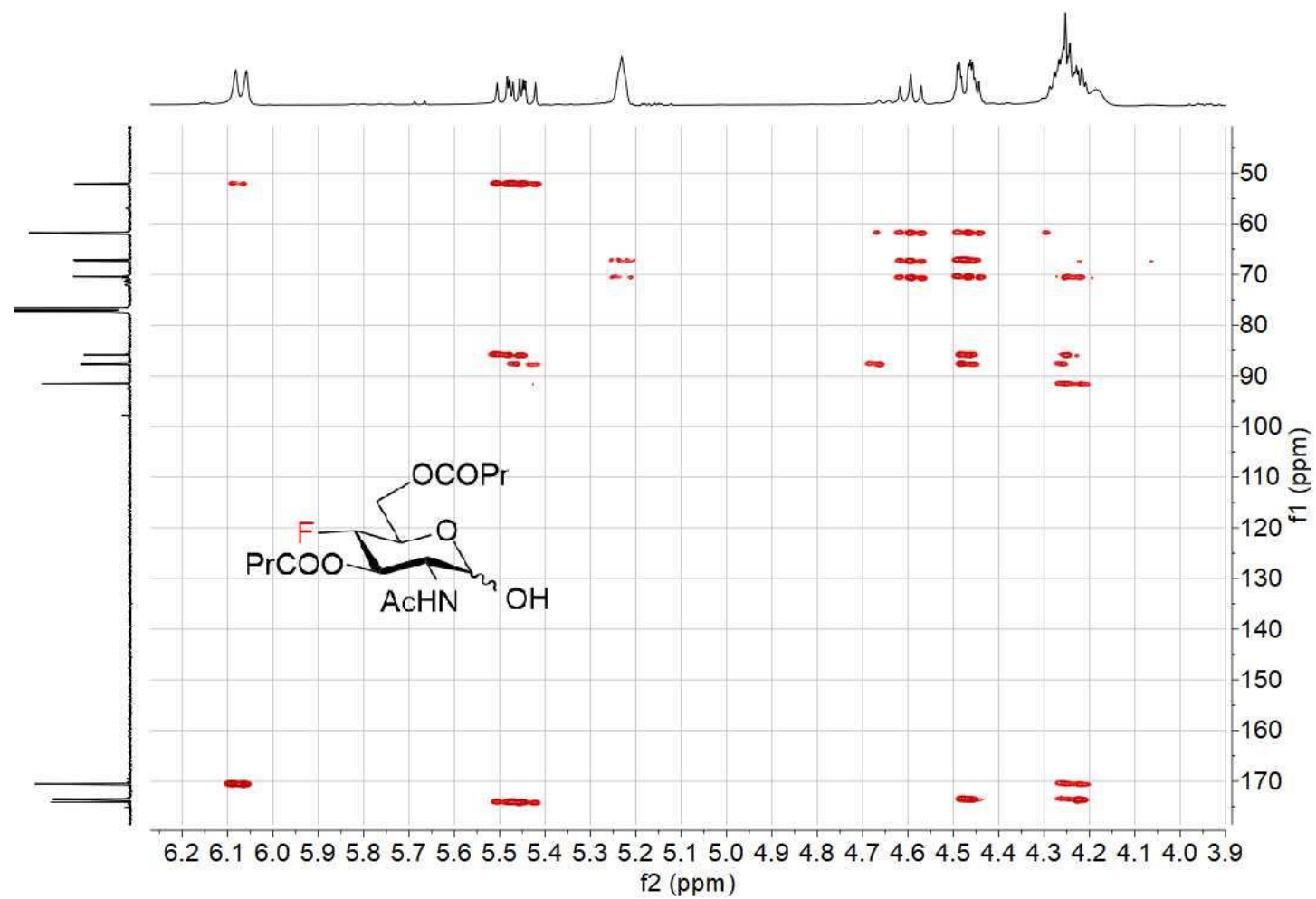
^{19}F NMR (376 MHz, CDCl_3) 17



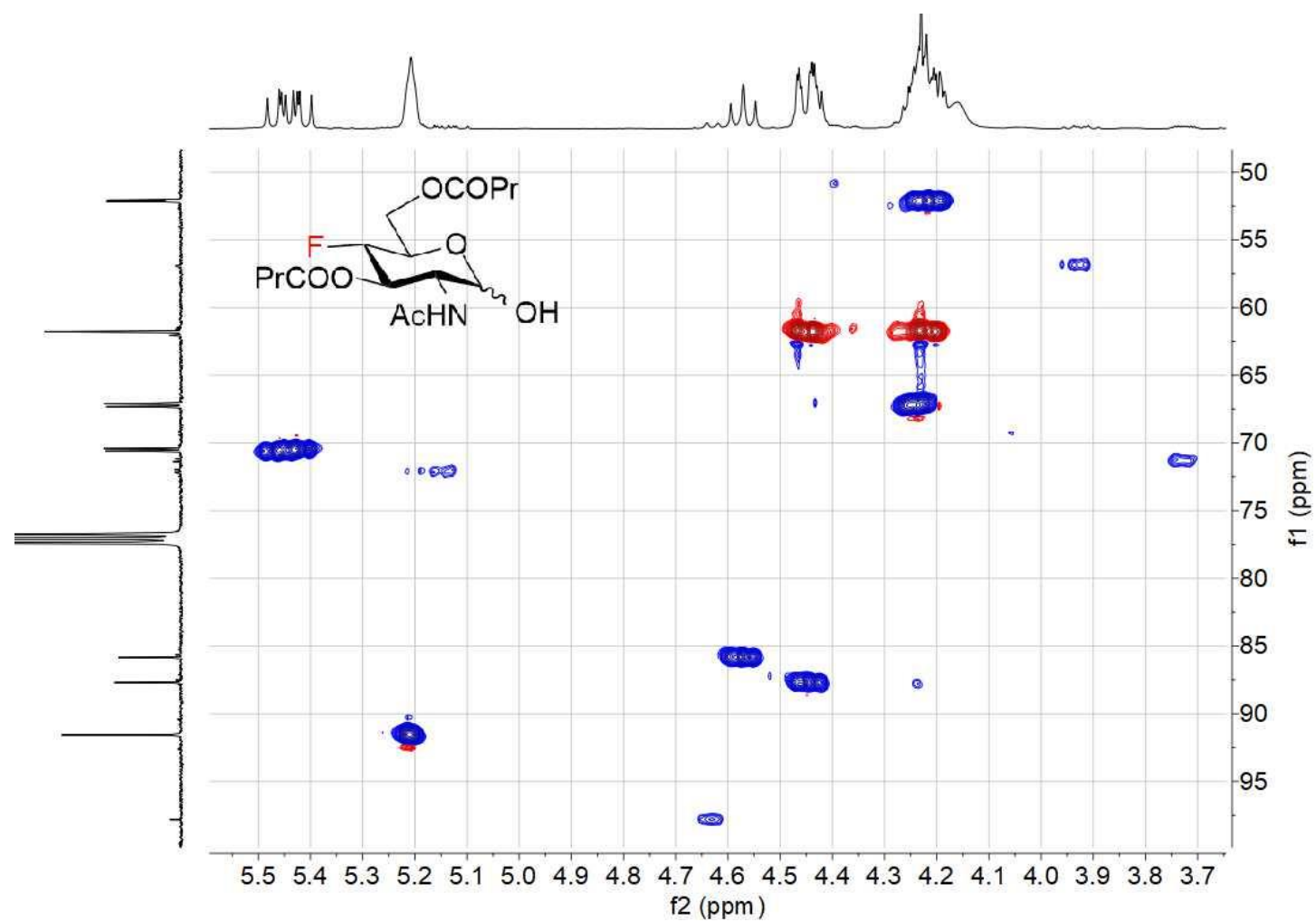
^1H - ^1H COSY 17



^1H - ^{13}C HMBC 17

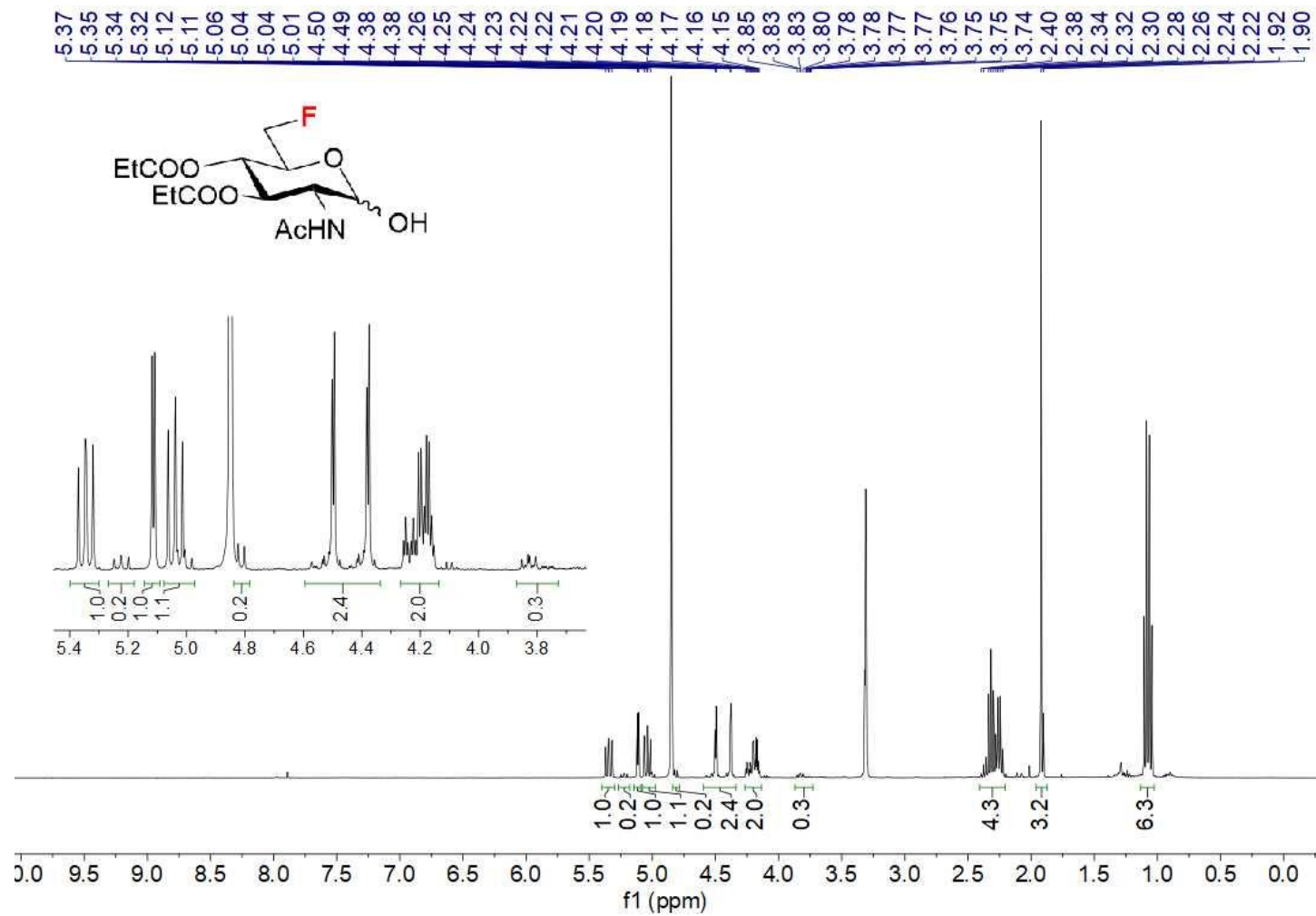


^1H - ^{13}C HSQC 17

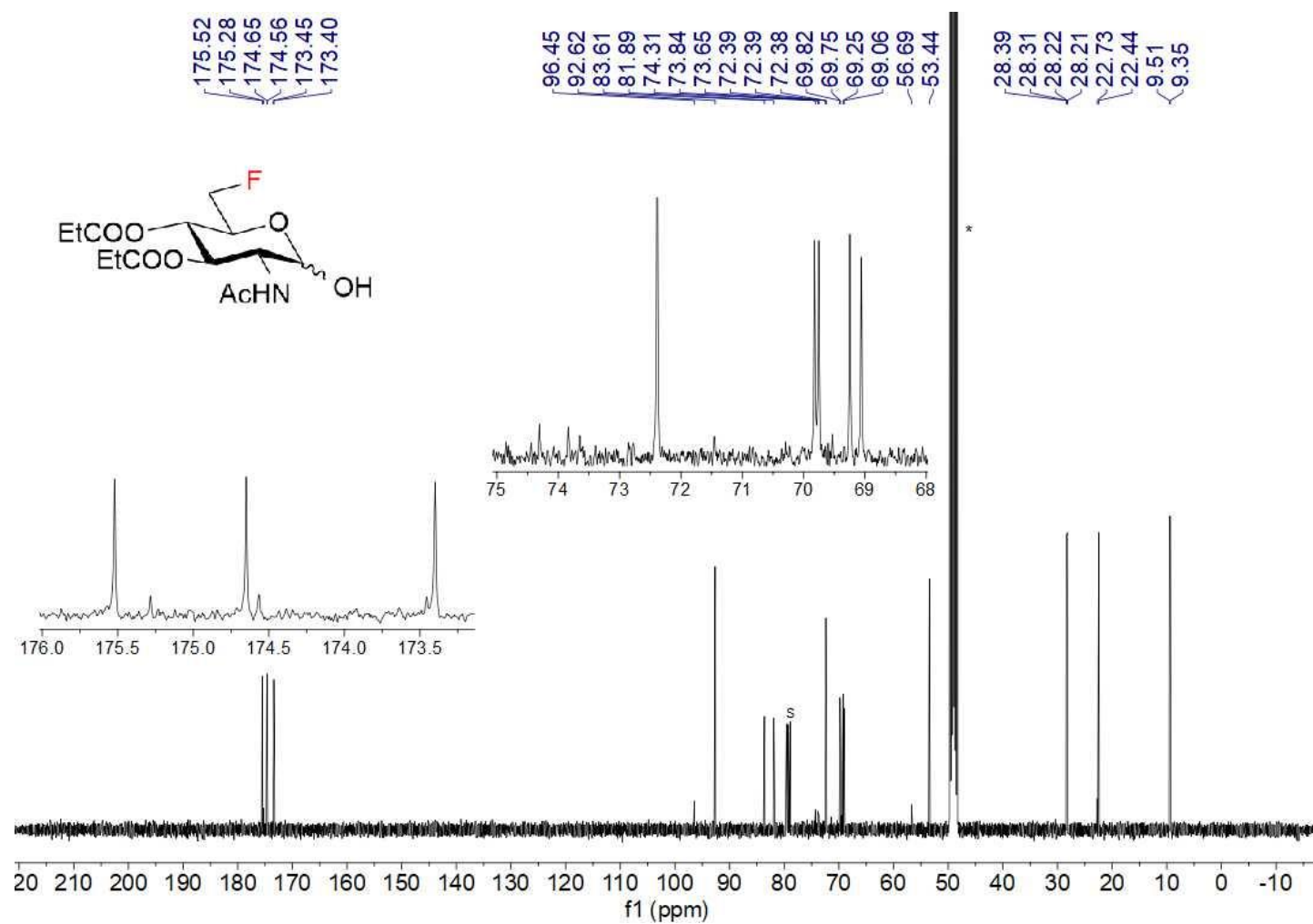


NMR COMPOUND 18 (prepared from compound 93)

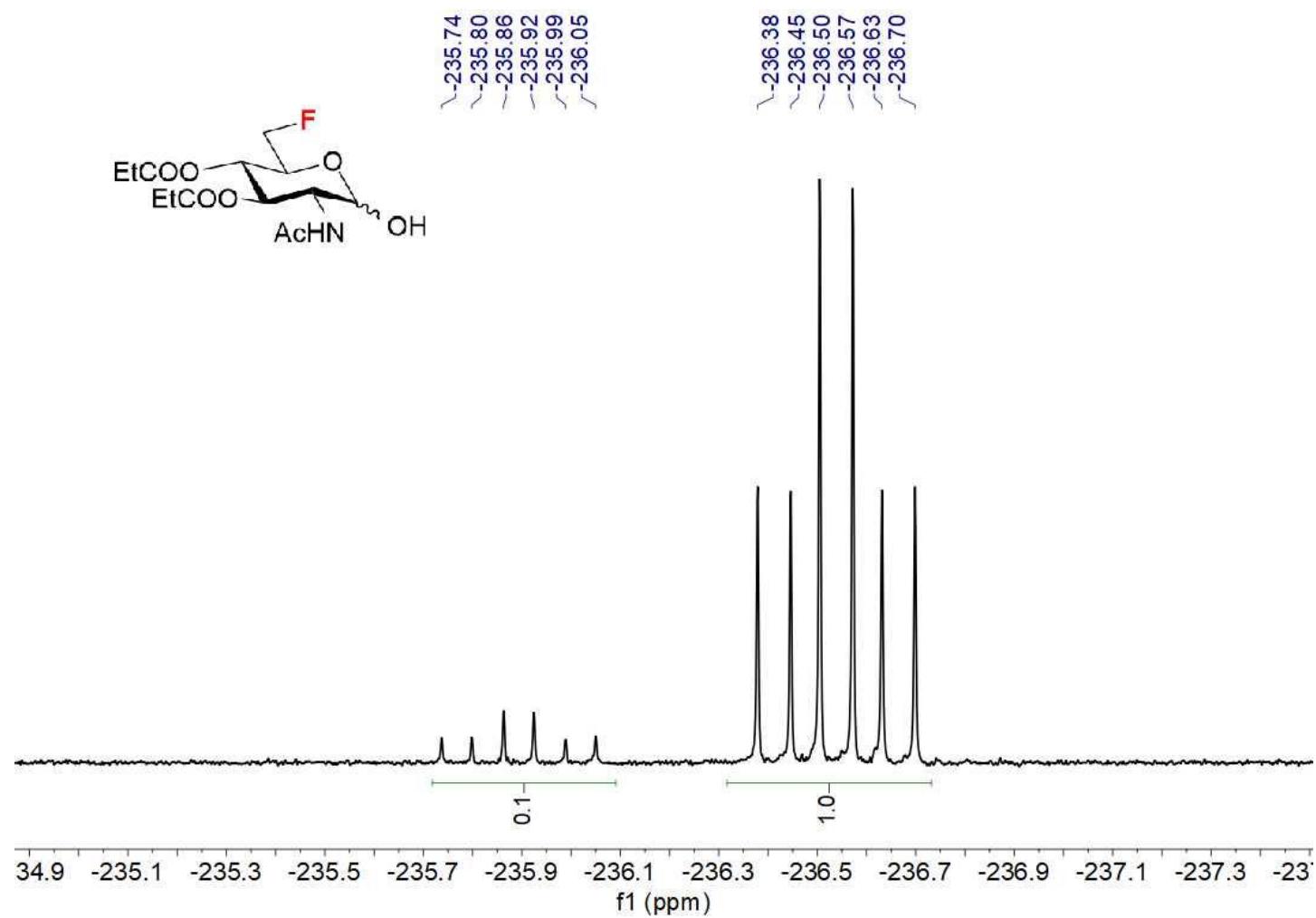
^1H NMR (400 MHz, CD_3OD) 18



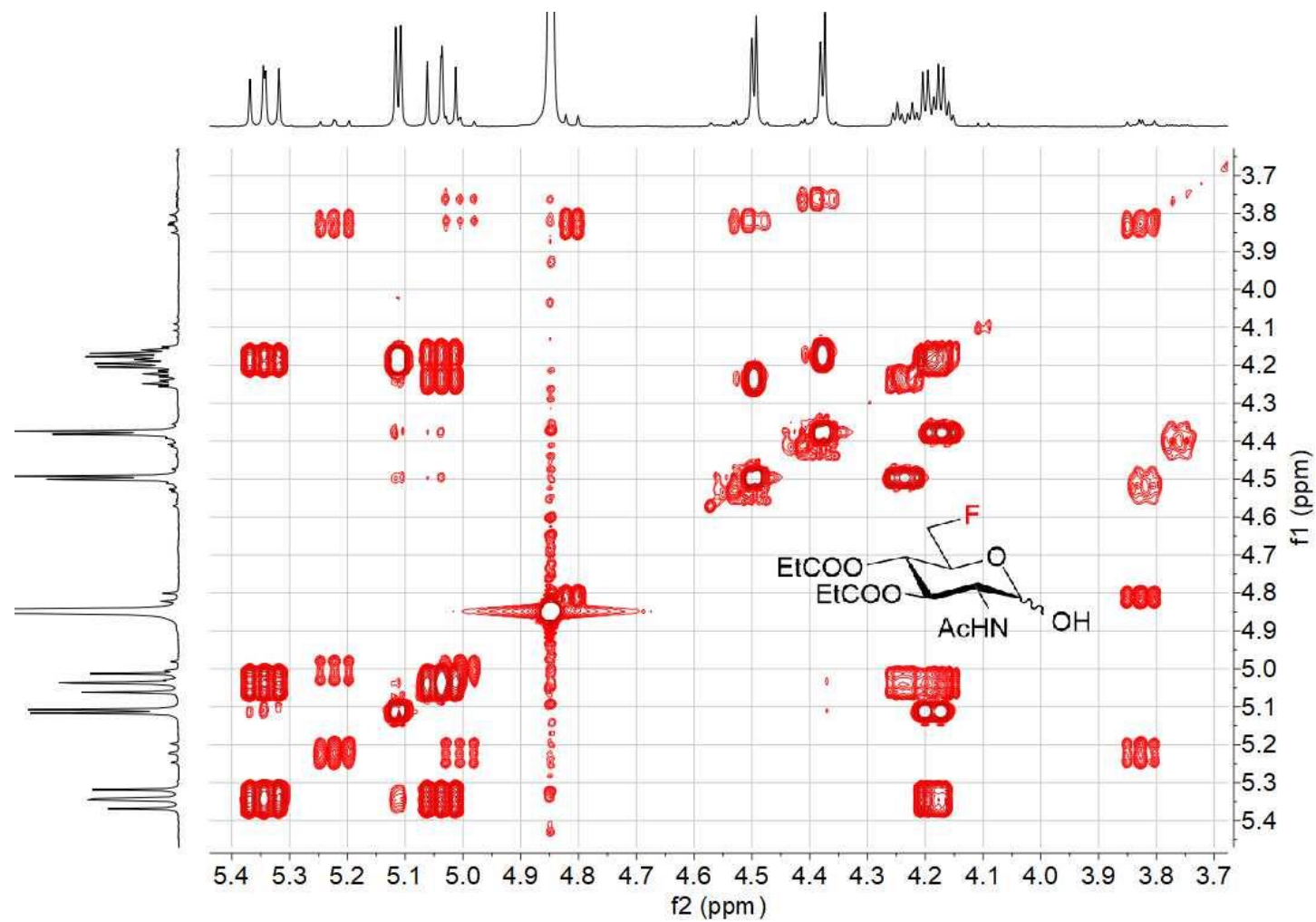
¹³C NMR (100 MHz, CD₃OD) 18



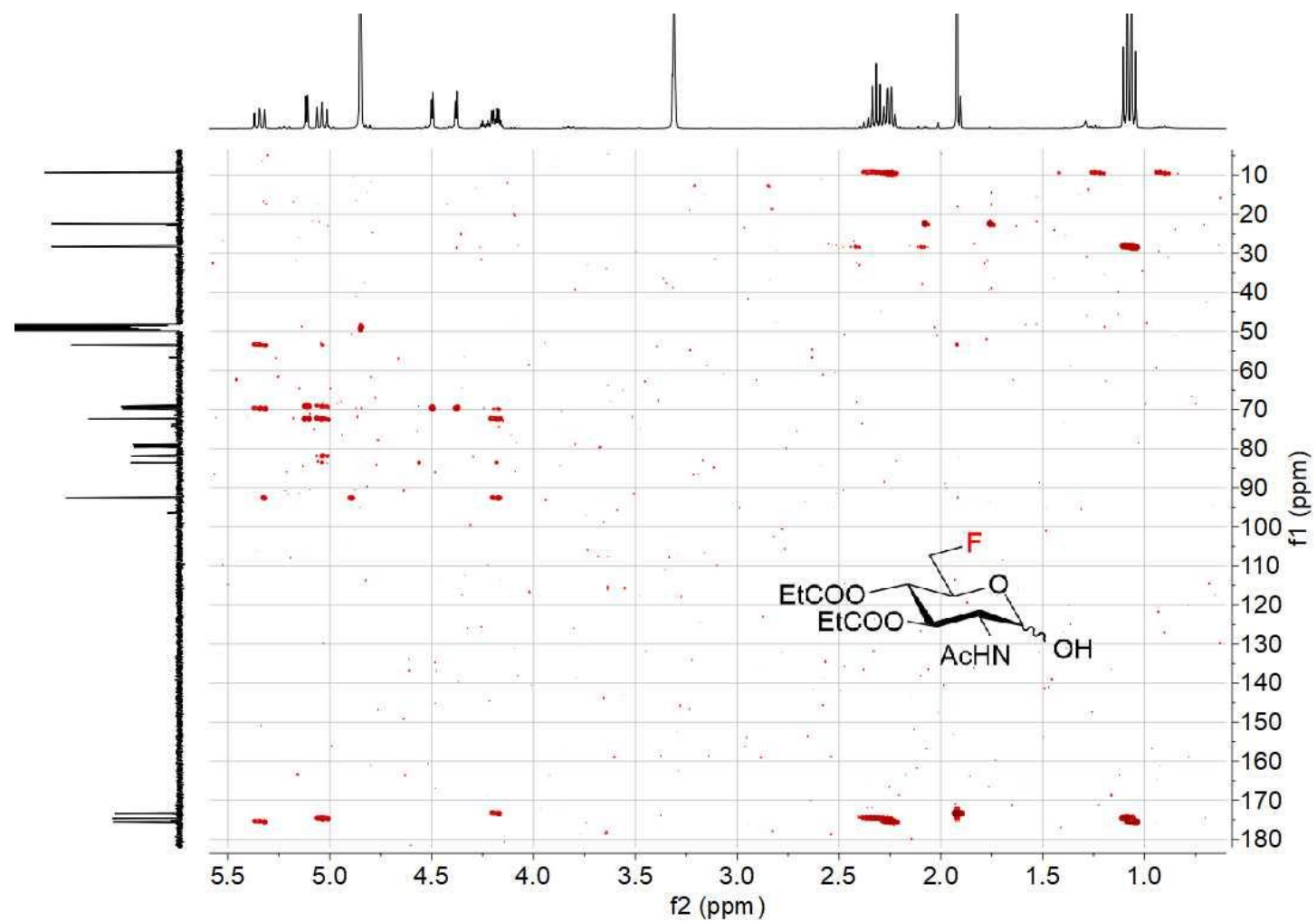
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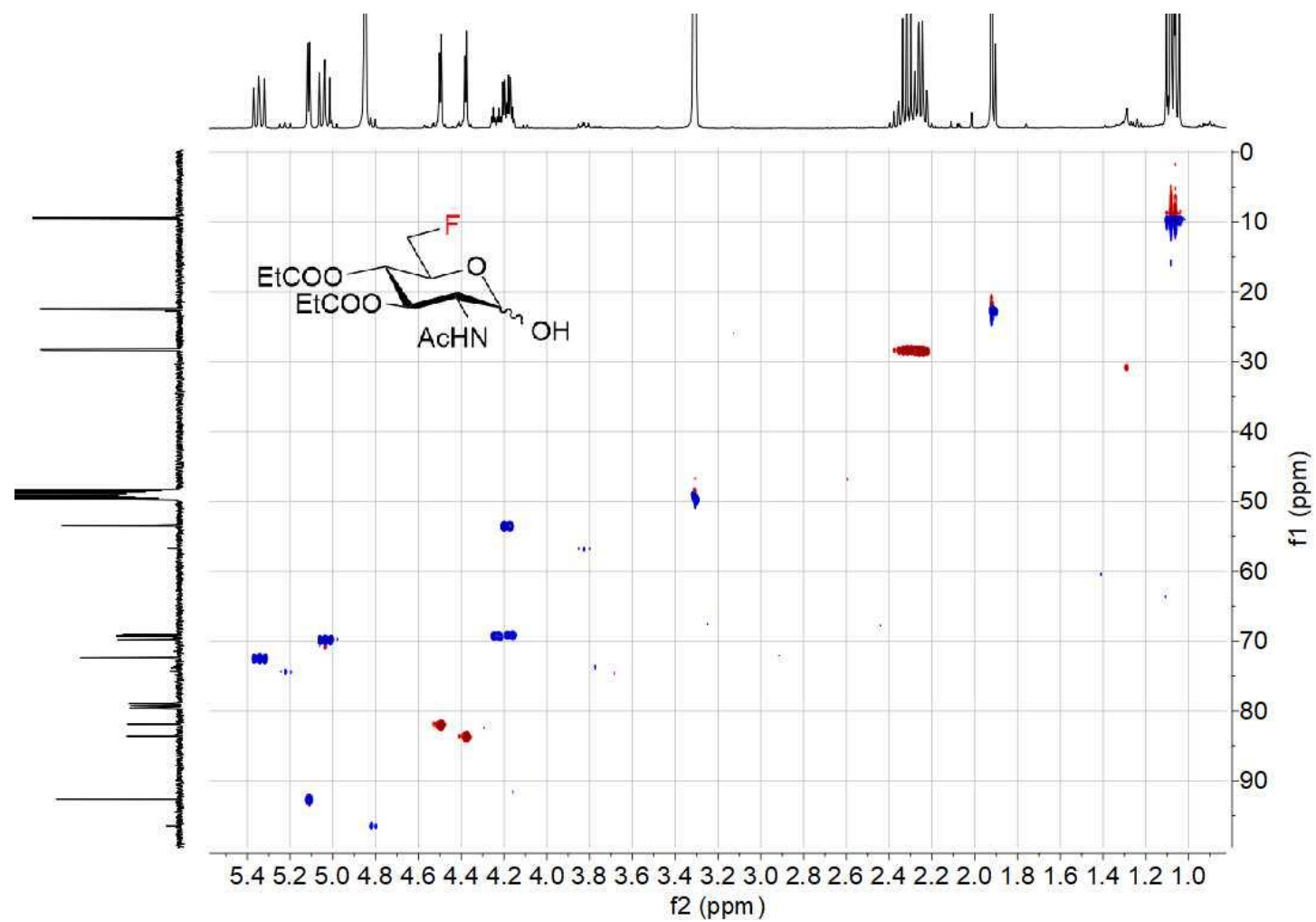
^1H - ^1H COSY 18



^1H - ^{13}C HMBC 18

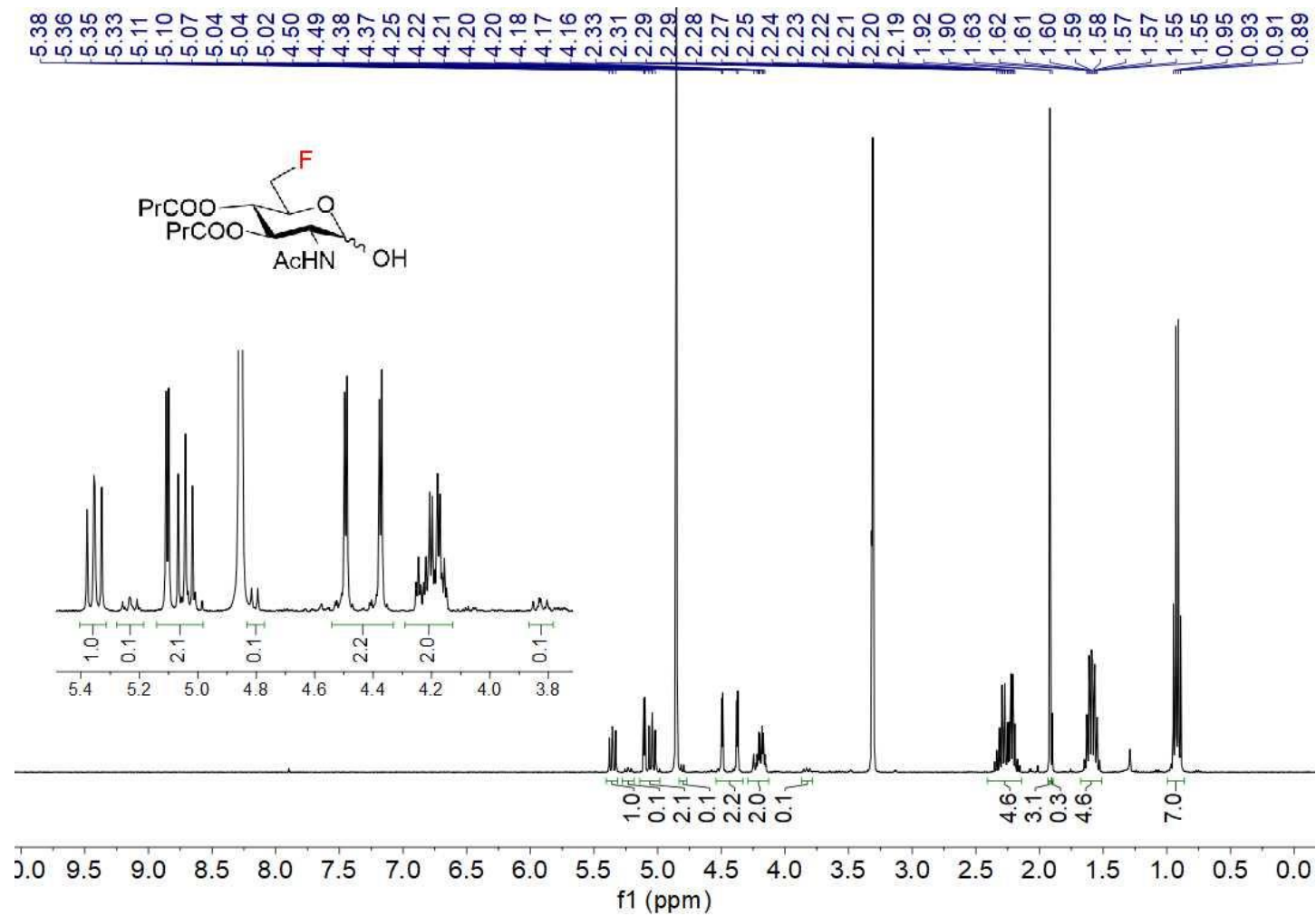


^1H - ^{13}C HSQC 18

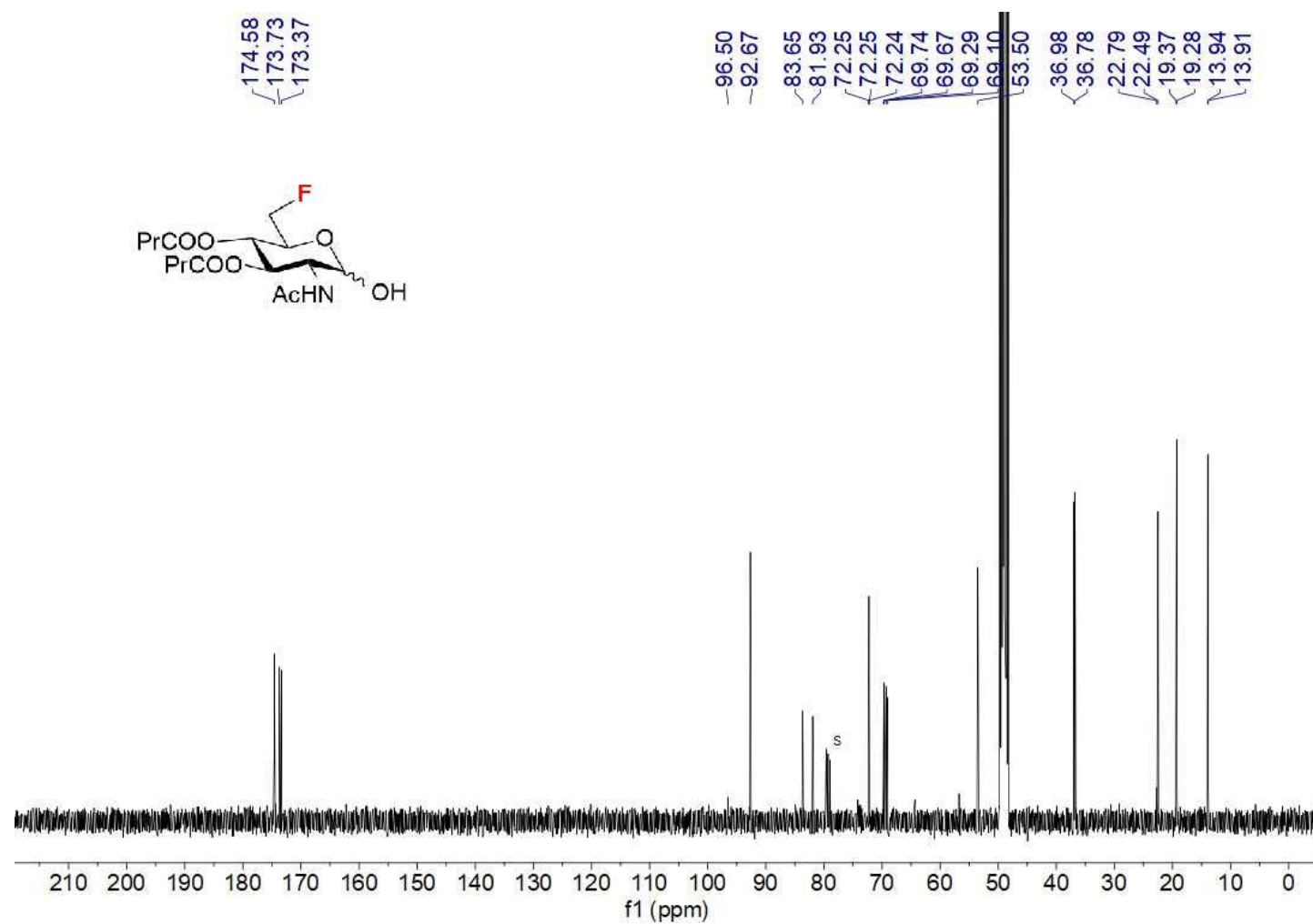


NMR COMPOUND 19 (prepared from compound 93)

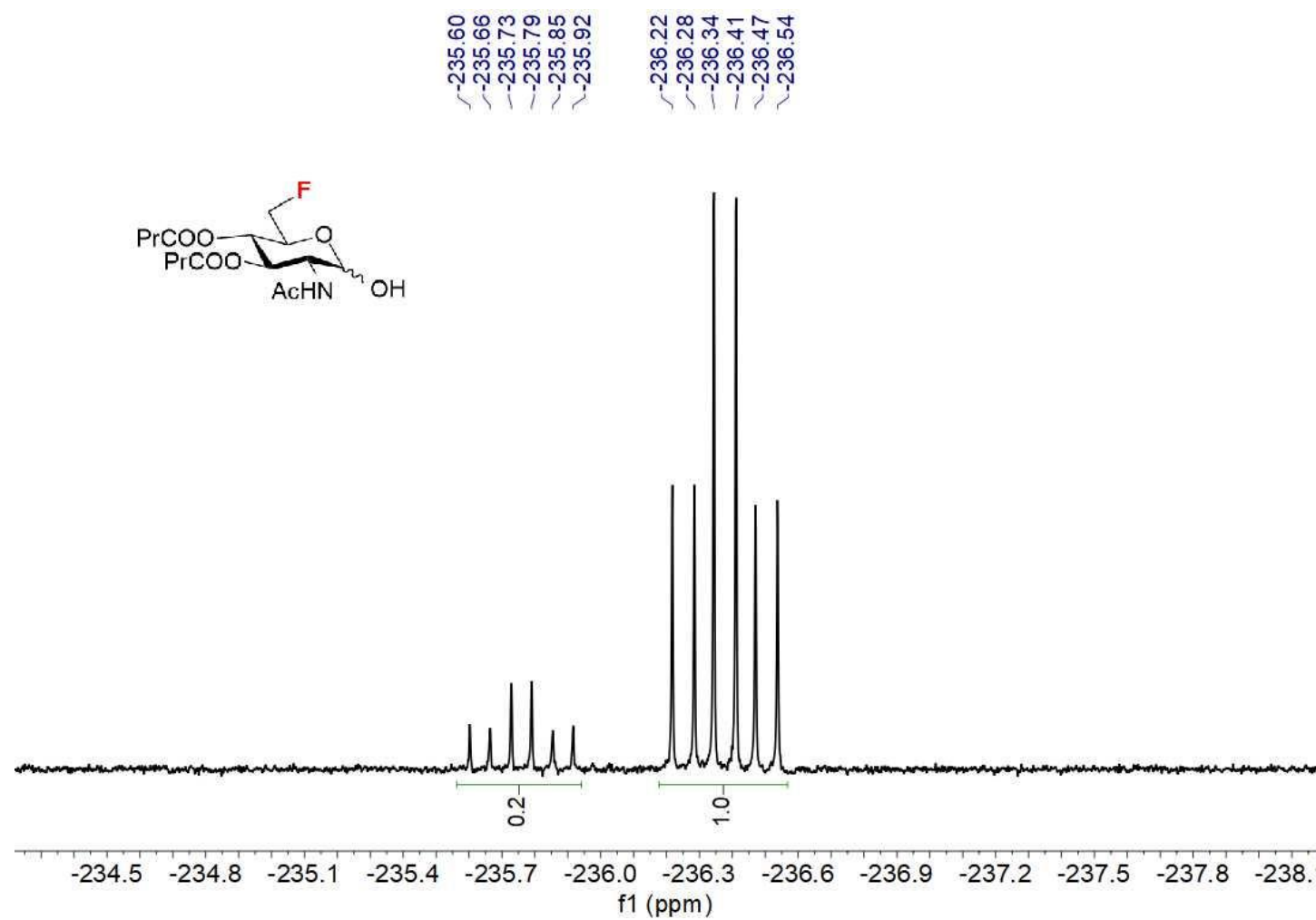
^1H NMR (400 MHz, CD_3OD) 19



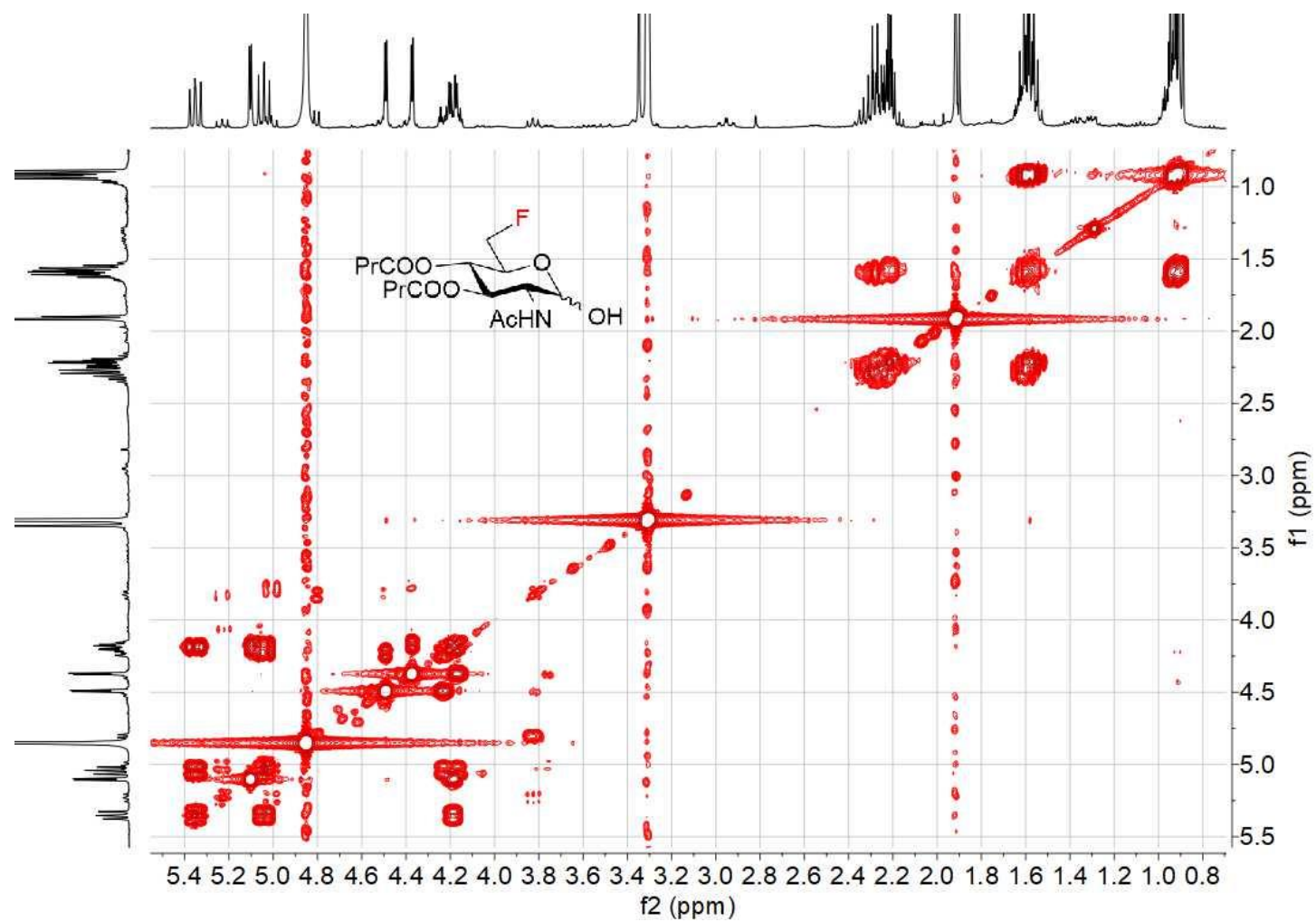
¹³C NMR (100 MHz, CD₃OD) 19



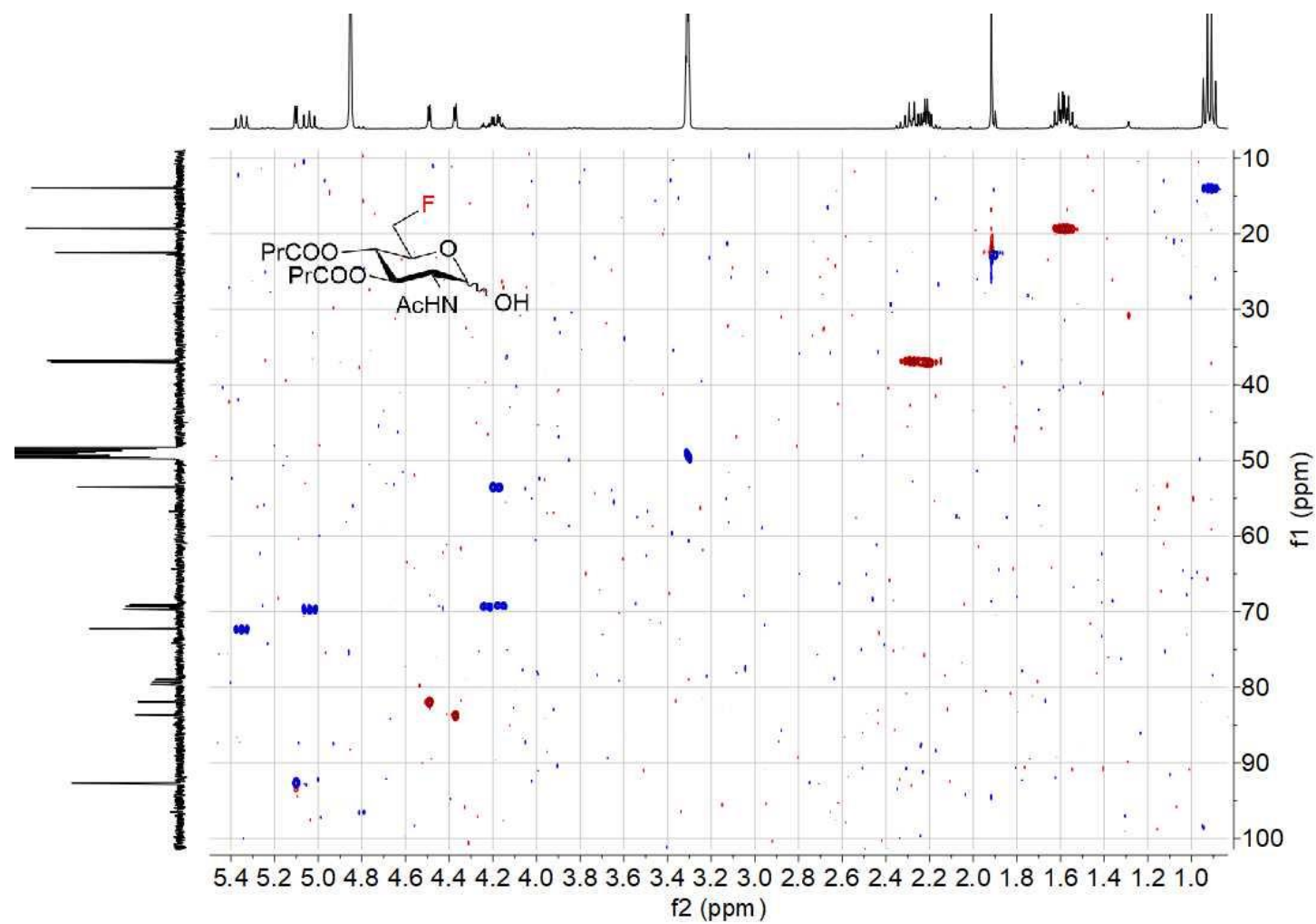
¹⁹F NMR (376 MHz, CD₃OD) 19



^1H - ^1H COSY 19

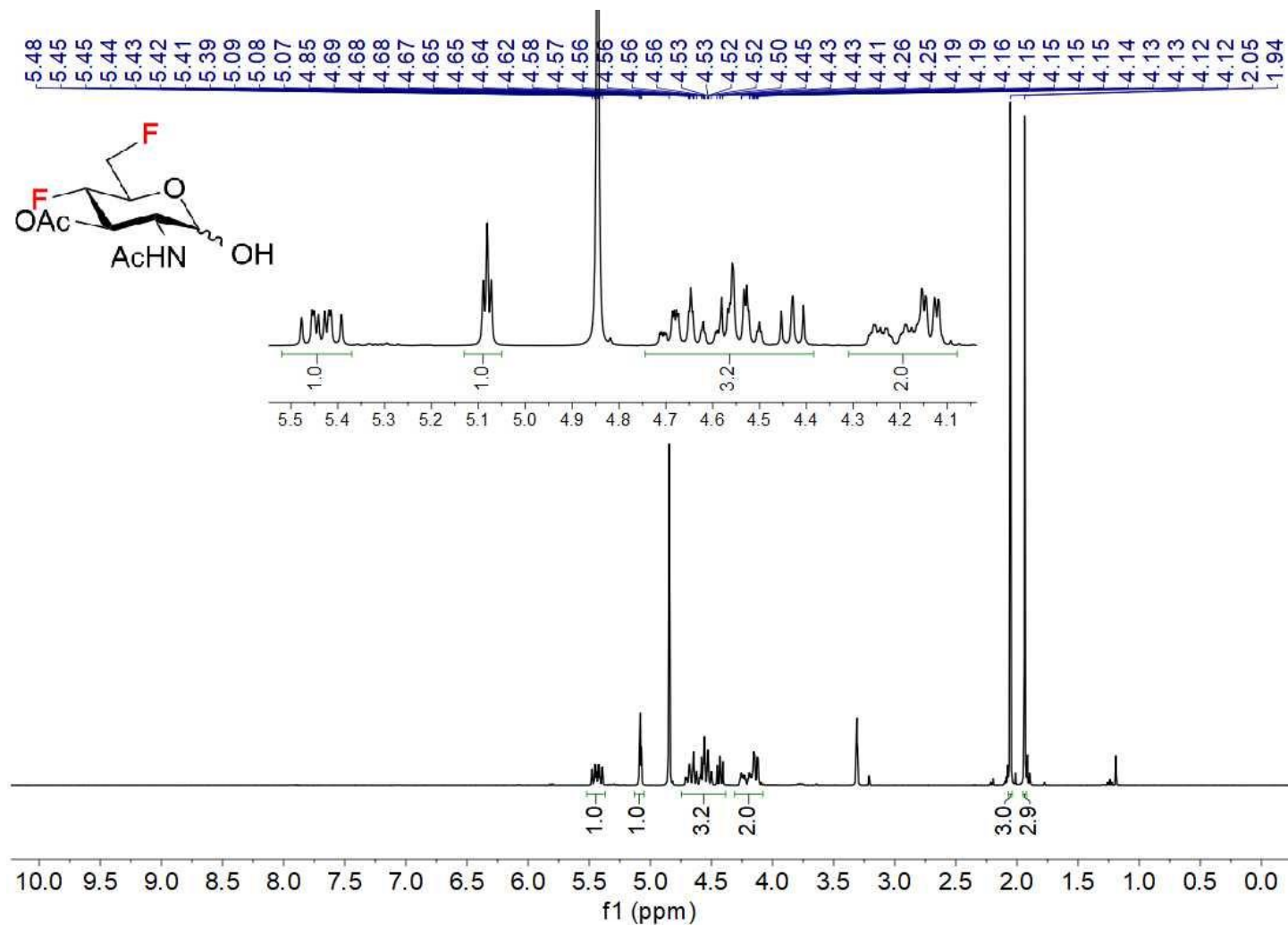


^1H - ^{13}C HSQC 19

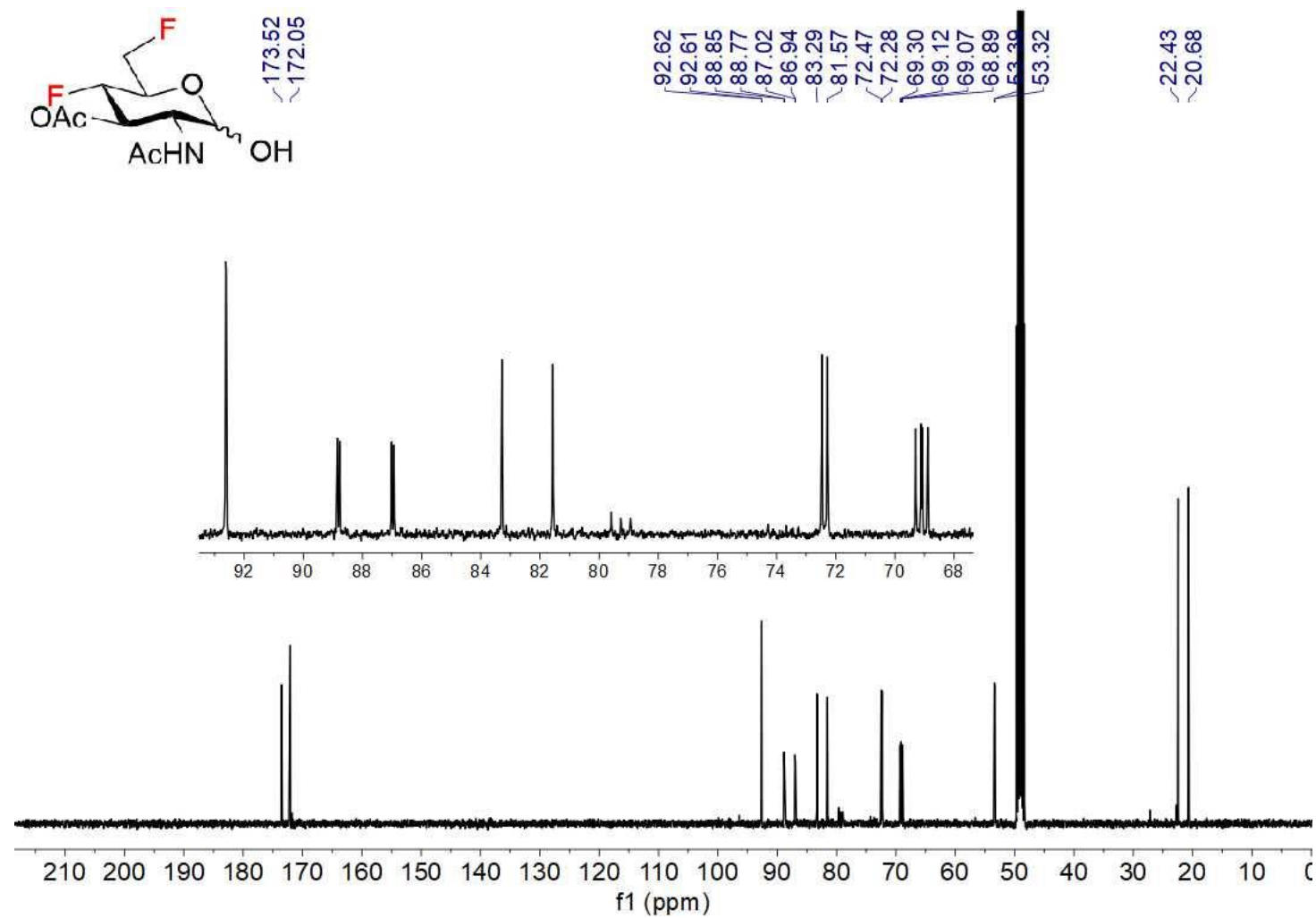


NMR COMPOUND 20

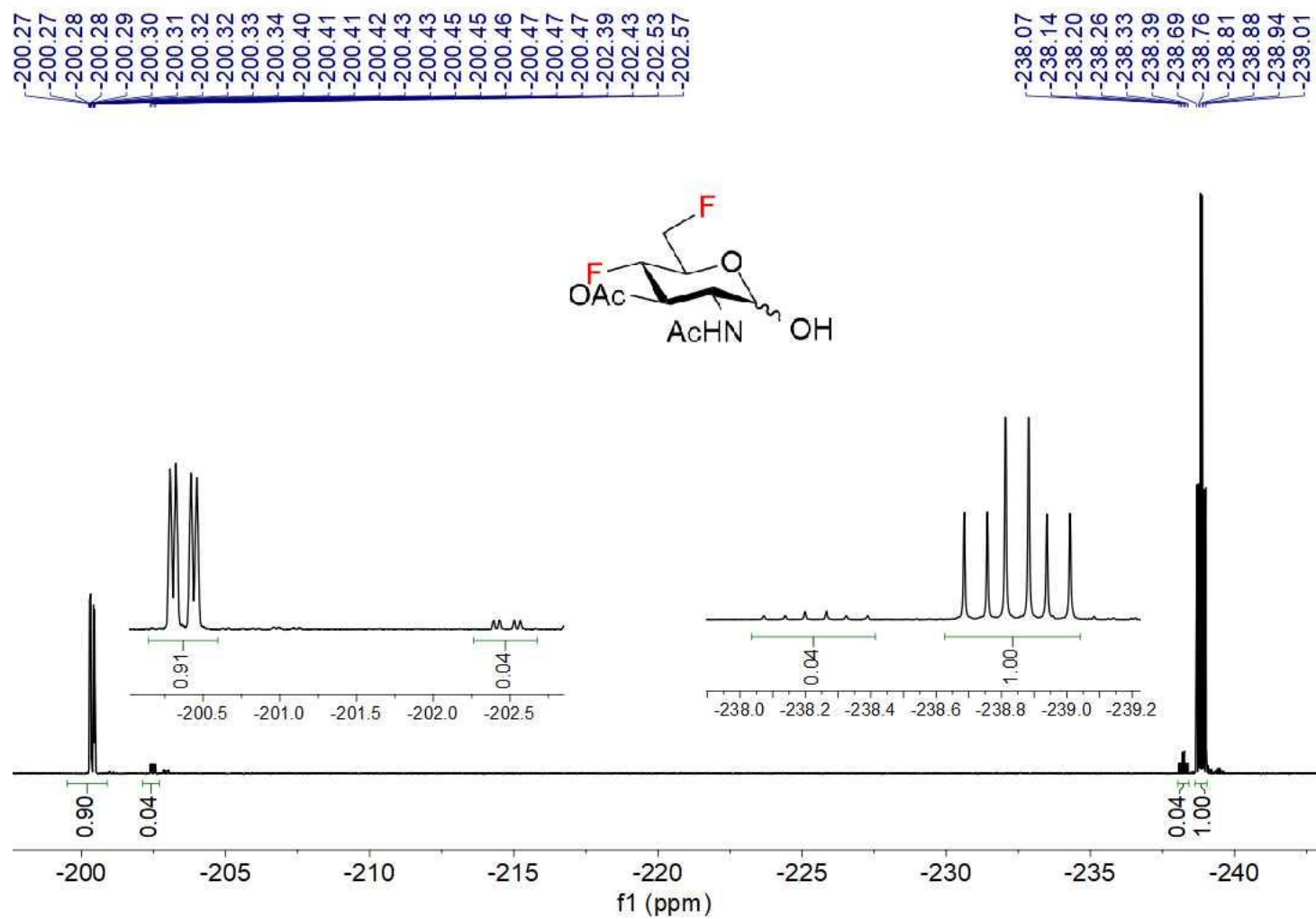
^1H NMR (400 MHz, CD_3OD) 20



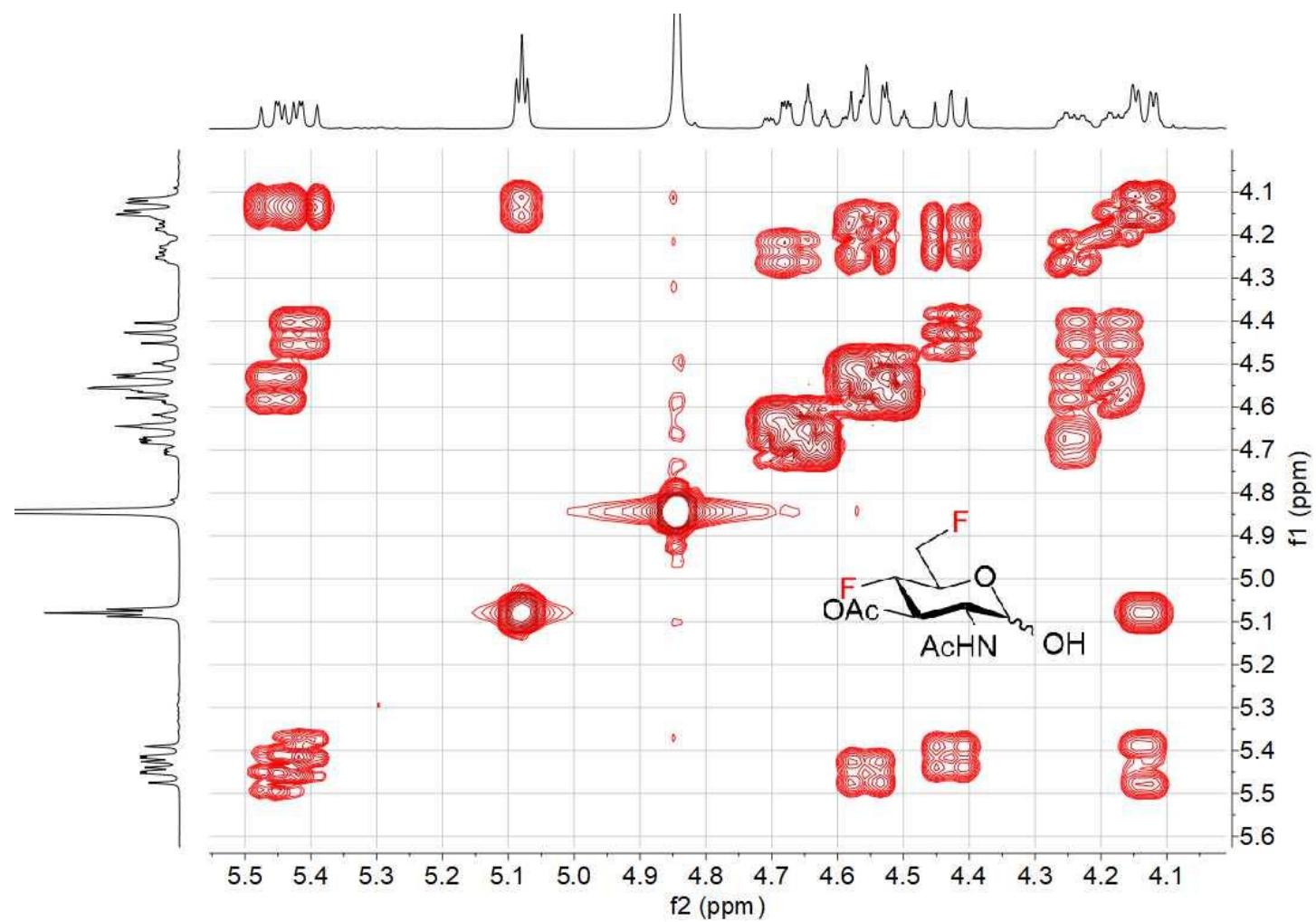
^{13}C NMR (100 MHz, CD_3OD) 20



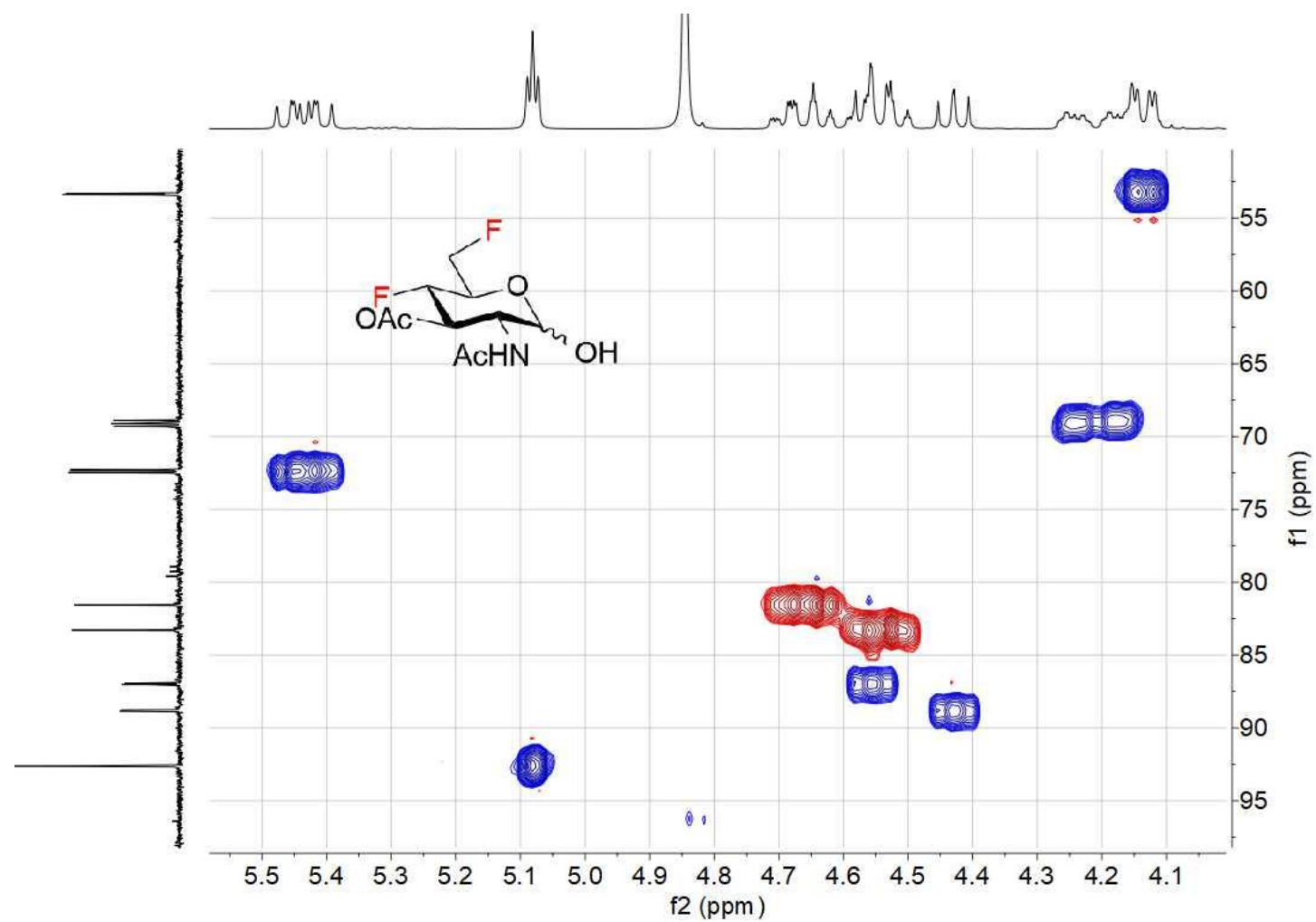
¹⁹F NMR (376 MHz, CD₃OD) 20



^1H - ^1H COSY 20

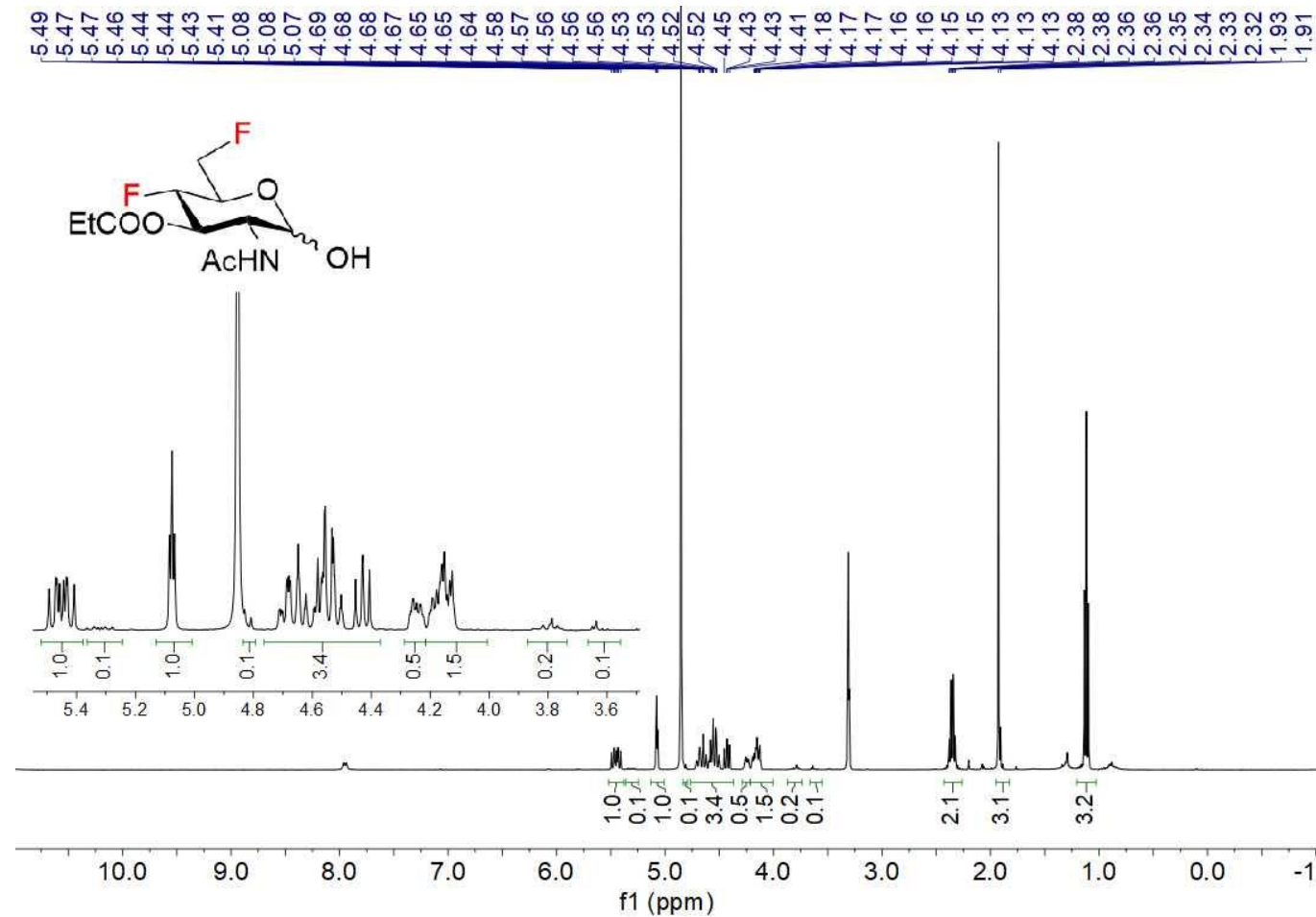


^1H - ^{13}C HSQC 20

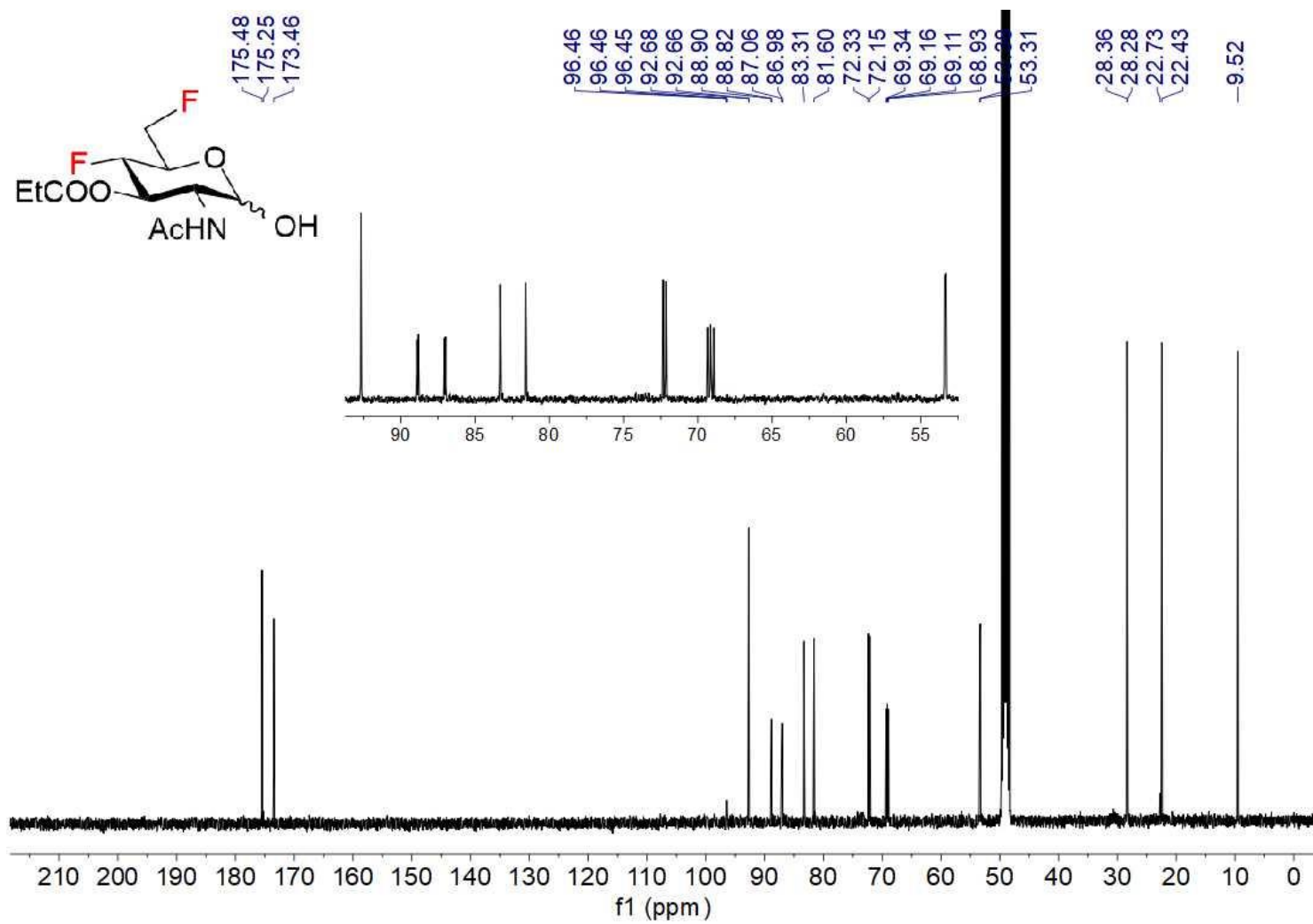


NMR COMPOUND 21

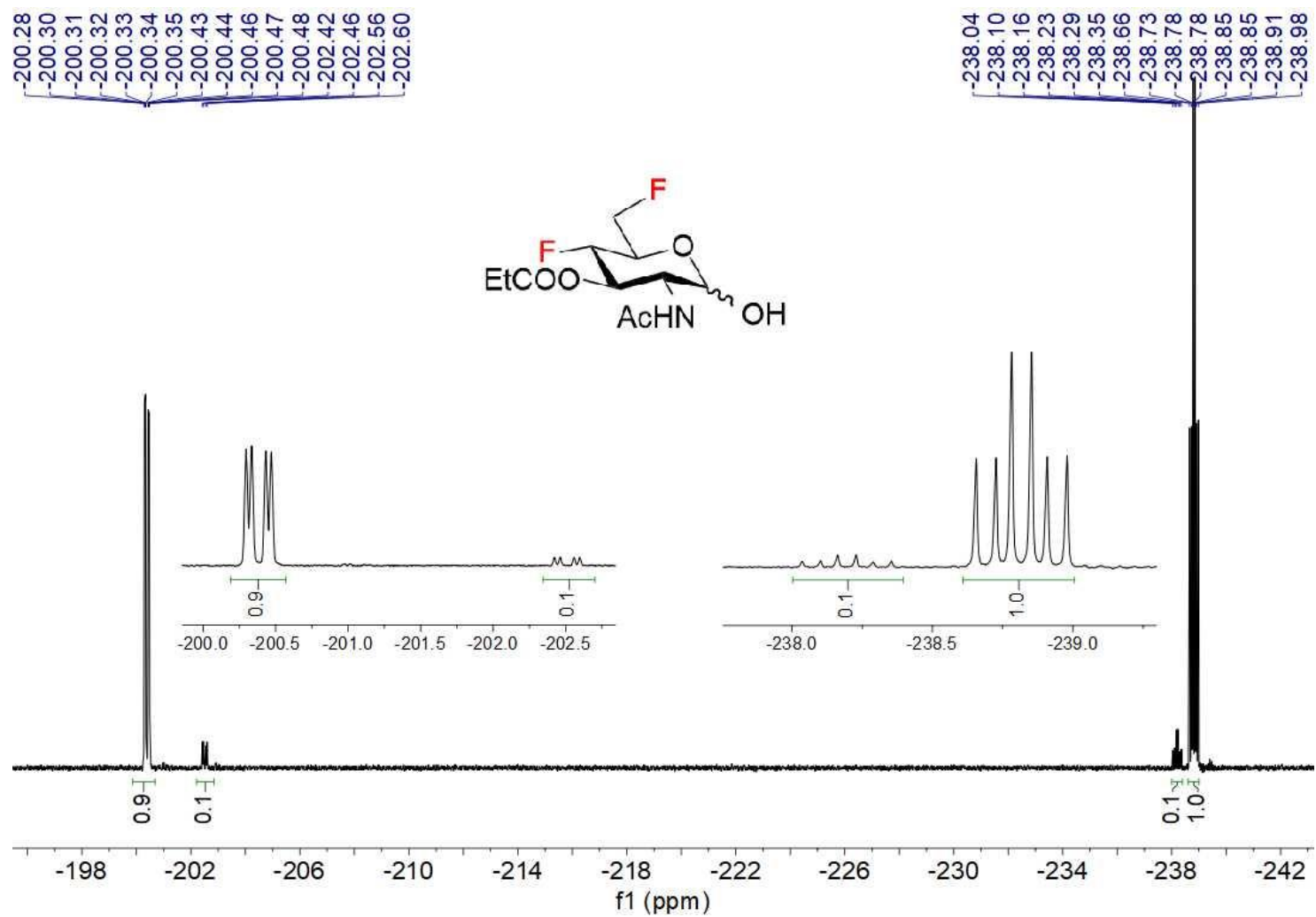
¹H NMR (400 MHz, CD₃OD) 21



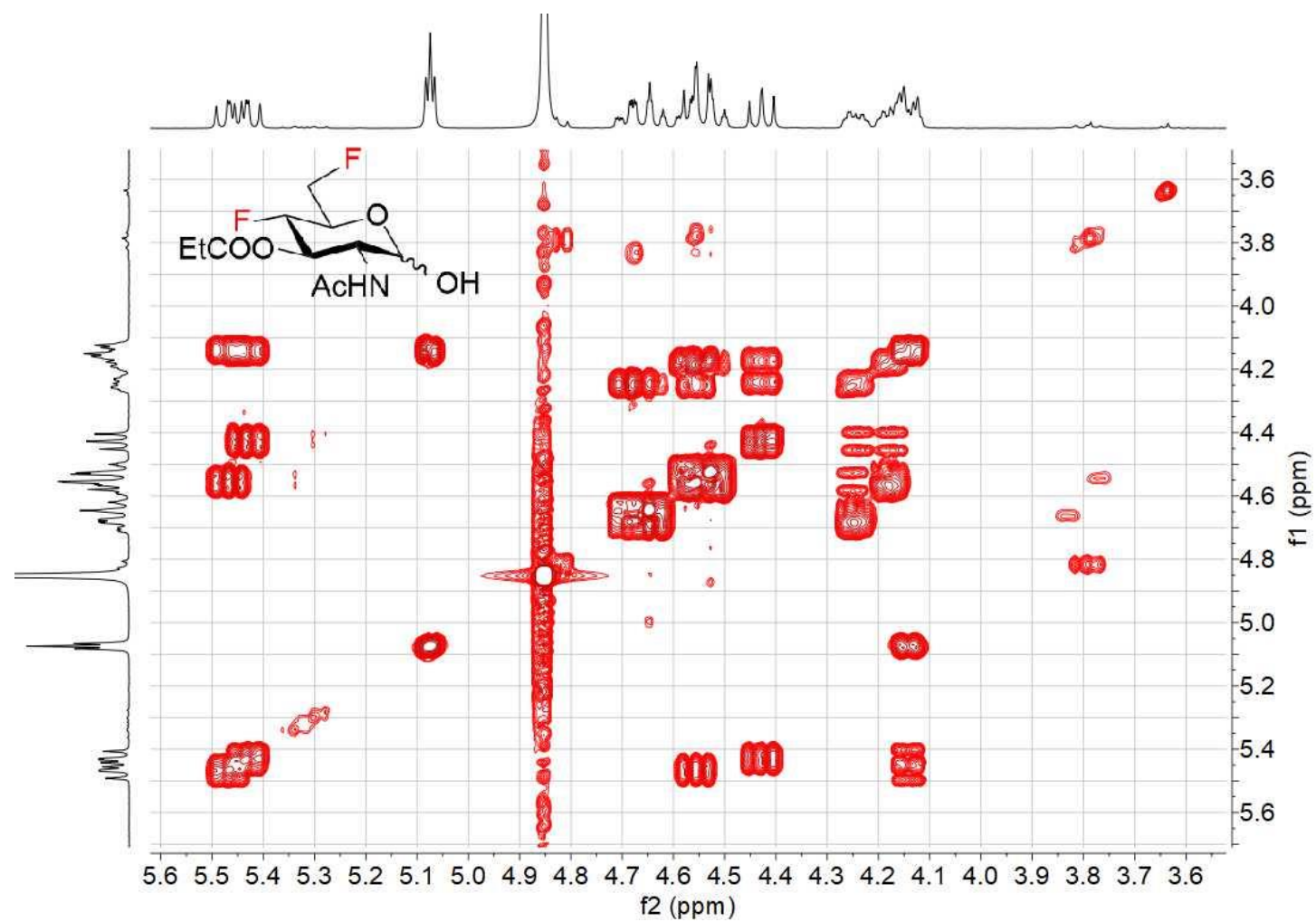
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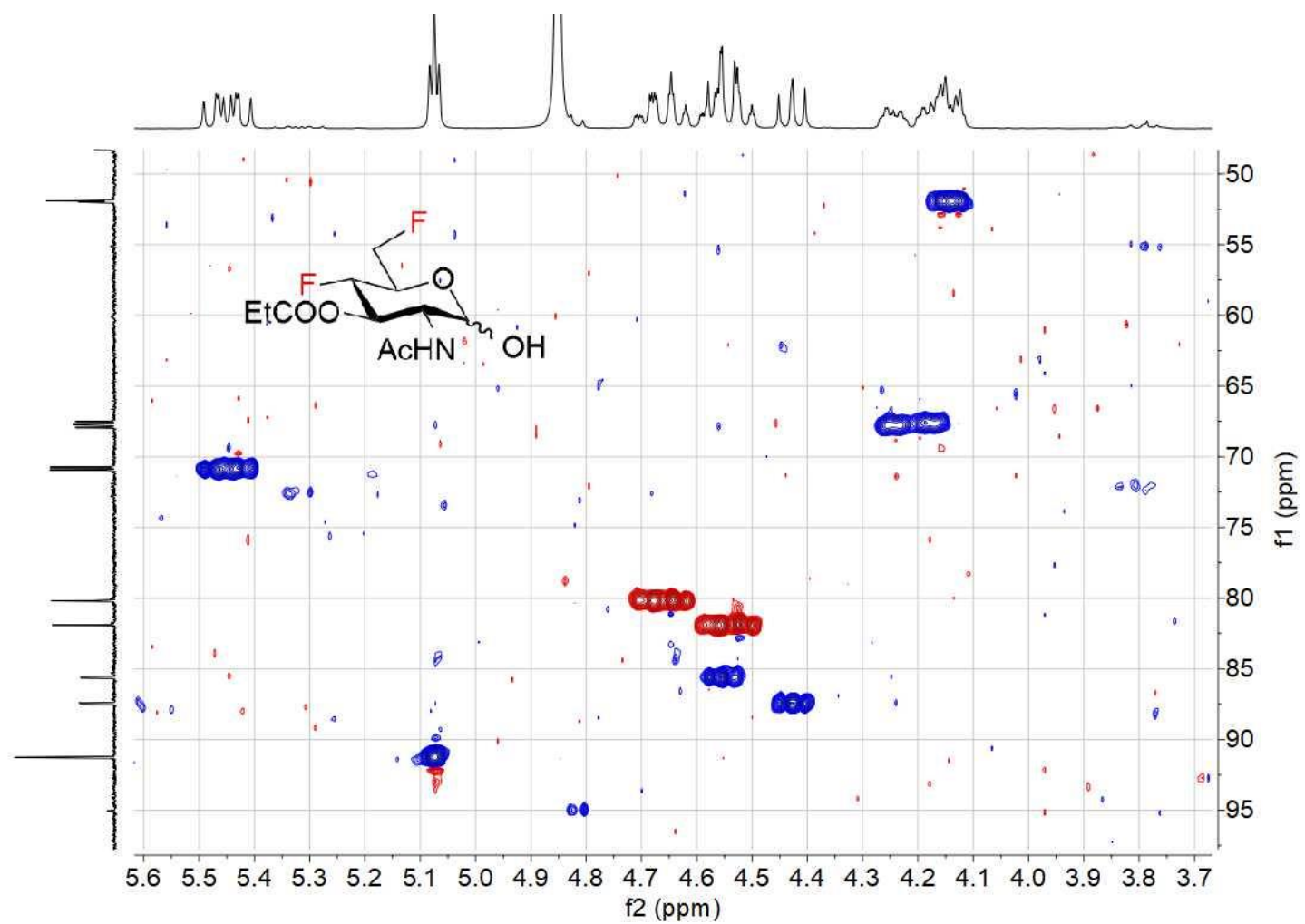
¹⁹F NMR (376 MHz, CD₃OD) 21



^1H - ^1H COSY 21

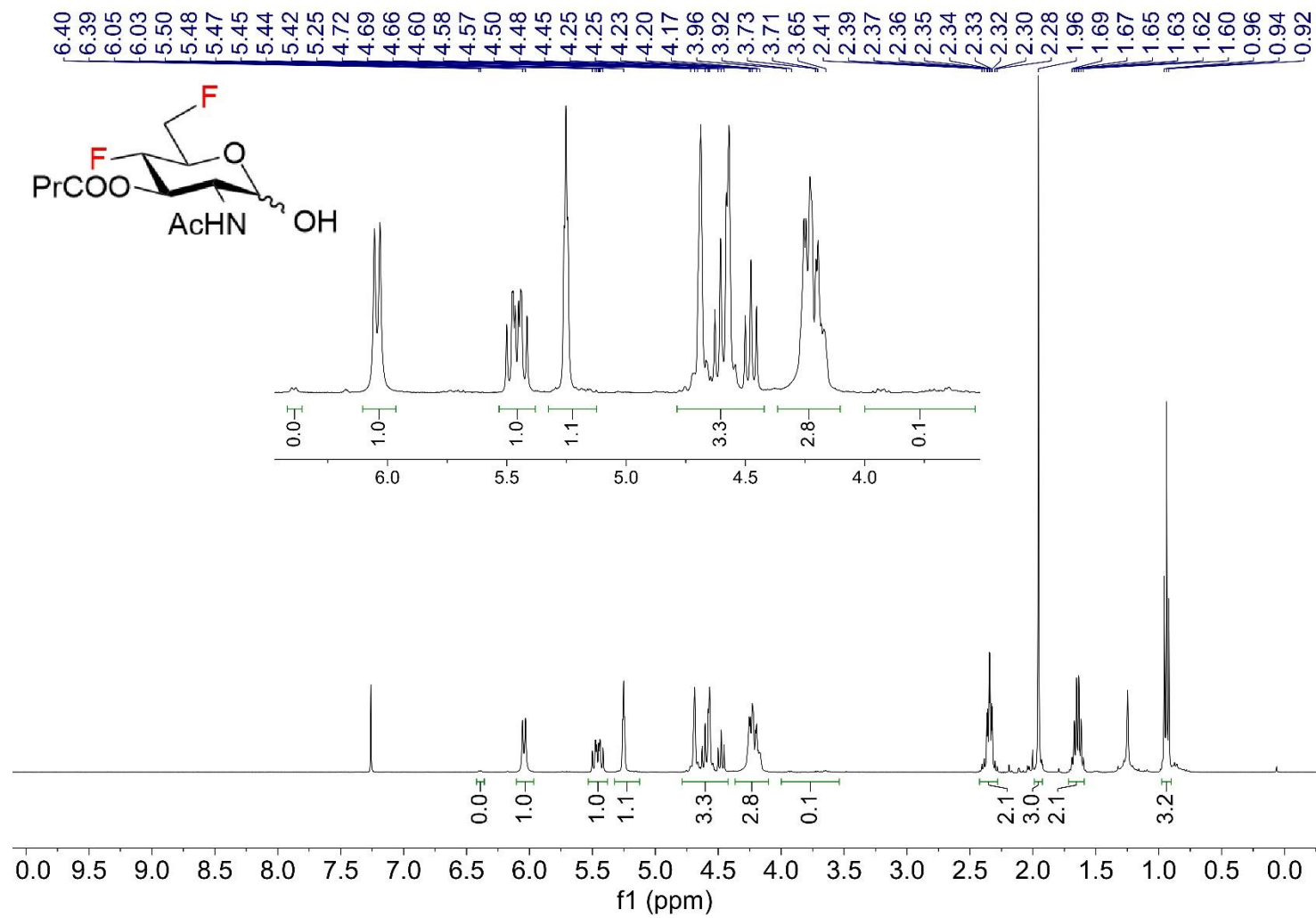


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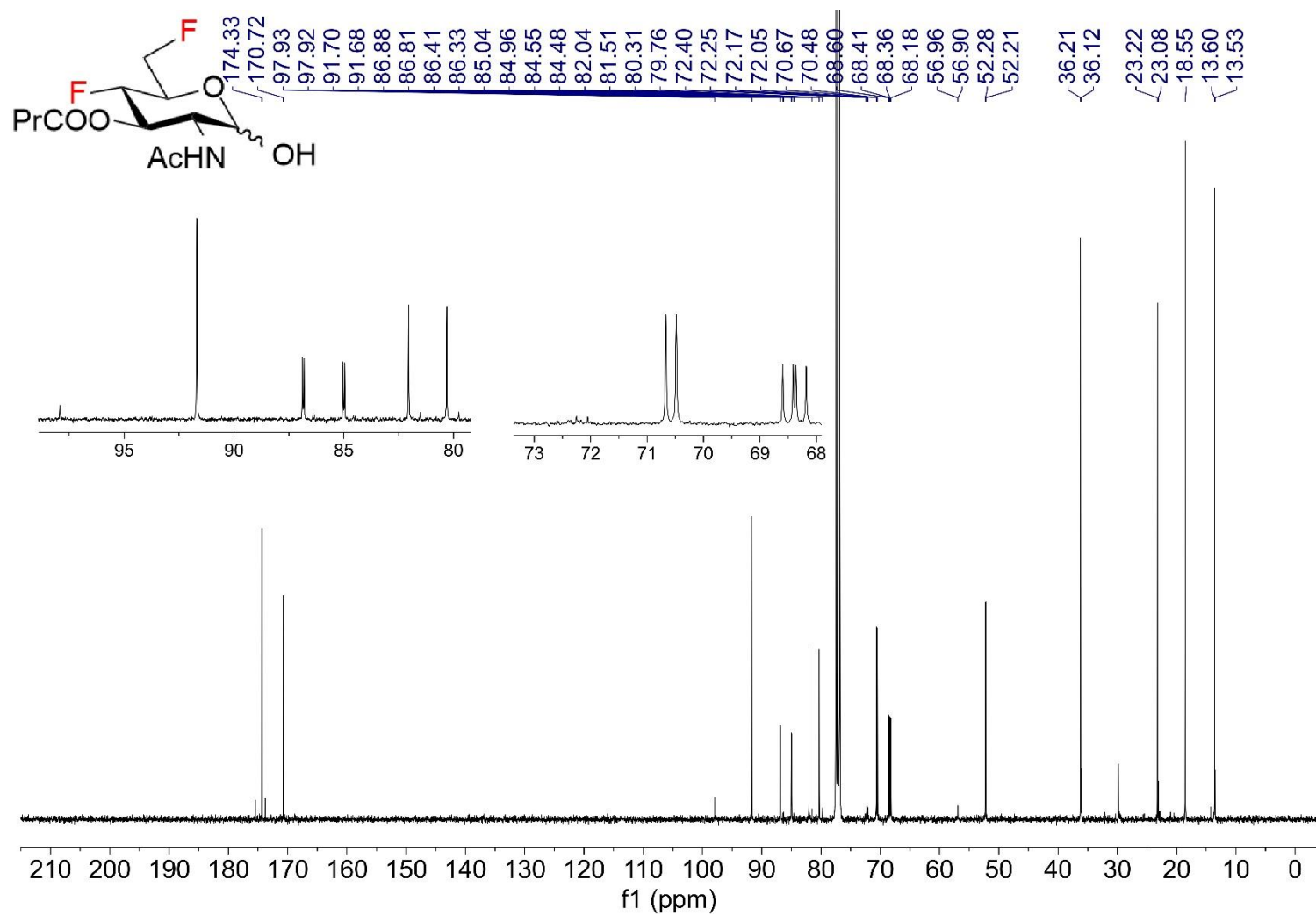


NMR COMPOUND 22

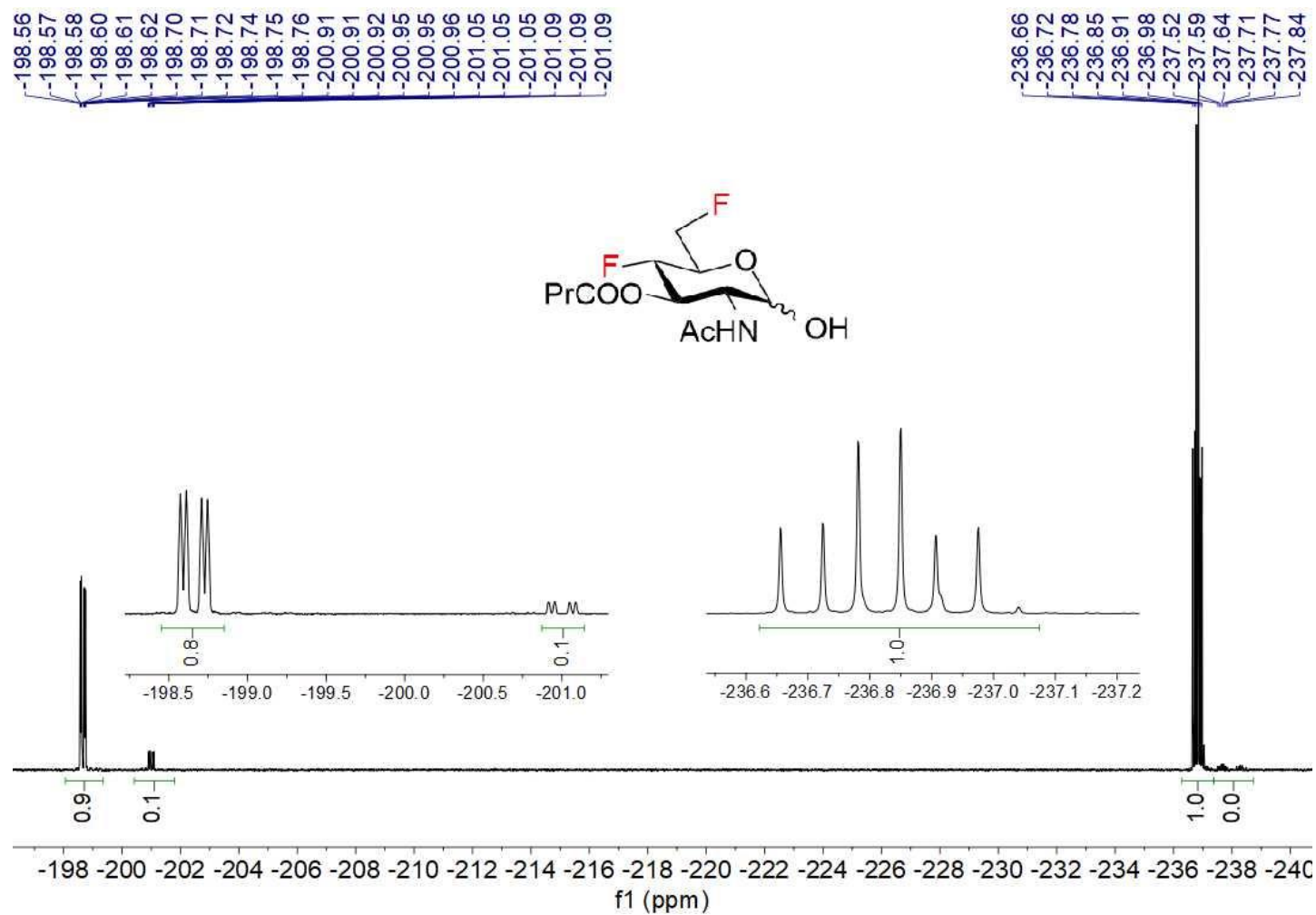
^1H NMR (400 MHz, CDCl_3) 22



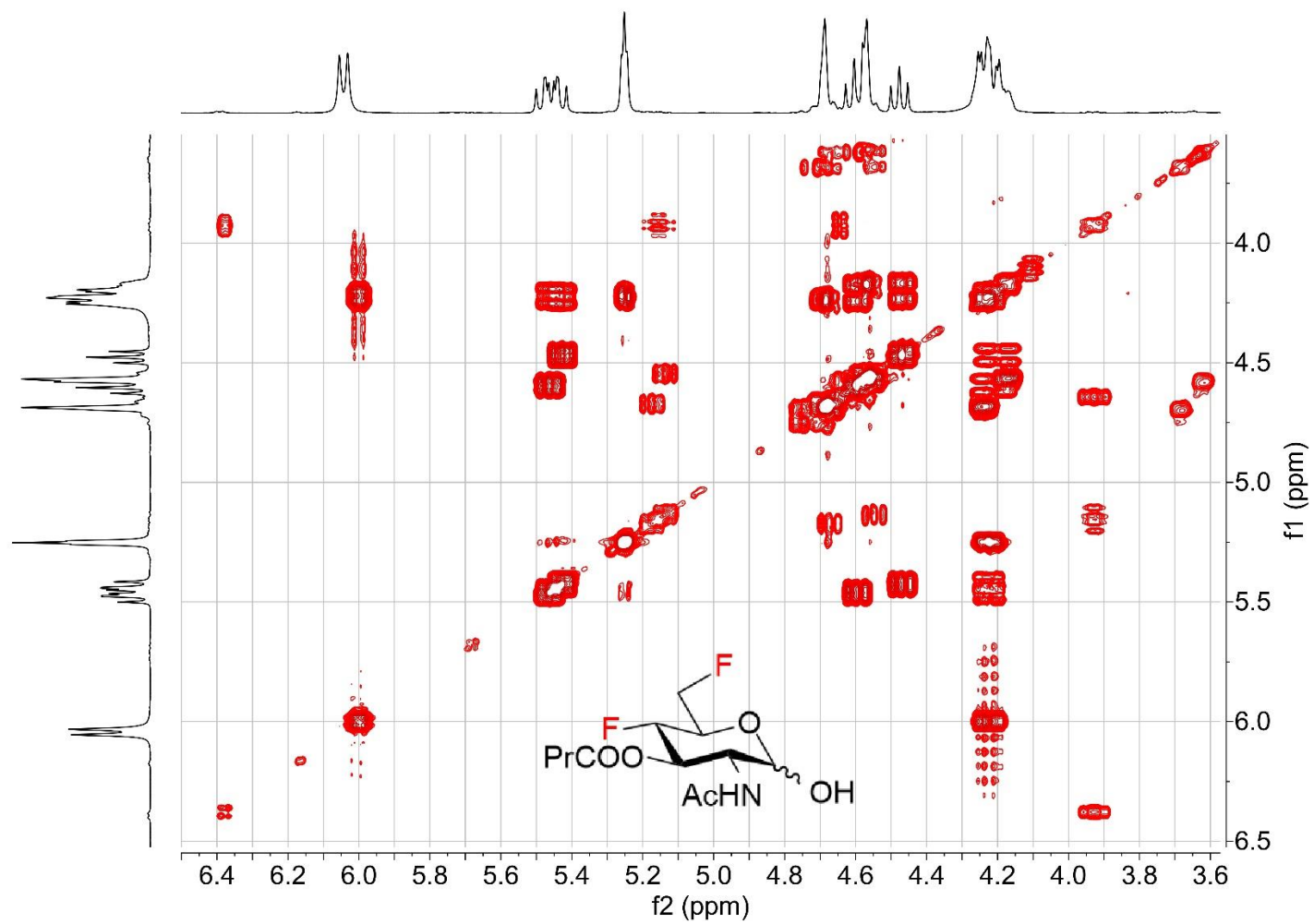
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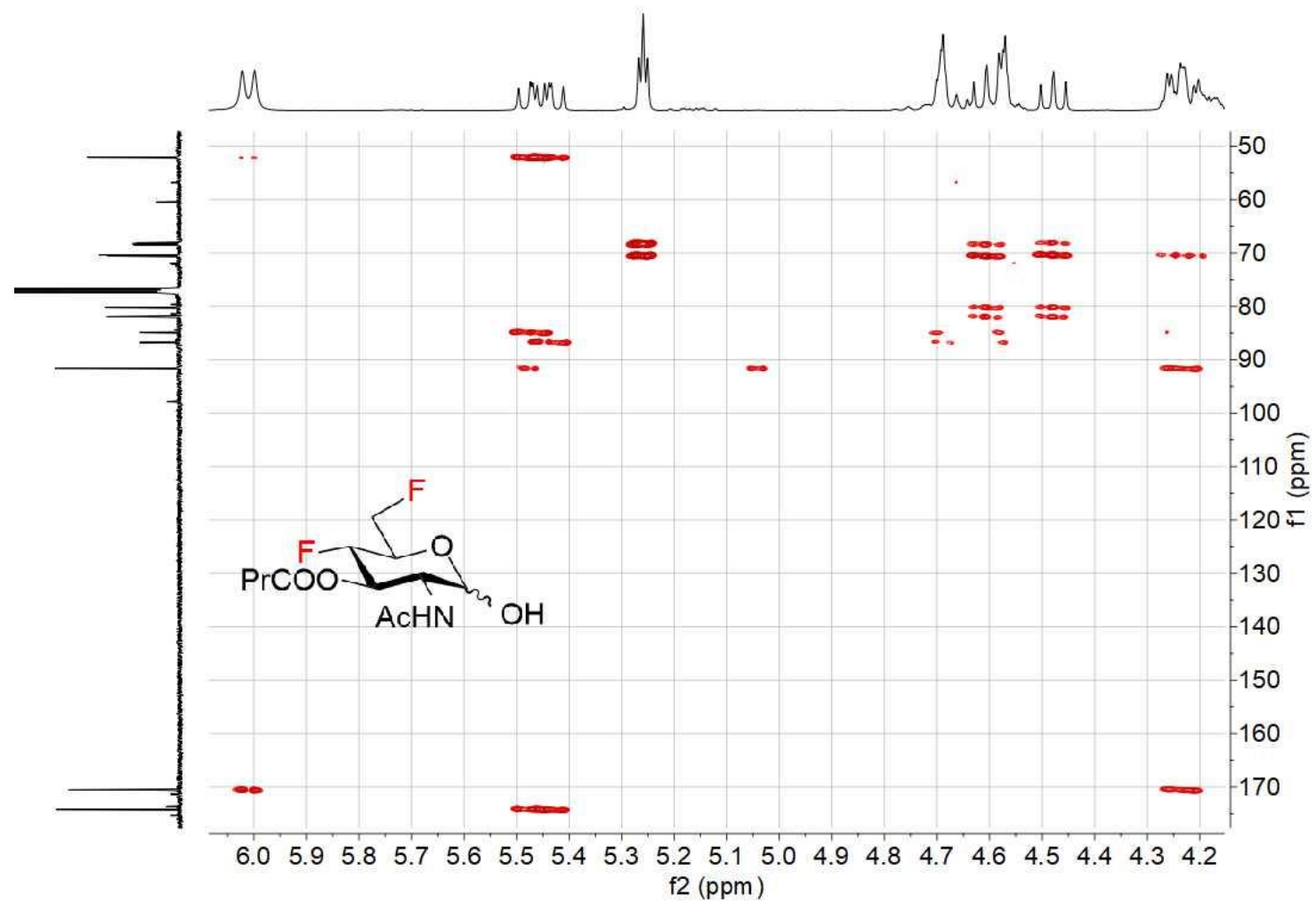
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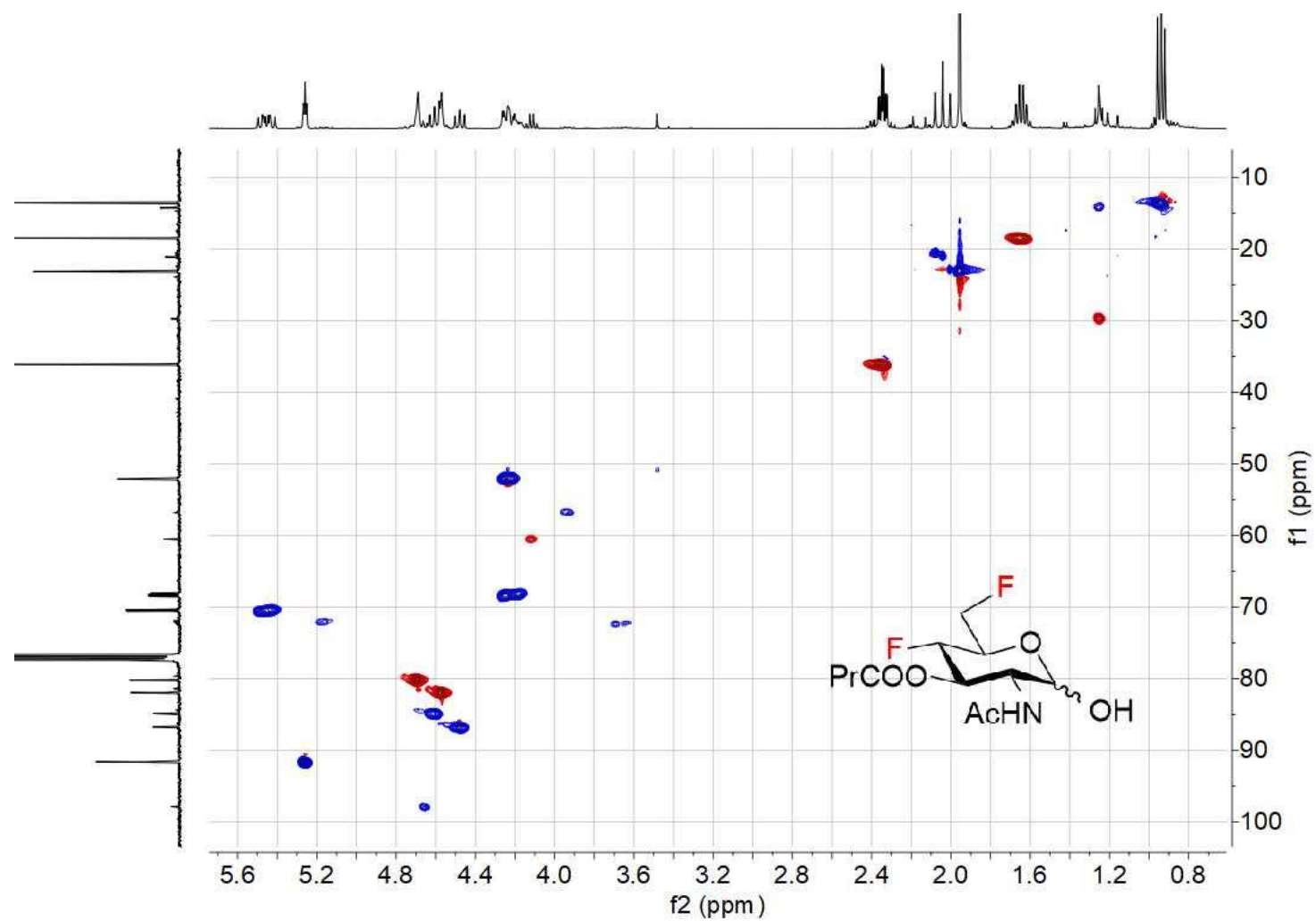
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^1H - ^{13}C HMBC 22

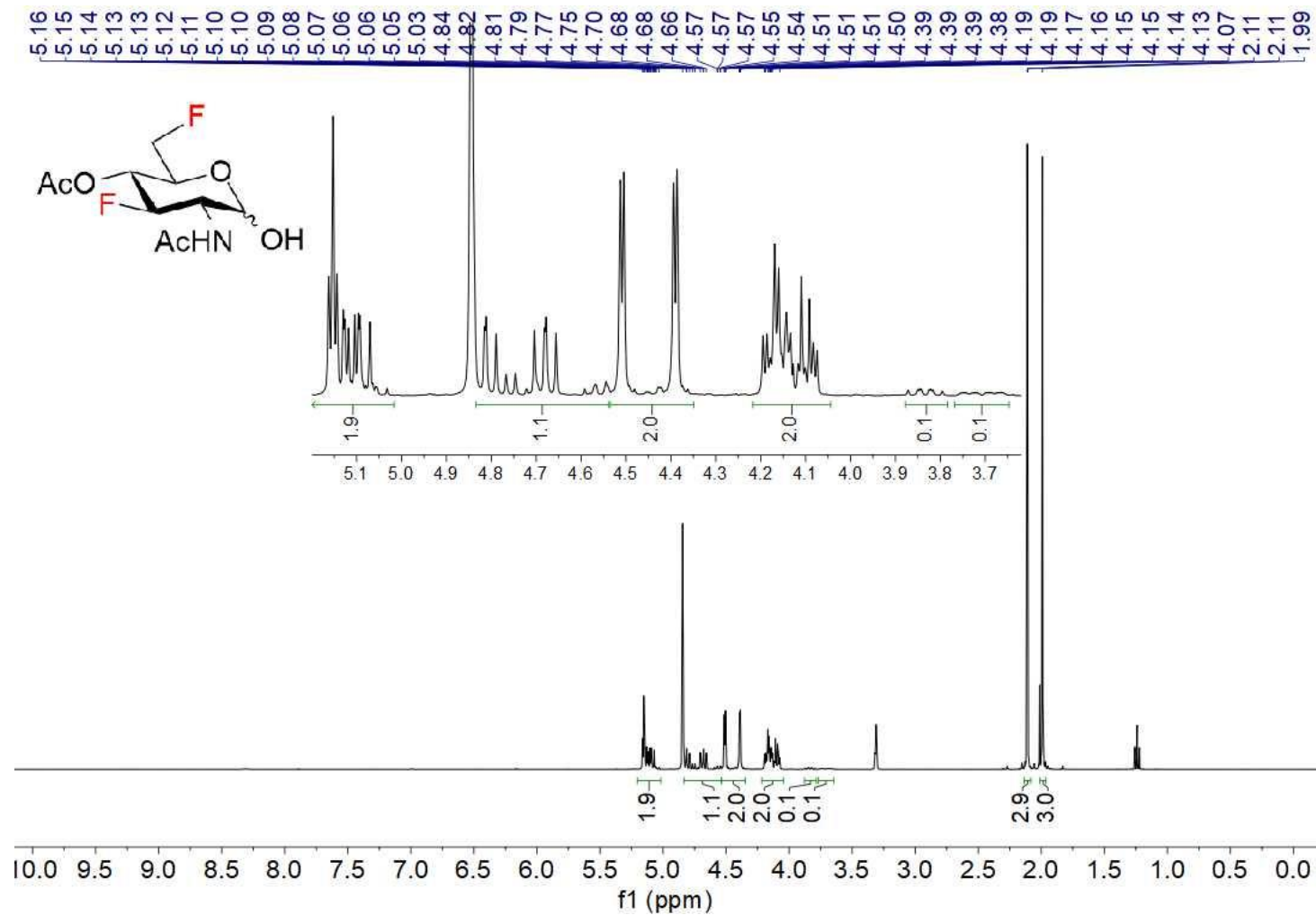


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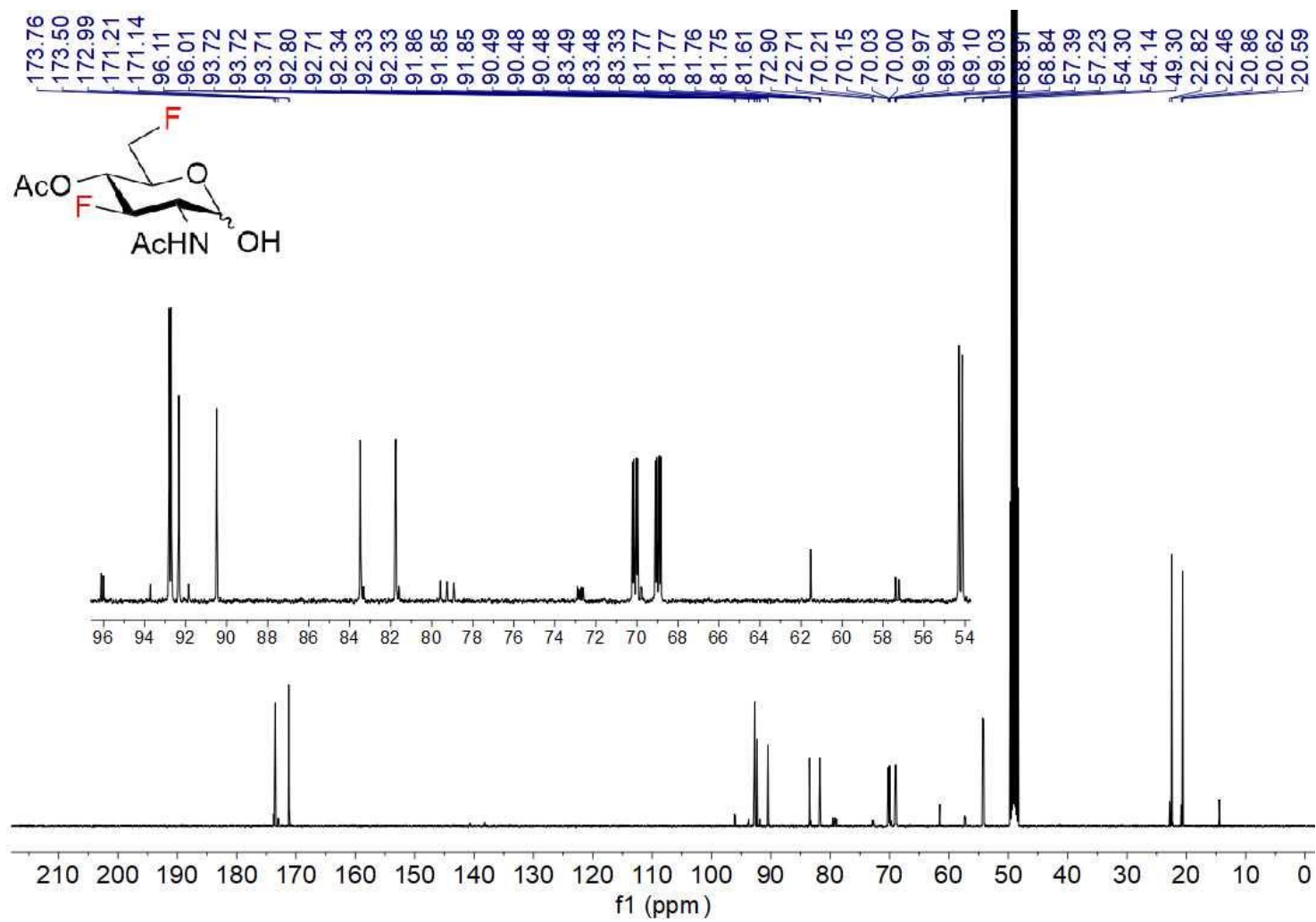


NMR COMPOUND 23

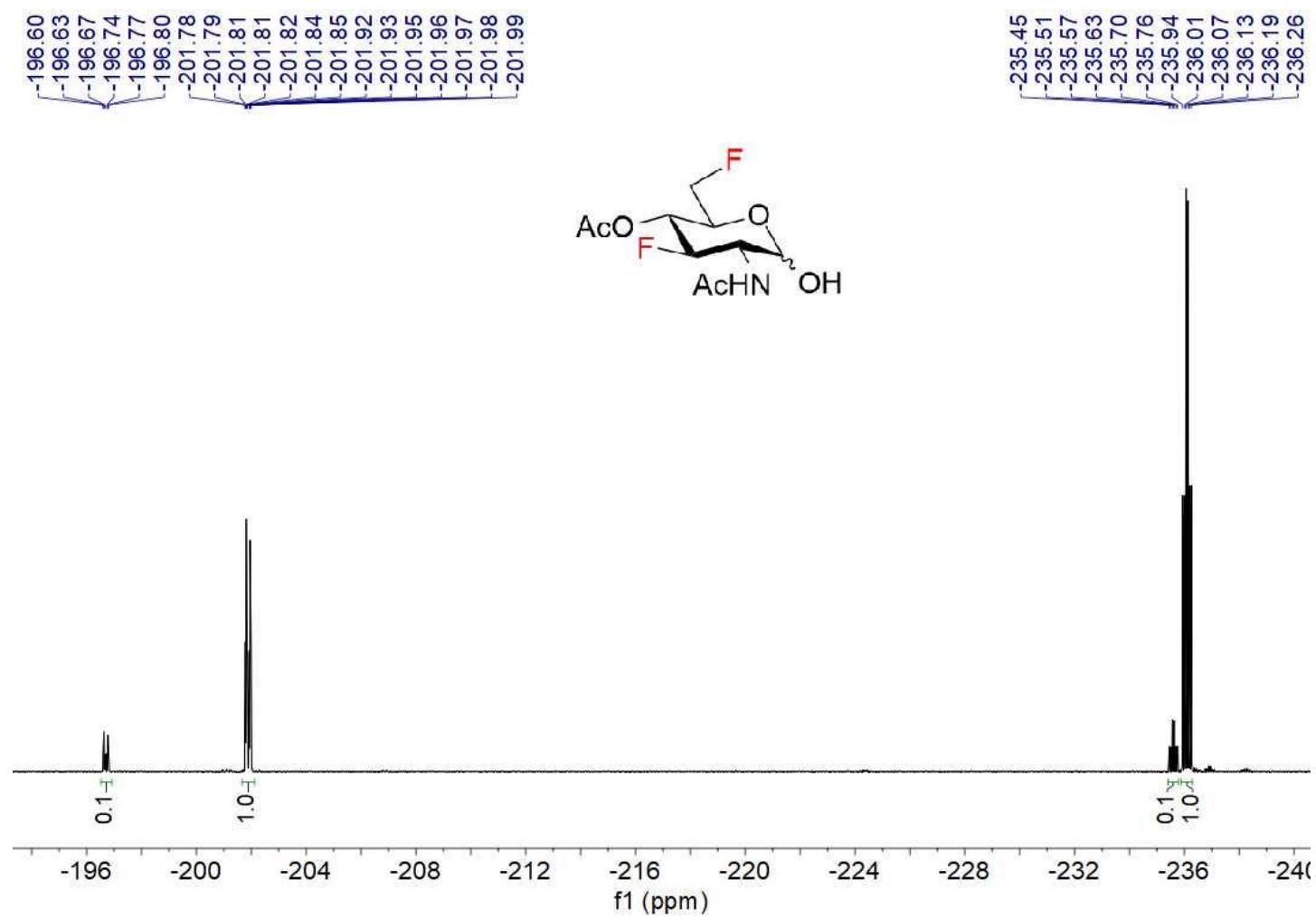
^1H NMR (400 MHz, CD_3OD) 23



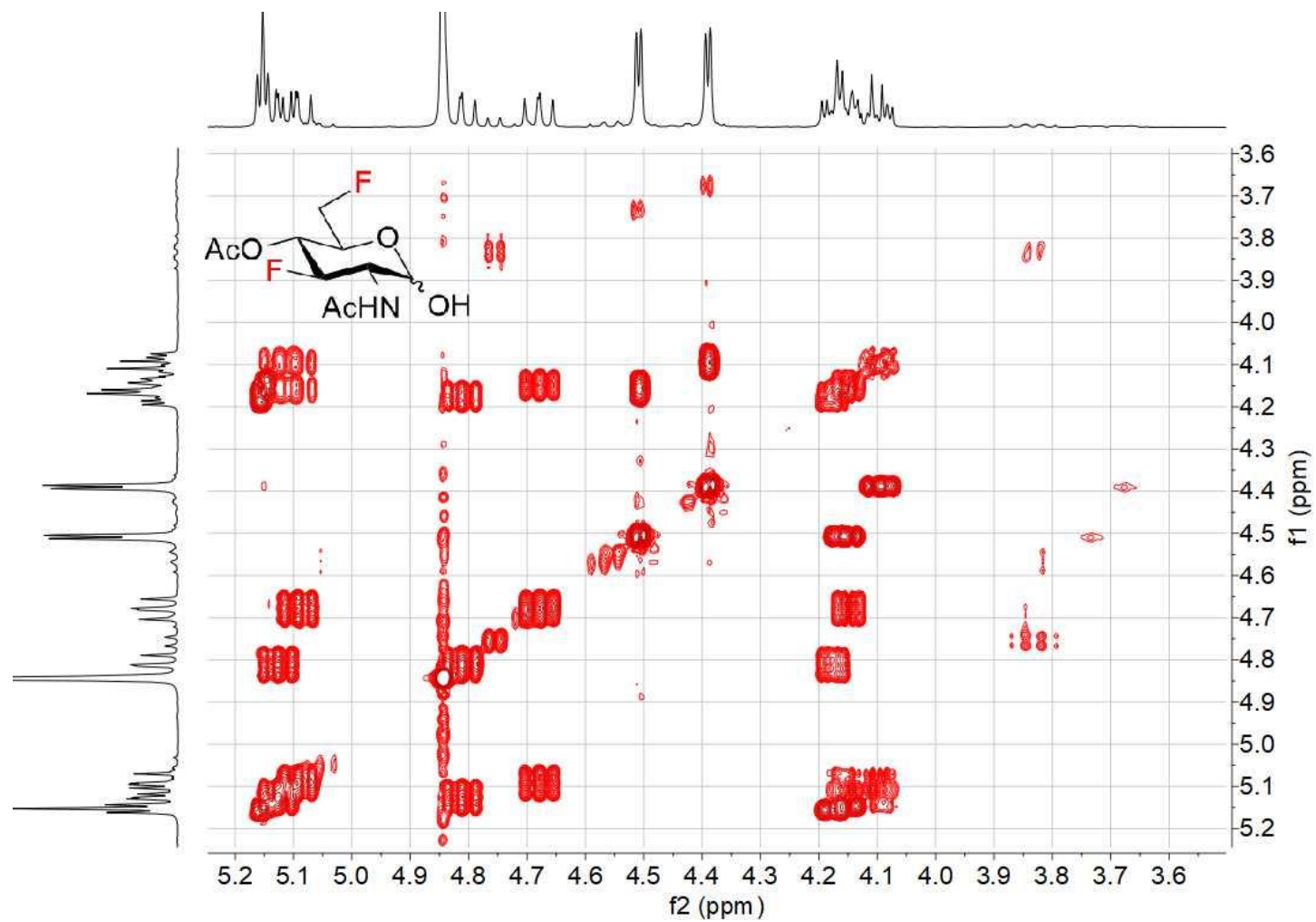
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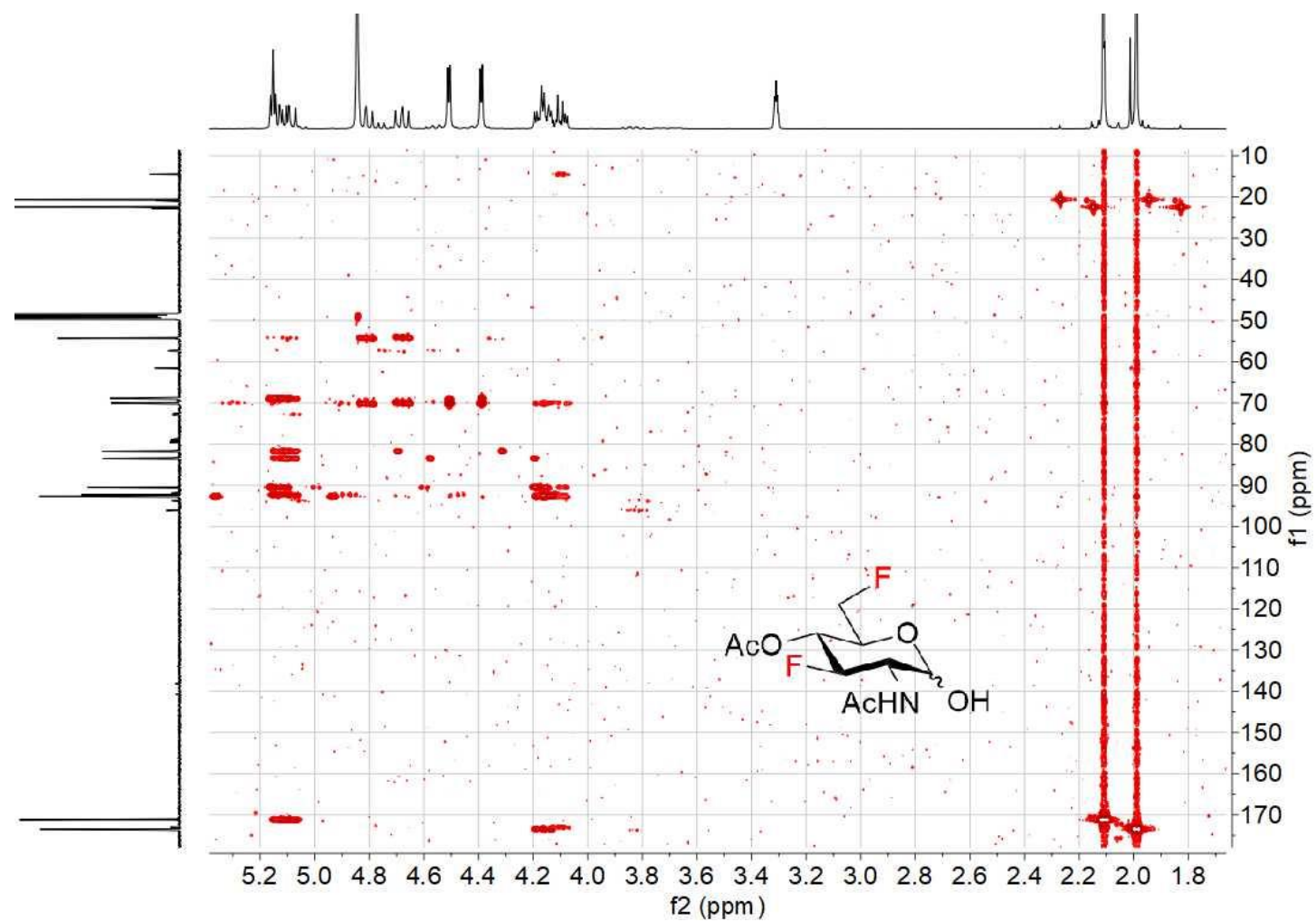
¹⁹F NMR (376 MHz, CD₃OD) 23



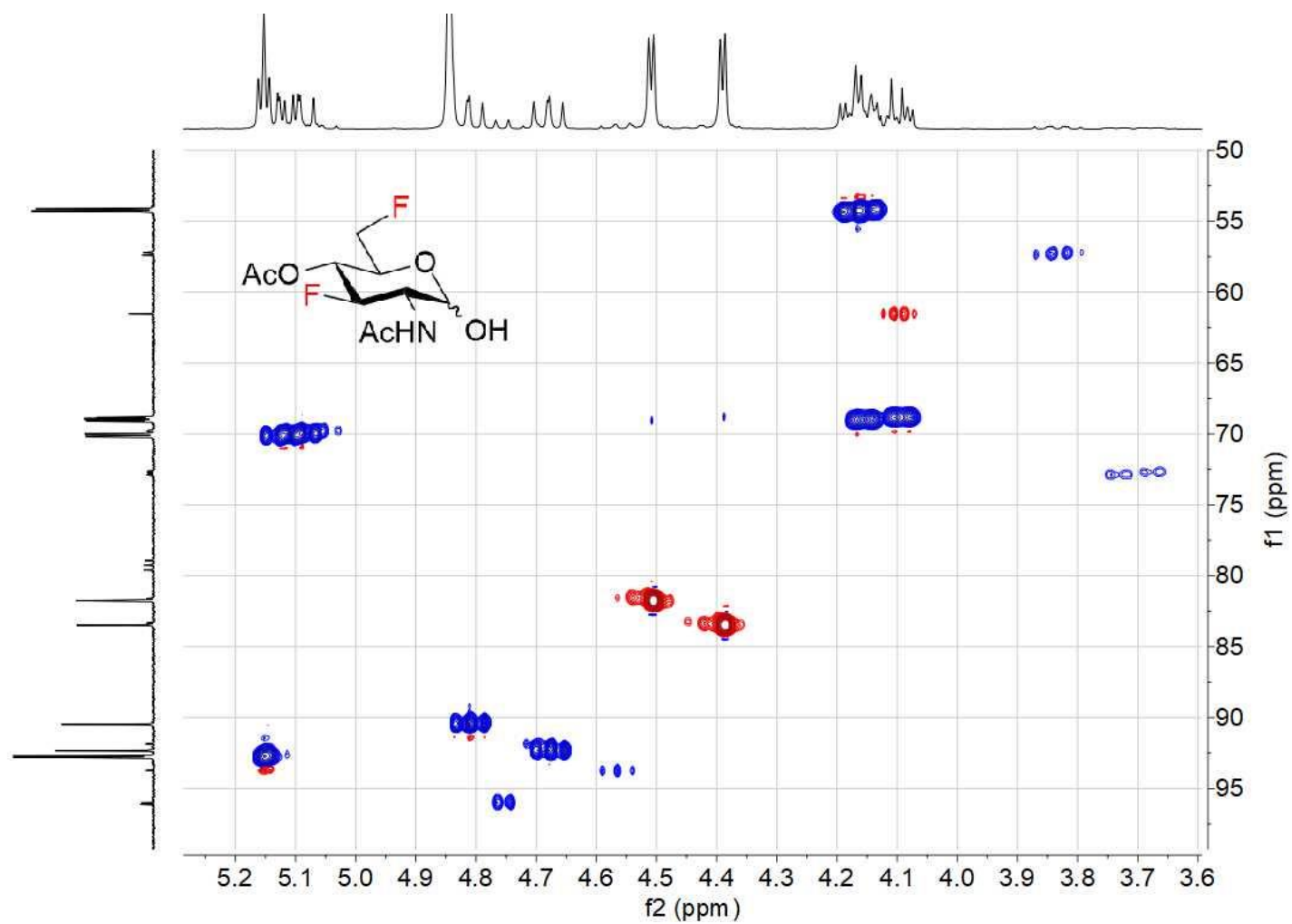
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^1H - ^{13}C HMBC 23

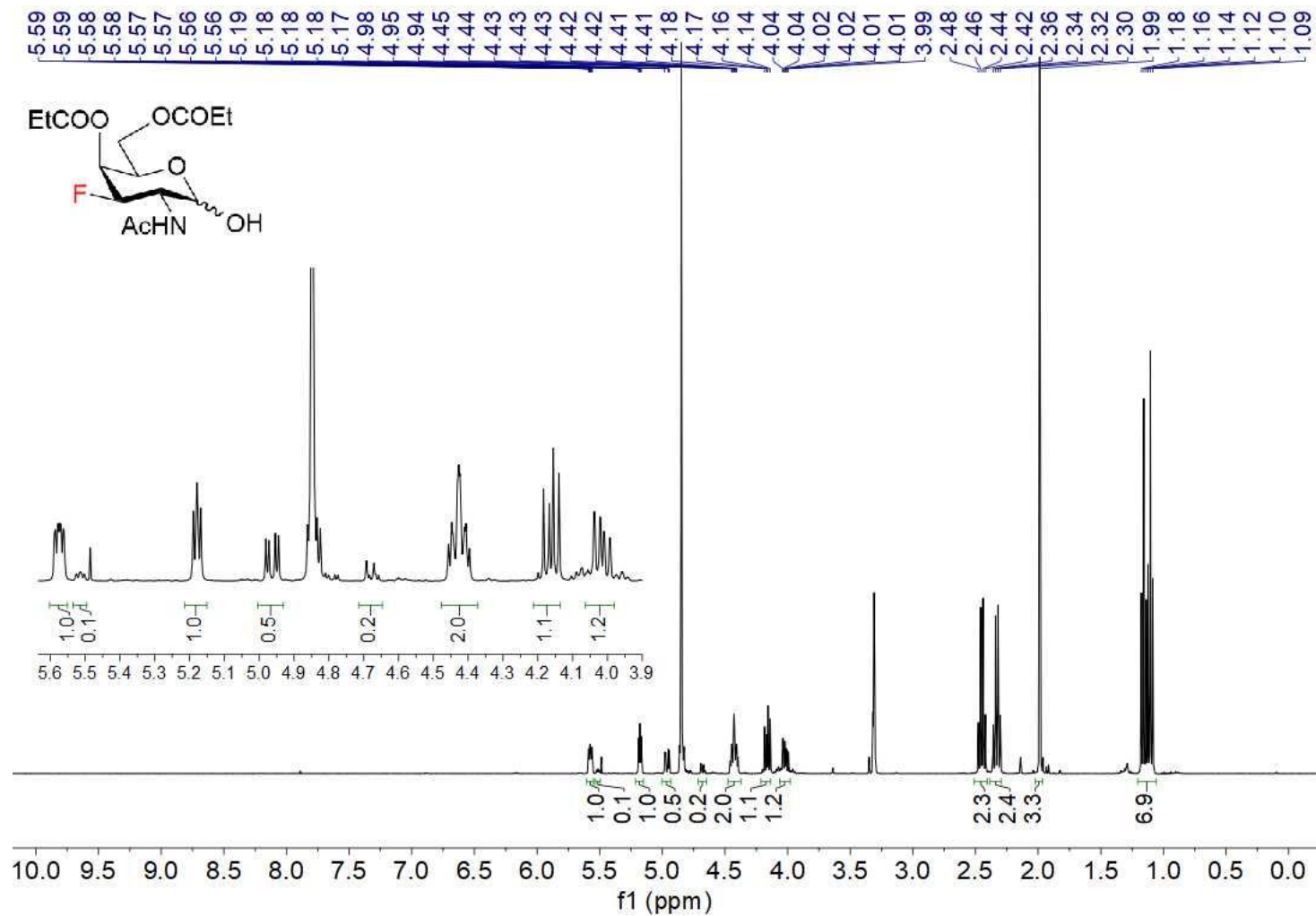


^1H - ^{13}C HSQC 23

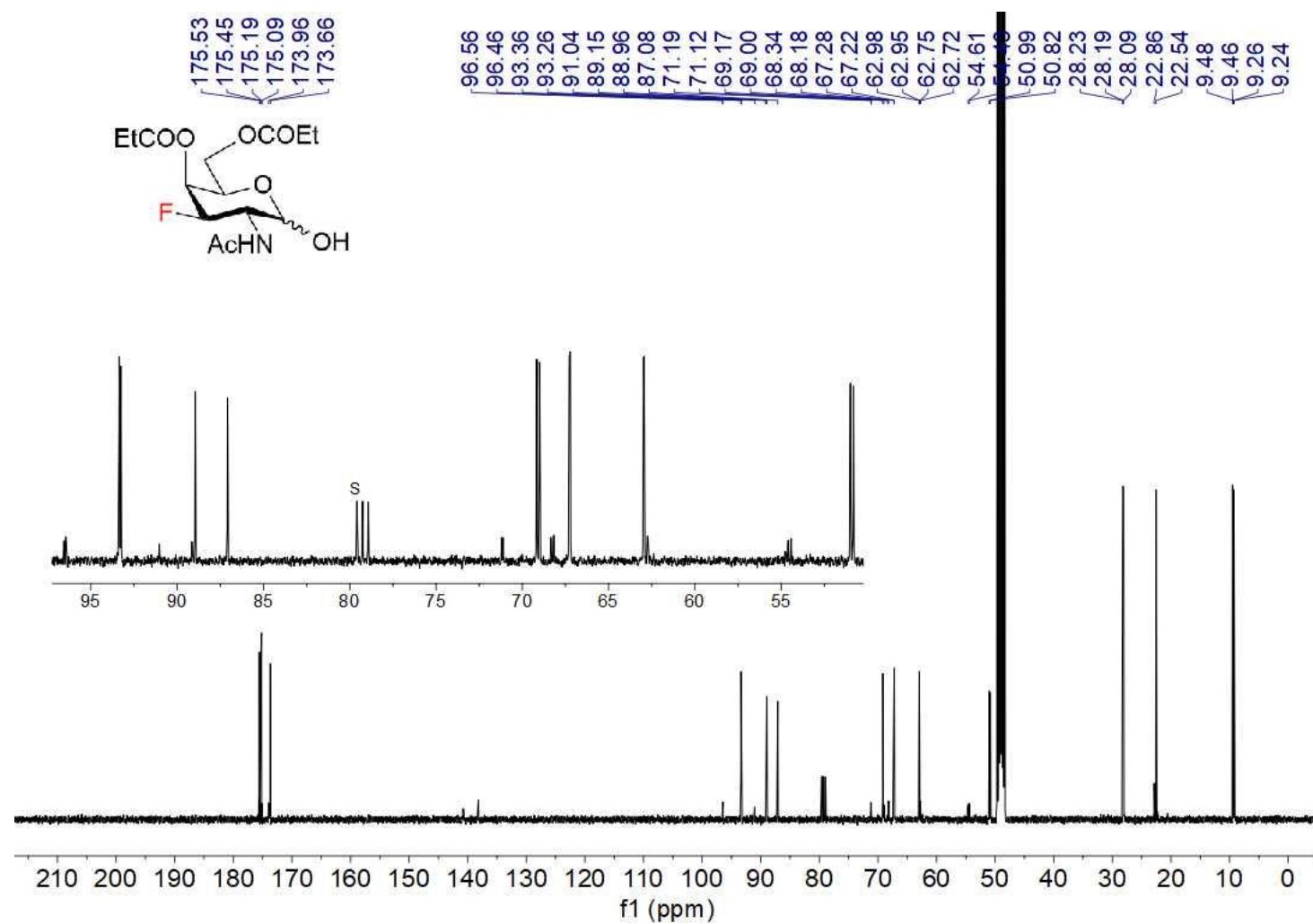


NMR COMPOUND 25

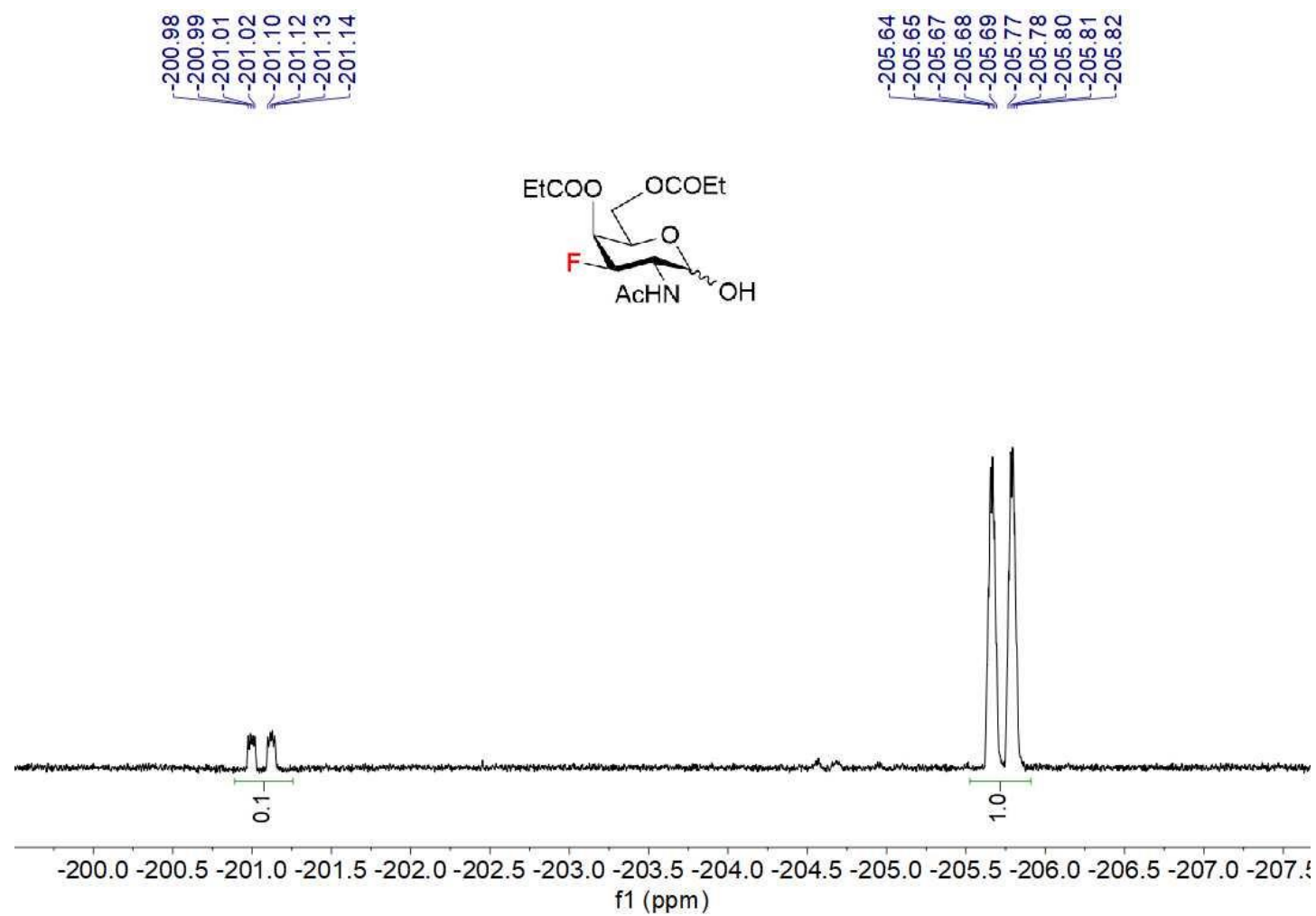
¹H NMR (400 MHz, CD₃OD) 25



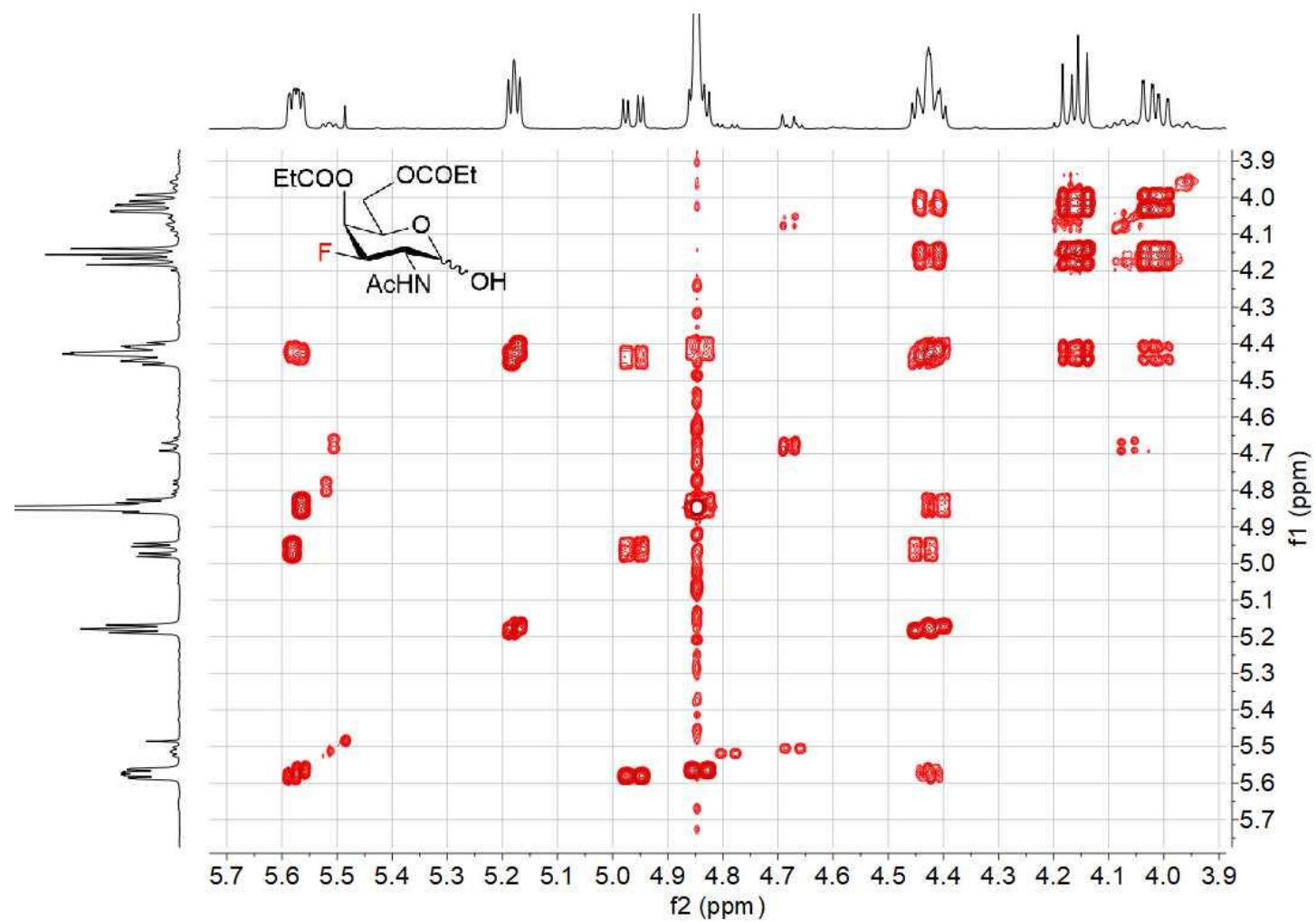
^{13}C NMR (100 MHz, CD_3OD) 25



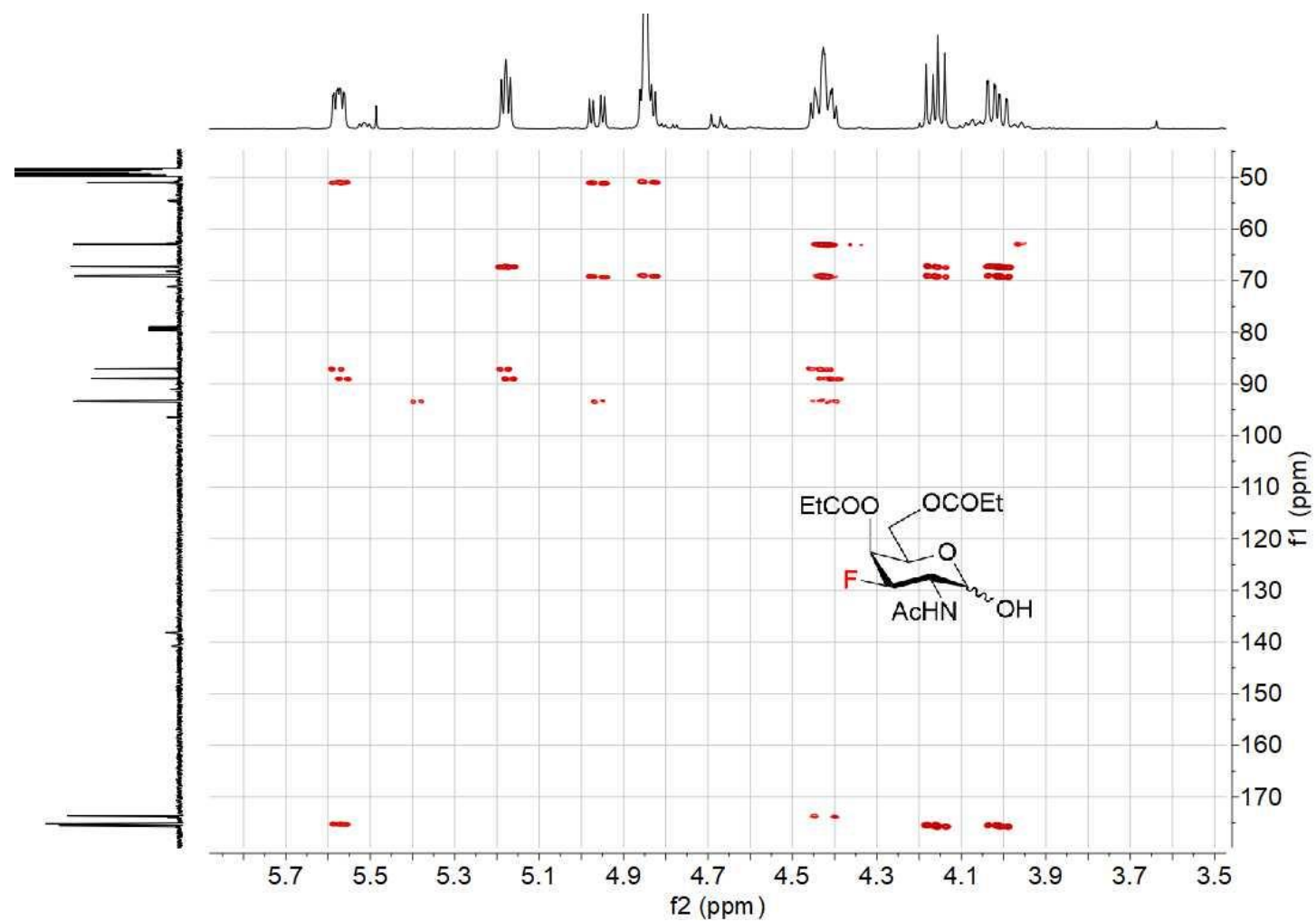
^{19}F NMR (376 MHz, CD_3OD) 25



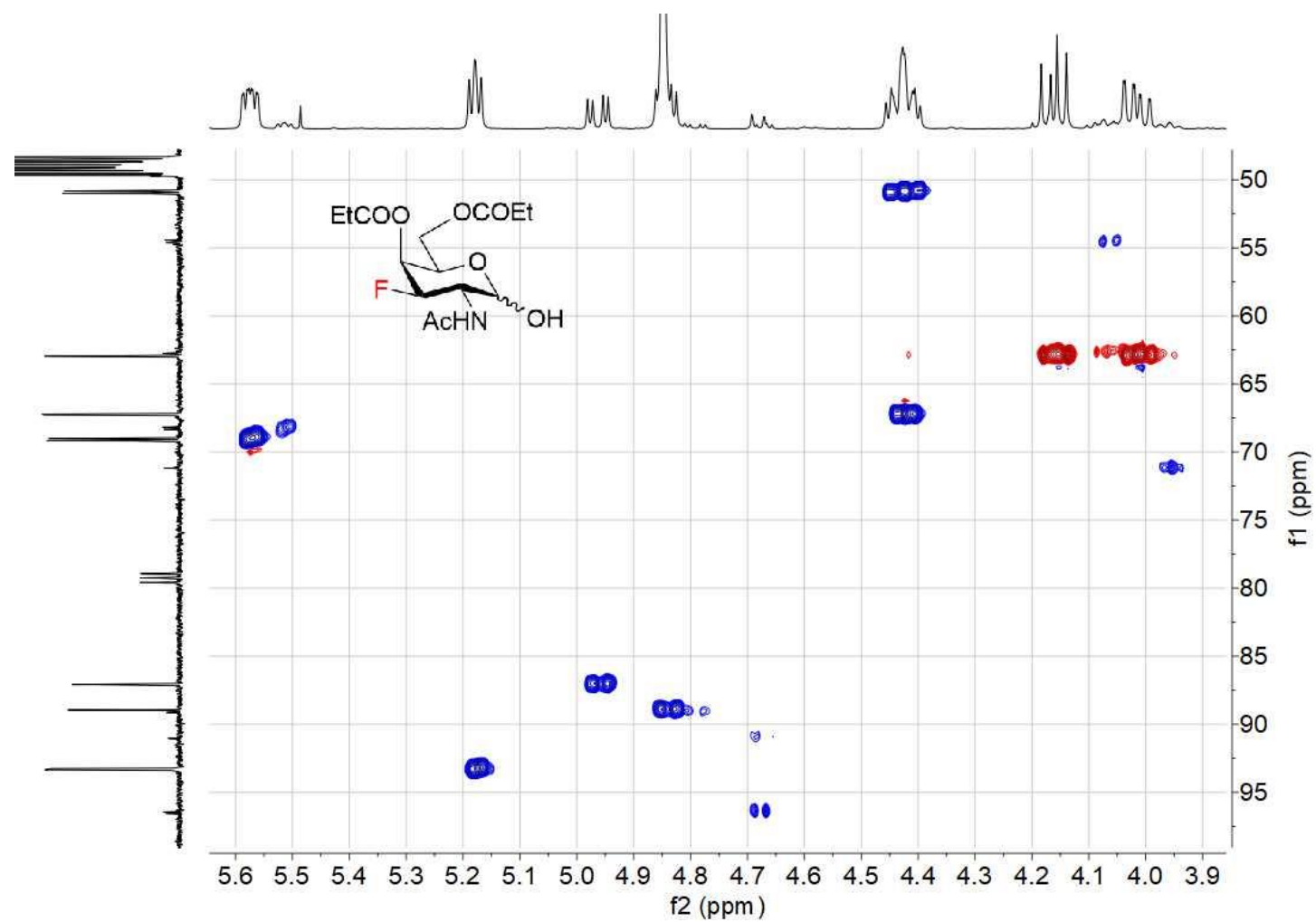
^1H - ^1H COSY 25



^1H - ^{13}C HMBC 25

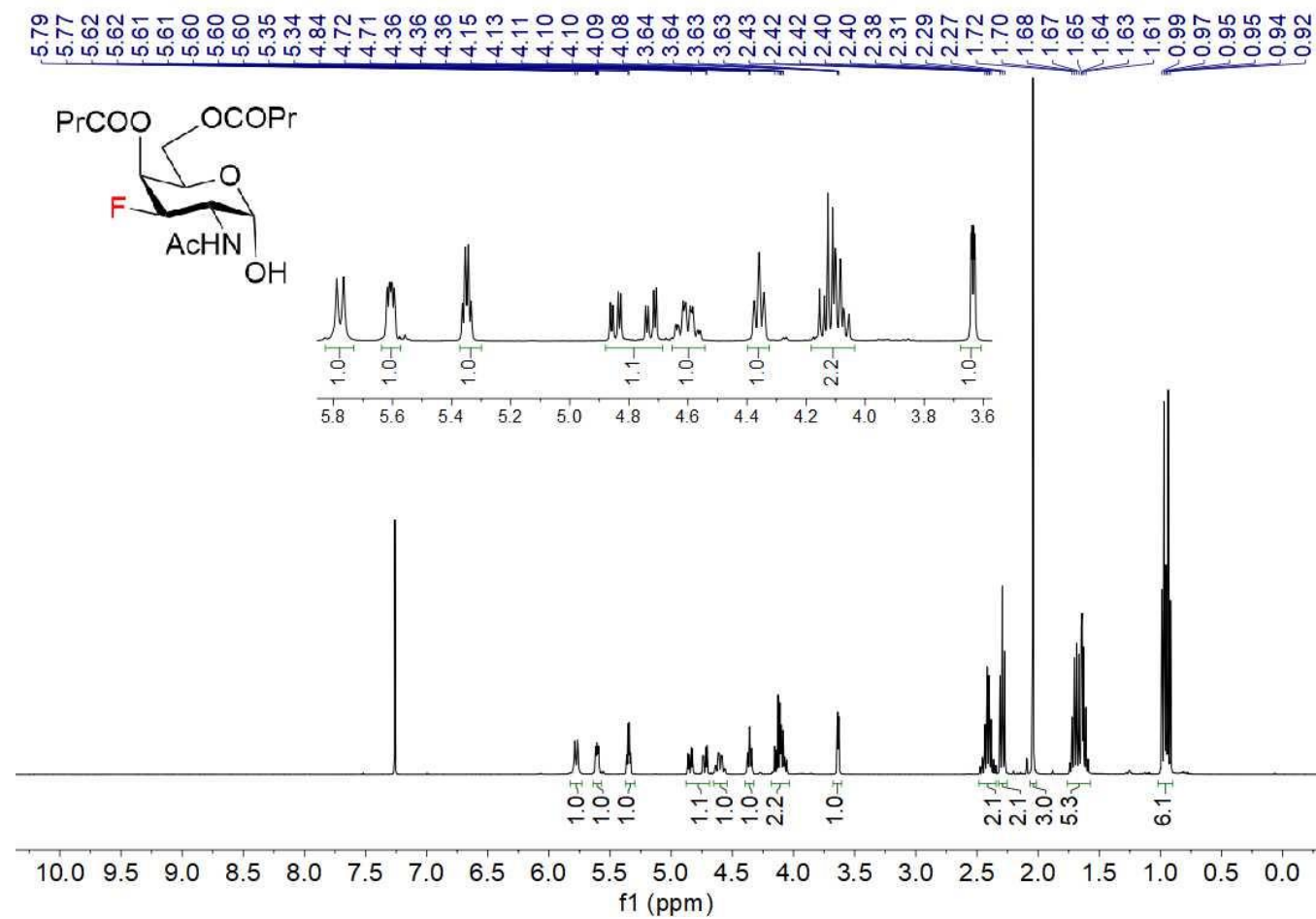


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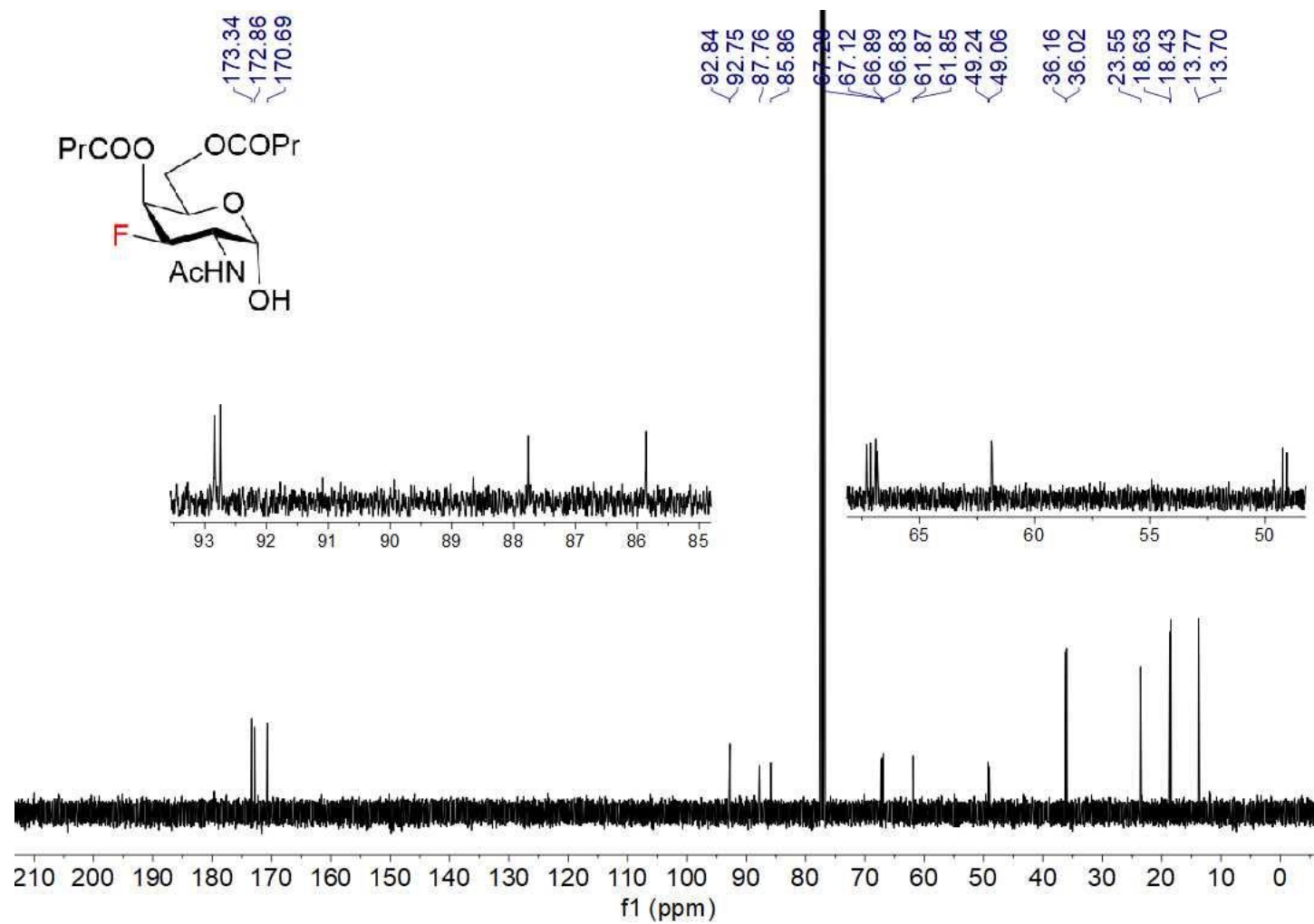


