Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Sustainable synthesis of acetals from glycerol as potential additives for biofuels under solvent-free conditions

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GENERAL TECHNIQUES

Analytical grade commercial solvents and reagents were purchased from Sigma-Aldrich, and used as received. Infrared spectra were recorded as neat using a FT-IR Varian 660 Fourier transform infrared spectrometer. Values are expressed in wavenumbers (cm^{-1}) and recorded in a range of 4000−400 cm^{-1}. NMR spectra were recorded at 25 °C in $CDCl_3$ on a Varian Mercury 300 spectrometer operating at 300 MHz for ^1H. All chemical shifts are reported in parts per million (ppm) and were measured relative to the solvent in which the sample was analyzed ($CDCl_3$ δ = 7.26). The percentage of acetals yield (%) were determined by using by ^1H NMR using TMB with internal standard.

EXPERIMENTAL PROCEDURES

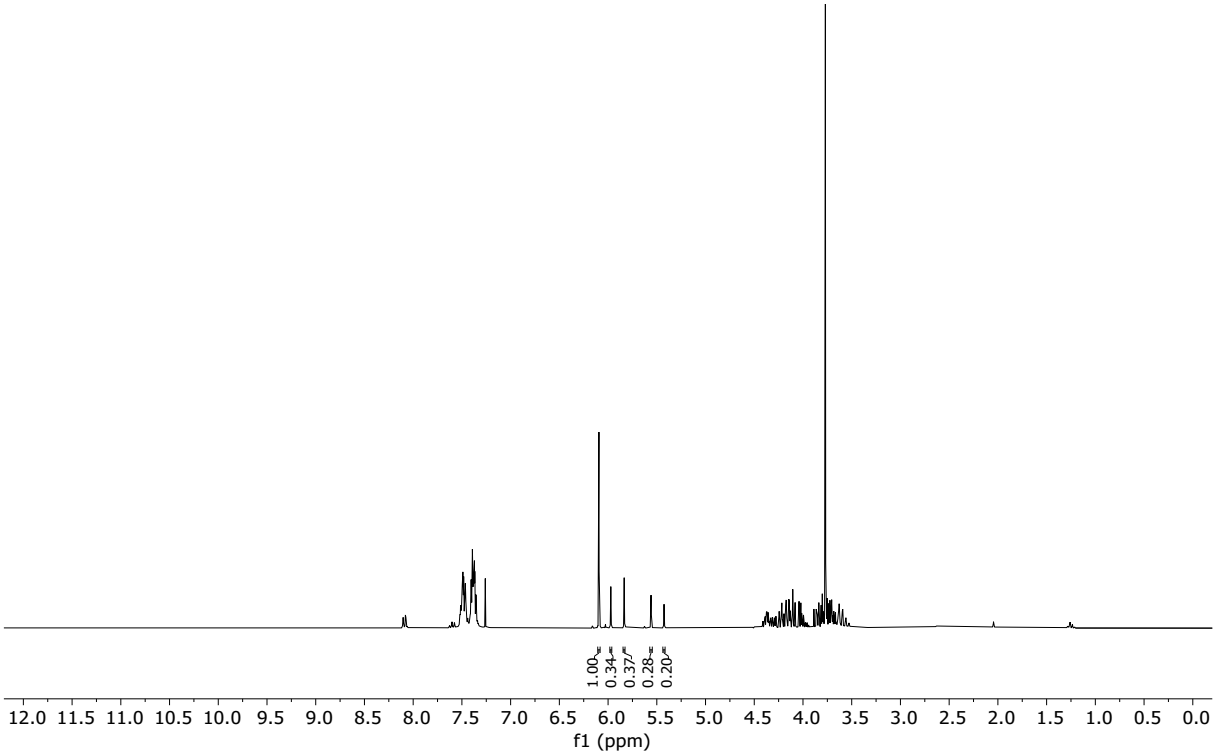

Fig. S1 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with benzaldehyde.

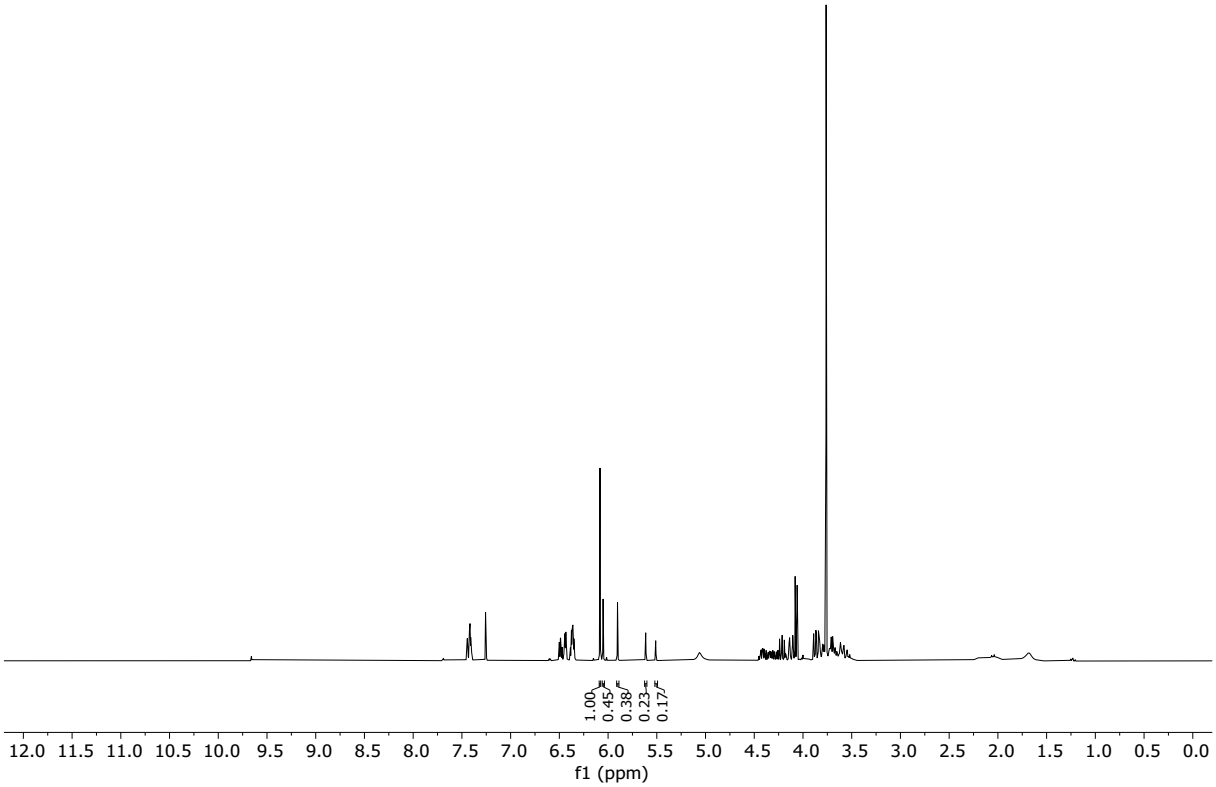

Fig. S2 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with furfural.

