Electronic Supplementary Information

Bio-based PBT copolyesters derived from D-glucose: influence of composition on properties

Cristina Japu,[a] Antxon Martínez de Ilarduya,[a] Abdelilah Alla,[a]
Mª Gracia García-Martín,[b] Juan A. Galbis[b] and Sebastián Muñoz-Guerra[a*]

[a]Universitat Politècnica de Catalunya, ETSEIB, Diagonal 647, 08028 Barcelona, Spain
[b]Universidad de Sevilla, Facultad de Farmacia, Francisco García González s/n, Sevilla, Spain

Corresponding author: sebastian.munoz@upc.edu

SI-Fig. 1. ^{1}H-^{1}H COSY NMR spectrum of $PB_{69}Glux_{31}T$ copolyester.

SI-Fig. 2. ^{1}H-^{13}C HETCOR NMR spectra of $PB_{69}Glux_{31}T$ copolyester (top) amplified region and all (bottom).

SI-Fig. 3. ^{1}H (top) and ^{13}C (bottom) NMR spectra of $PB_{69}Glux_{31}T$ copolyester.

SI-Fig. 4. ^{1}H-^{1}H COSY NMR spectrum of $PBT_{67}Glux_{33}$ copolyester.

SI-Fig. 5. ^{1}H-^{13}C HETCOR NMR spectra of $PBT_{67}Glux_{33}$ copolyester (top) all and (bottom) amplified region.

SI-Fig. 6. ^{1}H (top) and ^{13}C (bottom) NMR spectra of $PBT_{67}Glux_{33}$ copolyester.

SI-Fig. 7. DSC traces of PB_xGlux_yT (a) and PBT_xGlux_y (b) copolyesters recorded at heating from quenched samples for T_g observation.

SI-Fig. 8. Double logarithmic plots of the isothermal crystallization of $PB_{97}Glux_3T$, $PB_{94}Glux_6T$, $PB_{89}Glux_{11}T$, $PBT_{95}Glux_5$, $PBT_{90}Glux_{10}$ copolyesters and PBT homopolyester at the indicated temperatures.

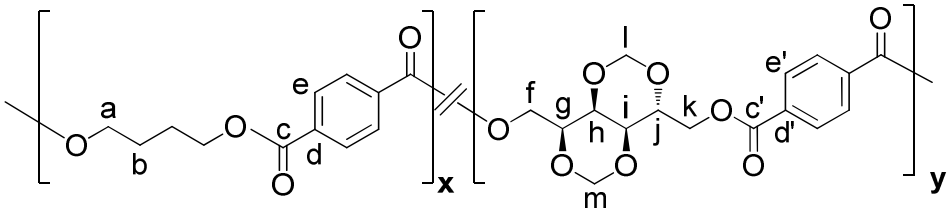
SI-Fig. 9. WAXS profiles of PB_xGlux_yT, PBT_xGlux_y copolymers and their parent homopolyesters recorded from powder samples without any previous thermal treatment.

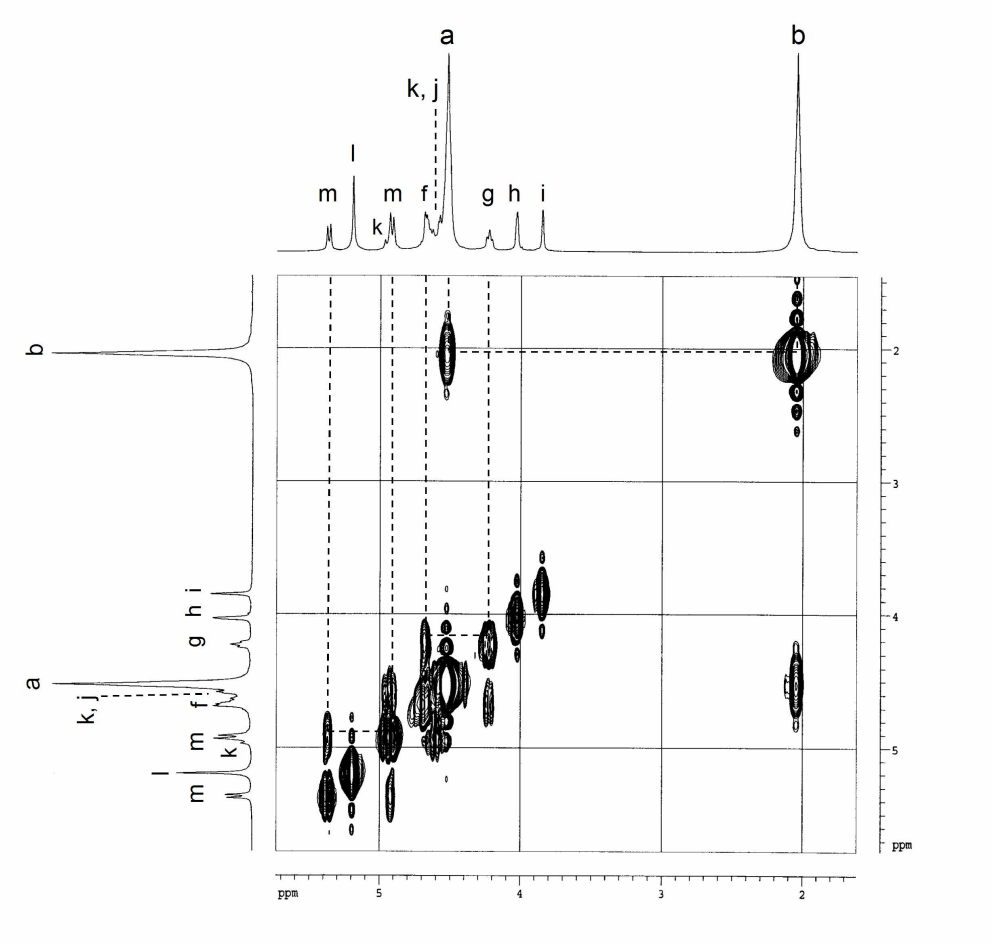
SI-Fig. 10. Compared ^{1}H NMR after incubation (residue) with water at pH 2.0 at 80 ºC and initial spectra of $PB_{59}Glux_{41}T$ (a) and $PBT_{55}Glux_{45}$ (b) copolyesters.

