

Supporting information for:

Isolation and Characterization of Galloylglucoses Effective against Multidrug-Resistant Strains of *Escherichia coli* and *Klebsiella pneumoniae*.

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Table S1: Summary of preparative HPLC parameters for isolation and purification of subfractions/compounds from the purified water fraction.

| Fraction to be Refined | Stationary phase | Mobile phase composition as %v/v of acetonitrile in water and other chromatographic conditions. (UV detection wavelength = 254 nm) | Recovered subfractions/ compounds |
|-------------------------|---|---|---|
| Purified water fraction | ZORBAX XDB-C18, 21.2 x 150 mm, 5 μ m (Agilent, US) | 20 – 20% (0 – 3 min), 20 – 45% (3 – 32 min), 45 – 45% (32 – 33 min), 45 – 95% (33 – 35 min), 95 – 95% (35 – 36 min), 95 – 20% (36 – 38 min). Sample conc. = 250 mg/ mL, injection volume = 50 μ L, Flow rate = 4 ml/min. | pooled first minor fractions, and major fractions A, B, C, D, E |
| A | | 20 – 20% (0 – 29 min), 20 – 50% (29 – 32 min), 50 – 50% (32 – 34 min), 50 – 20% (34 – 36 min), 20 – 20% (36 – 40 min). Sample conc. = 100 mg/ mL, injection volume = 100 μ L, Flow rate = 4 ml/min. | A1, A2 |
| B | | 0 – 20% (0 – 32 min), 20 – 75% (32 – 35 min), 75 – 75% (35 – 38 min), 75 – 20% (38 – 41 min), 20 – 20% (41 – 44 min). Sample conc. = 22.5 mg/ mL, injection volume = 8 μ L, Flow rate = 6 ml/min. | B1, B2, B3, B4&5, B6 |
| C | | 5 – 5 % (0 – 5 min), 5 – 26% (5 – 7 min), 26 – 26% (7 – 27 min), 26 – 5% (27 – 29 min), 5 – 5% (29 – 31 min). Sample conc. = 100 mg/ mL, injection volume = 20 μ L, Flow rate = 4 ml/min. | C1, C2, C3 |
| D | | 31 – 31% (0 – 32 min) Sample conc. = 100 mg/ mL, injection volume = 20 μ L, Flow rate = 2 ml/min. | D1, D2, D3&4 |
| E | | 31 – 31% (0 – 35 min) Sample conc. = 100 mg/ mL, injection volume = 35 μ L, Flow rate = 2 ml/min. | E1, E2, E3&4, E5 |
| B4&5 | ZORBAX Eclipse XDB-18, Semi-Preparative 9.4 x 250 mm, 5 μ m (Agilent, US) | 0 – 17.5% (0 – 34 min), 17.5 – 75% (34 – 37 min), 75 – 75% (37 – 41 min), 75 – 17.5% (41 – 43 min), 17.5 – 17.5 % (29 – 31 min). Sample conc. = 13.5 mg/ mL, injection volume = 50 μ L, Flow rate = 4 ml/min. | B4, B5 |

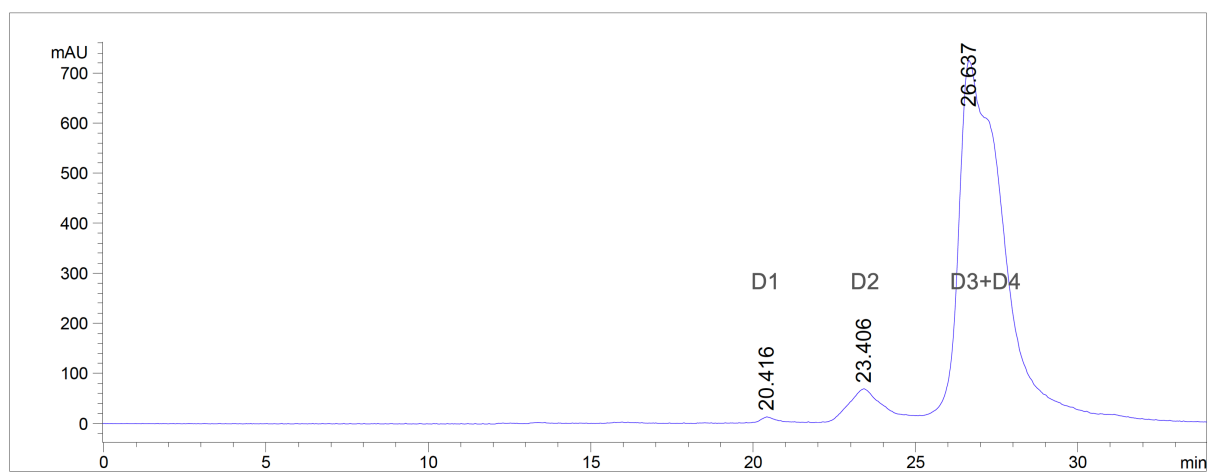


Figure S1: UV chromatogram subfraction D

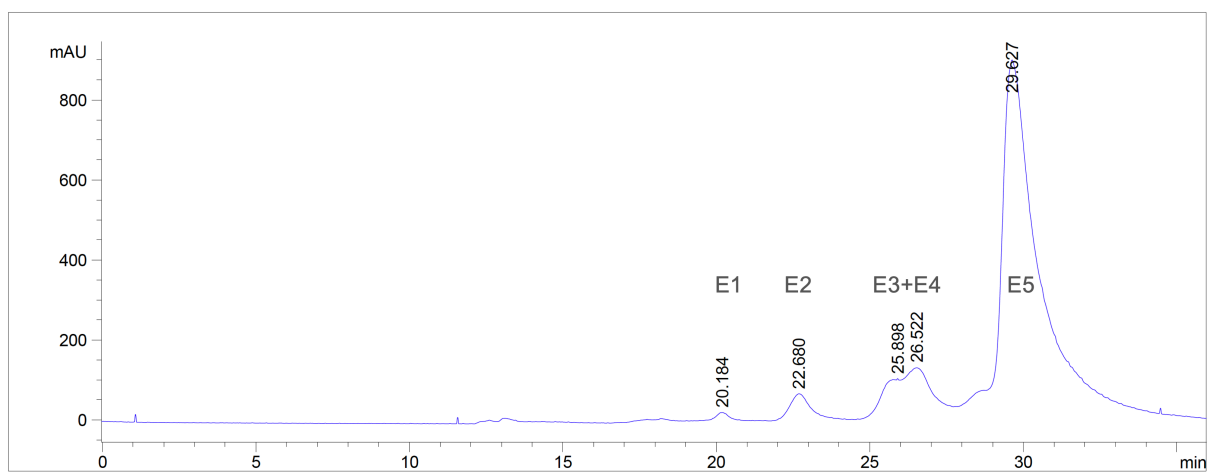


Figure S2: UV chromatogram of subfraction E

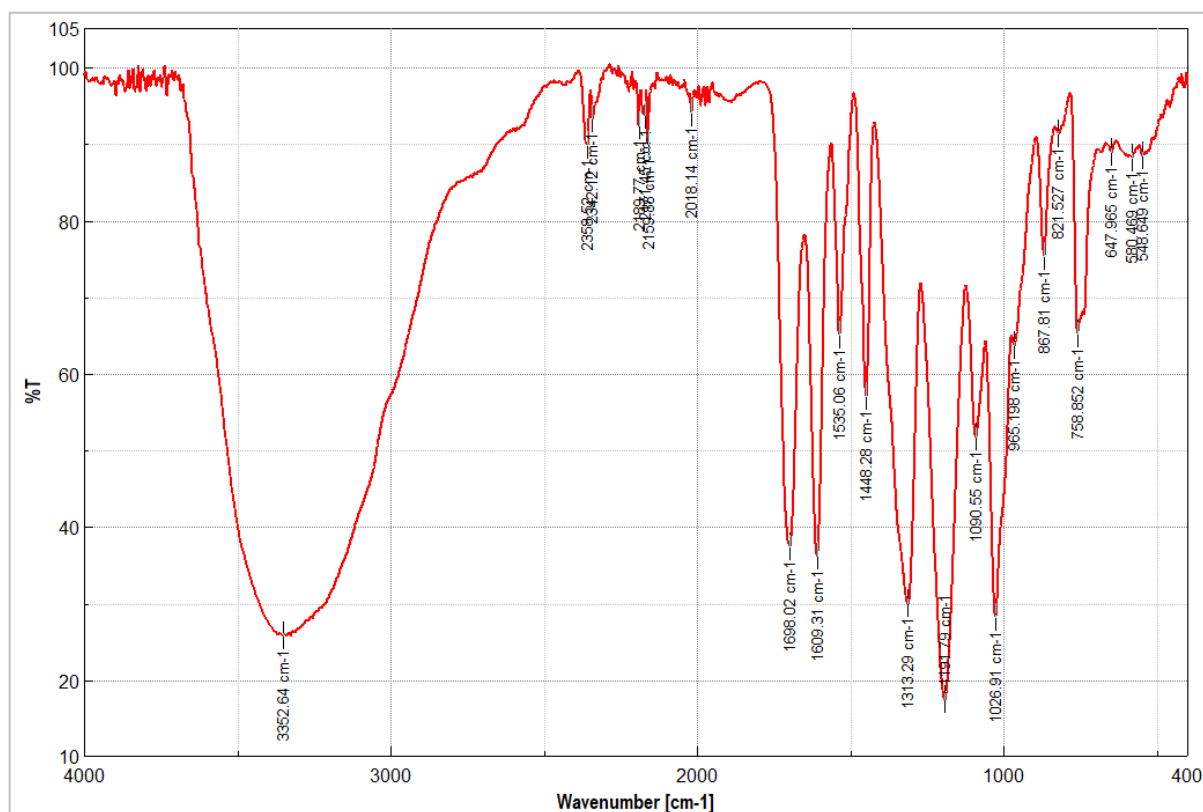


Figure S3: Infrared spectrum of 1,2,3,4,6-penta-O-galloyl-β-D-glucose (NMA2)

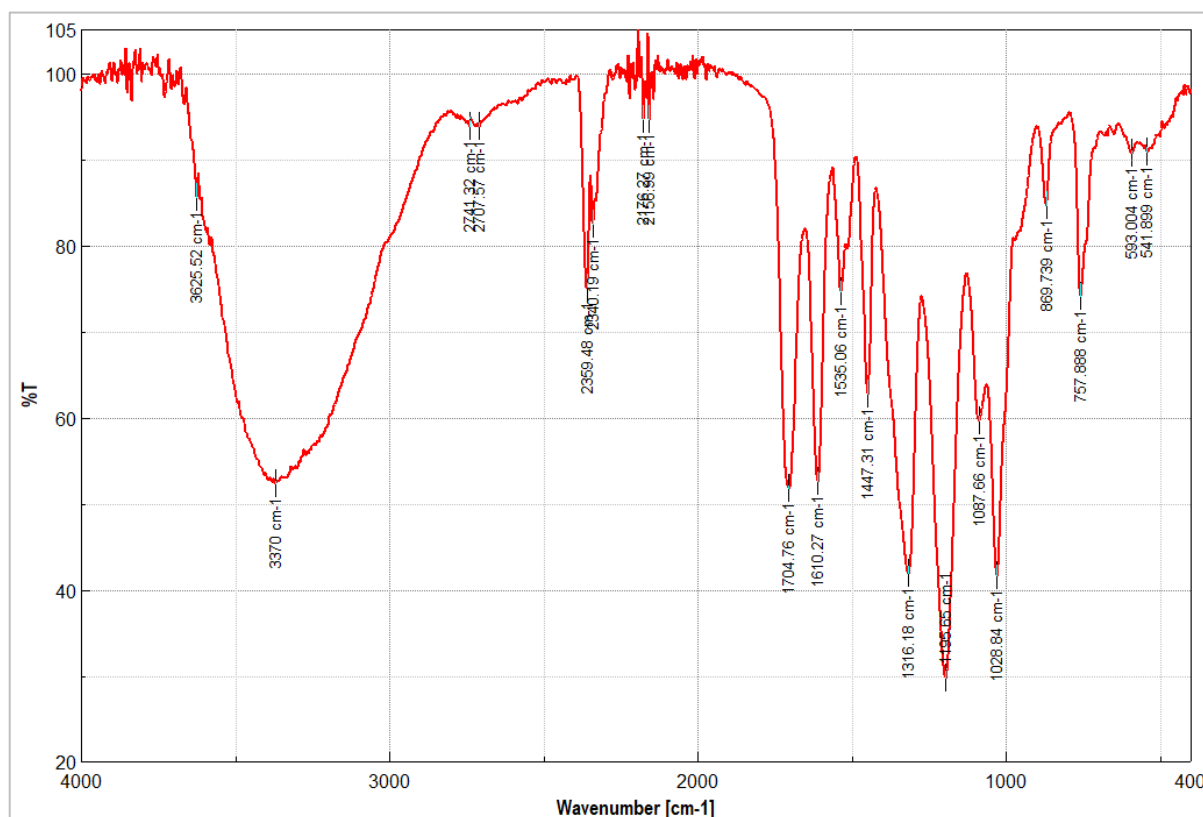


Figure S4: Infrared spectrum of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl-β-D-glucose (NMB4)

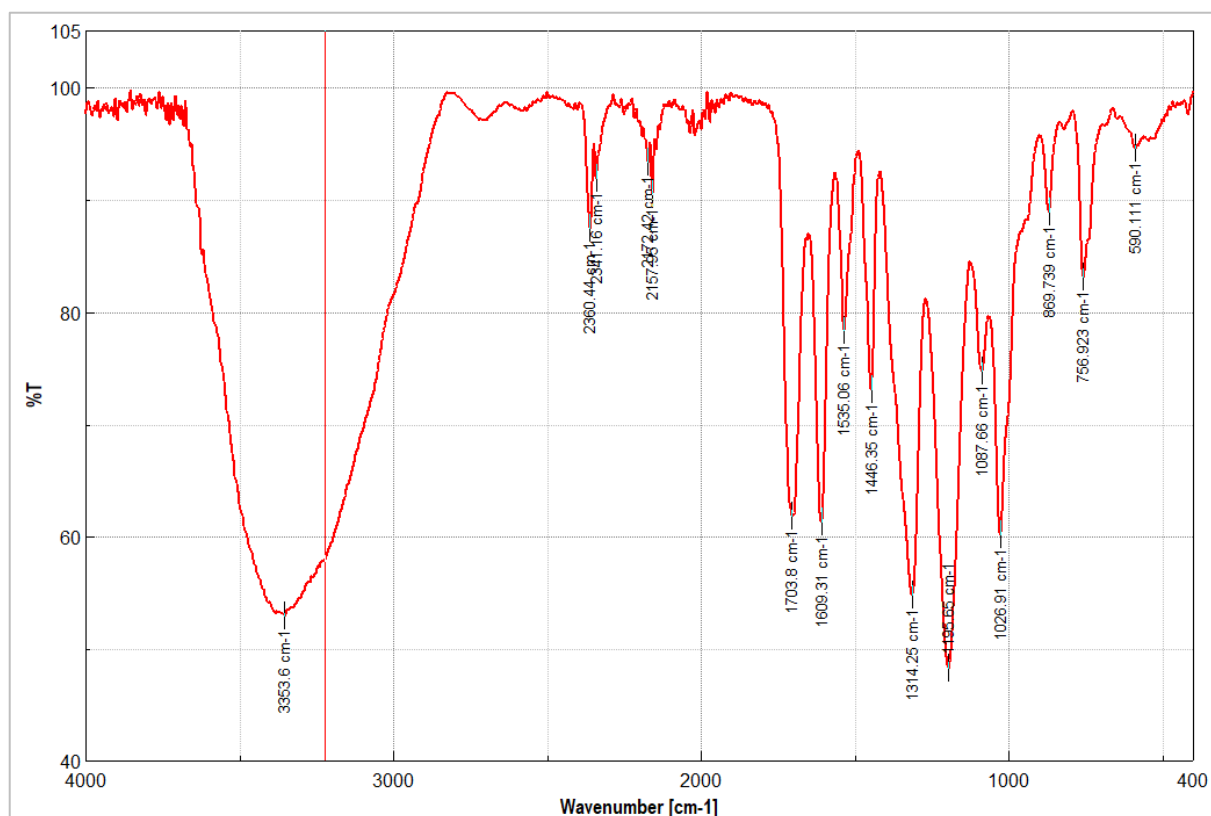


Figure S4: Infrared spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl-β-D-glucose (NMB6)

