

CuAAC Synthesis of Resorcin[4]arene-based glycoclusters as multivalent ligands of lectins

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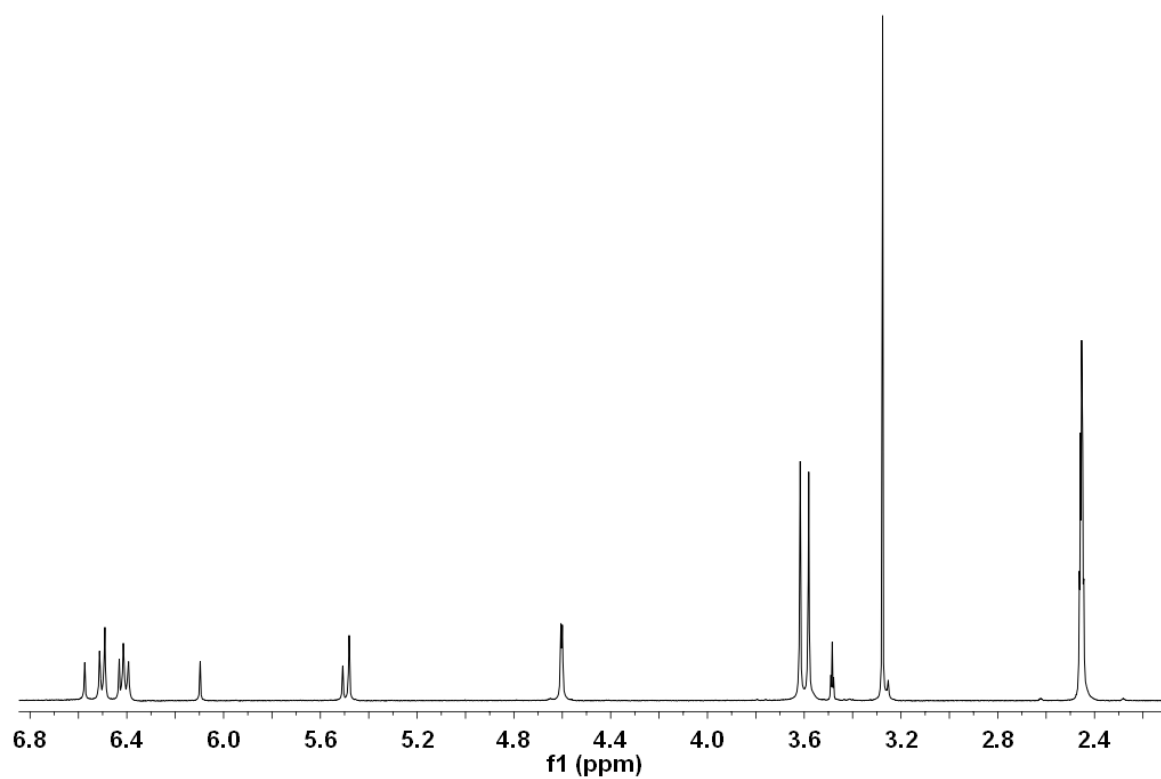


Figure 1: Full ¹H NMR (400 MHz, DMSO-*d*₆) of chair *rctt* **3a**

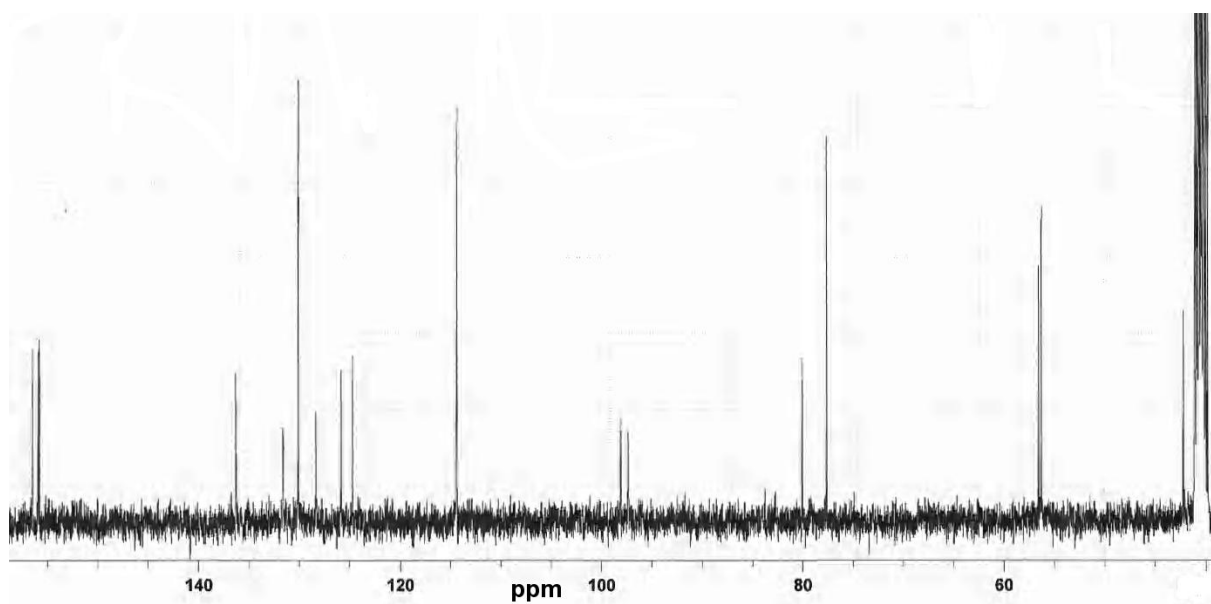


Figure 2: Full ¹³C NMR (100 MHz, DMSO-*d*₆ + ε DMF-*d*₇, 363K) of chair *rctt* **3a**

