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Host-guest blue light-emitting electrochemical cells

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1. Spectroscopy

Electronic absorption spectrum was recorded with an HP/Agilent 8453 Diode Array UV/VIS spectrophotometer under air in optical cells of 2 mm path length. The solutions in CH_2Cl_2 (Sigma-Aldrich, puriss p.a., ACS reagent) were freshly prepared before experiment.

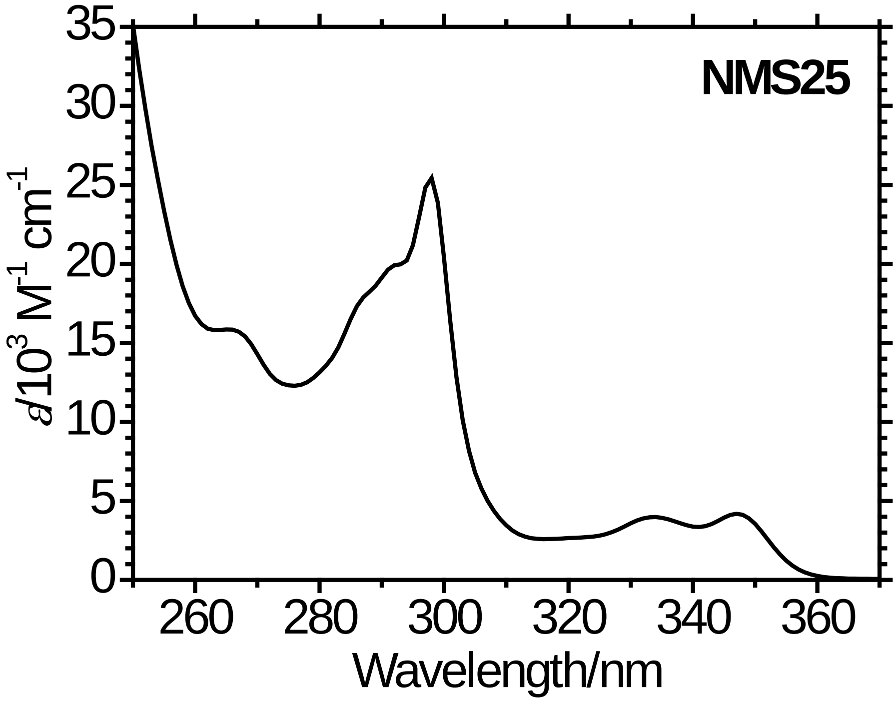


Fig. S1. Absorption spectrum of **NMS25** in dichloromethane (1.53×10^{-4} M). λ_{abs}/nm ($\varepsilon/10^3$ M^{-1} cm^{-1}): 265 (16, sh), 298 (25), 334 (4.0), 347 (4.2).

2. Electrochemistry

Electrochemical experiments were conducted in acetonitrile (99.9%, Extra Dry, over Molecular Sieves, AcroSeal®, Acros), with 0.1 M tetra-*n*-butylammonium hexafluorophosphate (Fluka, electrochemical grade) as the supporting electrolyte, with a PC controlled AutoLab PSTAT10 electrochemical workstation.

The experiments were carried out under argon in an electrochemical cell through which a stream of Ar was passed (the flow of Ar was stopped during the measurement to prevent stirring of the solution). Glassy-carbon disk (3 mm diameter), platinum spiral, and platinum wire served as working, counter, and quasi-reference electrodes. To clean, the working electrodes were polished on a pad in ethanol slurry of abrasive paste (Metrohm), briefly sonicated in ethanol, and rinsed with ethanol. At the end of each experiment, ferrocene was added as an internal reference. Estimated error: ±50 mV. Cyclic voltammetry was performed at scan rates of 0.02–5 V/s. Peak-to-peak separation for the ferrocene (reference) couple in acetonitrile was 83 mV at 1 V/s and 73 mV at 0.1 V/s.

