

Supplementary Informations

Water Soluble Extended Naphthalene Diimides as pH Fluorescent Sensors and G-Quadruplex Ligands

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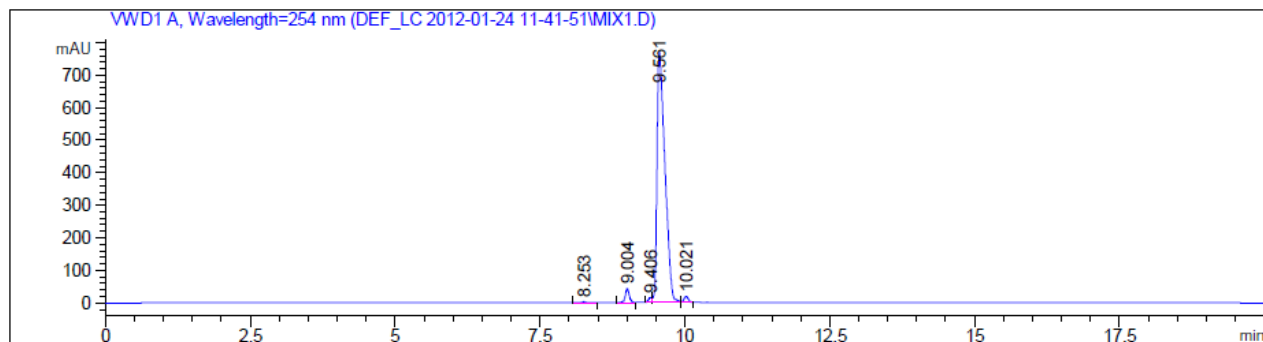
Supplemental Experimental Procedures

General Procedures.

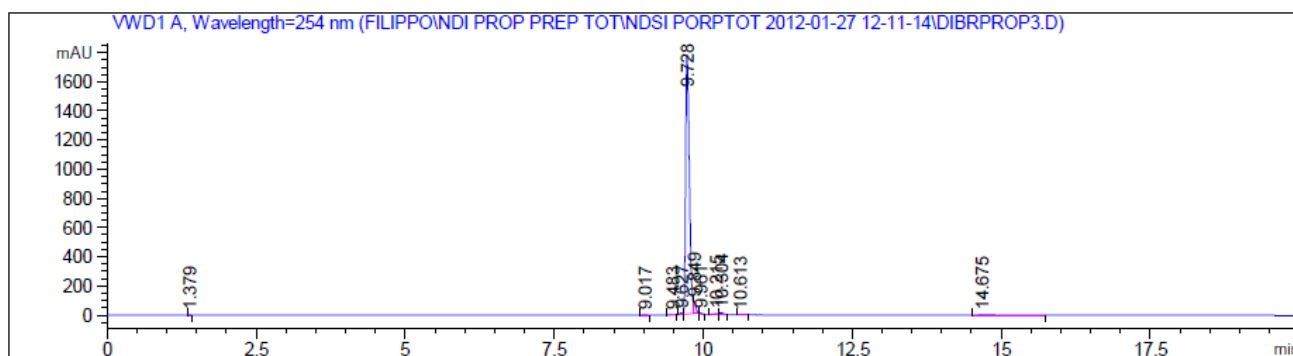
Reagents, solvents and chemicals were purchased from Alfa Aesar, or Sigma-Aldrich and were used as supplied without further purification. TLC analysis was carried out on silica gel (Merck 60F-254) with visualization at 254 and 366 nm. HPLC analysis and purifications were performed using two different HPLC: Waters system combining a Delta 600 PUMP, a 2489 UV/VIS detector and Fraction Collector III (for preparative and analytical) and an Agilent system SERIES 1260 (for analytical). The analytical column was XSelect CSH Phenyl-Hexyl (150 x 4.6 mm) (Waters). The preparative column was XSelect CSH Prep Phenyl-Hexyl 5 μ m (150 x 30 mm) (Waters). Flows were 1 ml/min for analytical and 27 ml/min for preparative. Two analytical methods were used: method A (Aqueous solvent: 0.1% trifluoroacetic acid in water; Organic solvent: Acetonitrile; Gradient: 95% aqueous for 2 minutes after injection, gradually to 60% aqueous over 14 minutes and at the end an isocratic flow over 4 minutes), method B (Aqueous solvent: 0.1% trifluoroacetic acid in water; Organic solvent: Acetonitrile; Gradient: 95% aqueous for 4 minutes after injection, gradually to 40% aqueous over 16 minutes and at the end an isocratic flow over 2 minutes). Preparative HPLC were performed using an upgrade of the method A and B. ^1H , ^{13}C -NMR spectra were recorded on a 300 MHz spectrometer and the chemical shifts are reported relative to TMS. The structures of new compounds were deduced from the results of ^1H , and ^{13}C NMR. Elemental analyses were made on a Carlo Erba CNH analyzer, model 19106.

