Electronic Supplementary Material (ESI) for RSC Advances.

Supercritical Carbon Dioxide Capture with Fusel Alcohols for Clean Preparation of Organic Carbonates

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Supporting Information

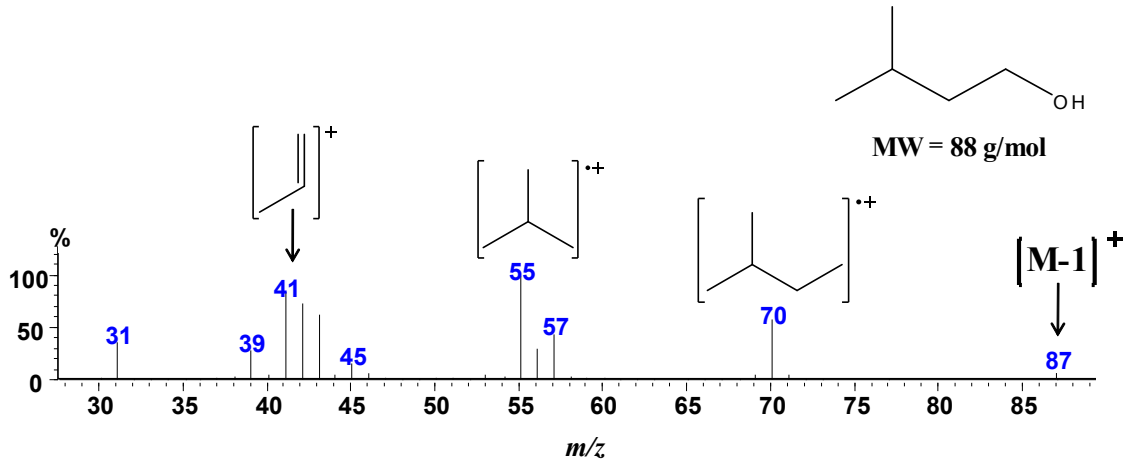

Figure S1. Mass spectrum of compound eluted at ~11 min which corresponds to isopentyl alcohol (Peak 1 from the chromatogram of the synthesis of butyl-isopentyl carbonate, Figure 1a).

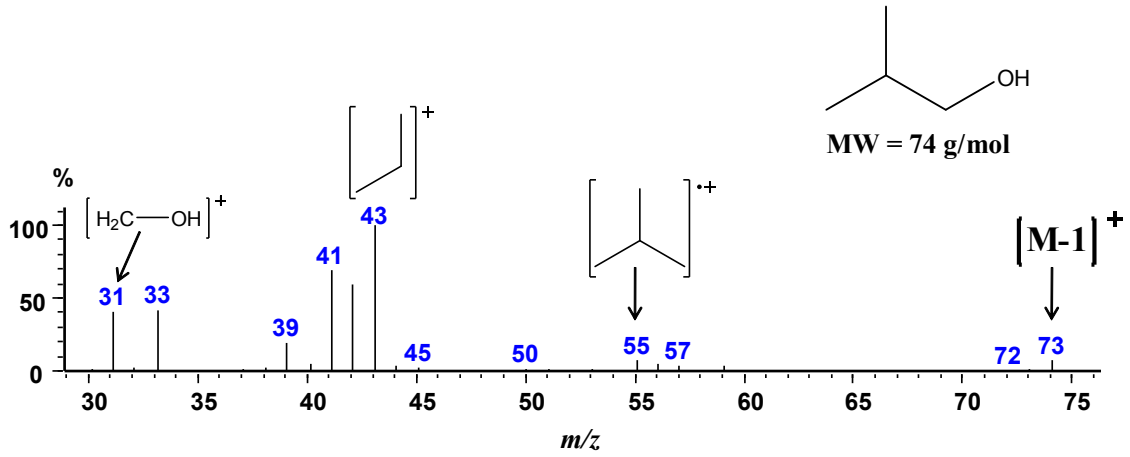

Figure S2. Mass spectrum of compound eluted at ~7 min associated to isobutyl alcohol (Peak 3 from the chromatogram of the synthesis of butyl-isobutyl carbonate, Figure 2a).

Figure S3 displays the chromatogram of crude fusel alcohols. Peak 3 (~3 min) corresponds to isobutyl alcohol and peak 1 (~5 min) is attributed to isopentyl alcohol.

The smaller peaks observed in the chromatogram are due to the presence of esters in fusel alcohols.

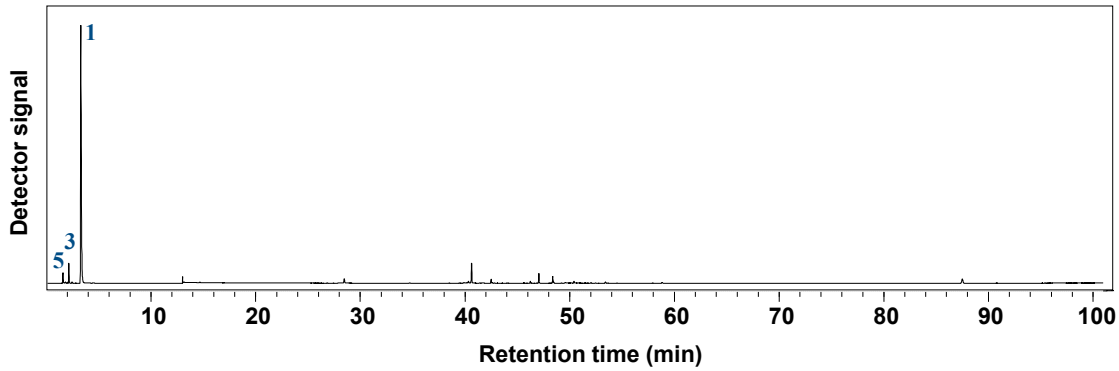

Figure S3. Chromatogram from crude fusel alcohols.

To confirm the peaks observed in the chromatogram from crude fusel alcohols observed in Figure S3, the analysis of this crude fusel alcohols and a fusel alcohol pattern was performed in the GC-FID. In both chromatograms, it can be observed the presence of ethyl alcohol (peak 5), propyl alcohol (peak 8), isobutyl alcohol (peak 2) and isopentyl alcohol (peak 1). In the chromatogram of fusel alcohol it can also be observed the butyl alcohol (peak 9), which is not seen in the chromatogram of the fusel alcohol pattern.

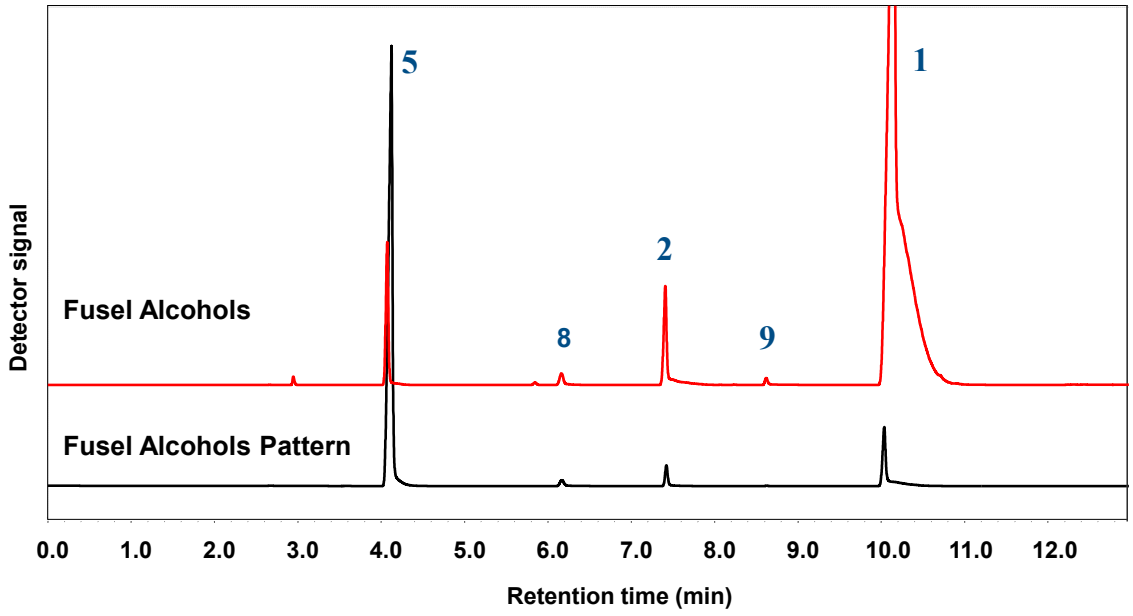

Figure S4. GC-FID chromatogram from crude fusel alcohols and GC-FID chromatogram from a crude fusel alcohol pattern.

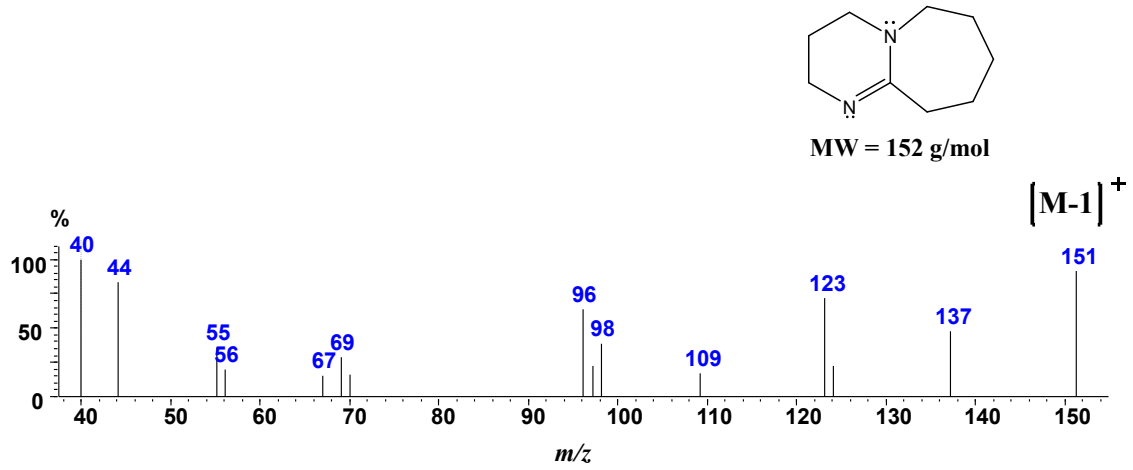

Figure S5. Mass spectrum of the base DBU.

DBU was extracted from the carbonate solution with water, which was later evaporated under reduced pressure. The spectra of DBU recovered as a free base is shown in Figure S5. Recycling of DBU will be further investigated.

