

Supporting Information

Unprecedented biodegradable cellulose-derived polyesters having pendant citronellol moieties: from monomer synthesis to enzymatic degradation

Aihemaiti Kayishaer, Sami Fadlallah,* Louis M. M. Mouterde,* Aurélien A. M. Peru, Yasmine Werghi, Quentin Carboué, Michel Lopez, Florent Allais*

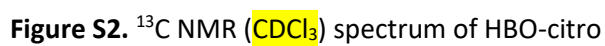
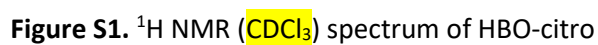
URD Agro-Biotechnologies Industrielles (ABI), CEBB, AgroParisTech, 51110 Pomacle.

* sami.fadlallah@agroparistech.fr, louis.mouterde@agroparistech.fr,
florent.allais@agroparistech.fr

Table of contents

NMR	2
LC-MS	16
SEC.....	17
FT-IR.....	21
DSC	22
TGA.....	24

a. HBO-citro



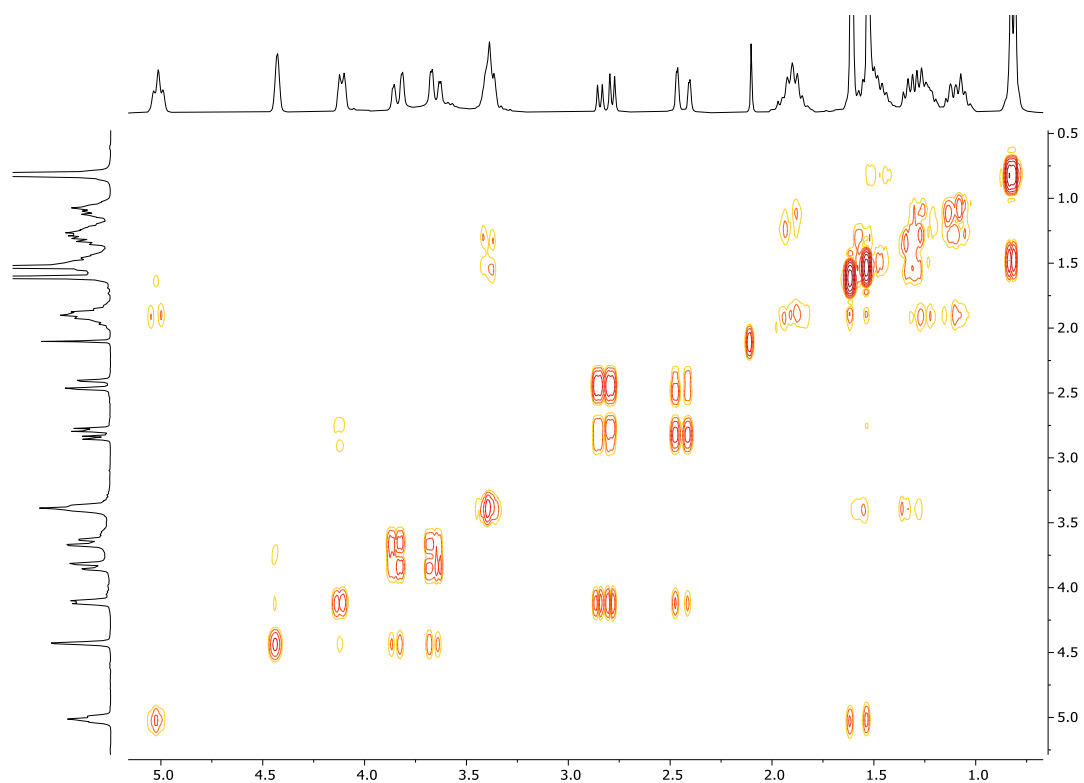


Figure S3. ^1H - ^1H COSY (CDCl_3) spectrum of HBO-citro

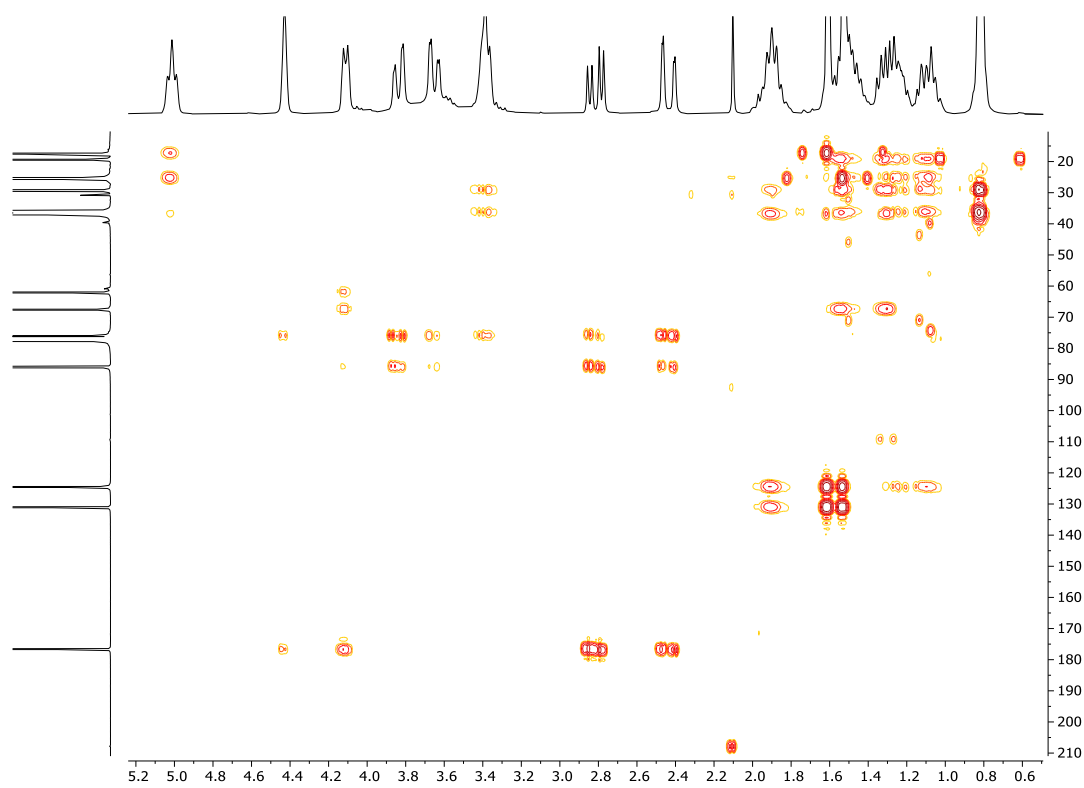


Figure S4. ^1H - ^{13}C HMBC (CDCl_3) spectrum of HBO-citro

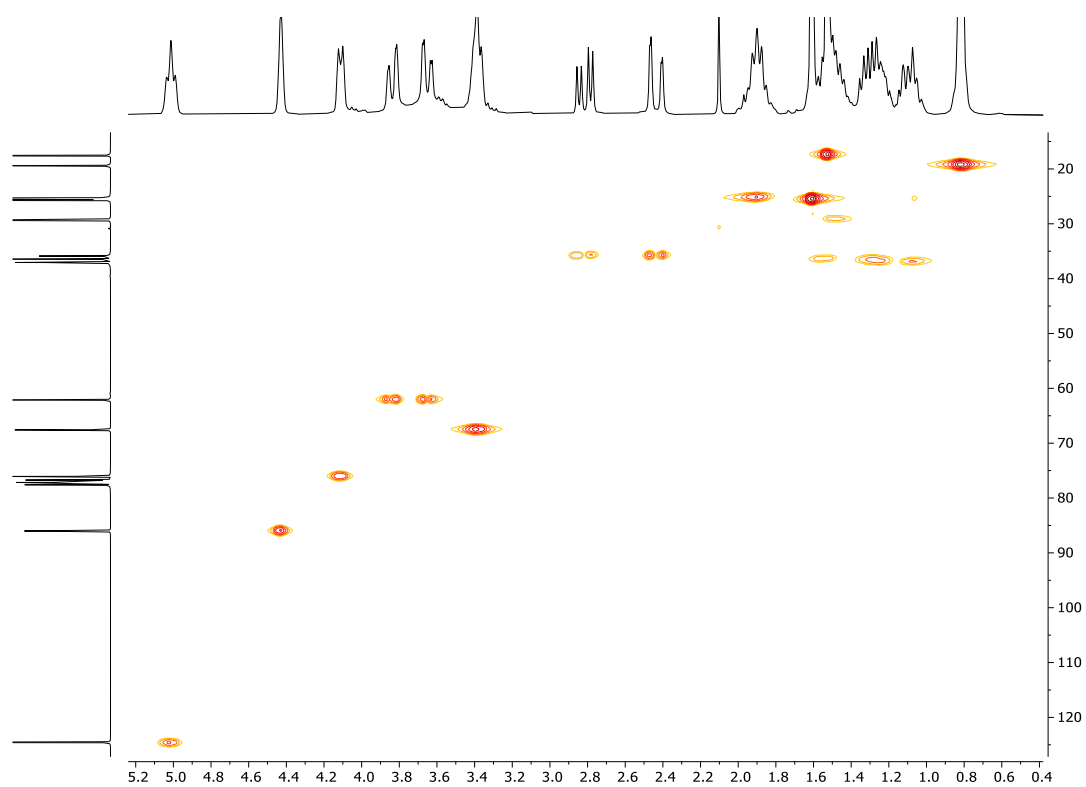


