Electronic Supplementary Information

Dicationic AC regioisomer cyclodextrins: mono-6^{A}-ammonium-6^{C}-alkylimidazolium-β-cyclodextrin chlorides as chiral selectors for enantioseparation

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Content

1. Materials

All chemical reagents and solvents were purchased from Sigma (St. Louis, MO, USA). Pyridine, ethanol and N,N-dimethylformamide (DMF) were freshly distilled over CaH_2 prior to use. All racemic analytes (Structure in Figure S1) were purchased either from Aldrich (Steinheim, Germany) or from Sigma (St. Louis, MO, USA).

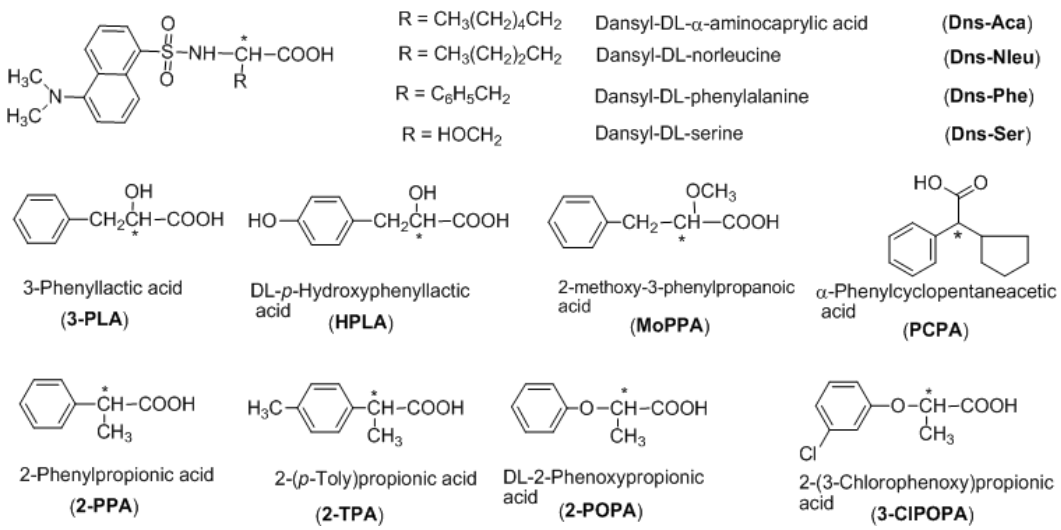


Figure S1. The chemical structures of racemates studied in this paper.

2. Instrumentation

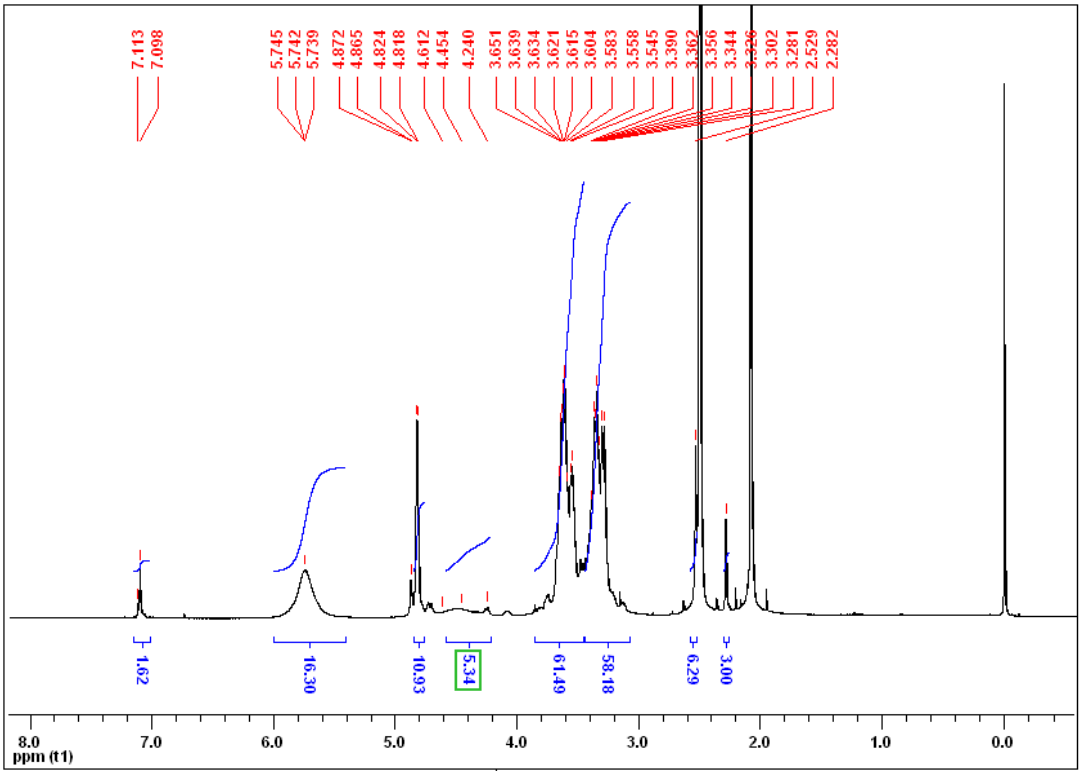
All synthetic intermediate compounds were routinely checked by infrared (IR) spectra (Shimadzu FT-IR 8101 M, Shimadzu Corporation, Kyoto, Japan). ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were obtained on a Bruker AVANCE 500 (Bruker Bio-Spin Corporation, Europe) working at 500 and 125 MHz, respectively; δ

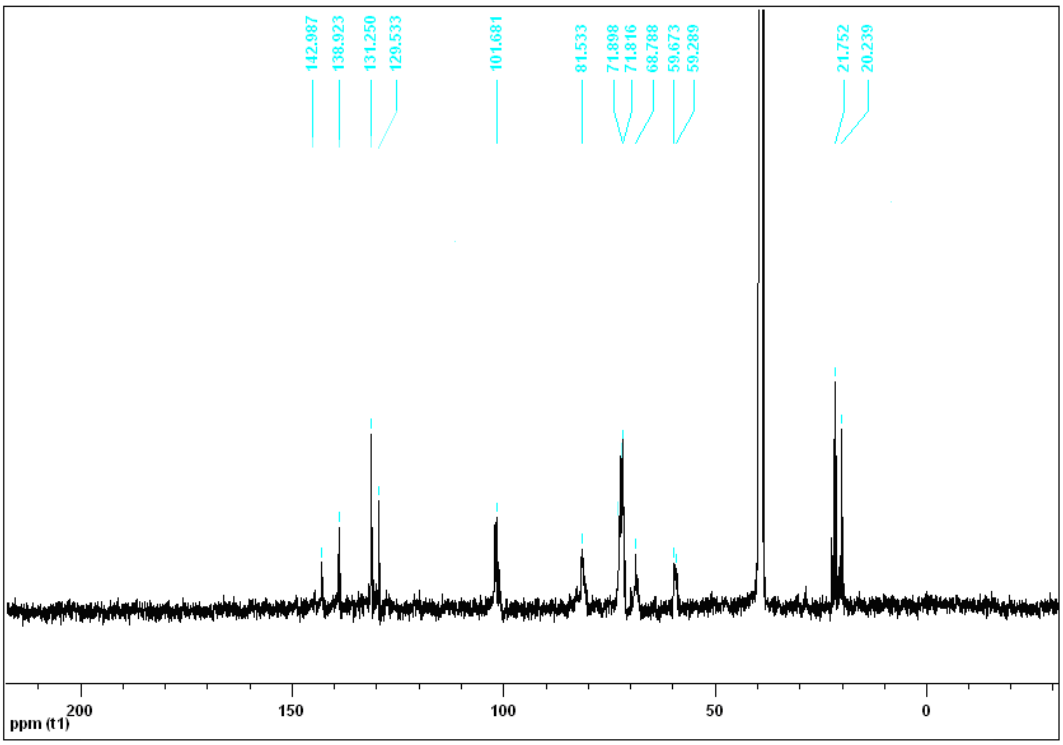
in ppm relative to $SiMe_4$ as internal standard; coupling constants *J* in Hz; ^{13}CNMR spectra were fully decoupled. The mass spectra of CD-cation were collected in positive modes in a single run from a Finniga/AM TSQ Quantum (Thermal, USA).

