Electronic Supplementary Material (ESI) for Polymer Chemistry.


# Model reactions for the evaluation of poly- and multifunctional molecules as potential interfacial agents for the compatibilization of polyethylene/poly(ethylene-*co*-vinyl alcohol) blends

*Elisa Gitzhofer,[a] Bertrand Vileno,[b] Michel Bouquey,[a] Delphine Chan-Seng[a]*

[a]Université de Strasbourg, CNRS, Institut Charles Sadron UPR 22, F-67000 Strasbourg, France

[b]Université de Strasbourg, CNRS, Institut de Chimie de Strasbourg UMR 7177, F-67000 Strasbourg, France

**TABLE OF CONTENT**

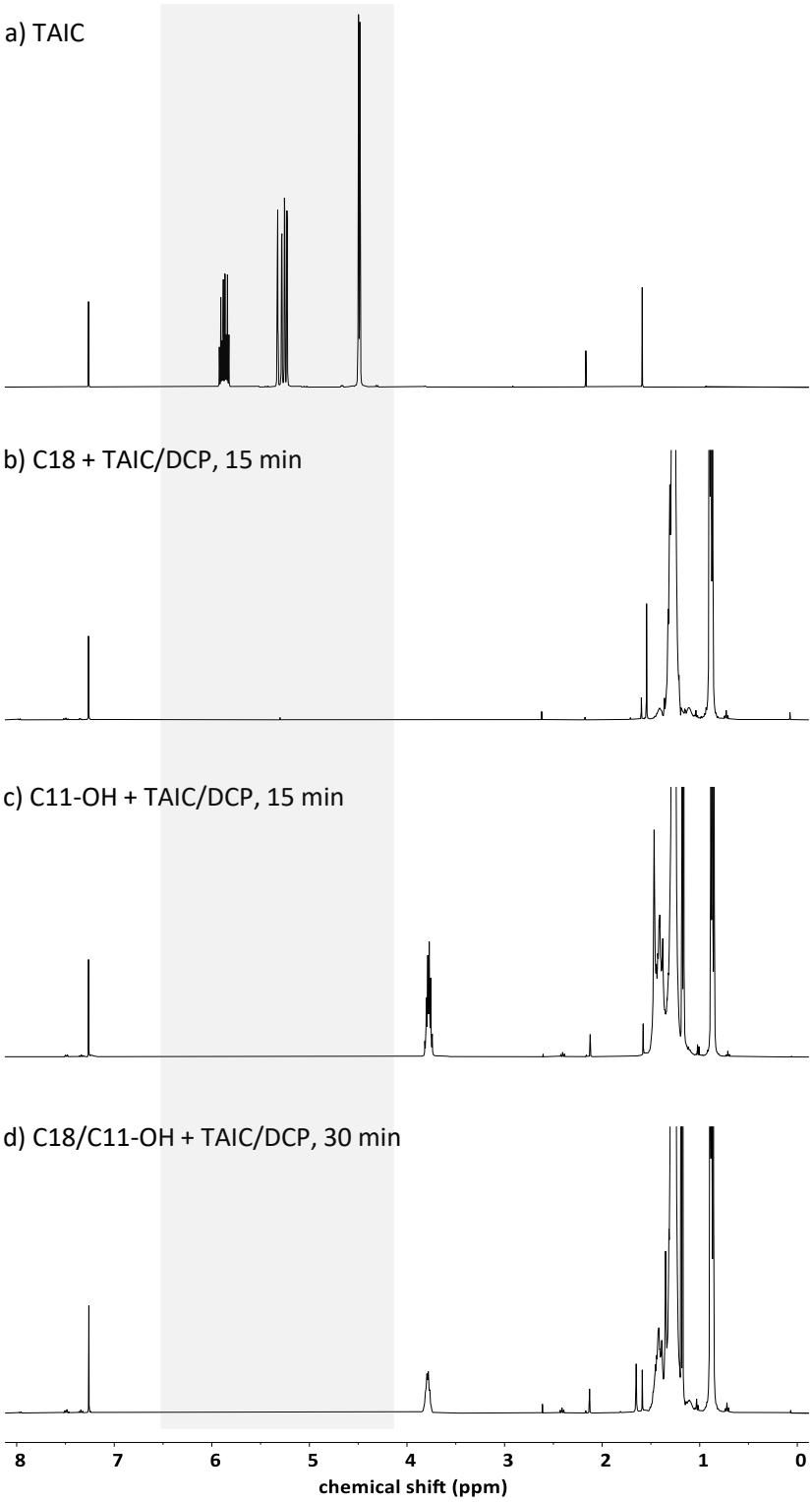
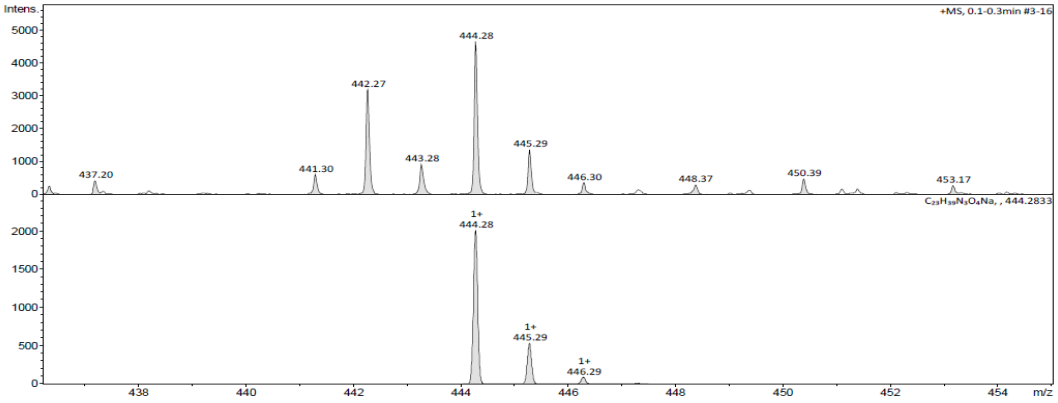
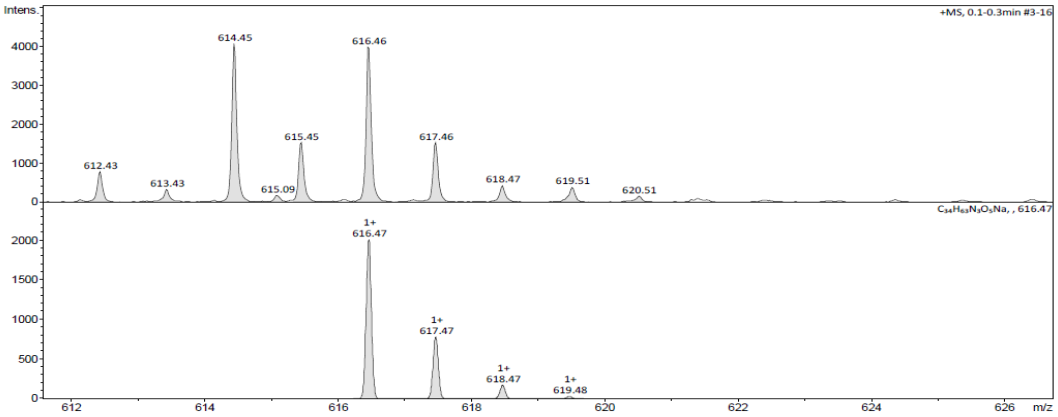



