The search for rigid, tough polyesters with high T_g - Renewable aromatic polyesters with high isosorbide content

Bruno Bottega Pergher[a] , Daniel H. Weinland[a] , Robert-Jan van Putten[b] and Gert-Jan M. Gruter[*a,b]

Supporting information

a. Industrial Sustainable Chemistry, van 't Hoff Institute of molecular sciences, University of Amsterdam, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands.

b. *Avantium N.V., Zekeringstraat 29, 1014 BV Amsterdam, The Netherlands;†*

* corresponding author: G.J.M.Gruter@uva.nl

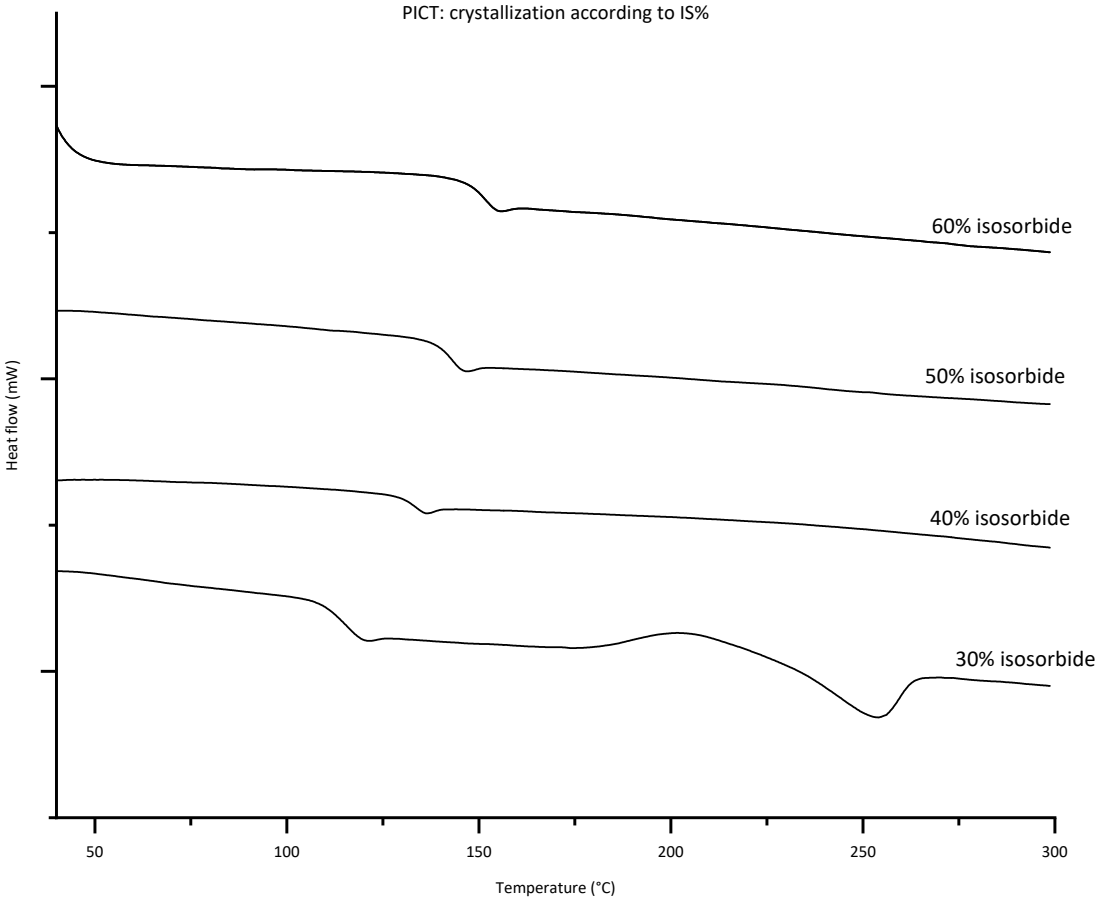
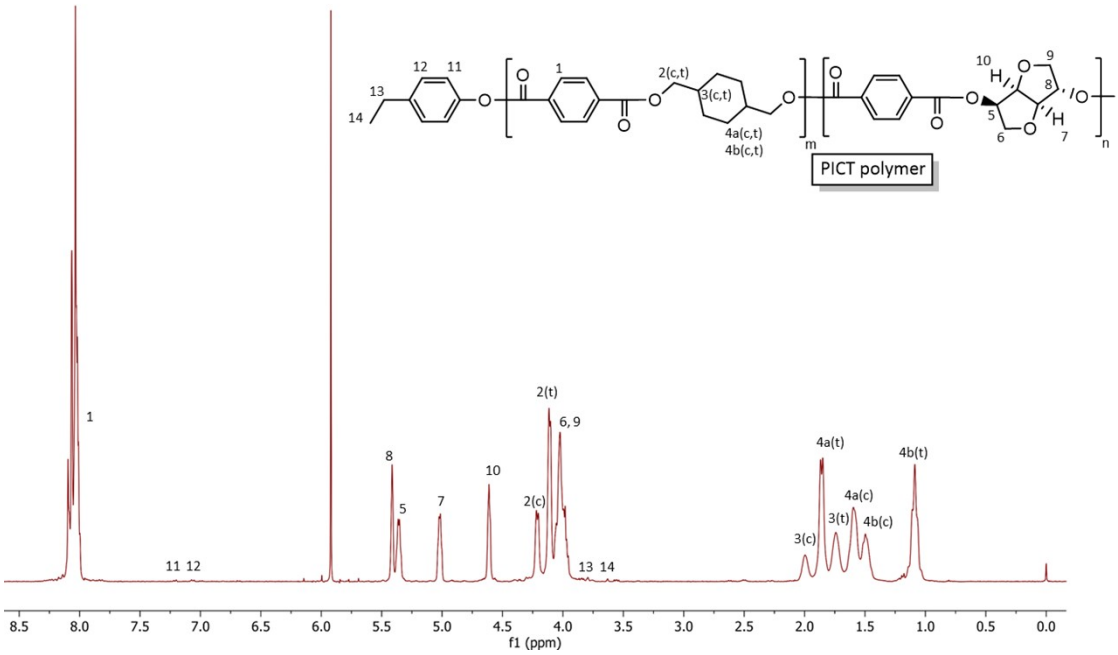
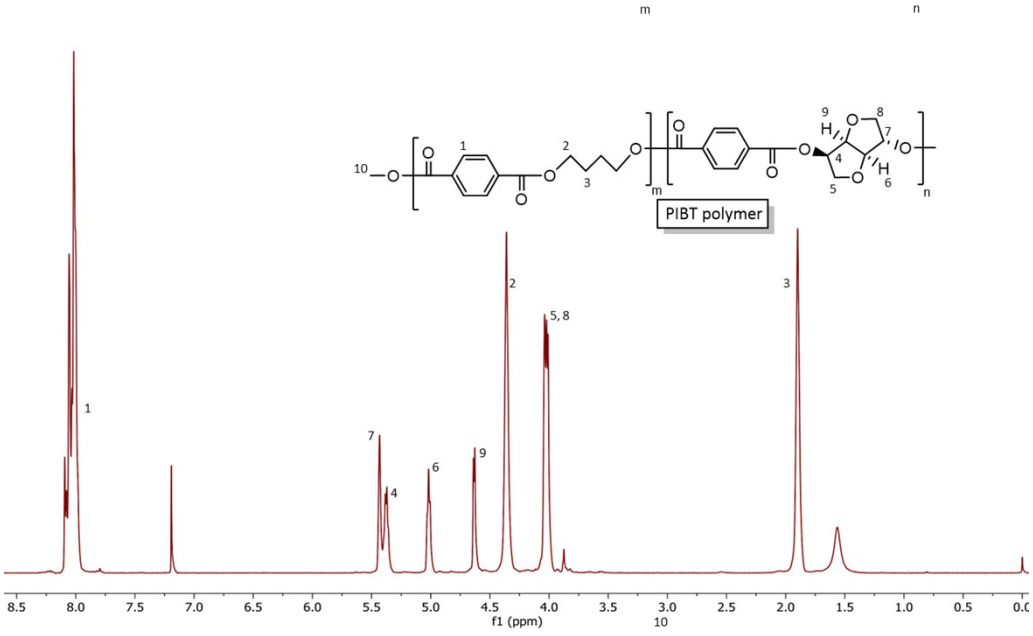
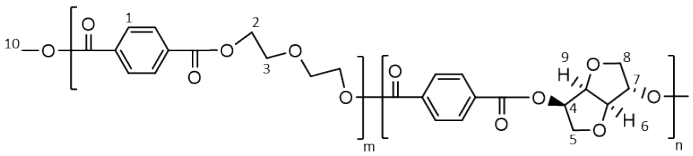


