

Supporting Information

A Chemoenzymatic Synthon Strategy for Synthesizing *N*-Acetyl Analogs of *O*-Acetylated *N. meningitidis* W Capsular Polysaccharide Oligosaccharides

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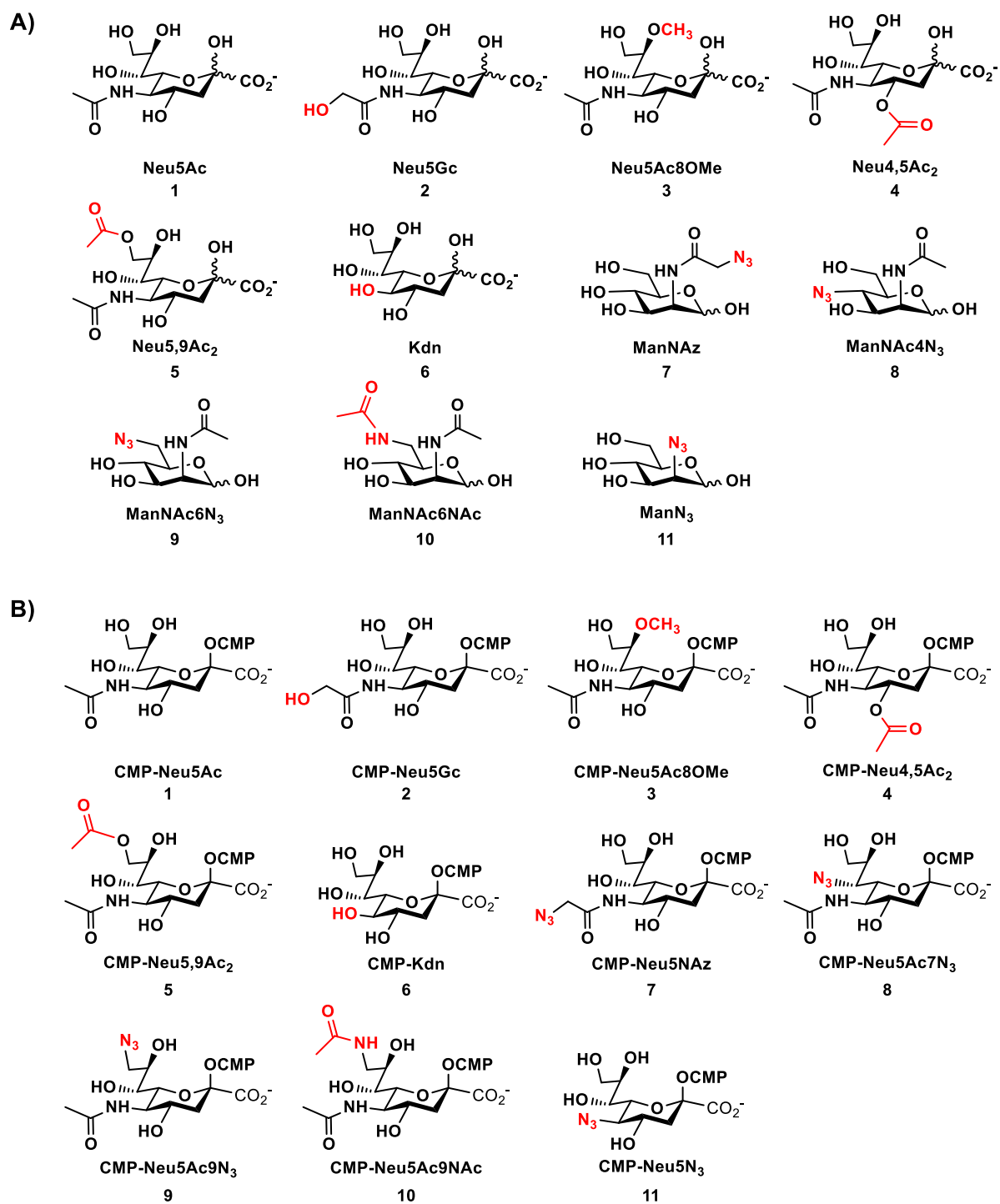


Figure S1. Structures of monosaccharides (A) that have been used in two-step one-pot multienzyme (OPME) donor substrate specific studies for the $\alpha 2$ -6-sialyltransferase activity of NmSiaD_W and the structures of the corresponding CMP-sialic acids (B). Galactosyl disaccharide **G2** was used as the acceptor substrate.

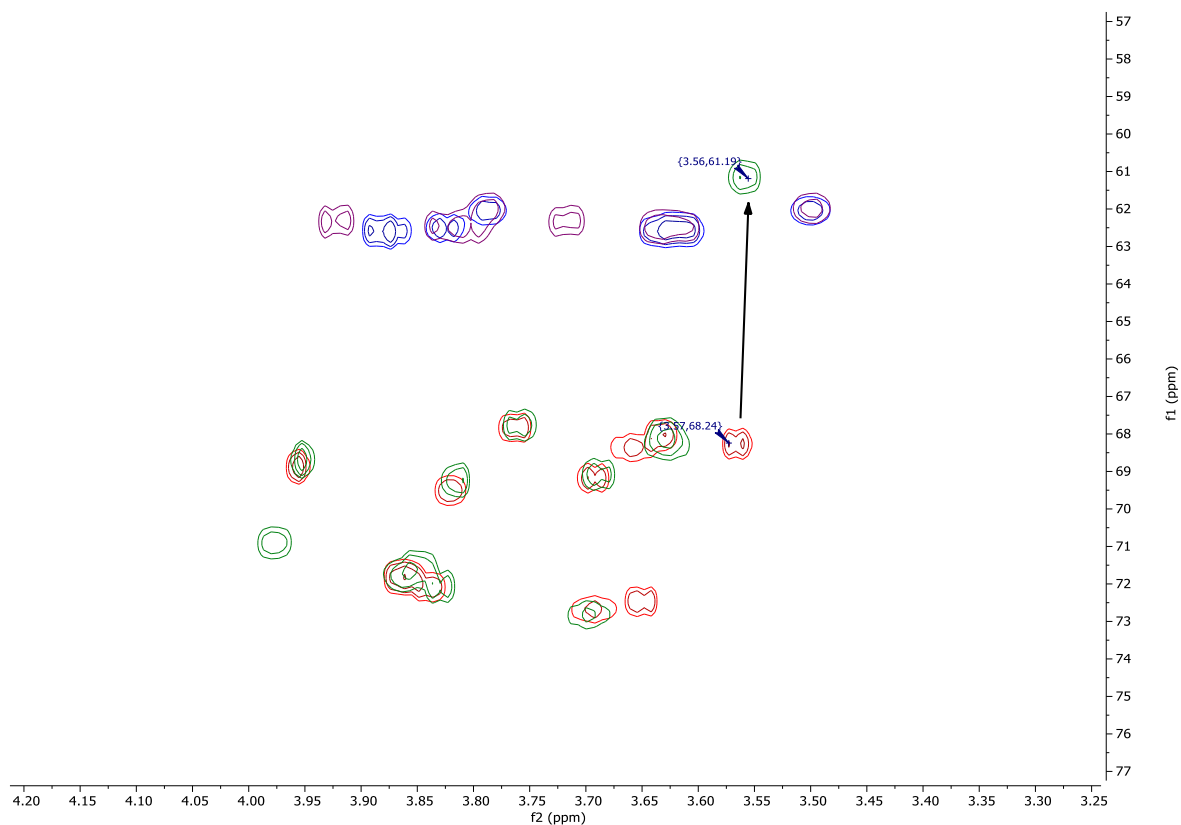


Figure S2. HSQC spectra comparison of the H^{'''}-7 and C^{'''}-7 in sialyltrisaccharides **7N₃-S3** (green/purple) and **S3** (red/blue).

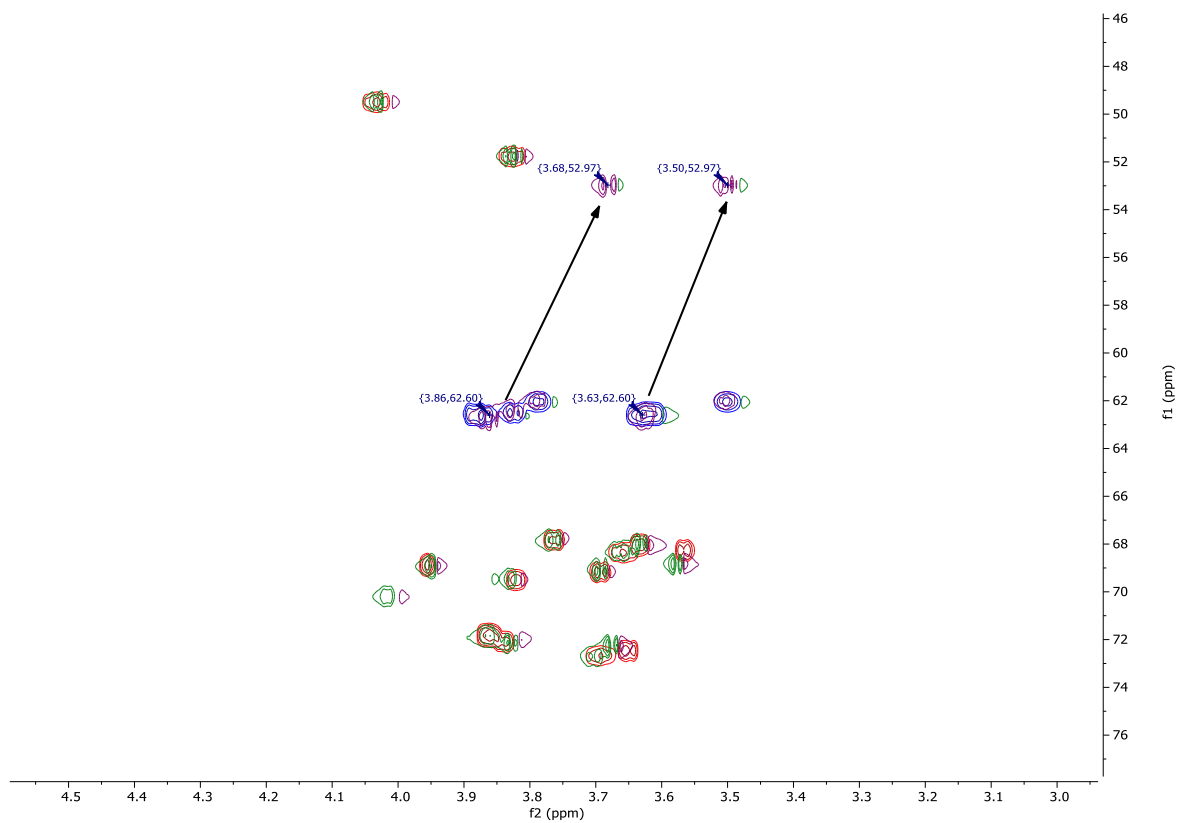
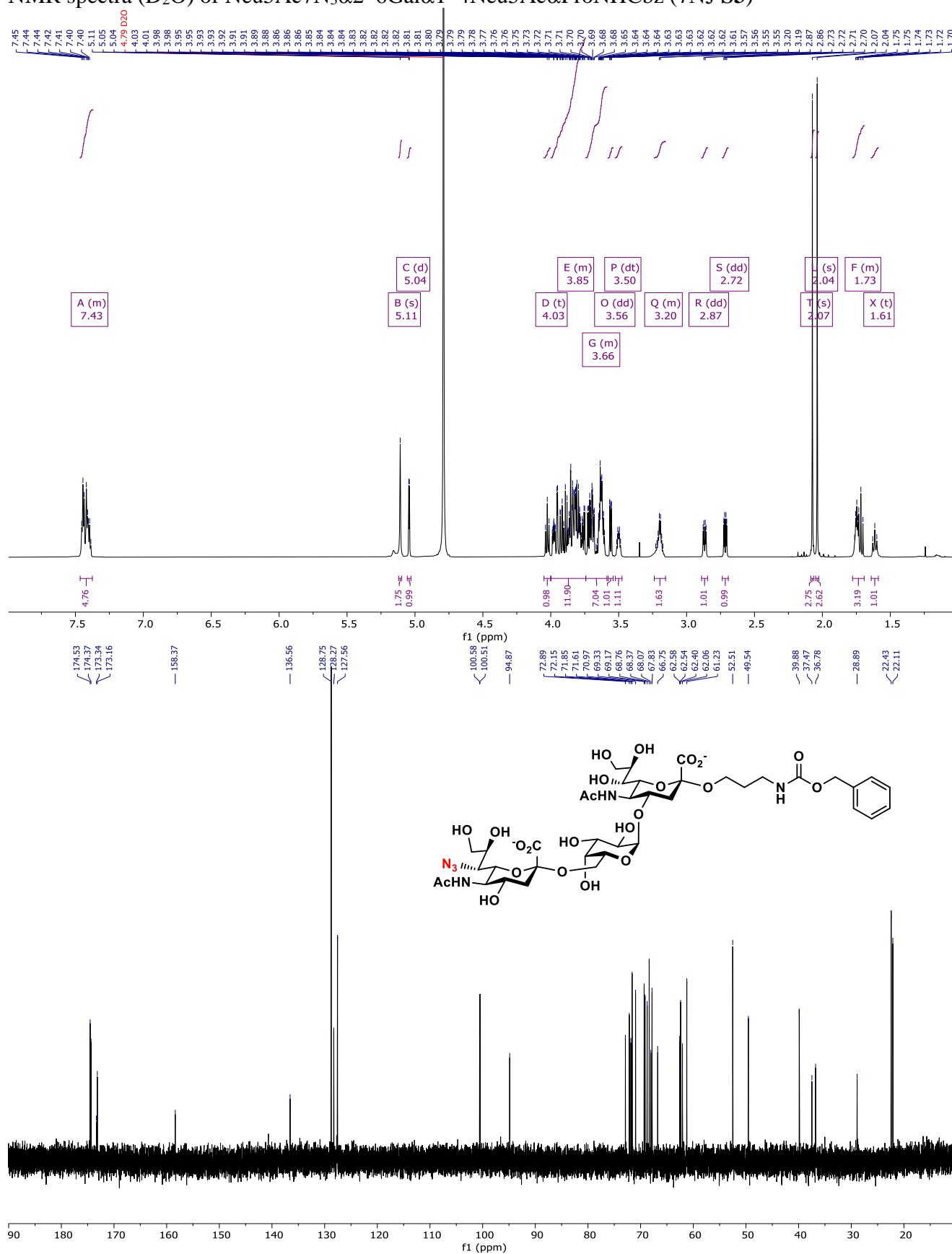
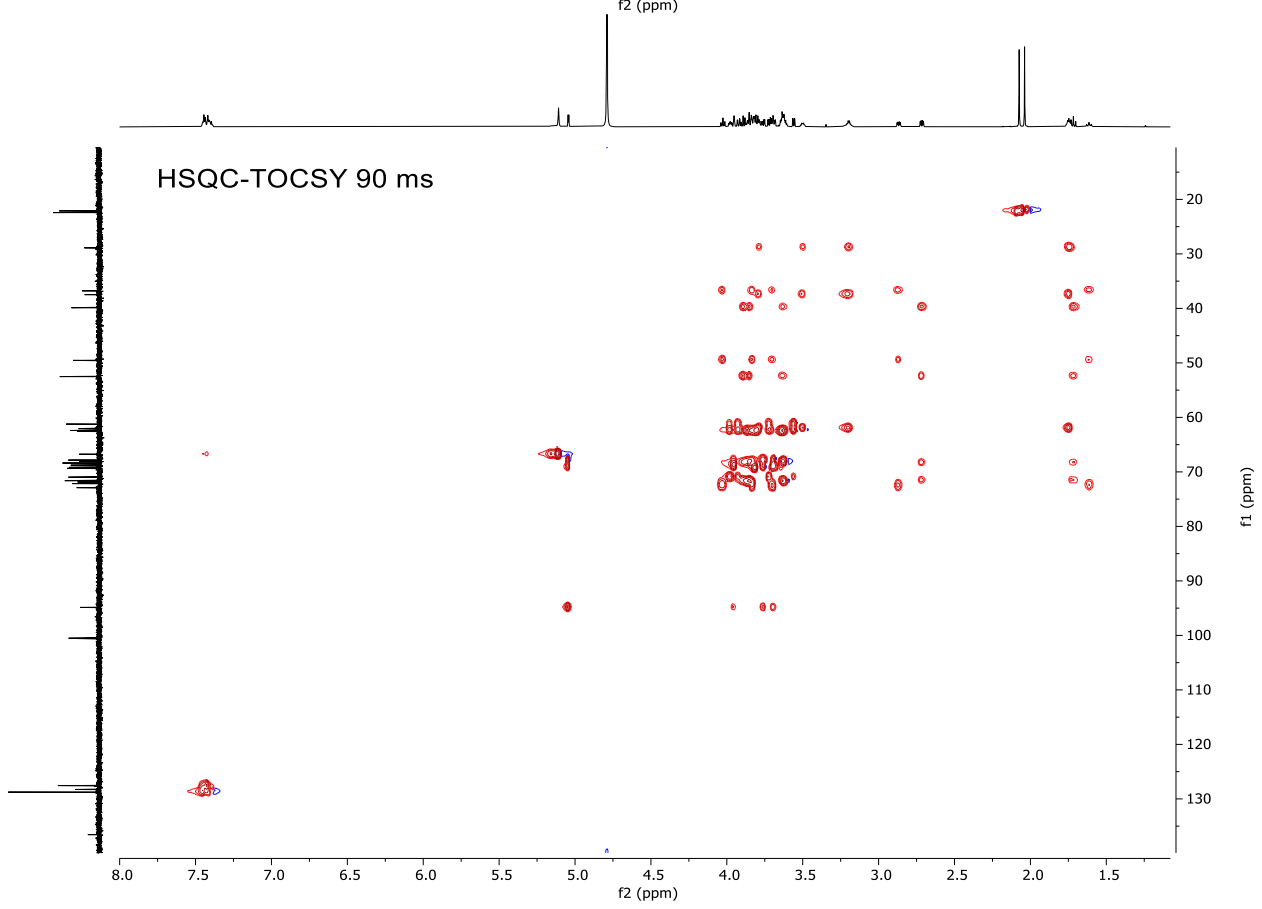
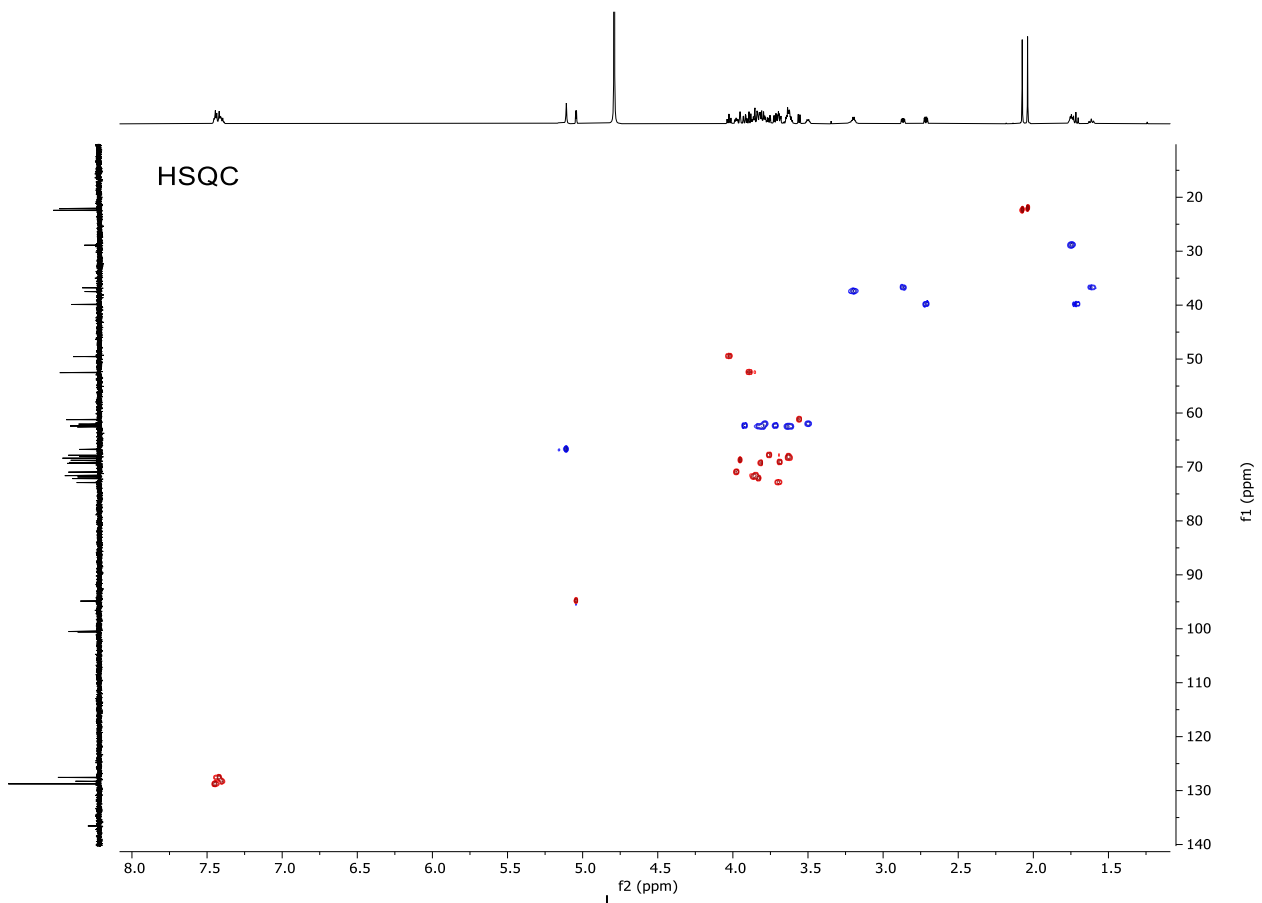
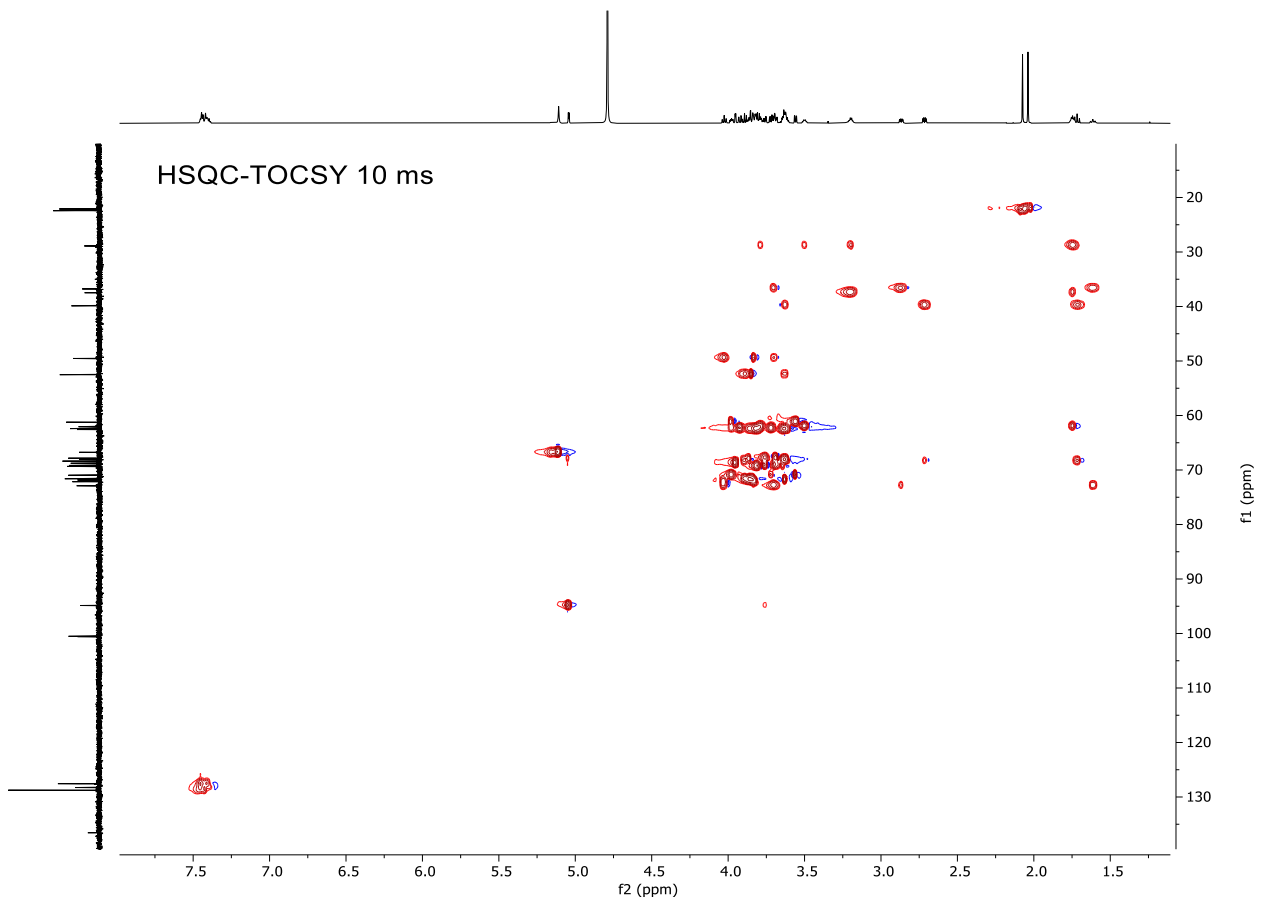


