

Supplementary Information

An Alternative Approach to Create N-substituted Cyclic Dipeptides

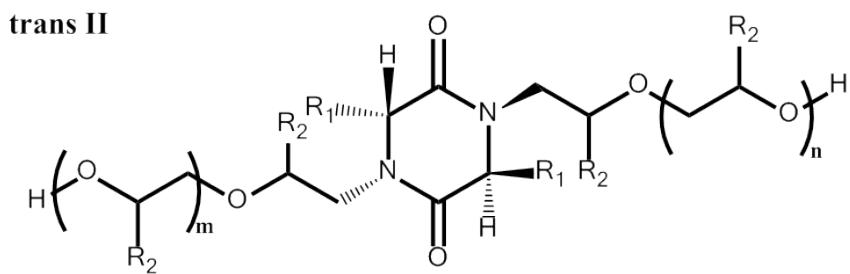
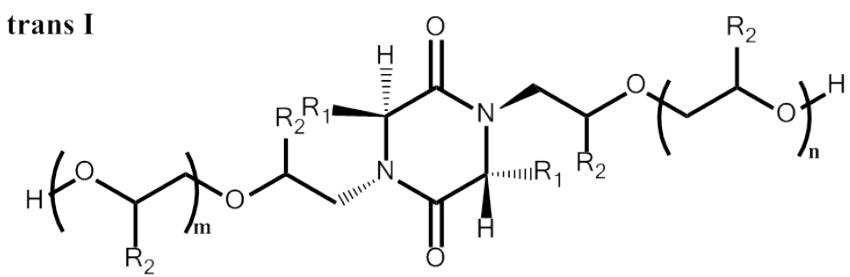
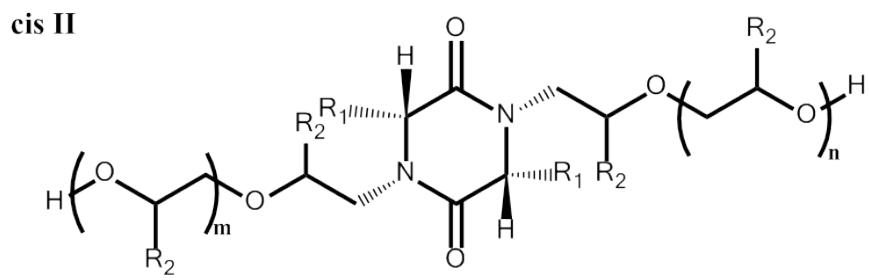
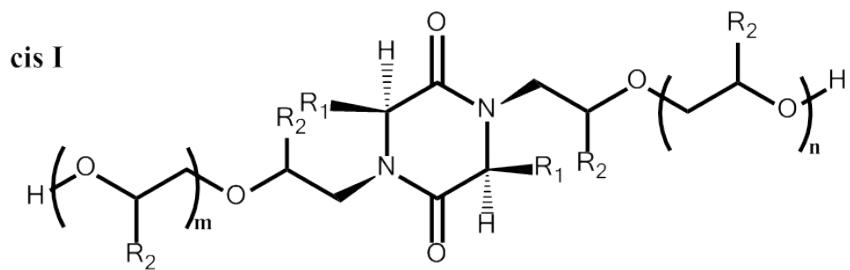
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Scheme S1: Isomers of N-Polyether-DKPs

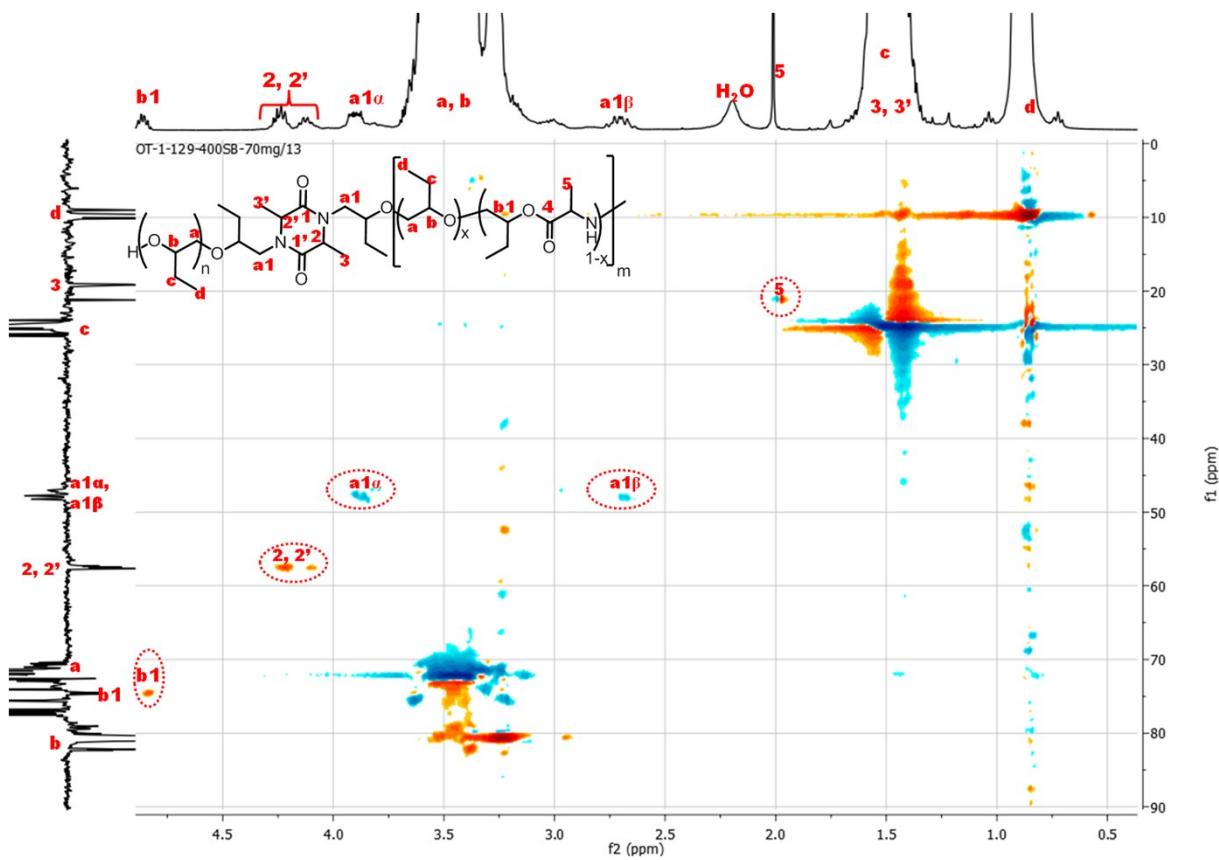


Figure S1: 2D-HSQC-NMR of P1-2.

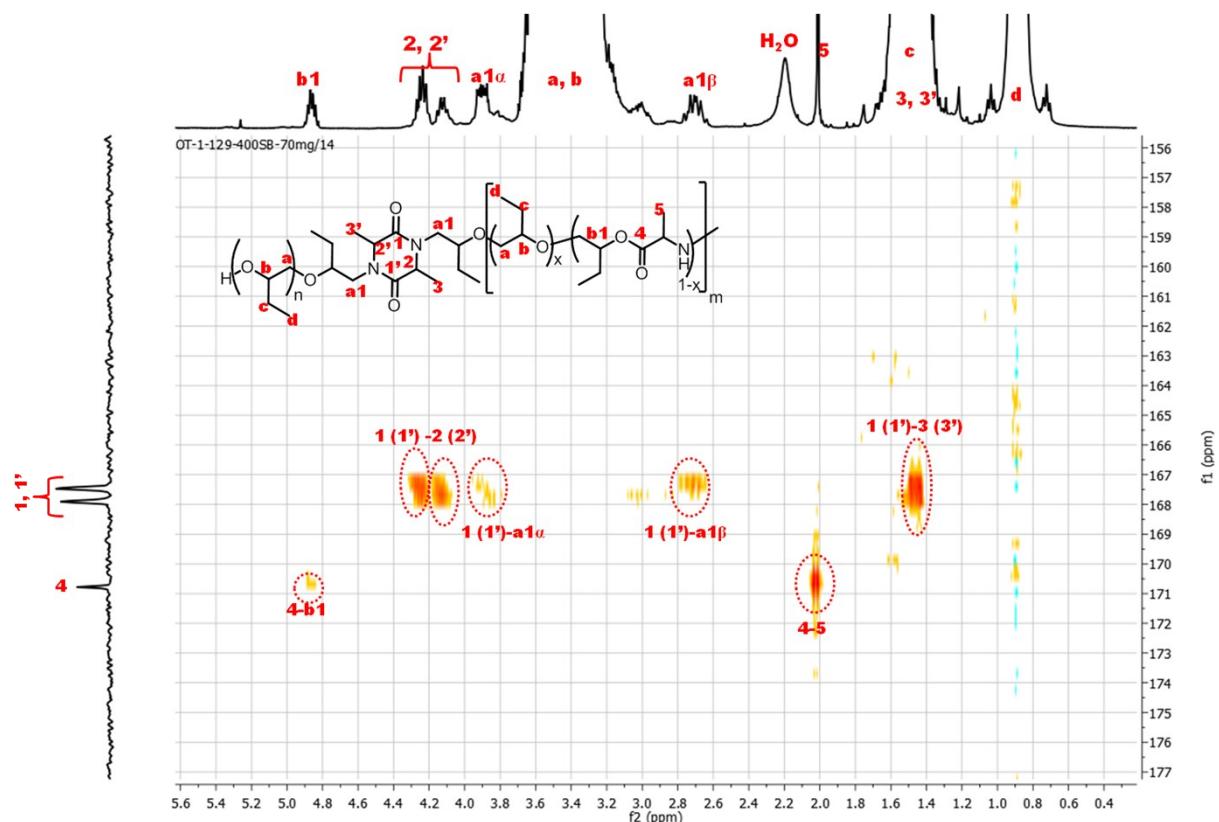


Figure S2: 2D-HMBC-NMR of P1-2.

