Supporting Information

9-Azido-9-deoxy-2,3-difluorosialic Acid as A Subnanomolar Inhibitor Against Bacterial Sialidases

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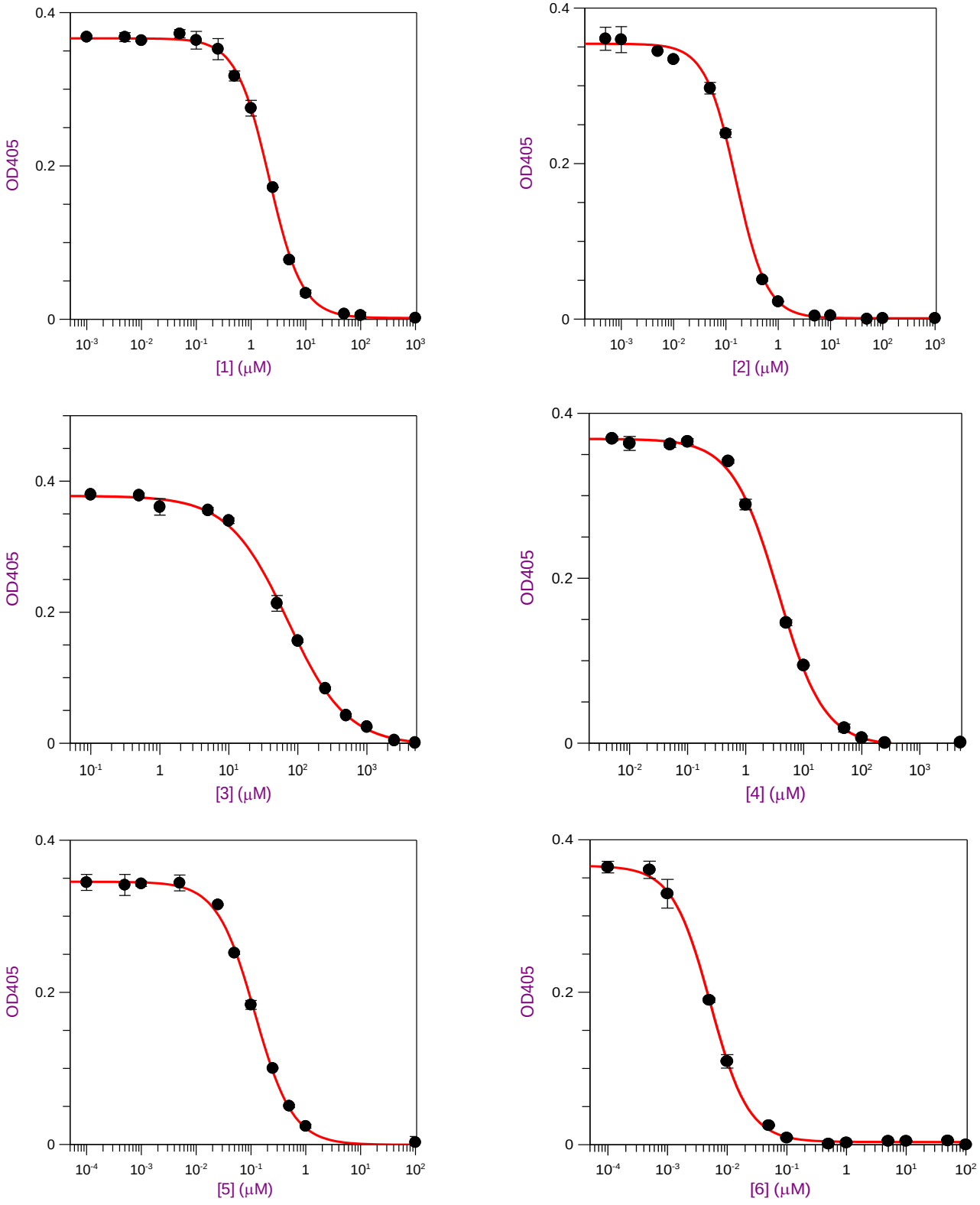
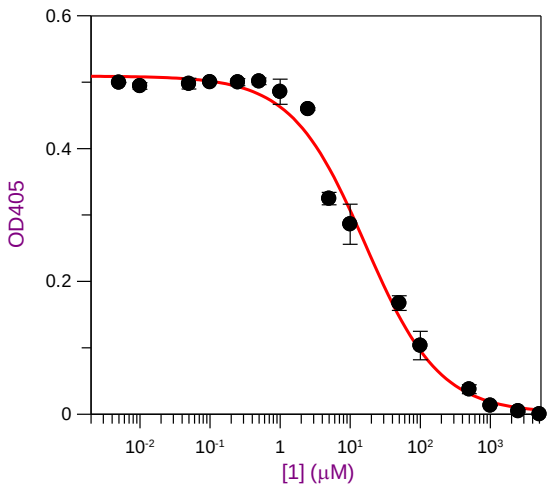
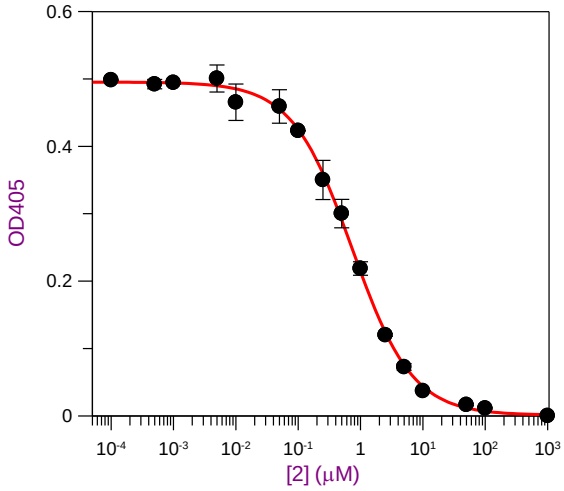
Figure S1. Sialidase inhibition IC_{50} plots for compounds **1**–**6**

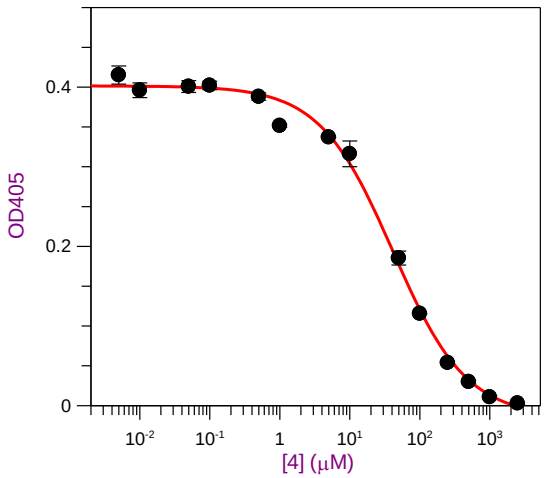
A) *A. ureafaciens* sialidase

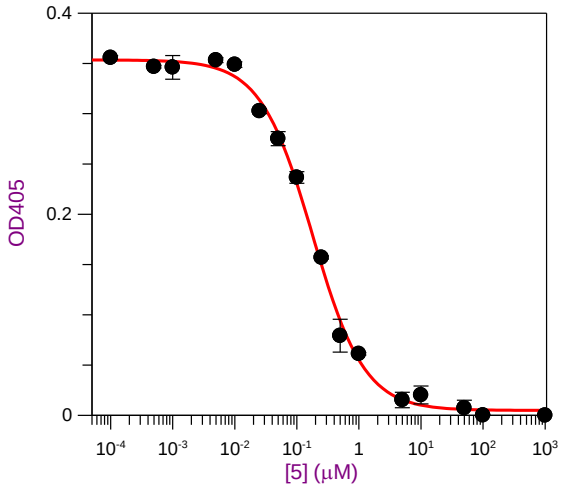


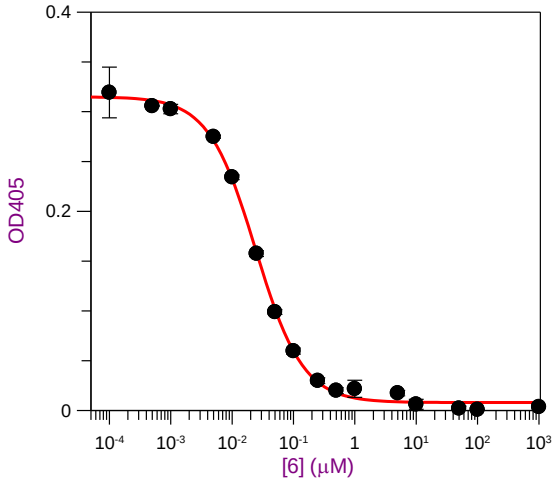
B) *C. perfringens* sialidase (CpNanI)



