

Supporting Information

Synthesis and Oligomerization of Fmoc/Boc-Protected PNA Monomers of 2,6-Diaminopurine, 2-Aminopurine and Thymine

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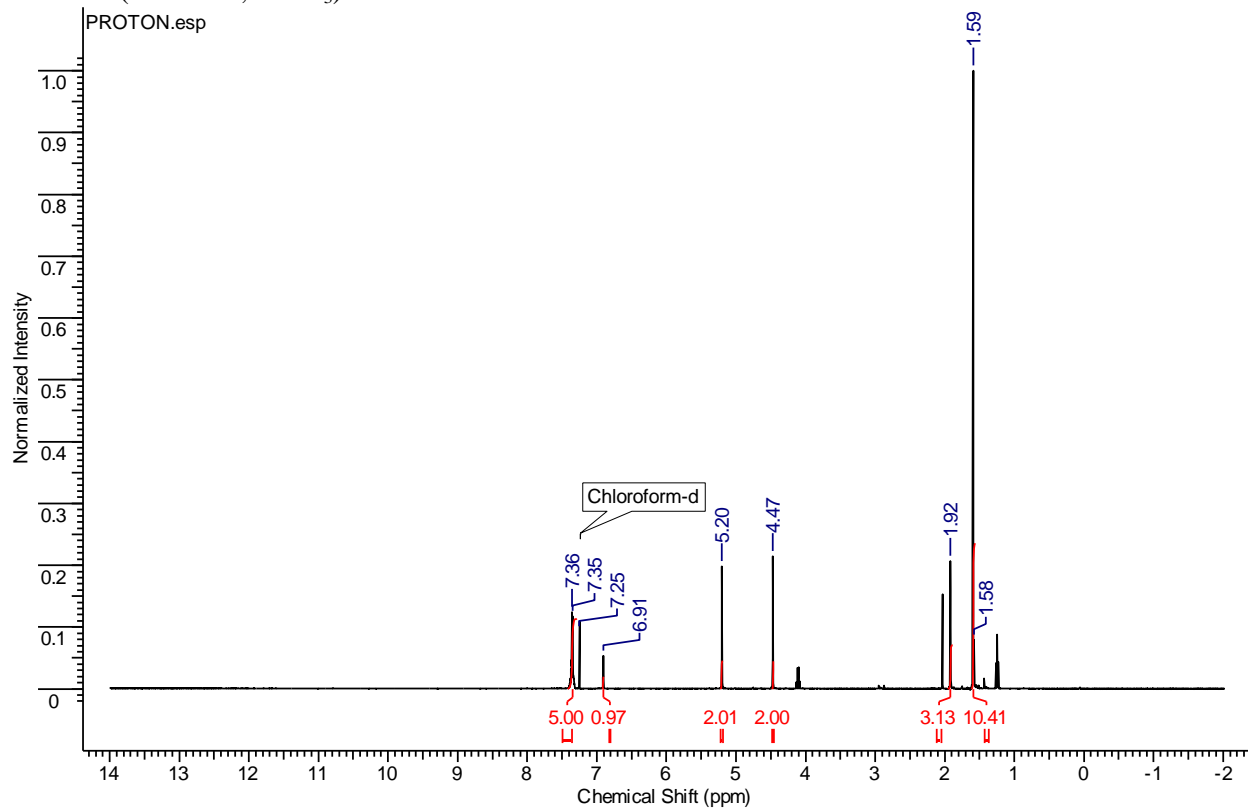
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General Remarks. All chemicals were obtained from commercial sources and were of ACS reagent grade or higher and were used without further purification. Solvents for solution-phase chemistry were dried by passing through activated alumina columns. Flash column chromatography (FCC) was performed on Merck Kieselgel 60, 230-400 mesh. Thin layer chromatography (TLC) was performed on Merck Kieselgel 60 TLC plates. Chemical shifts are reported in parts per million (δ), were measured from Tetramethylsilane (0 ppm) and are referenced to the solvent CDCl_3 (7.26 ppm), $\text{DMSO-}d_6$ (2.49 ppm), D_2O (4.79 ppm) for ^1H NMR and CDCl_3 (77.0 ppm), $\text{DMSO-}d_6$ (39.5 ppm) for ^{13}C NMR. Multiplicities are described as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br s (broad singlet). Coupling constants (J) are reported in Hertz (Hz). Resonances due to restricted rotation around the amide bond (rotamers) are reported as major (ma.) and minor (mi.). High resolution mass spectra (HRMS) were obtained using electron impact (EI) or electrospray ionization (ESI).

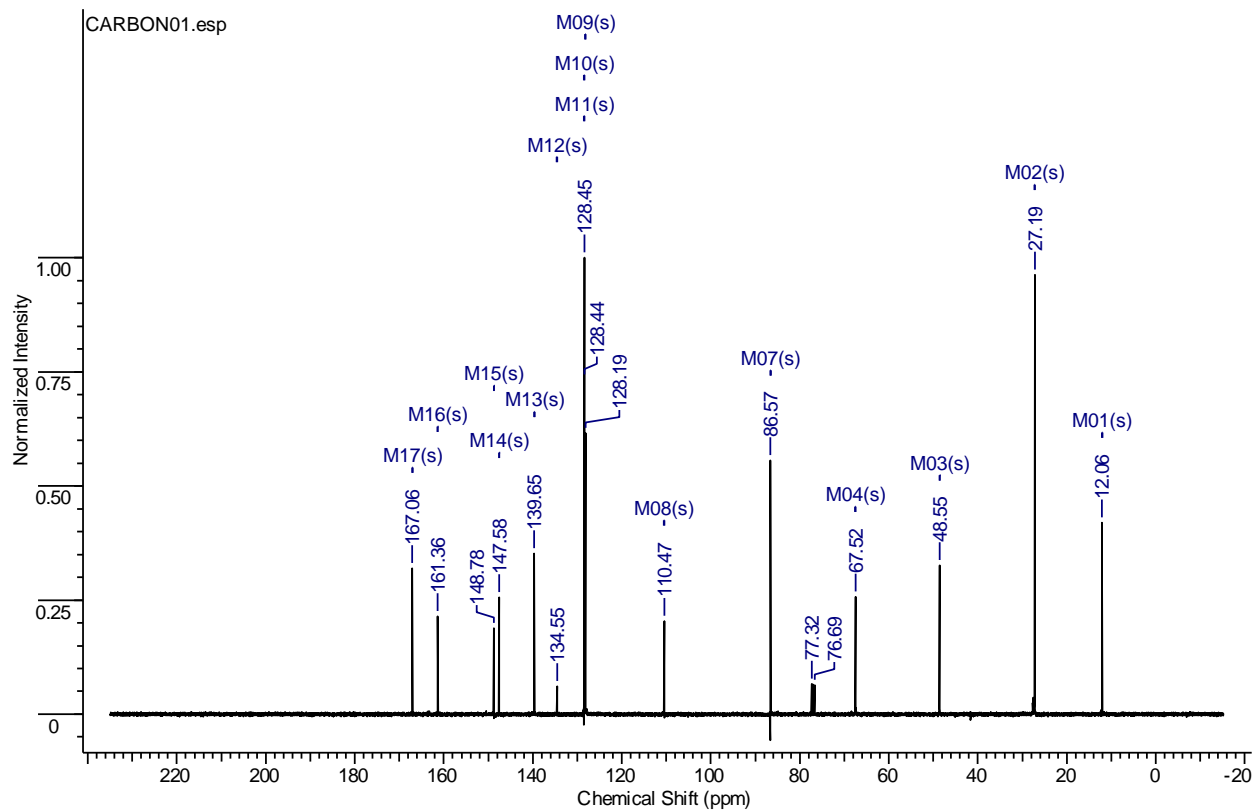
PNA1. HRMS (ESI) calculated for $\text{C}_{155}\text{H}_{204}\text{N}_{74}\text{O}_{47}$: $[\text{M} + 3\text{H}^+]$ 1285.5361, Found 1285.8582; $[\text{M} + 4\text{H}^+]$ 964.404, Found 964.6530.

PNA2. HRMS (ESI) calculated for $\text{C}_{125}\text{H}_{161}\text{N}_{67}\text{O}_{35}$: $[\text{M} + 3\text{H}^+]$ 1054.4371, Found 1054.7417; $[\text{M} + 4\text{H}^+]$ 791.0798, Found 791.3110.