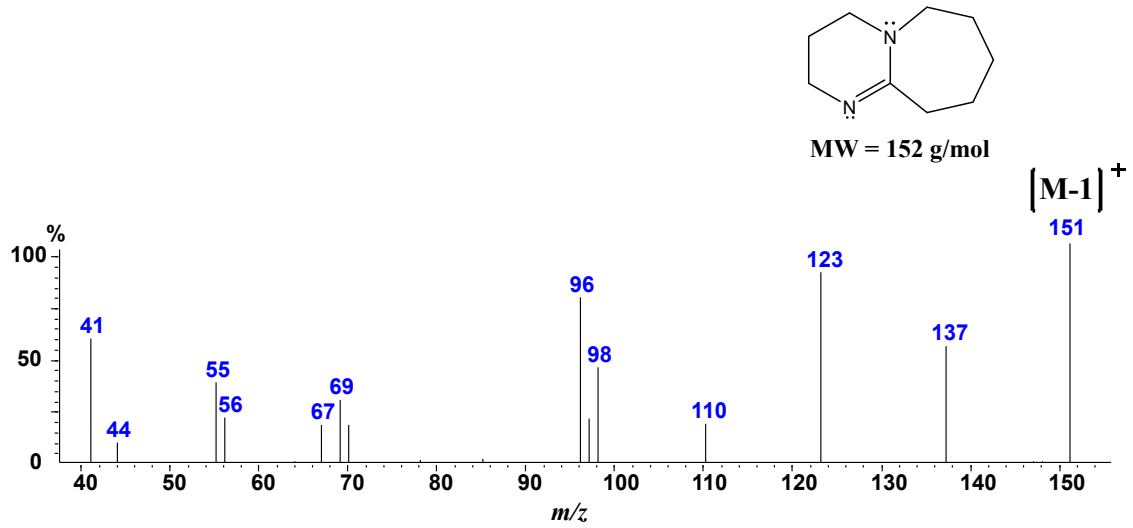

Figure S6. Mass spectrum of DBU recovered as a free base.

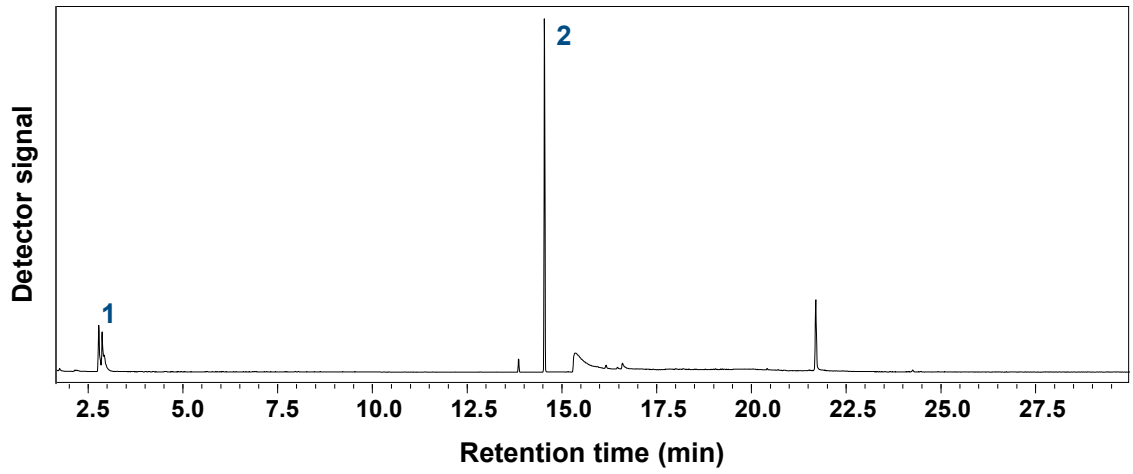

Figure S7. Chromatogram from the synthesis of butyl-isopentyl carbonate at 40 °C and 80 bar for 1 hour using DBN as promoter. Butyl-isopentyl carbonate was obtained in 86% of chromatographic conversion.

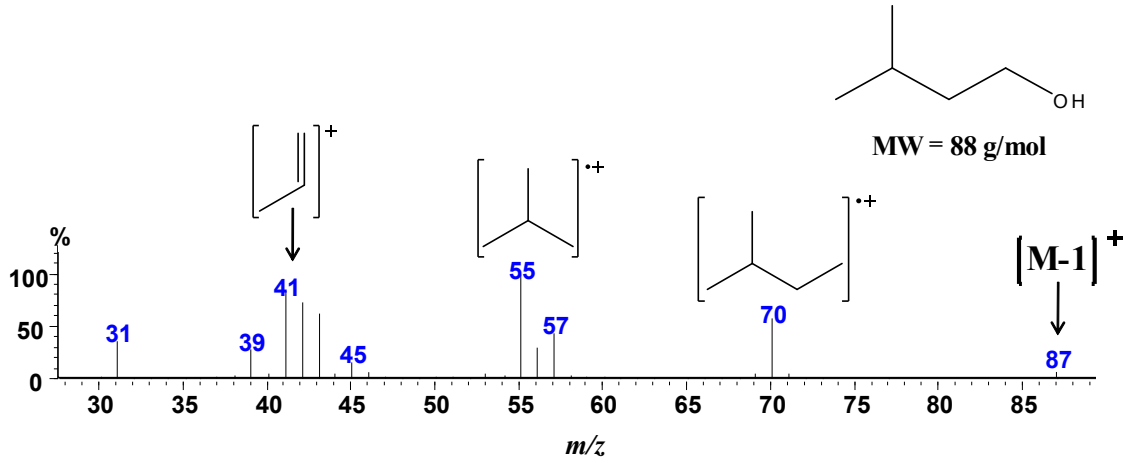

Figure S8. Mass spectrum of compound eluted at ~3 min which corresponds to isopentyl alcohol (Peak 1 from the chromatogram of the synthesis of butyl-isopentyl carbonate using DBN).

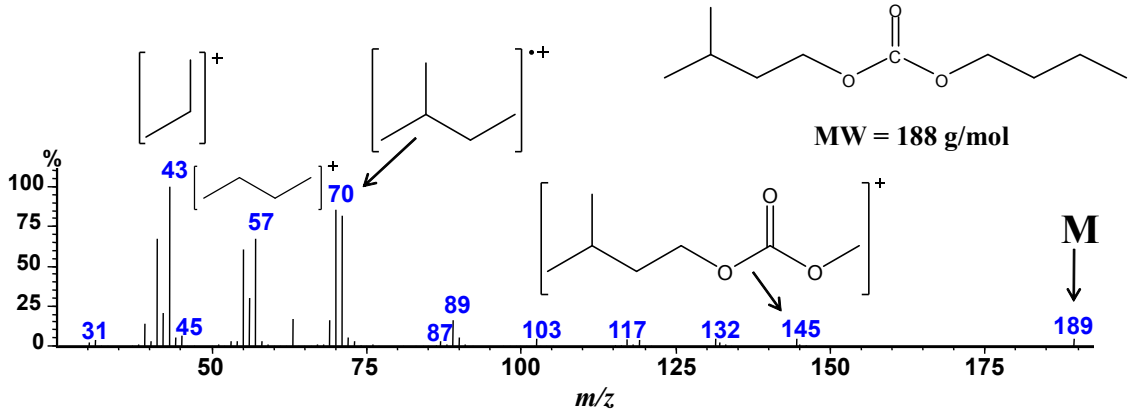

Figure S9. Mass spectrum of compound eluted at ~14 min which corresponds to butyl-isopentyl carbonate (Peak 2 from the chromatogram of the synthesis of butyl-isopentyl carbonate using DBN).

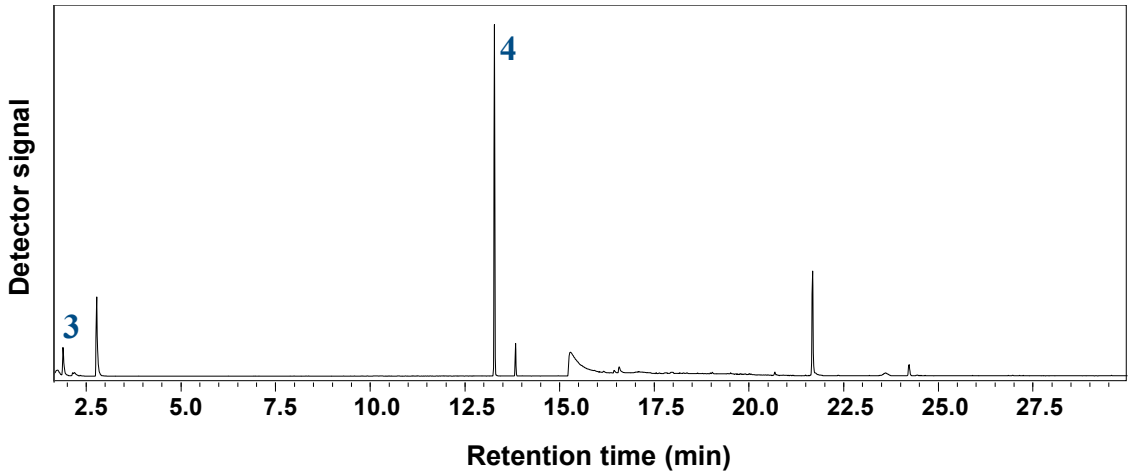

Figure S10. Chromatogram from the synthesis of butyl-isobutyl carbonate at 40 °C and 80 bar for 1 hour using DBN as promoter. Butyl-isobutyl carbonate was obtained in 89% of chromatographic conversion.

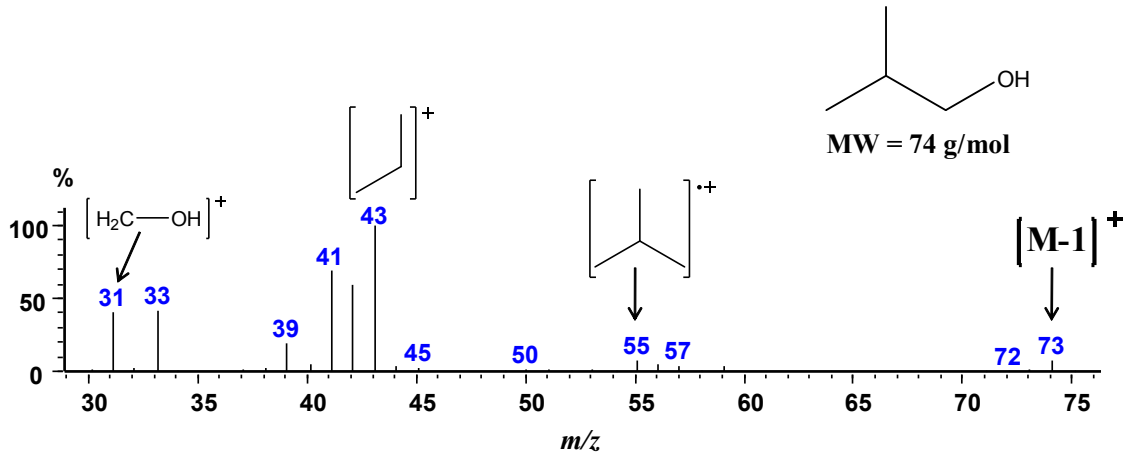

Figure S11. Mass spectrum of compound eluted at ~2 min associated to isobutyl alcohol (Peak 3 from the chromatogram of the synthesis of butyl-isobutyl carbonate using DBN).

