

Supporting Information

Bio-based Polycarbonates Derived from the Neolignan Honokiol

Kevin T. Wacker, Samantha L. Kristufek, Soon-Mi Lim, Sarosh Kahn, and Karen L. Wooley*

Departments of Chemistry, Chemical Engineering, Materials Science & Engineering, and the Laboratory for Synthetic-Biologic Interactions, Texas A&M University, College Station, Texas 77842-3012, United States

Contents

Additional Materials & Methods	S2
Figure S1. GPC – PHC in DMF (0.05 M LiBr)	S3
Figure S2. ATR-FTIR PHC – 55 kDa vs honokiol	S4
Figure S3. ATR-FTIR PHCs vs honokiol	S5
Figure S4. ¹ H (500 MHz) and ¹³ C (125 MHz) NMR spectrum for honokiol	S6
Figure S5. ¹ H (500 MHz) and ¹³ C (125 MHz) NMR spectrum for PHC – 15 kDa	S7
Figure S6. ¹ H (500 MHz) and ¹³ C (125 MHz) NMR spectrum for PHC – 33 kDa	S8
Figure S7. ¹ H (500 MHz) and ¹³ C (125 MHz) NMR spectrum for PHC – 55 kDa	S9
Figure S8. TGA of honokiol vs PHC – 40 kDa	S10
Figure S9. TGA of PHC – 15 kDa	S10
Figure S10. TGA of PHC – 33 kDa	S11
Figure S11. TGA of PHC – 55 kDa	S11
Figure S12. TGA of poly(bisphenol A carbonate) – 21 kDa	S12
Figure S13. TGA of polylactic acid – 30 kDa	S12
Figure S14. DMA of PHC – 23 kDa	S13
Figure S15. DMA of PHC – 31 kDa	S13
Figure S16. DMA of PHC – 37 kDa	S14
Figure S17. DMA composite overlay	S15
Figure S18. DSC of powder samples	S16
Figure S19. DSC of bar samples – 10 °C/min	S16
Figure S20. DSC of bar samples – 40 °C/min	S17
Figure S21. MTS Assay	S18

Additional Materials & Methods for Biological Assays

Coronary venular endothelial cells (CVEC) were kindly provided by Profs. Cynthia J. Meininger and Andreea Trache (Texas A&M Health Science Center, College Station, TX, USA). CVECs were cultured in GIBCO® Dulbecco's Modified Eagle Medium: Nutrient Mixture F-12 (DMEM/F-12) (Invitroge, Carlsbad, CA) mixed with 10% fetal bovine serum (Sigma Aldrich, St. Louis, MS), 100 U/mL penicillin - 100 U/mL streptomycin - 0.25 mg/mL amphotericin B (Lonza, Walkersville, MD), and 20 units/mL heparin (Midwest Vet Supply, Lakeville, MN). Cells (10×10^3 cells/well) were plated in 96-well plate (coated with 1% gelatin) and incubated at 37 °C in a humidified atmosphere containing 5% CO₂ for 24 h to adhere. Then, the medium was replaced with a fresh medium 1 h prior to the addition of 20 µL of poly(honokiol carbonate) stock solution (DMSO) to 100 µL of the medium (final concentrations ranged from 10 - 0.0048 µM). The cells were incubated with the formulations for 72 h, and then the medium was replaced with 100 µL of the fresh complete media. MTS combined reagent (20 µL) was added to each well (Cell Titer 96® Aqueous Non-Radioactive Cell Proliferation Assay, Promega Co., Madison, WI). The cells were incubated with the reagent for 2 h at 37 °C in a humidified atmosphere containing 5% CO₂ protected from light. Absorbance was measured at 490 nm using SpectraMax M5 (Molecular Devices Co., Sunnyvale, CA). The cell viability was calculated based on the relative absorbance to the control-untreated cells. IC₅₀ values of the polymer could not be determined because high cell-viabilities were observed at the range of the tested concentrations (10 - 0.0048 µM).

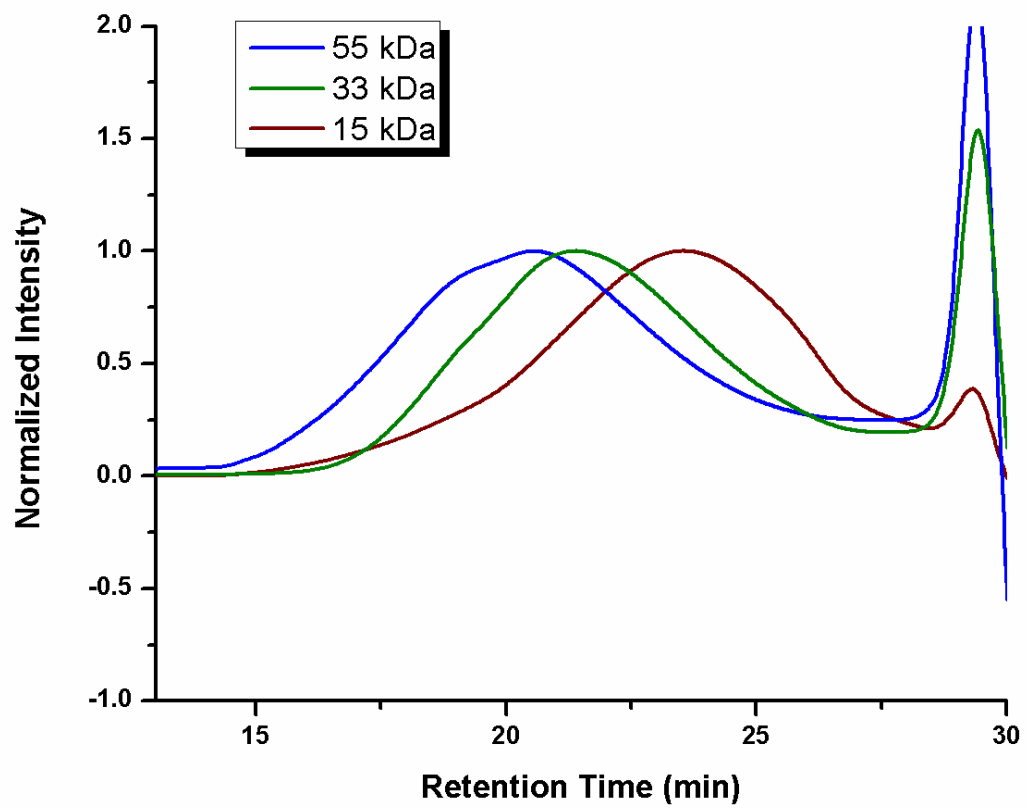


Figure S1. SEC traces of PHC in DMF (0.05 M LiBr) eluent.