Beckman P/ACE MDQ CE unit (Fullerton, CA, USA) was used for all CE separations. 50 μm ID, 375 μm OD fused silica capillary was used with a total length of 59.2 cm (49 cm to the detector). Detection of analytes was carried out simultaneously at 214 nm, 254 nm and 280nm by using variable-wavelength PDA (Photodiode Array, 190-300 nm) detector. The electrosmotic flow (EOF) was measured with methanol as neutral marker. Samples were introduced hydrodynamically into the capillary at 0.5 psi for 5 s. All experiments were performed under normal polarity with 15 kV applied voltage.

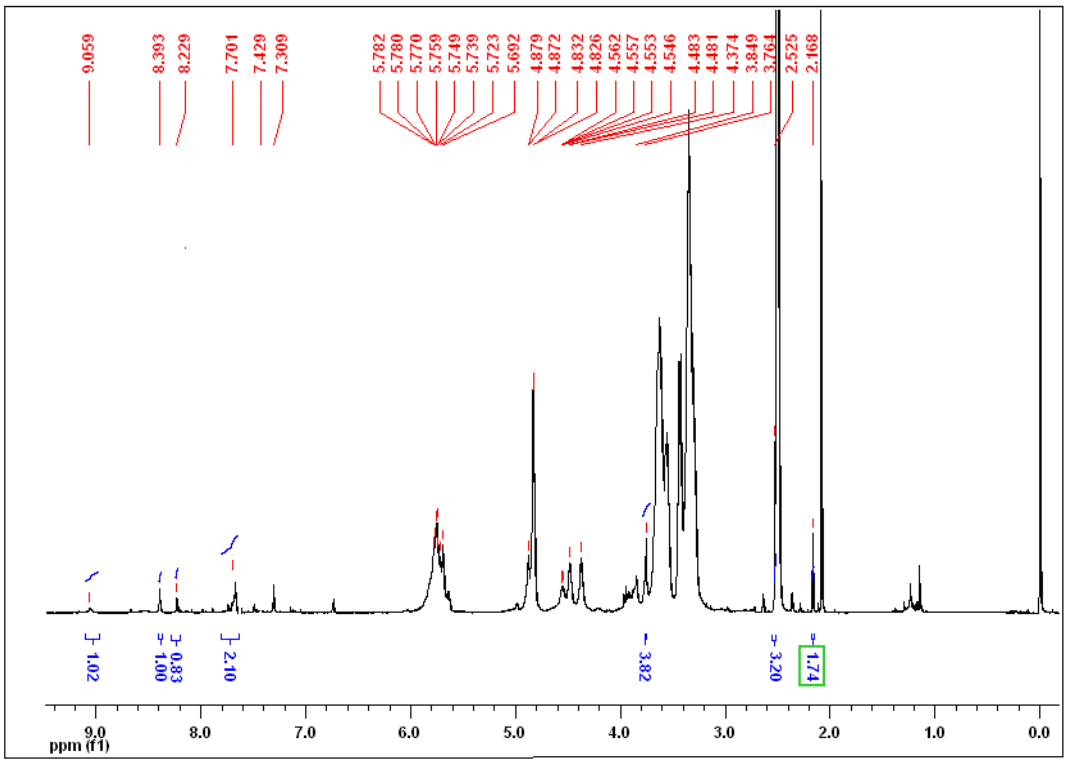
Background electrolytes (BGEs) were prepared with 50 mM acetate buffer (pH 5.5, 6.0) and sodium phosphate buffer (pH 6.5, 7.0). The stock racemates (structure shown in Figure S1) solution (50 μg ml^{-1}) was prepared with methanol/water (50:50, v/v) mixture solution, filtered with 0.45 μm syringe type Millipore membrane and sonicated prior to use. Acetate buffer was prepared by dissolving a desirable amount of sodium acetate in water, with its pH (5.5, 6.0) adjusted with acetic acid while sodium phosphate buffer was prepared with sodium phosphate and sodium hydroxide to get the required pH 6.5 and 7.0.

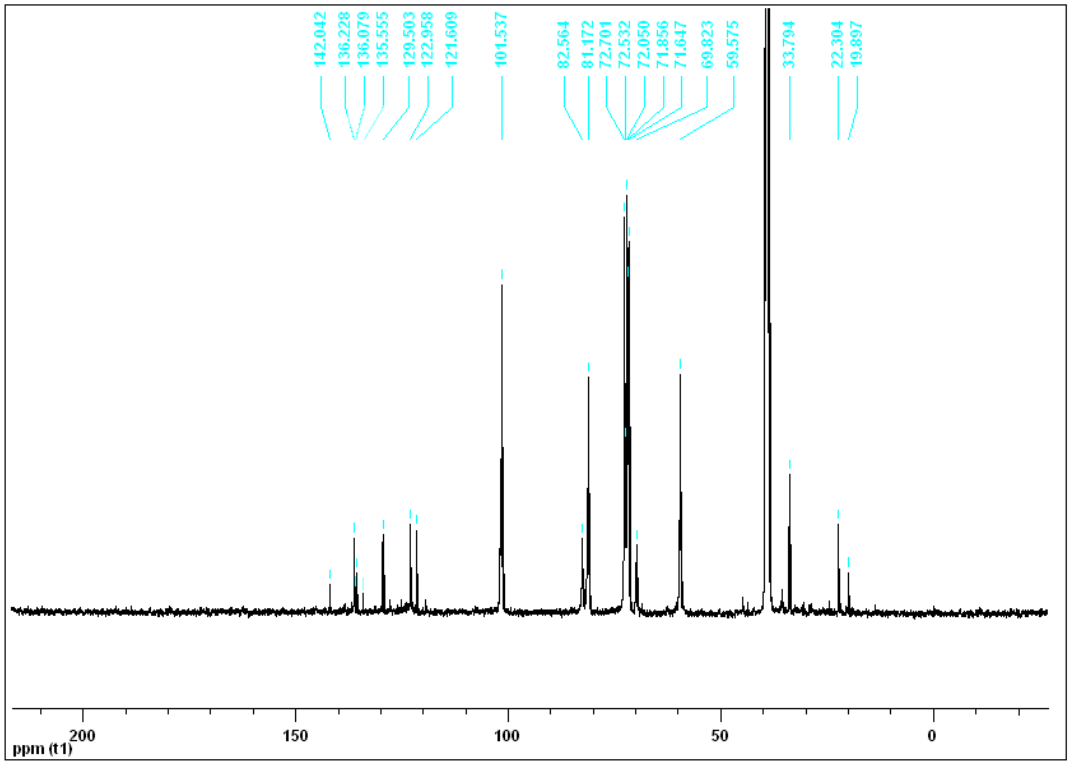
3. ^{1}H and ^{13}C NMR spectra of 6^{A}-azido-6^{C}-mesitylenesulfonyl-β-cyclodextrin (Mess-N_3-CD, **2**)



