Supplementary Information

Synthesis of a Multivalent α-1,2-Mannobiose Ligand for Targeting C-type Lectins

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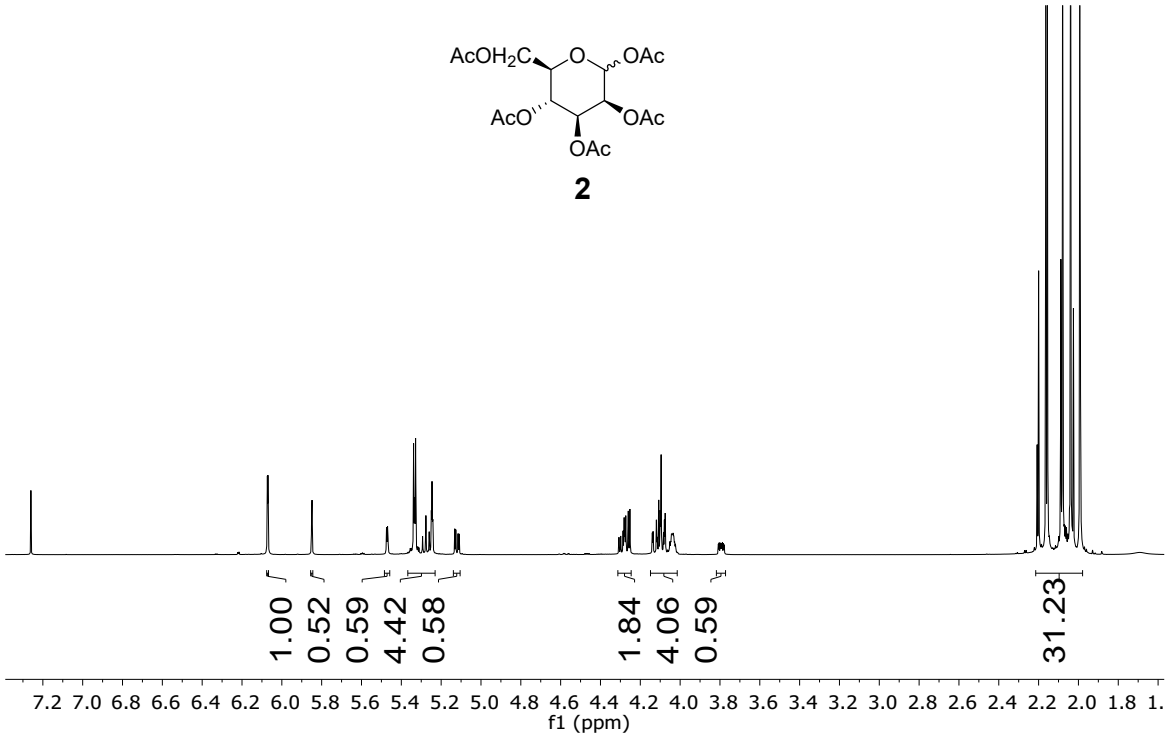

Figure 1: *^{1}H NMR ($CDCl_3$, 600MHz) of structure **2**.*

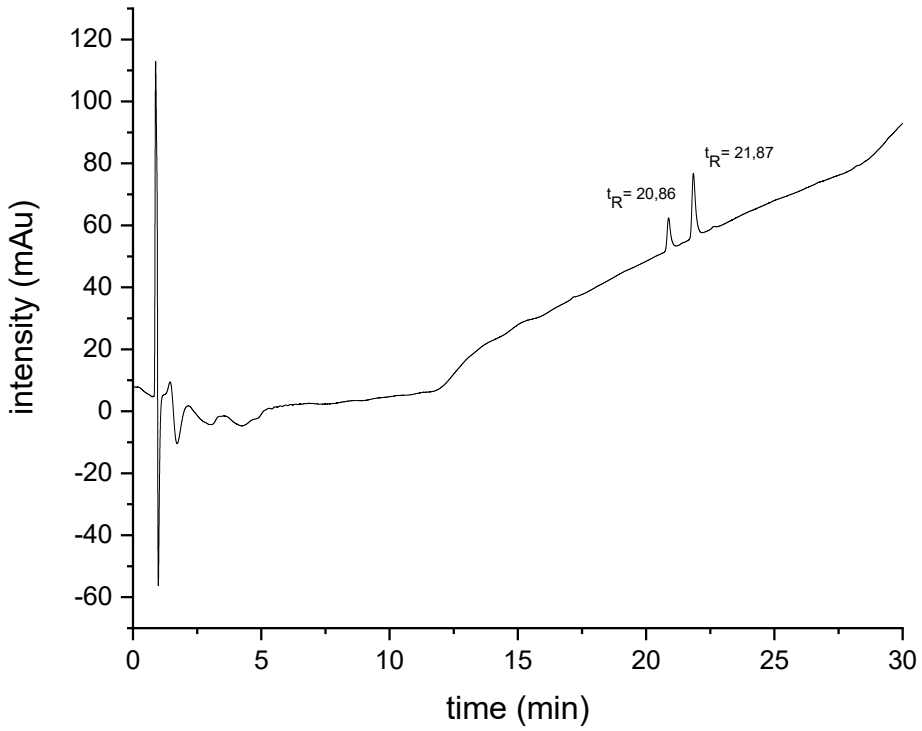

Figure 2: *RP HPLC chromatogram (linear gradient 0-50 Vol% MeCN in H_2O in 30 min at 25 °C) of structure **2**.*

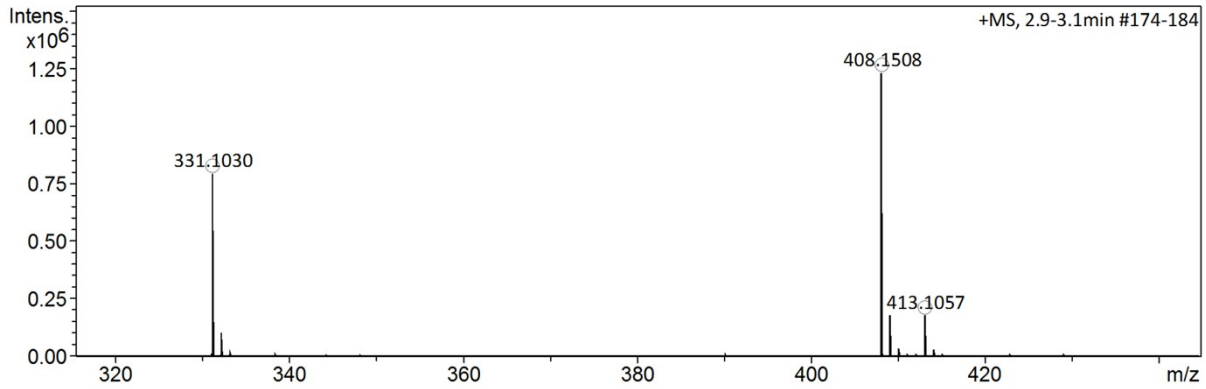

Figure 3: *HR MS of structure* ***2****.*

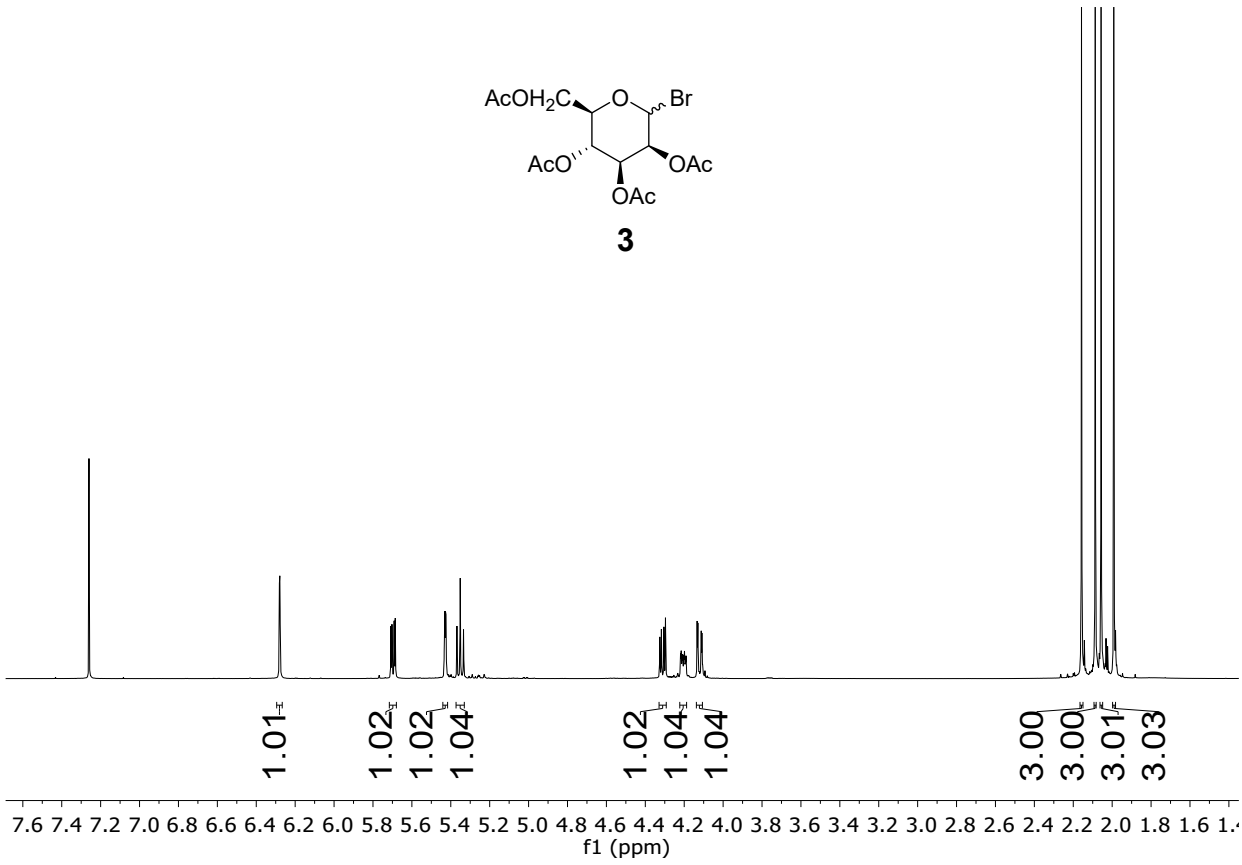

Figure 4: *^{1}H NMR ($CDCl_3$, 600MHz) of structure* ***3****.*

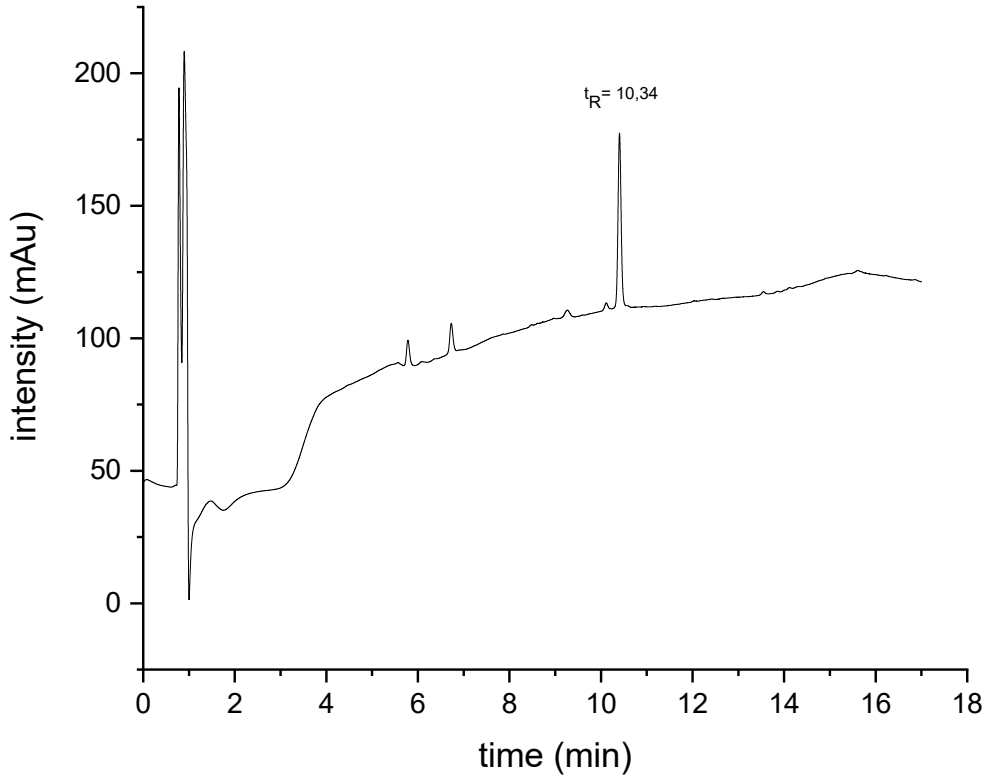

Figure 5: *RP HPLC chromatogram (linear gradient 0-50 Vol% MeCN in H_2O in 30 min at 25 °C) of structure **3**.*