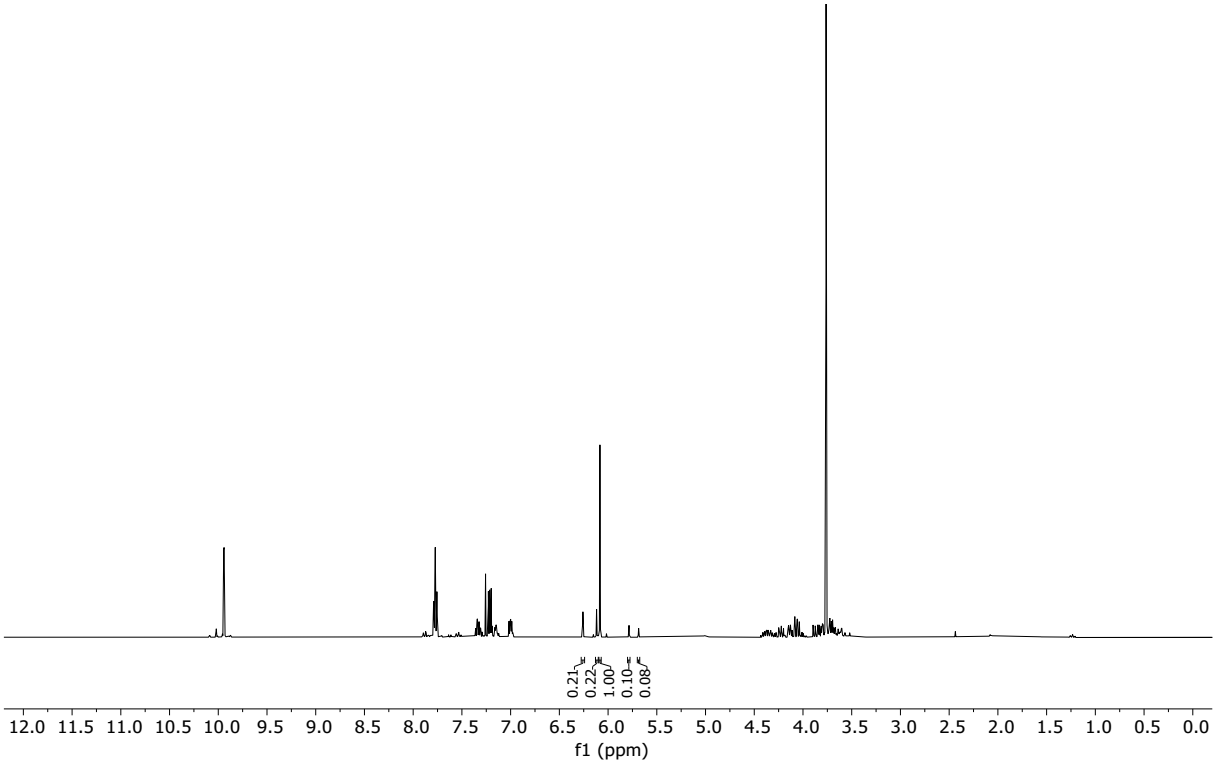

Fig. S3 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 2-thiophenecarboxaldehyde.

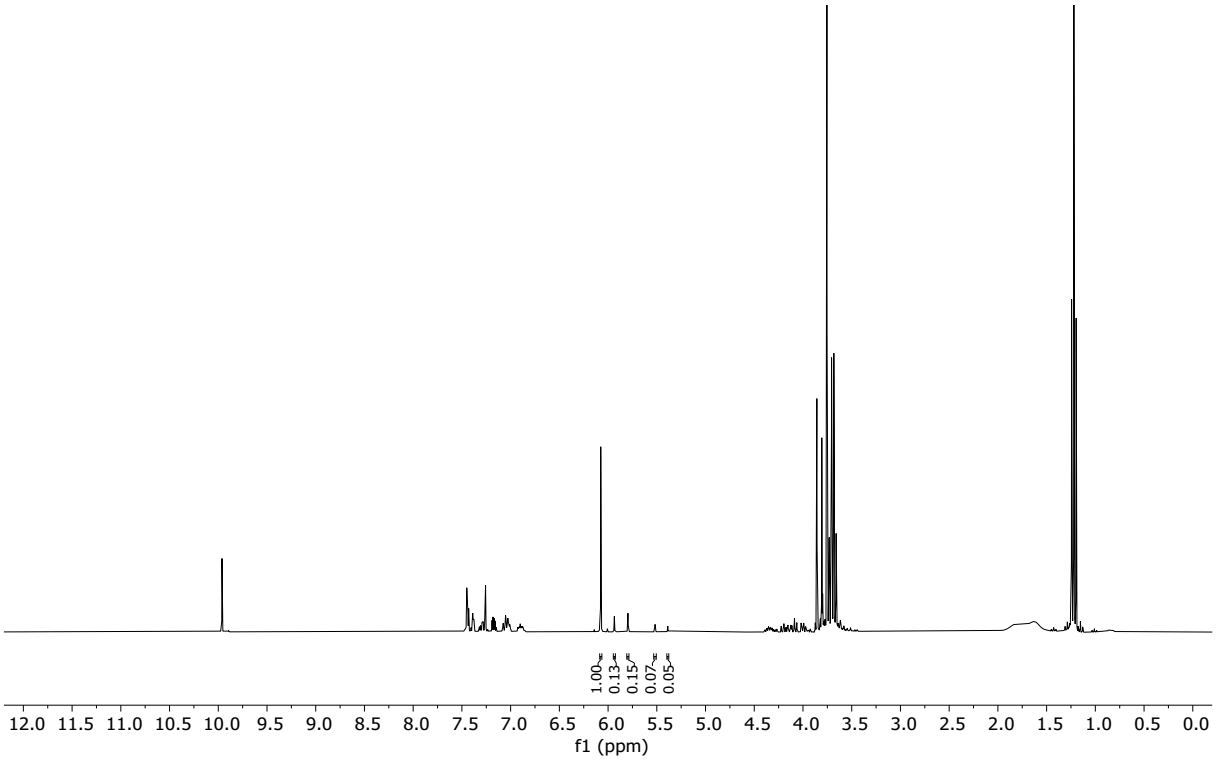

Fig. S4 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 3-methoxybenzaldehyde.

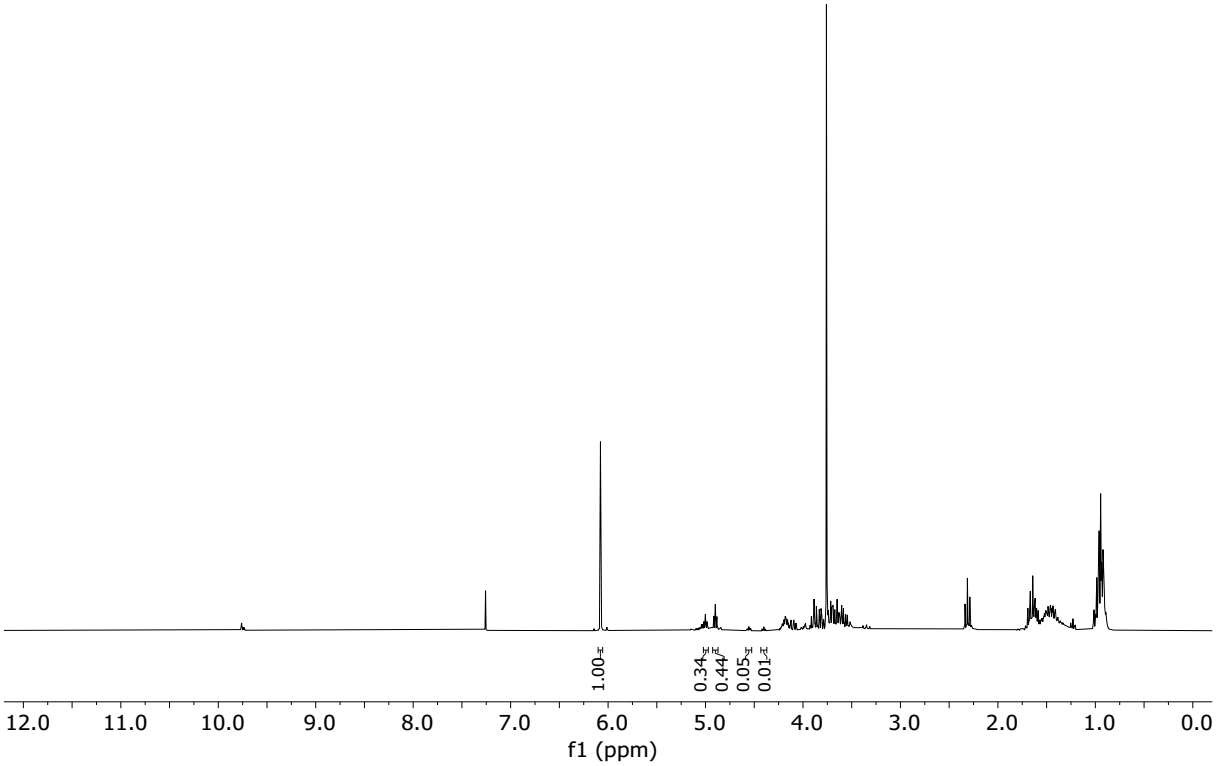

Fig. S5 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with butyraldehyde.