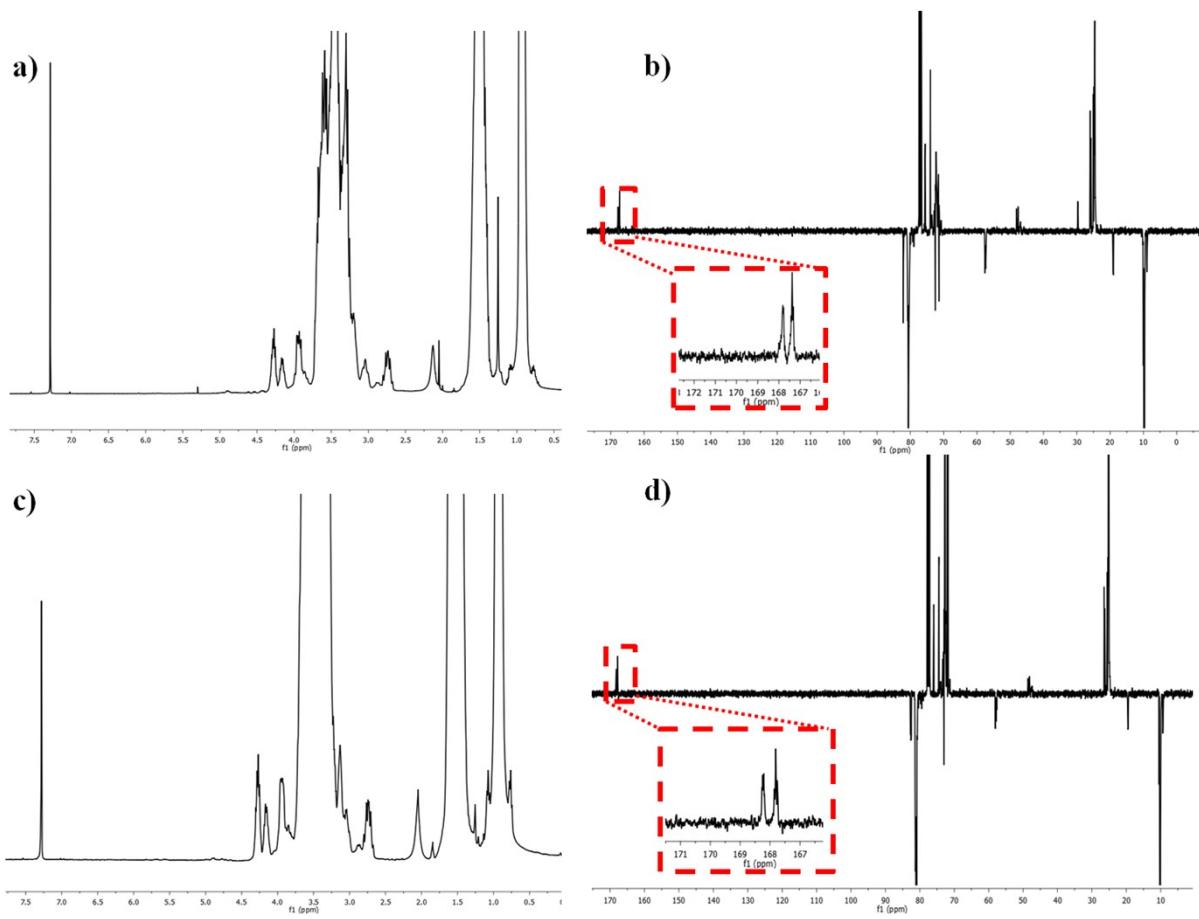


Figure S3: ^1H and ^{13}C NMR spectra of P1-3 and P1-4. a) ^1H NMR spectrum of P1-3. b) ^{13}C NMR spectrum of P1-3. c) ^1H NMR spectrum of P1-4. d) ^{13}C NMR spectrum of P1-4.

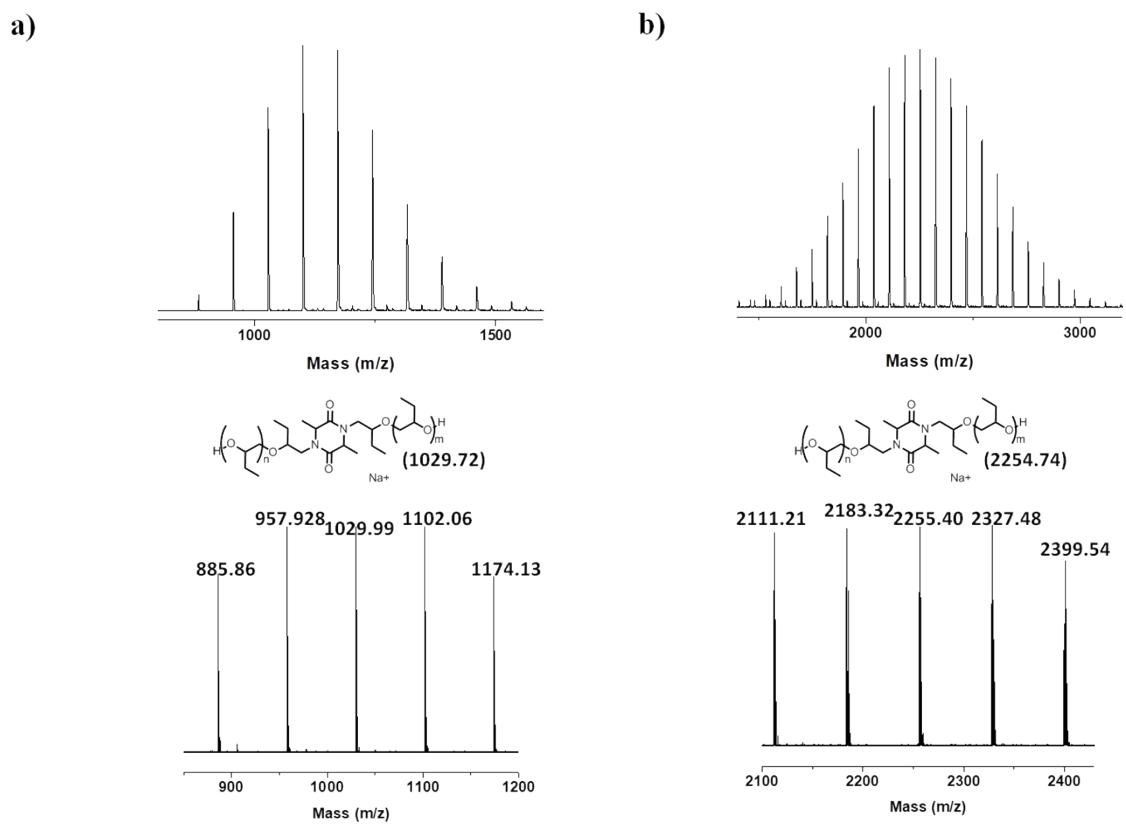


Figure S4: MALDI-Tof spectra of a) P1-3 and b) P1-4. Top spectra are collected in linear mode. Bottom ones are collected in reflectron mode.

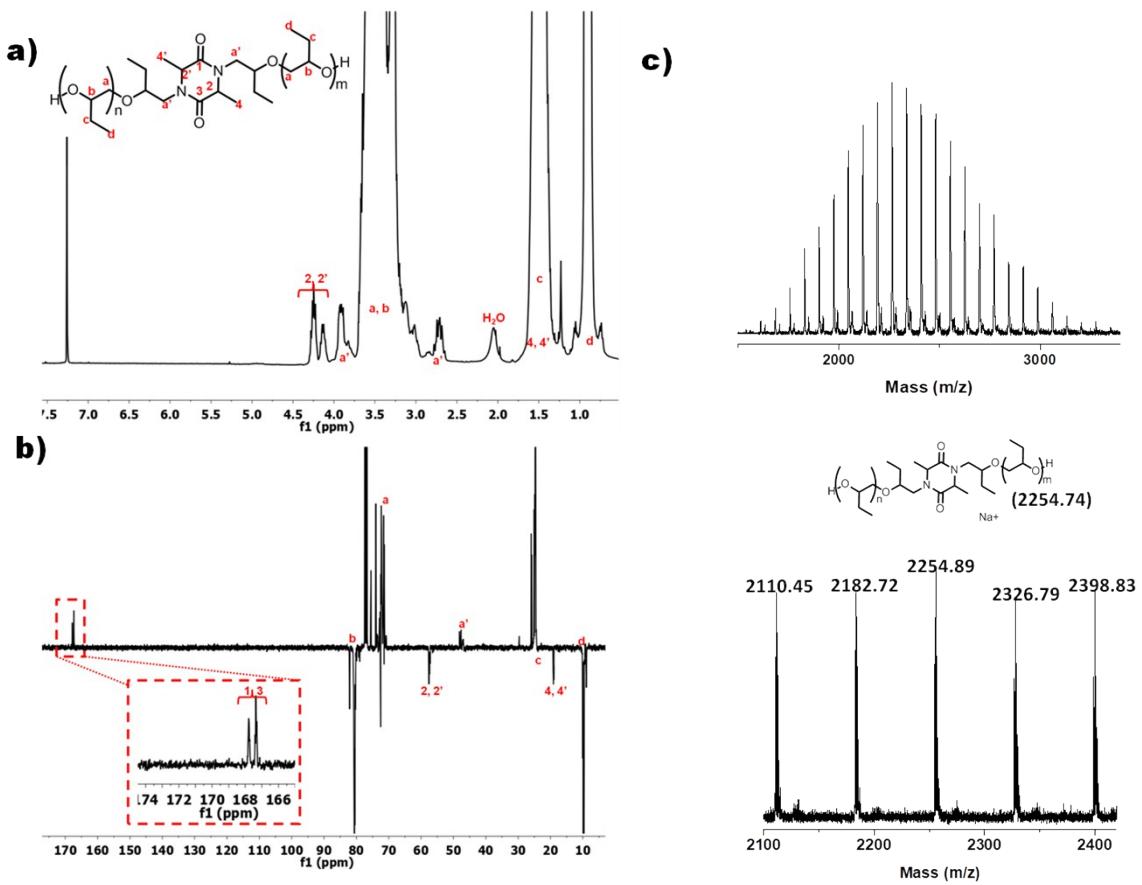


Figure S5: Analysis of P1-8 initiated by Cyclo(Ala-Ala), tBuP₂ and a catalytic amount of tBuP₄. a) ¹H NMR spectrum of P1-8 in CDCl₃. b) ¹³C NMR spectrum of P1-8 in CDCl₃. c) MALDI-ToF analysis, linear (top) and reflectron (bottom) modes.