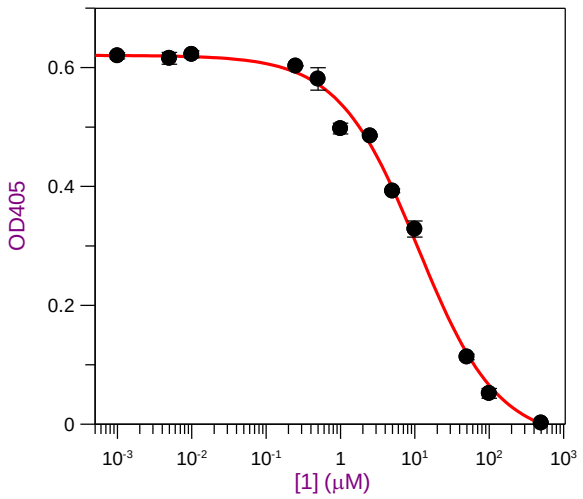








C) SpNanA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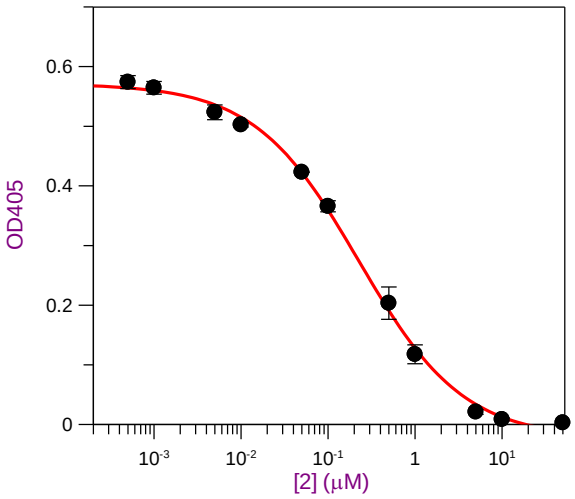
0.2
0
10-3 10-2 10-1 1 101 102 103
[1] (μM)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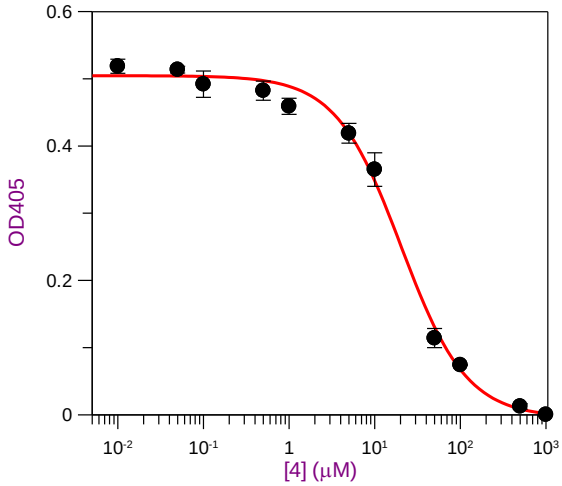
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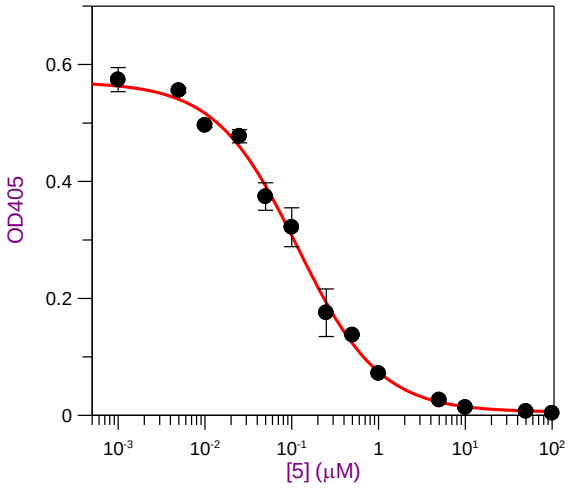
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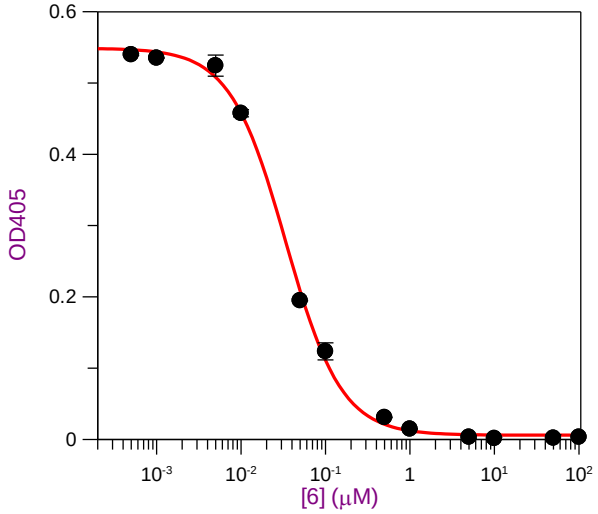
[5] (μM)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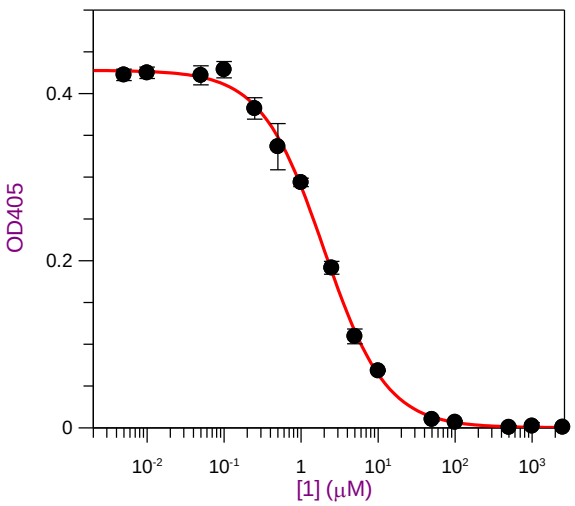
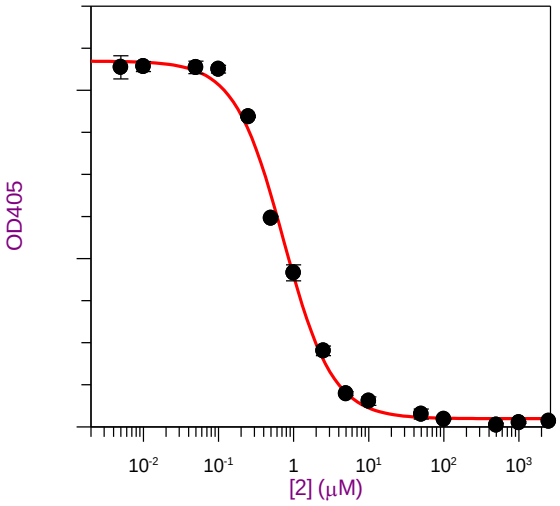
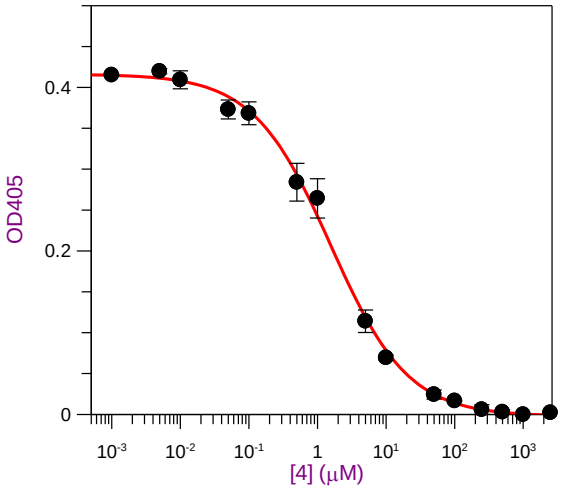
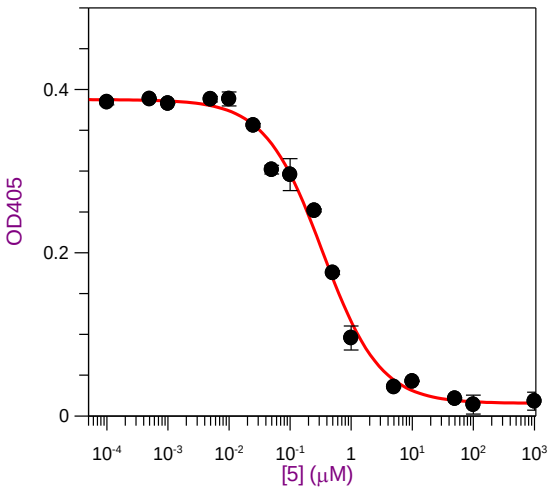
[6] (μM)

