

Supporting Information

Closed-loop chemically recyclable aromatic polyesters based on asymmetric dicarboxylates obtainable from lignocellulose

Nitin G. Valsange,¹ Niklas Warlin,¹ Smita V. Mankar,¹ Nicola Rehnberg,²
Baoyong Zhang,^{*1} and Patric Jannasch^{*1}

¹ *Centre for Analysis and Synthesis, Department of Chemistry, Lund University,
P.O. Box 124, SE-22100 Lund, Sweden.*

**E-mail: patric.jannasch@chem.lu.se, baoyong.zhang@chem.lu.se*

² *Bona Sweden AB, Box 210 74, 200 21 Malmö, Sweden*

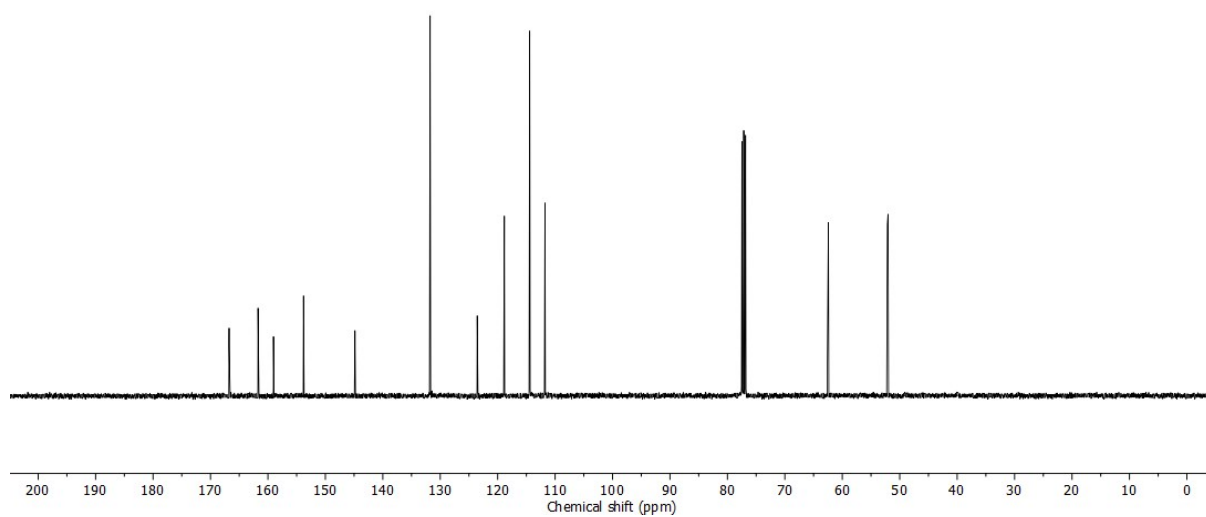


Figure S1. ^{13}C NMR spectrum of monomer M1.

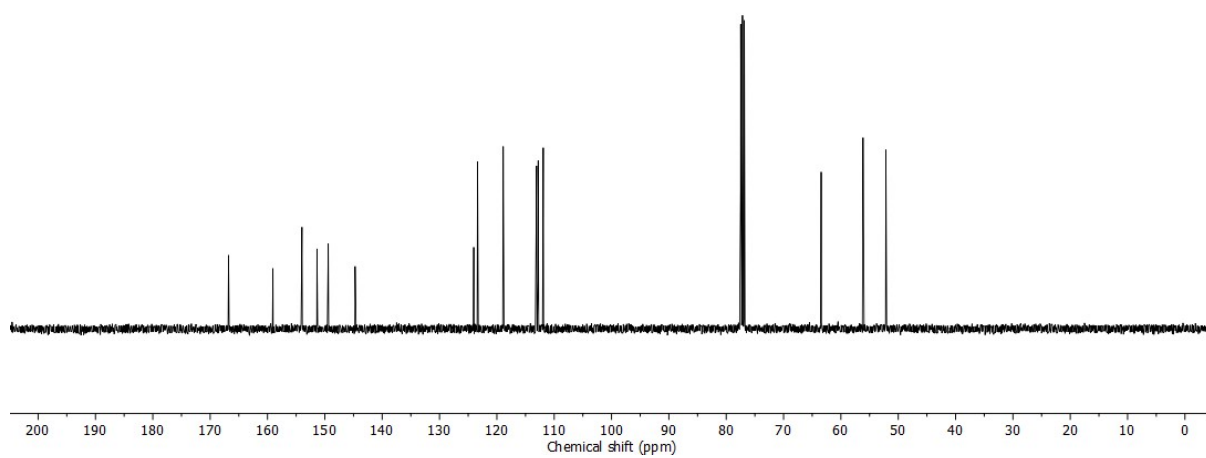


Figure S2. ^{13}C NMR spectrum of monomer M2.

