Electronic Supplementary Material (ESI) for Green Chemistry. This journal is © The Royal Society of Chemistry 2019

SUPPORTING INFORMATION

Synthesis of long-chain polyols from the Claisen condensation of $\gamma\textsc{-}$ valerolactone

Camila S. Santos^[a], Caio Soares^[b], Adriano Siqueira^[c] and Antonio C. B. Burtoloso^{*[a]}

Contents	Page
Derivatization of compound 3	2-3
¹ H and ¹³ C NMR spectra of all products	5-36

Derivatization of compound 3 for GC-MS analysis



Compound **3** (5 mg, 0,024 mmol), 0.5 mL of dry 2 Methyltetrahydrofuranand and 200 μ L of N,O-Bis(trimethylsilyl)trifluoroacetamide (BSTFA) were added to a 25 mL round bottom flask. Next, the reaction was heated at 60°C during 2h. The system was cooled to 25 °C and a 100 μ L aliquot of the reaction medium was diluted in 5 mL of dichloromethane. An aliquot of this solution was filtered off (Chromafil, Macherey-Nagel, pore size 0.45 μ m) and injected into GC-MS. GC-MS analyses were carried out on Shimadzu-CGMS QP 2010 ULTRA gas chromatography on RESTEK Rtx-5MS 5%diphenyl/95% dimethyl polysiloxane capillary Column 30 m × 0.25 mm, 0.25 μ m, split injector, entrained gas flow (He) 1.33 mL/min, injector 300 °C, interface 330 °C. Column temperature was started from 45 °C maintained for 1 minute and increased to 170 °C at the rate of 10 °C/min, remaining constant for 3 mim. Then, was heated to 330 °C at the rate of 10 °C/min.

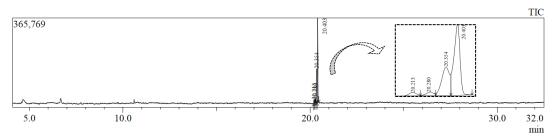
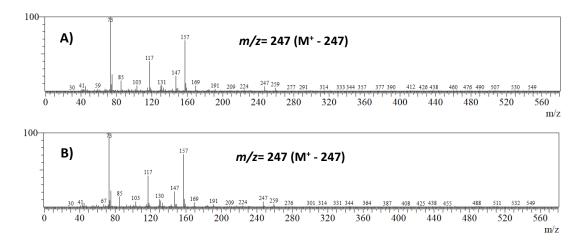


Figure 2. GC-MS chromatogram of silylated compound 3.



