

Supporting Information

α -Imino Iridium Carbenes from Imidoyl Sulfoxonium Ylides: Application in the One-step synthesis of Indoles

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Content

I. Setup for microwave experiments	S2
II. NMR Spectras of Imidoyl Sulfoxonium Ylides	S3
III. NMR Spectras of Indoles	S30

I. Setup for microwave experiments

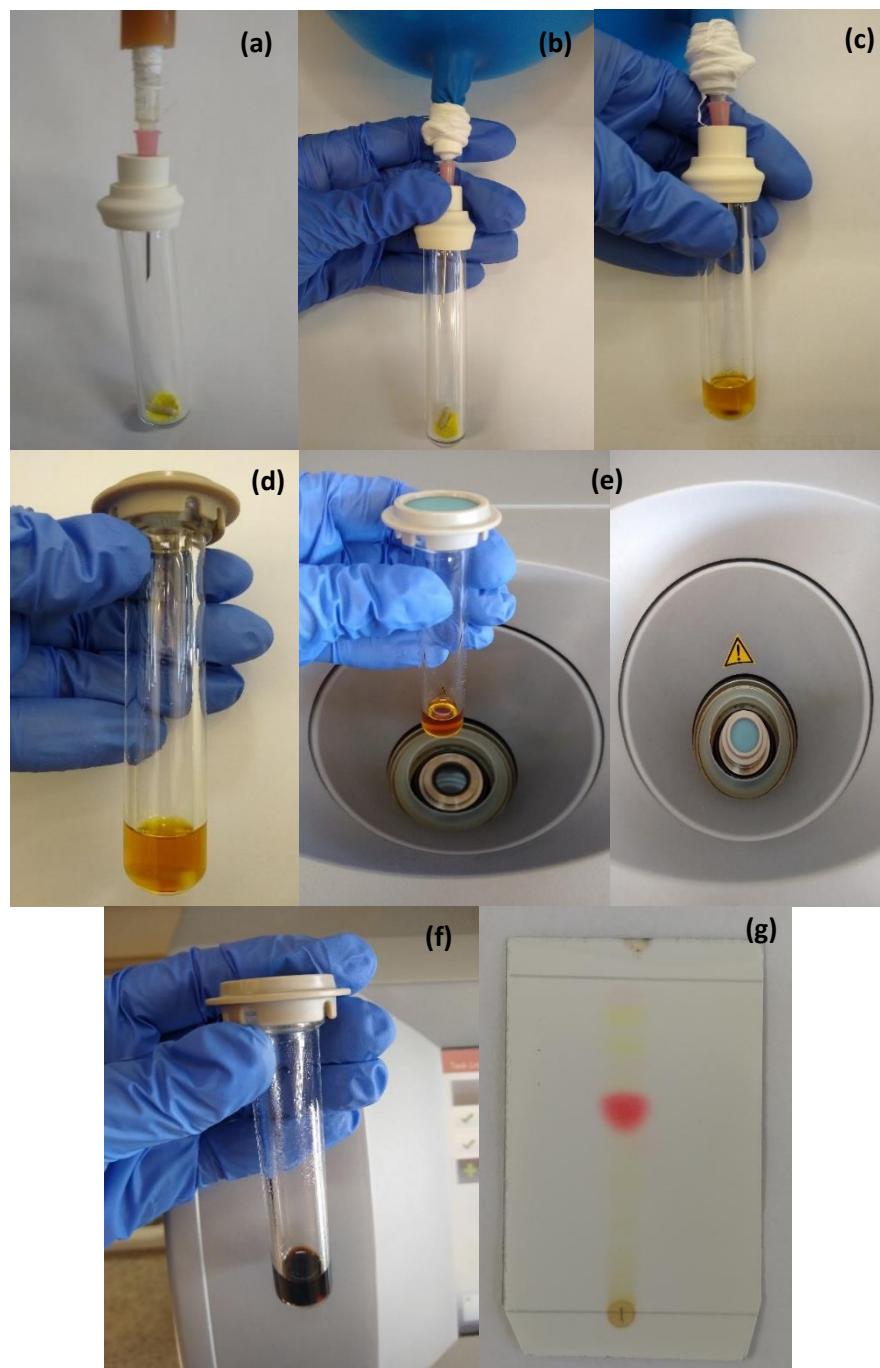


Figure S1. (a) Sulfur ylide **2a** + iridium catalyst in a microwave glass vial (10 mL) equipped with a magnetic stirrer, closed with a tightly fitted rubber septa and under a vacuum system. (b) The vacuum line was removed and the system filled with ultra-purified argon. (c) Dry solvents N,N-dimethylformamide (0.5 mL) and toluene (0.5 mL) were added with syringe. (d) The rubber septum was removed and the microwave vial was quickly capped with a teflon microwave cap. (e) Microwave equipment. (f) Mixture after the reaction time. (g) TLC of the crude rection to the formation of **5a**

II. NMR Spectra

Due to the possibility of rotamers, the signals of the NMR spectra at room temperature show broadened signals and low resolution (Figure S2 and S4). NMR spectra with better resolution can be acquired using DMSO as solvent at a temperature of 80 °C (Figure S3 and S5). For practical reasons, NMR characterization at 80 °C was applied to some selected ylides substrates as an example.

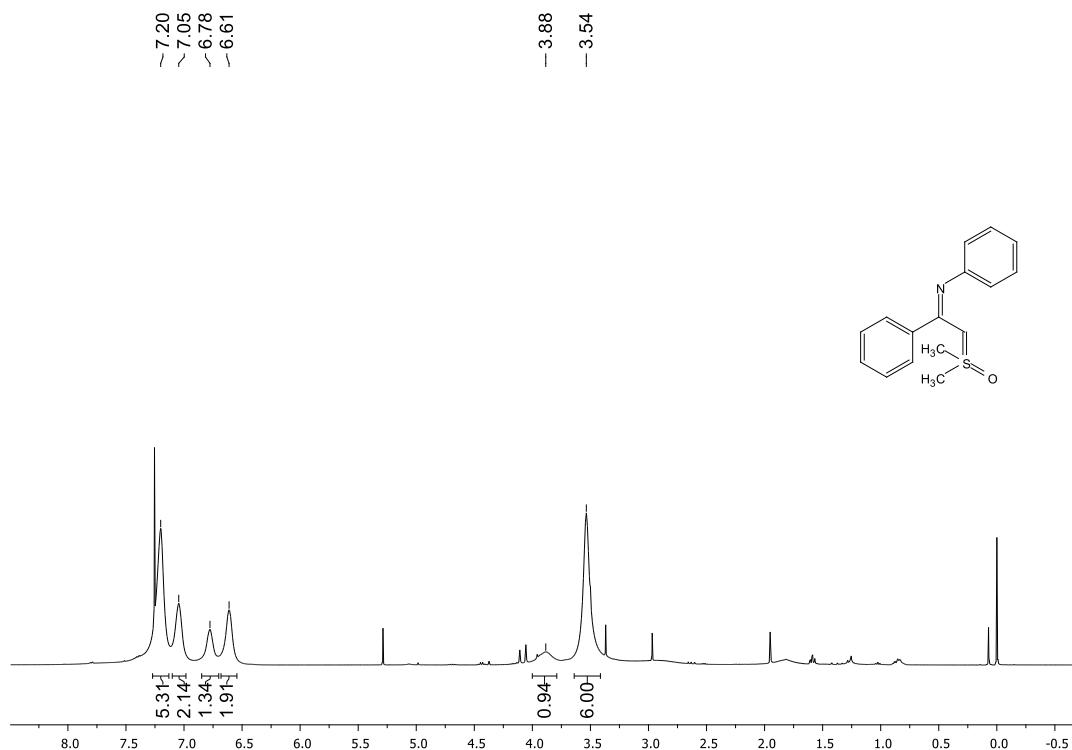


Figure S2. ¹H NMR spectra (400 MHz, CDCl₃) of **2a**.

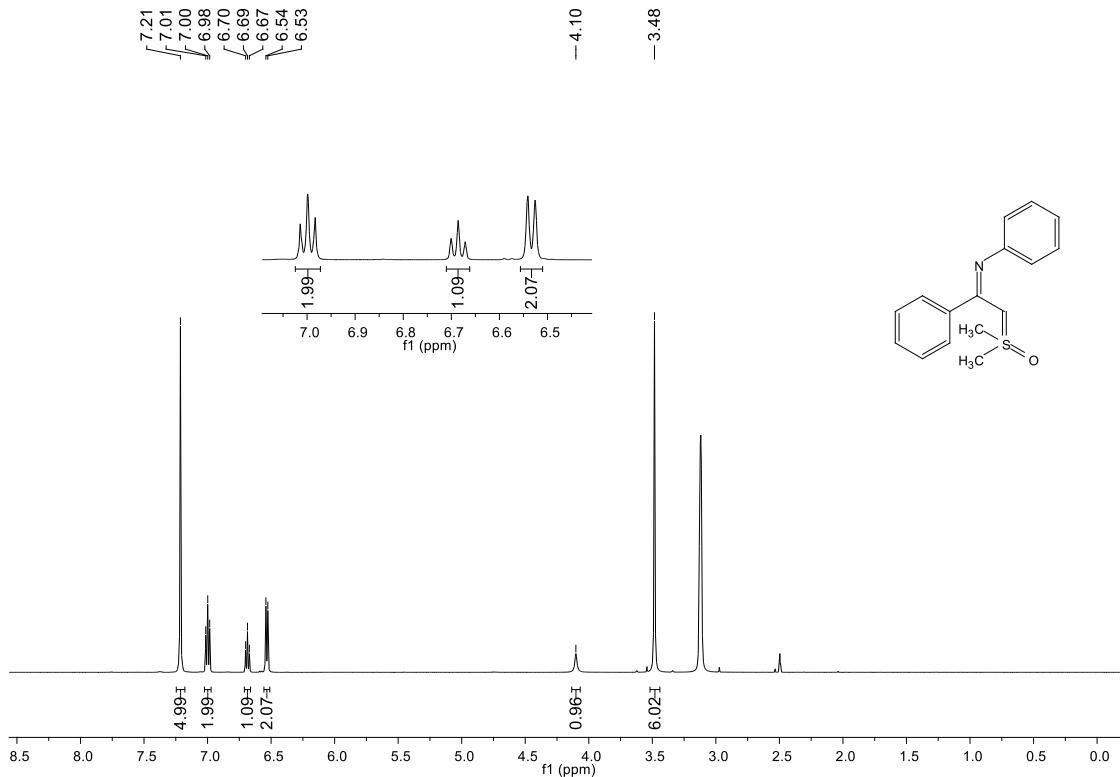


Figure S3. ^1H NMR spectra (500 MHz, DMSO, 80°C) de **2a**.

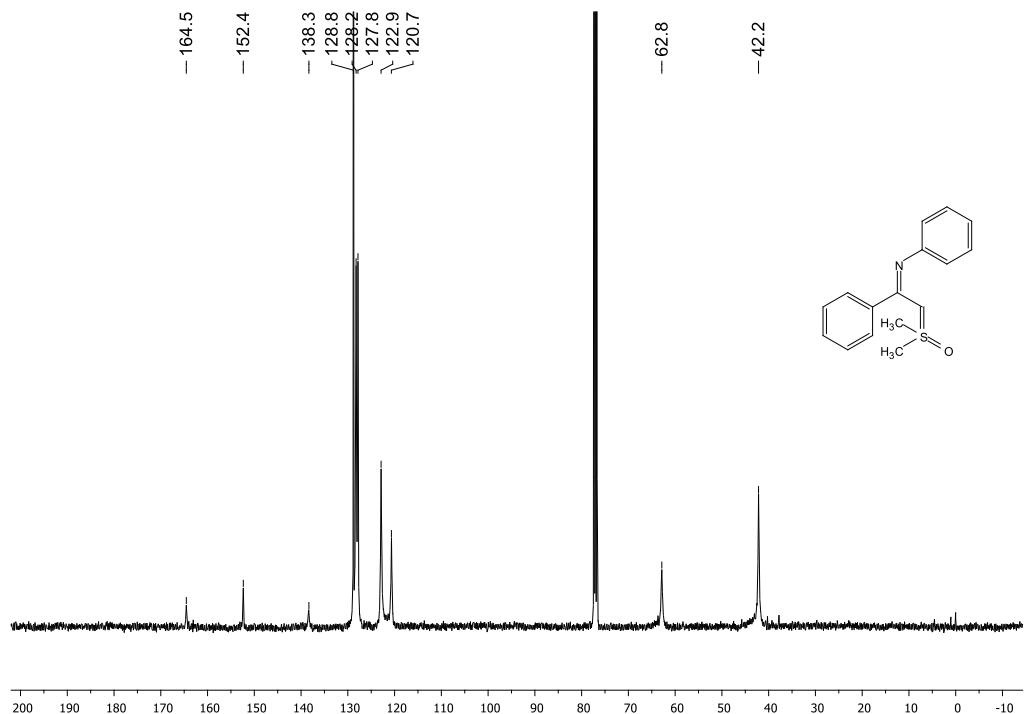


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra (100 MHz, CDCl_3) of **2a**.

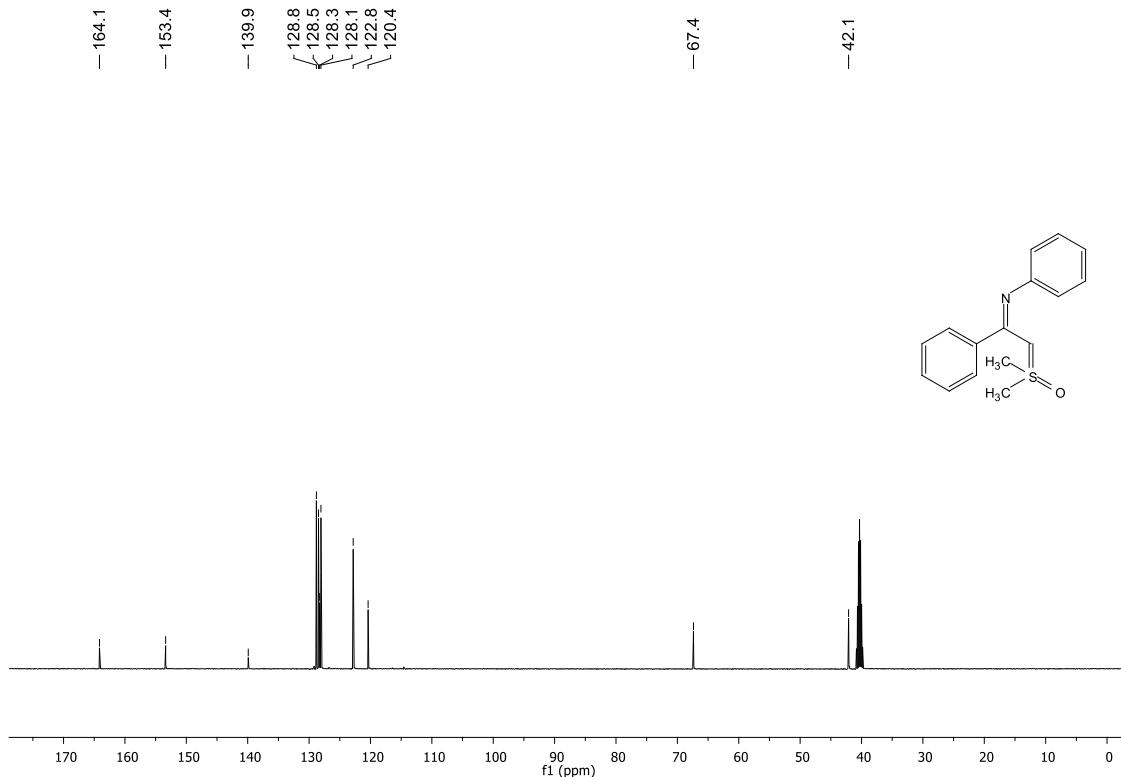
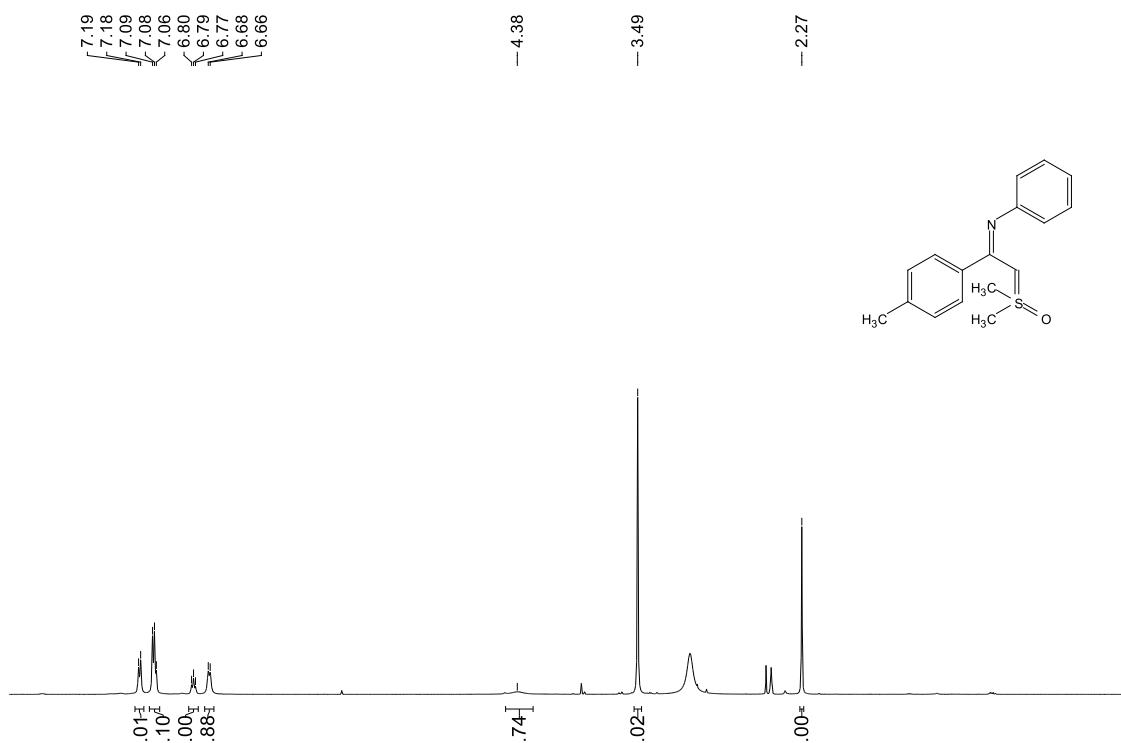
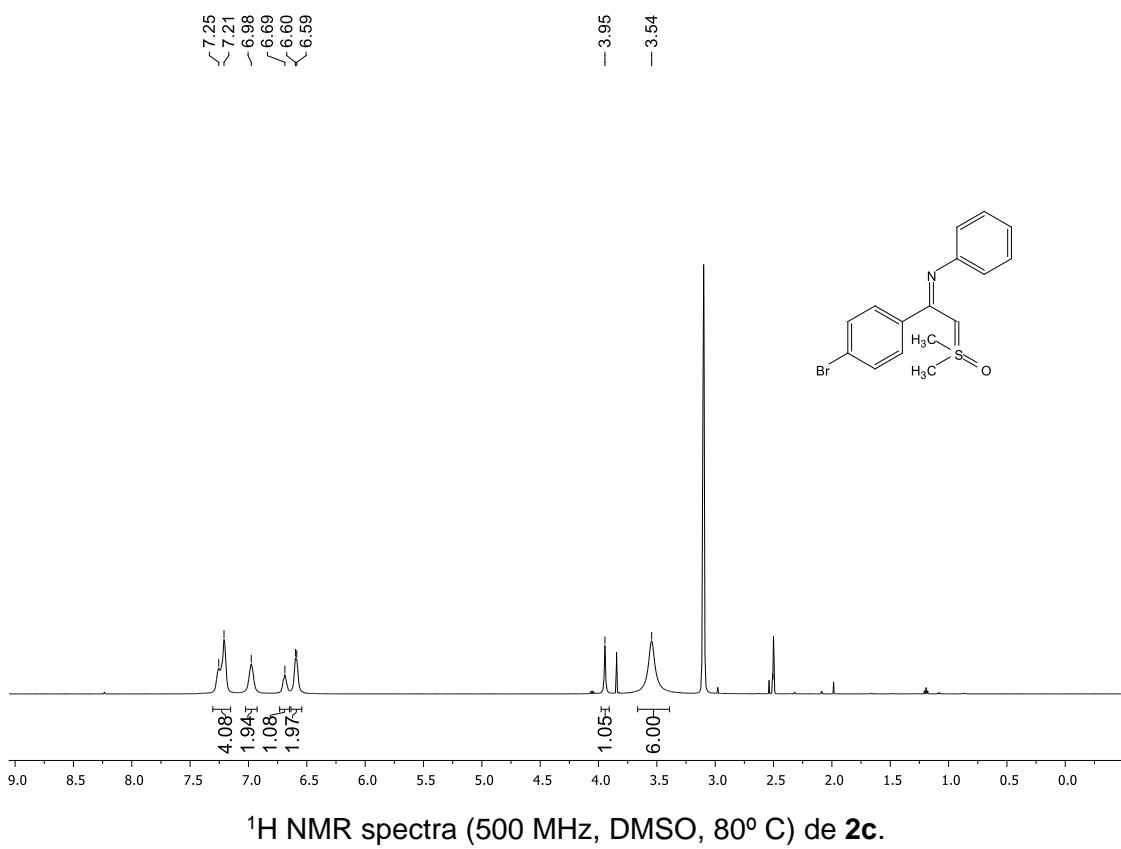
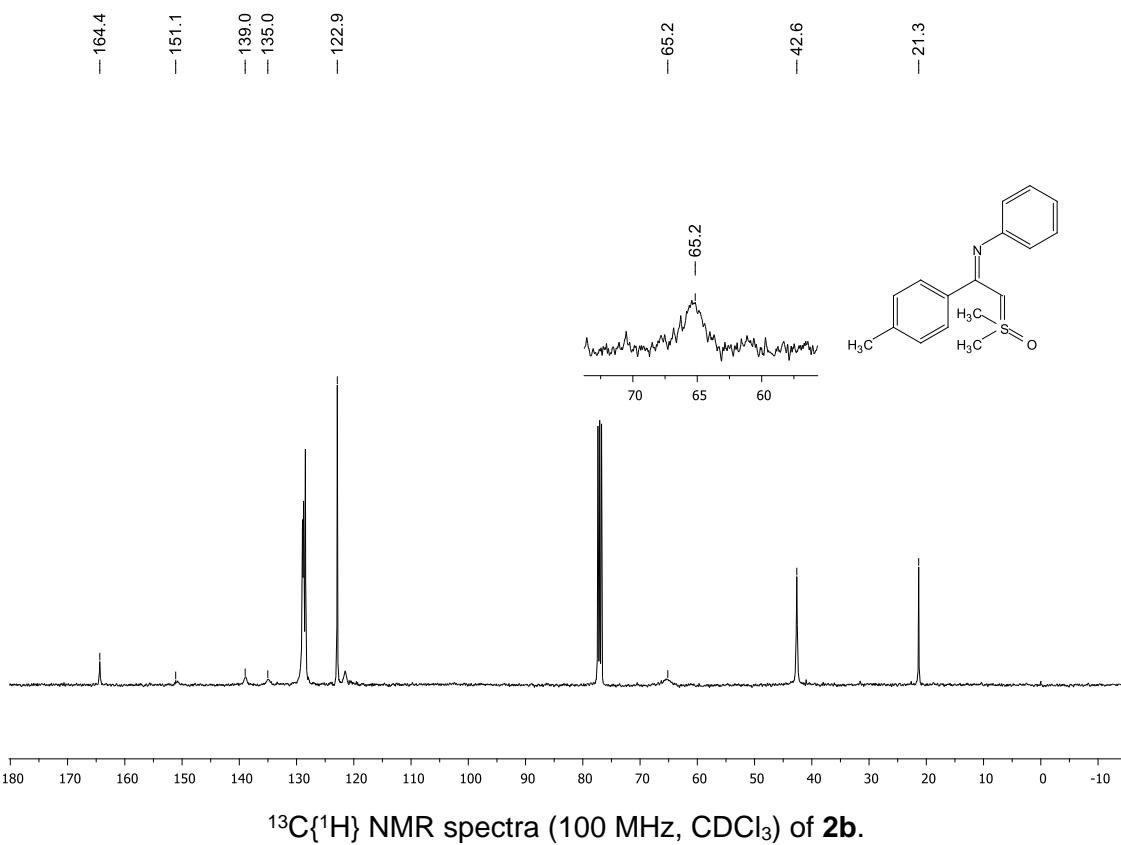
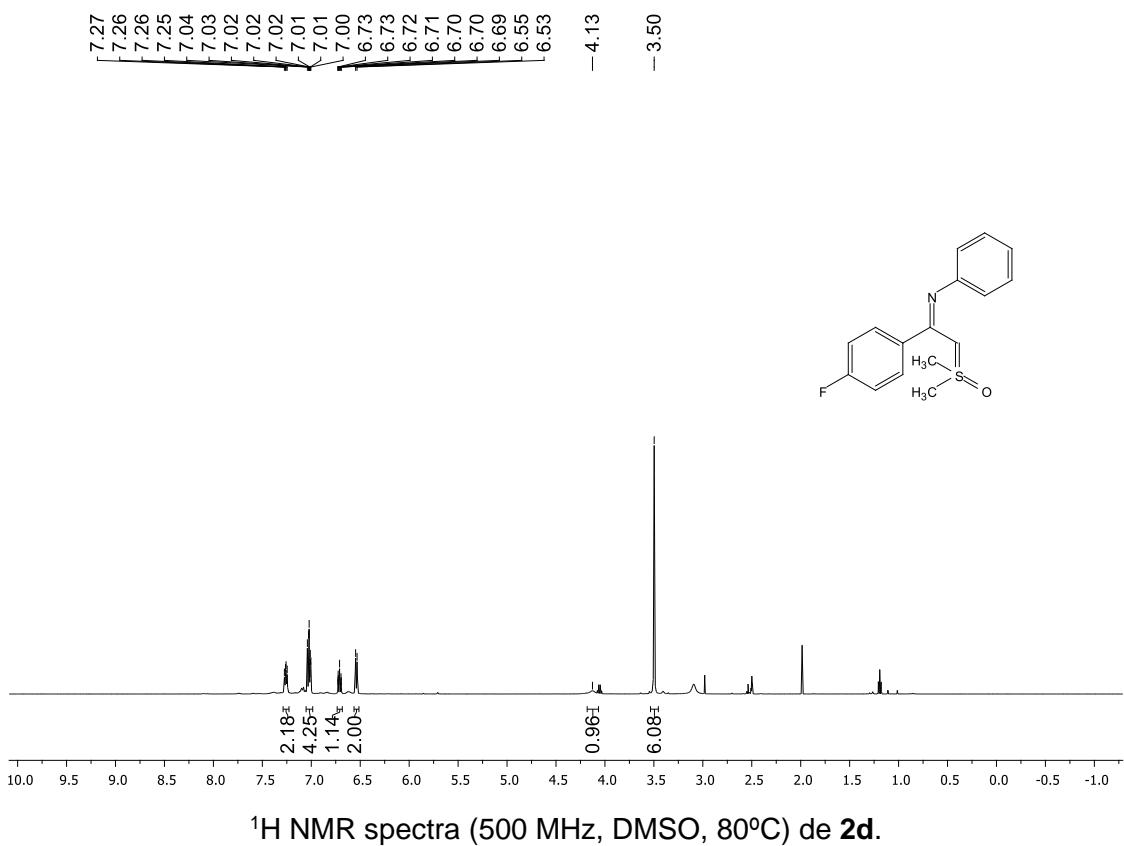
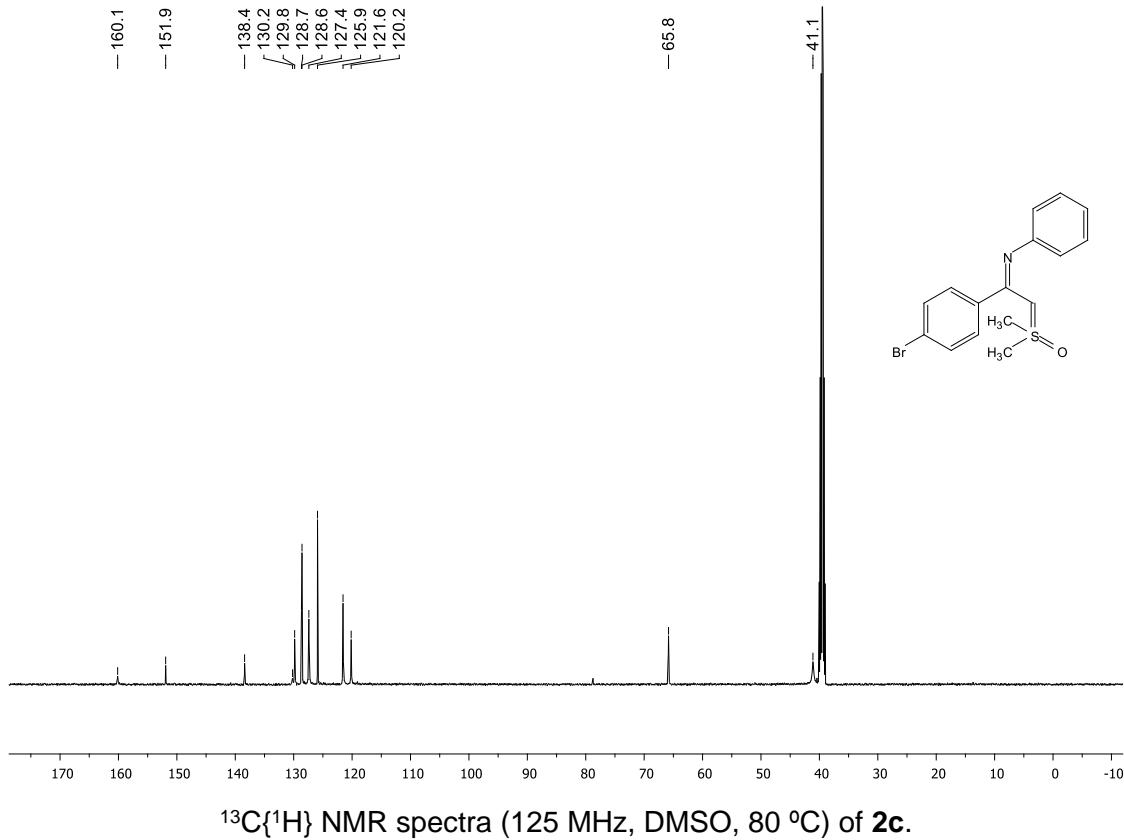