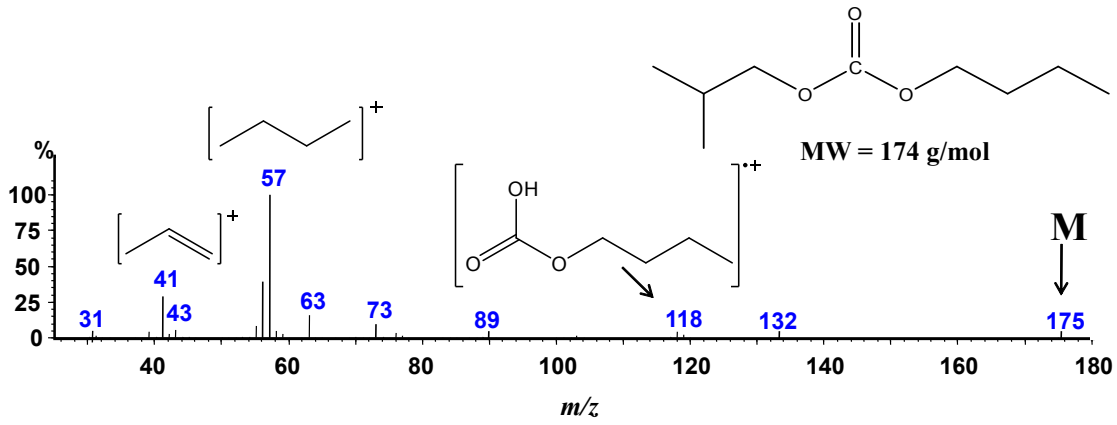

Figure S12. Mass spectrum of compound eluted at ~13 min which corresponds to butyl-isobutyl carbonate (Peak 4 from the chromatogram of the synthesis of butyl-isobutyl carbonate using DBN).

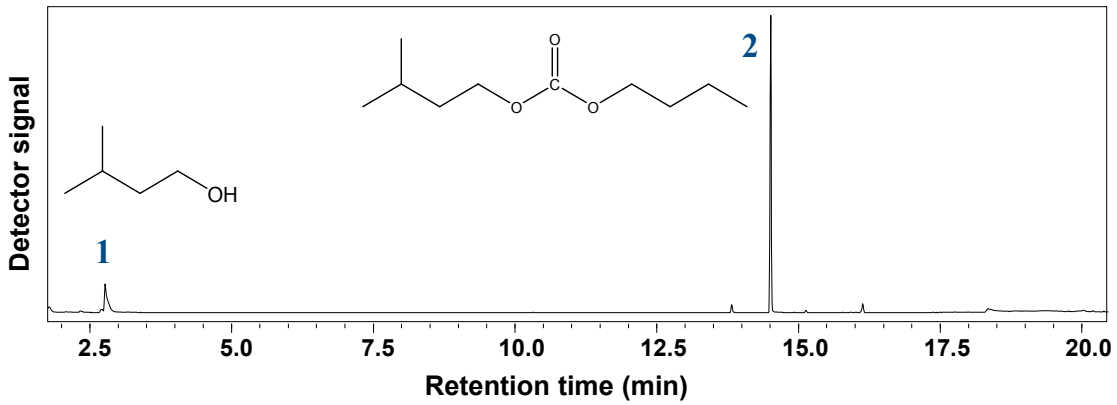

Figure S13. Chromatogram from the synthesis of butyl-isopentyl carbonate at 40 °C and 80 bar for 1 hour using TBD as promoter. Butyl-isopentyl carbonate was obtained in 49% of chromatographic conversion.

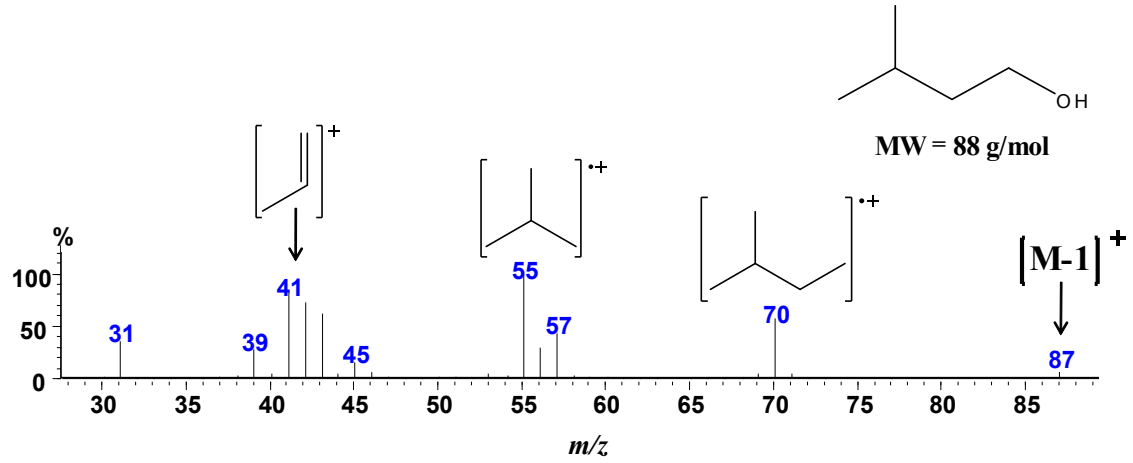

Figure S14. Mass spectrum of compound eluted at ~3 min which corresponds to isopentyl alcohol (Peak 1 from the chromatogram of the synthesis of butyl-isopentyl carbonate using TBD).

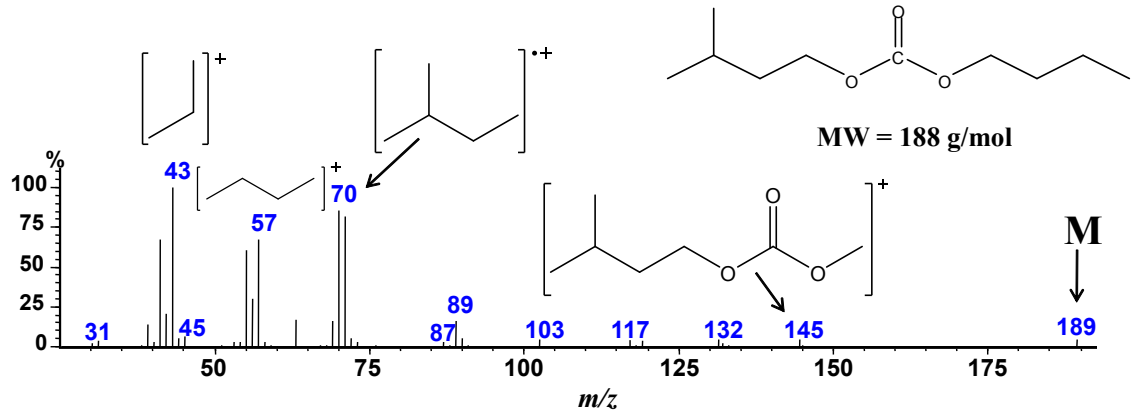

Figure S15. Mass spectrum of compound eluted at ~14 min which corresponds to butyl-isopentyl carbonate (Peak 2 from the chromatogram of the synthesis of butyl-isopentyl carbonate using TBD).

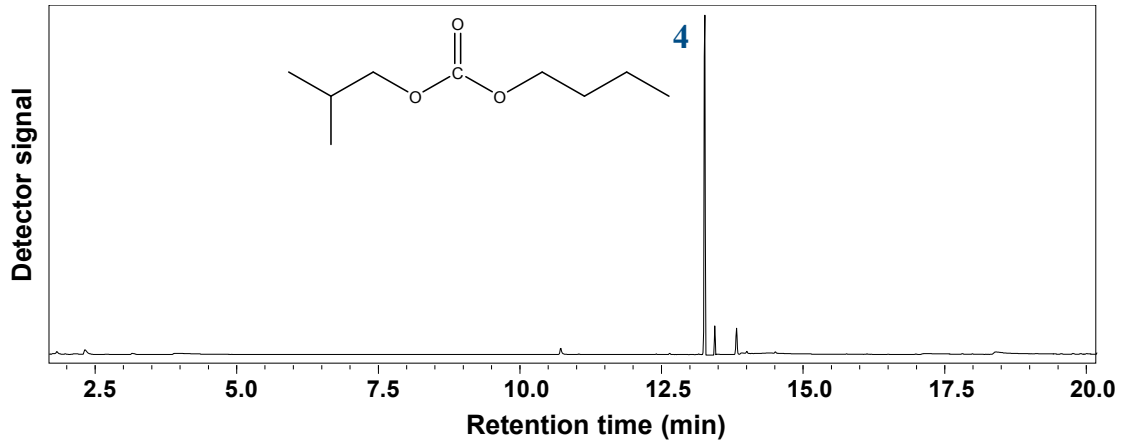

Figure S16. Chromatogram from the synthesis of butyl-isobutyl carbonate at 40 °C and 80 bar for 1 hour using TBD as promoter. Butyl-isobutyl carbonate was obtained in 45% of chromatographic conversion.

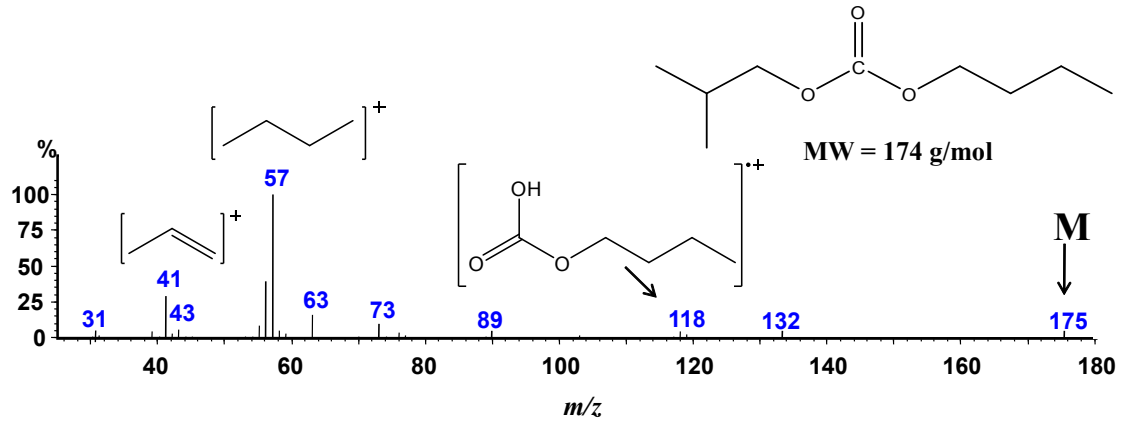

Figure S17. Mass spectrum of compound eluted at ~13 min which corresponds to butyl-isobutyl carbonate (Peak 4 from the chromatogram of the synthesis of butyl-isobutyl carbonate using TBD).

