Supporting Information

for

Cyclodextrins tethered with oligolactides – green synthesis and structural assessment

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Analytical Data

Contents

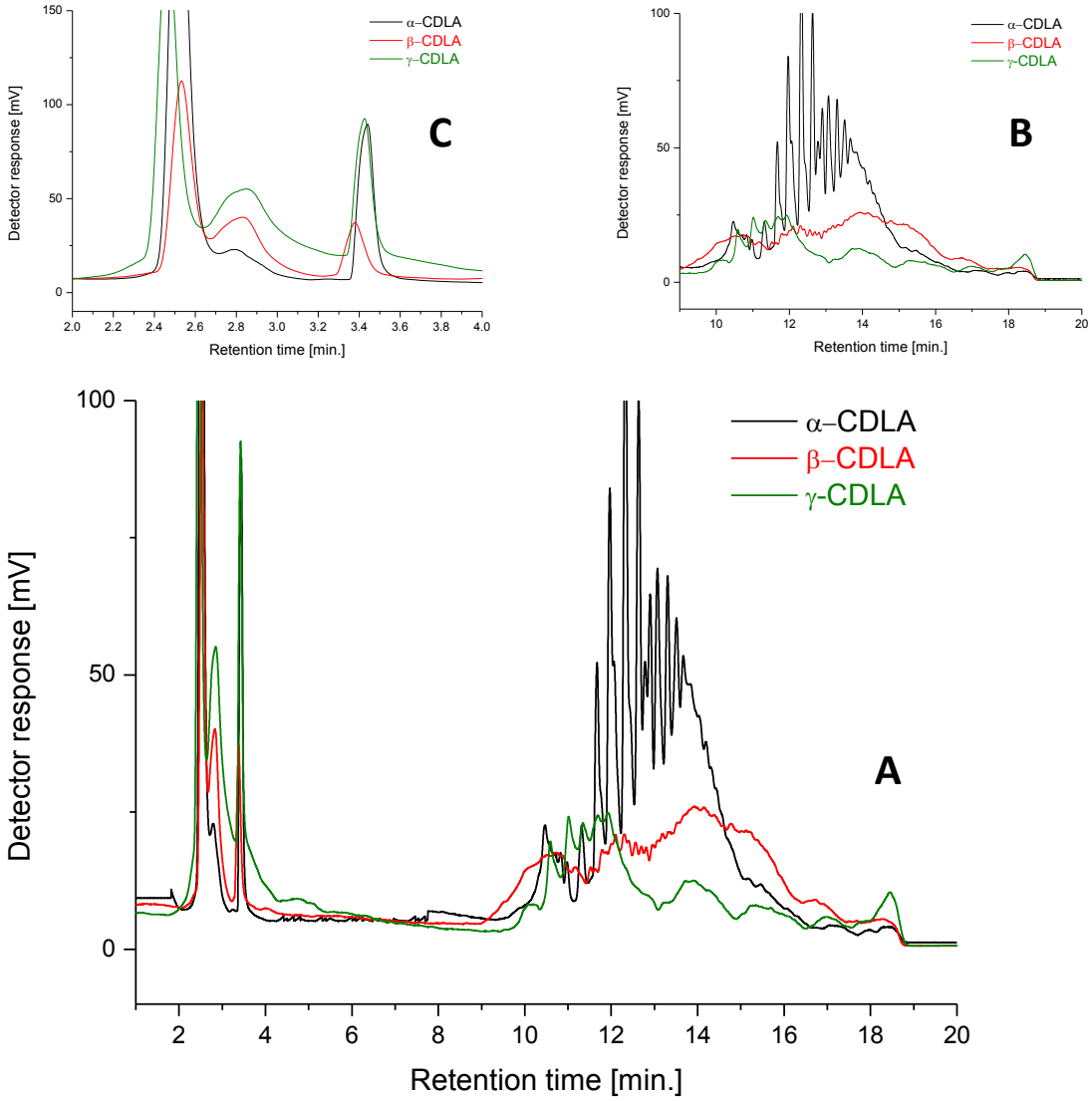

Figure S1: LC–ESLD chromatograms of α-, β- and γ-CD-LA (A), highlights of 9–20 min region (B) and 2–4 min region (C).

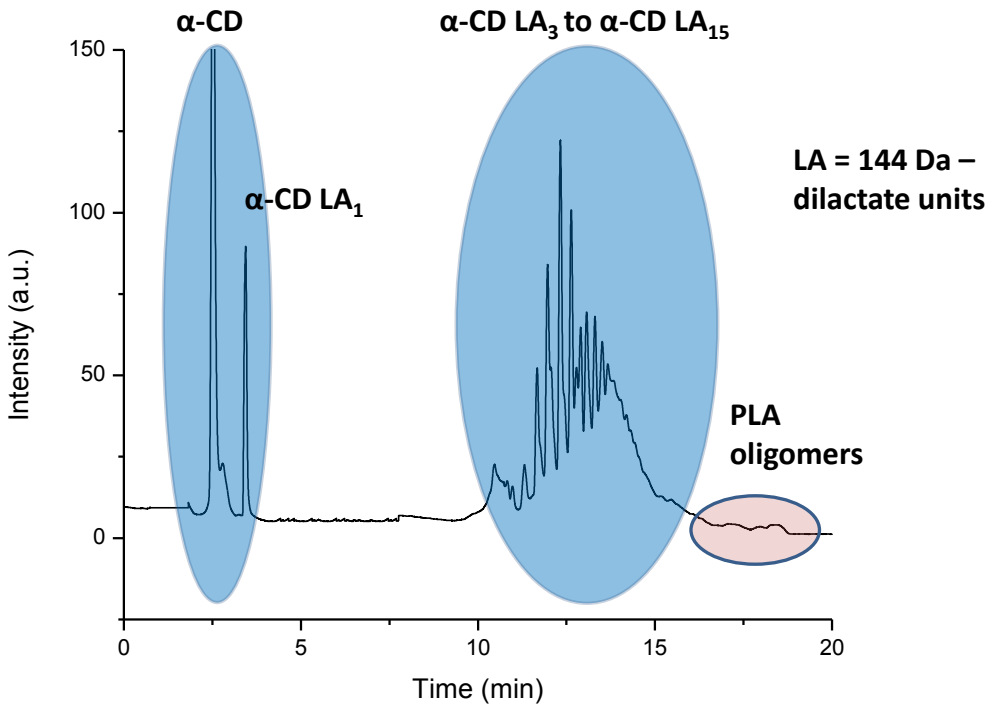

Figure S2: LC–ESLD chromatogram of α-CD-LA(f1 - 2.3 – 3 min; f2 – 3 – 4.2 min; f3 – 9.8 – 12 min; f4 – 12 – 14 min; f5 – 14 – 16 min; f6 – 16 – 19 min).

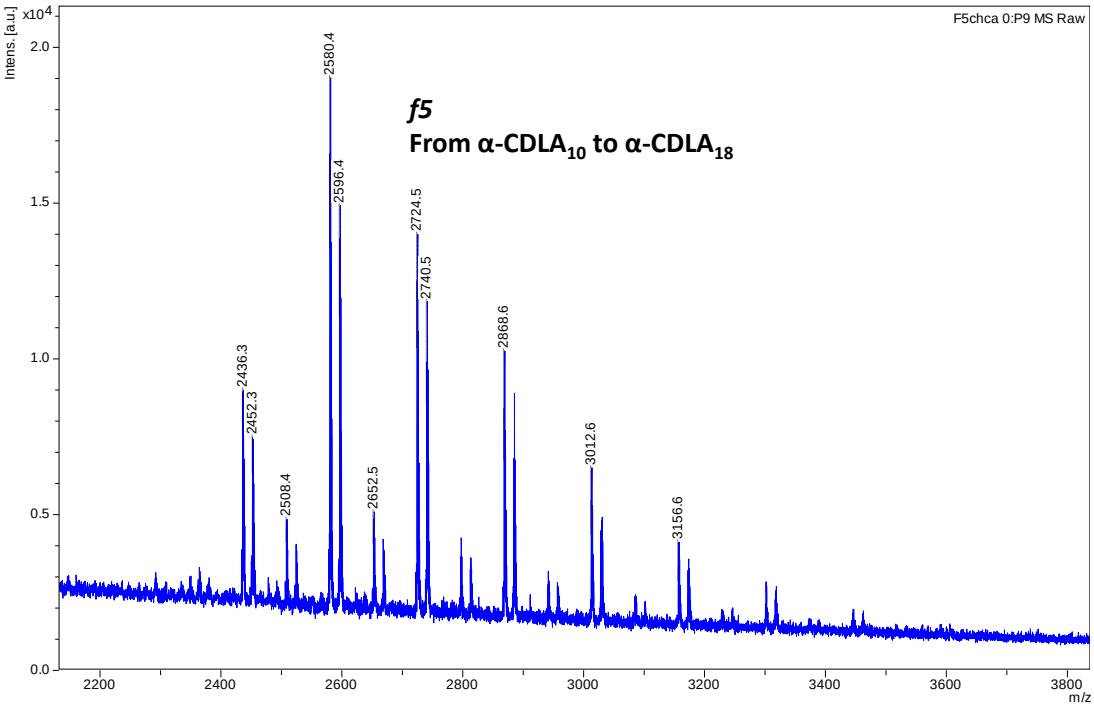

Figure S3: MALDI–MS spectrum of fraction f5 from α-CD-LA separation.

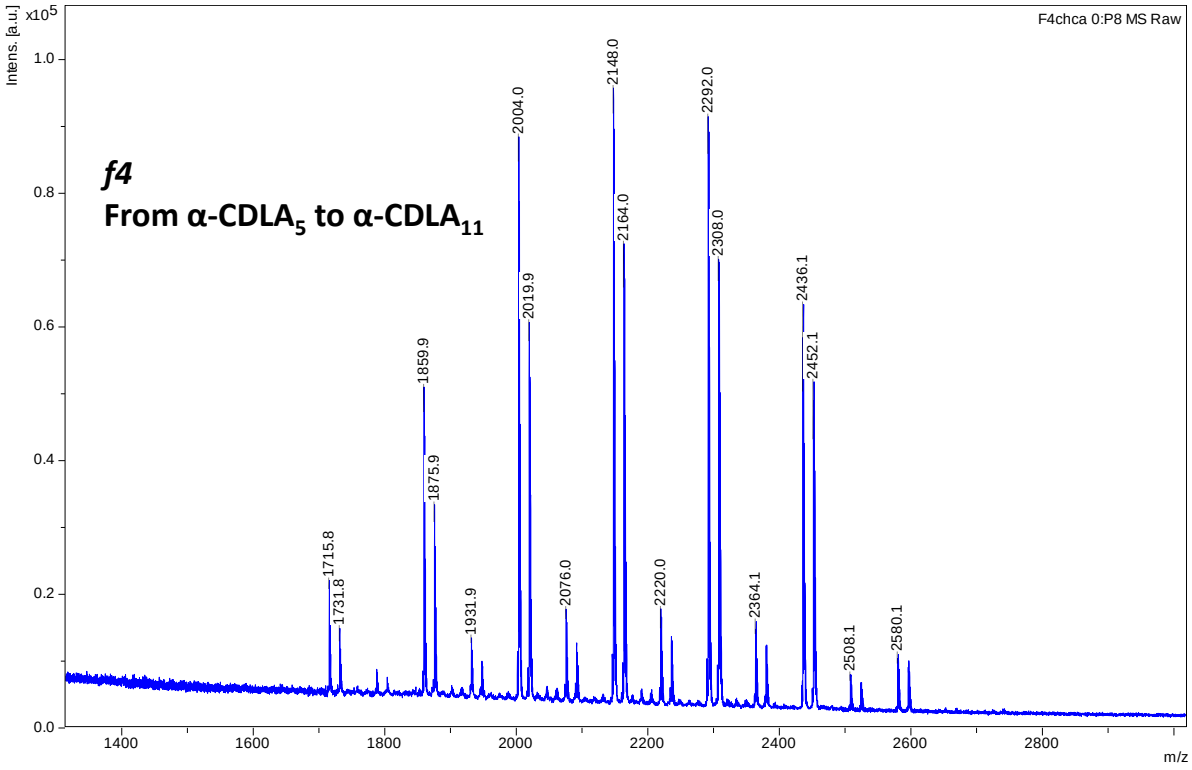

Figure S4: MALDI–MS spectrum of fraction f4 from α-CD-LA separation.

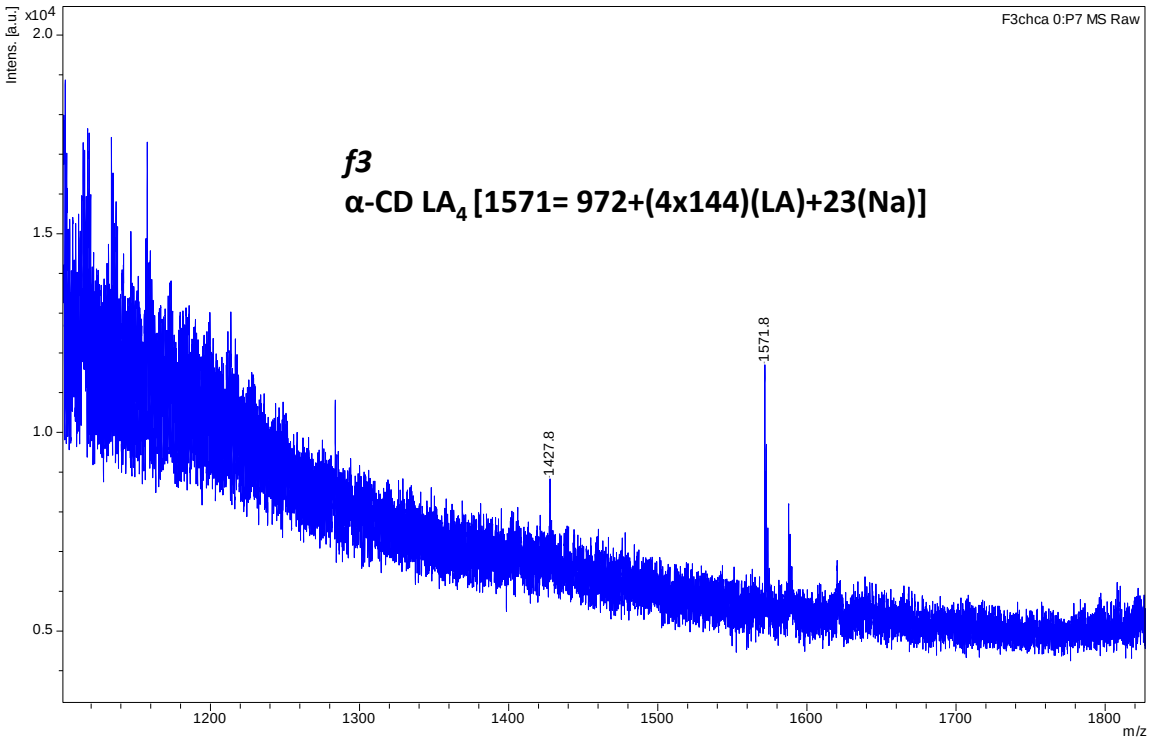

Figure S5: MALDI–MS spectrum of fraction f3 from α-CD-LA separation.