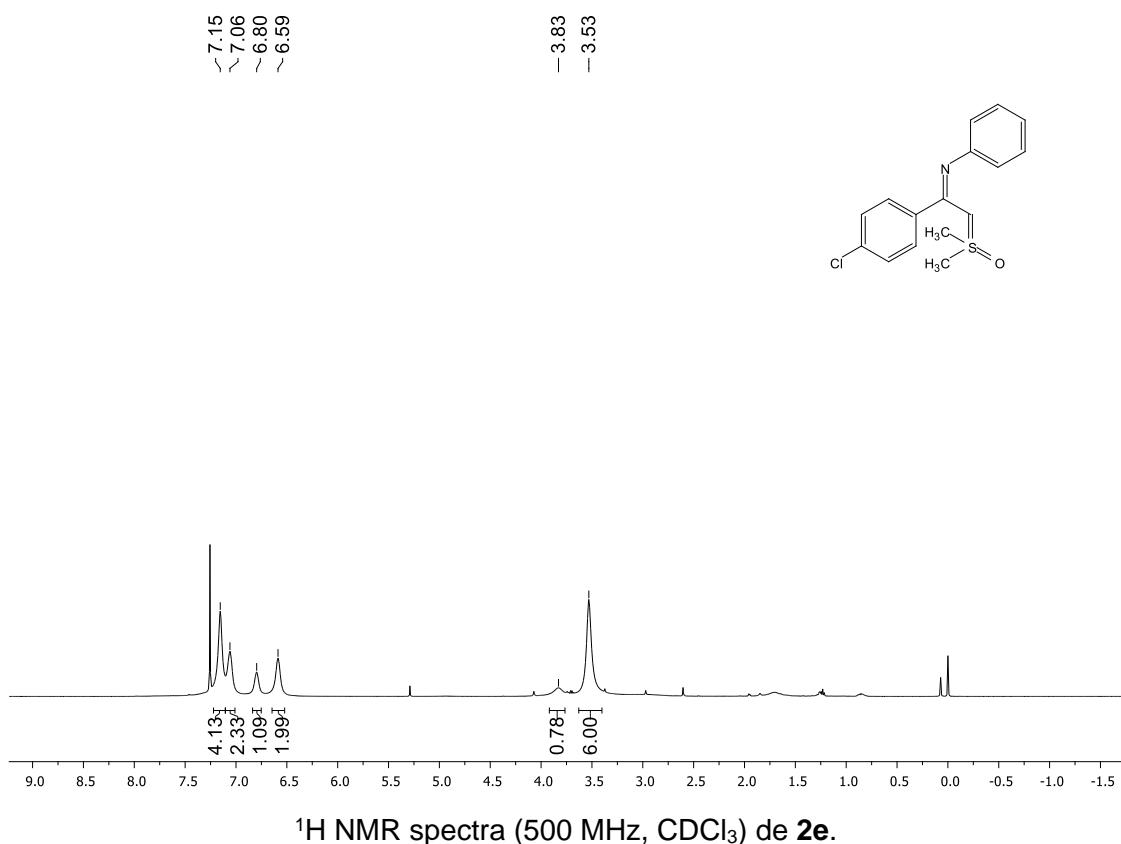
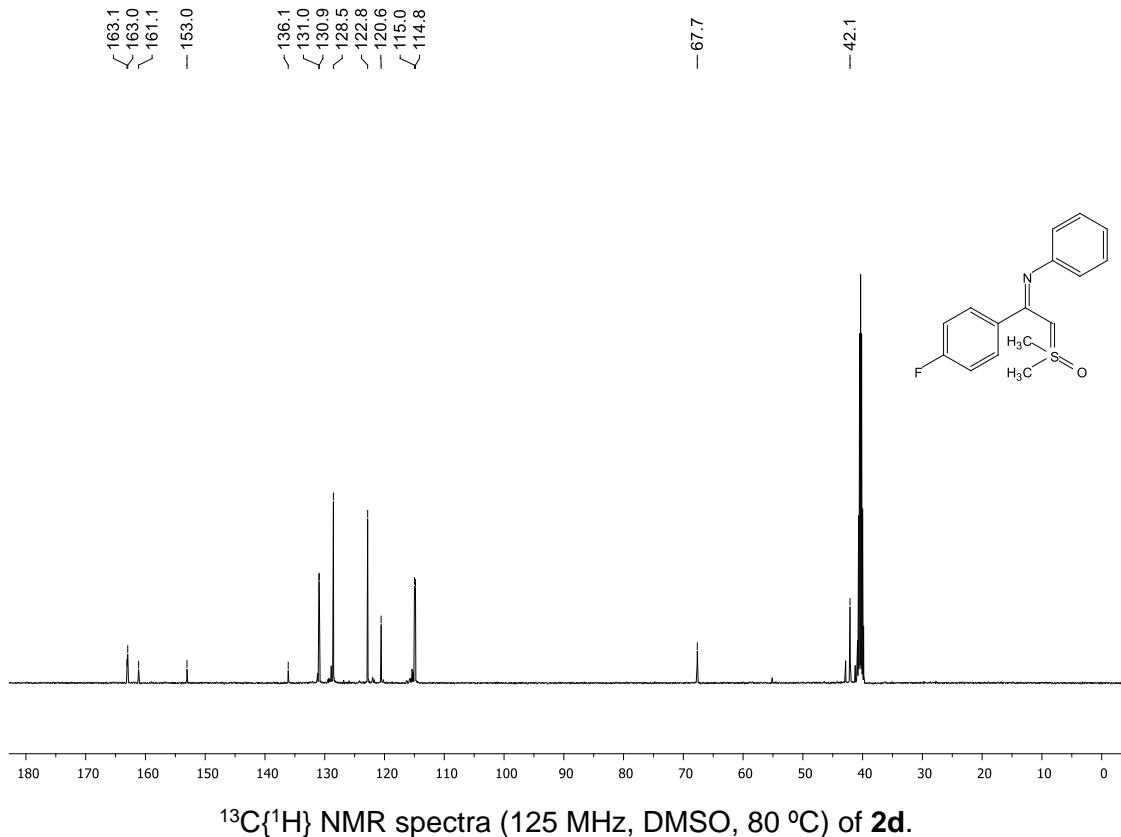
Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra (125 MHz, DMSO, 80°C) de **2a**.

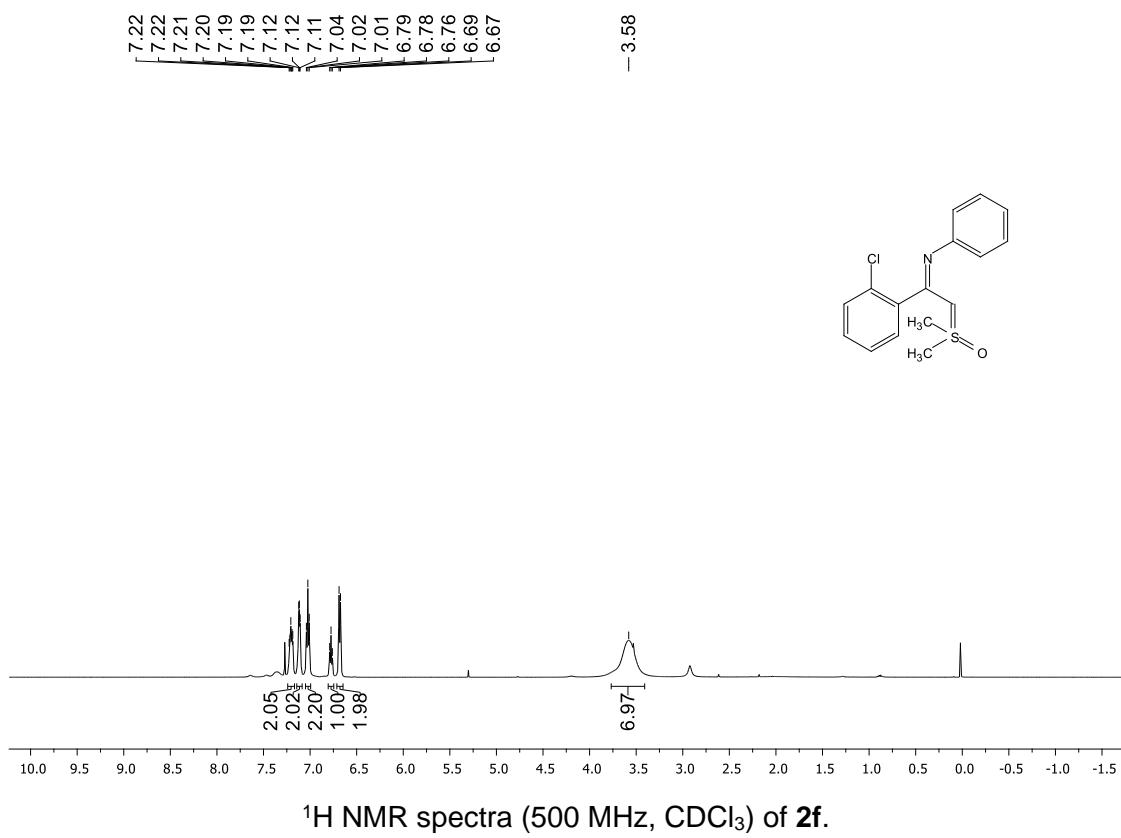
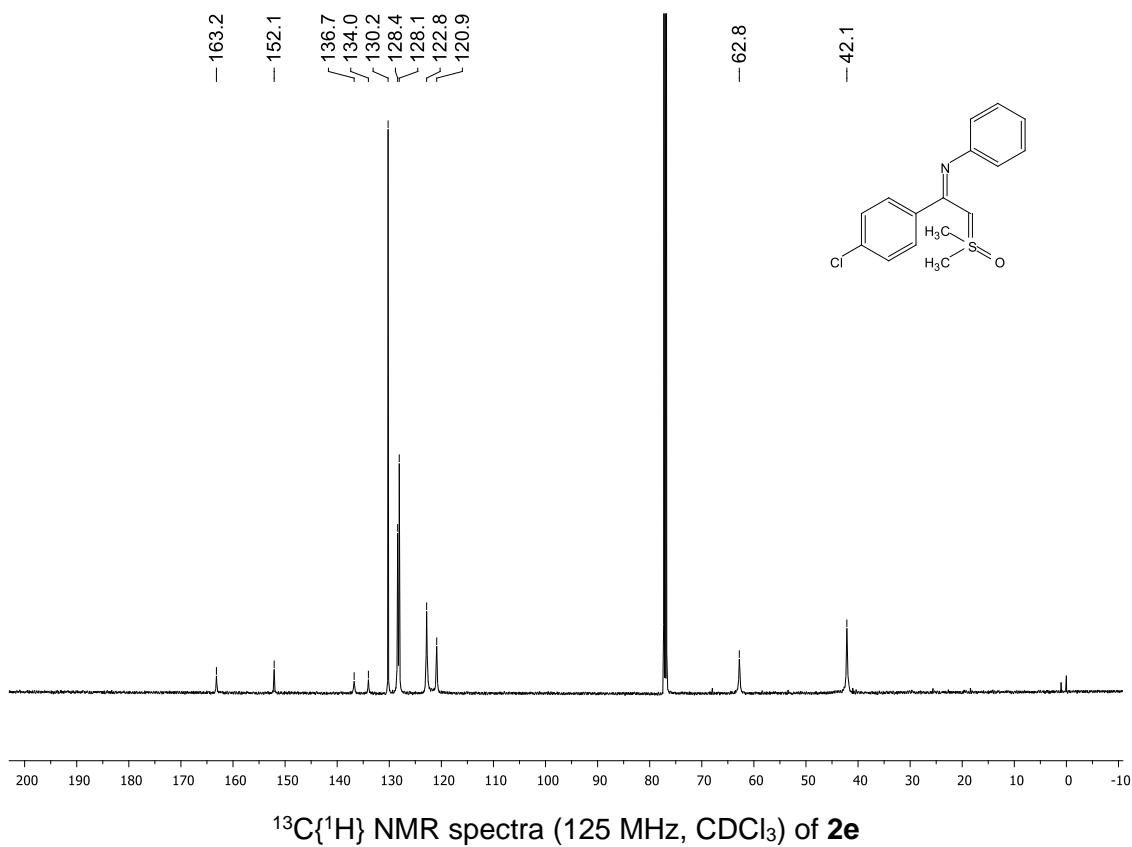


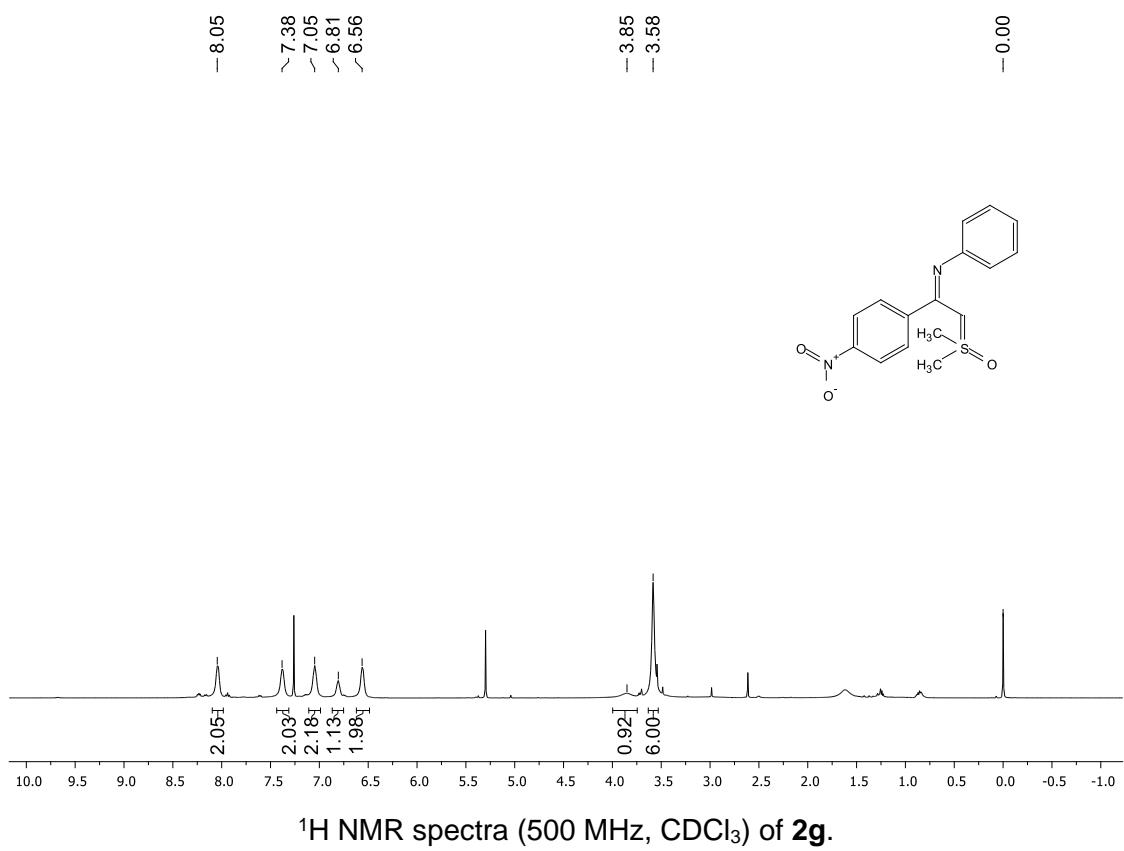
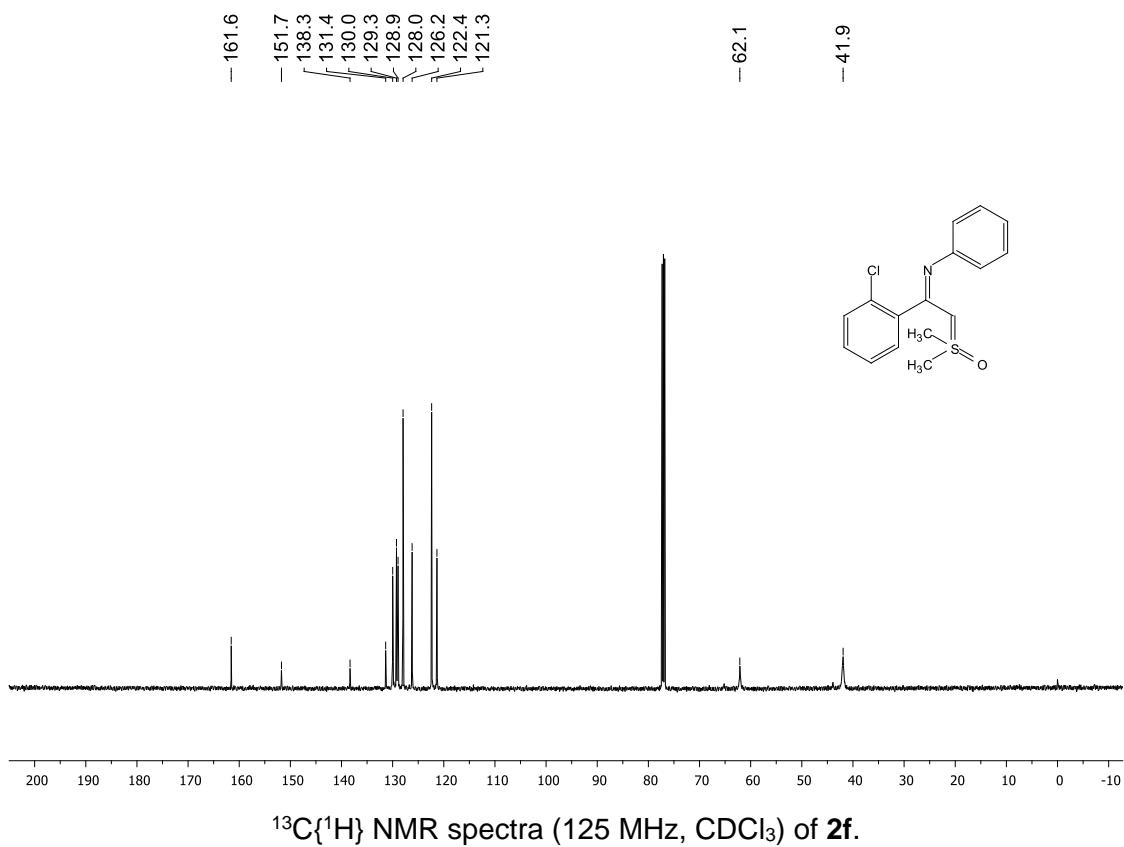
^1H NMR spectra (500 MHz, DMSO, 80°C) de **2b**.

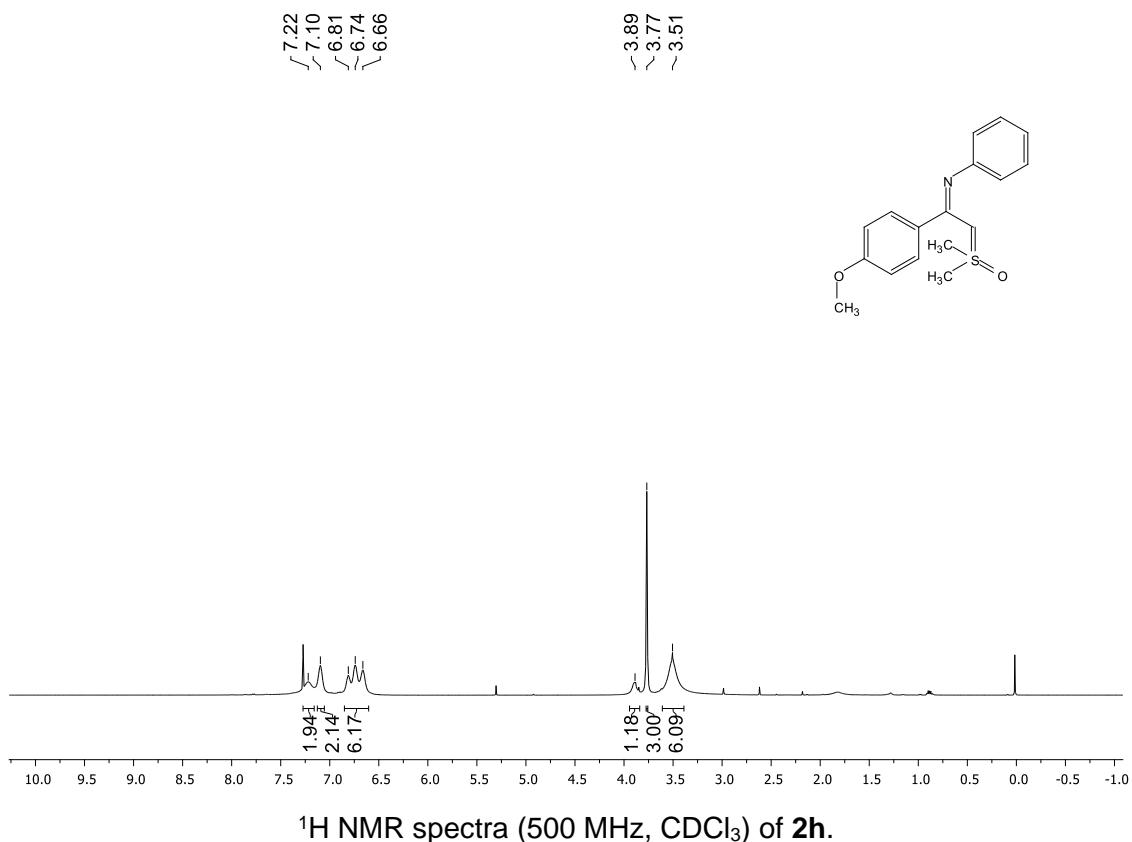
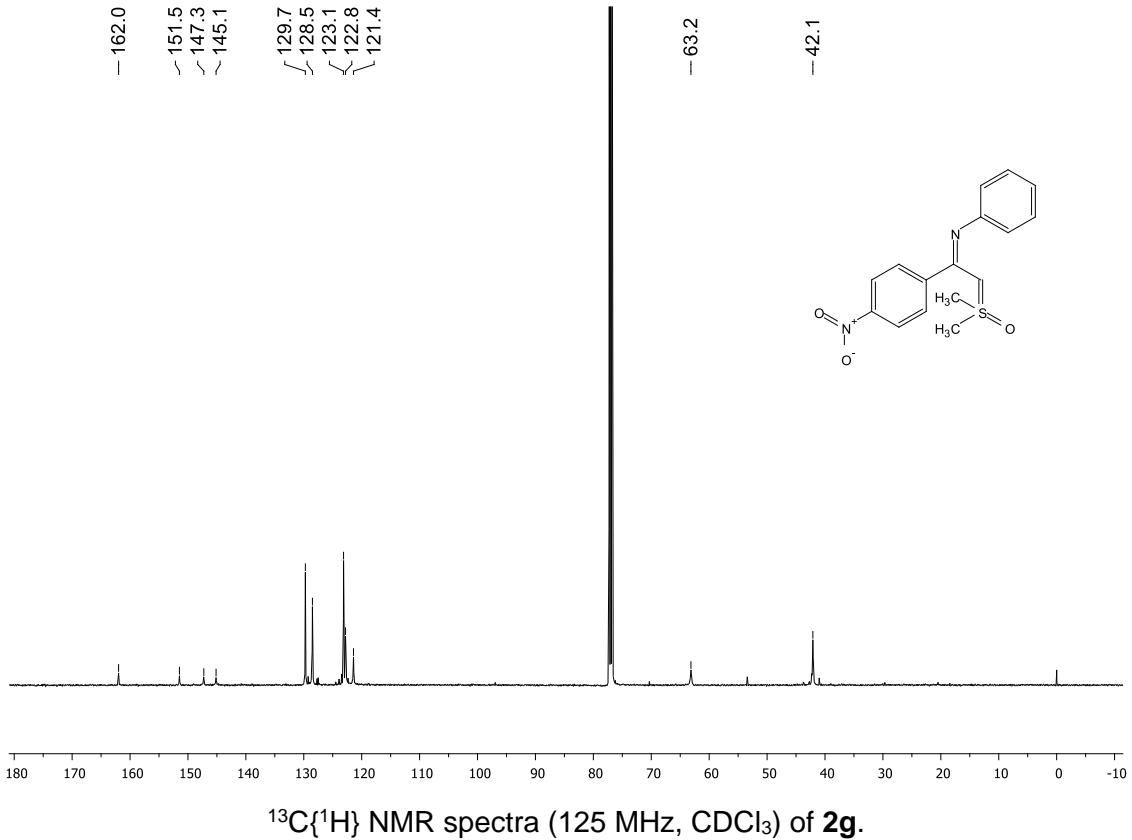


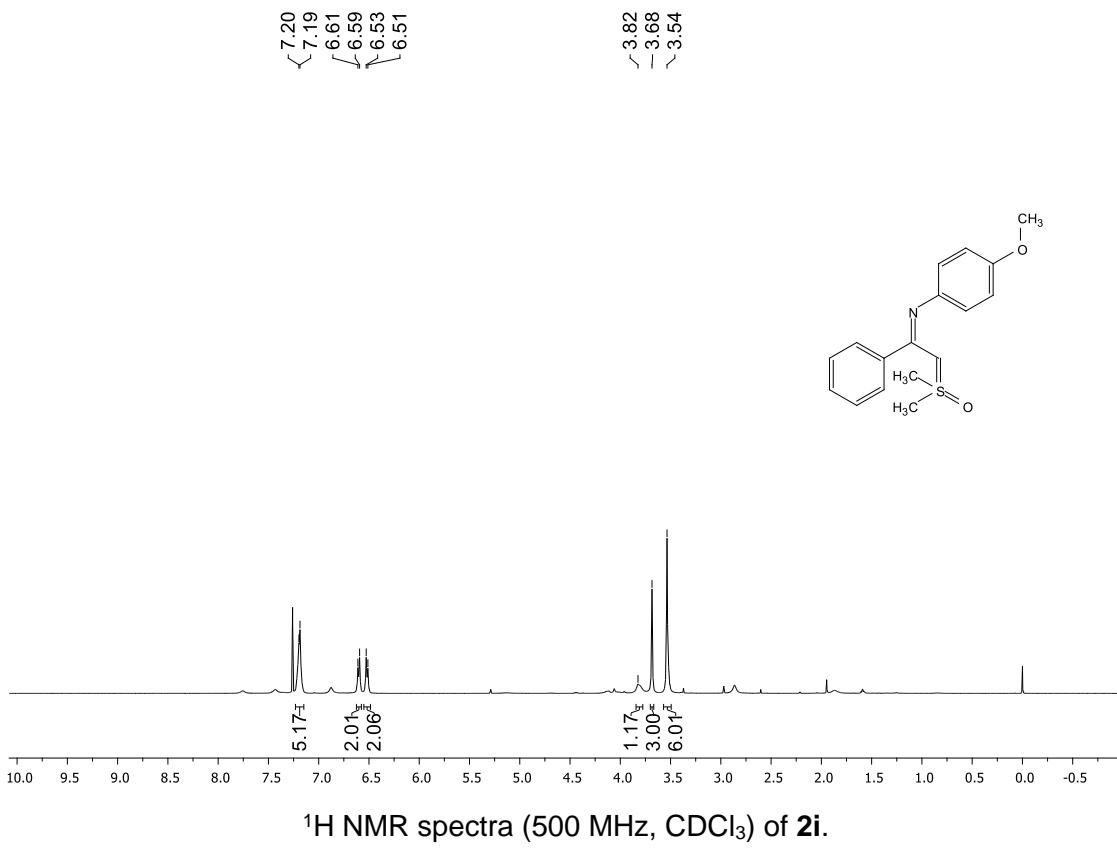
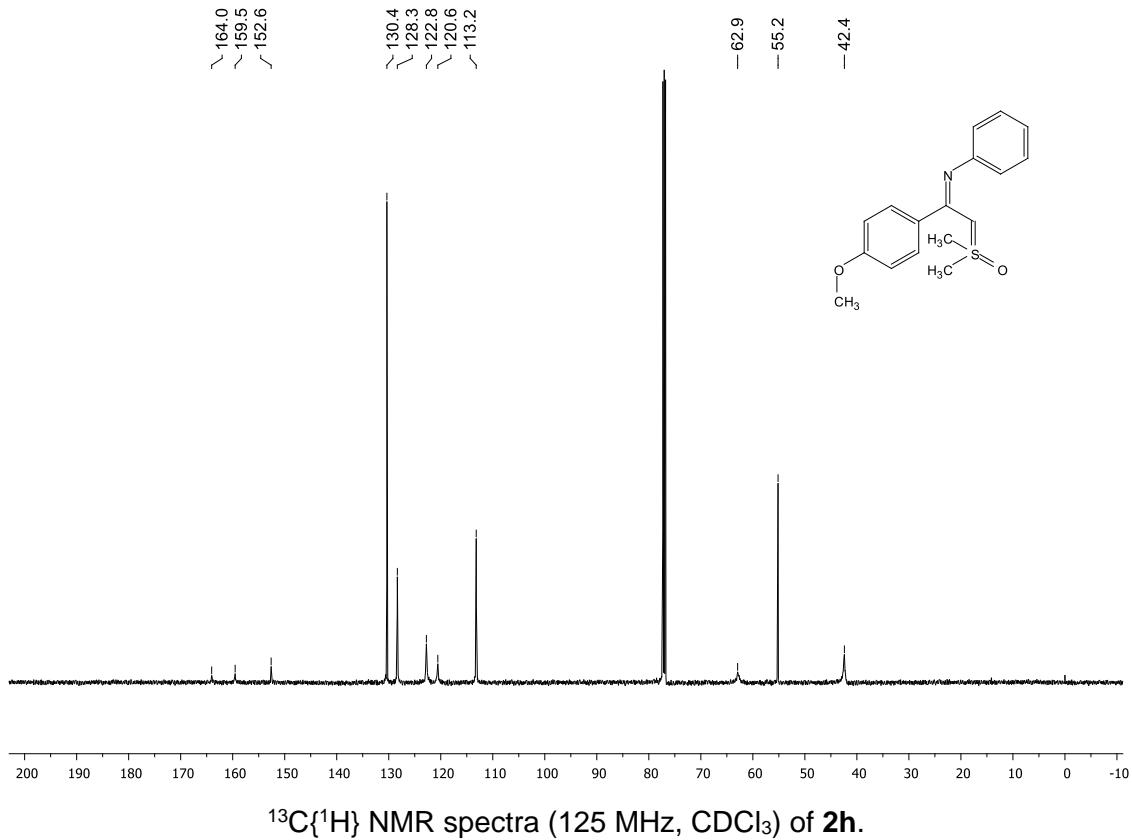