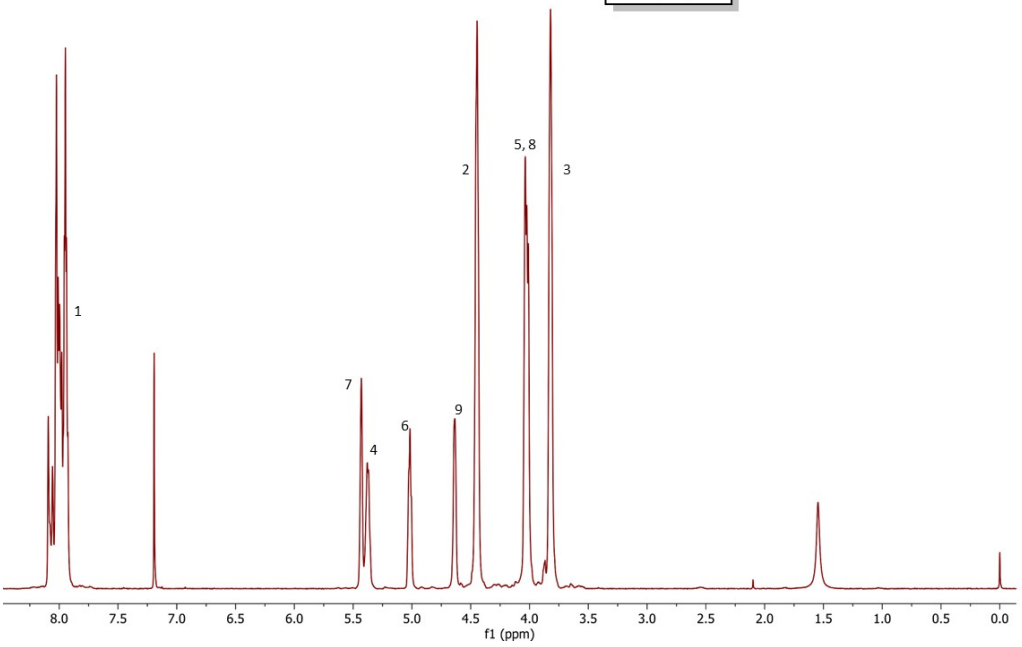
Figure 1 - DSC graphs of PICT with different isosorbide composition.

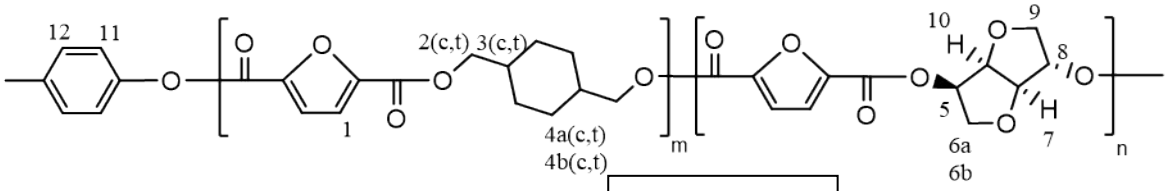

PICT polymer
f1 (ppm)


PIBT polymer
f1 (ppm)

