

SUPPLEMENTARY MATERIAL

Theoretical Calculations for Highly Selective Direct Heteroarylation Polymerization: New Nitrile-Substituted Dithienyl-Diketopyrrolopyrrole-Based Polymers

Thomas Bura ^{1,†}, Serge Beaupré ^{1,†}, Marc-André Légaré ², Olzhas A. Ibraikulov ³, Nicolas Leclerc ⁴ and Mario Leclerc ^{1,*}

¹ Canada Research Chair on Electroactive and Photoactive Polymers, Department of Chemistry, Université Laval, G1V 0A6 Quebec City, Canada; thomas.bura.1@ulaval.ca (T.B.); serge.beaupre.1@ulaval.ca (S.B.)

² Institut für Anorganische Chemie, Julius-Maximilians Universität Würzburg, Am Hubland, 97074 Würzburg, Germany; marcandrelegare@gmail.com

³ Laboratoire ICube, DESSP, Université de Strasbourg, CNRS, 23 rue du Loess, 67037 Strasbourg, France; ibraikulov@unistra.fr

⁴ Institut de Chimie et Procédés pour l'Énergie, l'Environnement et la Santé, ICPEES, Université de Strasbourg, CNRS, 67087 Strasbourg, France; leclercn@unistra.fr

* Correspondence: Mario.Leclerc@chm.ulaval.ca

Figures S1-S13: ¹H-and ¹³C-NMR spectra 2-8

Figures S14-S17: Infrared spectra 9-10

Figures S18-S20: GPC chromatograms for polymers **P6, P7a and P7b** 11-12

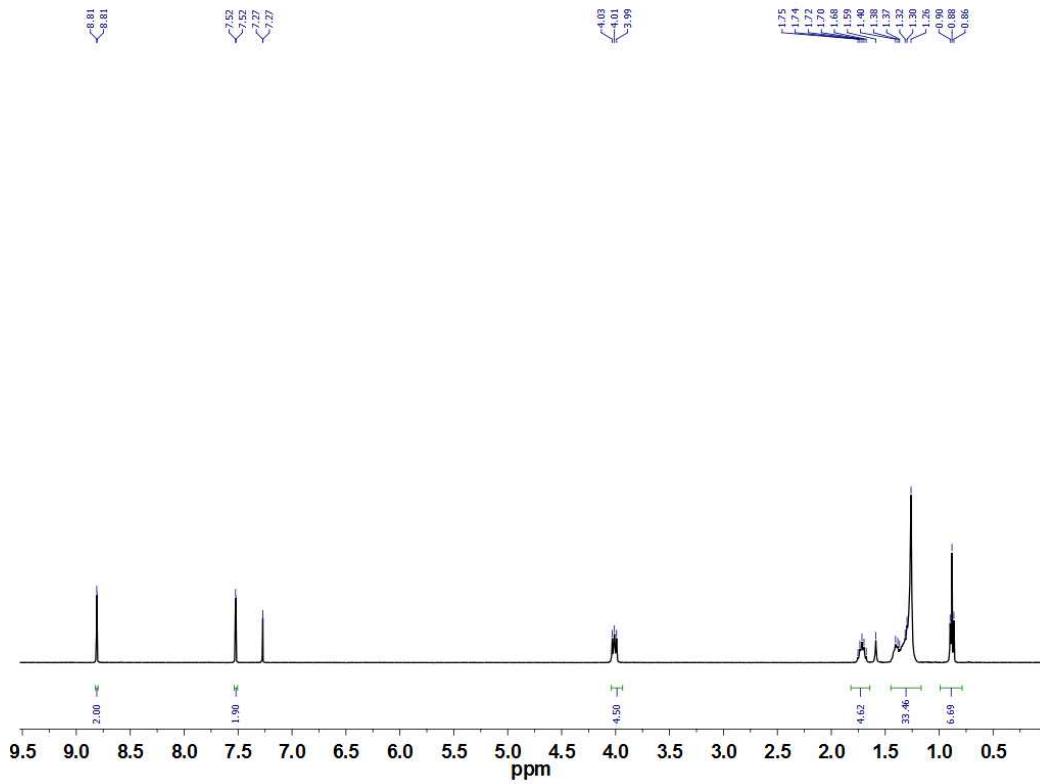


Figure S1 : ^1H -NMR spectrum in CDCl_3 of compound 3.

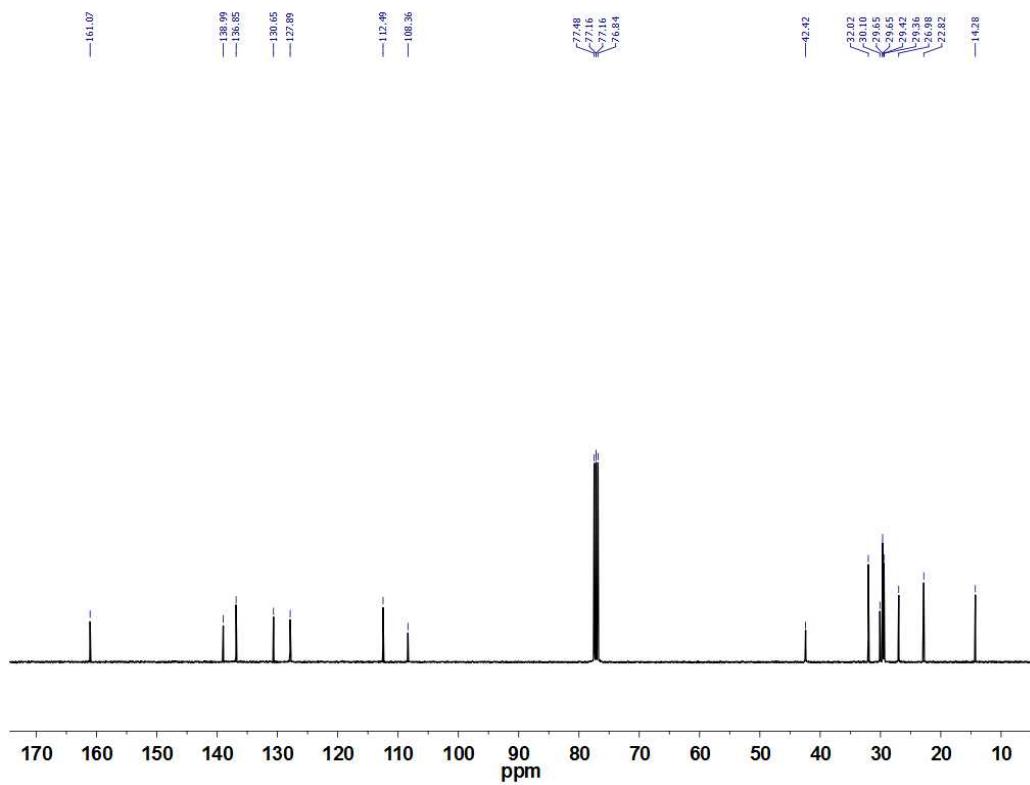


Figure S2 : ^{13}C -NMR spectrum in CDCl_3 of compound 3.