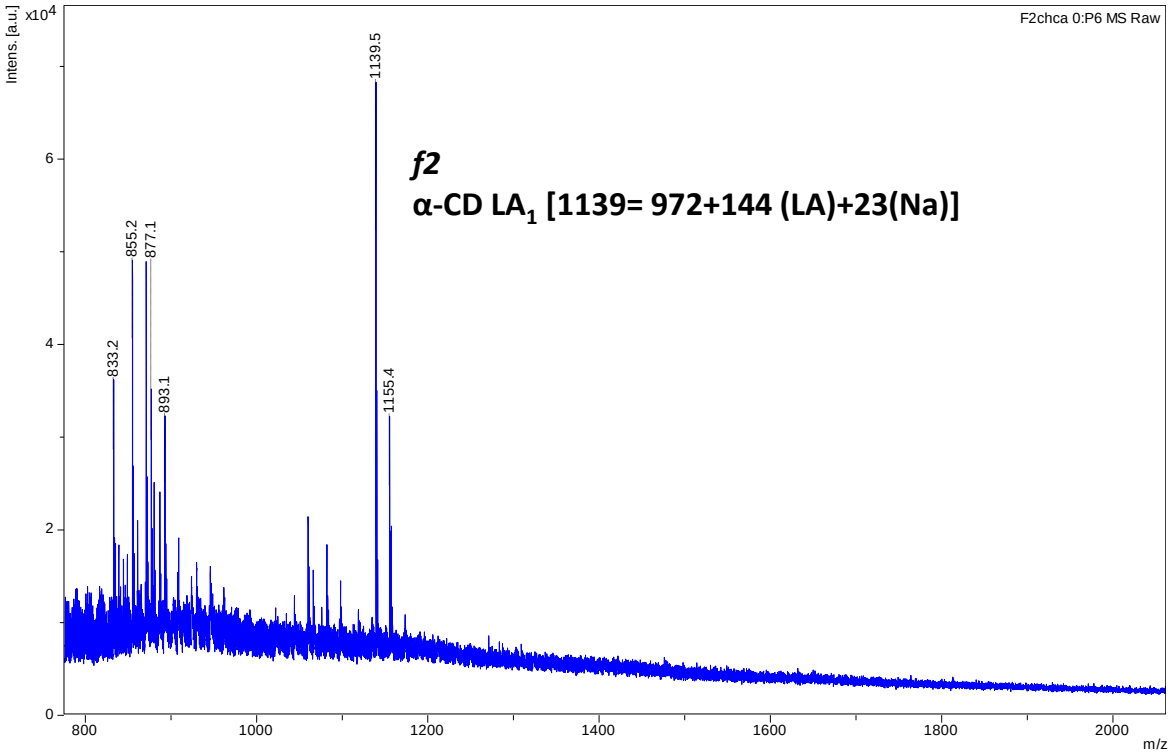

Figure S6: MALDI–MS spectrum of fraction f2 from α-CD-LA separation.

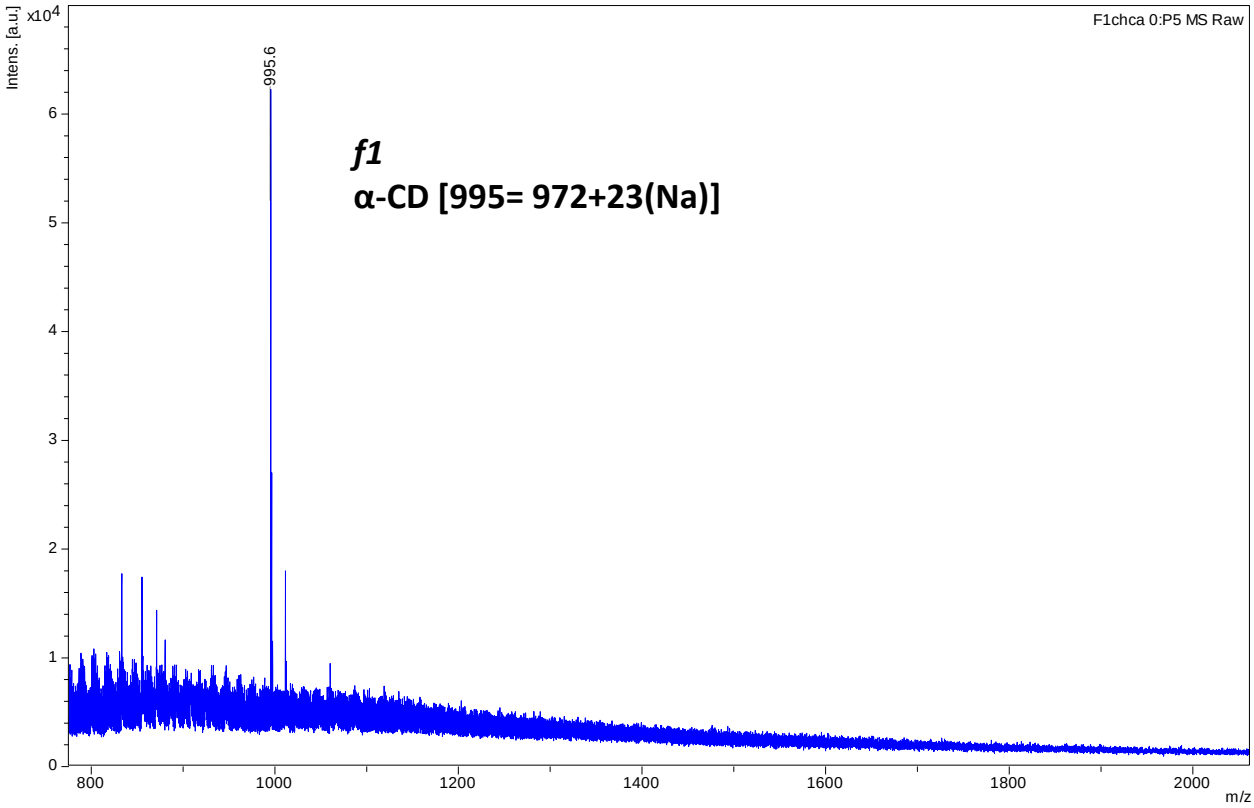

Figure S7: MALDI–MS spectrum of fraction f1 from α-CD-LA separation.

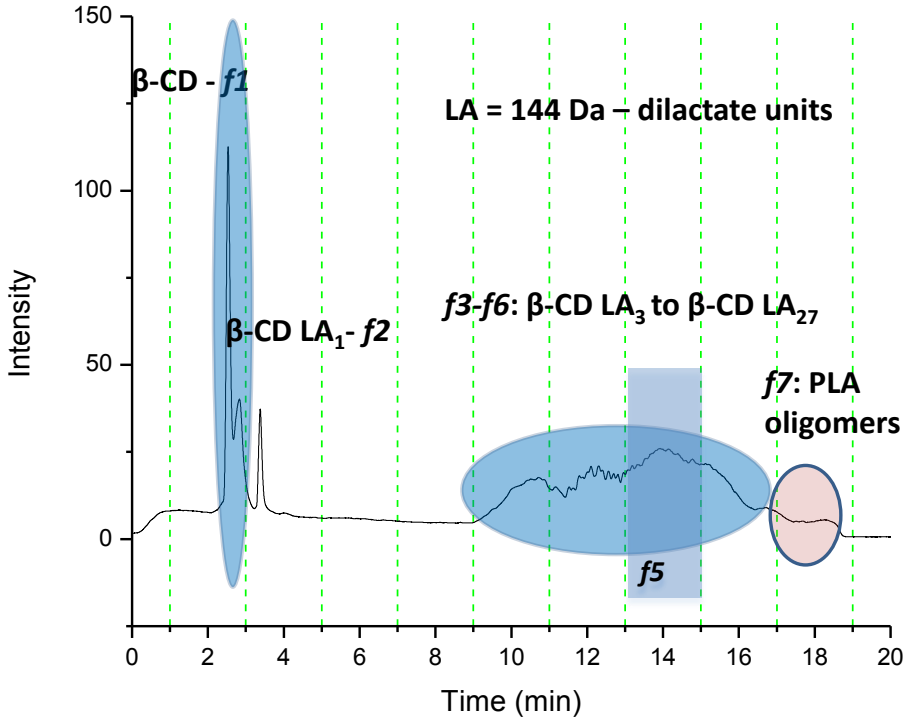

Figure S8: LC–ESLD chromatogram of β-CD-LA (f1 - 2– 3 min; f2 – 3 – 4 min; f3 – 9 – 11 min; f4 – 11 – 13 min; f5 – 13 – 15 min; f6 – 15 – 17 min; f7 – 17 – 19 min).

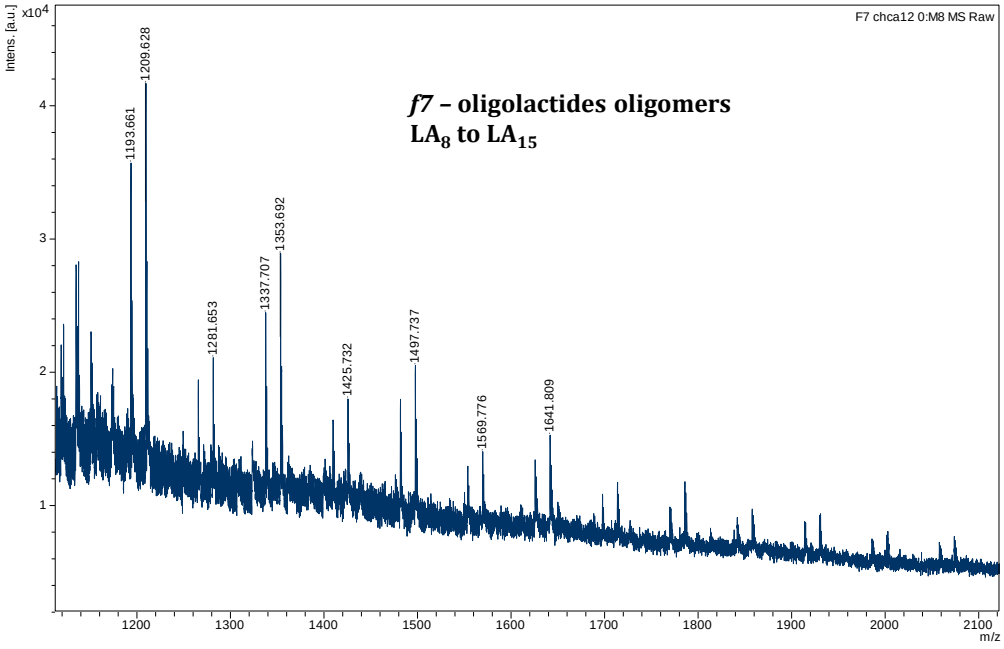

Figure S9: MALDI–MS spectrum of fraction *f7* from β-CD-LA separation.

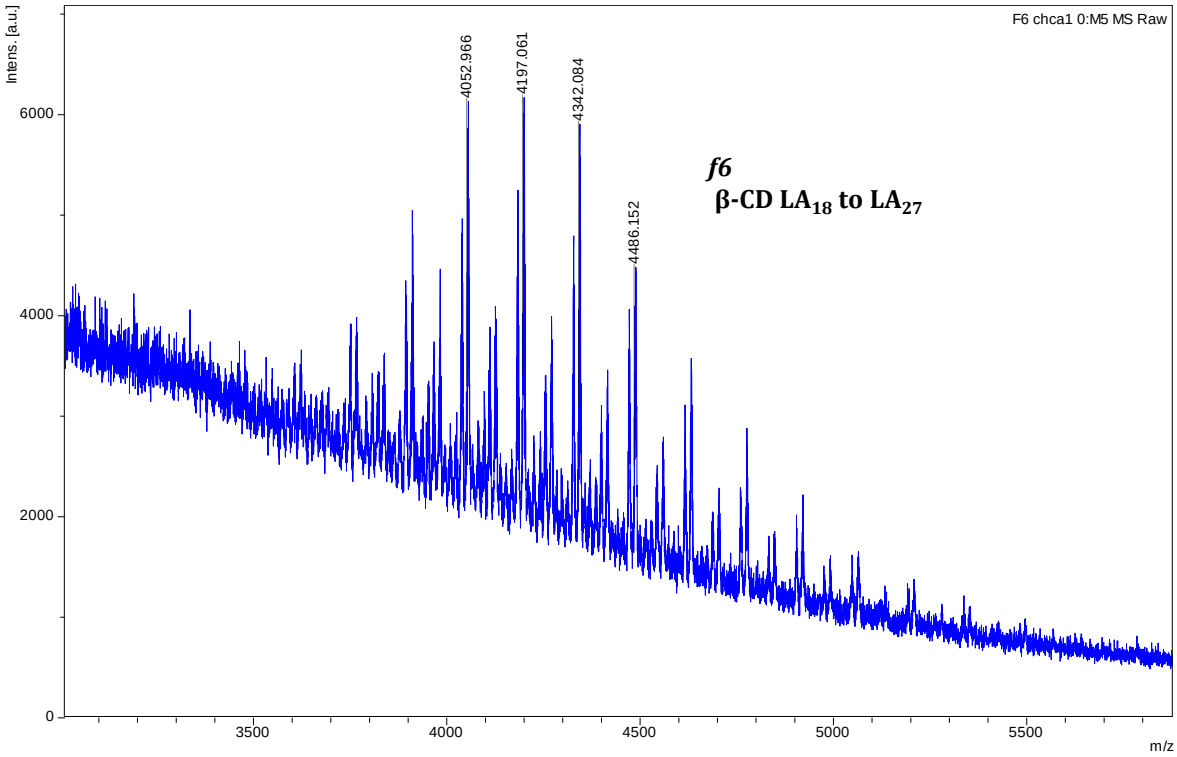

Figure S10: MALDI–MS spectrum of fraction *f6* from β-CD-LA separation.