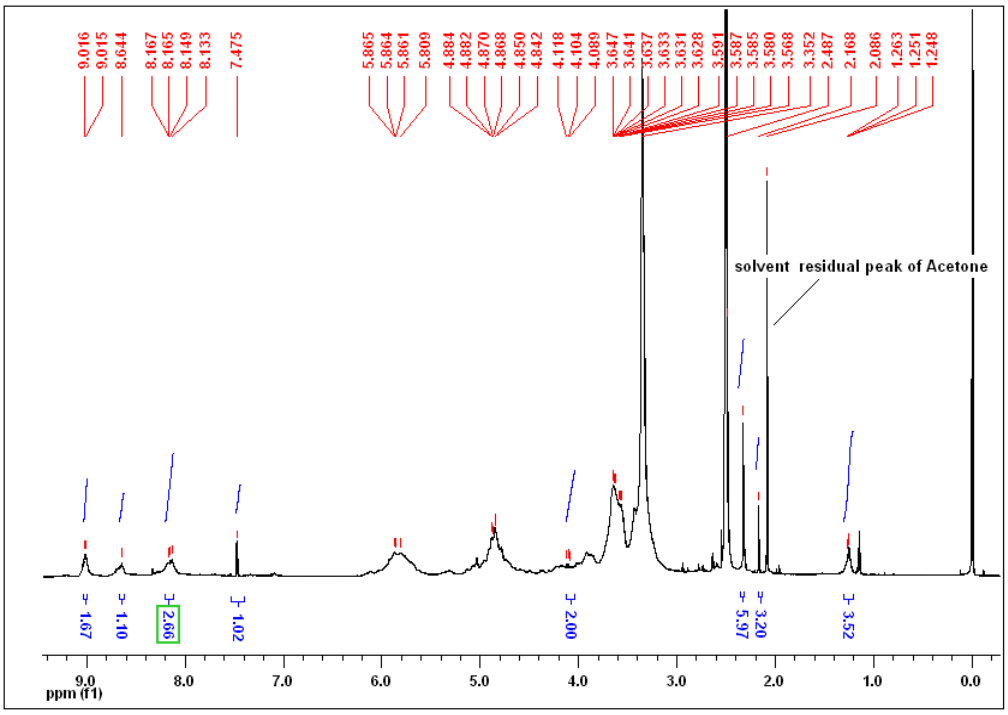


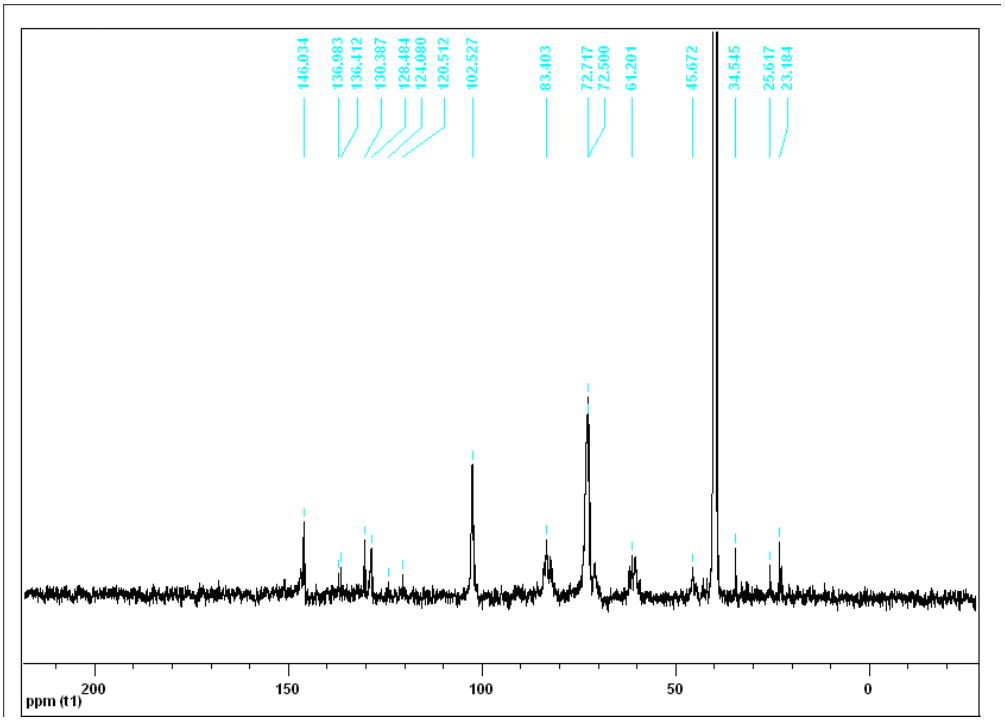
4. ^{1}H and ^{13}C NMR spectra of 6^{A}-azido-6^{C}-methylimidazolium -β-cyclodextrin mesitylene sulfonate **4a**



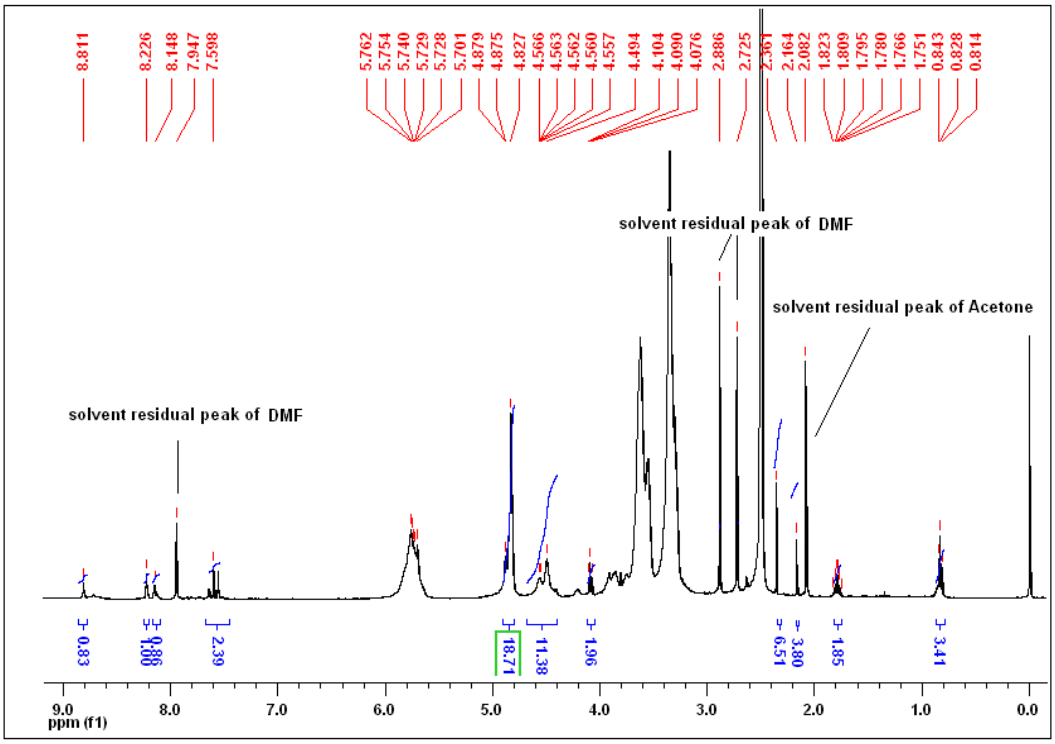


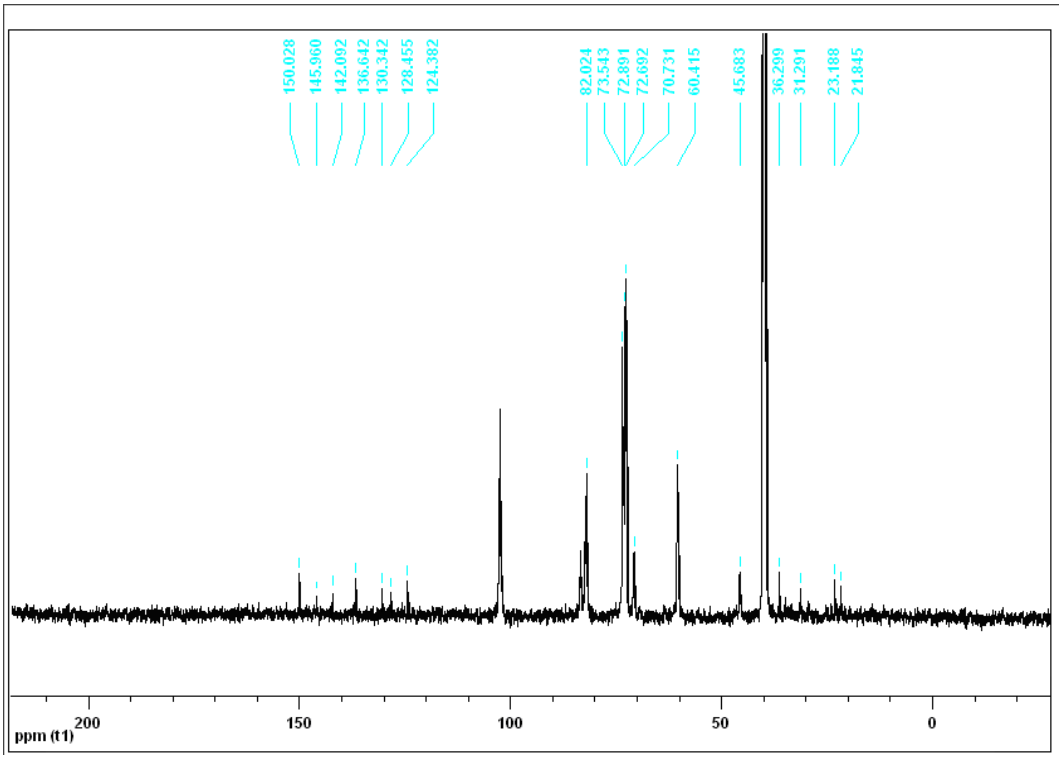
5. ^{1}H and ^{13}C NMR spectra of 6^{A}-azido-6^{C}-ethylimidazolium-β-cyclodextrin mesitylene sulfonate **4b**