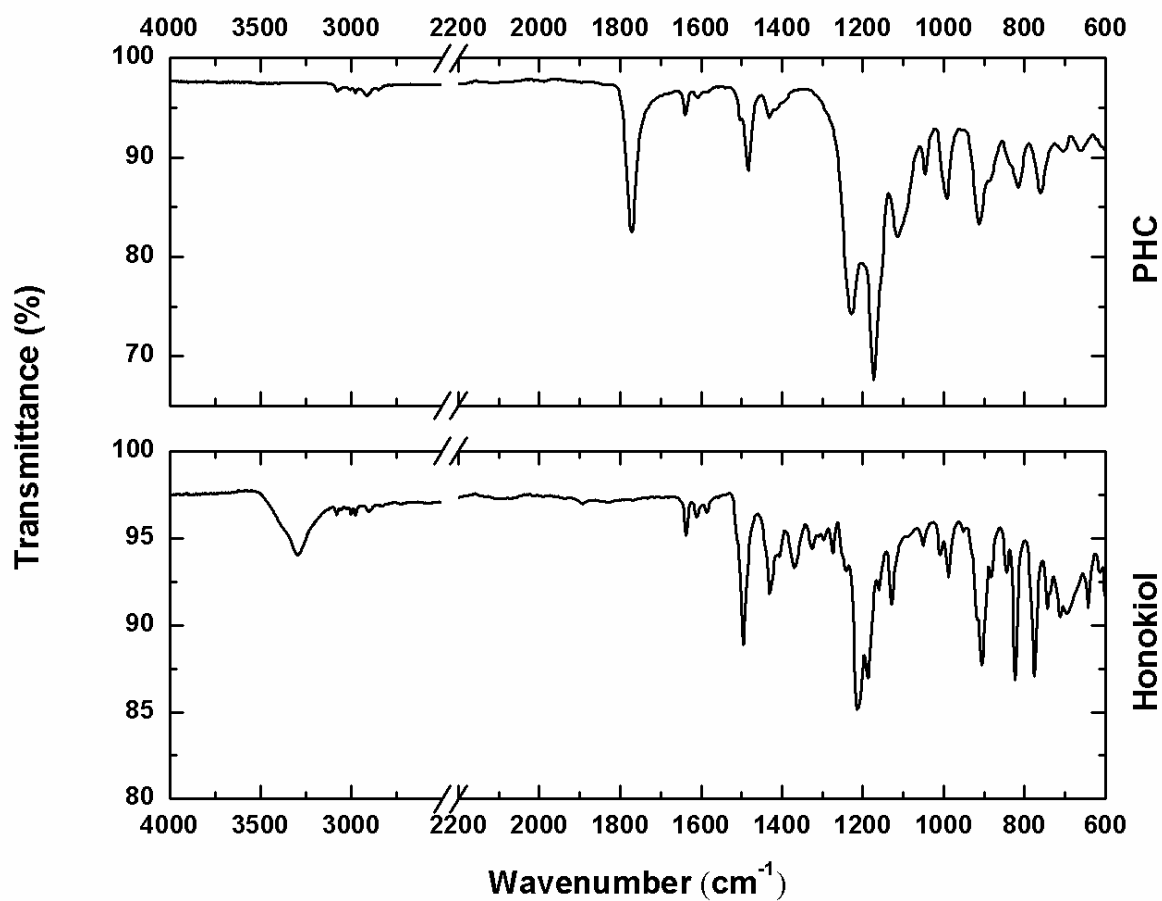


Figure S2. ATR-FTIR spectra comparing PHC-55 kDa and honokiol.

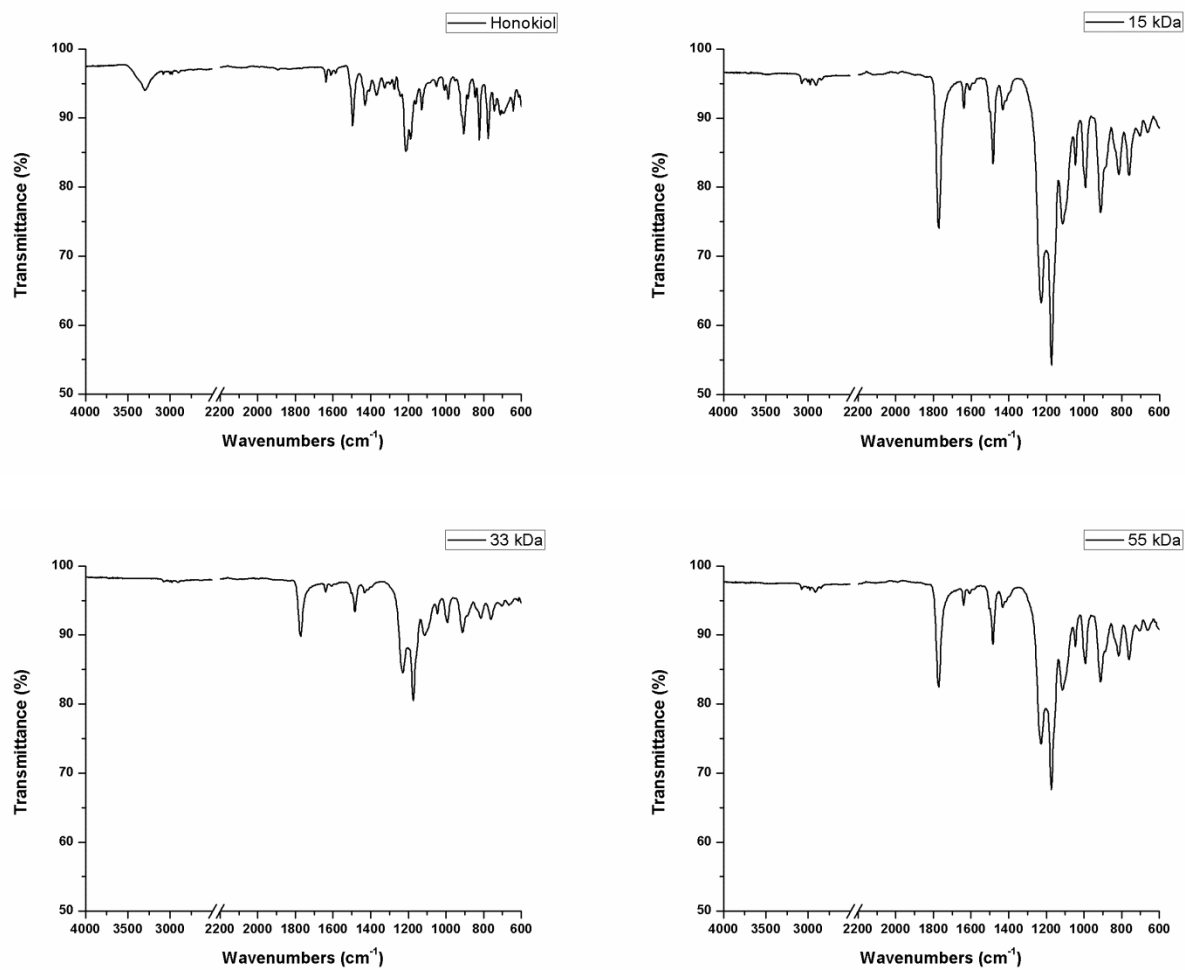


Figure S3. ATR-FTIR spectra comparing PHC and honokiol.