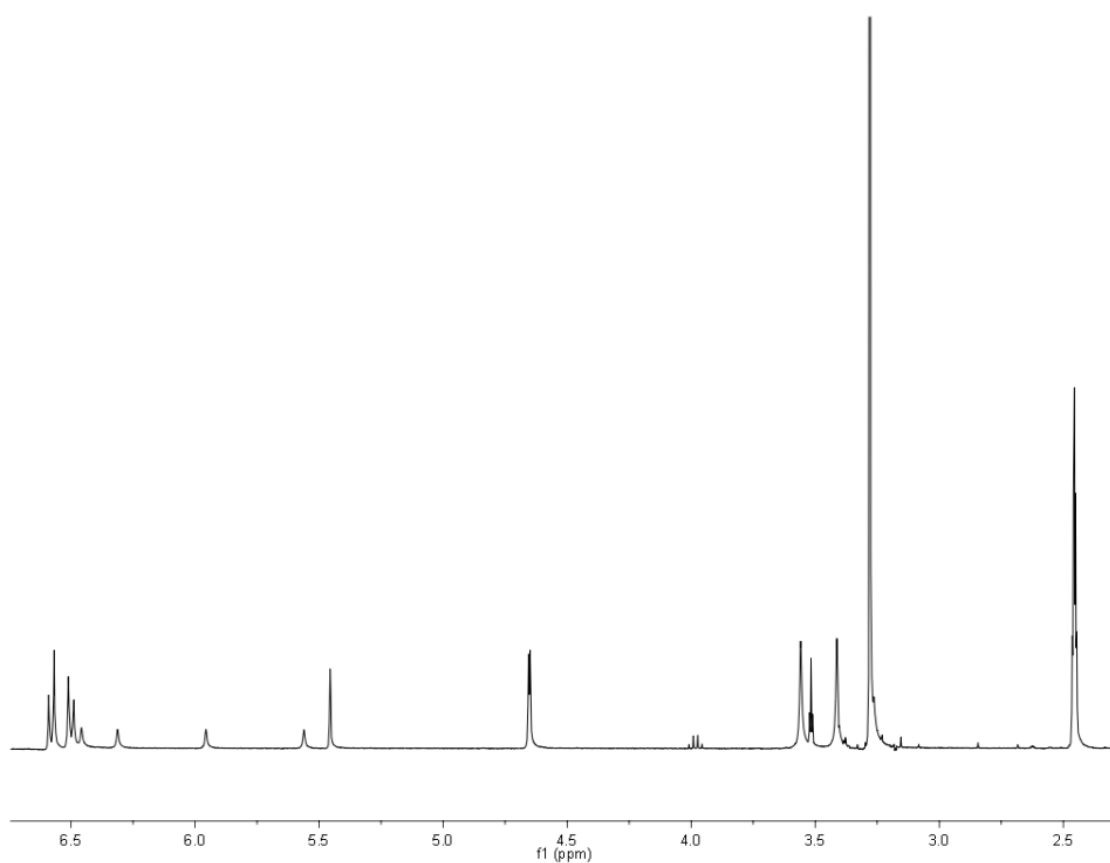


Figure 3: Full ¹H NMR (400 MHz, DMSO-*d*₆) of flattened boat *rccc* **3b**

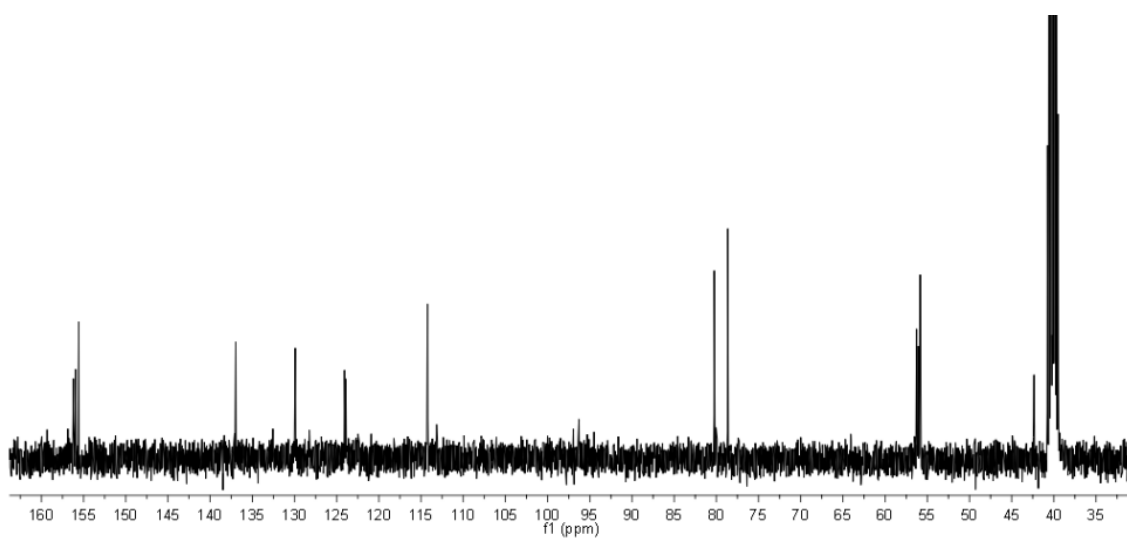


Figure 4: Full ¹³C NMR (100 MHz, DMSO-*d*₆) of flattened boat *rccc* **3b**

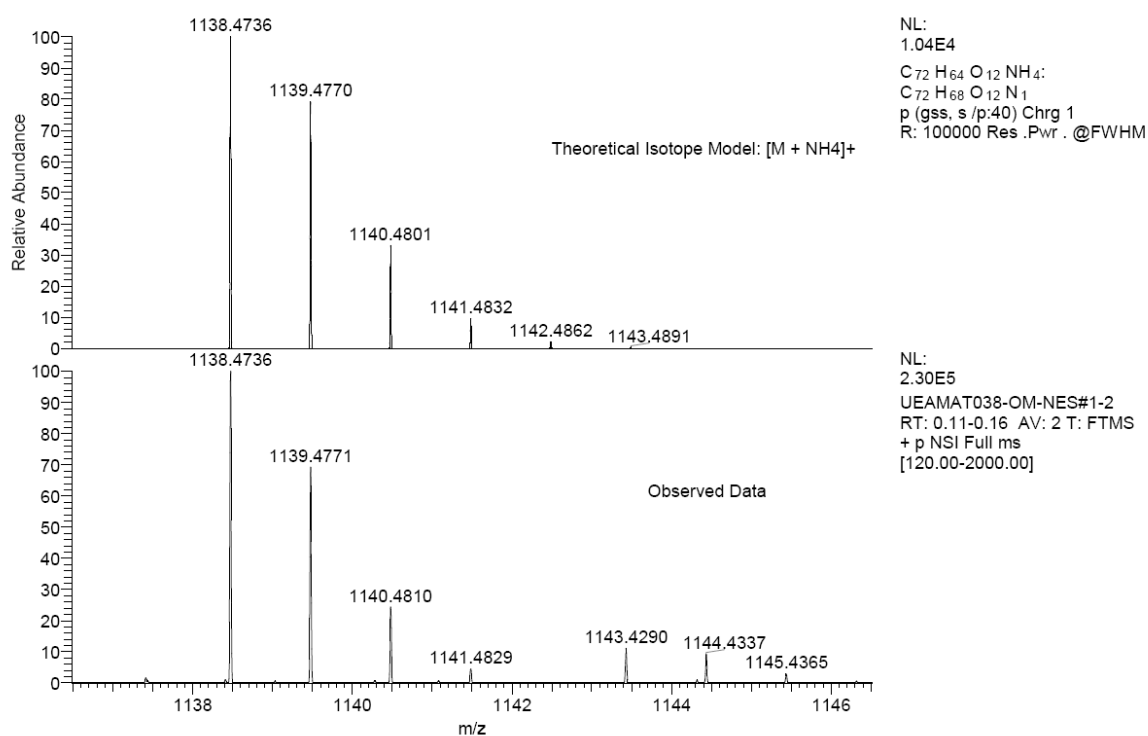


Figure 5: ESI-MS of chair *rctt* **3a**

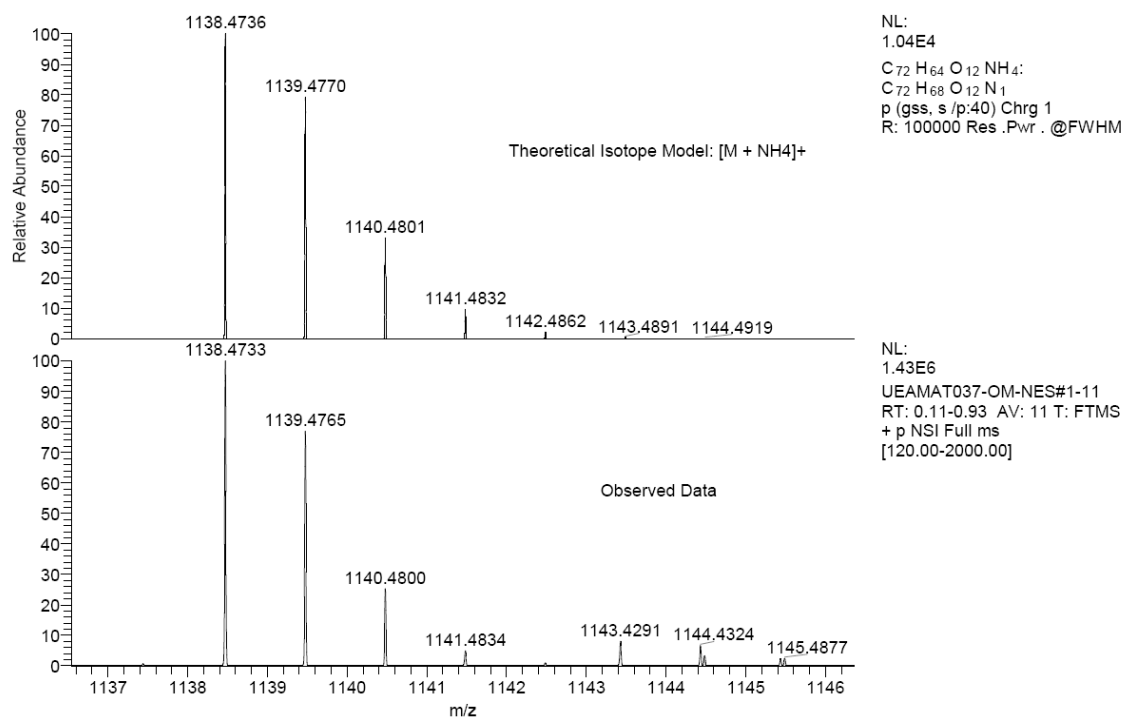


Figure 6: ESI-MS of flattened boat *rcc* **3b**

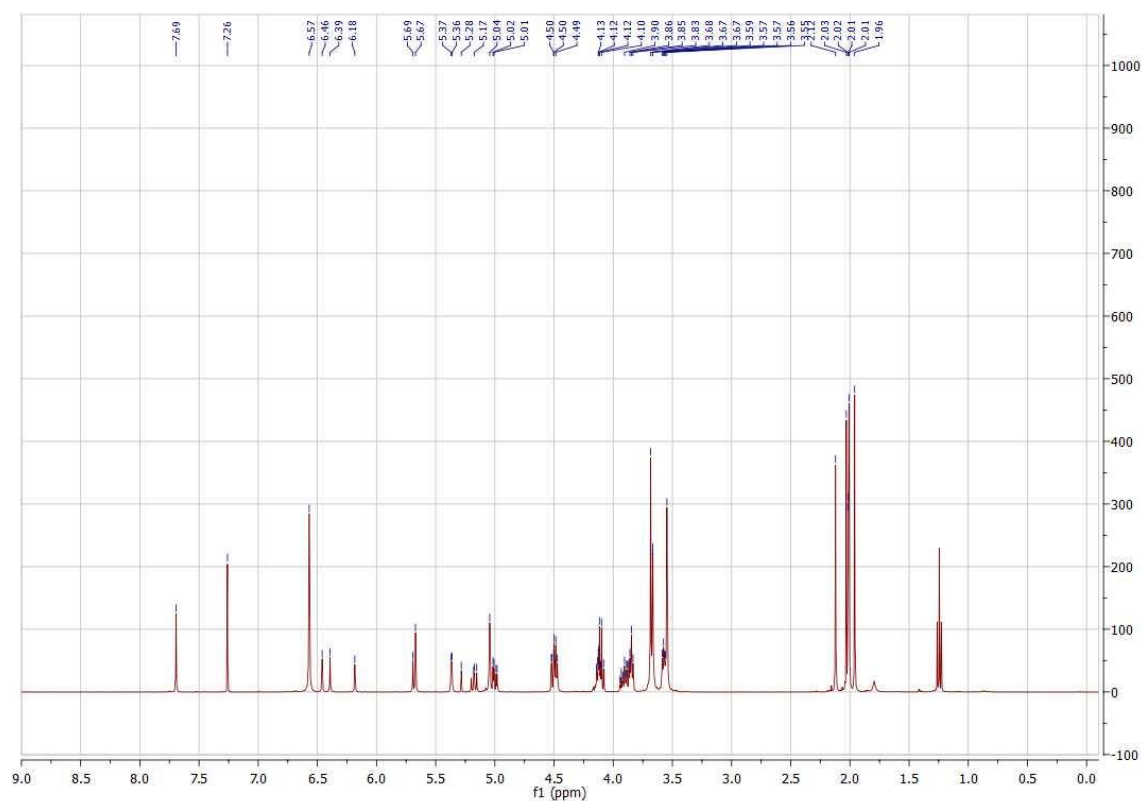


Figure 7: Full ^1H NMR (400 MHz, CDCl_3) Tetra $(\text{AcO})_4\text{GalEG}_3$ Resorcinarene chair - Acetylated Glycocluster **5a_G**