NMR COMPOUND 26

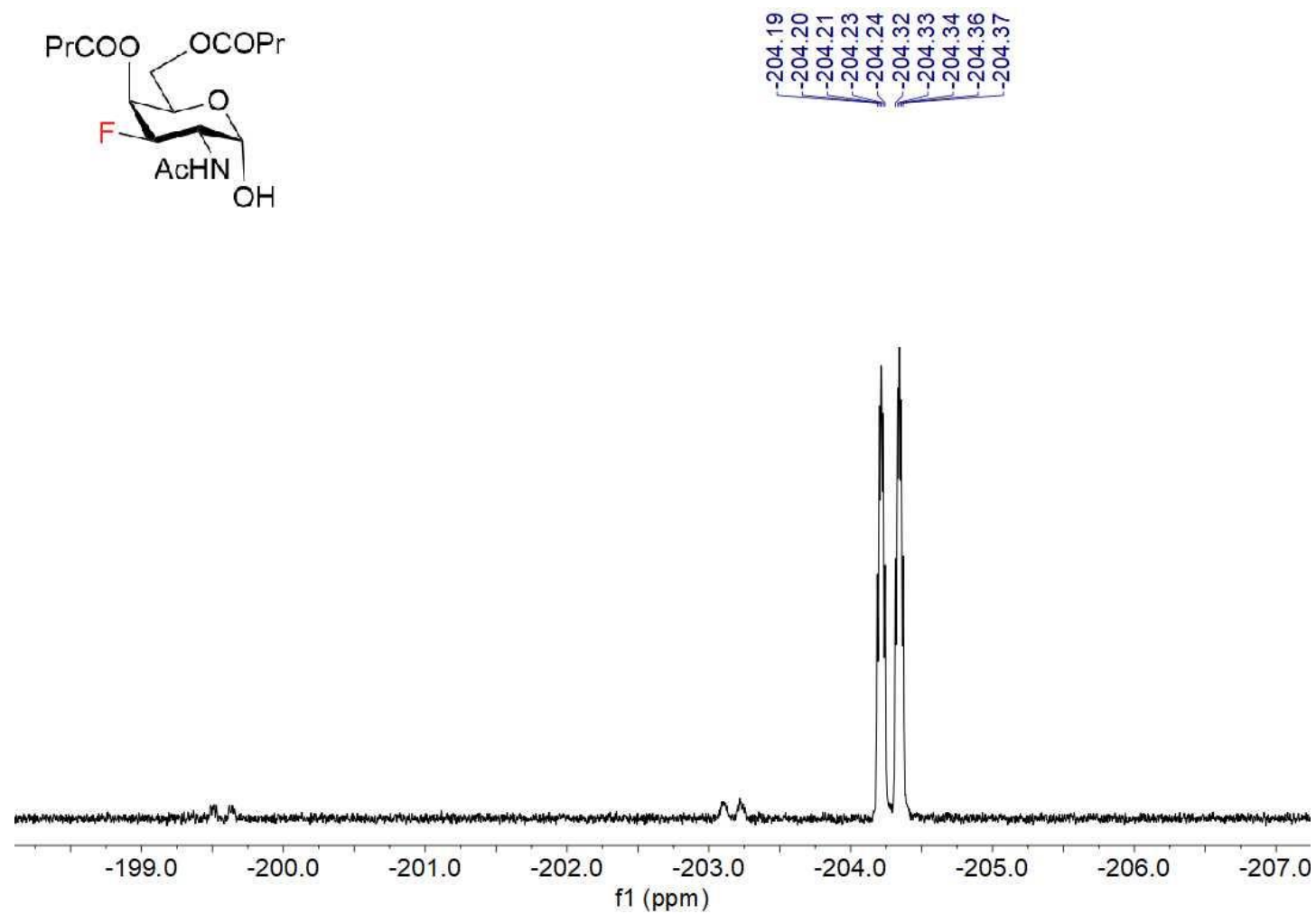
^1H NMR (400 MHz, CDCl_3) 26



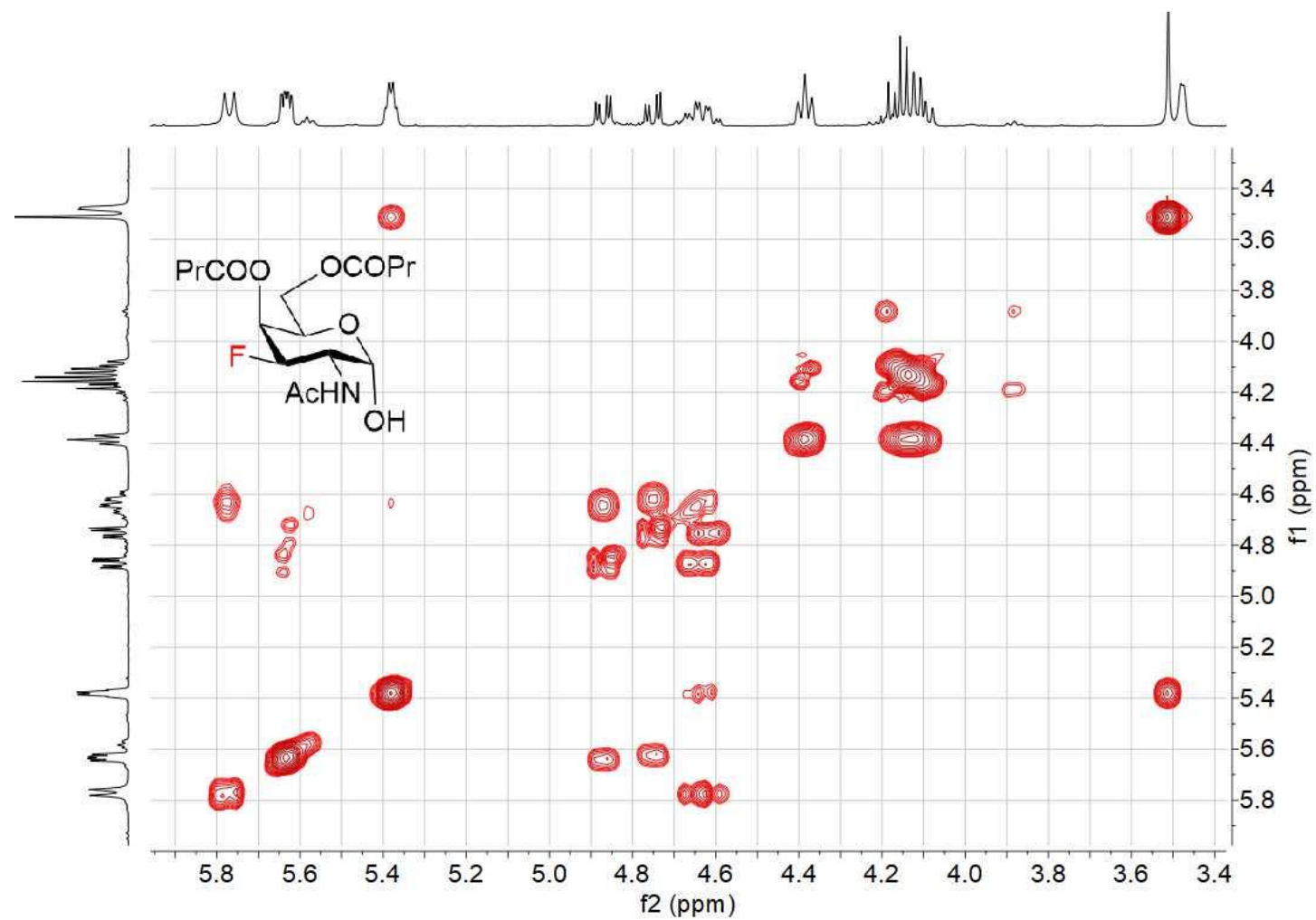
^{13}C NMR (100 MHz, CDCl_3) 26



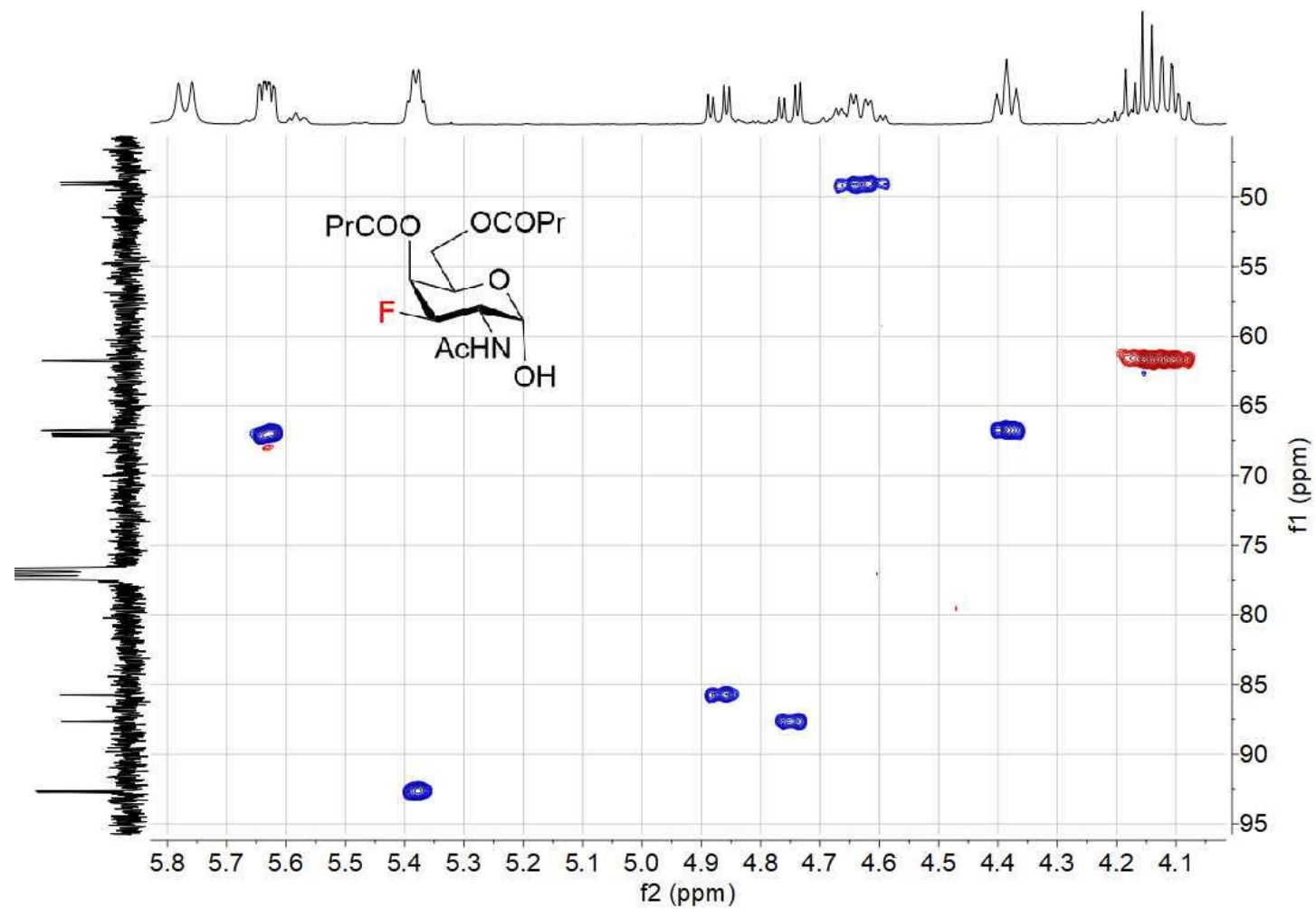
^{19}F NMR (376 MHz, CDCl_3) 26



^1H - ^1H COSY 26

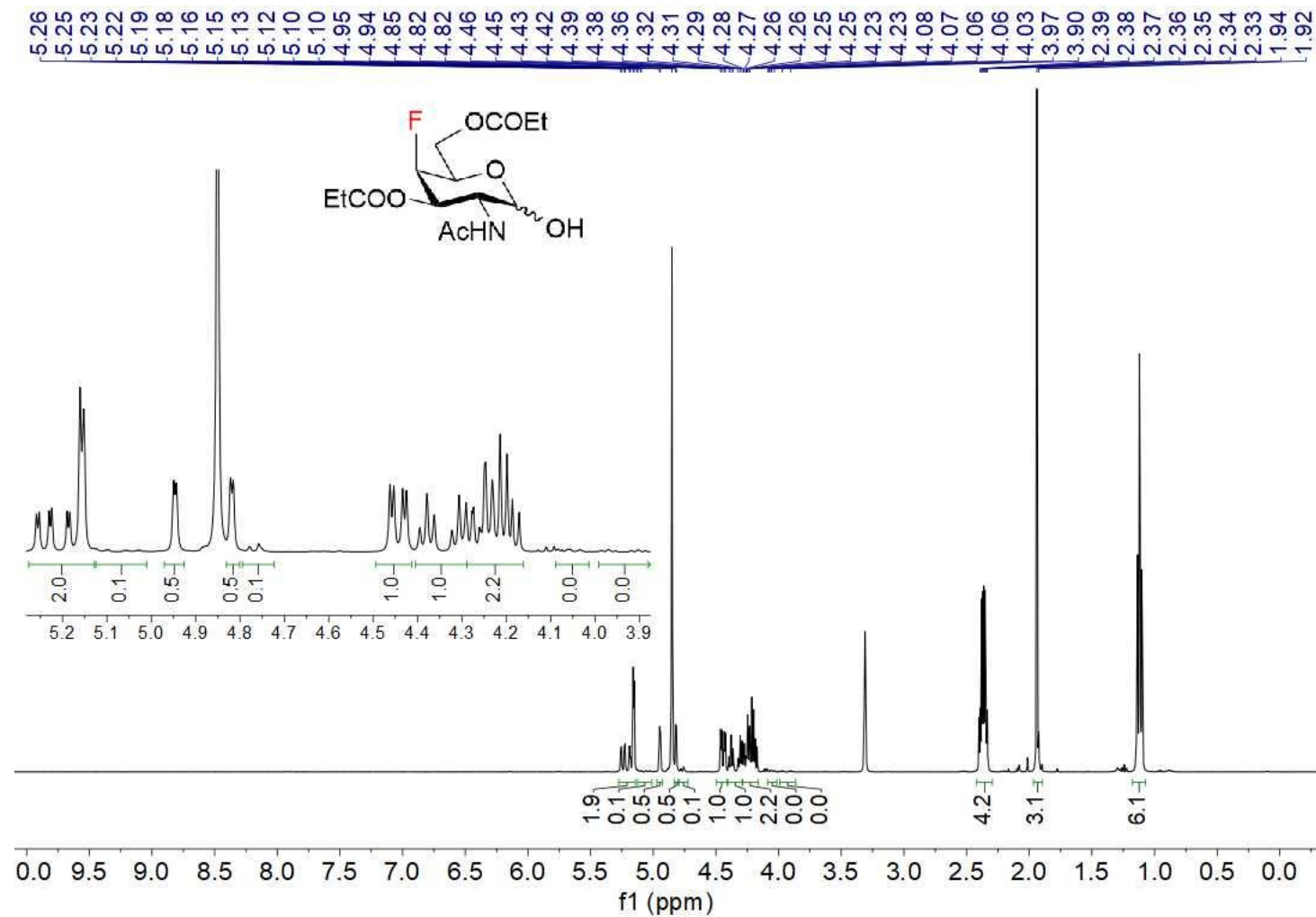


^1H - ^{13}C HSQC 26

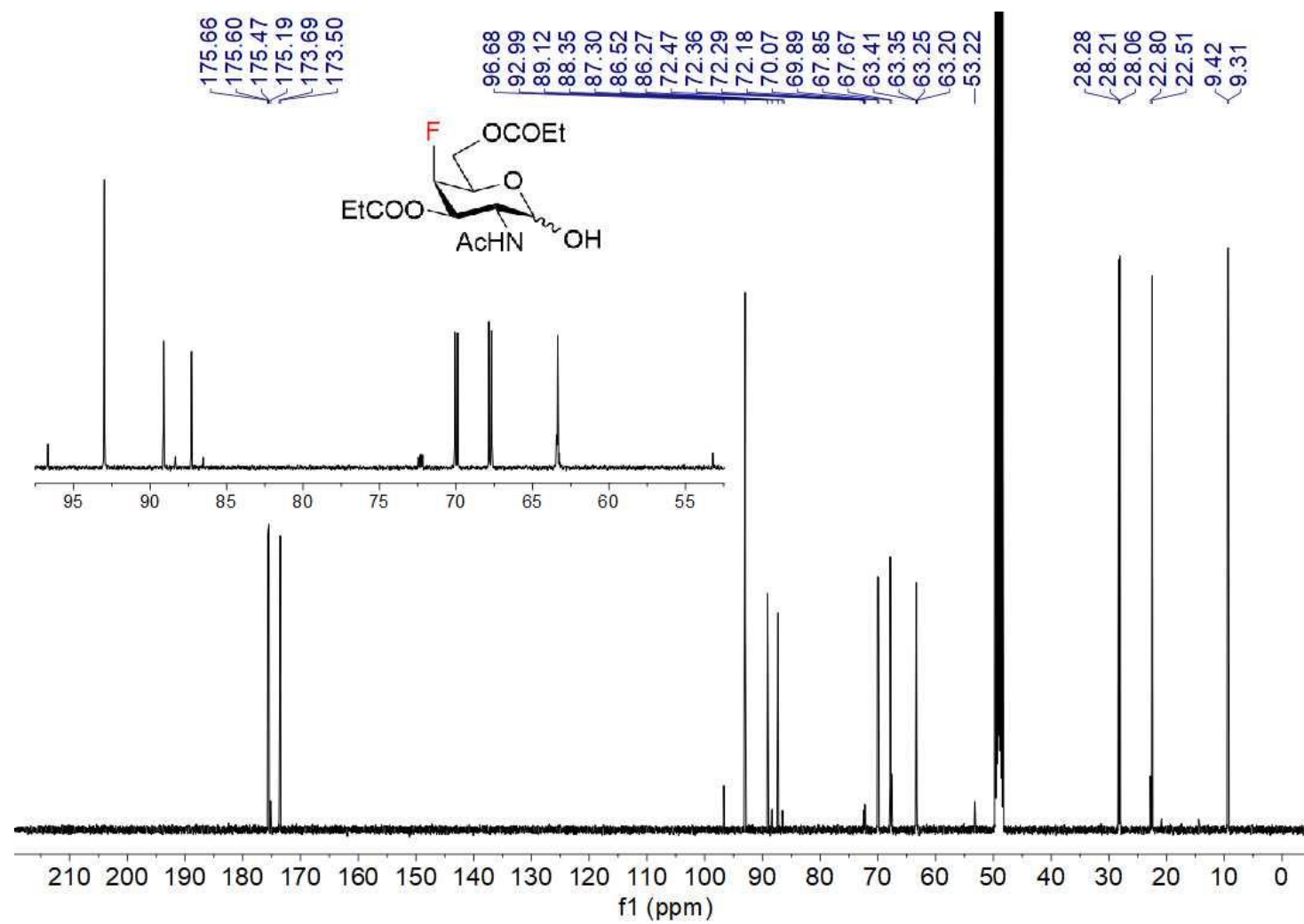


NMR COMPOUND 27

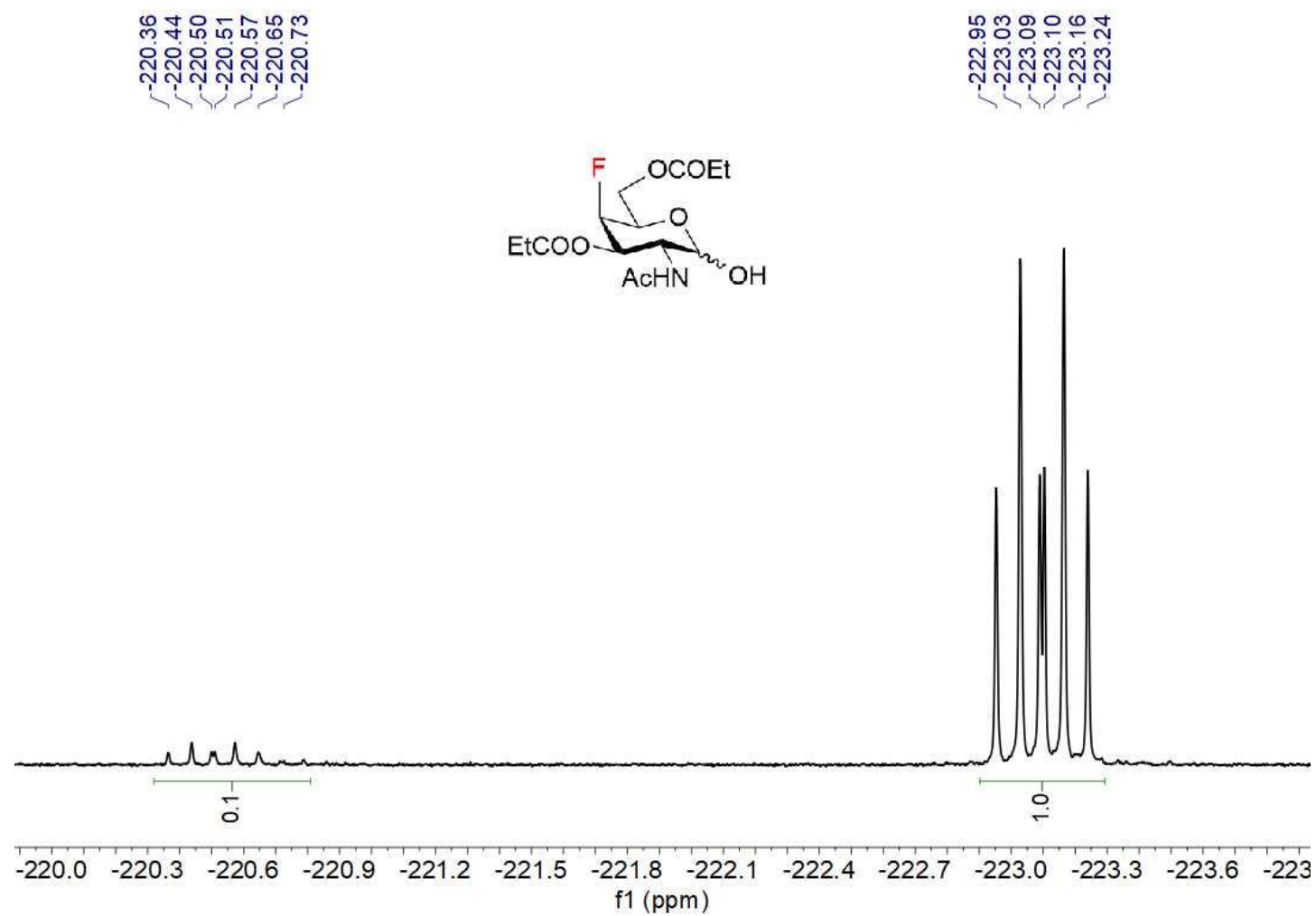
^1H NMR (400 MHz, CD_3OD) 27



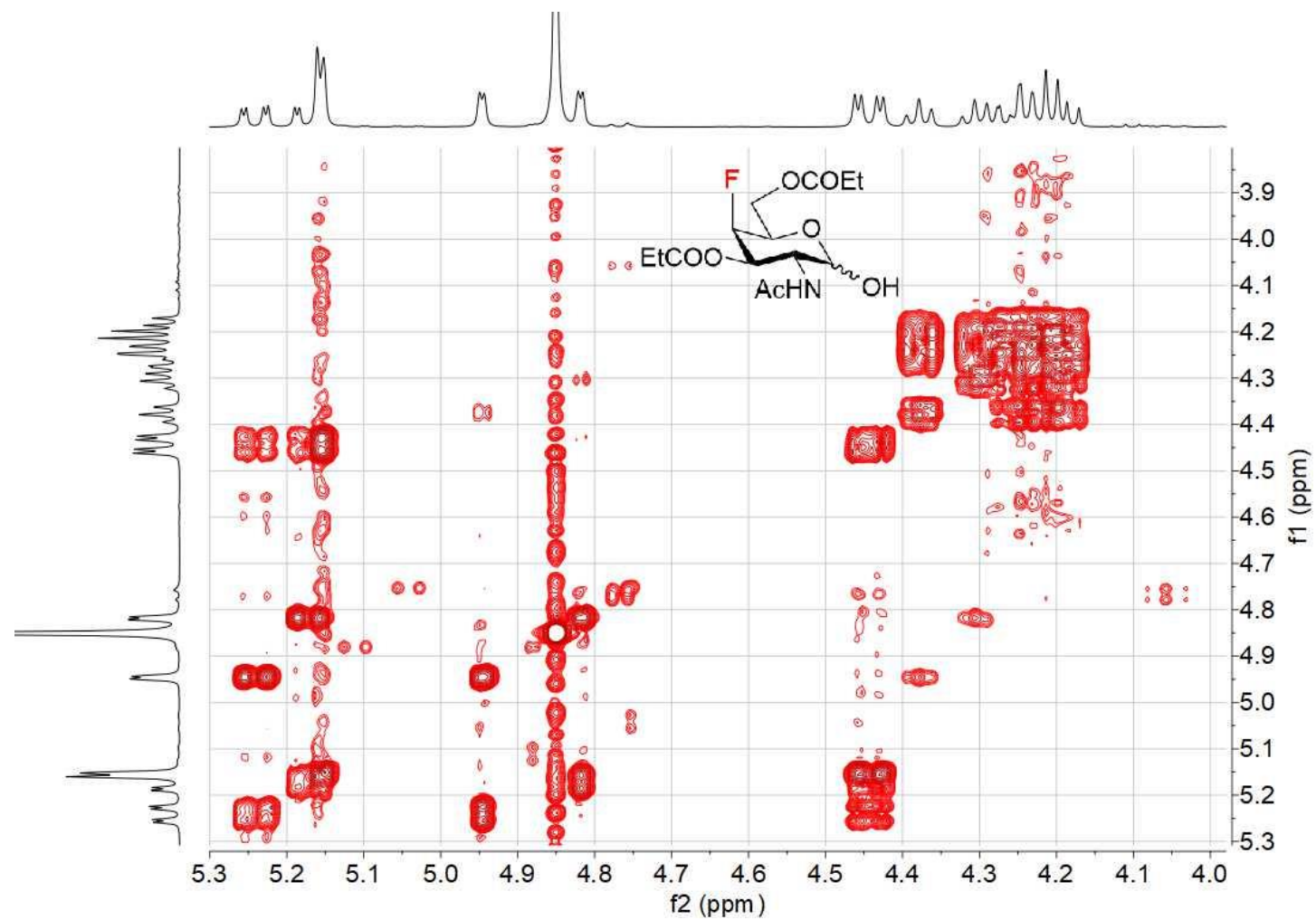
^{13}C NMR (100 MHz, CD_3OD) 27



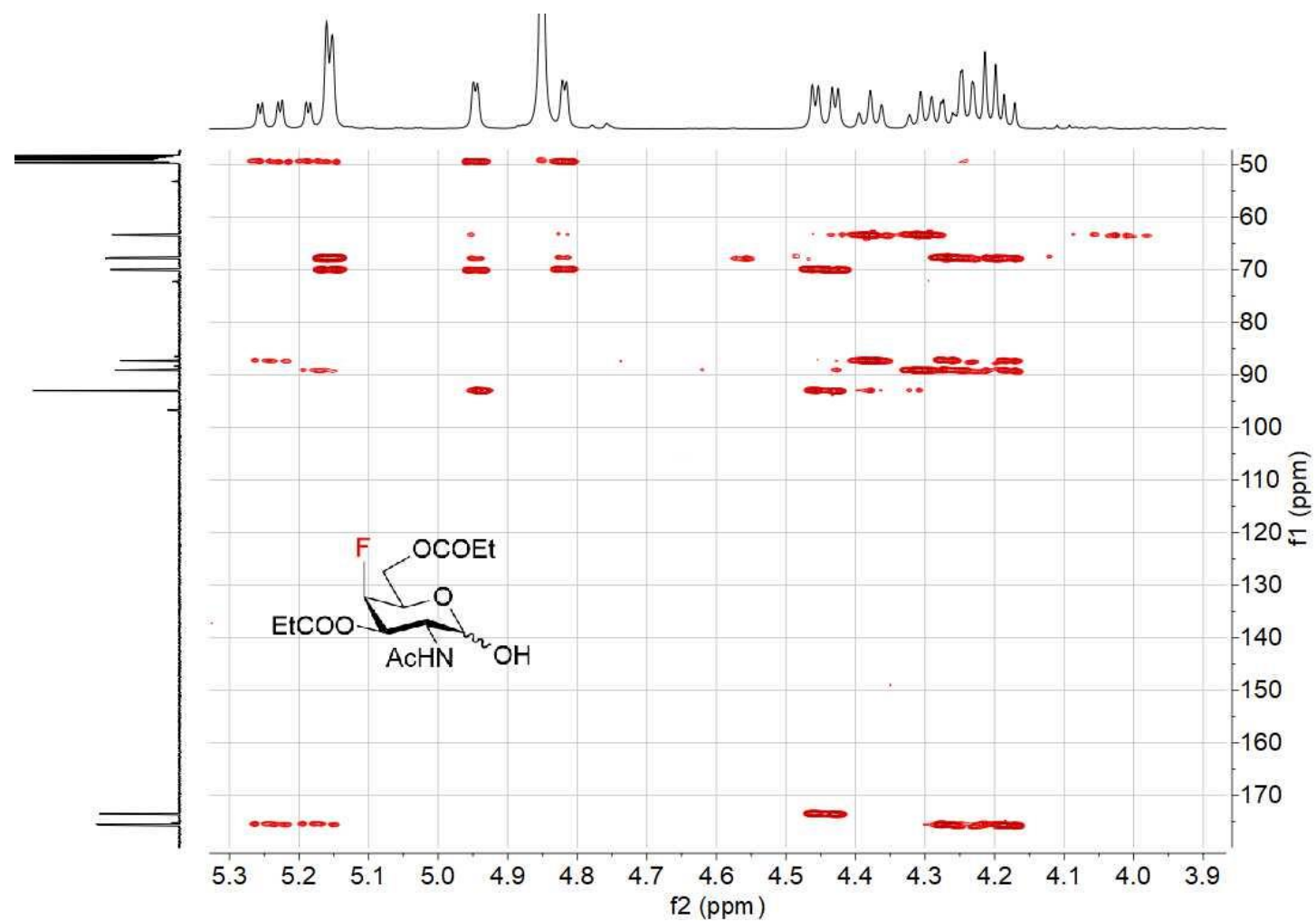
^{19}F NMR (376 MHz, CD_3OD) 27



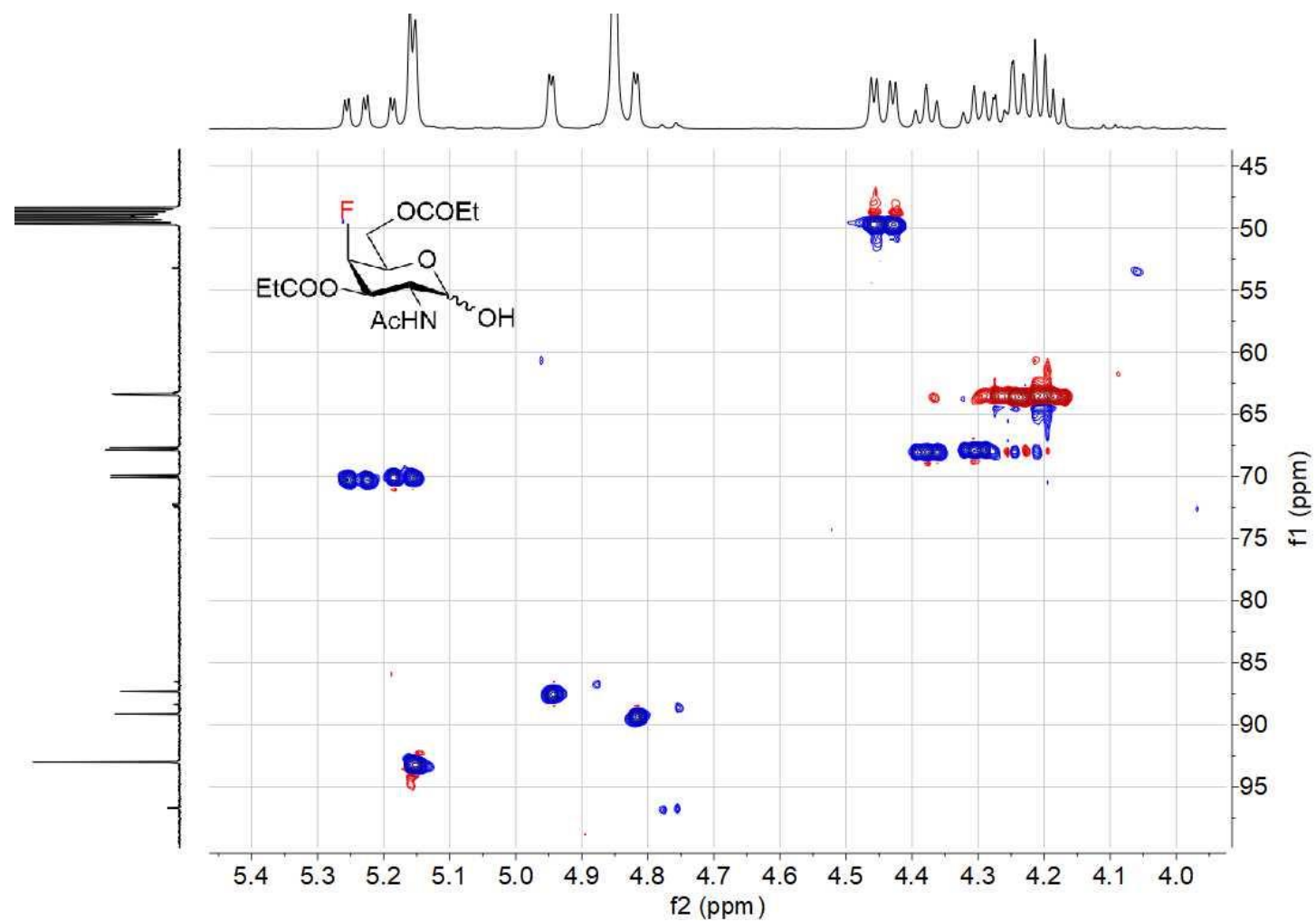
^1H - ^1H COSY 27



^1H - ^{13}C HMBC 27

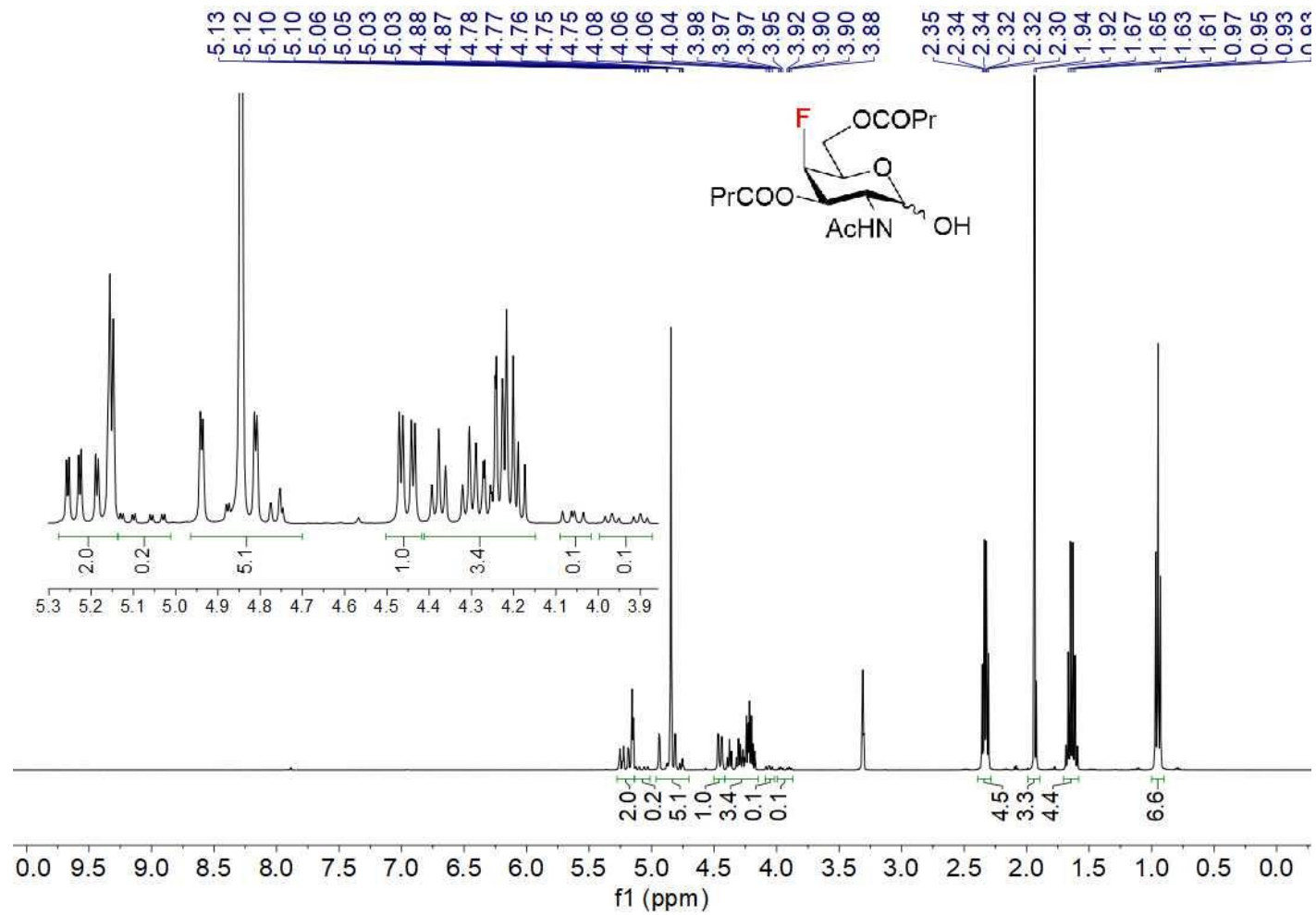


^1H - ^{13}C HSQC 27

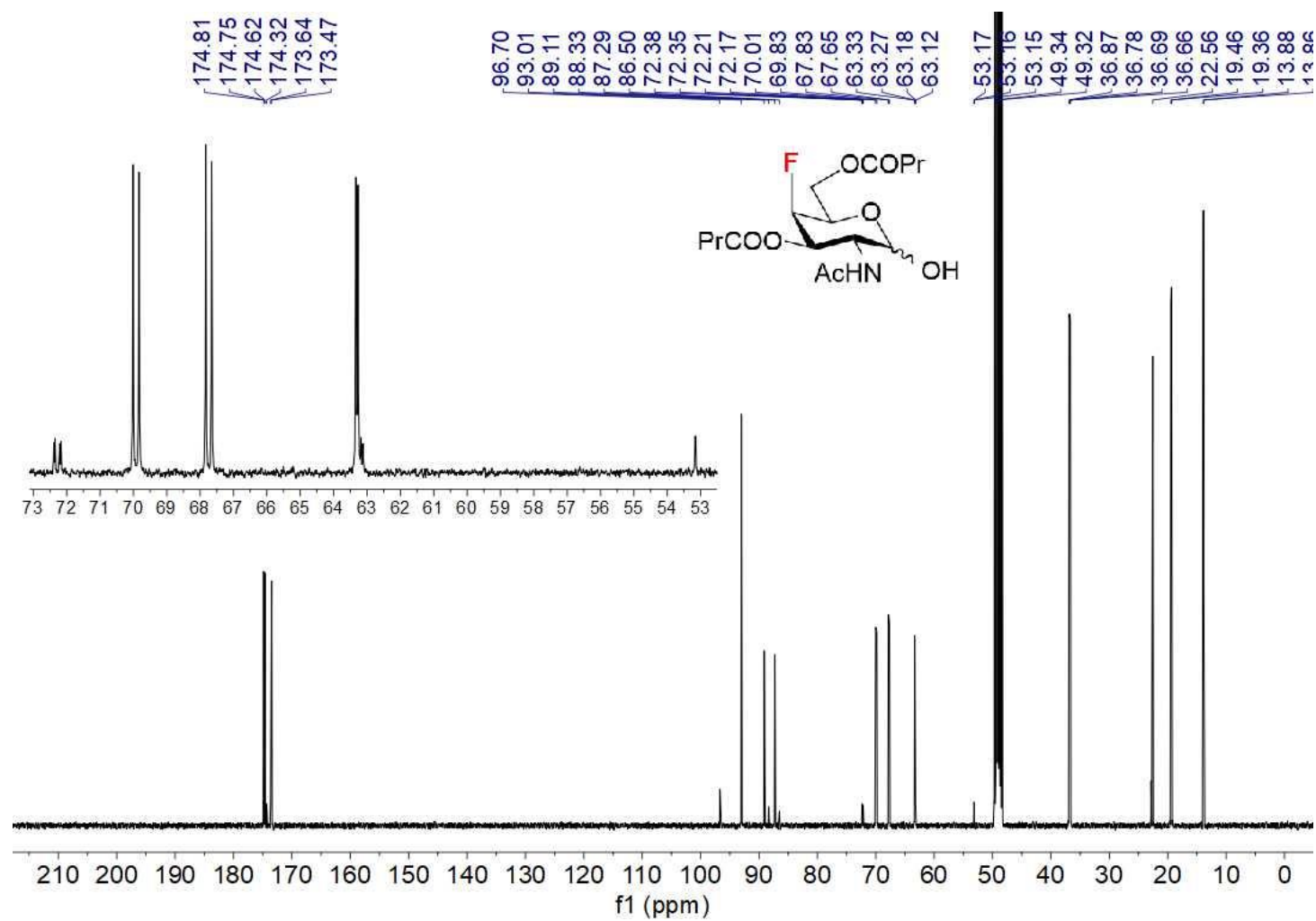


NMR COMPOUND 28

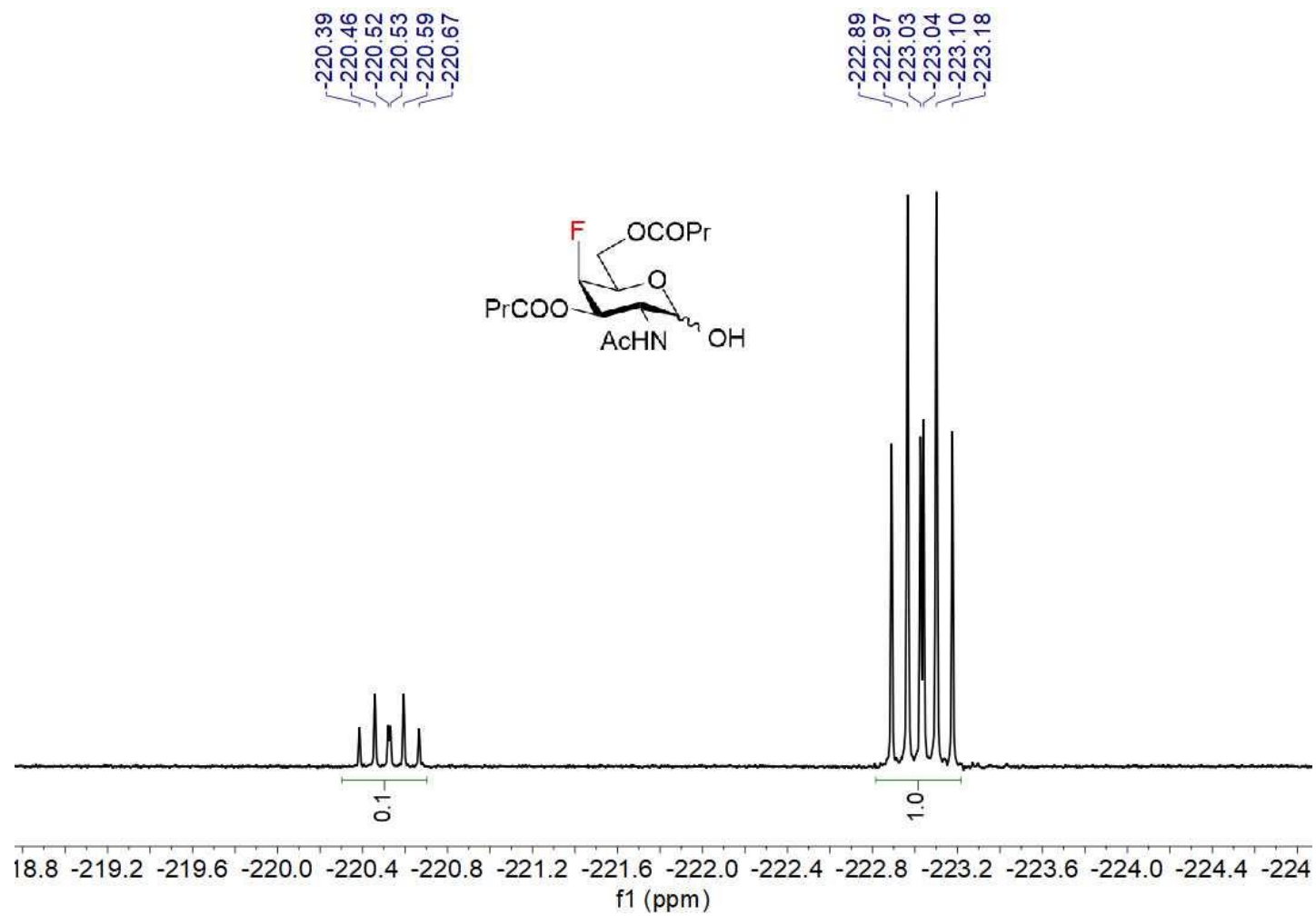
¹H NMR (400 MHz, CD₃OD) 28



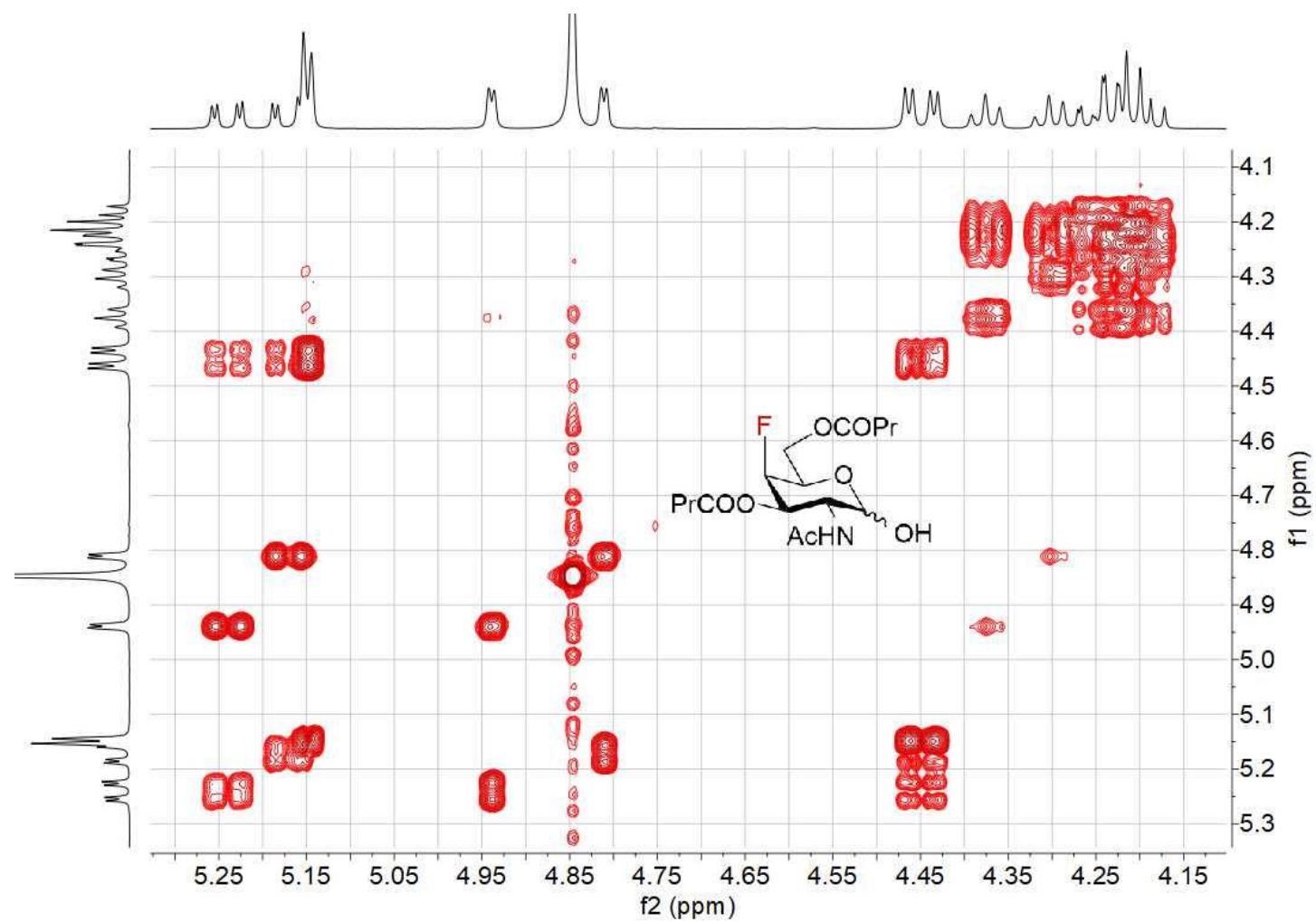
^{13}C NMR (100 MHz, CD_3OD) 28



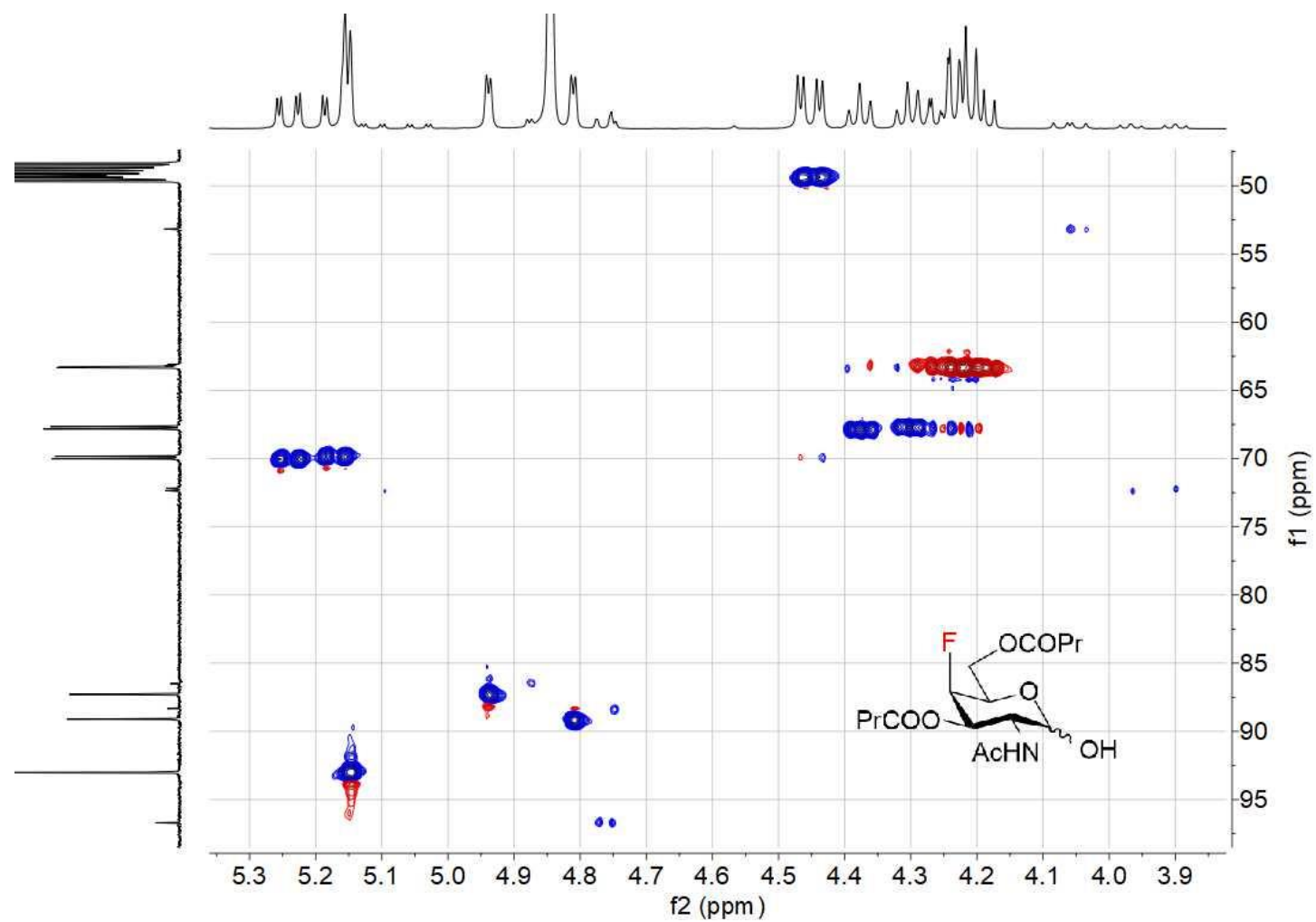
^{19}F NMR (376 MHz, CD_3OD) 28



^1H - ^1H COSY 28

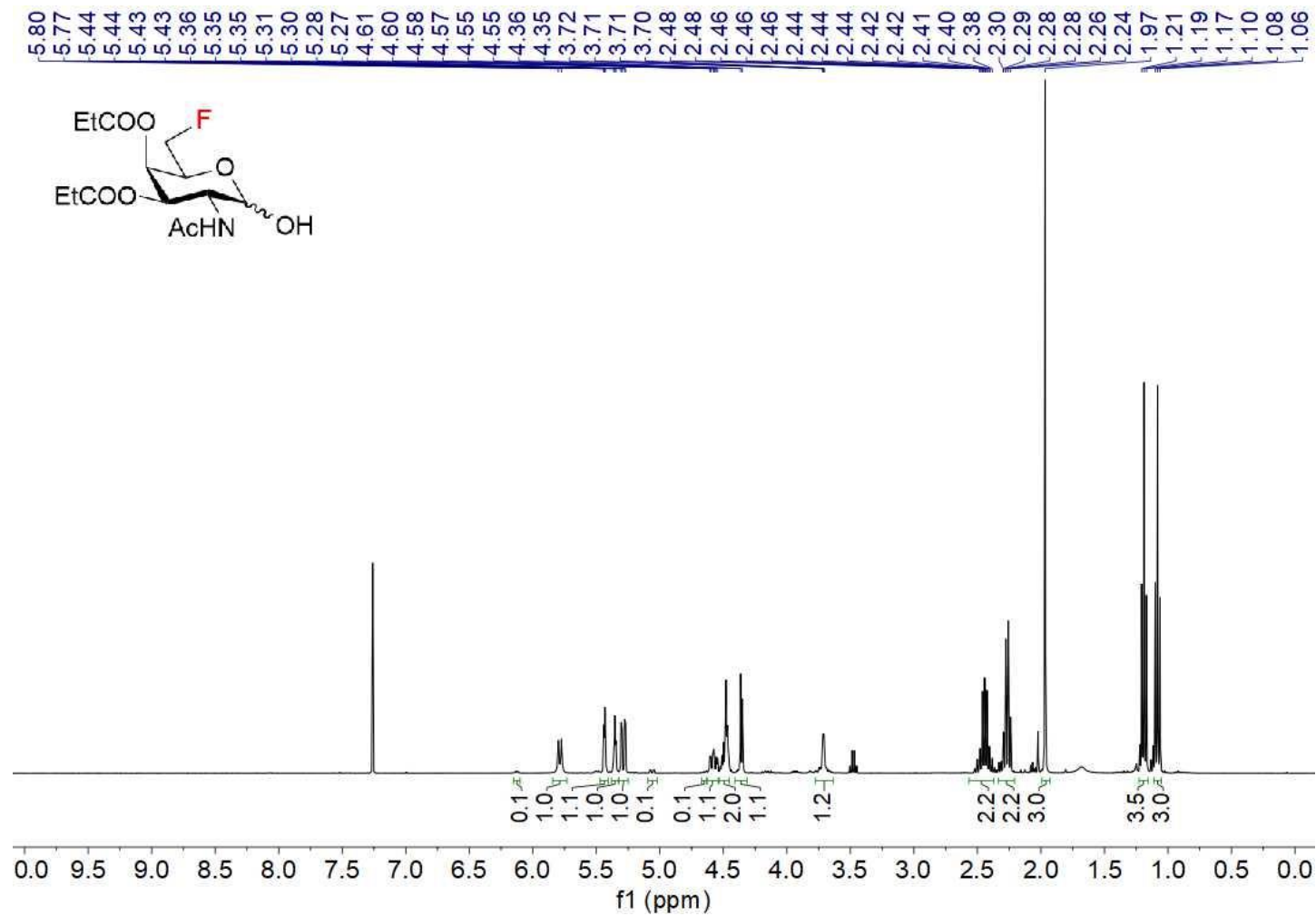


^1H - ^{13}C HSQC 28

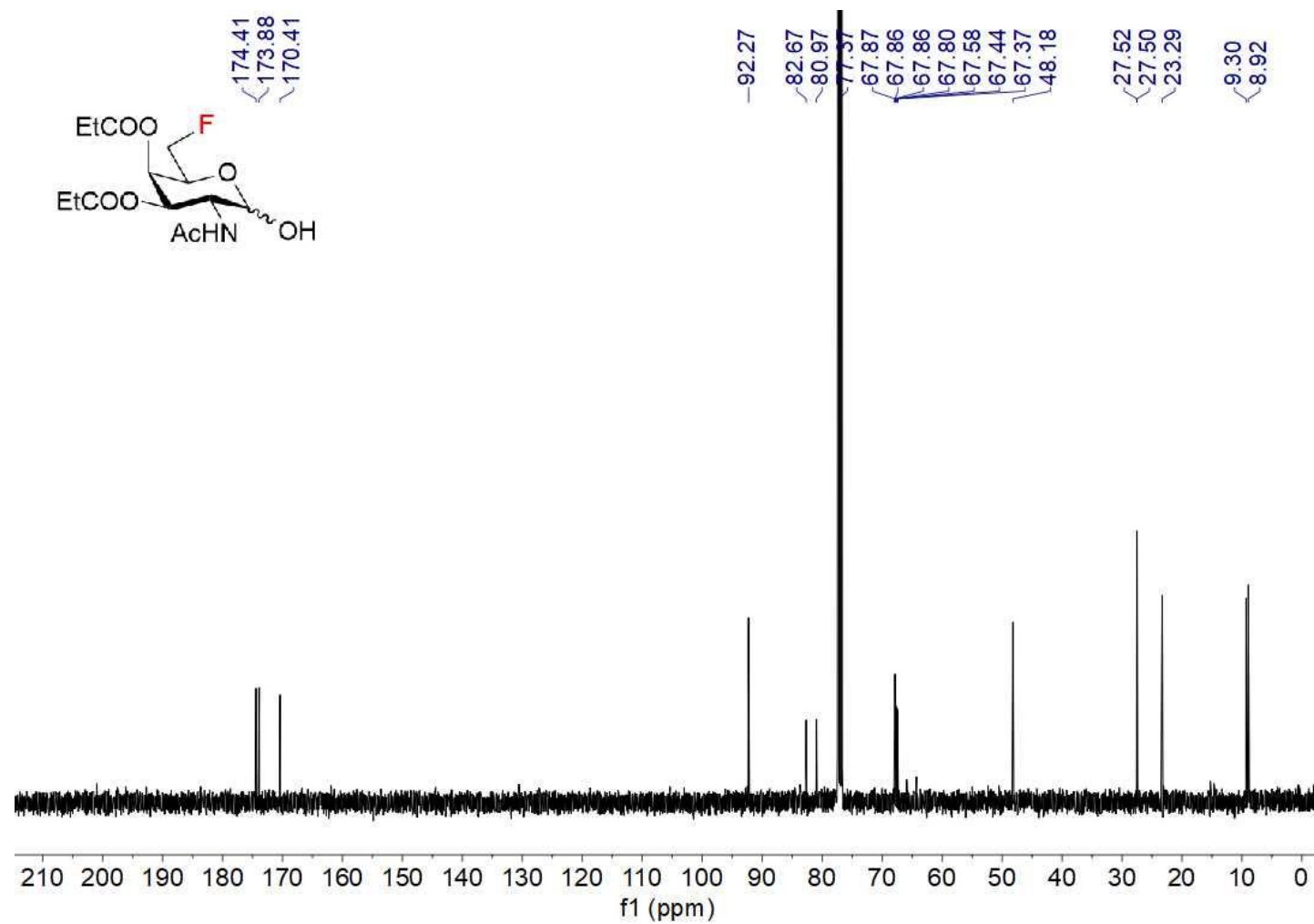


NMR COMPOUND 29

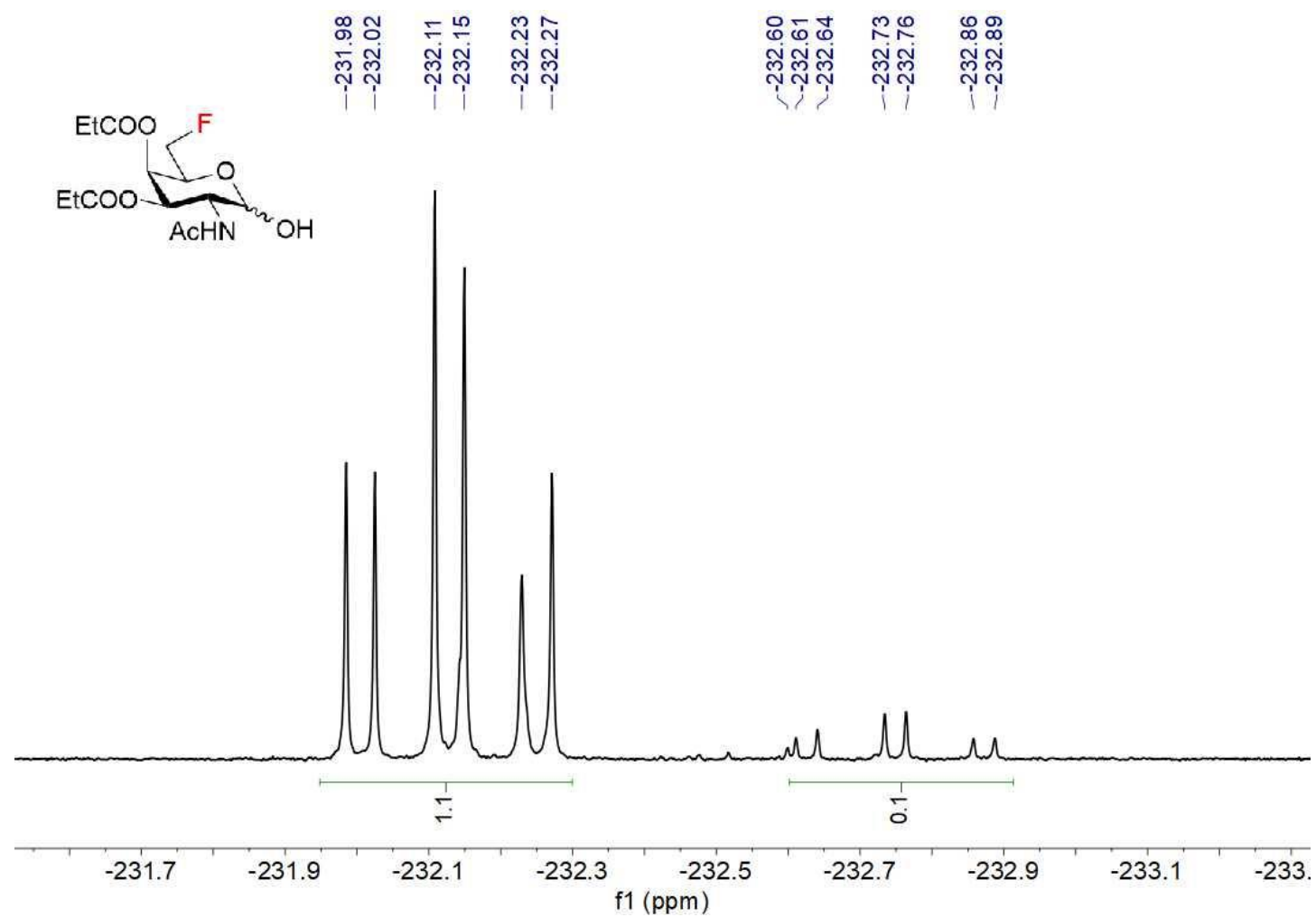
¹H NMR (400 MHz, CDCl₃) 29



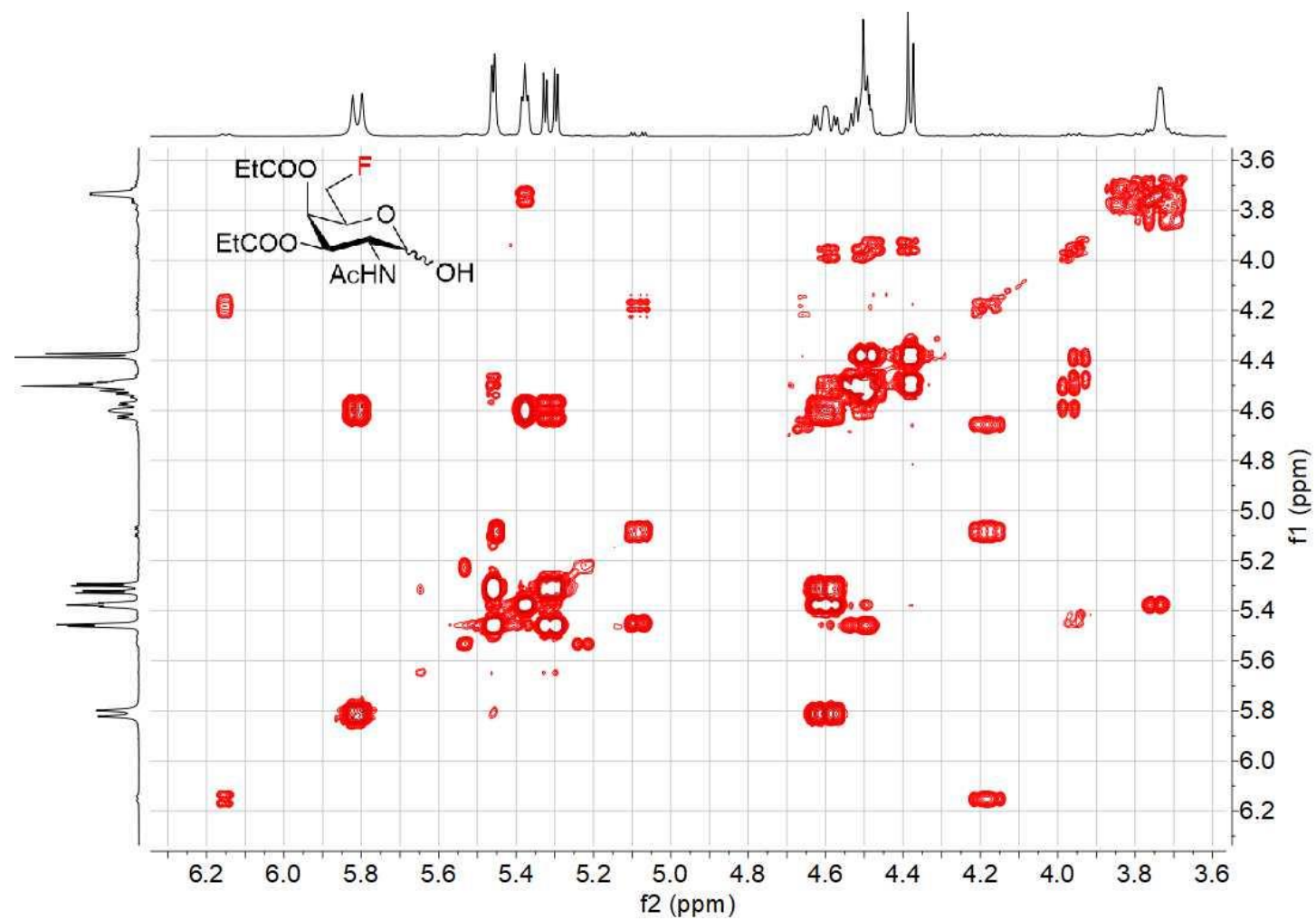
^{13}C NMR (100 MHz, CDCl_3) 29



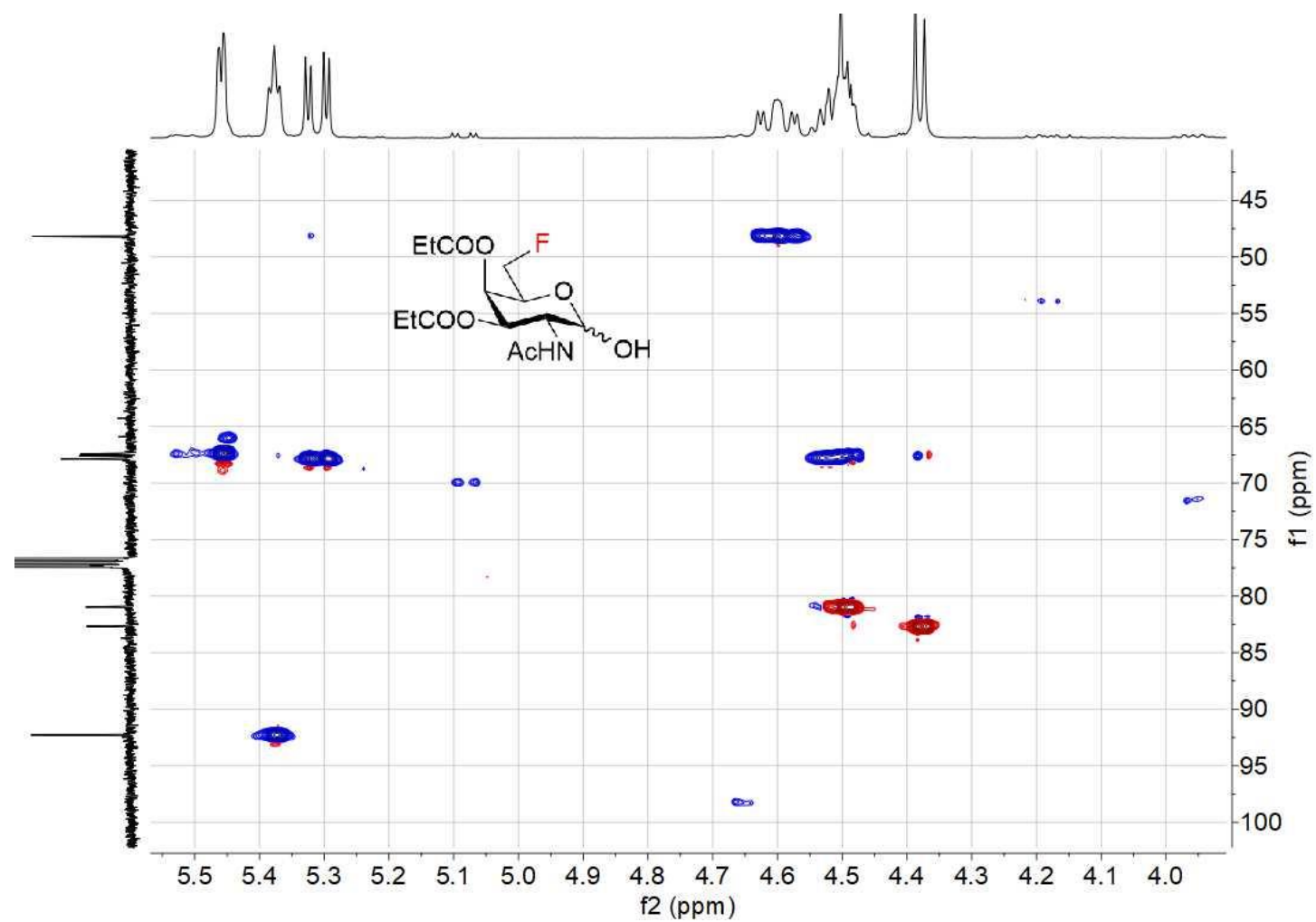
¹⁹F NMR (376 MHz, CDCl₃) 29



^1H - ^1H COSY 29

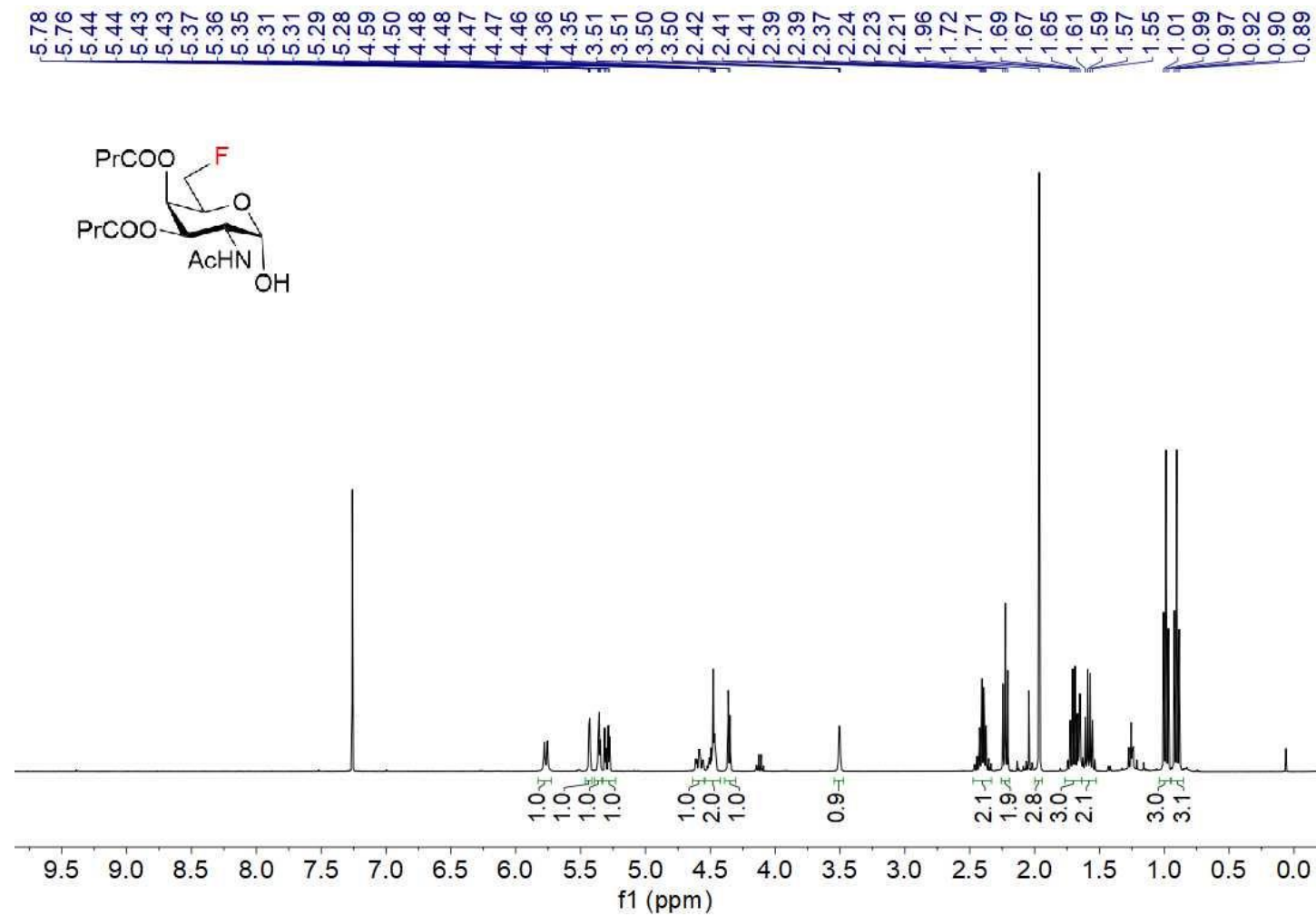


^1H - ^{13}C HSQC 29

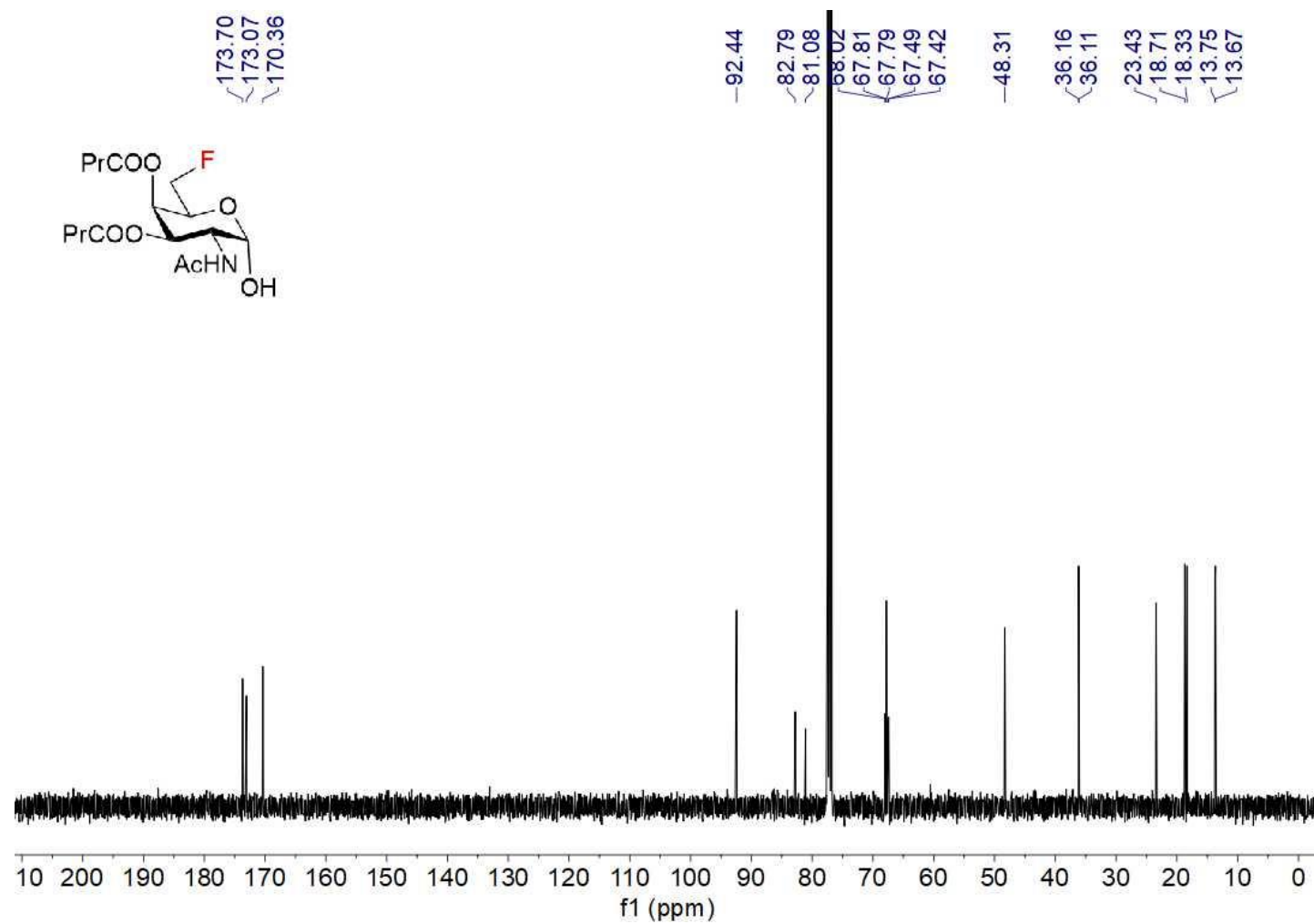


NMR COMPOUND 30

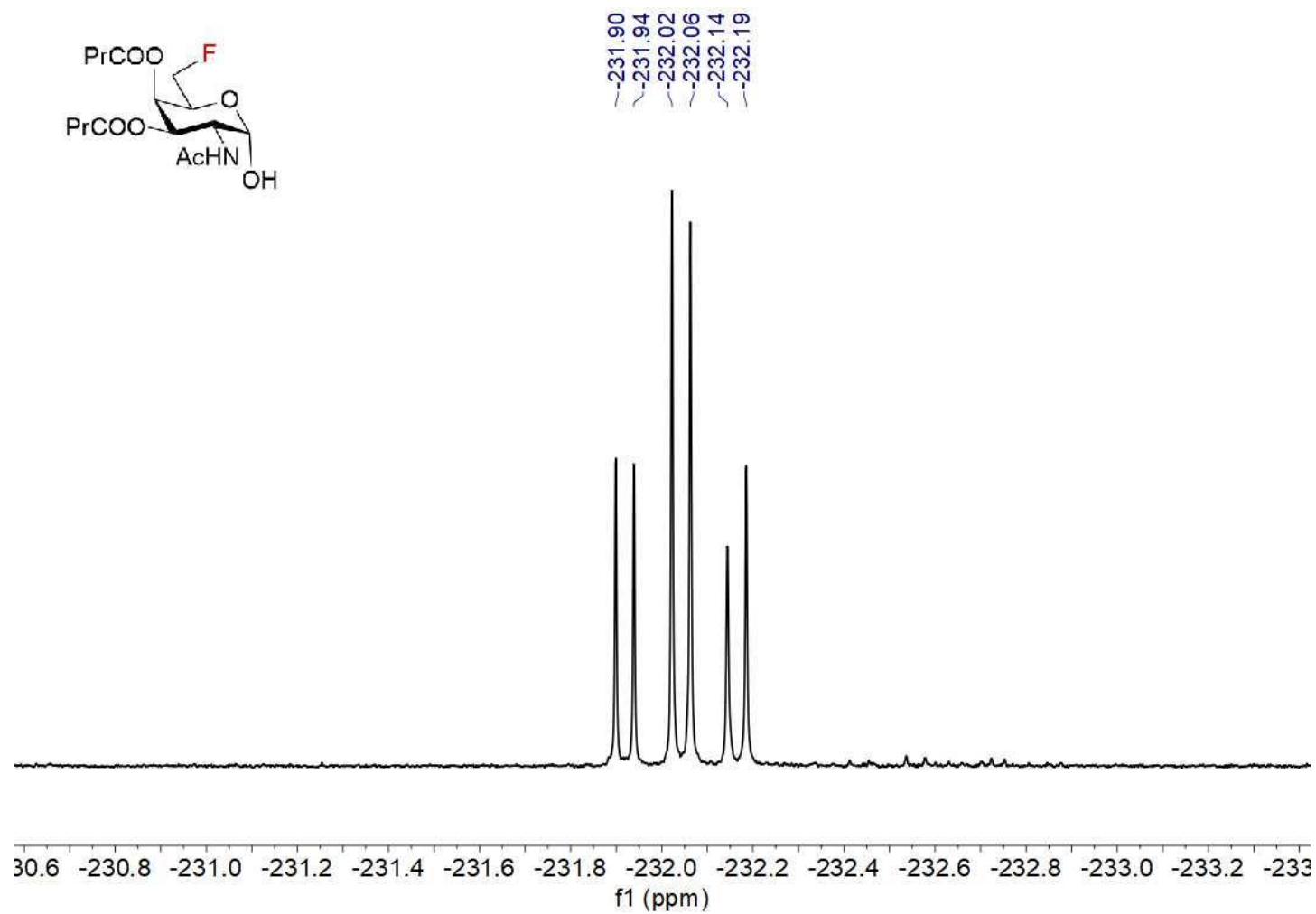
¹H NMR (400 MHz, CDCl₃) 30



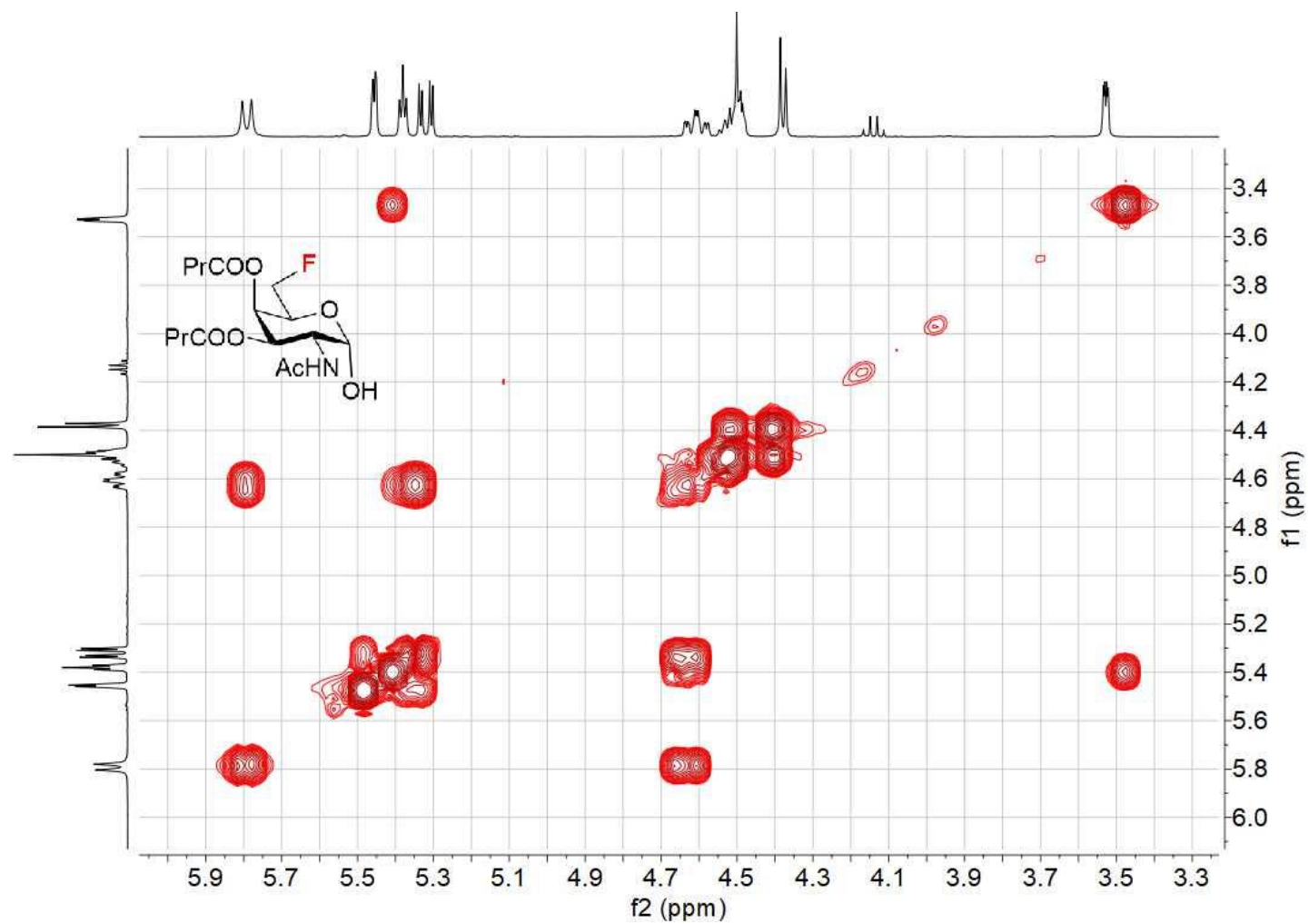
^{13}C NMR (100 MHz, CDCl_3) 30



^{19}F NMR (376 MHz, CDCl_3) 30

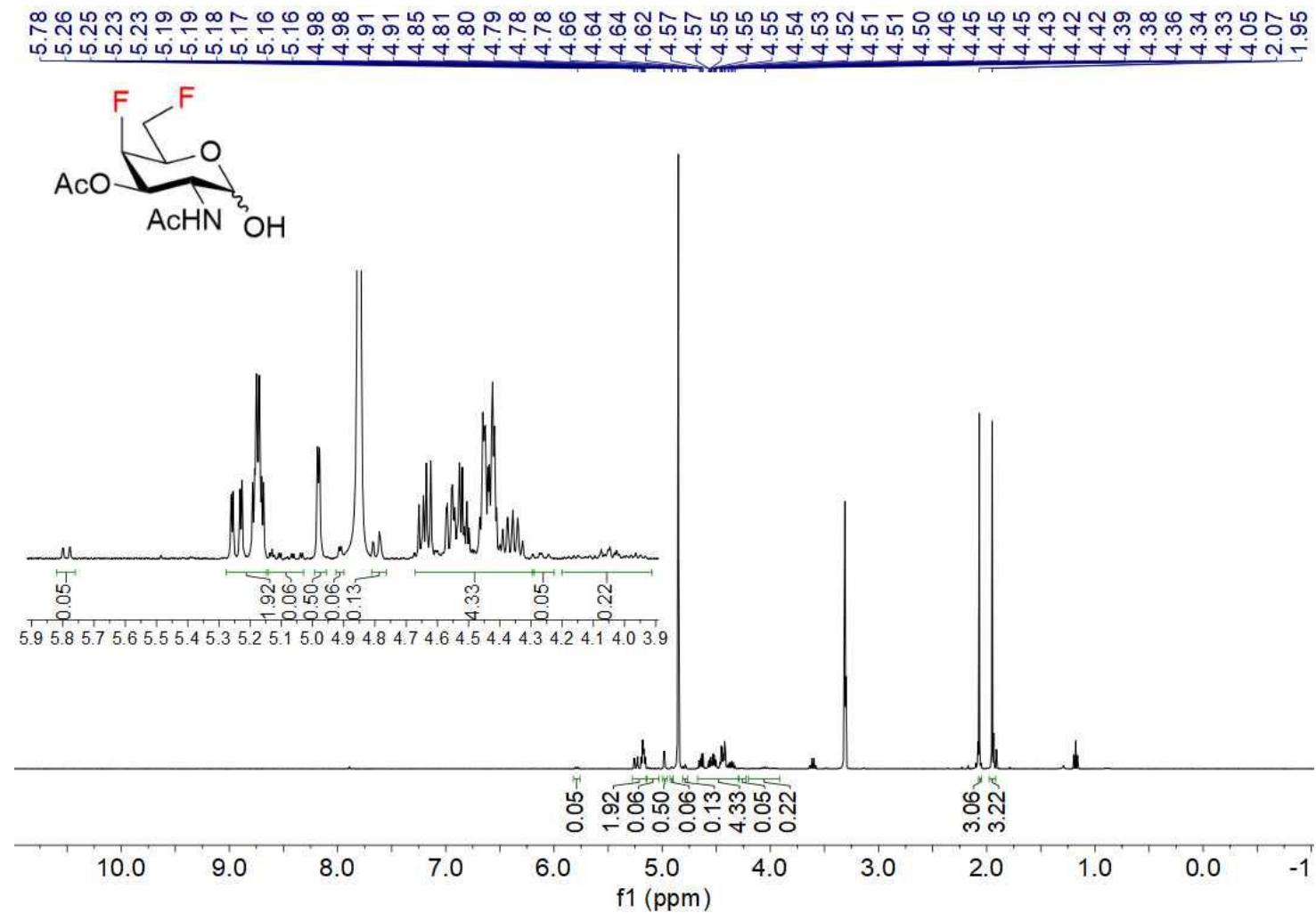


^1H - ^1H COSY 30

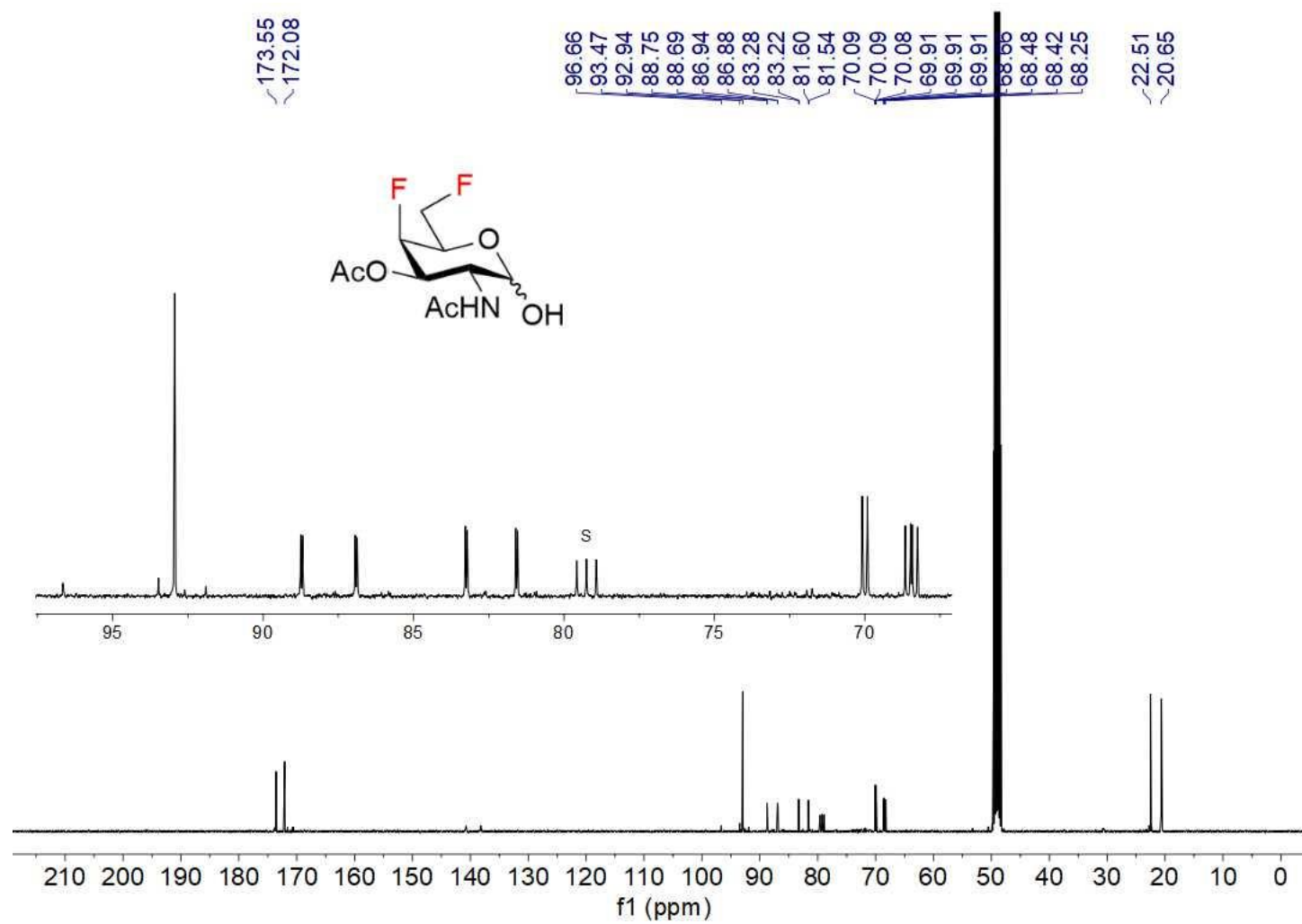


NMR COMPOUND 31

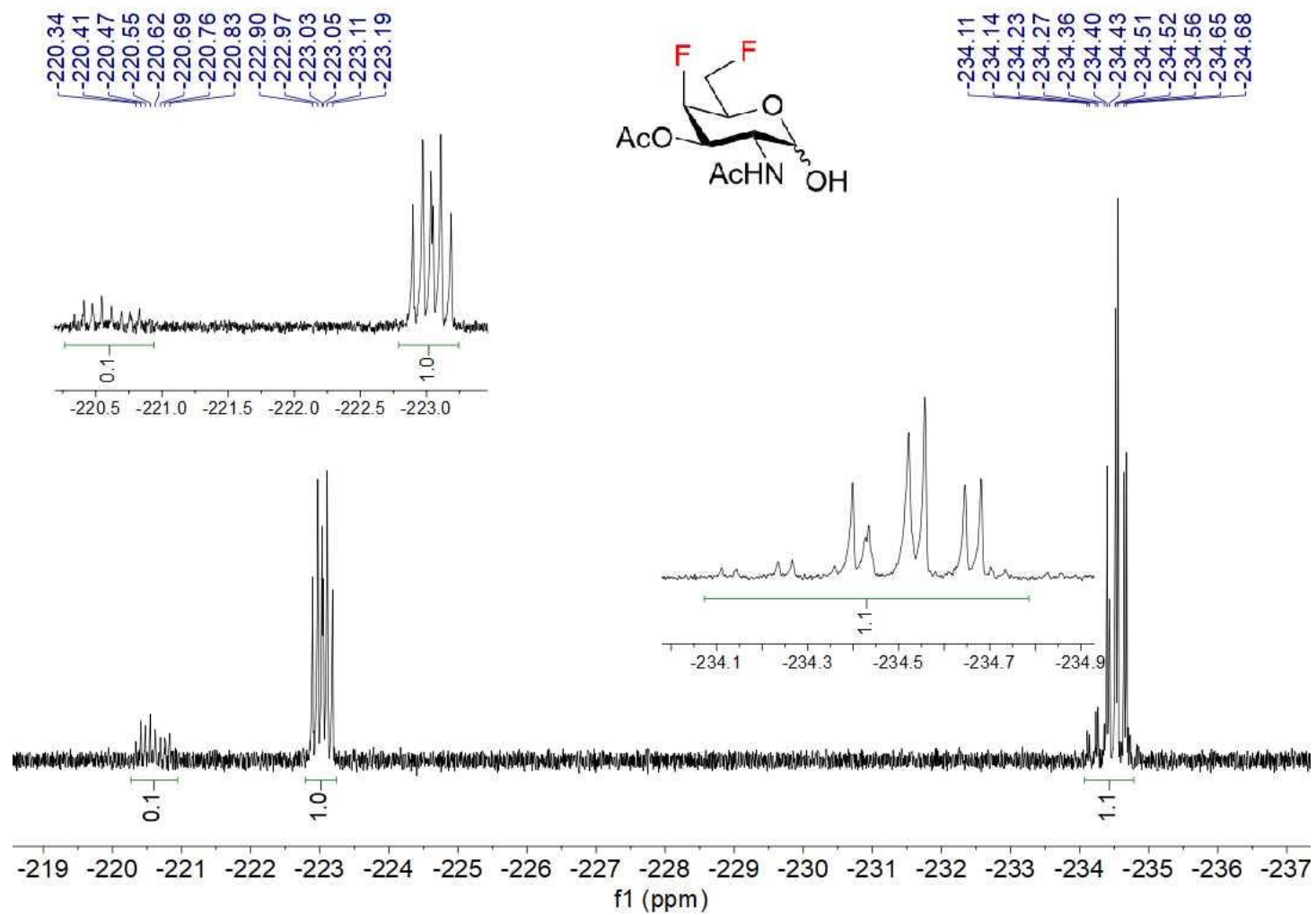
¹H NMR (400 MHz, CD₃OD) 31



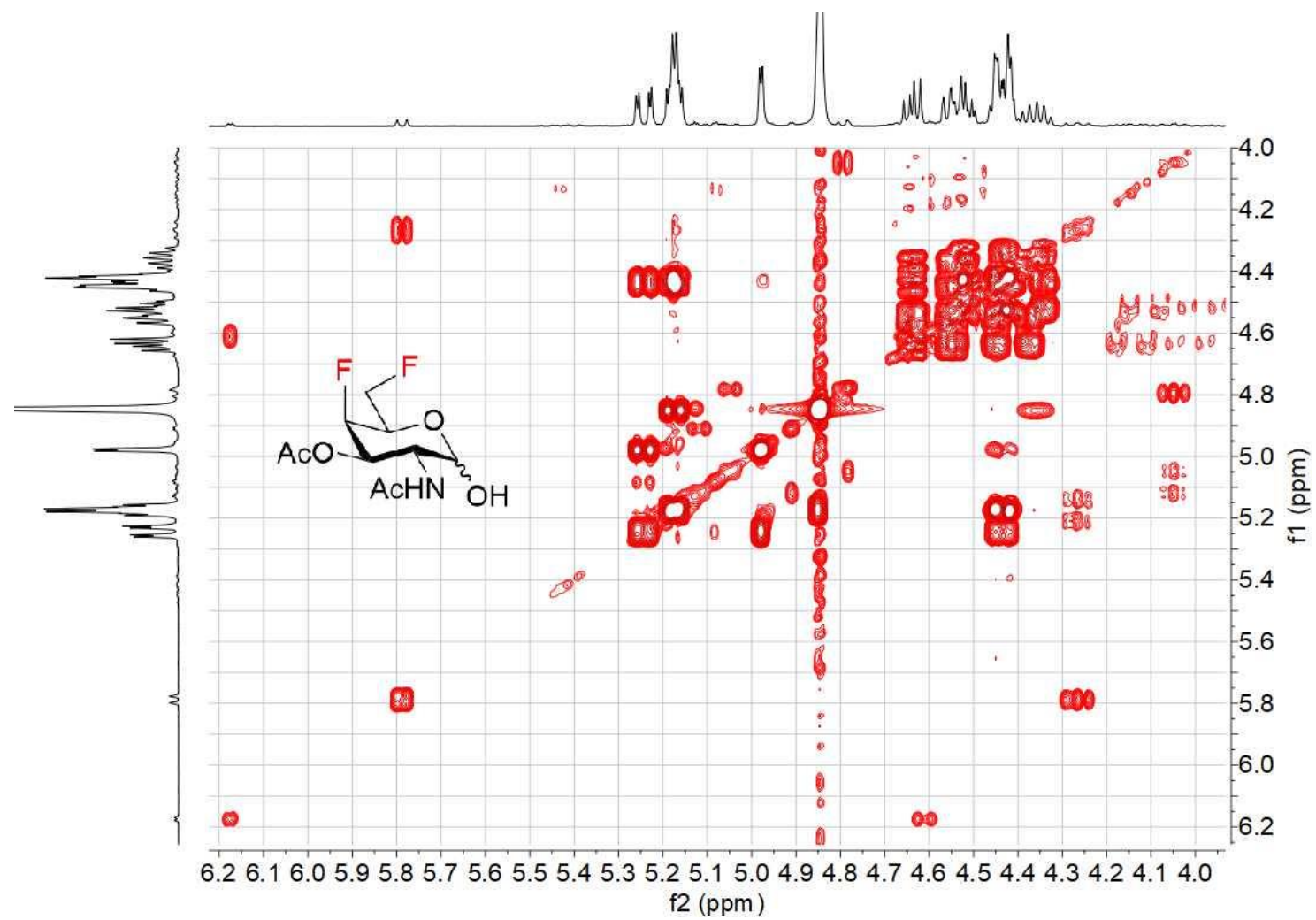
^{13}C NMR (100 MHz, CD_3OD) 31



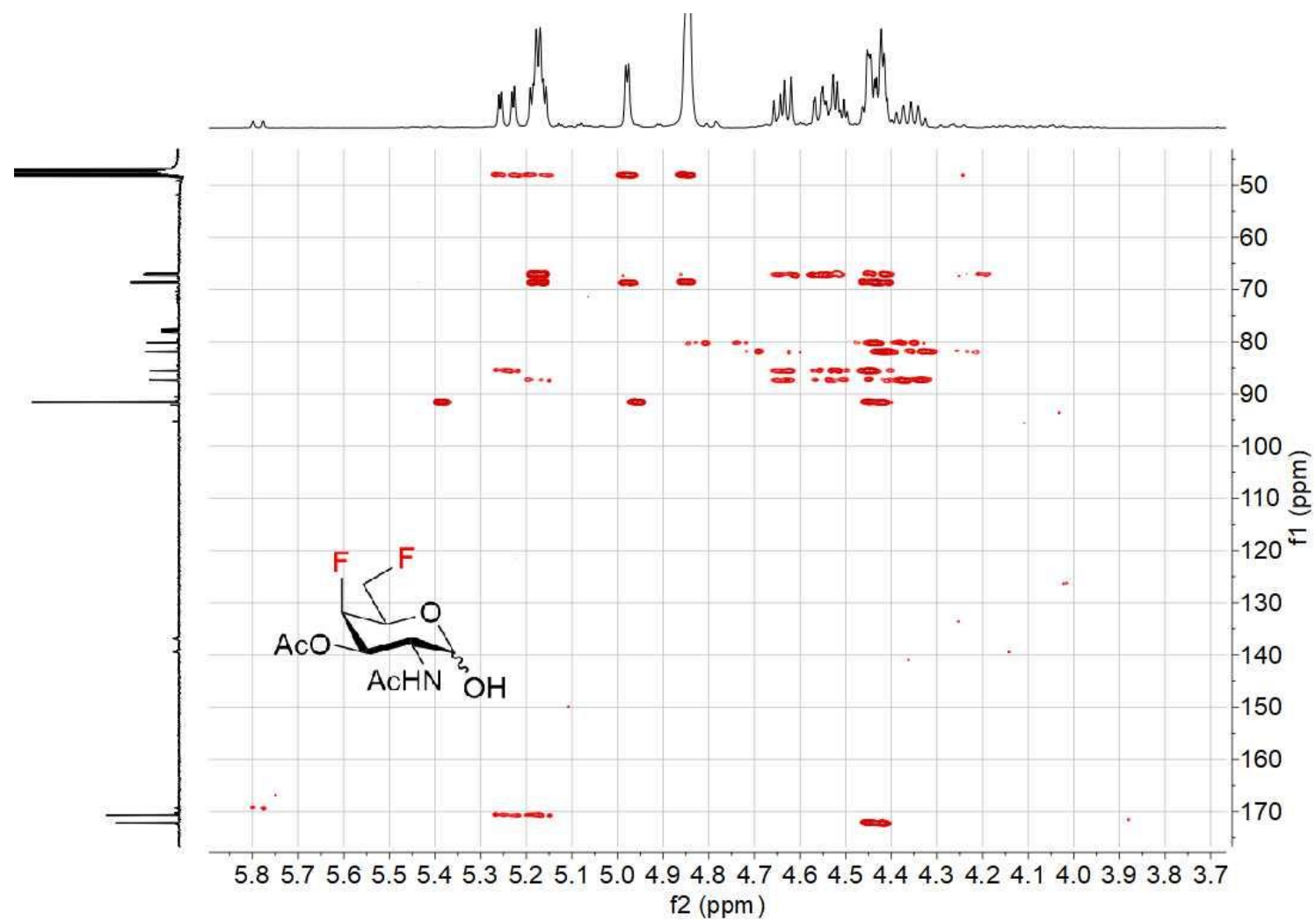
¹⁹F NMR (376 MHz, CD₃OD) 31



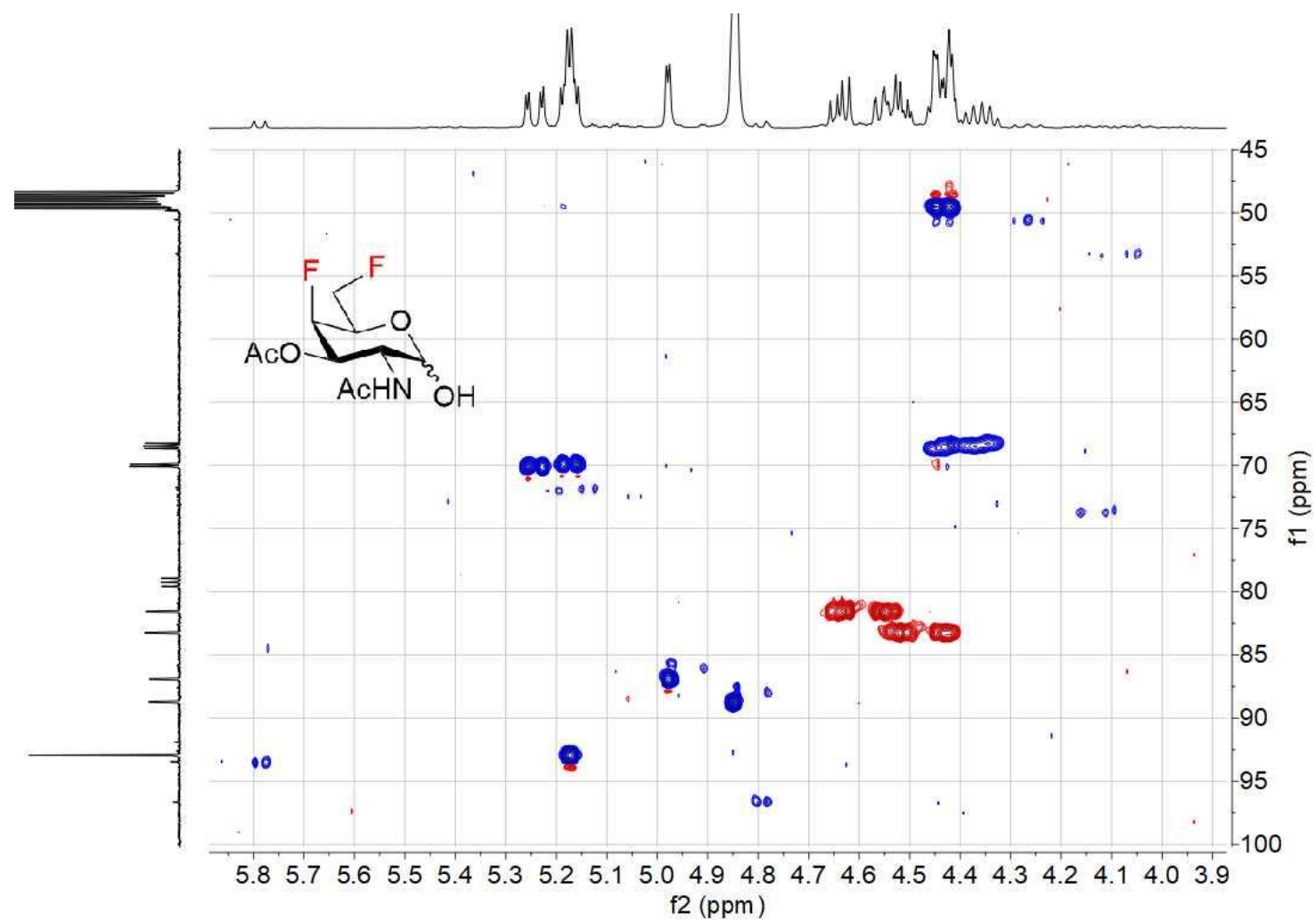
^1H - ^1H COSY 31



^1H - ^{13}C HMBC 31

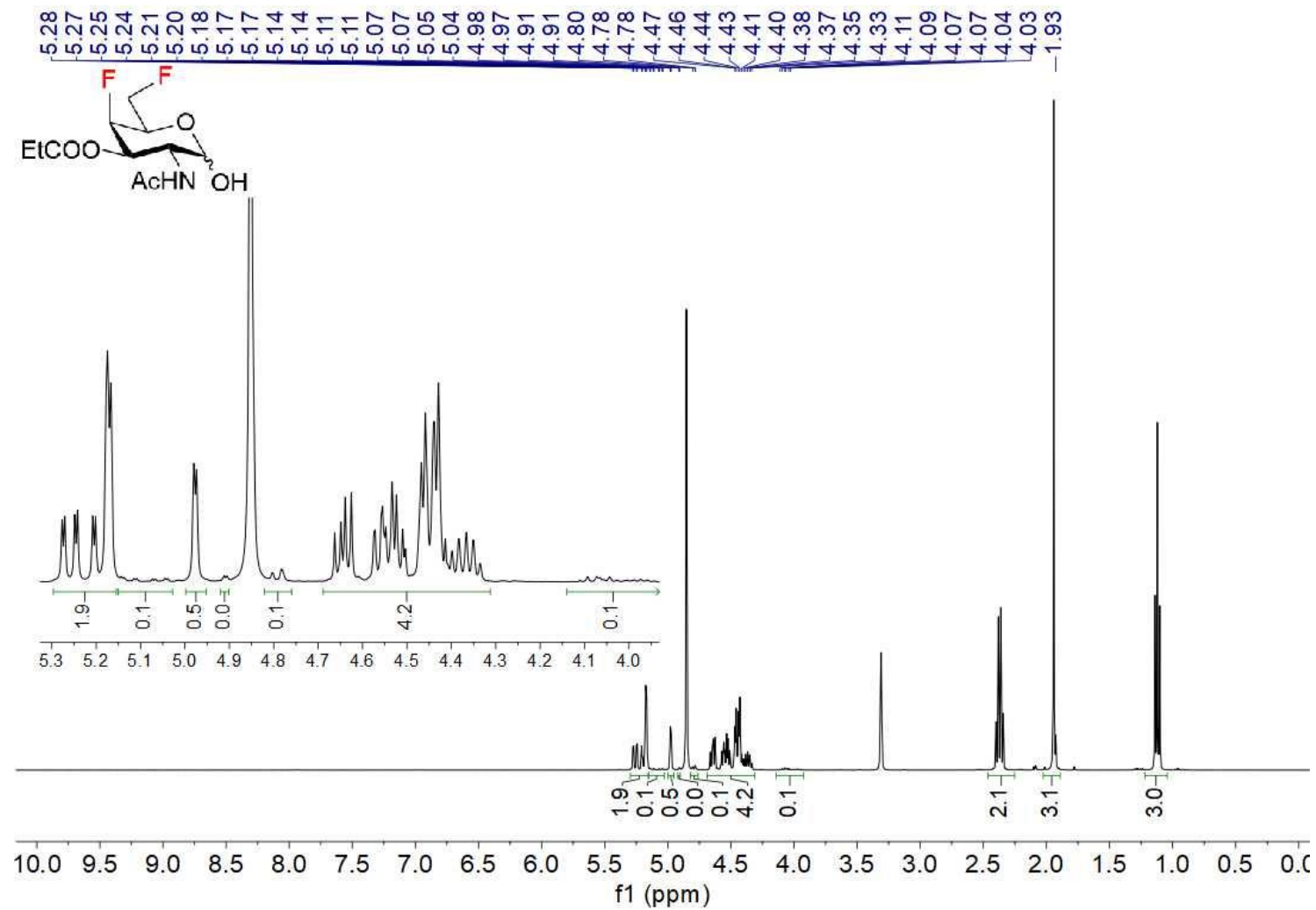


^1H - ^{13}C HSQC 31

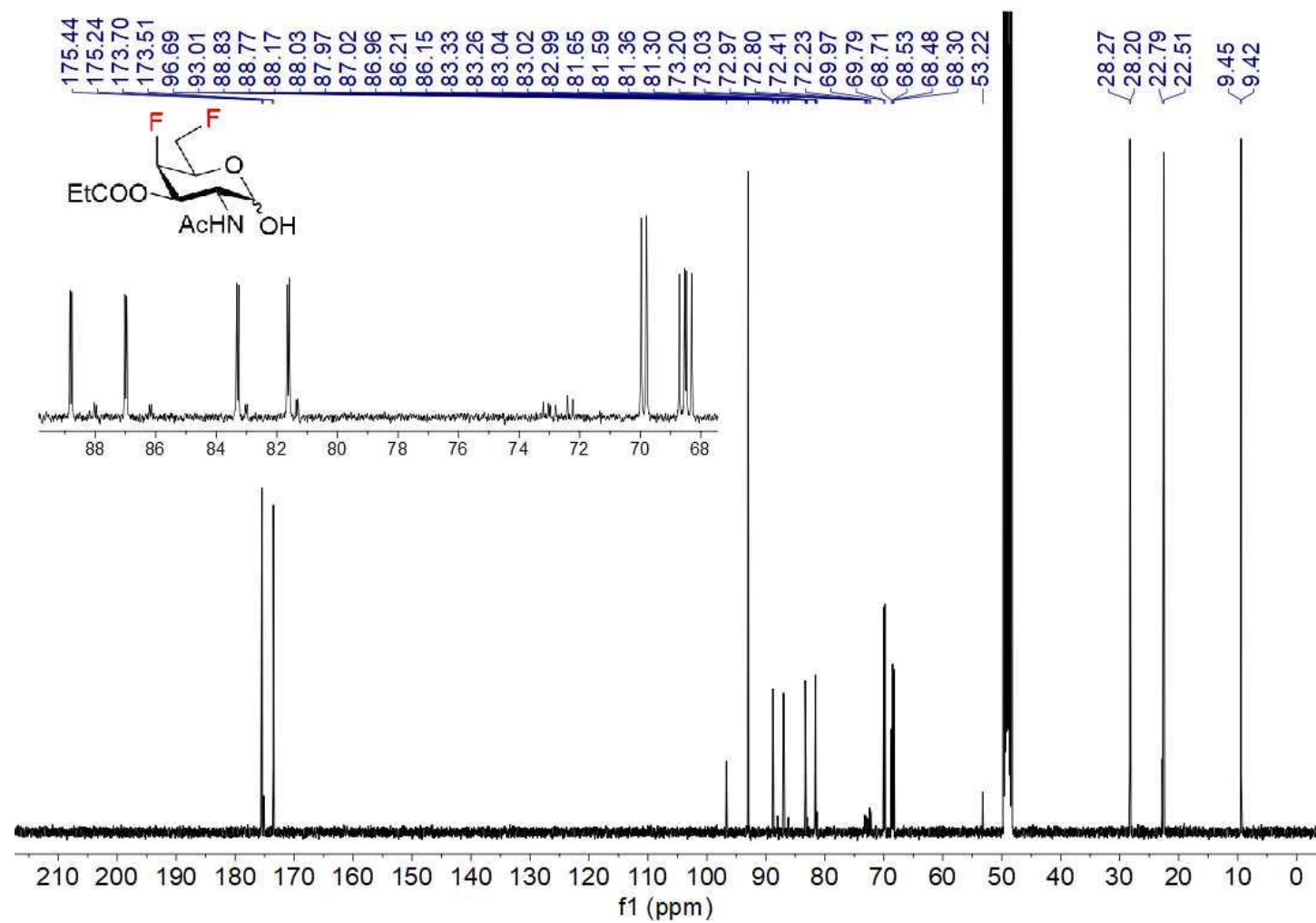


NMR COMPOUND 32

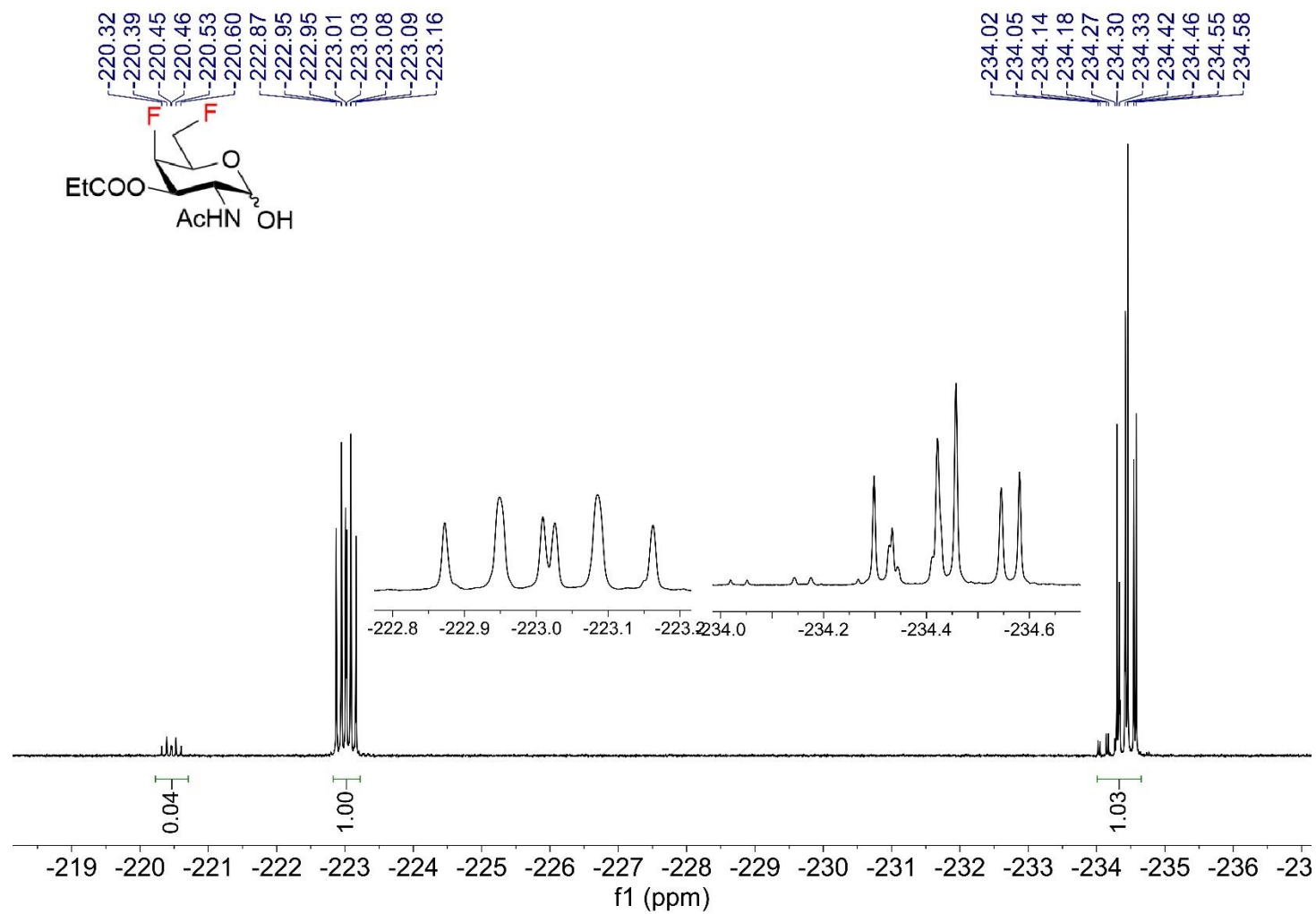
¹H NMR (400 MHz, CD₃OD) 32



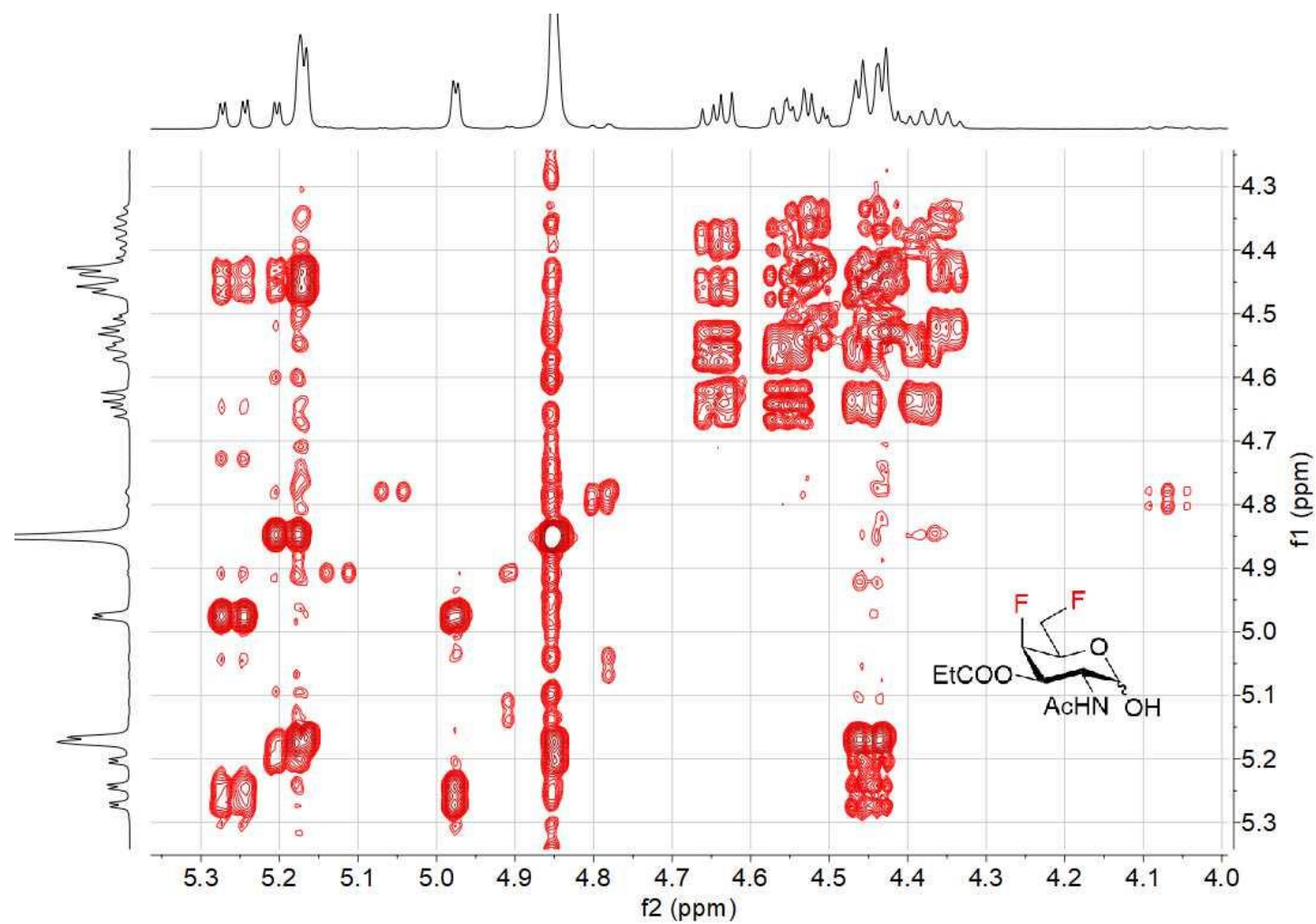
¹³C NMR (100 MHz, CD₃OD) 32



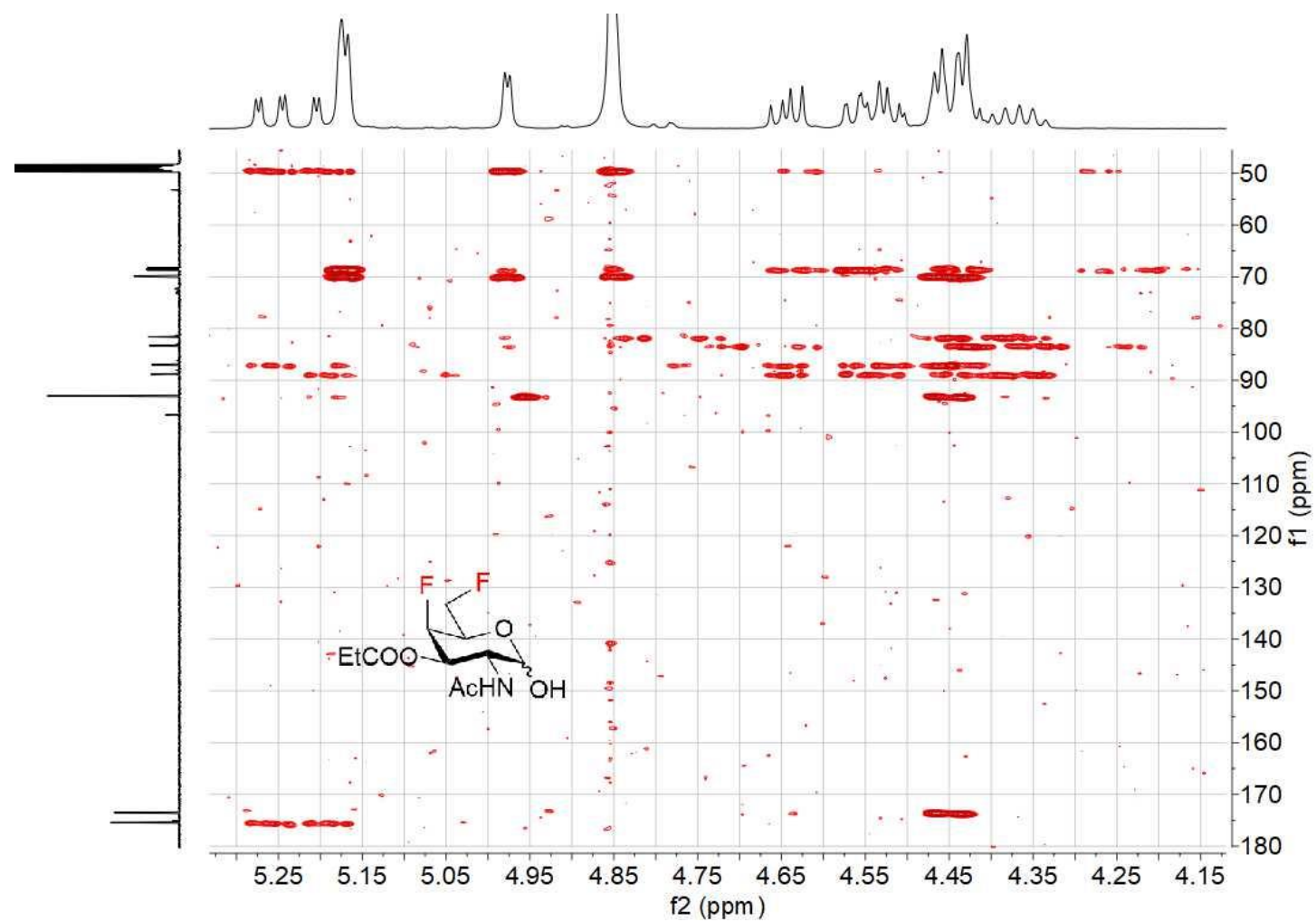
¹⁹F NMR (376 MHz, CD₃OD) 32



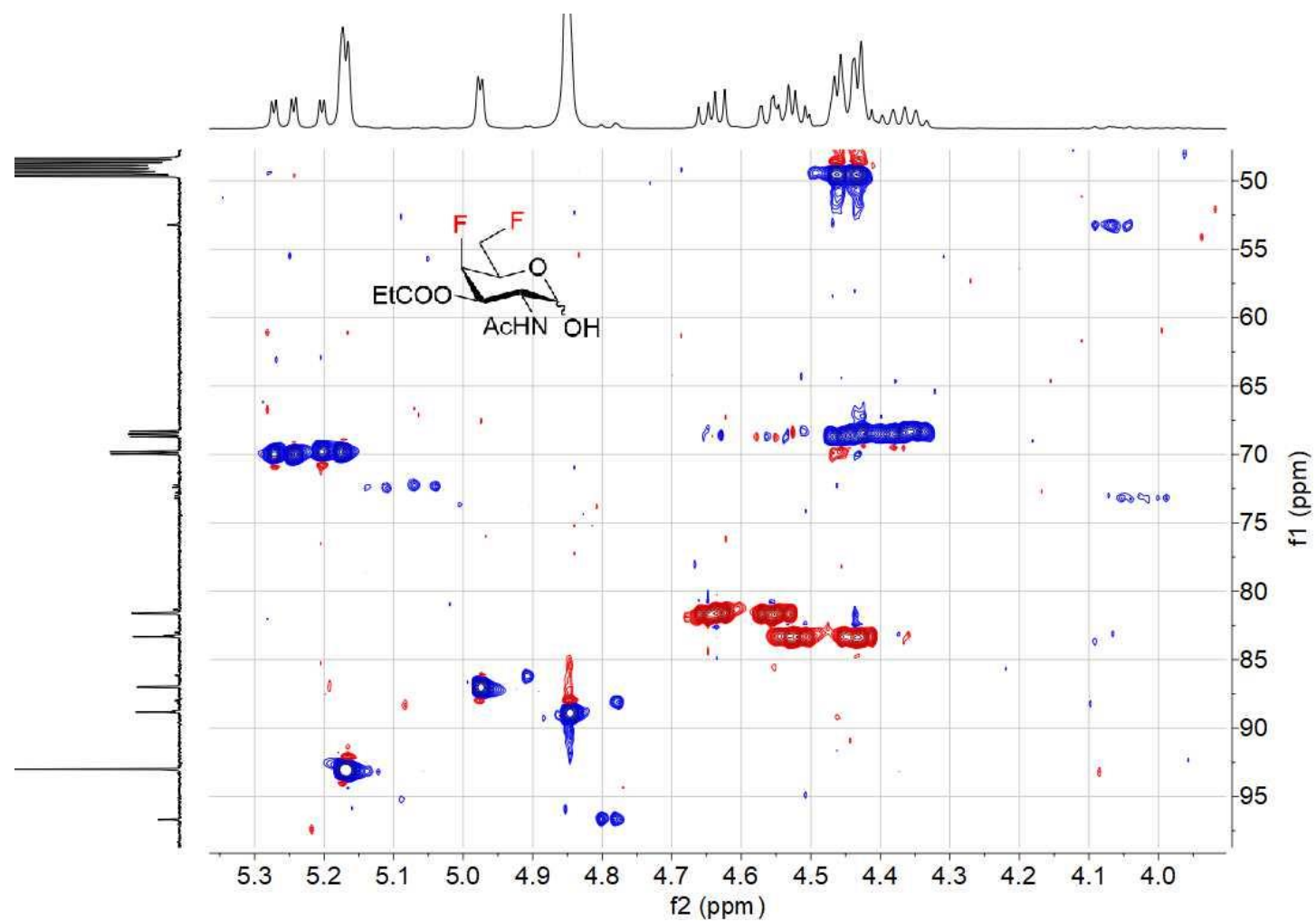
^1H - ^1H COSY 32



^1H - ^{13}C HMBC 32

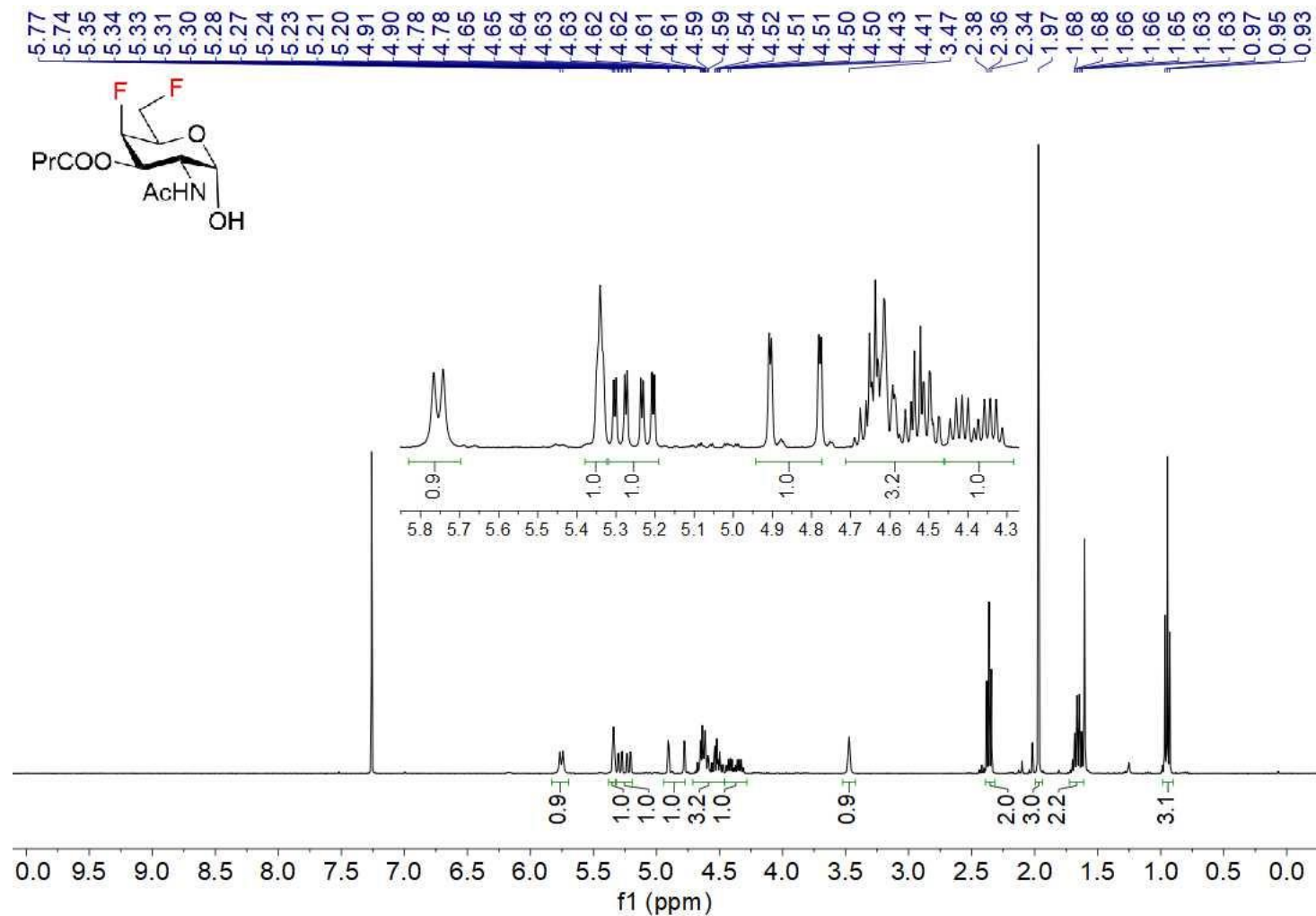


^1H - ^{13}C HSQC 32

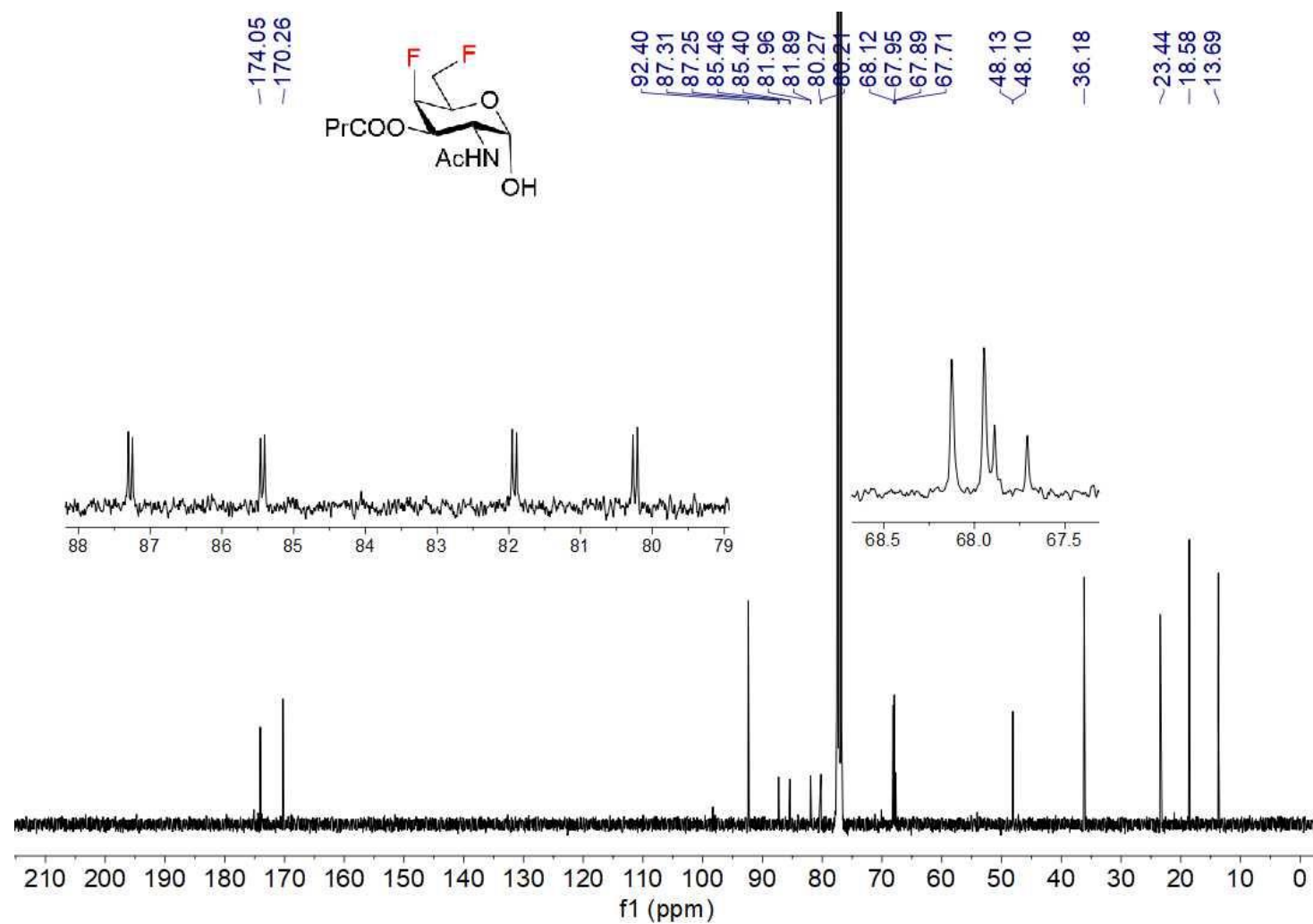


NMR COMPOUND 33

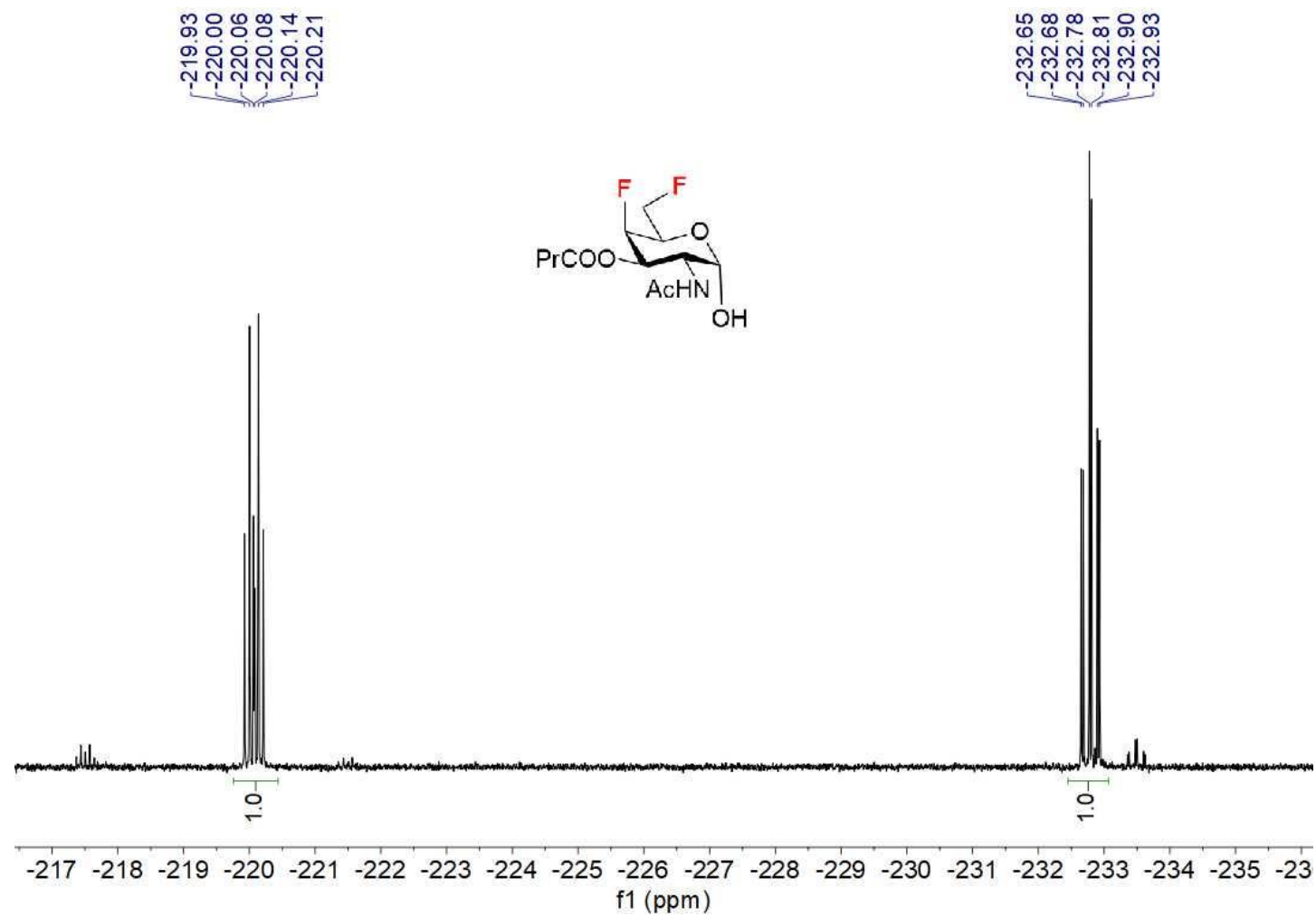
¹H NMR (400 MHz, CDCl₃) 33



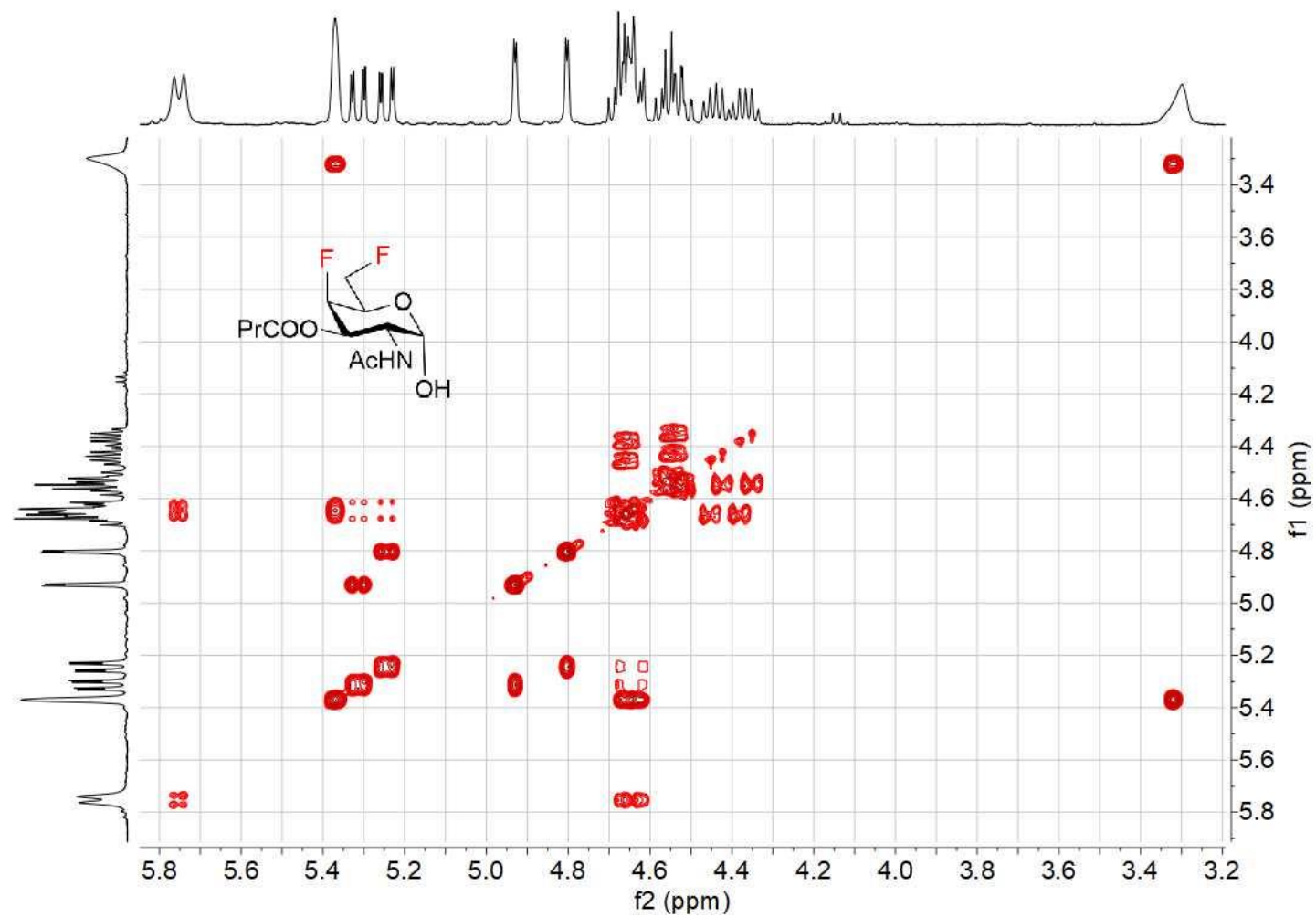
^{13}C NMR (100 MHz, CDCl_3) 33



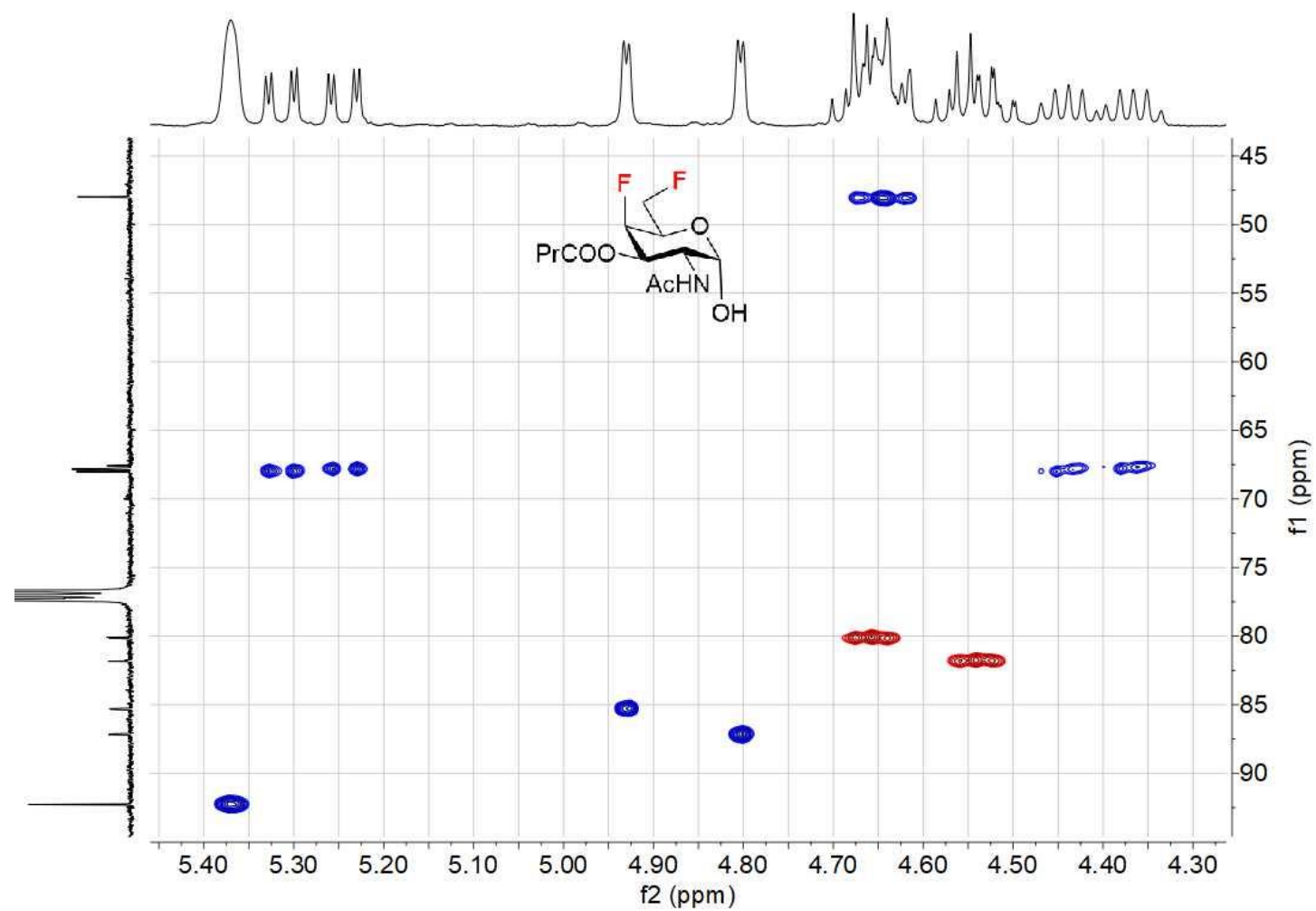
^{19}F NMR (376 MHz, CDCl_3) 33



^1H - ^1H COSY 33

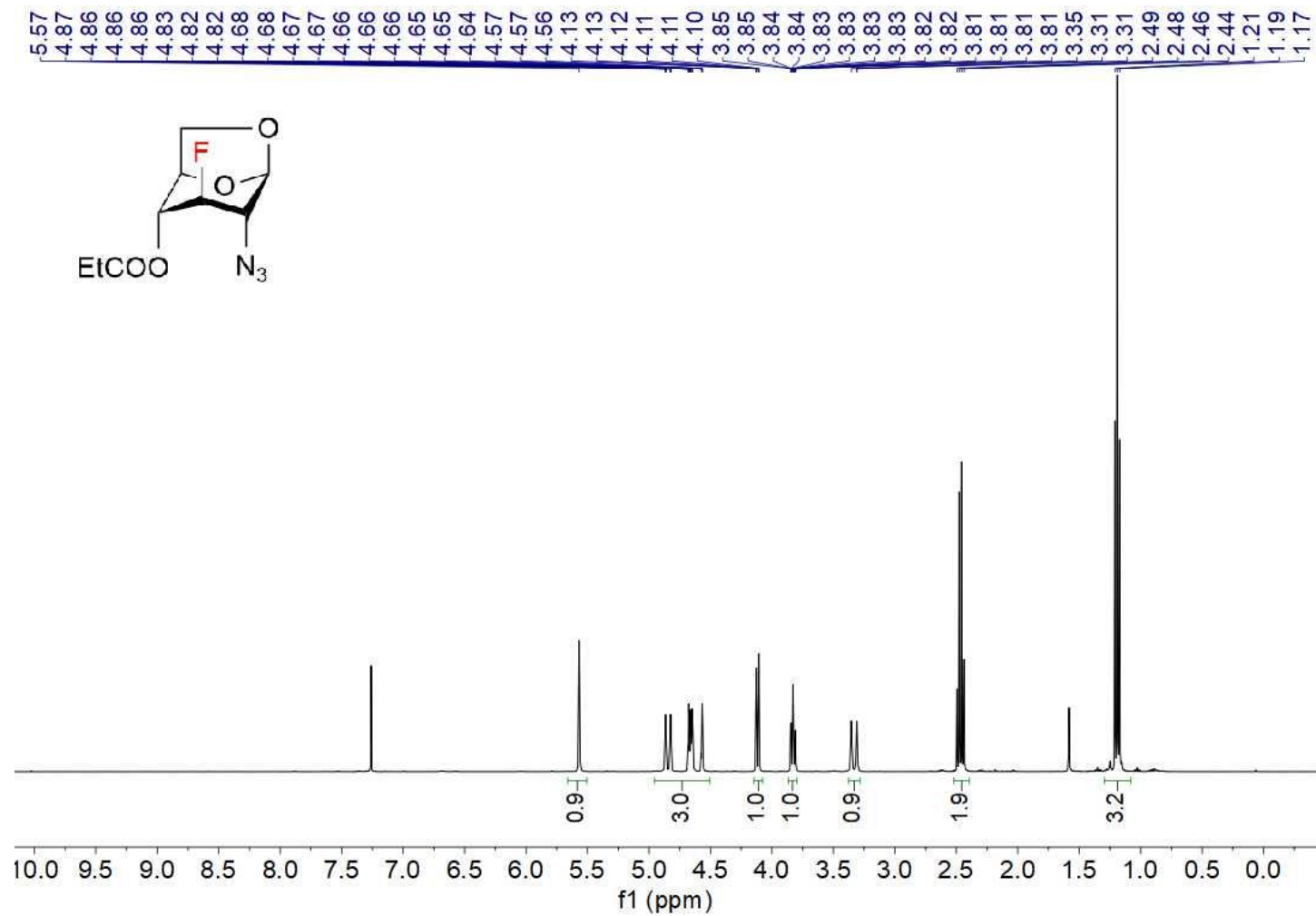


^1H - ^{13}C HSQC 33

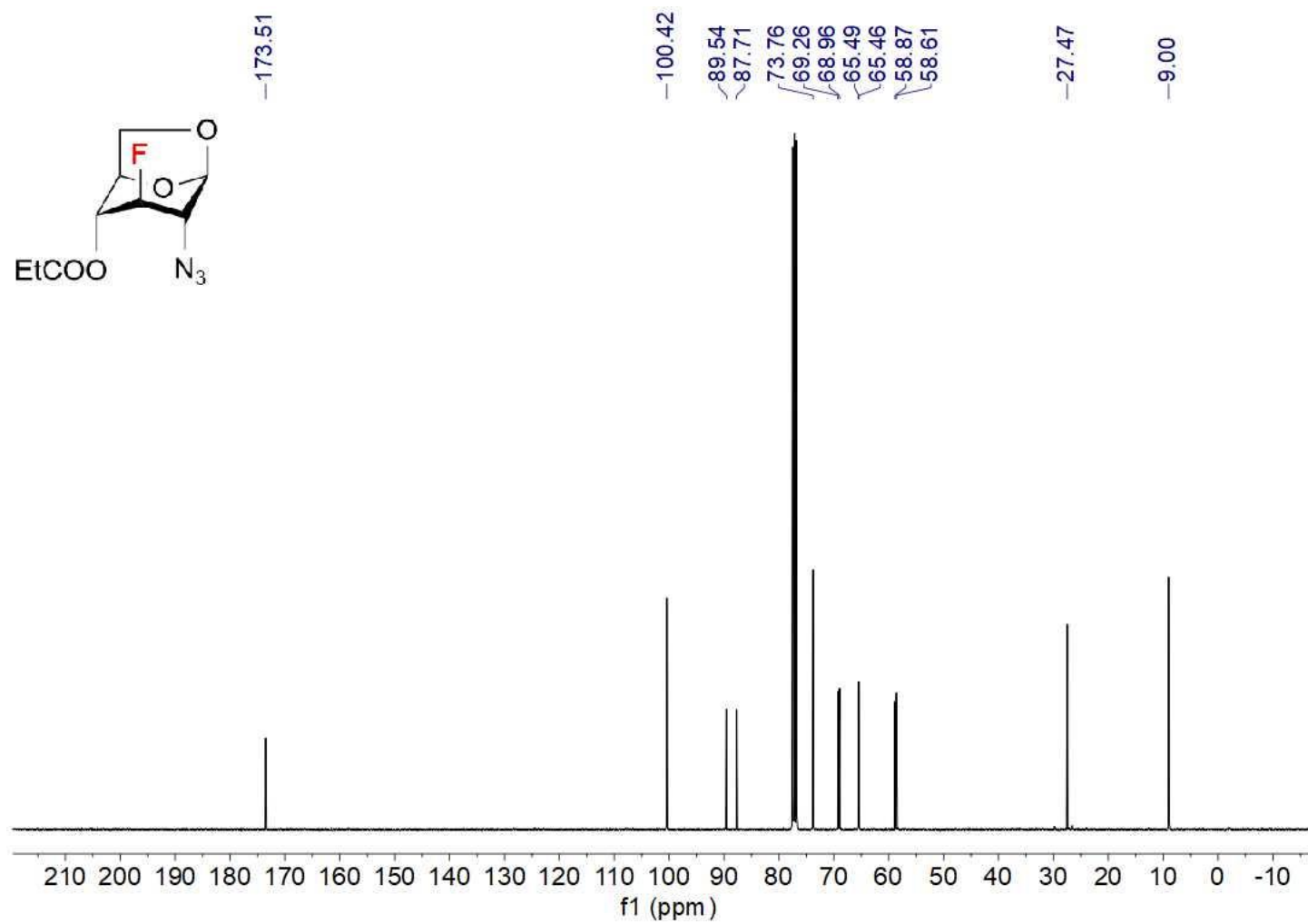


NMR COMPOUND 40

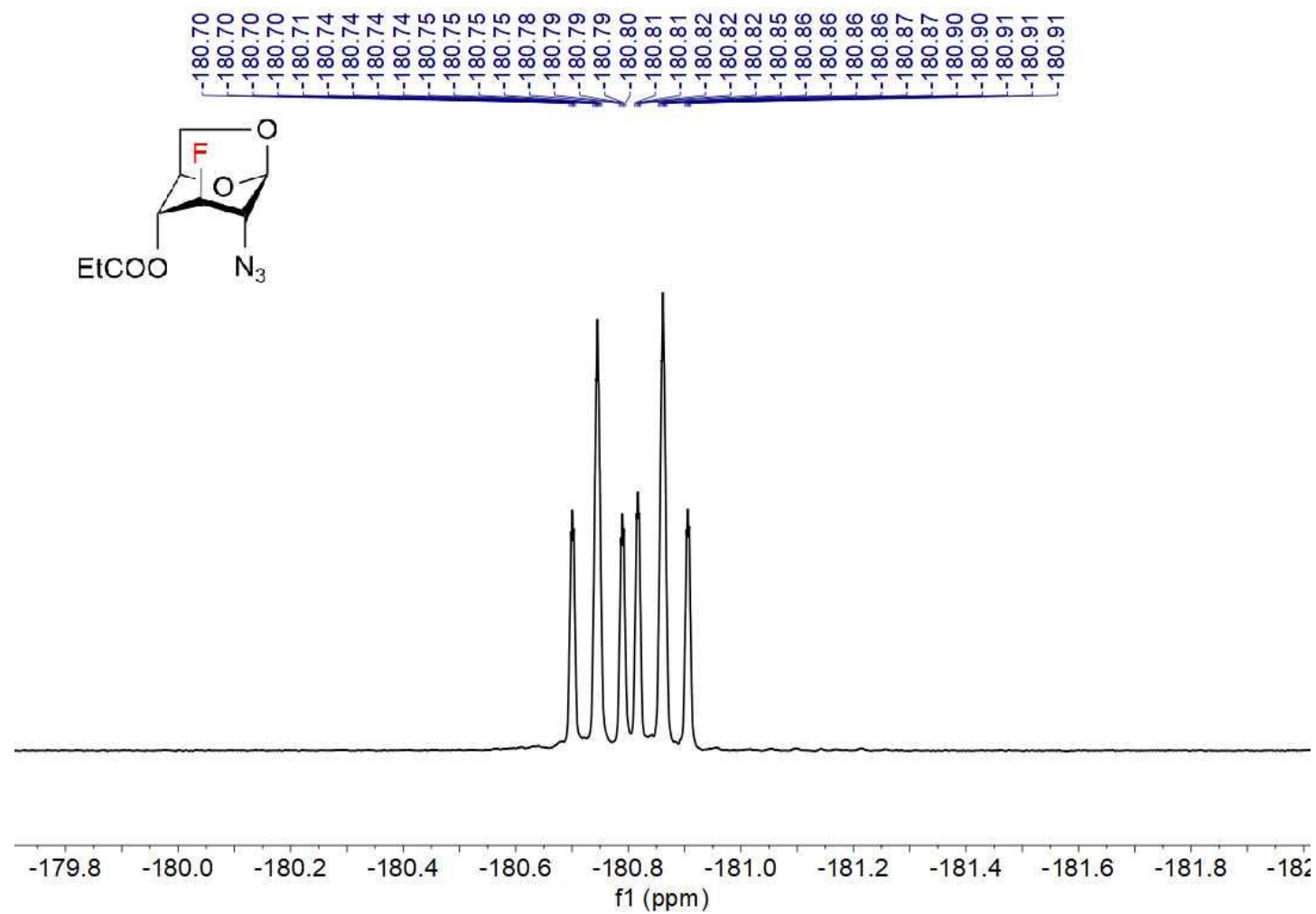
^1H NMR (400 MHz, CDCl_3) 40



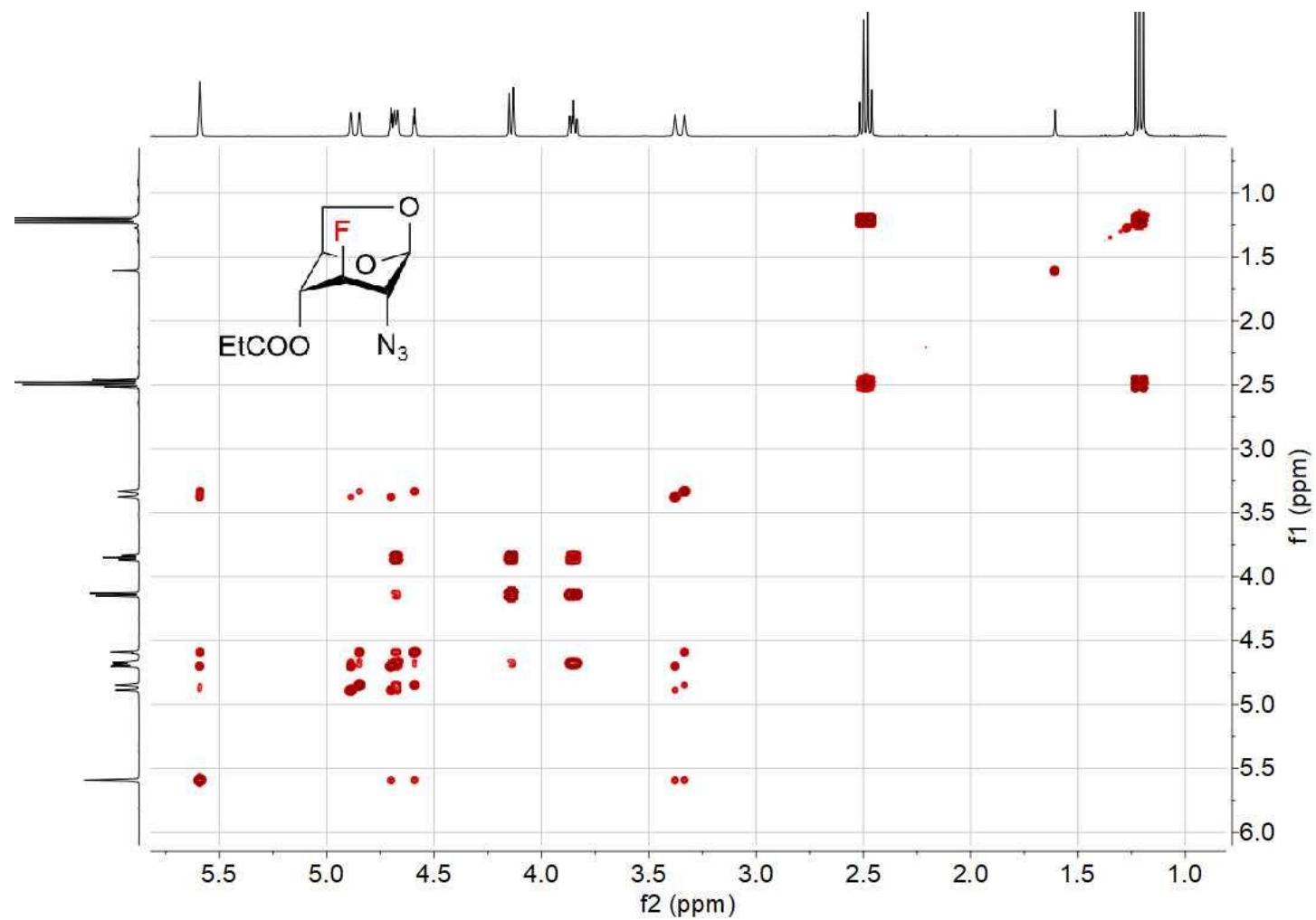
^{13}C NMR (100 MHz, CDCl_3) 40



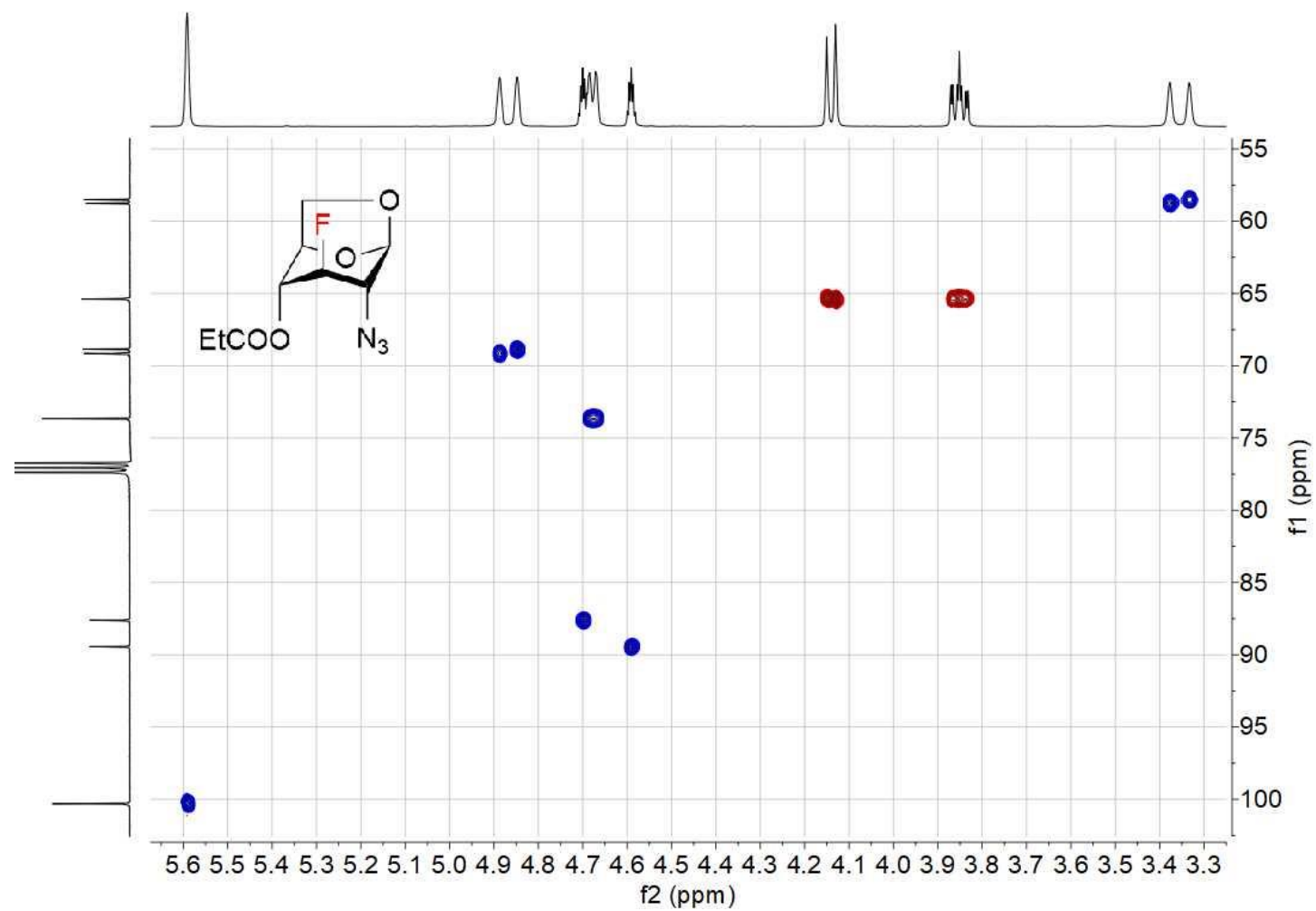
¹⁹F NMR (376 MHz, CDCl₃) 40



^1H - ^1H COSY 40

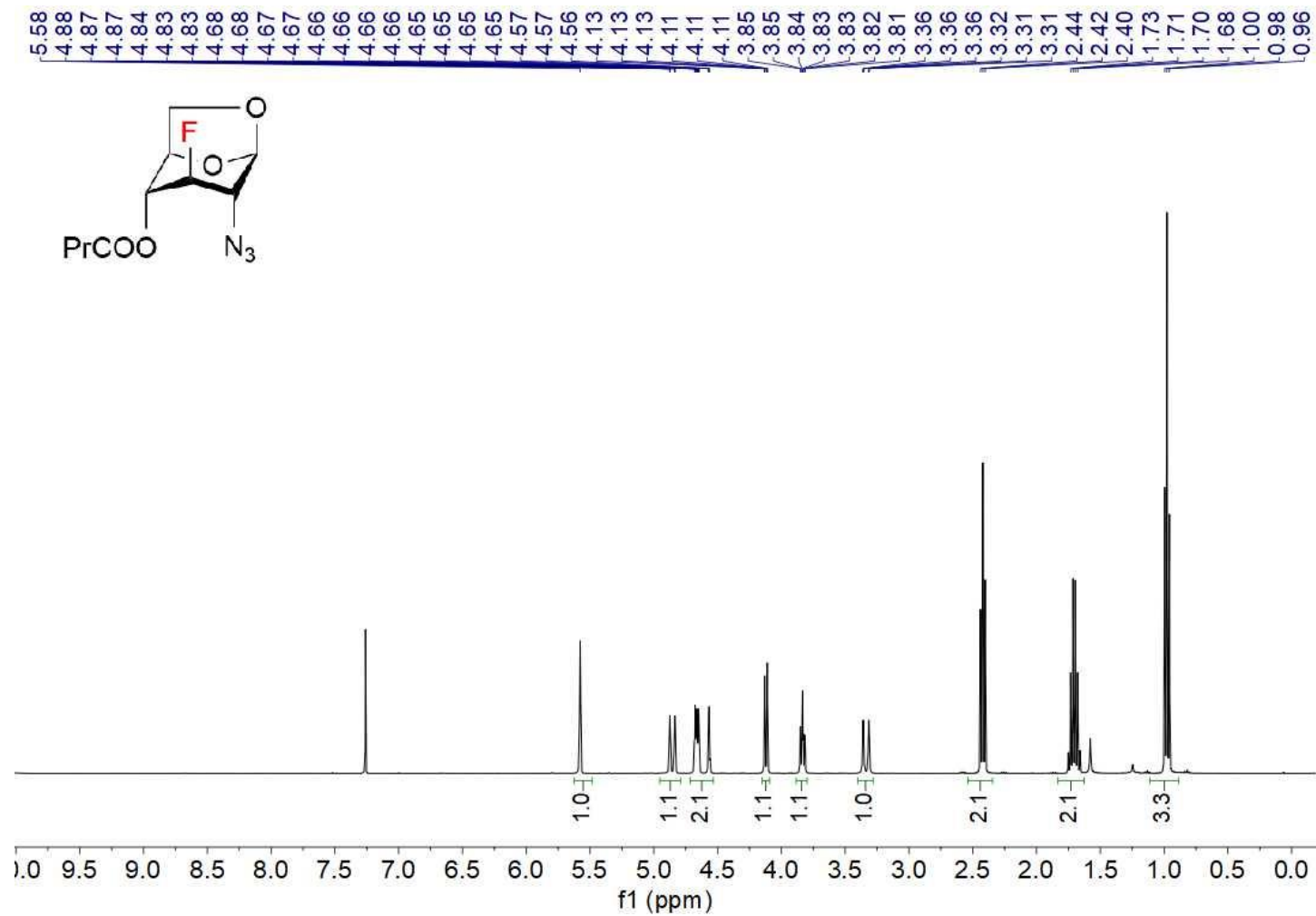


^1H - ^{13}C HSQC 40

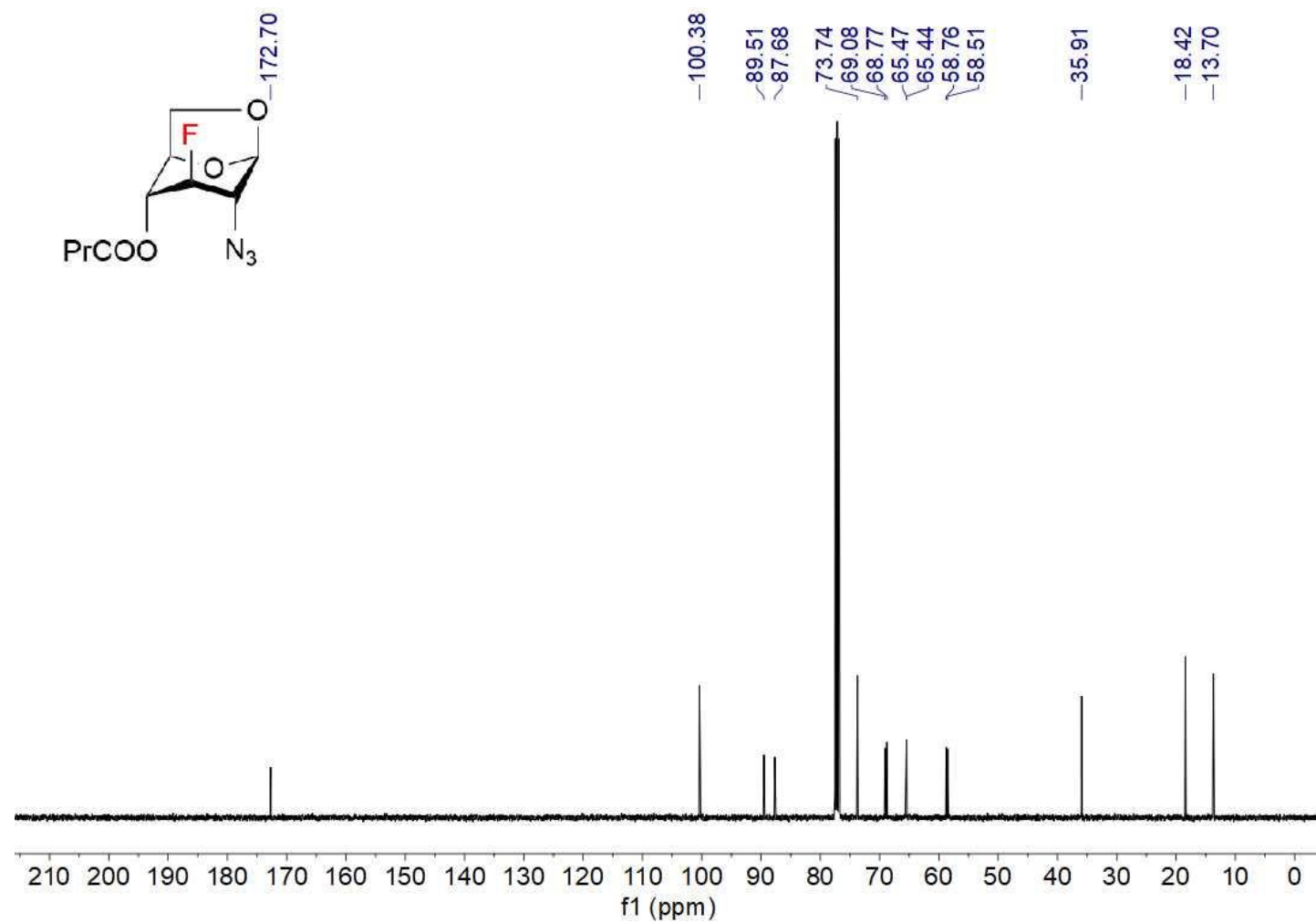


NMR COMPOUND 41

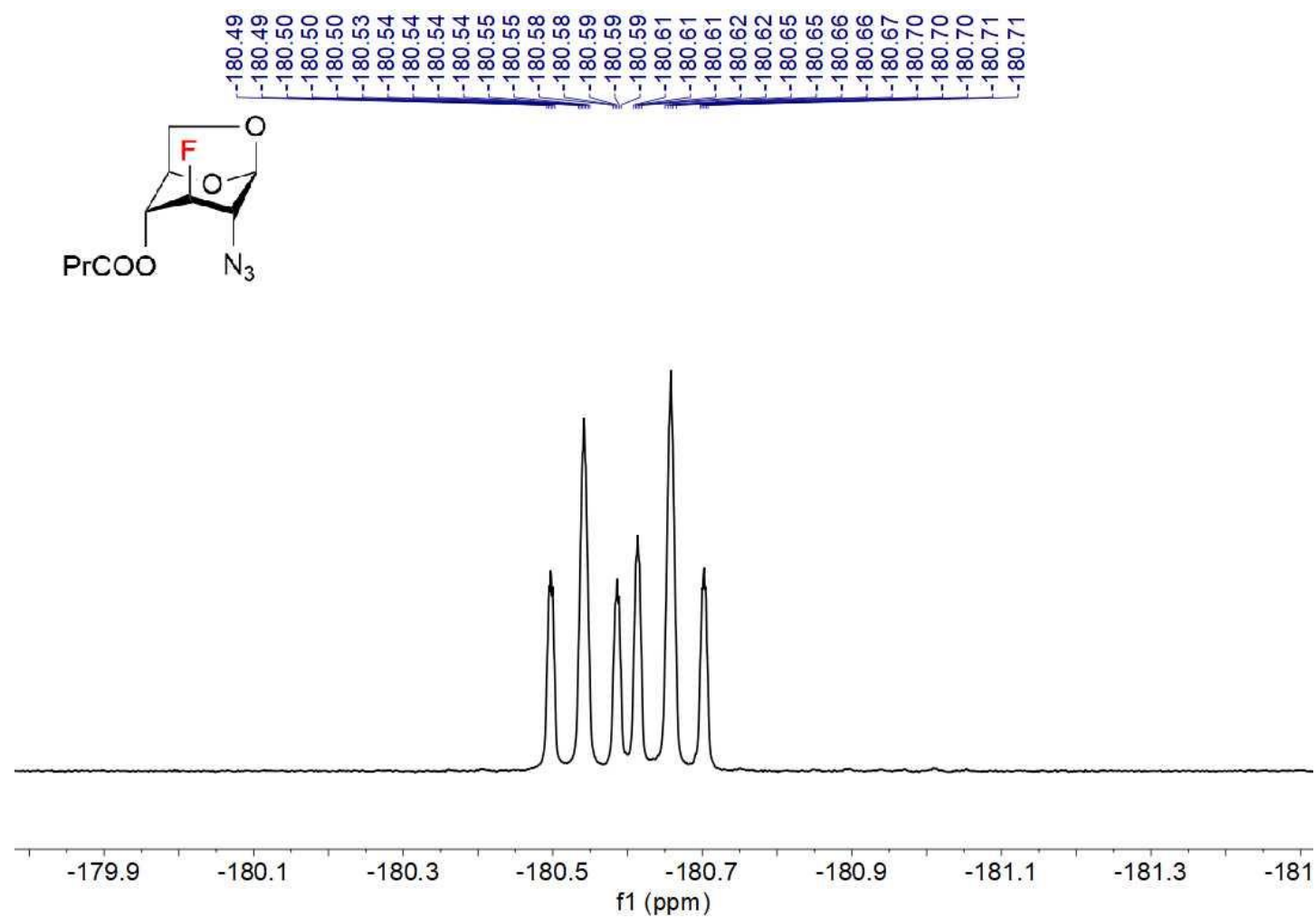
¹H NMR (400 MHz, CDCl₃) 41



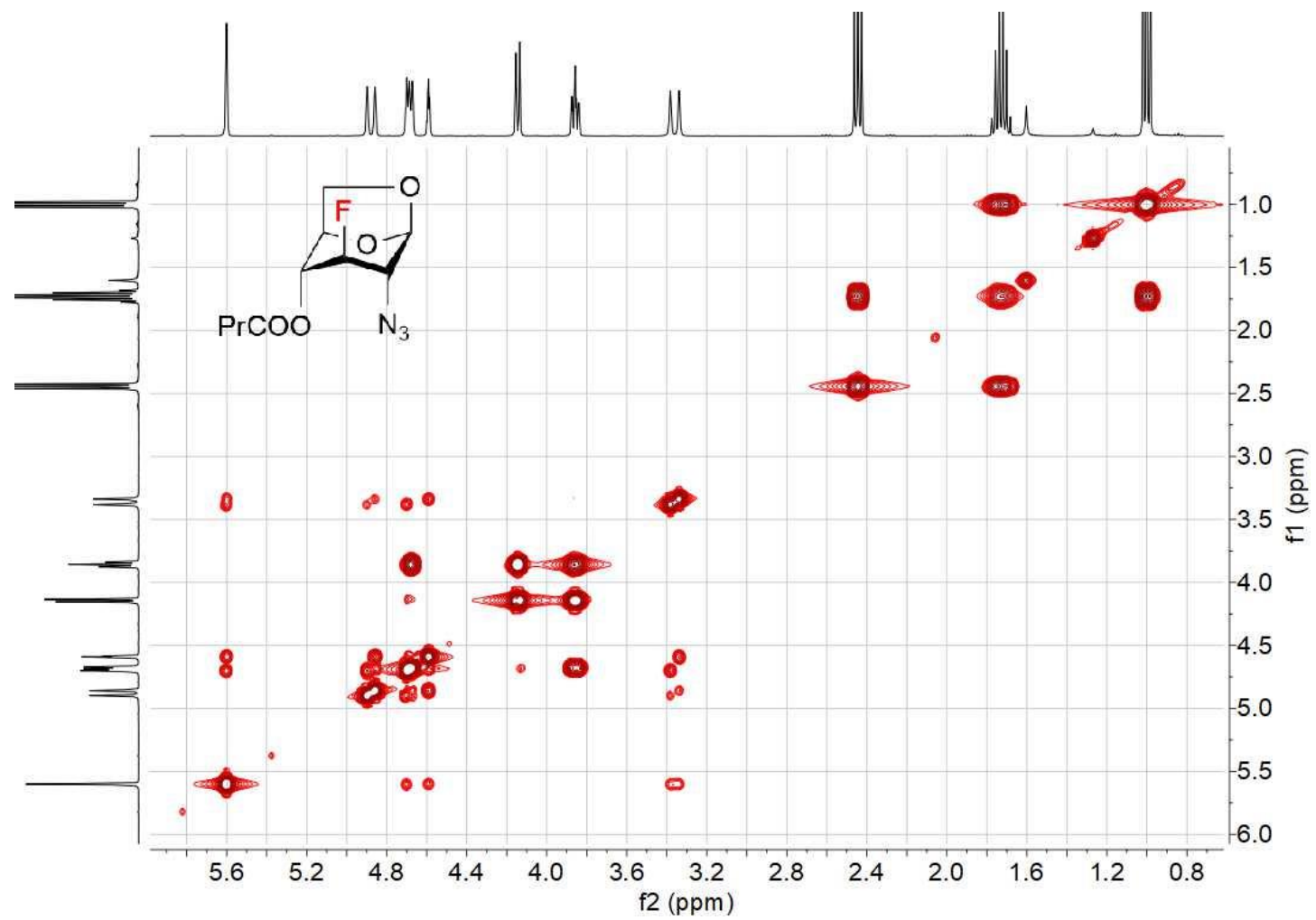
^{13}C NMR (100 MHz, CDCl_3) 41



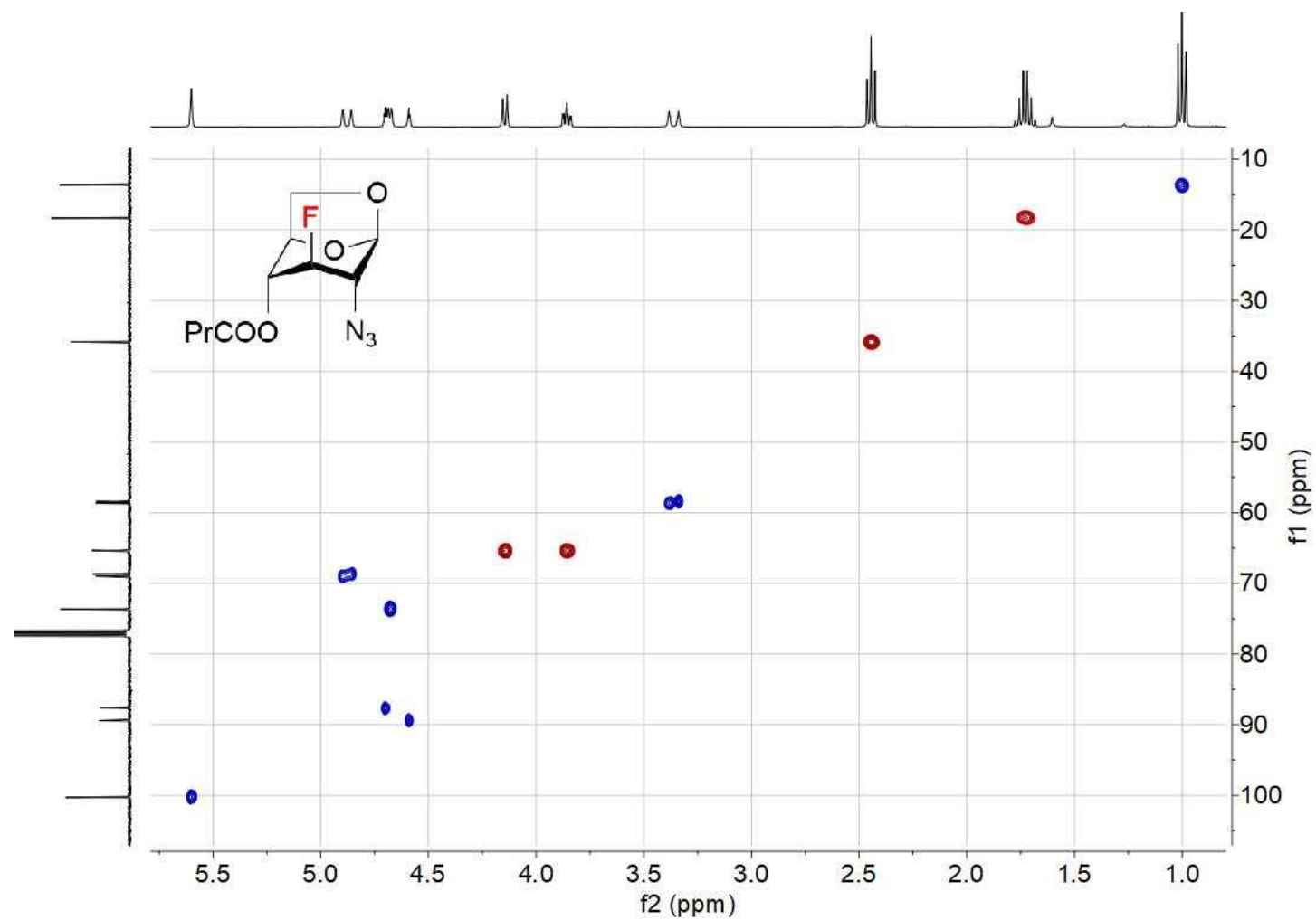
¹⁹F NMR (376 MHz, CDCl₃) 41



^1H - ^1H COSY 41

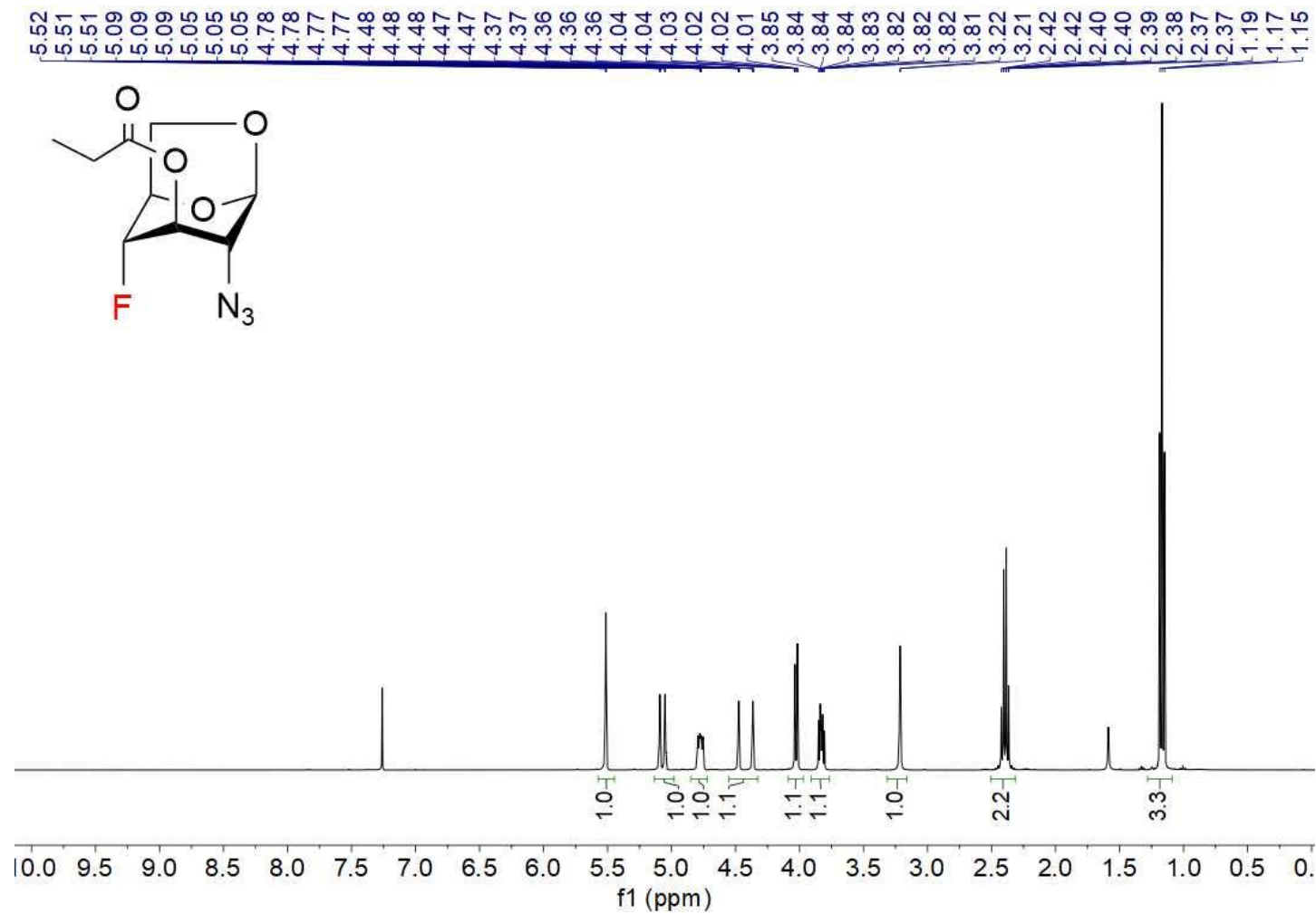


^1H - ^{13}C HSQC 41

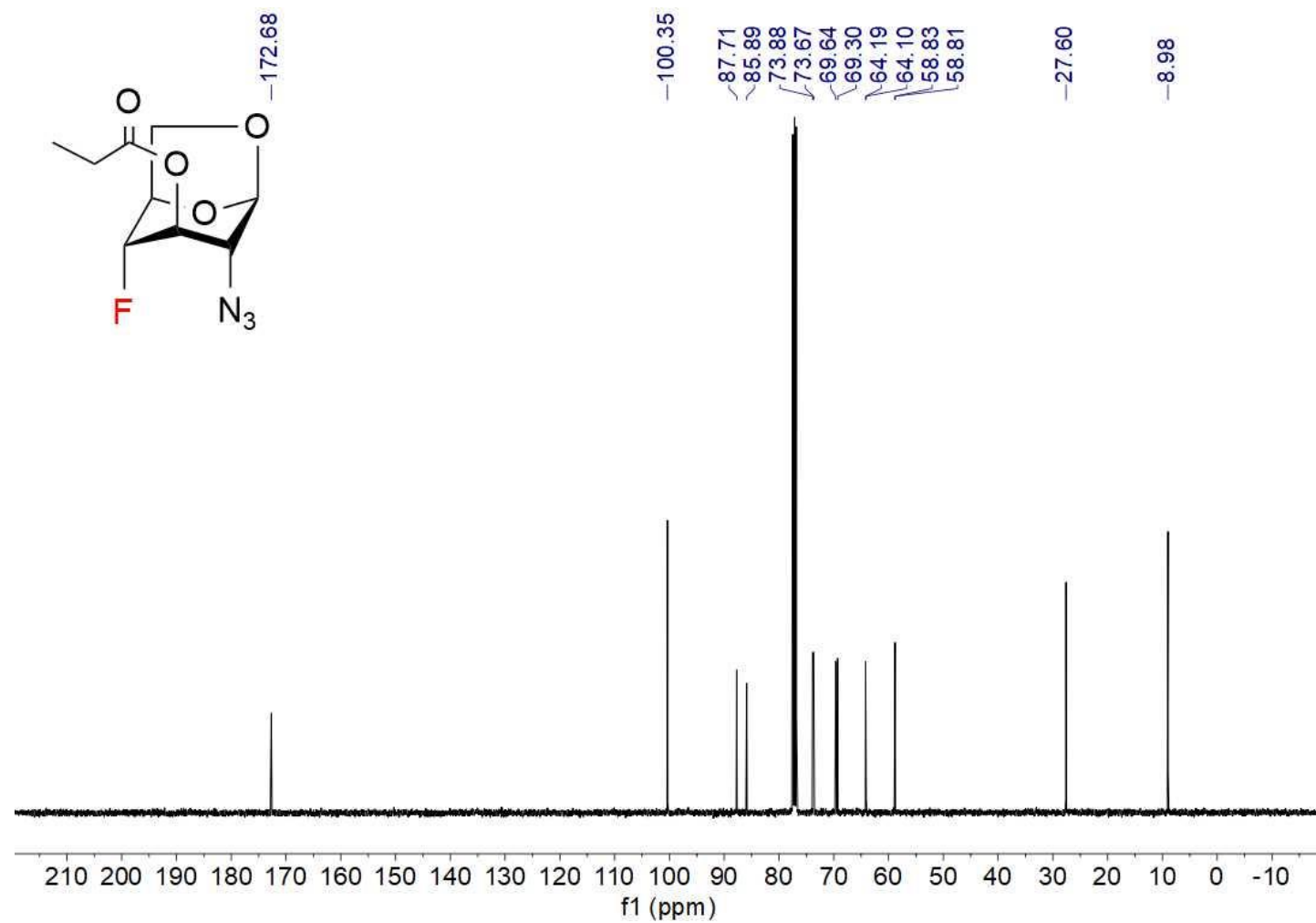


NMR COMPOUND 43

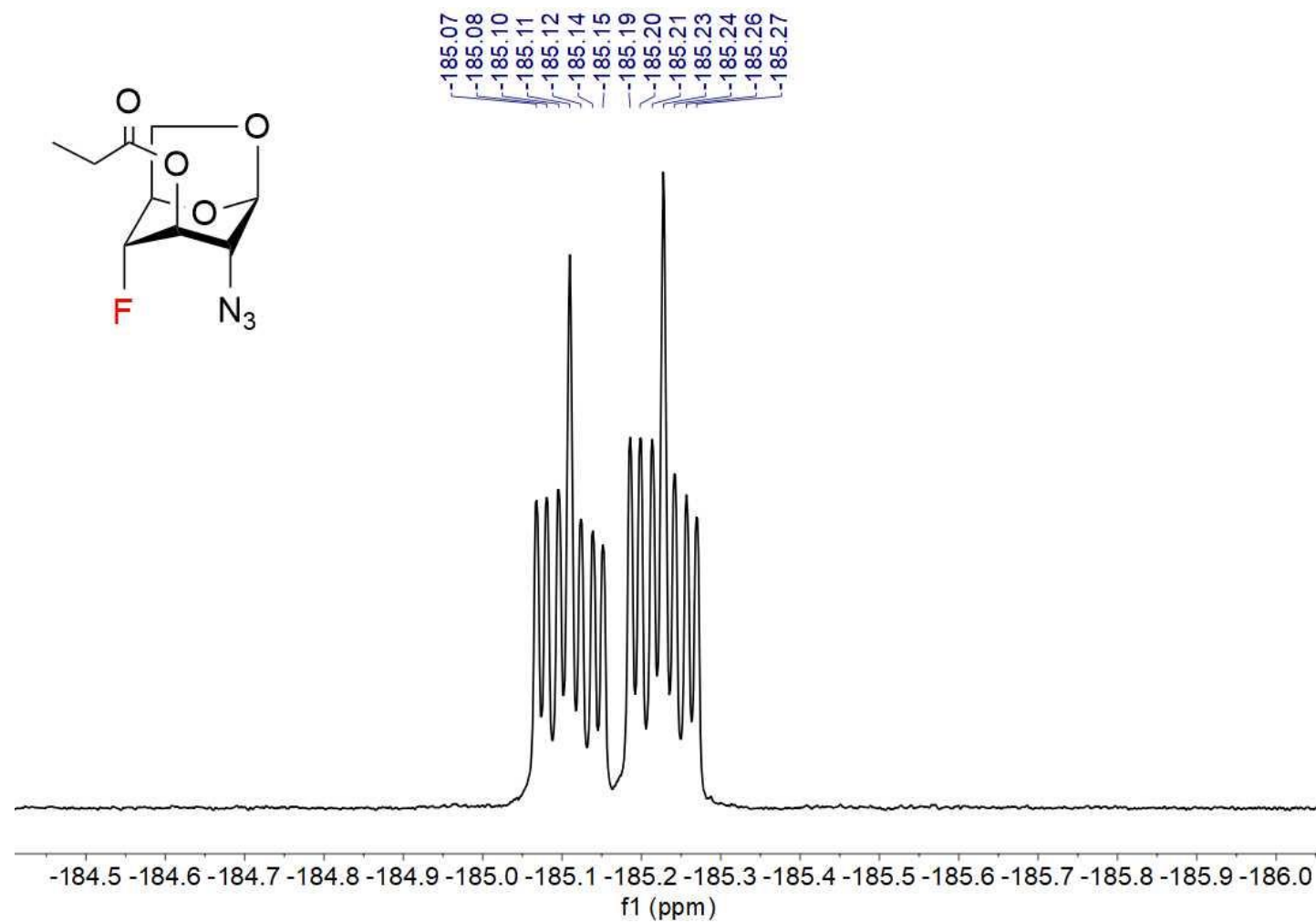
¹H NMR (400 MHz, CDCl₃) 43



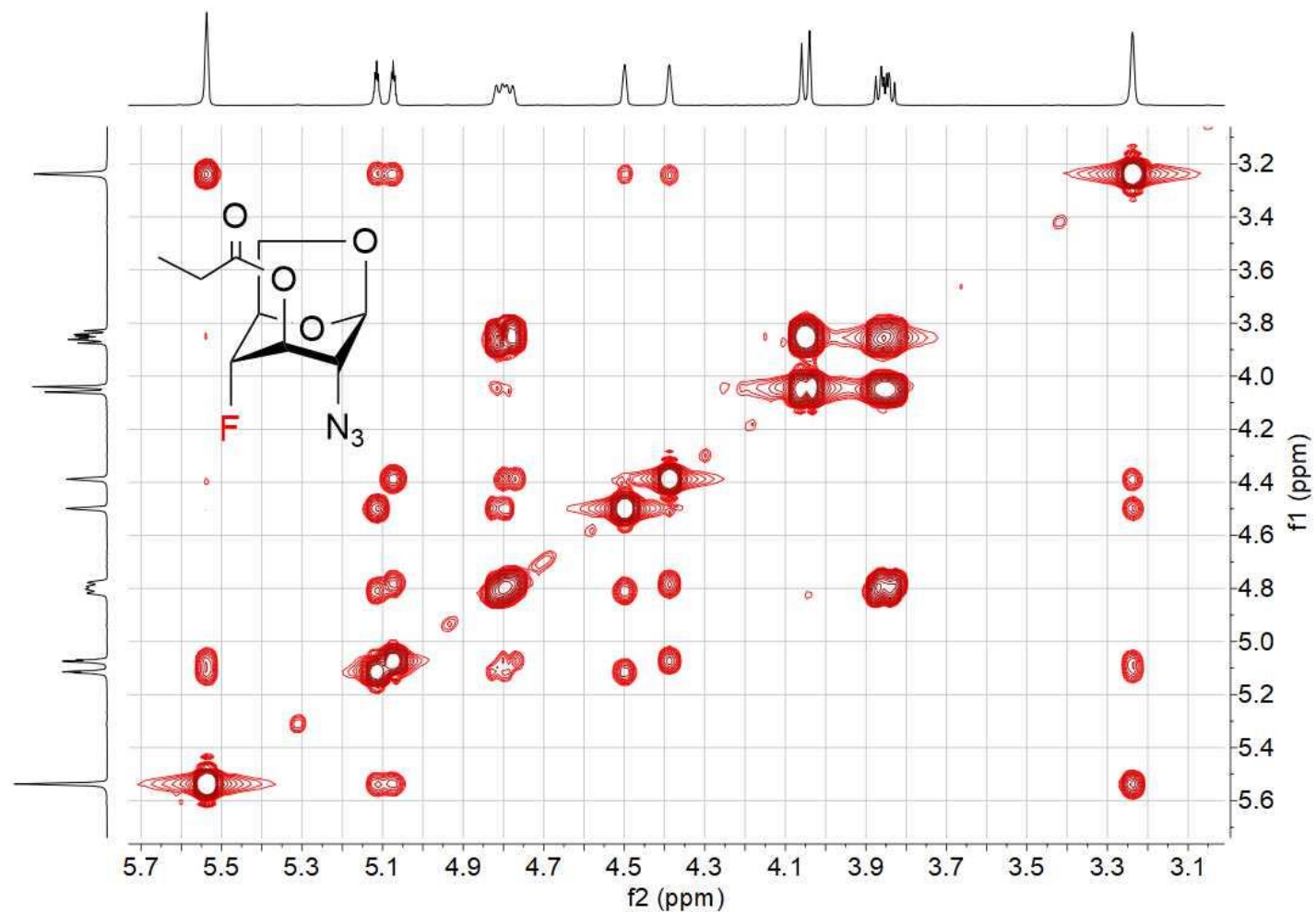
^{13}C NMR (100 MHz, CDCl_3) 43



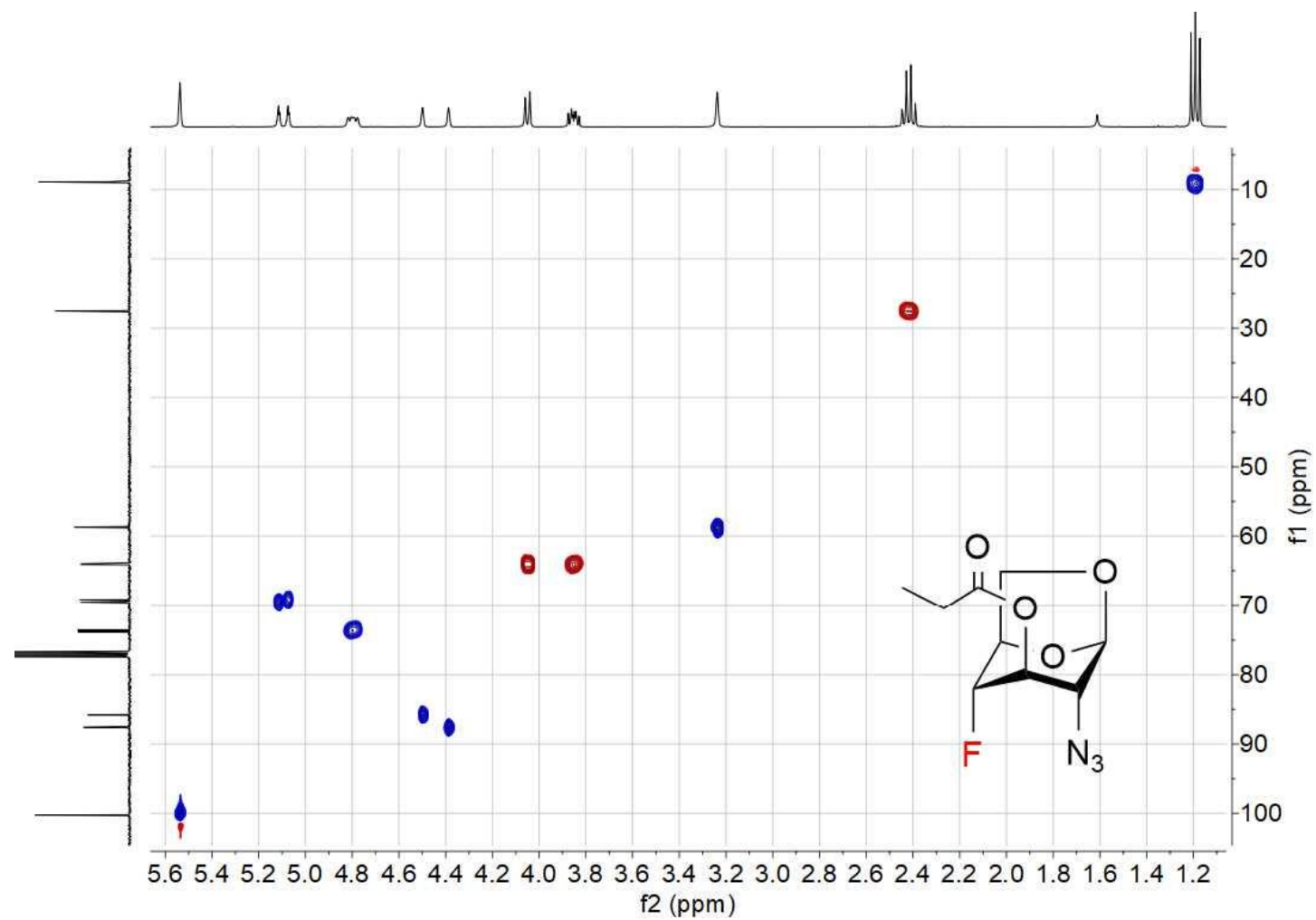
^{19}F NMR (376 MHz, CDCl_3) 43



^1H - ^1H COSY 43