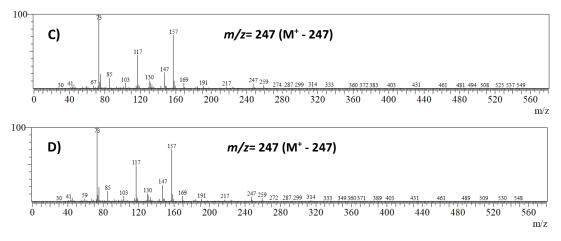
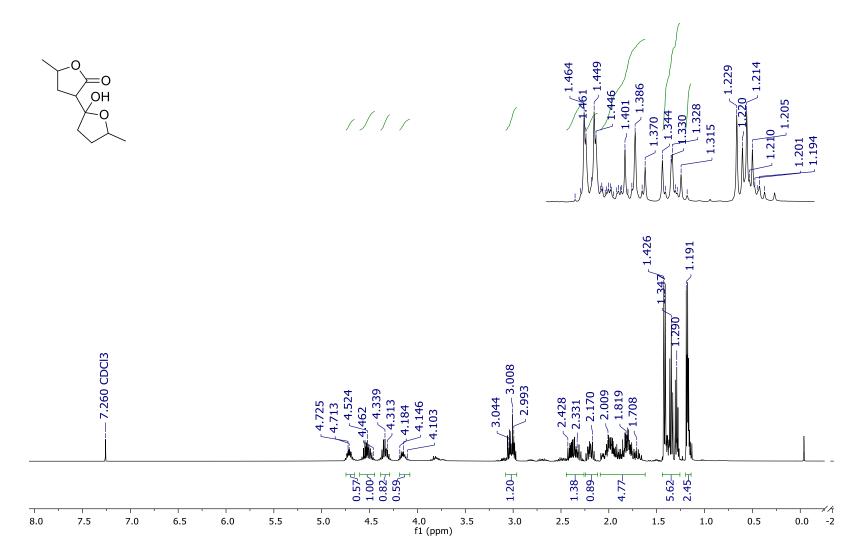
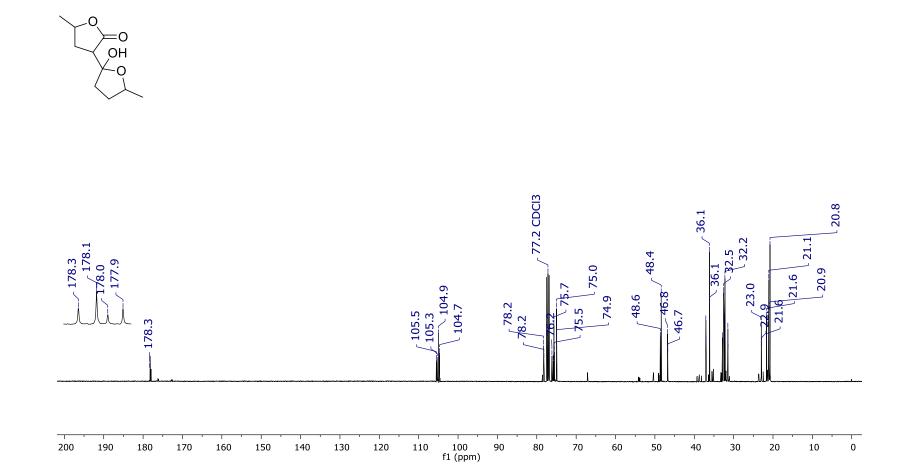
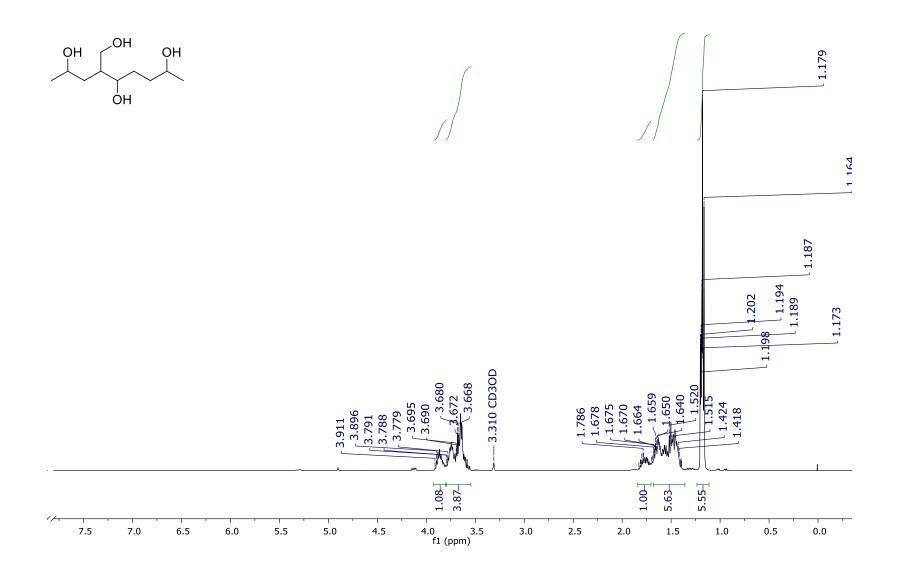
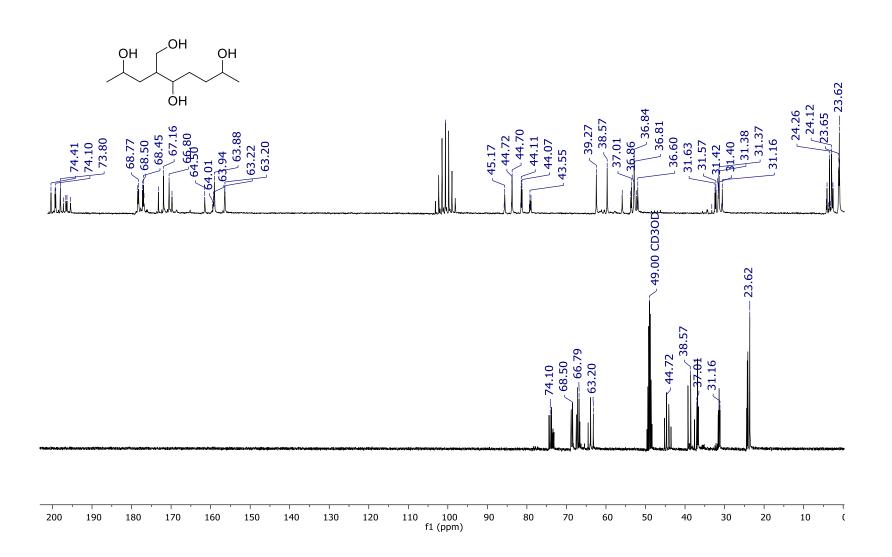


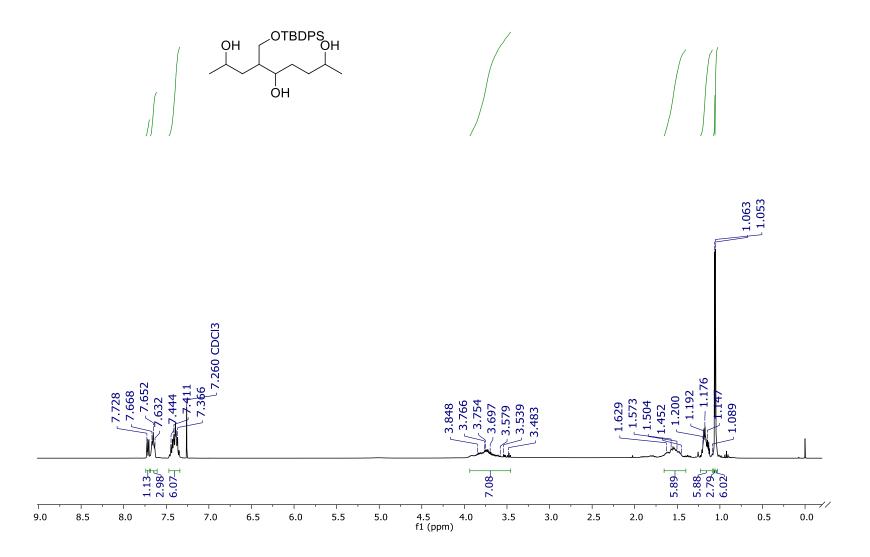
Figure 3. Fragmentation of peaks with retention time A) 20.213, B) 20.280, C) 20.354, D)20.403.