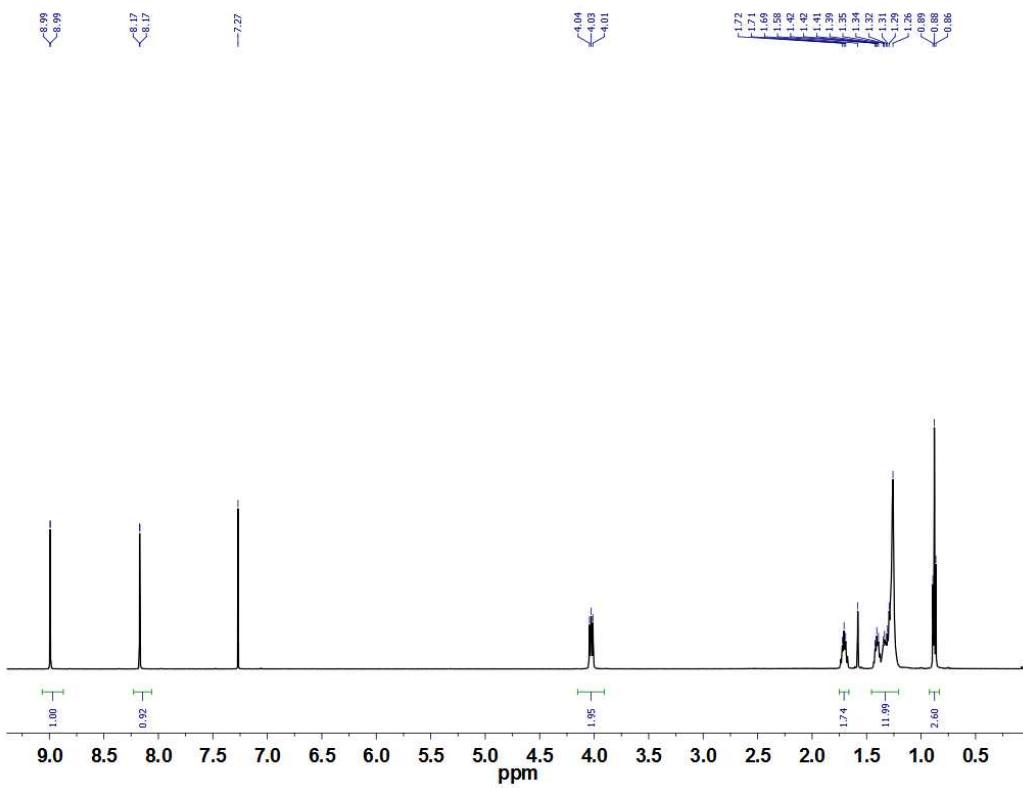


Figure S3 : ^1H -NMR spectrum in CDCl_3 of compound M7.

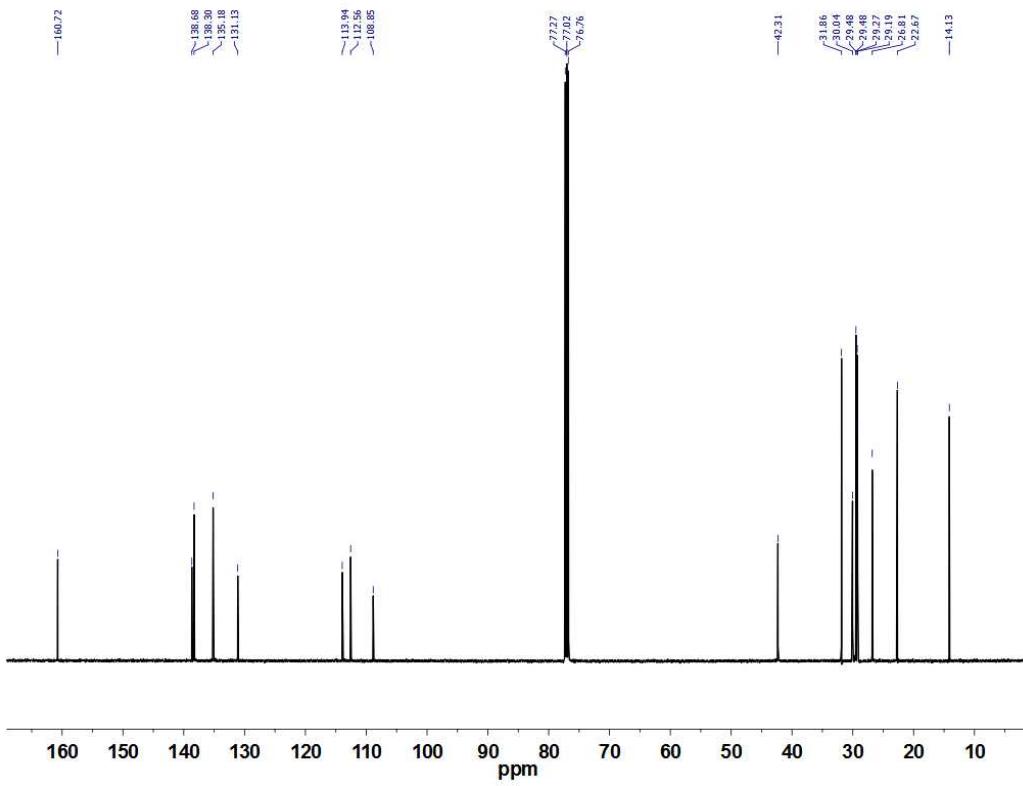


Figure S4 : ^{13}C -NMR spectrum in CDCl_3 of compound M7.