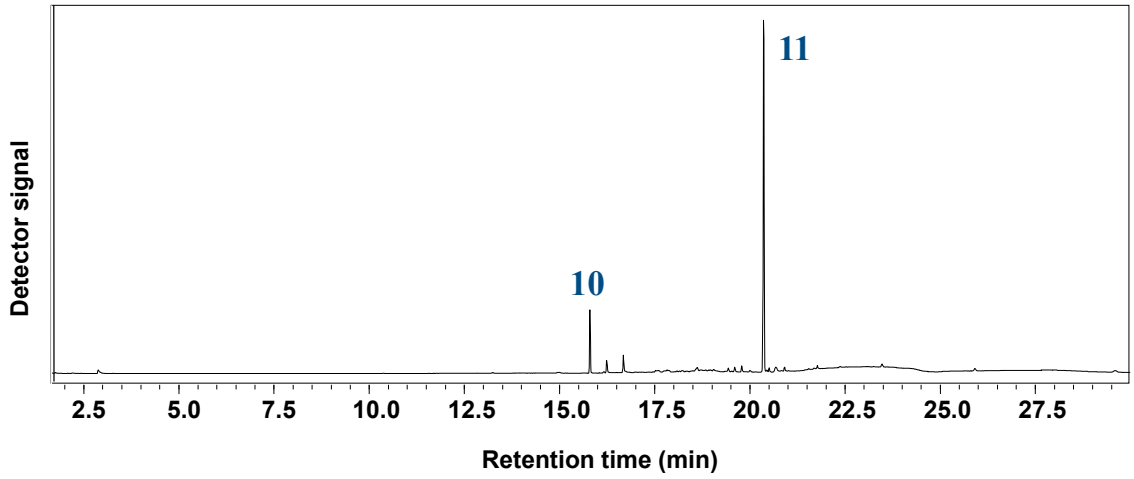

Figure S18. Chromatogram from the synthesis of 2.4-dichlorobenzyl-isopentyl carbonate at 40 °C and 80 bar for 1 hour using DBU as promoter. Peak 10 corresponds to the remaining alkylating agent and peak 8 is associated to the carbonate.

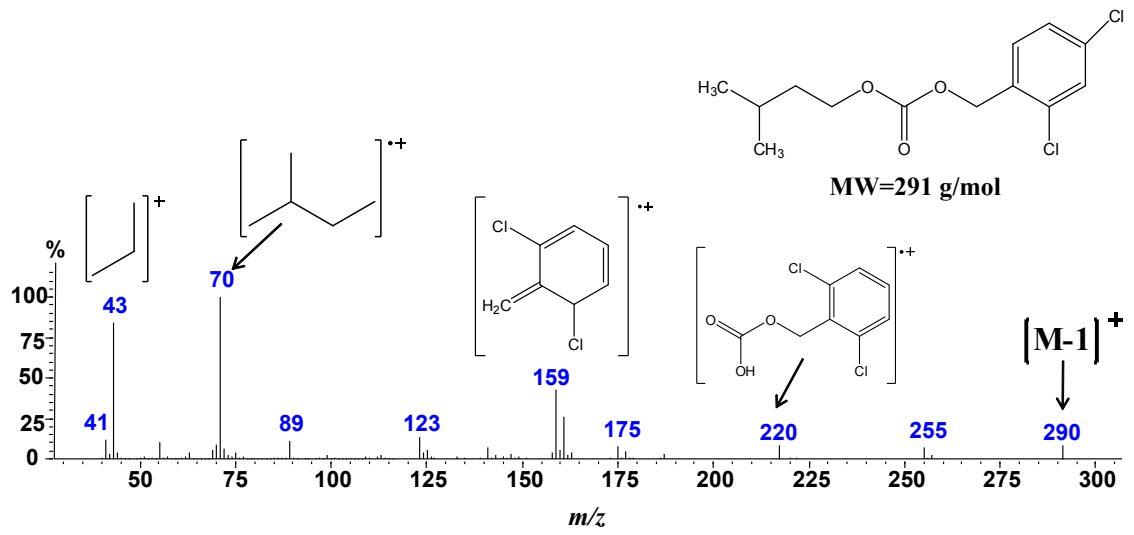

Figure S19. Mass spectrum corresponding to 2.4-dichlorobenzyl-isopentyl carbonate eluted at ~21 min. The carbonate was obtained in 99% of chromatographic conversion.

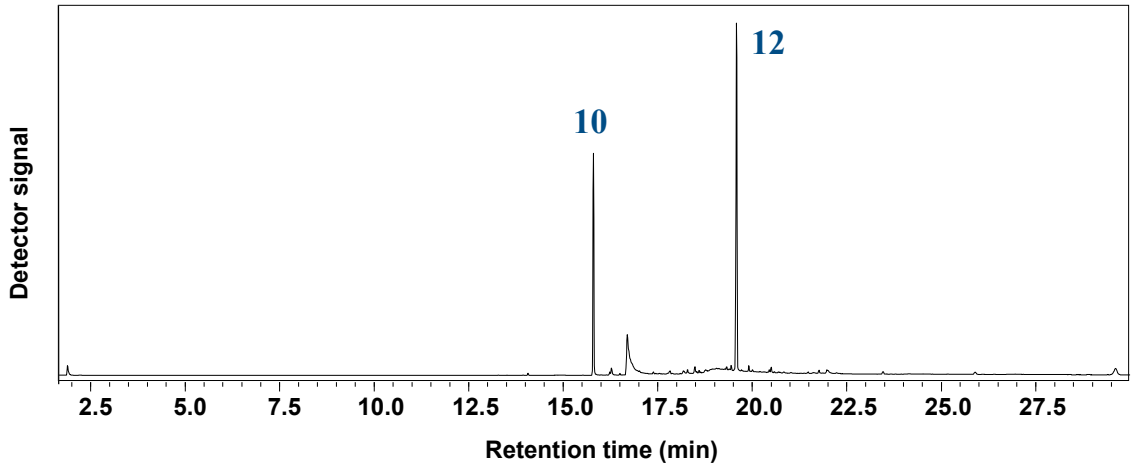

Figure S20. Chromatogram from the synthesis of 2.4-dichlorobenzyl-isobutyl carbonate at 40 °C and 80 bar for 1 hour using DBU as promoter. Peak 10 corresponds to the remaining alkylating agent and peak 12 is associated to the carbonate.

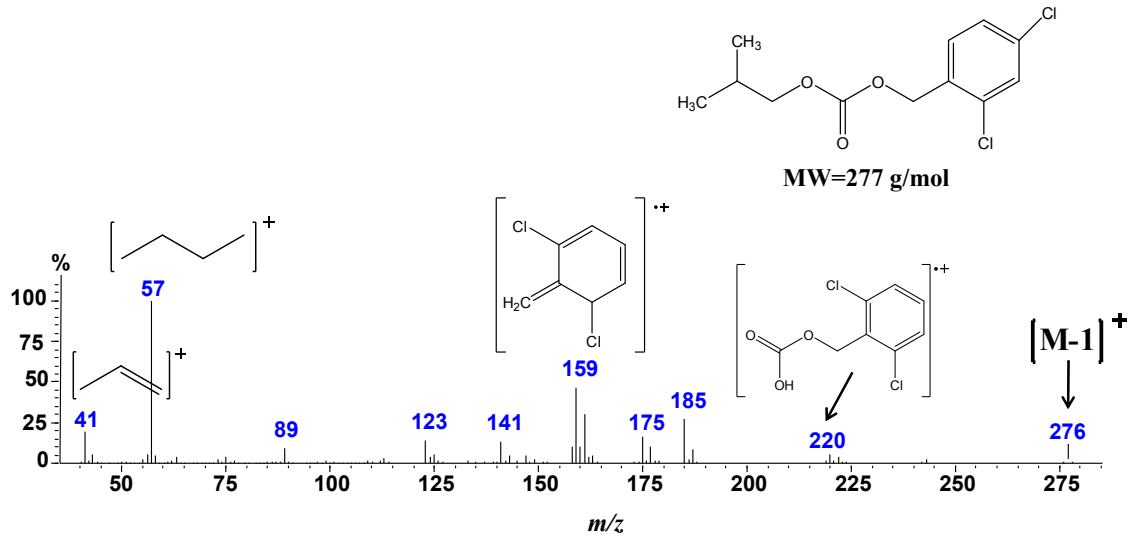

Figure S21. Mass spectrum corresponding to 2.4-dichlorobenzyl-isobutyl carbonate eluted at ~19 min. The carbonate was obtained in 97% of chromatographic conversion.