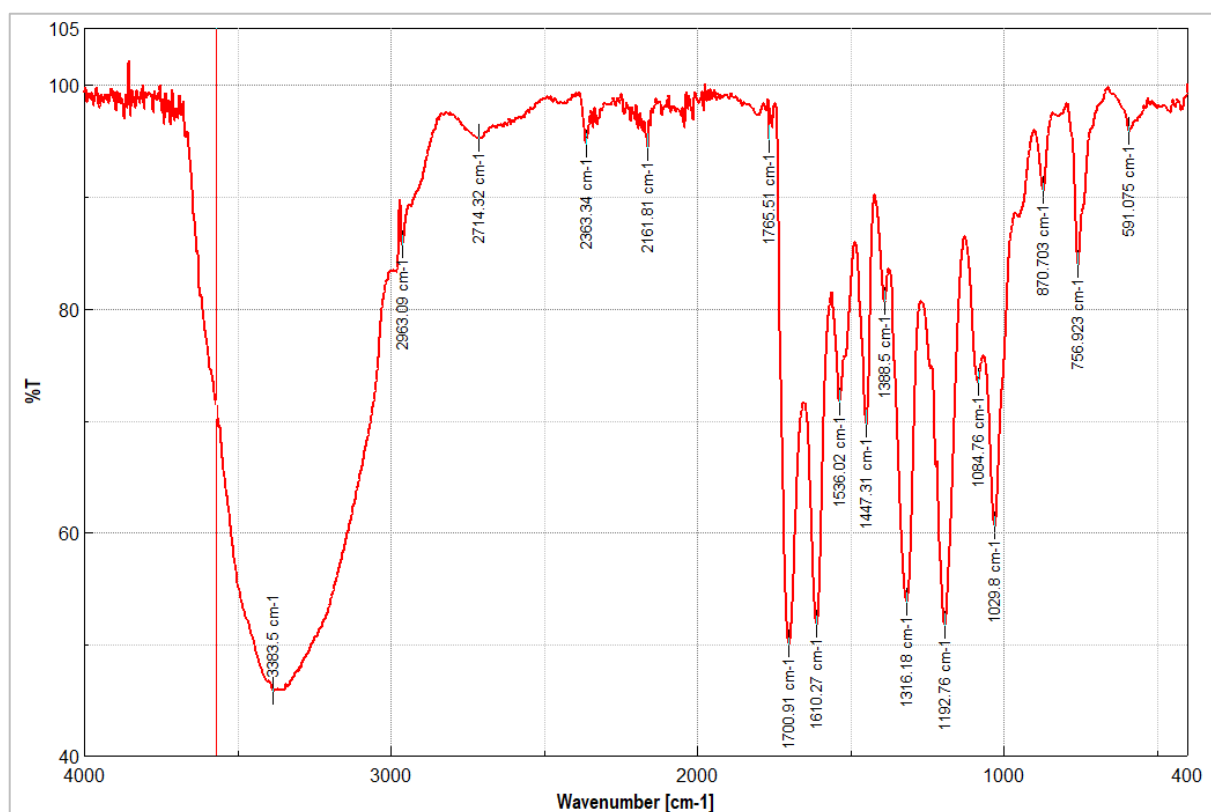


Figure S6: Infrared spectrum of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl-β-D-glucose (NMC3)

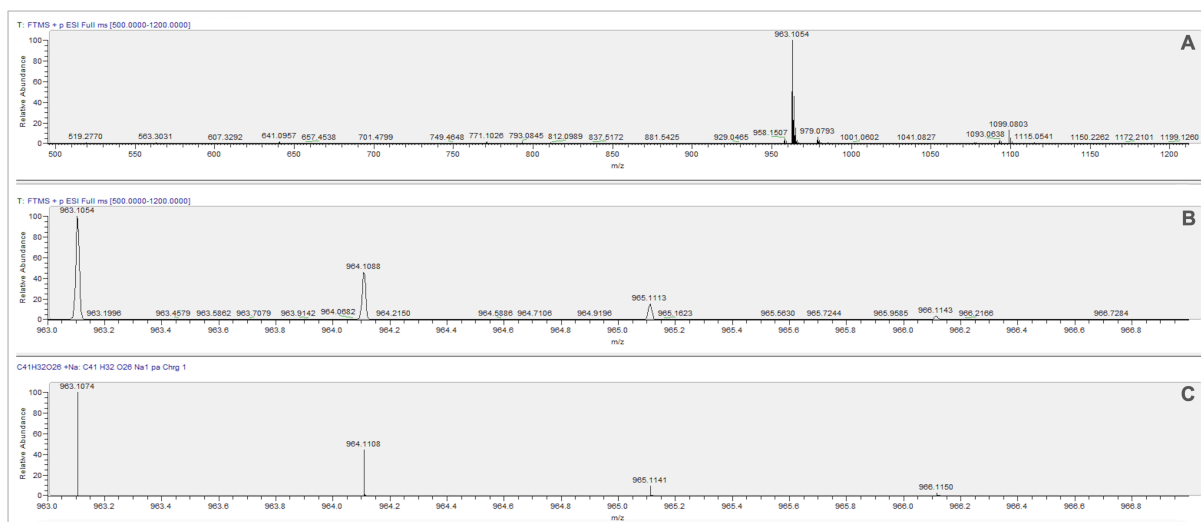


Figure S7: HR-ESI-MS spectra of 1,2,3,4,6-penta-O-galloyl-β-D-glucose (NMA2) showing the full mass spectrum (A), zoom in of the major peak region (B) and simulated spectrum for the shown molecular formula (C).

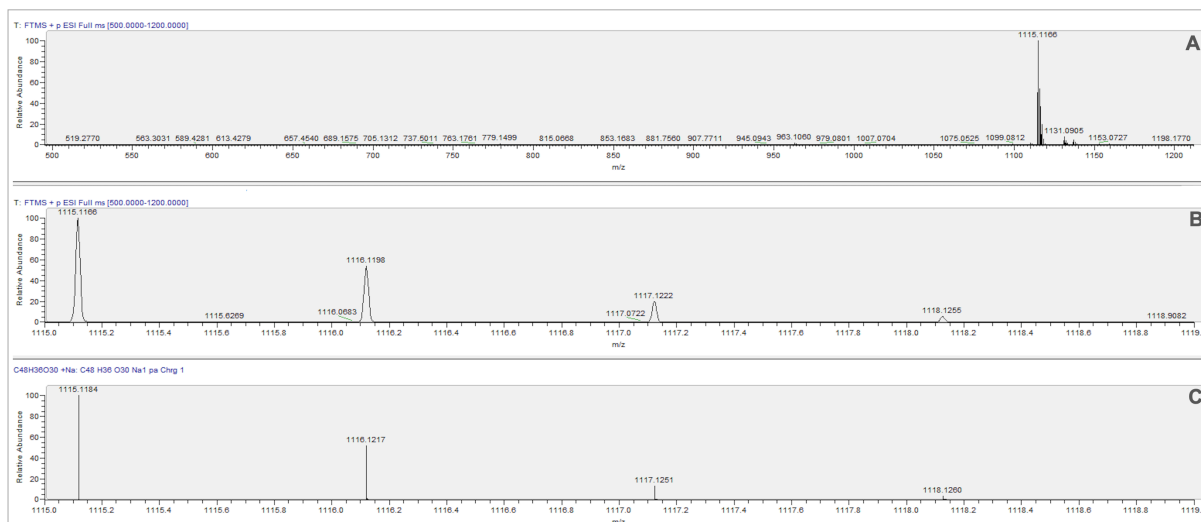


Figure S8: HR-ESI-MS spectra of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl-β-D-glucose (NMB4) showing the full mass spectrum (A), zoom in of the major peak region (B) and simulated spectrum for the shown molecular formula (C).

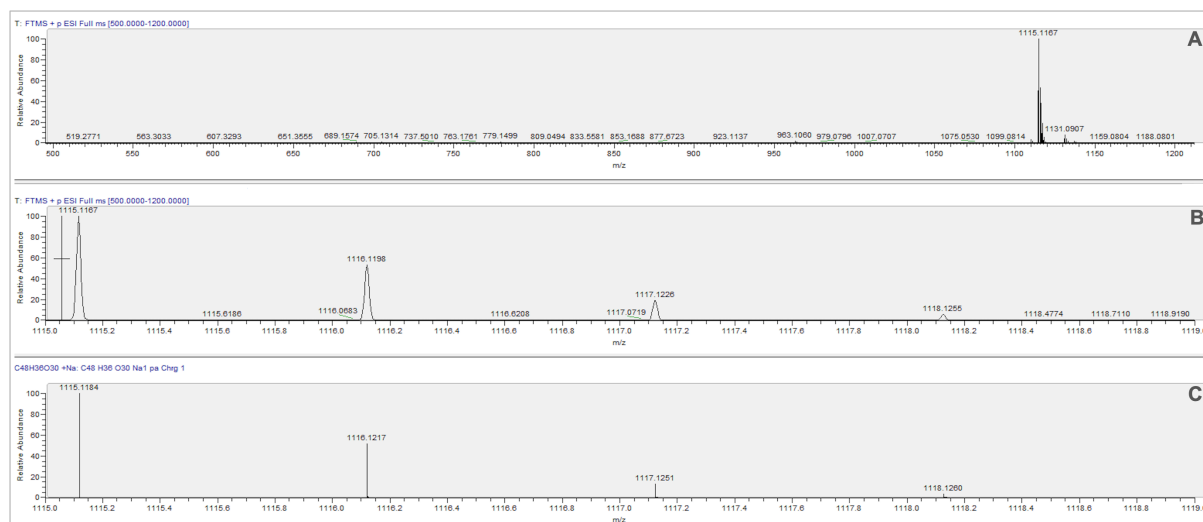


Figure S9: HR-ESI-MS spectra of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl-β-D-glucose (NMB6) showing the full mass spectrum (A), zoom in of the major peak region (B) and simulated spectrum for the shown molecular formula (C).

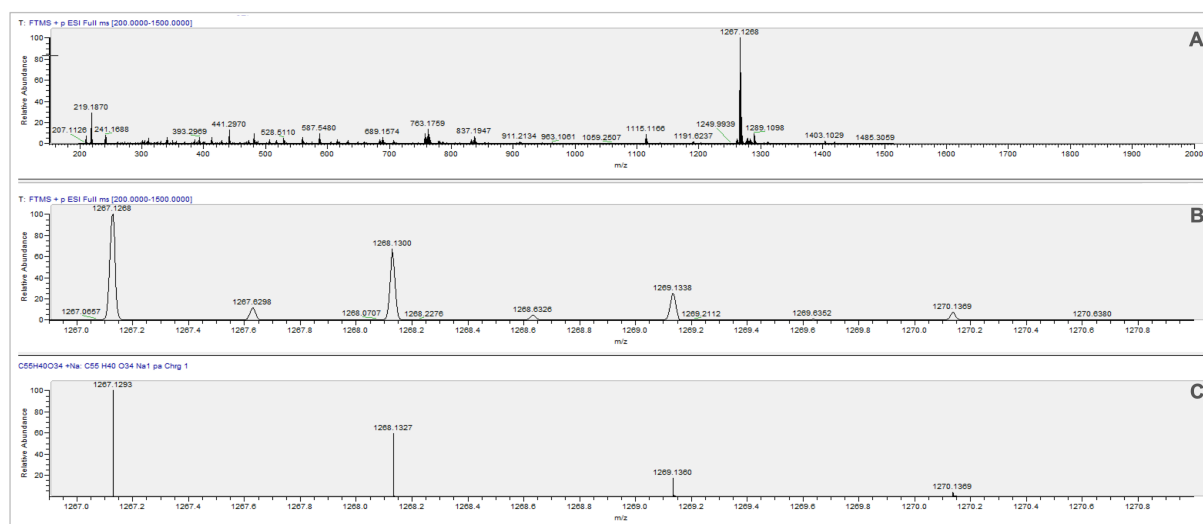


Figure S10: HR-ESI-MS spectra of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl-β-D-glucose (NMC3) showing the full mass spectrum (A), zoom in of the major peak region (B) and simulated spectrum for the shown molecular formula (C).

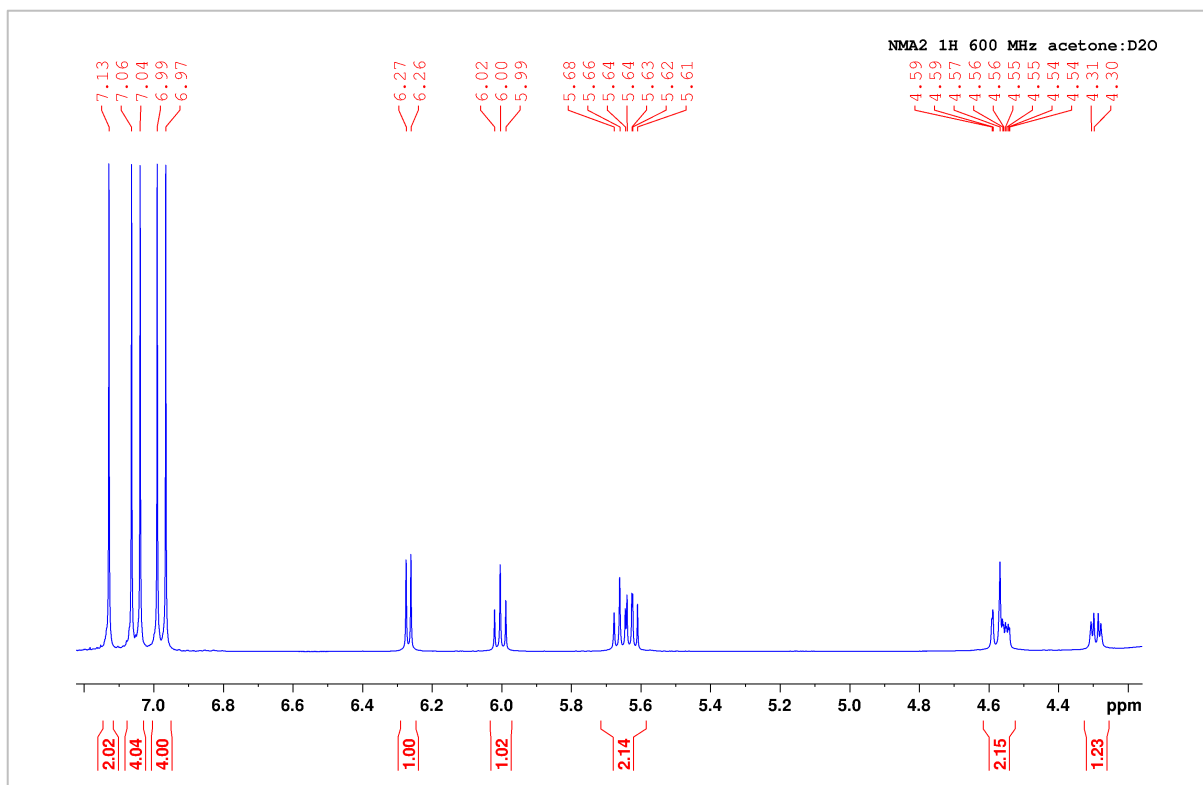


Figure S11: ^1H spectrum of 1,2,3,4,6-penta-O-galloyl- β -D-glucose (NMA2)