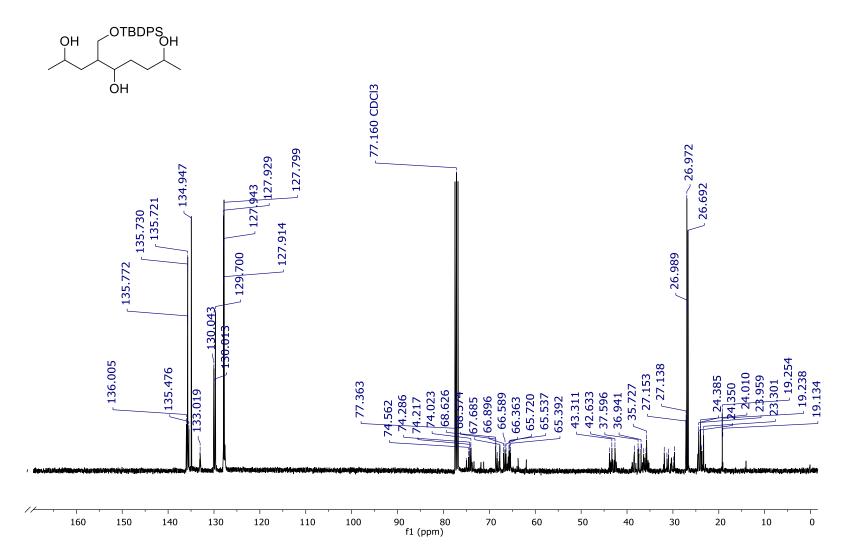


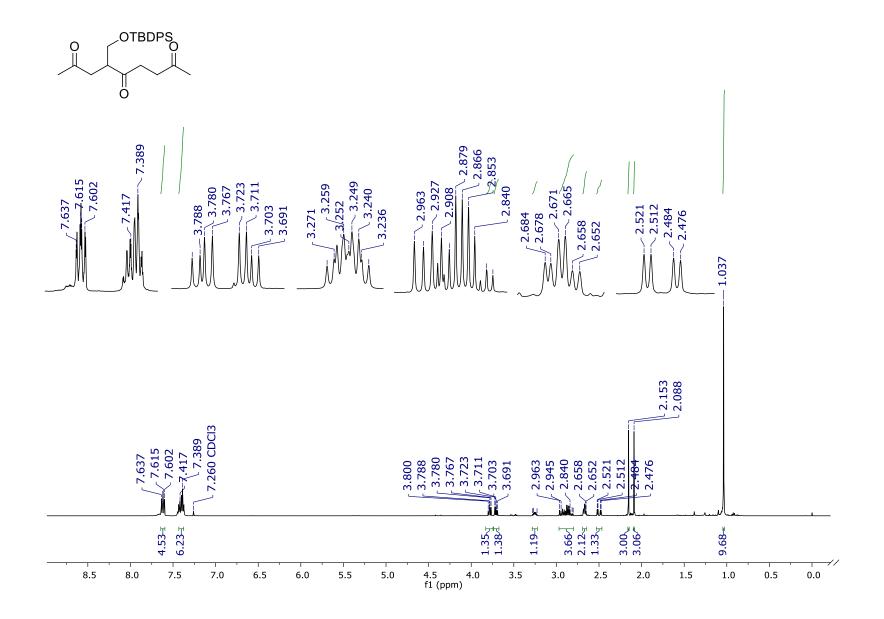


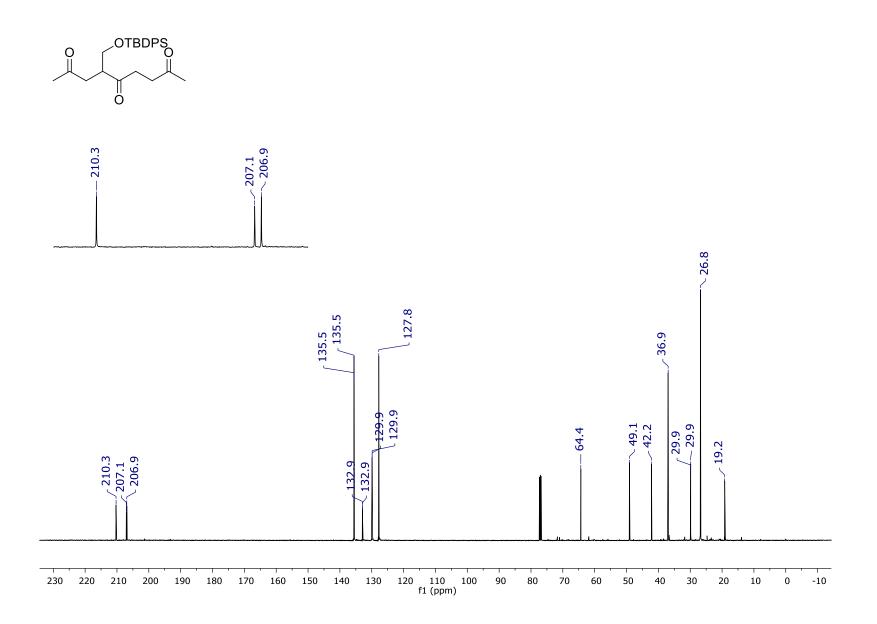


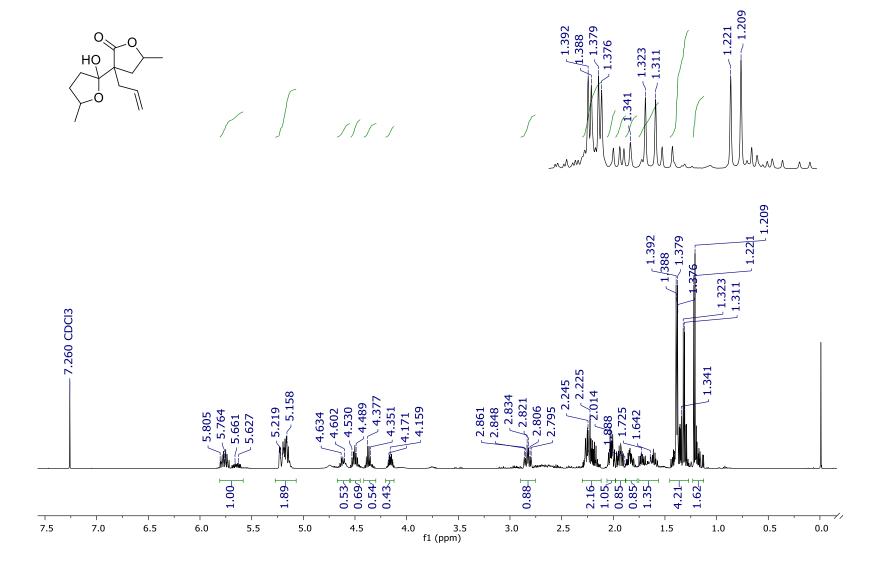




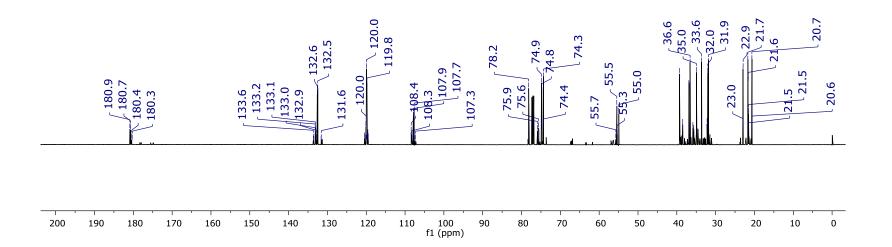