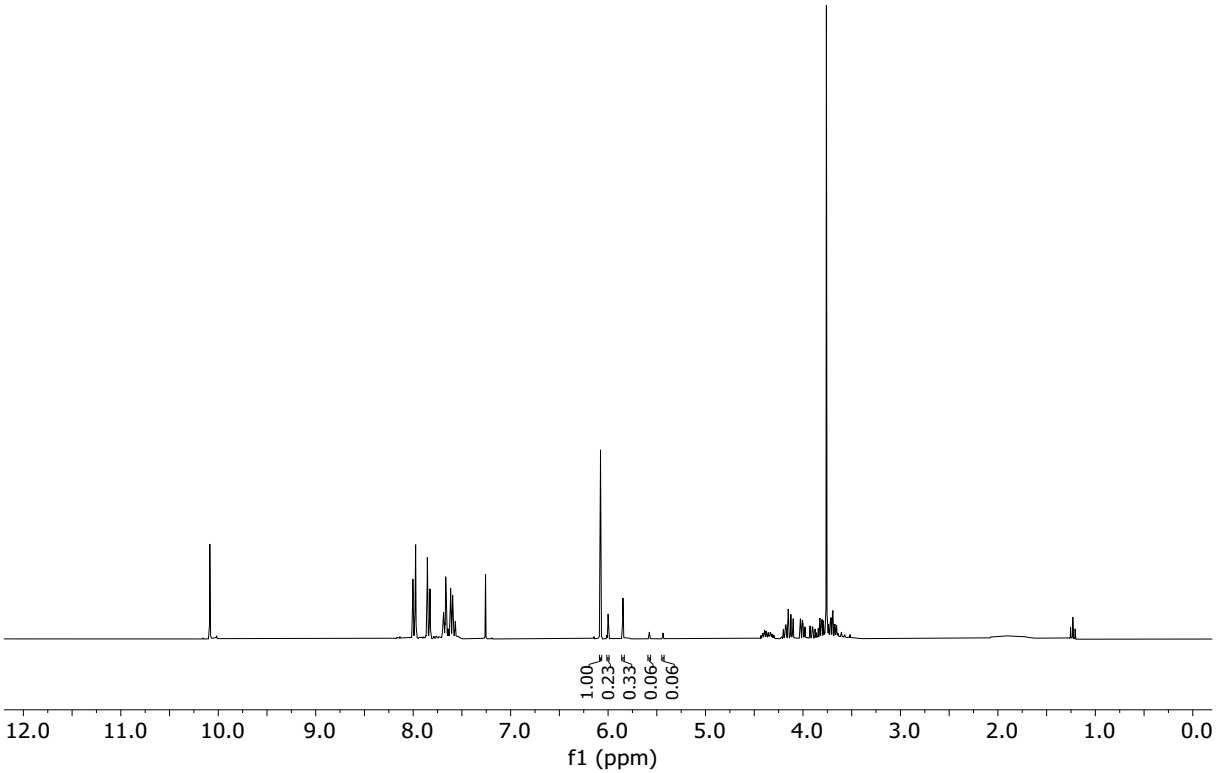

Fig. S6 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-cyanobenzaldehyde.

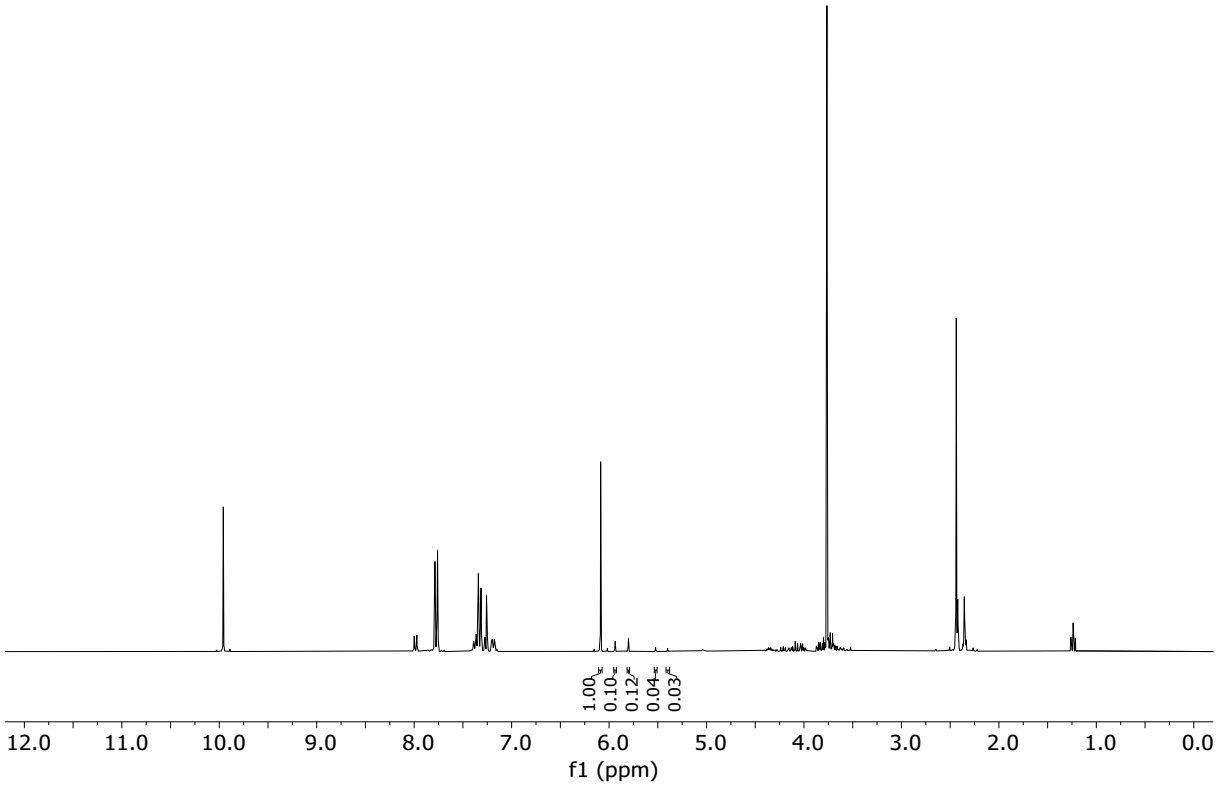

Fig. S7 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-methylbenzaldehyde.