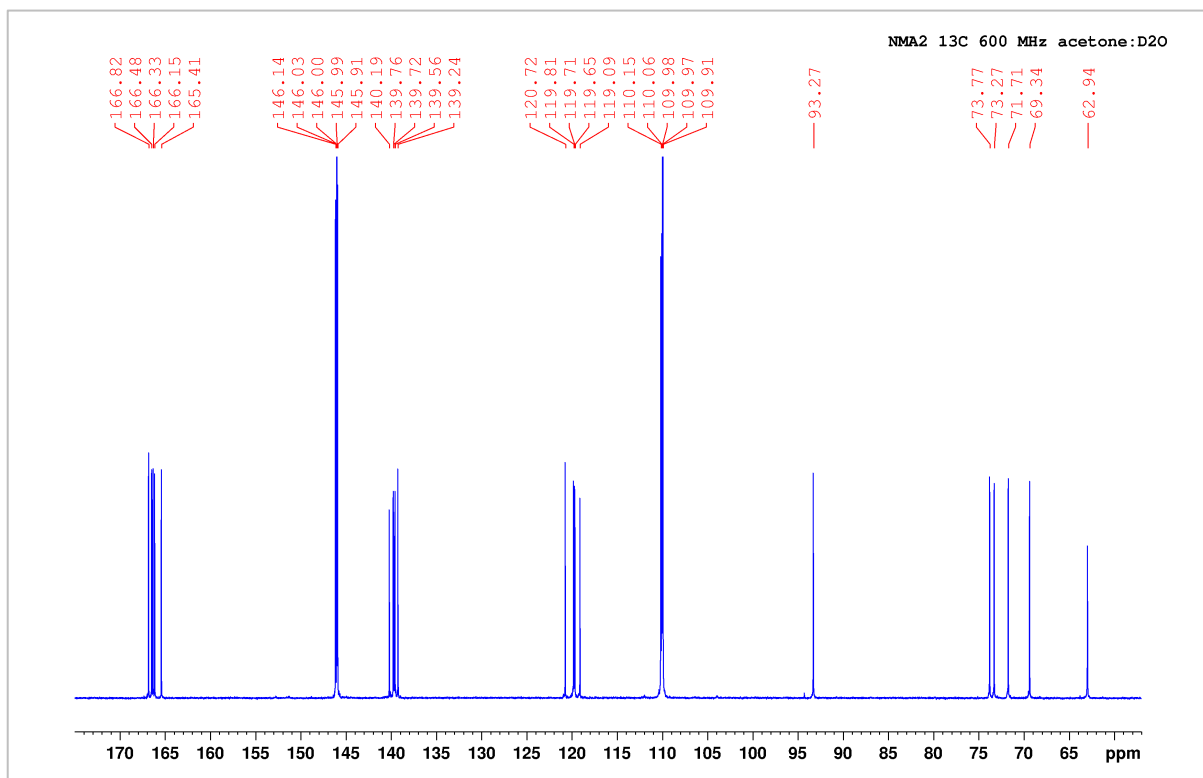


Figure S12: ^{13}C spectrum of 1,2,3,4,6-penta-O-galloyl- β -D-glucose (NMA2)

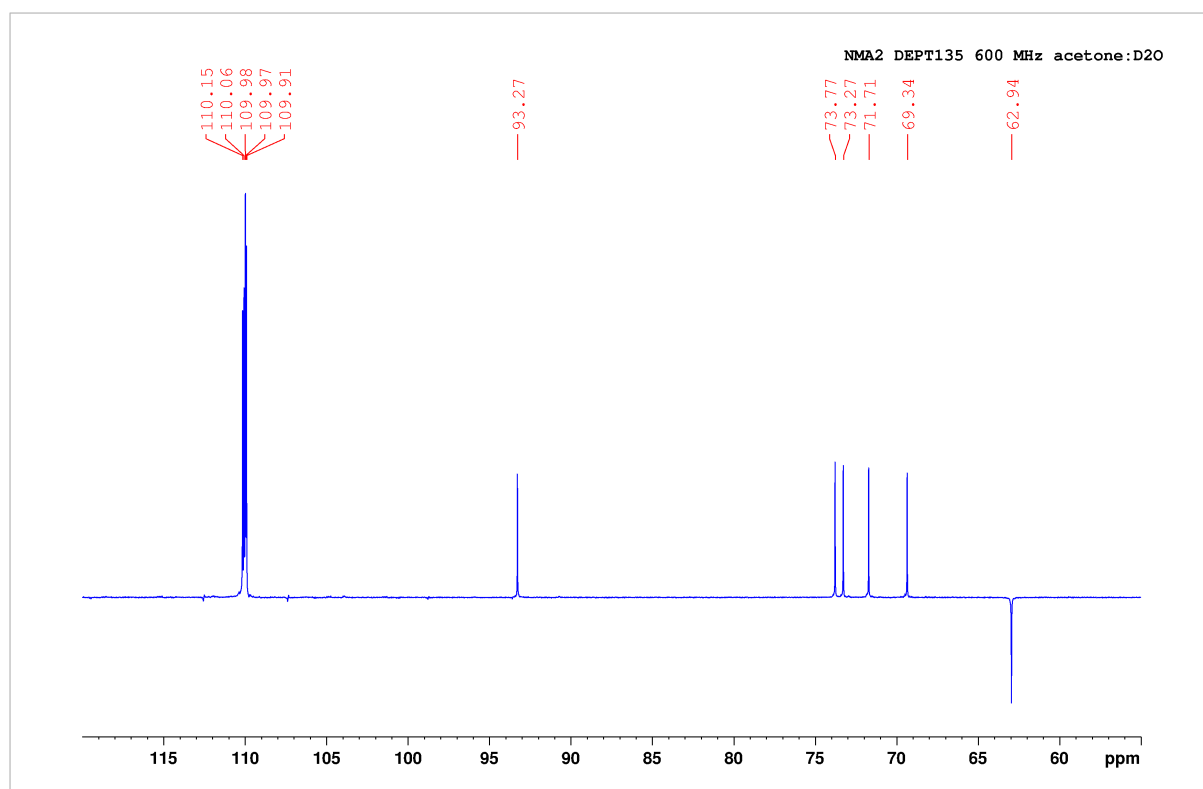


Figure S13: DEPT- 135 spectrum of 1,2,3,4,6-penta-O-galloyl- β -D-glucose (NMA2)

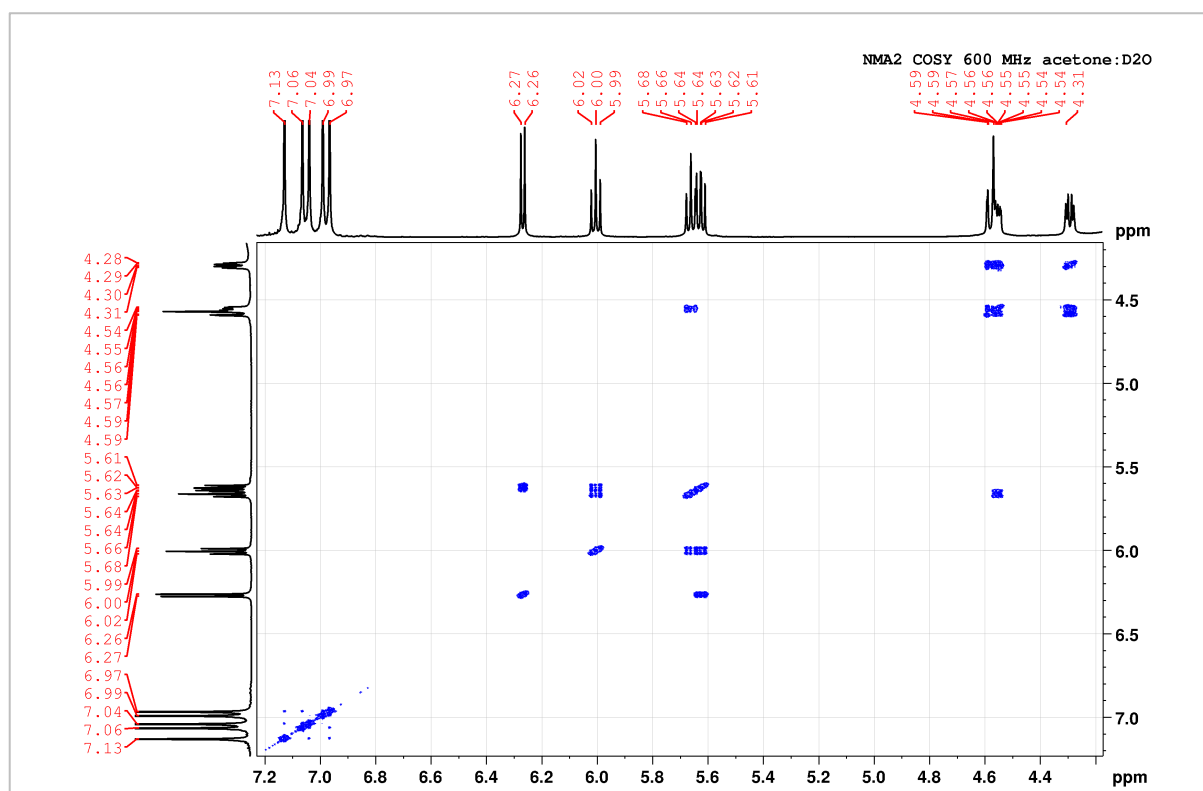


Figure S14: COSY spectrum of 1,2,3,4,6-penta-O-galloyl- β -D-glucose (NMA2)

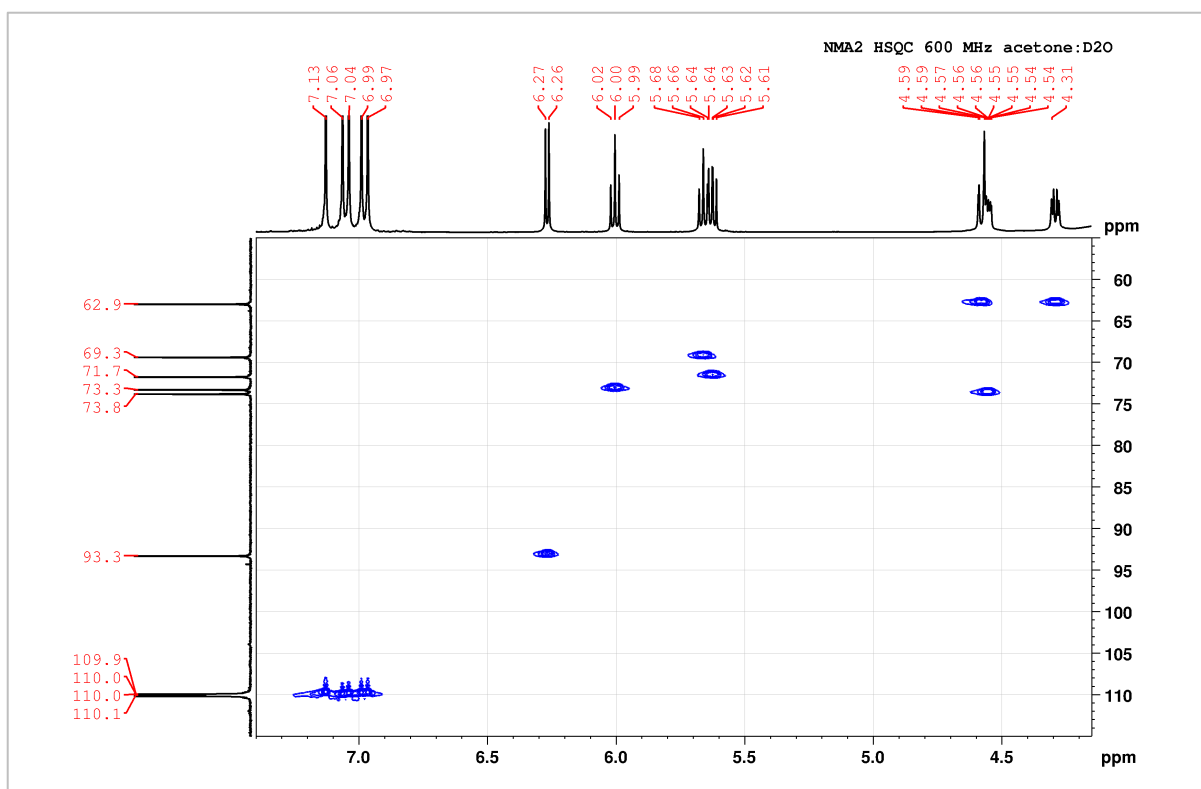


Figure S15: HSQC spectrum of 1,2,3,4,6-penta-O-galloyl- β -D-glucose (NMA2)

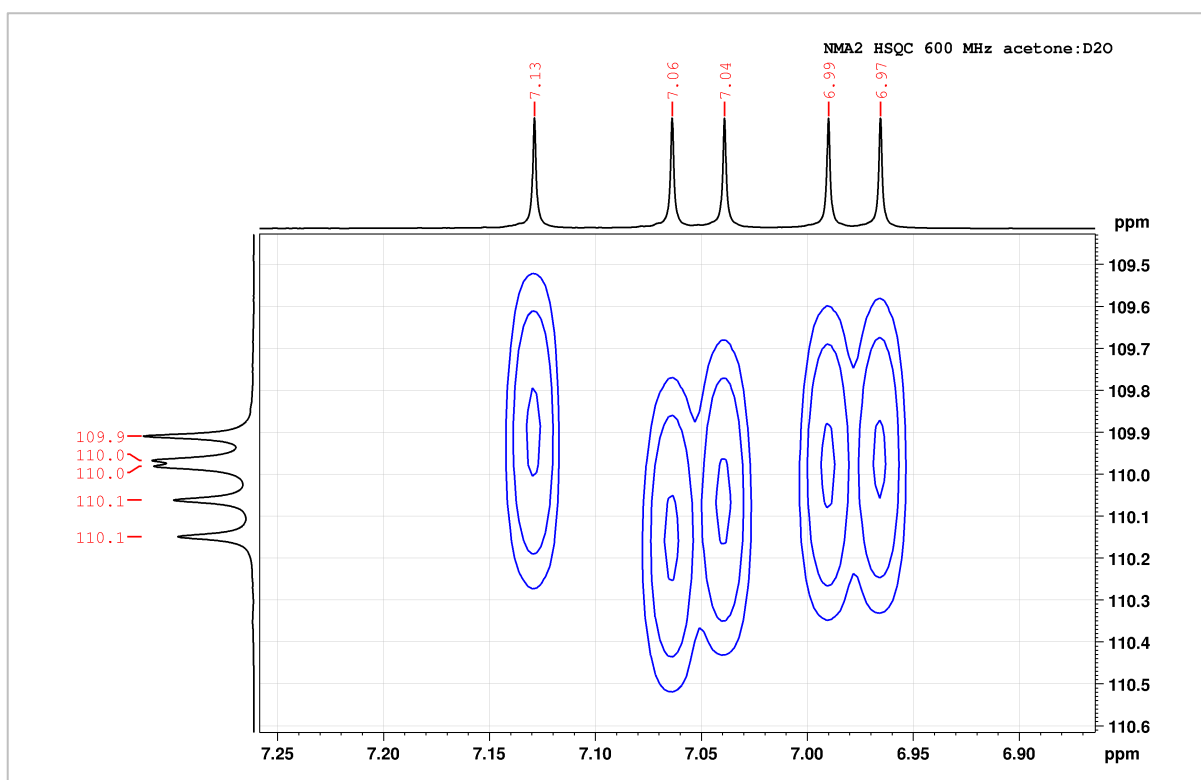


Figure S16: Zoom in of the aromatic aromatic region of HSQC spectrum of 1,2,3,4,6-penta-O-galloyl- β -D-glucose (NMA2)