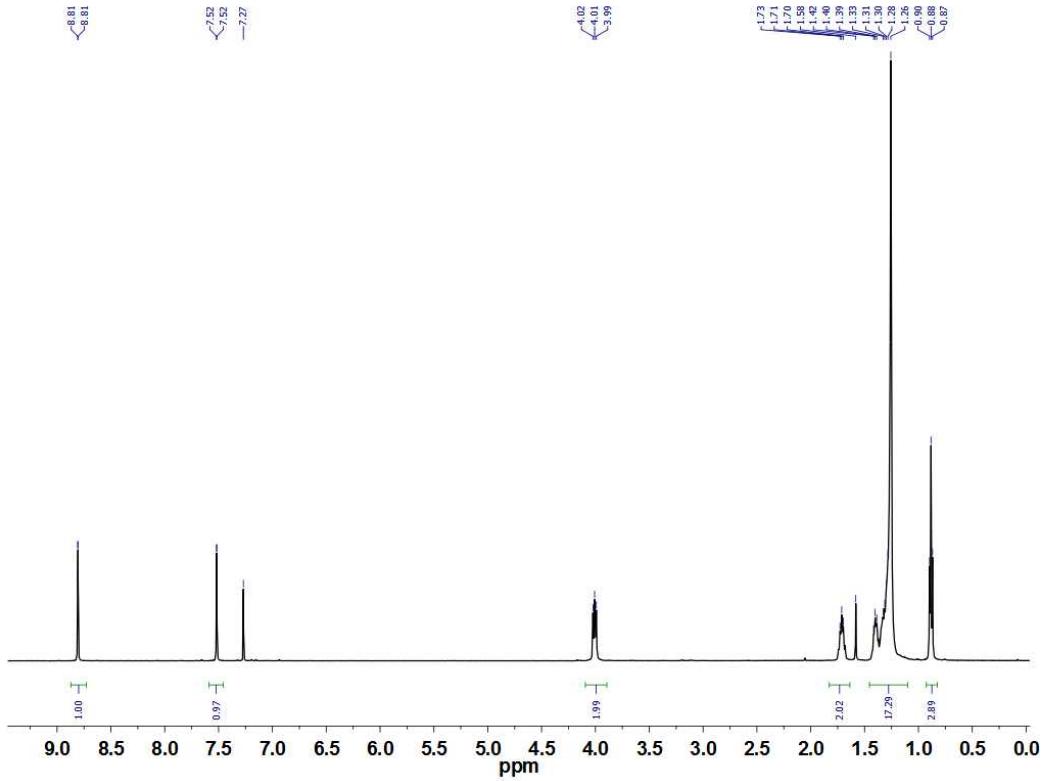


Figure S5 : ^1H -NMR spectrum in CDCl_3 of compound 4.

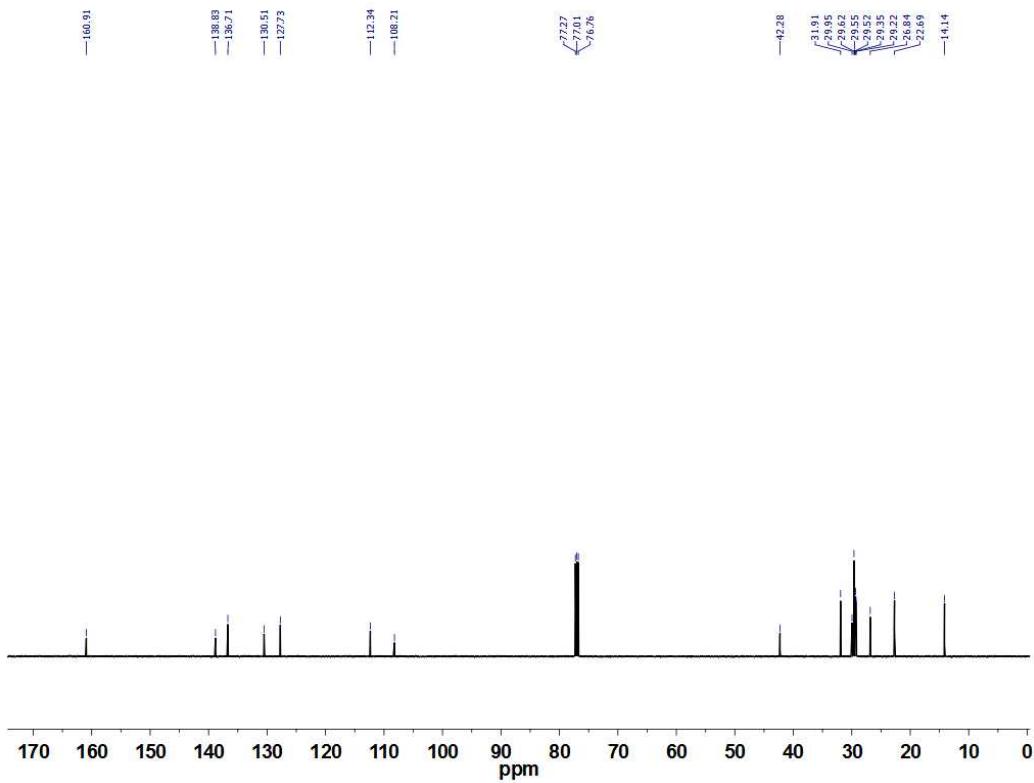


Figure S6 : ^{13}C -NMR spectrum in CDCl_3 of compound 4.

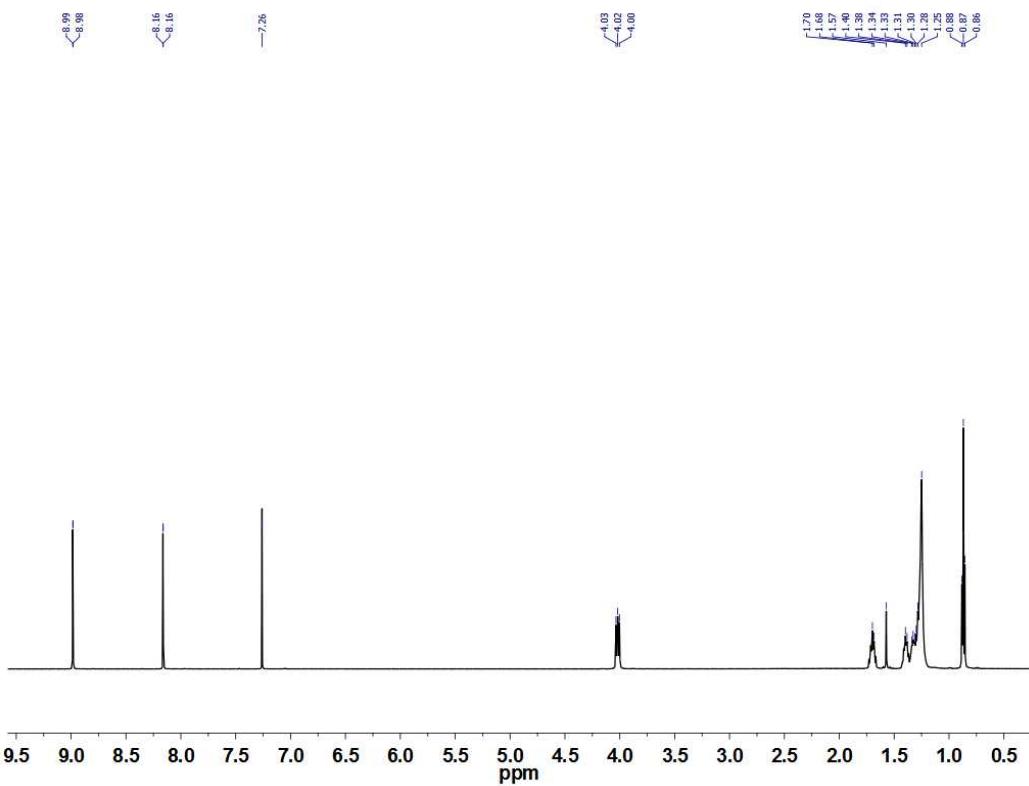


Figure S7: ^1H -NMR spectrum in CDCl_3 of compound **M8**.