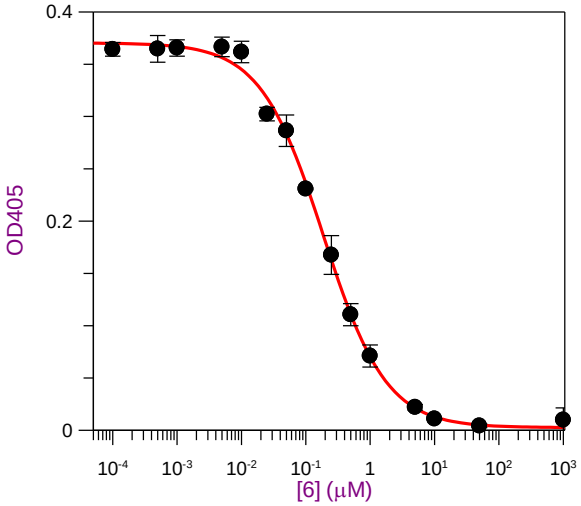
D) *V. cholerae* sialidase











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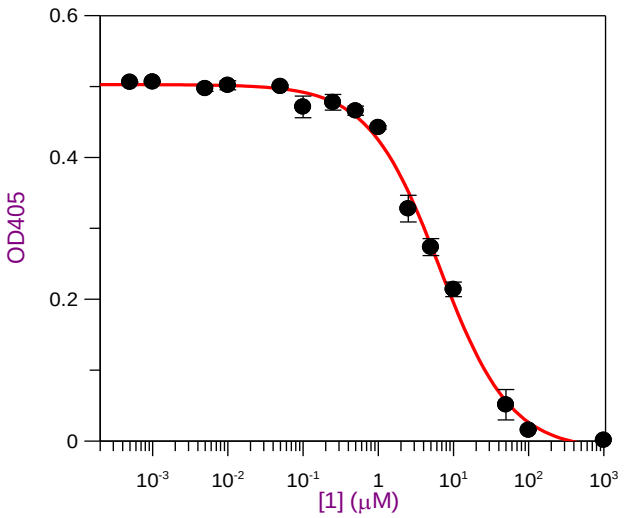
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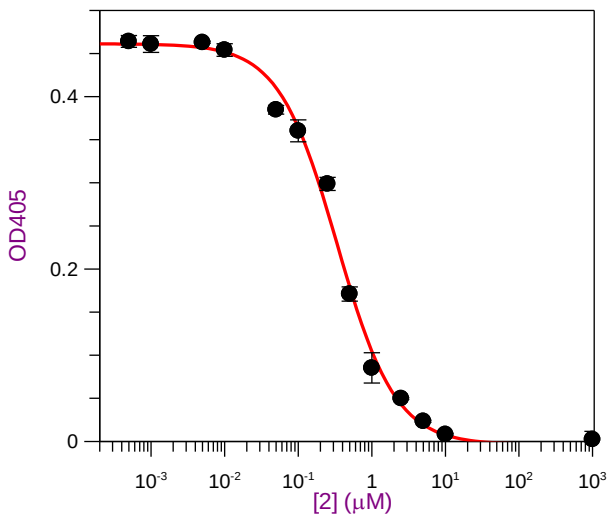
[1] (μM)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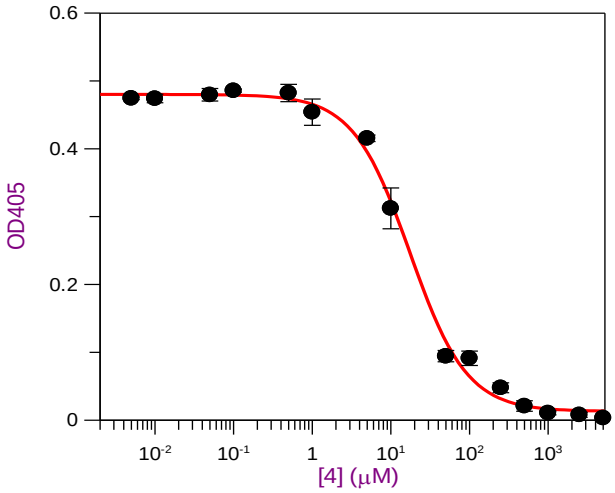
[2] (μM)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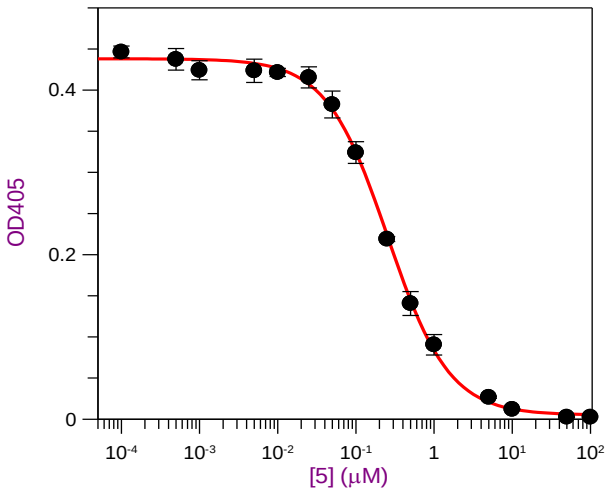
10-2 10-1 1 101 102 103
[4] (μM)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0.2
0
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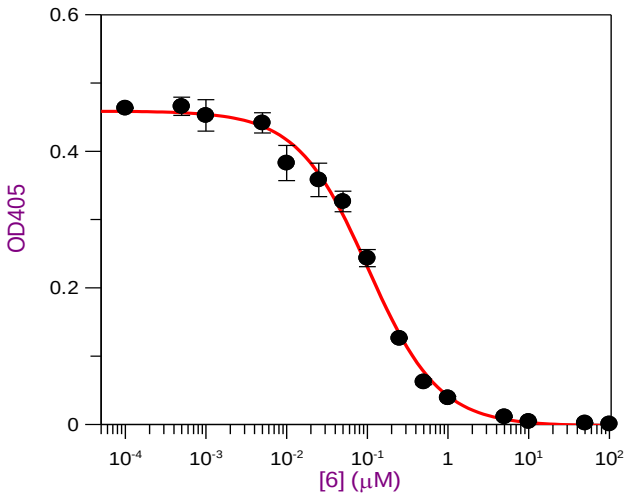
[5] (μM)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0.4
0.2
0
10-4 10-3 10-2 10-1 1 101 102
[6] (μM)