1. HPLC PURITY DATA

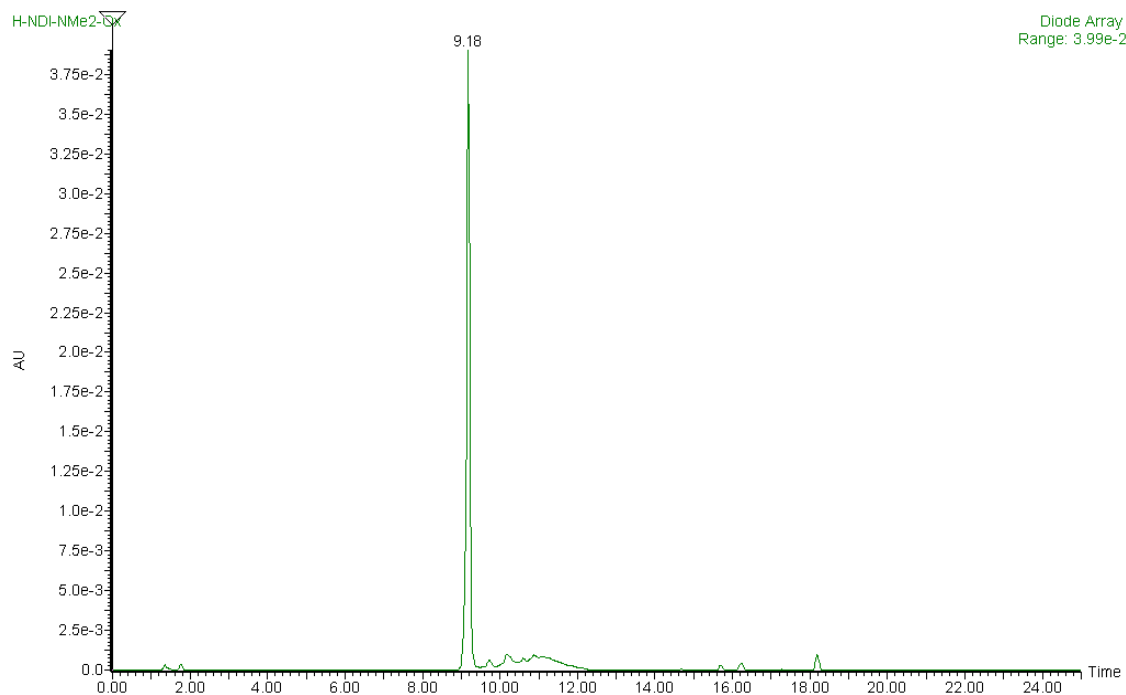
3a Method A



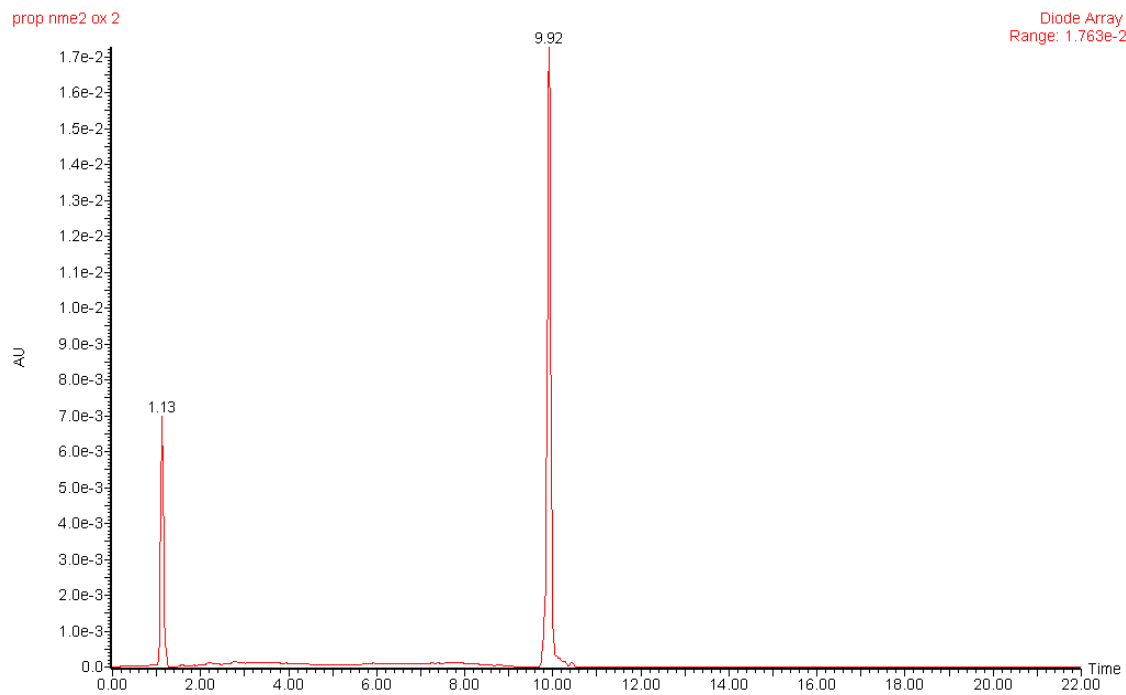
3b Method A



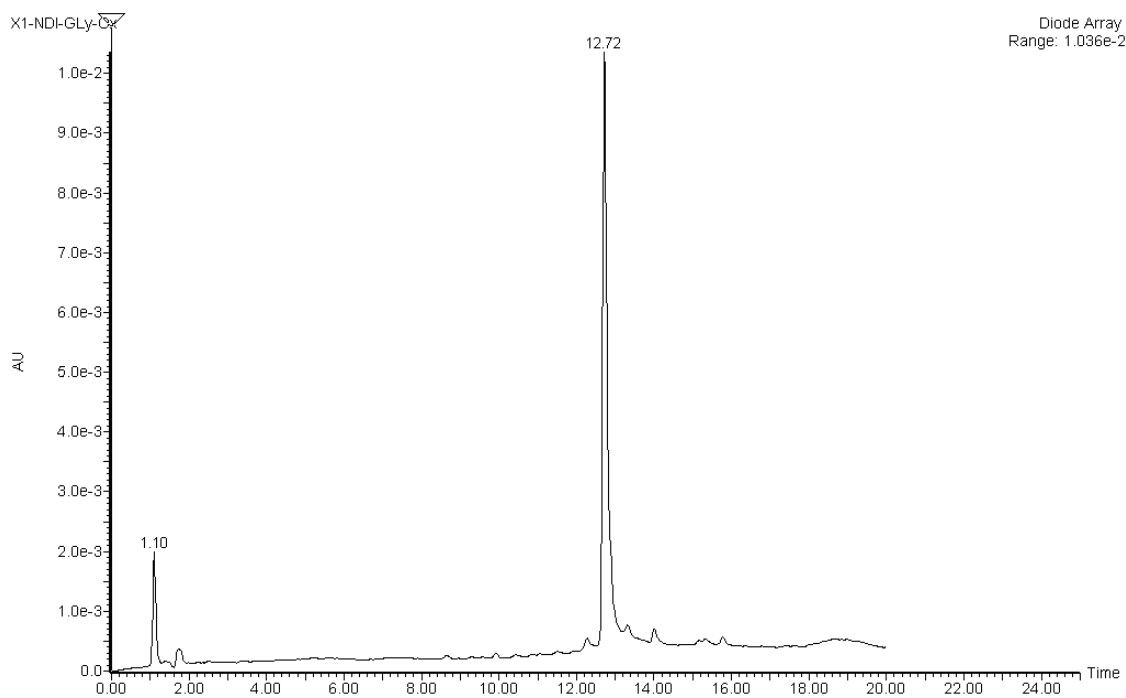
