Supplementary Material for Organic & Biomolecular Chemistry

Supporting Information for

Synthesis of 1,2,3-triazole and 1,2,3,4-tetrazole-fused glycosides and nucleosides by an intramolecular 1,3-dipolar cycloaddition reaction

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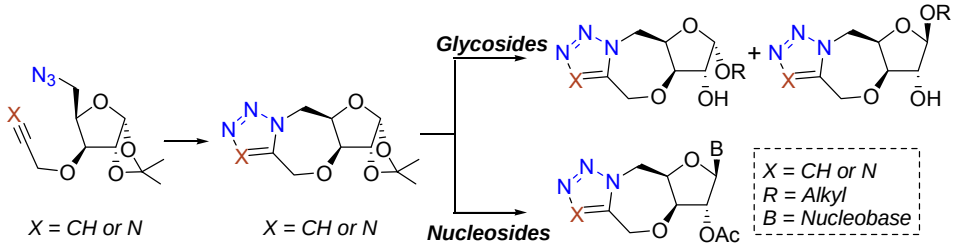
ABSTRACT

Various 1,2,3-triazole and 1,2,3,4-tetrazole fused multi-cyclic compounds were synthesized from carbohydrate derived azido-alkyne and azido-cyanide substrates. The acid sensitive 1,2-*O*-isopropylidene group of the furanosyl sugar was utilized for diversification to glycosides and nucleosides under Fischer glycosidation and Vorbruggen's conditions, respectively.

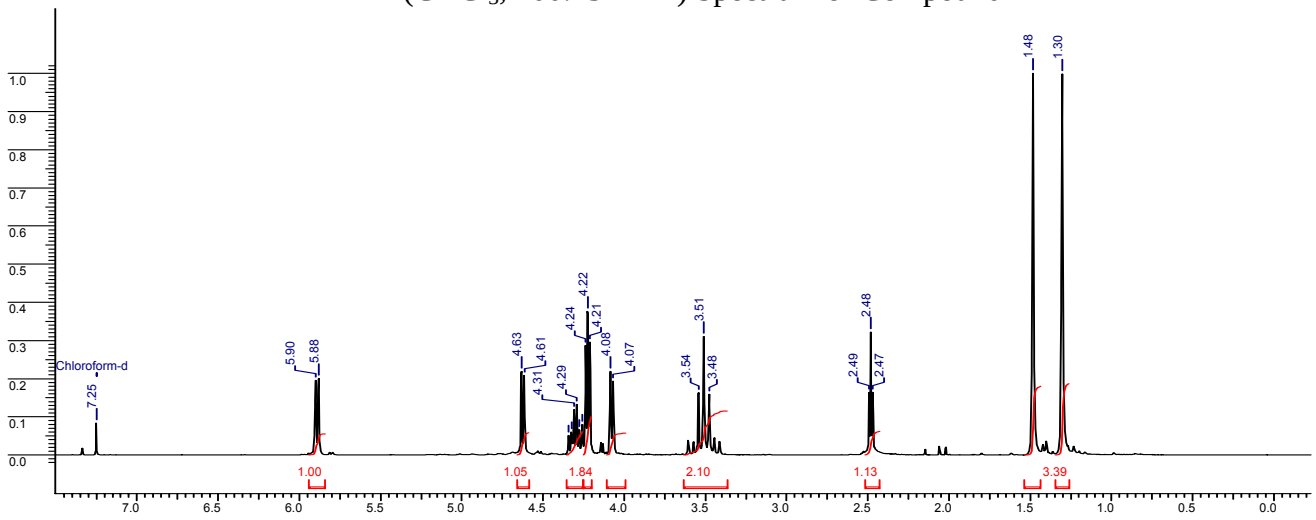


General Experimental Techniques and Apparatus

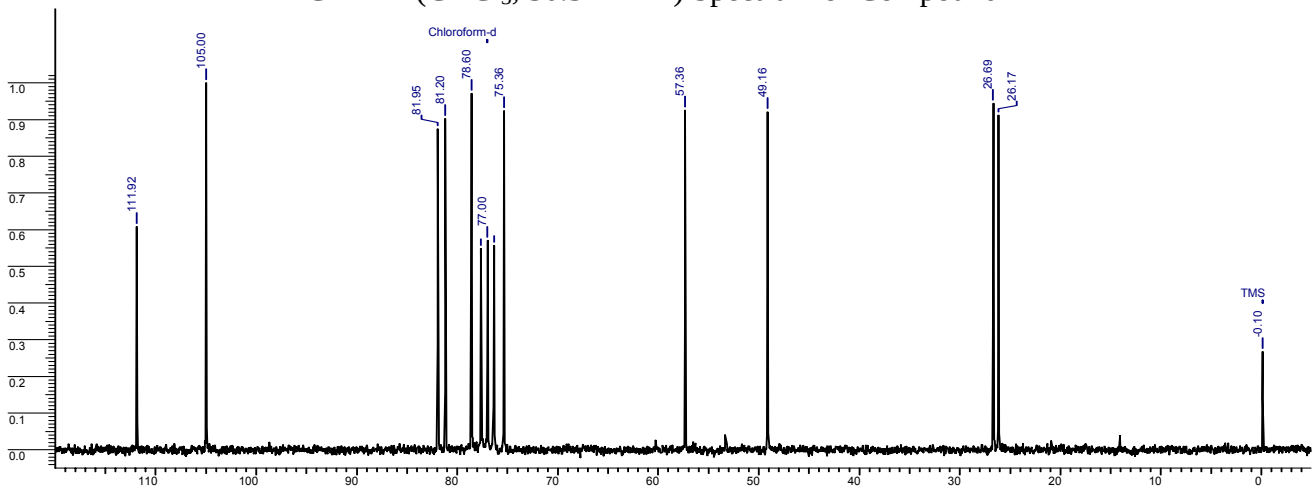
Unless otherwise noted, materials were obtained from commercial suppliers and were used without further purification. Unless otherwise reported all reactions were performed under argon atmosphere. Removal of solvent *in vacuo* refers to distillation using a rotary evaporator attached to an efficient vacuum pump. Products obtained as solids or syrups were dried under high vacuum. $AuBr_3$ was purchased from Aldrich. Analytical thin-layer chromatography was performed on pre-coated silica plates (F_{254}, 0.25 mm thickness); compounds were visualized by UV light or by staining with anisaldehyde spray. ^1H, ^{13}C NMR spectra were recorded on 200 MHz for ^1H and 50 MHz for ^{13}C NMR or 300 MHz for ^1H and 75 MHz for ^{13}C NMR spectrometers. Chemical shifts (δ_H) are quoted in ppm and are referenced to tetramethylsilane (internal). IR spectra were recorded on FT-IR spectrophotometer.

Supporting Information

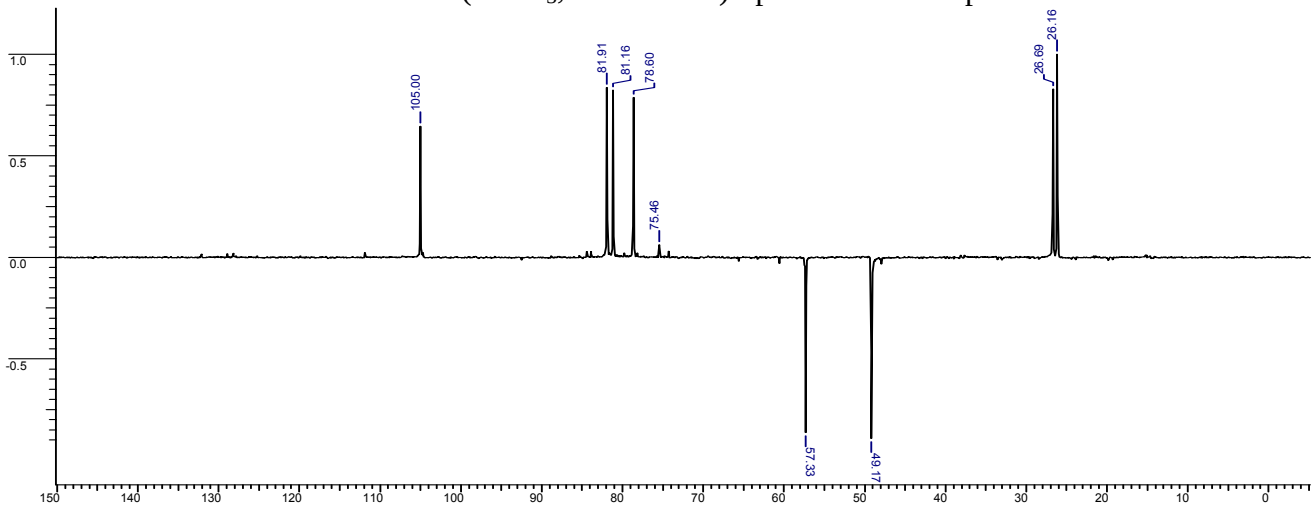
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **4**



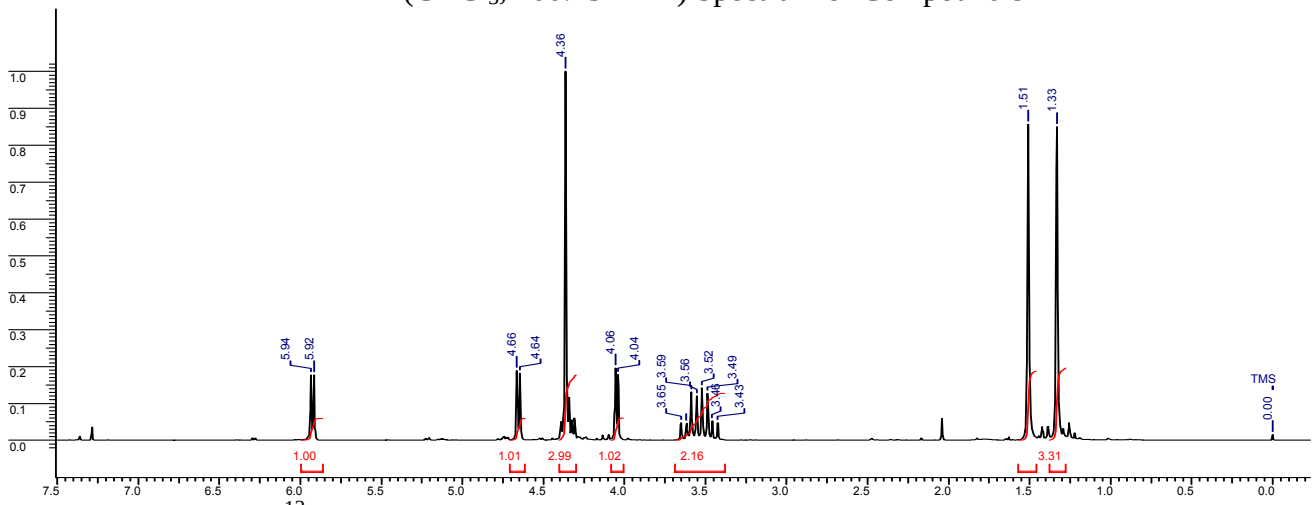
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **4**



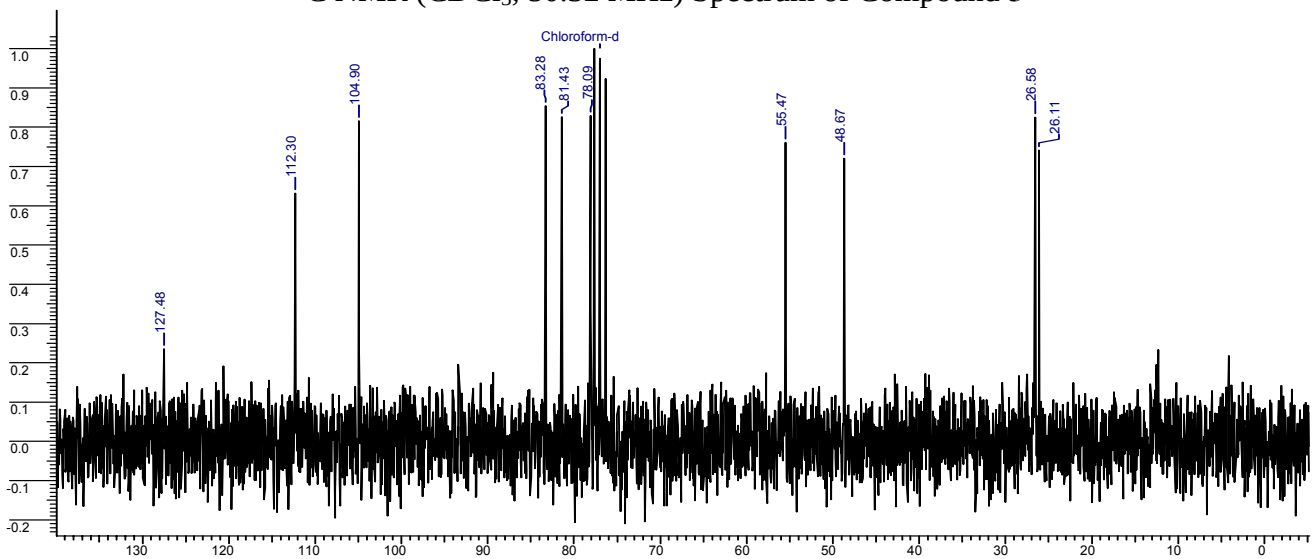
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **4**



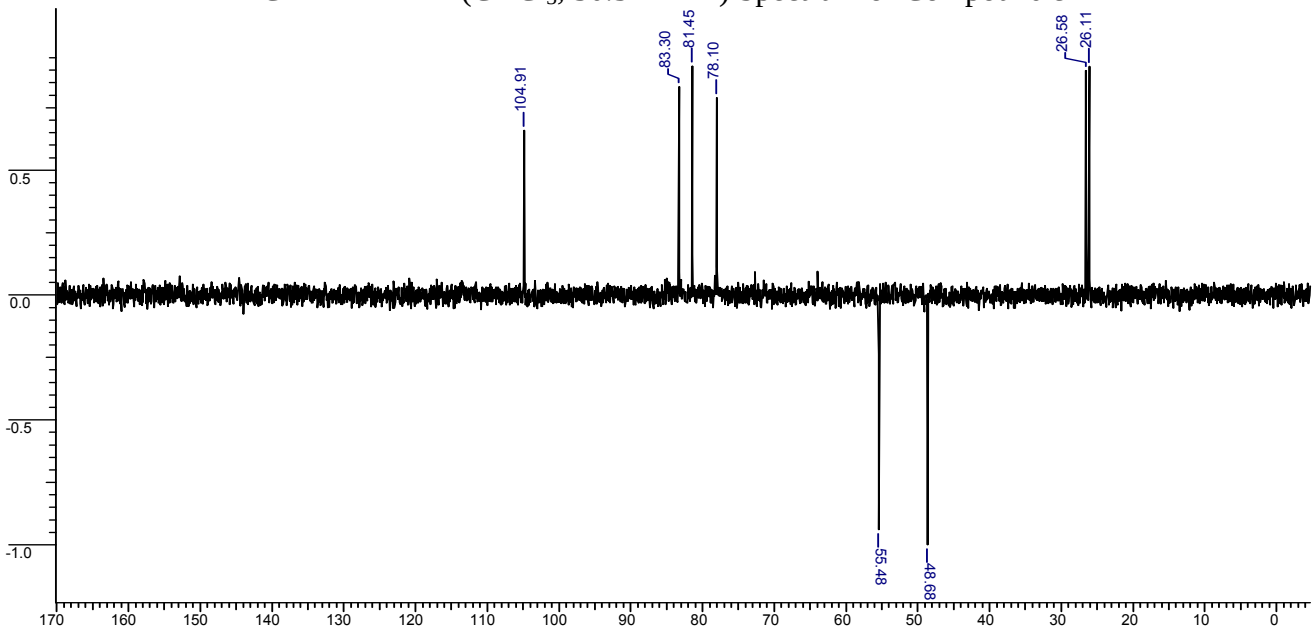
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **5**



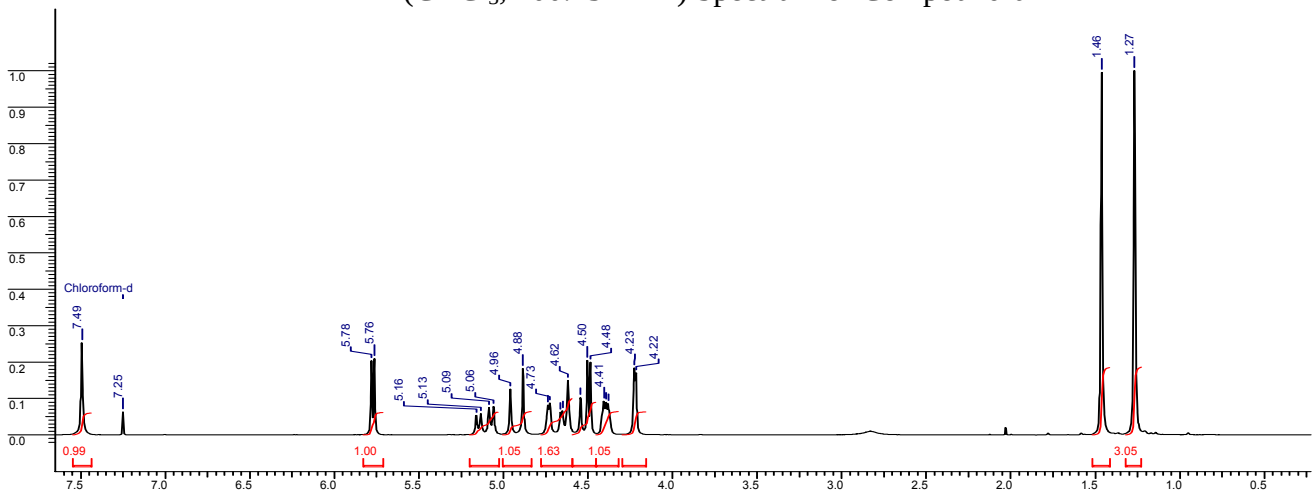
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **5**



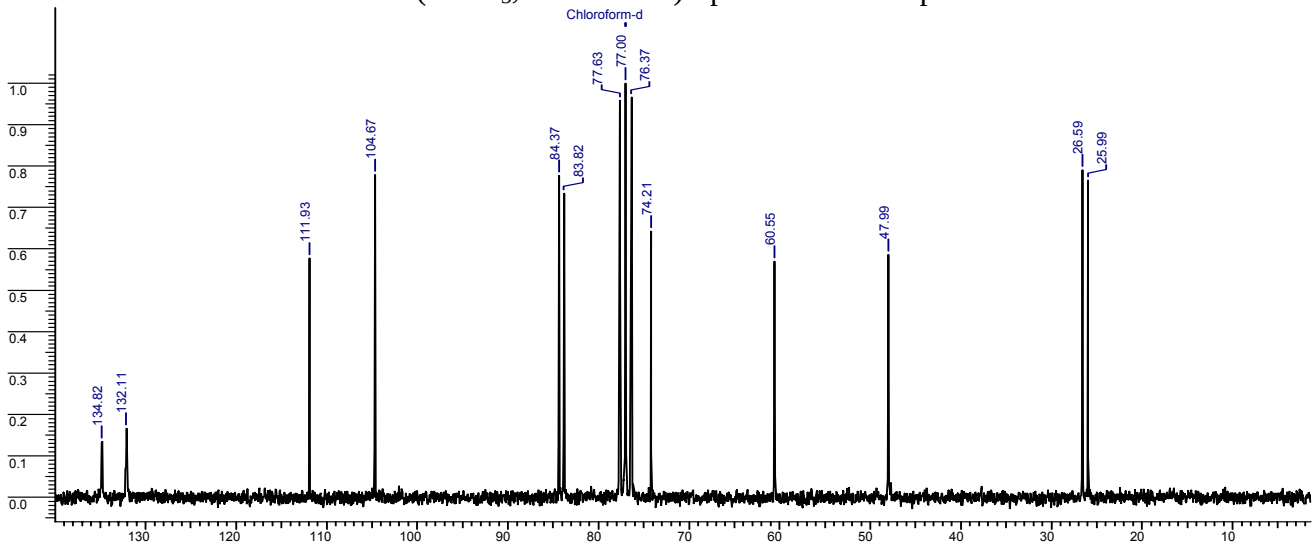
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **5**



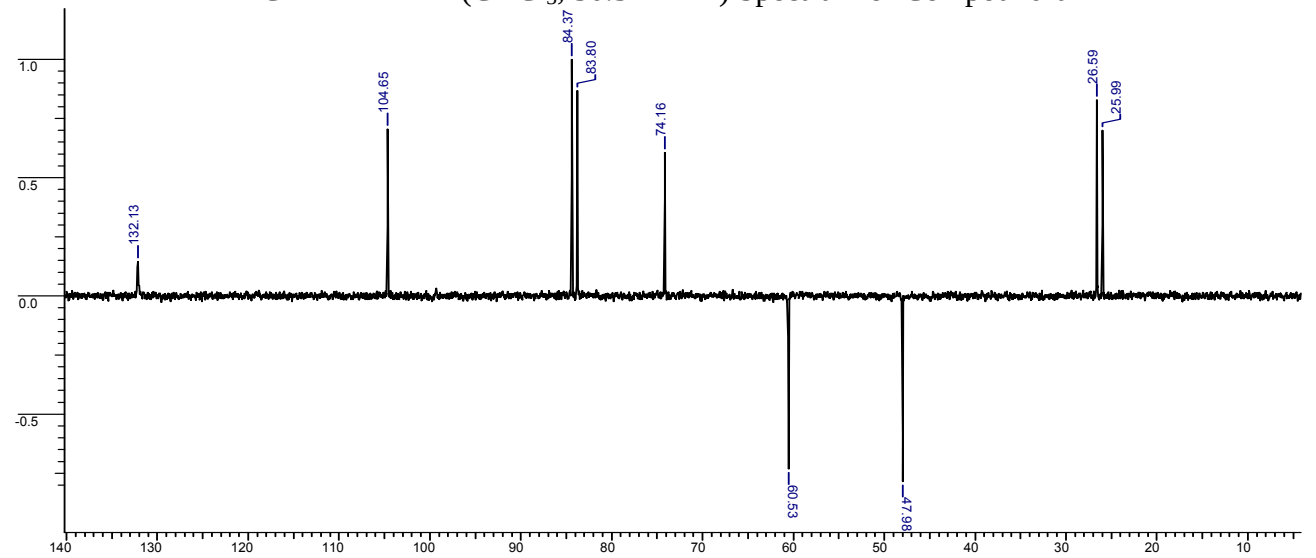
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **6**