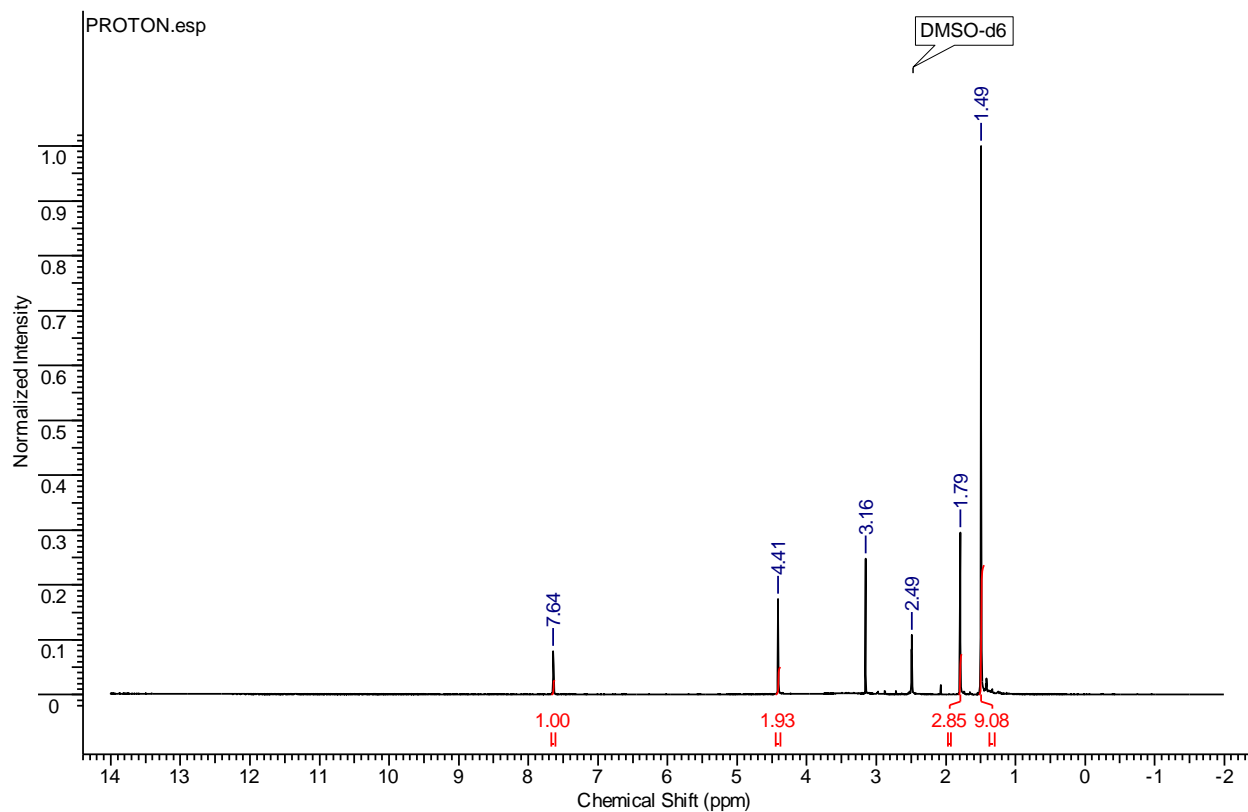
^1H NMR (400 MHz, CDCl_3) of **1**



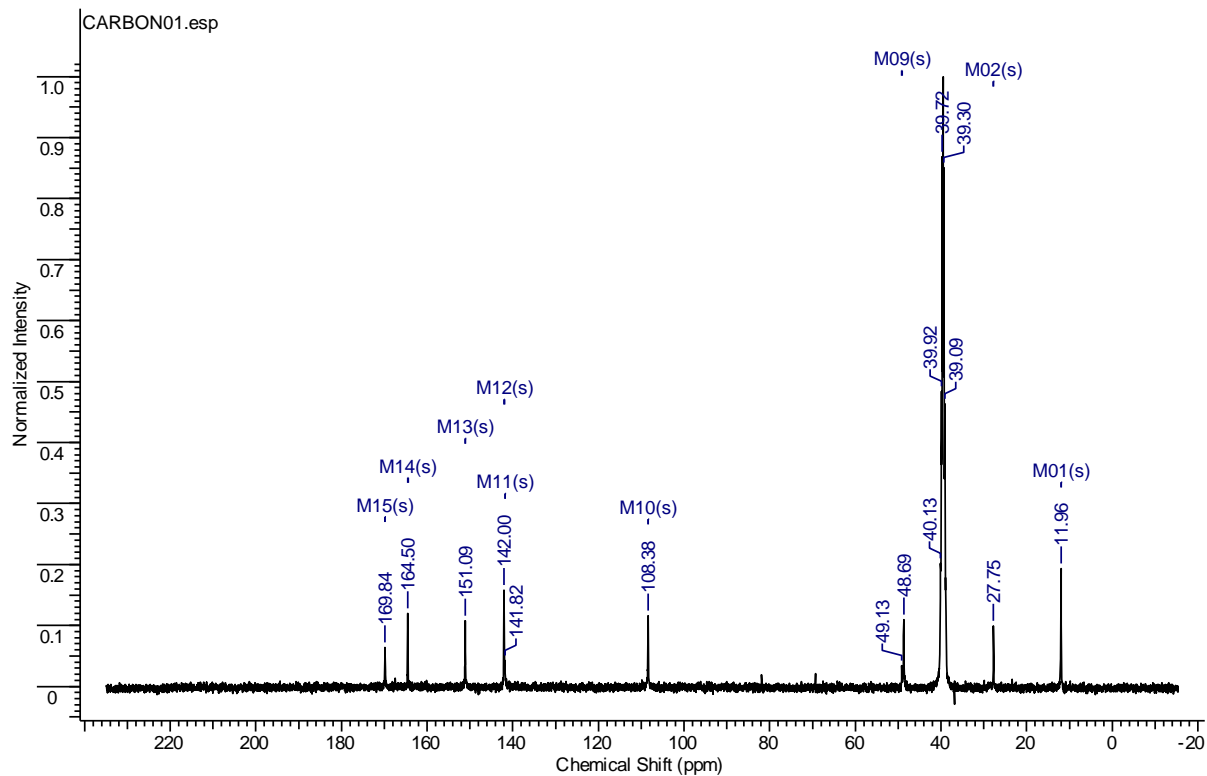
^{13}C NMR (101 MHz, CDCl_3) of **1**



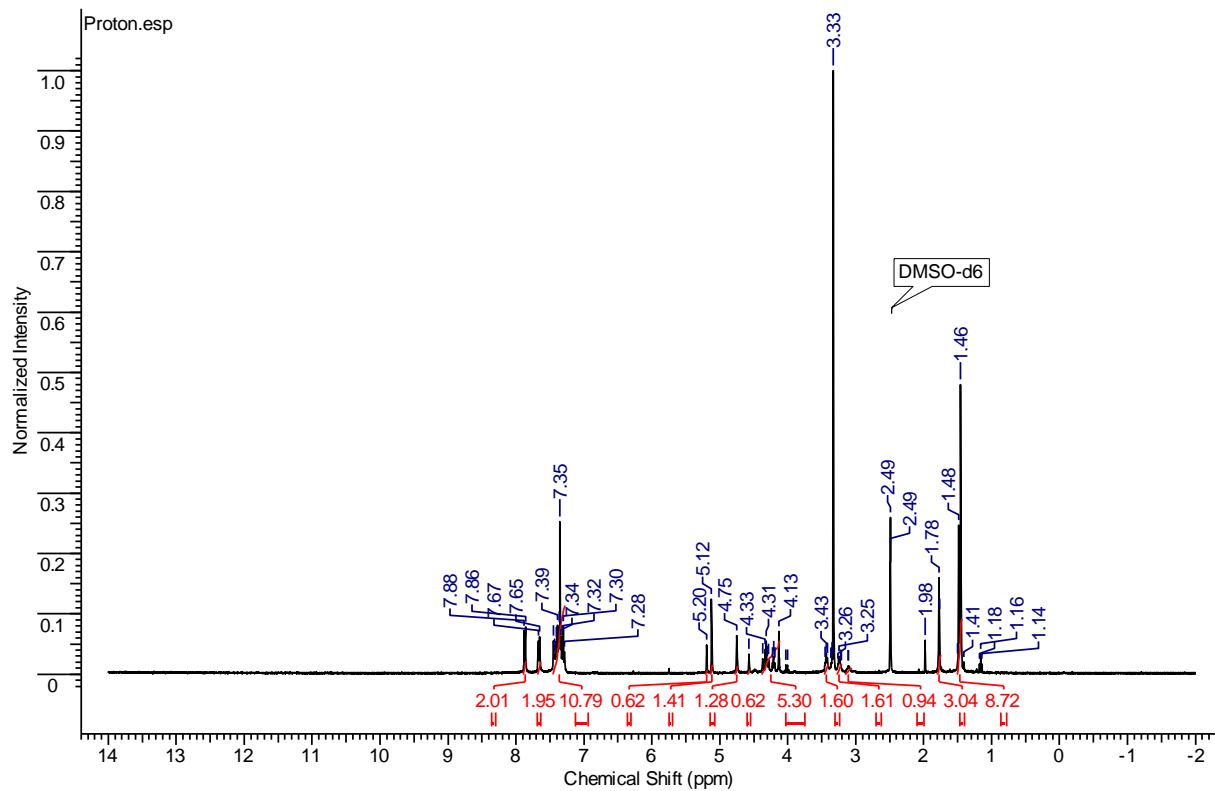
^1H NMR (400 MHz, DMSO- d_6) of **2**



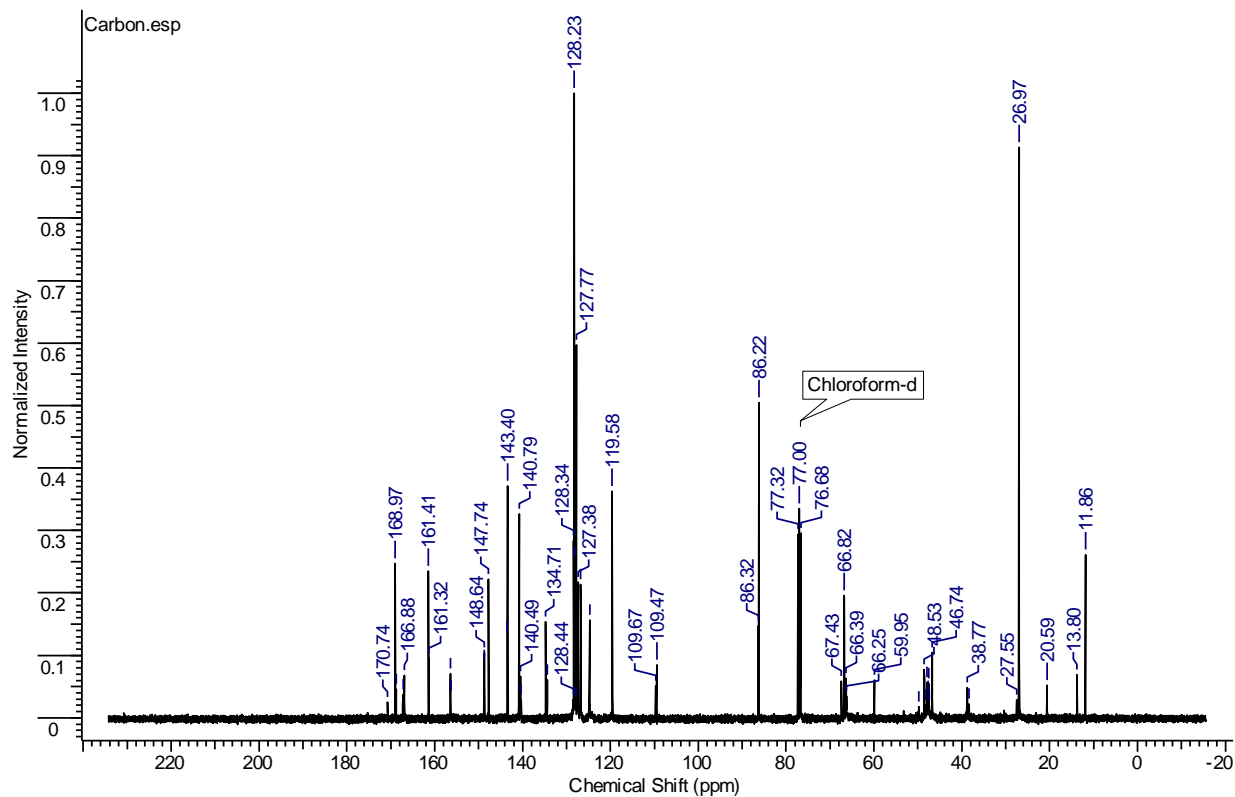
^{13}C NMR (101 MHz, DMSO- d_6) of **2**



