Biobased furandicarboxylic acids (FDCAs): effects of isomeric substitution on polyester synthesis and properties

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Supporting information:

Contents:

Note:

1. All the NMR spectra were recorded using $CDCl_3$ and TFA-d (6:1) mixture.

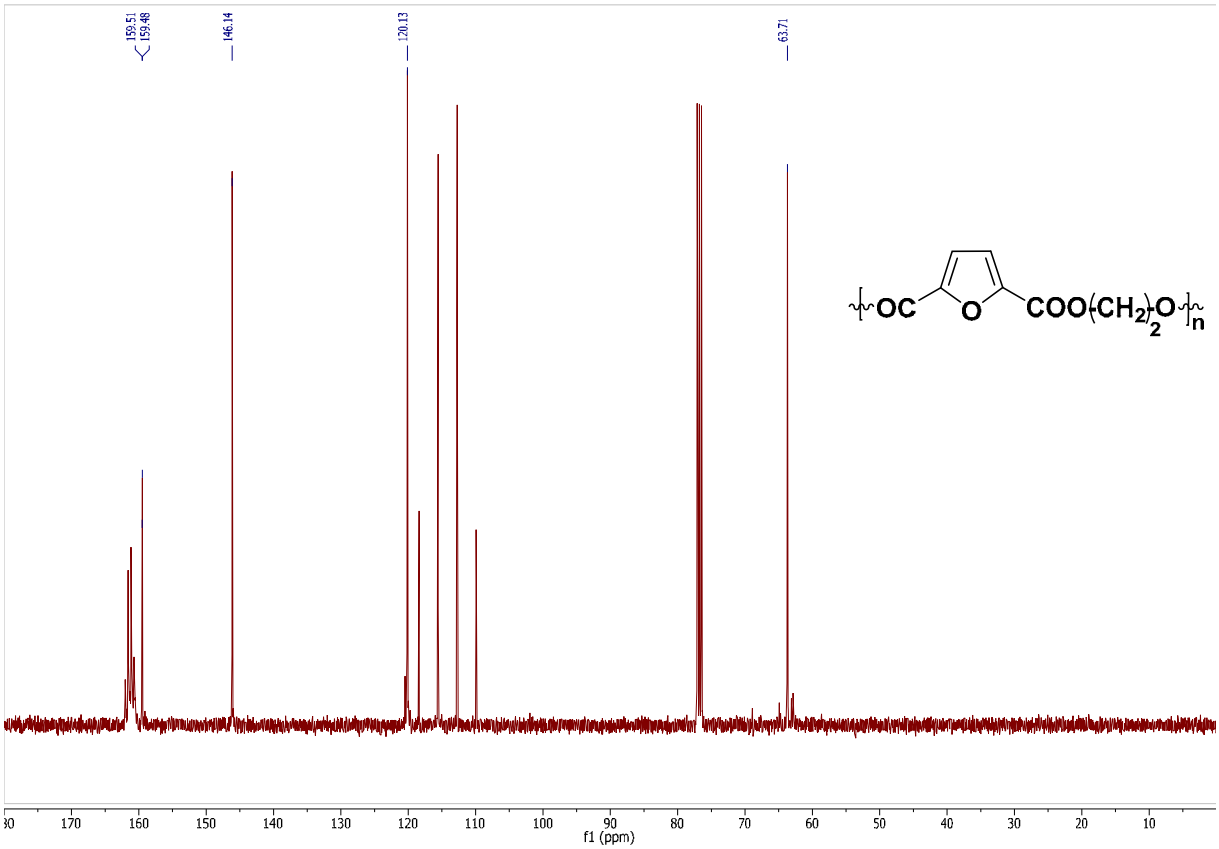

Figure 1: ^{13}C NMR spectrum of Poly(1,2-ethylene-2,5-furandicarboxylate) (2,5-PEF)

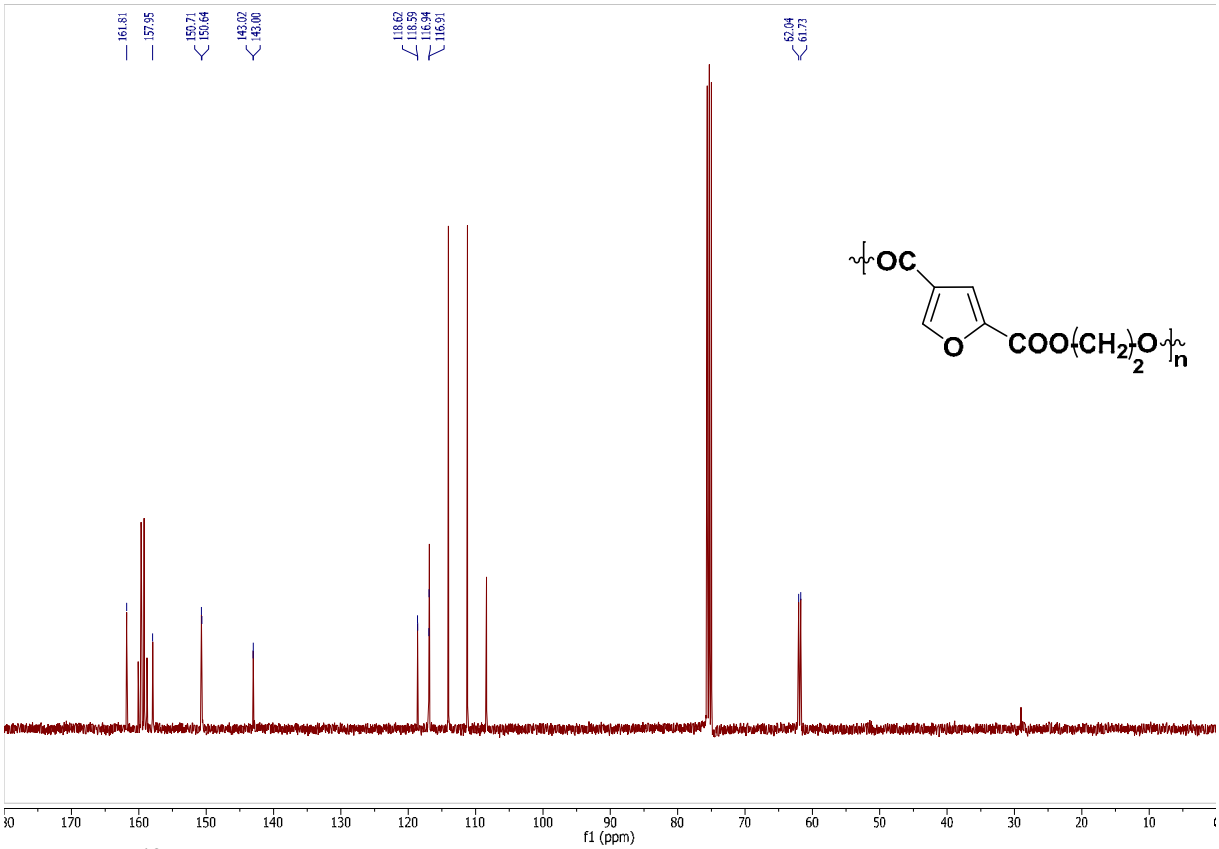

Figure 2: ^{13}C NMR spectrum of Poly(1,2-ethylene-2,4-furandicarboxylate) (2,4-PEF)

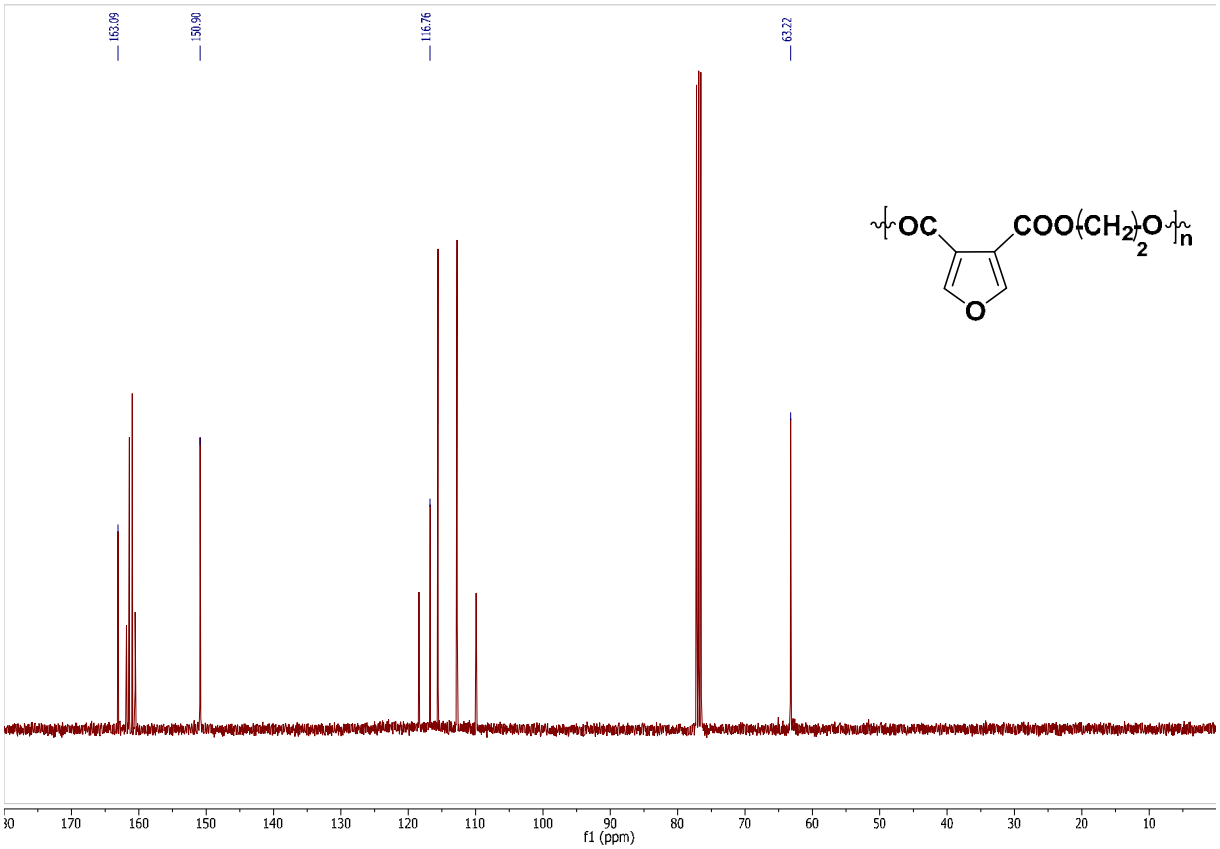

Figure 3: ^{13}C NMR spectrum of Poly(1,2-ethylene-3,4-furandicarboxylate) (3,4-PEF)