**Figure S1.** $^{1}H$ NMR spectra in $CDCl_3$ of a) TAIC and product formed after reaction of b) C18, c) C11-OH, and d) a mixture of C18 and C11-OH (1/1) with TAIC (1 mol%) in the presence of DCP (0.5 mol%) at 150 °C. The area highlighted in gray corresponds to the zoom presented in **Figure 1b**.

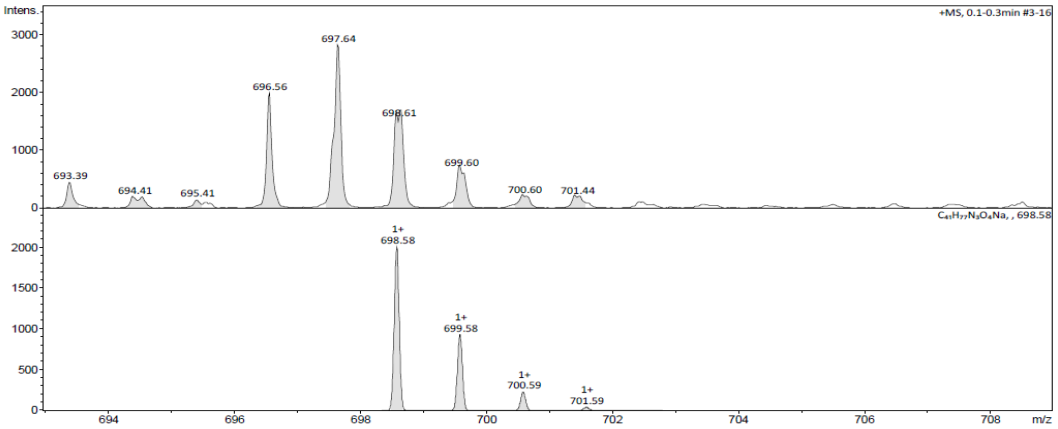
[TAIC+C11-OHx1+Na]+



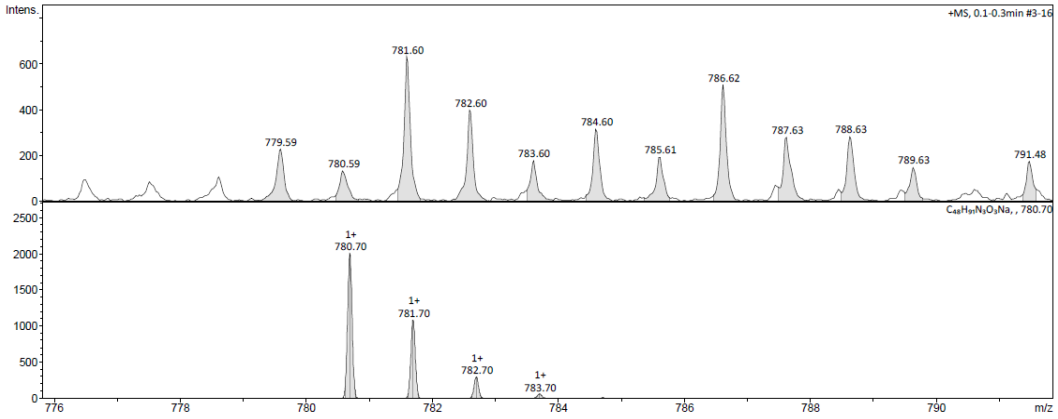

[TAIC+C11-OHx2+Na]+




TAIC+C18x1+C11-OHx1+Na]+




[TAIC+C18x2+Na]+



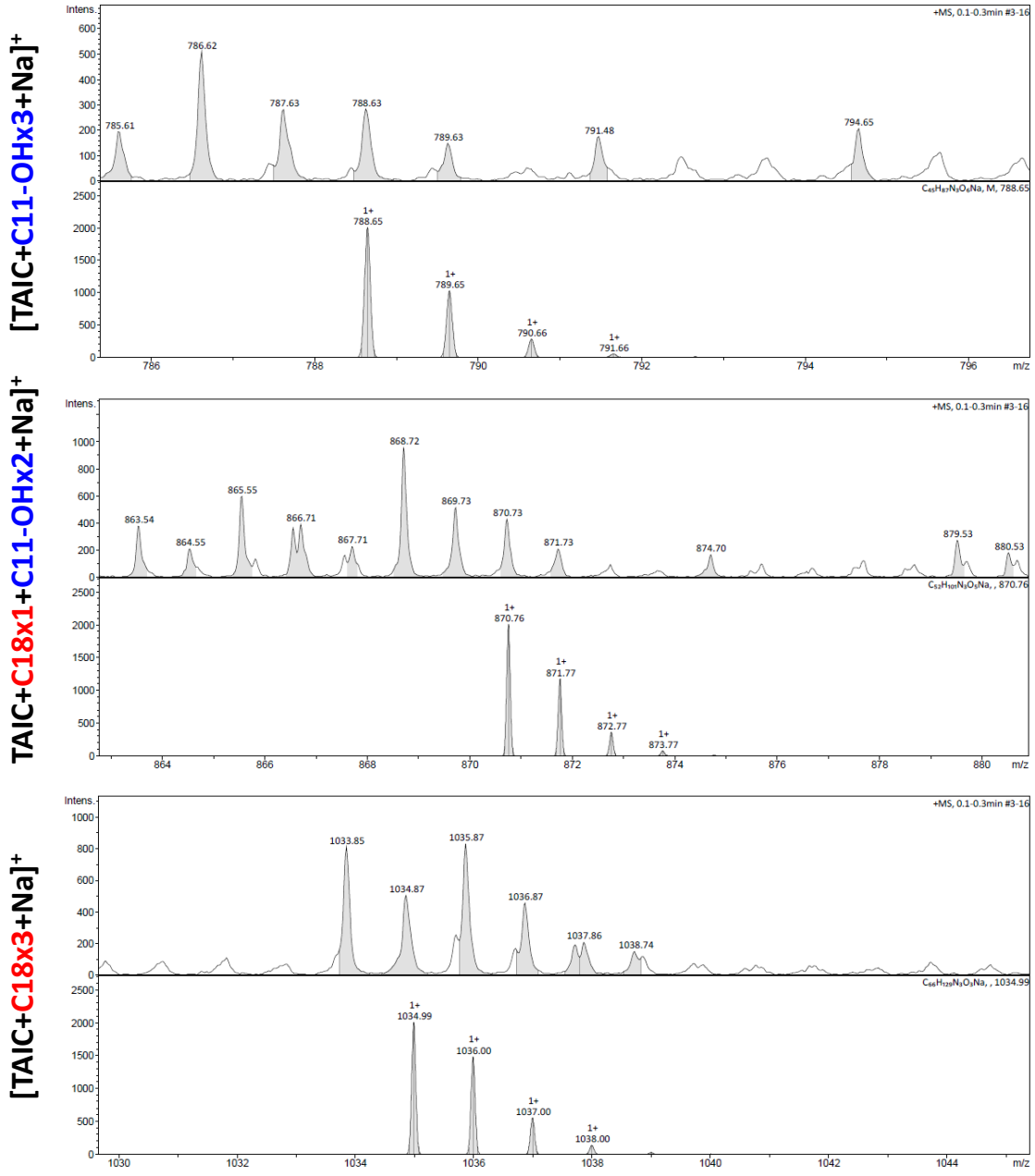



**Figure S2.** Zoom on the molecular peaks observed by ESI-MS (**Figure 1c**) corresponding to the different products formed from the reaction of C18 and C11-OH (1/1) with TAIC (1 mol%) in the presence of DCP (0.5 mol%) at 150 °C after 30 min of reaction. For each molecular peak, the spectrum on the top corresponds to the experimental one, and on the bottom the simulated one according to the molecular formula.