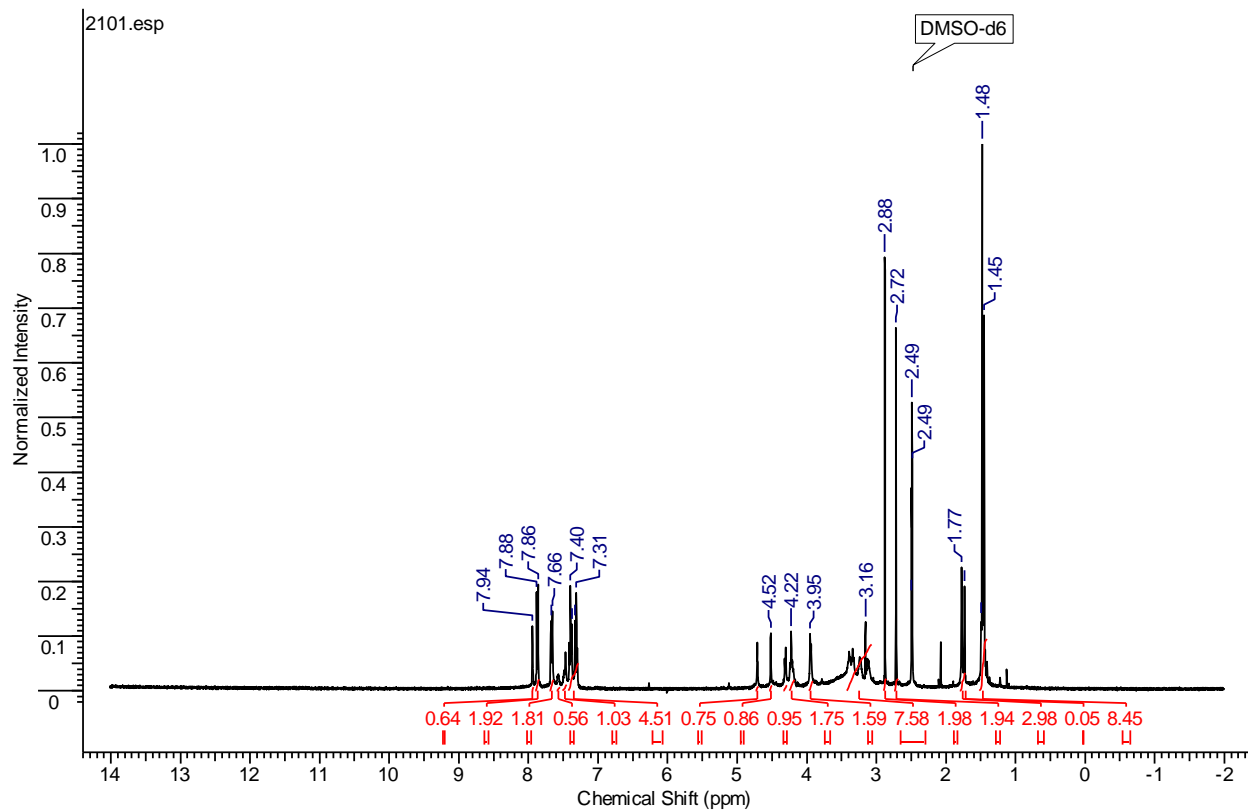
^1H NMR (400 MHz, DMSO-*d*₆) of **3**



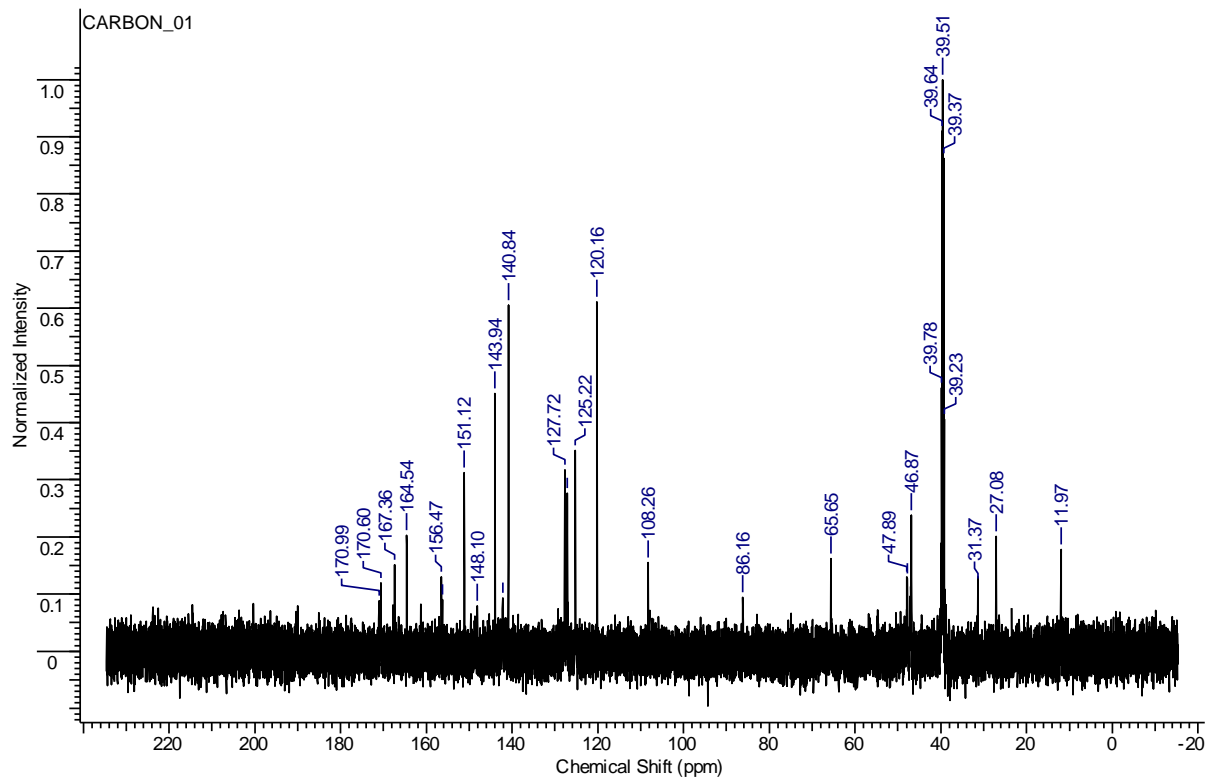
^{13}C NMR (101 MHz, CDCl₃) of **3**



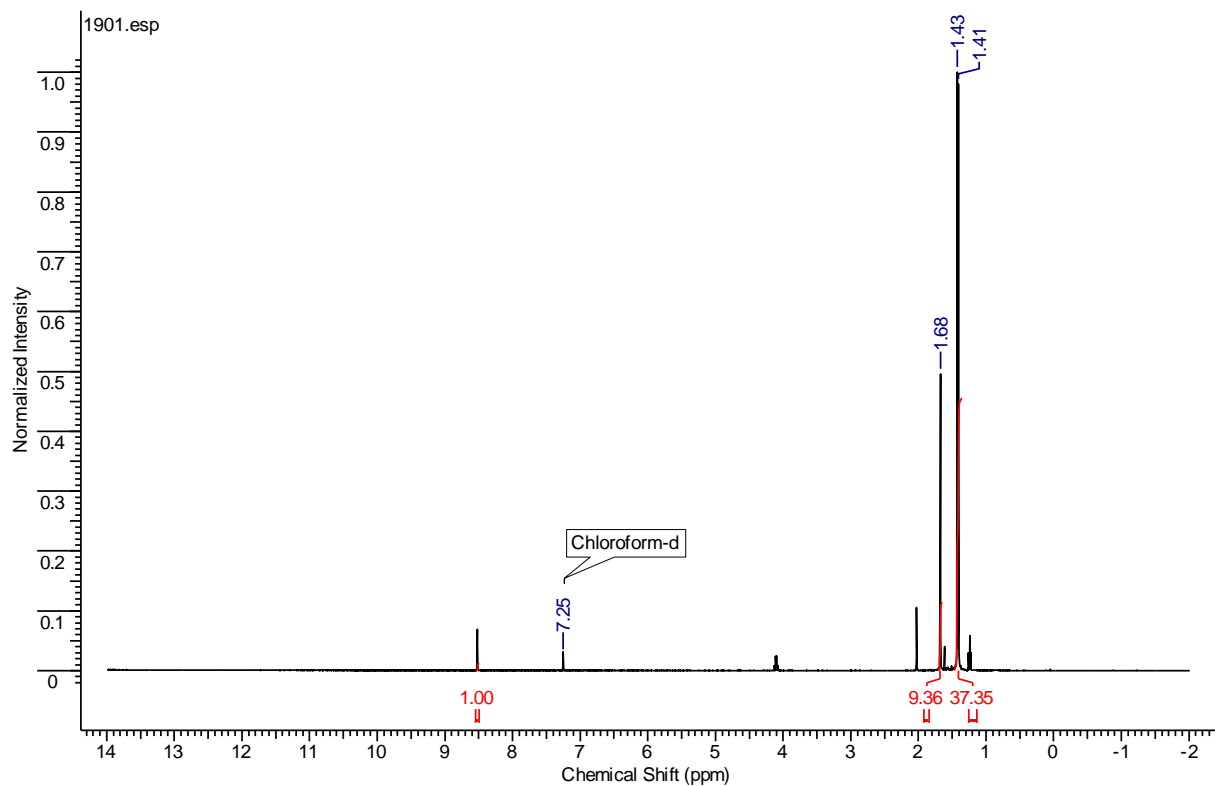
^1H NMR (400 MHz, DMSO-*d*₆) of **4**



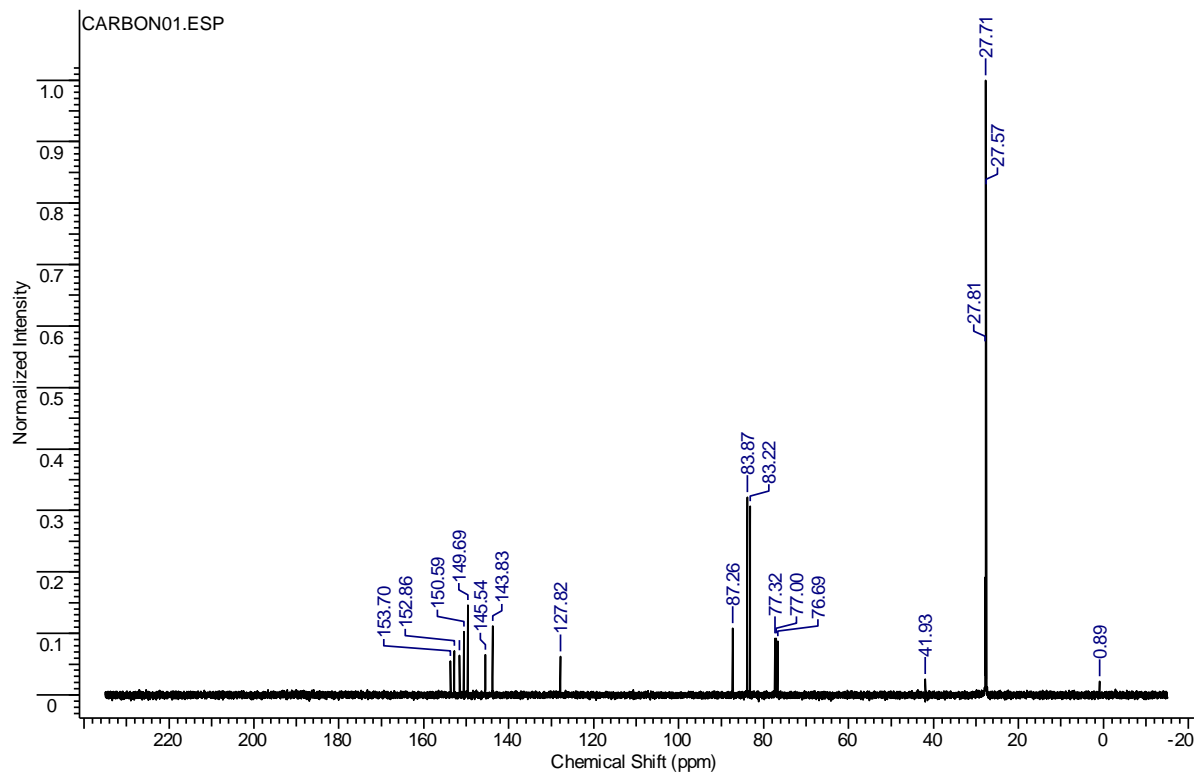
^{13}C NMR (151 MHz, CDCl₃) of **4**



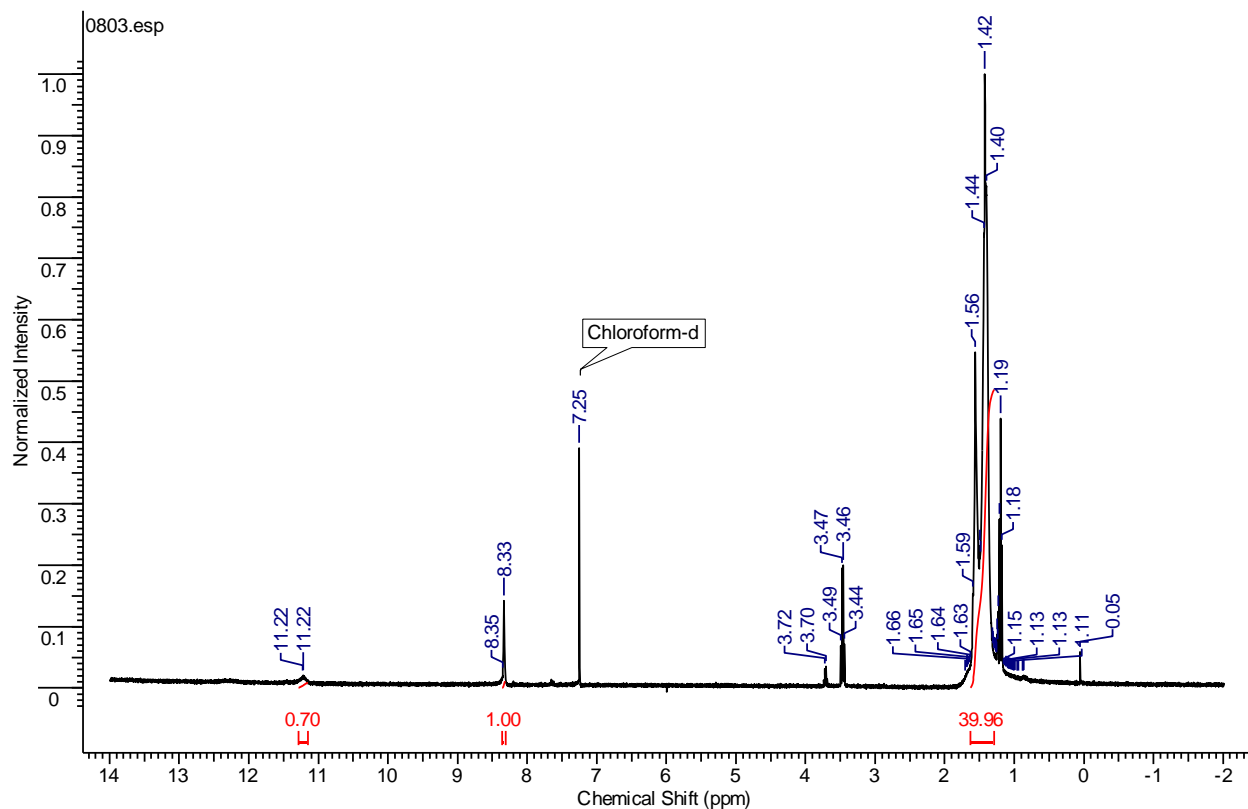