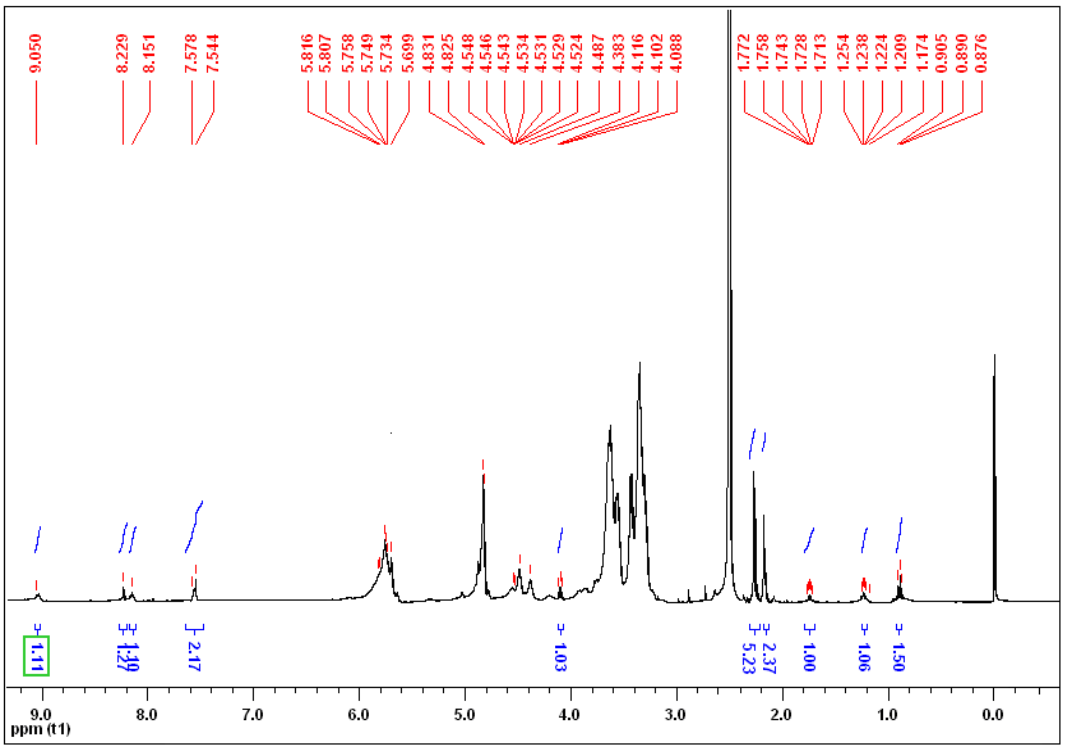


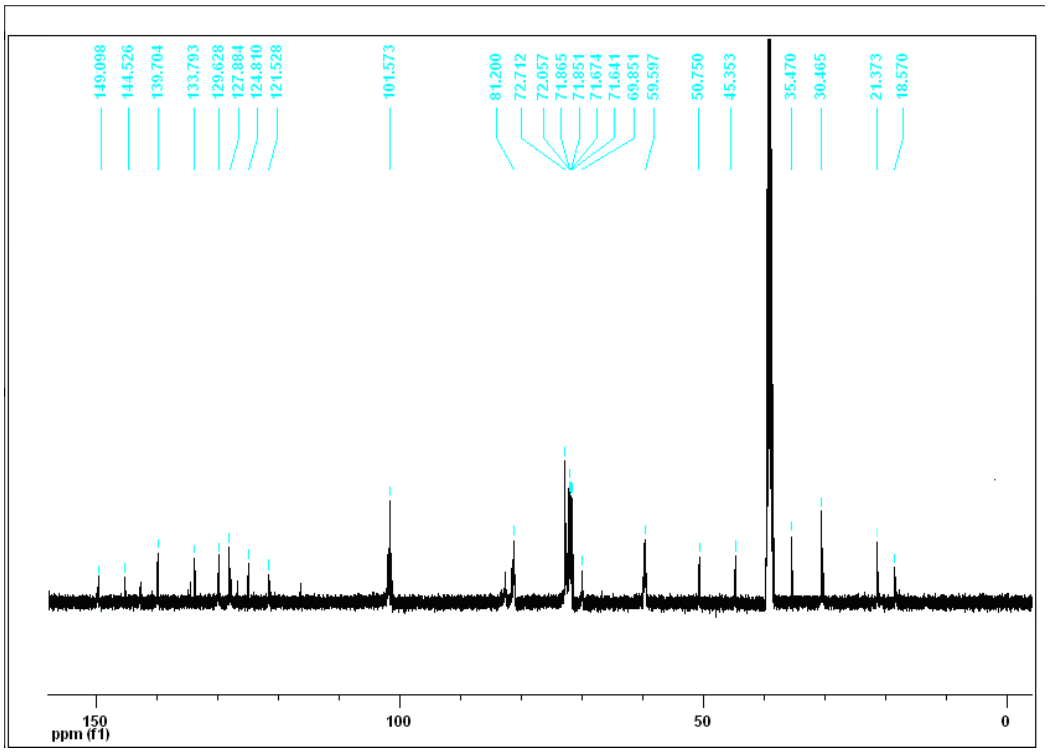
6. ^{1}H and ^{13}C NMR spectra of 6^{A}-azido-6^{C}-propylimidazolium-β-cyclodextrin mesitylene sulfonate **4c**