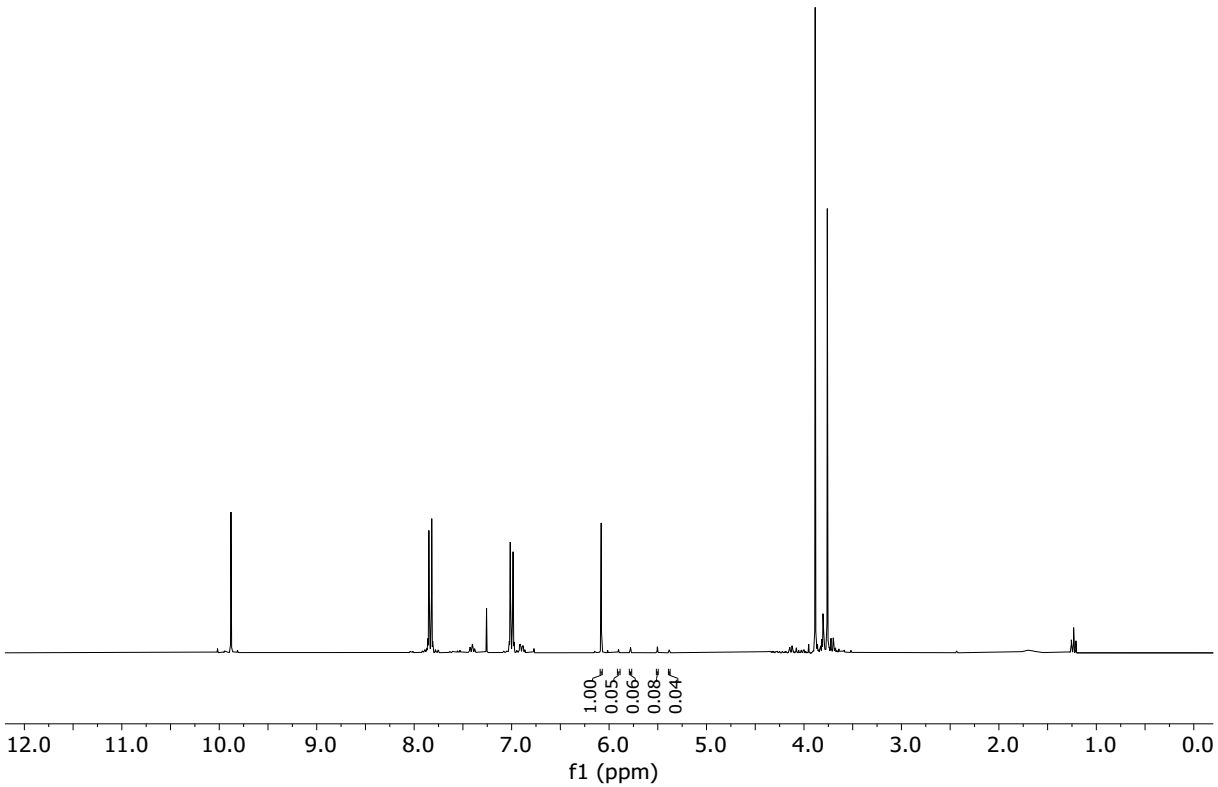

Fig. S8 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-methoxybenzaldehyde.

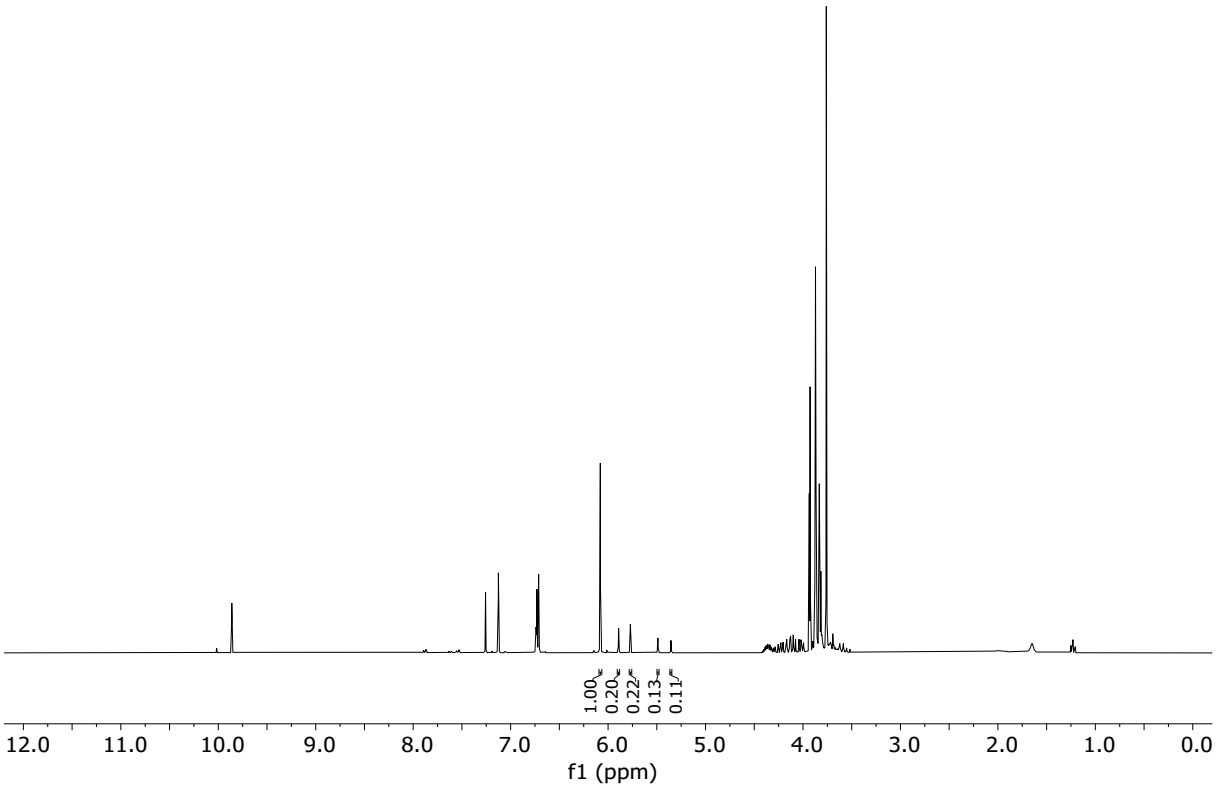

Fig. S9 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 3,4,5-trimethoxybenzaldehyde.

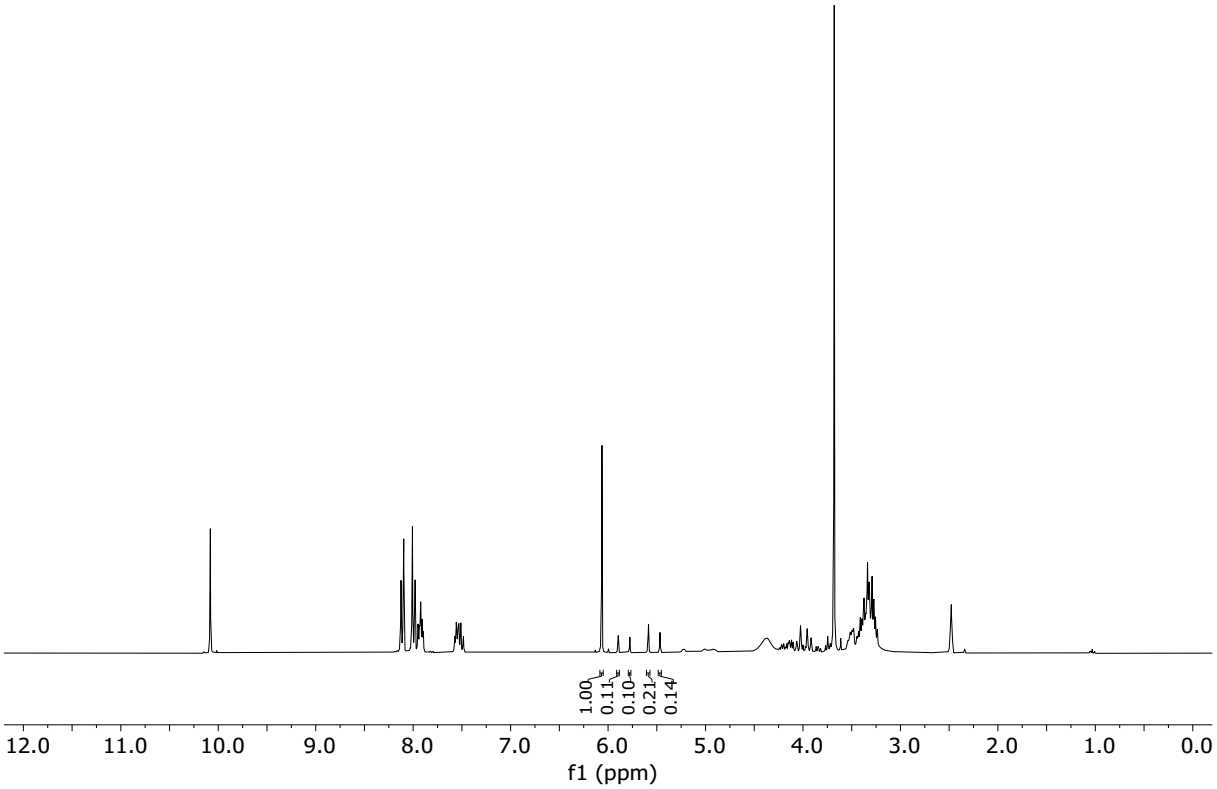

Fig. S10 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-carboxybenzaldehyde.