^1H NMR (400 MHz, CDCl_3) of **5**



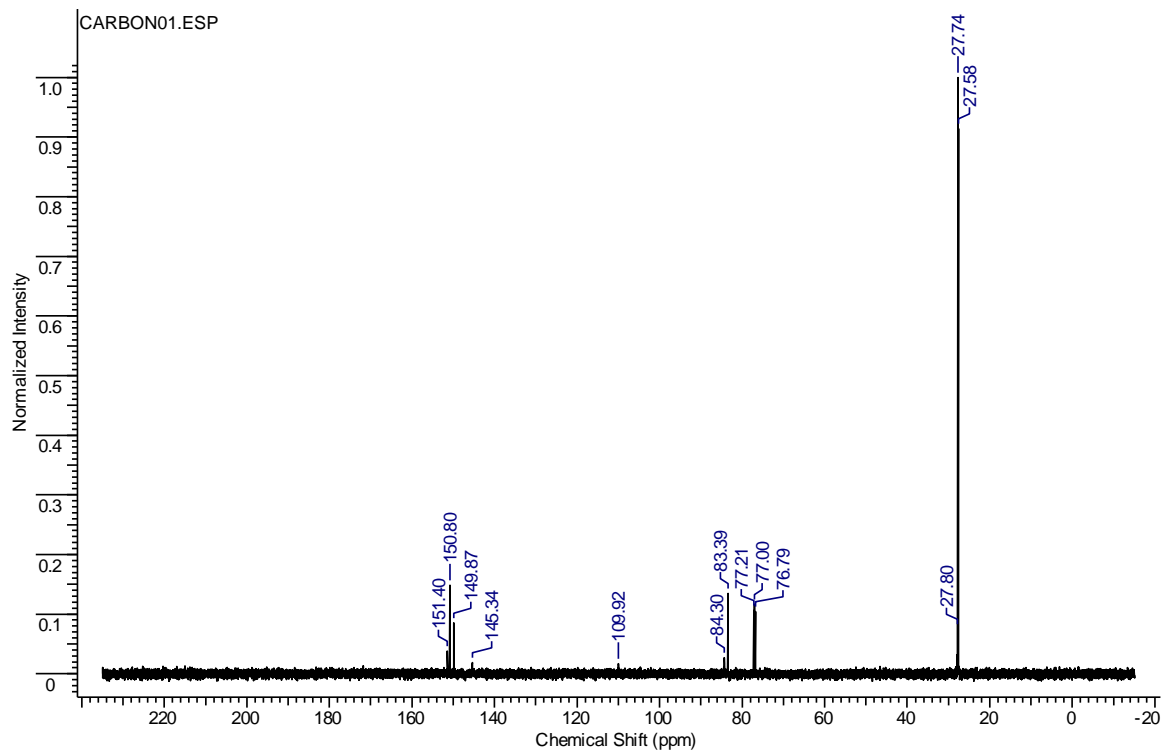
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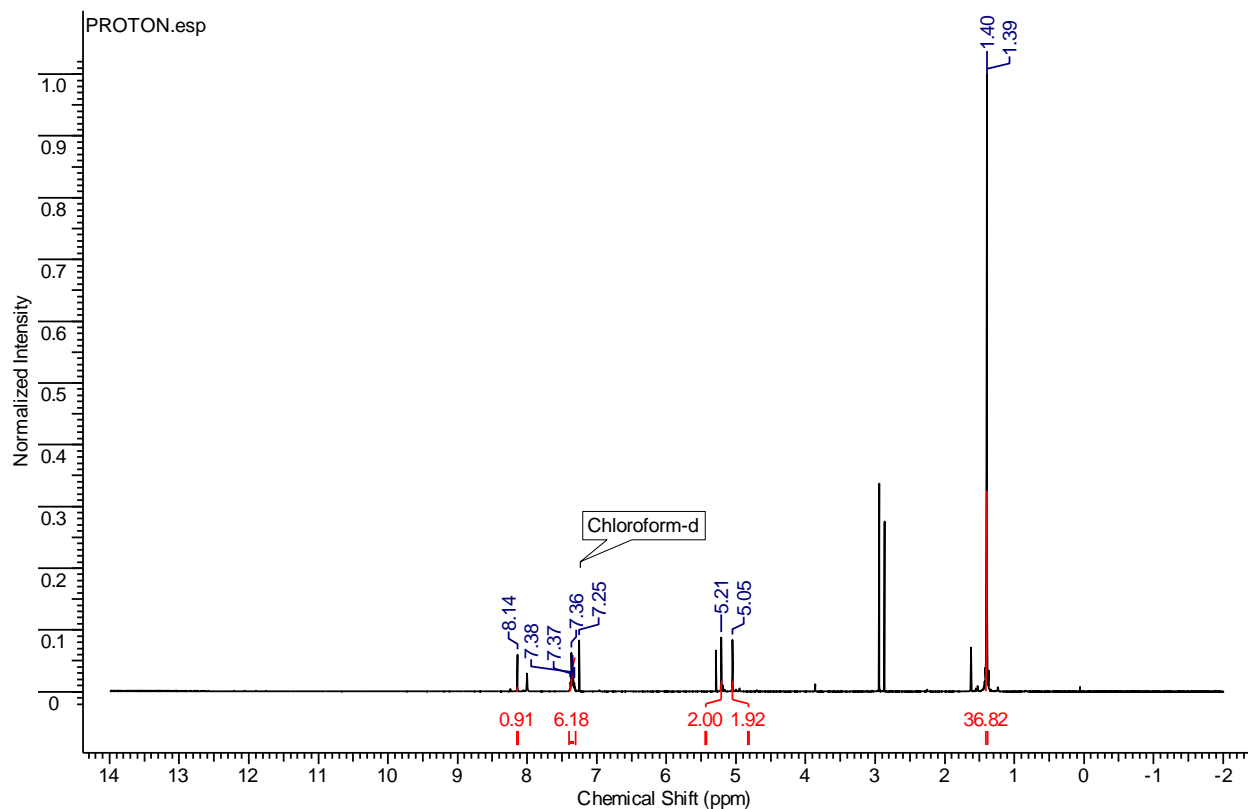
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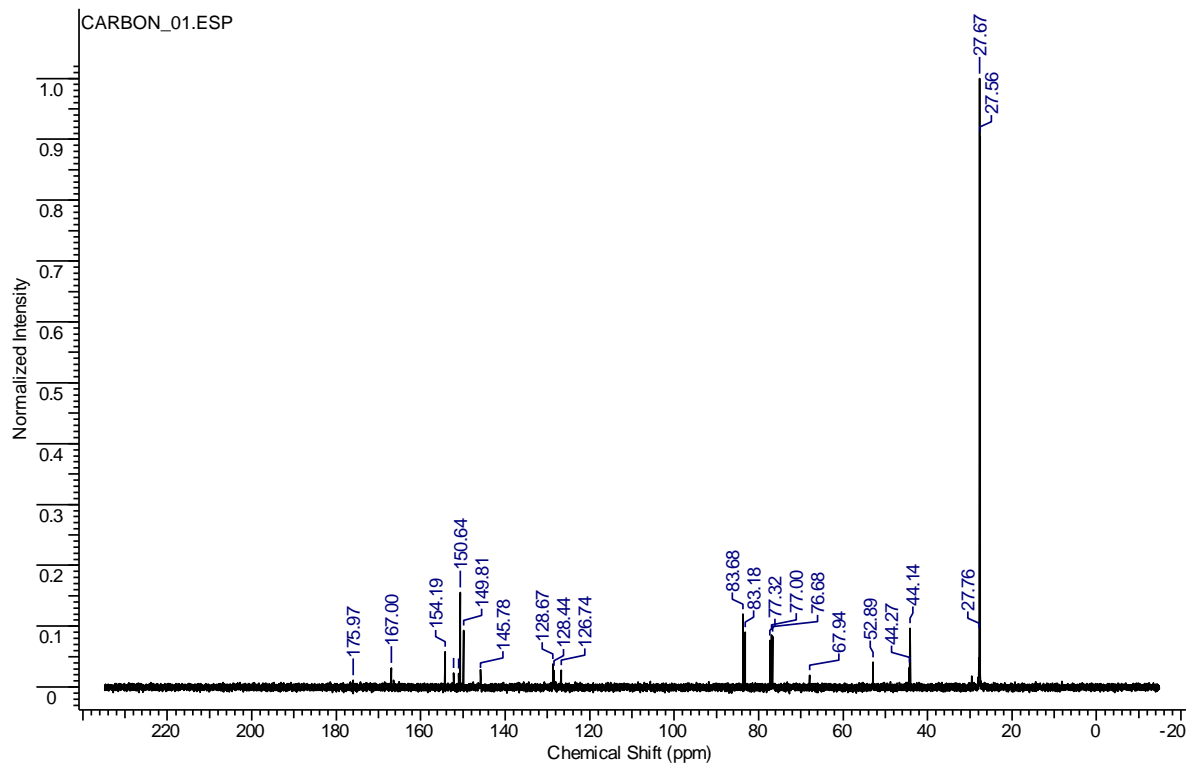
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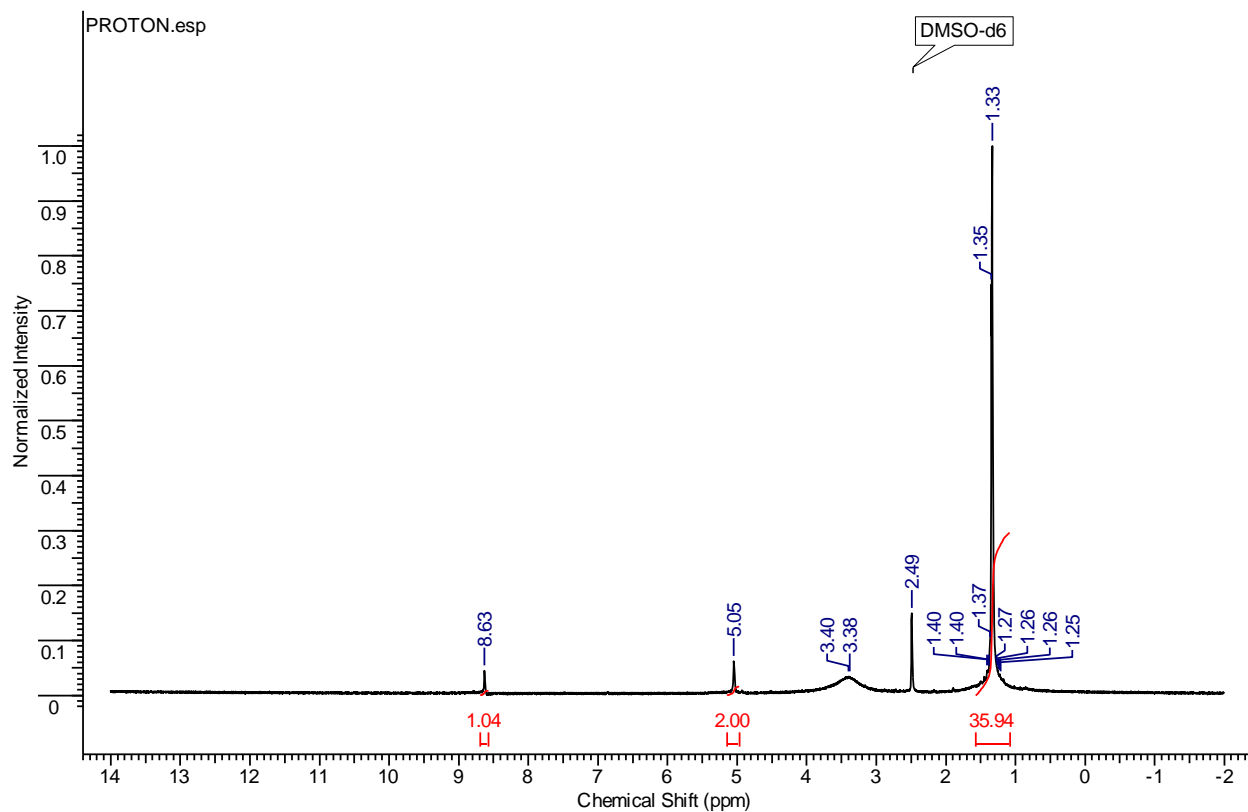
^1H NMR (400 MHz, DMSO-*d*₆) of **7**