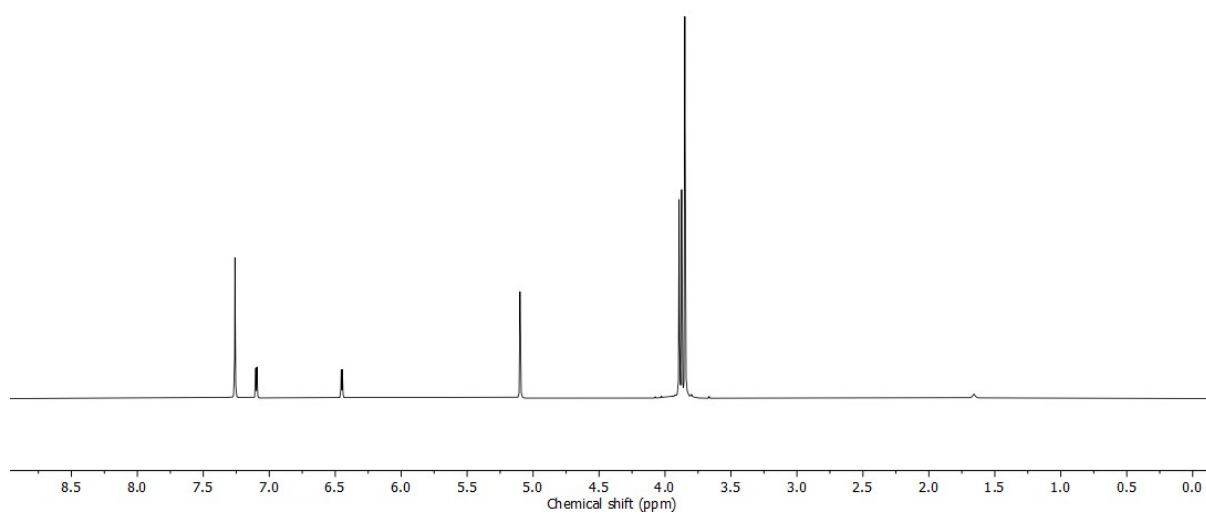


Figure S3. ^1H NMR spectrum of monomer M3.

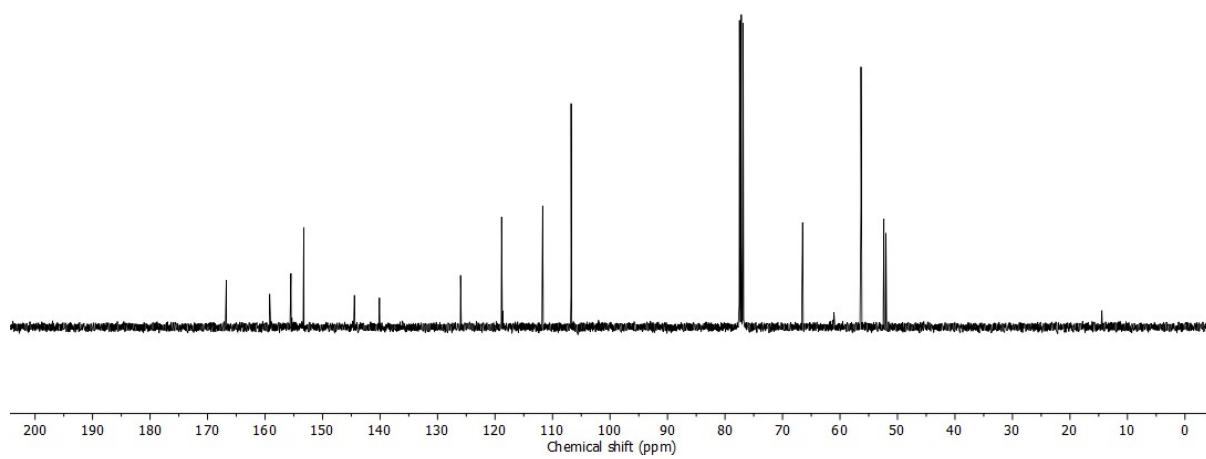


Figure S4. ^{13}C NMR spectrum of monomer M3.