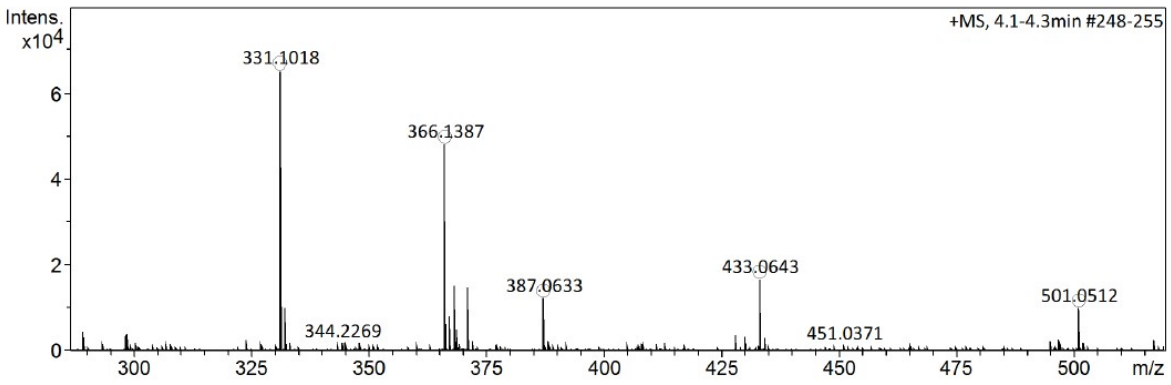

*Figure 6: HRMS of structure **3**.*

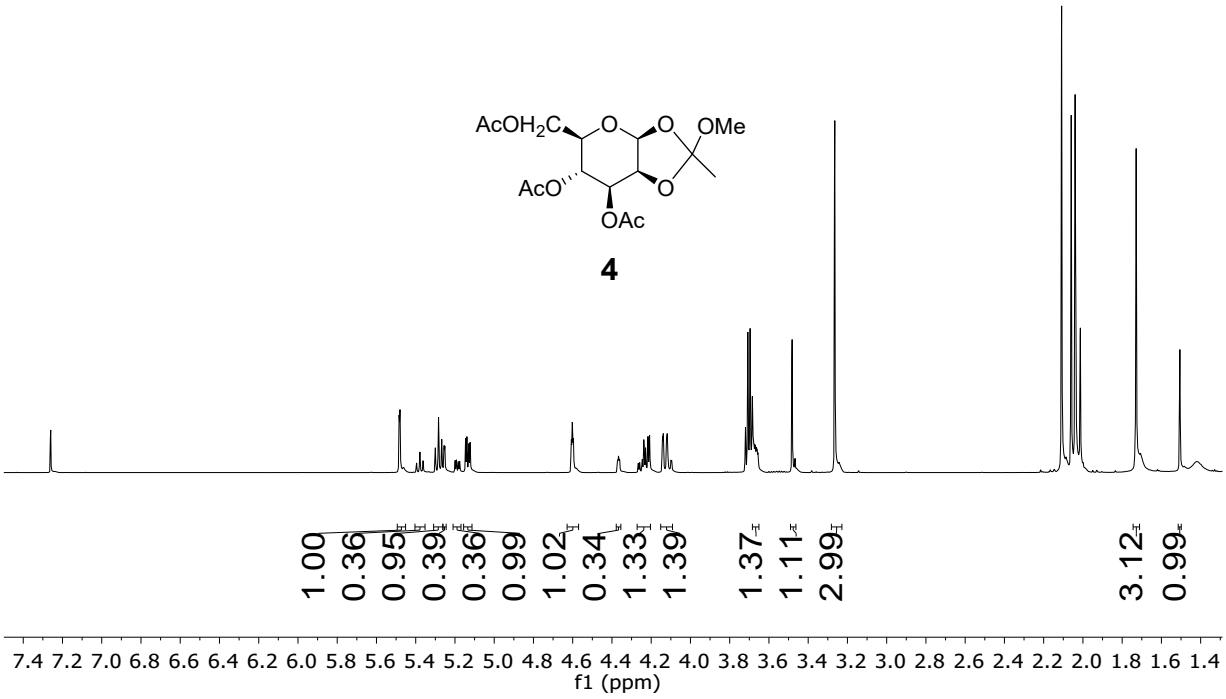

Figure 7: *^{1}H NMR ($CDCl_3$, 600MHz) of structure **4**.*

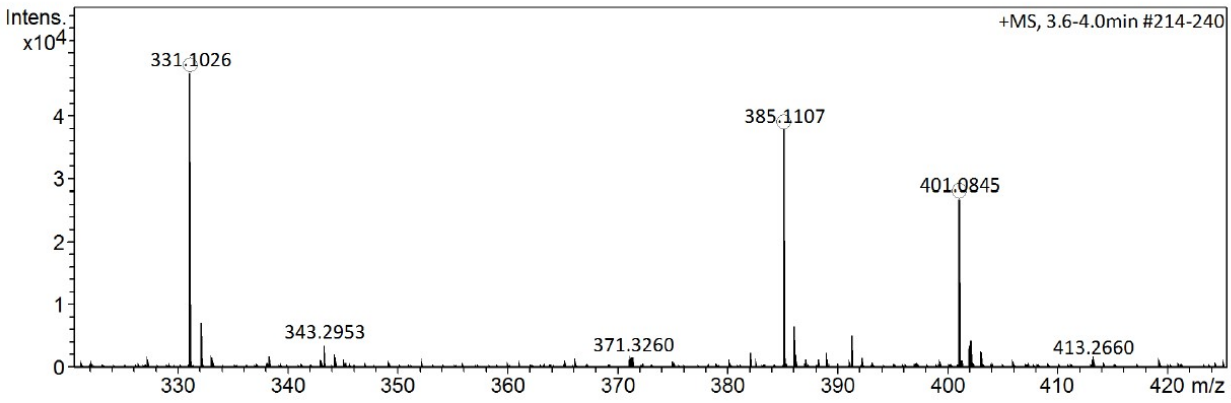

Figure 8: *HRMS of structure **4**.*

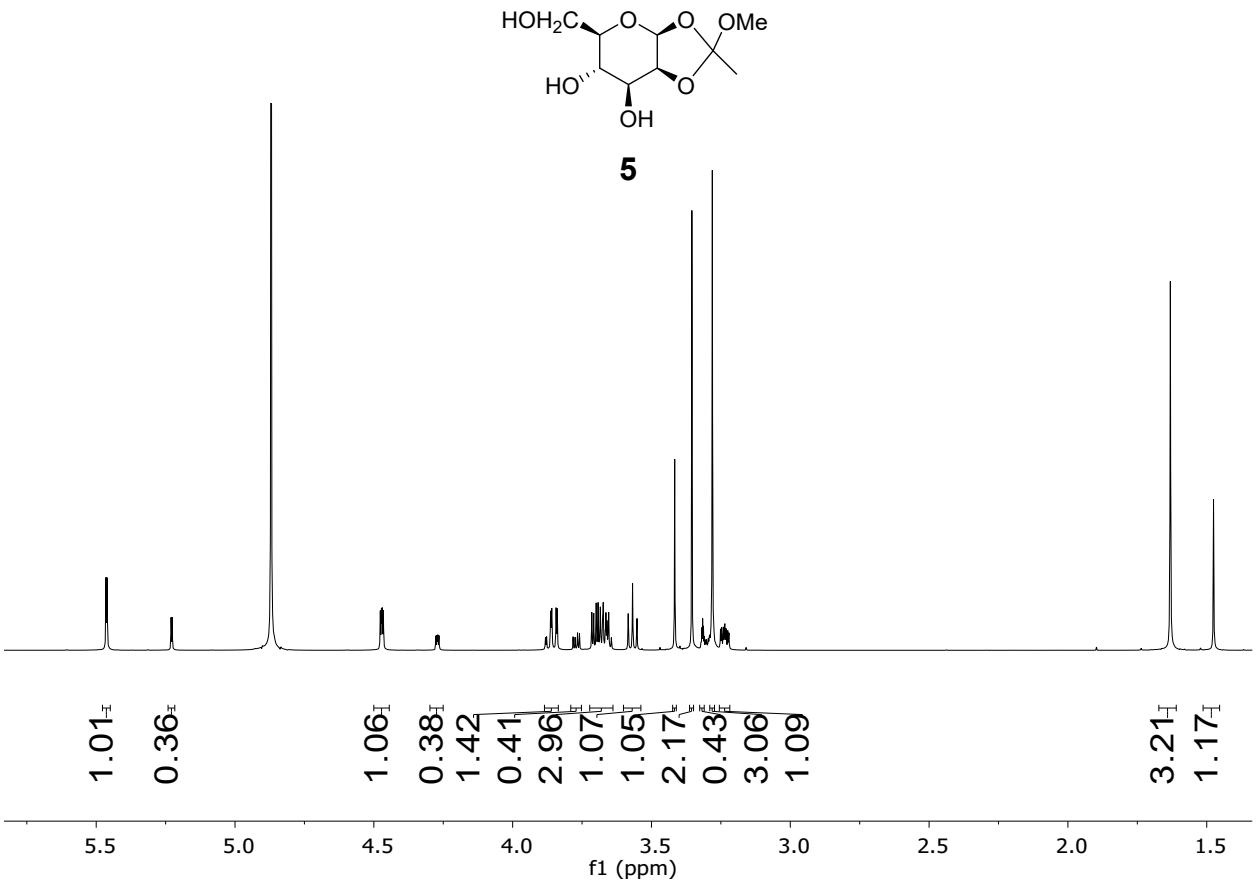

Figure 9: *^{1}H NMR (MeOH-d_4, 600MHz) of structure **5**.*

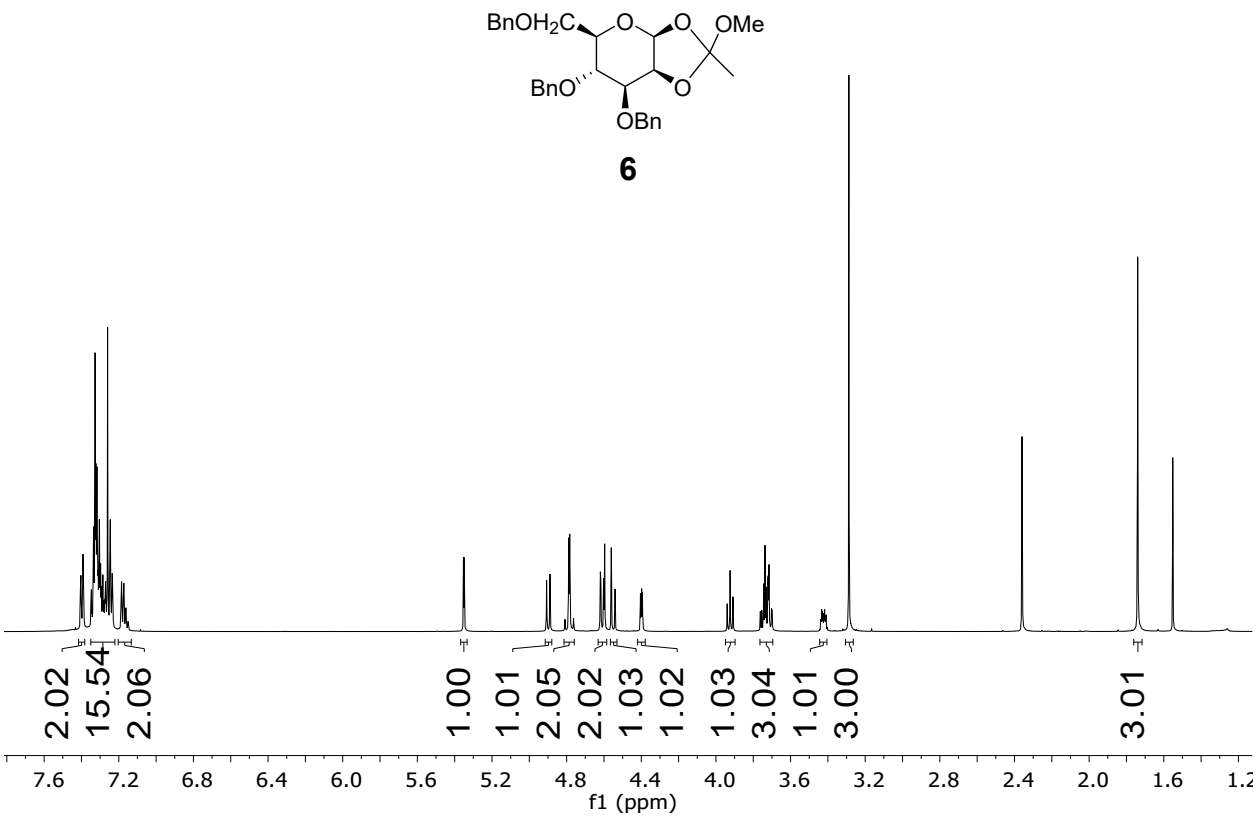