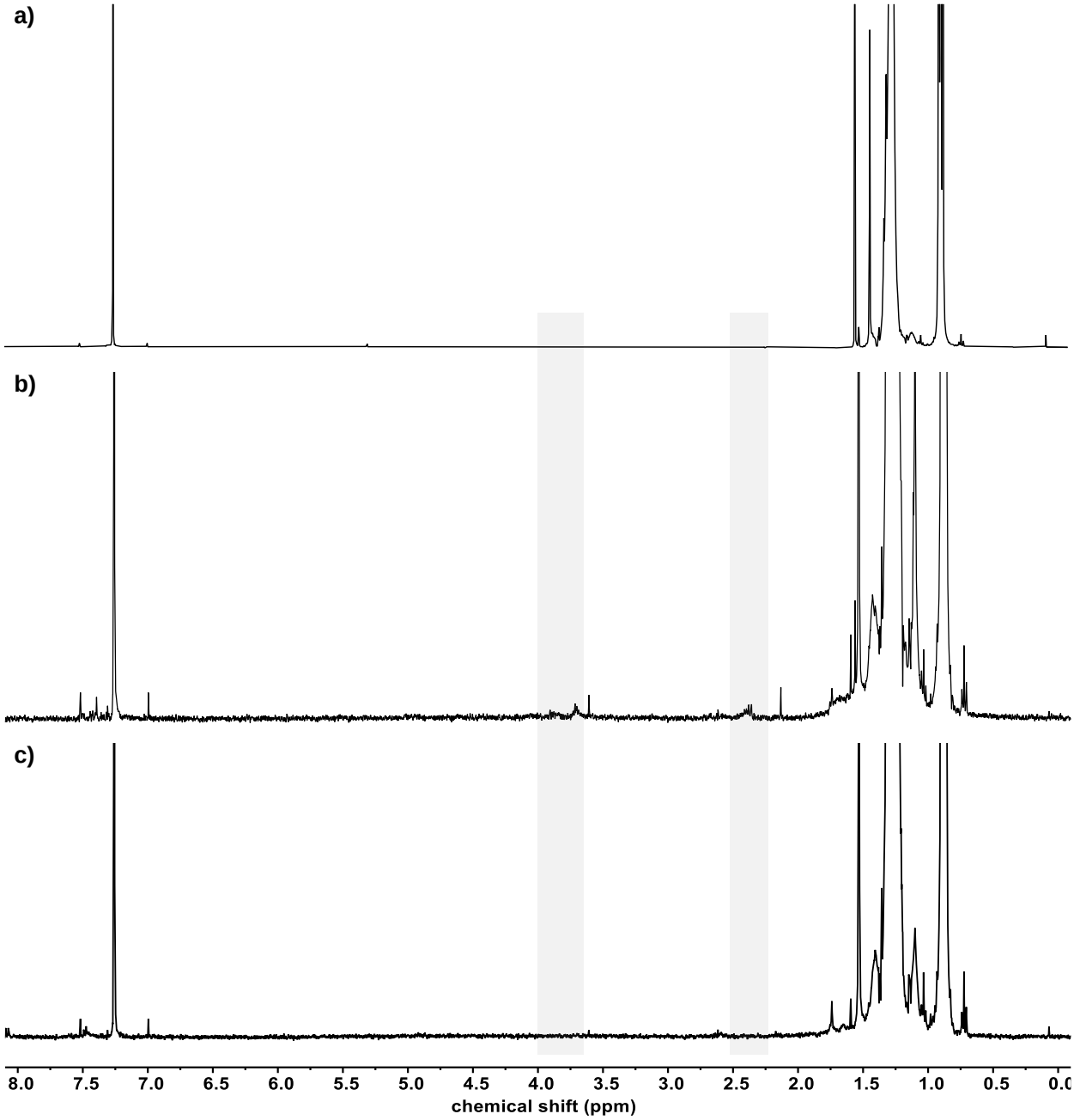



**Figure S3.** $^{1}H$ NMR spectra in $CDCl_3$ of a) C18, and the reaction conducted on C18 for 22 h in the presence of 4 mol% of TEMPO and 2 mol% of either b) DCP or c) BPO. The areas highlighted in gray showed the peaks attributed to the grafting of TEMPO on the model molecules.