Figure S5. ^1H - ^{13}C HSQC (CDCl_3) spectrum of HBO-citro

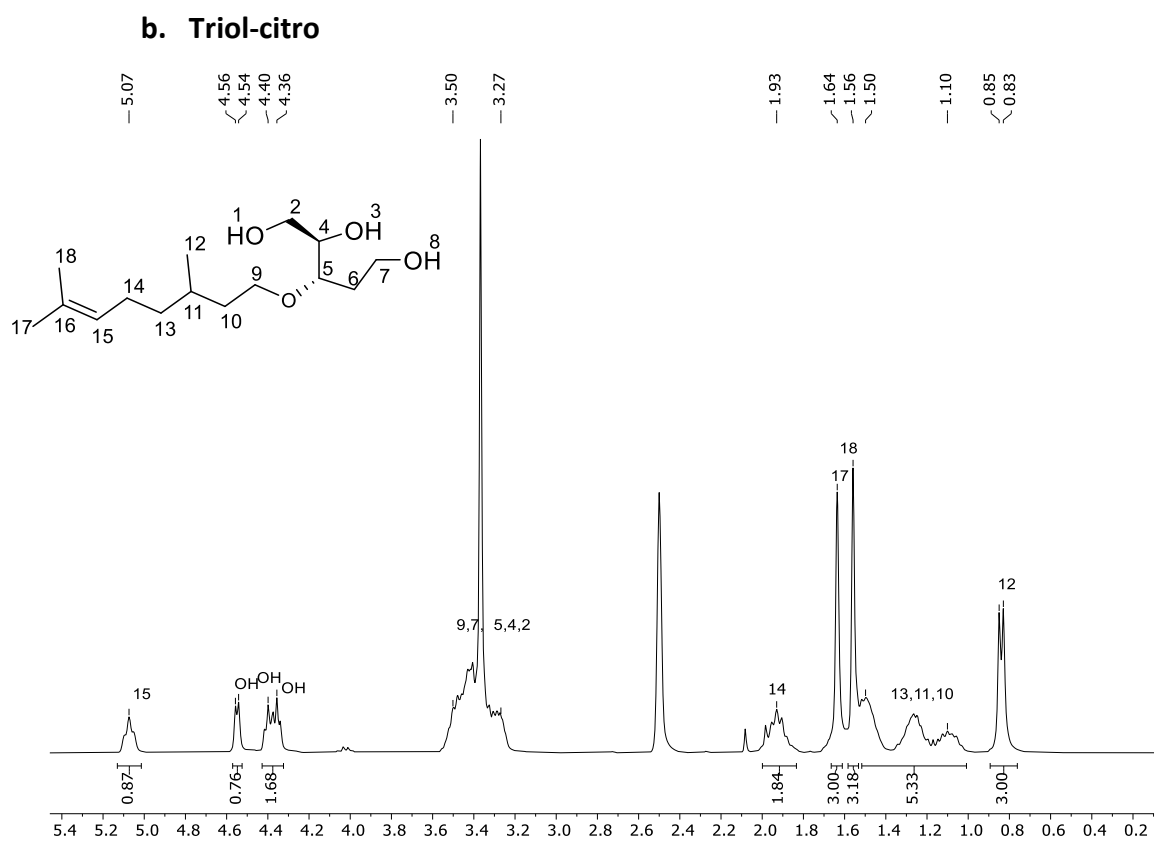


Figure S6. ^1H NMR ($\text{DMSO}-d_6$) spectrum of Triol-citro

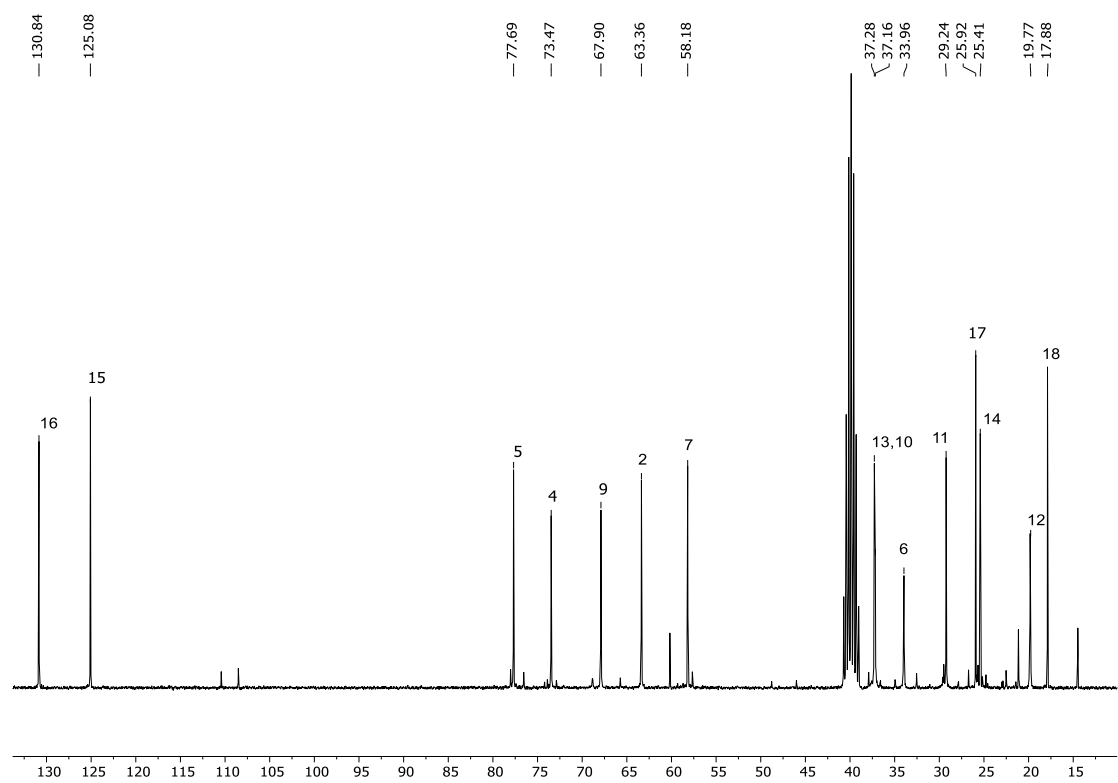


Figure S7. ^{13}C NMR ($\text{DMSO}-d_6$) spectrum of Triol-citro

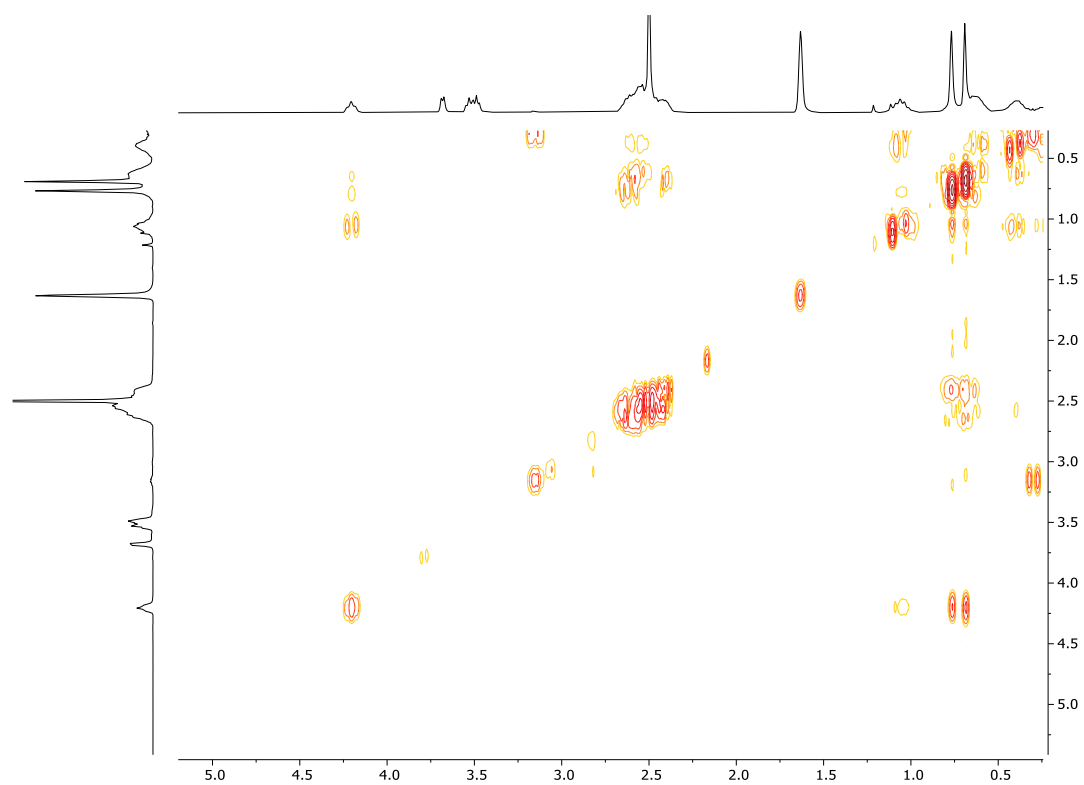


Figure S8. ^1H - ^1H COSY (DMSO- d_6) spectrum of Triol-citro

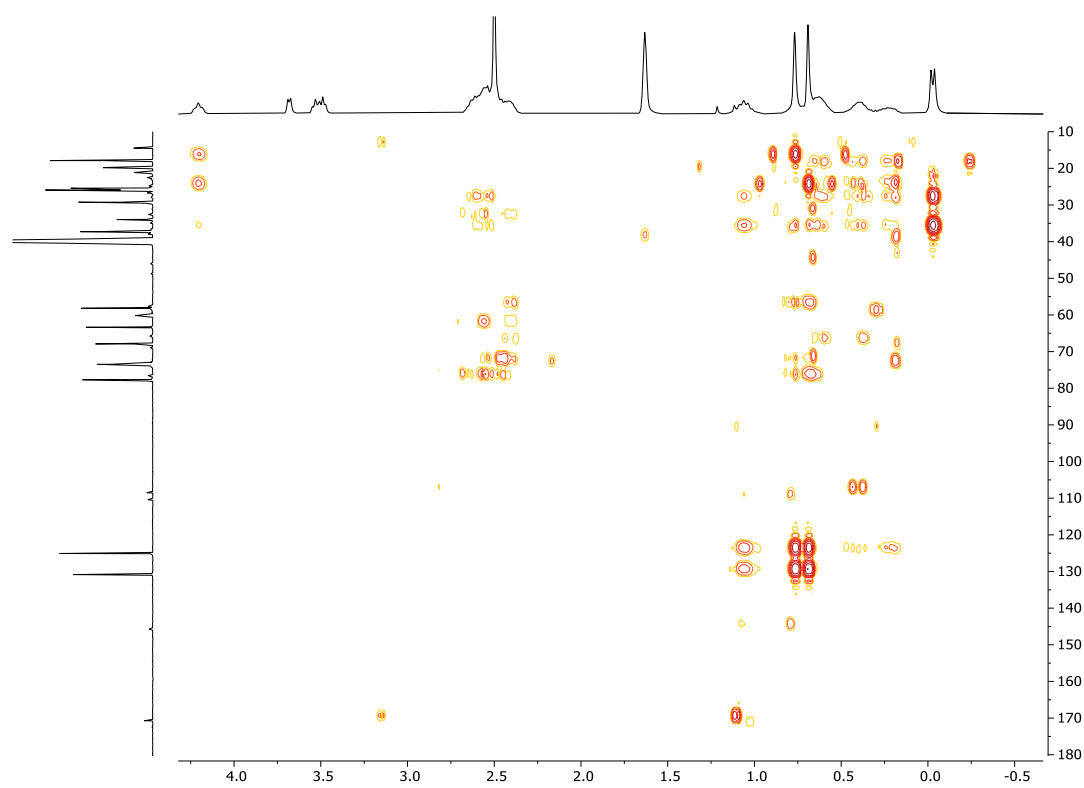


Figure S9. ^1H - ^{13}C HMBC (DMSO- d_6) spectrum of Triol-citro

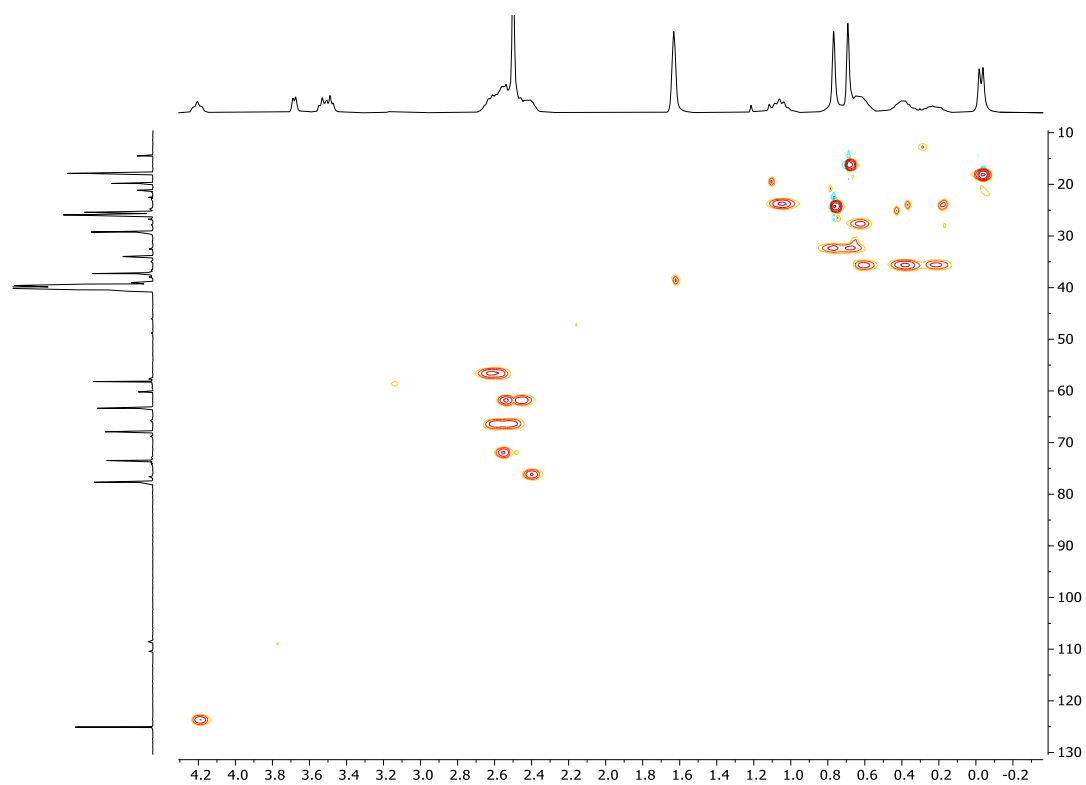


Figure S10. ^1H - ^{13}C HSQC (DMSO- d_6) spectrum of Triol-citro

c. Lactol-citro mixture

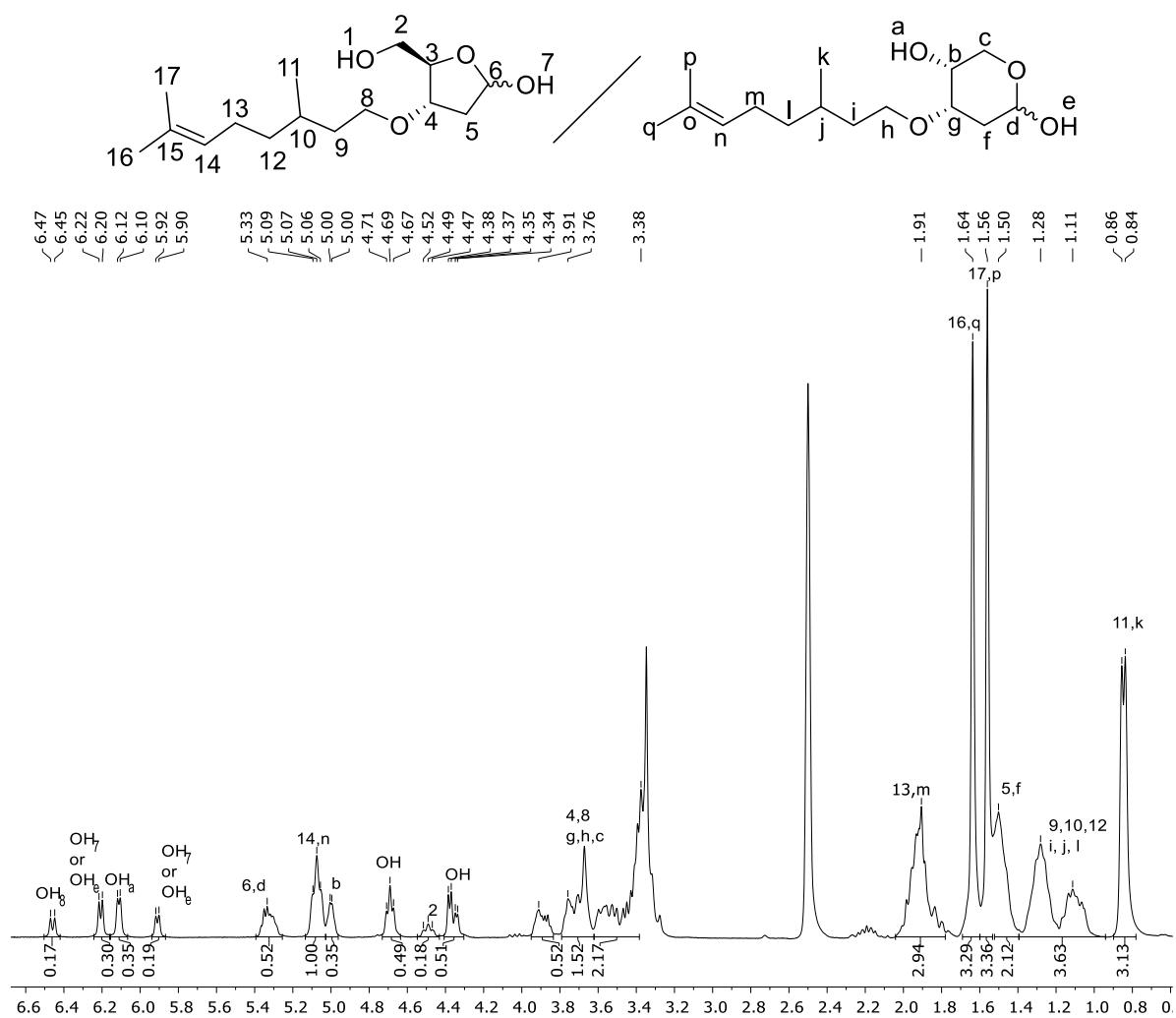


Figure S11. ^1H NMR (DMSO- d_6) spectrum of Lactol-citro

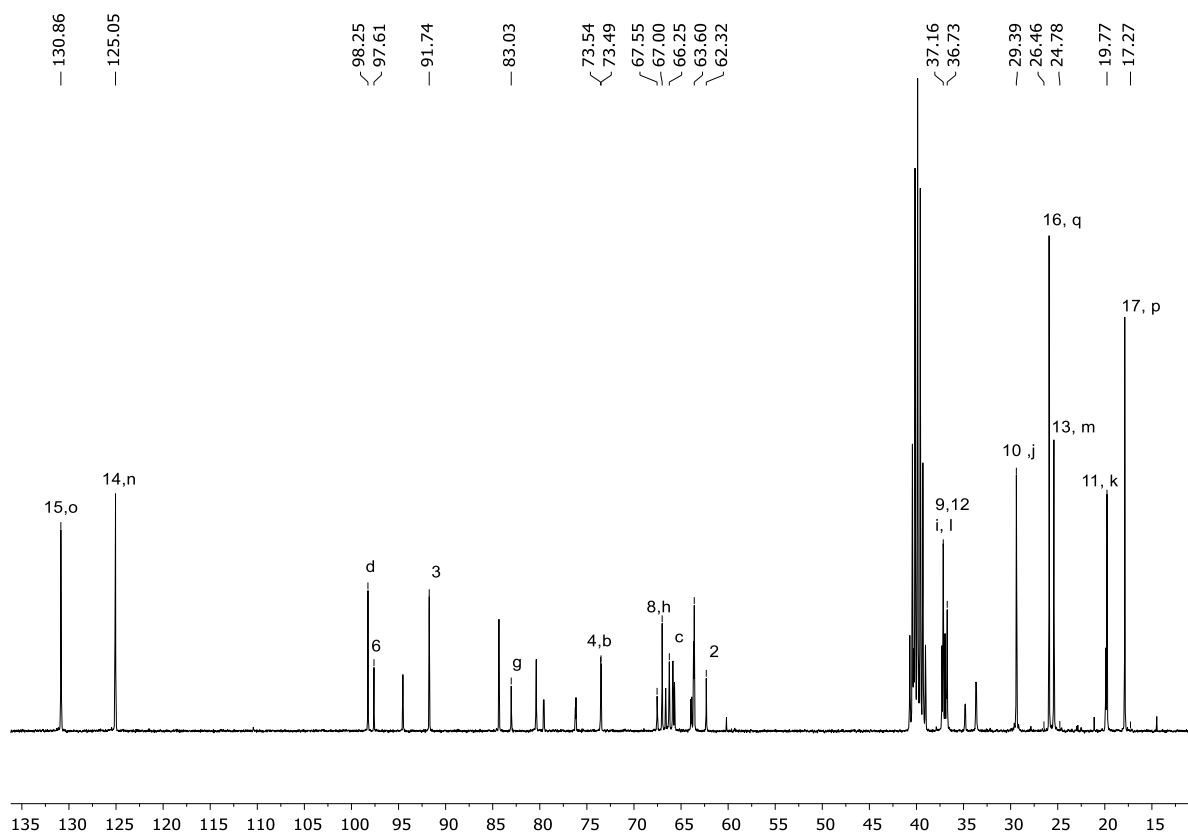


Figure S12. ^{13}C NMR ($\text{DMSO}-d_6$) spectrum of Lactol-citro

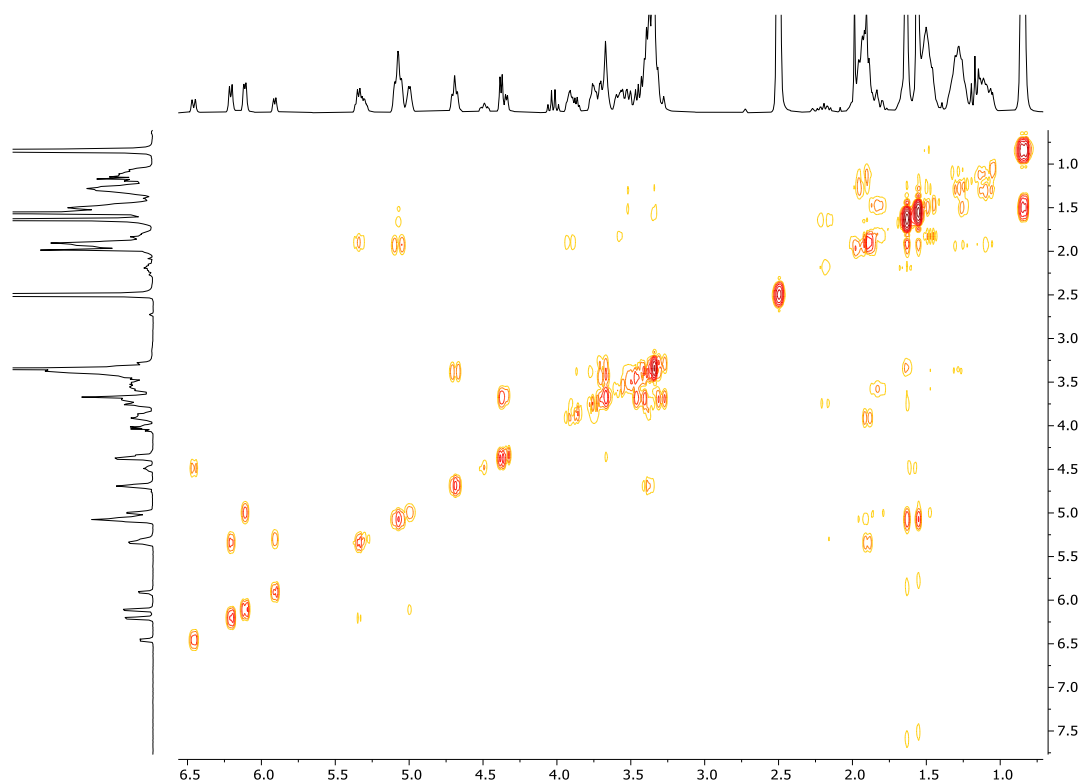


Figure S13. $^1\text{H}-^1\text{H}$ COSY ($\text{DMSO}-d_6$) spectrum of Lactol-citro