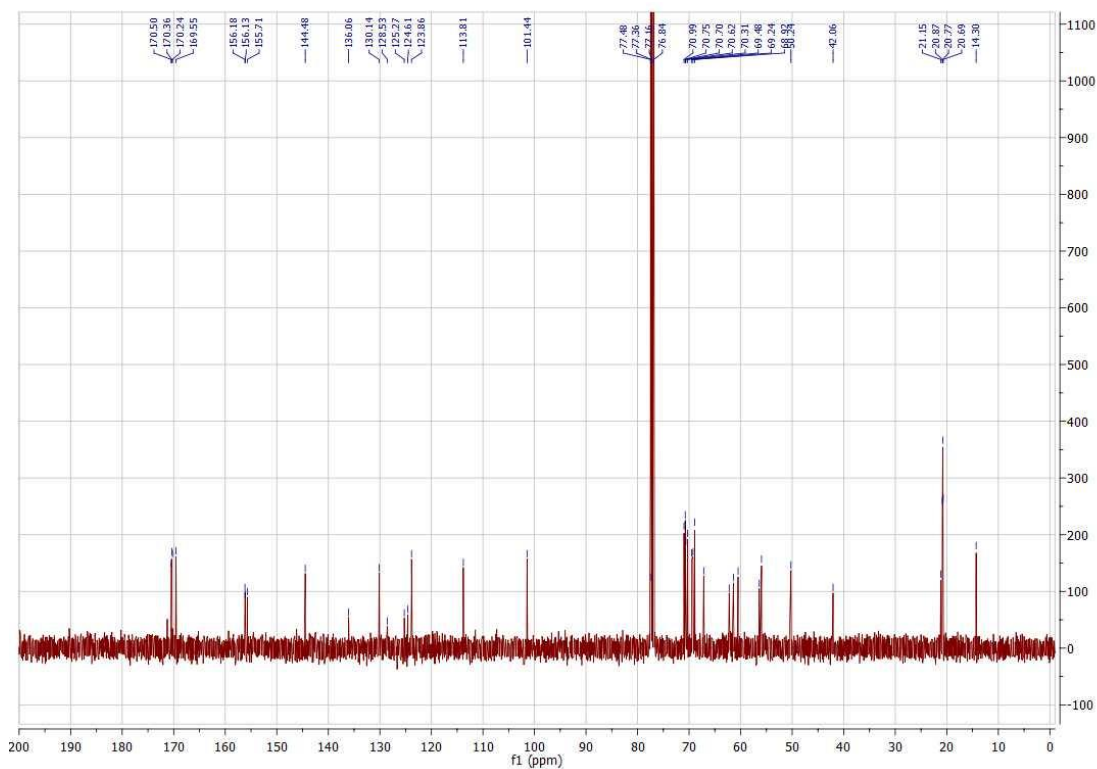


Figure 8: Full ^{13}C NMR (100 MHz, CDCl_3) Tetra $(\text{AcO})_4\text{GalEG}_3$ Resorcinarene chair - Acetylated Glycocluster **5a_G**

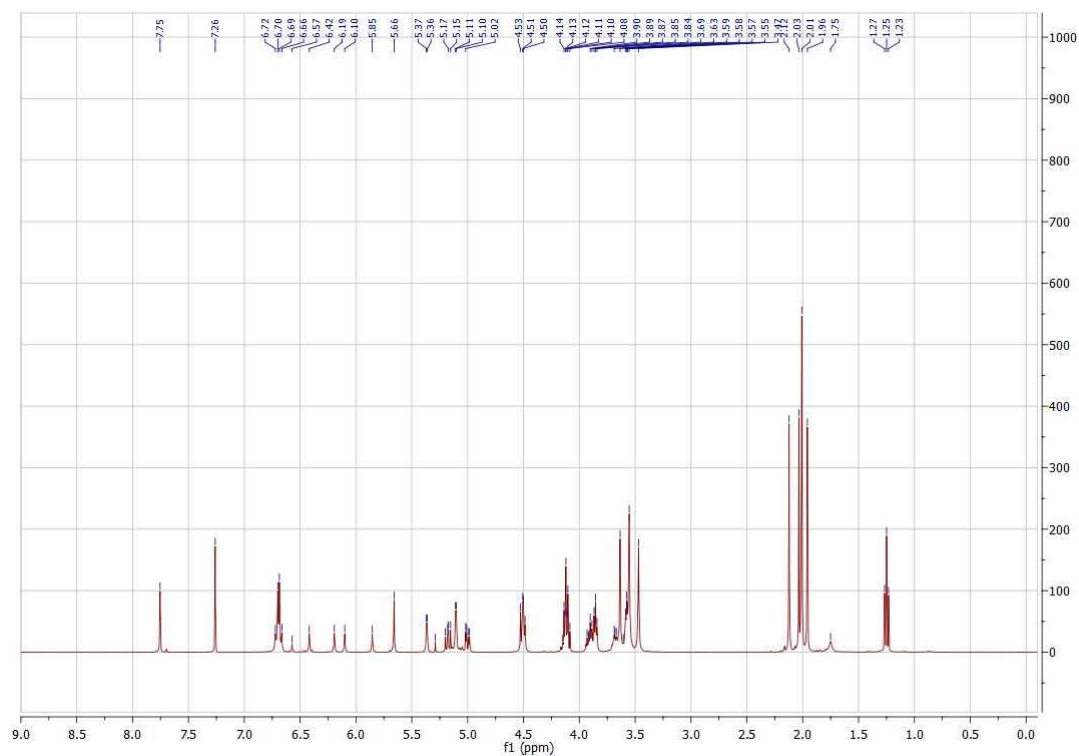


Figure 9: Full ^1H NMR (400 MHz, CDCl_3) Tetra $(\text{AcO})_4\text{GalEG}_3$ Resorcinarene boat - Acetylated Glycocluster **5b_G**

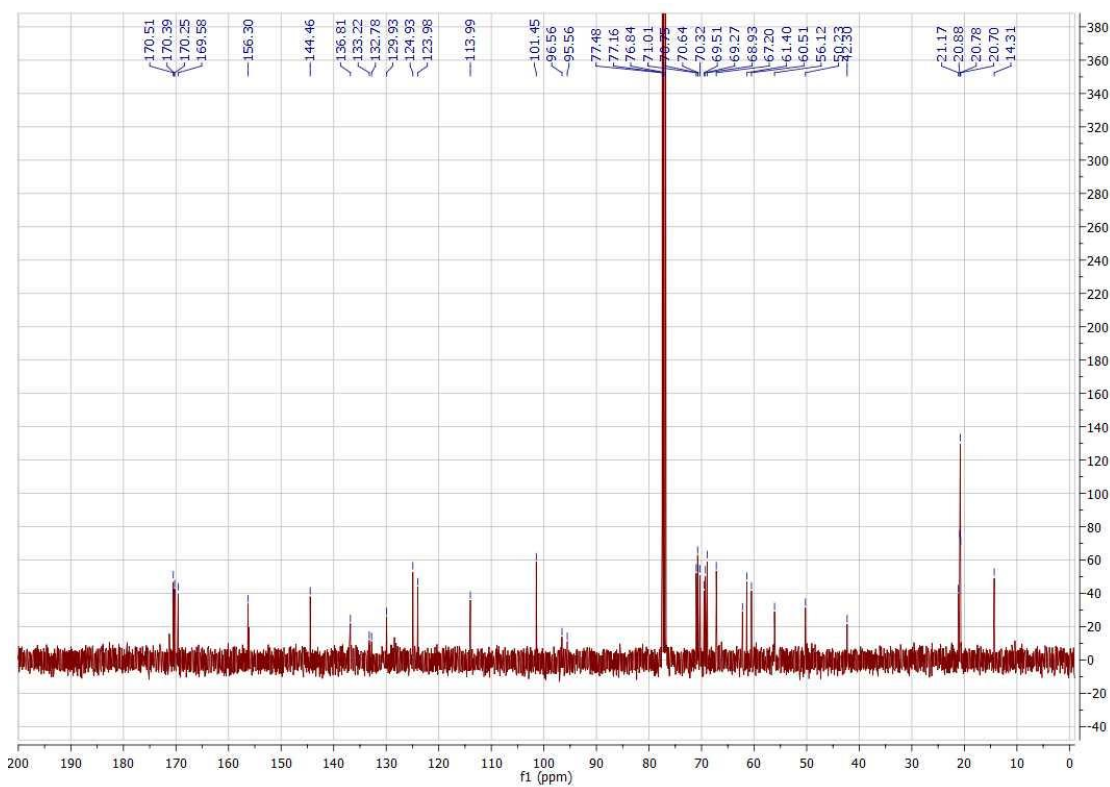


Figure 10: Full ^{13}C NMR (100 MHz, CDCl_3) Tetra (AcO) $_4$ GalEG $_3$ Resorcinarene boat - Acetylated Glycocluster **5b_G**

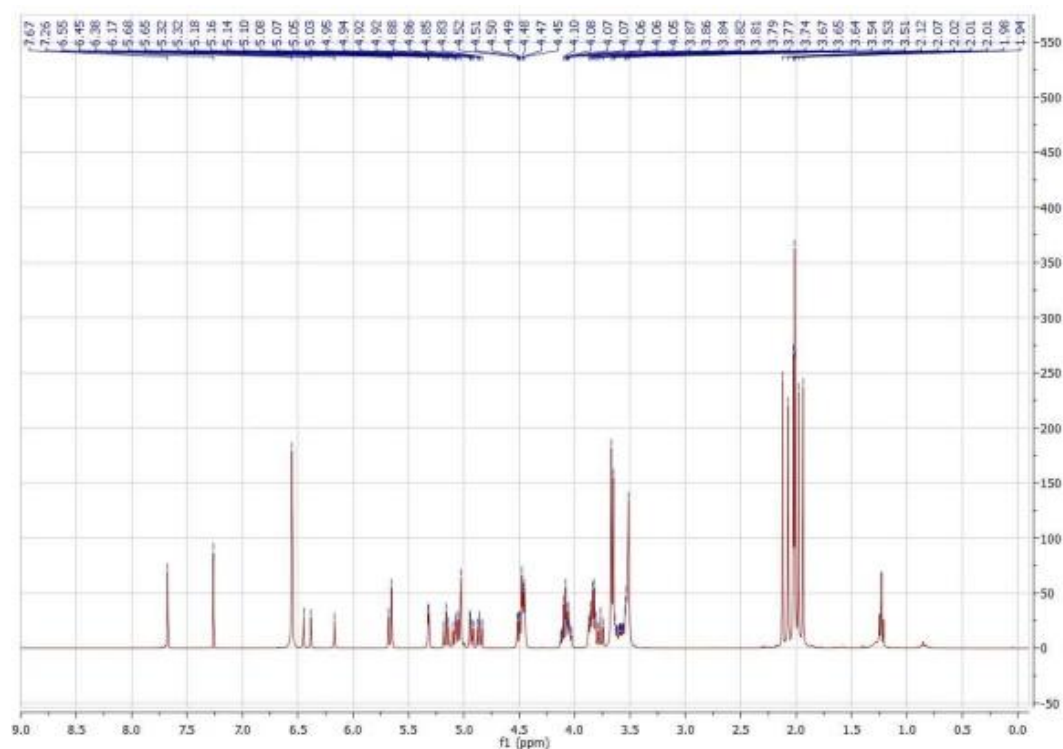


Figure 11: Full ^1H NMR (400 MHz, CDCl_3) Tetra (AcO) $_7$ LacEG $_3$ Resorcinarene chair - Acetylated Glycocluster **5a_L**