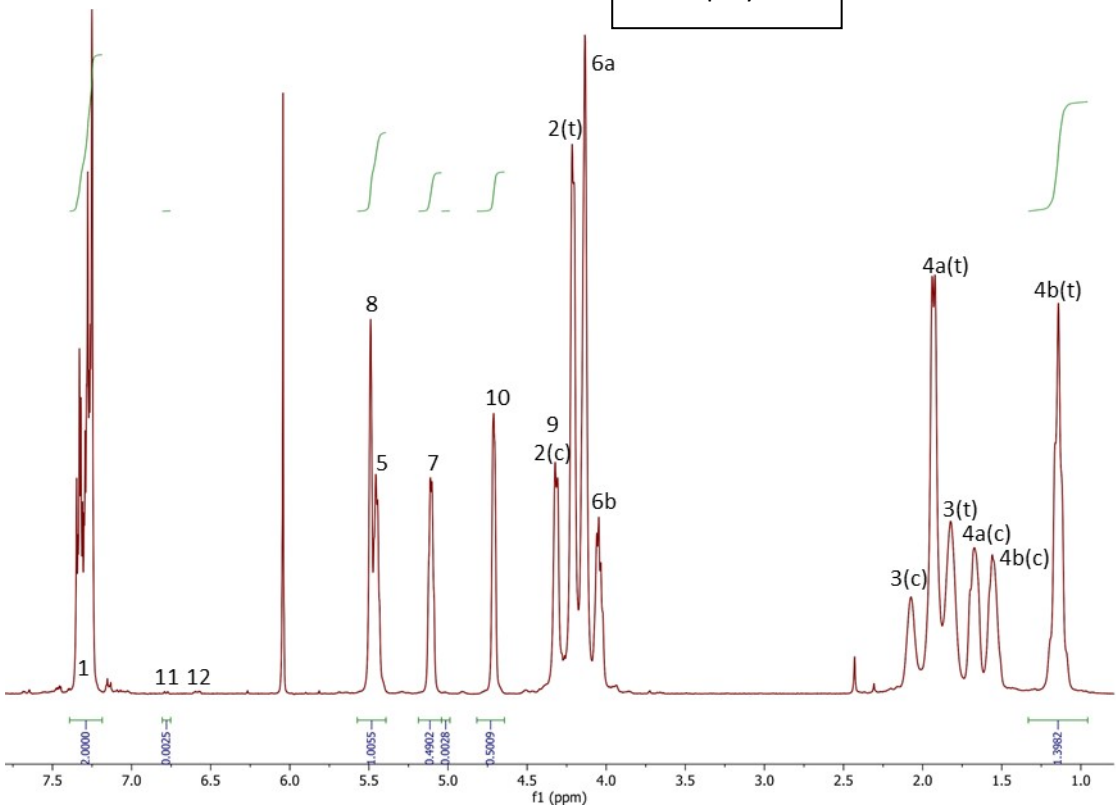


PIDT polymer





PICF polymer