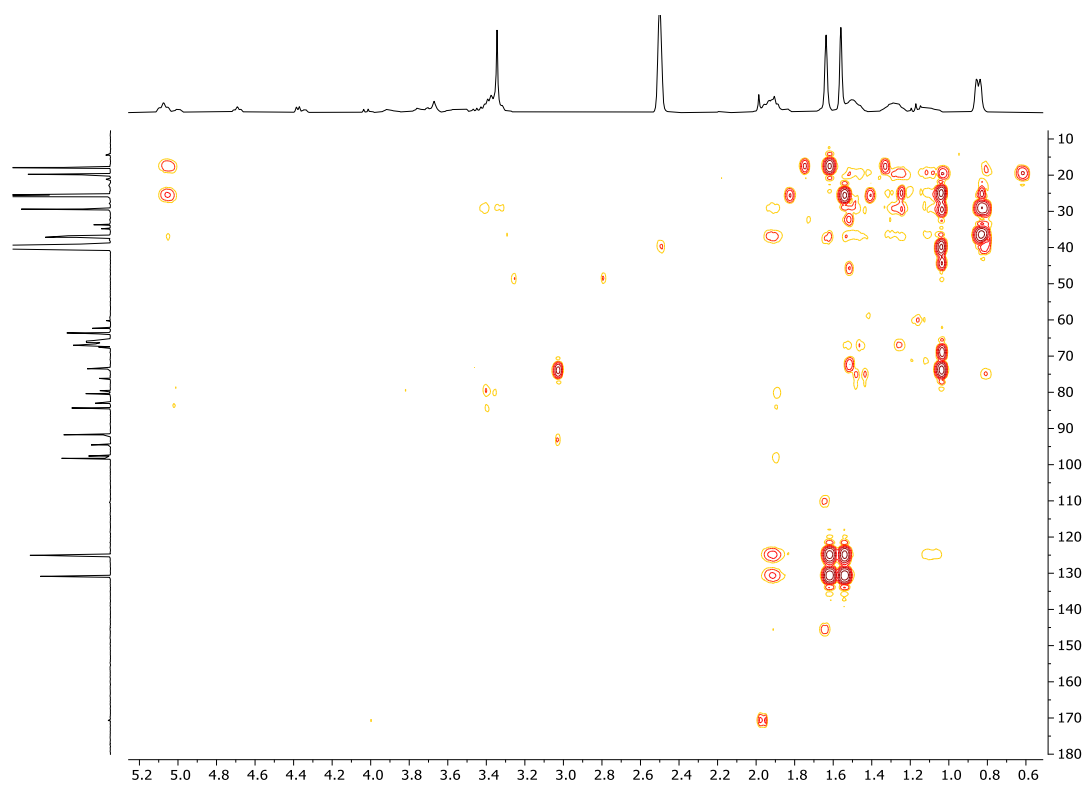


Figure S14. ^1H - ^{13}C HMBC (DMSO- d_6) spectrum of Lactol-citro

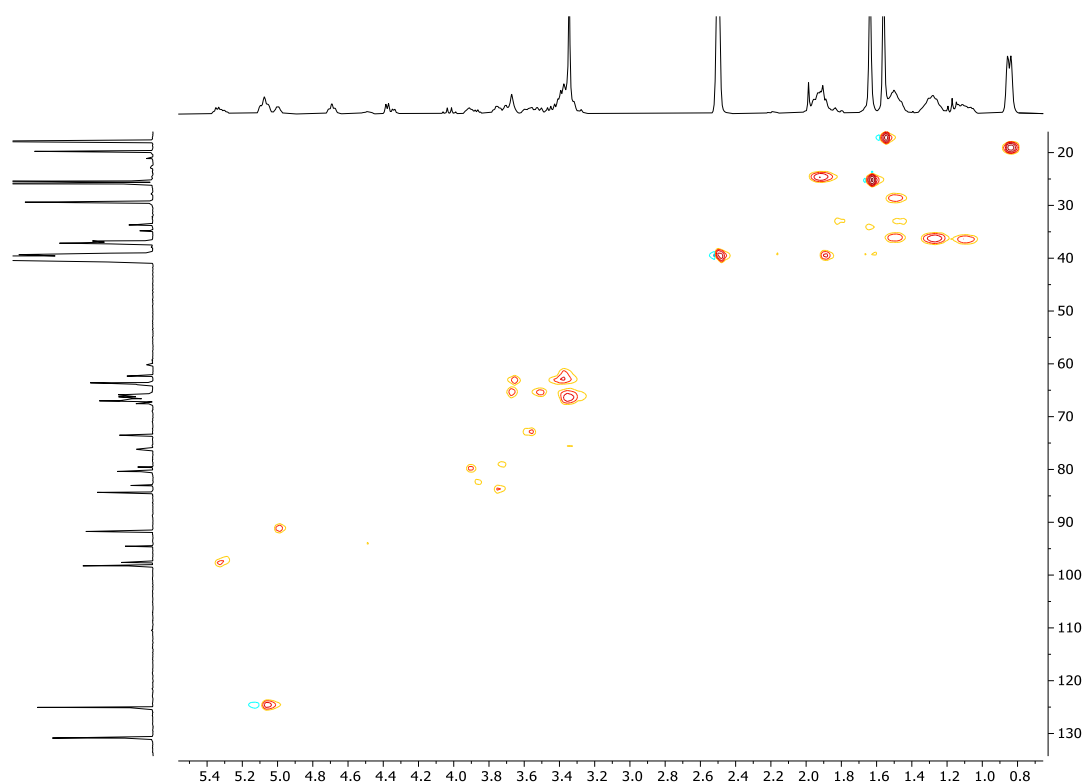


Figure S15. ^1H - ^{13}C HSQC (DMSO- d_6) spectrum of Lactol-citro

d. P1

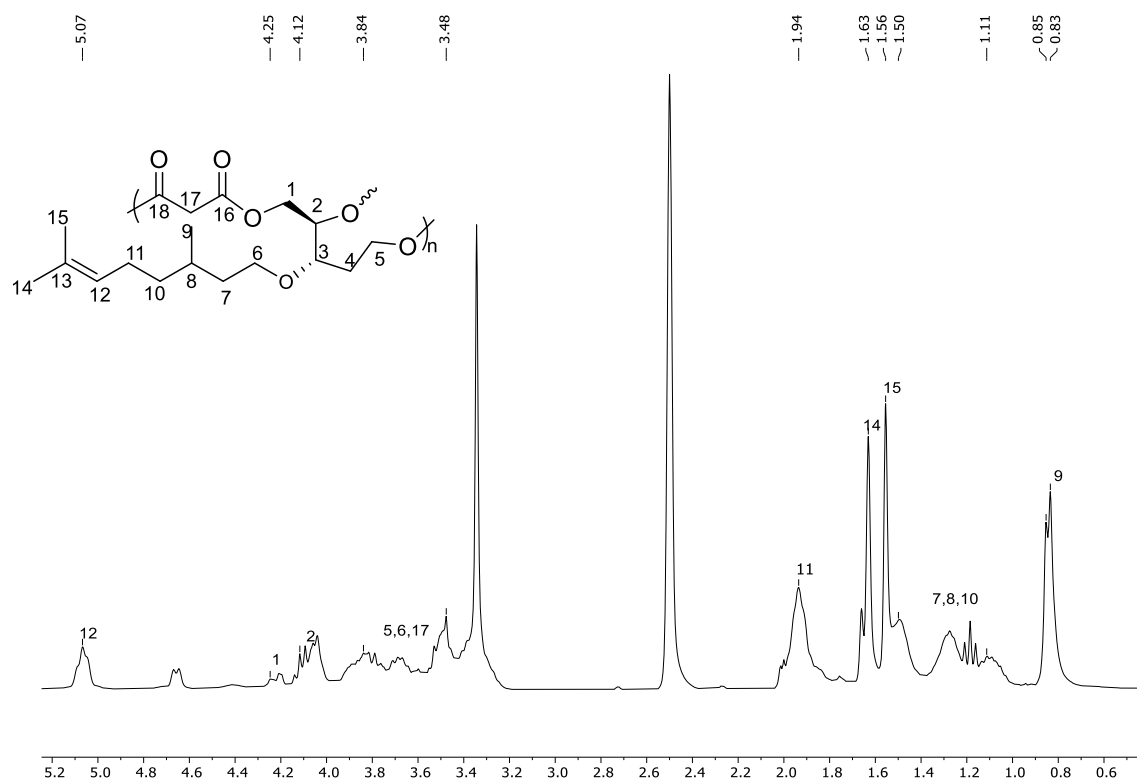


Figure S16. Typical ^1H NMR (DMSO- d_6) spectrum of P1

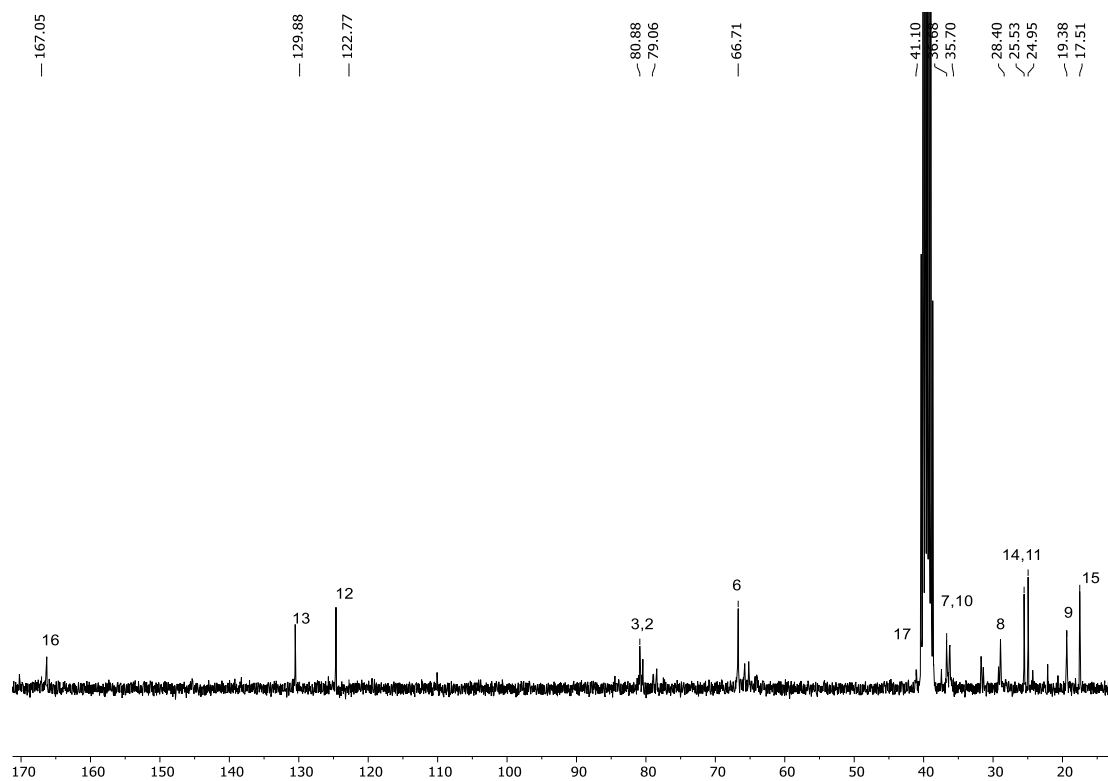


Figure S17. Typical ^{13}C NMR (DMSO- d_6) spectrum of P1

e. P2

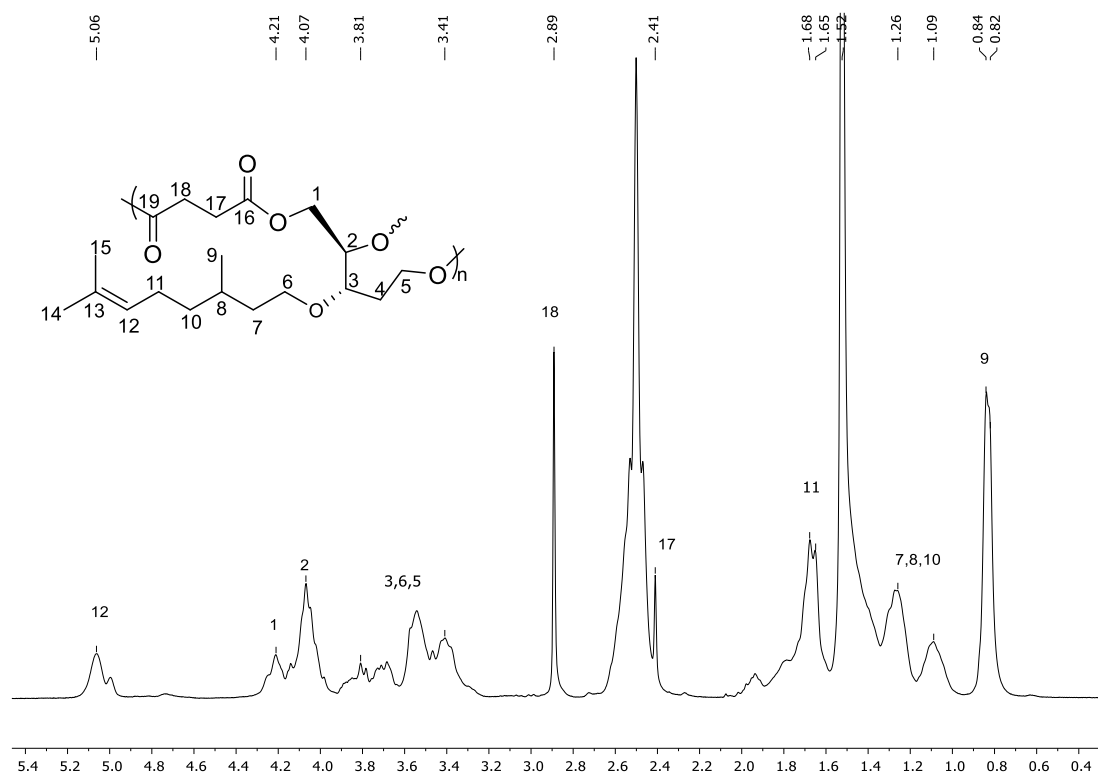


Figure S18. Typical ^1H NMR (DMSO- d_6) spectrum of P2

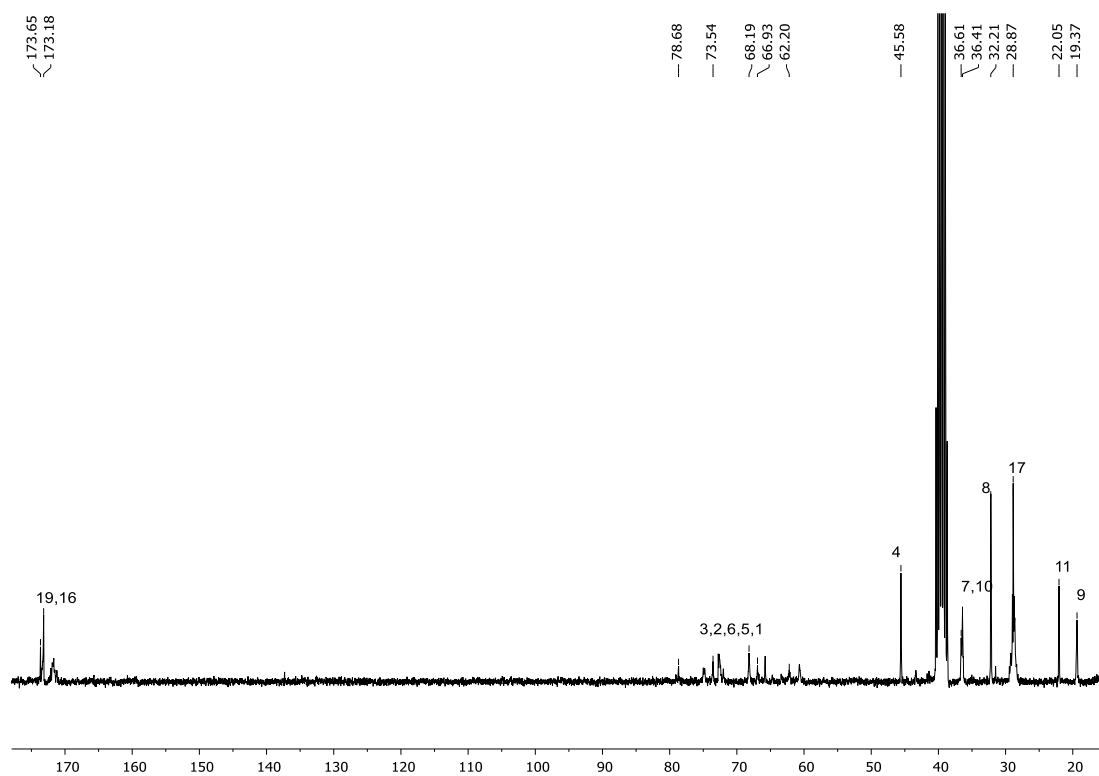


Figure S19. Typical ^{13}C NMR (DMSO- d_6) spectrum of P2

f. P3

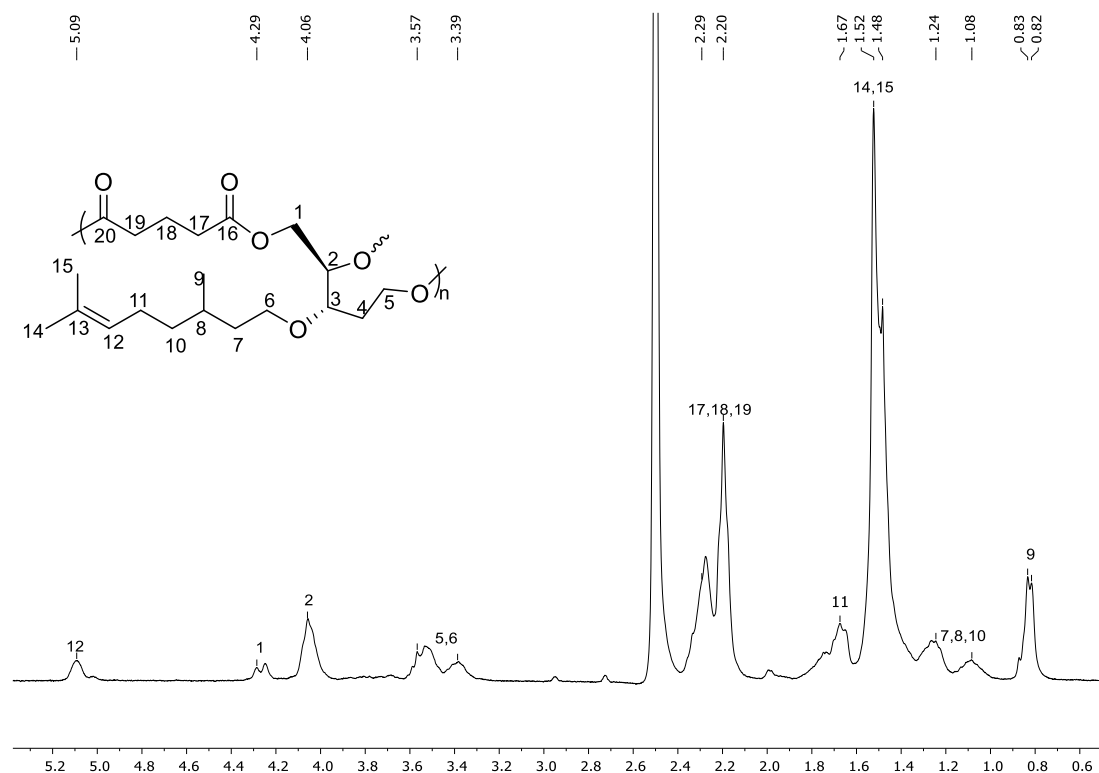


Figure S20. Typical ^1H NMR (DMSO- d_6) spectrum of P3