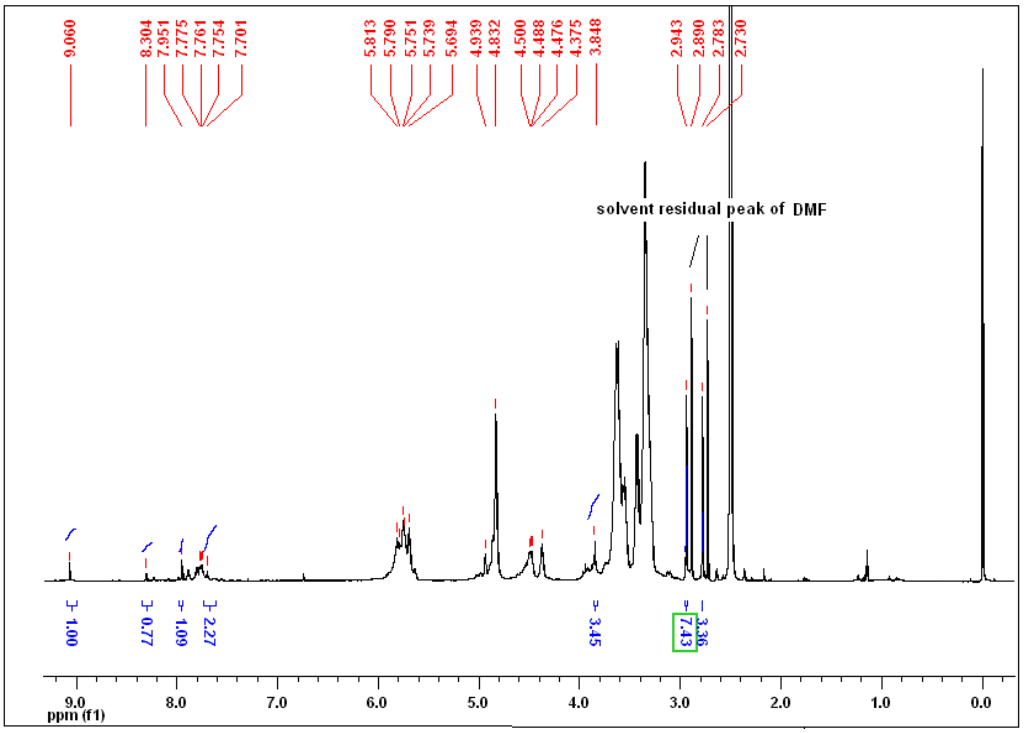


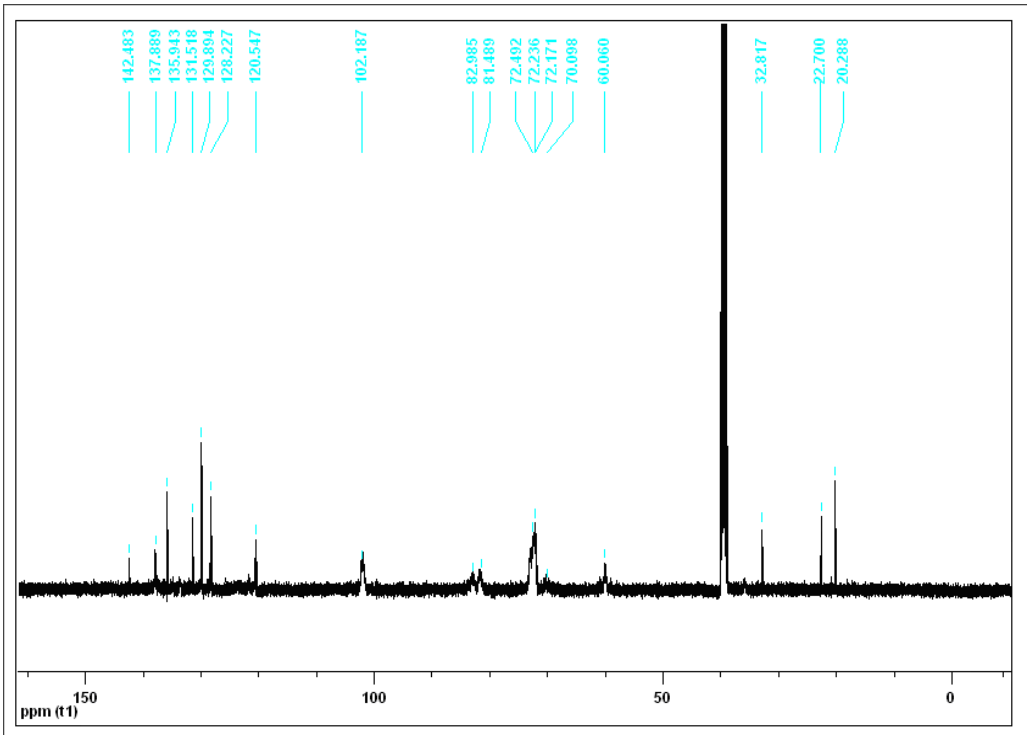
7. ^{1}H and ^{13}C NMR spectra of 6^{A}-azido-6^{C}-butylimidazolium-β-cyclodextrin mesitylene sulfonate **4d**



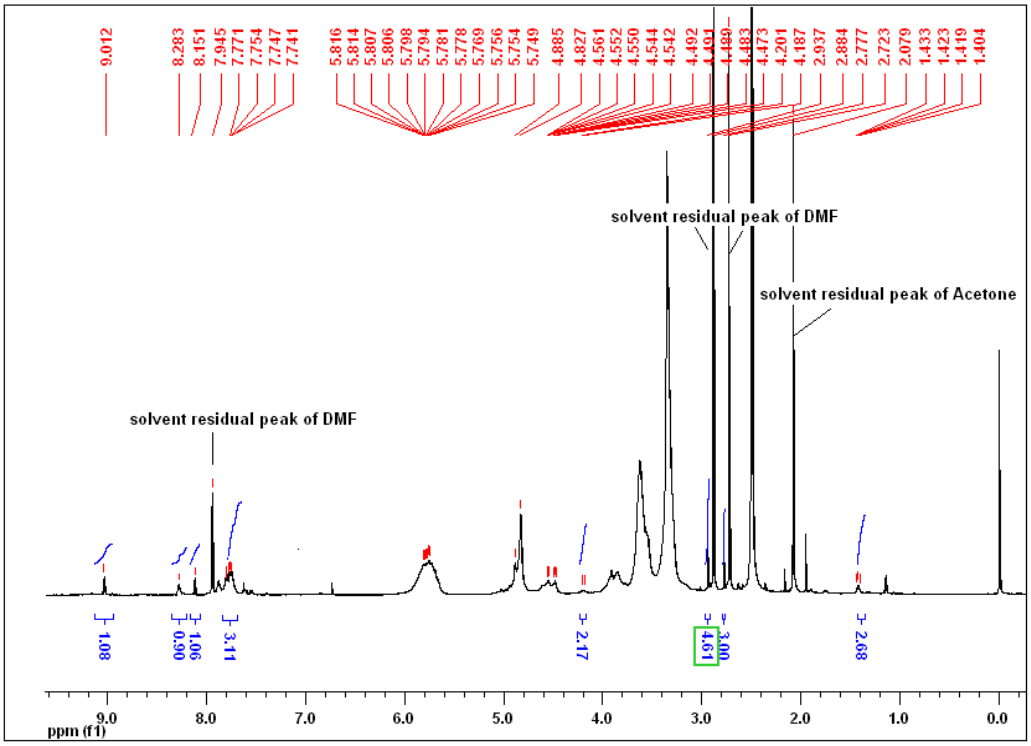


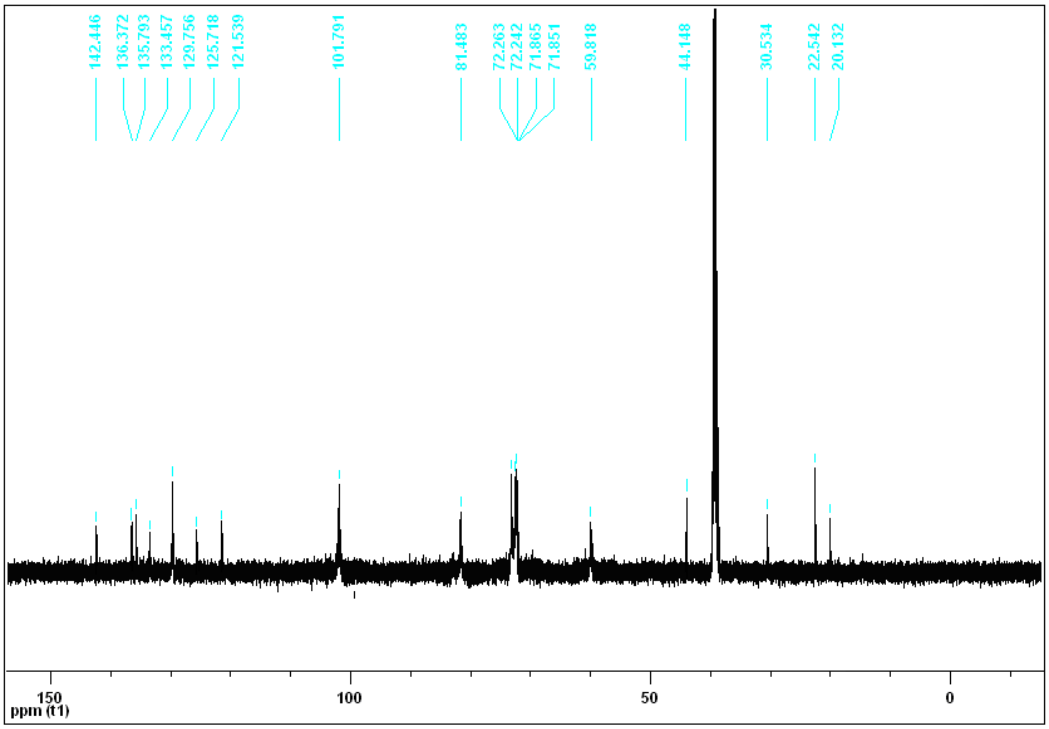
8. ^{1}H and ^{13}C NMR spectra of 6^{A}-amino-6^{C}-methylimidazolium-β-cyclodextrin mesitylene sulfonate **5a**