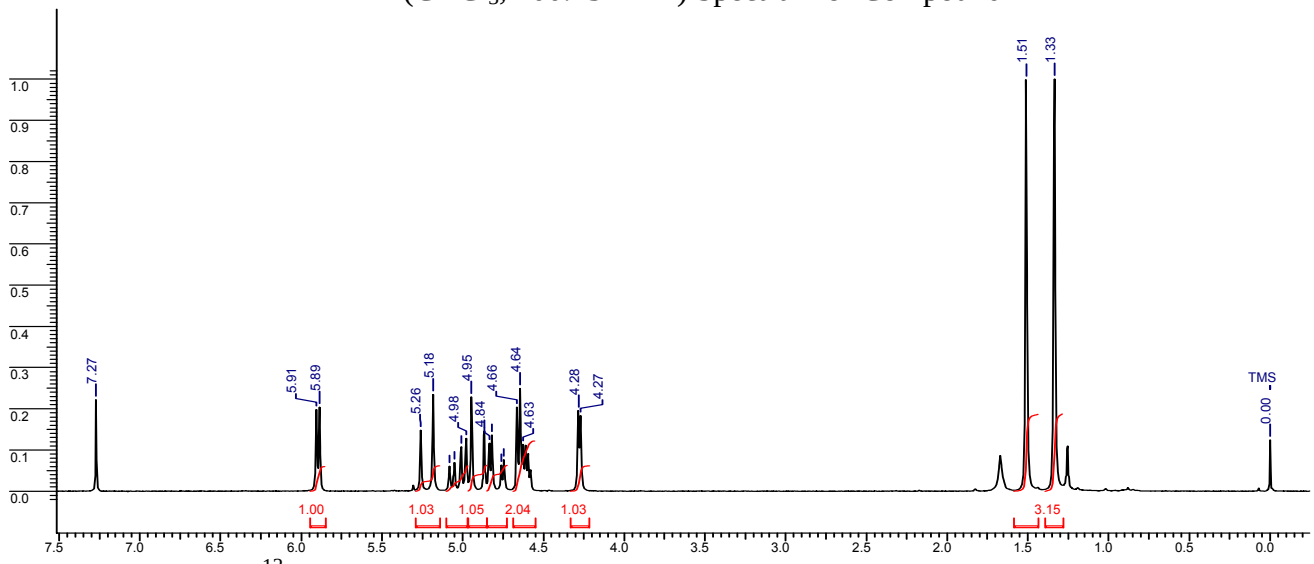
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **6**



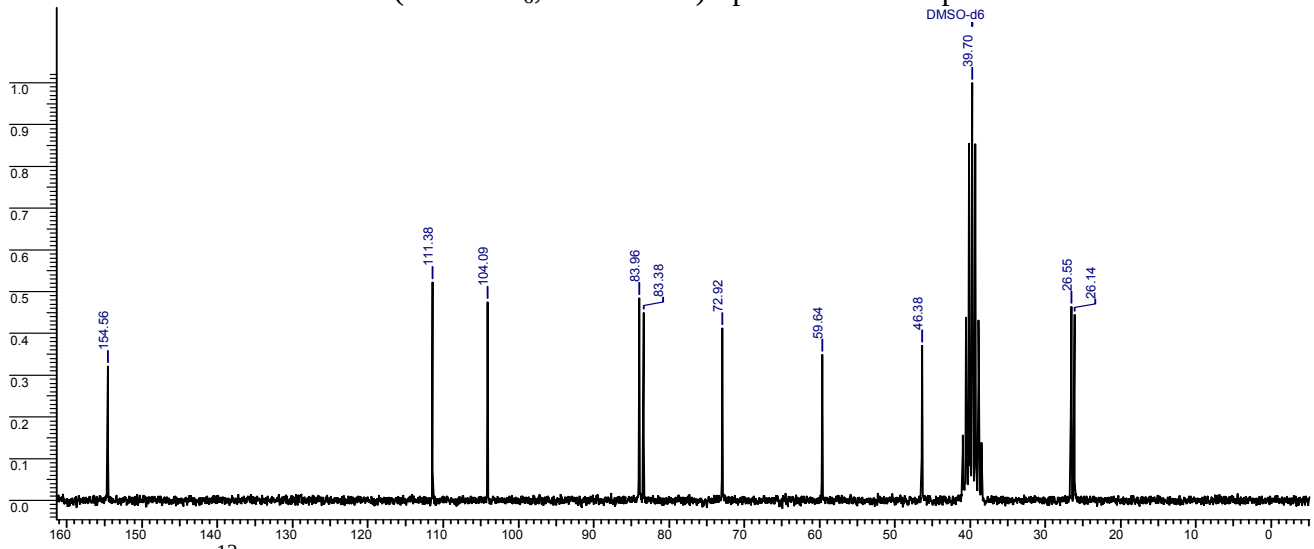
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **6**



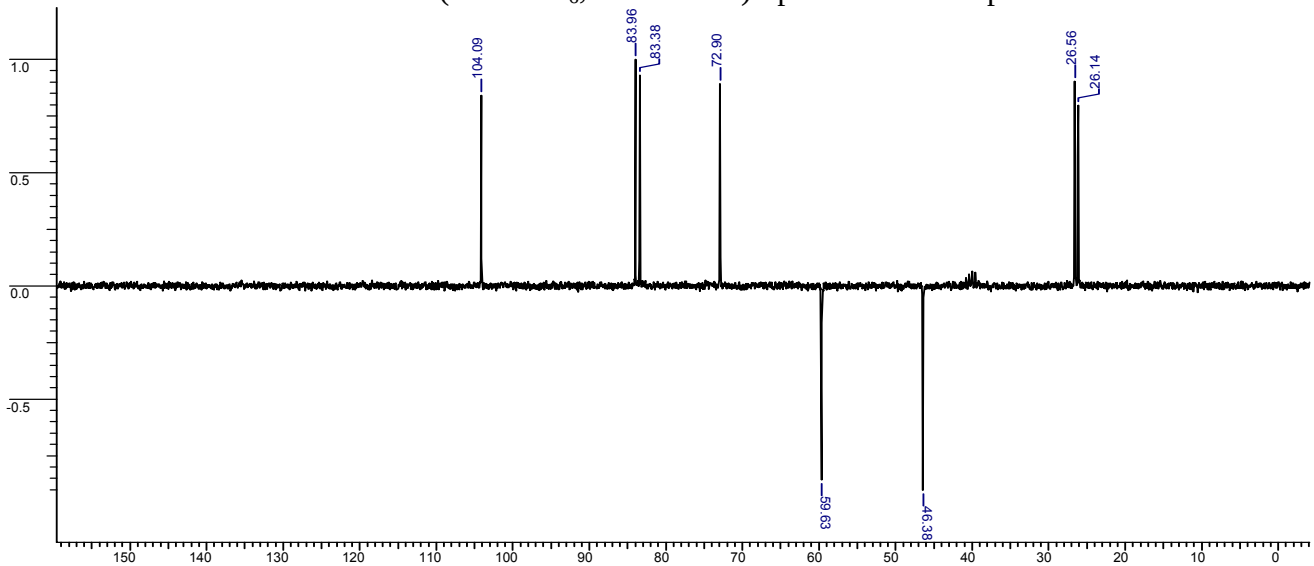
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **7**



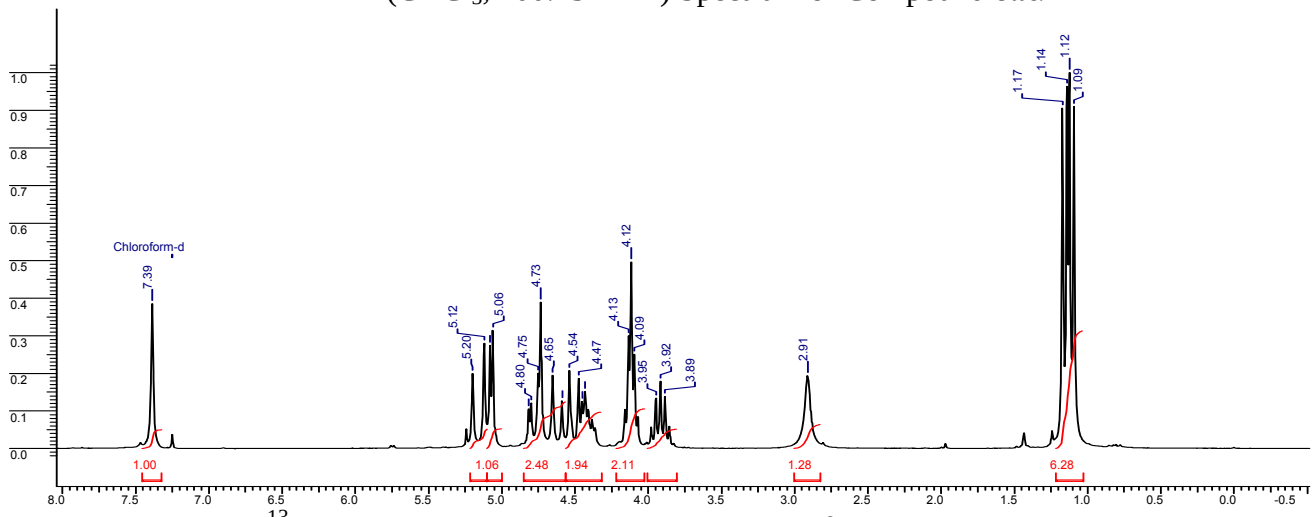
^{13}C NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **7**



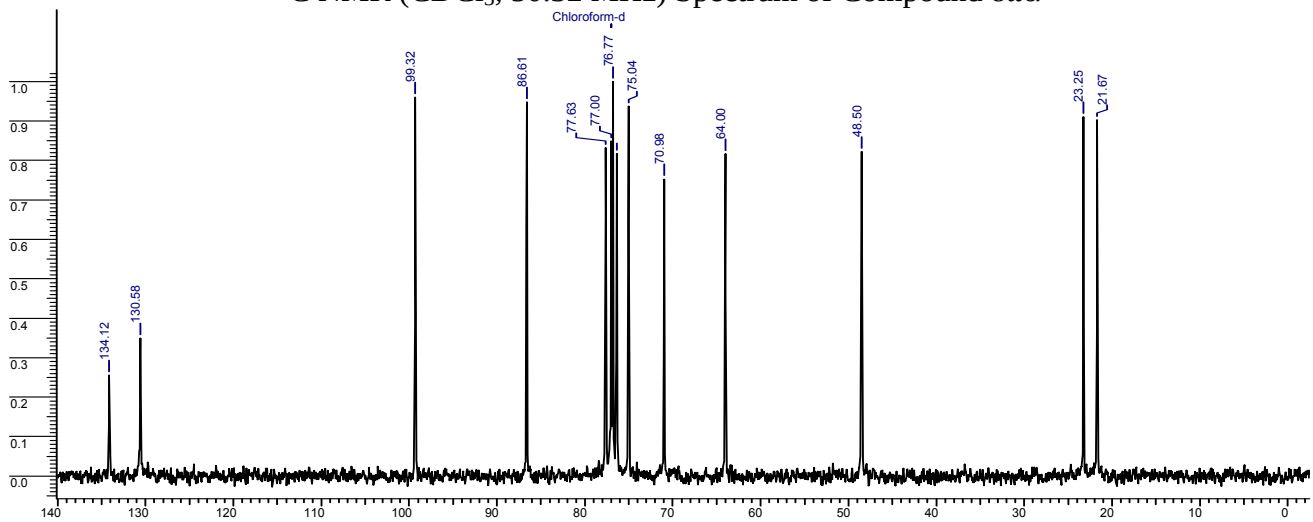
^{13}C-DEPT NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **7**



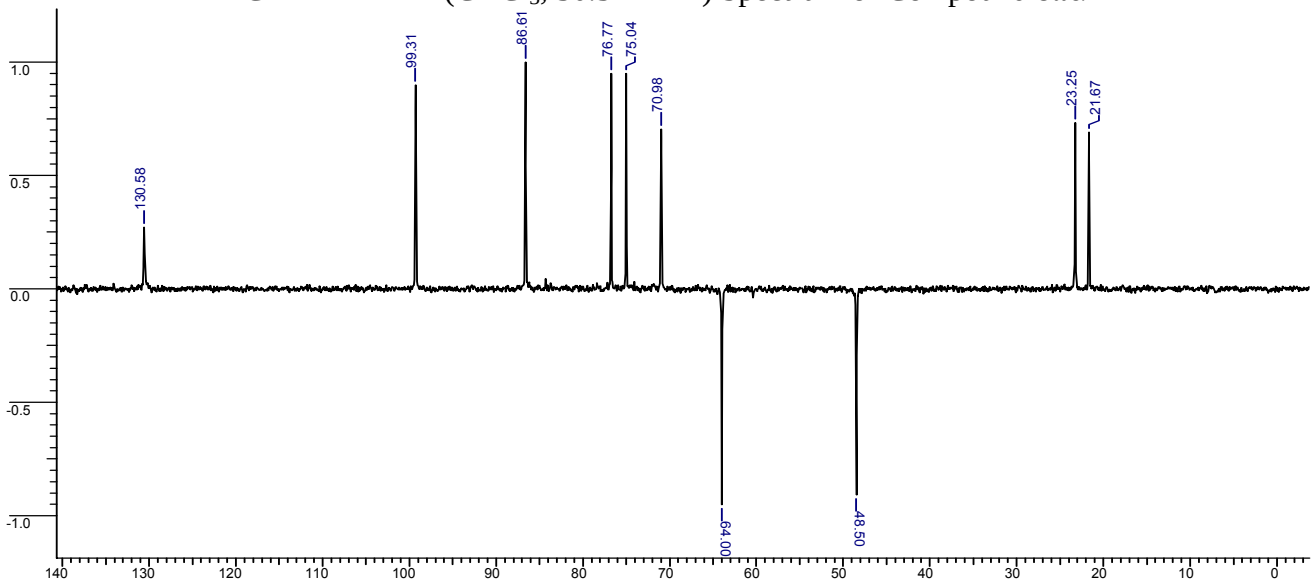
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **8aα**



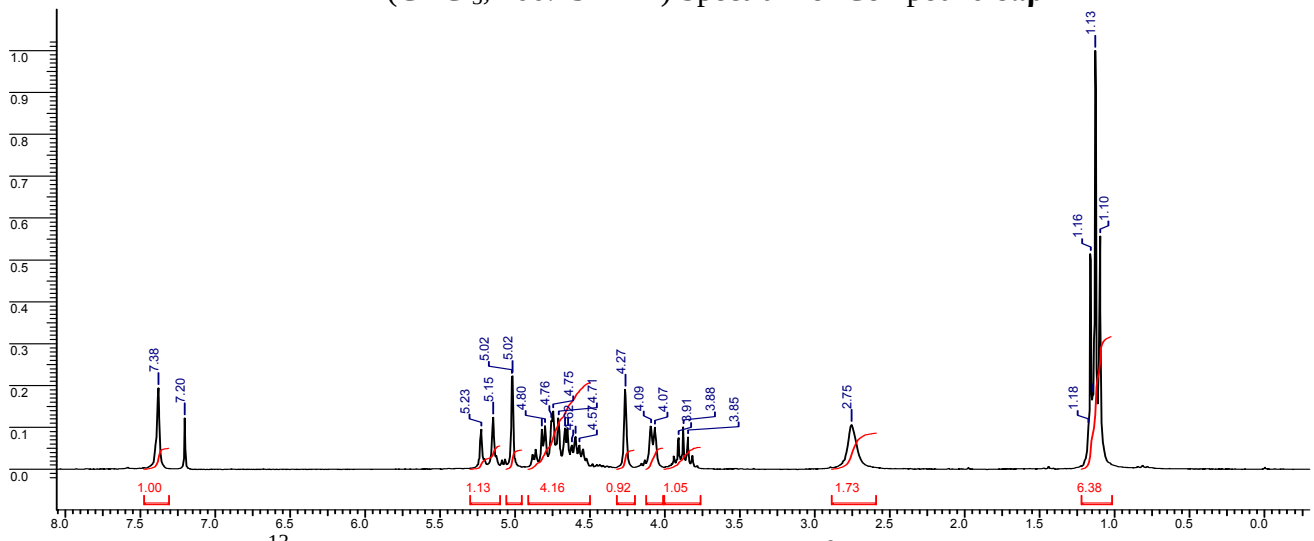
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8aα**



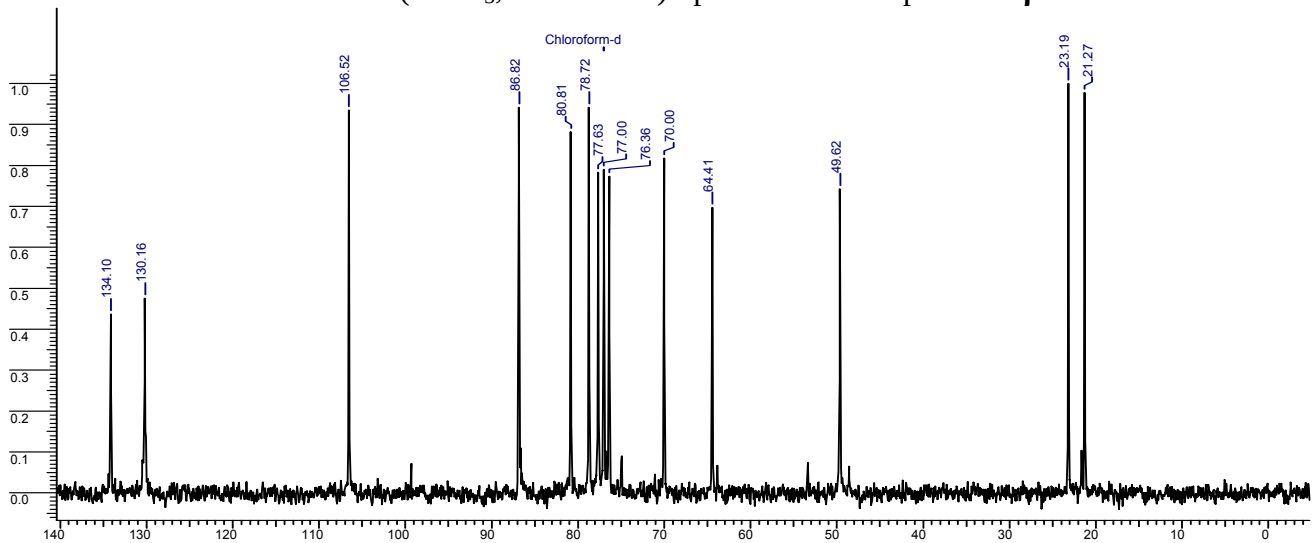
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8aα**



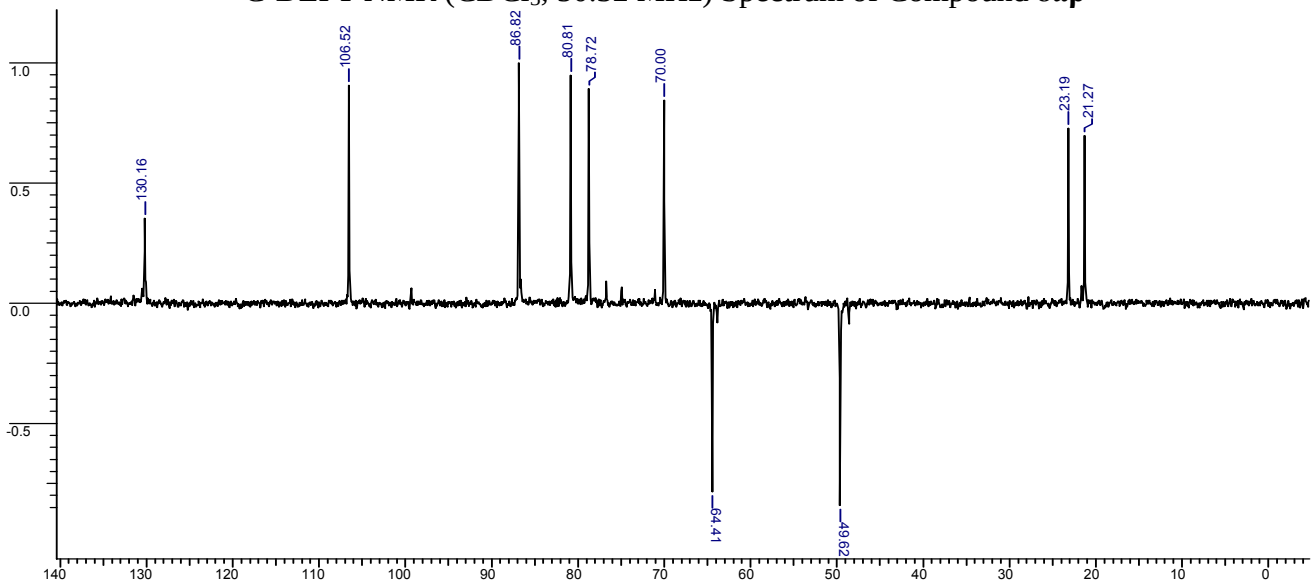
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **8aβ**



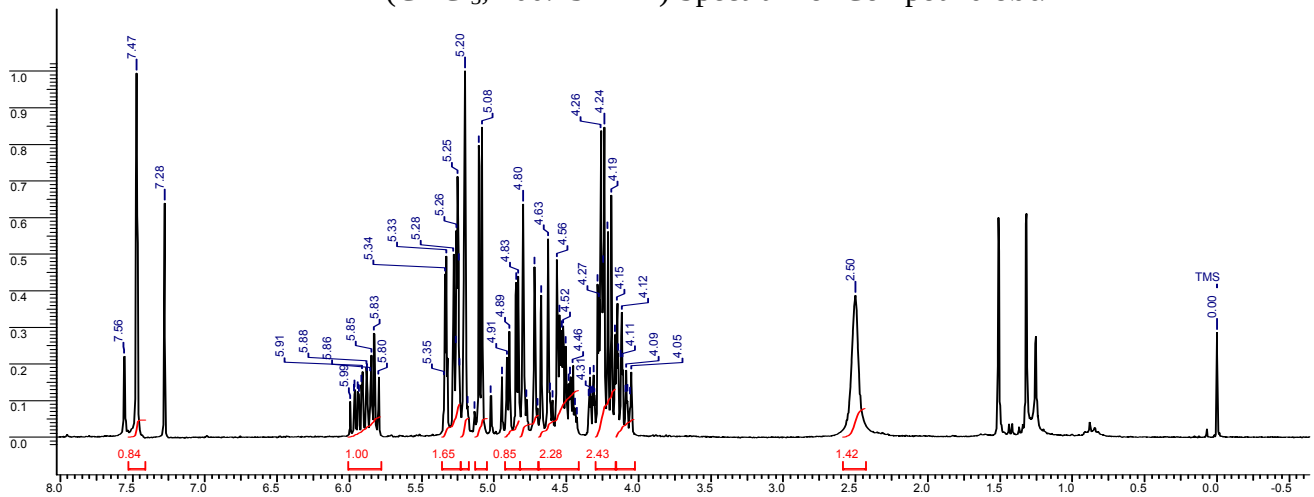
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8aβ**