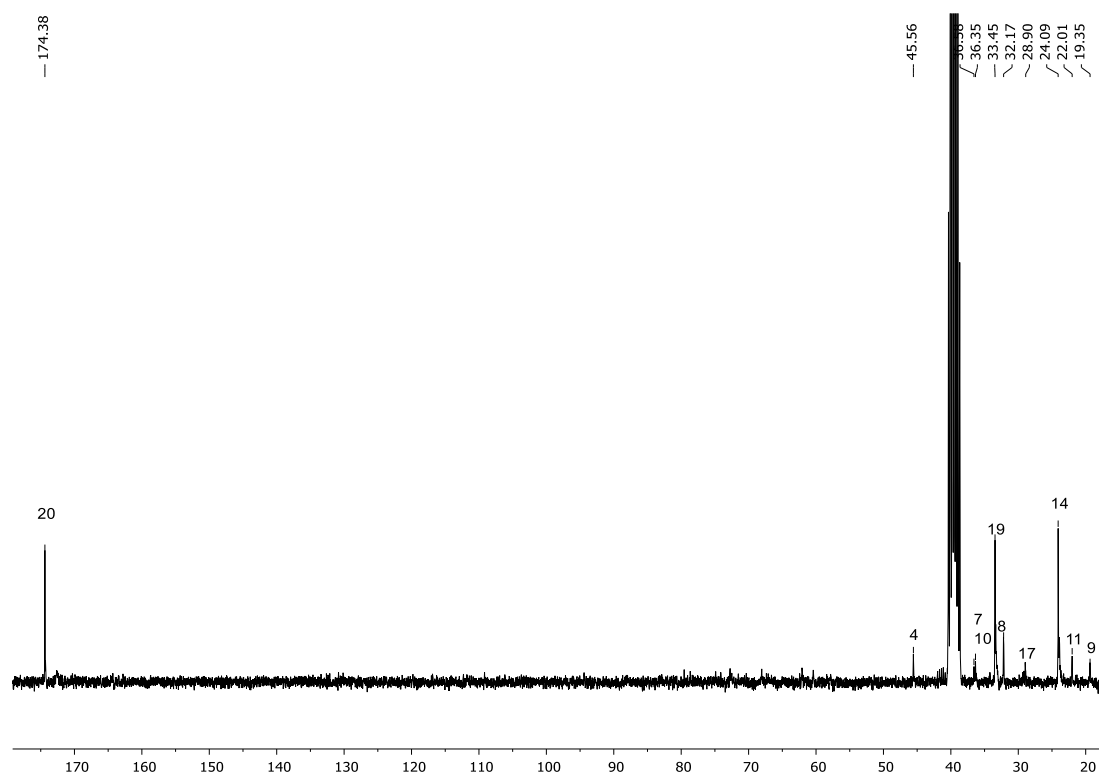


Figure S21. Typical ^{13}C NMR (DMSO- d_6) spectrum of P3

g. P4

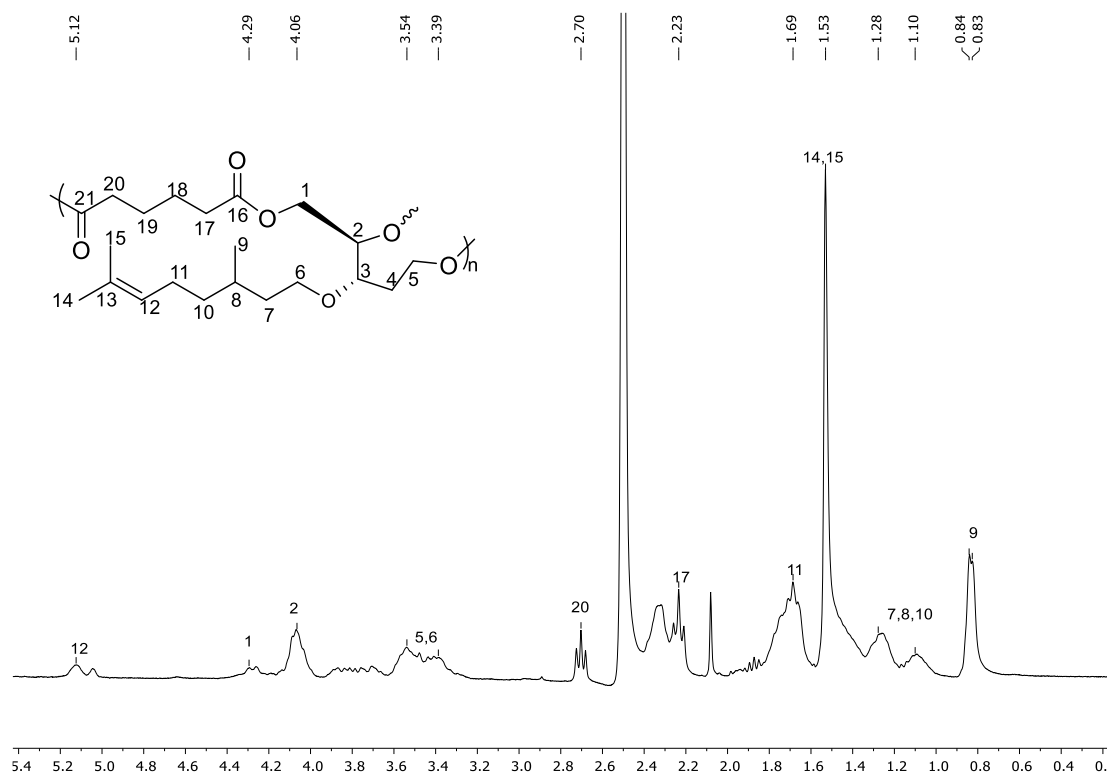


Figure S22. Typical ^1H NMR (DMSO- d_6) spectrum of P4

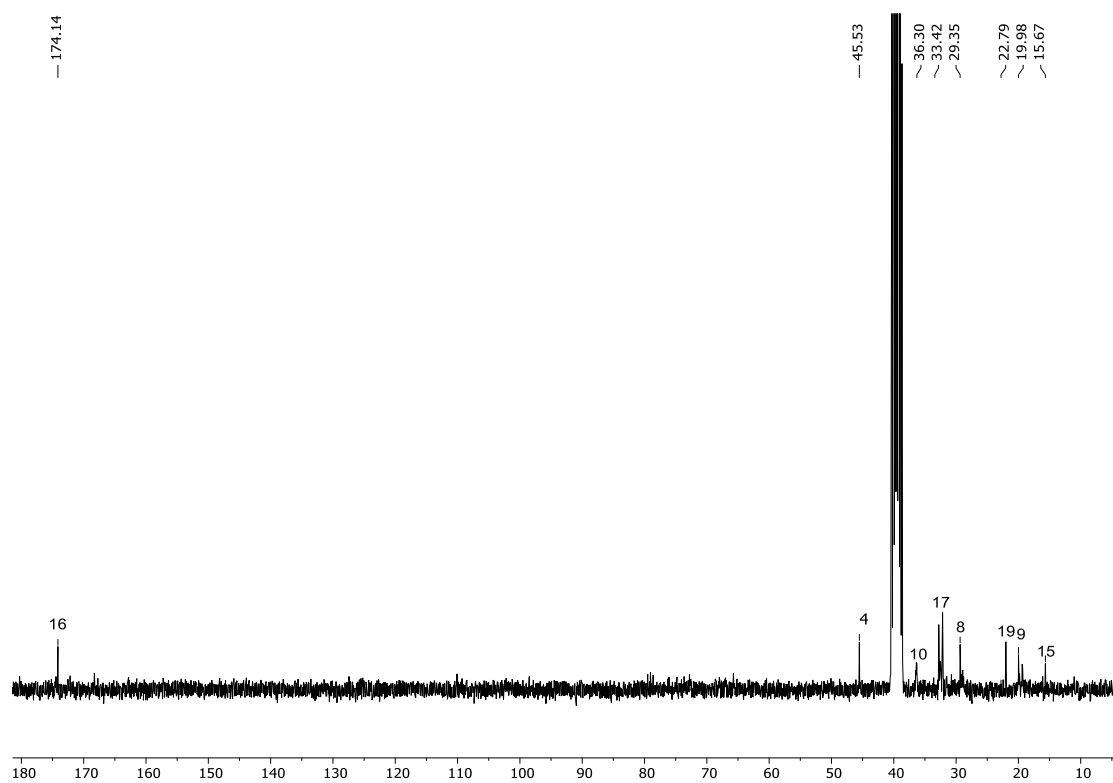


Figure S23. Typical ^{13}C NMR (DMSO- d_6) spectrum of P4

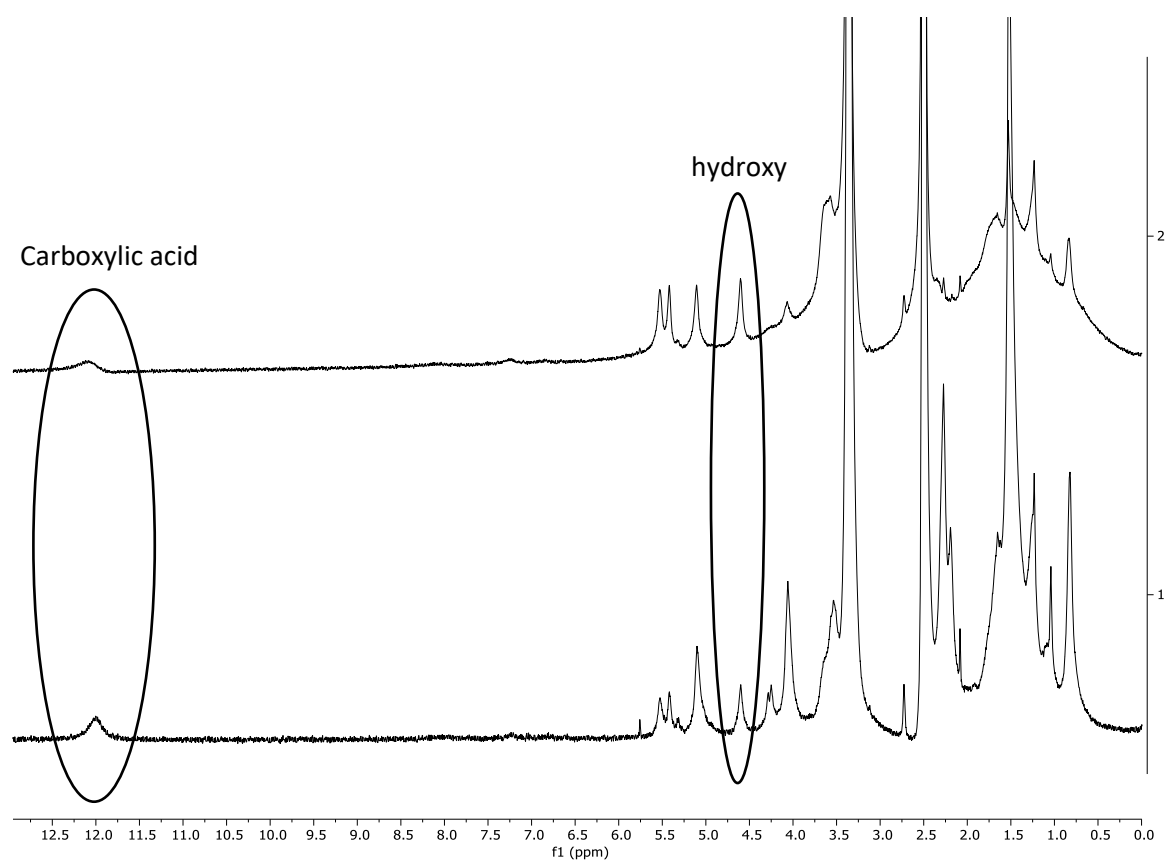


Figure S24. ^1H NMR ($\text{DMSO-}d_6$) spectra of the hydrolyzed products of P3 (below) and P4 (above) after enzymatic degradation

II. LC-MS

a. HBO-citro

$C_{15}H_{26}O_4$ (270.1831 g/mol)

271.1897 g/mol identified at 10 min

The theoretical mass of $[M+H]^+$ is 271.1904 g/mol

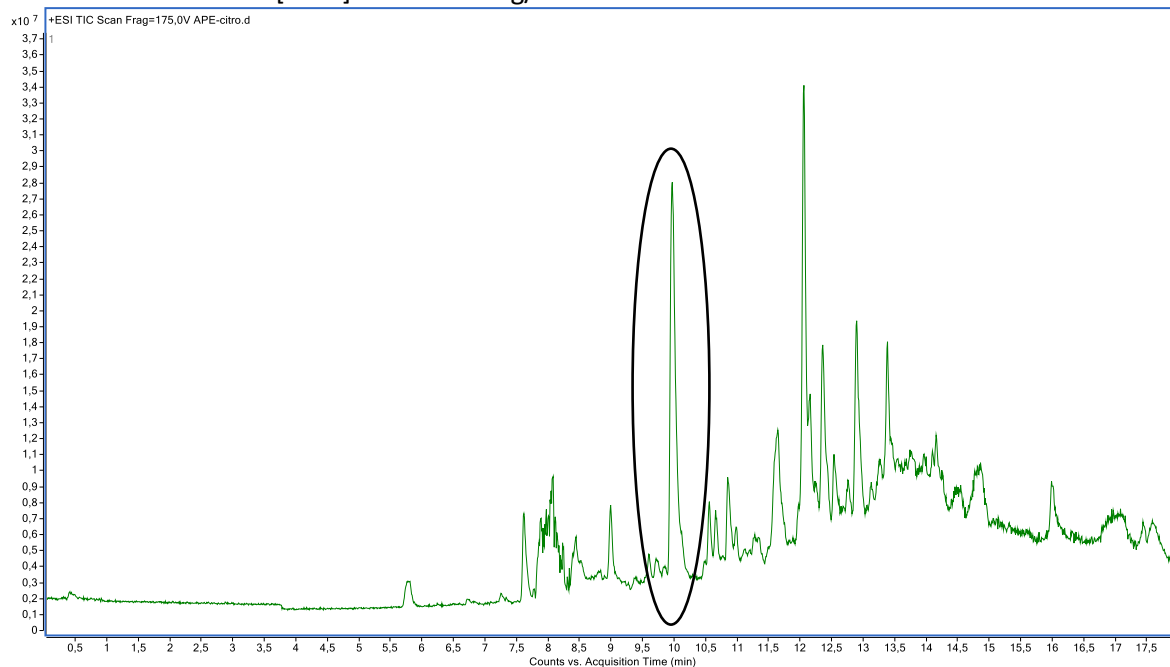


Figure S25. LC-MS chromatogram of HBO-citro

b. Triol-citro

$C_{15}H_{30}O_4$ (274.2144 g/mol)