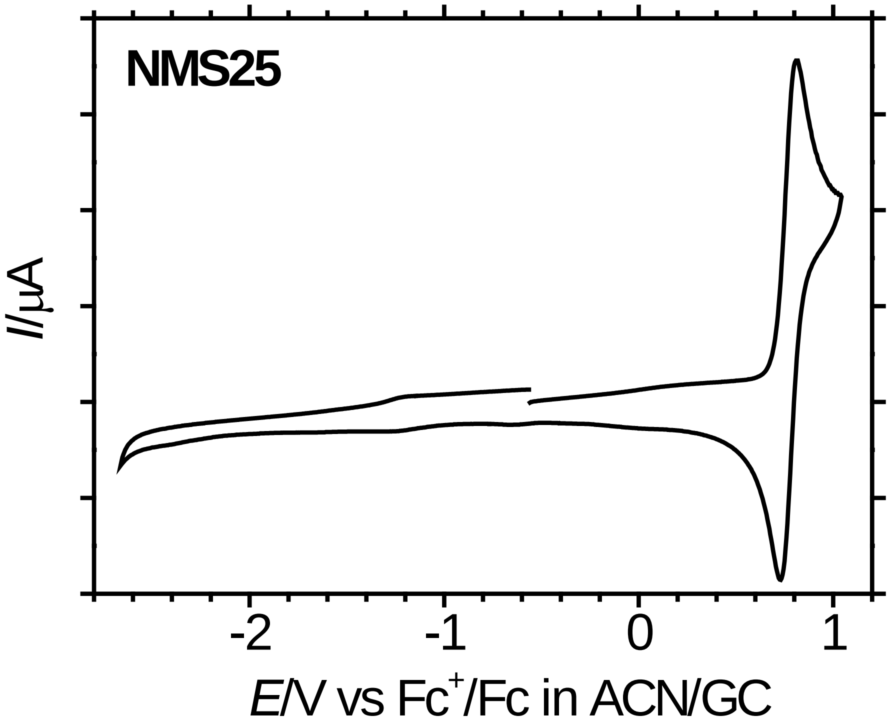
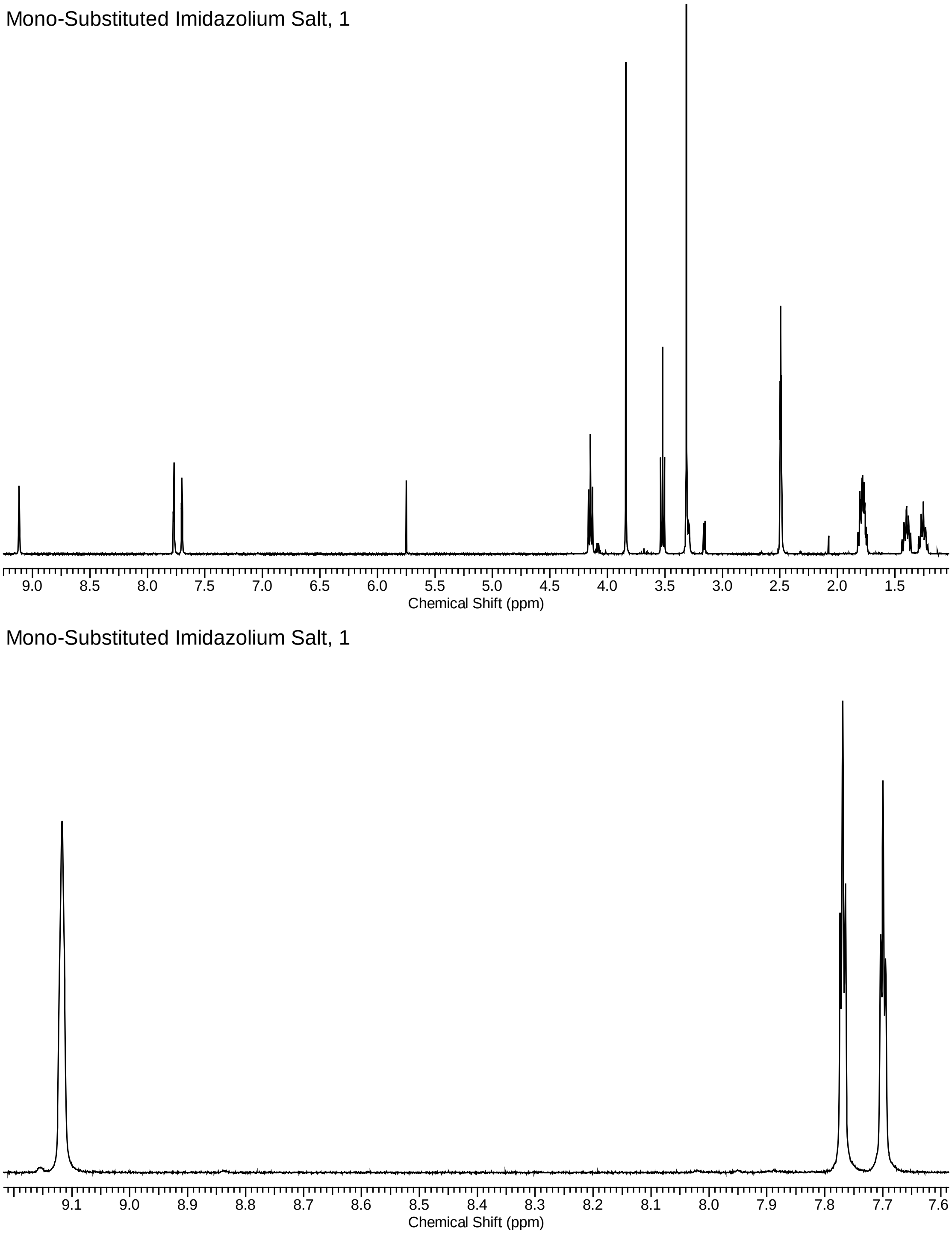
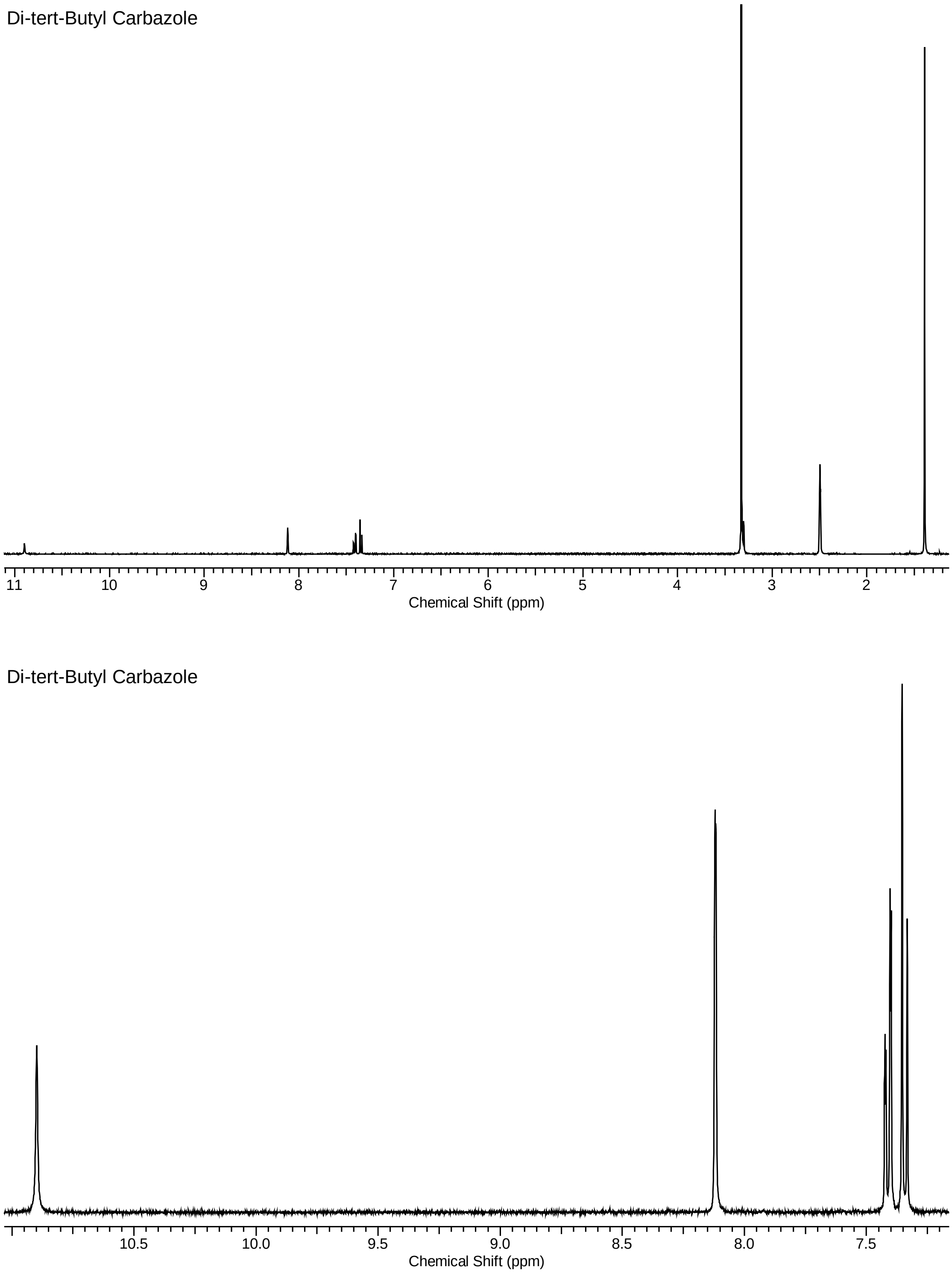