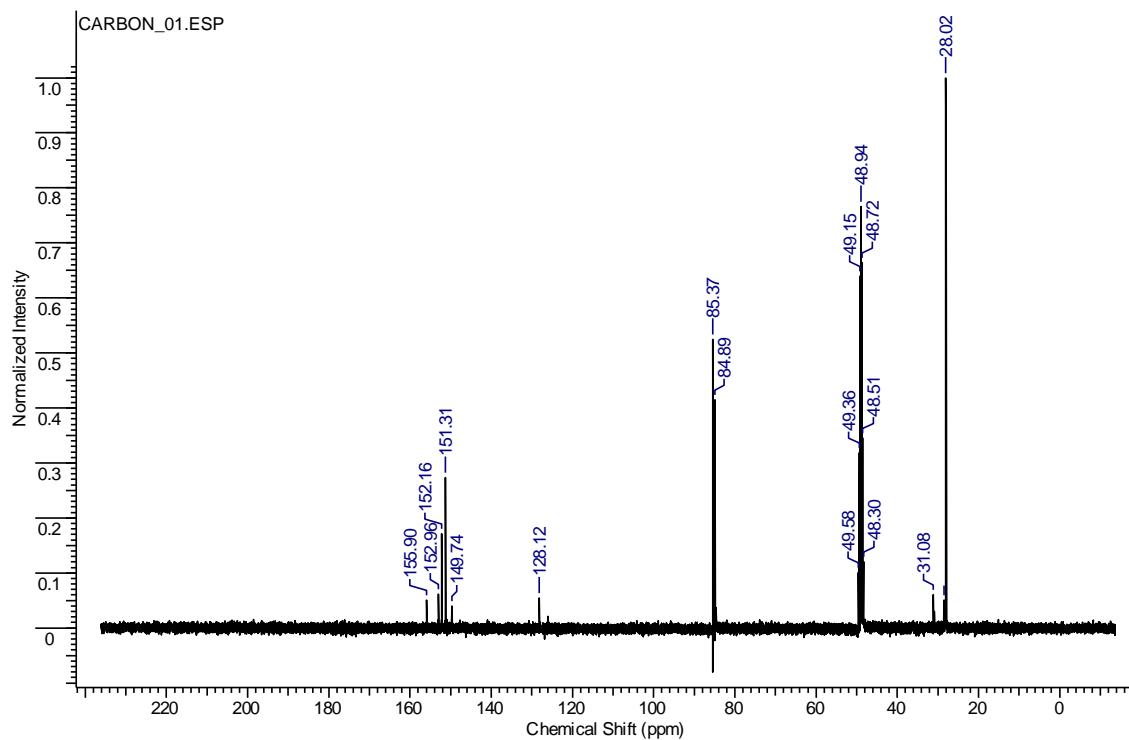
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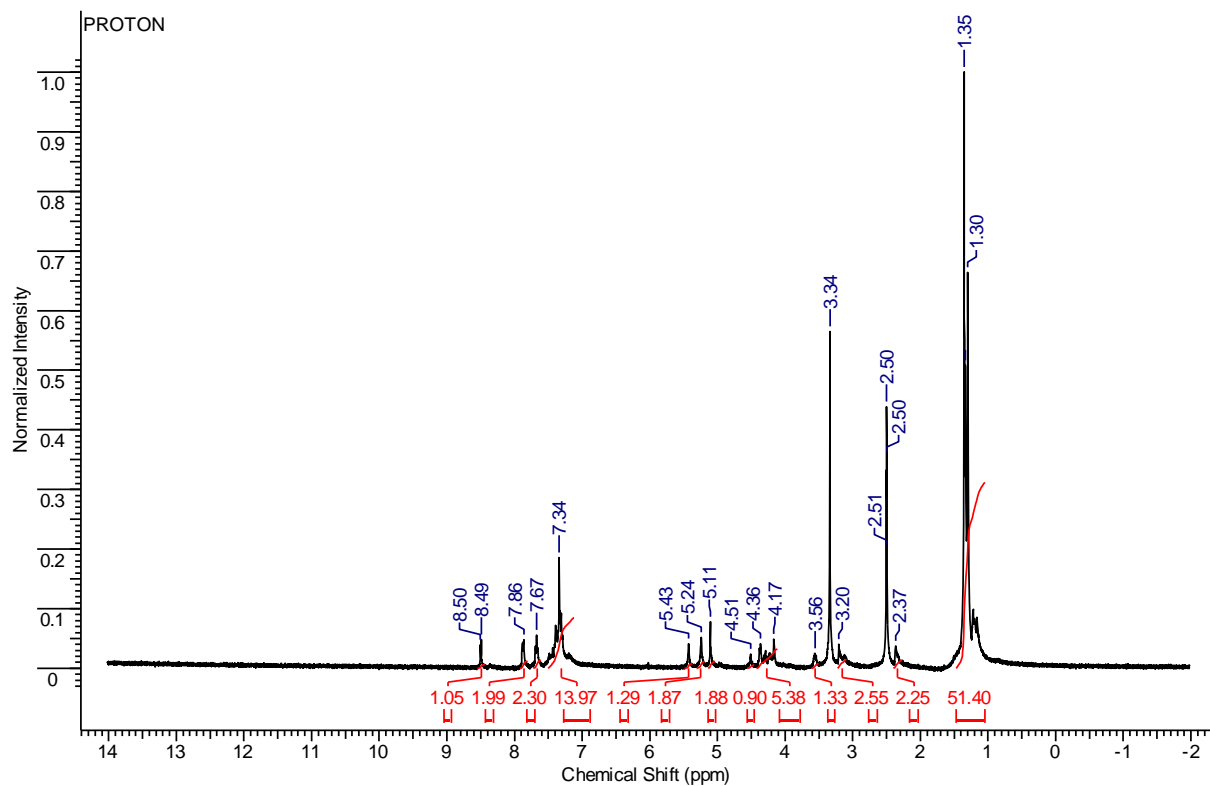
^1H NMR (400 MHz, DMSO-*d*₆) of **8**



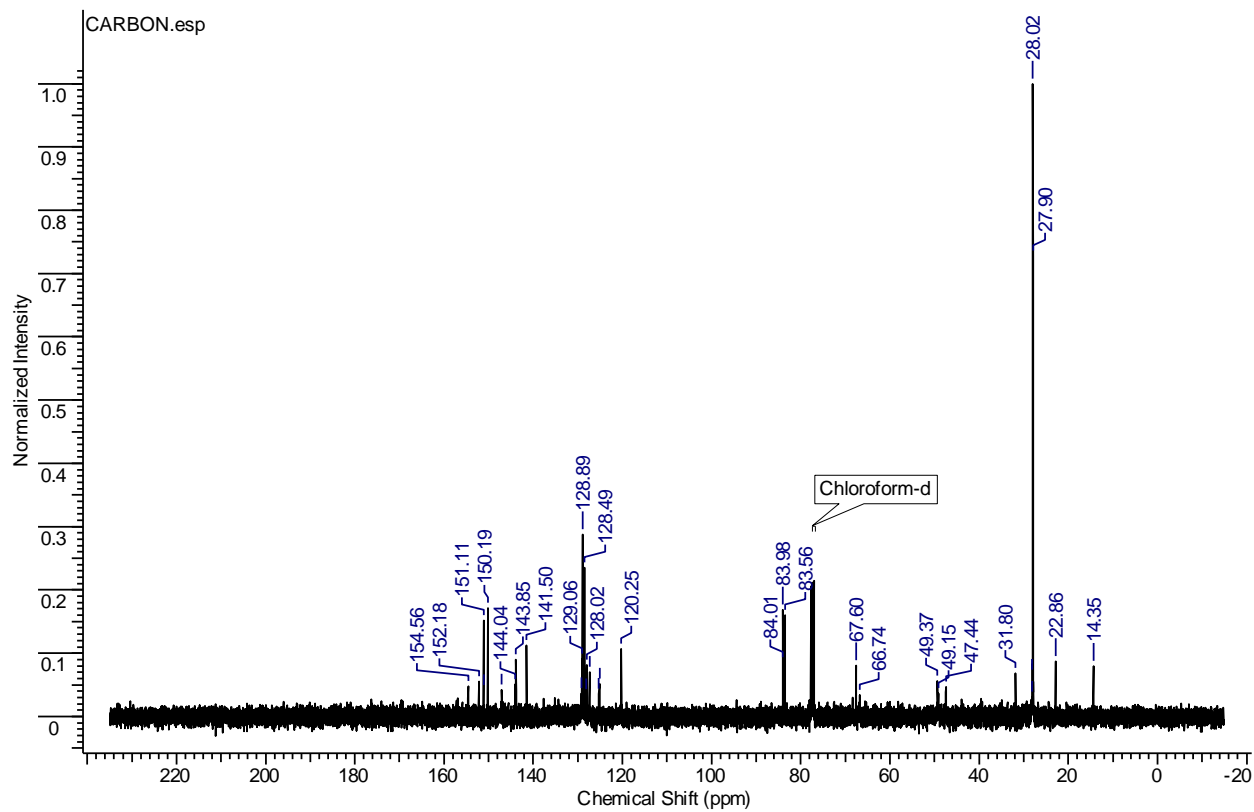
^{13}C NMR (101 MHz, MeOD-*d*₄) of **8**