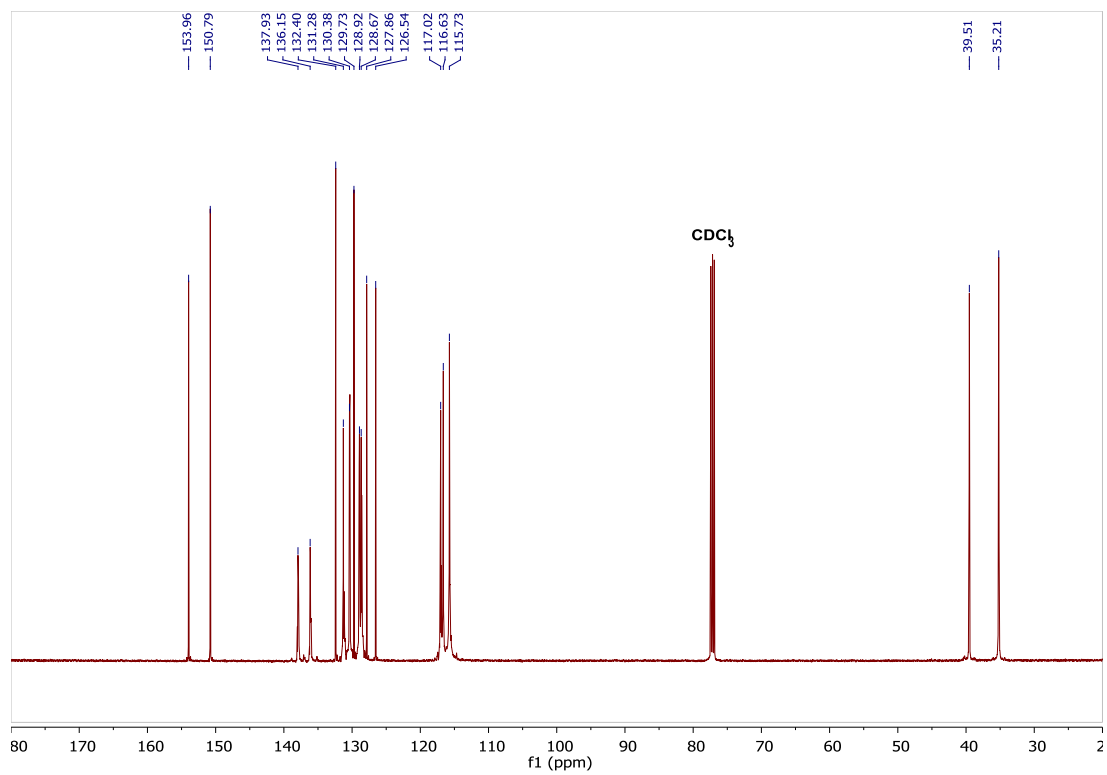
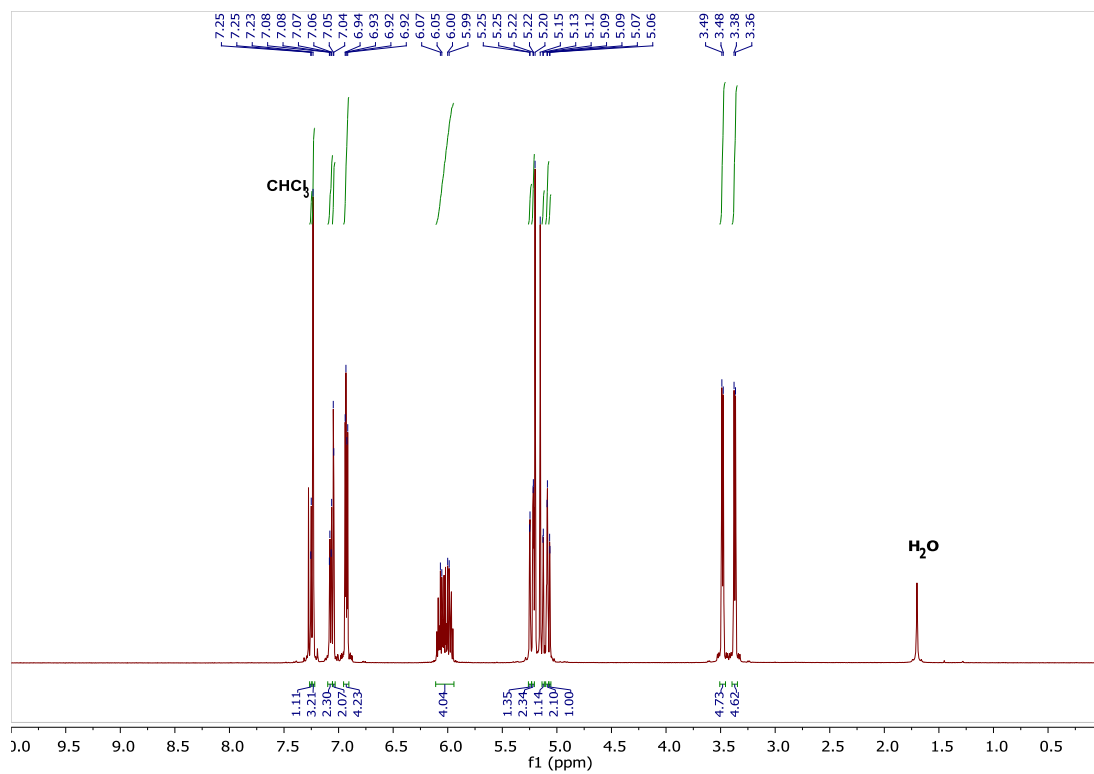


Figure S4. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra for honokiol.

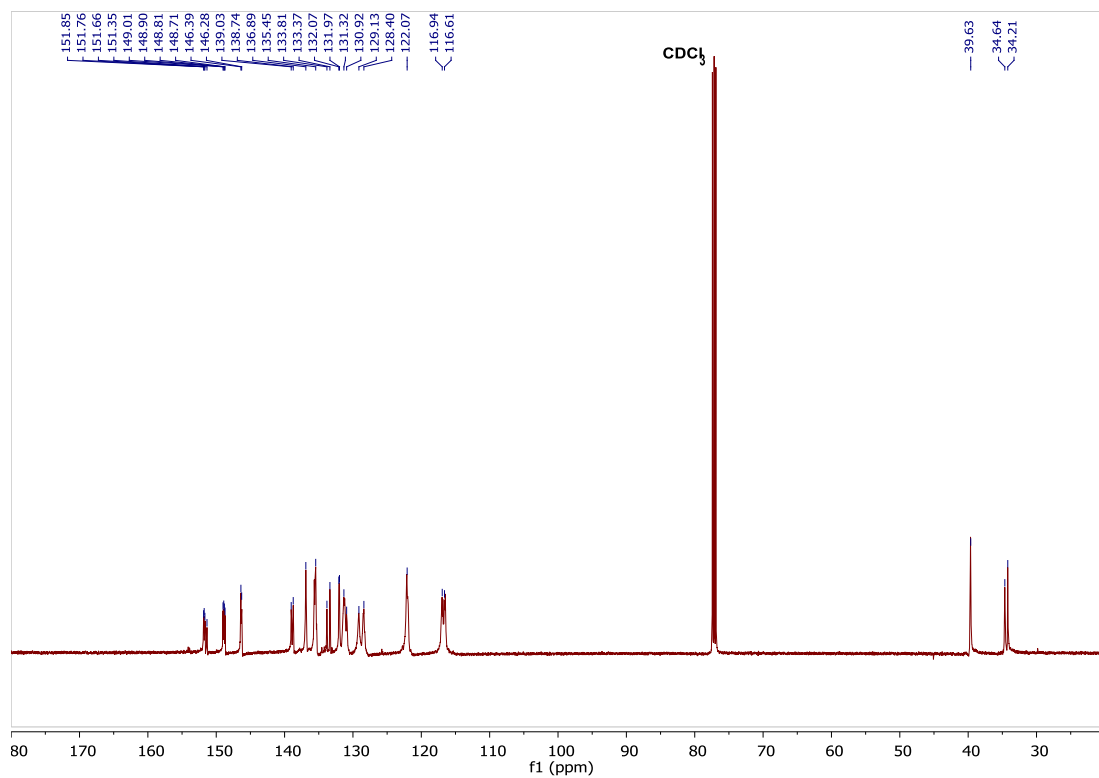
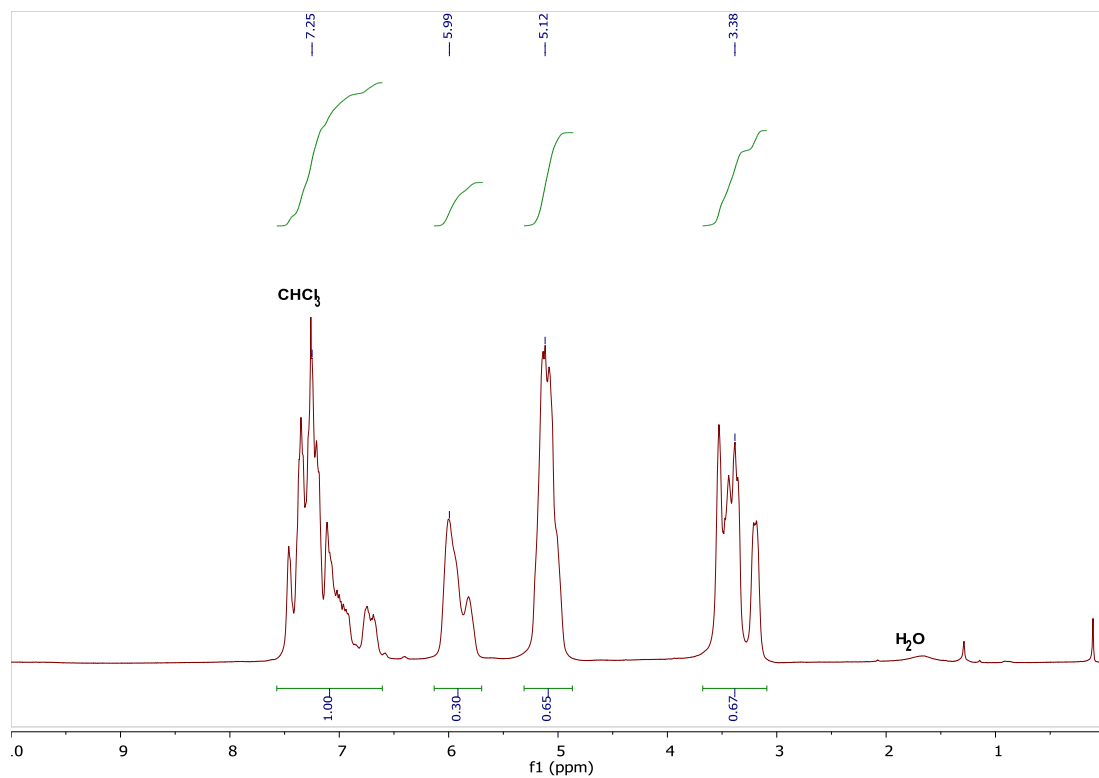


Figure S5. ¹H (500 MHz) and ¹³C (125 MHz) NMR spectra for poly(honokiol carbonate) having a *M_n* of 15 kDa.