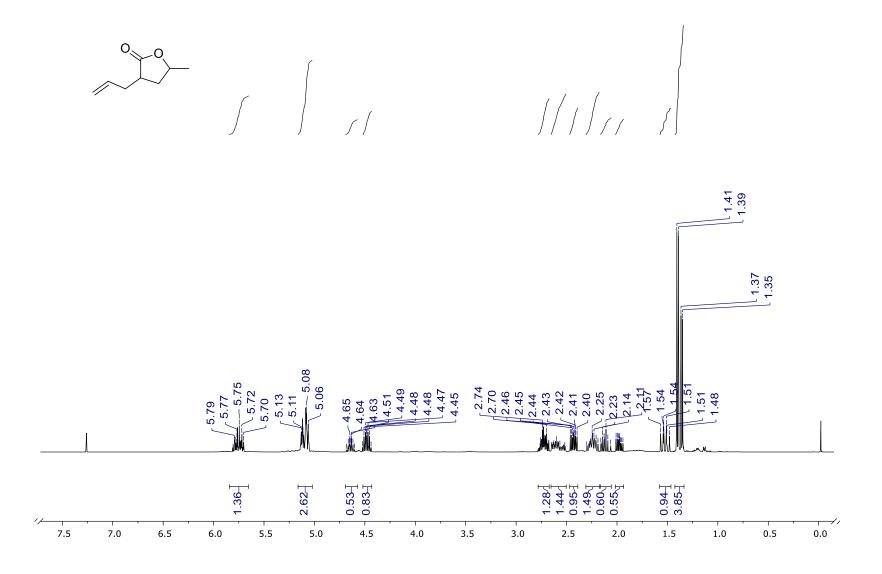






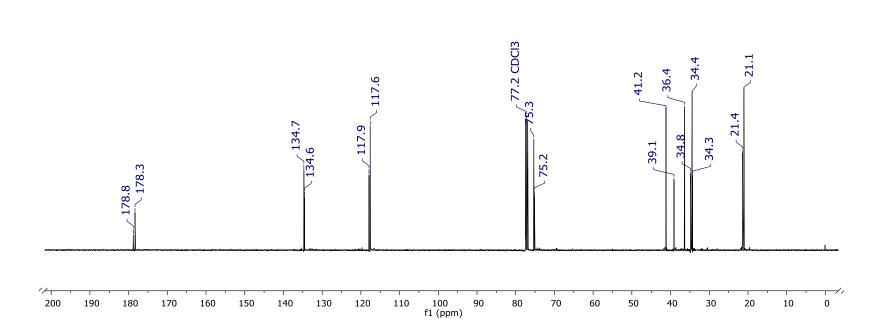
HO



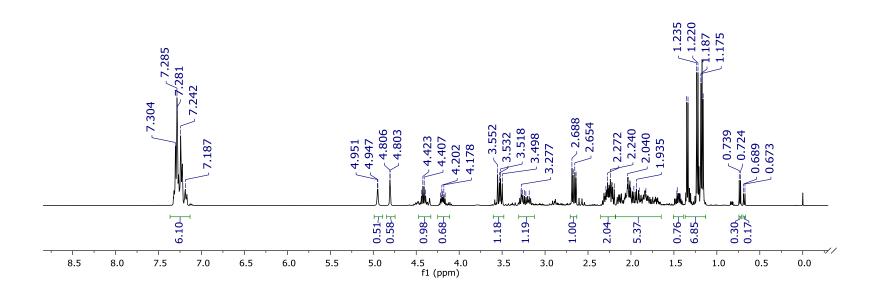


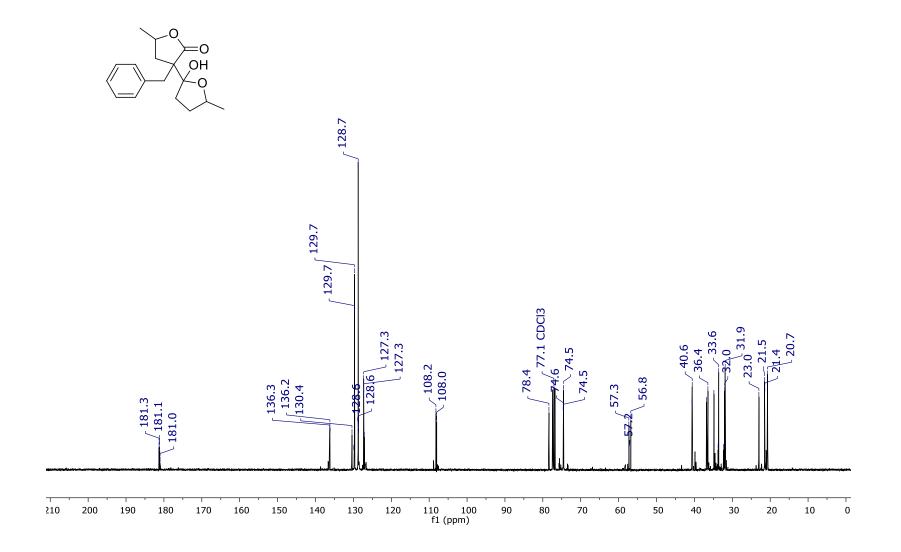