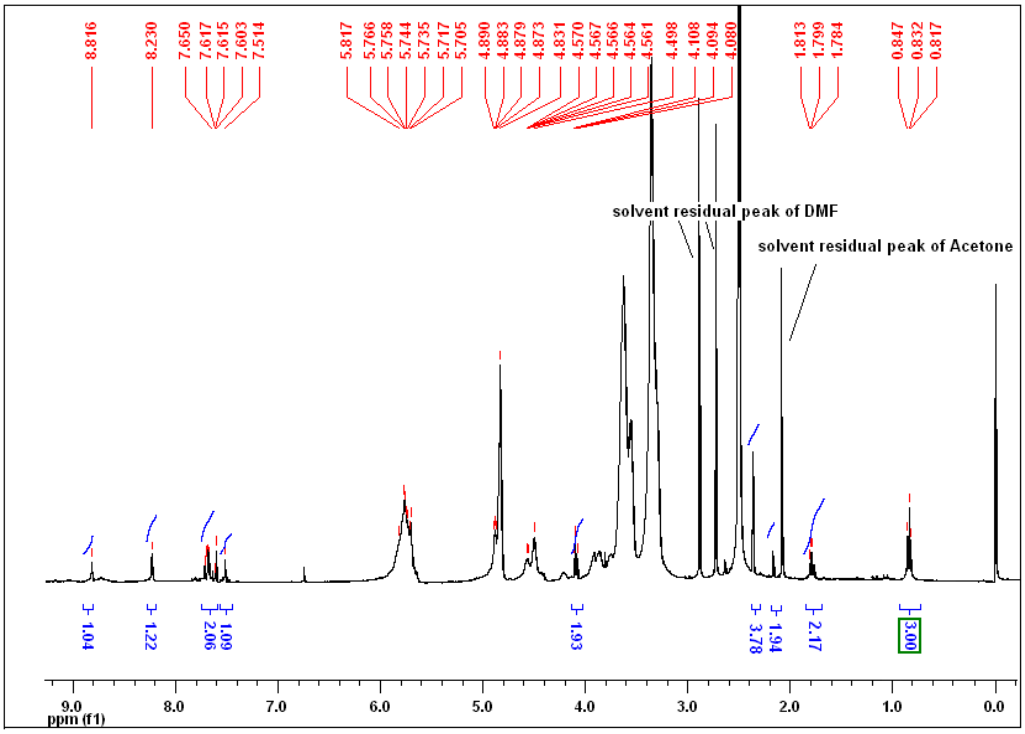


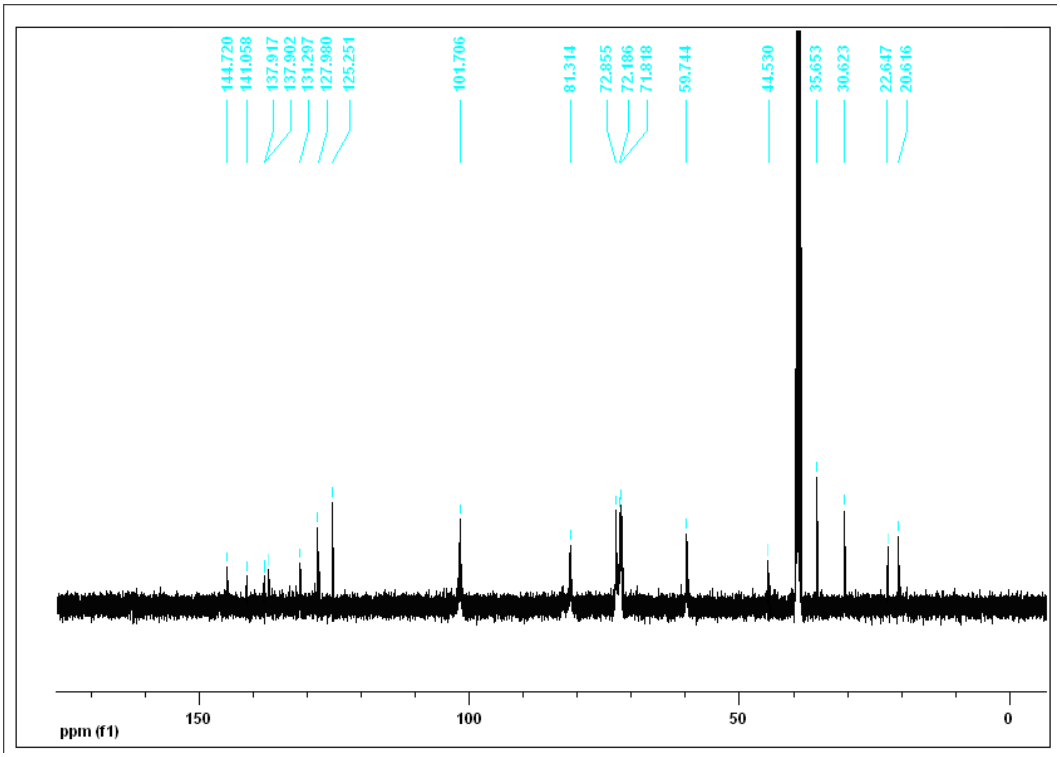
9. ^{1}H and ^{13}C NMR spectra of 6^{A}-amino-6^{C}-ethylimidazolium-β-cyclodextrin mesitylene sulfonate **5b**



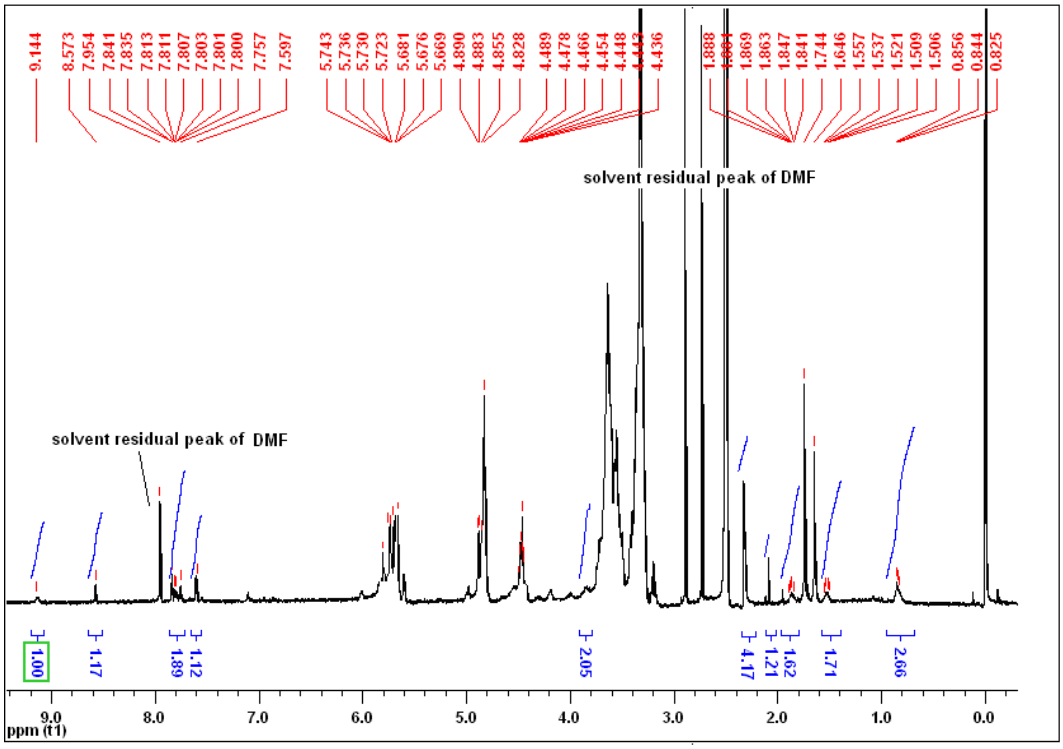


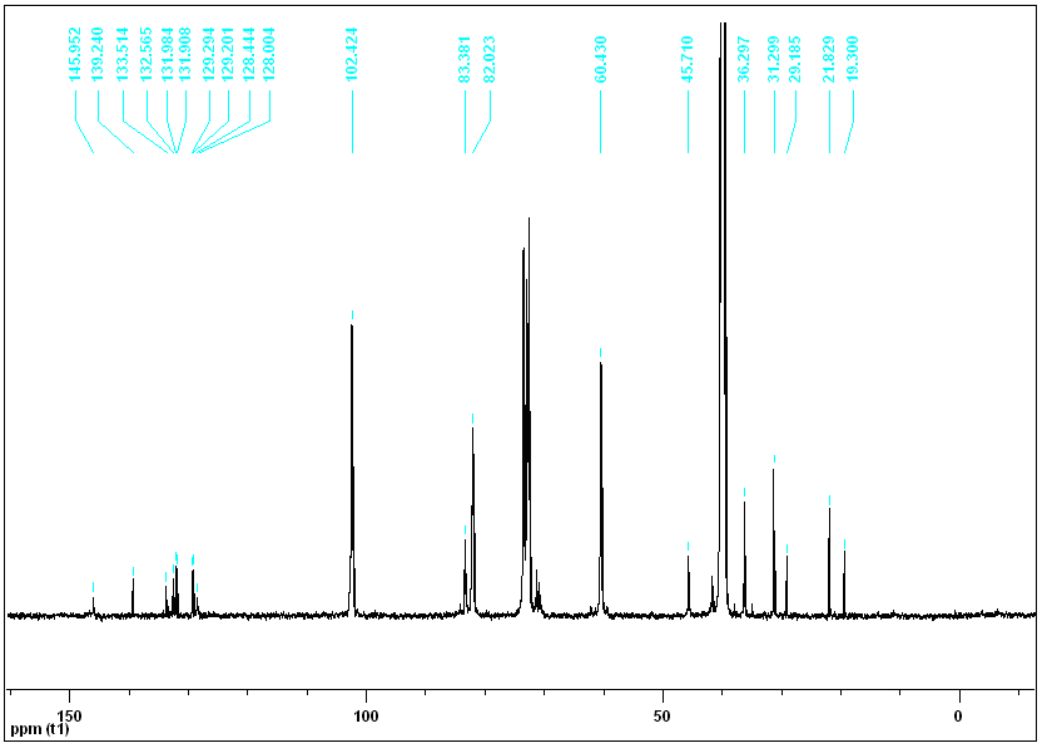
10. ^{1}H and ^{13}C NMR spectra of 6^{A}-amino-6^{C}-propylimidazolium-β-cyclodextrin mesitylene sulfonate **5c**