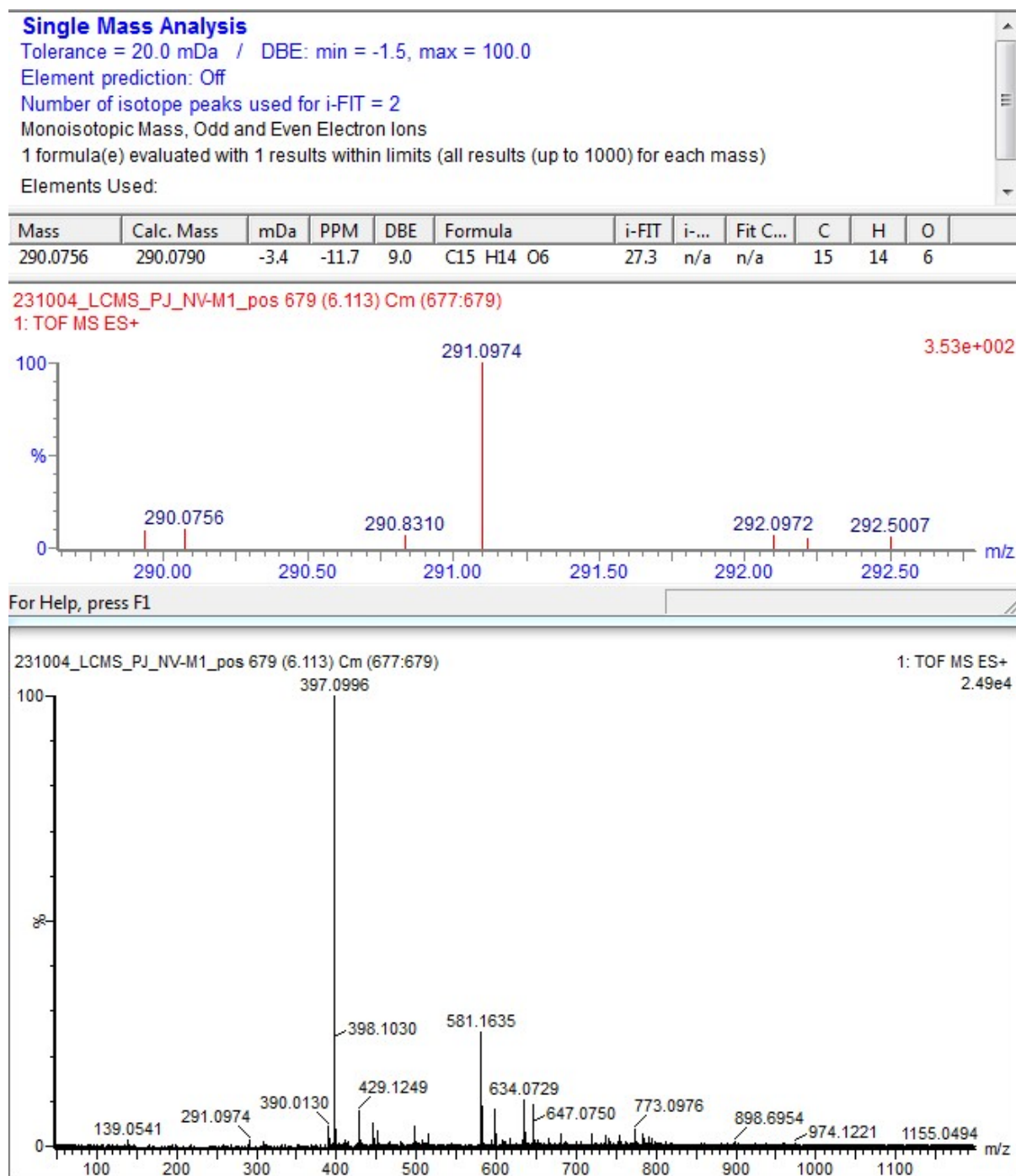


Figure S5. HRMS data of monomer M1.