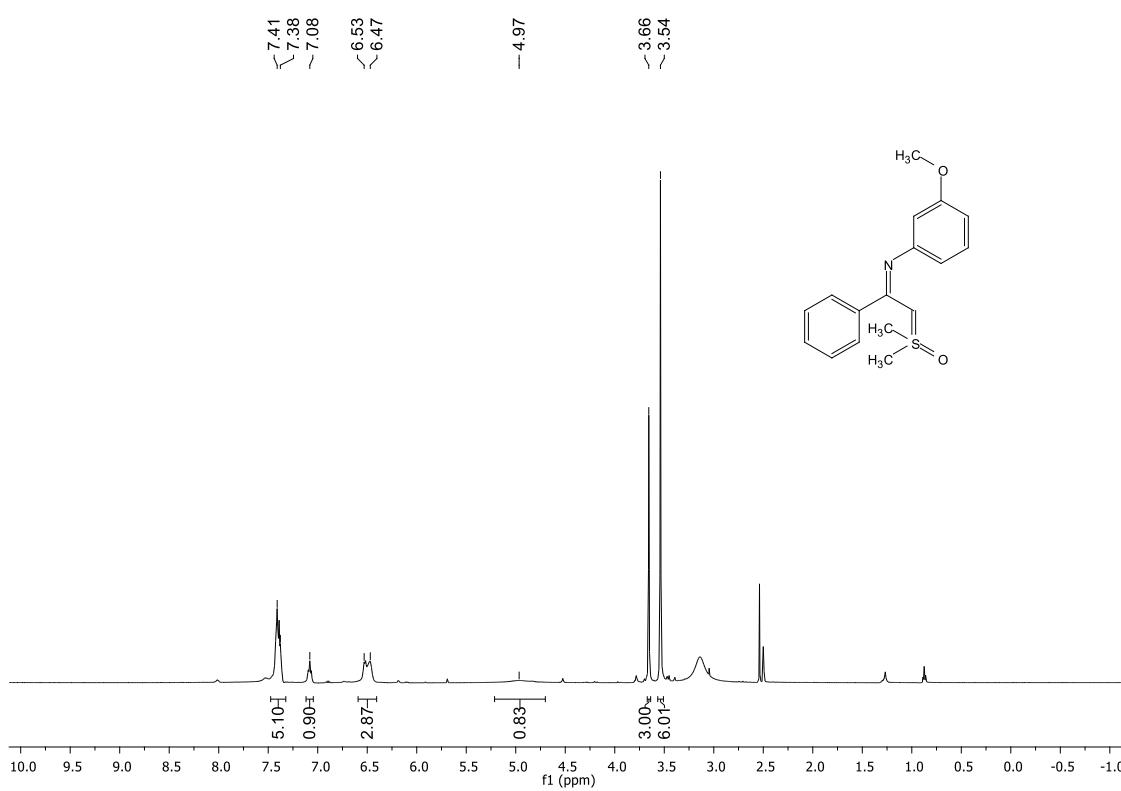
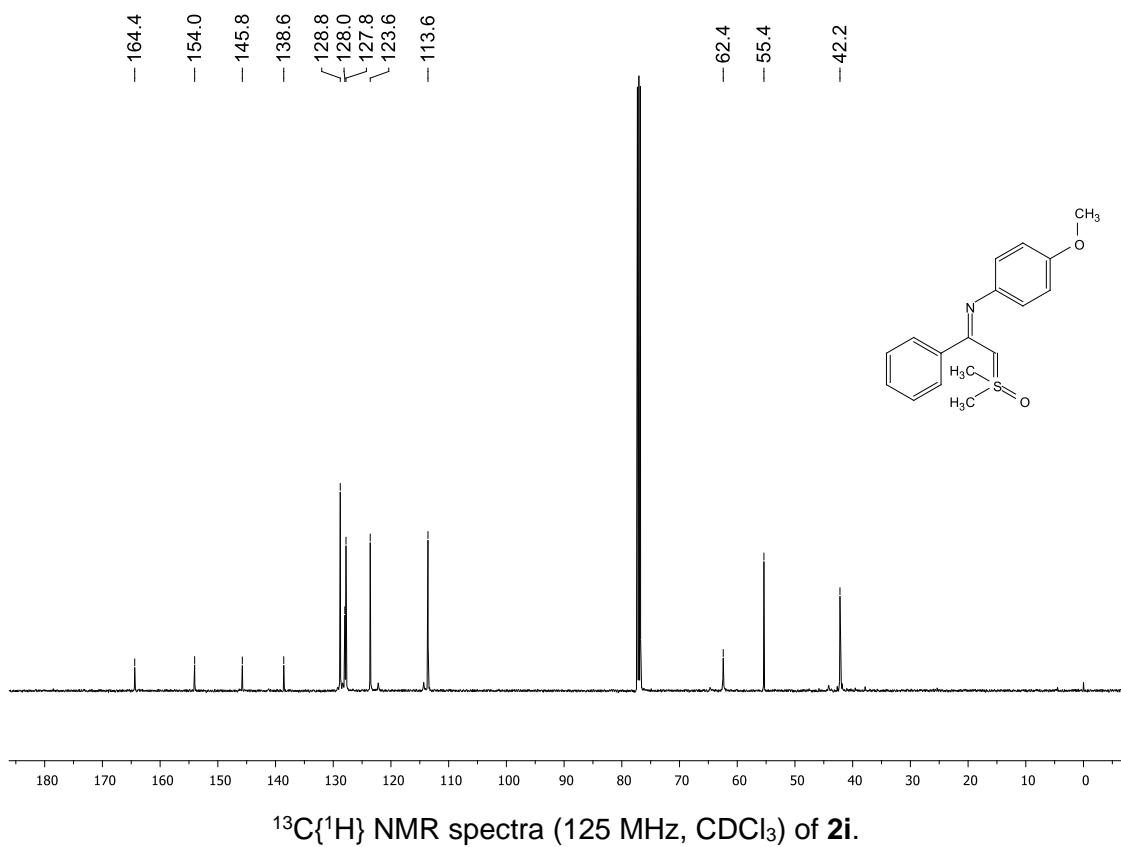




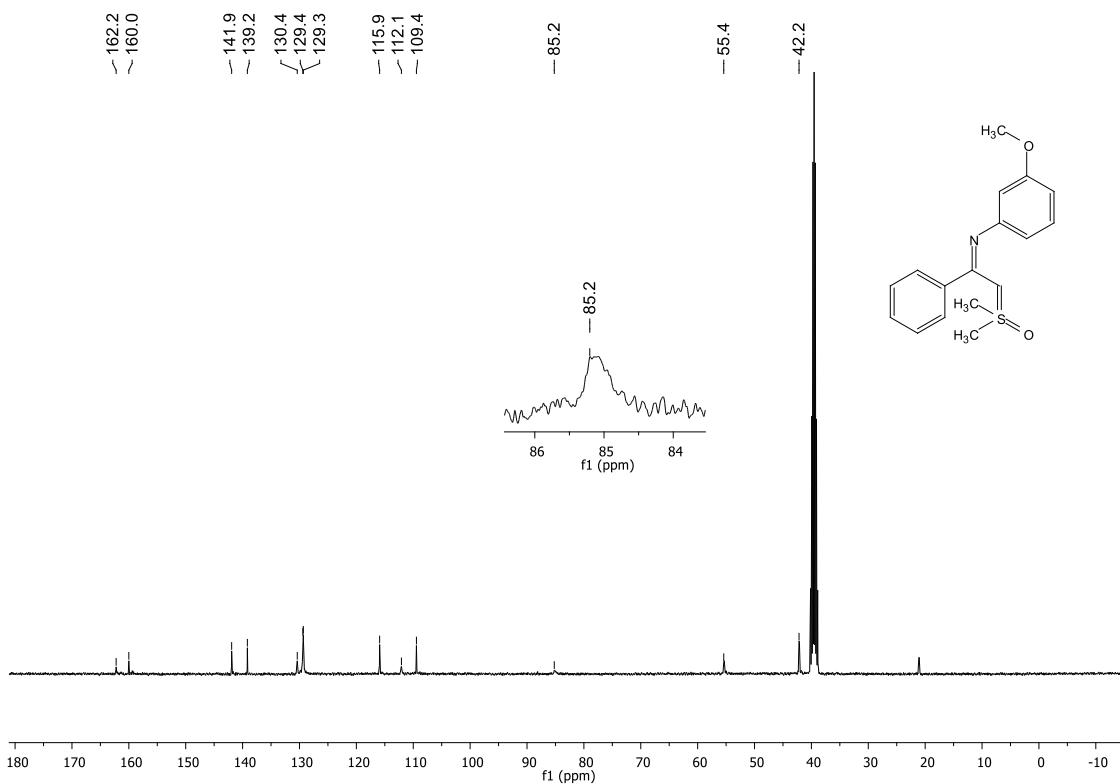




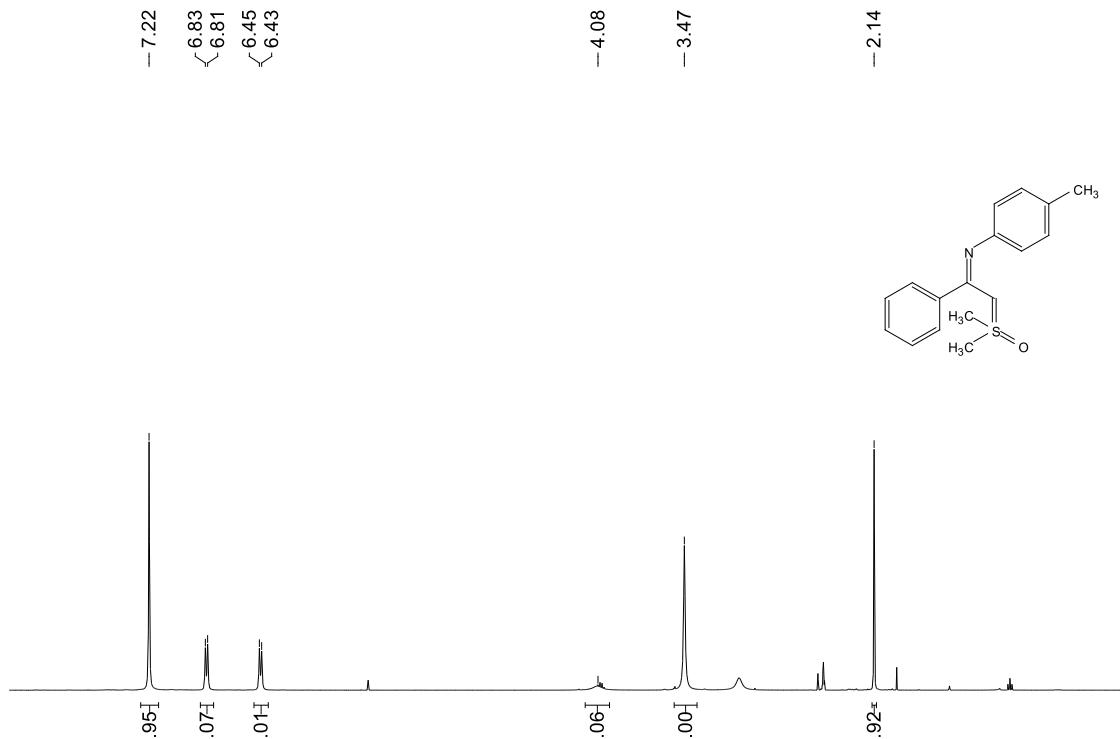




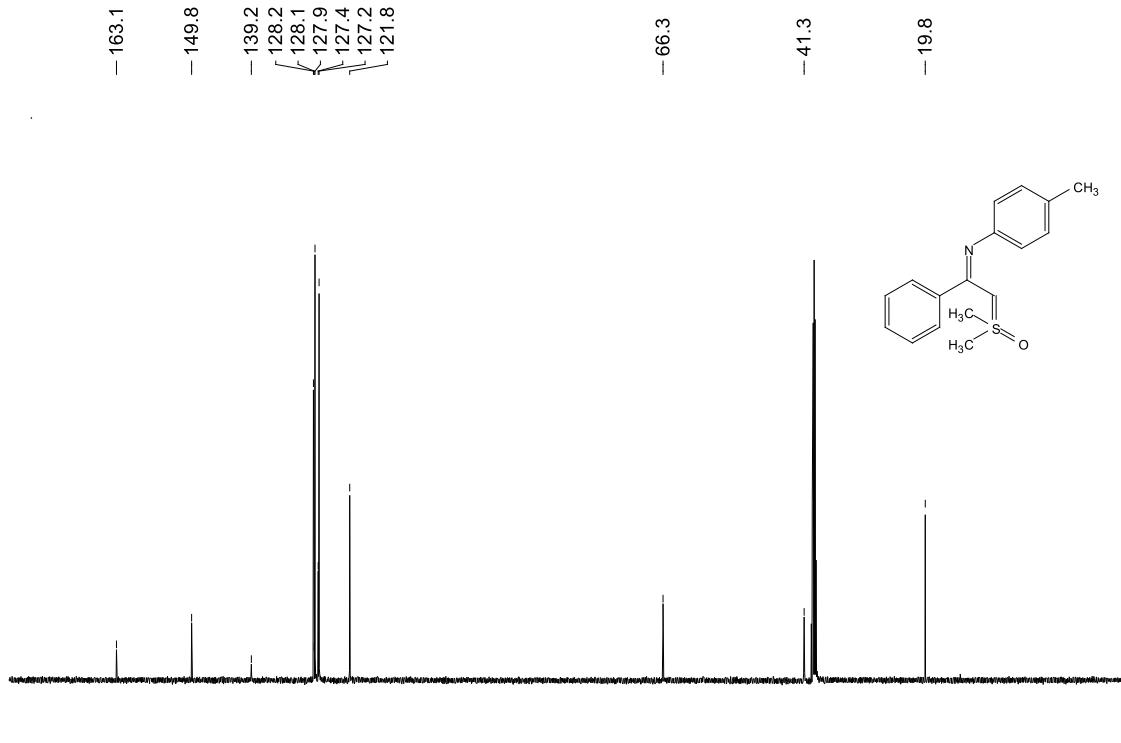
^1H NMR spectra (500 MHz, DMSO, 80°C) of **2j**.



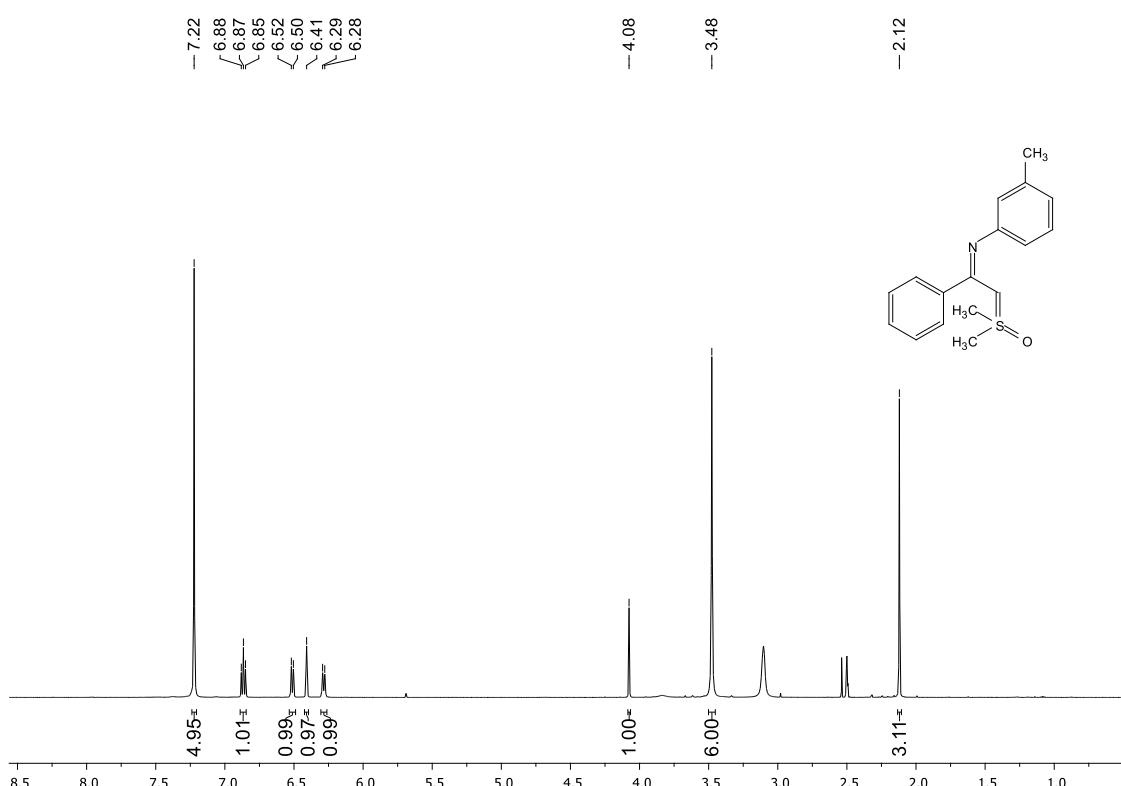
$^{13}\text{C}\{^1\text{H}\}$ NMR spectra (100 MHz, DMSO) of **2j**.



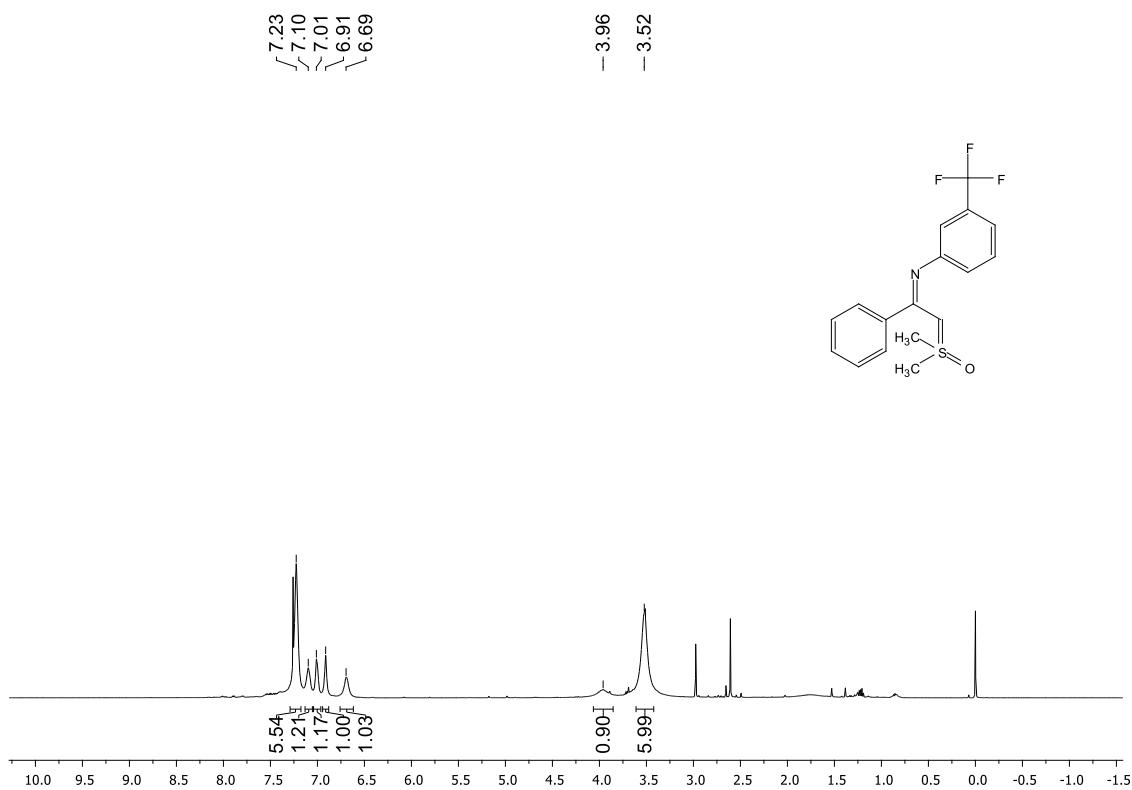
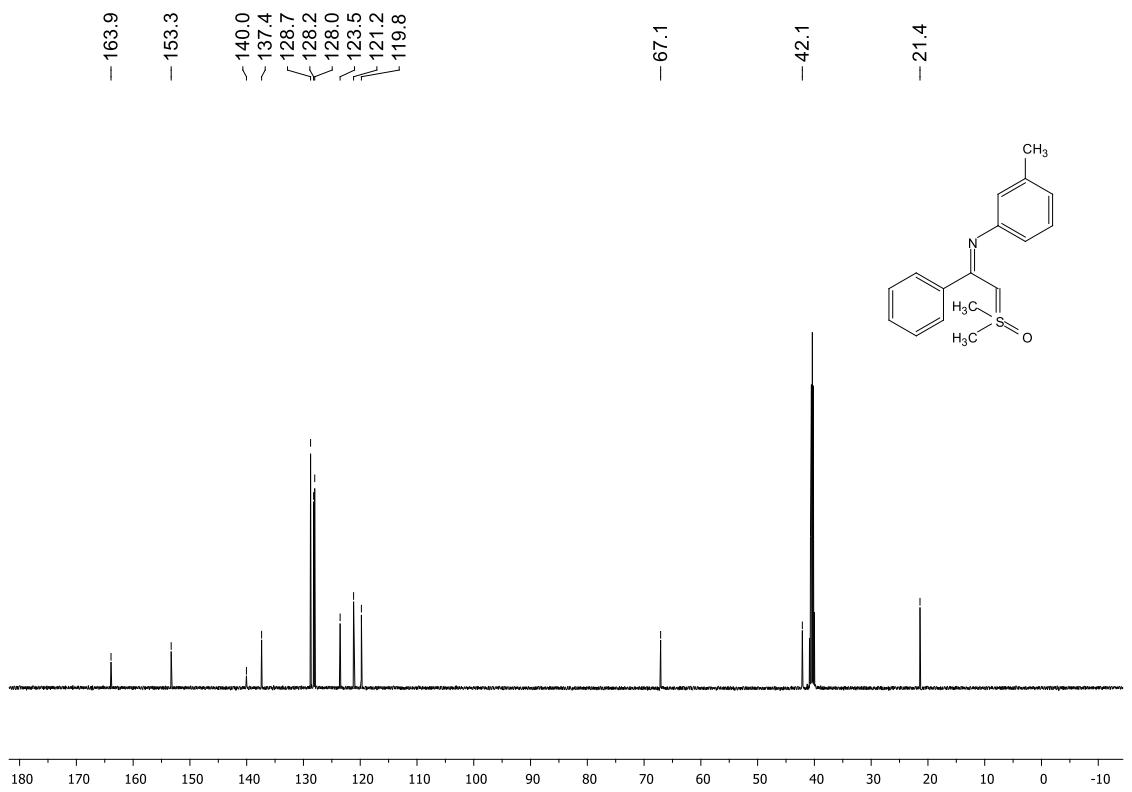
^1H NMR spectra (500 MHz, DMSO, 80°C) of **2k**.

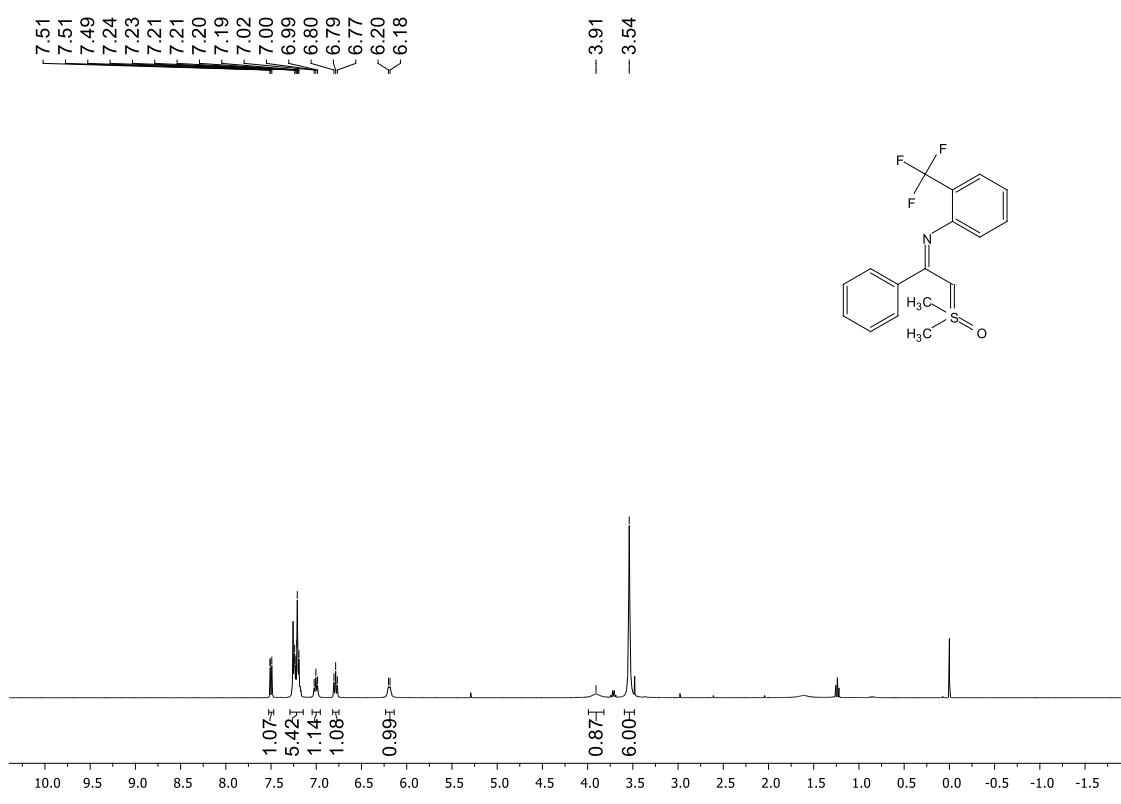
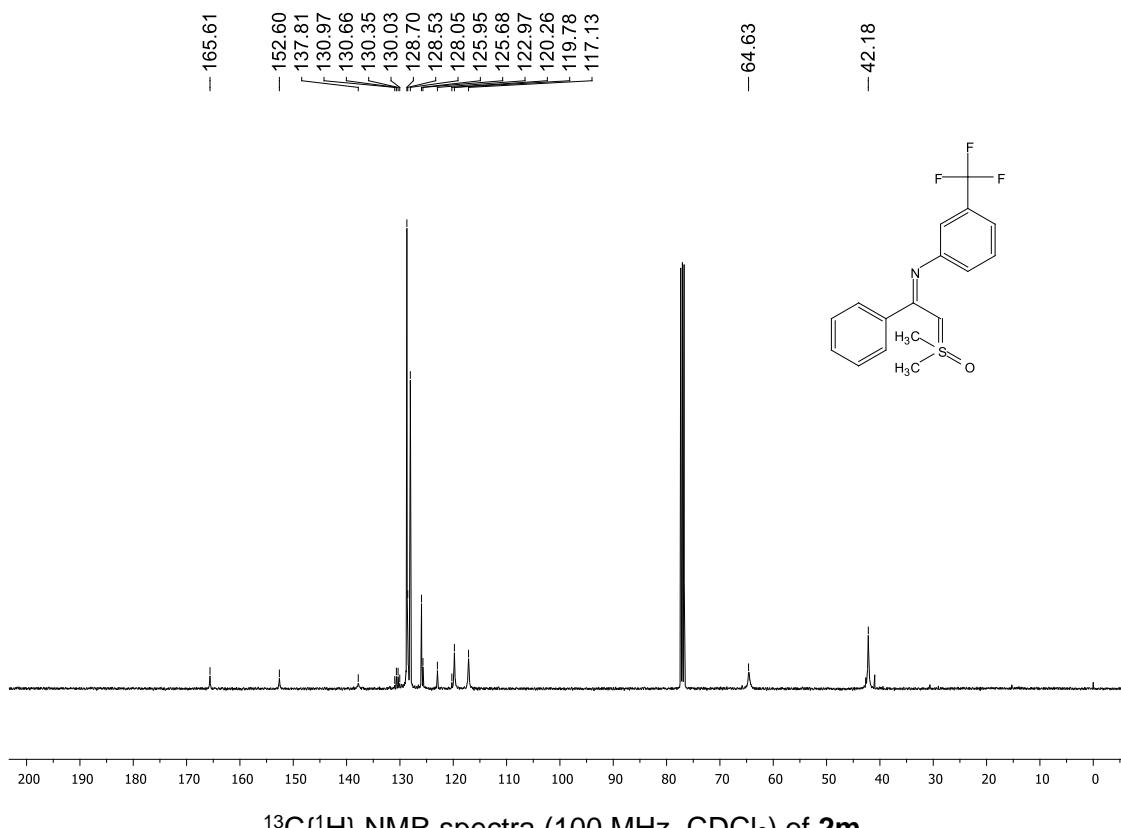