F) hNEU2

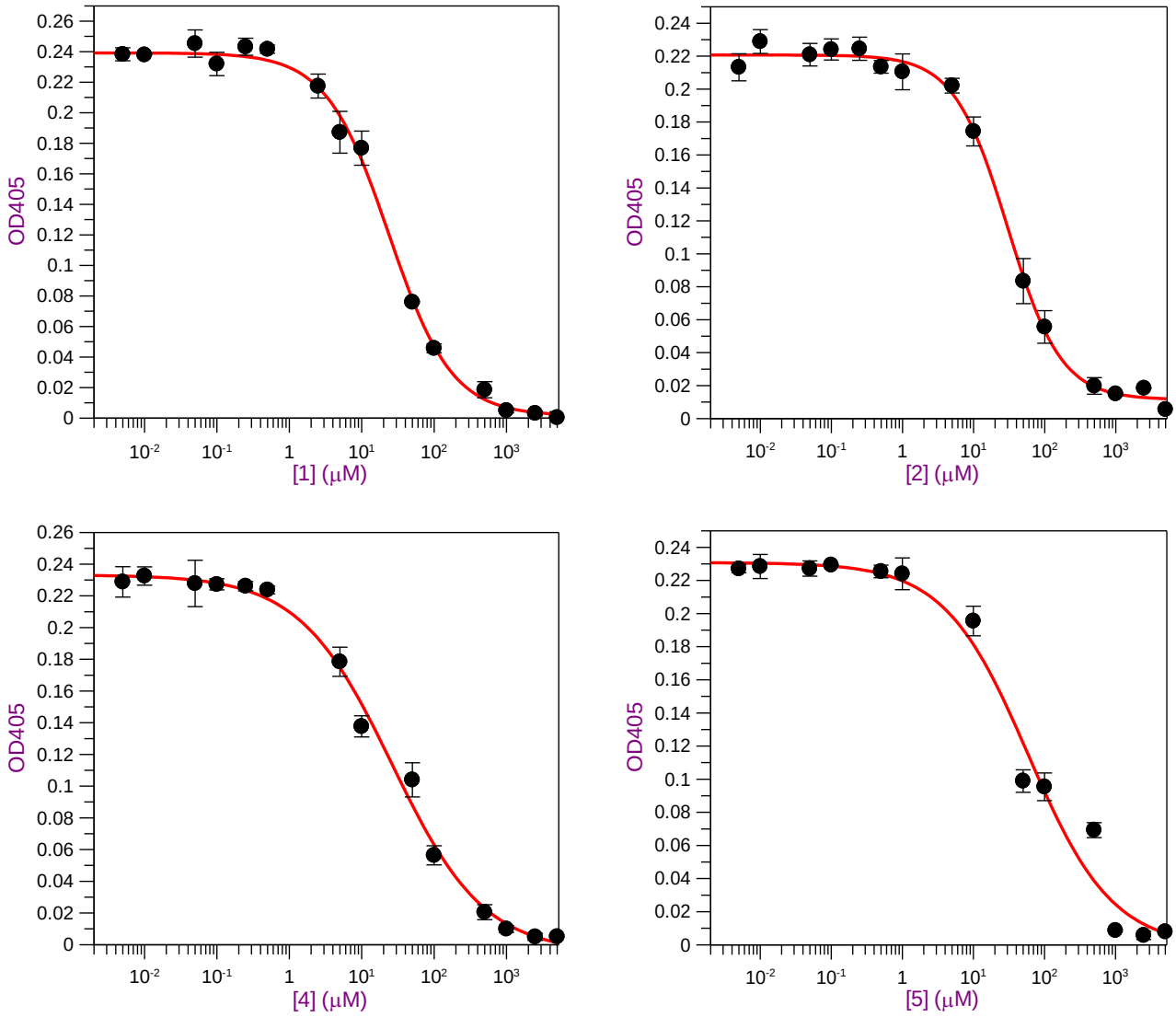
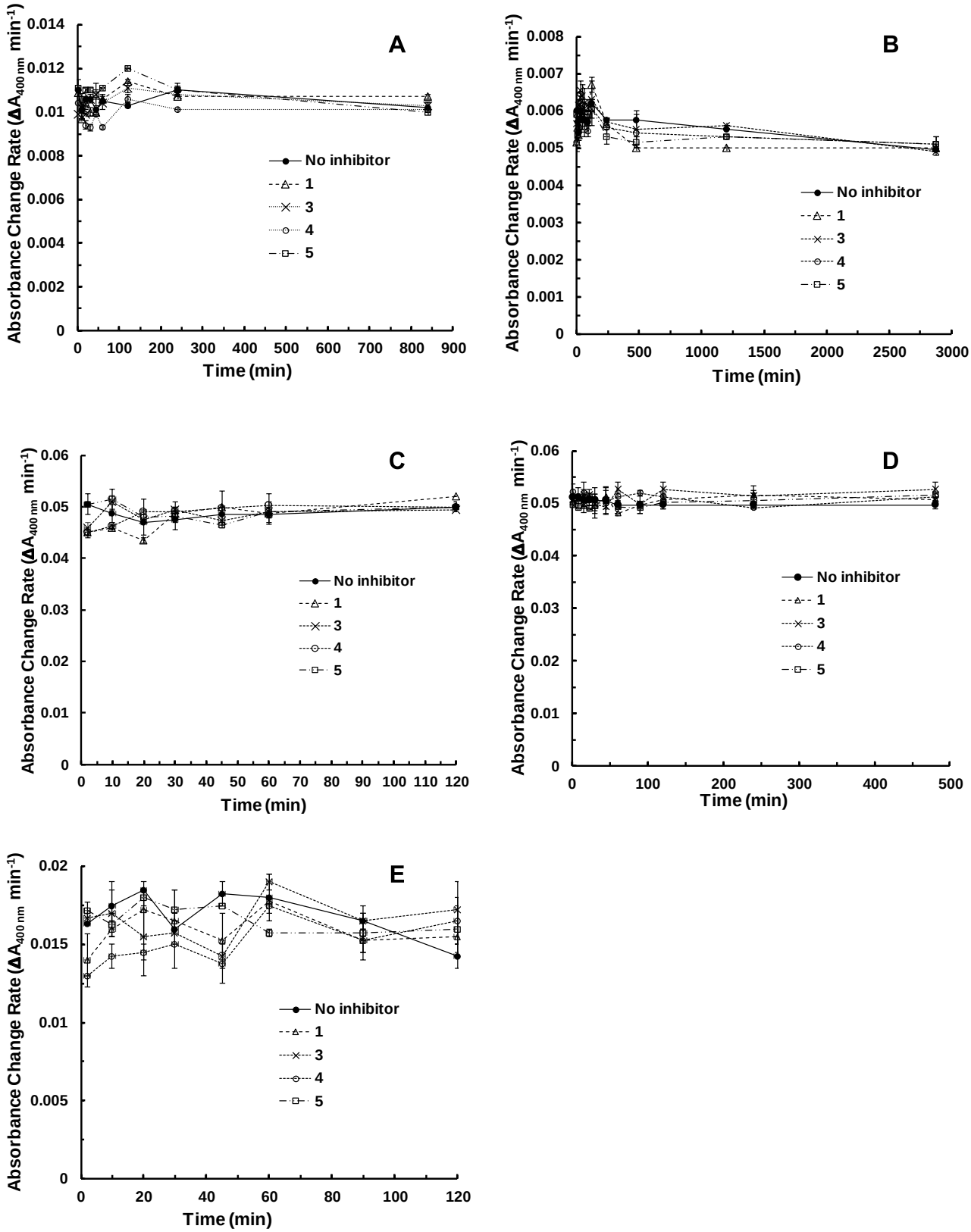
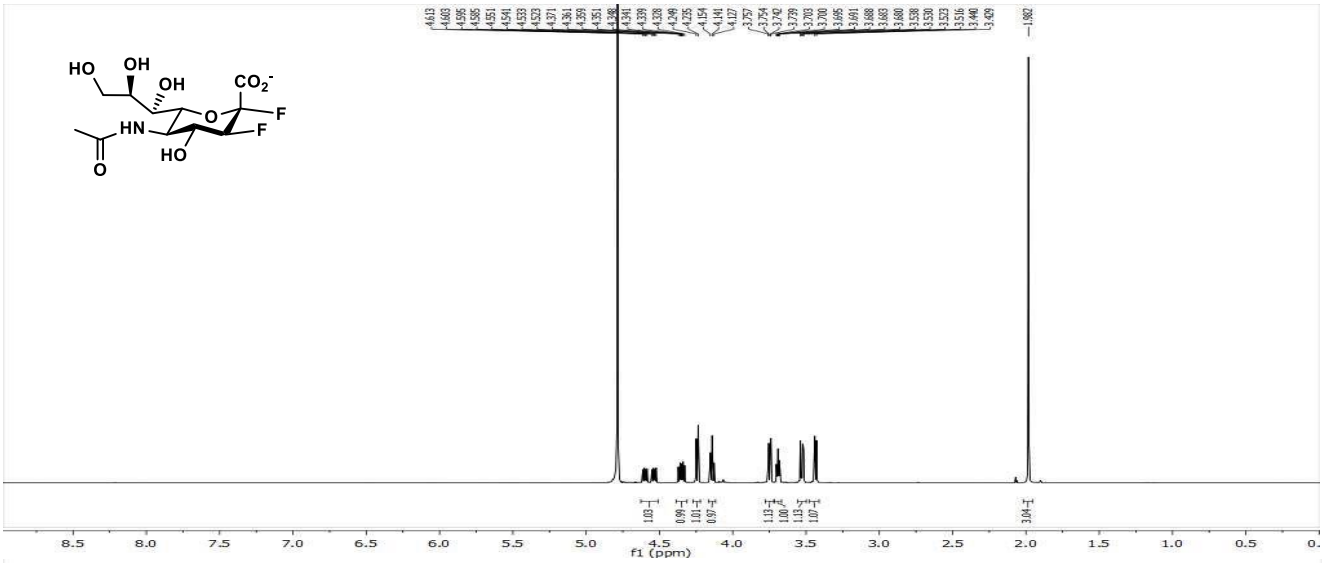
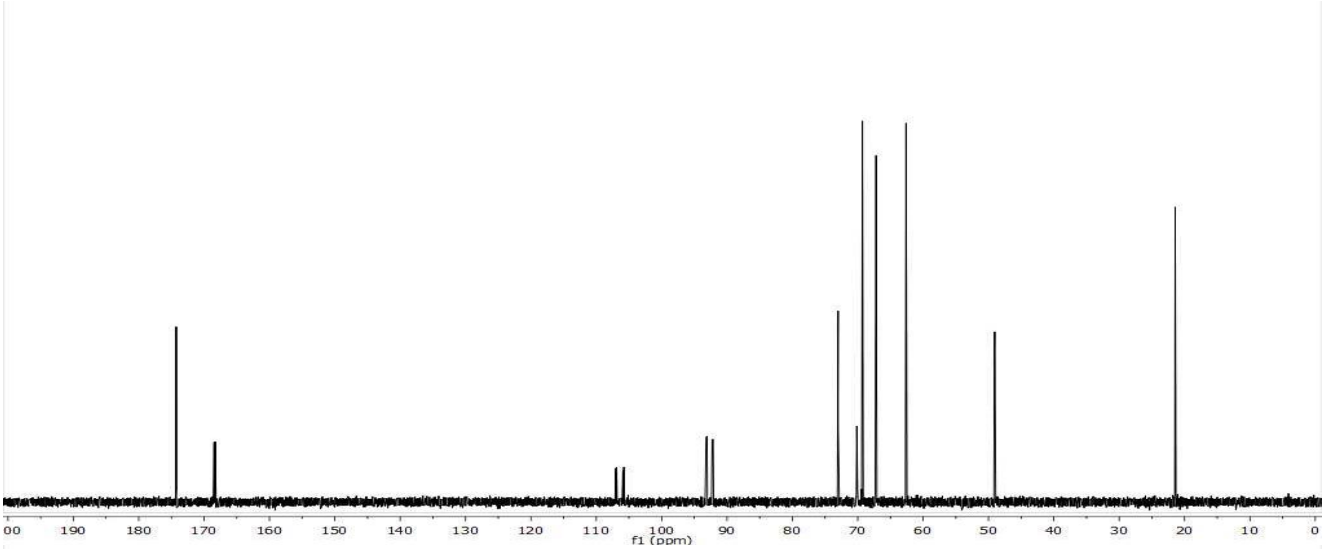


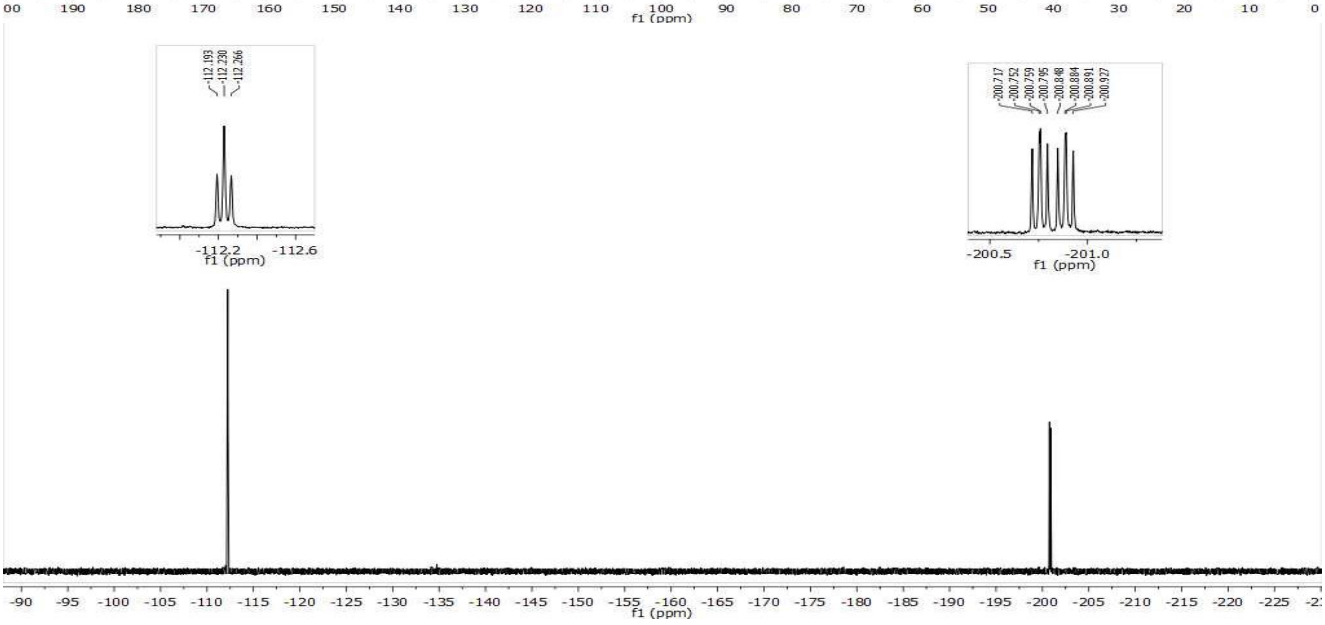
Figure S2. Time course study results for sialidase de-activation and re-activation in the presence or the absence of a covalent inhibitor (**1** or **3–5**). **A**, *C. perfringens* sialidase CpNanI; **B**, *V. cholerae* sialidase; **C**, SpNanA; **D**, BiNanH2; **E**, hNEU2.