Fig. S2. Cyclic voltammogram of **NMS25** on glassy-carbon electrode in acetonitrile with 0.1 M NBu_4PF_6 at 1 V/s on clockwise scan. The unit on the vertical axis is 5 μA. $E_{1/2}^{ox}$ = 0.77 V (78 mV). The anodic/cathodic peak separation for the oxidation process of **NMS25** was 78–107 mV at scan rates of 0.02–5 V/s.

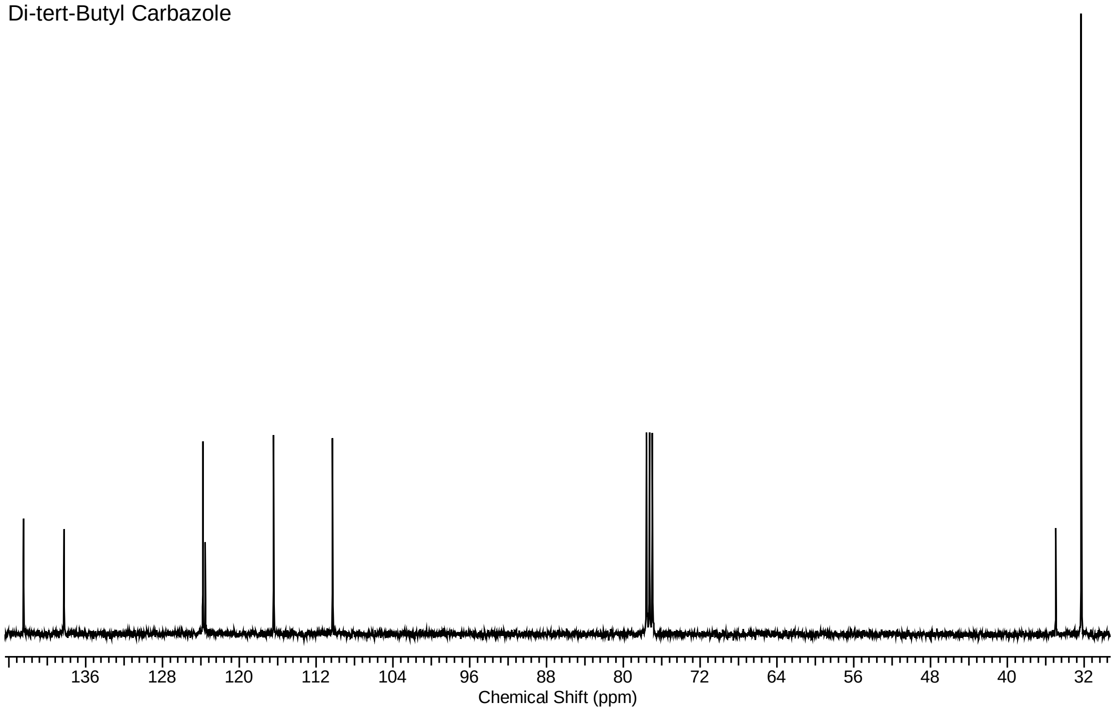
3. NMR Spectra



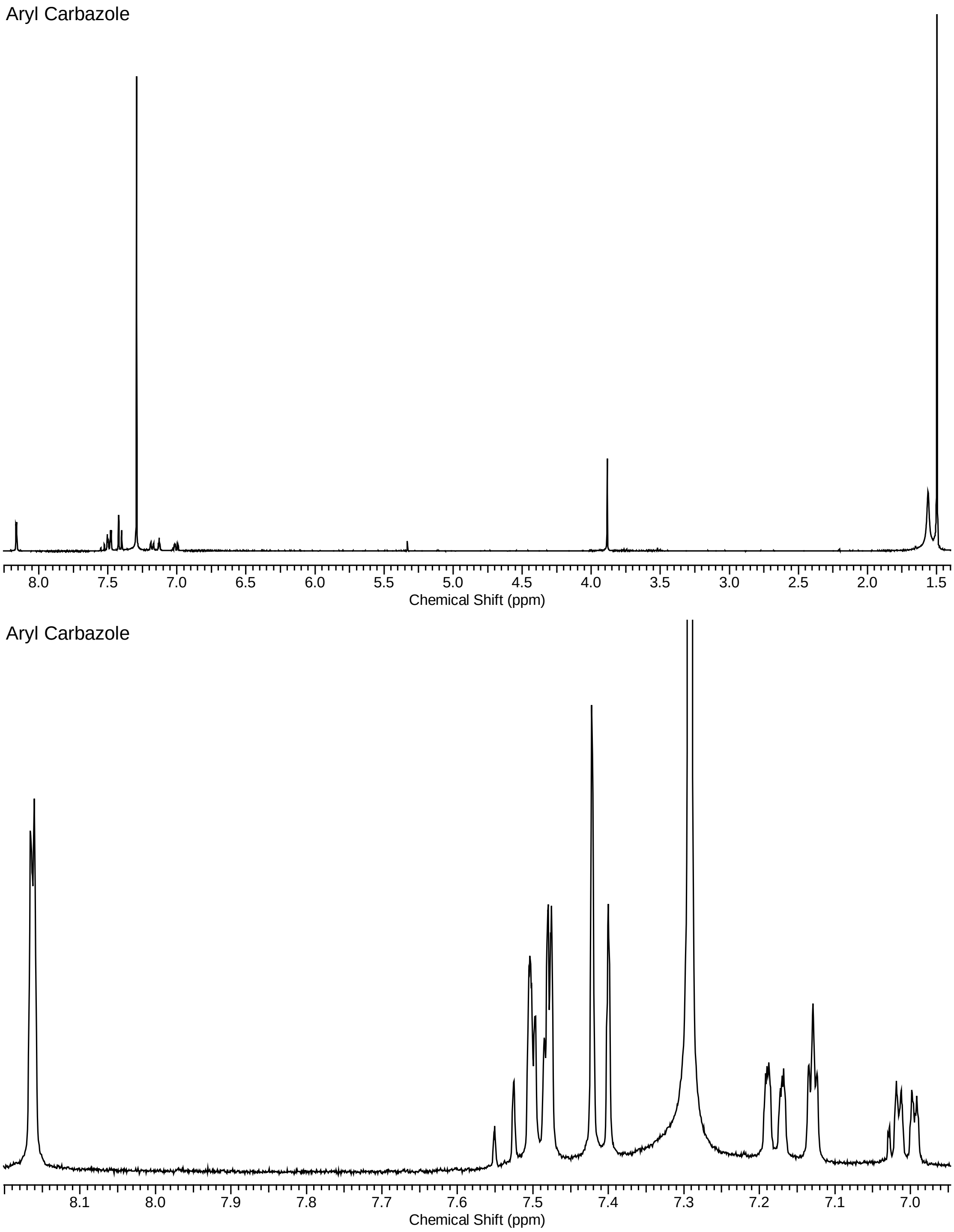
^{1}**H NMR Spectrum** of **1** in DMSO-*d*$_6$ (top, complete; bottom, arom. H). **1** contained residual acetone, dichloromethane, and methanol.