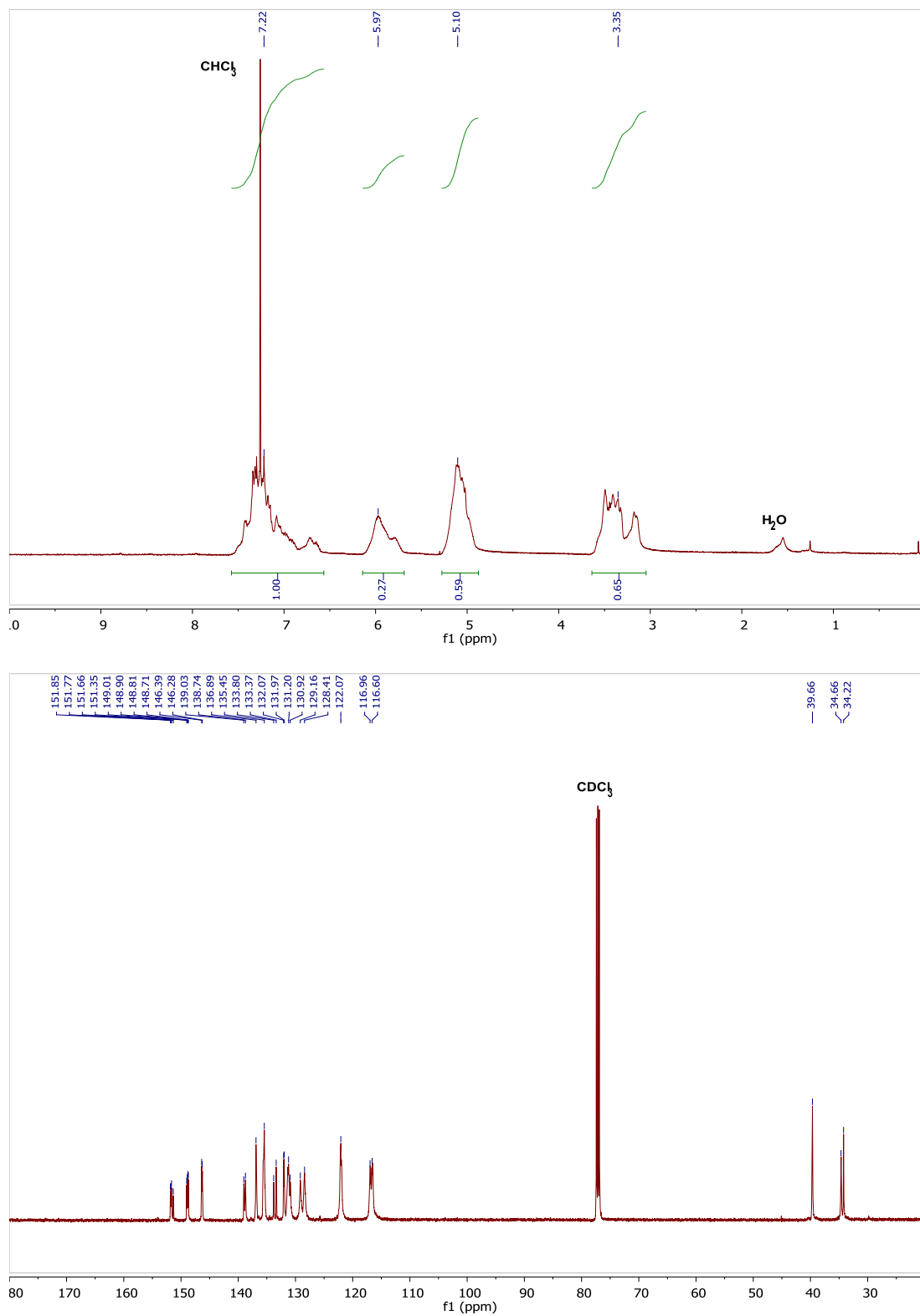


Figure S6. ^1H (500 MHz) and ^{13}C (125 MHz) NMR spectra for poly(honokiol carbonate) having a M_n of 33 kDa.

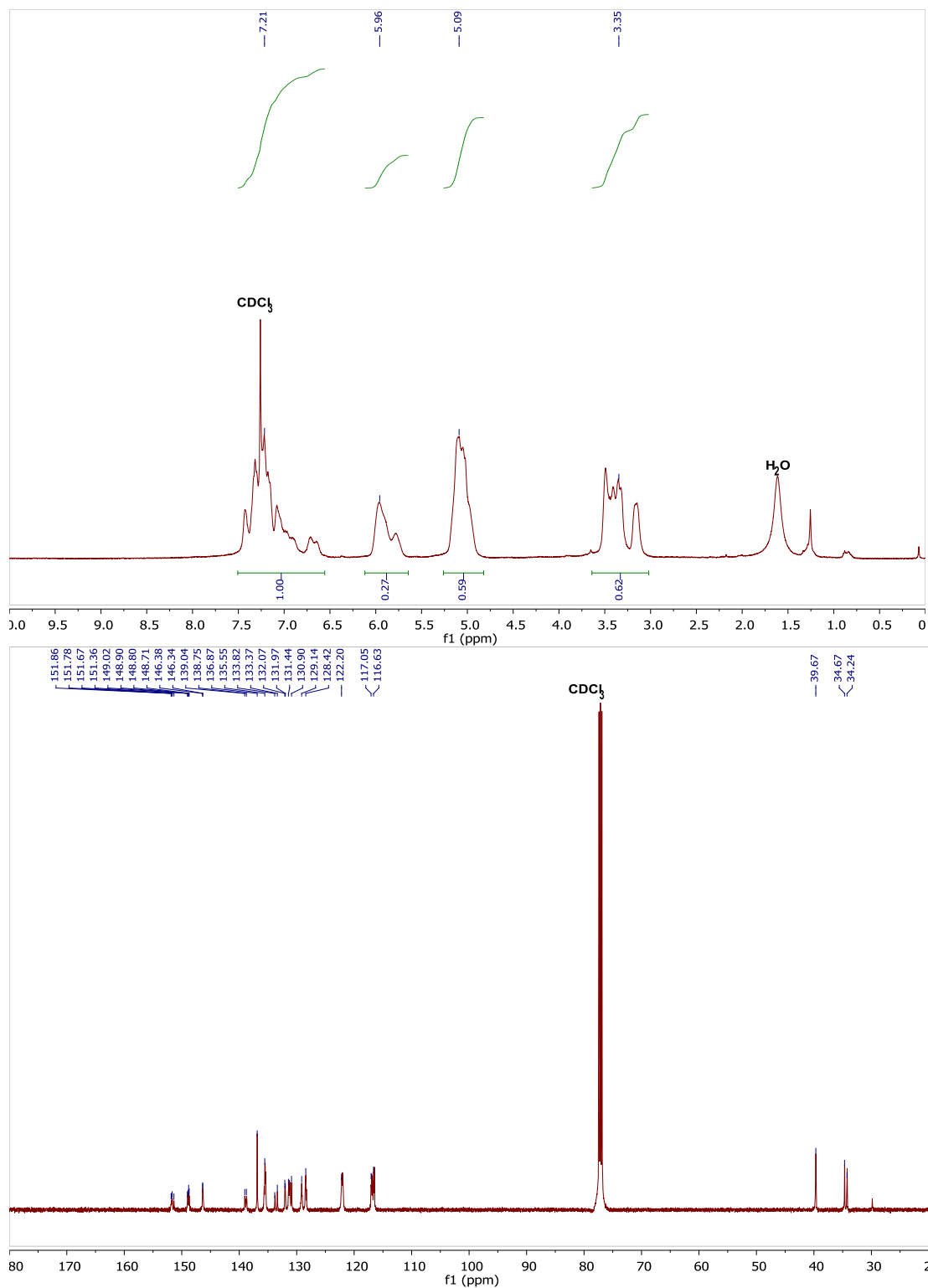


Figure S7. ^1H (500 MHz) and ^{13}C (125 MHz) NMR spectra for poly(honokiol carbonate) having a M_n of 55 kDa.