SI-Fig. 11. ^{1}H NMR spectra in D_2O of the products released to the aqueous medium after incubation of $PBT_{55}Glux_{45}$ at pH 2.0 at 80 ºC for four weeks.

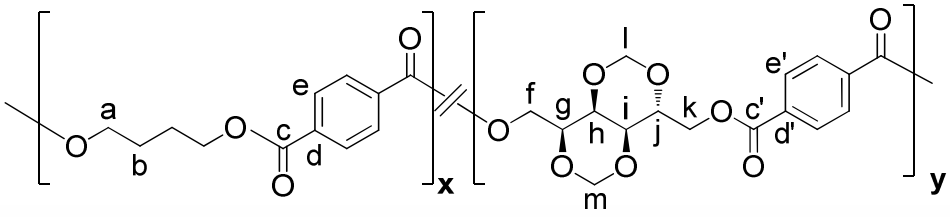
SI-Table 1. Powder X-ray diffraction data of polyesters.

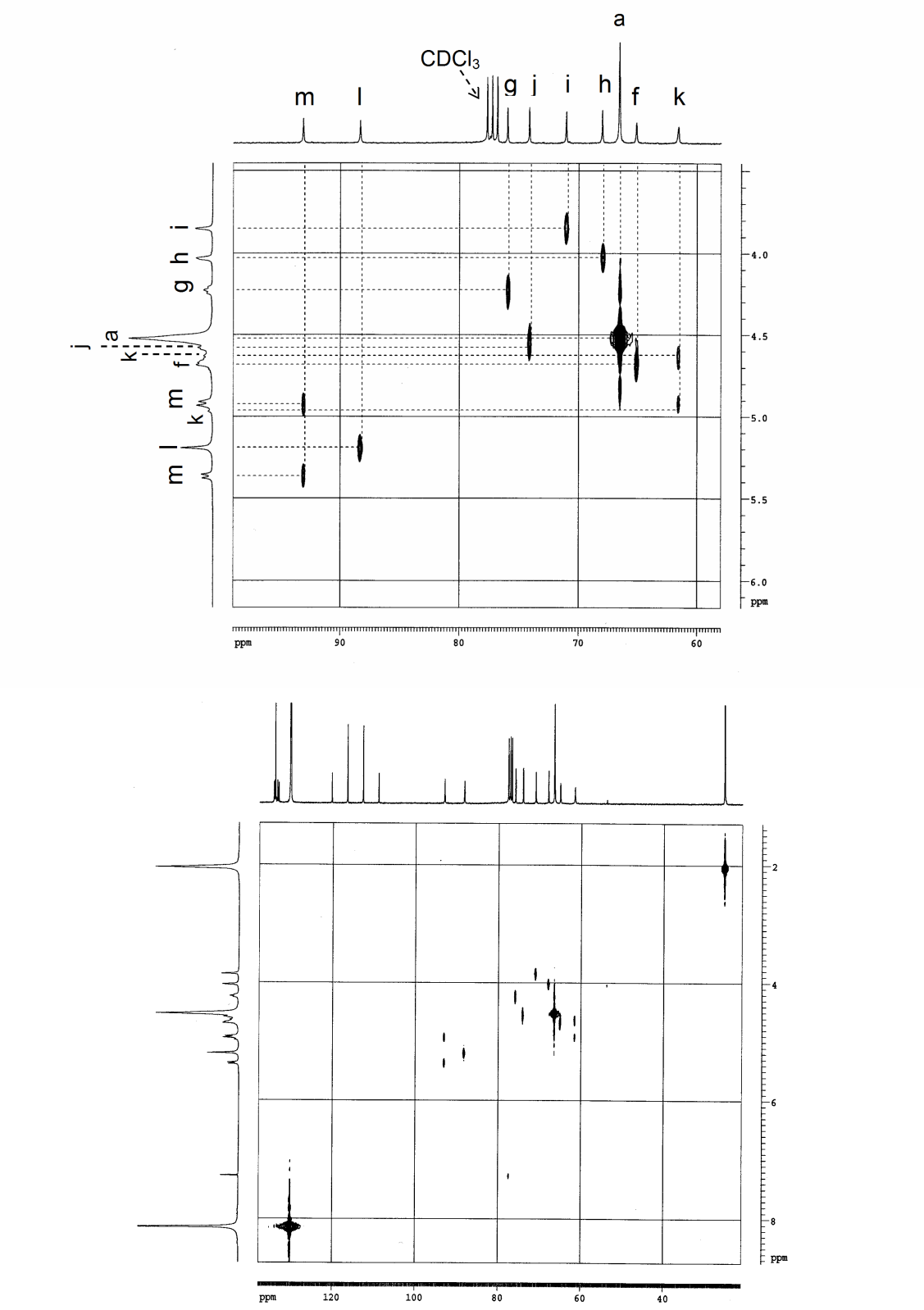
SI-Table 2. Mechanical properties.