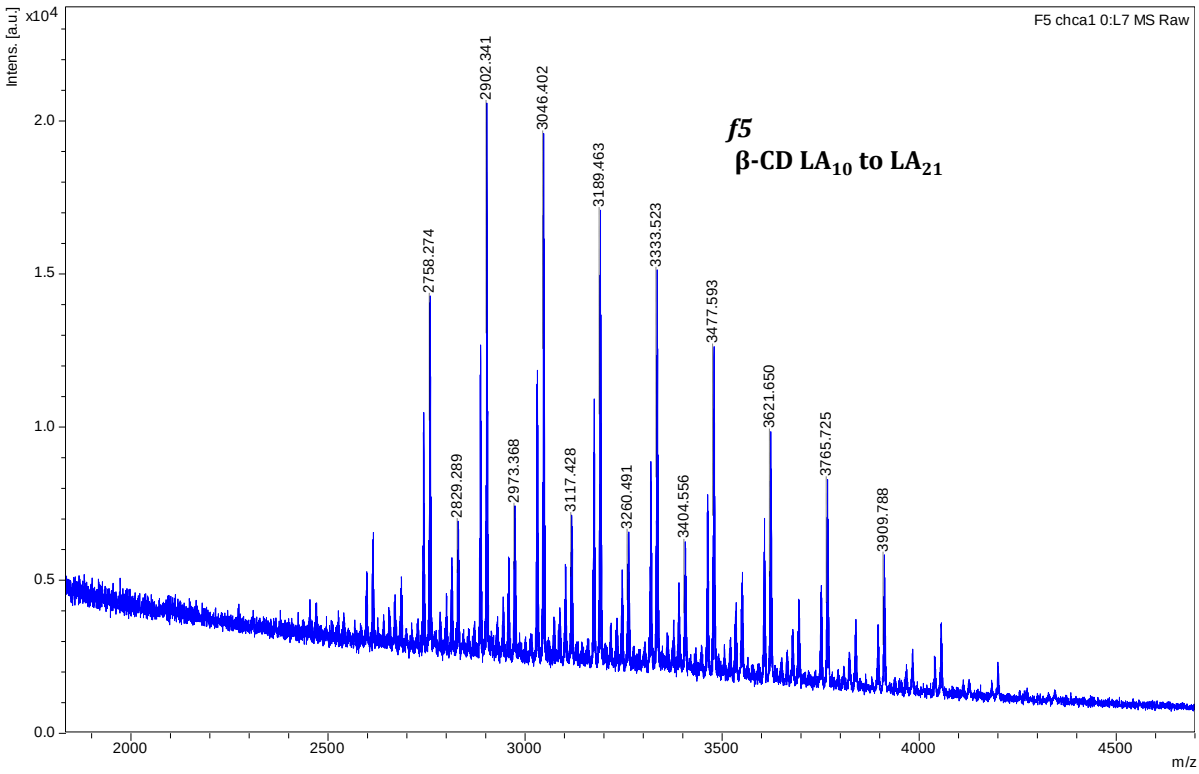

Figure S11: MALDI–MS spectrum of fraction *f5* from β-CD-LA separation.

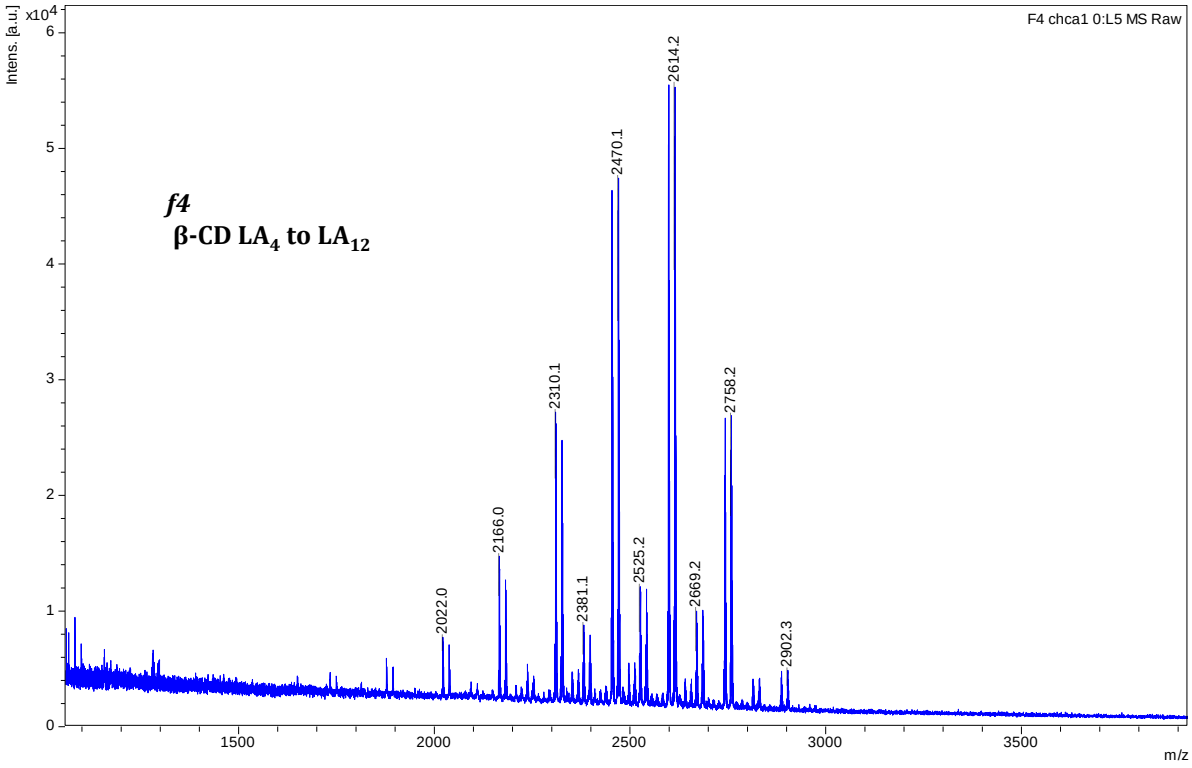

Figure S12: MALDI–MS spectrum of fraction *f4* from β-CD-LA separation.

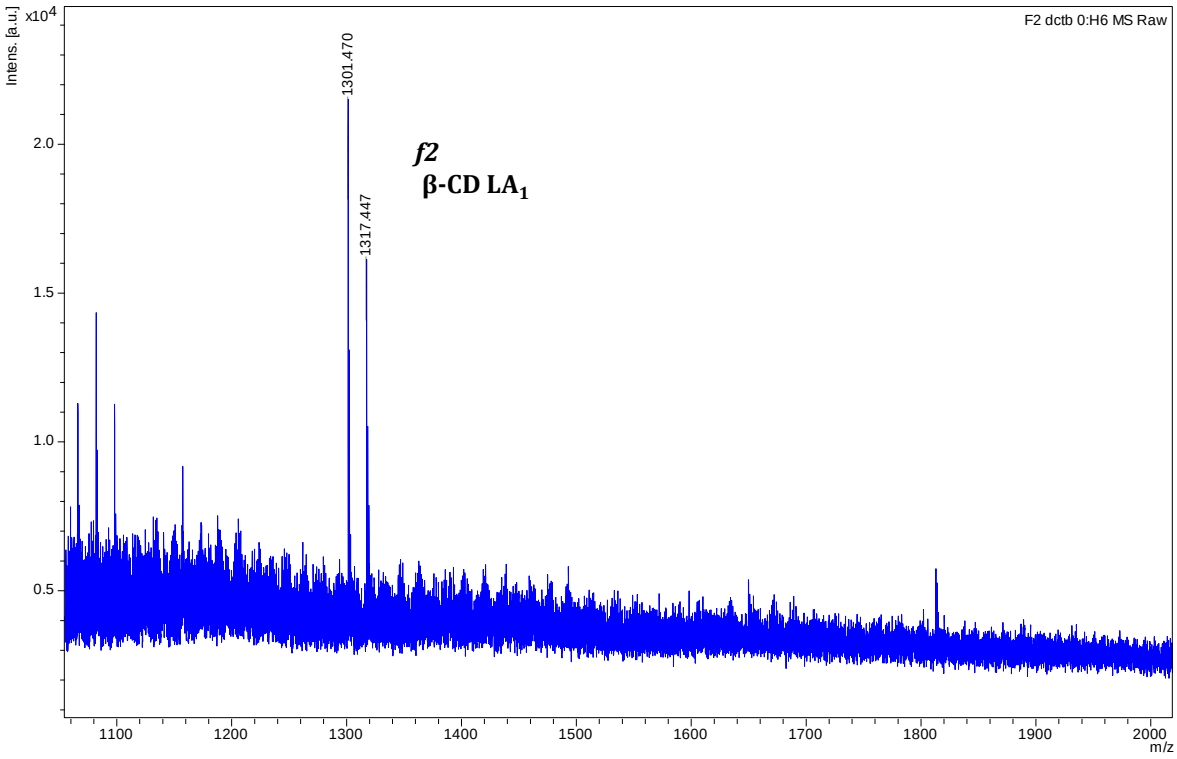

Figure S13: MALDI–MS spectrum of fraction *f2* from β-CD-LA separation.

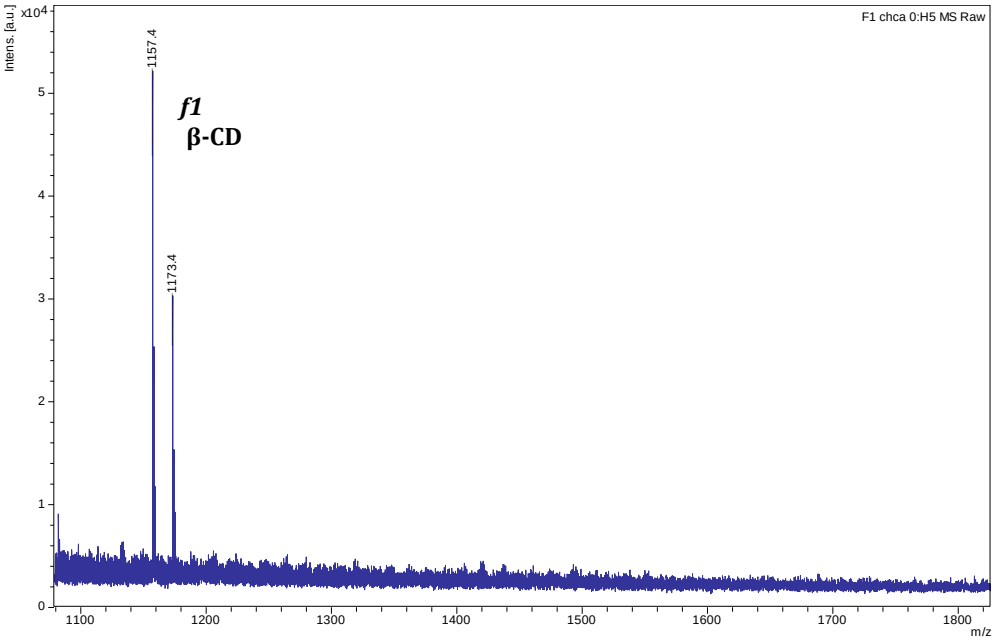

Figure S14: MALDI–MS spectrum of fraction *f1* from β-CD-LA separation.

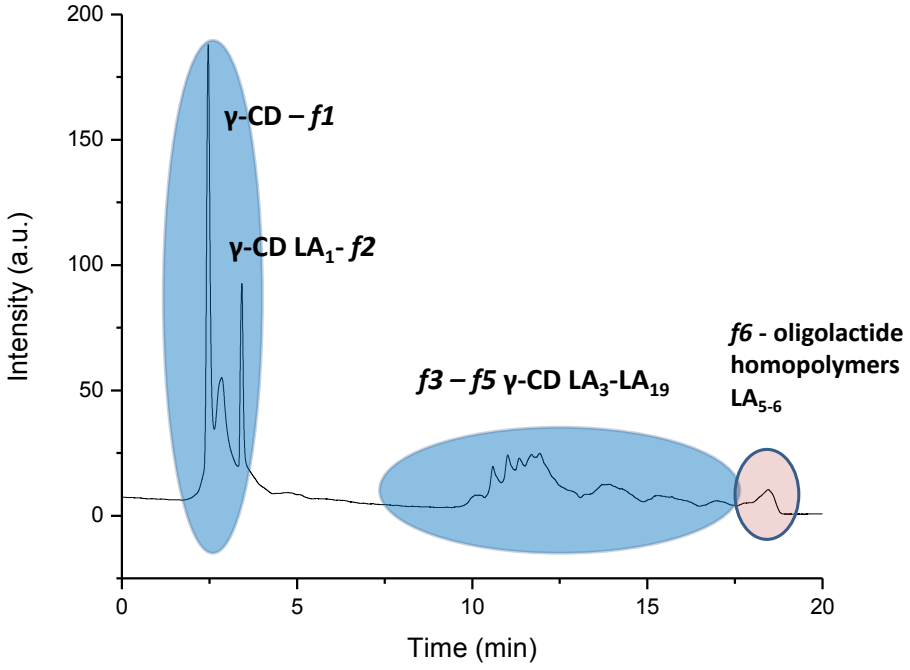

Figure S15: LC–ESLD chromatogram of γ-CD-LA (f1 - 2.3 – 3 min; f2 – 3 – 4.2 min; f3 – 10 – 12.5 min; f4 – 12.5 – 15 min; f5 – 15 – 17.5 min; f6 – 17.5 – 19 min).

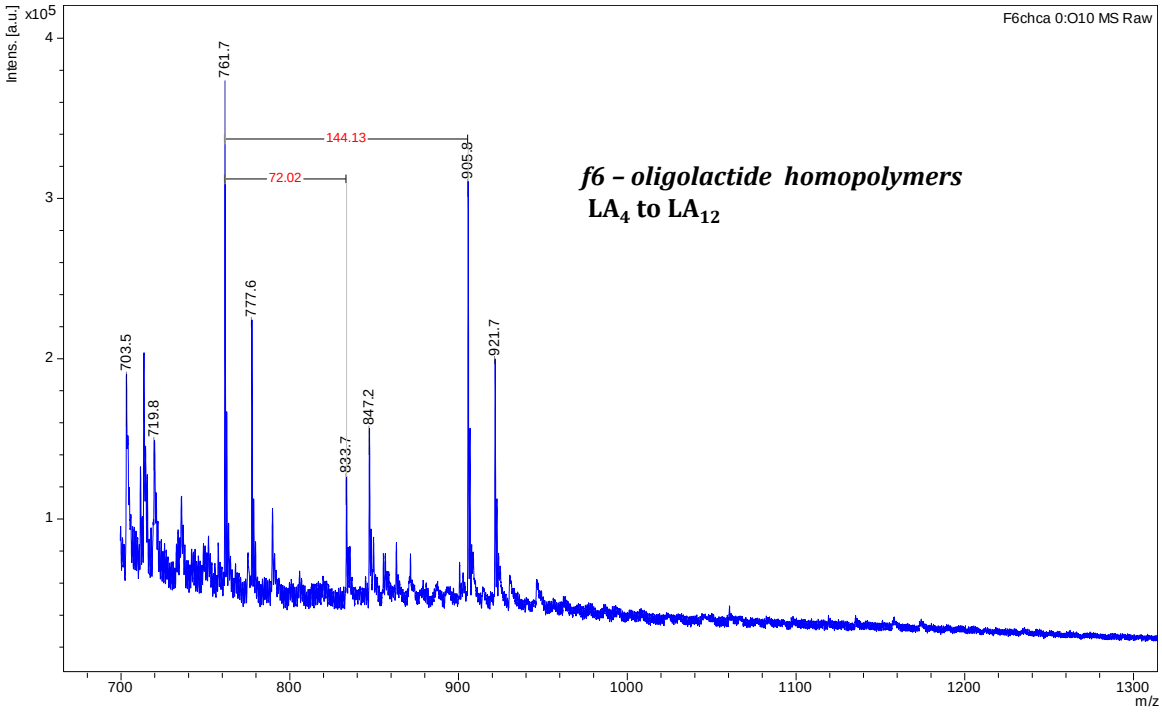

Figure S16: MALDI–MS spectrum of fraction *f6* from γ-CD-LA separation.