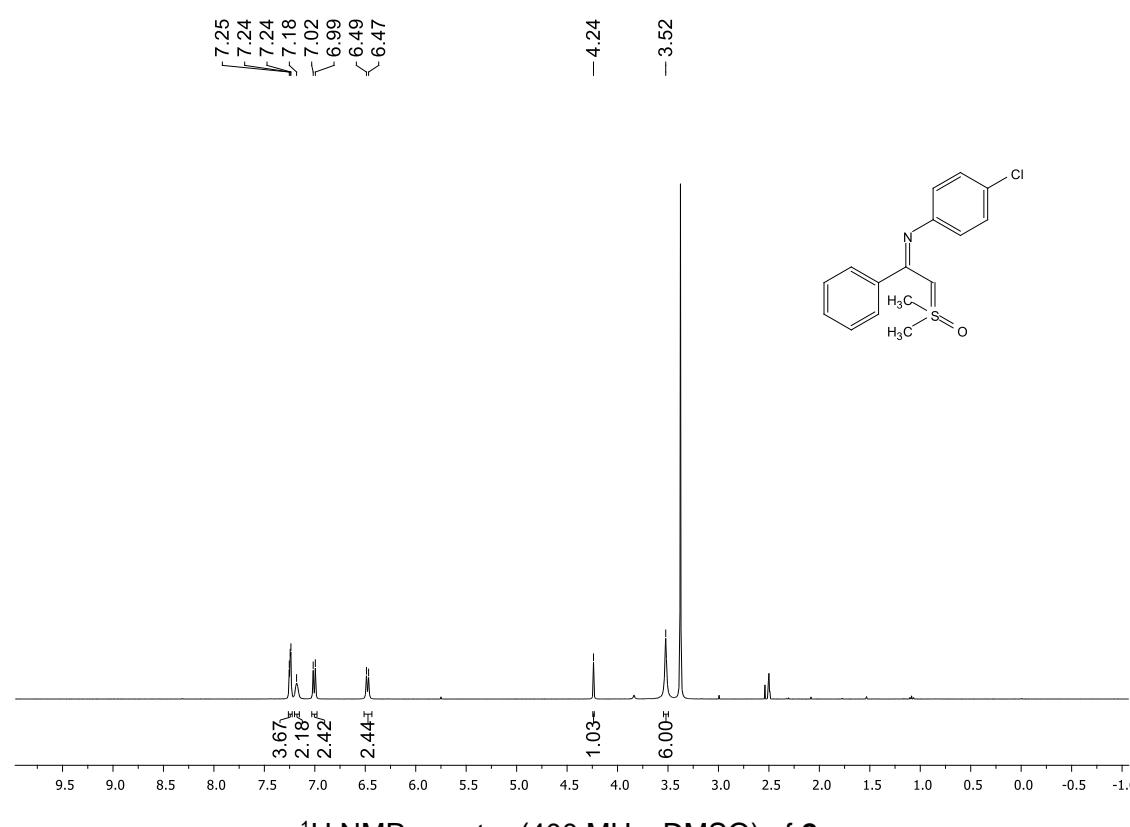
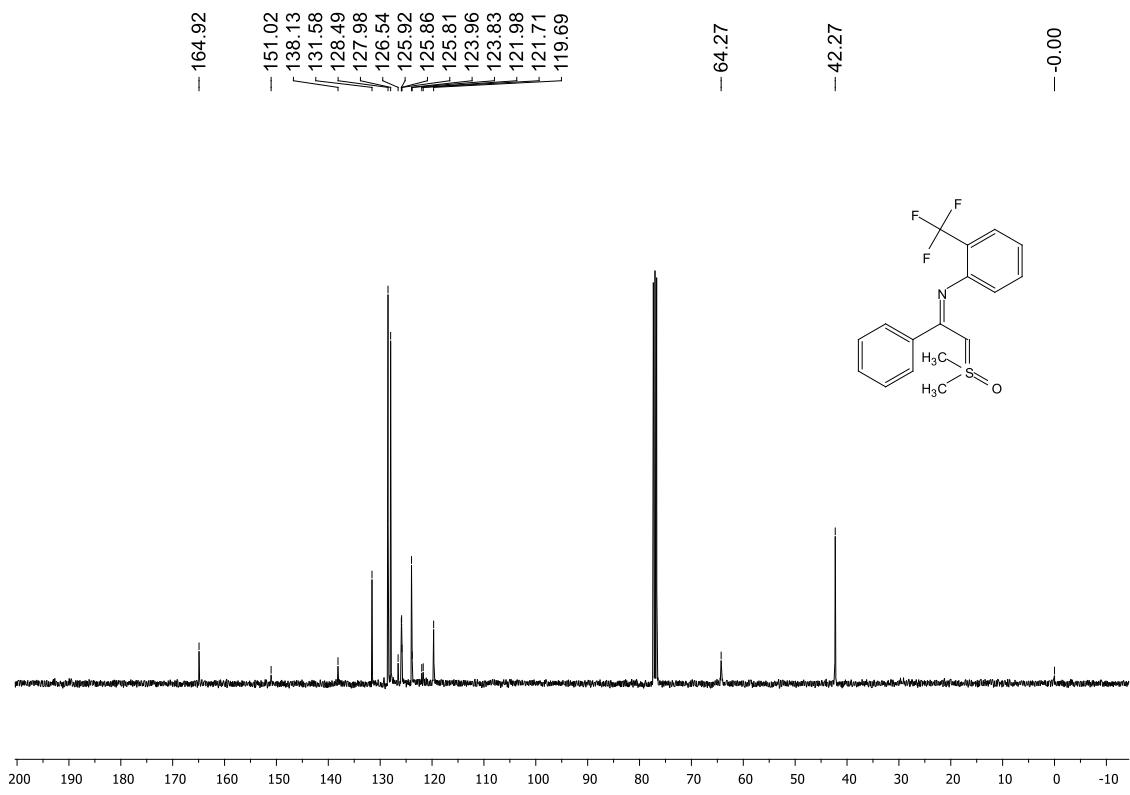
$^{13}\text{C}\{^1\text{H}\}$ NMR spectra (125 MHz, DMSO, 80 °C) of **2k**.

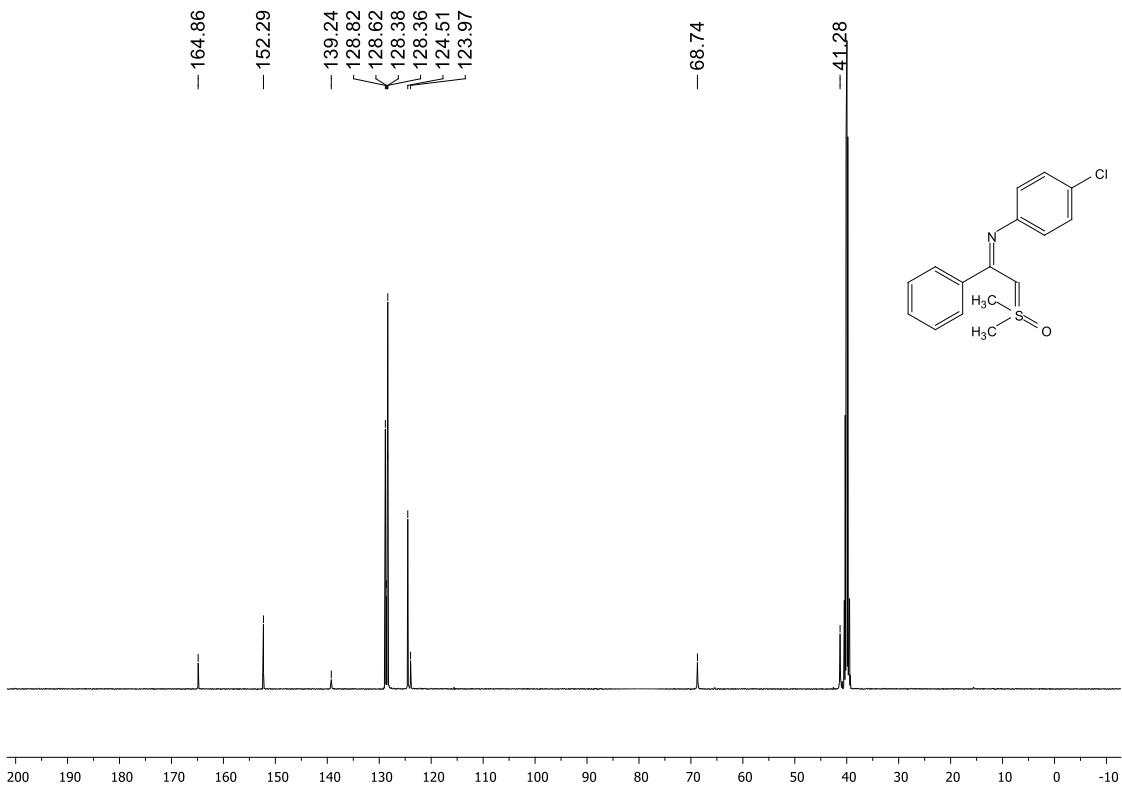


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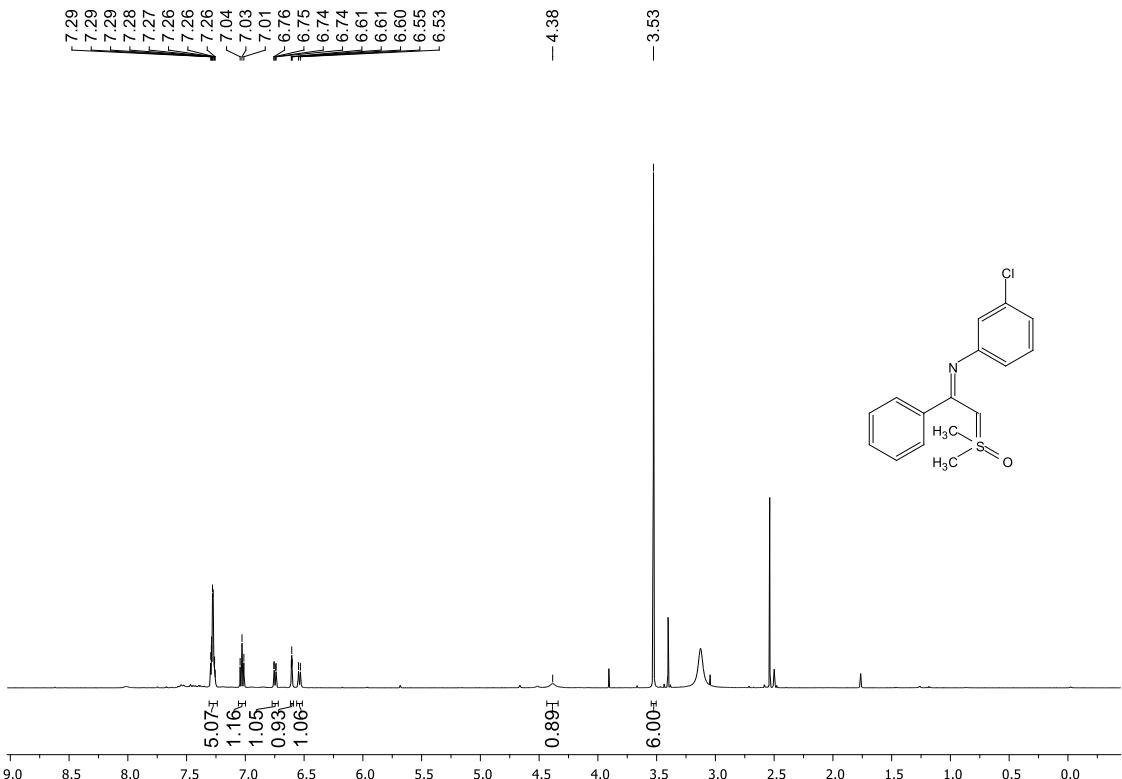




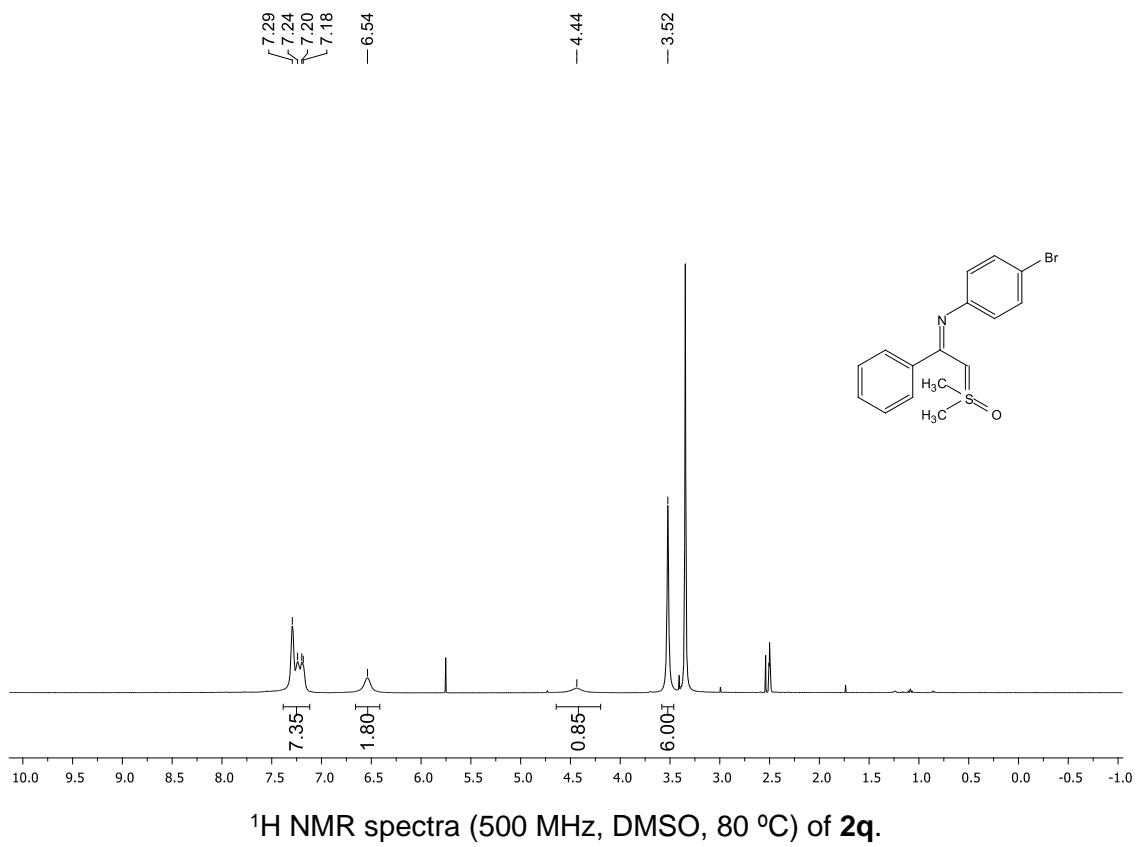
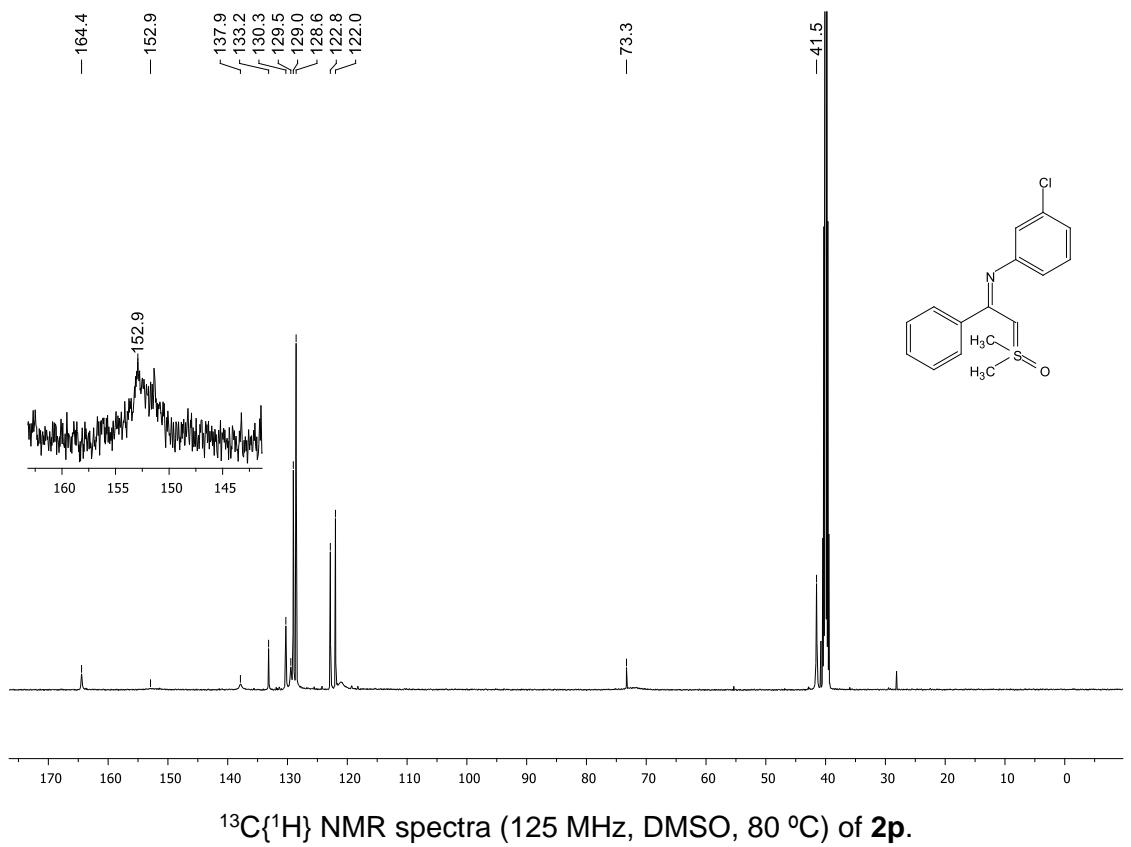


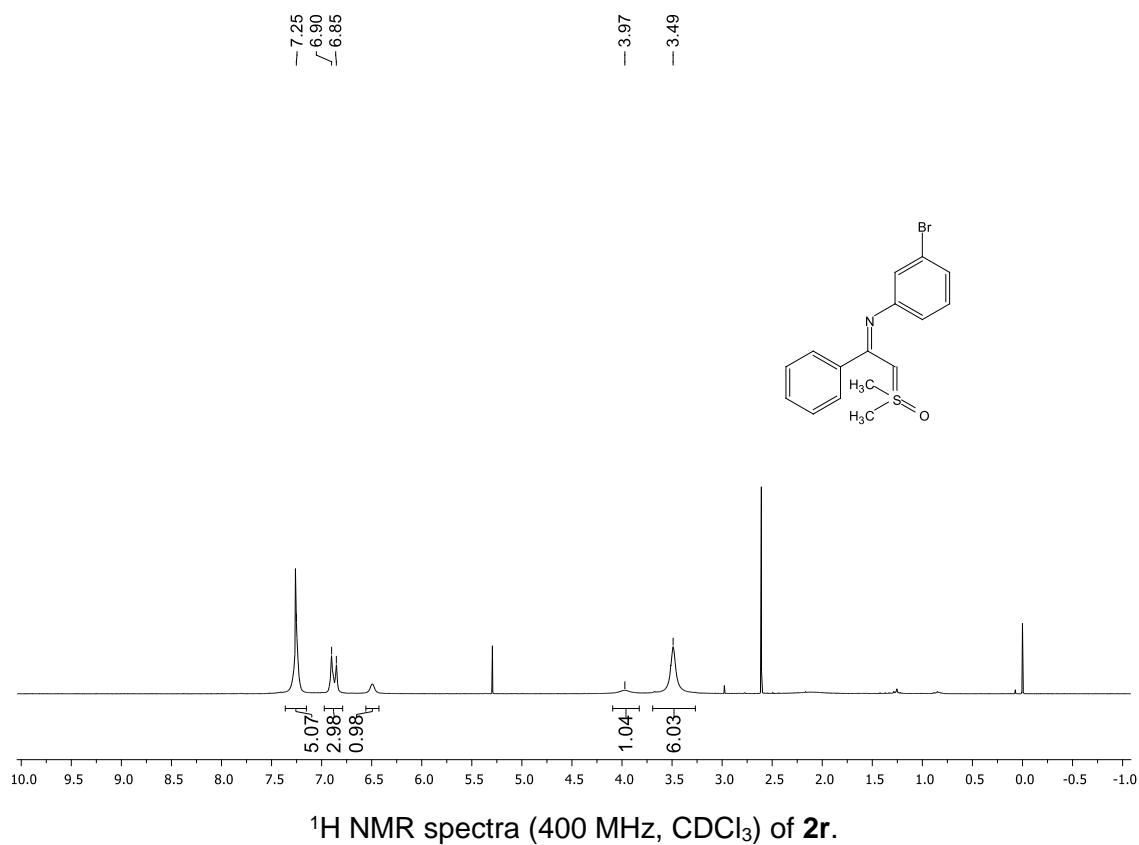
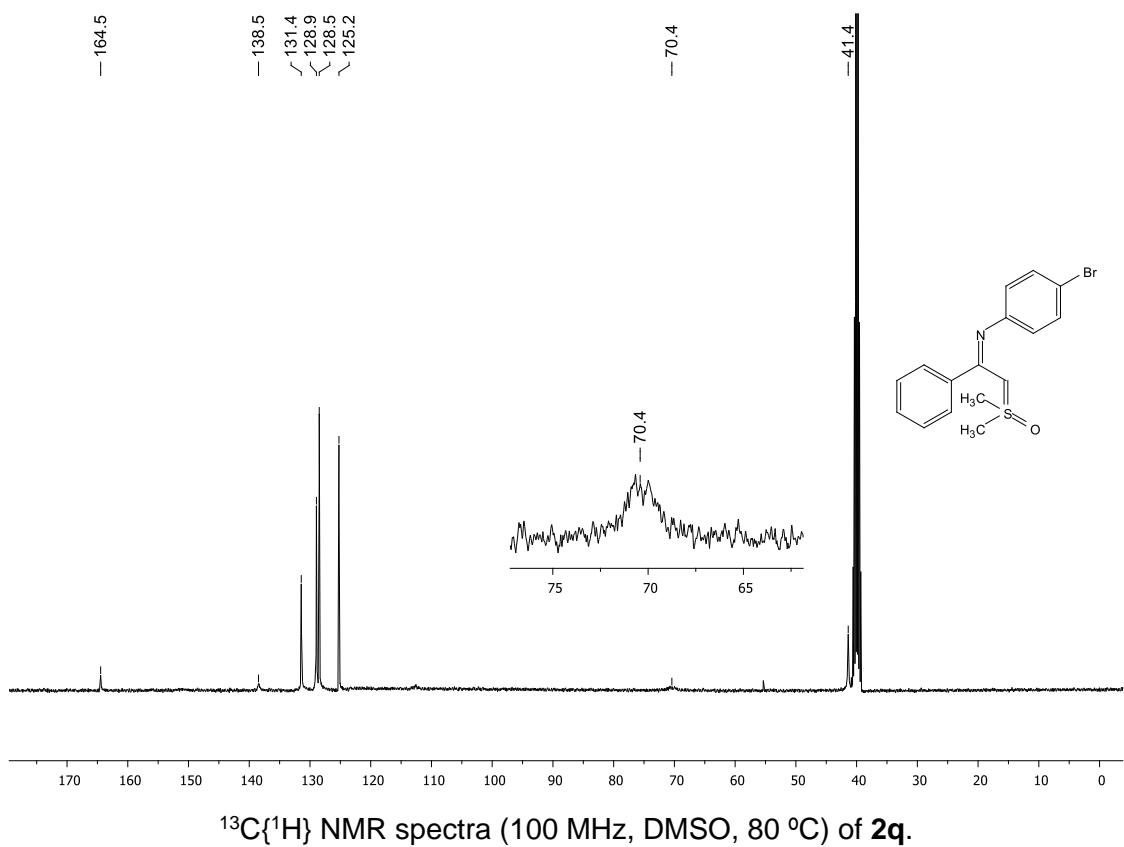


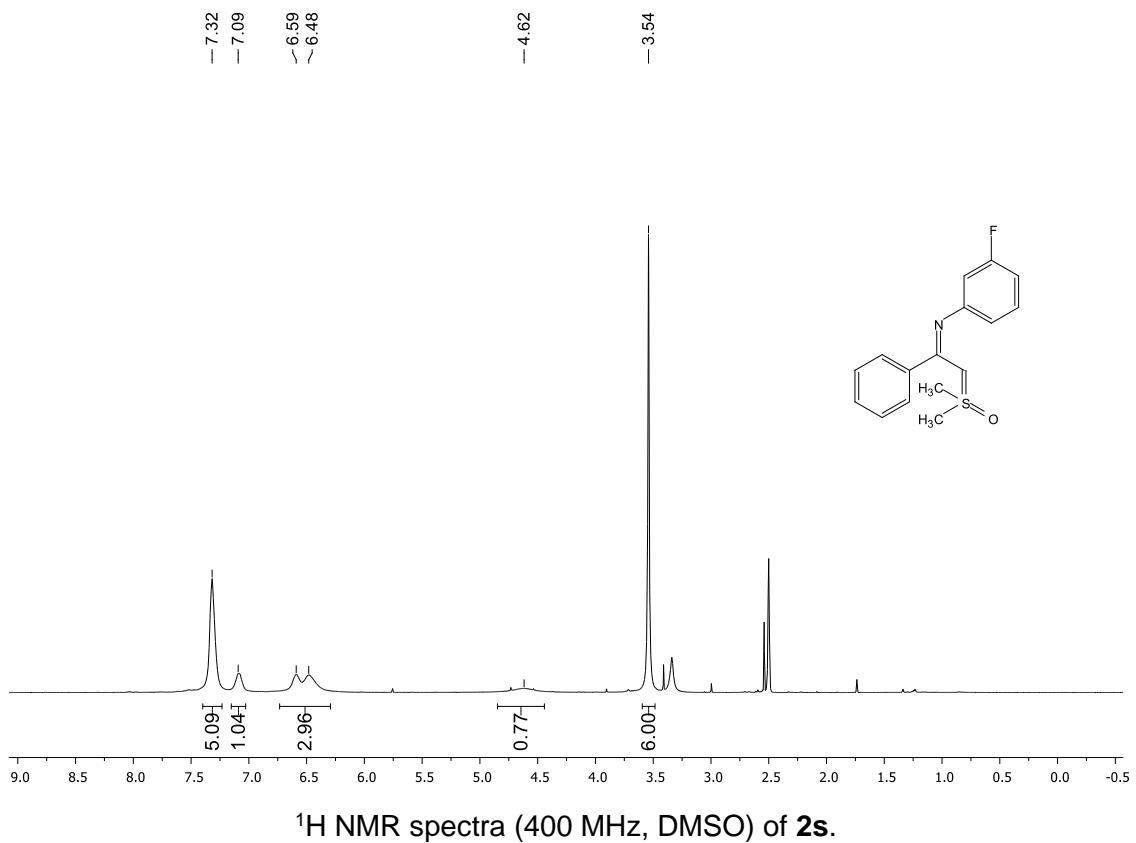
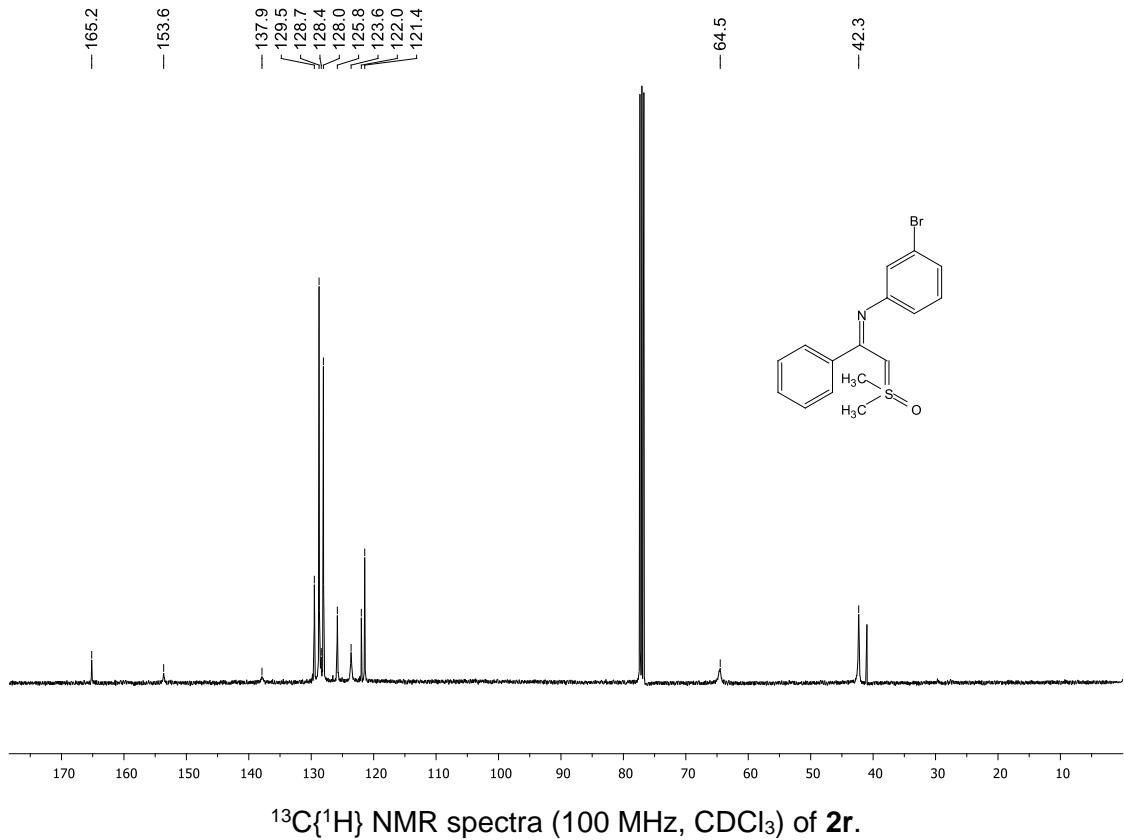
¹³C{¹H} NMR spectra (125 MHz, DMSO) of **2o**.