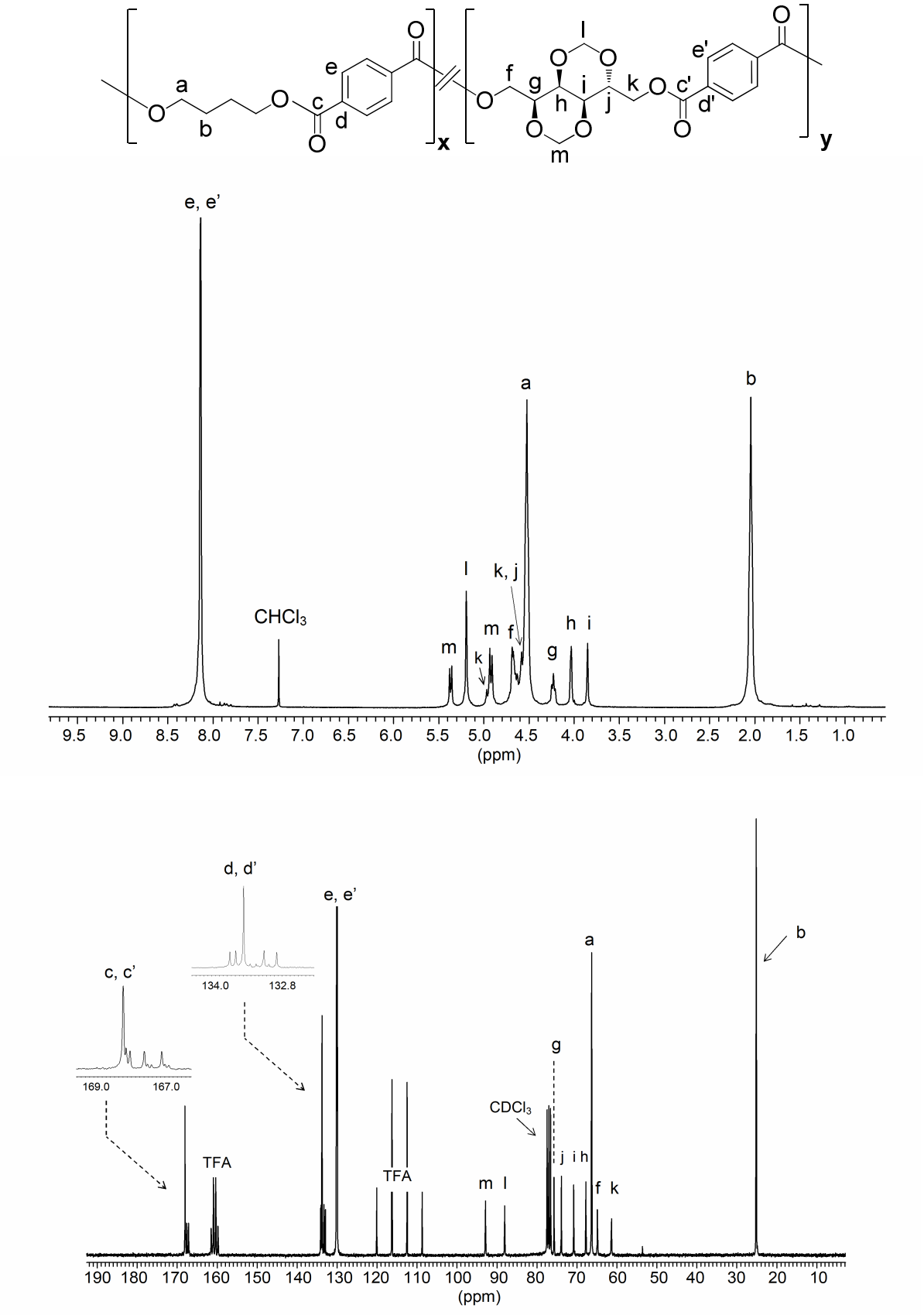


SI-Fig. 1. ^{1}H-^{1}H COSY NMR spectrum of $PB_{69}Glux_{31}T$ copolyester.