Figure 10: *[1]H NMR (CDCl3, 600MHz) of structure* ***6****.*

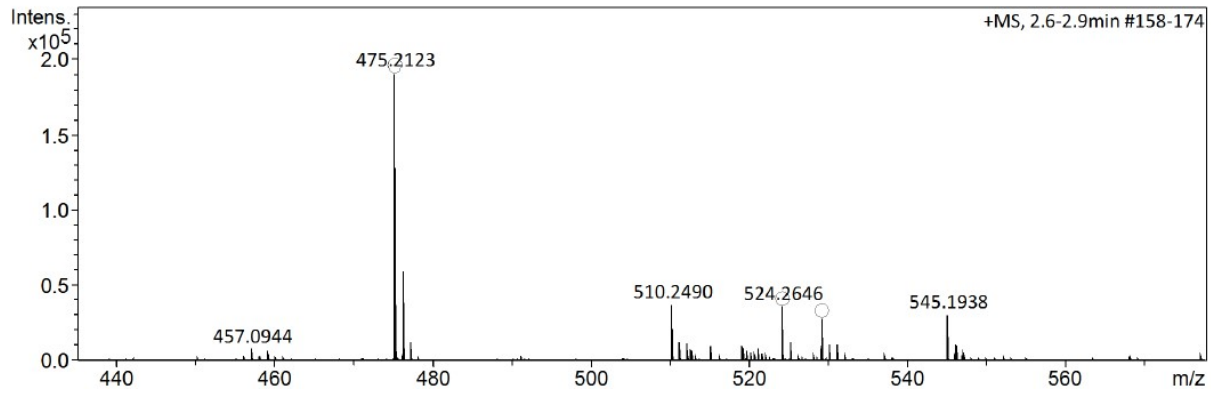

Figure 11: *HRMS of structure* ***6****.*

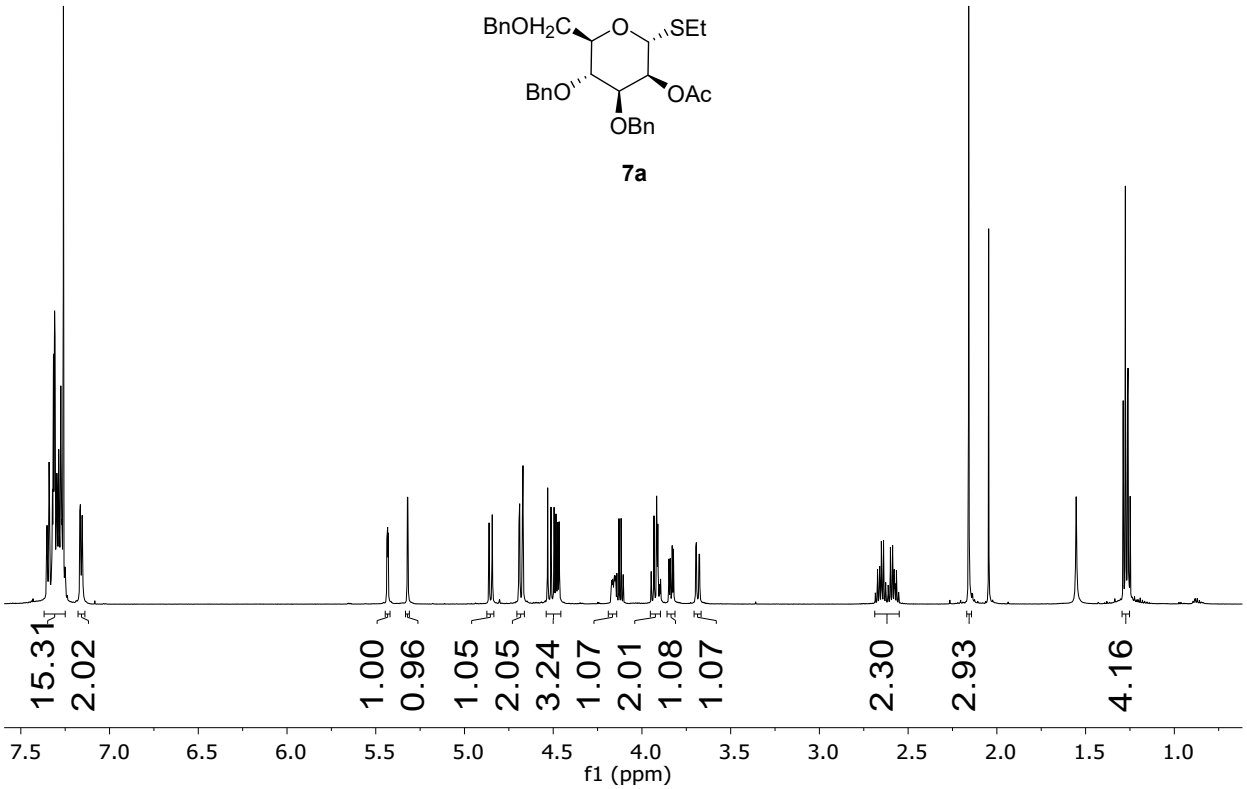

Figure 12: *^{1}H NMR ($CDCl_3$, 600MHz) of structure **7a**.*

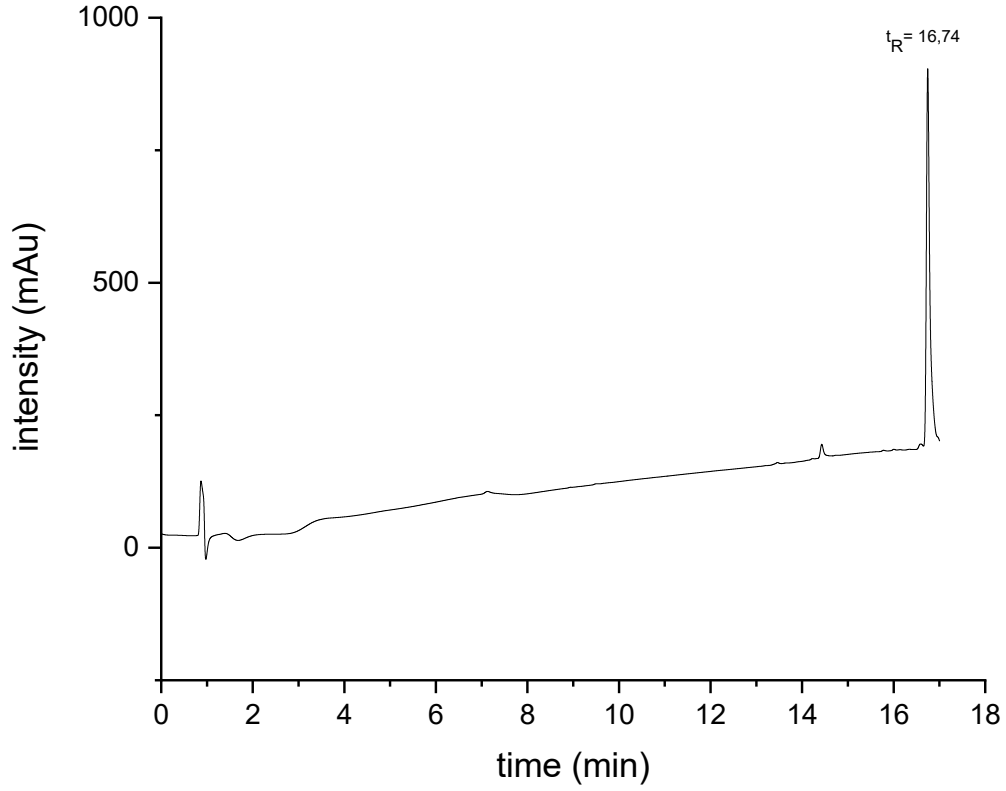

Figure 13: *RP HPLC chromatogram (linear gradient 0-50 Vol% MeCN in H_2O in 18 min at 25 °C) of structure **7a**.*