Figure S3. HSQC spectra comparison of the H^{'''}-9 and C^{'''}-9 in sialyltrisaccharides **9N₃-S3** (green/purple) and **S3** (red/blue).

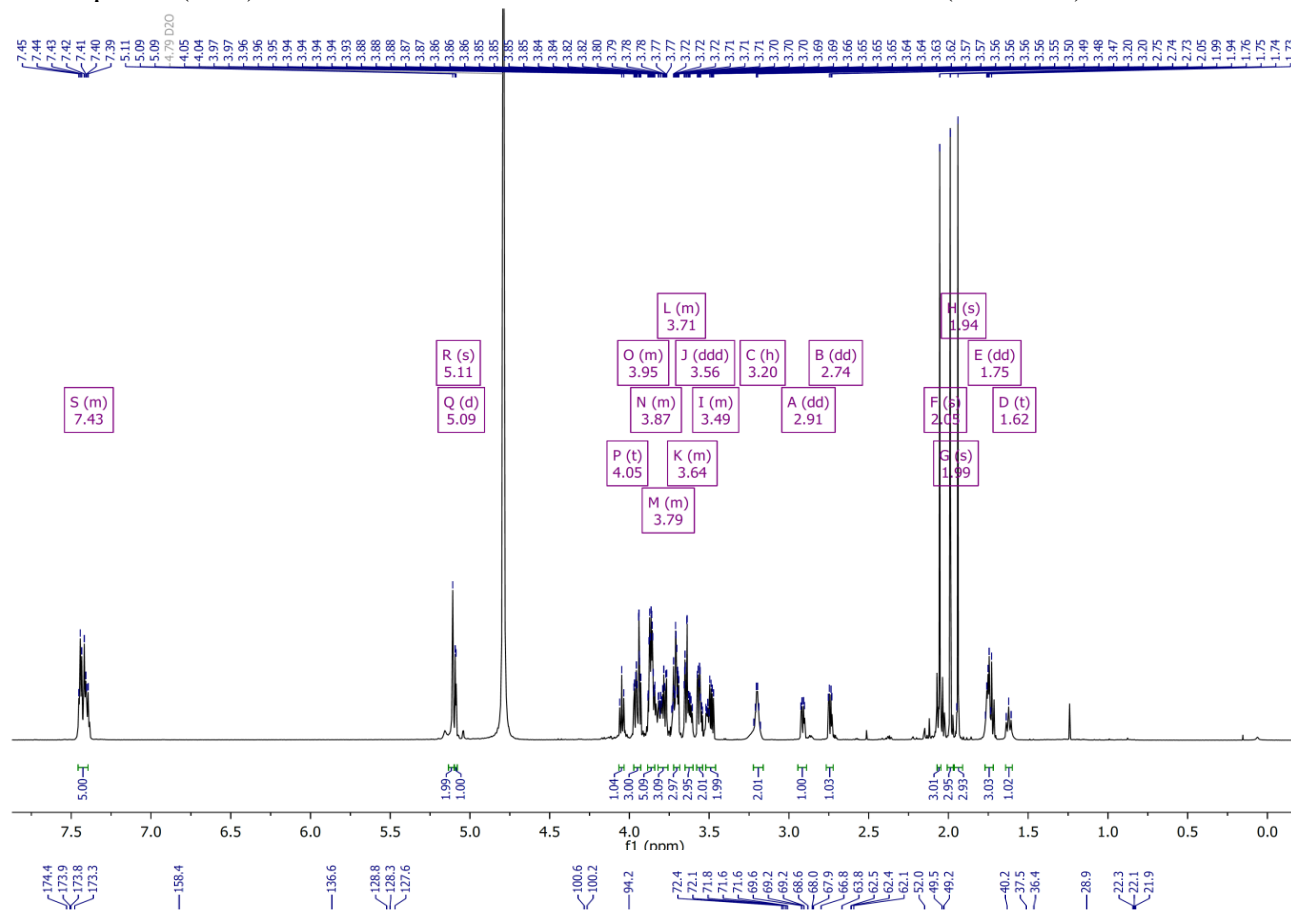
^1H (800 MHz), ^{13}C (200 MHz), HSQC (800 MHz), and HSQC-TOCSY (90 ms and 10 ms, 800 MHz) NMR spectra (D_2O) of Neu5Ac7N α 2-6Gal α 1-4Neu5Ac α ProNHCBz (7N α 3-S3)



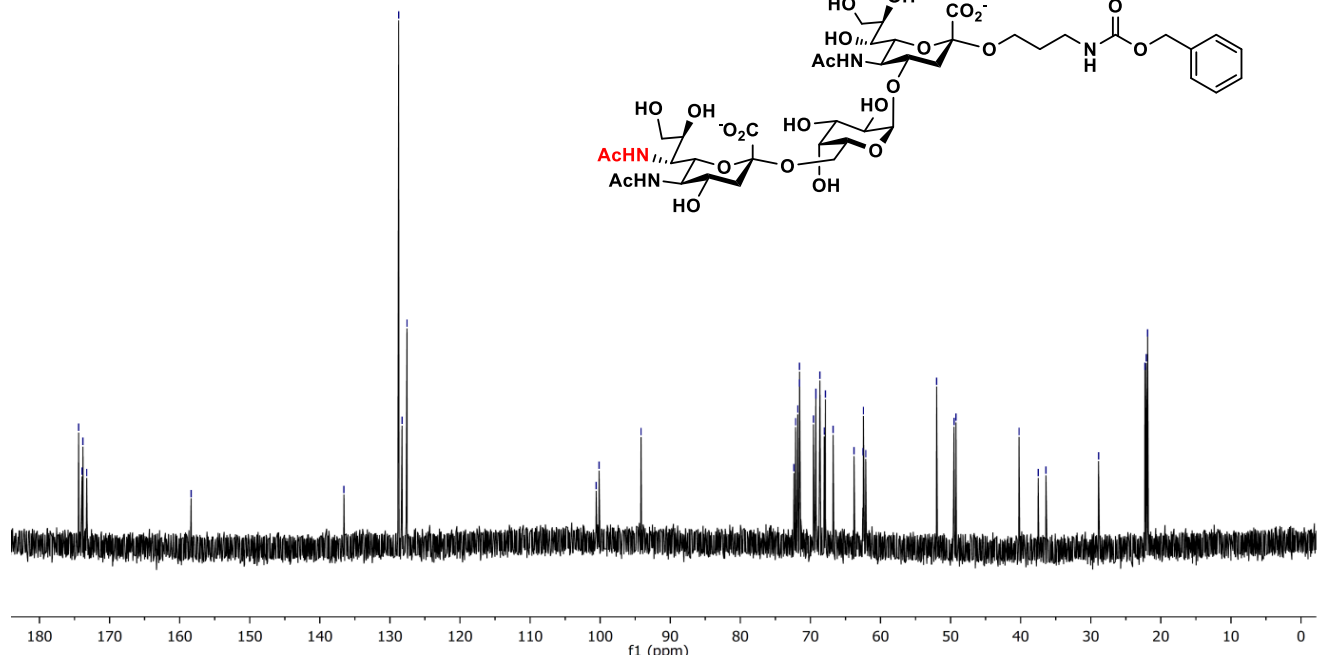
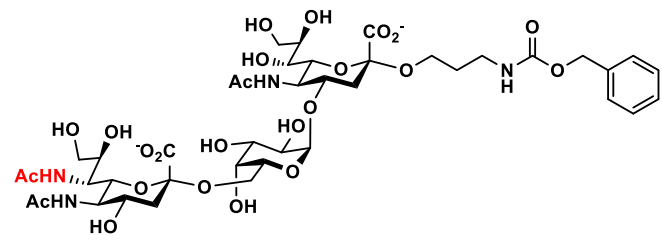