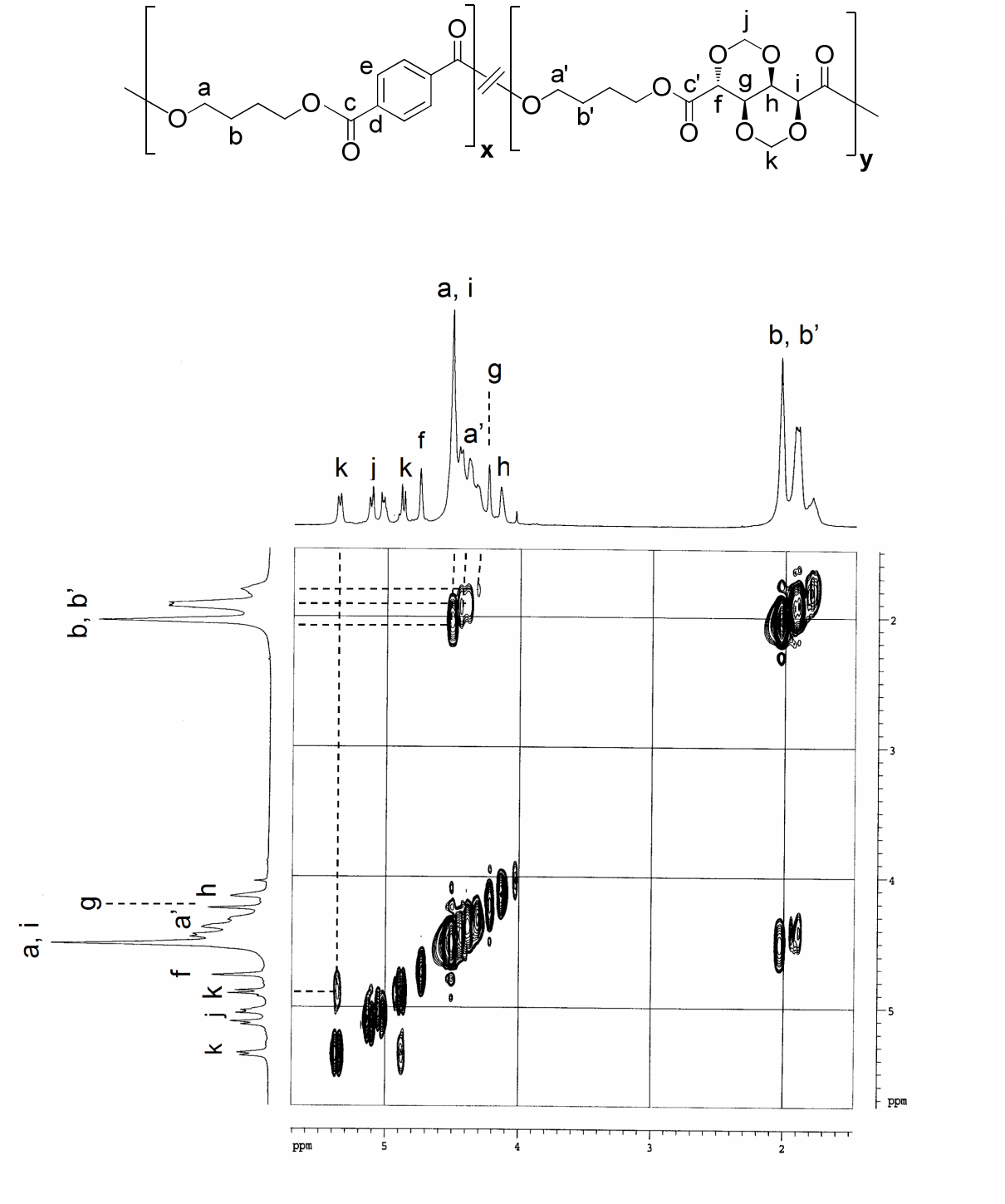




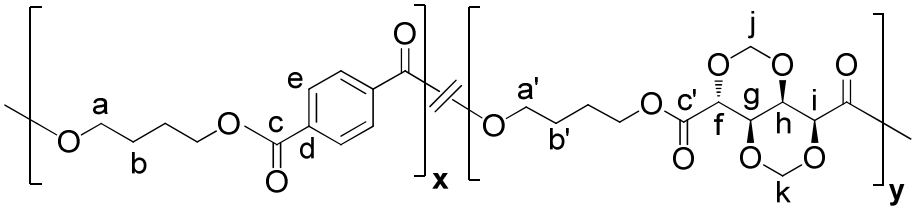
SI-Fig. 2. ^{1}H-^{13}C HETCOR NMR spectrum of $PB_{69}Glux_{31}T$ copolyester (bottom) and enlarged region (top).

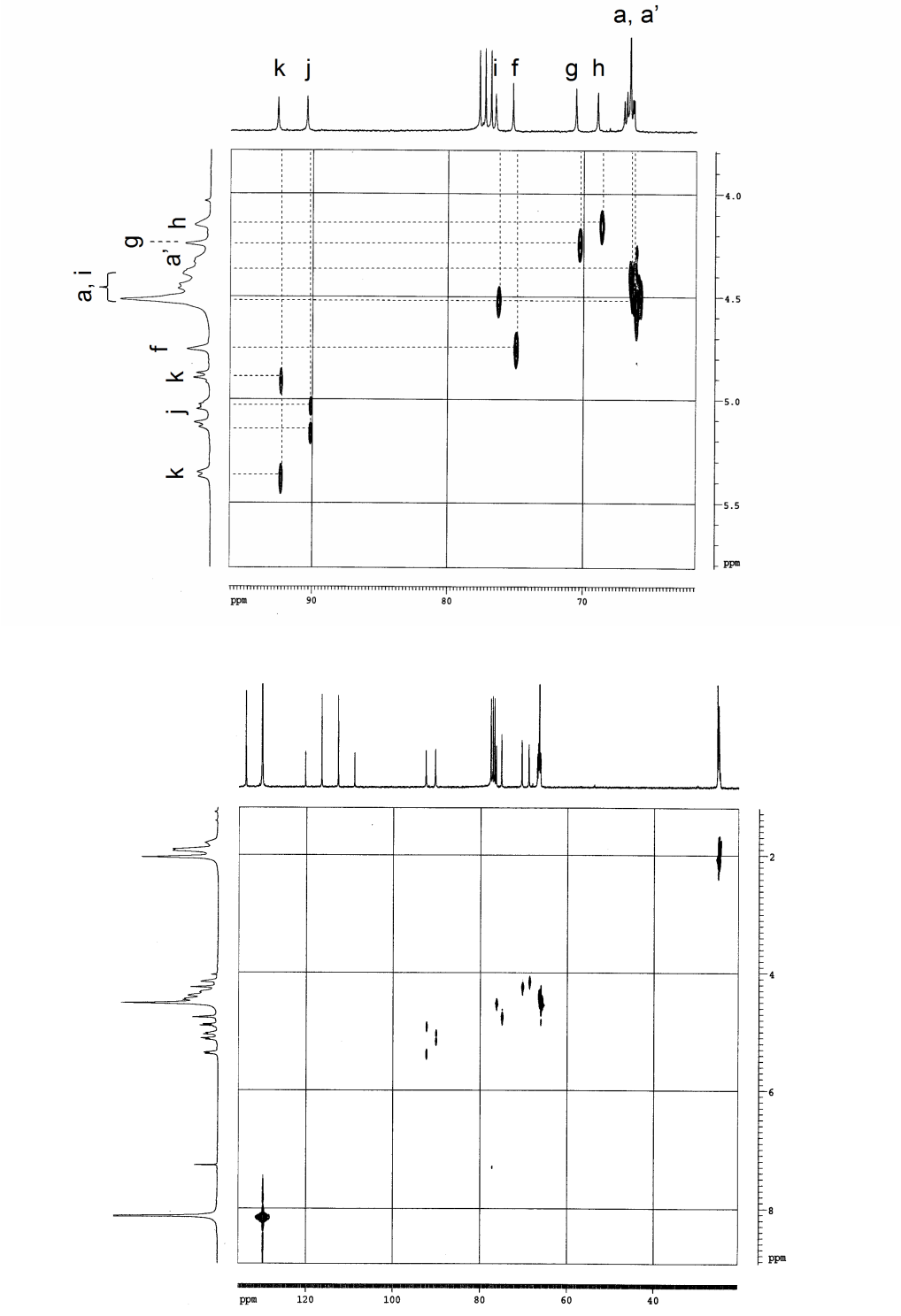


SI-Fig. 3. ^{1}H (top) and ^{13}C (bottom) NMR spectra of $PB_{69}Glux_{31}T$ copolyester.