275.2213 g/mol identified at 8.6 min

The theoretical mass of $[M+H]^+$ is 275.2217 g/mol

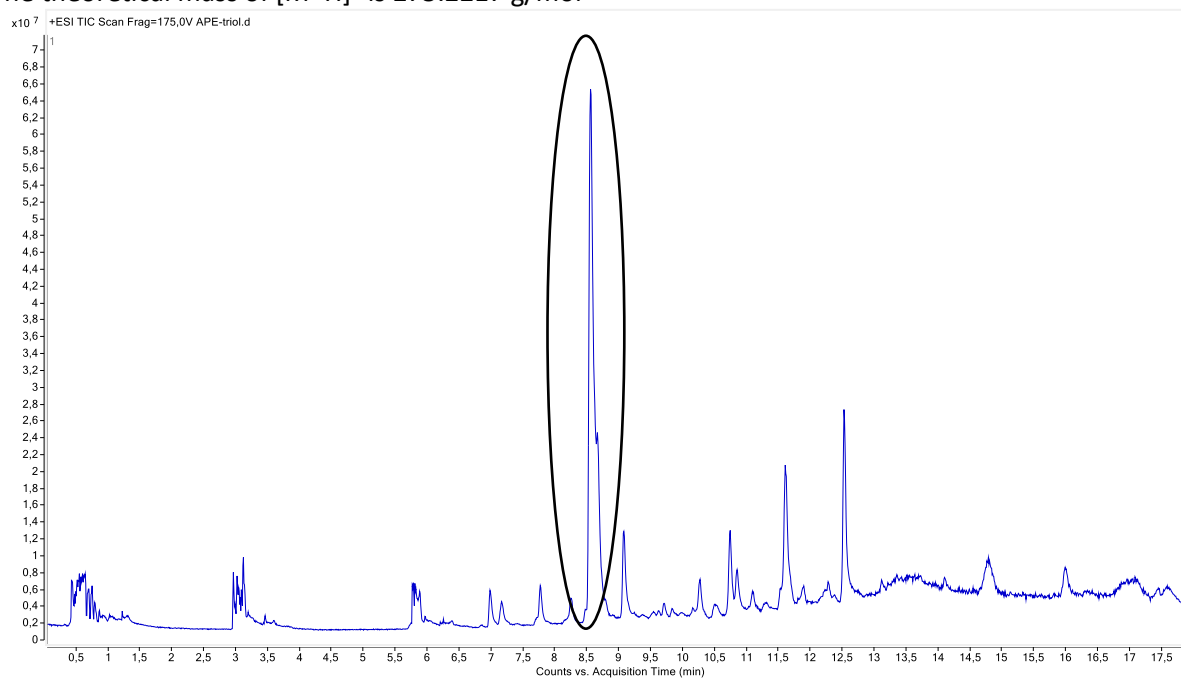


Figure S26. LC-MS chromatogram of Triol-citro

III. SEC

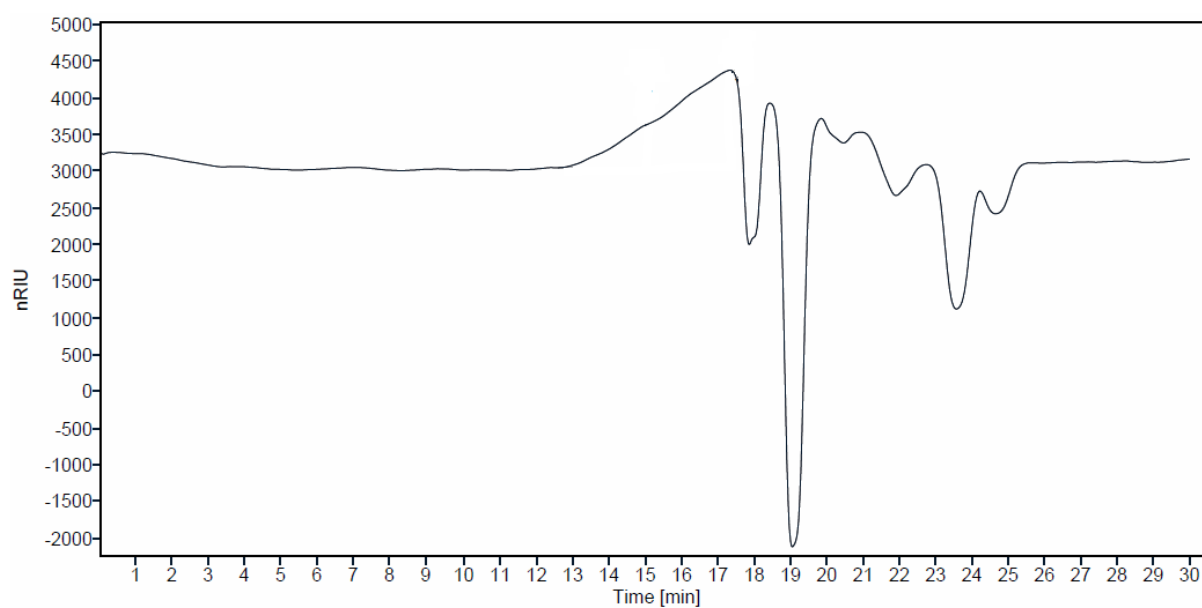


Figure S27. SEC trace of P1, Table 2

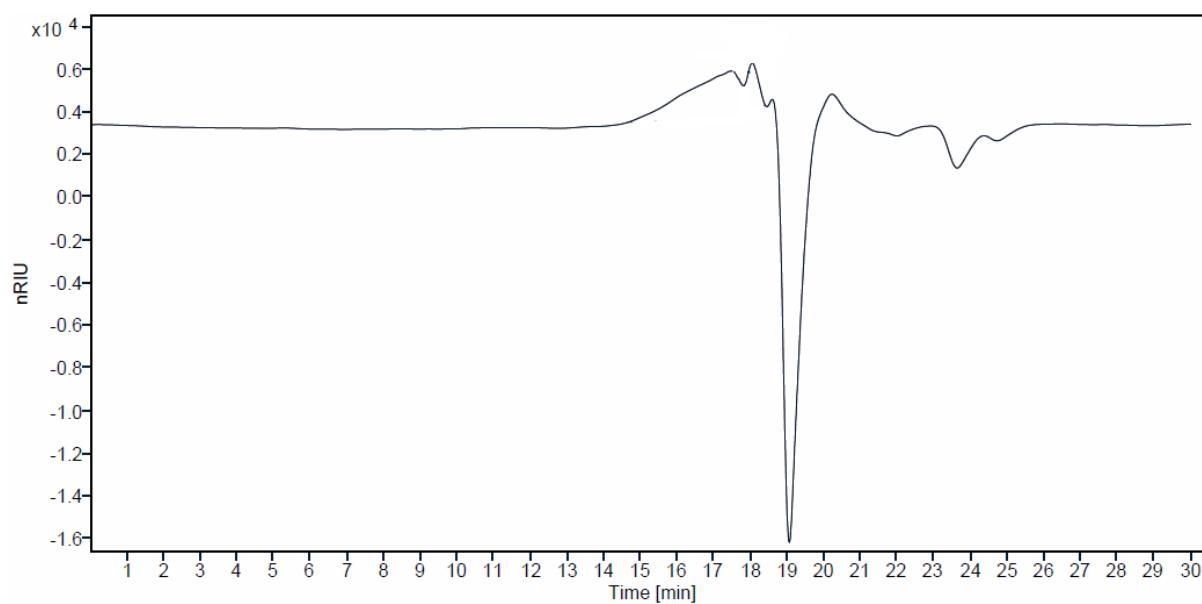


Figure S28. SEC trace of P2, Table 2

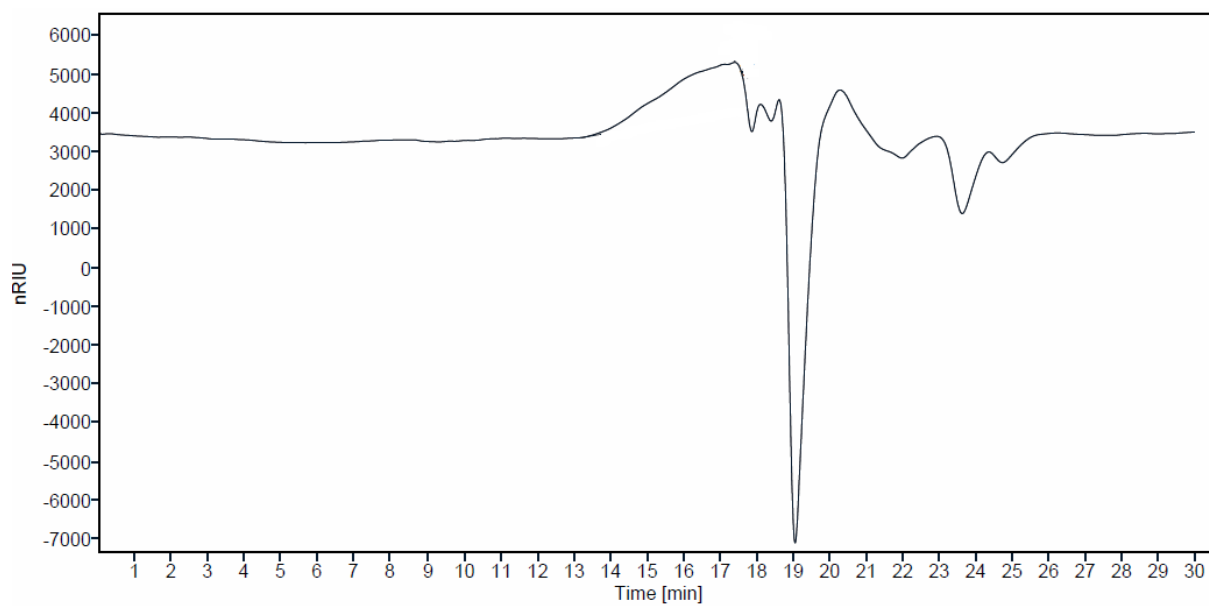


Figure S29. SEC trace of P3, Table 2

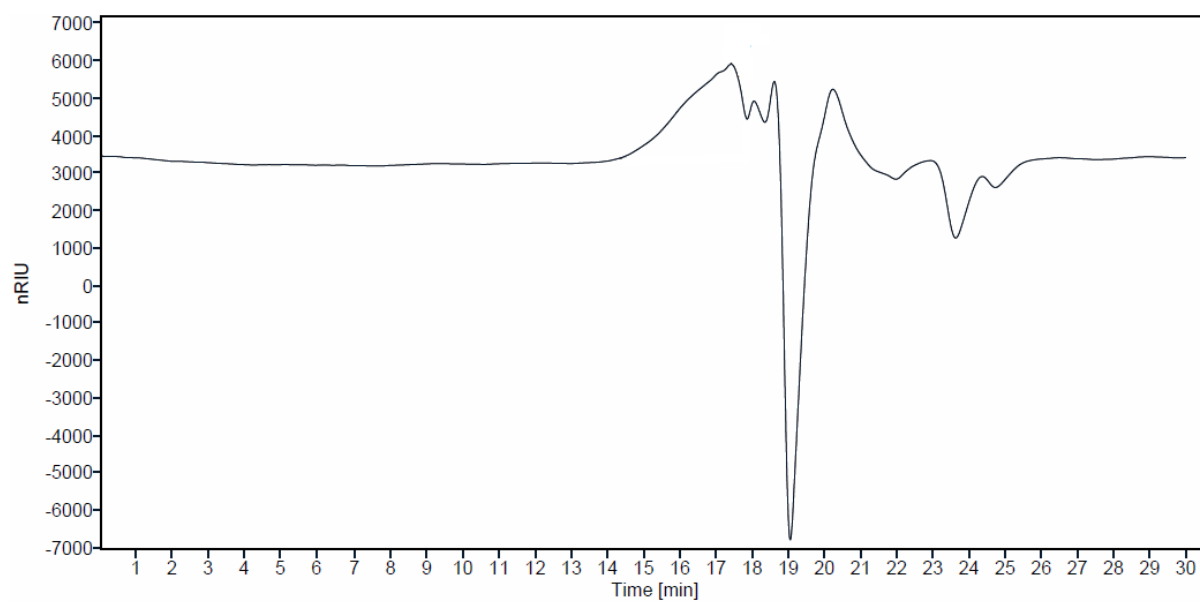


Figure S30. SEC trace of P4, Table 2

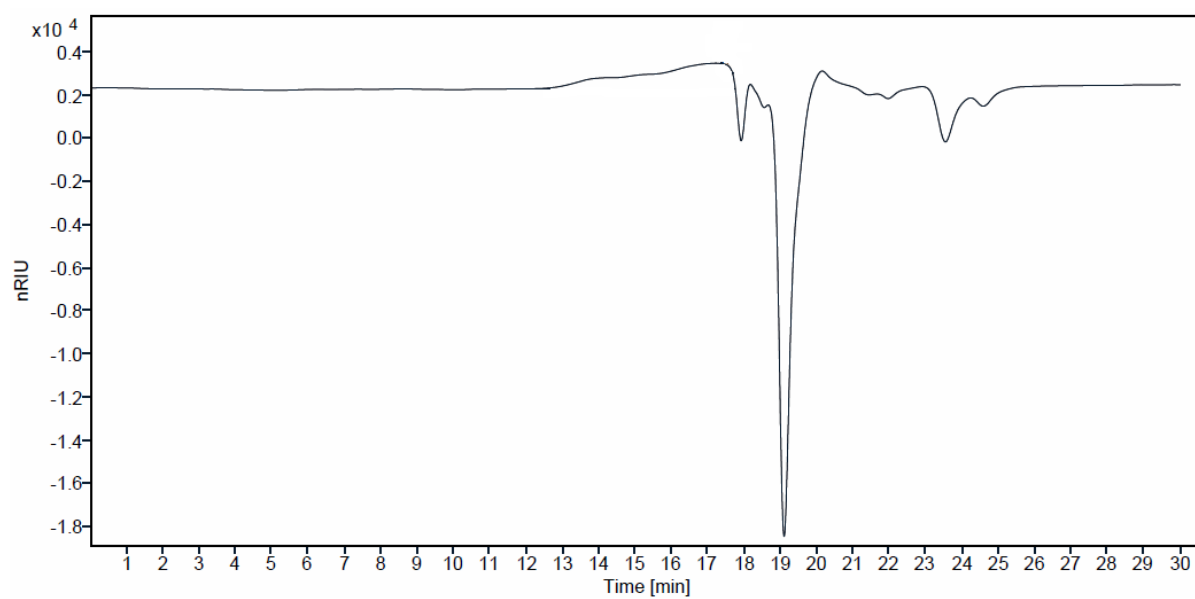


Figure S31. SEC trace of the resulting product of P1 (run 1, Table 2) after enzymatic degradation

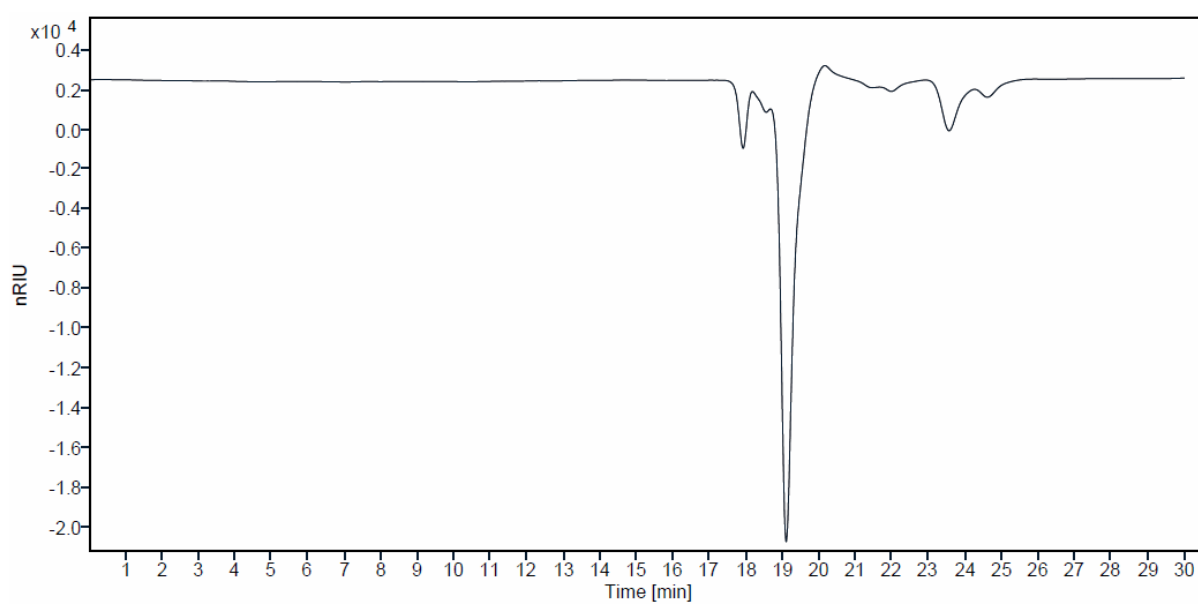


Figure S32. SEC trace of the resulting product of P2 (run 2, Table 2) after enzymatic degradation

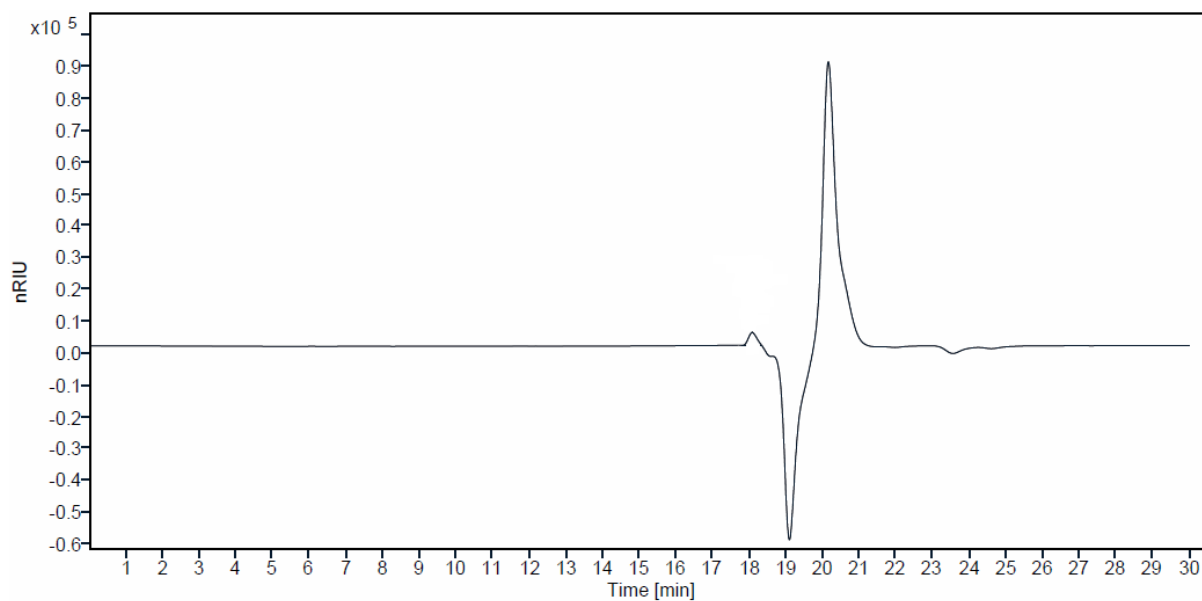


Figure S33. SEC trace of the resulting product of P3 (run 3, Table 2) after enzymatic degradation

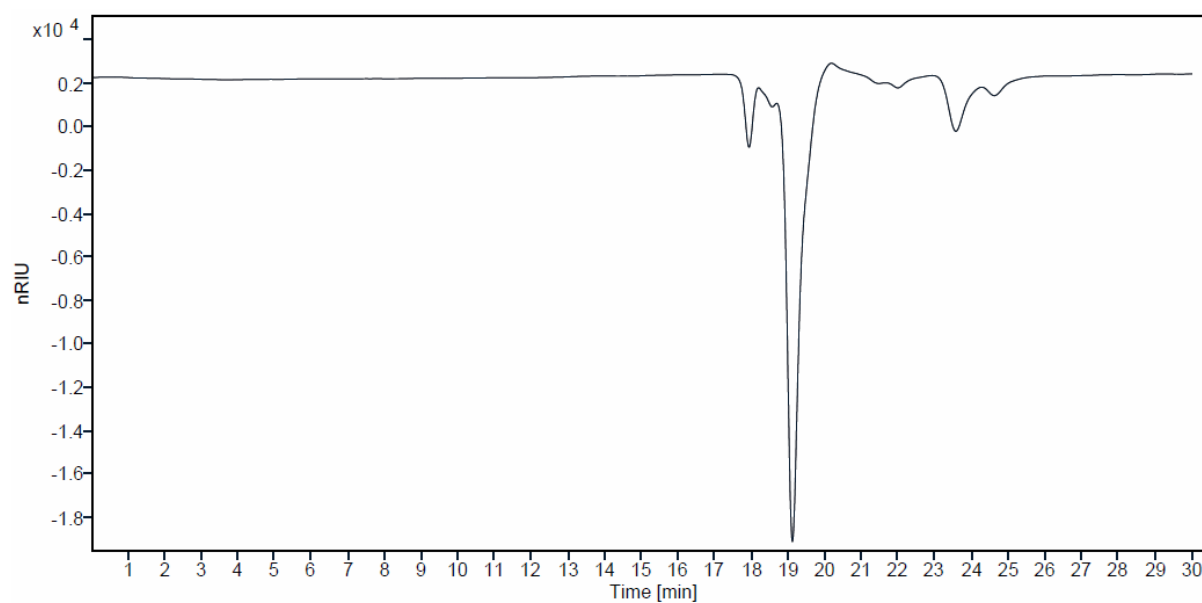


Figure S34. SEC trace of the resulting product of P4 (run 4, Table 2) after enzymatic degradation