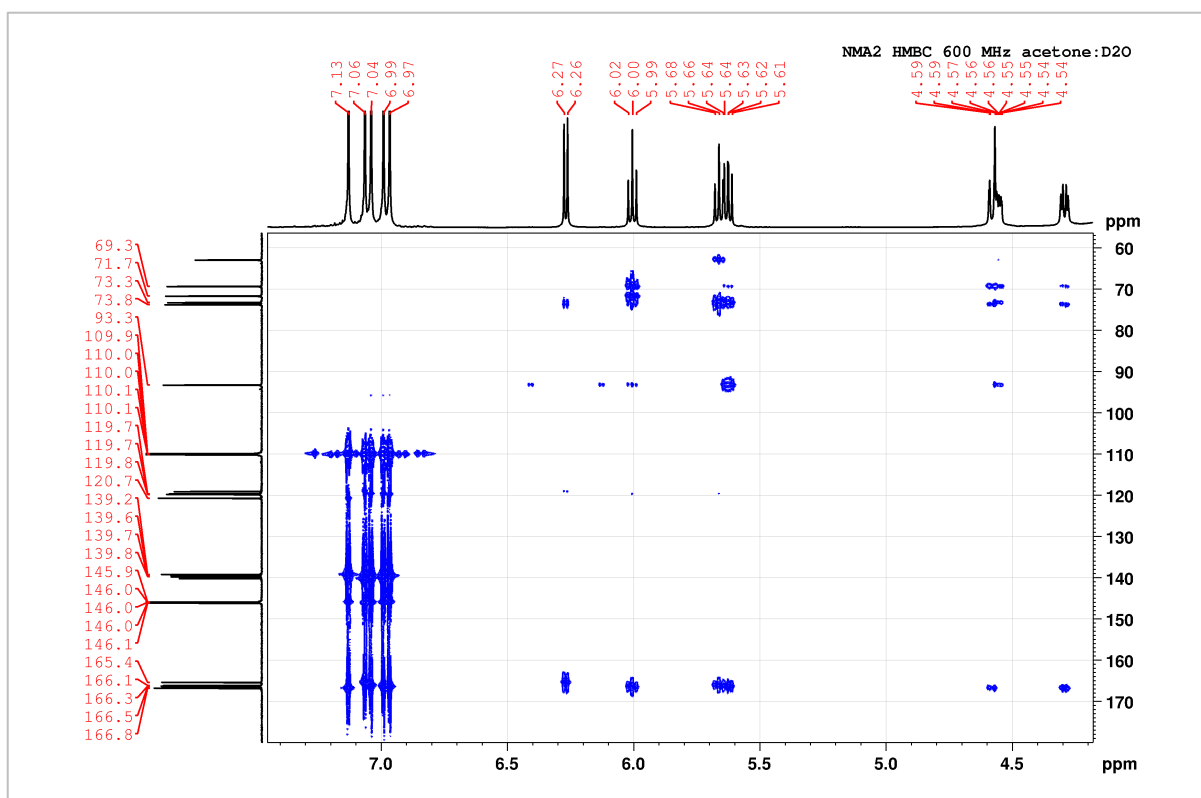


Figure S17: HMBC spectrum of 1,2,3,4,6-penta-O-galloyl- β -D-glucose (NMA2)

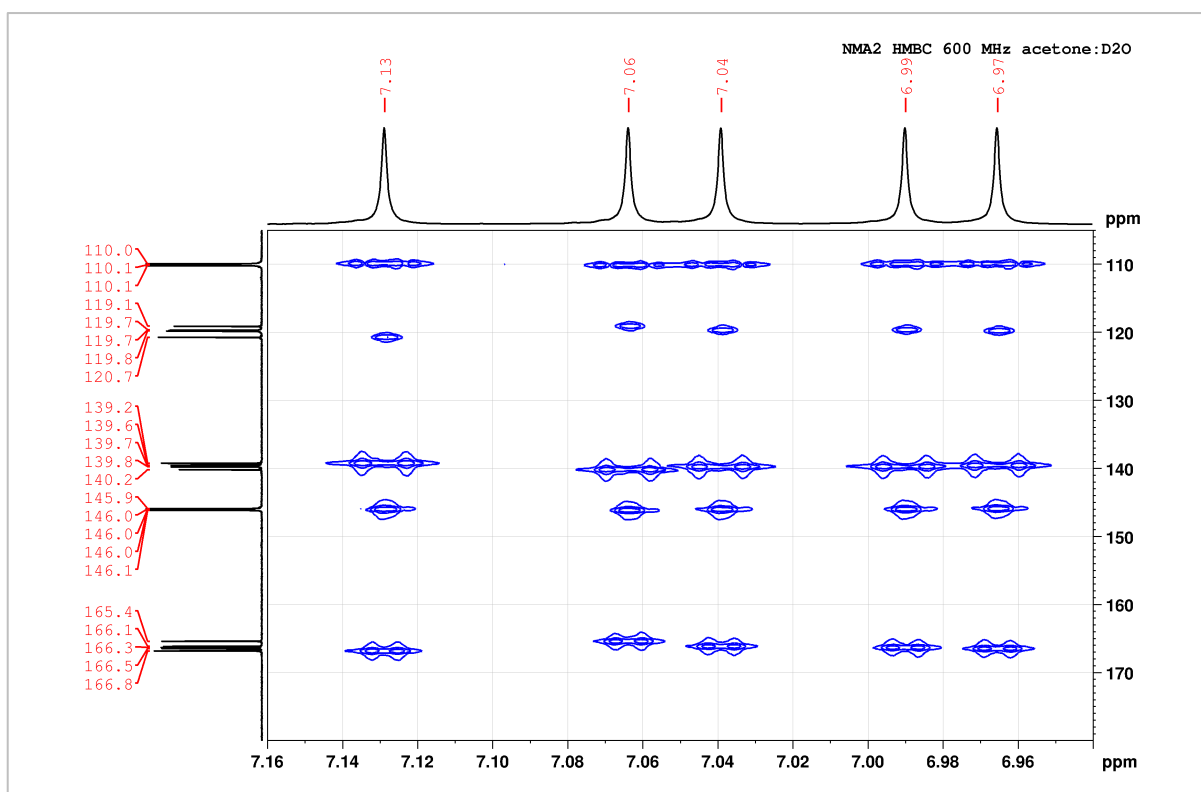


Figure S18: Zoom in of the aromatic region of HMBC spectrum of 1,2,3,4,6-penta-O-galloyl- β -D-glucose (NMA2)

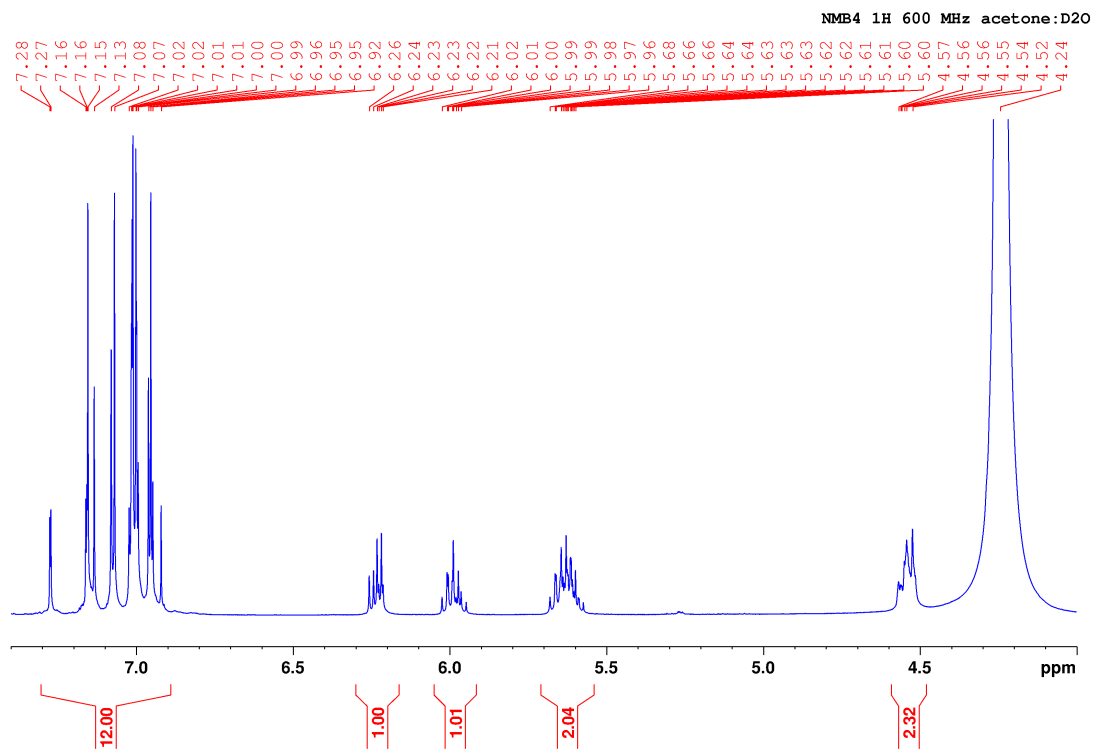


Figure S19: ^1H spectrum of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl- β -D-glucose (NMB4)

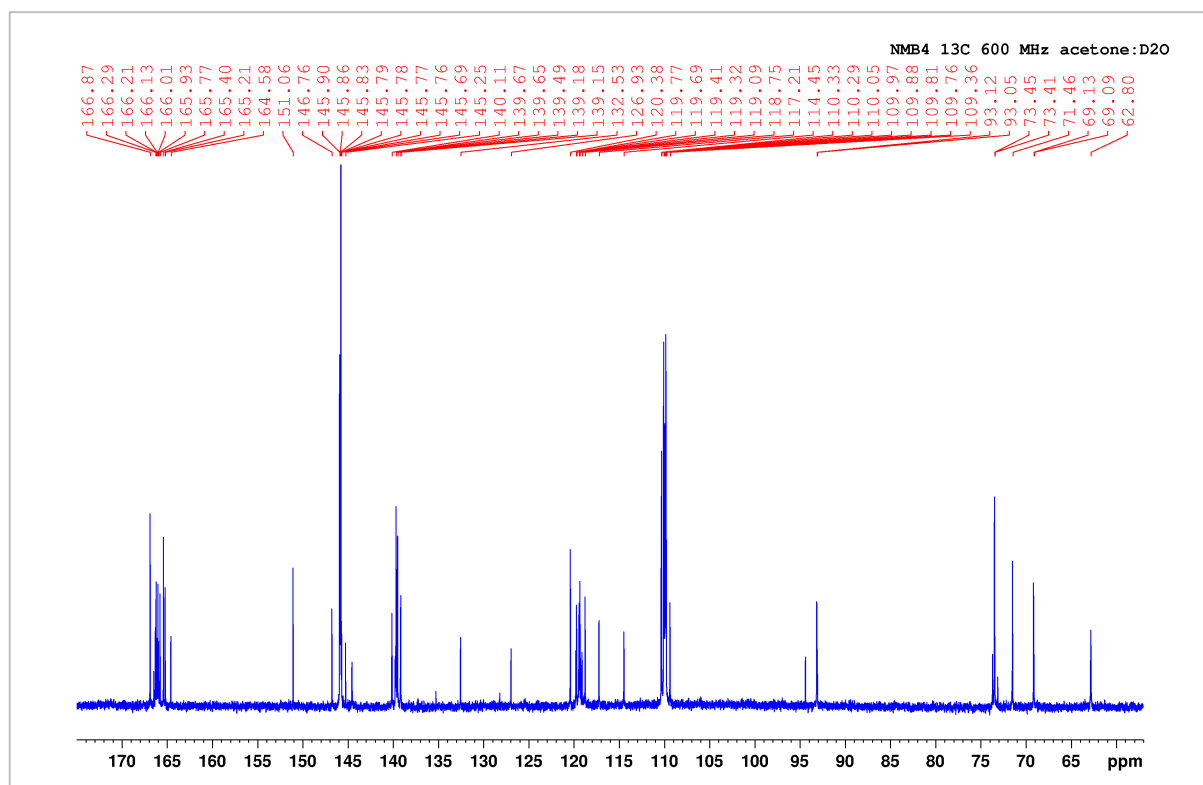


Figure S20: ^{13}C spectrum of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl- β -D-glucose (NMB4)

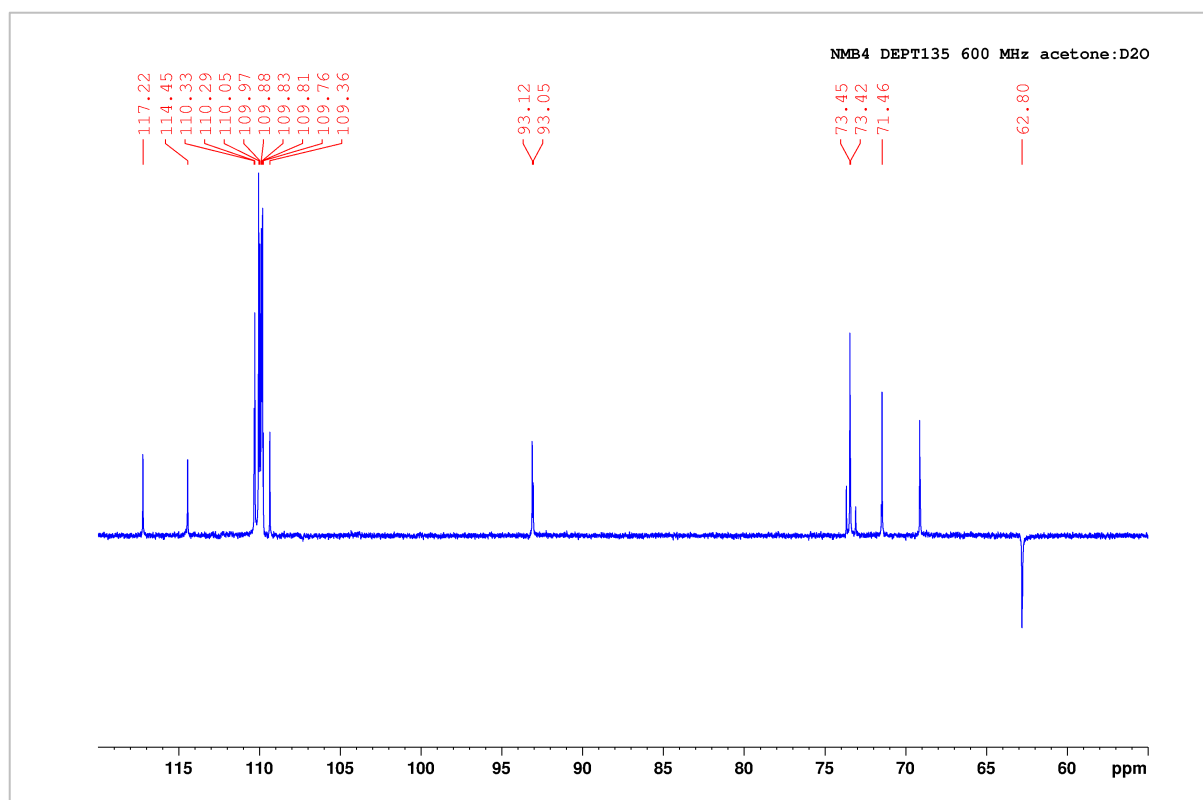


Figure S21: DEPT-135 of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl- β -D-glucose (NMB4)

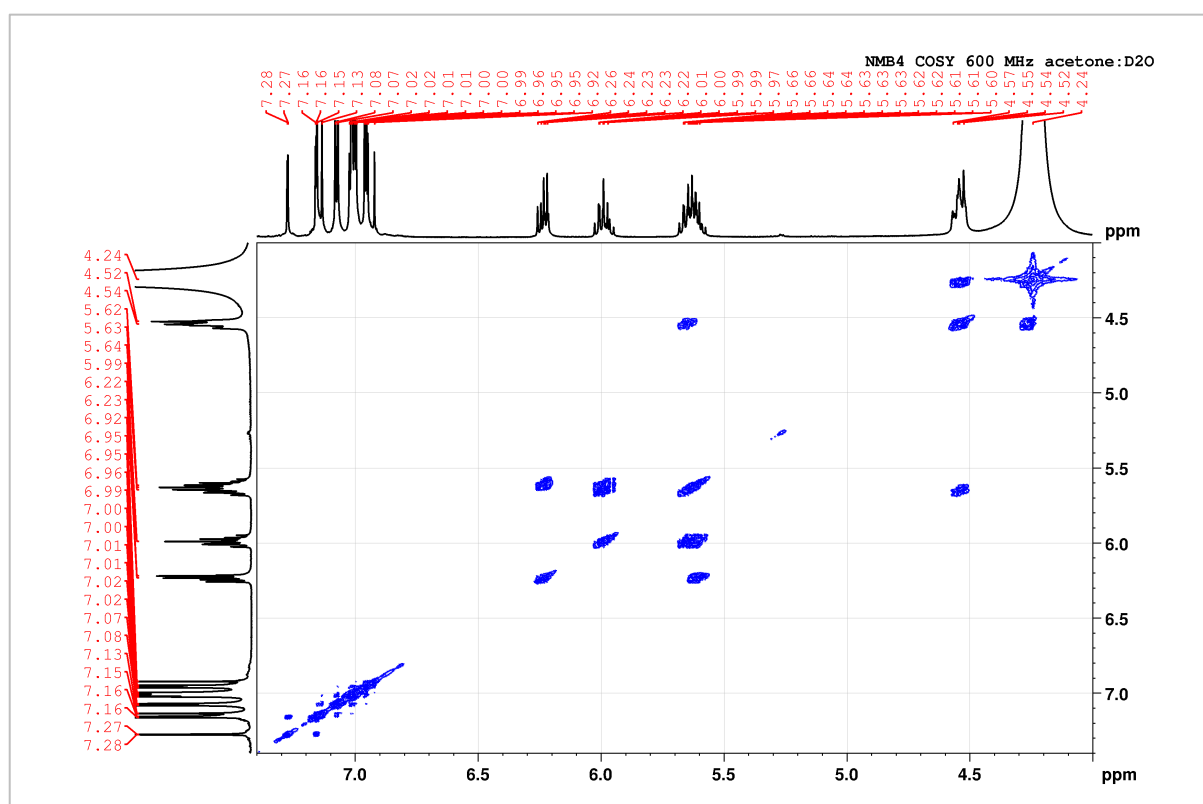


Figure S22: COSY Spectrum of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl- β -D-glucose (NMB4)