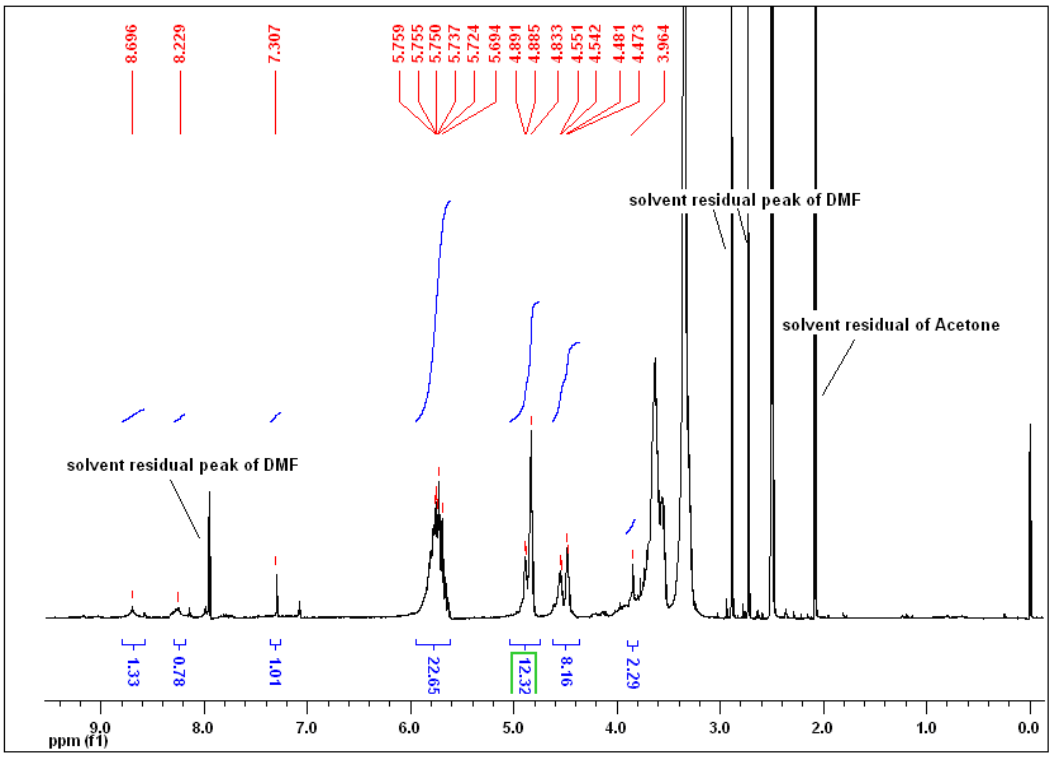


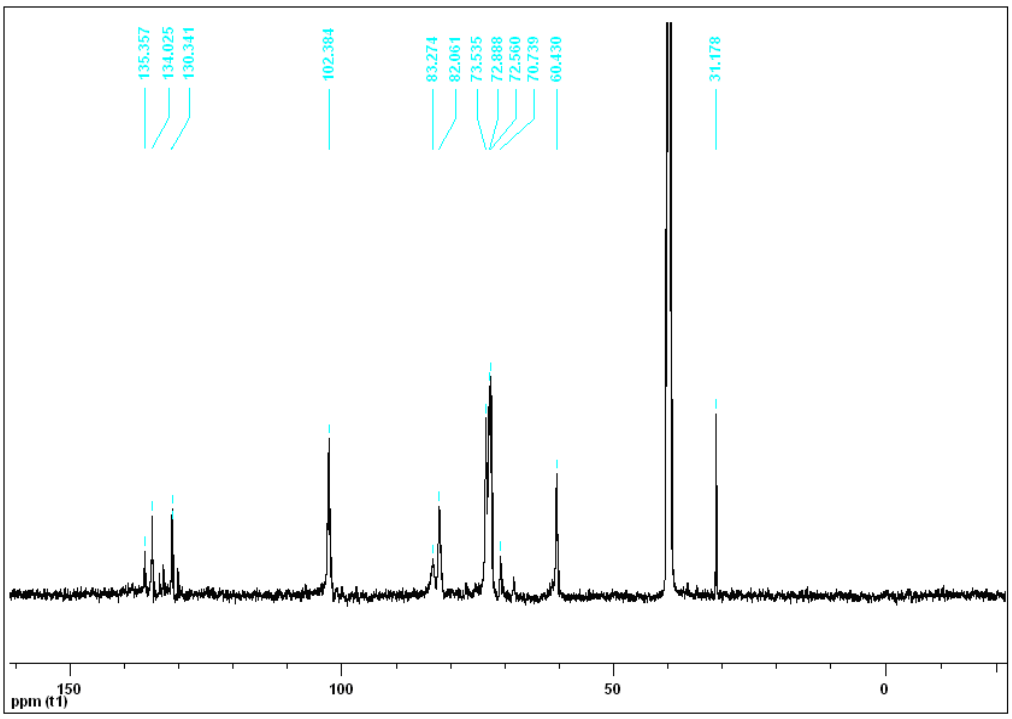
11. ^{1}H and ^{13}C NMR spectra of 6^{A}-amino-6^{C}-butylimidazolium-β-cyclodextrin mesitylene sulfonate **5d**