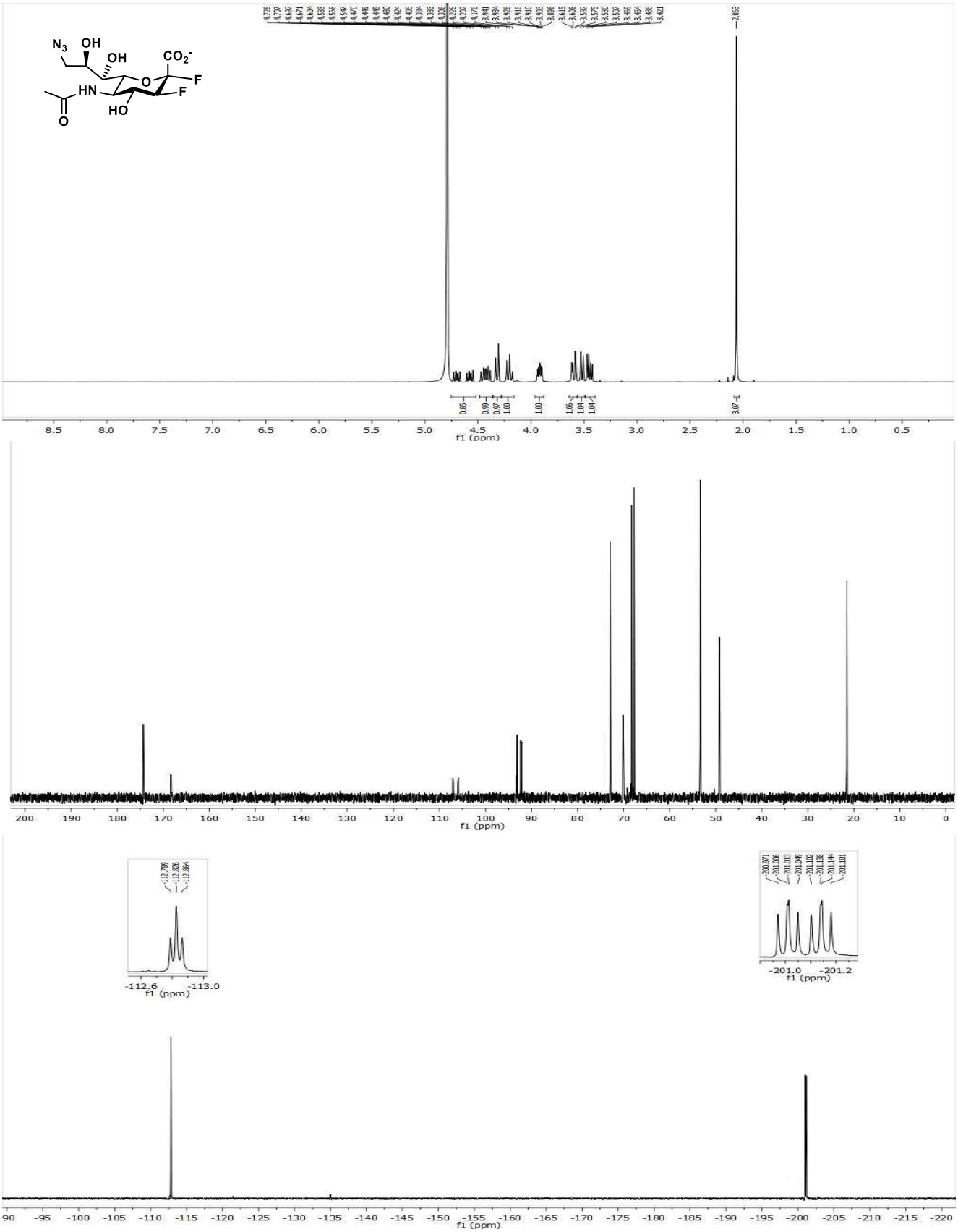
^{1}H, ^{13}C, an d ^{19}F NMR spectra of 5-acetamido-2,3,5-trideoxy-3-fluoro-D-*erythro*-α-L-*gluco*-non-2-ulopyranosylonic fluoride (2*e*3*e*DFNeu5Ac) (**1**)