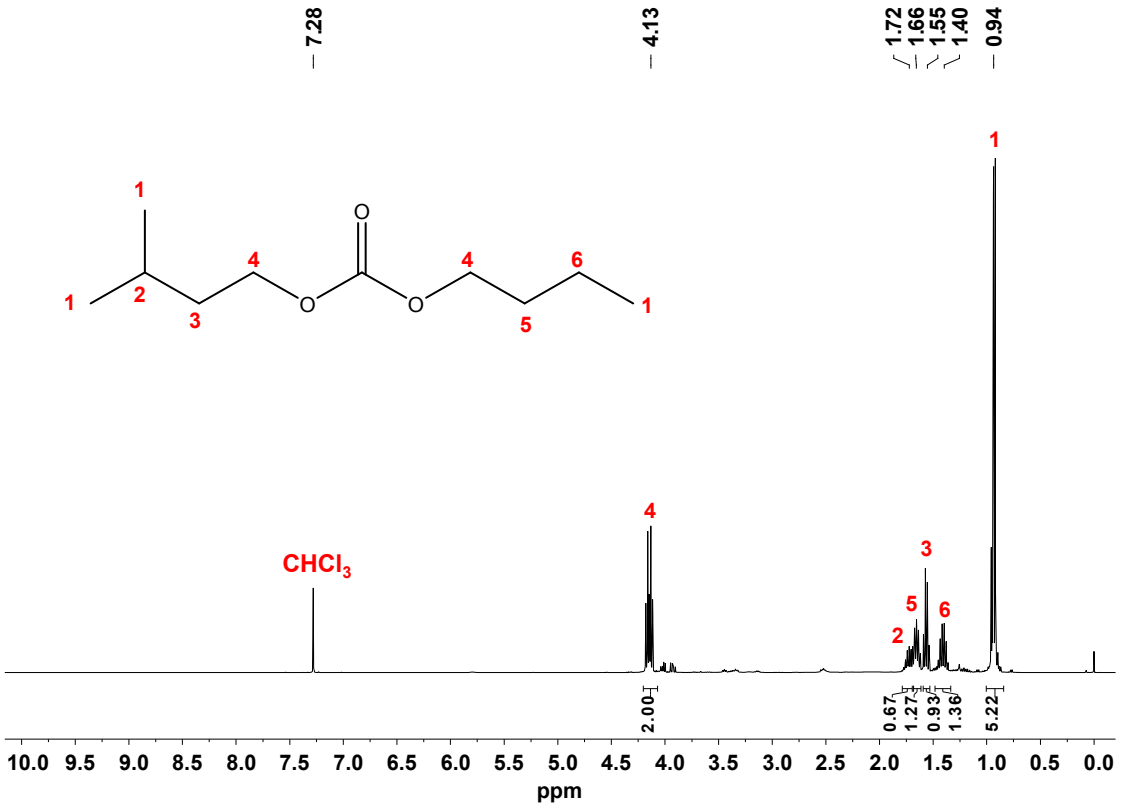

Figure S22. ^{1}H-NMR spectrum ($CDCl_3$, 500 MHz) of butyl-isopentyl carbonate.

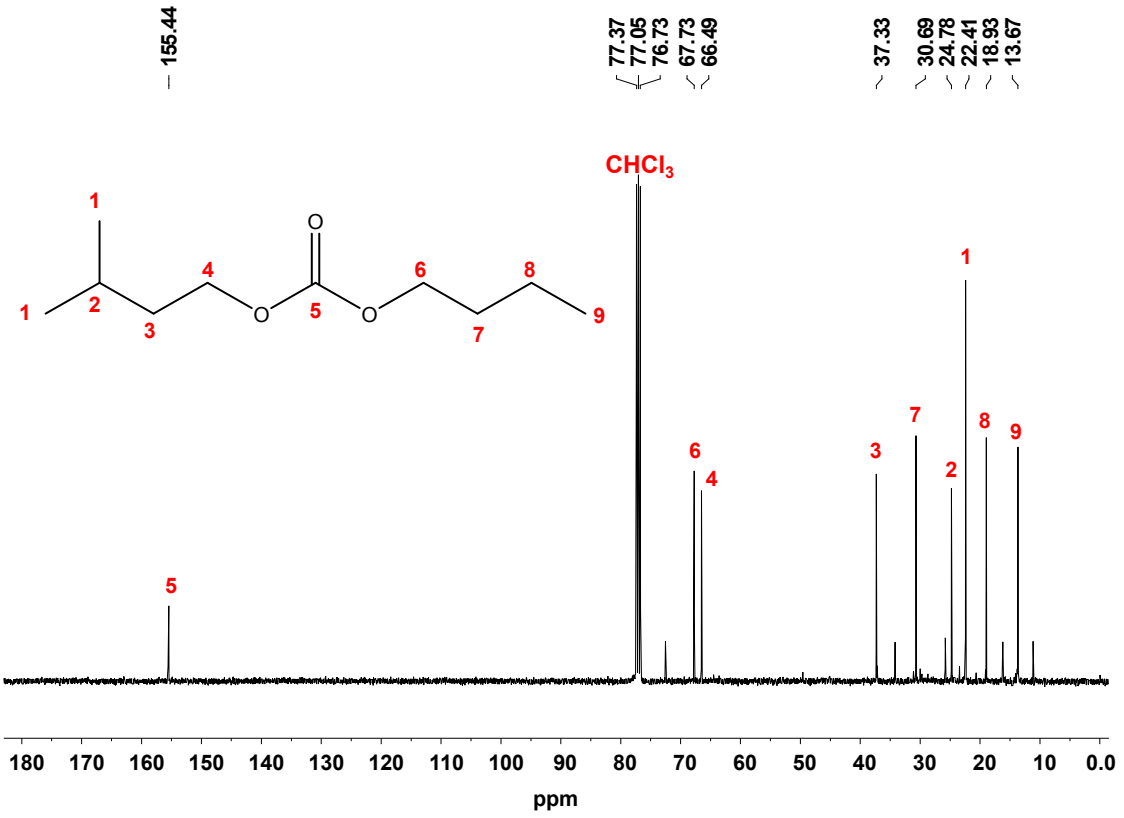

Figure S23. ^{13}C-NMR spectrum ($CDCl_3$, 500 MHz) of butyl-isopentyl carbonate.

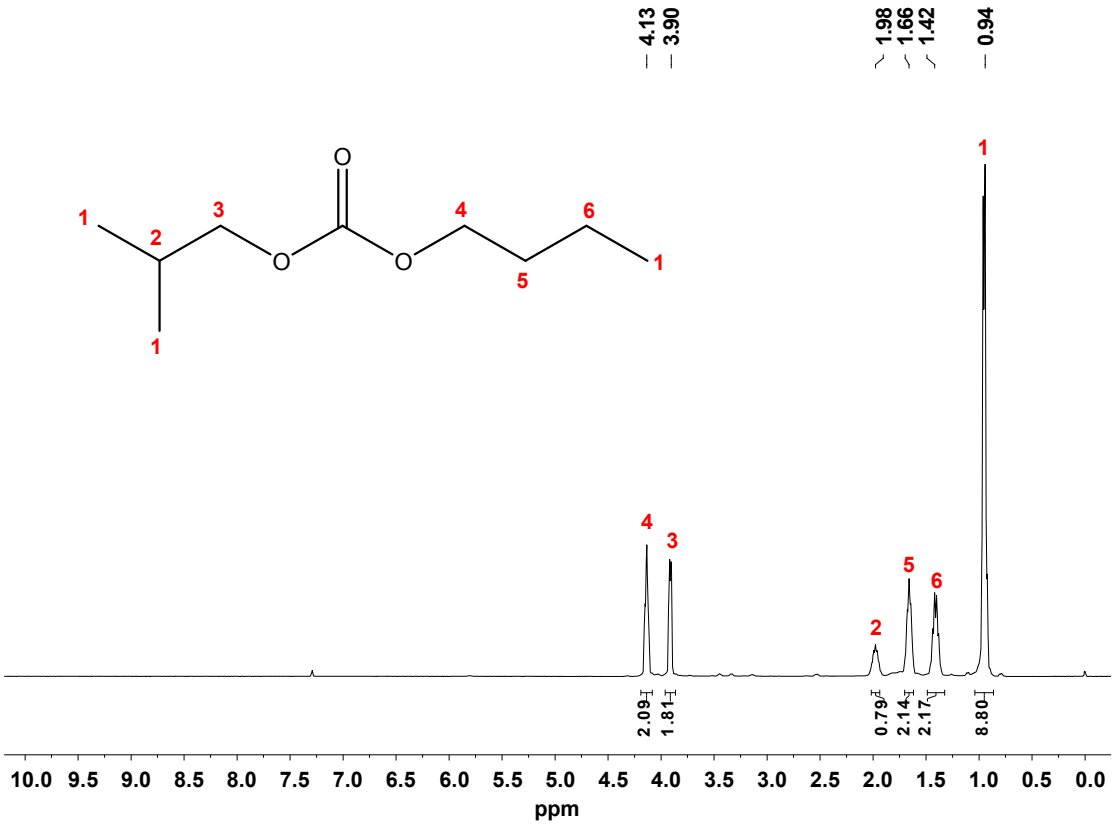

Figure S24. ^{1}H-NMR spectrum ($CDCl_3$, 500 MHz) of butyl-isobutyl carbonate.

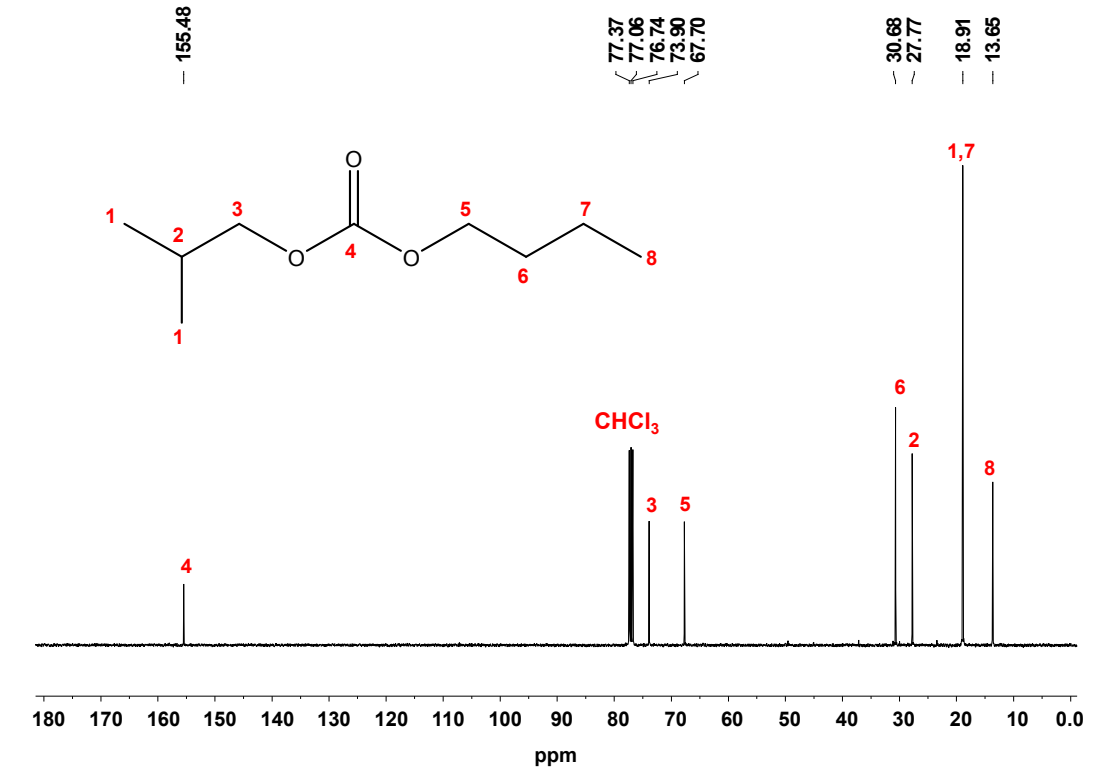

Figure S25. ^{13}C-NMR spectrum ($CDCl_3$, 500 MHz) of butyl-isobutyl carbonate.