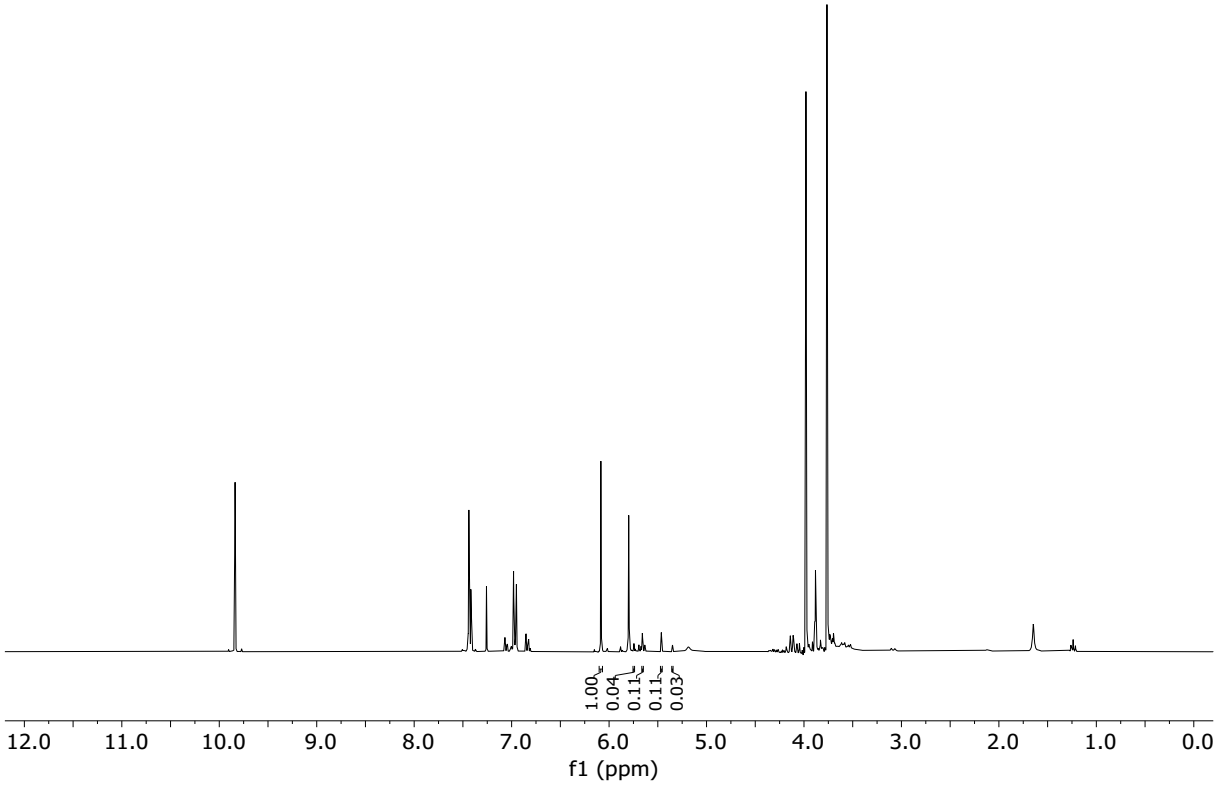

Fig. S11 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-hydroxy-3-methoxybenzaldehyde.

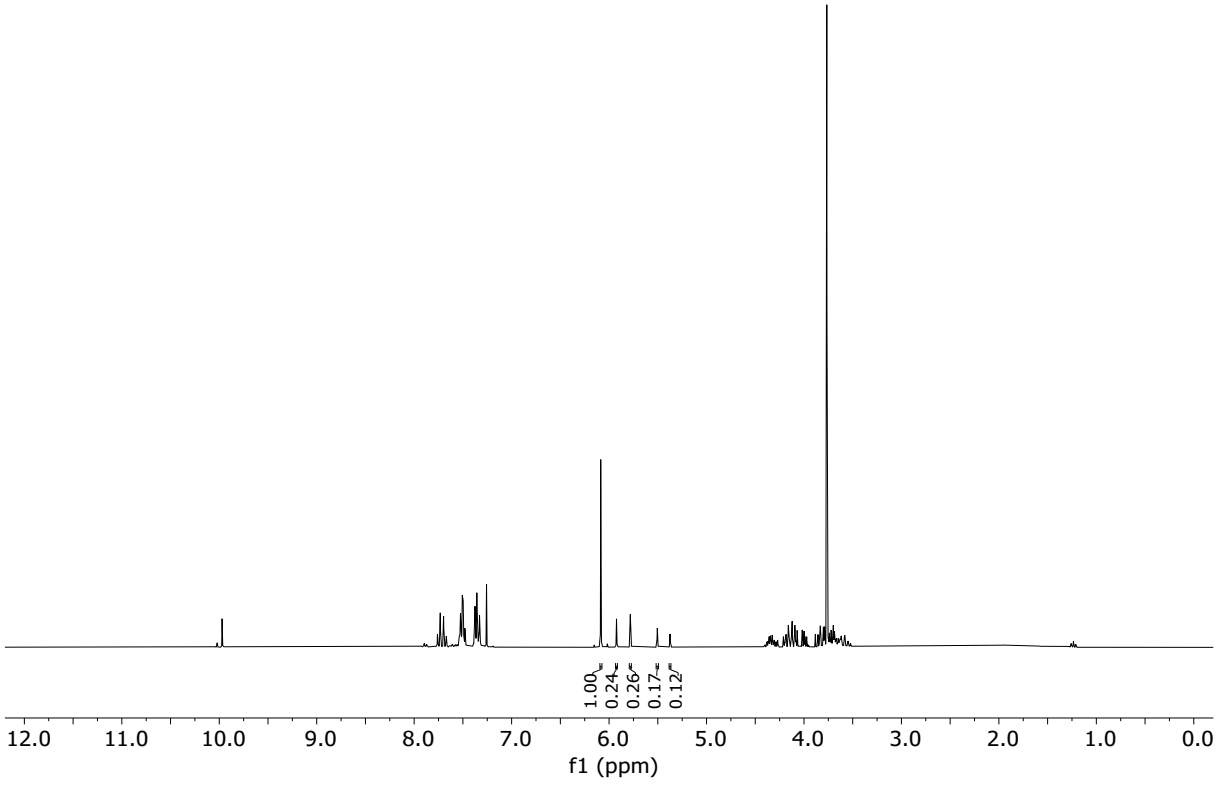

Fig. S12 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-bromobenzaldehyde.