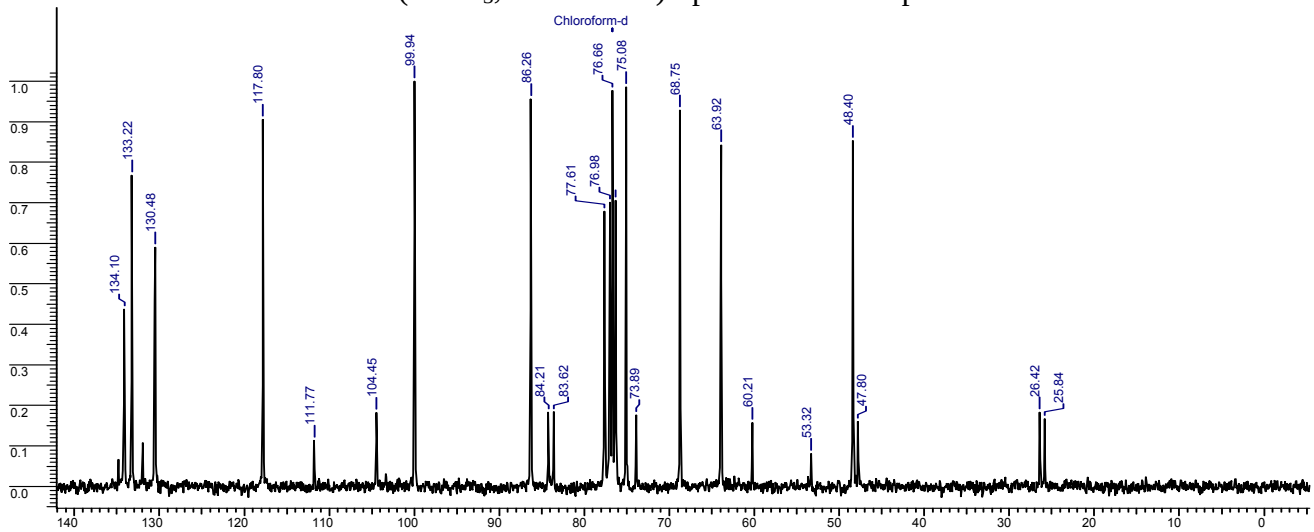
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8aβ**



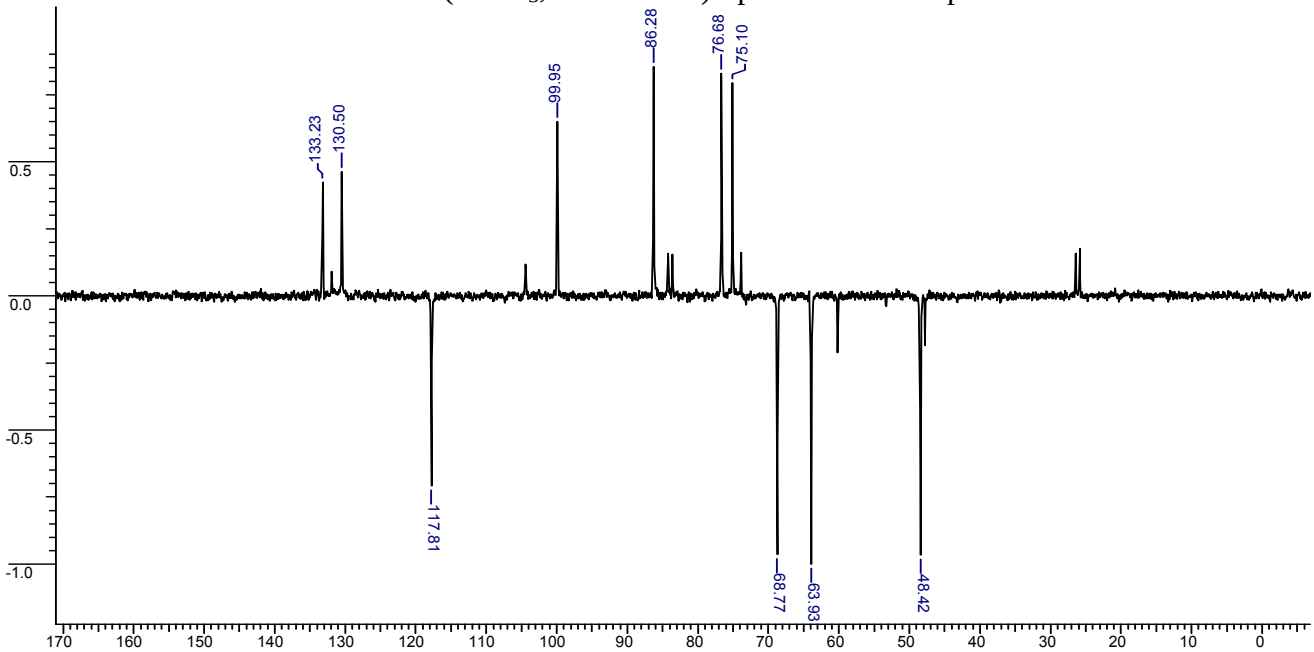
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **8bα**



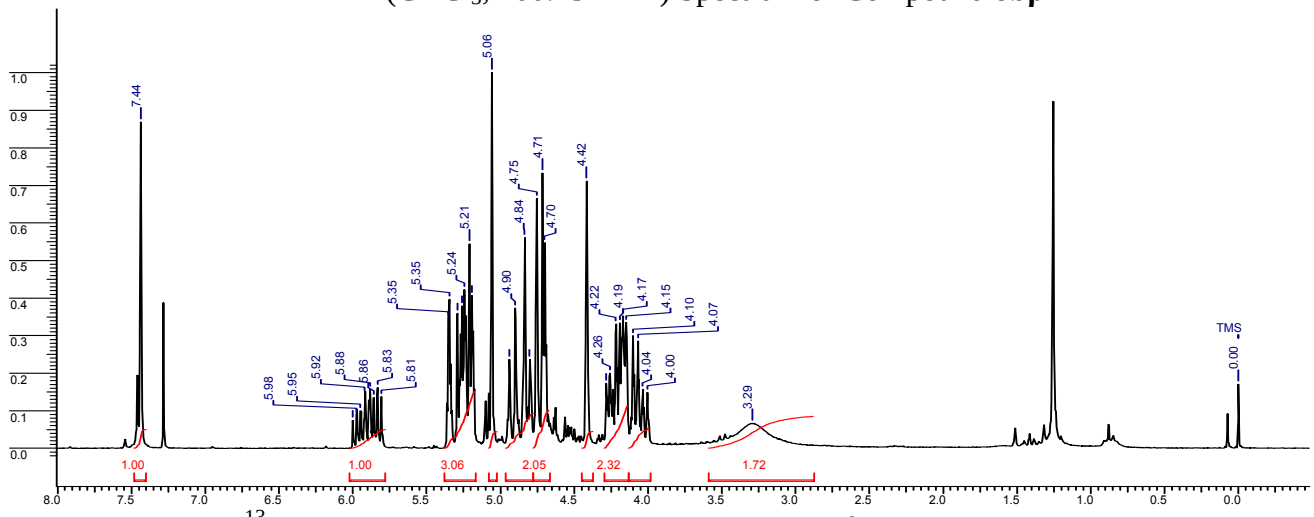
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8bα**



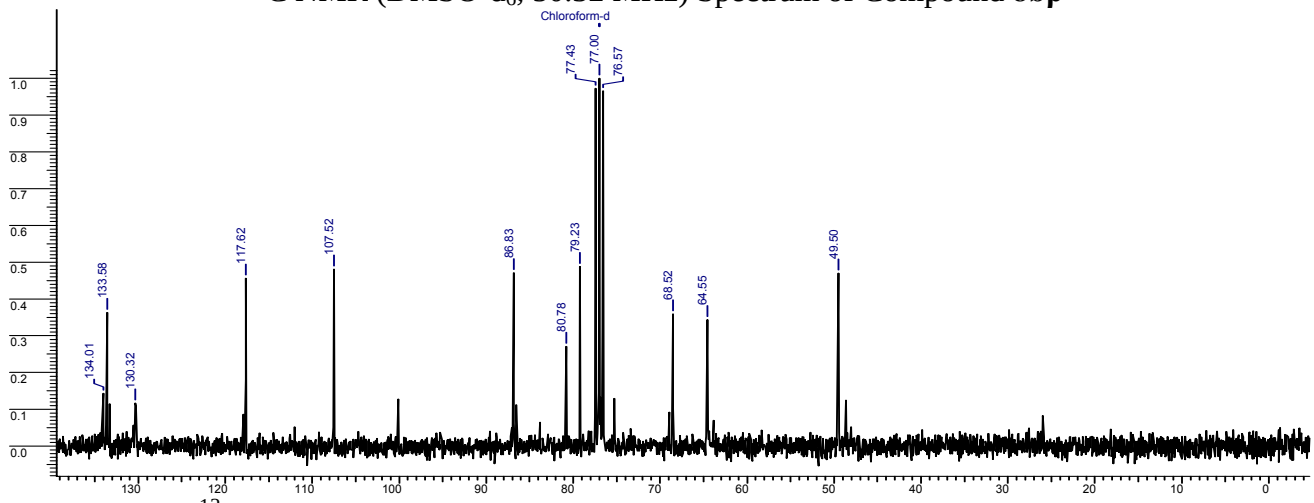
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8bα**



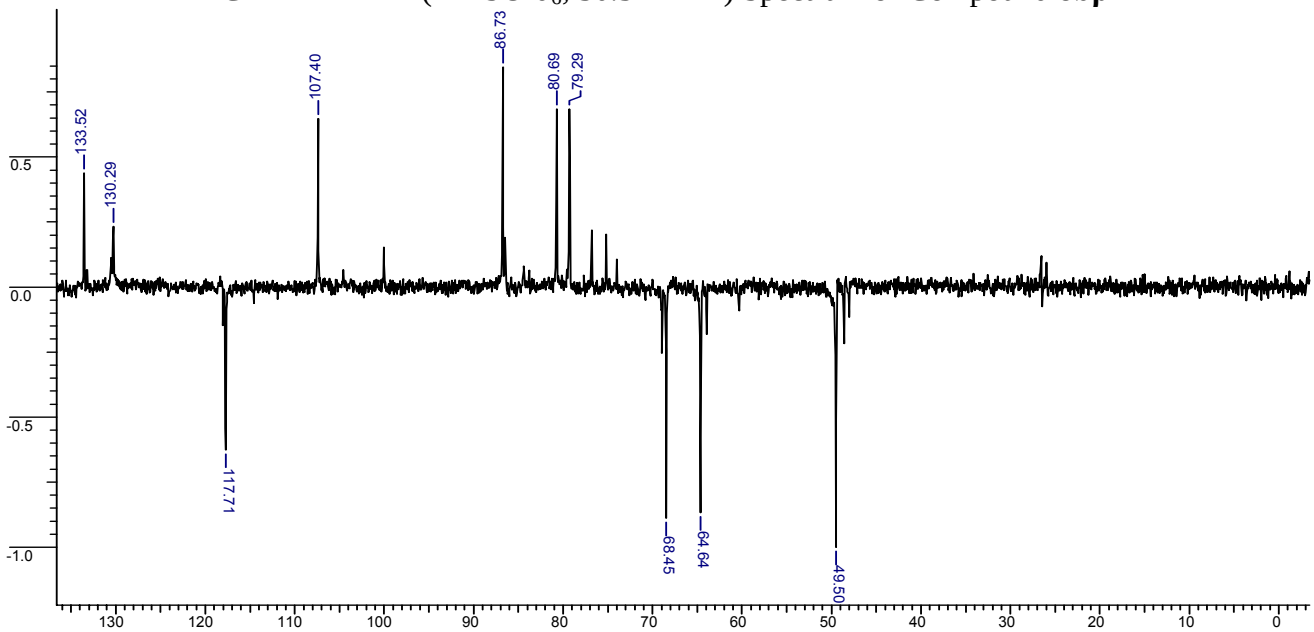
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **8bβ**



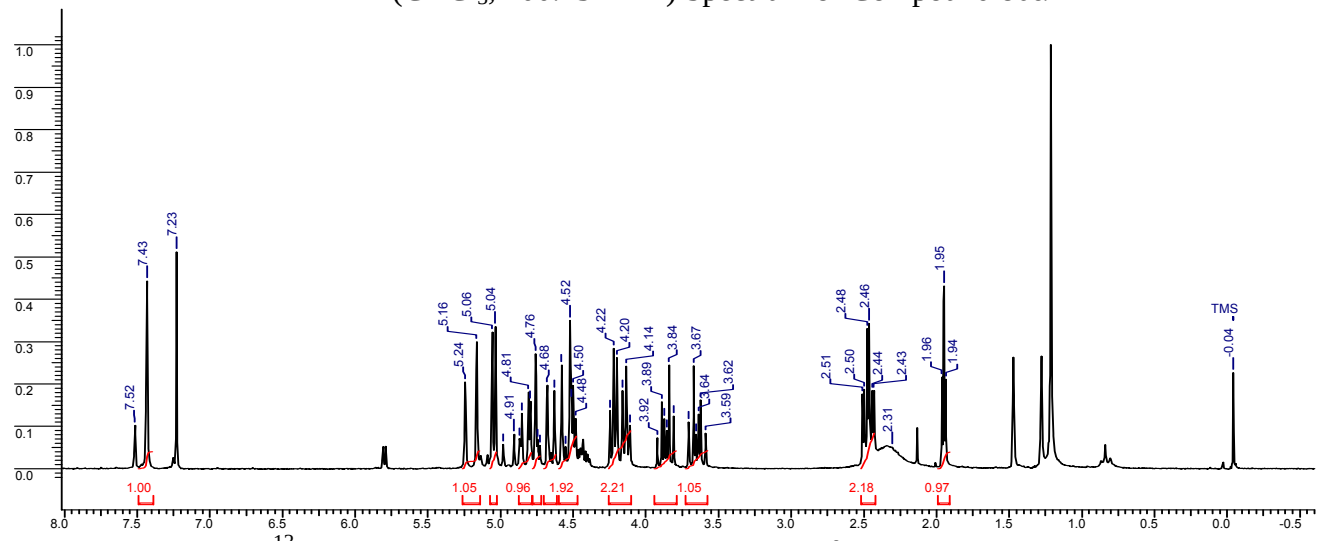
^{13}C NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **8bβ**



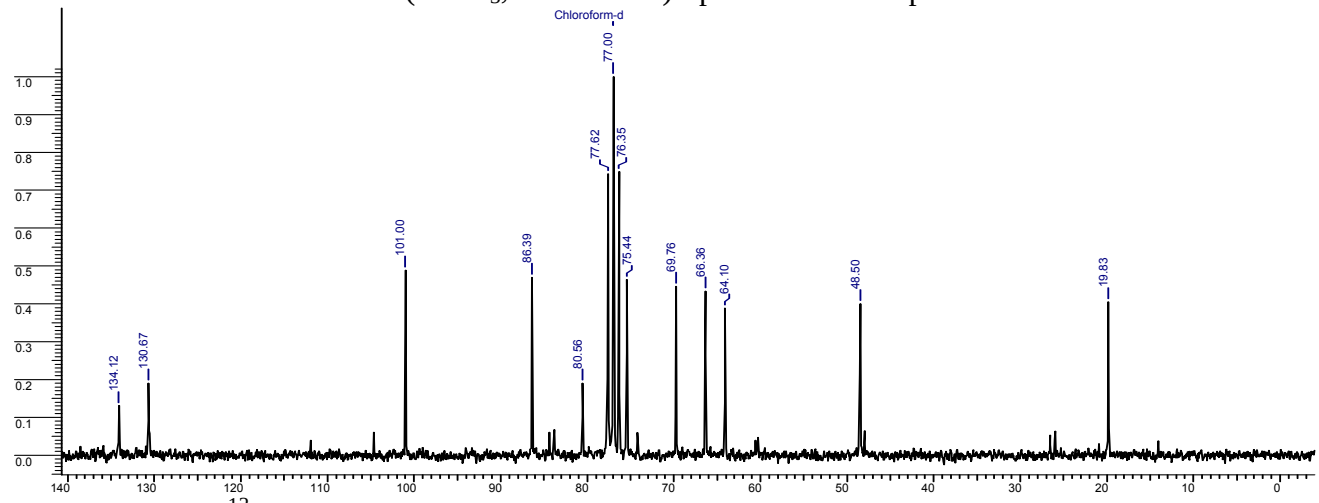
^{13}C-DEPT NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **8bβ**



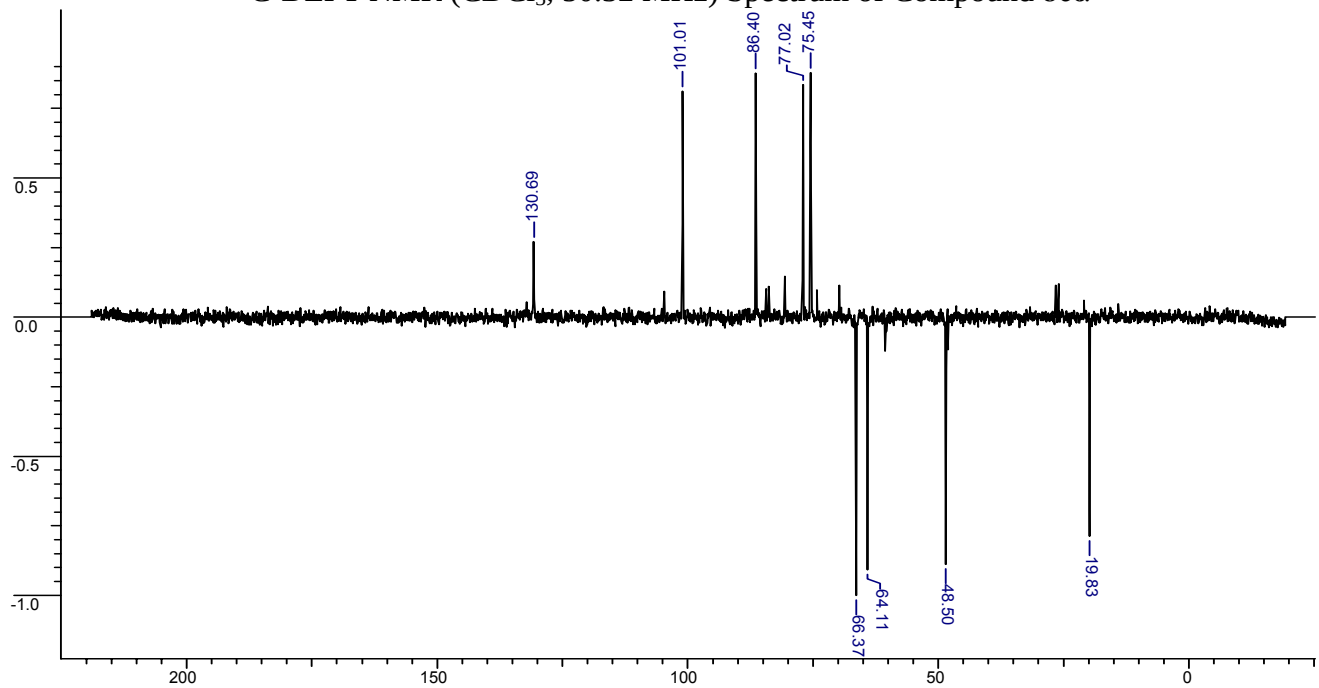
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **8cα**



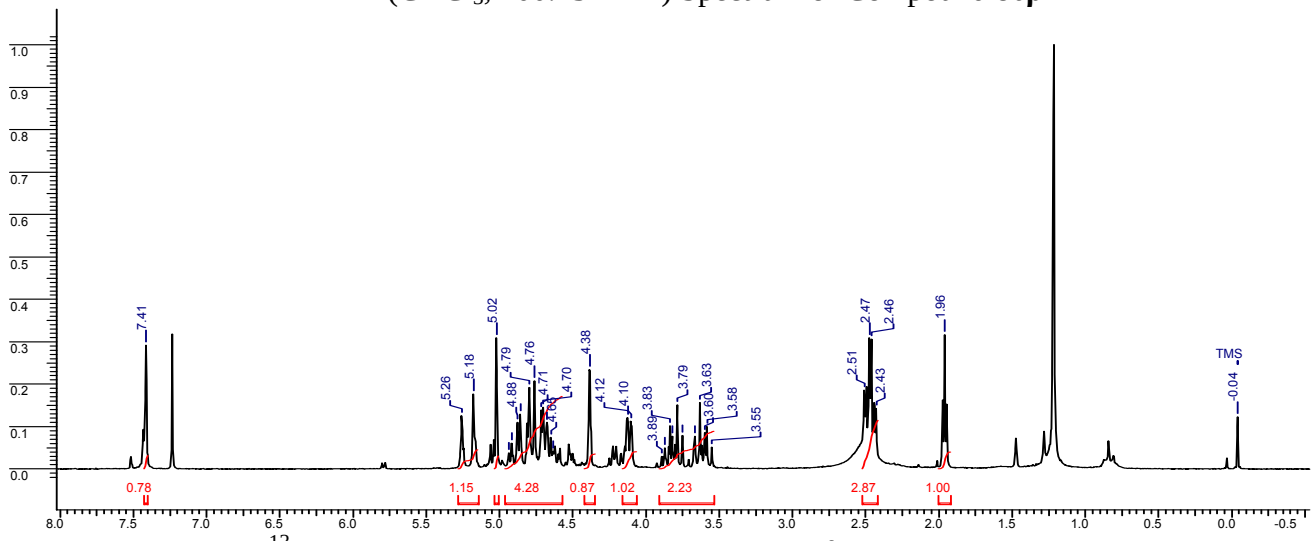
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8cα**