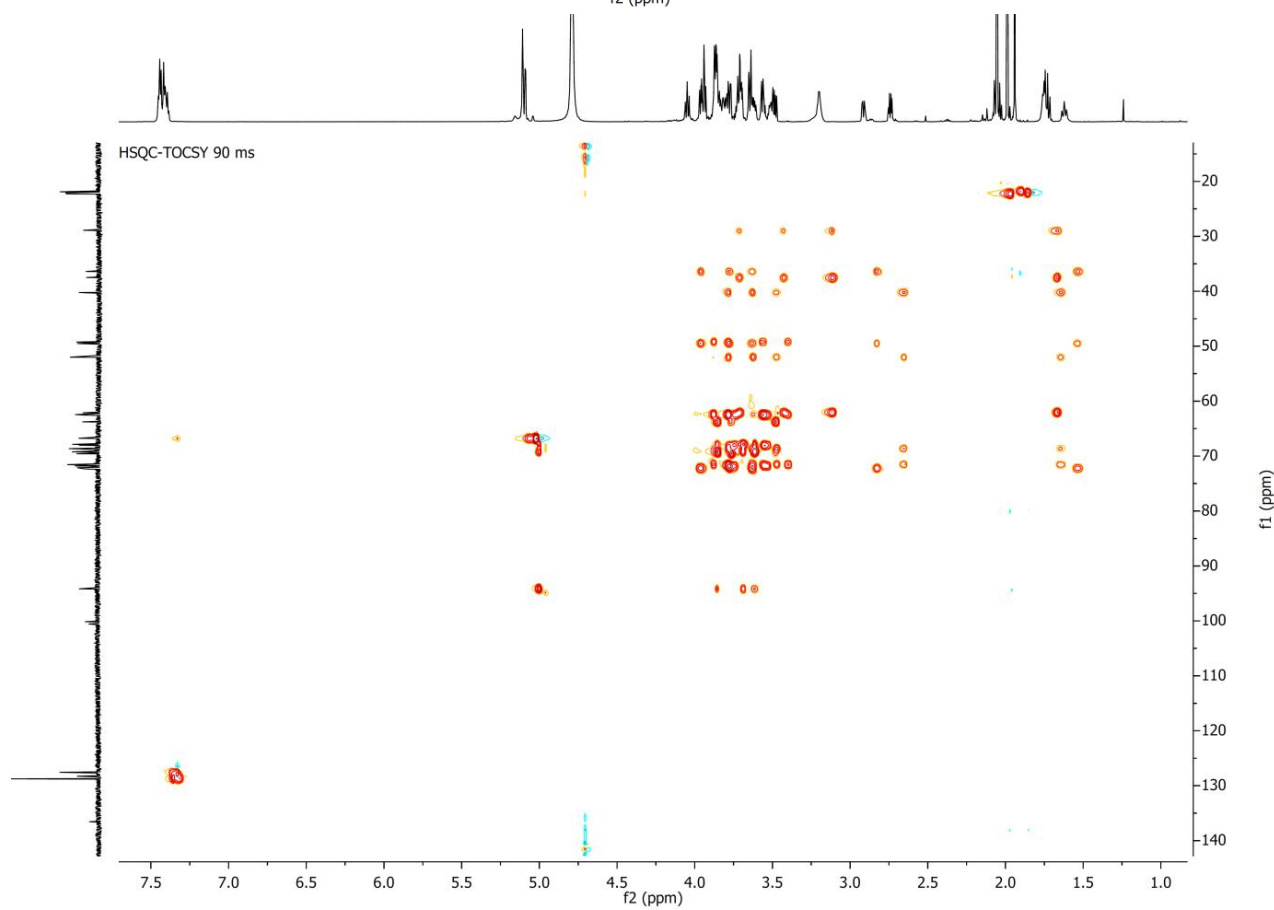
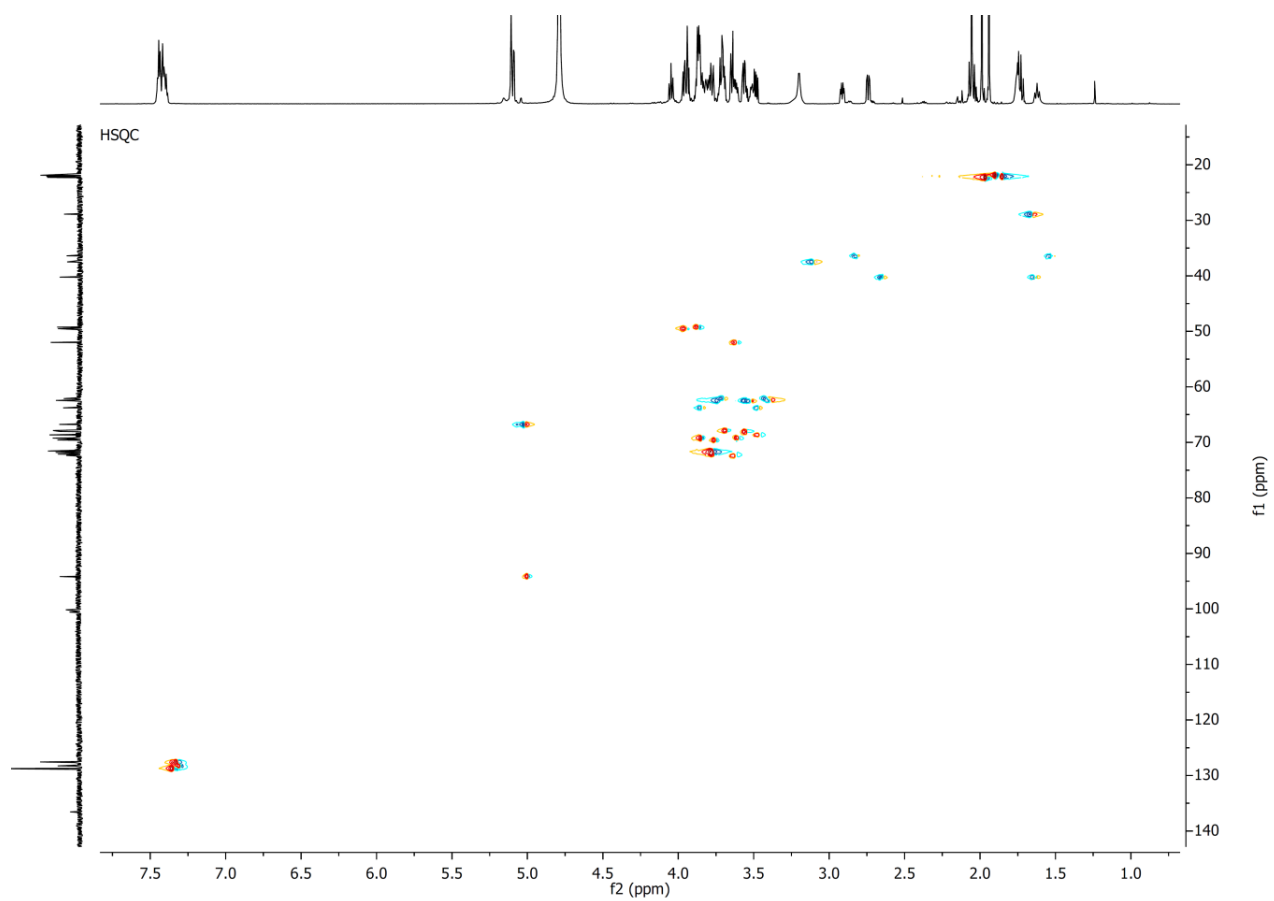


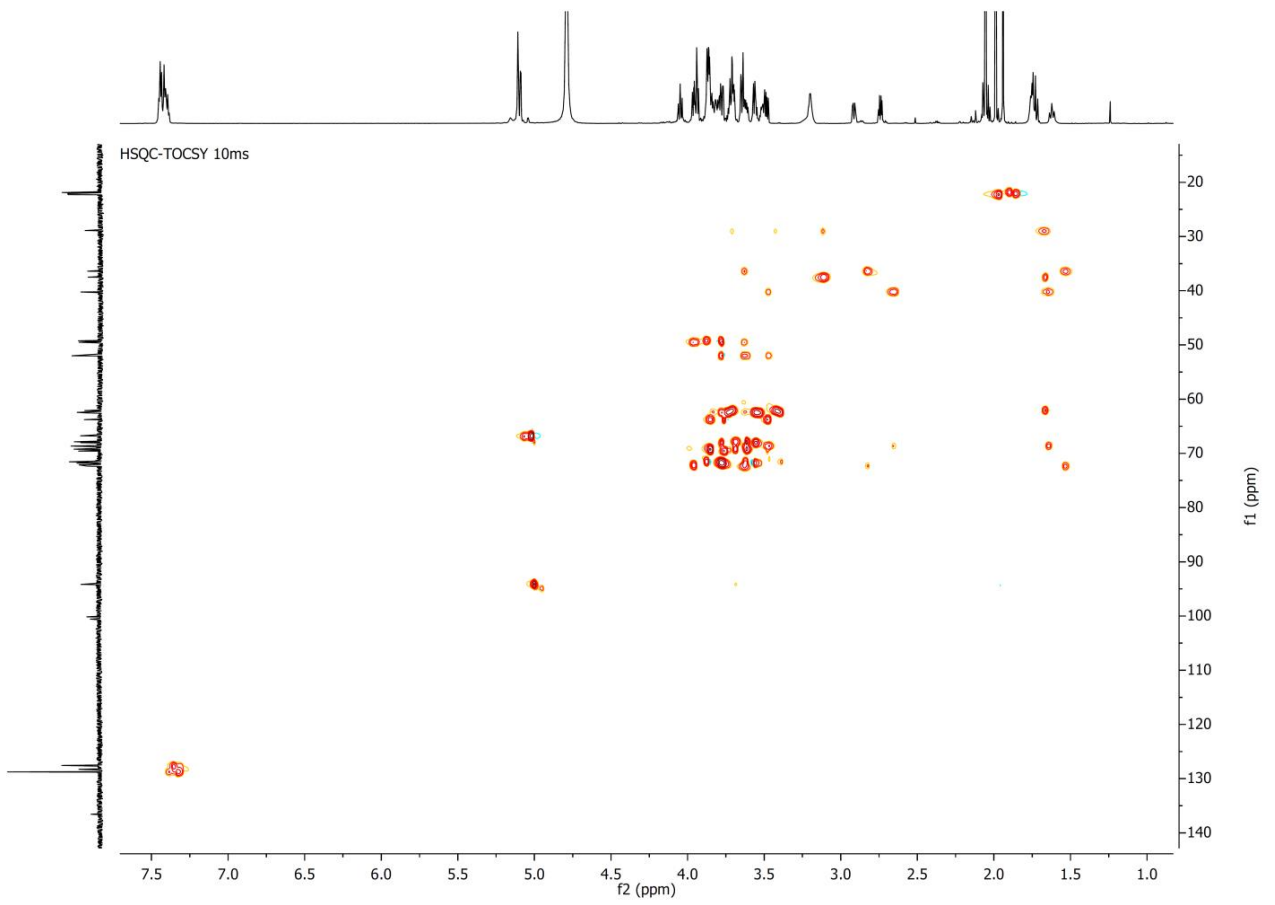
^1H (800 MHz), ^{13}C (200 MHz), HSQC (800 MHz), and HSQC-TOCSY (90 ms and 10 ms, 800 MHz) NMR spectra (D_2O) of Neu5Ac7NAc α 2-6Gal α 1-4Neu5Ac α ProNHcbz (**7NAc-S3**)



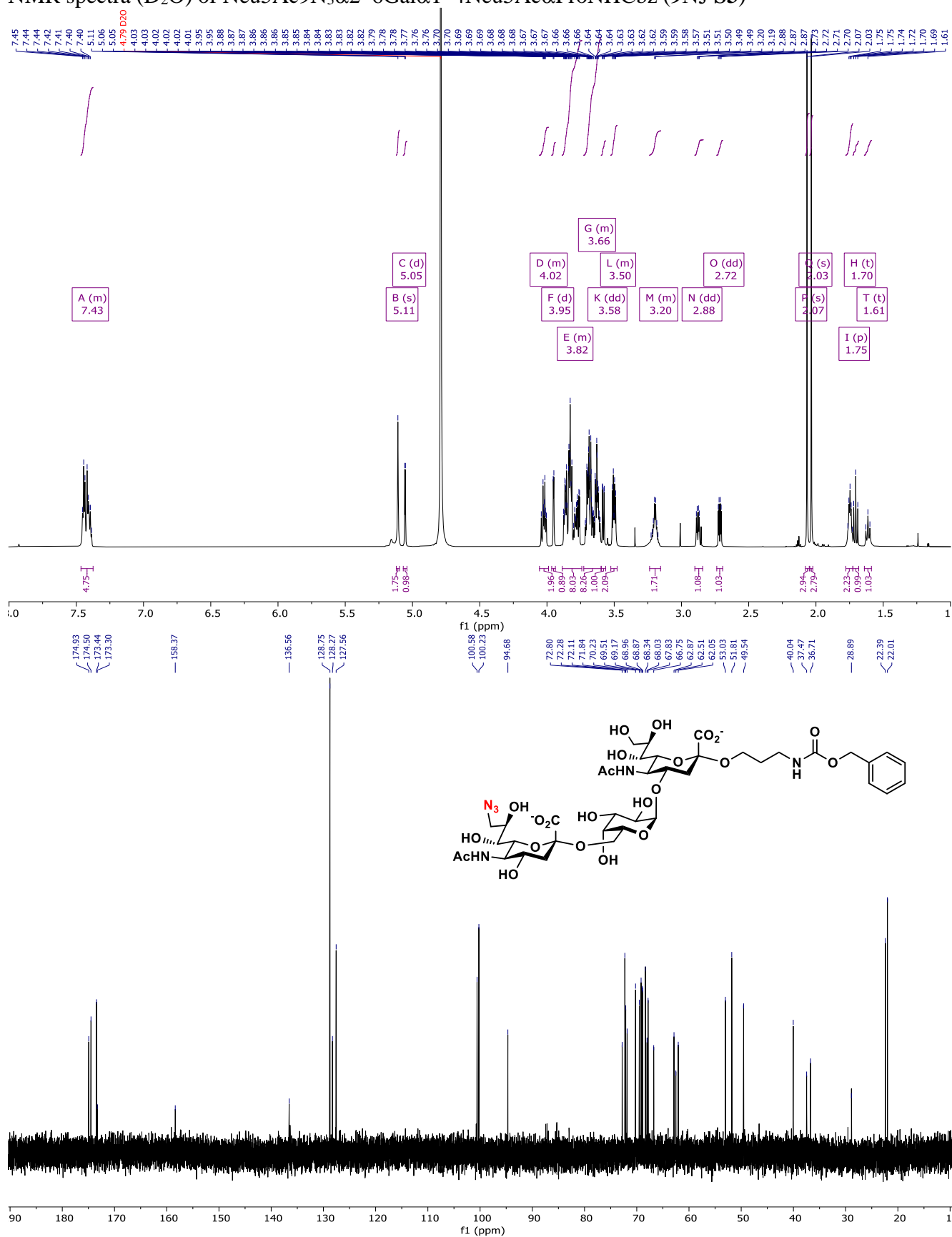
^{13}C NMR spectrum of Neu5Ac7NAc α 2-6Gal α 1-4Neu5Ac α ProNHcbz (**7NAc-S3**) in D_2O . The x-axis is chemical shift in ppm (f1) from 0 to 180. The spectrum shows several peaks with labels: 174.4, 173.9, 173.8, 173.3, 158.4, 136.6, 128.8, 128.2, 127.8, 100.6, 100.2, 94.2, 72.4, 72.1, 71.8, 71.6, 71.6, 69.6, 69.2, 69.2, 68.6, 68.0, 66.8, 62.5, 62.4, 62.1, 49.5, 49.2, 40.2, 37.5, 36.4, 28.9, 22.3, 22.1, 21.9.