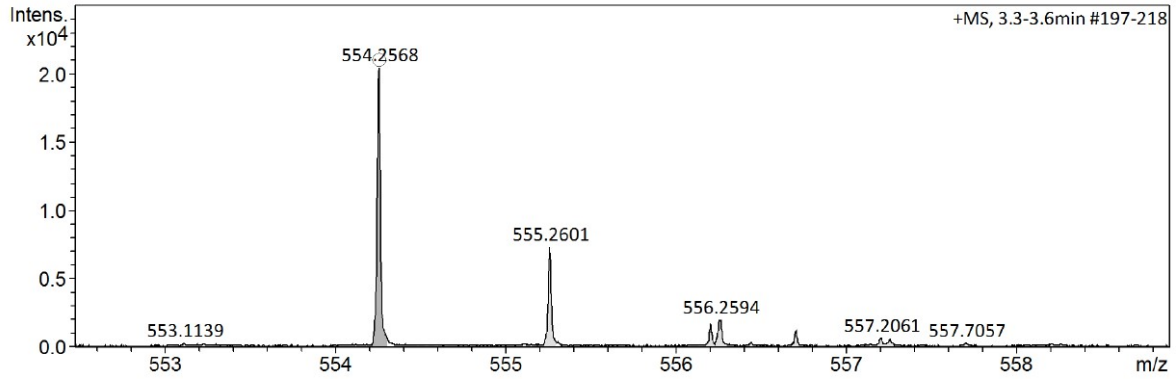

Figure 14: *HR MS of structure* ***7a****.*

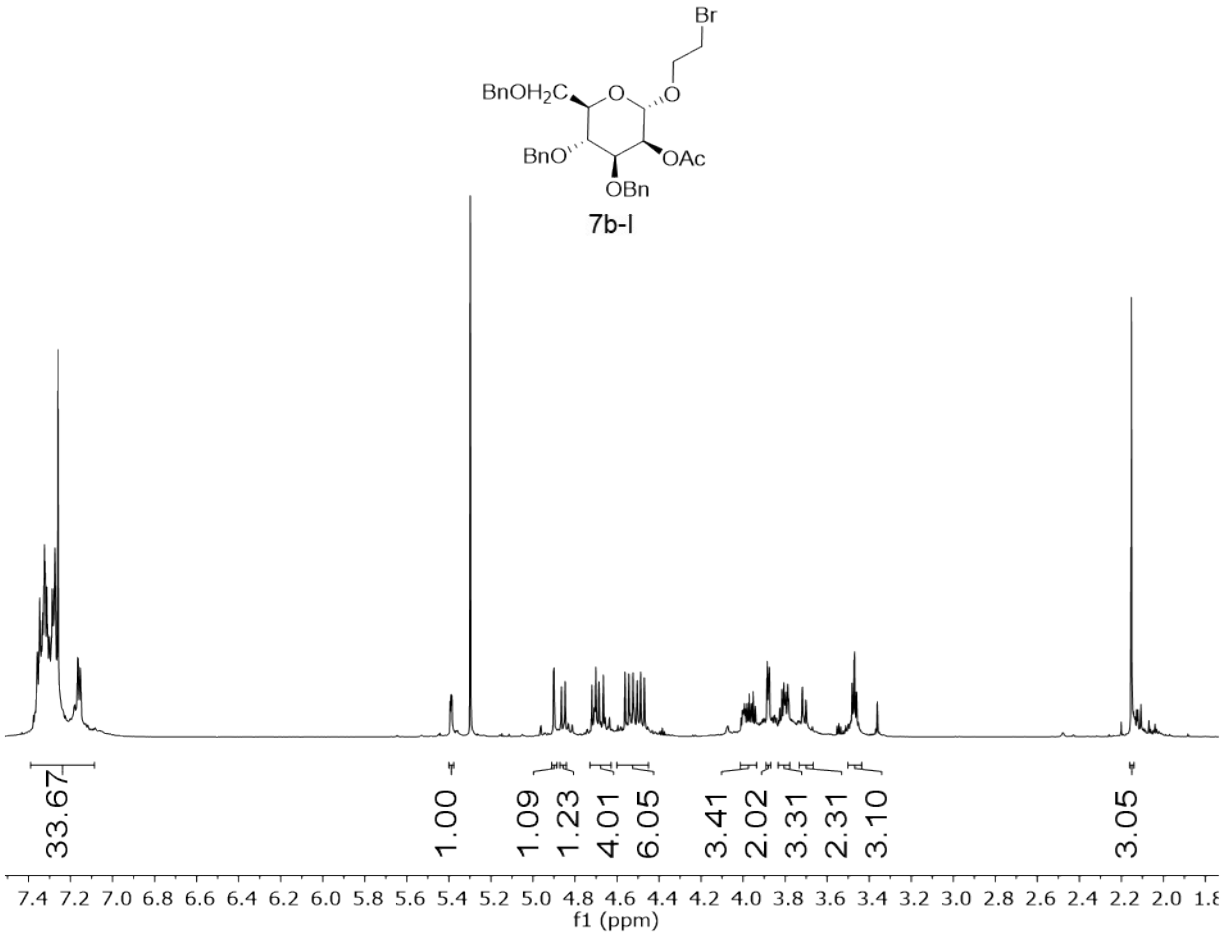

Figure 15: *^{1}H NMR ($CDCl_3$, 600MHz) of structure* ***7b-I****.*

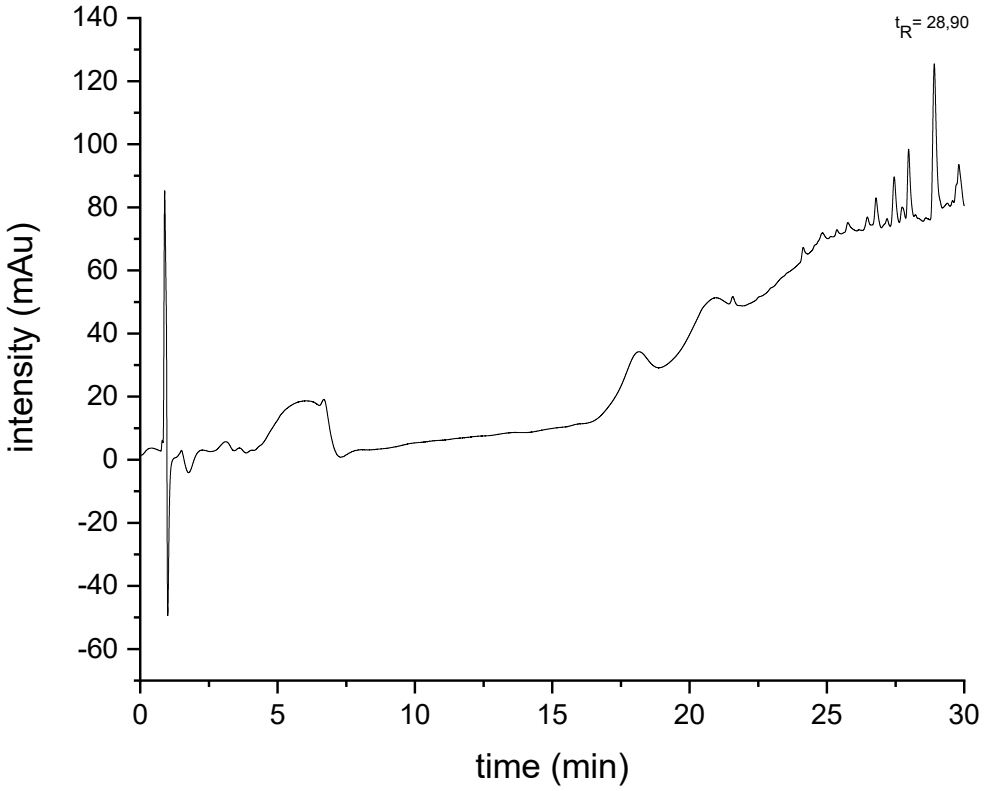

Figure 16: *RP HPLC chromatogram (linear gradient 0-50 Vol% MeCN in H_2O in 30 min at 25 °C) of structure* ***7b-I****.*

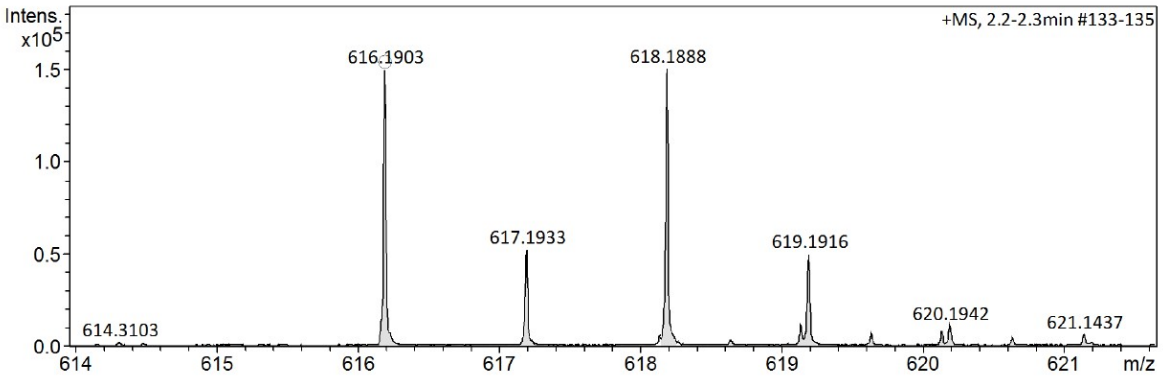

Figure 17: *HR-MS of structure* ***7b-I****.*

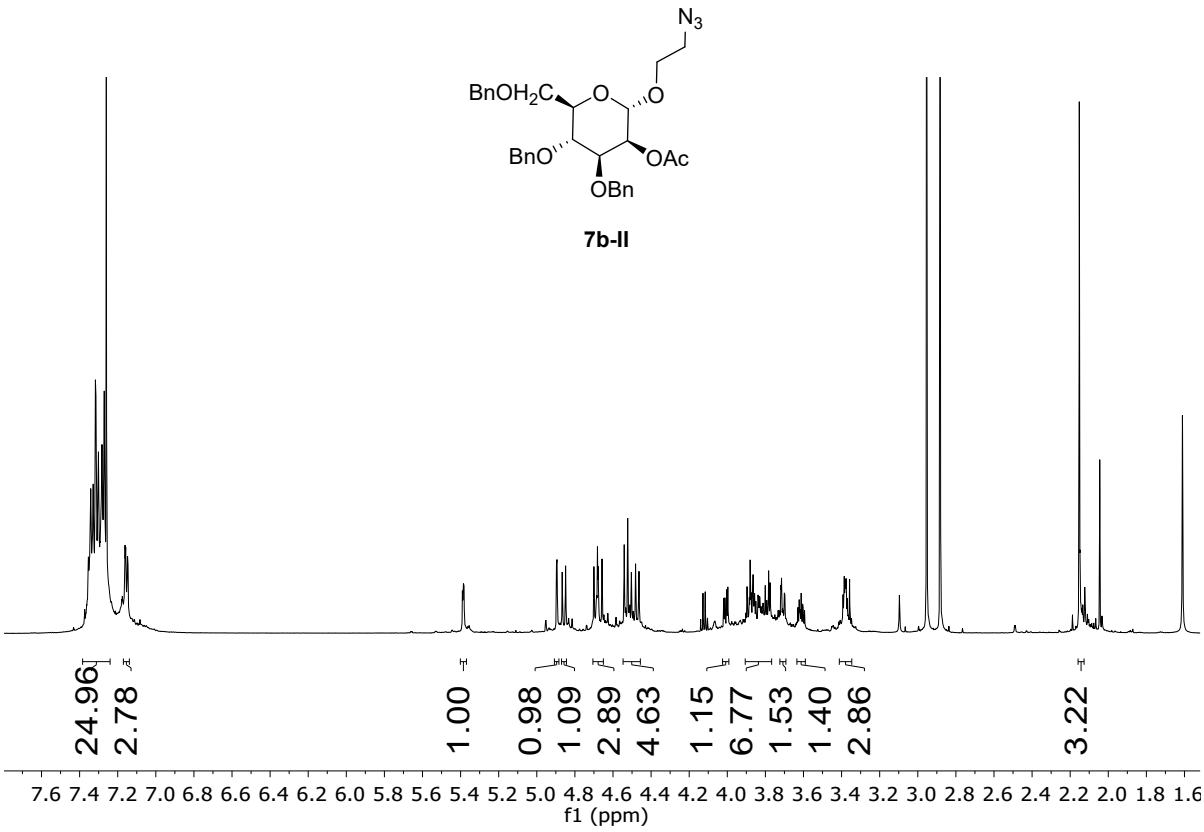

Figure 18: *^{1}H NMR ($CDCl_3$, 600MHz) of structure* ***7b-II****.*

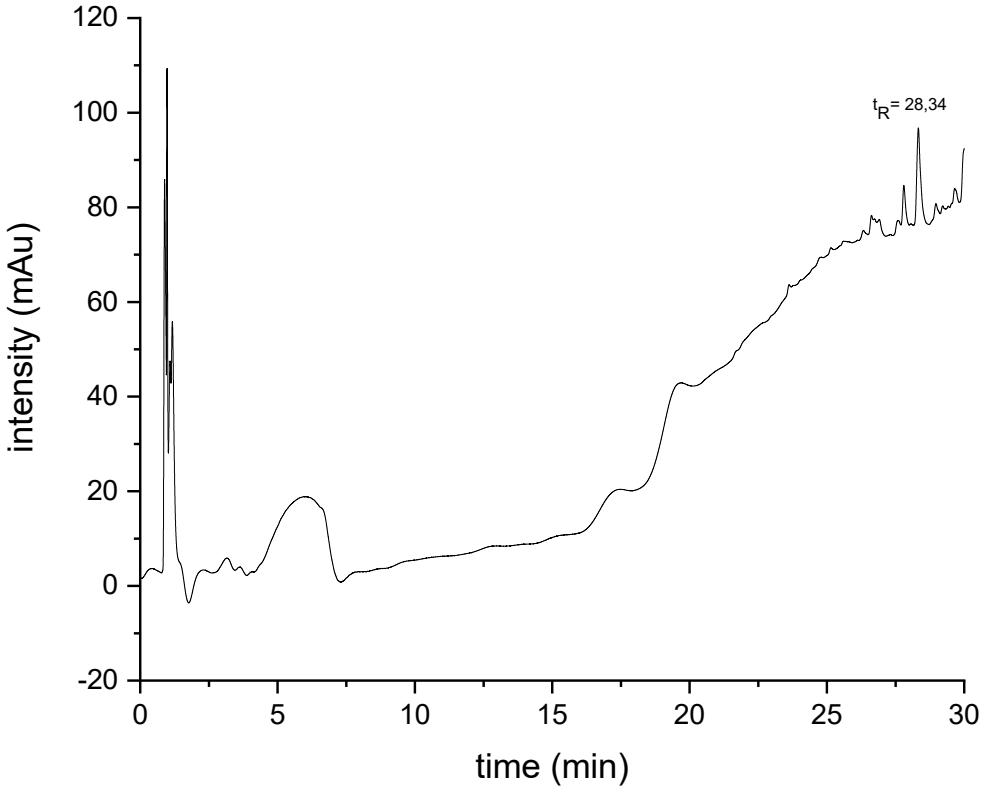

Figure 19: *RP HPLC chromatogram (linear gradient 0-50 Vol% MeCN in H_2O in 30 min at 25 °C) of structure* ***7b-II****.*