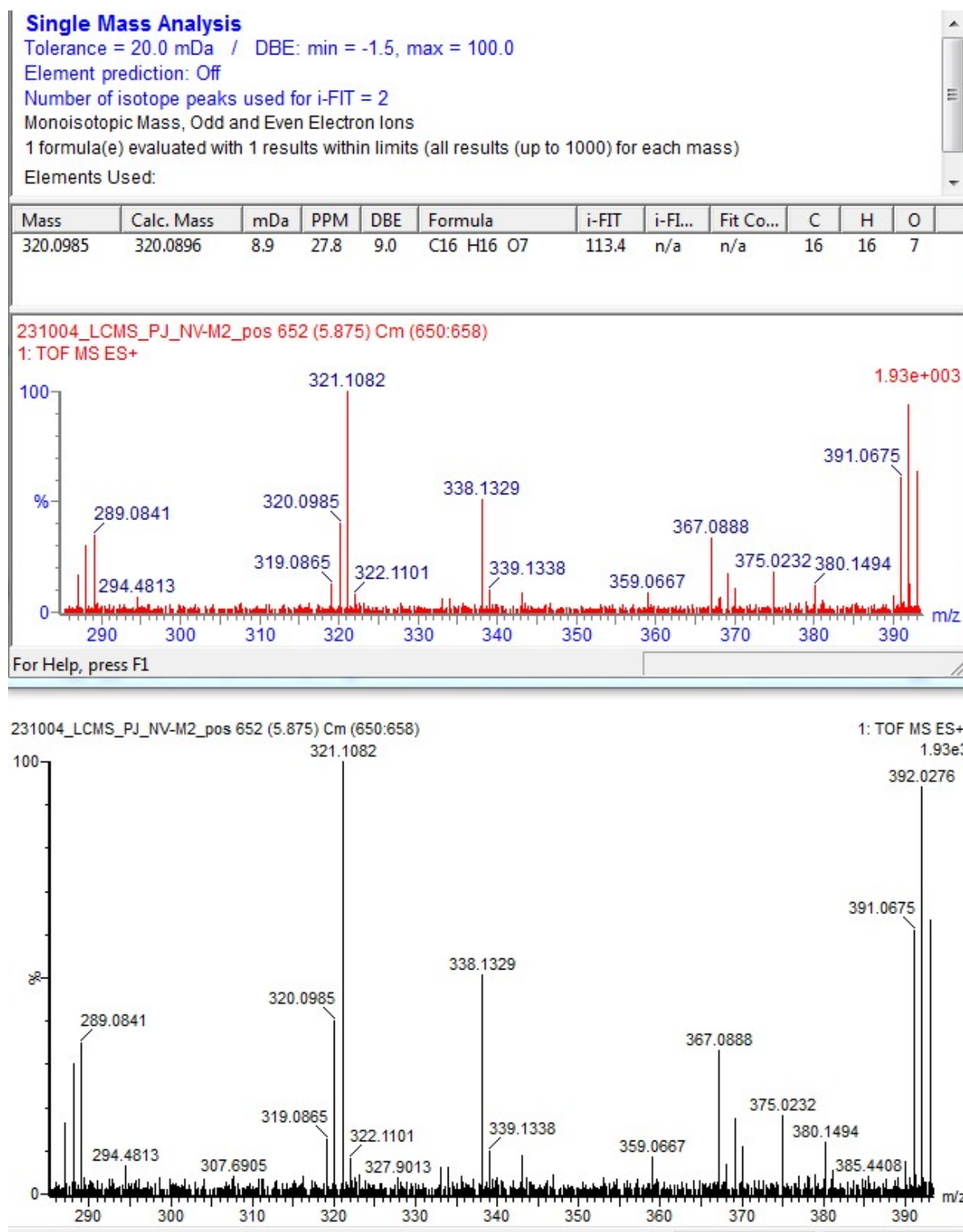


Figure S6. HRMS data of monomer M2.

Single Mass Analysis

Tolerance = 20.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Odd and Even Electron Ions

1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FL...	Fit...	C	H	O
350.1106	350.1002	10.4	29.7	9.0	C17 H18 O8	117.0	n/a	n/a	17	18	8

231004_LCMS_PJ_NV-M3_pos 666 (5.995) Cm (663:674)

1: TOF MS ES+



Spectrum - [231004_LCMS_PJ_NV-M3_pos]