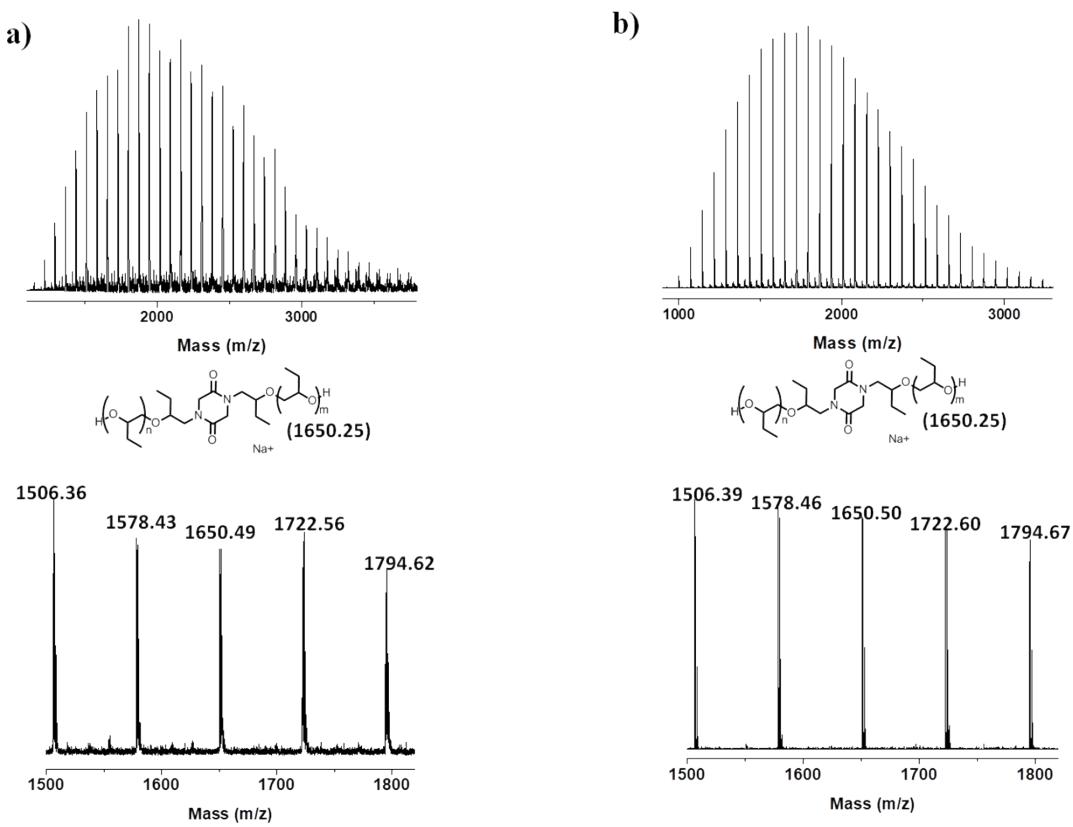


Figure S6: MALDI-ToF spectra of a) P2-1 and b) P2-2. Top spectra are collected in linear mode. Bottom ones are collected in reflectron mode.

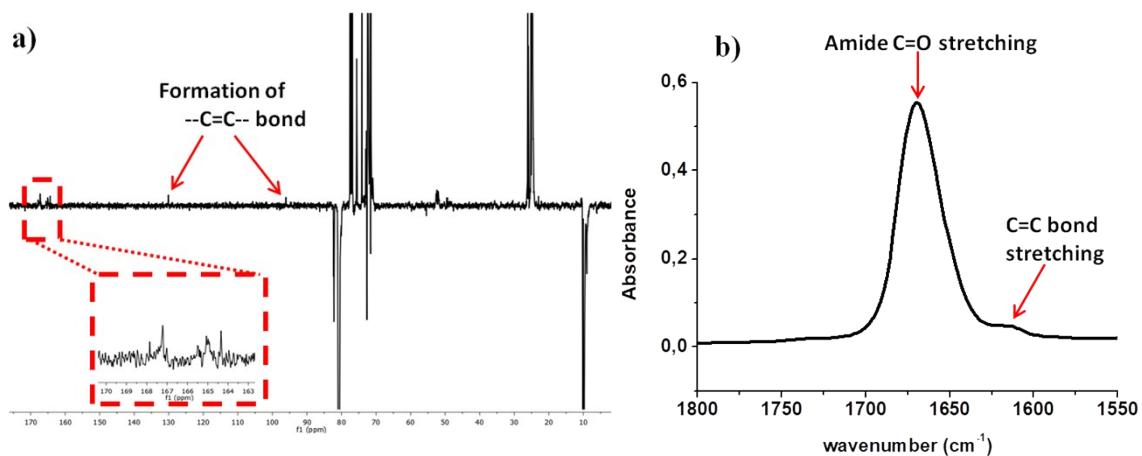


Figure S7: Characterization of P2-2 by a) ¹³C NMR in CDCl₃ and b) ATR-FITR.

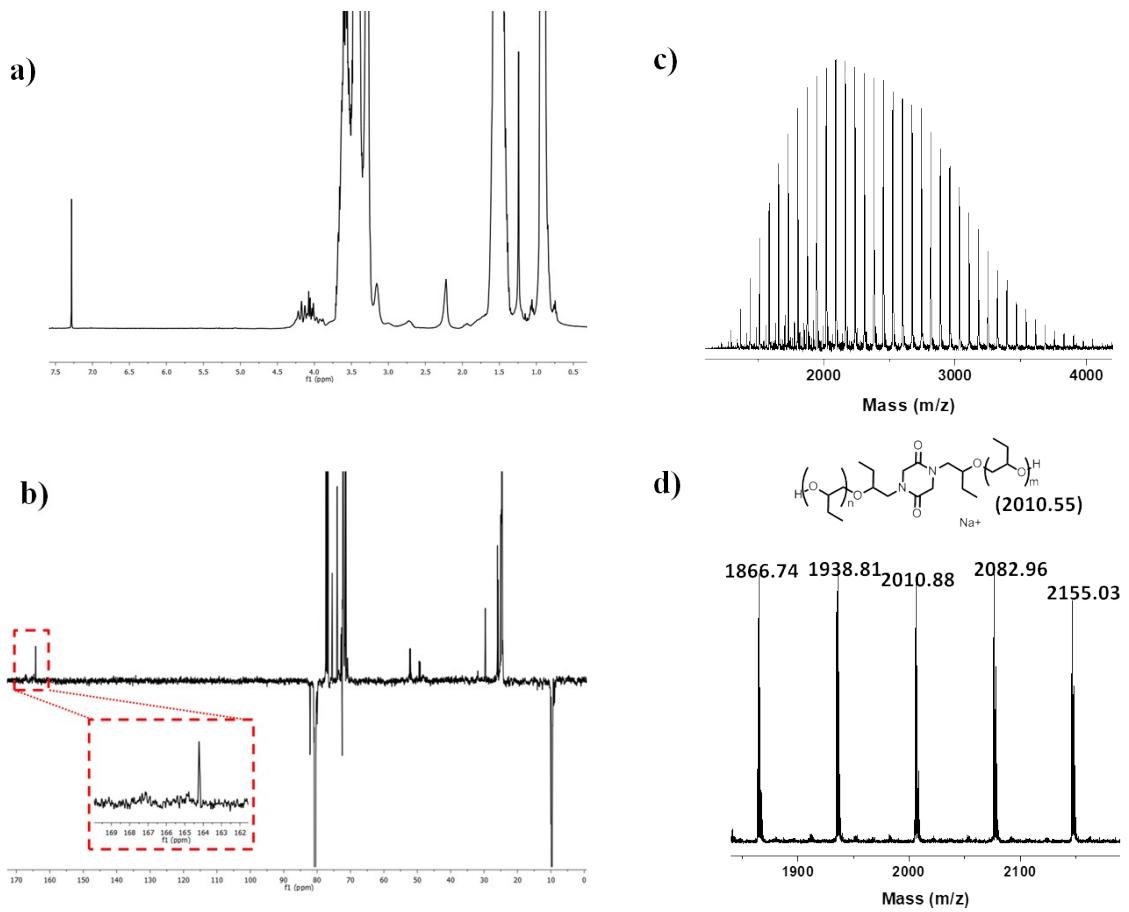


Figure S8: Analysis of P2-5. a) ^1H NMR spectrum of P2-5 in CDCl_3 . b) ^{13}C NMR spectrum of P2-5 in CDCl_3 . c) MALDI-Tof analysis in linear mode. d) MALDI-Tof analysis in reflectron mode.