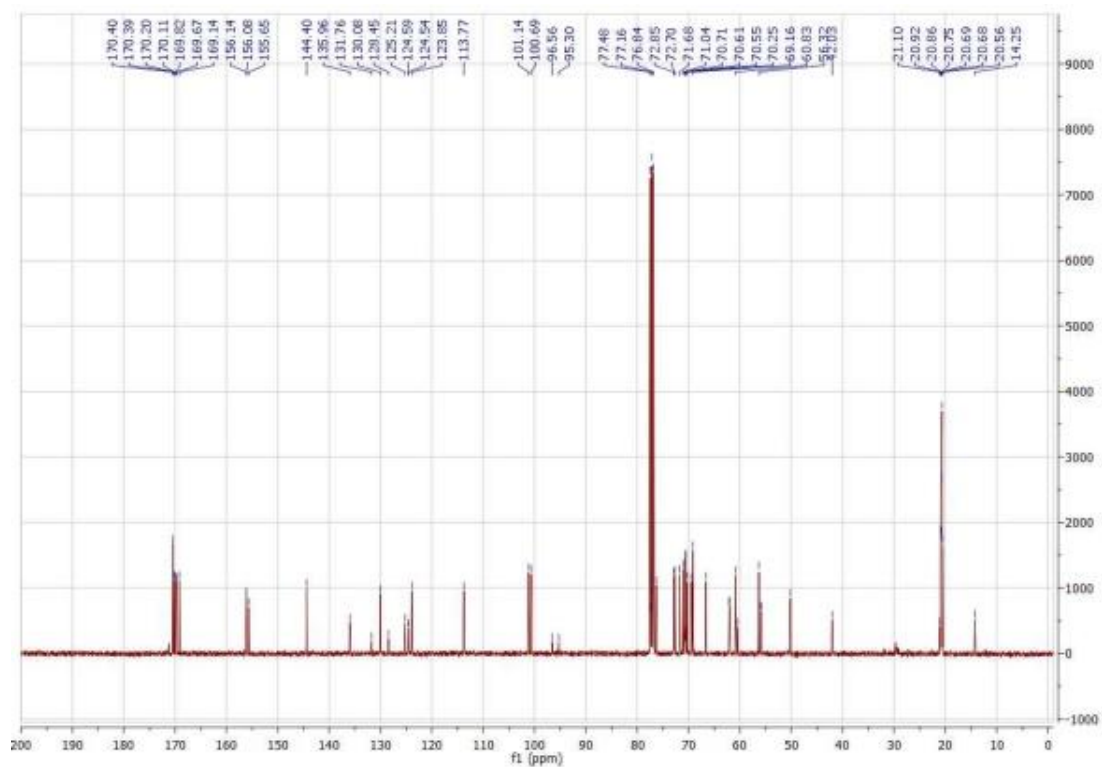


Figure 12: Full ^{13}C NMR (100 MHz, CDCl_3) Tetra (AcO) $_7$ LacEG $_3$ Resorcinarene chair - Acetylated Glycocluster **5a_L**

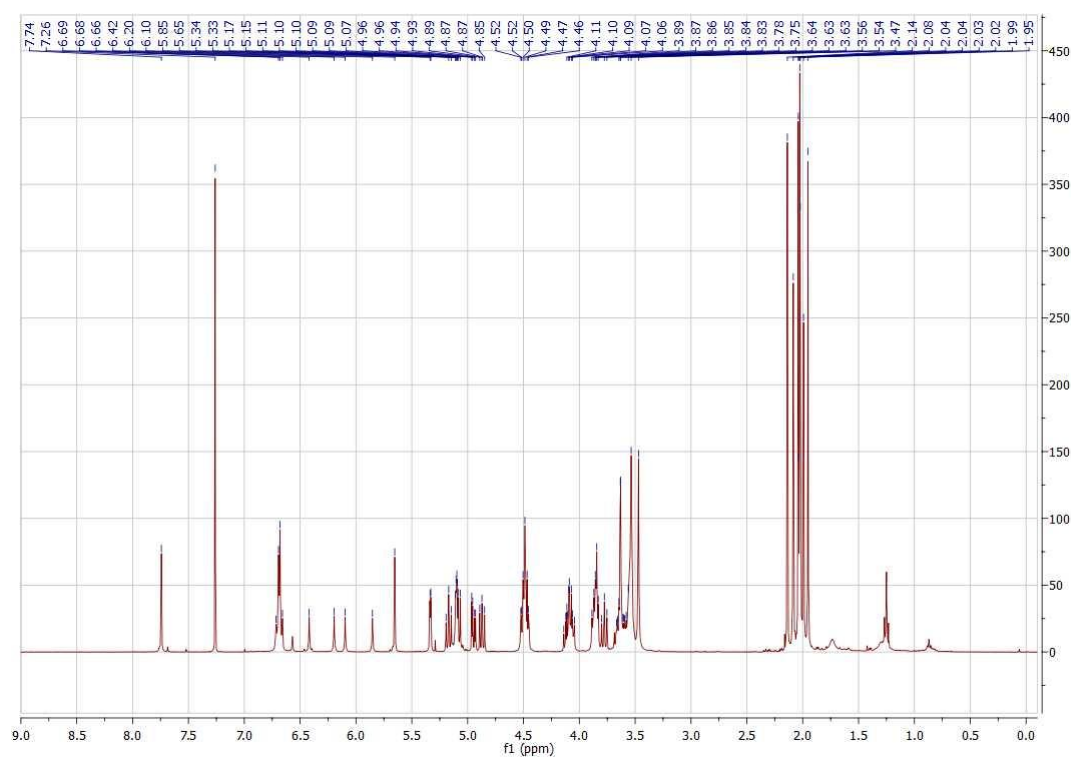


Figure 13: Full ^1H NMR (400 MHz, CDCl_3) Tetra (AcO) $_7$ LacEG $_3$ Resorcinarene boat - Acetylated Glycocluster **5b_L**

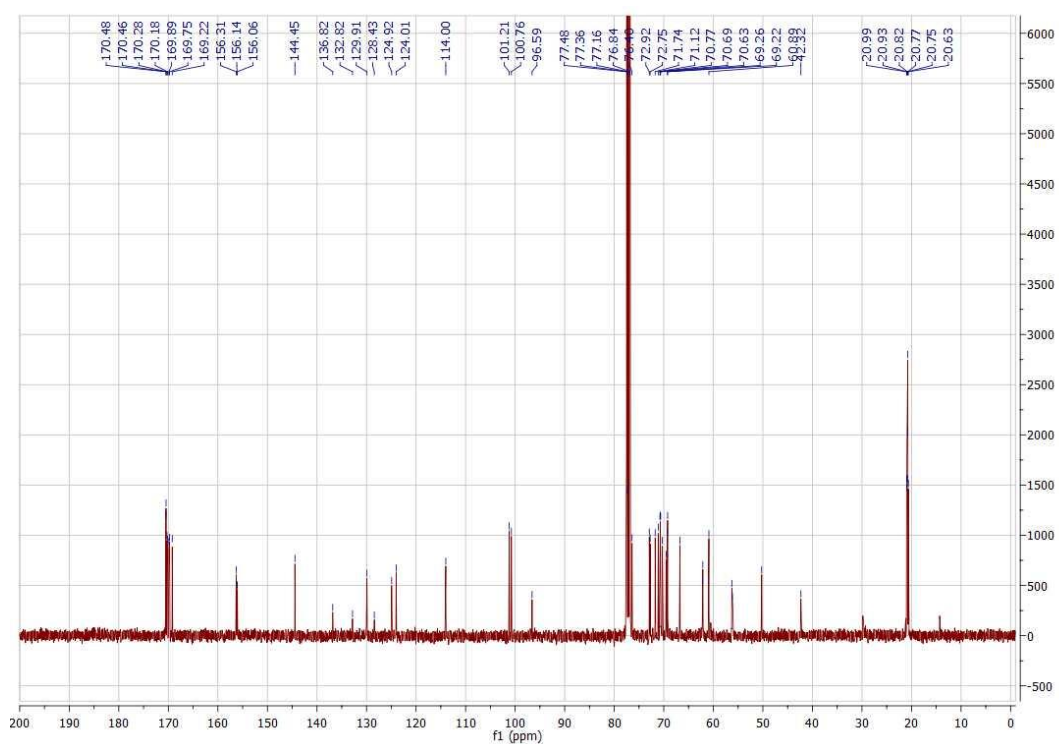


Figure 14: Full ^{13}C NMR (100 MHz, CDCl_3) Tetra (AcO) $_7$ LacEG $_3$ Resorcinarene boat - Acetylated Glycocluster **5b_L**