^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8cα**



^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **8cβ**



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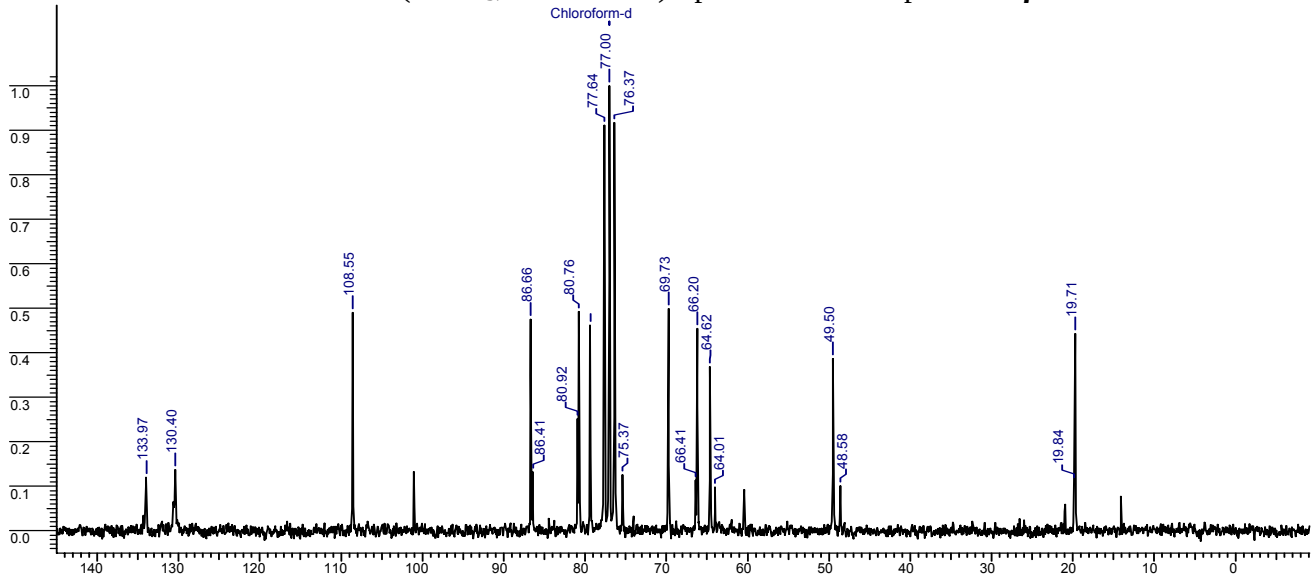
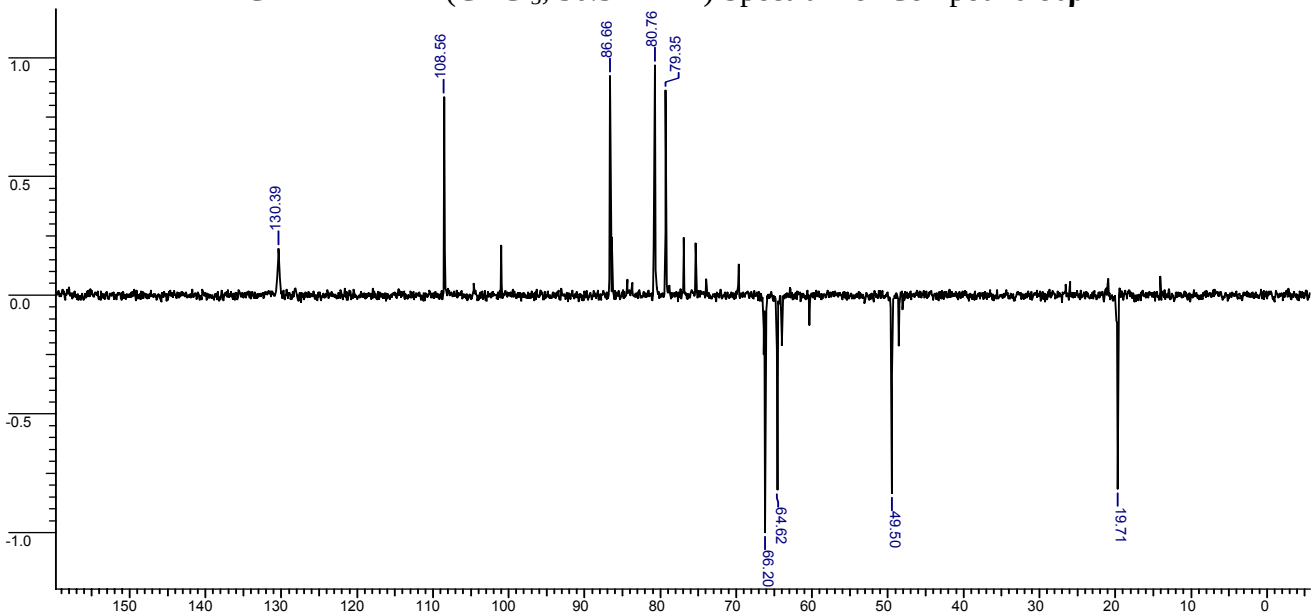
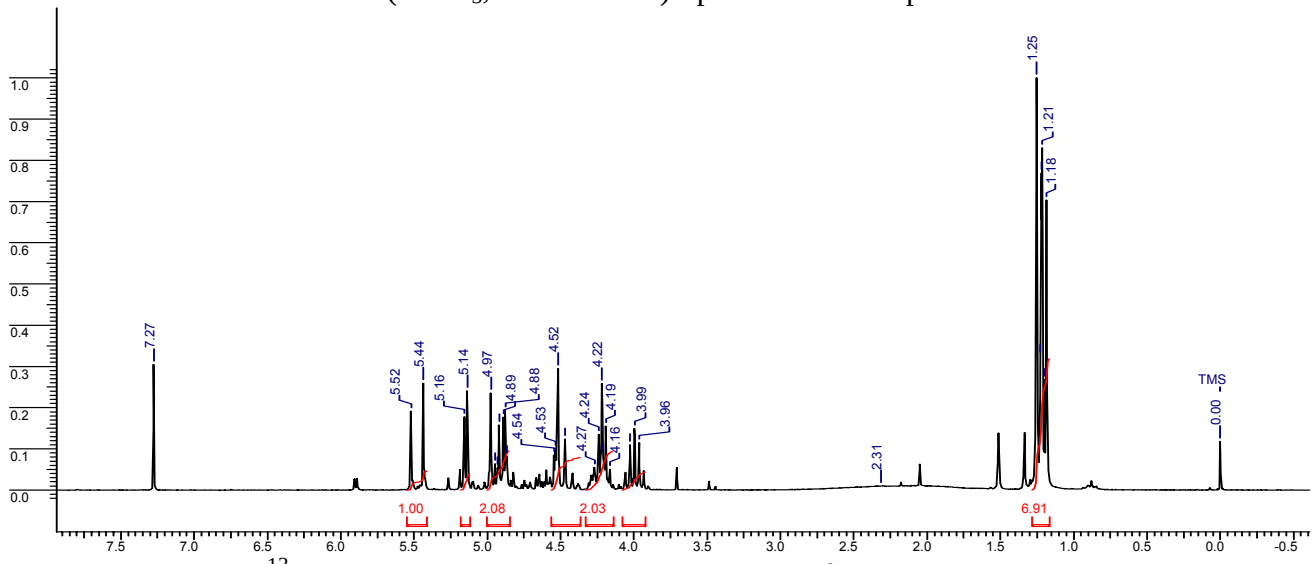


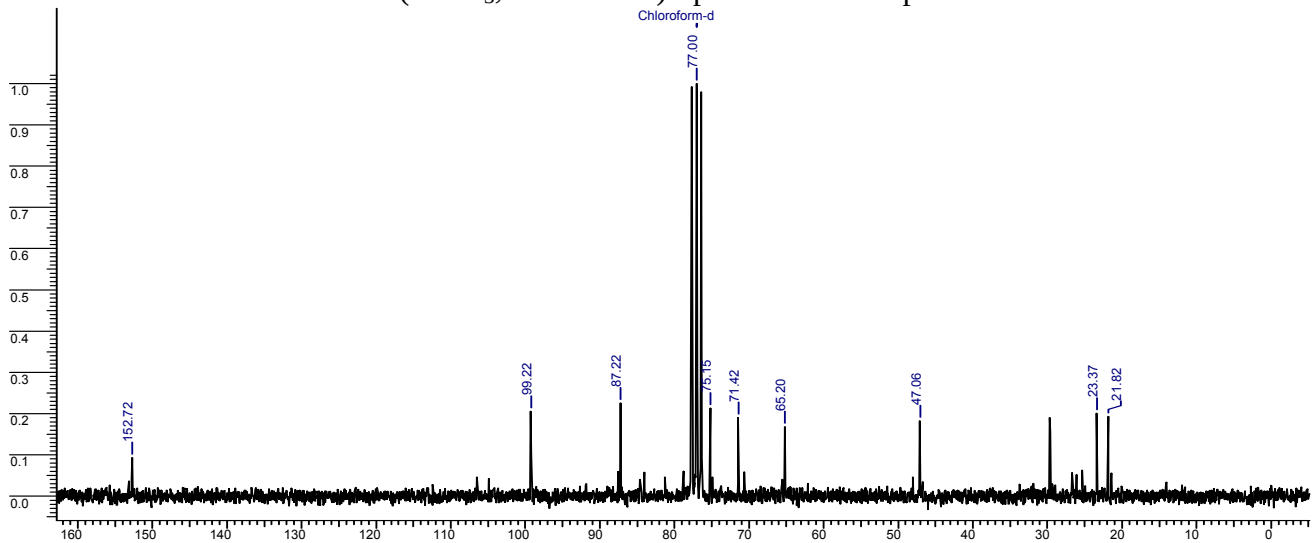
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **8cβ**



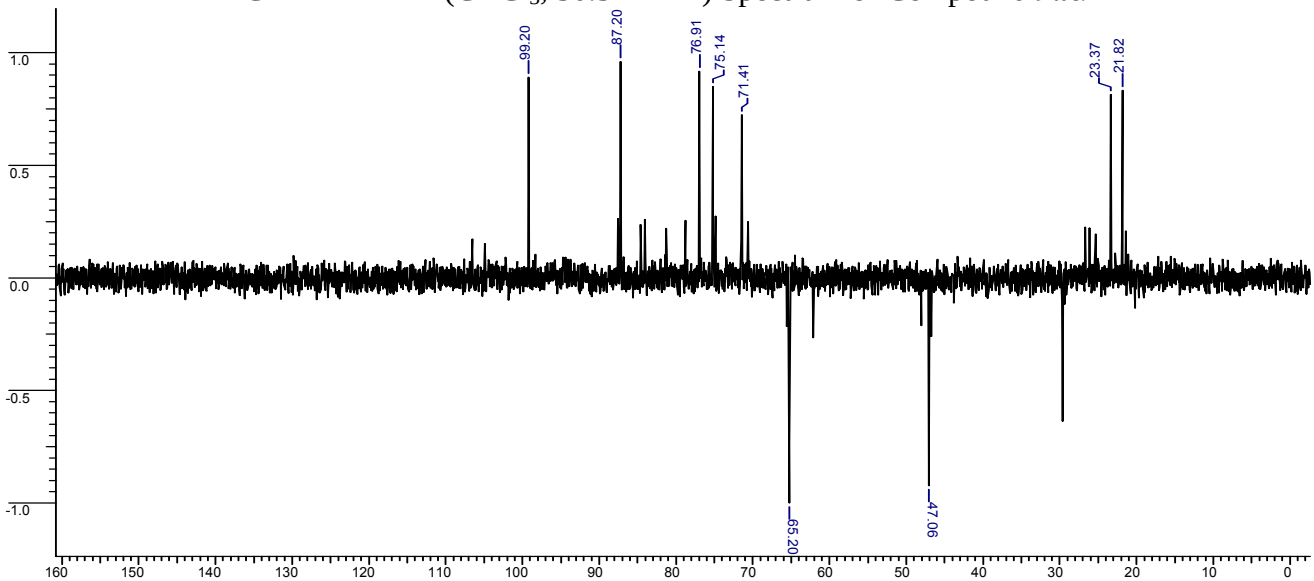
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **9aα**



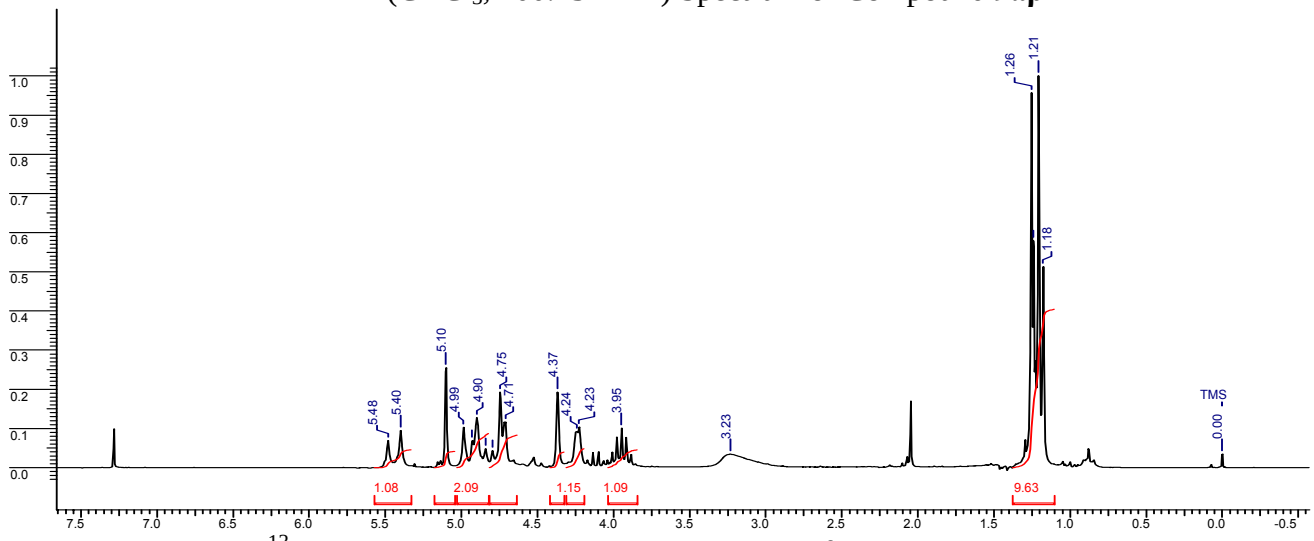
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **9aα**



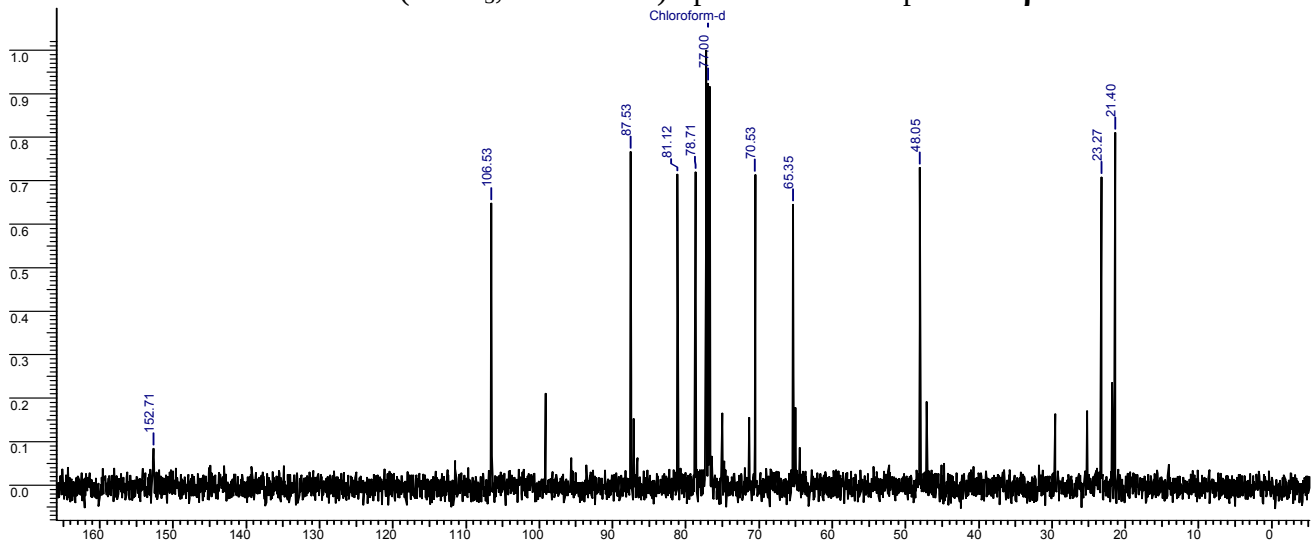
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **9aα**



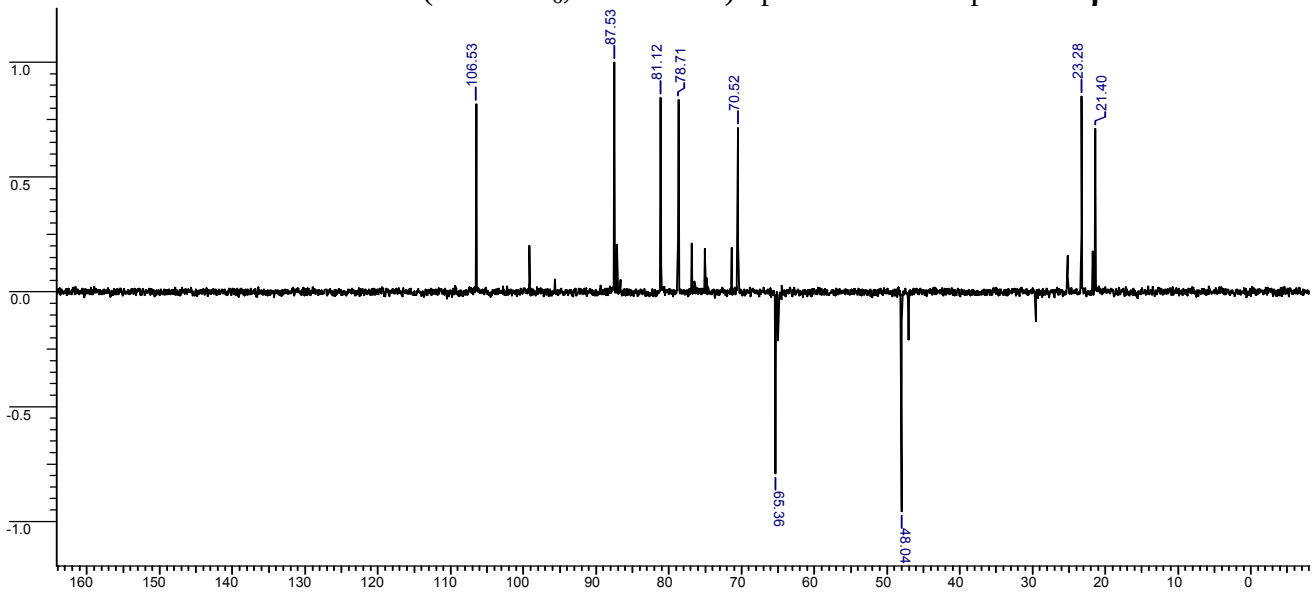
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **9aβ**



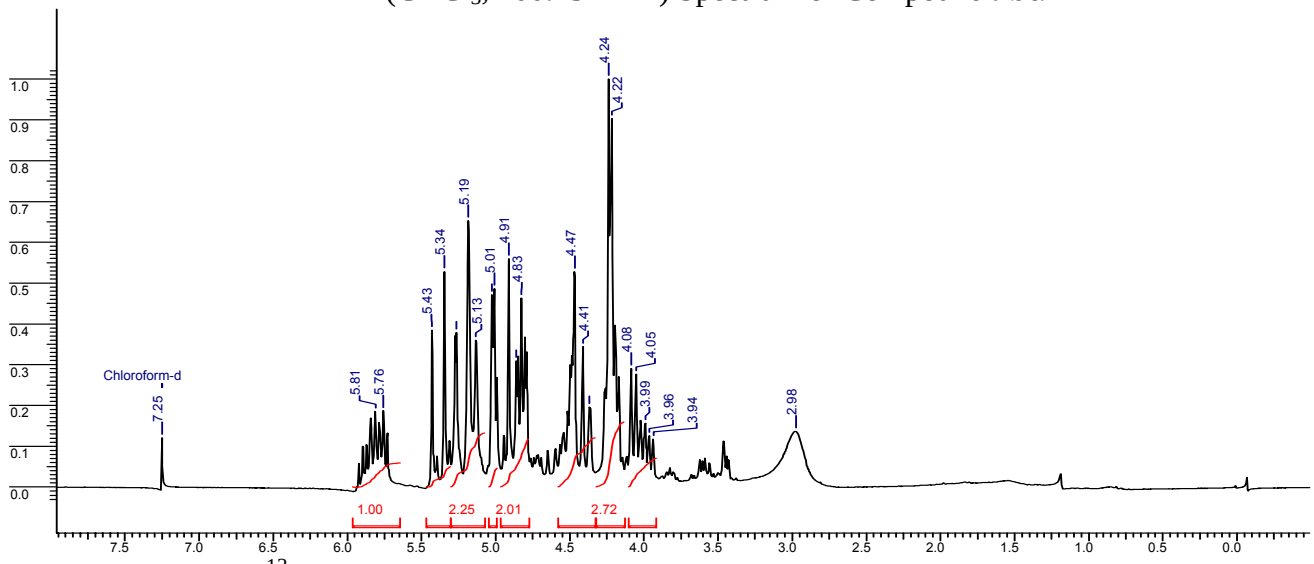
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **9aβ**