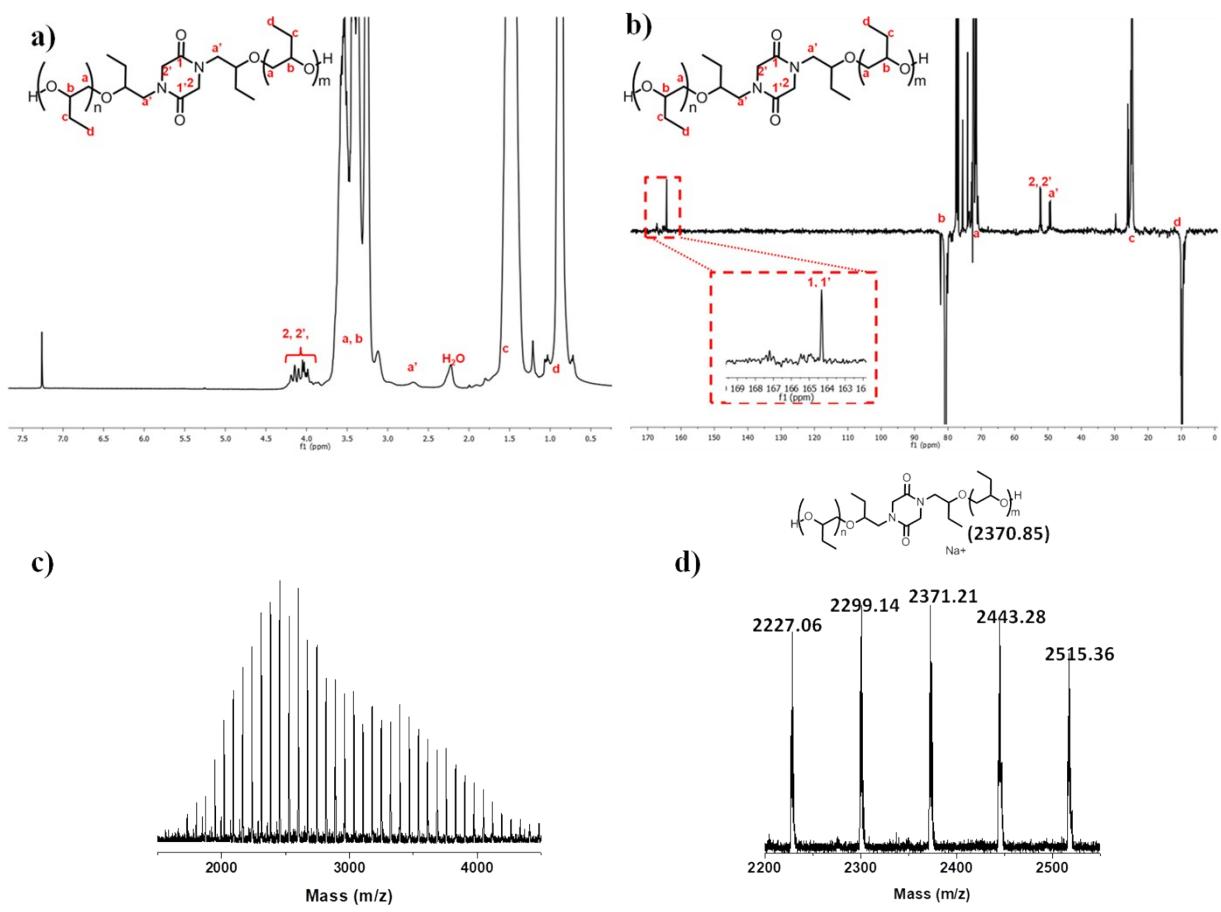


Figure S9: Analysis of P2-7. a) ^1H NMR spectrum of P2-7 in CDCl_3 . b) ^{13}C NMR spectrum of P2-7 in CDCl_3 . c) MALDI-Tof analysis in linear mode. d) MALDI-Tof analysis in reflectron mode.

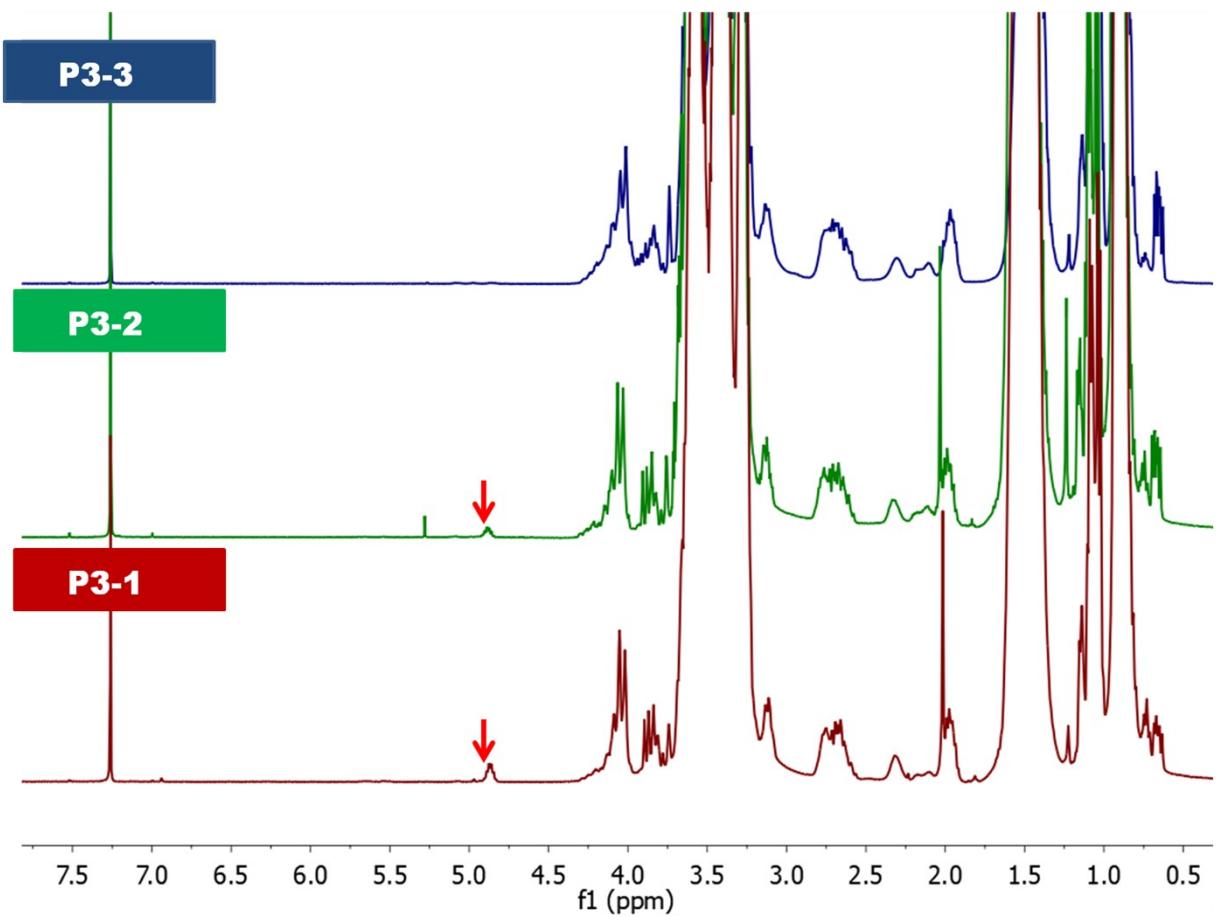


Figure S10: ¹H-NMR spectra of P3-1, P3-2 and P3-3.

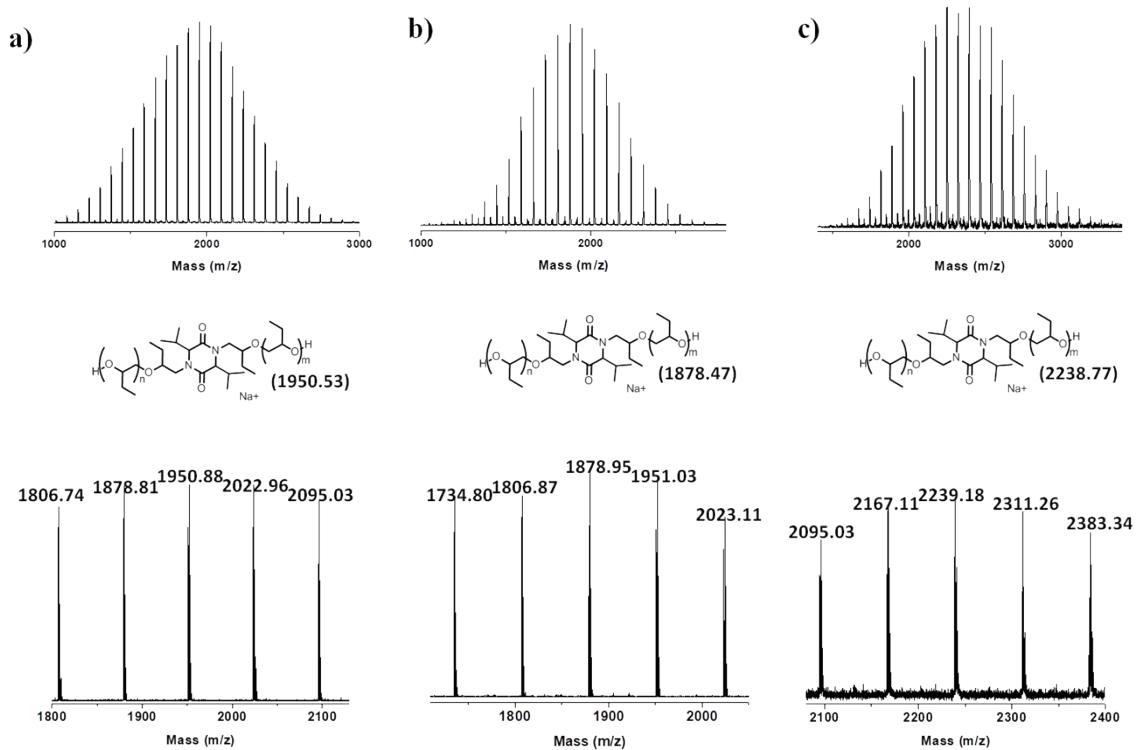


Figure S11: MALDI-ToF spectra of a) P3-1, b) P3-2 and c) P3-3. Top spectra are collected in linear mode. Bottom ones are collected in reflectron mode.