4a Method A



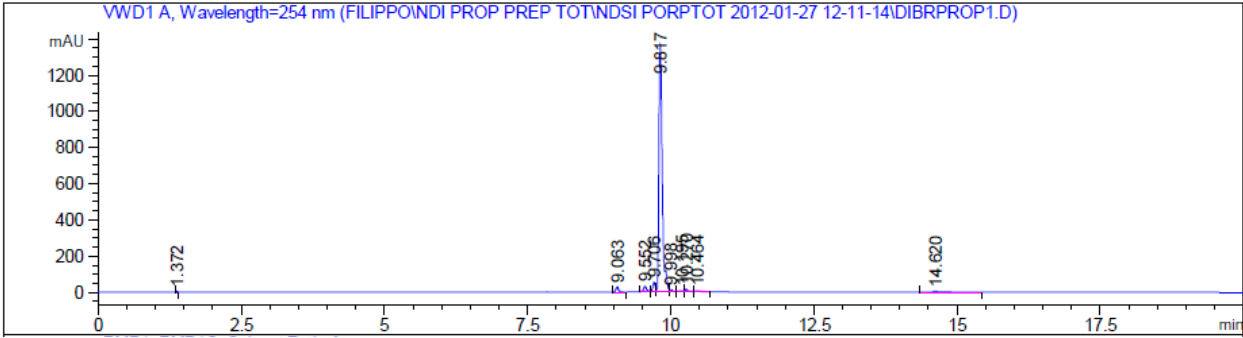
4b Method A



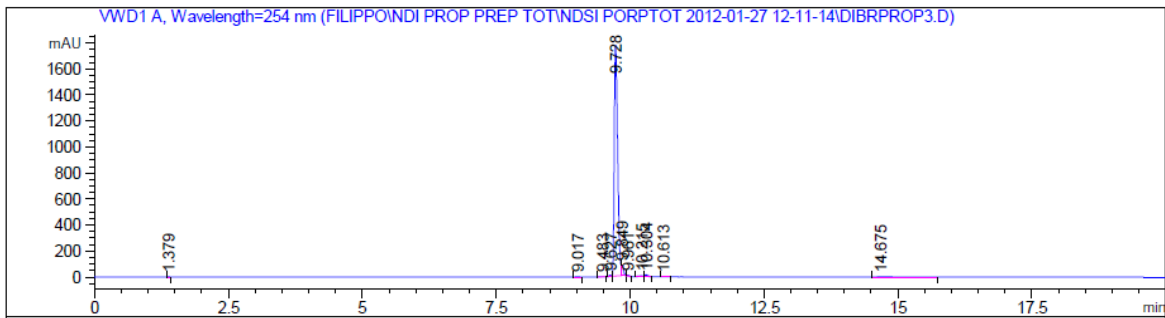
4c Method B