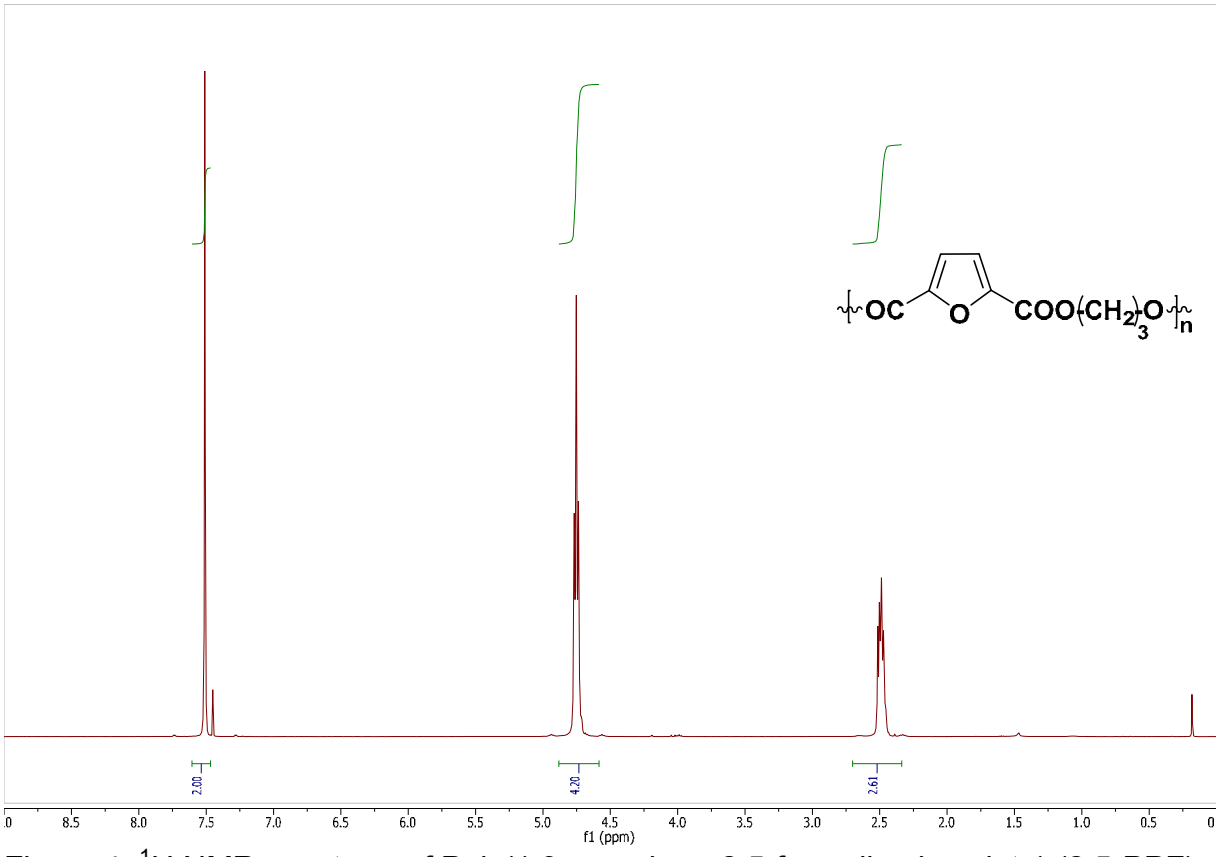

Figure 4: ^{1}H NMR spectrum of Poly(1,3-propylene-2,5-furandicarboxylate) (2,5-PPF)

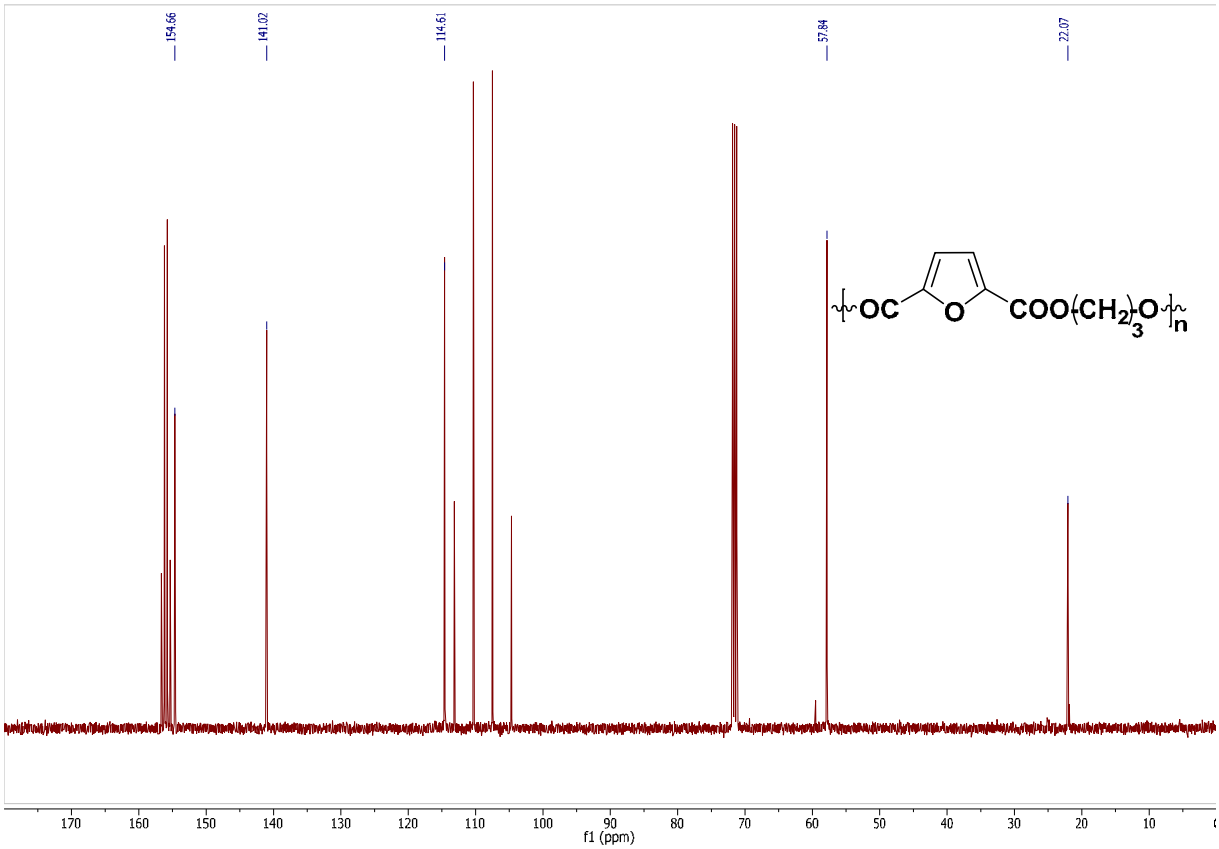

Figure 5: ^{13}C NMR spectrum of Poly(1,3-propylene-2,5-furandicarboxylate) (2,5-PPF)

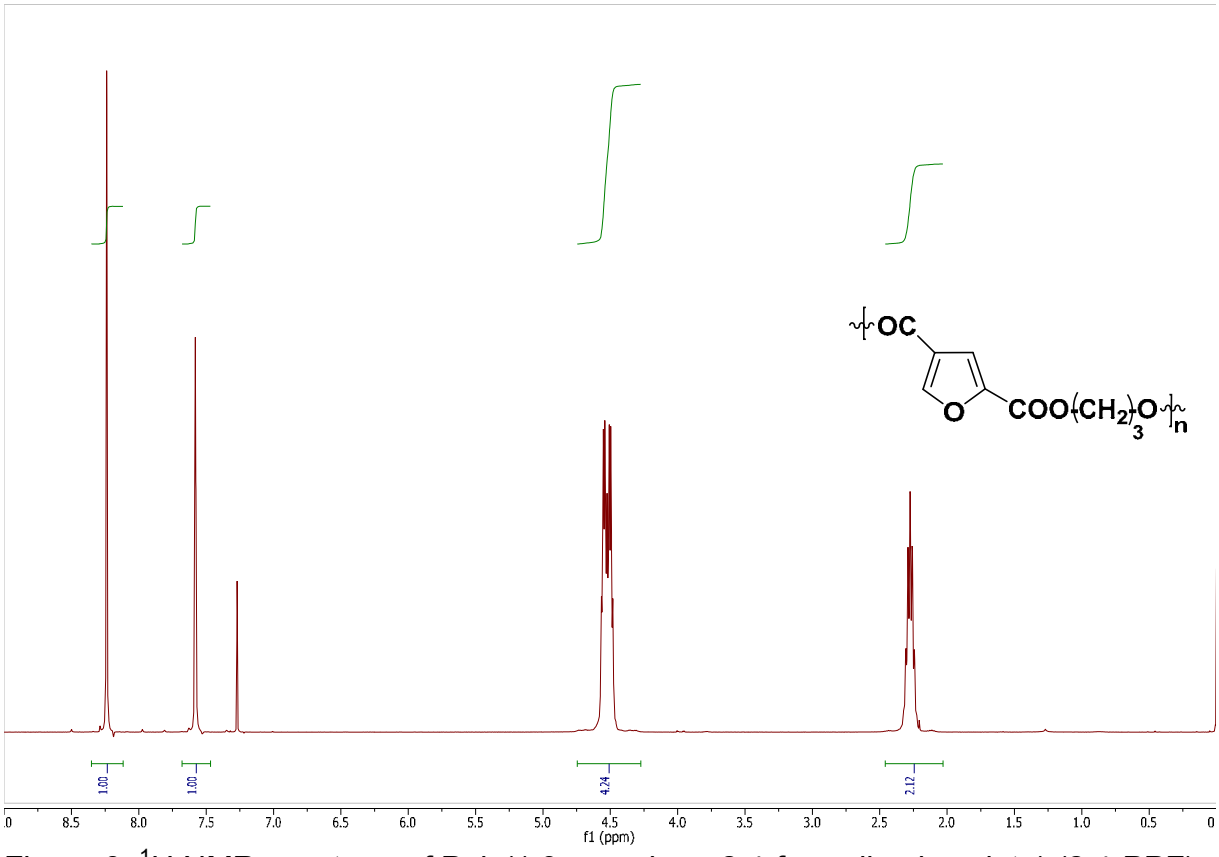

Figure 6: ^{1}H NMR spectrum of Poly(1,3-propylene-2,4-furandicarboxylate) (2,4-PPF)

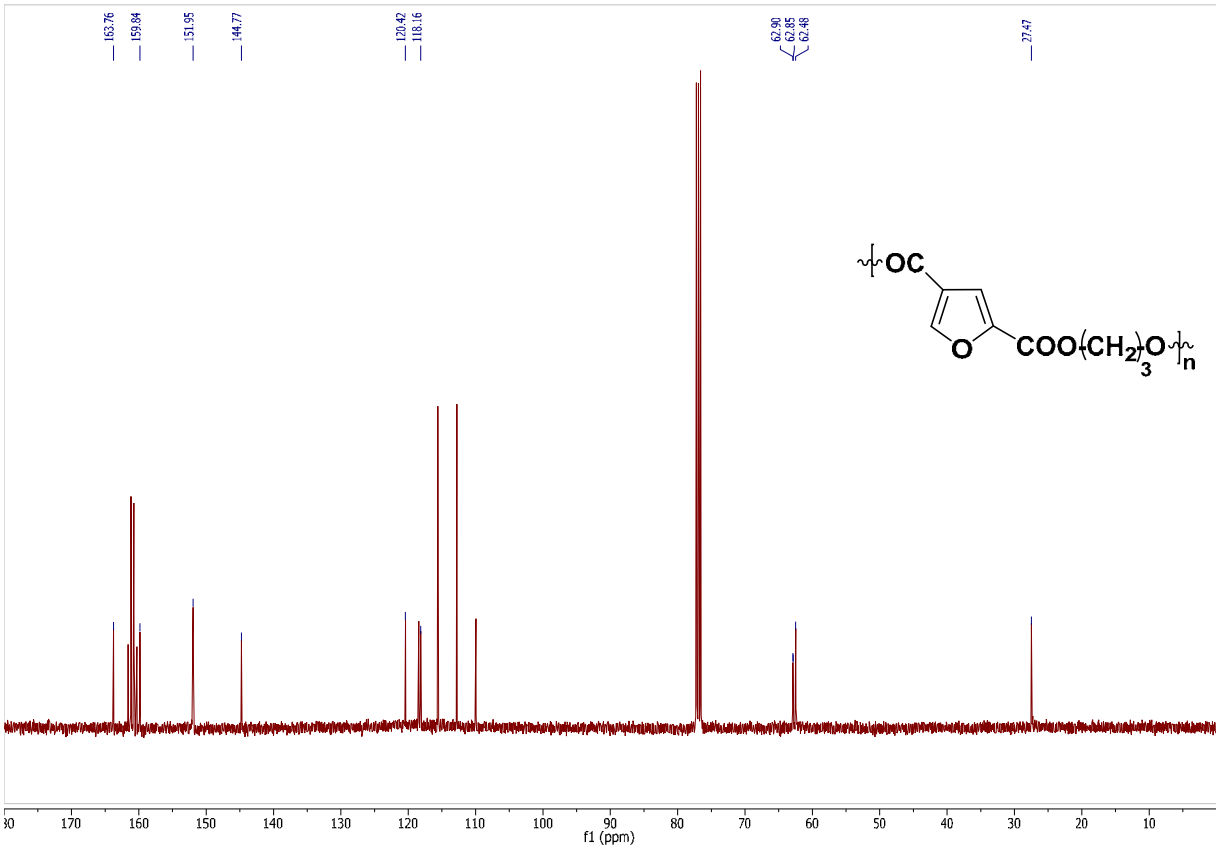

Figure 7: ^{13}C NMR spectrum of Poly(1,3-propylene-2,4-furandicarboxylate) (2,4-PPF)