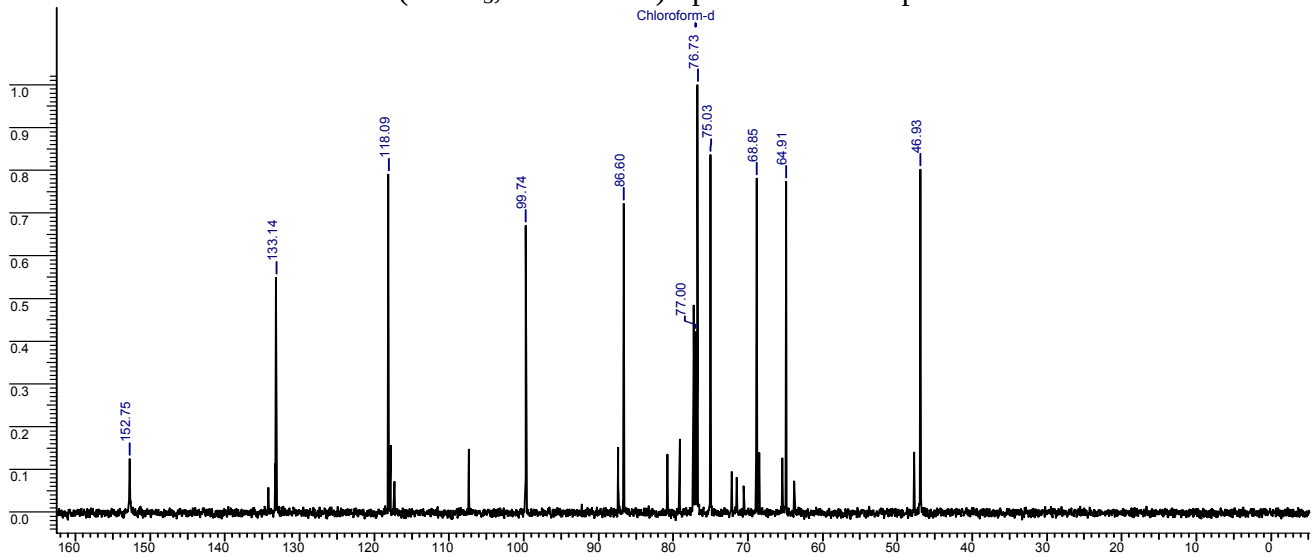
^{13}C-DEPT NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **9aβ**



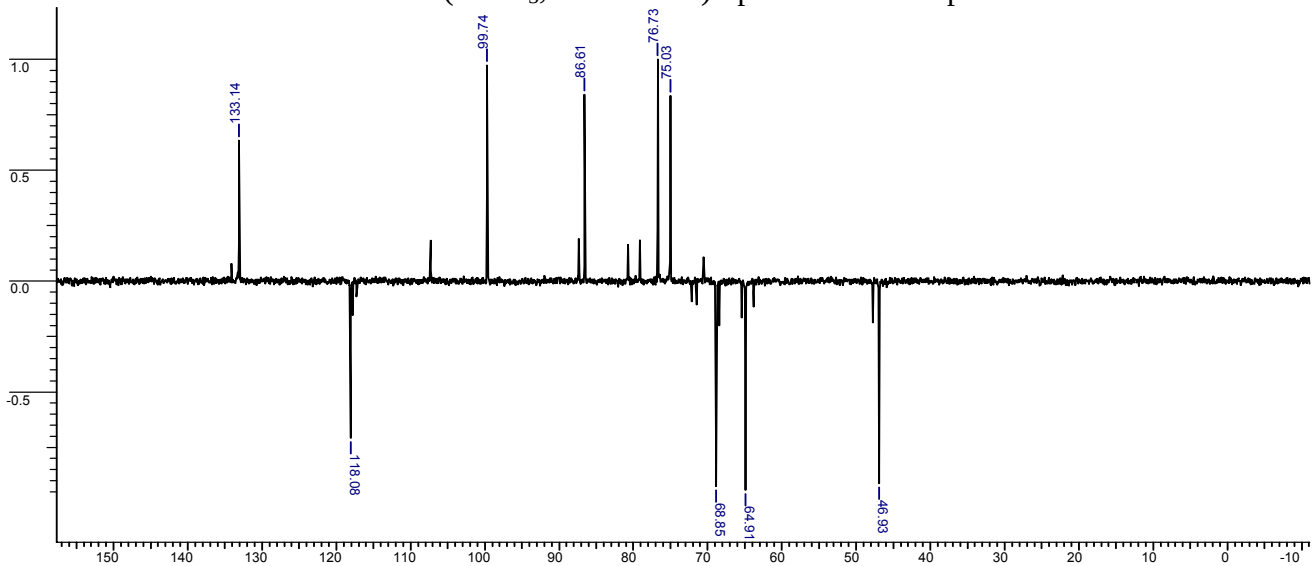
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **9bα**



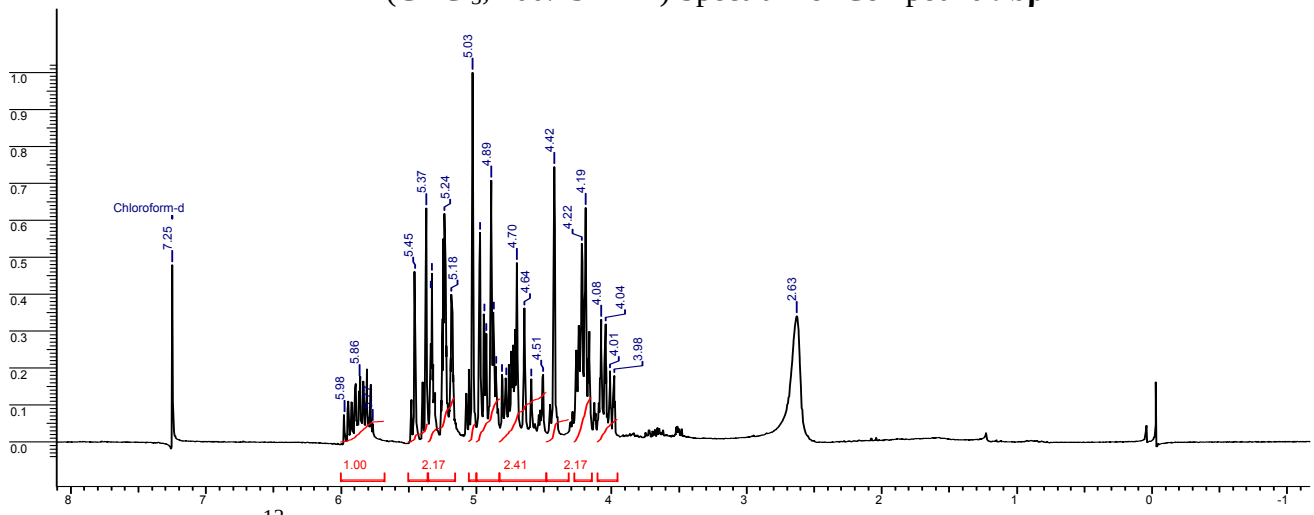
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **9bα**



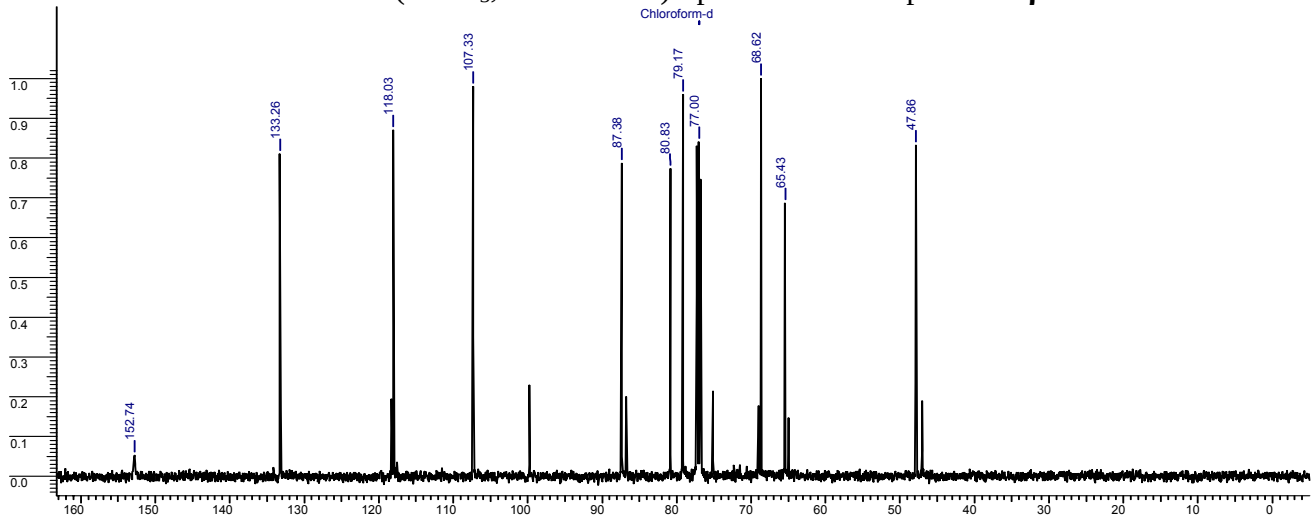
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **9bα**



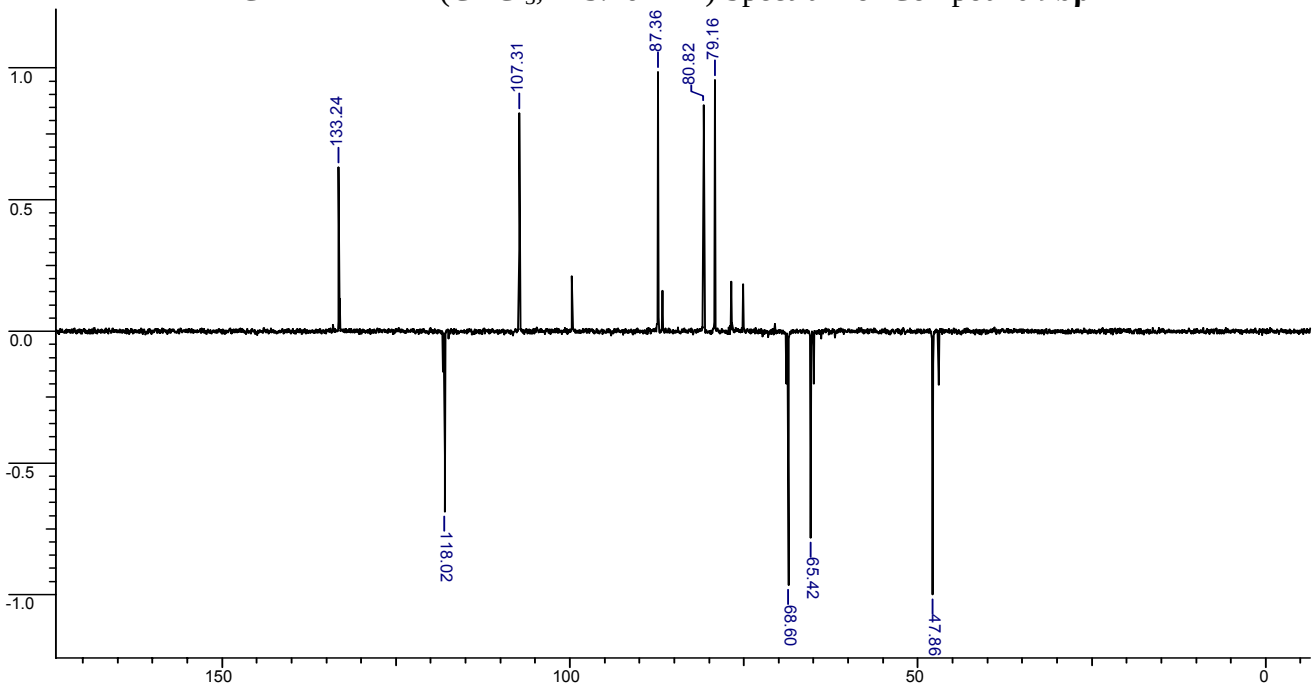
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **9bβ**



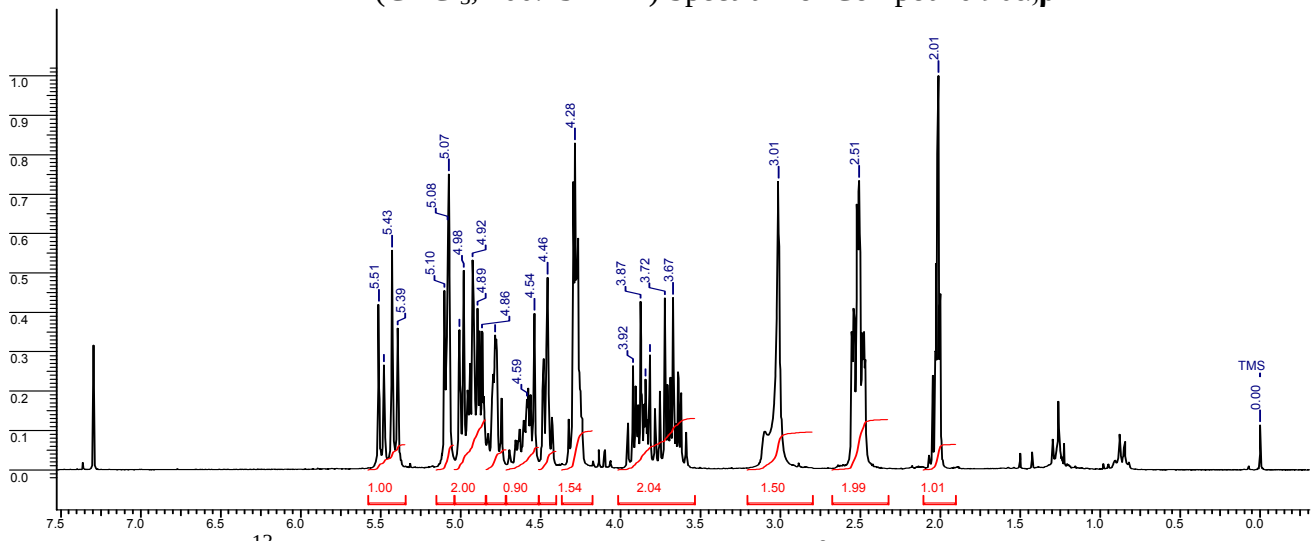
^{13}C NMR ($CDCl_3$, 125.76MHz) Spectrum of Compound **9bβ**



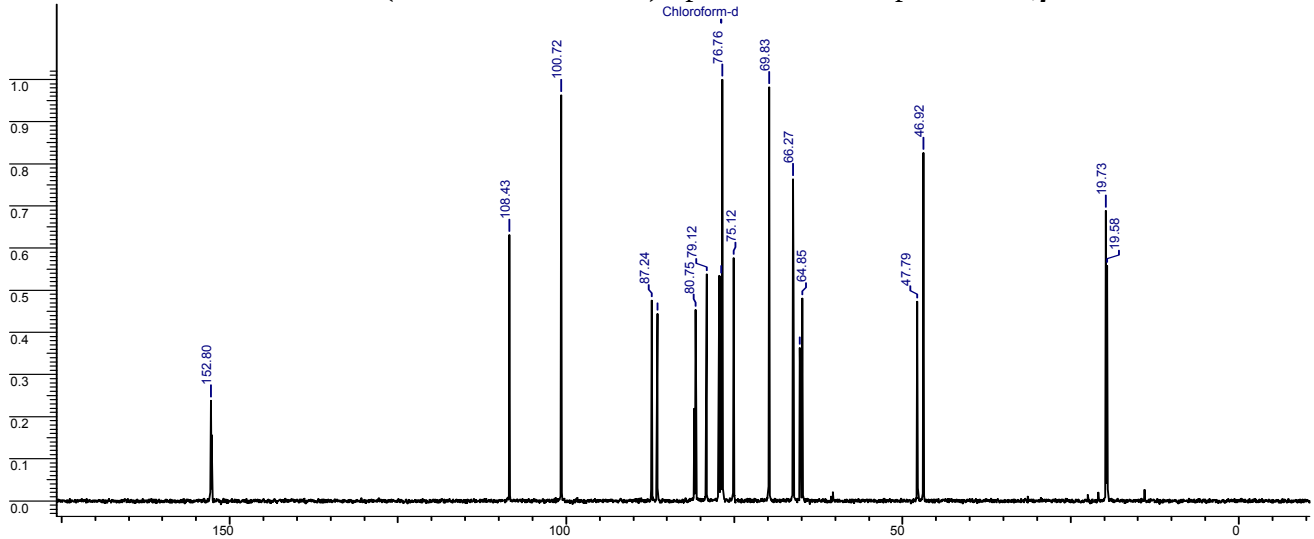
^{13}C-DEPT NMR ($CDCl_3$, 125.76MHz) Spectrum of Compound **9bβ**



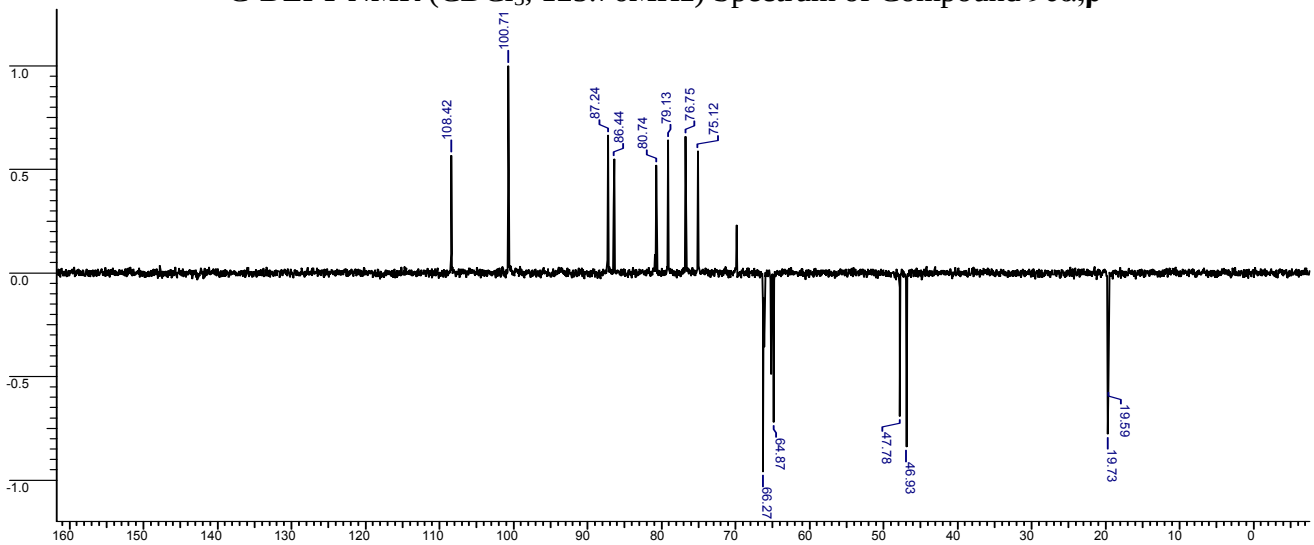
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **9cα,β**



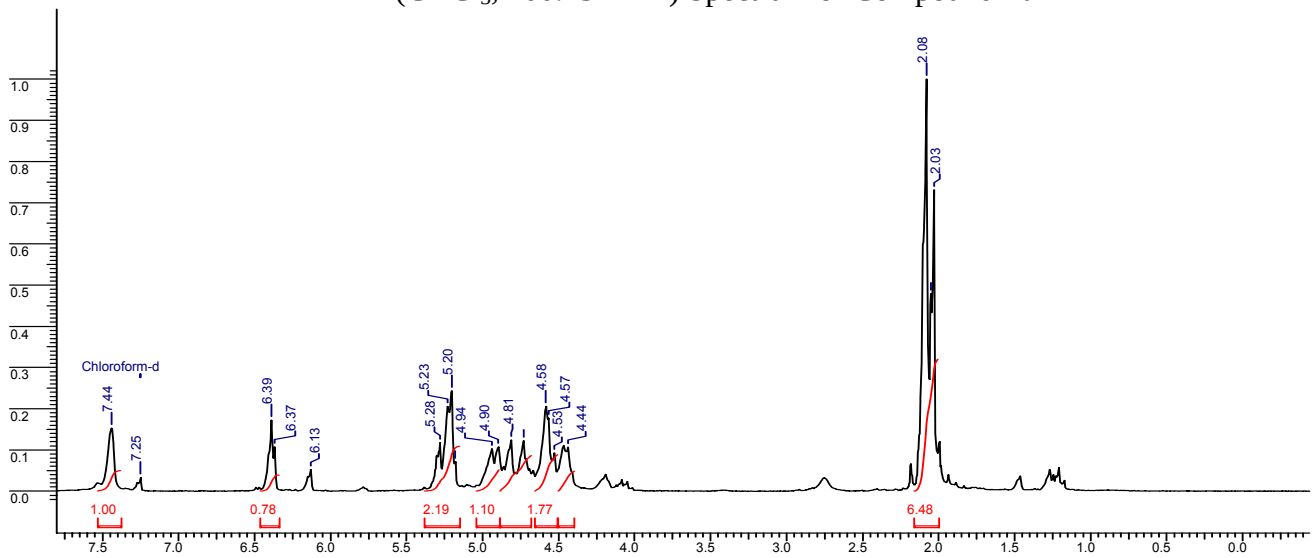
^{13}C NMR ($CDCl_3$, 125.76MHz) Spectrum of Compound **9cα,β**



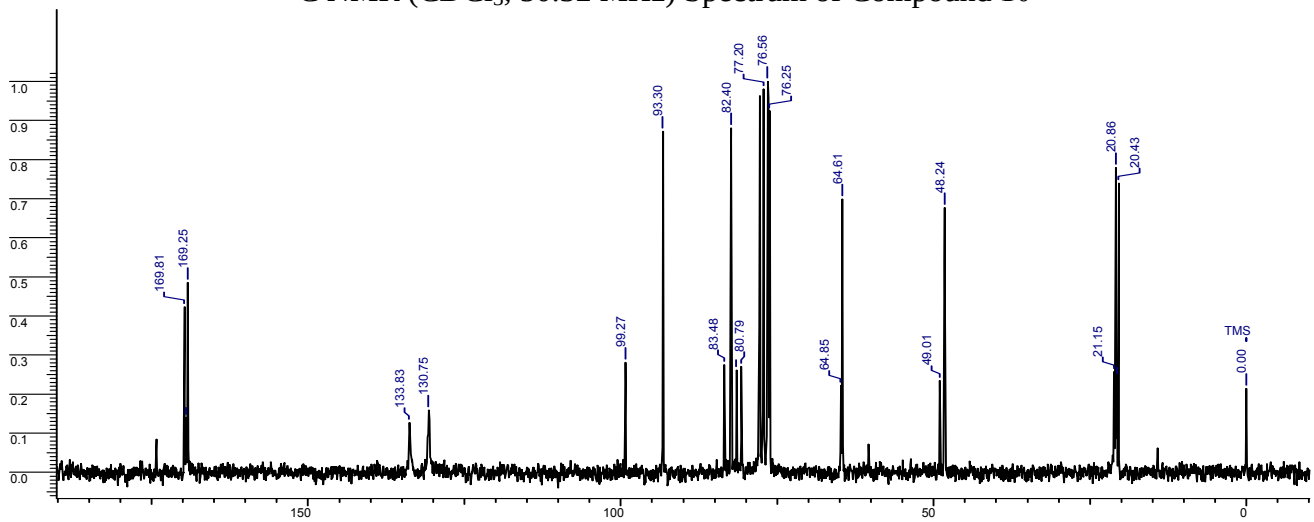
^{13}C-DEPT NMR ($CDCl_3$, 125.76MHz) Spectrum of Compound **9cα,β**