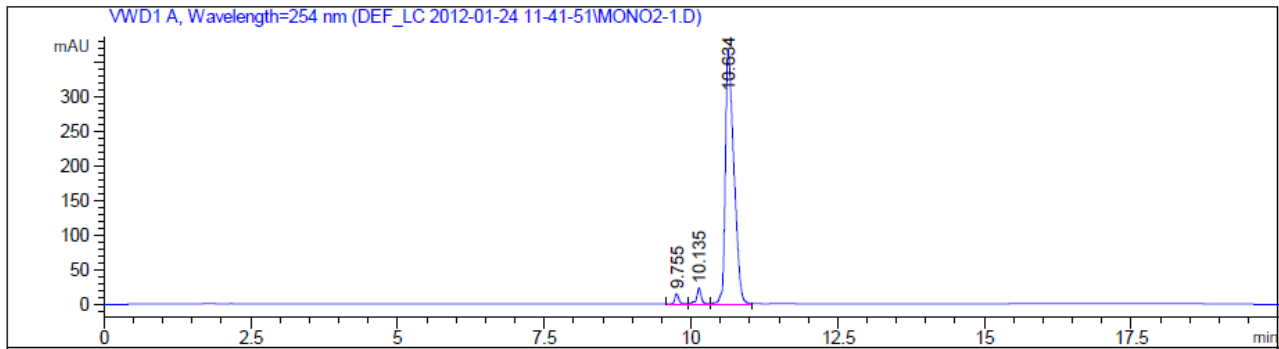
6b Method A



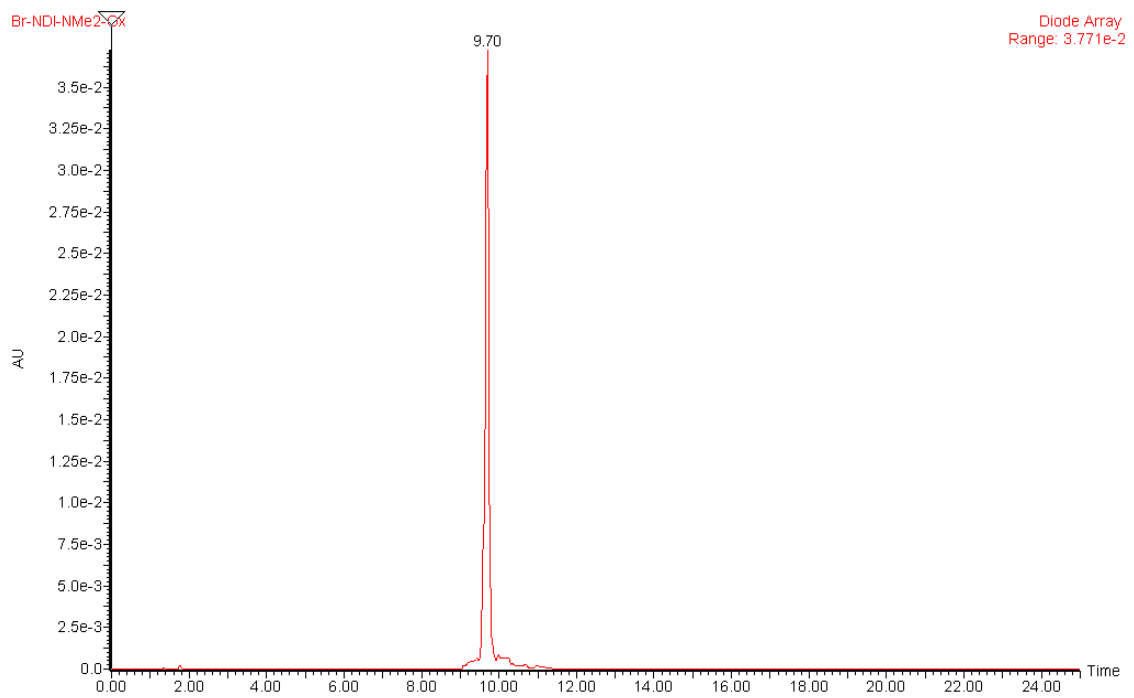
7a Method A



7b Method A

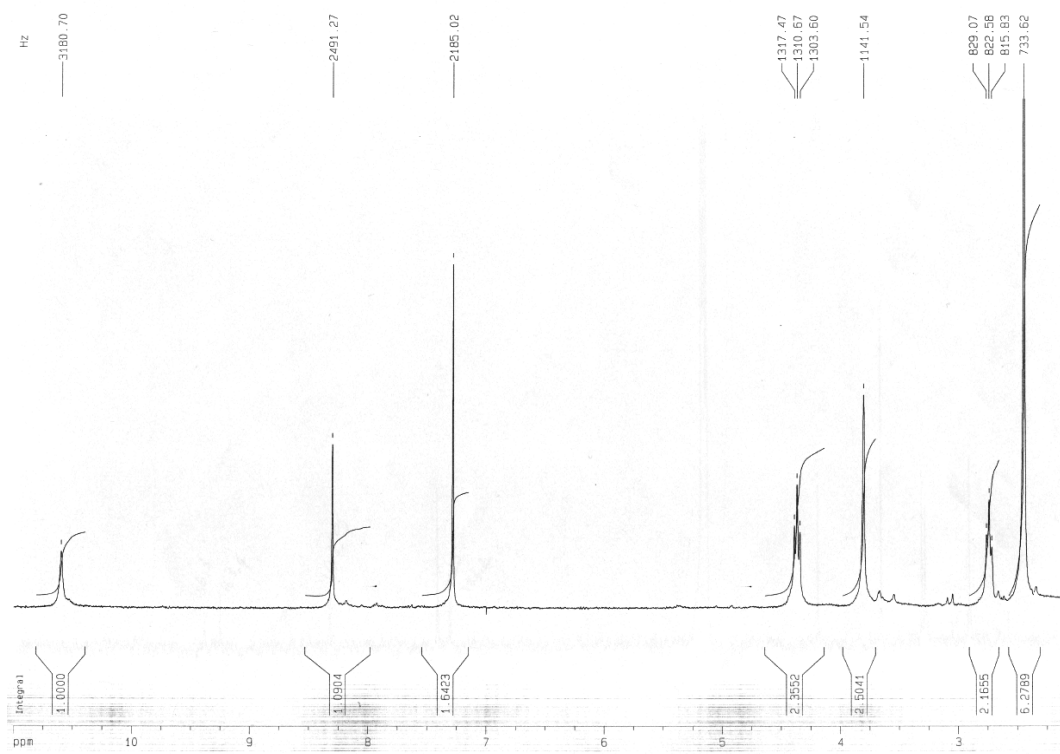