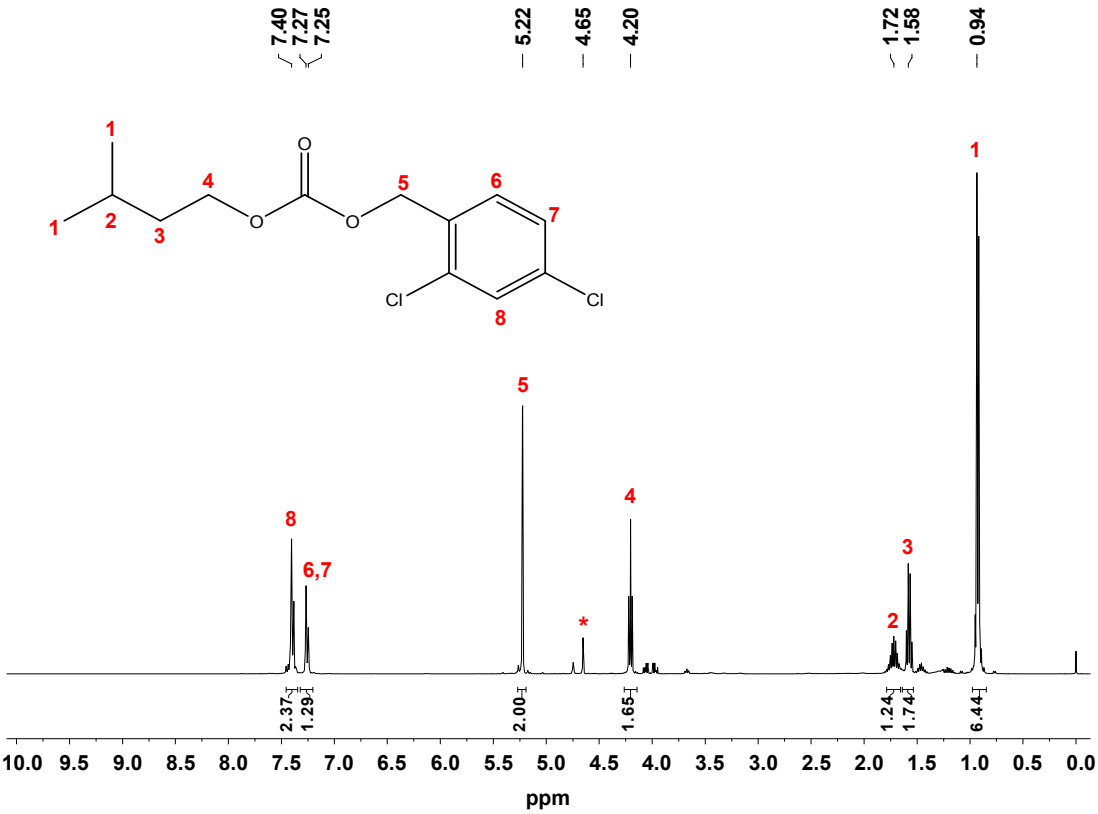

Figure S26. ^{1}H-NMR spectrum ($CDCl_3$, 500 MHz) of 2,4-dichlorobenzyl-isopentyl carbonate. The signal with * symbol corresponds to methylene of the remaining alkylating agent.

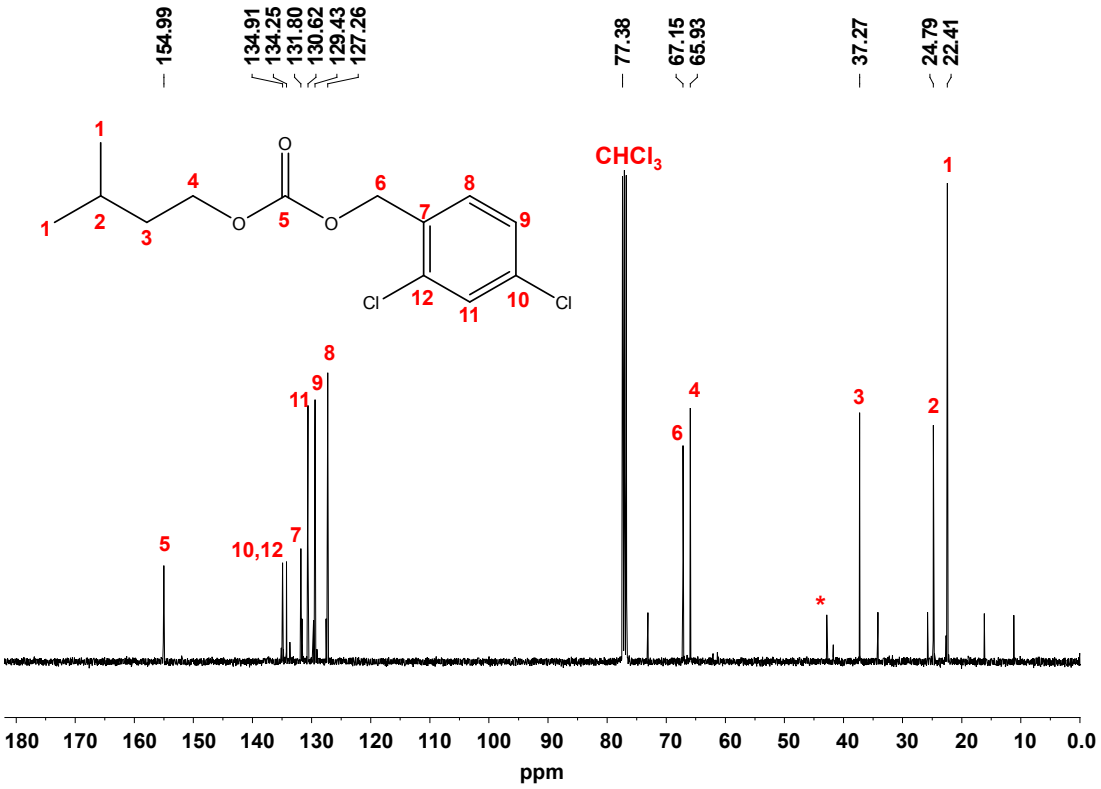

Figure S27. ^{13}C-NMR spectrum ($CDCl_3$, 500 MHz) of 2,4-dichlorobenzyl-isopentyl carbonate. The signal with * symbol corresponds to methylene of the remaining alkylating agent.

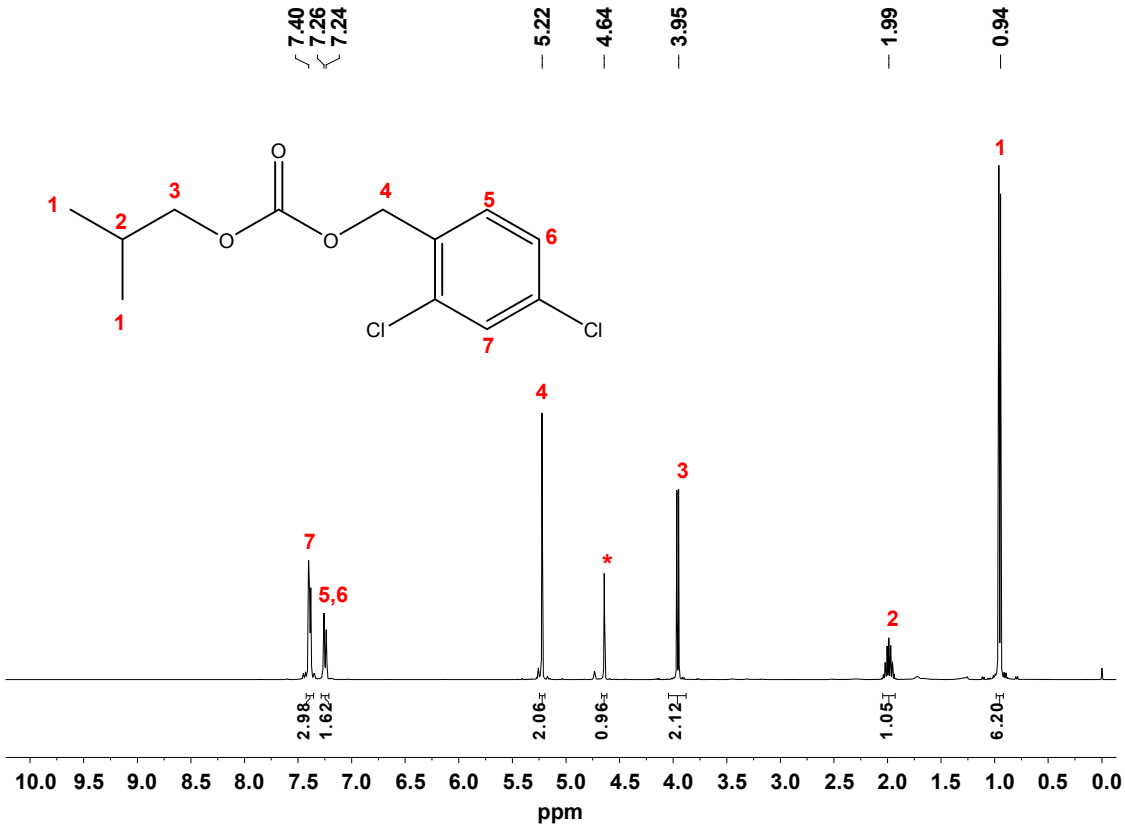

Figure S28. ^{1}H-NMR spectrum ($CDCl_3$, 500 MHz) of 2,4-dichlorobenzyl-isobutyl carbonate. The signal with * symbol corresponds to methylene of the remaining alkylating agent.