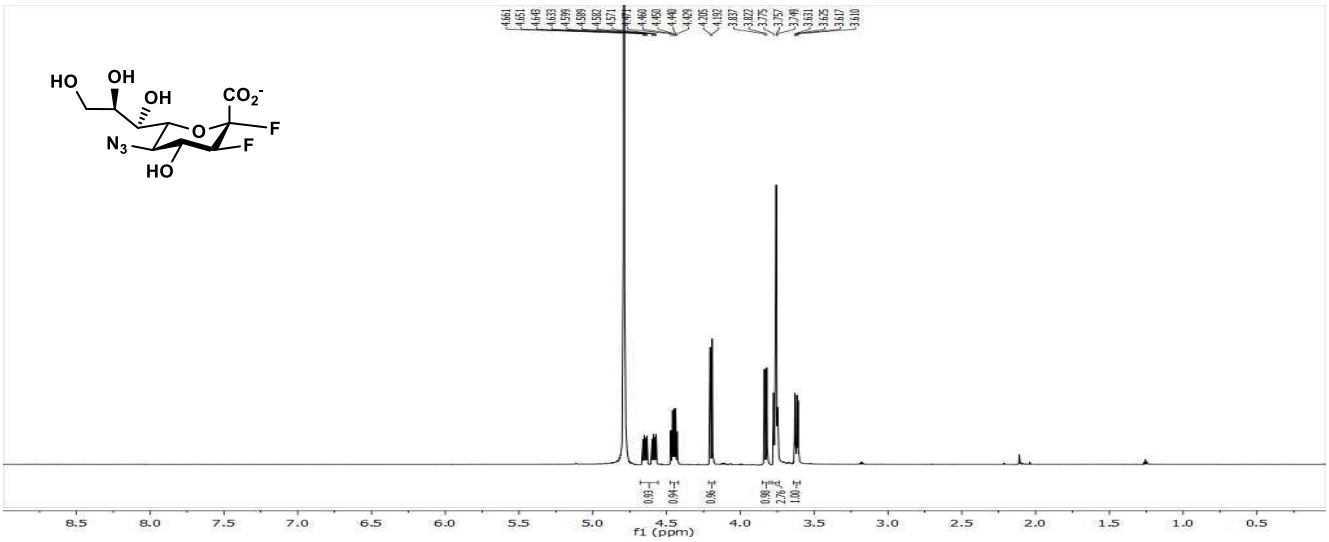


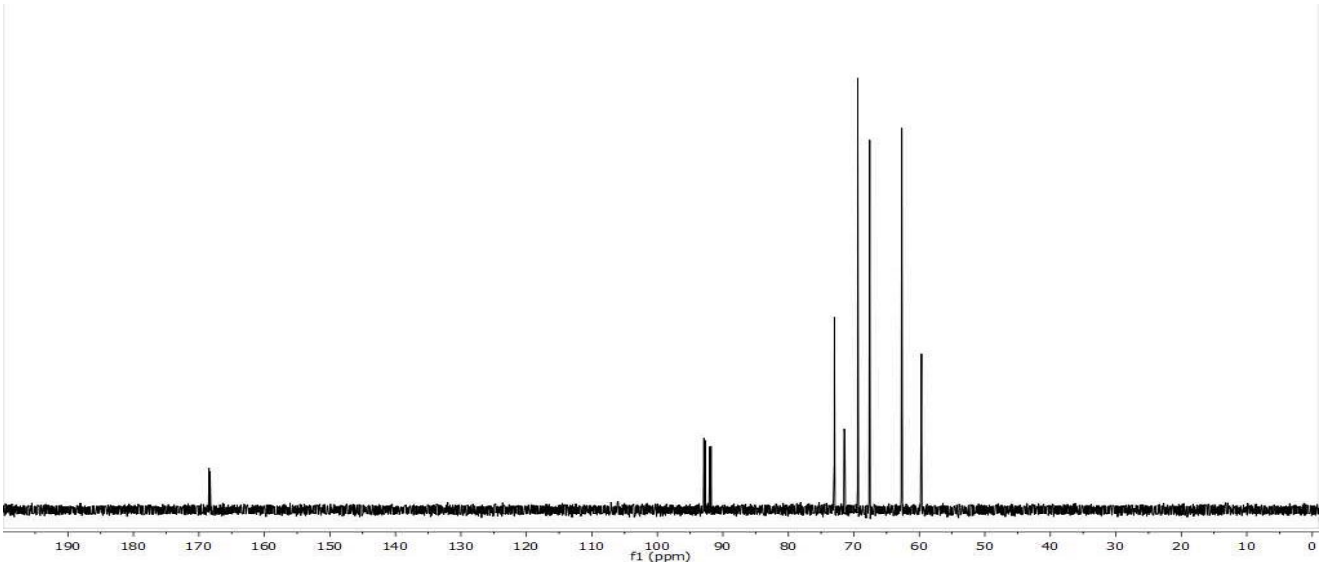


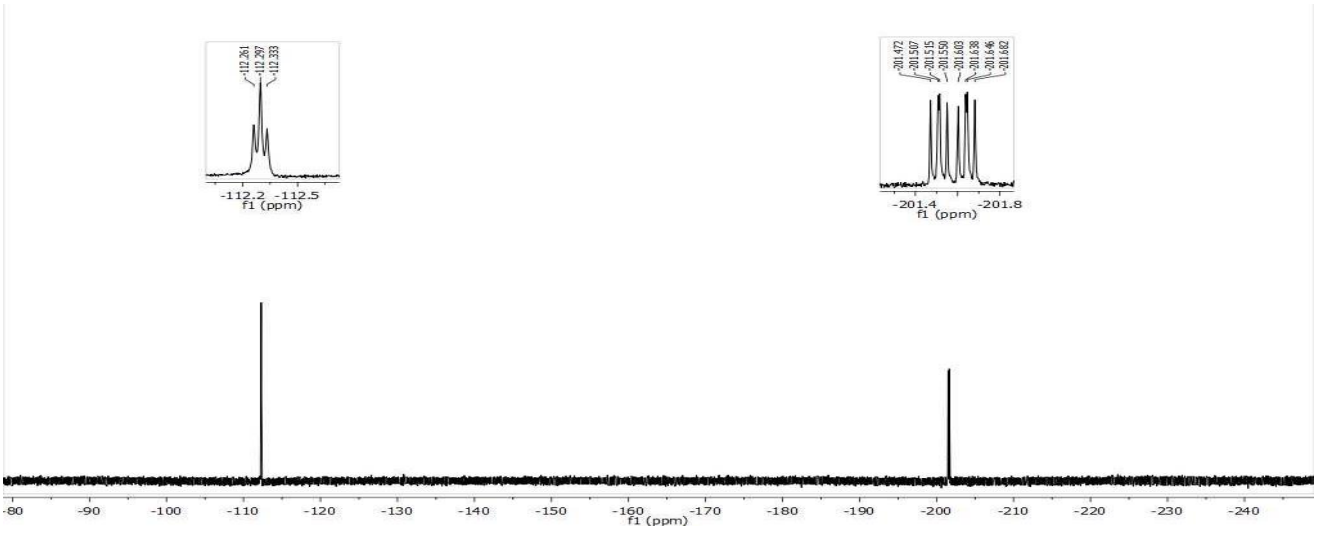
^{1}H, ^{13}C, ^{19}F NMR spectra of 5-acetamido-9-azido-2,3,5,9-tetradeoxy-3-fluoro-D-*erythro*-α-L-*gluco*-non-2-ulopyranosylonic fluoride (2*e*3*e*DFNeu5Ac9N_3) (**2**)



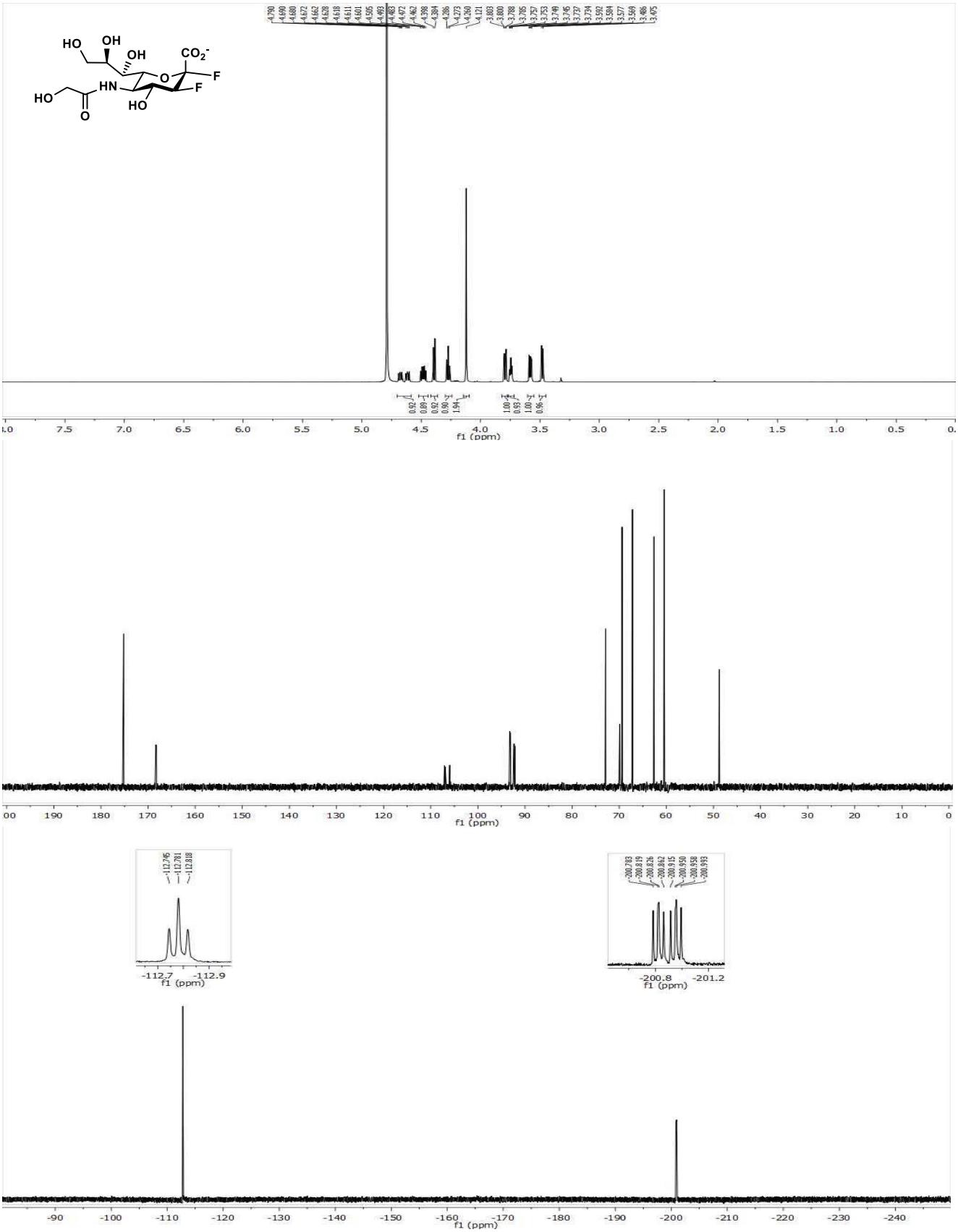
^{1}H, ^{13}C, and ^{19}F NMR spectra of 5-azido-2,3,5-trideoxy-3-fluoro-D-*erythro*-α-L-*gluco*-non-2-ulopyranosylonic fluoride (2*e*3*e*Neu5N$_3$) (**3**)