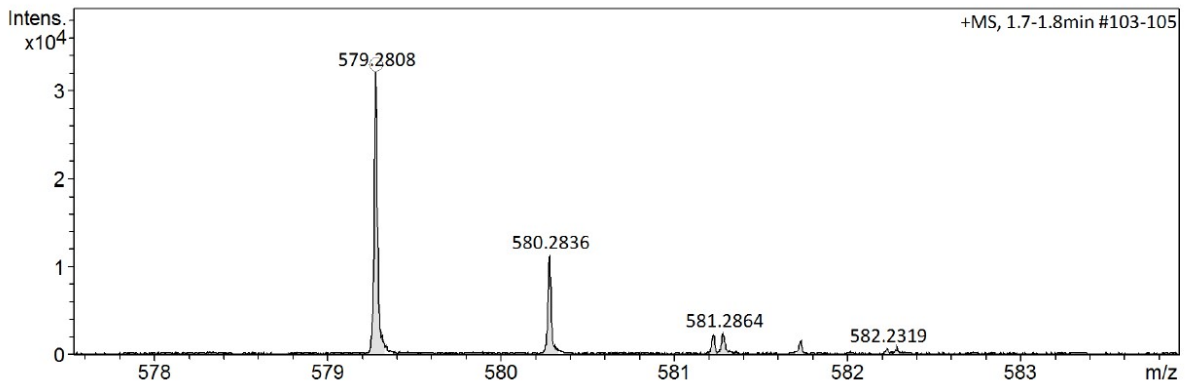

Figure 20: *HR-MS of structure* ***7b-II****.*

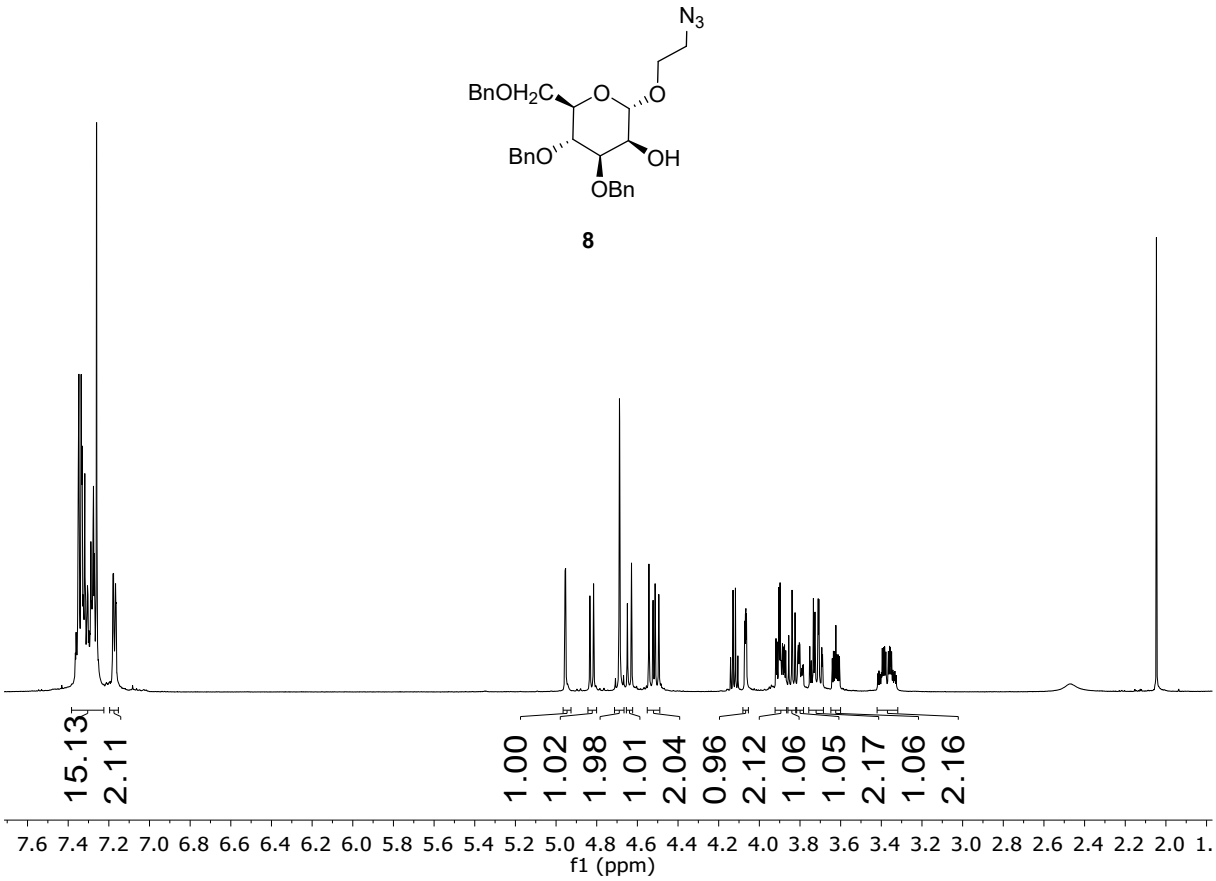

***Figure 21**: [1]H NMR ($CDCl_3$, 600MHz) of structure **8**.*

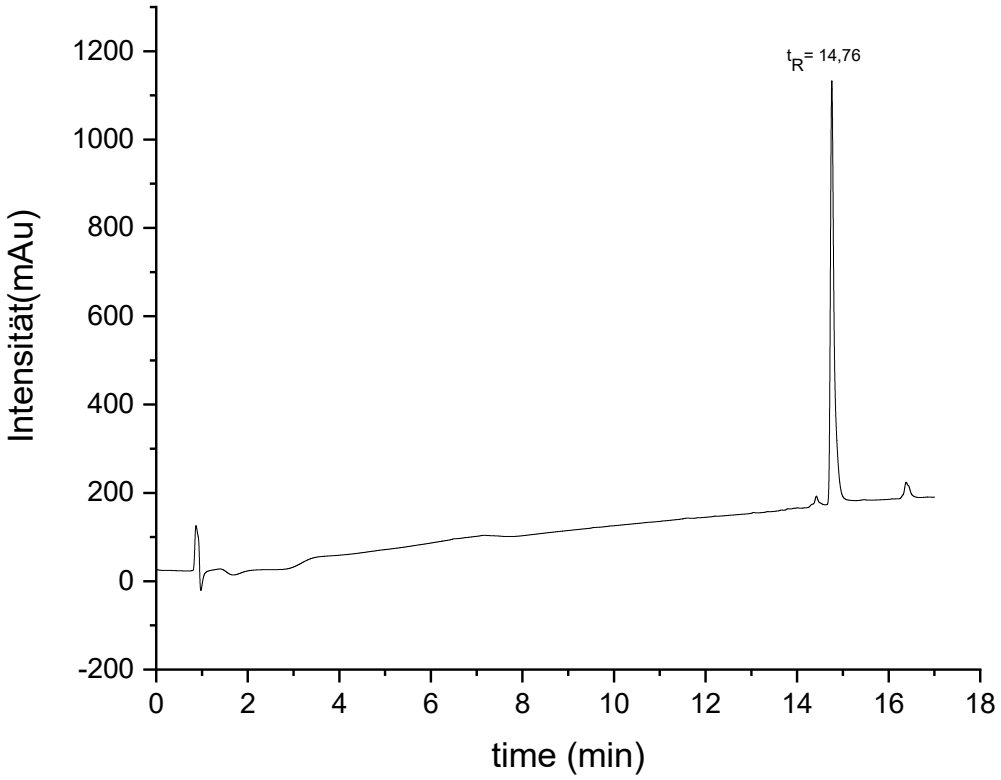

Figure 22: *RP HPLC chromatogram (linear gradient 0-50 Vol% MeCN in H_2O in 18 min at 25 °C) of structure **8**.*