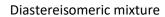
Ο

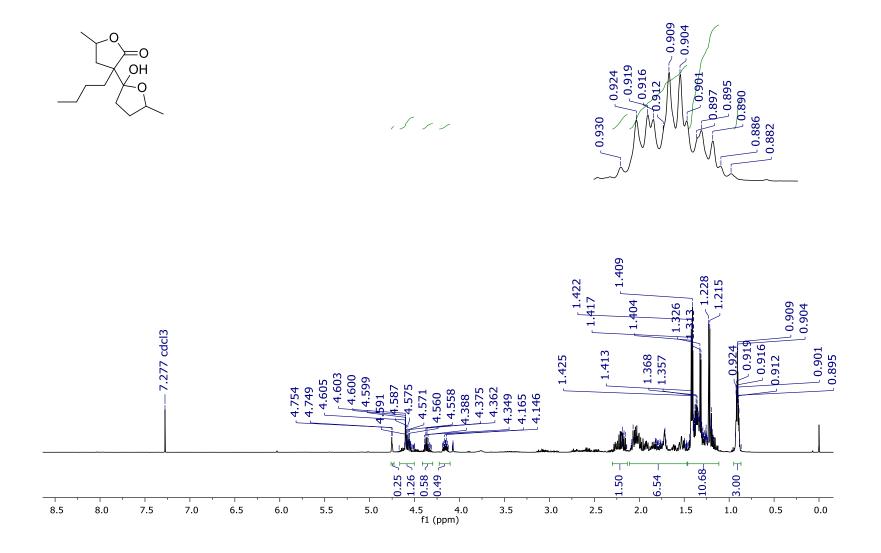


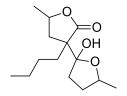


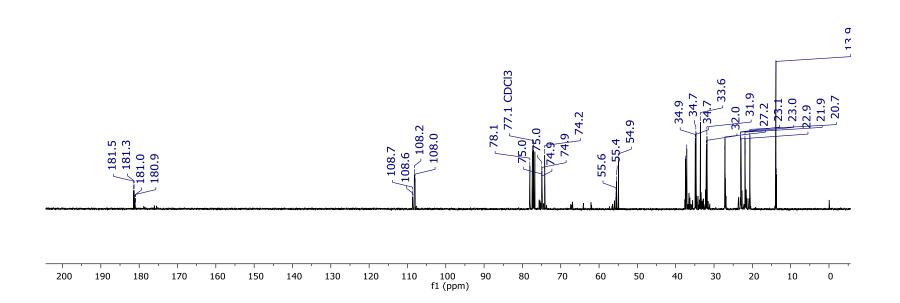