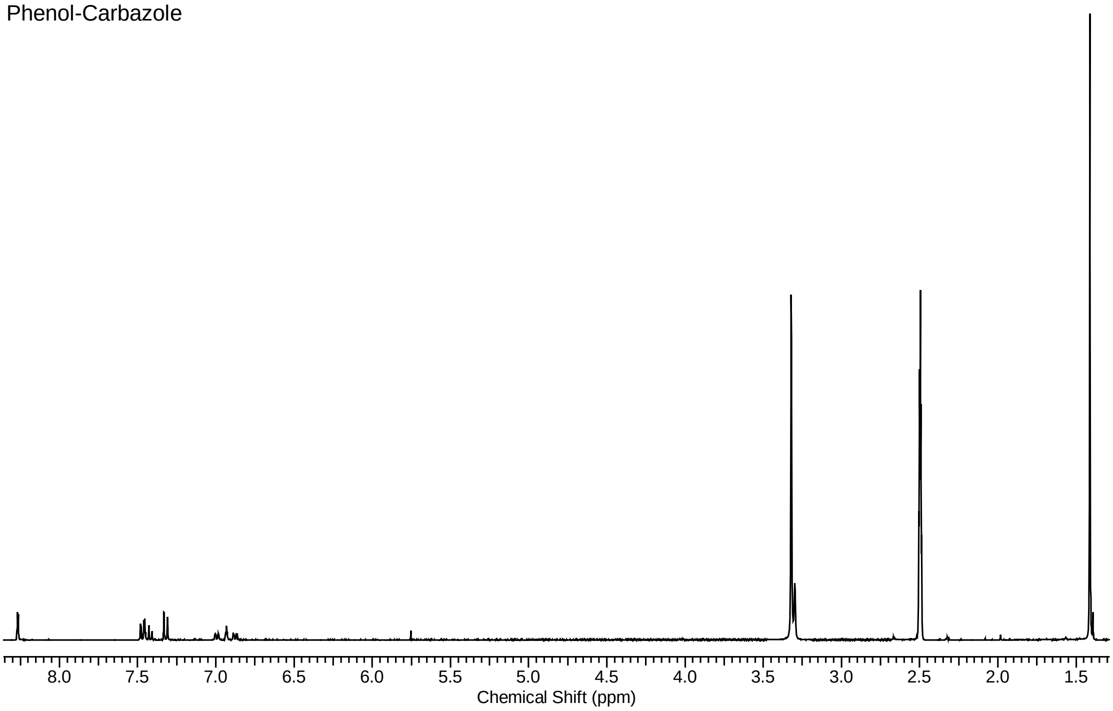
^{1}**H NMR Spectrum** of di-tert-butyl carbazole **2** in DMSO-d_6 (top, complete; bottom, arom. H).

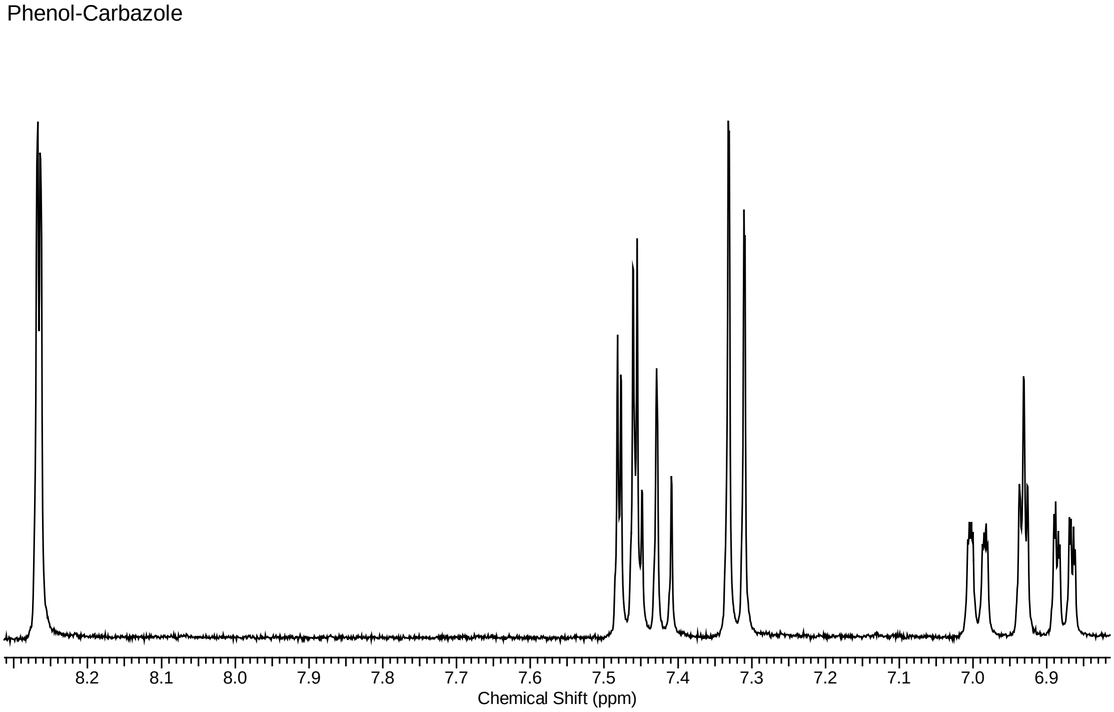


^{13}C NMR Spectrum of di-tert-butyl carbazole **2** in $CDCl_3$.