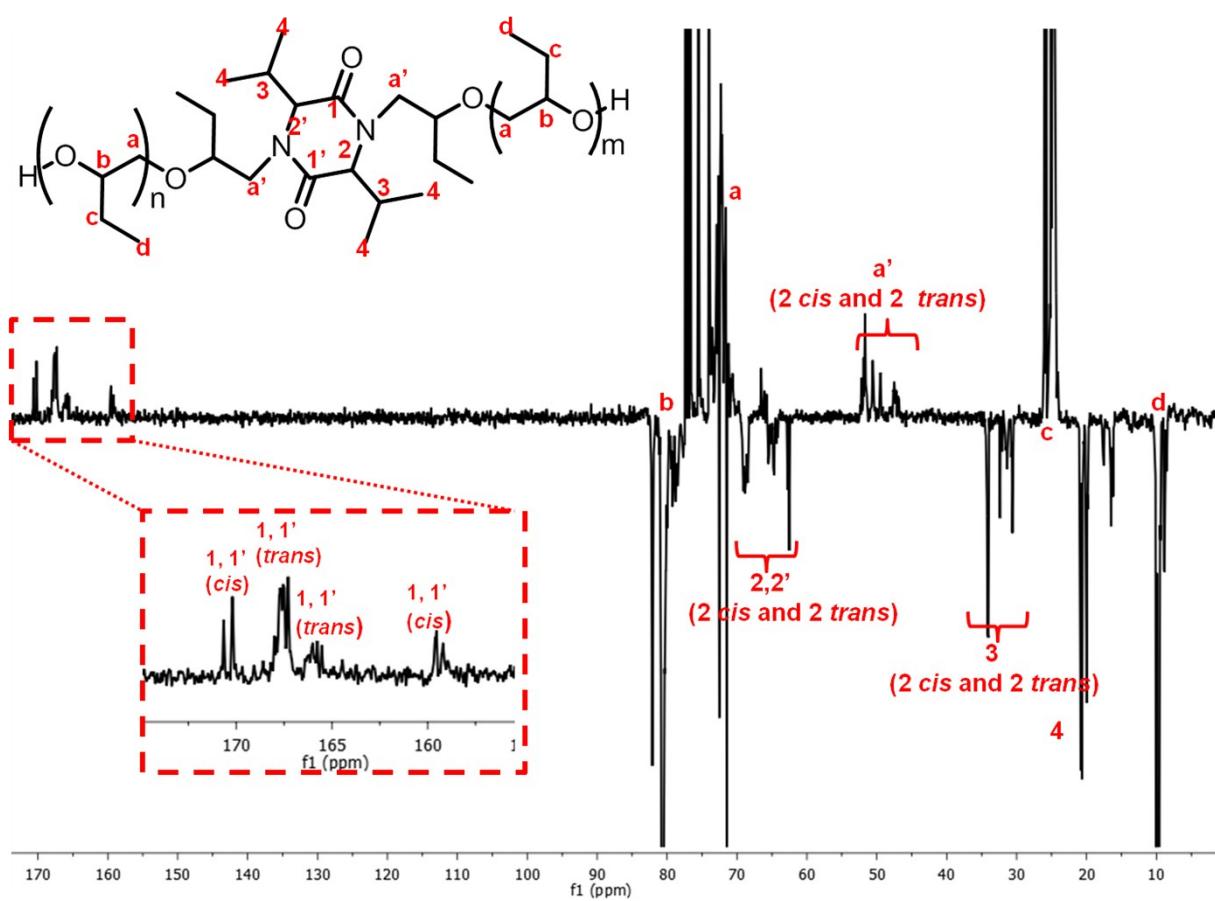


Figure S12: ^{13}C NMR spectrum of P3-3 in CDCl_3 .

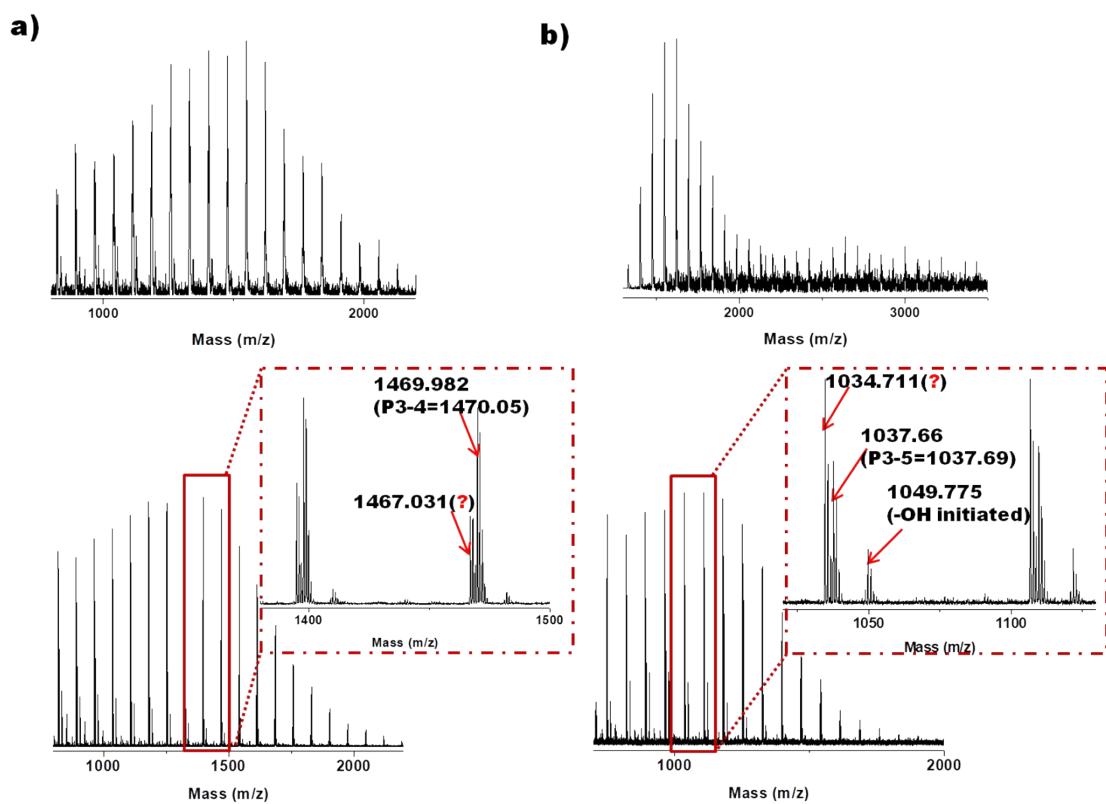


Figure S13: MALDI-Tof analysis of a) P3-4 and b) P3-5.

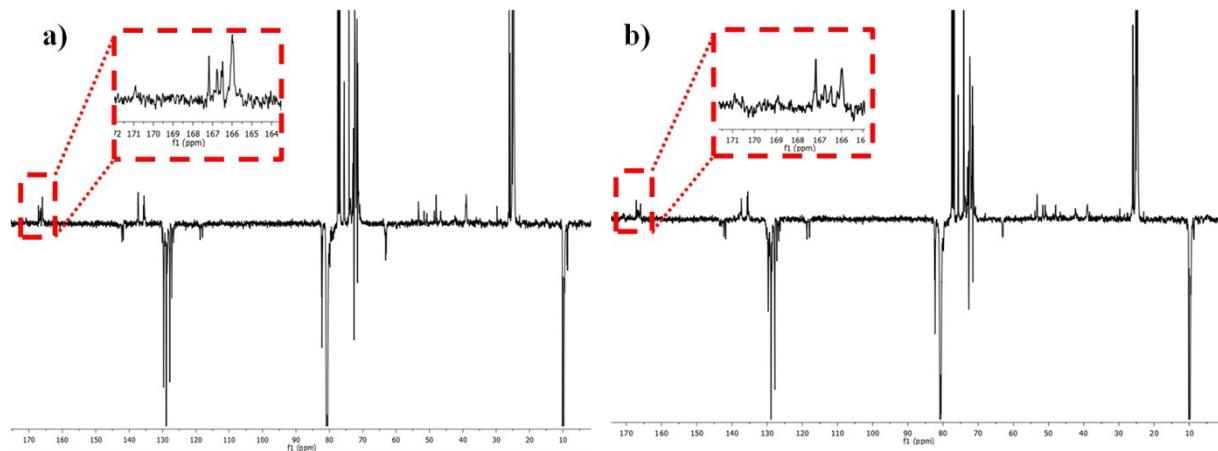


Figure S14: ^{13}C NMR analysis of a) P3-4 and b) P3-5 in CDCl_3 .