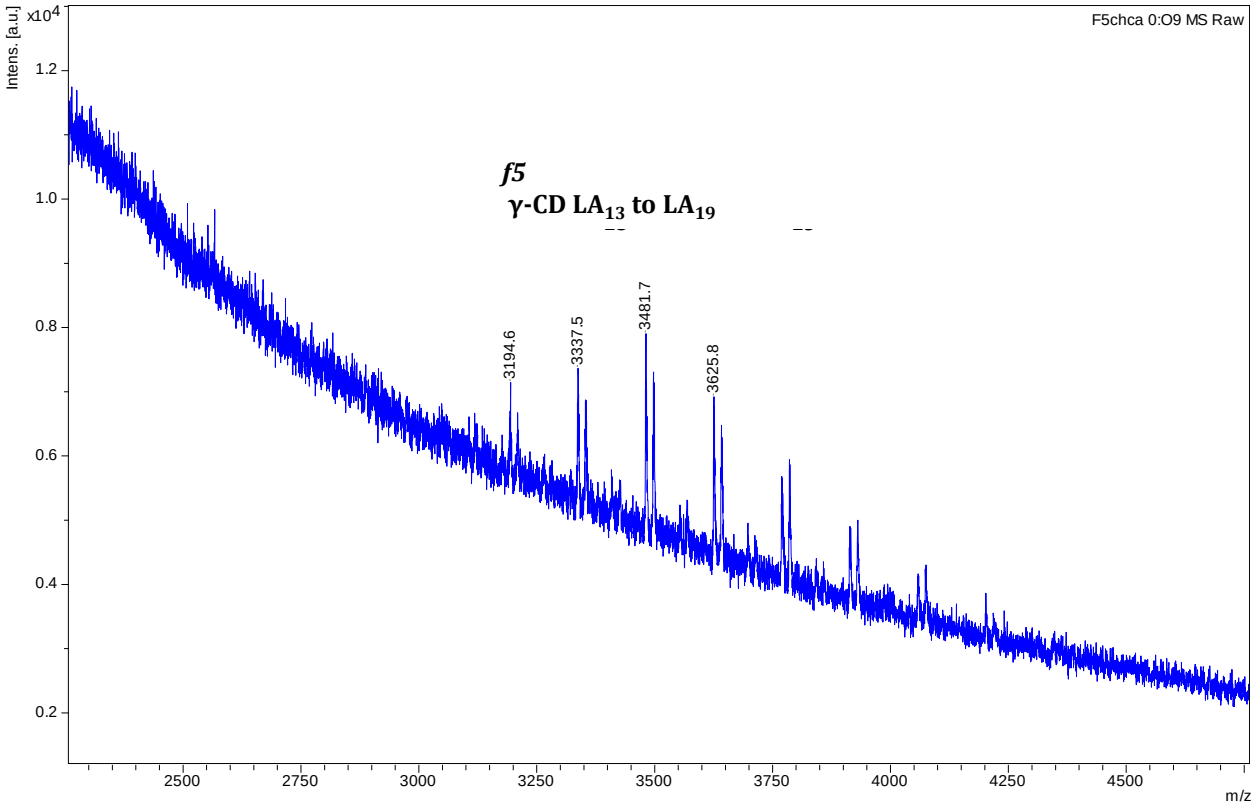

Figure S17: MALDI–MS spectrum of fraction *f5* from γ-CD-LA separation.

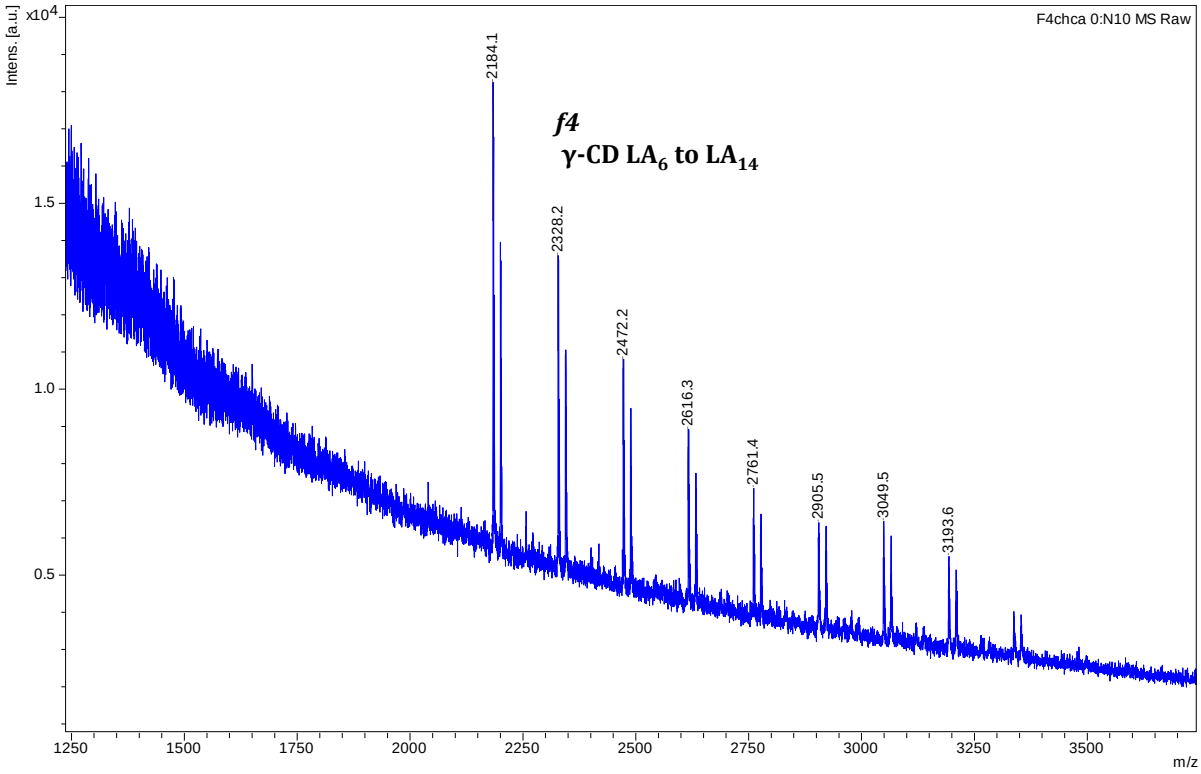

Figure S18: MALDI–MS spectrum of fraction *f4* from γ-CD-LA separation.

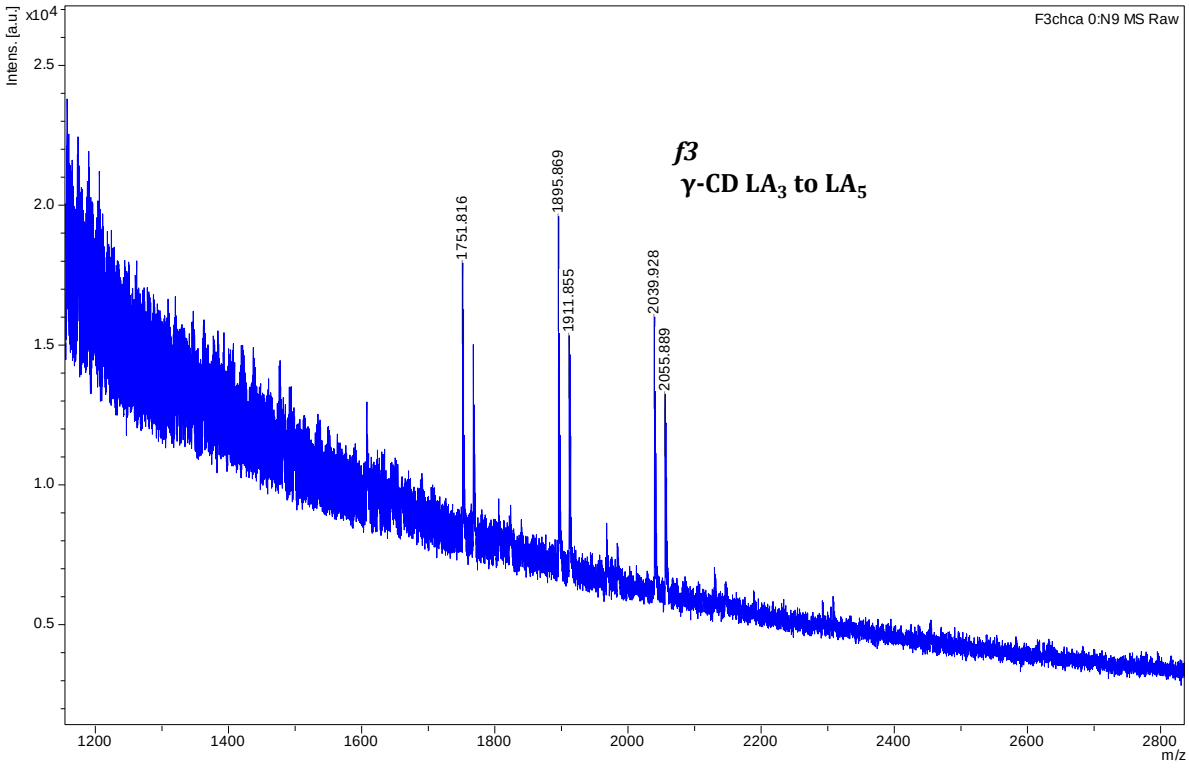

Figure S19: MALDI–MS spectrum of fraction *f3* from γ-CD-LA separation.

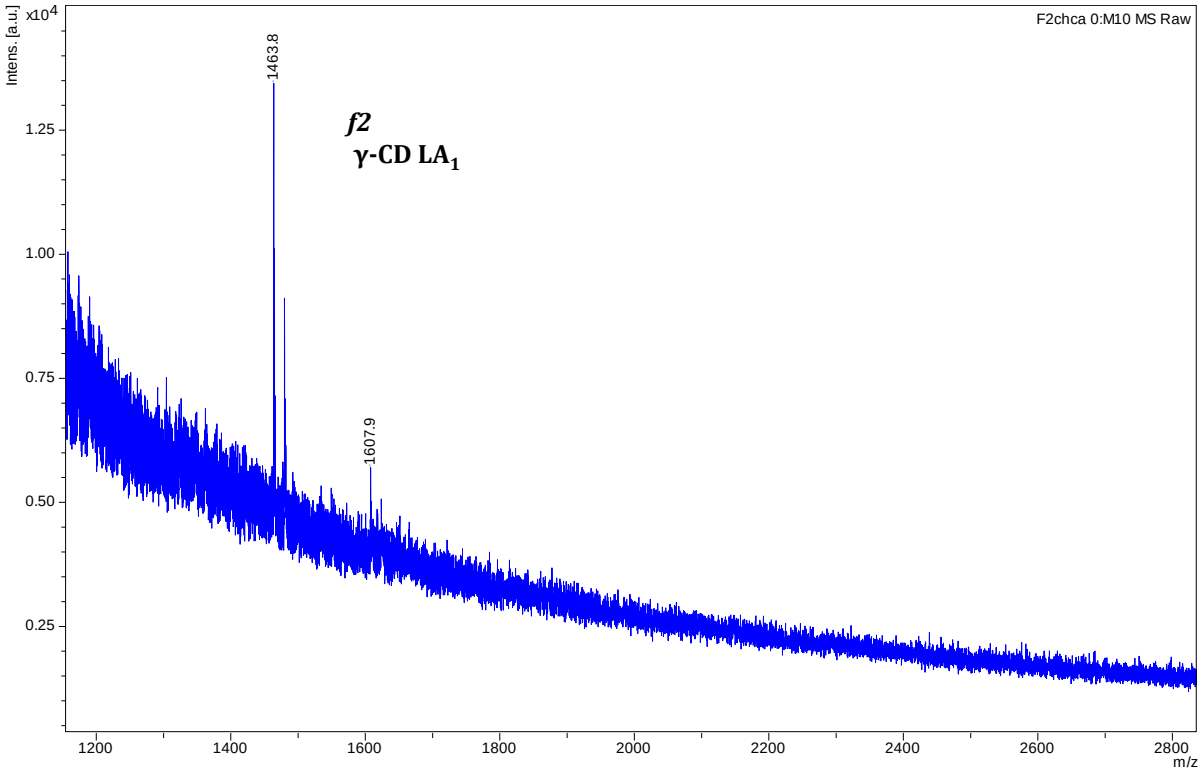

Figure S20: MALDI–MS spectrum of fraction *f2* from γ-CD-LA separation.

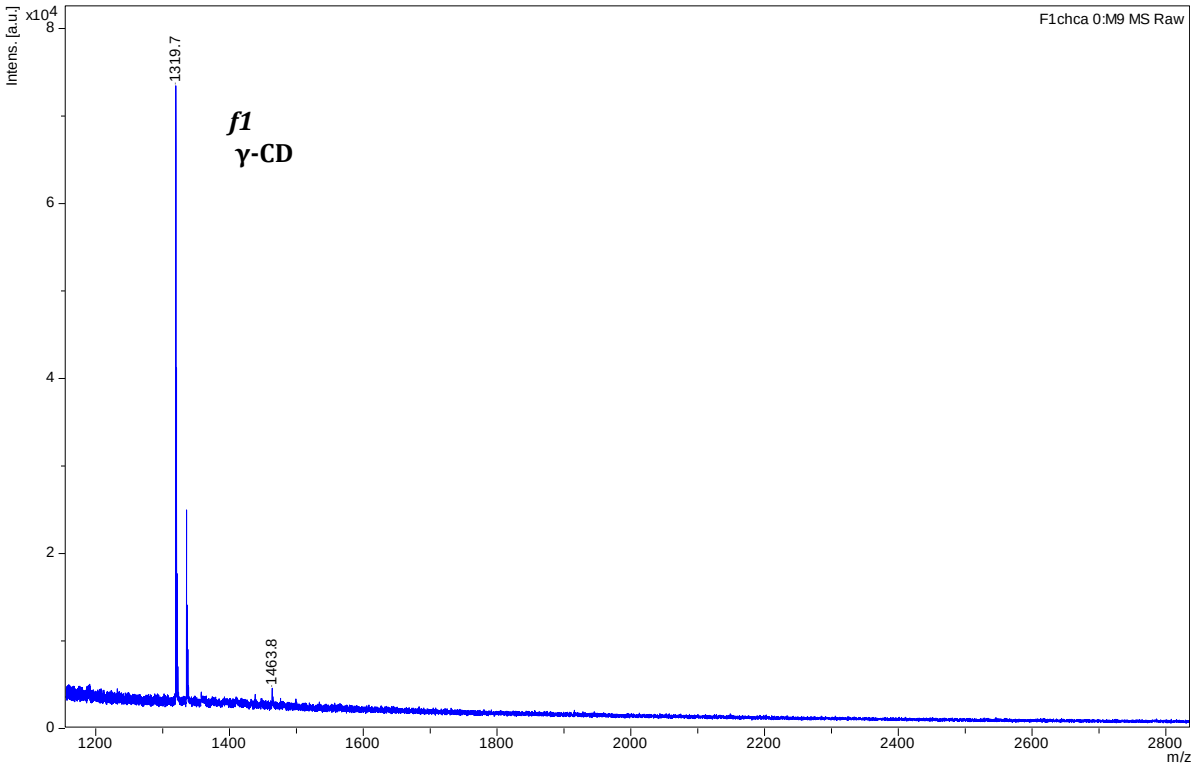

Figure S21: MALDI–MS spectrum of fraction *f1* from γ-CD-LA separation.