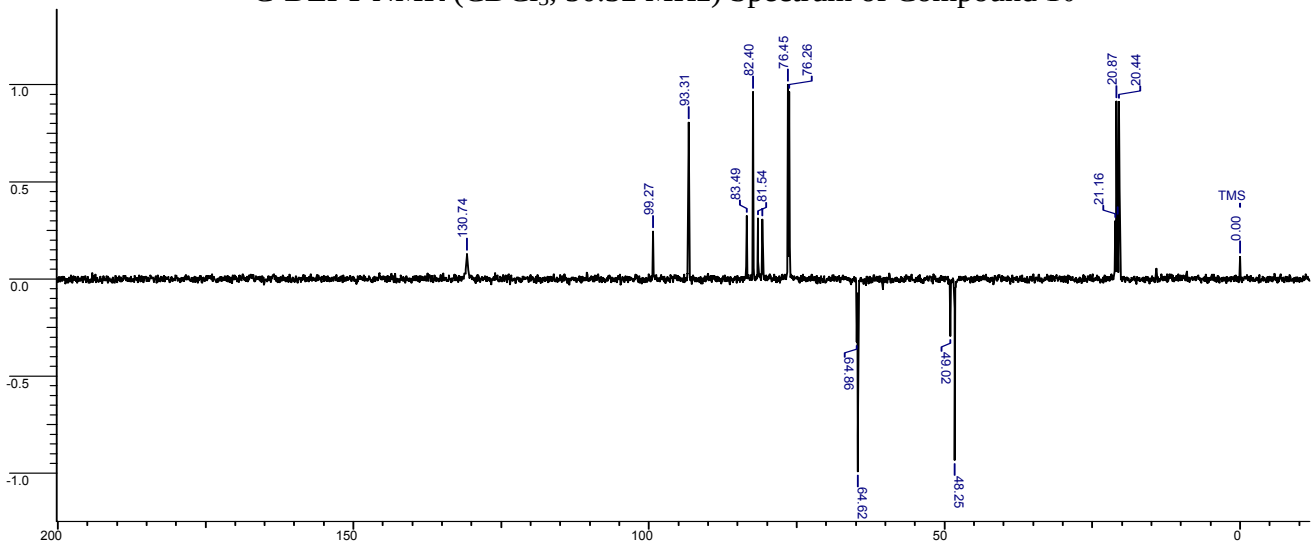
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **10**



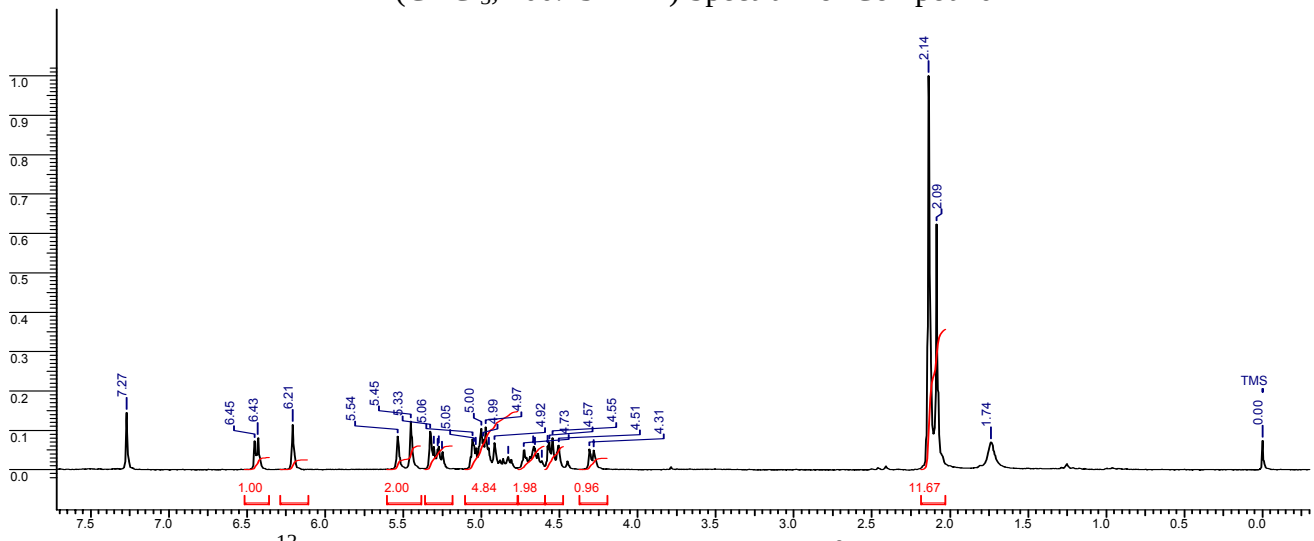
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **10**



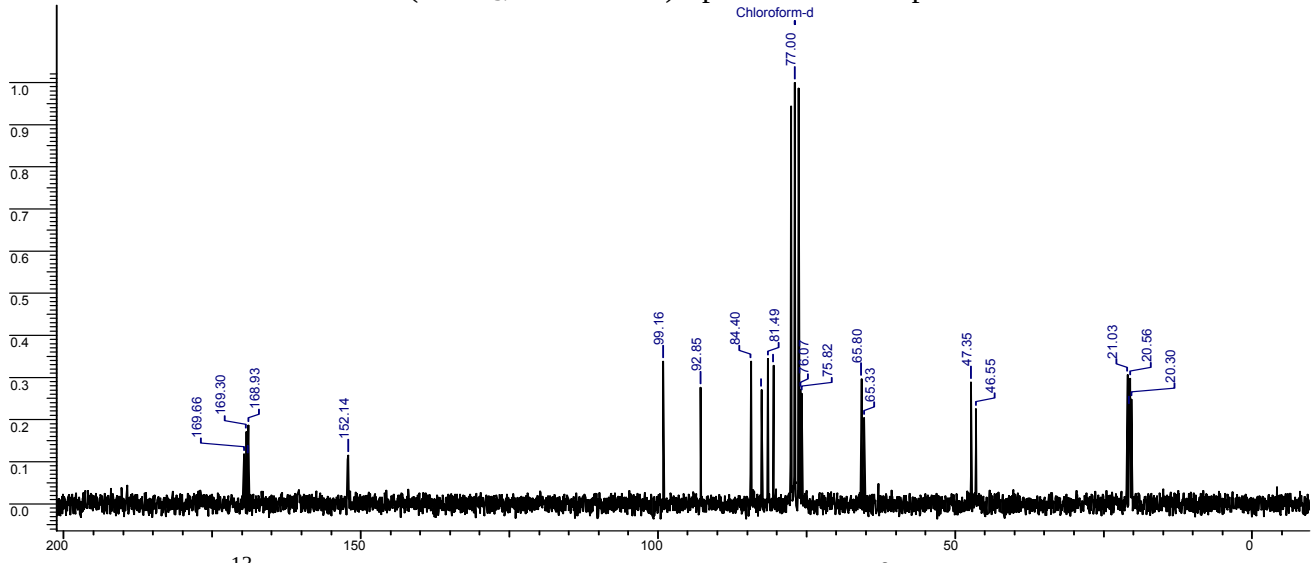
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **10**



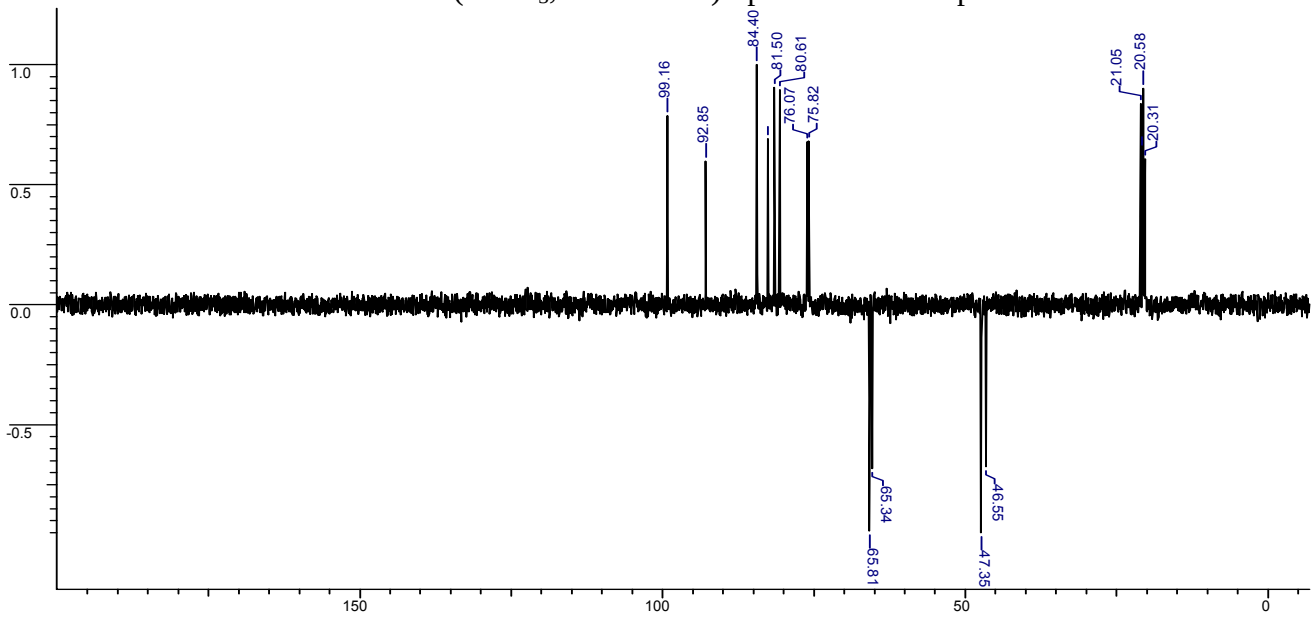
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **11**



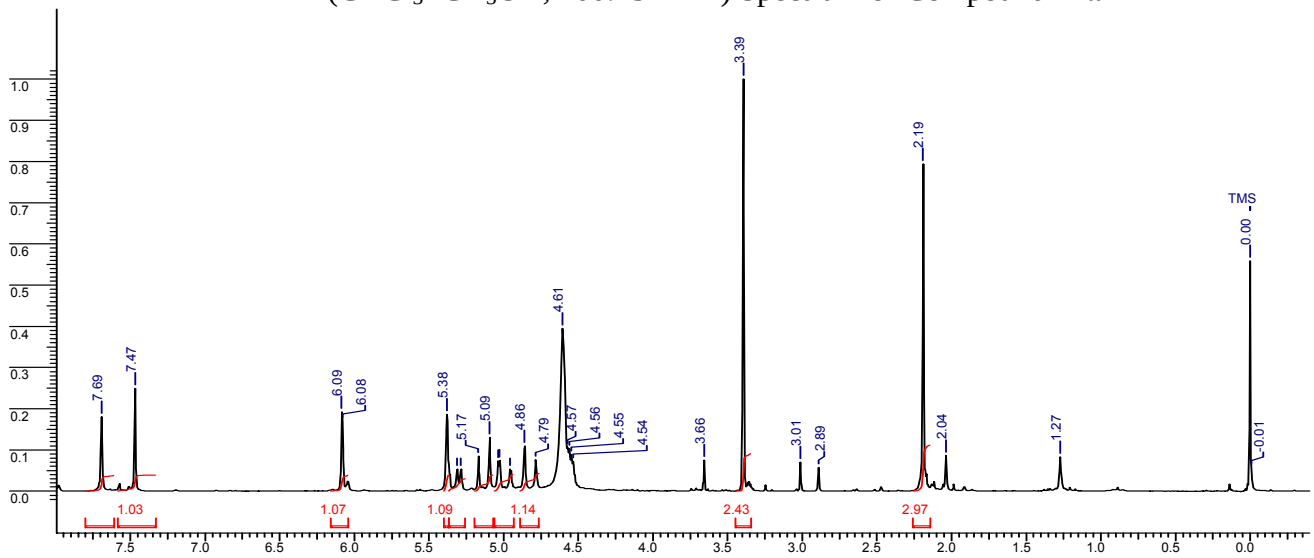
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **11**



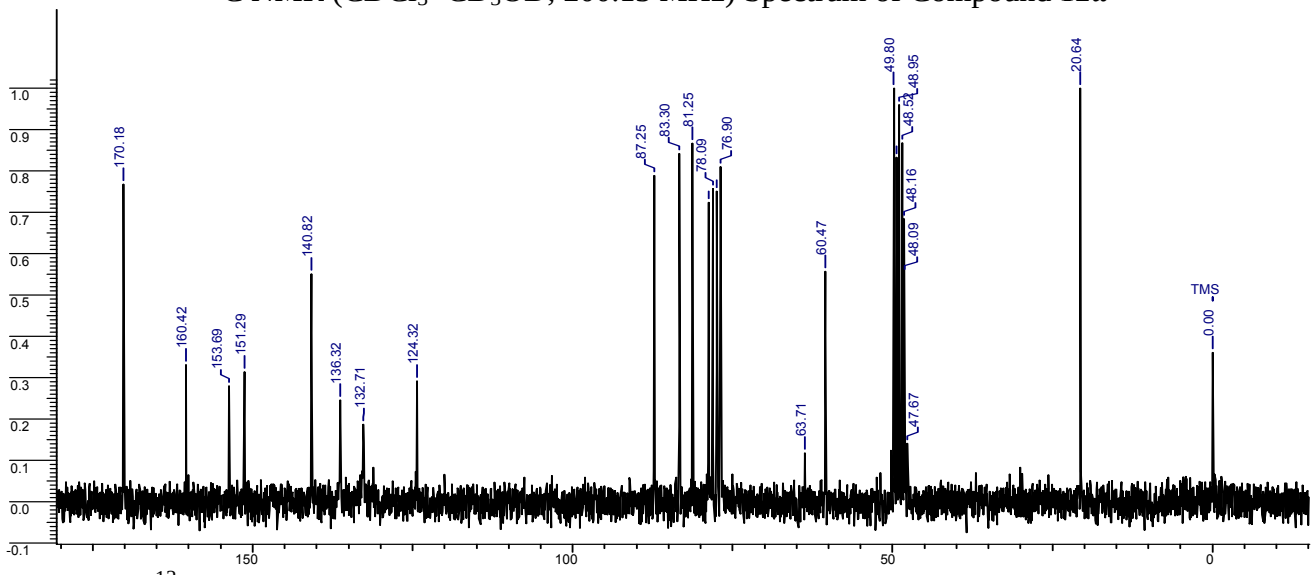
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **11**



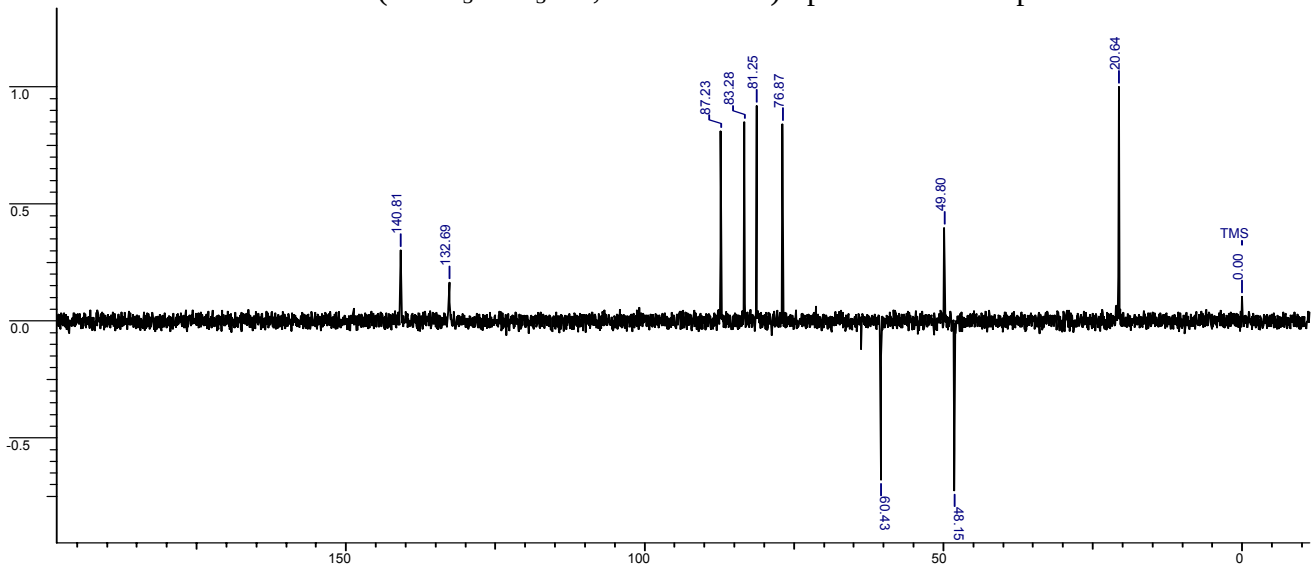
^{1}H NMR ($CDCl_3$+CD_3OD, 200.13 MHz) Spectrum of Compound **12a**



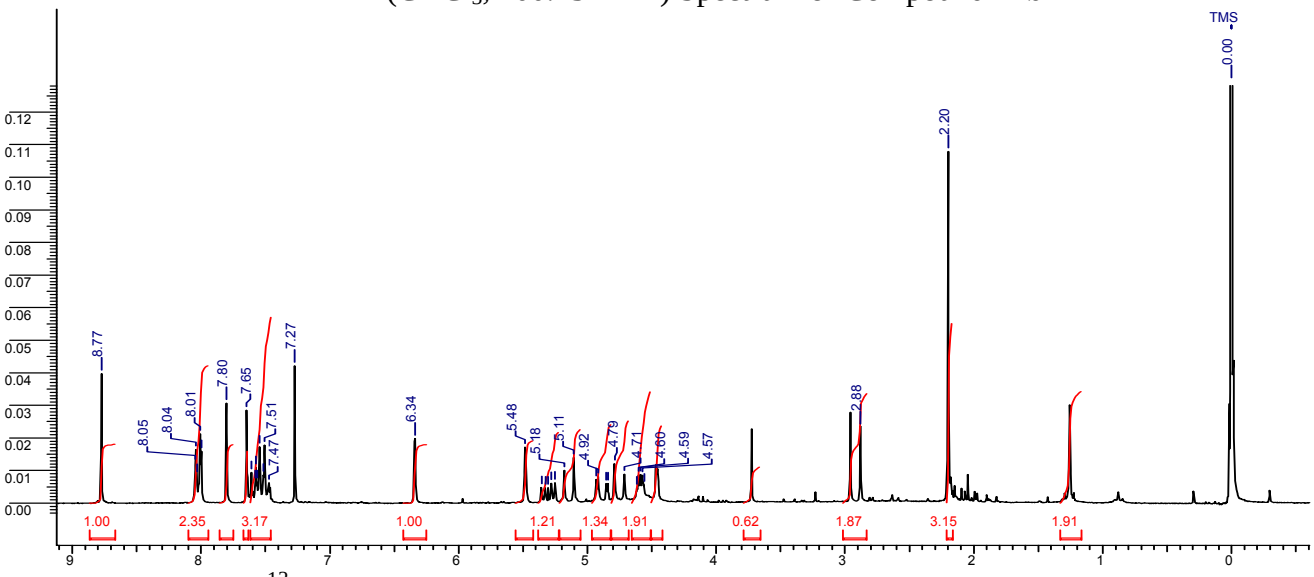
^{13}C NMR ($CDCl_3$+CD_3OD, 200.13 MHz) Spectrum of Compound **12a**



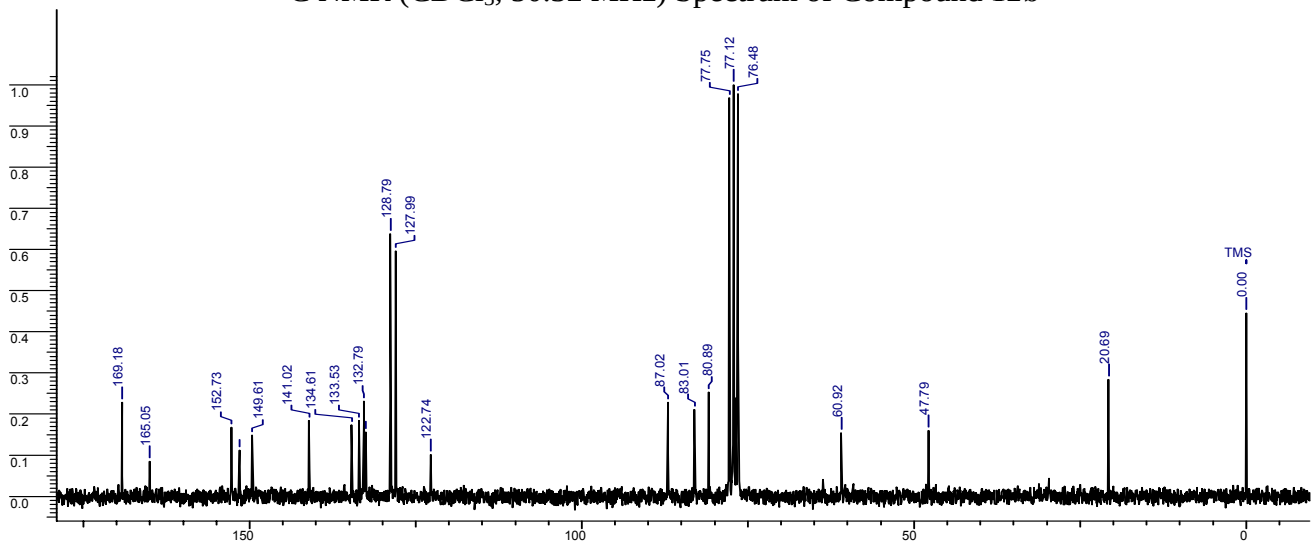
^{13}C-DEPT NMR ($CDCl_3$+CD_3OD, 200.13 MHz) Spectrum of Compound **12a**