8a Method A

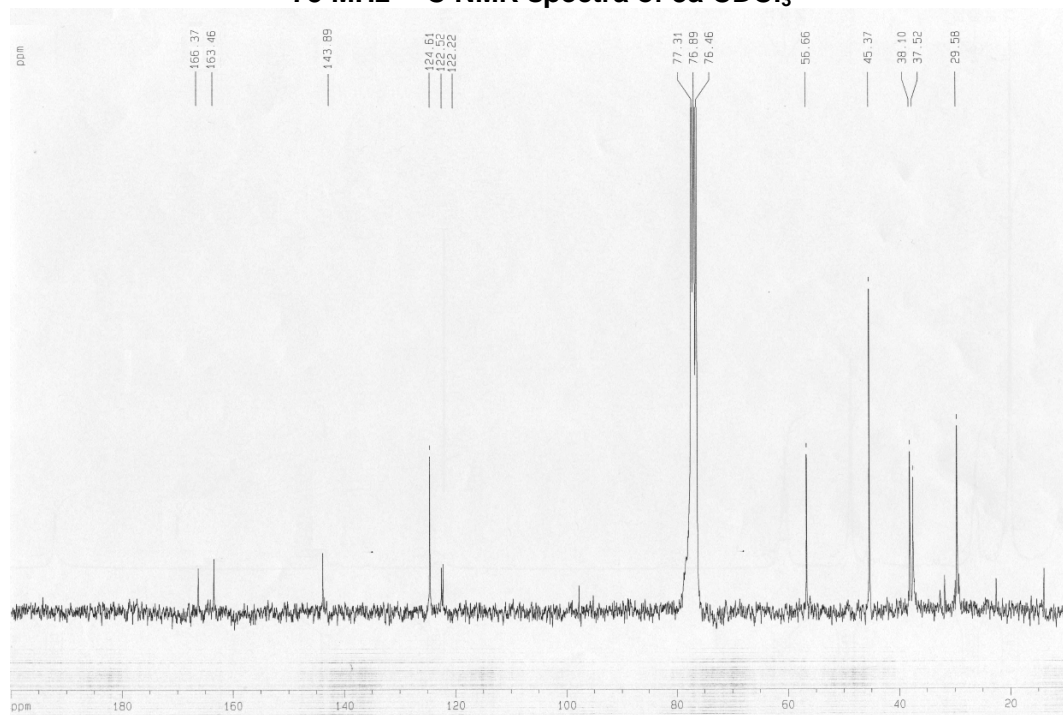


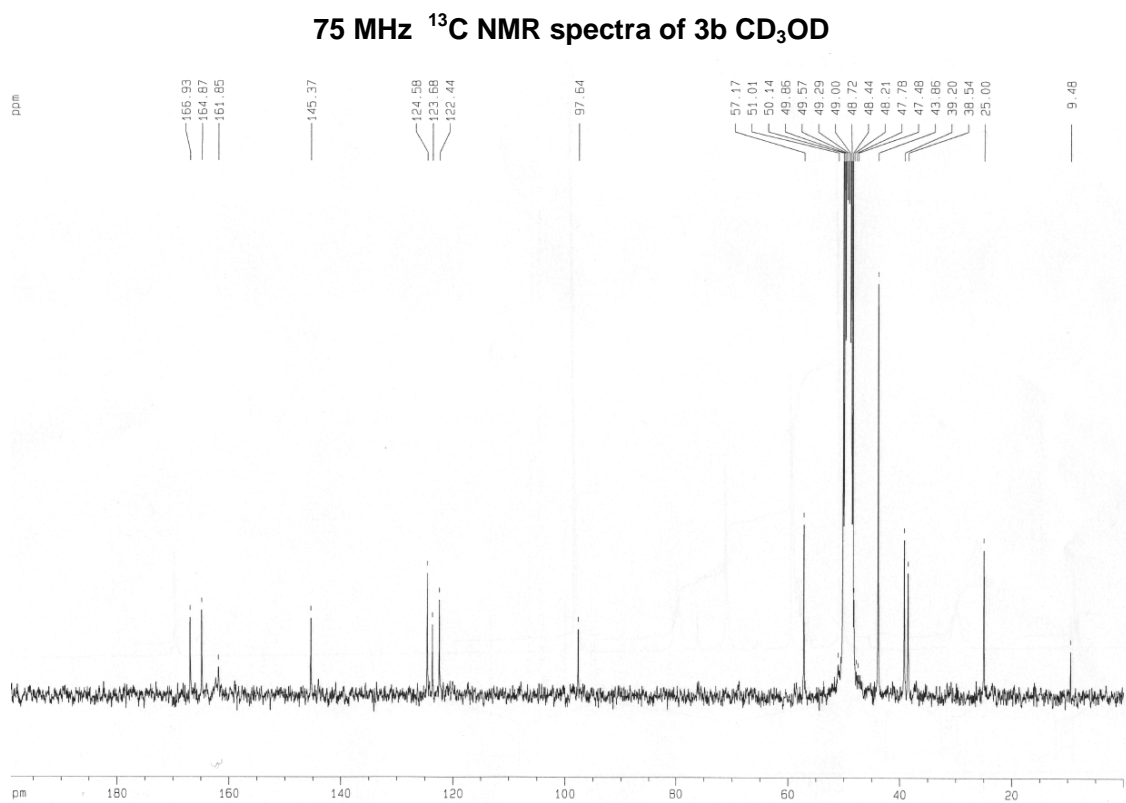
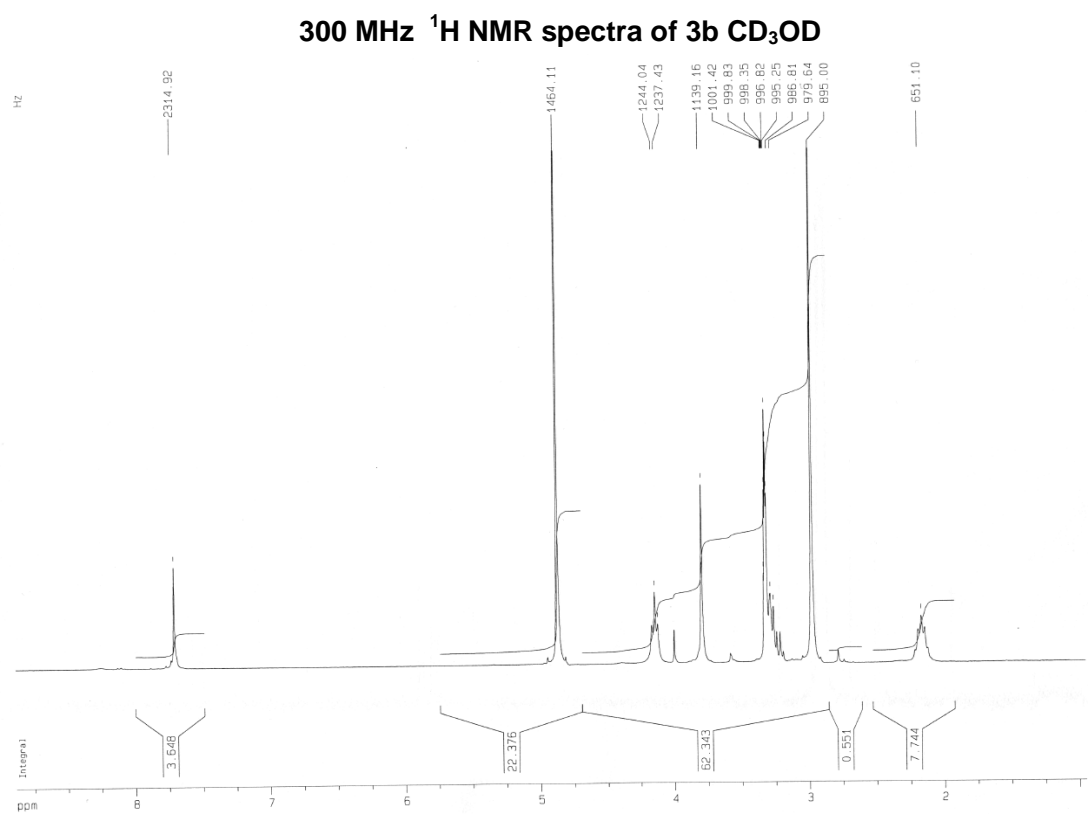
2. NMR spectra