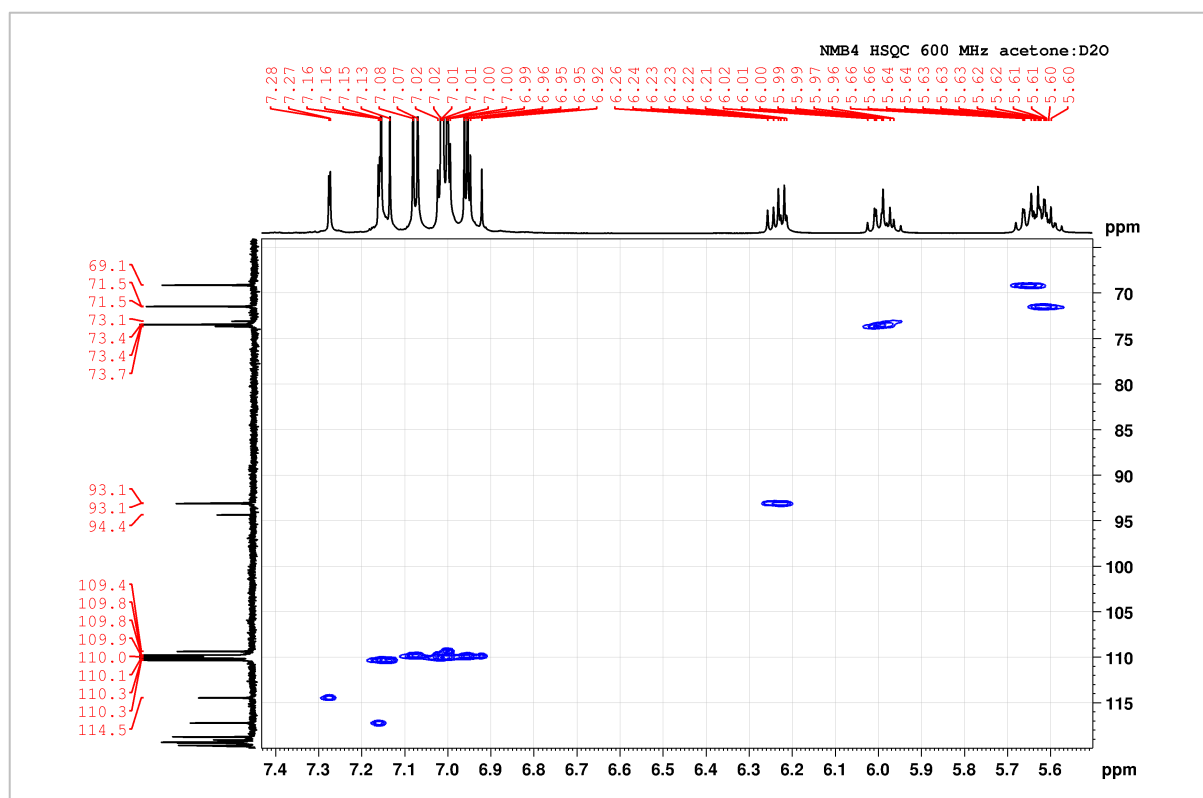


Figure S23: HSQC spectrum of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl-β-D-glucose (NMB4)

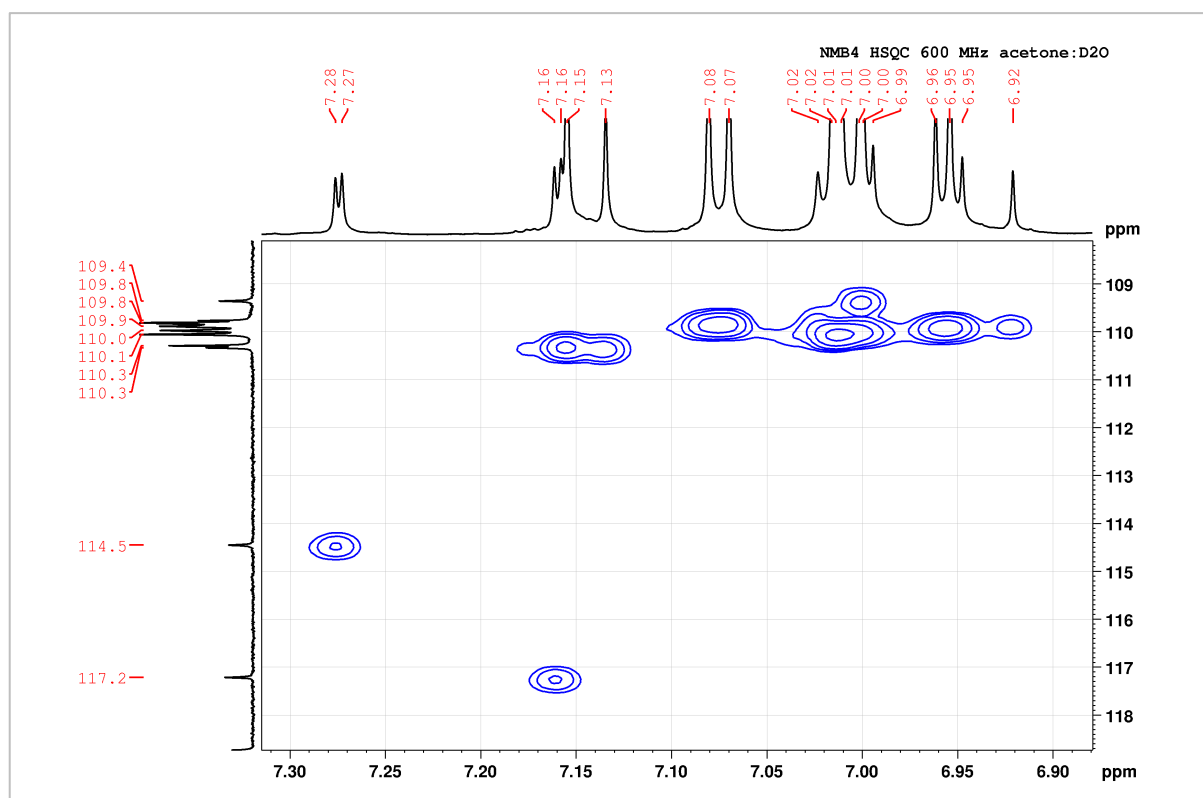


Figure S24: Zoom in of the aromatic region of HSQC spectrum of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl-β-D-glucose (NMB4)

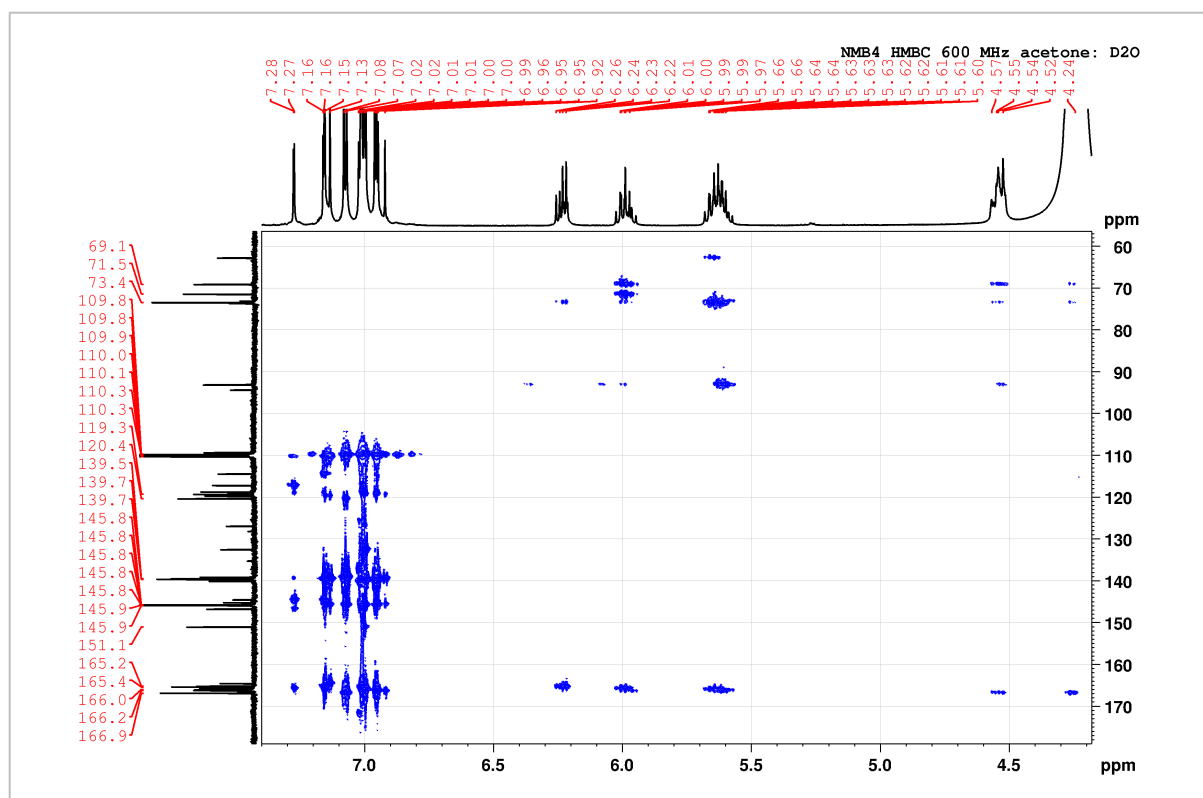


Figure S25: HMBC spectrum of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl- β -D-glucose (NMB4)

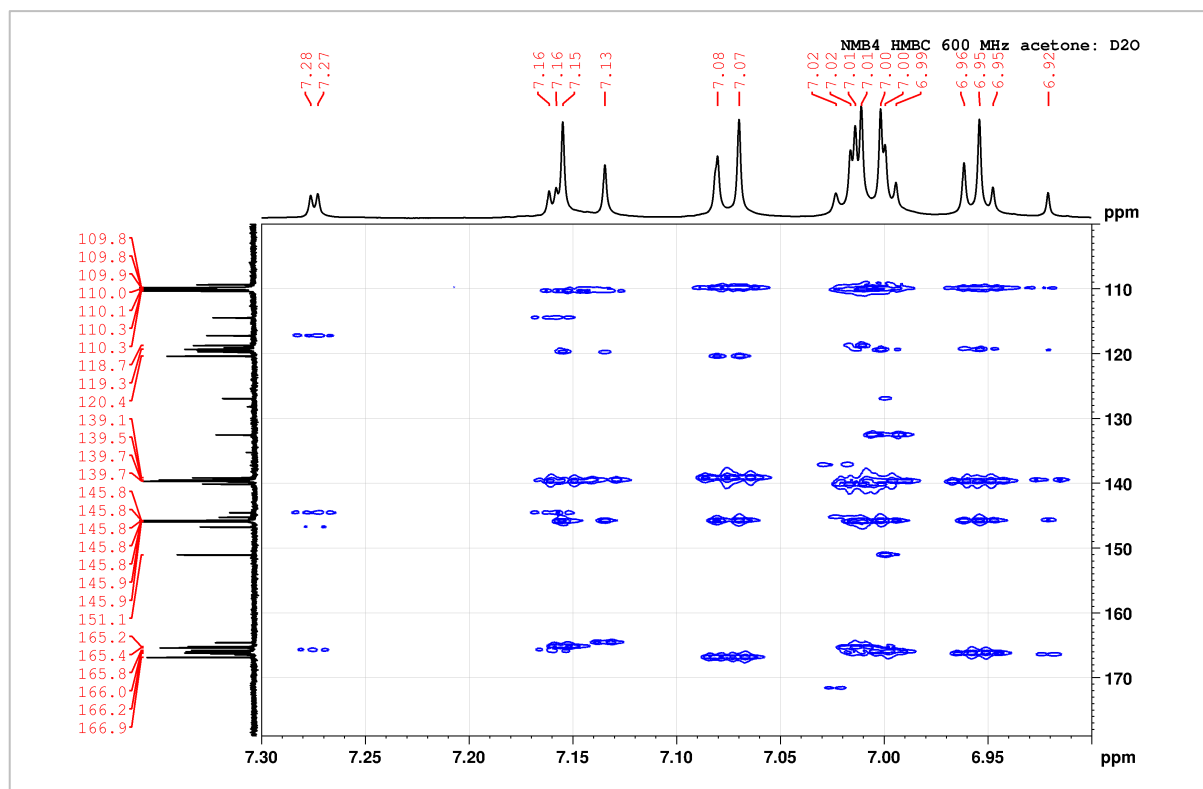


Figure S26: Zoom in of the aromatic region of HMBC spectrum of 3-O-digalloyl-1,2,4,6-tetra-O-galloyl- β -D-glucose (NMB4)

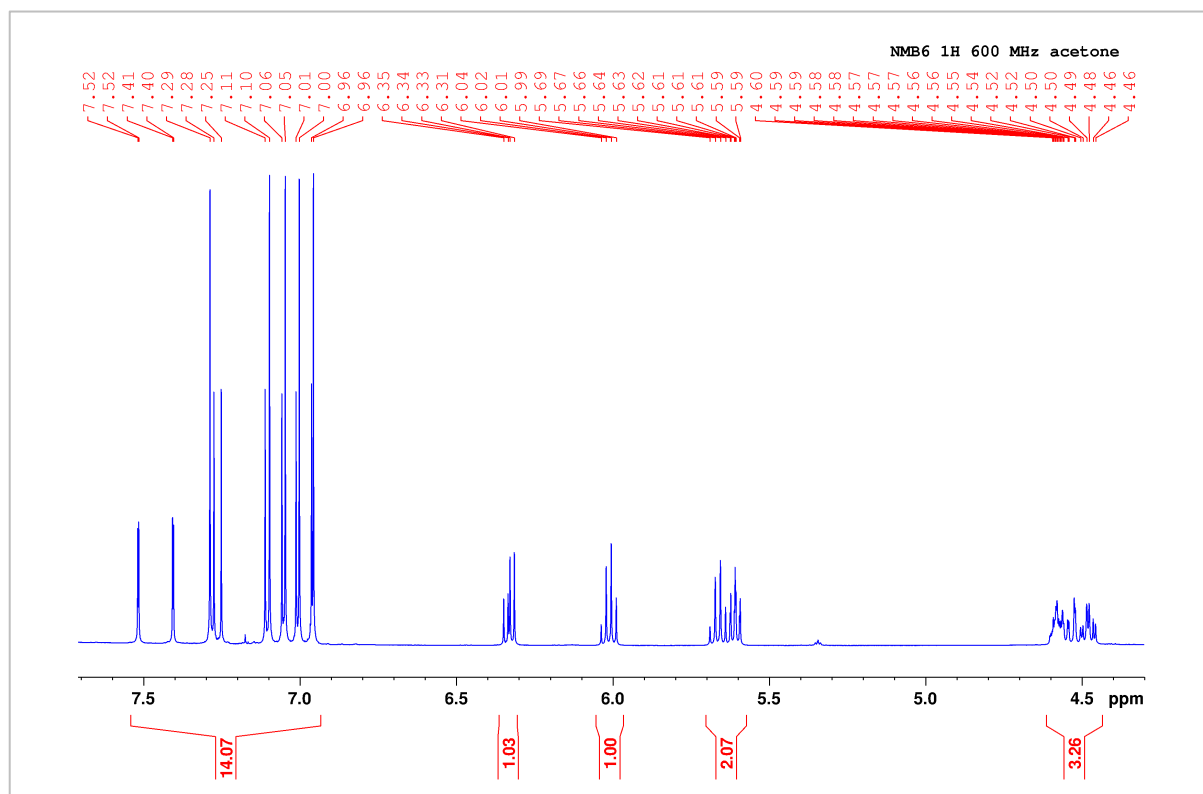


Figure S27: ^1H spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl- β -D-glucose (NMB6)