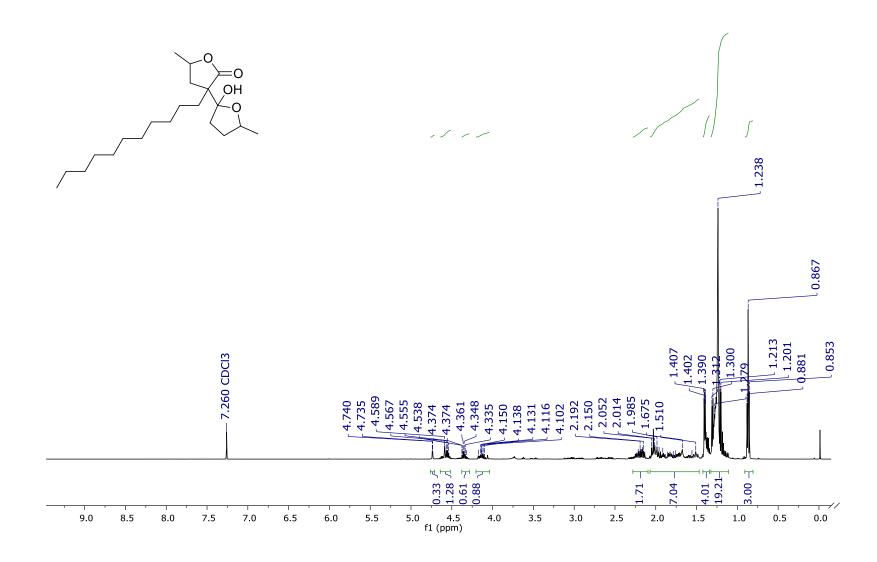


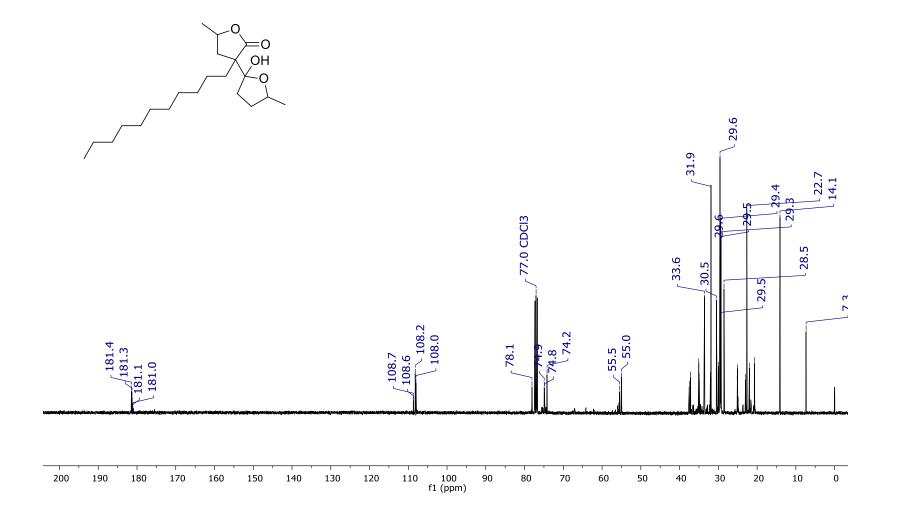


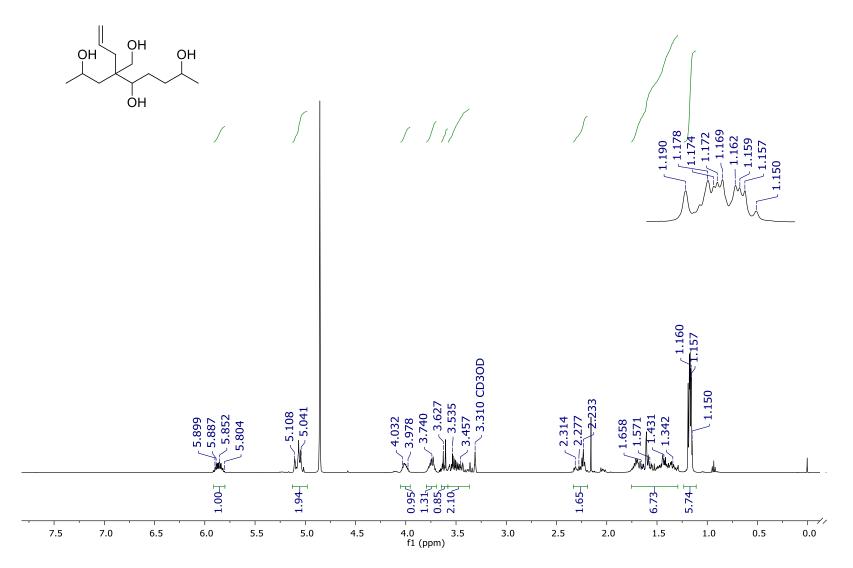




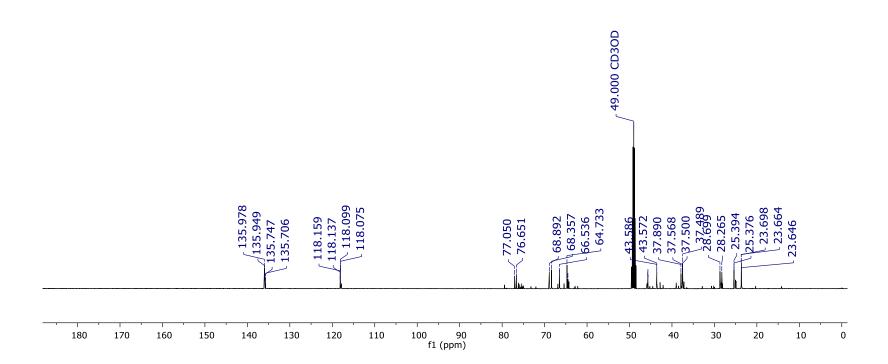




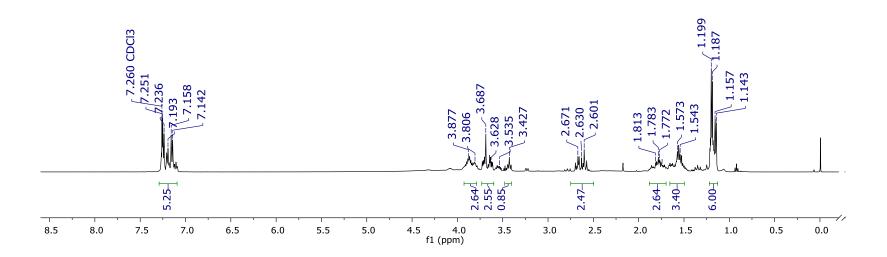