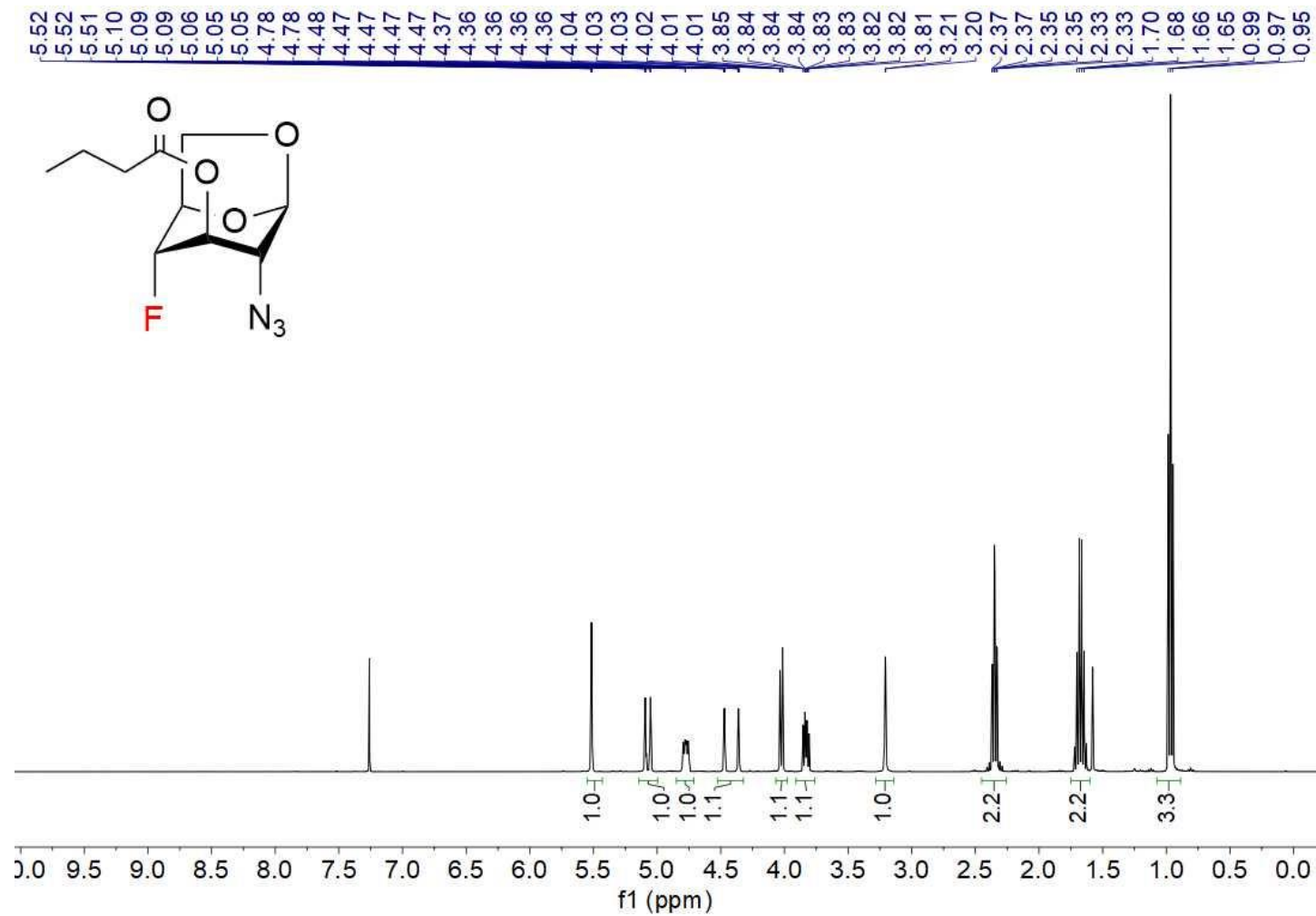


^1H - ^{13}C HSQC 43

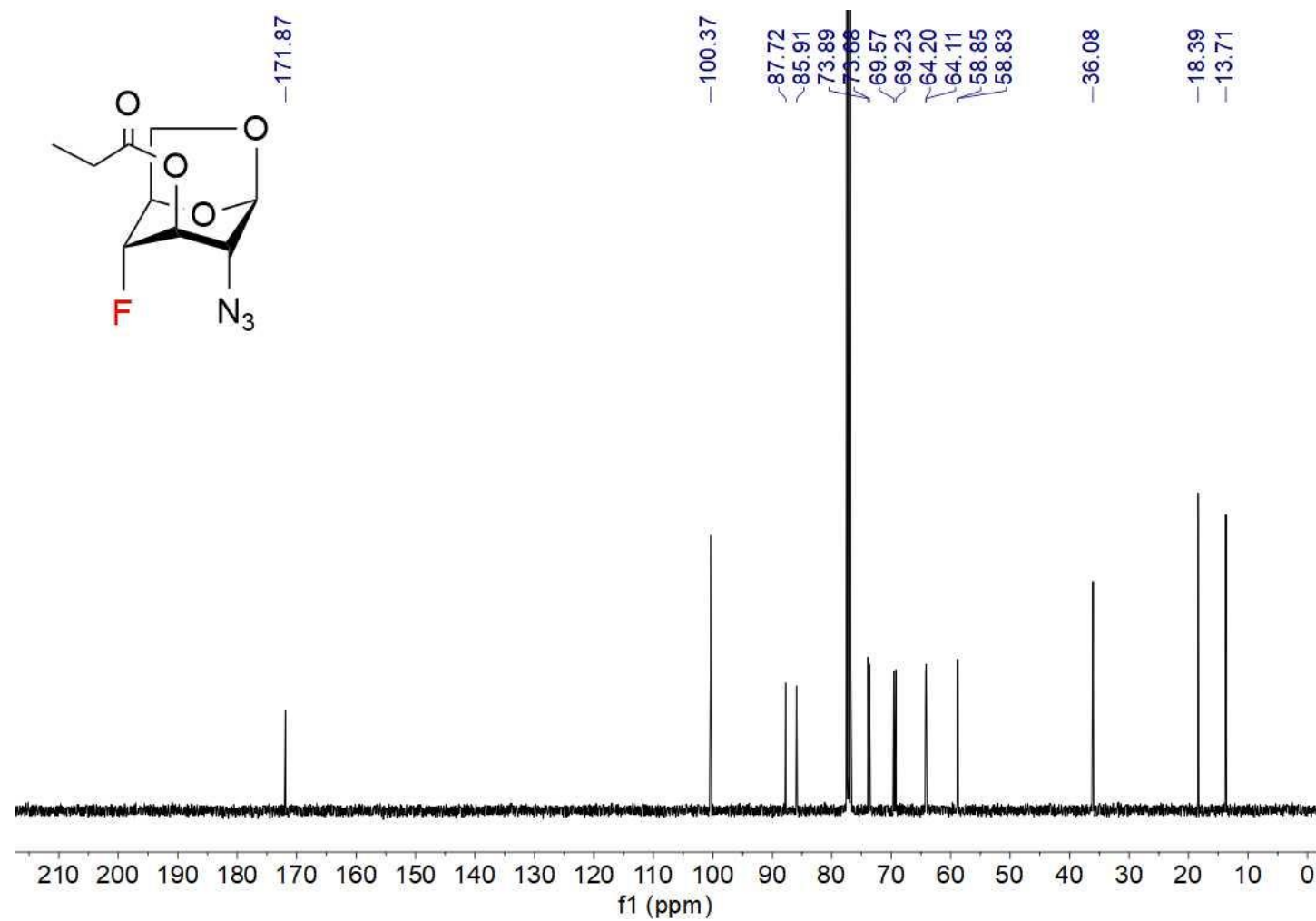


NMR COMPOUND 44

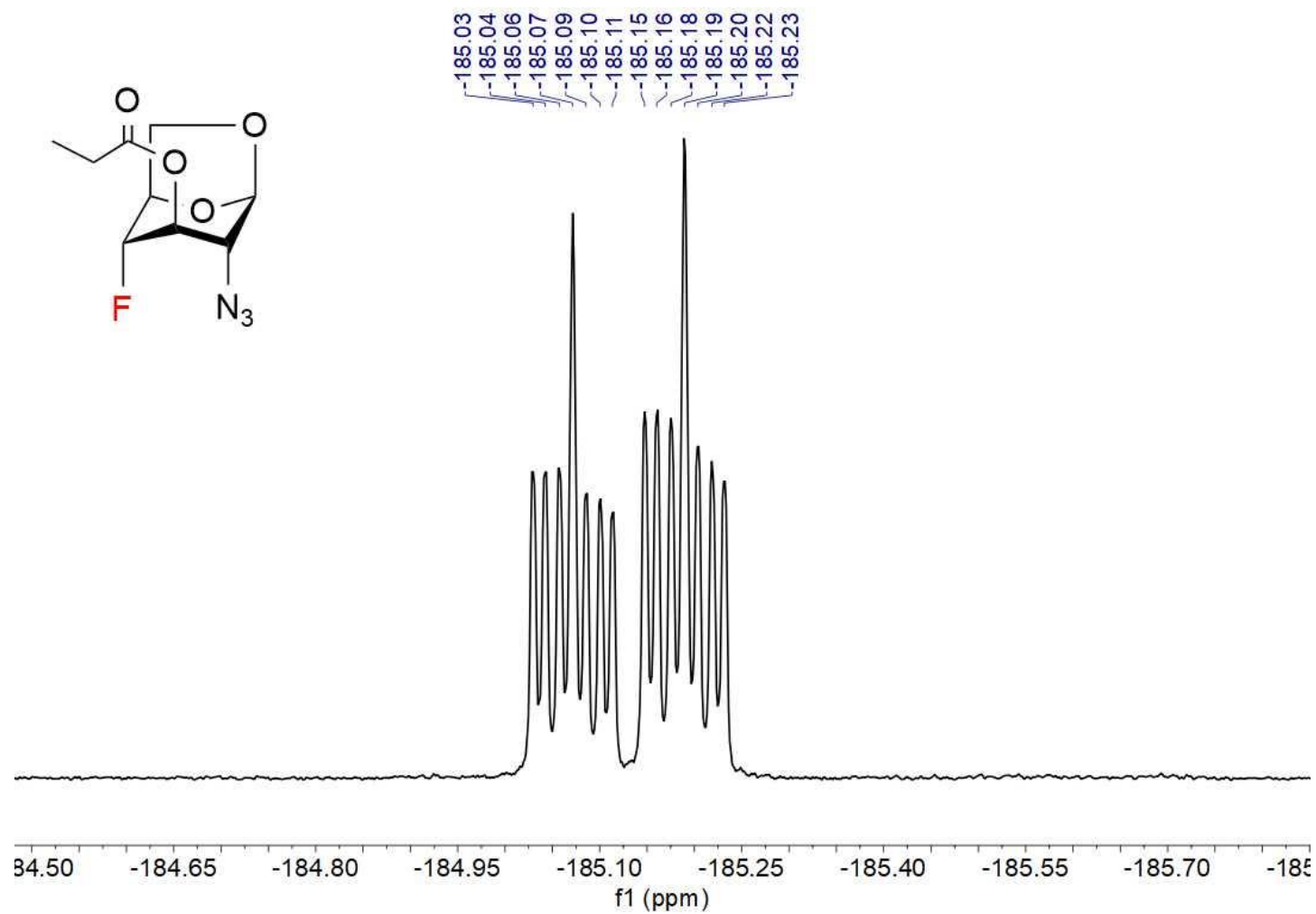
^1H NMR (400 MHz, CDCl_3) 44



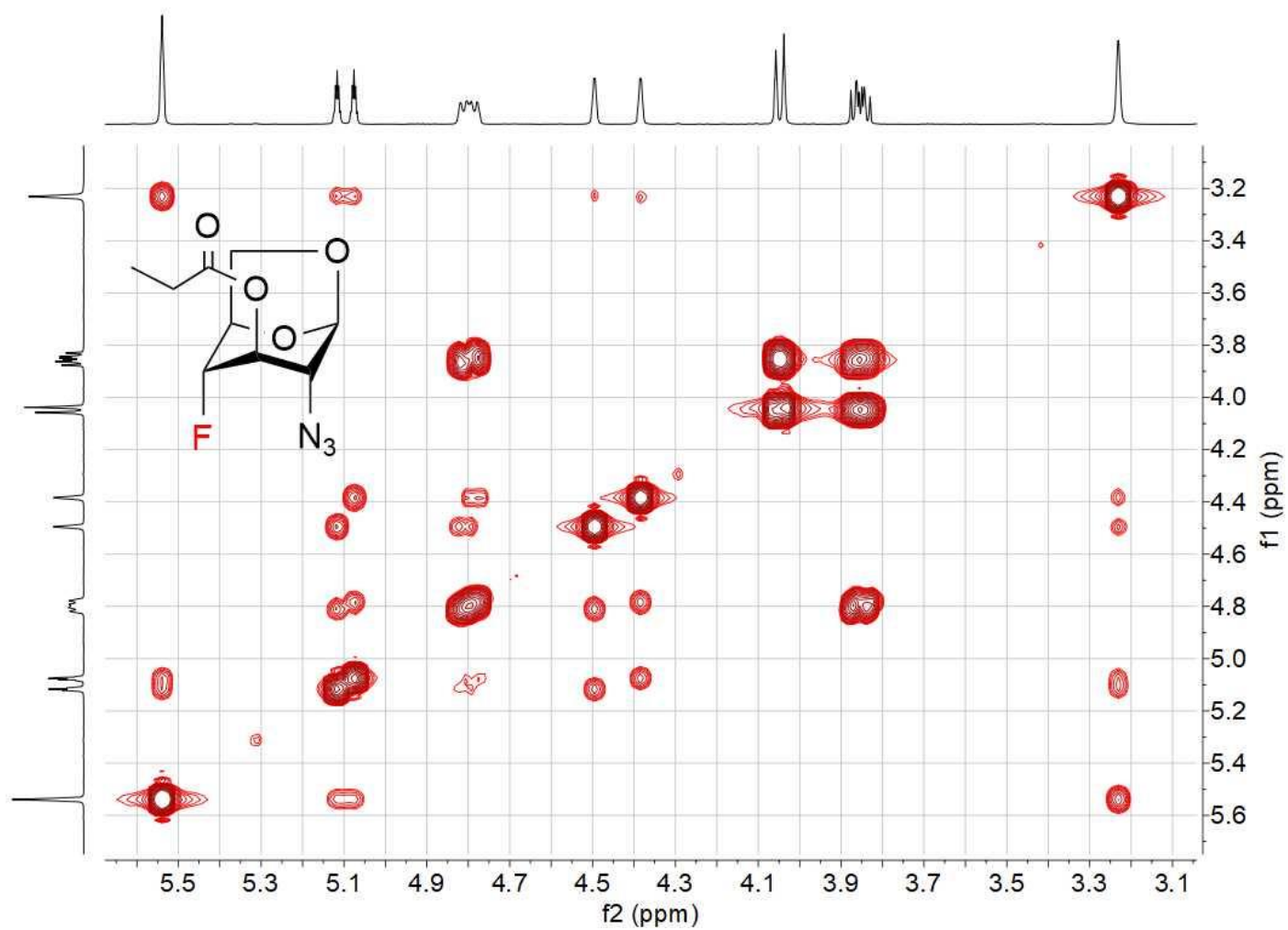
^{13}C NMR (100 MHz, CDCl_3) 44



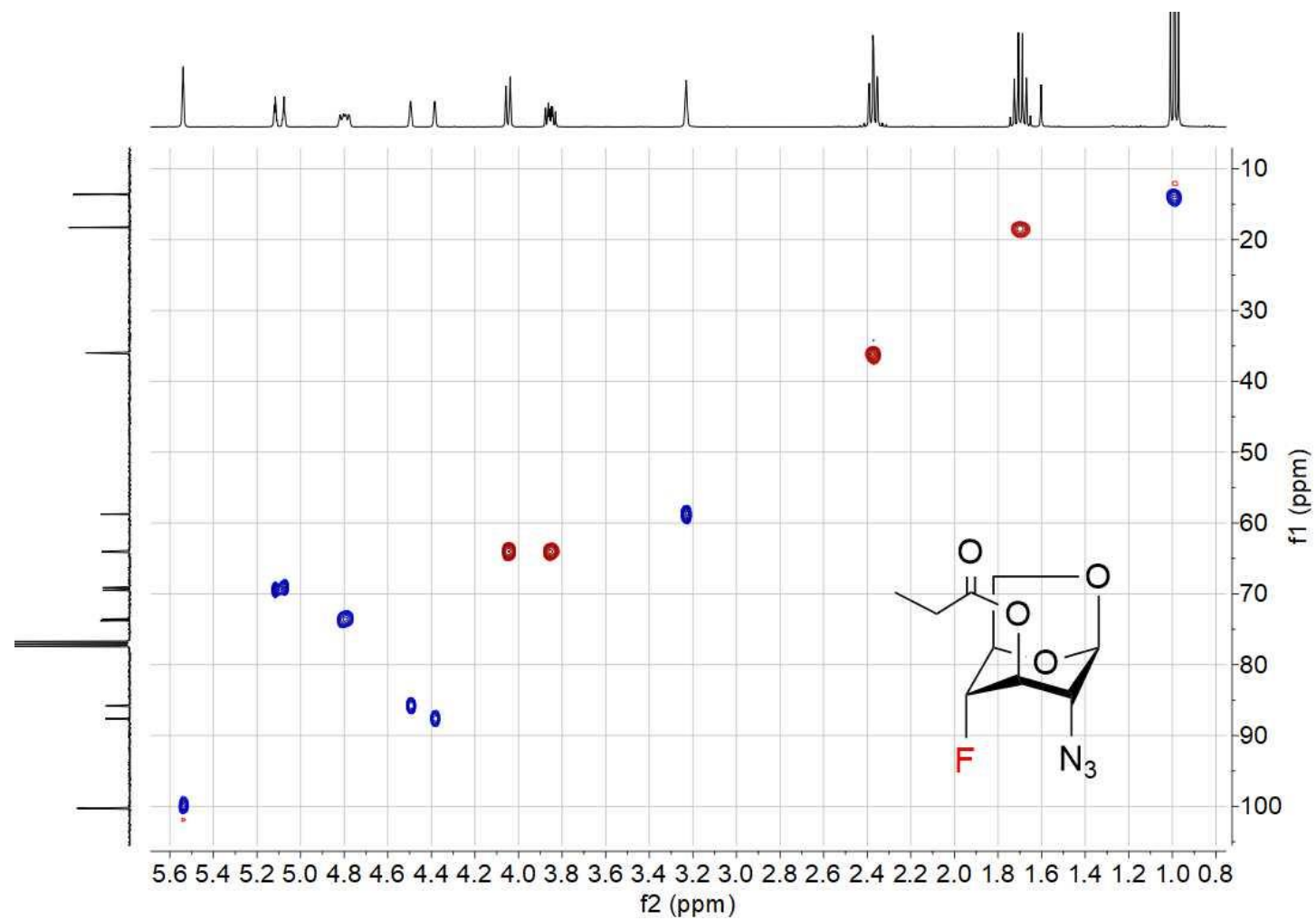
^{19}F NMR (376 MHz, CDCl_3) 44



^1H - ^1H COSY 44

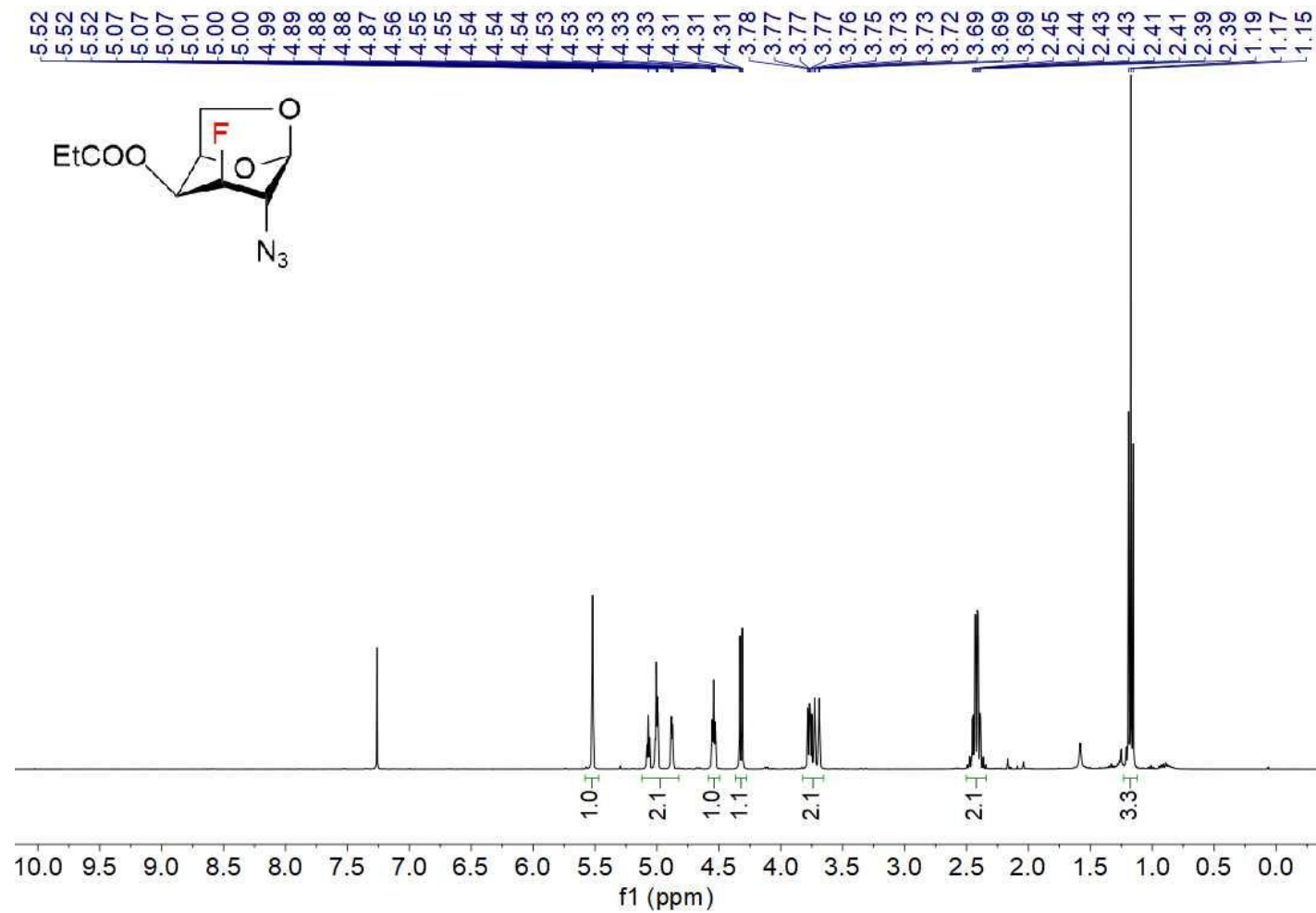


^1H - ^{13}C HSQC 44

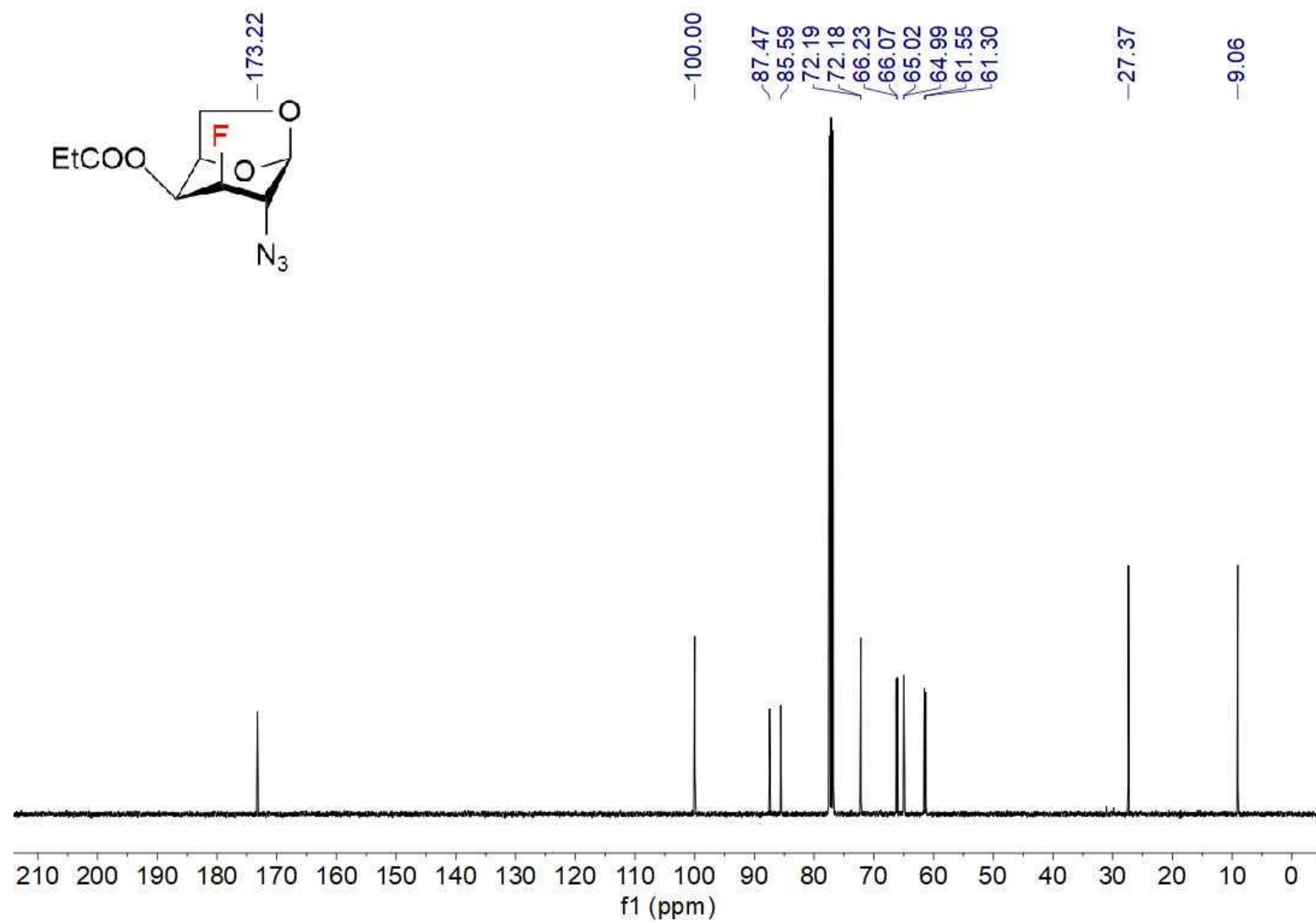


NMR COMPOUND 45

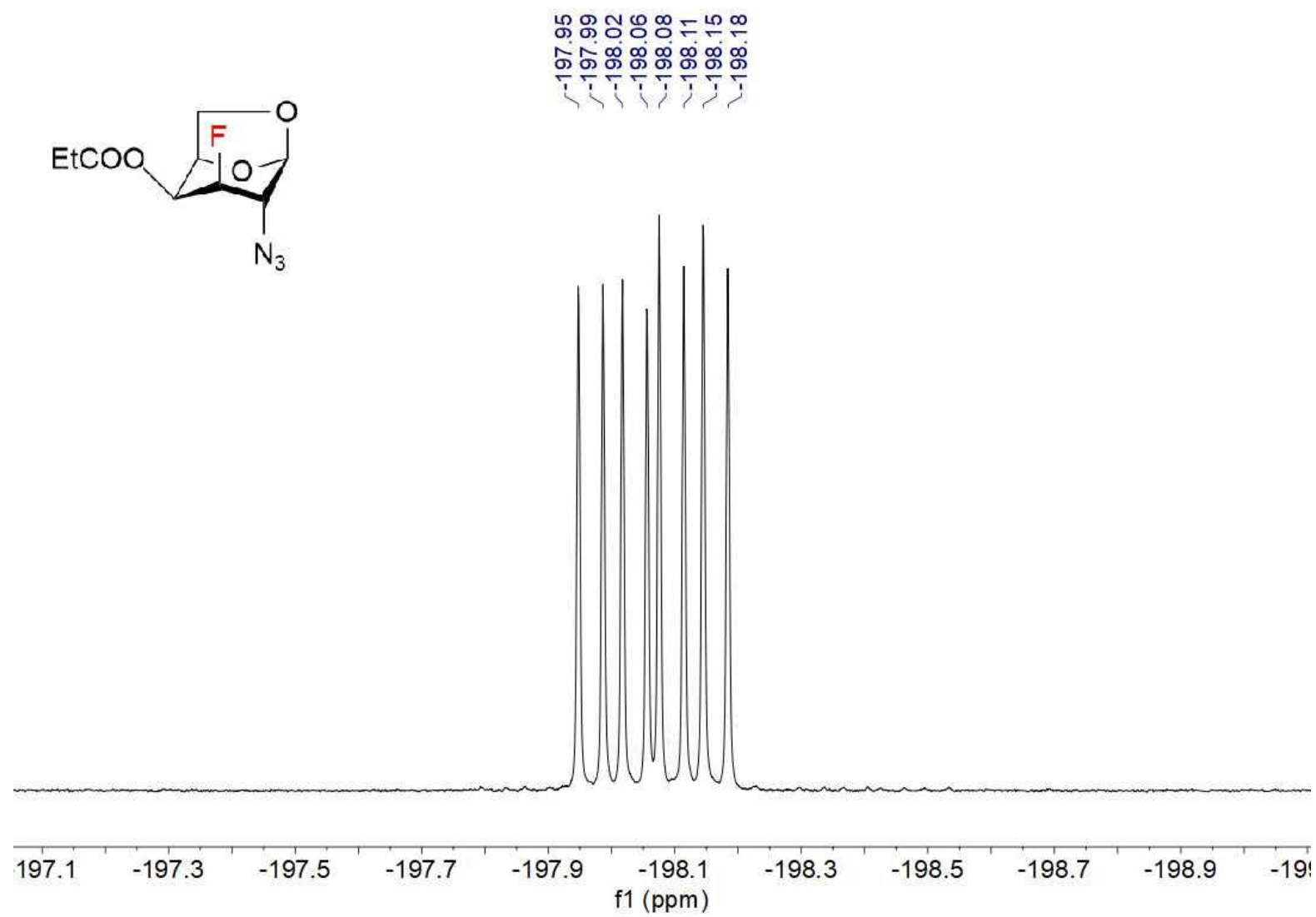
^1H NMR (400 MHz, CDCl_3) 45



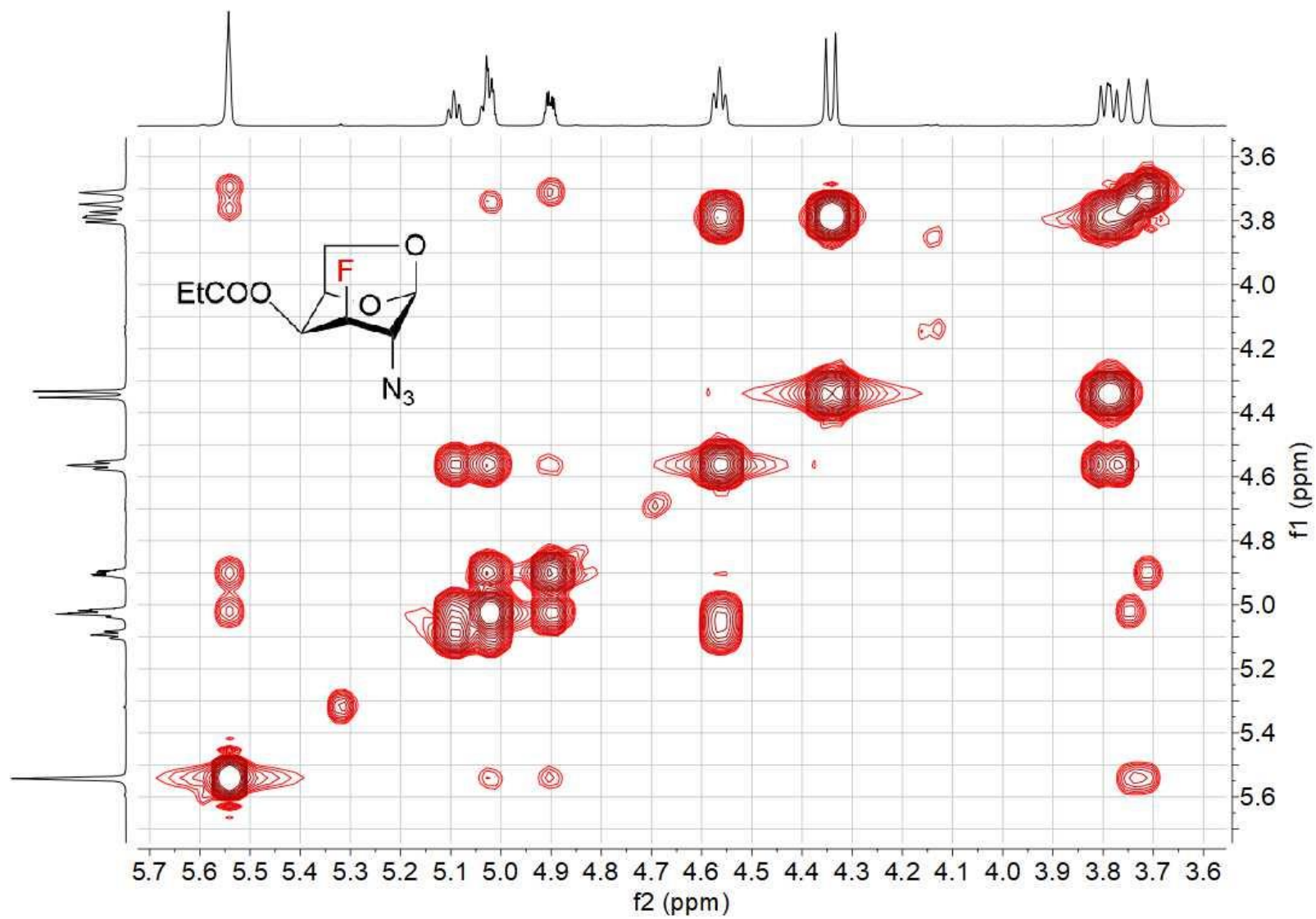
^{13}C NMR (100 MHz, CDCl_3) 45



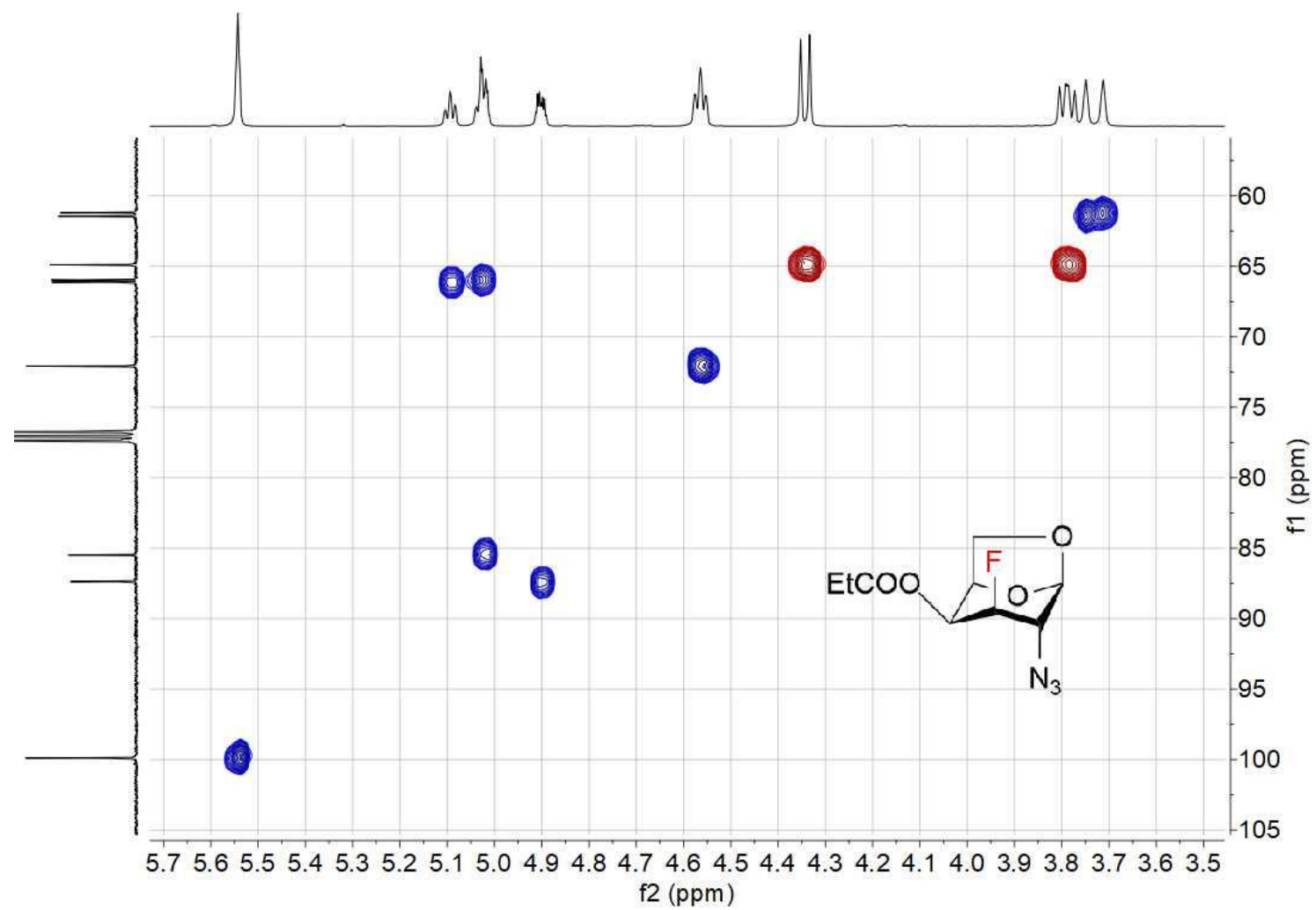
^{19}F NMR (376 MHz, CDCl_3) 45



^1H - ^1H COSY 45

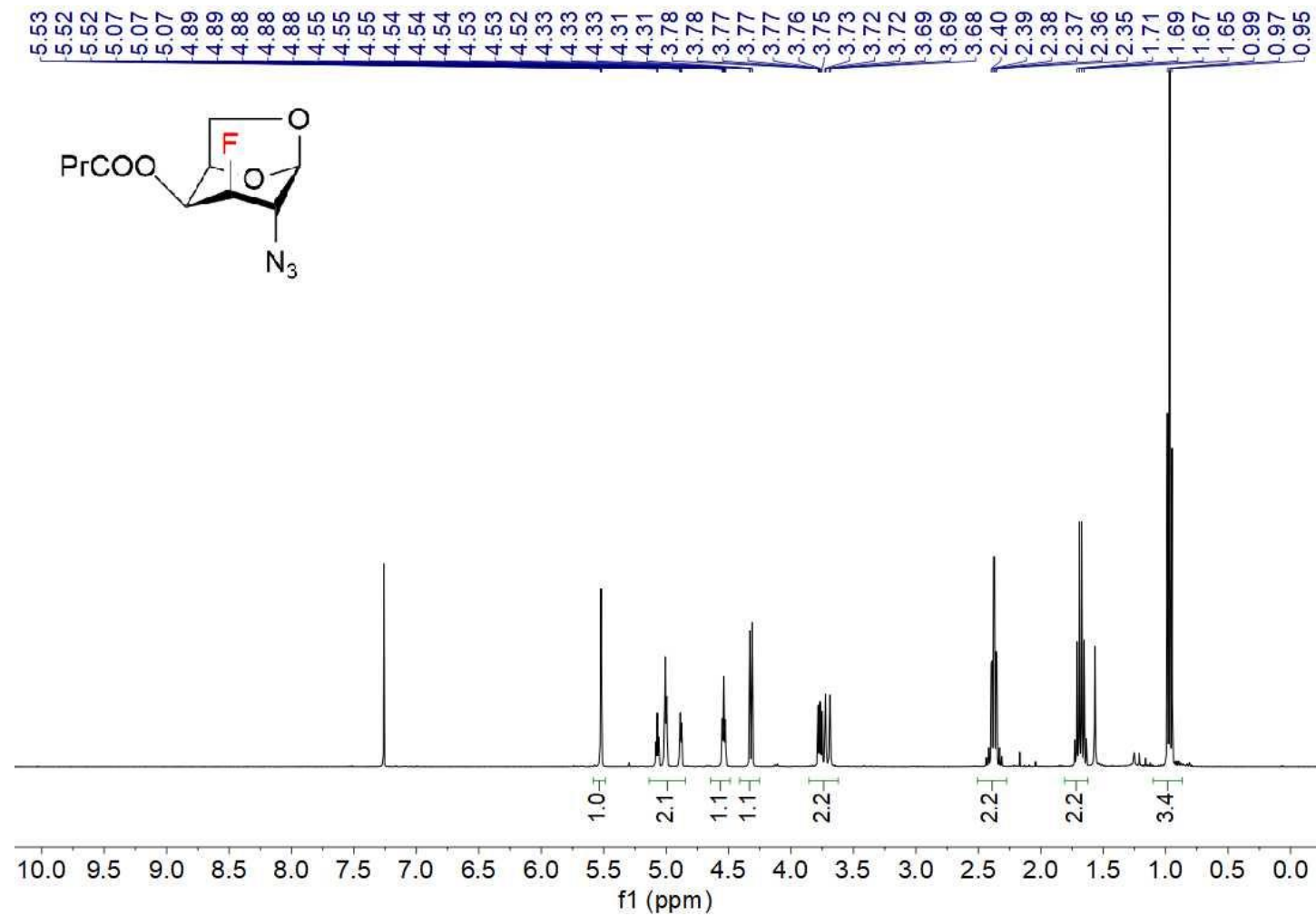


^1H - ^{13}C HSQC 45

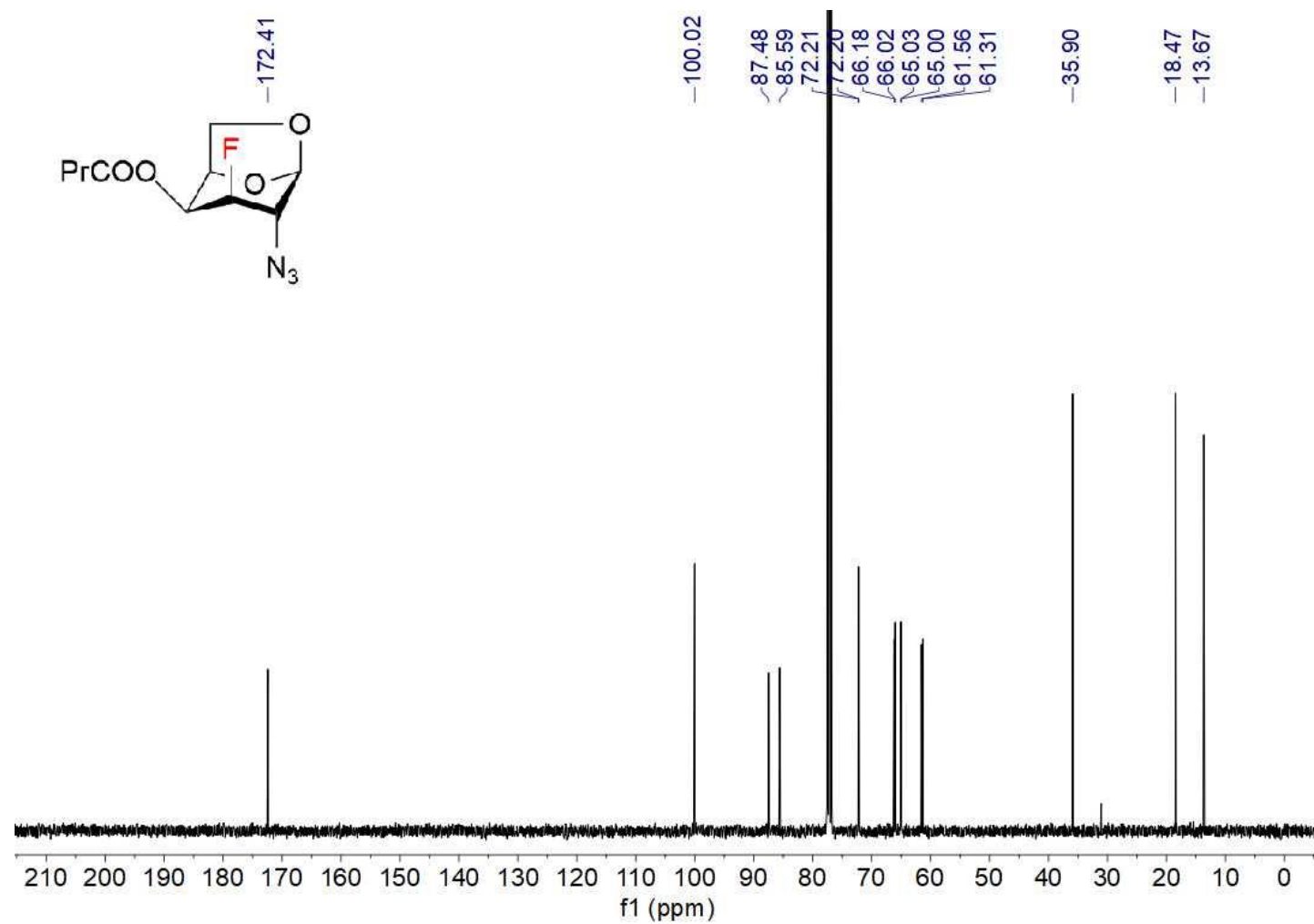


NMR COMPOUND 46

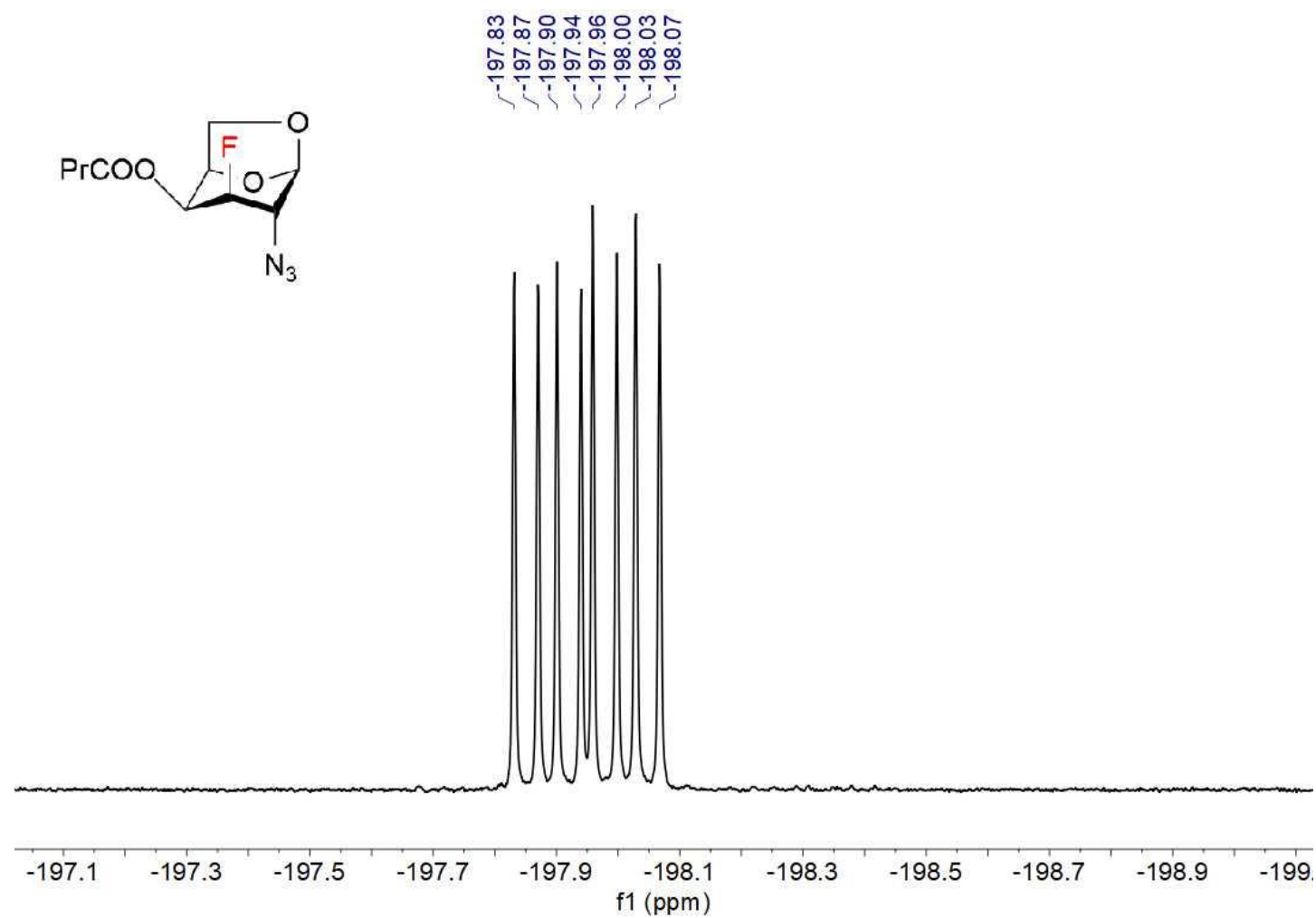
^1H NMR (400 MHz, CDCl_3) 46



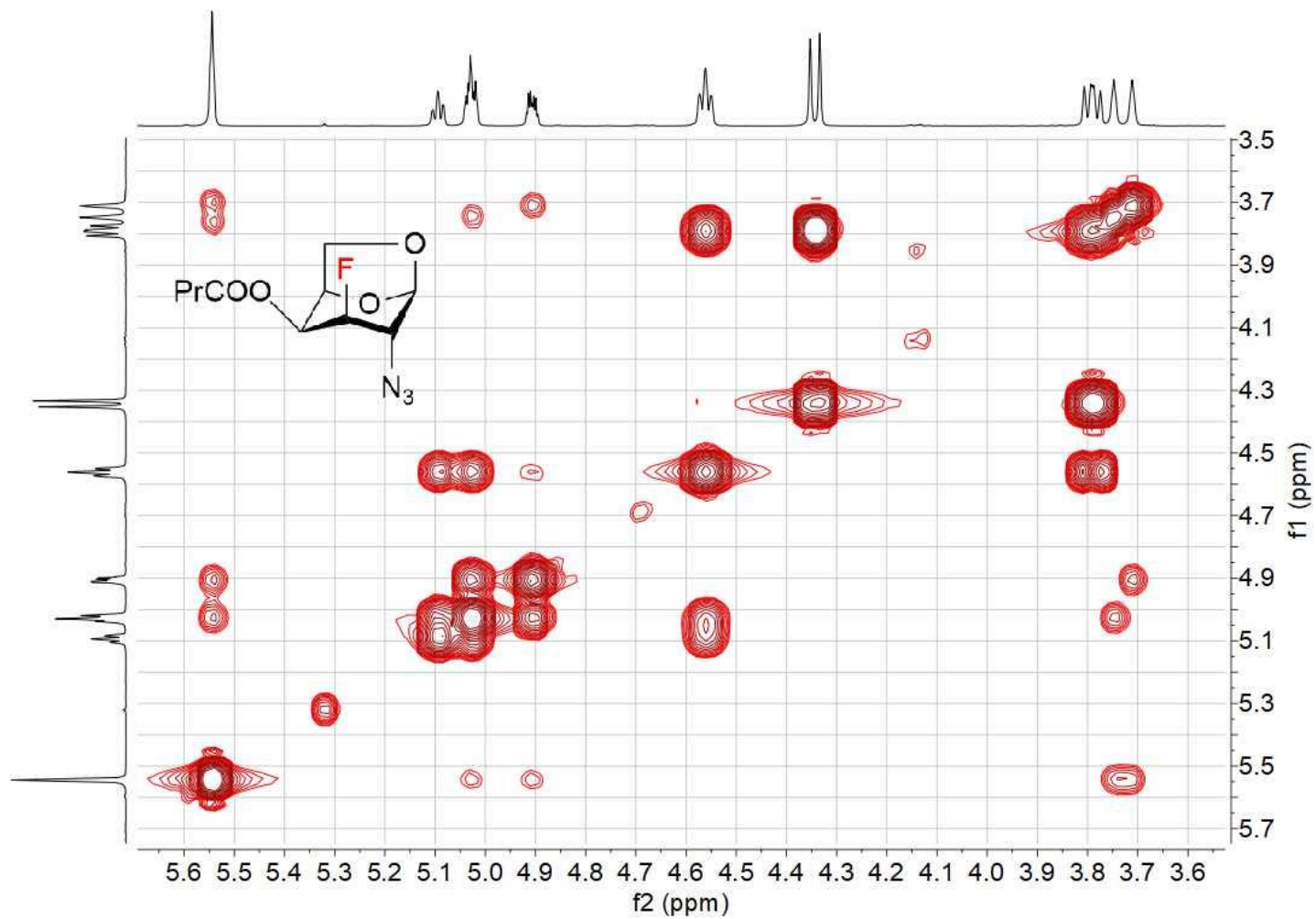
^{13}C NMR (100 MHz, CDCl_3) 46



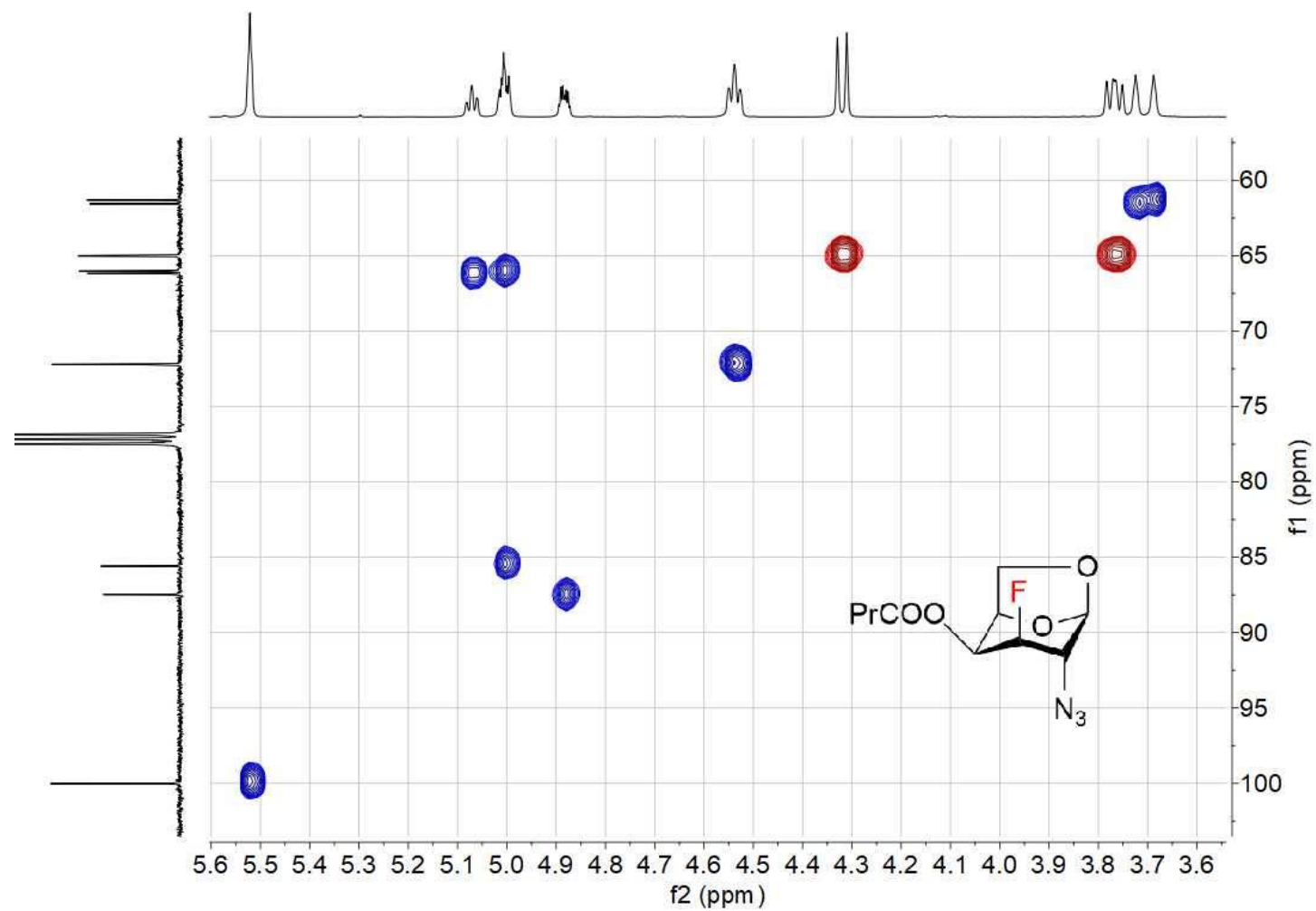
^{19}F NMR (376 MHz, CDCl_3) 46



¹H-¹H COSY 46

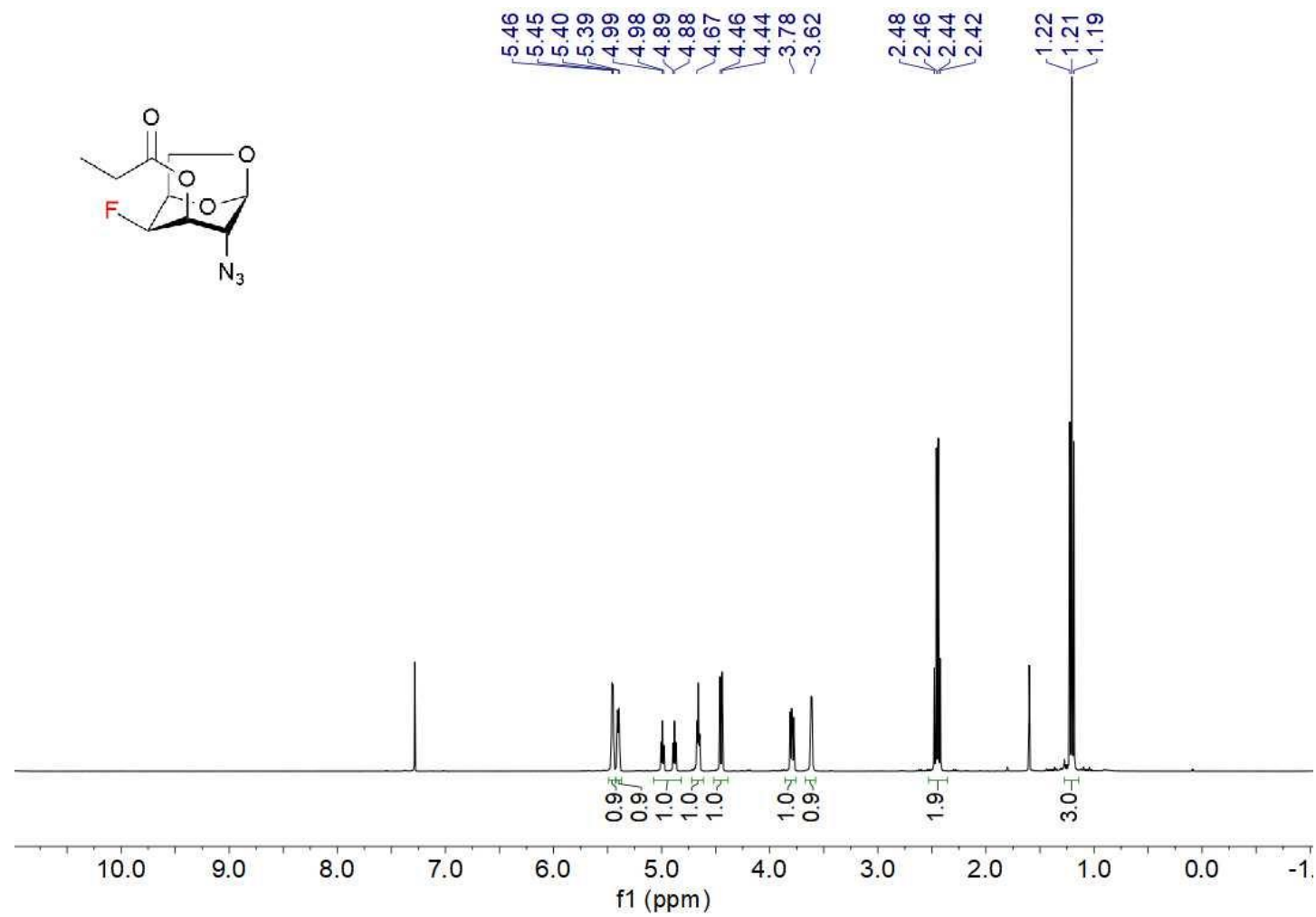


^1H - ^{13}C HSQC 46

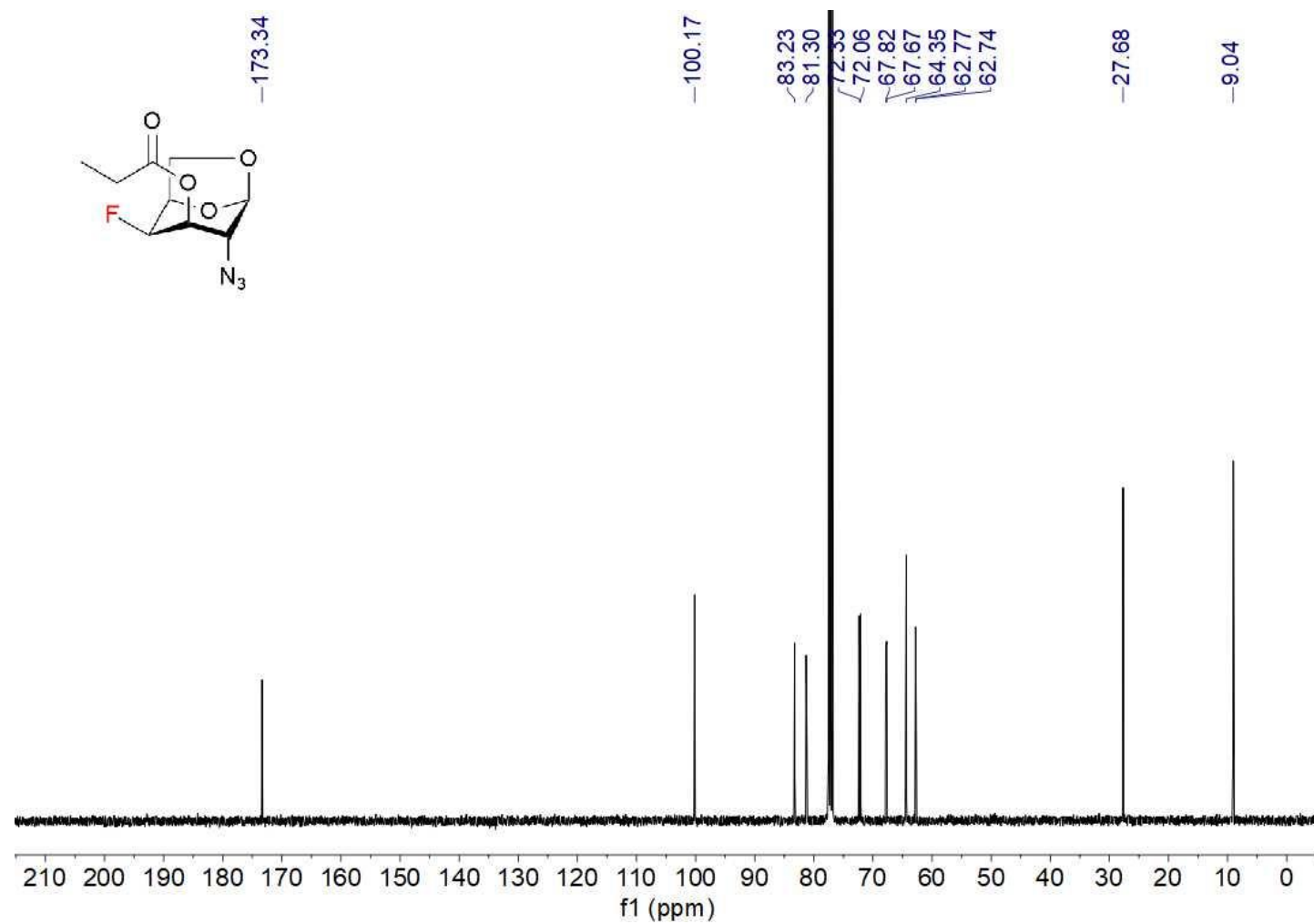


NMR COMPOUND 48

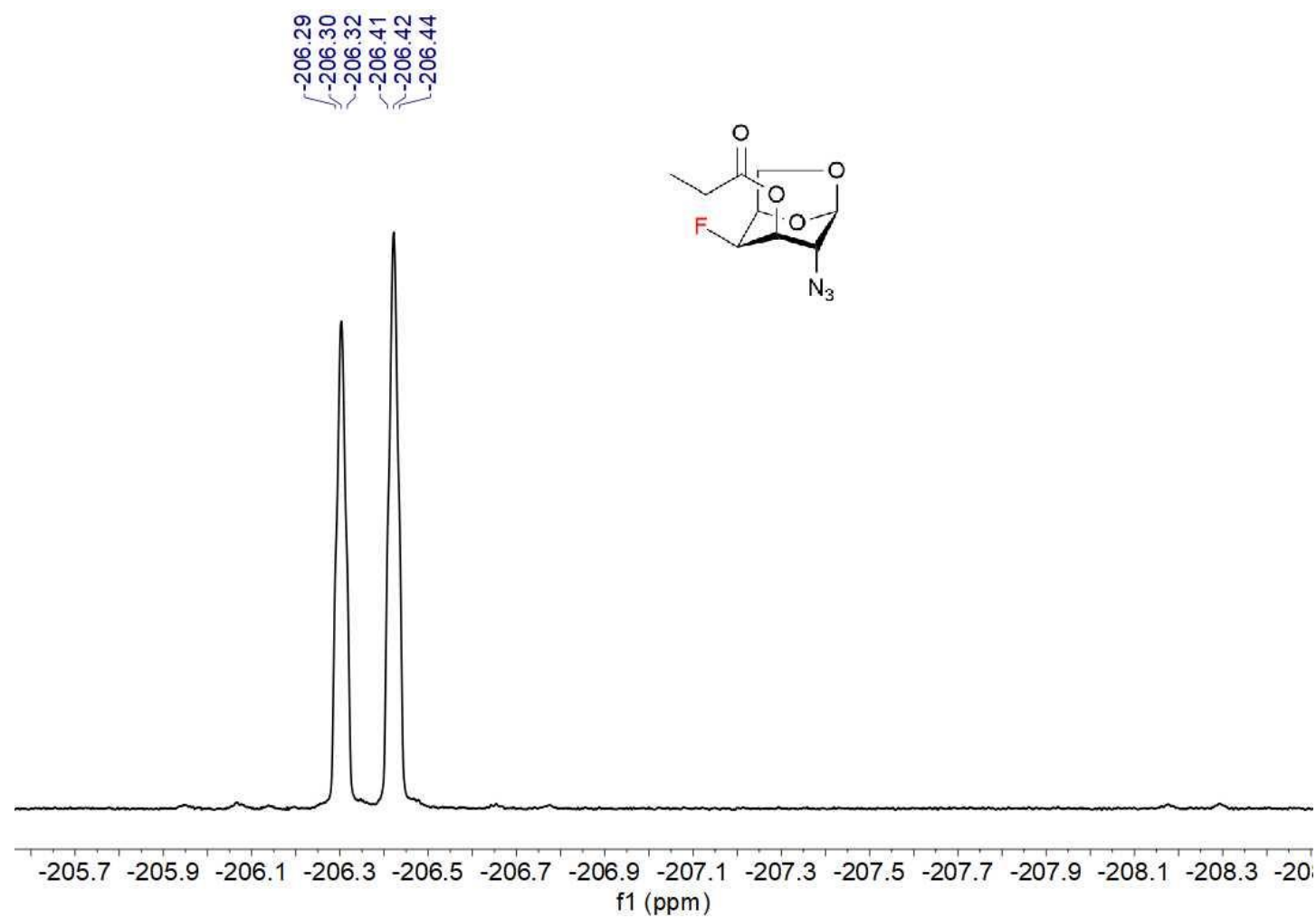
^1H NMR (400 MHz, CDCl_3) 48



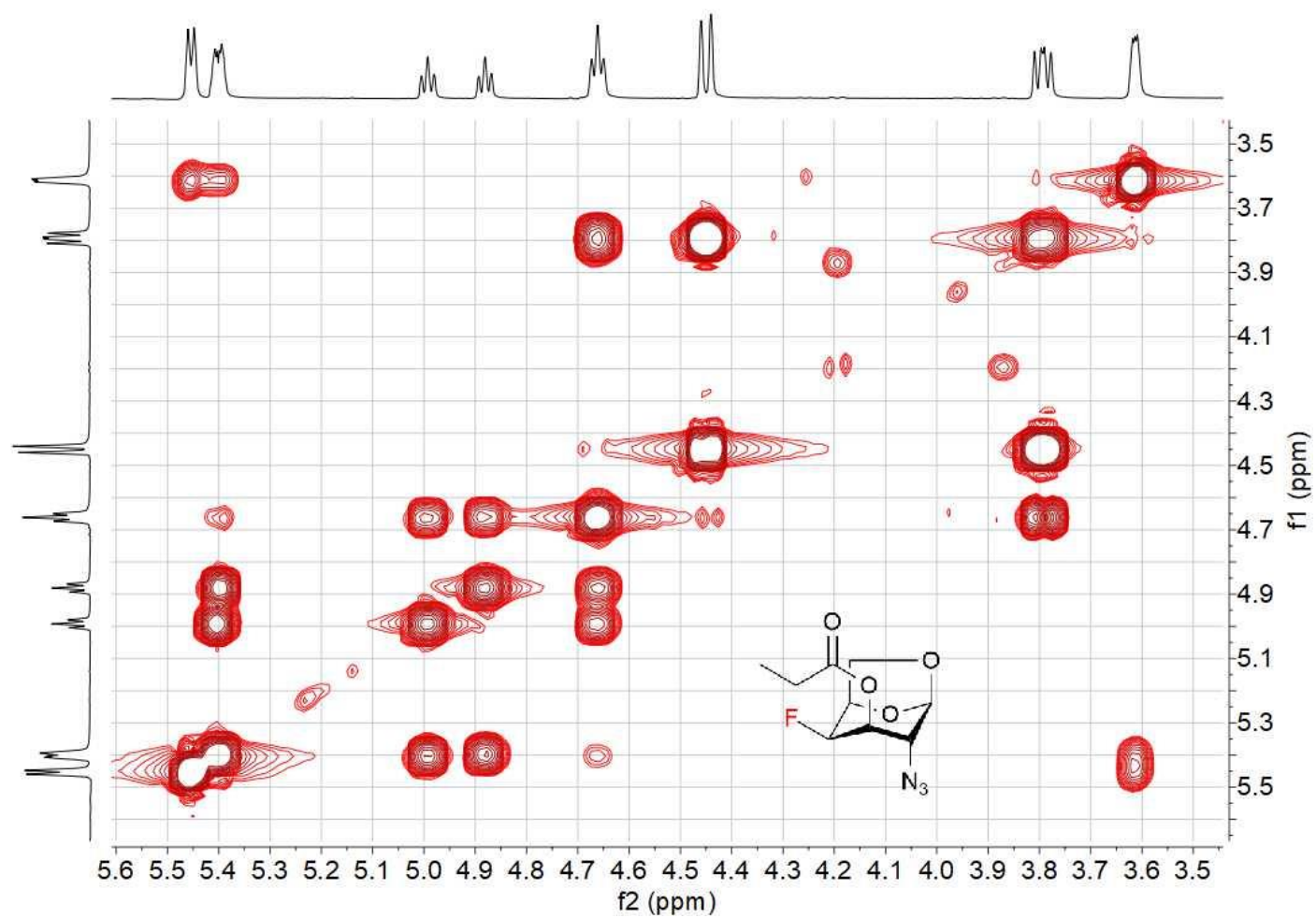
^{13}C NMR (100 MHz, CDCl_3) 48



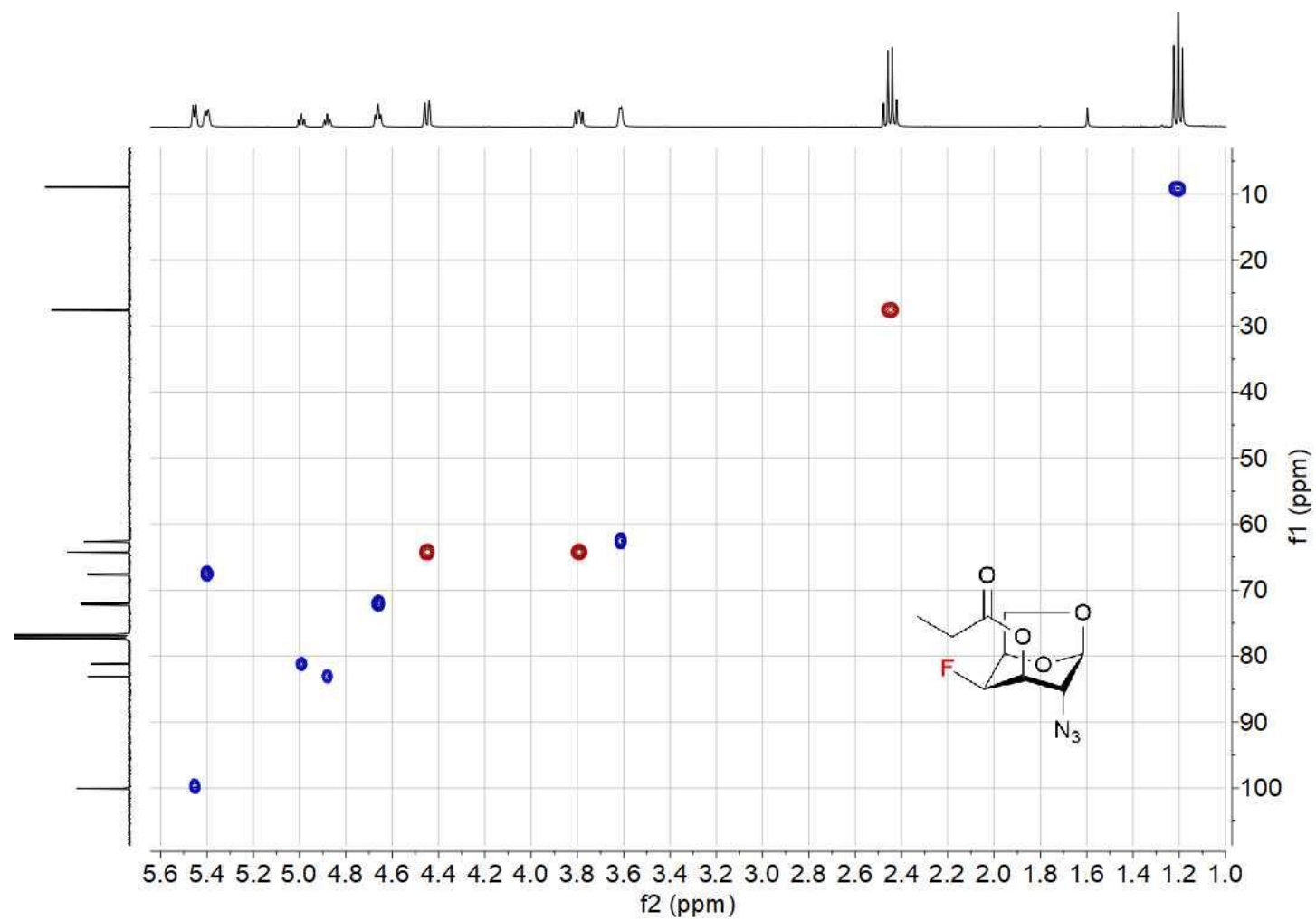
^{19}F NMR (376 MHz, CDCl_3) 48



^1H - ^1H COSY 48

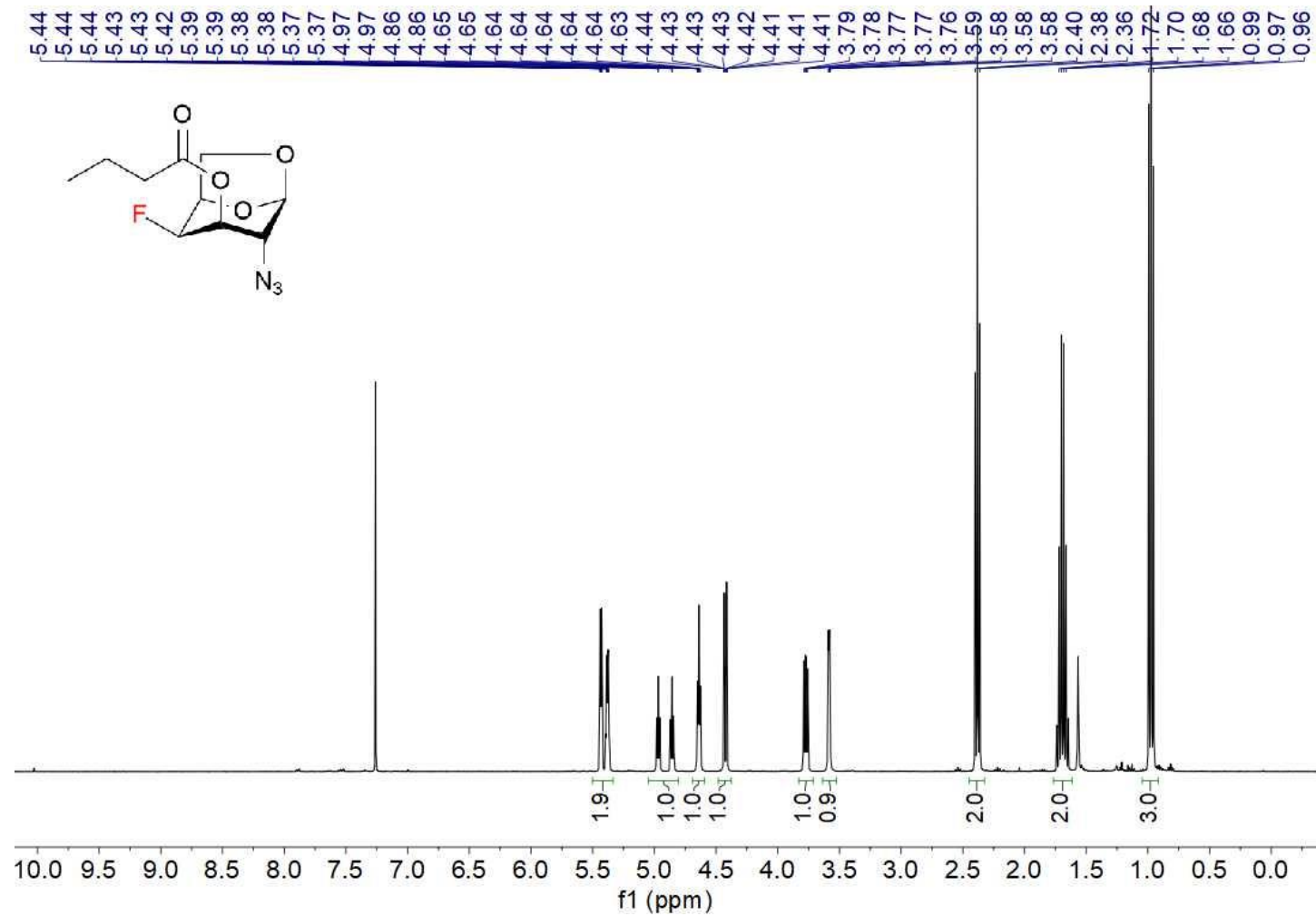


^1H - ^{13}C HSQC 48

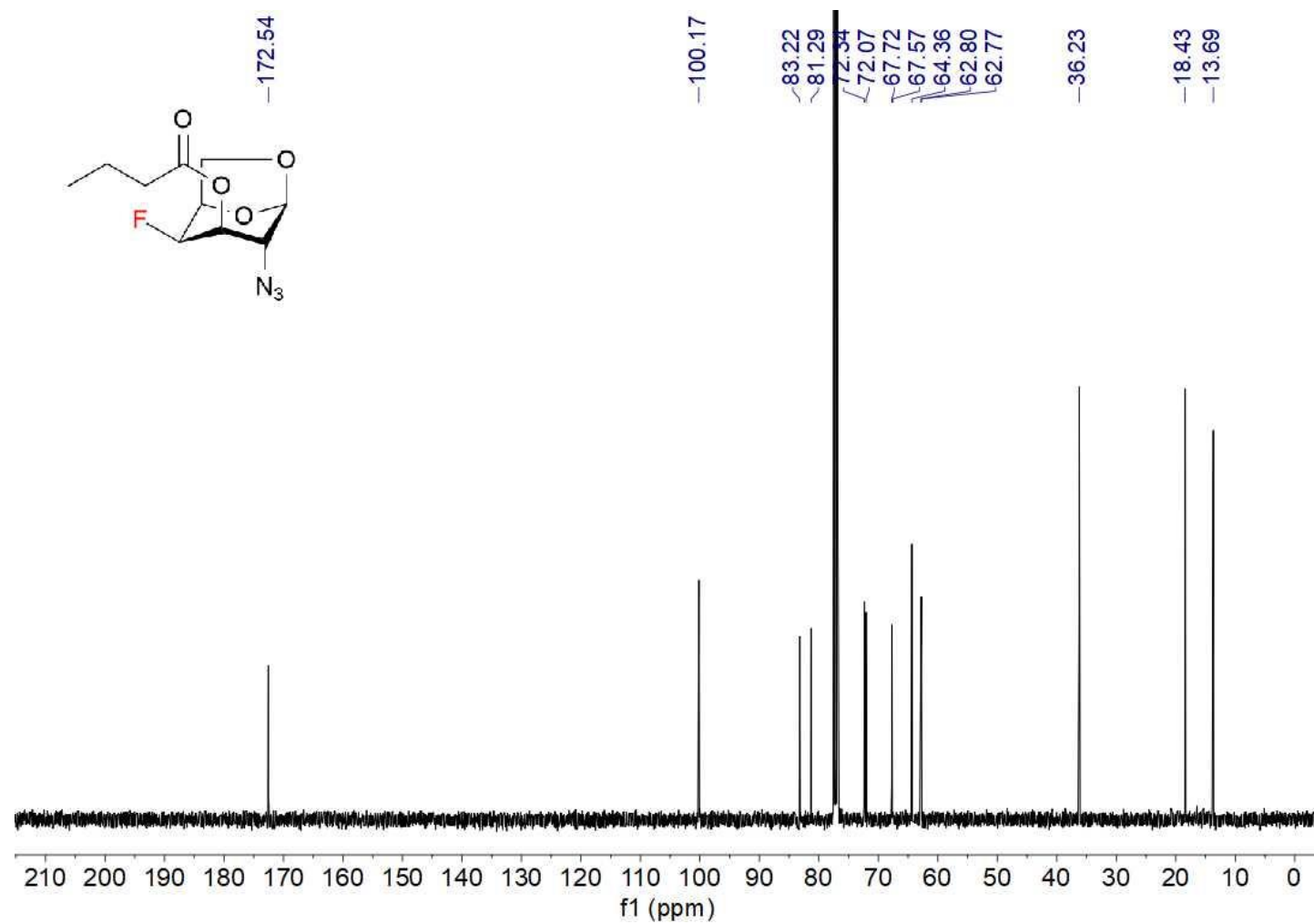


NMR COMPOUND 49

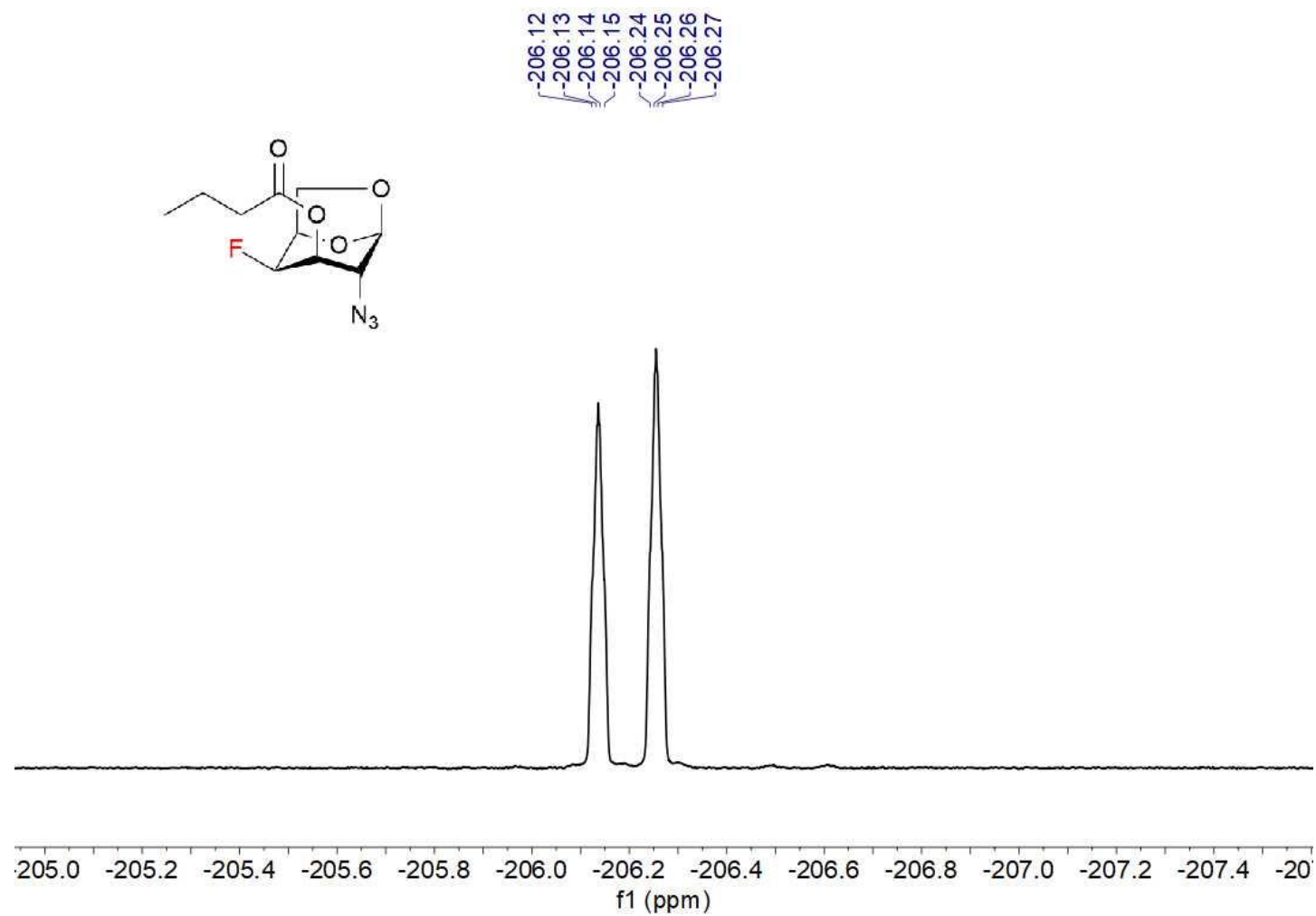
¹H NMR (400 MHz, CDCl₃) 49



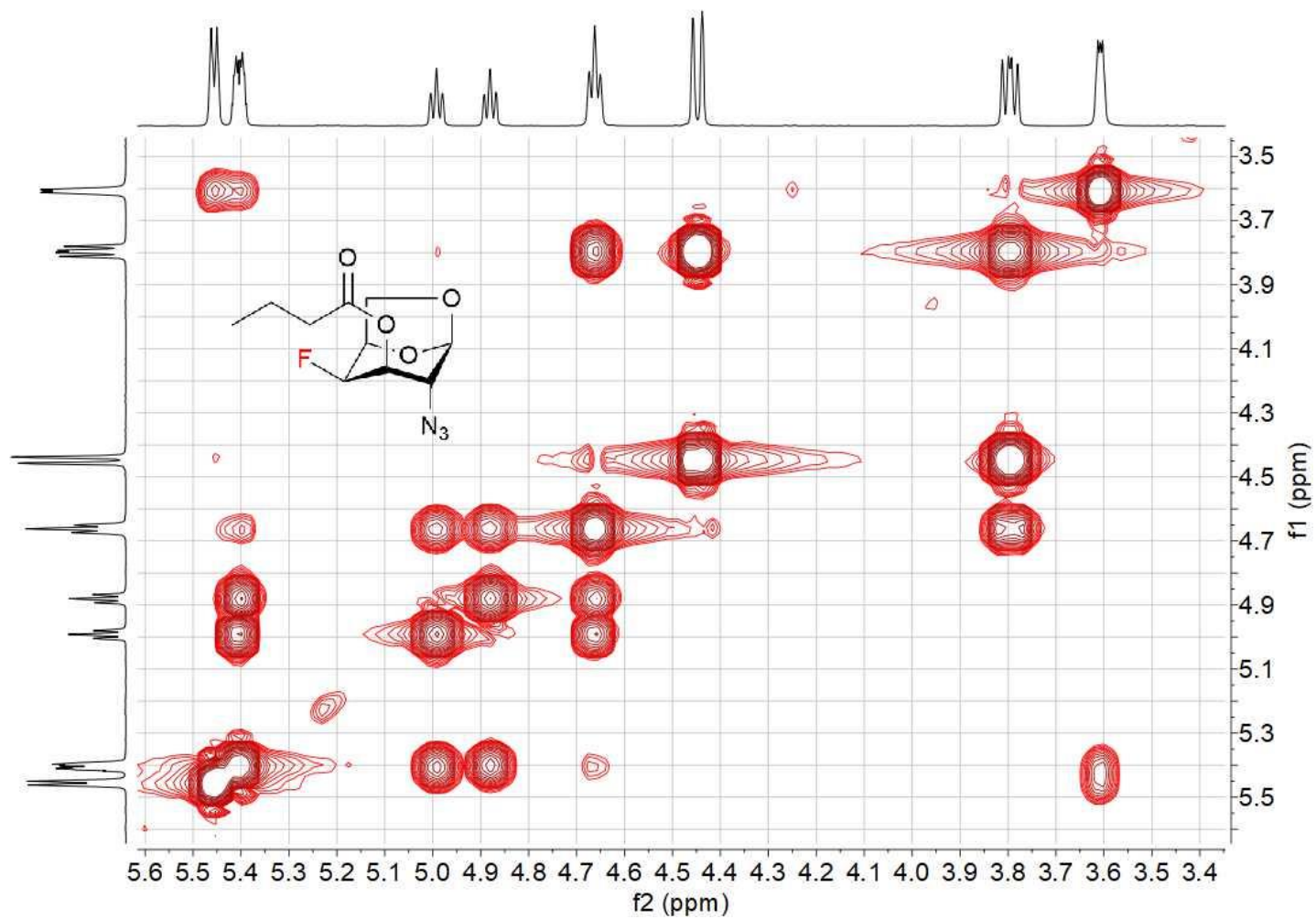
^{13}C NMR (100 MHz, CDCl_3) 49



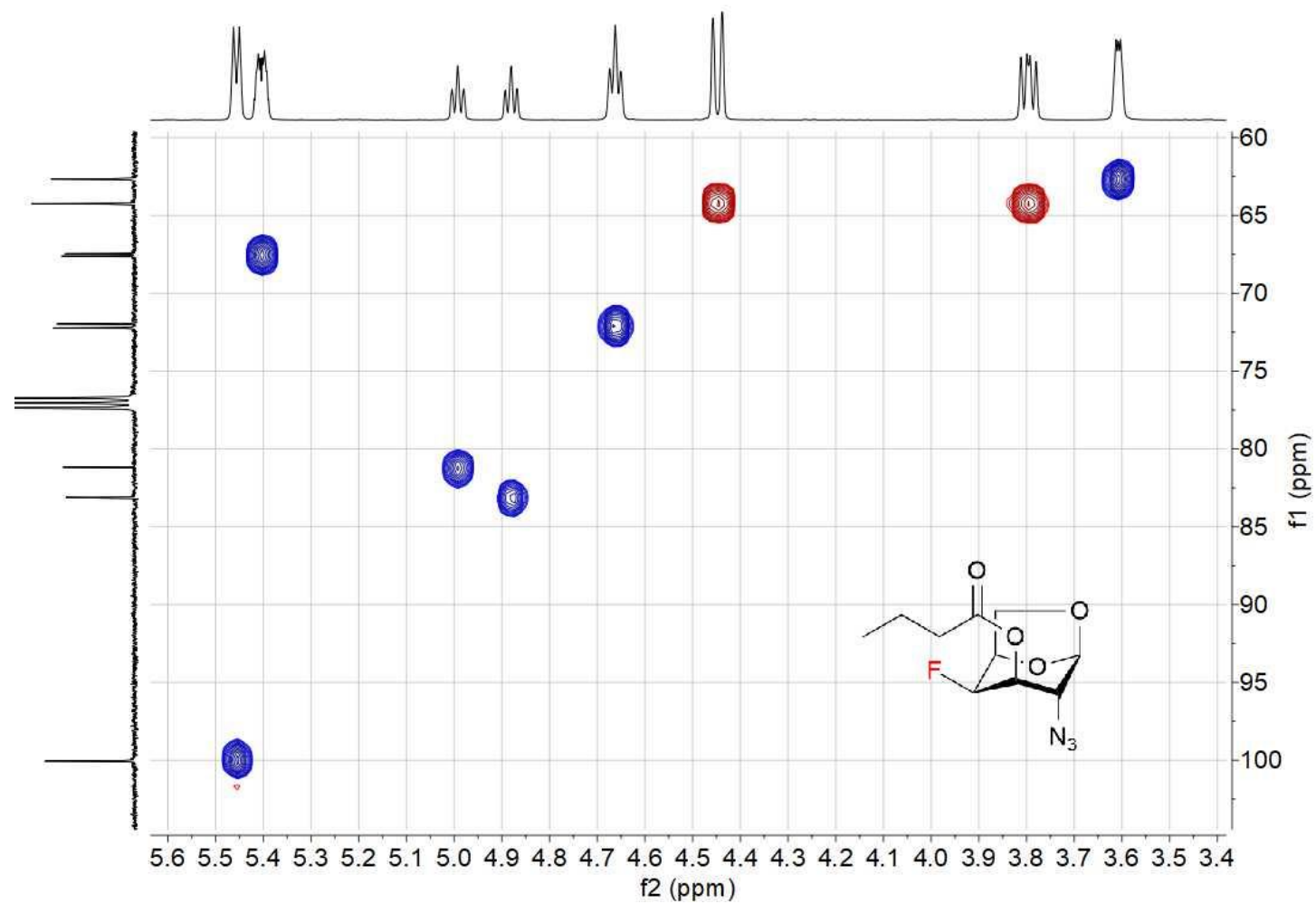
^{19}F NMR (376 MHz, CDCl_3) 49



¹H-¹H COSY 49

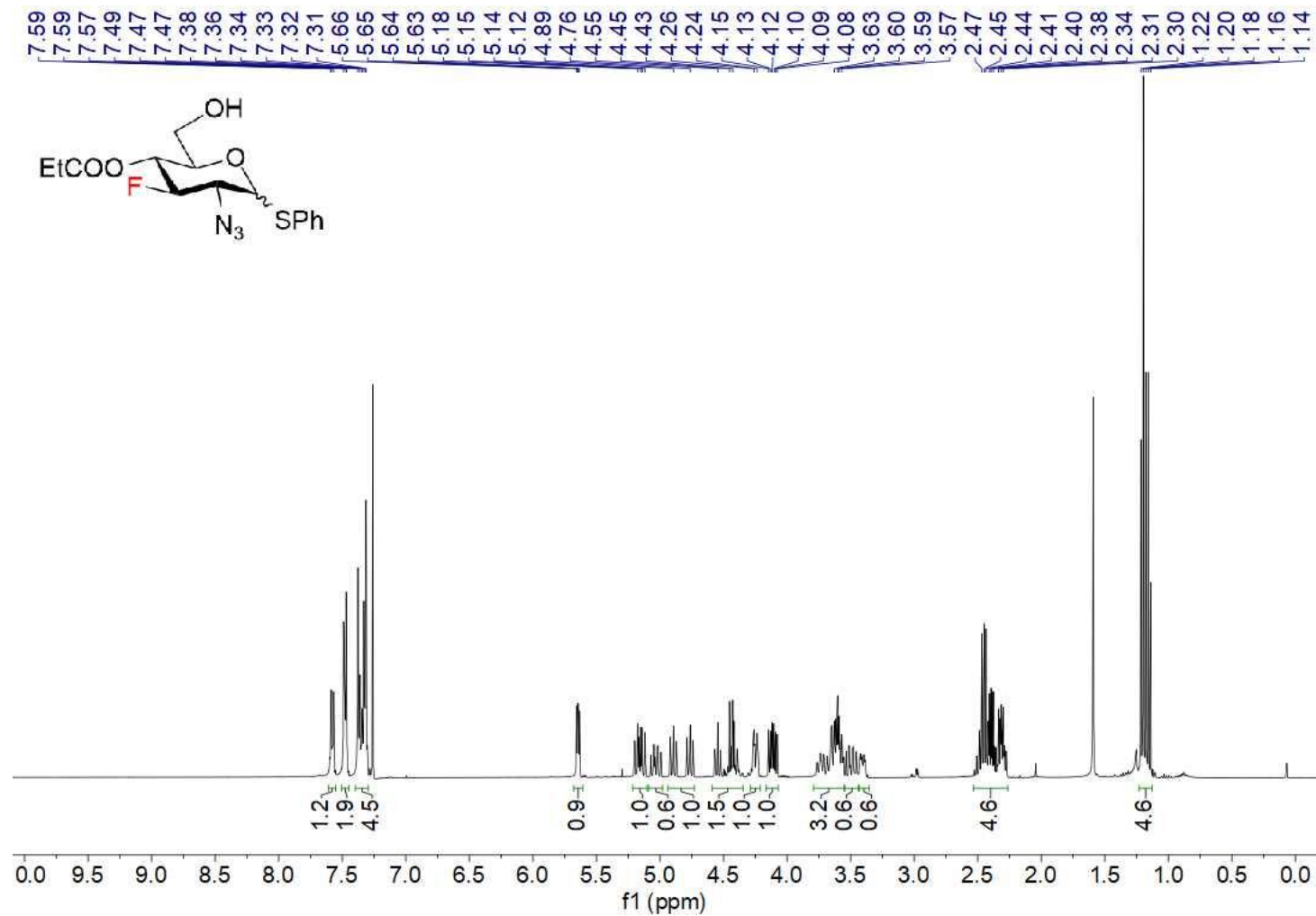


^1H - ^{13}C HSQC 49

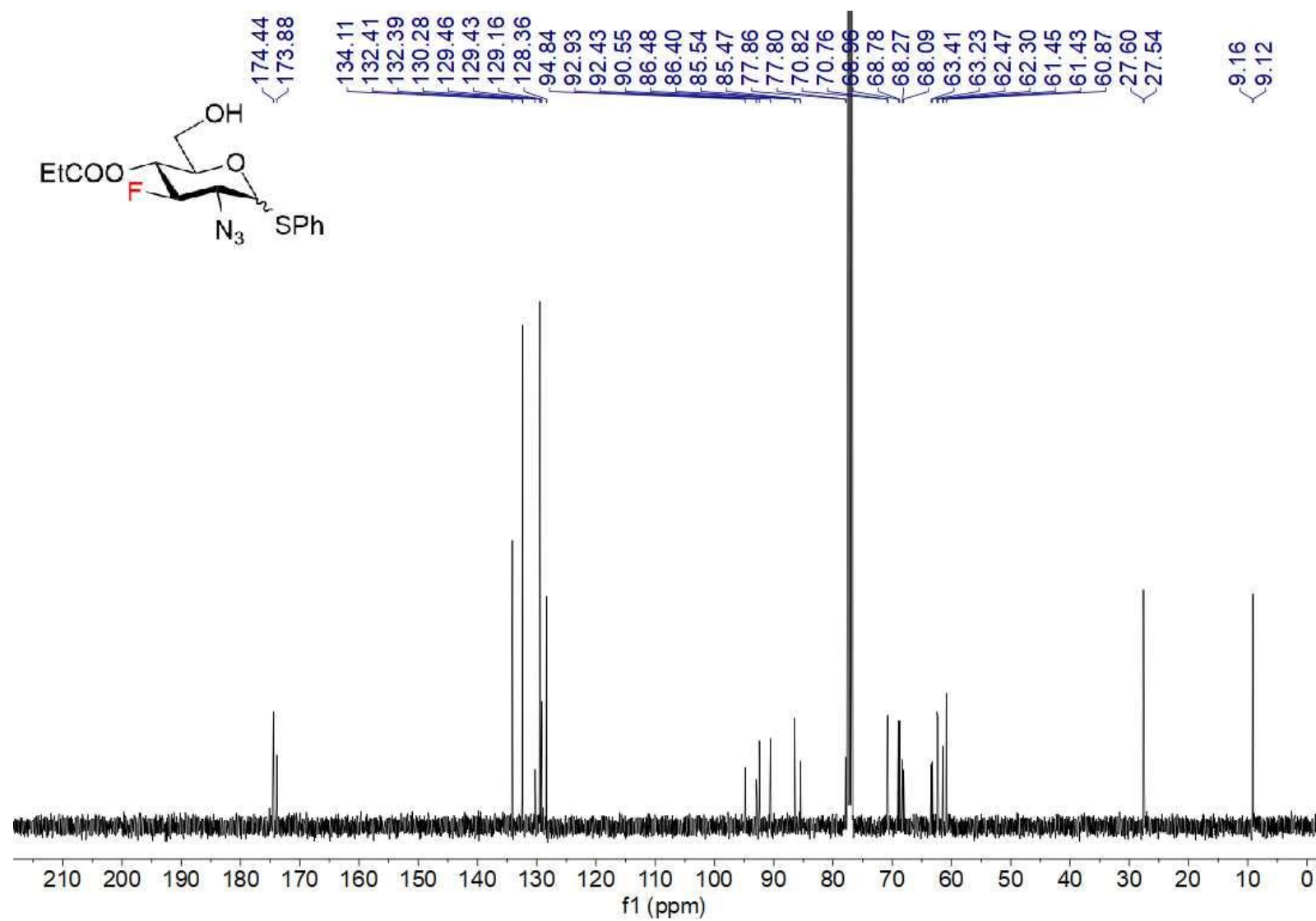


NMR COMPOUND 51

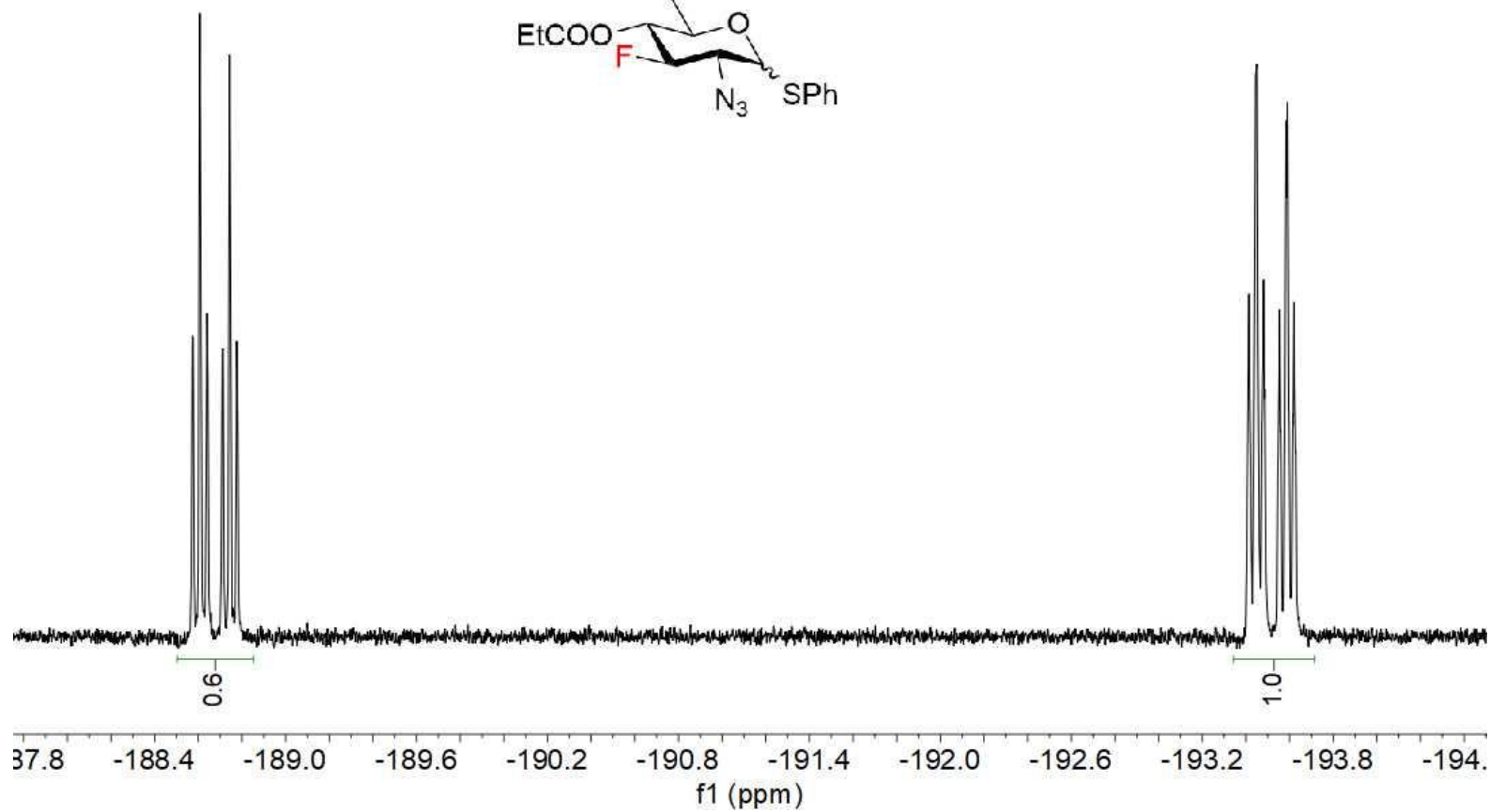
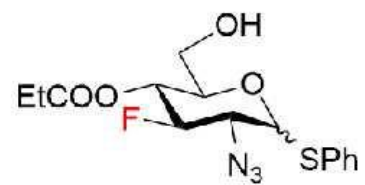
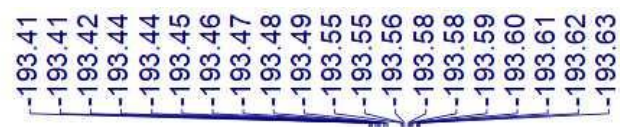
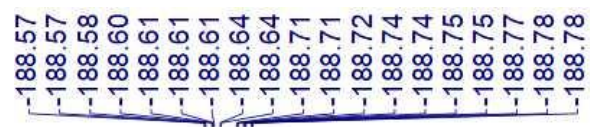
¹H NMR (400 MHz, CDCl₃) 51



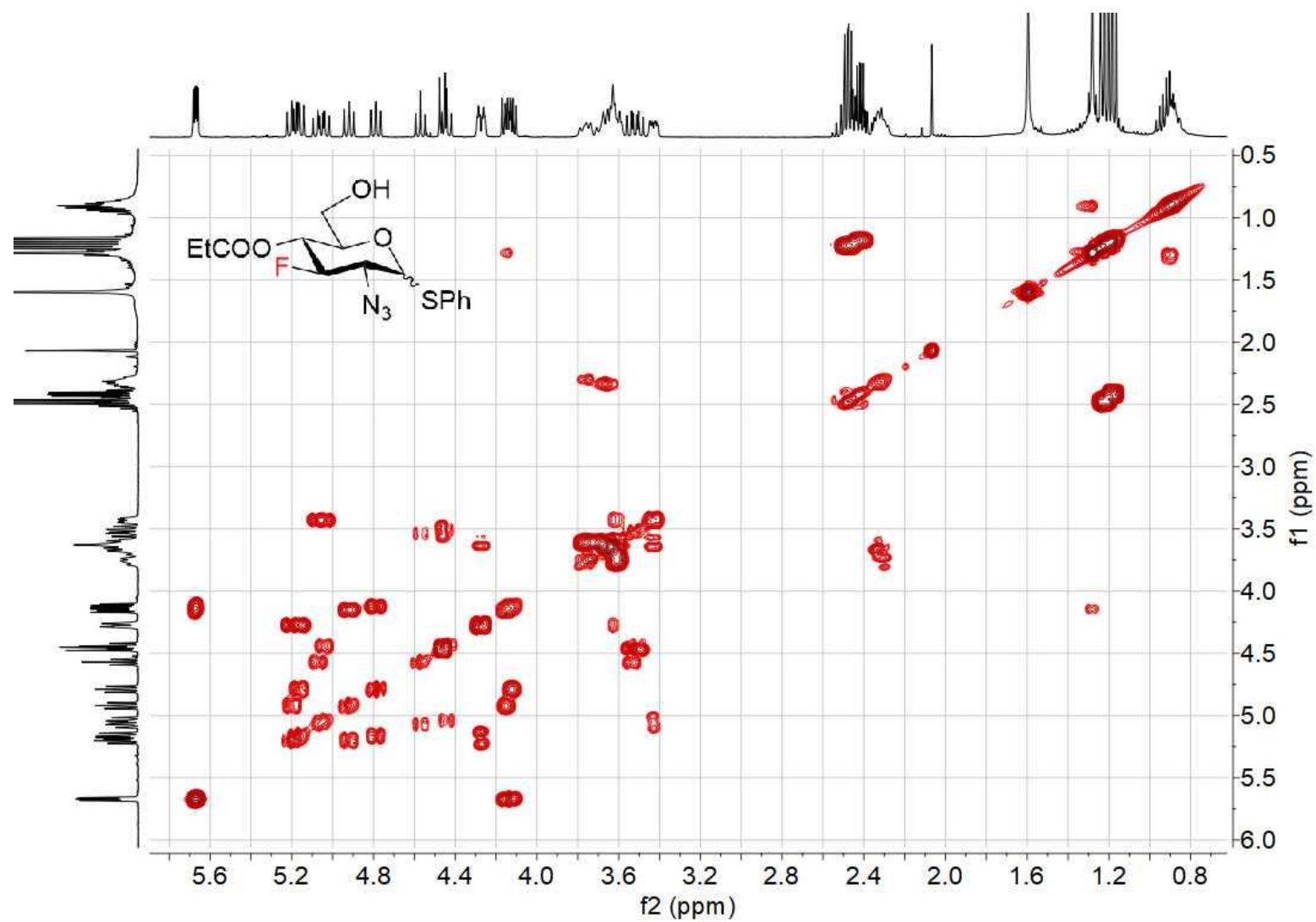
¹³C NMR (100 MHz, CDCl₃) 51



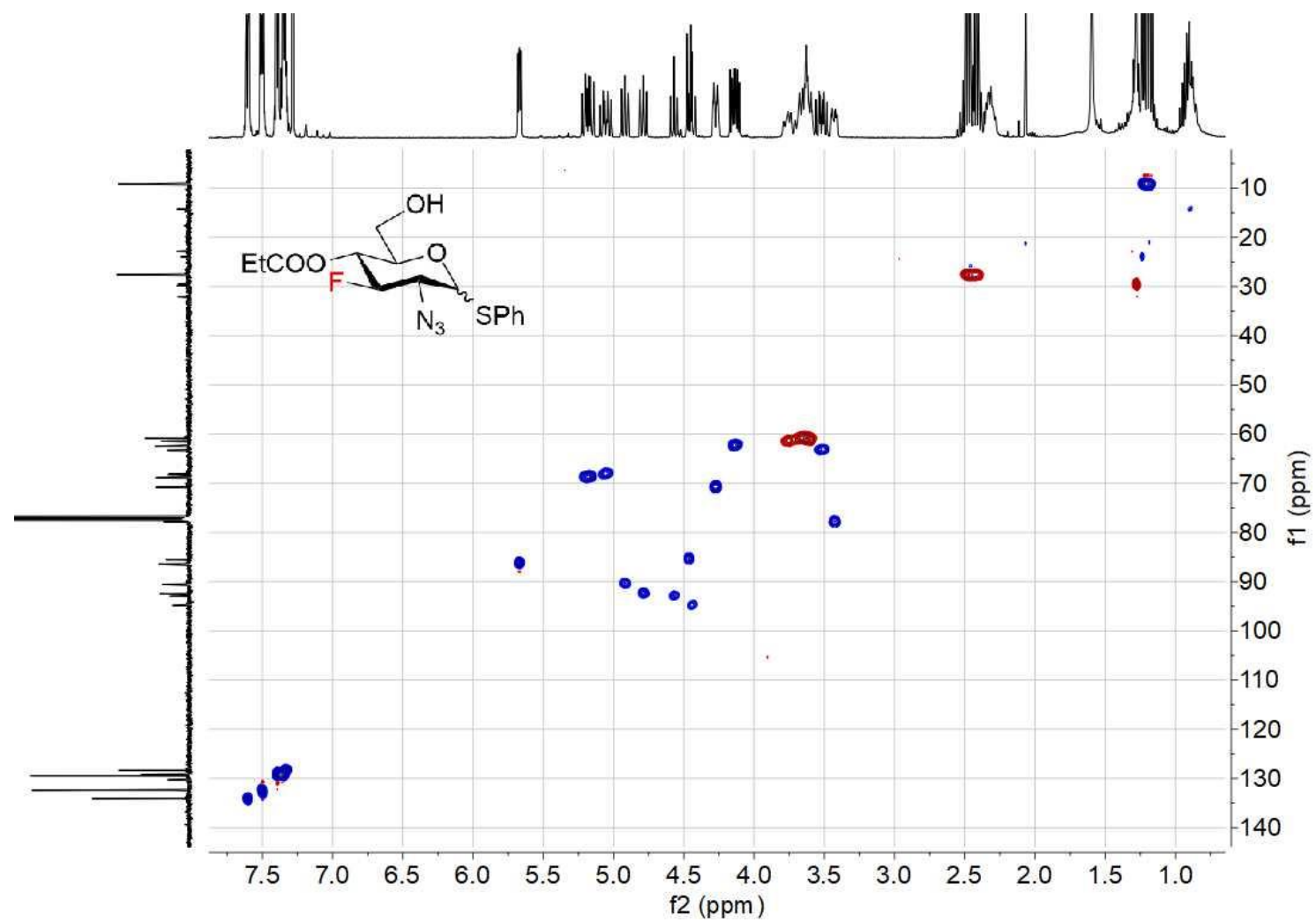
¹⁹F NMR (376 MHz, CDCl₃) 51



¹H-¹H COSY 51

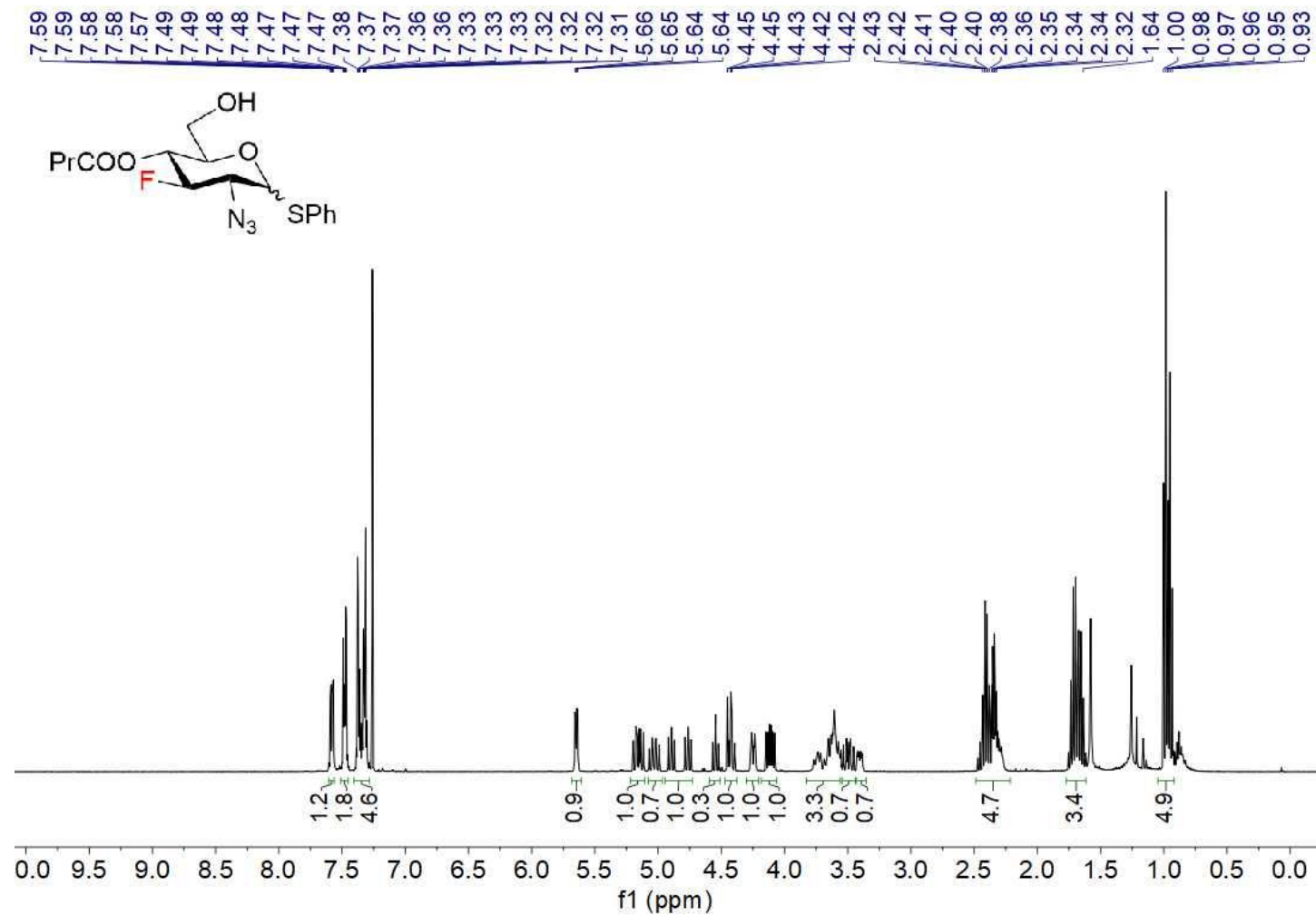


^1H - ^{13}C HSQC 51

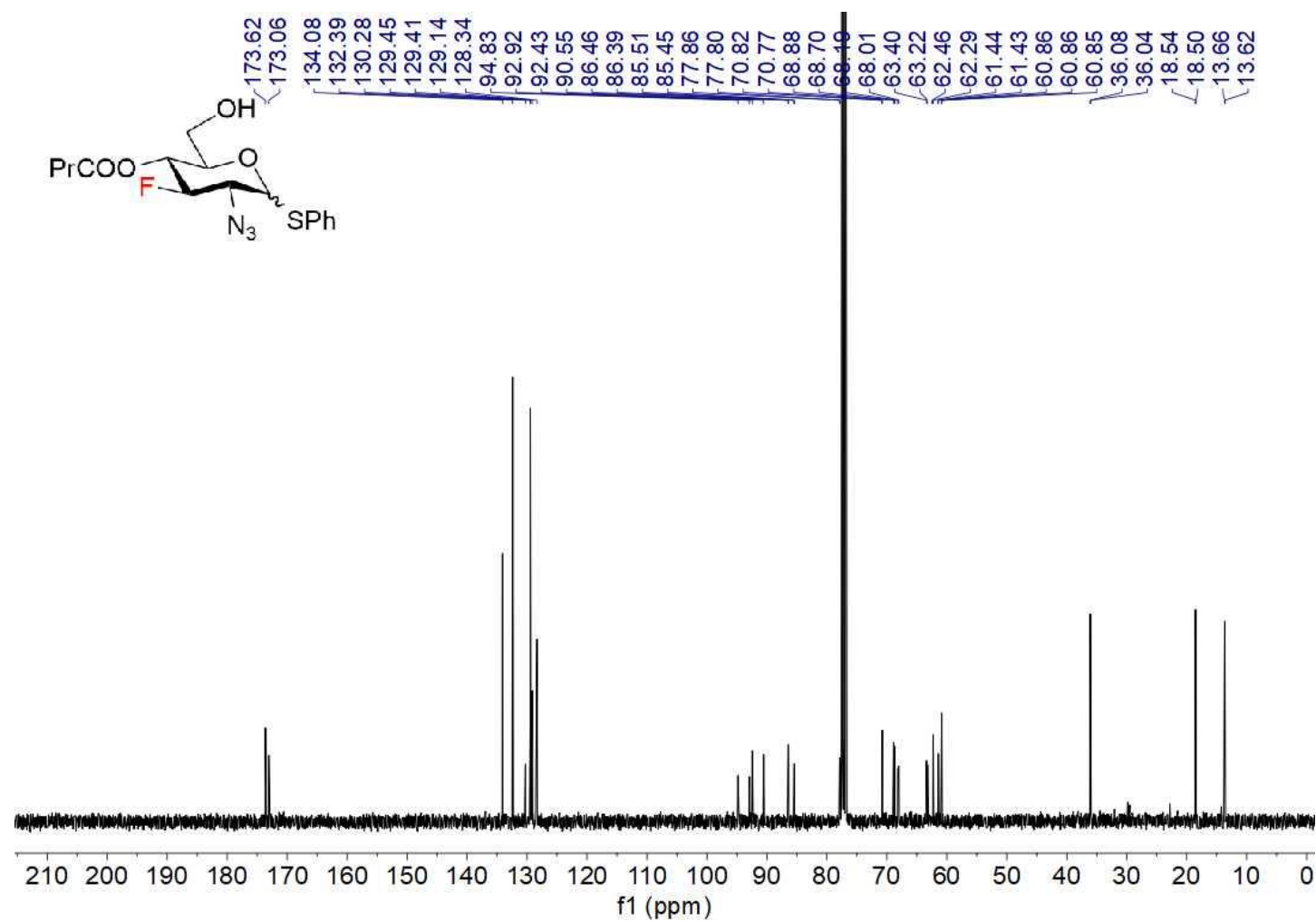


NMR COMPOUND 52

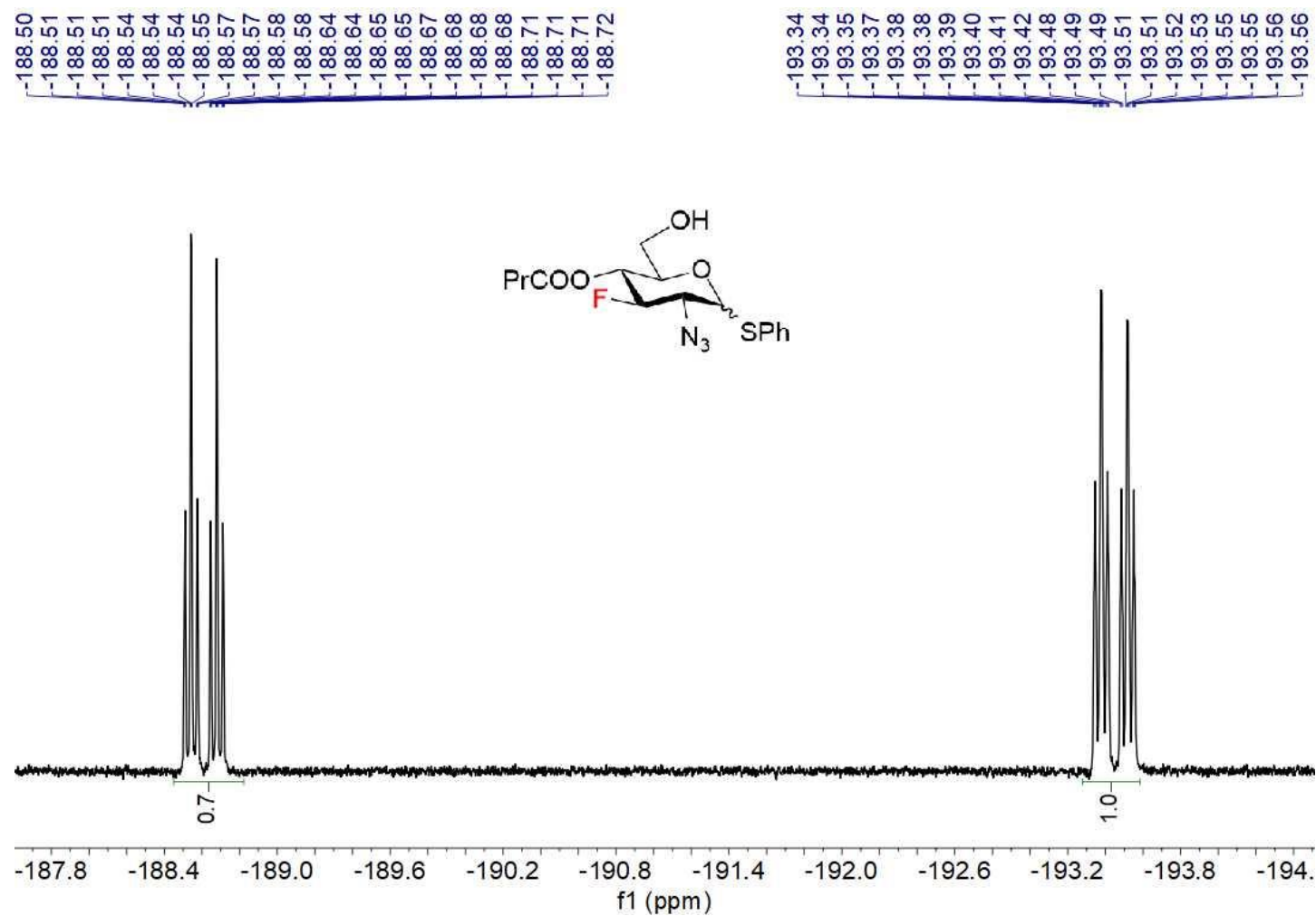
¹H NMR (400 MHz, CDCl₃) 52



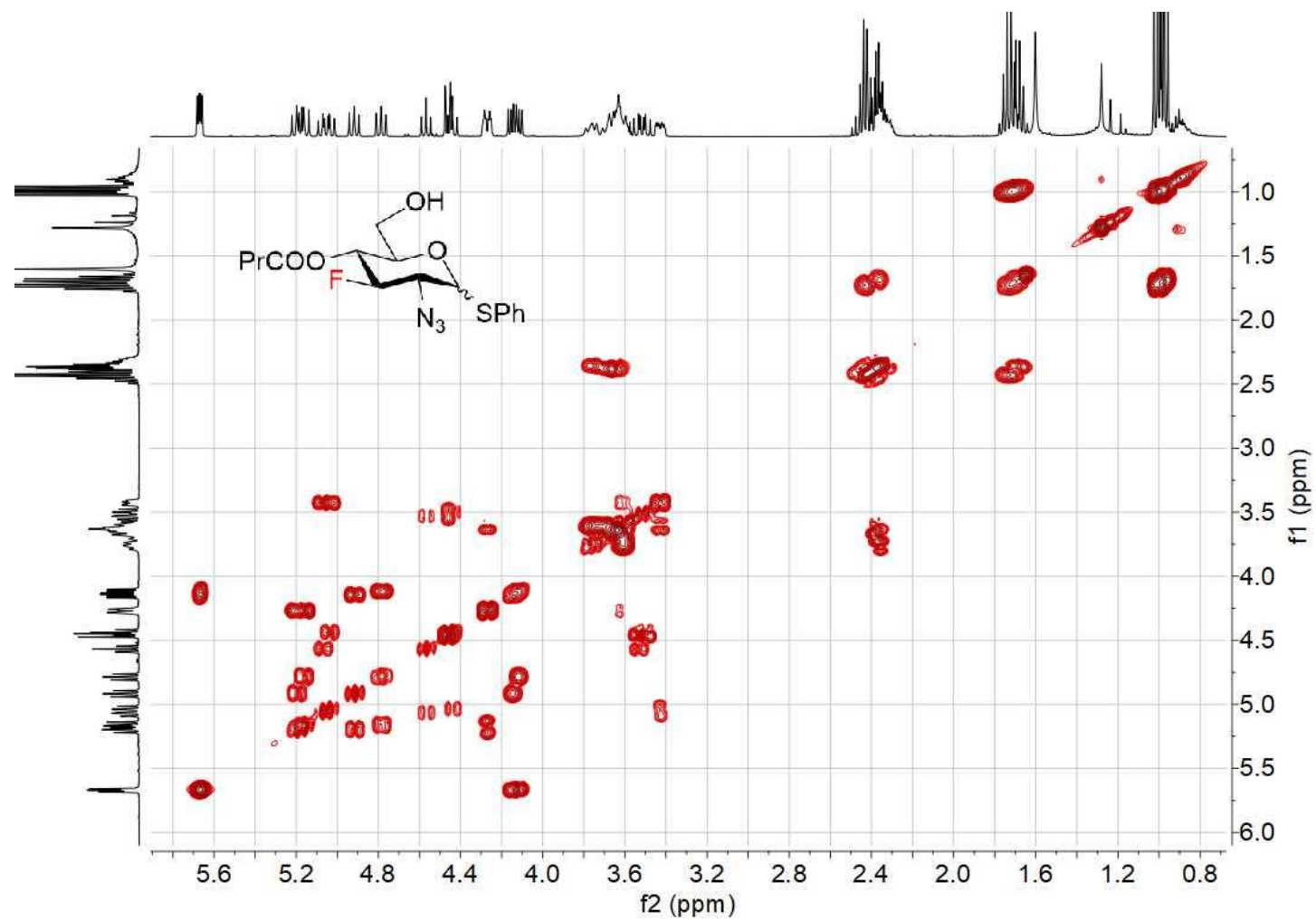
¹³C NMR (100 MHz, CDCl₃) 52



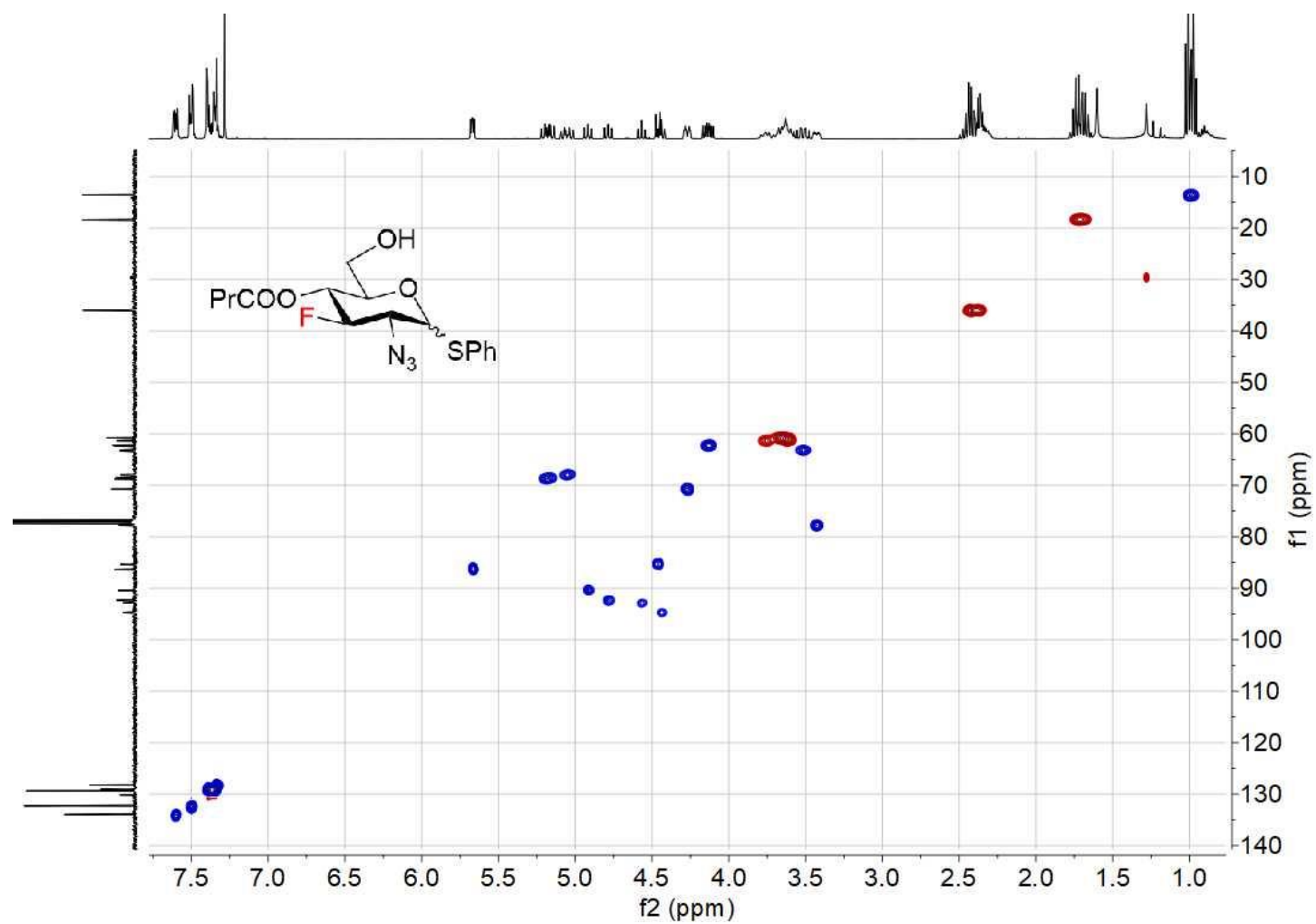
¹⁹F NMR (376 MHz, CDCl₃) 52



^1H - ^1H COSY 52

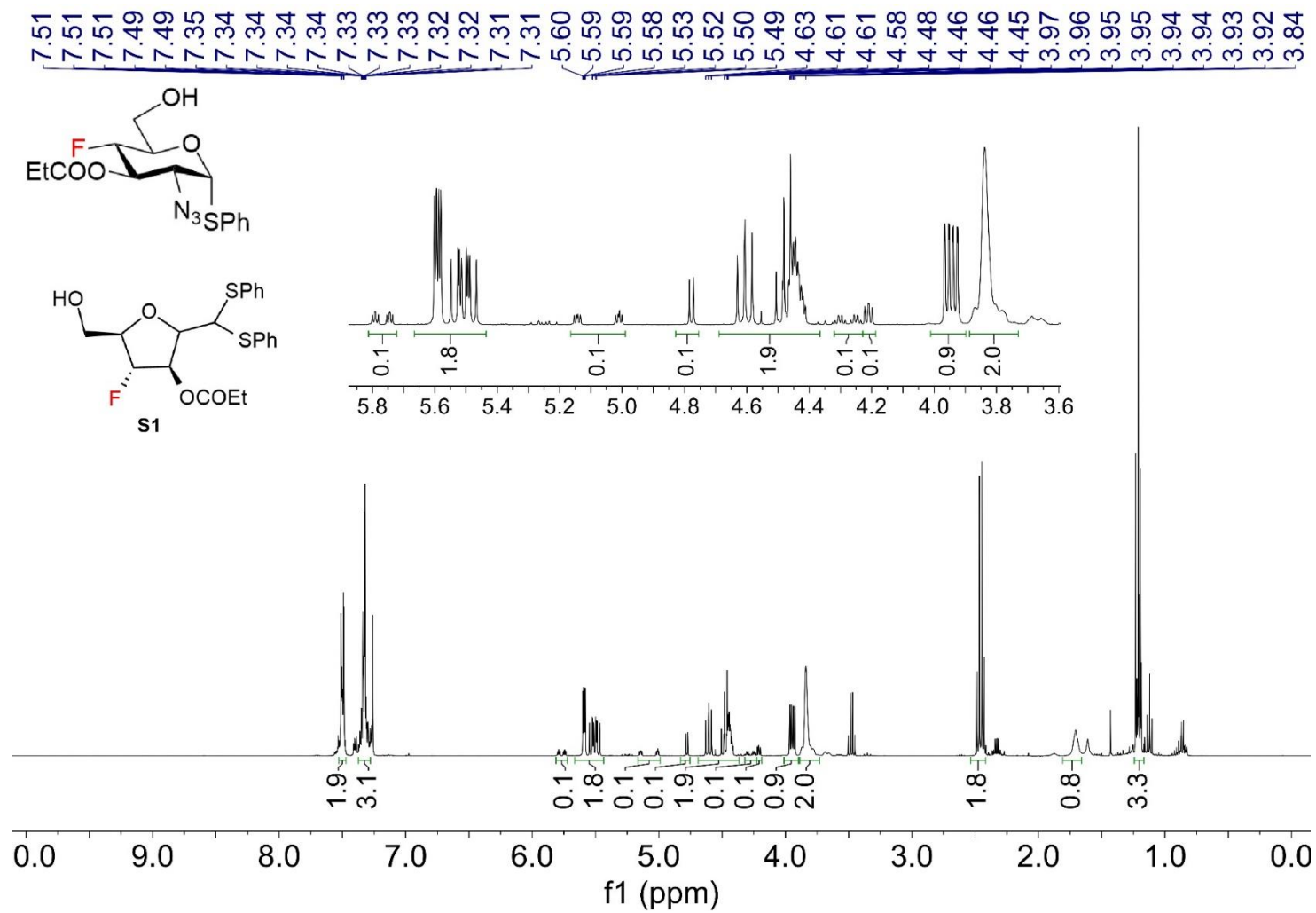


^1H - ^{13}C HSQC 52

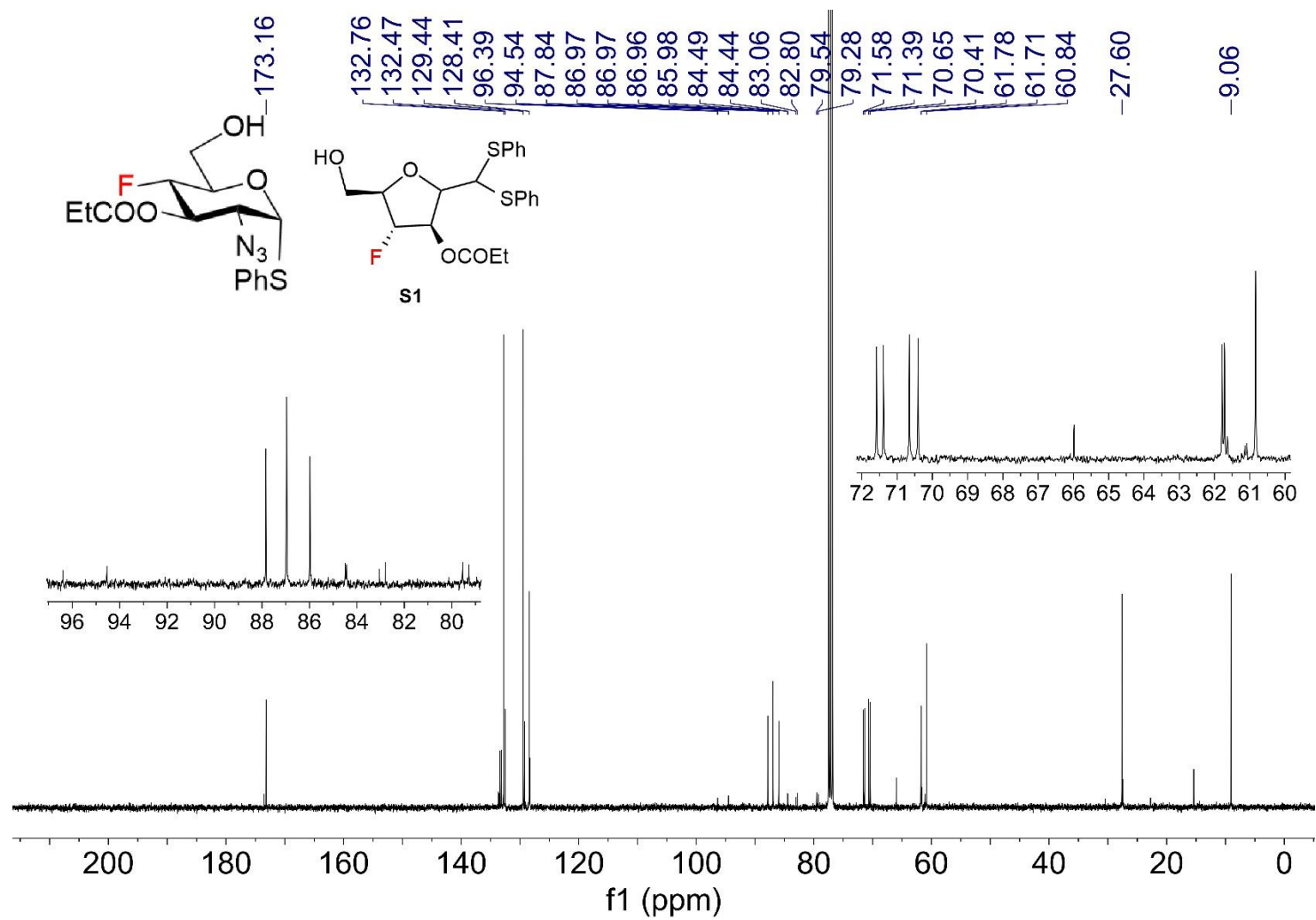


NMR COMPOUND α -54

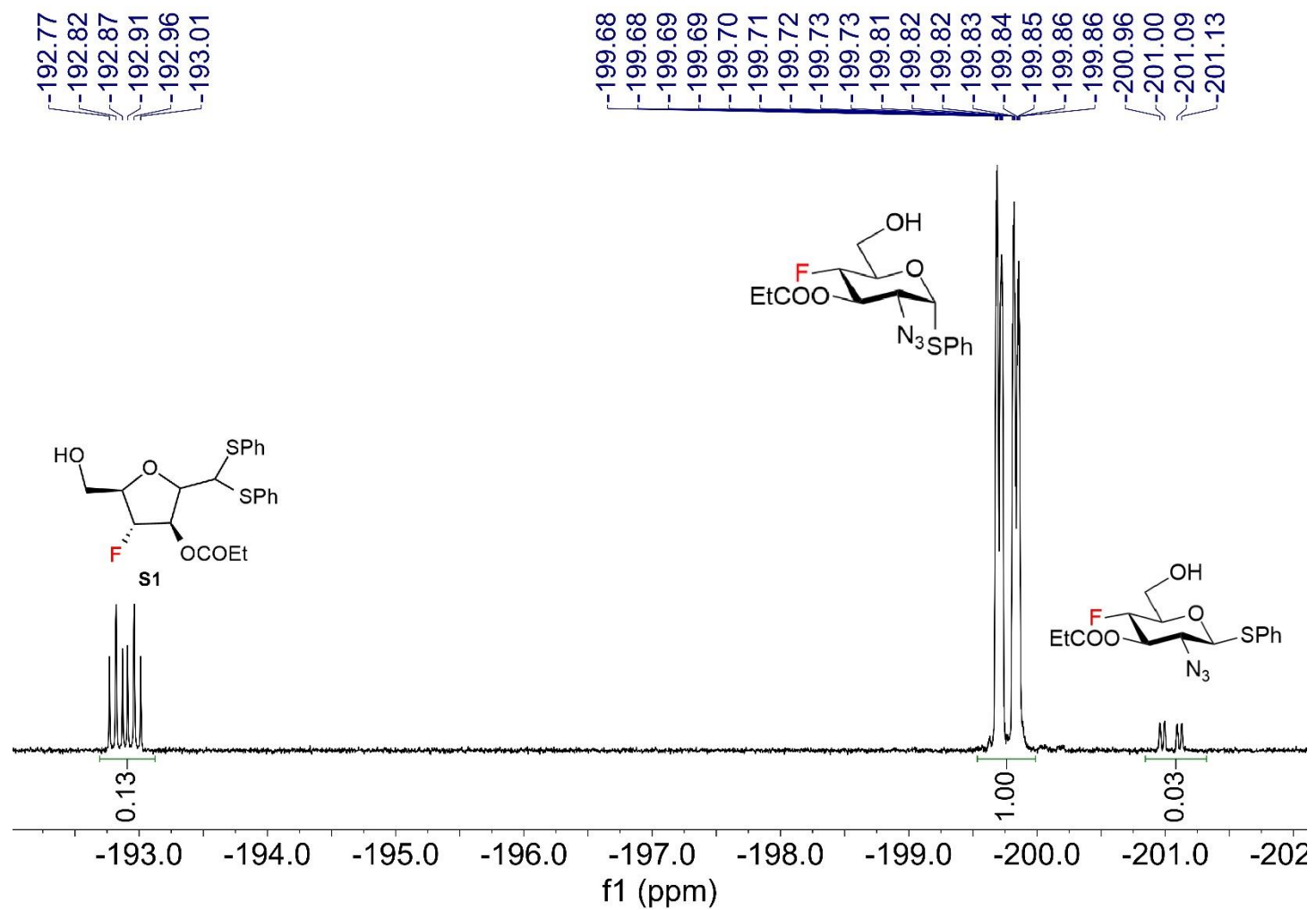
^1H NMR (400 MHz, CDCl_3) α -54 and 9% of S1



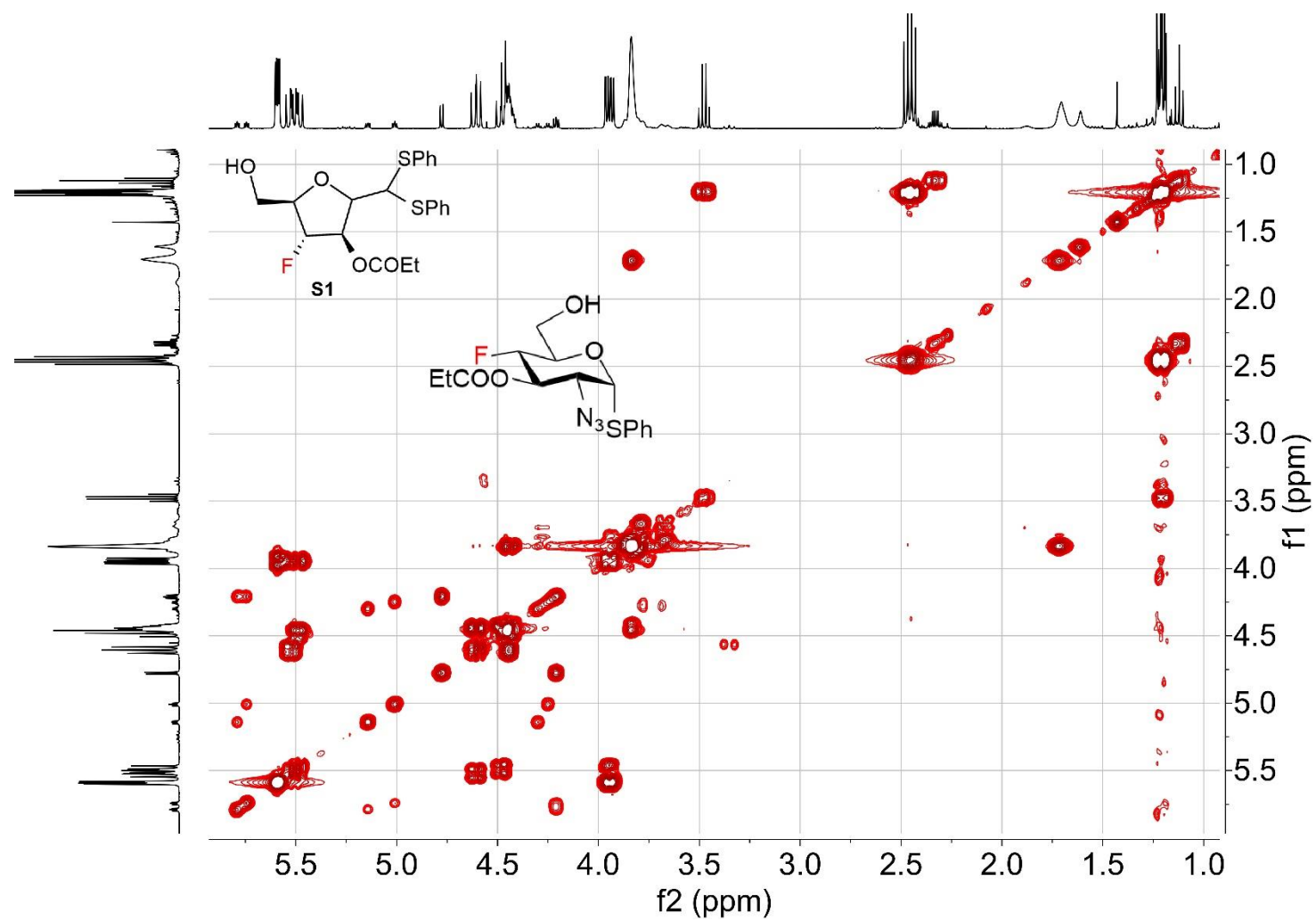
¹³C NMR (100 MHz, CDCl₃) α-54 and S1

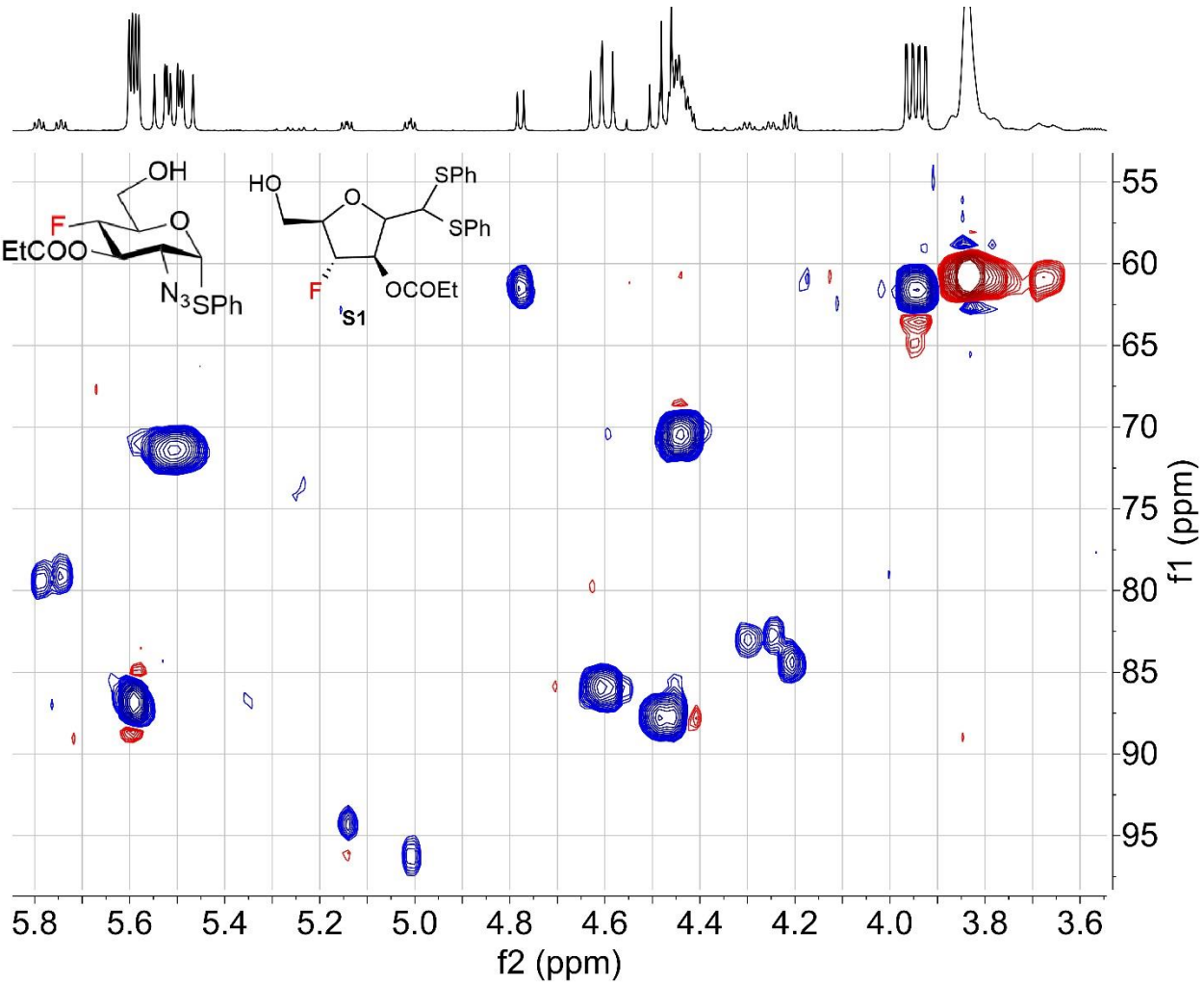


^{19}F NMR (376 MHz, CDCl_3) α -54, 9% S1 and 3% β -23



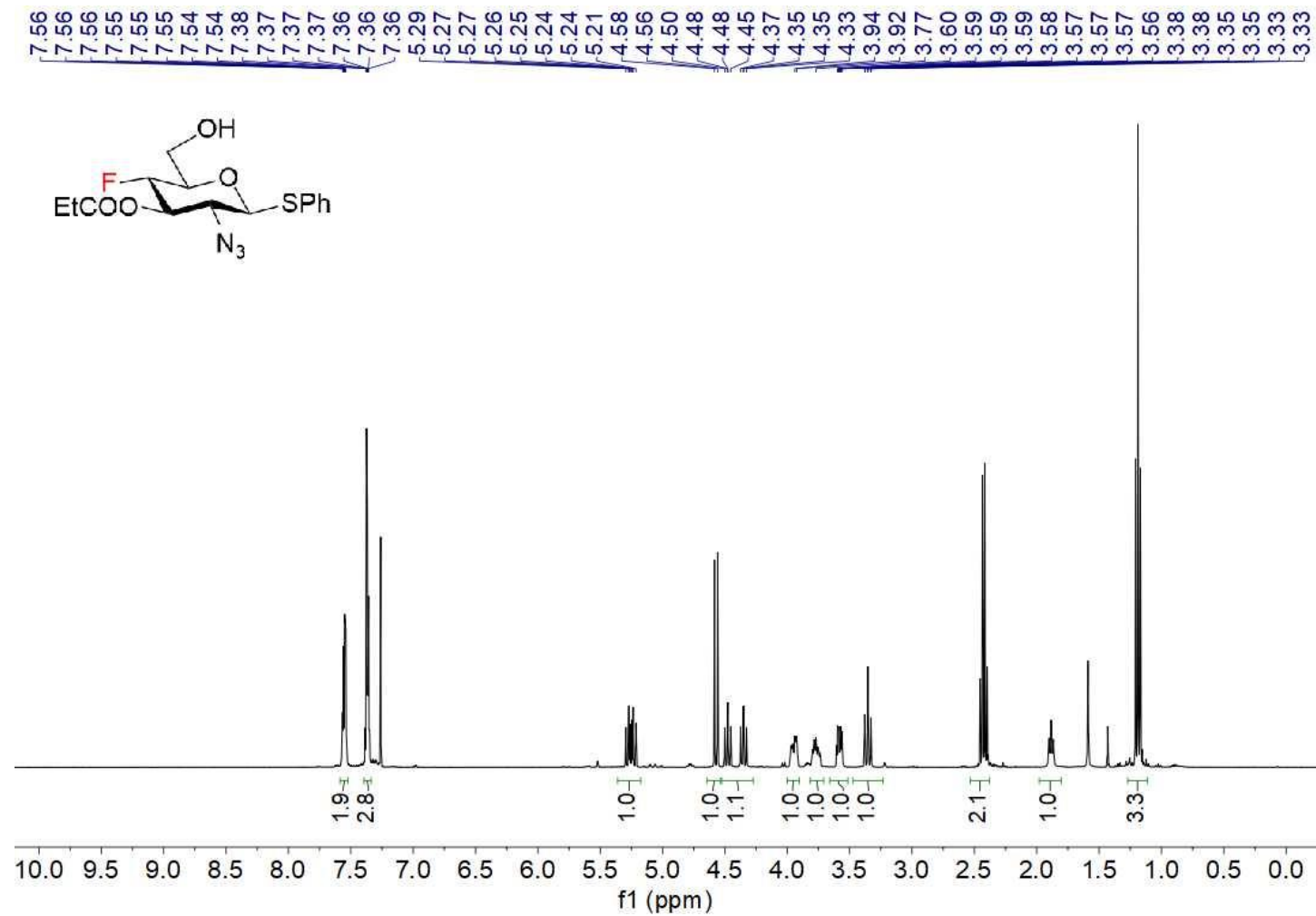
^1H - ^1H COSY α -54



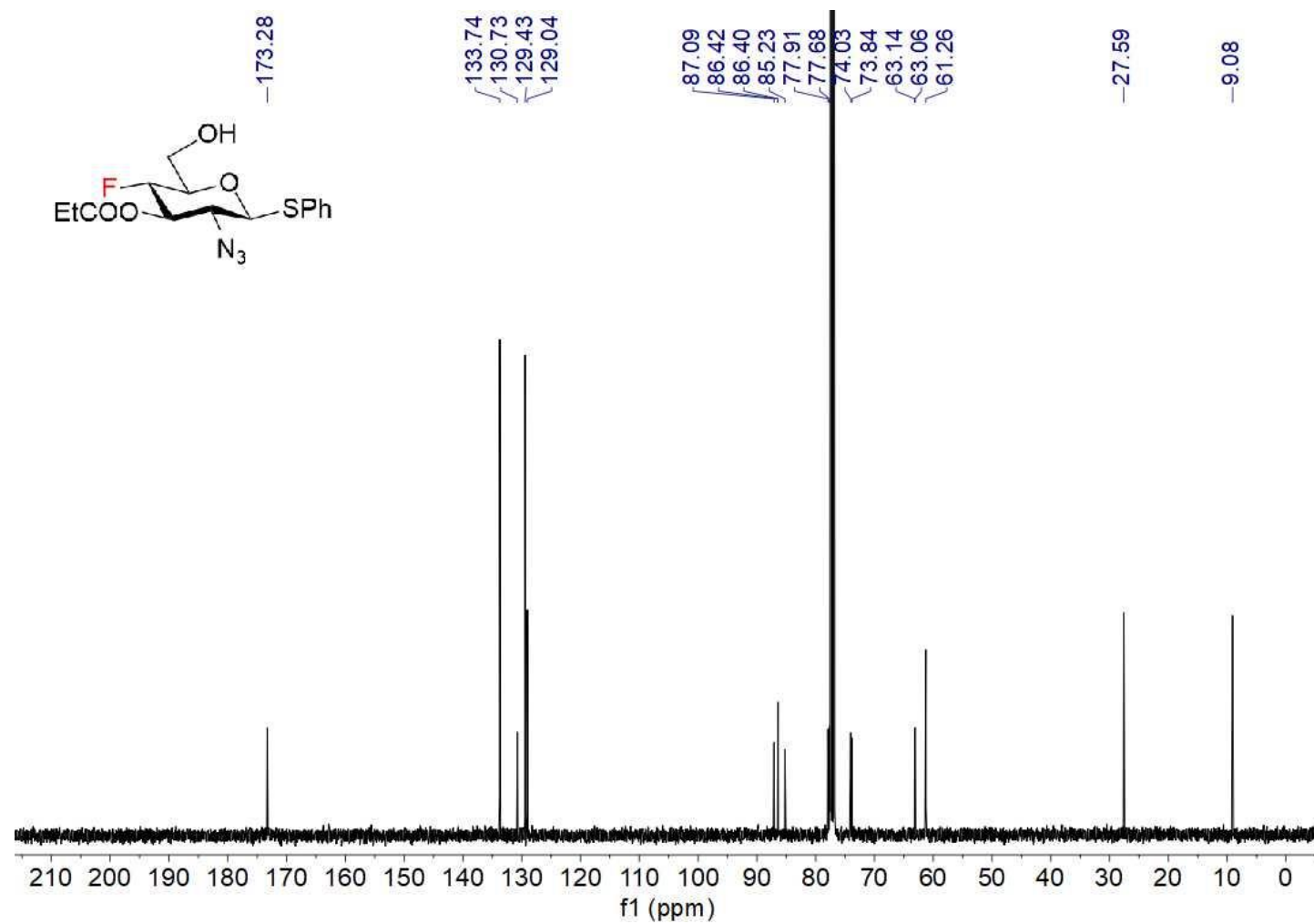
^1H - ^{13}C HSQC α -54

NMR COMPOUND β -54

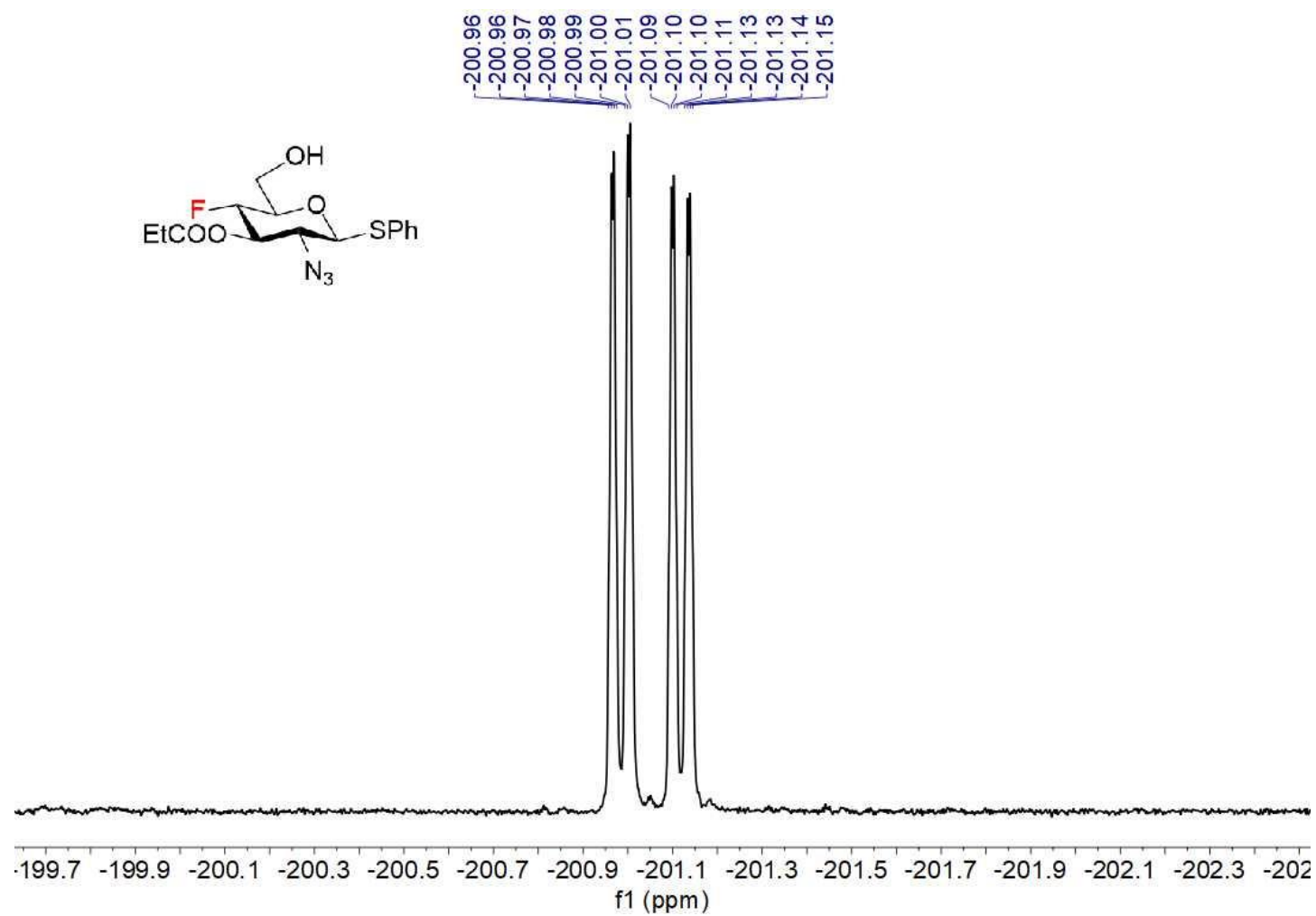
^1H NMR (400 MHz, CDCl_3) β -54



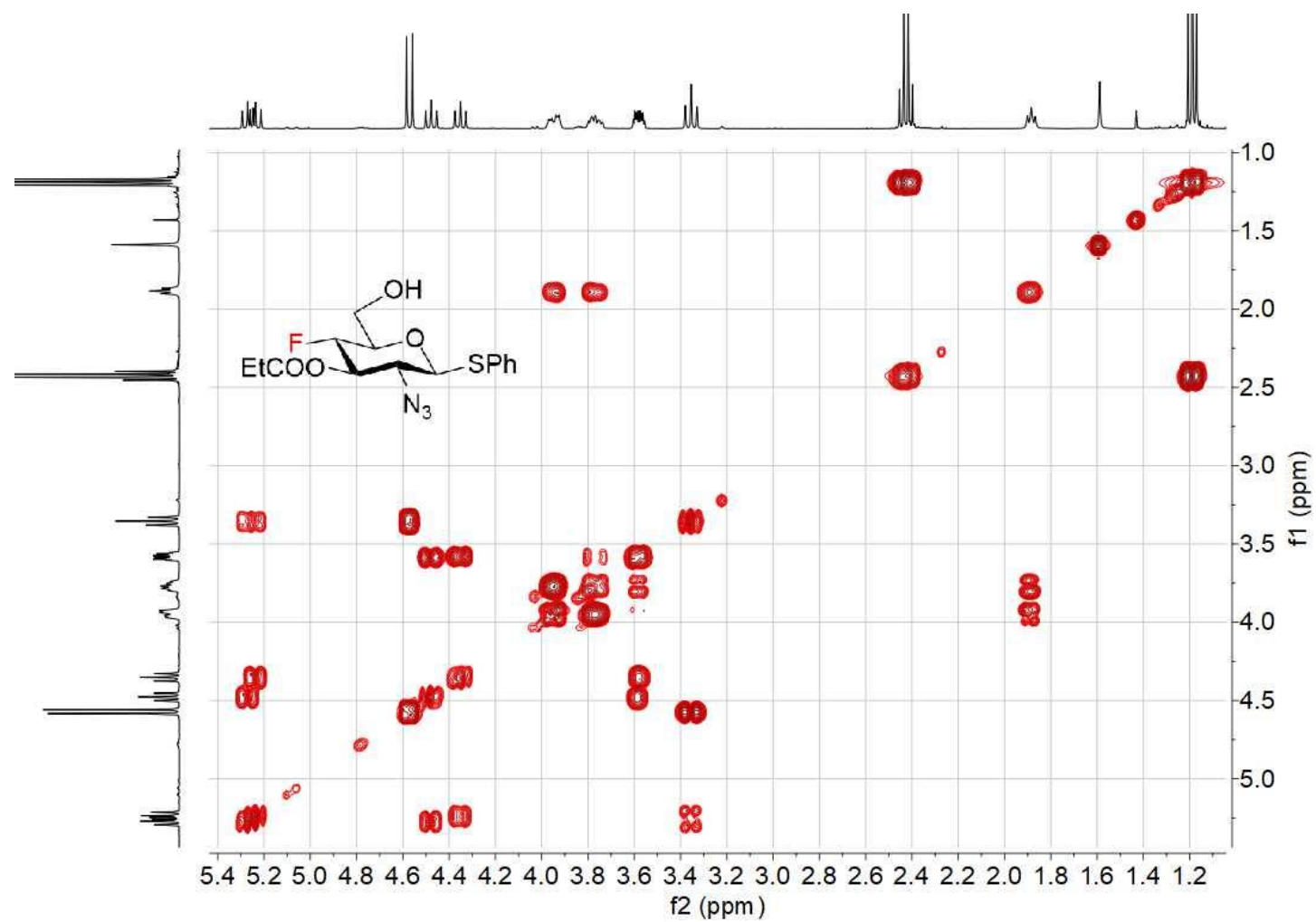
¹³C NMR (100 MHz, CDCl₃) β-54



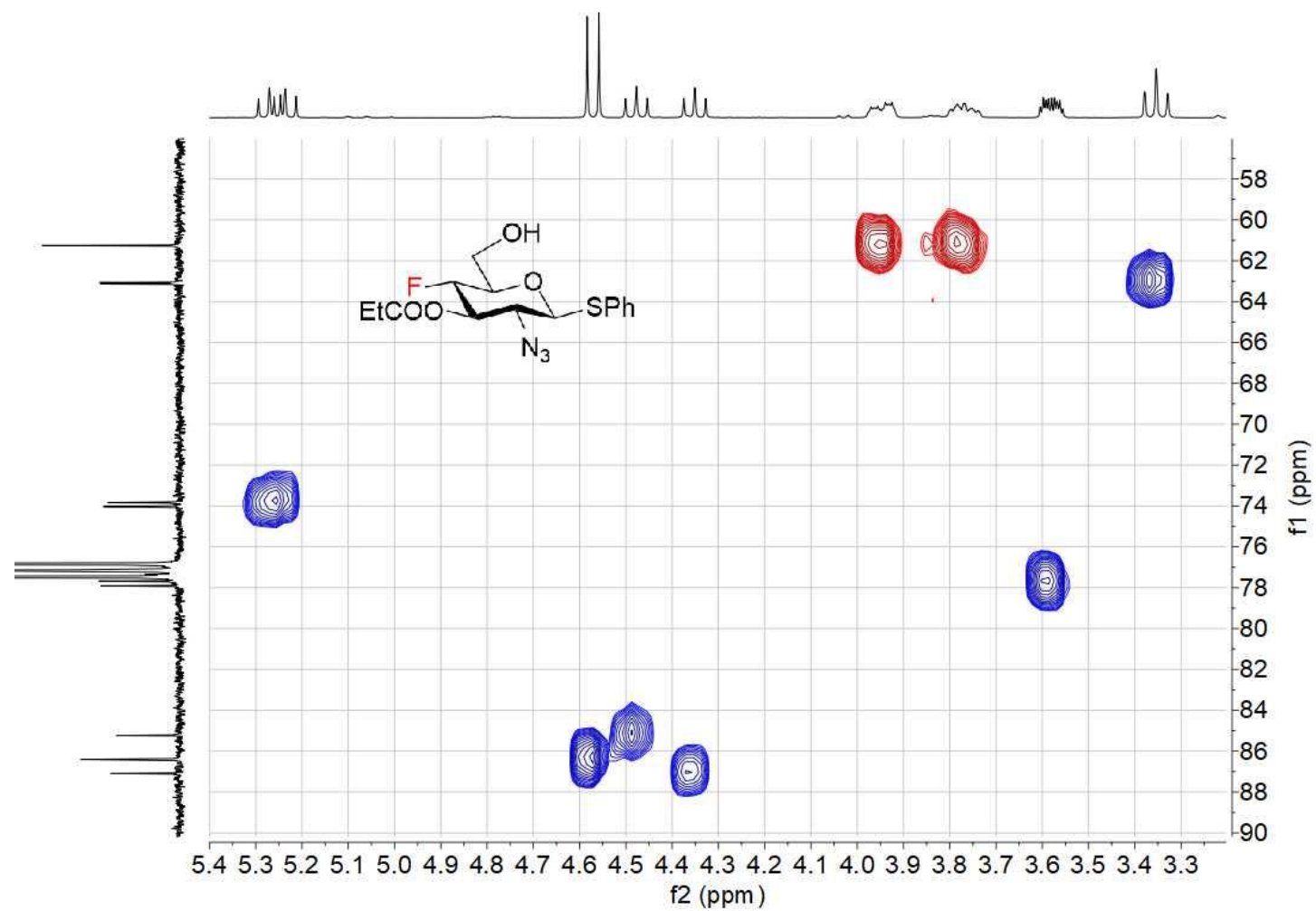
^{19}F NMR (376 MHz, CDCl_3) β -54



^1H - ^1H COSY β -54

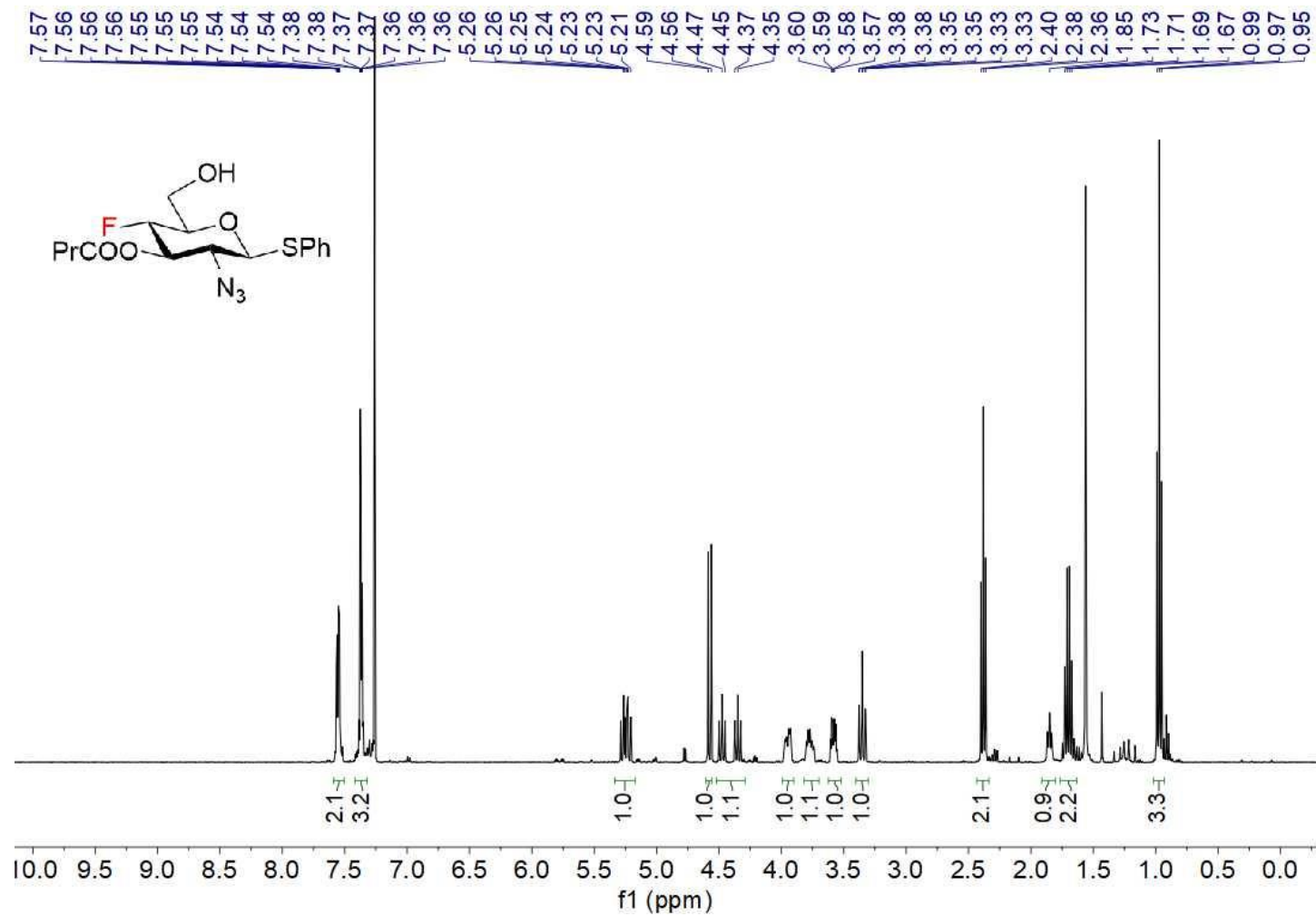


^1H - ^{13}C HSQC β -54

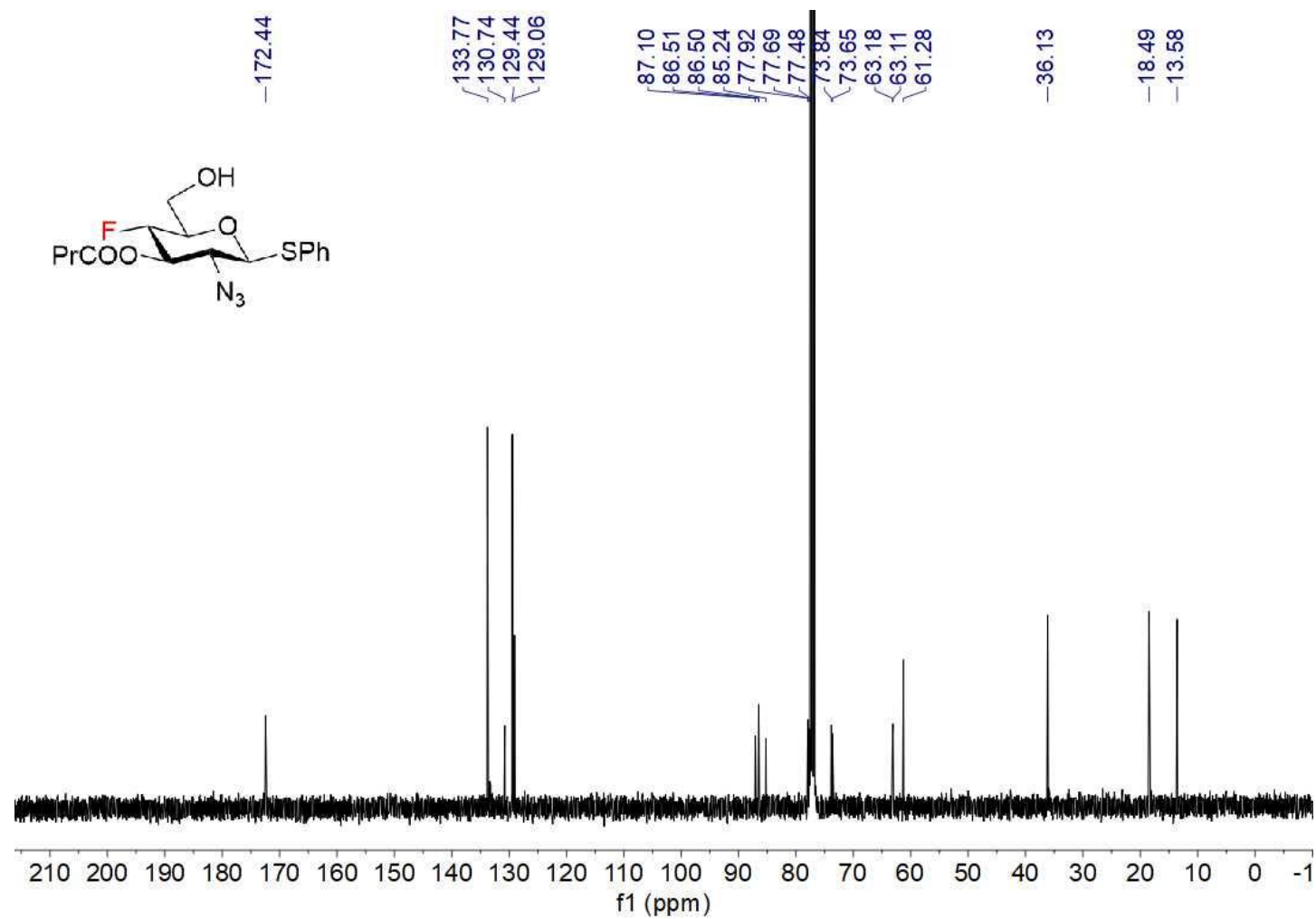


NMR COMPOUND β -55

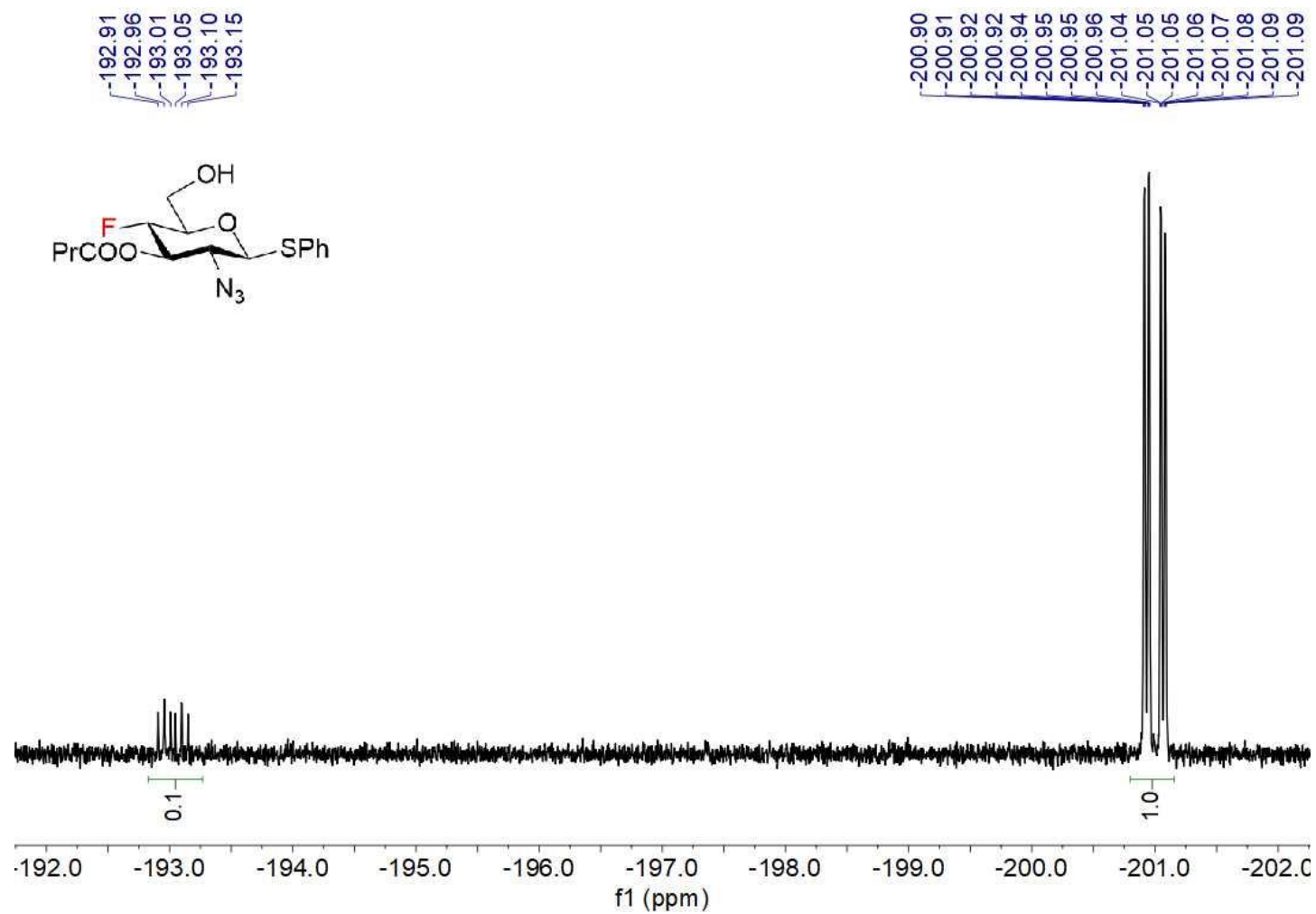
^1H NMR (400 MHz, CDCl_3) β -55



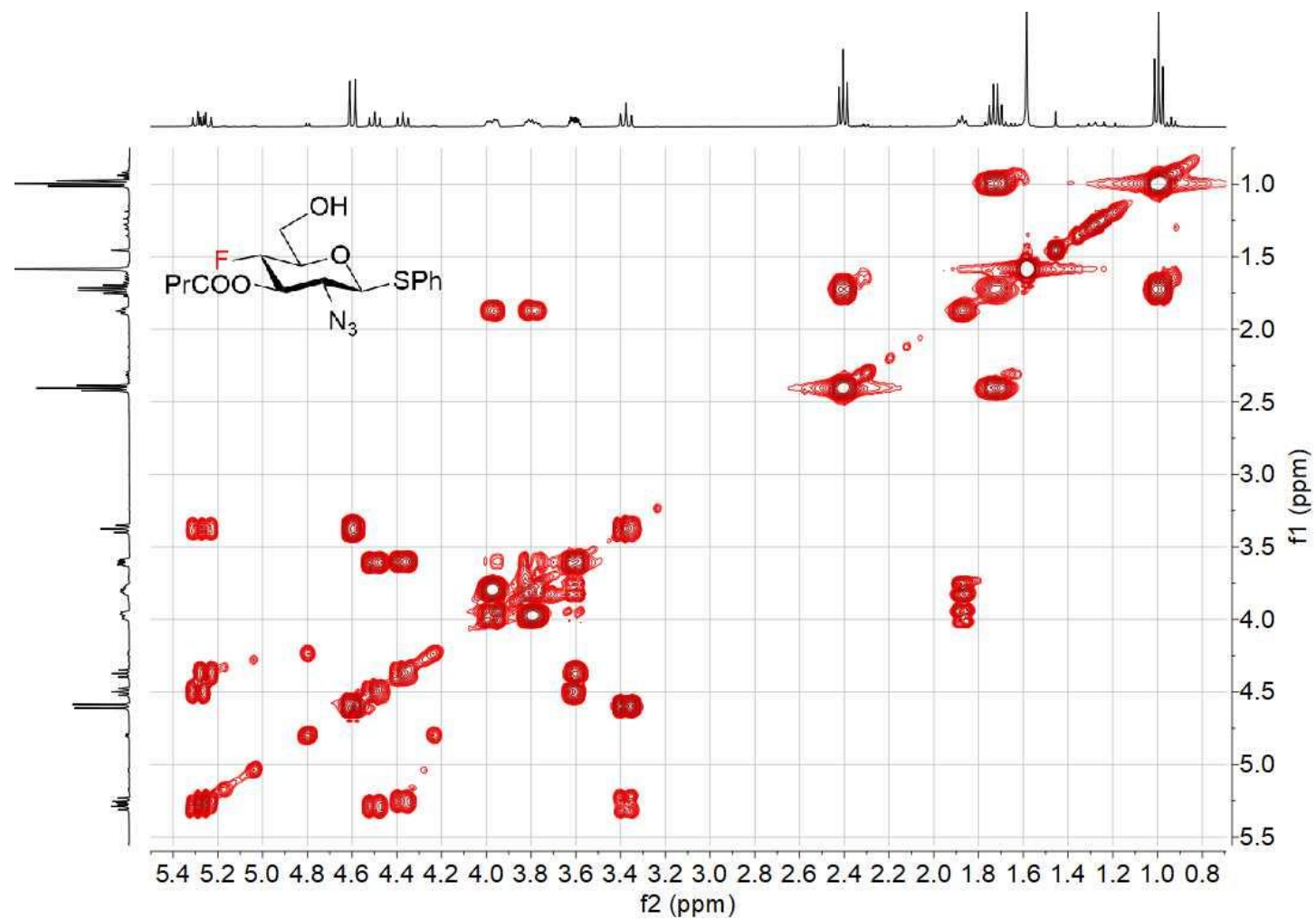
¹³C NMR (100 MHz, CDCl₃) β-55



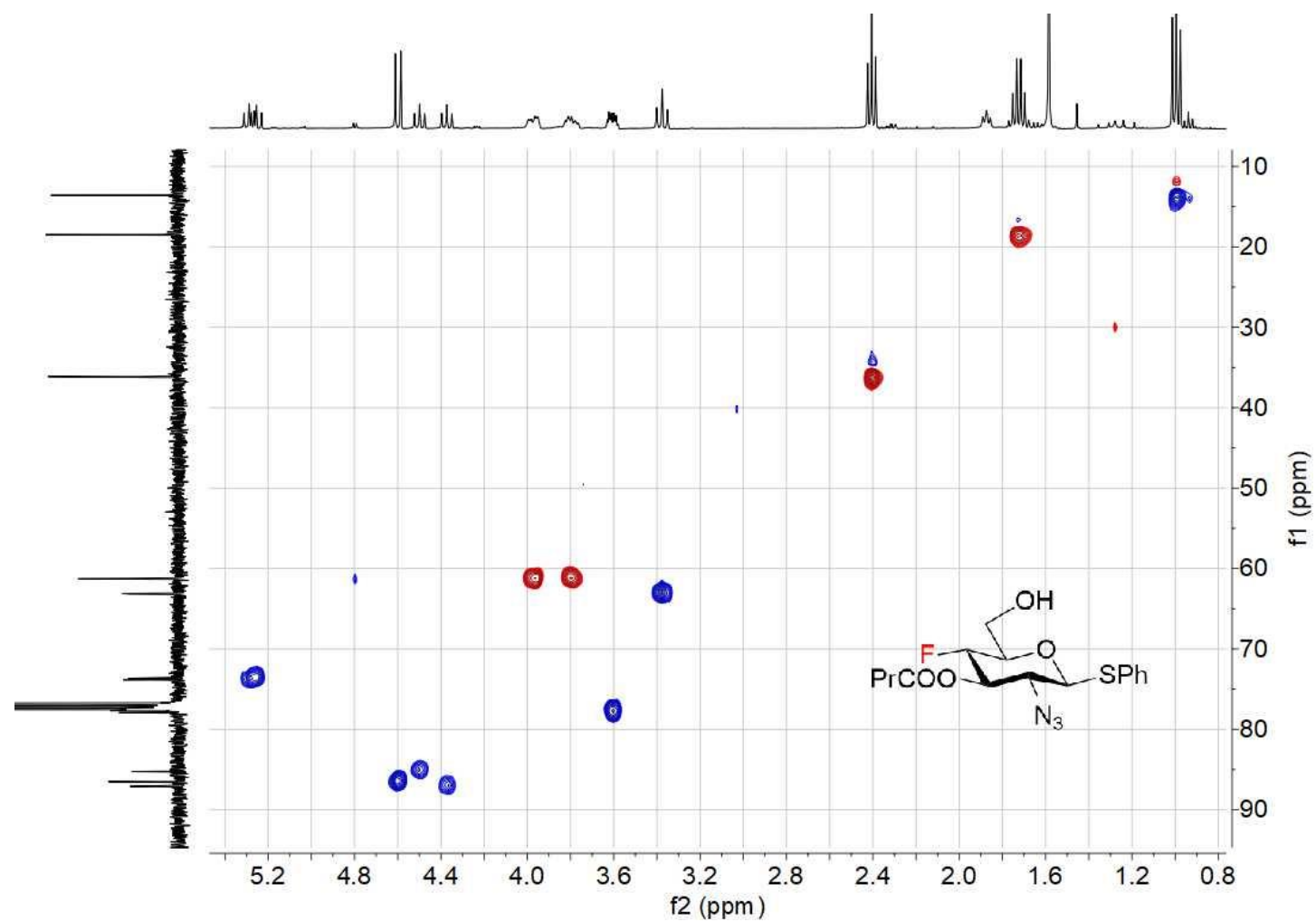
¹⁹F NMR (376 MHz, CDCl₃) β-55



^1H - ^1H COSY β -55

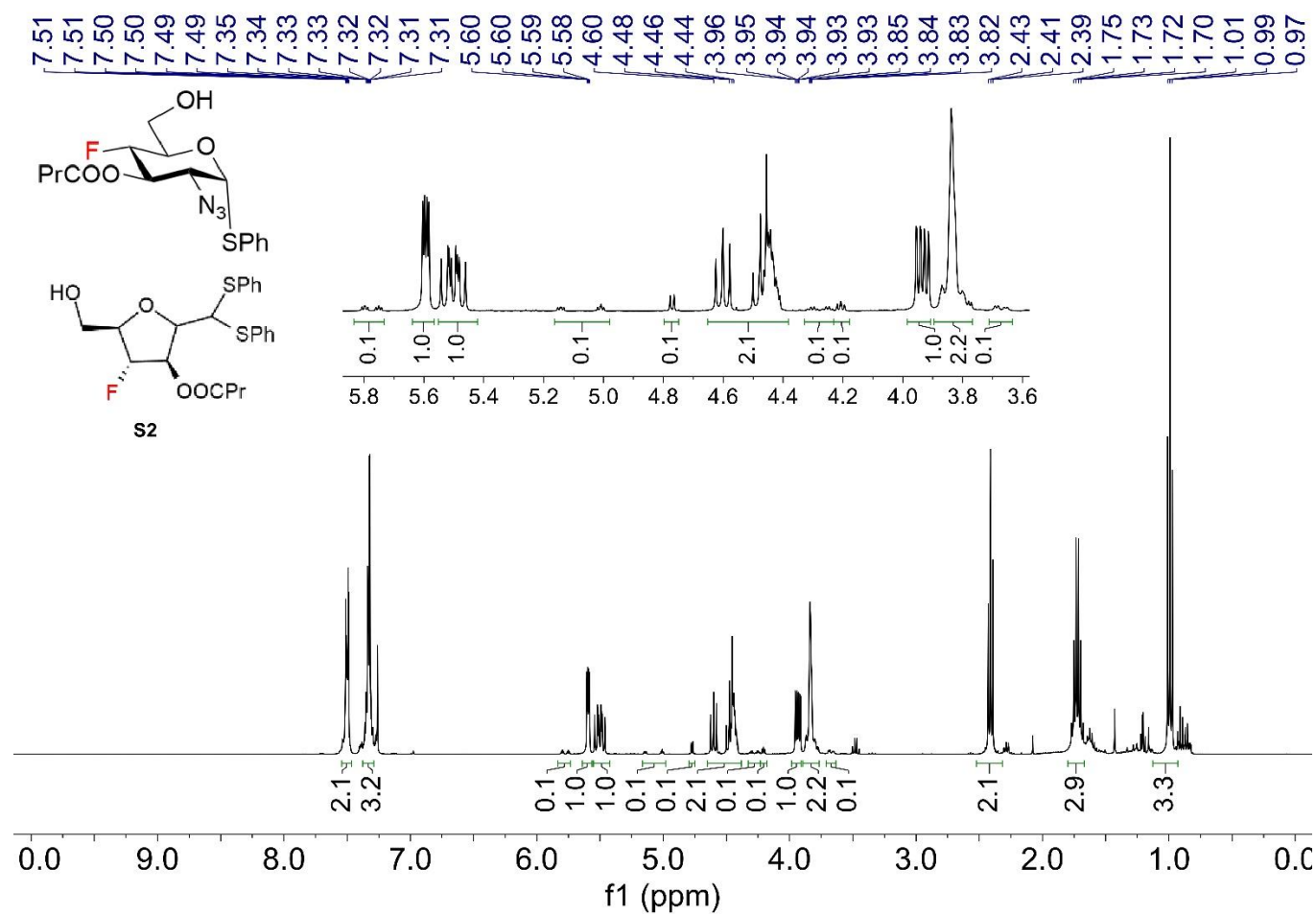


^1H - ^{13}C HSQC β -55

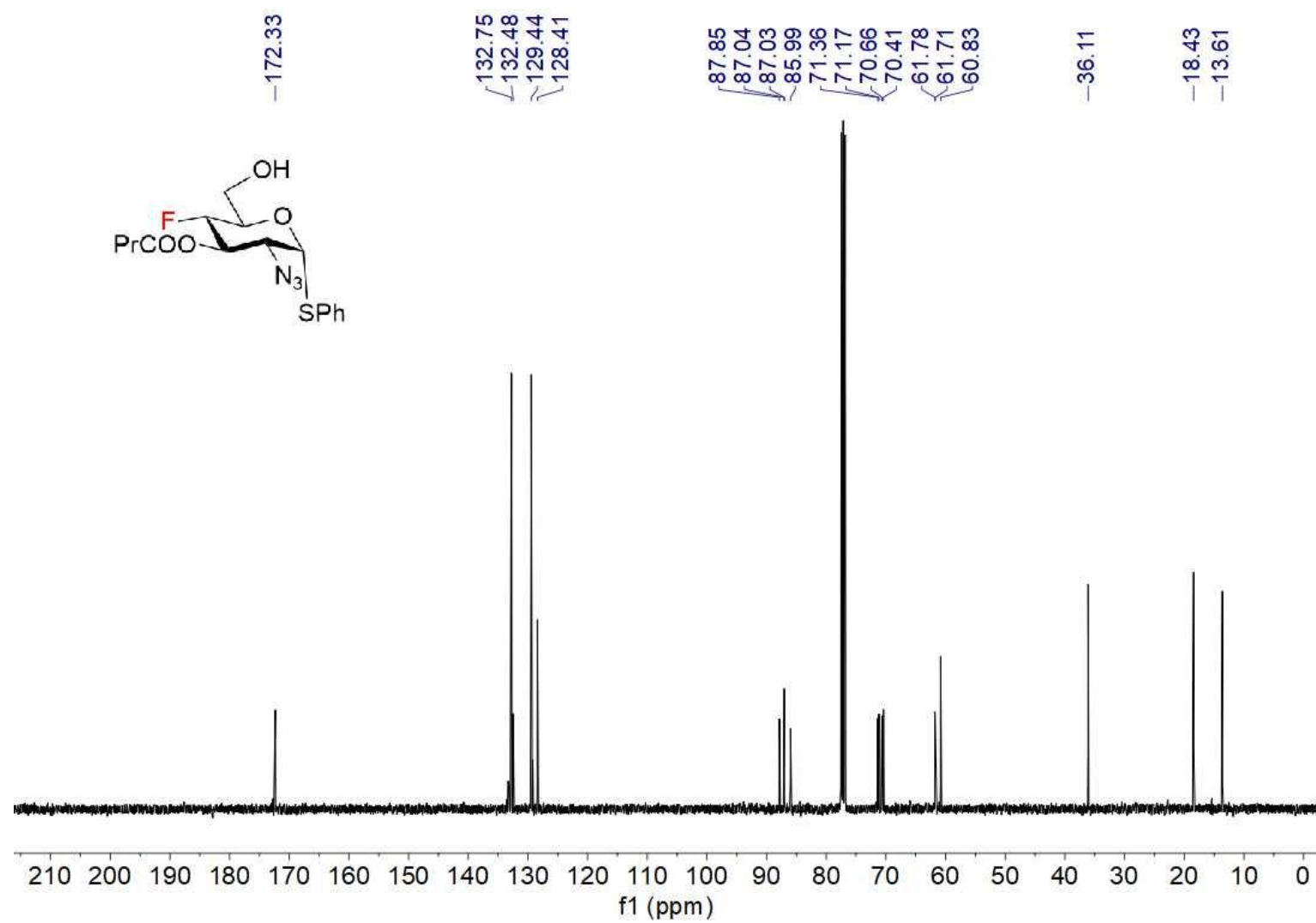


NMR COMPOUND α -55

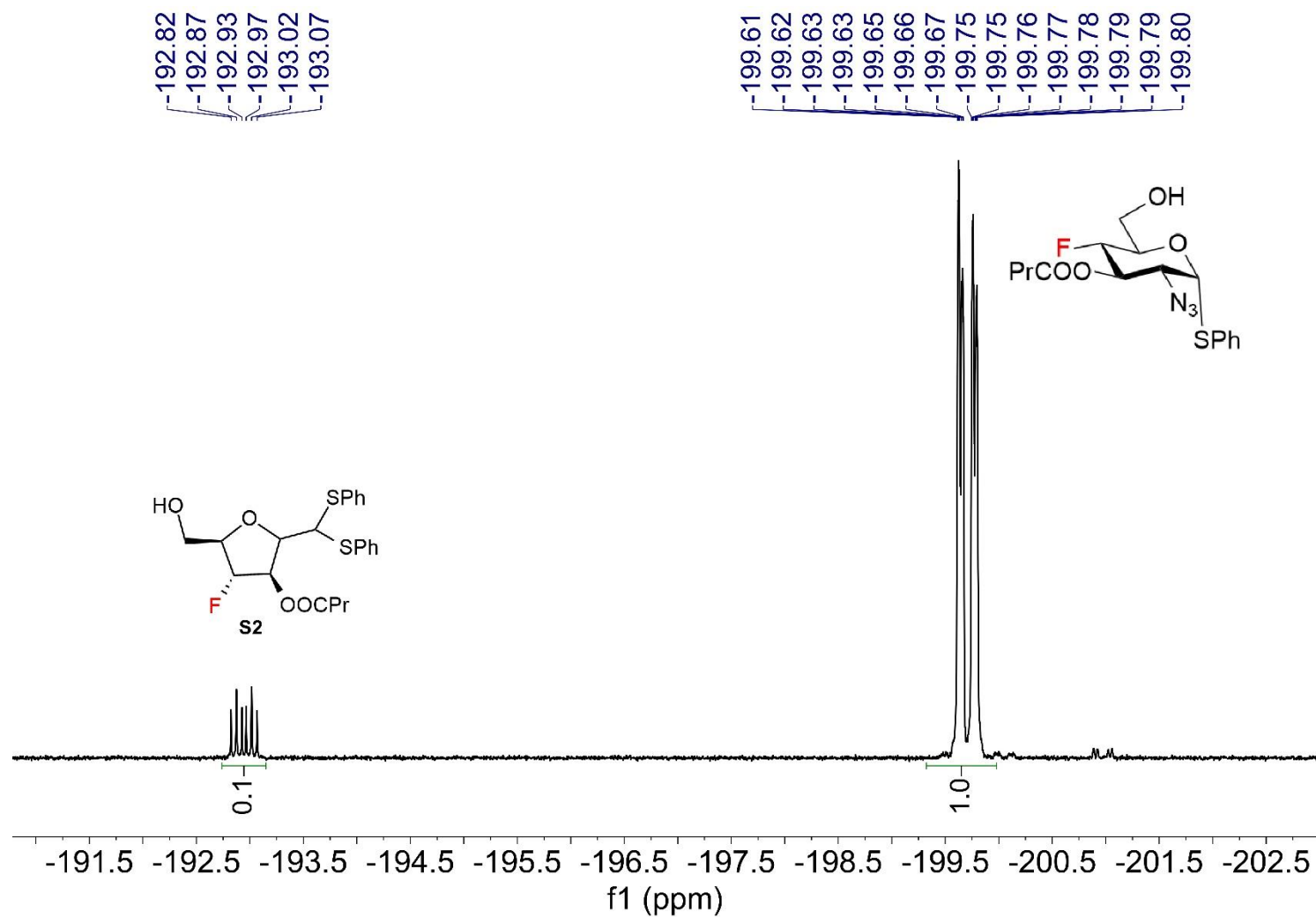
^1H NMR (400 MHz, CDCl_3) α -55 and 9% of S2