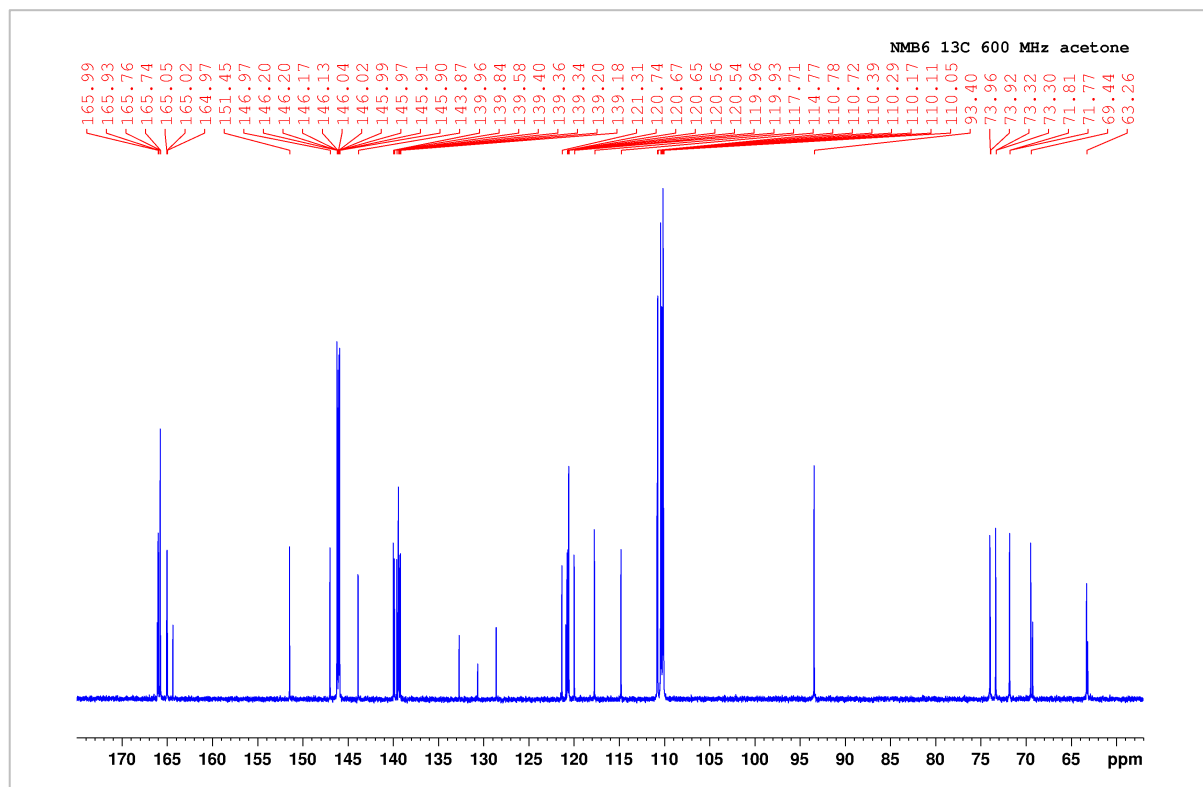


Figure S28: ^{13}C spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl- β -D-glucose (NMB6)

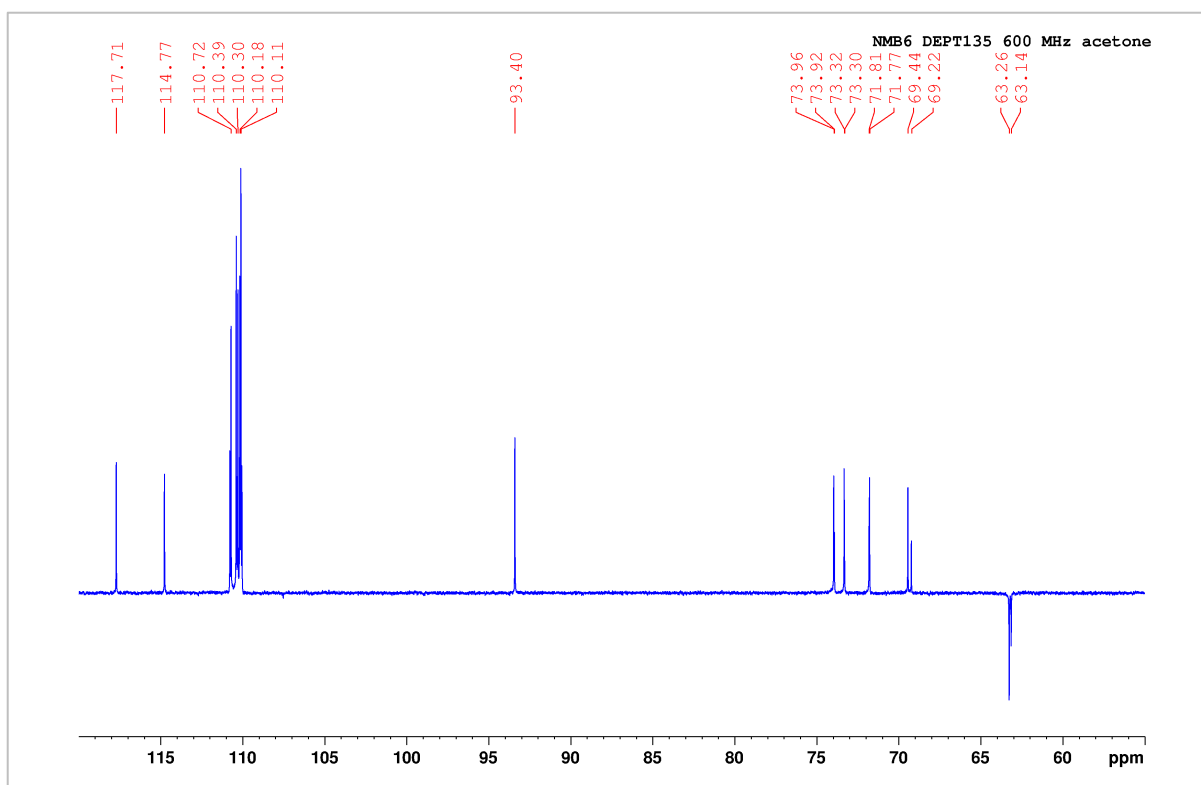


Figure S29: DEPT135 spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl-β-D-glucose (NMB6)

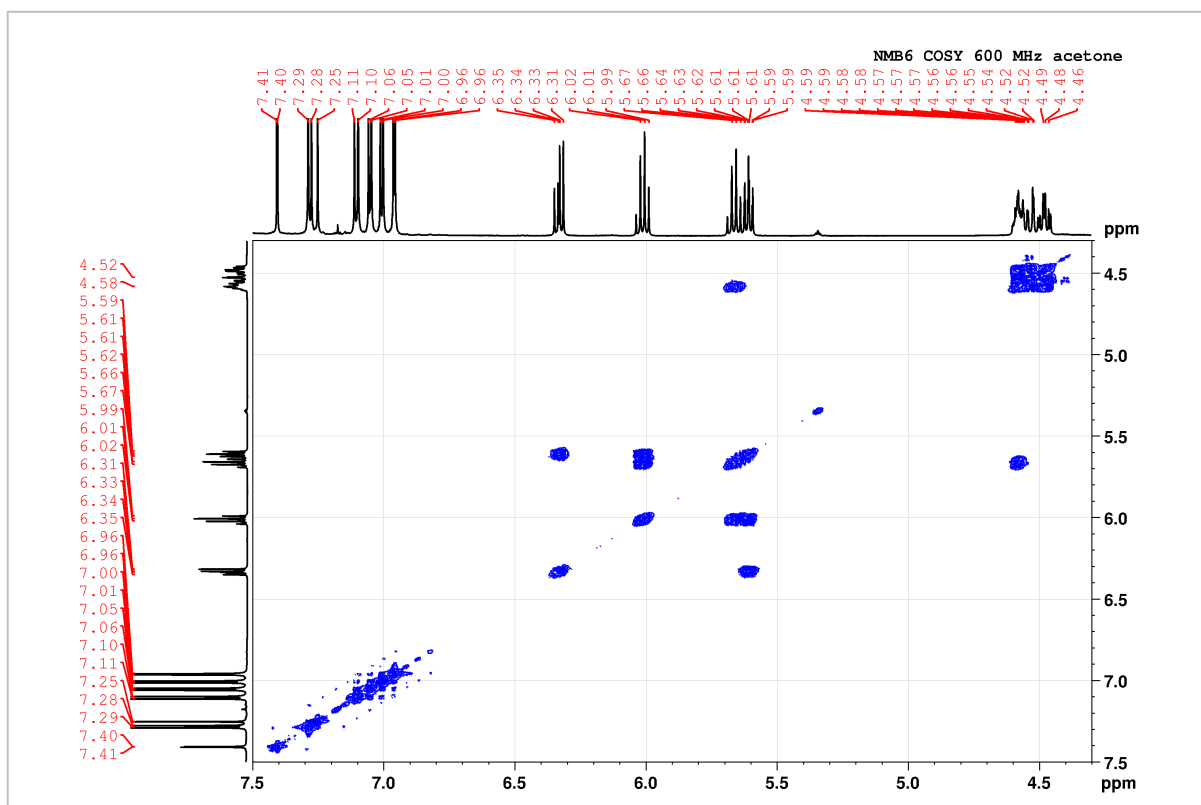


Figure S30: COSY spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl-β-D-glucose (NMB6)

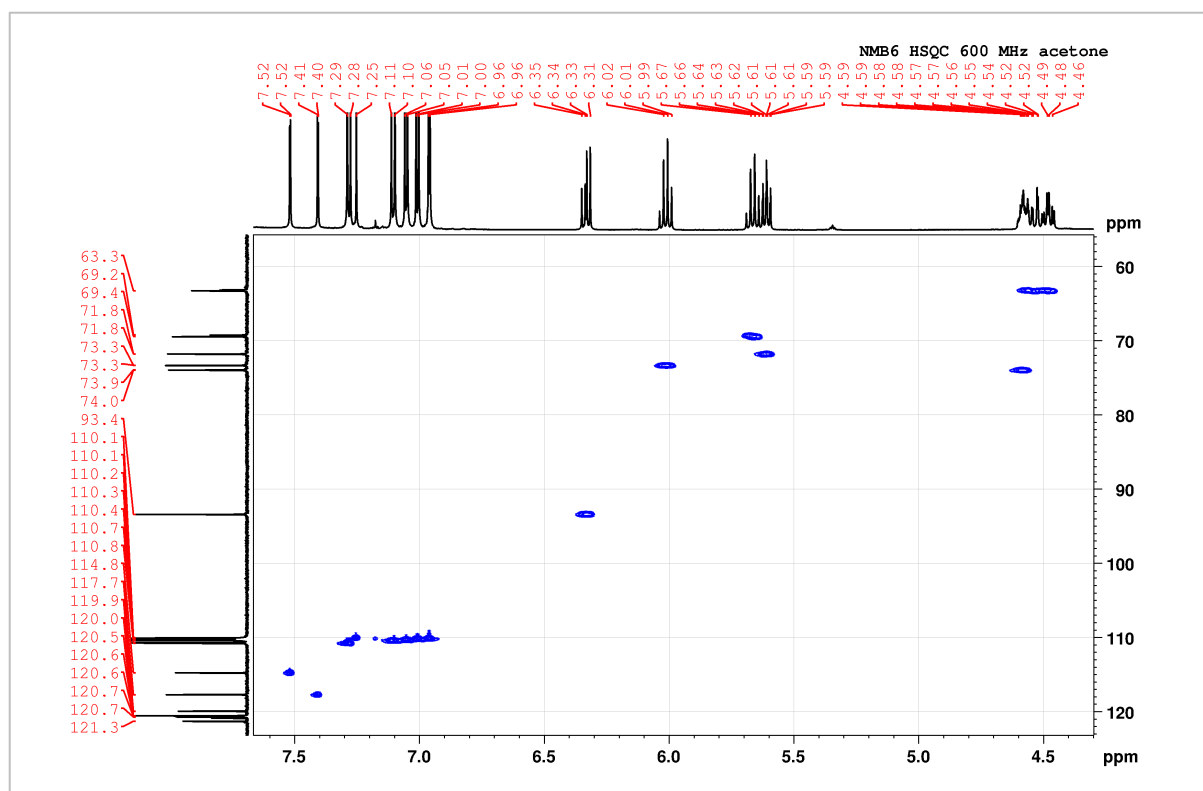


Figure S31: HSQC spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl- β -D-glucose (NMB6)

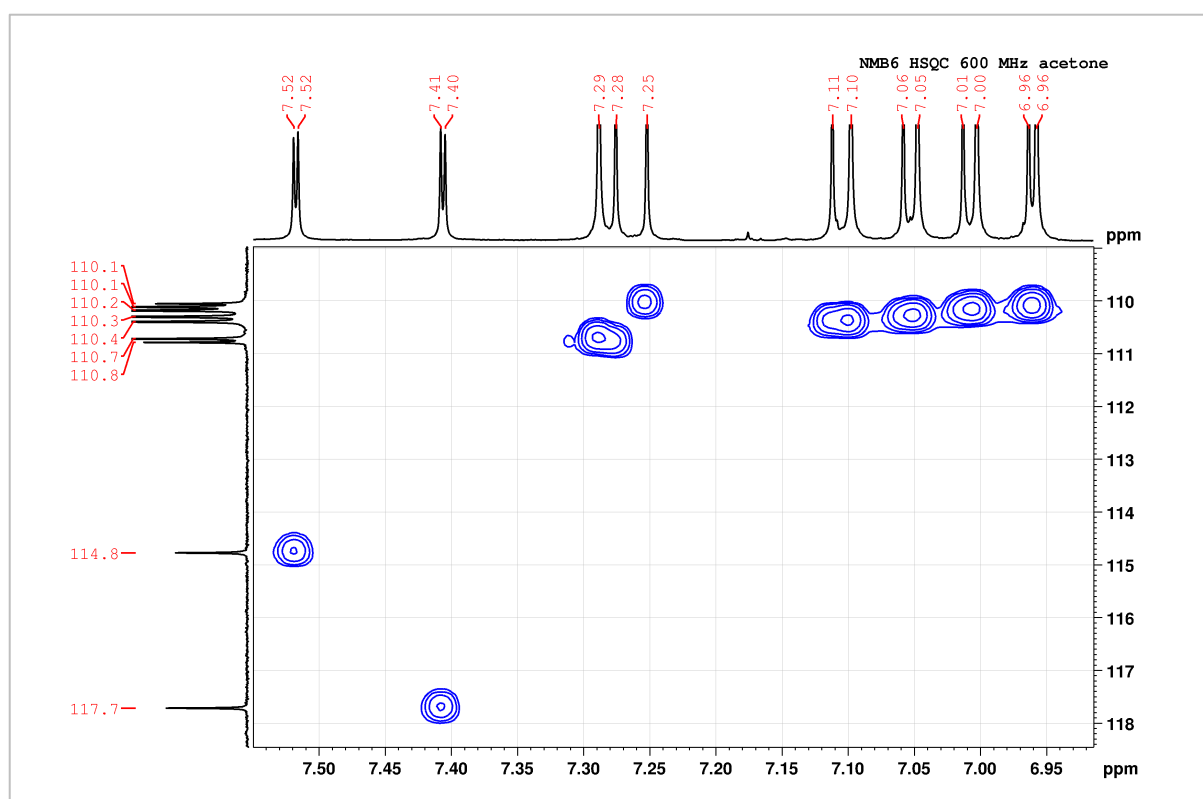


Figure S32: Zoom in of the aromatic region of HSQC spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl- β -D-glucose (NMB6)