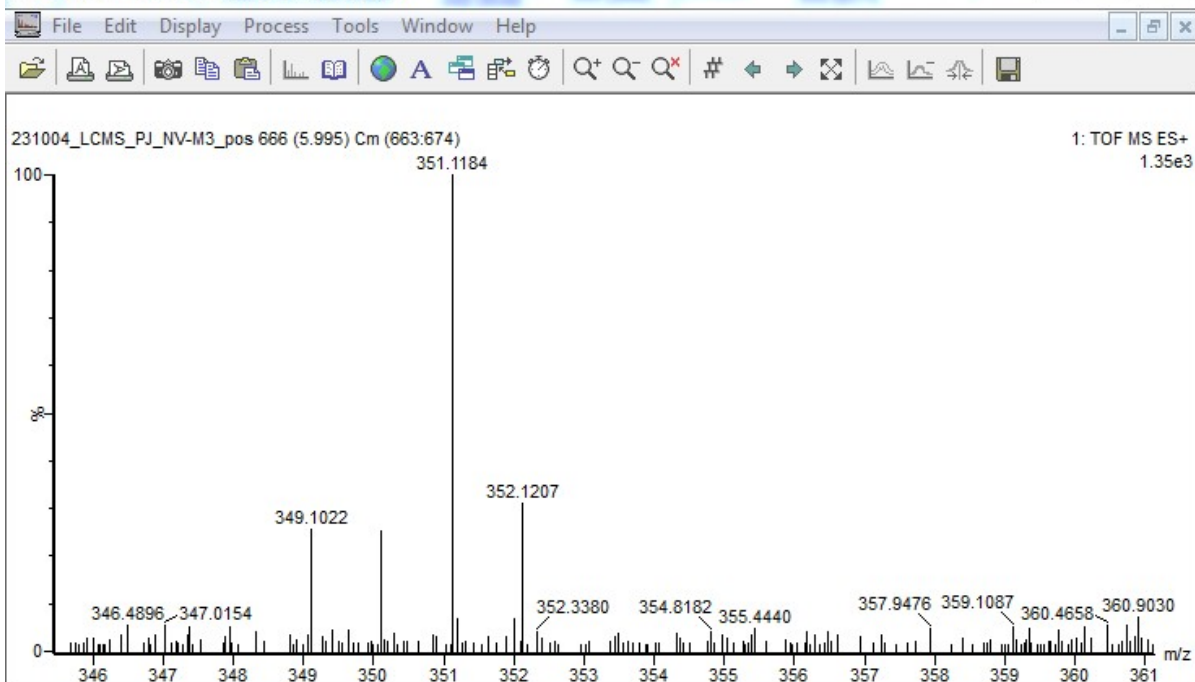


Figure S7. HRMS data of monomer M3.

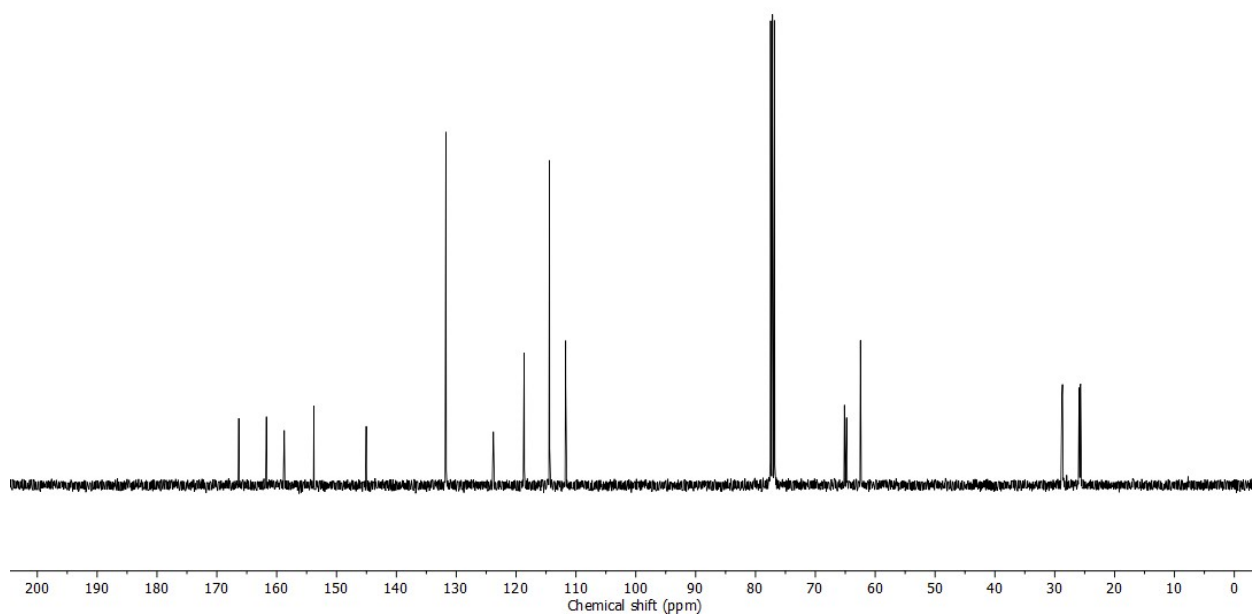


Figure S8. ^{13}C NMR spectrum of polyester P1a.