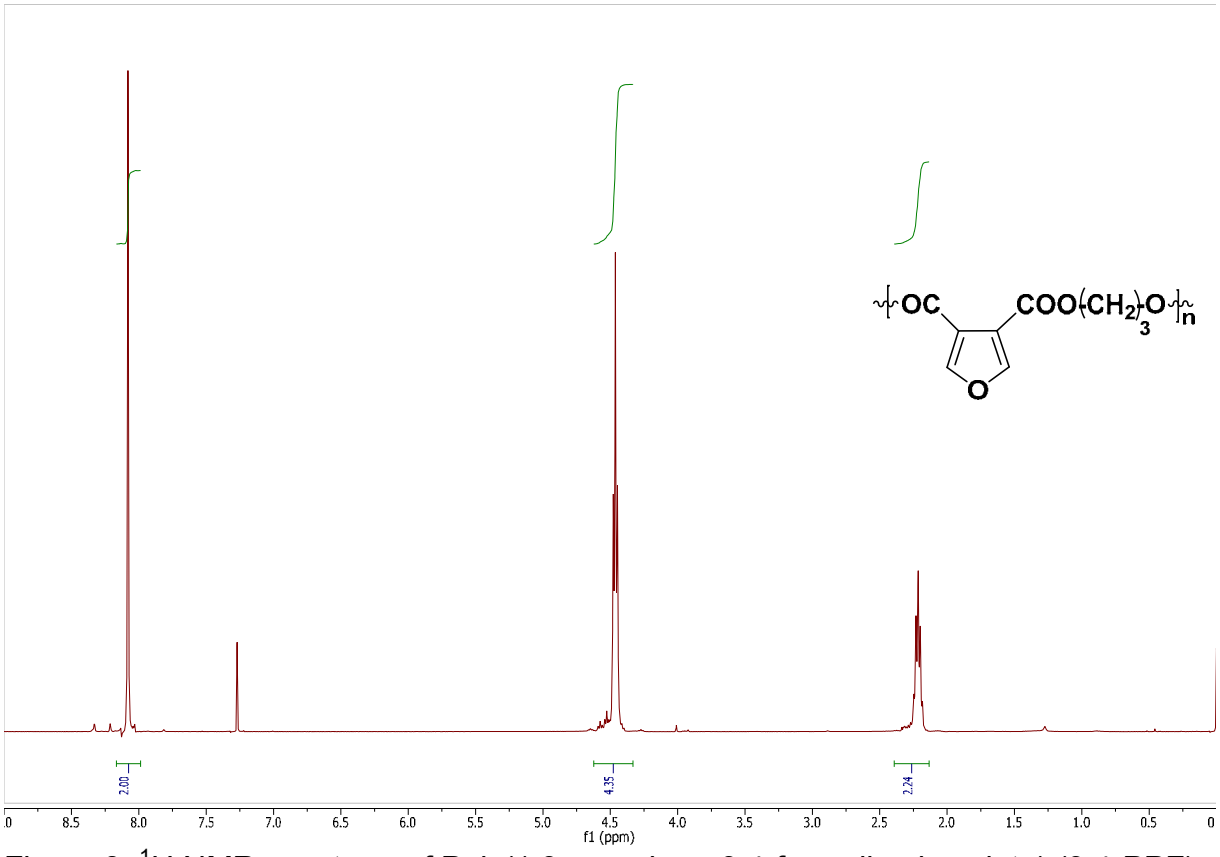

Figure 8: ^{1}H NMR spectrum of Poly(1,3-propylene-3,4-furandicarboxylate) (3,4-PPF)

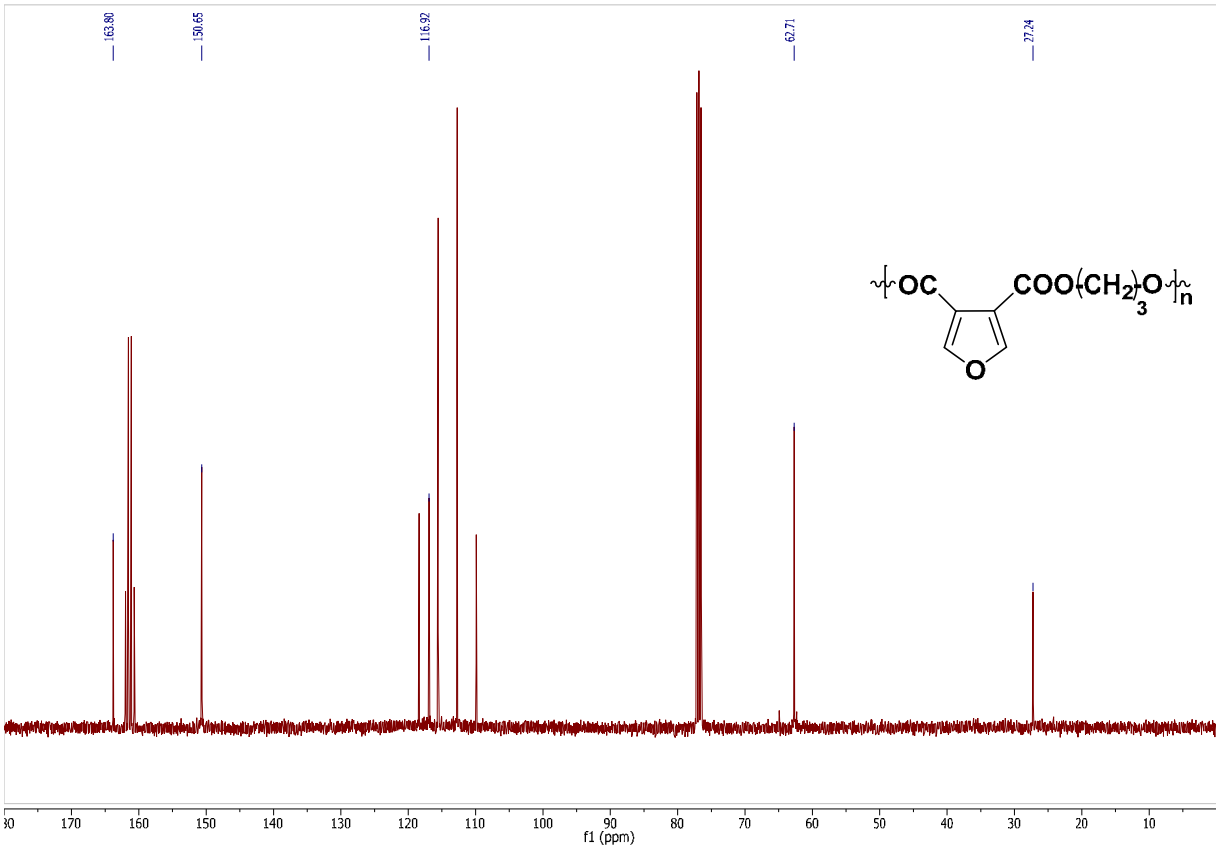

Figure 9: ^{13}C NMR spectrum of Poly(1,3-propylene-3,4-furandicarboxylate) (3,4-PPF)

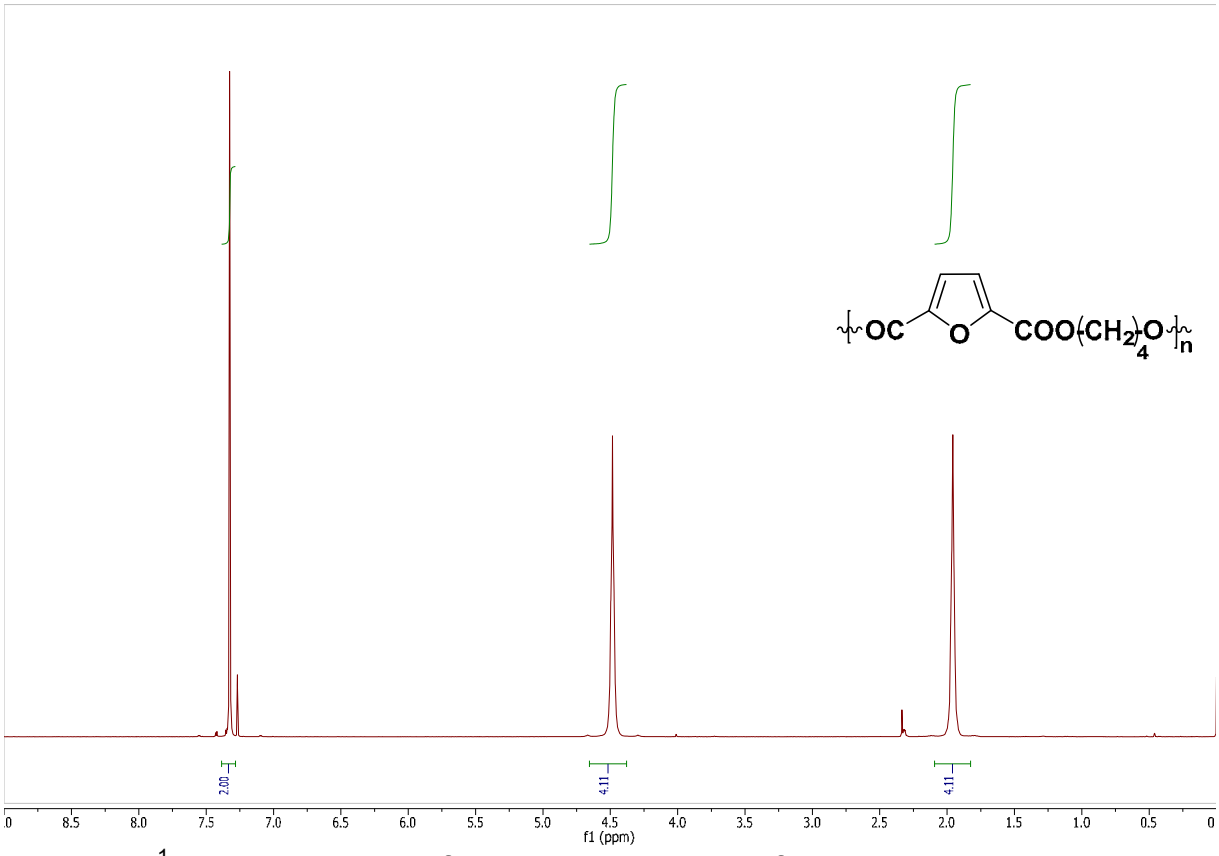

Figure 10: ^{1}H NMR spectrum of Poly(1,4-butylene-2,5-furandicarboxylate) (2,5-P14BF)