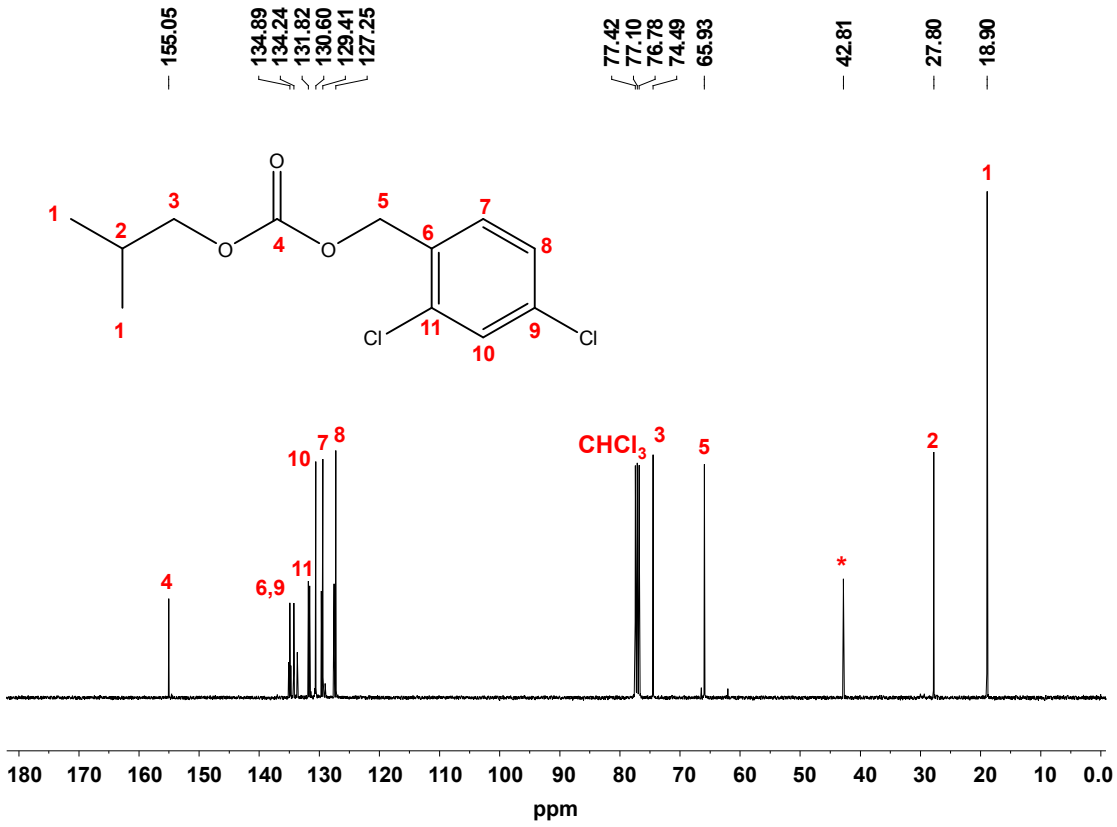

Figure S29. ^{13}C-NMR spectrum ($CDCl_3$, 500 MHz) of 2,4-dichlorobenzyl-isobutyl carbonate. The signal with * symbol corresponds to methylene of the remaining alkylating agent.

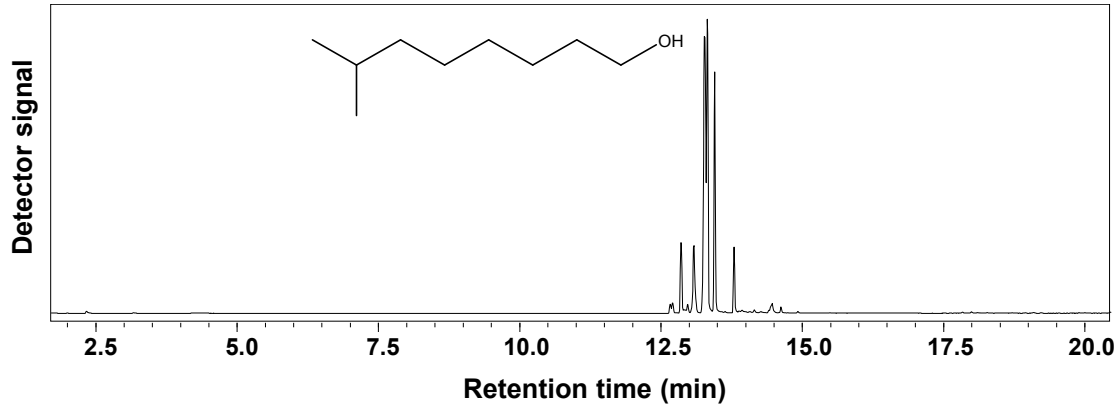

Figure S30. Chromatogram of isononyl alcohol. The peaks correspond to alcohol isomers.

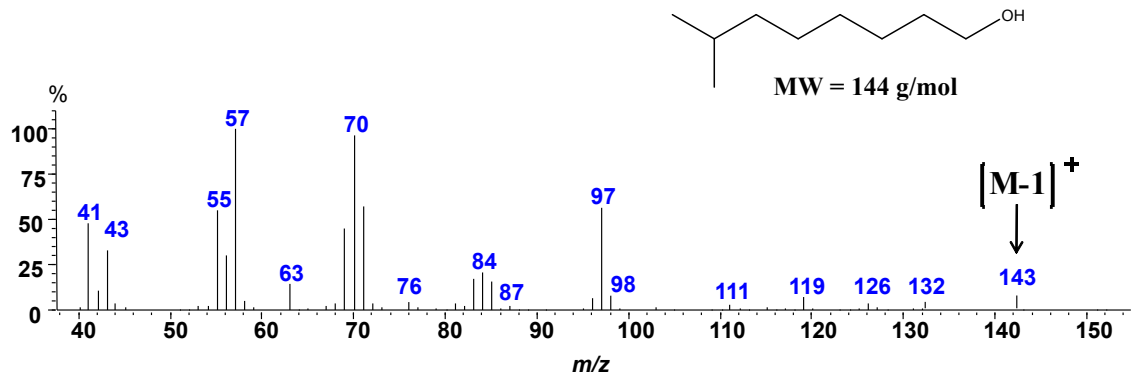

Figure S31. Mass spectrum of compound eluted at ~13 min associated to isononyl alcohol.

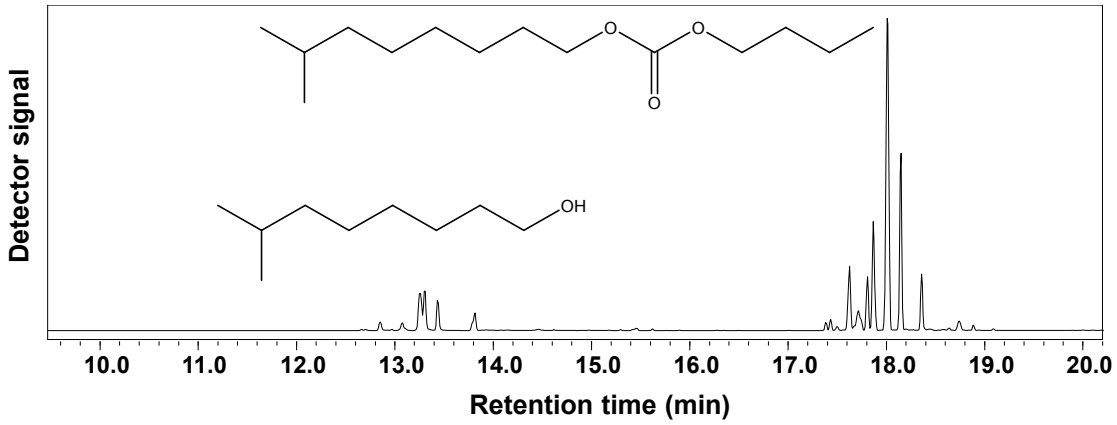

Figure S32. Chromatogram from the synthesis of butyl-isononyl carbonate at 40 °C and 80 bar for 1 hour using DBU as promoter. It is seen the remaining alcohol isomers from ~13 min to ~14 min and the formation of carbonates of each isomer from ~17.5 min to ~19 min.

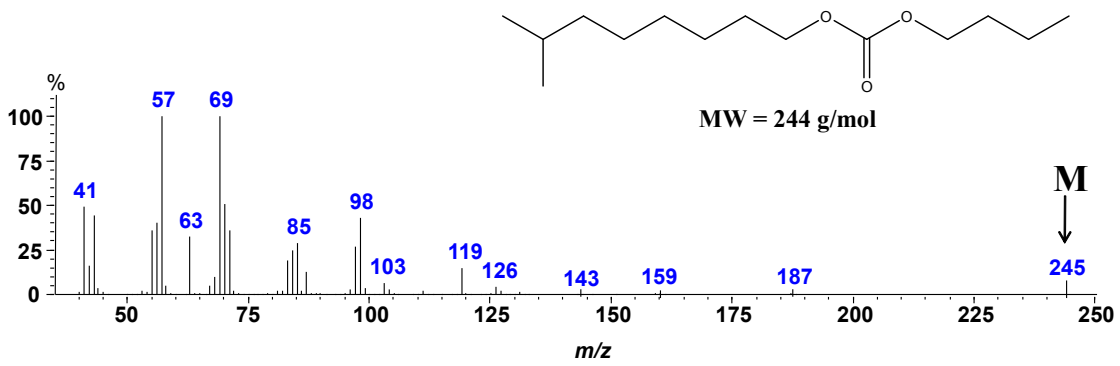

Figure S33. Mass spectrum of butyl-isononyl carbonate eluted at ~18 min.

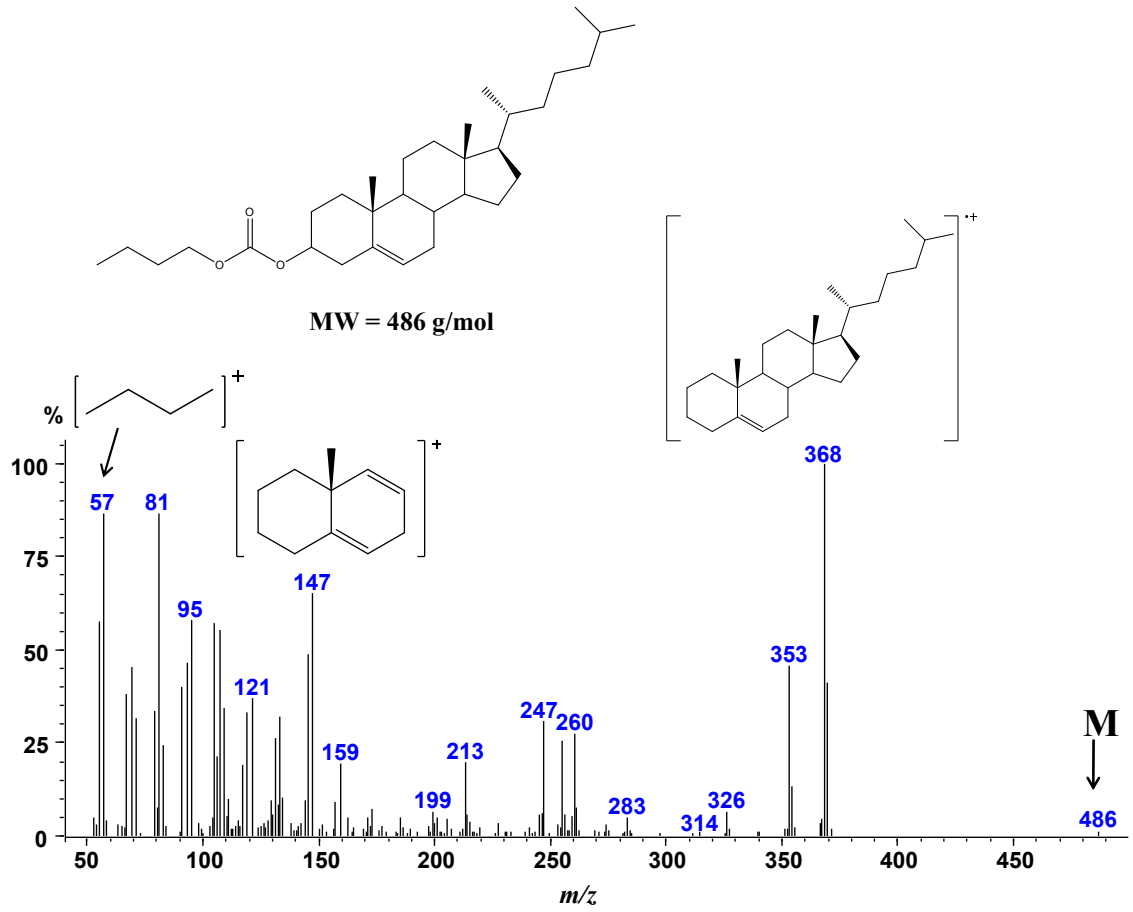

Figure S34. Mass spectrum of cholesteryl-butyl carbonate.