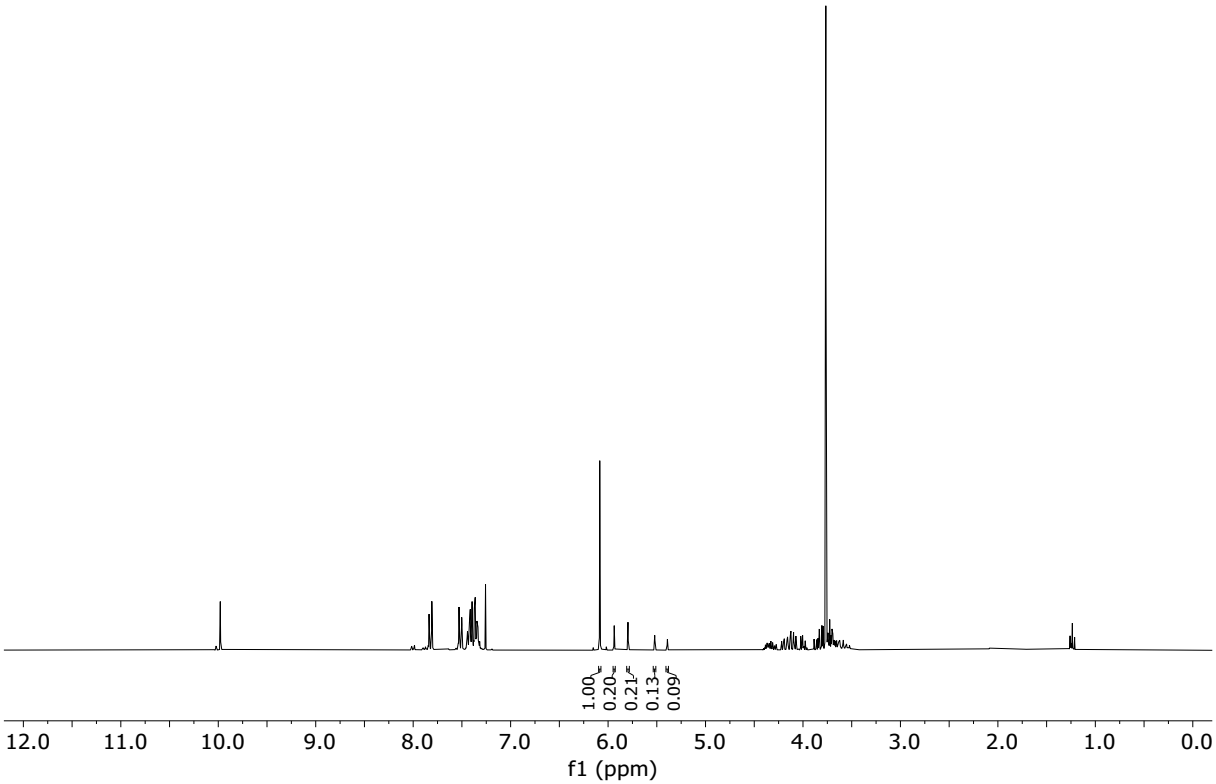

Fig. S13 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-chlorobenzaldehyde.

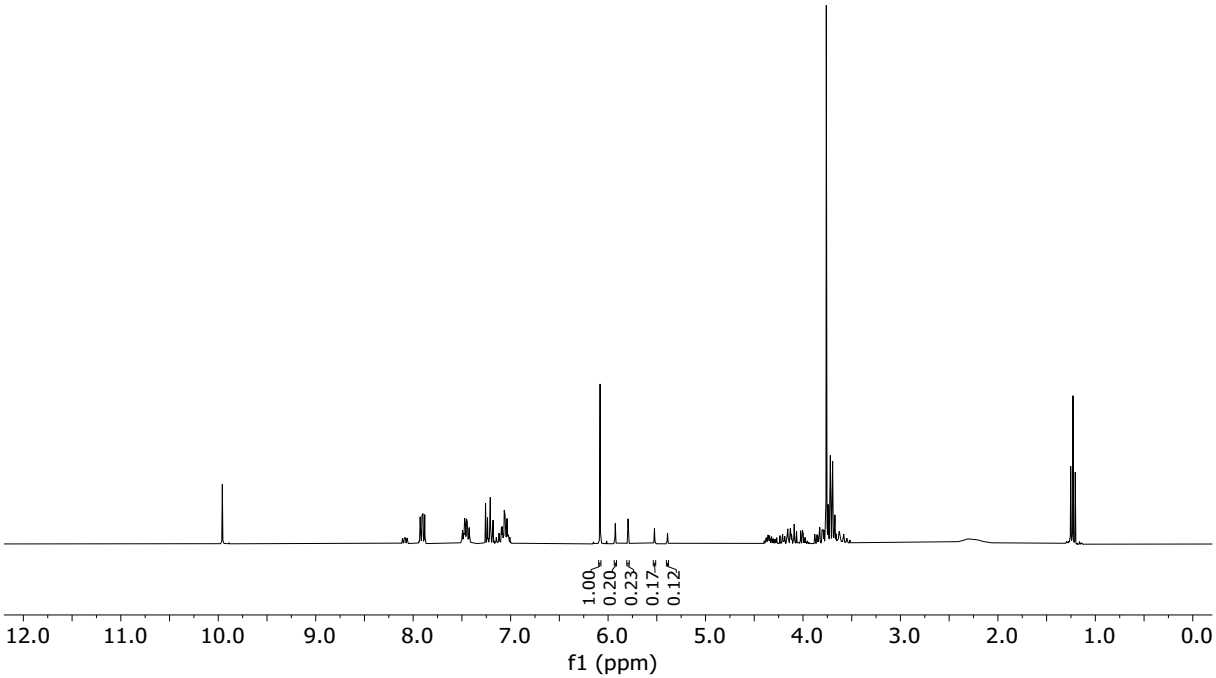

Fig. S14 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-fluorobenzaldehyde.

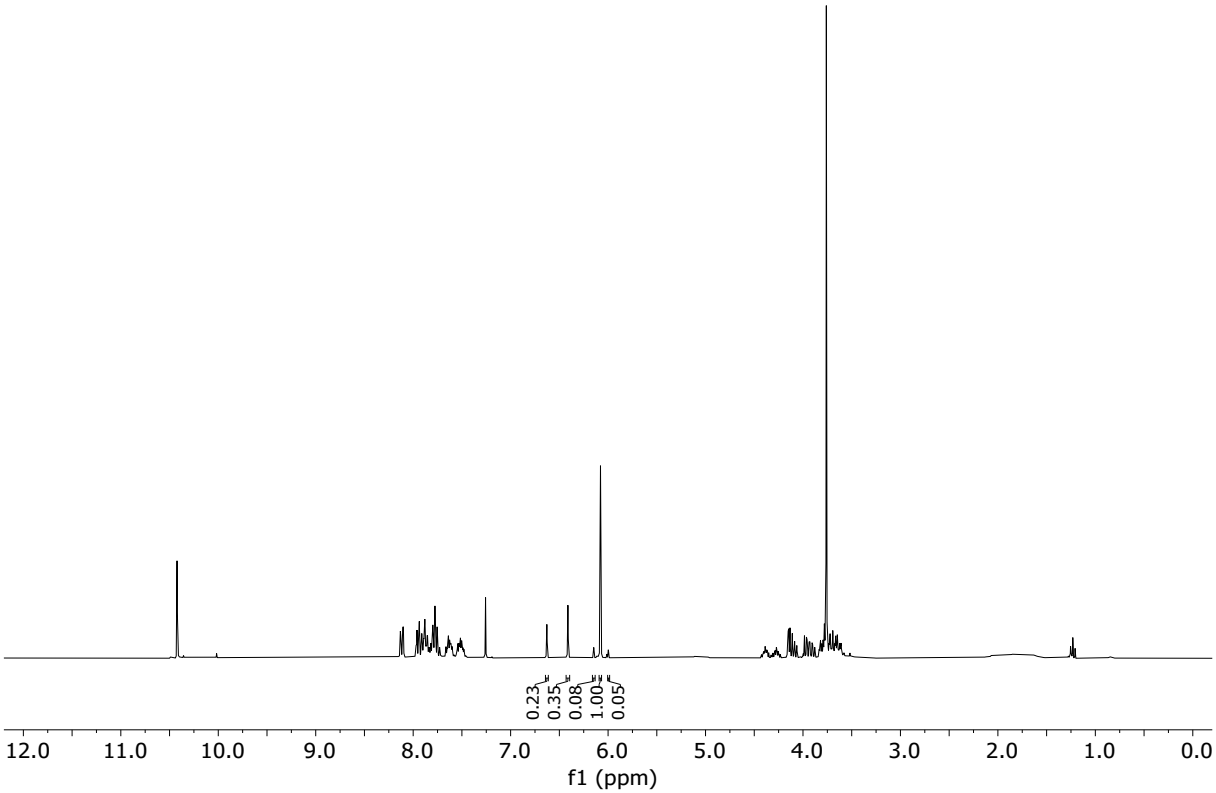

Fig. S15 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 2-nitrobenzaldehyde.