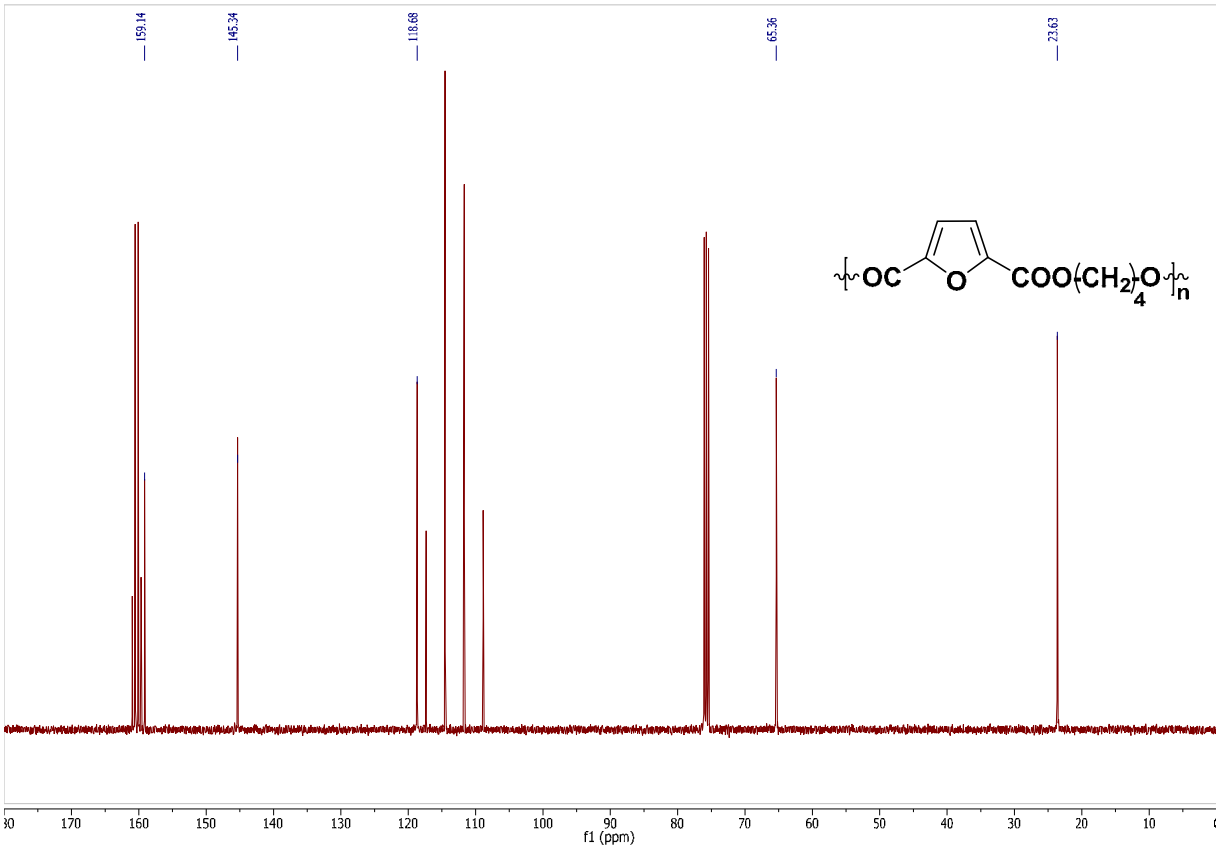

Figure 11: ^{13}C NMR spectrum of Poly(1,4-butylene-2,5-furandicarboxylate) (2,5-P14BF)

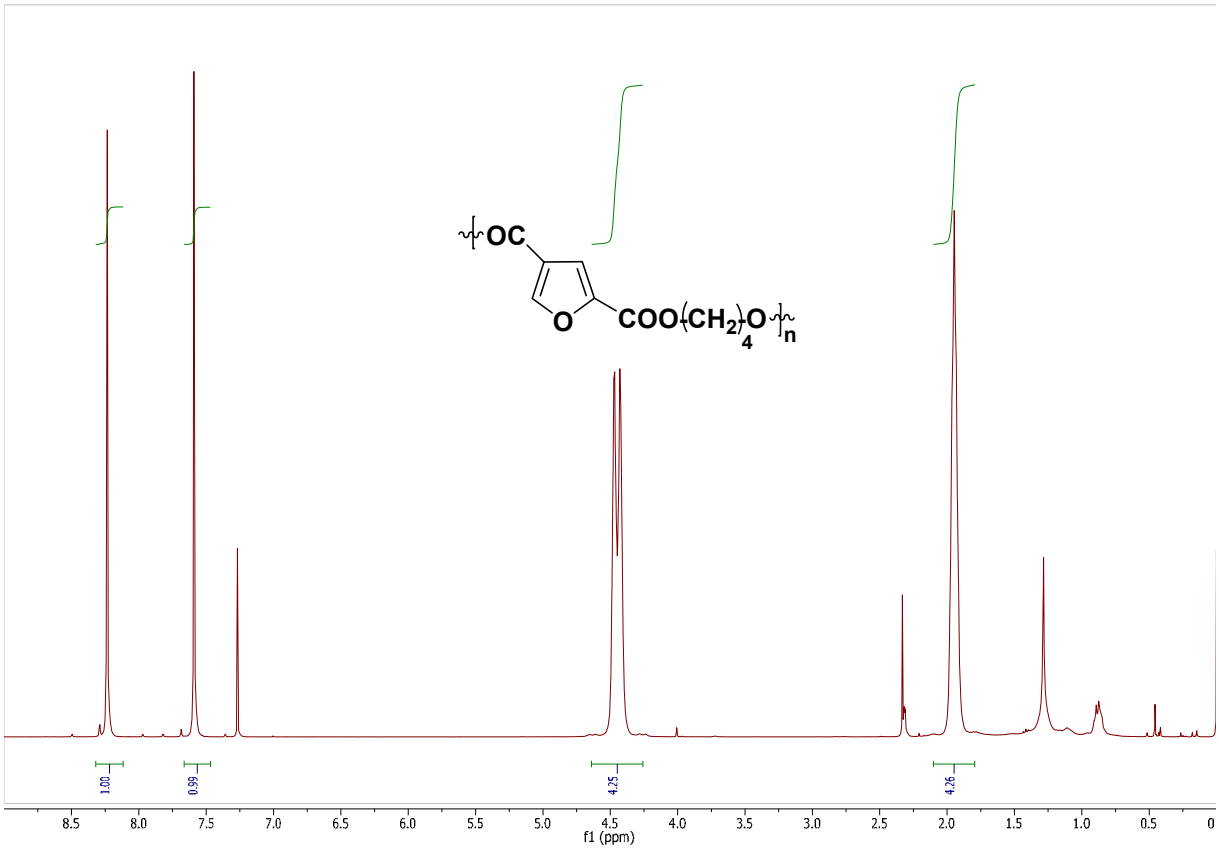

Figure 12: ^{1}H NMR spectrum of Poly(1,4-butylene-2,4-furandicarboxylate) (2,4-P14BF)

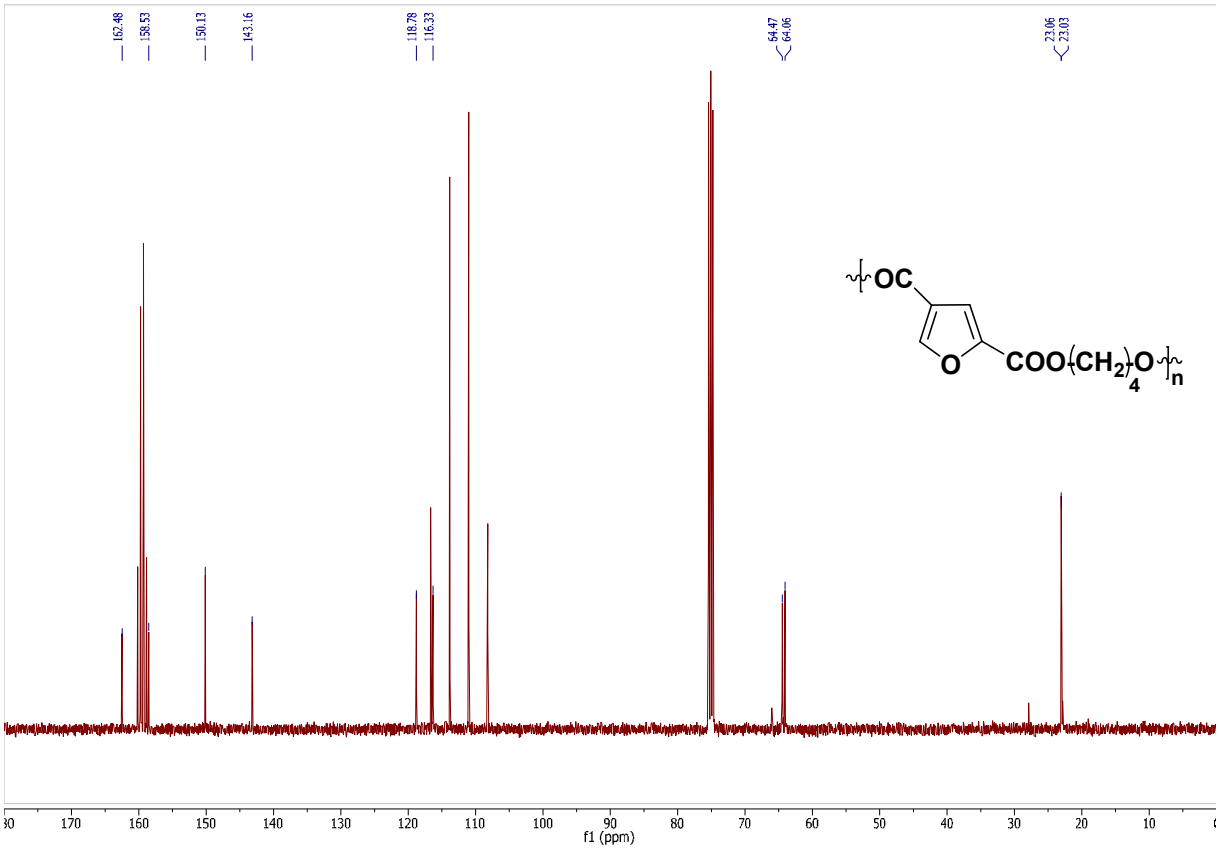

Figure 13: ^{13}C NMR spectrum of Poly(1,4-butylene-2,4-furandicarboxylate) (2,4-P14BF)

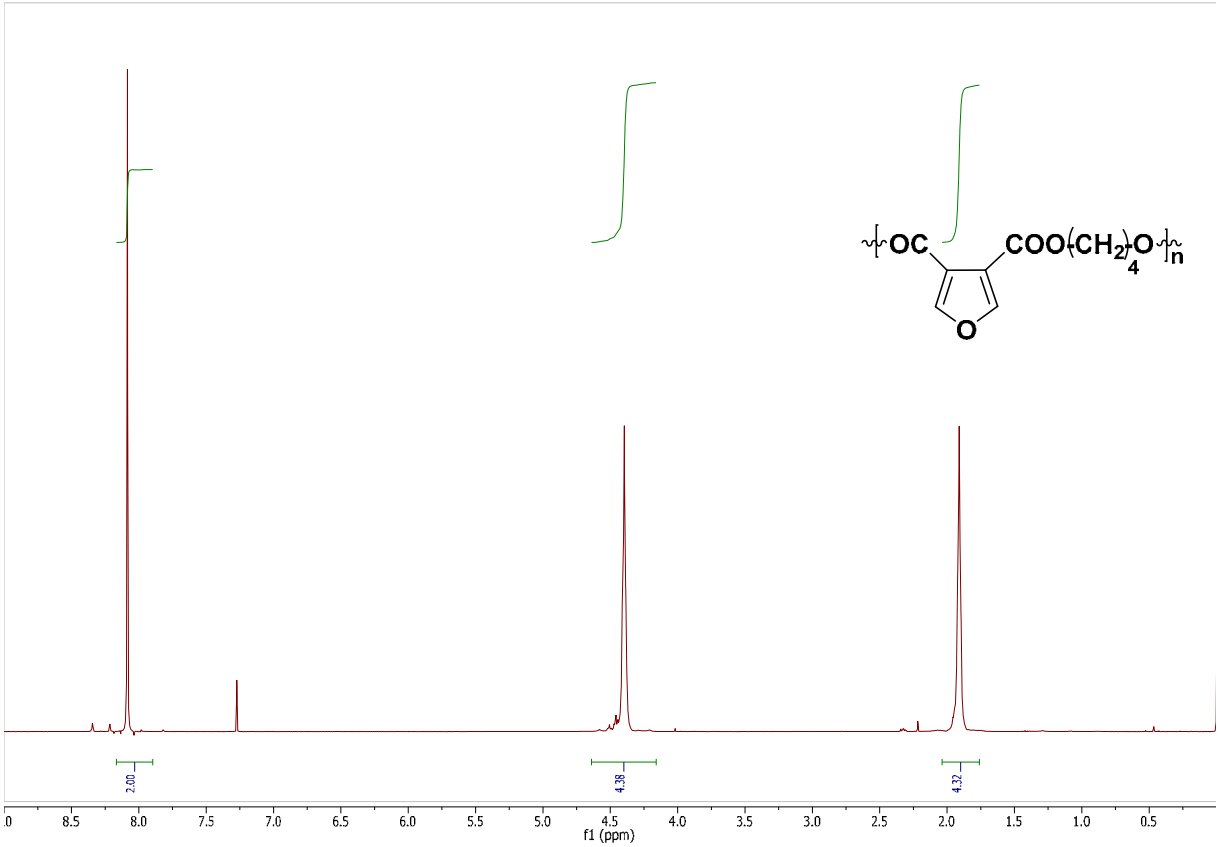

Figure 14: ^{1}H NMR spectrum of Poly(1,4-butylene-3,4-furandicarboxylate) (3,4-P14BF)