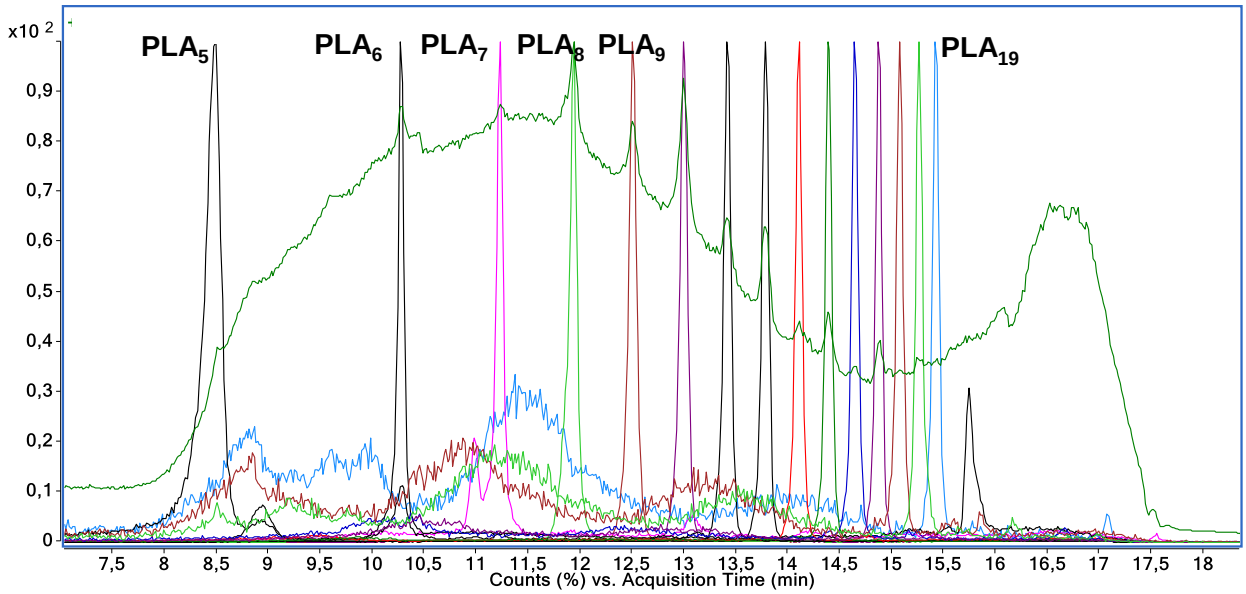

Figure S22: LC–MS separation of β-CD-LA (total ion chromatogram from 8 to 17.5 min and extracted ion chromatograms of PLA oligomers from 5 to 19 lactate units).

In Figure S22 are overlapped the extracted ion chromatograms for PLA homopolymers; each extracted ion chromatogram is scaled to the highest peak, giving only qualitative information when compared with all other chromatograms.

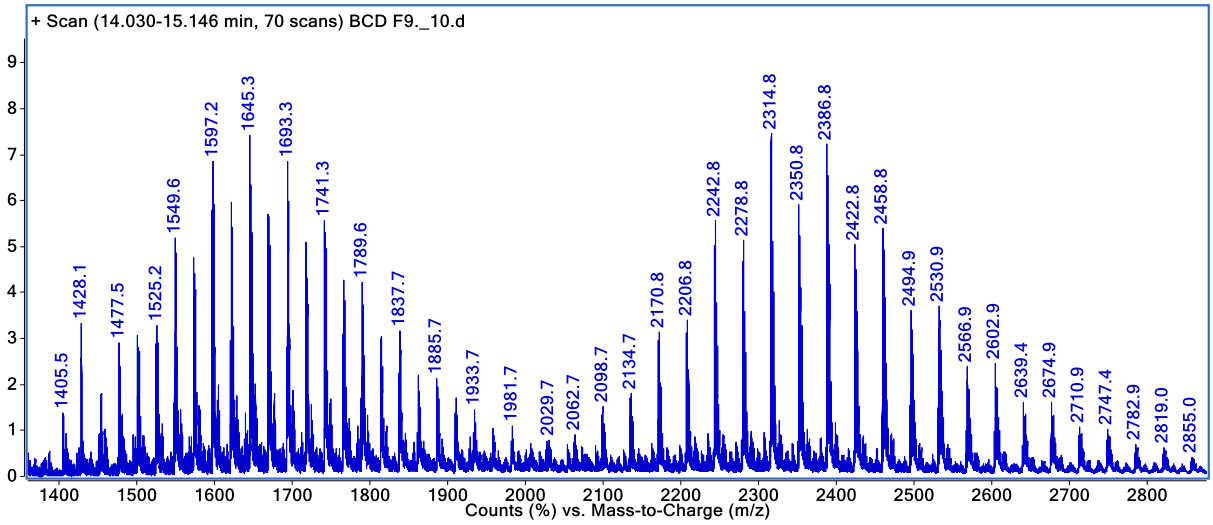

Figure S23: LC–ESI–MS spectrum β-CD-LA collected between 14 and 15 min; contains double charged (left) and triple charged (right) species of β-CD-LA (average mass of this fraction is close to 5000 Da).

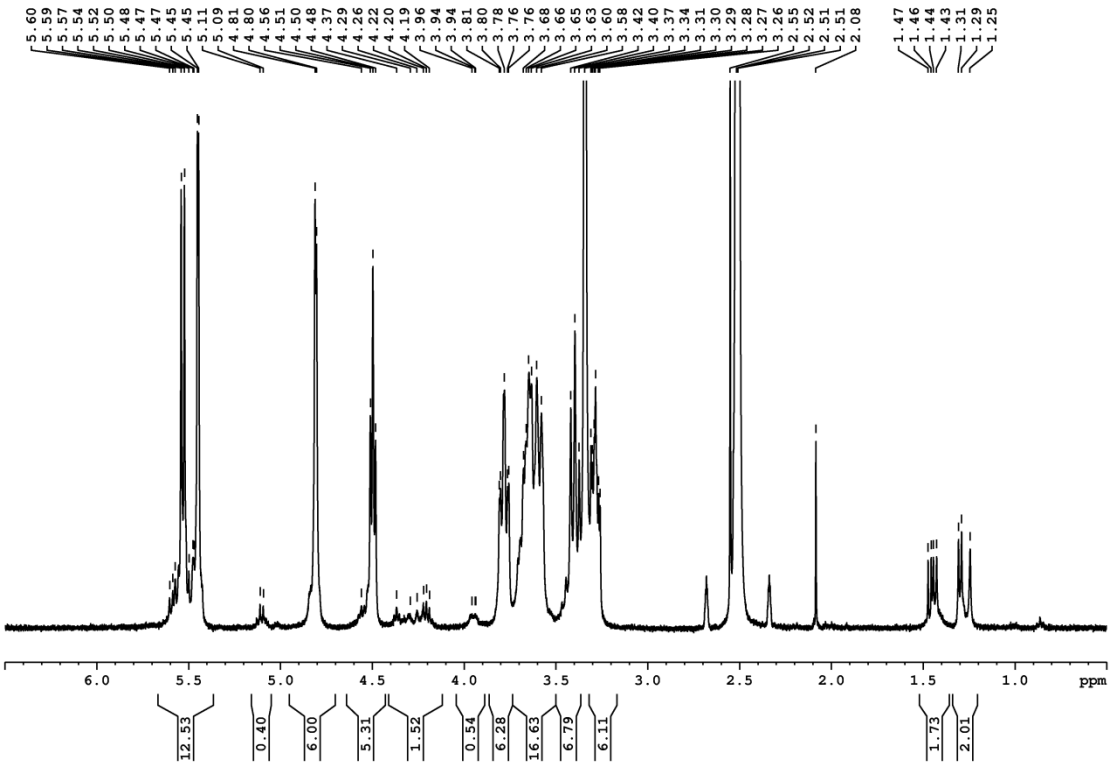

Figure S24: ^{1}H NMR spectrum of α-CD-LA F1 fraction.

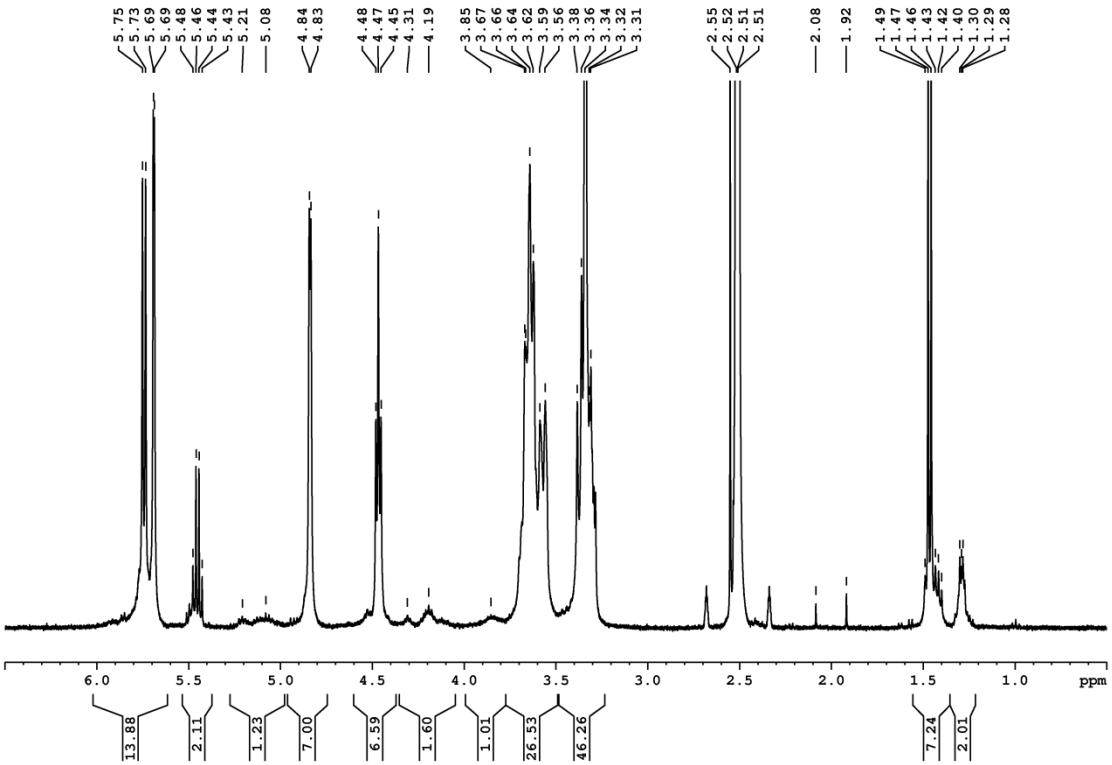

Figure S25: ^{1}H NMR spectrum of β-CD-LA F1 fraction.

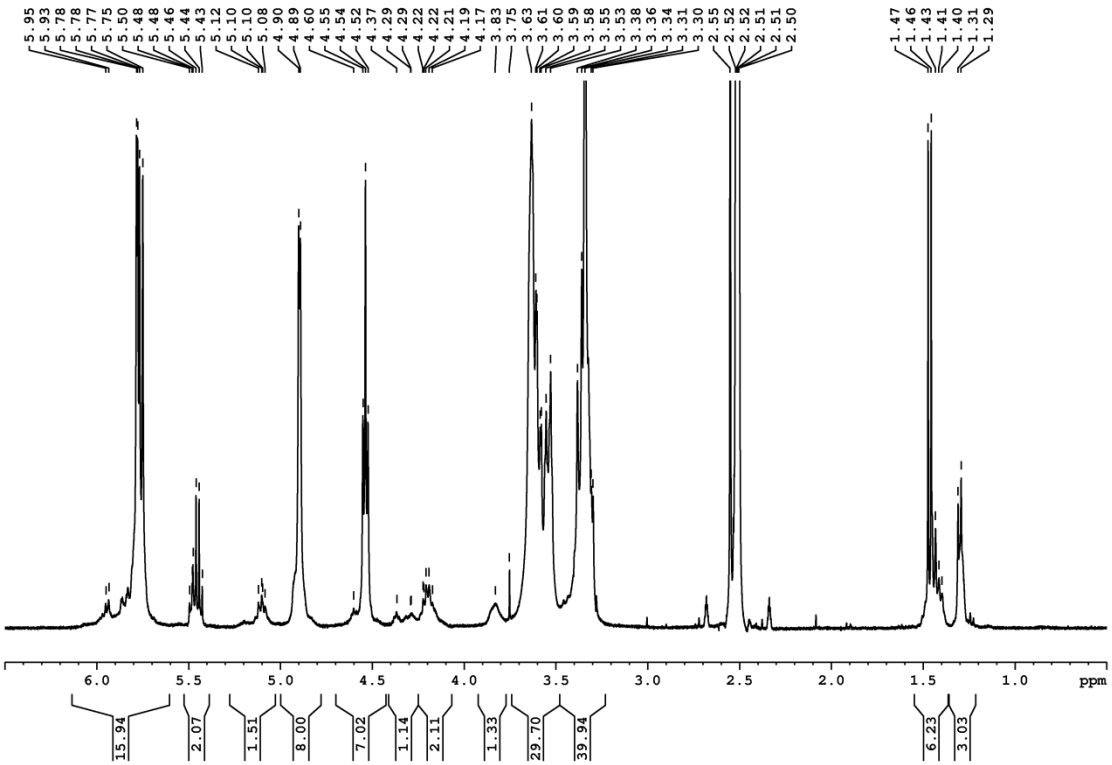

Figure S26: ^{1}H NMR spectrum of γ-CD-LA F1 fraction.