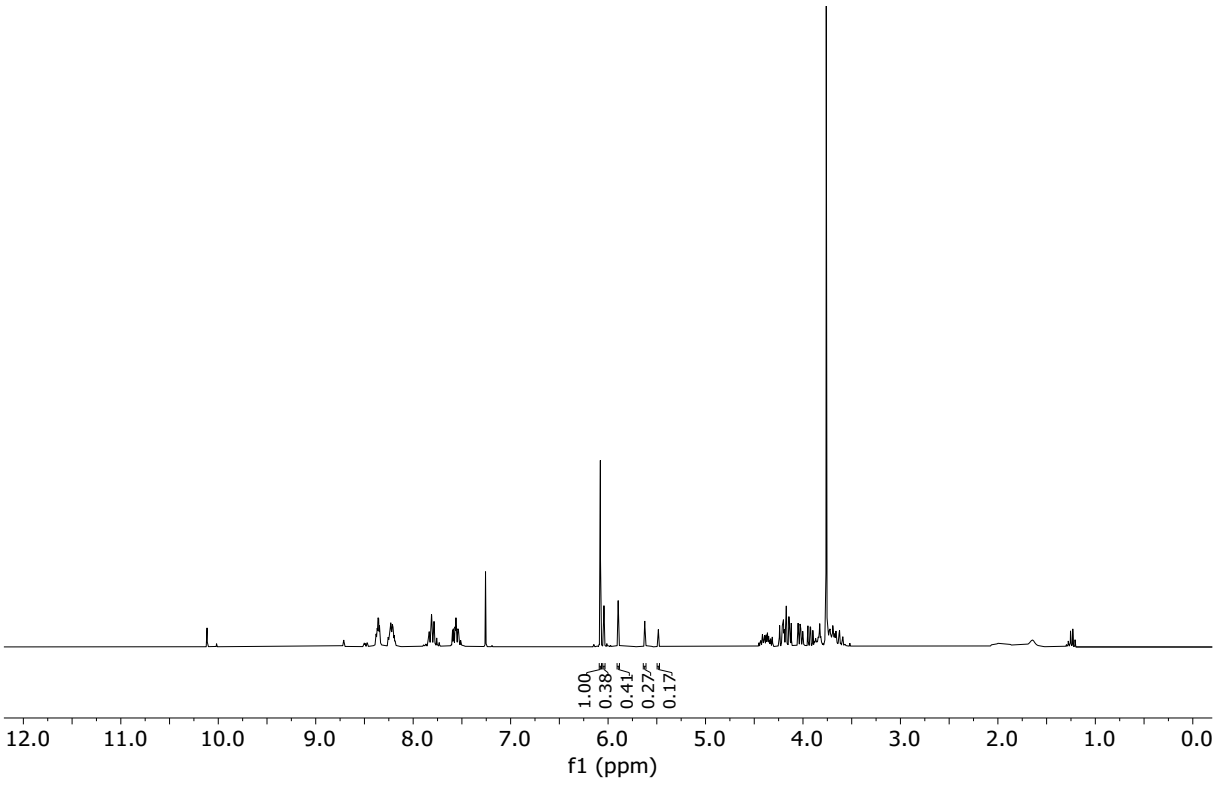

Fig. S16 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 3-nitrobenzaldehyde.

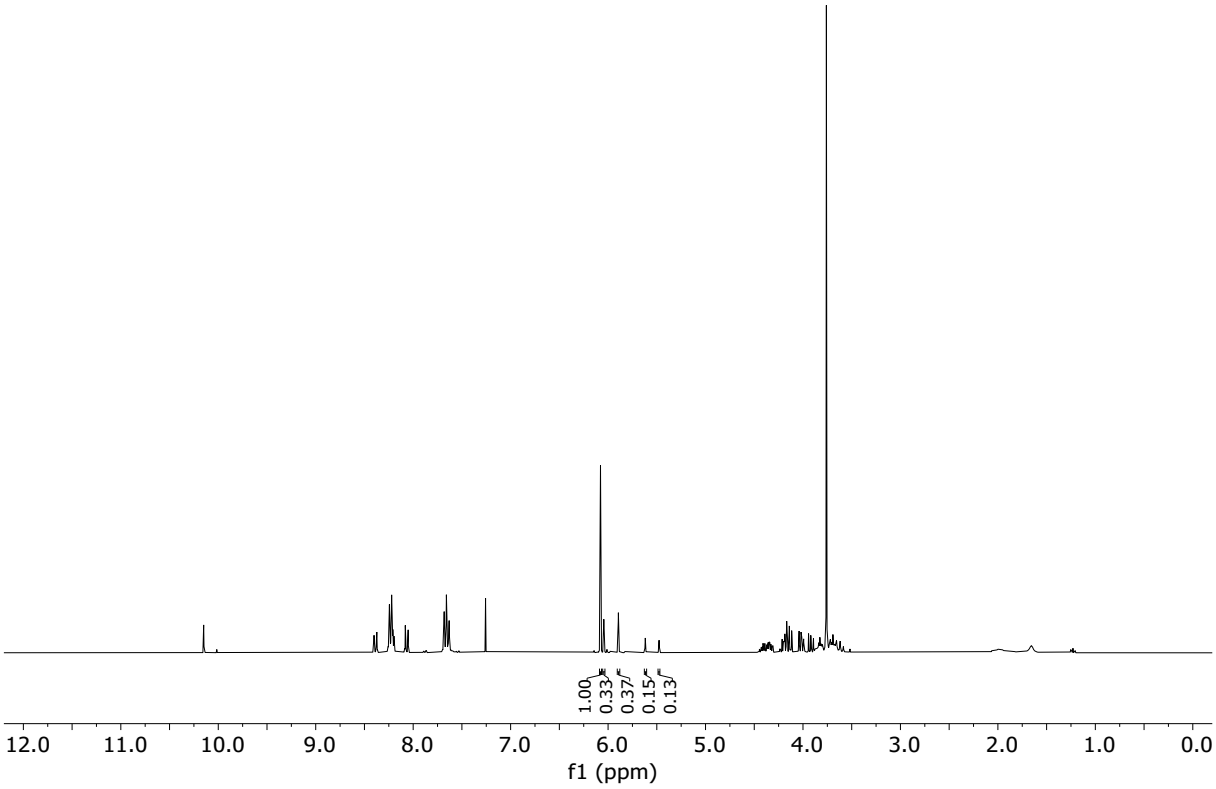

Fig. S17 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-nitrobenzaldehyde.