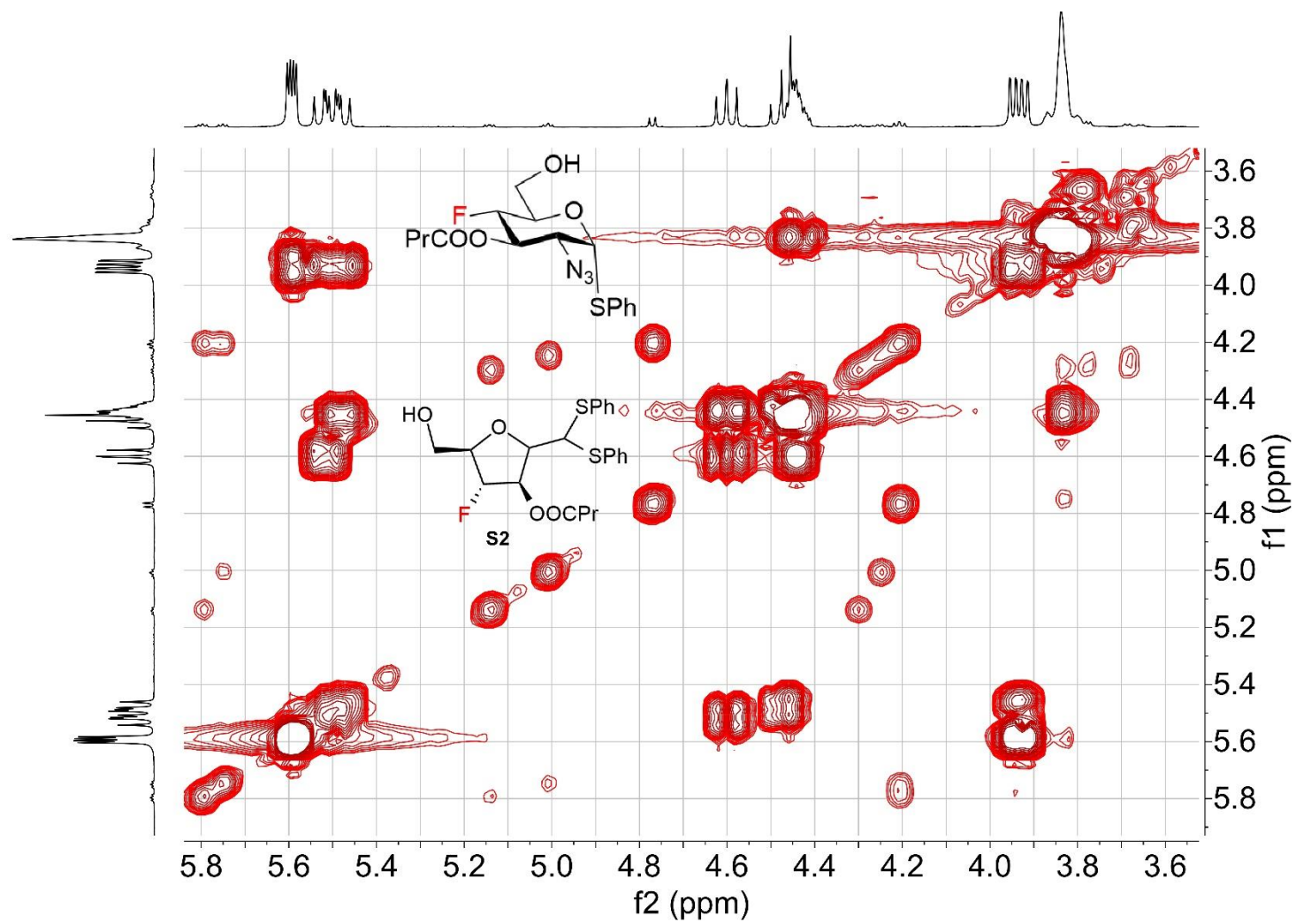
^{13}C NMR (100 MHz, CDCl_3) α -55



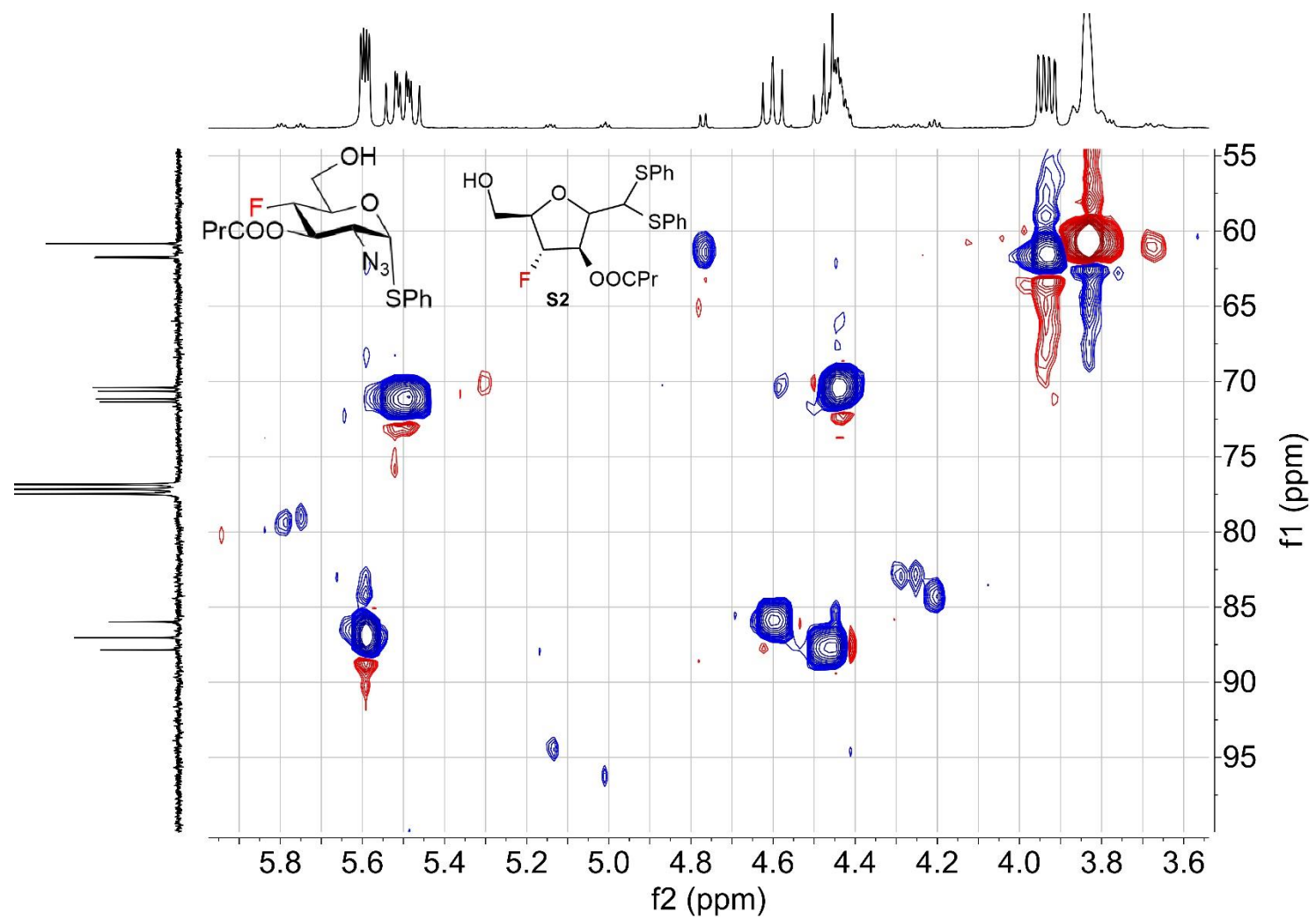
^{19}F NMR (376 MHz, CDCl_3) α -55 and 9% of S2



^1H - ^1H COSY α -55

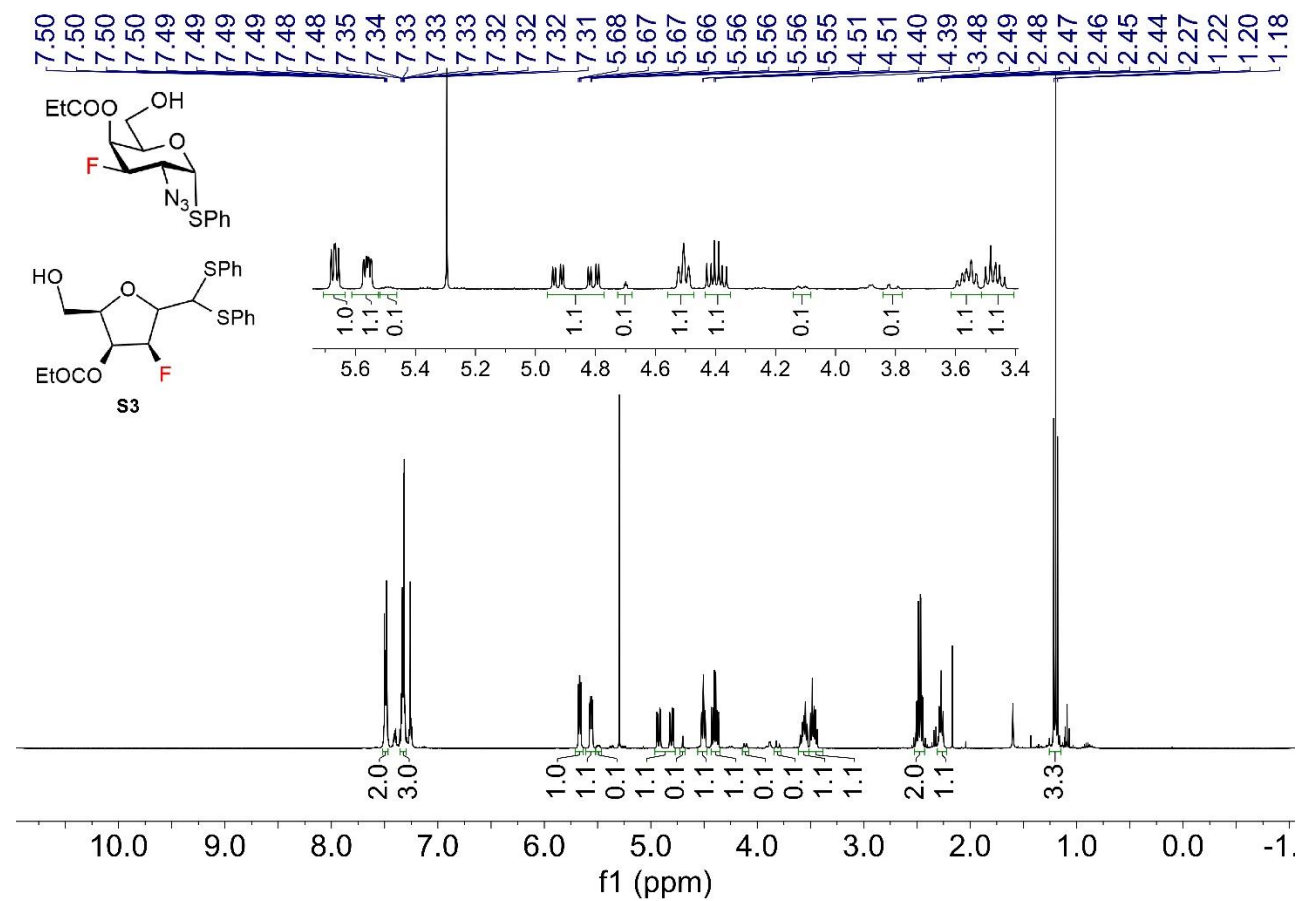


^1H - ^{13}C HSQC α -55

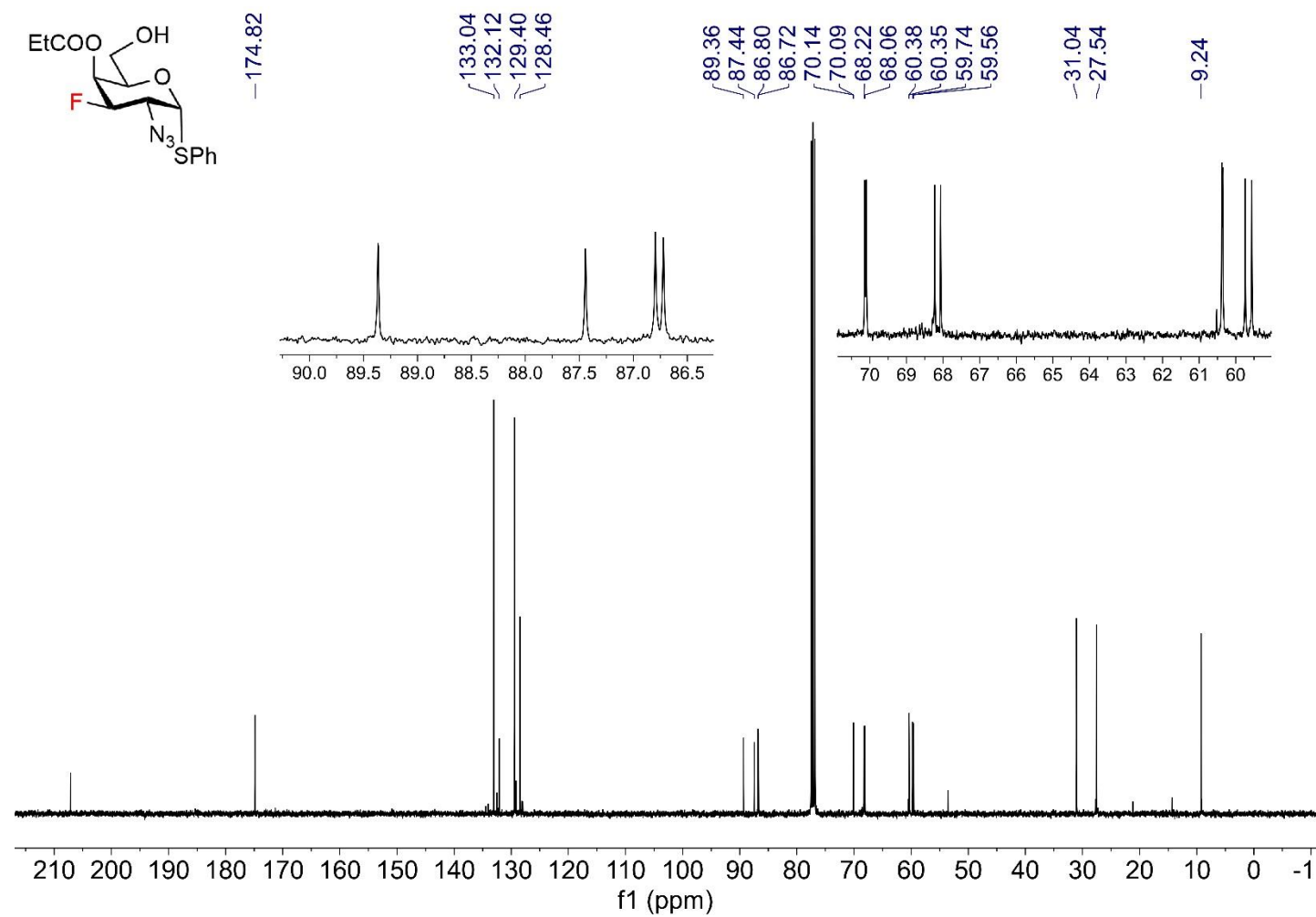


NMR COMPOUND α -56

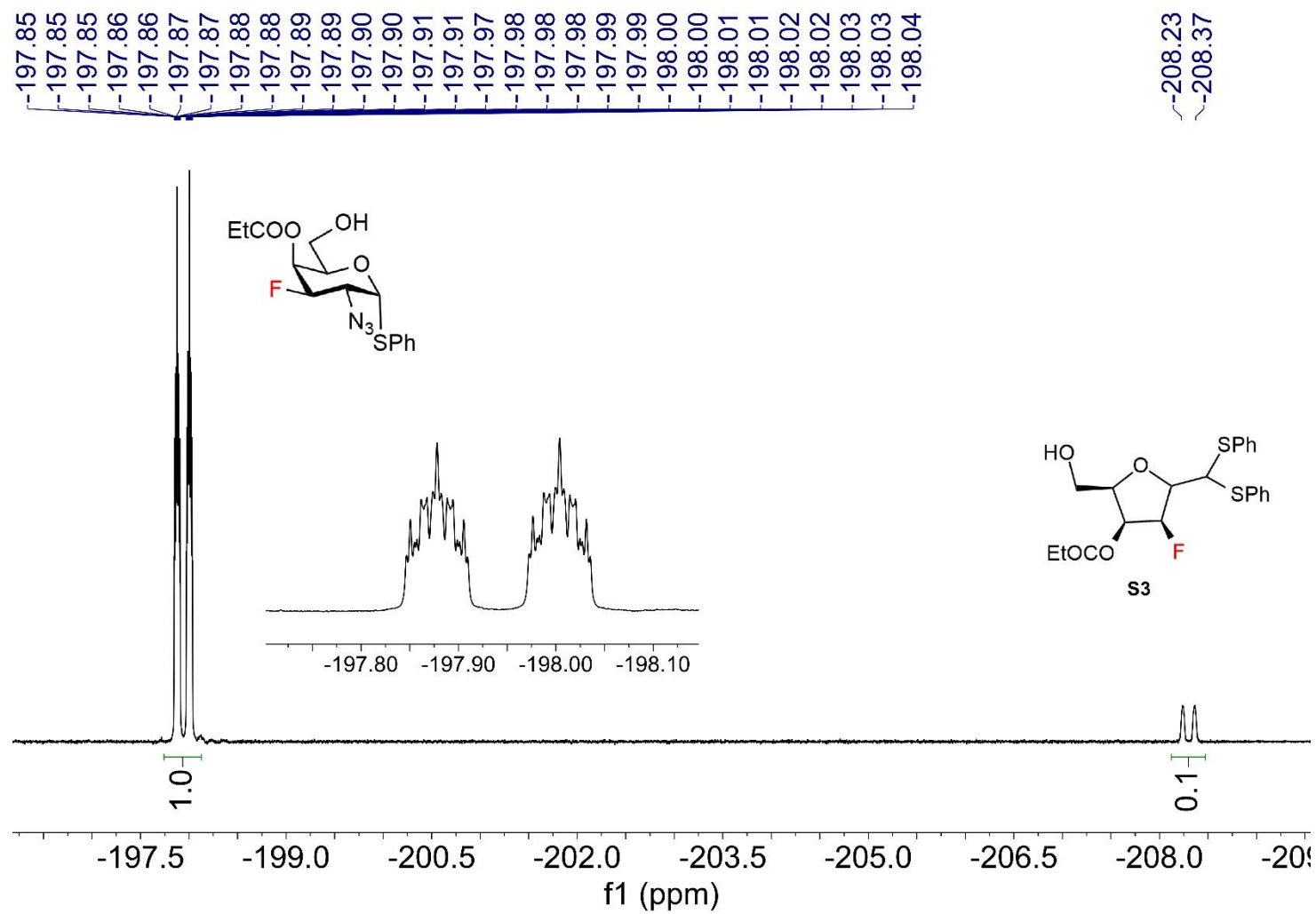
^1H NMR (400 MHz, CDCl_3) α -56 and ca 9% S3



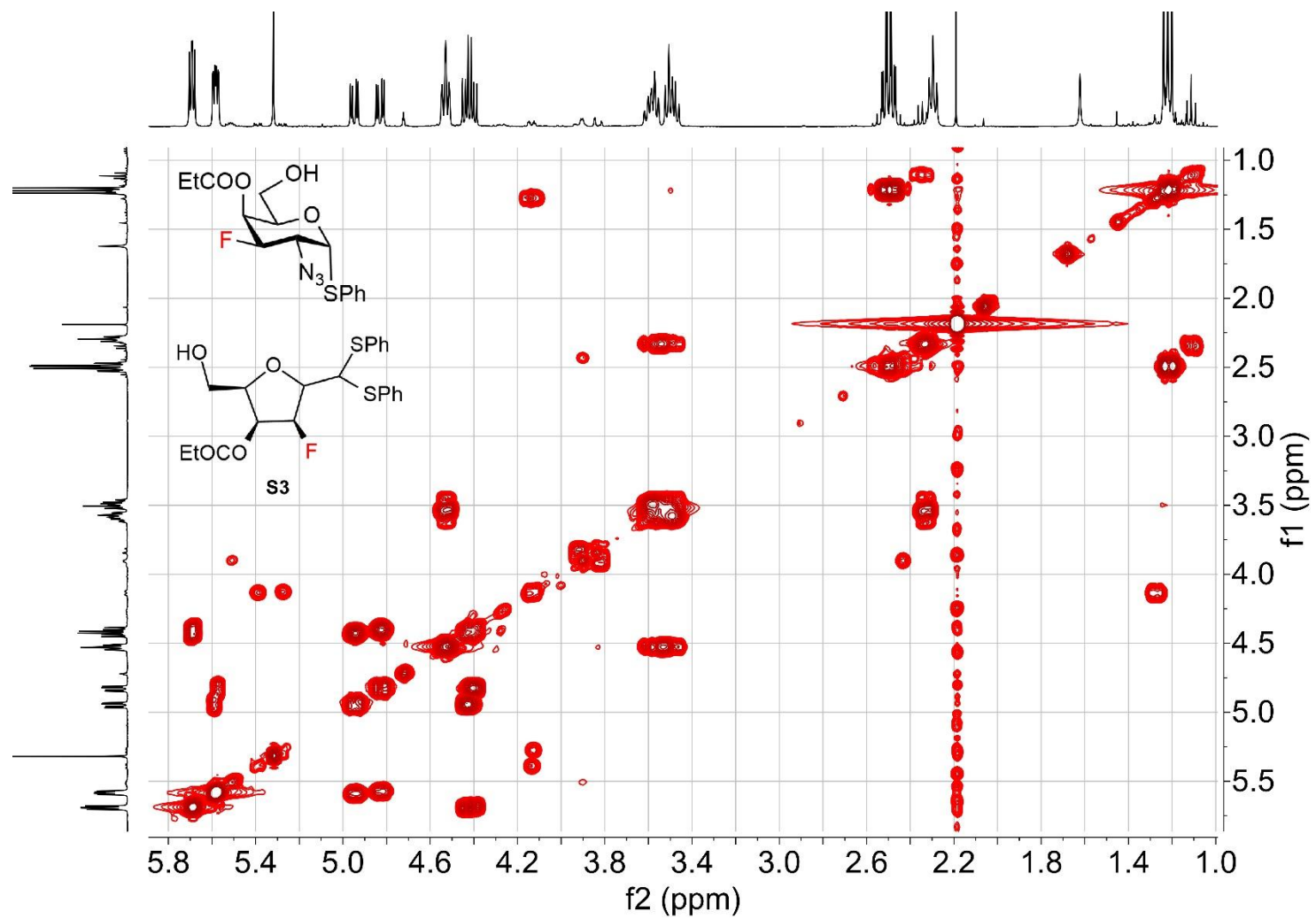
¹³C NMR (100 MHz, CDCl₃) α-56



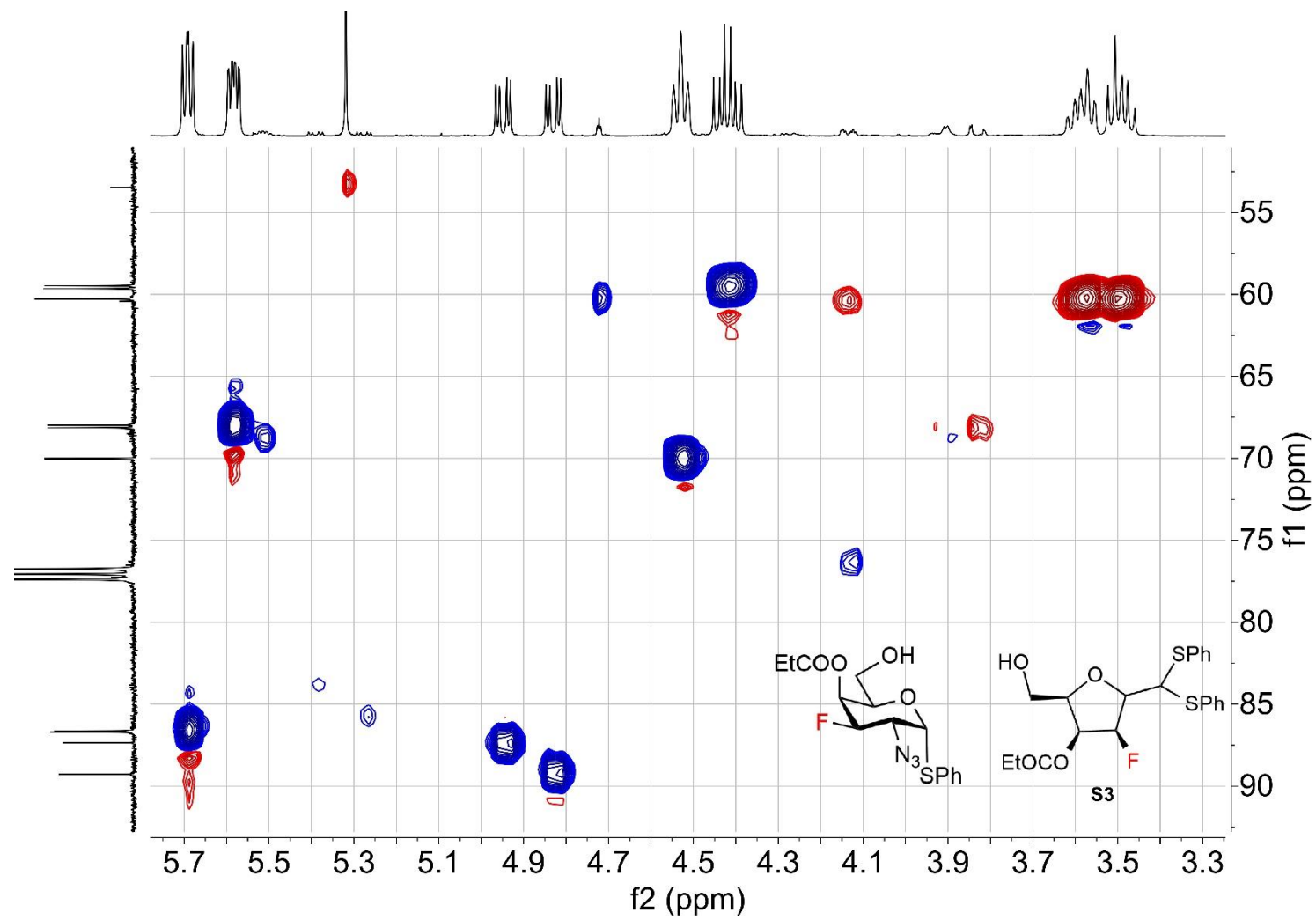
¹⁹F NMR (376 MHz, CDCl₃) α-56 and 9% of S3



^1H - ^1H COSY α -56

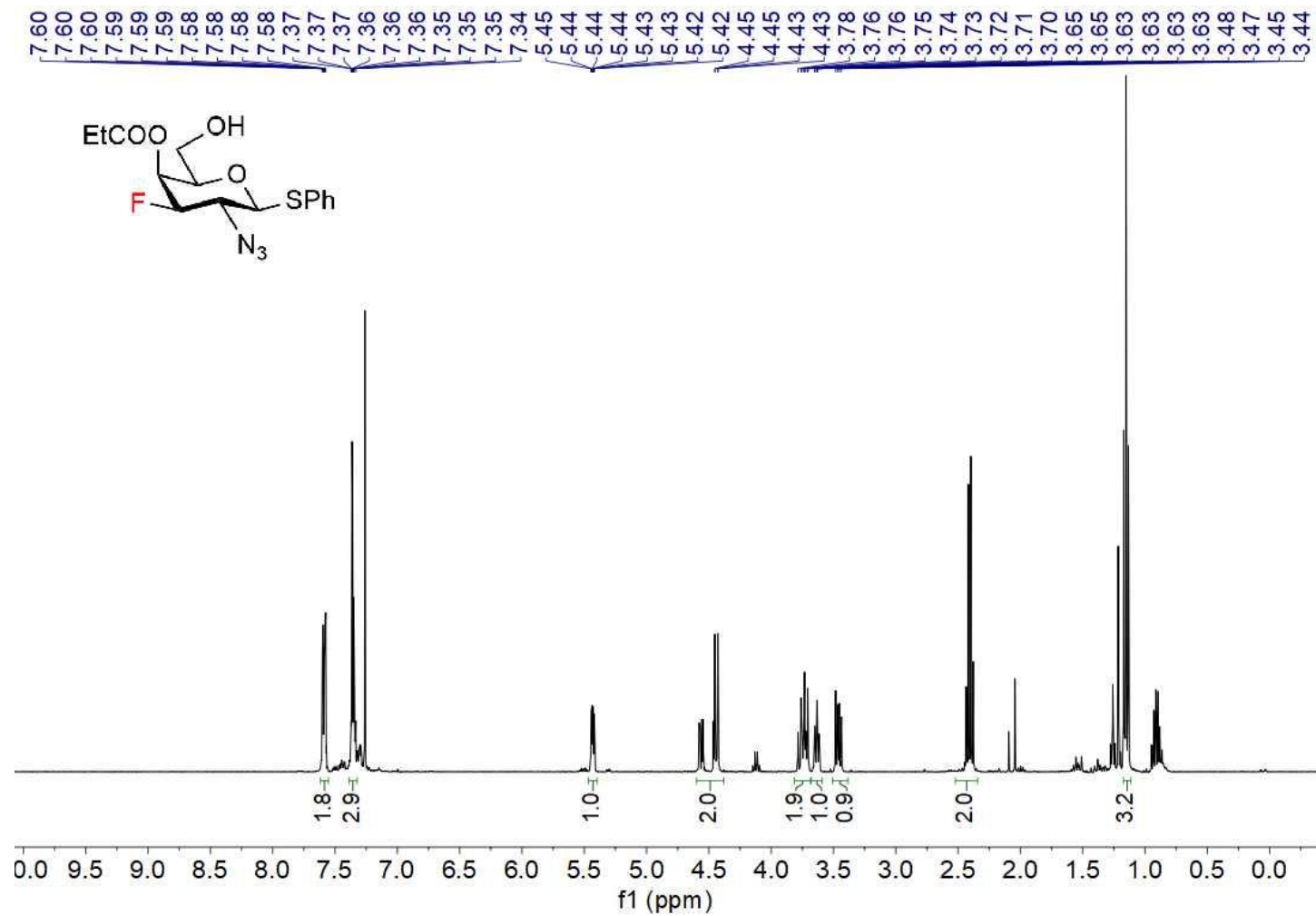


^1H - ^{13}C HSQC α -56

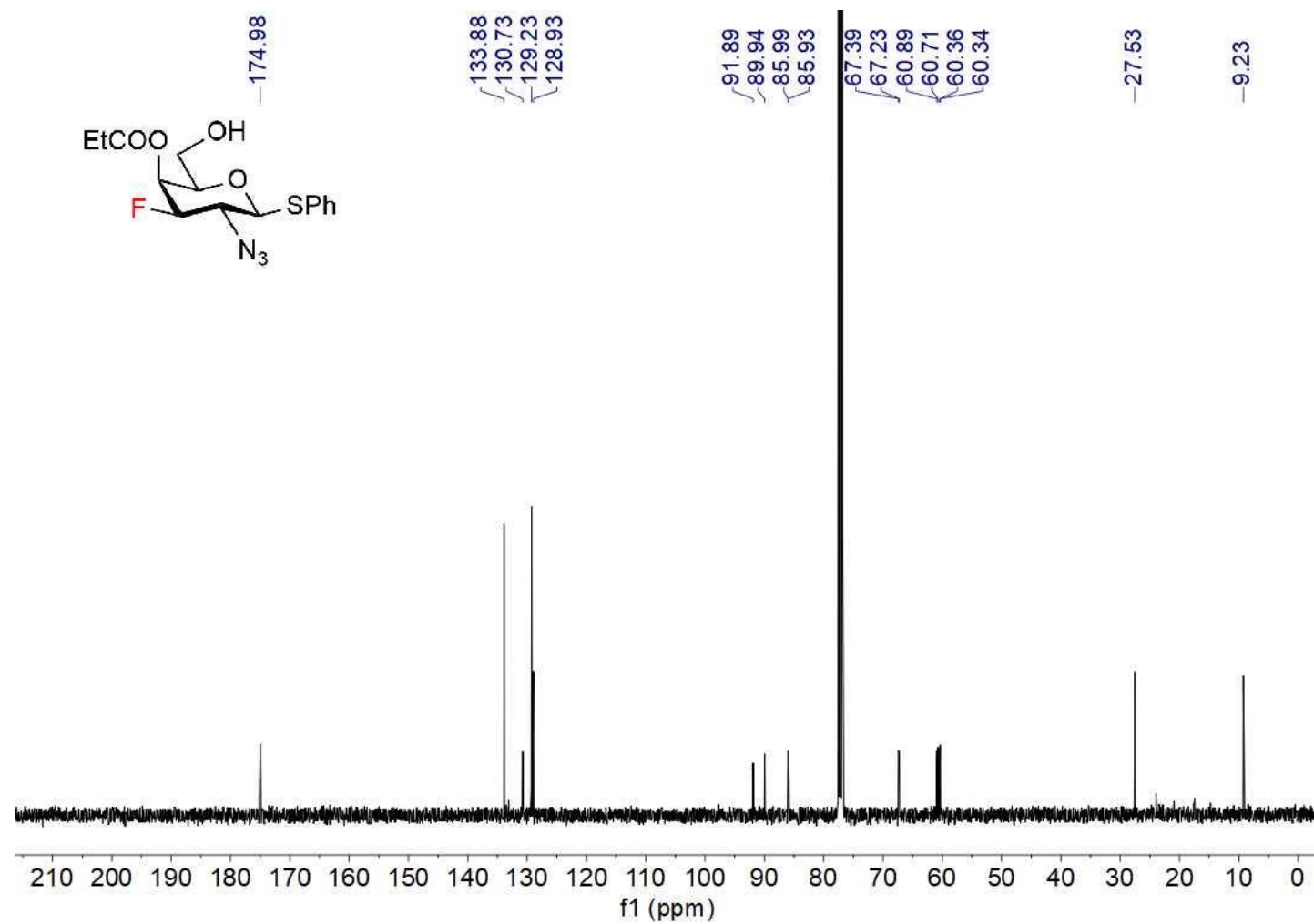


NMR COMPOUND β -56

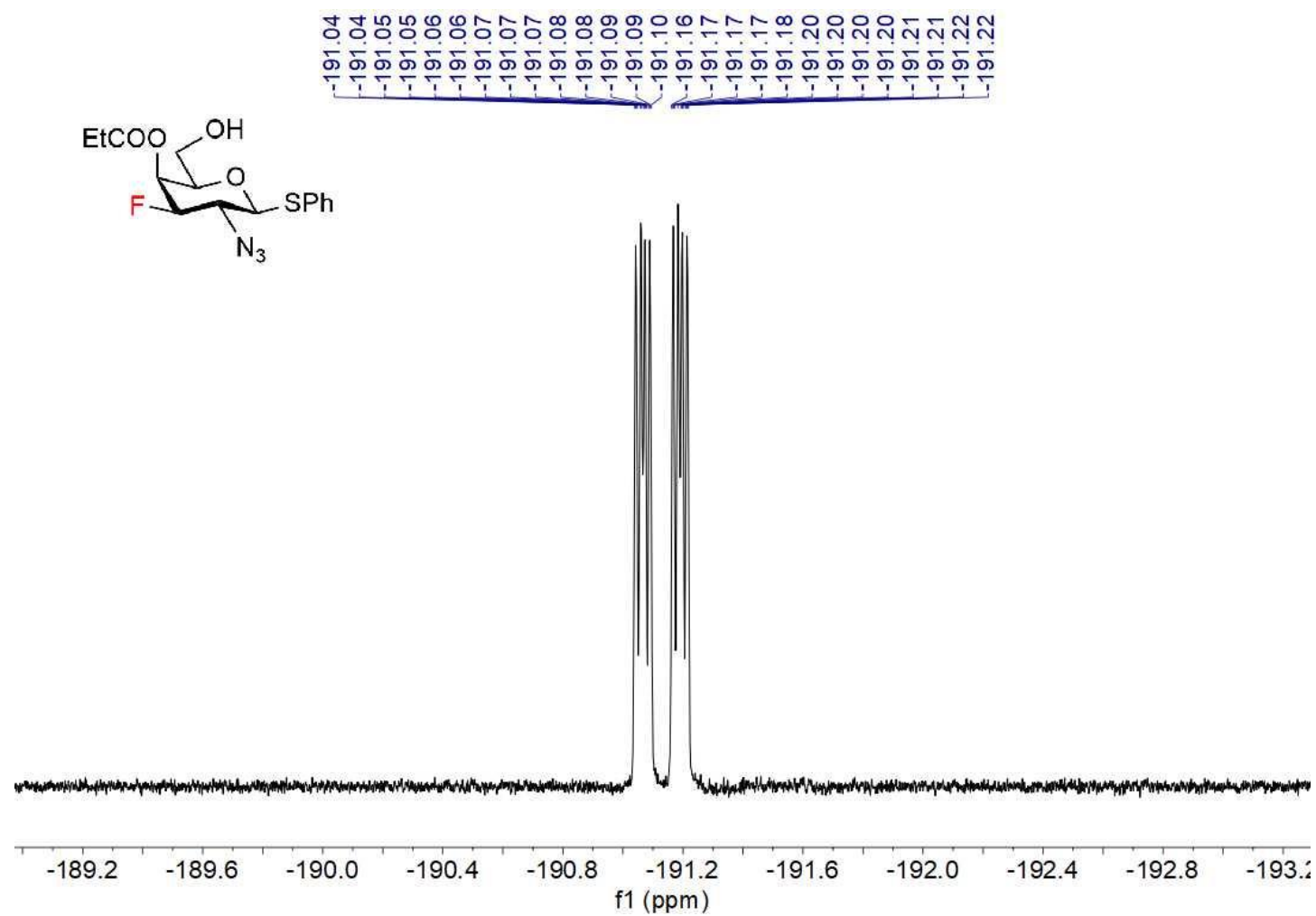
^1H NMR (400 MHz, CDCl_3) β -56



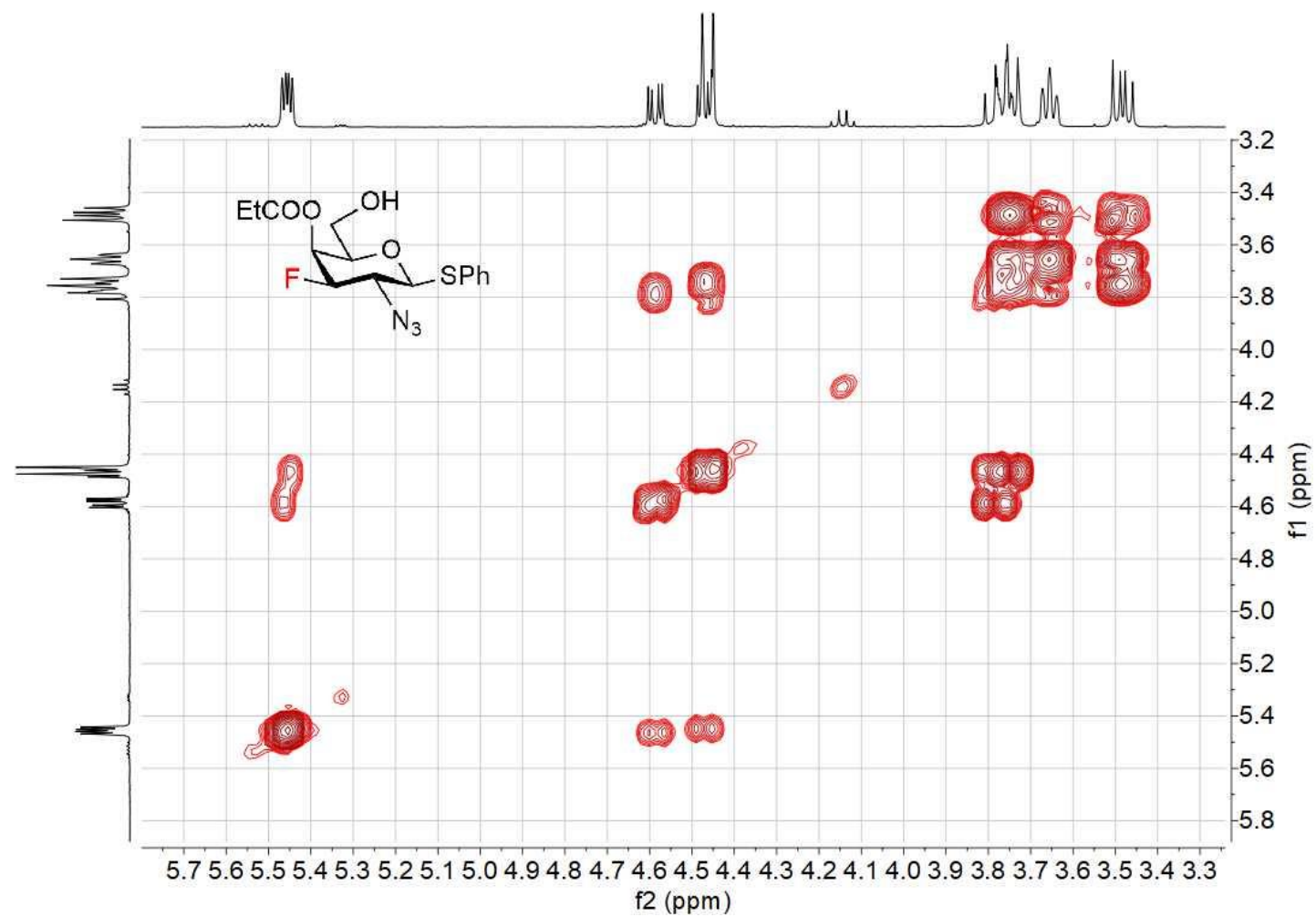
¹³C NMR (100 MHz, CDCl₃) β-56



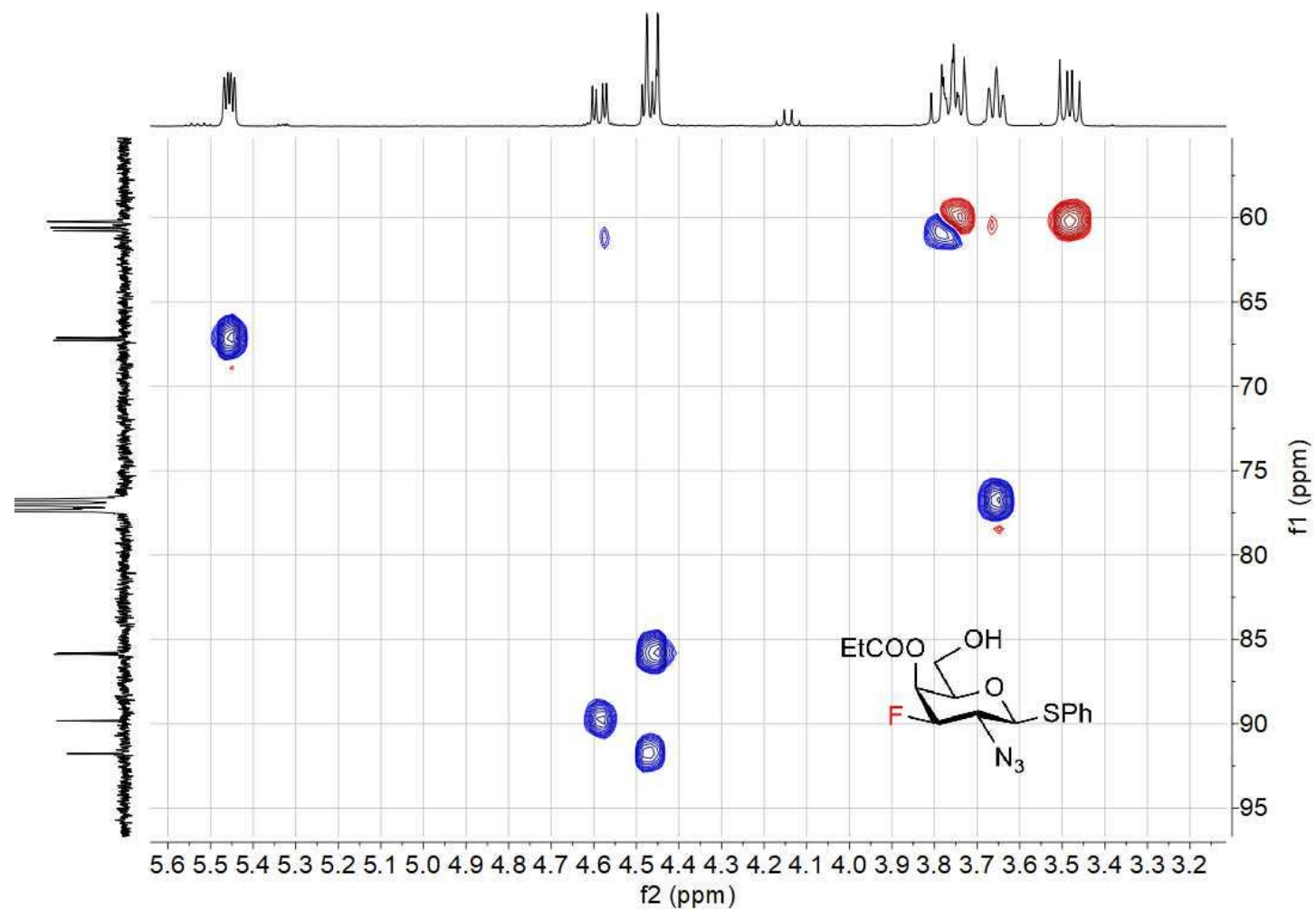
¹⁹F NMR (376 MHz, CDCl₃) β-56



^1H - ^1H COSY β -56

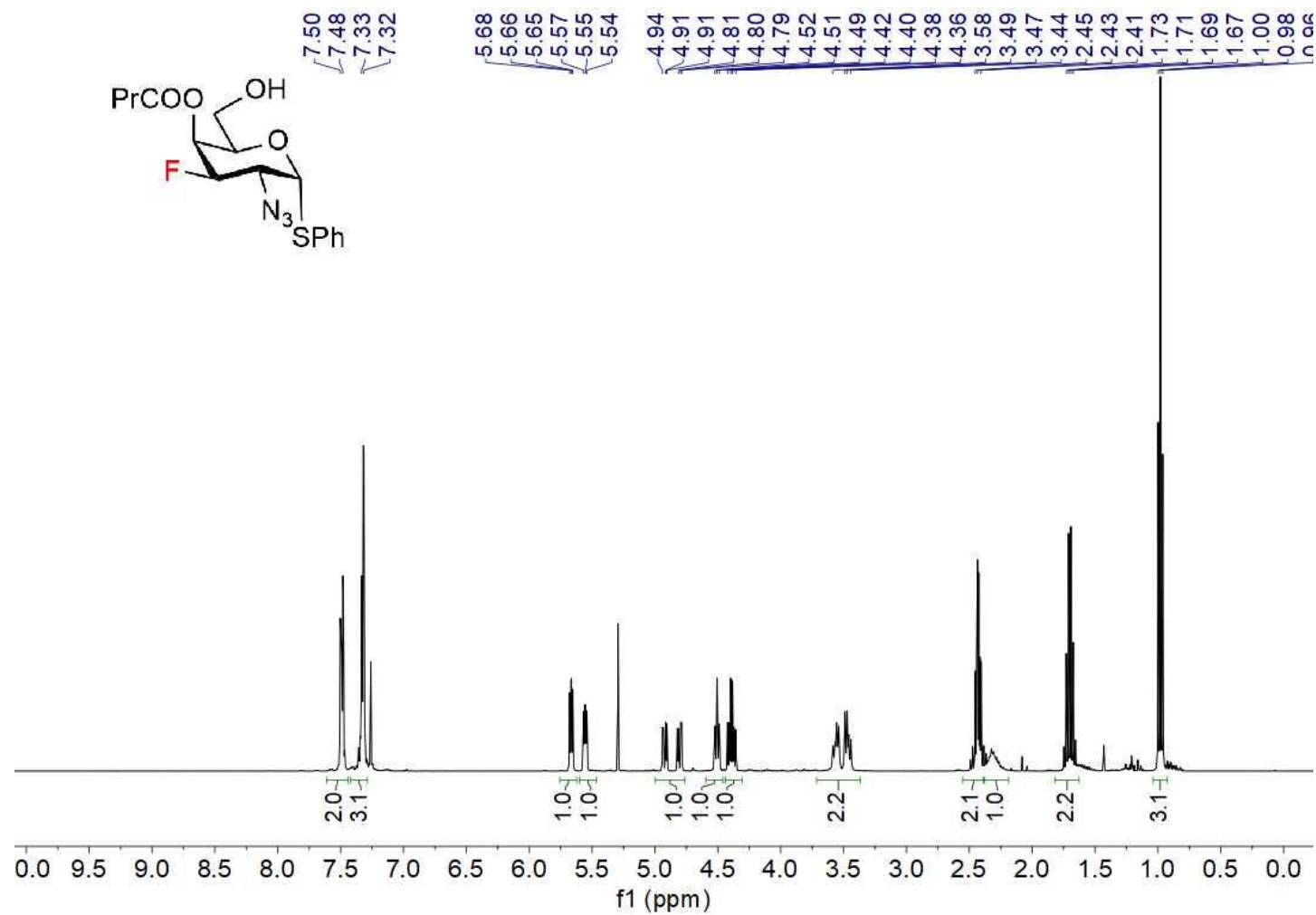


^1H - ^{13}C HSQC β -56

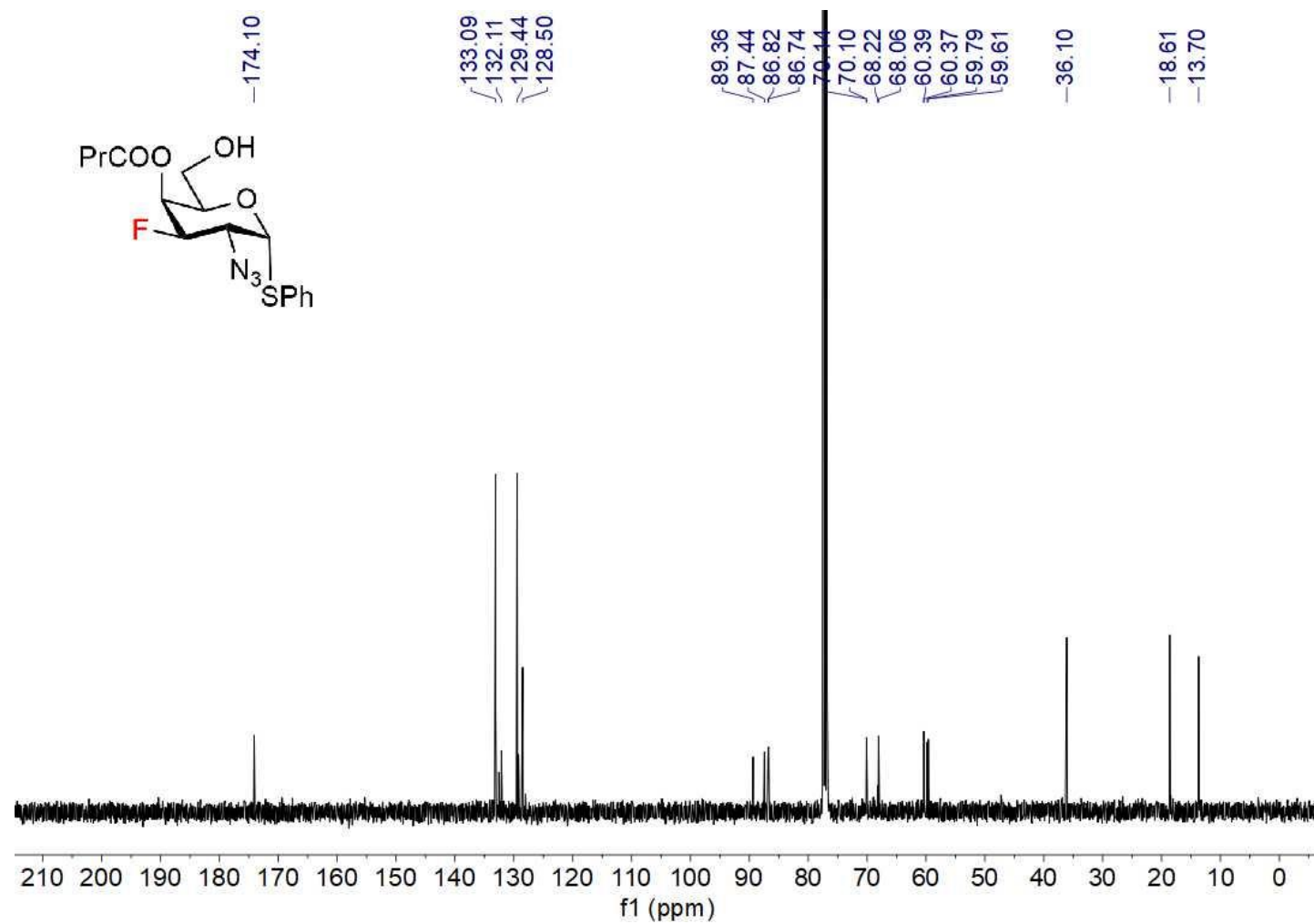


NMR COMPOUND α -57

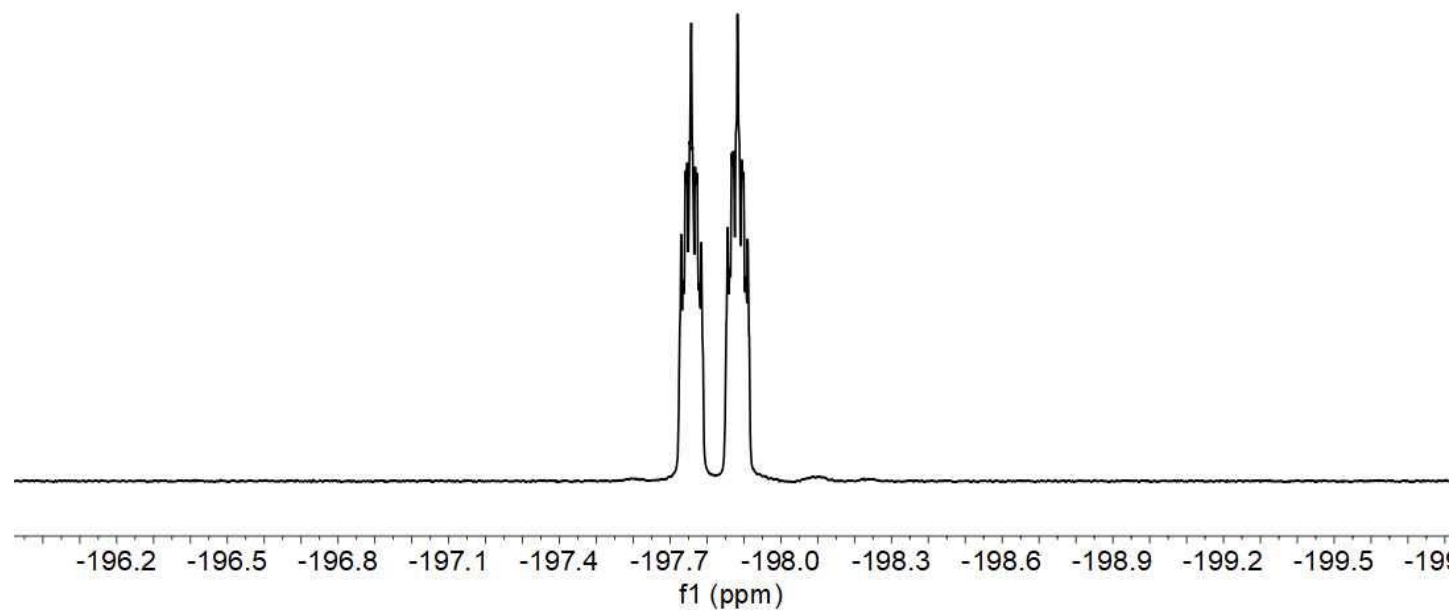
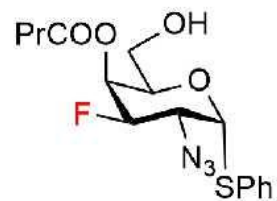
^1H NMR (400 MHz, CDCl_3) α -57



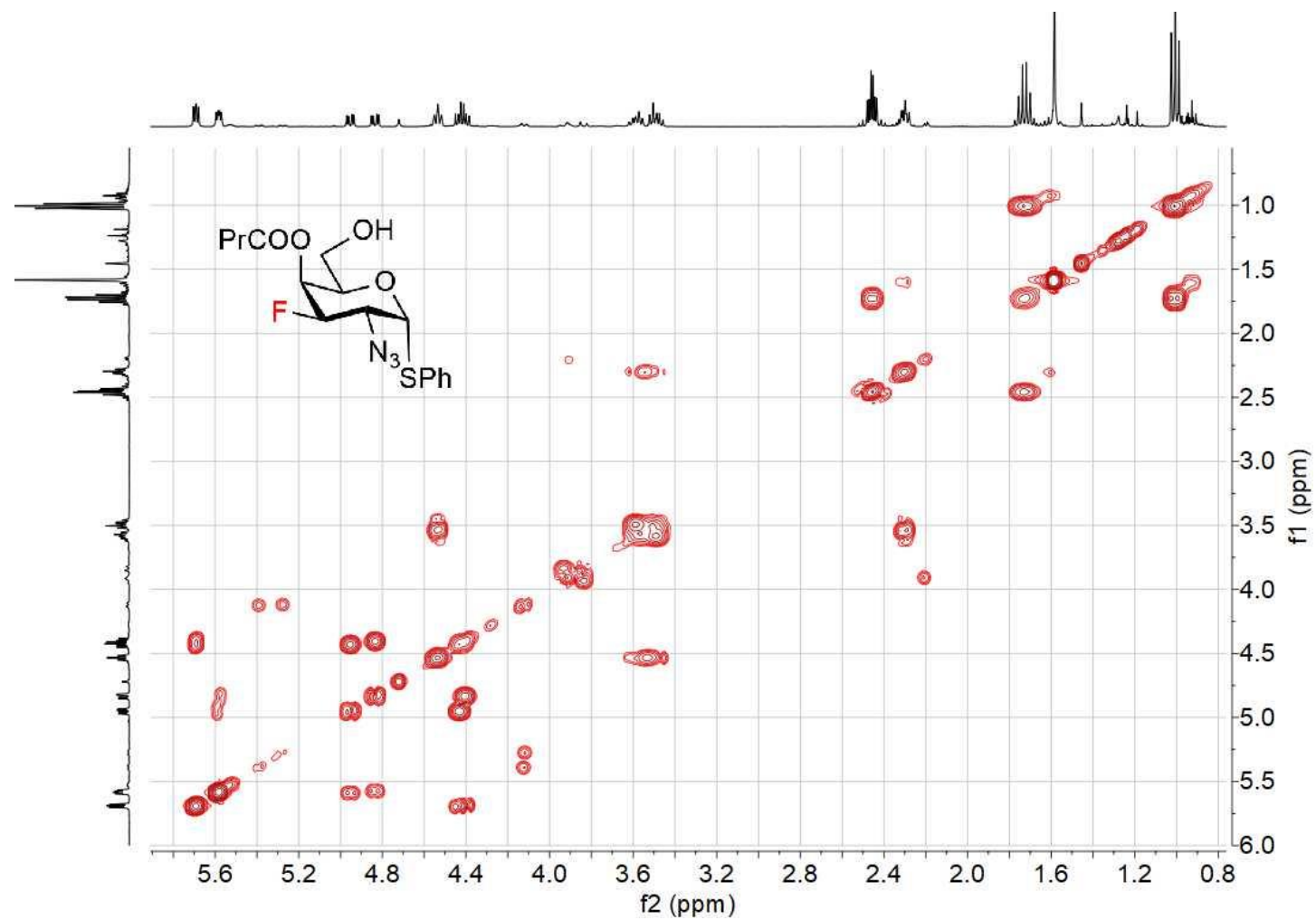
^{13}C NMR (100 MHz, CDCl_3) α -57



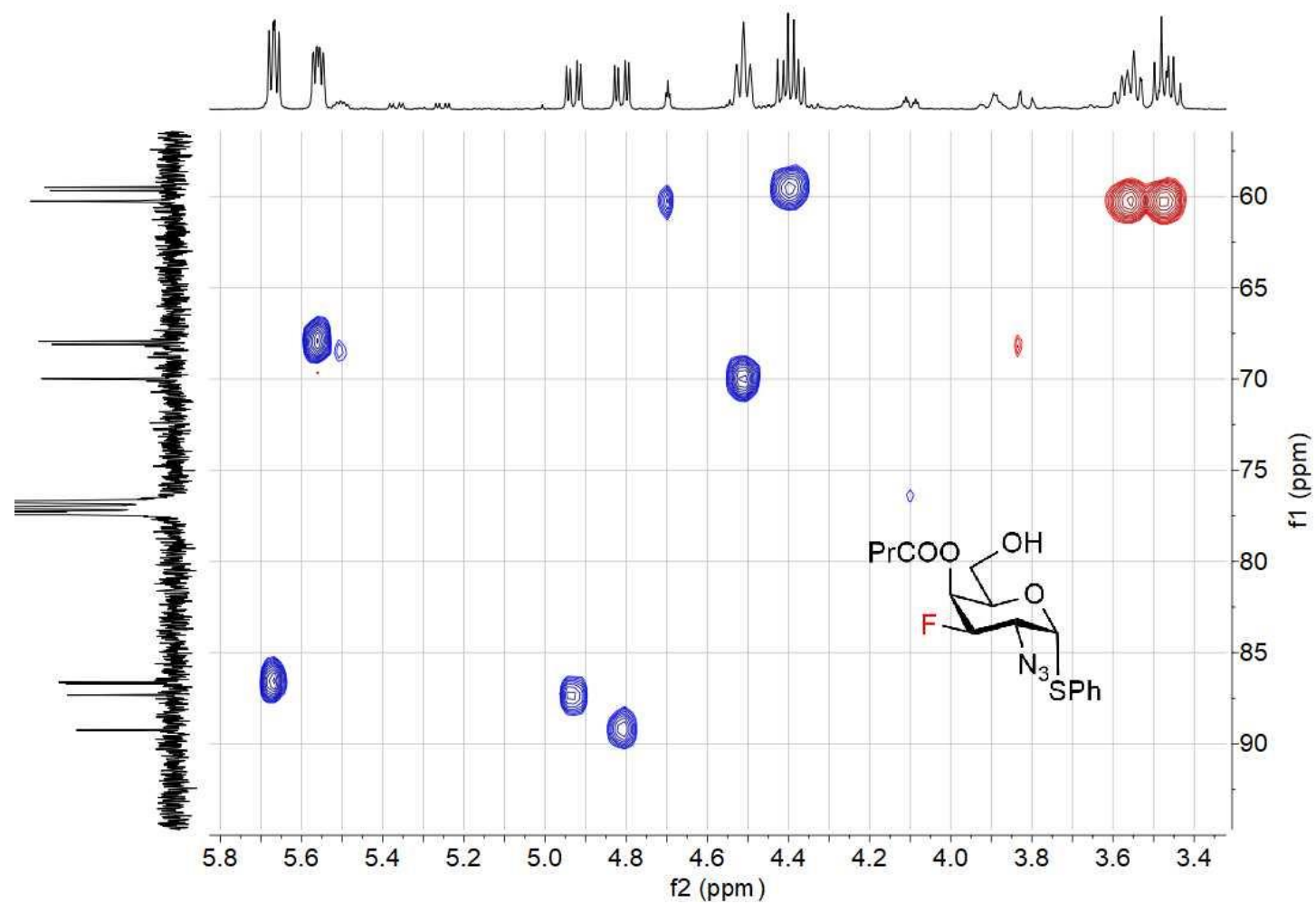
^{19}F NMR (376 MHz, CDCl_3) α -57



^1H - ^1H COSY α -57

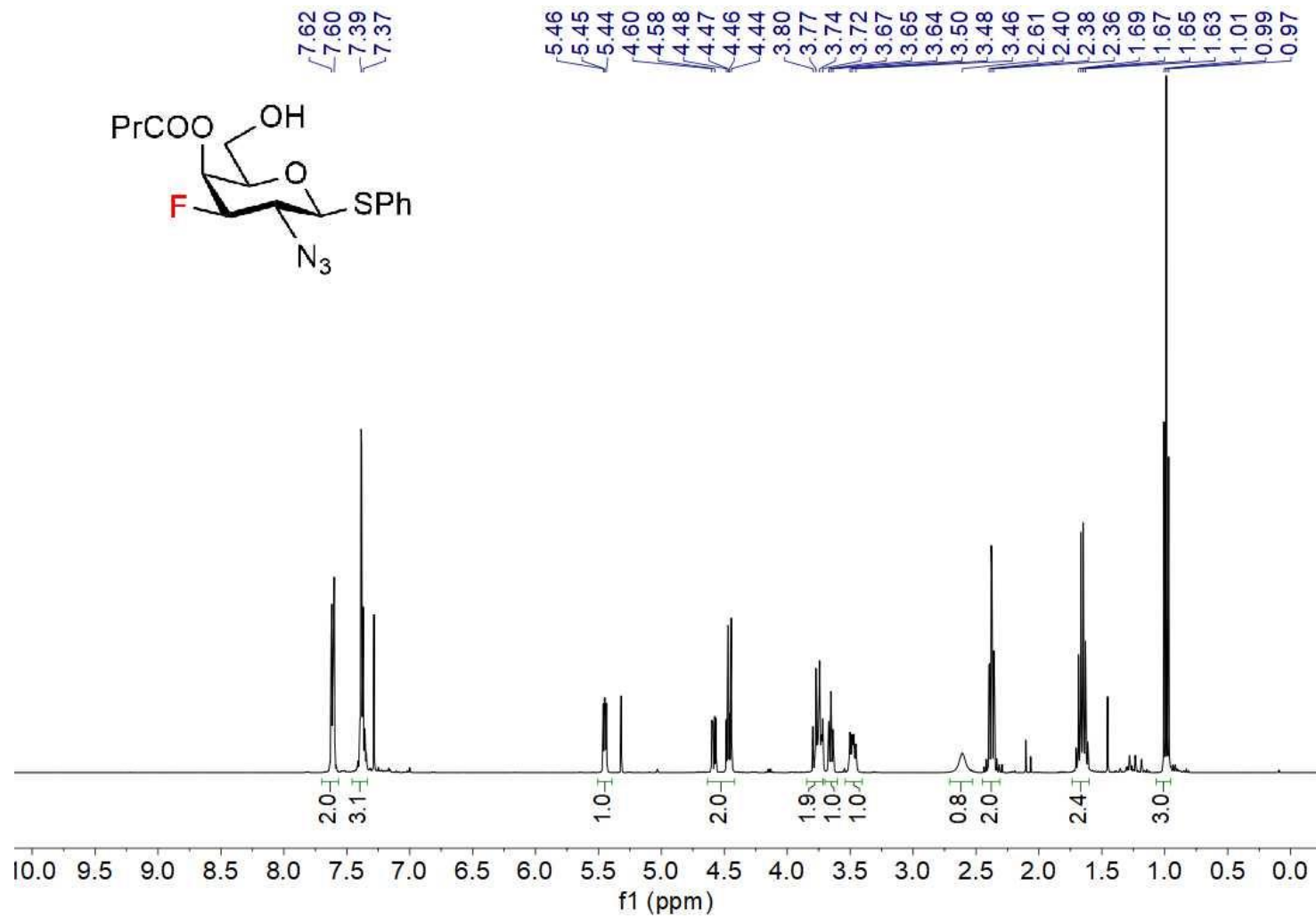


^1H - ^{13}C HSQC α -57

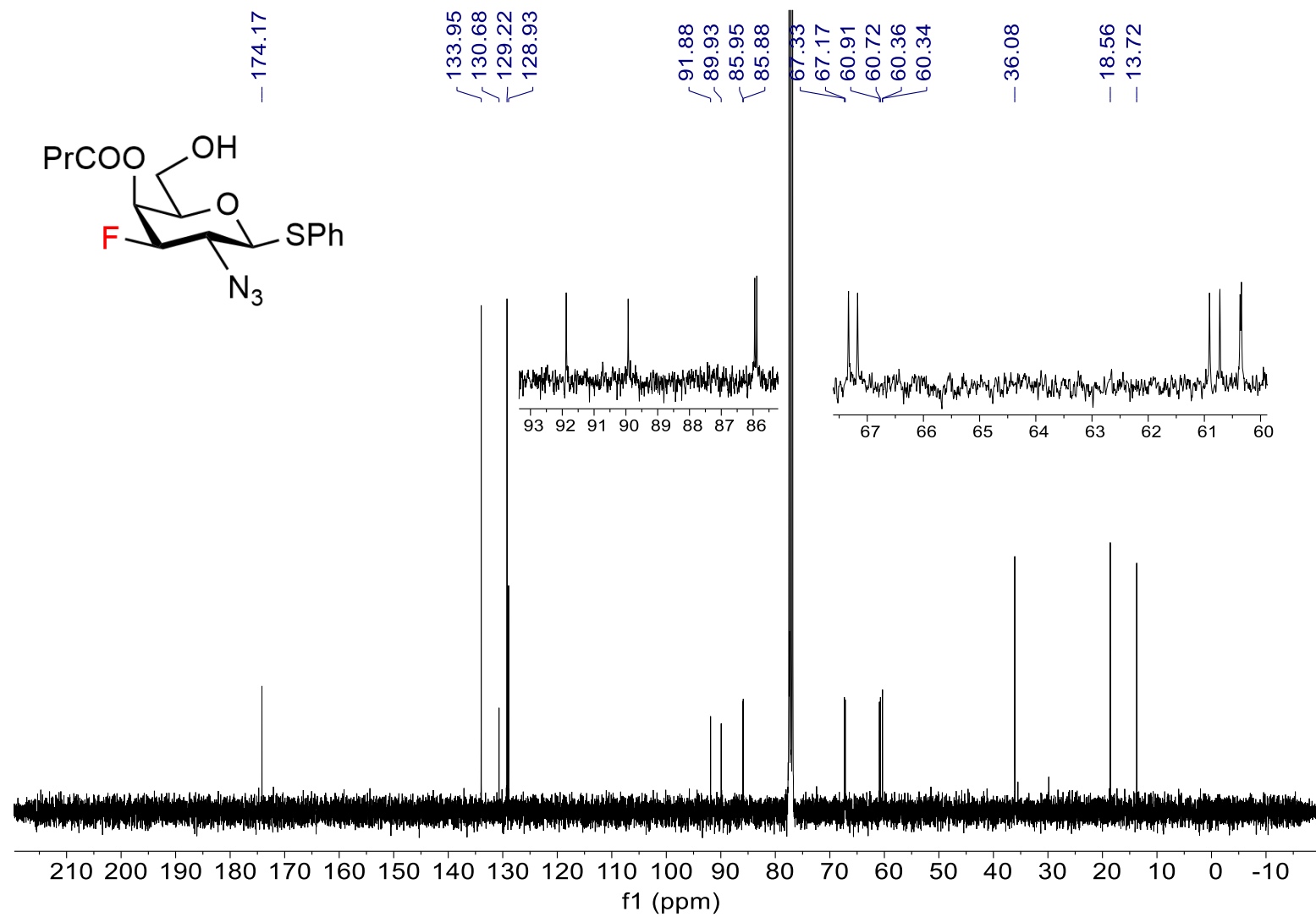


NMR COMPOUND β -57

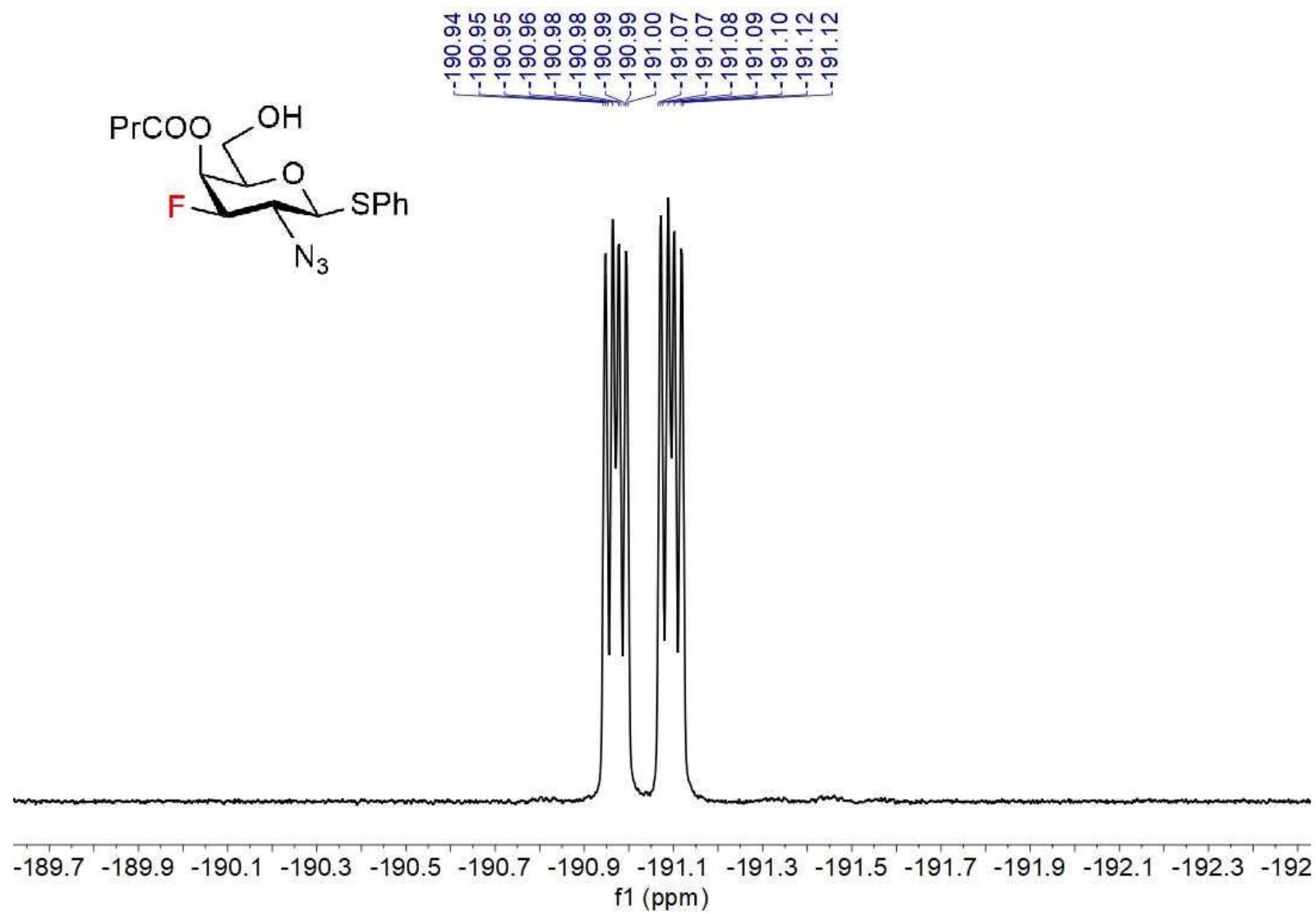
^1H NMR (400 MHz, CDCl_3) β -57



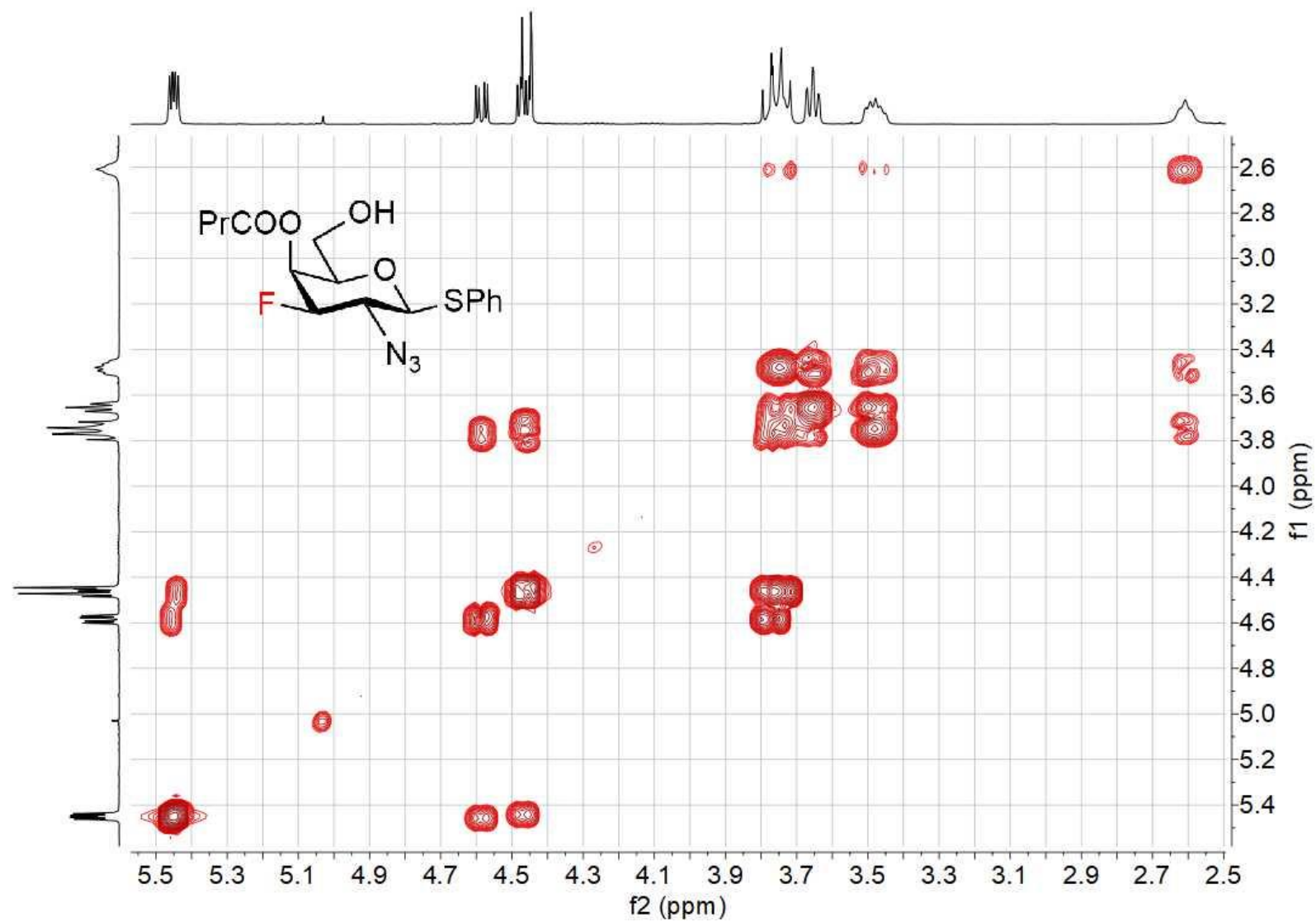
¹³C NMR (100 MHz, CDCl₃) β-57



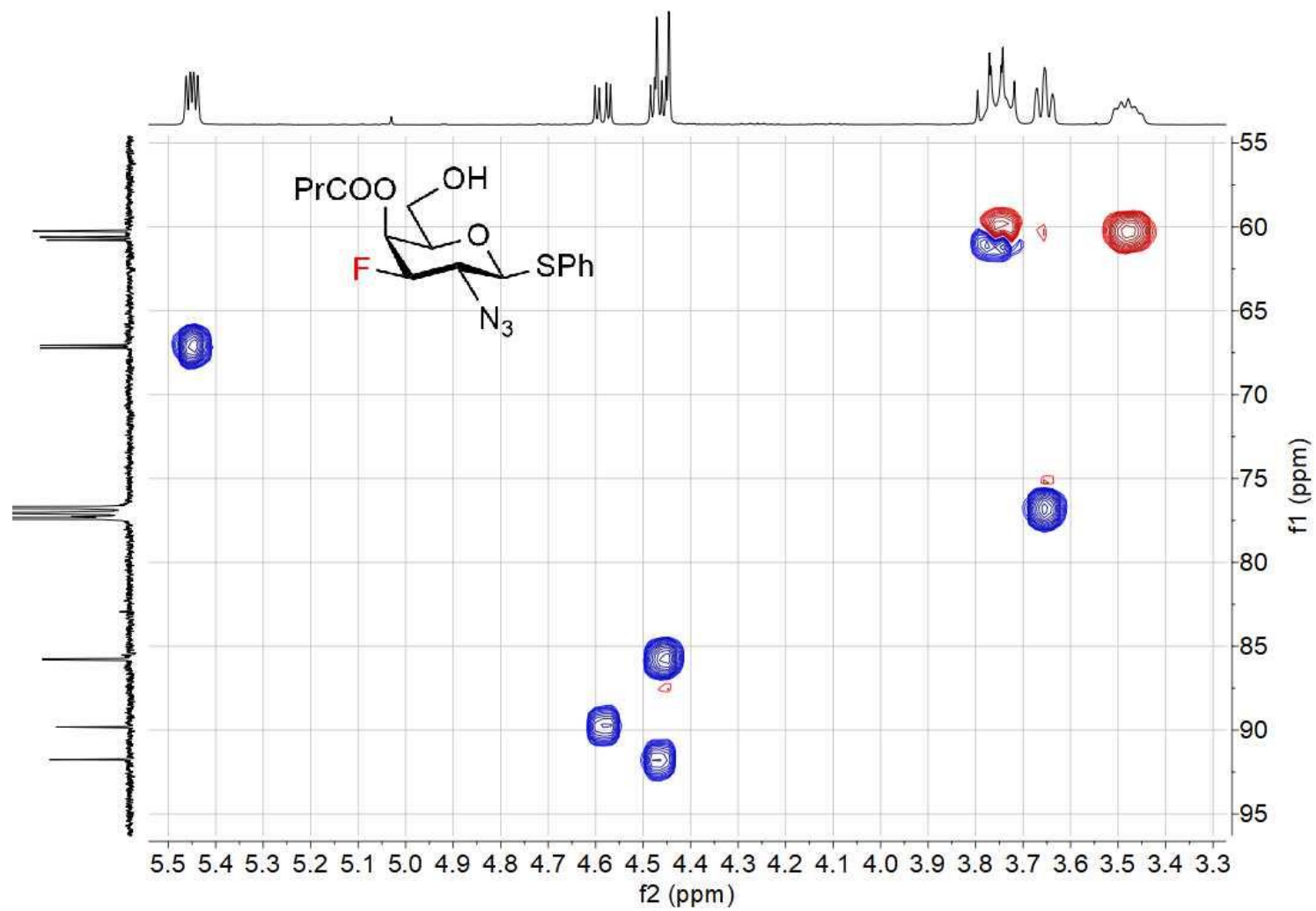
^{19}F NMR (376 MHz, CDCl_3) β -57



^1H - ^1H COSY β -57

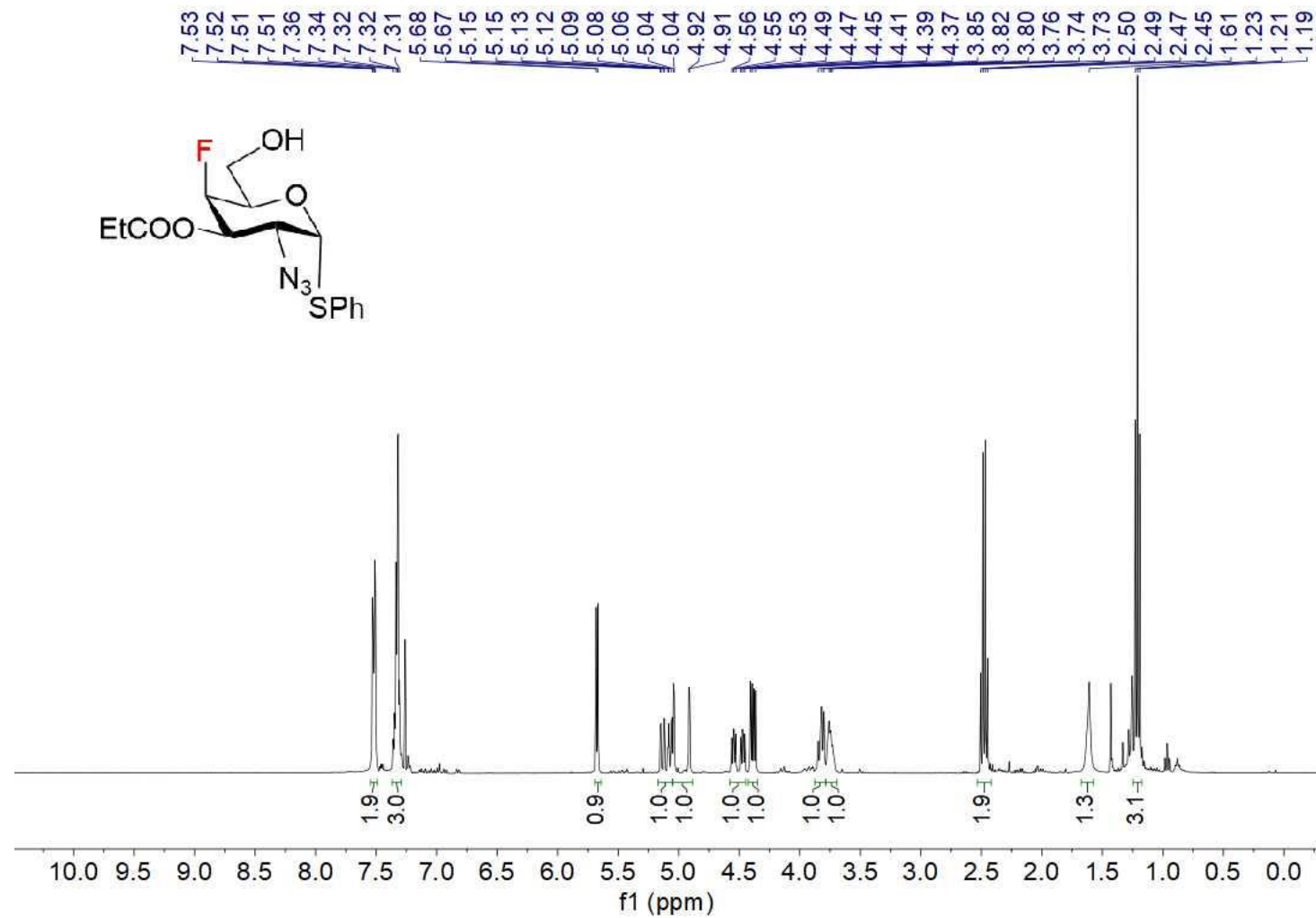


^1H - ^{13}C HSQC β -57

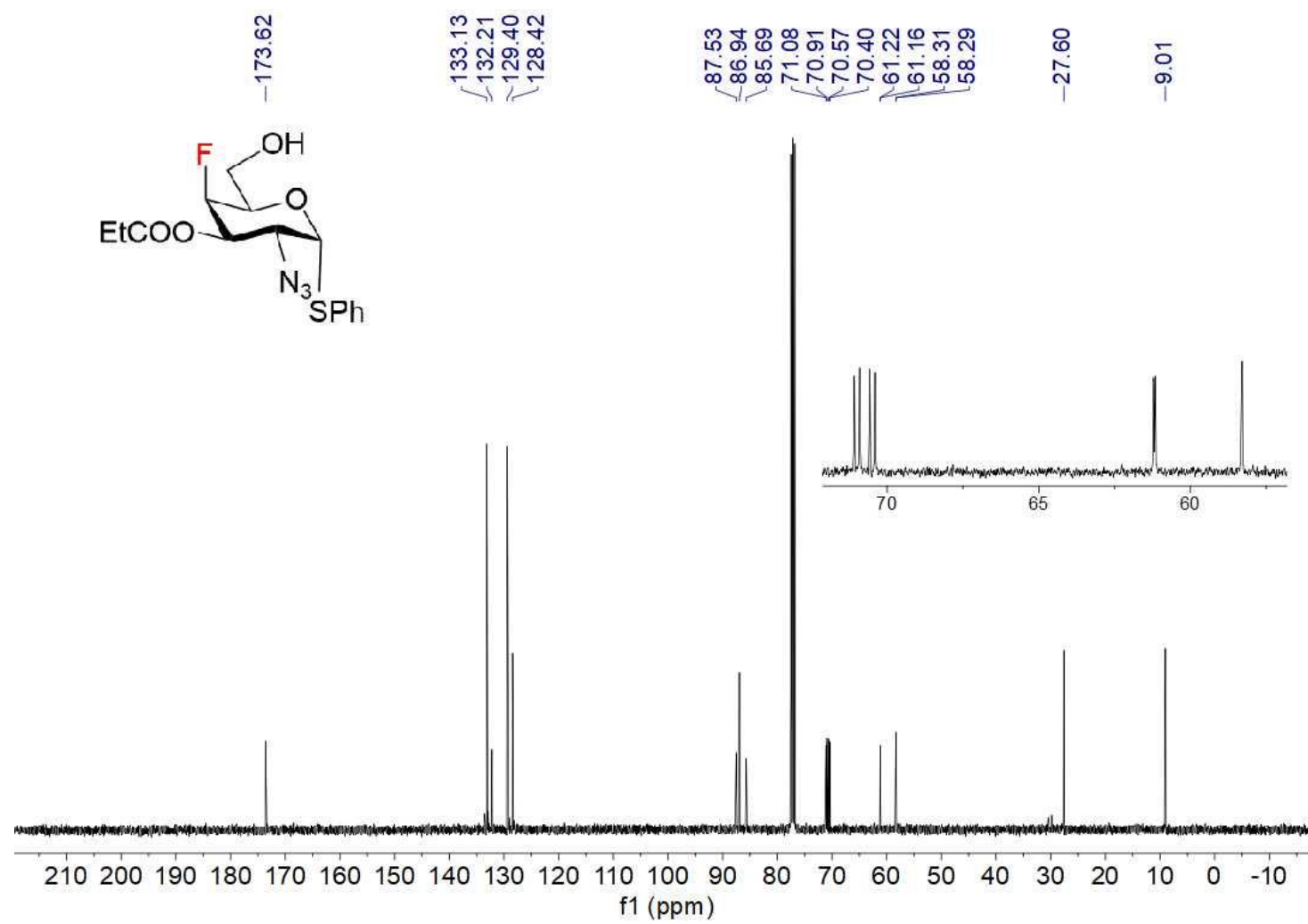


NMR COMPOUND α -59

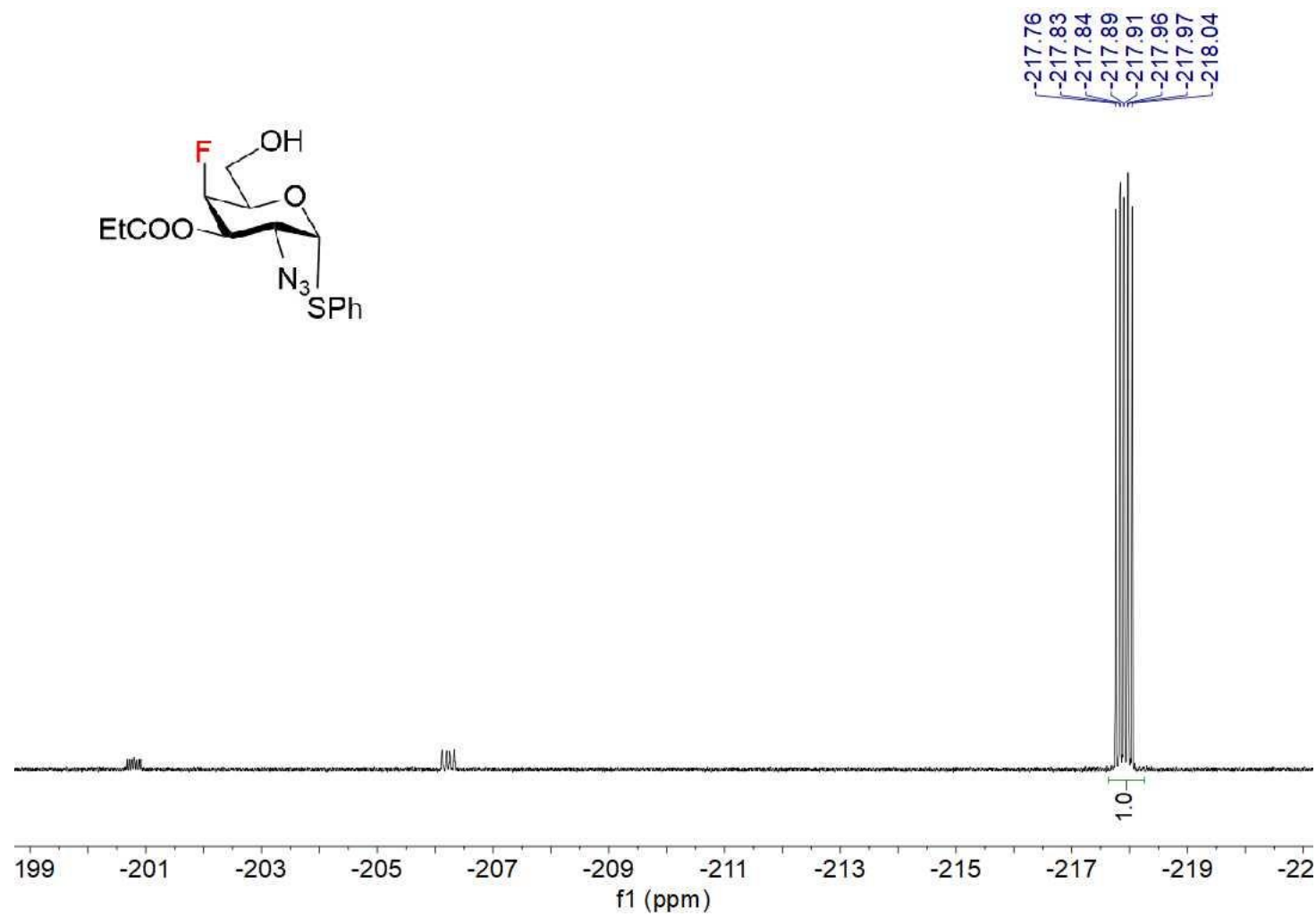
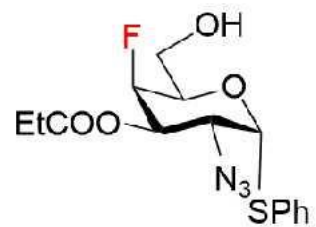
^1H NMR (400 MHz, CDCl_3) α -59