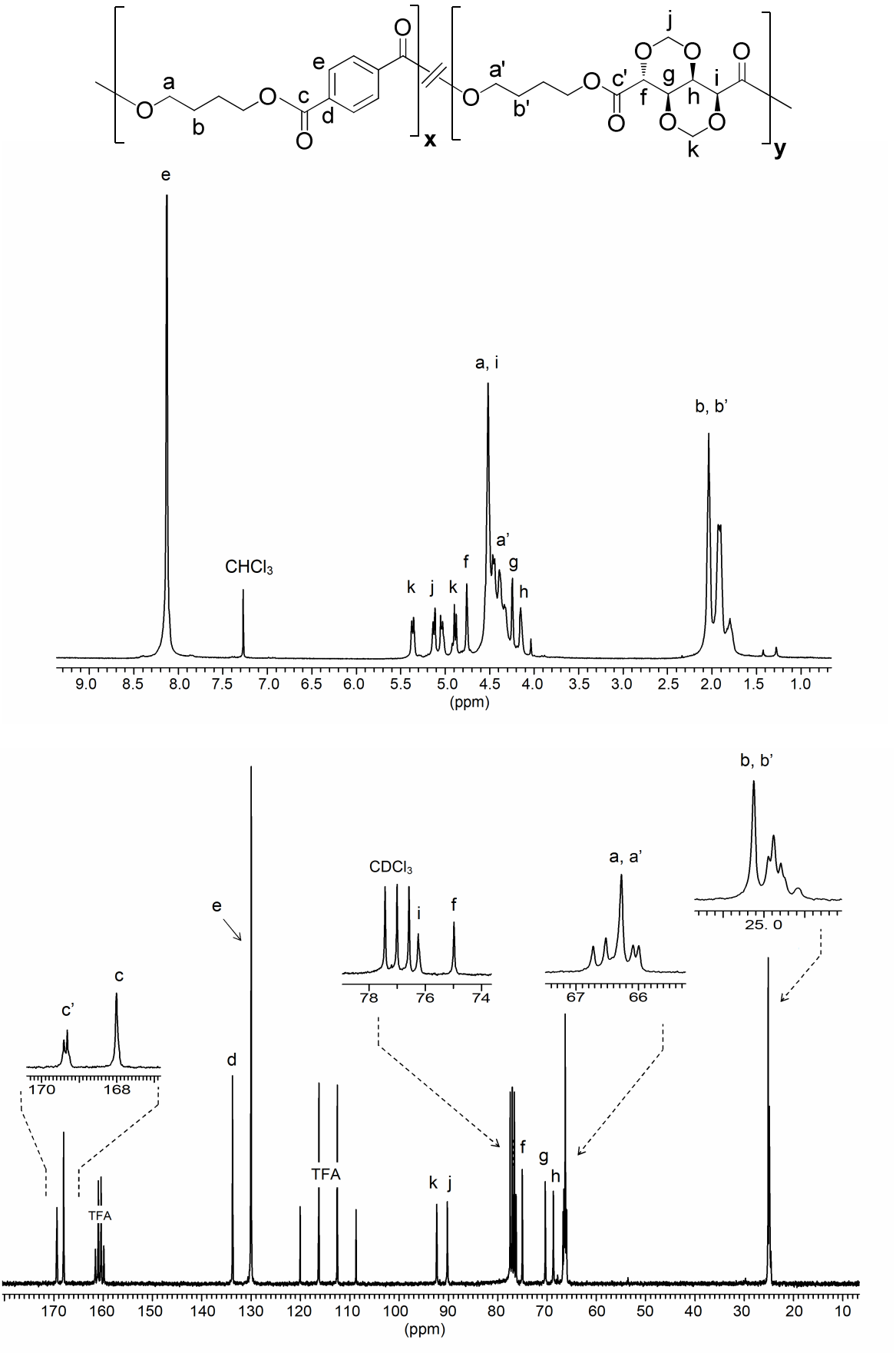


SI-Fig. 4. ^{1}H-^{1}H COSY NMR spectrum of $PBT_{67}Glux_{33}$ copolyester.