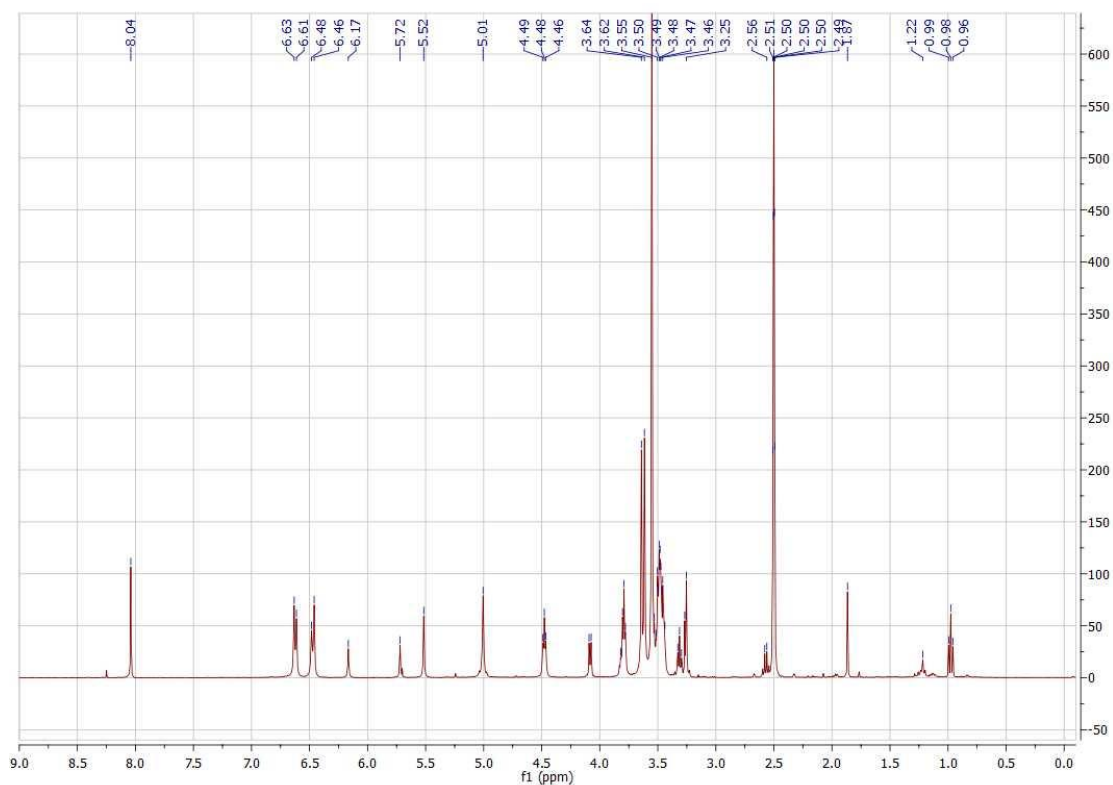


Figure 15: Full ^1H NMR (400 MHz, $\text{DMSO}-d_6 + \varepsilon \text{D}_2\text{O}$) Tetra (HO) $_4$ GalEG $_3$ Resorcinarene chair - Hydroxylated Glycocluster **6a_G**

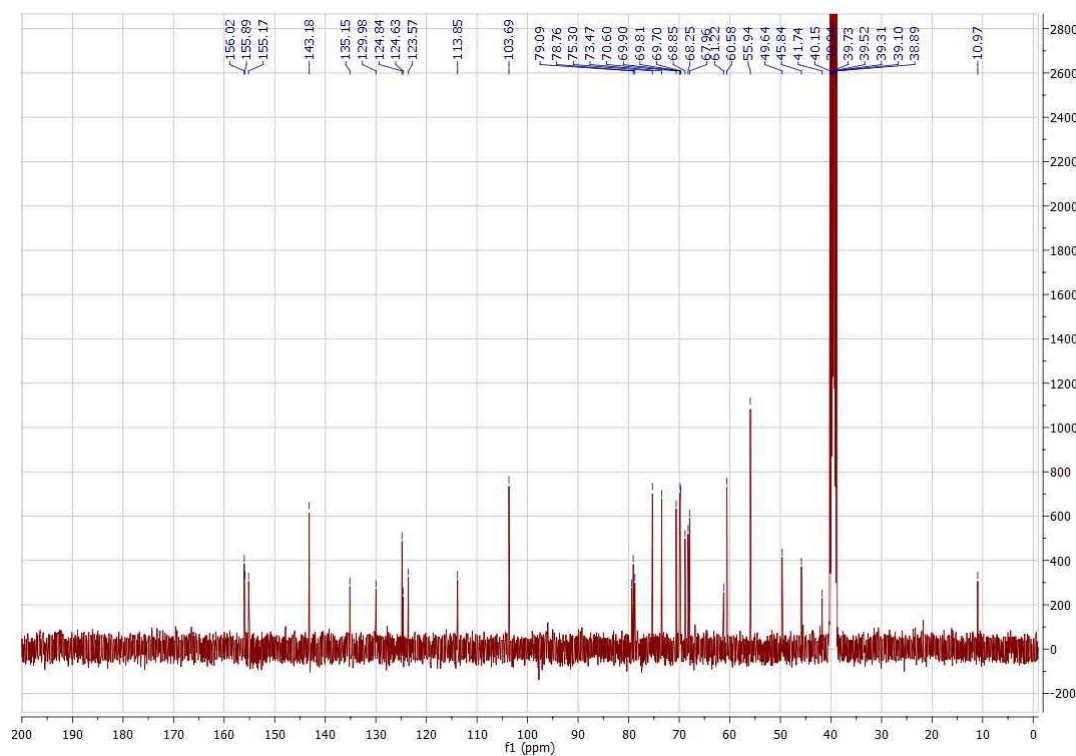


Figure 16: Full ^{13}C NMR (100 MHz, $\text{DMSO-}d_6 + \varepsilon \text{D}_2\text{O}$) Tetra $(\text{HO})_4\text{GalEG}_3$ Resorcinarene chair - Hydroxylated Glycocluster **6a_C**

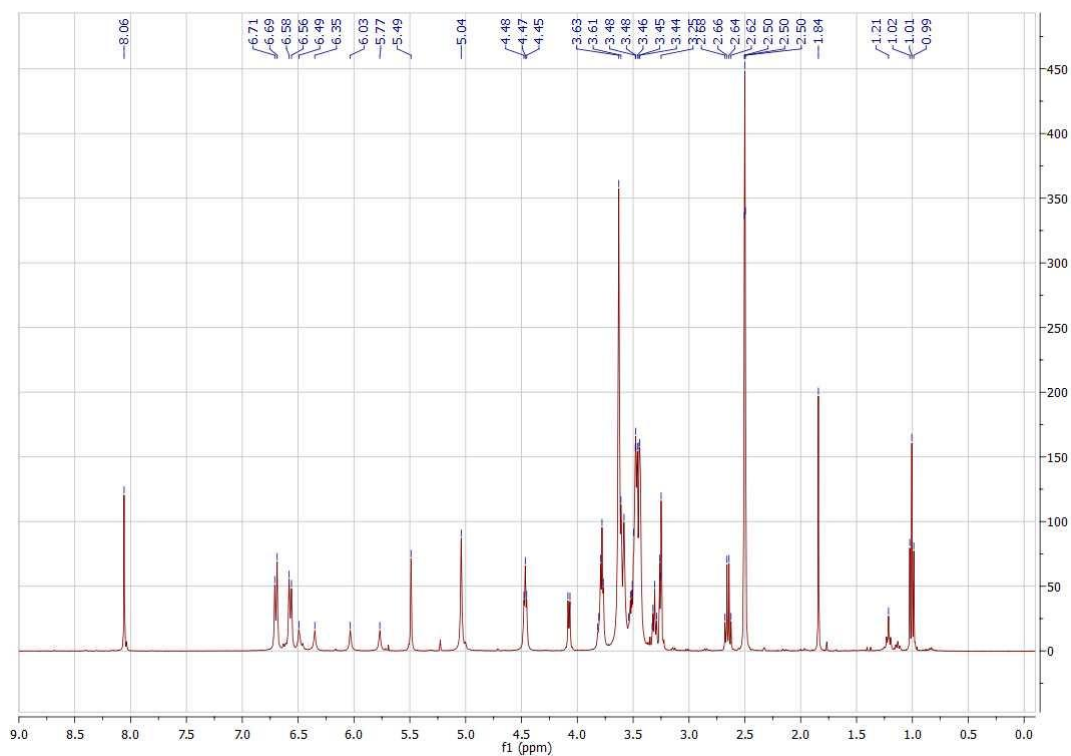
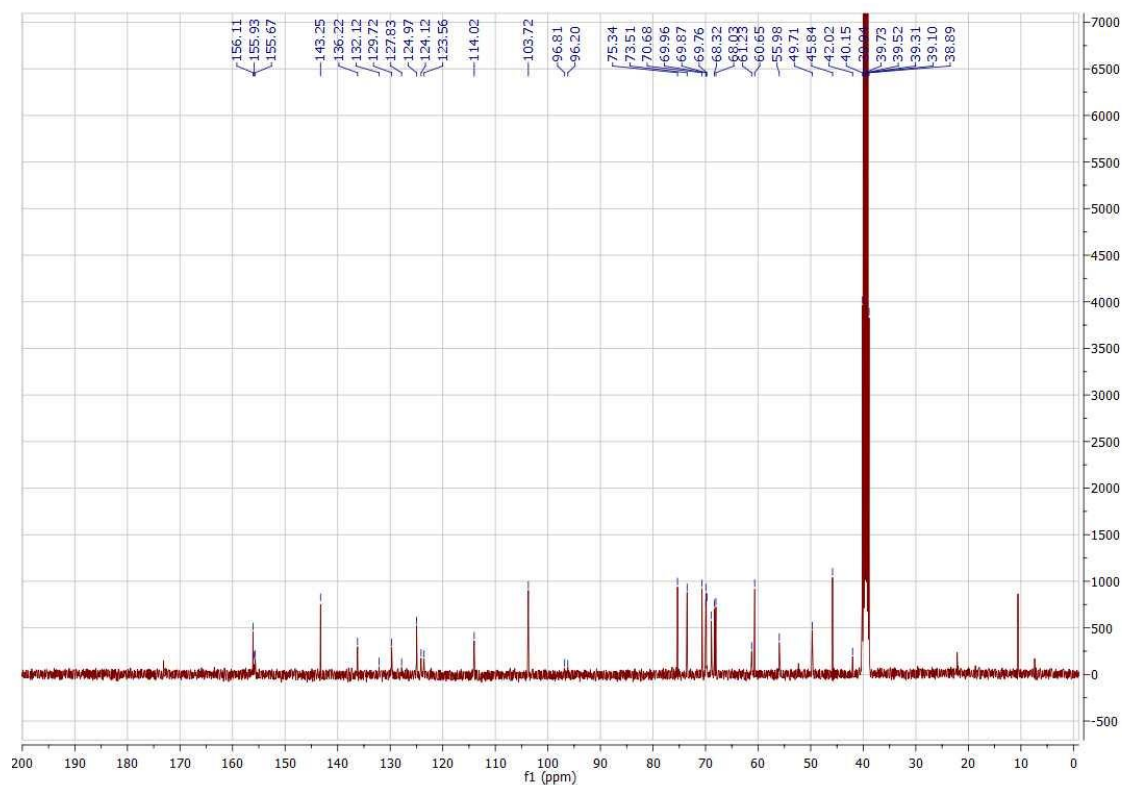