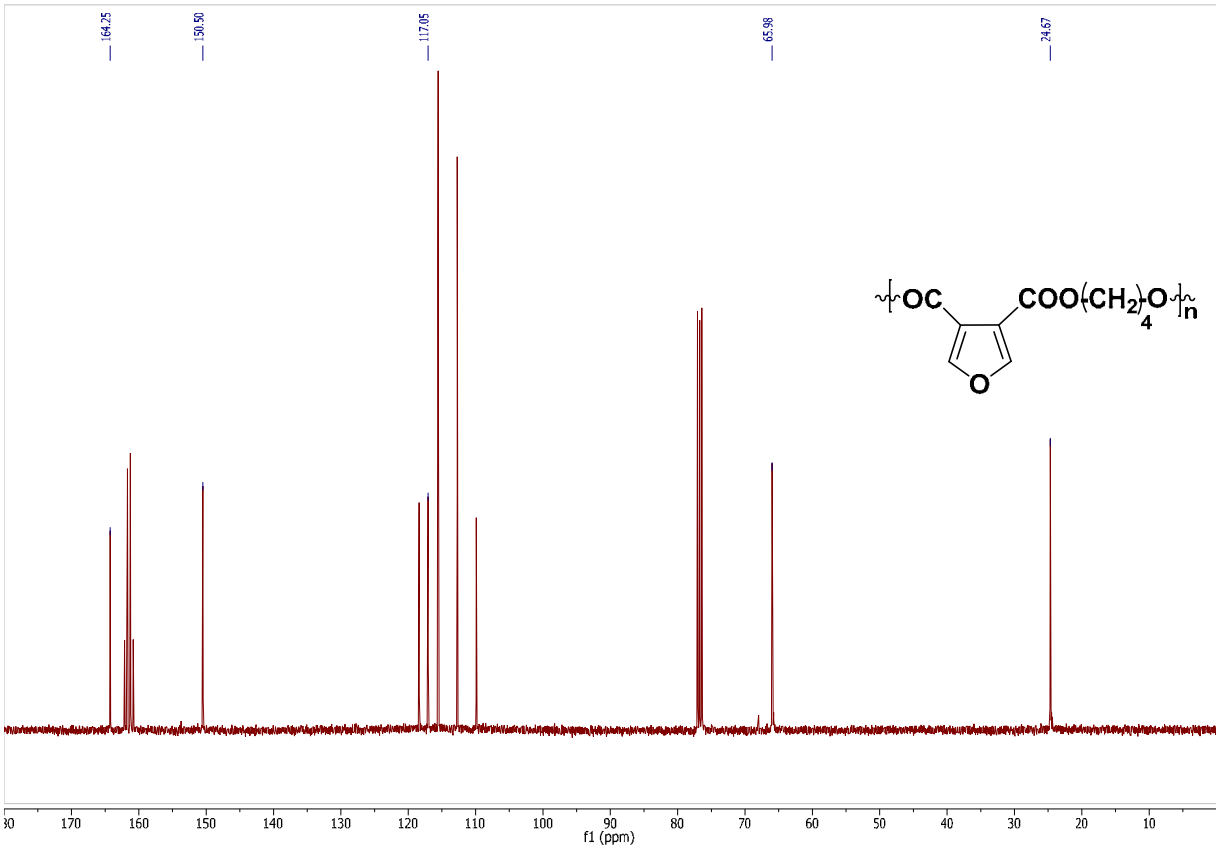

Figure 15: ^{13}C NMR spectrum of Poly(1,4-butylene-3,4-furandicarboxylate) (3,4-P14BF)

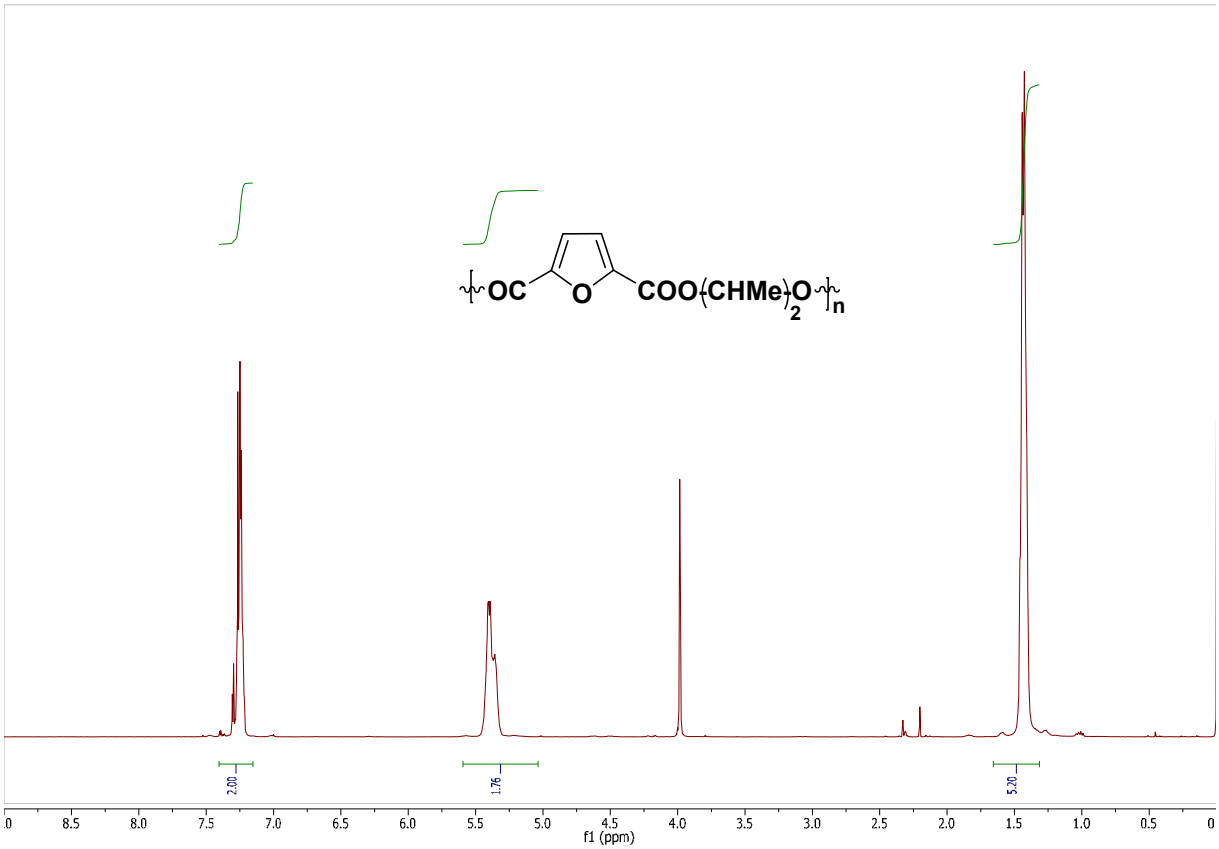

Figure 16: ^{1}H NMR spectrum of Poly(2,3-butylene-2,5-furandicarboxylate) (2,5-P23BF)

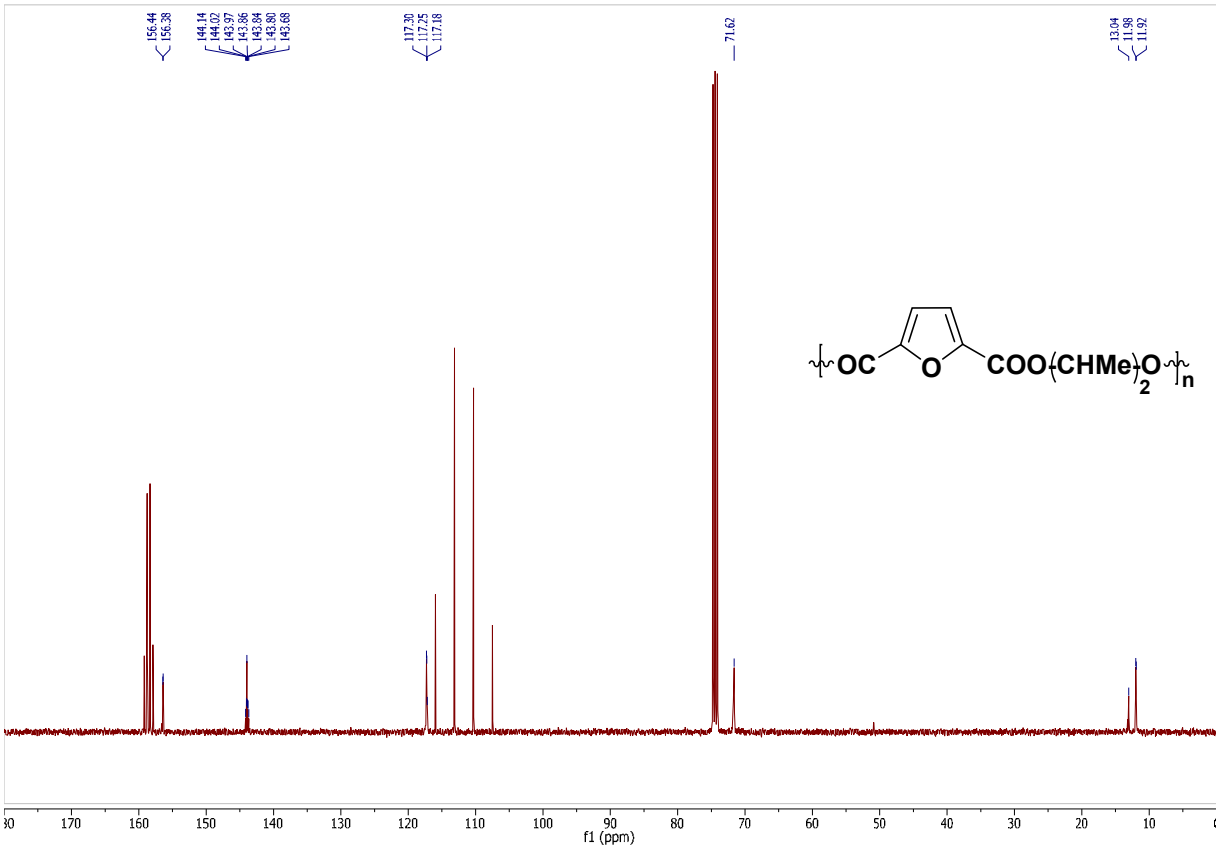

Figure 17: ^{13}C NMR spectrum of Poly(2,3-butylene-2,5-furandicarboxylate) (2,5-P23BF)