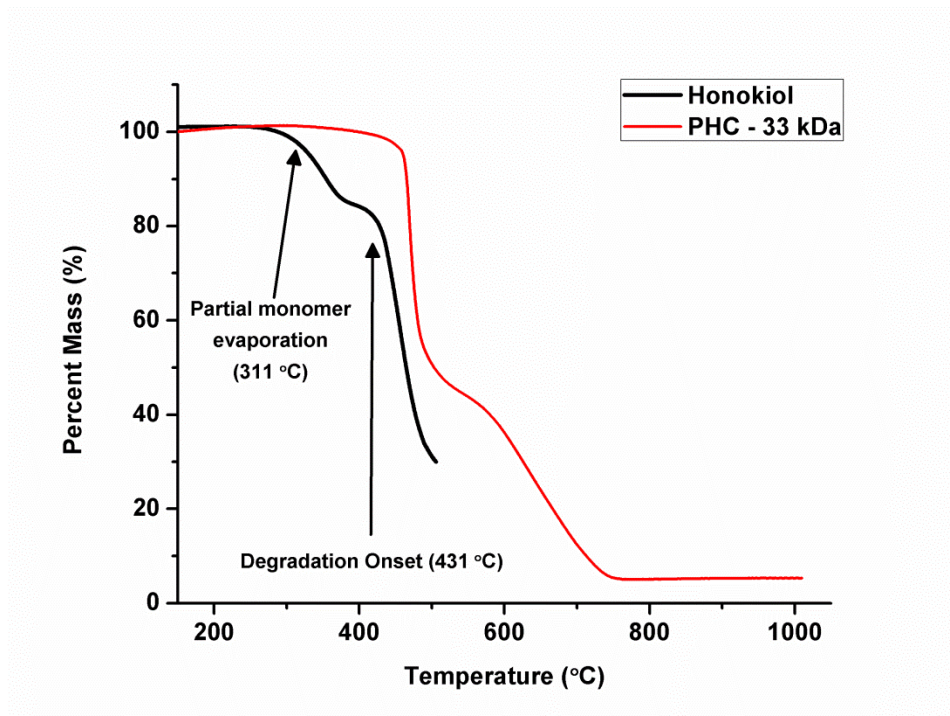


Figure S8. TGA – Thermal degradation of honokiol and PHC having a M_n of 33 kDa.

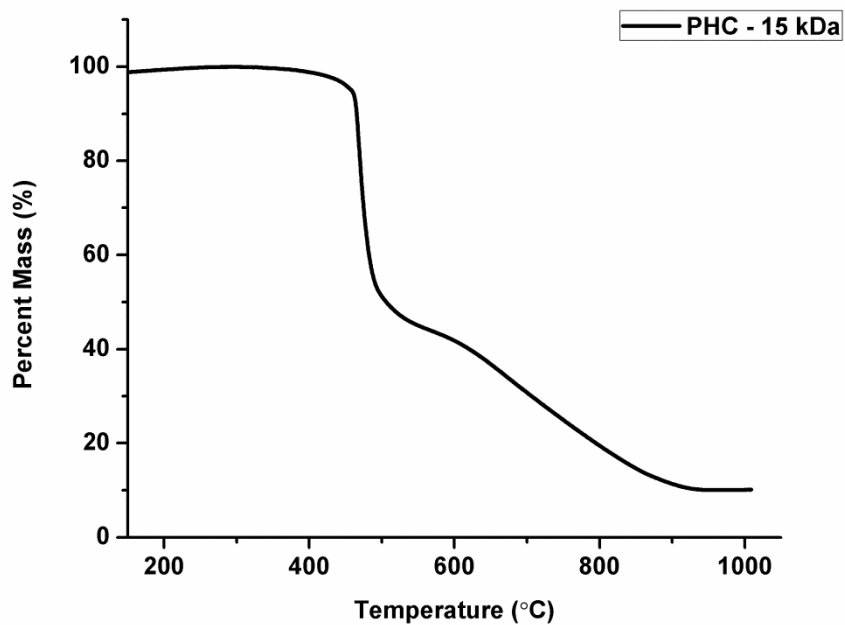


Figure S9. TGA – Thermal degradation of PHC having a M_n of 15 kDa.

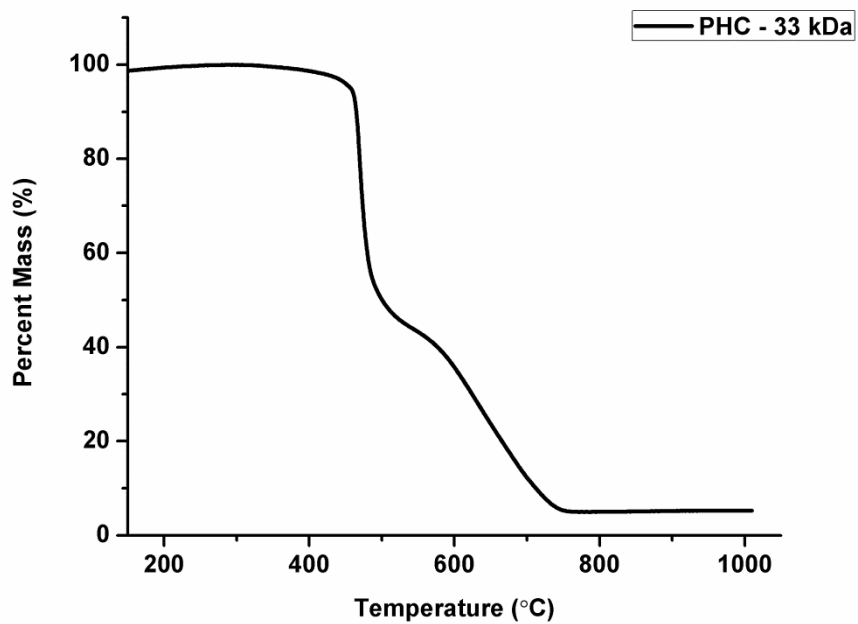


Figure S10. TGA – Thermal degradation of PHC having a M_n of 33 kDa.

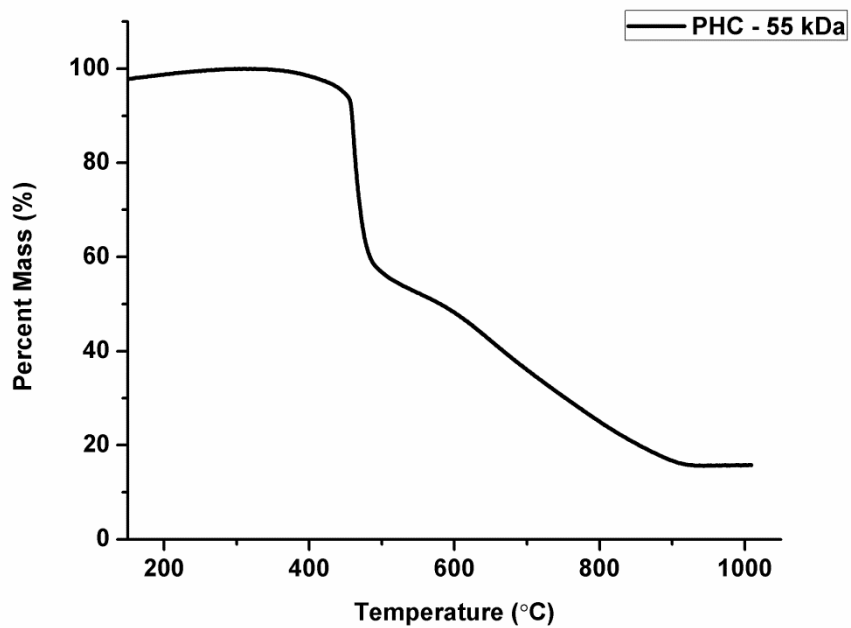


Figure S11. TGA – Thermal degradation of PHC having a M_n of 55 kDa.