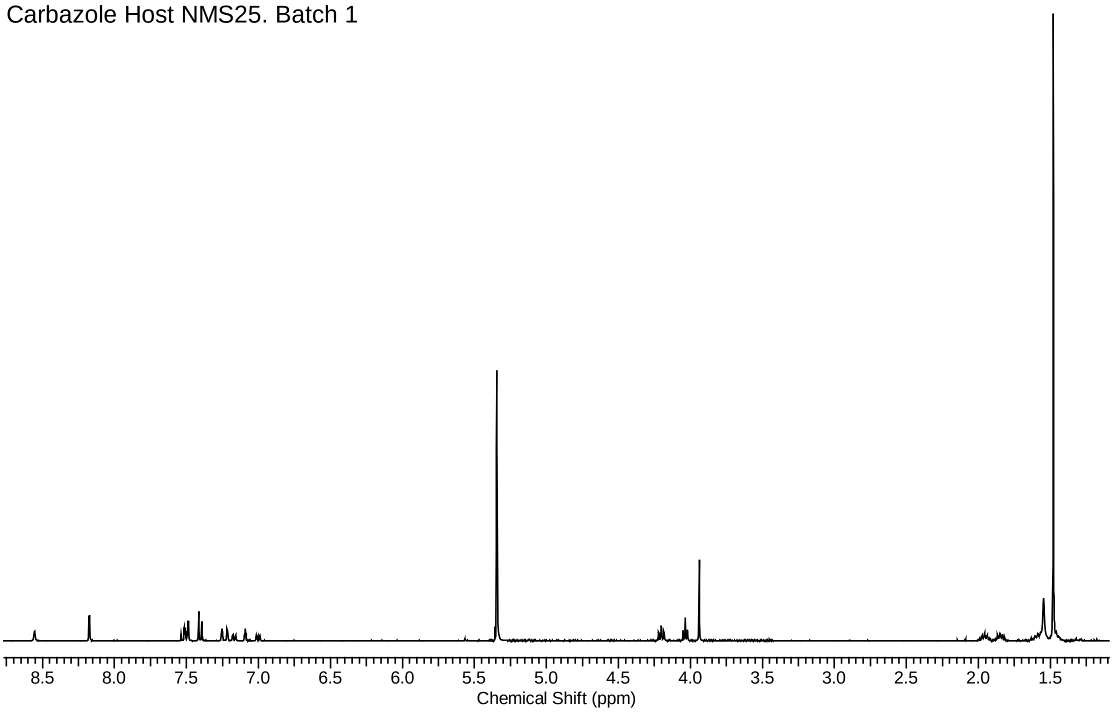


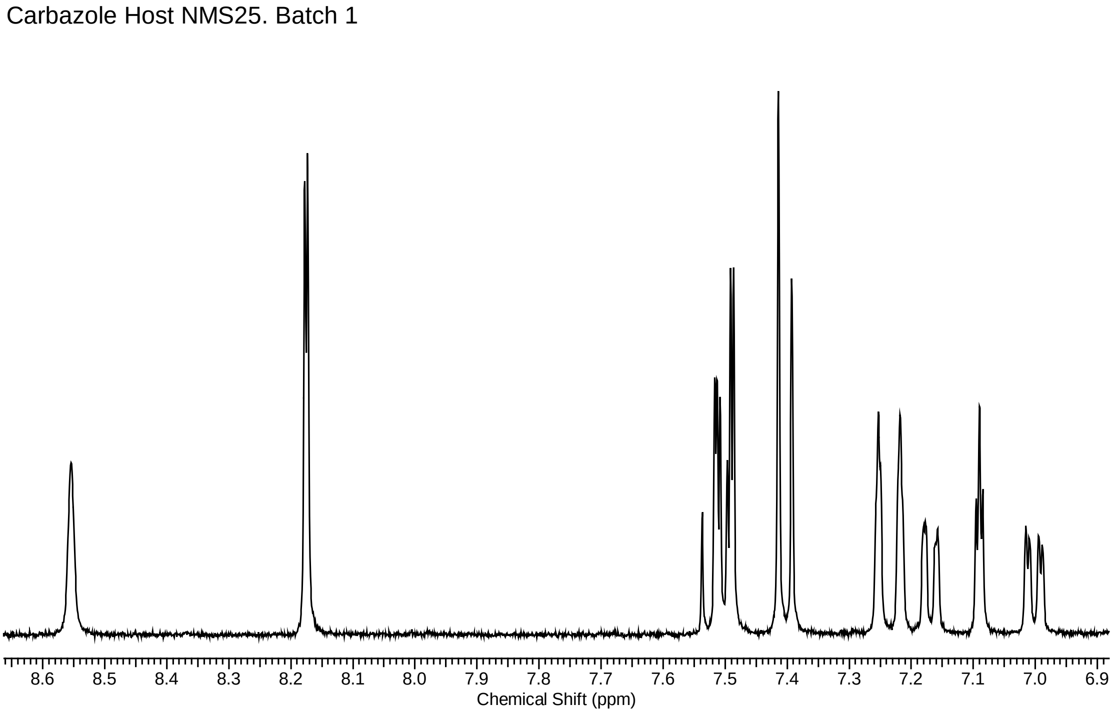
^{1}H NMR Spectrum of aryl carbazole **3** in $CDCl_3$ (top, complete; bottom, arom. H).