Figure 17: Full ^1H NMR (400 MHz, $\text{DMSO-}d_6 + \varepsilon \text{D}_2\text{O}$) Tetra $(\text{HO})_4\text{GalEG}_3$ Resorcinarene boat - Hydroxylated Glycocluster **6b_C**



Figur

e 18: Full ^{13}C NMR (100 MHz, $\text{DMSO-}d_6 + \varepsilon \text{D}_2\text{O}$) Tetra $(\text{HO})_4\text{GalEG}_3$ Resorcinarene boat - Hydroxylated Glycocluster **6b_G**

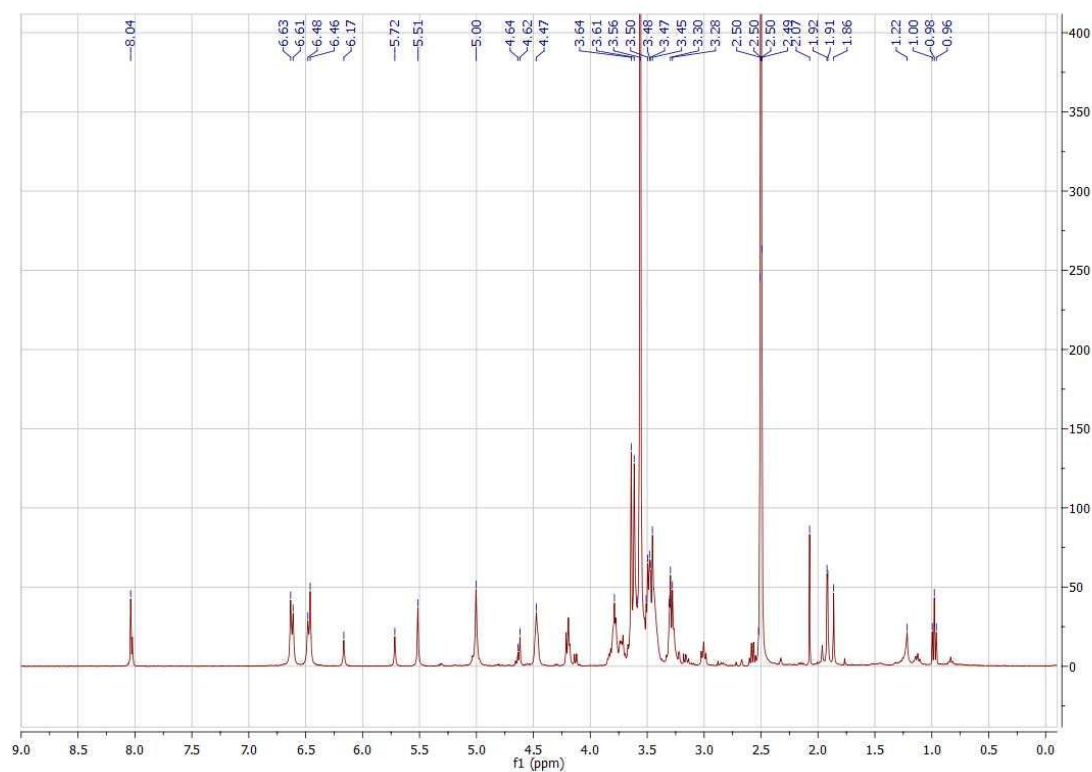


Figure 19: Full ^1H NMR (400 MHz, $\text{DMSO-}d_6 + \varepsilon \text{D}_2\text{O}$) Tetra $(\text{HO})_7\text{LacEG}_3$ Resorcinarene chair - Hydroxylated Glycocluster **6a_L**

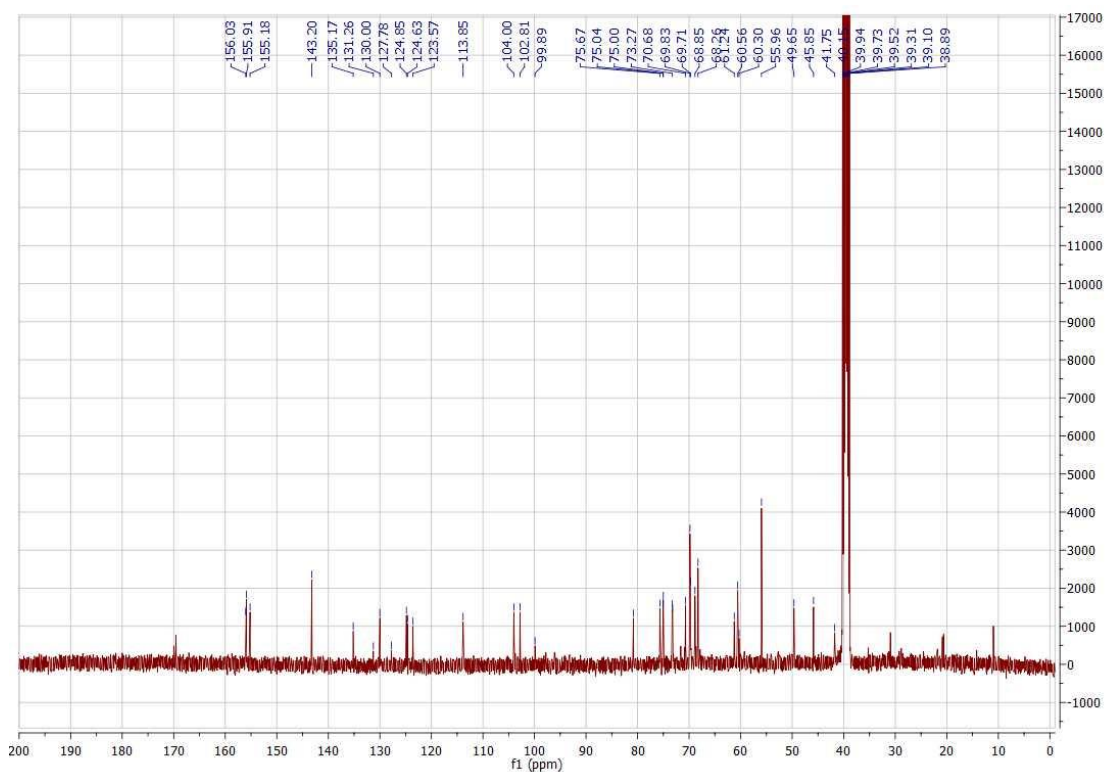


Figure 20: Full ^{13}C NMR (100 MHz, $\text{DMSO-}d_6 + \varepsilon \text{D}_2\text{O}$) Tetra (HO) $_7$ LacEG $_3$ Resorcinarene chair - Hydroxylated Glycocluster **6a_L**

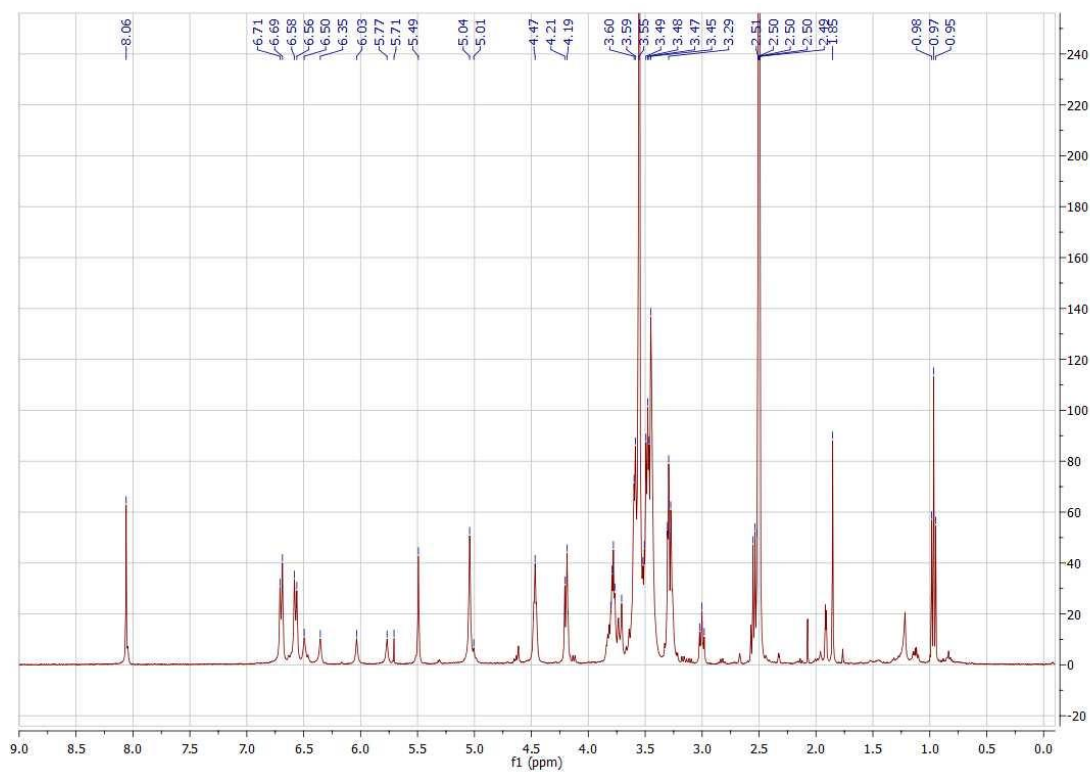


Figure 21: Full ^1H NMR (400 MHz, $\text{DMSO-}d_6 + \varepsilon \text{D}_2\text{O}$) Tetra (HO) $_7$ LacEG $_3$ Resorcinarene boat - Hydroxylated Glycocluster **6b_L**