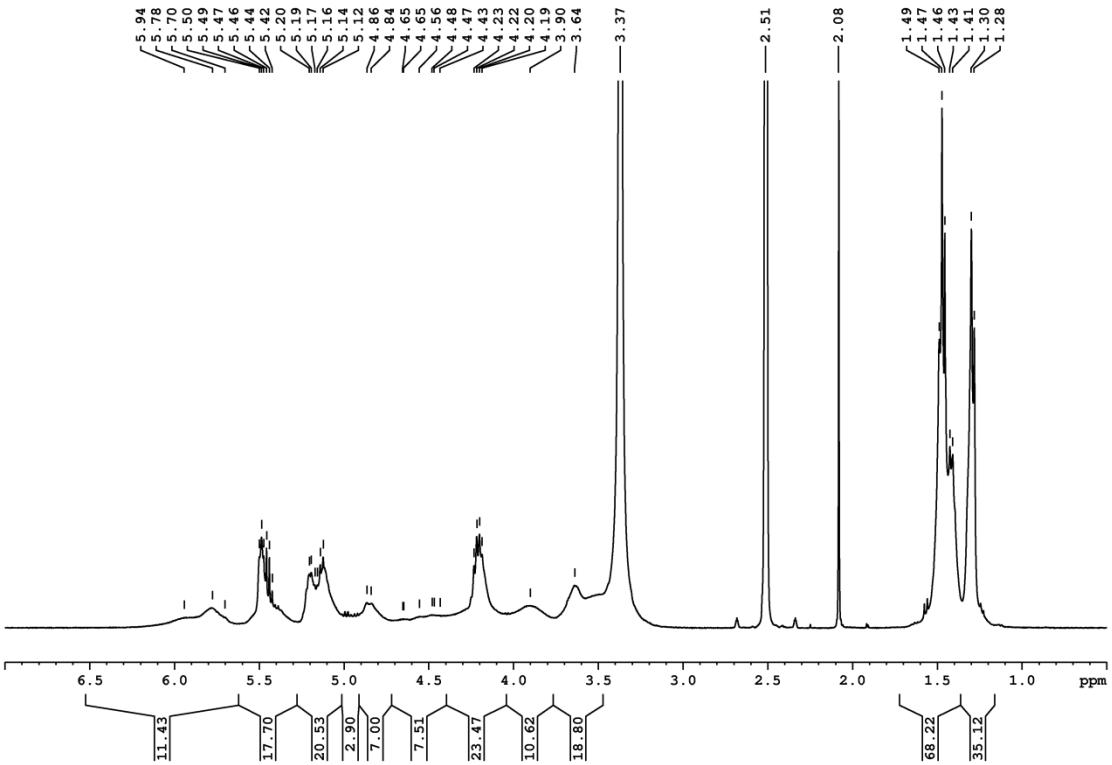

Figure S27: ^{1}H NMR spectrum of β-CD-LA F2 fraction.

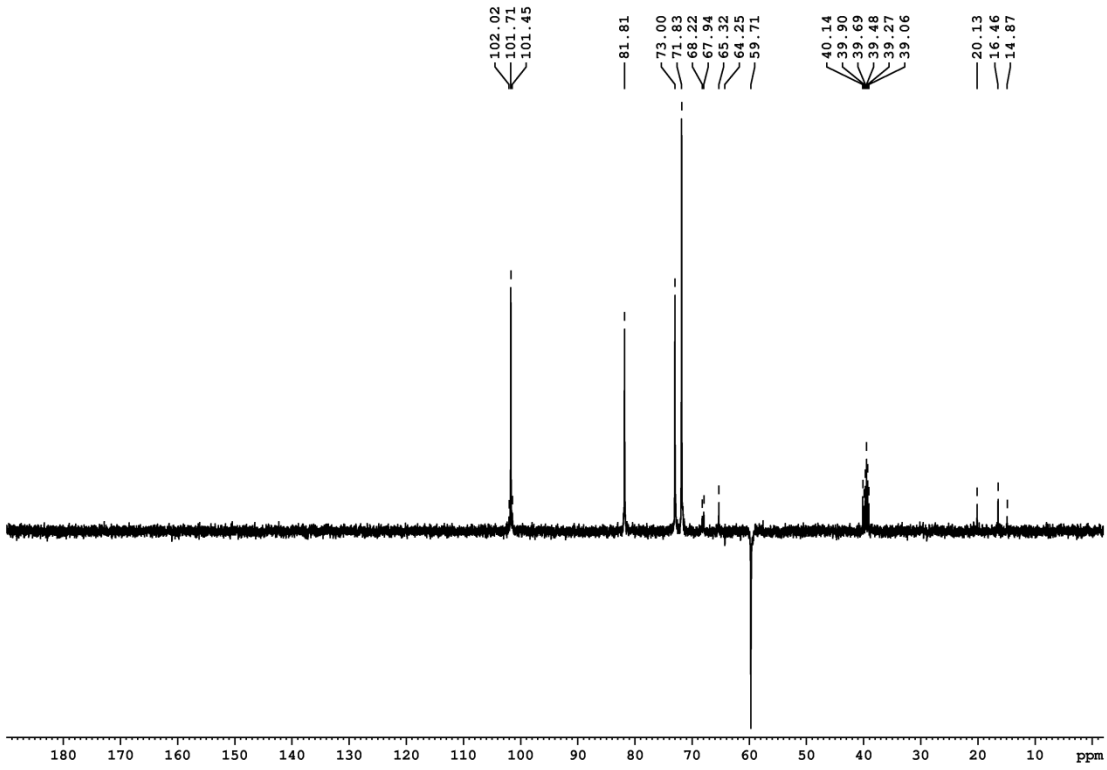

Figure S28: DEPT135-NMR spectrum of α-CD-LA F1 fraction.

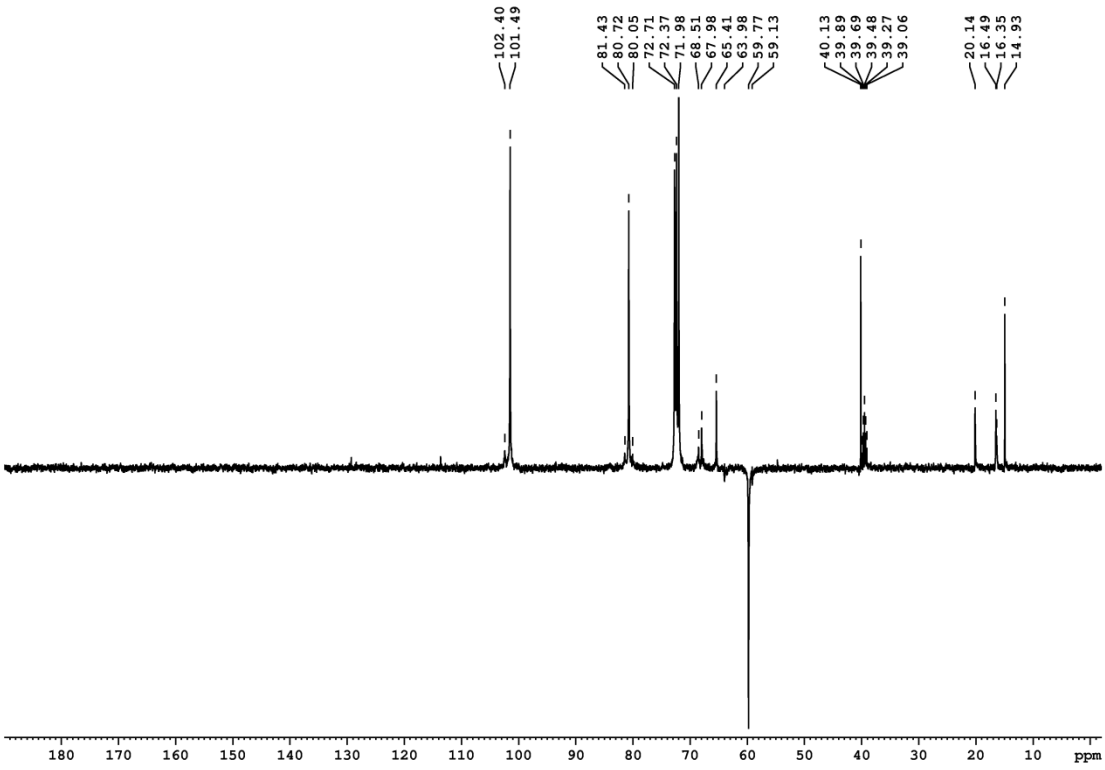

Figure S29: DEPT135-NMR spectrum of γ-CD-LA F1 fraction.

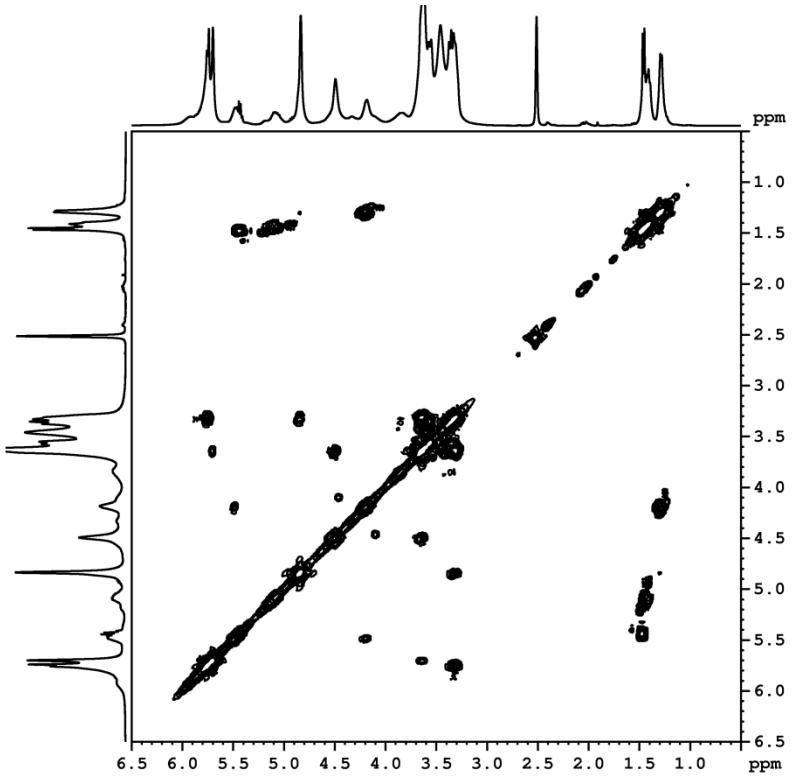

Figure S30: 2D-COSY-NMR spectrum of β-CD-LA F1 fraction.

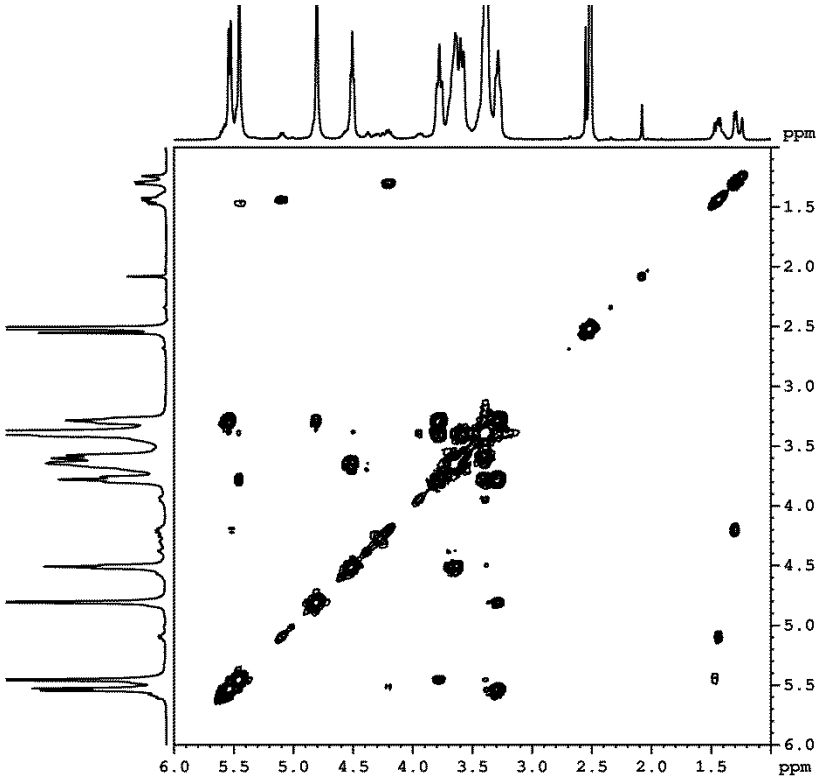

Figure S31: 2D-COSY-NMR spectrum of α-CD-LA F1 fraction.

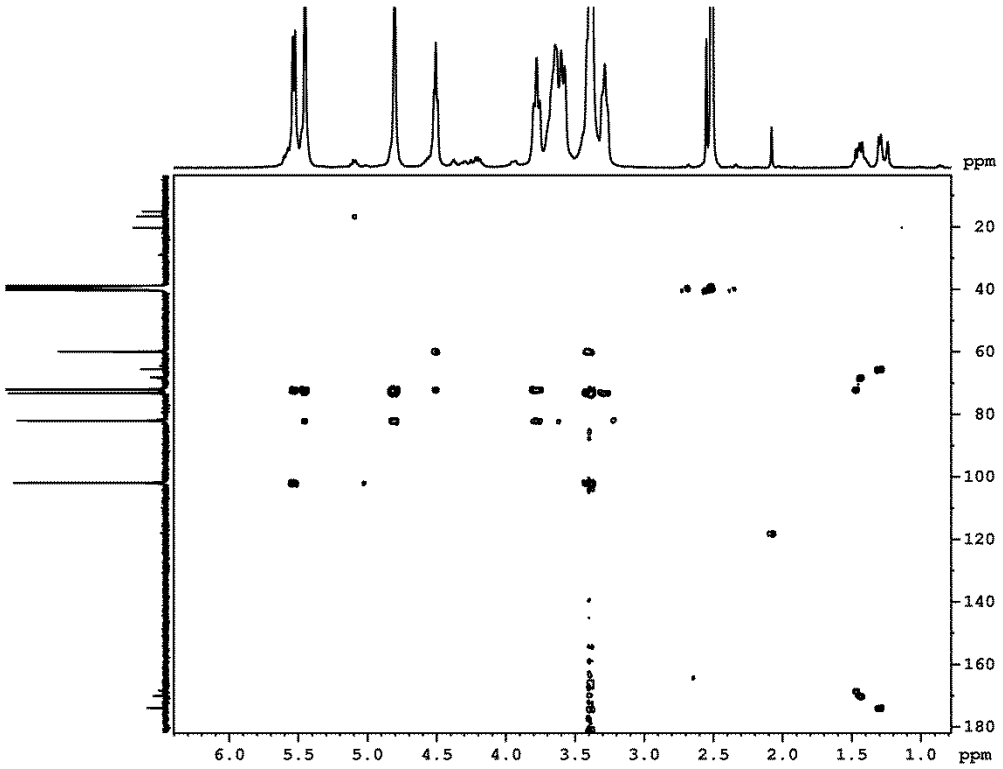

Figure S32: 2D-HMBC-NMR spectrum of α-CD-LA F1 fraction.