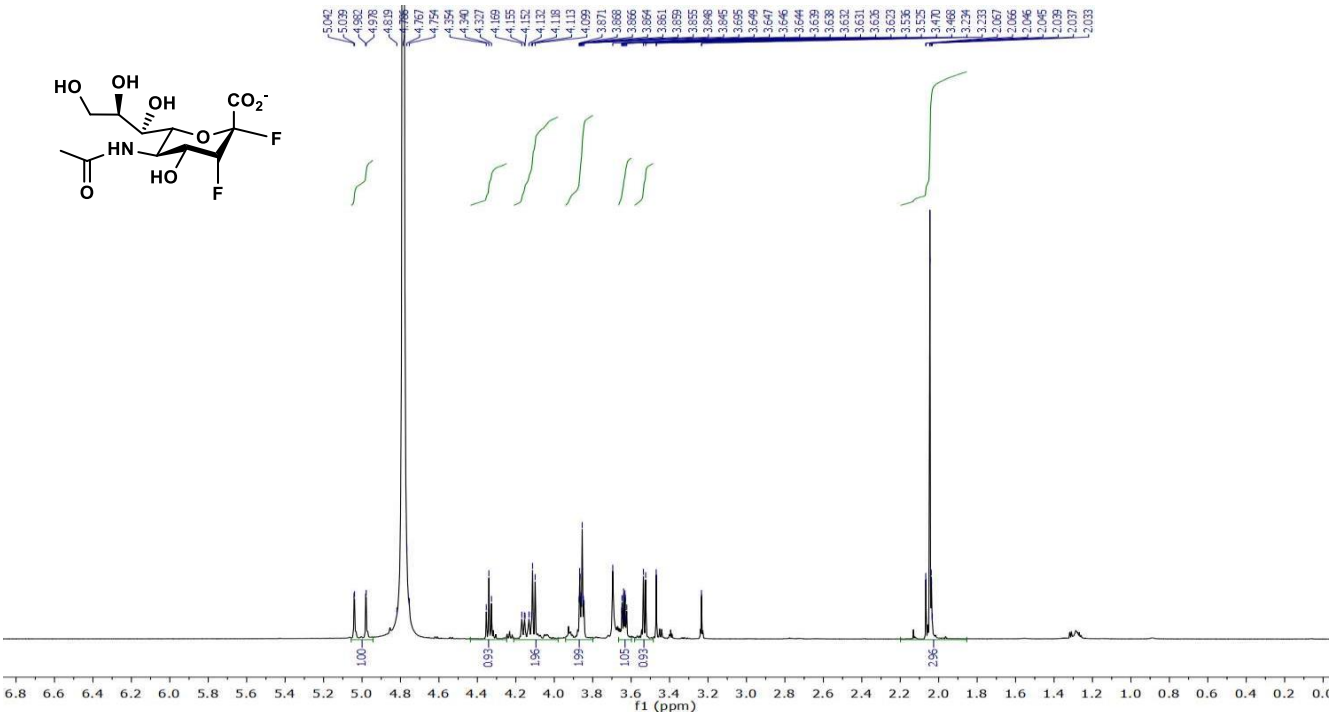


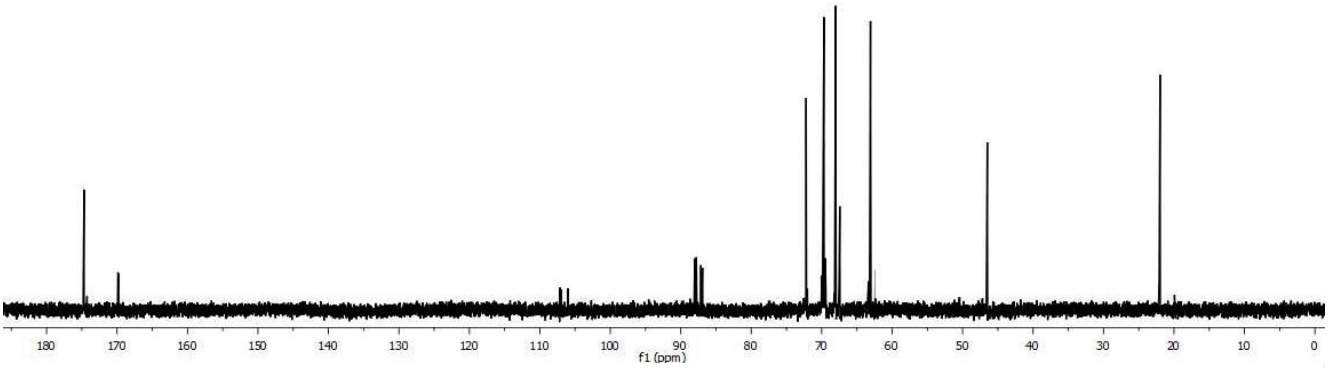


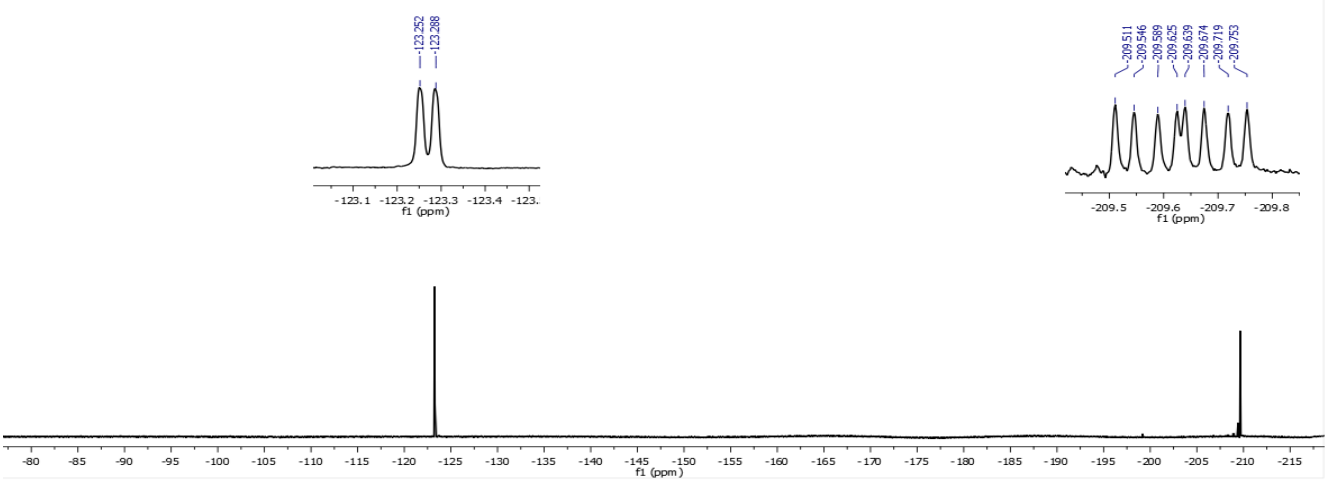
^{1}H, ^{13}C, and ^{19}F NMR spectra of 5-glycolamido-2,3,5-trideoxy-3-fluoro-D-*erythro*-α-L-*gluco*-non-2-ulopyranosylonic fluoride (2*e*3*e*DFNeu5Gc) (**4**)



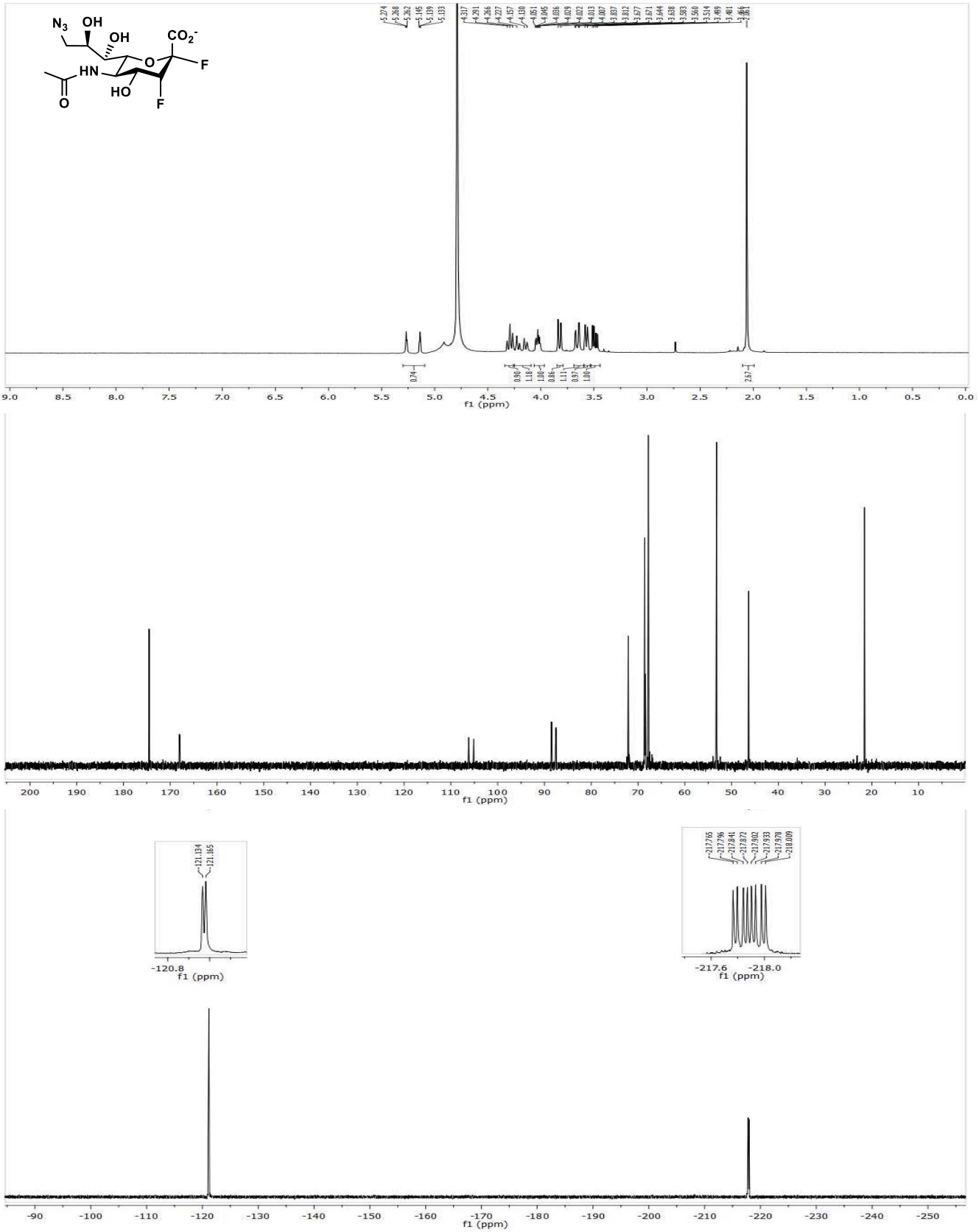
^{1}H, ^{13}C, and ^{19}F NMR spectra of 5-acetamido-2,3,5-trideoxy-3-fluoro-D-*erythro*-α-L-*manno*-non-2-ulopyranosylonic fluoride (2*e*3*a*DFNeu5Ac) (**5**)