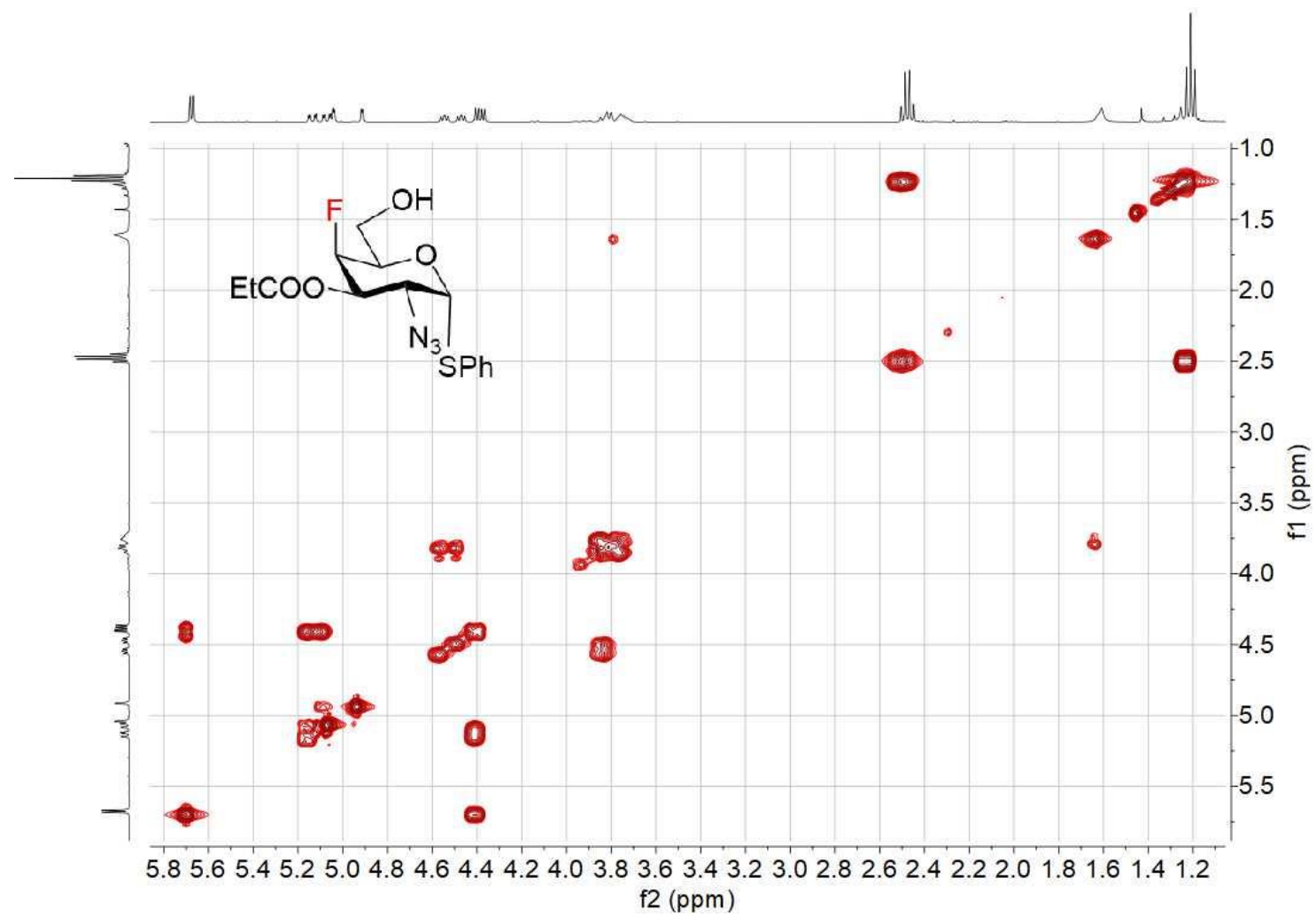
^{13}C NMR (100 MHz, CDCl_3) α -59



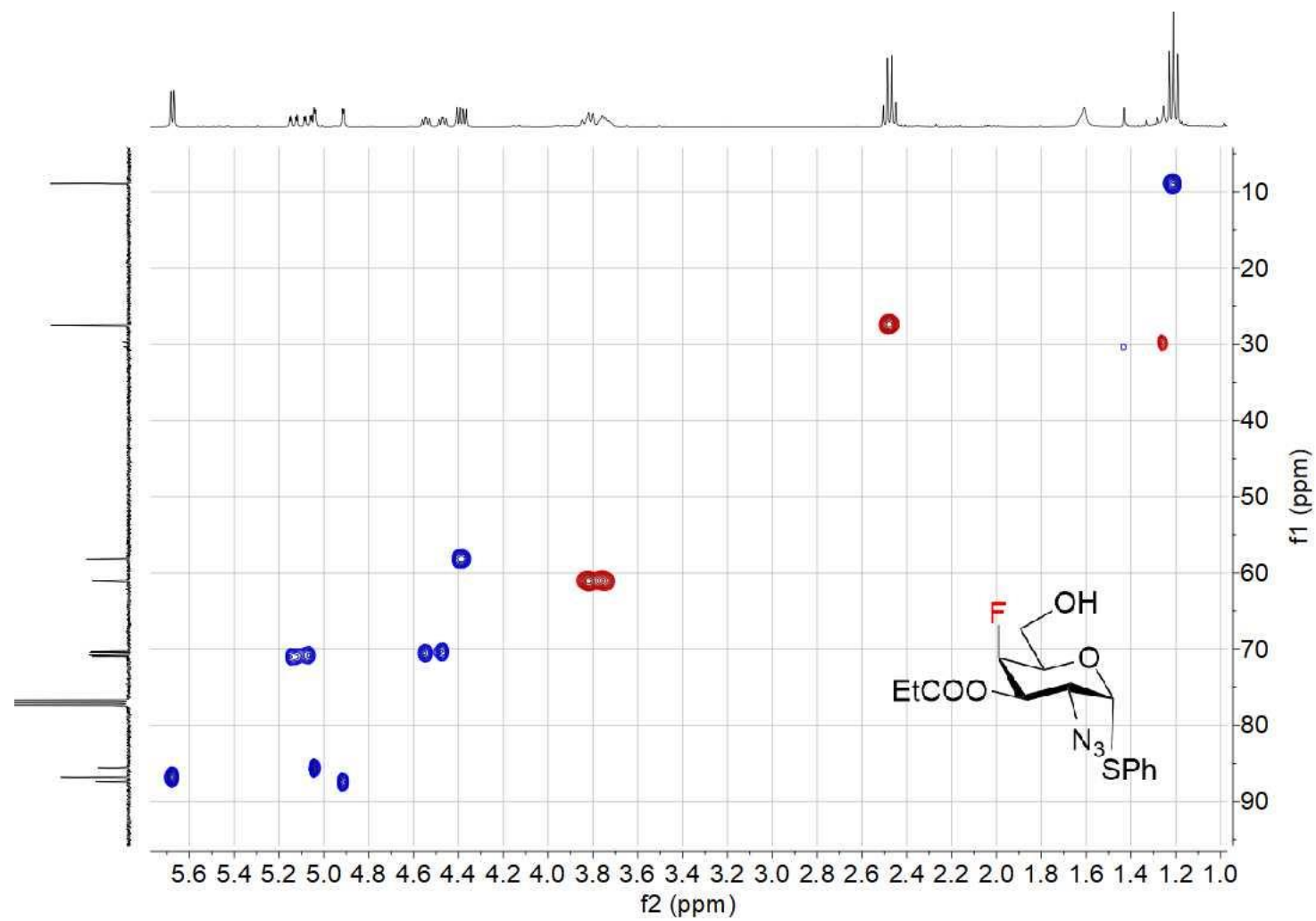
^{19}F NMR (376 MHz, CDCl_3) α -59



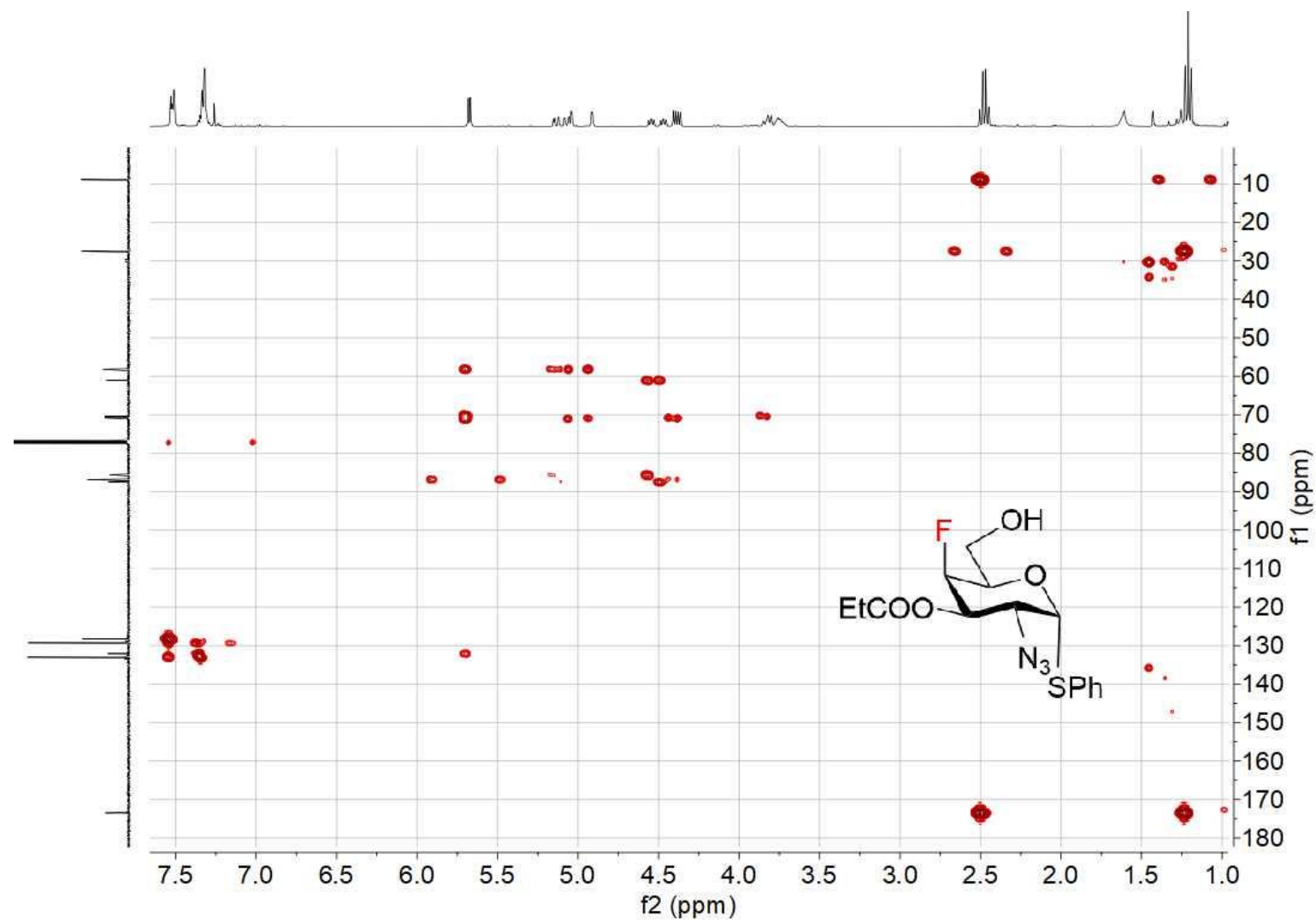
^1H - ^1H COSY α -59



^1H - ^{13}C HSQC α -59

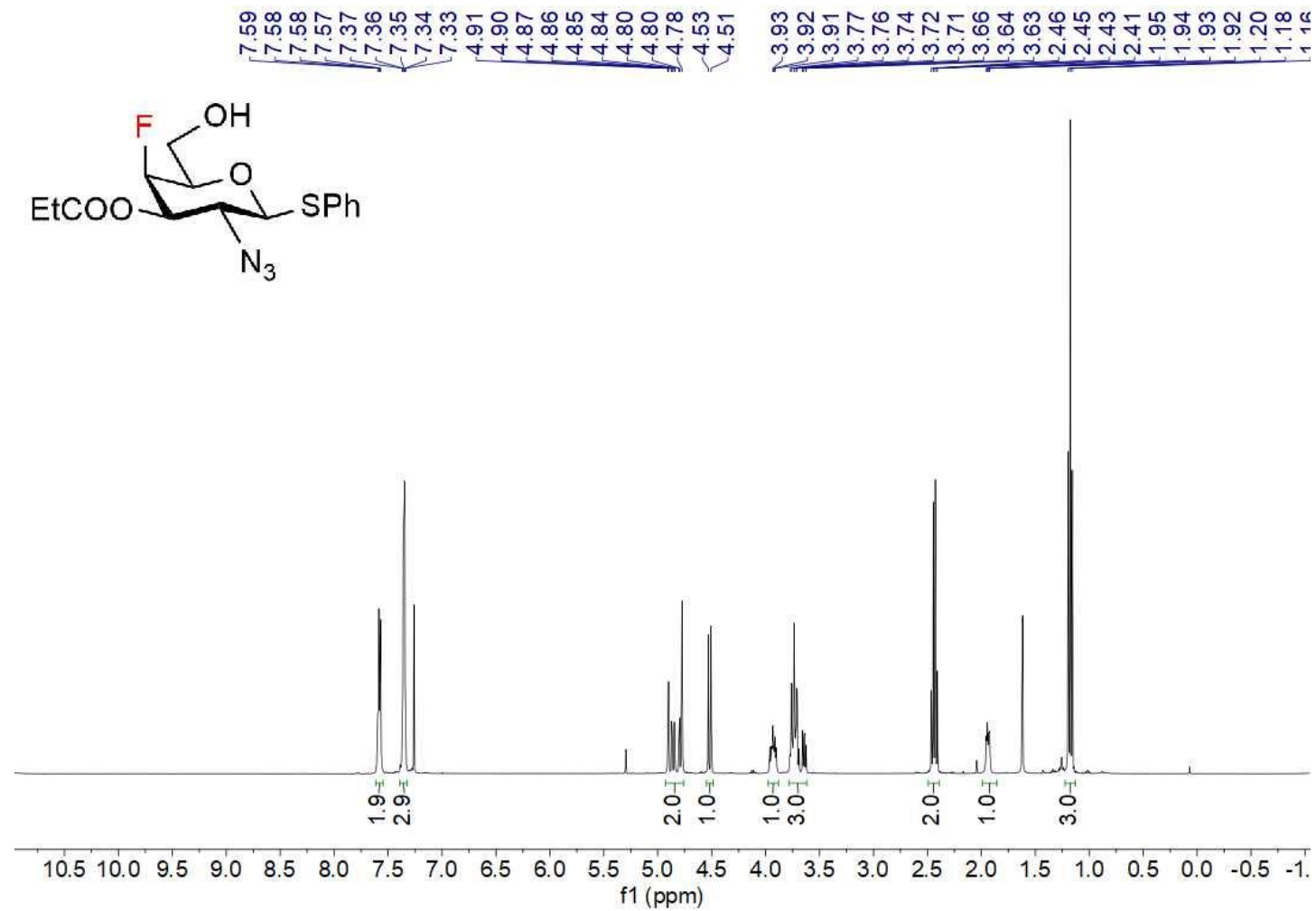


^1H - ^{13}C HMBC α -59

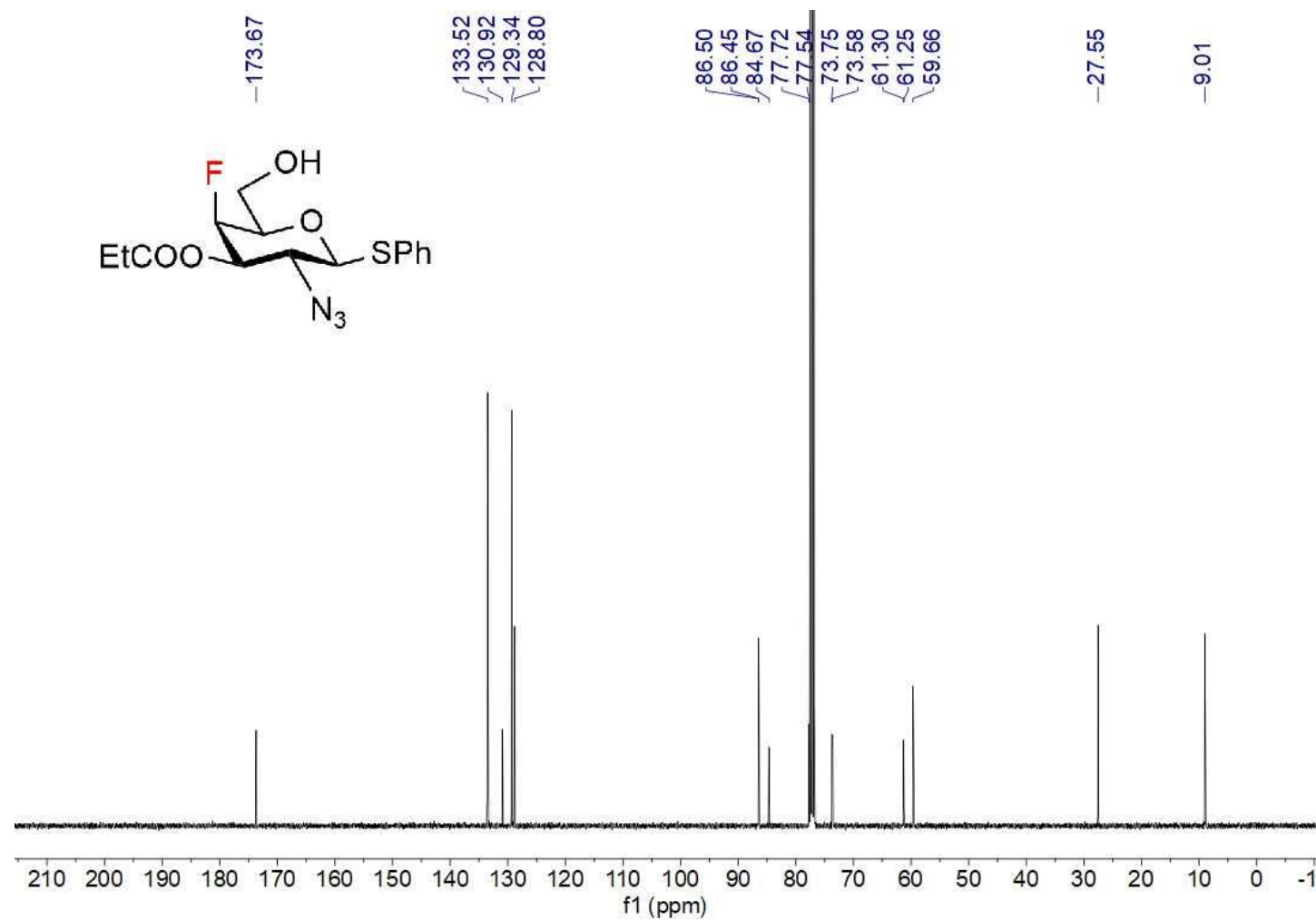


NMR COMPOUND β -59

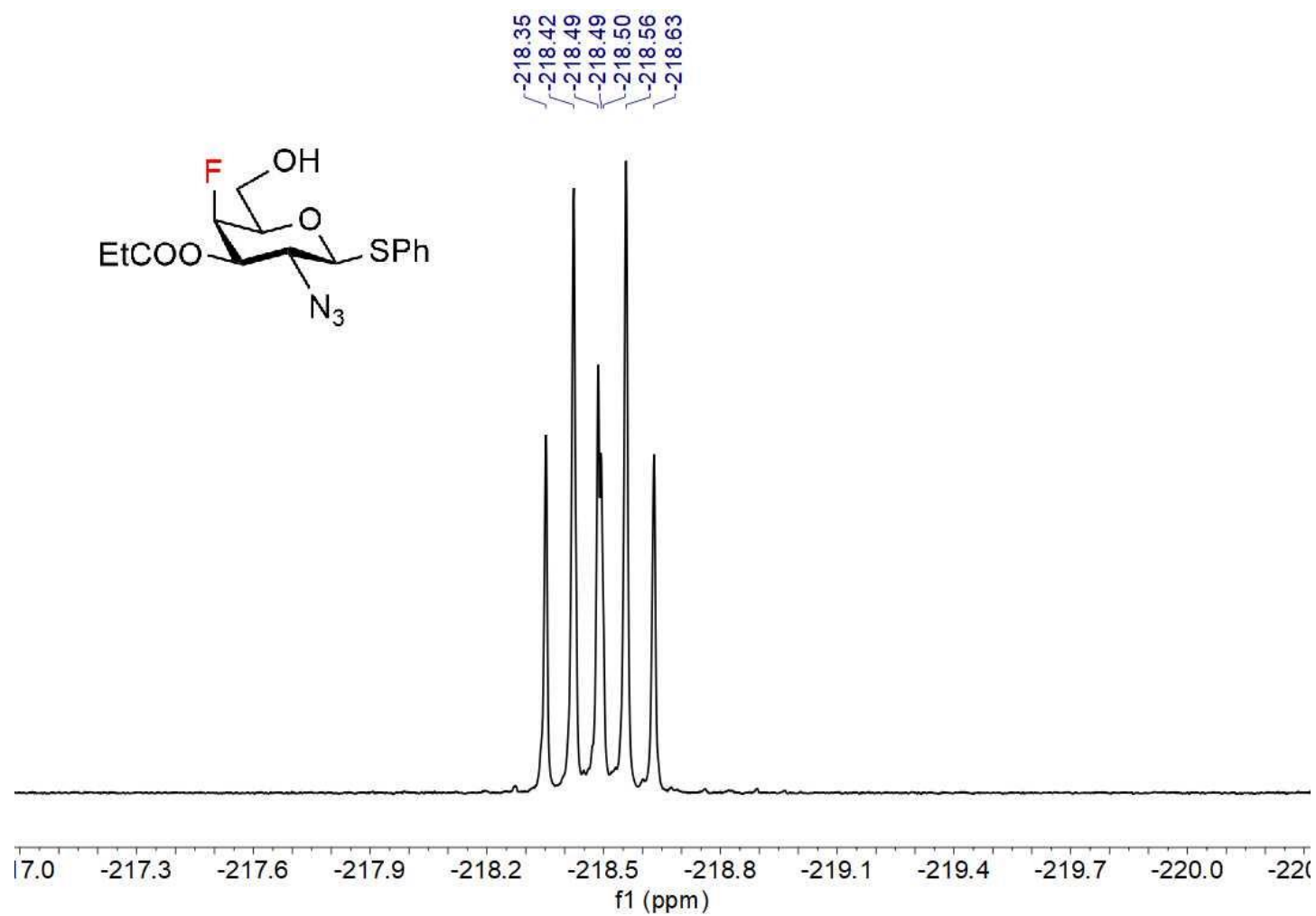
^1H NMR (400 MHz, CDCl_3) β -59



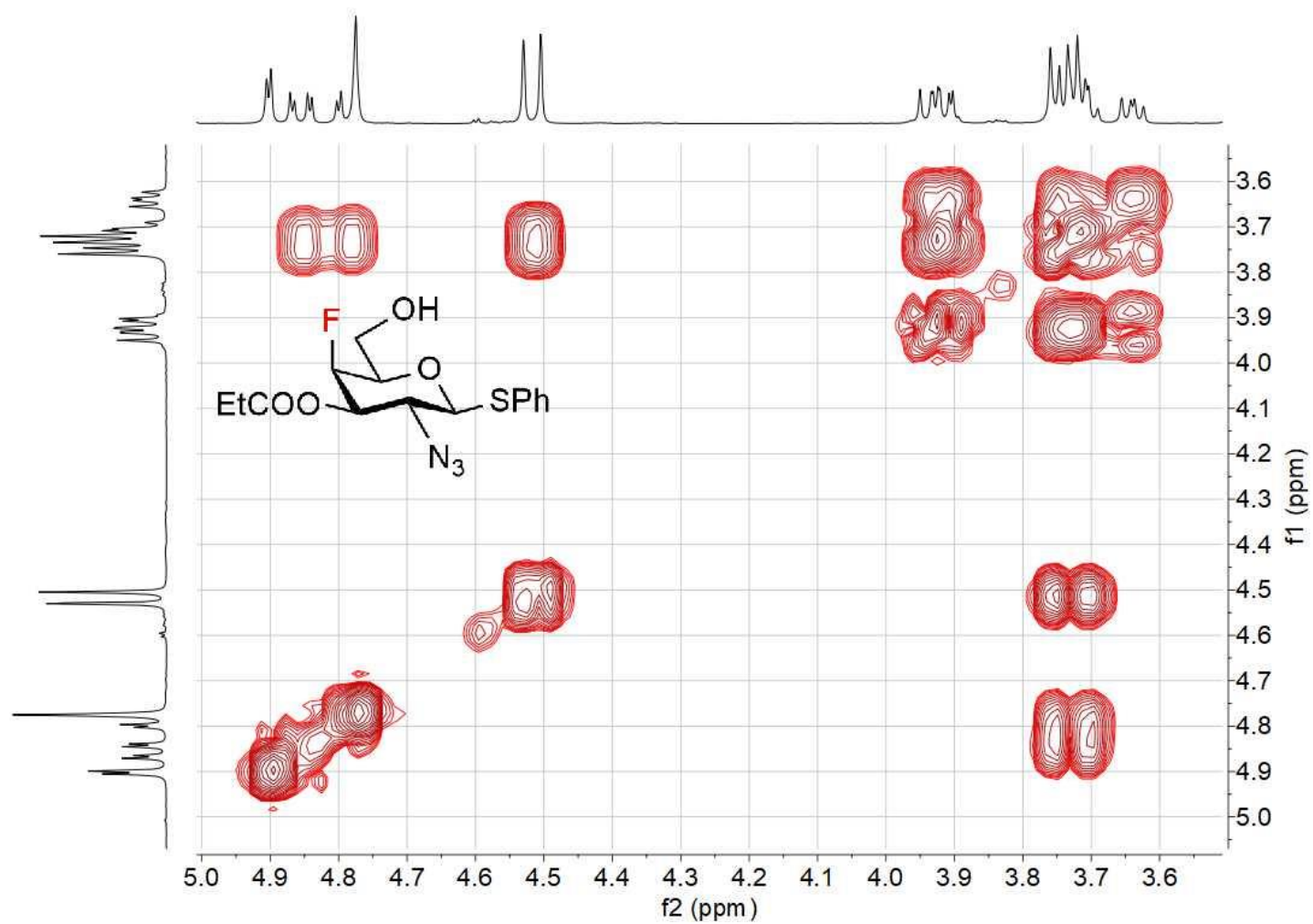
^{13}C NMR (100 MHz, CDCl_3) β -59



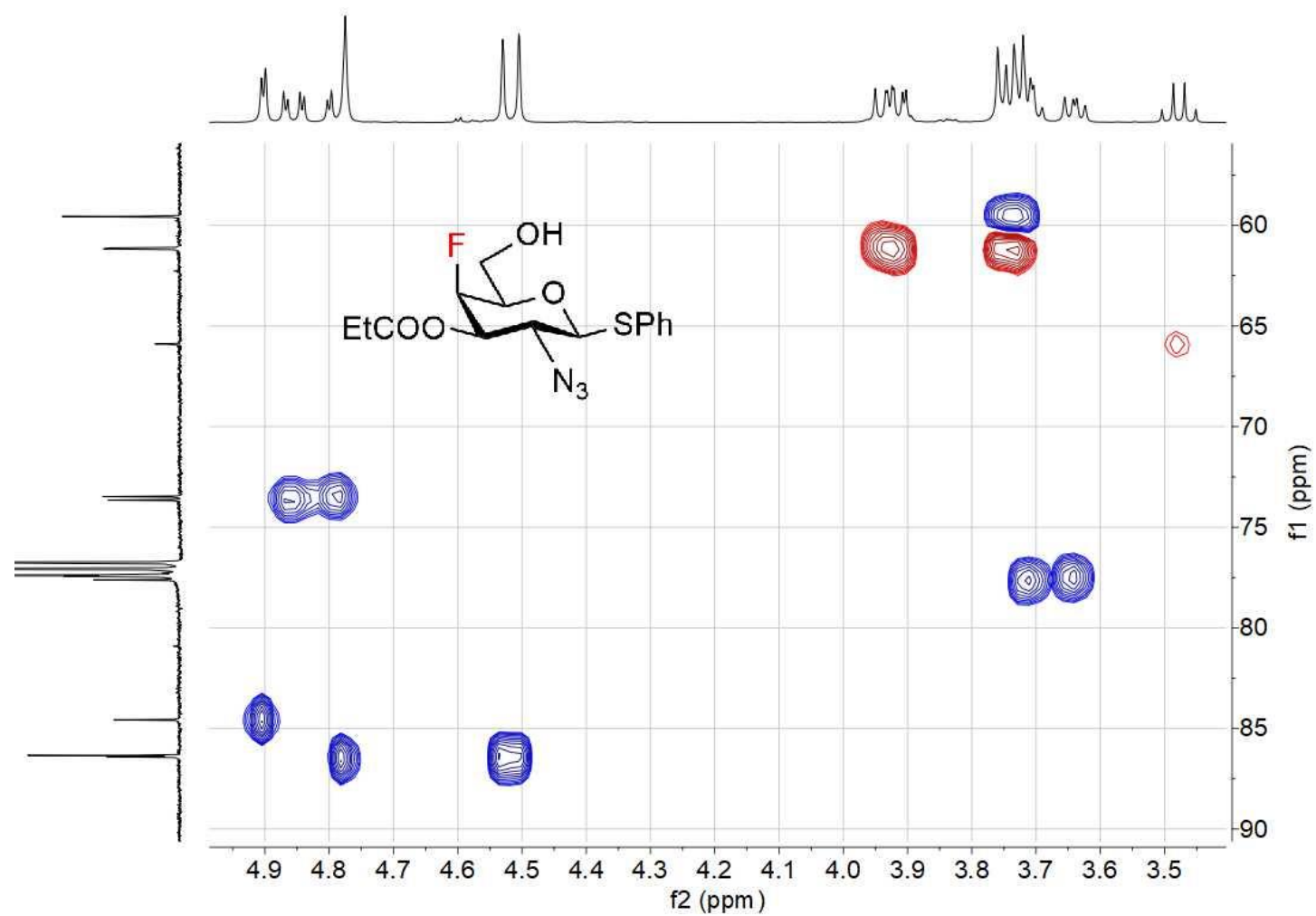
^{19}F NMR (376 MHz, CDCl_3) β -59



^1H - ^1H COSY β -59

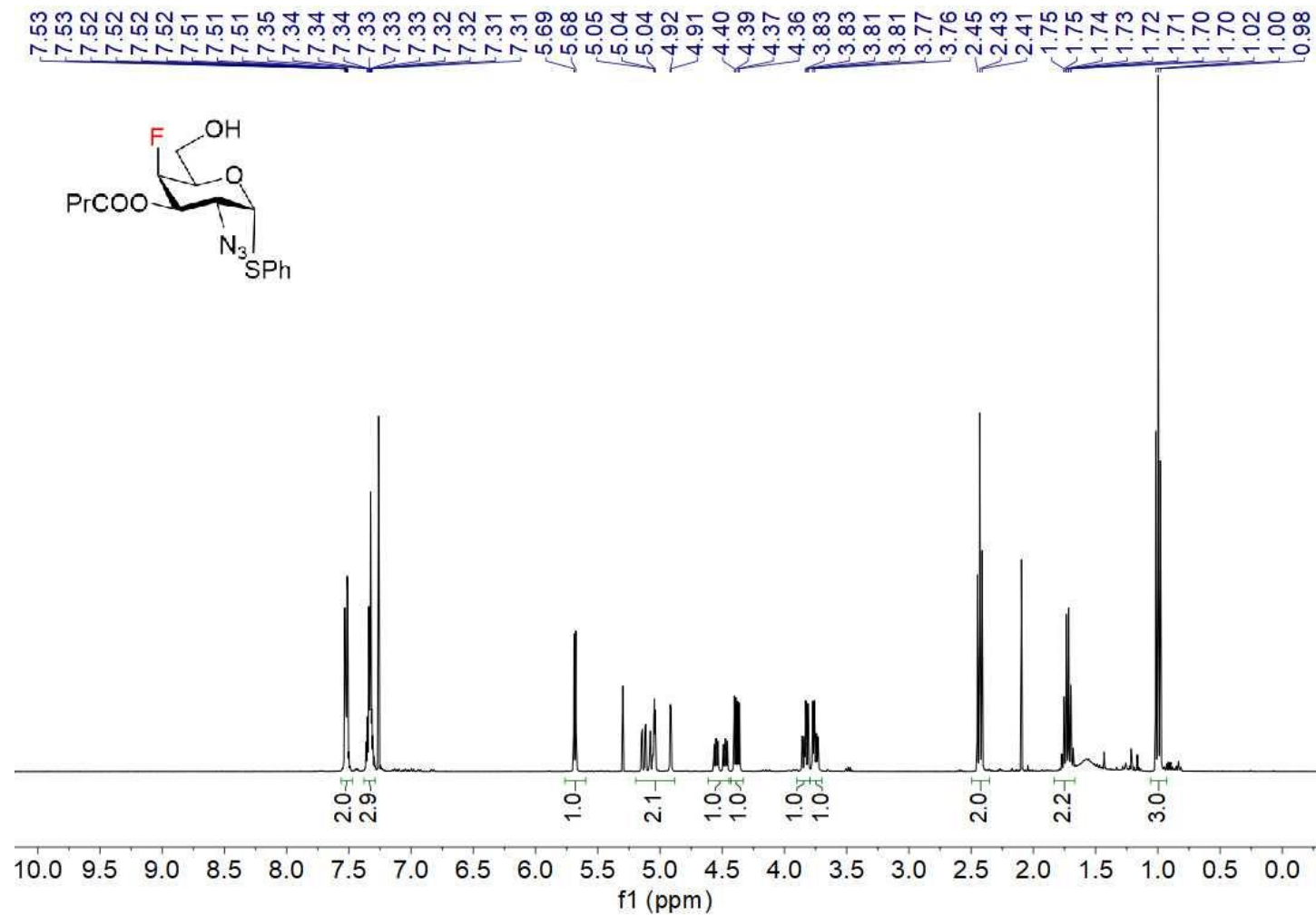


^1H - ^{13}C HSQC β -59

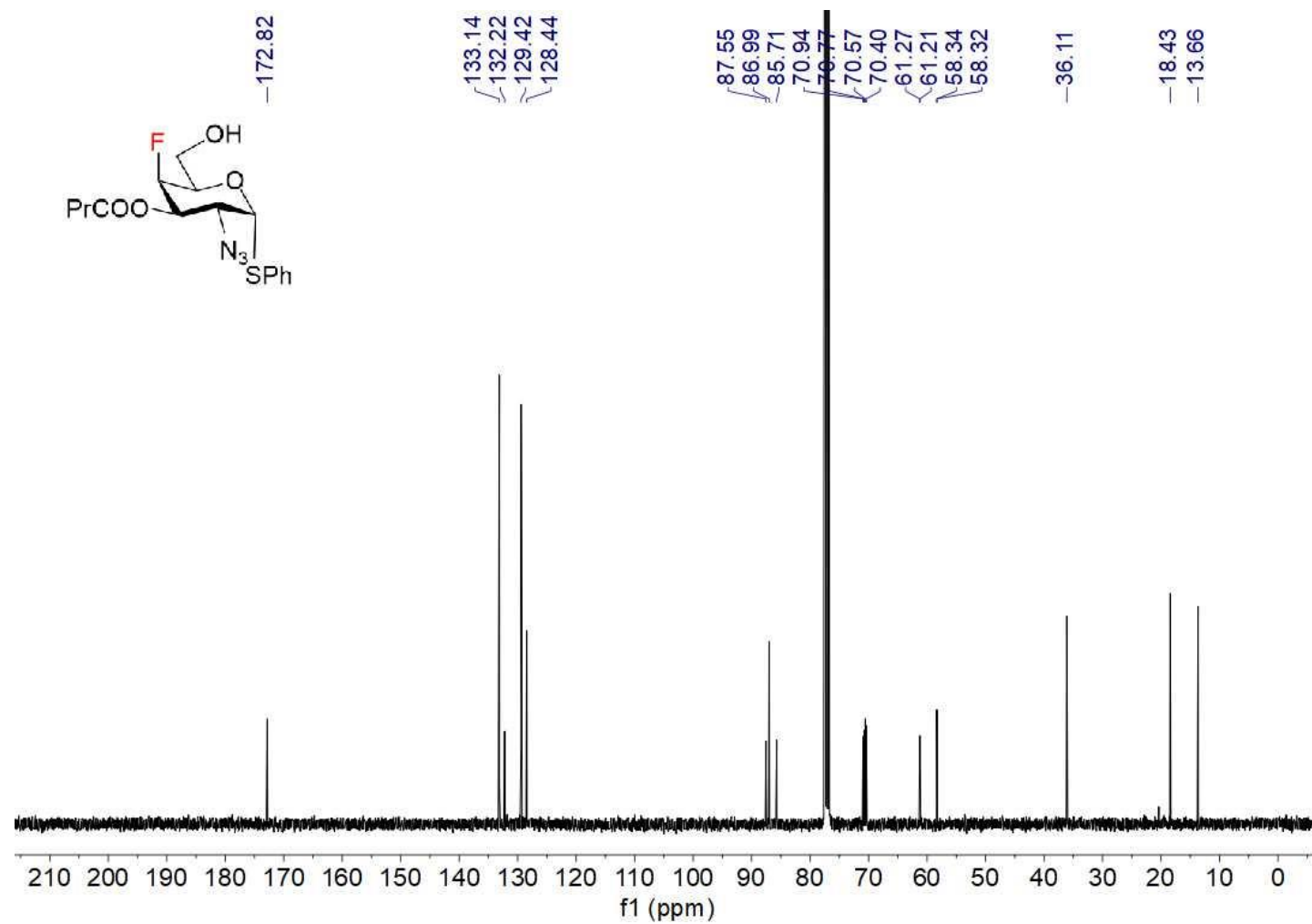


NMR COMPOUND α -60

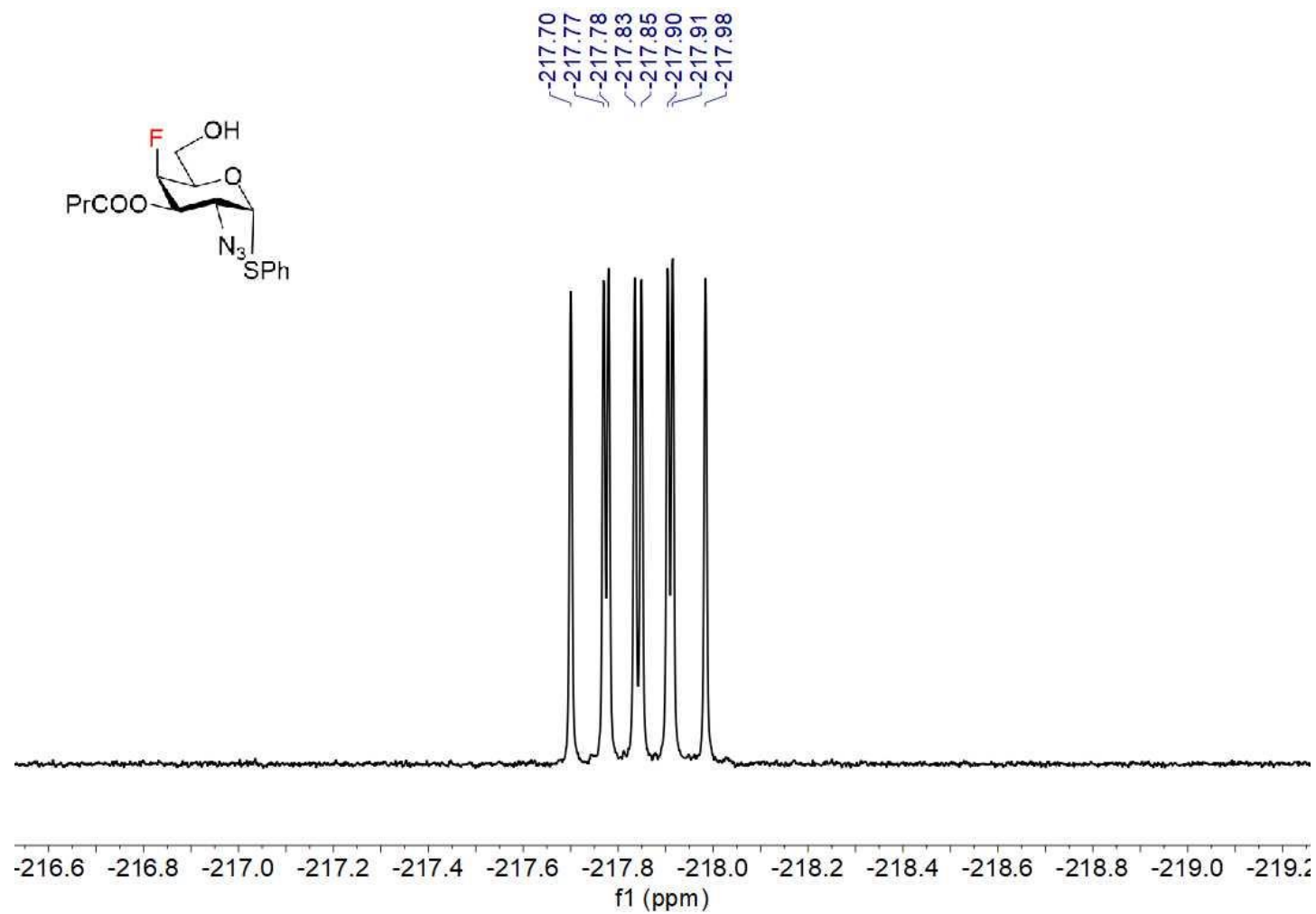
^1H NMR (400 MHz, CDCl_3) α -60



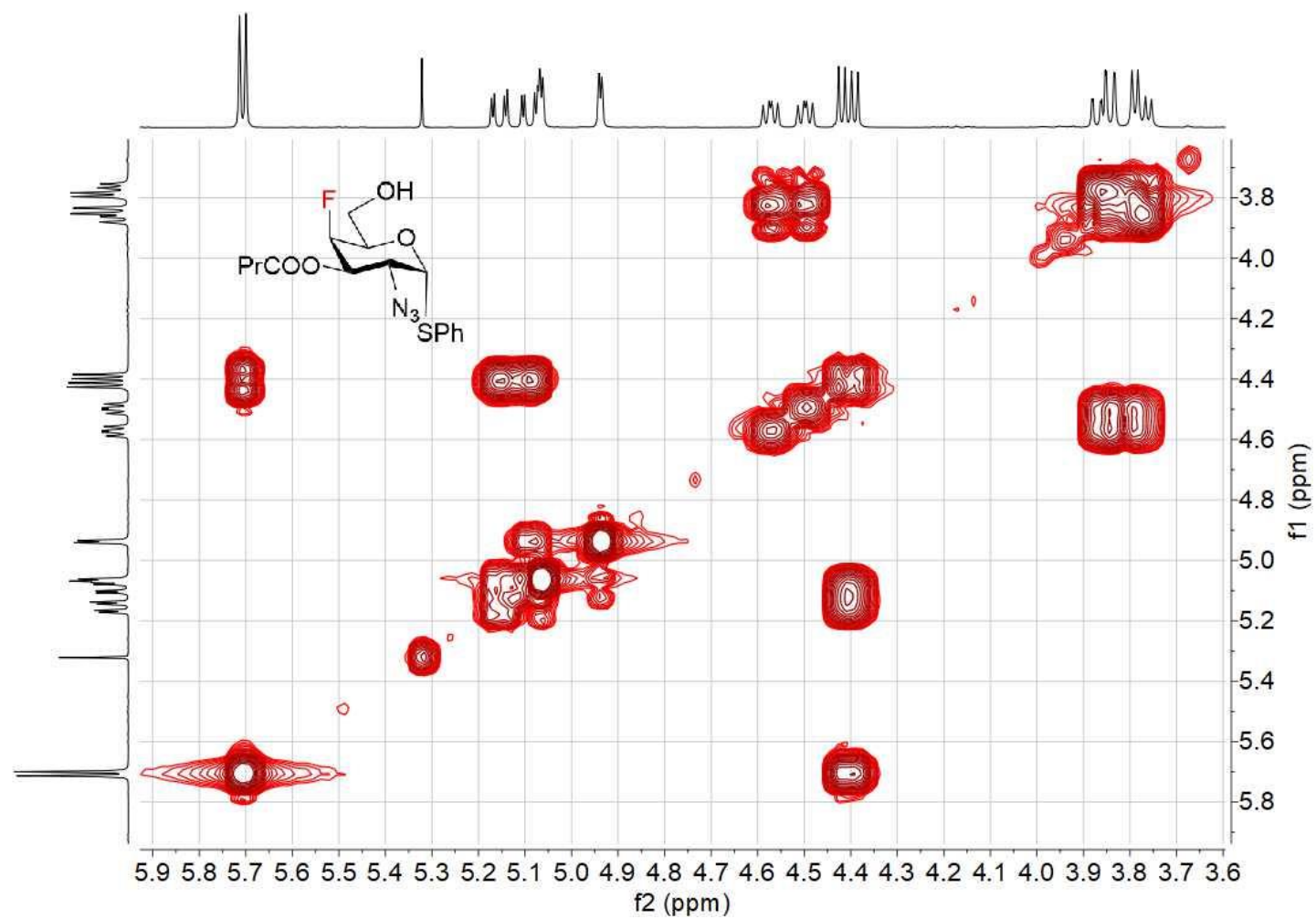
^{13}C NMR (100 MHz, CDCl_3) α -60



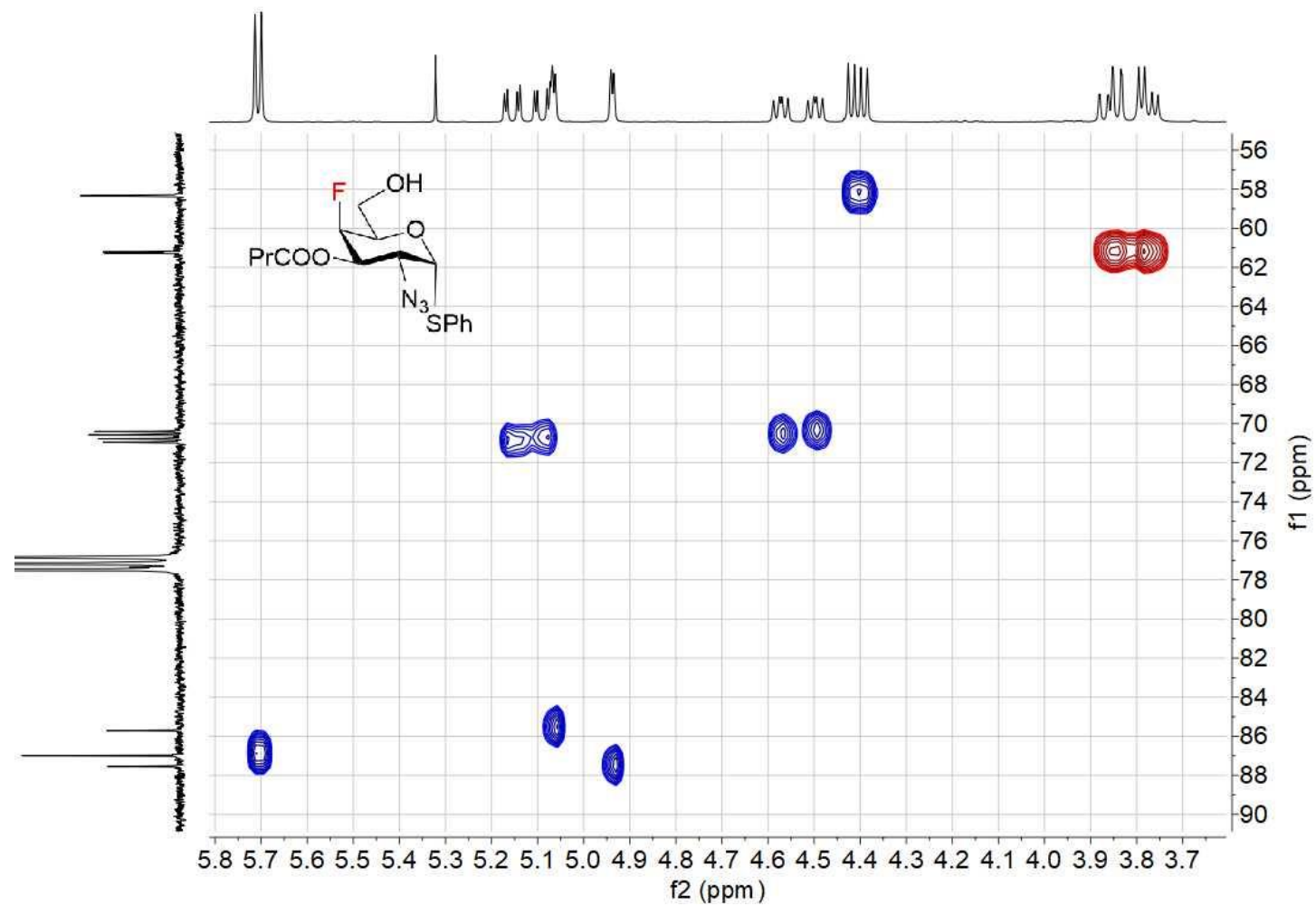
^{19}F NMR (376 MHz, CDCl_3) α -60



^1H - ^1H COSY α -60

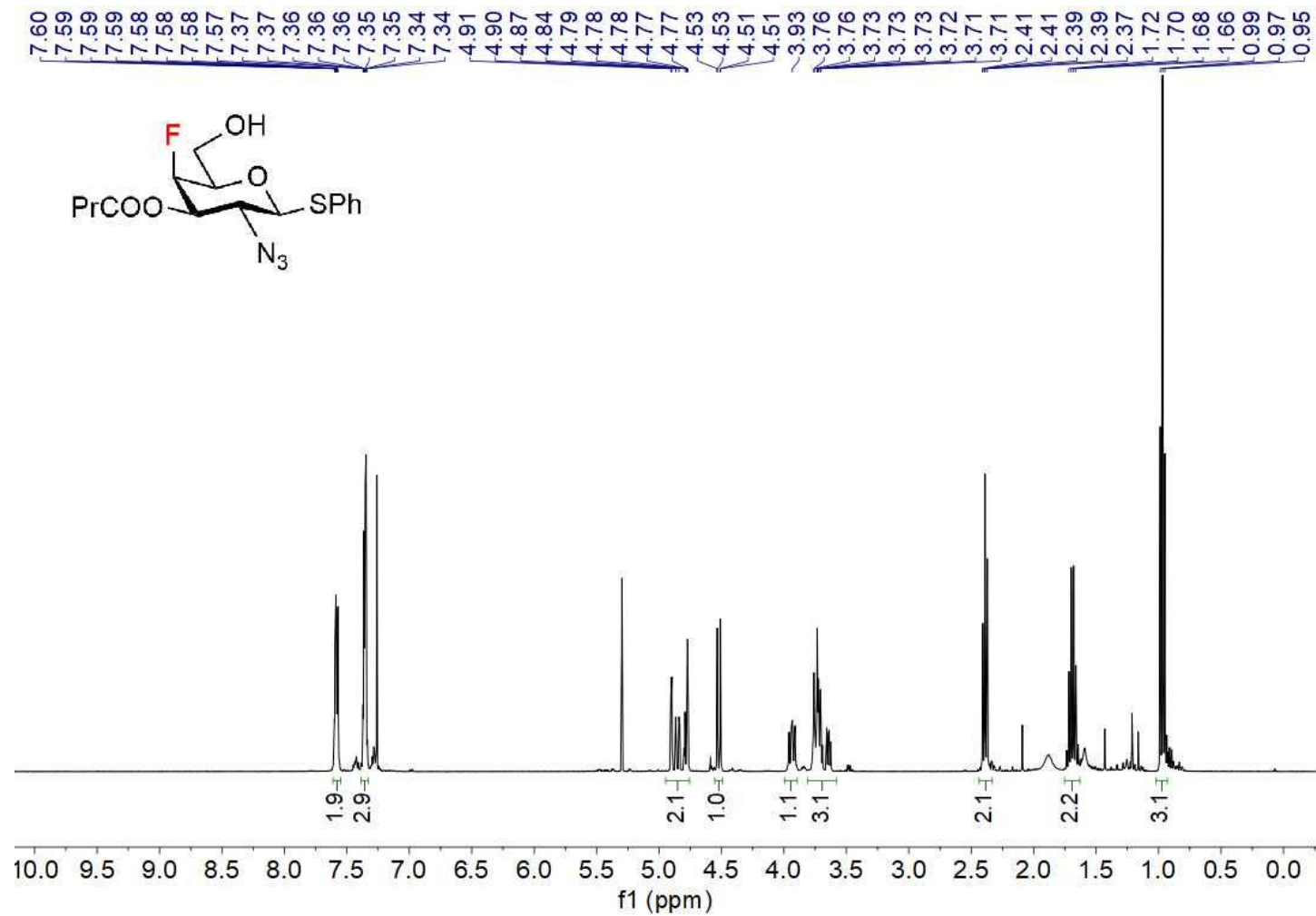


^1H - ^{13}C HSQC α -60

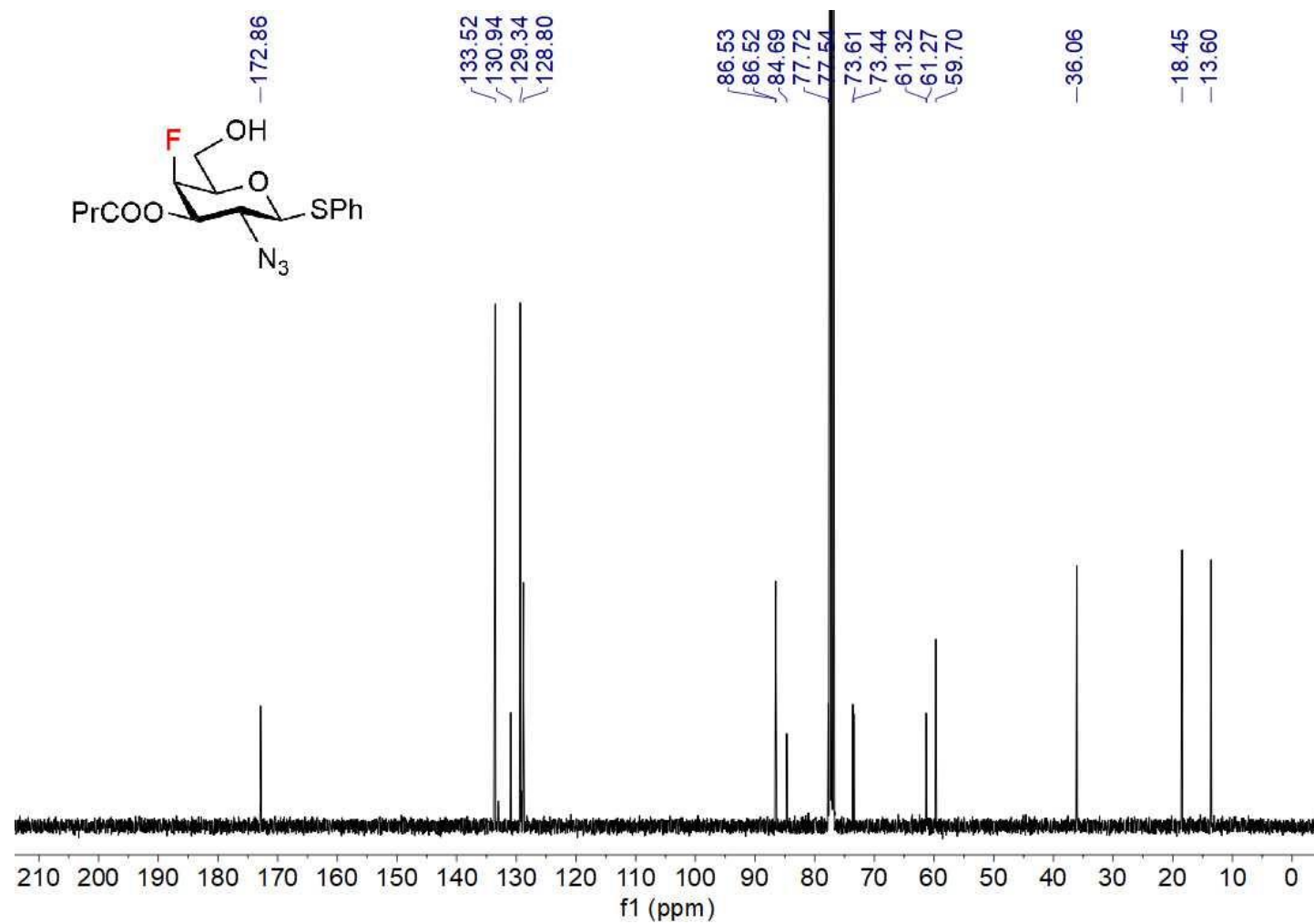


NMR COMPOUND β -60

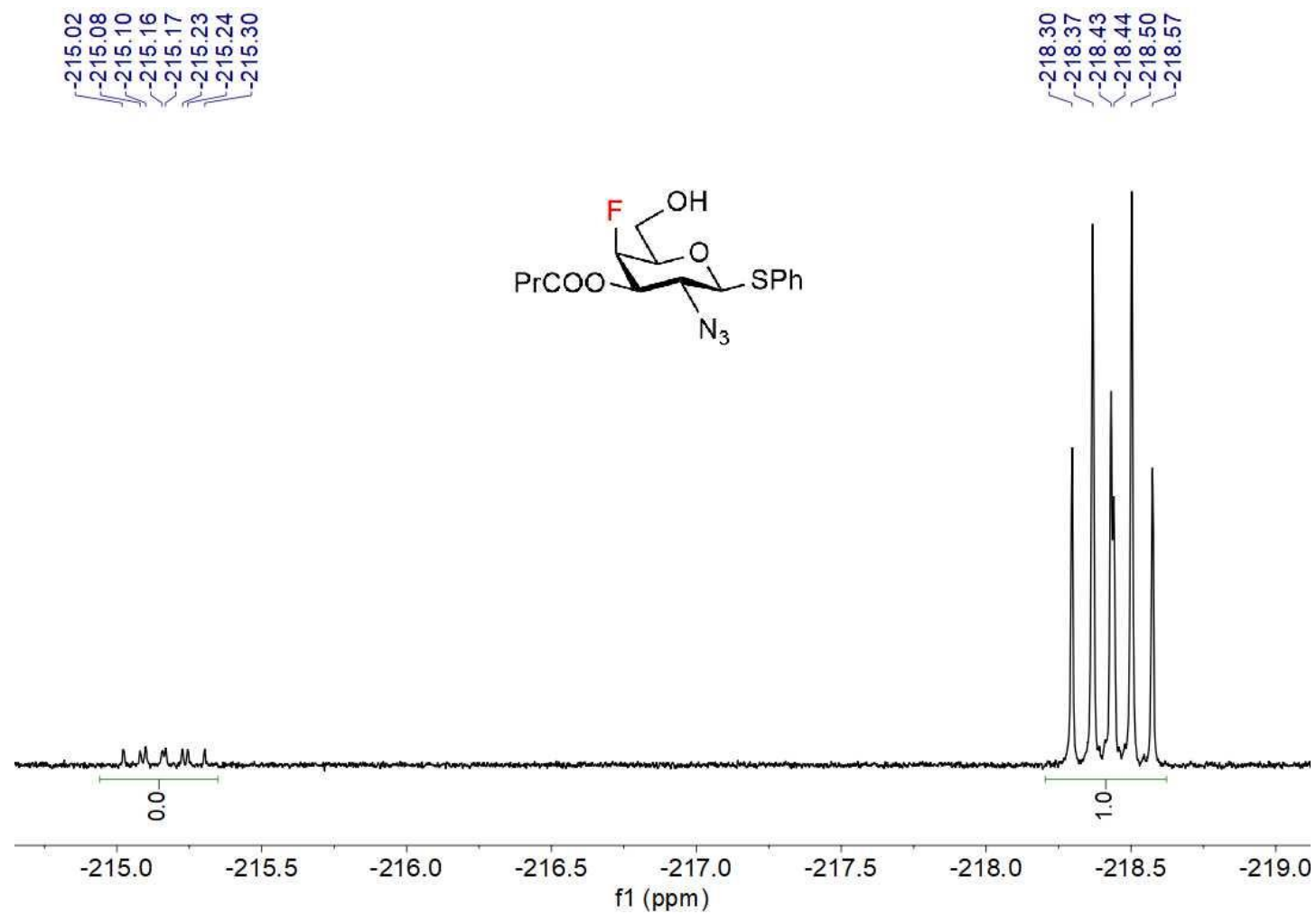
^1H NMR (400 MHz, CDCl_3) β -60



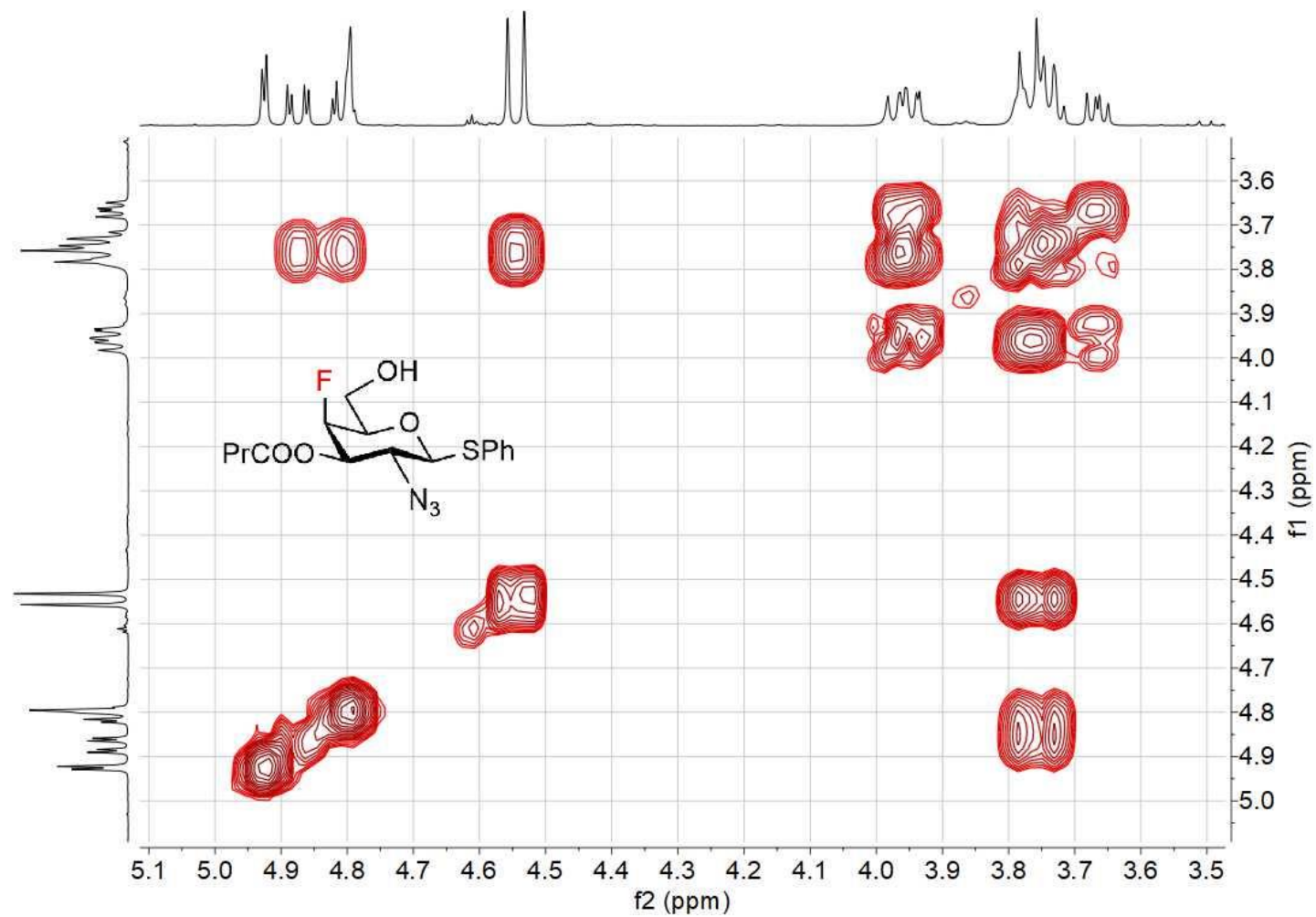
¹³C NMR (100 MHz, CDCl₃) β-60



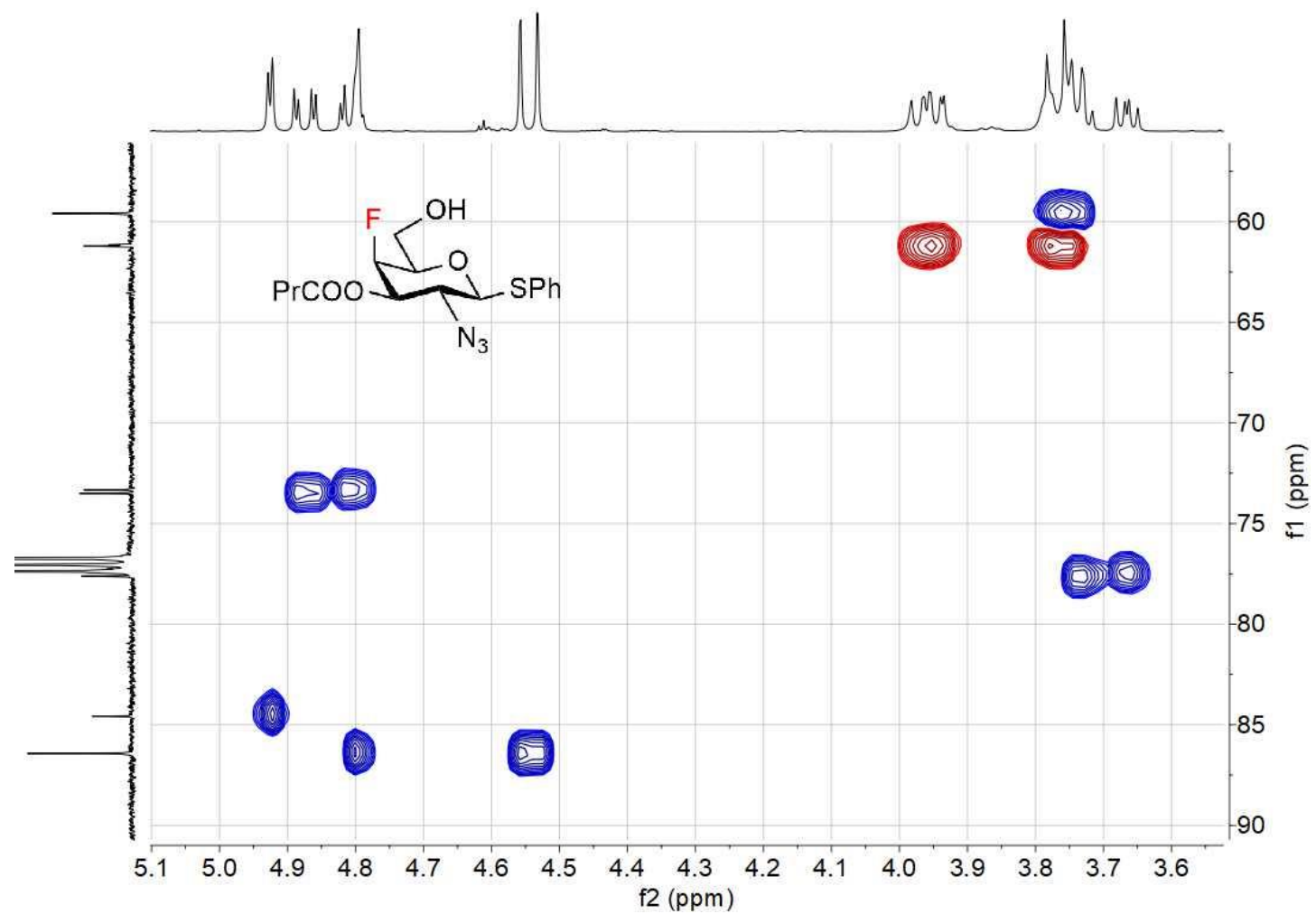
¹⁹F NMR (376 MHz, CDCl₃) β-60



^1H - ^1H COSY β -60

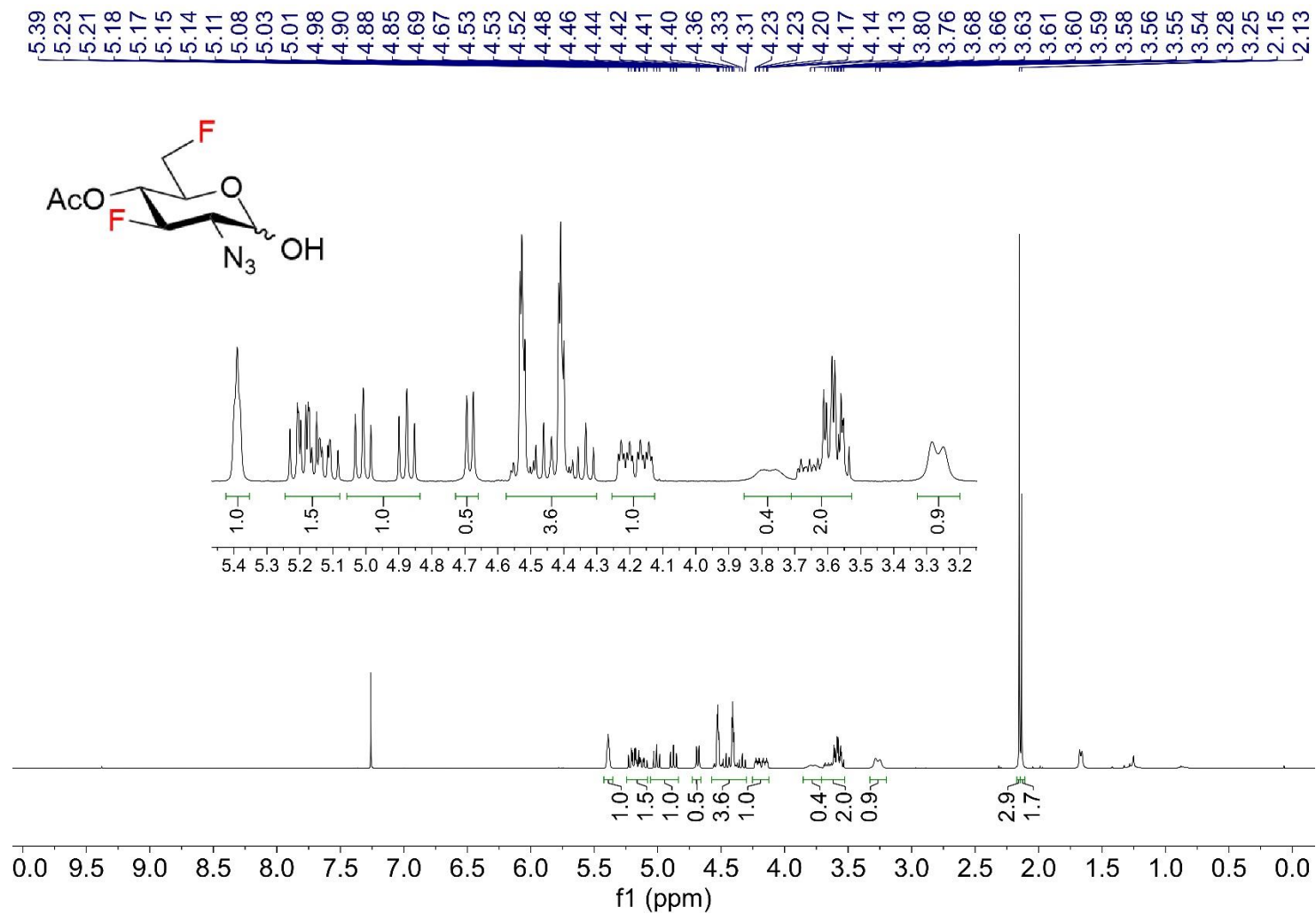


^1H - ^{13}C HSQC 60

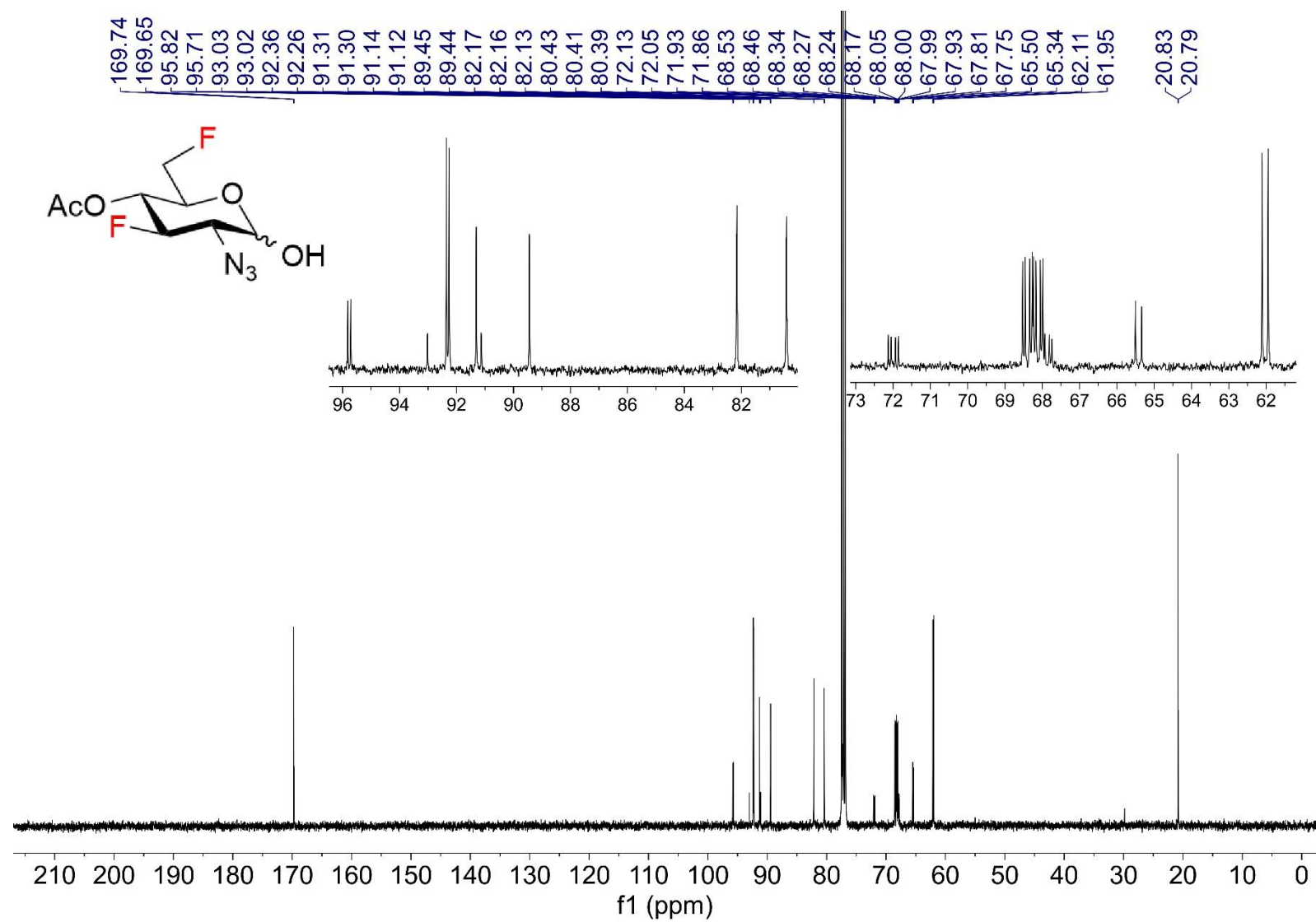


NMR COMPOUND 61

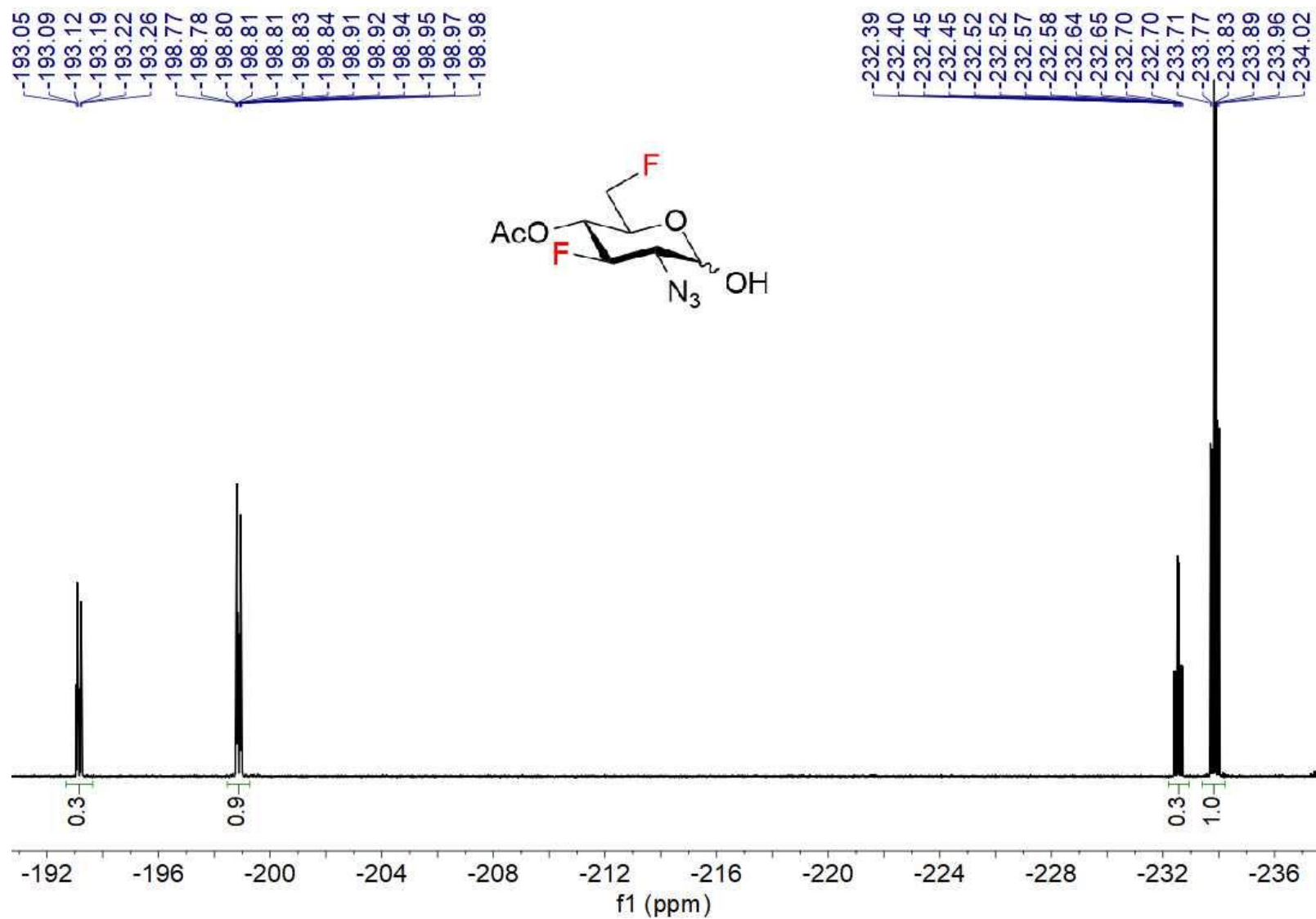
¹H NMR (400 MHz, CDCl₃) 61



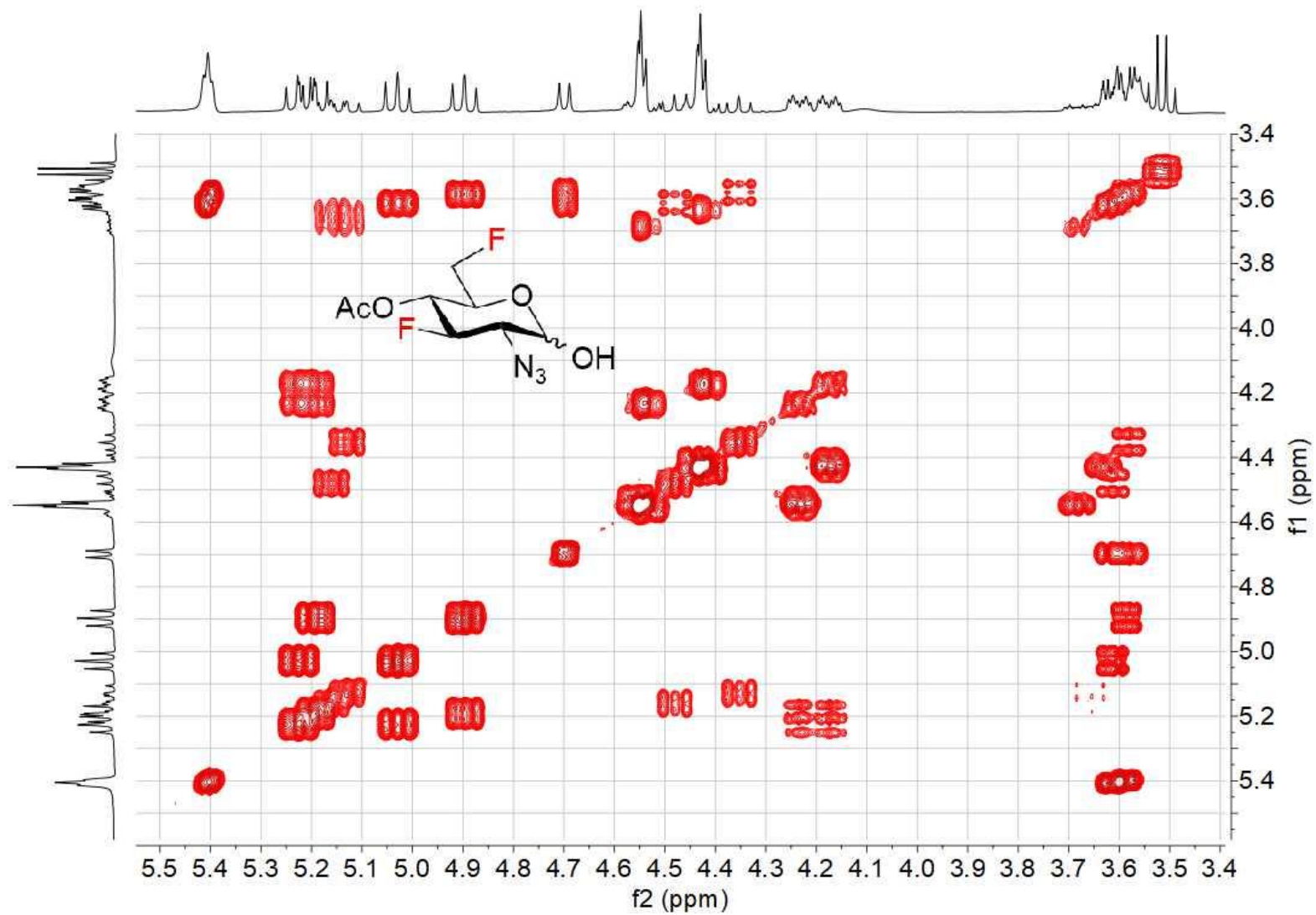
¹³C NMR (100 MHz, CDCl₃) 61



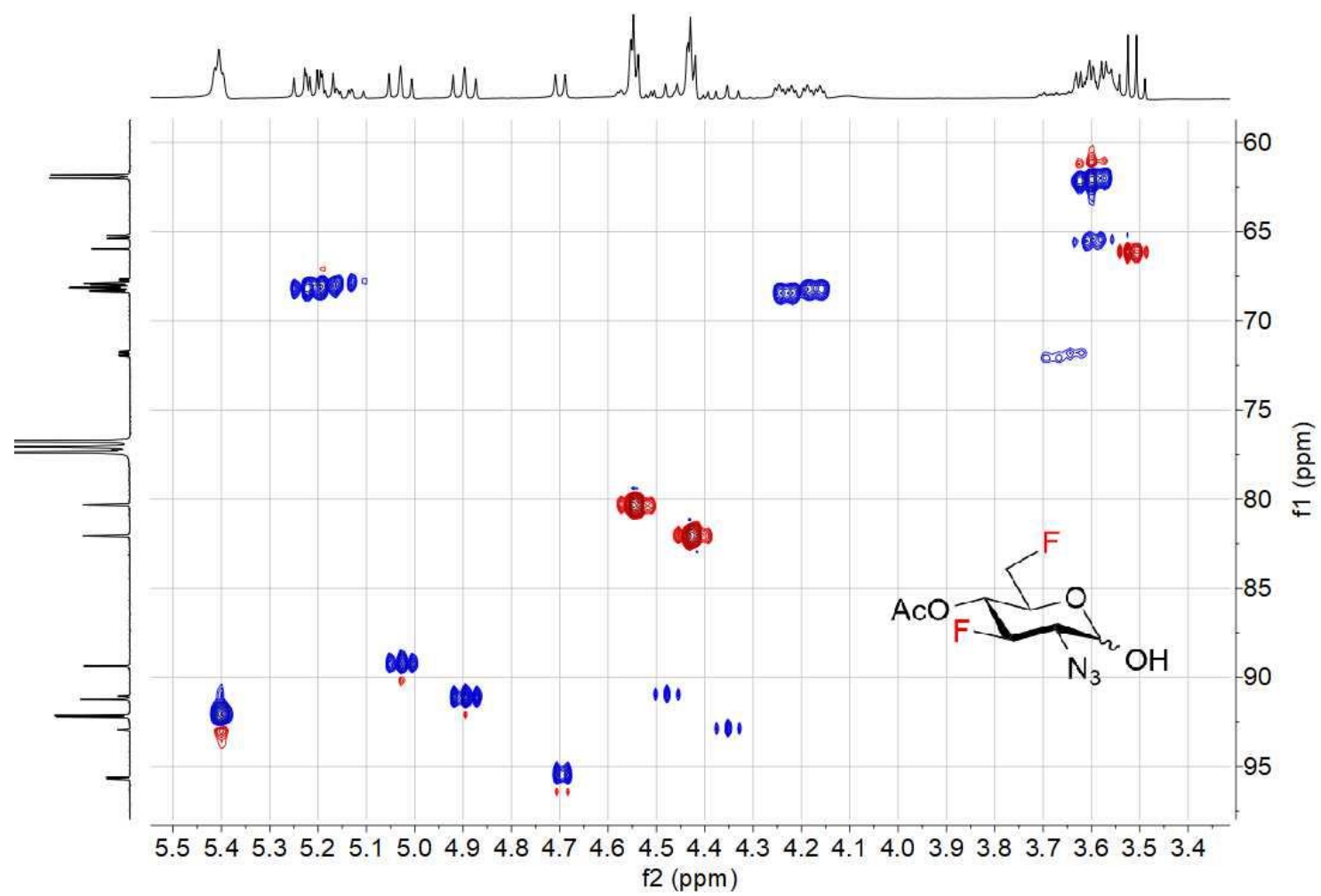
¹⁹F NMR (376 MHz, CDCl₃) 61



¹H-¹H COSY 61

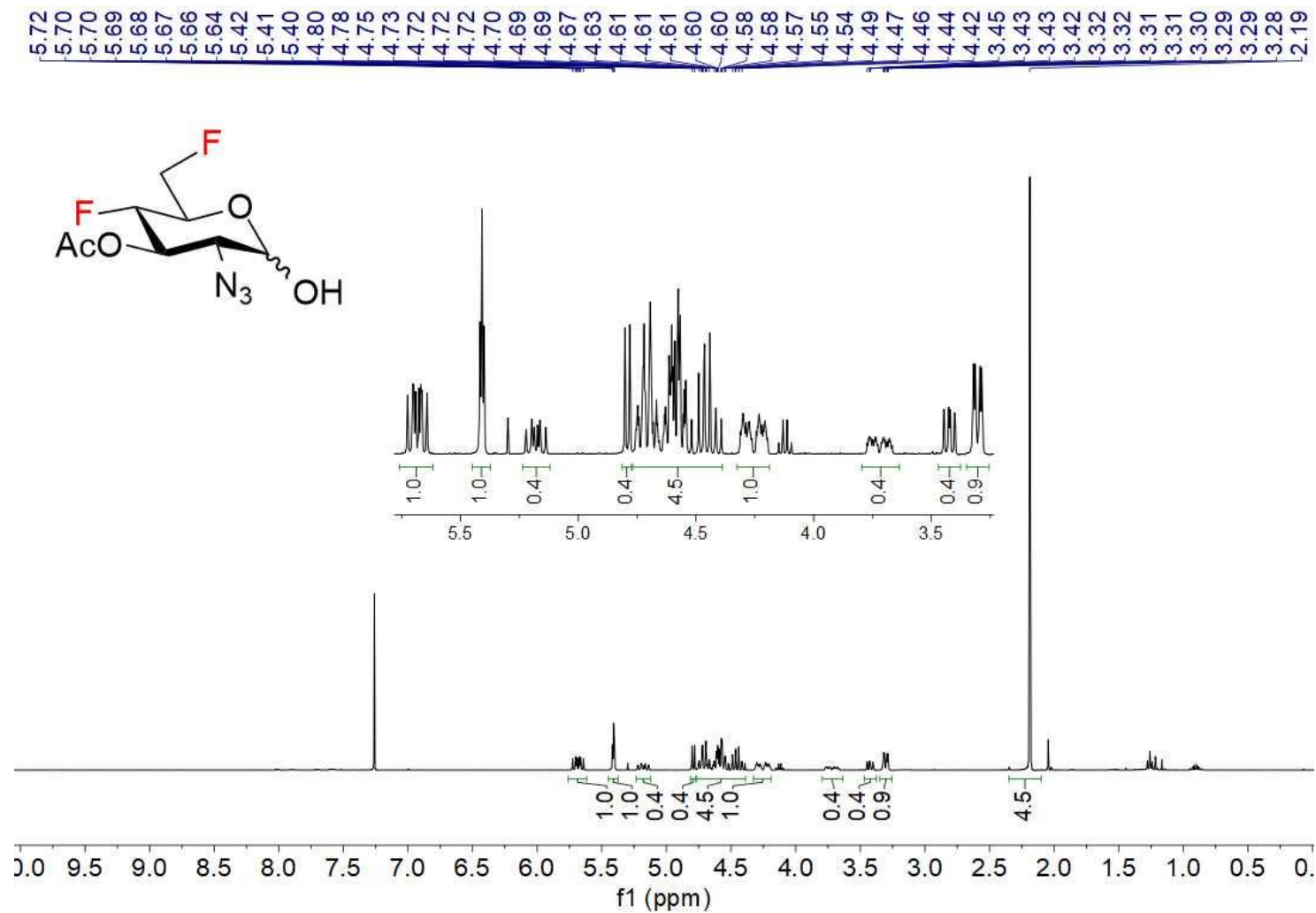


^1H - ^{13}C HSQC 61

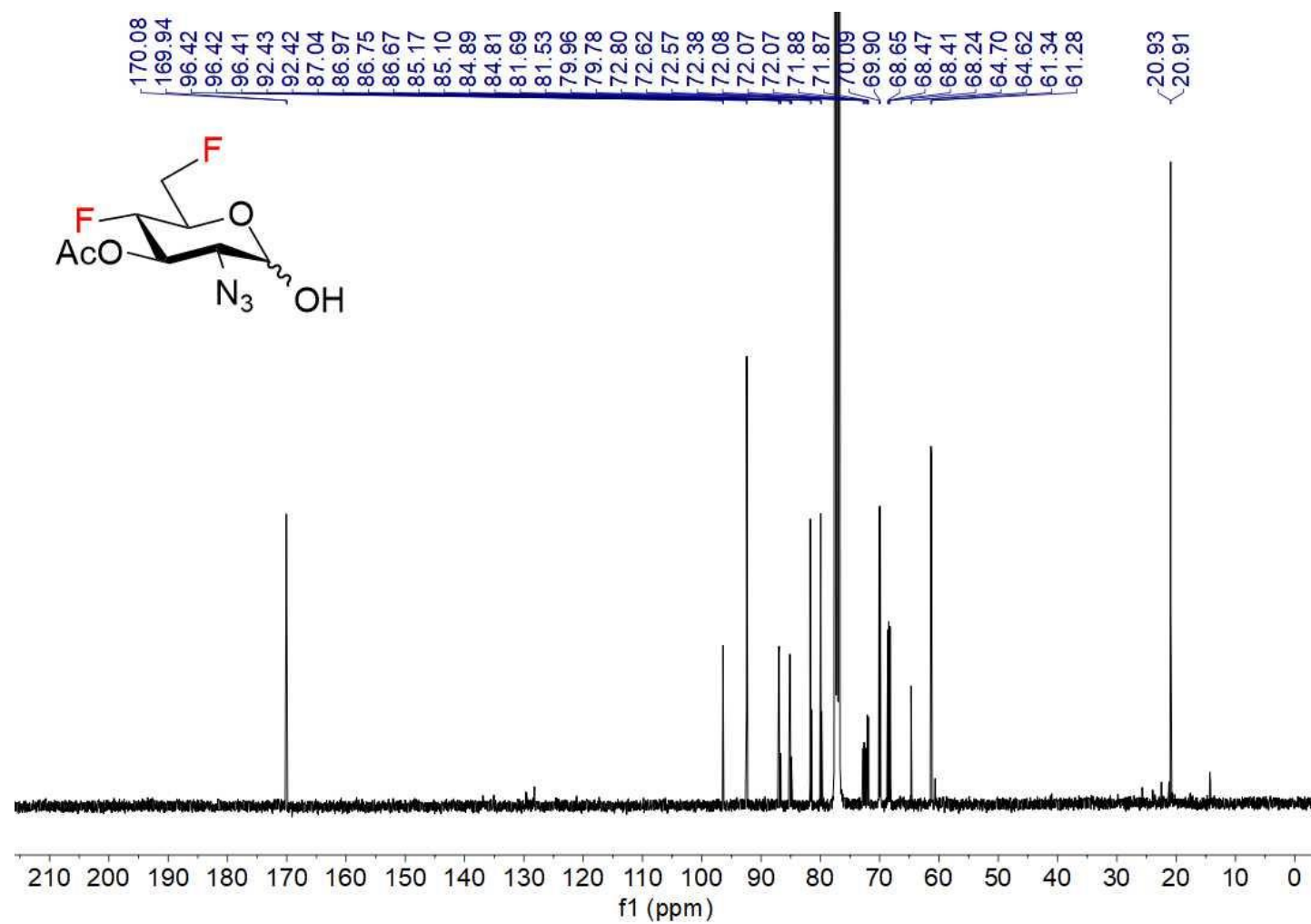


NMR COMPOUND 62

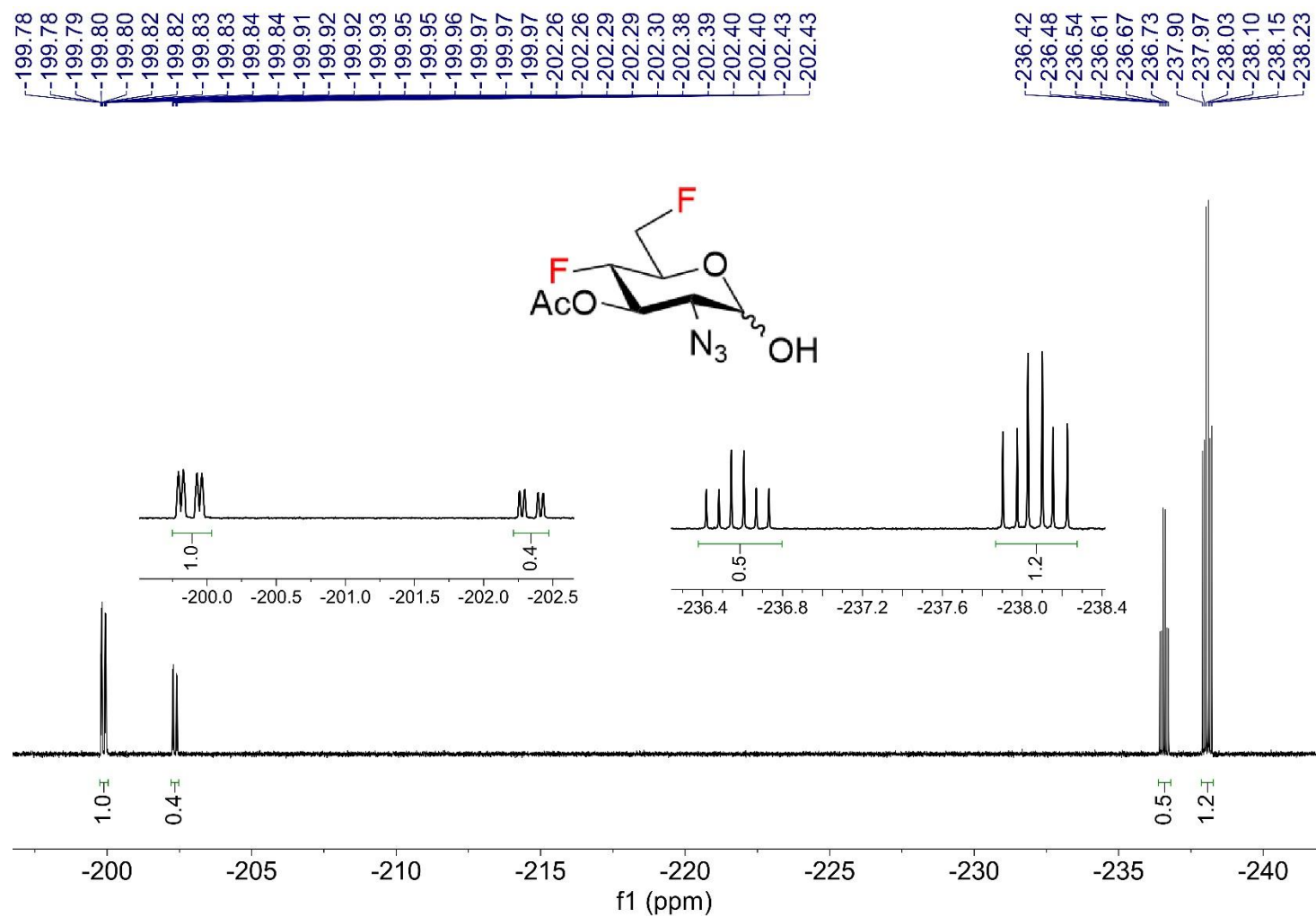
¹H NMR (400 MHz, CDCl₃) 62



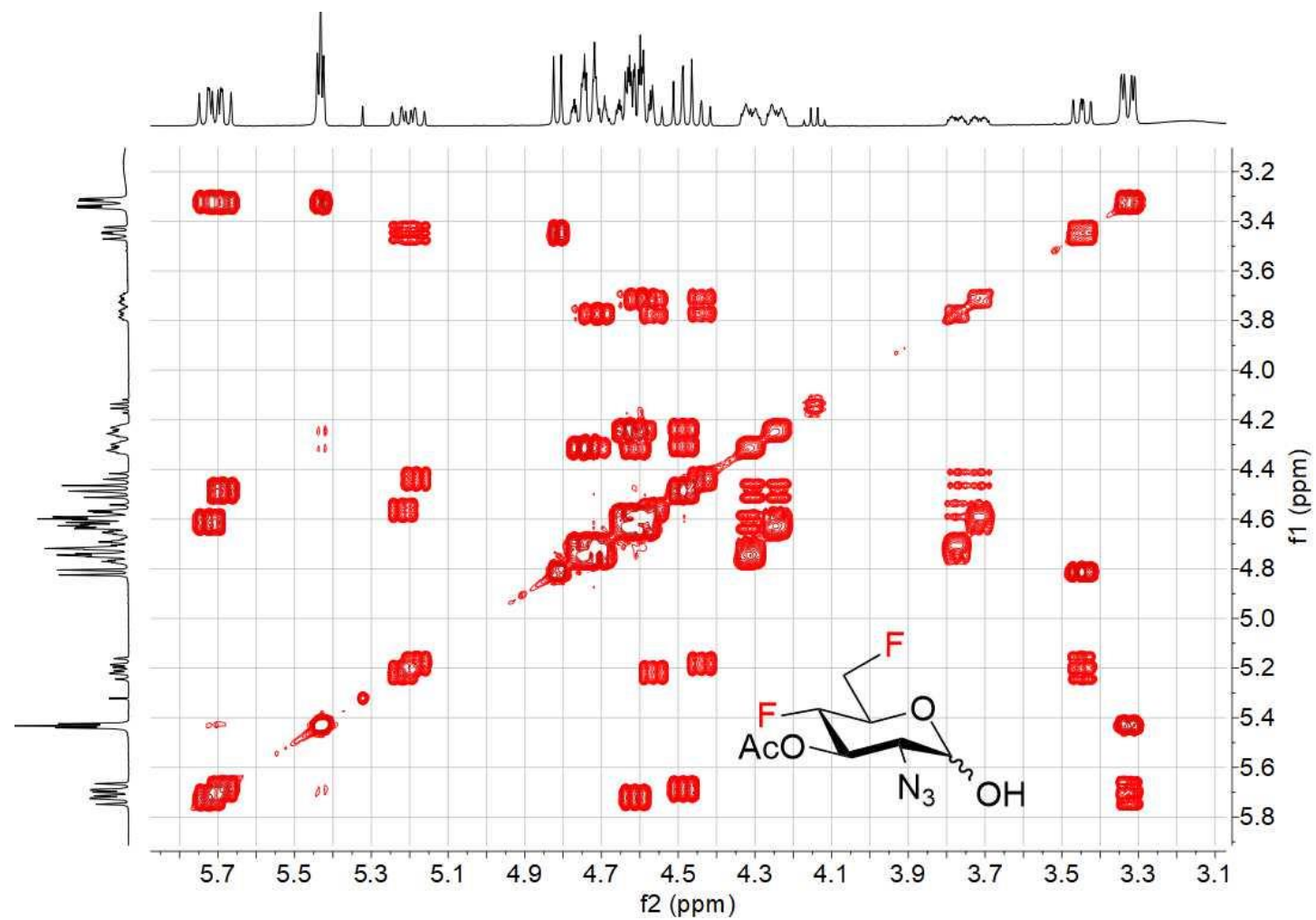
^{13}C NMR (100 MHz, CDCl_3) 62



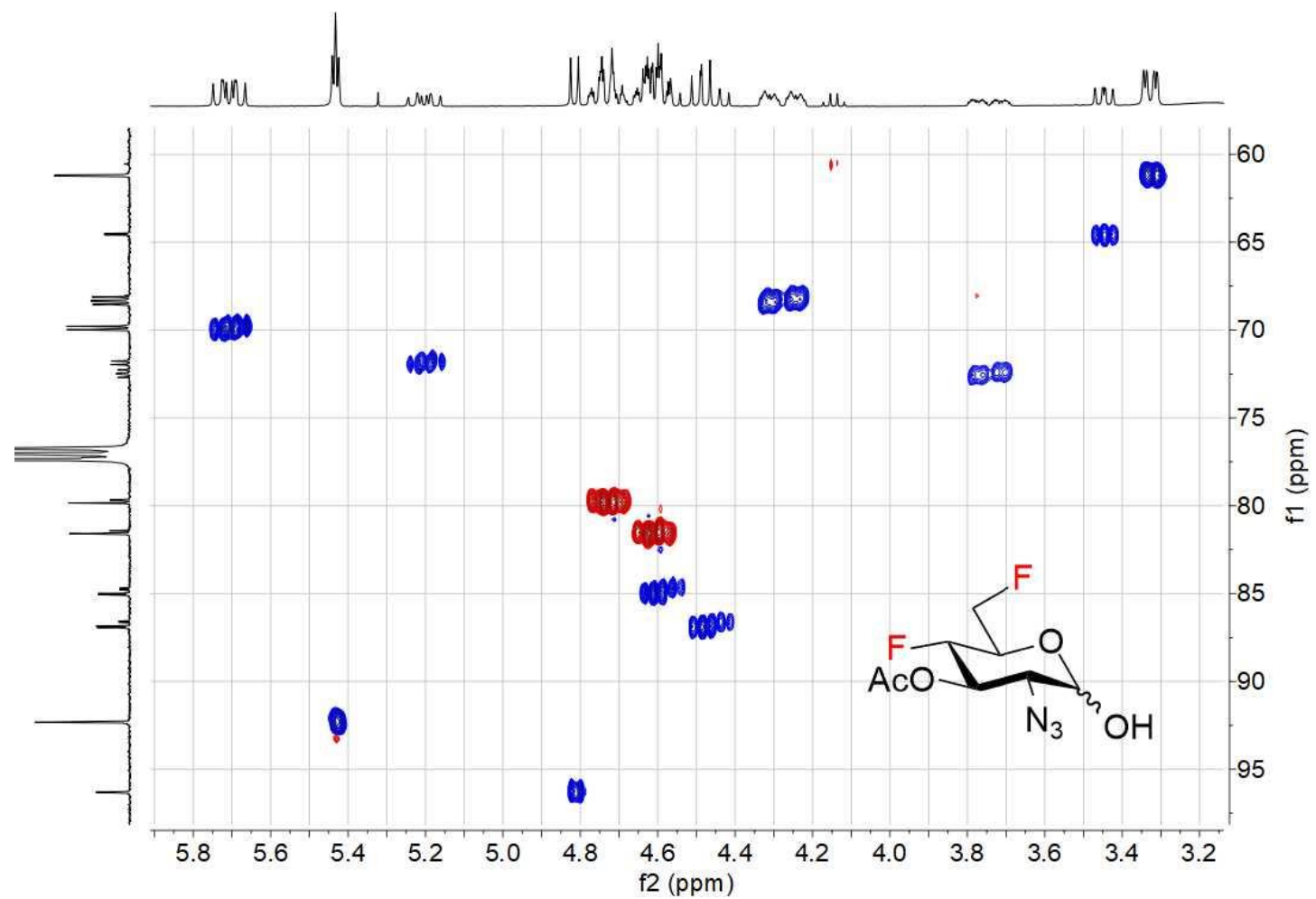
¹⁹F NMR (376 MHz, CDCl₃) 62



^1H - ^1H COSY 62

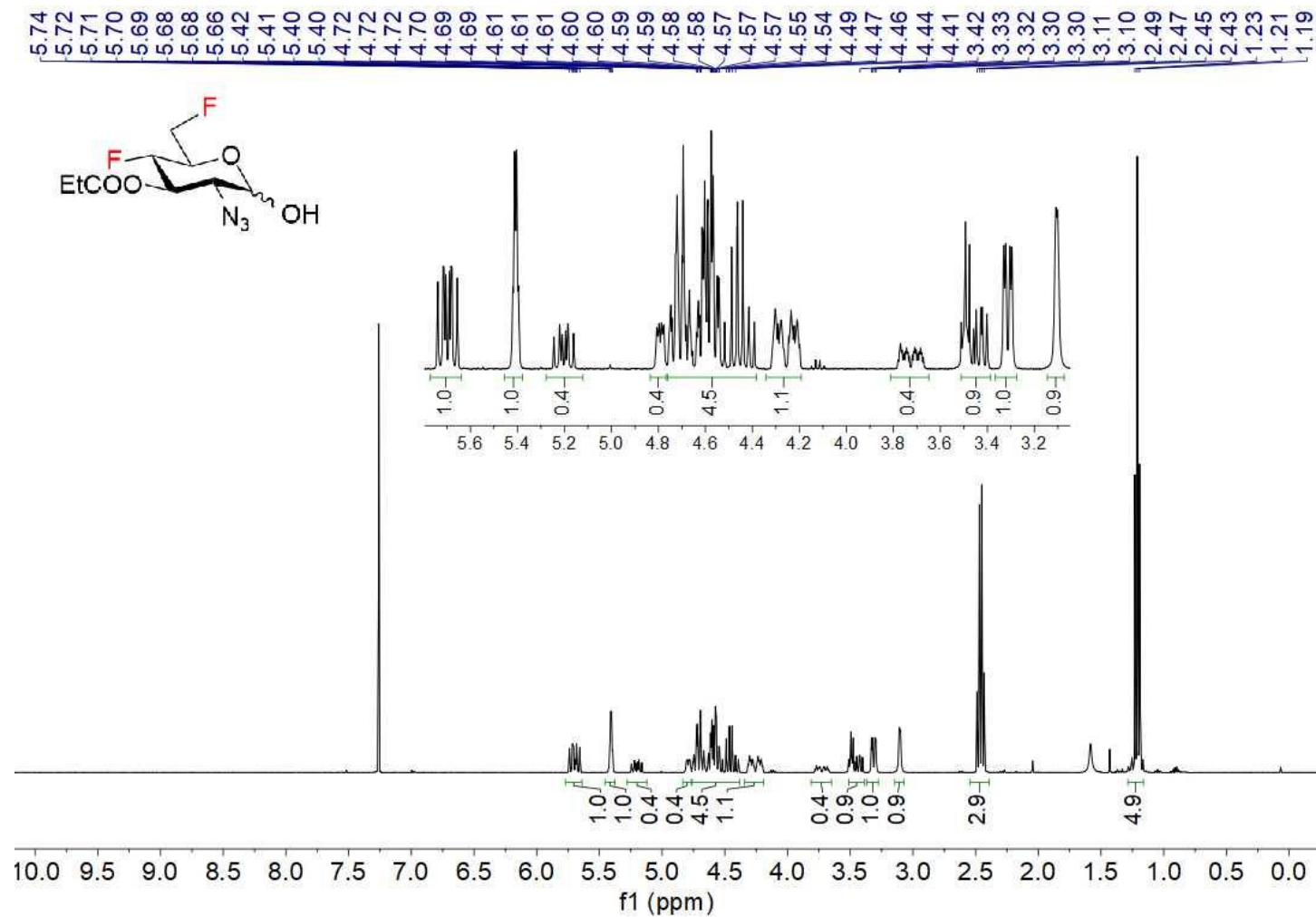


^1H - ^{13}C HSQC 62

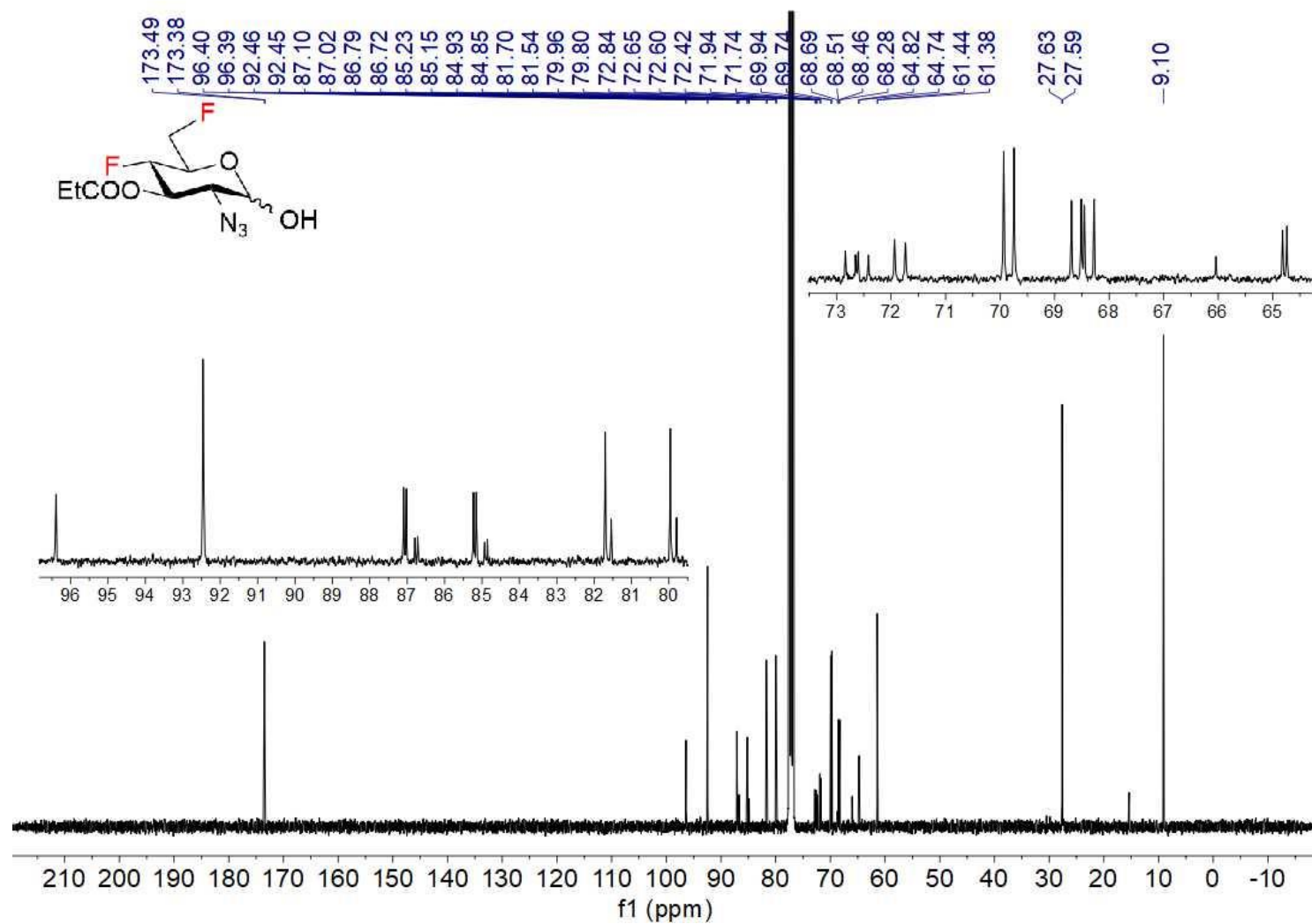


NMR COMPOUND 63

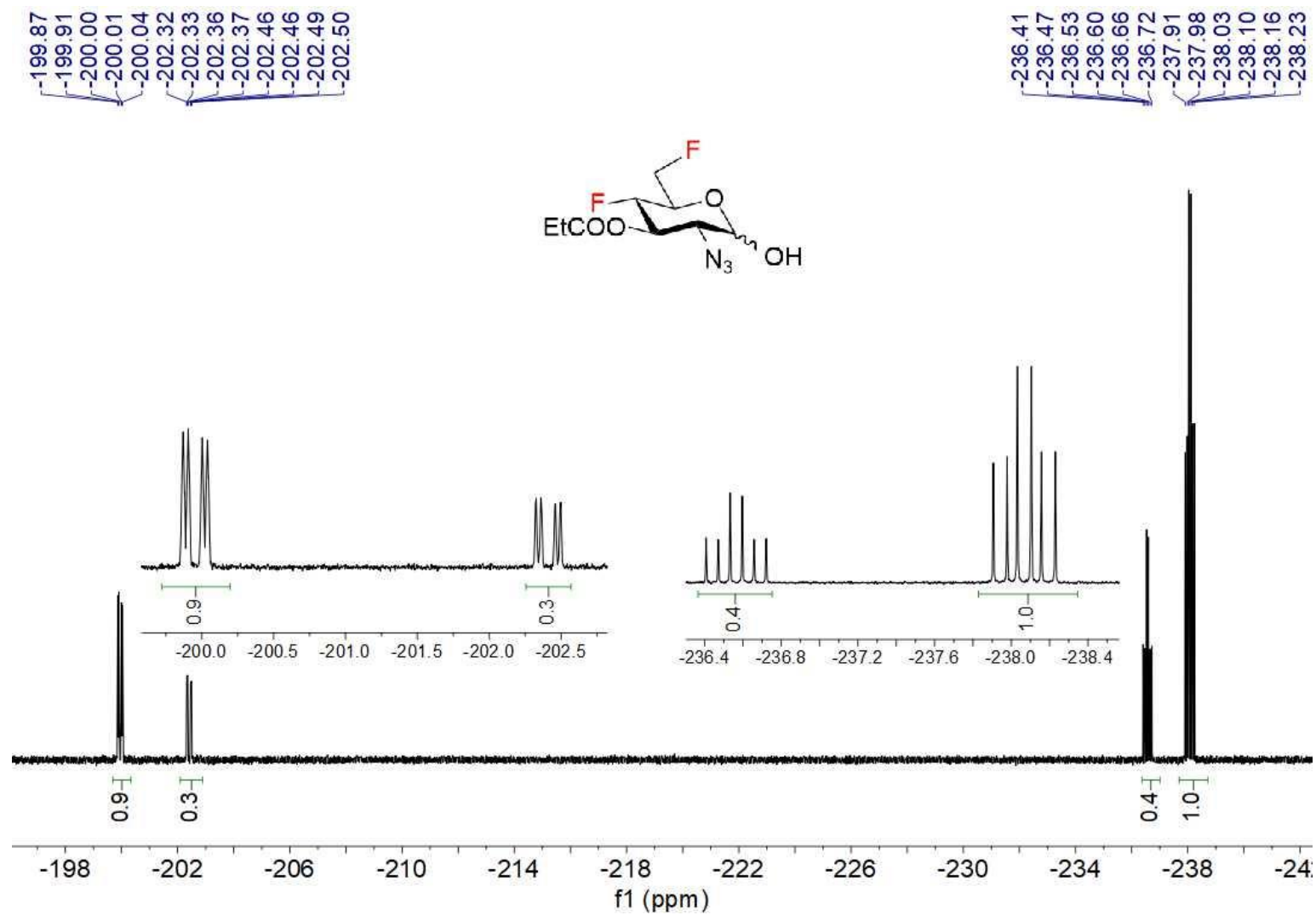
¹H NMR (400 MHz, CDCl₃) 63



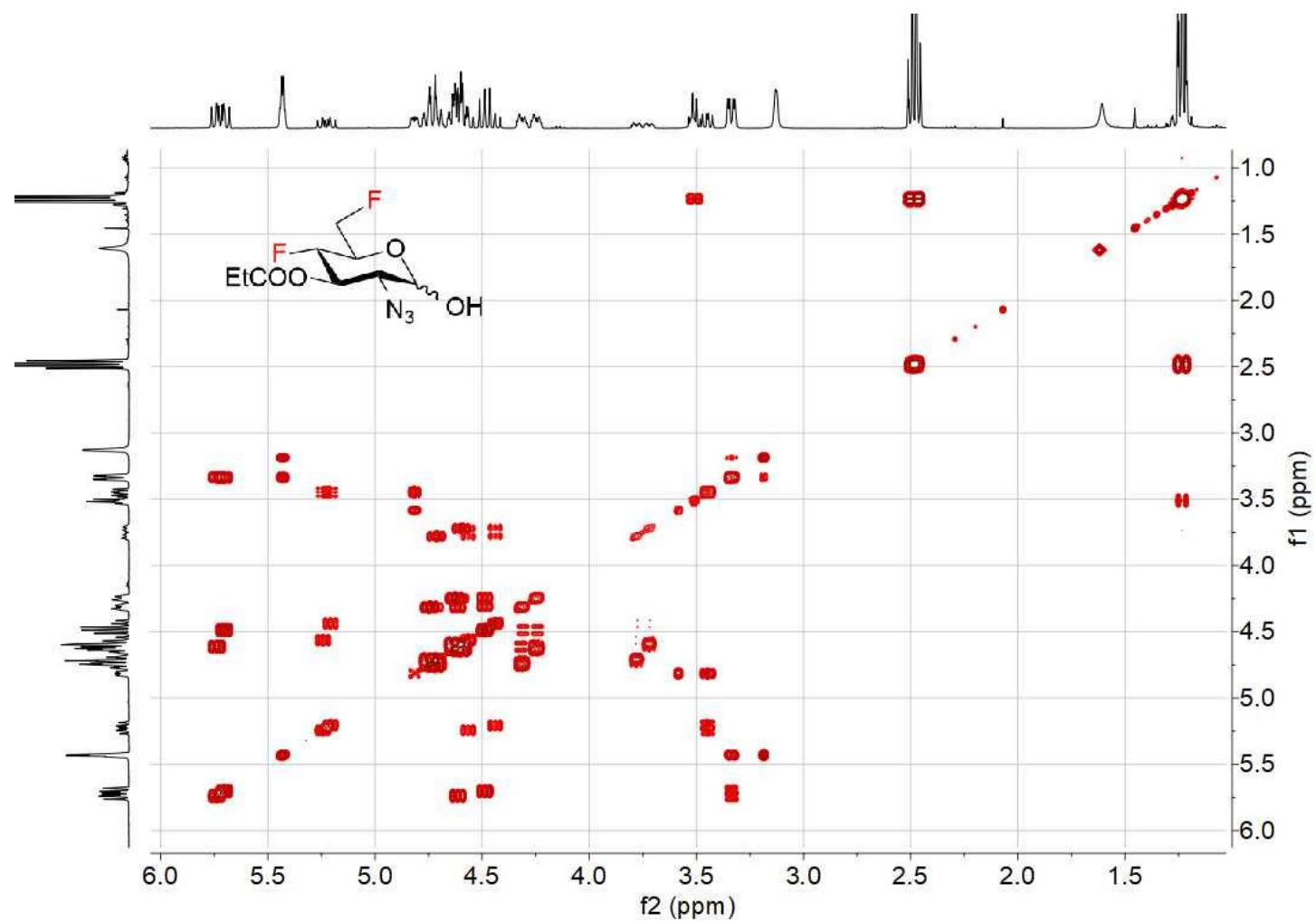
^{13}C NMR (100 MHz, CDCl_3) 63



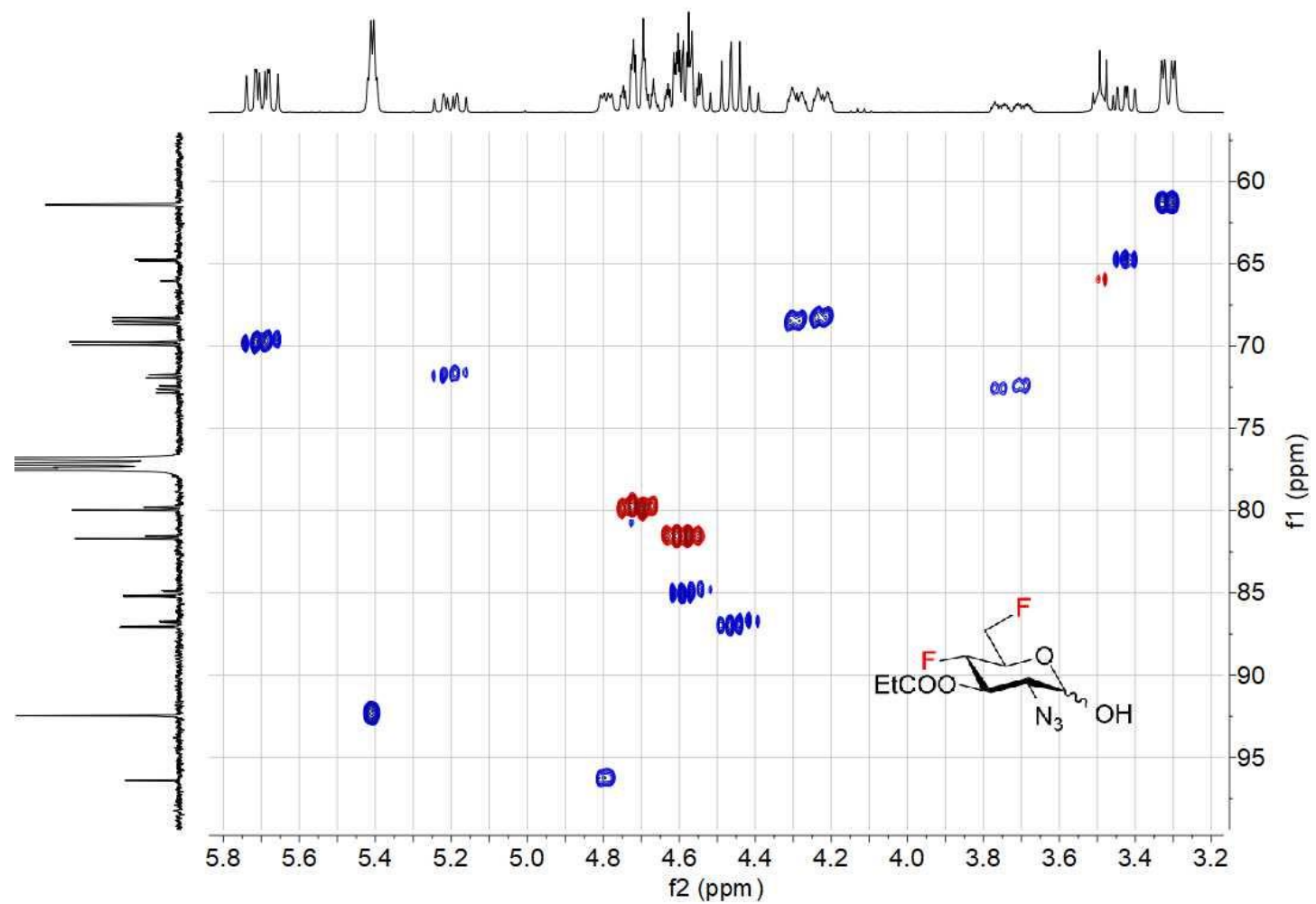
^{19}F NMR (376 MHz, CDCl_3) 63



¹H-¹H COSY 63

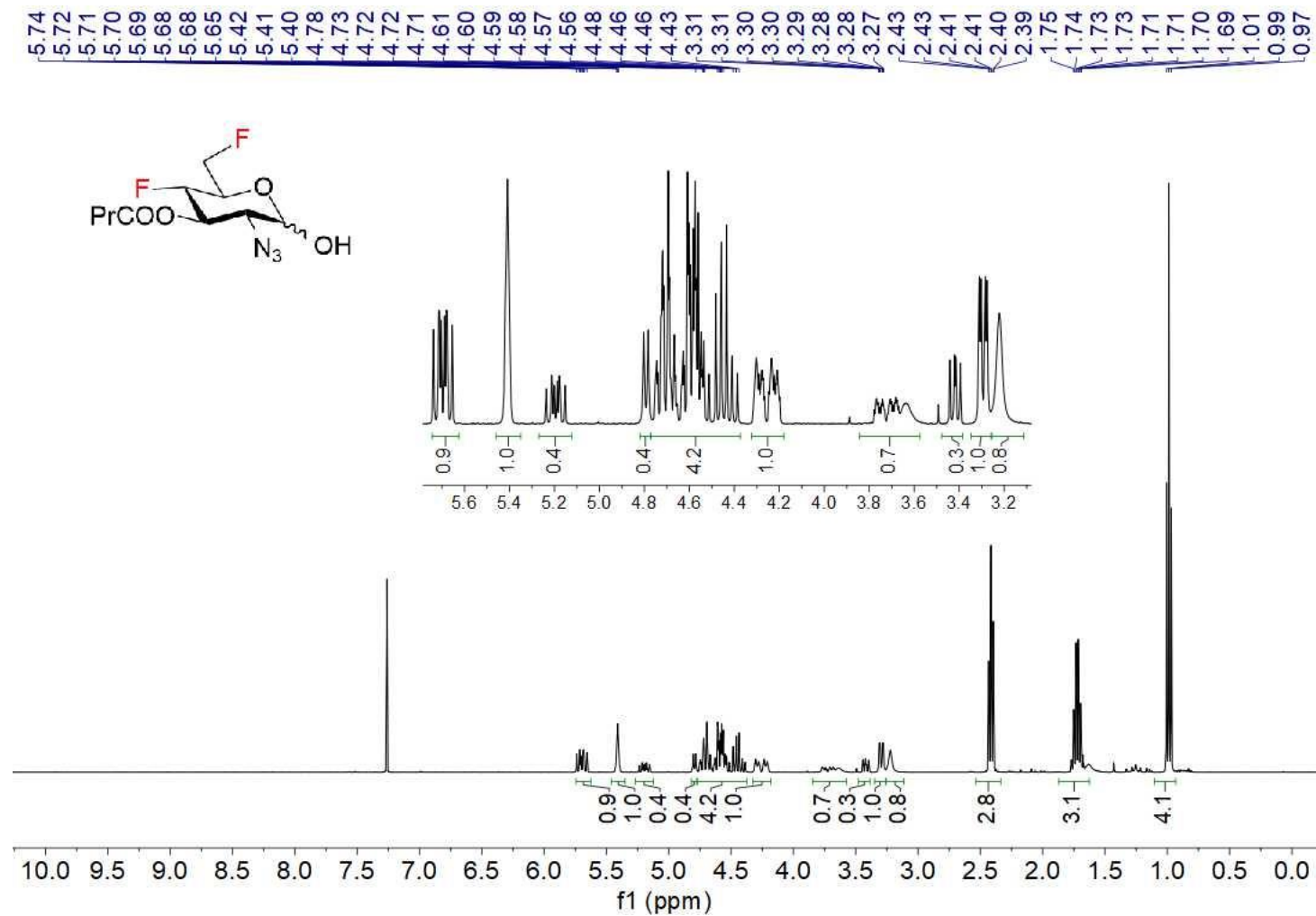


^1H - ^{13}C HSQC 63

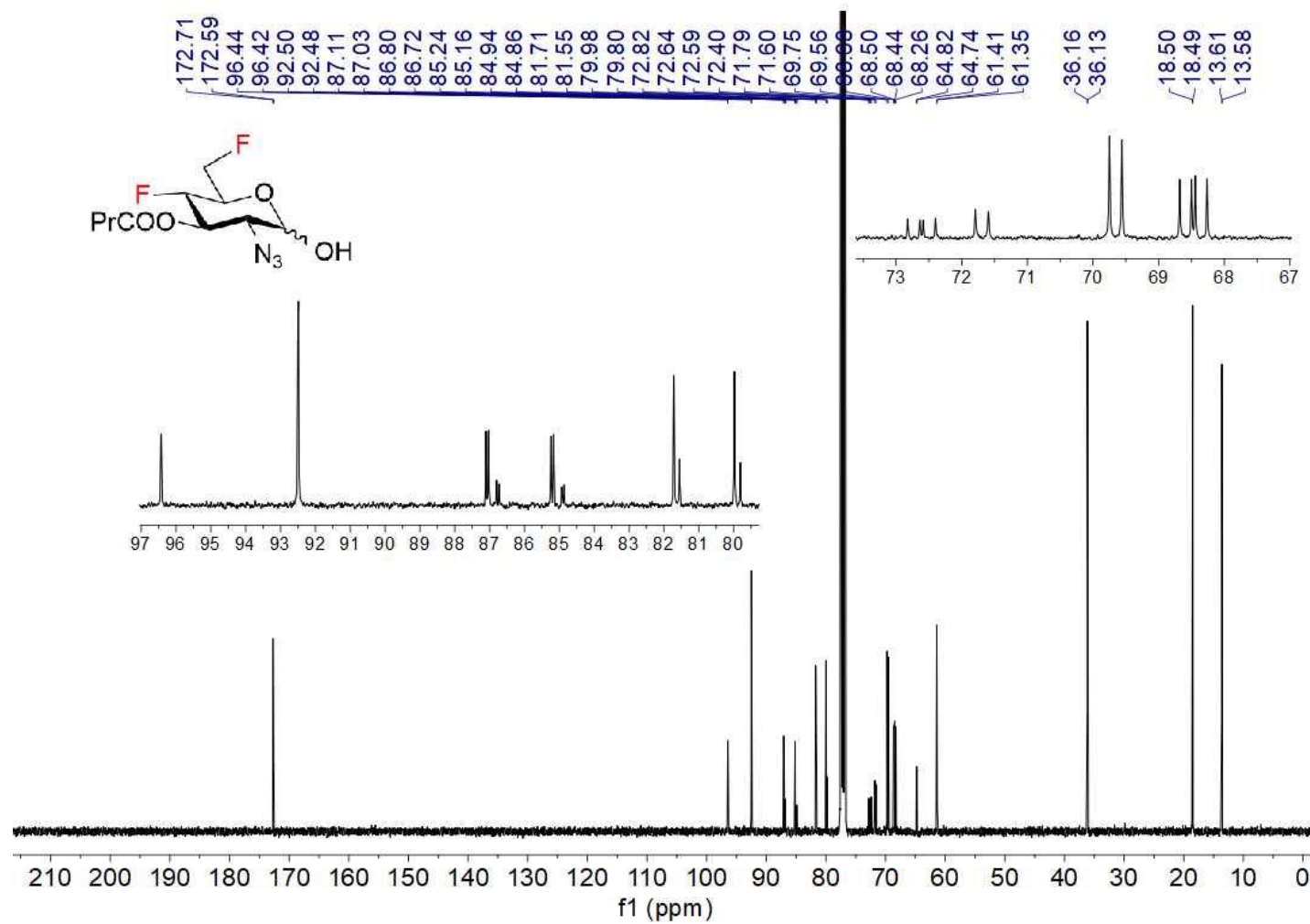


NMR COMPOUND 64

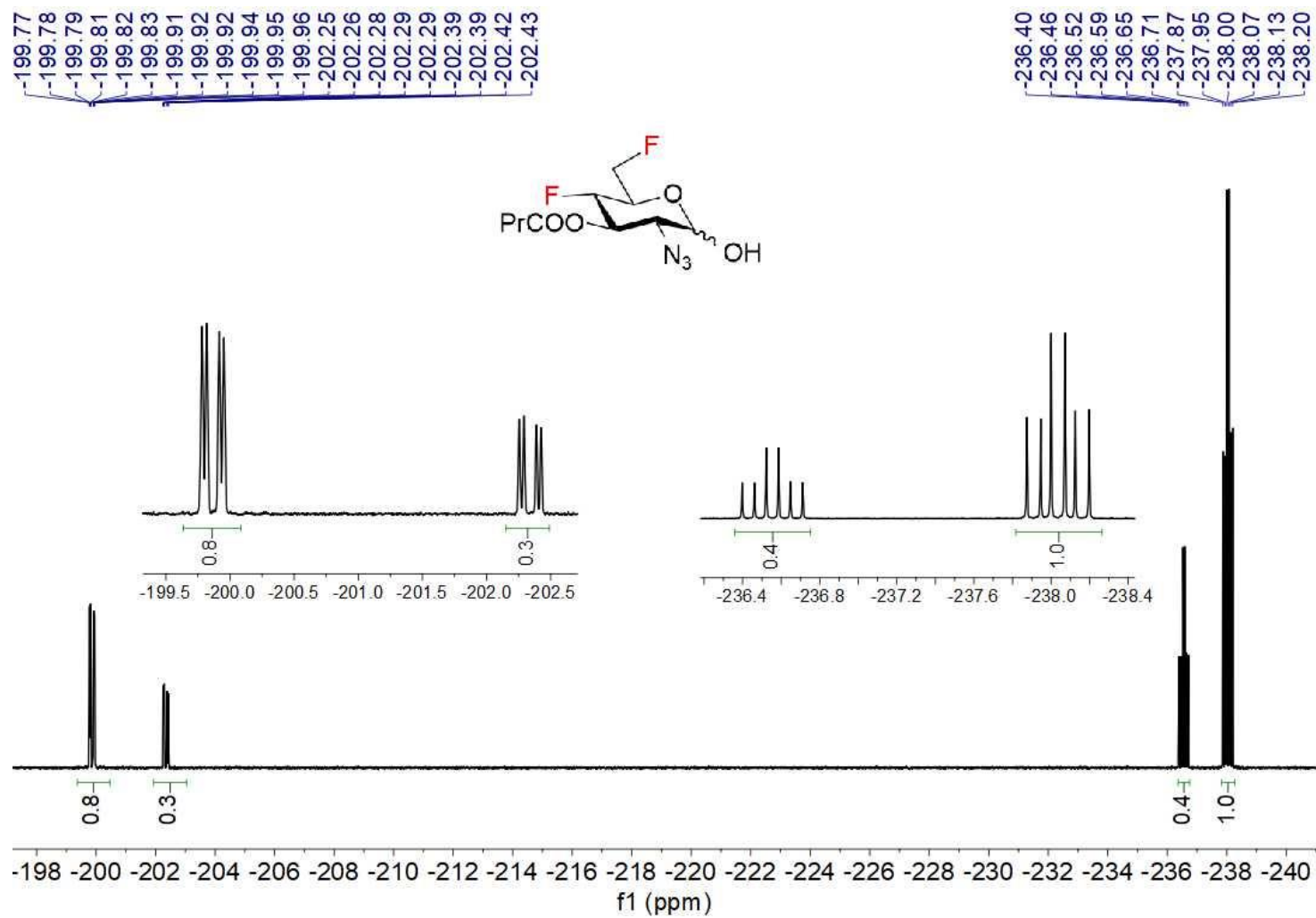
¹H NMR (400 MHz, CDCl₃) 64



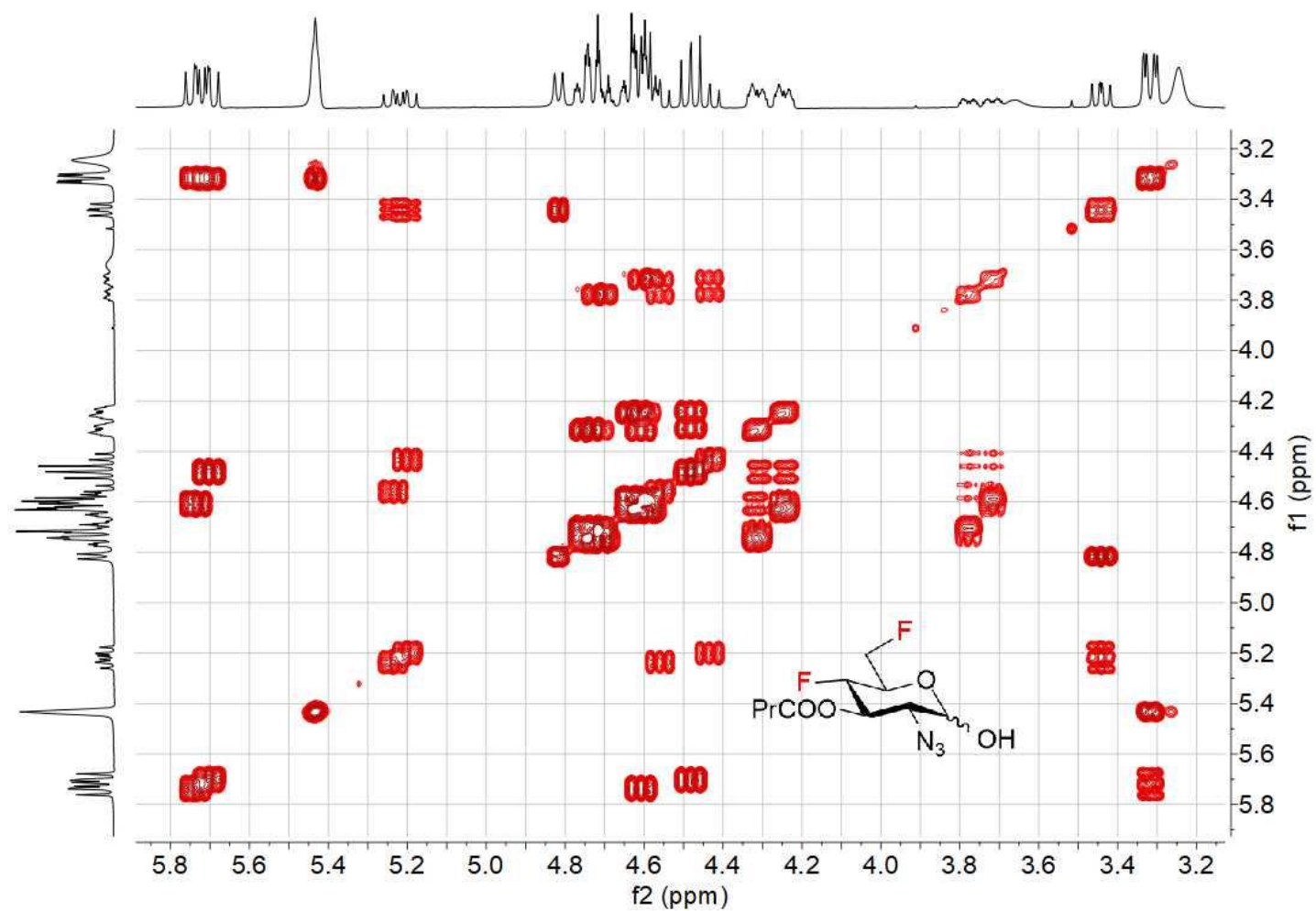
^{13}C NMR (100 MHz, CDCl_3) 64



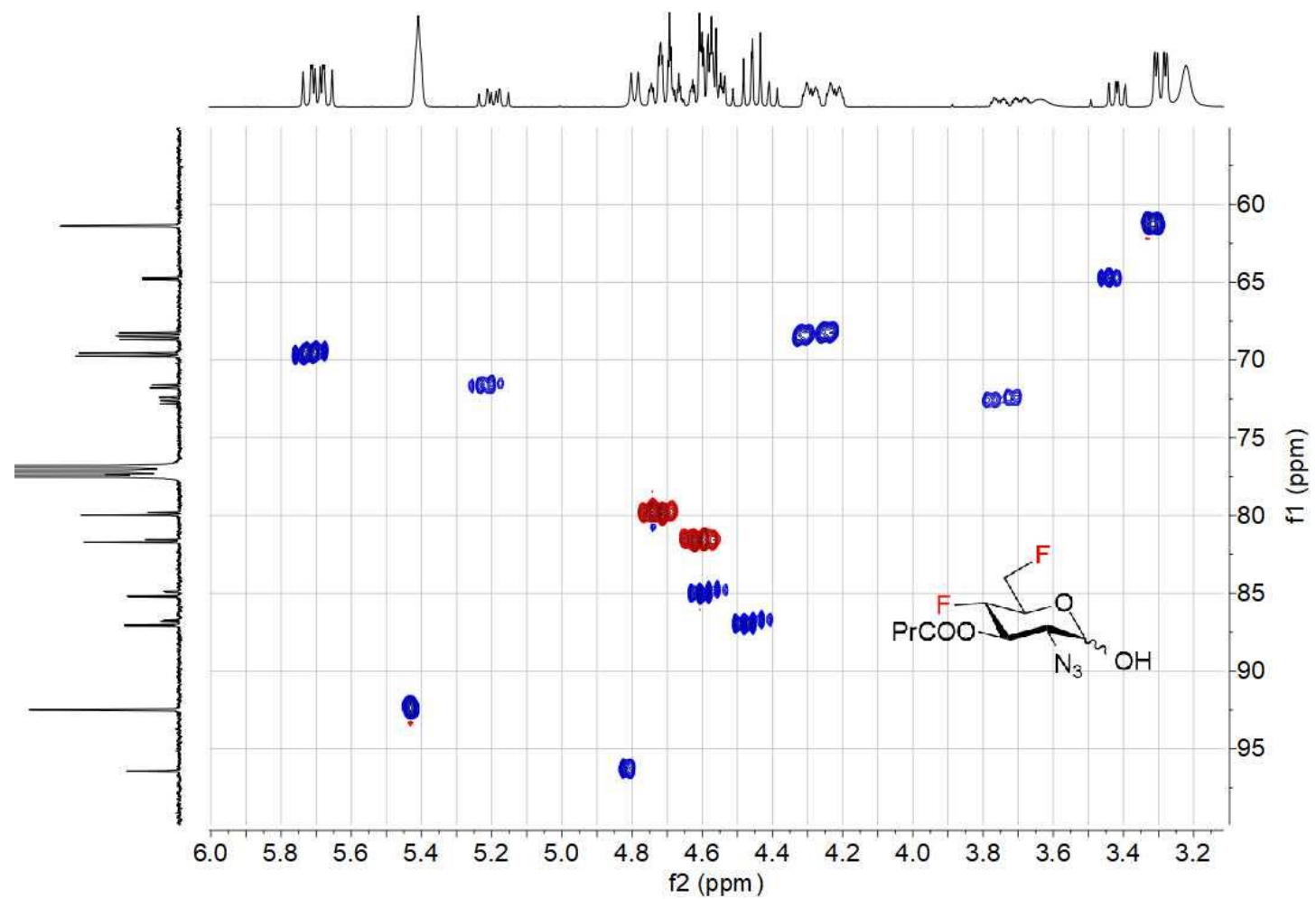
¹⁹F NMR (376 MHz, CDCl₃) 64



¹H-¹H COSY 64

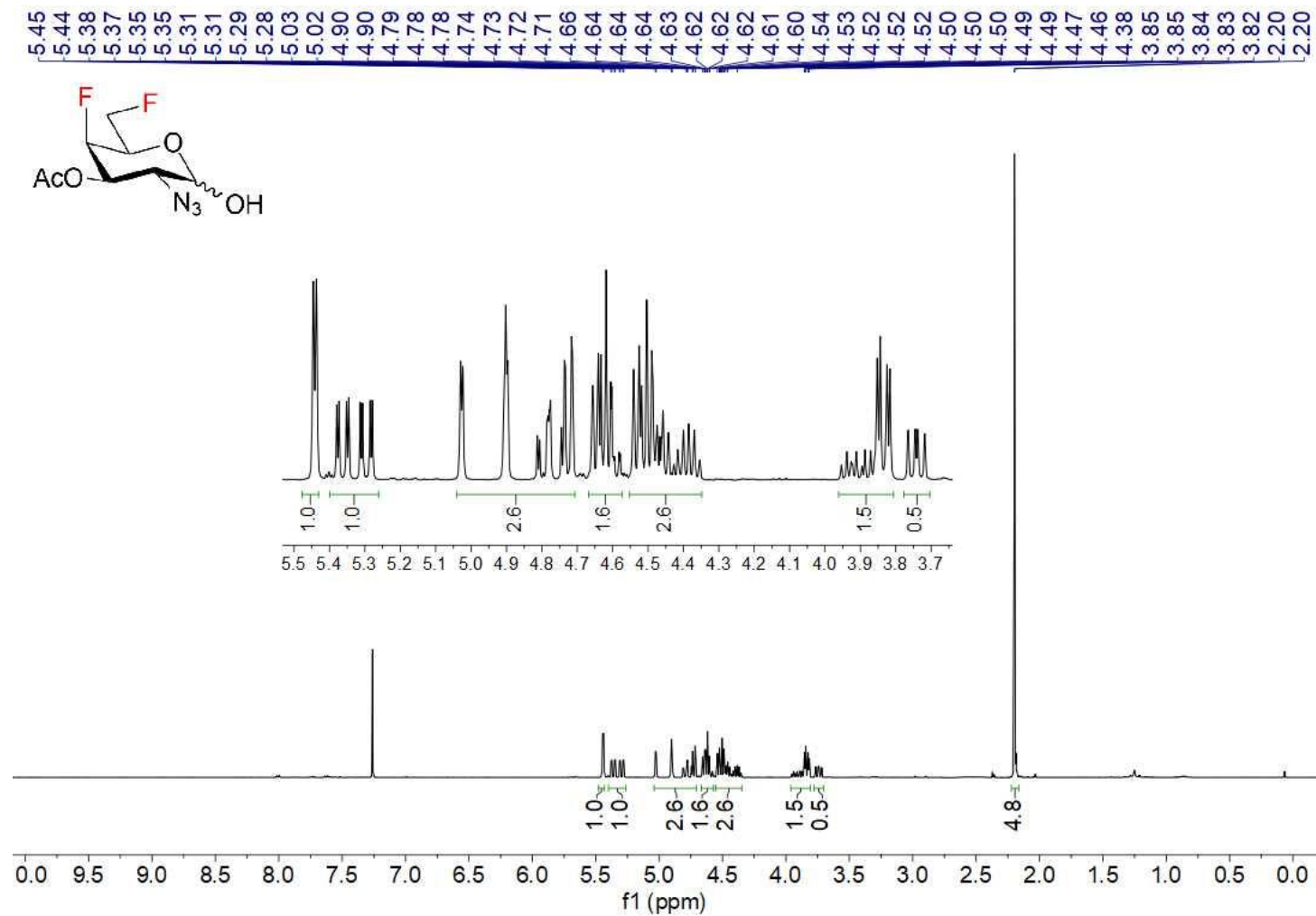


^1H - ^{13}C HSQC 64

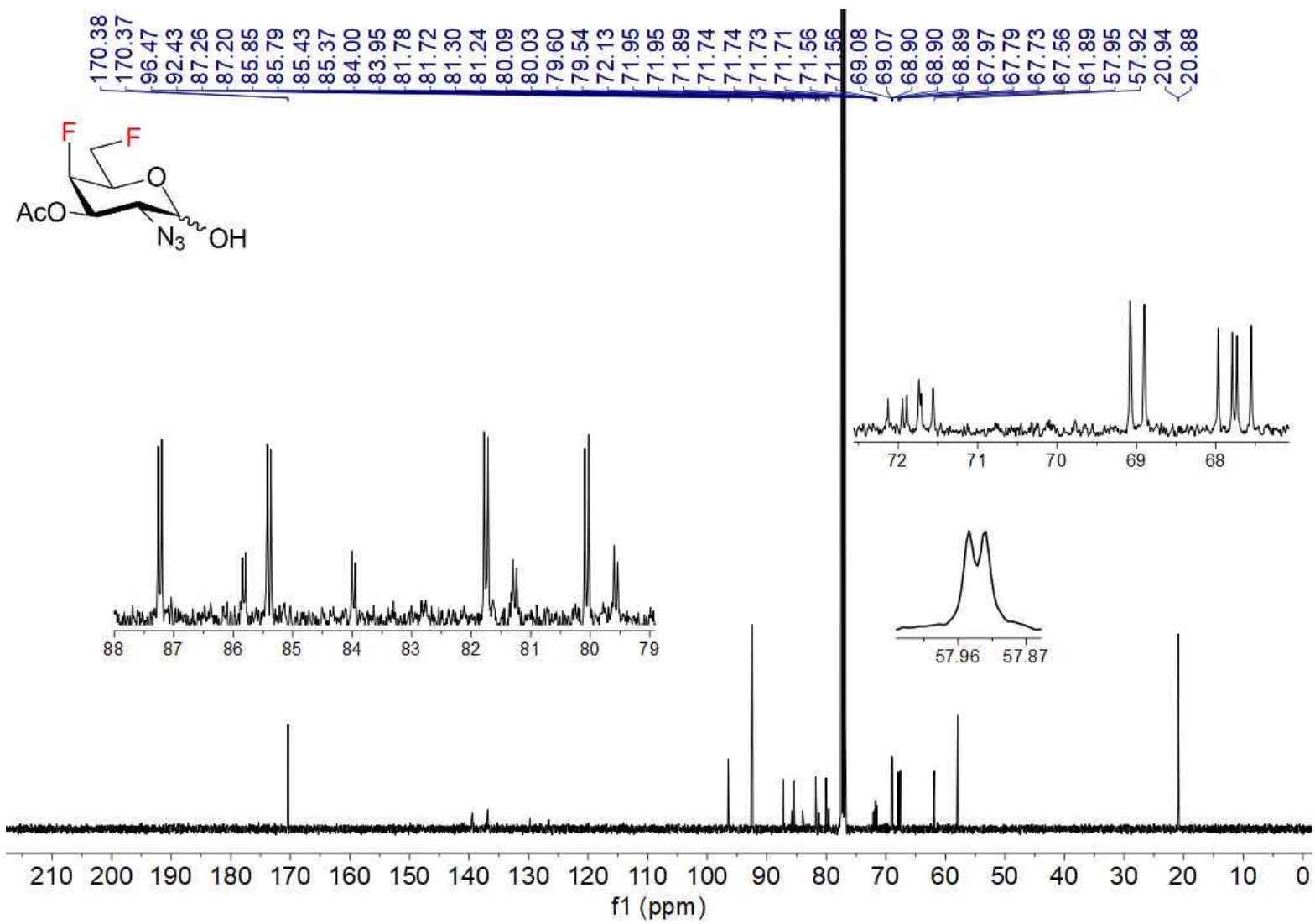


NMR COMPOUND 65

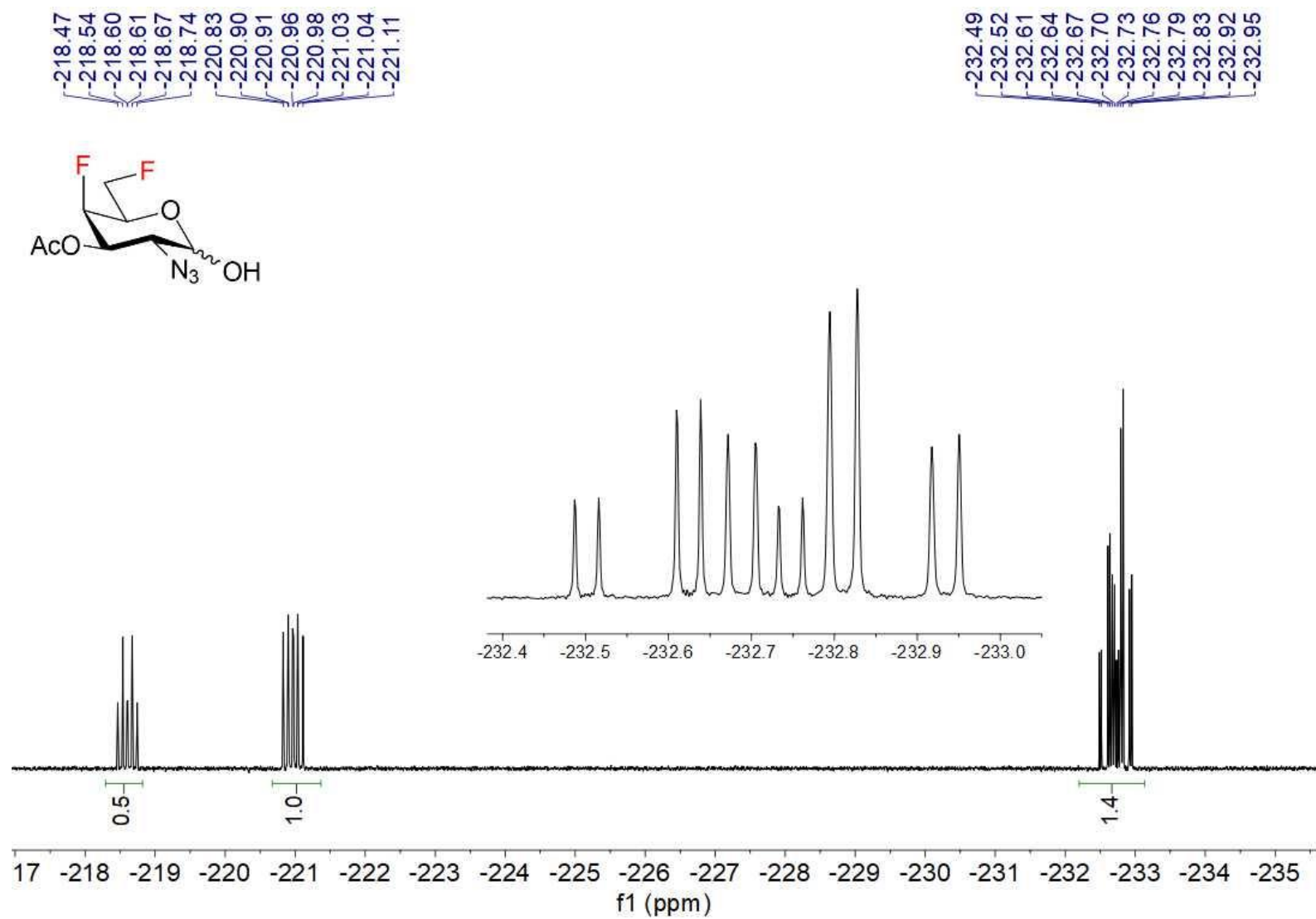
¹H NMR (400 MHz, CDCl₃) 65



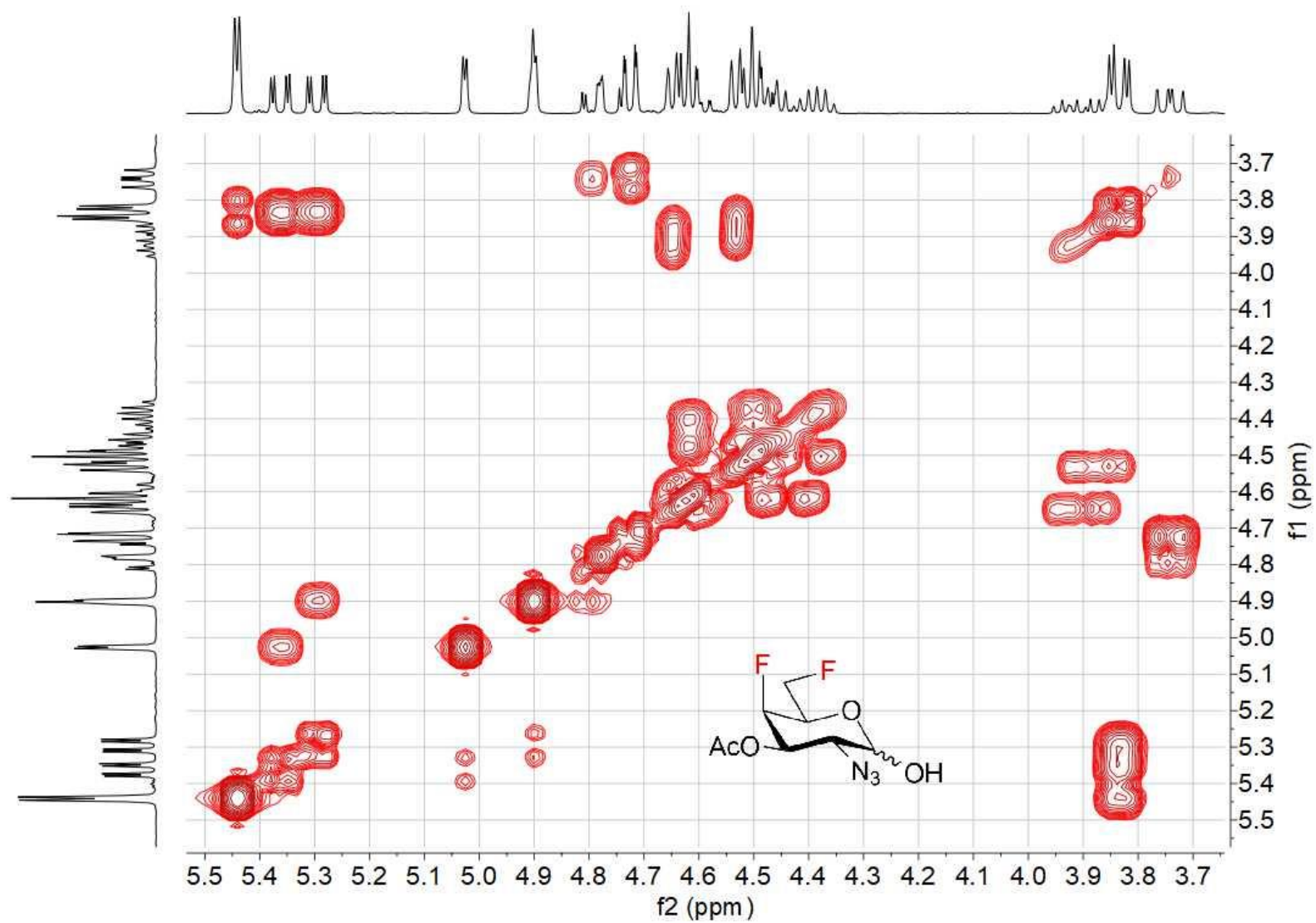
¹³C NMR (100 MHz, CDCl₃) 65



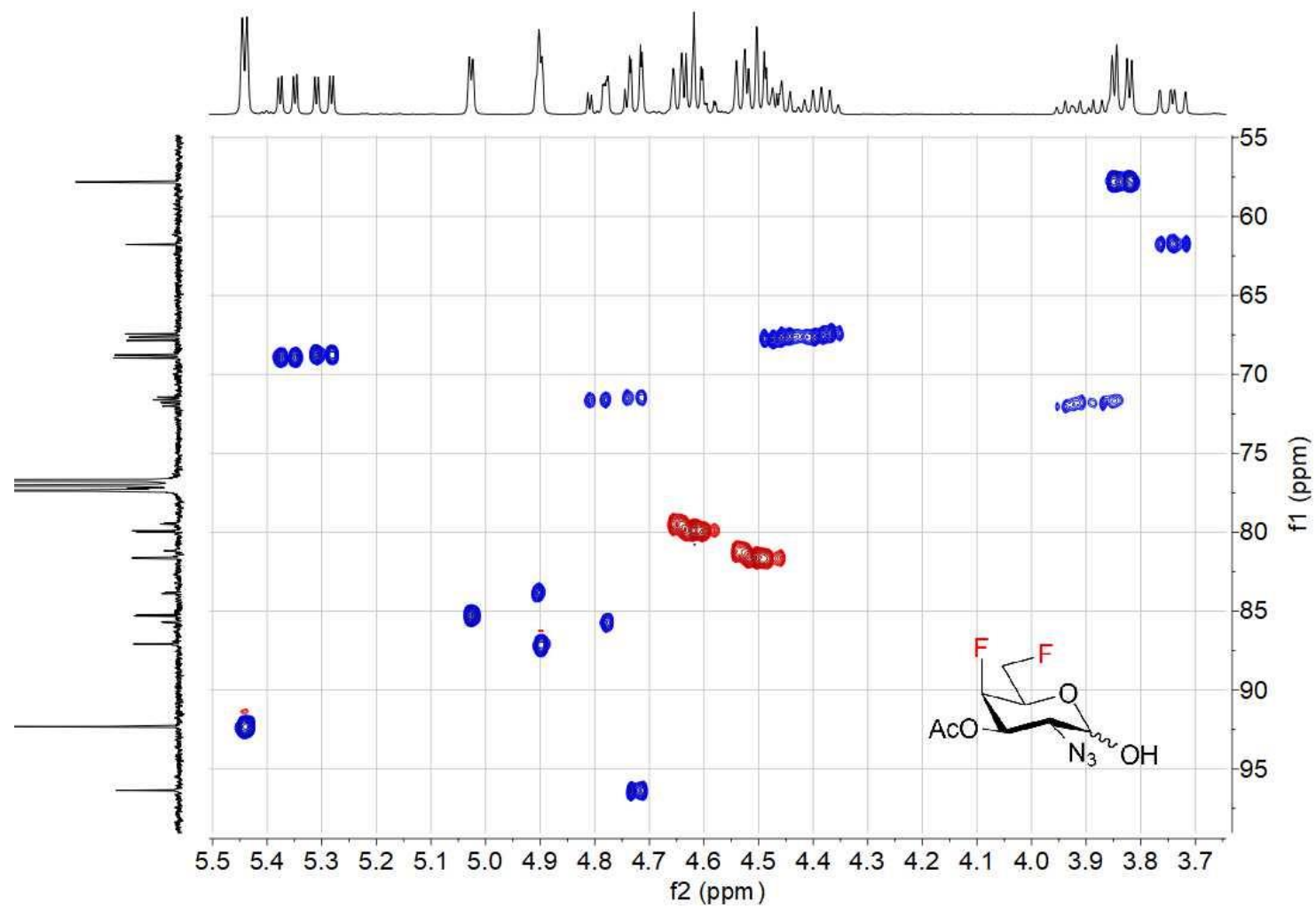
¹⁹F NMR (376 MHz, CDCl₃) 65



¹H-¹H COSY 65

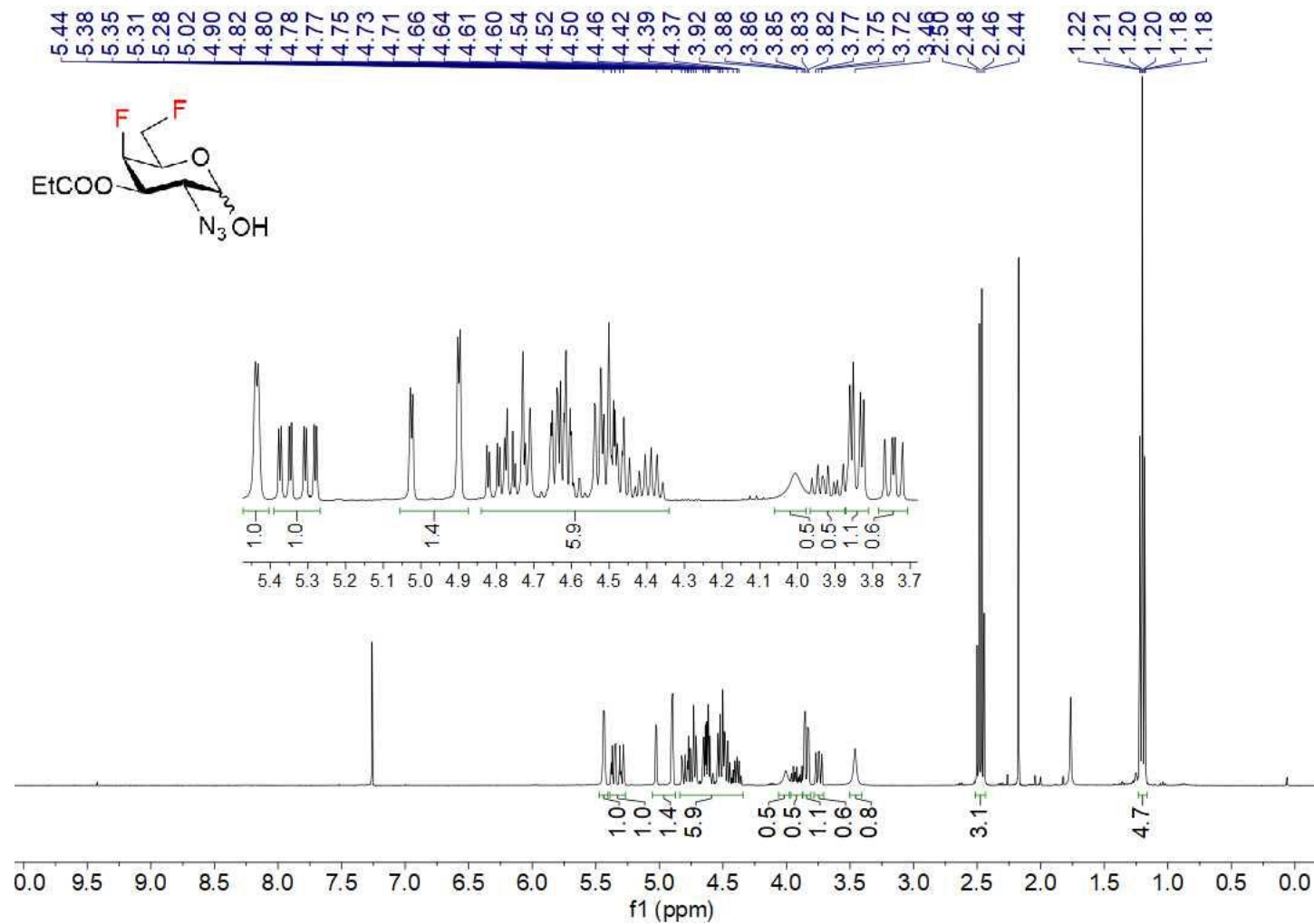


^1H - ^{13}C HSQC 65

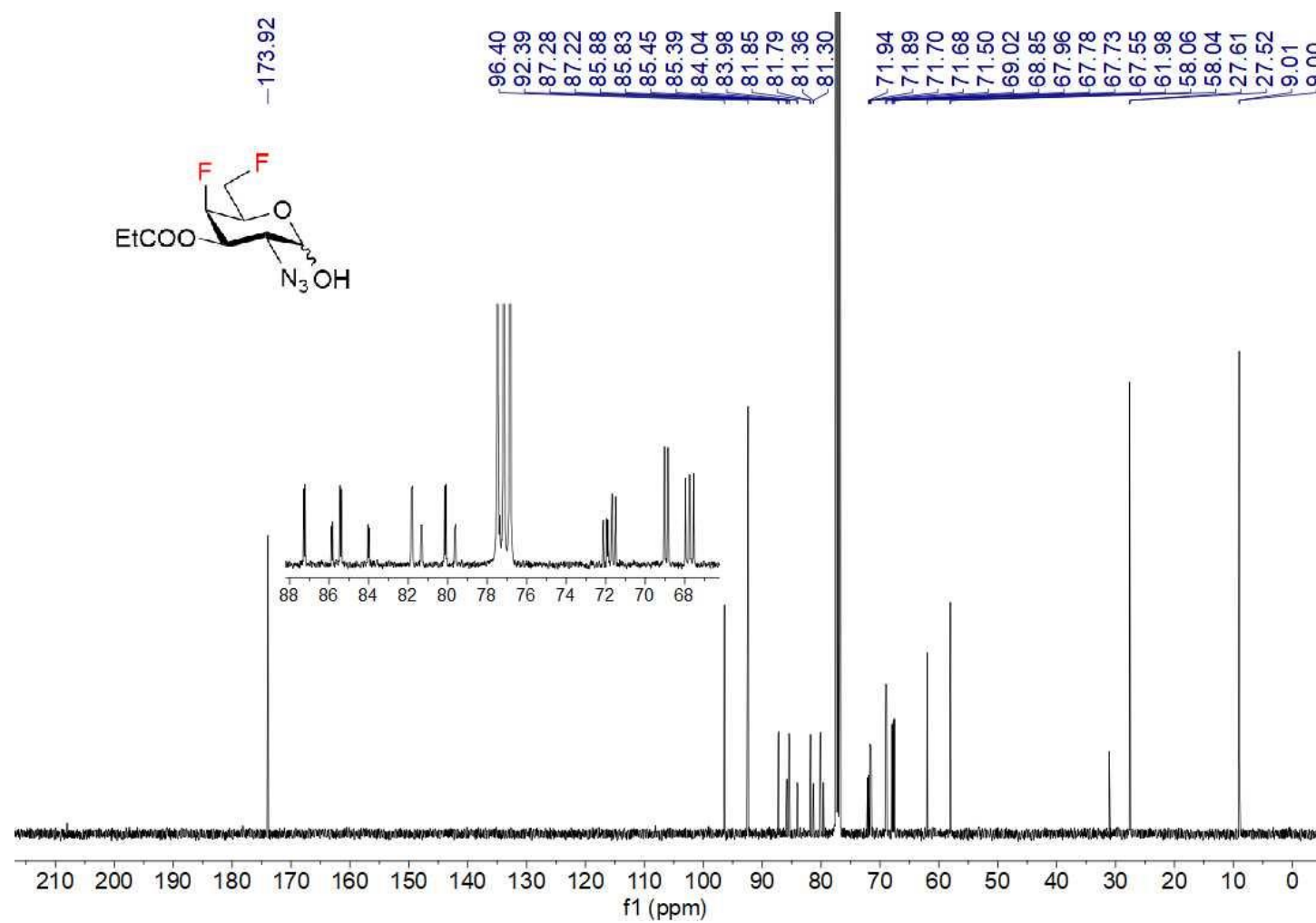


NMR COMPOUND 66

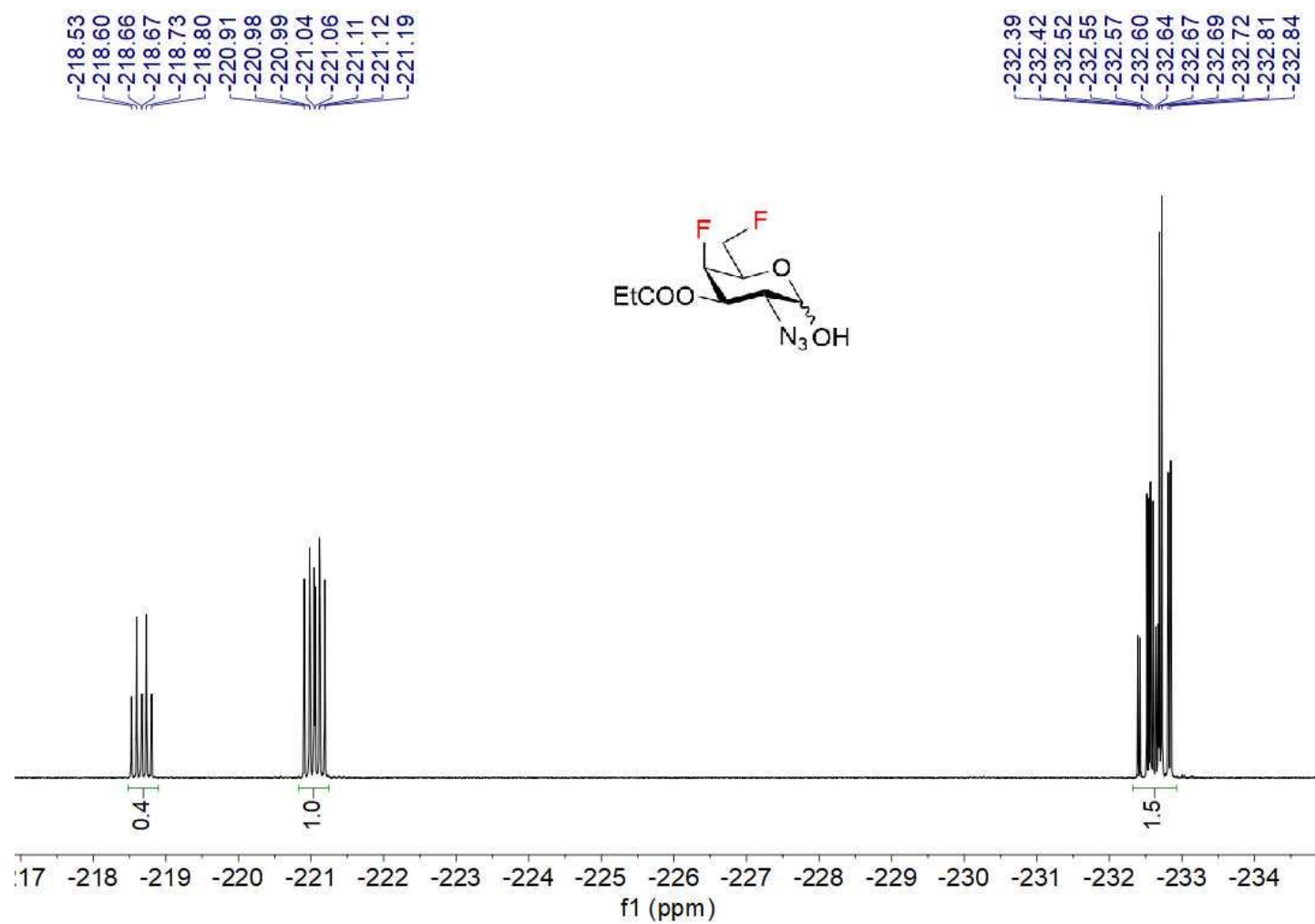
¹H NMR (400 MHz, CDCl₃) 66



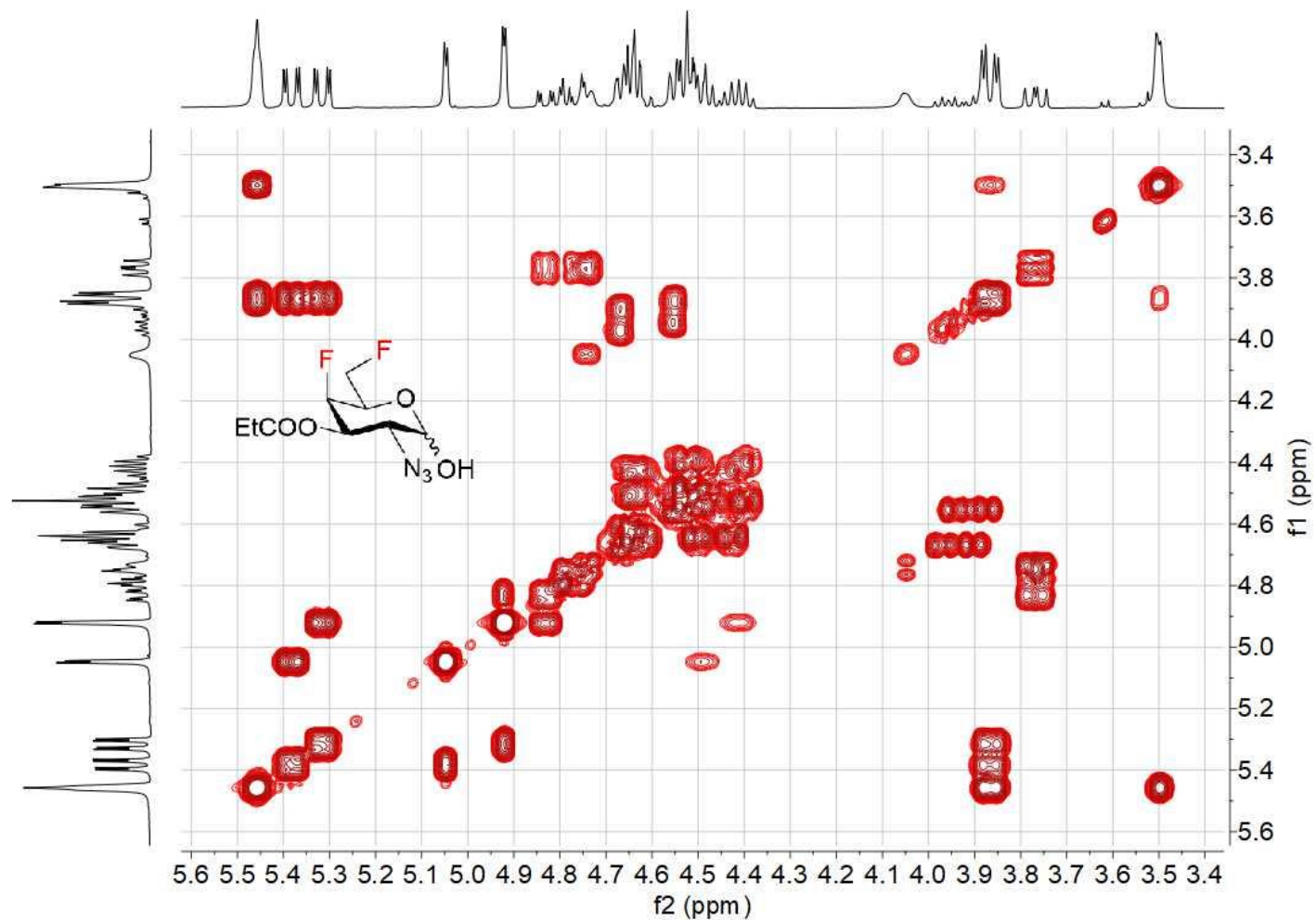
^{13}C NMR (100 MHz, CDCl_3) 66



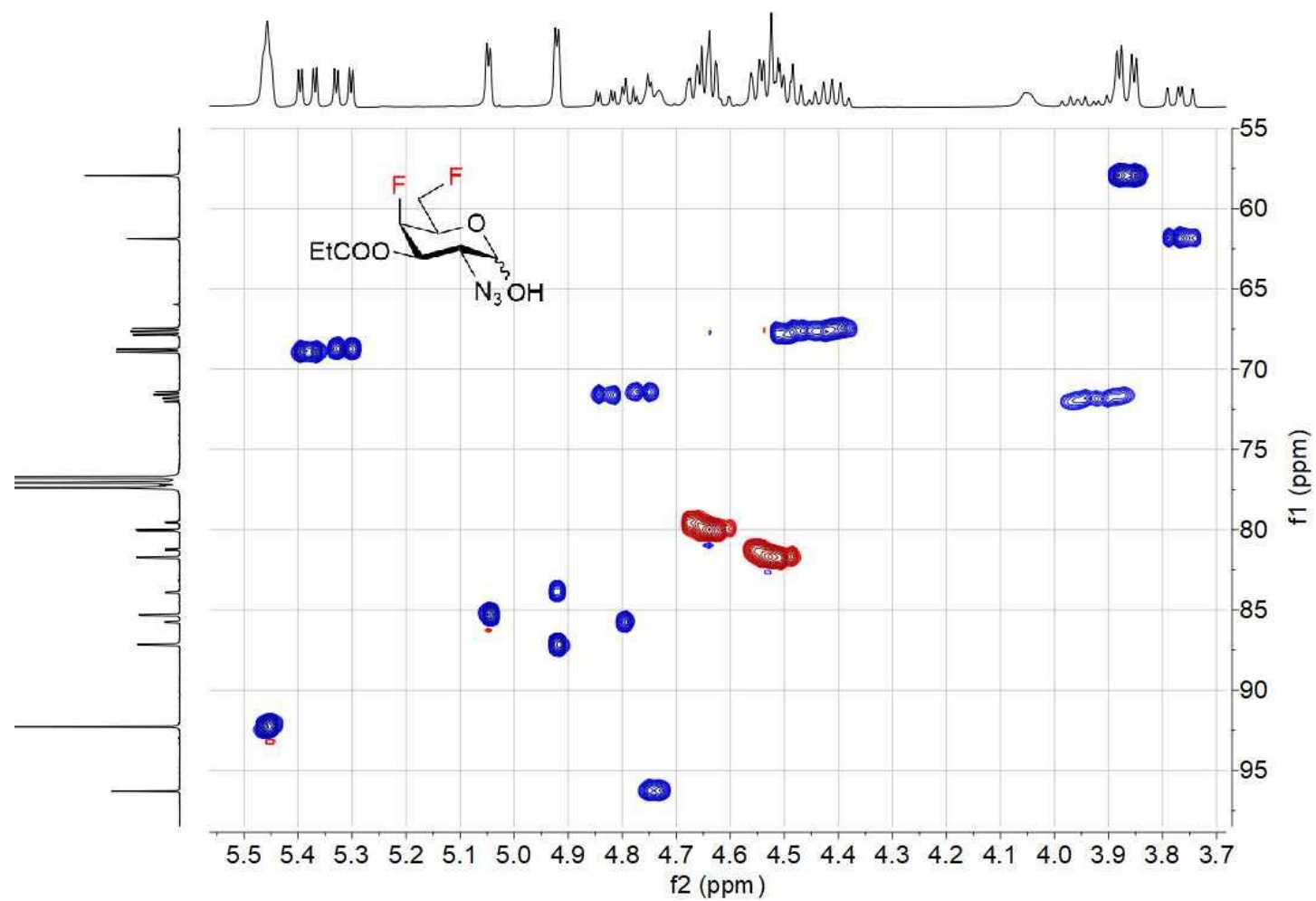
¹⁹F NMR (376 MHz, CDCl₃) 66



¹H-¹H COSY 66

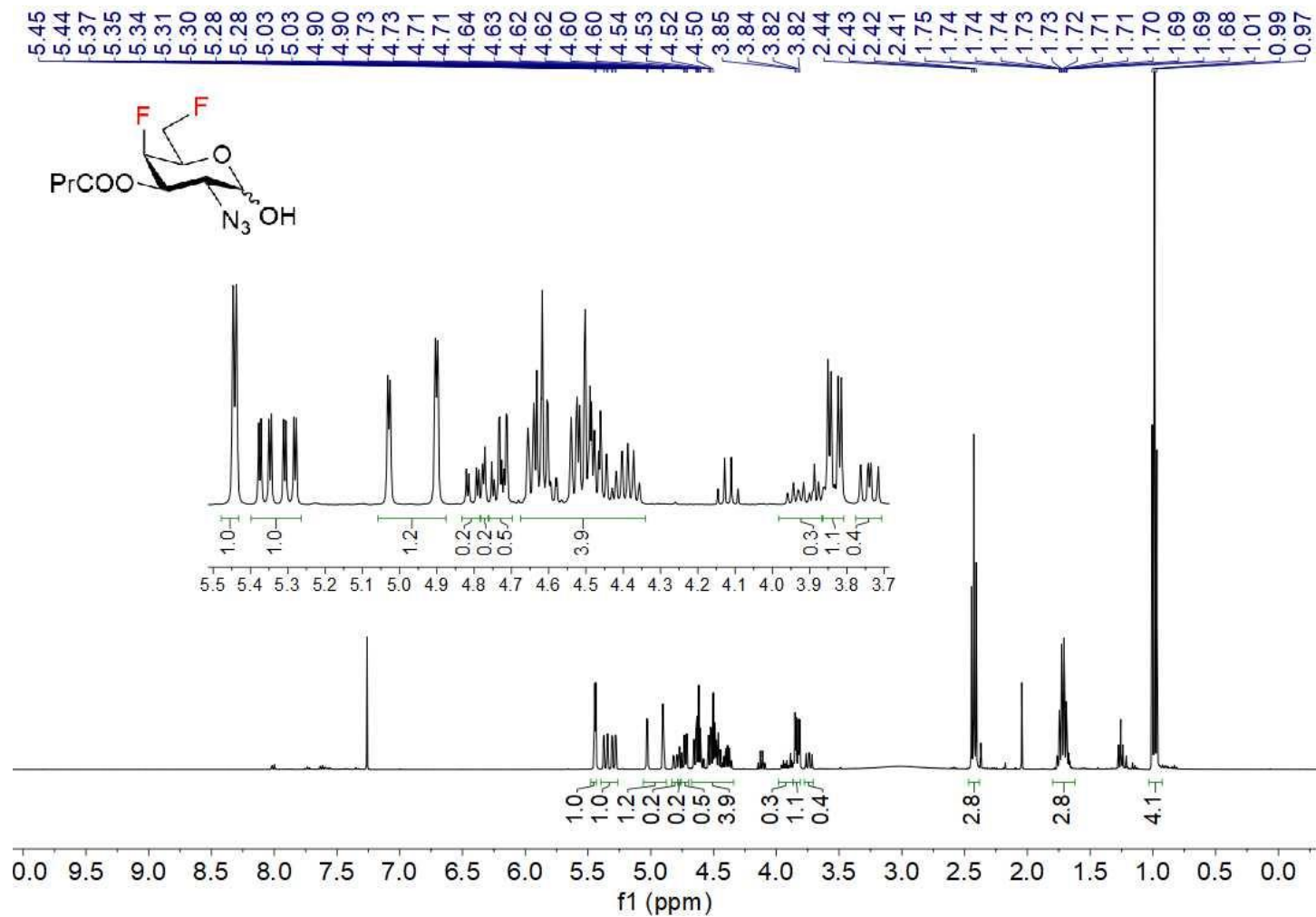


^1H - ^{13}C HSQC 66

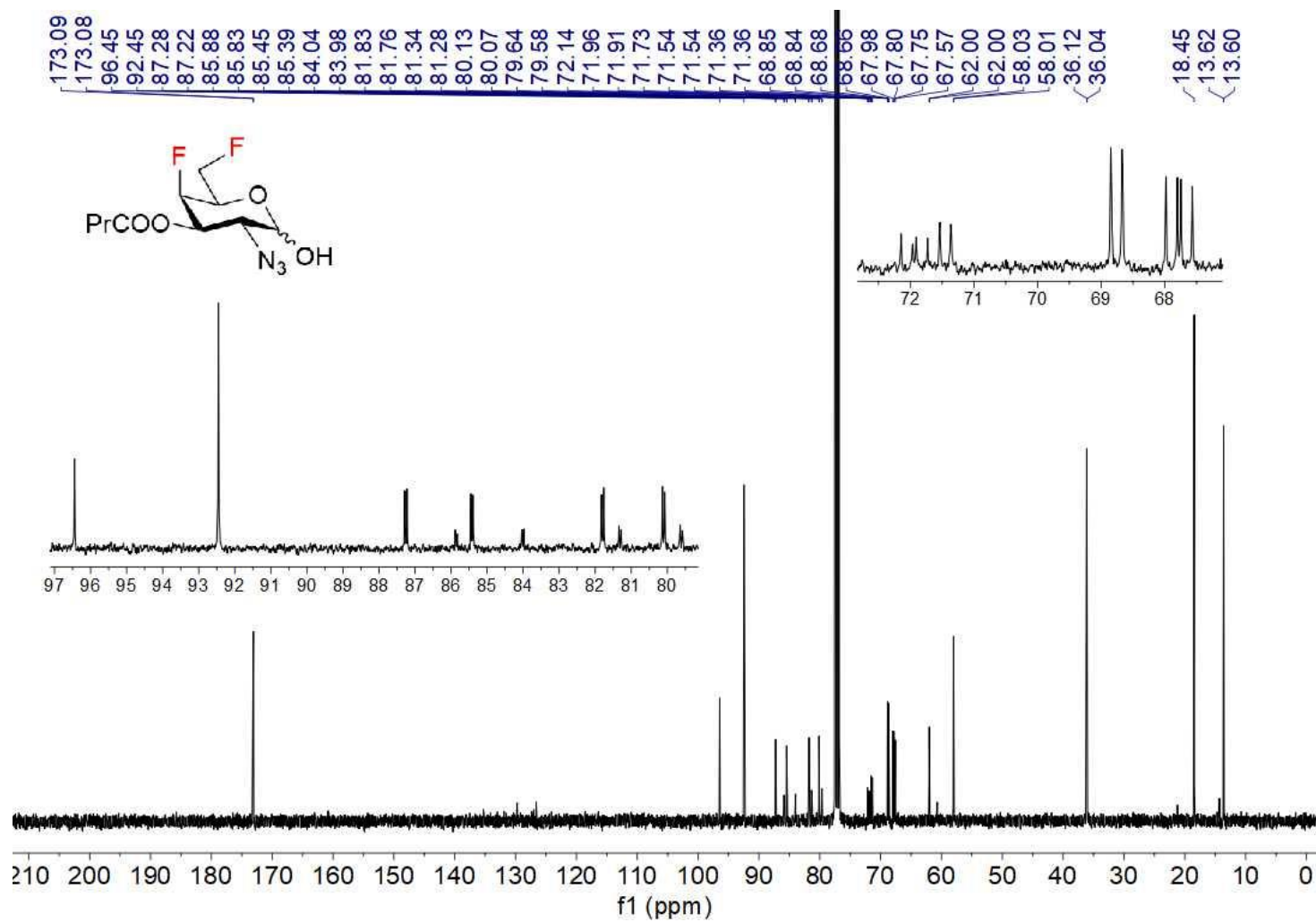


NMR COMPOUND 67

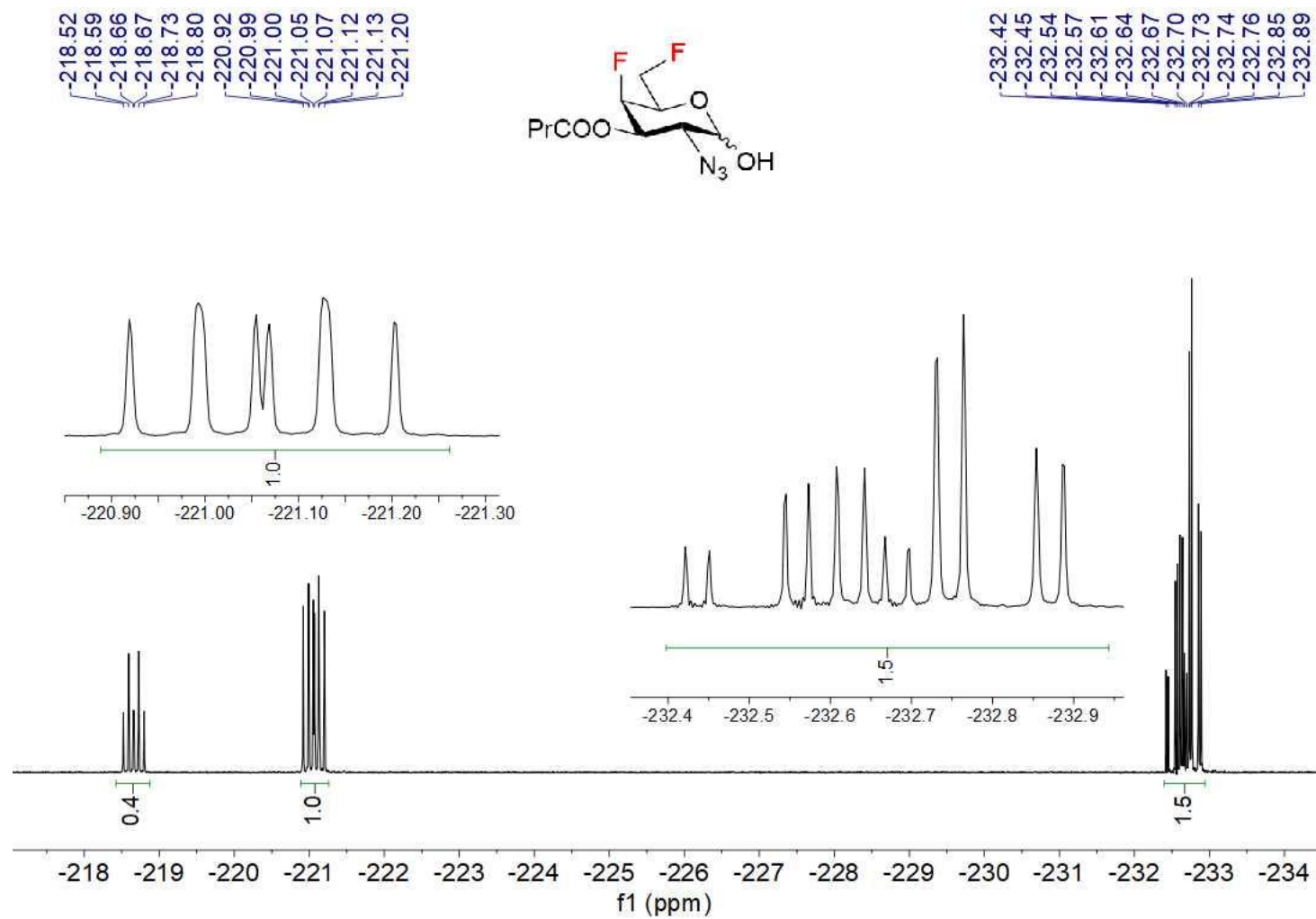
¹H NMR (400 MHz, CDCl₃) 67



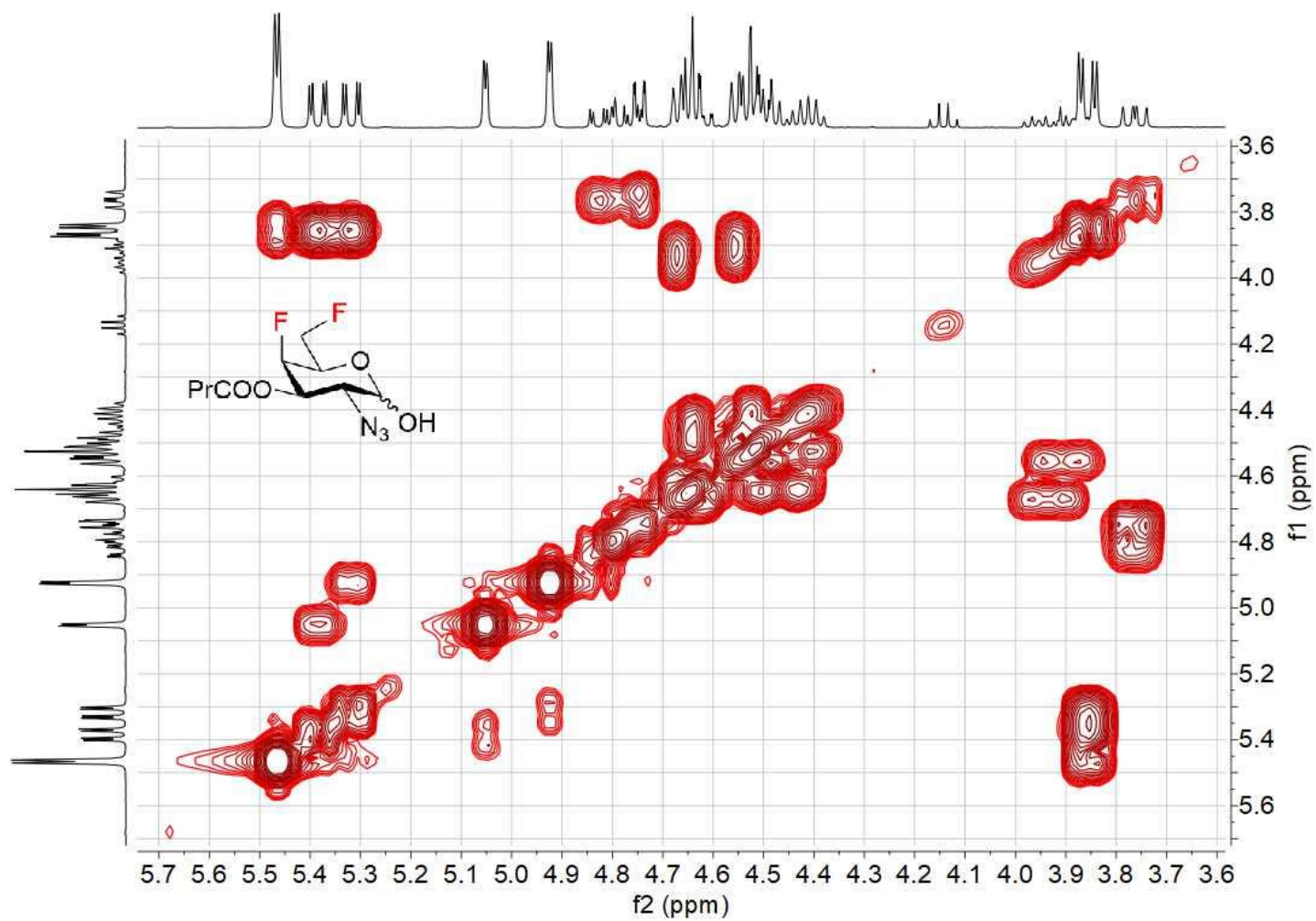
^{13}C NMR (100 MHz, CDCl_3) 67



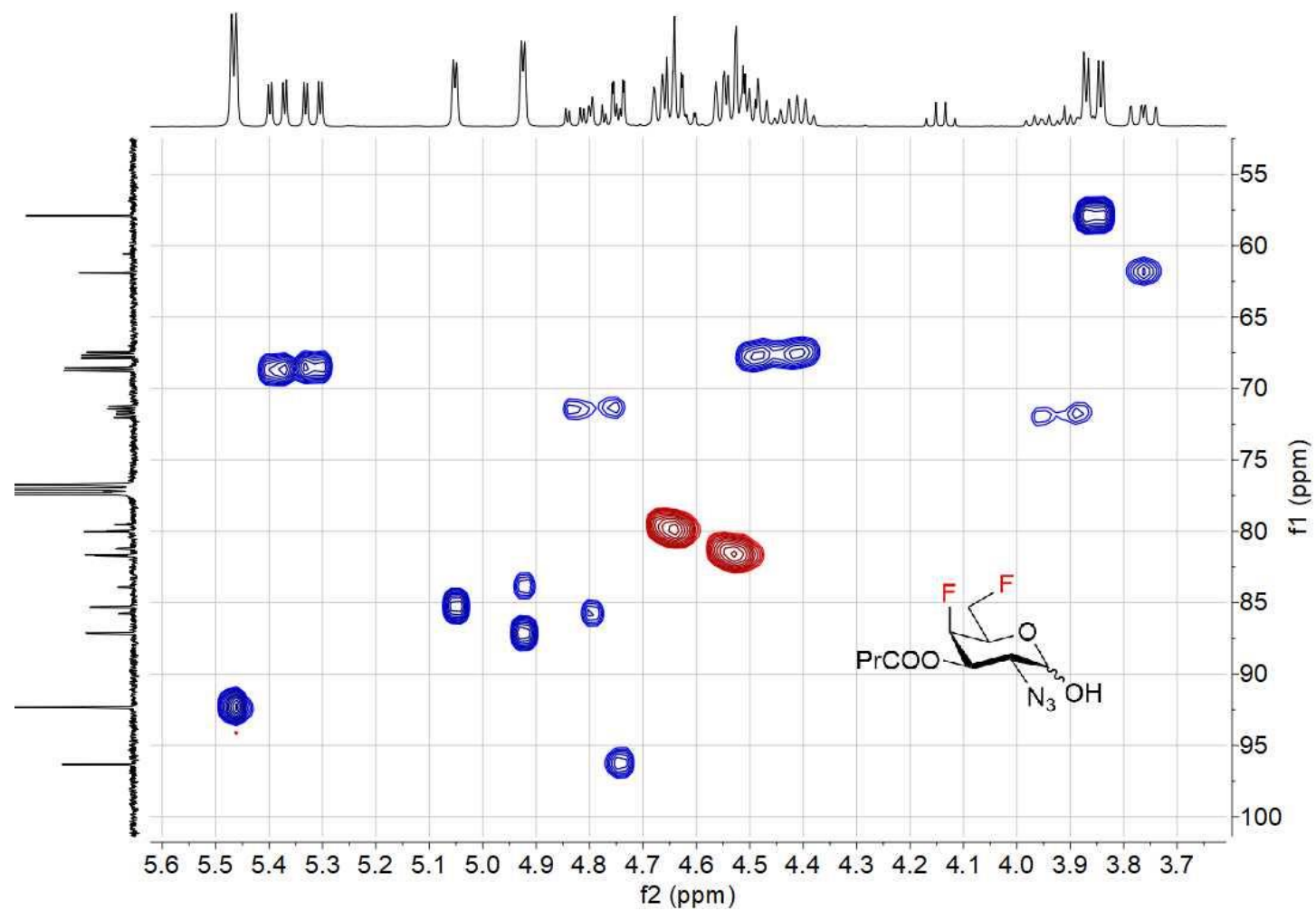
¹⁹F NMR (376 MHz, CDCl₃) 67



¹H-¹H COSY 67

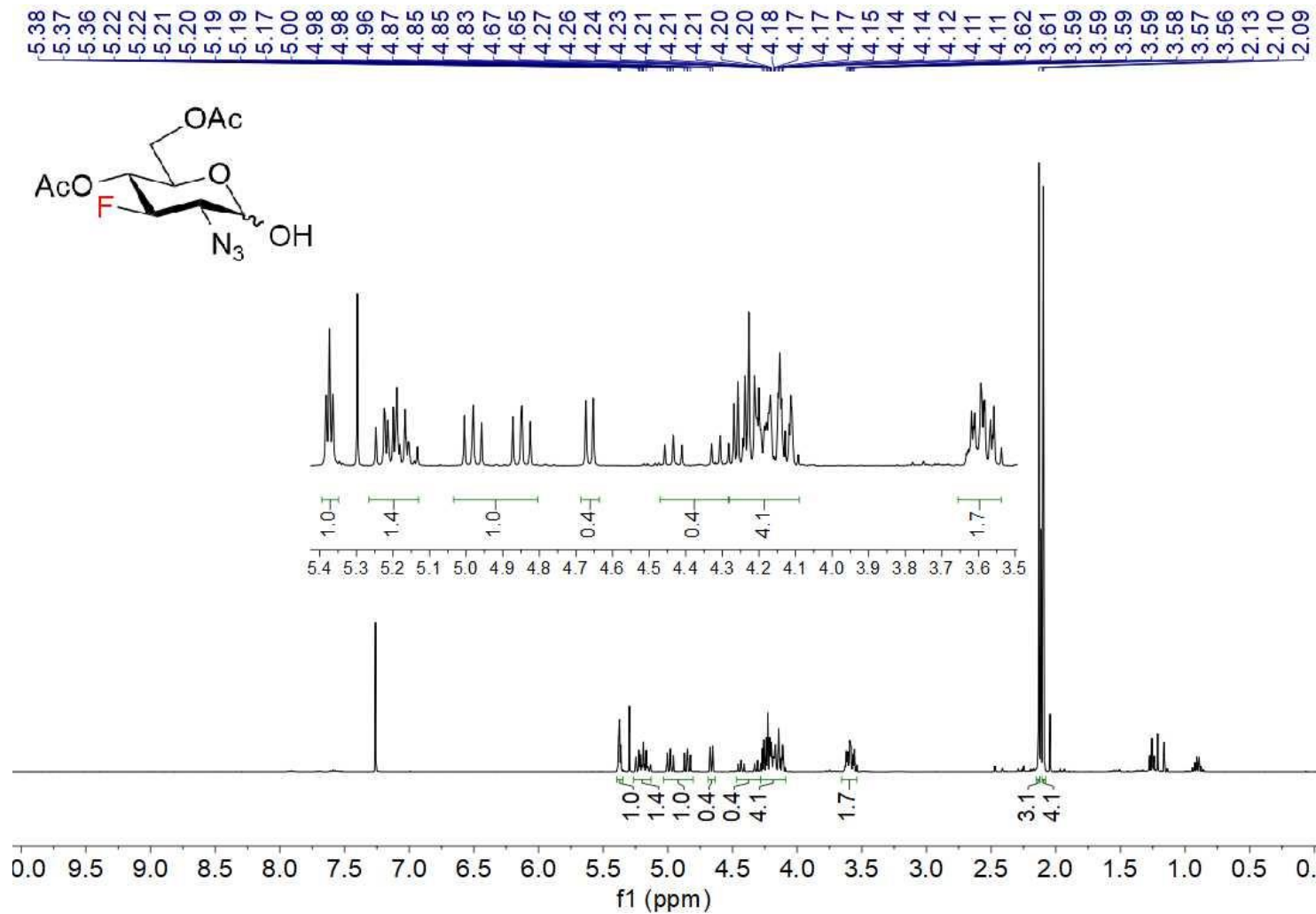


^1H - ^{13}C HSQC 67

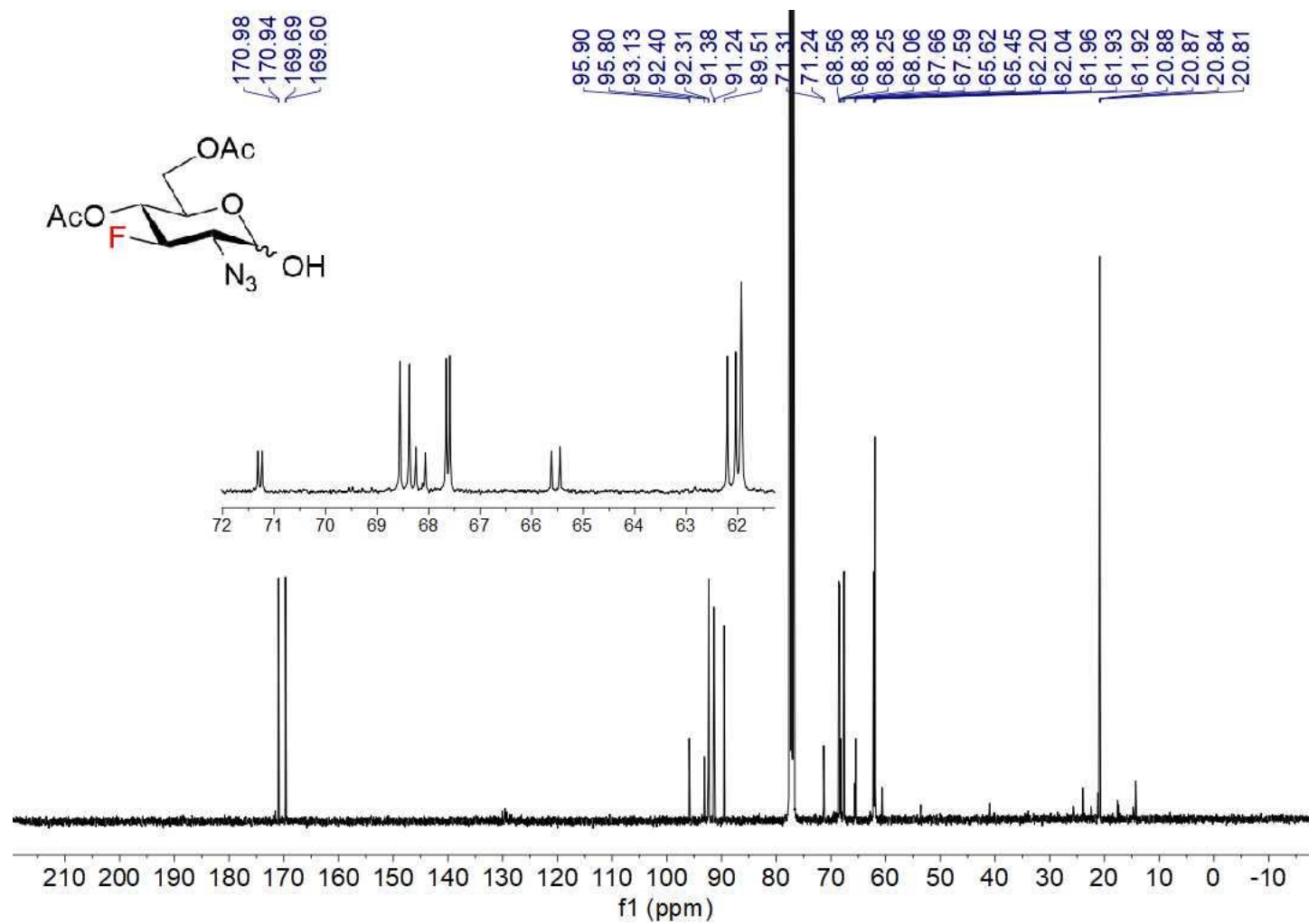


NMR COMPOUND 68

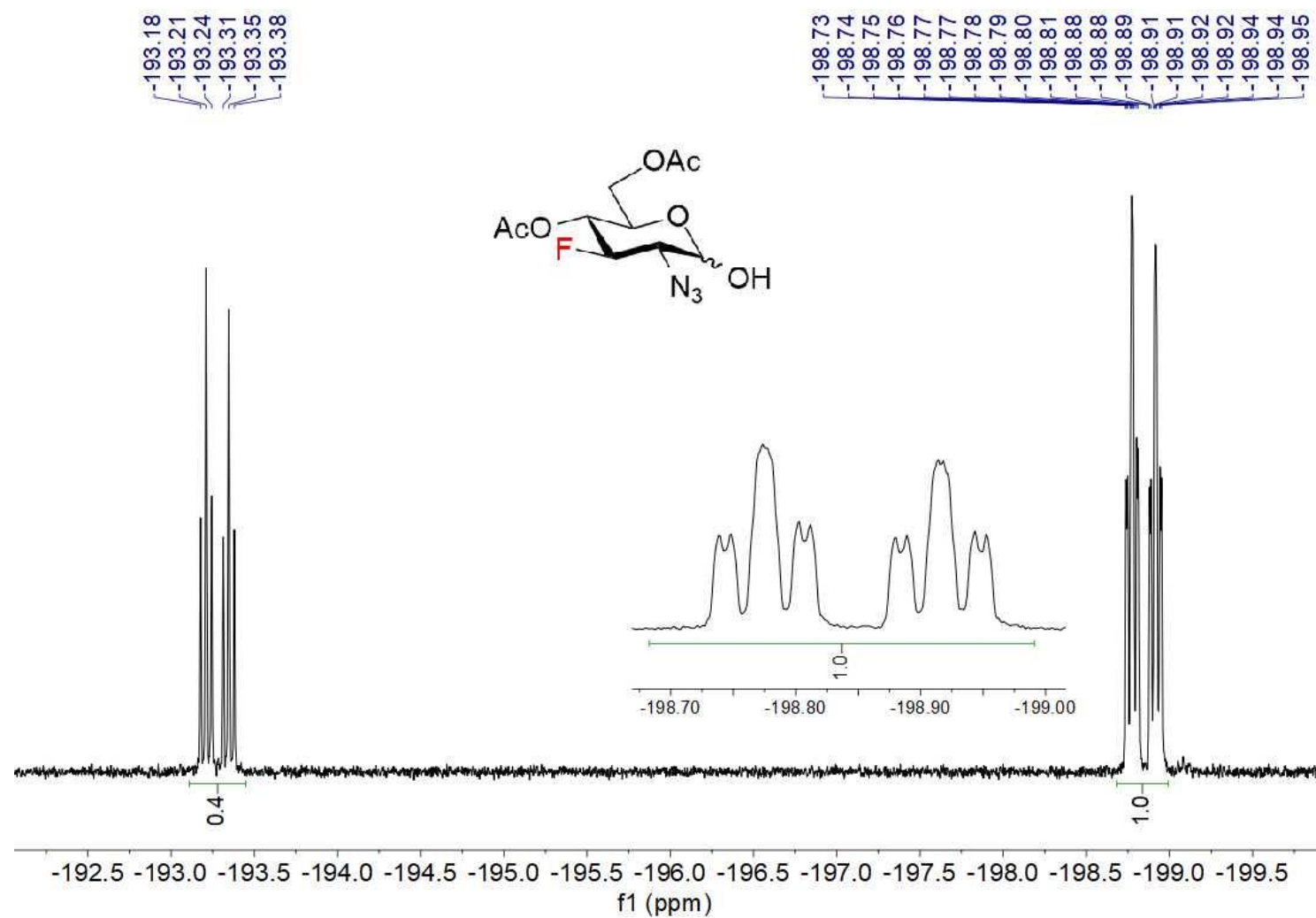
¹H NMR (400 MHz, CDCl₃) 68



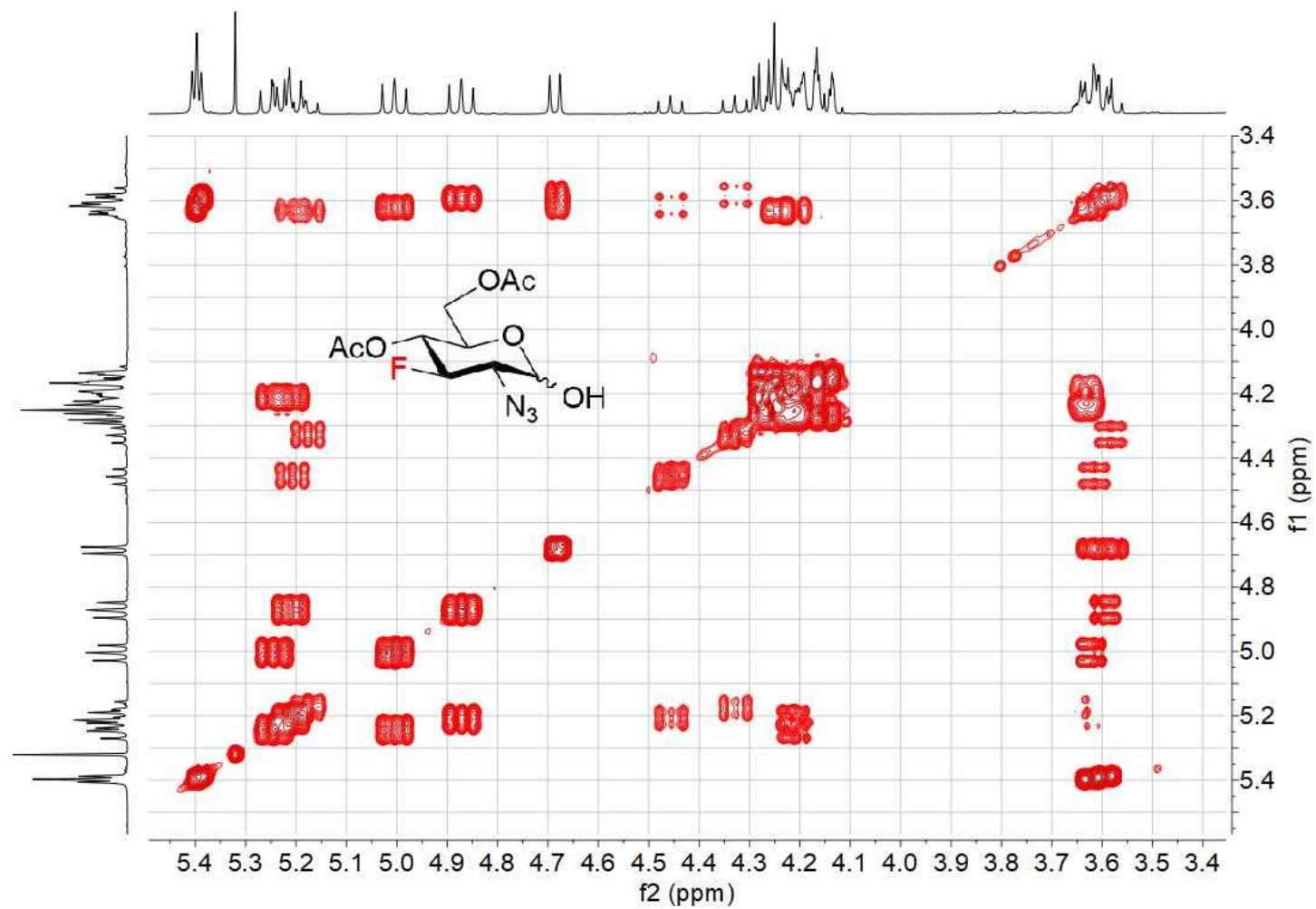
^{13}C NMR (100 MHz, CDCl_3) 68



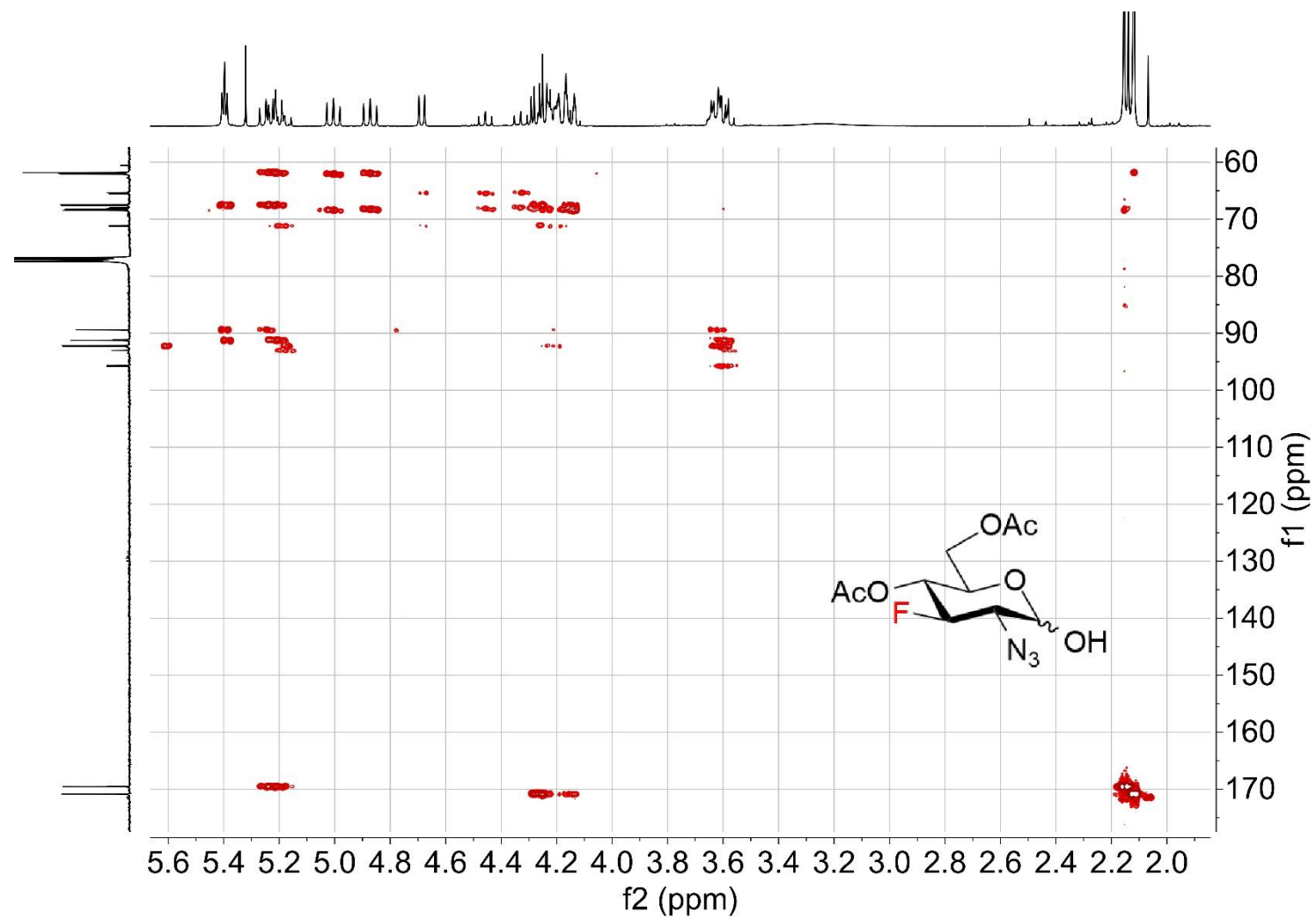
¹⁹F NMR (376 MHz, CDCl₃) 68



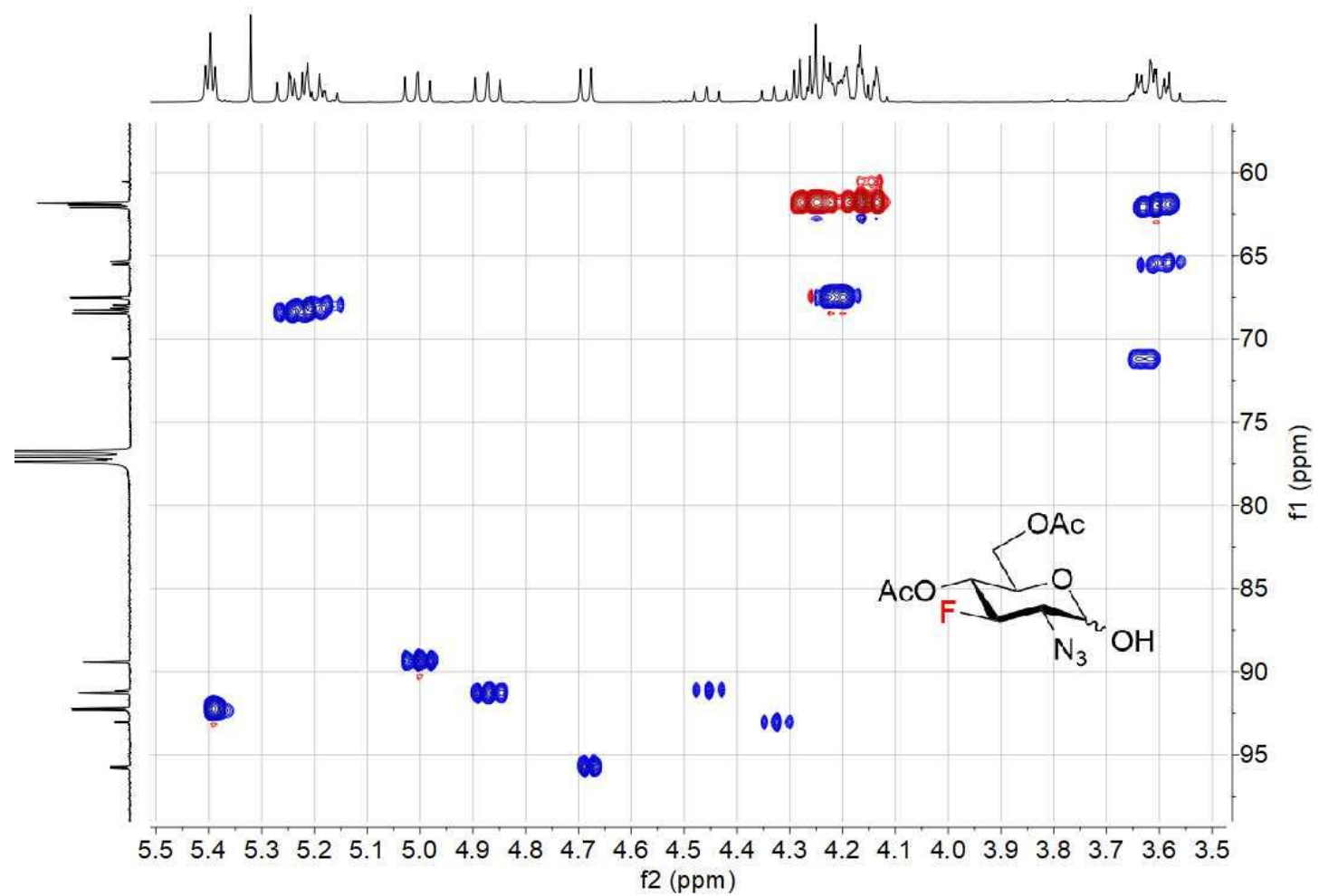
¹H-¹H COSY 68



^1H - ^{13}C HMBC 68

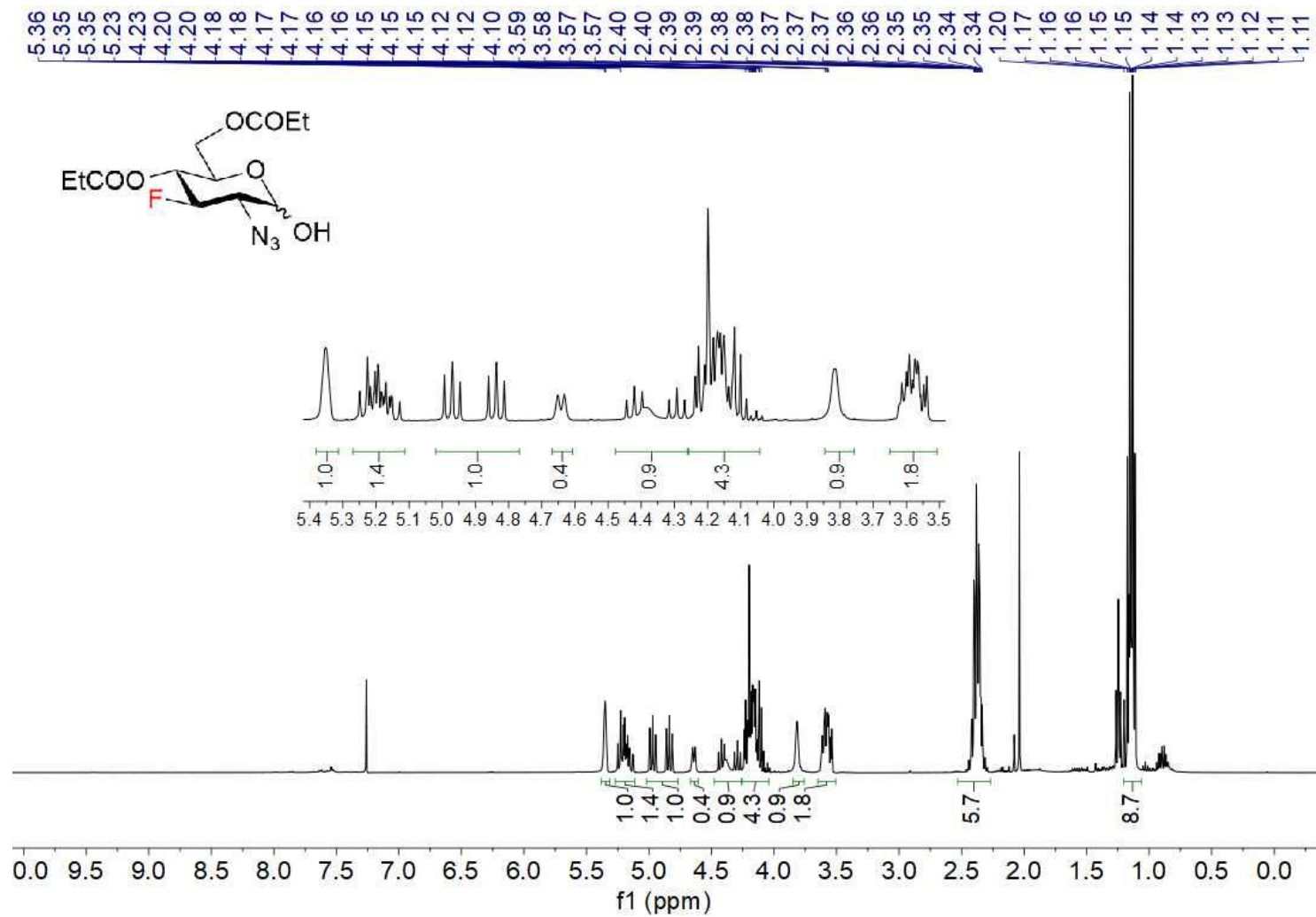


^1H - ^{13}C HSQC 68

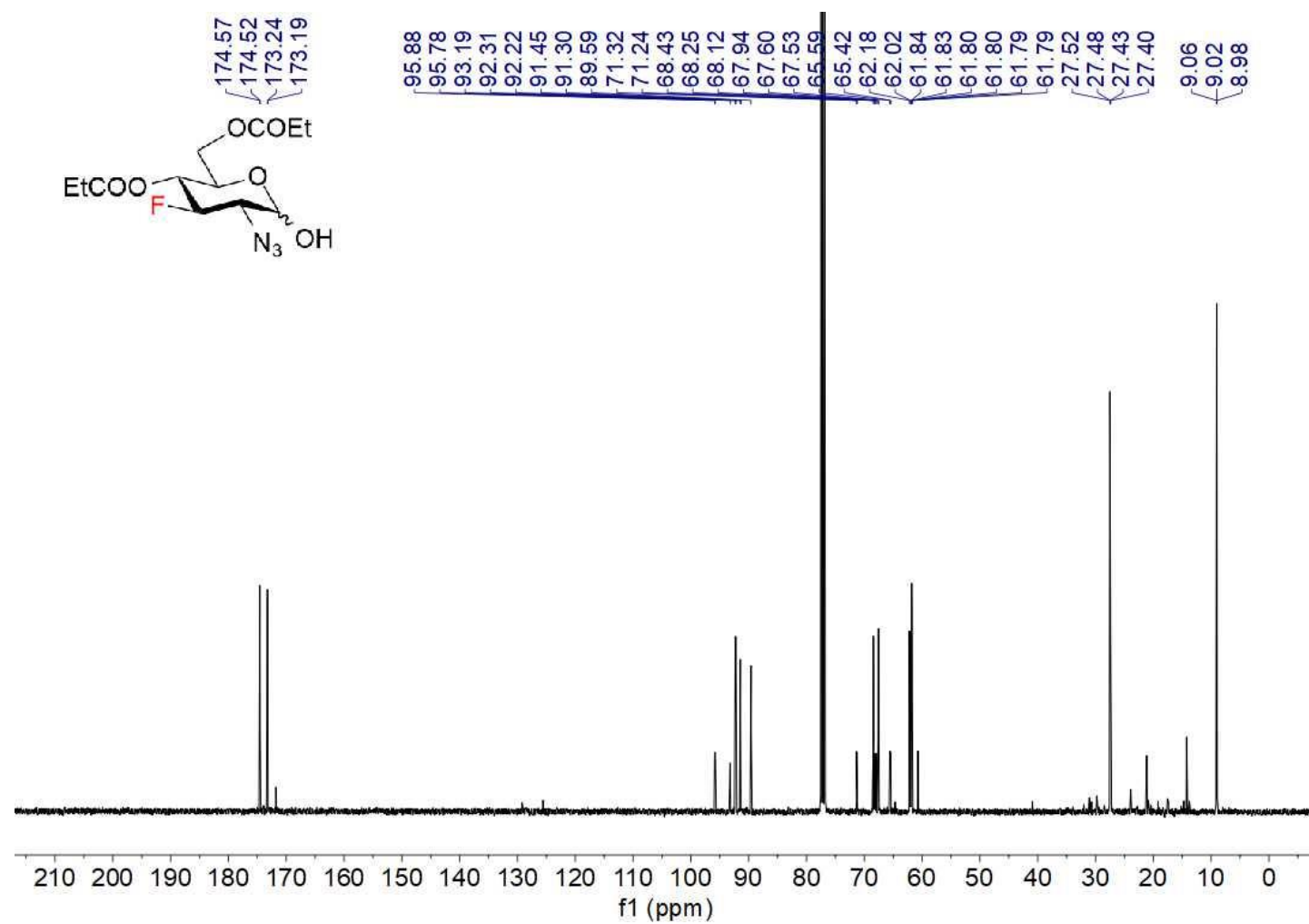


NMR COMPOUND 69

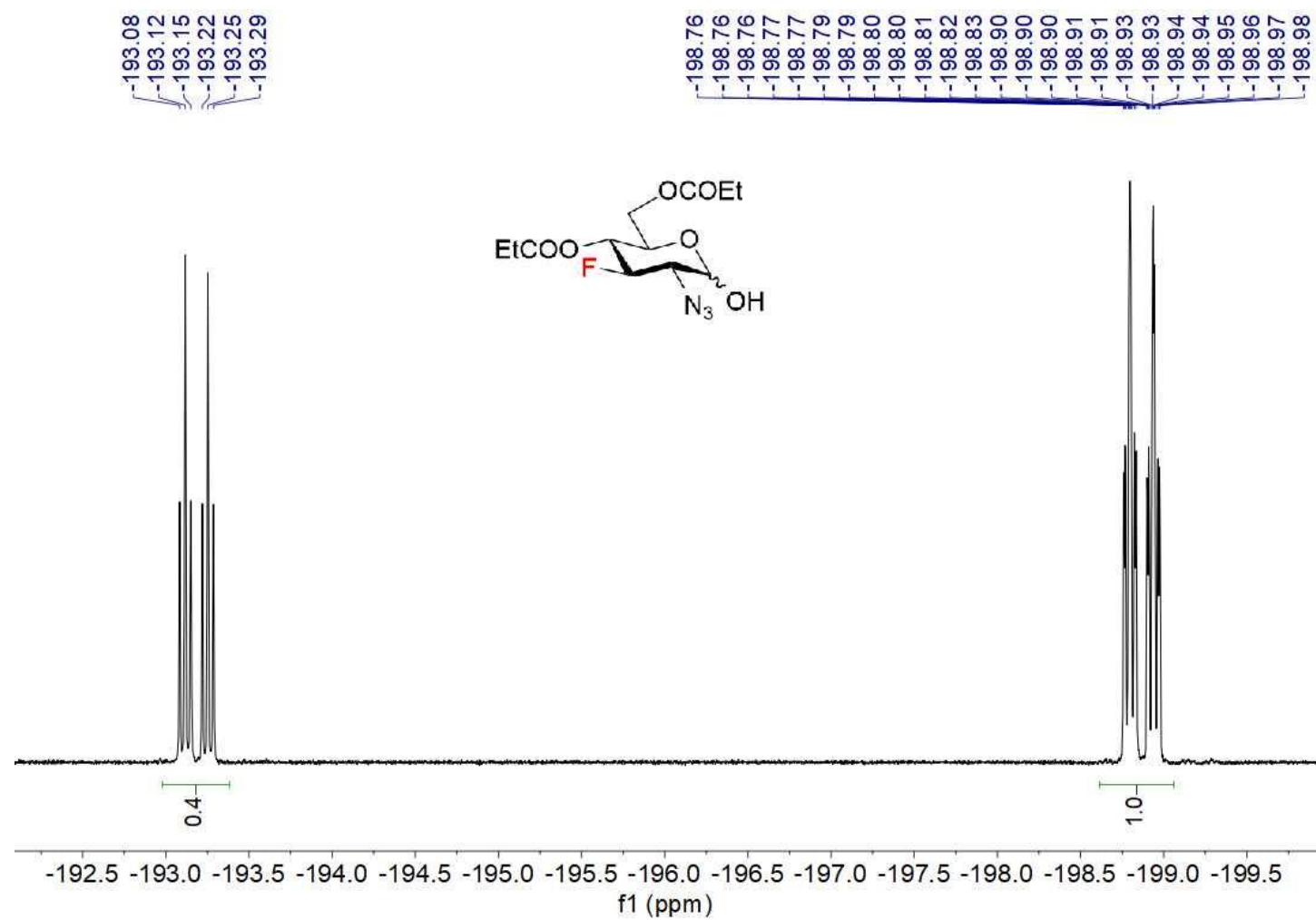
^1H NMR (400 MHz, CDCl_3) 69



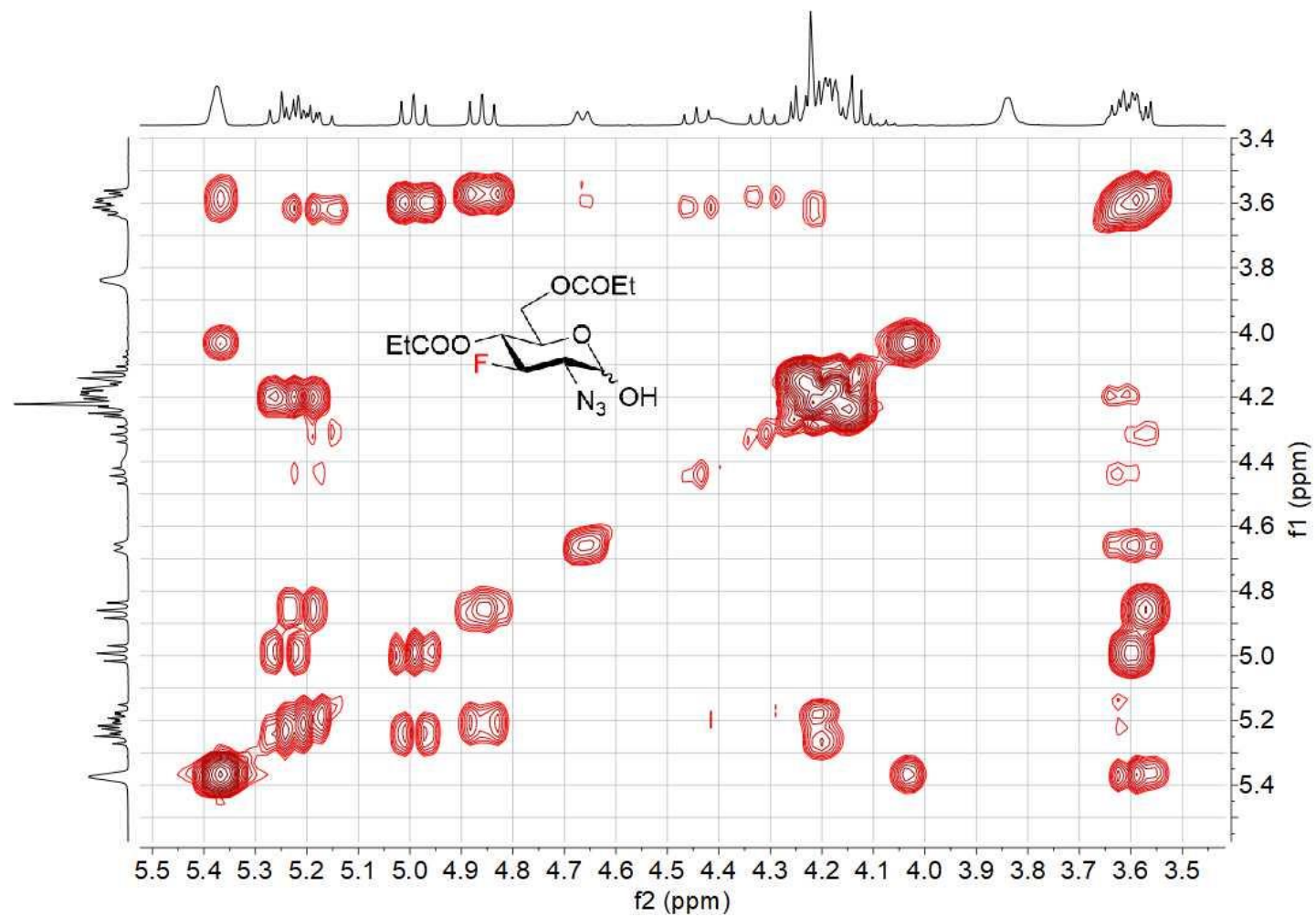
^{13}C NMR (100 MHz, CDCl_3) 69



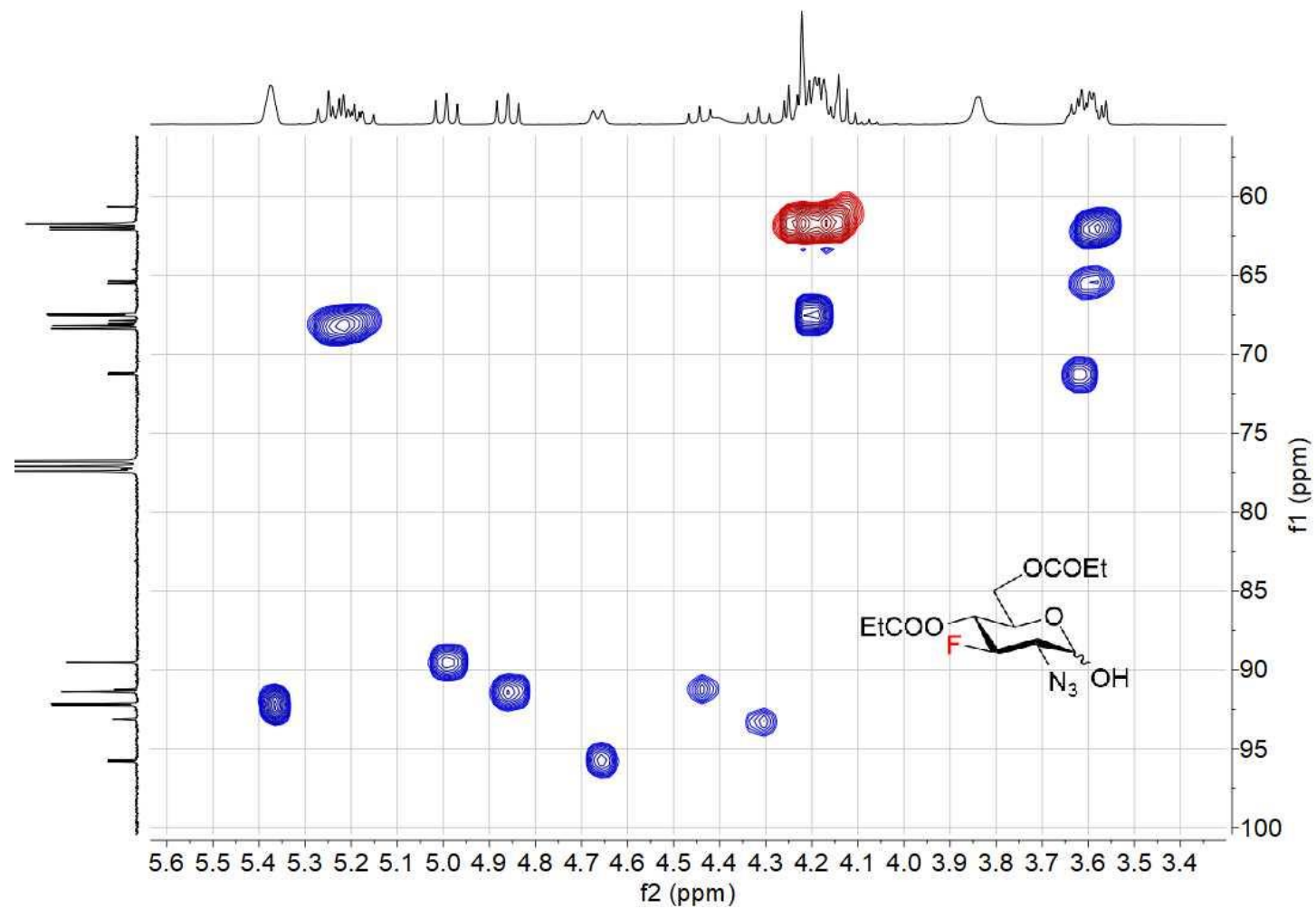