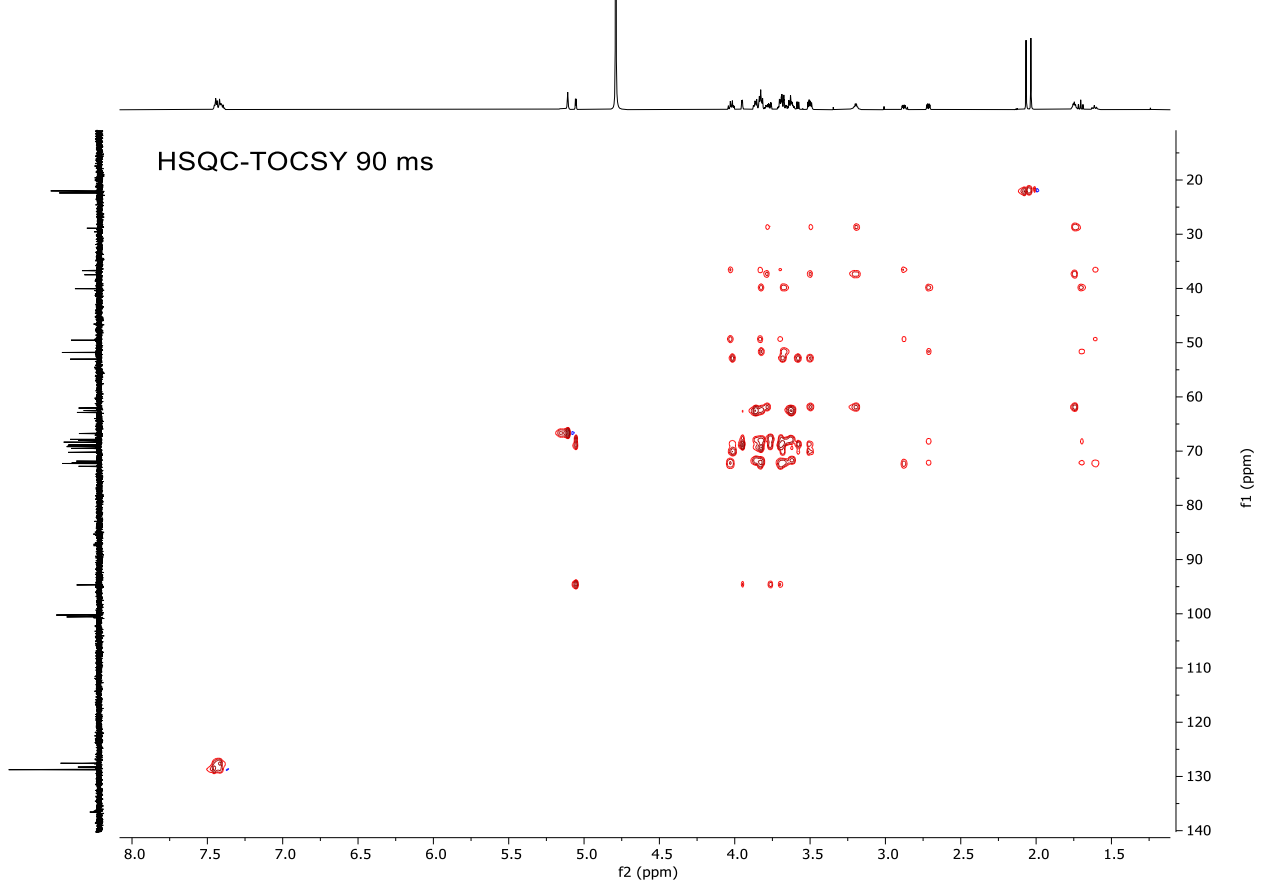
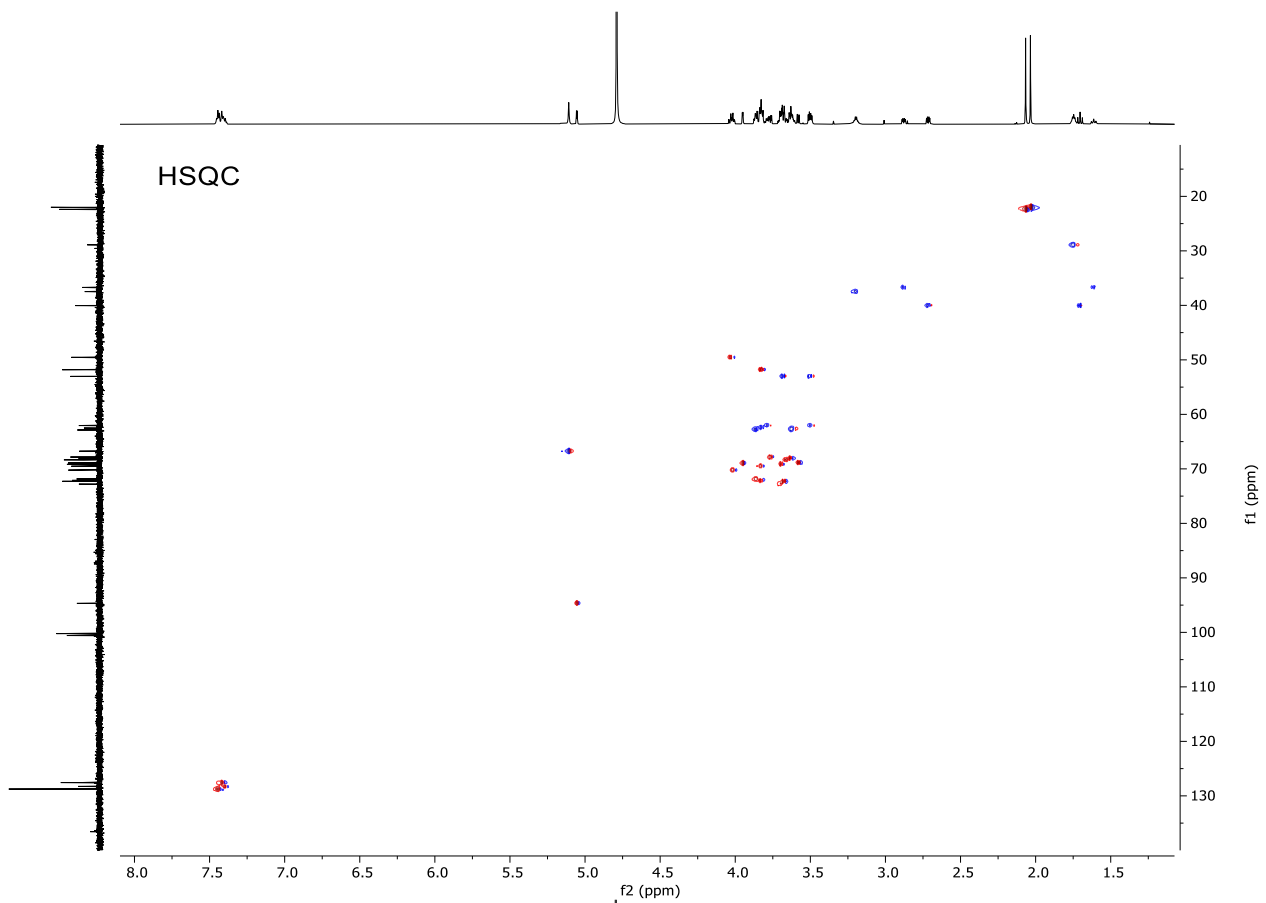


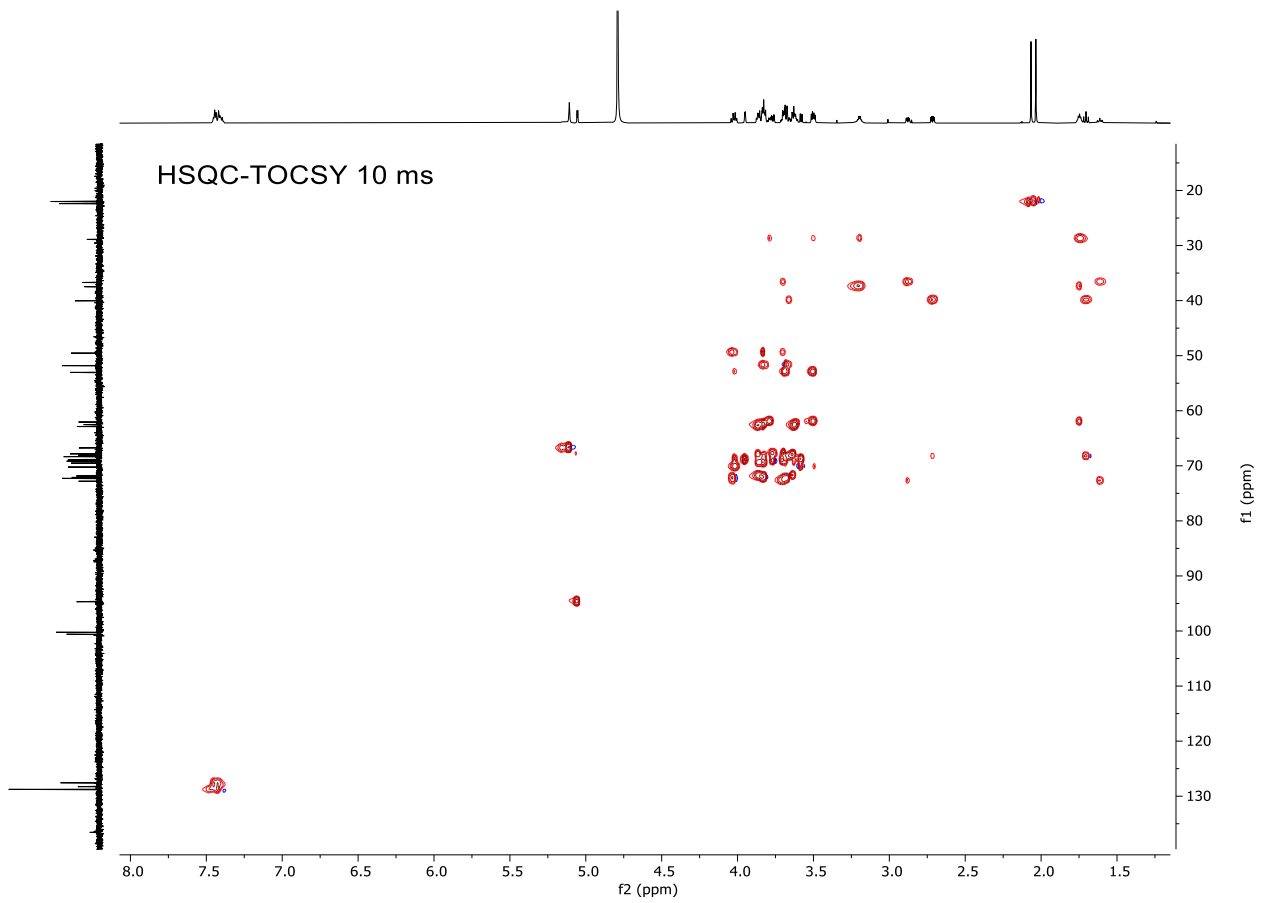




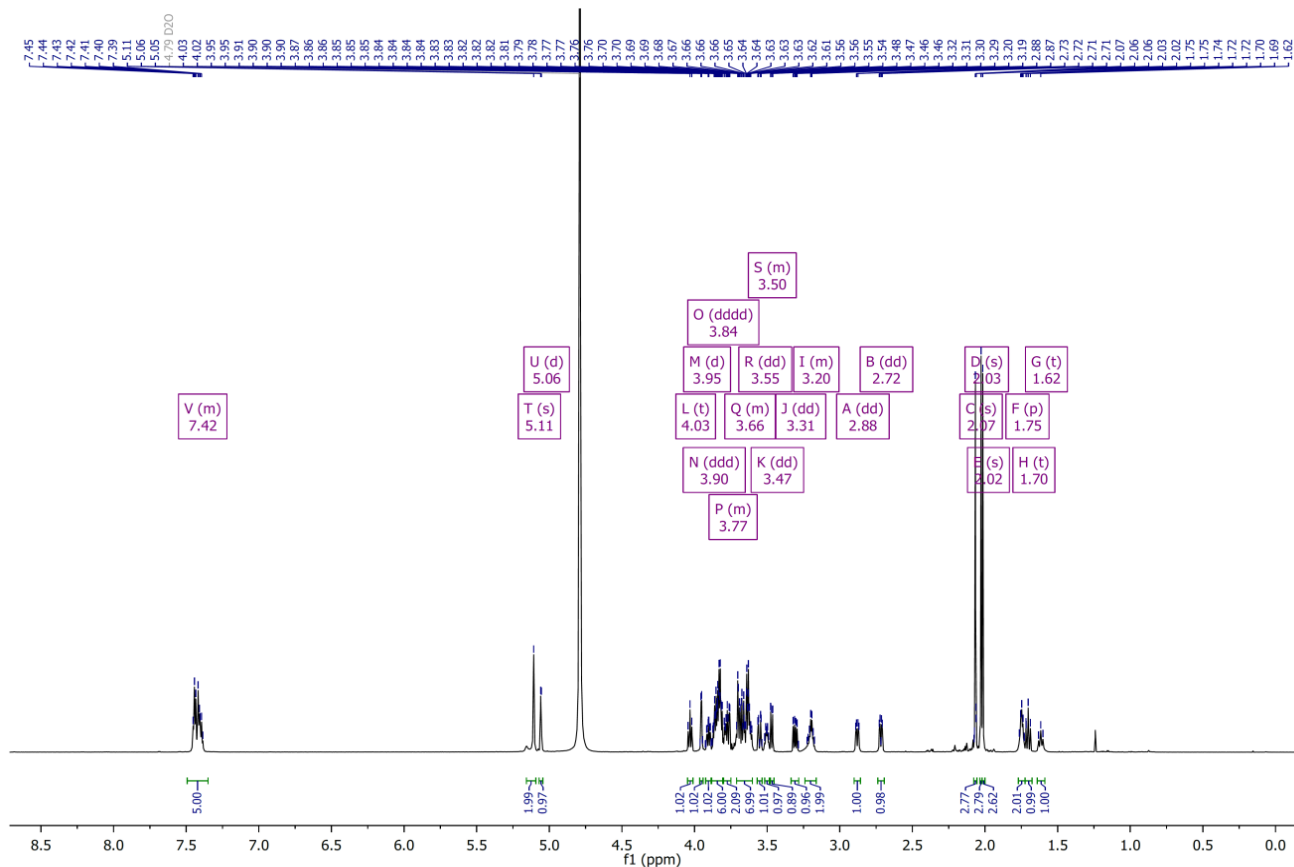
^1H (800 MHz), ^{13}C (200 MHz), HSQC (800 MHz), and HSQC-TOCSY (90 ms and 10 ms, 800 MHz) NMR spectra (D_2O) of Neu5Ac α Neu3 α 2-6Gal α 1-4Neu5Ac α ProNHCBz (**9N₃-S3**)







^1H (800 MHz), ^{13}C (200 MHz), HSQC (800 MHz), and HSQC-TOCSY (90 ms and 10 ms, 800 MHz) NMR spectra (D_2O) of Neu5Ac9NAc α 2-6Gal α 1-4Neu5Ac α ProNHcbz (**9NAc-S3**)



174.9
174.3
174.4
173.5

158.4

136.1
128.8
128.3
127.6

100.3

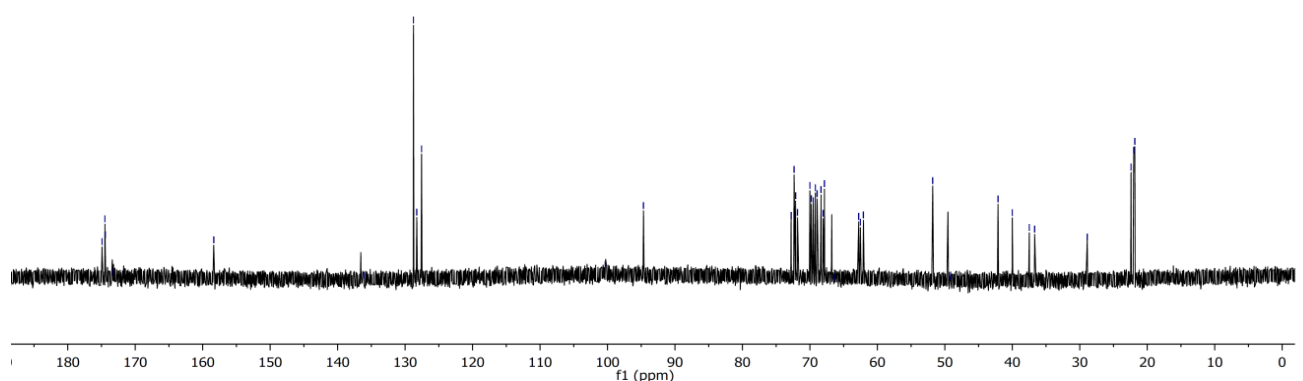
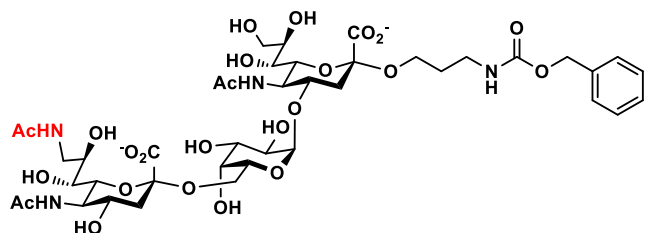
94.7