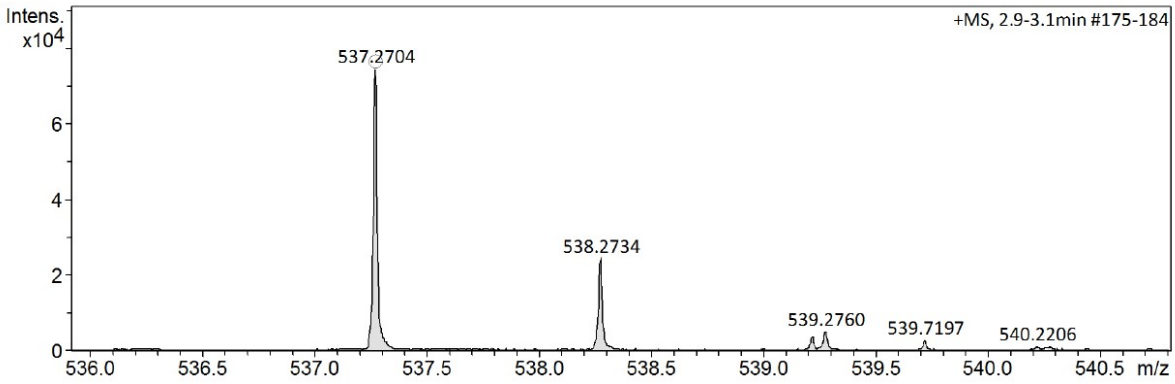

Figure 23: *HRMS of structure **8**.*

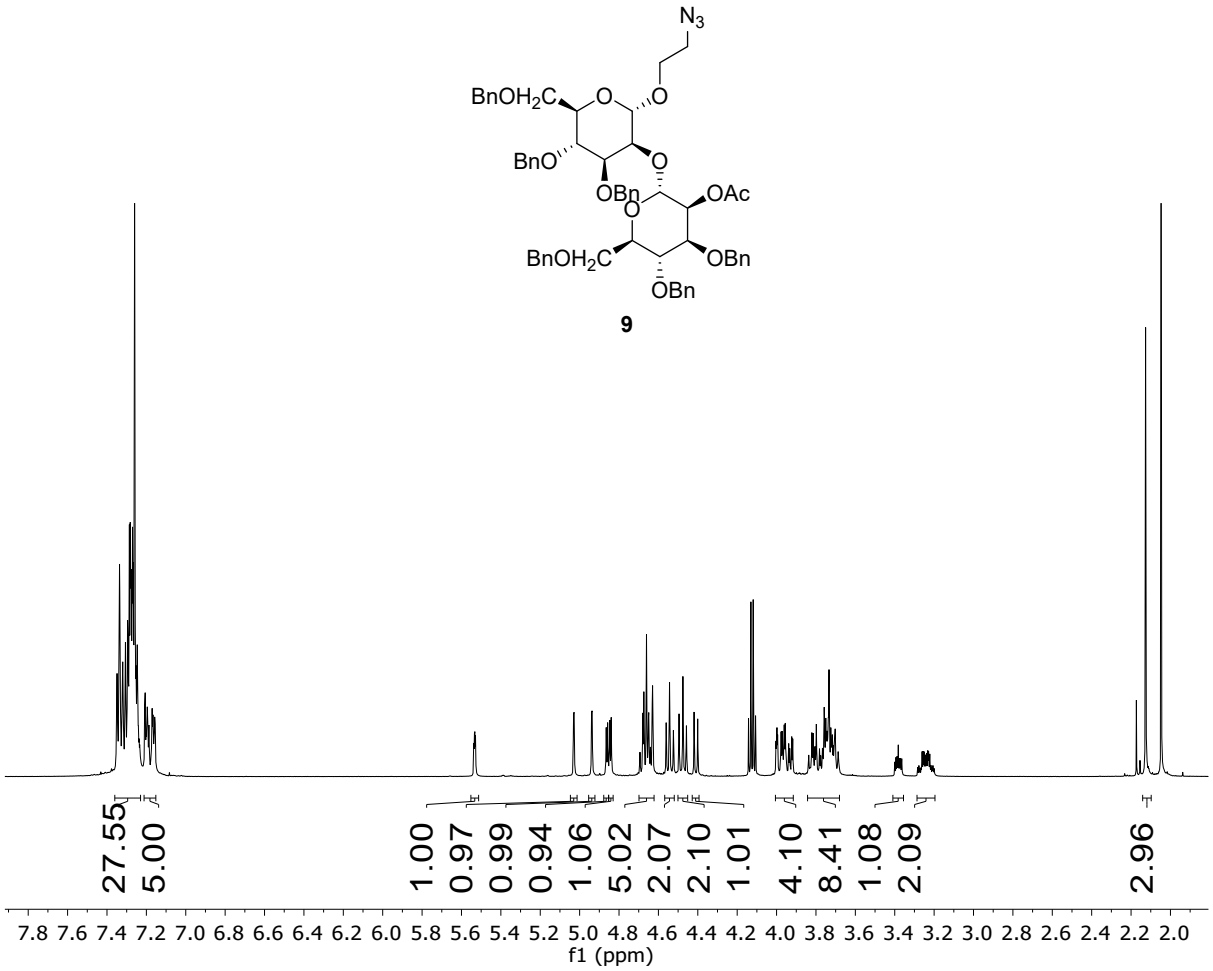

Figure 24: *^{1}H NMR ($CDCl_3$, 600MHz) of structure **9**.*

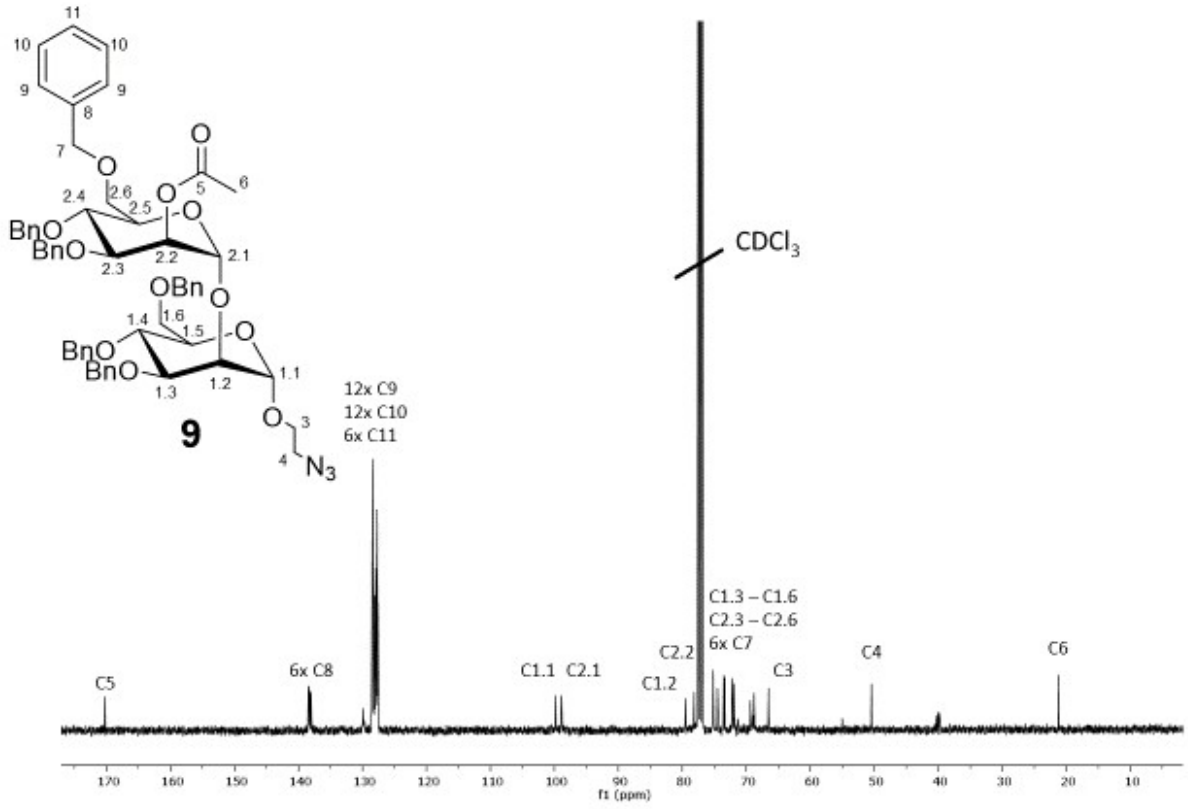

Figure 25: *^{13}C NMR ($CDCl_3$ 100 MHz) of structure **9**.*

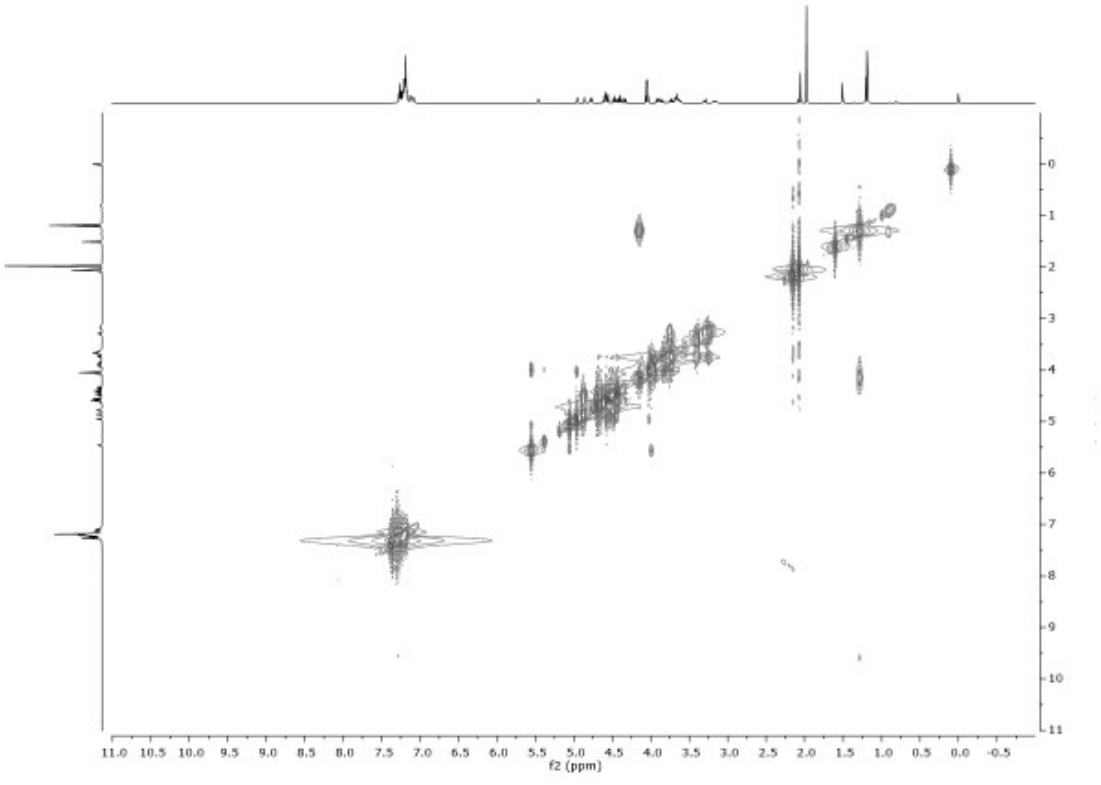

Figure 26: *COSY ($CDCl_3$ 600MHz) of structure **9**.*

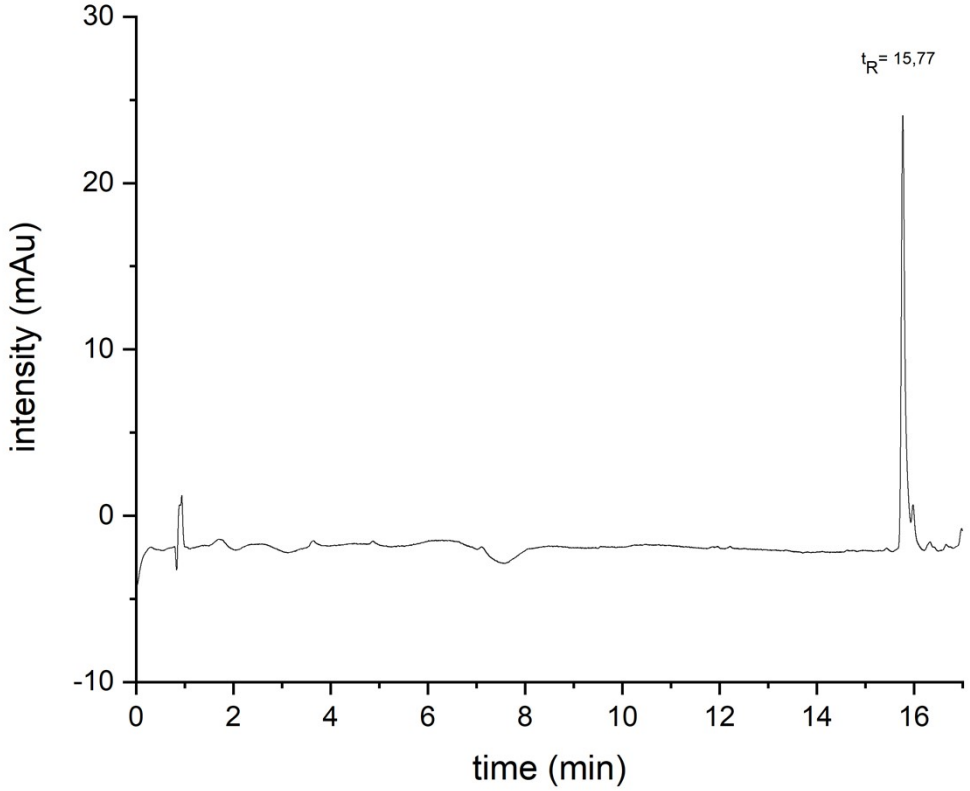

Figure 27: *RP HPLC chromatogram (linear gradient 0-50 Vol% MeCN in H_2O in 18 min at 25 °C) of structure* ***9****.*