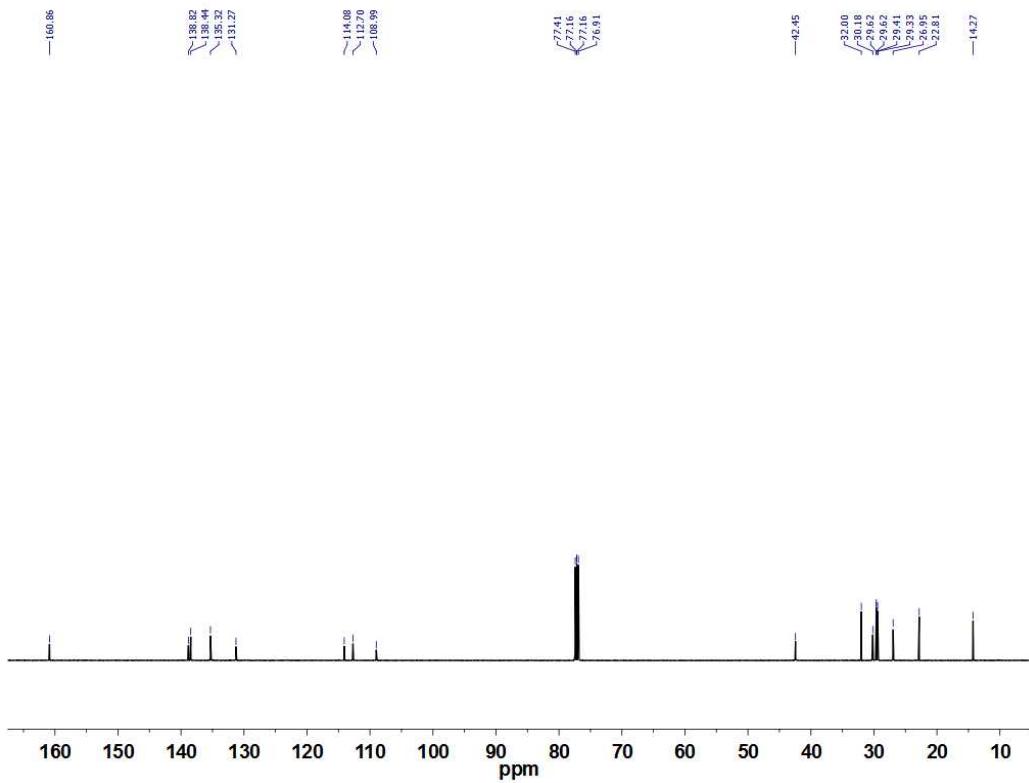


Figure S8 : ^{13}C -NMR spectrum in CDCl_3 of compound **M8**.

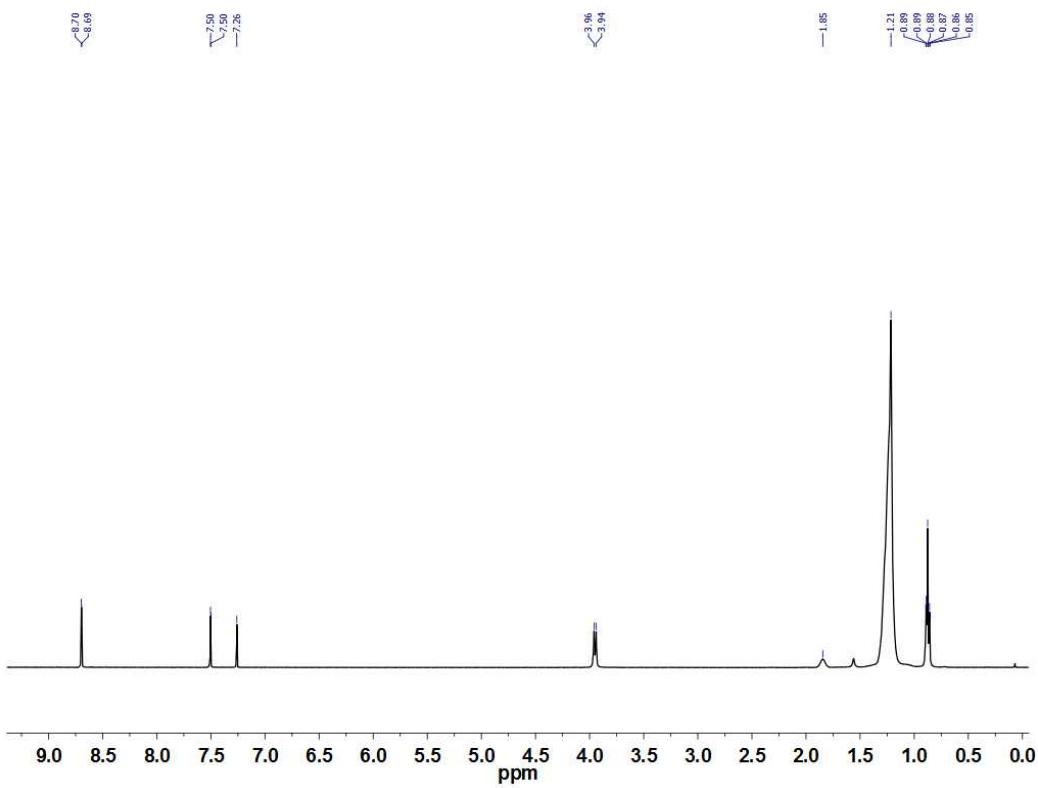


Figure S9 : ¹H-NMR spectrum in CDCl_3 of compound 5.