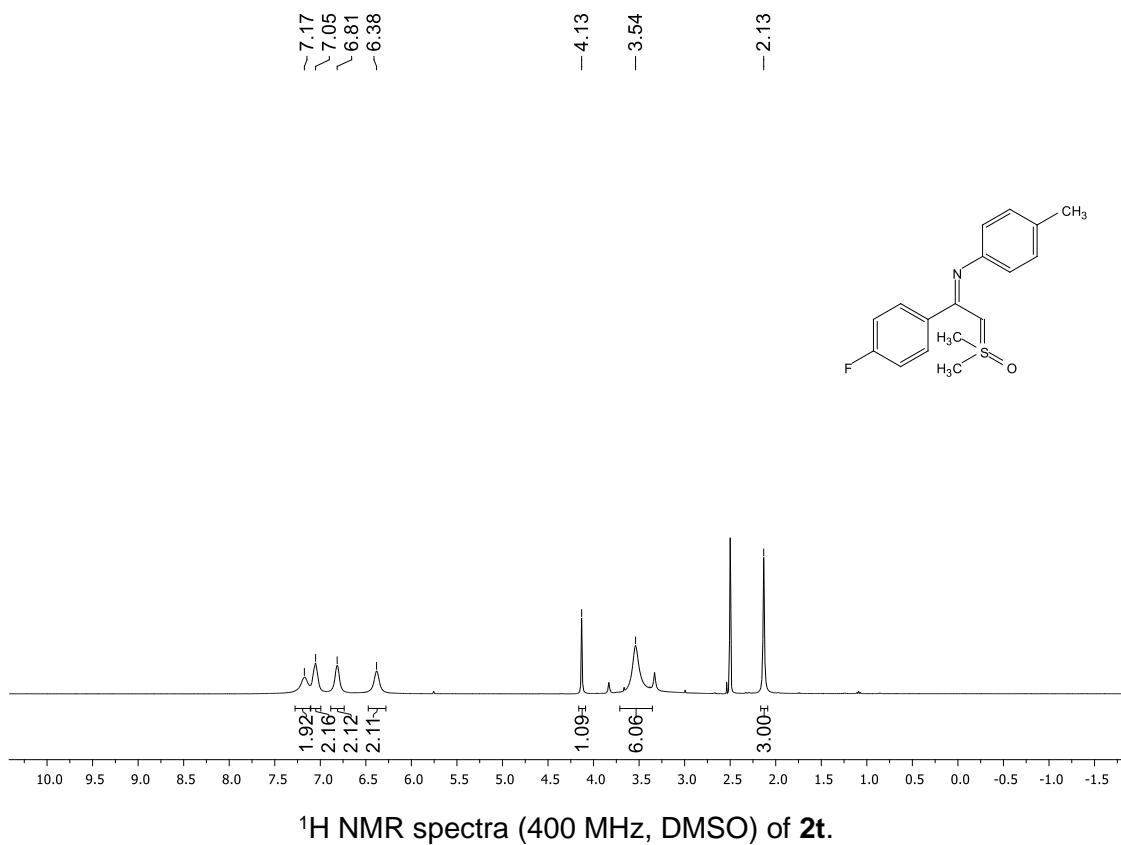
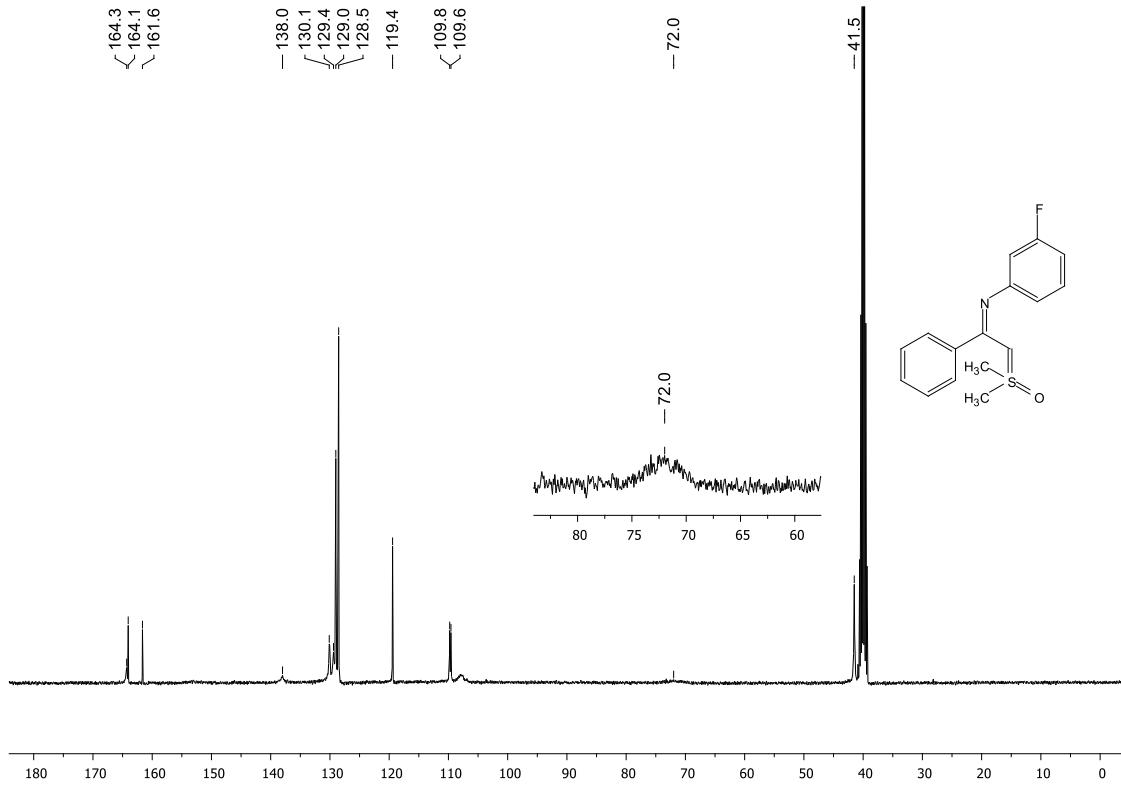


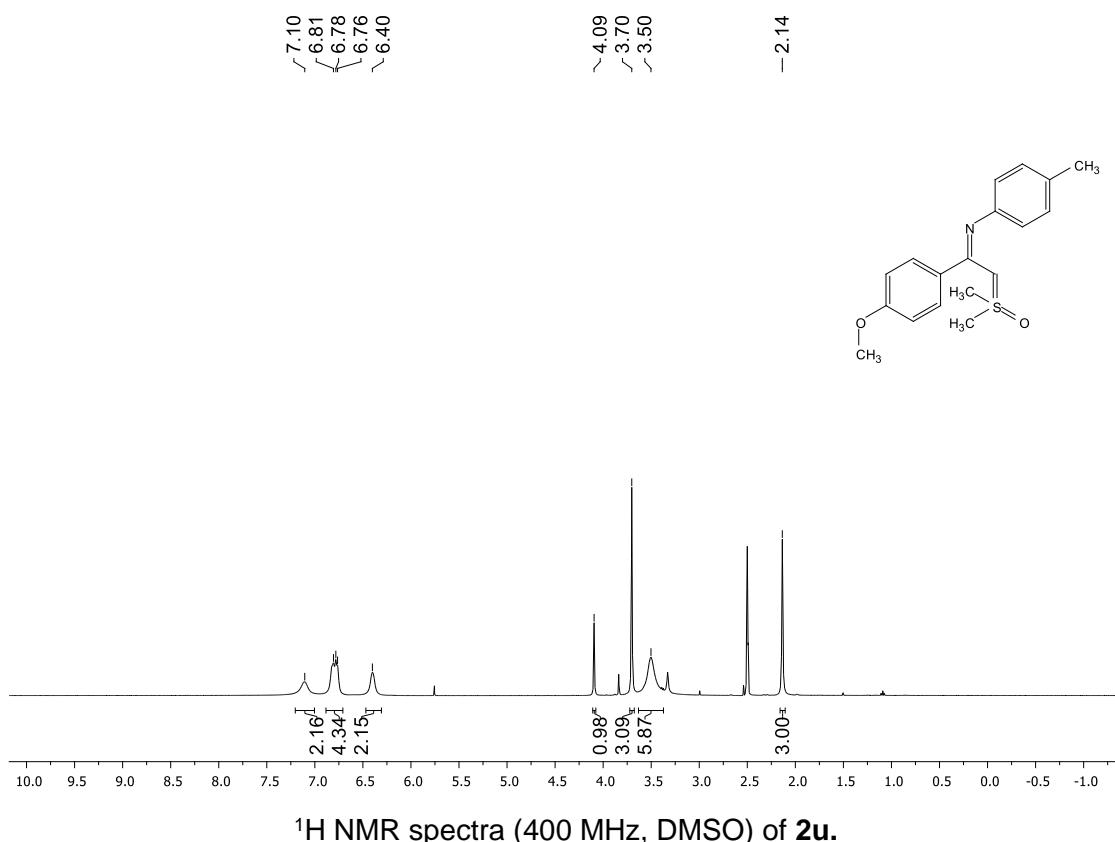
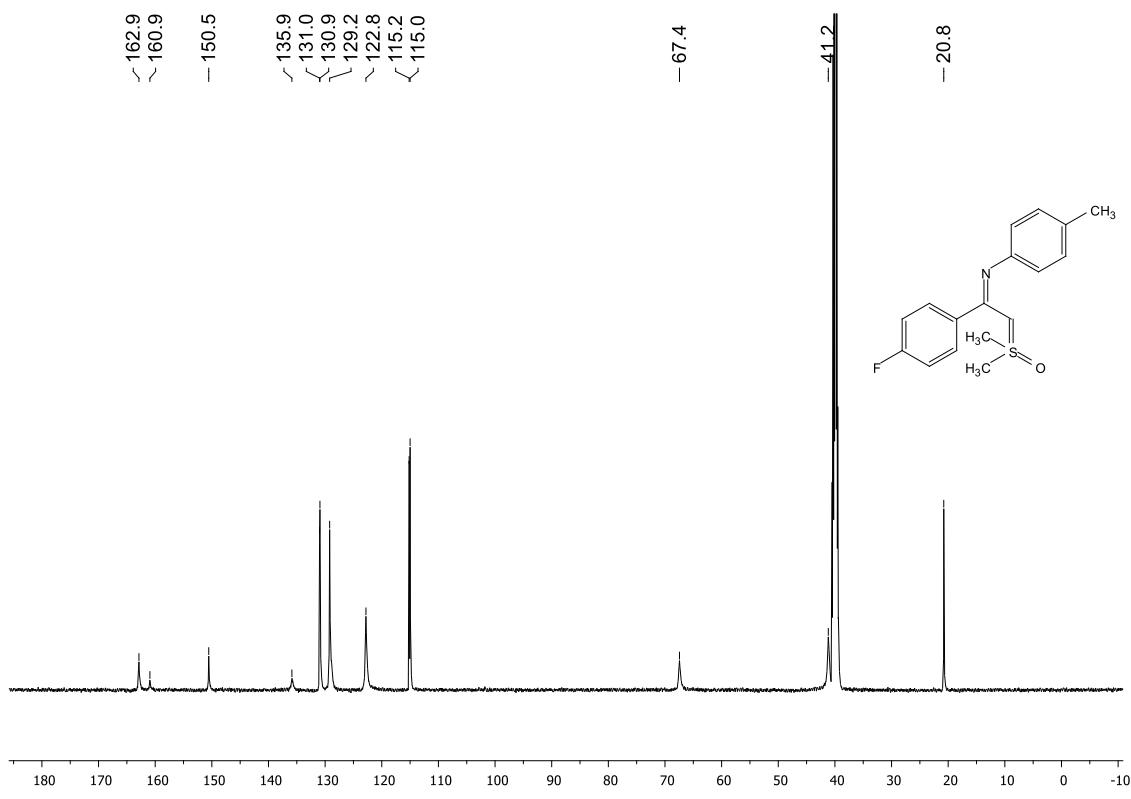
¹H NMR spectra (500 MHz, DMSO, 80 °C) of **2p**.

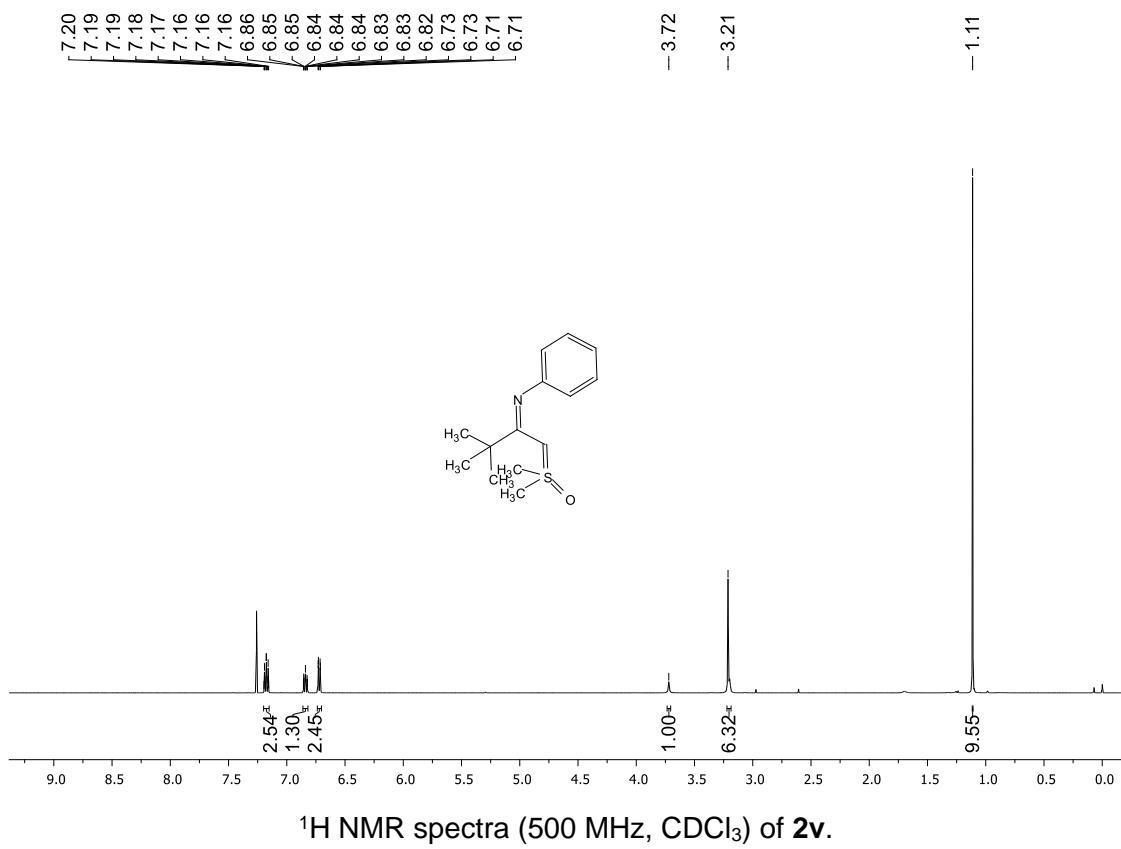
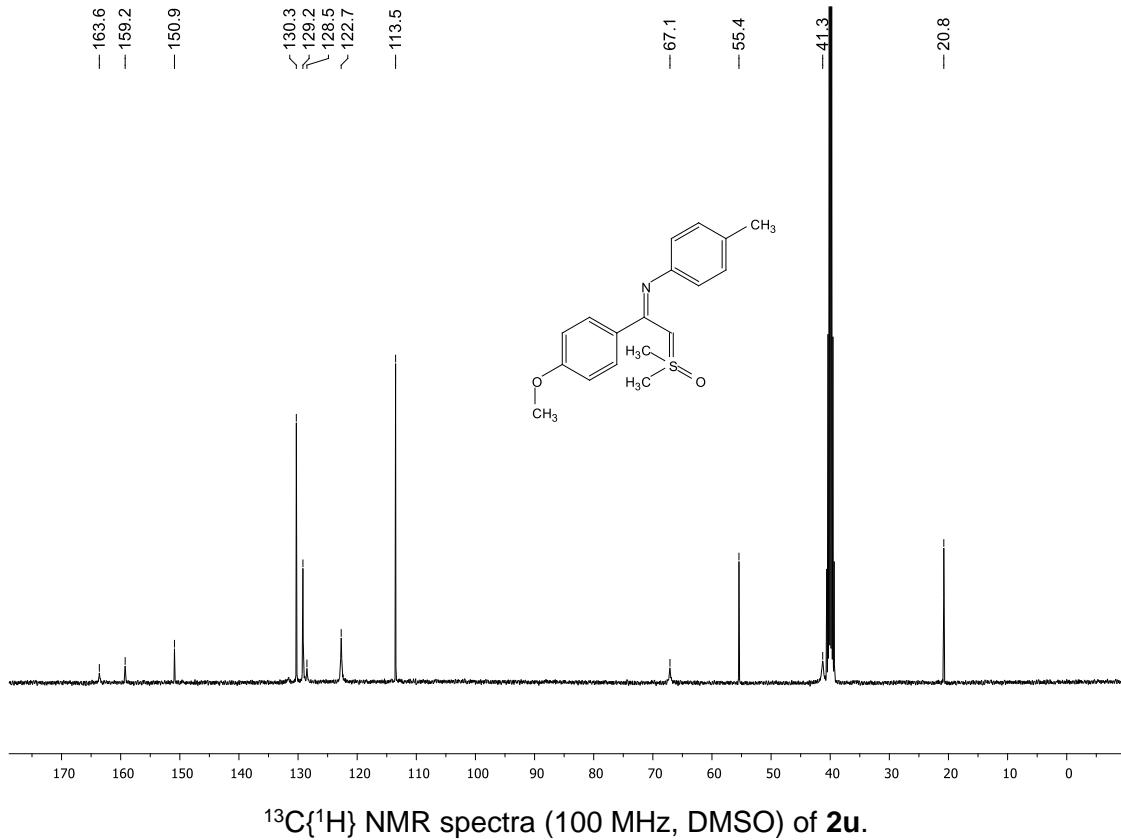


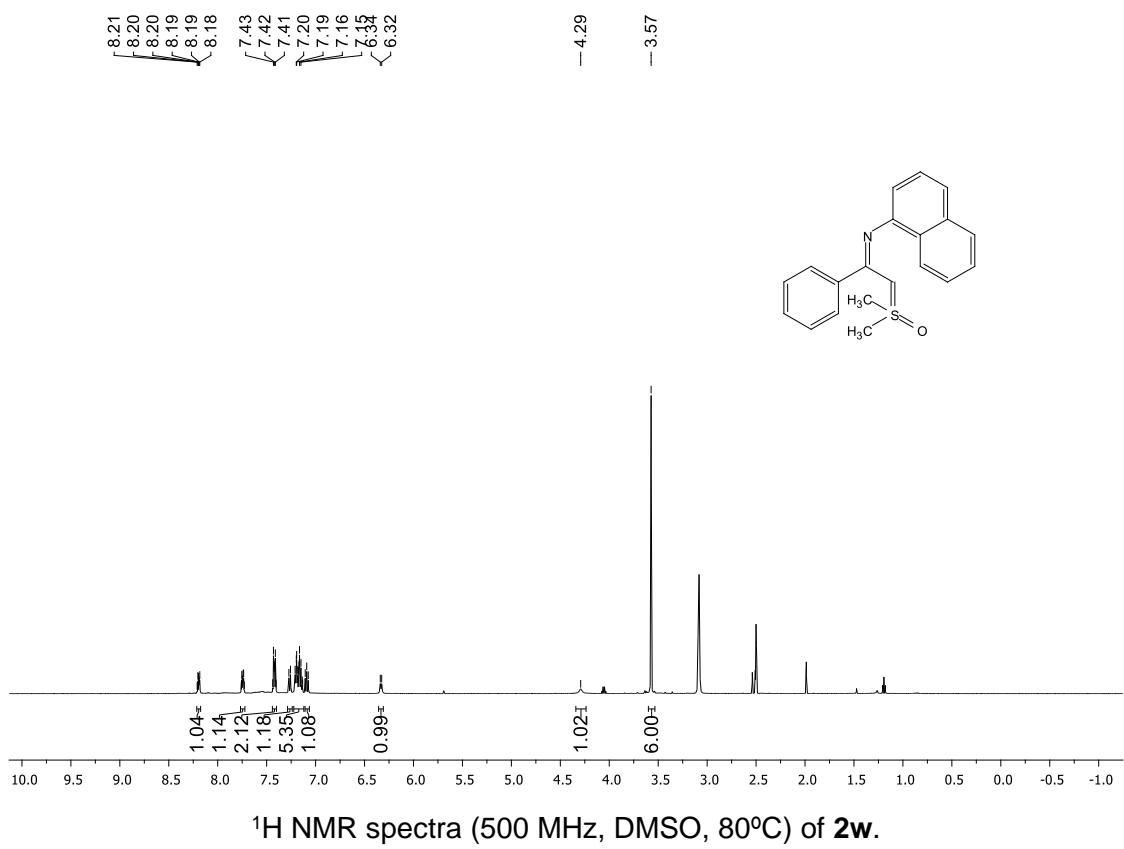
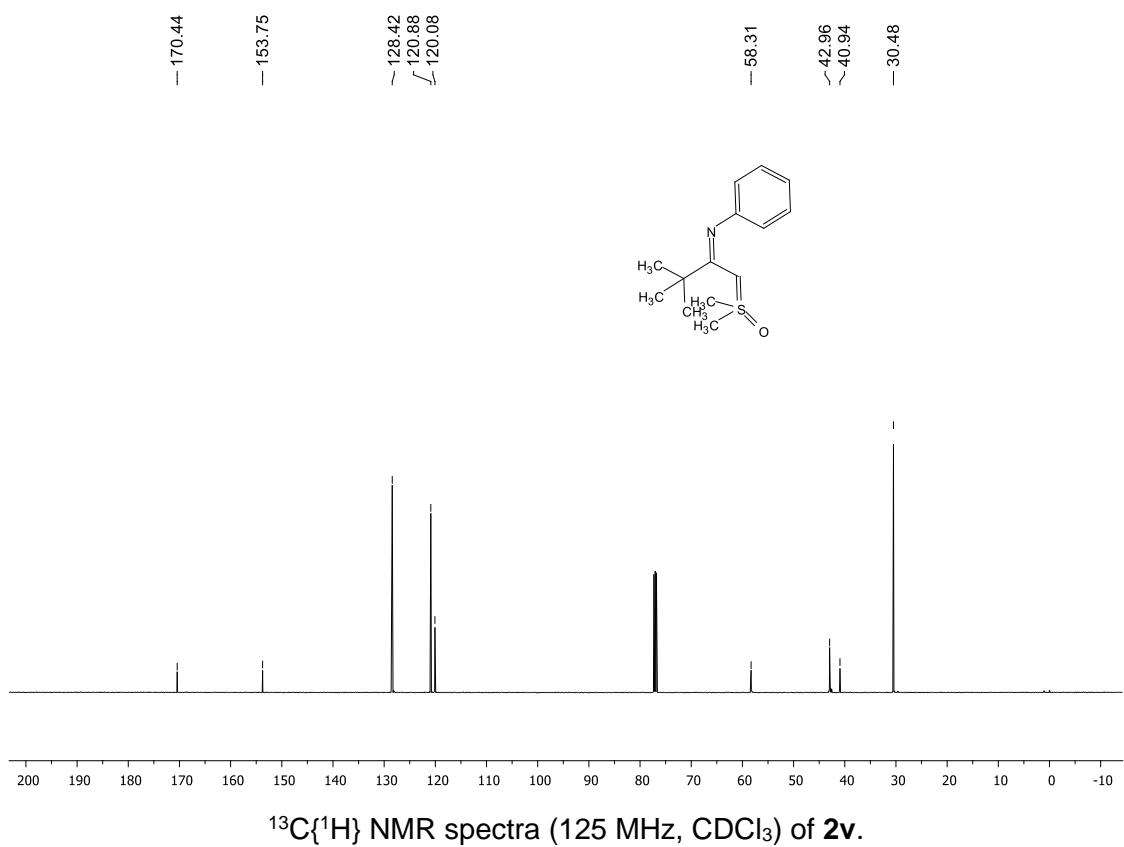


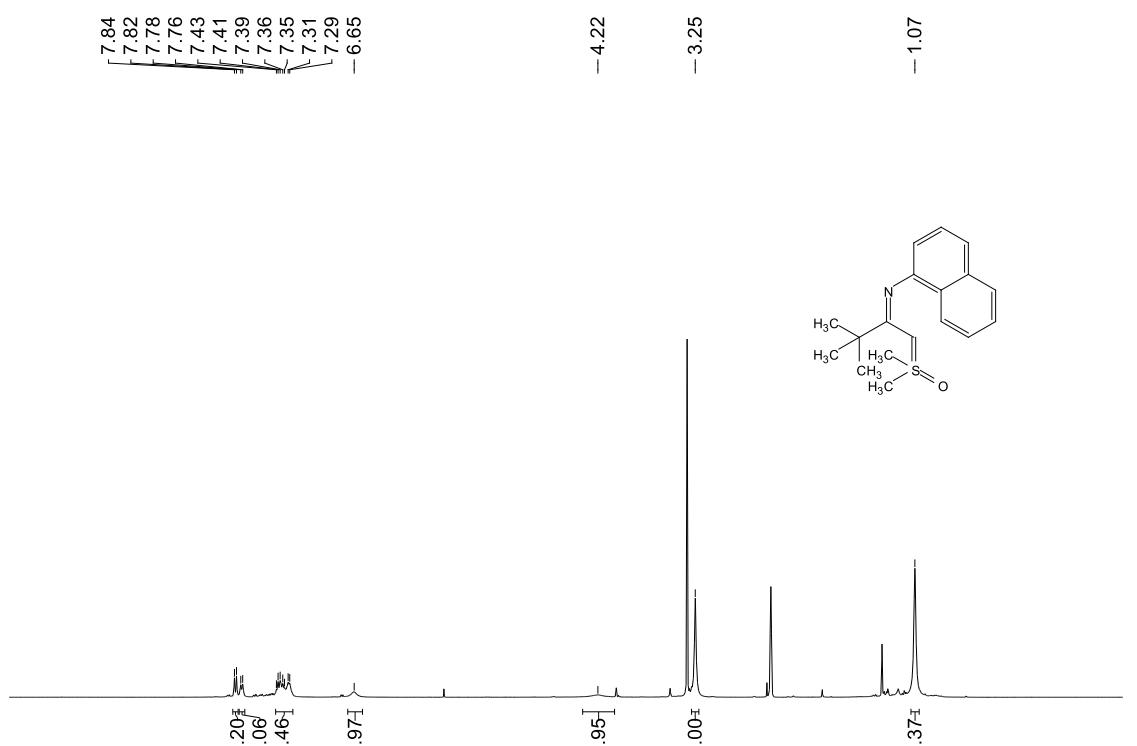
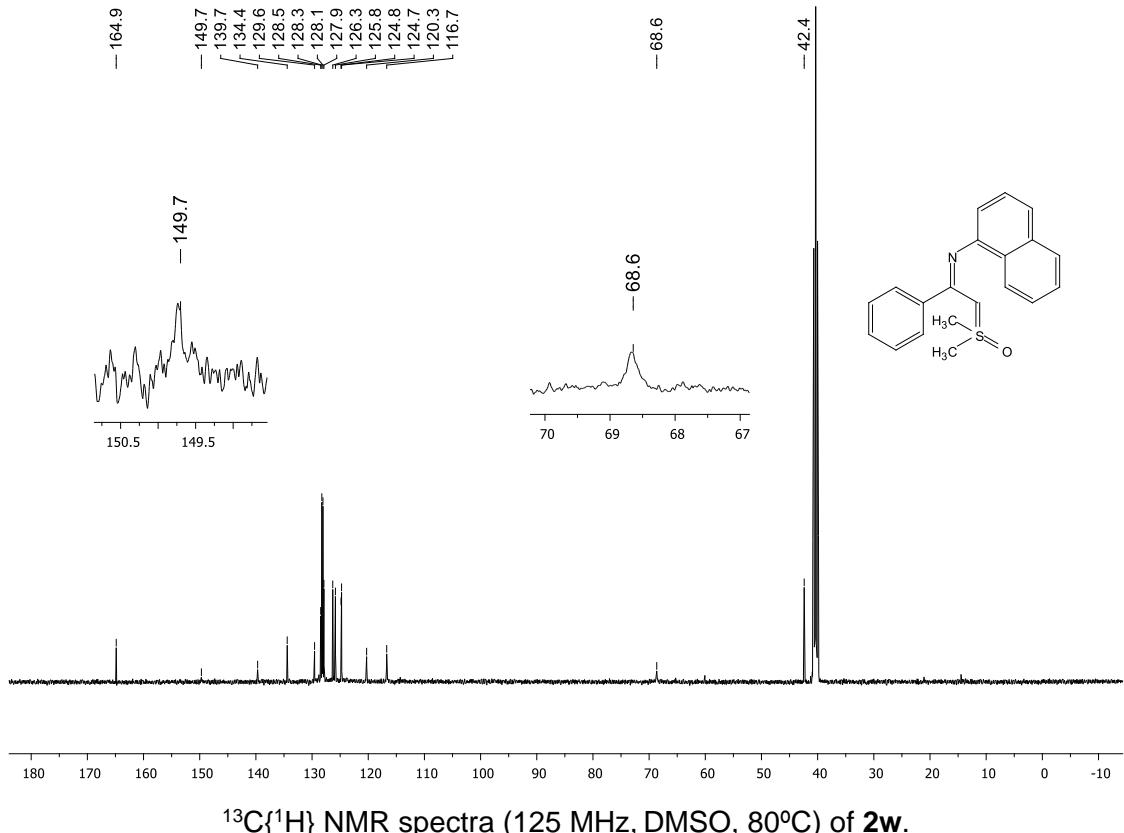