300 MHz ^1H NMR spectra of 3a CDCl_3

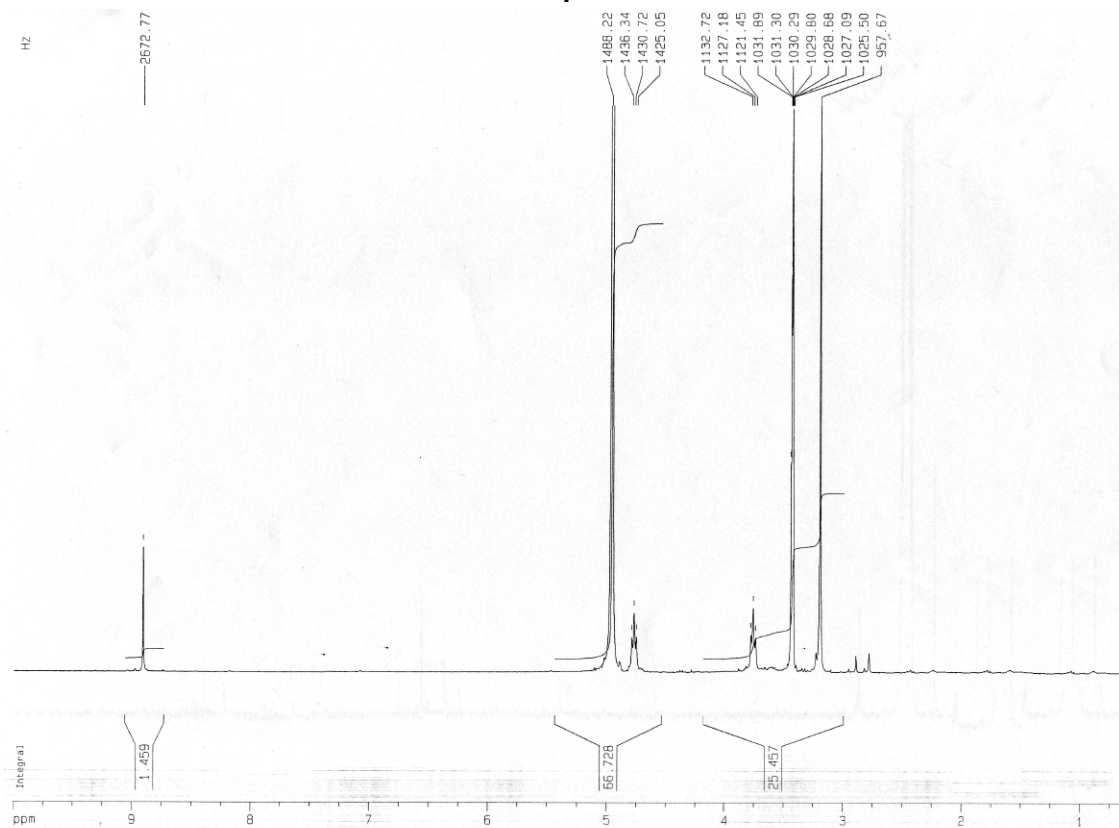


75 MHz ^{13}C NMR spectra of 3a CDCl_3

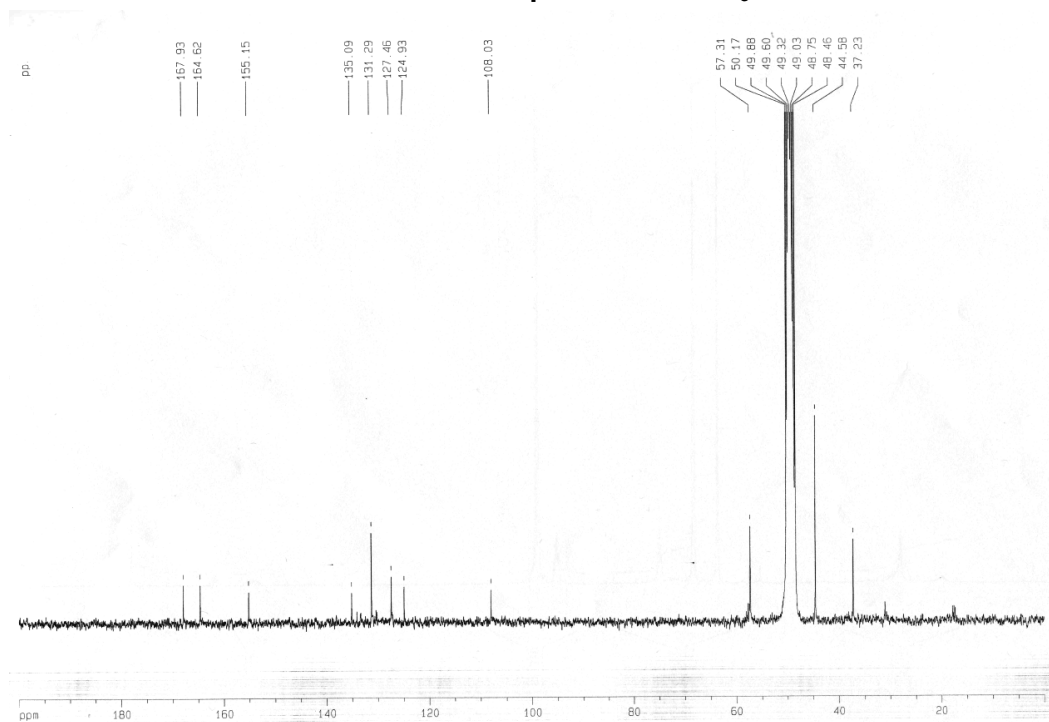




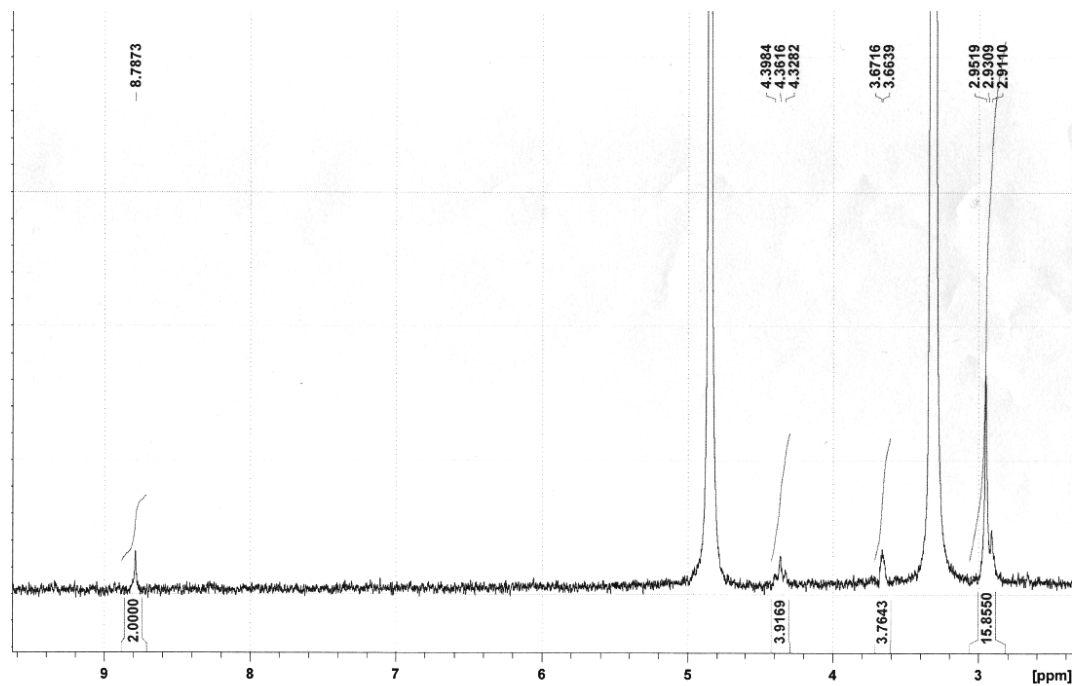
300 MHz ^1H NMR spectra of 4a CD_3OD