IV. FTIR

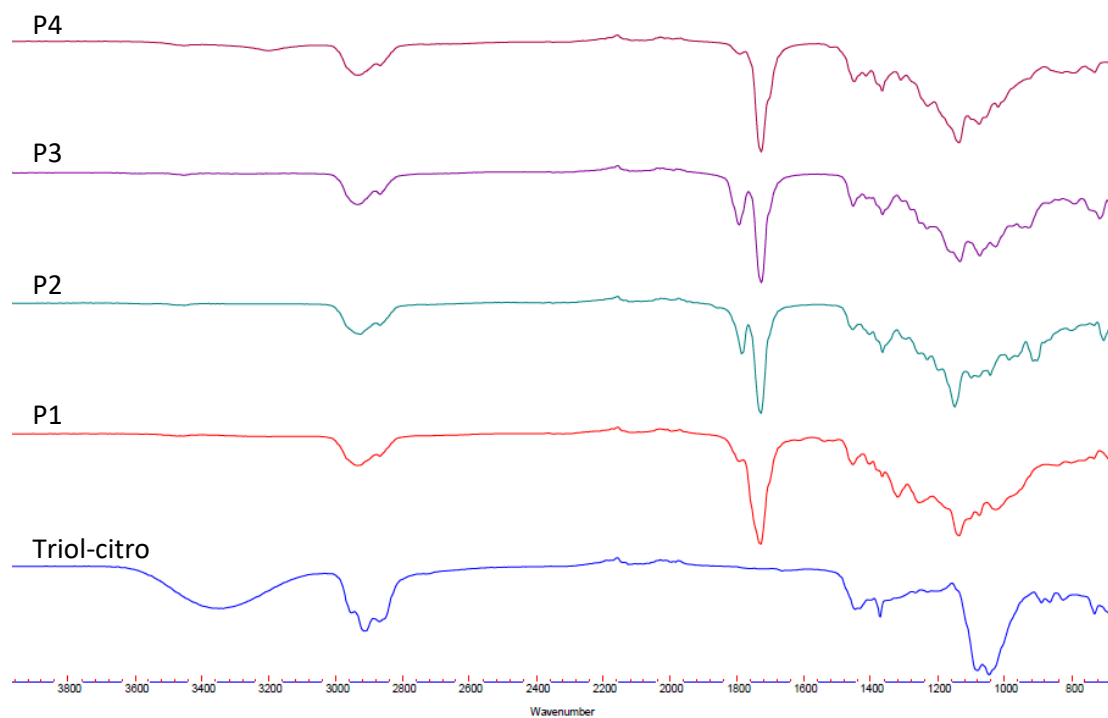


Figure S35. Typical FTIR spectra of P1-P4 (runs 1-4, Table 2)

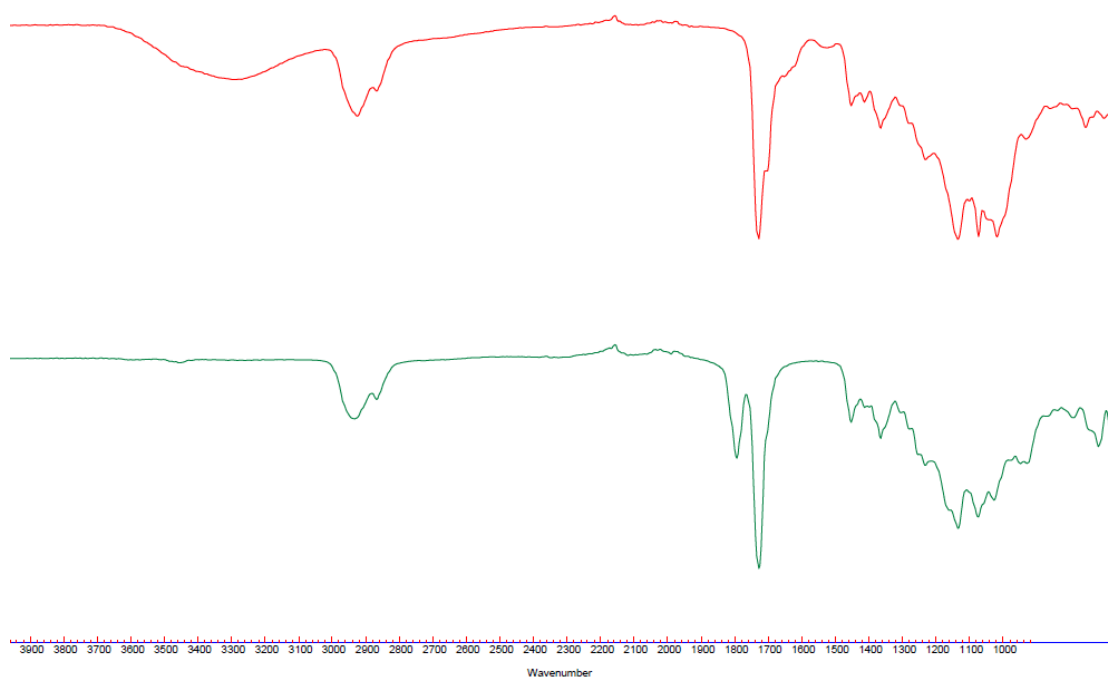


Figure S36. Typical FTIR spectra of P3 (taken as an example) before and after enzymatic degradation (before: green and after: red, respectively)