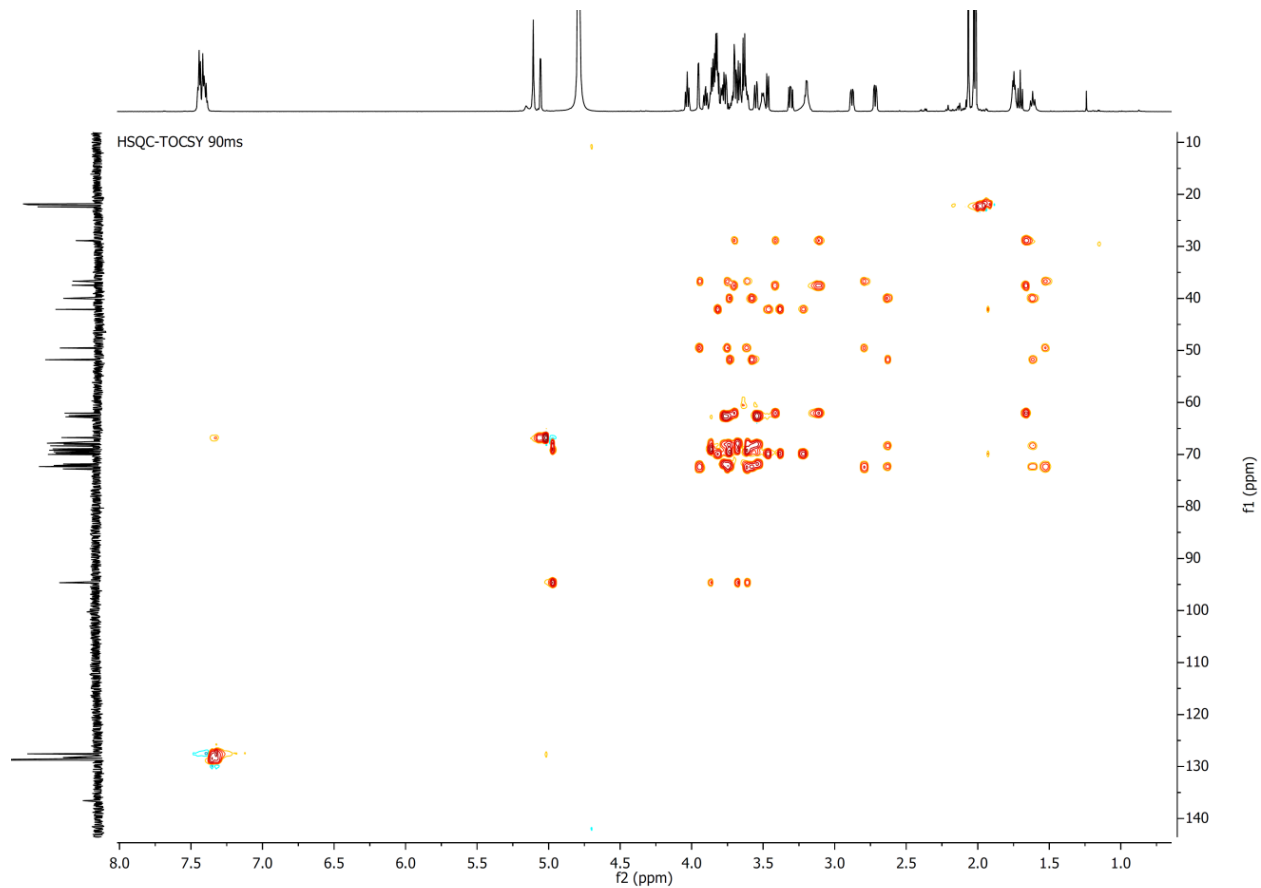
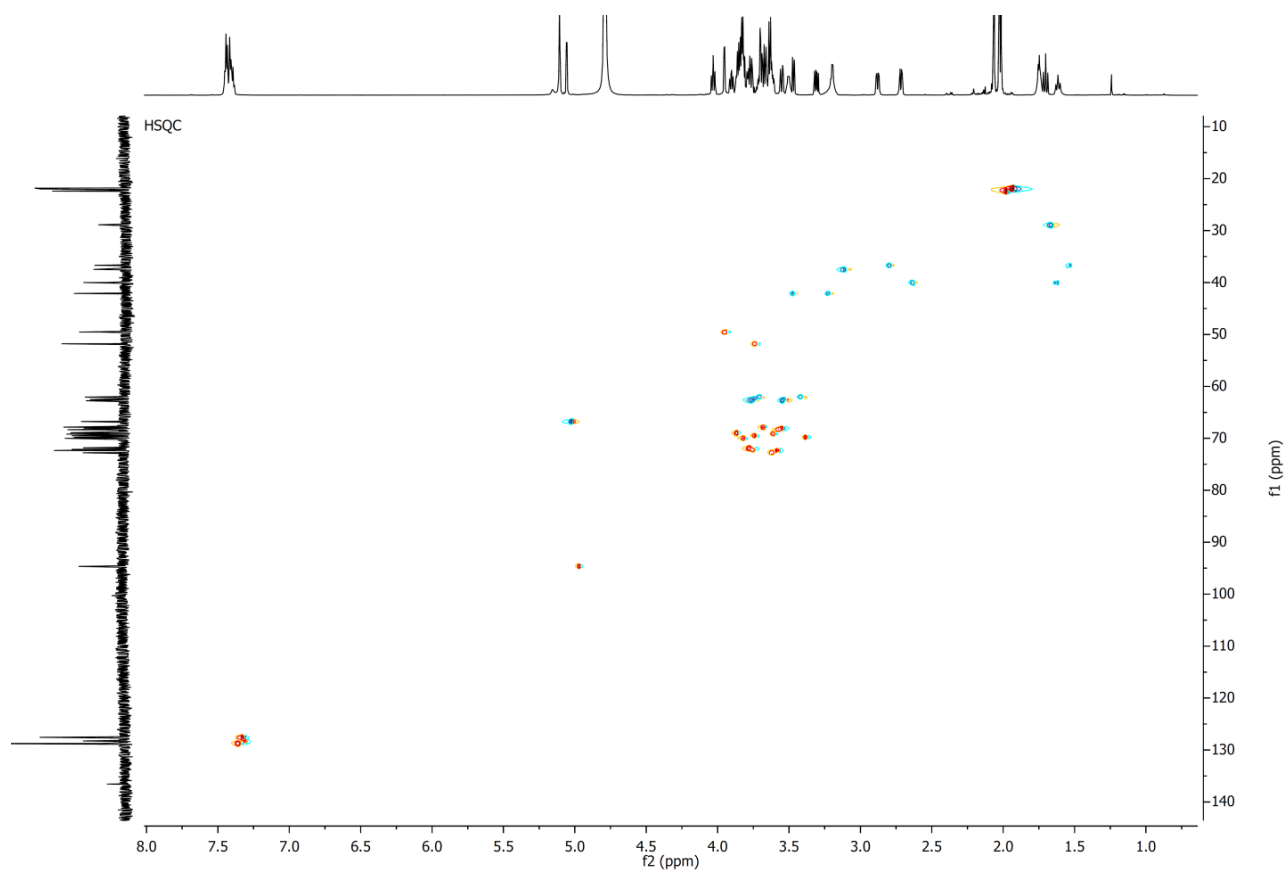
72.8
72.1
72.1
71.8
70.0
69.8
69.5
69.2
68.9
68.3
68.3
67.8
66.4
62.8
62.5
62.1
51.8
49.1

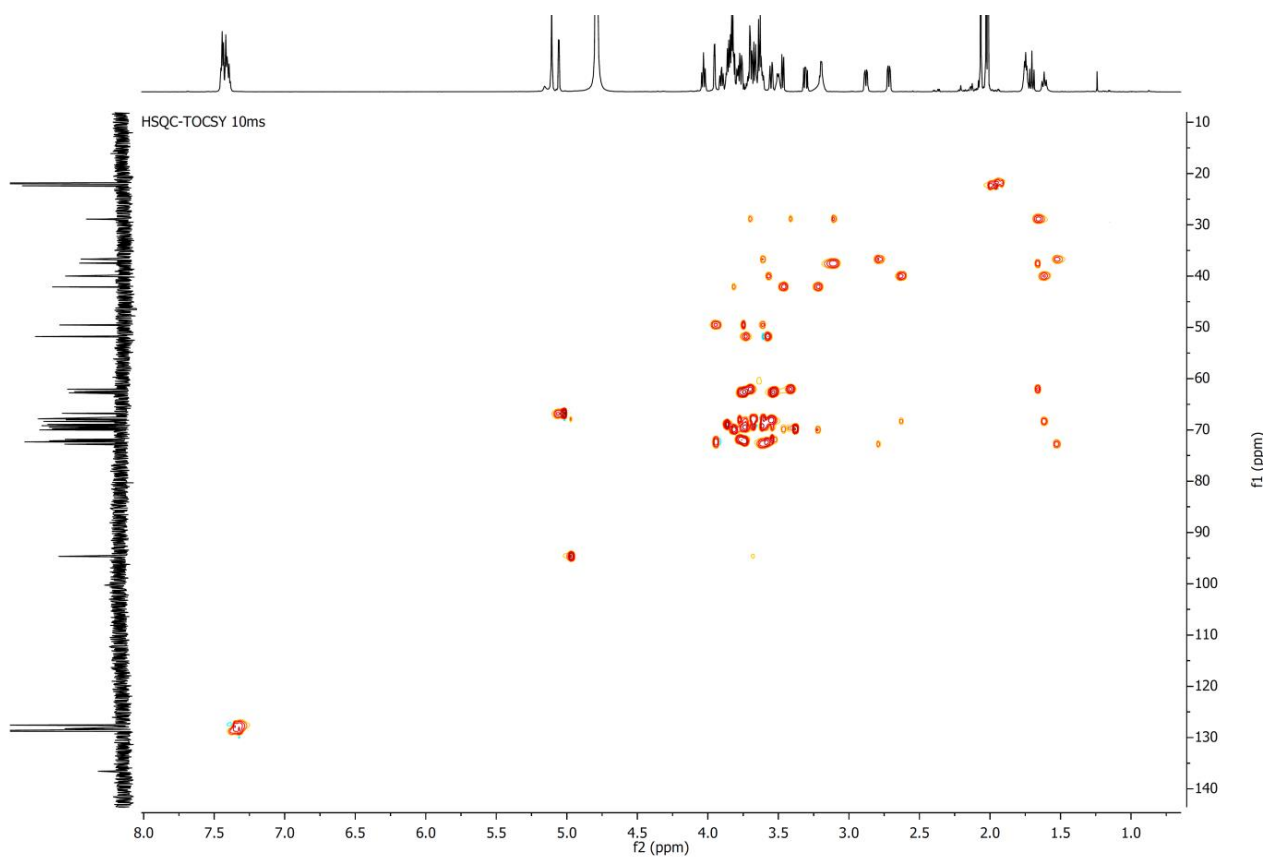
43.1
40.0
37.5
36.7

28.9

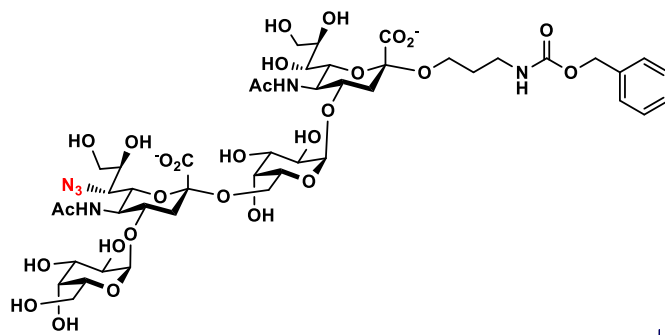
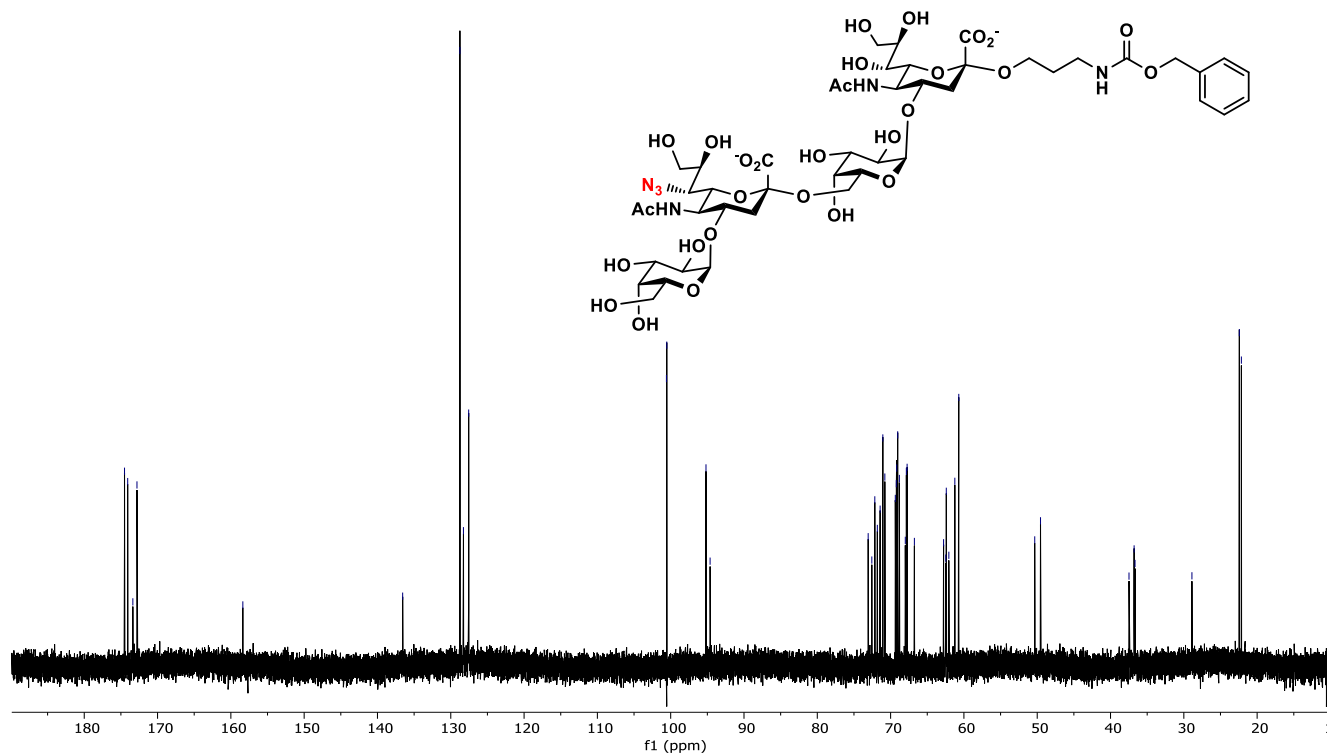
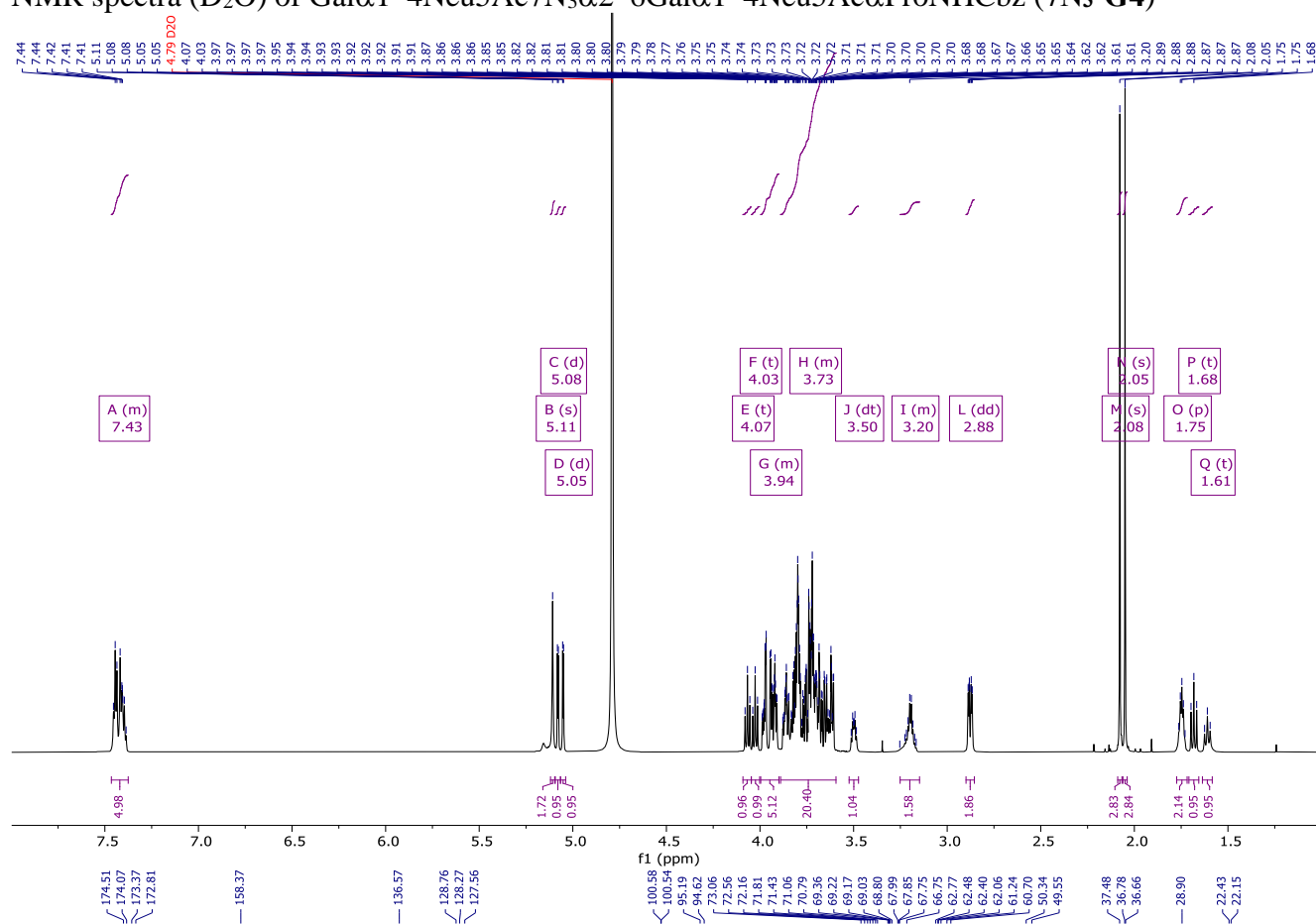
22.4
22.0
21.8