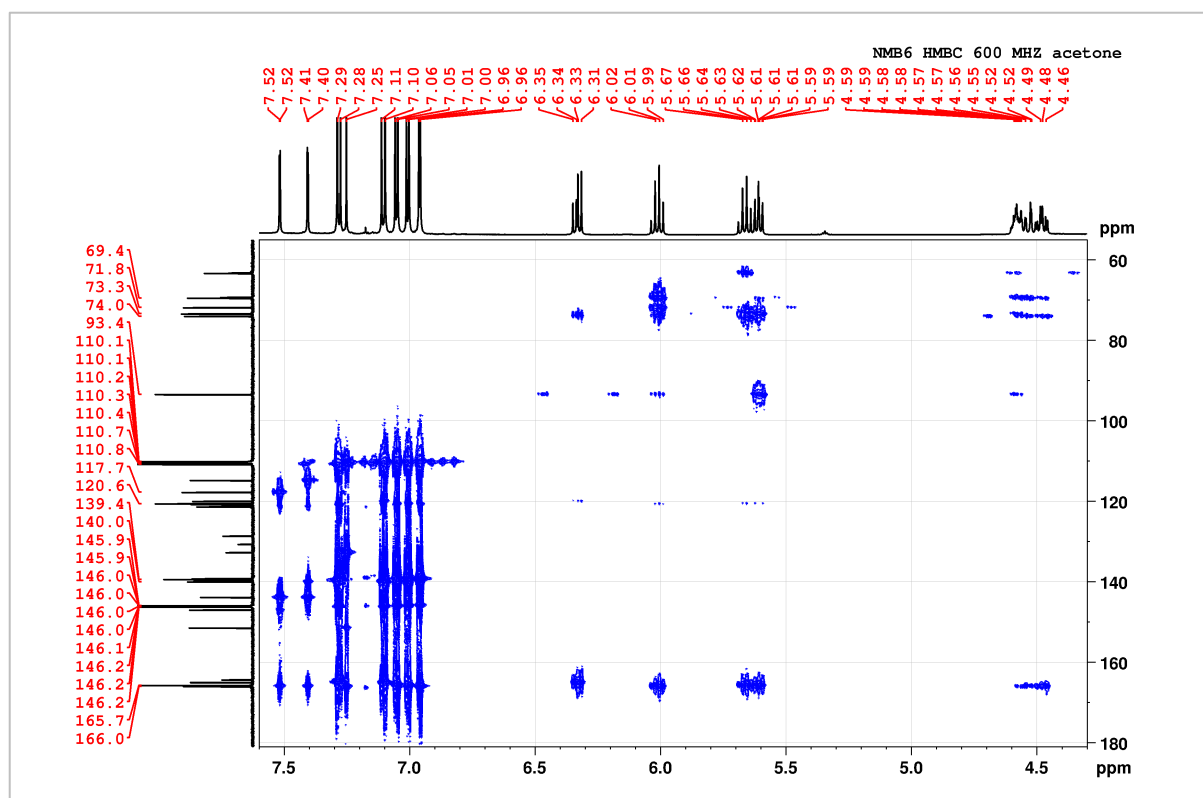


Figure S33: HMBC spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl- β -D-glucose (NMB6)

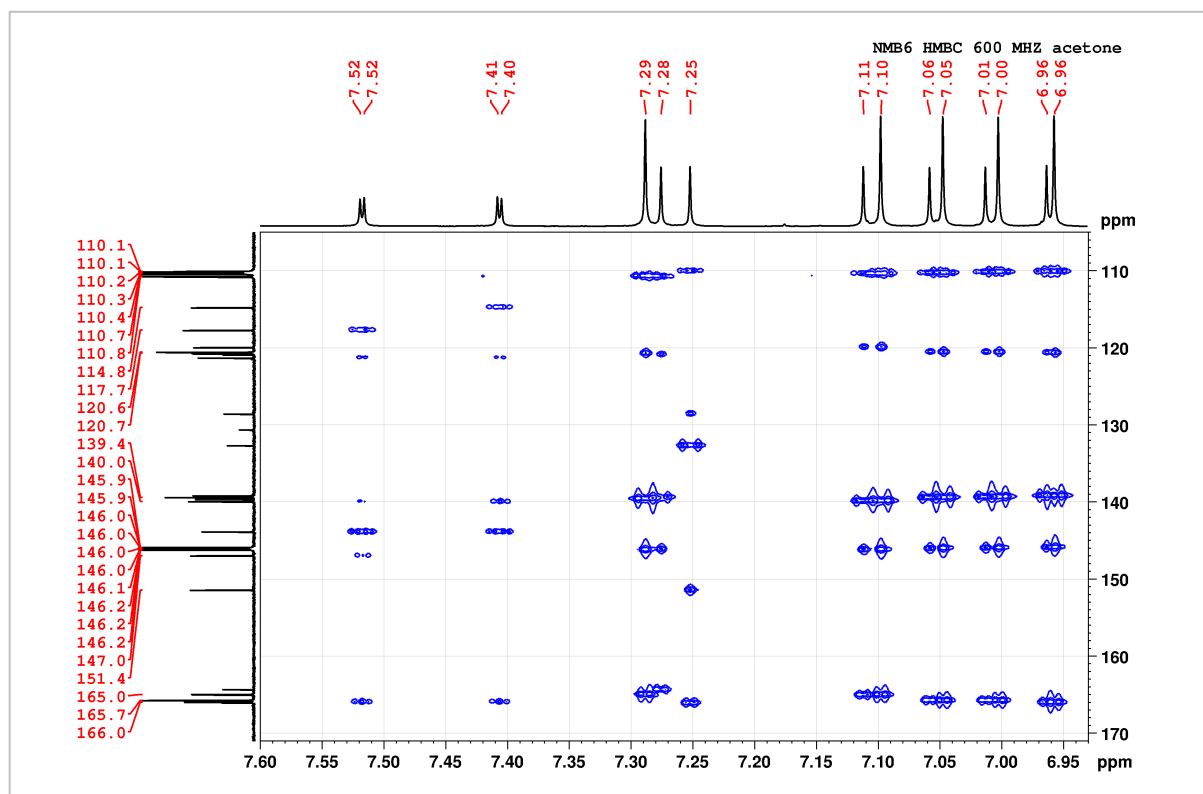


Fig S34: Zoom in of the aromatic region of HMBC spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl- β -D-glucose (NMB6)

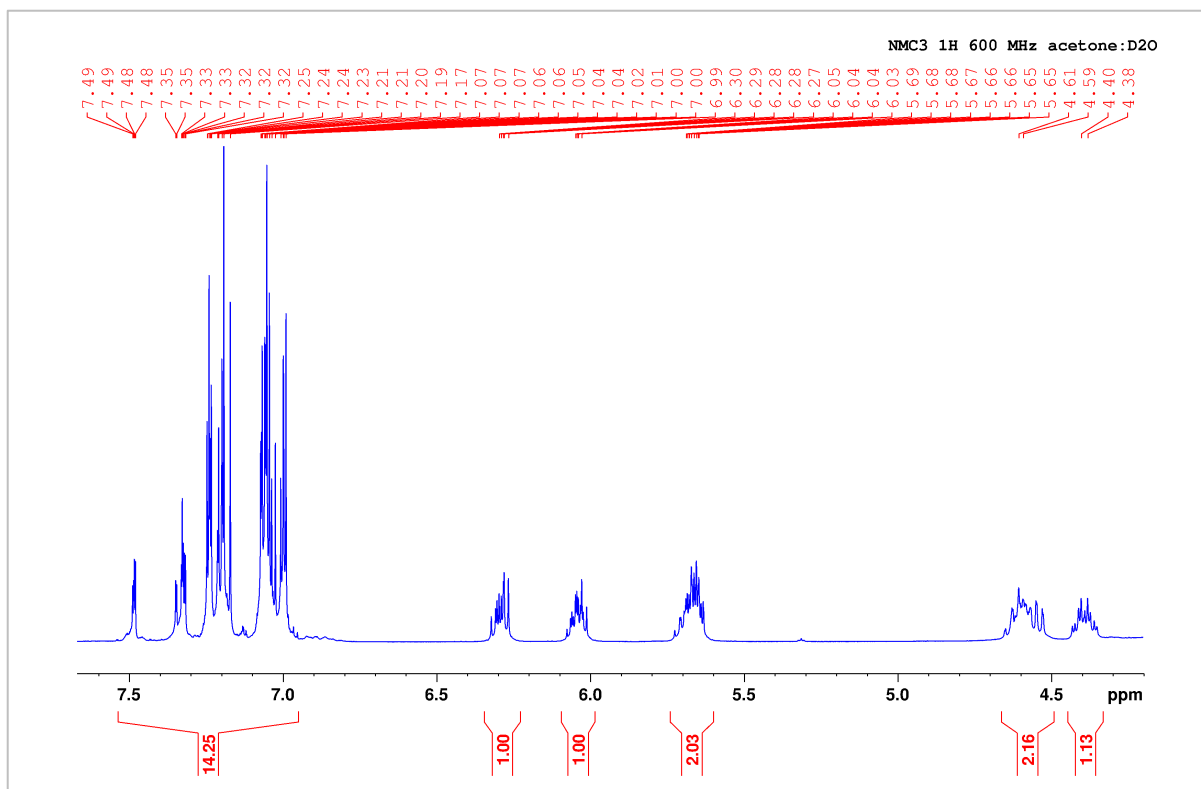


Figure S35: ^1H spectrum of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl- β -D-glucose (NMC3)

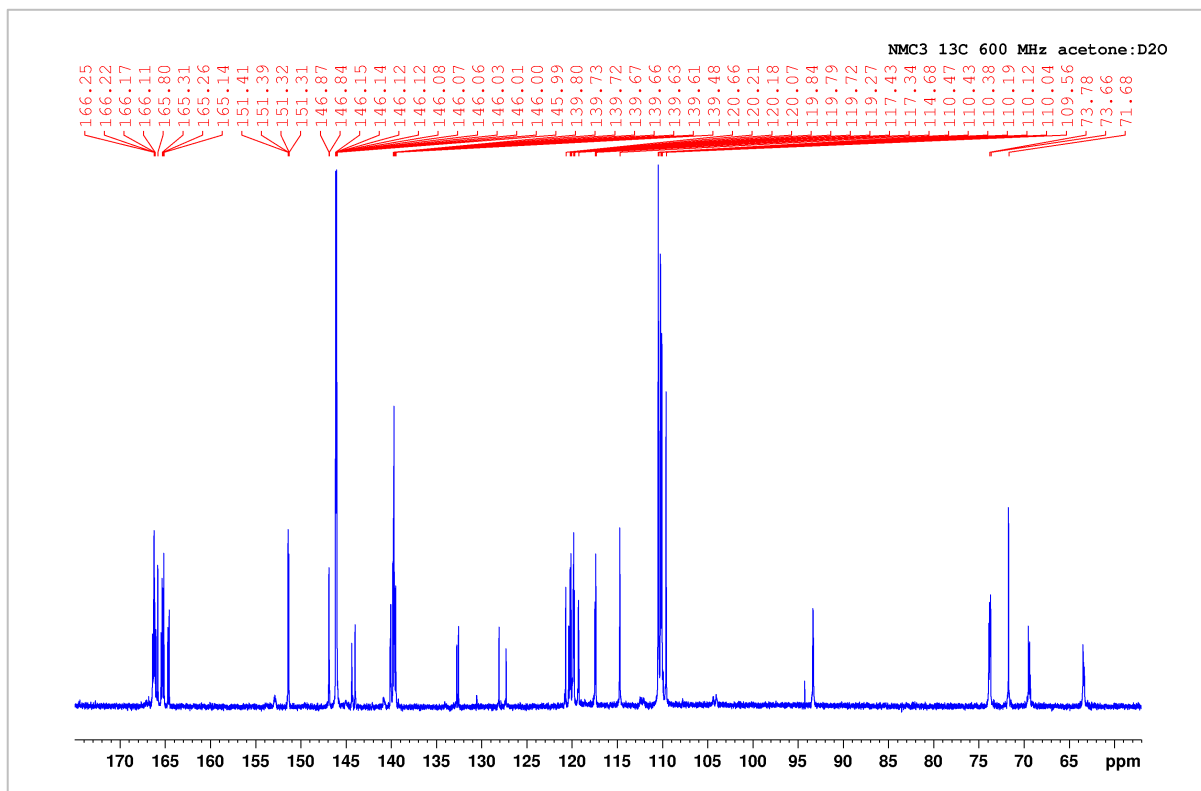


Figure S36: ^{13}C spectrum of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl- β -D-glucose (NMC3)

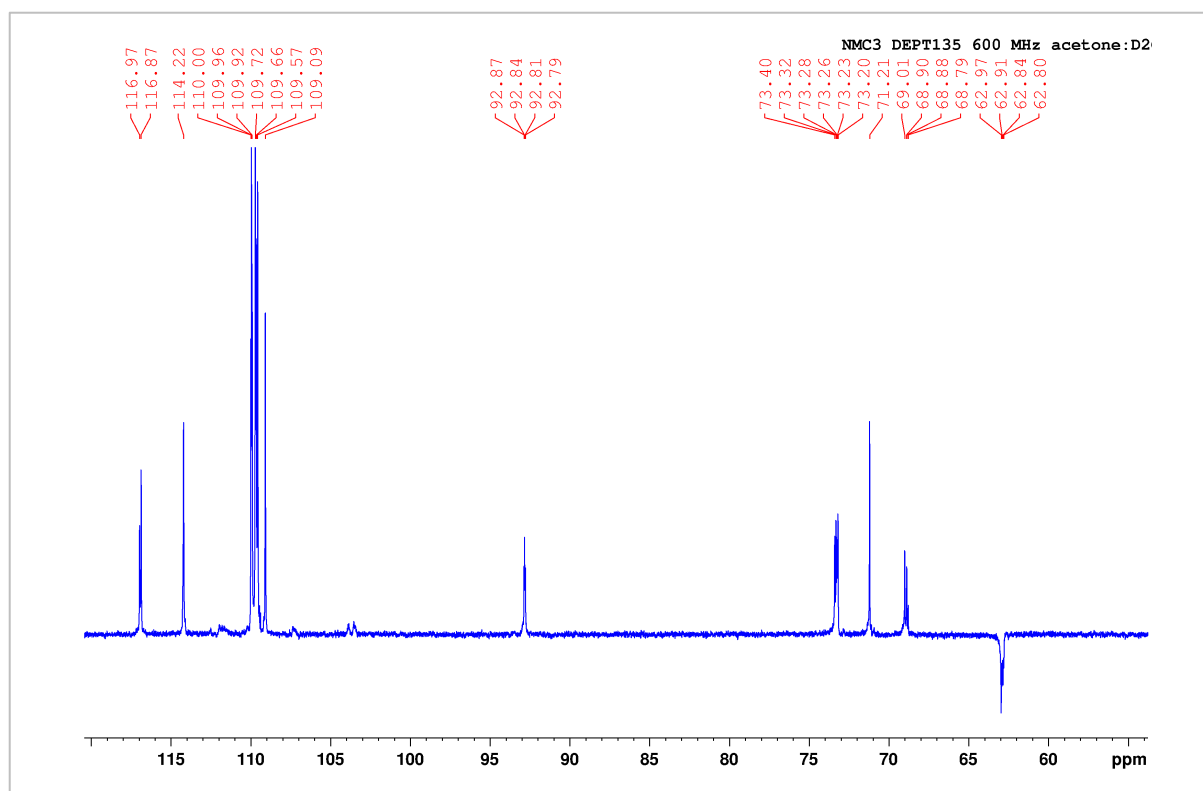


Figure S37: DEPT-135 spectrum of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl-β-D-glucose (NMC3)