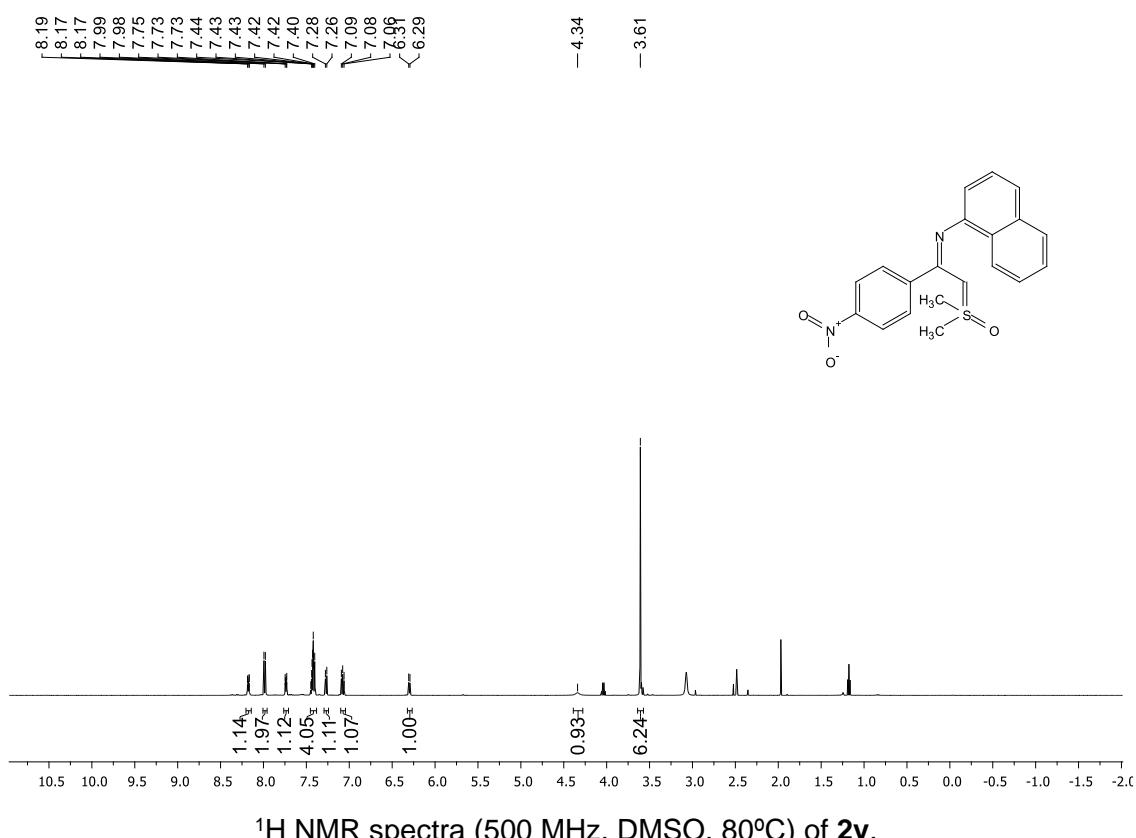
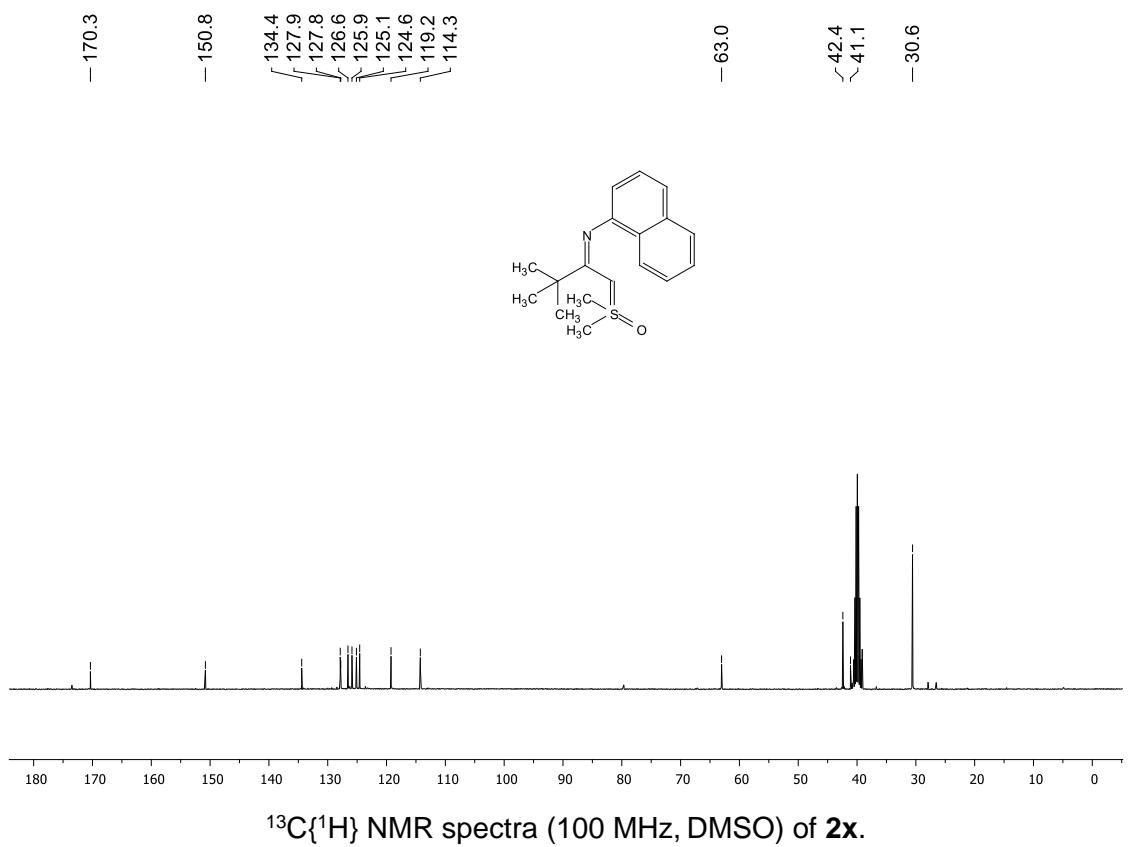


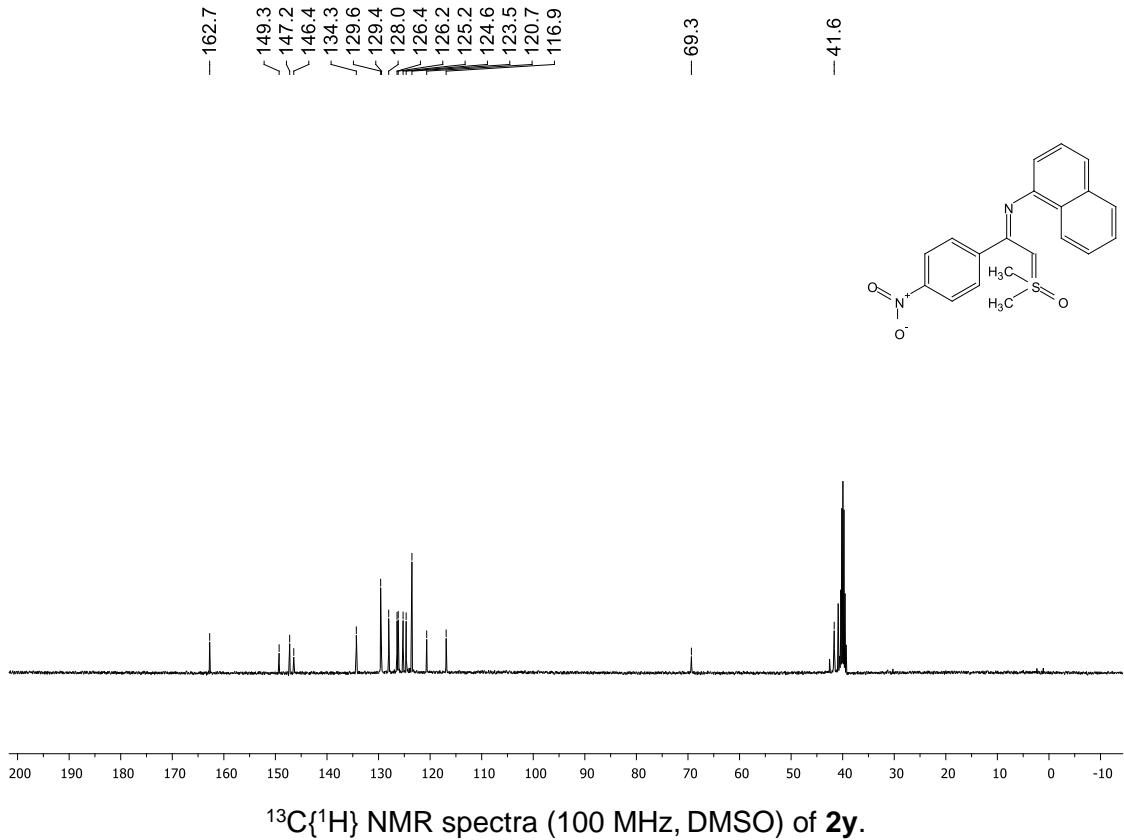




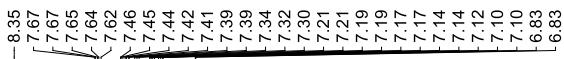


^1H NMR spectra (400 MHz, DMSO) of **2x**.





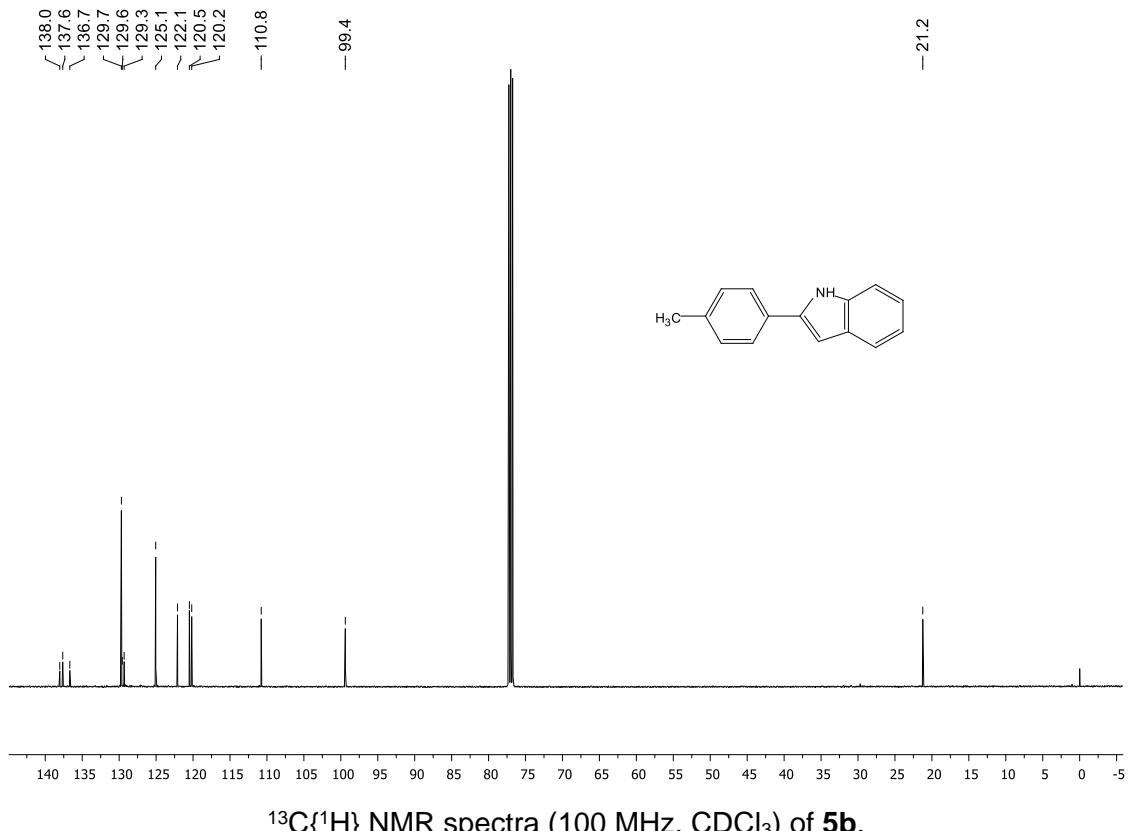
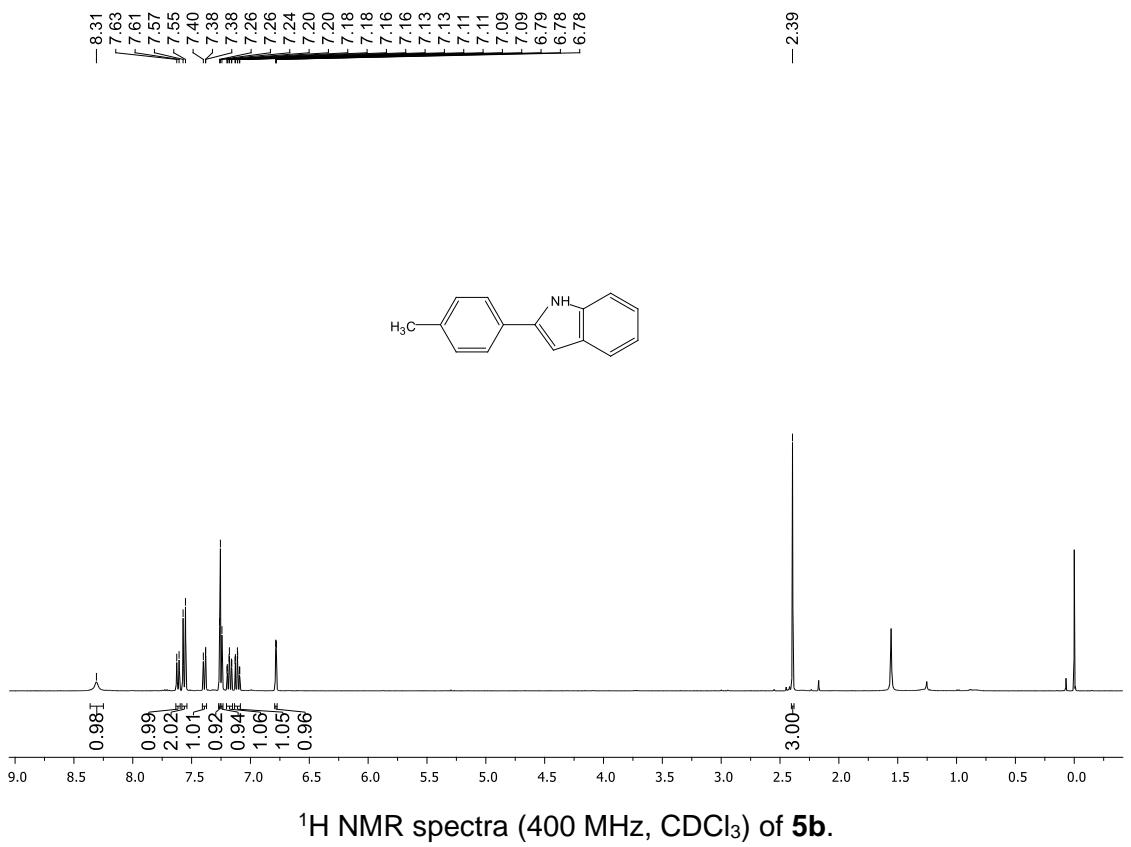
III. NMR spectra of indoles

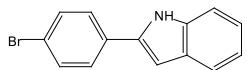
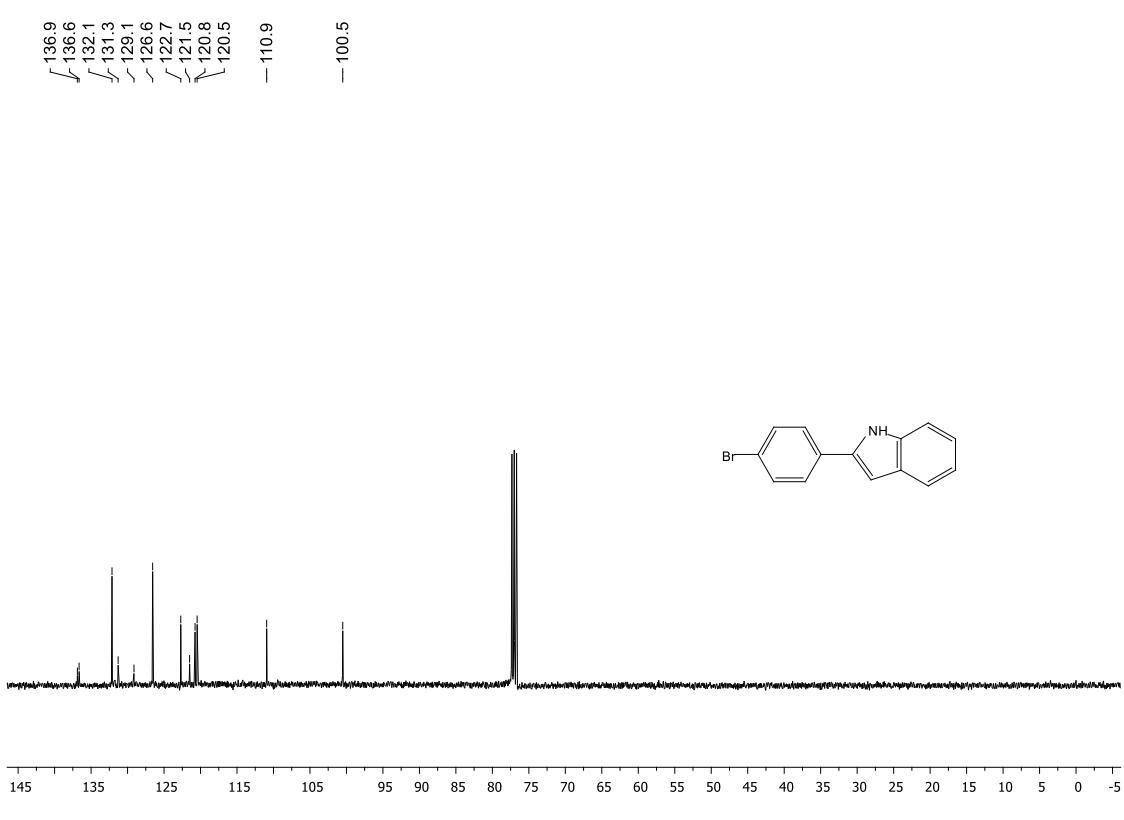
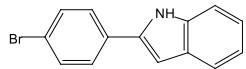
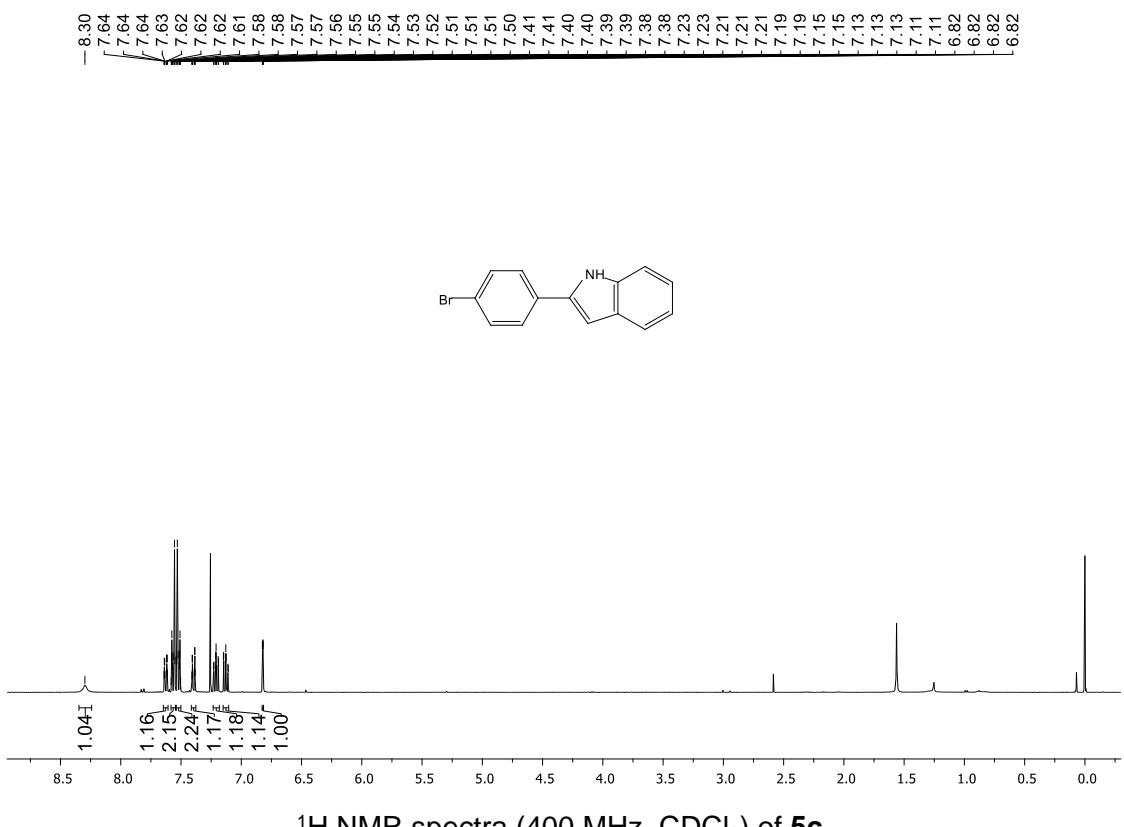


¹H NMR spectra (400 MHz, CDCl₃) of **5a**.



¹³C{¹H} NMR spectra (100 MHz, CDCl₃) of **5a**.

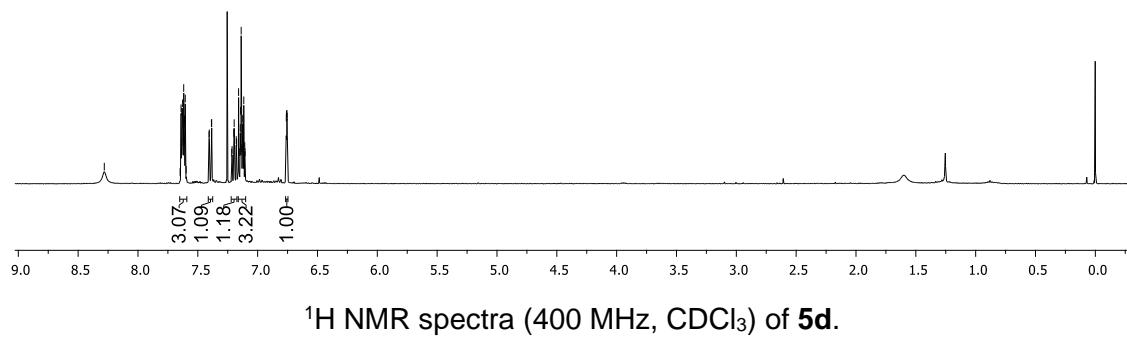
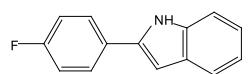




$^{13}\text{C}\{\text{H}\}$ NMR spectra (100 MHz, CDCl_3) of **5c**.

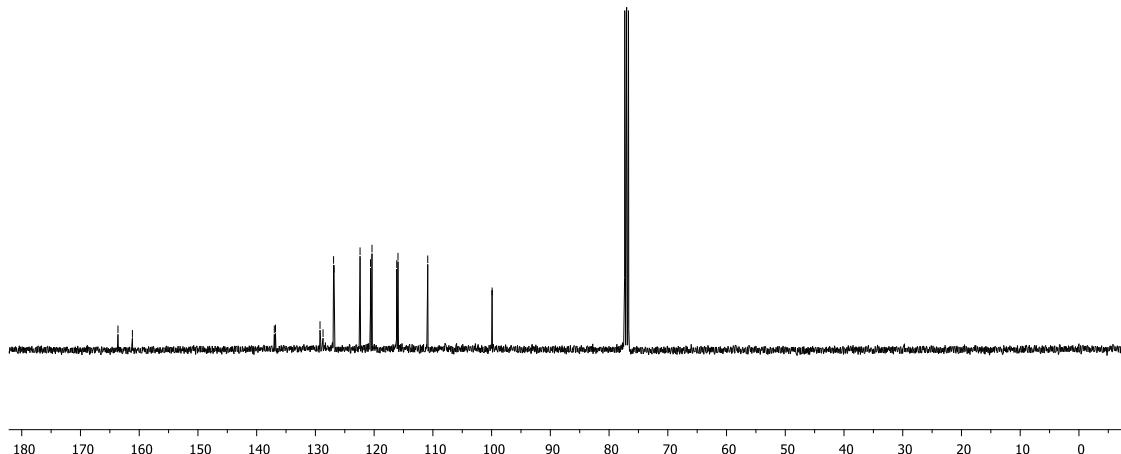
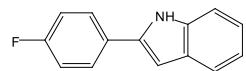
— 8.28

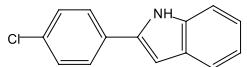
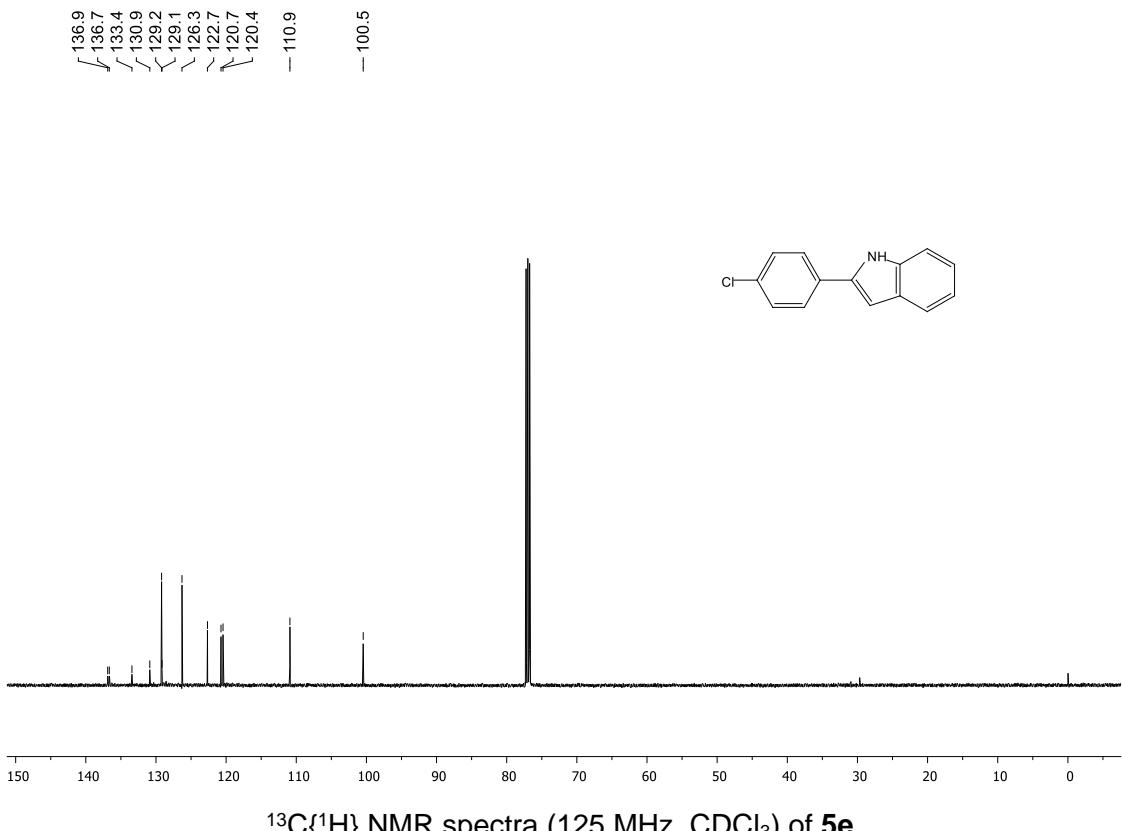
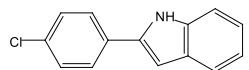
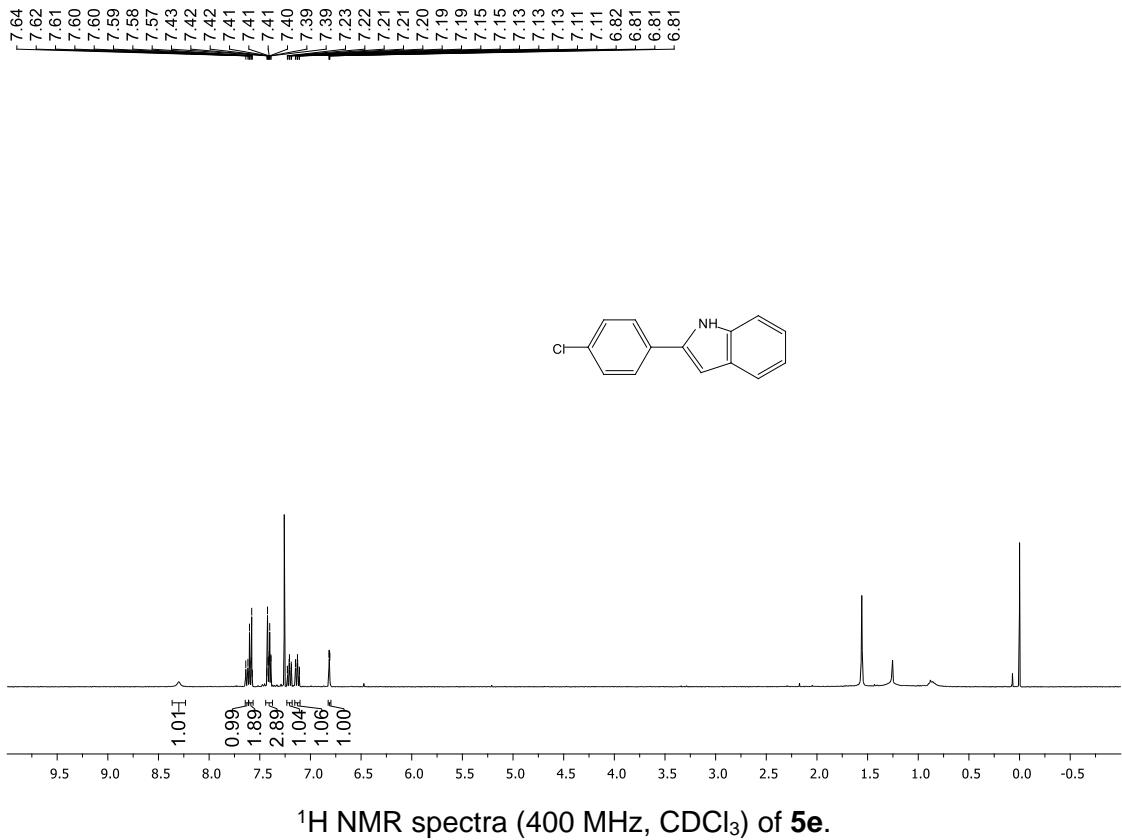
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6.75