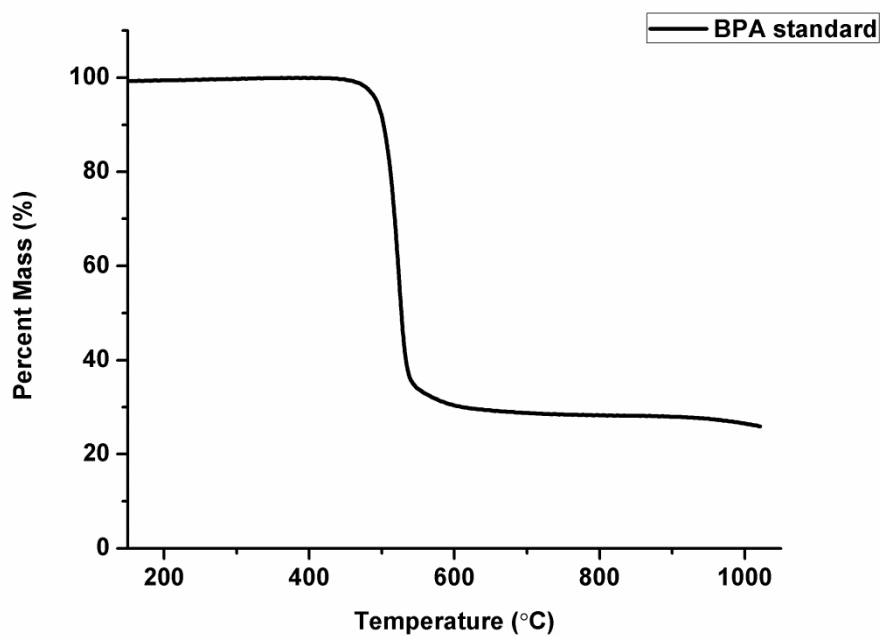


Figure S12. TGA – Thermal degradation of poly(BPA carbonate) having a M_n of 21 kDa.

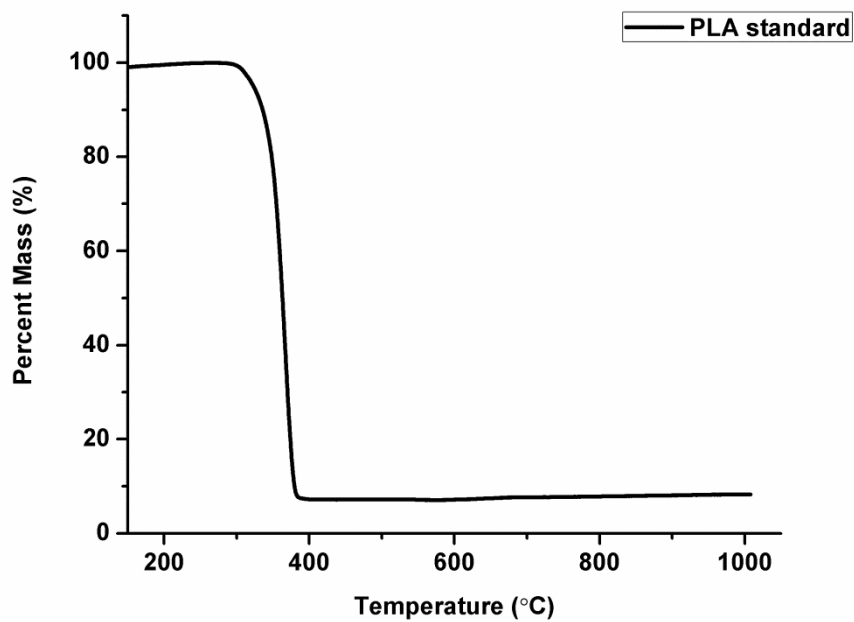


Figure S13. TGA – Thermal degradation of poly(lactic acid) having a M_n of 30 kDa.

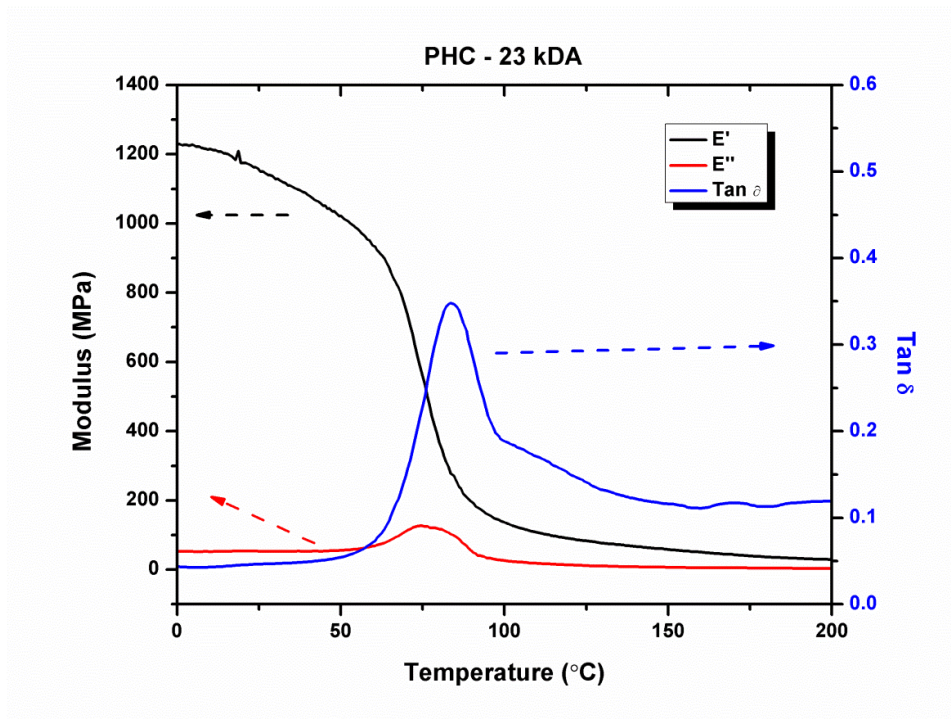


Figure S14. DMA – Representative dynamic mechanical analysis of PHC having a M_n of 23 kDa.

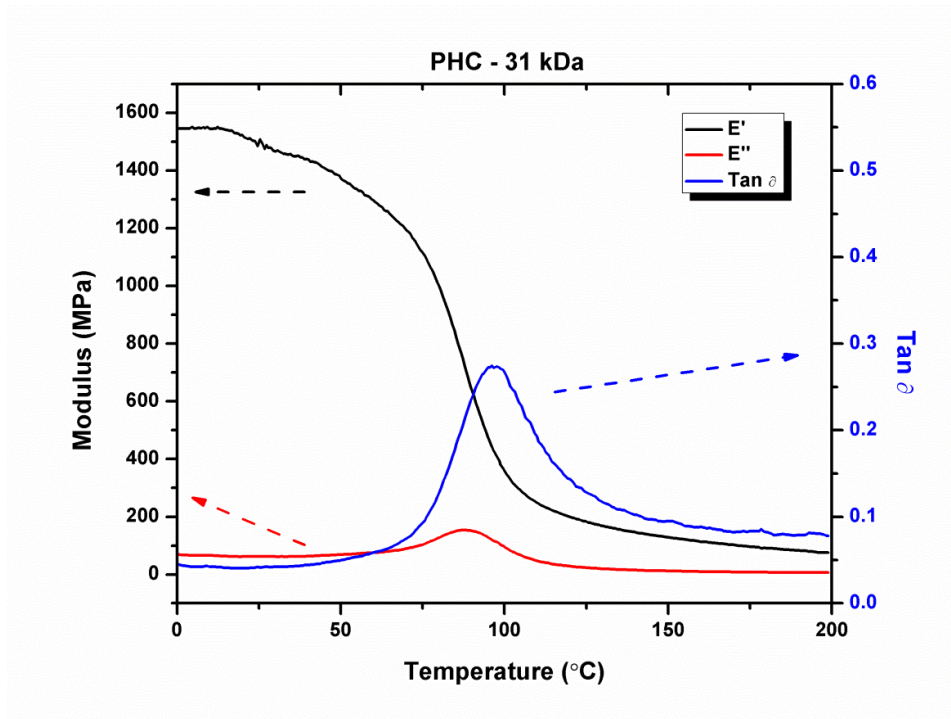


Figure S15. DMA – Representative dynamic mechanical analysis of PHC having a M_n of 31 kDa.