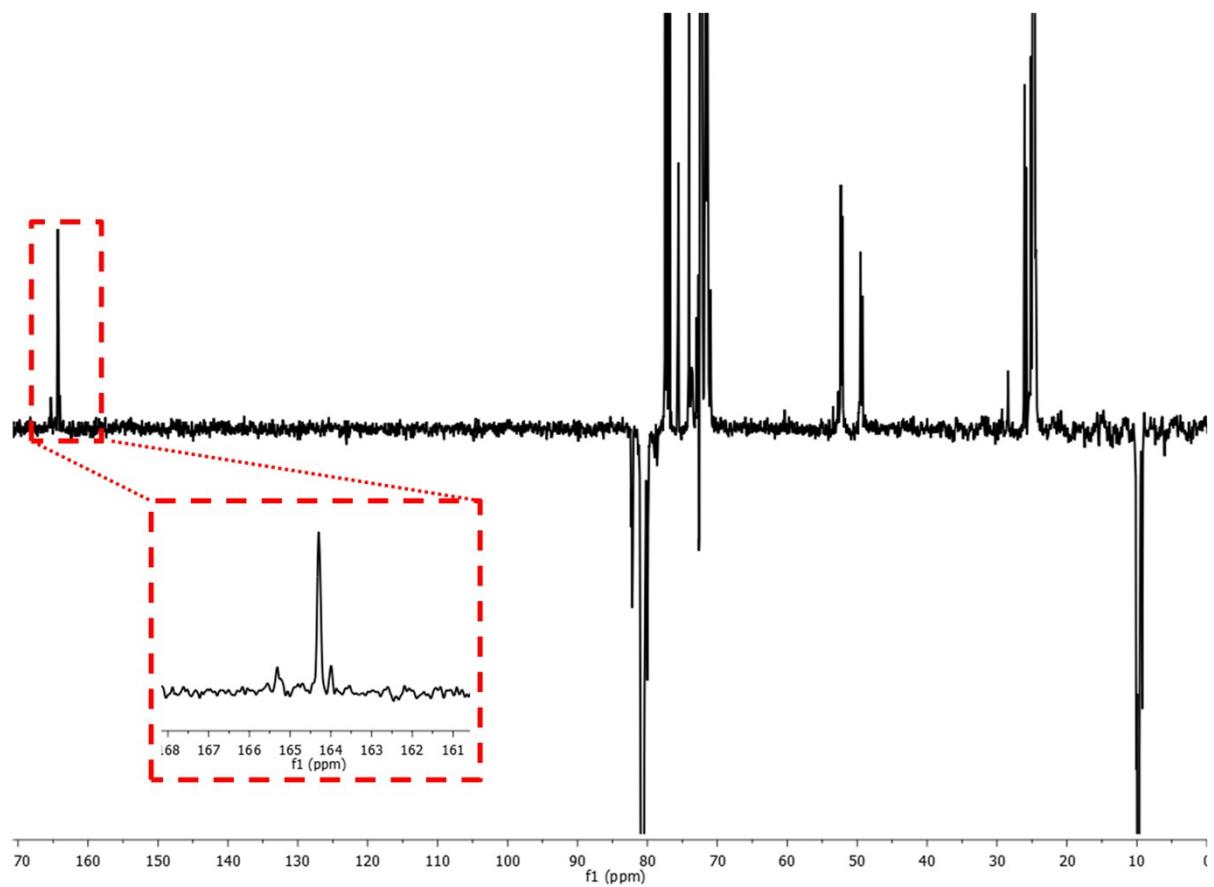


Figure S15: ^{13}C NMR spectrum of P4-3 in CDCl_3 .

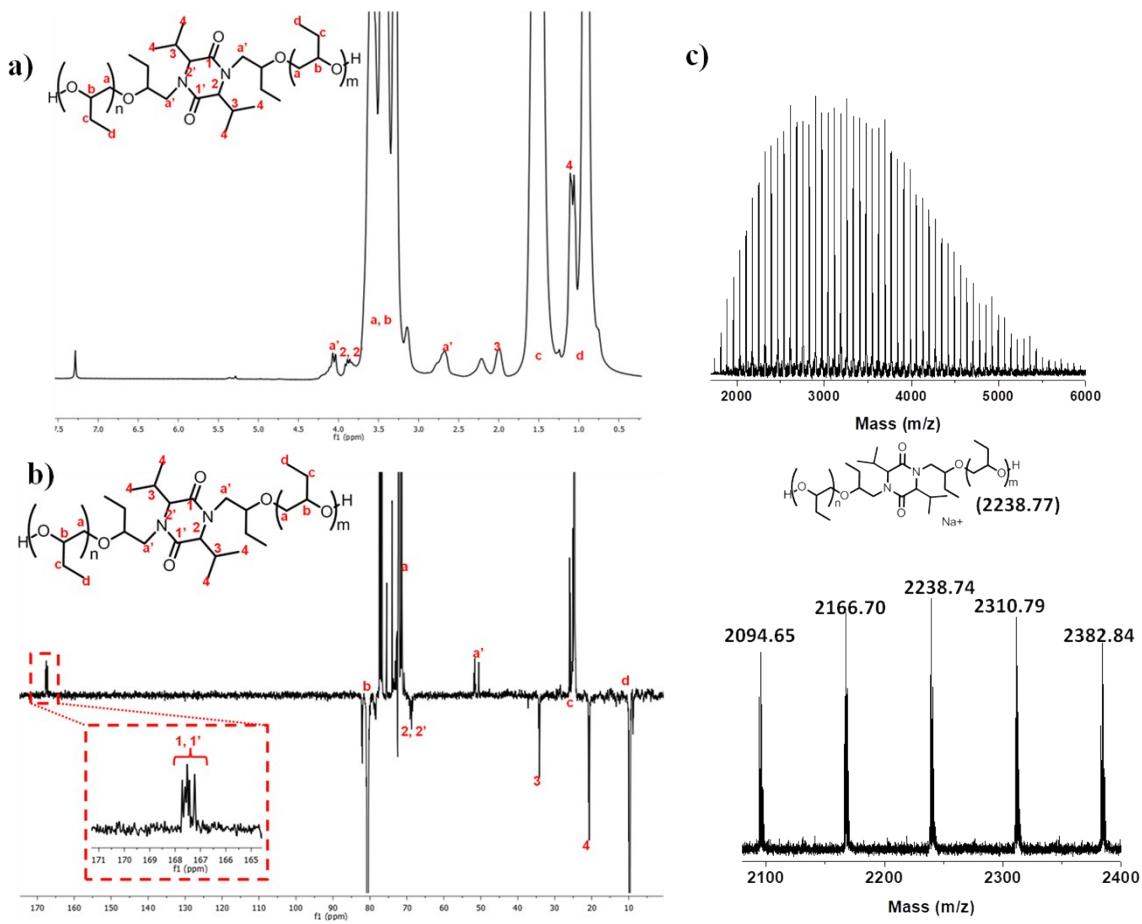


Figure S16: Analysis of P4-5 a) ^1H NMR spectrum of P4-5 in CDCl_3 . b) ^{13}C NMR spectrum of P4-5 in CDCl_3 . c) MALDI-Tof analysis, linear (top) and reflectron (bottom) modes.

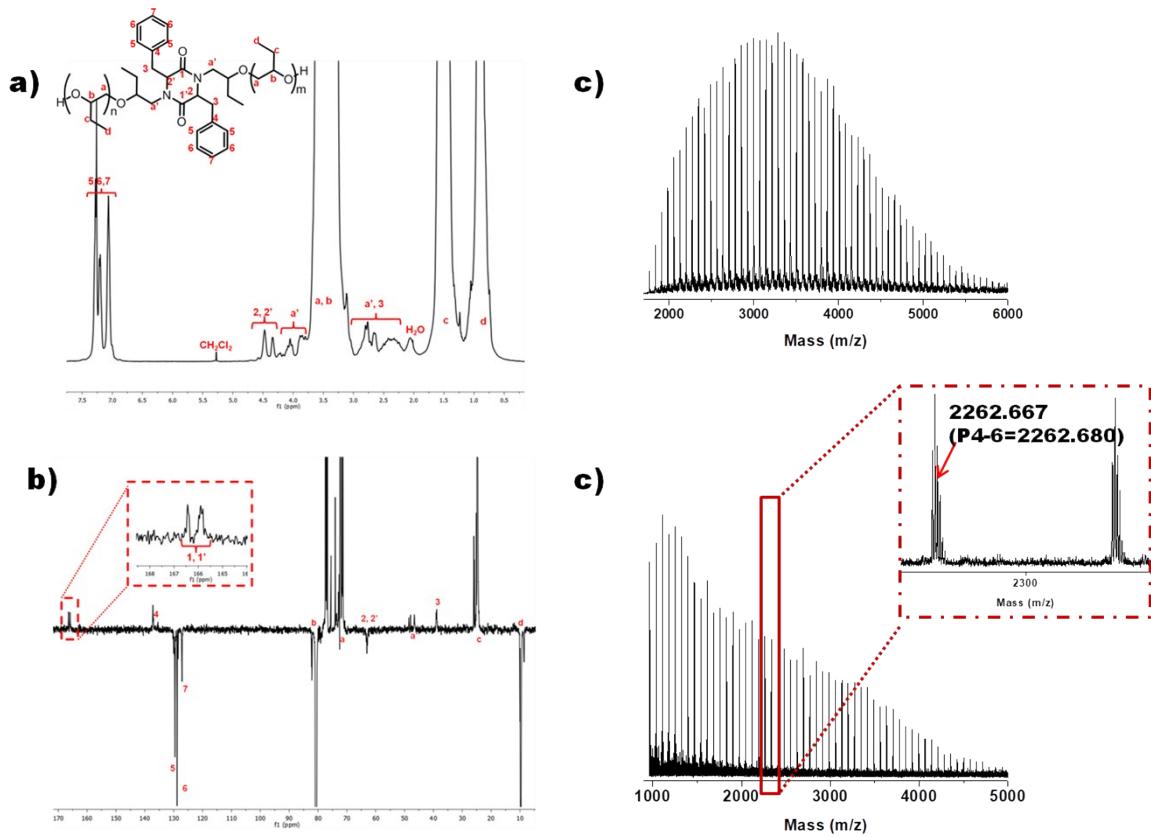


Figure S17: Analysis of P4-6 a) ^1H NMR spectrum of P4-6 in CDCl_3 . b) ^{13}C NMR spectrum of P4-6 in CDCl_3 . c) MALDI-Tof analysis, linear (top) and reflectron (bottom) modes.