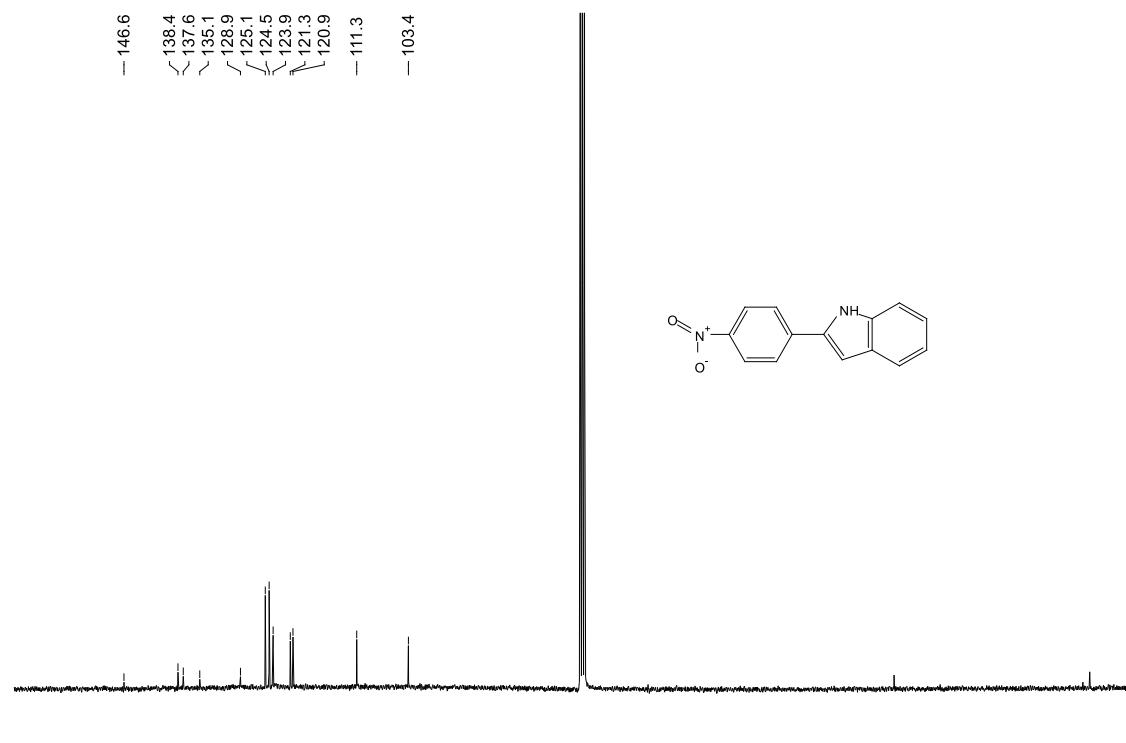
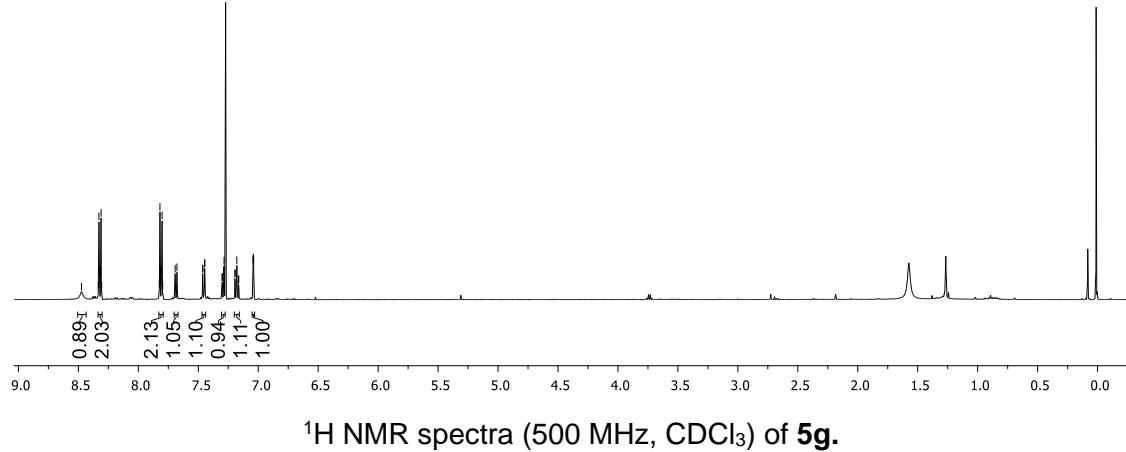


— 163.6
— 161.2

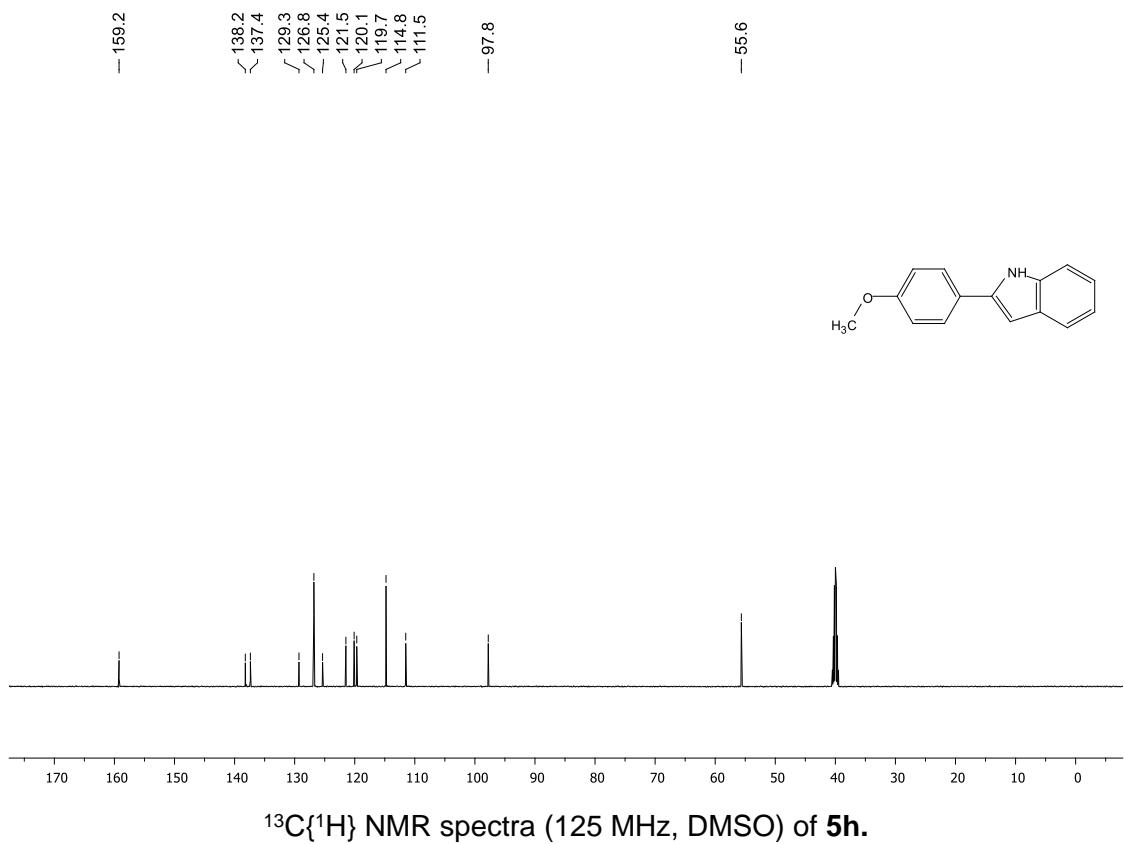
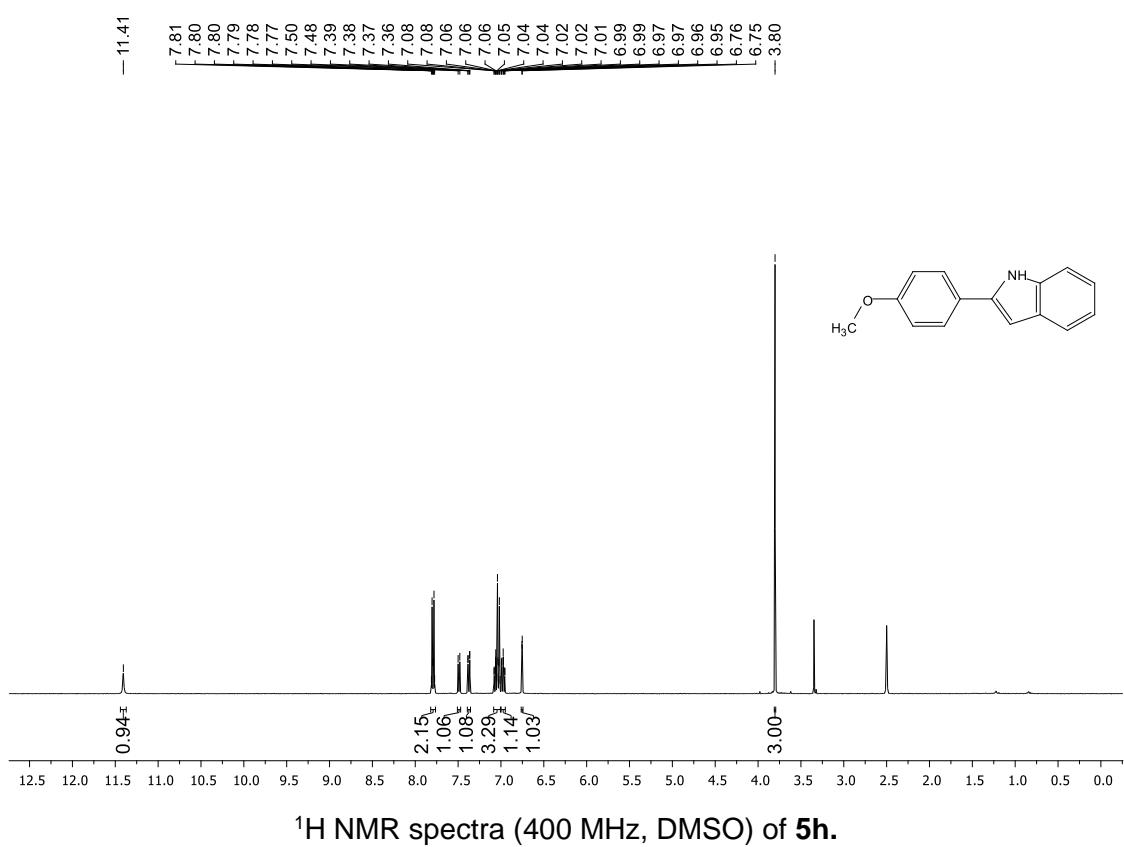
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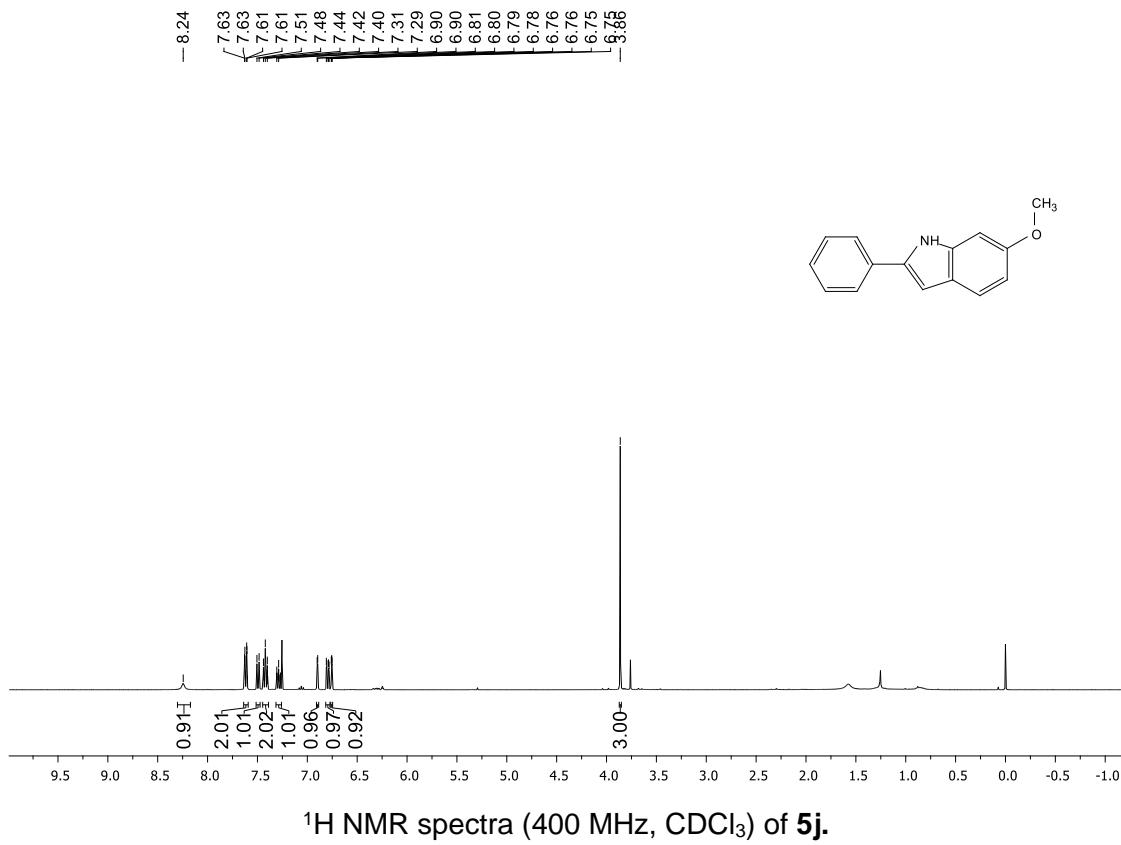
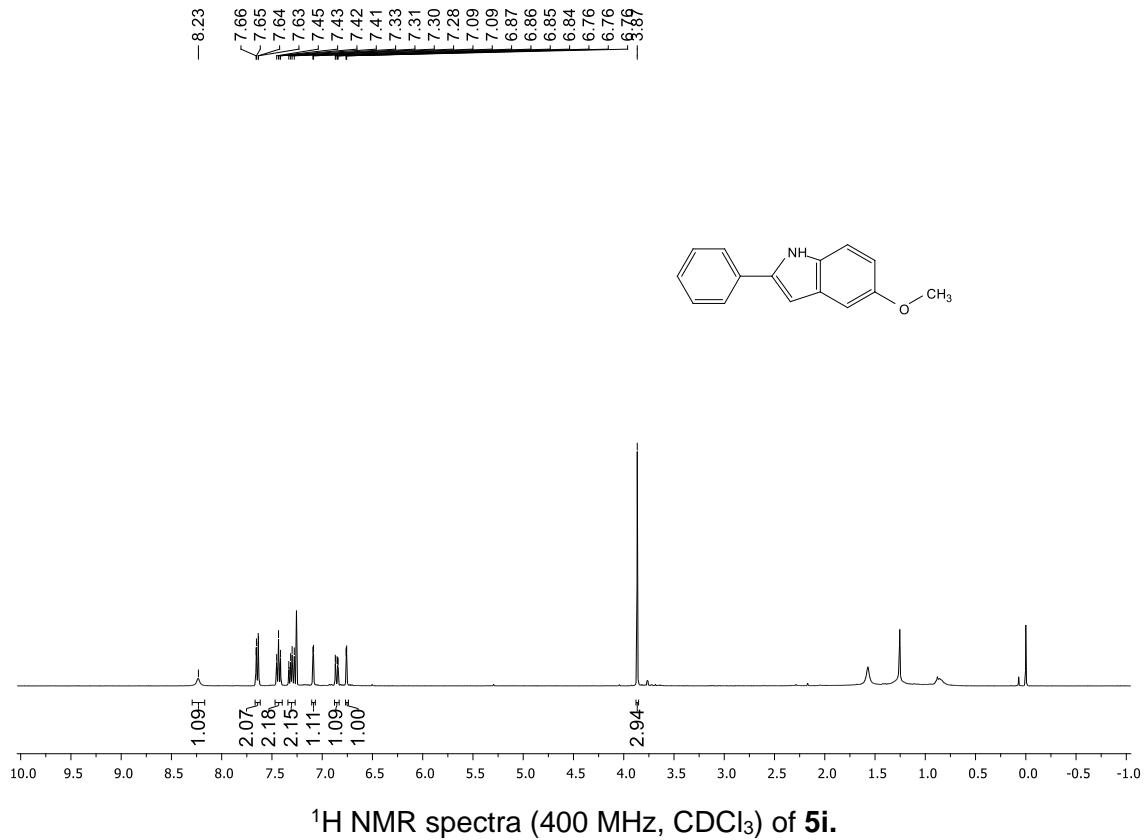


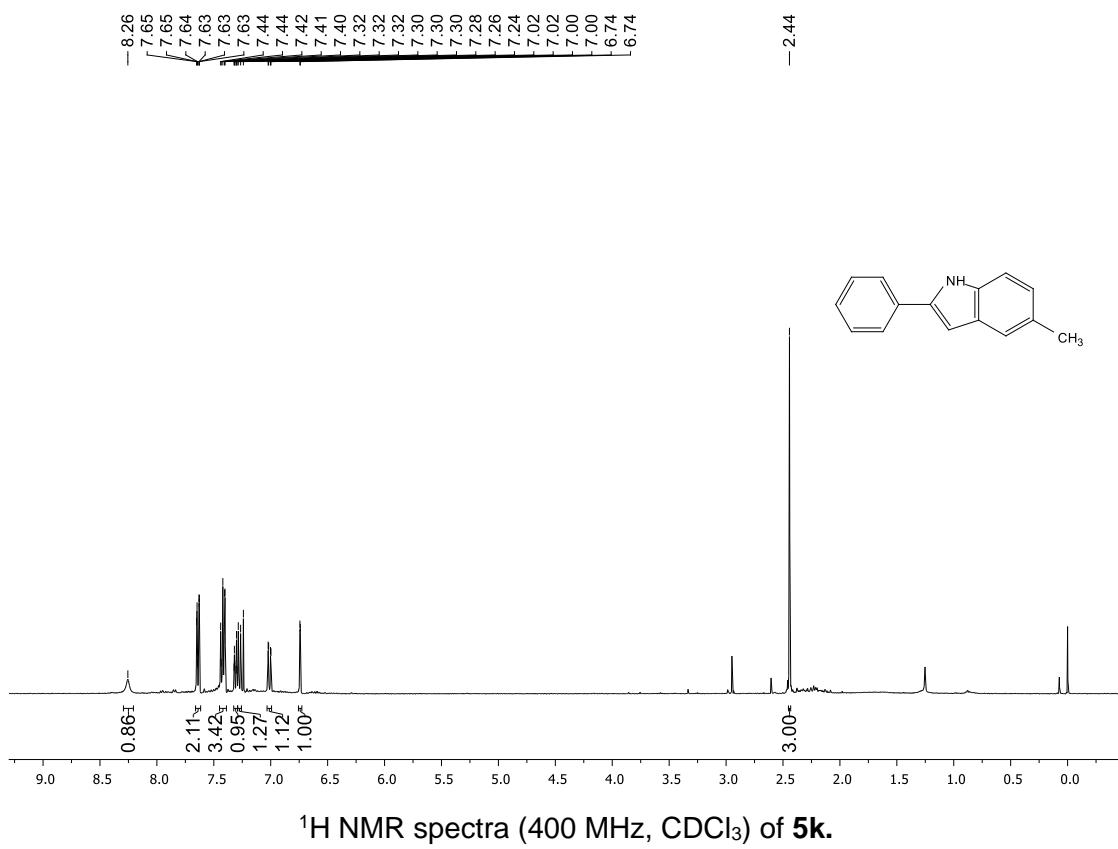
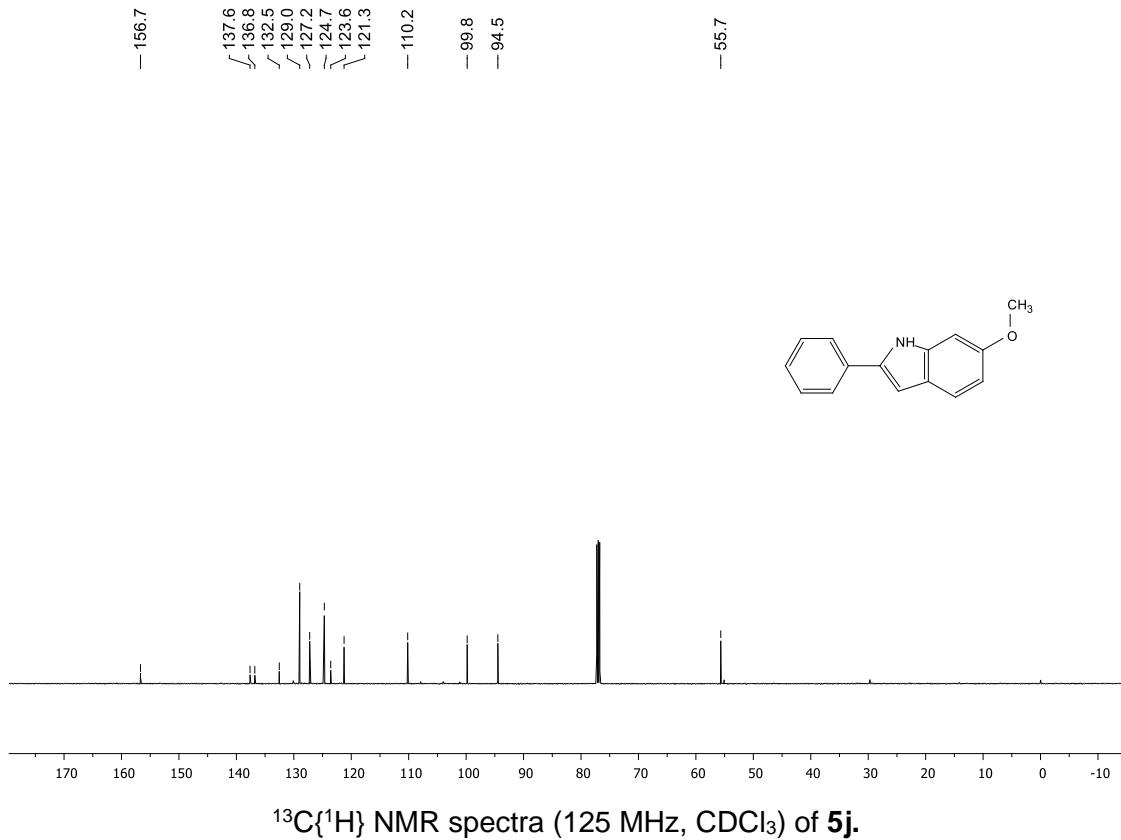


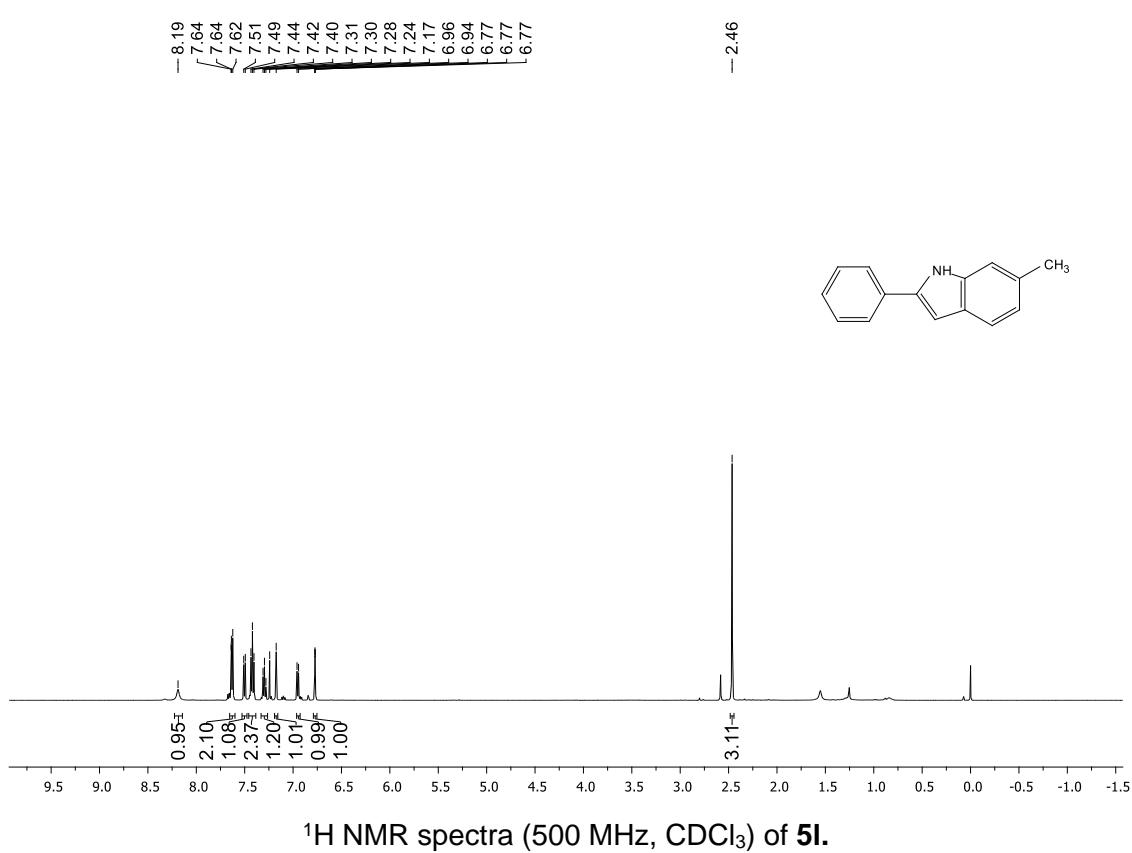
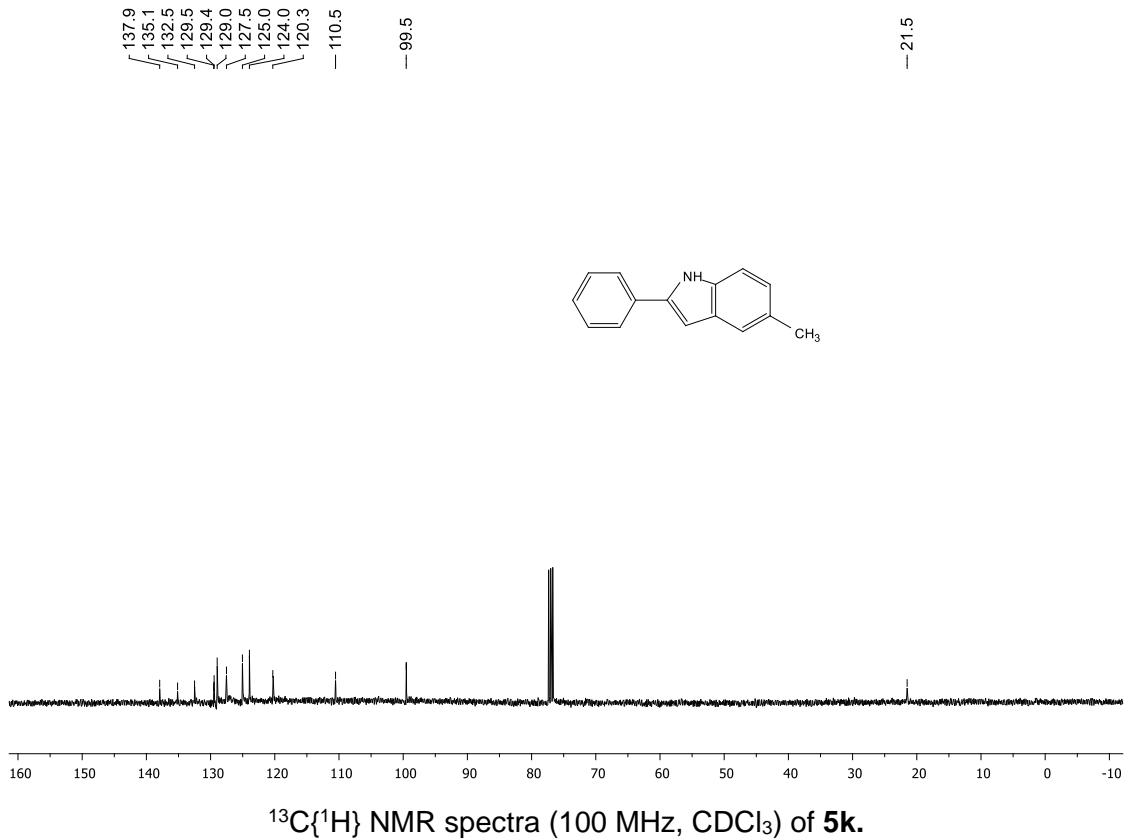


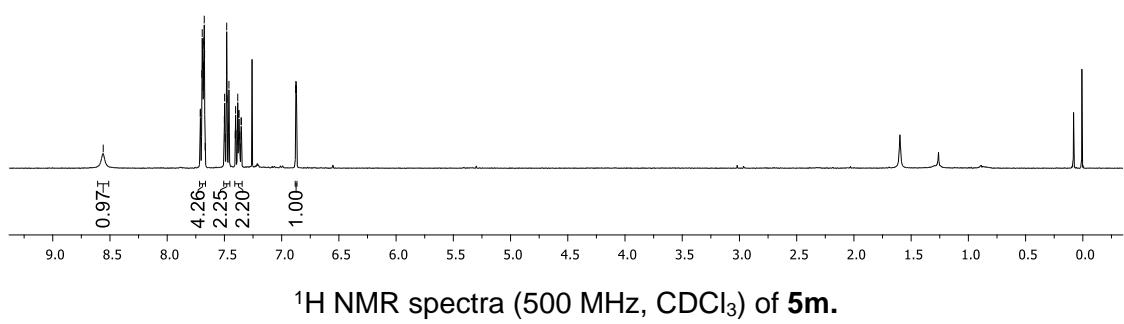
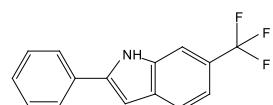
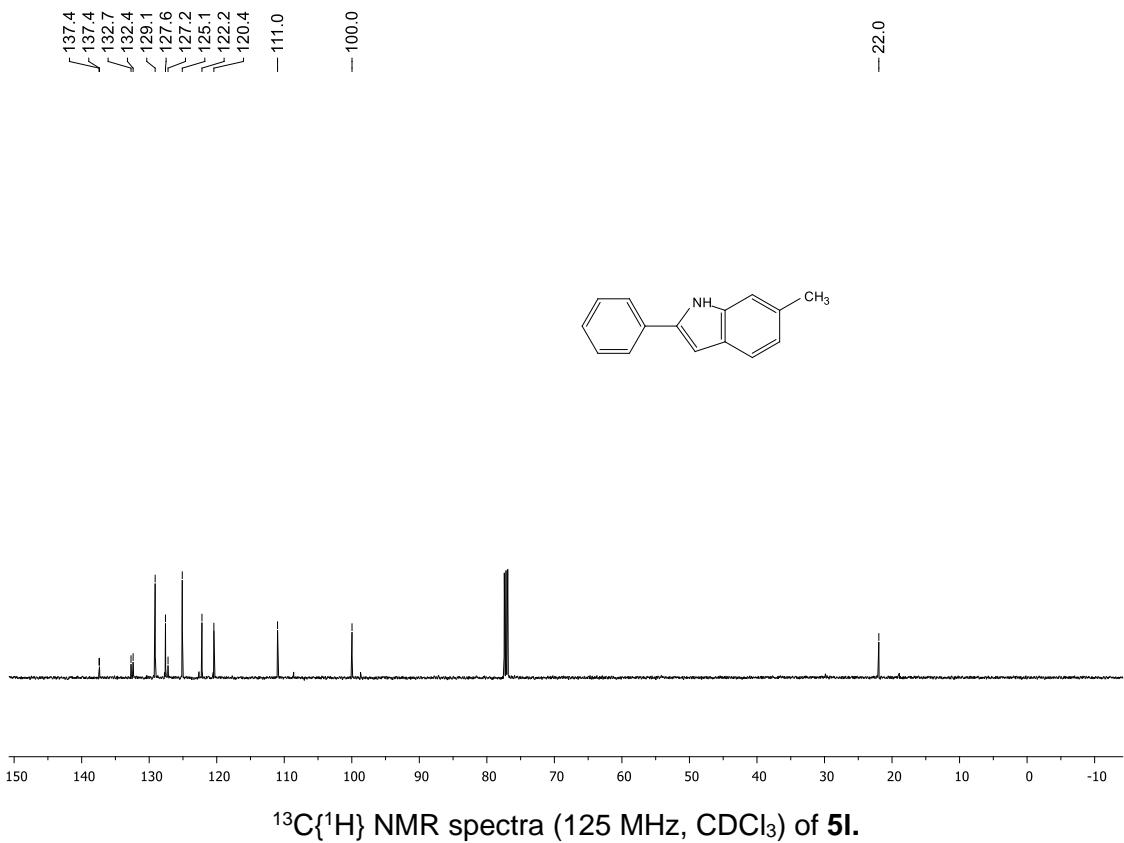
¹³C{¹H} NMR spectra (100 MHz, CDCl₃) of **5g**.