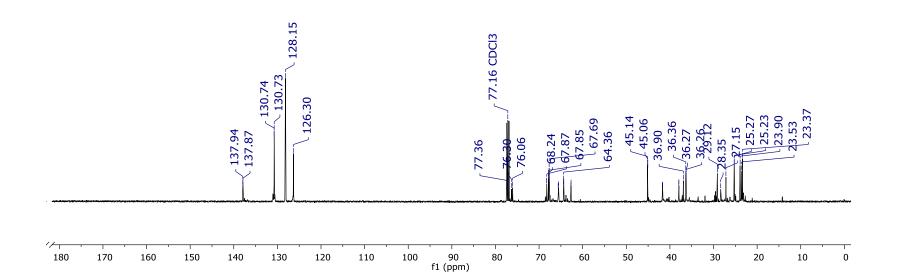
ОН ОН OH ÓН

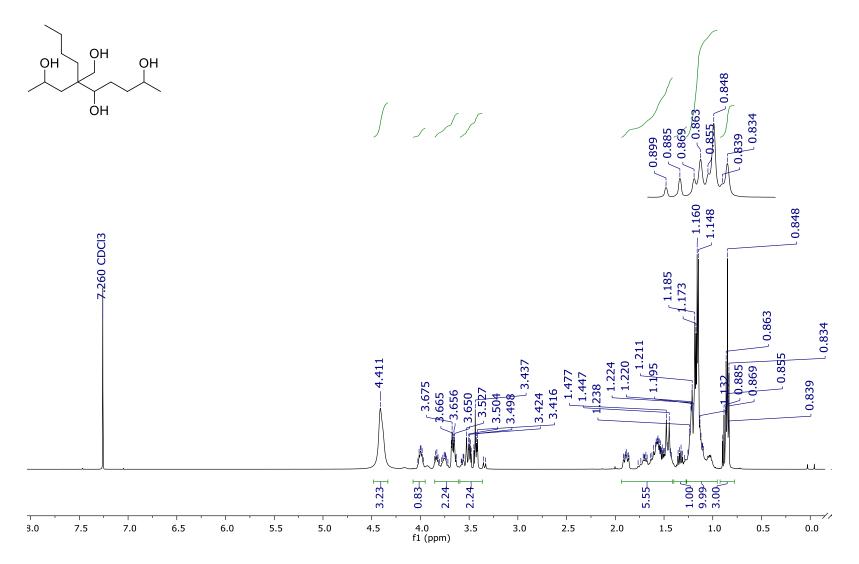




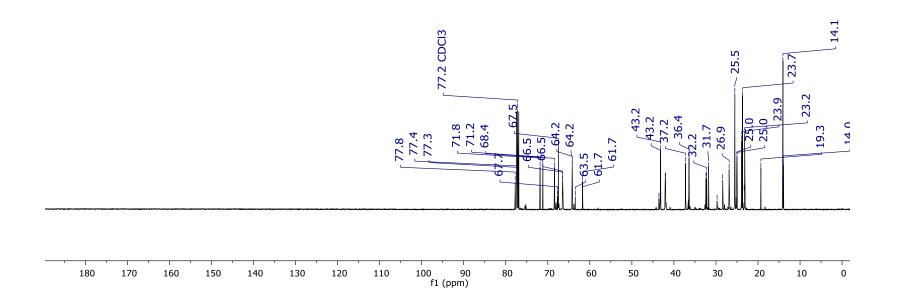


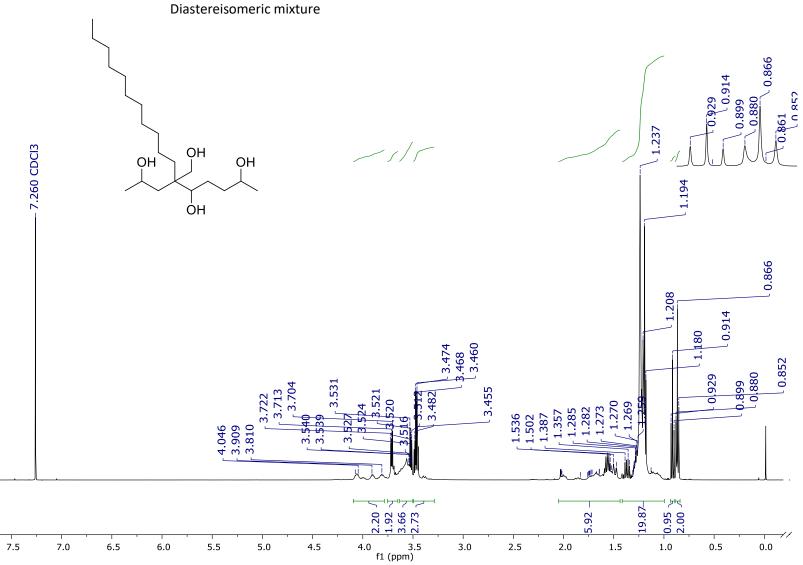
ŌН QН ÓН HΟ