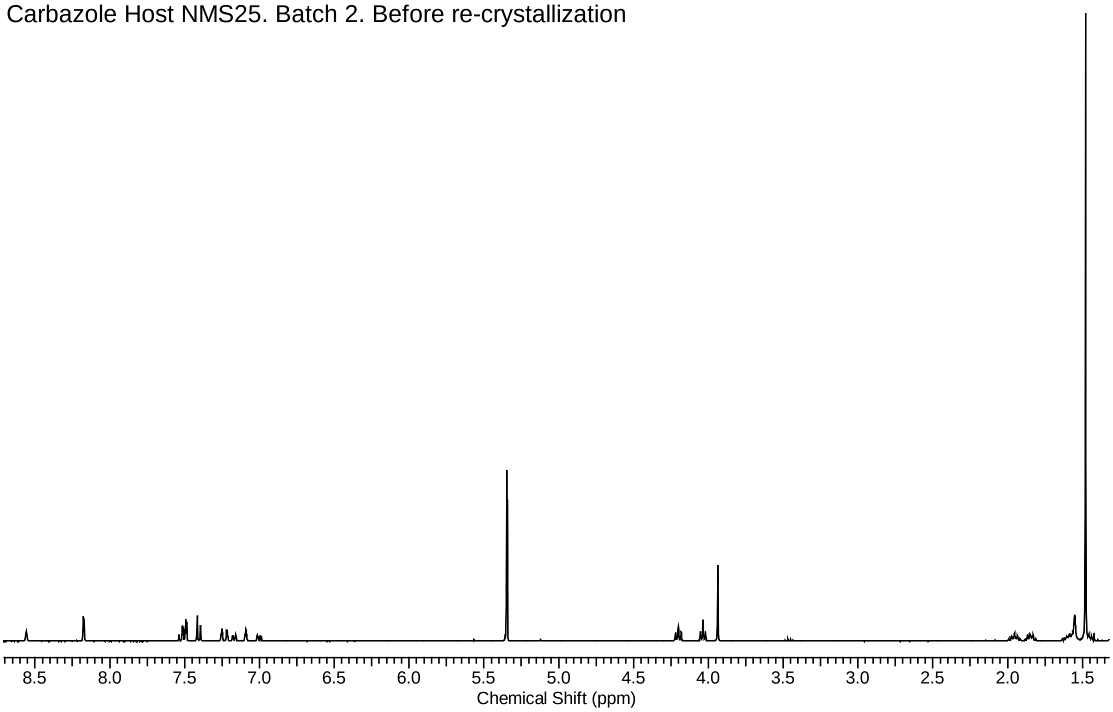


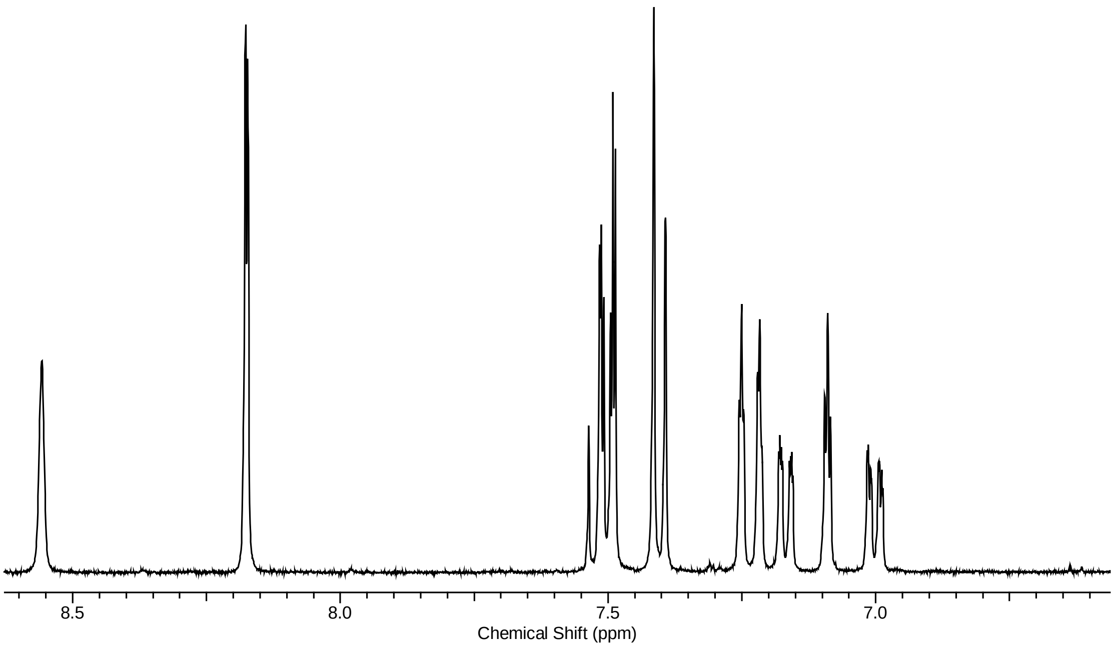
^{1}**H NMR Spectrum** of phenol-carbazole **4** in DMSO-d_6 (top, complete; bottom, arom. H).