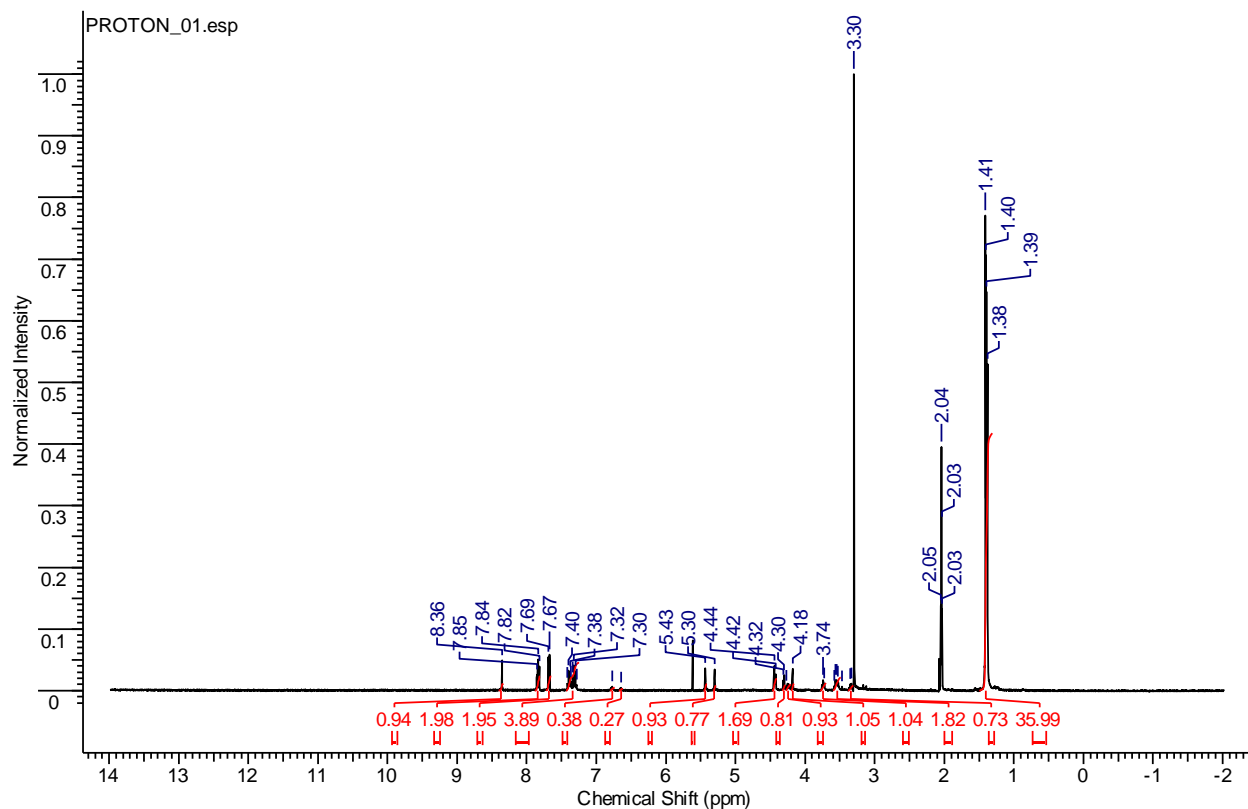
^1H NMR (400 MHz, DMSO-*d*₆) of **9**



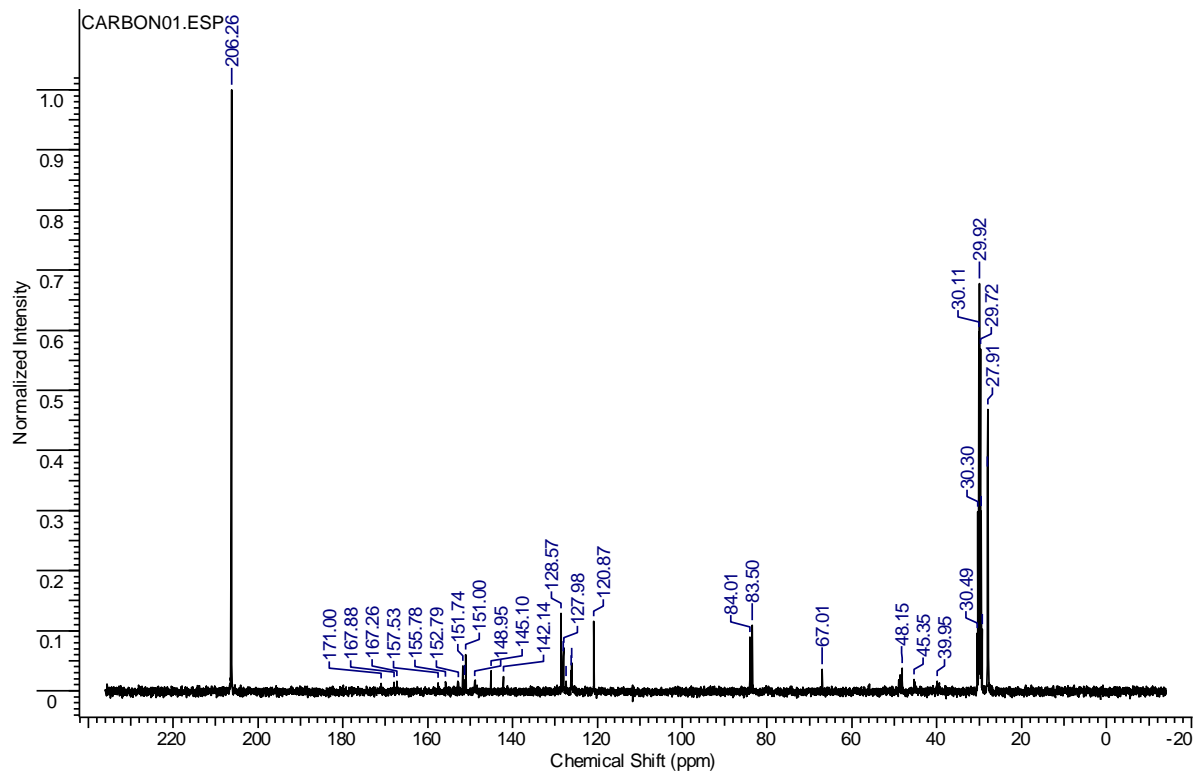
^{13}C NMR (101 MHz, CDCl₃) of **9**



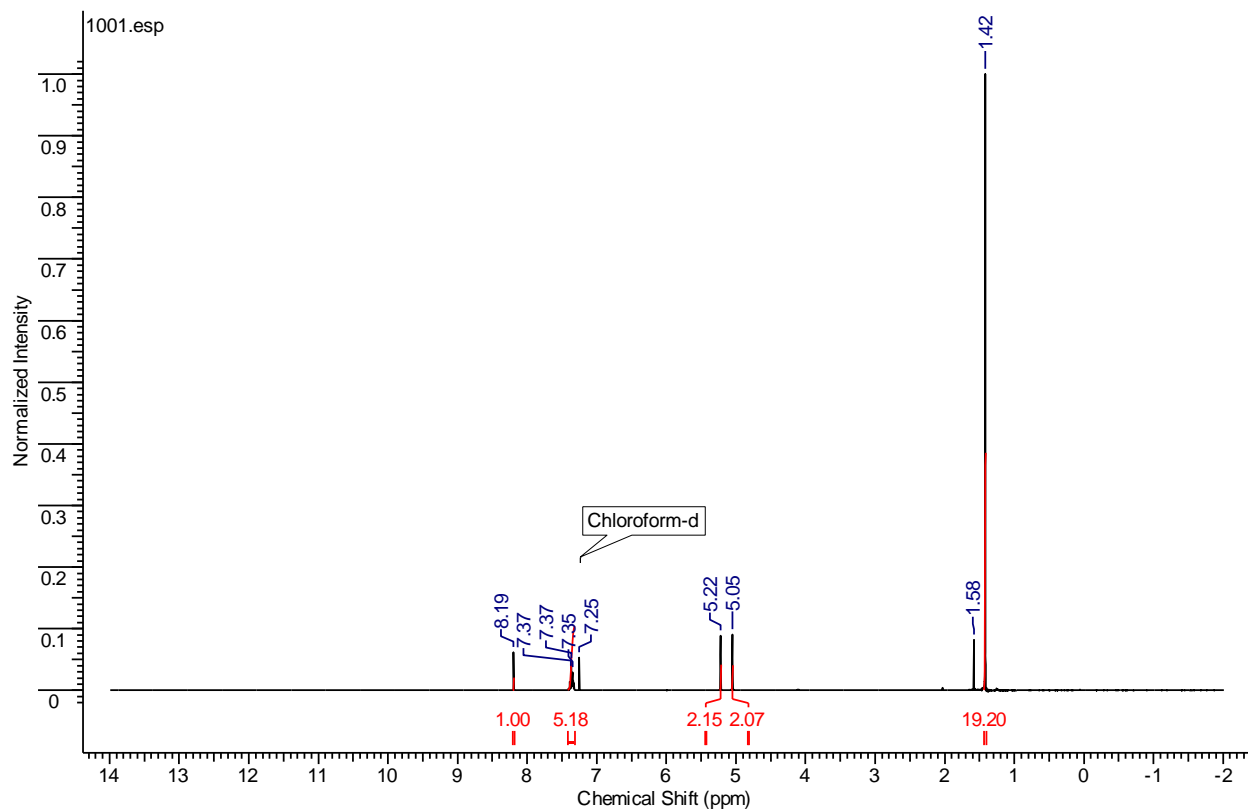
^1H NMR (400 MHz, acetone- d_6) of **10**



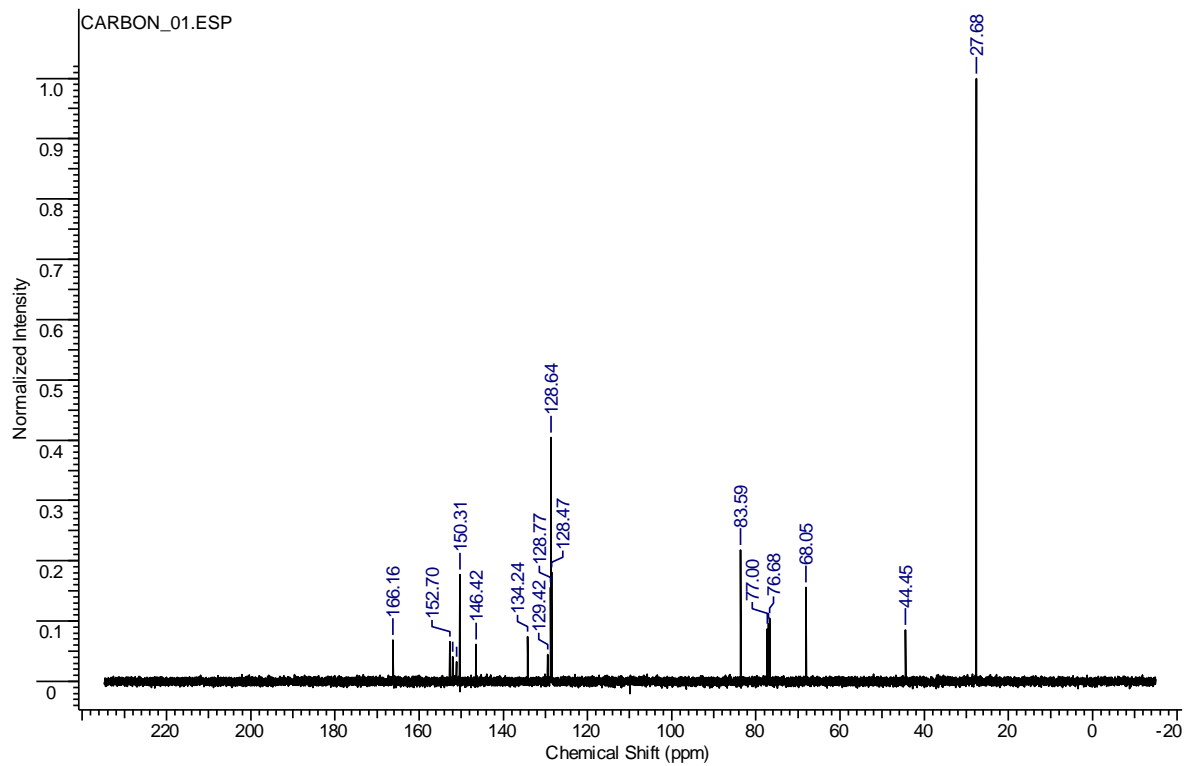
^{13}C NMR (101 MHz, acetone- d_6) of **10**