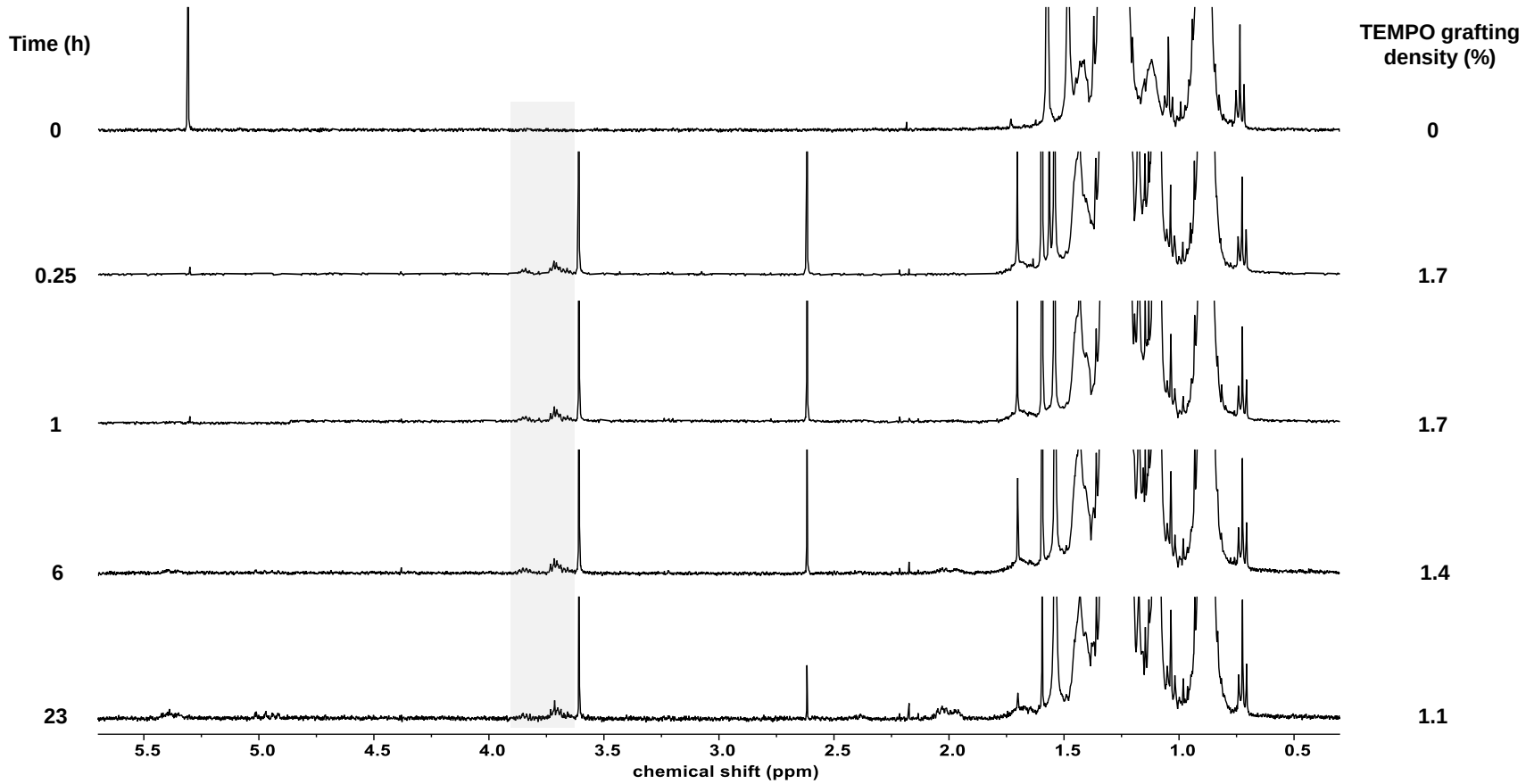



**Figure S4.** Monitoring of the formation of TEMPO-grafted C12 (4 mol% TEMPO, 2 mol% DCP, 150 °C) by $^{1}$H NMR spectroscopy ($CDCl_3$) over time. The area highlighted in gray shows the peak corresponding to the proton on the aliphatic chain on which TEMPO is grafted. The decrease of grafting