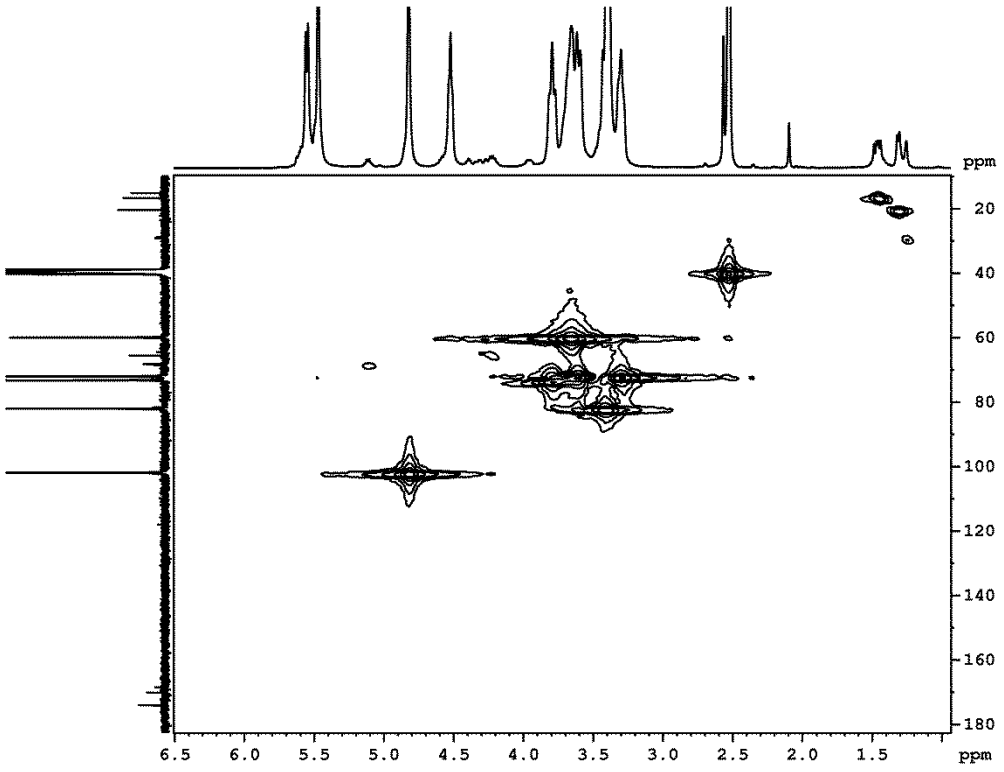

Figure S33: 2D-HMQC-NMR spectrum of α-CD-LA F1 fraction.

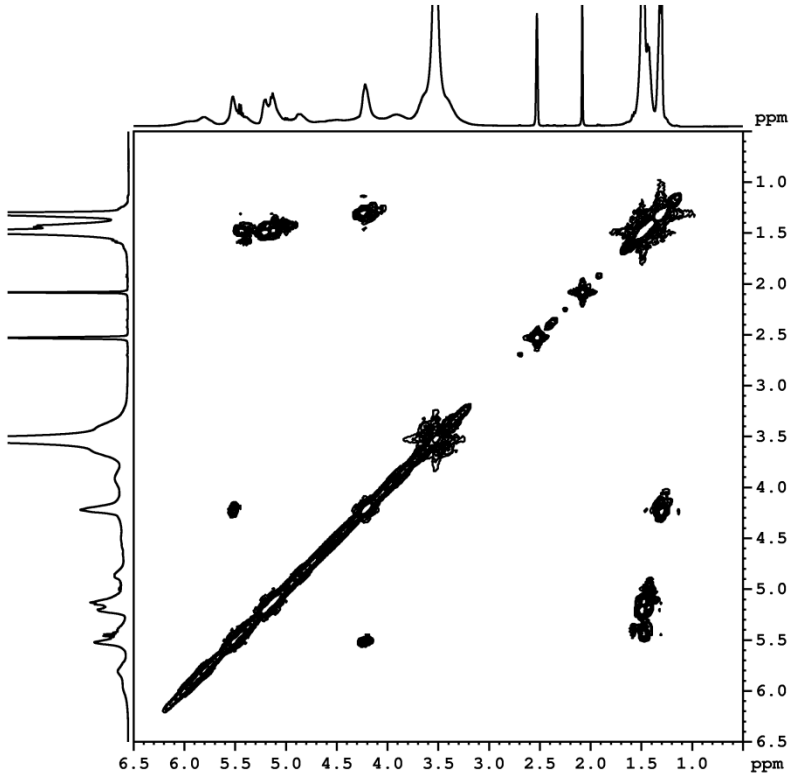

Figure S34: 2D-COSY-NMR spectrum of β-CD-LA F2 fraction.

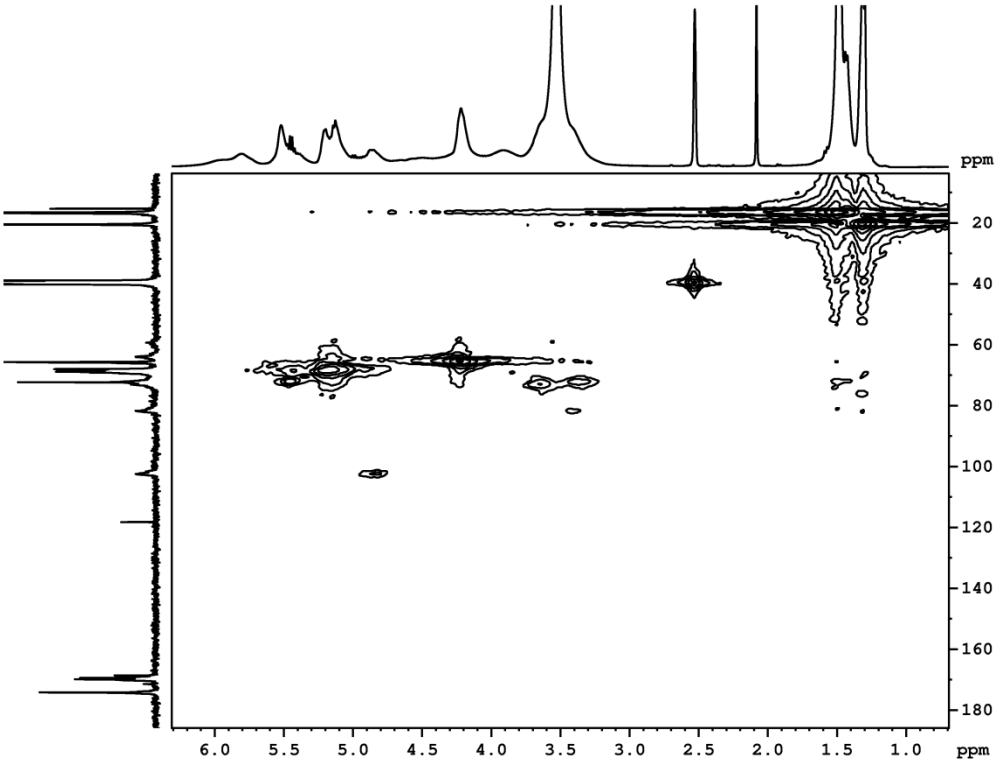

Figure S35: 2D-HMQC-NMR spectrum of β-CD-LA F2 fraction.

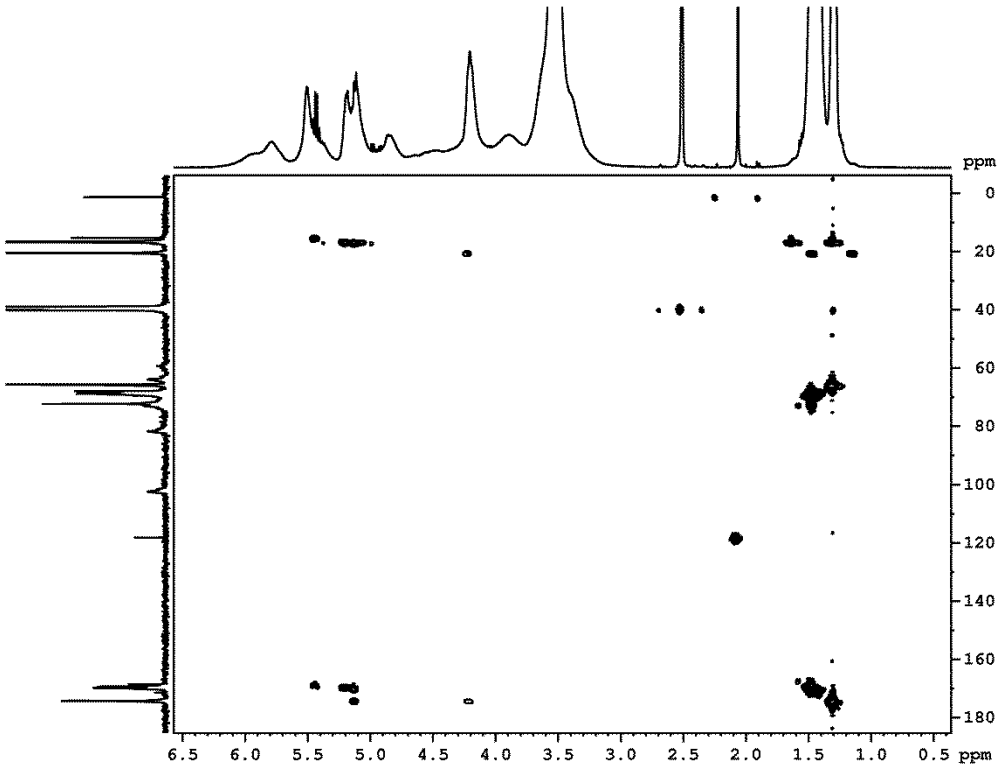

Figure S36: 2D-HMBC-NMR spectrum of β-CD-LA F2 fraction.

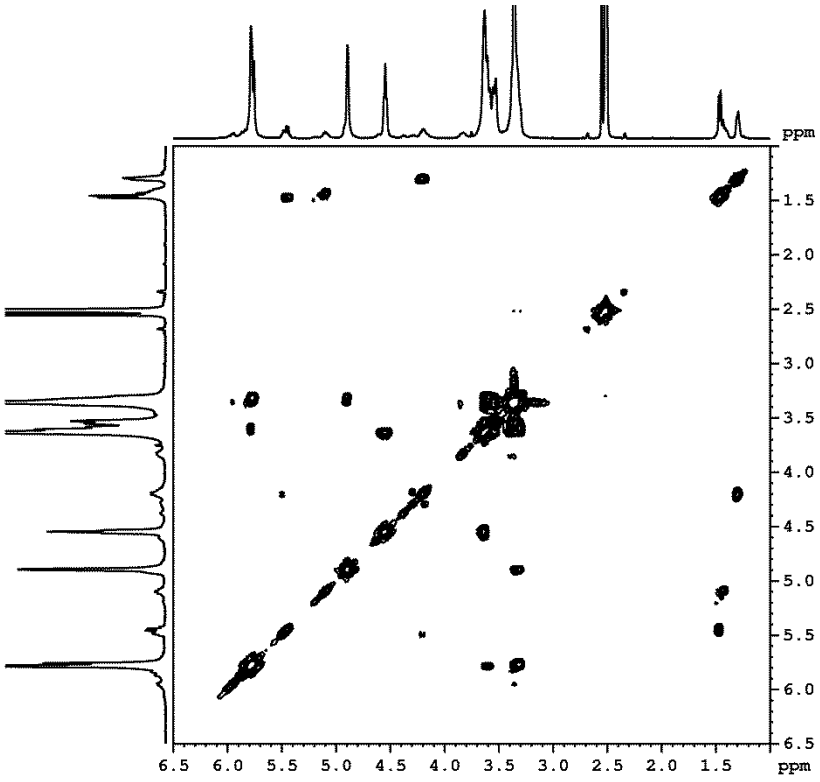

Figure S37: 2D-COSY-NMR spectrum of γ-CD-LA F1 fraction.

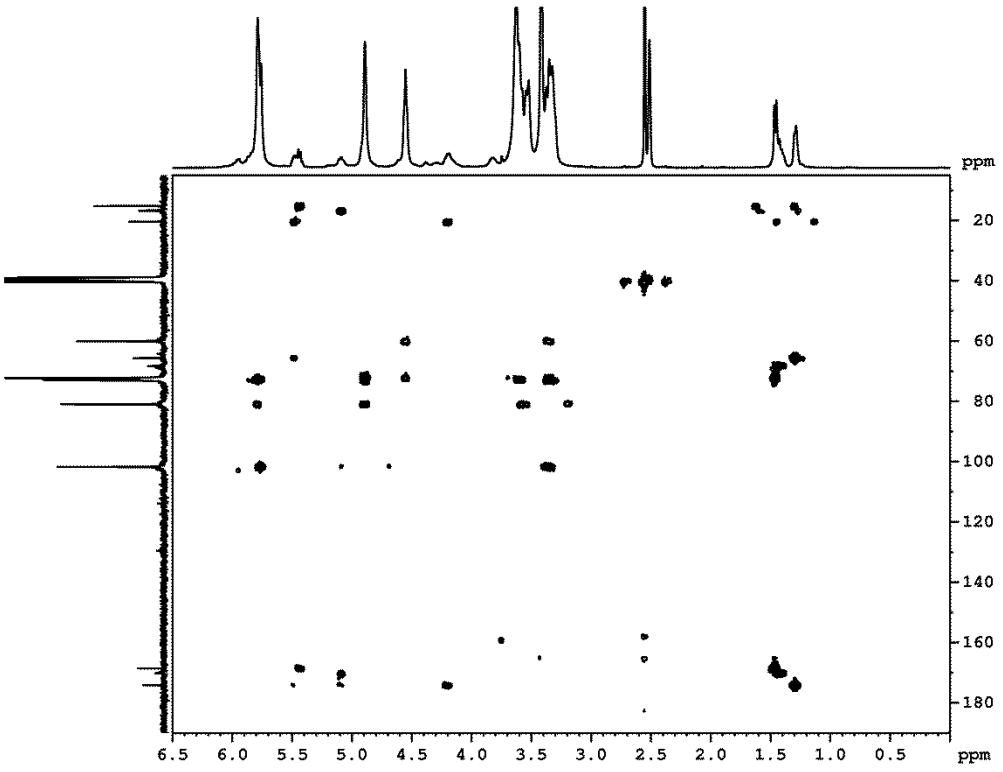

Figure S38: 2D-HMBC-NMR spectrum of γ-CD-LA F1 fraction.

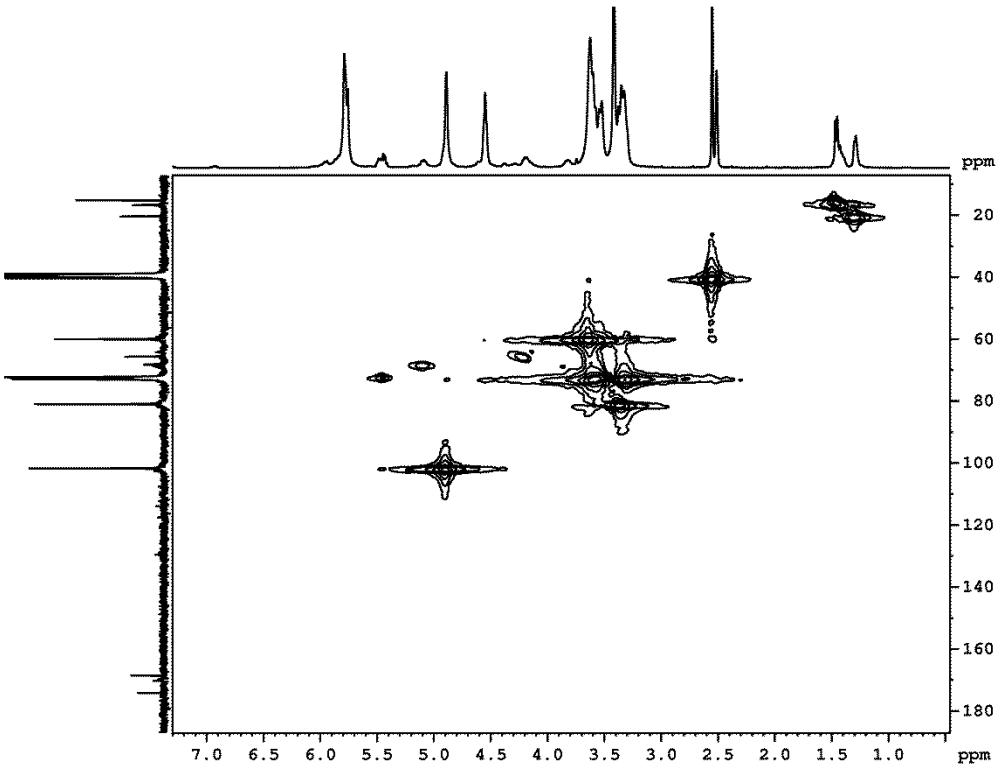

Figure S39: 2D-HMQC-NMR spectrum of γ-CD-LA F1 fraction.