¹⁹F NMR (376 MHz, CDCl₃) 69



¹H-¹H COSY 69

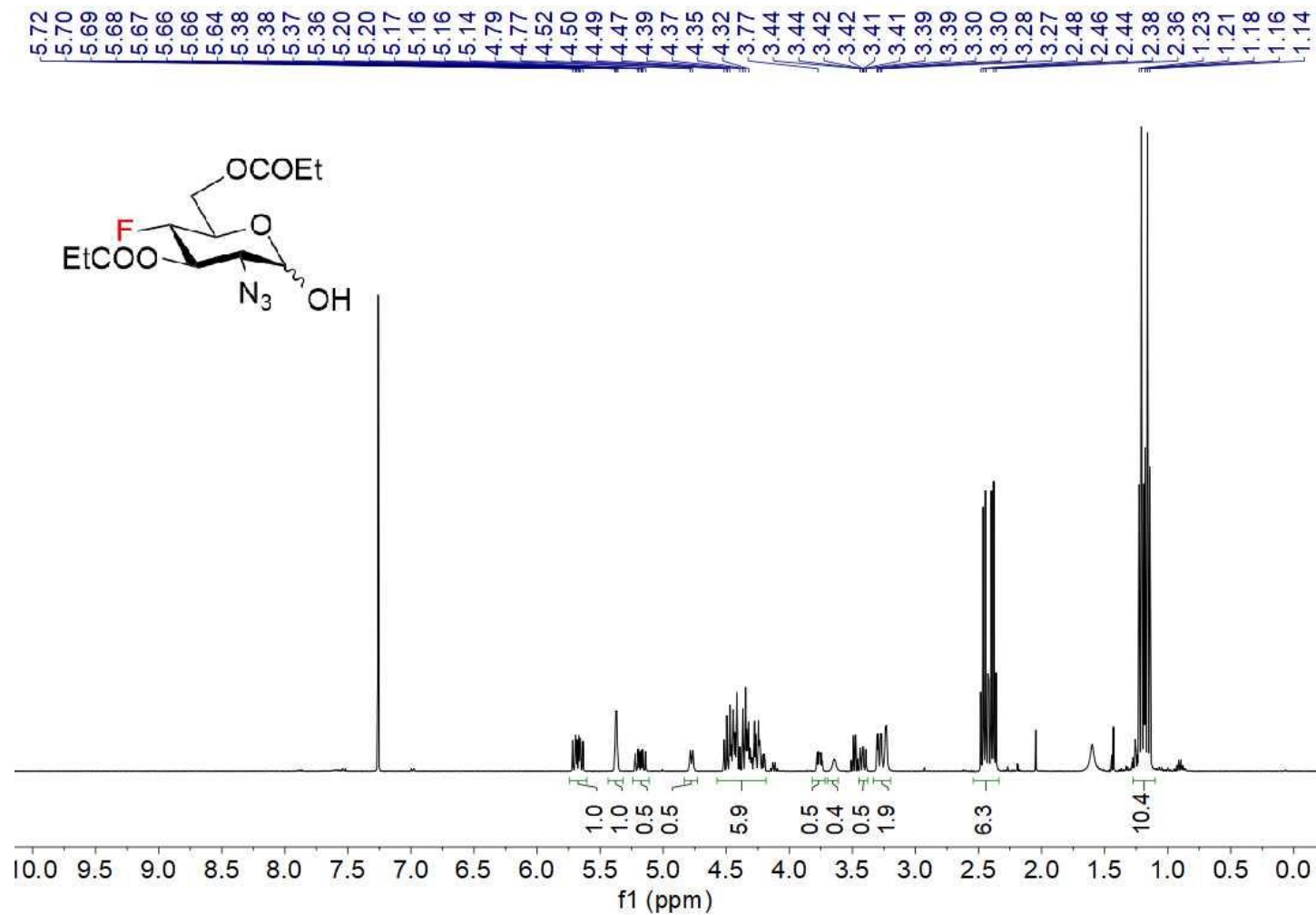


^1H - ^{13}C HSQC 69

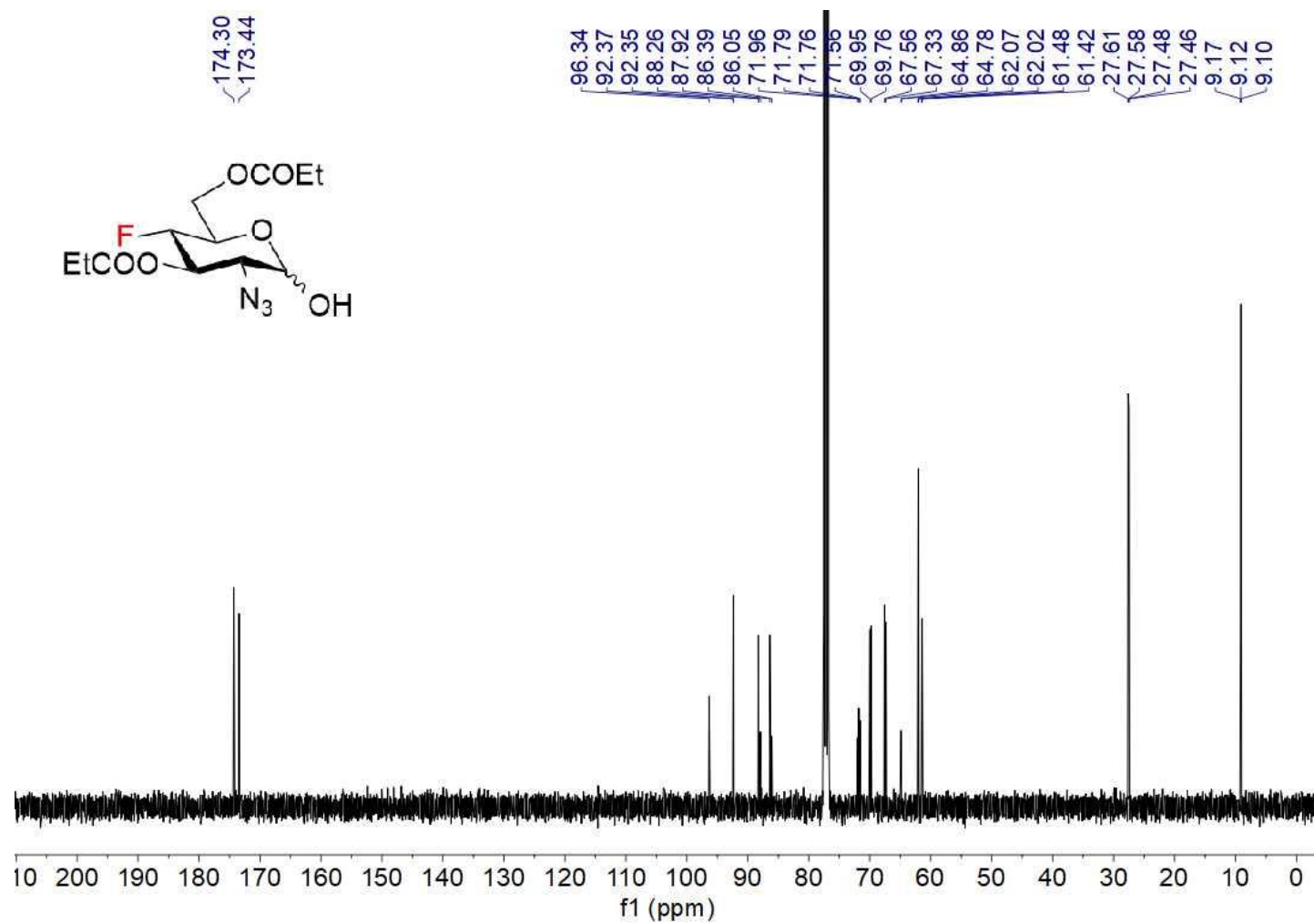


NMR COMPOUND 70

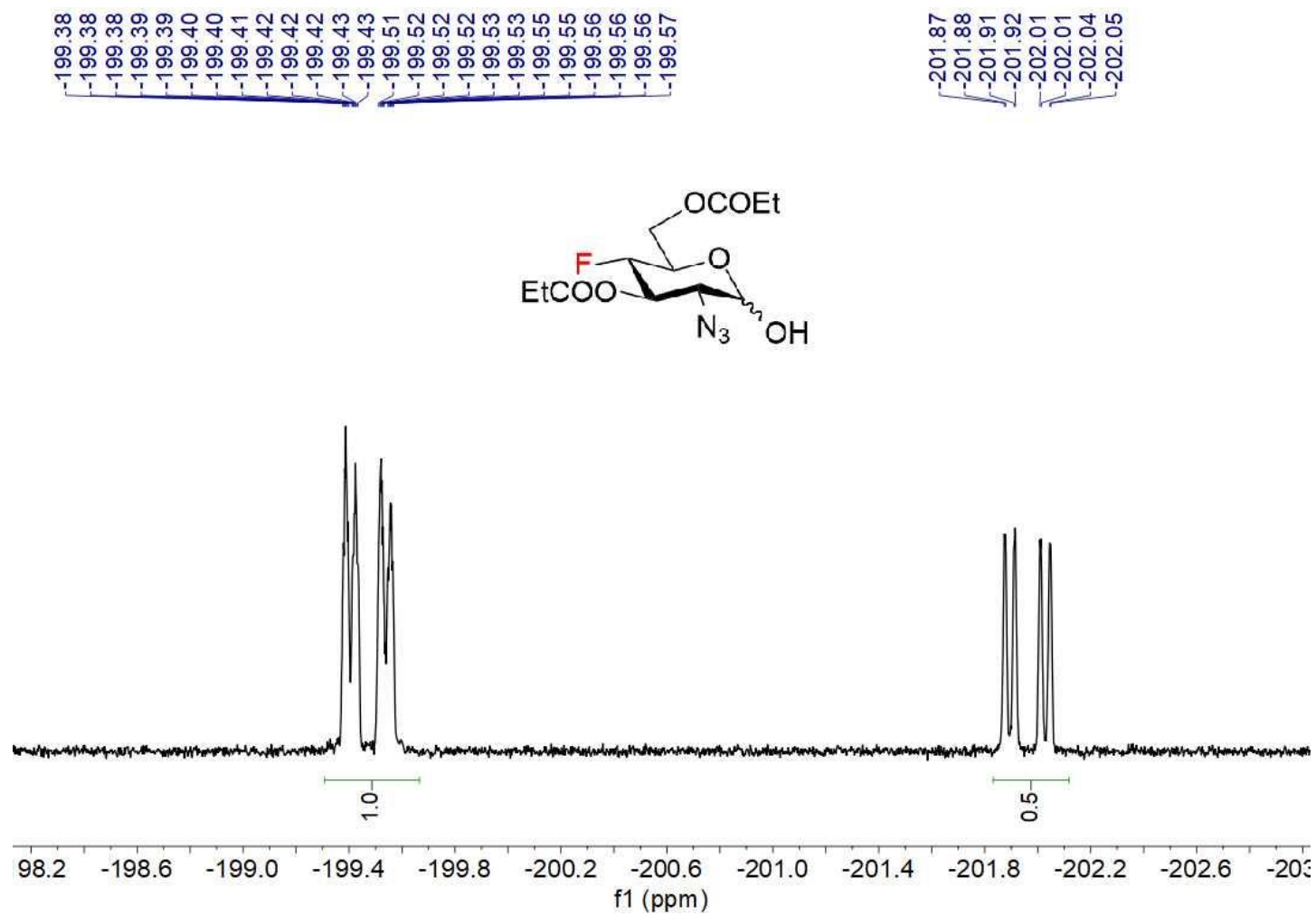
¹H NMR (400 MHz, CDCl₃) 70



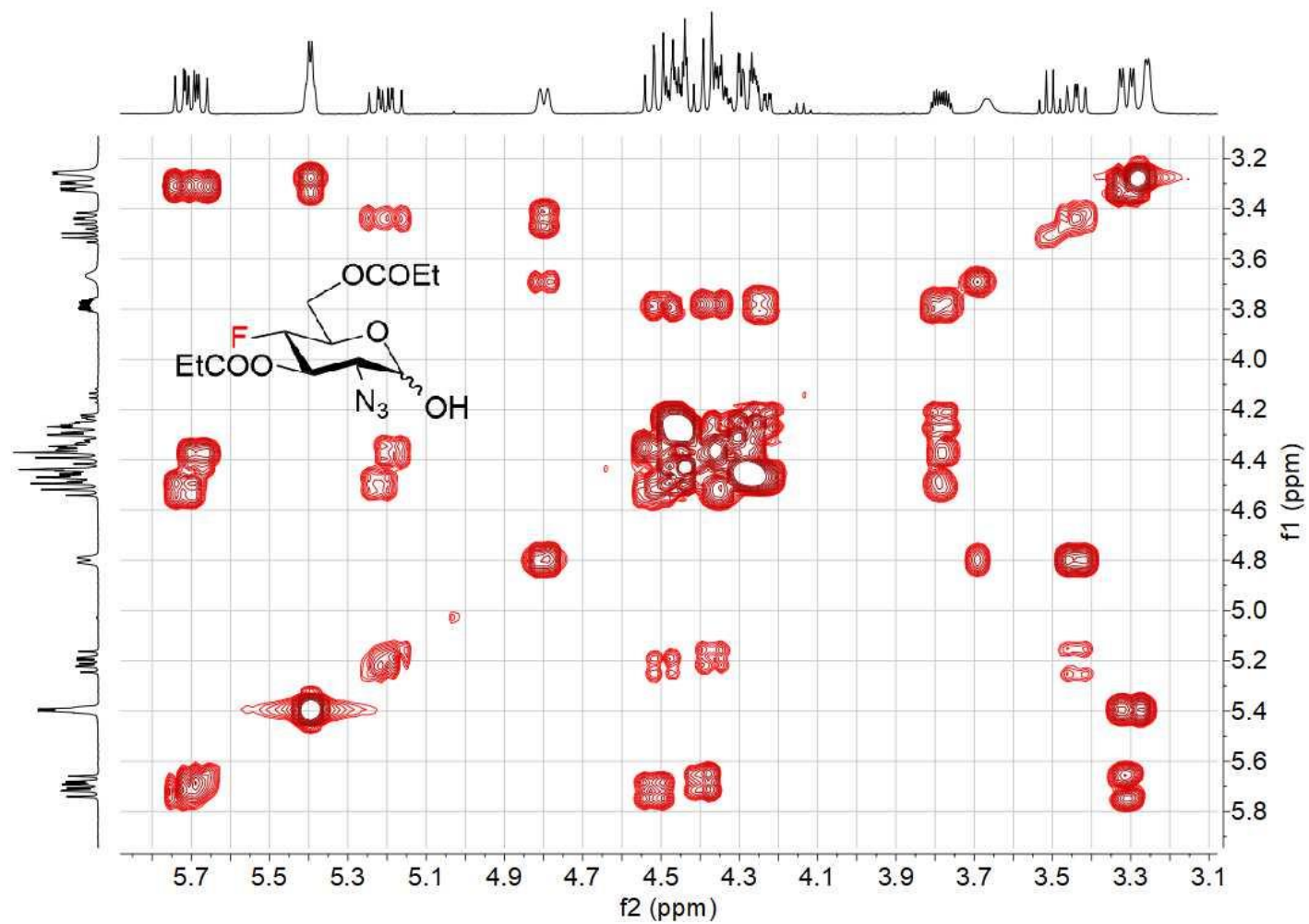
^{13}C NMR (100 MHz, CDCl_3) 70



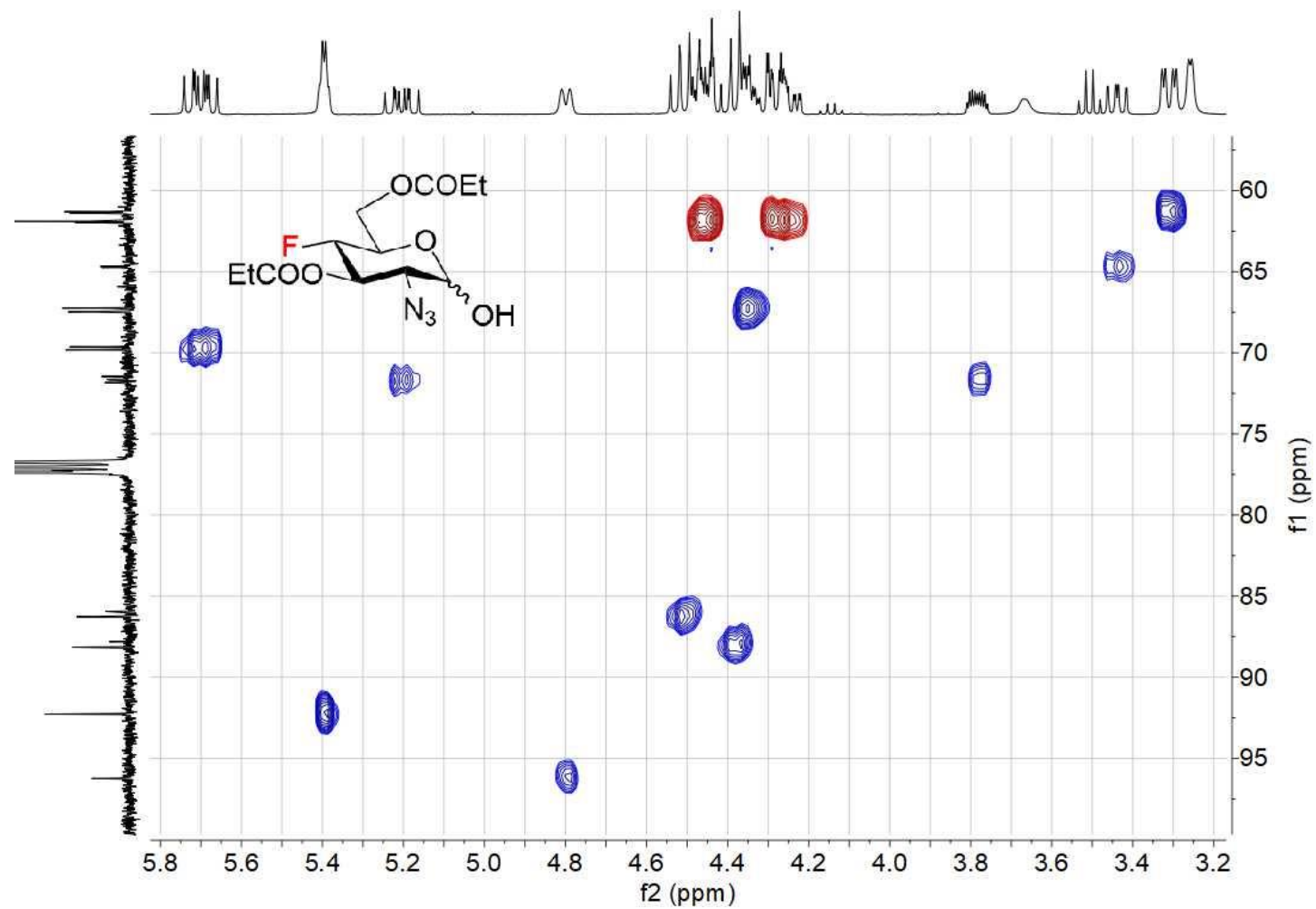
^{19}F NMR (376 MHz, CDCl_3) 70



^1H - ^1H COSY 70

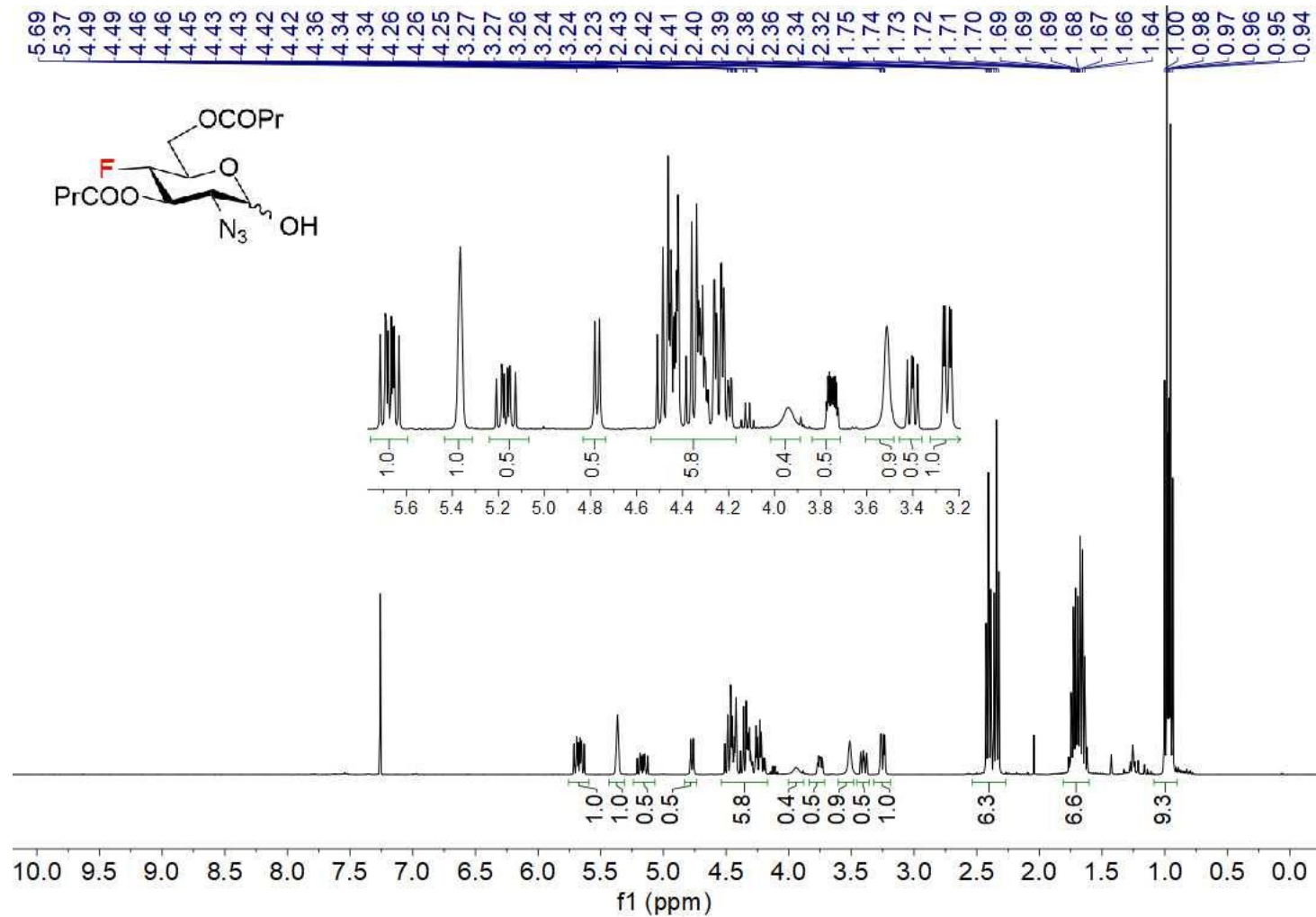


^1H - ^{13}C HSQC 70

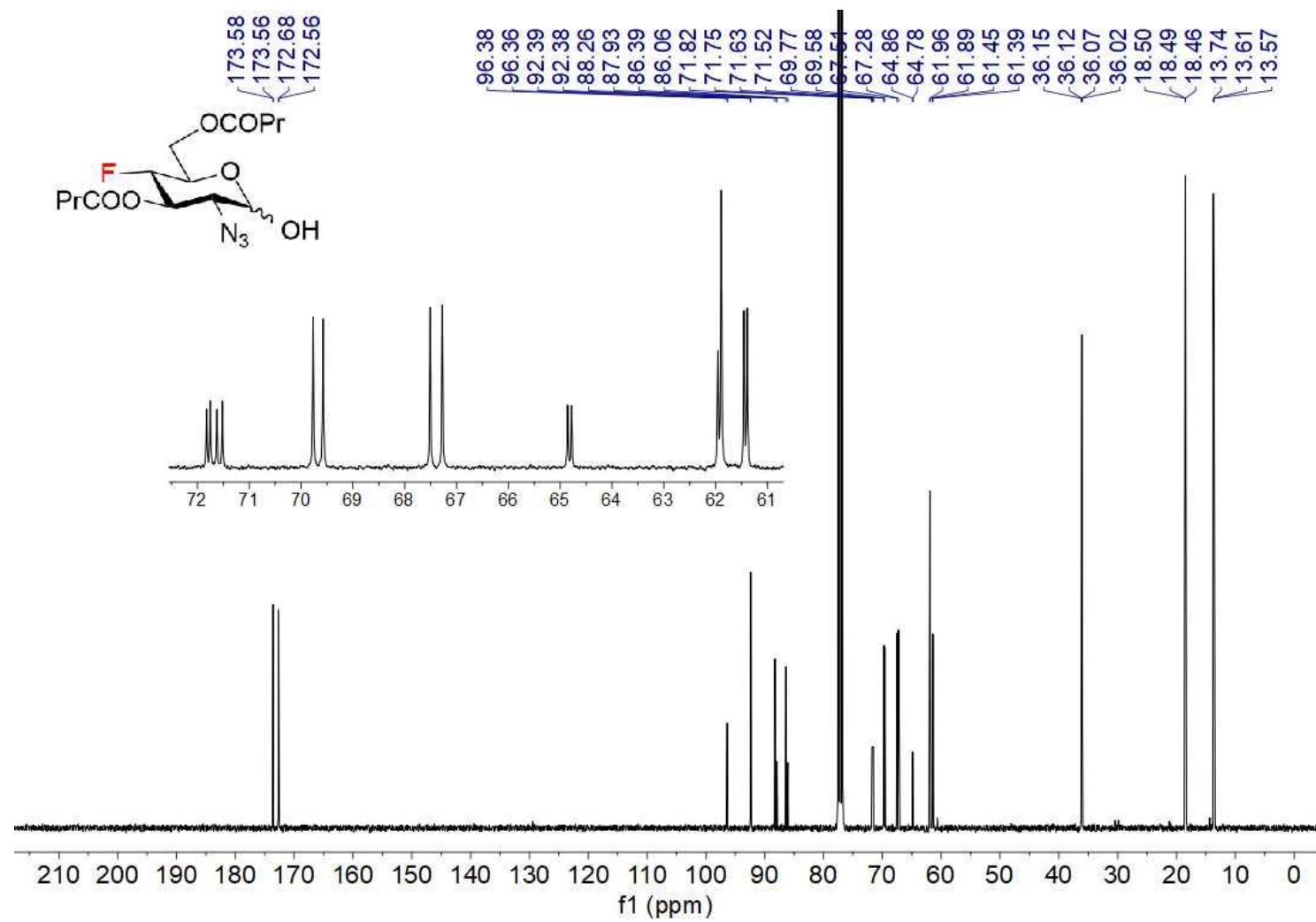


NMR COMPOUND 71

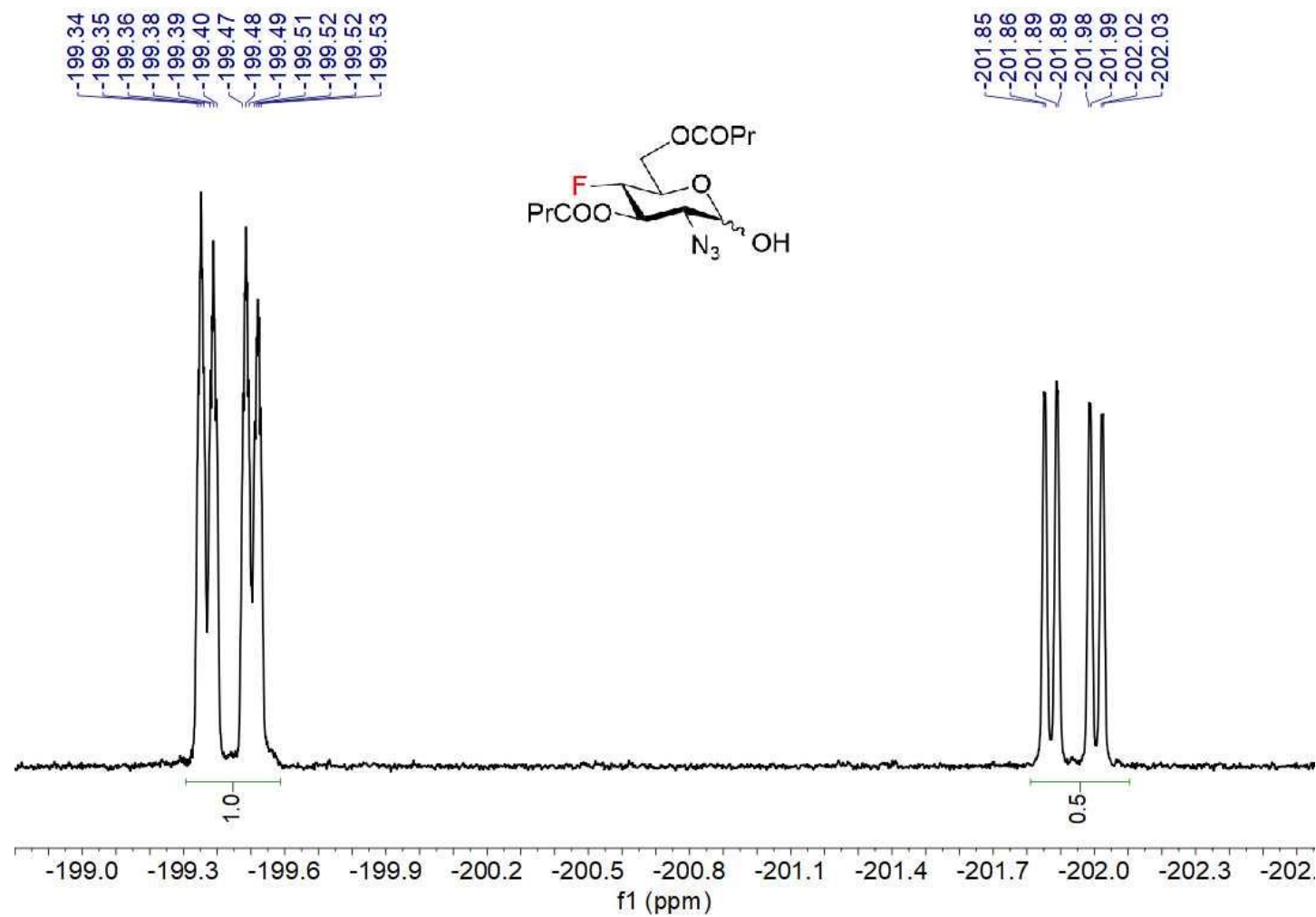
¹H NMR (400 MHz, CDCl₃) 71



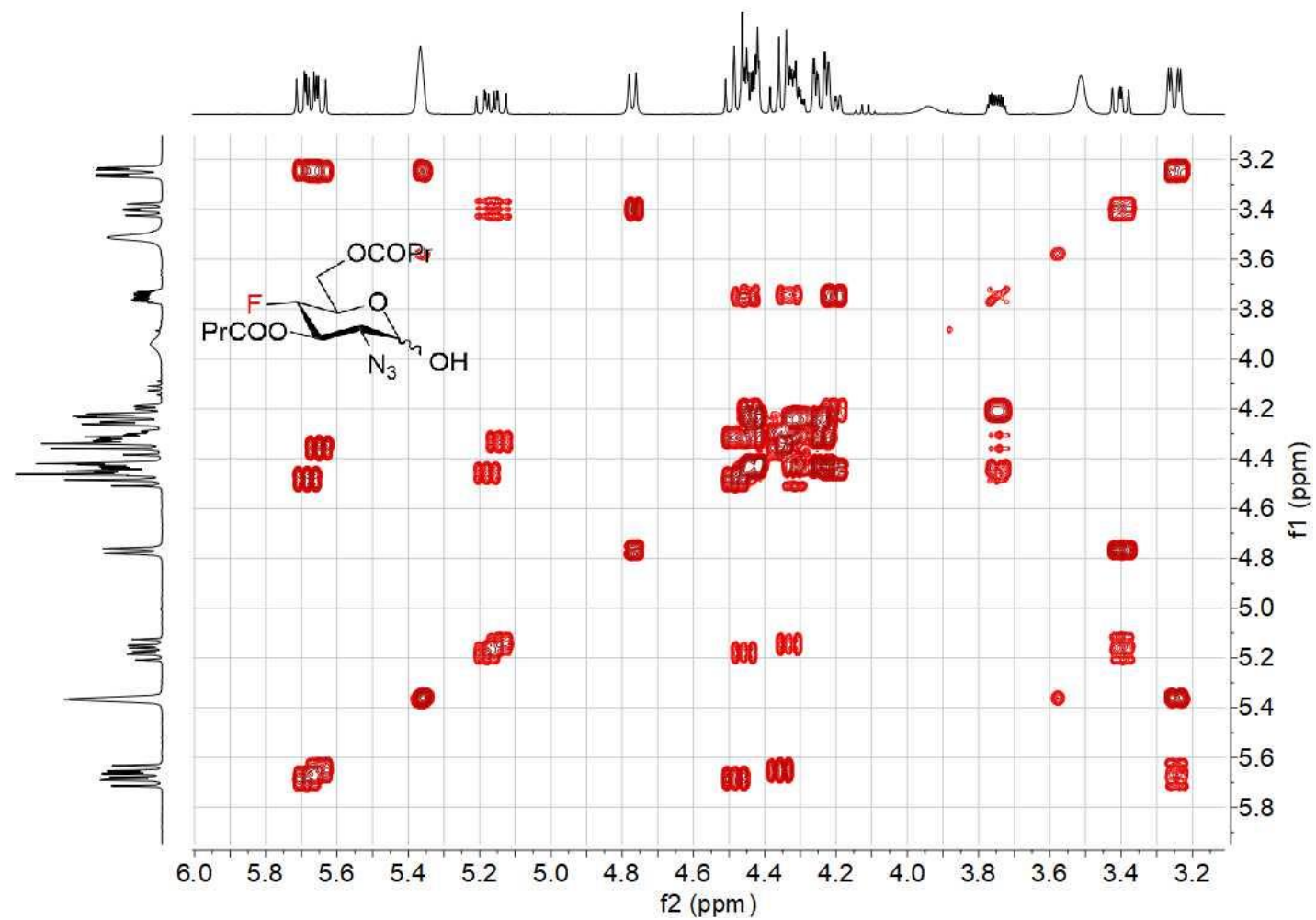
¹³C NMR (100 MHz, CDCl₃) 71



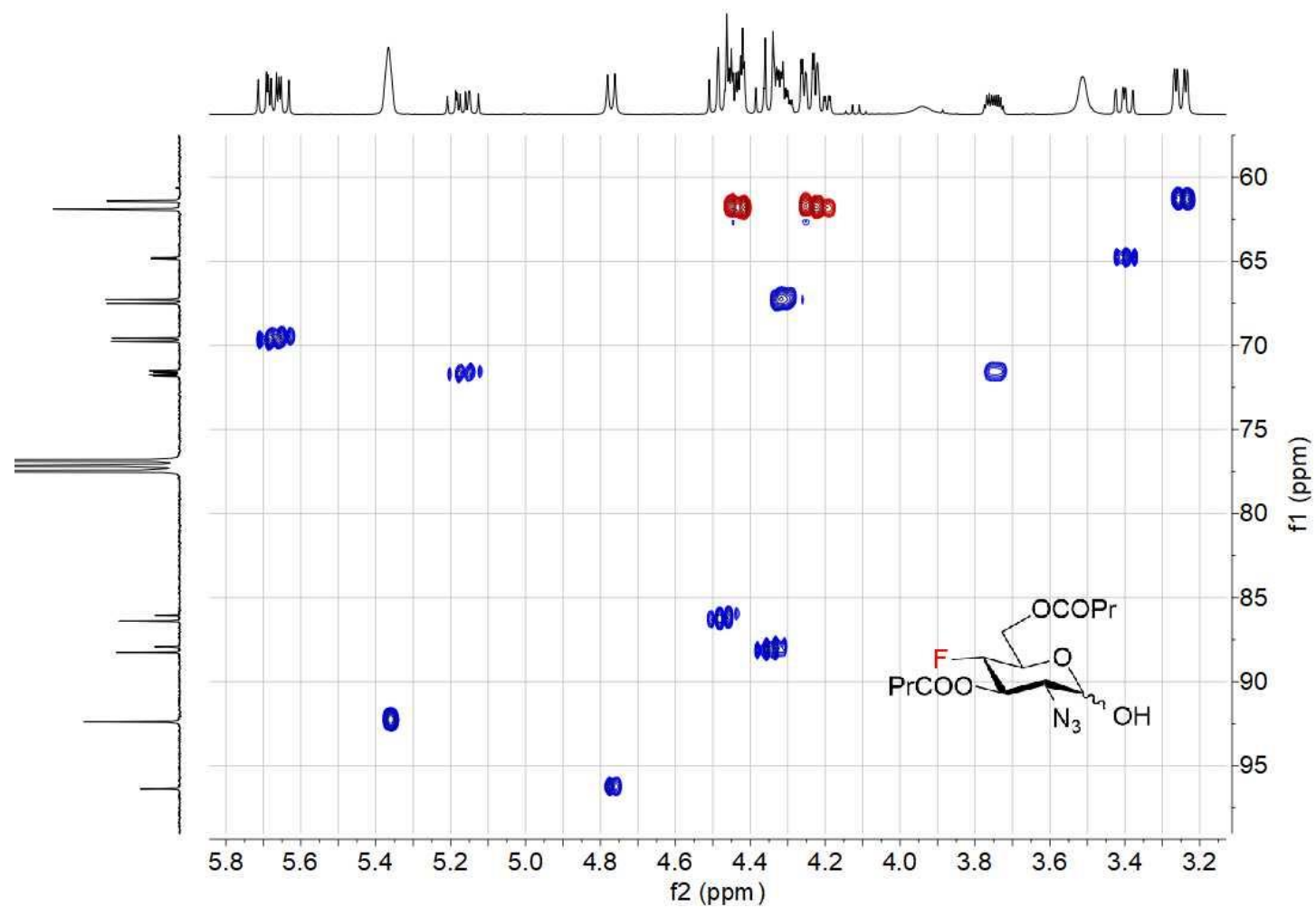
^{19}F NMR (376 MHz, CDCl_3) 71



^1H - ^1H COSY 71

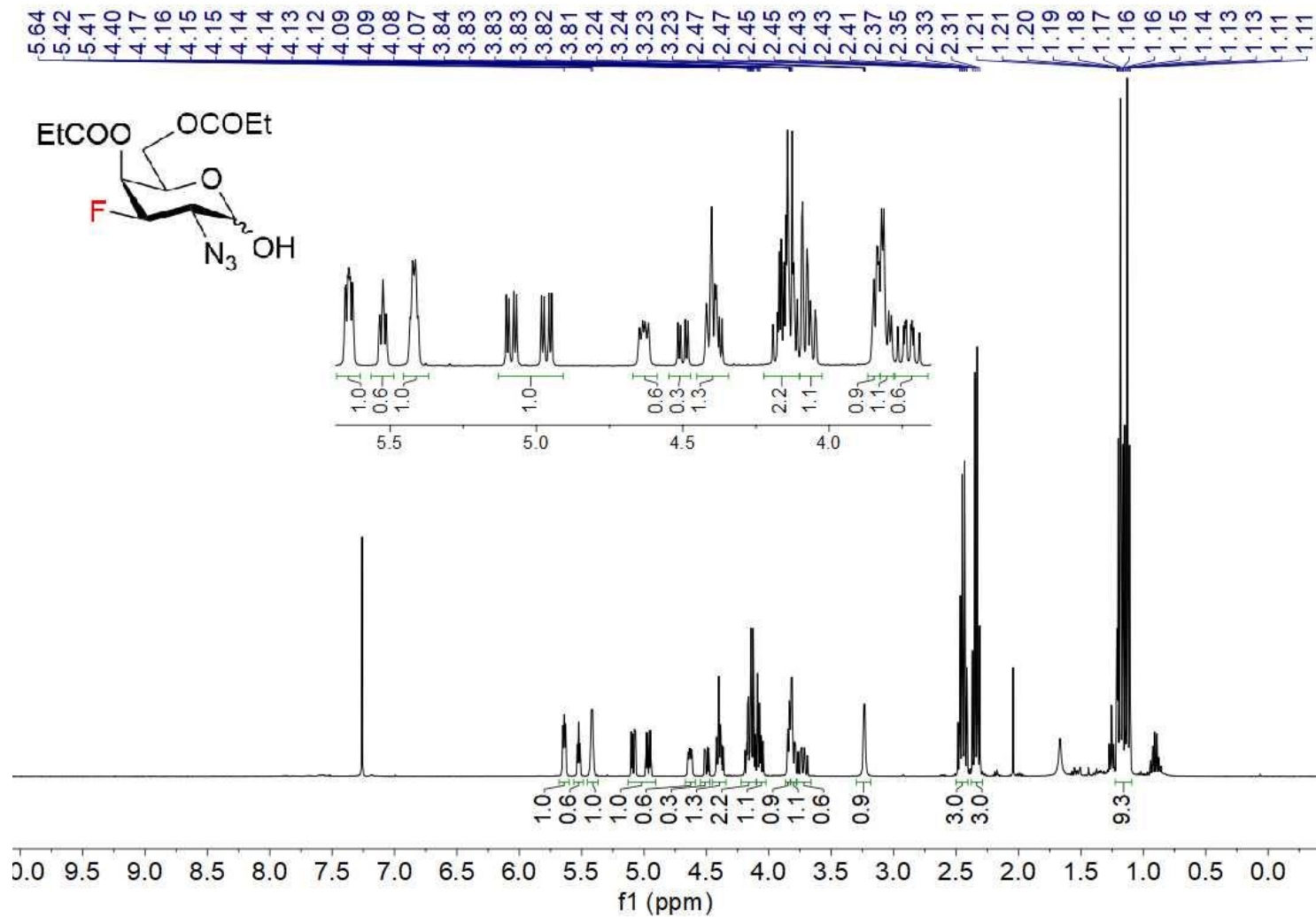


^1H - ^{13}C HSQC 71

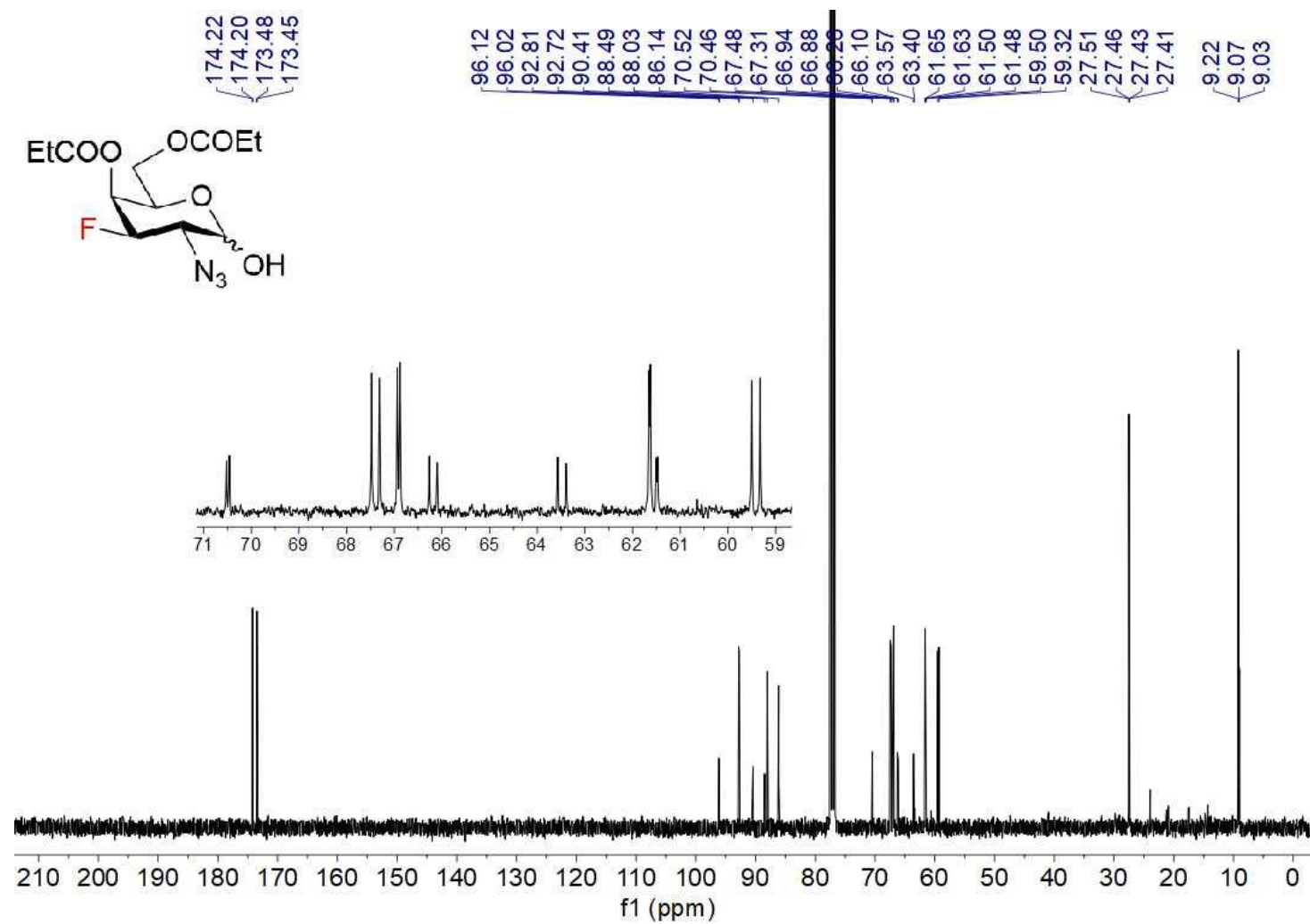


NMR COMPOUND 72

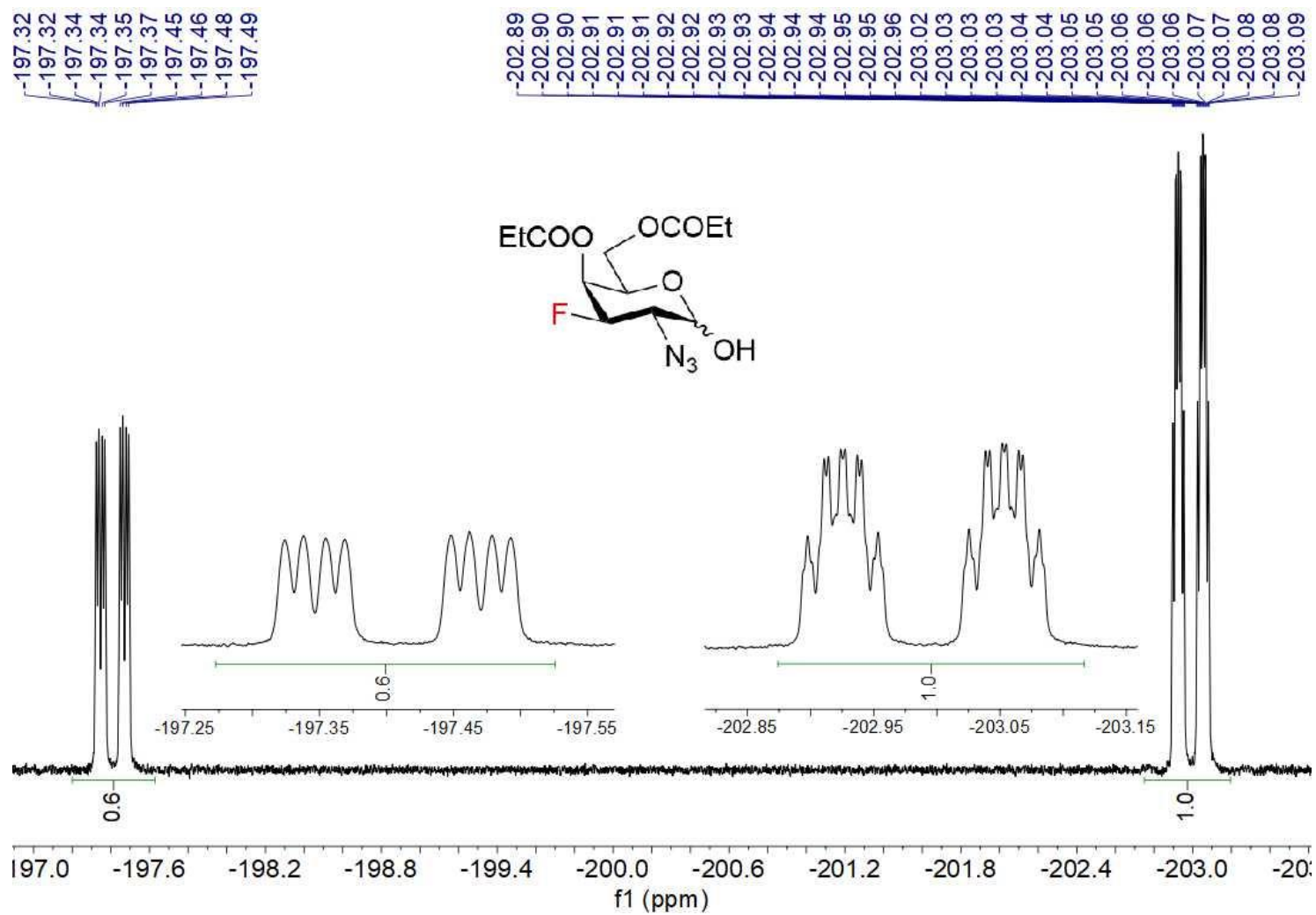
^1H NMR (400 MHz, CDCl_3) 72



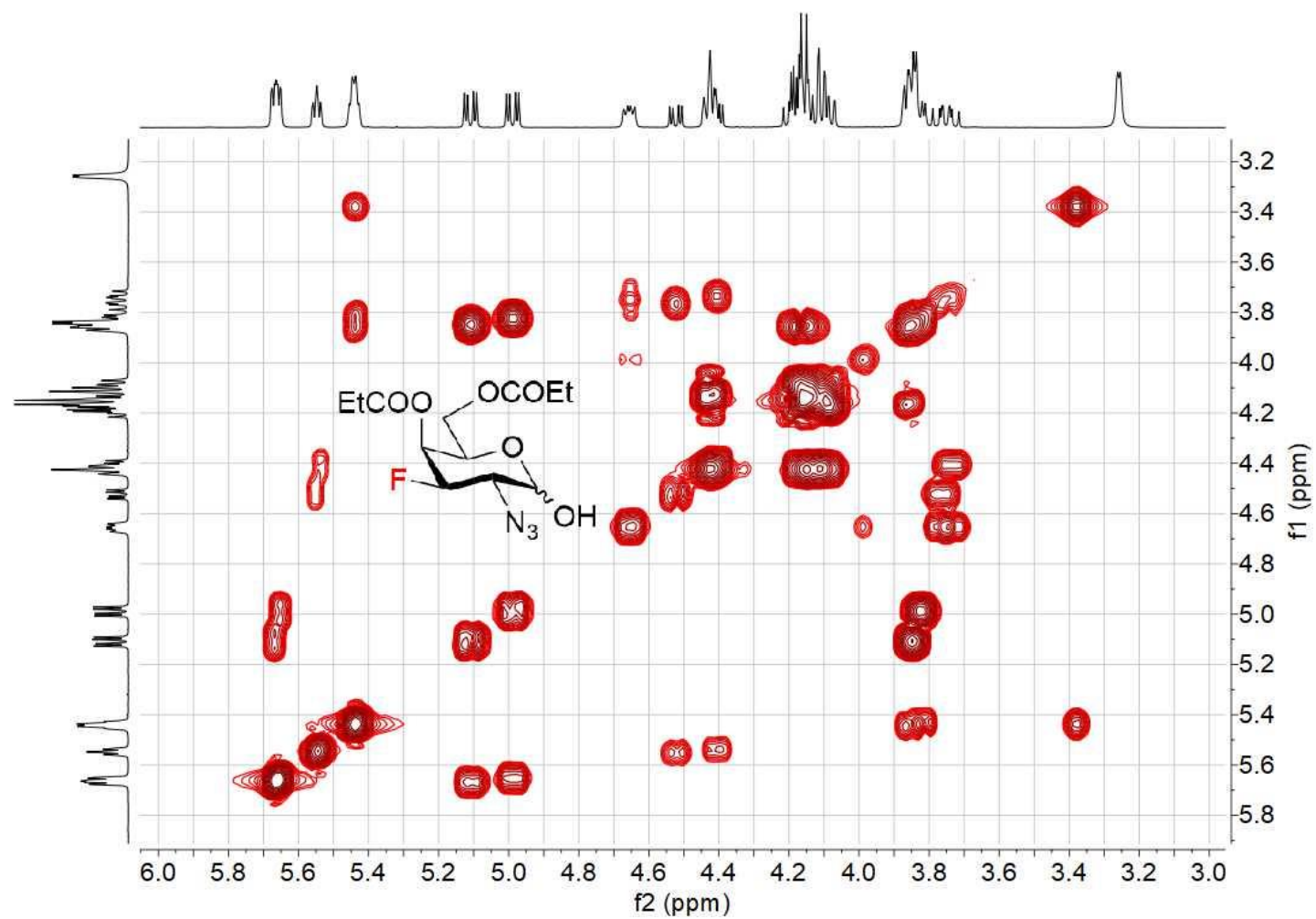
^{13}C NMR (100 MHz, CDCl_3) 72



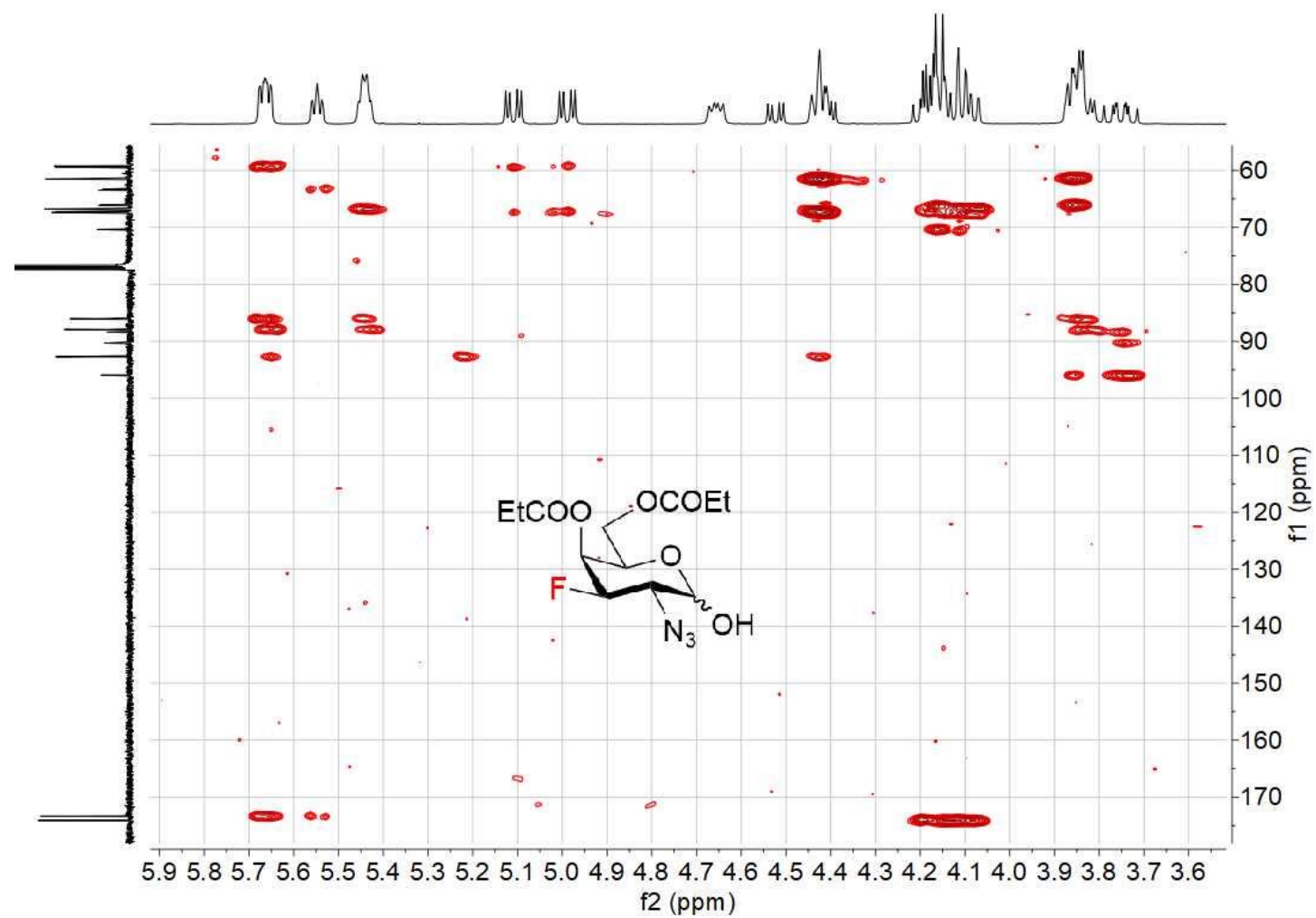
¹⁹F NMR (376 MHz, CDCl₃) 72



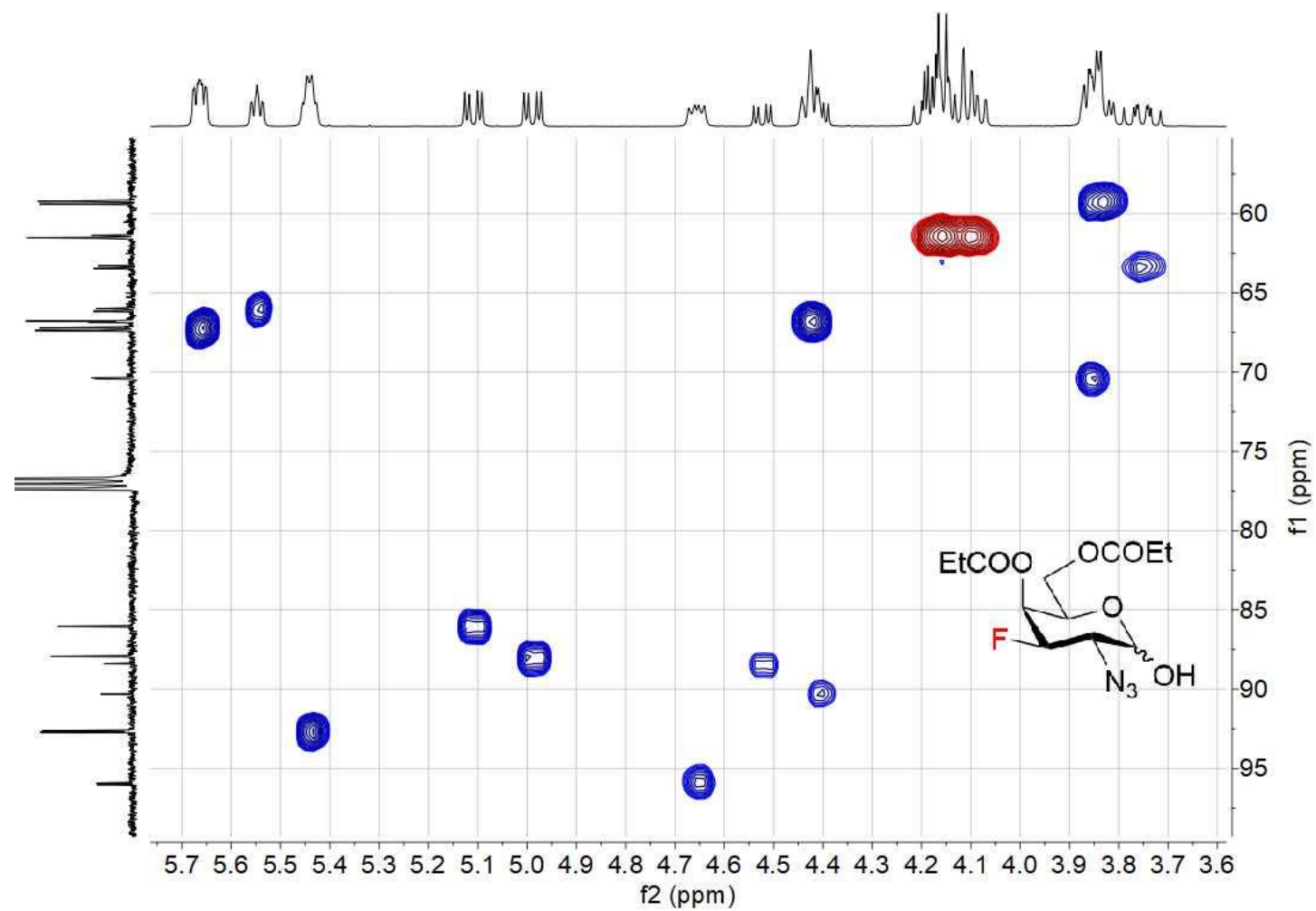
^1H - ^1H COSY 72



^1H - ^{13}C HMBC 72

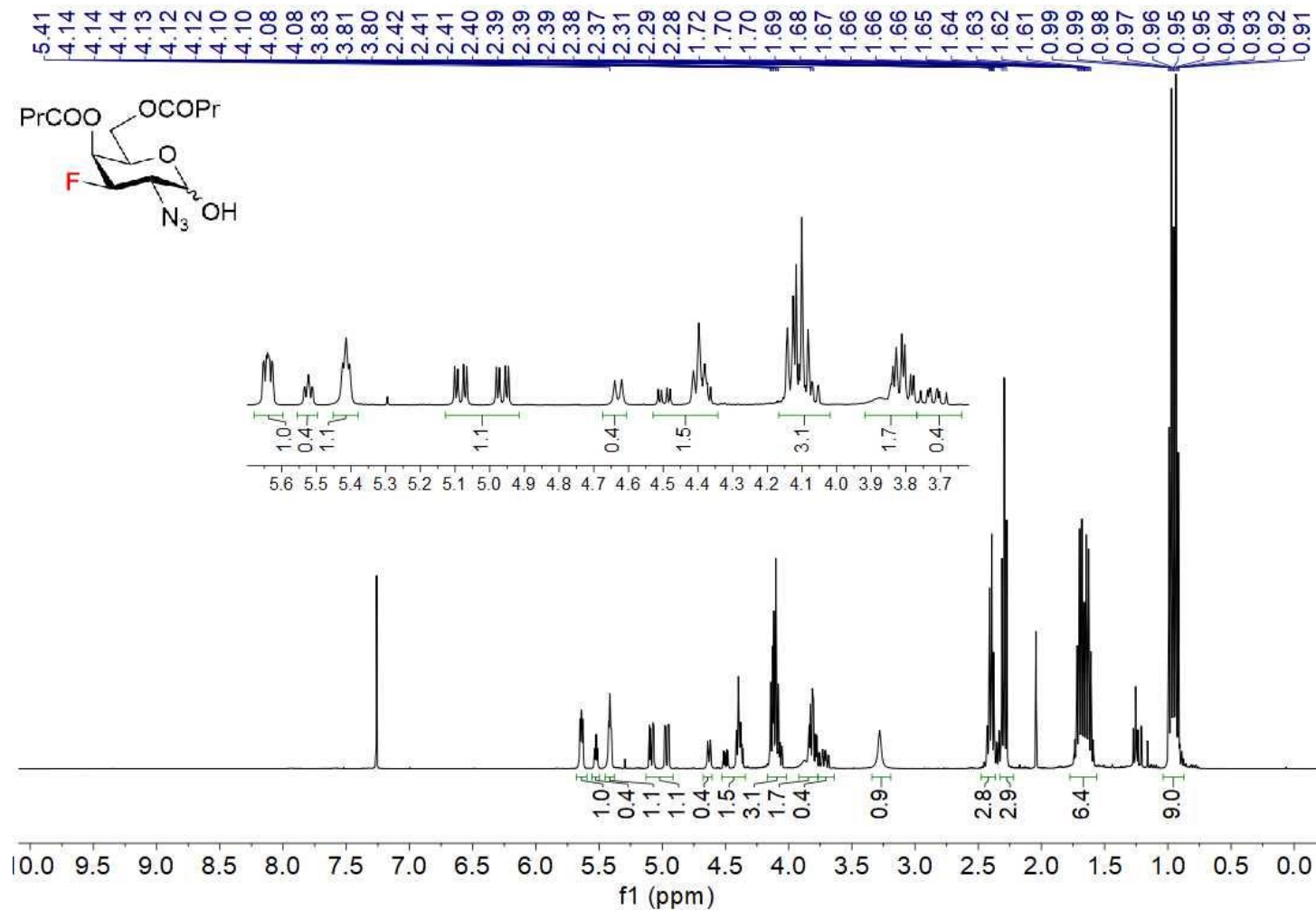


^1H - ^{13}C HSQC 72

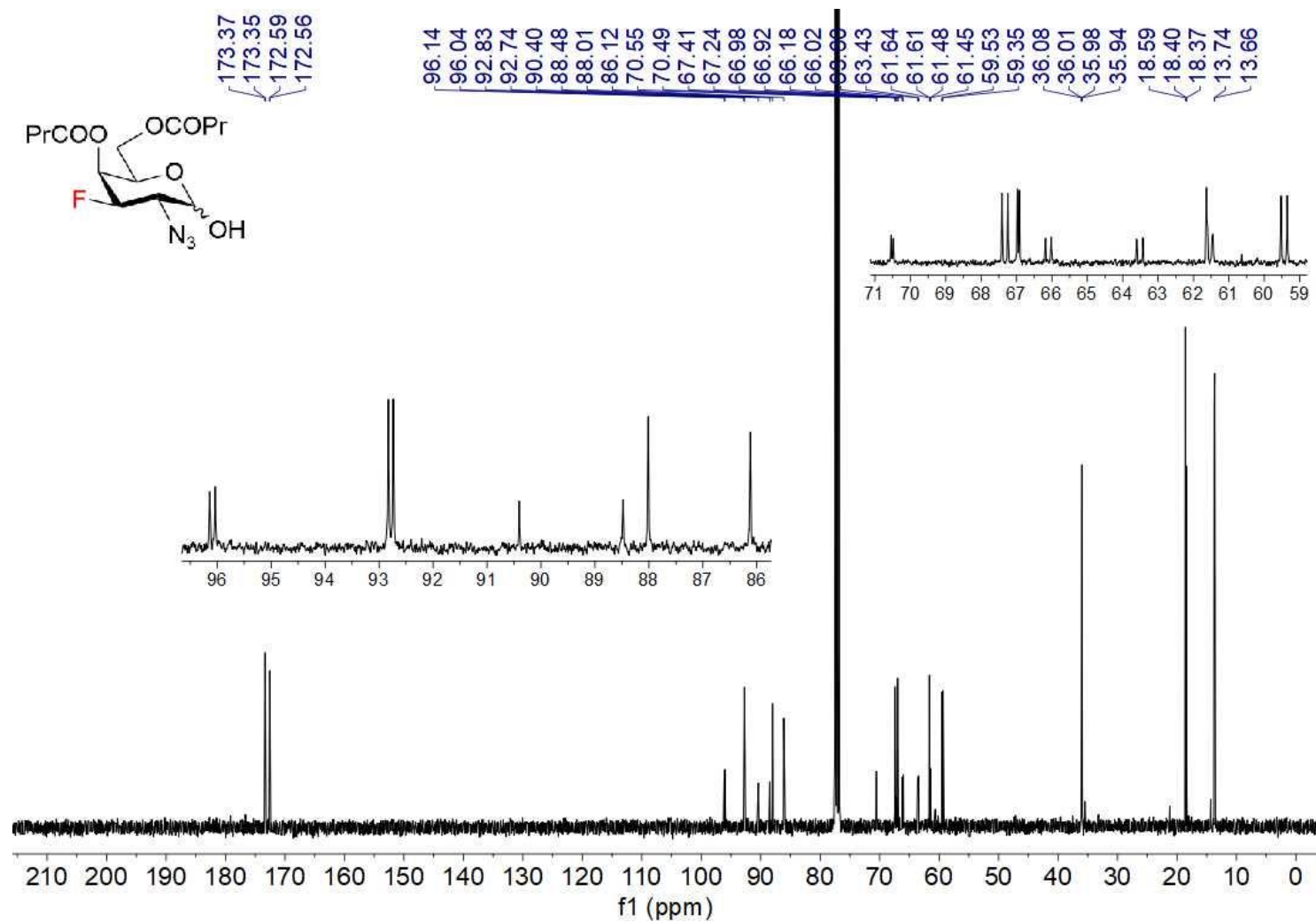


NMR COMPOUND 73

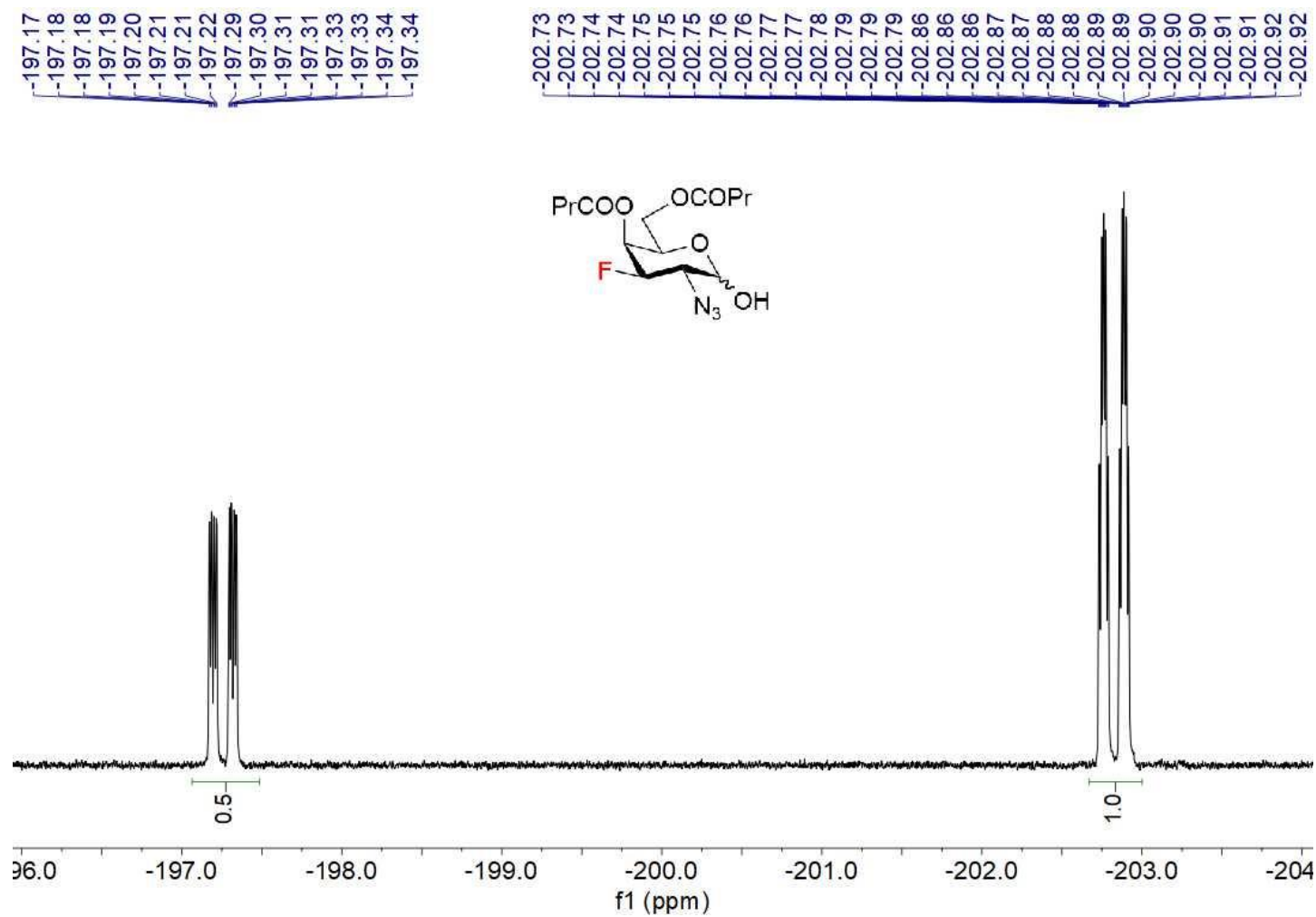
¹H NMR (400 MHz, CDCl₃) 73



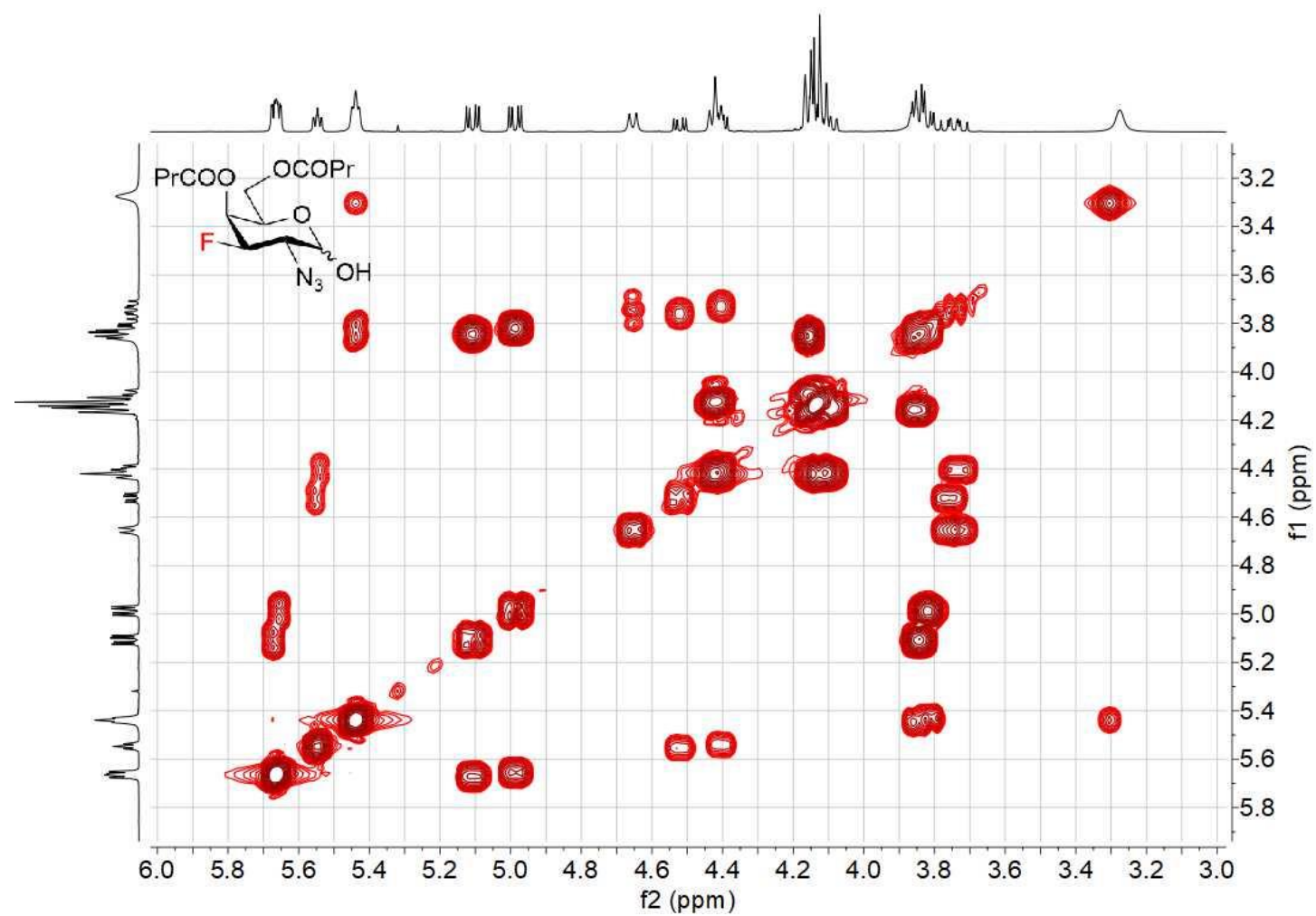
^{13}C NMR (100 MHz, CDCl_3) 73



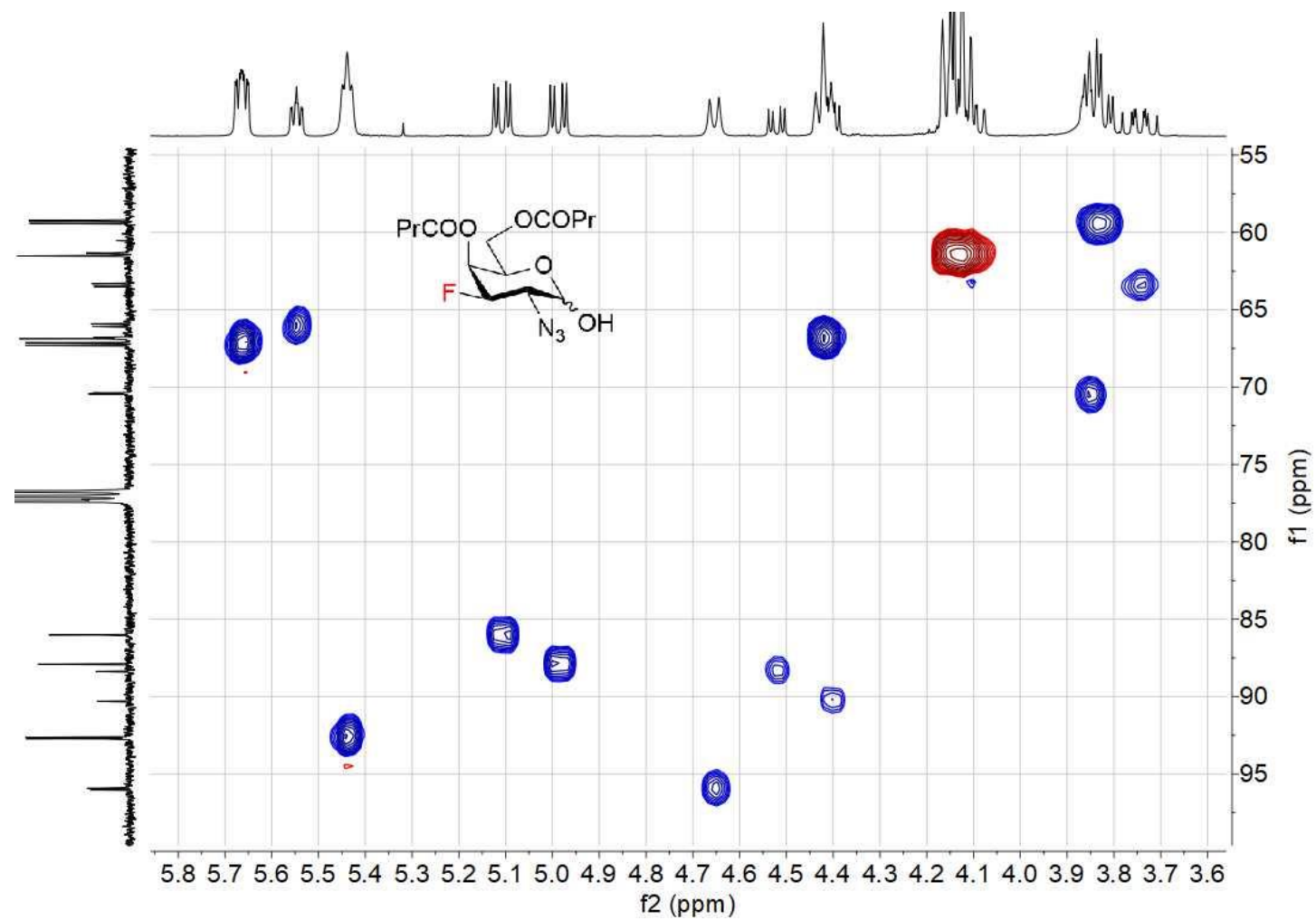
¹⁹F NMR (376 MHz, CDCl₃) 73



^1H - ^1H COSY 73

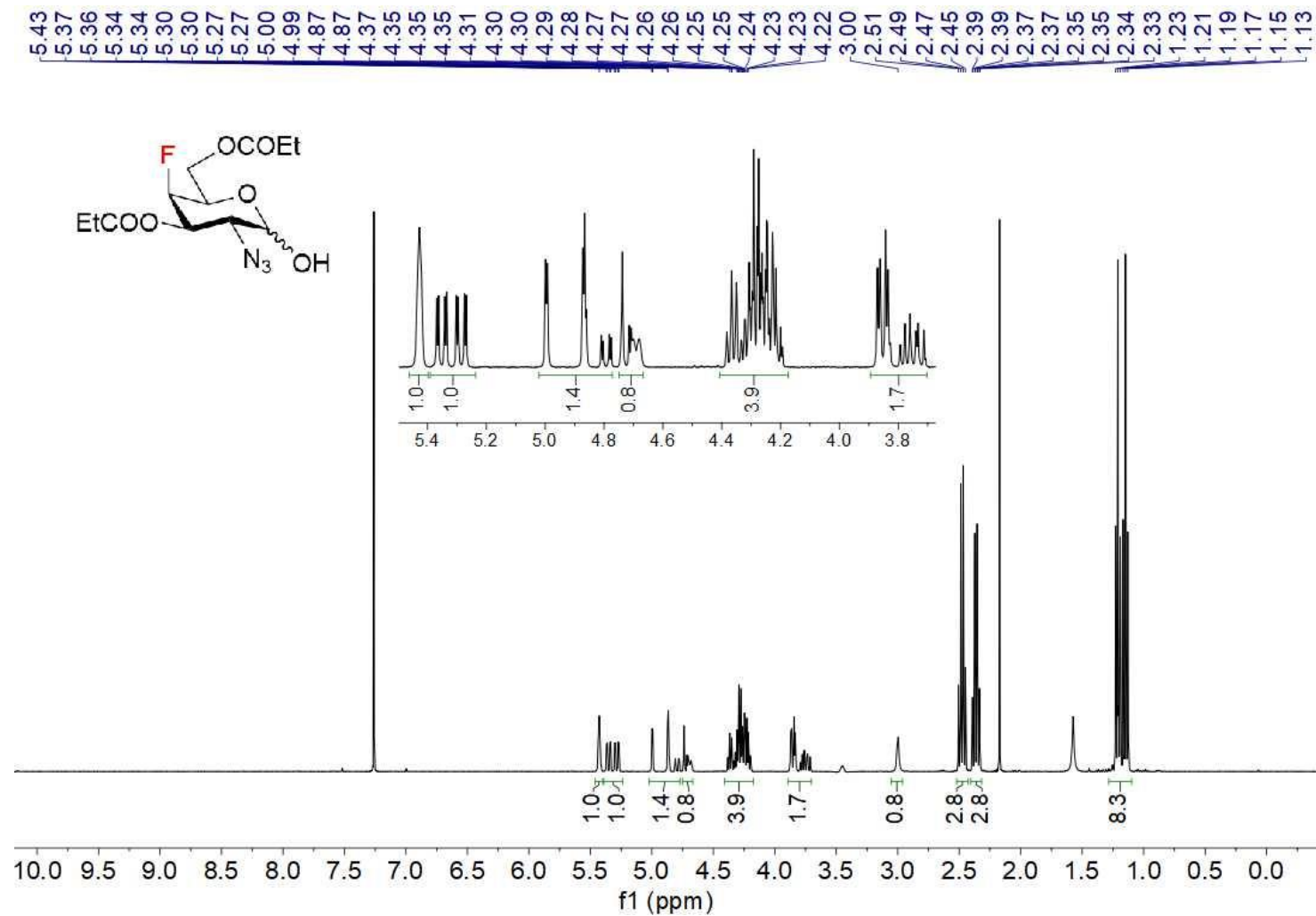


^1H - ^{13}C HSQC 73

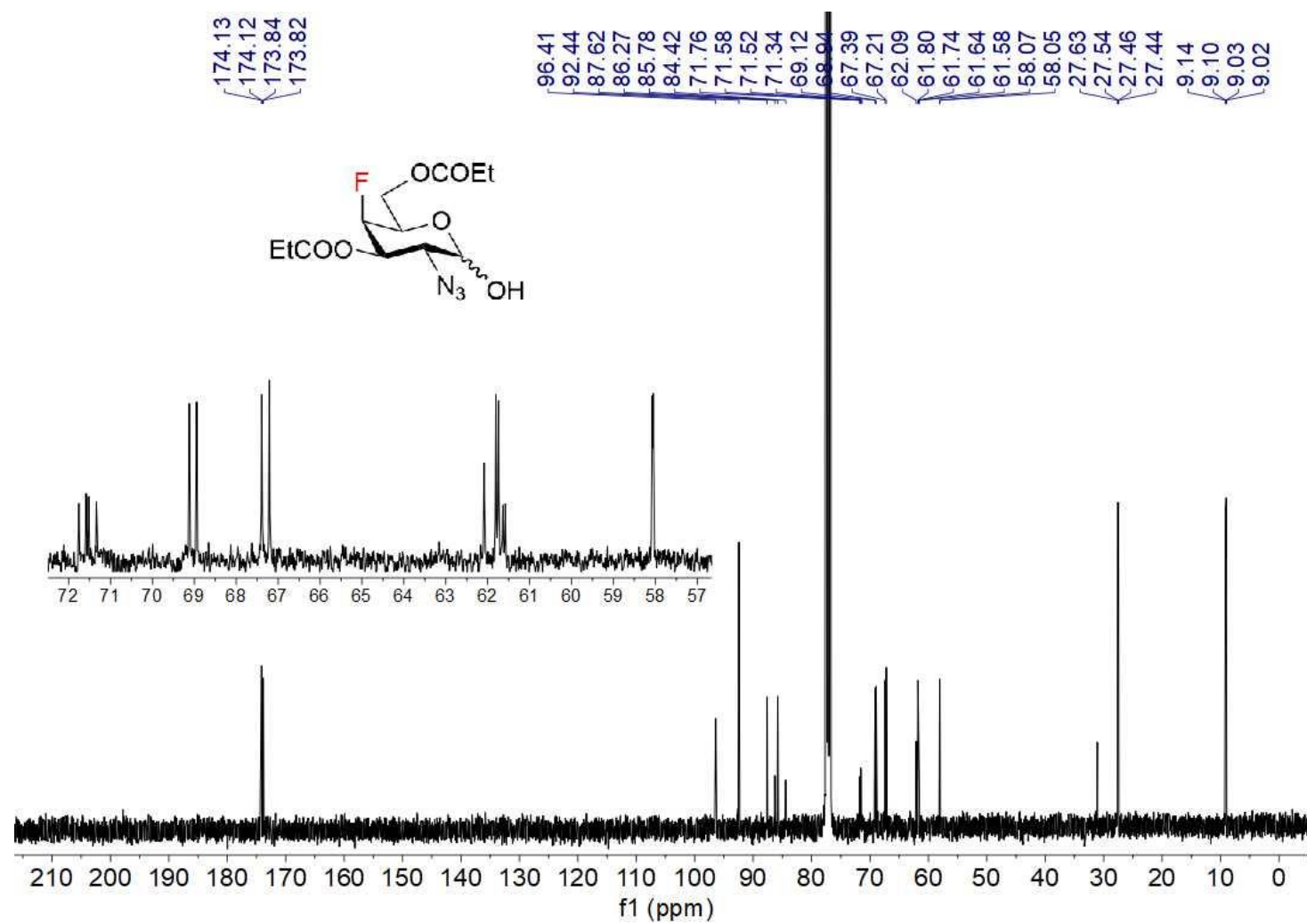


NMR COMPOUND 74

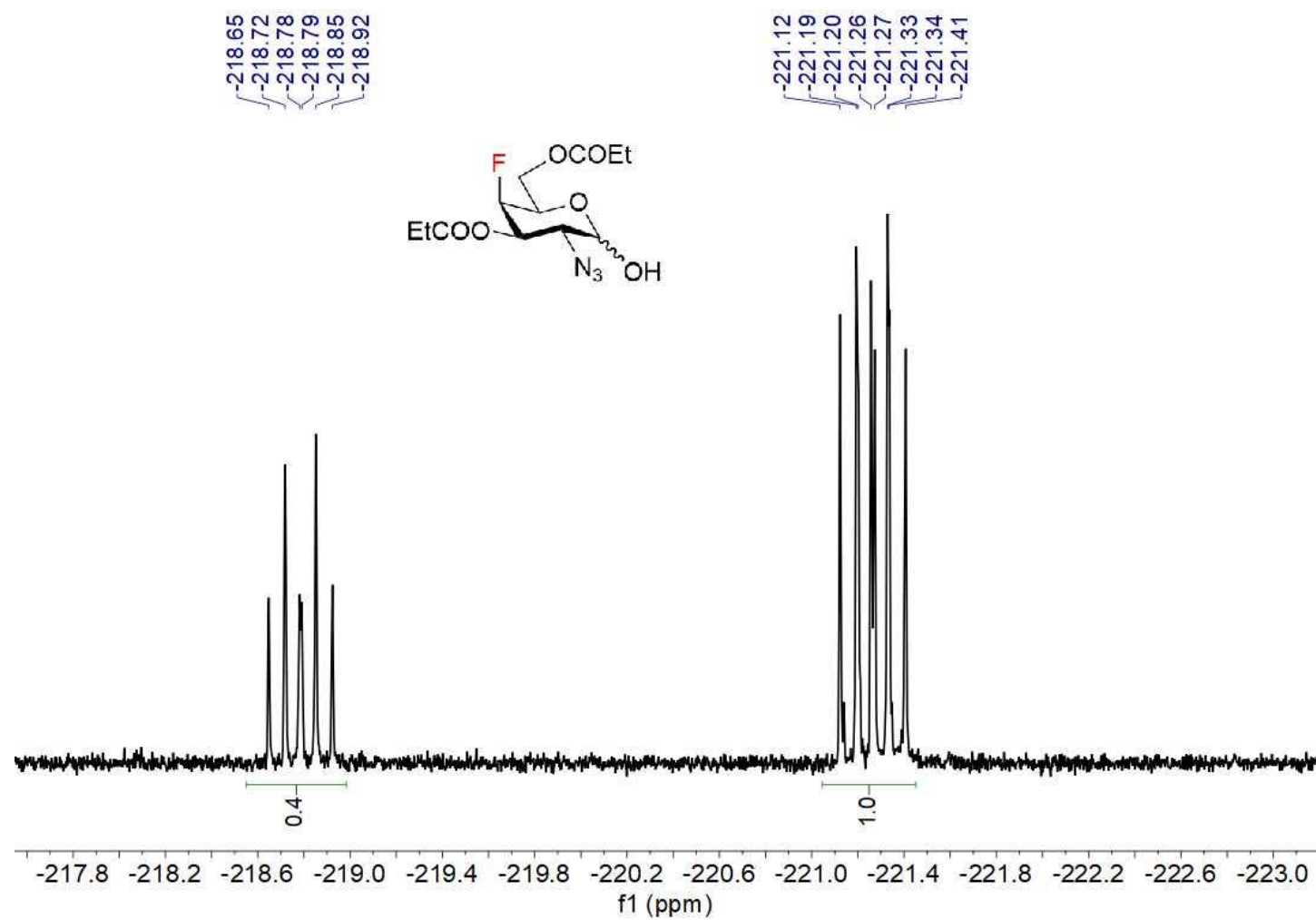
¹H NMR (400 MHz, CDCl₃) 74



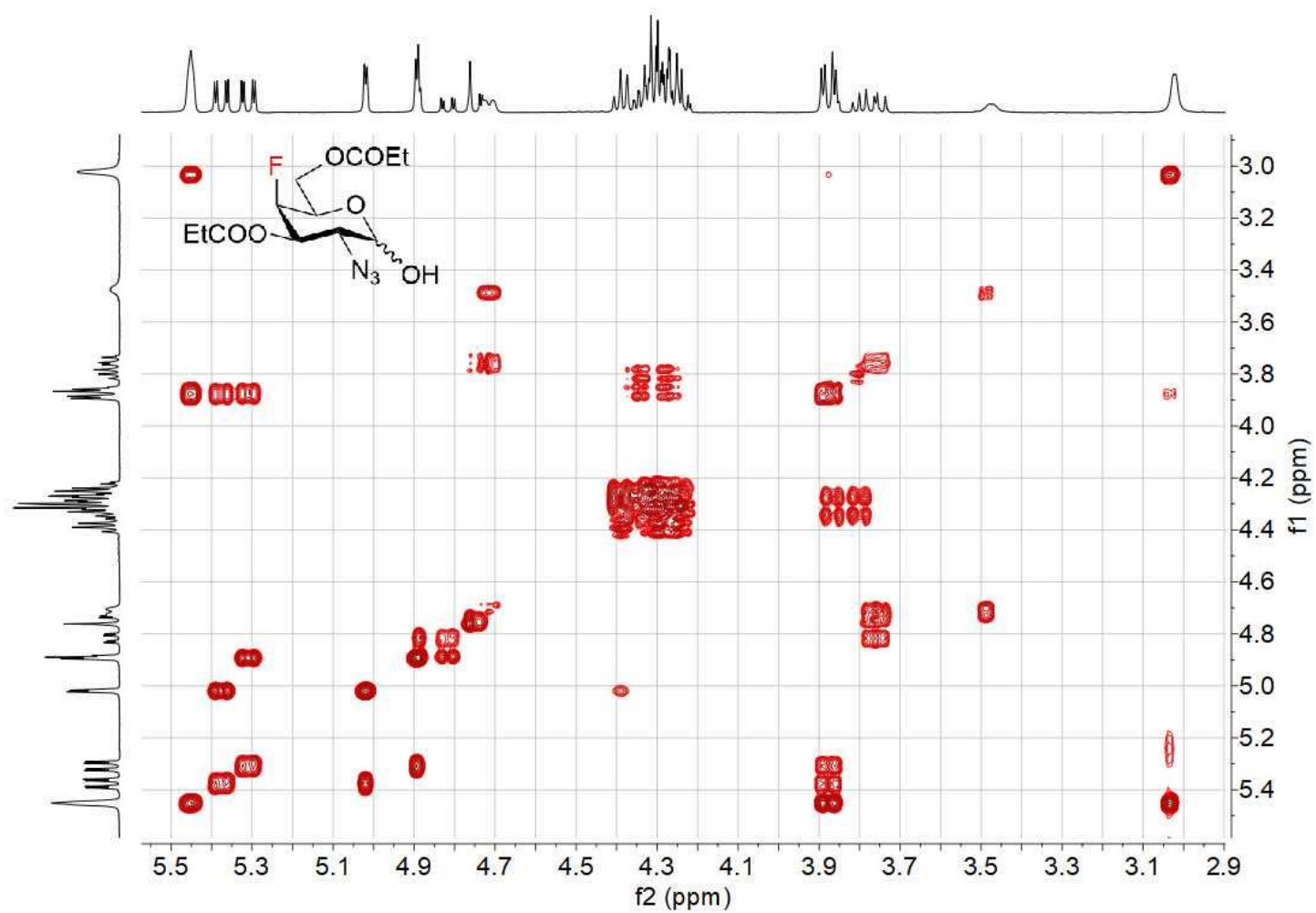
^{13}C NMR (100 MHz, CDCl_3) 74

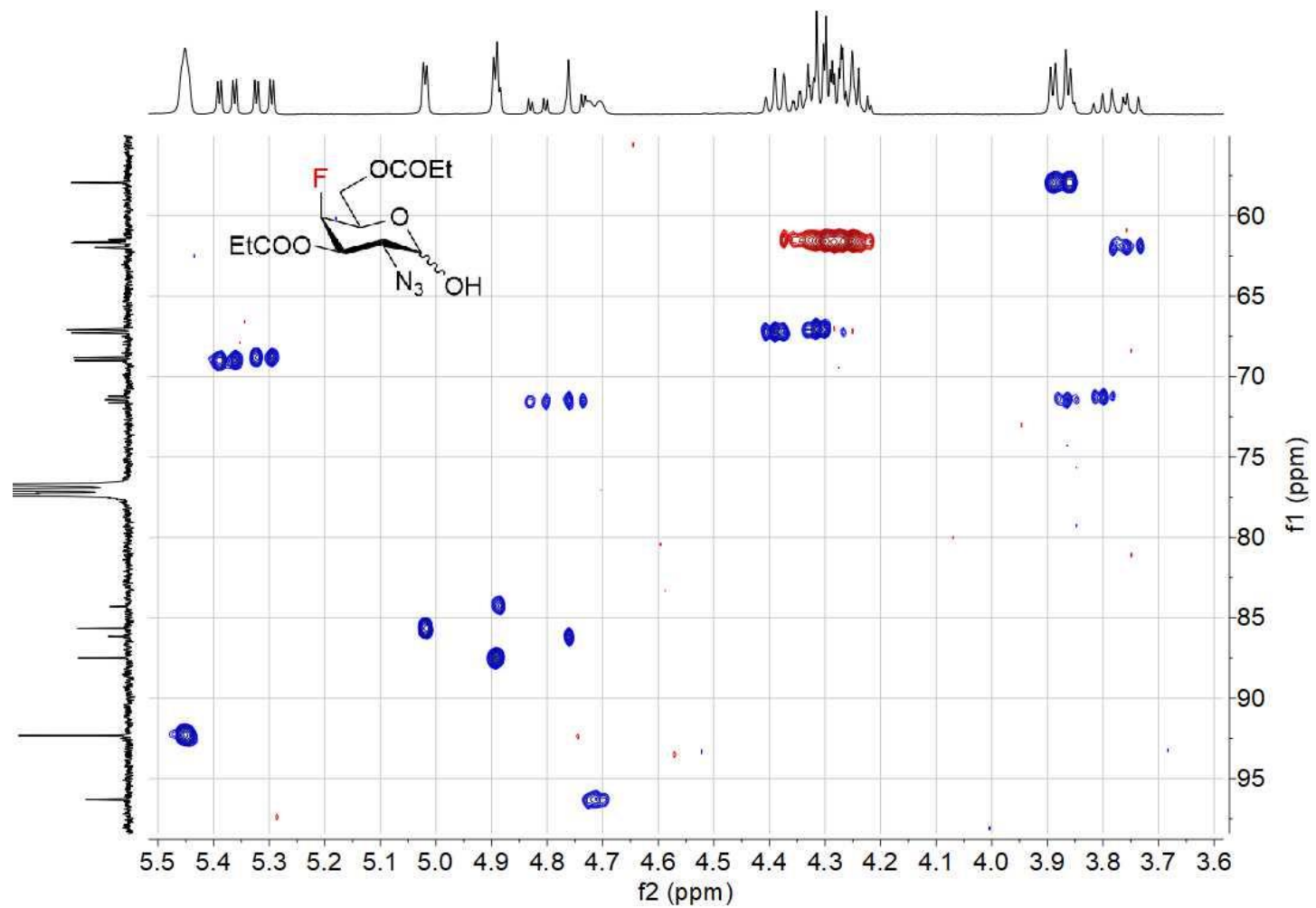


¹⁹F NMR (376 MHz, CDCl₃) NMR 74



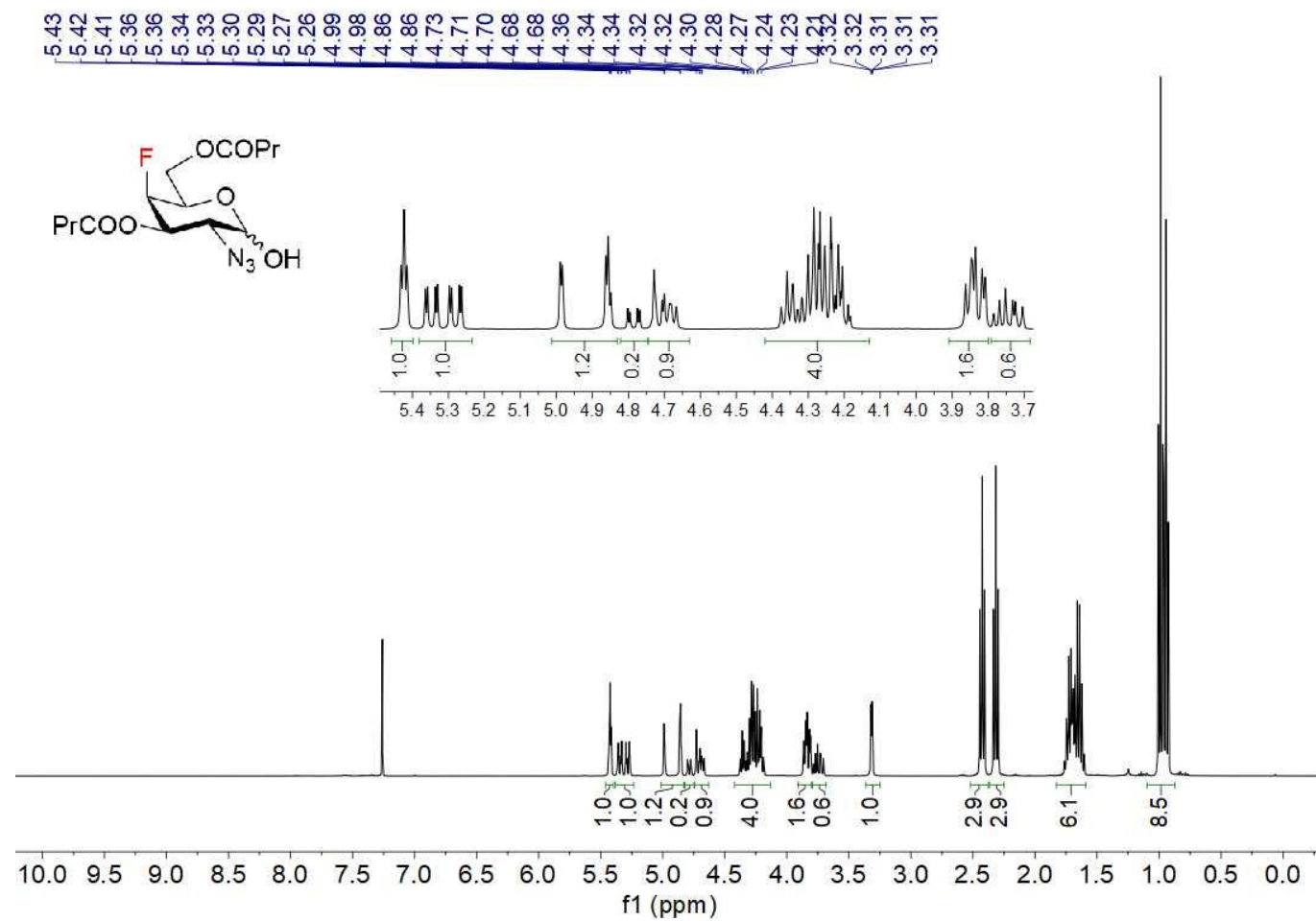
¹H-¹H COSY 74



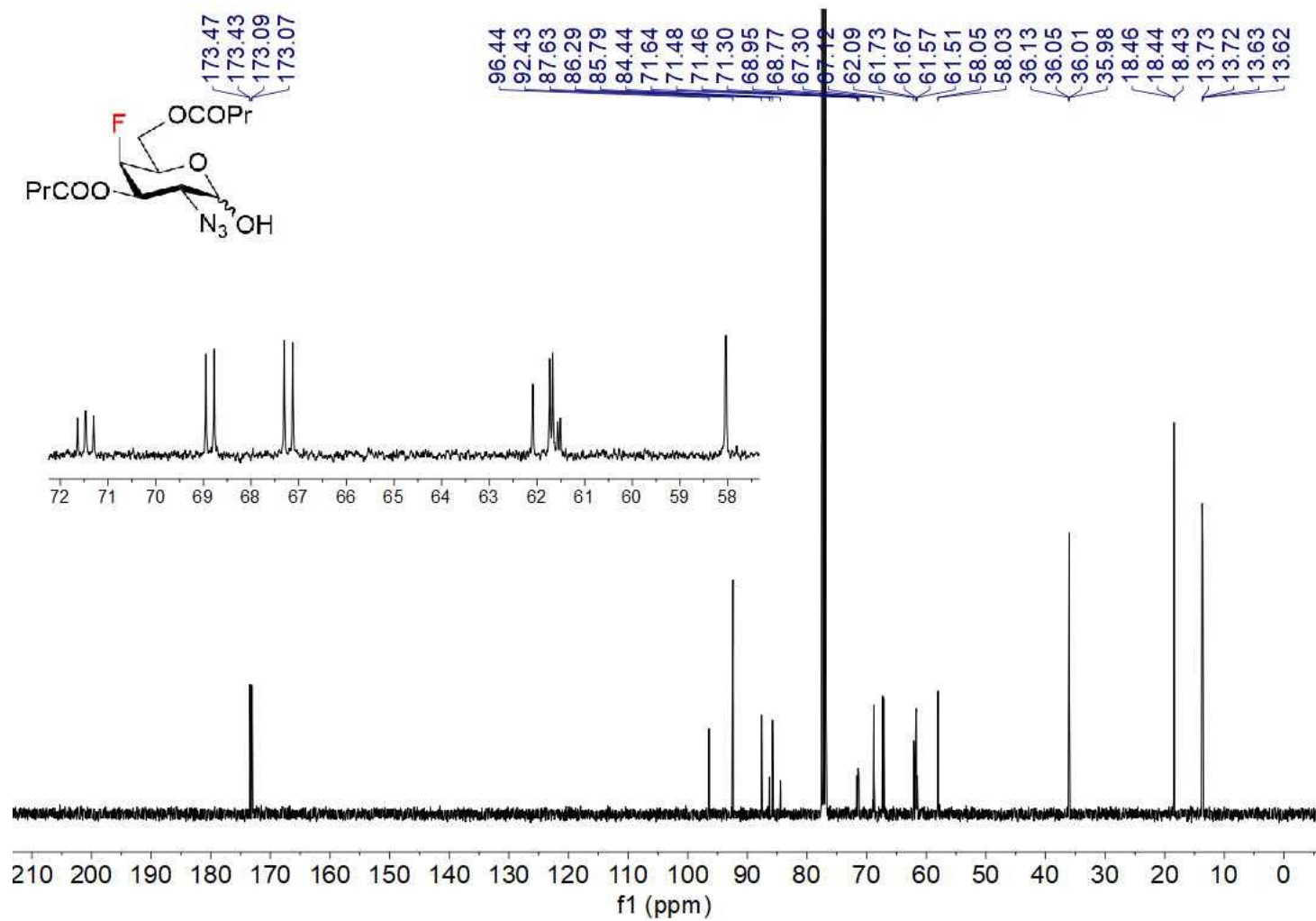
¹H-¹³C HSQC 74

NMR COMPOUND 75

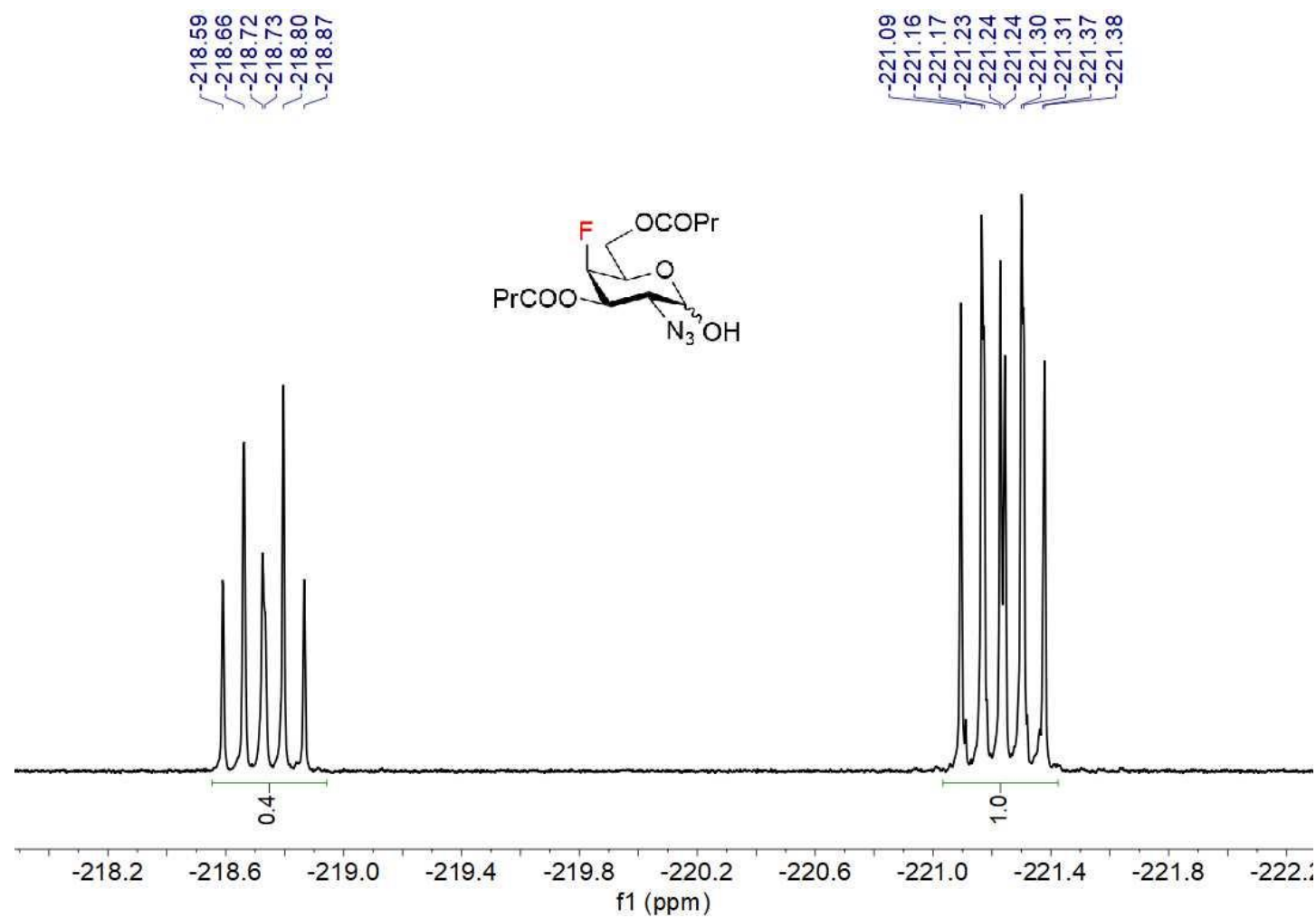
¹H NMR (400 MHz, CDCl₃) 75



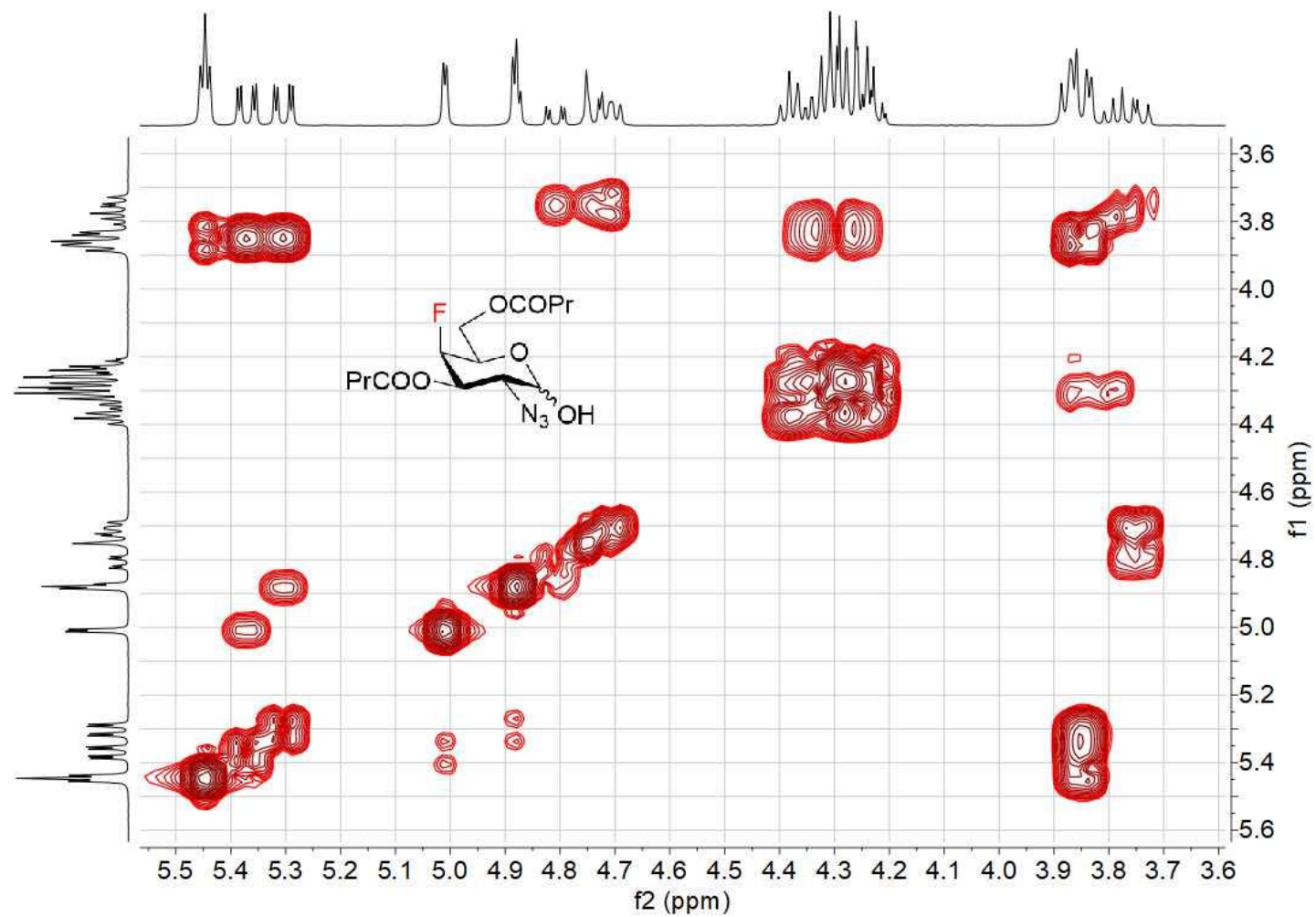
^{13}C NMR (100 MHz, CDCl_3) 75



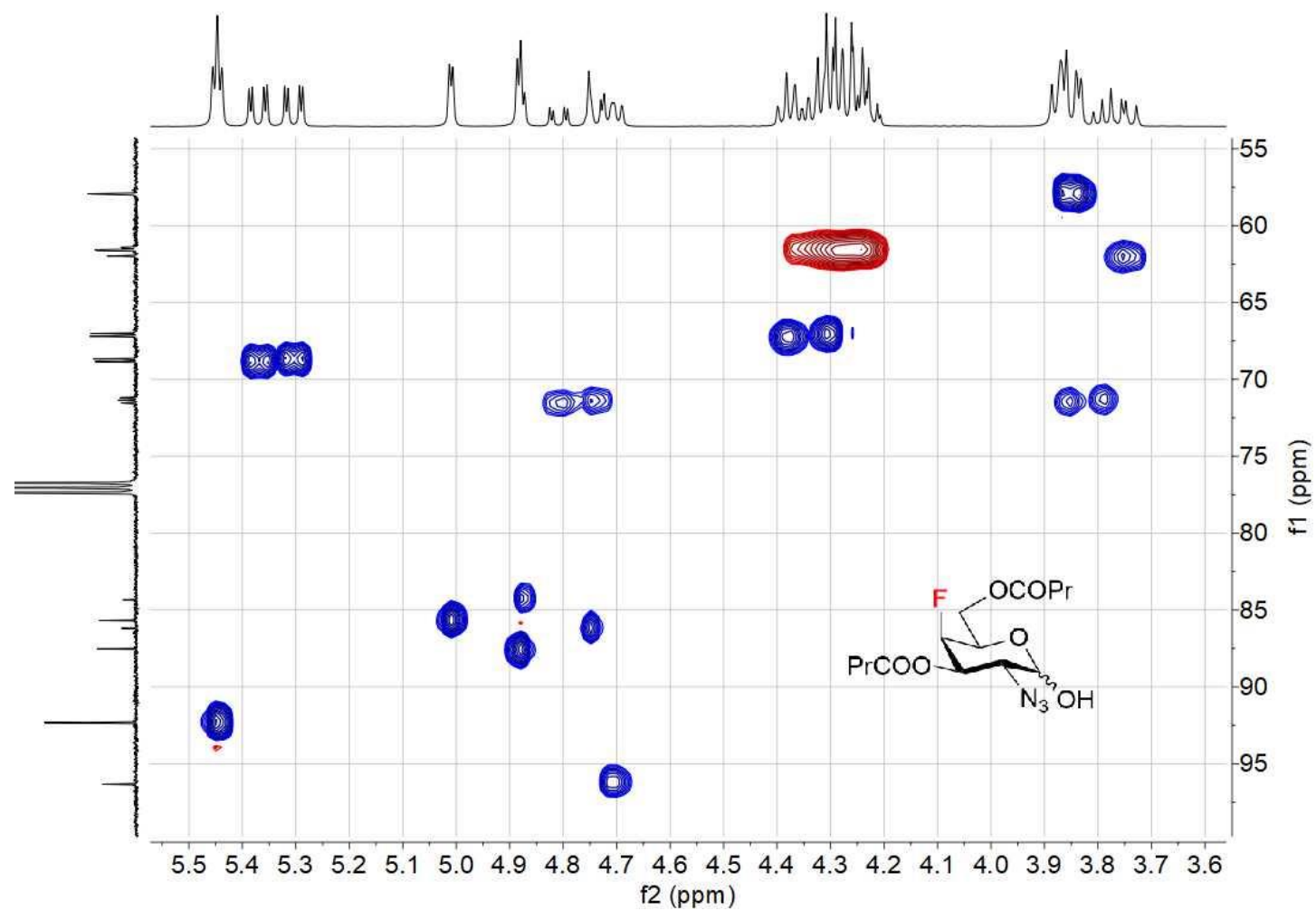
^{19}F NMR (376 MHz, CDCl_3) NMR 75



^1H - ^1H COSY 75

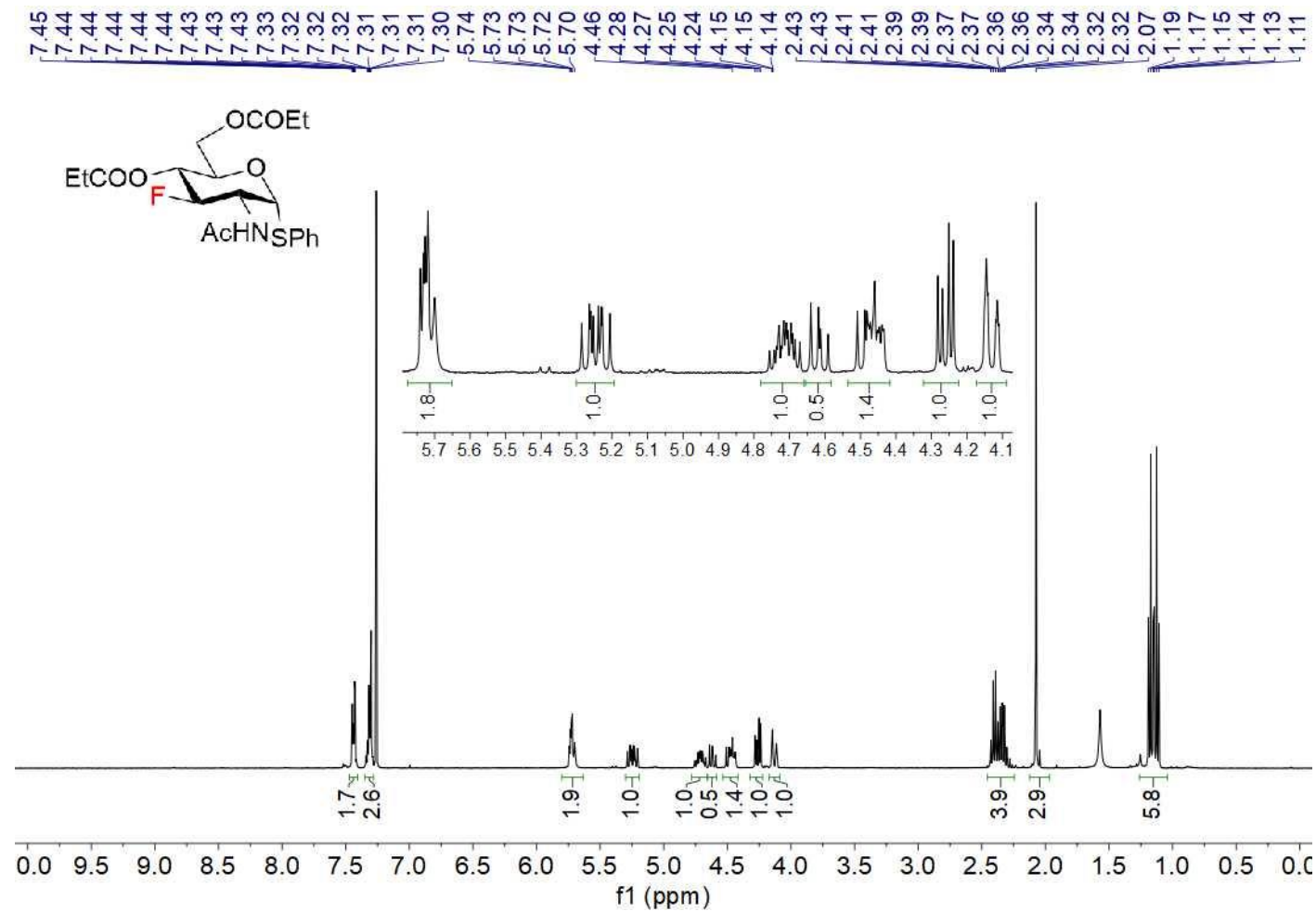


^1H - ^{13}C HSQC 75

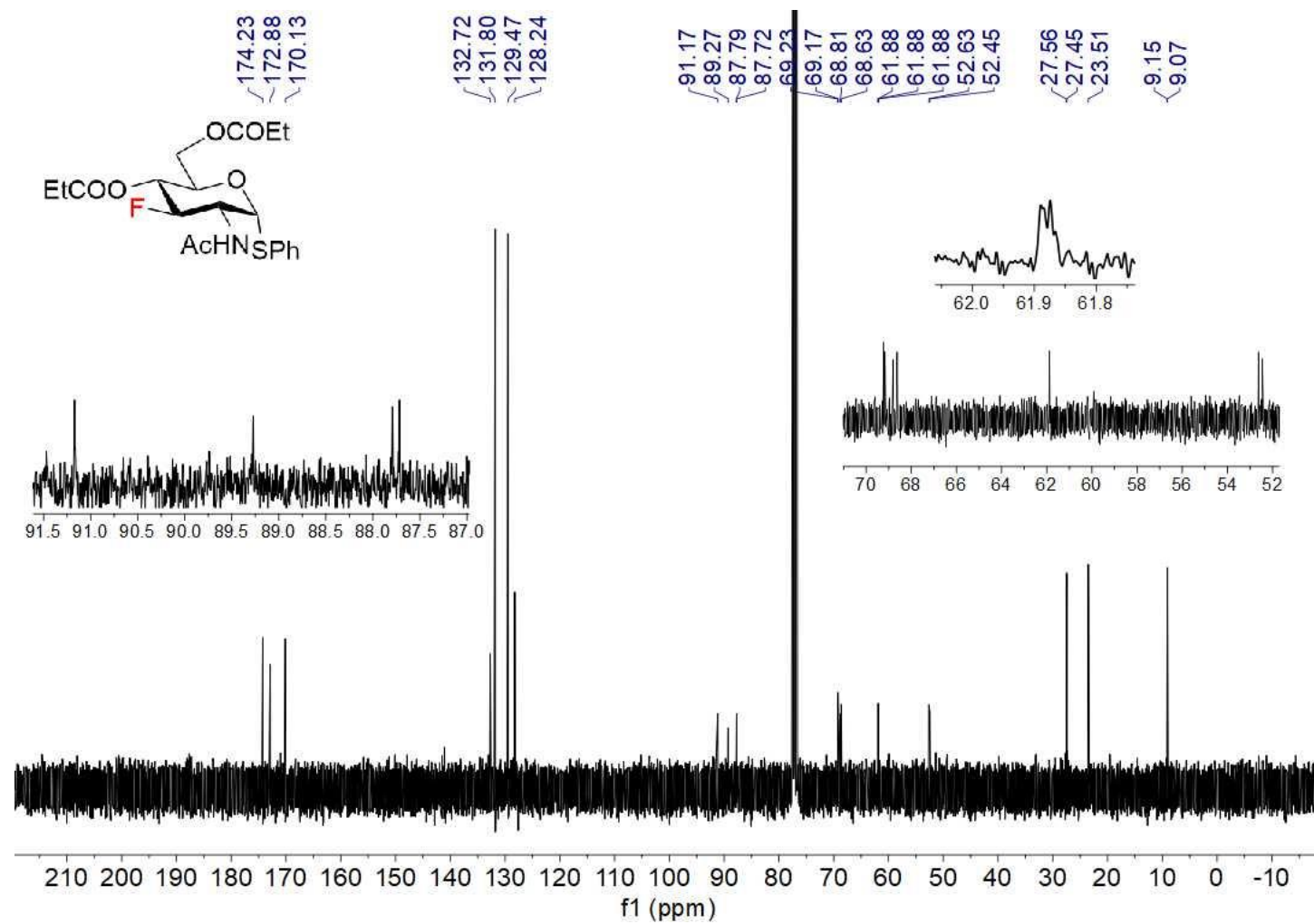


NMR COMPOUND 76

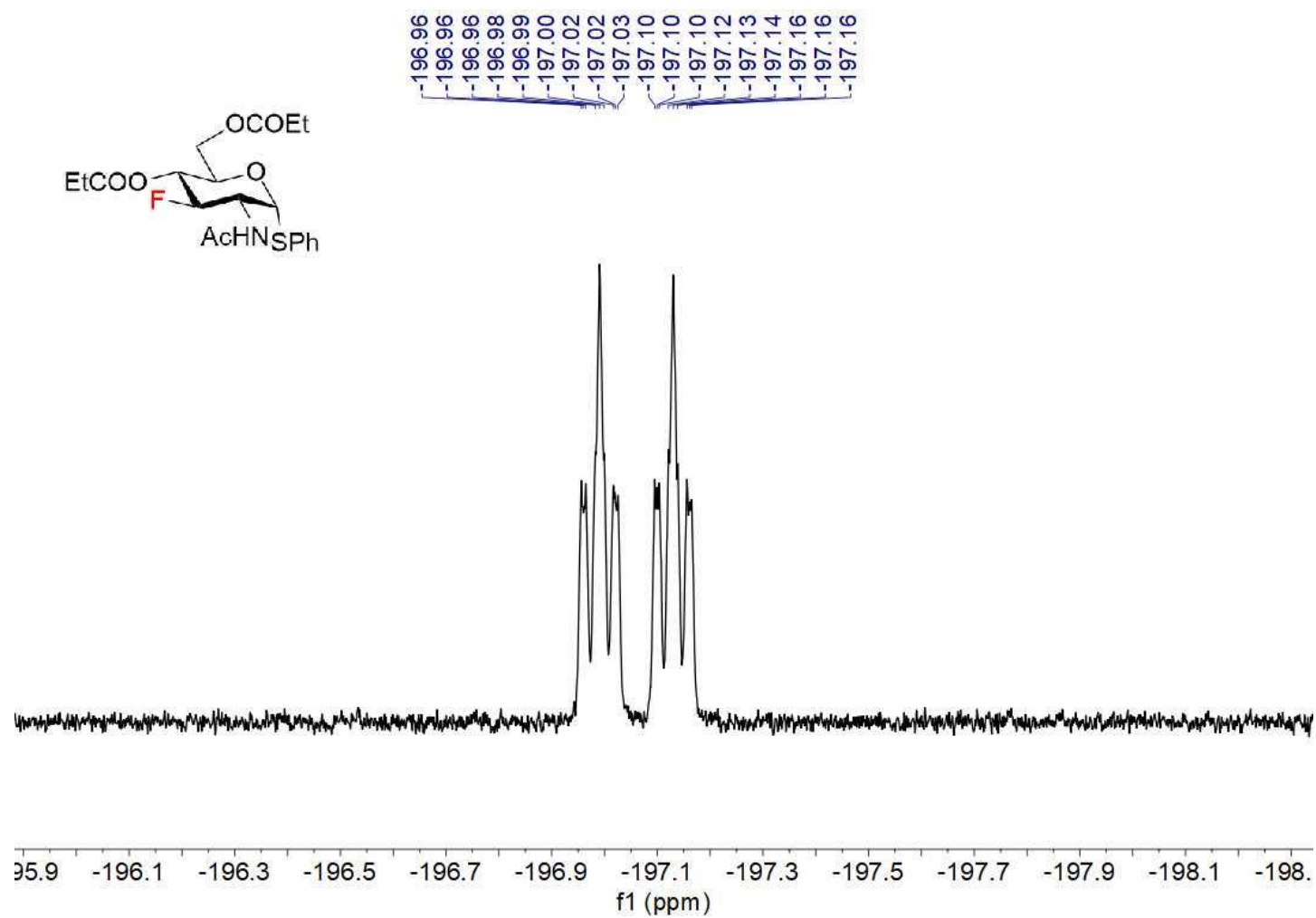
¹H NMR (400 MHz, CDCl₃) 76



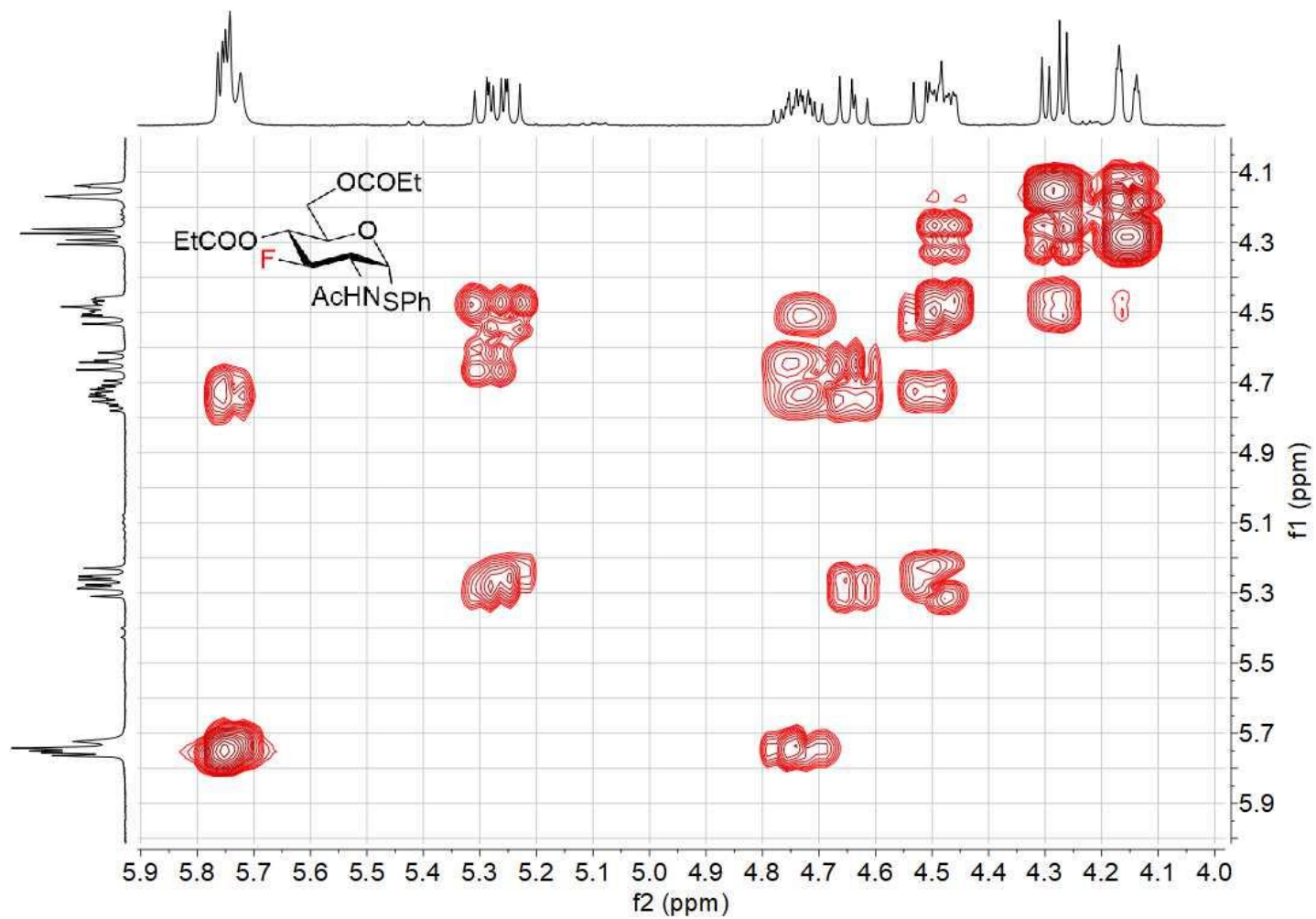
^{13}C NMR (100 MHz, CDCl_3) 76



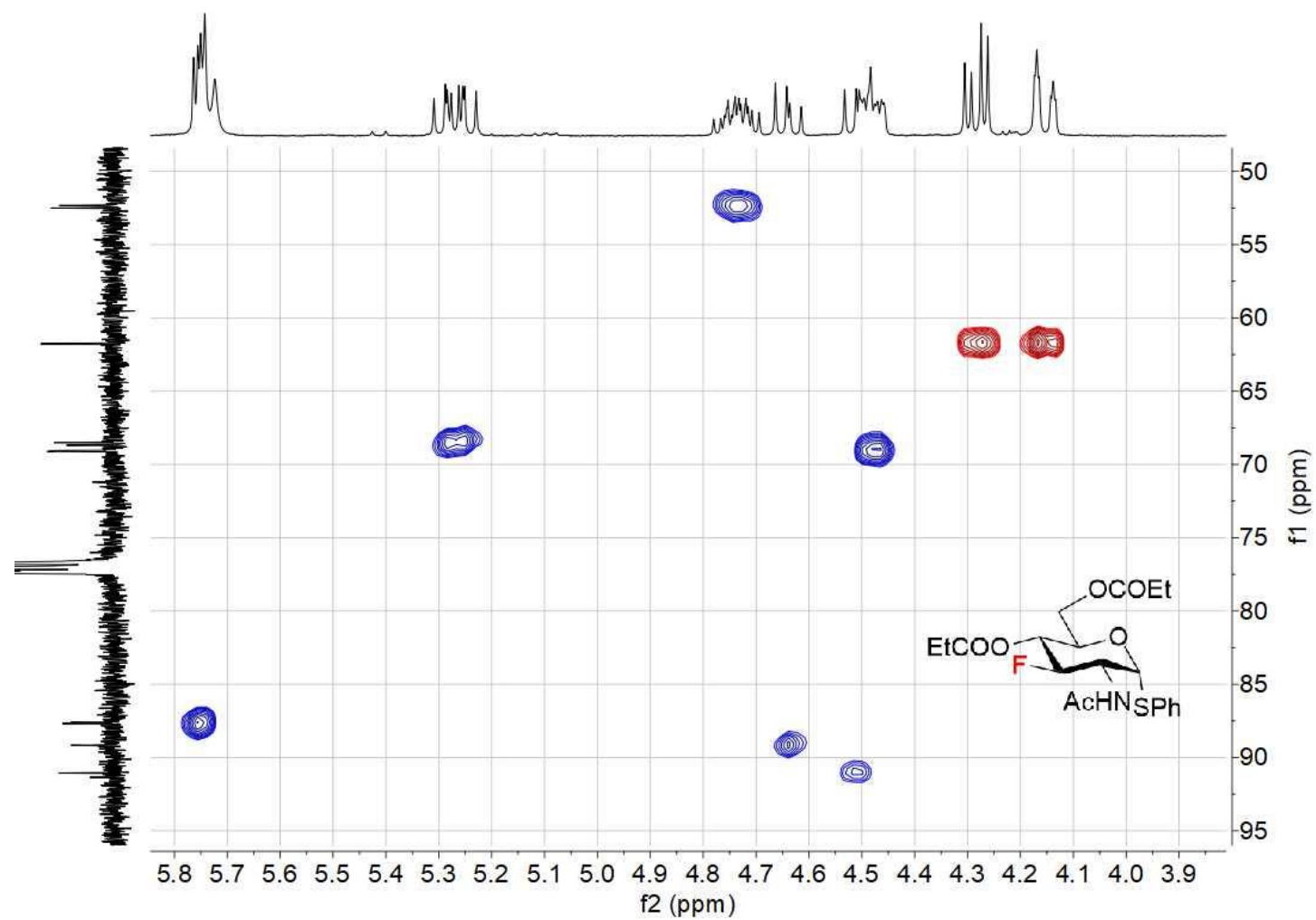
^{19}F NMR (376 MHz, CDCl_3) 76



^1H - ^1H COSY 76

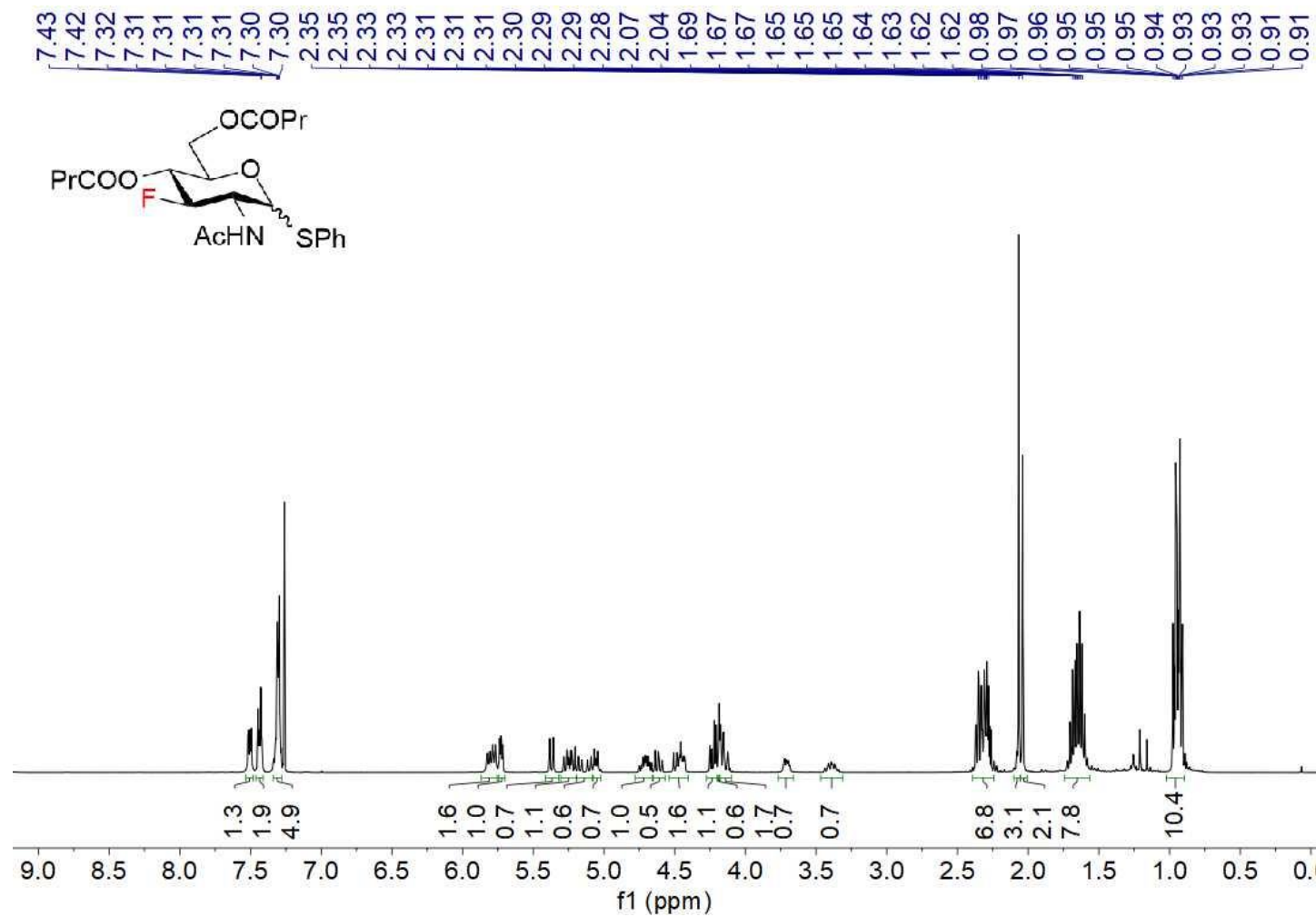


^1H - ^{13}C HSQC 76

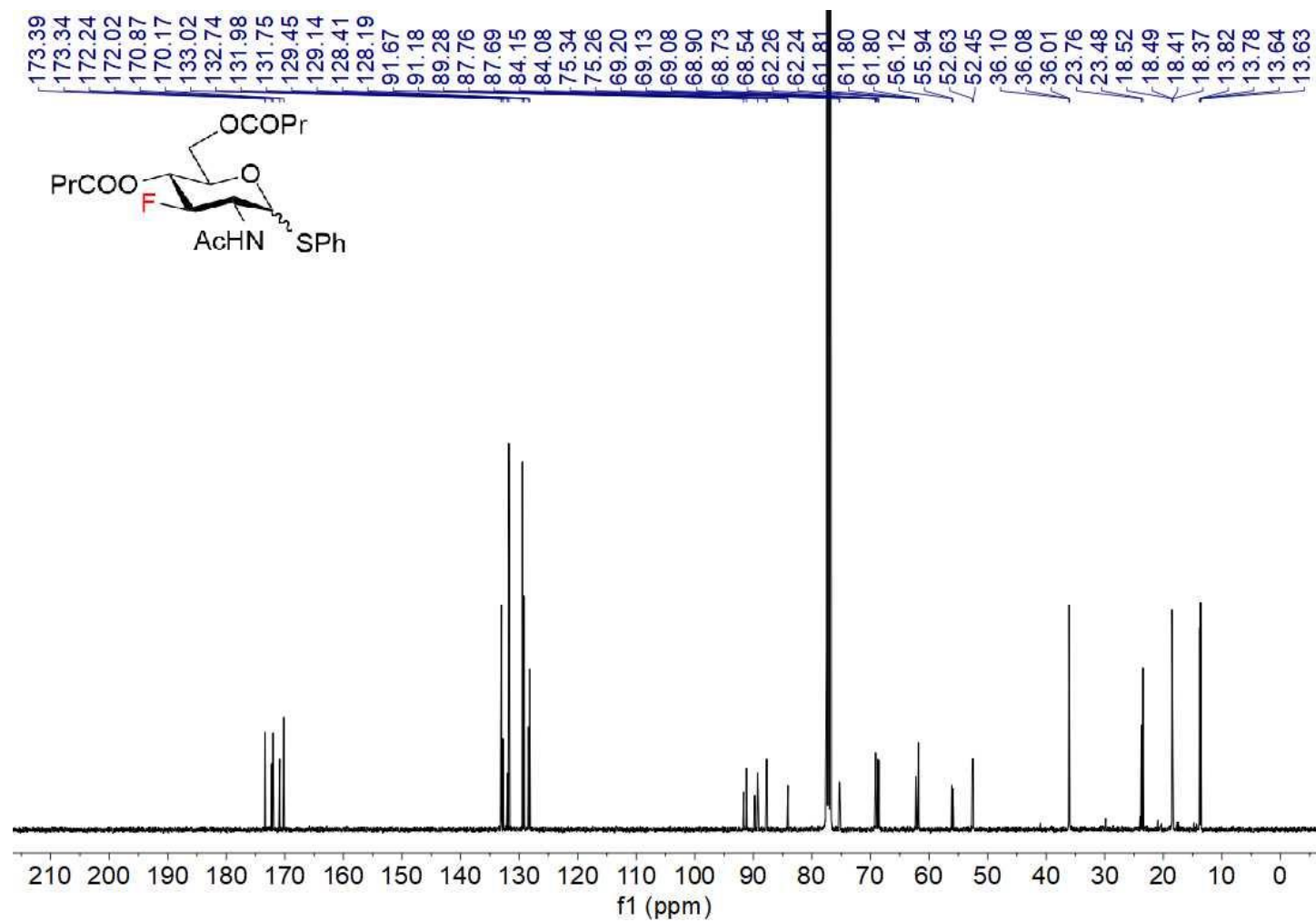


NMR COMPOUND 77

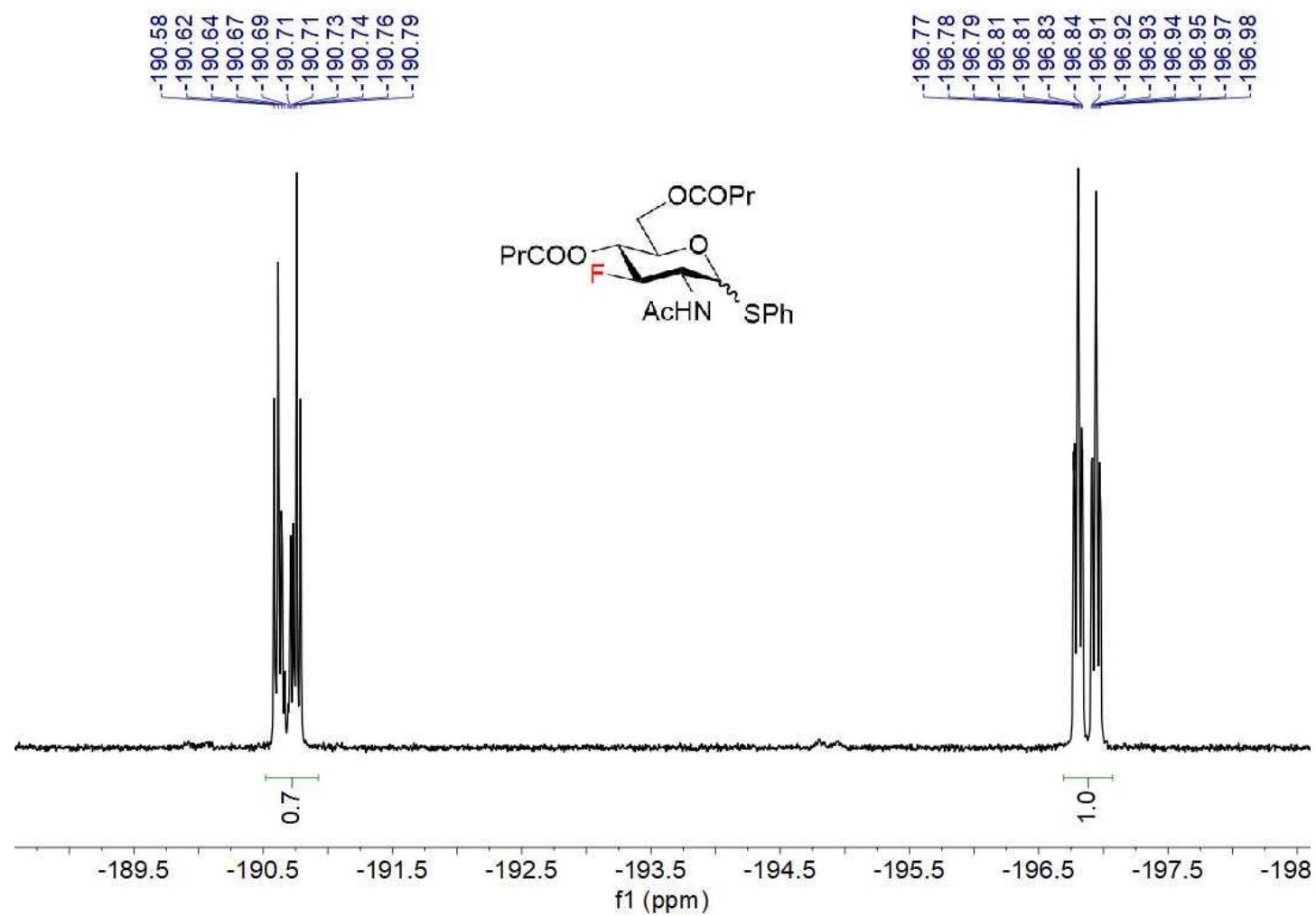
^1H NMR (400 MHz, CDCl_3) 77



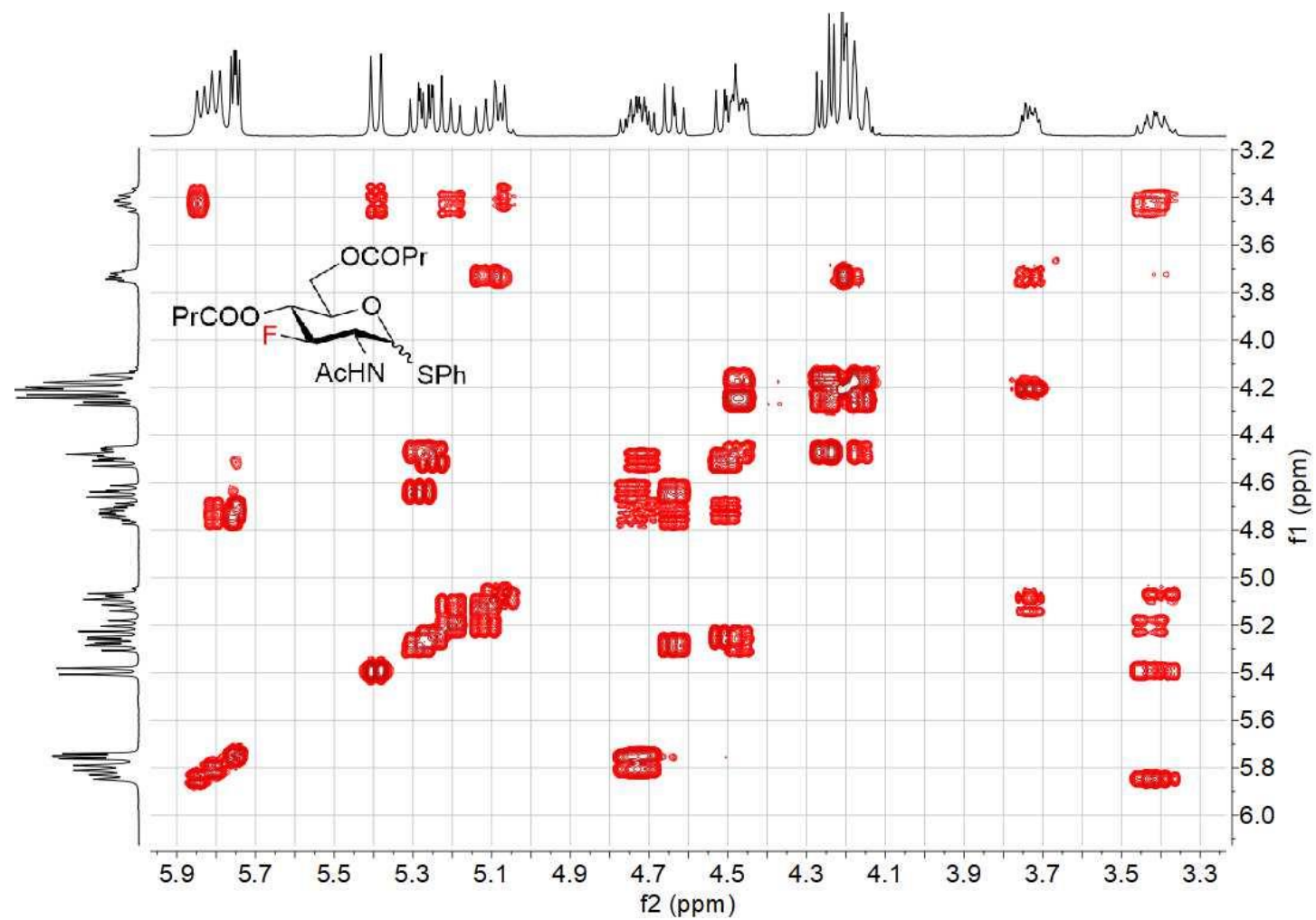
¹³C NMR (100 MHz, CDCl₃) 77



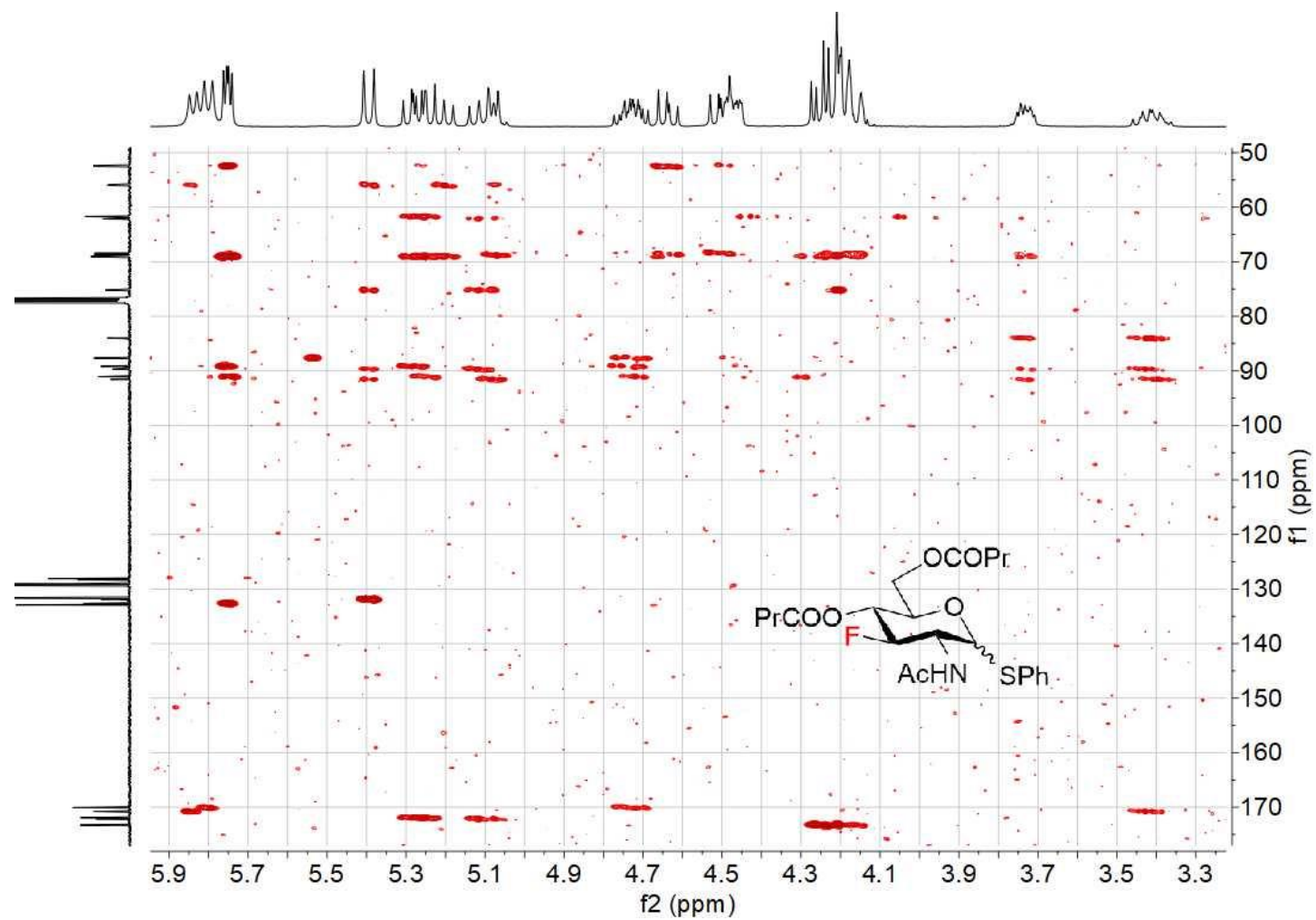
^{19}F NMR (376 MHz, CDCl_3) 77



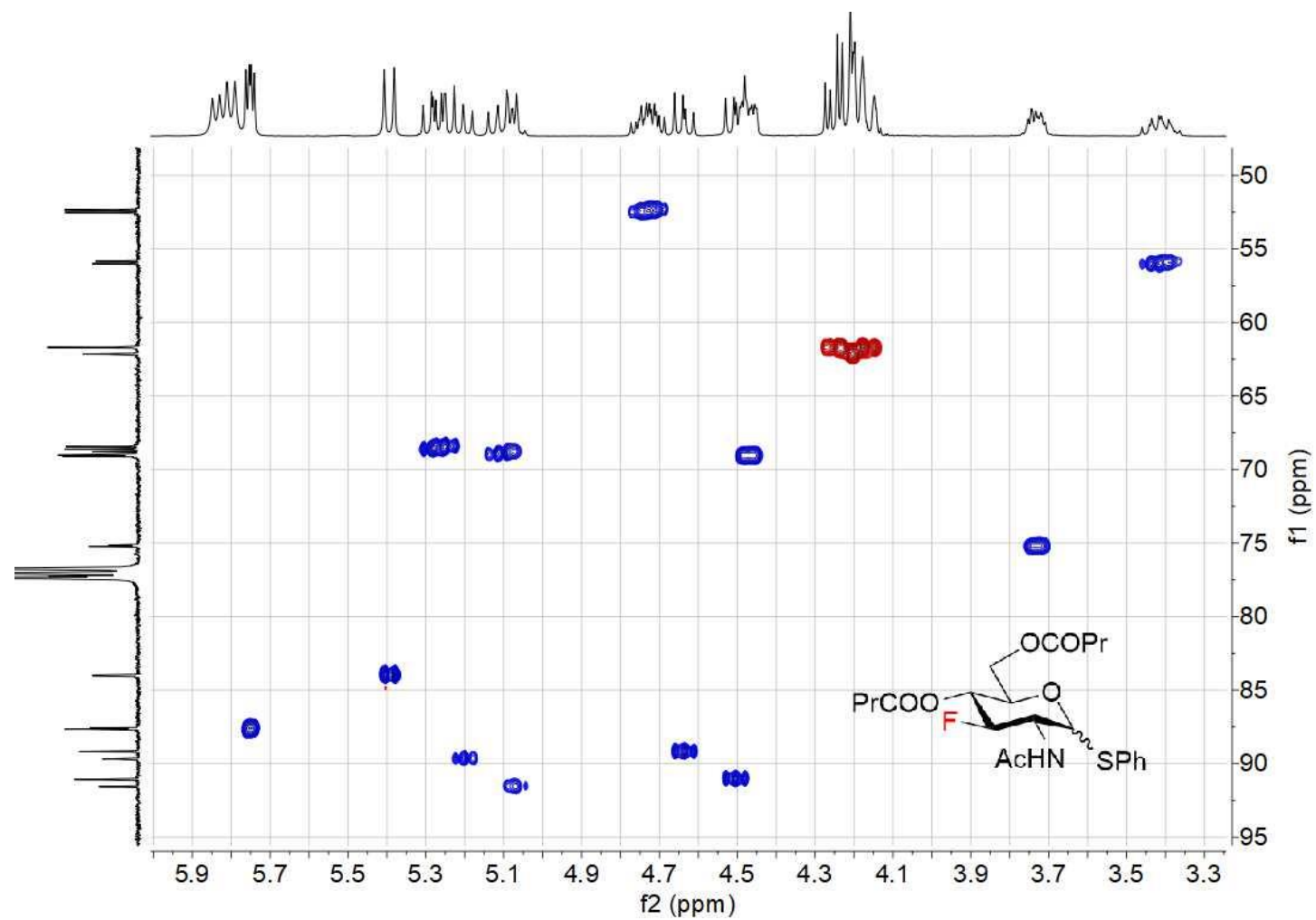
^1H - ^1H COSY 77



^1H - ^{13}C HMBC 77

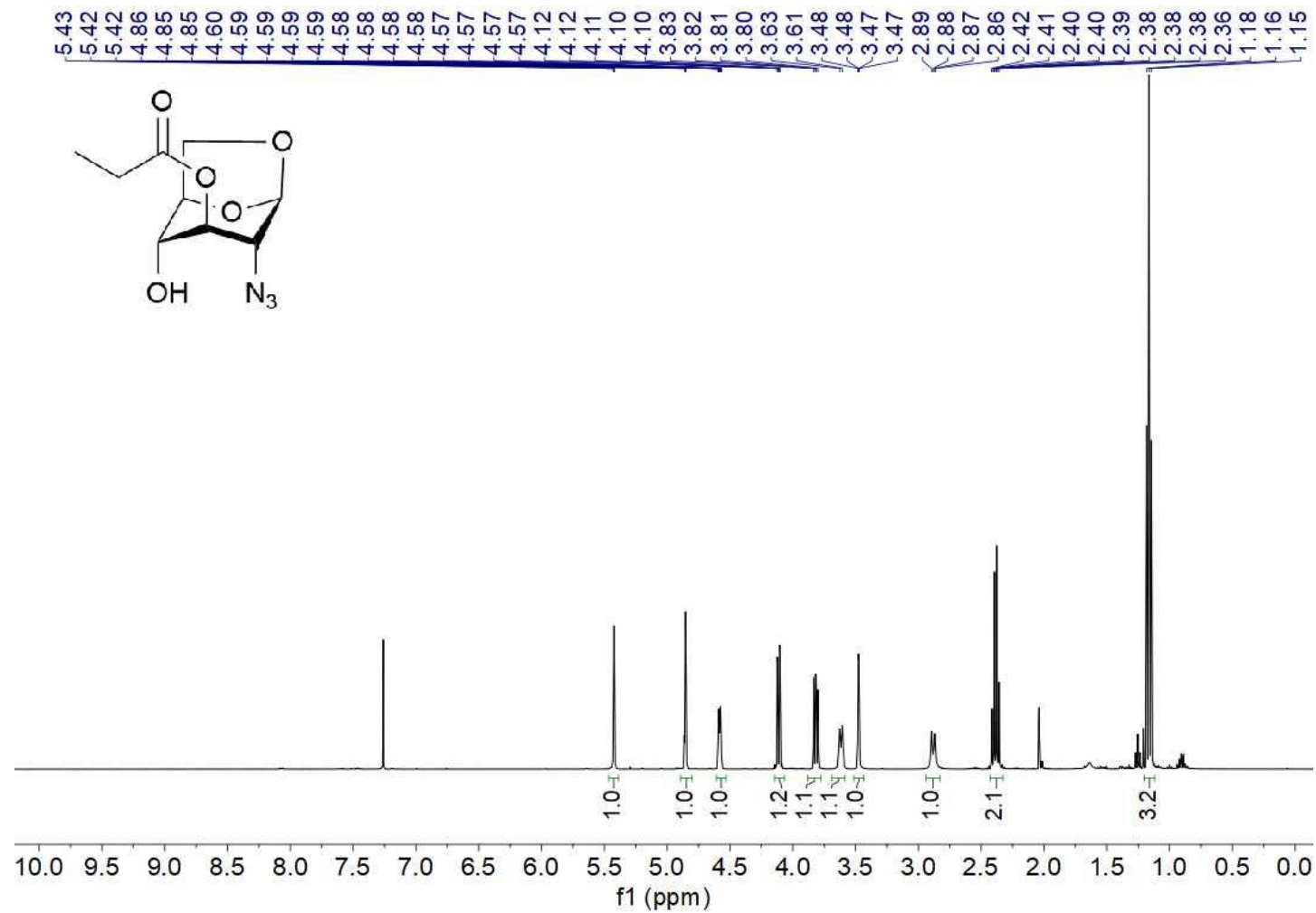


^1H - ^{13}C HSQC 77

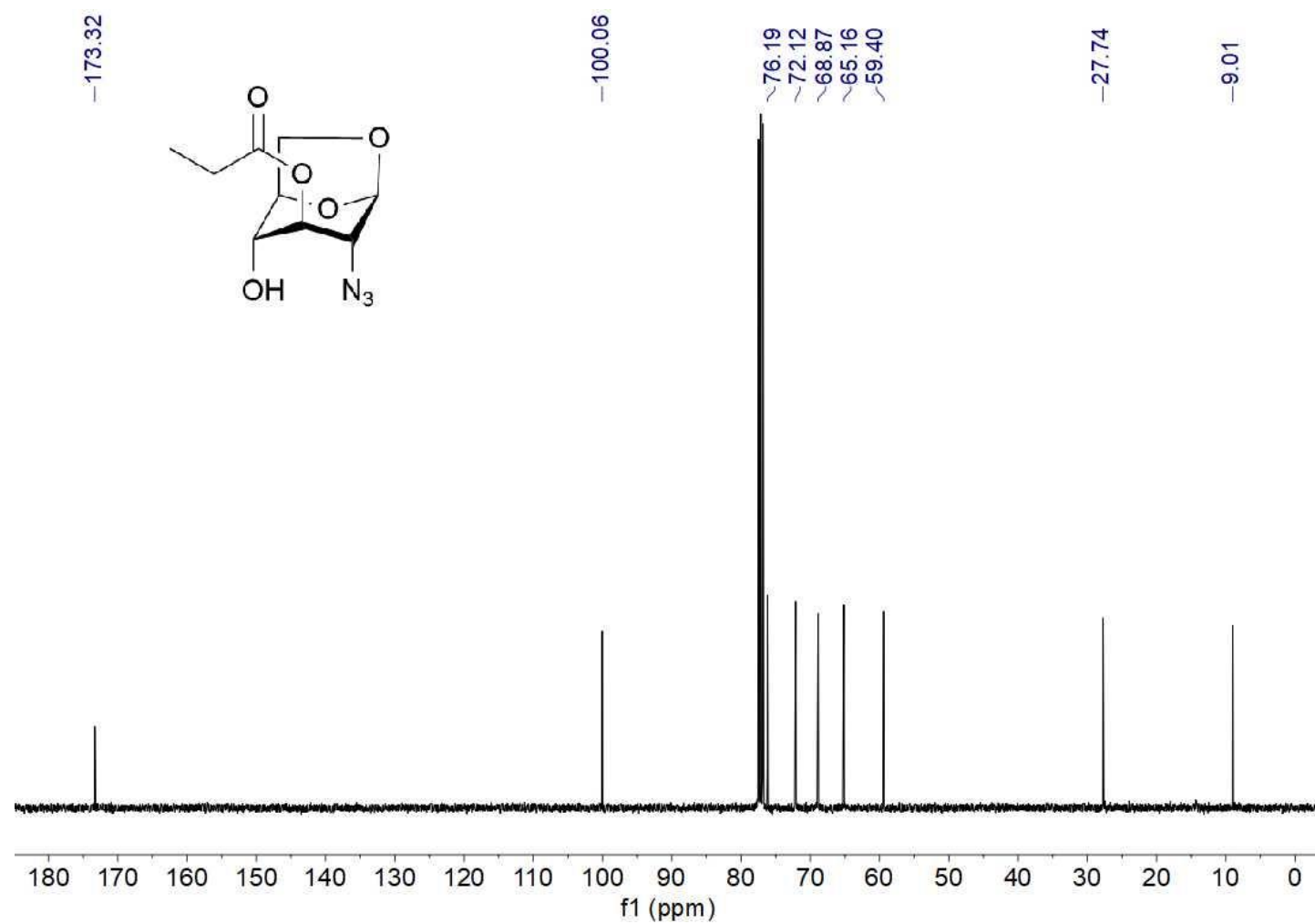


NMR COMPOUND 79

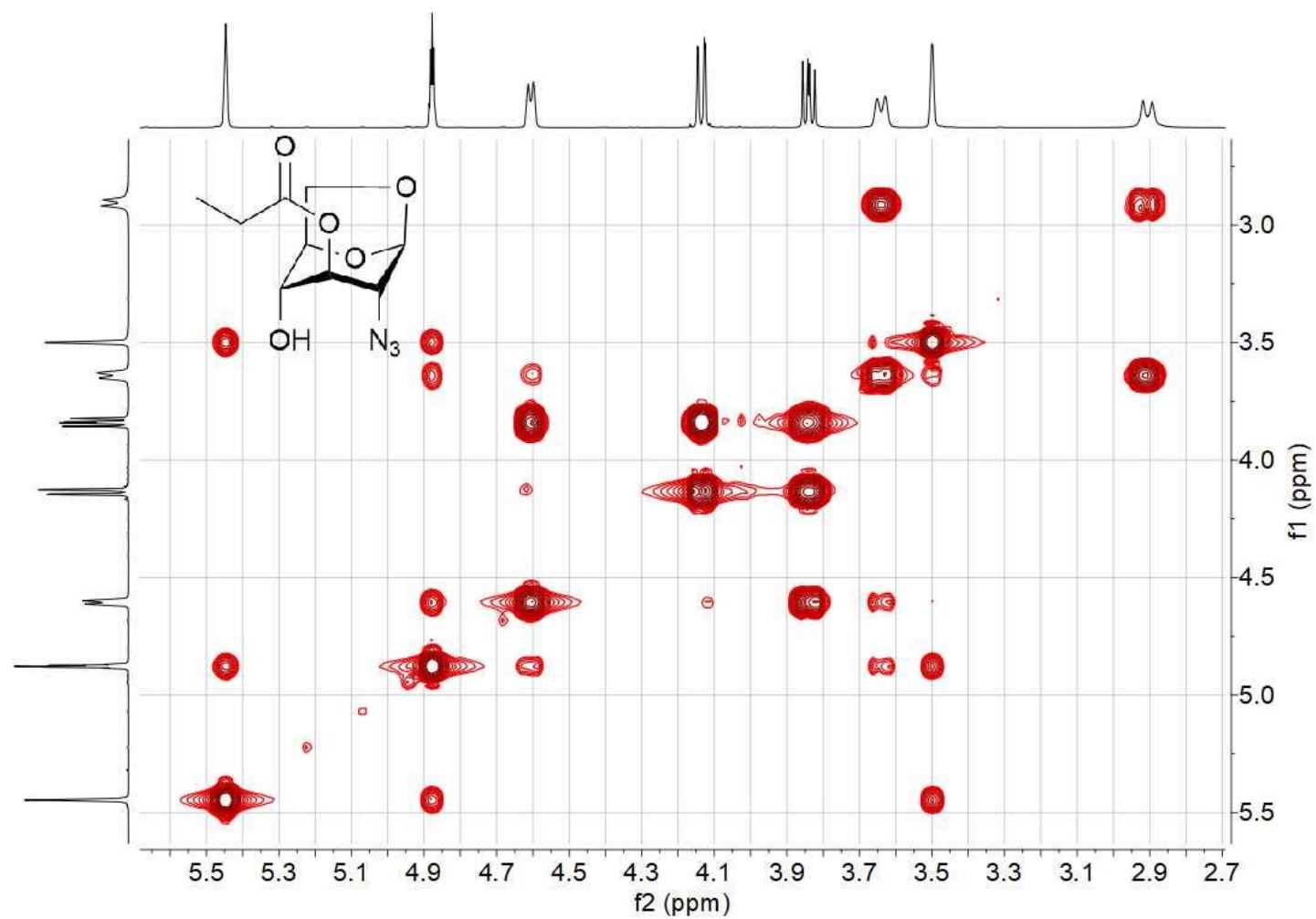
¹H NMR (400 MHz, CDCl₃) 79



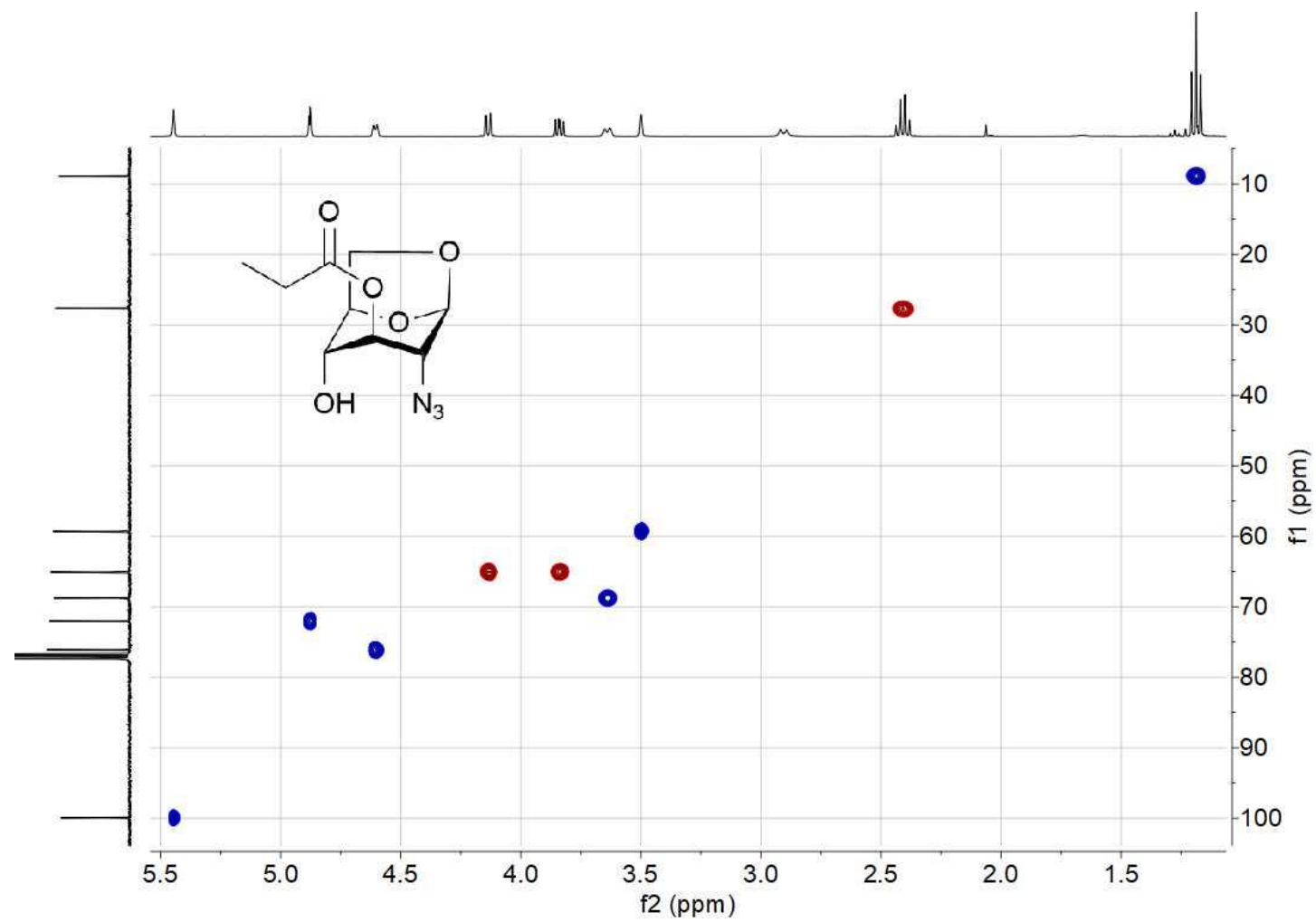
^{13}C NMR (100 MHz, CDCl_3) 79



¹H-¹H COSY 79

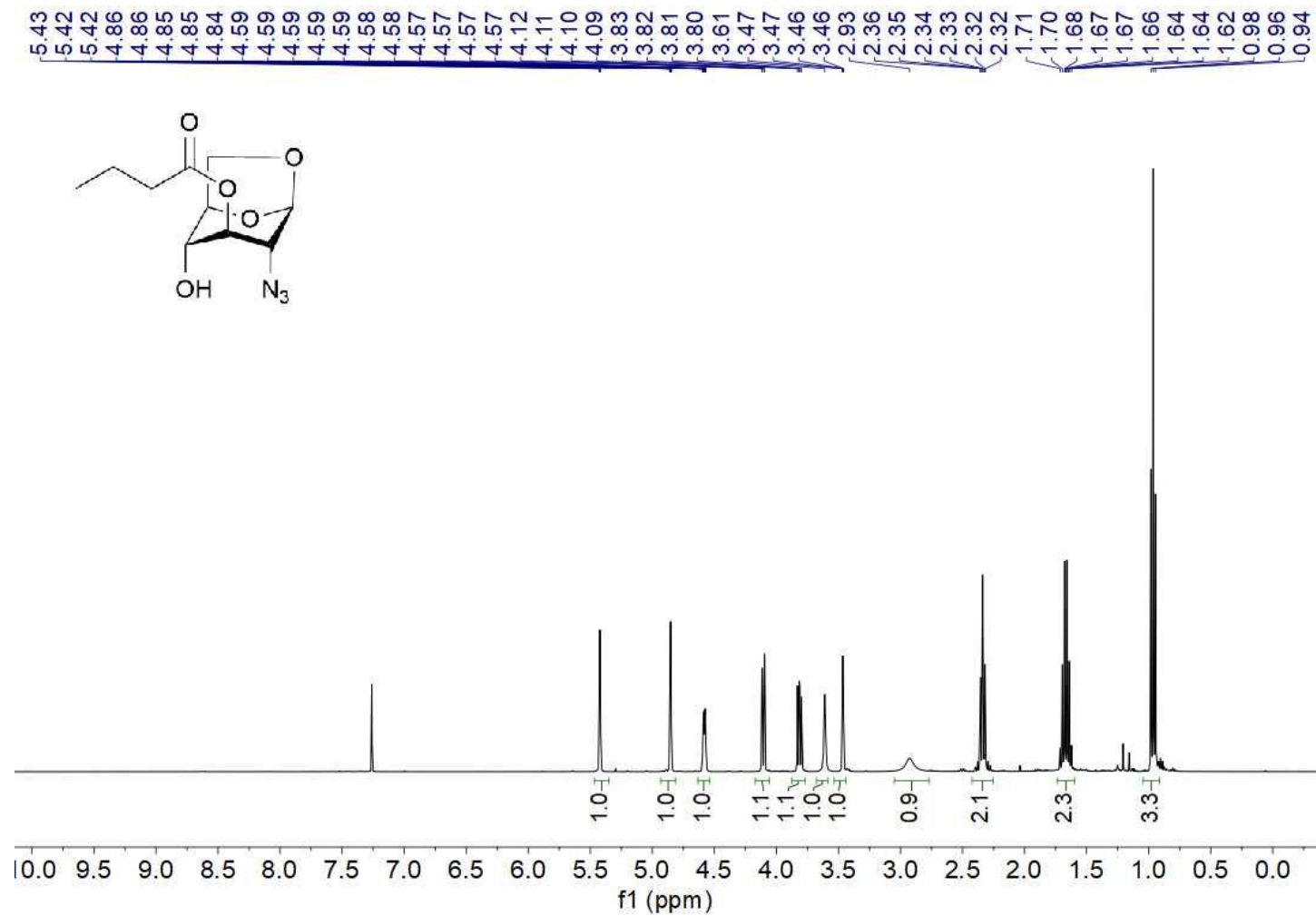


^1H - ^{13}C HSQC 79

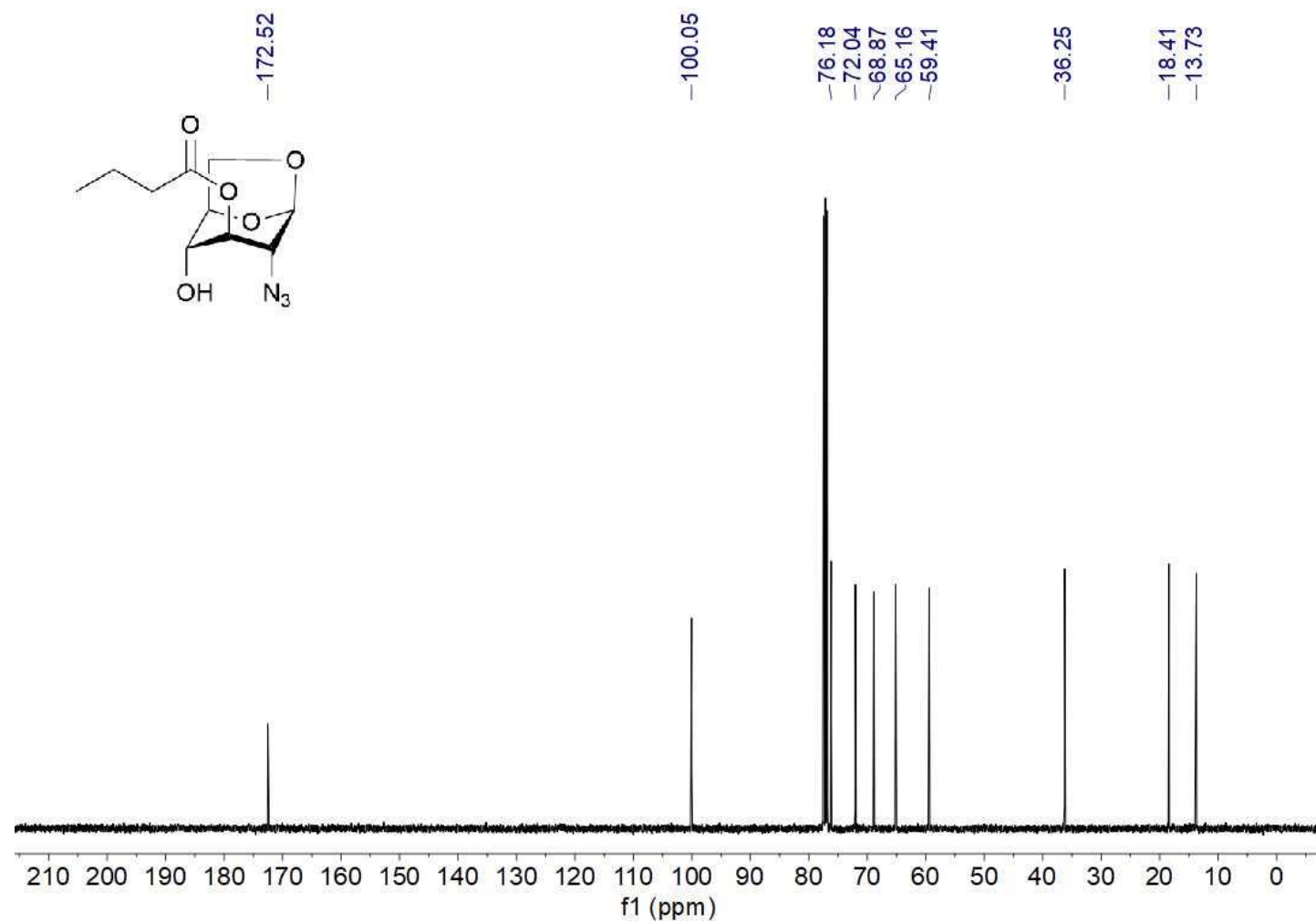


NMR COMPOUND 80

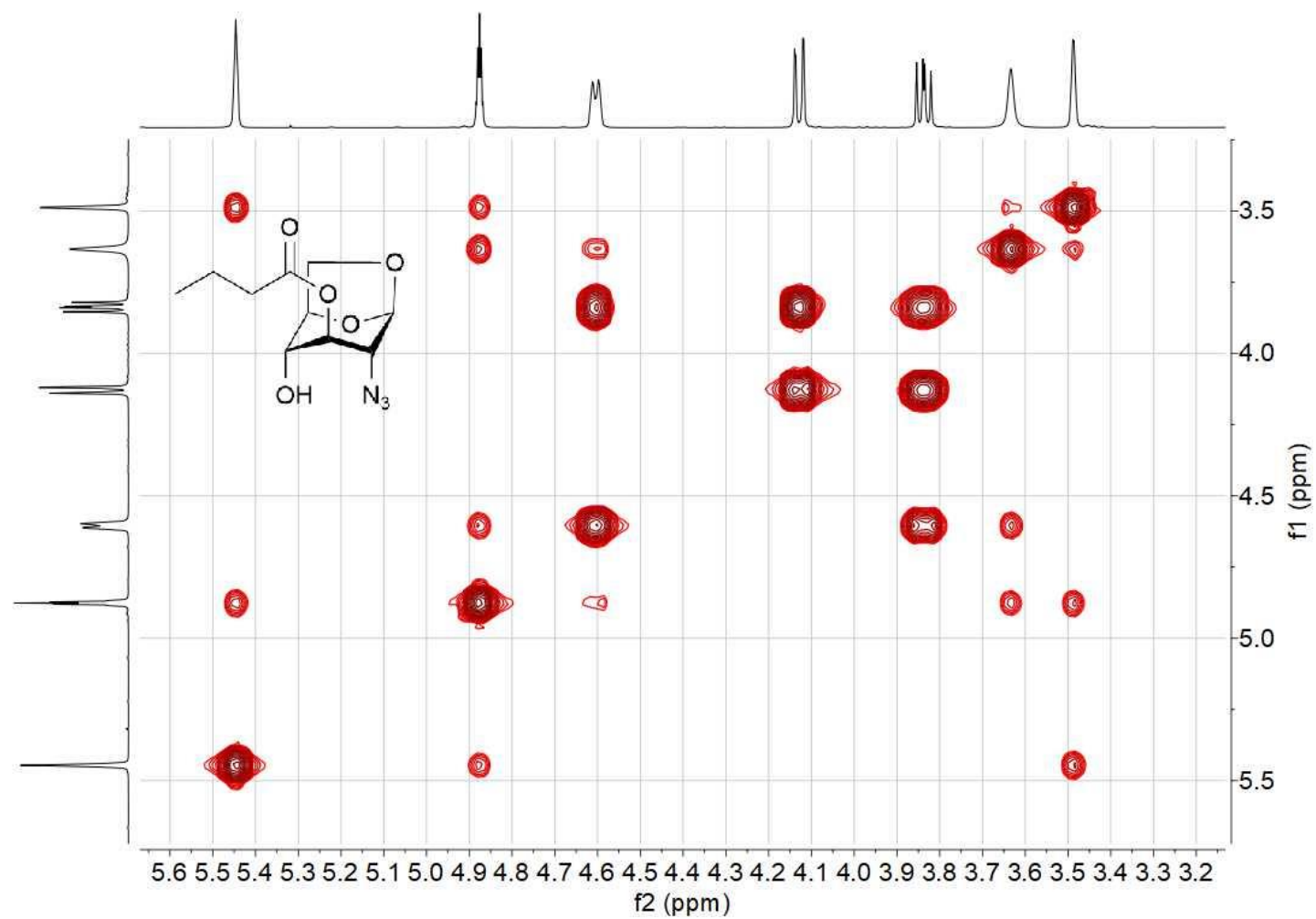
¹H NMR (400 MHz, CDCl₃) 80



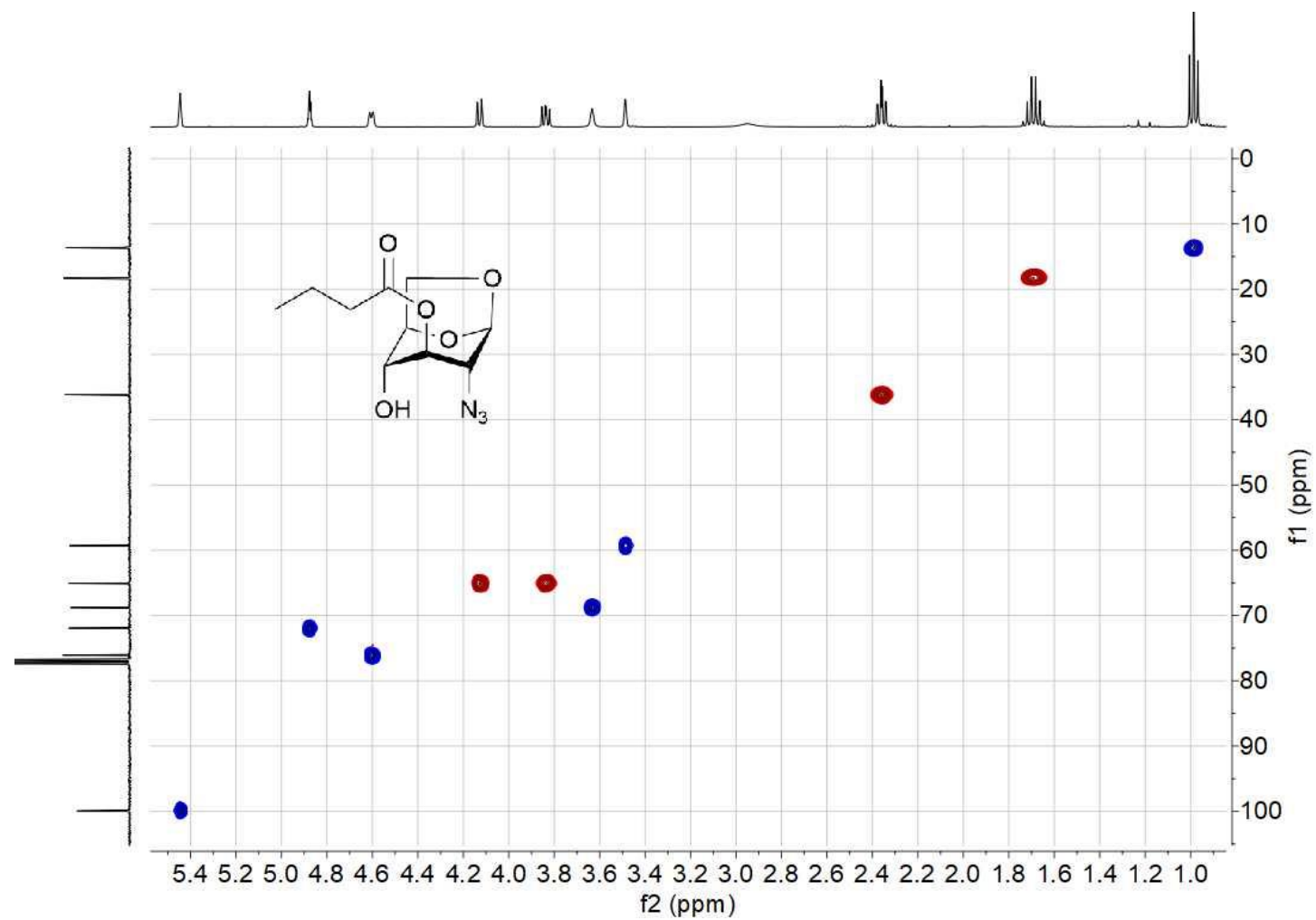
^{13}C NMR (100 MHz, CDCl_3) 80



¹H-¹H COSY 80

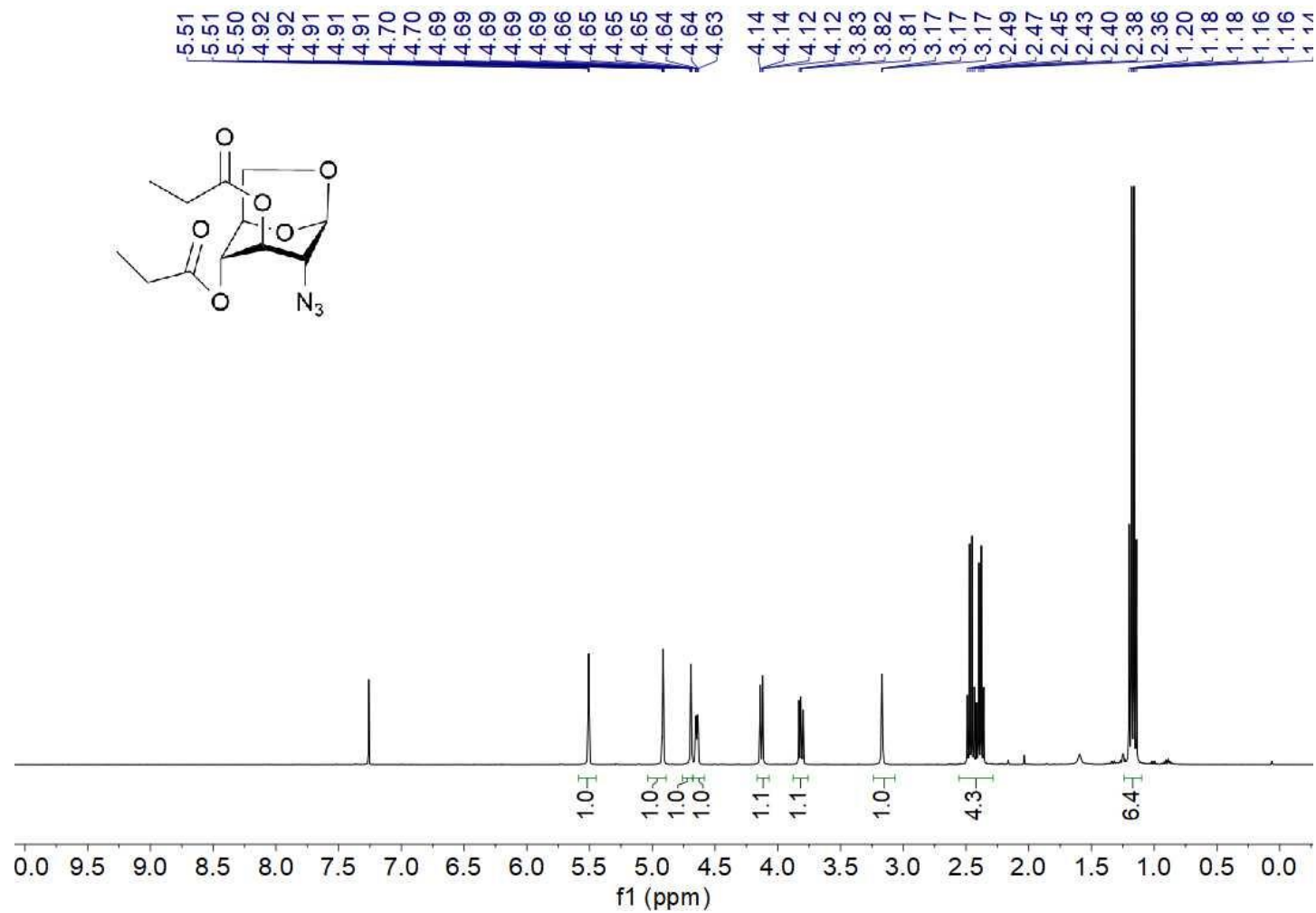


^1H - ^{13}C HSQC 80

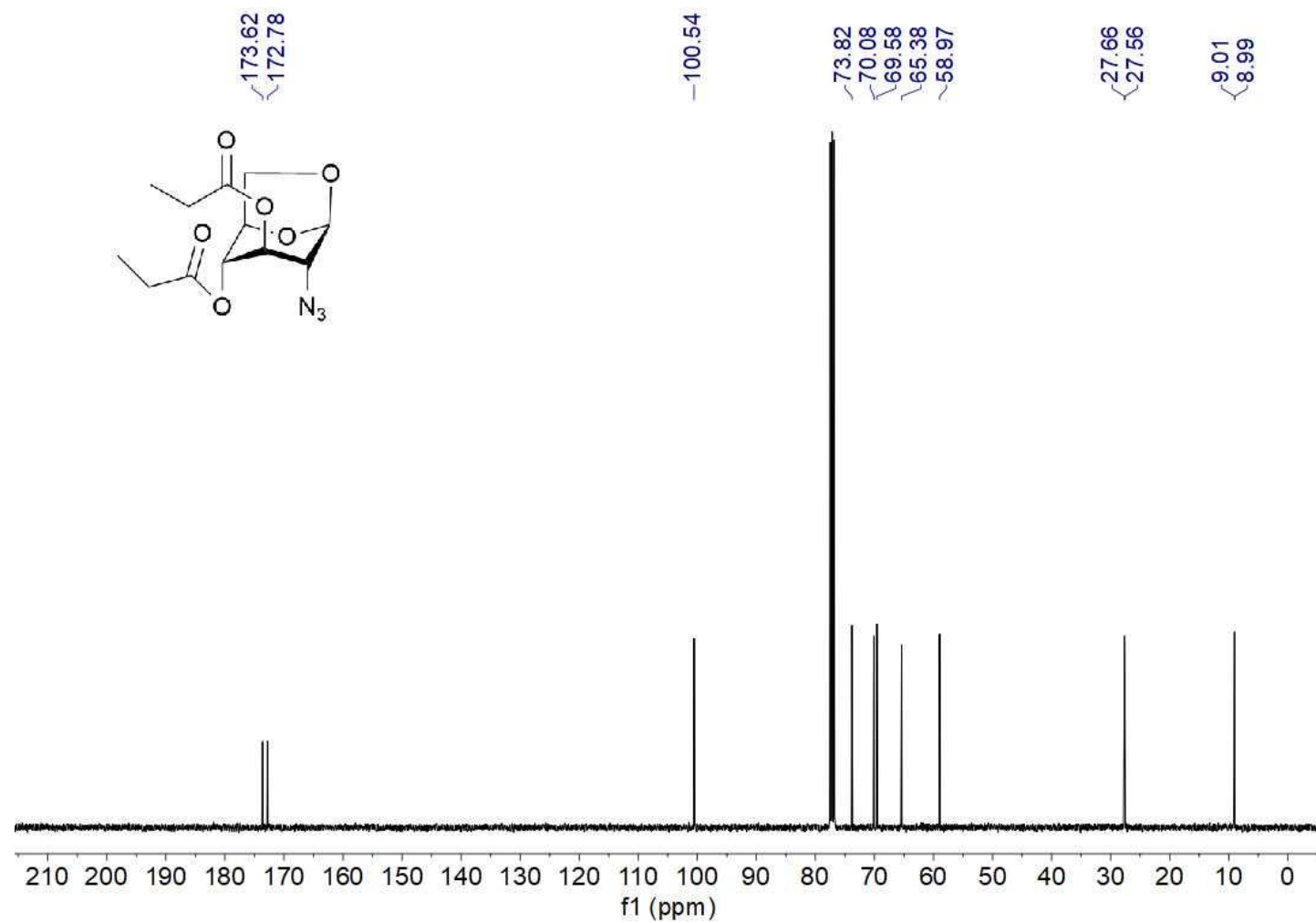


NMR COMPOUND 81

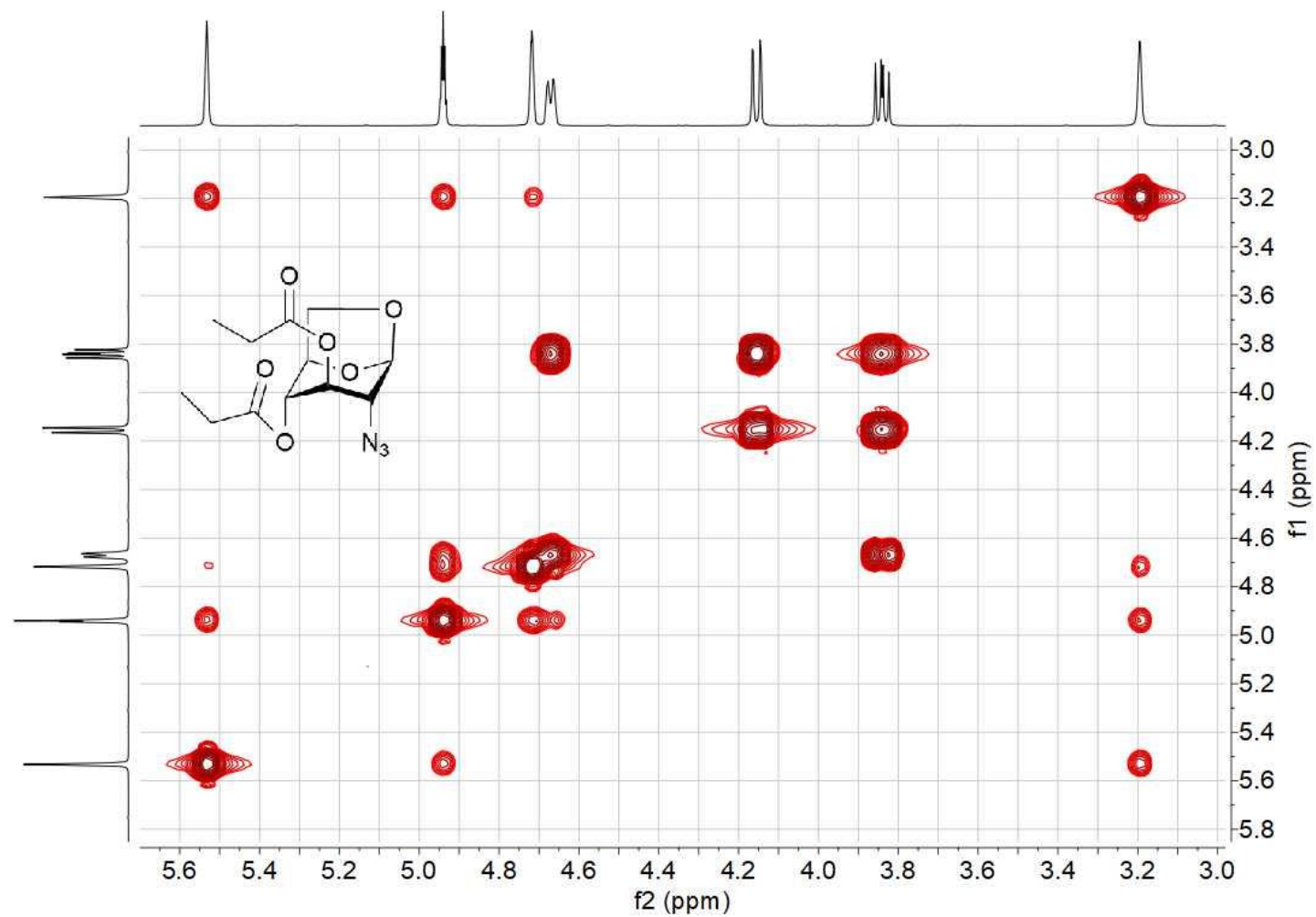
¹H NMR (400 MHz, CDCl₃) 81



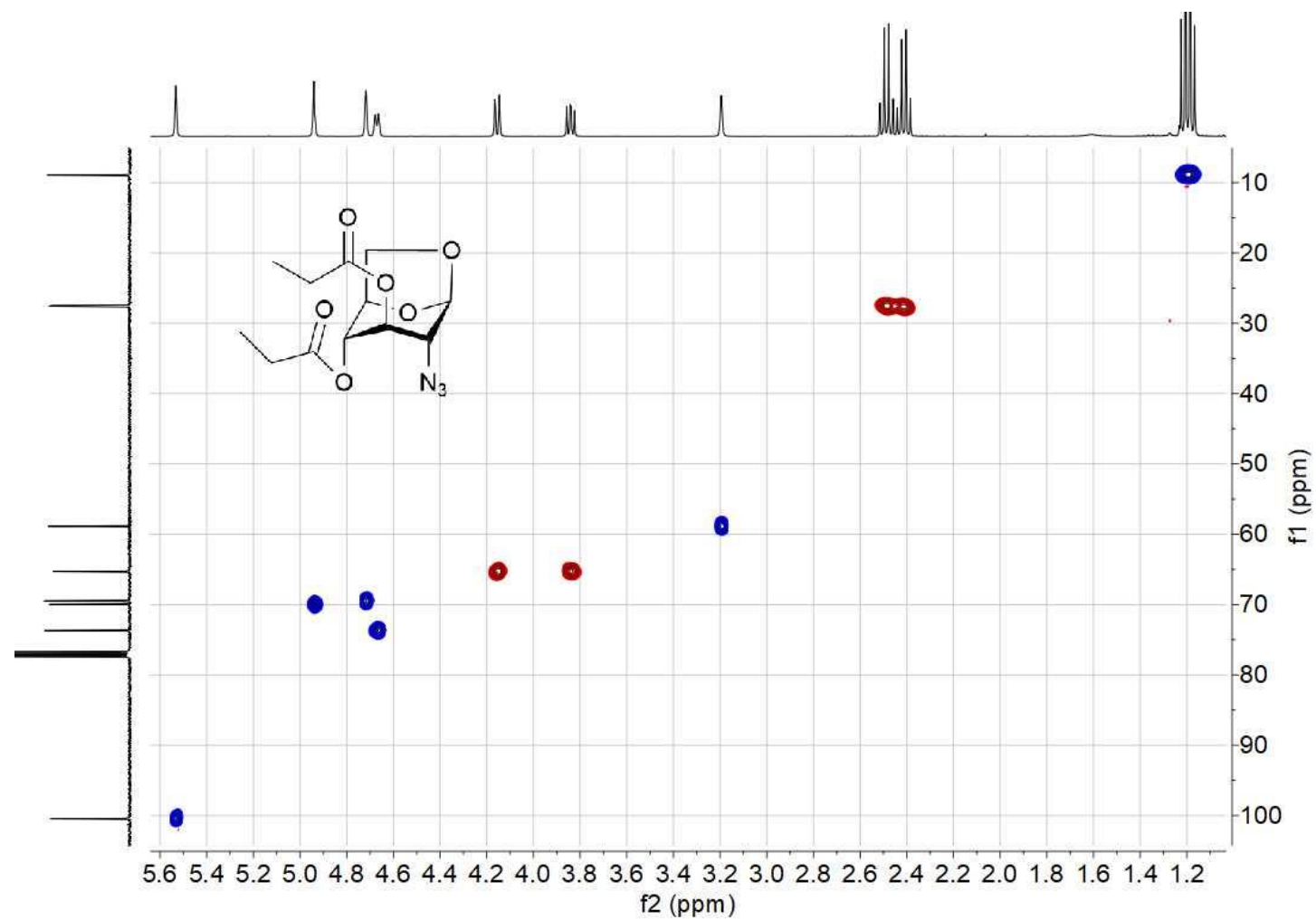
^{13}C NMR (100 MHz, CDCl_3) 81



¹H-¹H COSY 81

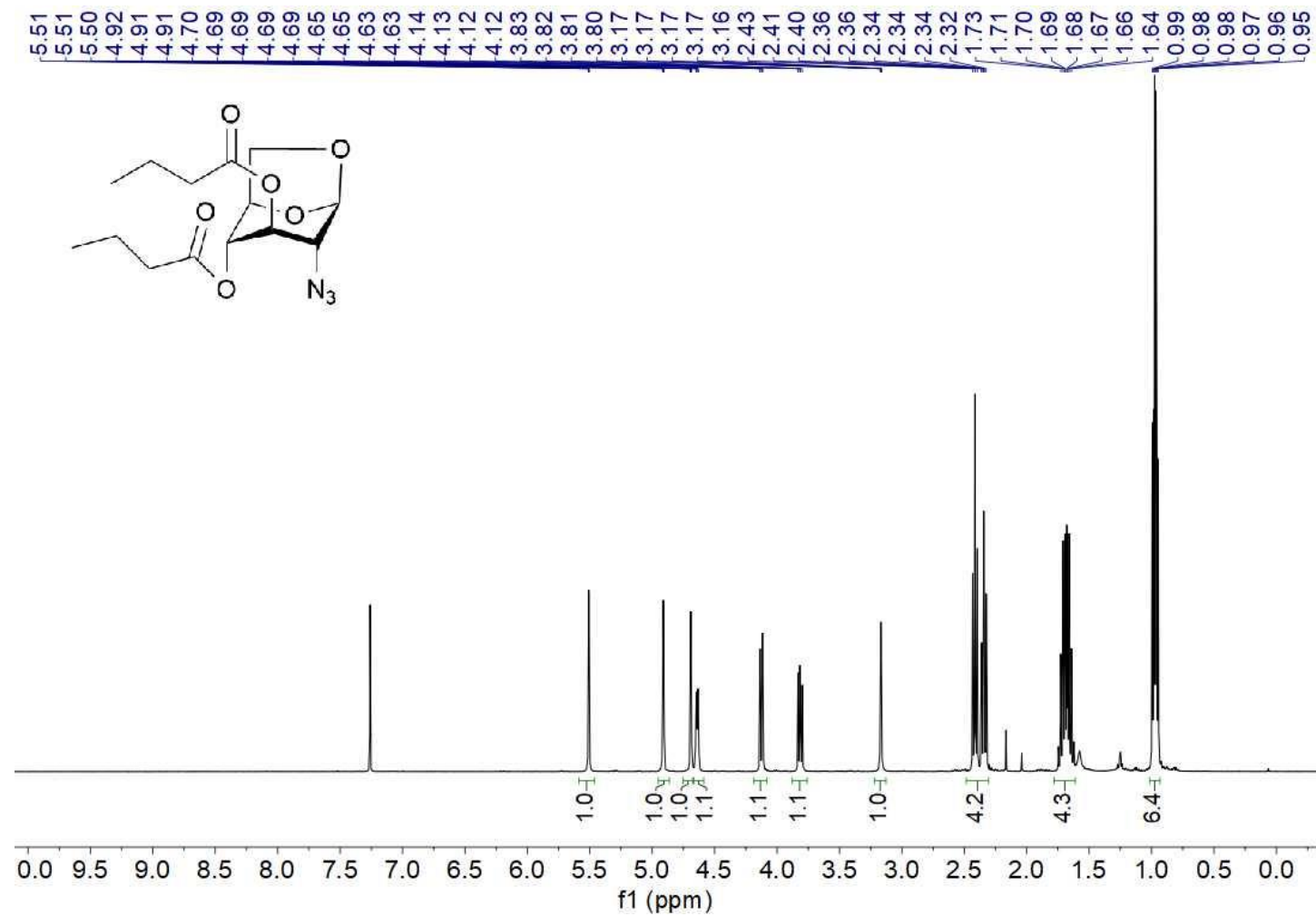


^1H - ^{13}C HSQC 81

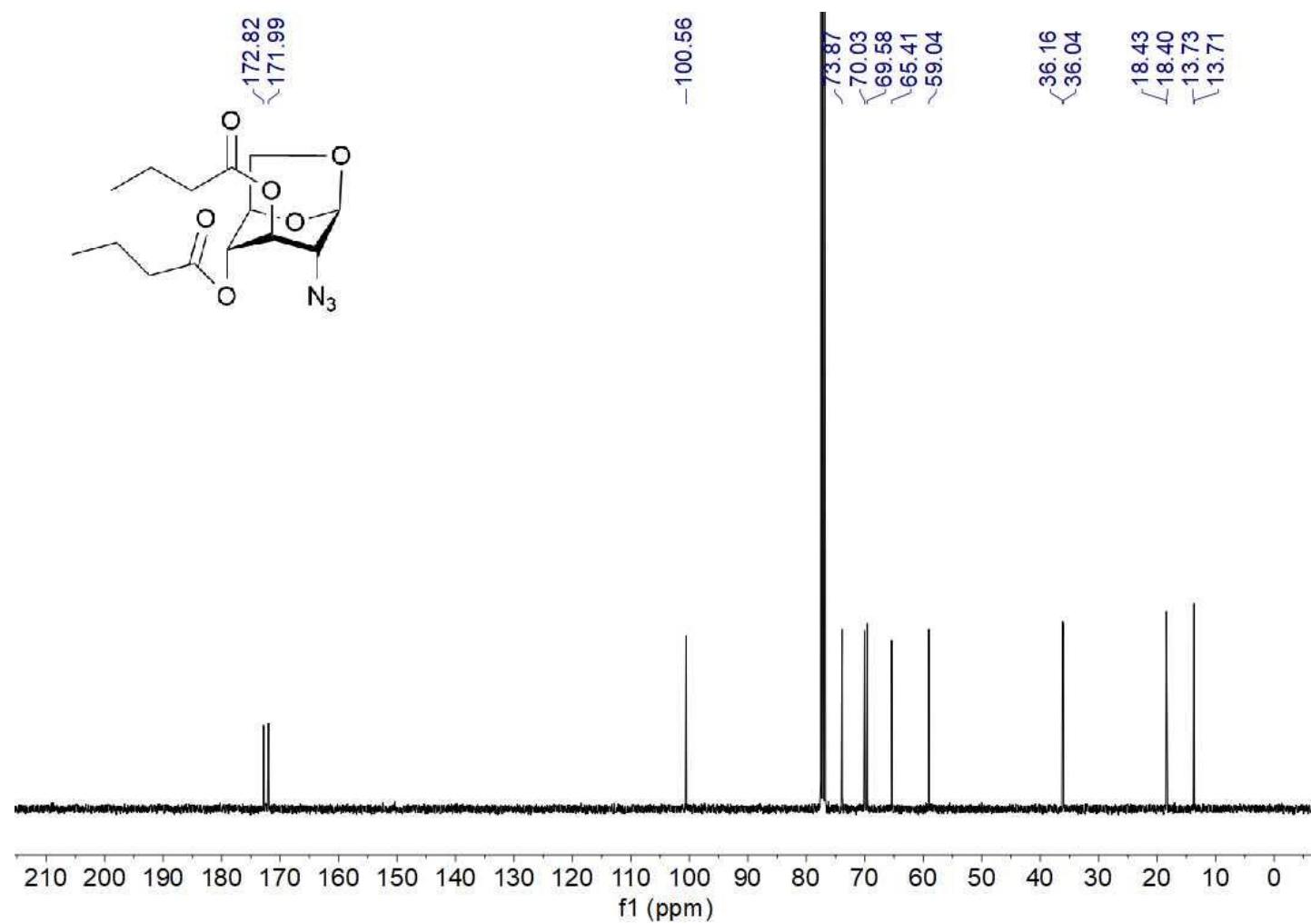


NMR COMPOUND 82

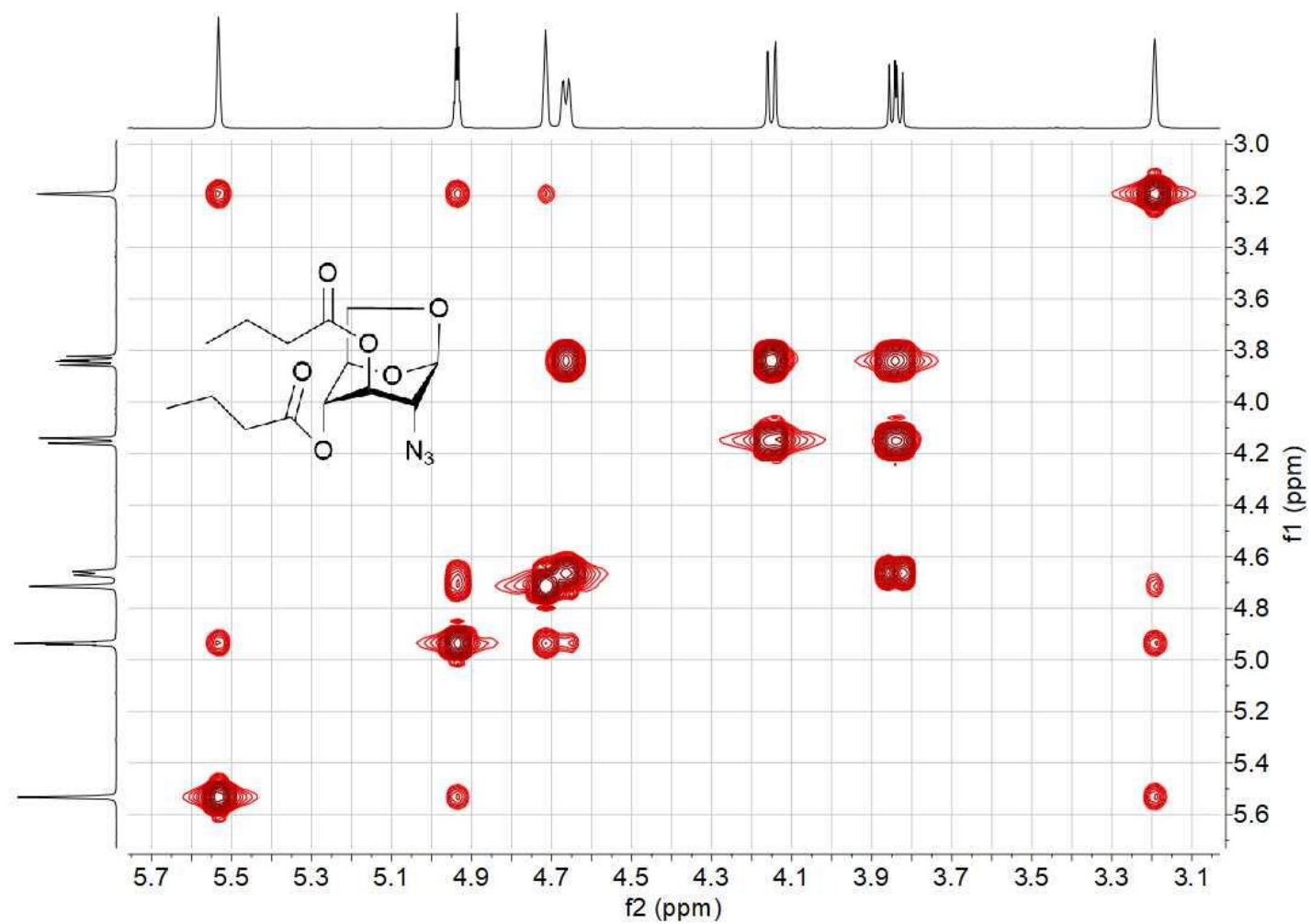
¹H NMR (400 MHz, CDCl₃) 82



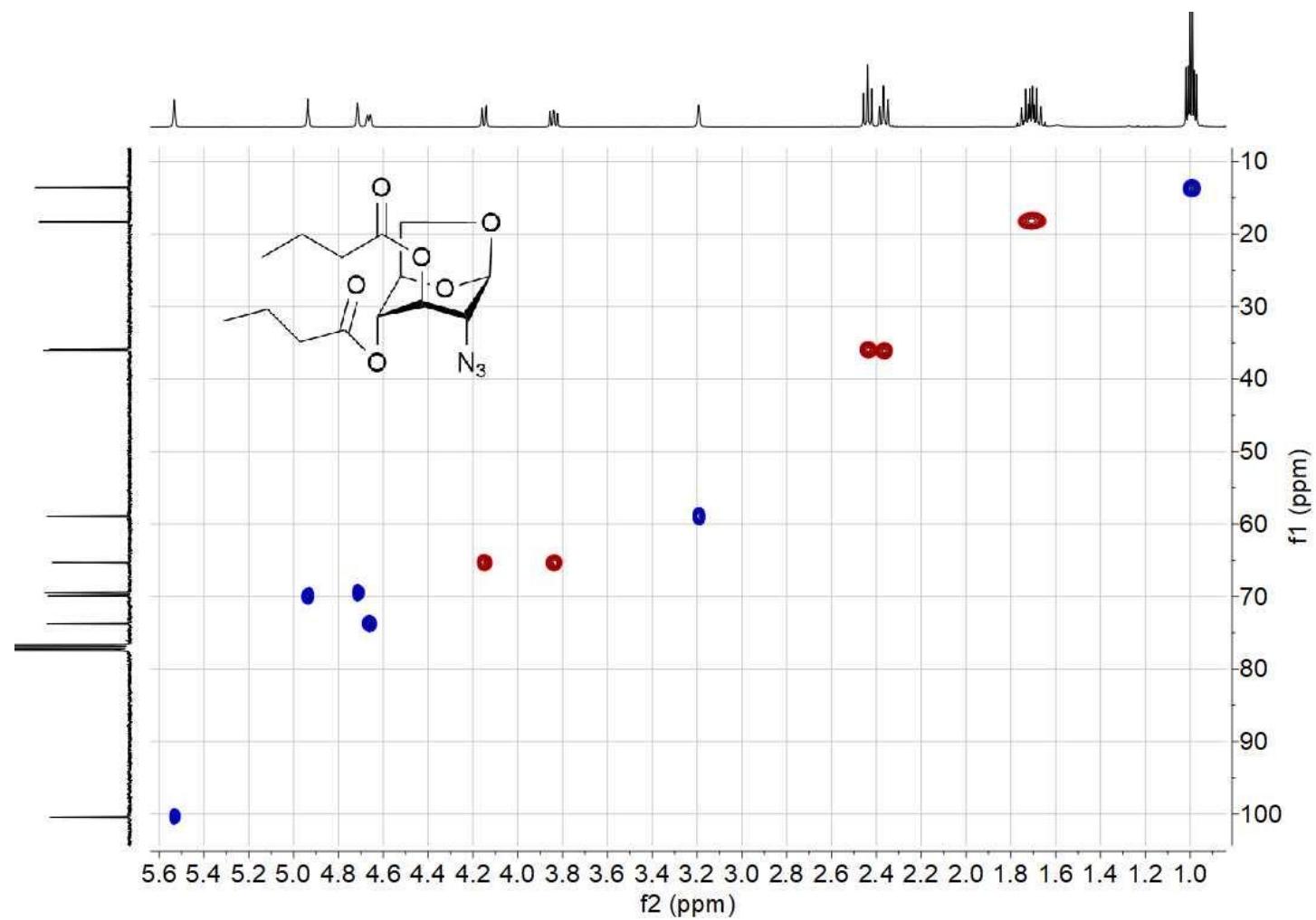
^{13}C NMR (100 MHz, CDCl_3) 82



^1H - ^1H COSY 82

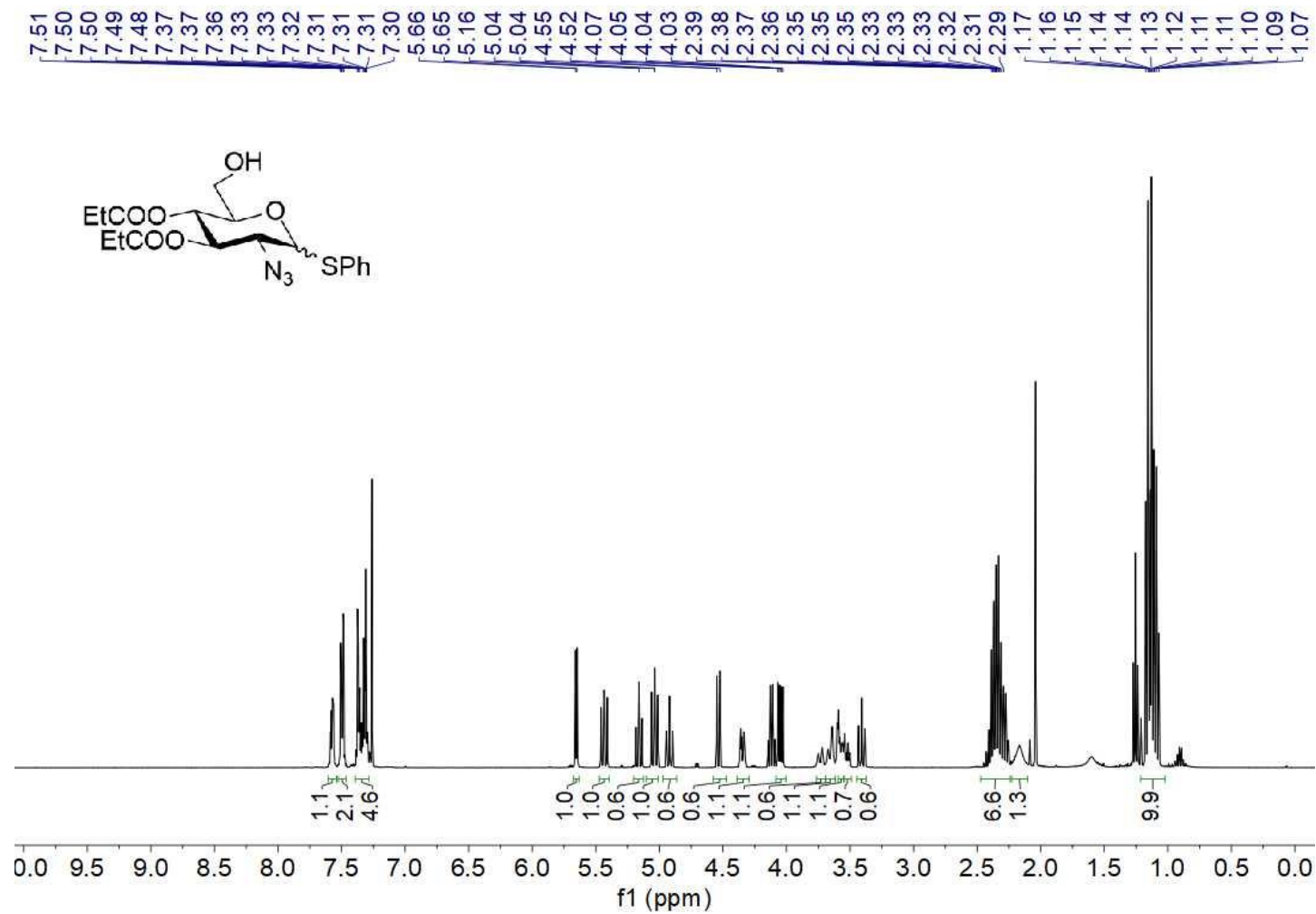


^1H - ^{13}C HSQC 82

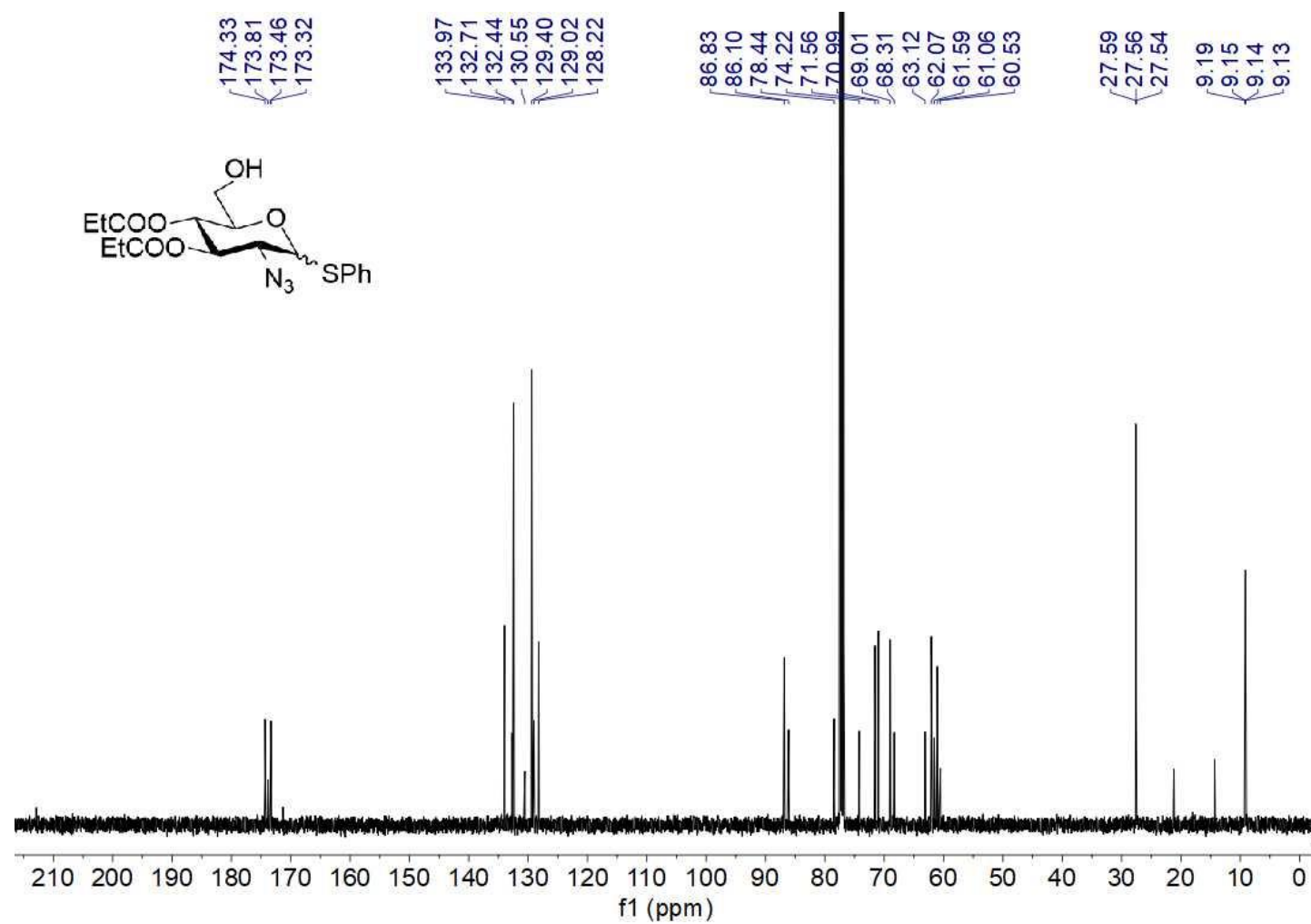


NMR COMPOUND 83

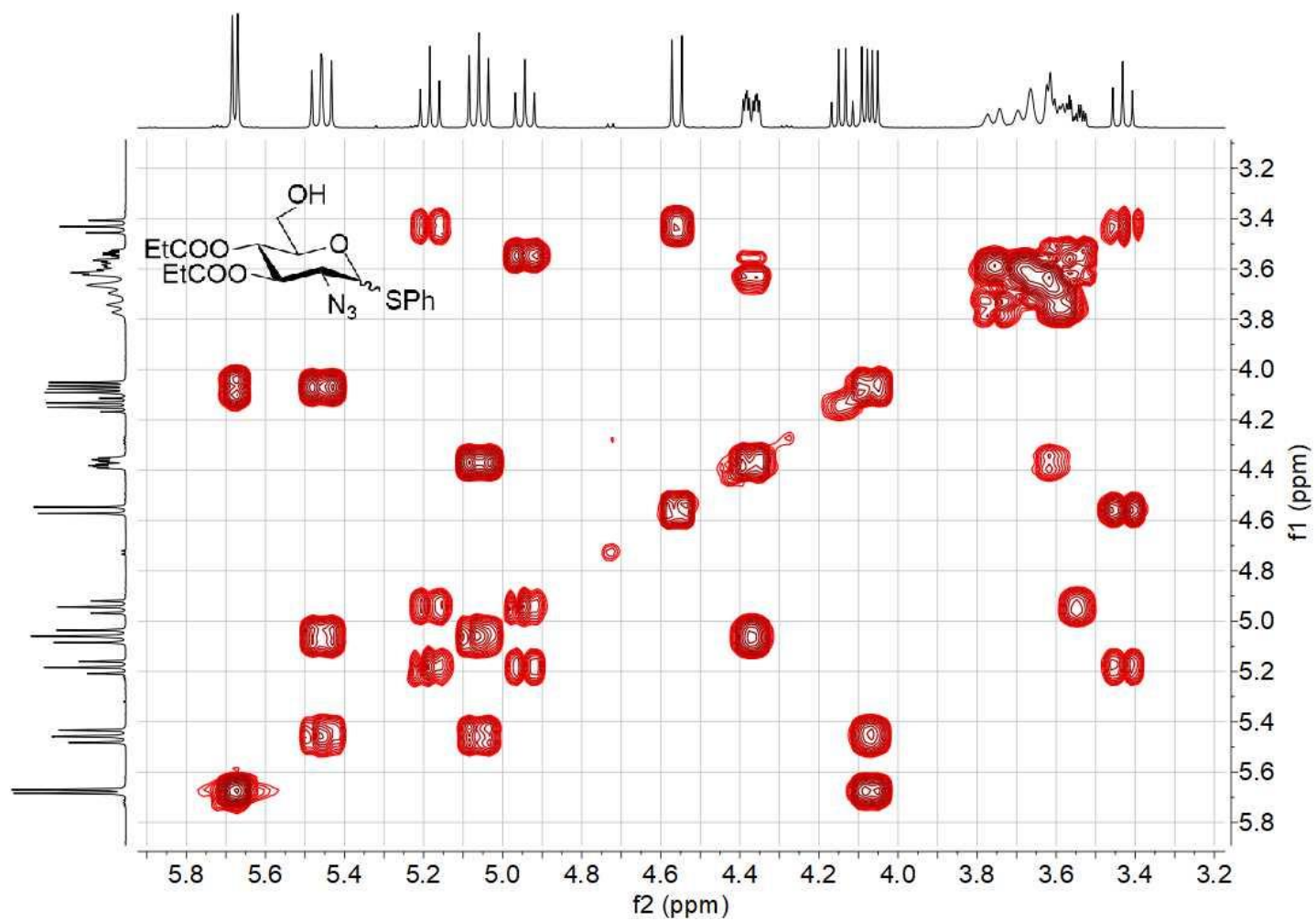
¹H NMR (400 MHz, CDCl₃) 83



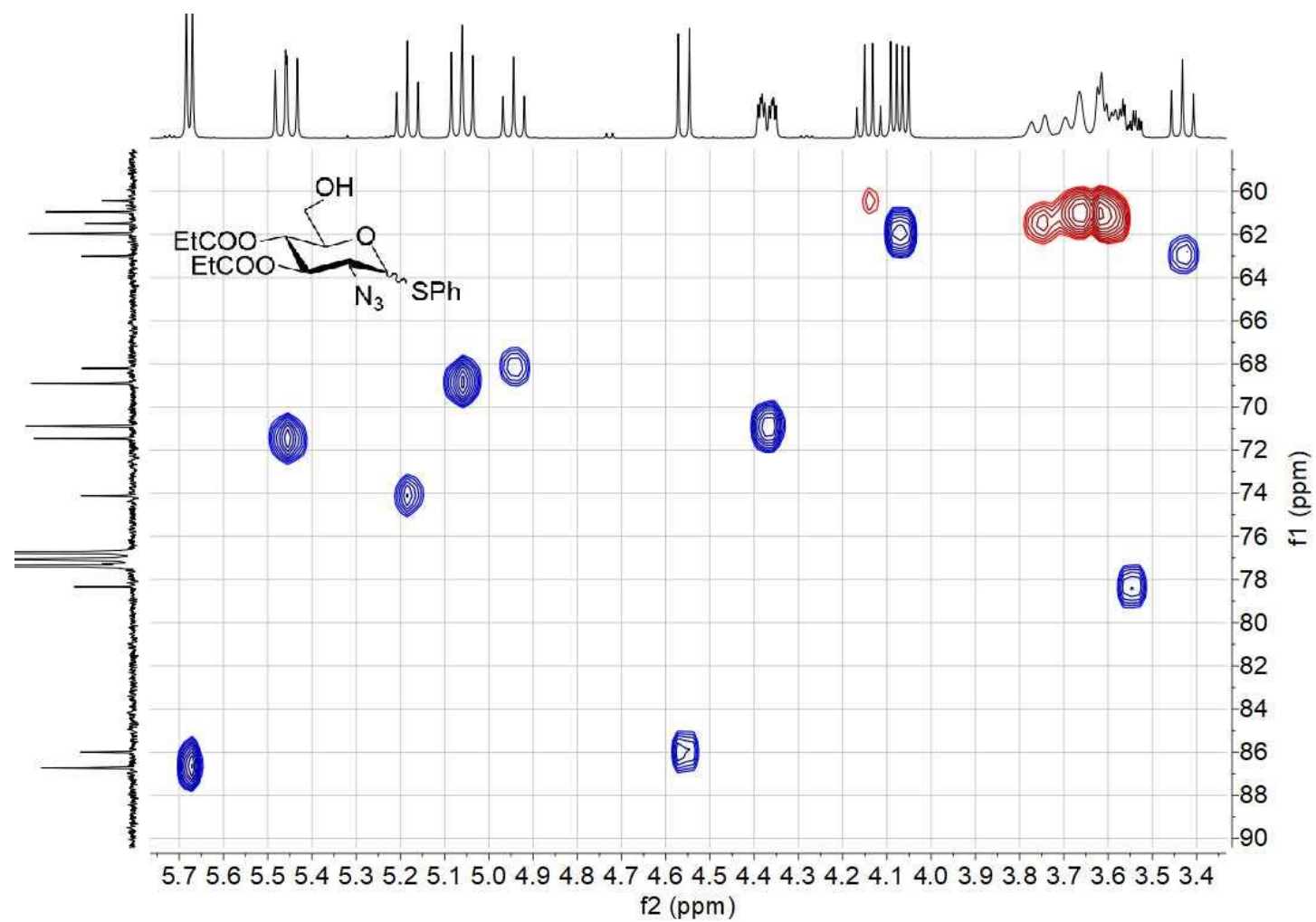
¹³C NMR (100 MHz, CDCl₃) 83



^1H - ^1H COSY 83

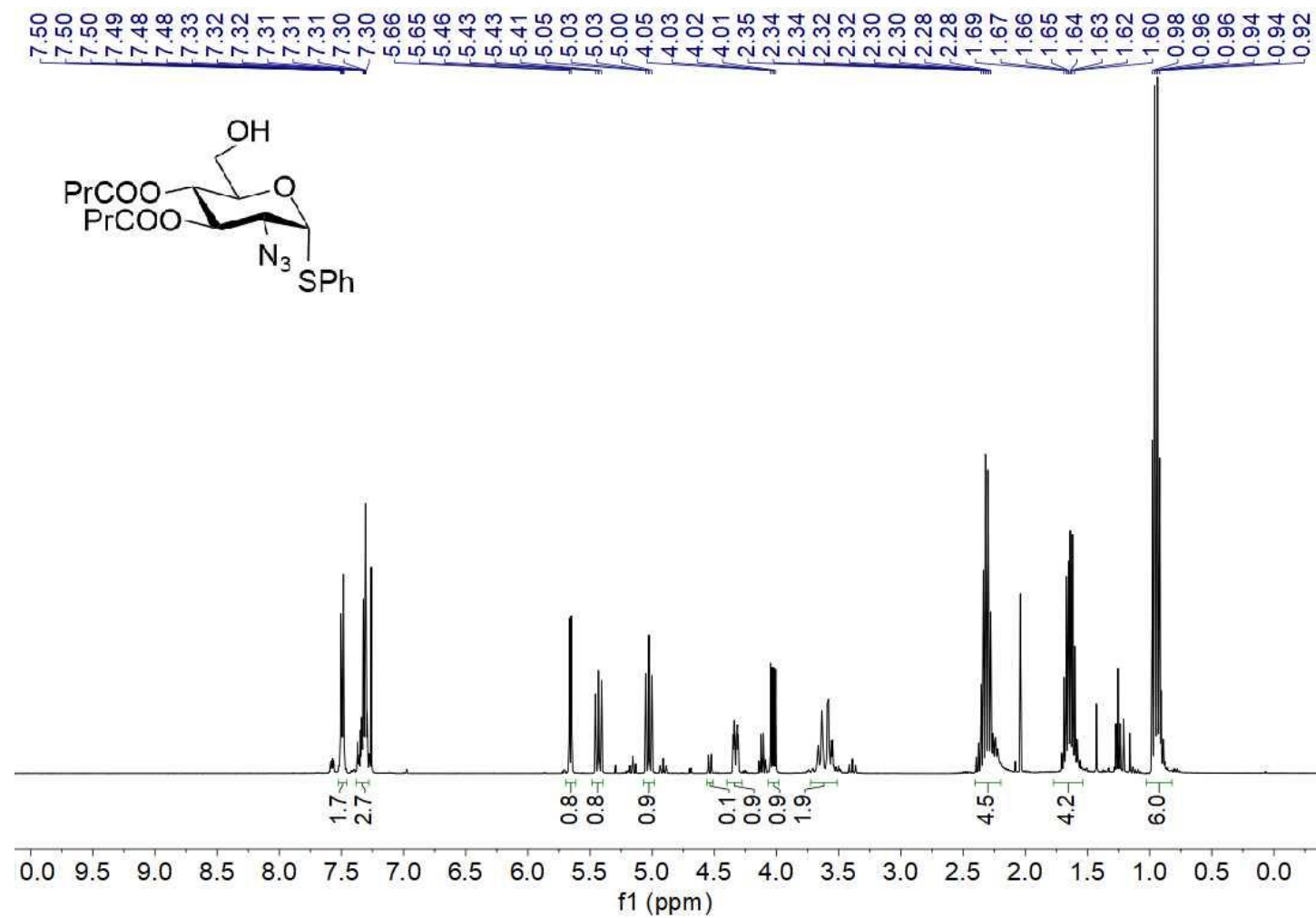


^1H - ^{13}C HSQC 83

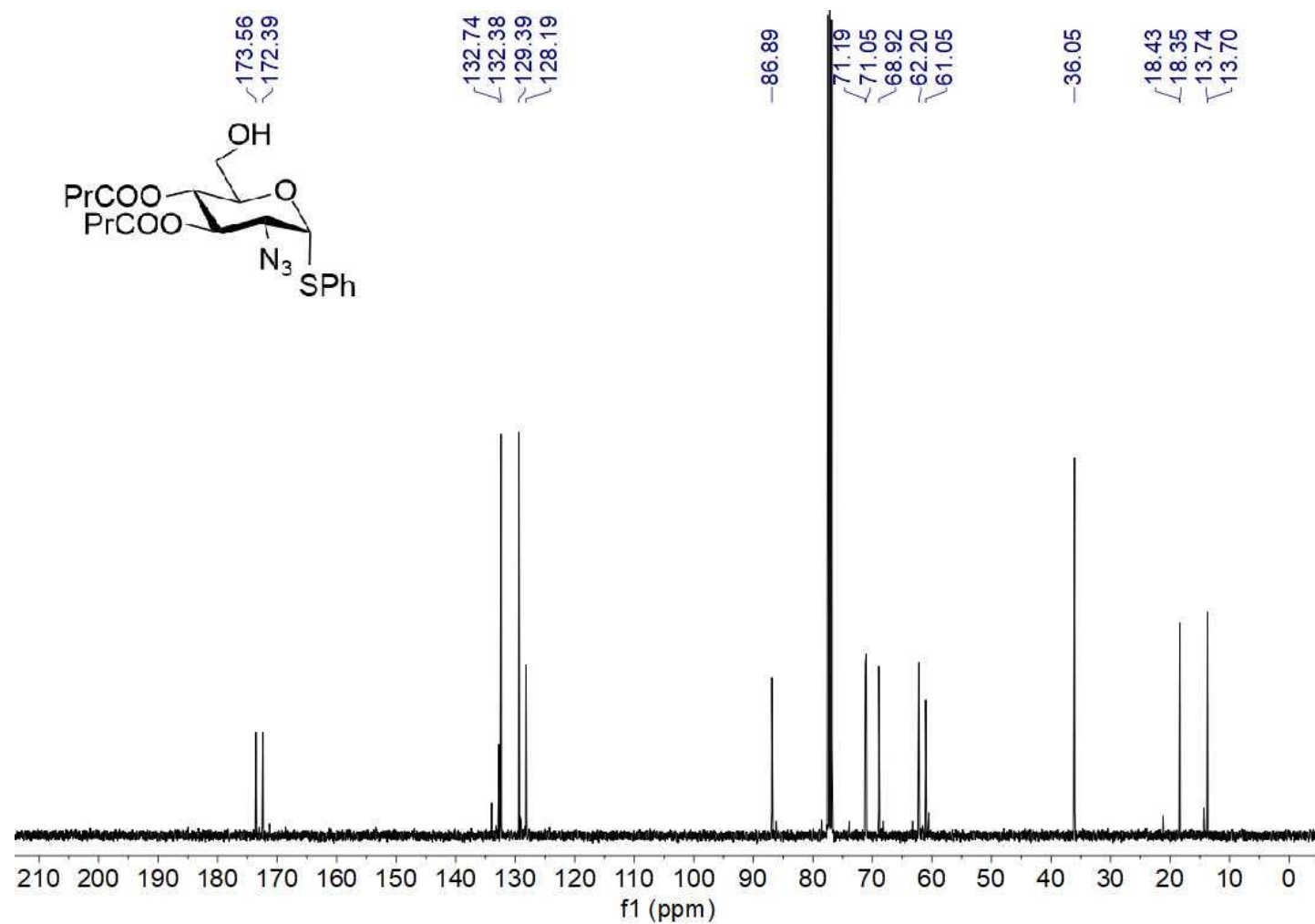


NMR COMPOUND 84 (enriched α -anomer)