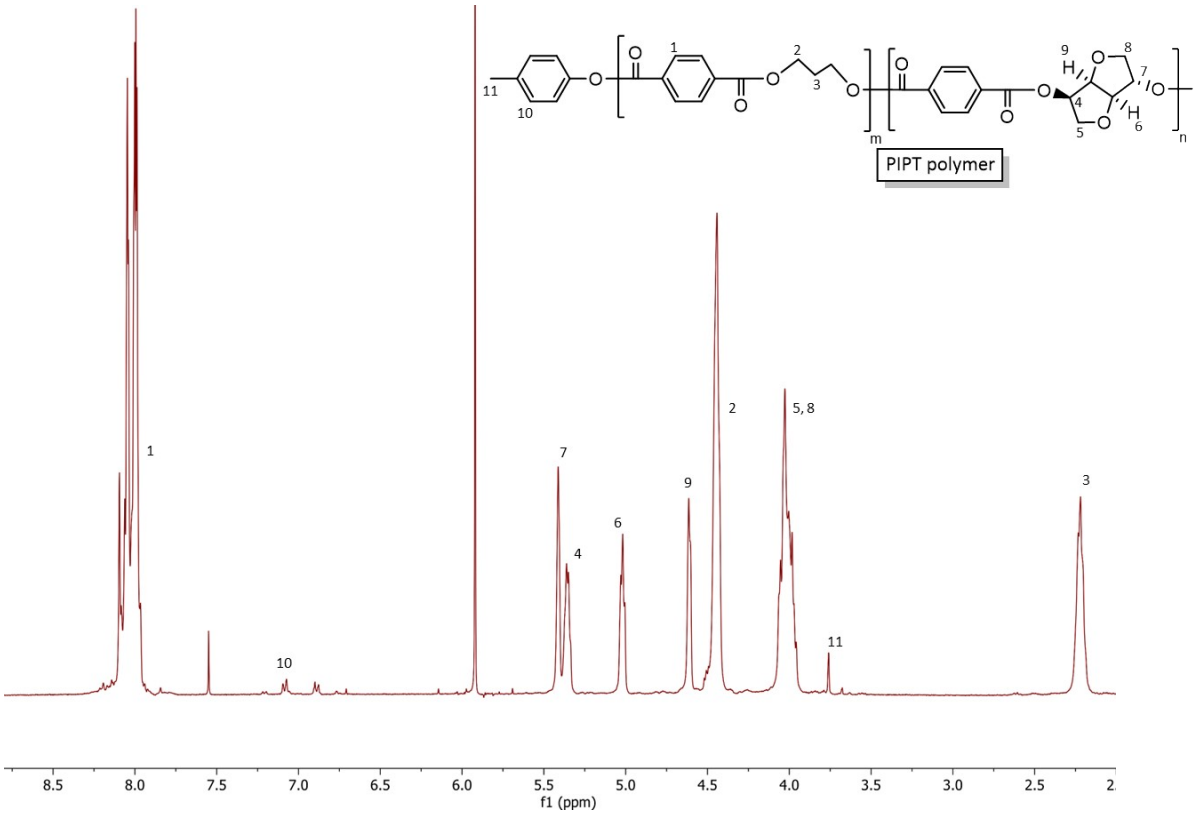
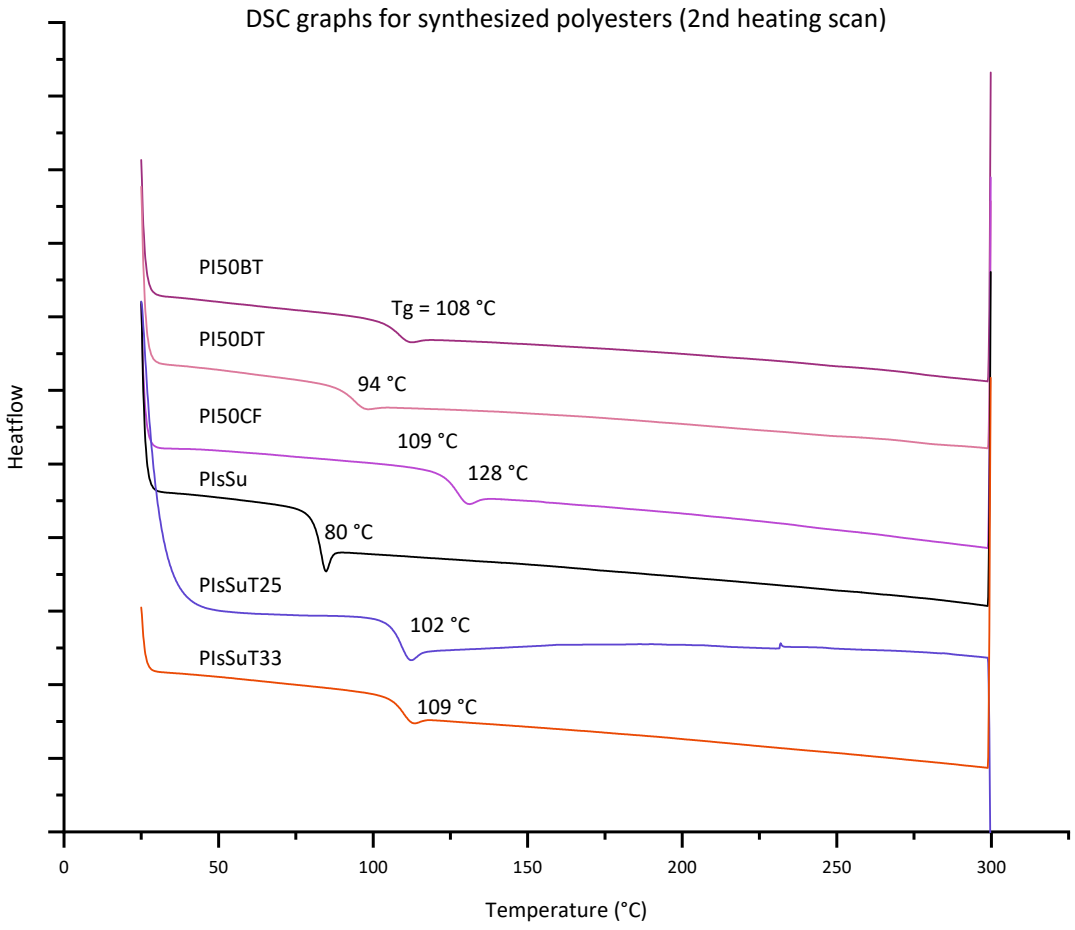