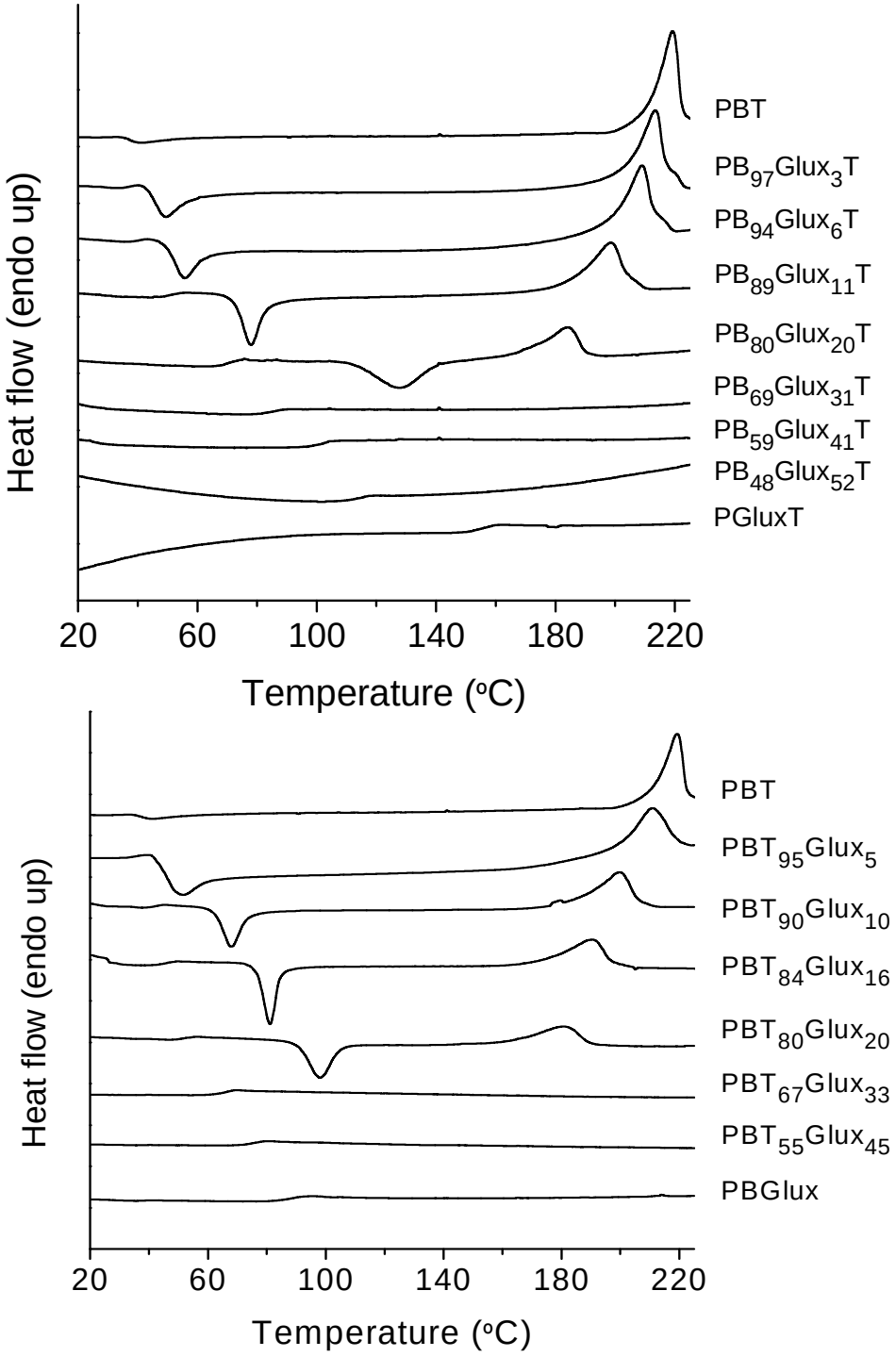




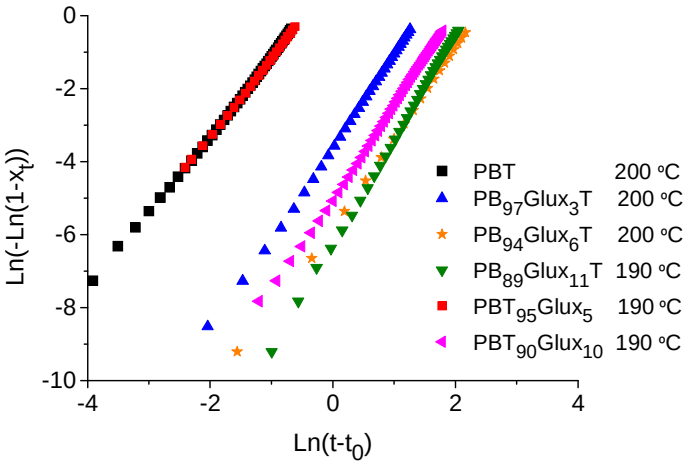
SI-Fig. 5. ^{1}H-^{13}C HETCOR NMR spectrum of $PBT_{67}Glux_{33}$ copolyester (top) and amplified region (bottom).



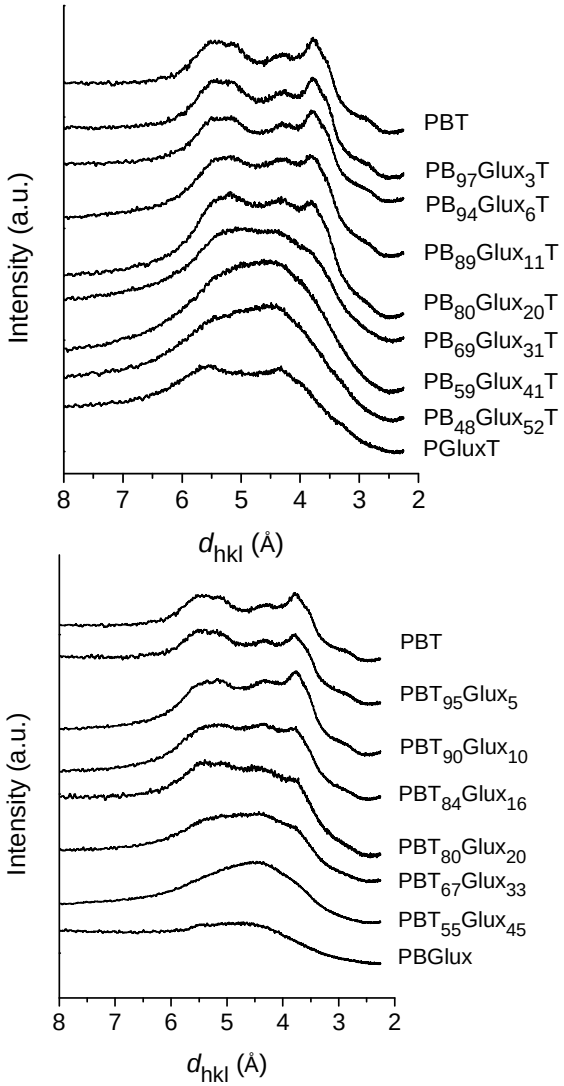
SI-Fig. 6. ^{1}H (top) and ^{13}C (bottom) NMR spectra of $PBT_{67}Glux_{33}$ copolyester.