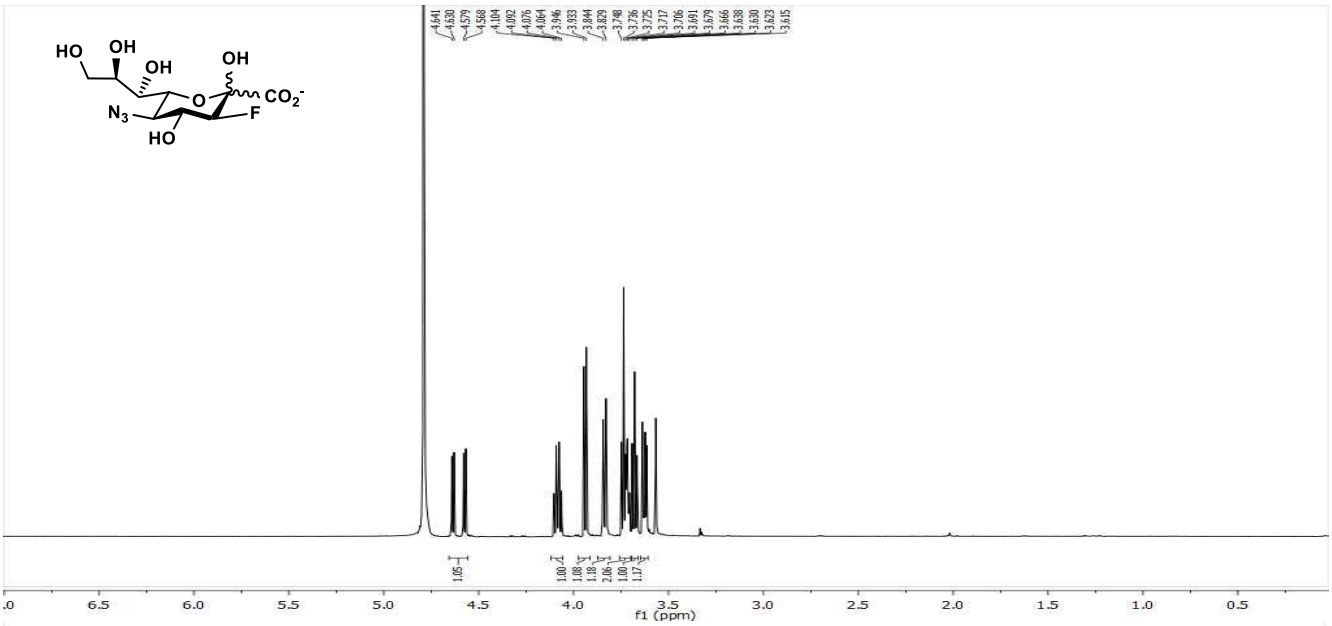


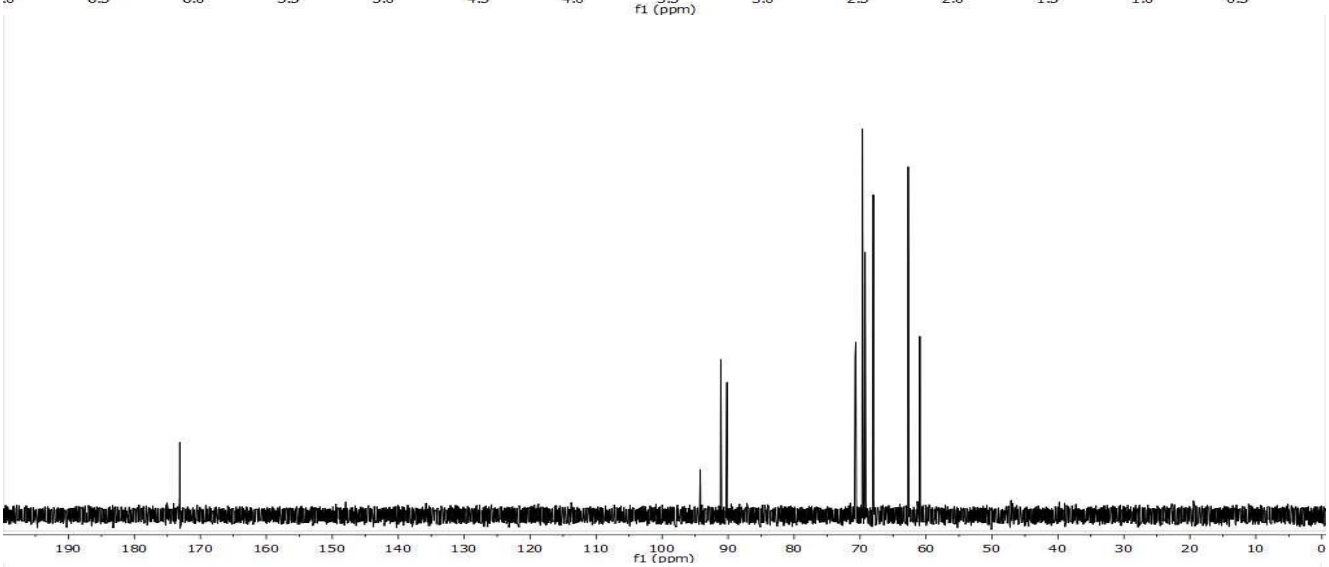


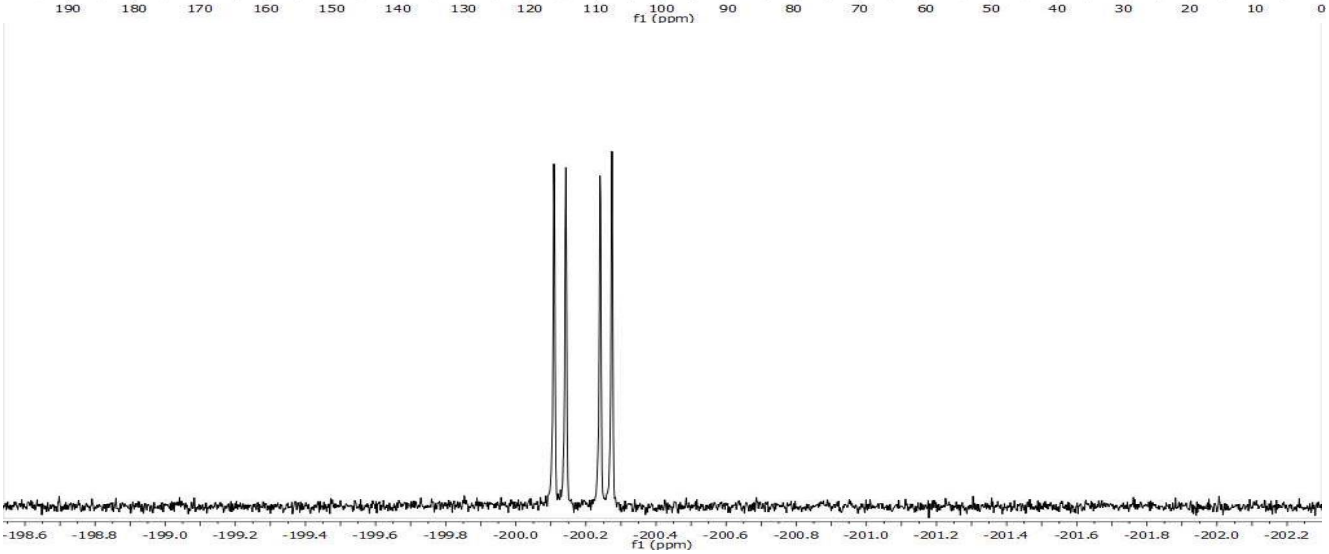
^{1}H, ^{13}C, ^{19}F NMR spectra of 5-acetamido-9-azido-2,3,5,9-tetradeoxy-3-fluoro-D-*erythro*-α-L-*manno*-non-2-ulopyranosylonic fluoride (2*e*3*a*DFNeu5Ac9N$_3$) (**6**)



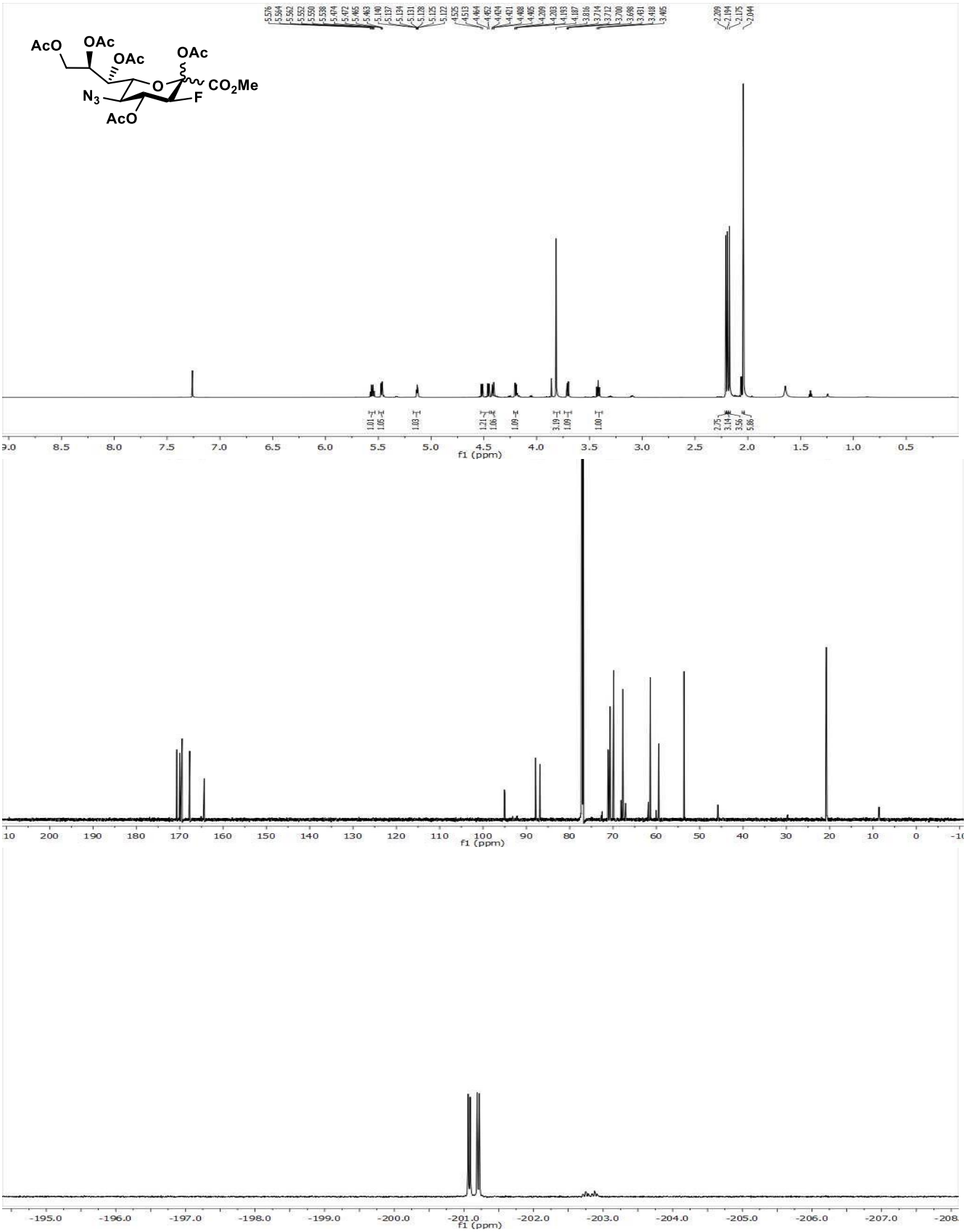
^{1}H, ^{13}C, and ^{19}F NMR spectra of 5-azido-3,5-dideoxy-3-fluoro-D-*erythro*-L-*gluco*-2-nonulopyranosonic acid 3F(*e*)Neu5N$_3$ (**11**)







^{1}H, ^{13}C, and ^{19}F NMR spectra of methyl 5-azido-2,4,7,8,9-penta-*O*-acetyl-3,5-dideoxy-3-fluoro-D-*erythro*-L-*gluco*-non-2-ulopyranosonate (**12**)



^{1}H, ^{13}C, and ^{19}F NMR spectra of methyl 5-acetamido-4,7,8,9-tetra-*O*-acetyl-2,3,5-trideoxy-3-fluoro-D-*erythro*-α-L-*gluco*-non-2-ulopyranosylonate fluoride (**13**)