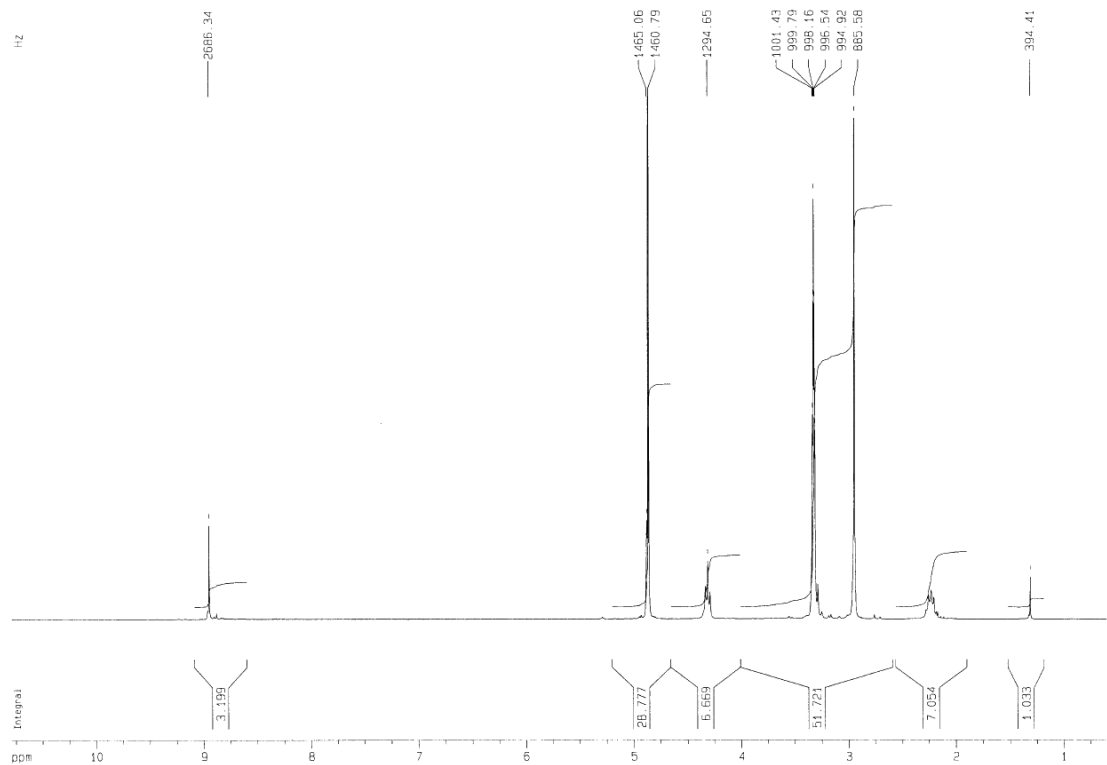
75 MHz ^{13}C NMR spectra of 4a CD_3OD



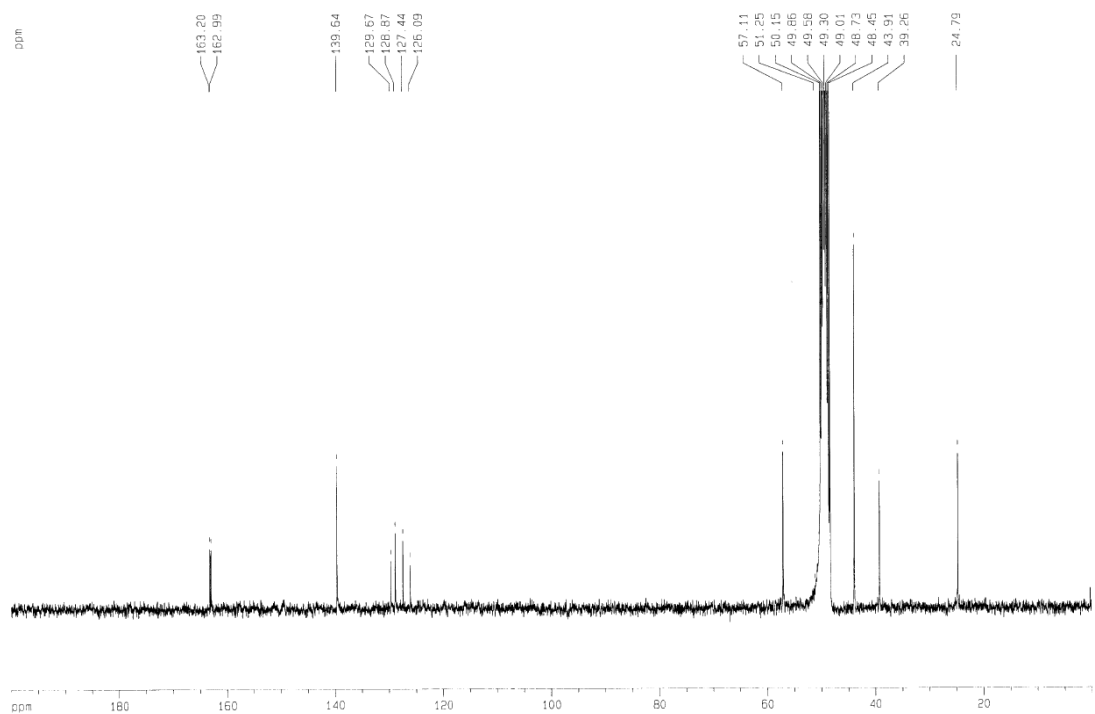
300 MHz ¹H NMR spectra of 4b CDCl₃



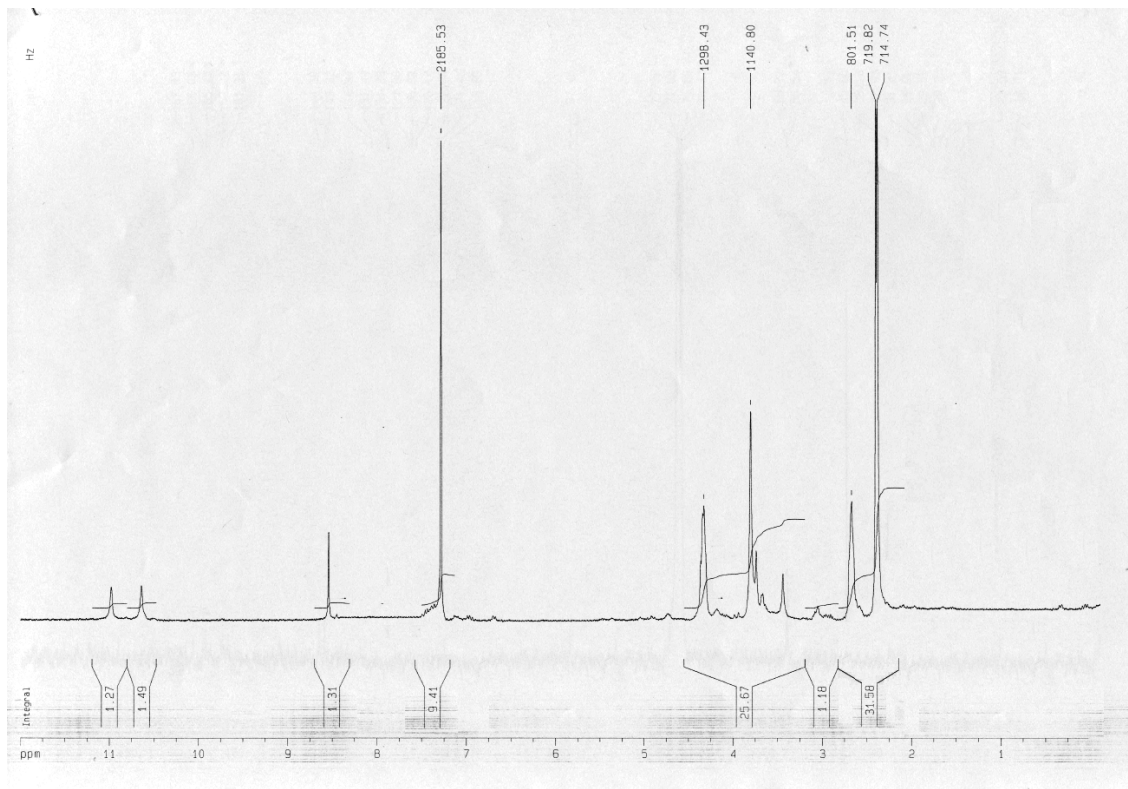