SI-Fig. 7. DSC traces of PB_xGlux_yT (a) and PBT_xGlux_y (b) copolyesters recorded at heating from quenched samples for T_g observation.

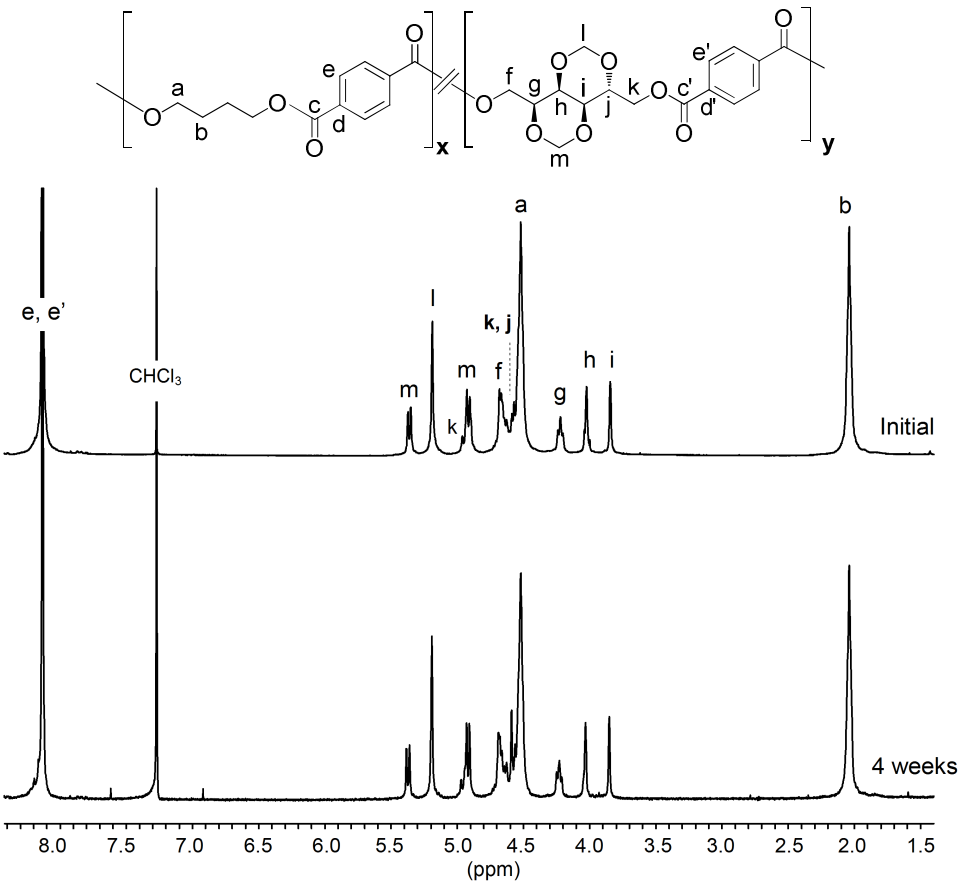


SI-Fig. 8. Double logarithmic plots of the isothermal crystallization of $PB_{97}Glux_3T$, $PB_{94}Glux_6T$, $PB_{89}Glux_{11}T$, $PBT_{95}Glux_5$, $PBT_{90}Glux_{10}$ copolyesters and PBT homopolyester at the indicated temperatures.

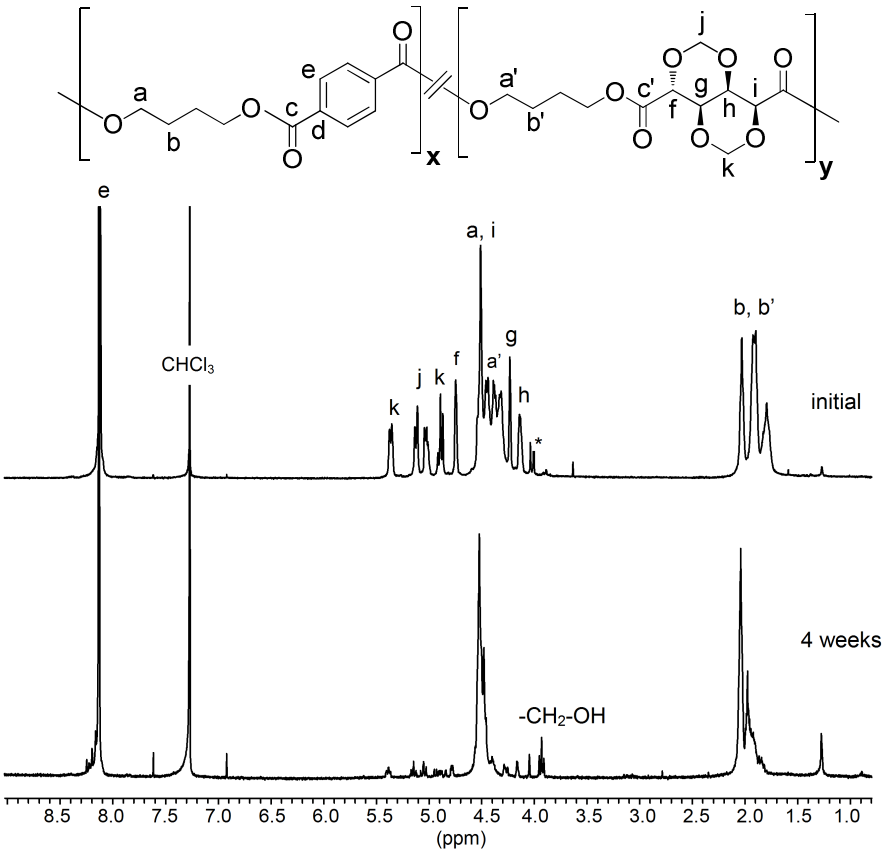


SI-Fig. 9. WAXS profiles of PB_xGlux_yT (top) PBT_xGlux_y (bottom) copolymers and their respective parent homopolyesters recorded from powder samples without any previous thermal treatment.