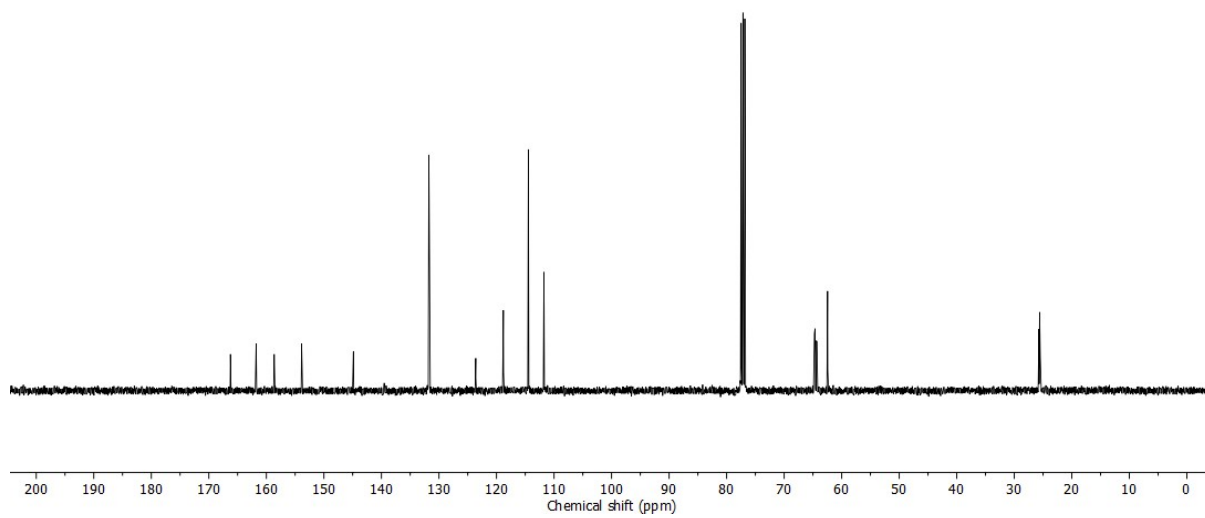


Figure S9. ^{13}C NMR spectrum of polyester P1b.

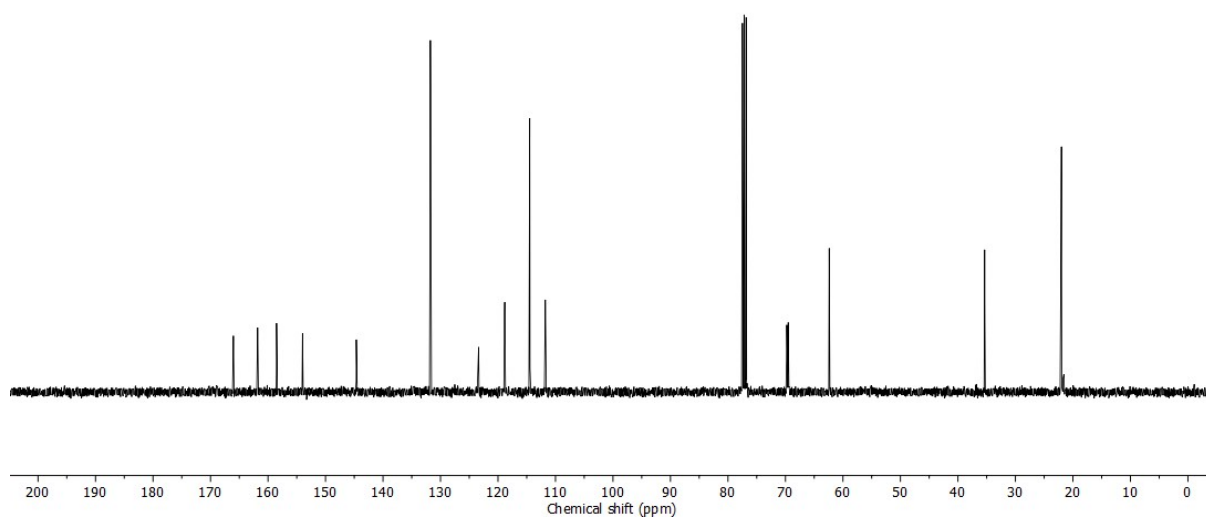


Figure S10. ^{13}C NMR spectrum of polyester P1c.