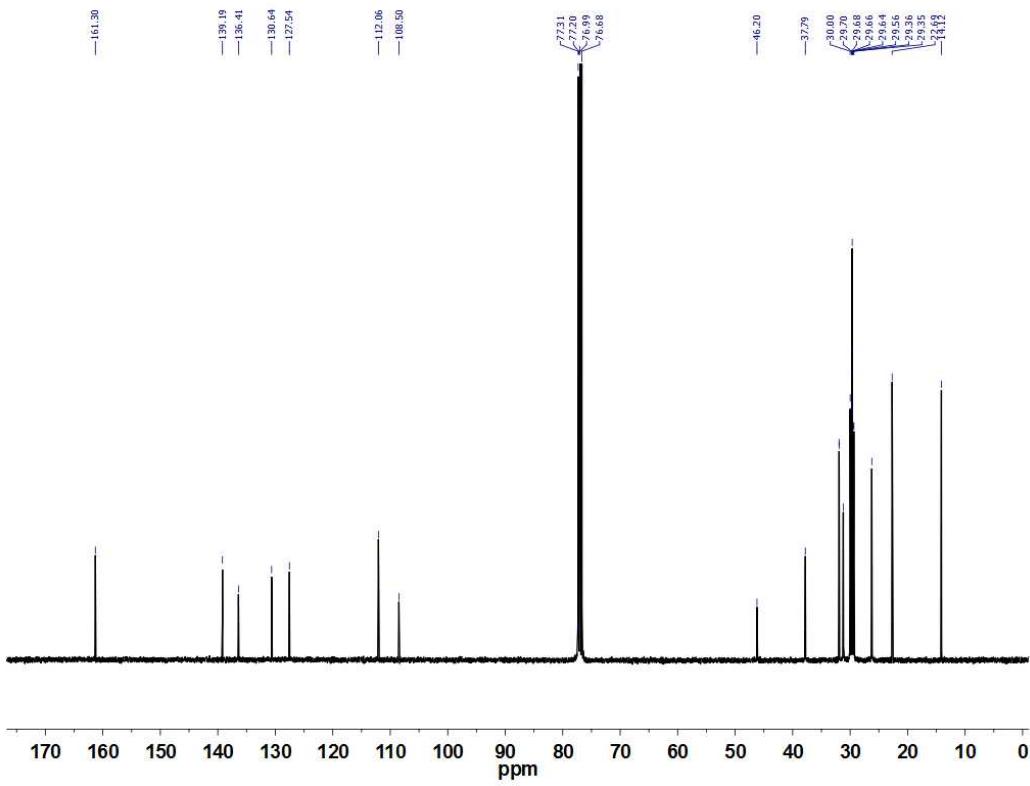


Figure S10 : ¹³C-NMR spectrum in CDCl_3 of compound 5.

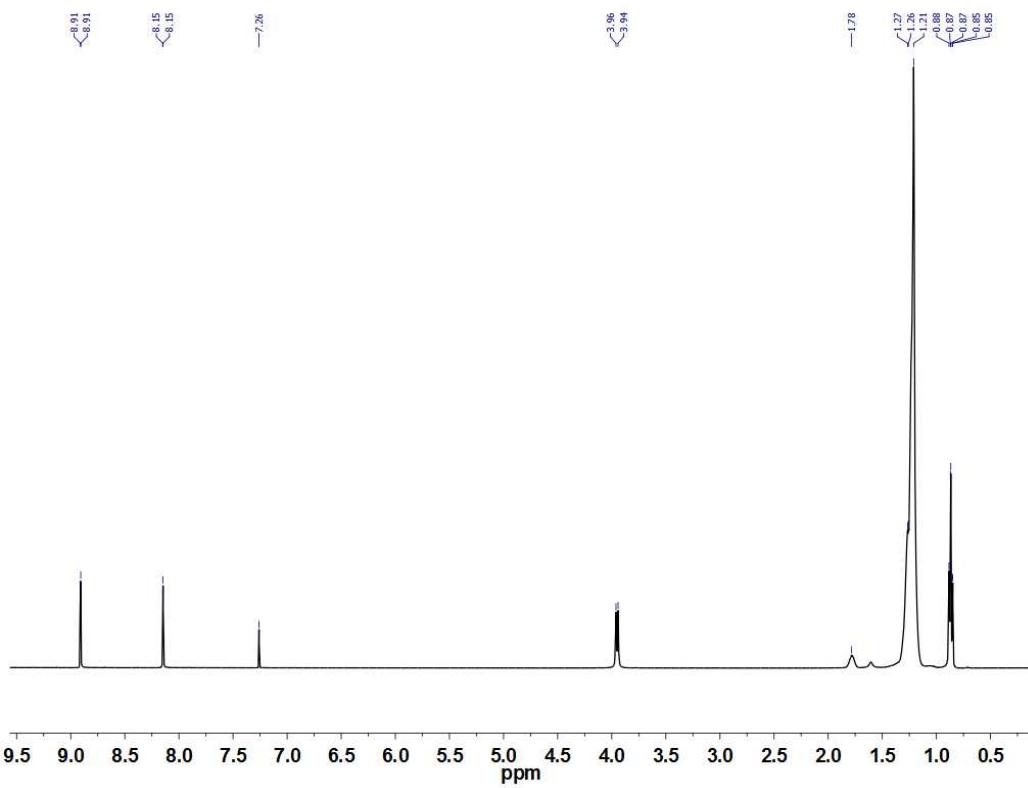


Figure S11 : ¹H-NMR spectrum in CDCl_3 of compound M9.

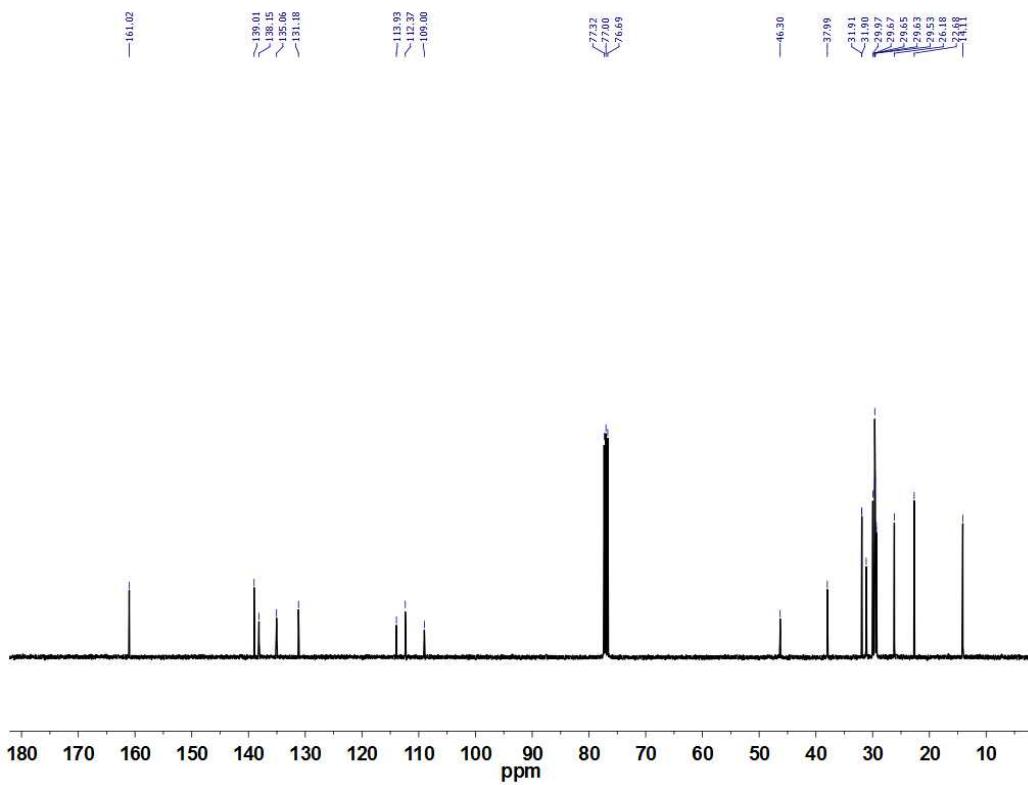


Figure S12 : ¹³C-NMR spectrum in CDCl_3 of compound M9.