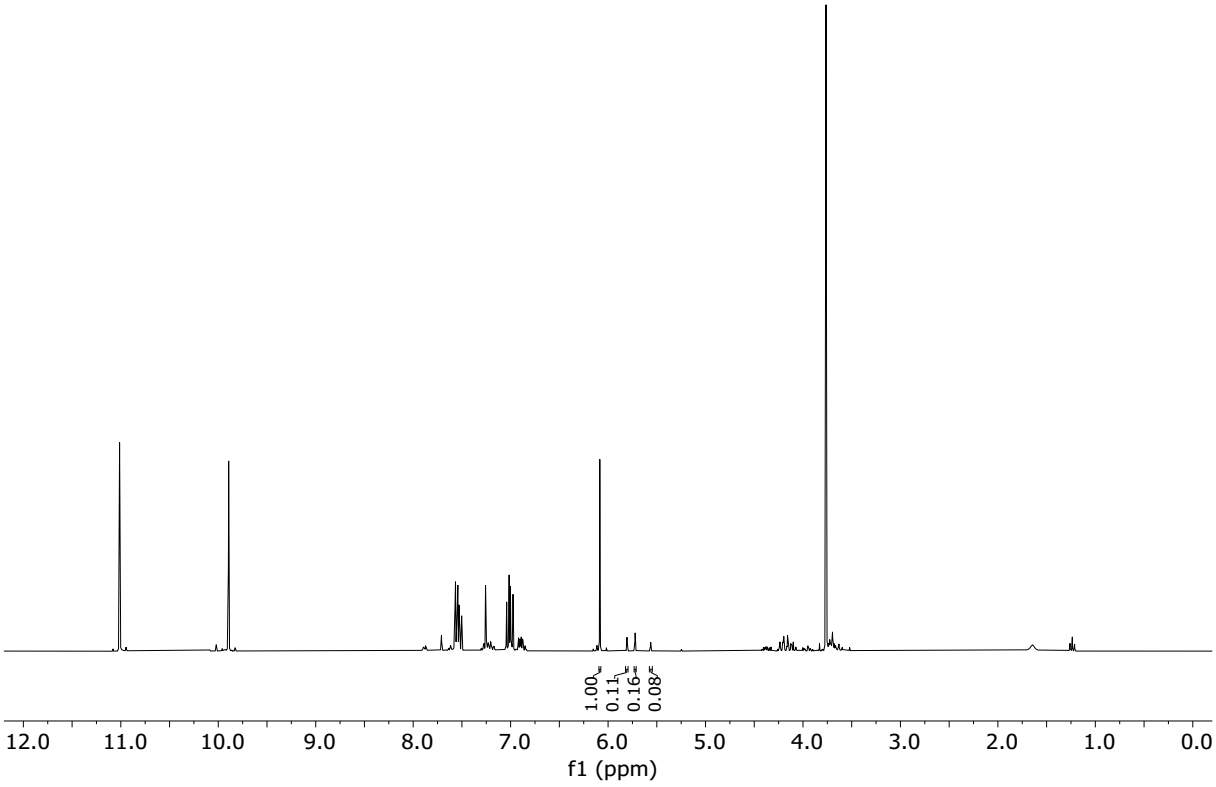

Fig. S18 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 2-hydroxybenzaldehyde.

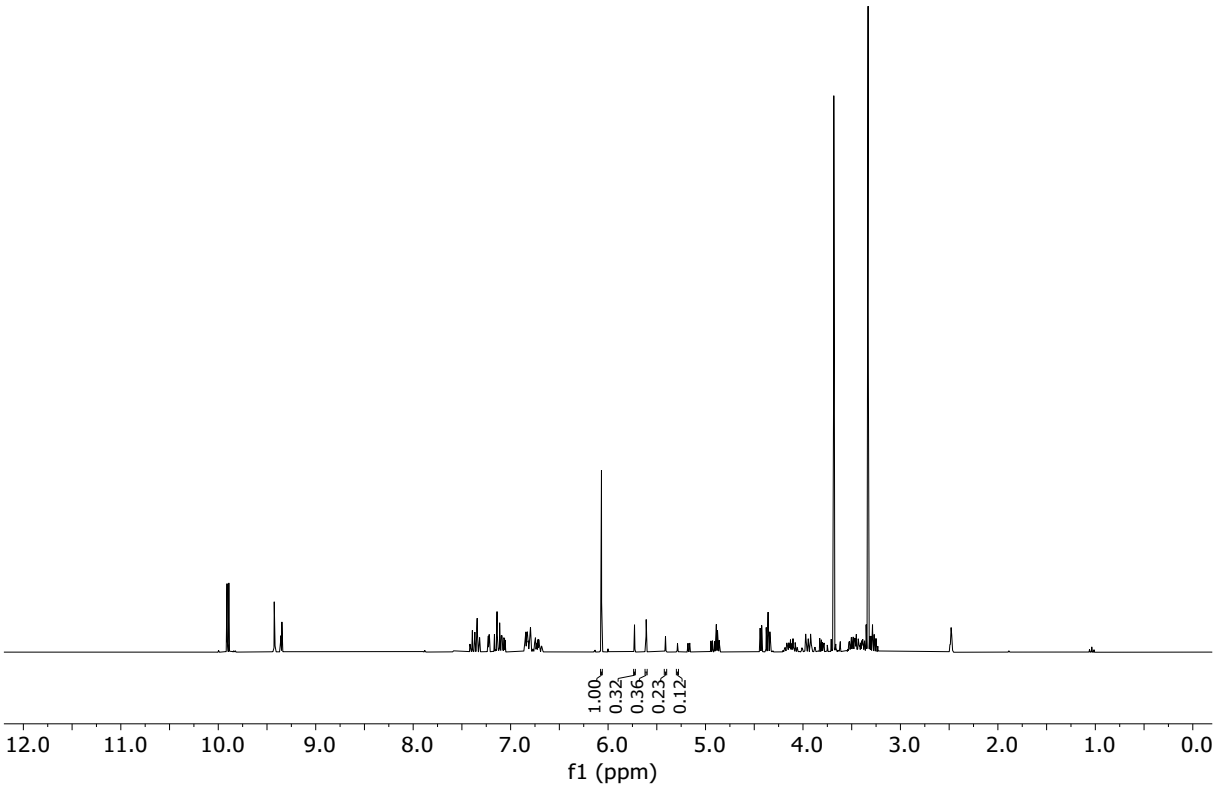

Fig. S19 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 3-hydroxybenzaldehyde.

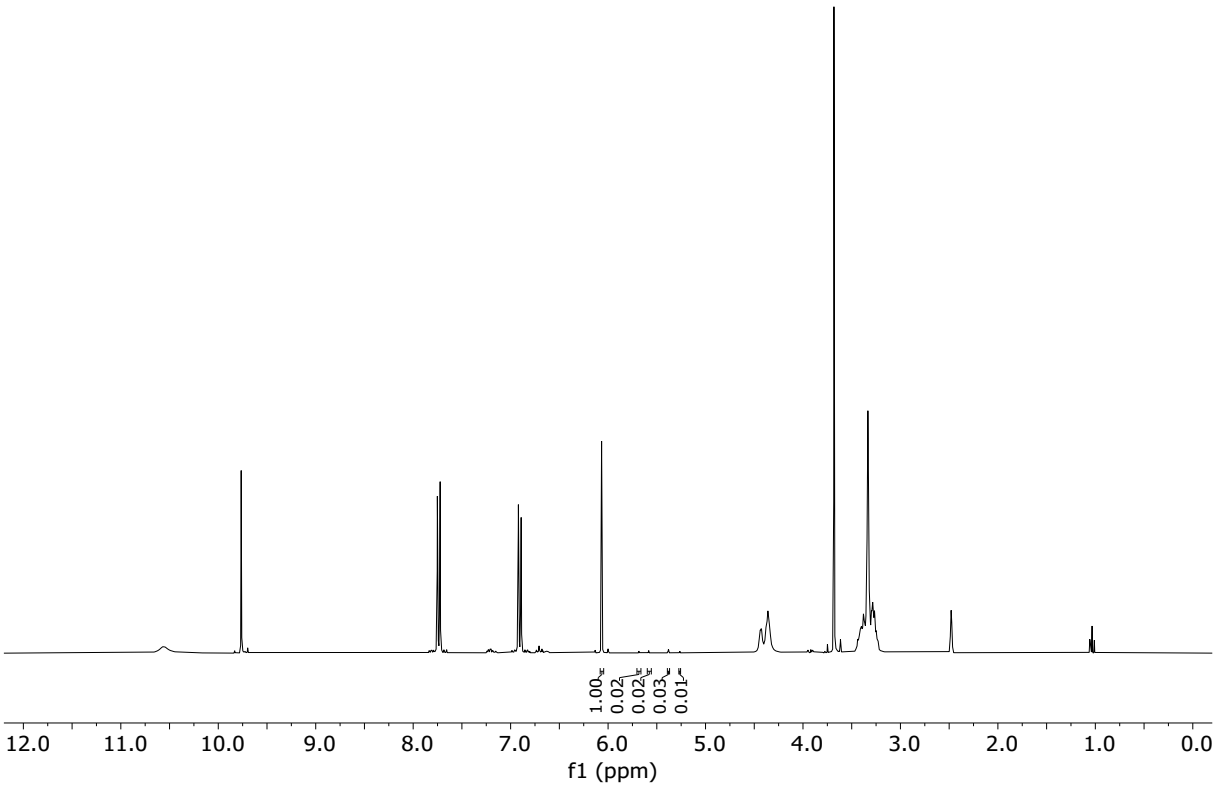

Fig. S20 ^{1}H NMR spectrum (300.069 MHz, $CDCl_3$, δ_{CHCl3} 7.26, δ_{TMB} 6.09), reaction mixture of the acetalization of glycerol with 4-hydroxybenzaldehyde.