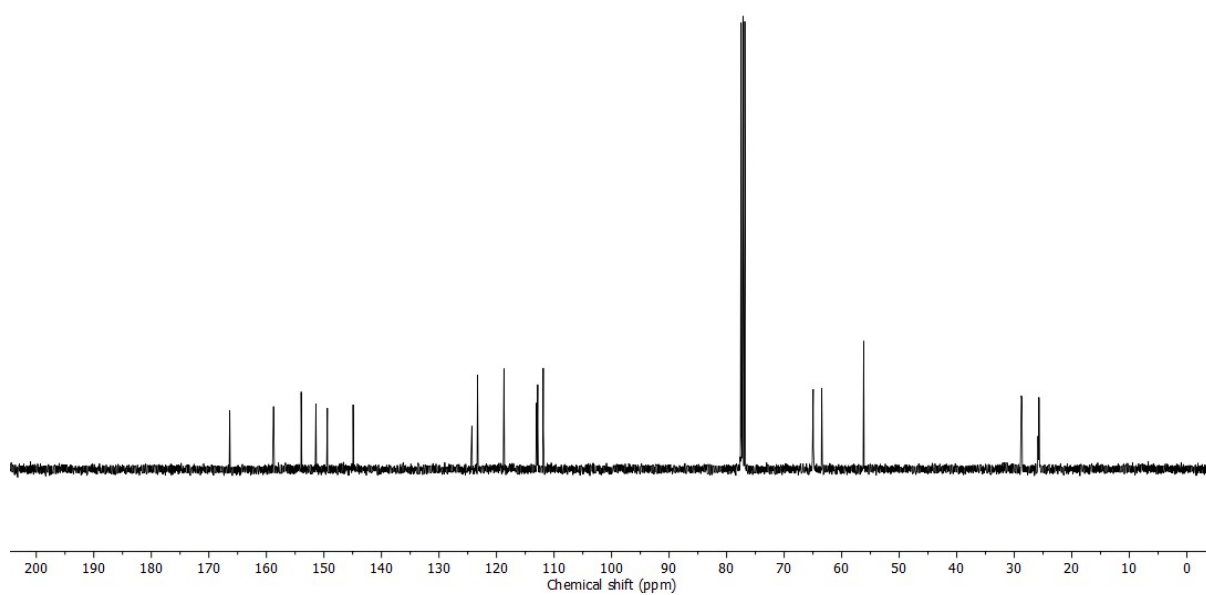


Figure S11. ^{13}C NMR spectrum of polyester P2a.

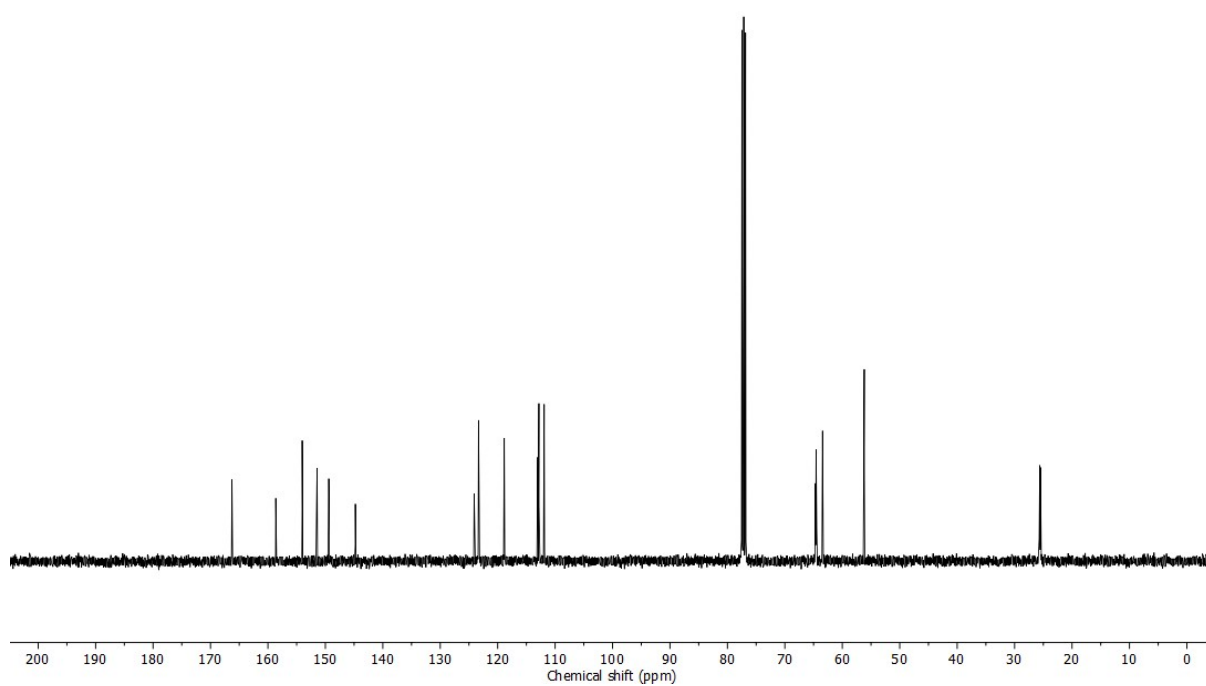


Figure S12. ^{13}C NMR spectrum of polyester P2b.