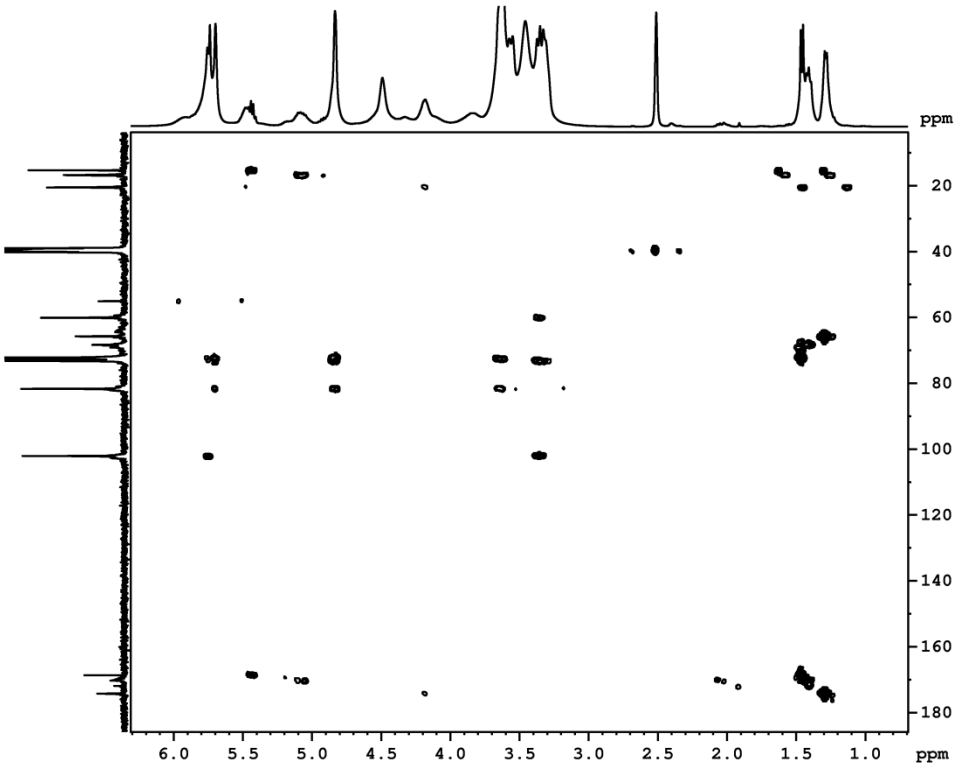

Figure S40: 2D-HMBC-NMR spectrum of γ-CD-LA F1 fraction.

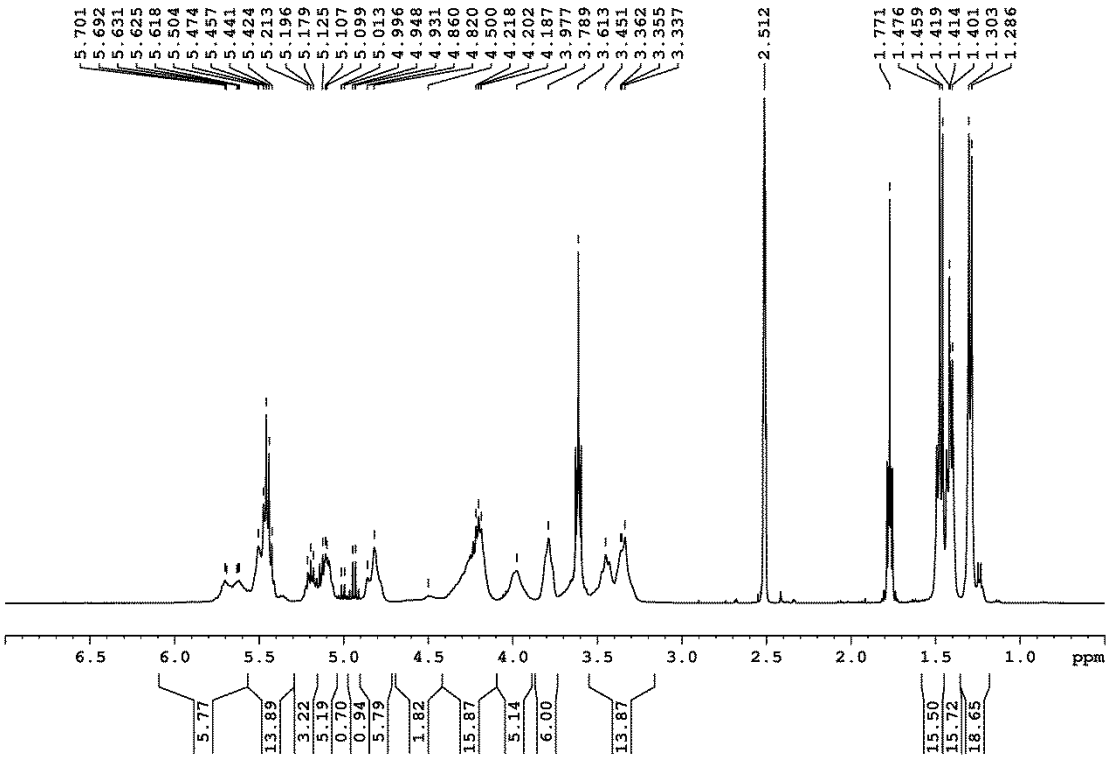

Figure S41: ^{1}H NMR spectrum of α-CD-LA F2 fraction.

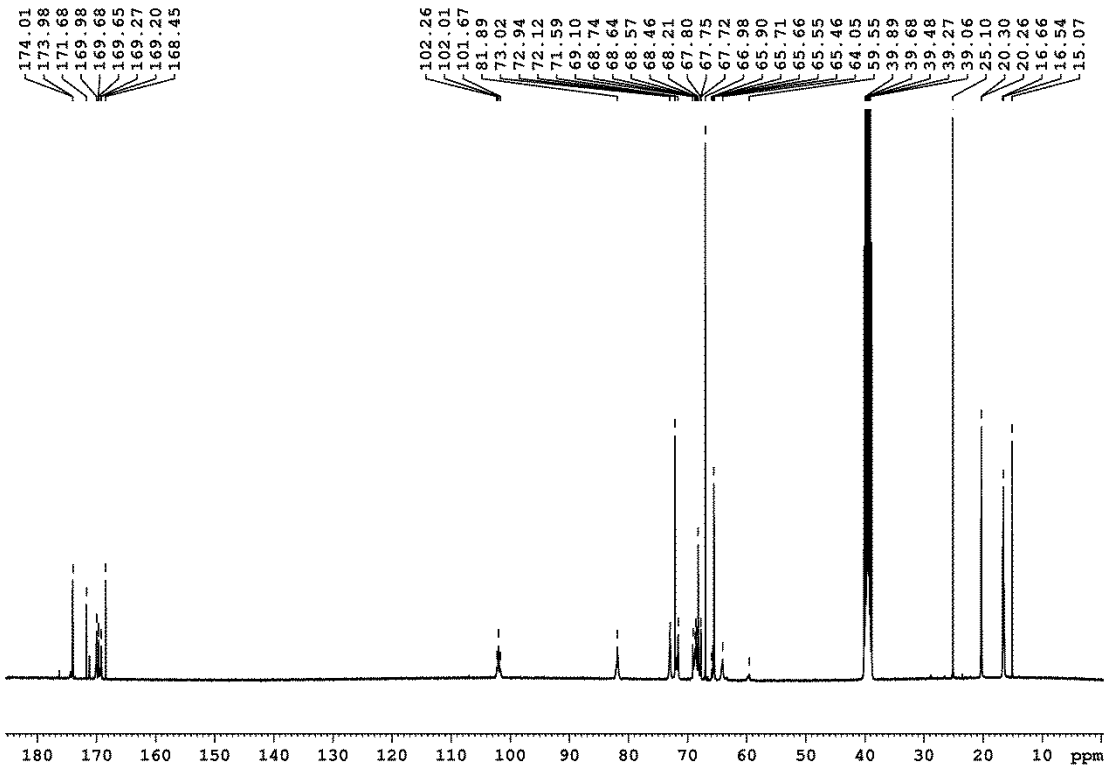

Figure S42: ^{13}C NMR spectrum of α-CD-LA F2 fraction.

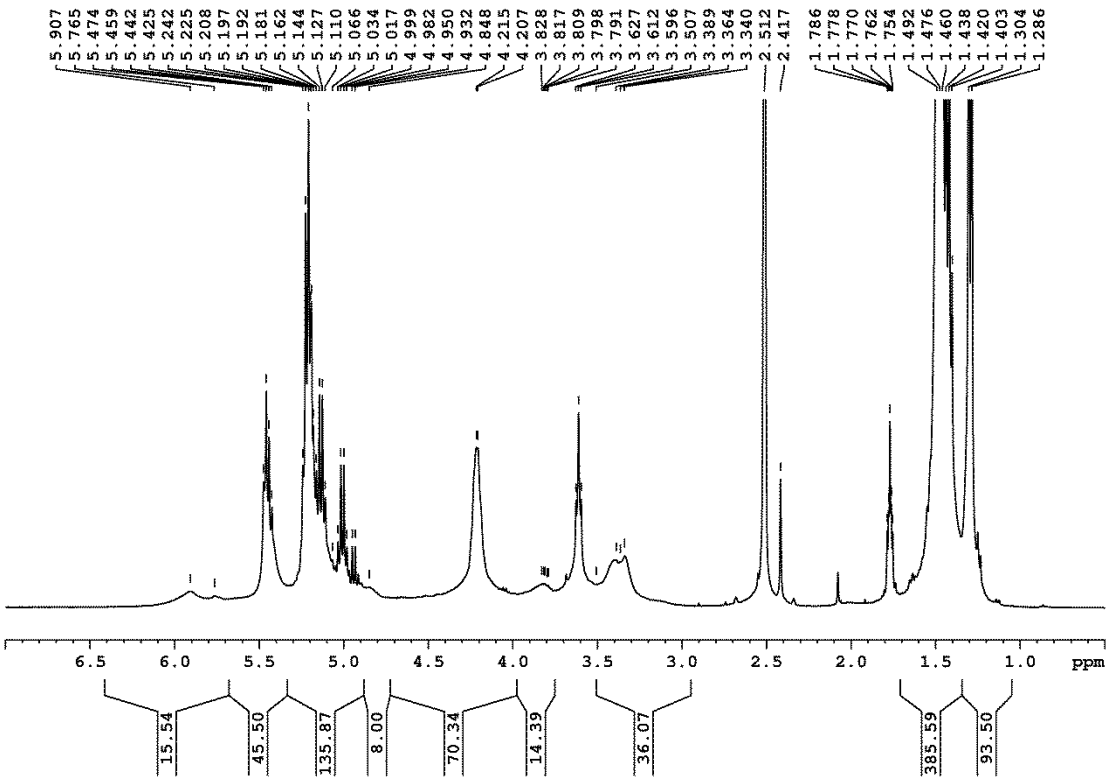

Figure S43: ^{1}H NMR spectrum of γ-CD-LA F2 fraction.

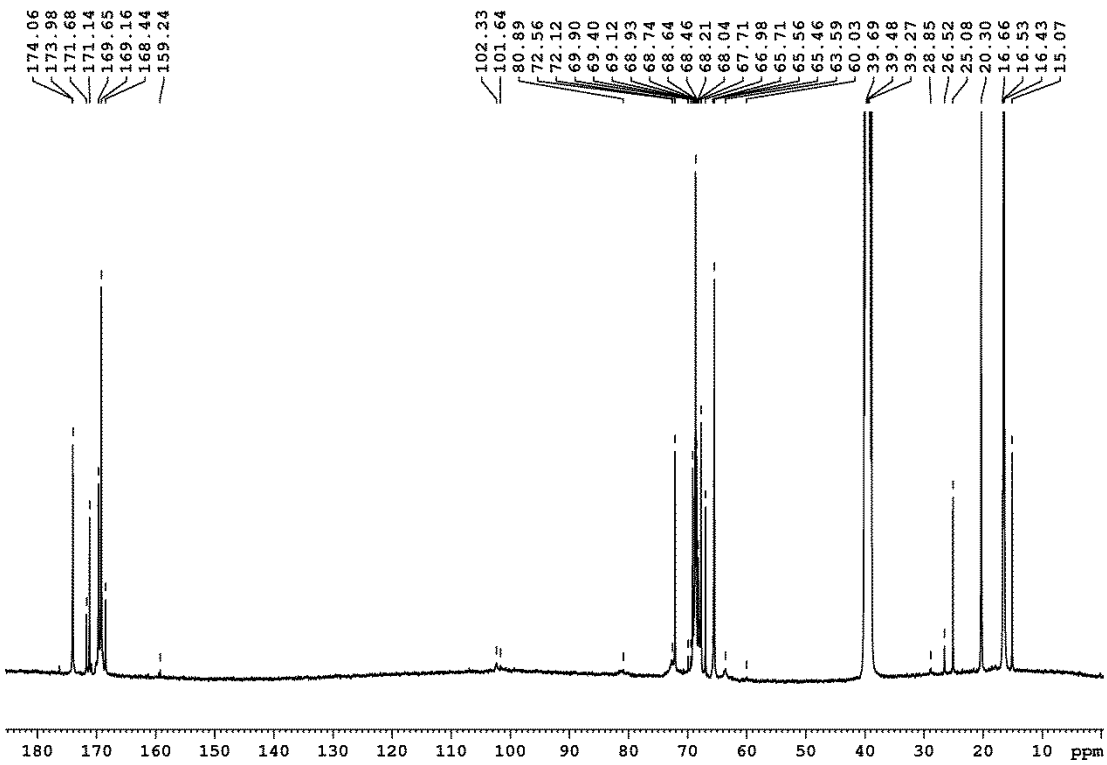

Figure S44: ^{13}C NMR spectrum of γ-CD-LA F2 fraction.