Figure 2 - Proton NMR of synthesized polyesters.



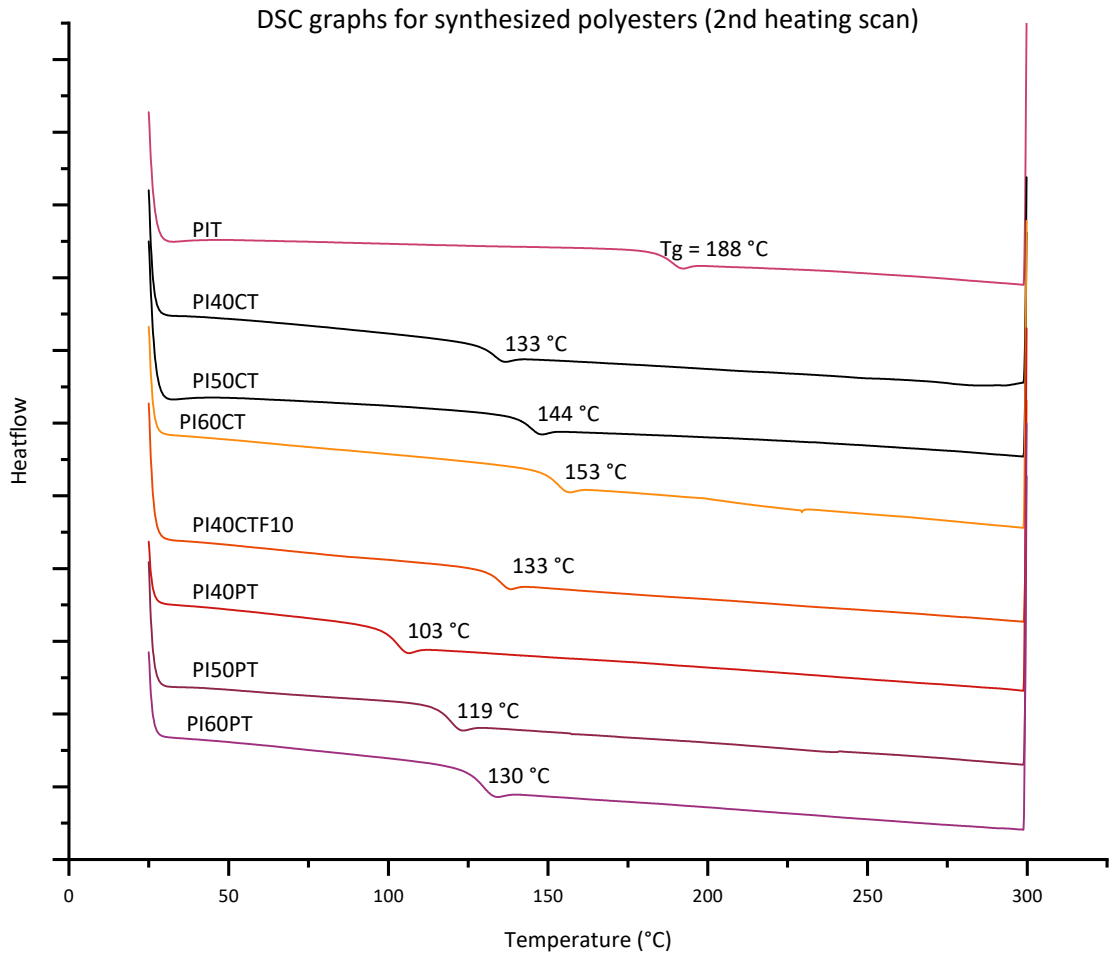
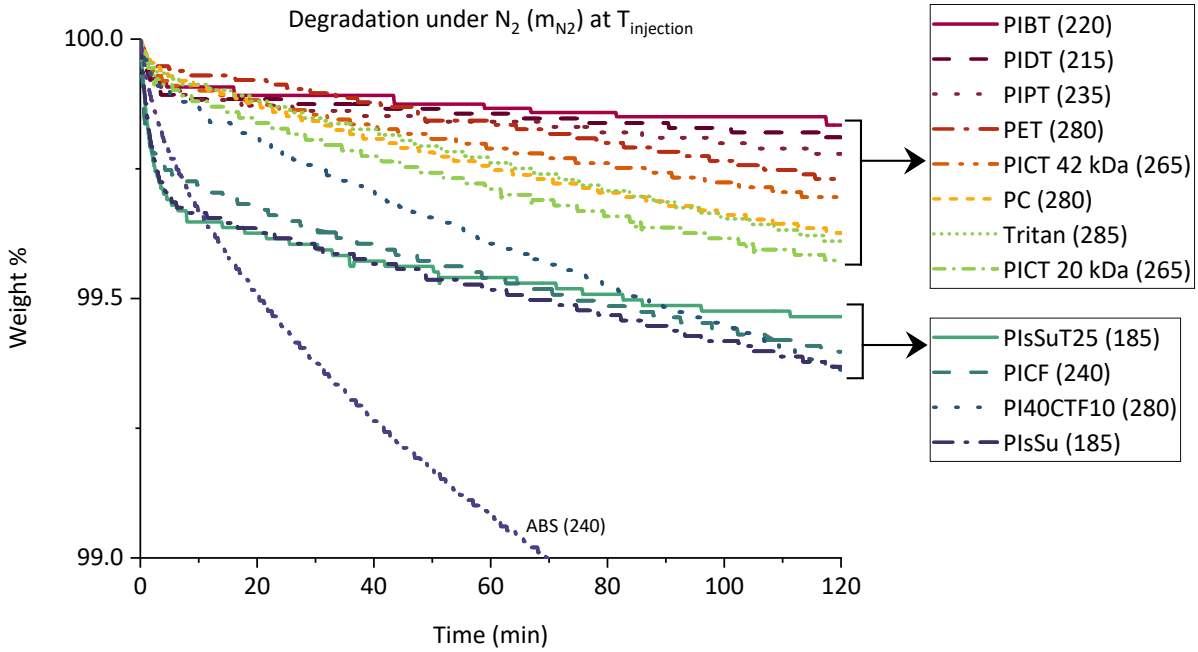


Figure 4 - DSC scans (2nd heating) for synthesized polyesters, with T_g indicated.