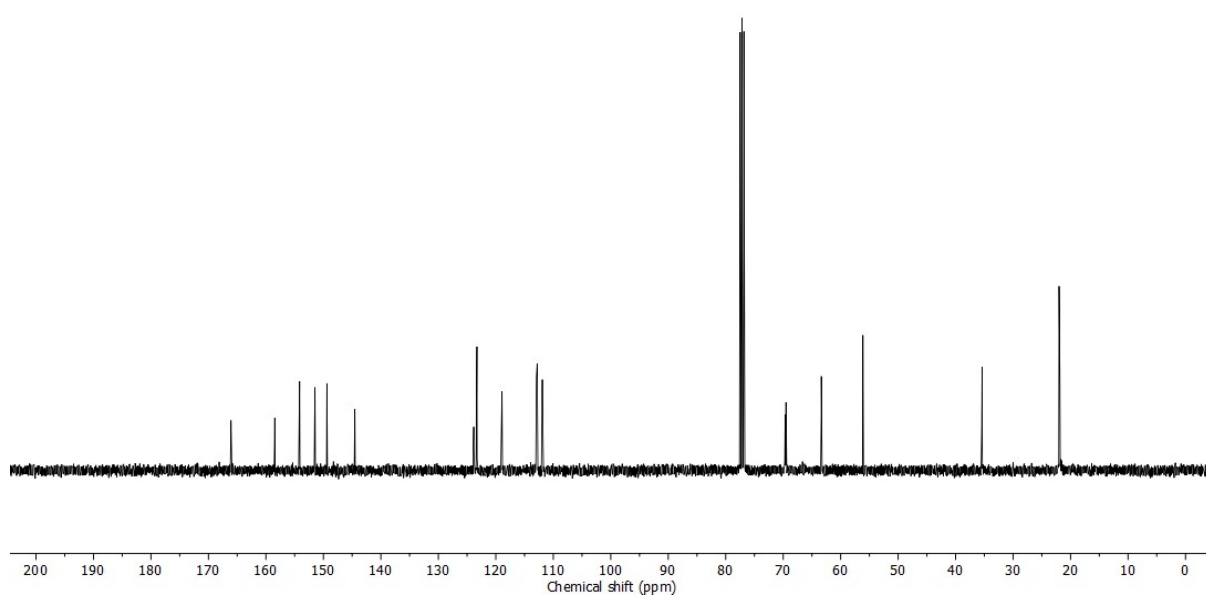


Figure S13. ^{13}C NMR spectrum of polyester P2c.

Calculation of the monomer recovery yields:

Diester monomer (r-M2):

$$\text{Theoretical wt.} = \frac{\text{Wt. of the polymer}}{\text{MW of the repeating unit}} \times \text{MW of the } r - M2$$

$$\text{Theoretical wt.} = \frac{4.0}{374.39} \times 320.3$$

$$\text{Theoretical wt.} = 3.42 \text{ gm}$$

$$\text{Yield of the } r - M2 = \frac{\text{Wt. of } r - M2}{\text{Theoretical wt. of } r - M2} \times 100$$

$$\text{Yield of the } r - M2 = \frac{2.53}{3.42} \times 100$$

$$\text{Yield of the } r - M2 = 74\%$$

Diol monomer (r-1,6-HD):

$$\text{Theoretical wt.} = \frac{\text{Wt. of the polymer}}{\text{MW of the repeating unit}} \times \text{MW of the } r - 1,6 - HD$$

$$\text{Theoretical wt.} = \frac{4.0}{374.39} \times 118.18$$

$$\text{Theoretical wt.} = 1.26 \text{ gm}$$

$$\text{Yield of the } r - 1,6 - HD = \frac{\text{Wt. of the } r - 1,6 - HD}{\text{Theoretical wt. of } r - 1,6 - HD} \times 100$$

$$\text{Yield of the } r - 1,6 - HD = \frac{0.91}{1.26} \times 100$$

$$\text{Yield of the } r - 1,6 - HD = 72\%$$