V. DSC

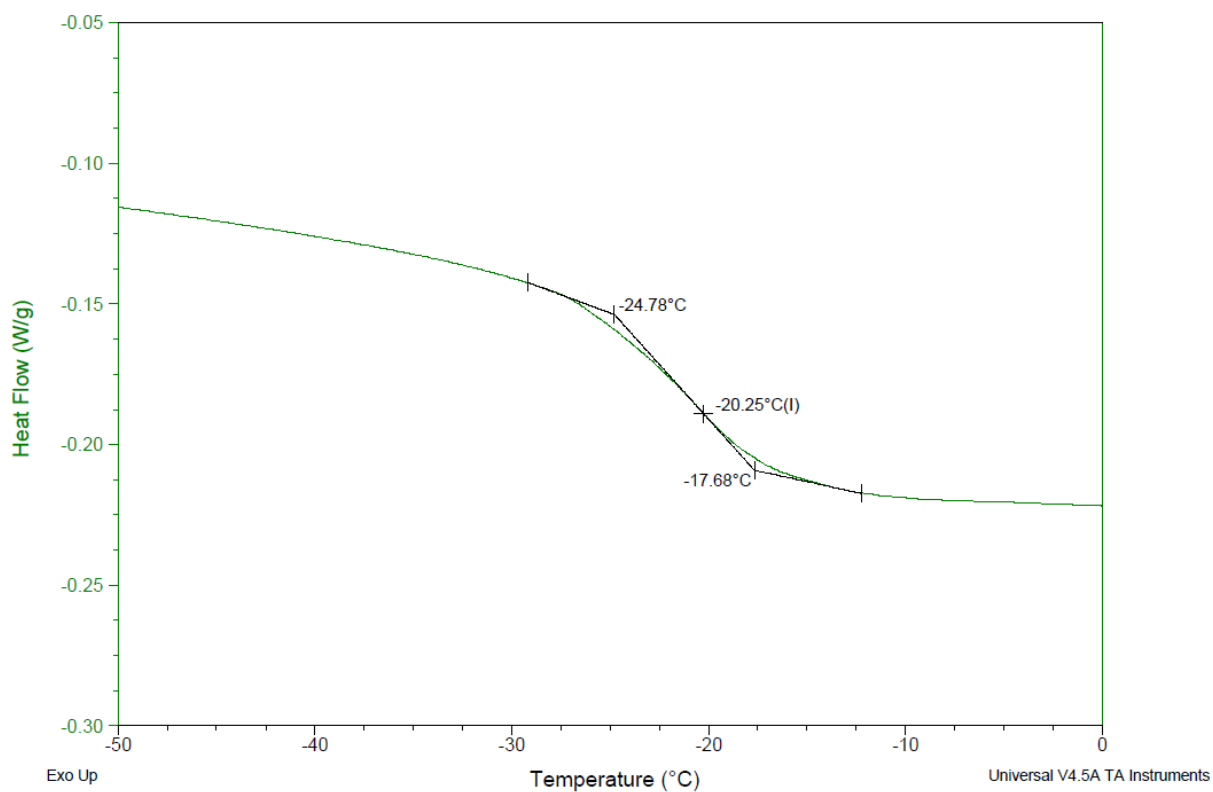


Figure S37. DSC thermogram (3rd heat cycle) of P1, run 1, Table 2

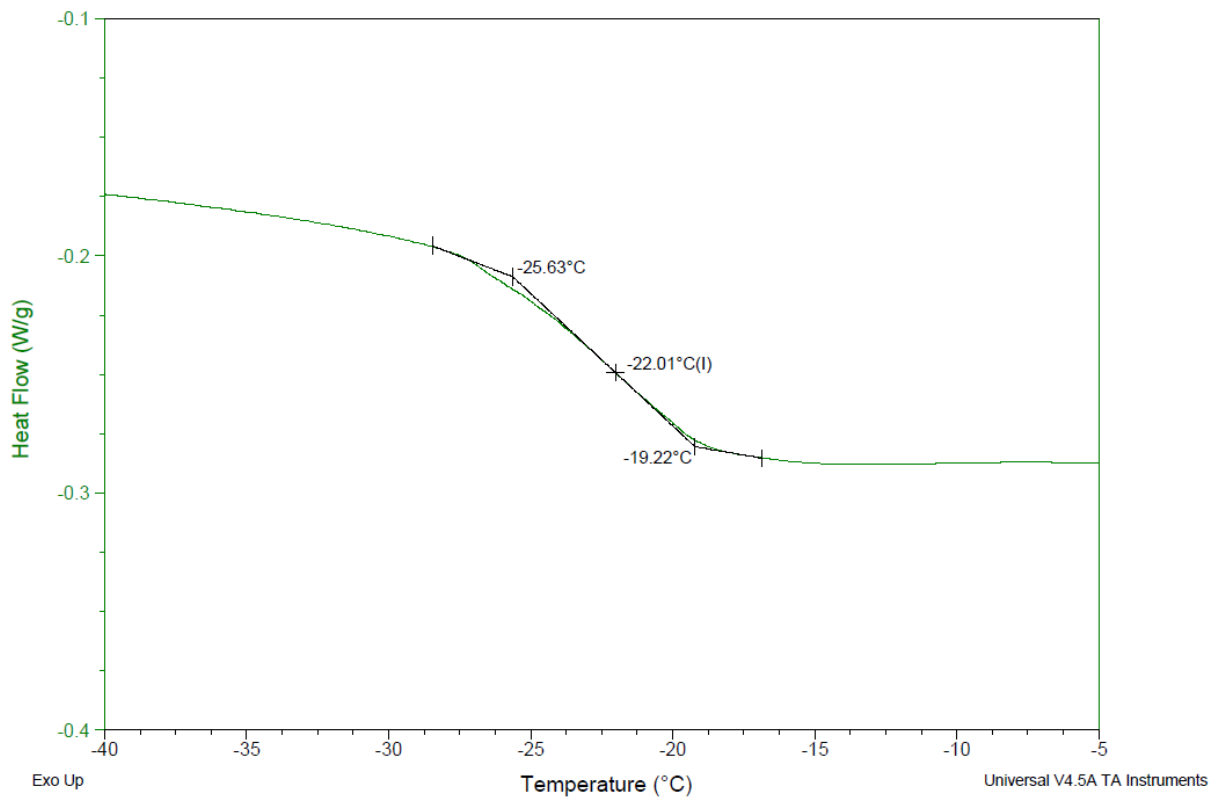


Figure S38. DSC thermogram (3rd heat cycle) of P2, run 2, Table 2

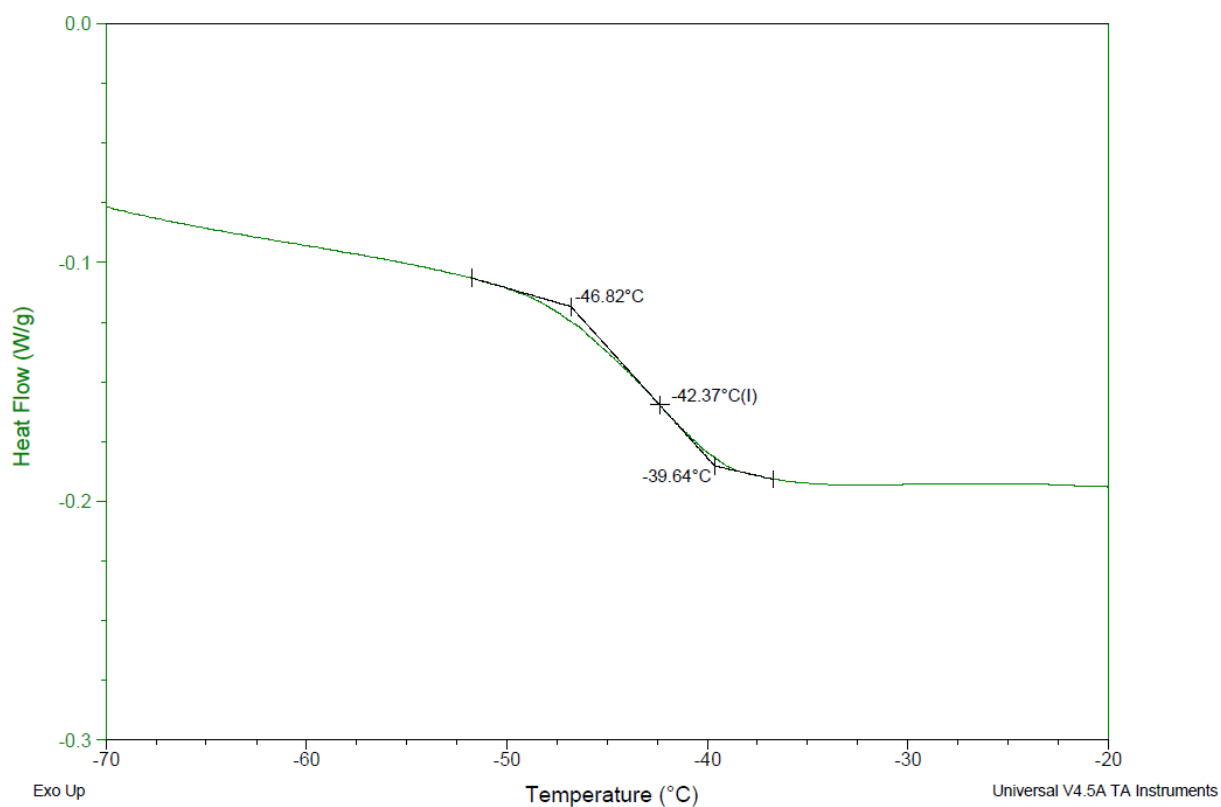


Figure S39. DSC thermogram (3rd heat cycle) of P3, run 3, Table 2

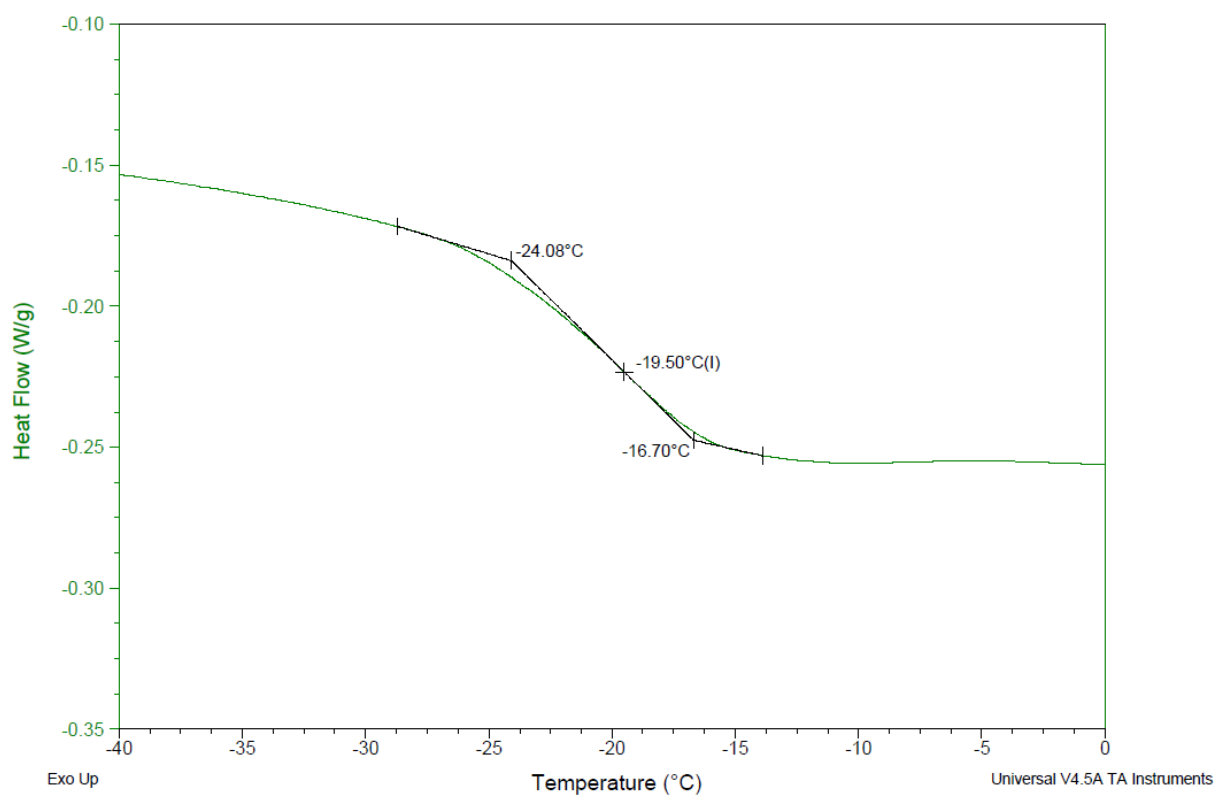