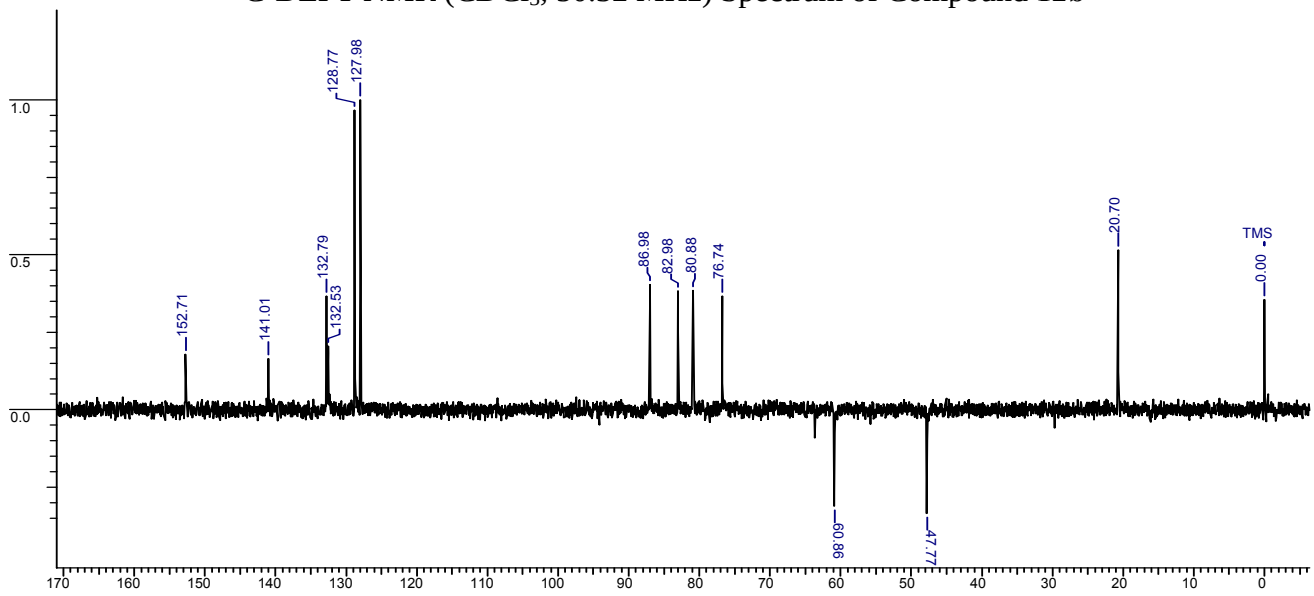
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **12b**



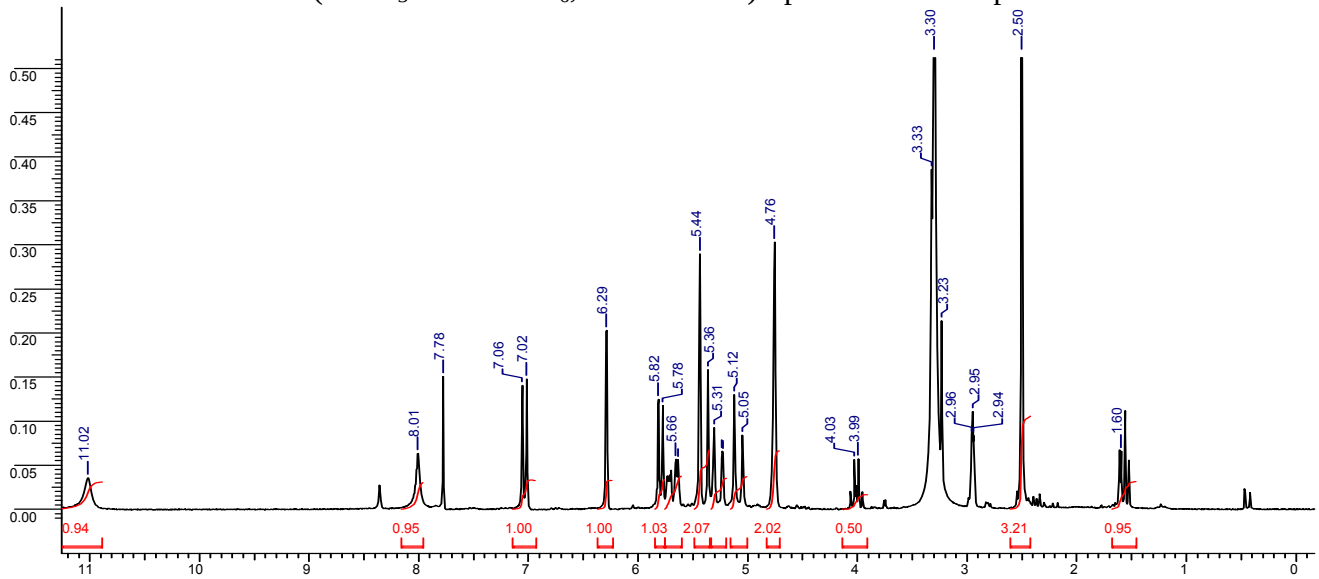
^{13}C NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **12b**



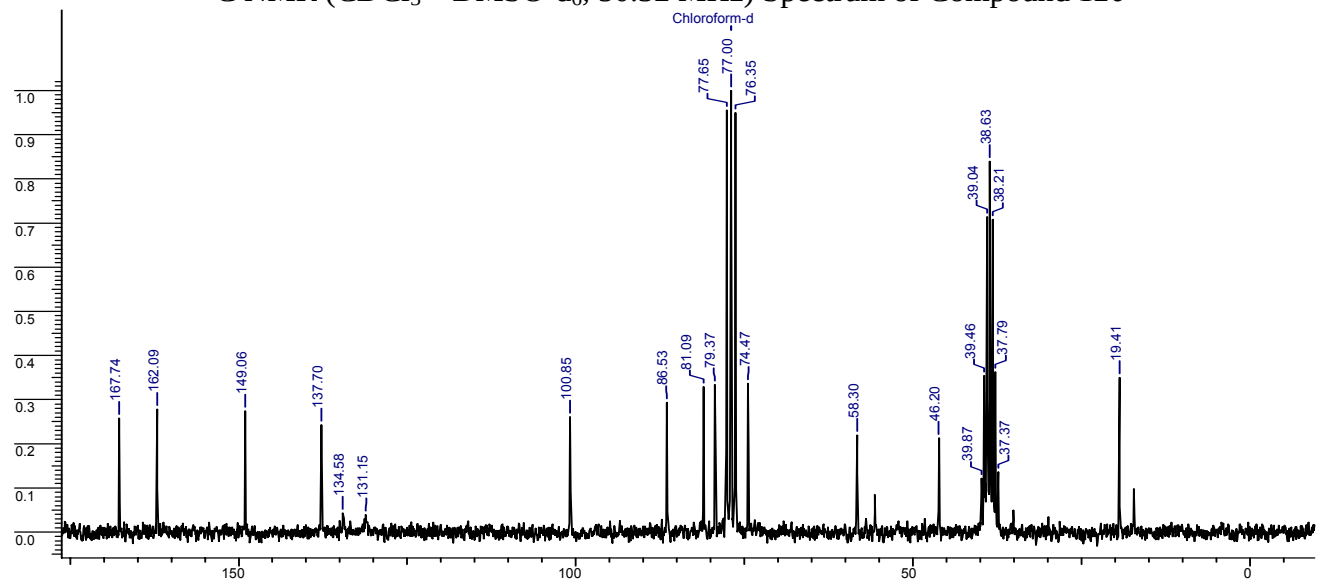
^{13}C-DEPT NMR ($CDCl_3$, 50.32 MHz) Spectrum of Compound **12b**



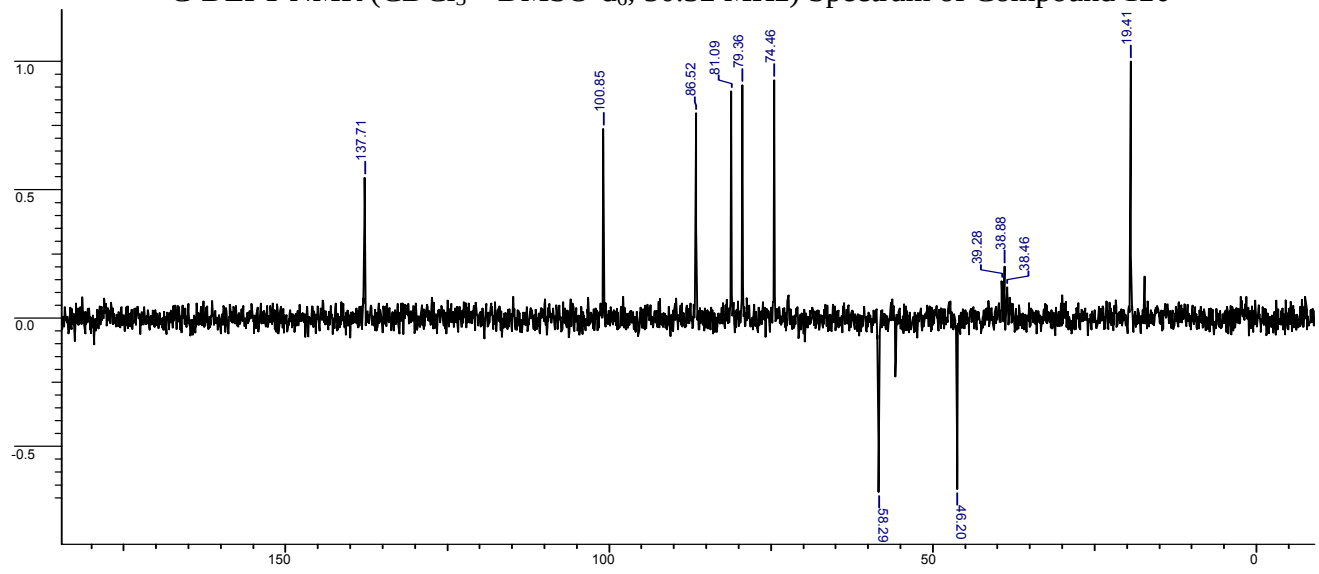
^{1}H NMR ($CDCl_3$ + DMSO-d_6, 200.13 MHz) Spectrum of Compound **12c**



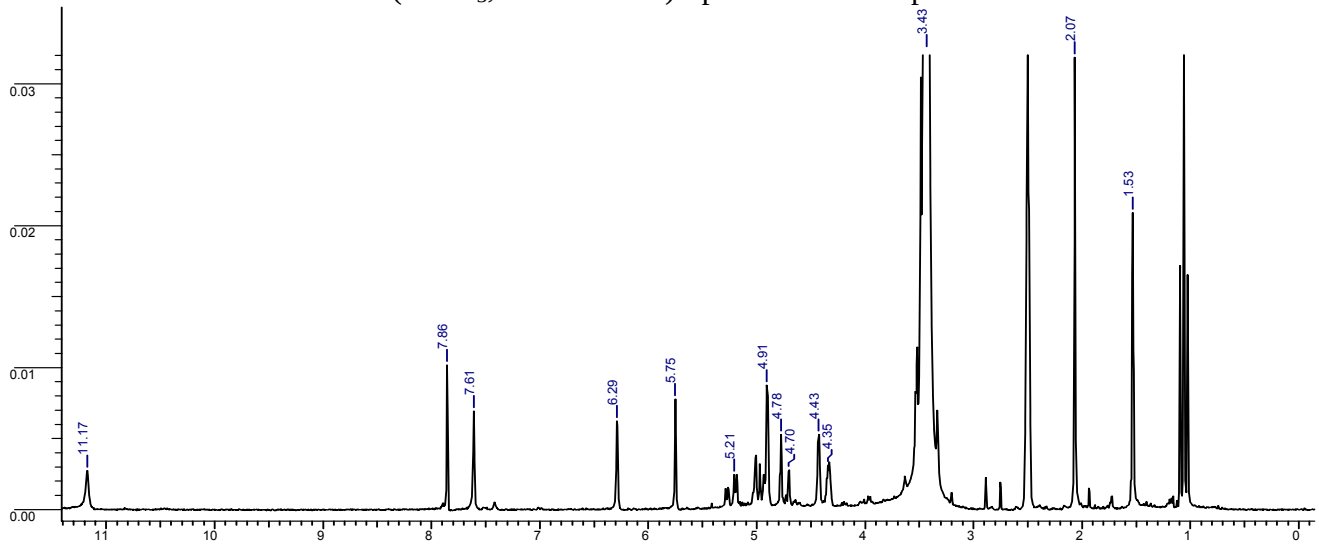
^{13}C NMR ($CDCl_3$ + DMSO-d_6, 50.32 MHz) Spectrum of Compound **12c**



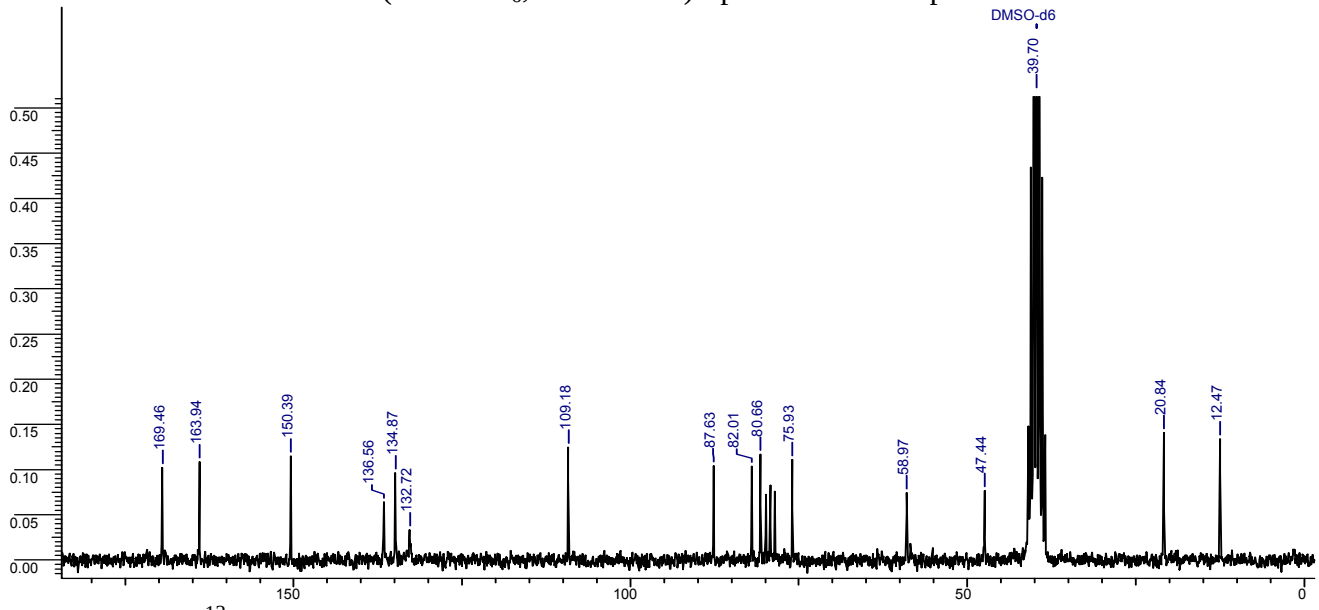
^{13}C-DEPT NMR ($CDCl_3$ + DMSO-d_6, 50.32 MHz) Spectrum of Compound **12c**



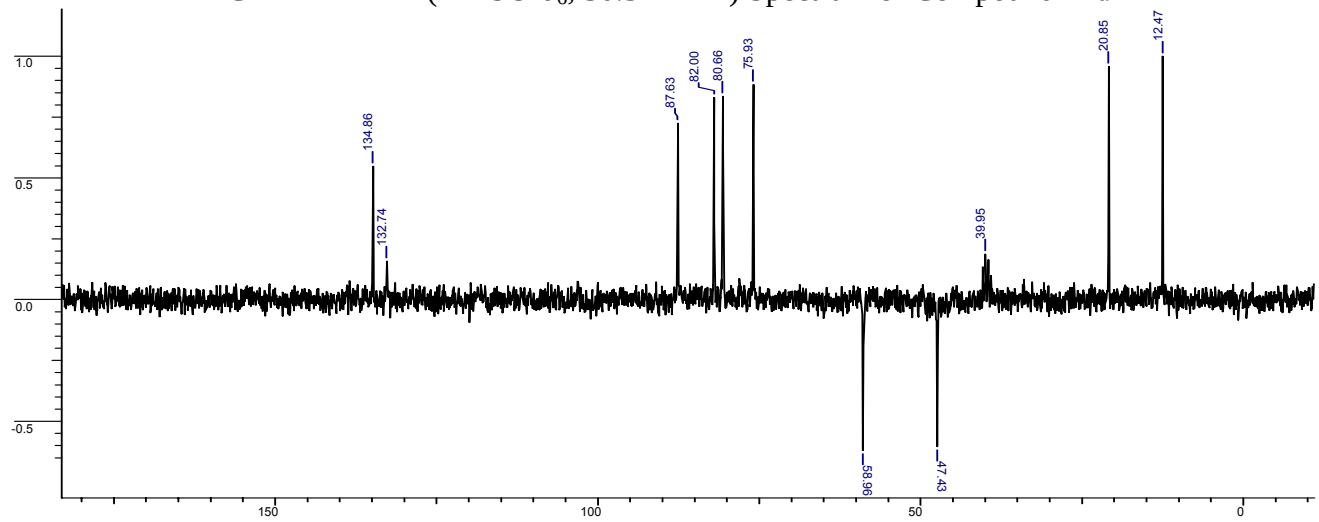
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **12d**



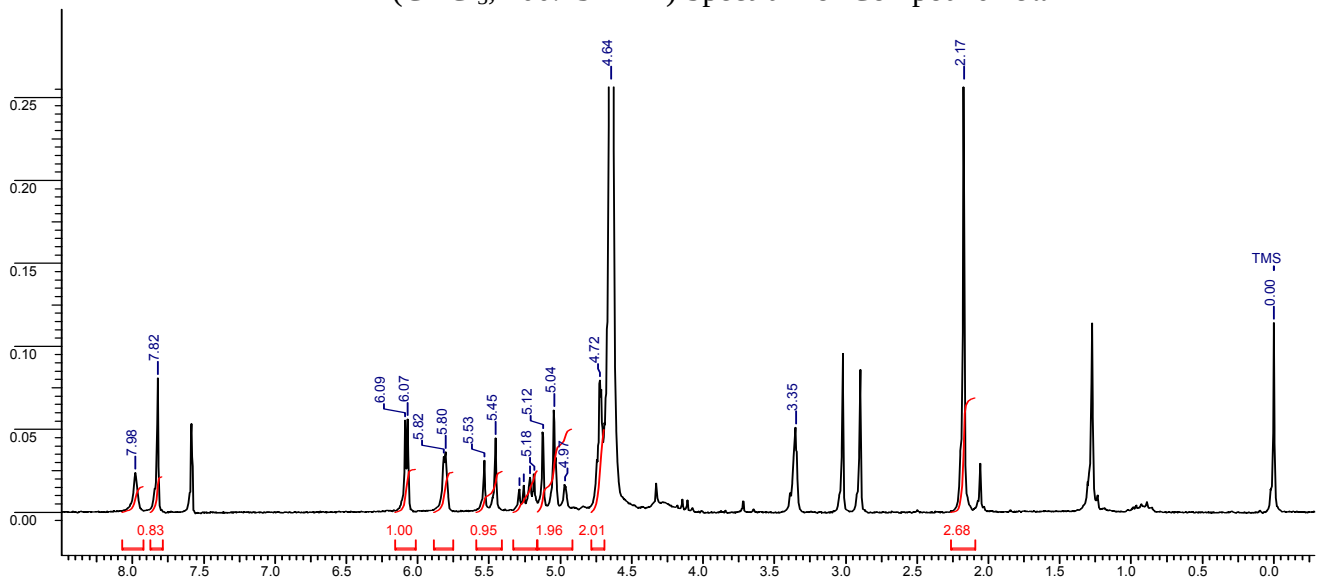
^{13}C NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **12d**



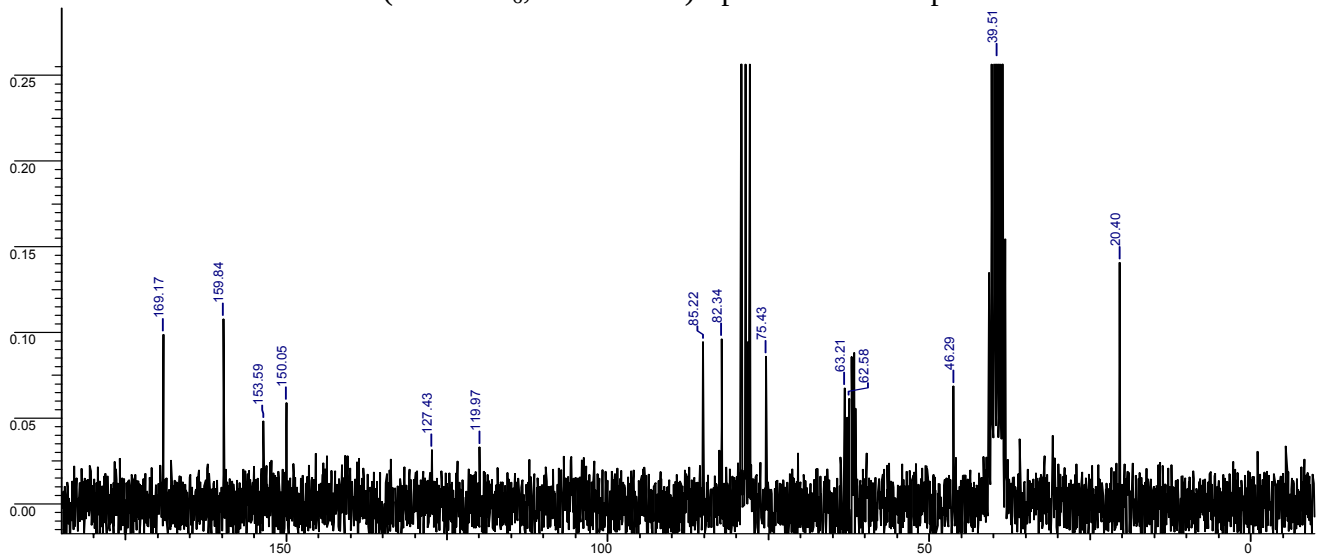
^{13}C-DEPT NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **12d**