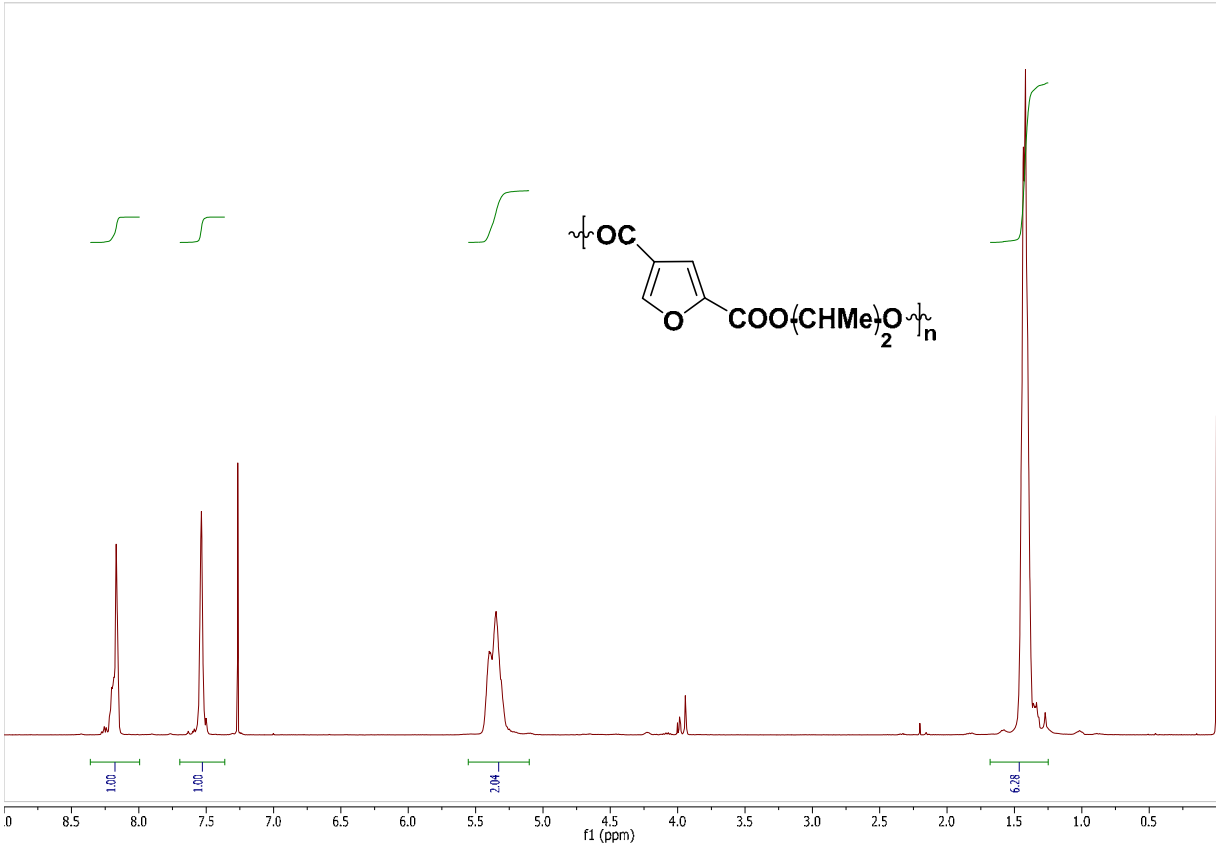

Figure 18: ^{1}H NMR spectrum of Poly(2,3-butylene-2,4-furandicarboxylate) (2,4-P23BF)

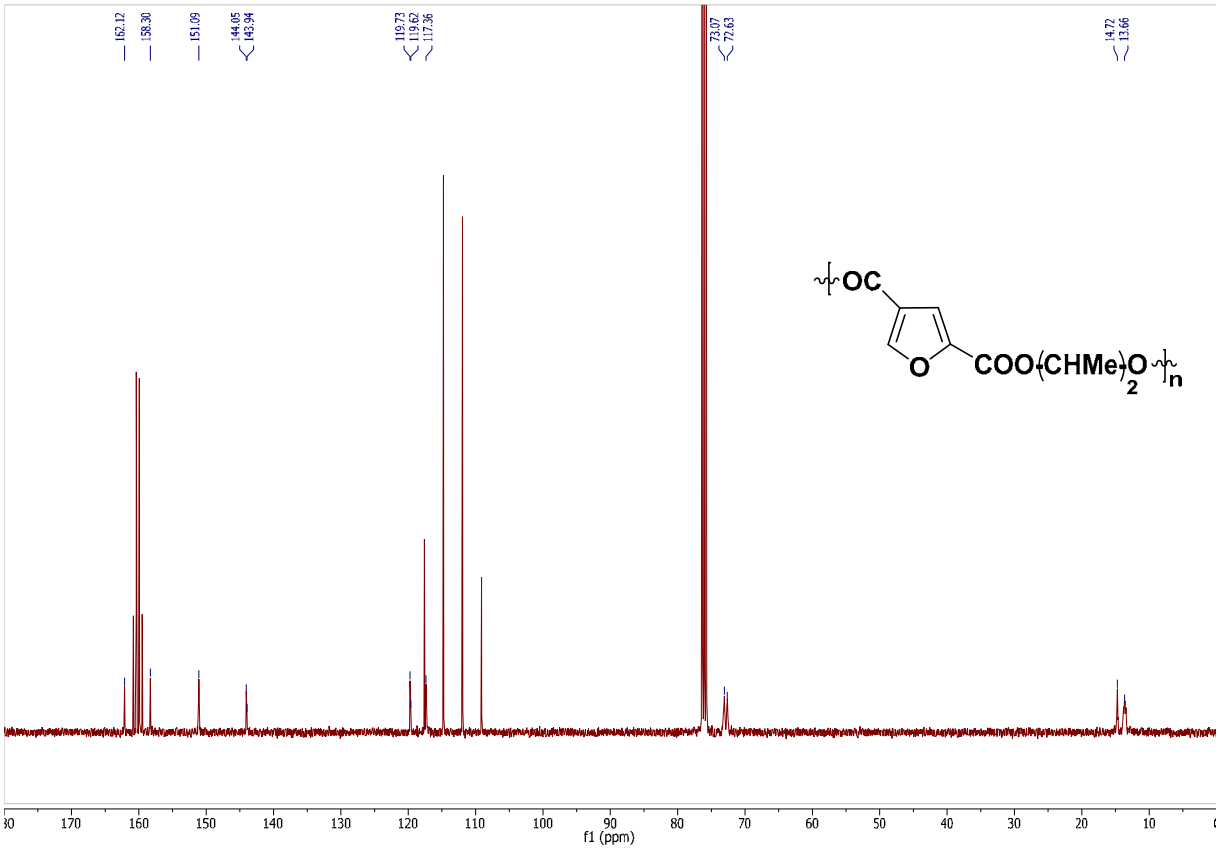

Figure 19: ^{13}C NMR spectrum of Poly(2,3-butylene-2,4-furandicarboxylate) (2,4-P23BF)

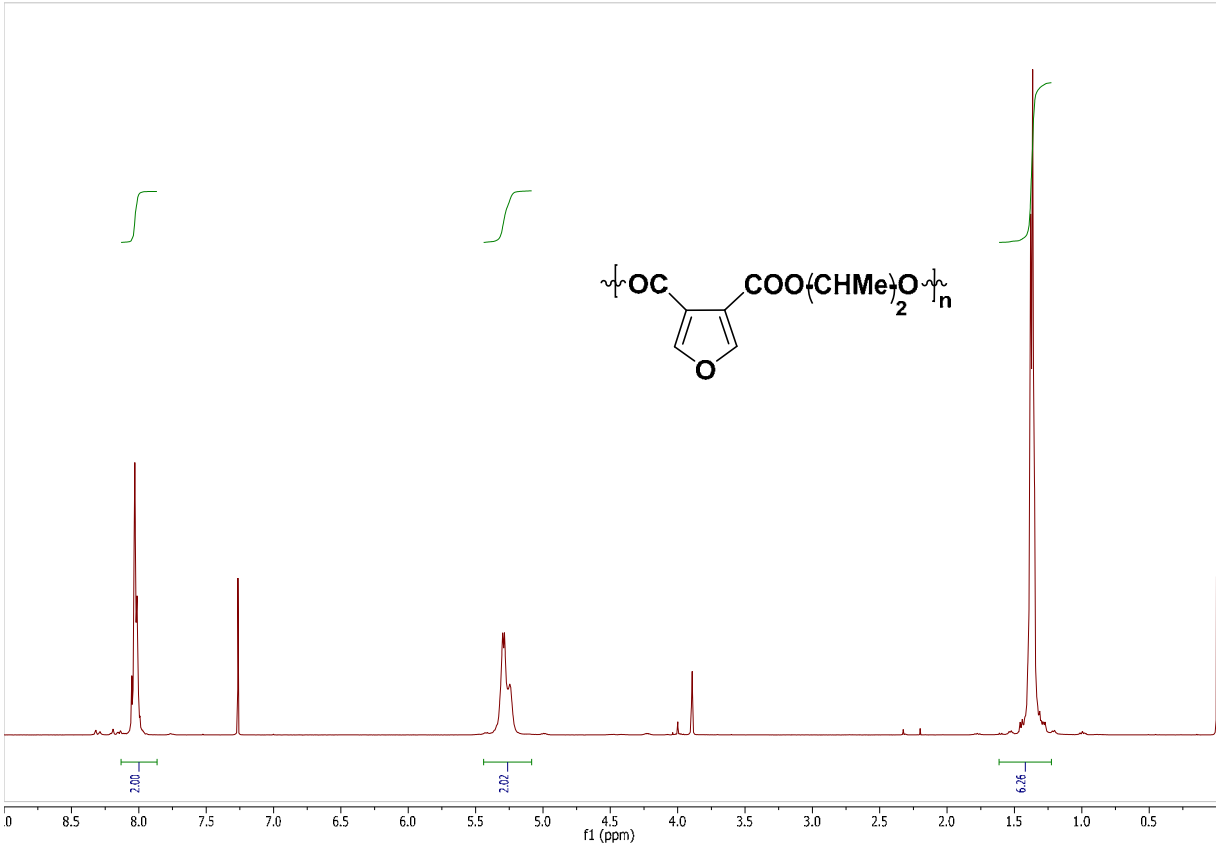

Figure 20: ^{1}H NMR spectrum of Poly(2,3-butylene-3,4-furandicarboxylate) (3,4-P23BF)