density in TEMPO over time was attributed to the elimination of TEMPO leading to the formation of unsaturations observed between 4.8 and 5.6 ppm.

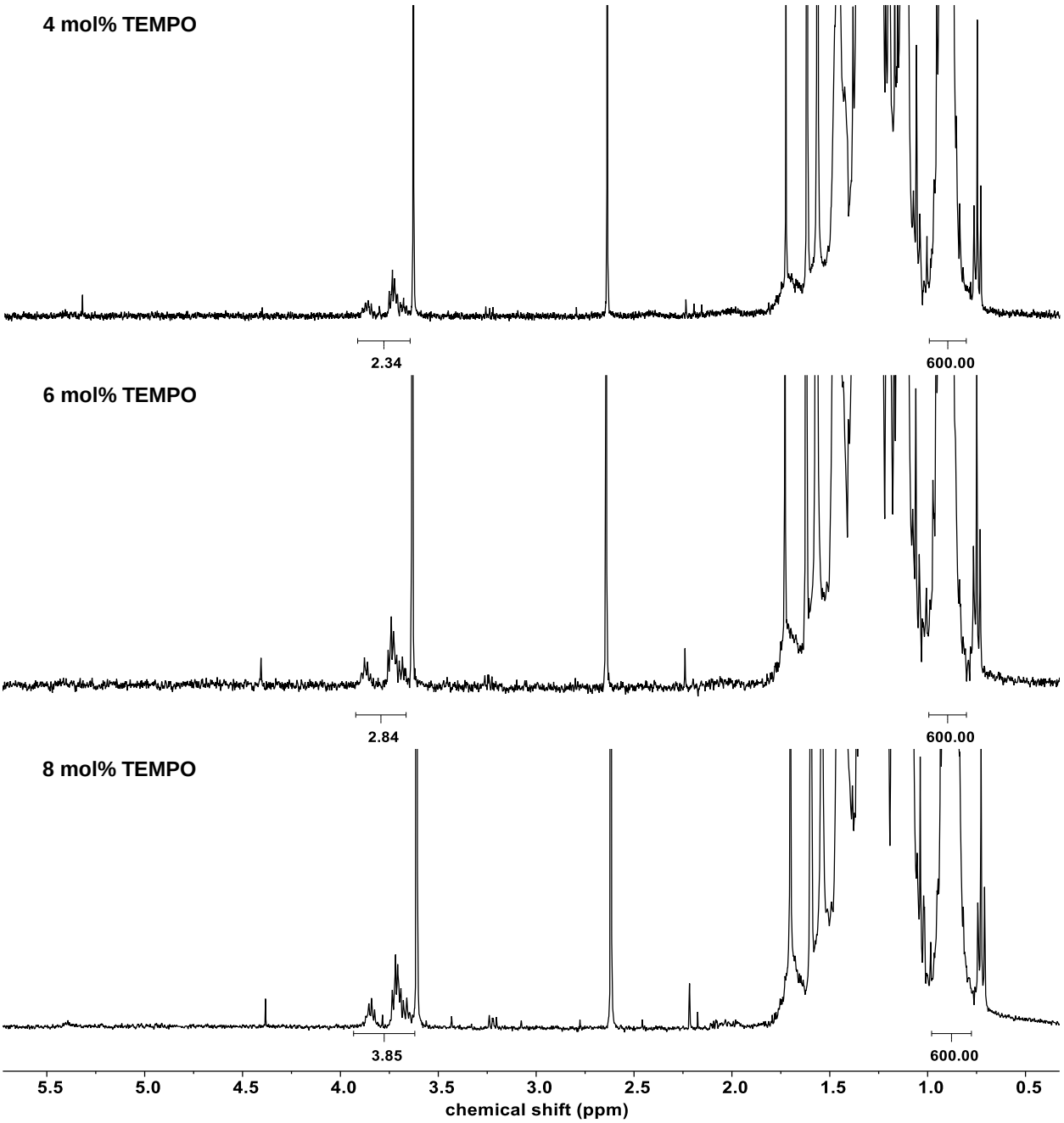



**Figure S5.** Effect of the concentration in TEMPO ([TEMPO]:[DCP] = 2:1, 150 °C, 1 h) on its grafting on C12 by $^{1}H$ NMR spectroscopy ($CDCl_3$).