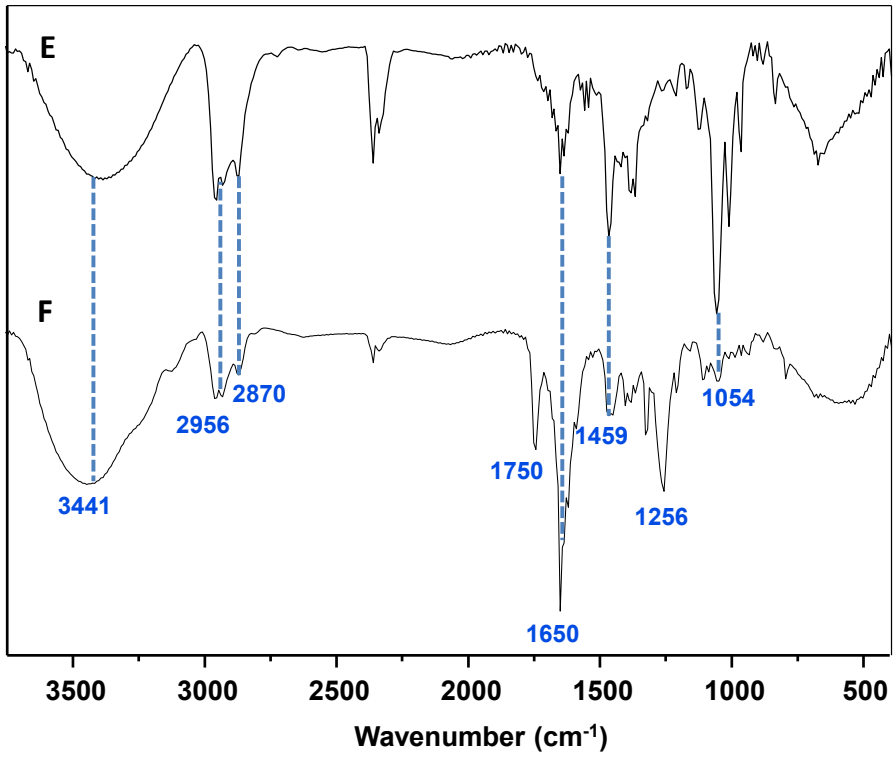

Figure S35. FT-IR spectra of a crude fusel oil sample (**E**) and its corresponding NPOCs (**F**).

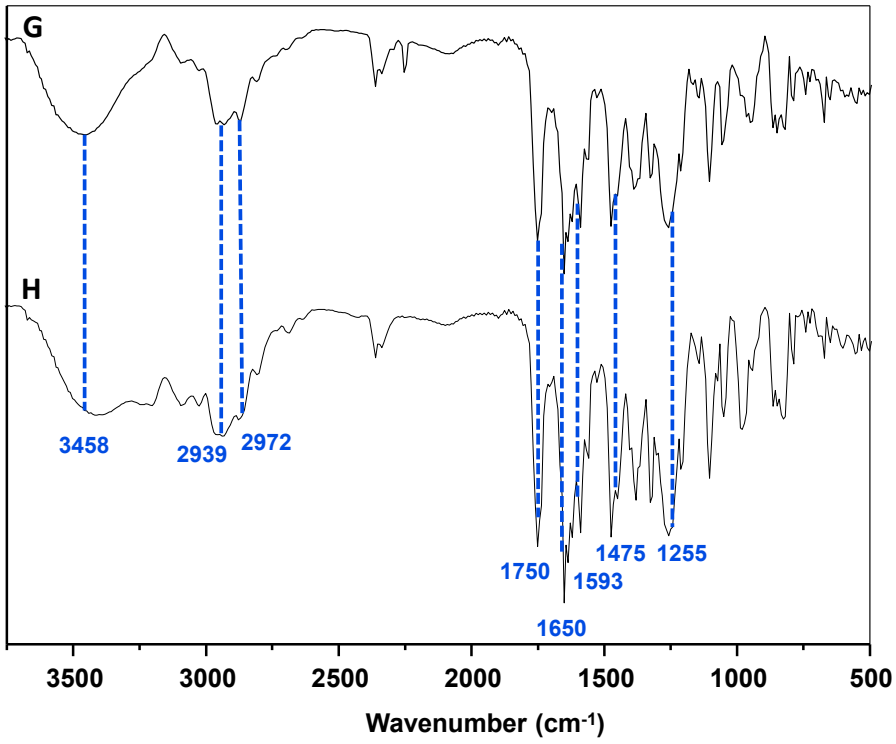

Figure S36. FT-IR spectra of 2,4-dichlorobenzyl-isopentyl carbonate (**G**) and 2,4-dichlorobenzyl-isobutyl carbonate (**H**).

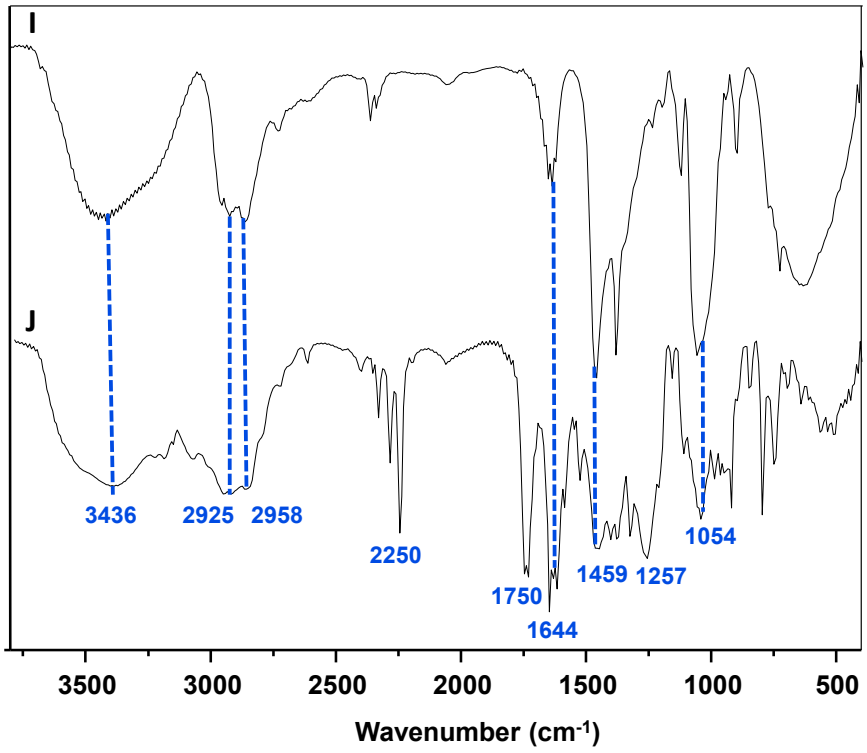

Figure S37. FT-IR spectra of isononyl alcohol (**I**) and butyl-isononyl carbonate (**J**).

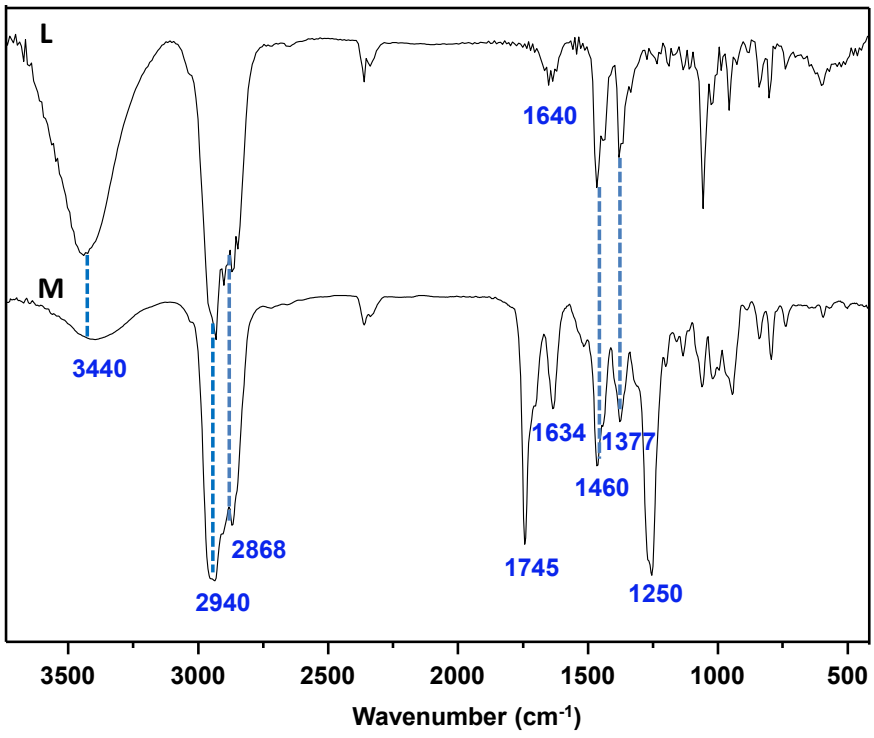

Figure S38. FT-IR spectra of cholesterol (**L**) and cholesteryl-butyl carbonate (**M**).