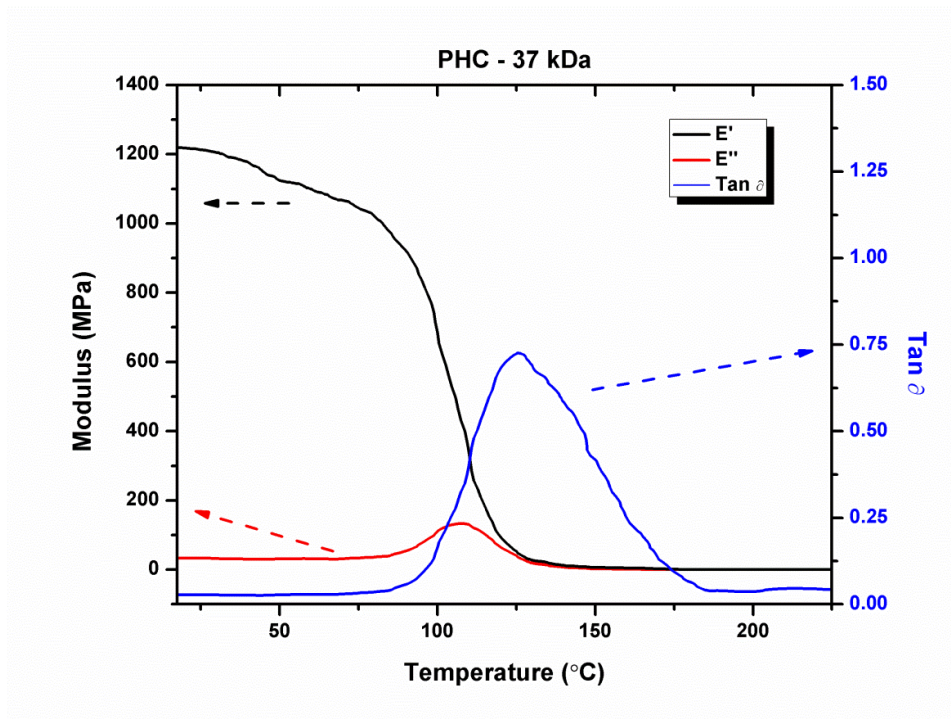


Figure S16. DMA – Representative dynamic mechanical analysis of PHC having a M_n of 37 kDa.

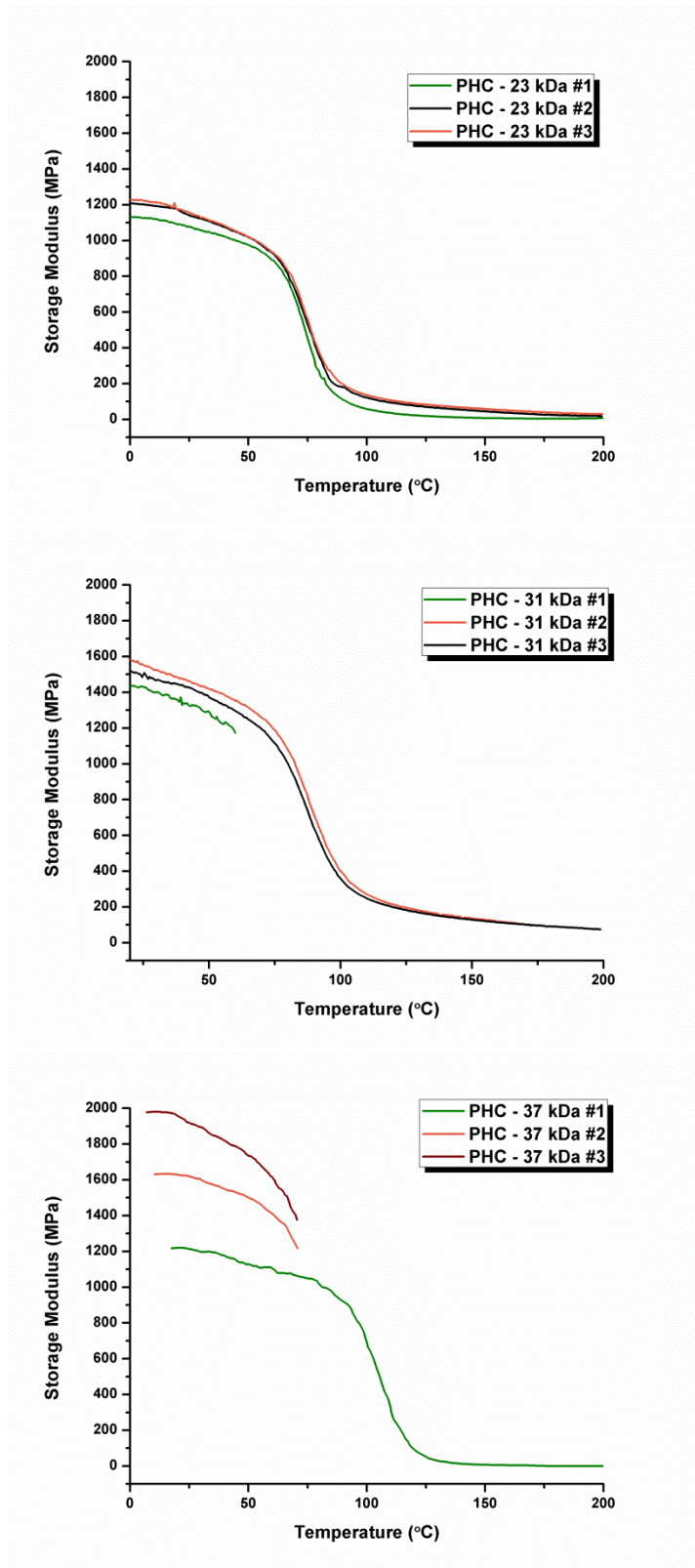


Figure S17. DMA – Composite of storage moduli traces collected for each of the PHC samples having M_n values of (a) 23 kDa, (b) 31 kDa, (c) 37 kDa.

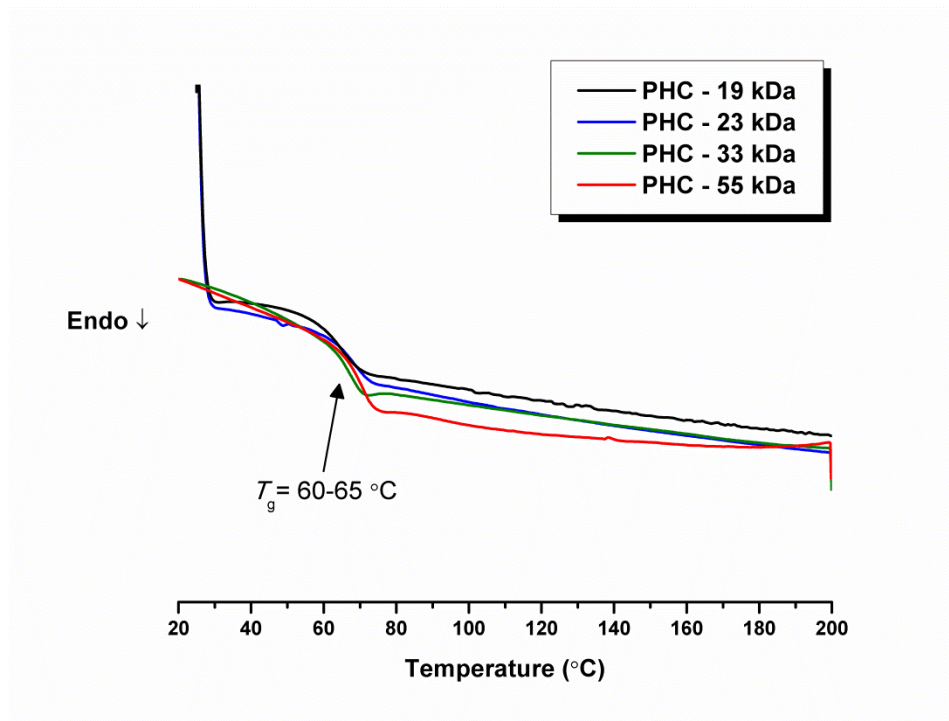


Figure S18. DSC traces of powder PHC samples showing T_g s all in the range of 60-65 °C.