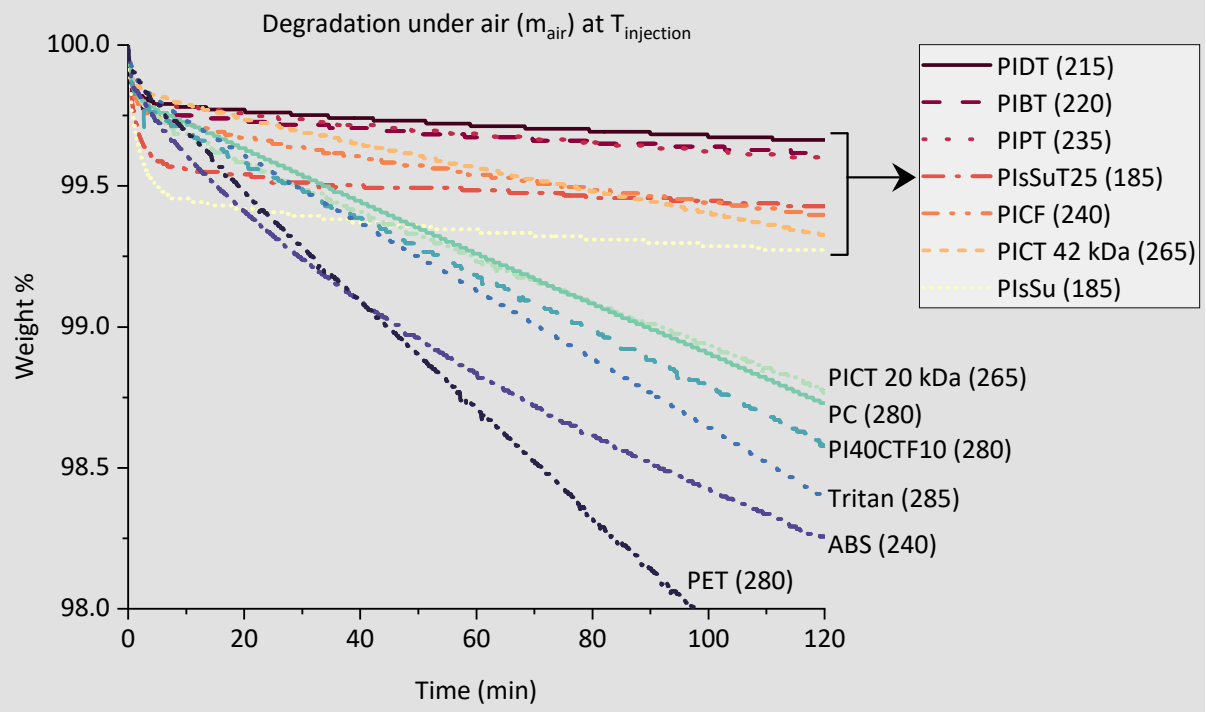
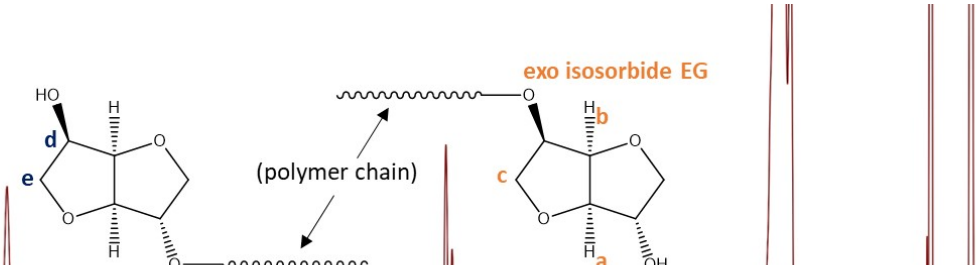


Figure 4 - TGA stability of samples under air (first graph) and nitrogen flow (second). Injection temperatures shown in brackets.