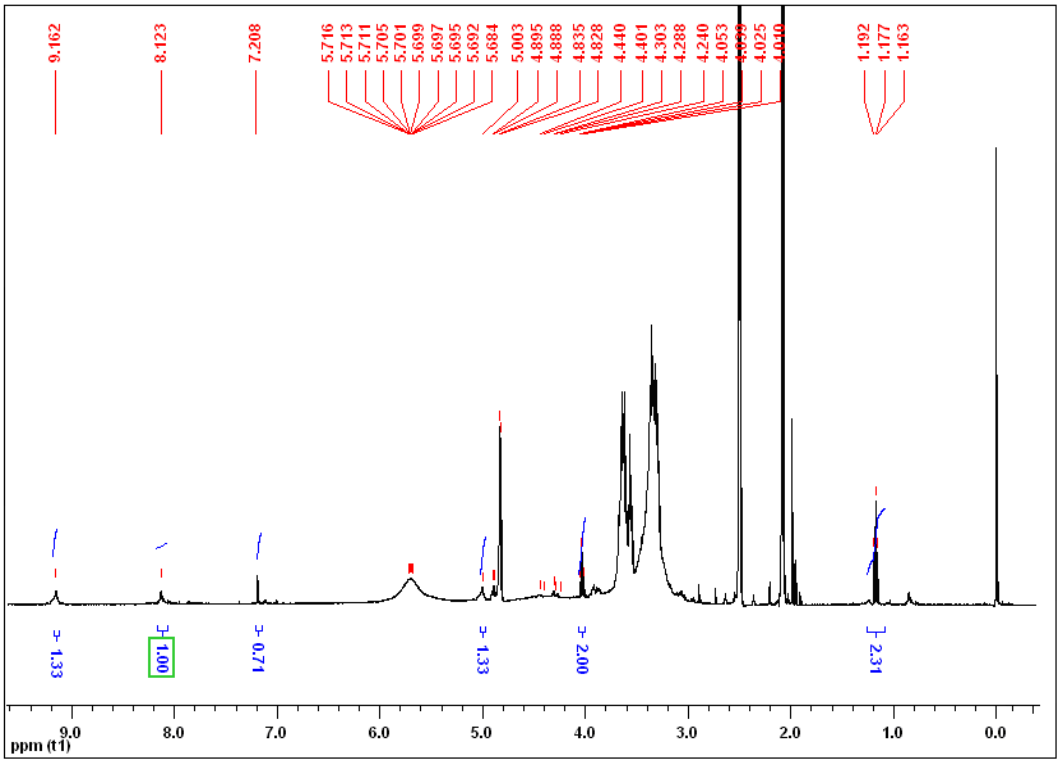


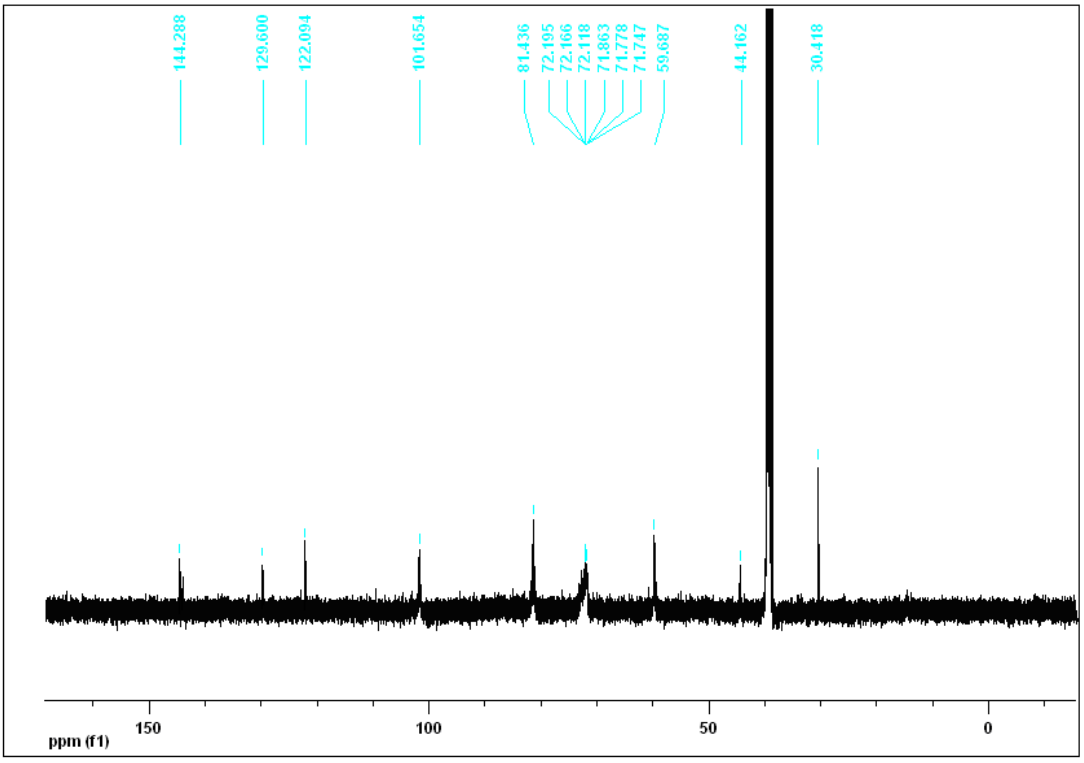
12. ^{1}H and ^{13}C NMR spectra of 6^{A}-ammonium-6^{C}-methylimidazolium-β-cyclodextrin chloride **7a**



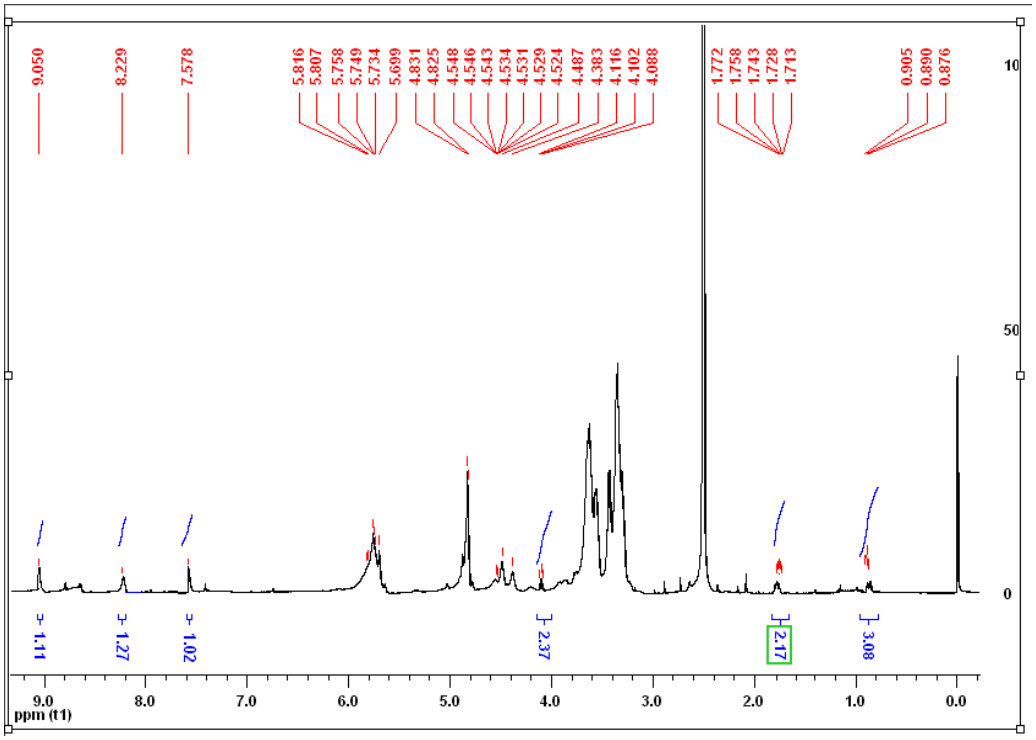


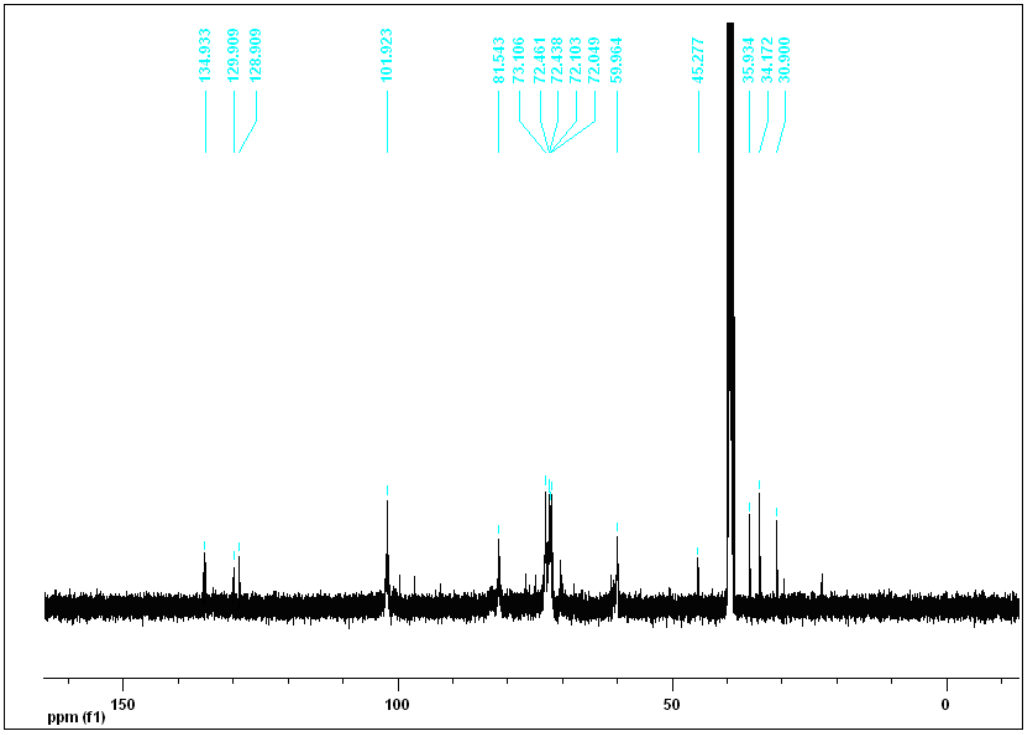
13. ^{1}H and ^{13}C NMR spectra of 6^{A}-ammonium-6^{C}-ethylimidazolium-β-cyclodextrin chloride **7b**





14. ^{1}H and ^{13}C NMR spectra of 6^{A}-ammonium-6^{C}-propylimidazolium-β-cyclodextrin chloride **7c**





15. ^{1}H and ^{13}C NMR spectra of 6^{A}-ammonium-6^{C}-butylimidazolium-β-cyclodextrin chloride **7d**