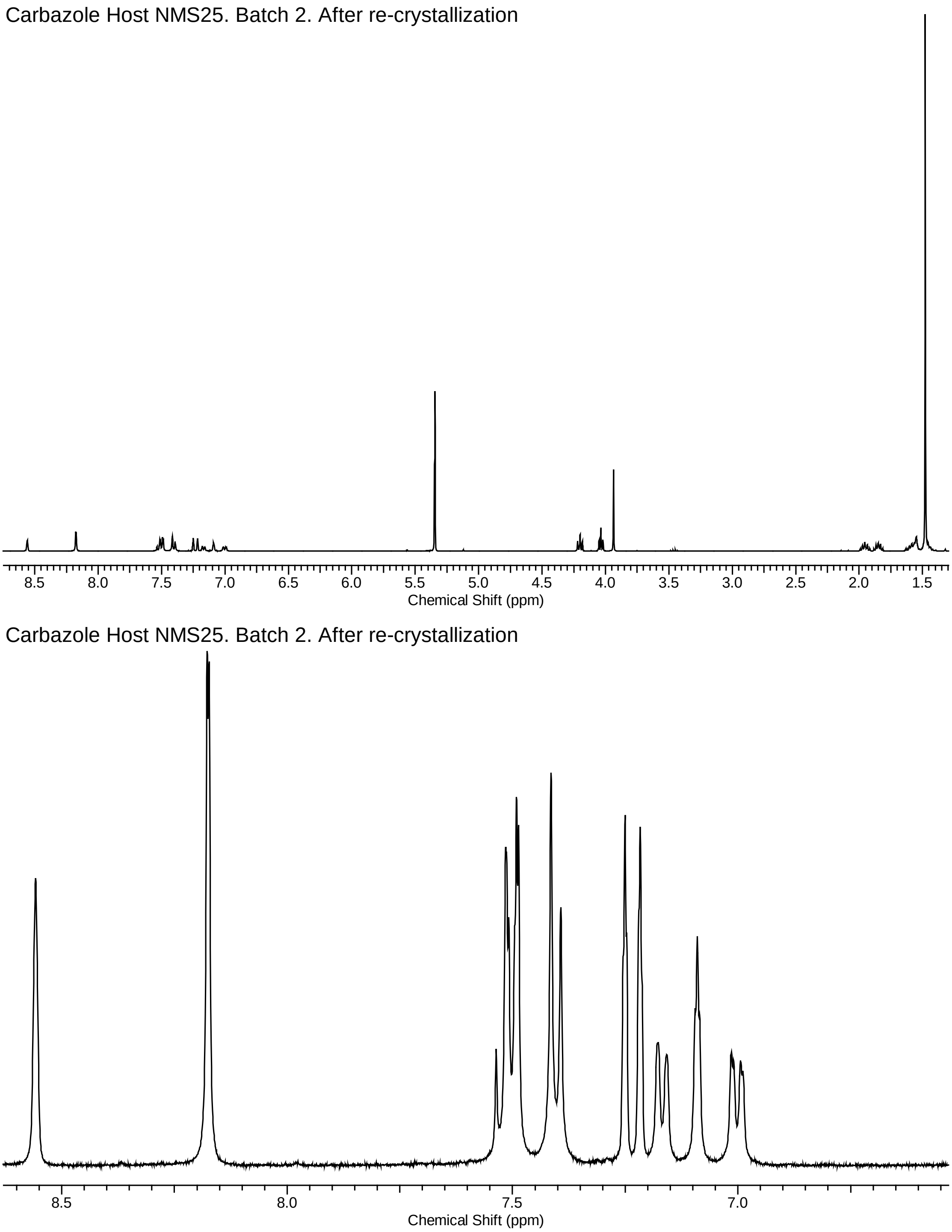


^{1}**H NMR Spectrum** of **NMS25** (Batch 1) in CD_2Cl_2 (top, complete; bottom, arom. H).