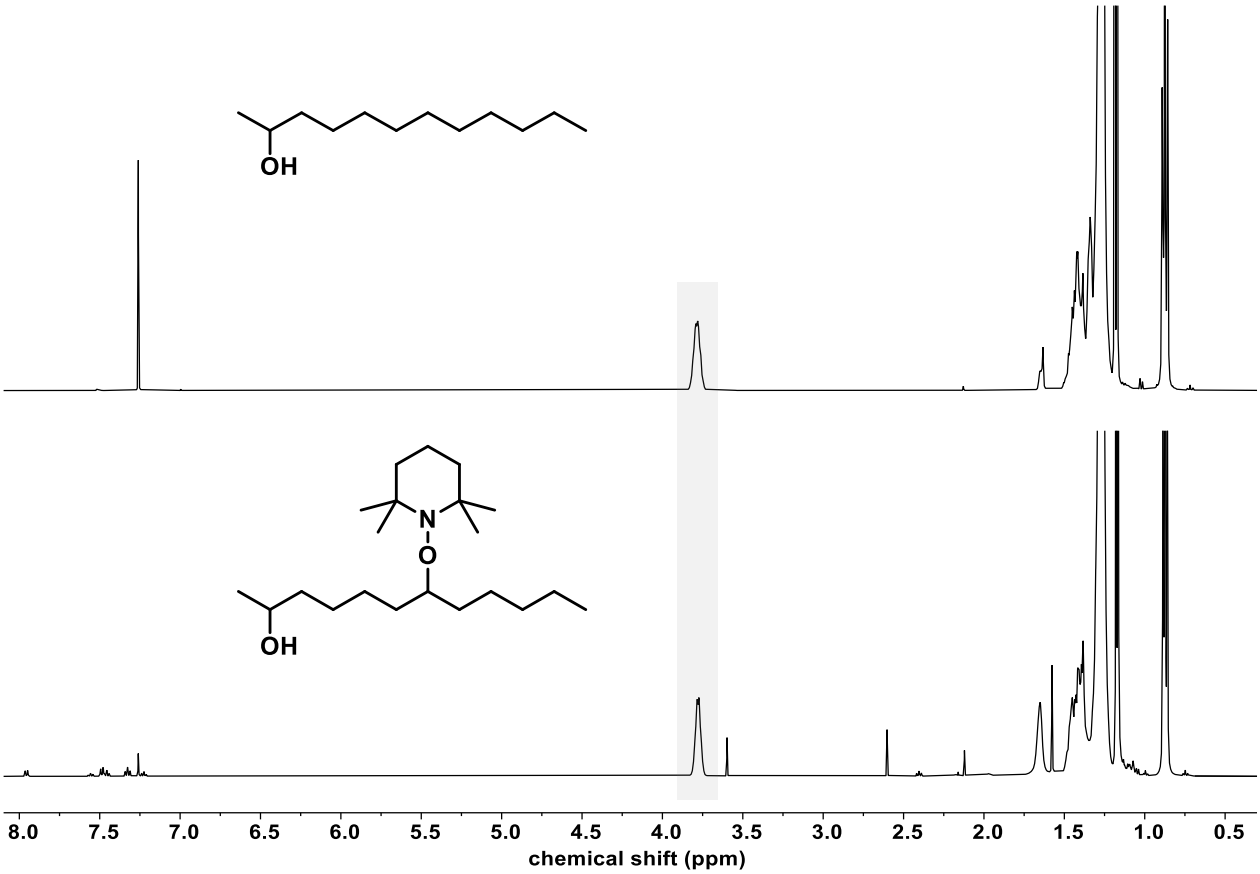



**Figure S6.** $^{1}H$ NMR spectra ($CDCl_3$) of 2-undecanol (top) and the product obtained after reaction with TEMPO (4 mol%) and DCP (2 mol%) at 150 °C (bottom). The area highlighted in gray shows the area in which was expected the peak of the proton on the carbon on which TEMPO would be grafted. The structure of TEMPO-grafted C11-OH was drawn with TEMPO in the center, but it could be on any carbon of the aliphatic chain.