Figure S40. DSC thermogram (3rd heat cycle) of P4, run 4, Table 2

VI. TGA

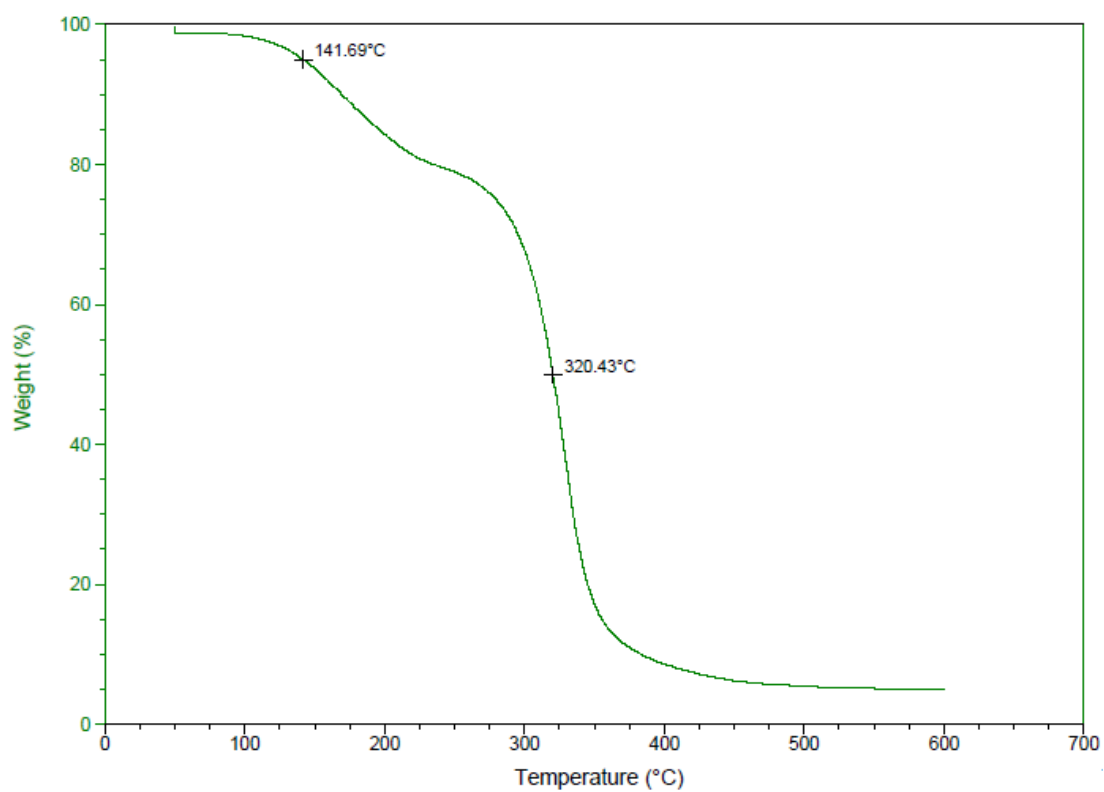


Figure S41. TGA thermogram of P1, run 1, Table 2

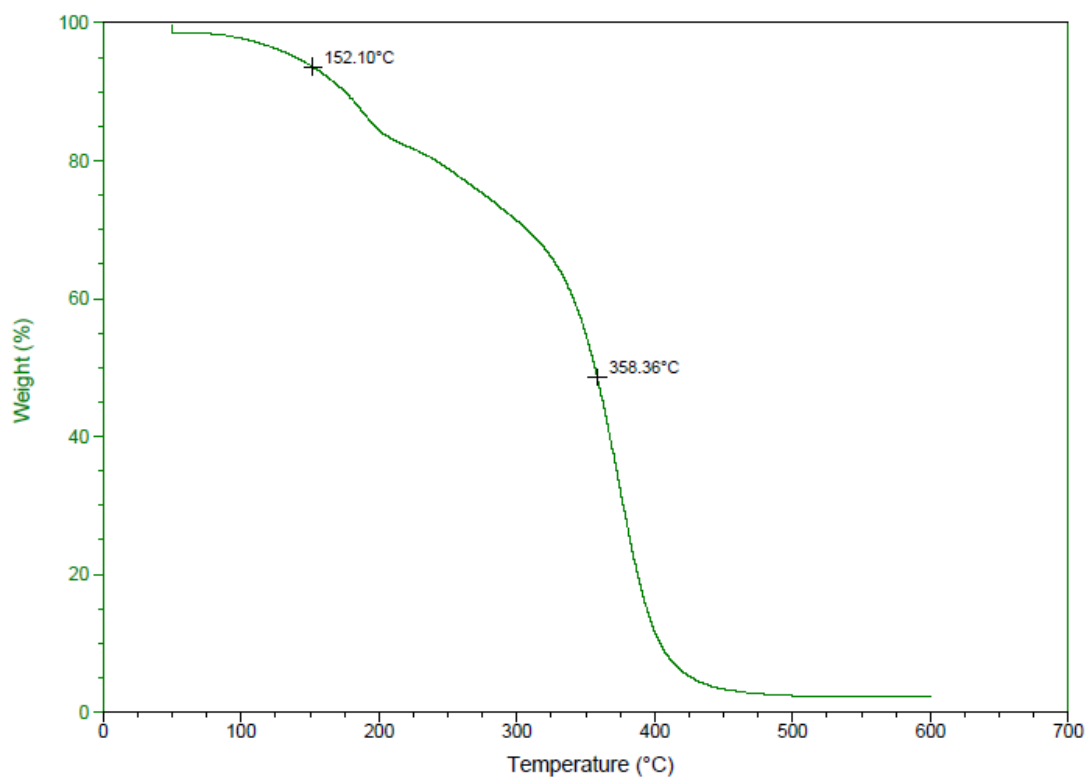


Figure S42. TGA thermogram of P2, run 2, Table 2

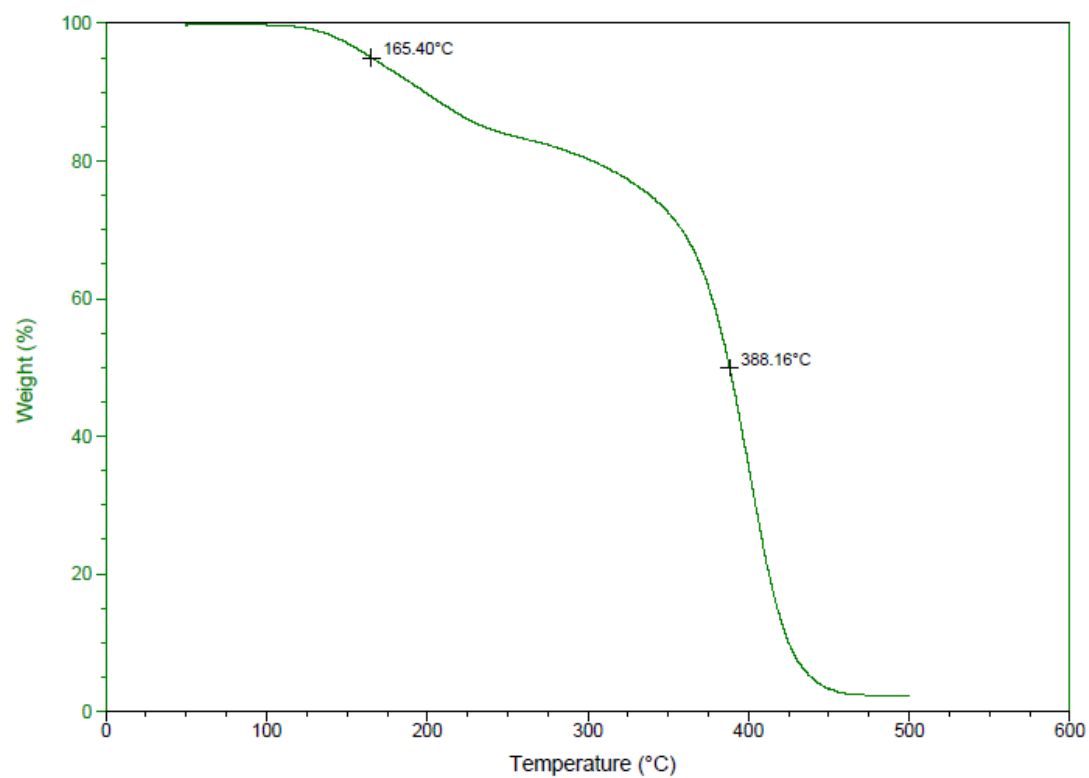


Figure S43. TGA thermogram of P3, run 3, Table 2

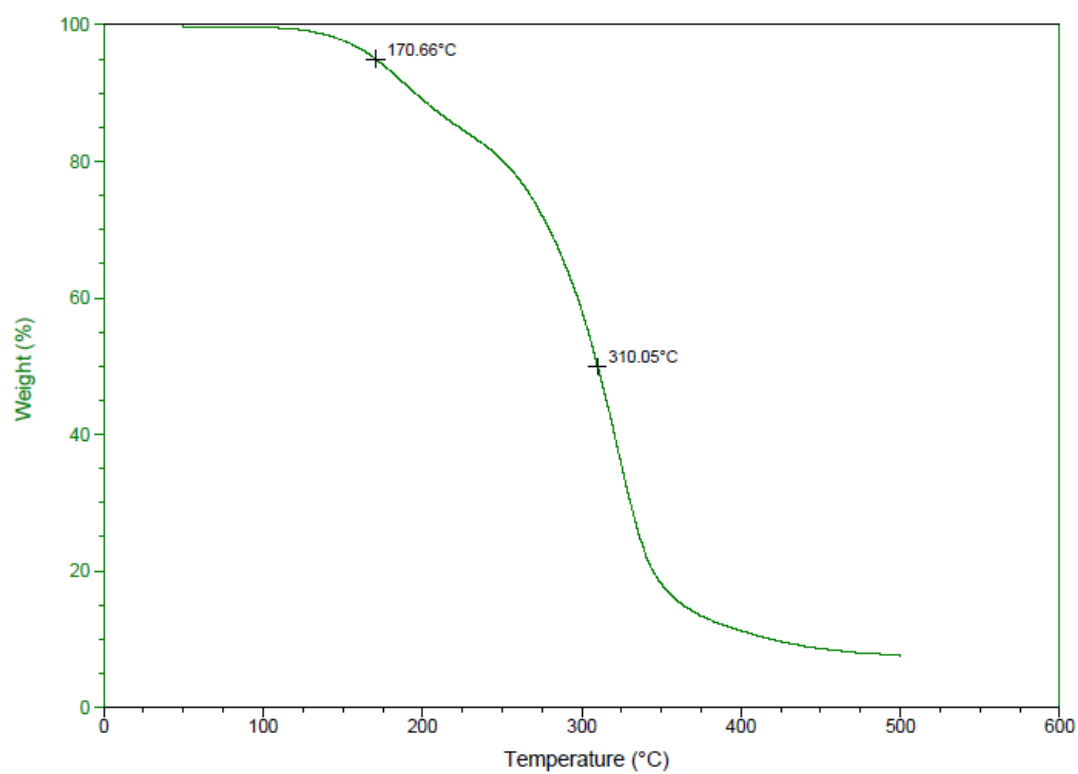


Figure S44. TGA thermogram of P4, run 4, Table 2