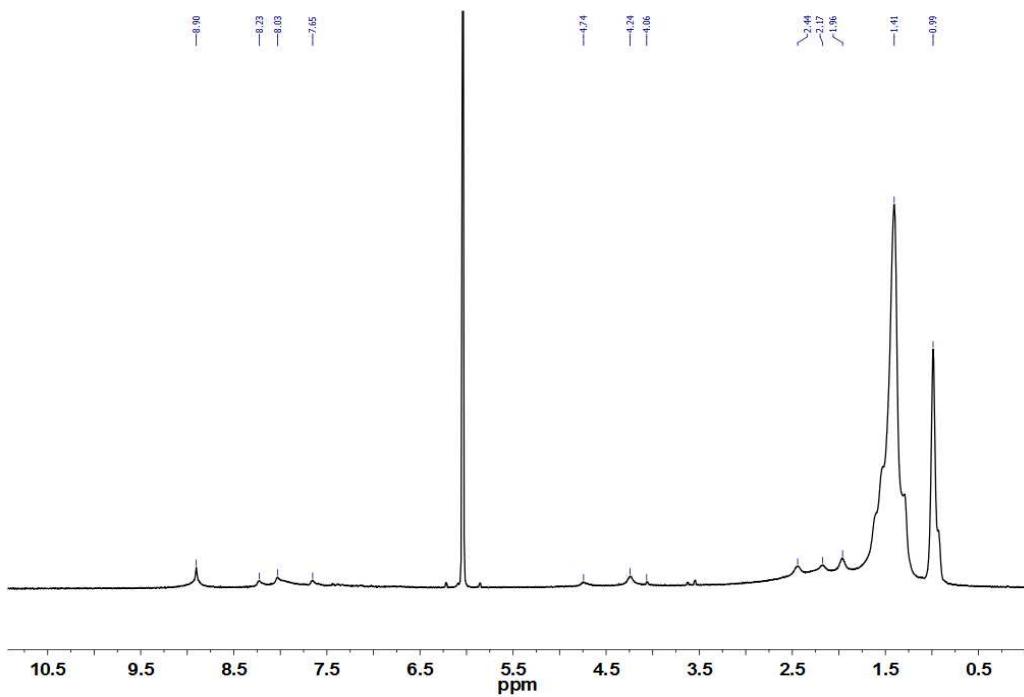


Figure S13 : ¹H-NMR spectrum in TCE at 110°C of polymer **P6**.

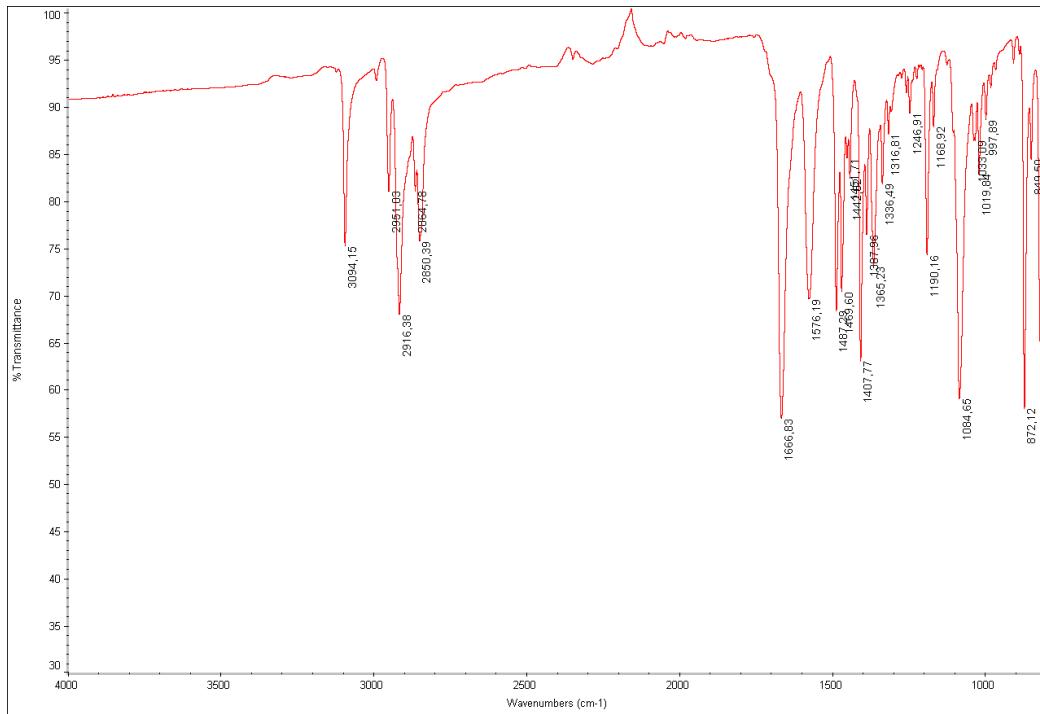


Figure S14 : Infrared spectrum of compound **3**.