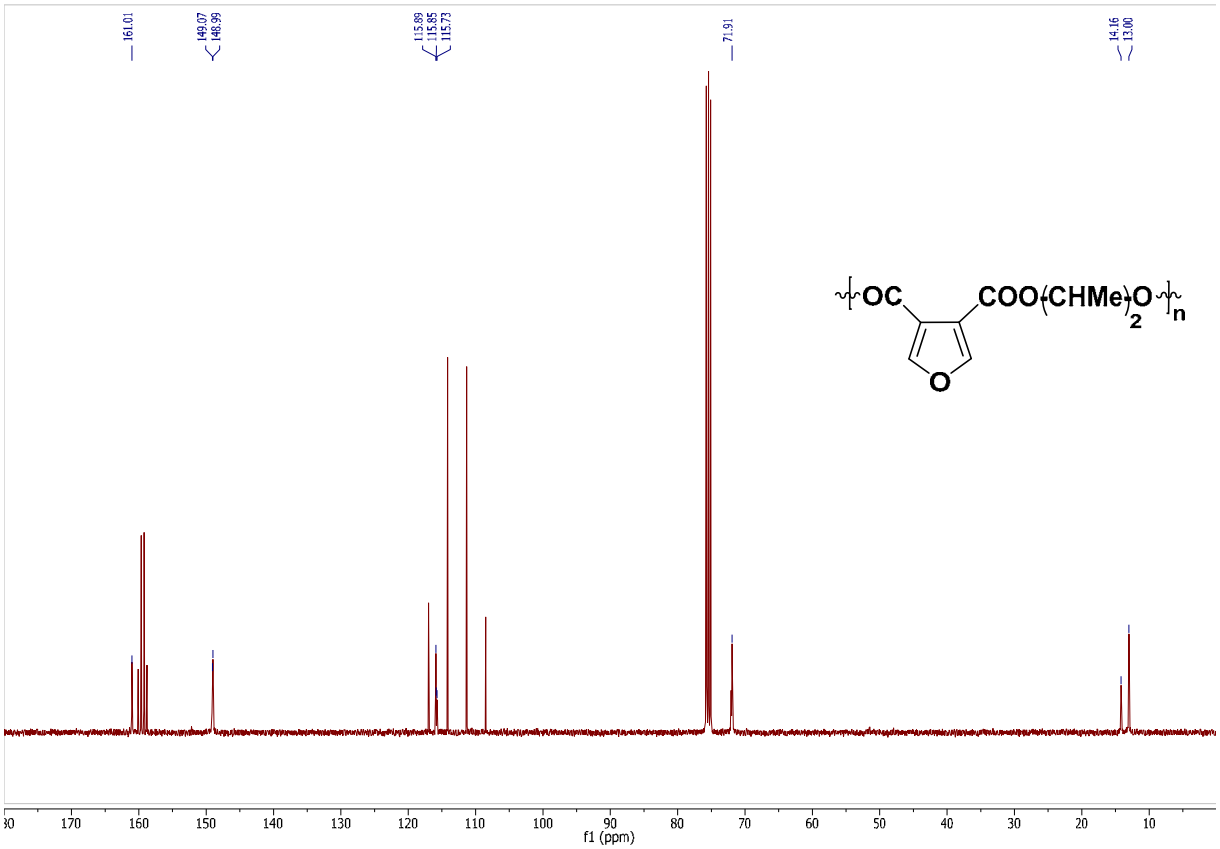

Figure 21: ^{13}C NMR spectrum of Poly(2,3-butylene-3,4-furandicarboxylate) (3,4-P23BF)

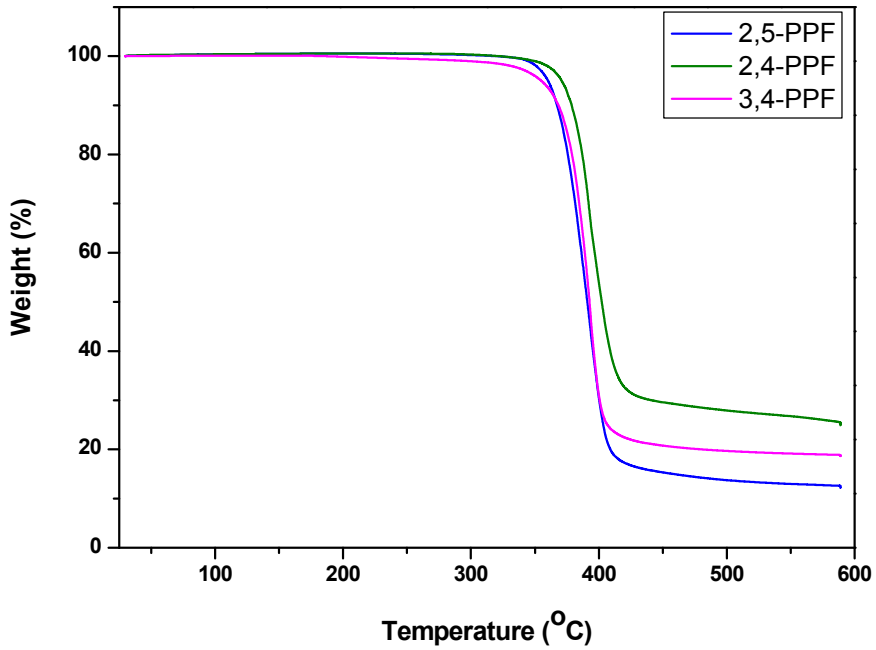

Figure 22: TGA traces of poly(1,3-propylene-furandicarboxylate)s recorded from 30-600 °C at 10 °C/min under N_2 atmosphere.

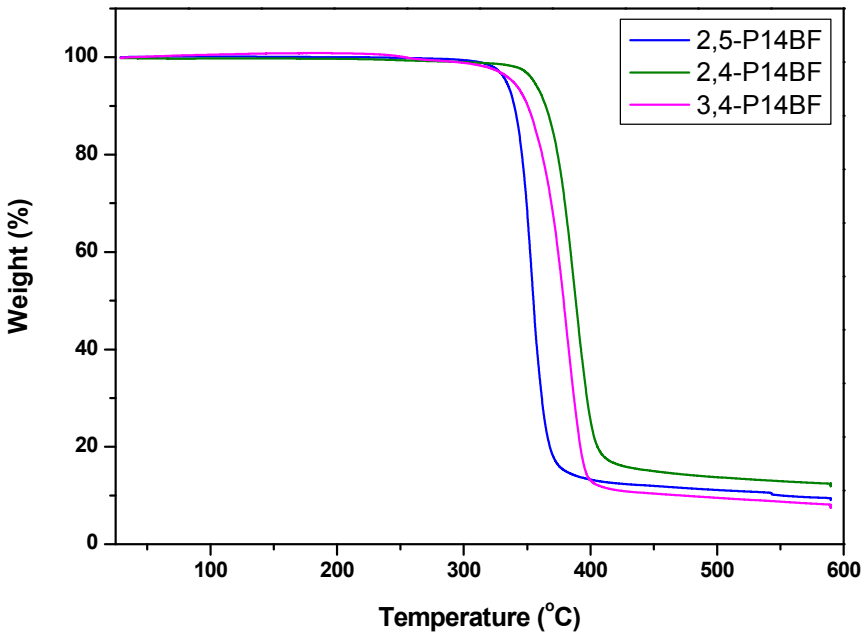

Figure 23: TGA traces of poly(1,4-butylene-furandicarboxylate)s recorded from 30-600 °C at 10 °C/min under N_2 atmosphere.

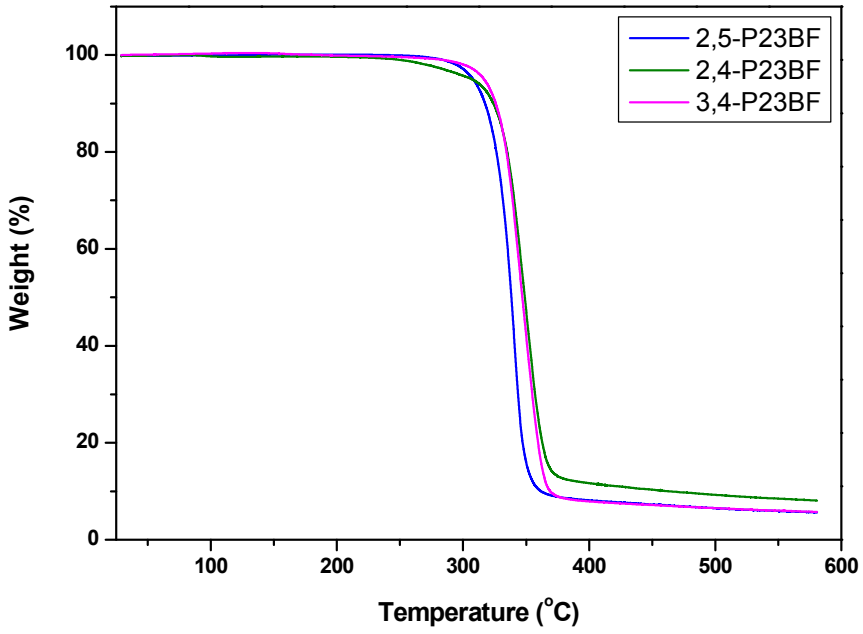

Figure 24: TGA traces of poly(2,3-butylene-furandicarboxylate)s recorded from 30-600 °C at 10 °C/min under N_2 atmosphere.

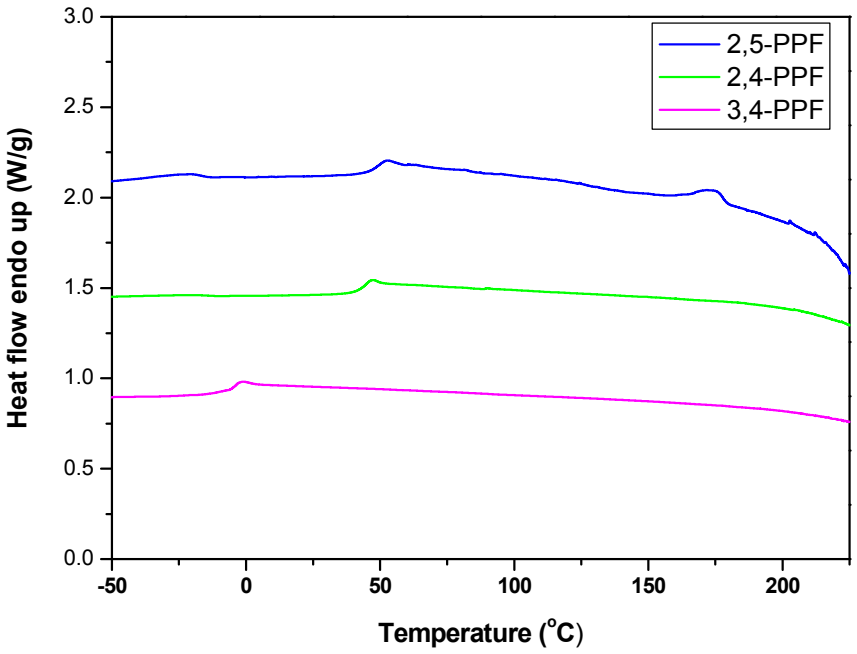

Figure 25. Second heating DSC curves of poly(1,3-propylene-furandicarboxylate)s derived from FDCA analogues. The experiments were carried out from −60 to 230 °C at a heating/cooling rate of 10 °C/min.

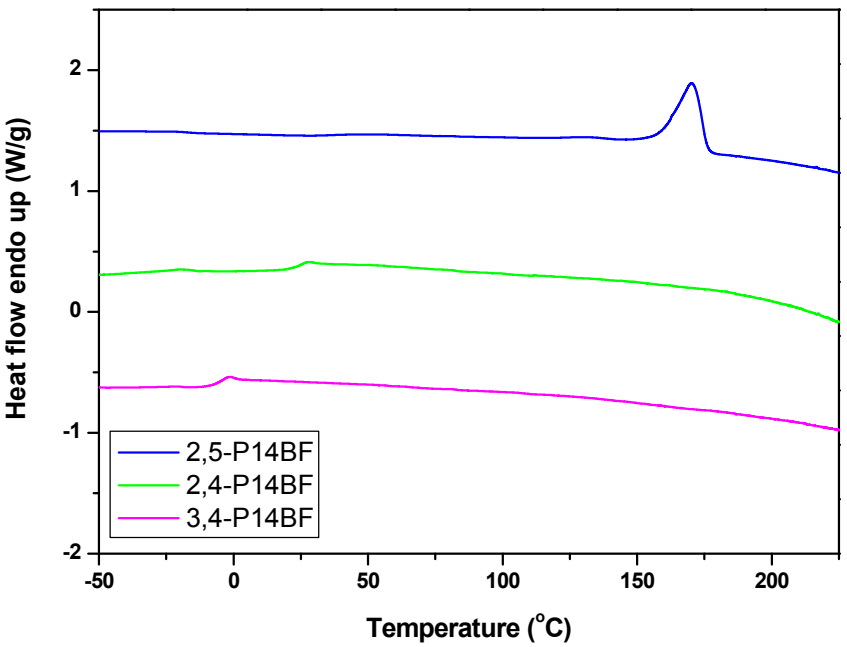

Figure 26. Second heating DSC curves of poly(1,4-butylene-furandicarboxylate)s derived from FDCA analogues. The experiments were carried out from −60 to 230 °C at a heating/cooling rate of 10 °C/min.