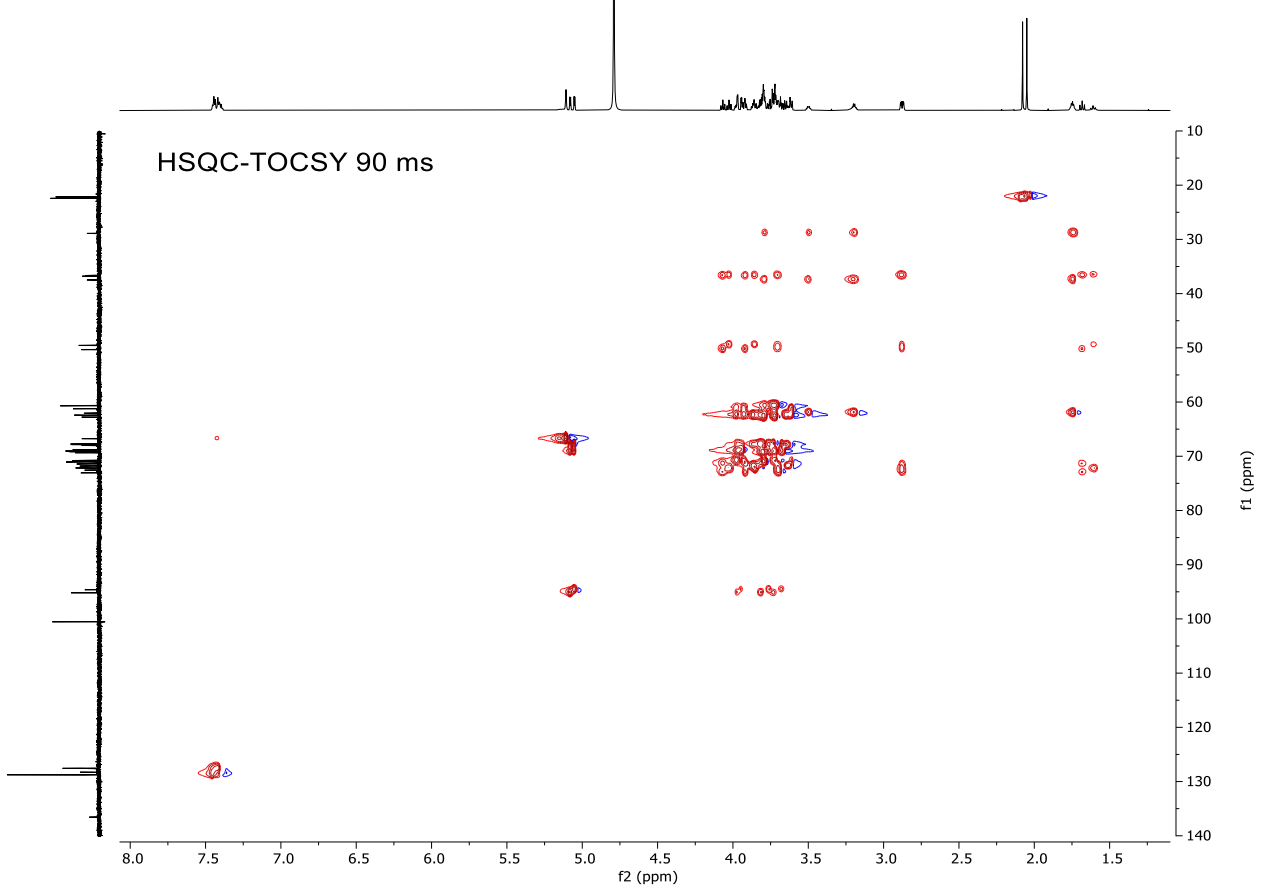
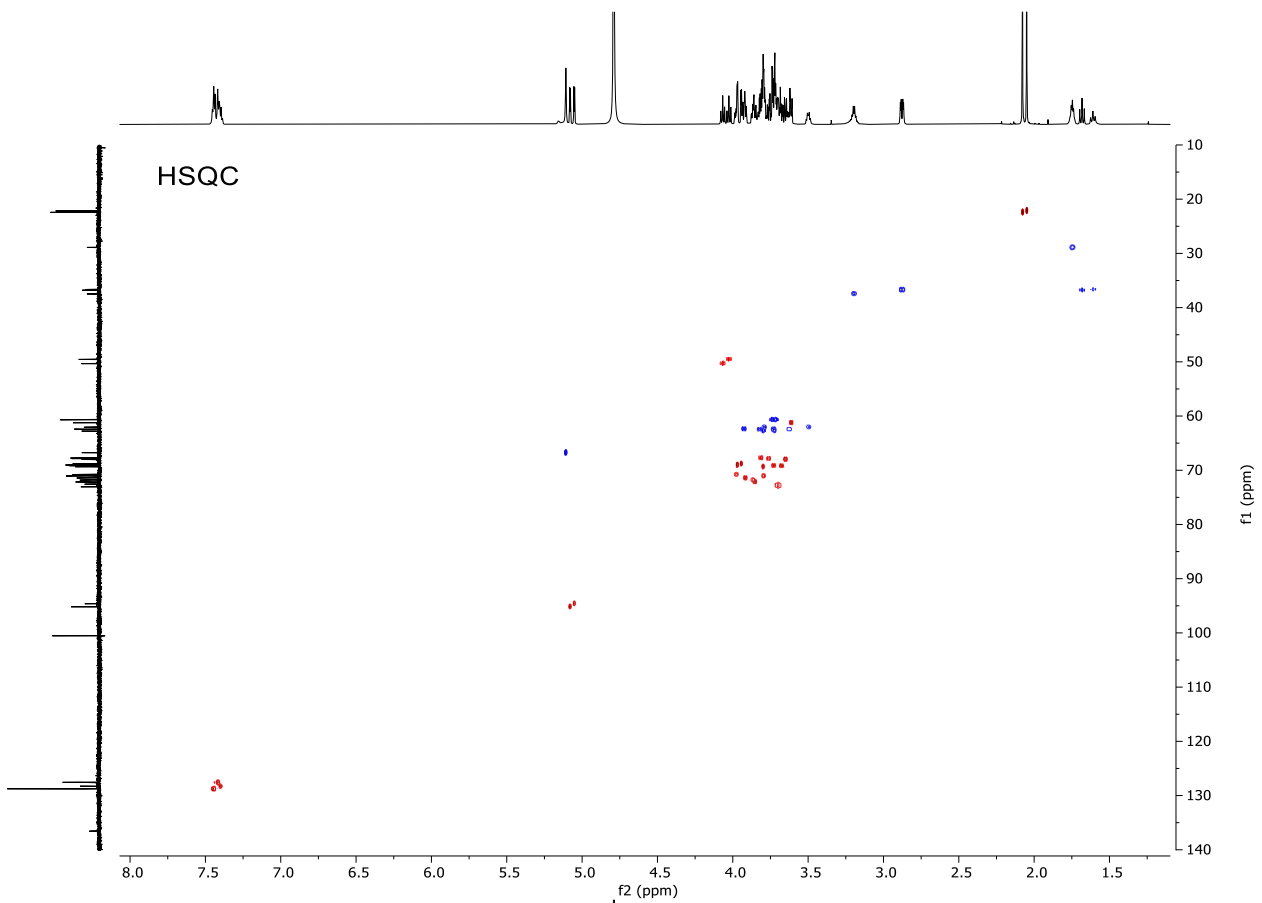