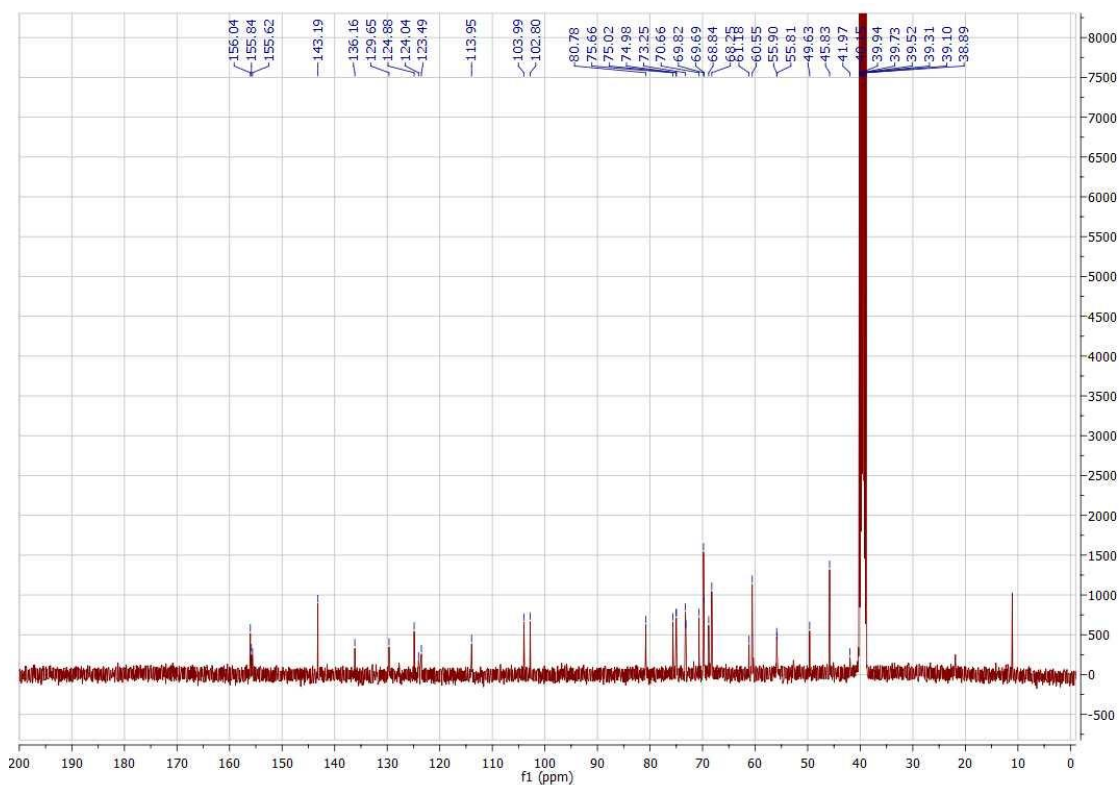


Figure 22: Full ^{13}C NMR (100 MHz, $\text{DMSO-}d_6 + \varepsilon \text{D}_2\text{O}$) Tetra (HO) $_7$ LacEG $_3$ Resorcinarene boat - Hydroxylated Glycocluster **6b_L**

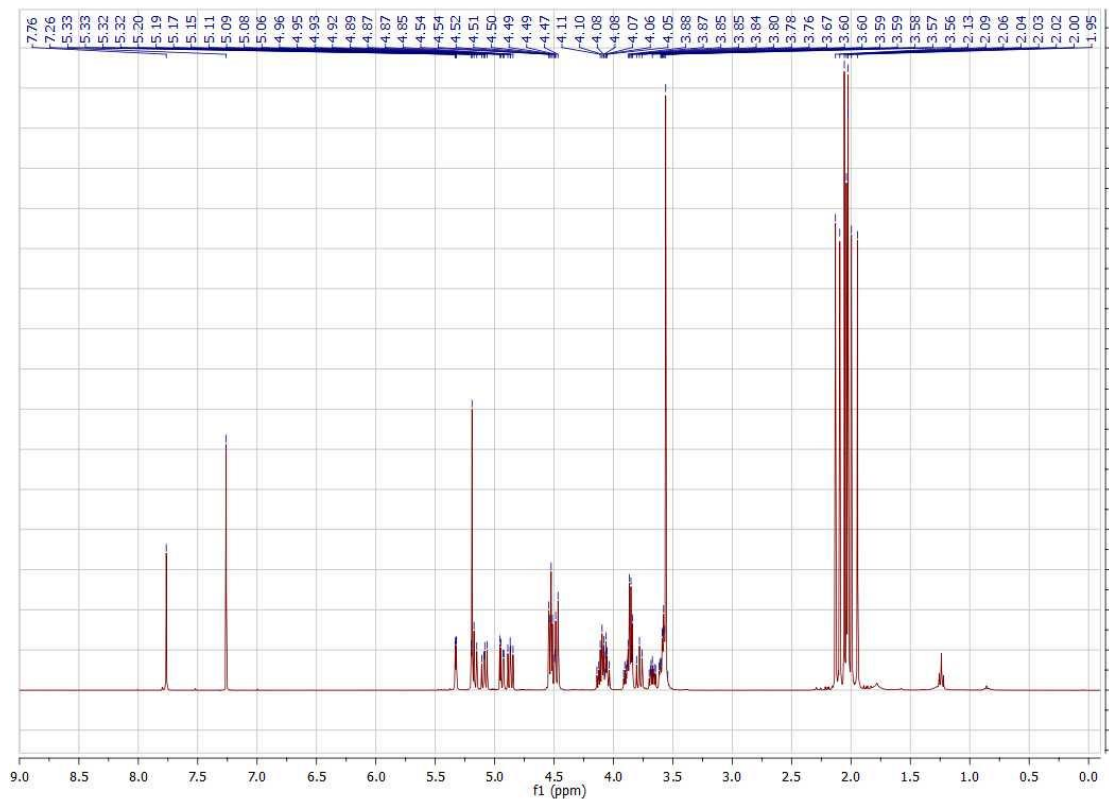


Figure 23: Full ^1H NMR (400 MHz, CDCl_3) 1-[1,2,3-Triazol-4-yl-(acetoxy)methyl]-3,6-dioxaoct-8-yl 2,3,6,2',3',4',6'-hepta-*O*-acetyl- β -D-lactoside **8_L**

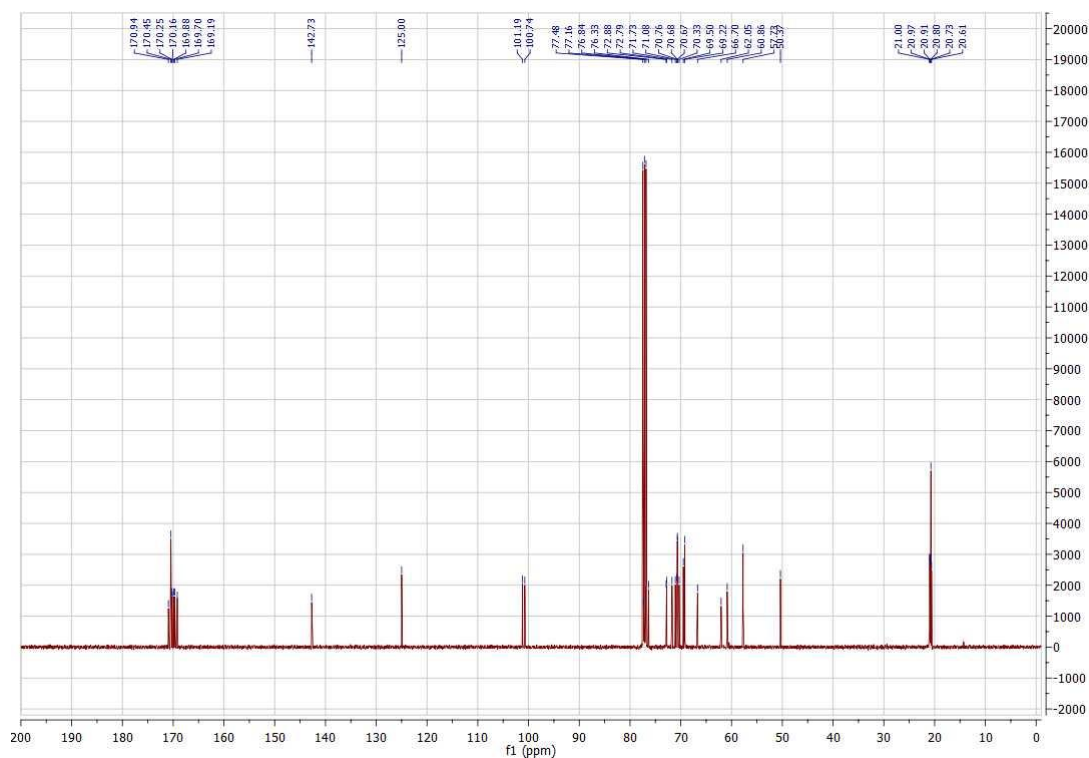


Figure 24: Full ^{13}C NMR (100 MHz, CDCl_3) 1-[1,2,3-Triazol-4-yl-(acetoxy)methyl]-3,6-dioxaoct-8-yl 2,3,6,2',3',4',6'-hepta-*O*-acetyl- β -D-lactoside **8_L**