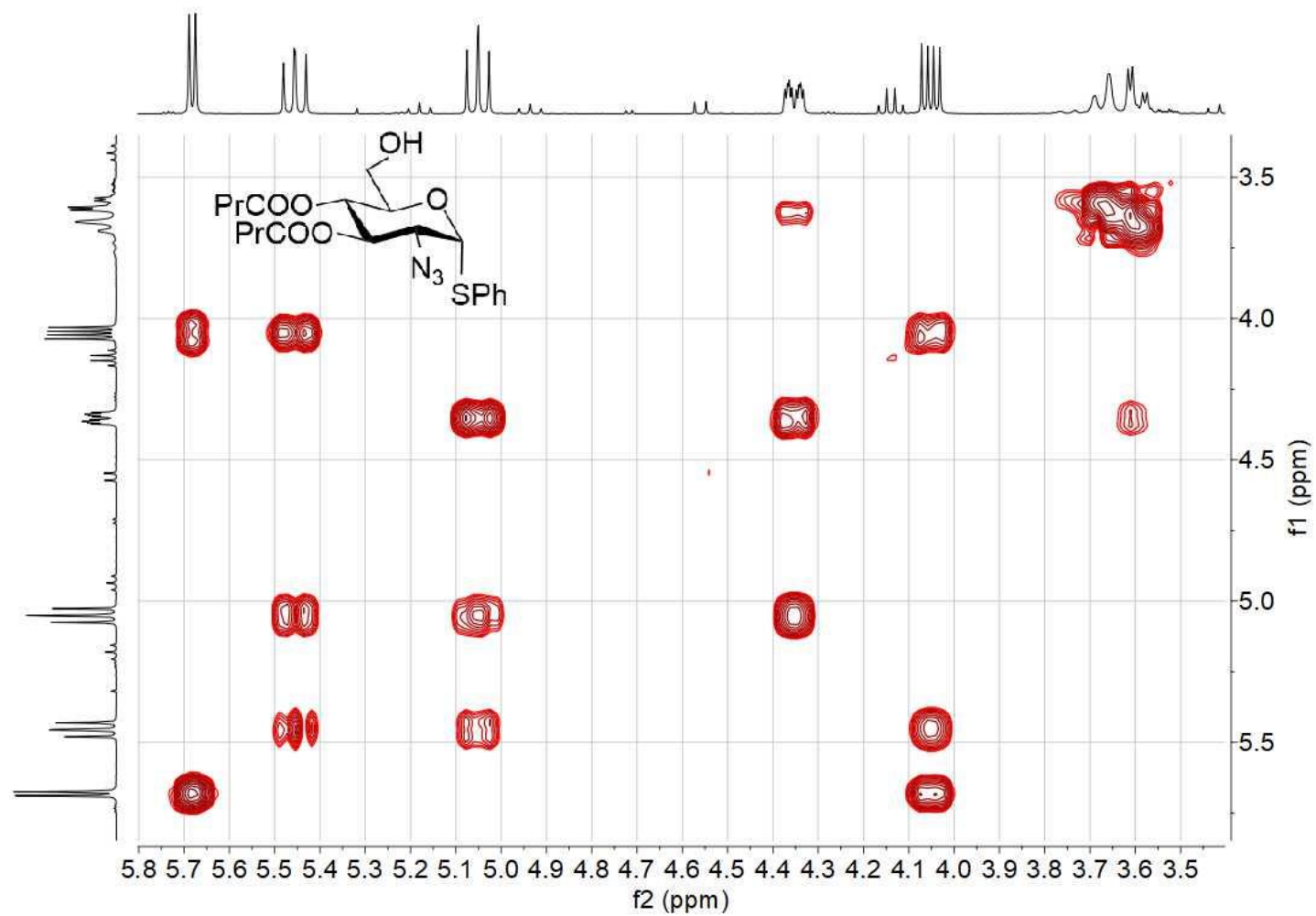
^1H NMR (400 MHz, CDCl_3) 84 (enriched α -anomer)



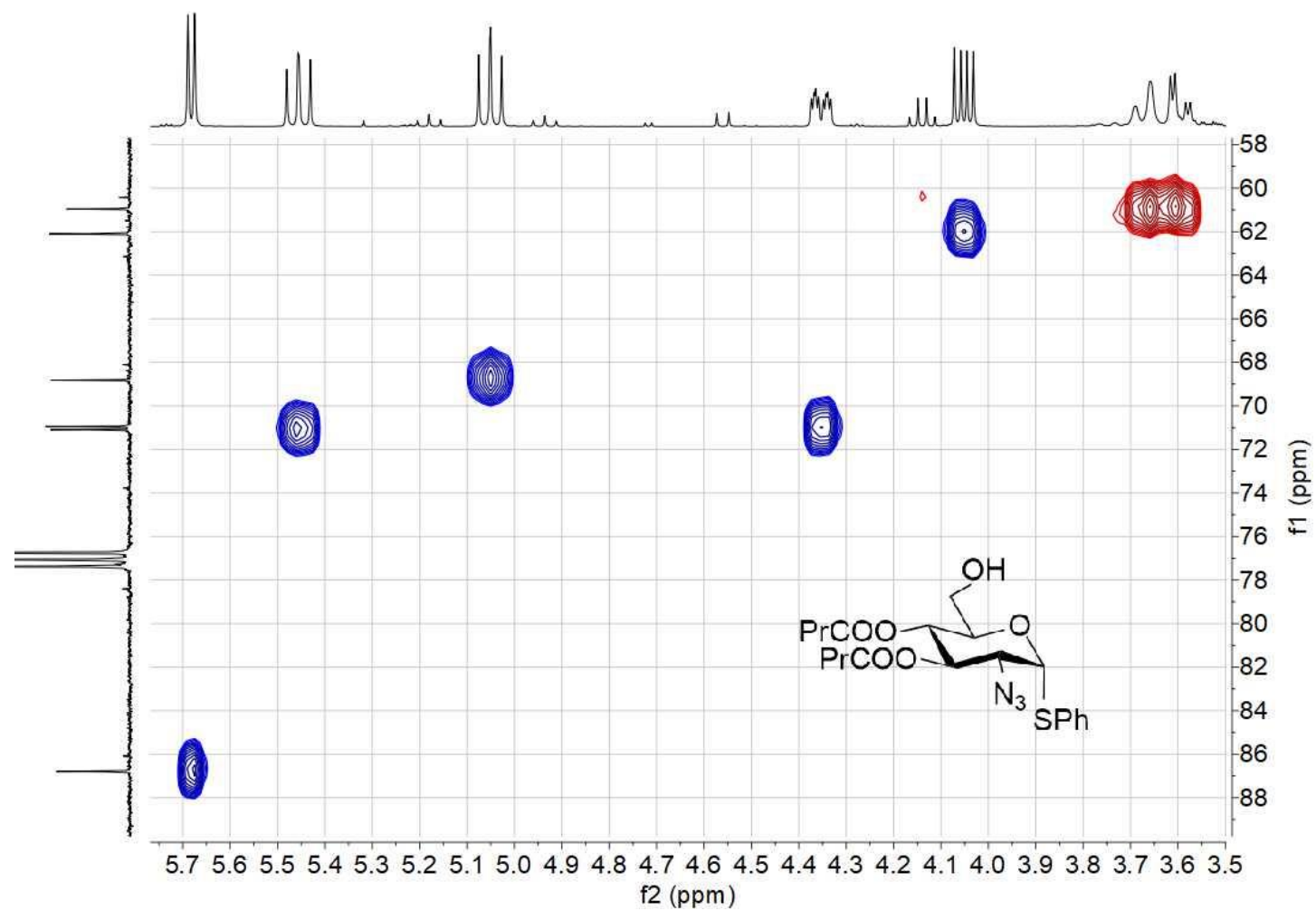
¹³C NMR (100 MHz, CDCl₃) 84 (enriched α-anomer)



^1H - ^1H COSY 84 (enriched α -anomer)

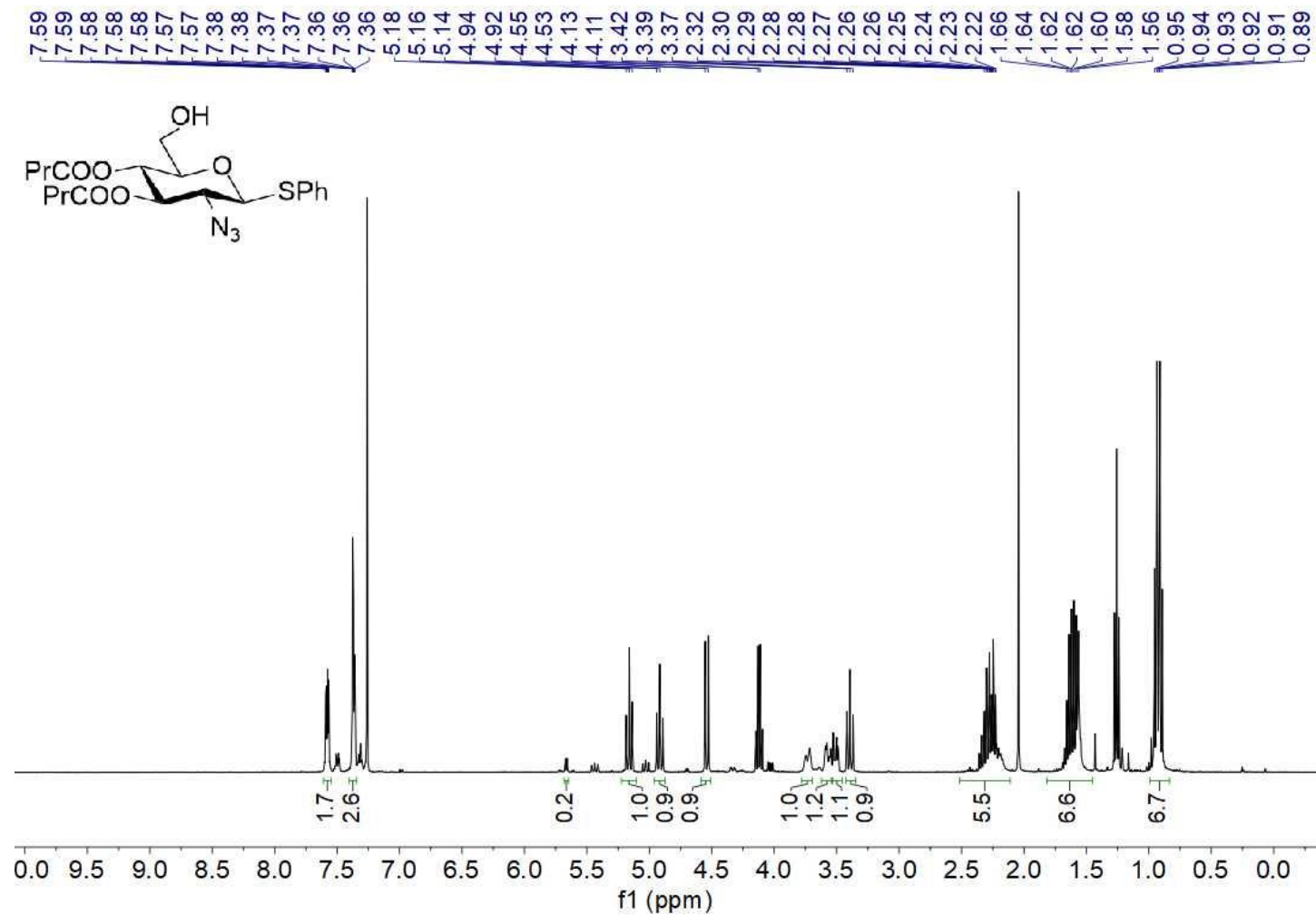


^1H - ^{13}C HSQC 84 (enriched α -anomer)

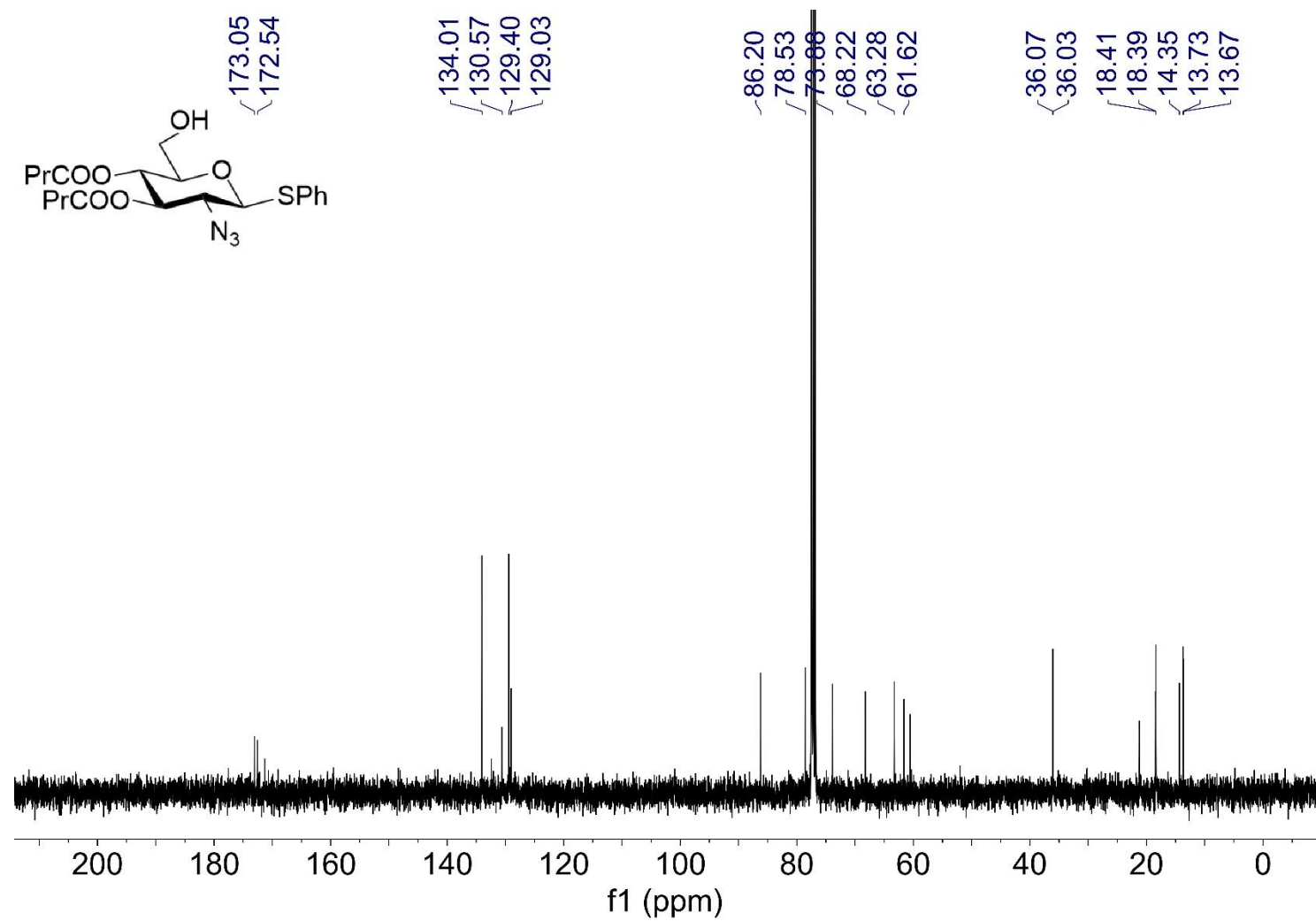


NMR COMPOUND 84 (enriched β -anomer)

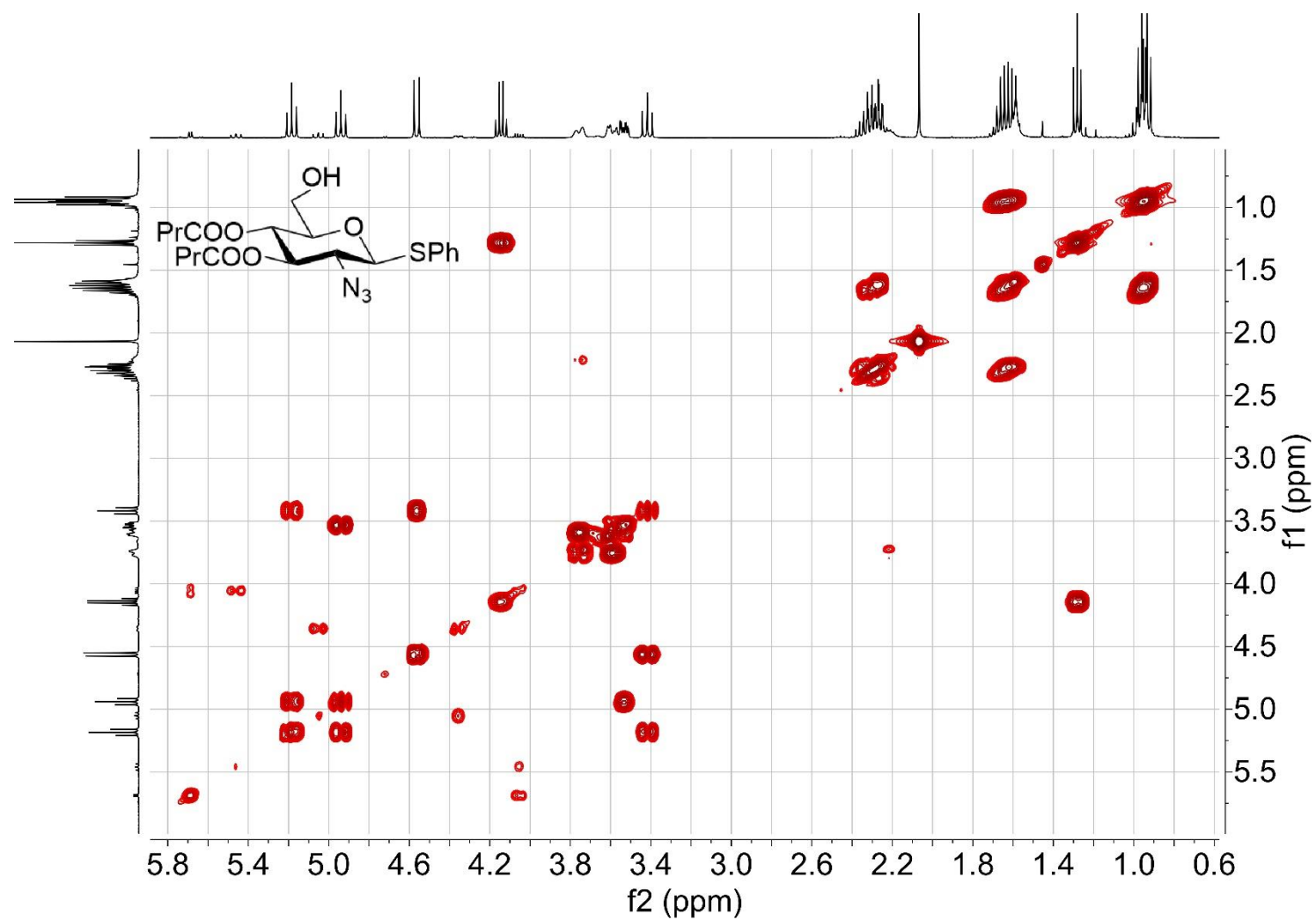
^1H NMR (400 MHz, CDCl_3) 84 (enriched β -anomer)



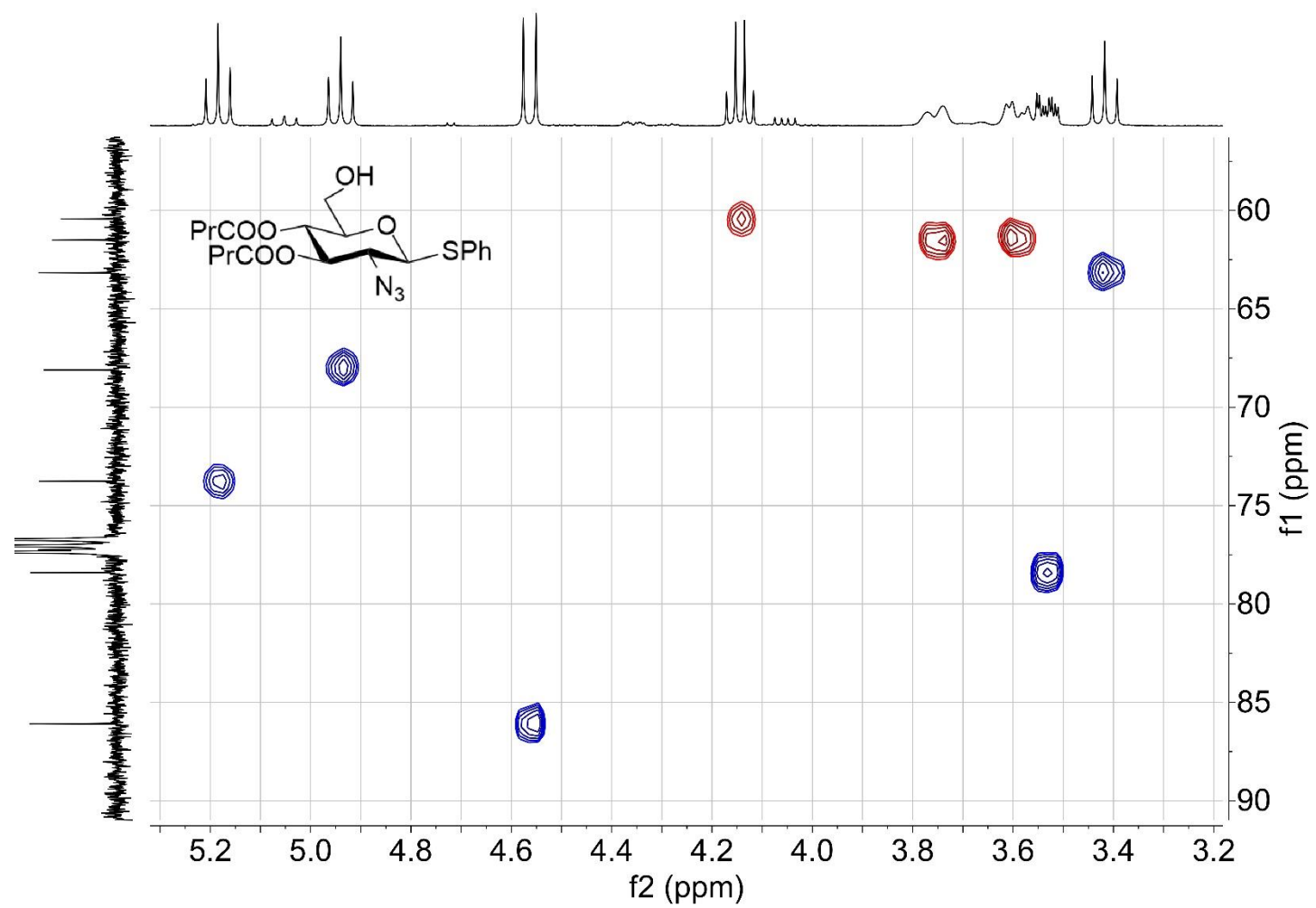
¹³C NMR (100 MHz, CDCl₃) 84 (enriched β-anomer)



^1H - ^1H COSY 84 (enriched β -anomer)

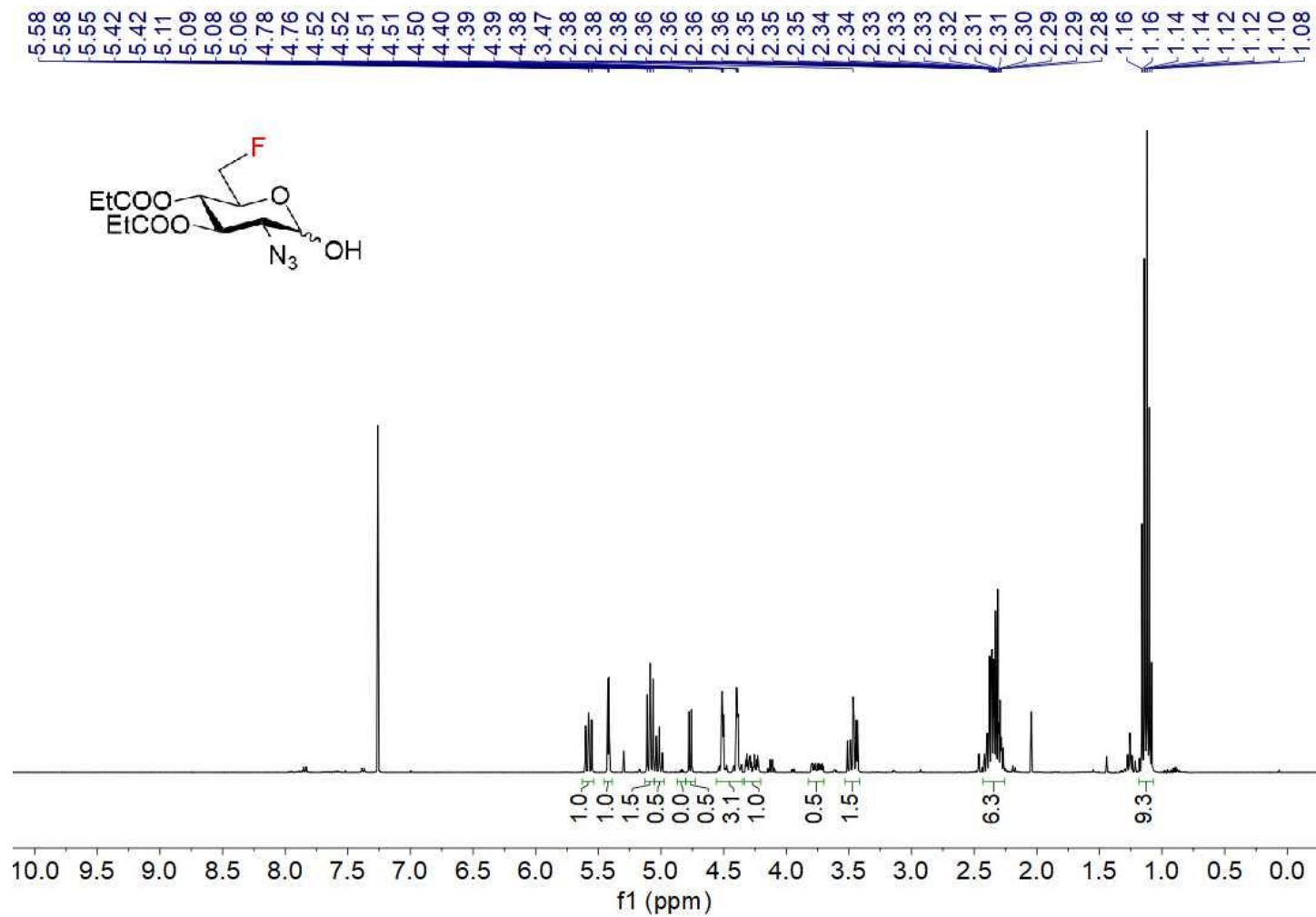


^1H - ^{13}C HSQC 84 (enriched β -anomer)