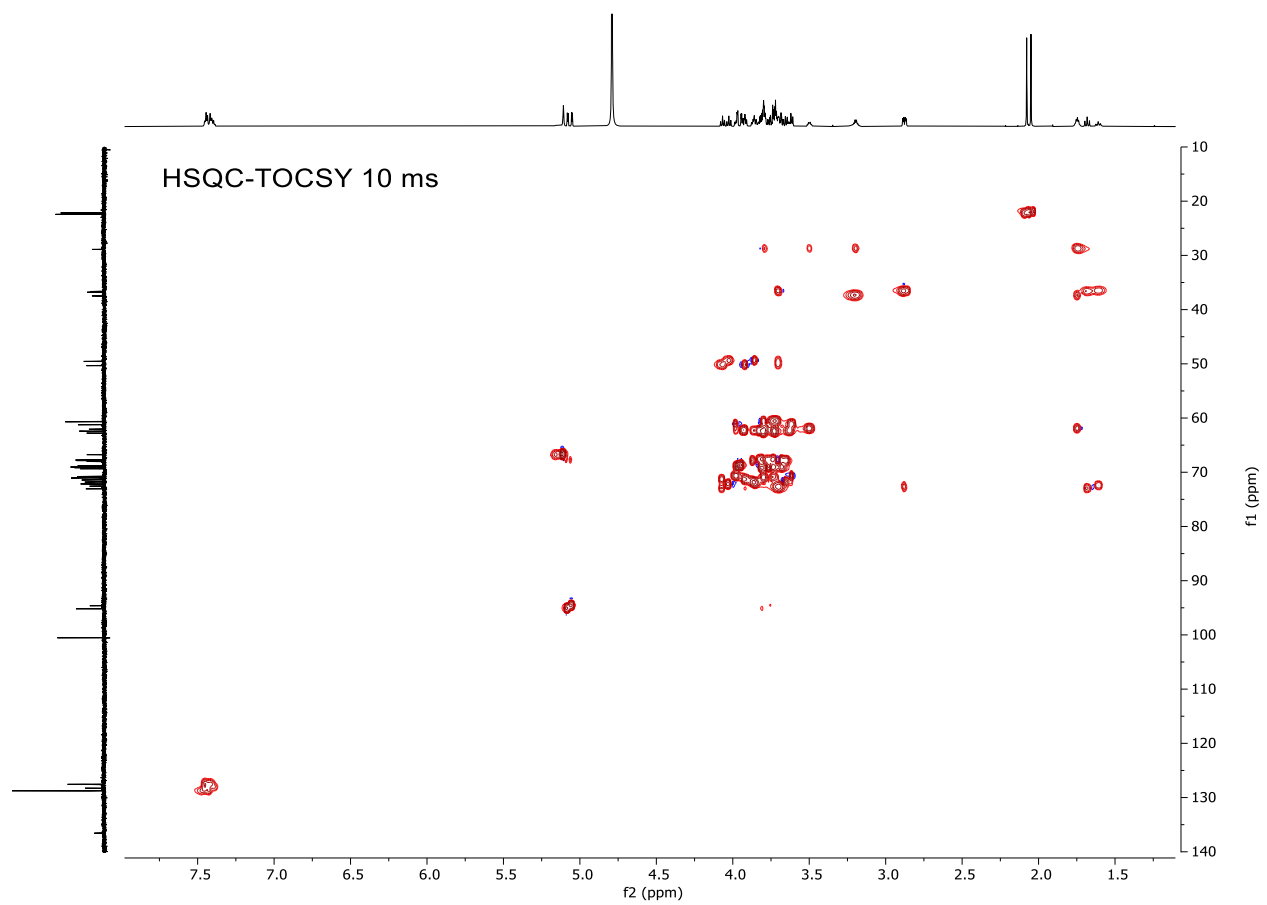




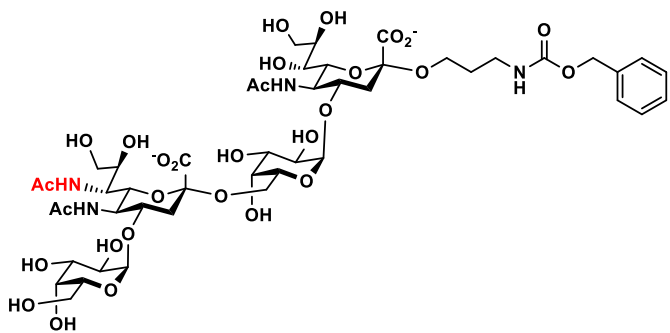
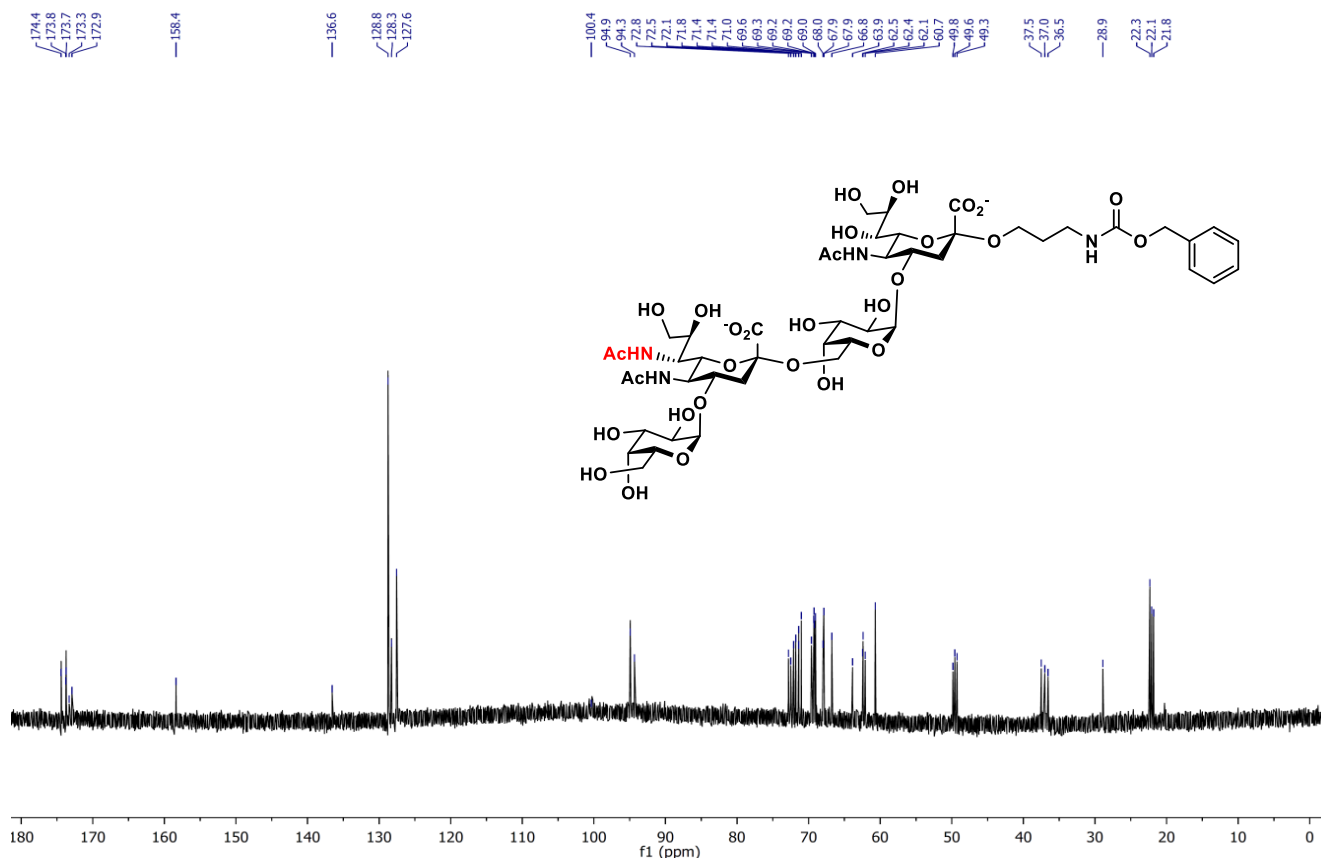
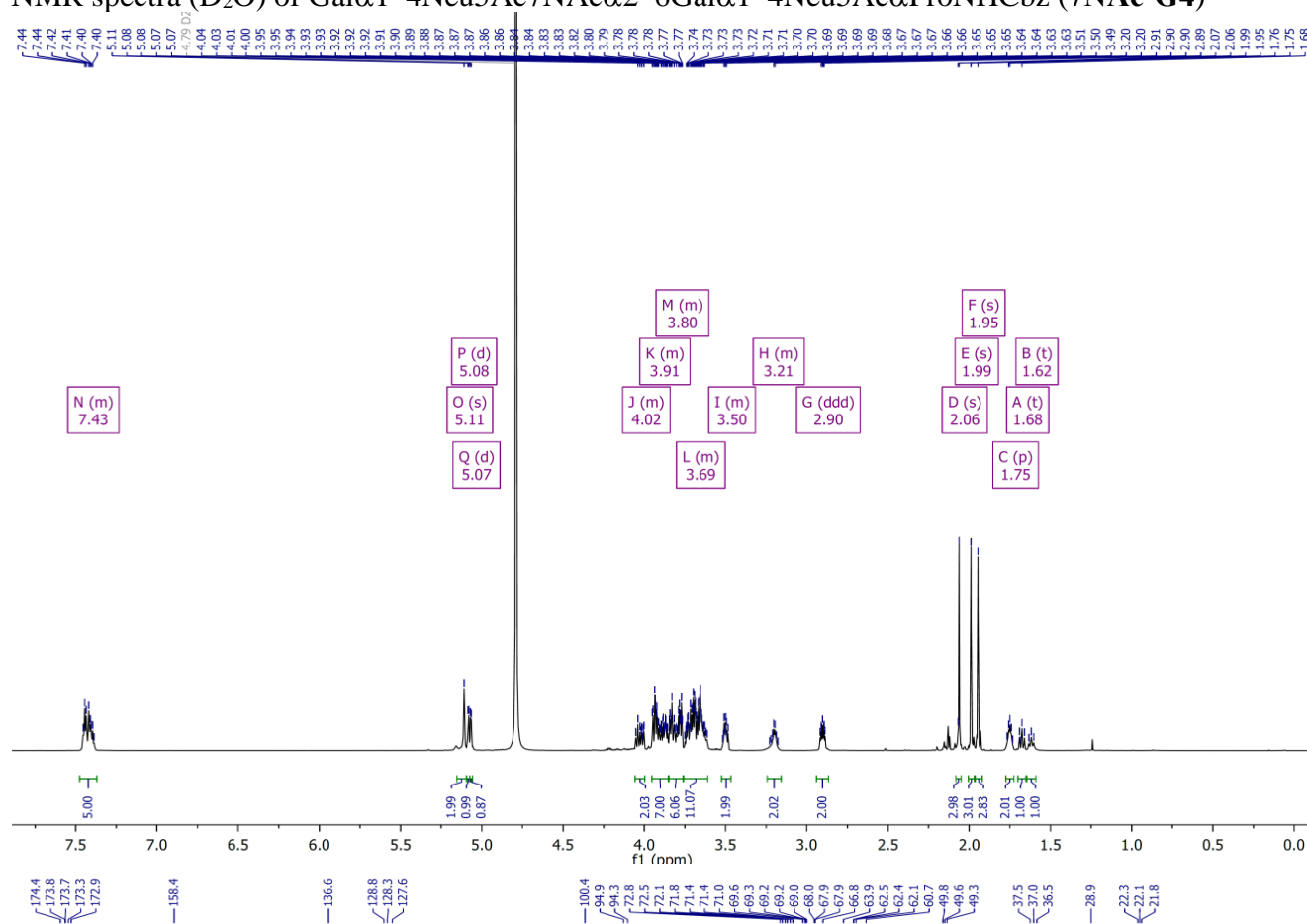
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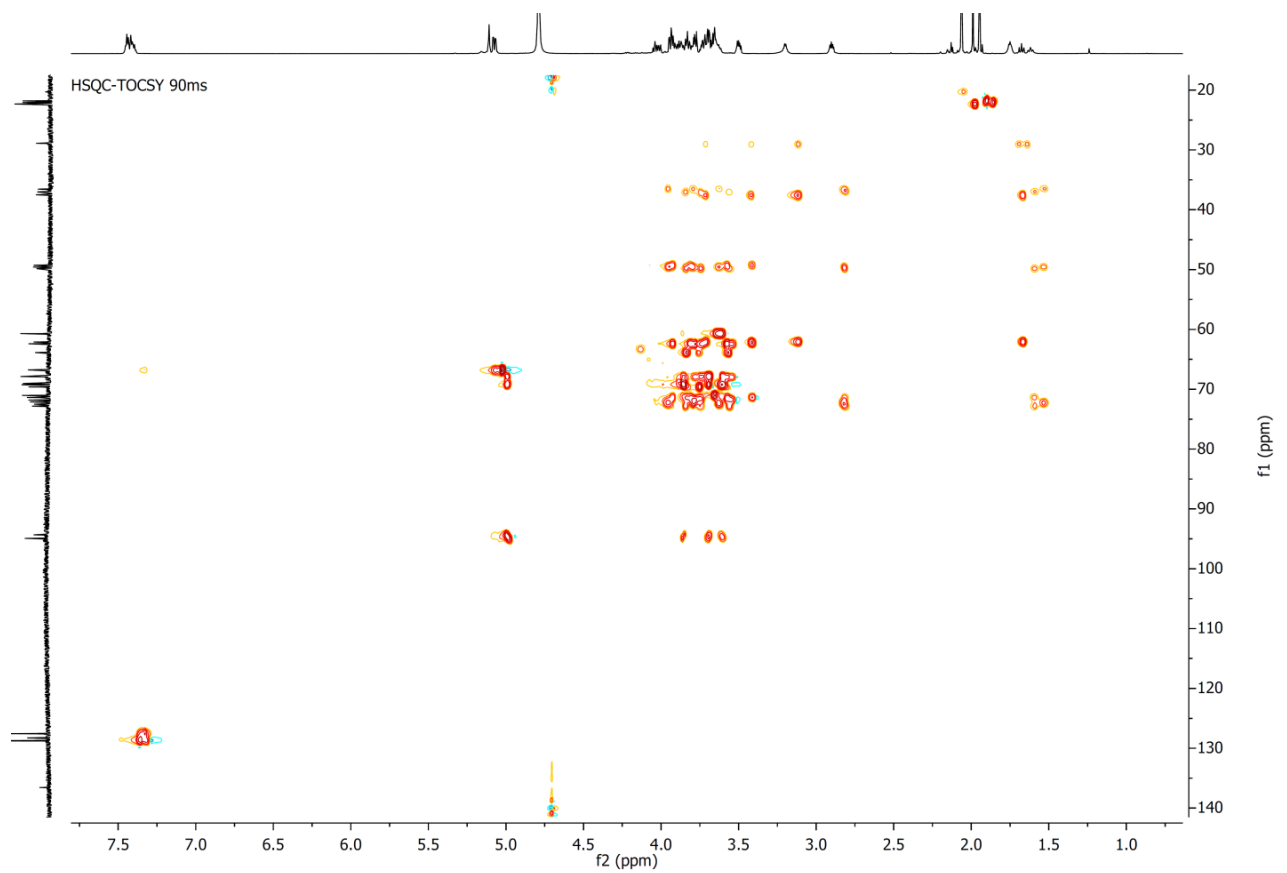
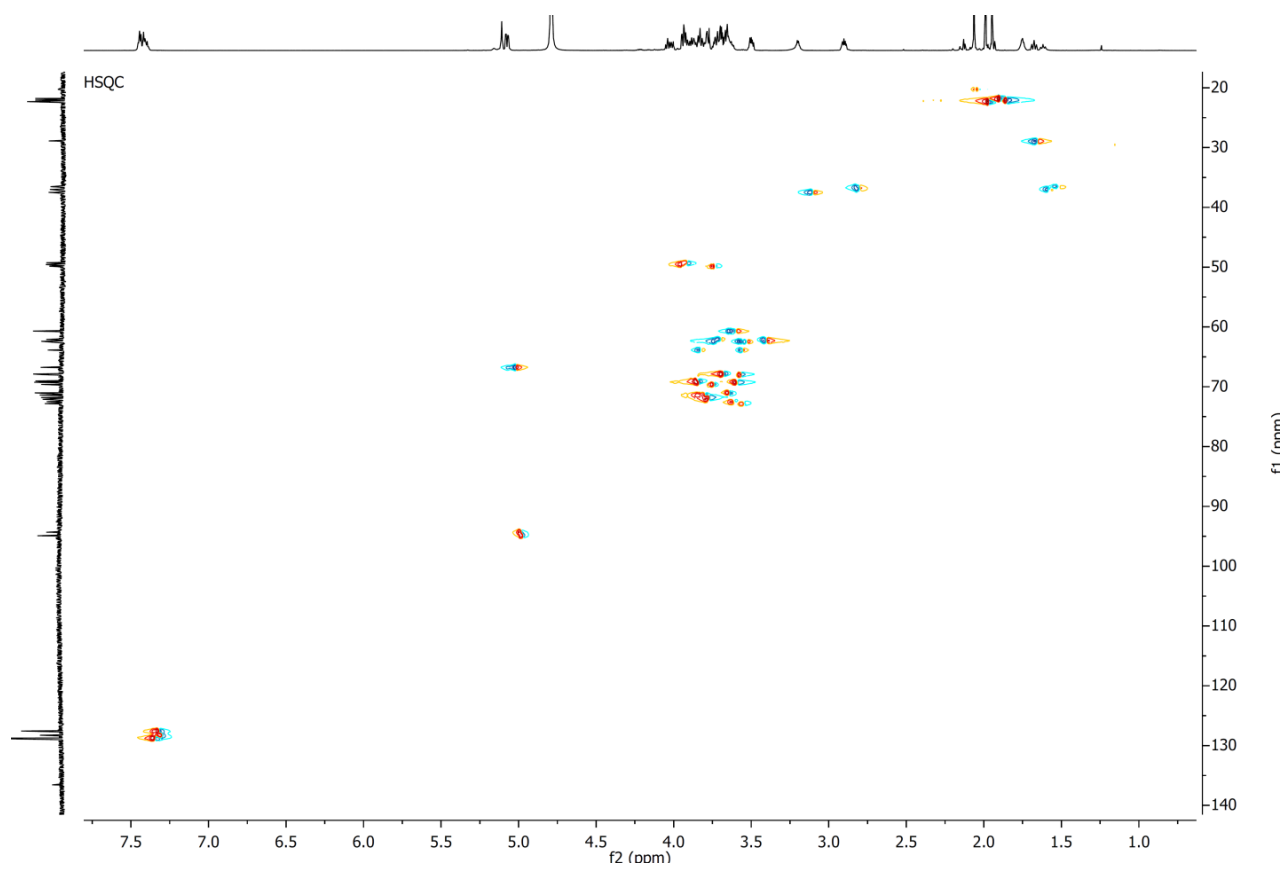