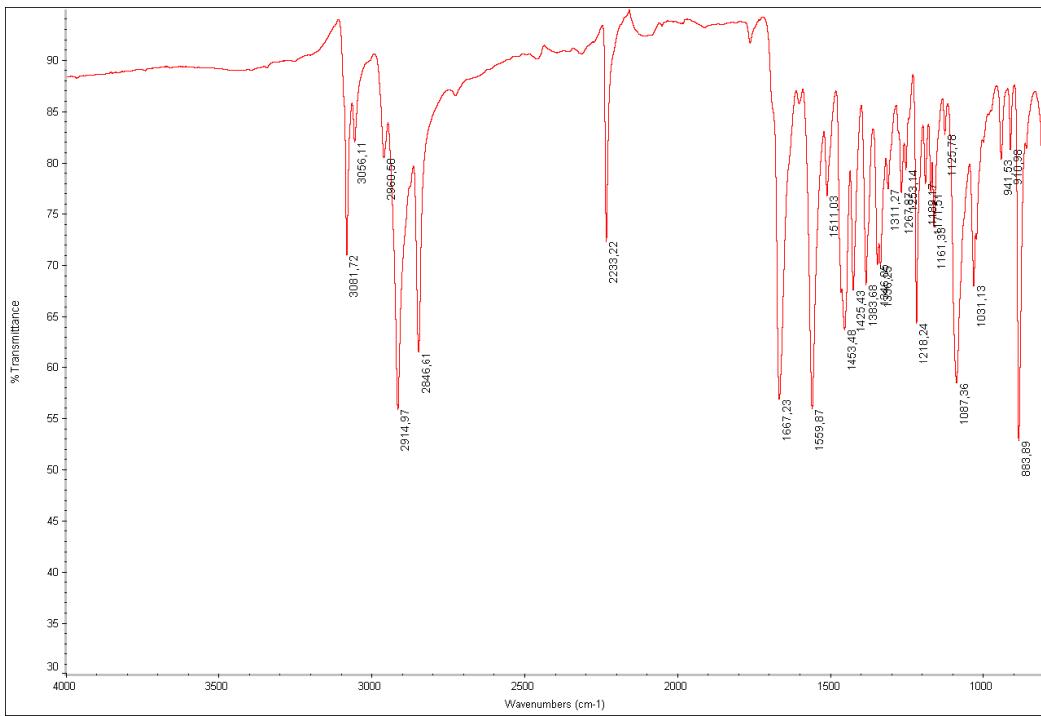


Figure S15 : Infrared spectrum of compound **M7**.

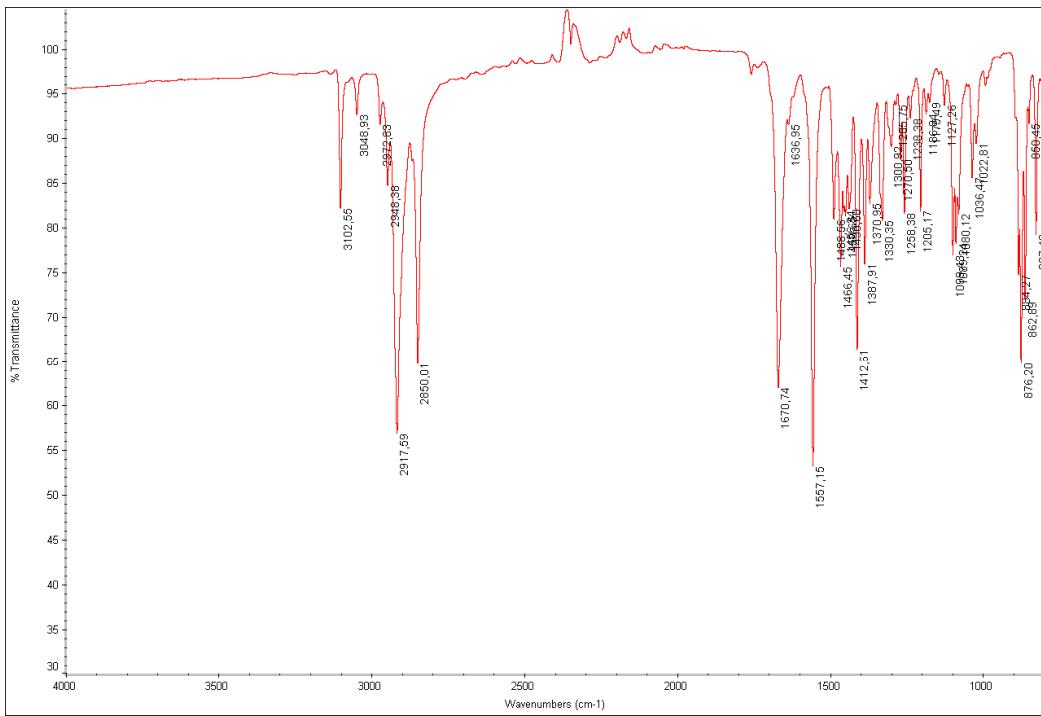


Figure 16 : Infrared spectrum of compound **4**.

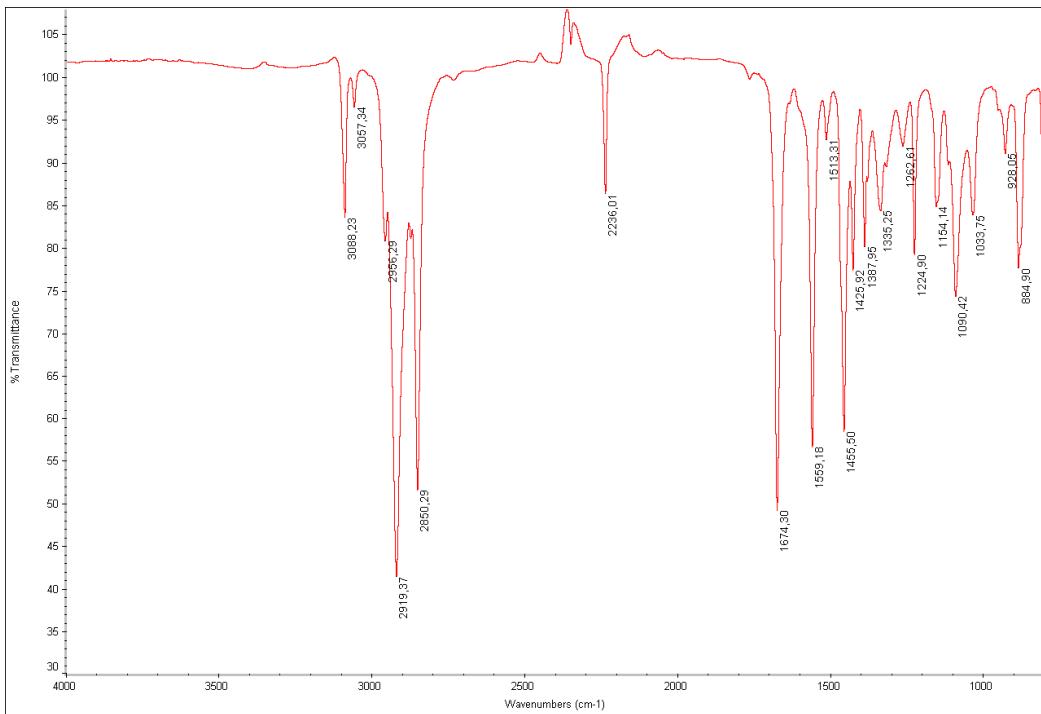


Figure S17 : Infrared spectrum of compound M8.