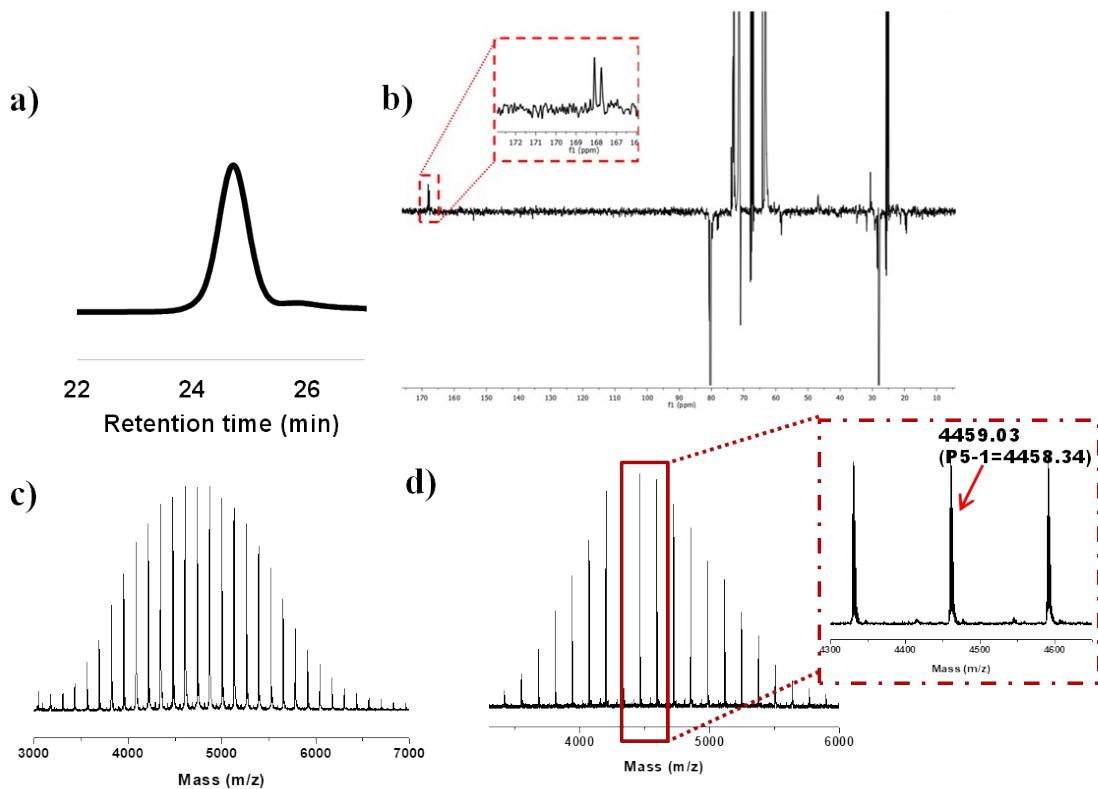


Figure S18: Analysis of P5-1. a) GPC IR trace of P5-1, THF used as eluent. b) ^{13}C NMR spectrum collected in THF-d8. c) MALDI-Tof spectrum in linear mode. d) MALDI-Tof spectrum in reflectron mode.

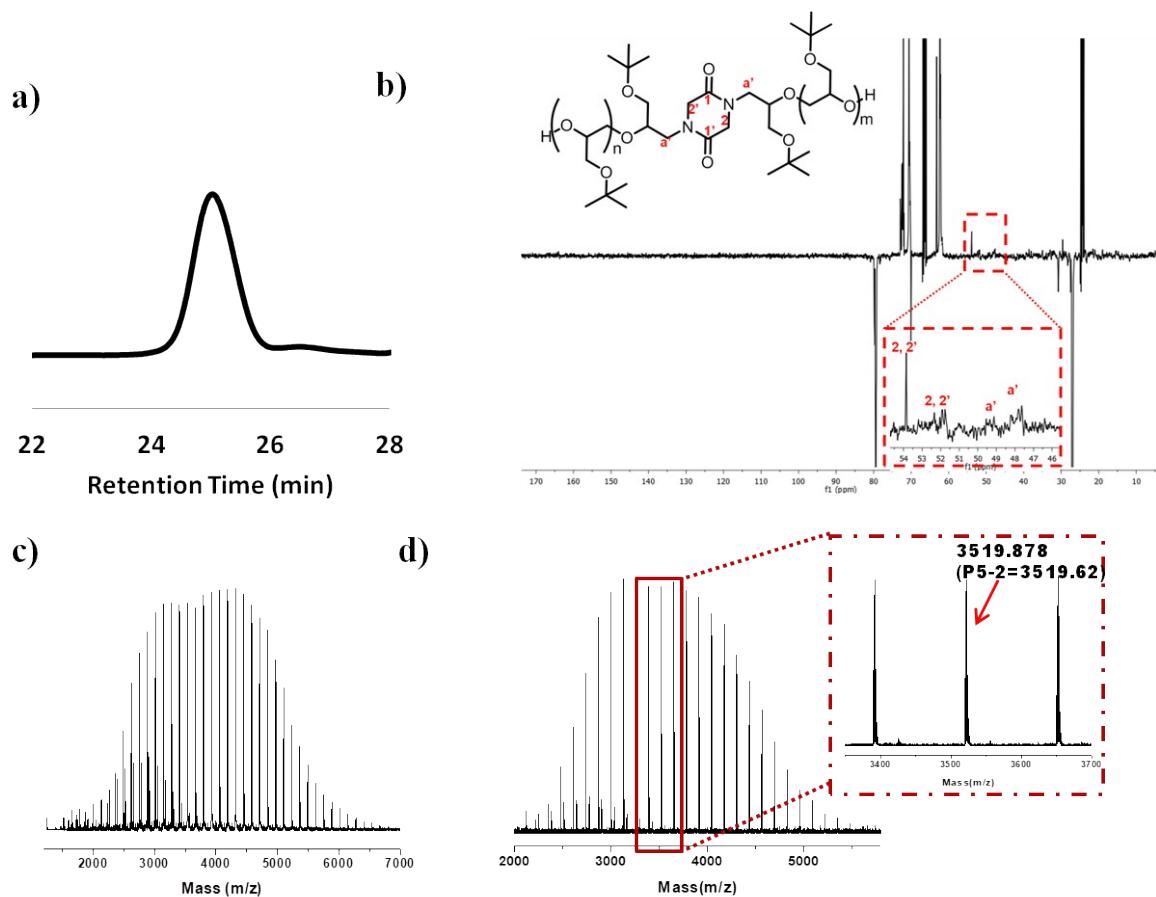


Figure S19: Analysis of P5-2. a) GPC IR trace of P5-2, THF used as eluent. b) ^{13}C NMR spectrum collected in THF-d8. c) MALDI-Tof spectrum in linear mode. d) MALDI-Tof spectrum in reflectron mode.

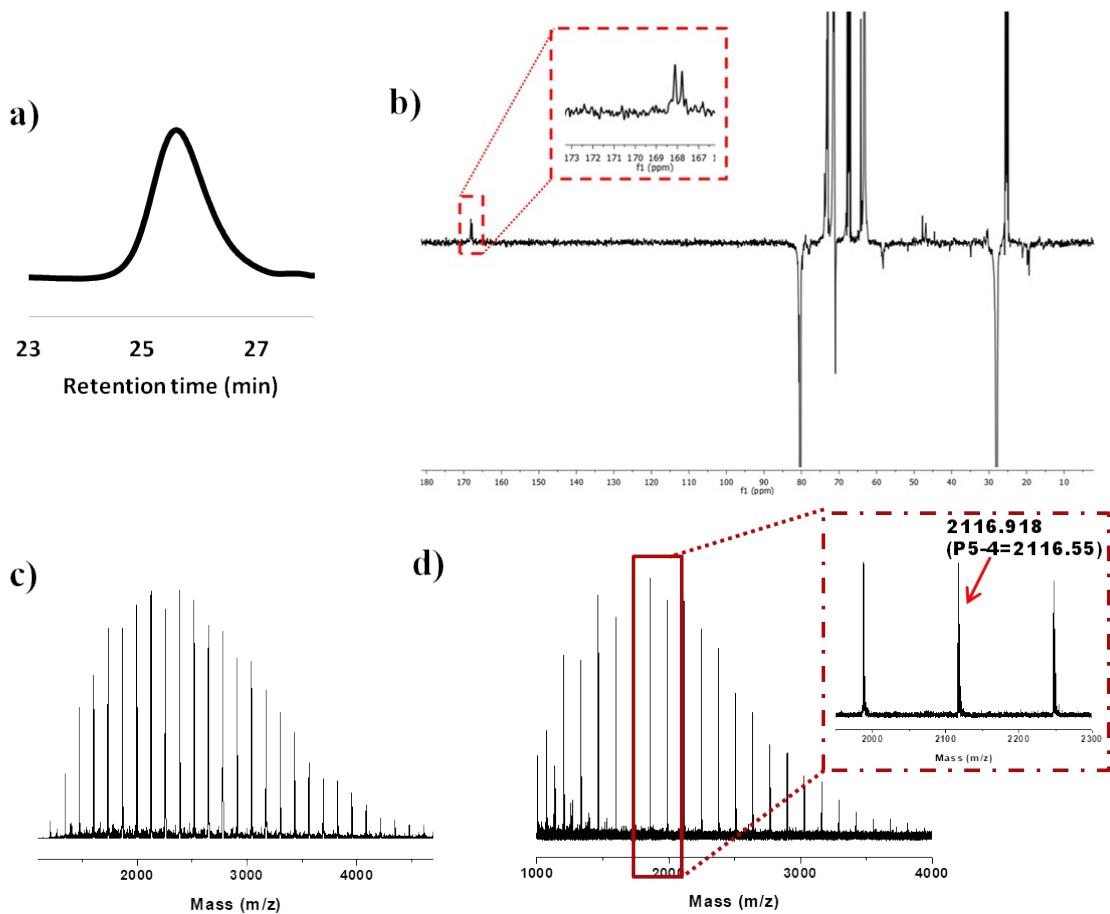


Figure S20: Analysis of P5-4. a) GPC IR trace of P5-4, THF used as eluent. b) ^{13}C NMR spectrum collected in THF-d8. c) MALDI-Tof spectrum in linear mode. d) MALDI-Tof spectrum in reflectron mode.