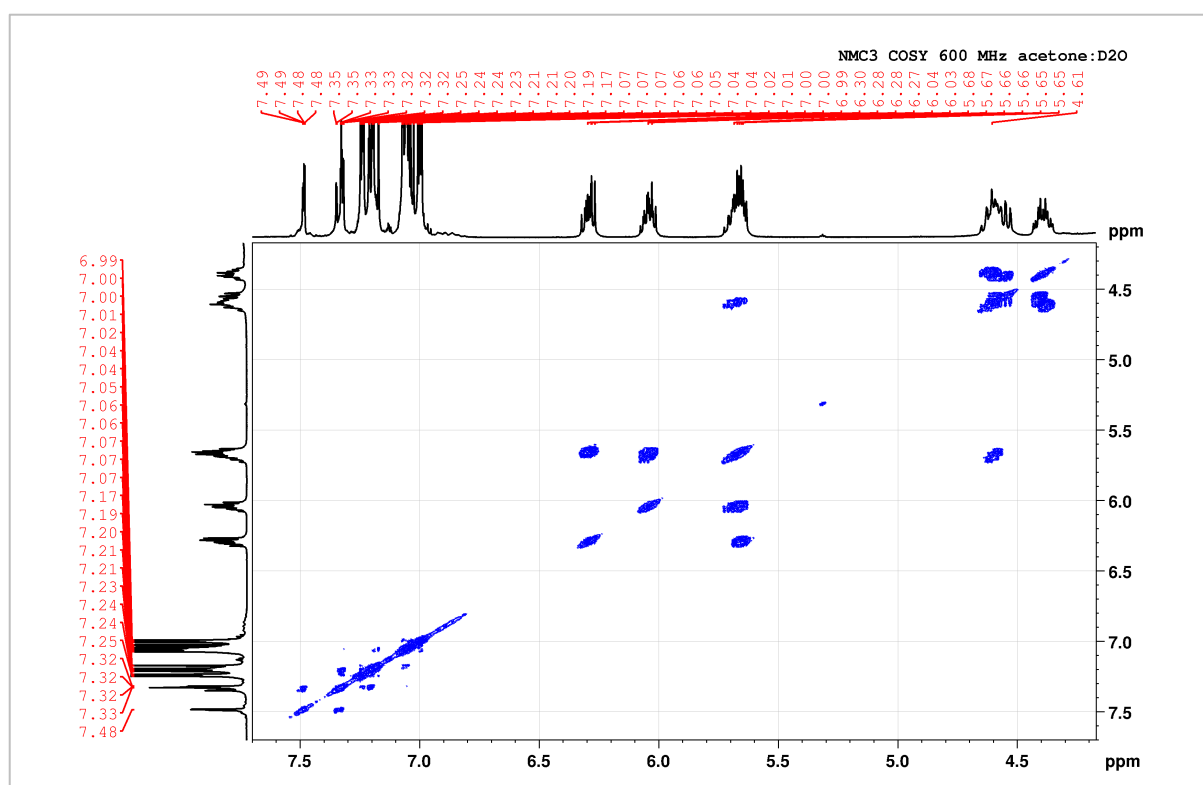


Figure S38: COSY spectrum of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl-β-D-glucose (NMC3)

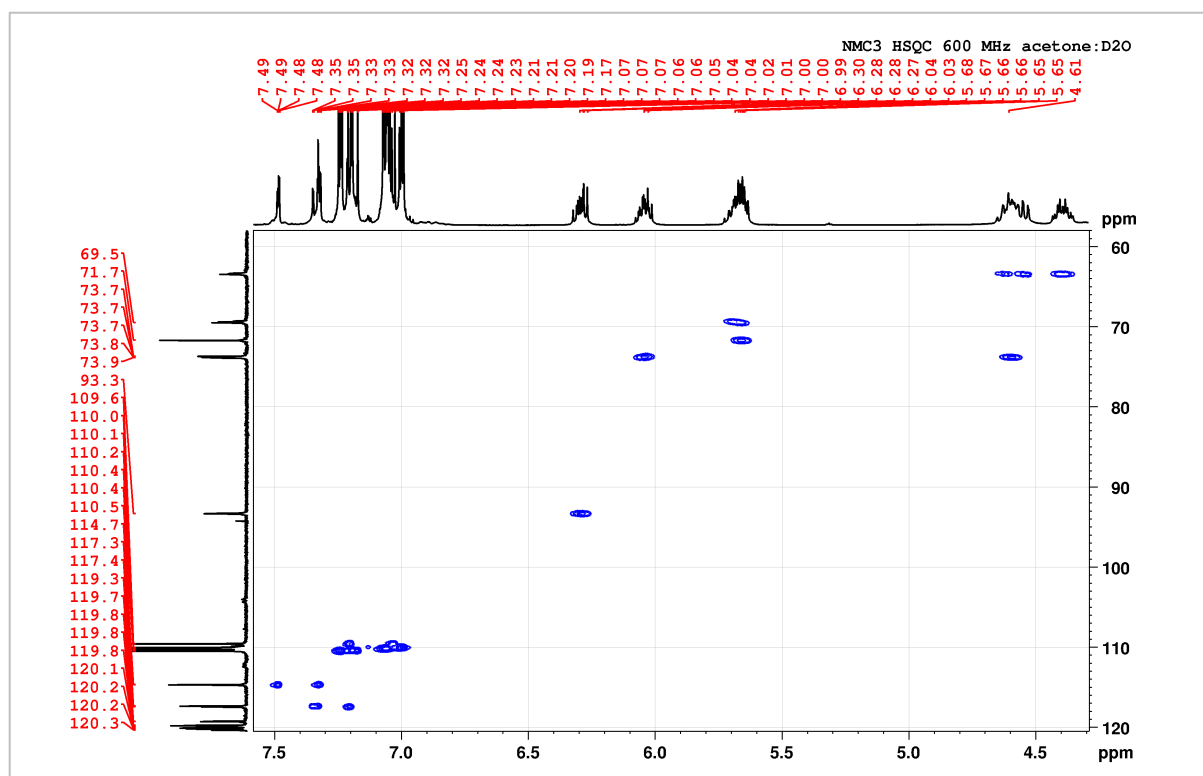


Figure S39: HSQC spectrum of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl- β -D-glucose (NMC3)

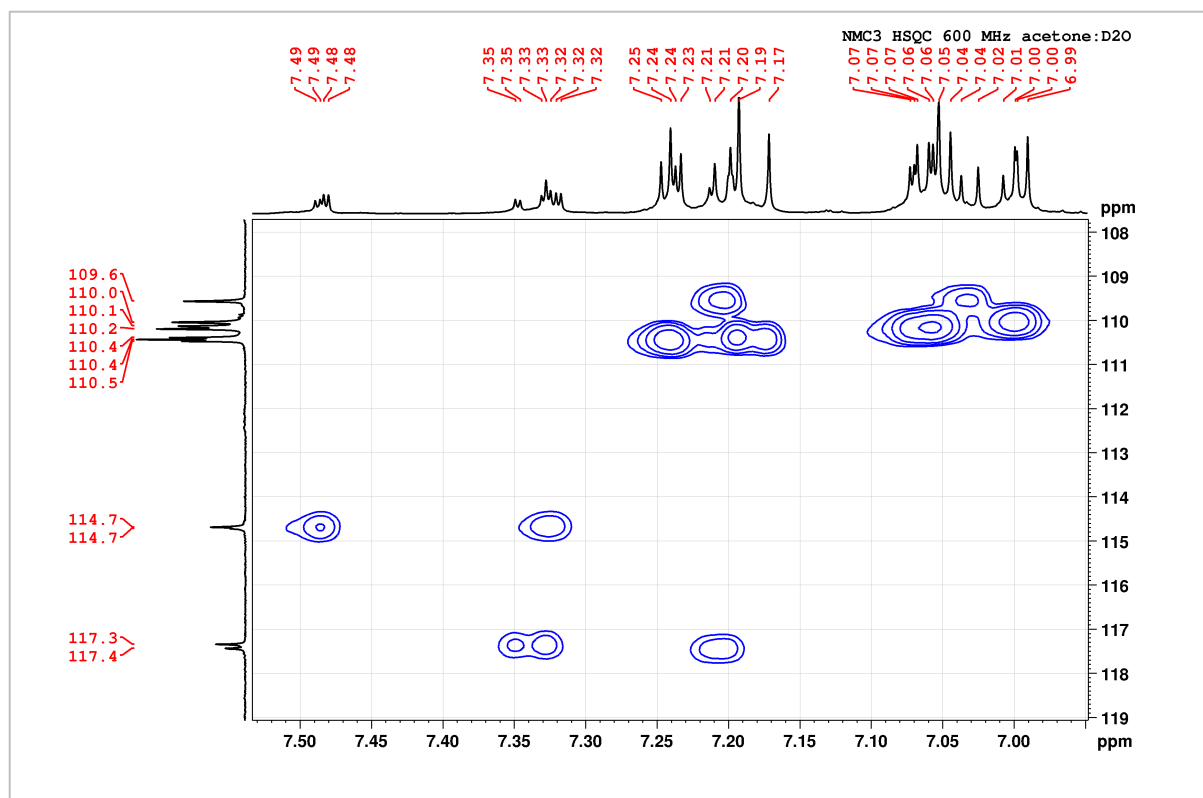


Figure S40: Zoom in of the aromatic region of the HSQC spectrum of 6-O-digalloyl-1,2,3,4-tetra-O-galloyl- β -D-glucose (NMB6)

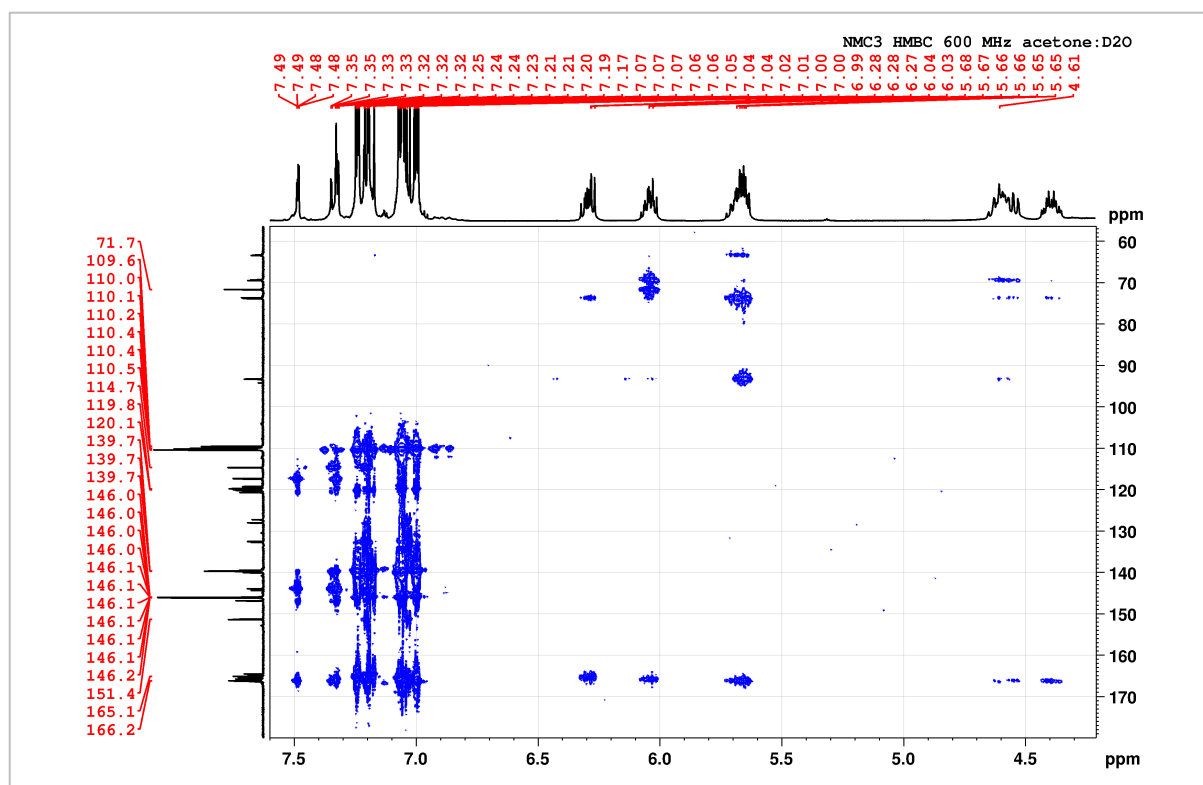


Figure S41: HMBC spectrum of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl- β -D-glucose (NMC3)

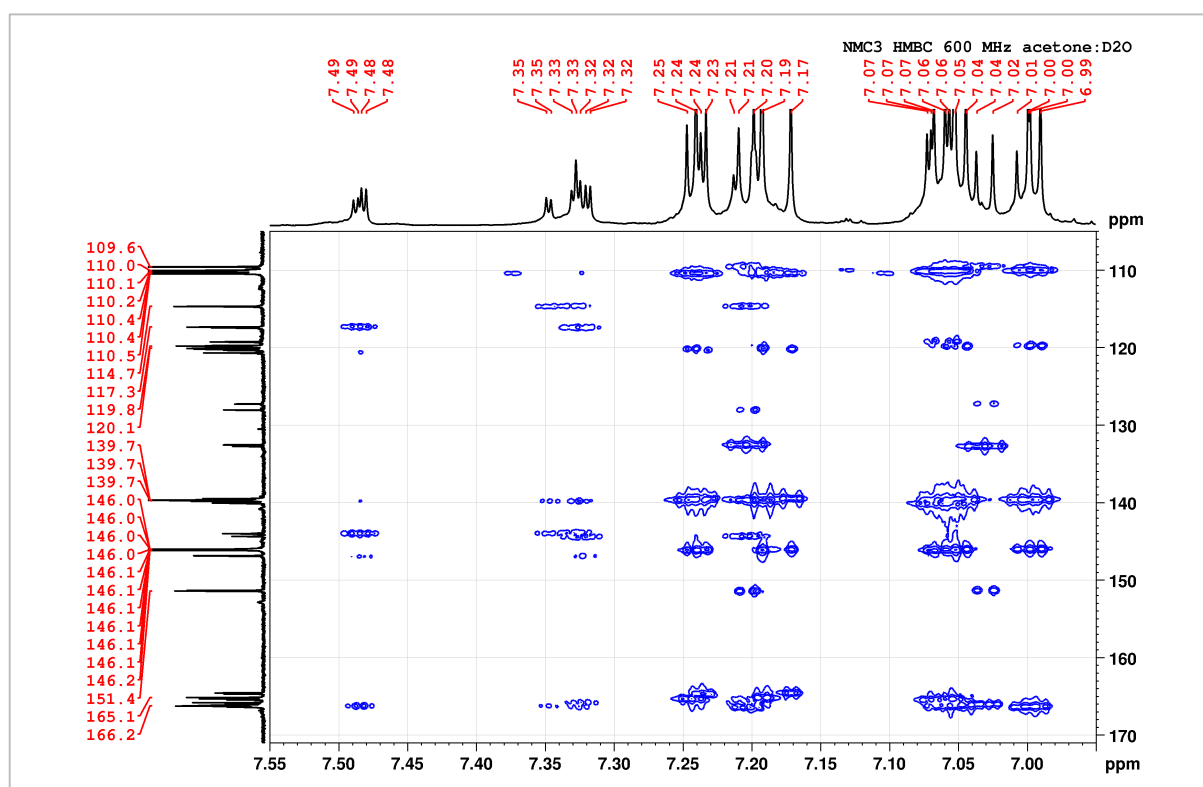


Figure S42: Zoom in of the aromatic region of HMBC spectrum of 3,6-bis-O-digalloyl-1,2,4-tri-O-galloyl- β -D-glucose (NMC3)