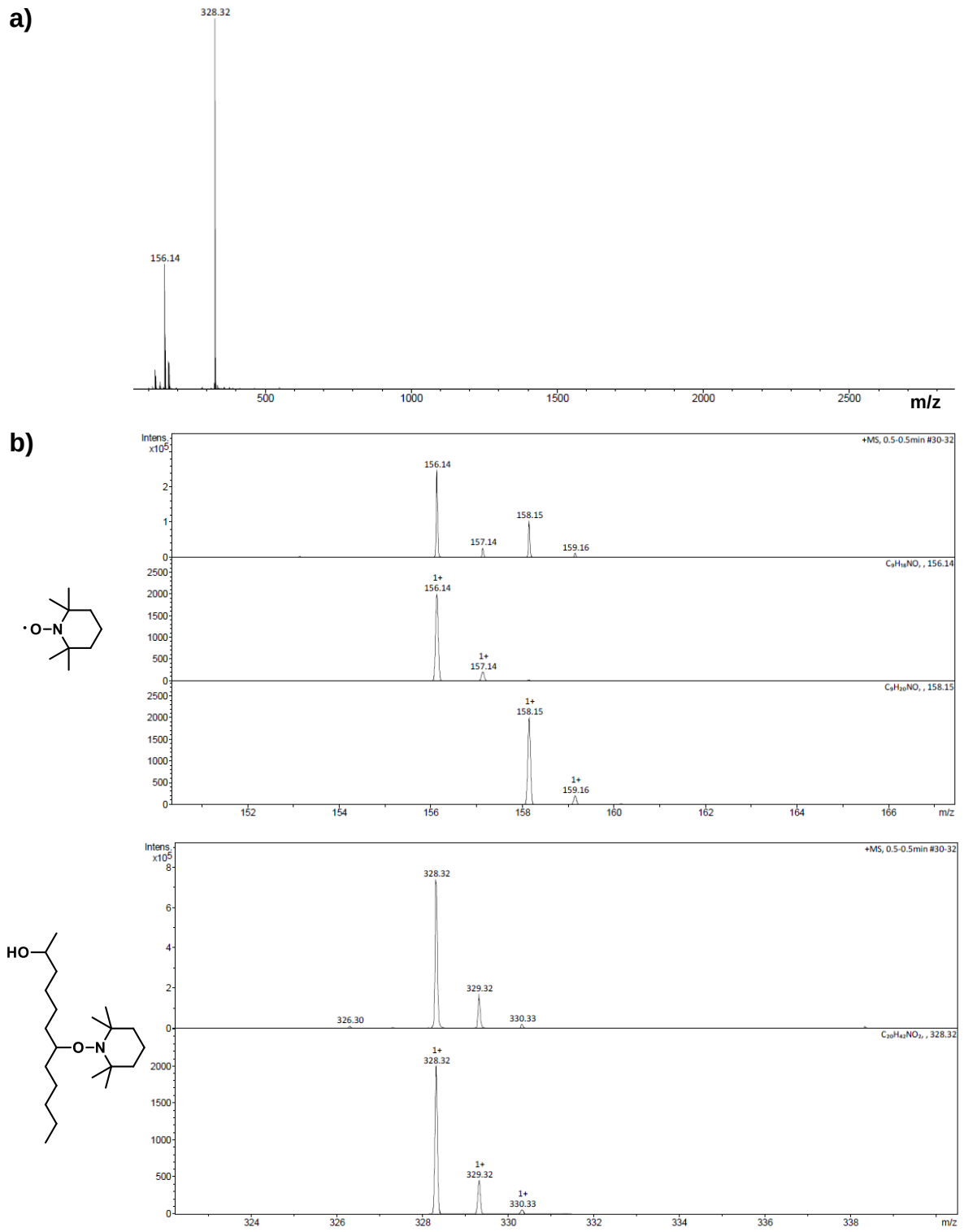



**Figure S7.** Mass spectrum and zooms on the molecular peaks obtained by ESI-MS of the reaction of 2-undecanol with 4 mol% TEMPO and 2 mol% DCP at 150 °C after 1 h. For each molecular peak, the spectrum on the top corresponds to the experimental one, and on the bottom the simulated one according to the molecular formula. The structure of TEMPO-grafted C11-OH as drawn with TEMPO in the center, but it could be on any carbon of the aliphatic chain.