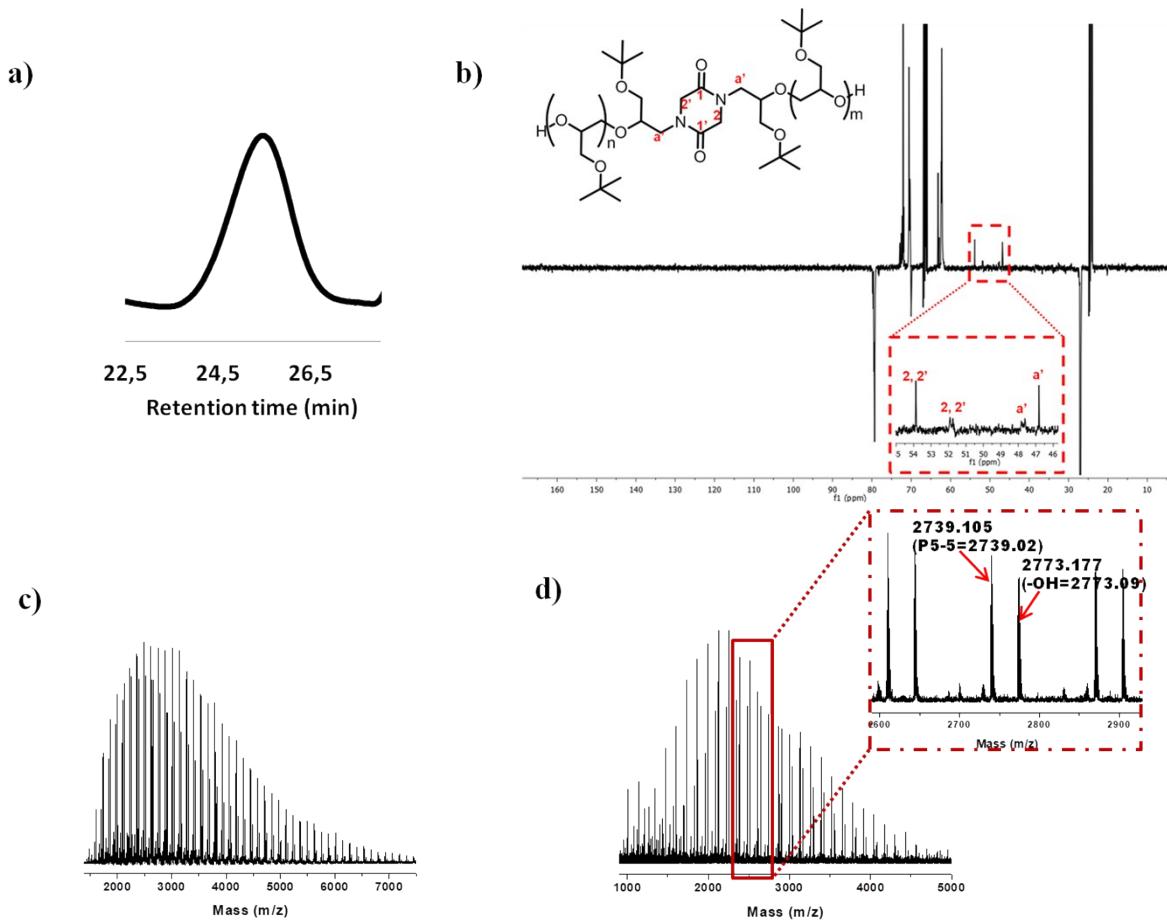


Figure S21: Analysis of P5-5. a) GPC IR trace of P5-5, THF used as eluent. b) ^{13}C NMR spectrum collected in THF-d8. c) MALDI-Tof spectrum in linear mode. d) MALDI-Tof spectrum in reflectron mode.

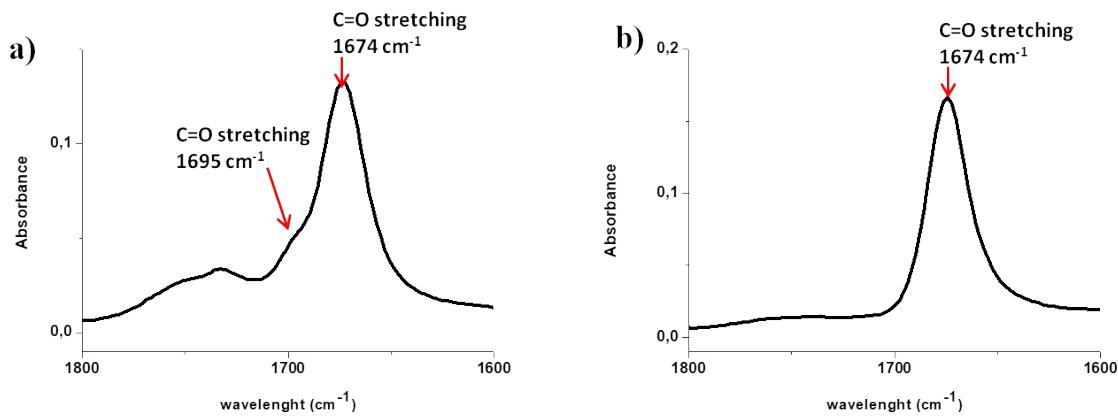


Figure S22: ATR-FTIR analysis of a) P5-2 and b) P5-5, demonstrating the presence of amide C=O group on the polymers.

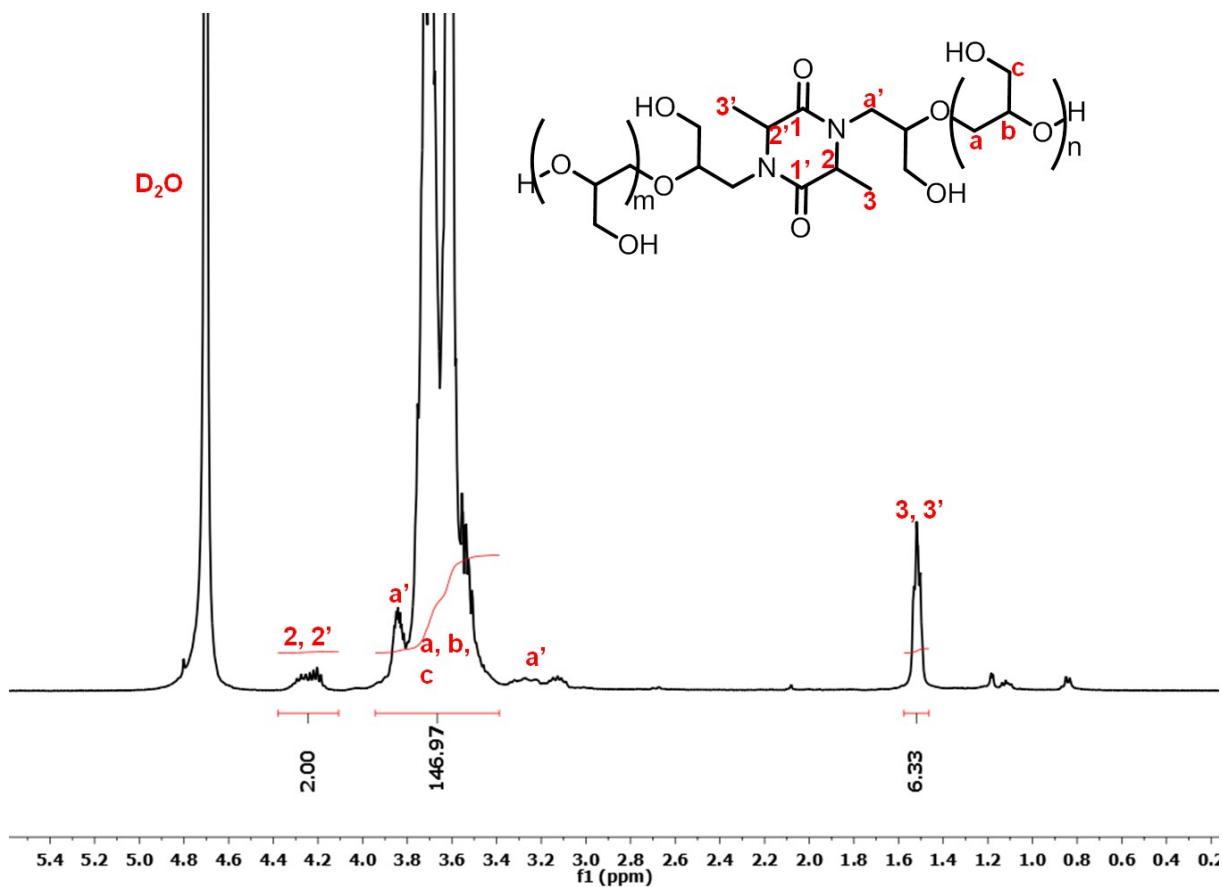


Figure S23: ^1H NMR analysis of N-PG-Cyclo(Ala-Ala) in D_2O .