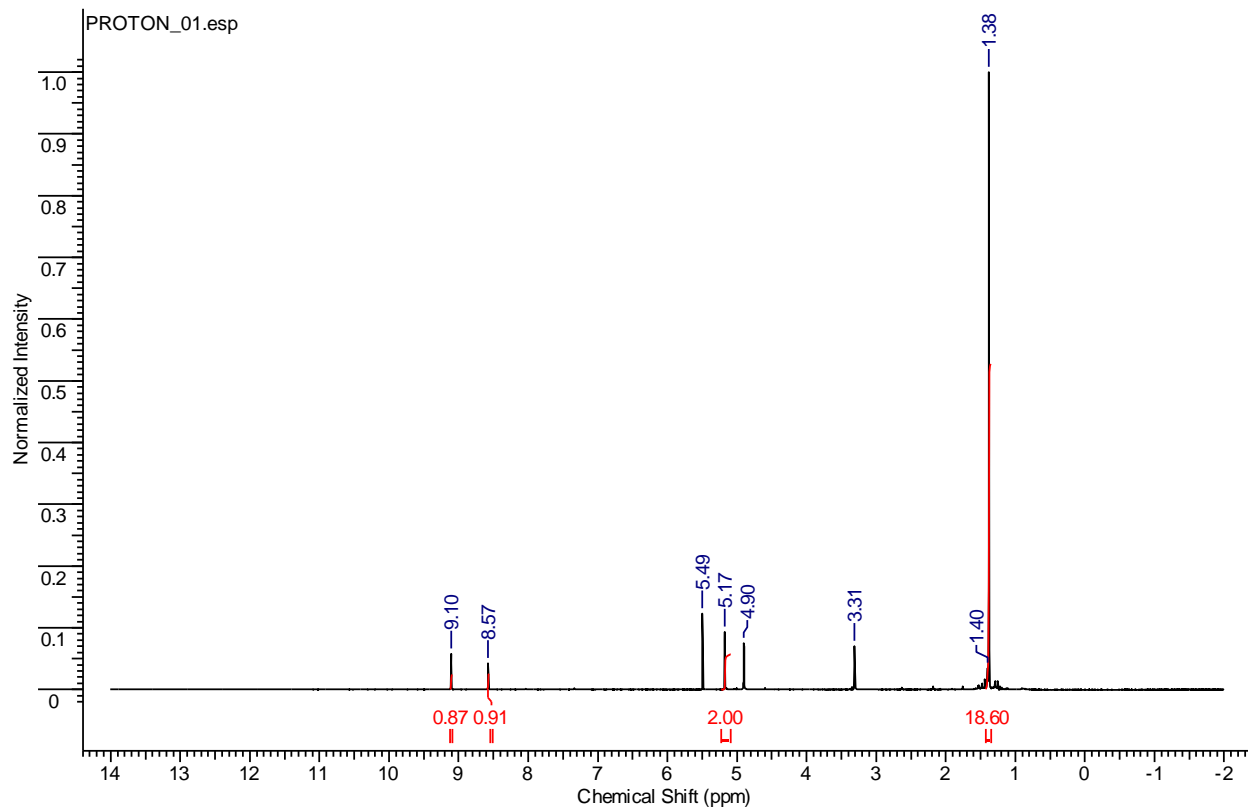
^1H NMR (400 MHz, CDCl_3) of **11a**



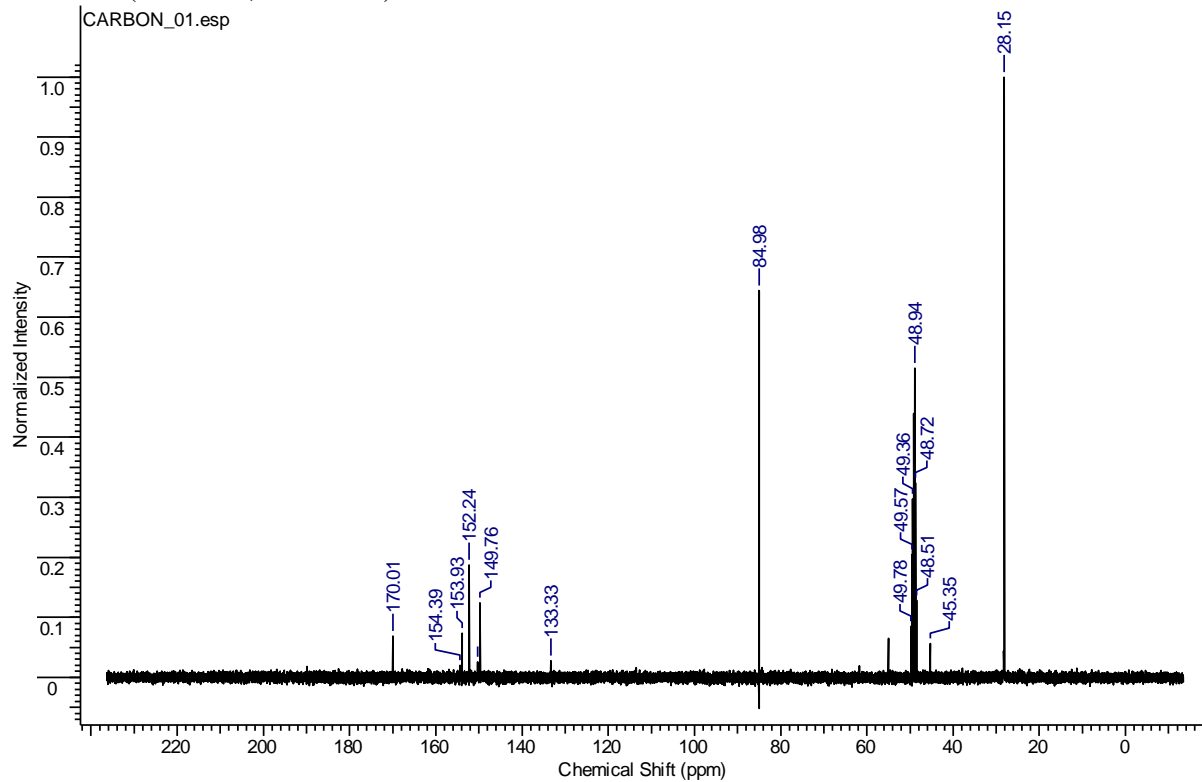
^{13}C NMR (101 MHz, CDCl_3) of **11a**



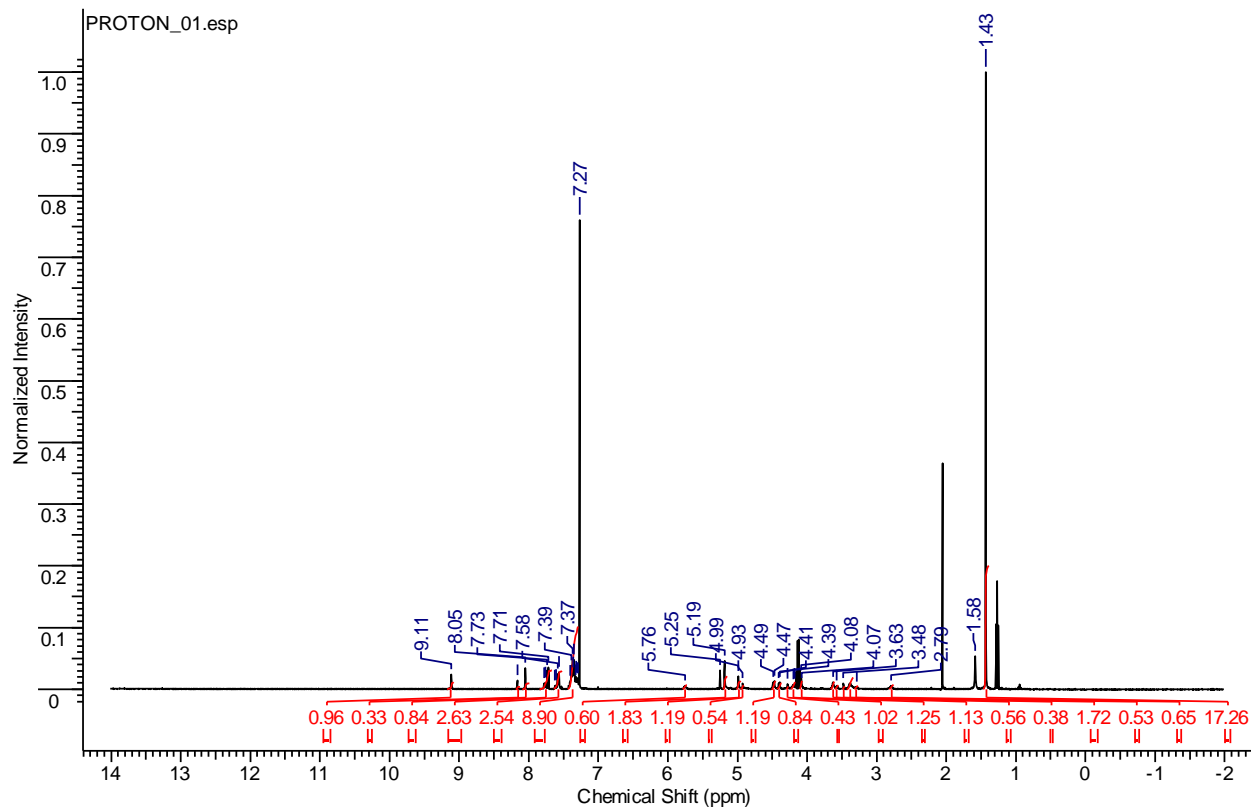
^1H NMR (400 MHz, MeOH- d_4) of **12**



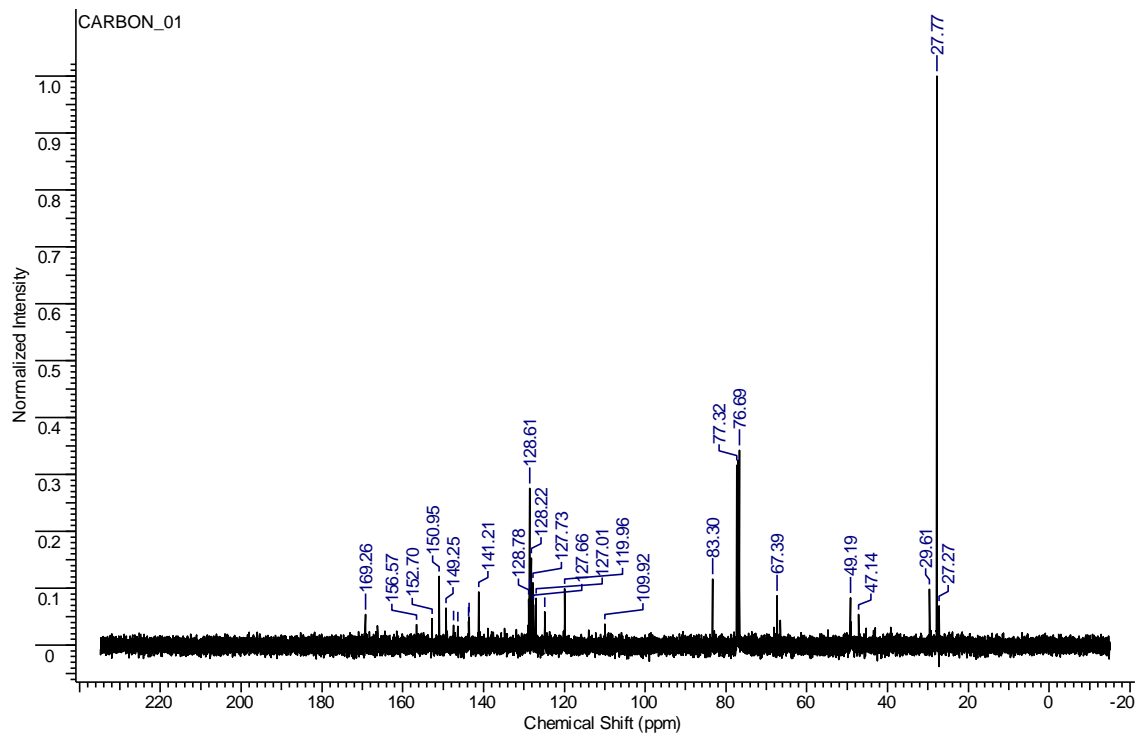
^{13}C NMR (101 MHz, MeOH- d_4) of **12**