300 MHz ¹H NMR spectra of 6b CD₃OD



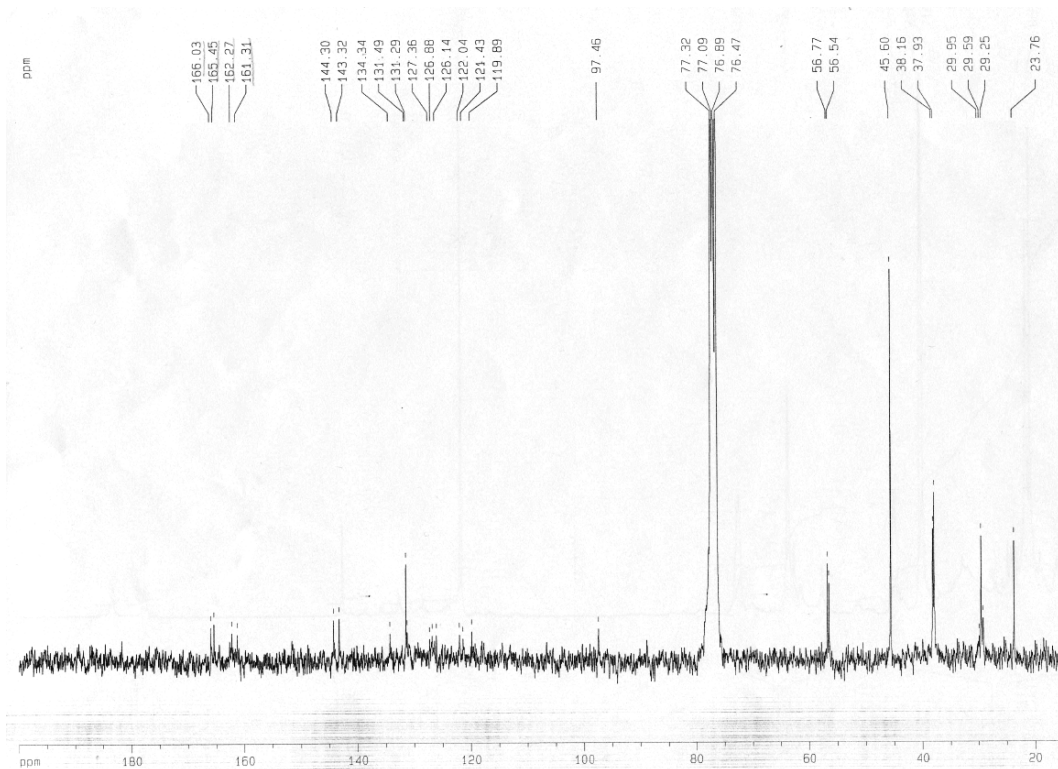
300 MHz ¹H NMR spectra of 6b CD₃OD



300 MHz ¹H NMR spectra of 7a CDCl₃



75 MHz ^{13}C NMR spectra of 7a CDCl_3



300 MHz ^1H NMR spectra of 7b CDCl_3