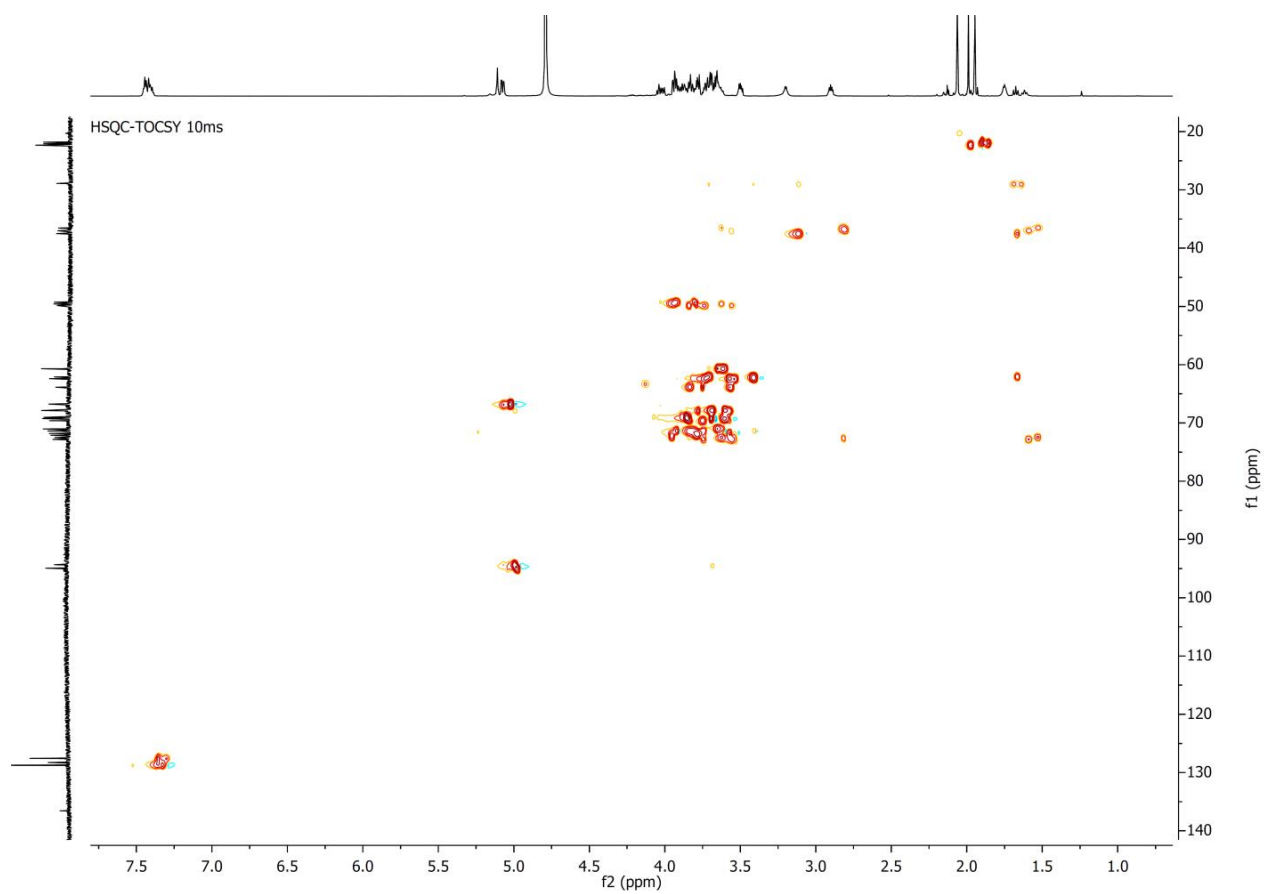




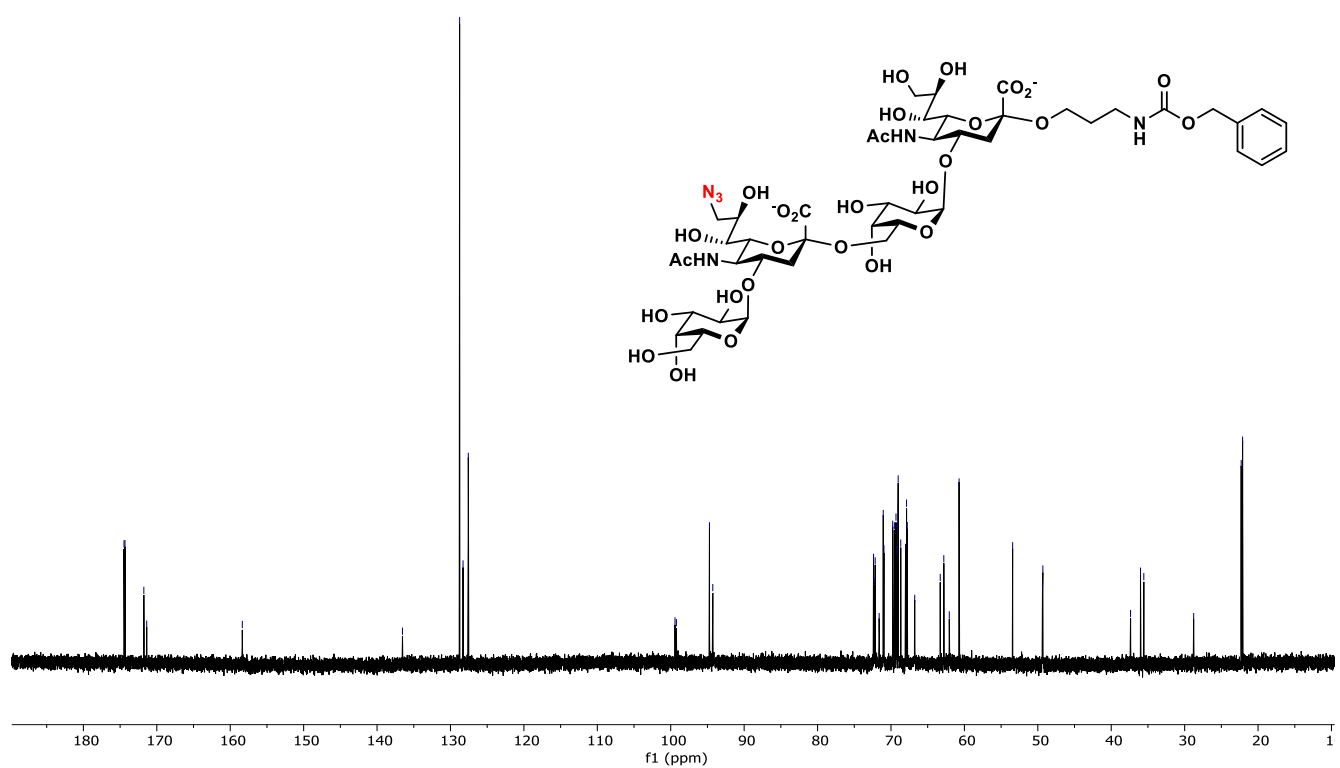
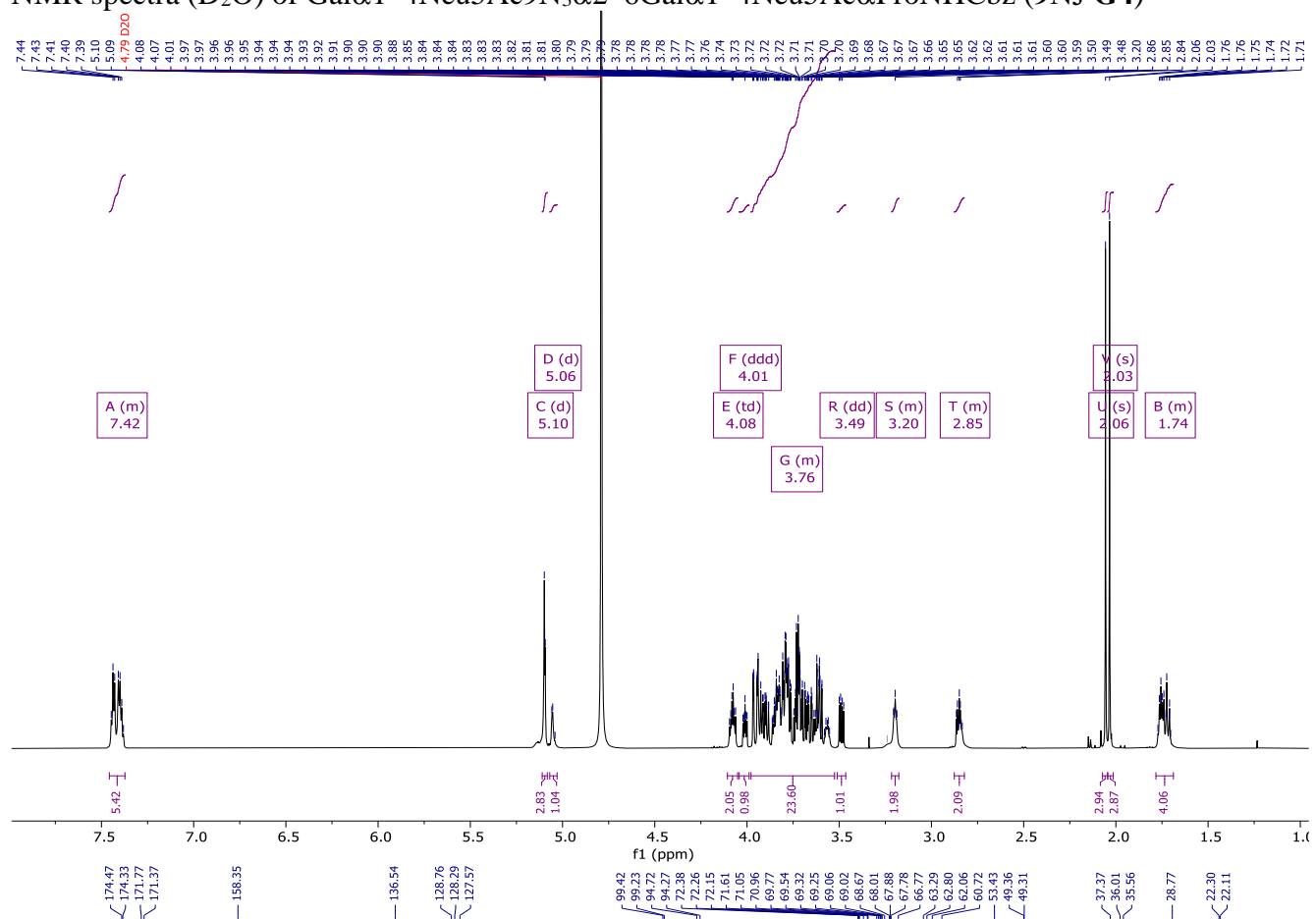
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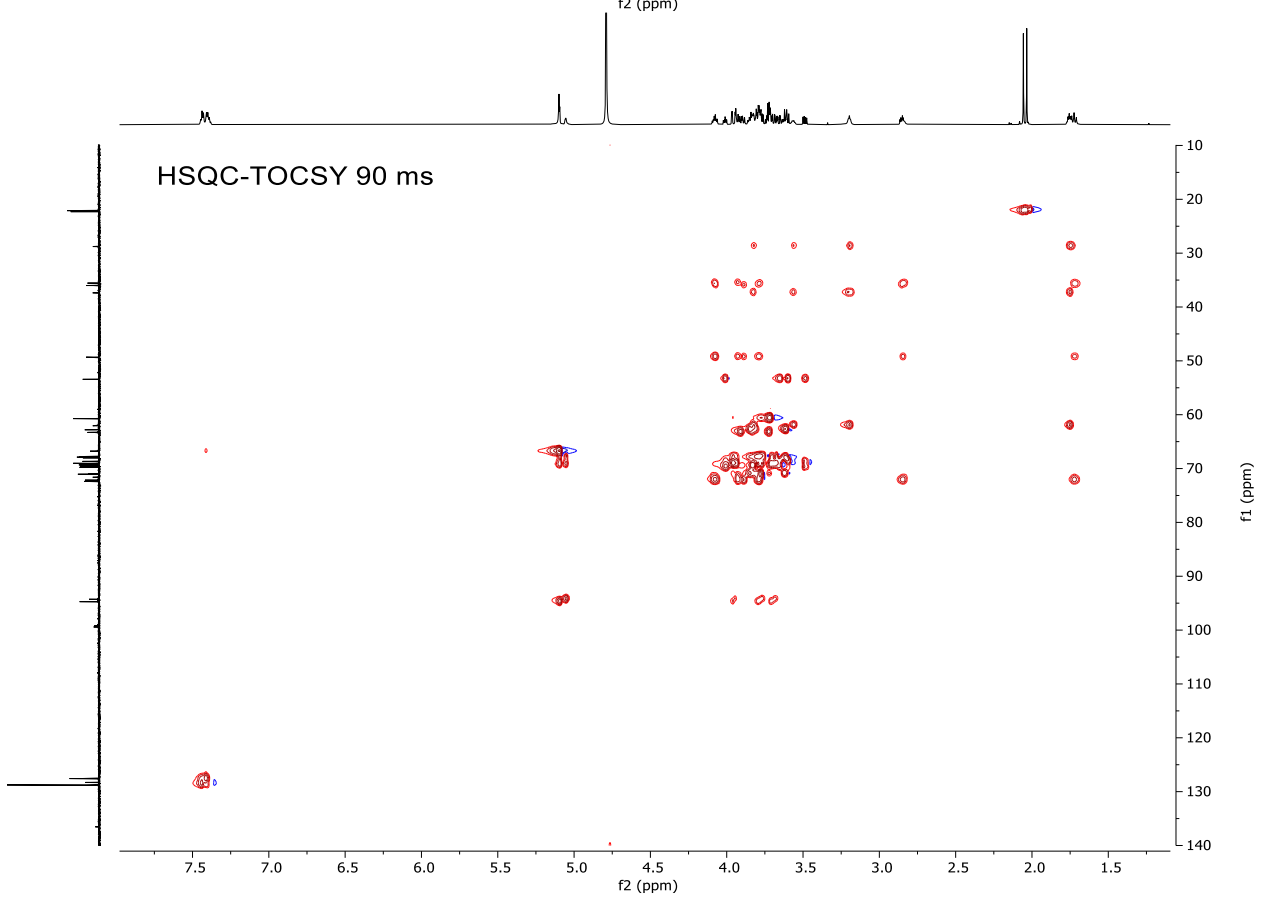
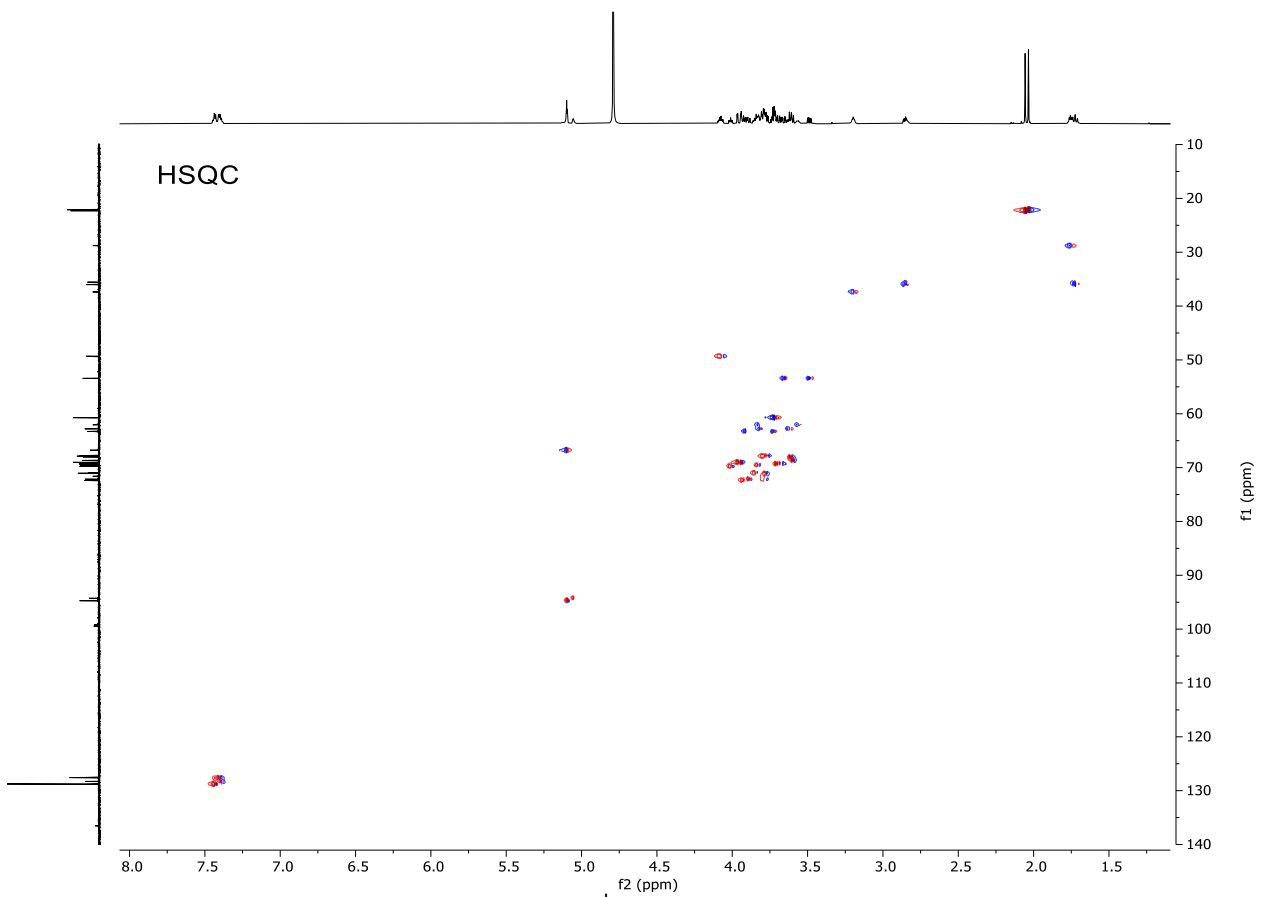


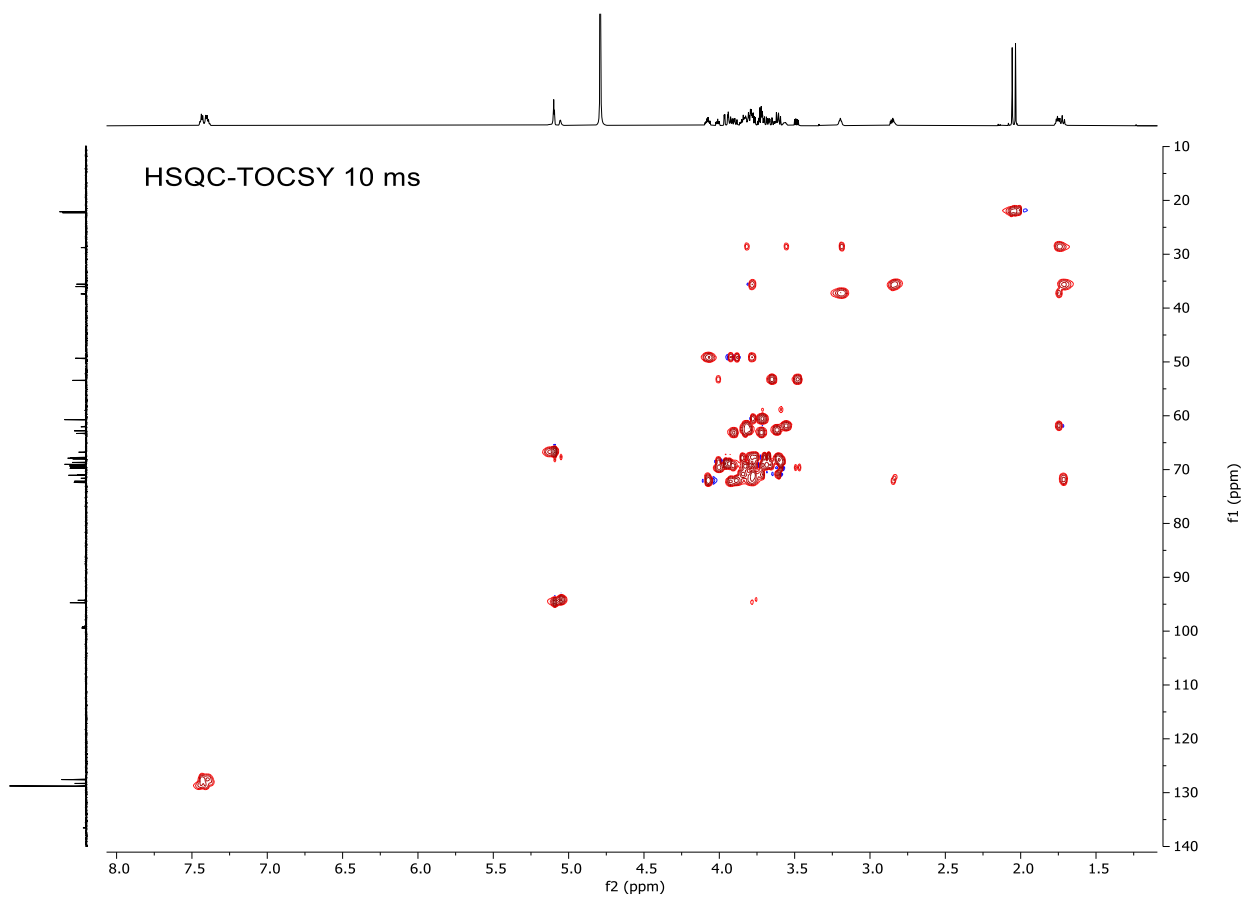




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