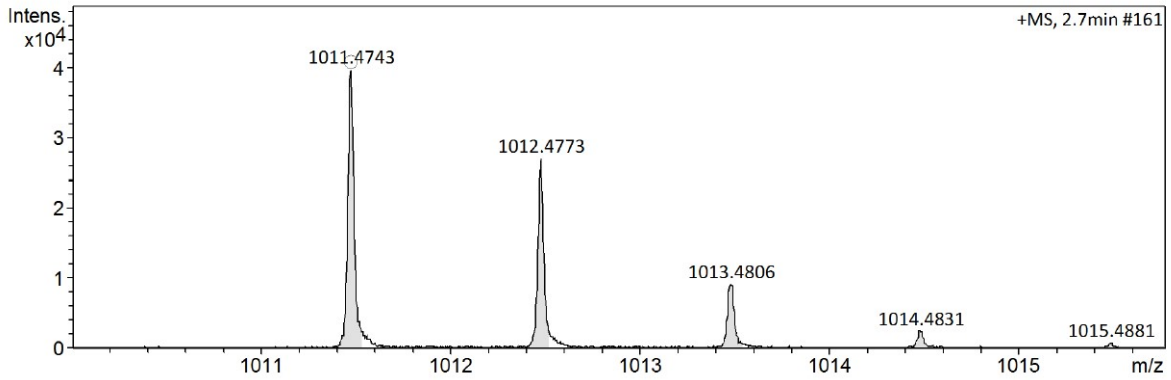

Figure 28: *HRMS of structure* ***9****.*

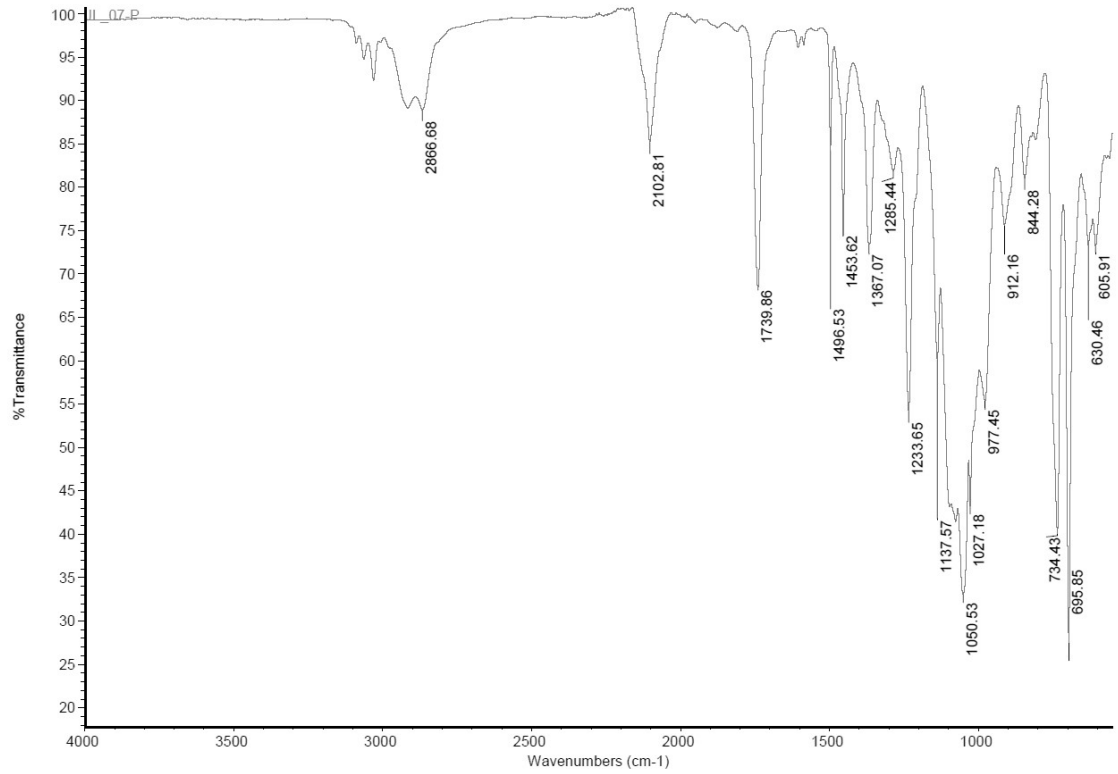

Figure 29: *IR-Spectrum of structure* ***9****.*

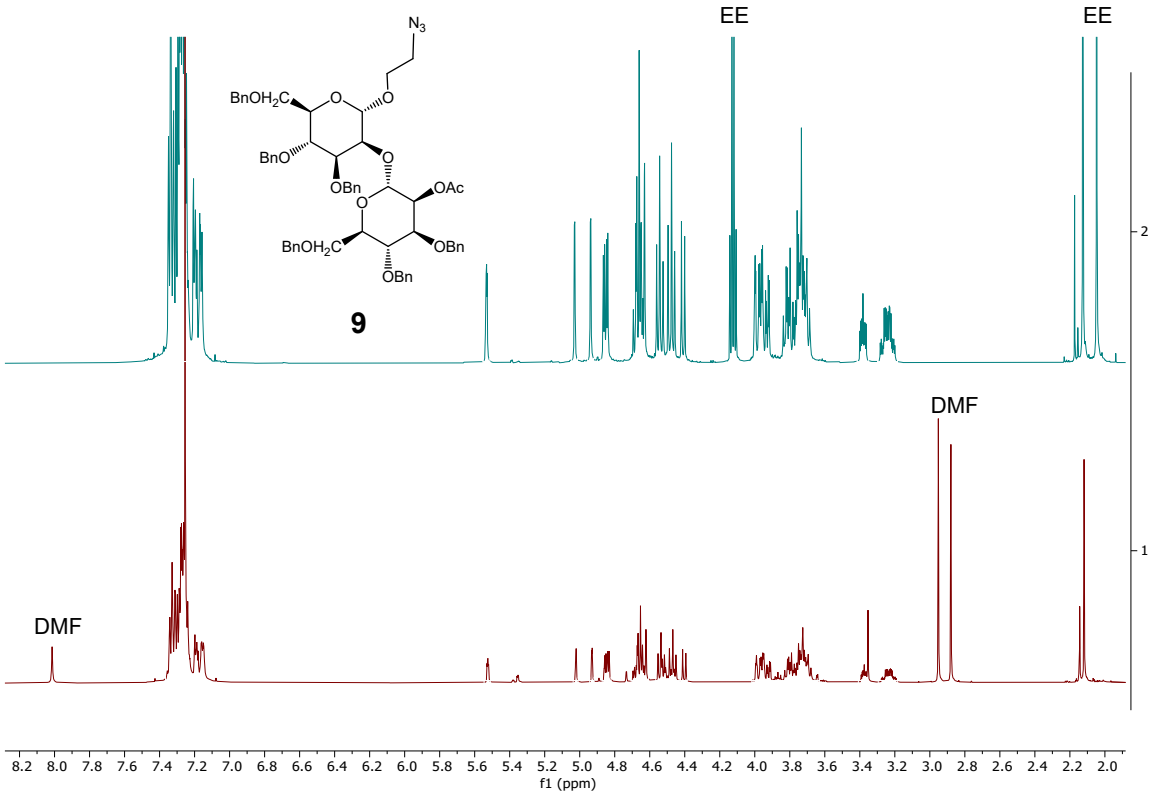

Figure 30: *Comparison of the* ^{1}*H NMR spectra of* ***9*** *after synthesis (blue) and after recovery from the coupling solution of CuAAC (red).*

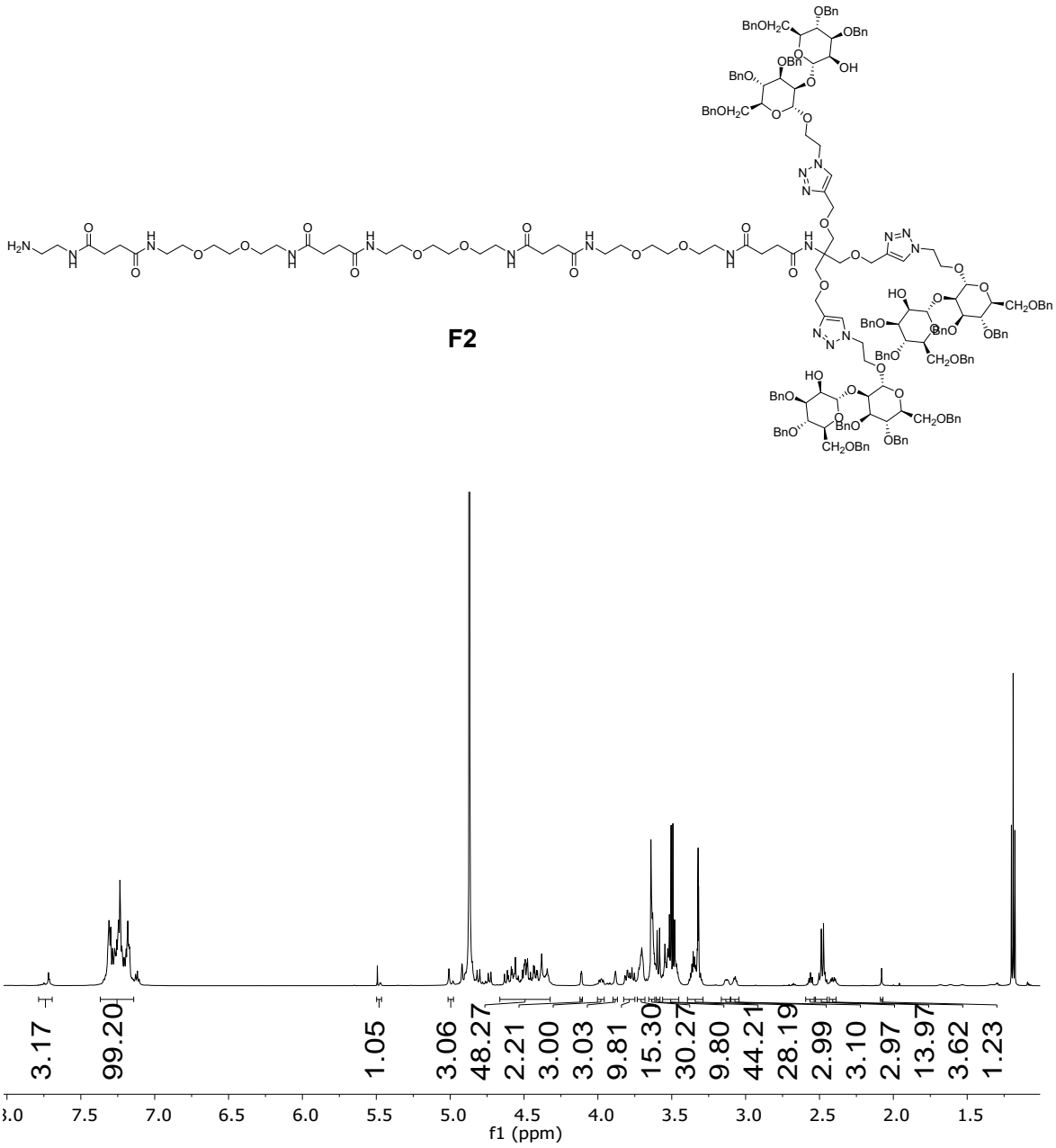

Figure 31: *^{1}H NMR (MeOH-d_4, 600MHz) of structure **F2** before benzyl group deprotection.*