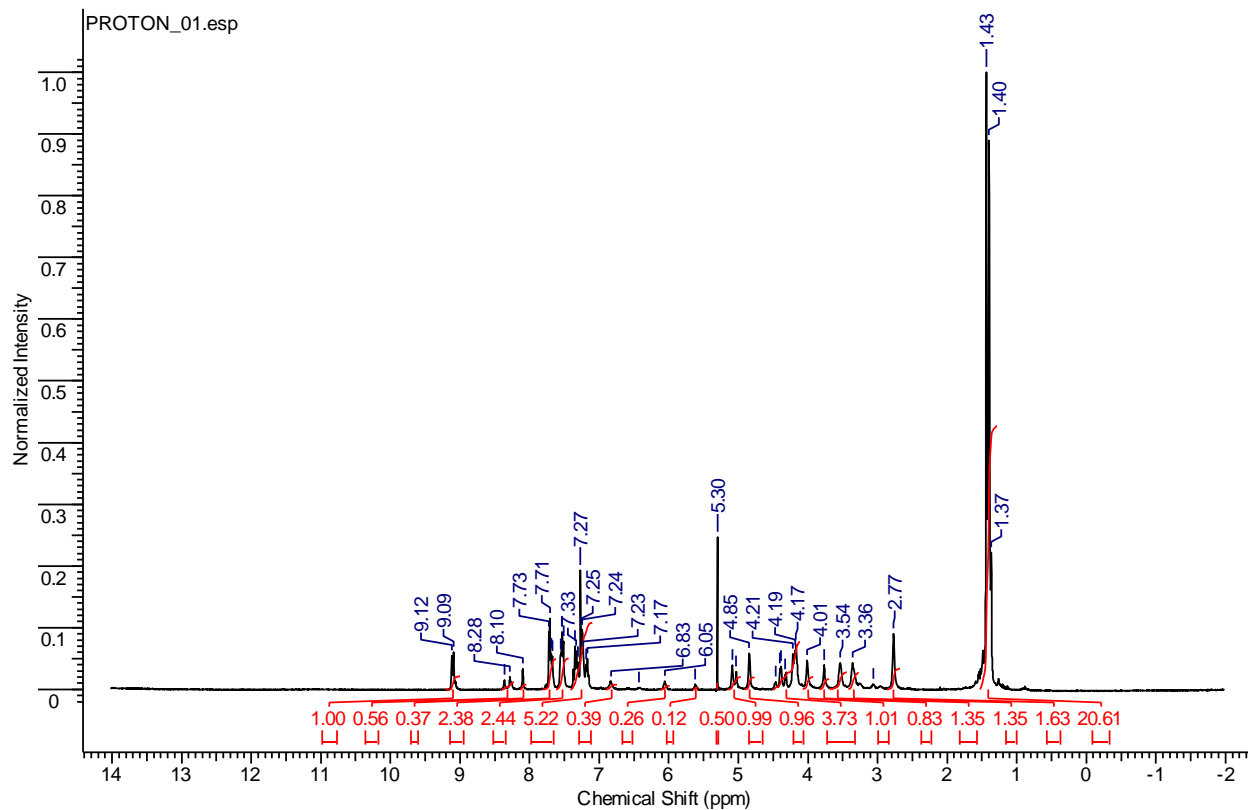
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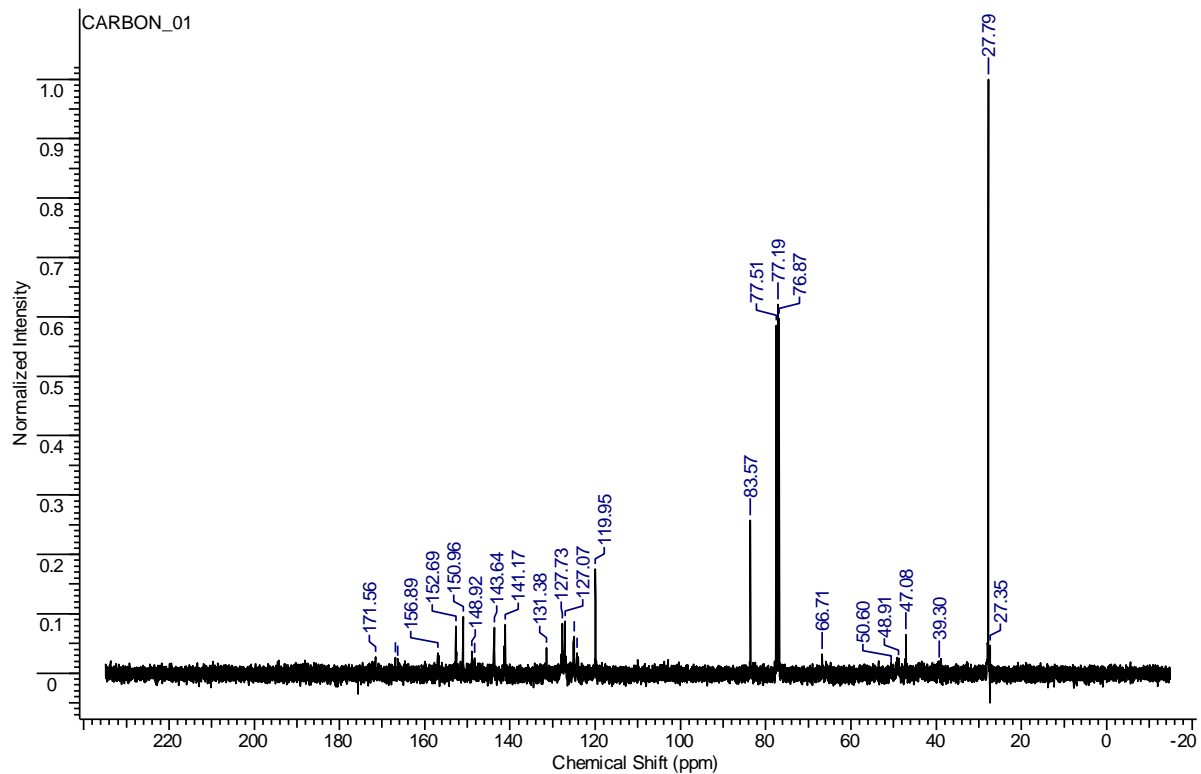
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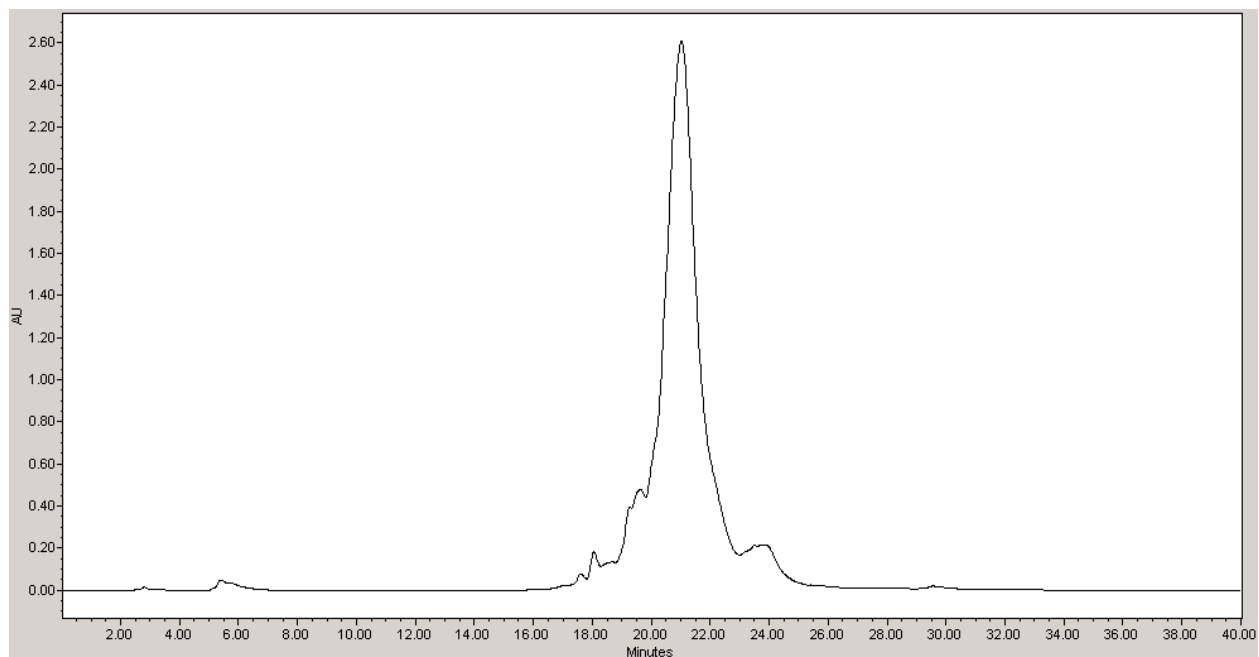
^1H NMR (400 MHz, CDCl_3) of **14**



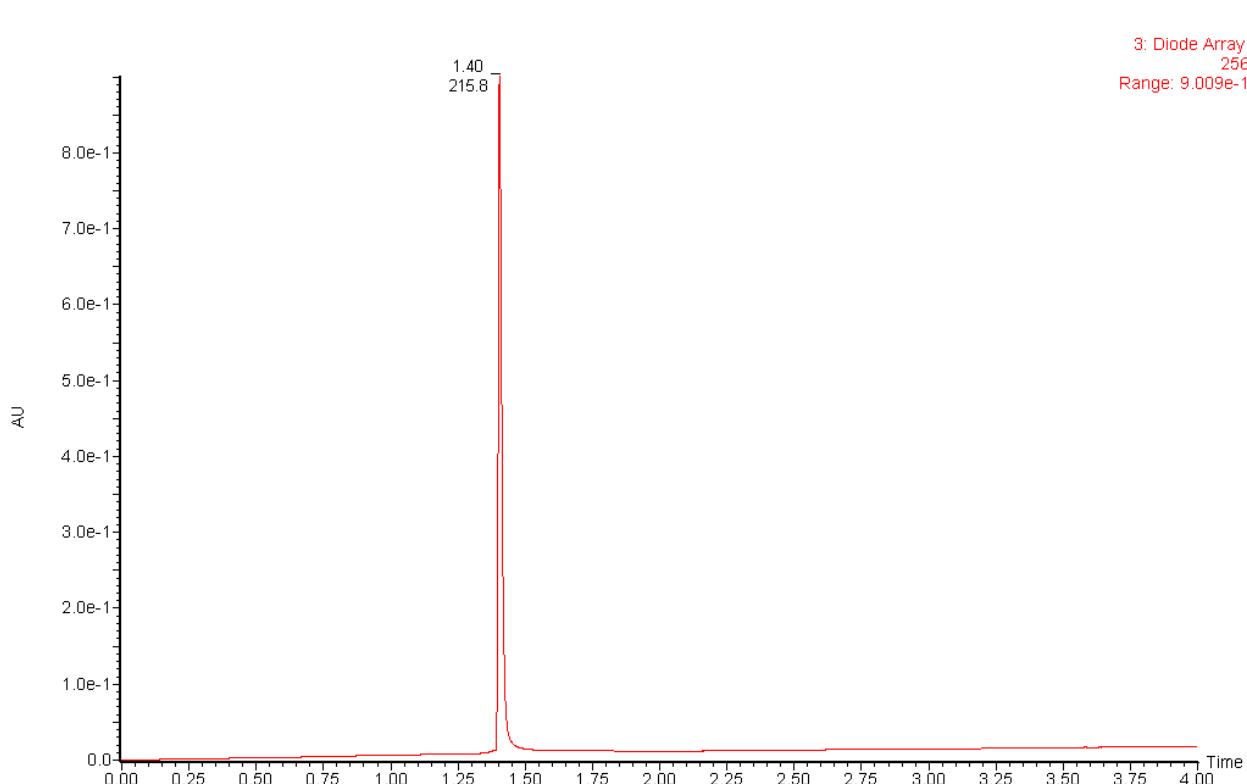
^{13}C NMR (101 MHz, CDCl_3) of **14**



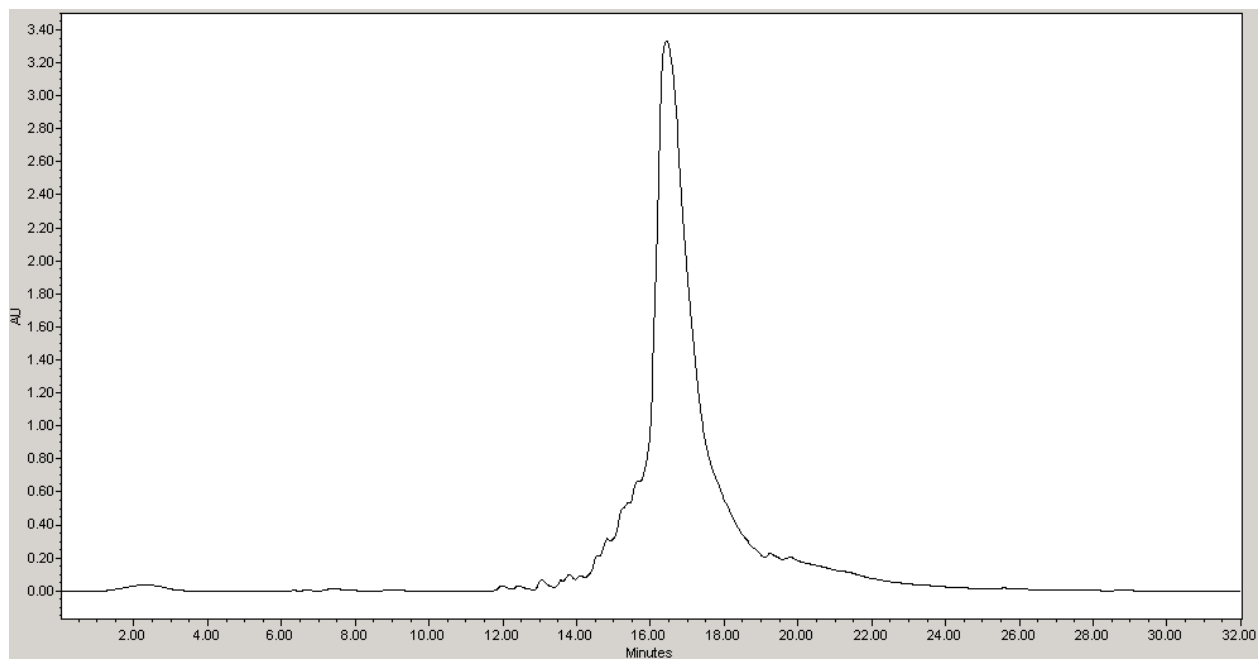
HPLC trace of crude PNA1



UPLC trace of purified PNA1



HPLC trace of crude PNA2



UPLC trace of purified PNA2