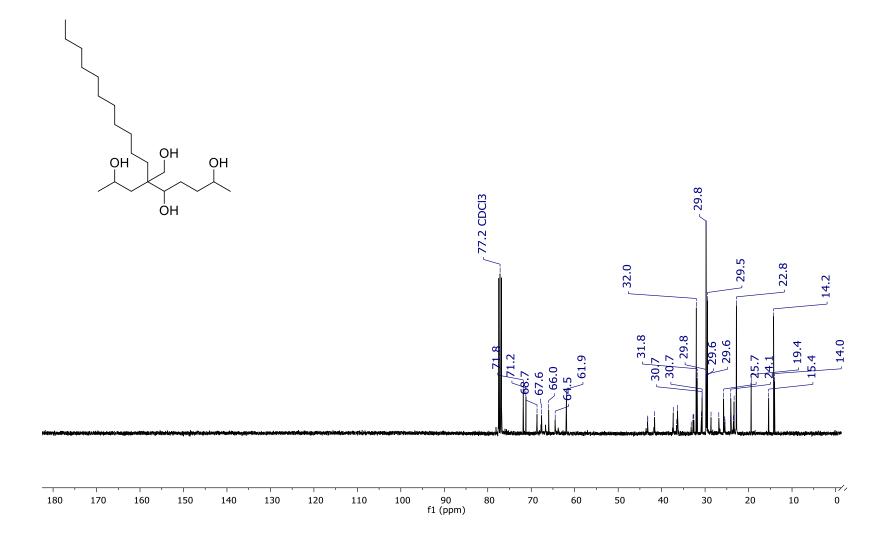


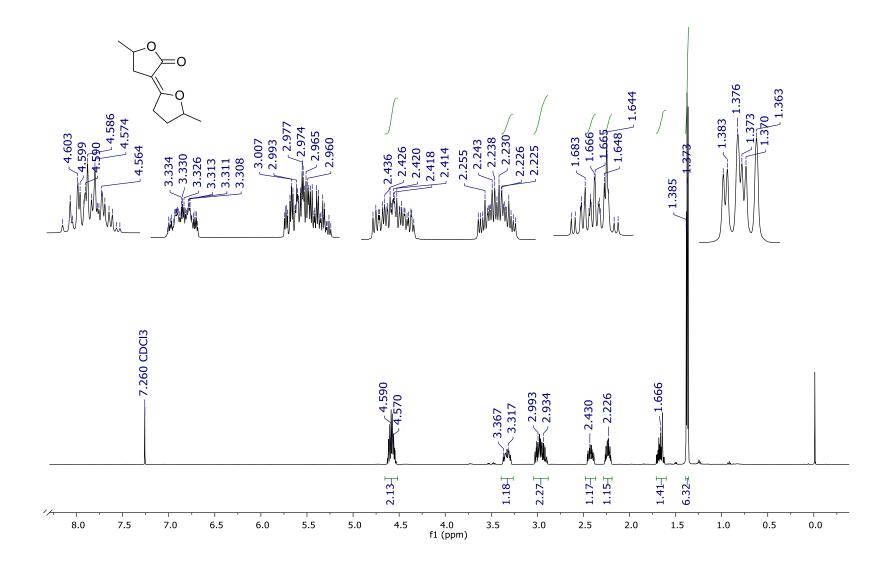


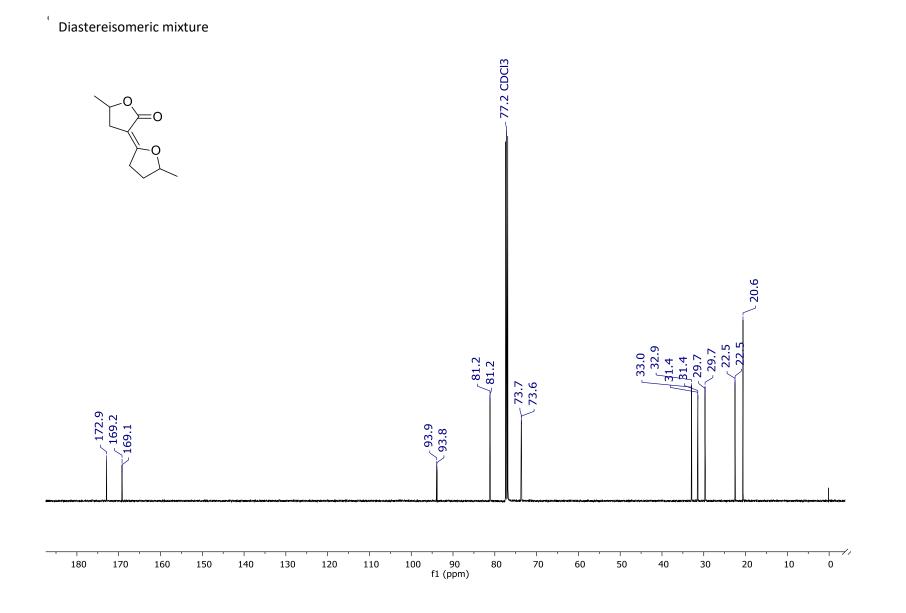
ОН QН ŌН ÓН

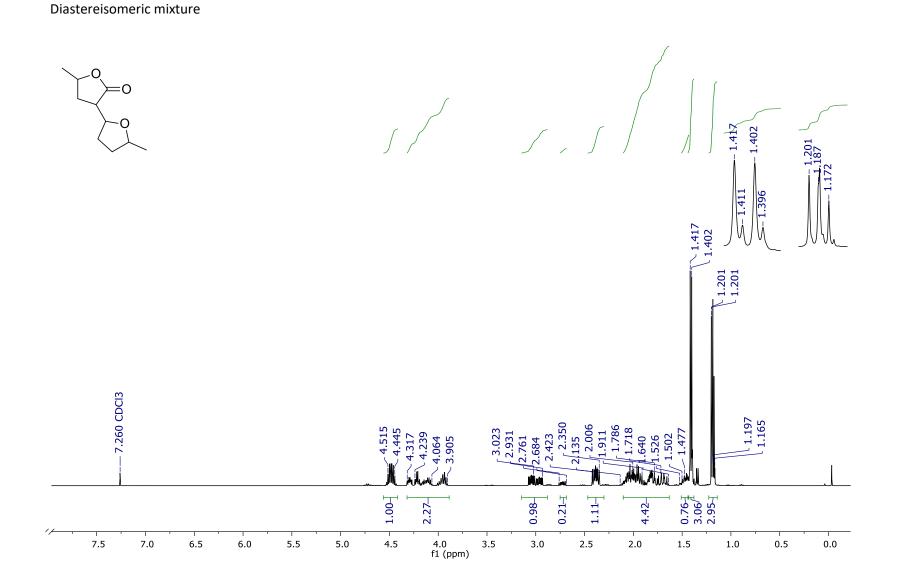












O