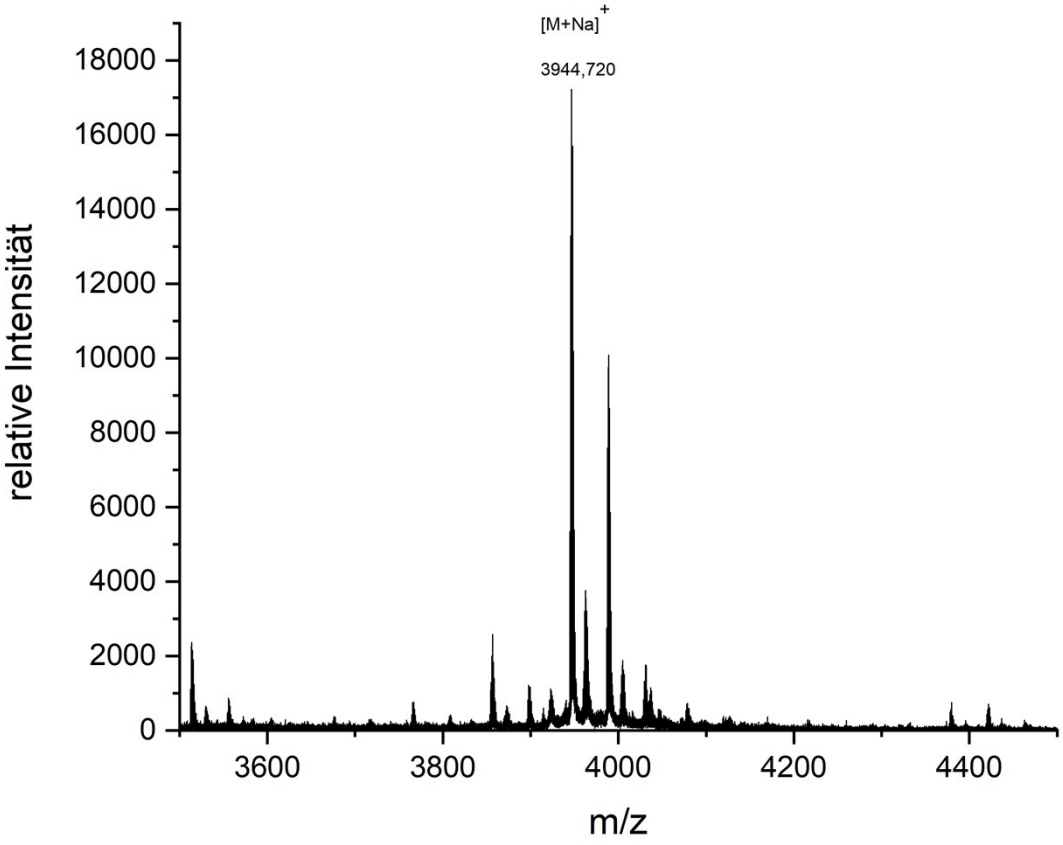

Figure 32: *MALDI TOF MS spectrum of structure* ***F2*** *before benzyl group deprotection.*

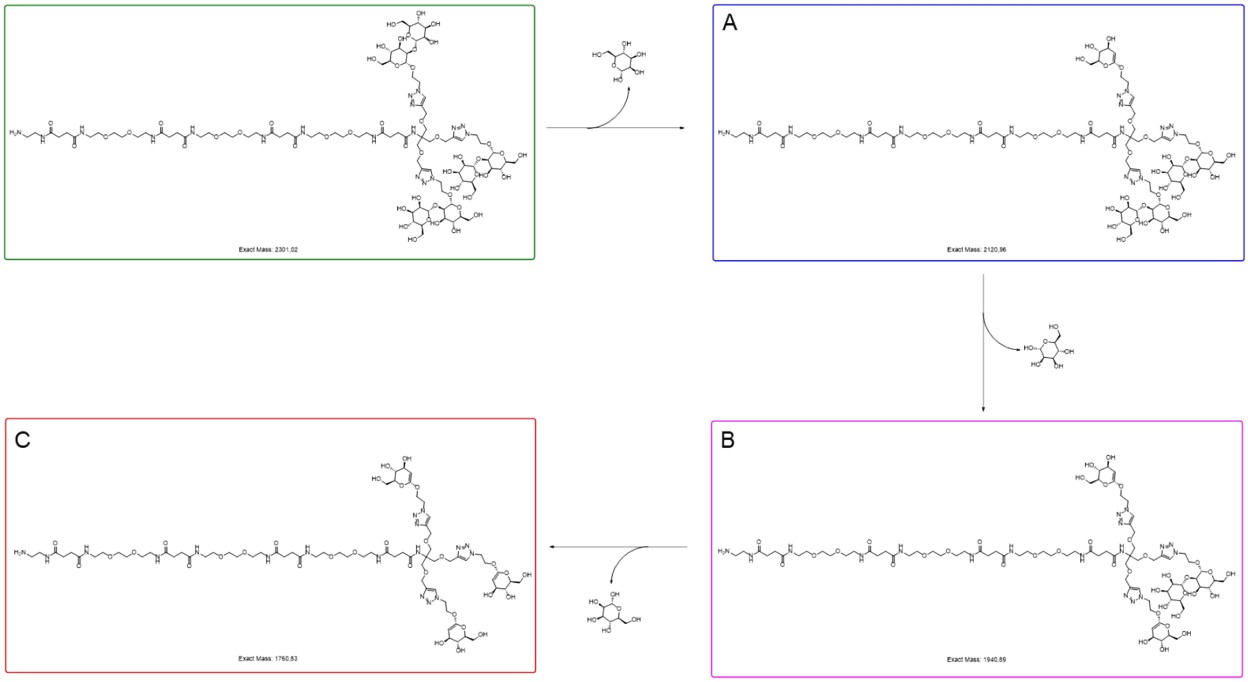

Figure 33: *Fragmentation of* ***F2*** *in HRMS measurement. (Green = no fragmentation, blue = fragmentation of one mannobiose (A), pink = fragmentation of two mannobiose (B), red = fragmentation of three mannobiose (C))*

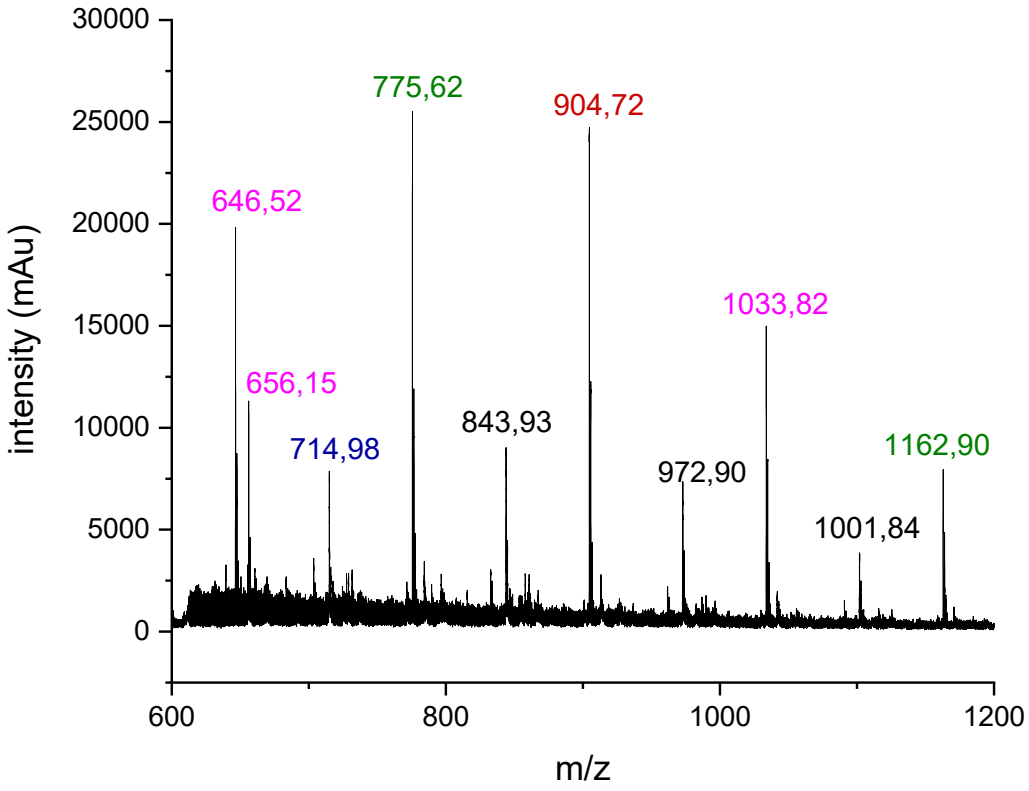

Figure 34: *HRMS Spectrum of* ***F2*** *after complete deprotection. (Green = no fragmentation, blue = fragmentation of one mannobiose, pink = fragmentation of two mannobiose, red= framentation of three mannobiose)*

Table 1: *Corresponding fragments and ion adducts of* Figure 35

m/z	Fragment	Adduct
646,52	Fragment B	M+3H
656,15	Fragment B	M+2H+Na
714,98	Fragment A	M+2H+Na
775,62	Product	M+2H+Na
904,72	Fragment C	M+2Na
1033,82	Fragment B	M+3ACN+2H
1162,9	Product	M+H+Na

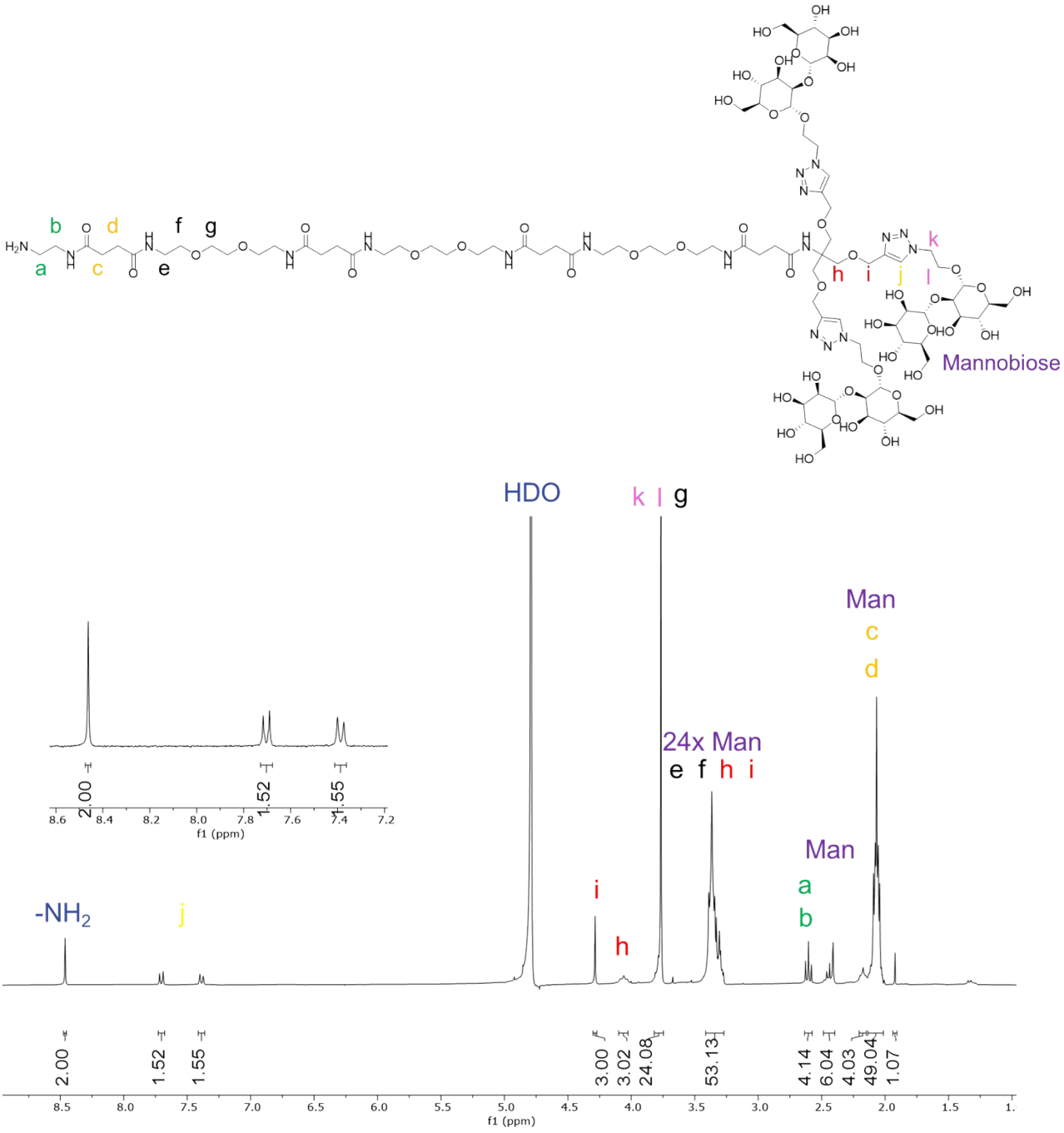

Figure 35: *^{1}H NMR (D_2O, 600MHz) of* ***F2*** *after complete deprotection.*