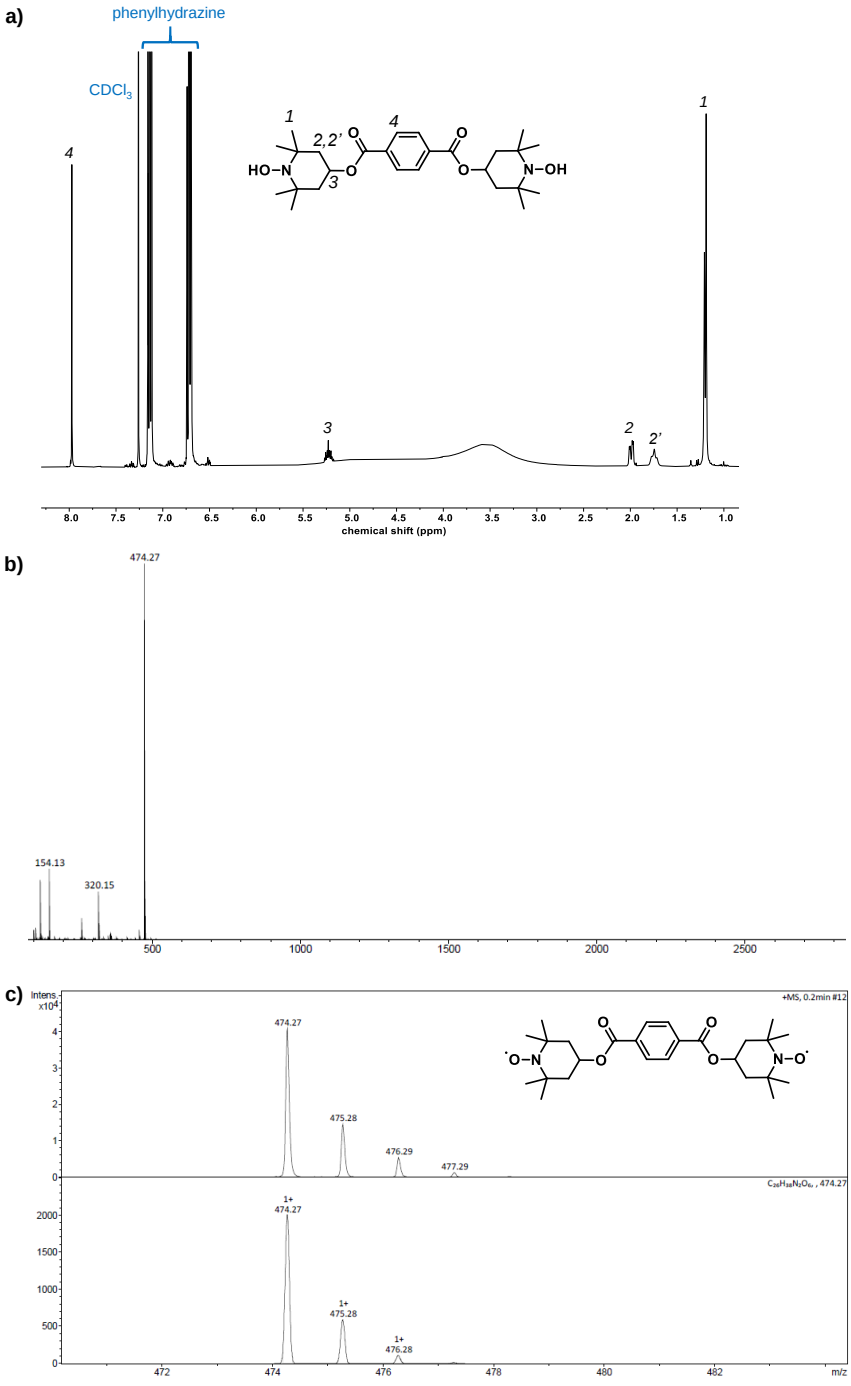



**Figure S8.** diTEMPO: a) $^{1}H$ NMR spectrum in $CDCl_3$ upon addition of one drop of phenylhydrazine and b) mass spectrum by ESI-MS (the spectrum on the top corresponds to the experimental one, and on the bottom the simulated one according to the molecular formula).

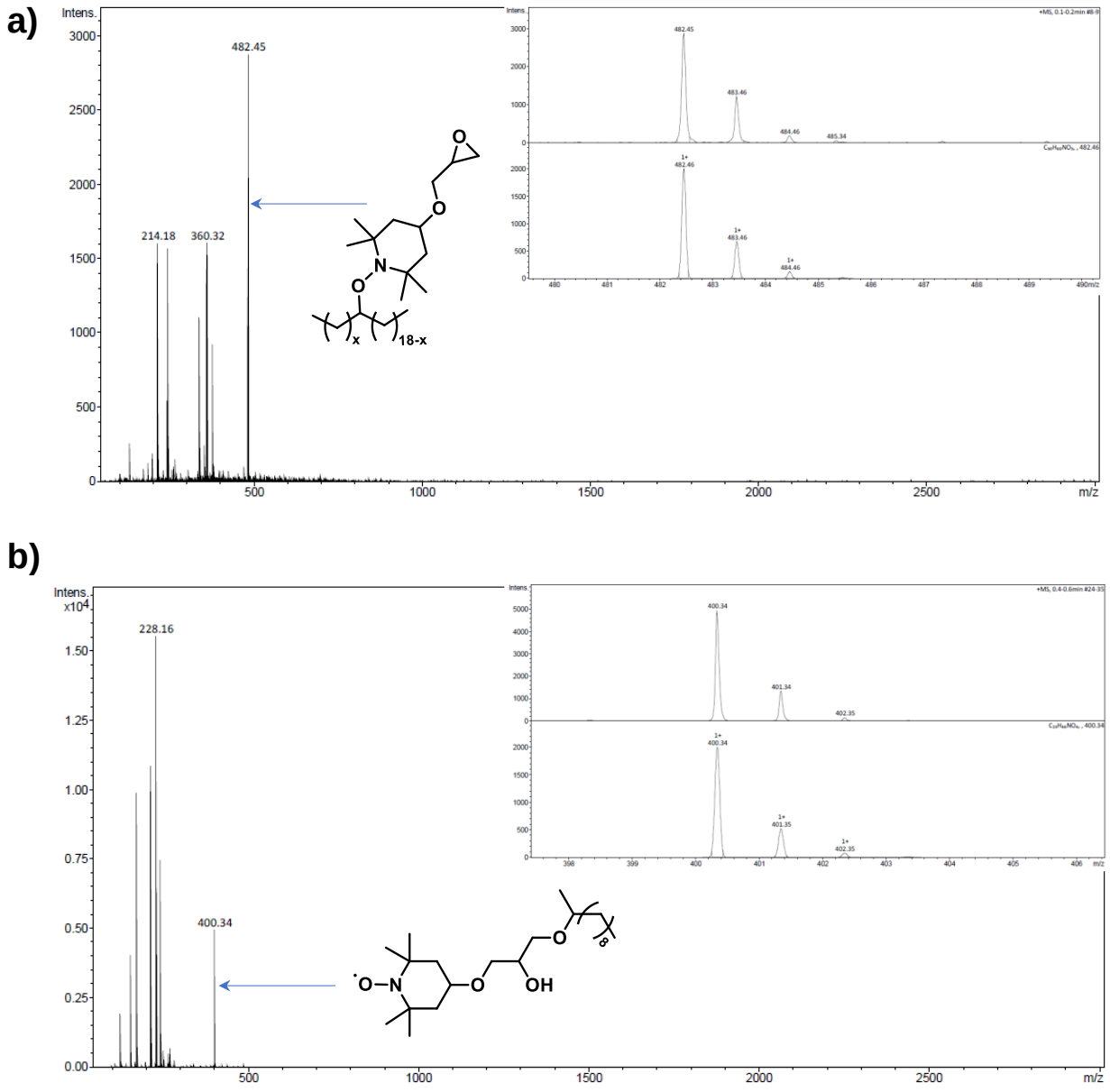



**Figure S9.** Mass spectra of the reaction crude product of TEMPO-epoxy (4 mol%) in the presence of DCP (2 mol%) at 150 °C for 15 min for a) C18 and b) C11-OH. For each molecular peak in inset, the spectrum on the top corresponds to the experimental one, and on the bottom the simulated one according to the molecular formula.