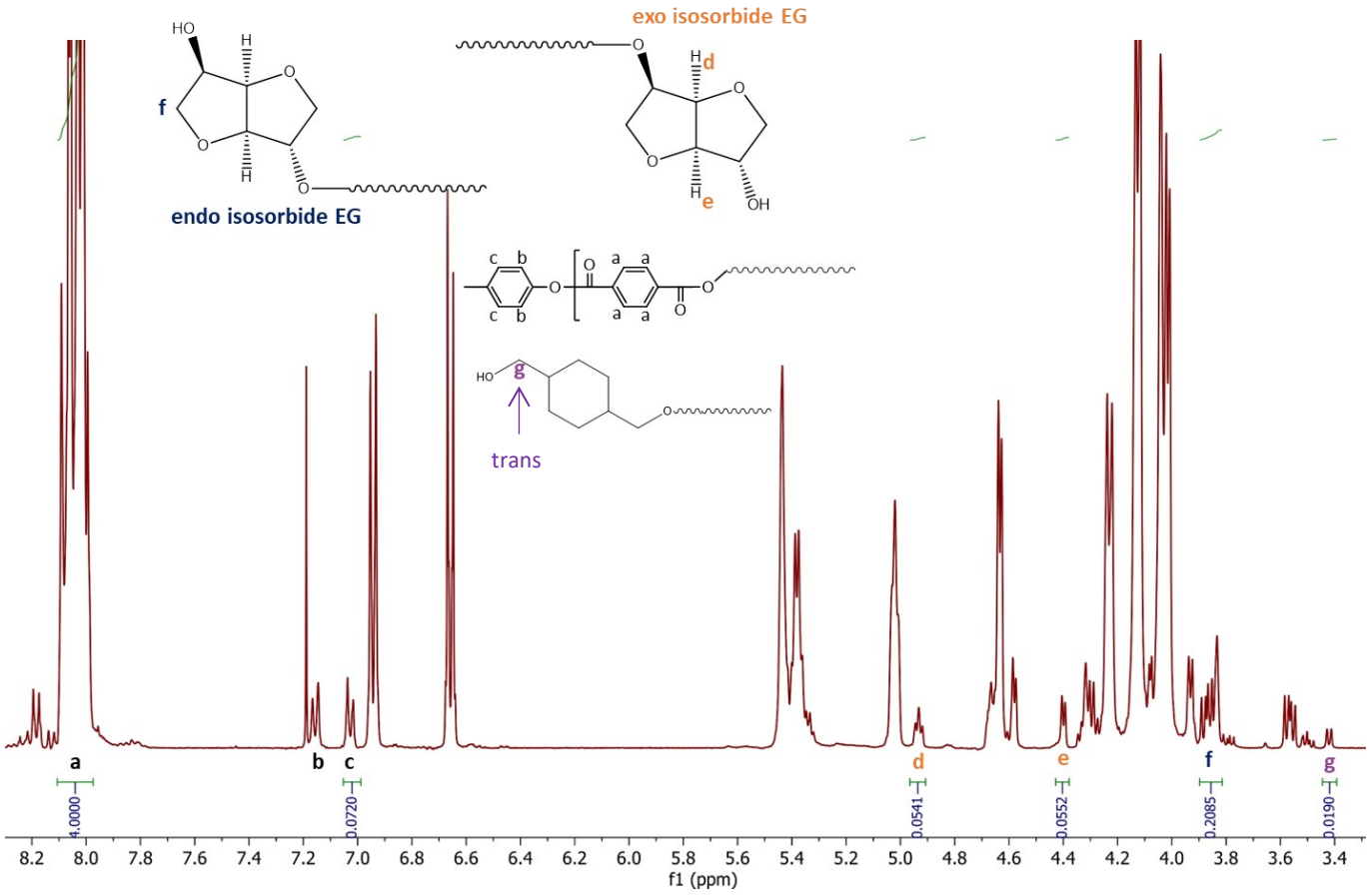


Figure 6 - End groups in PICT highlighted for calculation example. Same reaction as ^{13}C-NMR spectrum, in autoclave with 0.3 equivalent of p-cresol. Current time: 18 h of esterification (pre-vacuum). The integrals are normalized in comparison to the terephthalate group at 8.1 ppm, with 4 protons.This image can be used as an example of the calculations presented in the paper: peak ‘c’ has 2 protons, so a total of 3.60 mol% of end groups of p-cresol relative to the repeat unit. Analogously, ‘d’ and ‘e’ have 1 proton each, totaling ~5.4 mol% of isosorbide endo end groups and ‘f’ has two protons, which totals ~10.4 mol% of exo end groups – summing the two values, isosorbide end groups represent ~15.8 mol% compared to the repeat unit. At last, ‘g’ has 2 protons for the trans CHDM phase (70% of total), so in total 0.95 mol%/70% = 1.36 mol% total for CHDM.