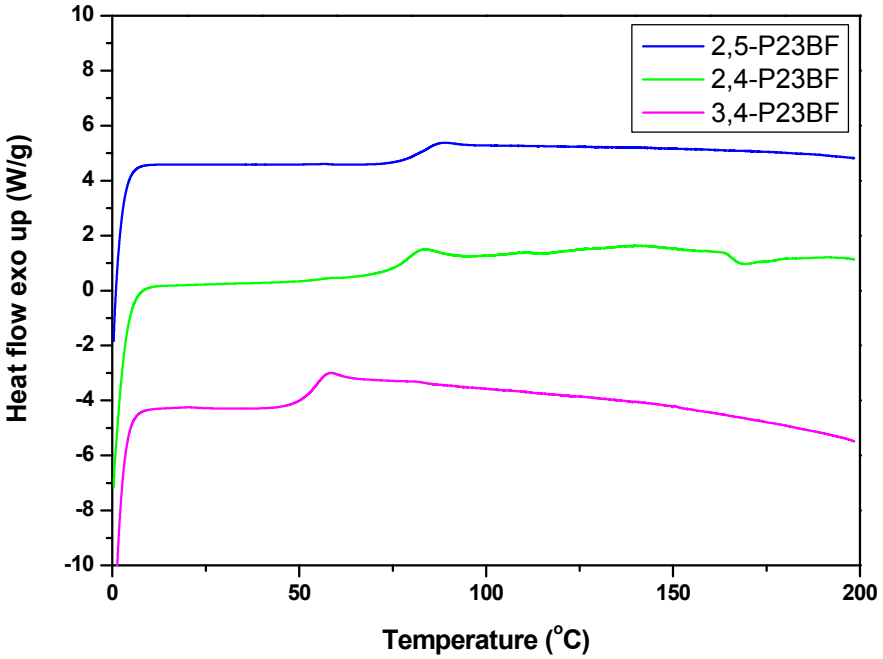

Figure 27. Second heating DSC curves of poly(2,3-butylene-furandicarboxylate)s derived from FDCA analogues. The experiments were carried out from 0 to 200 °C at a heating/cooling rate of 10 °C/min.

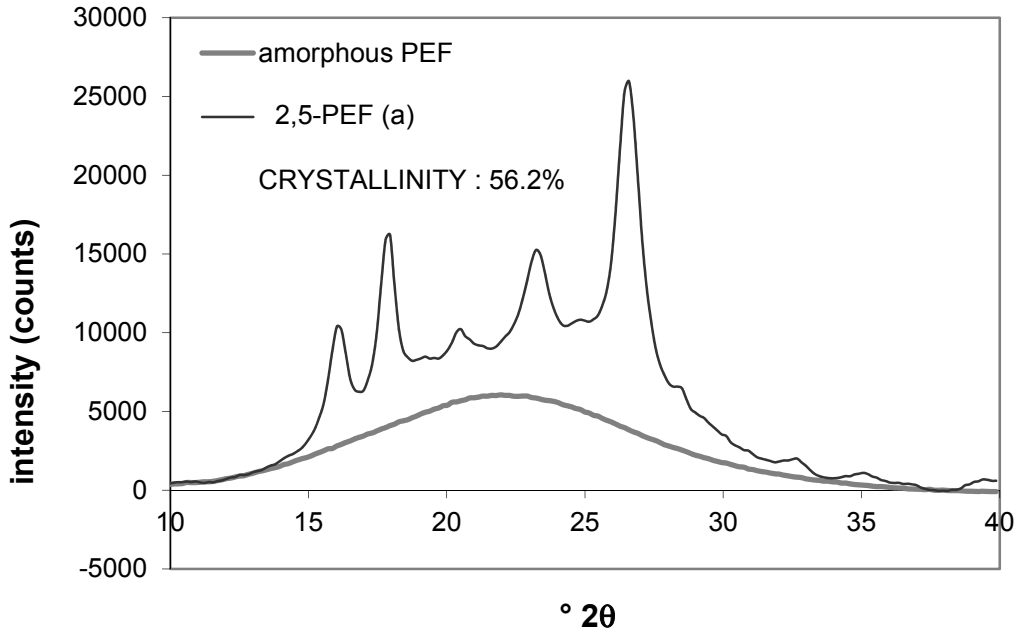

Figure 28. Wide angle X-ray powder diffraction profiles of annealed 2,5-PEF (a) and amorphous 2,5-PEF (obtained by quench cooling from the melt), for comparison and calculating the degree of crystallinity.

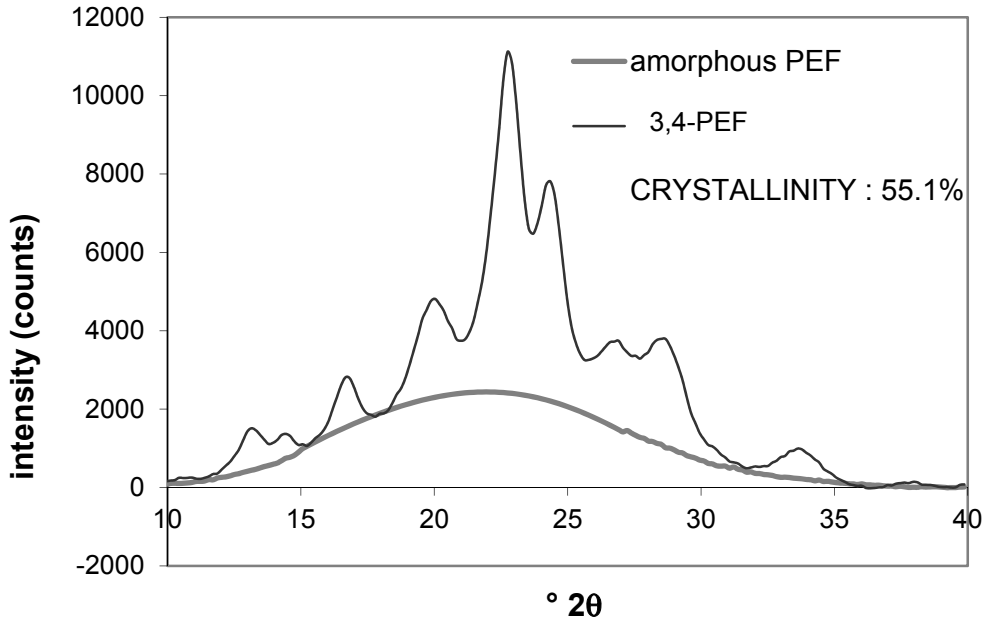

Figure 29. Wide angle X-ray powder diffraction profiles of precipitated 3,4-PEF and amorphous 3,4-PEF (obtained by quench cooling from the melt), for comparison and calculating the degree of crystallinity.

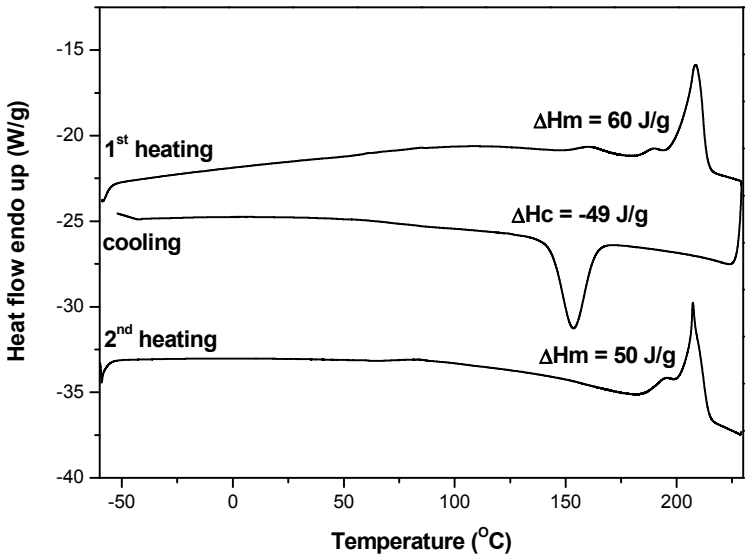

Figure 30. DSC curves of 2,5-PEF (a), annealed at 175 °C for 15 h. DSC runs were performed from -60 to 230 °C at a heating/cooling rate of 10 °C/min.

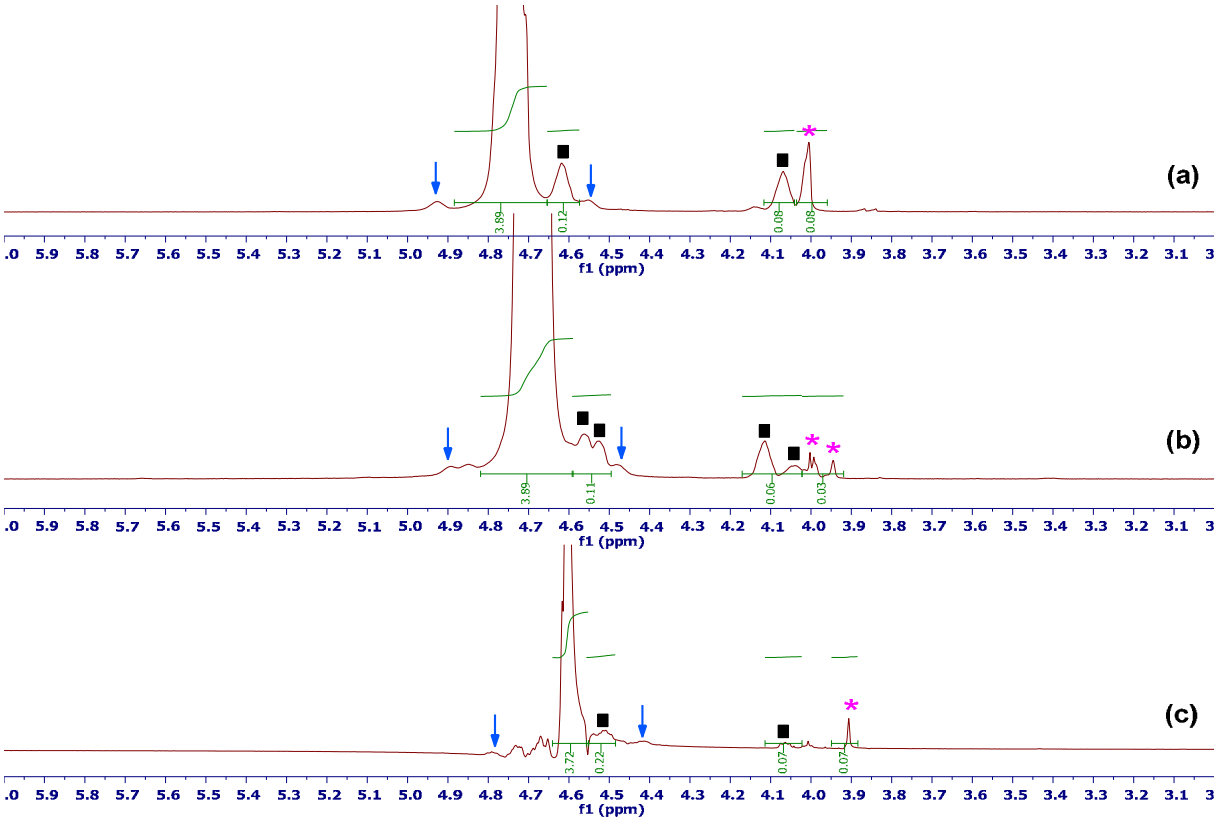

Figure 31. Zoom-in (3-6 ppm) of ^{1}H NMR spectra of (a) 2,5-PEF; (b) 2,4-PEF and (c) 3,4-PEF in $CDCl_3$/TFA-d (6:1). The pink asterisk indicate end groups, the black square indicate the presence of DEG groups and the blue arrow indicate the ^{13}C satellites shouldering the main peaks.