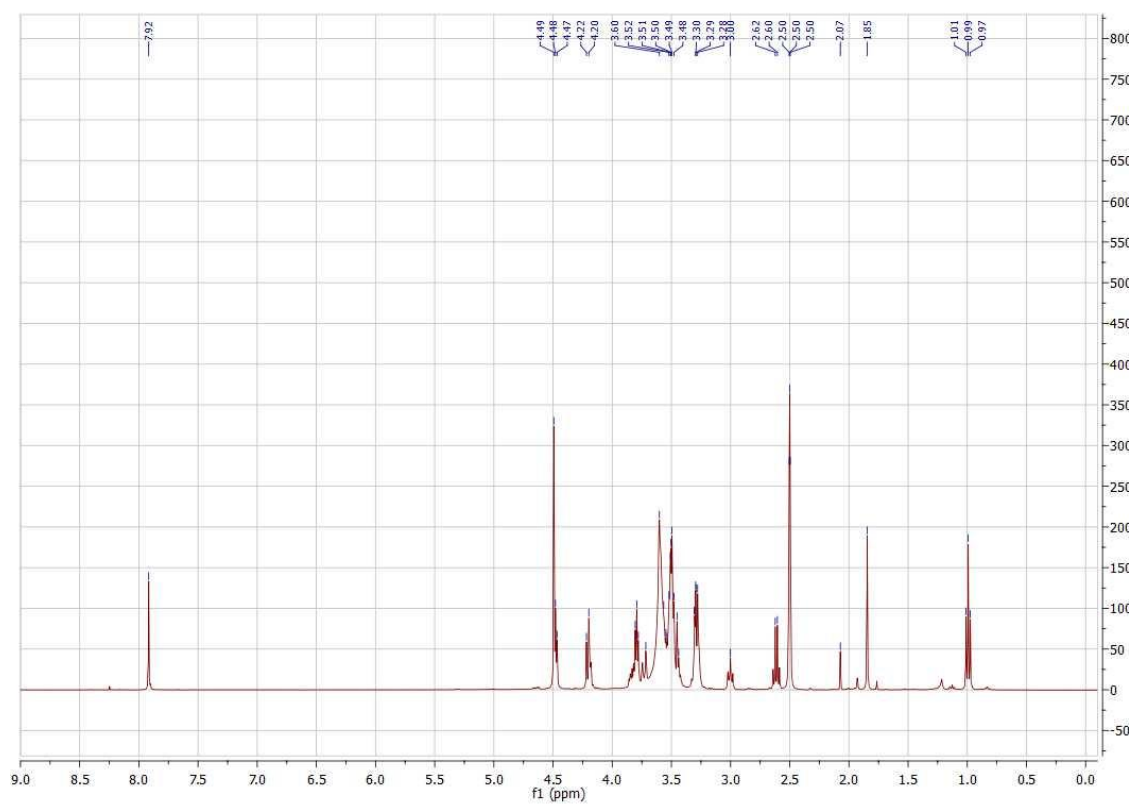


Figure 25: Full ^1H NMR (400 MHz, $\text{DMSO-}d_6 + \epsilon \text{ D}_2\text{O}$) 1-[1,2,3-Triazol-4-yl-(hydroxy)methyl]-3,6-dioxaoct-8-yl β -D-lactoside **9_L**

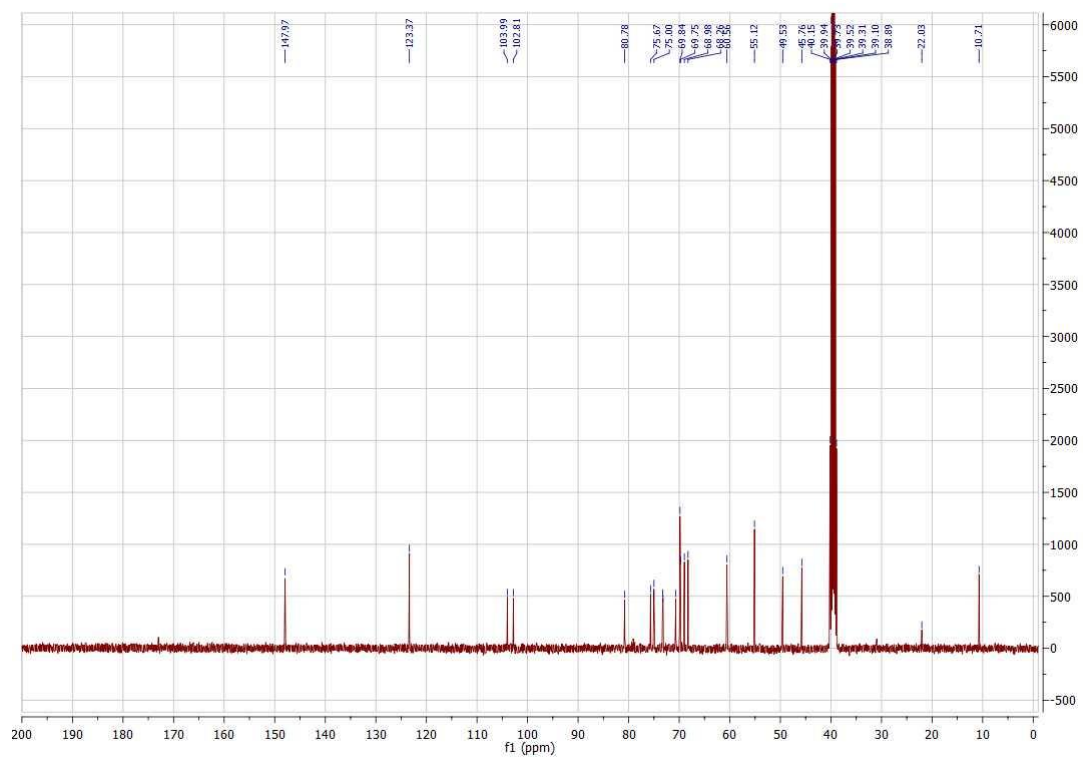


Figure 26: Full ^{13}C NMR (100 MHz, $\text{DMSO-}d_6 + \epsilon \text{D}_2\text{O}$) 1-[1,2,3-Triazol-4-yl-(hydroxy)-methyl]-3,6-dioxaoct-8-yl β -D-lactoside **9_L**

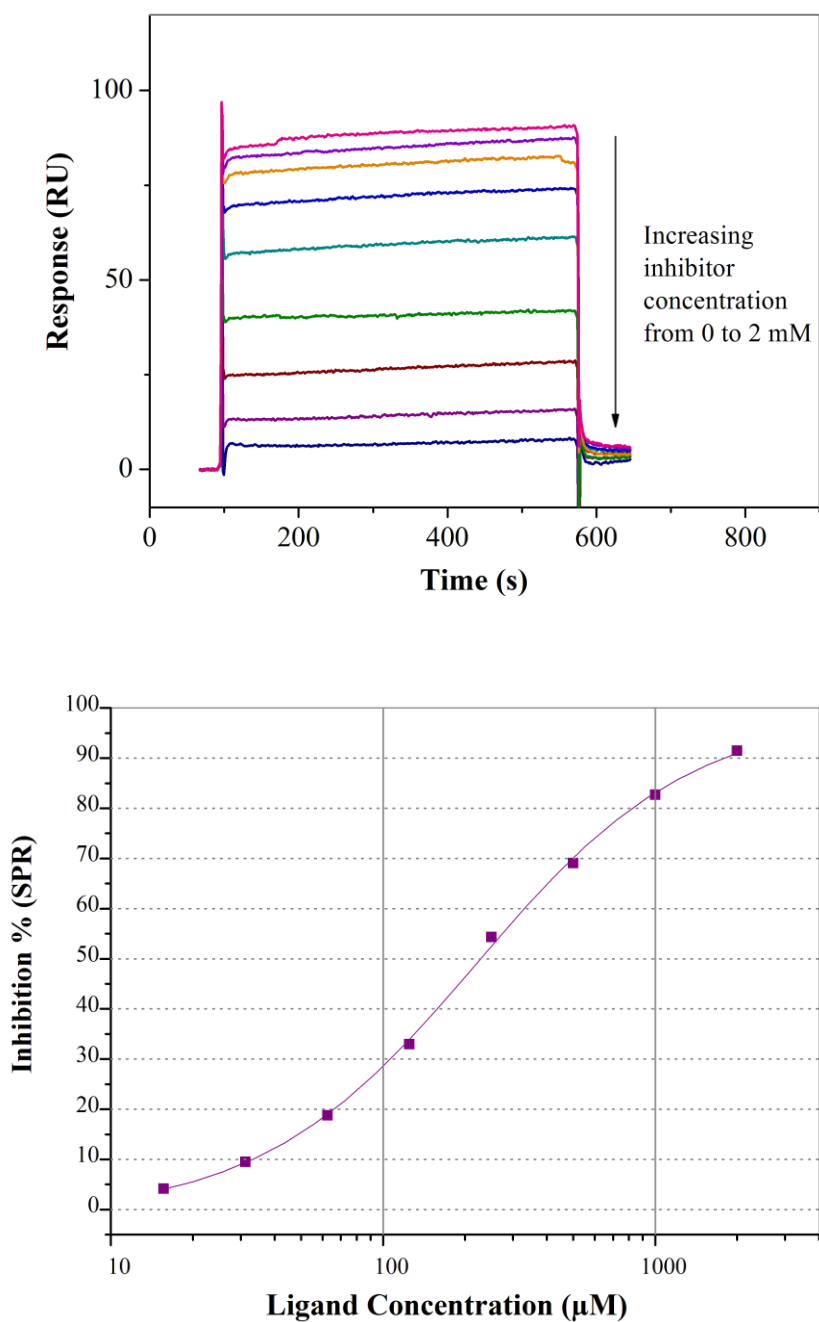


Figure 27: SPR sensorgram measured for $\mathbf{9_L}$ incubated with PA-IL (5 μM) and injected on a CM5 chip coated with Streptavidin/Biotin-PAA- α -D-Galactose. a) sensorgram, b) corresponding inhibition curve. PAA=Polyacrylamide