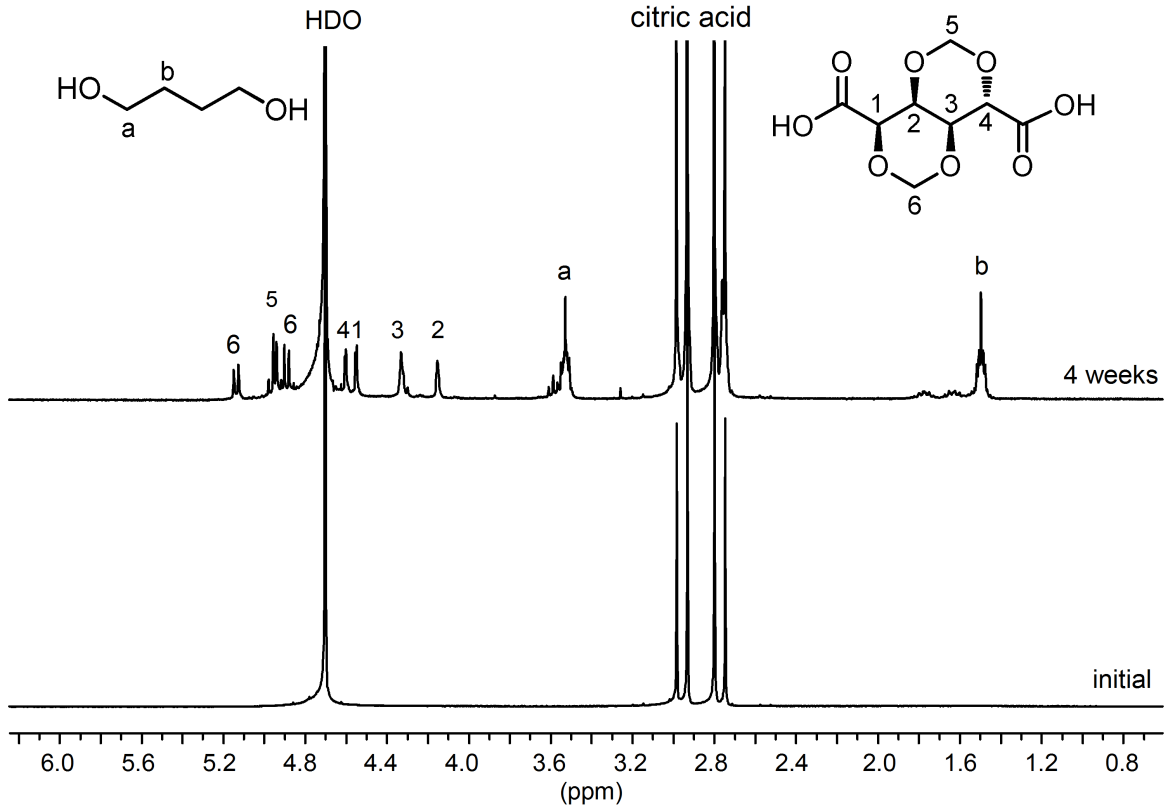
a)



b)



SI-Fig.10. Compared ^{1}H NMR spectra of $PB_{59}Glux_{41}T$ (a) and $PBT_{55}Glux_{45}$ (b) copolyesters before and after incubation (residue) in water at pH 2.0 at 80 ºC.



SI-Fig.11. ^{1}H NMR spectra in D_2O of the products released to the aqueous medium by $PBT_{55}Glux_{45}$ after incubation in water at pH 2.0 at 80 ºC for four weeks.

SI-Table 1. Powder X-ray diffraction data of polyesters.

Polyester	d_{hkl} [a] (Å)										X_c [b]
PBT	5.50 s	5.13 s	4.45 w	4.29 s	3.95 m	3.81 s	3.69 w	3.52 s	3.04 w	2.84 m	0.70
$PBT_{95}Glux_5$	5.53 s	5.13 s	4.46 vw	4.29 s	3.95 m	3.82 s	3.69 w	3.52 s	3.04 w	2.84 m	0.66
$PBT_{90}Glux_{10}$	5.53 s	5.13 s	-	4.31 s	3.95 m	3.82 s	3.69 vw	3.52 s	3.04 w	2.85 m	0.60
$PB_{94}Glux_6T$	5.50 s	5.13 s	4.45 vw	4.31 s	3.95 m	3.82 s	3.69 w	3.52 s	3.04 w	2.85 m	0.63
$PB_{89}Glux_{11}T$	5.50 s	5.13 s	-	4.31 s	3.95 m	3.82 s	3.69 vw	3.52 s	3.04 w	2.85 m	0.49

[a]Bragg spacings measured in powder diffraction patterns obtained from annealed samples. Intensities visually estimated as follows: m, medium; s, strong; w, weak; vw, very weak.
[b]Crystallinity index calculated as the quotient between crystalline area and total area. Crystalline and amorphous areas in the X-ray diffraction pattern were quantified using PeakFit v4.12 software.

SI-Table 2. Mechanical properties.

Polyester	Elastic modulus (MPa)	Tensile strength (MPa)	Elongation at break (%)
PBT	863±25	33±4	15±4
$PB_{69}Glux_{31}T$	885±17	41±5	79±9
$PB_{59}Glux_{41}T$	892±22	47±6	105±16
$PBT_{67}Glux_{33}$	590±20	27±5	121±15
$PBT_{55}Glux_{45}$	582±15	24±5	131±18