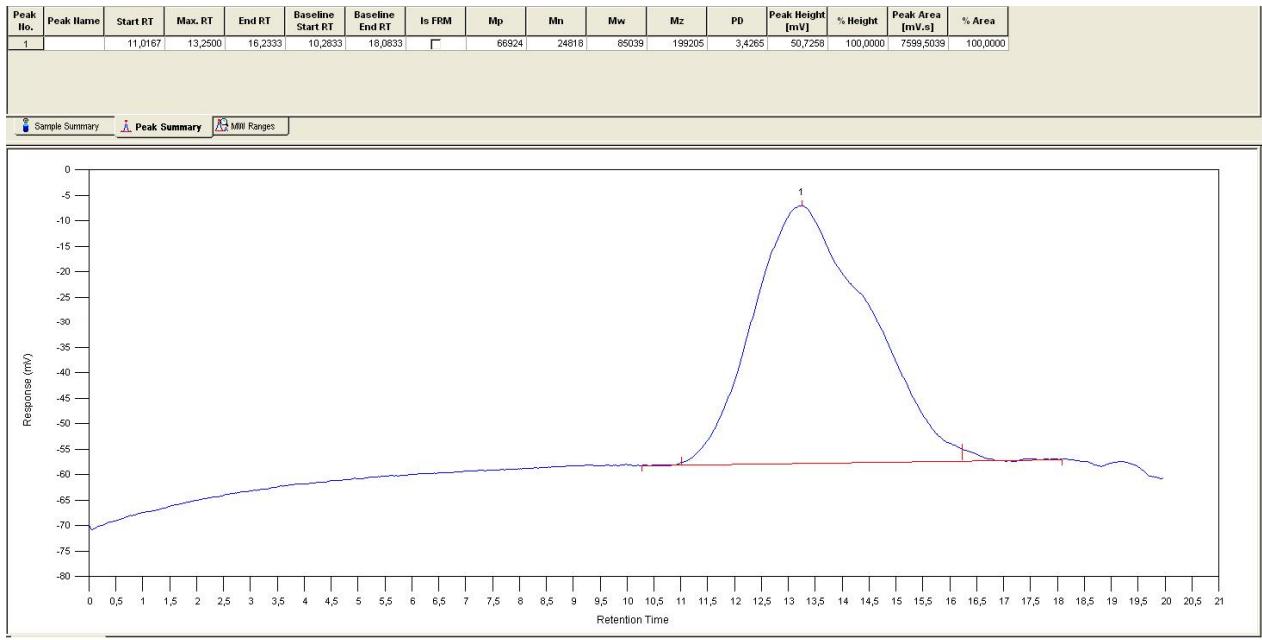


Figure S18 : GPC chromatogram for polymer P6

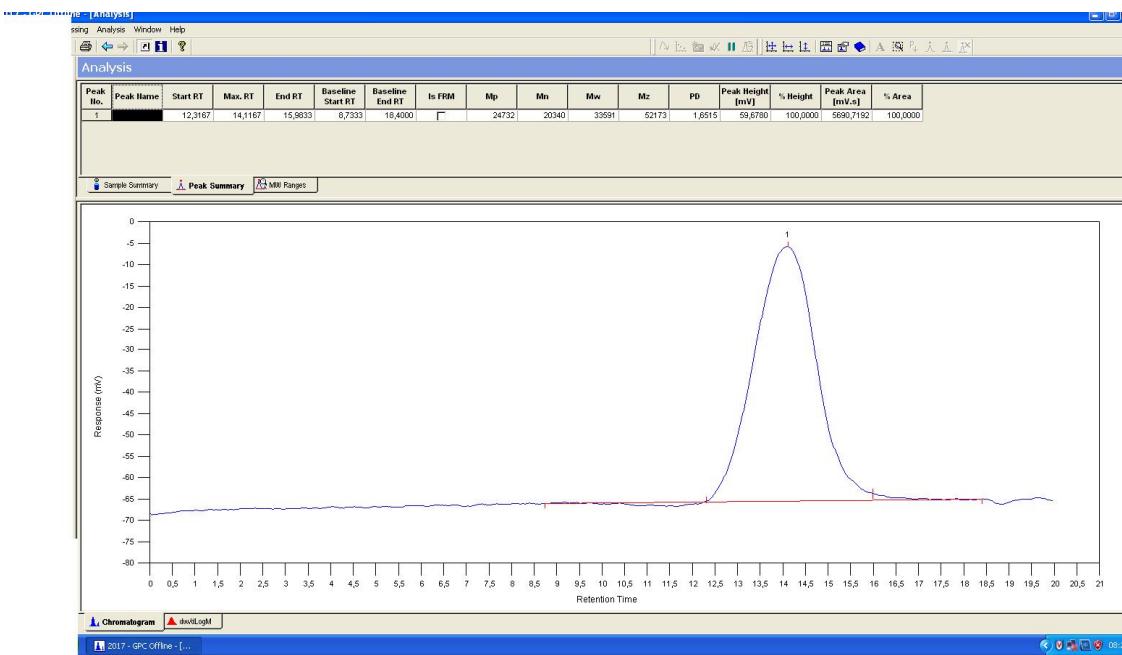


Figure S19 : GPC chromatogram for polymer P7a

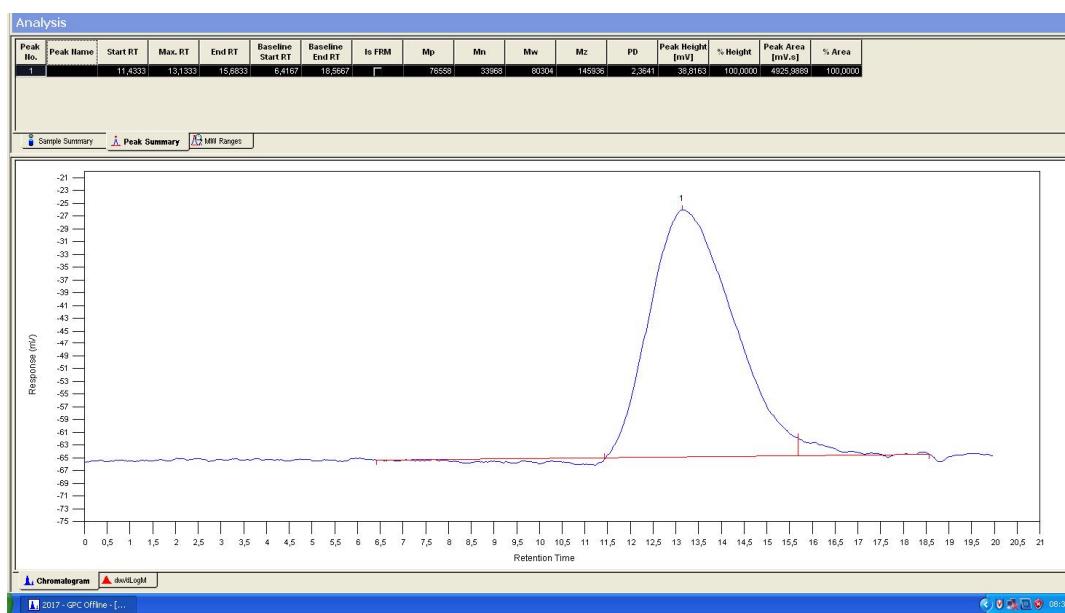


Figure S20 : GPC chromatogram for polymer P7b.