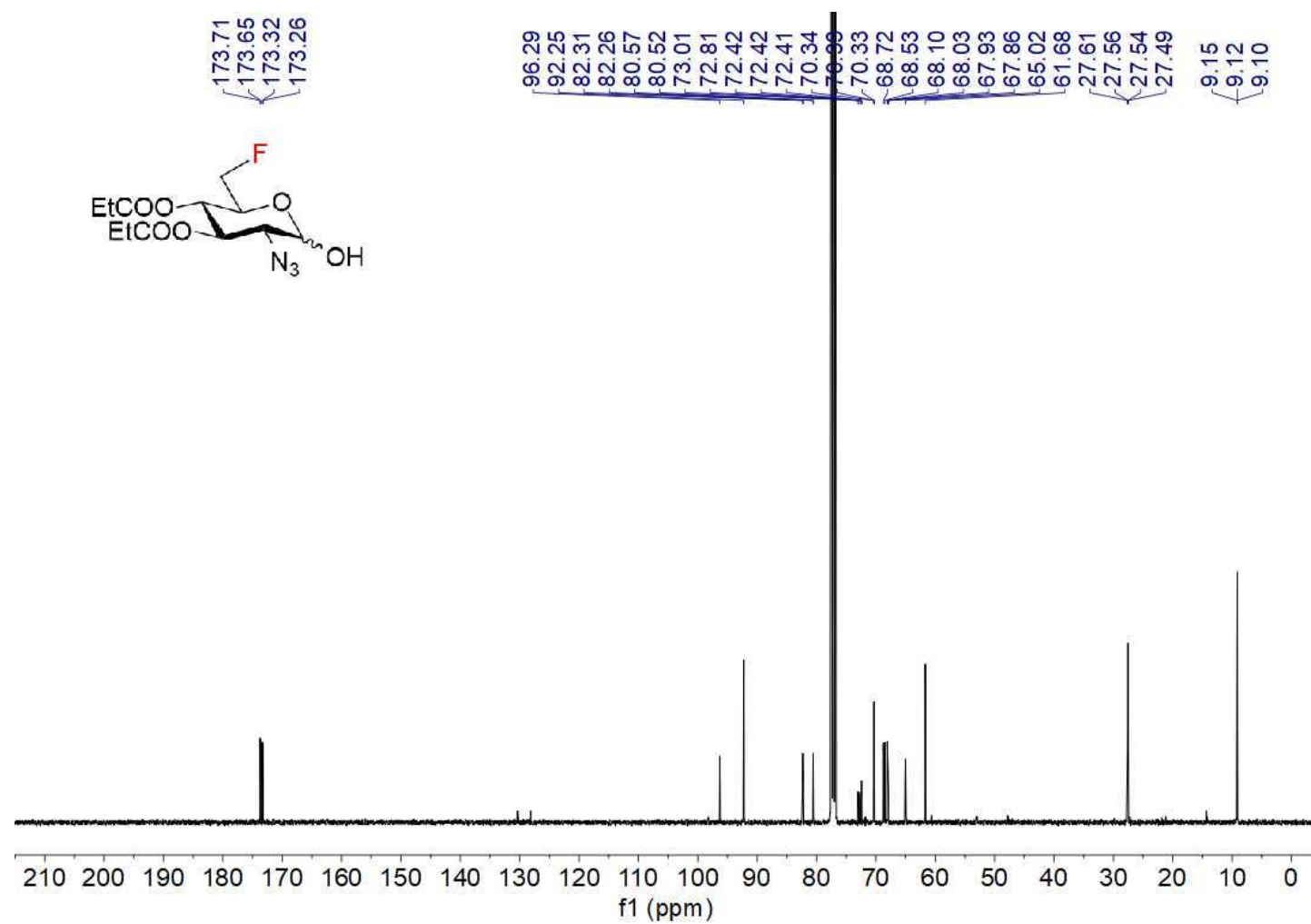


NMR COMPOUND 85

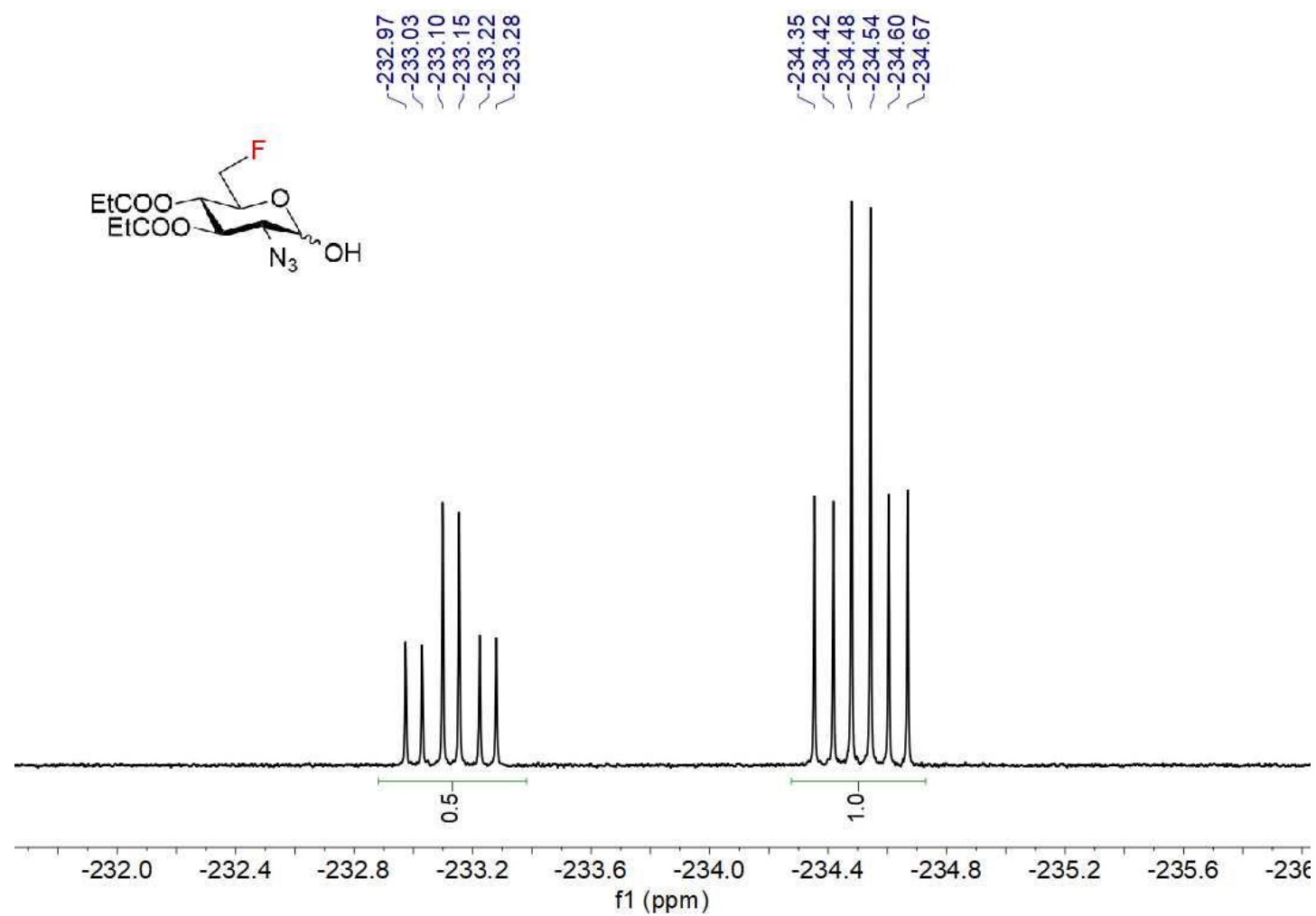
^1H NMR (400 MHz, CDCl_3) 85



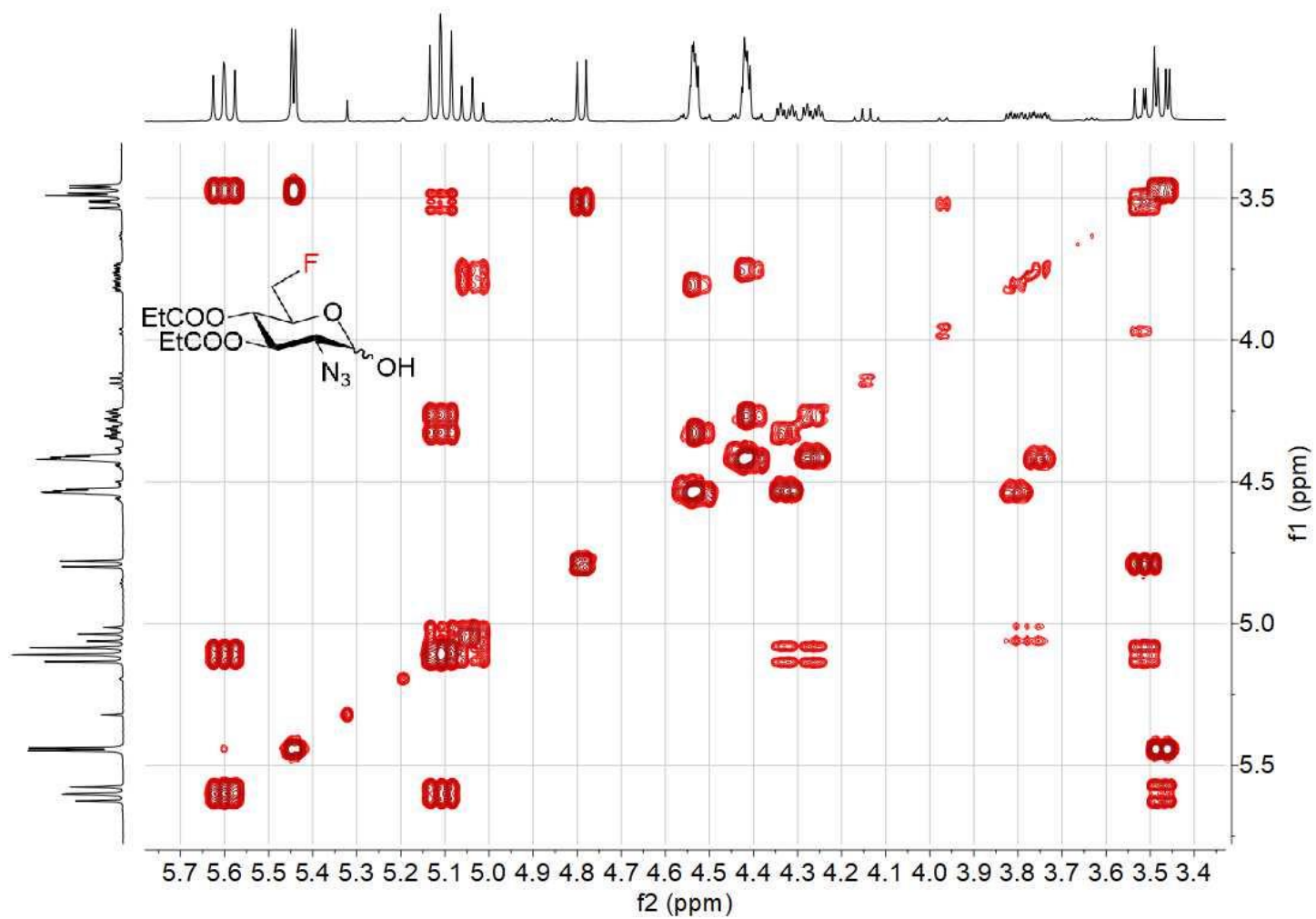
^{13}C NMR (100 MHz, CDCl_3) 85



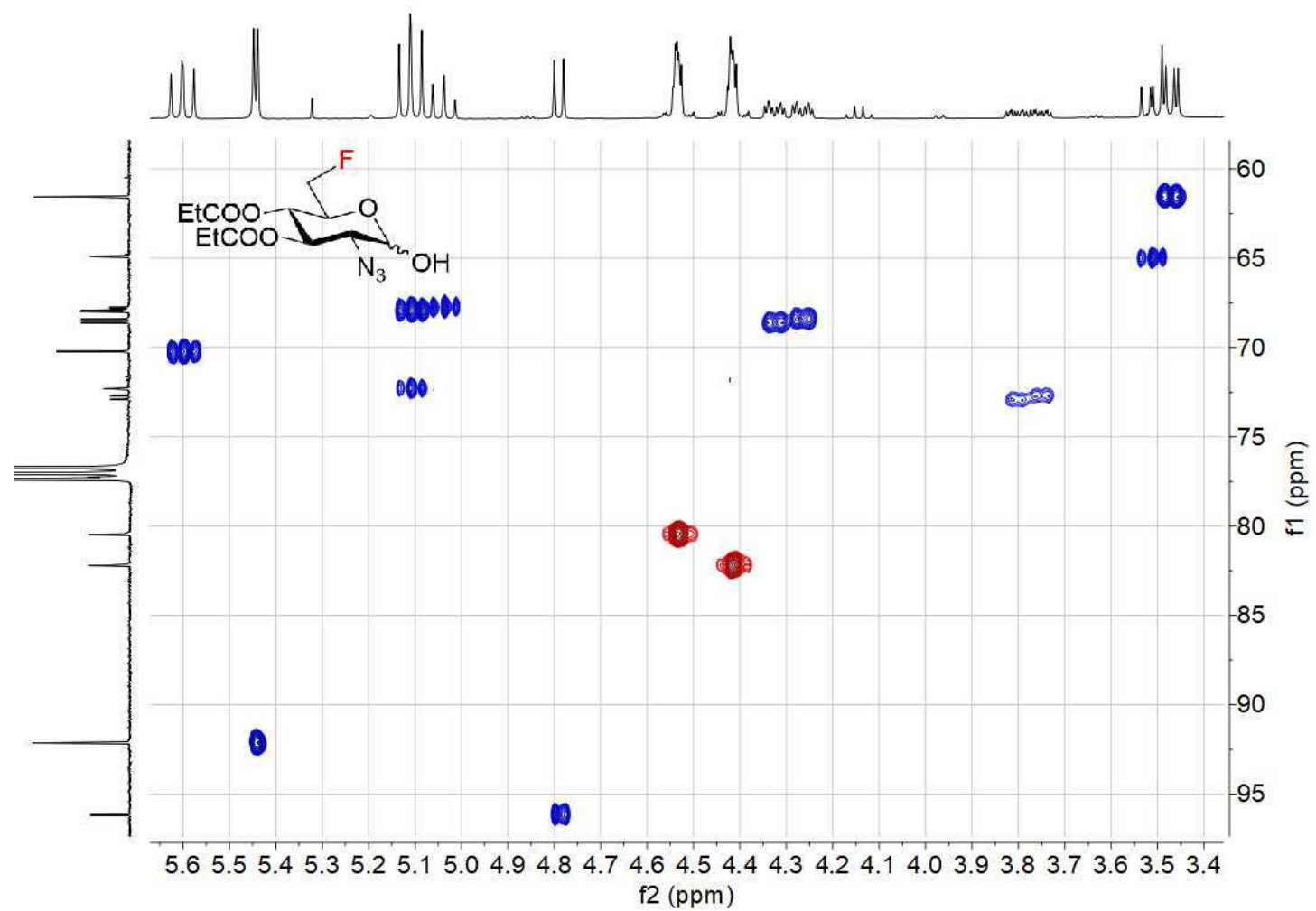
¹⁹F NMR (376 MHz, CDCl₃) 85



^1H - ^1H COSY 85

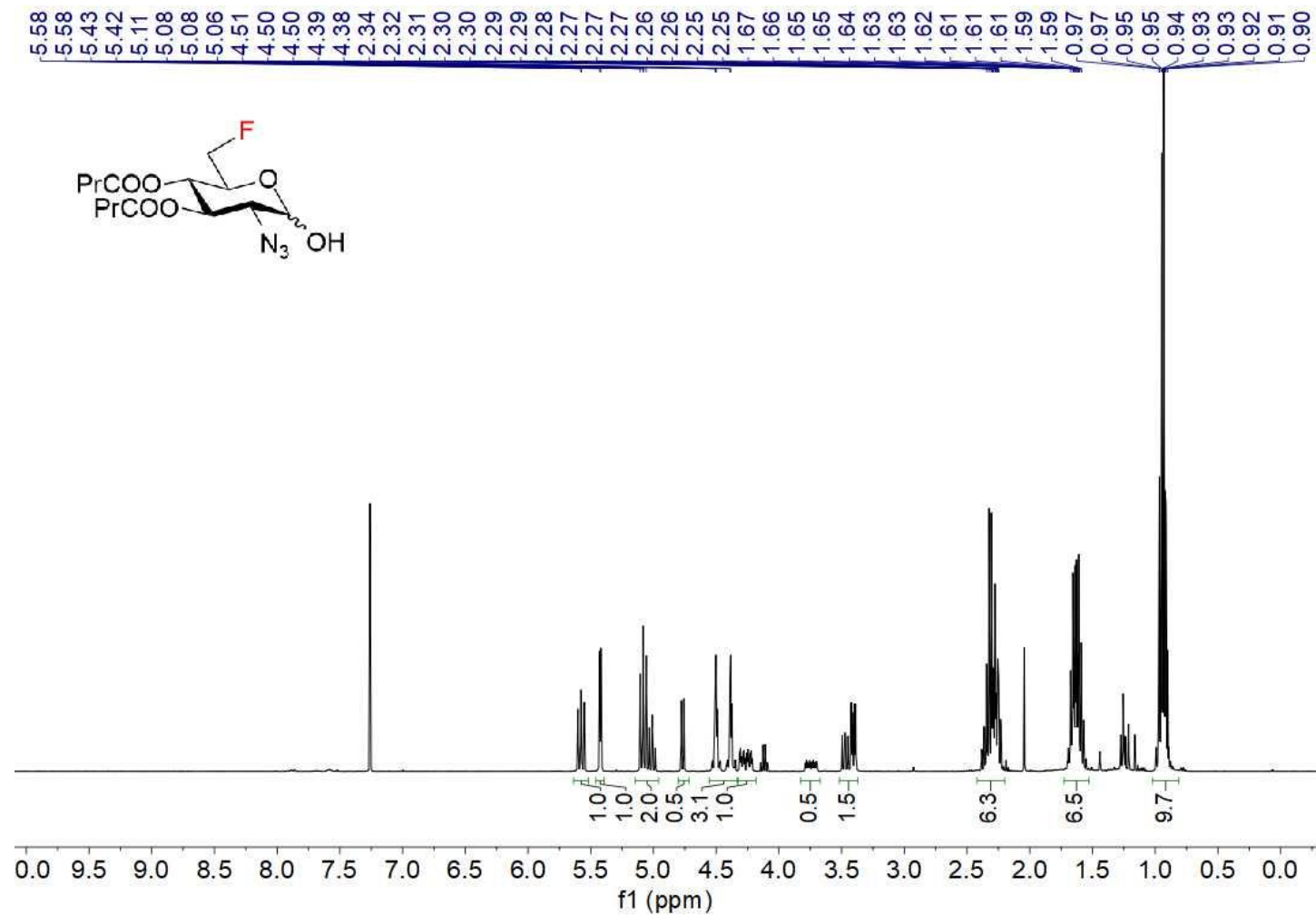


^1H - ^{13}C HSQC 85

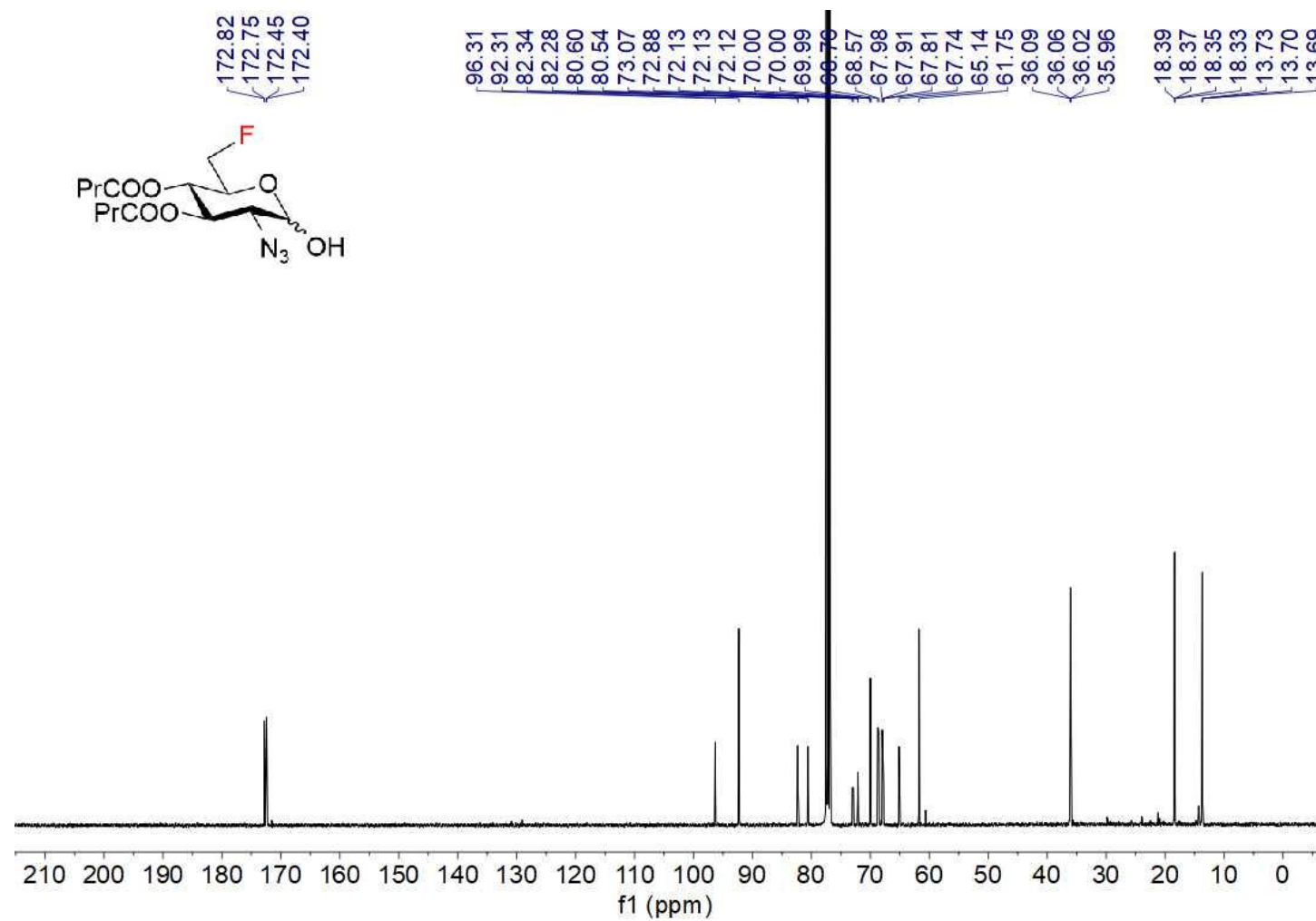


NMR COMPOUND 86

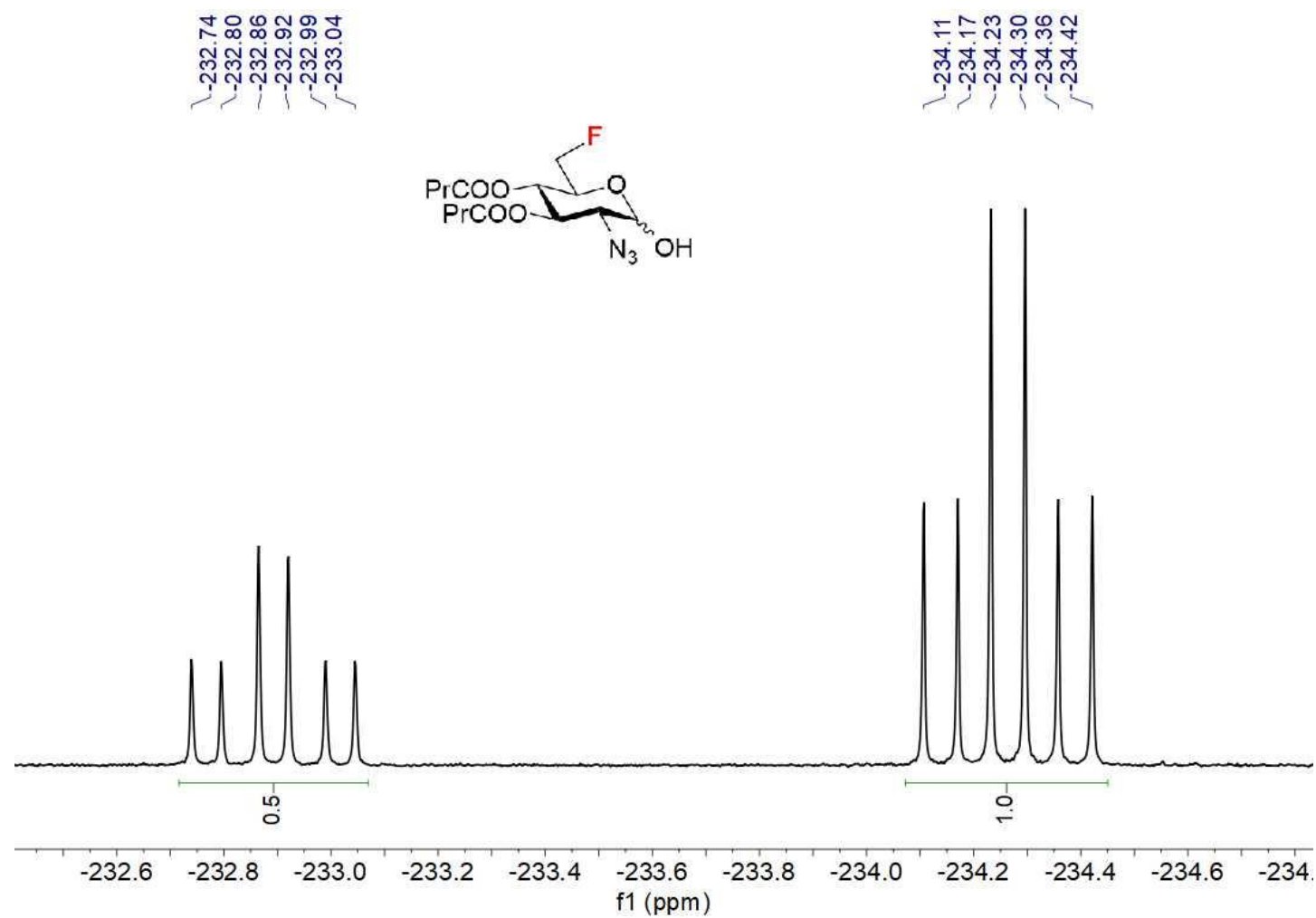
¹H NMR (400 MHz, CDCl₃) 86



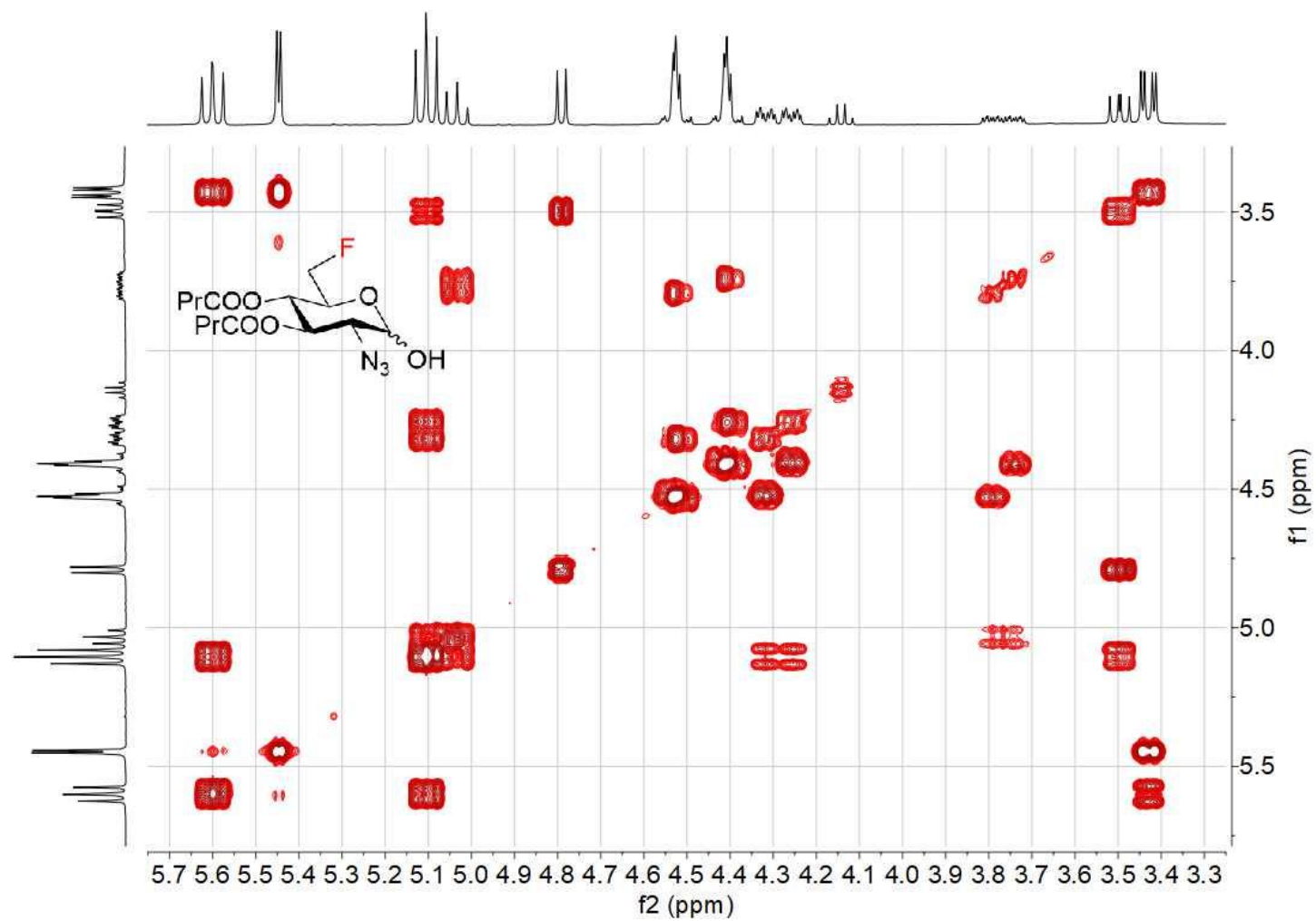
^{13}C NMR (100 MHz, CDCl_3) 86



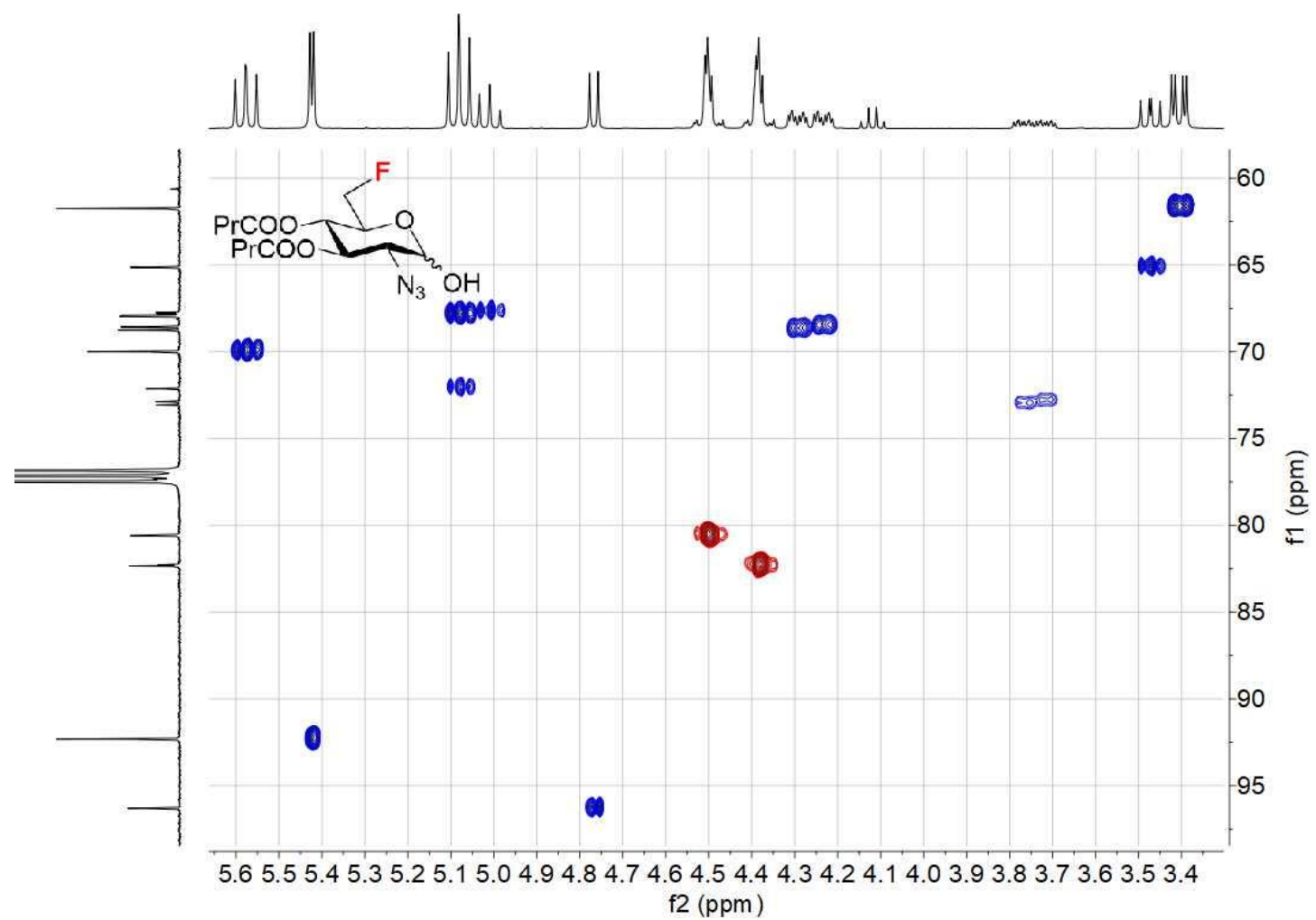
^{19}F NMR (376 MHz, CDCl_3) 86



^1H - ^1H COSY 86

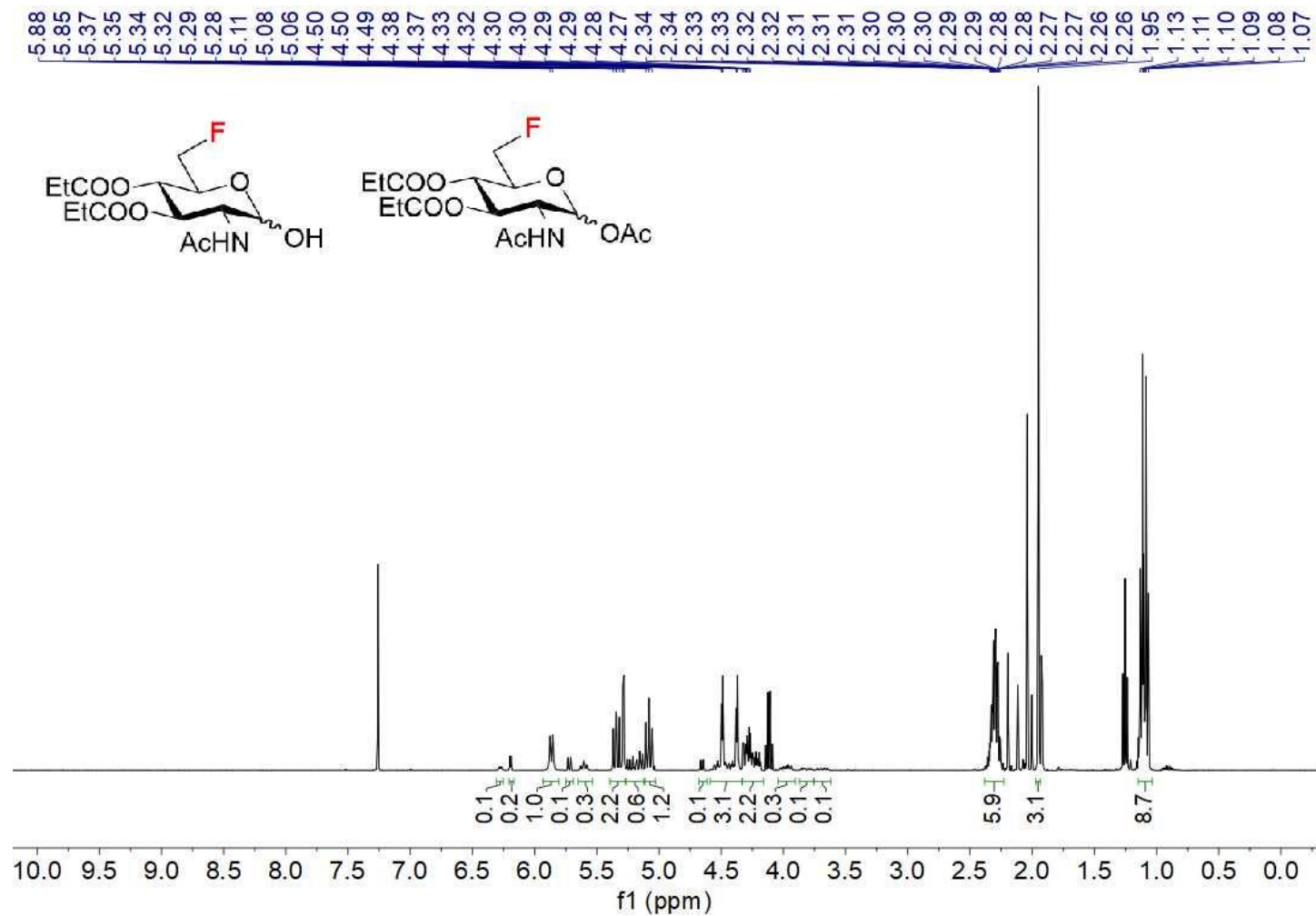


^1H - ^{13}C HSQC 86

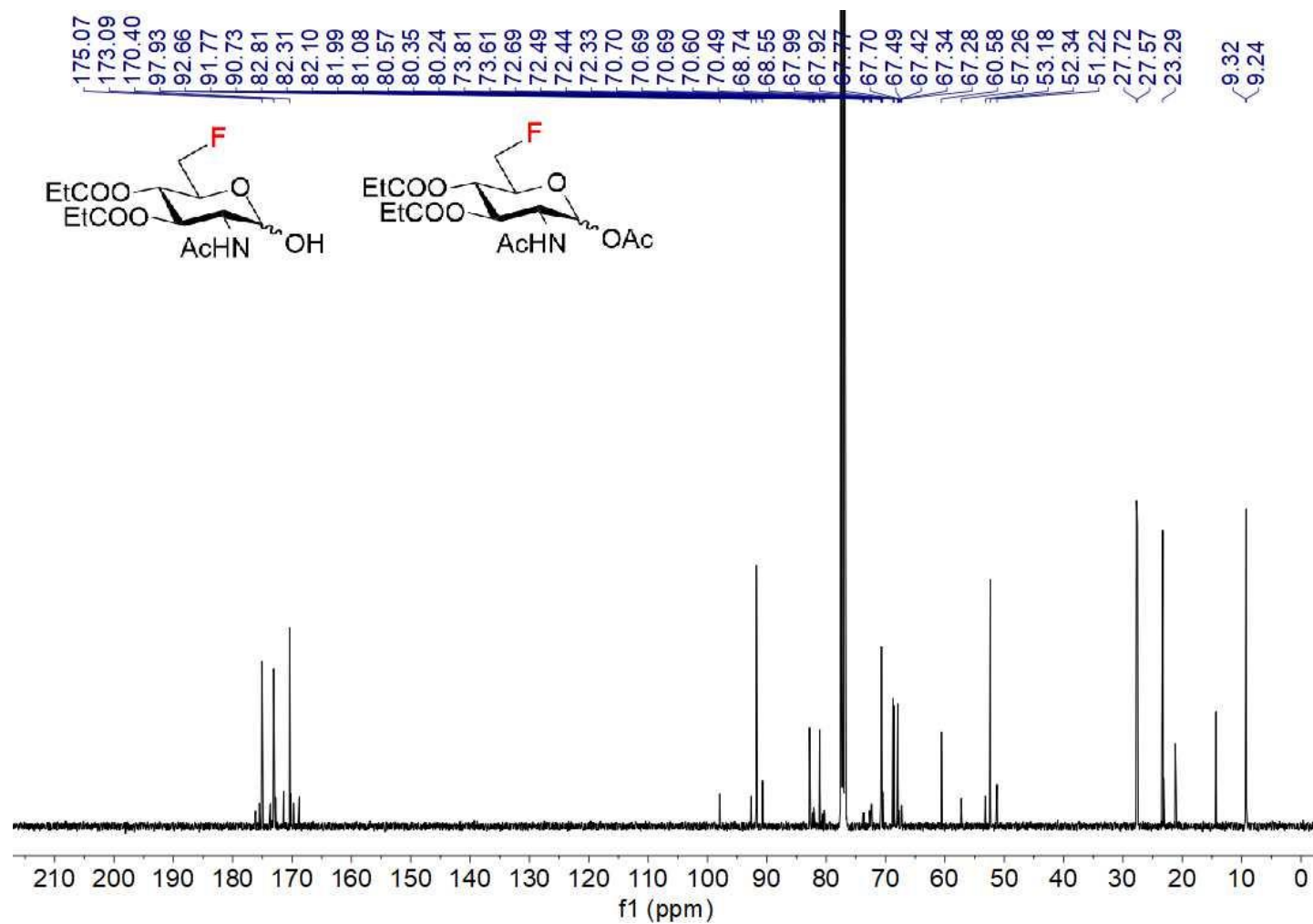


NMR MIXTURE OF COMPOUNDS 18 AND 87

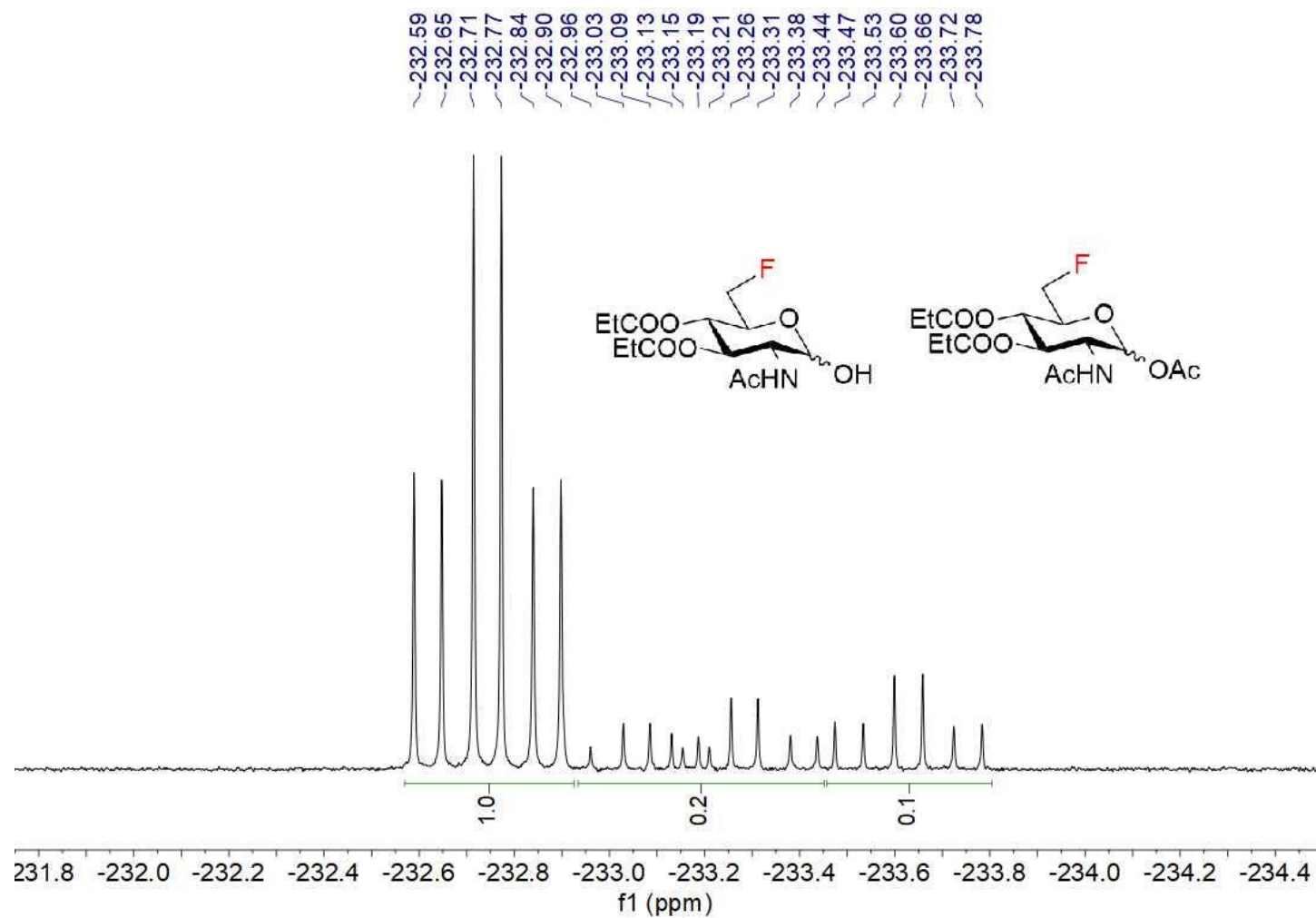
¹H NMR (400 MHz, CDCl₃) 18 AND 87



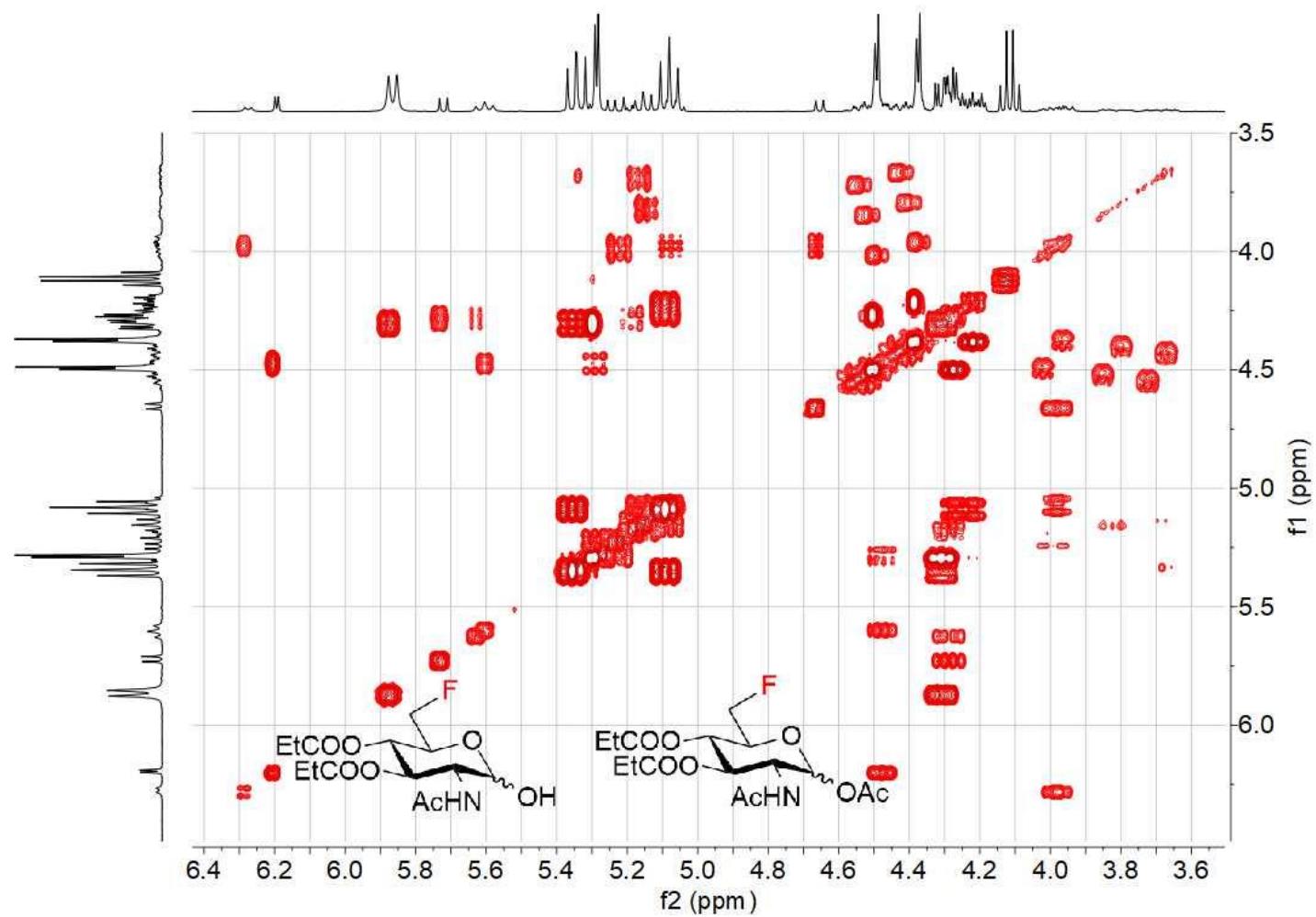
¹³C NMR (100 MHz, CDCl₃) 18 AND 87



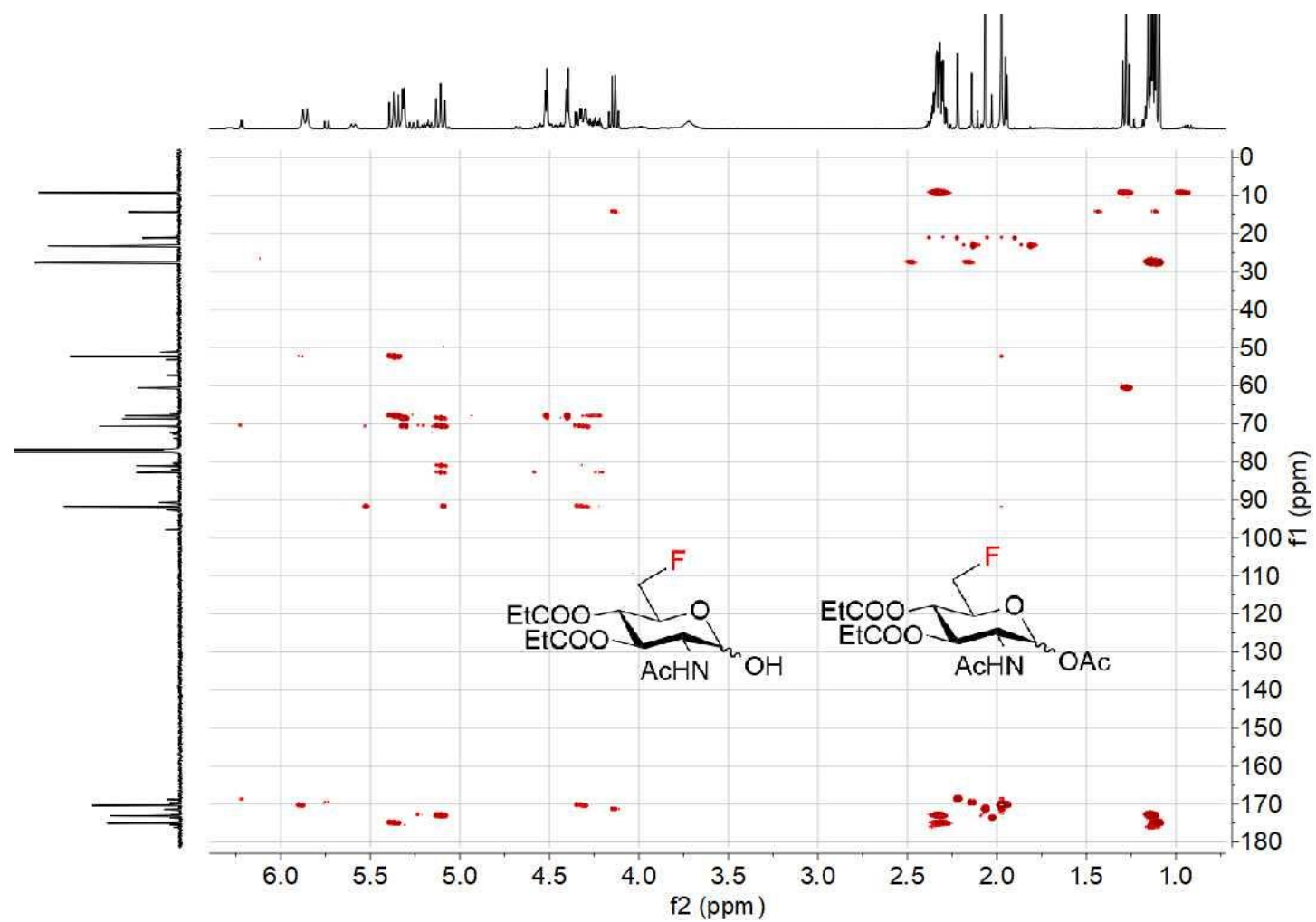
¹⁹F NMR (376 MHz, CDCl₃) 18 AND 87



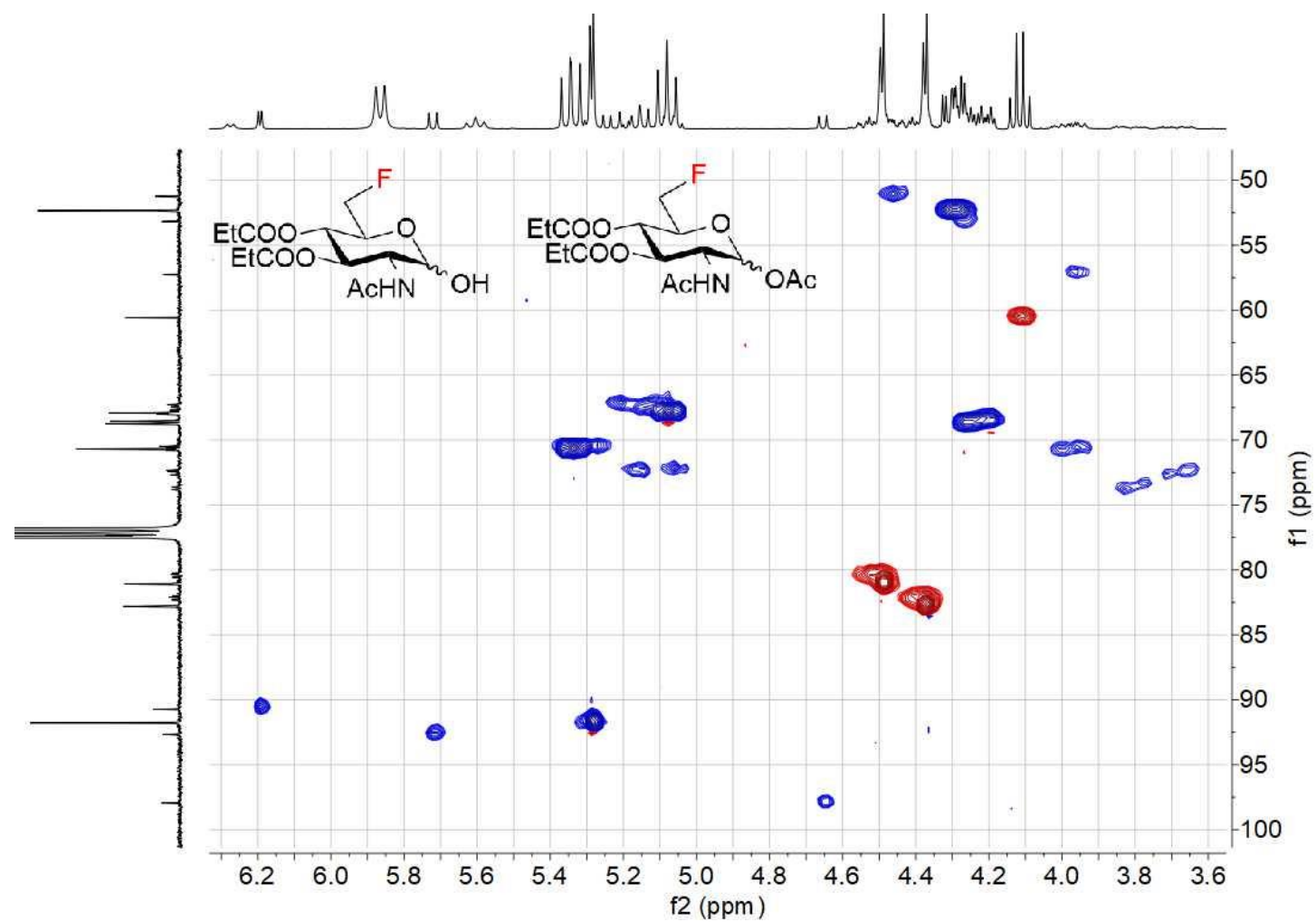
^1H - ^1H COSY 18 AND 87



^1H - ^{13}C HMBC 18 AND 87

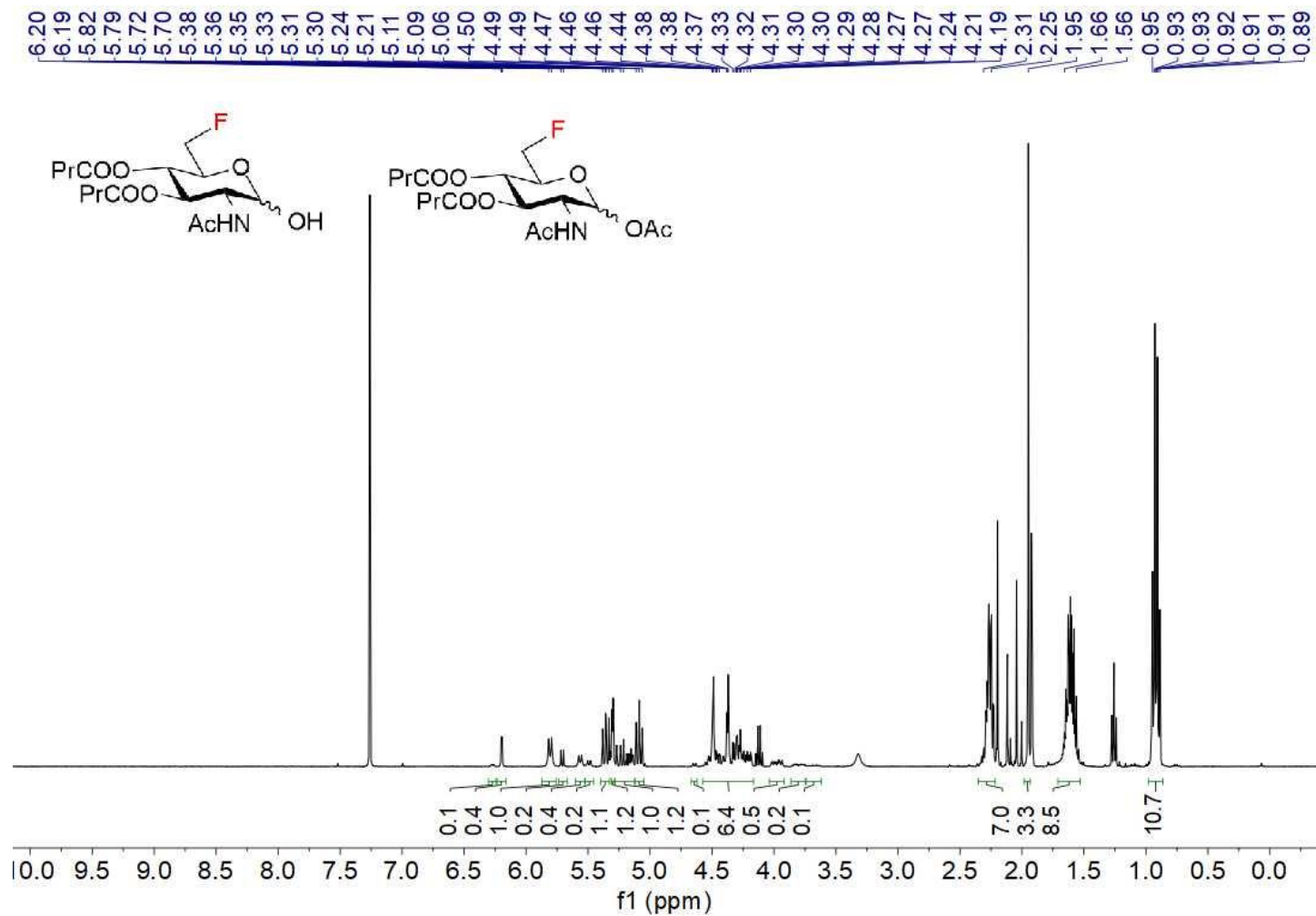


^1H - ^{13}C HSQC 18 AND 87

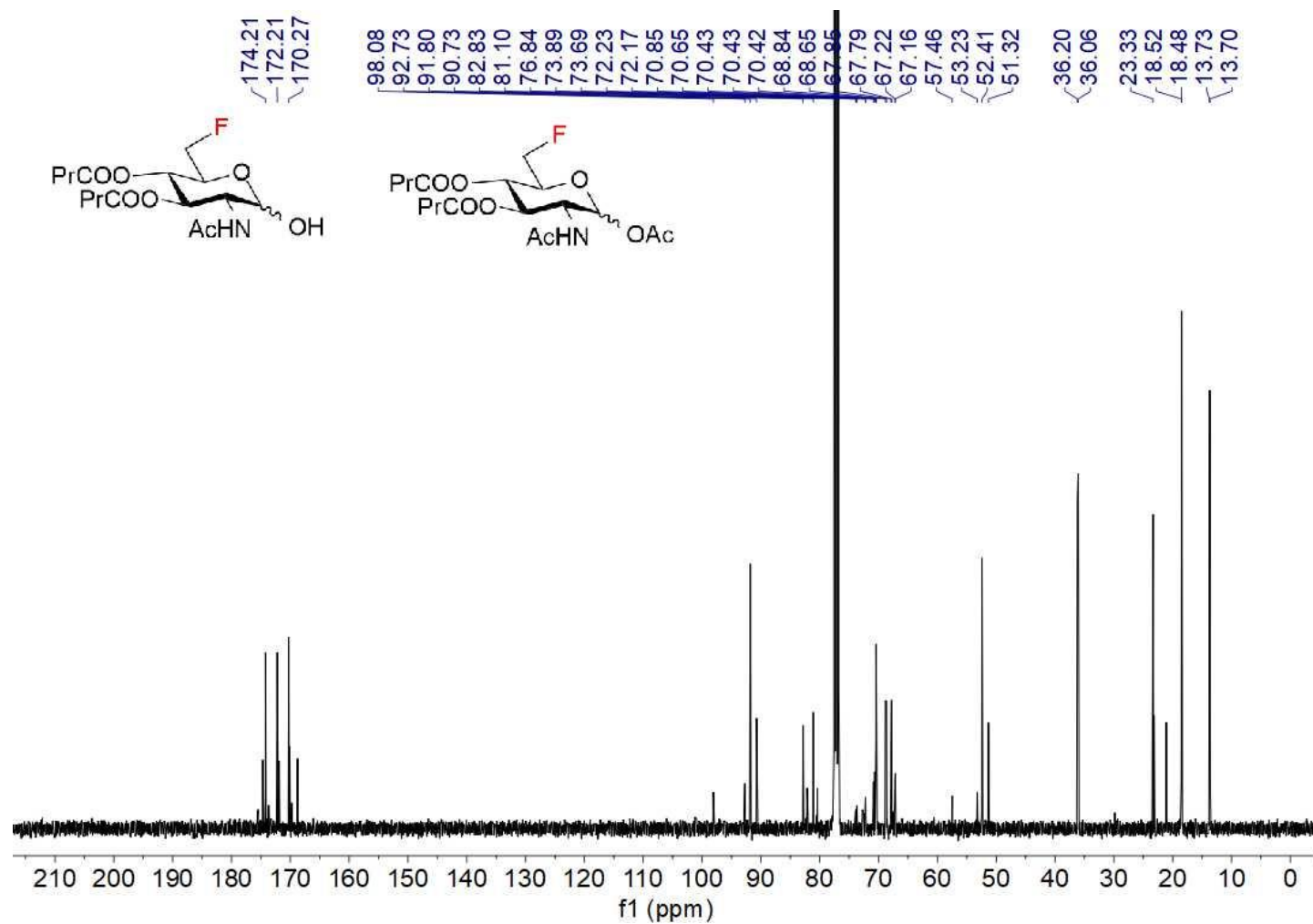


NMR MIXTURE OF COMPOUNDS 19 AND 88

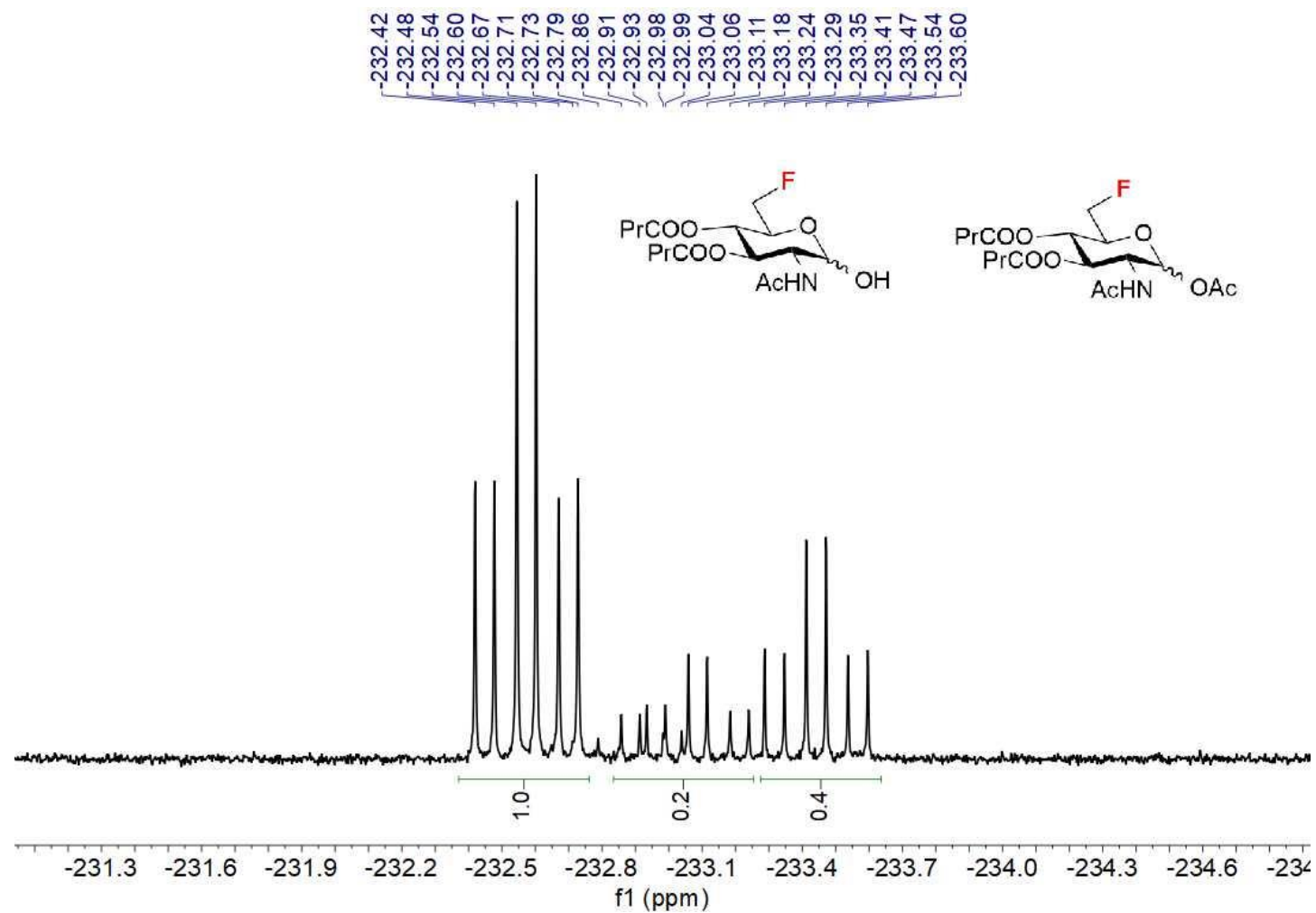
¹H NMR (400 MHz, CDCl₃) 19 AND 88



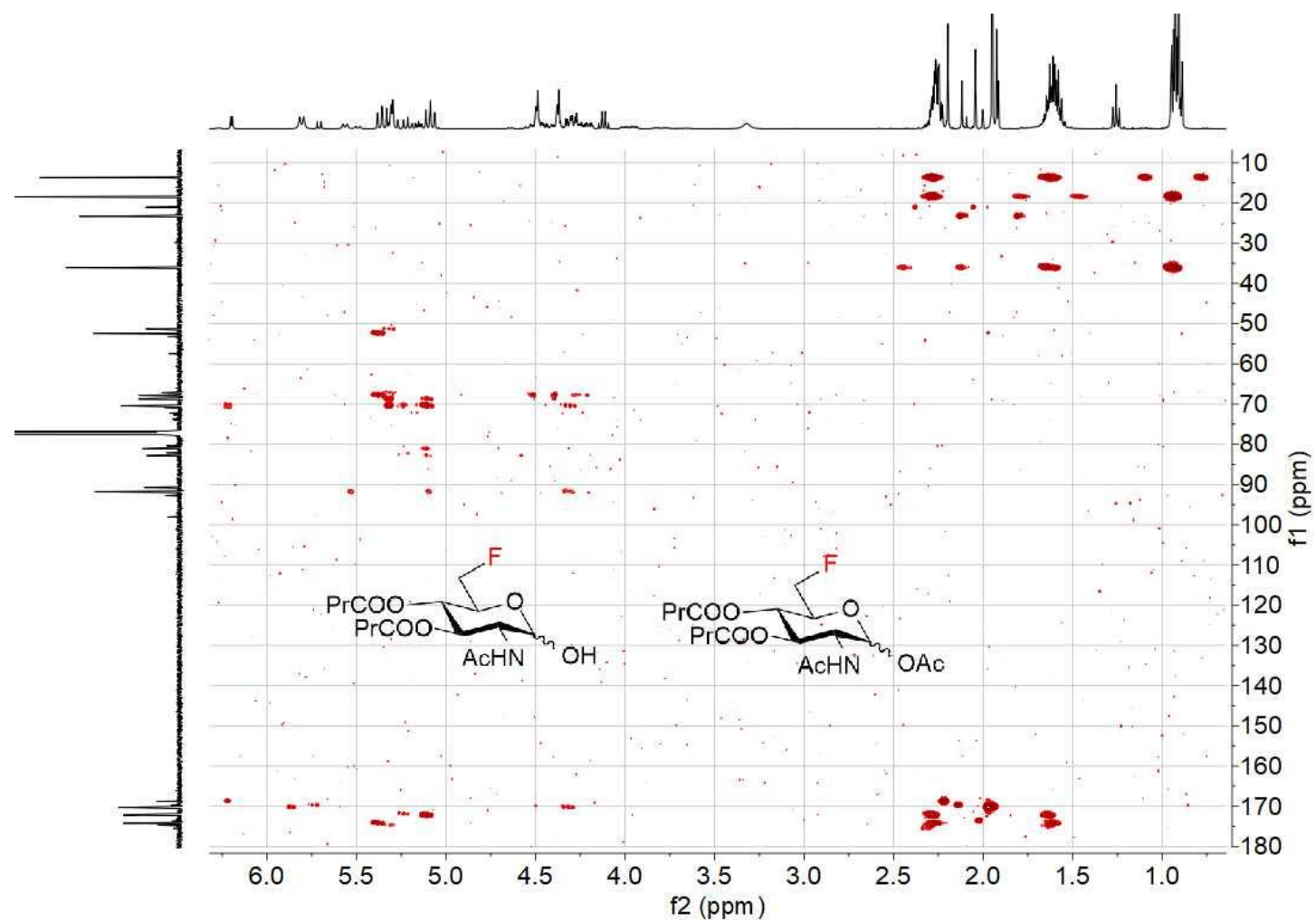
¹³C NMR (100 MHz, CDCl₃) 19 AND 88



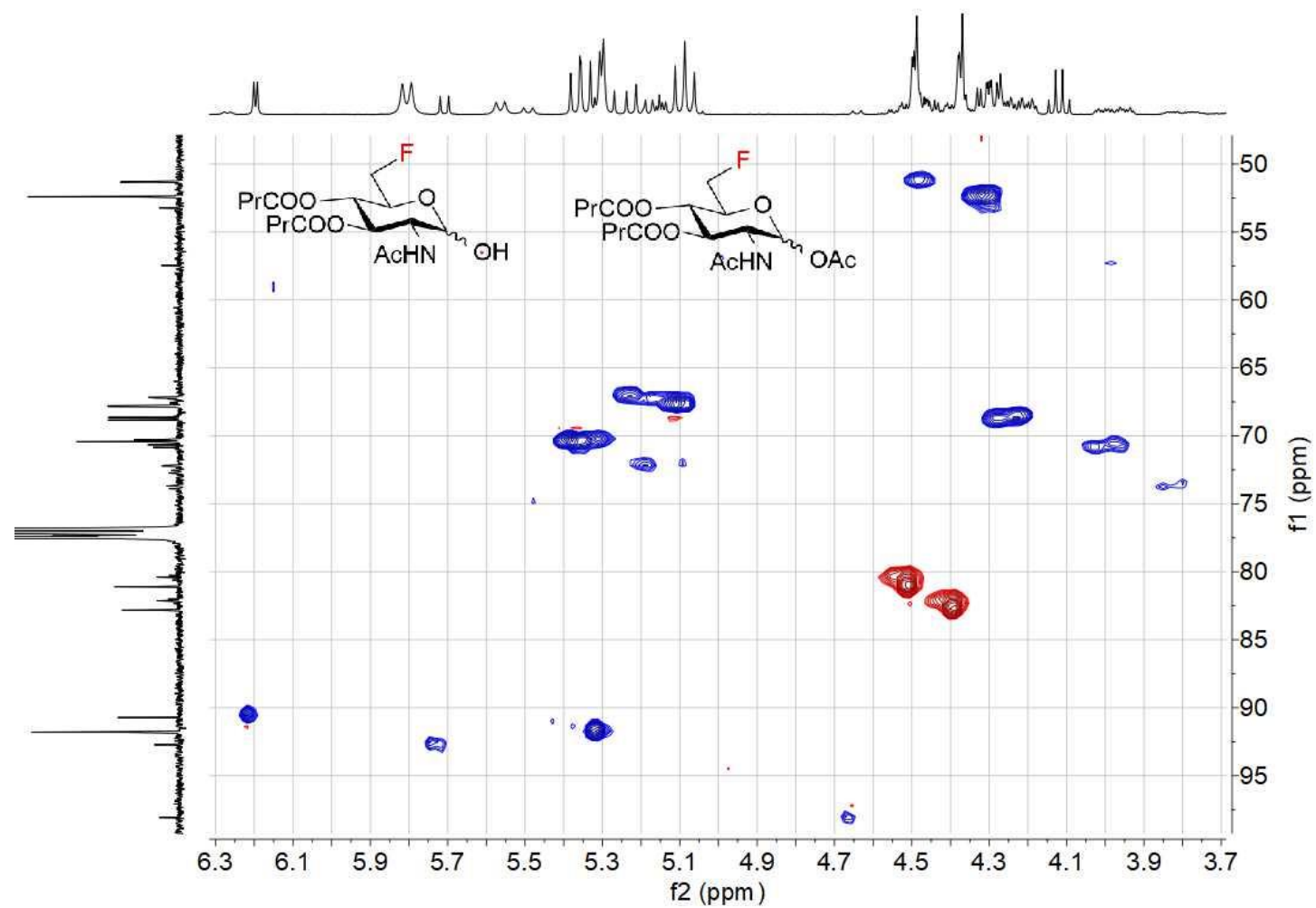
^{19}F NMR (376 MHz, CDCl_3) 19 AND 88



^1H - ^{13}C HMBC 19 AND 88

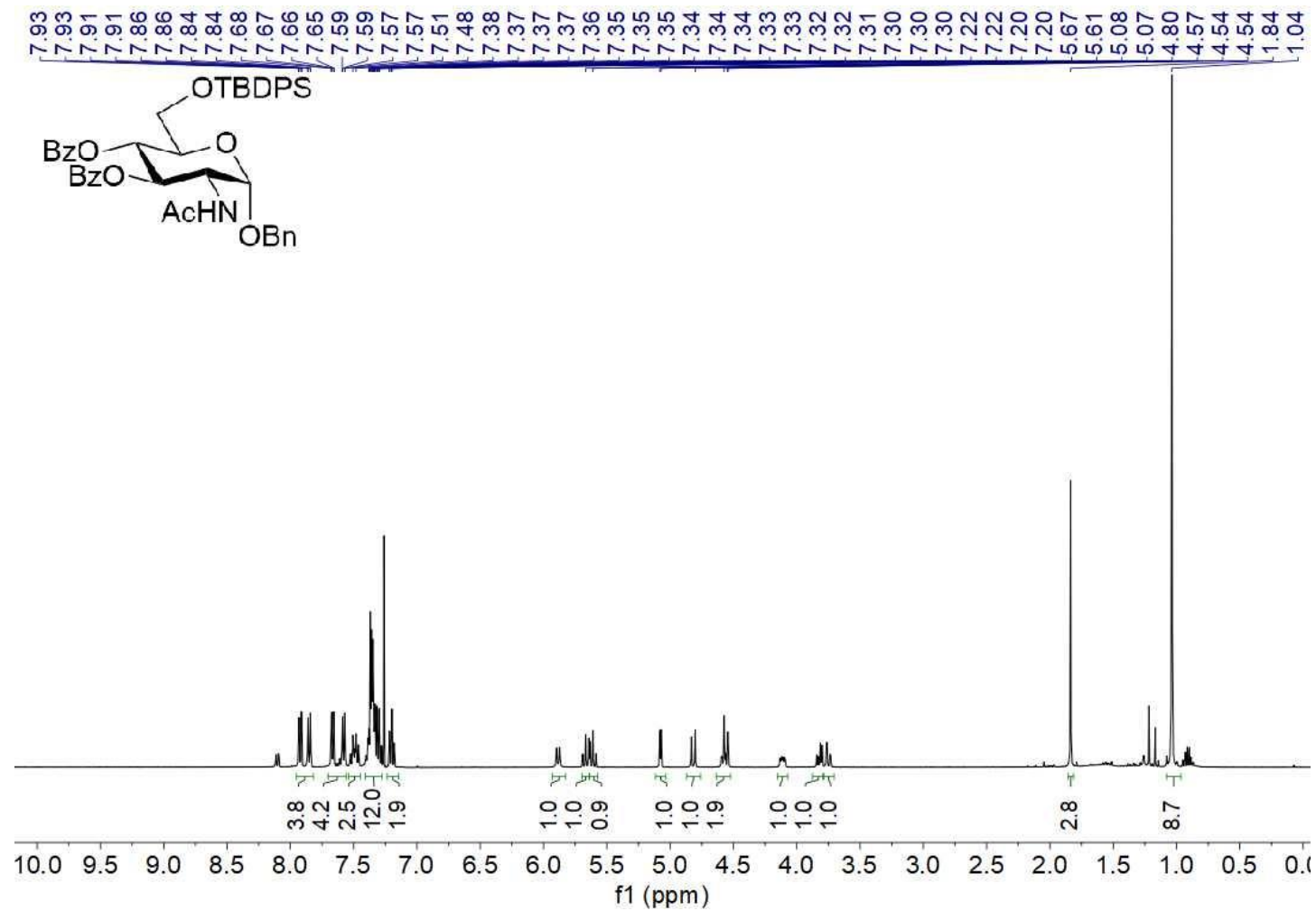


^1H - ^{13}C HSQC 19 AND 88

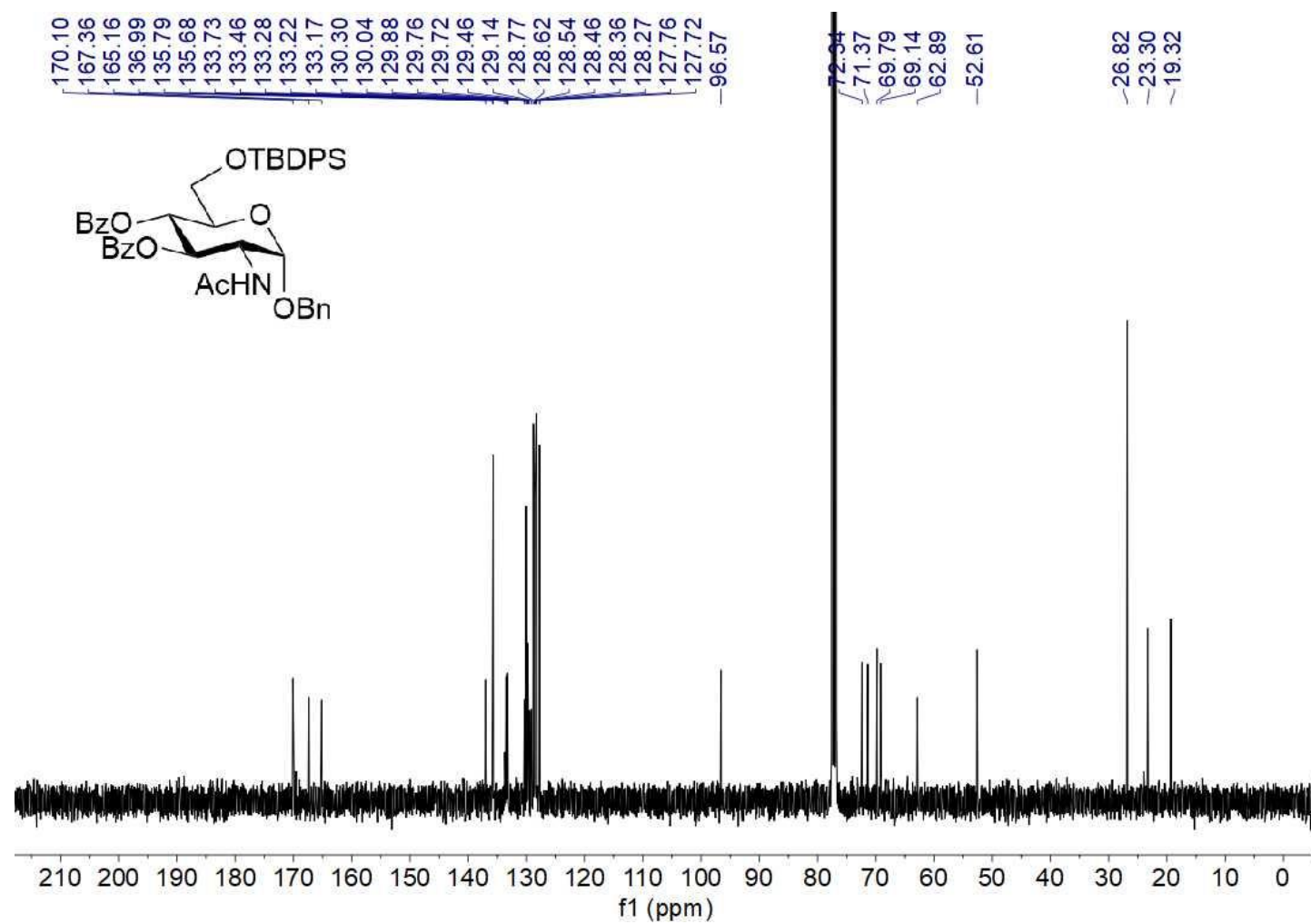


NMR COMPOUND 90

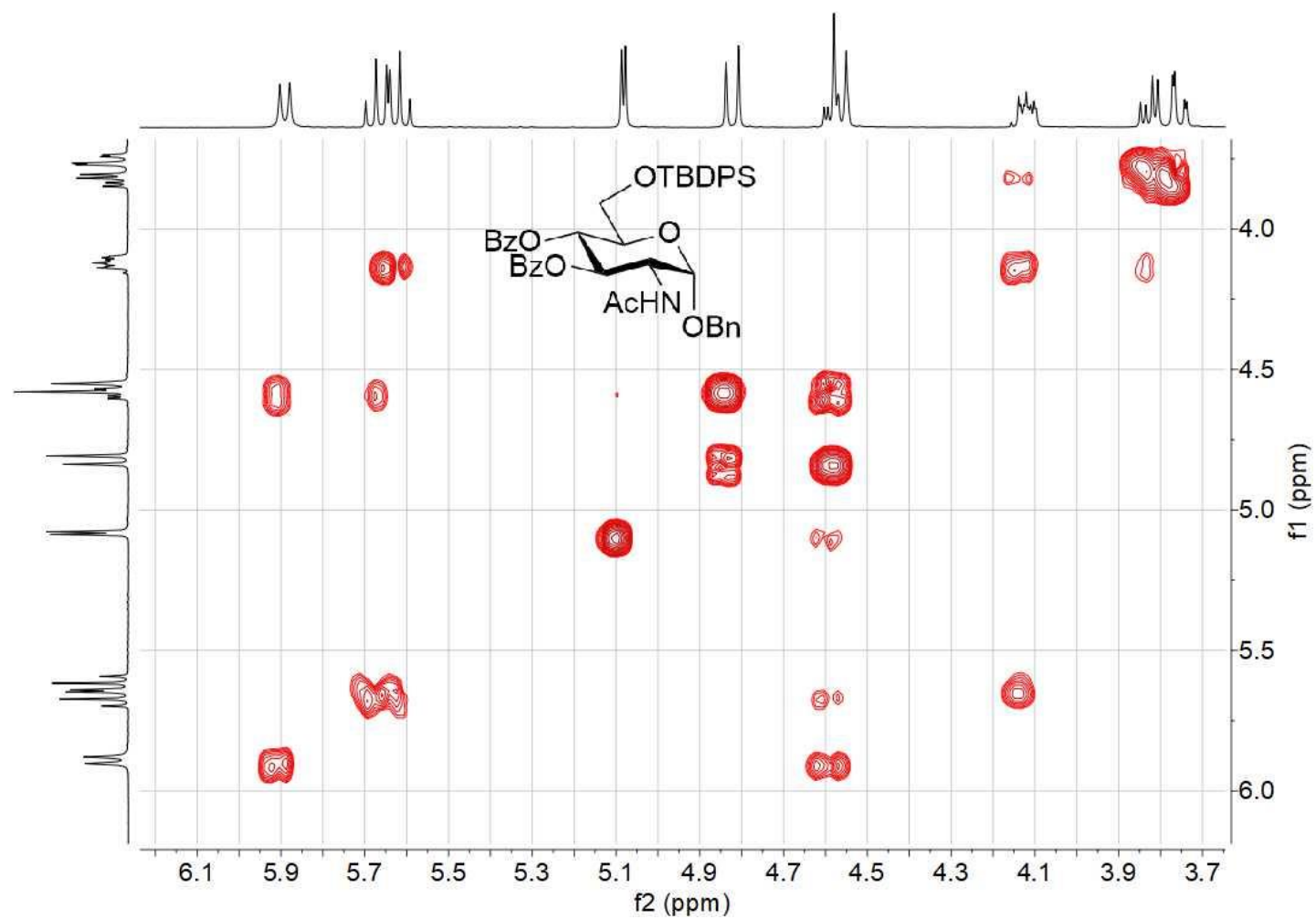
¹H NMR (400 MHz, CDCl₃) 90



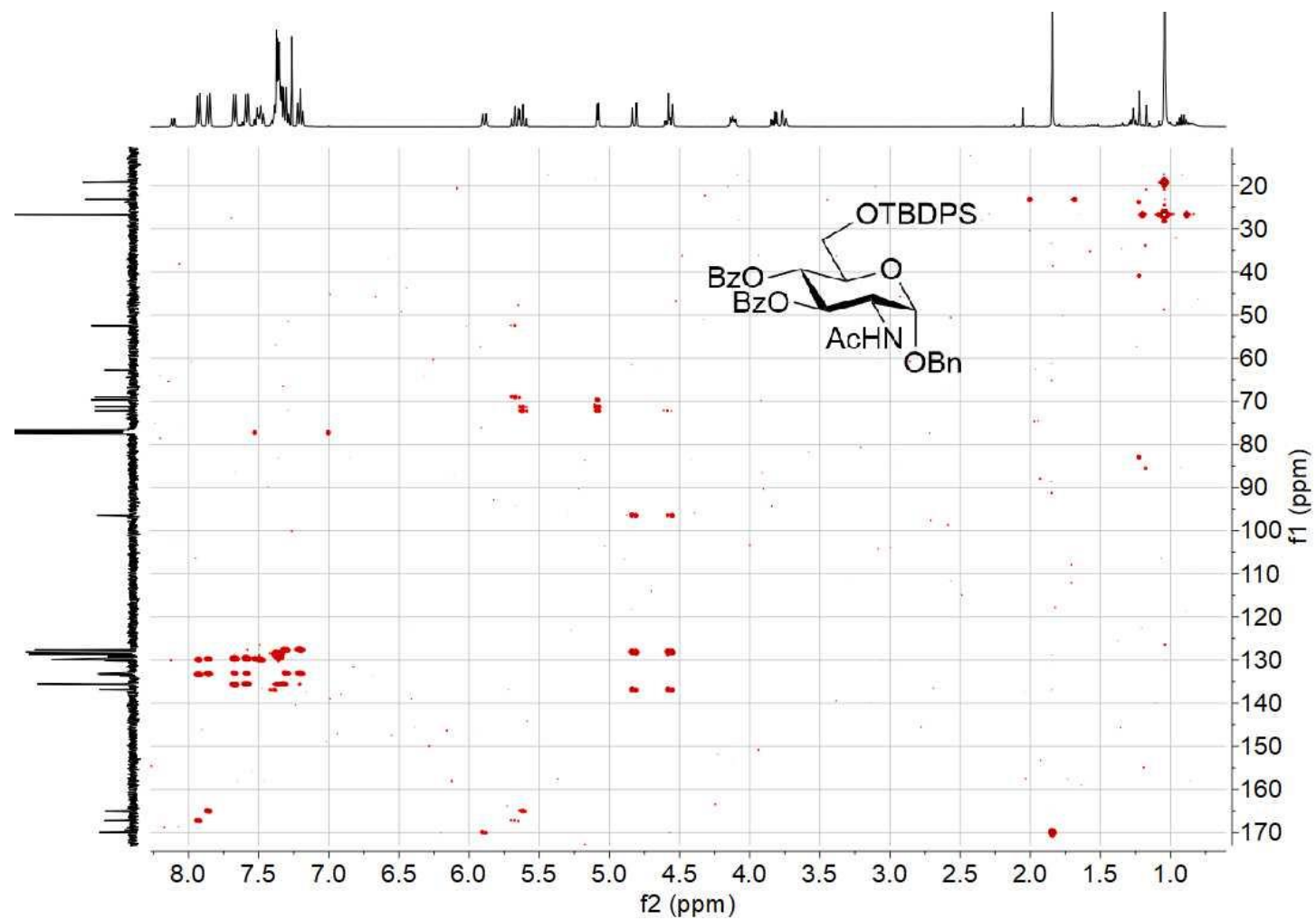
^{13}C NMR (100 MHz, CDCl_3) 90



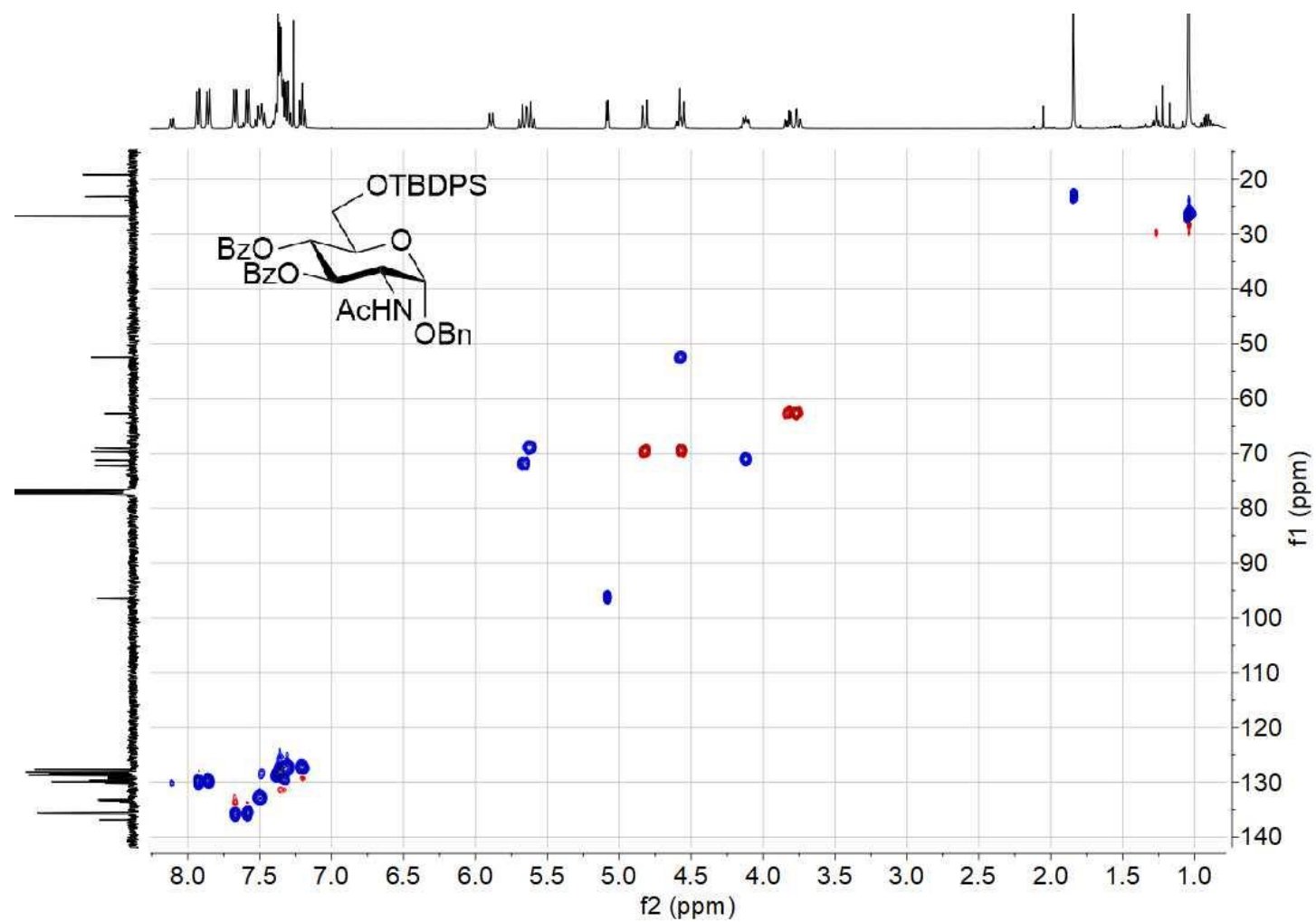
^1H - ^1H COSY 90



^1H - ^{13}C HMBC 90

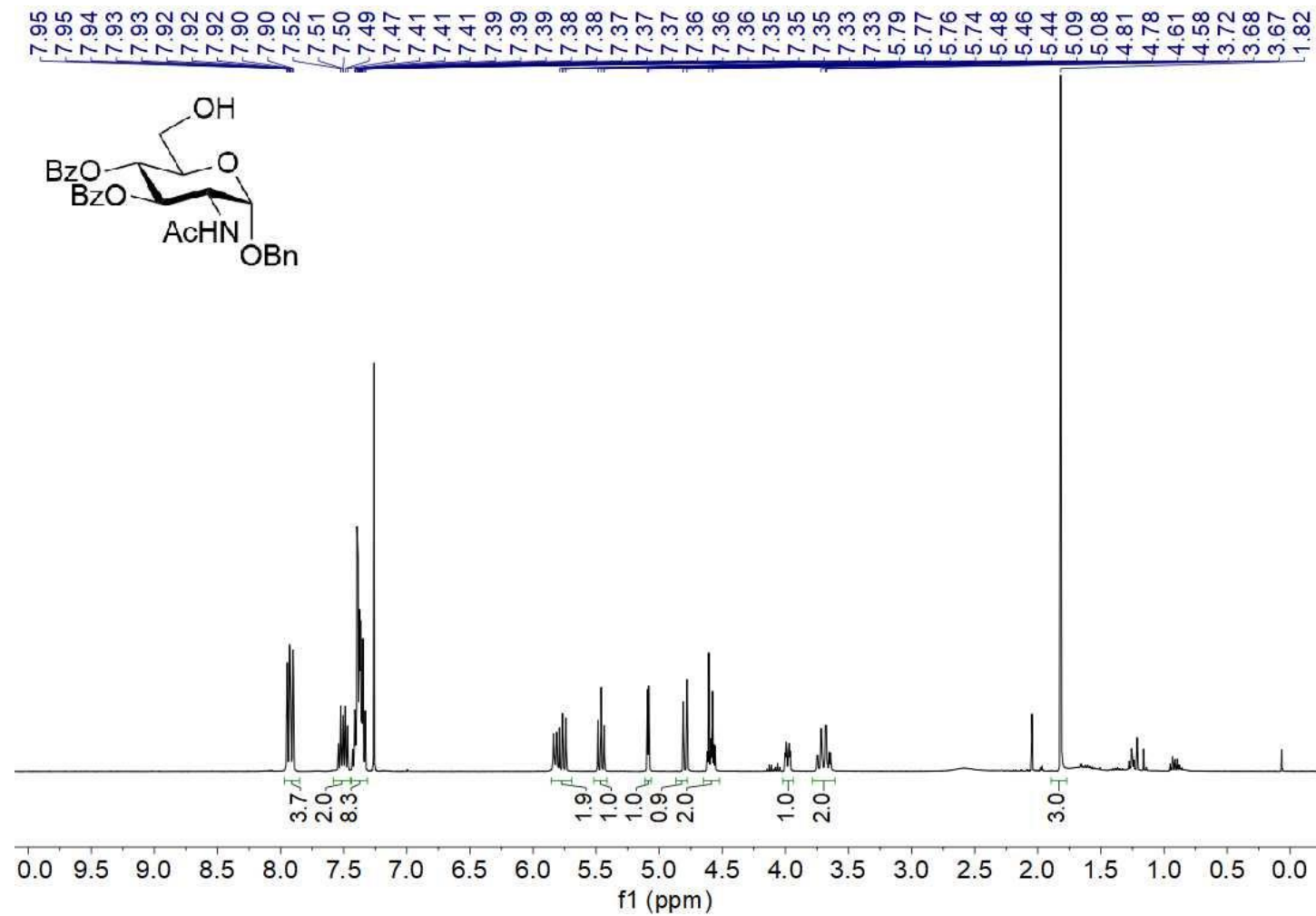


^1H - ^{13}C HSQC 90

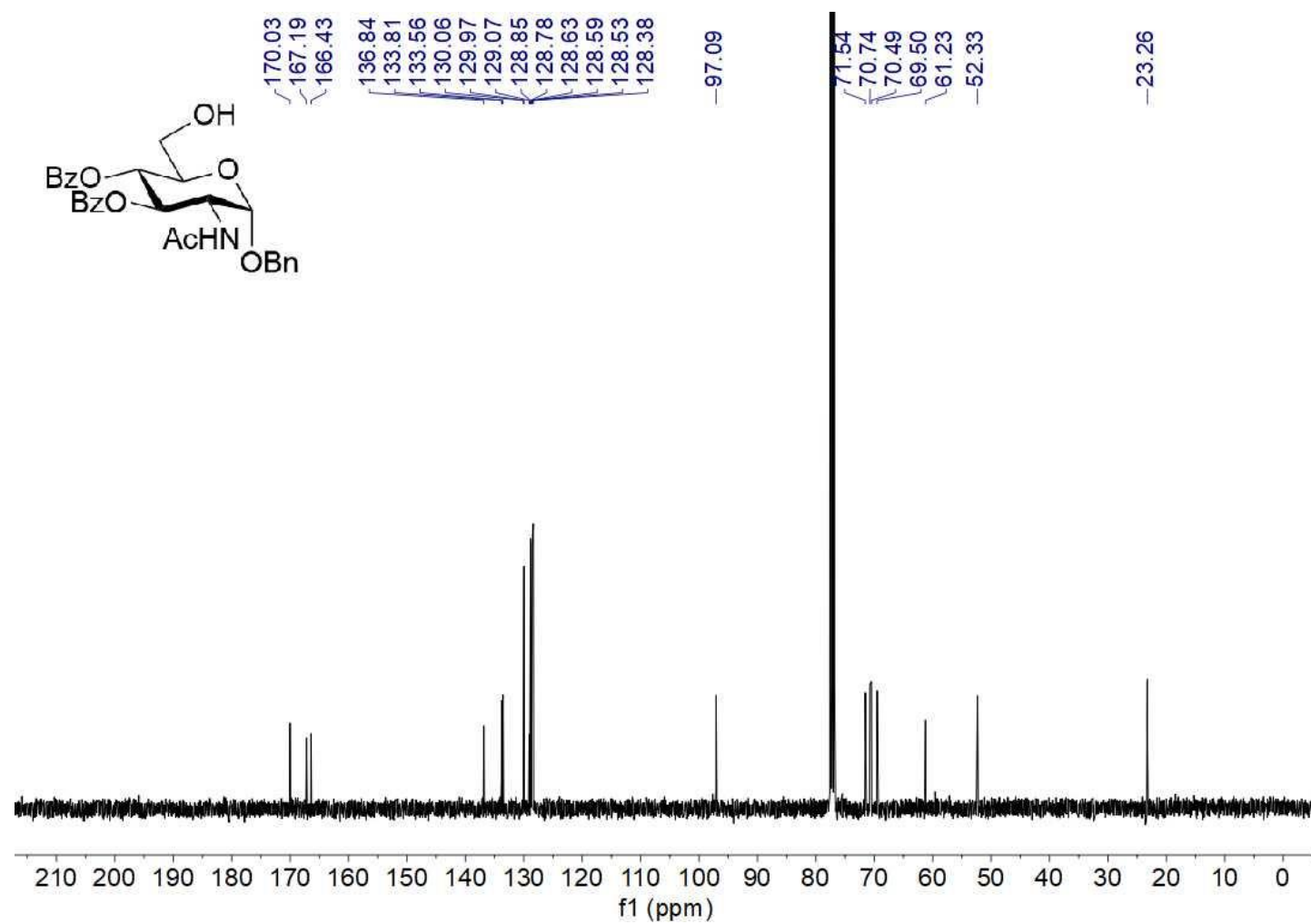


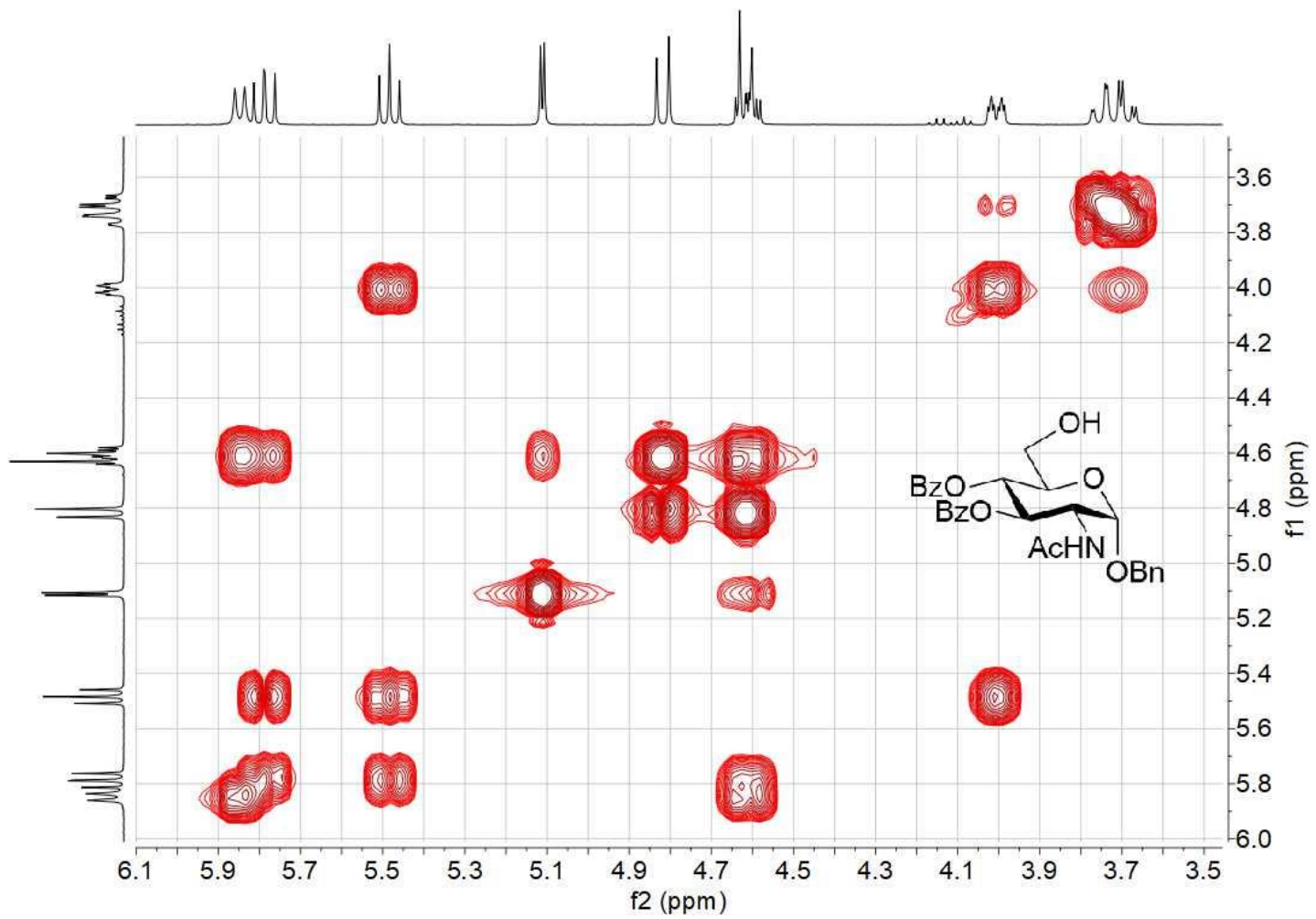
NMR COMPOUND 91

^1H NMR (400 MHz, CDCl_3) 91

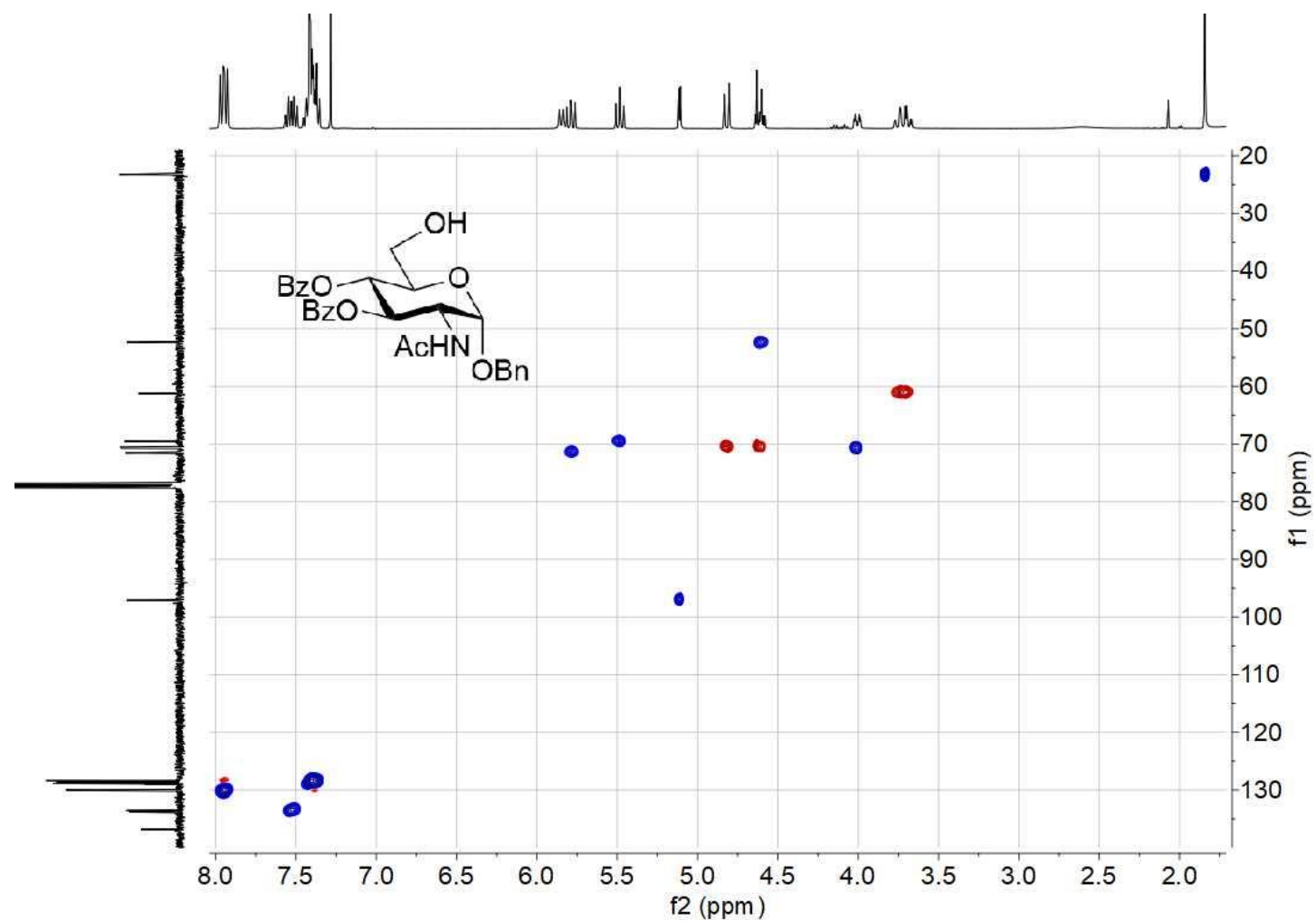


¹³C NMR (100 MHz, CDCl₃) 91



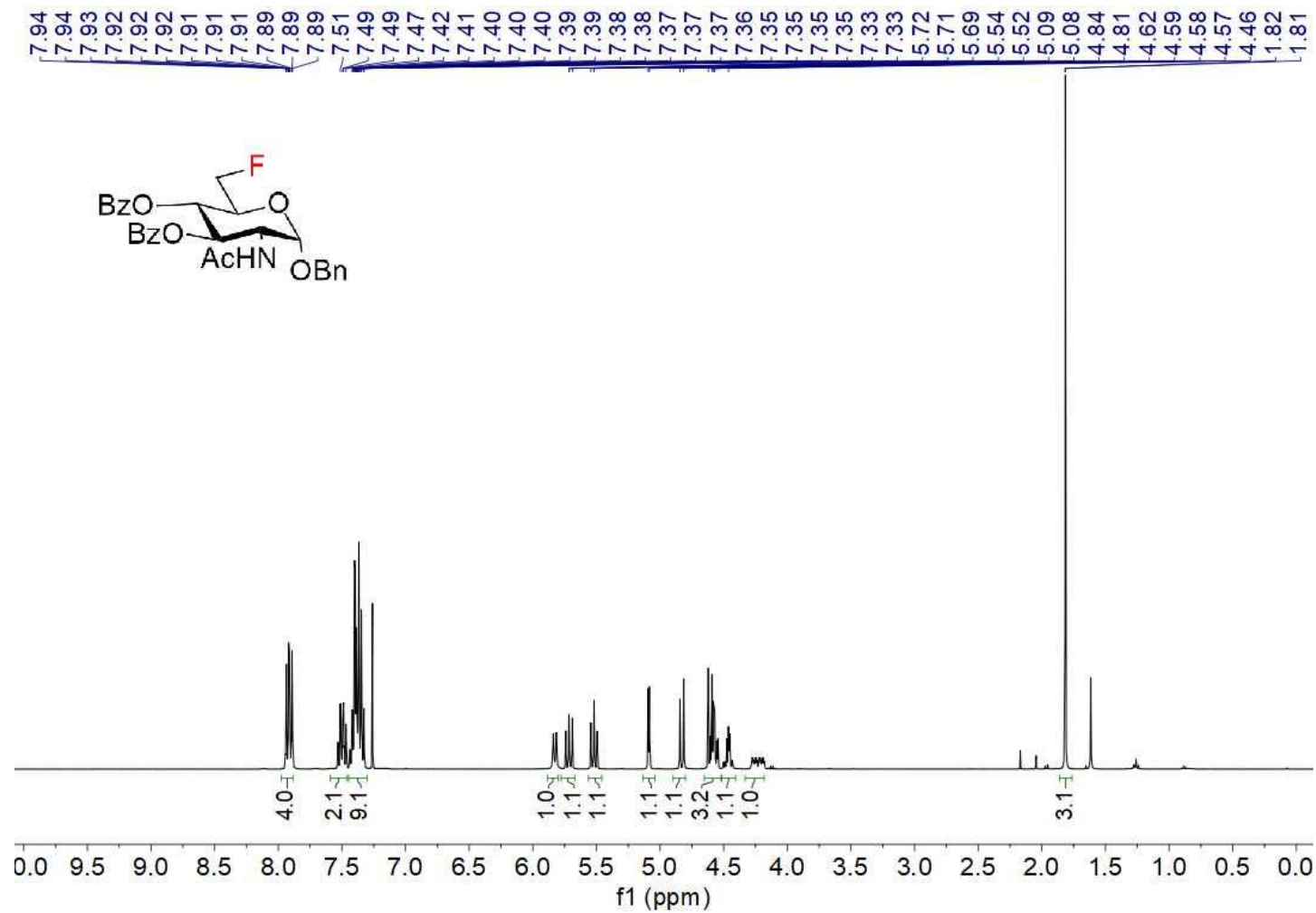
¹H-¹H COSY 91

^1H - ^{13}C HSQC 91

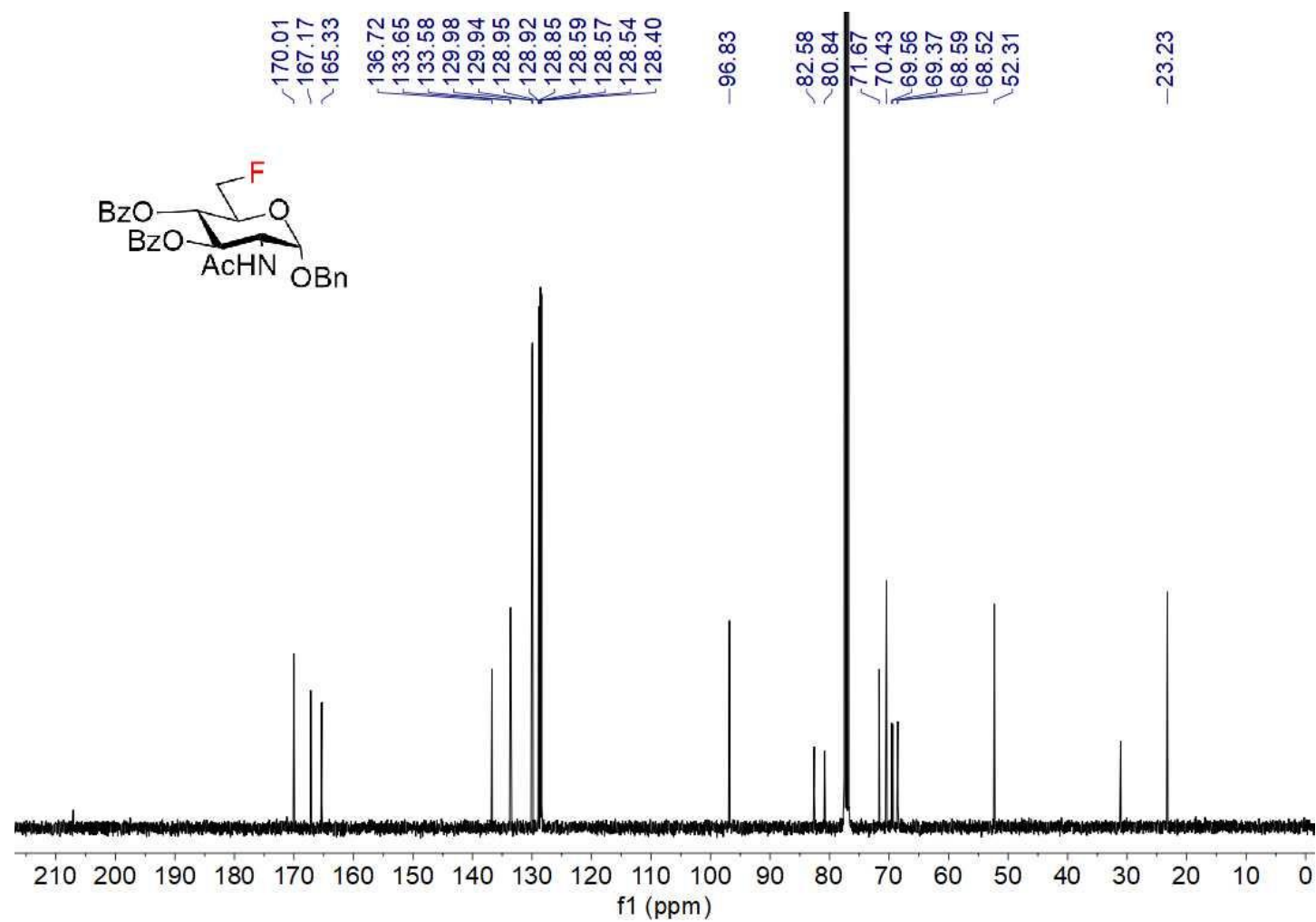


NMR COMPOUND 92

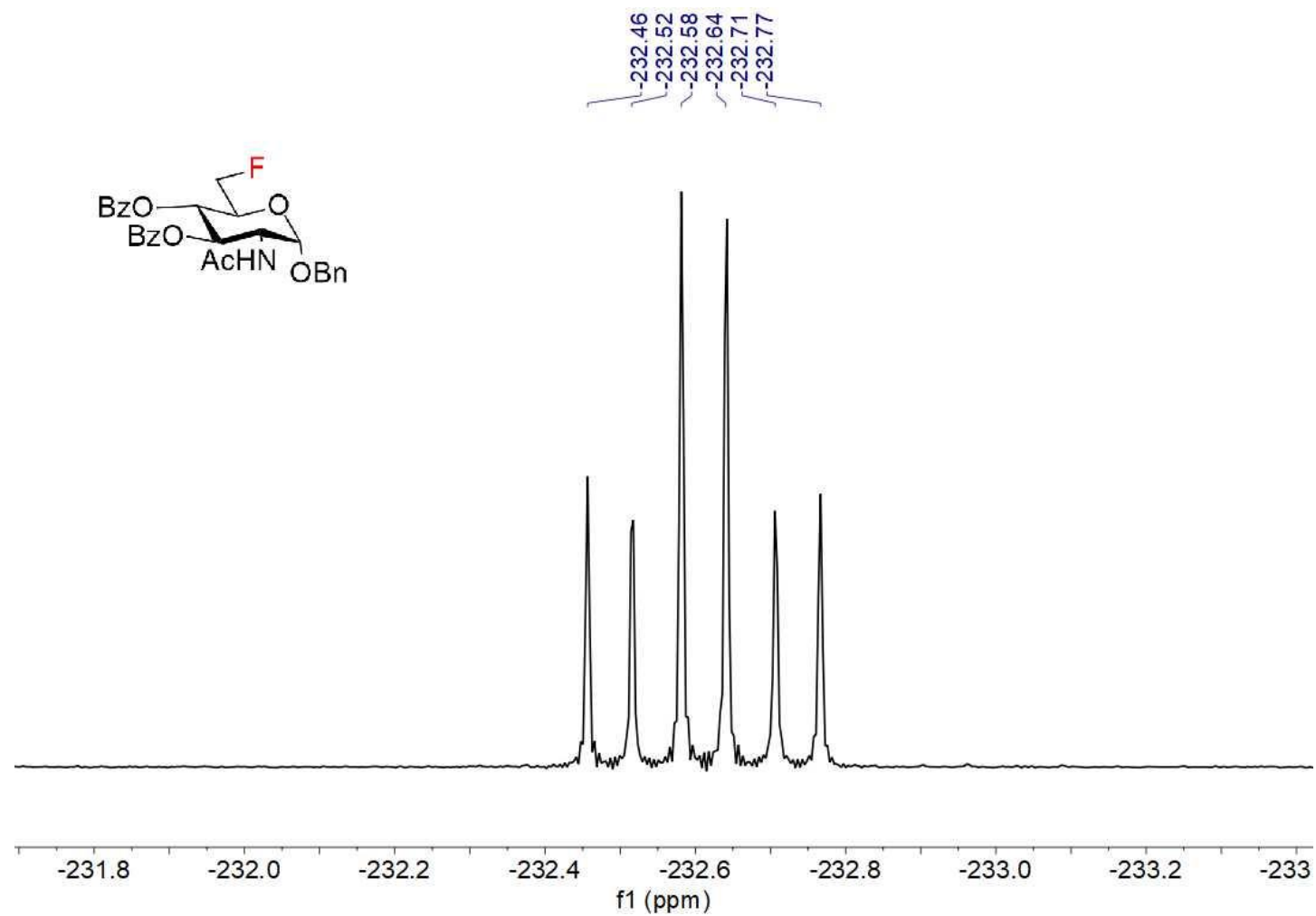
¹H NMR (400 MHz, CDCl₃) 92



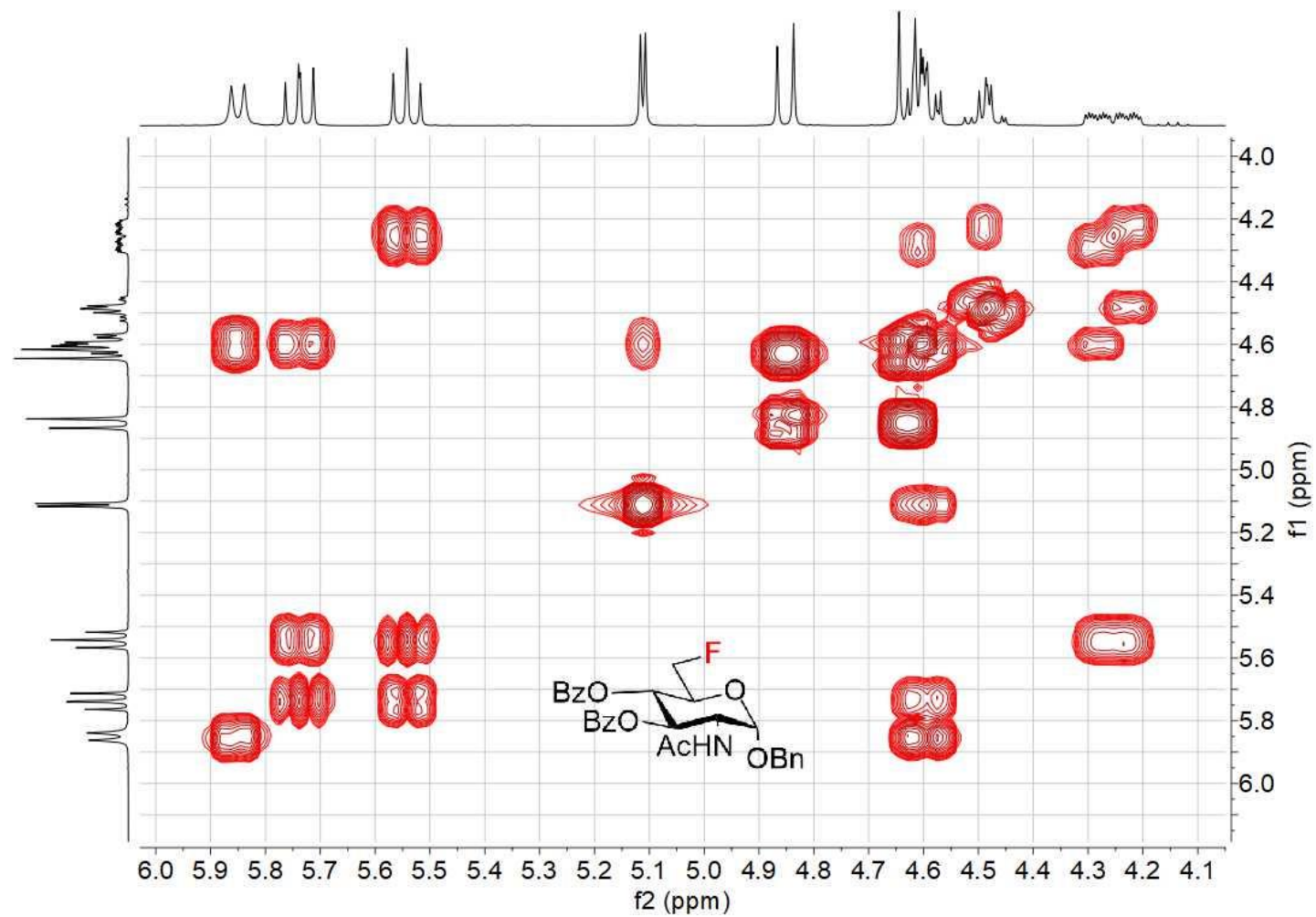
^{13}C NMR (100 MHz, CDCl_3) 92



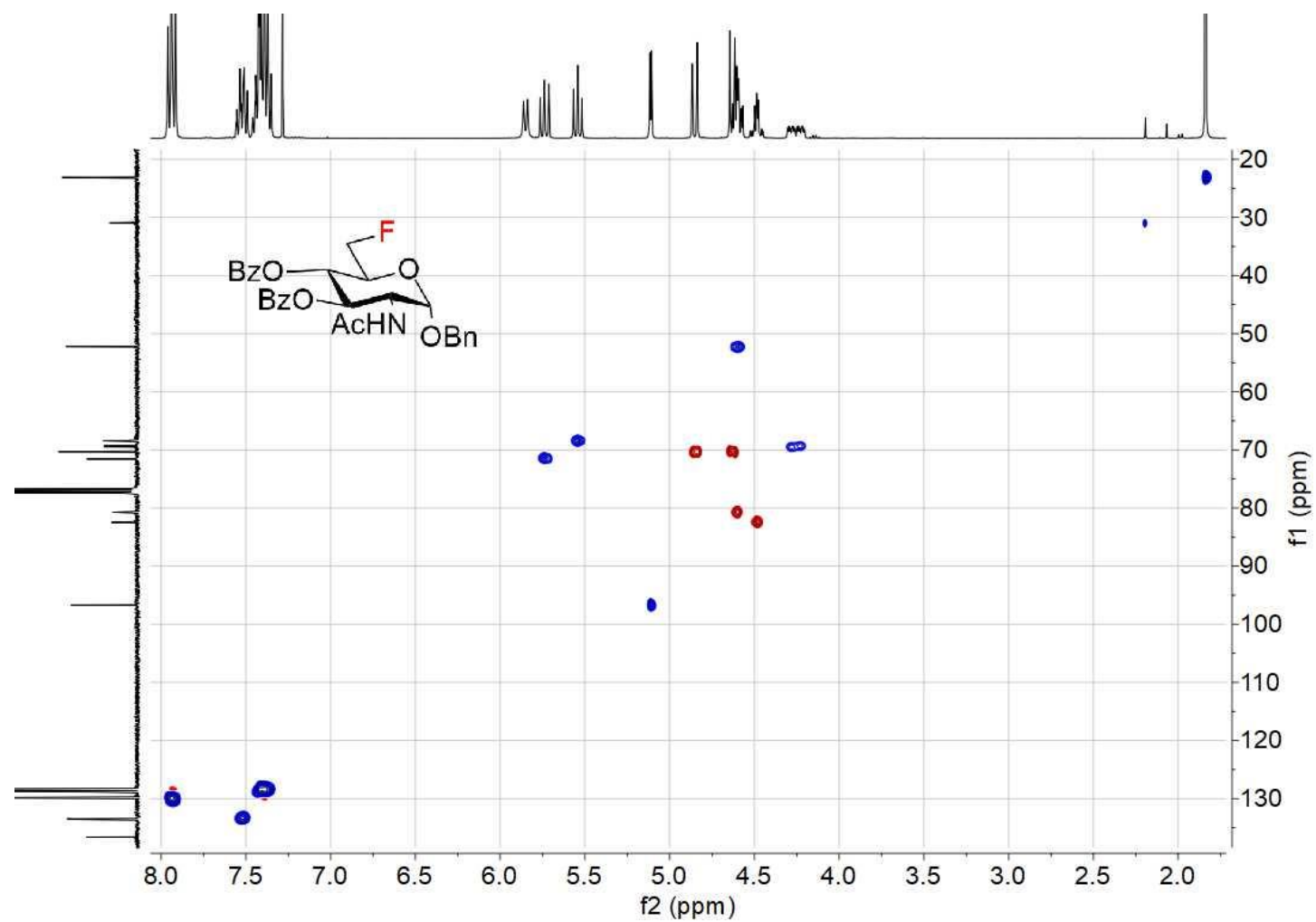
^{19}F NMR (376 MHz, CDCl_3) 92



^1H - ^1H COSY 92

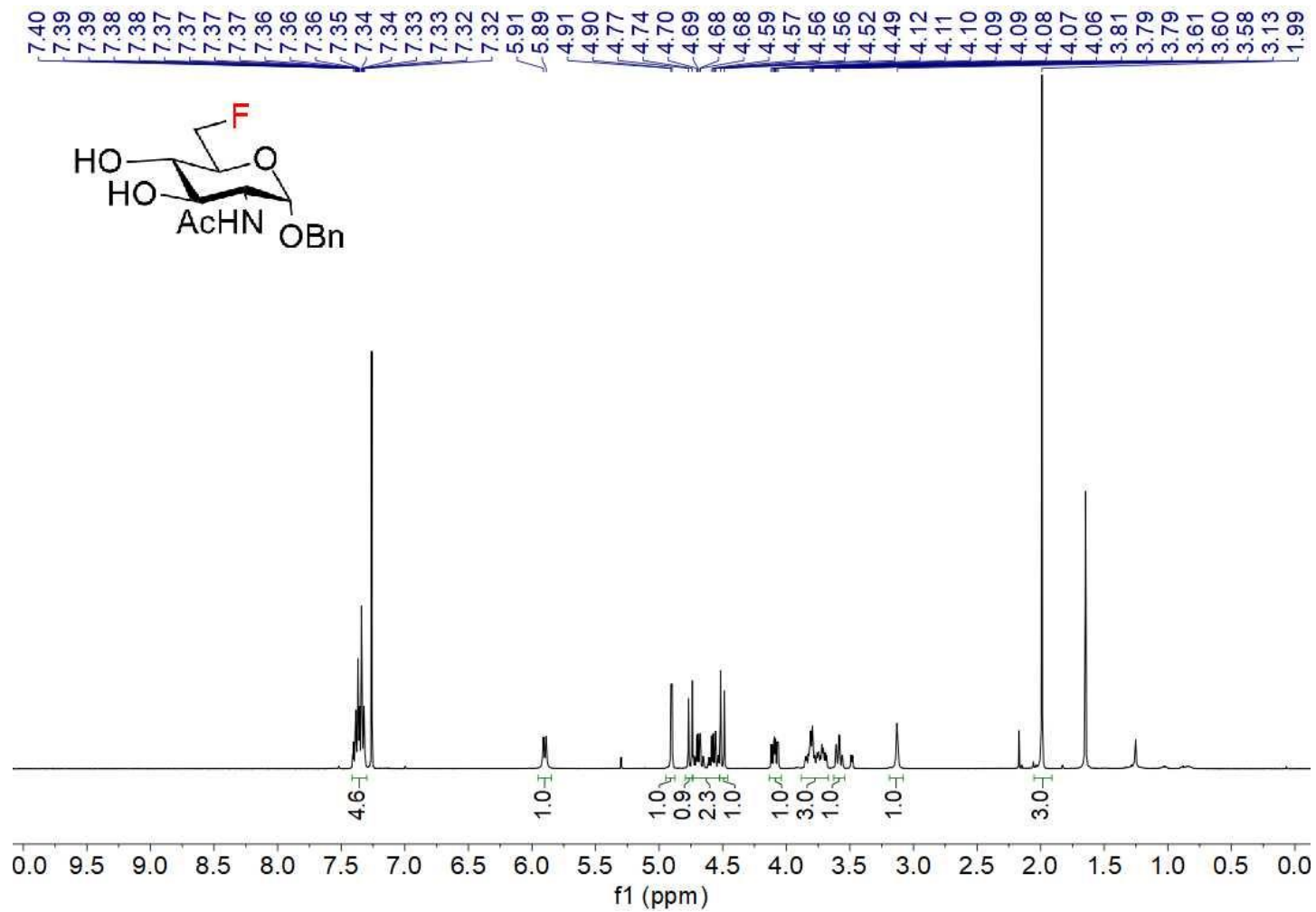


^1H - ^{13}C HSQC 92

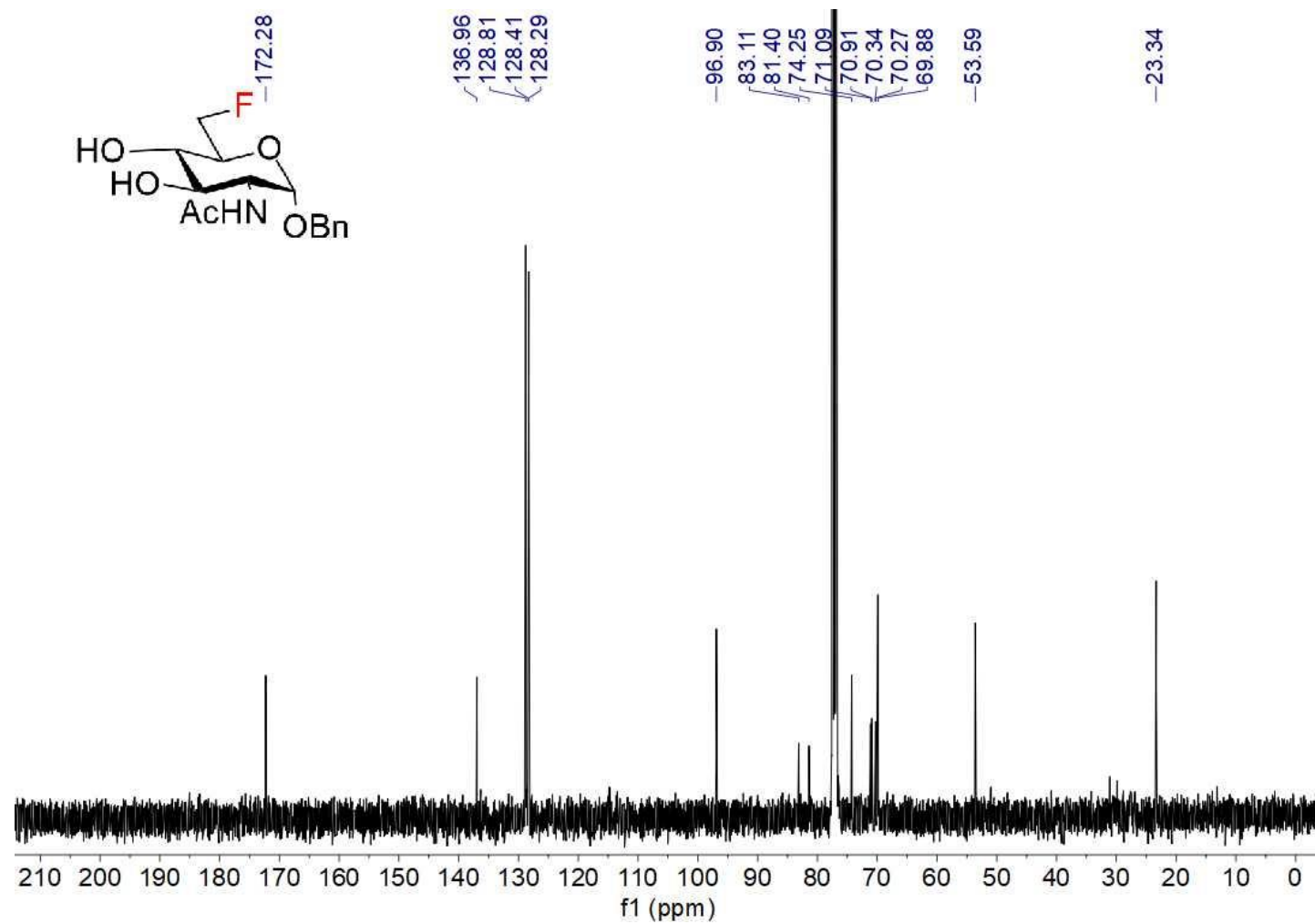


NMR COMPOUND 93

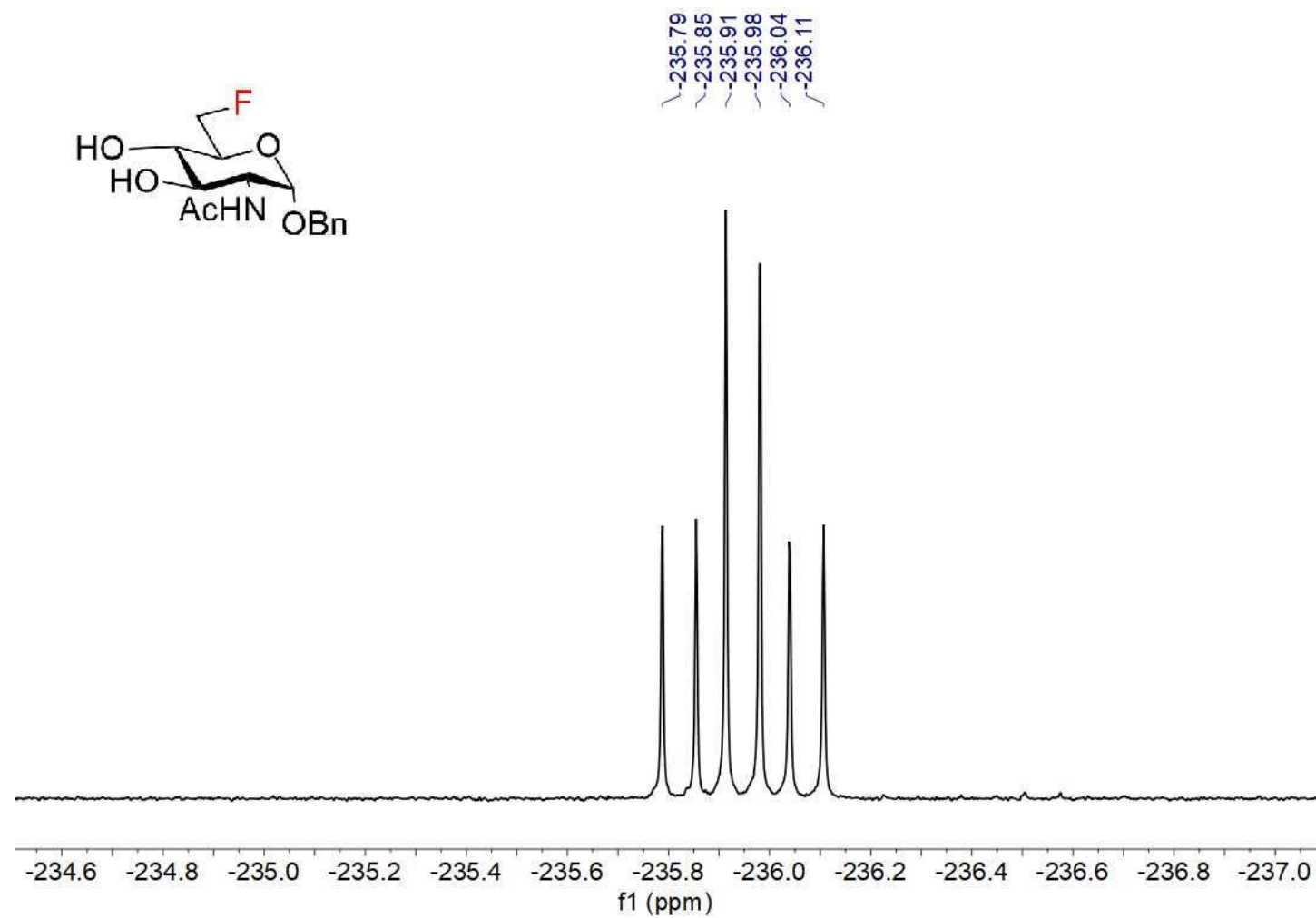
¹H NMR (400 MHz, CDCl₃) 93



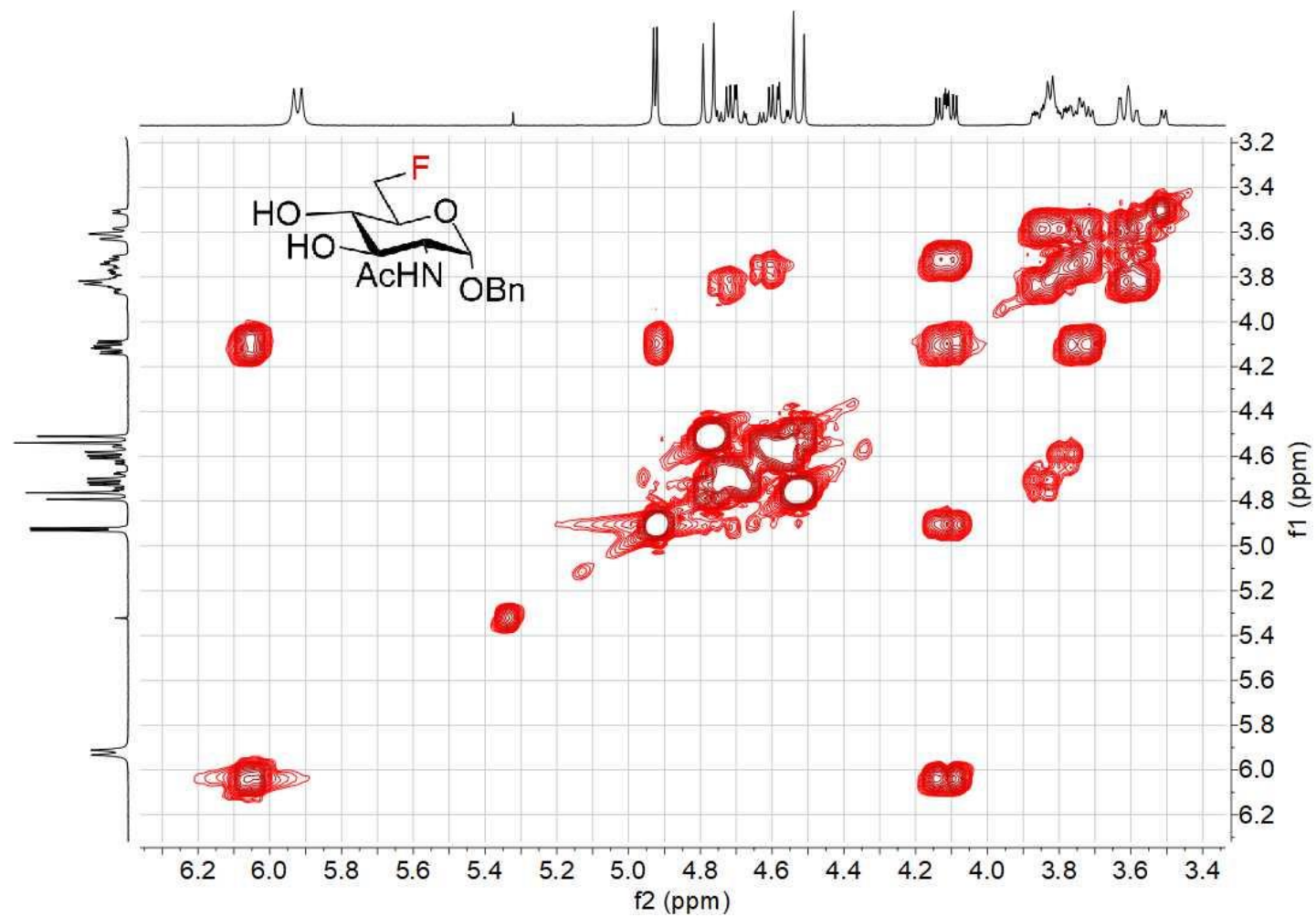
^{13}C NMR (100 MHz, CDCl_3) 93



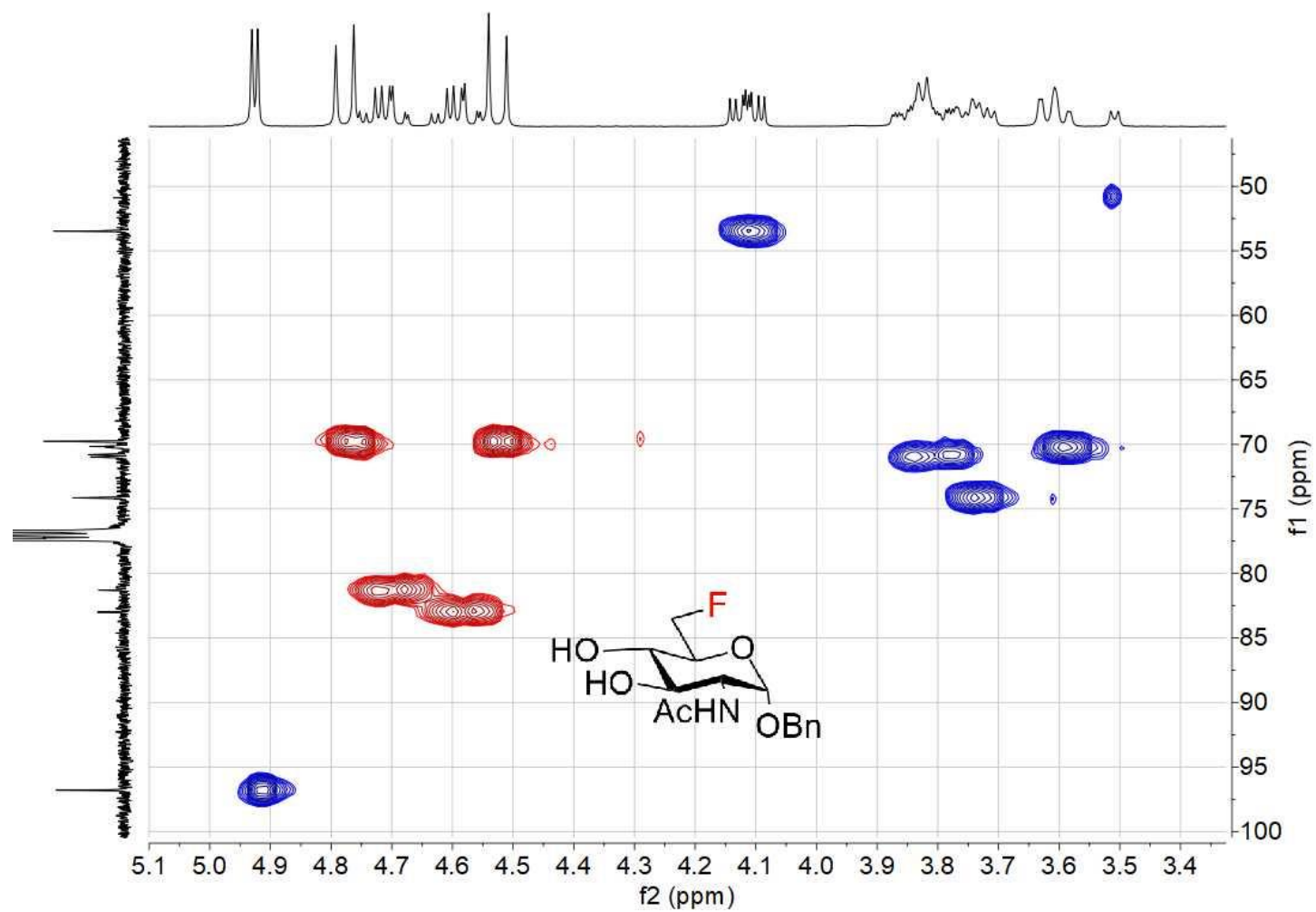
^{19}F NMR (376 MHz, CDCl_3) 93



^1H - ^1H COSY 93

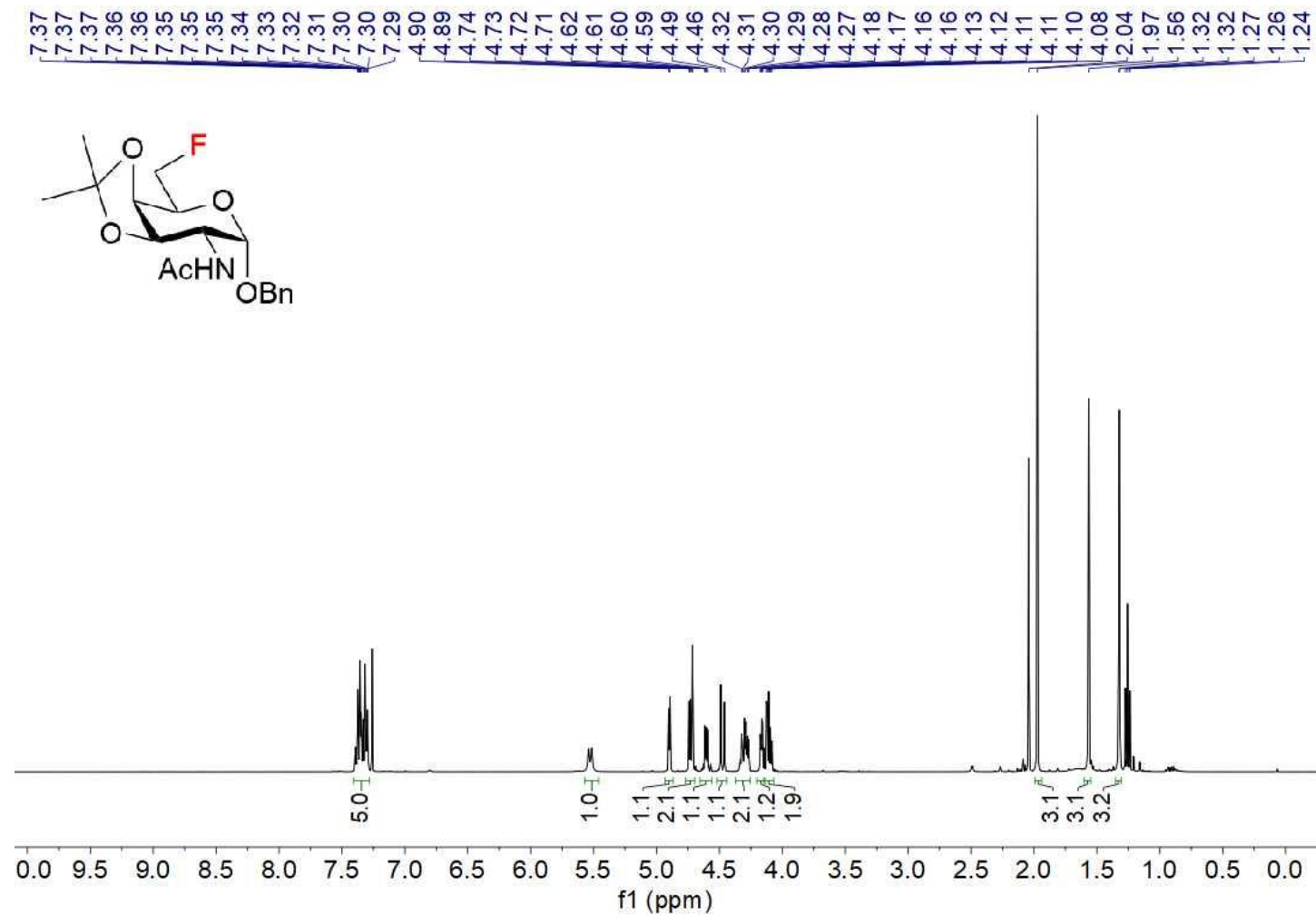


^1H - ^{13}C HSQC 93

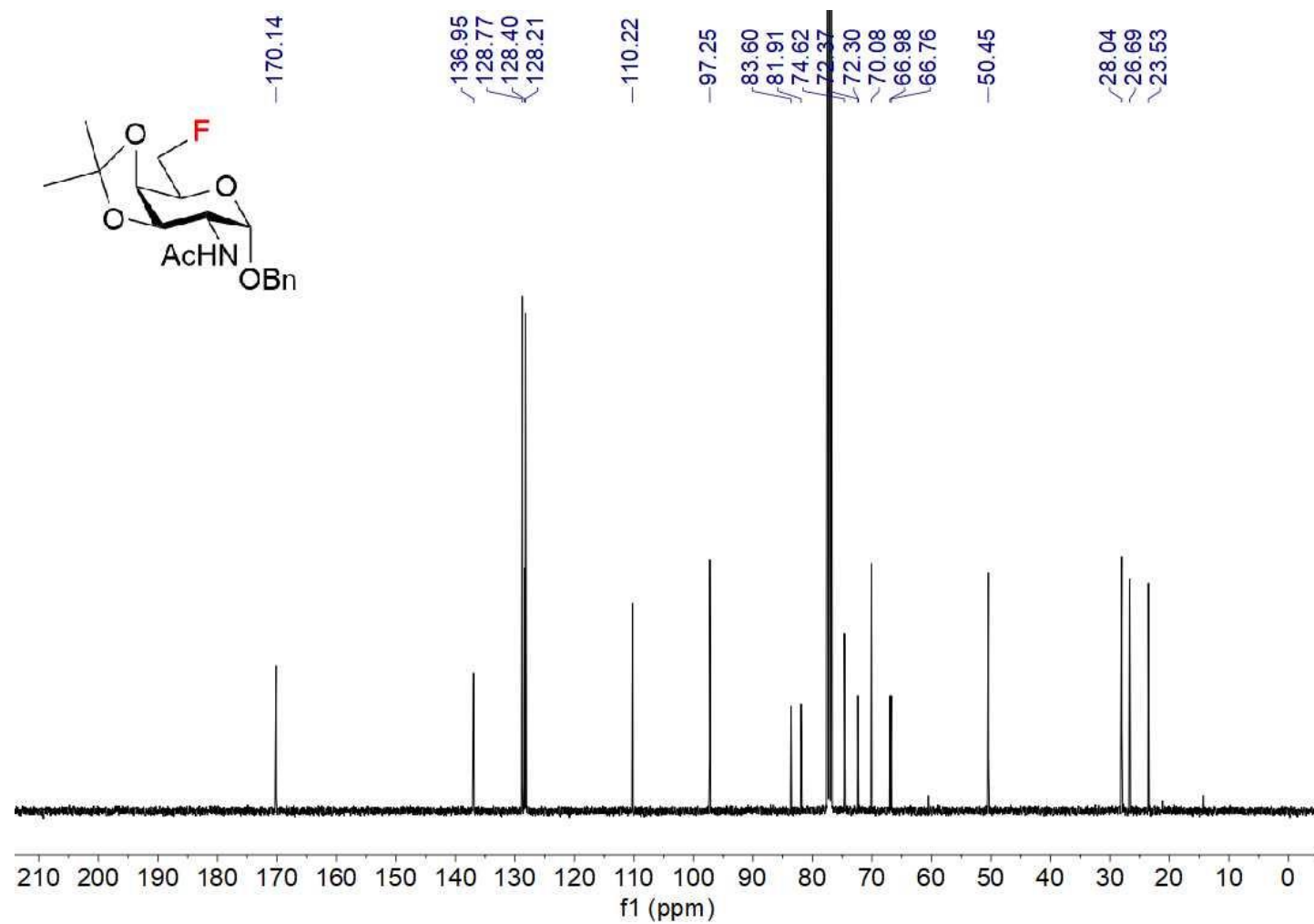


NMR COMPOUND 95

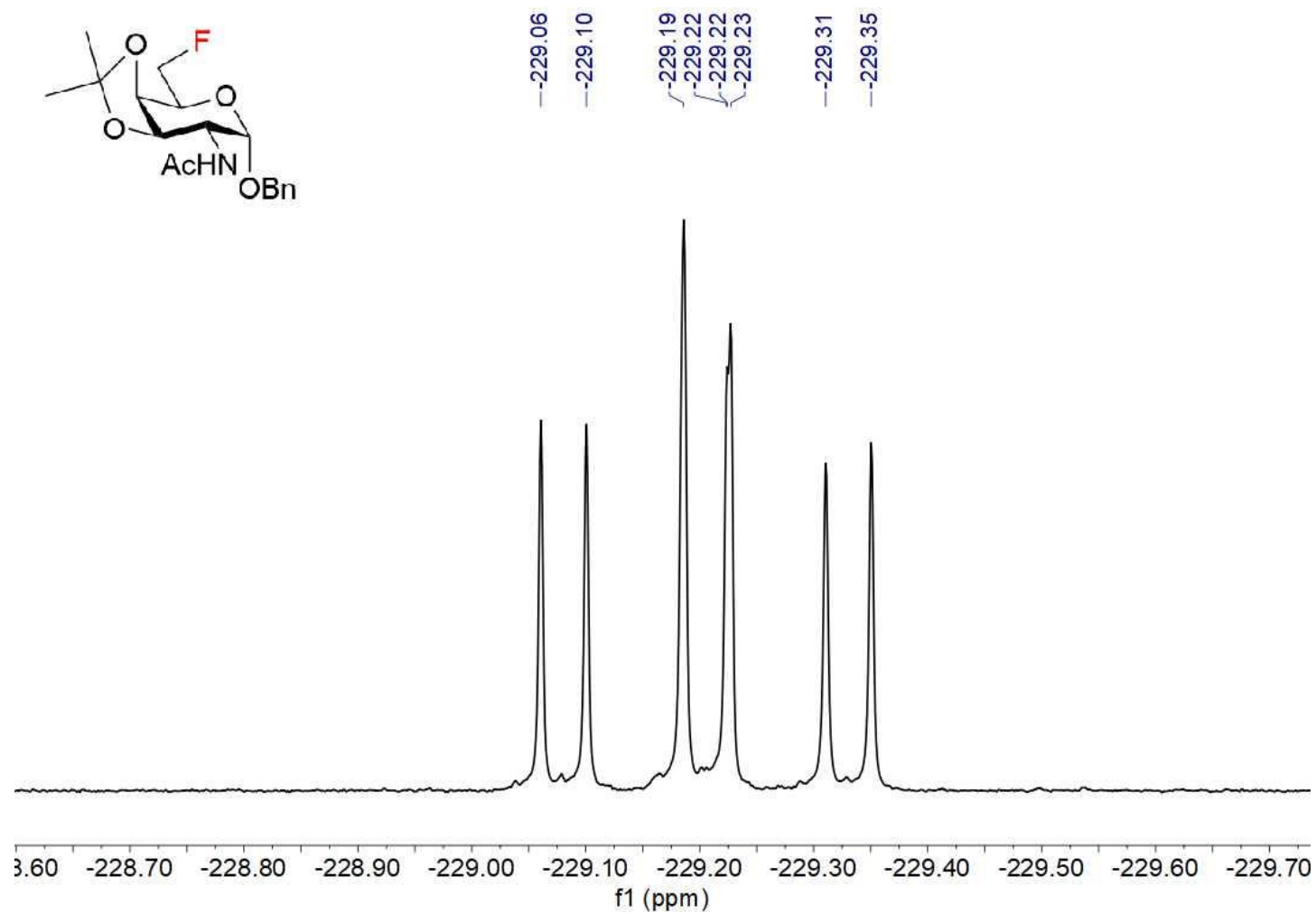
¹H NMR (400 MHz, CDCl₃) 95



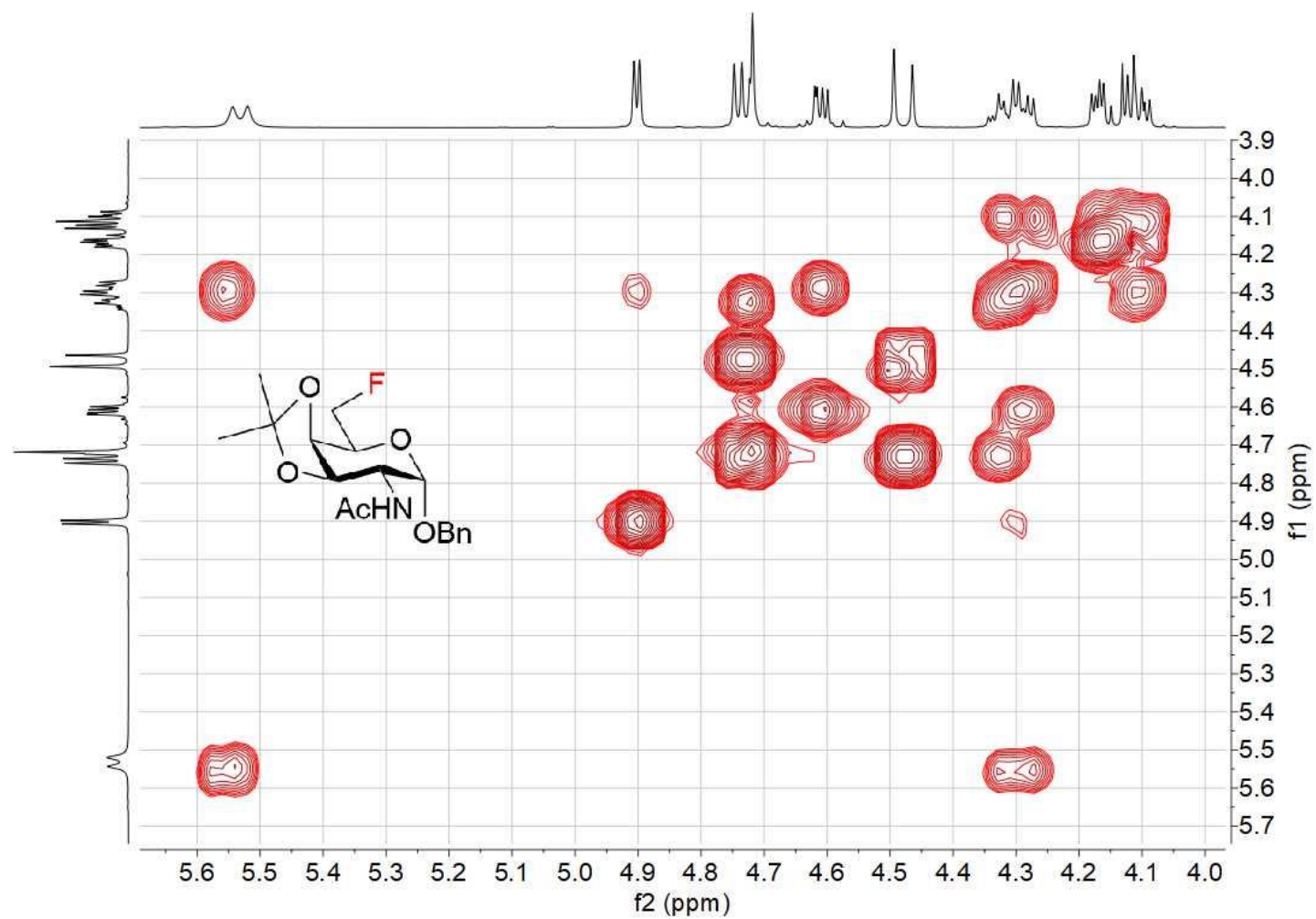
^{13}C NMR (100 MHz, CDCl_3) 95



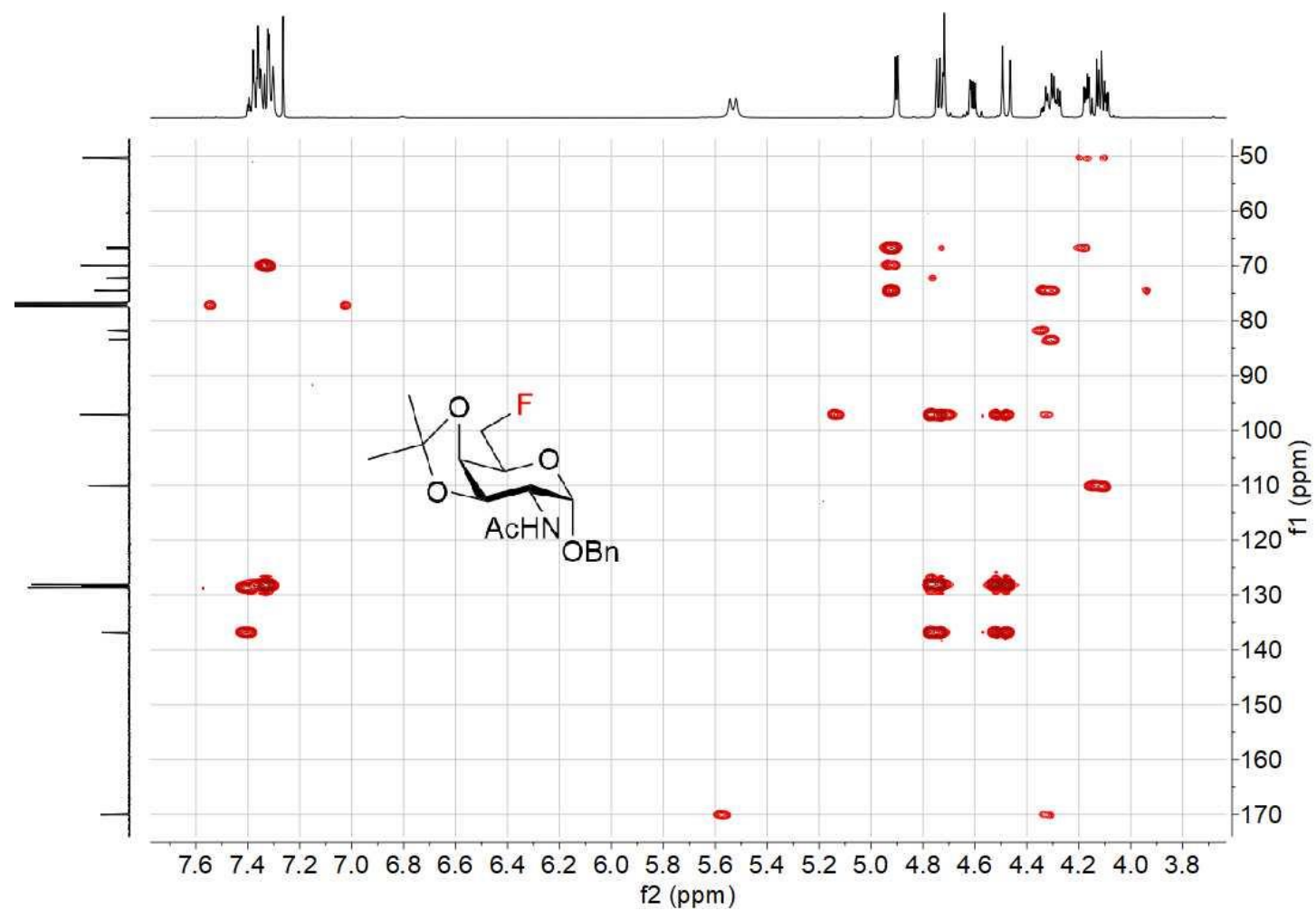
^{19}F NMR (376 MHz, CDCl_3) 95



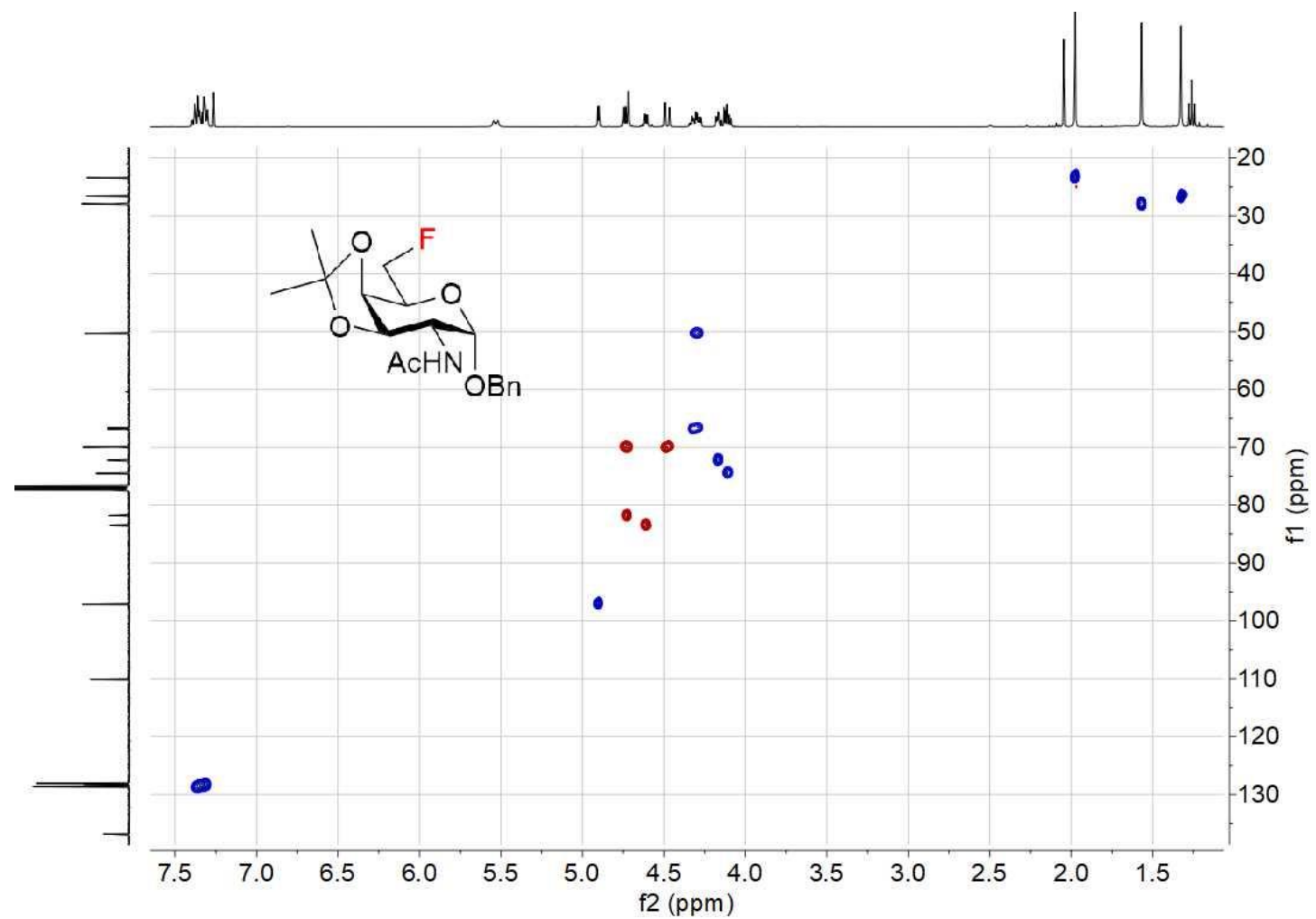
^1H - ^1H COSY 95



^1H - ^{13}C HMBC 95

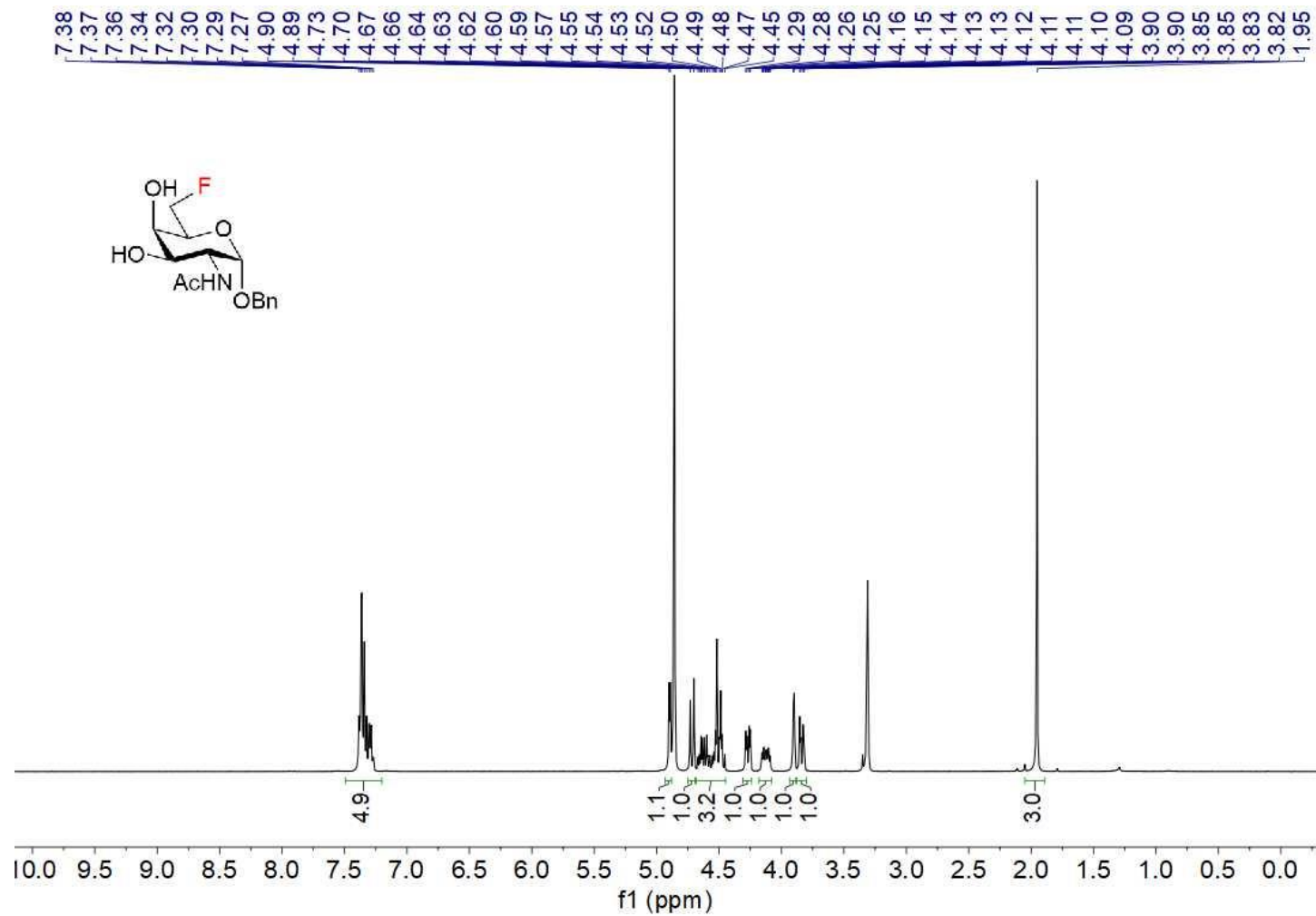


^1H - ^{13}C HSQC 95

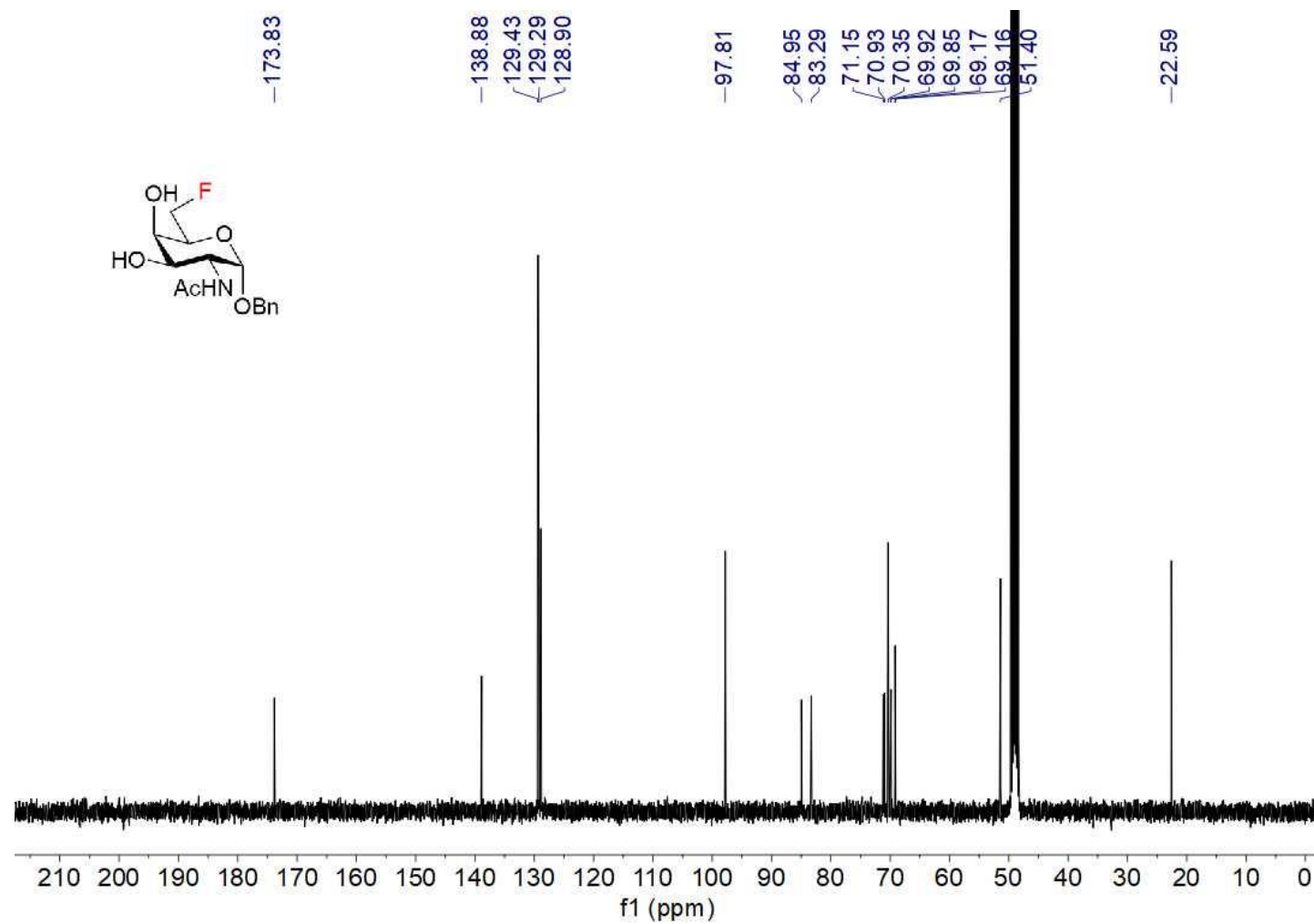


NMR COMPOUND 96

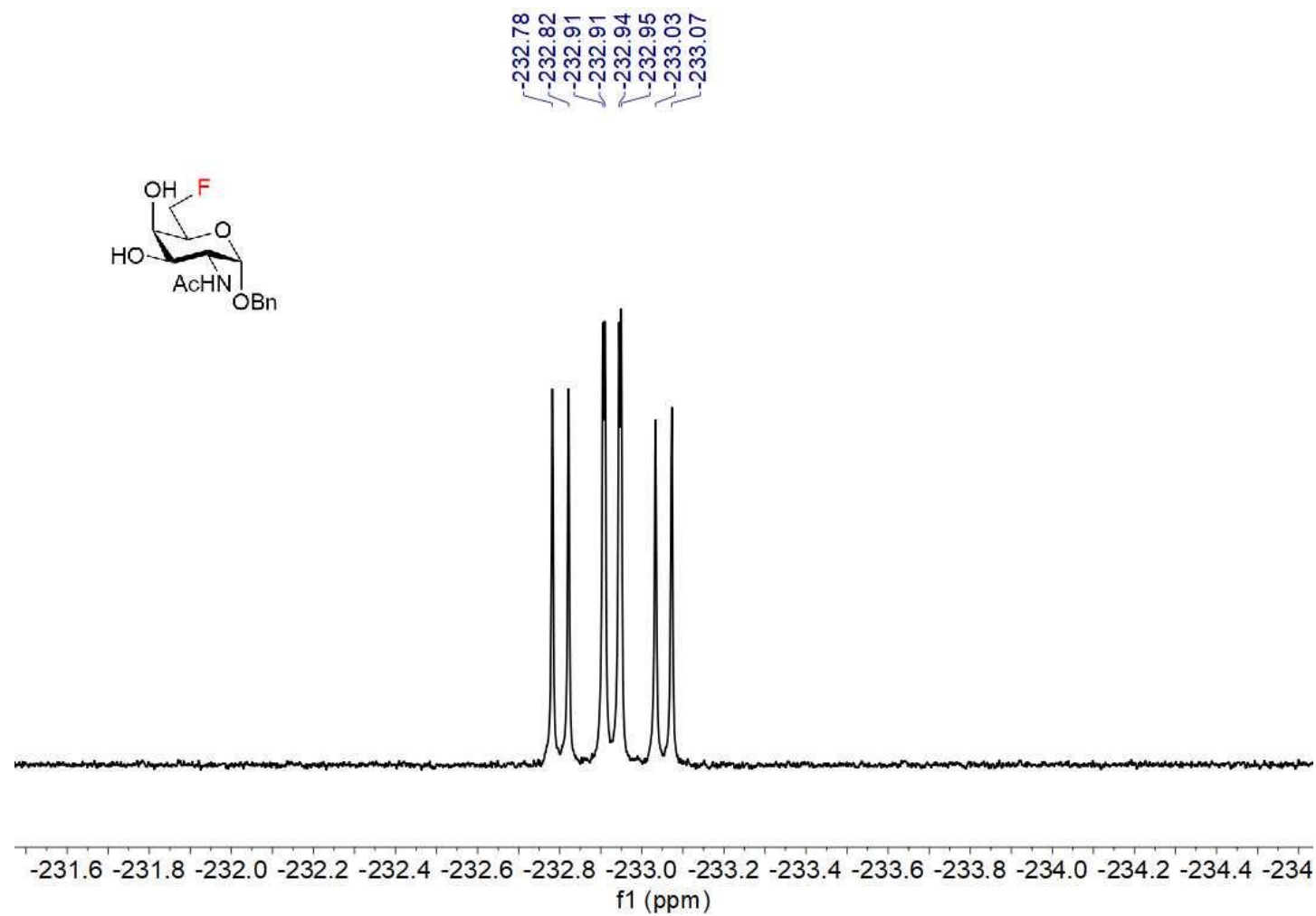
¹H NMR (400 MHz, CD₃OD) 96



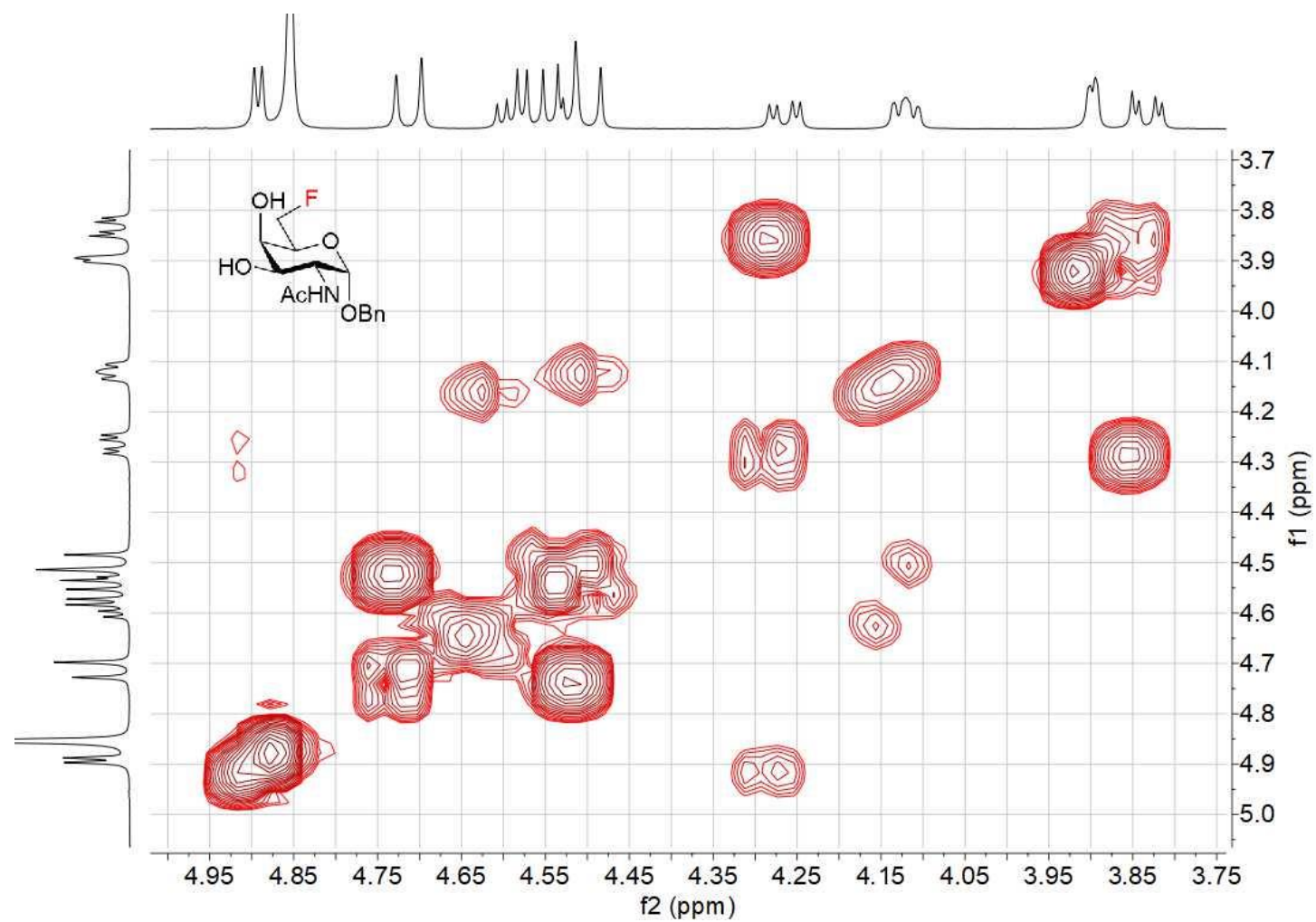
¹³C NMR (100 MHz, CD₃OD) 96



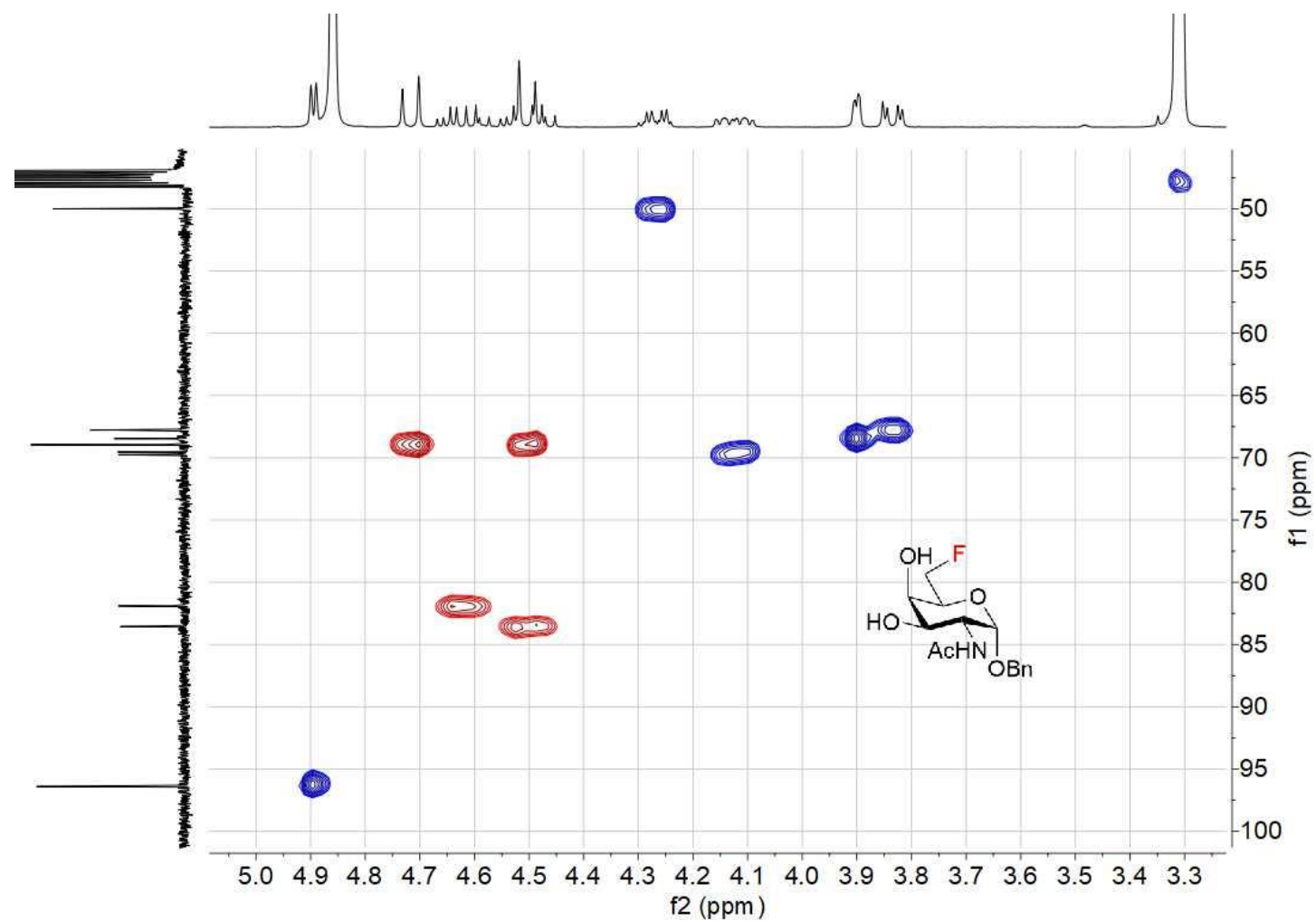
^{19}F NMR (376 MHz, CD_3OD) 96



¹H-¹H COSY 96

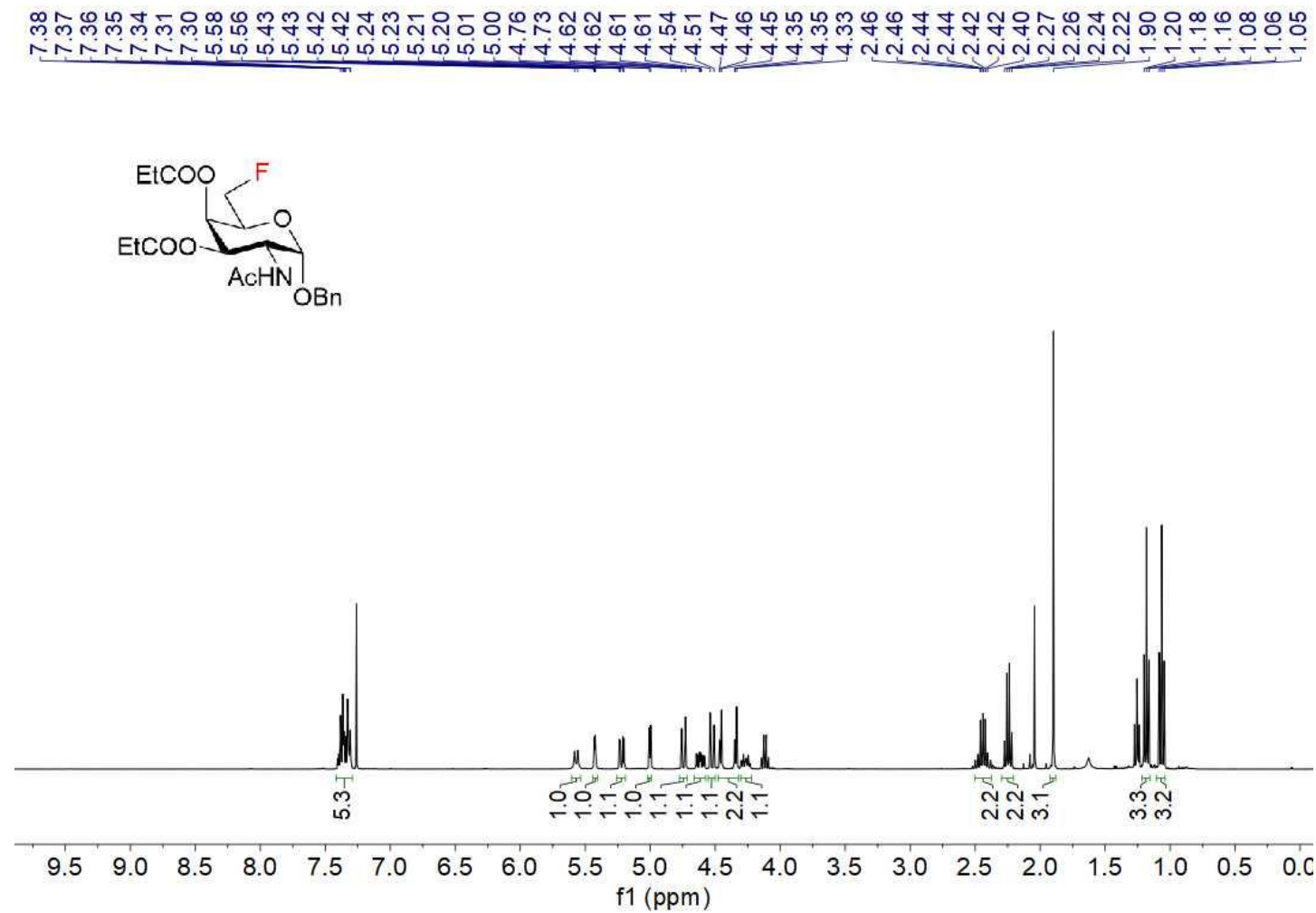


^1H - ^{13}C HSQC 96

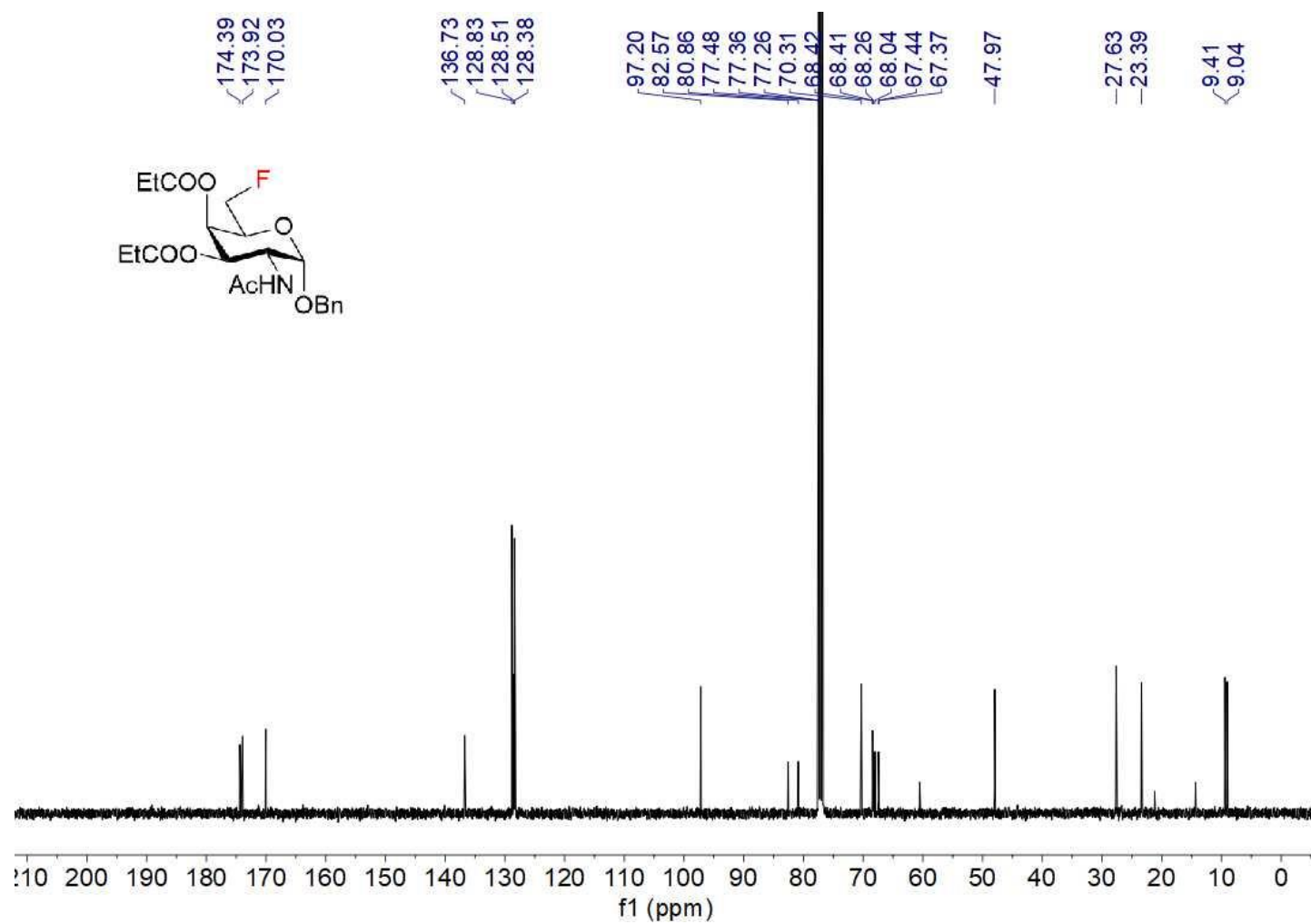


NMR COMPOUND 97

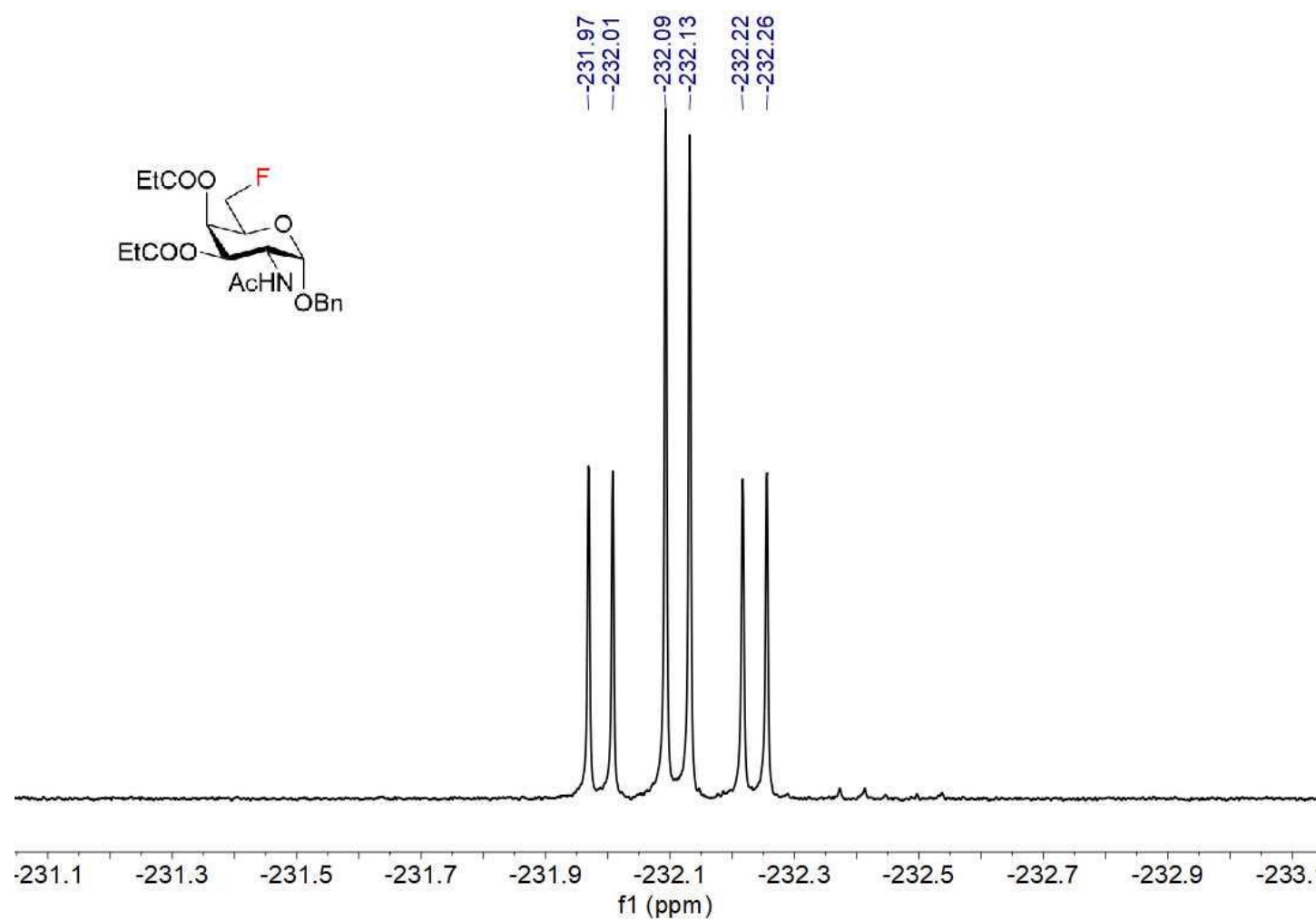
¹H NMR (400 MHz, CDCl₃) 97



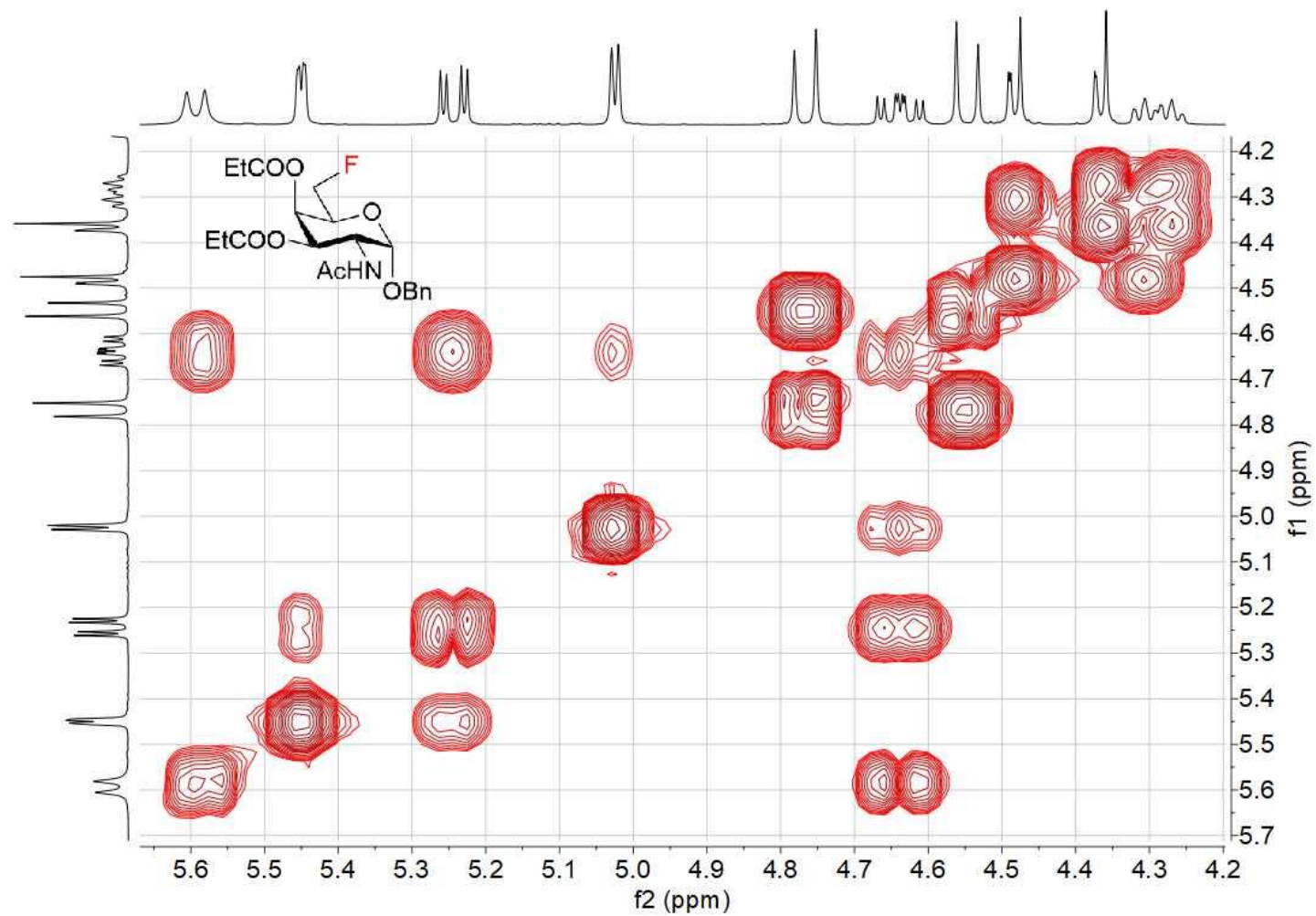
^{13}C NMR (100 MHz, CDCl_3) 97



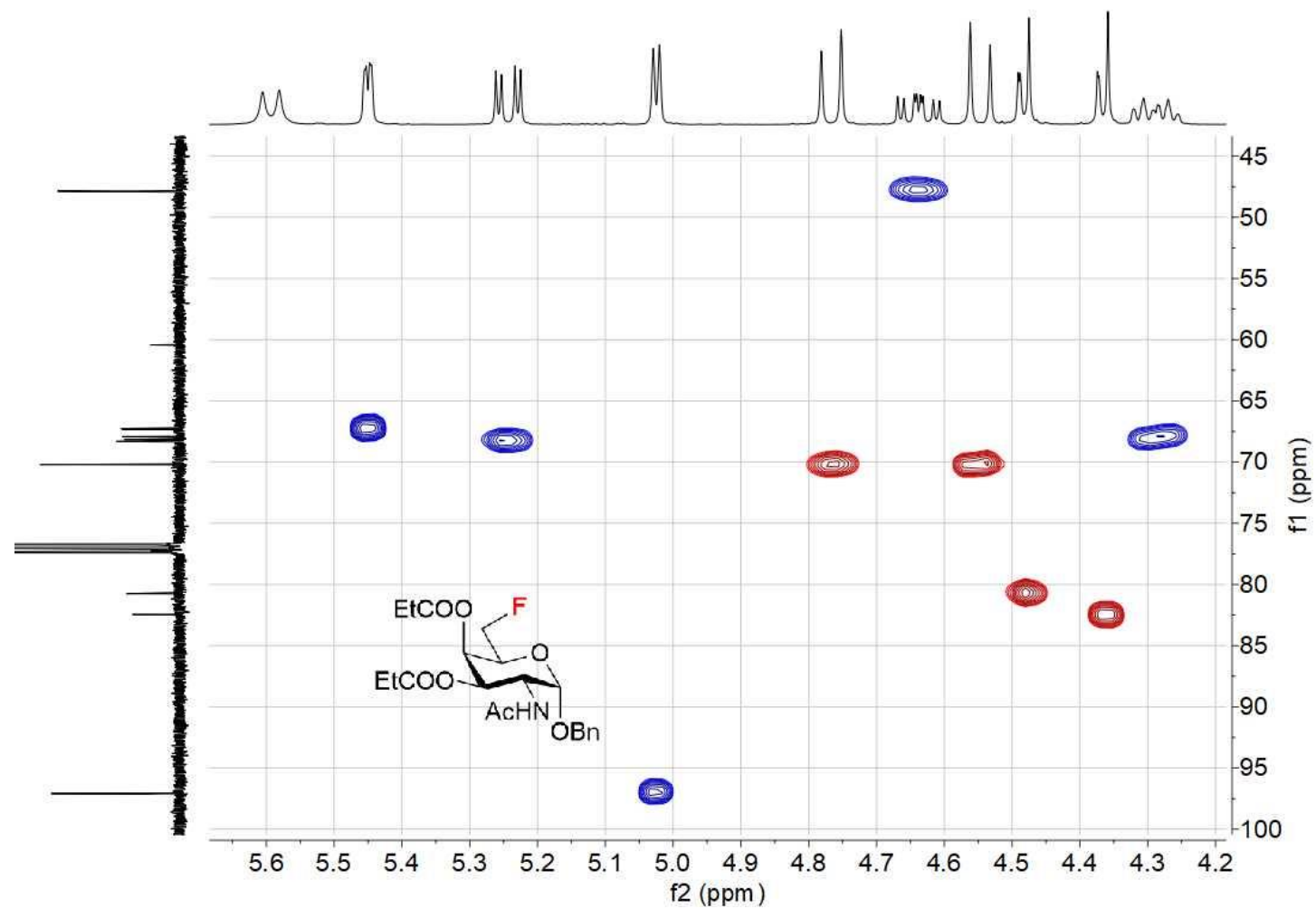
^{19}F NMR (376 MHz, CDCl_3) 97



^1H - ^1H COSY 97

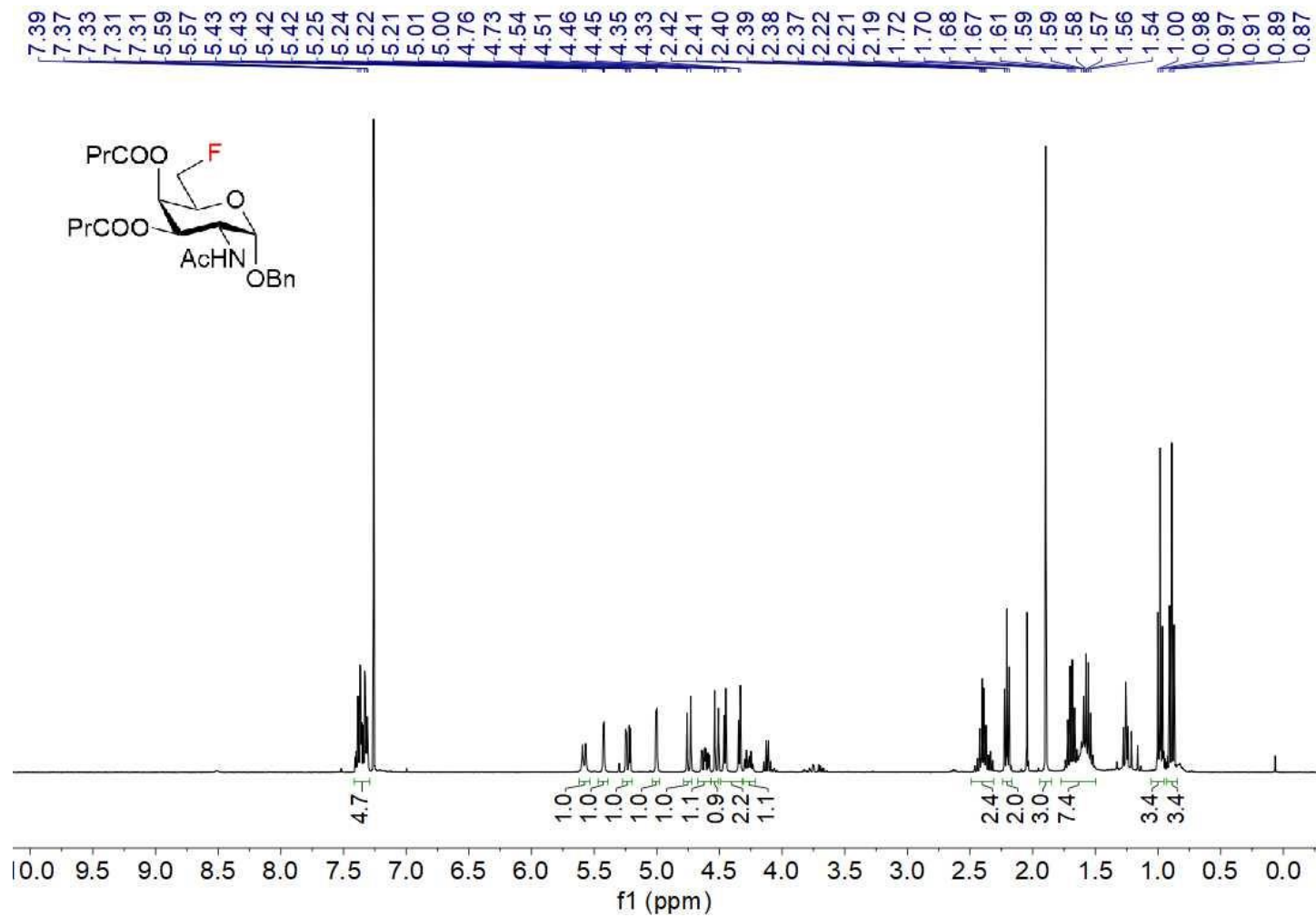


^1H - ^{13}C HSQC 97

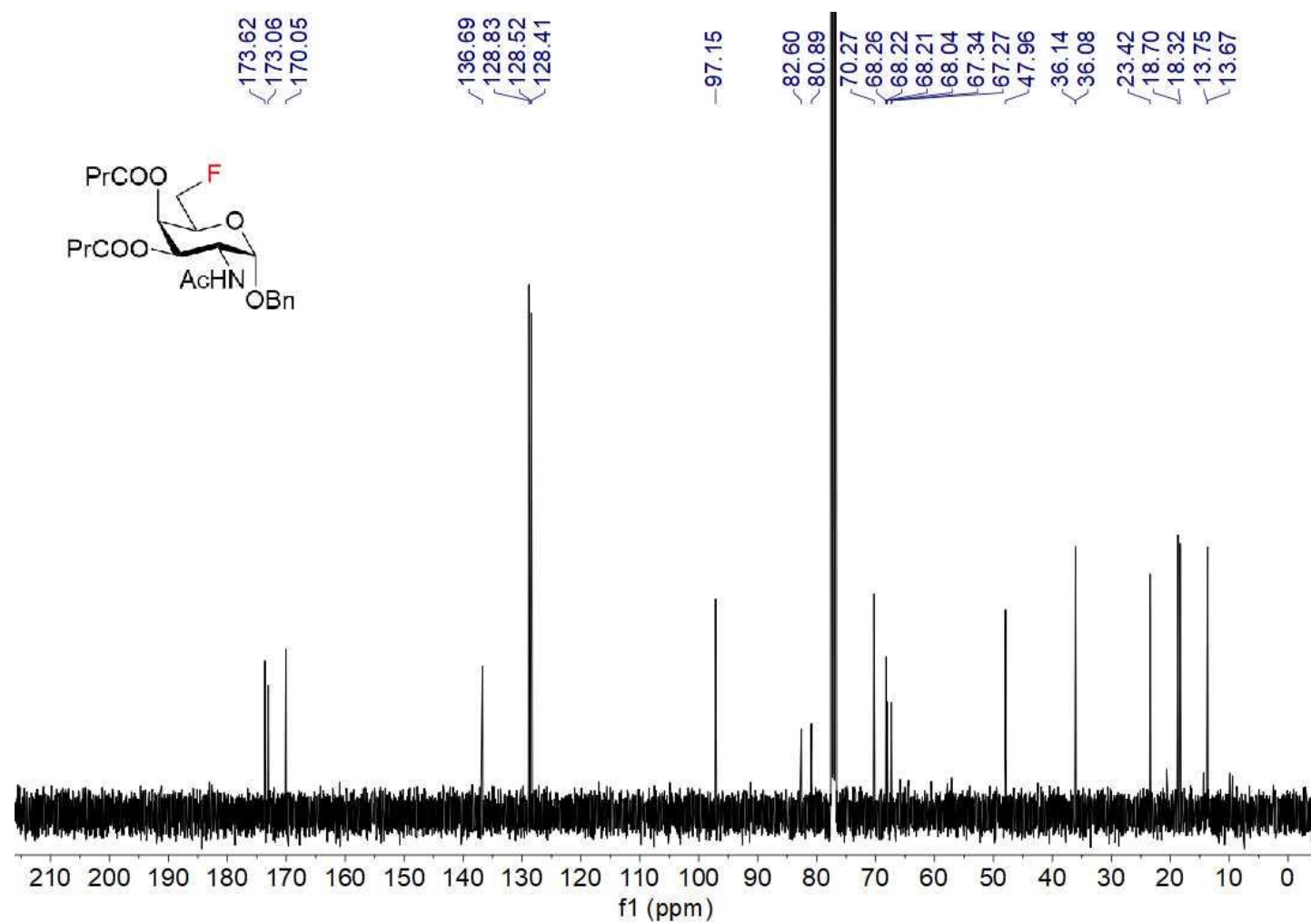


NMR COMPOUND 98

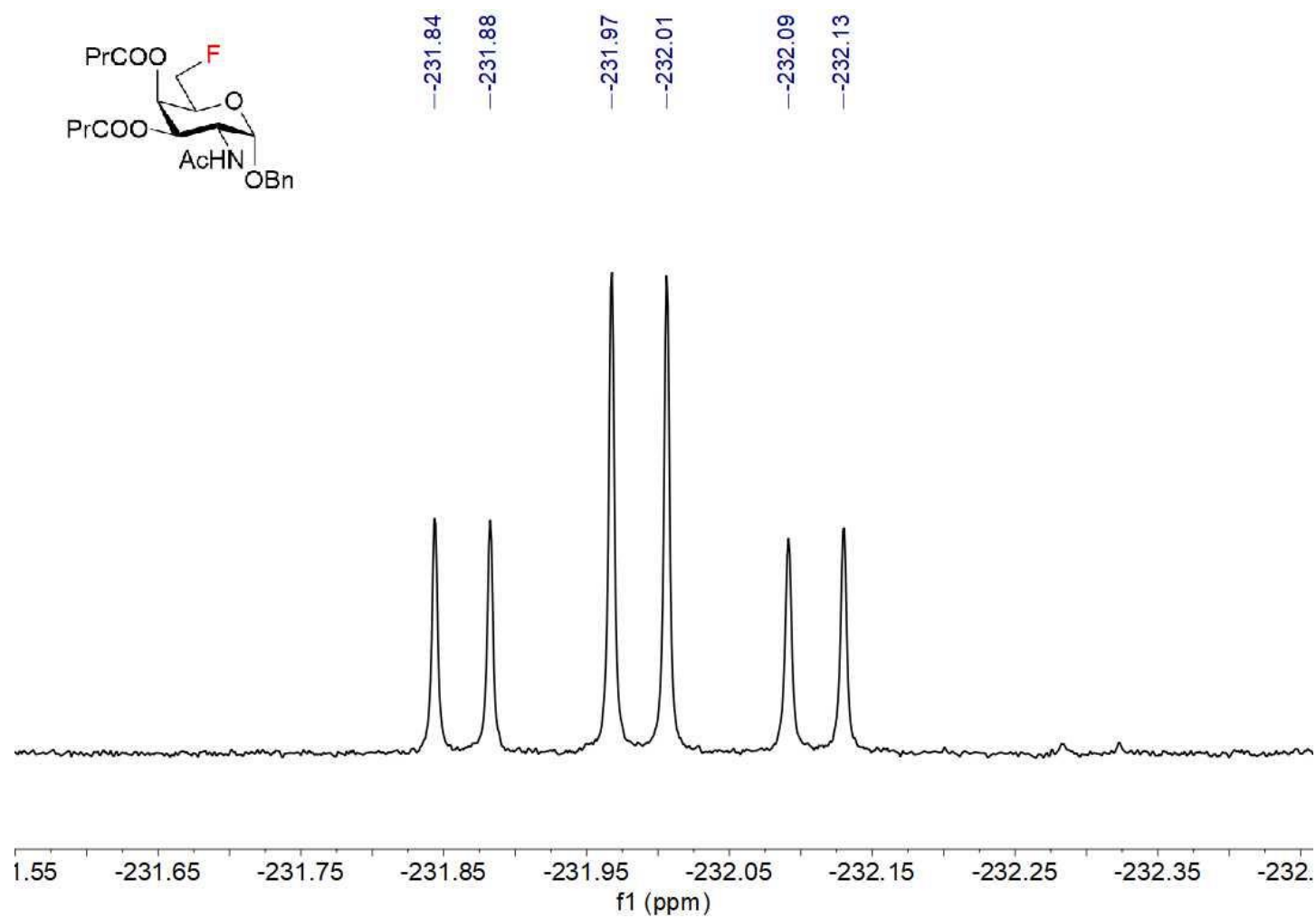
¹H NMR (400 MHz, CDCl₃) 98



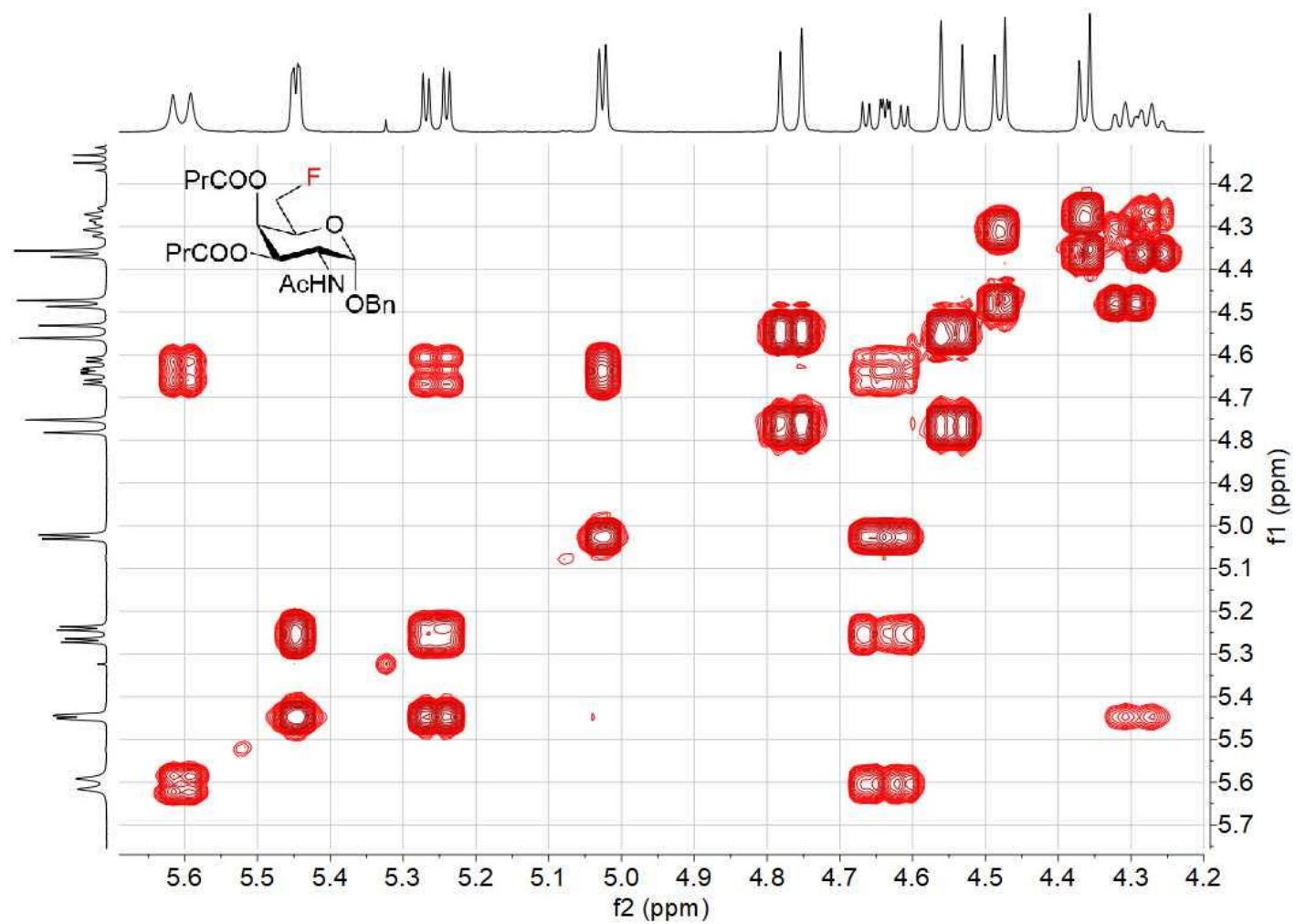
¹³C NMR (100 MHz, CDCl₃) 98



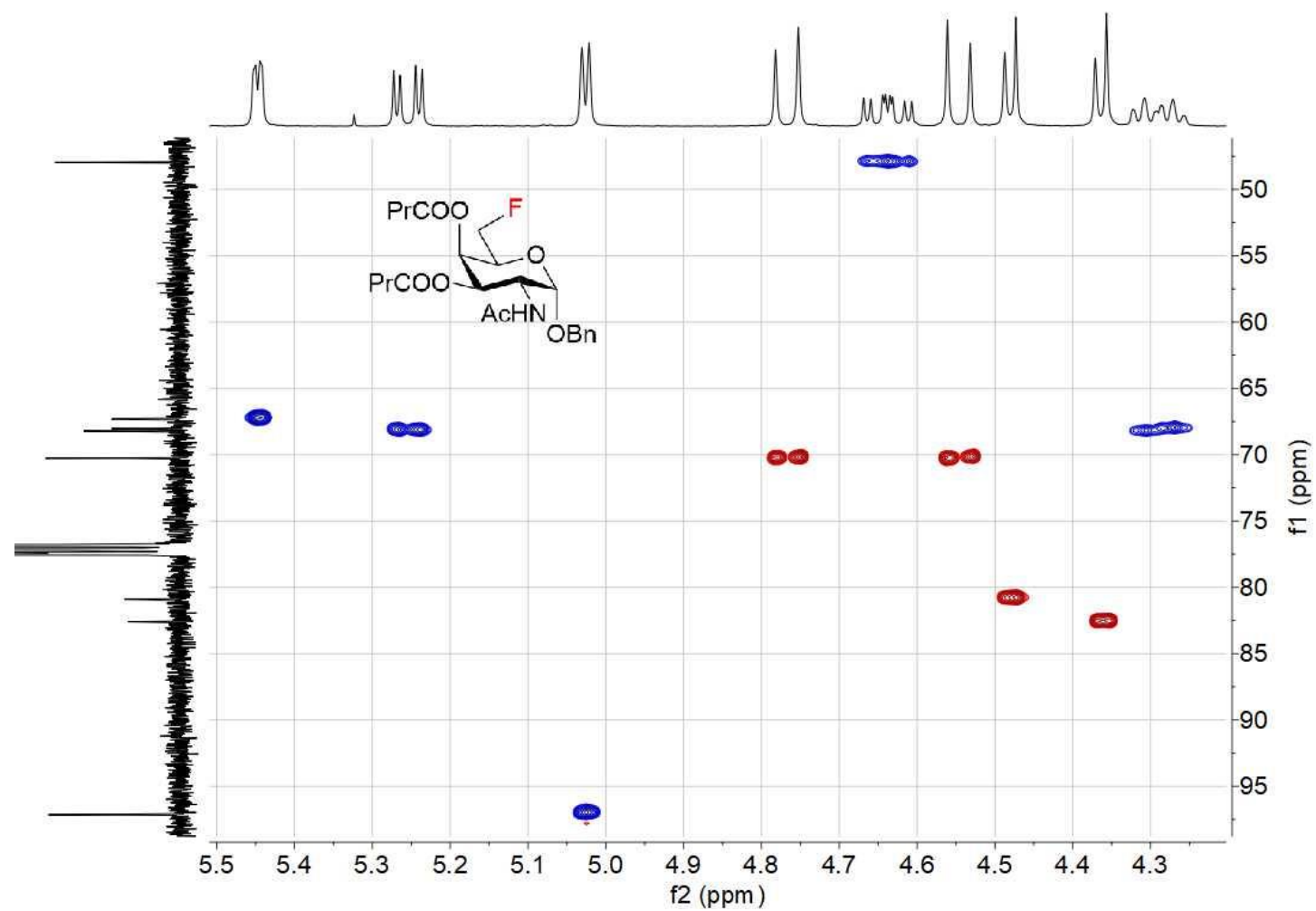
¹⁹F NMR (376 MHz, CDCl₃) 98



^1H - ^1H COSY 98

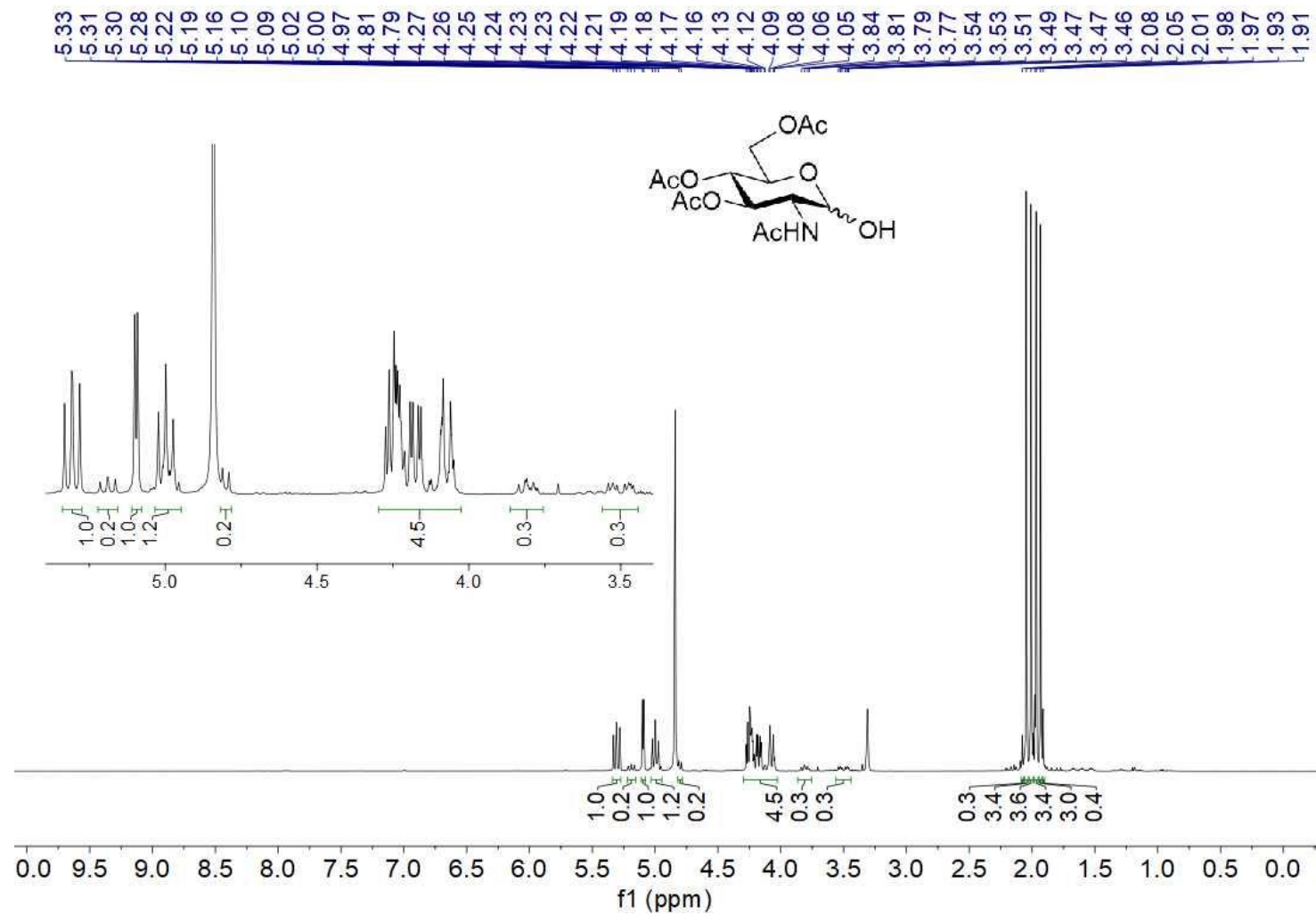


^1H - ^{13}C HSQC 98

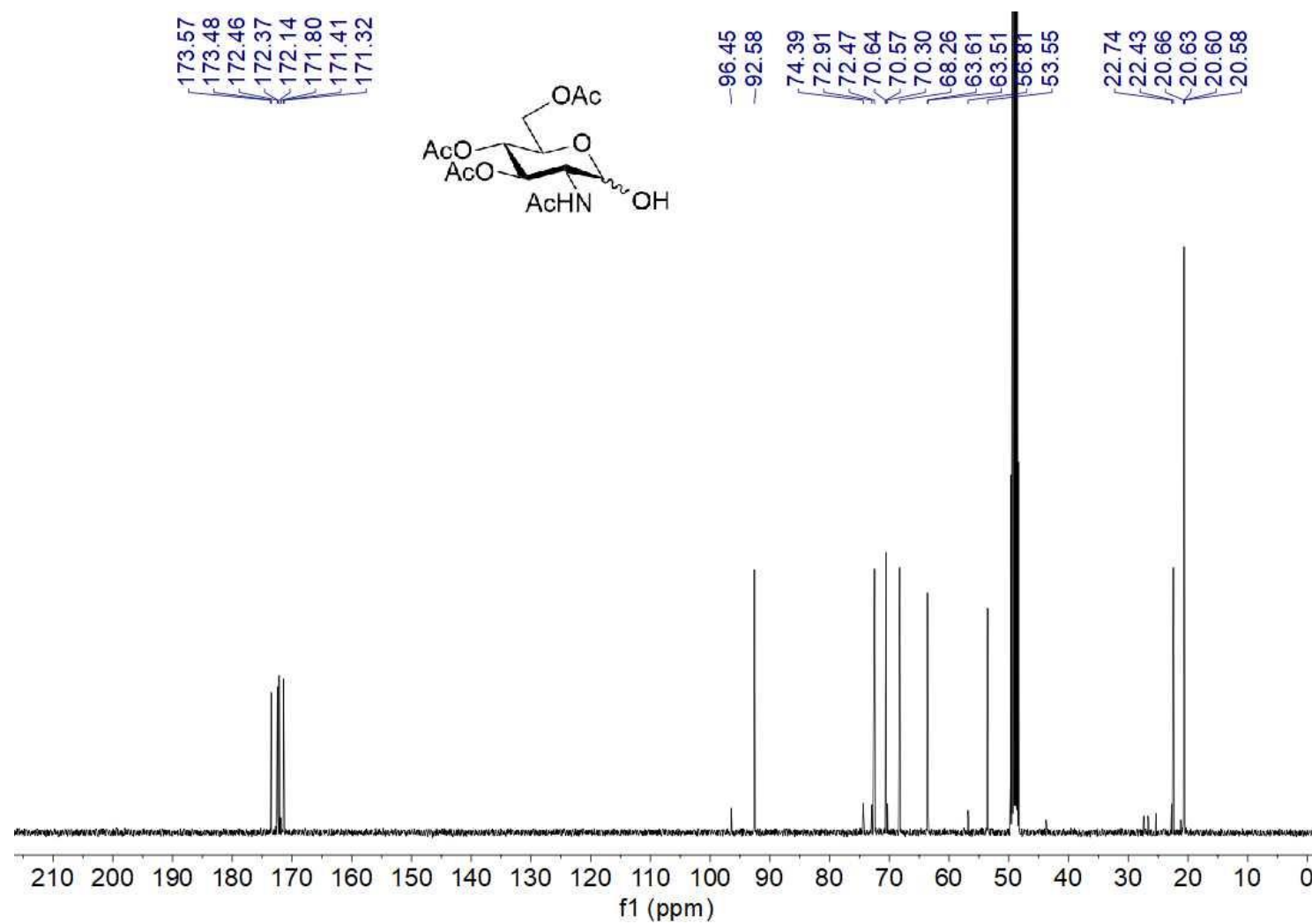


NMR COMPOUND 99

¹H NMR (400 MHz, CDCl₃) 99

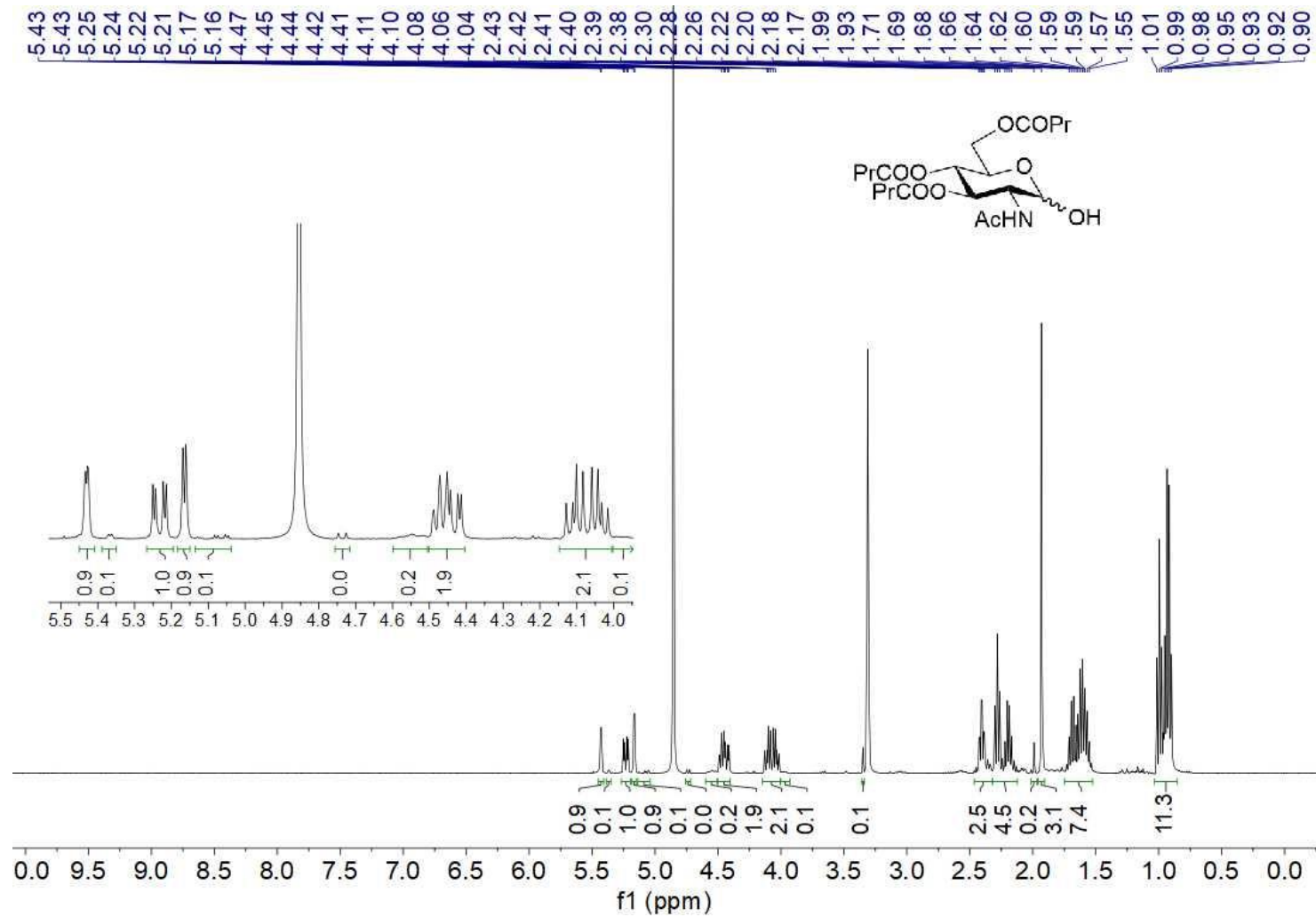


^{13}C NMR (100 MHz, CDCl_3) 99

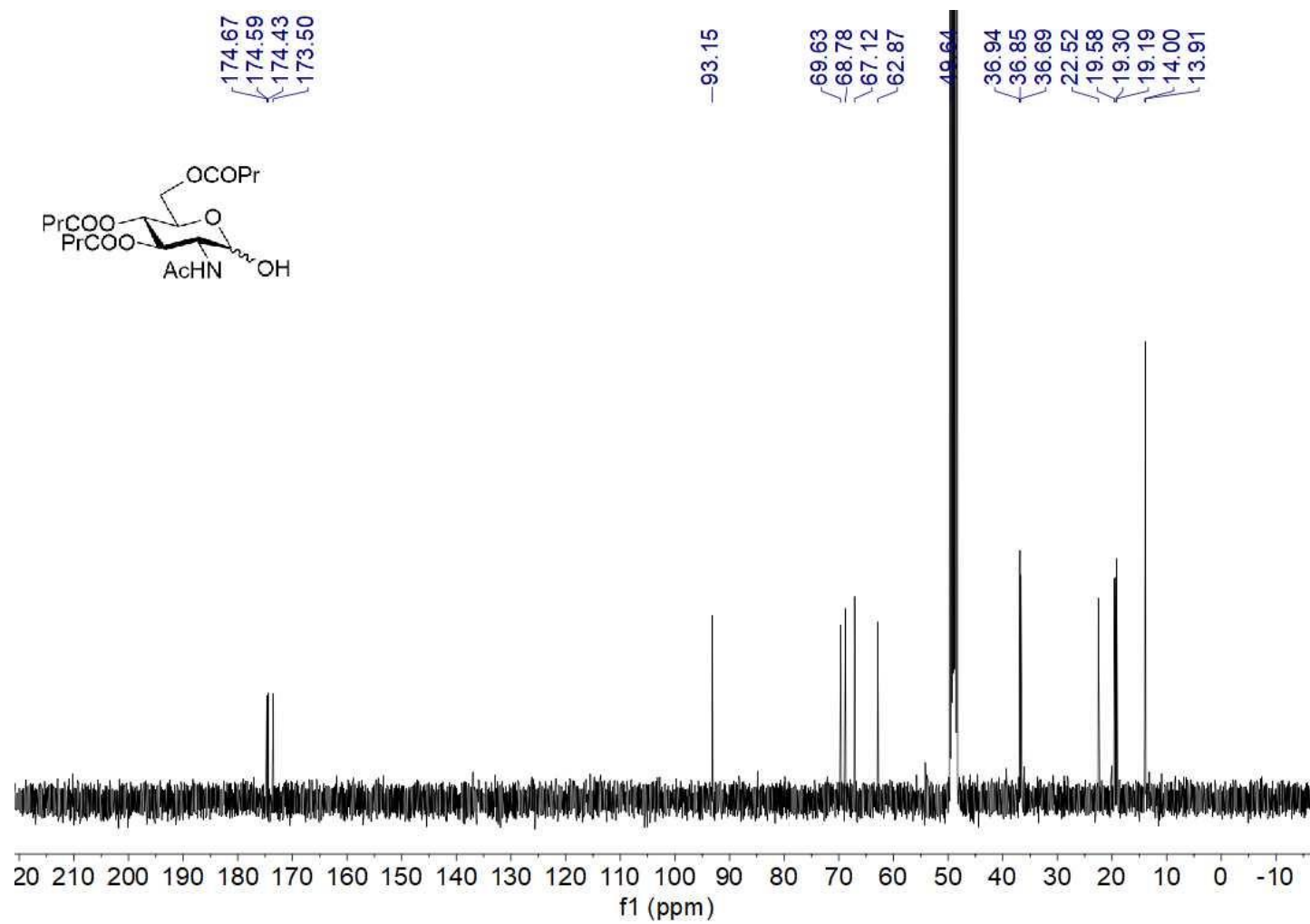


NMR COMPOUND 100

¹H NMR (400 MHz, CDCl₃) 100

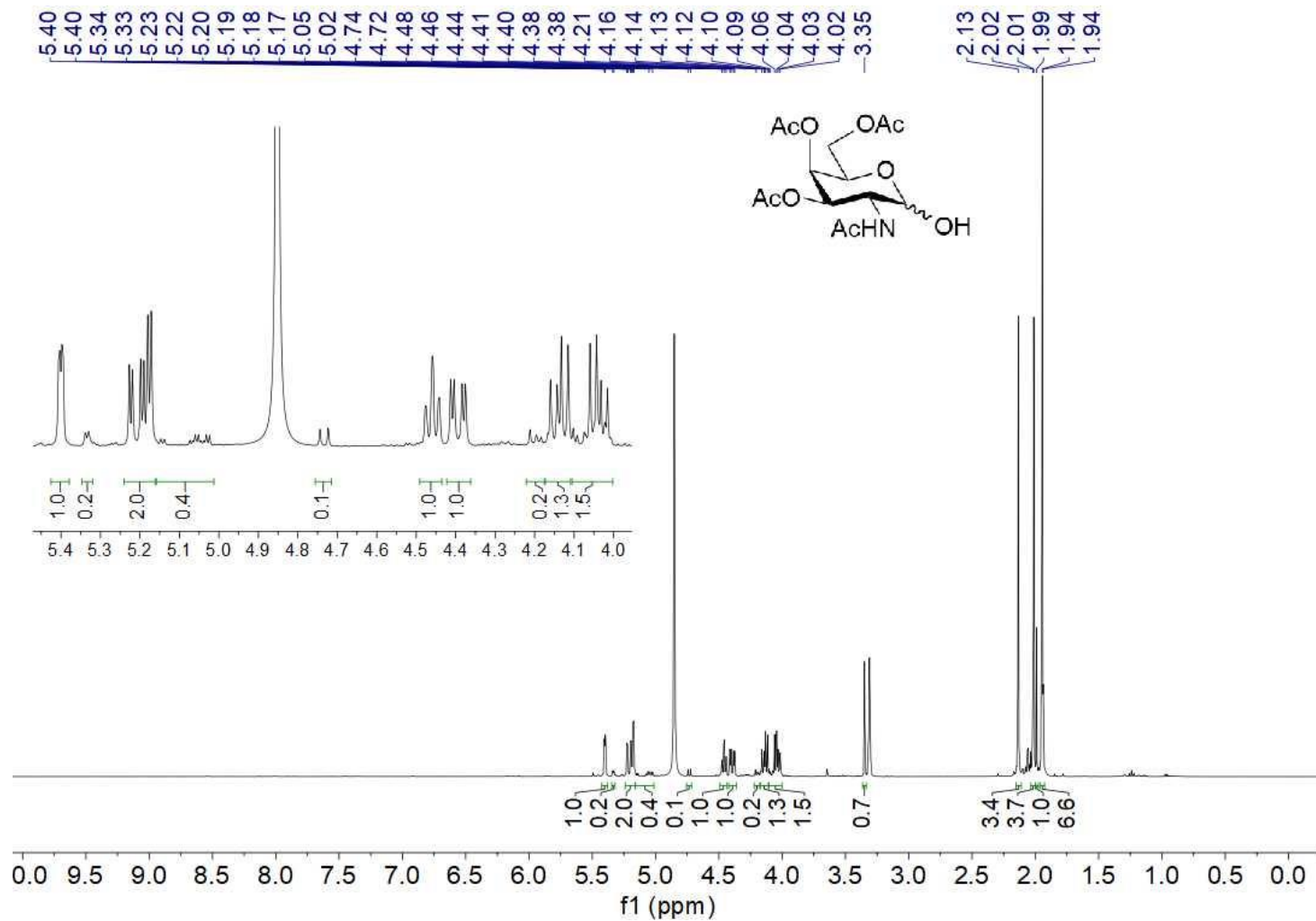


^{13}C NMR (100 MHz, CDCl_3) 100

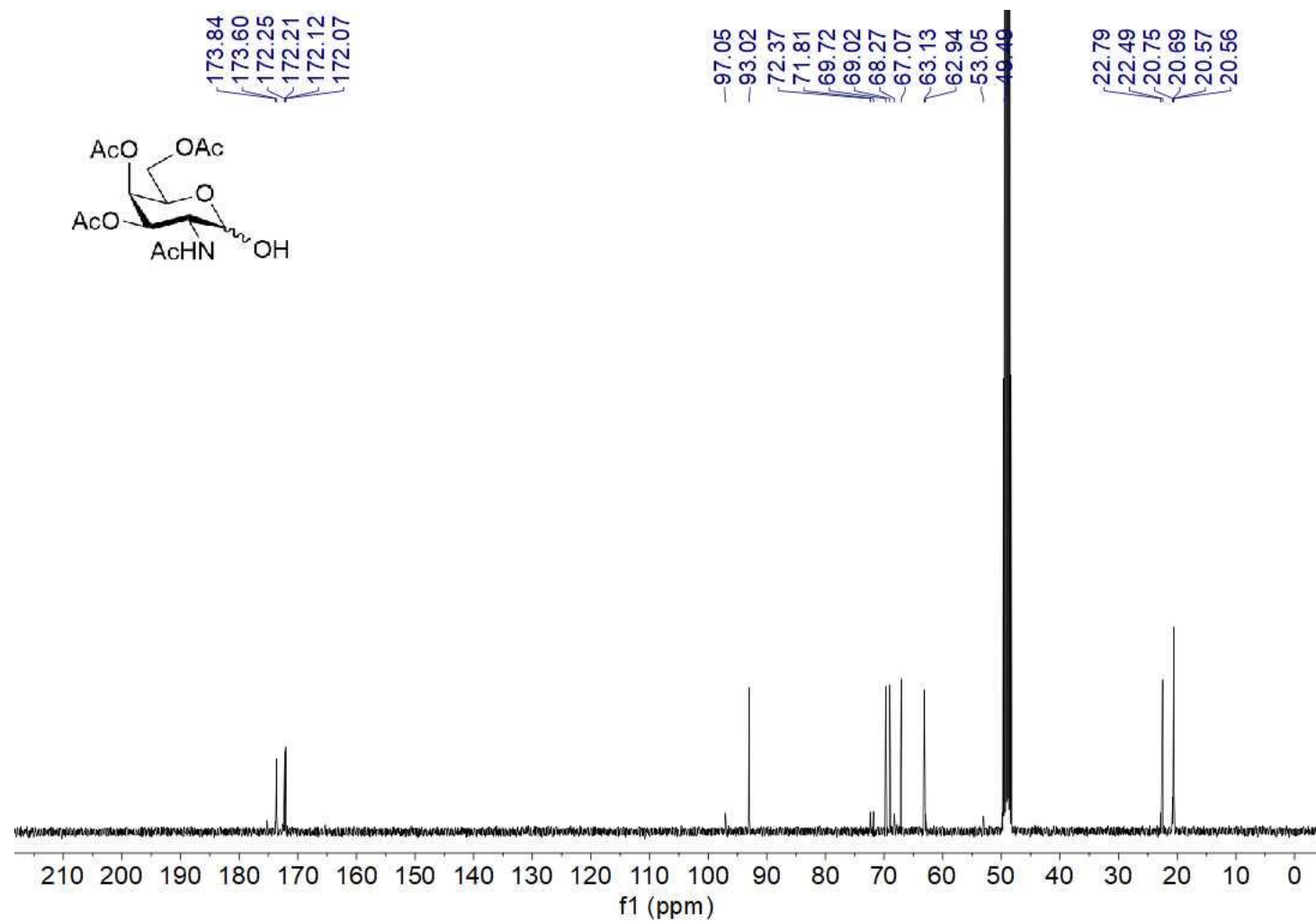


NMR COMPOUND 102

¹H NMR (400 MHz, CDCl₃) 102

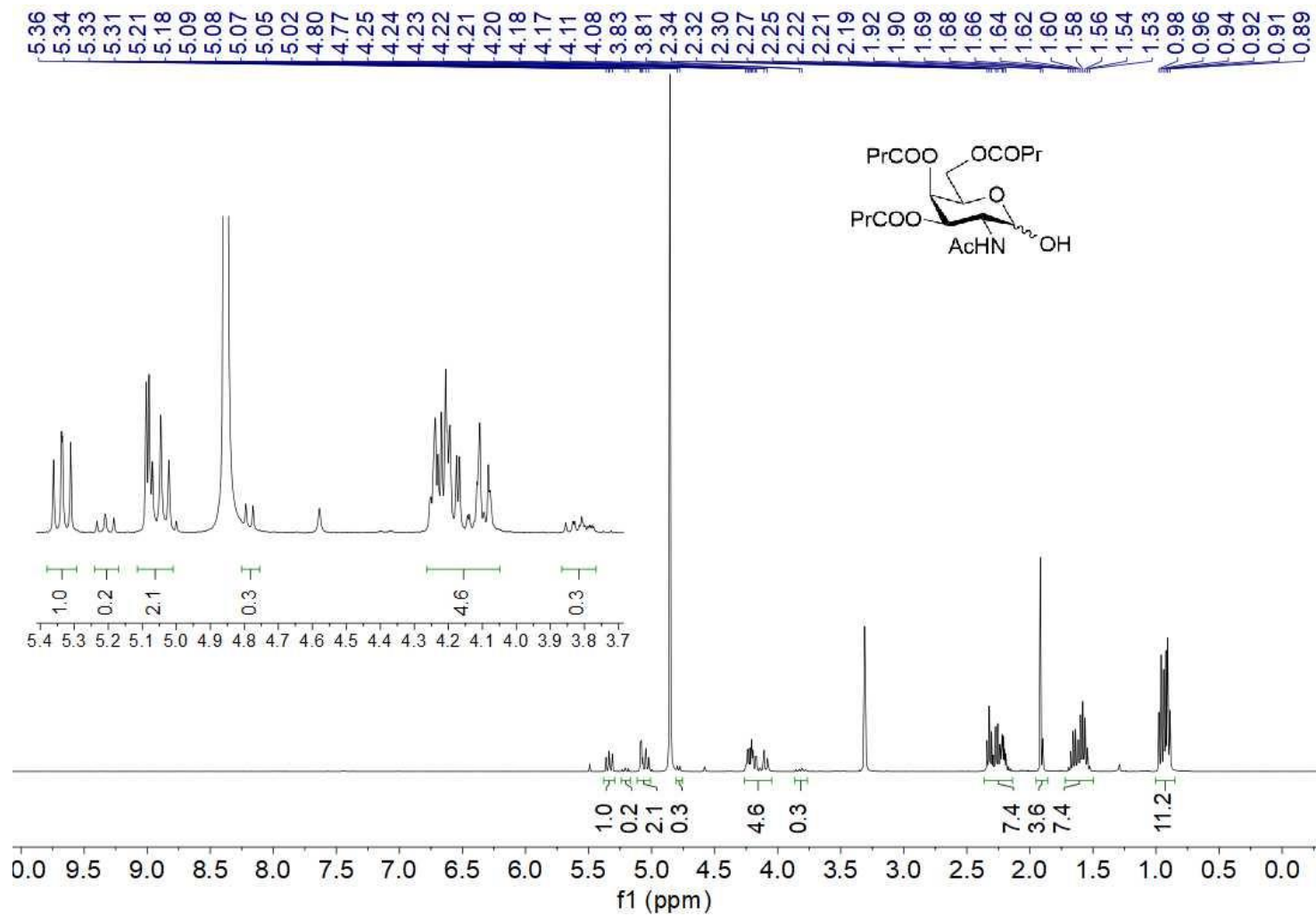


¹³C NMR (100 MHz, CDCl₃) 102

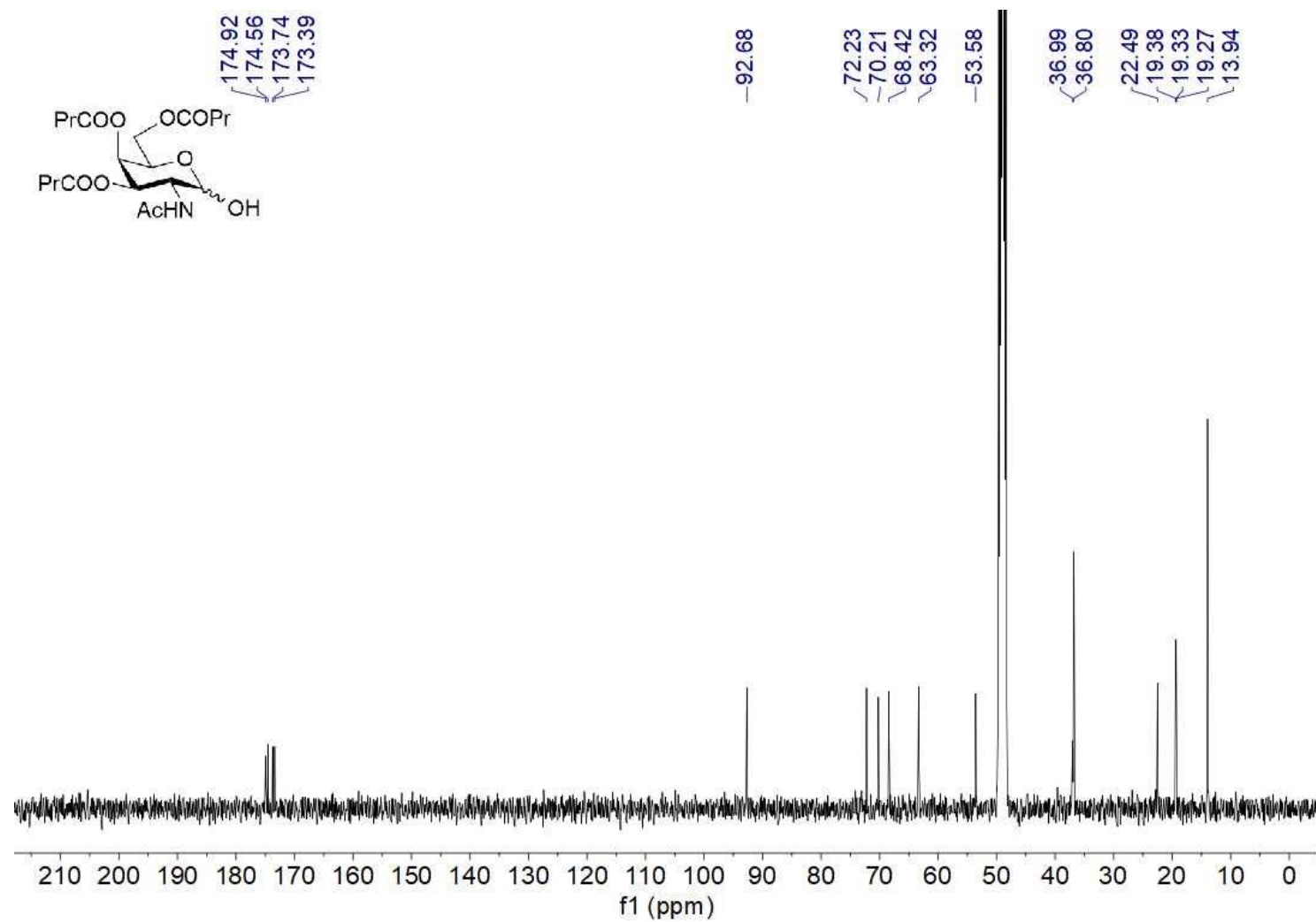


NMR COMPOUND 103

¹H NMR (400 MHz, CDCl₃) 103

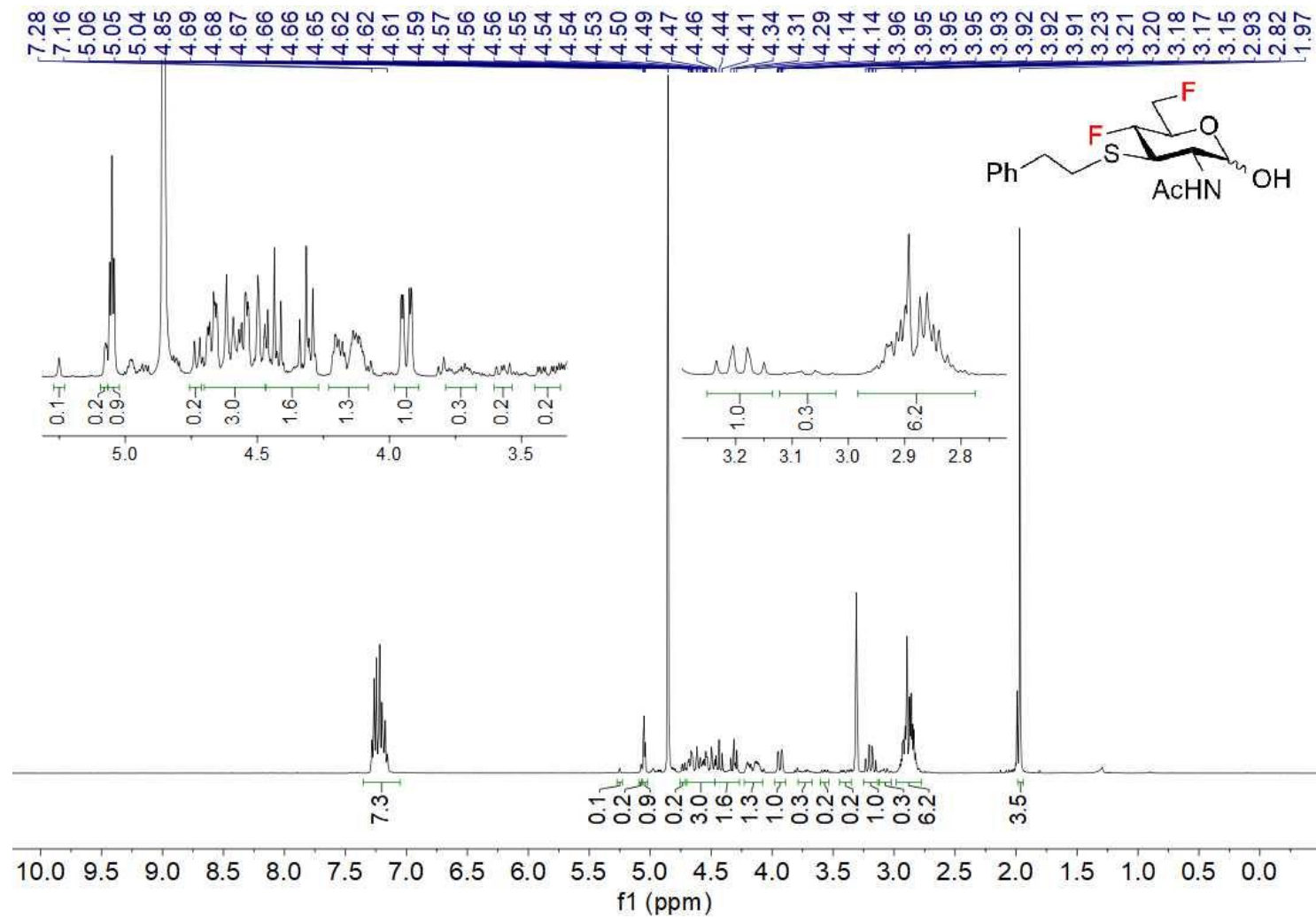


¹³C NMR (100 MHz, CDCl₃) 103

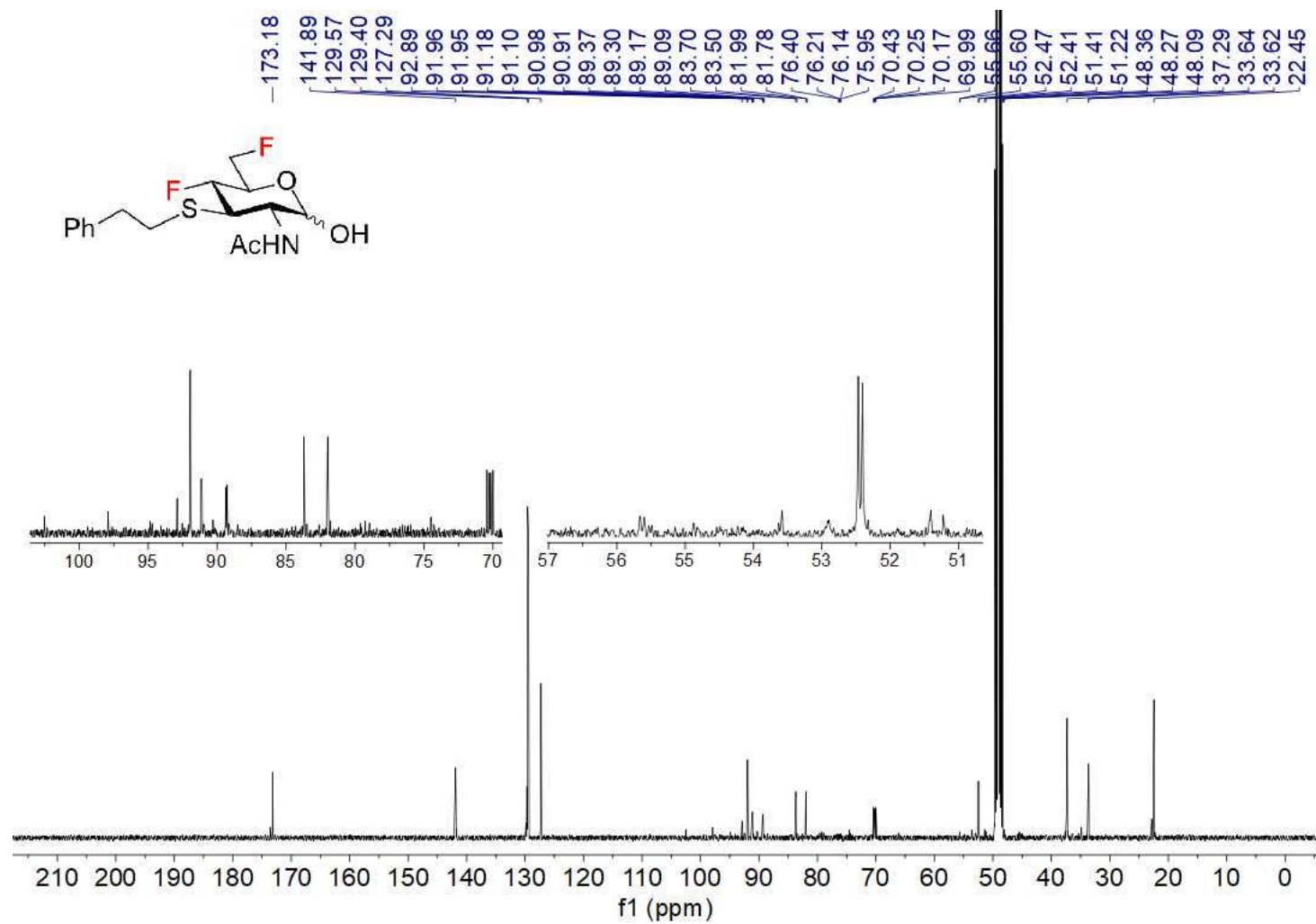


NMR COMPOUND 110

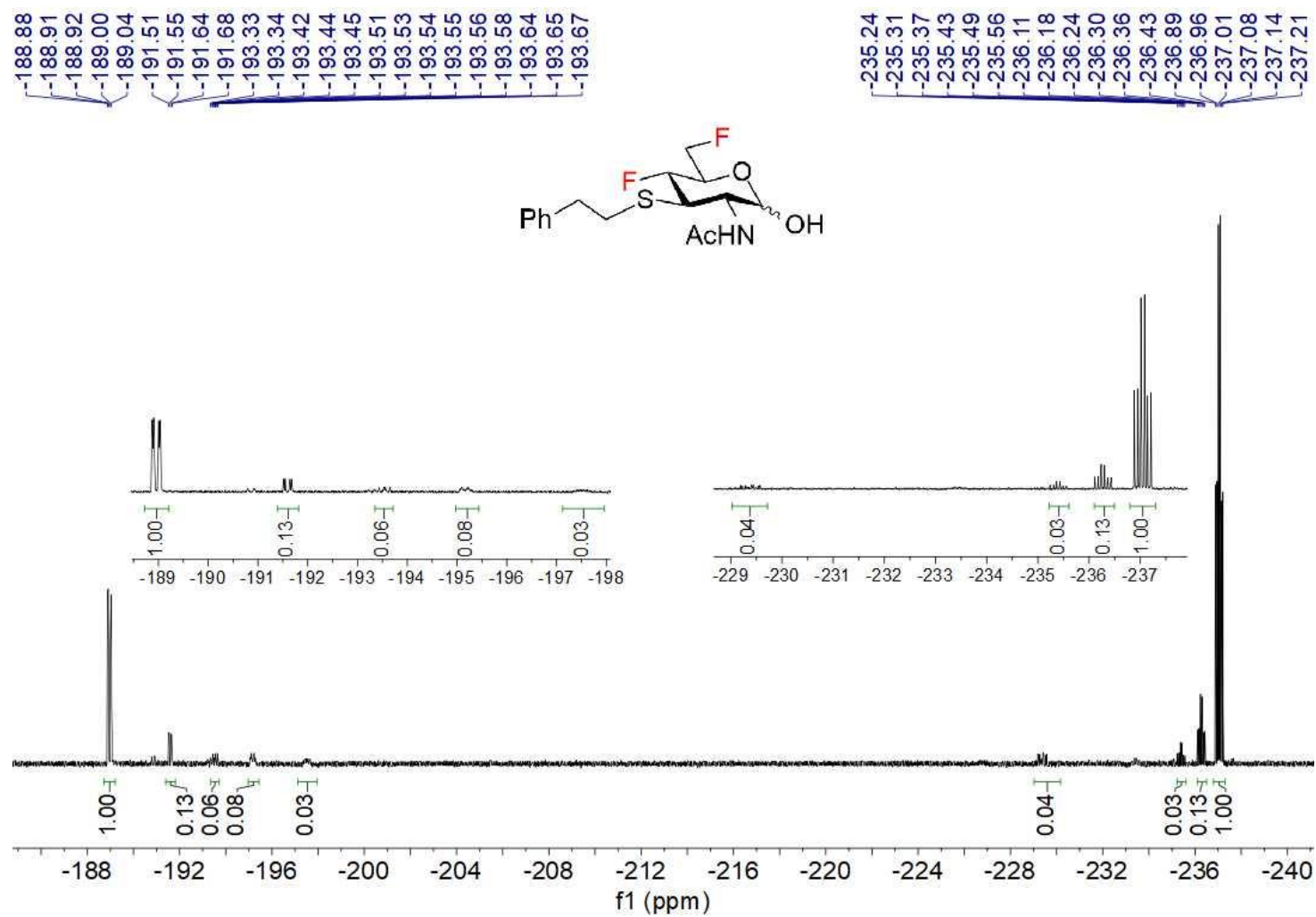
¹H NMR (400 MHz, CD₃OD) 110



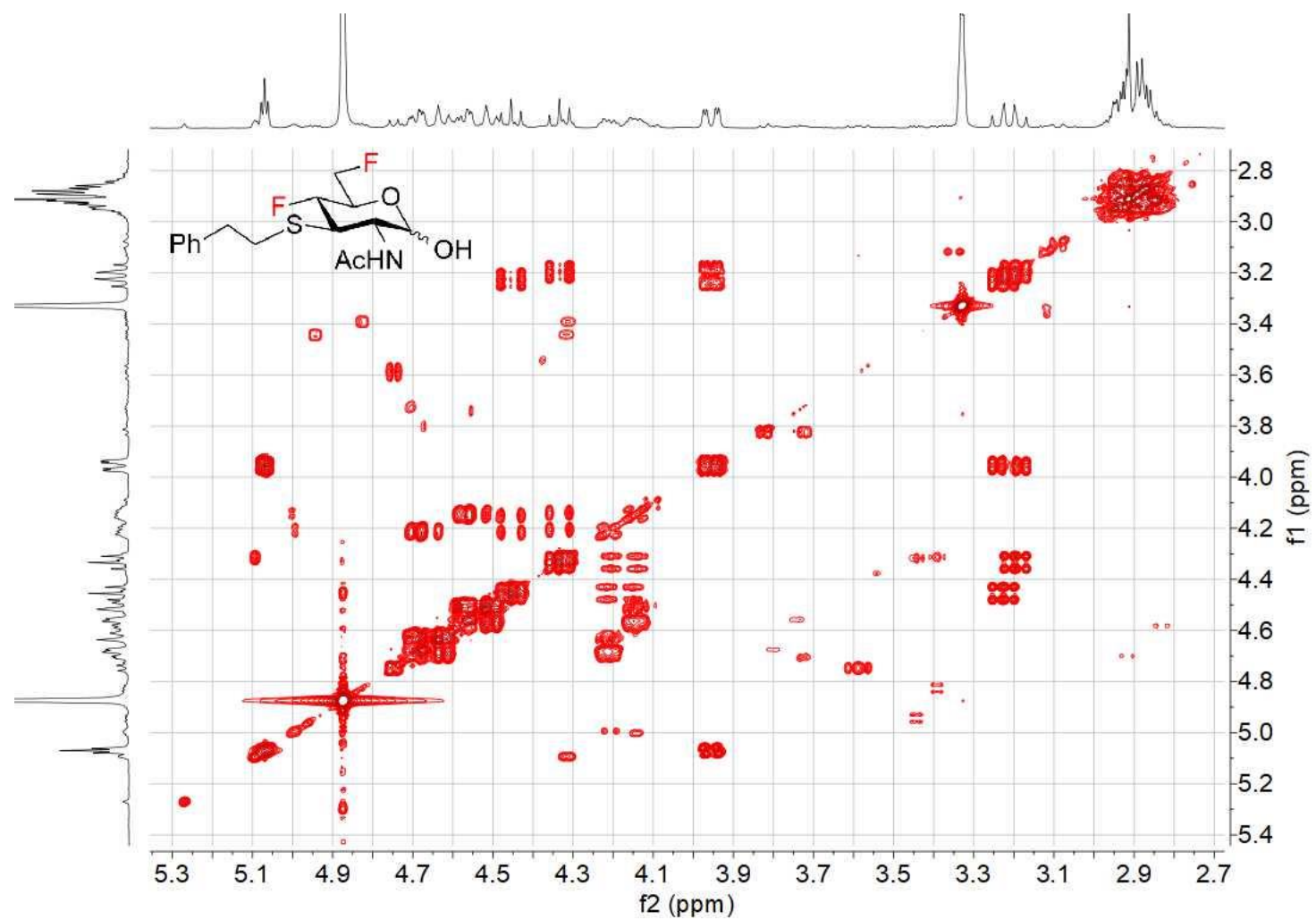
^{13}C NMR (100 MHz, CD_3OD) 110



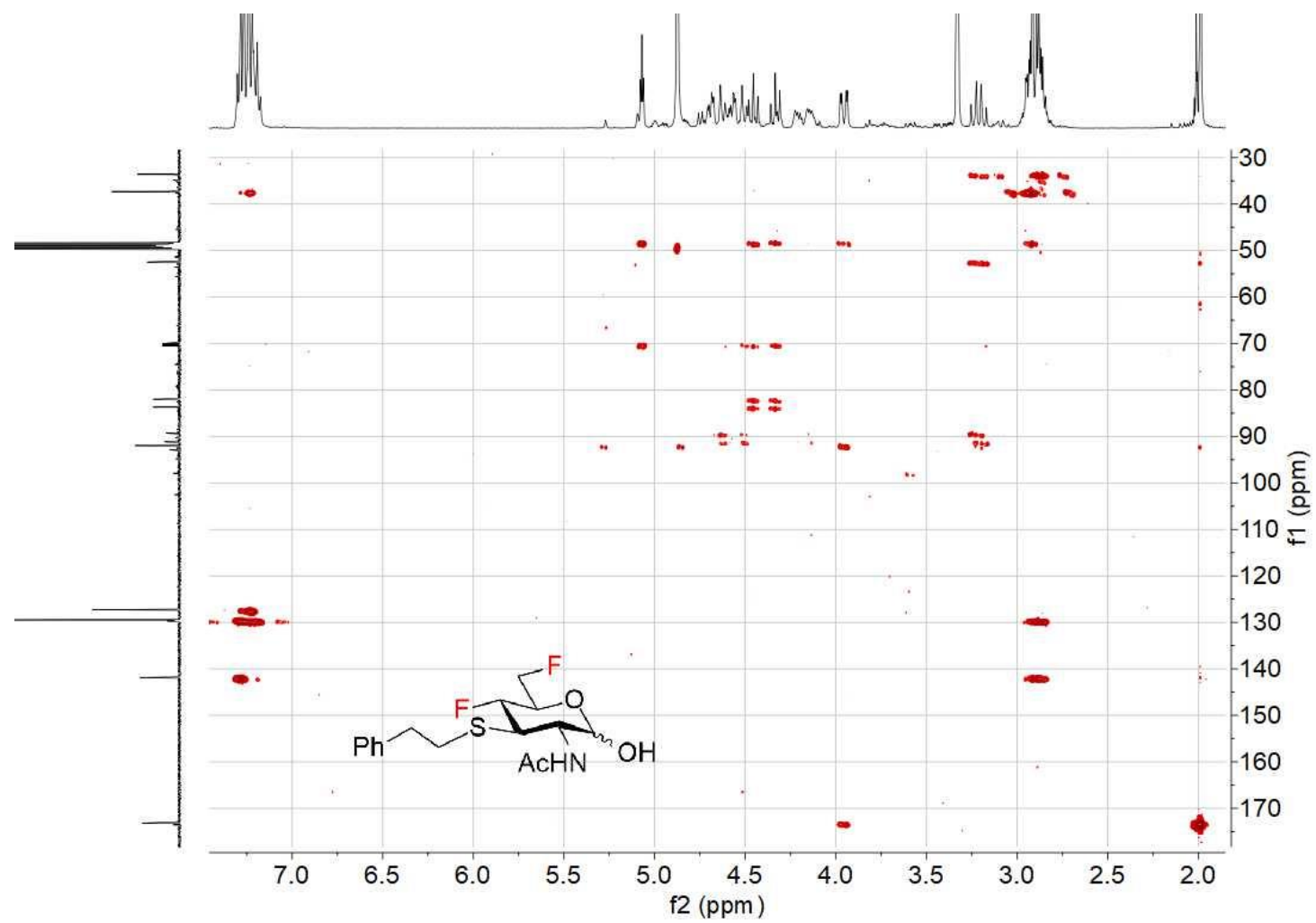
¹⁹F NMR (376 MHz, CD₃OD) 110



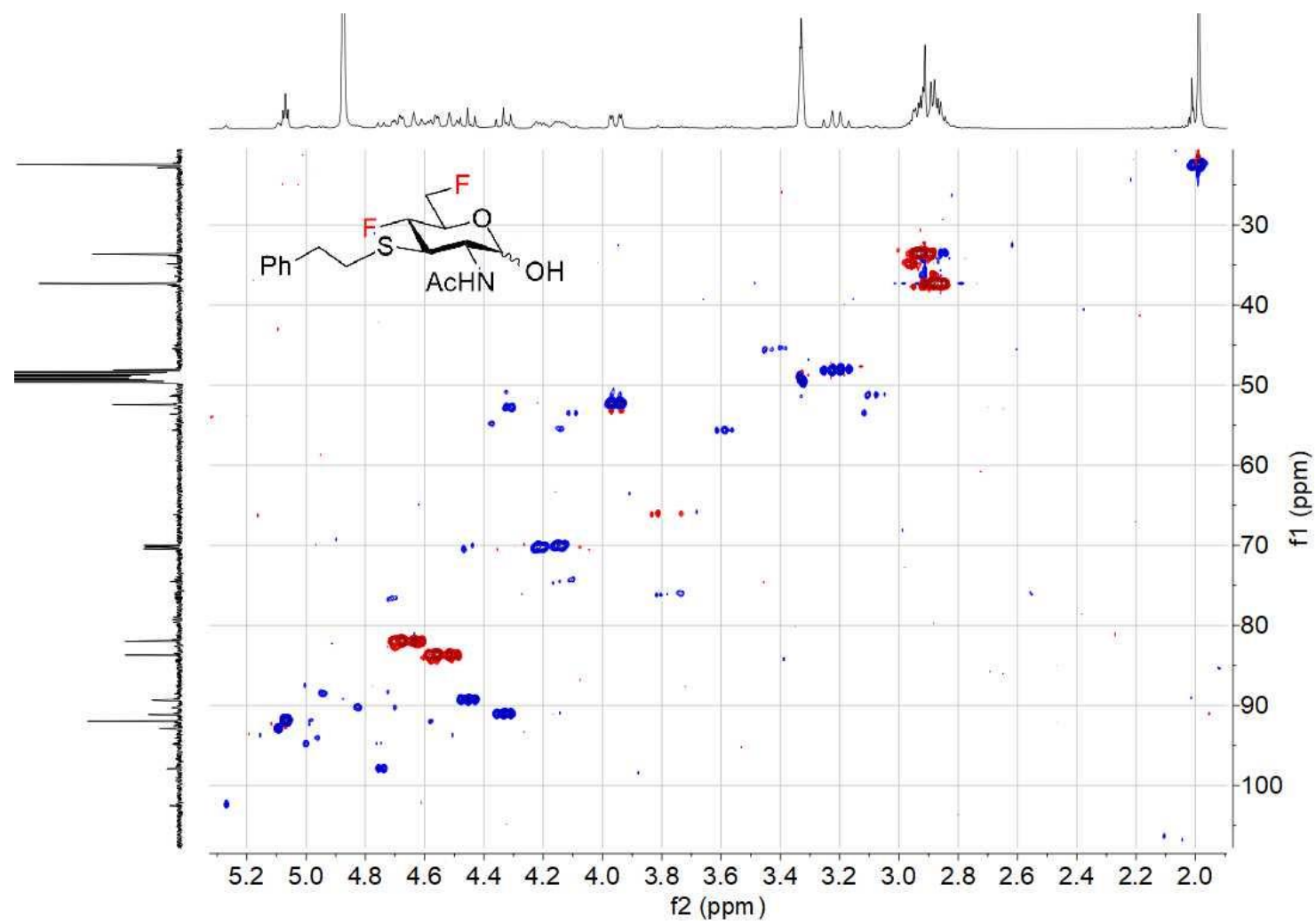
^1H - ^1H COSY 110



^1H - ^{13}C HMBC 110

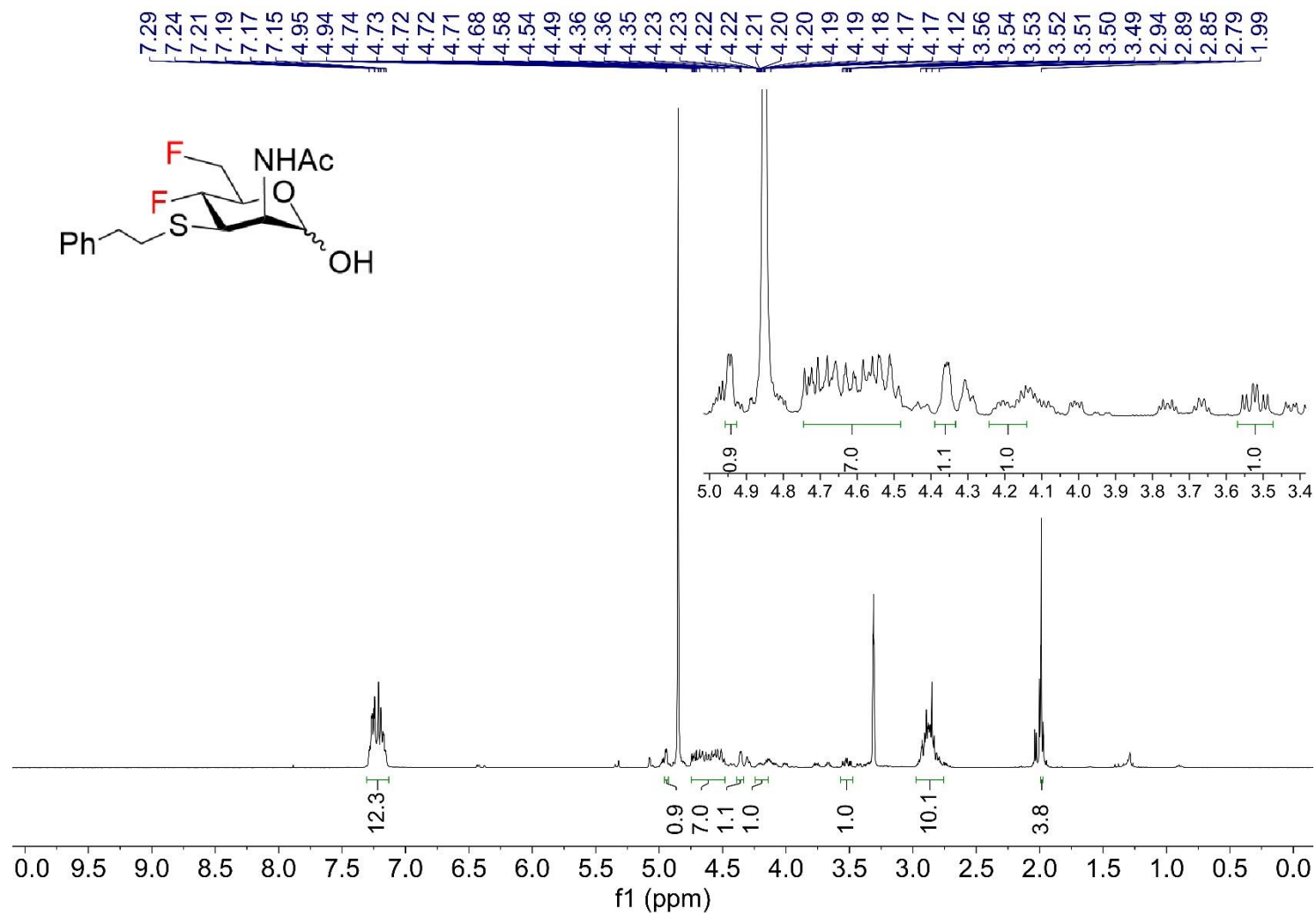


^1H - ^{13}C HSQC 110

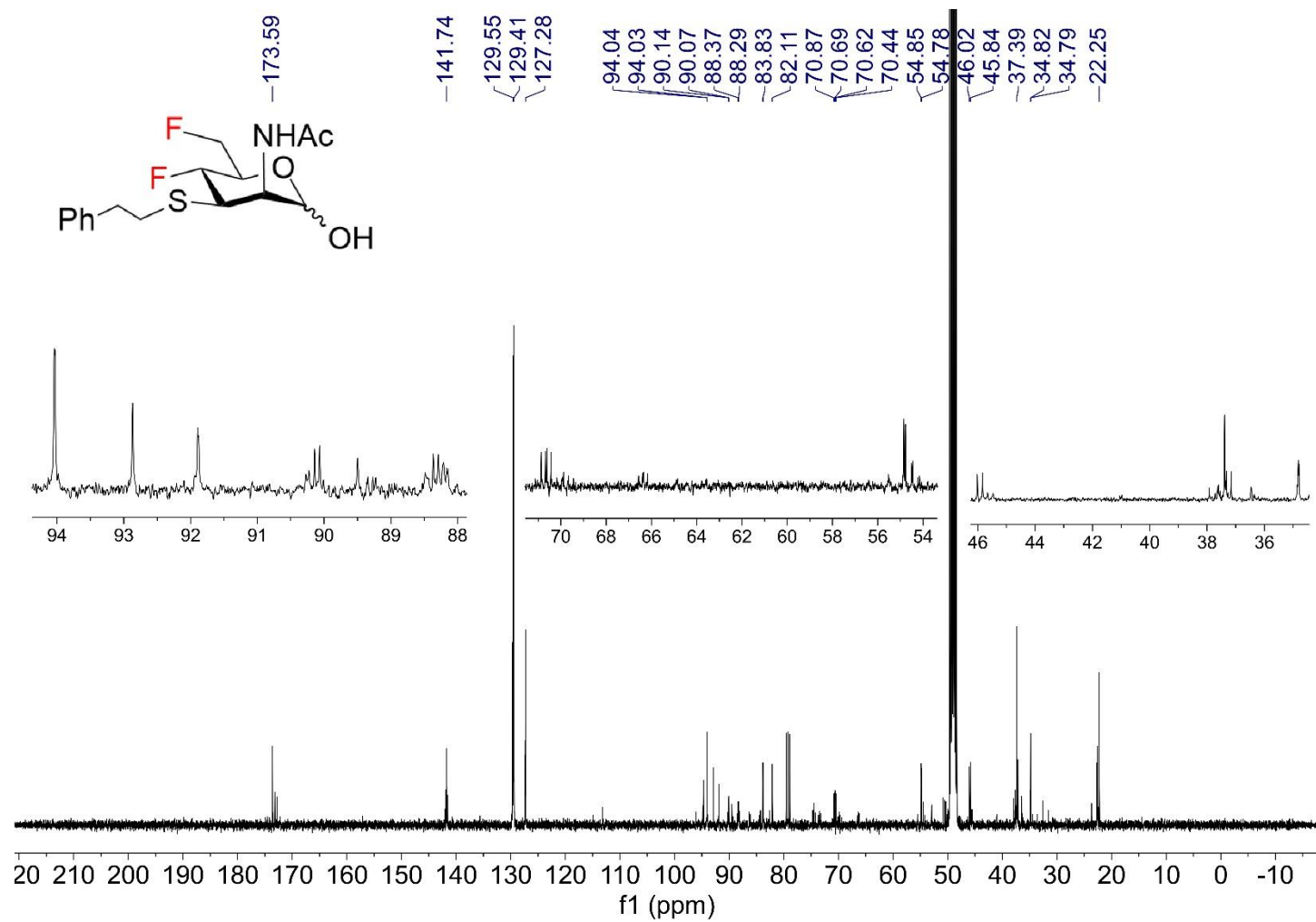


NMR COMPOUND 111 (in a mixture with ca 40% of unidentified compounds)

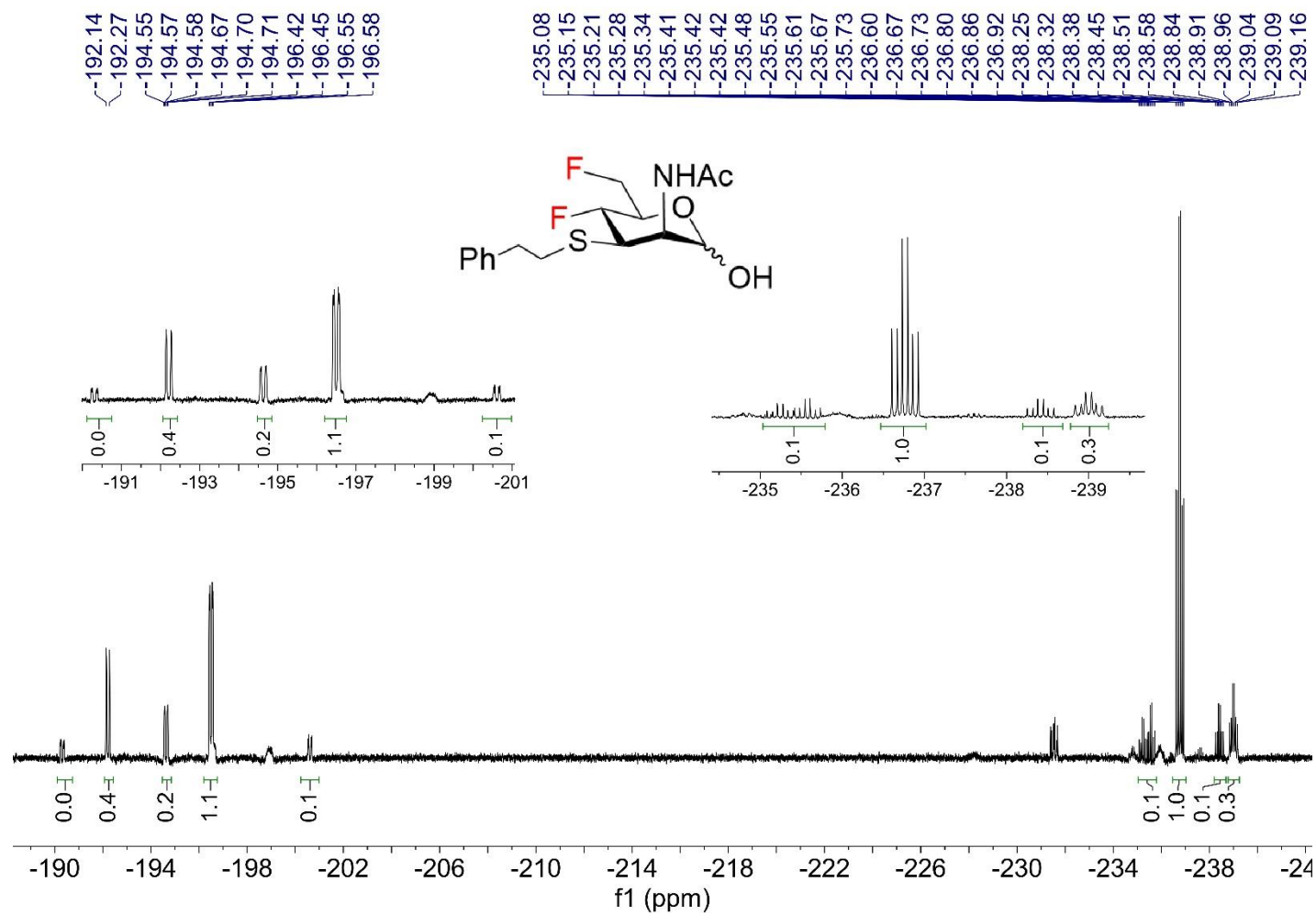
¹H NMR (400 MHz, CD₃OD) 111



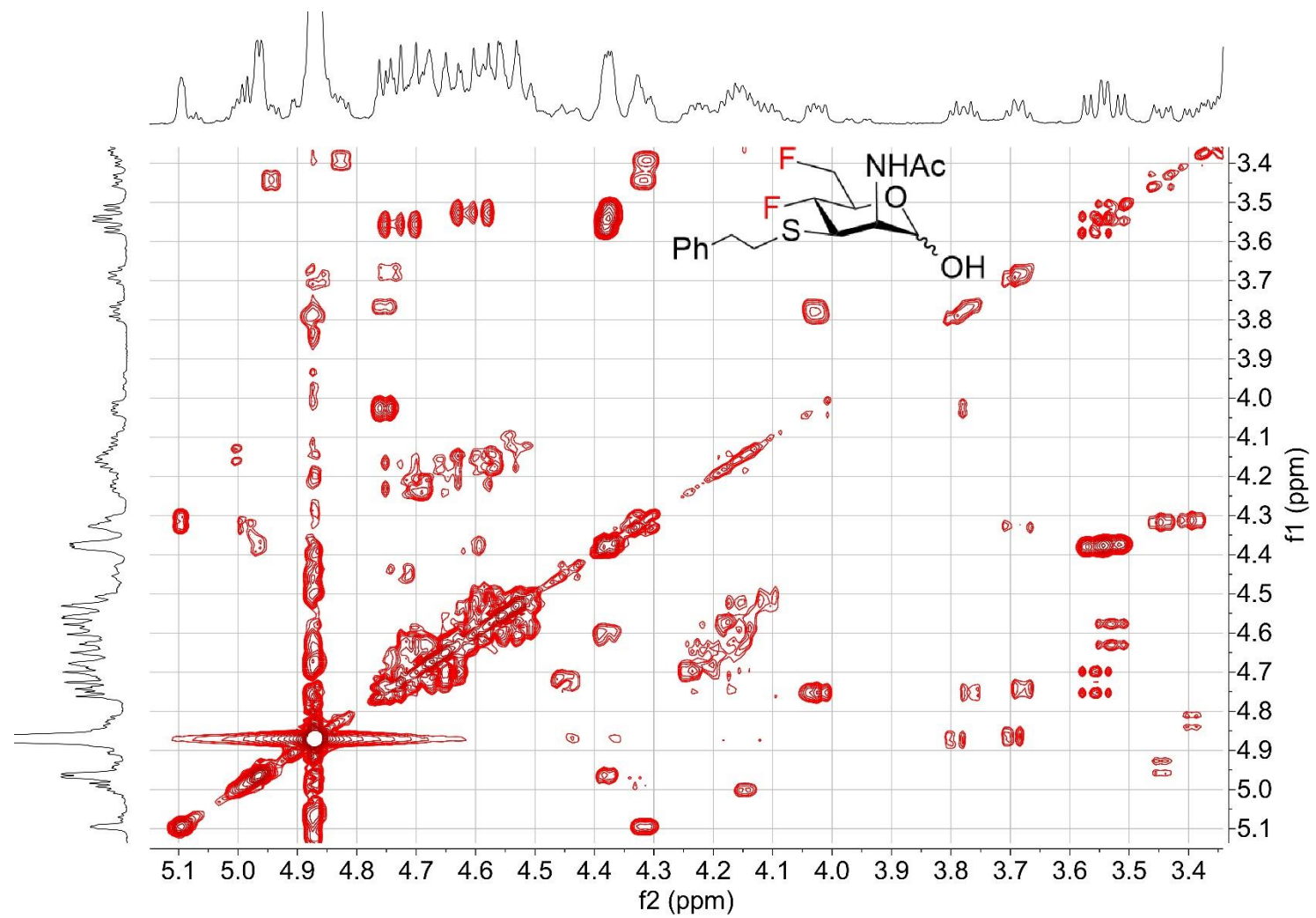
¹³C NMR (100 MHz, CD₃OD) 111



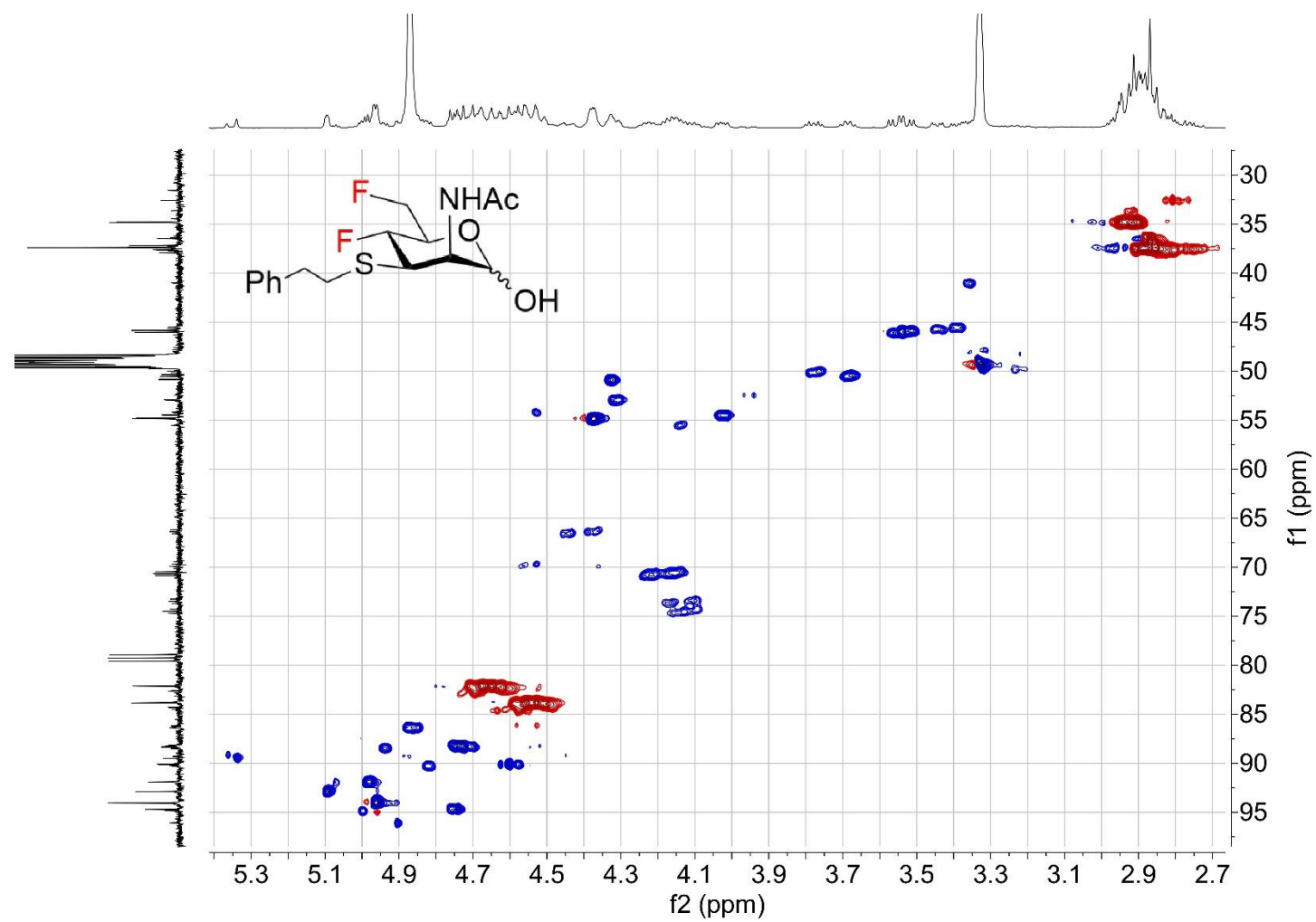
^{19}F NMR (376 MHz, CD_3OD) 111



¹H-¹H COSY 111

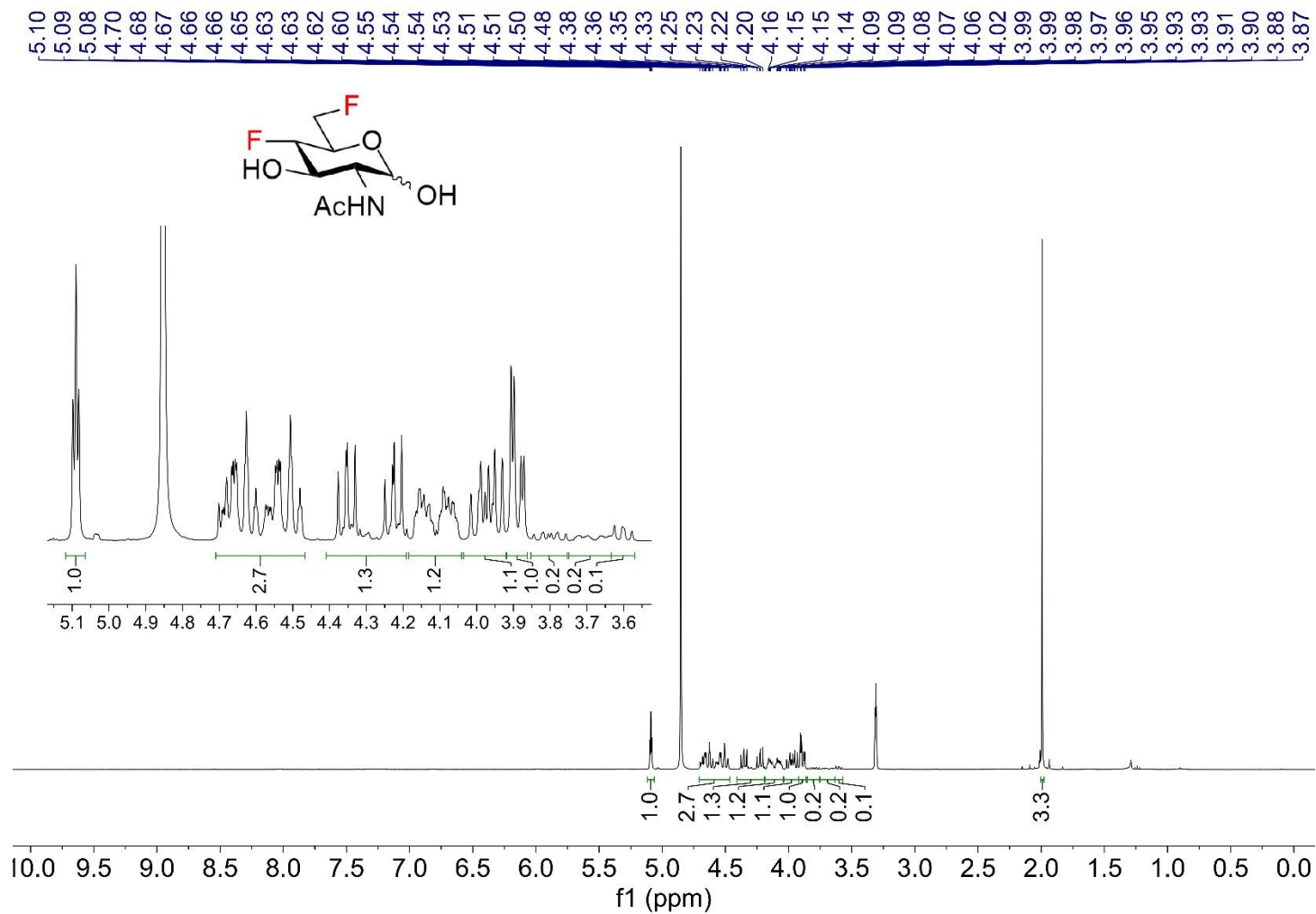


^1H - ^{13}C HSQC 111

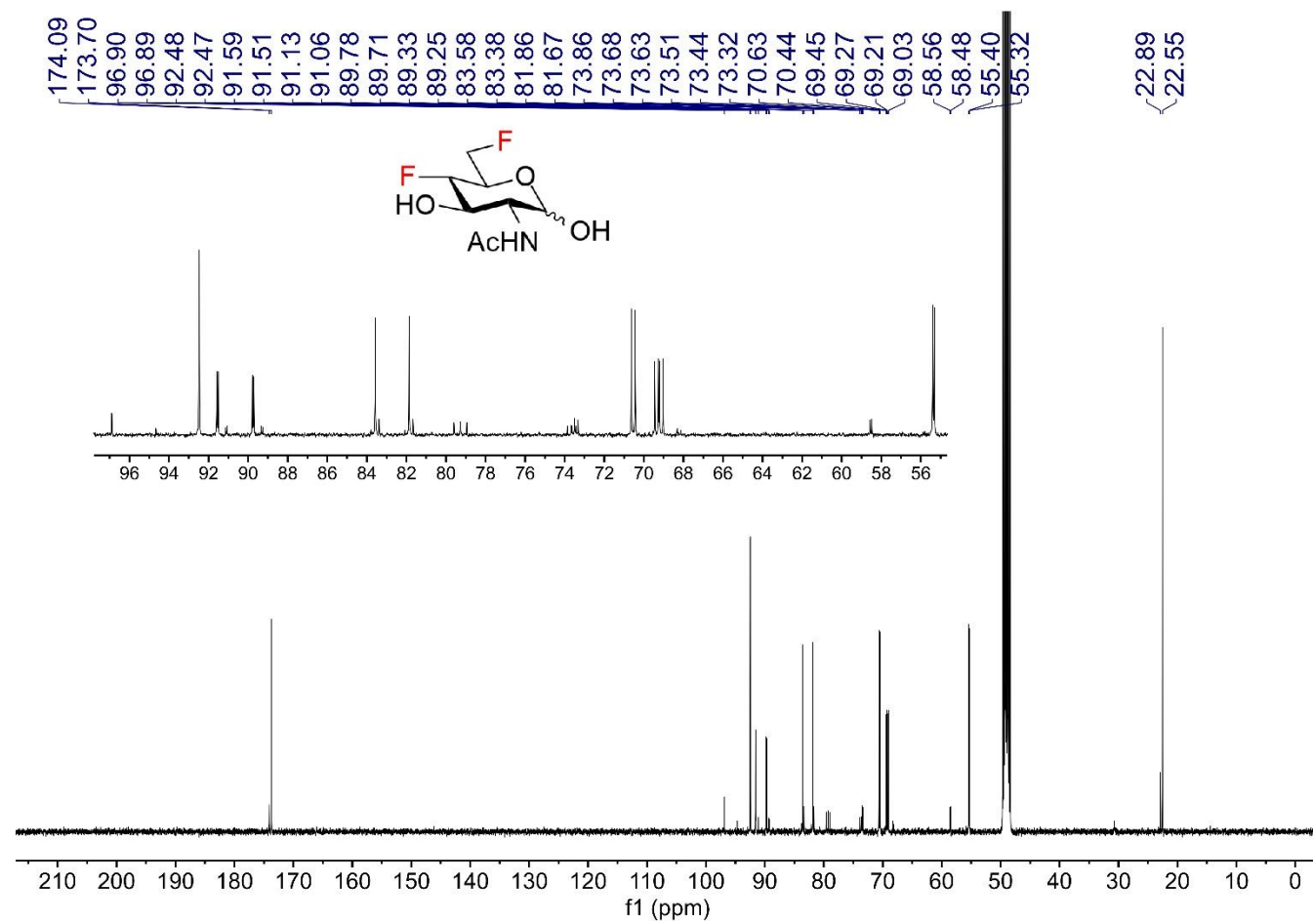


NMR COMPOUND 112

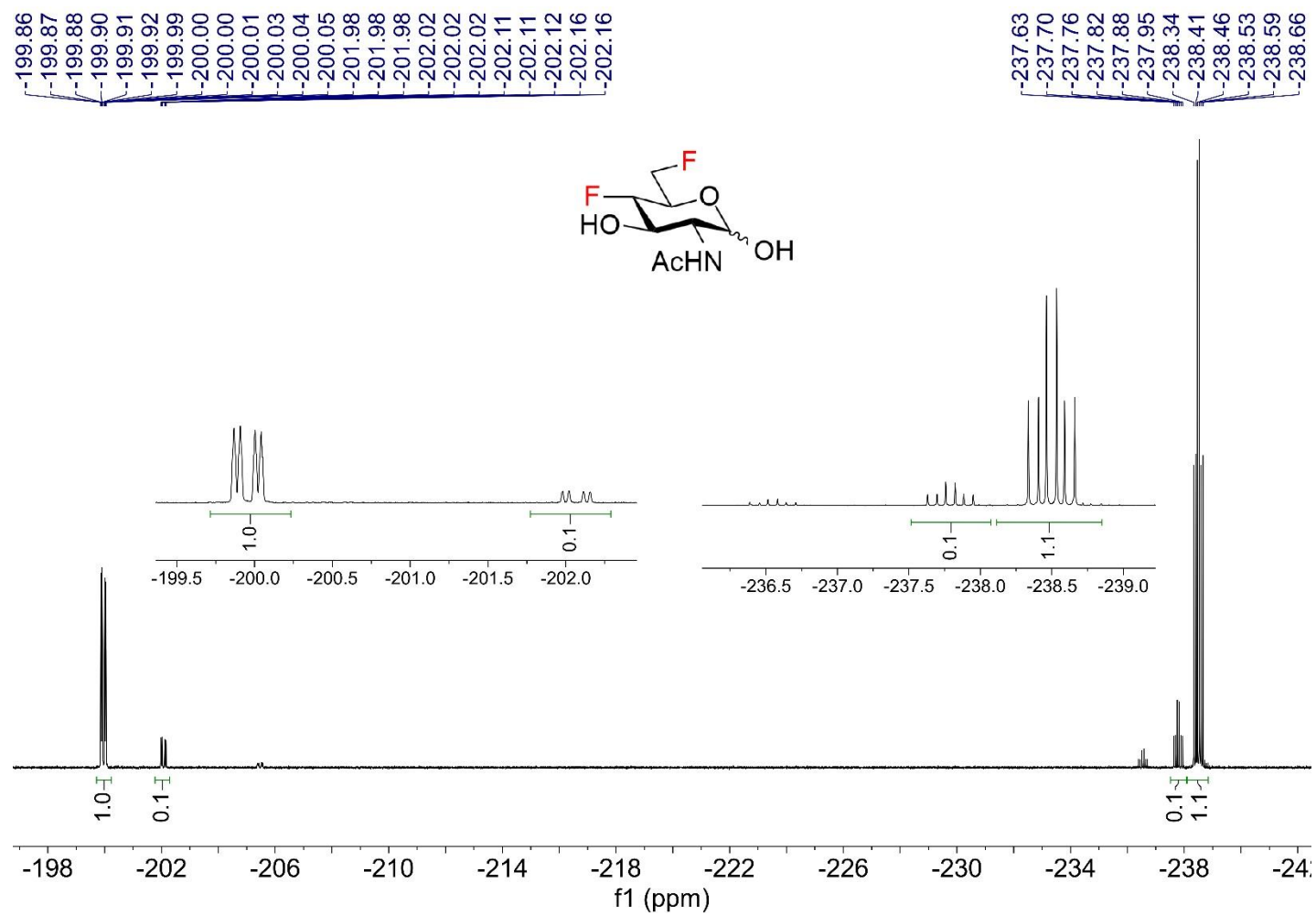
¹H NMR (400 MHz, CD₃OD) 112



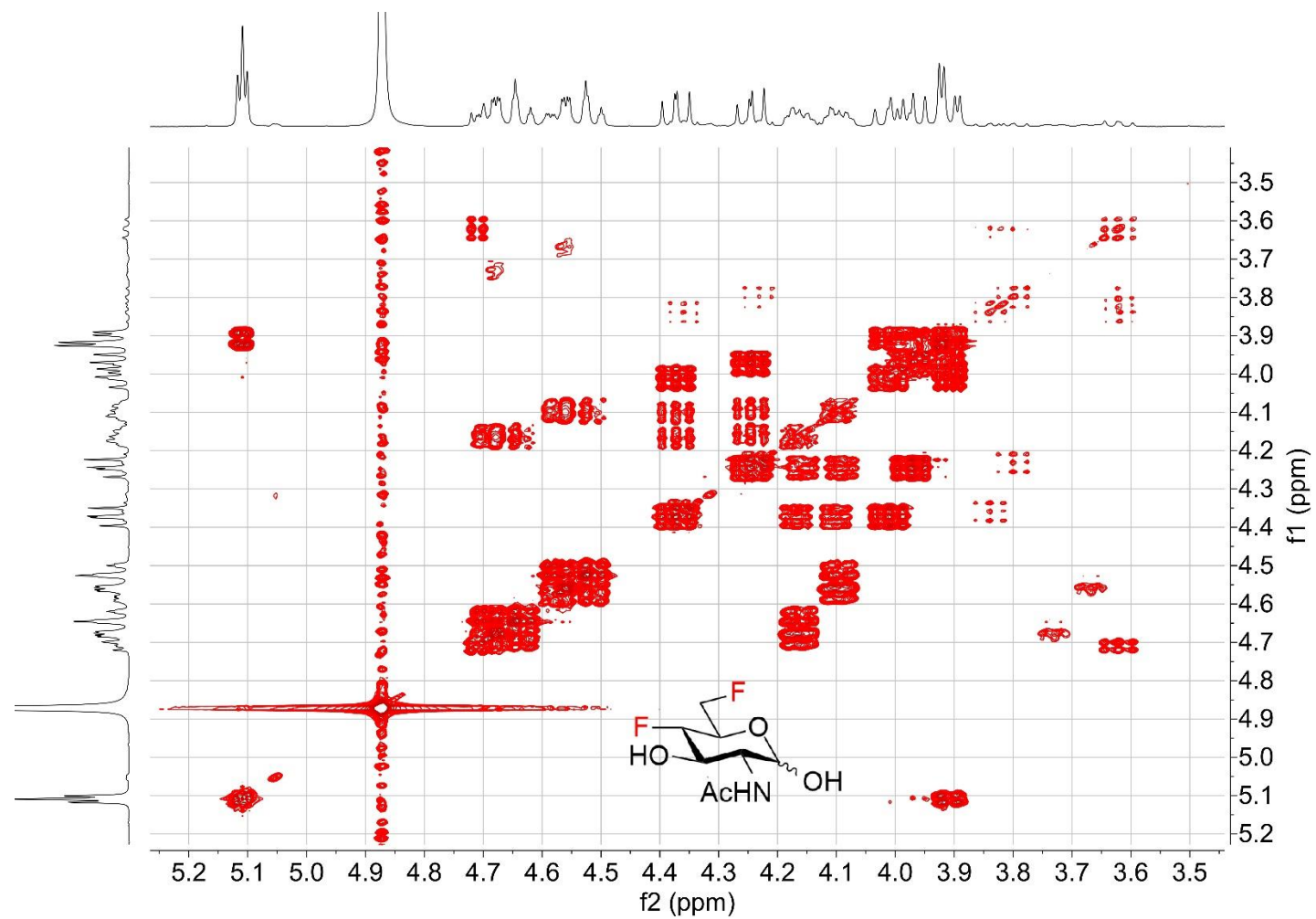
¹³C NMR (100 MHz, CD₃OD) 112



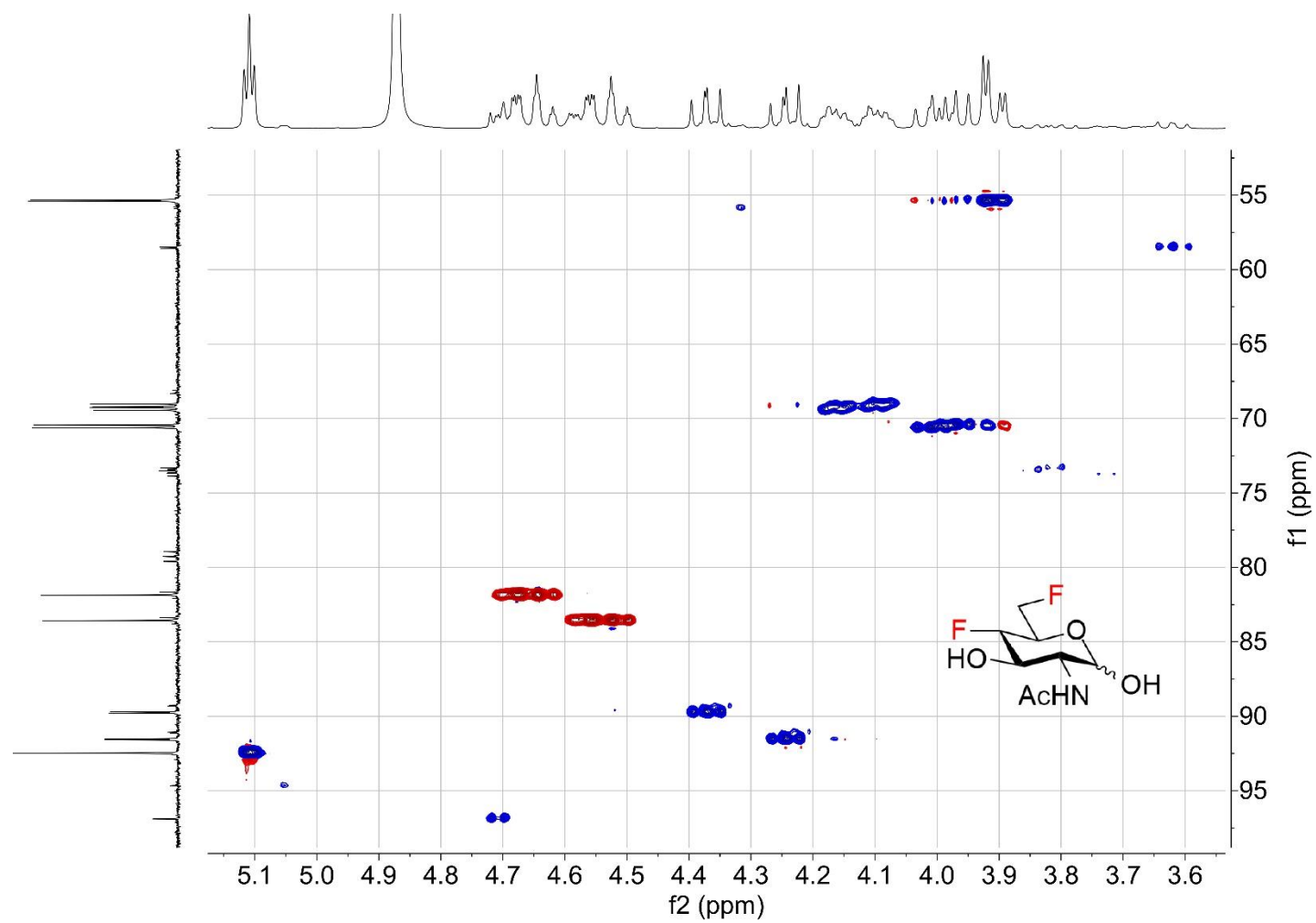
¹⁹F NMR (376 MHz, CD₃OD) 112



^1H - ^1H COSY 112

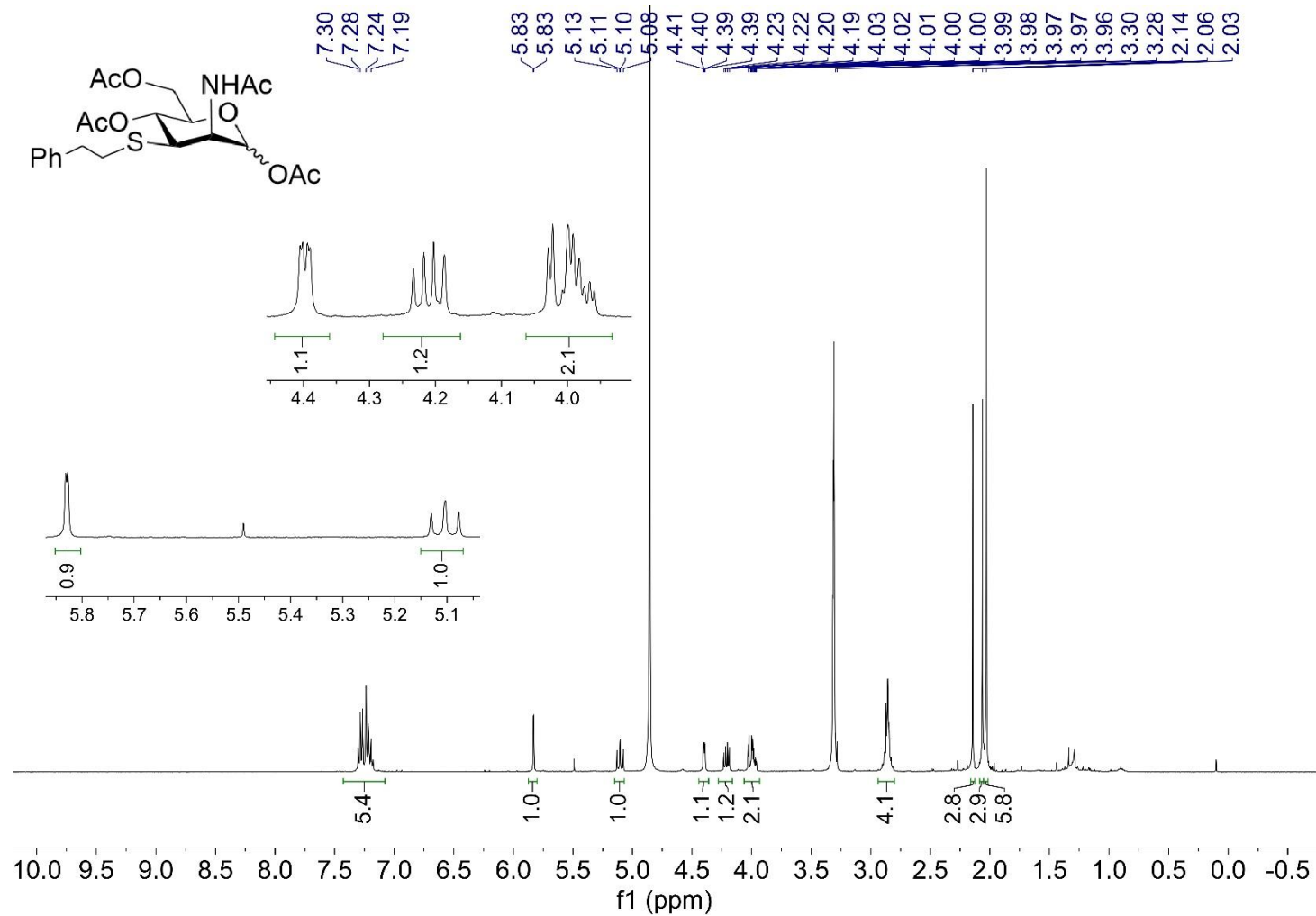


^1H - ^{13}C HSQC 112

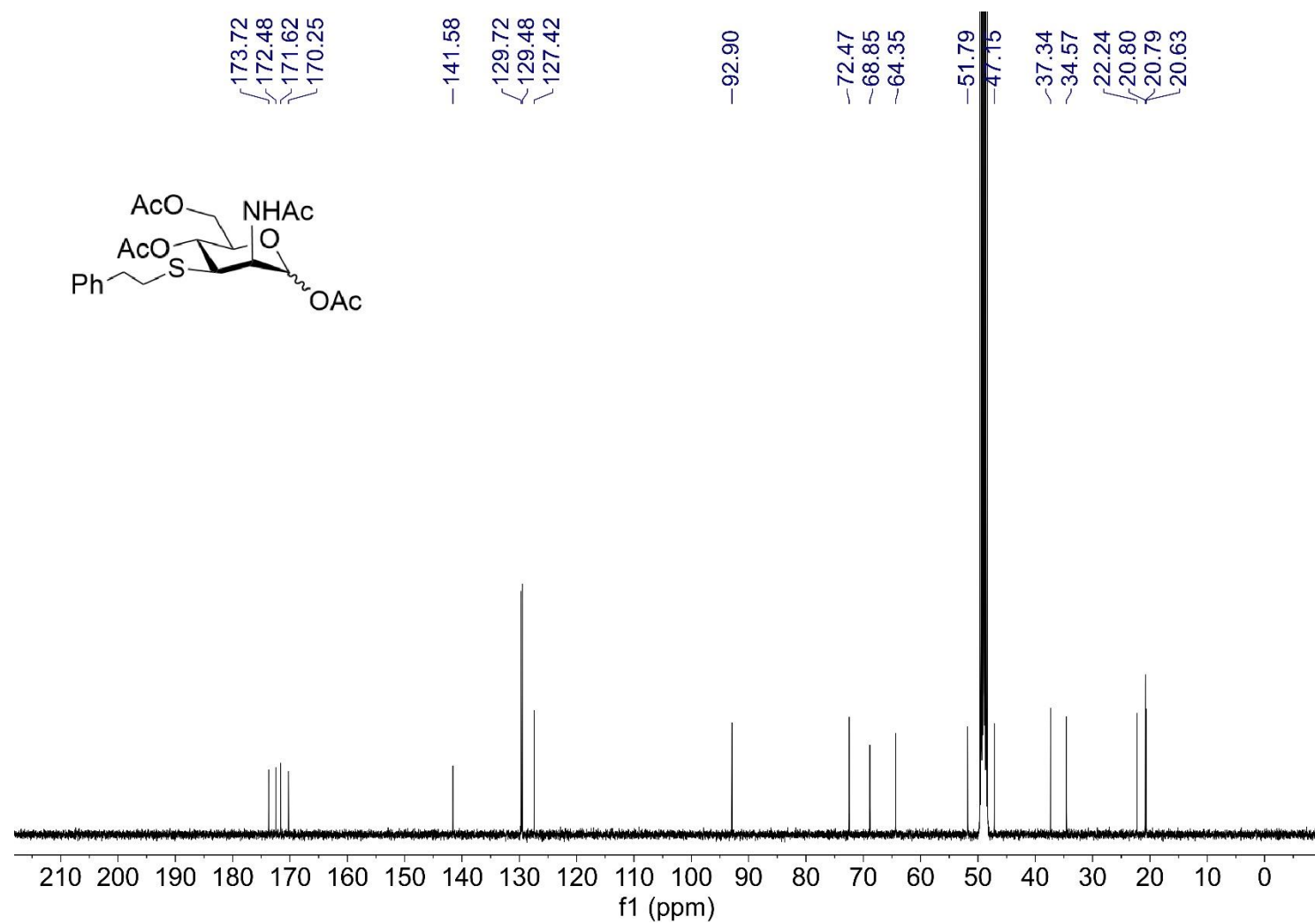


NMR COMPOUND 113

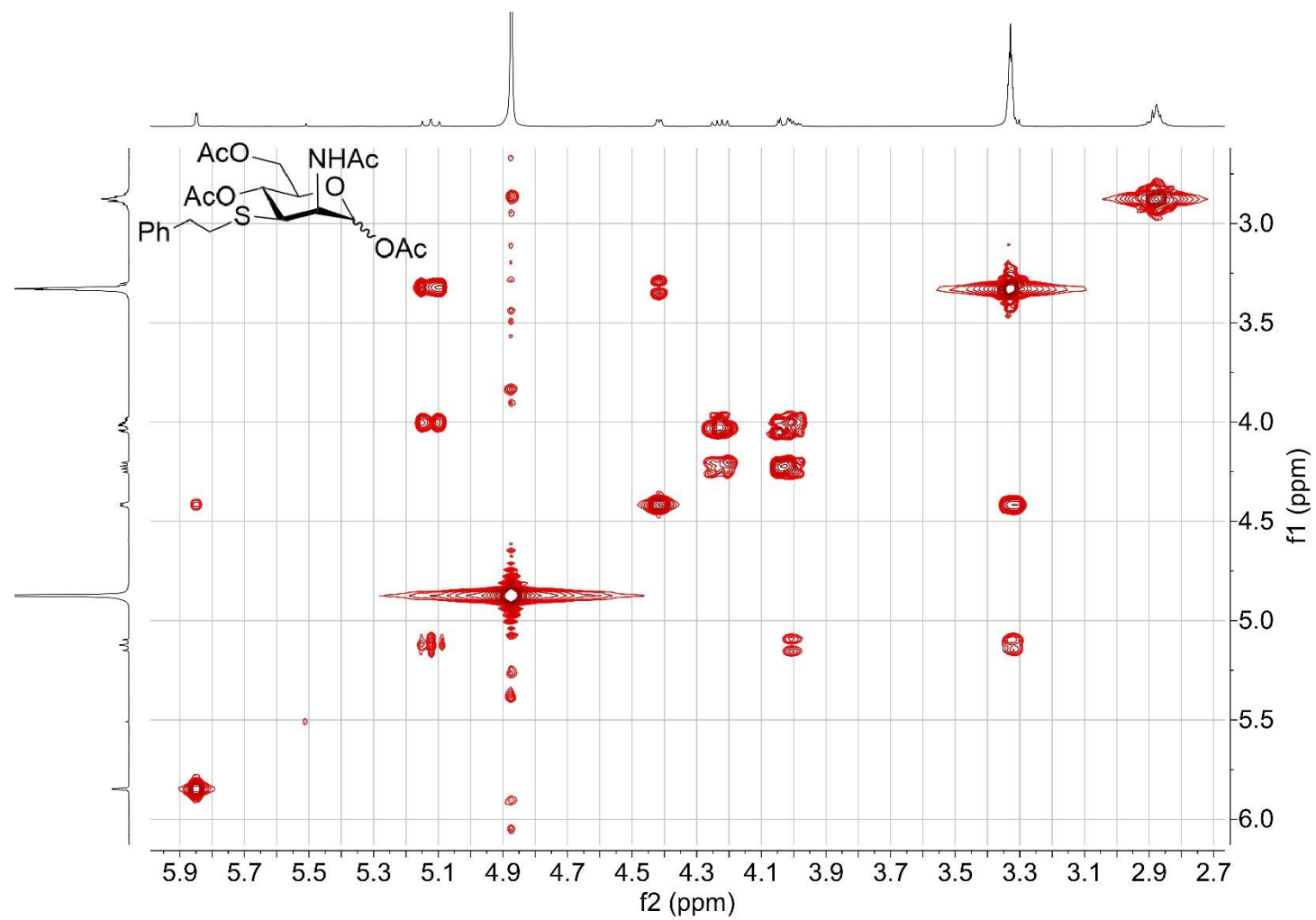
¹H NMR (400 MHz, CD₃OD) 113



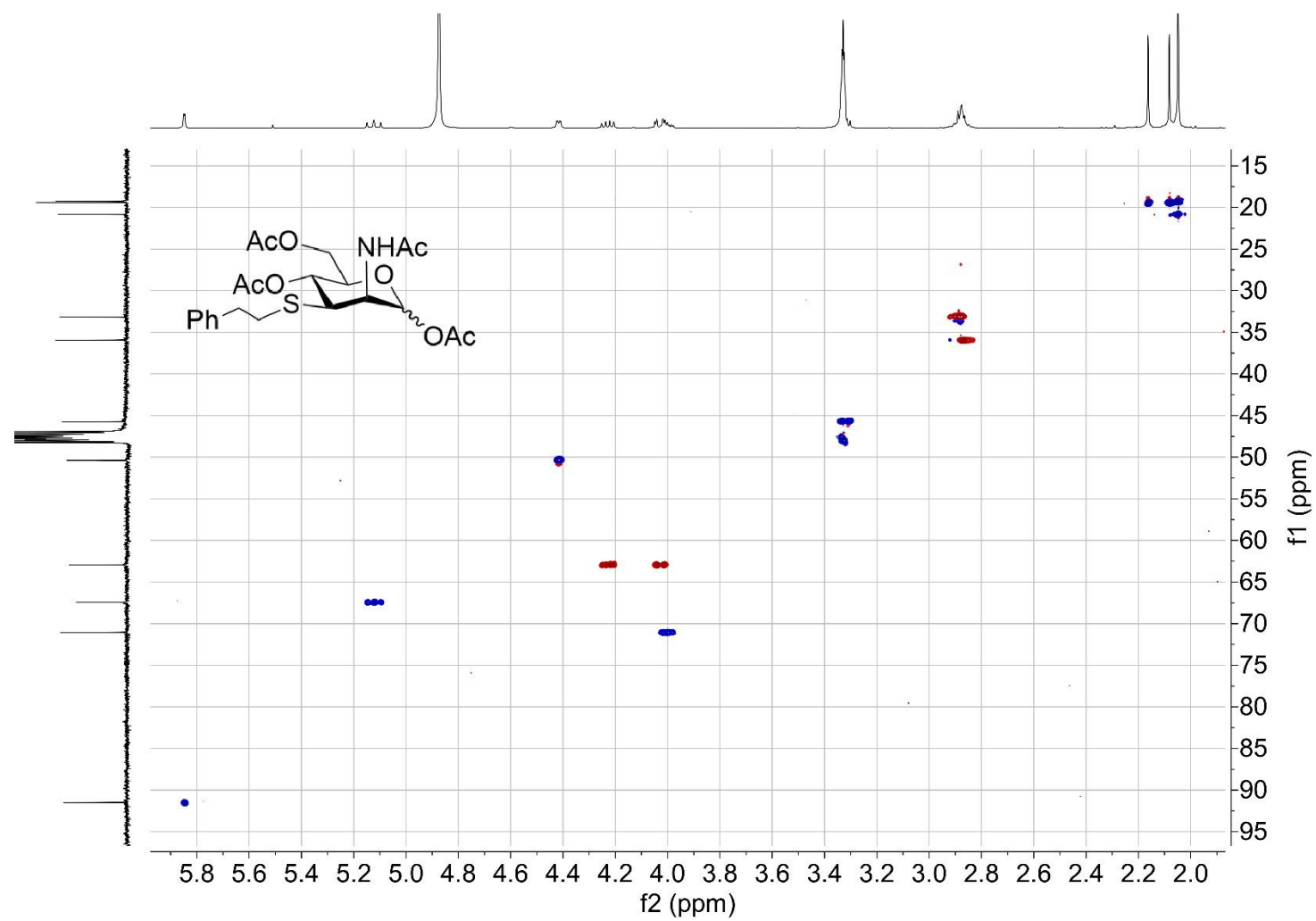
¹³C NMR (100 MHz, CD₃OD) 113



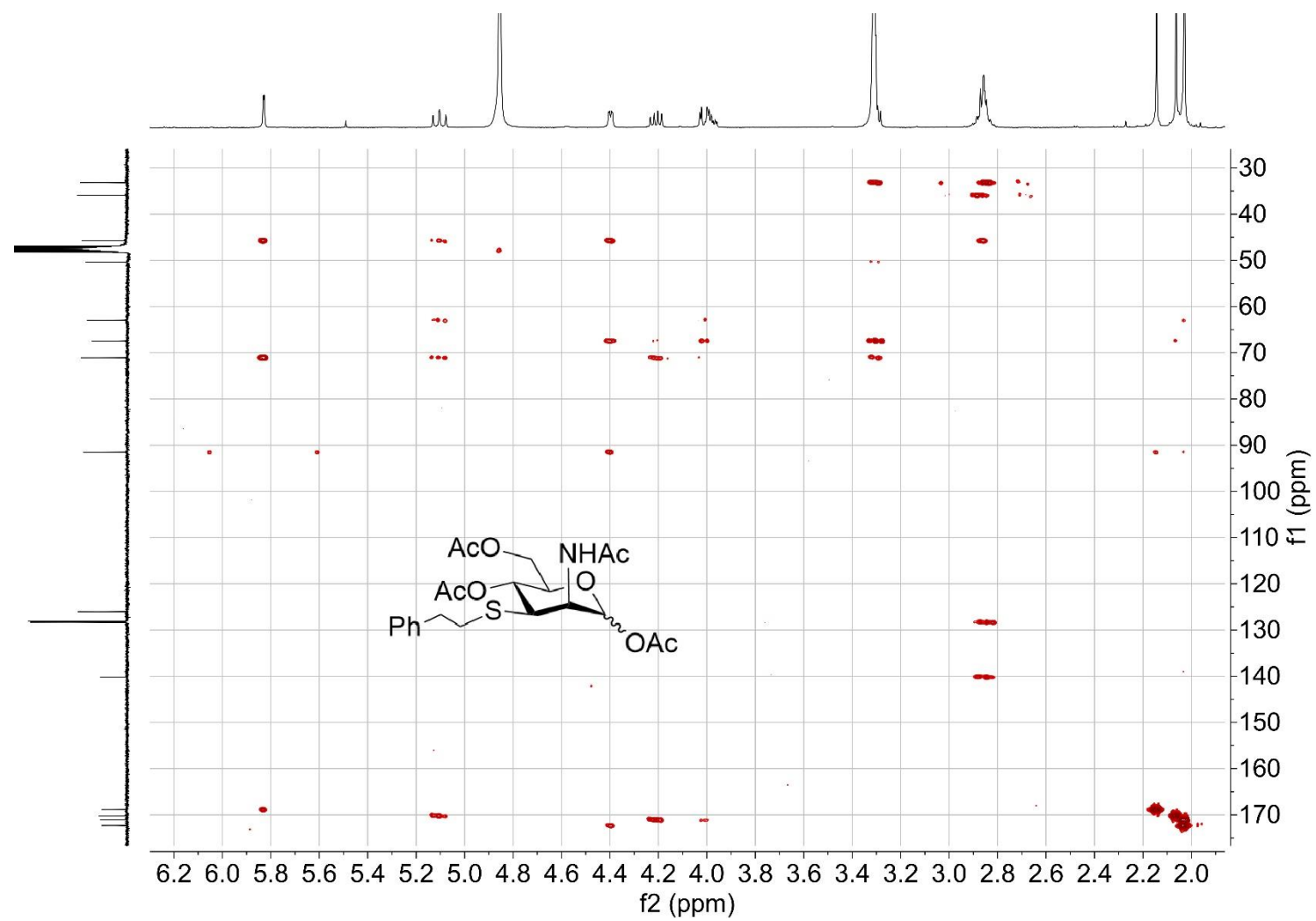
¹H-¹H COSY 113



^1H - ^{13}C HSQC 113



^1H - ^{13}C HMBC 113



^{19}F NMR OF PRODUCTS FORMED ON REACTION OF 20 WITH 2-PHENYLETHANTHIOL UNDER DIFFERENT CONDITIONS

^{19}F NMR $\{^1\text{H}\}$ (376 MHz, CD_3OD), reaction conditions: MeONa/MeOH (1) and $\text{Na}_2\text{CO}_3/\text{H}_2\text{O}$ (2)