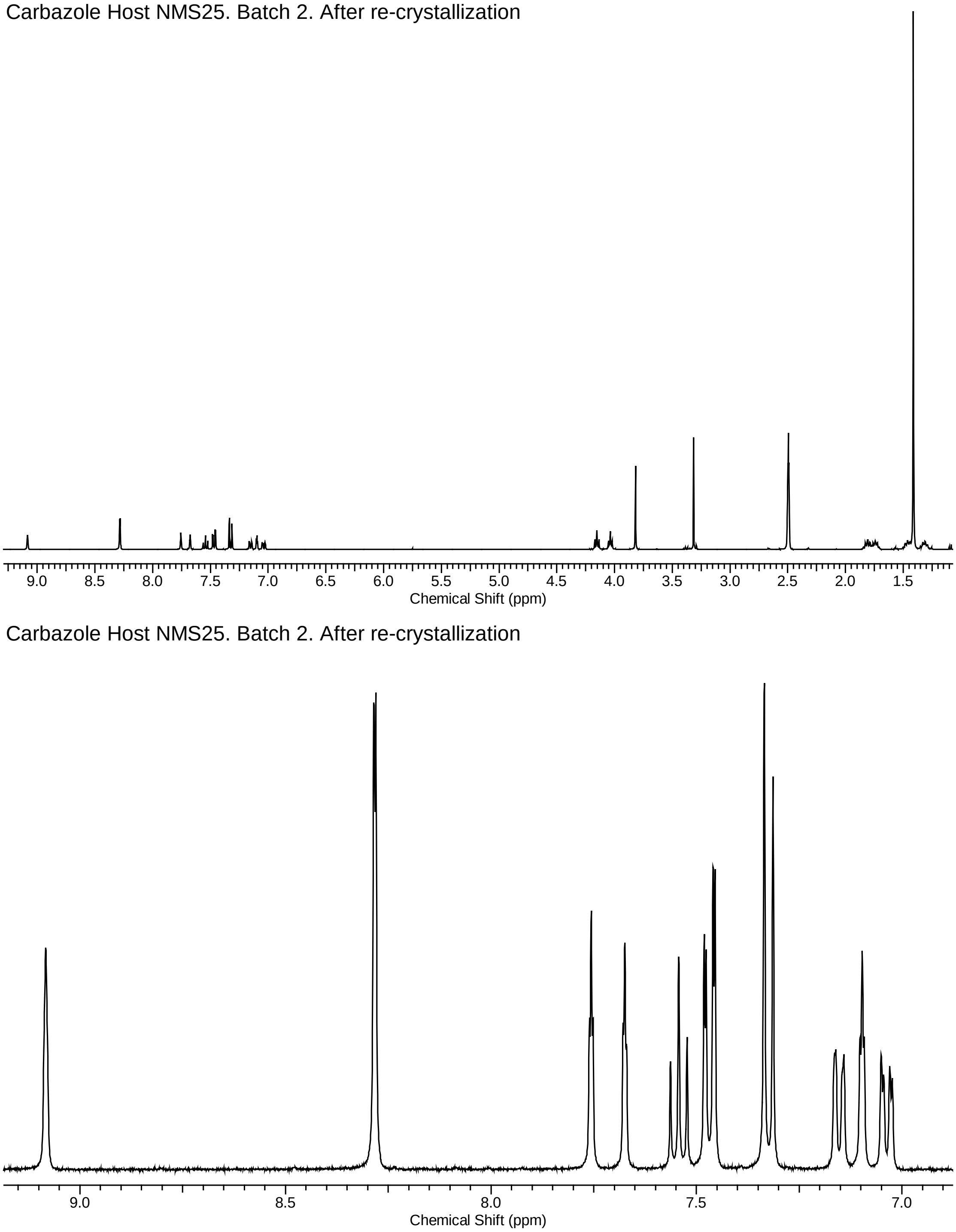

Carbazole Host NMS25. Batch 2. Before re-crystallization


Carbazole Host NMS25. Batch 2. Before re-crystallization

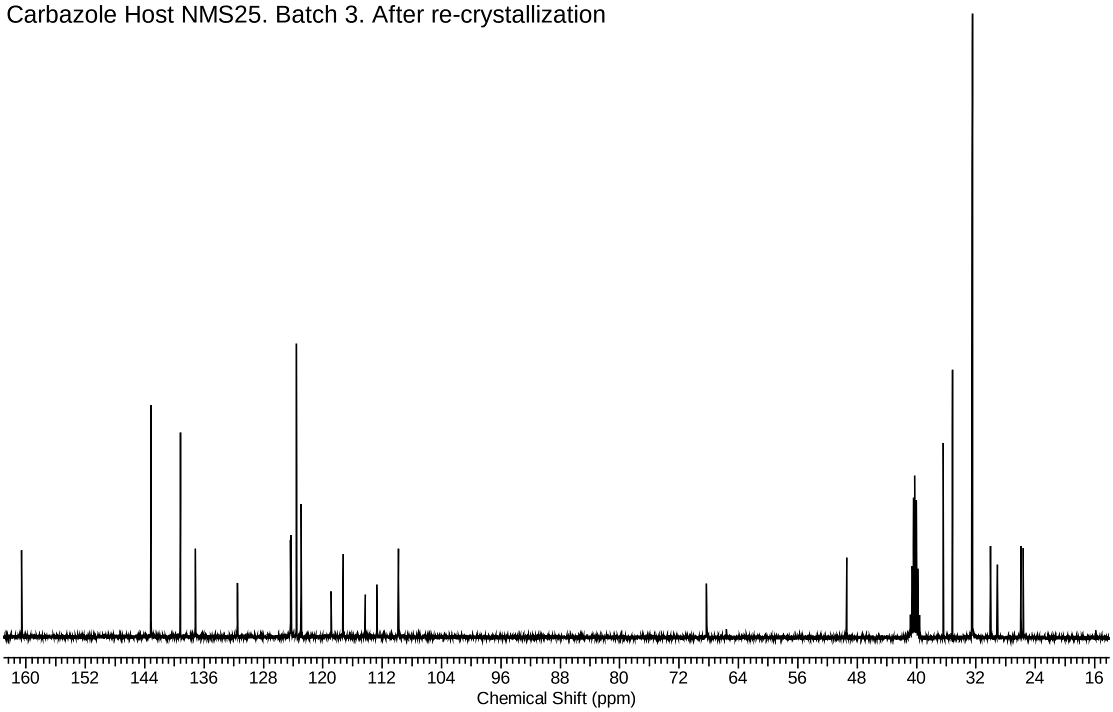
^{1}**H NMR Spectrum** of **NMS25** (Batch 2, before re-crystallization) in CD_2Cl_2 (top, complete; bottom, arom. H). The signals of impurity are observed at δ = 7.30 and 6.60–6.65 ppm.

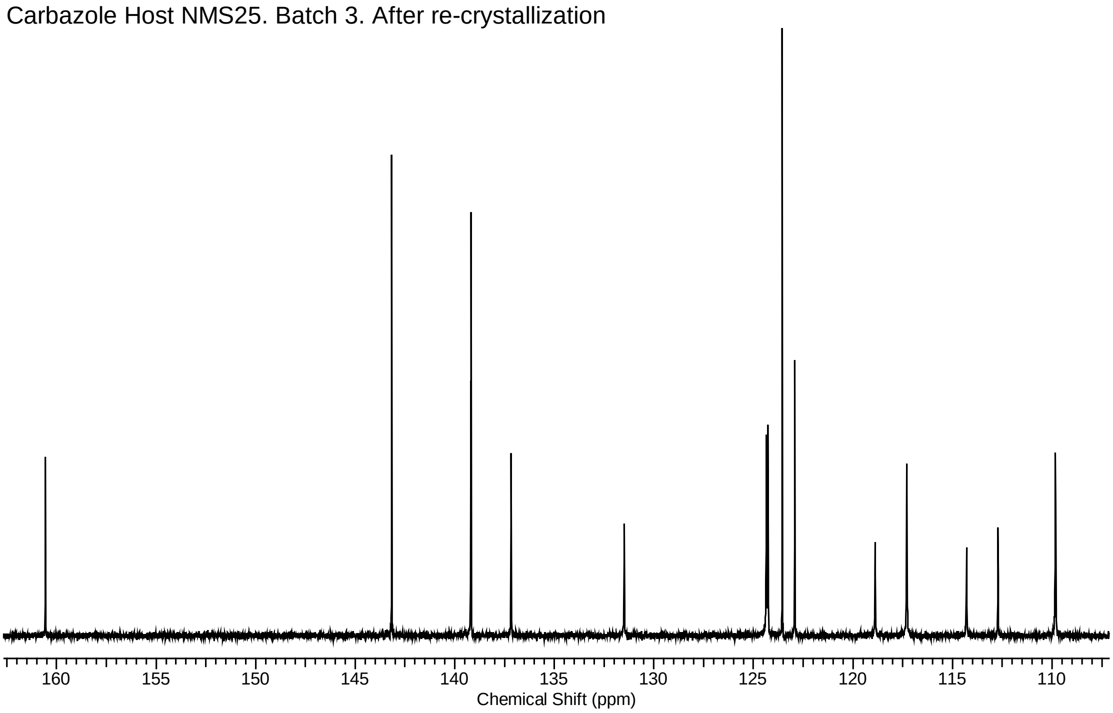


^{1}H NMR Spectrum of **NMS25** (Batch 2, after re-crystallization) in CD_2Cl_2 (top, complete; bottom, arom. H). The signals of impurity at δ = 7.30 and 6.60–6.65 ppm are nearly absent (compare with Batch 2, before re-crystallization).



^{1}H NMR Spectrum of **NMS25** (Batch 2, after re-crystallization) in DMSO-d_6 (top, complete; bottom, arom. H).





^{13}C NMR Spectrum of **NMS25** (Batch 3, after re-crystallization) in DMSO-d_6 (top, complete; bottom, arom. C). **NMS25** contained residual ether.