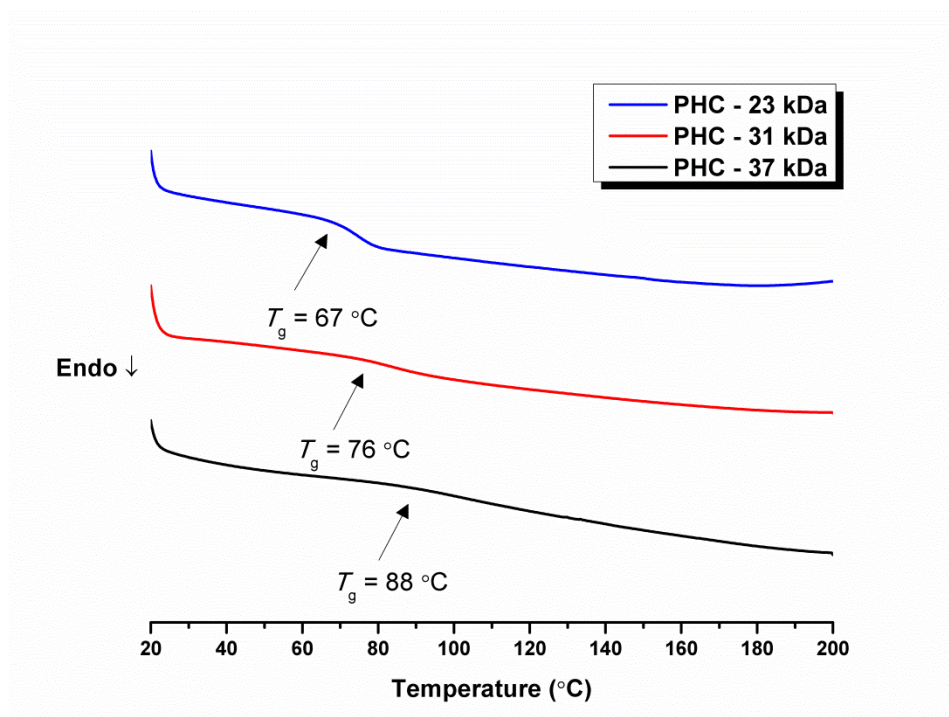


Figure S19. DSC traces of PHC bars used in DMA analyses showing an increase in T_g higher than powder samples. Heating rate: 10 °C/min.

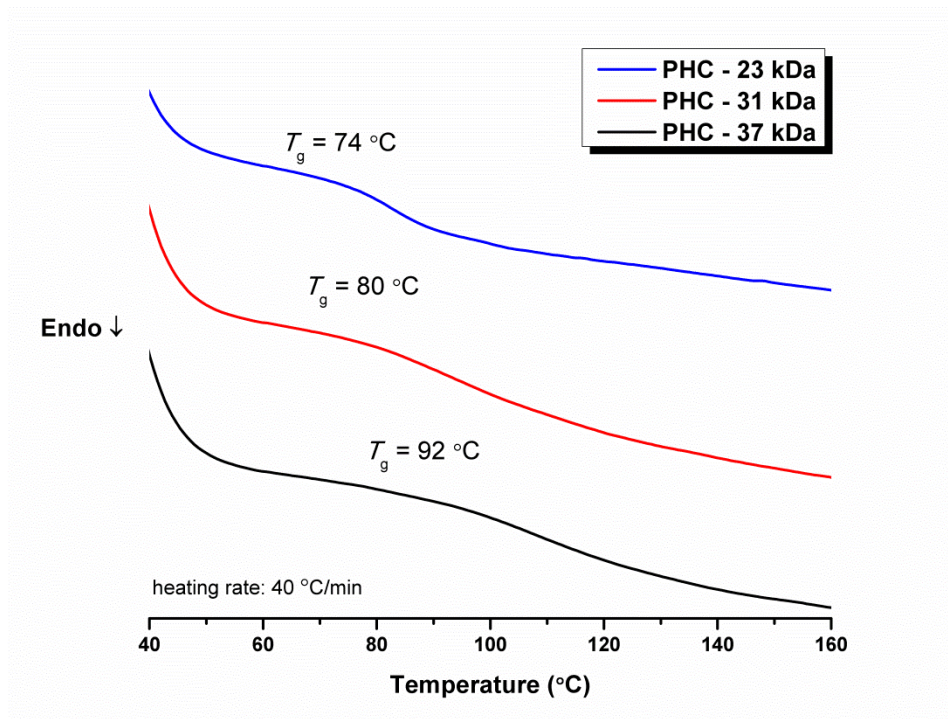


Figure S20. DSC traces of PHC bars used in DMA analyses showing an increase in T_g with increase in molecular weight. Heating rate: 40 °C/min.

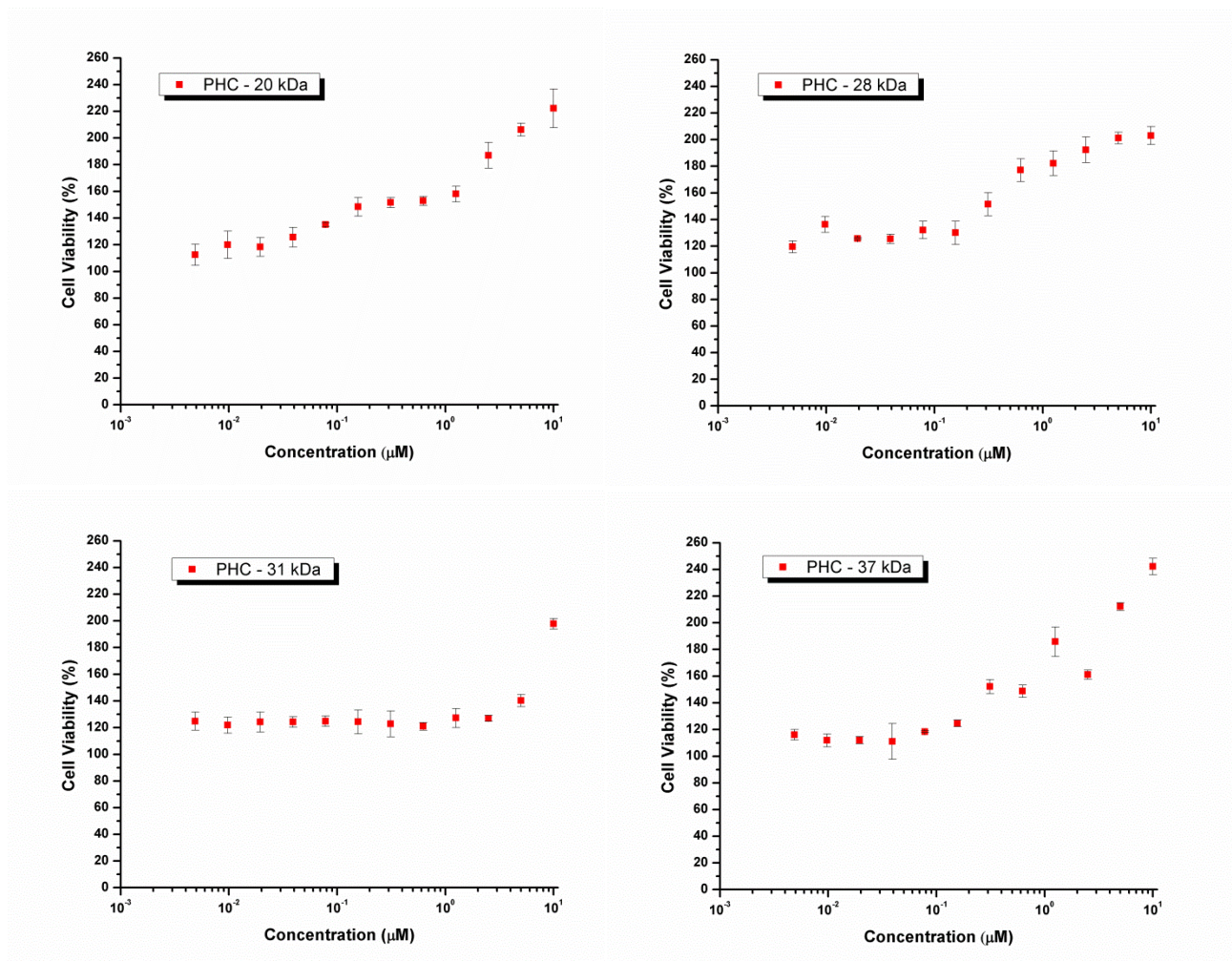


Figure S21. MTS cytotoxicity assays comparing cell viability to control group.