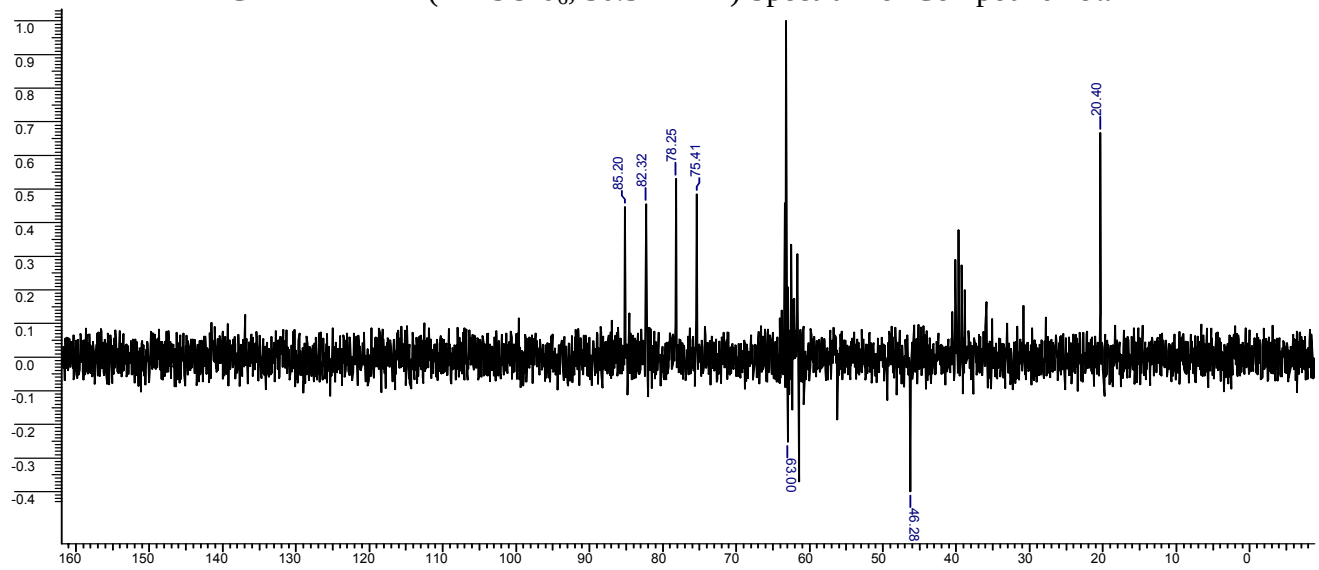
^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **13a**



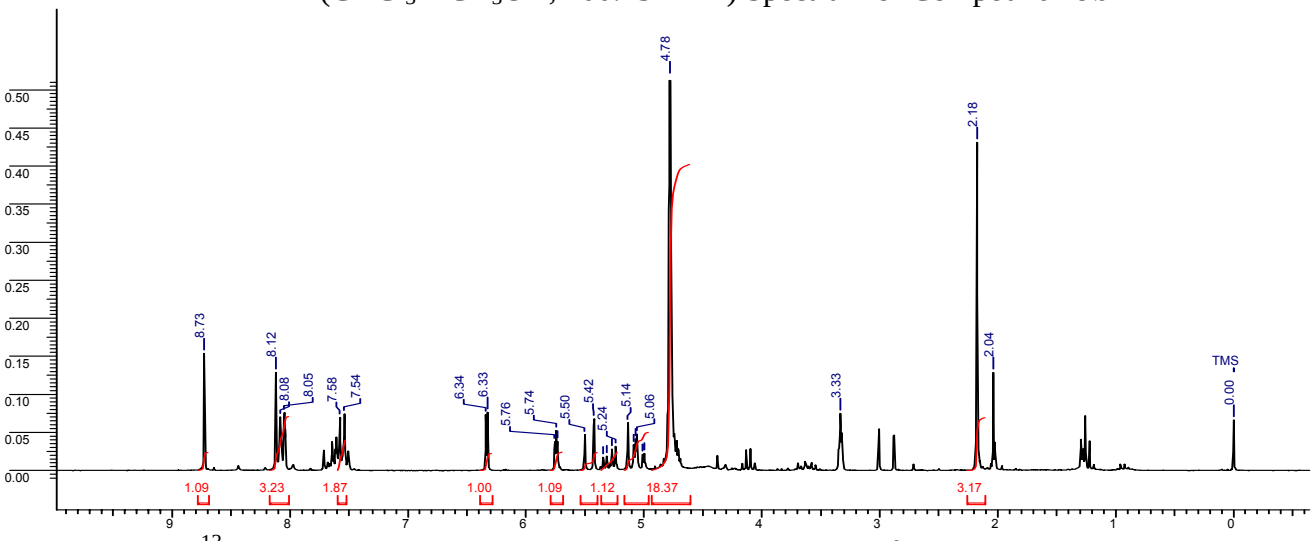
^{13}C NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **13a**



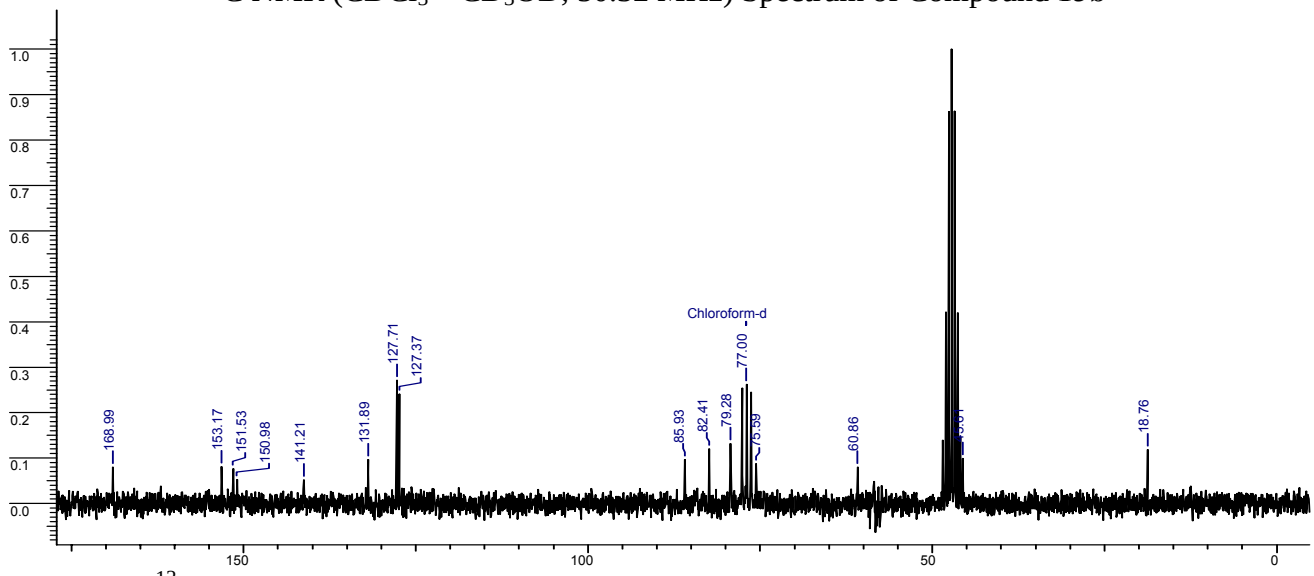
^{13}C-DEPT NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **13a**



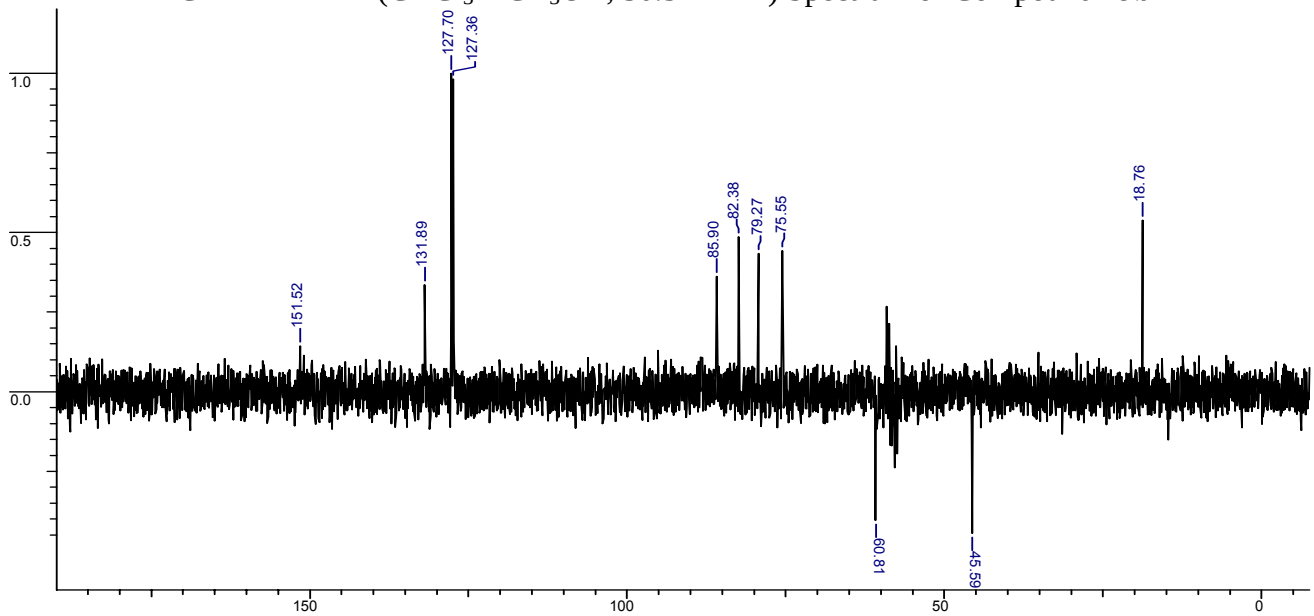
^{1}H NMR ($CDCl_3$ + CD_3OD, 200.13 MHz) Spectrum of Compound **13b**



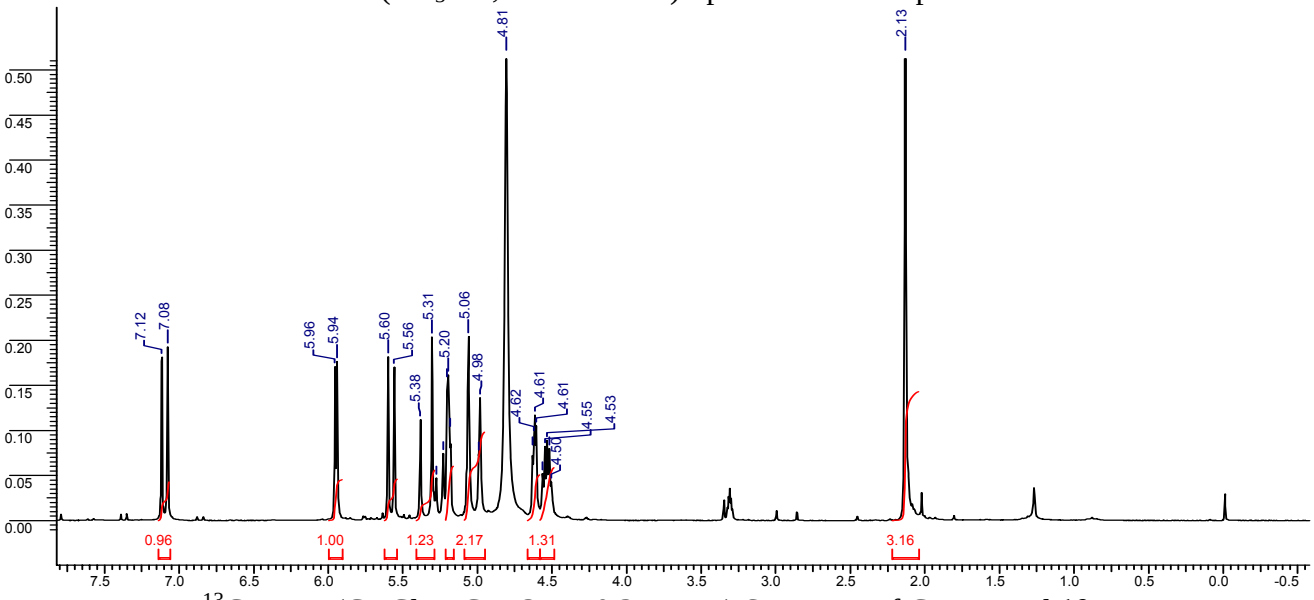
^{13}C NMR ($CDCl_3$ + CD_3OD, 50.32 MHz) Spectrum of Compound **13b**



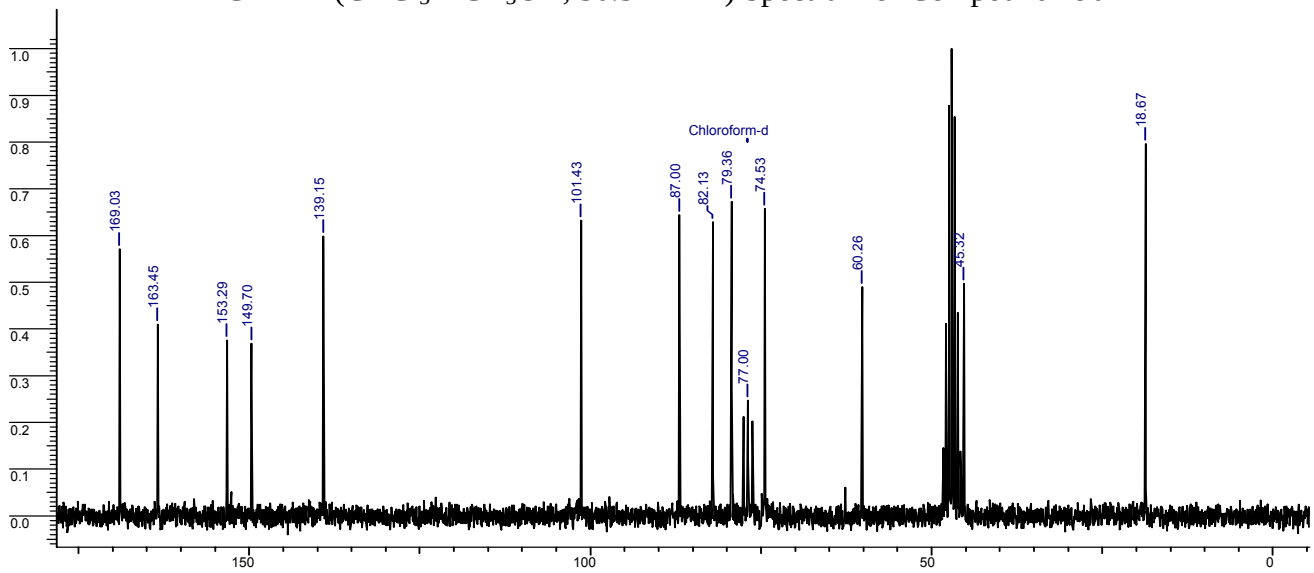
^{13}C-DEPT NMR ($CDCl_3$ + CD_3OD, 50.32 MHz) Spectrum of Compound **13b**



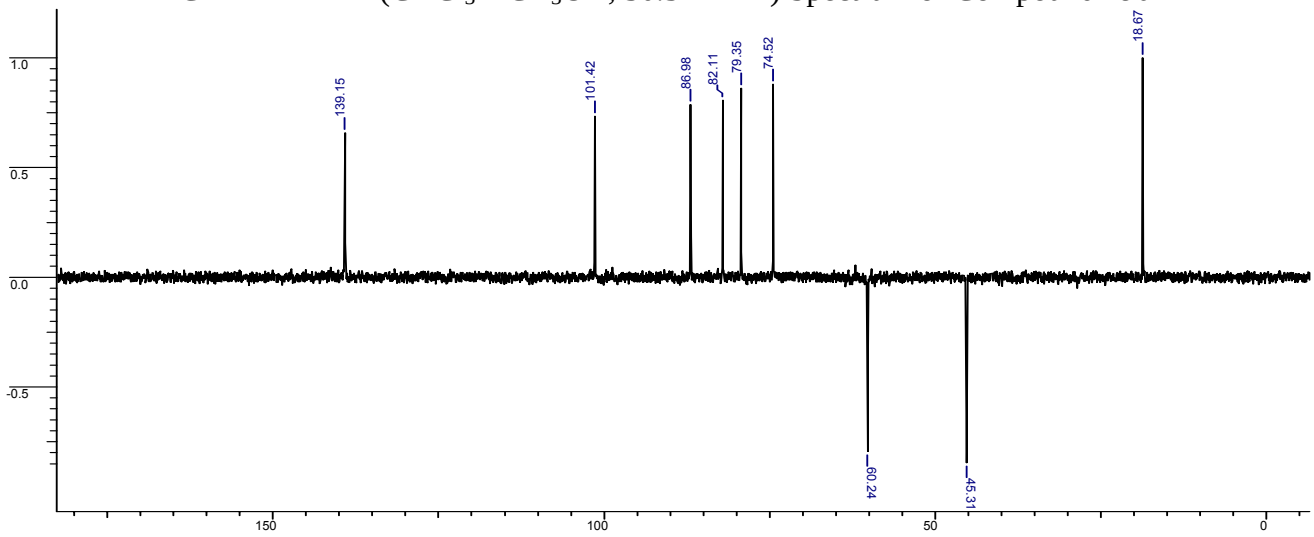
^{1}H NMR (CD_3OD, 200.13 MHz) Spectrum of Compound **13c**



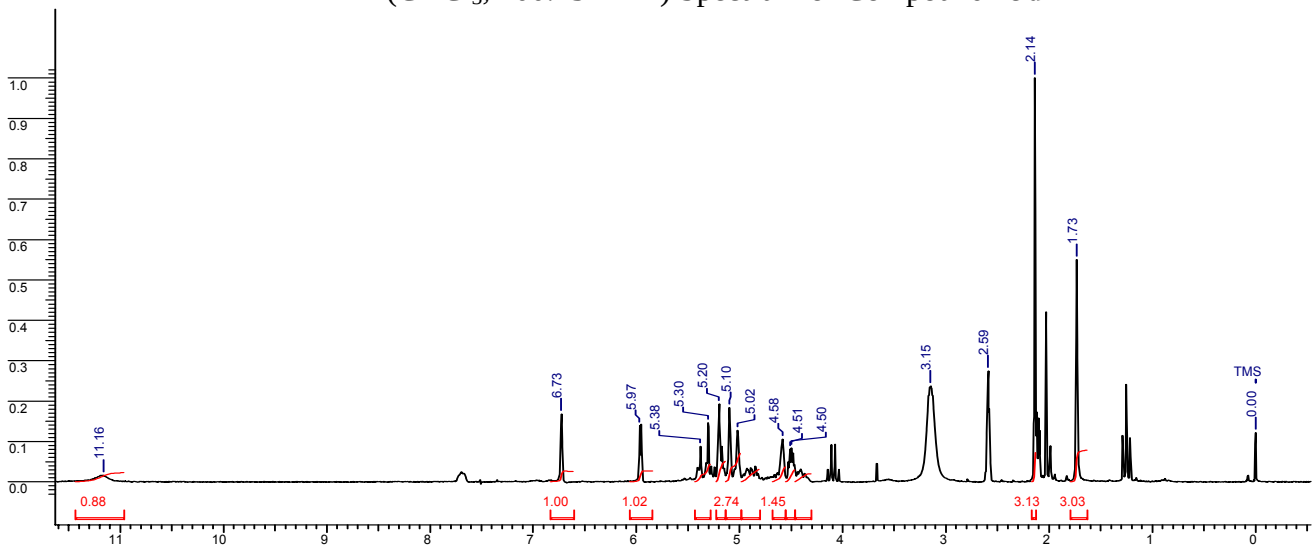
^{13}C NMR ($CDCl_3$ + CD_3OD, 50.32 MHz) Spectrum of Compound **13c**



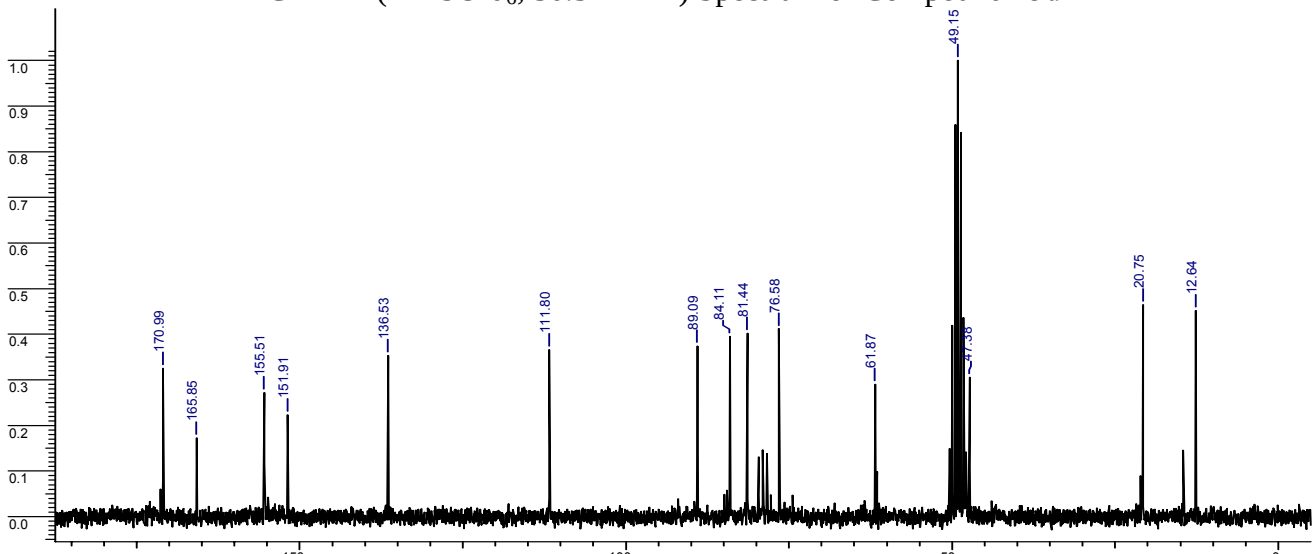
^{13}C-DEPT NMR ($CDCl_3$ + CD_3OD, 50.32 MHz) Spectrum of Compound **13c**



^{1}H NMR ($CDCl_3$, 200.13 MHz) Spectrum of Compound **13d**



^{13}C NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **13d**



^{13}C-DEPT NMR (DMSO-d_6, 50.32 MHz) Spectrum of Compound **13d**