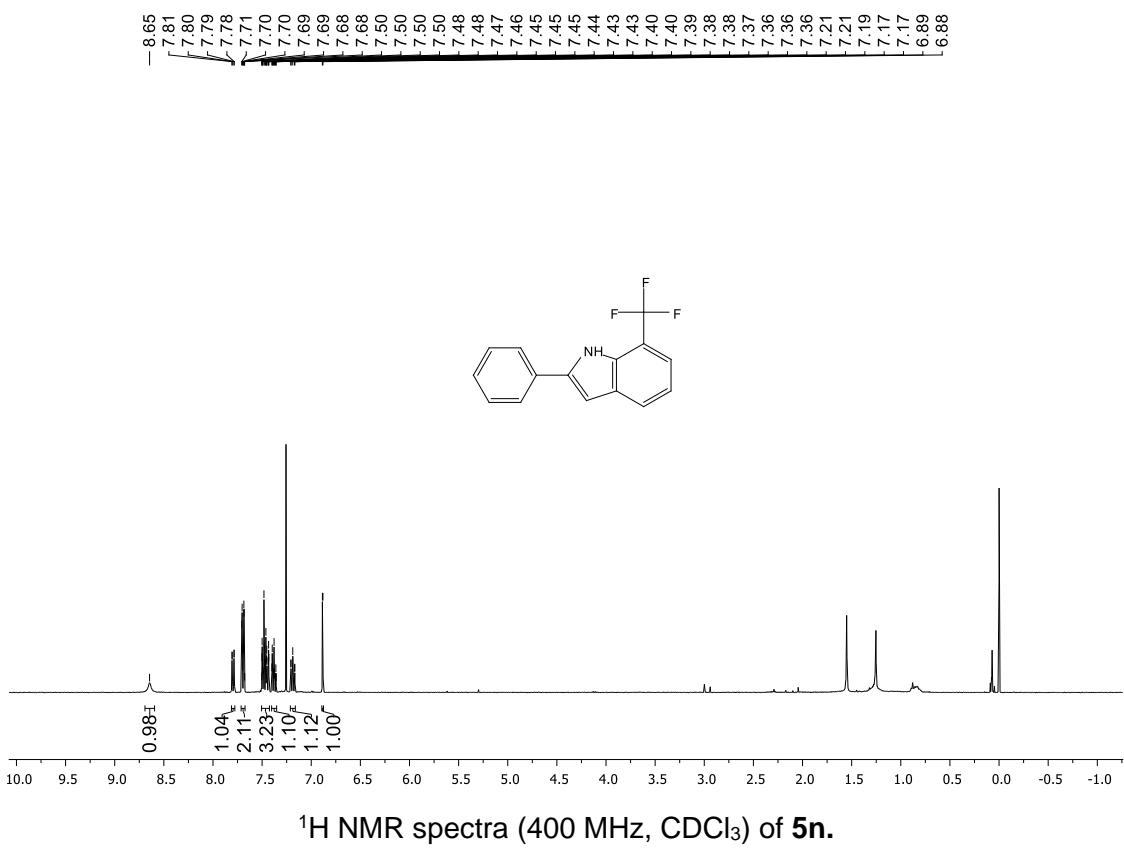
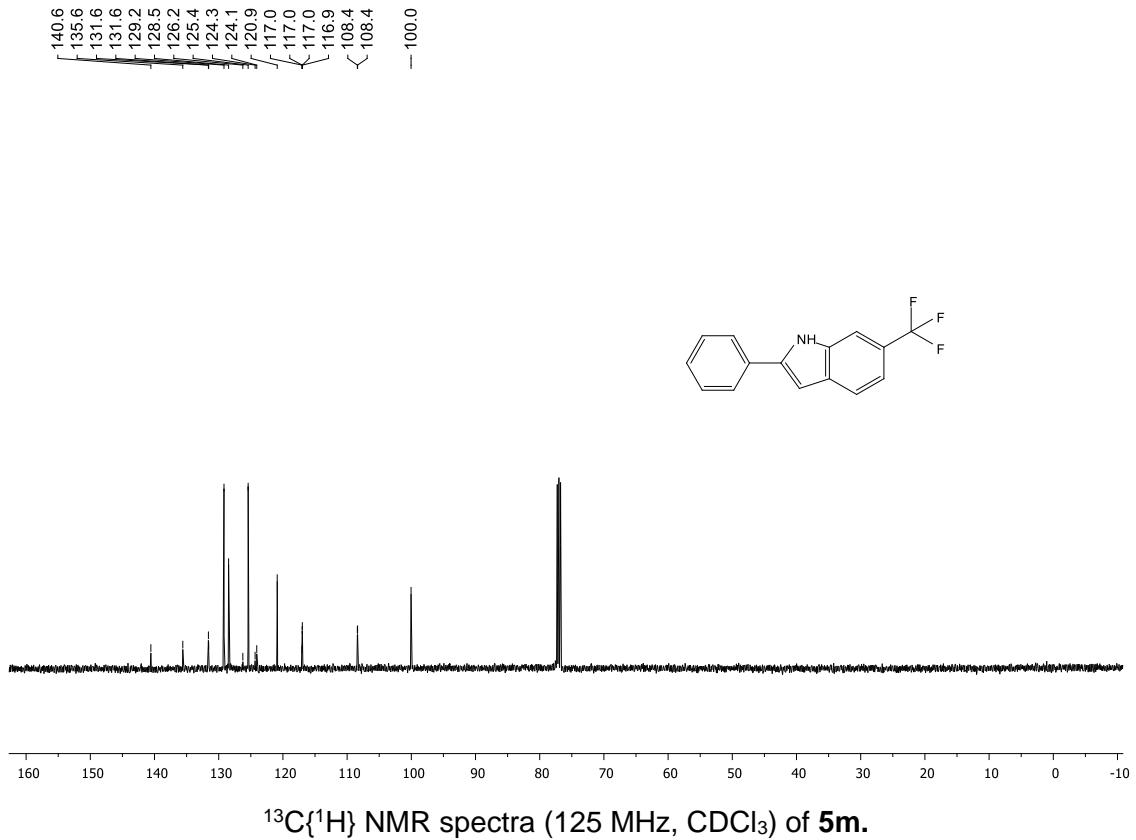


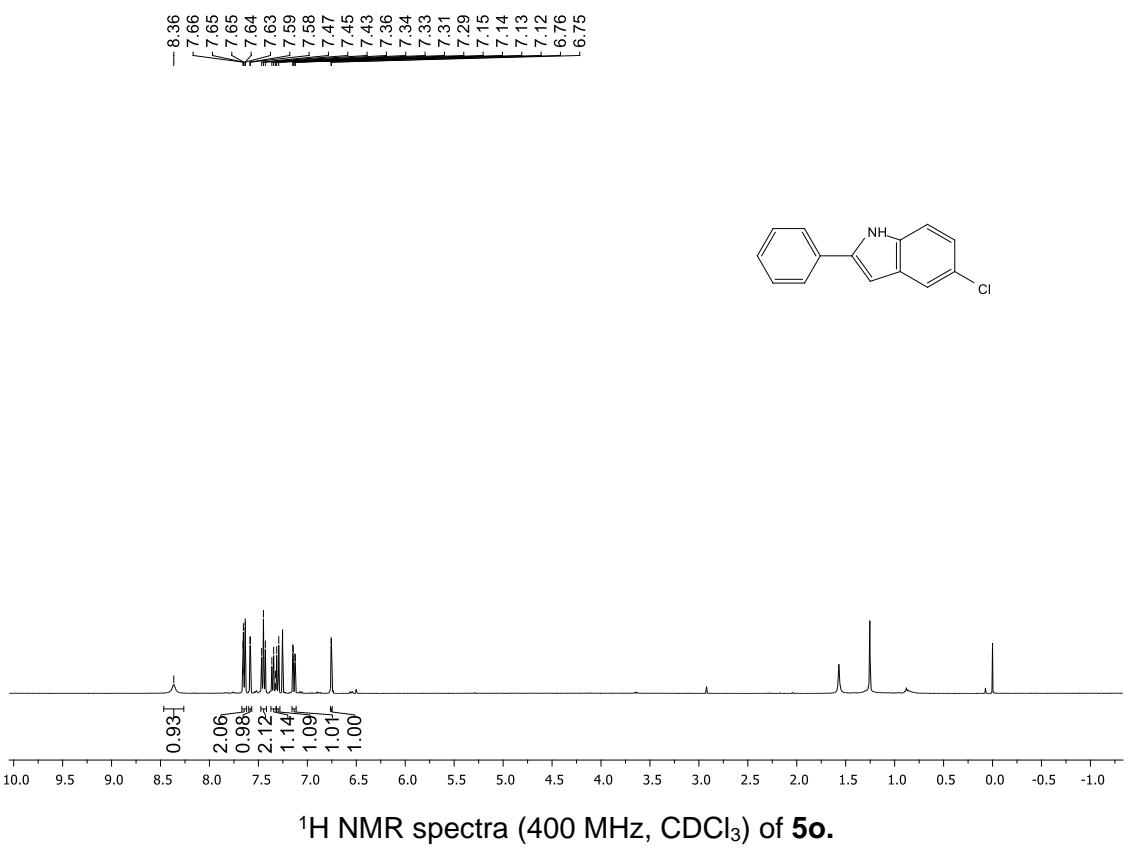
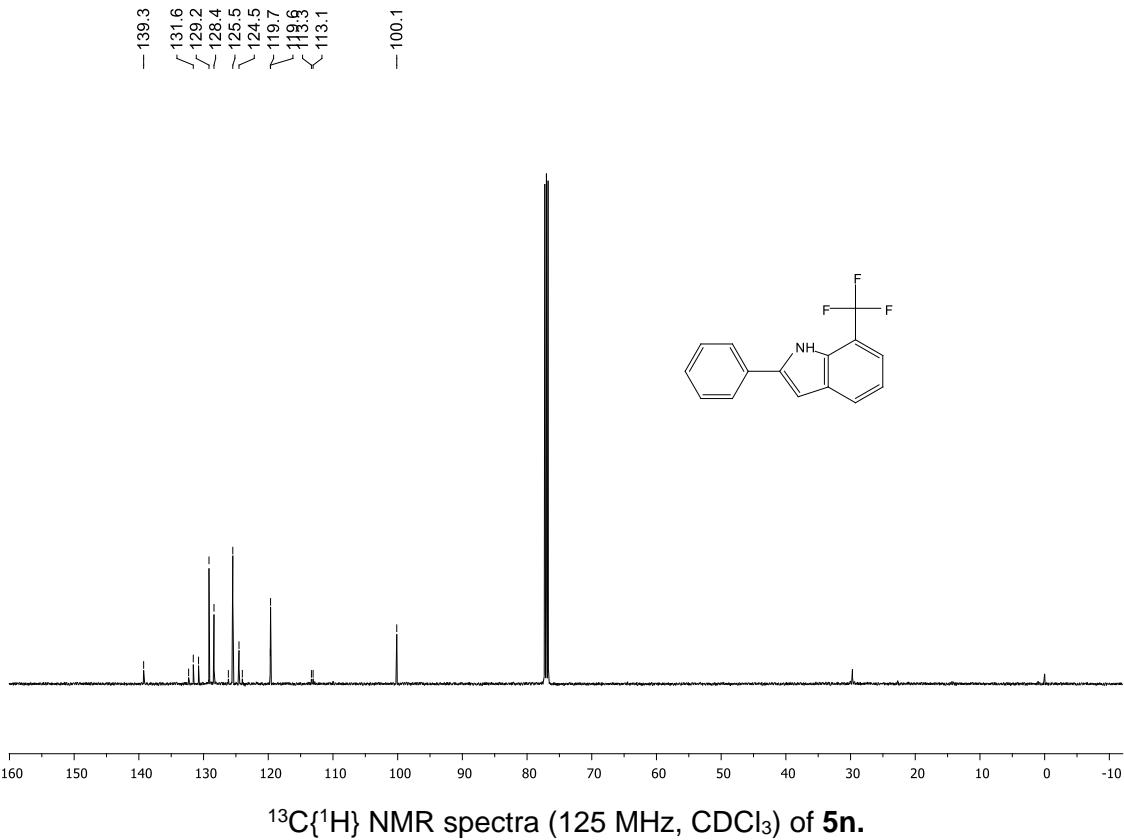


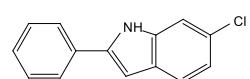
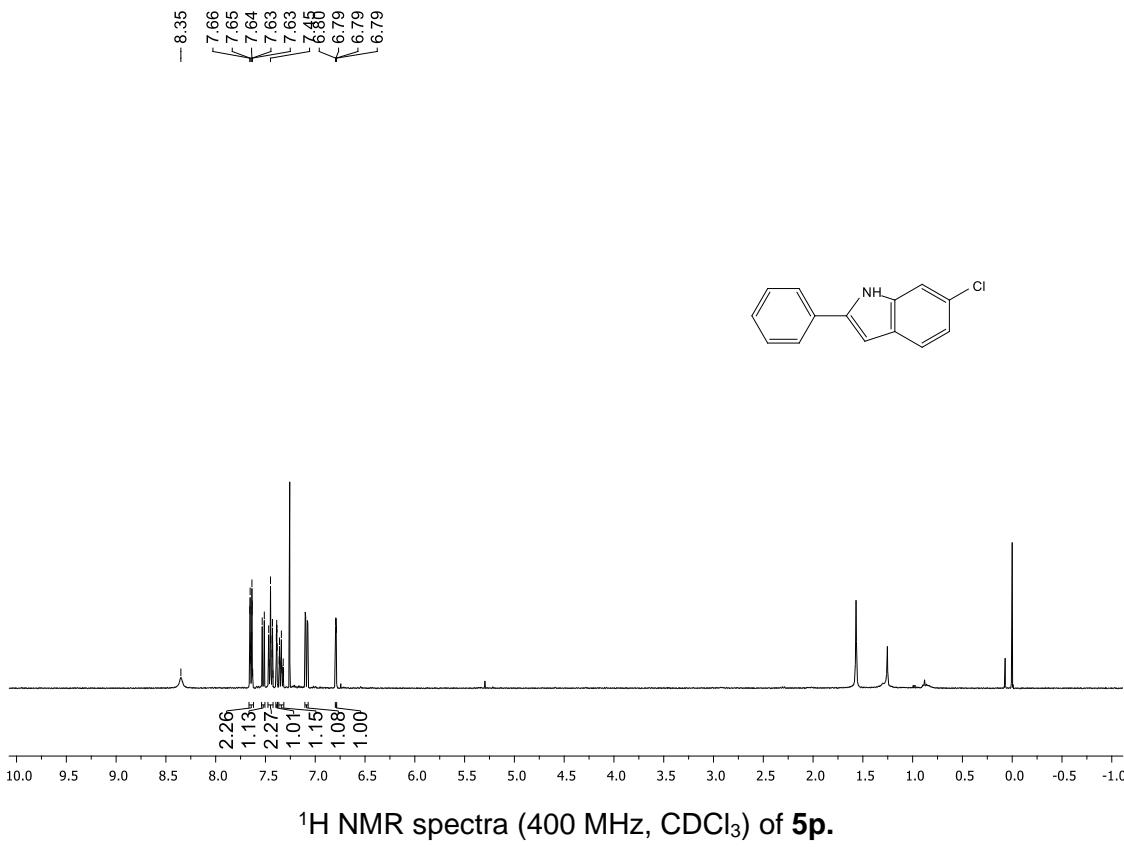
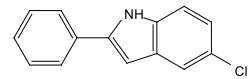
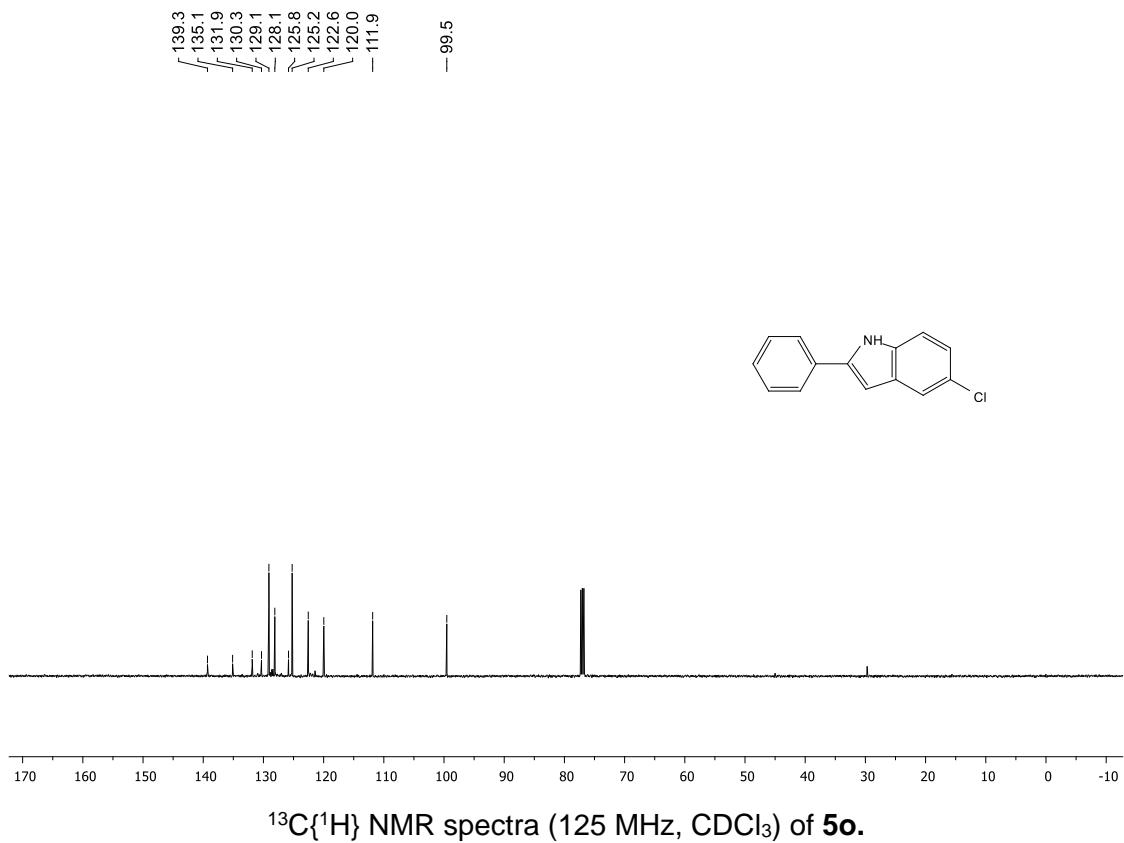


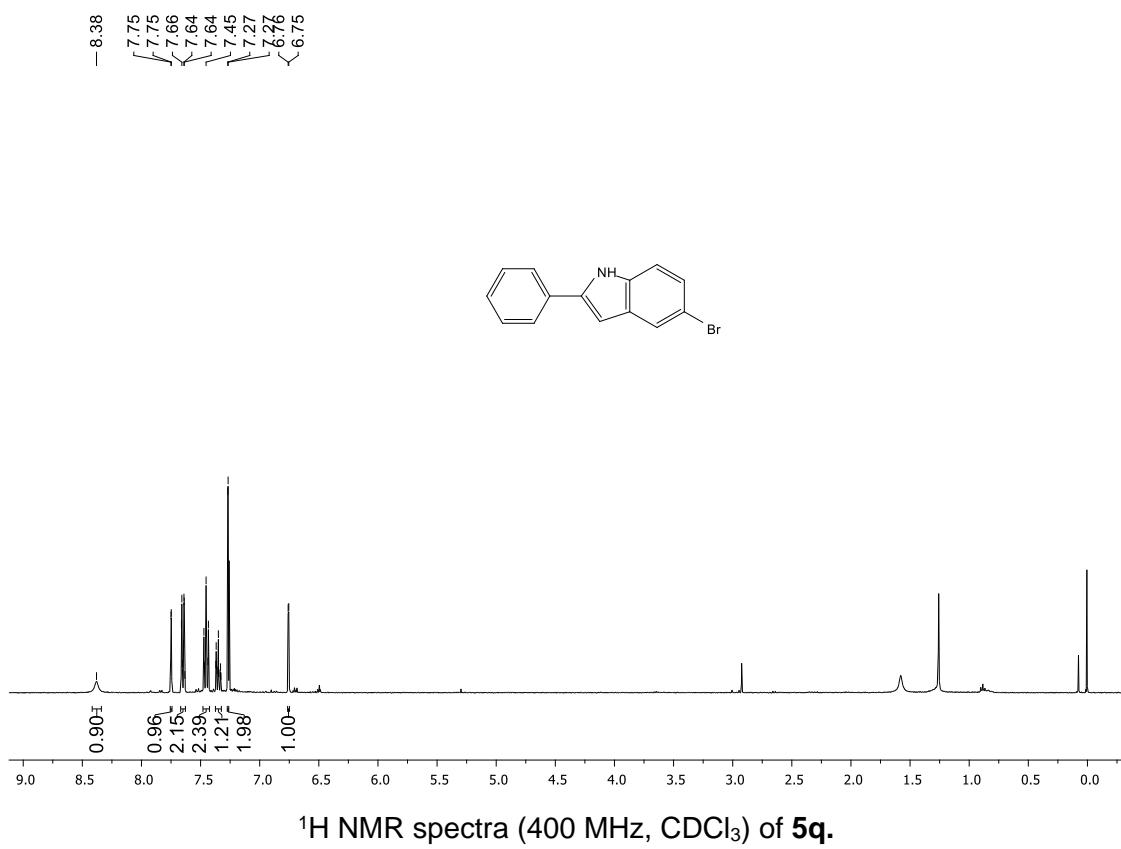
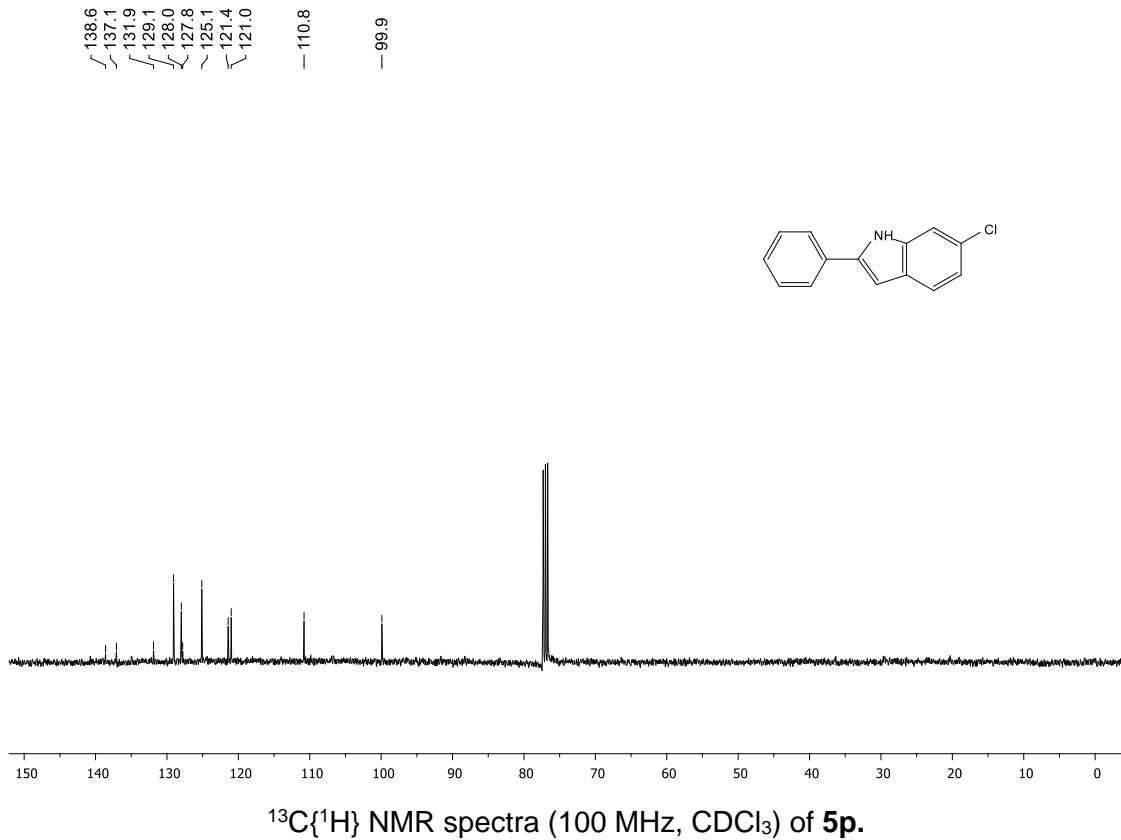


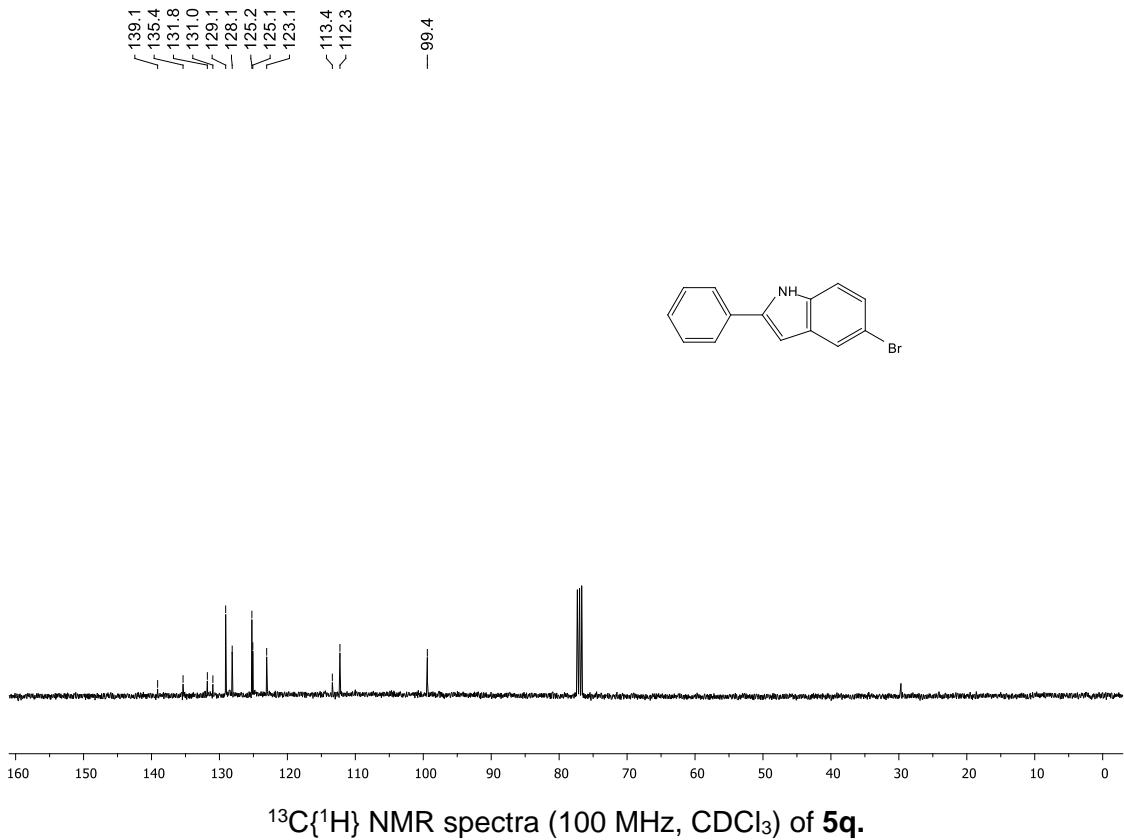




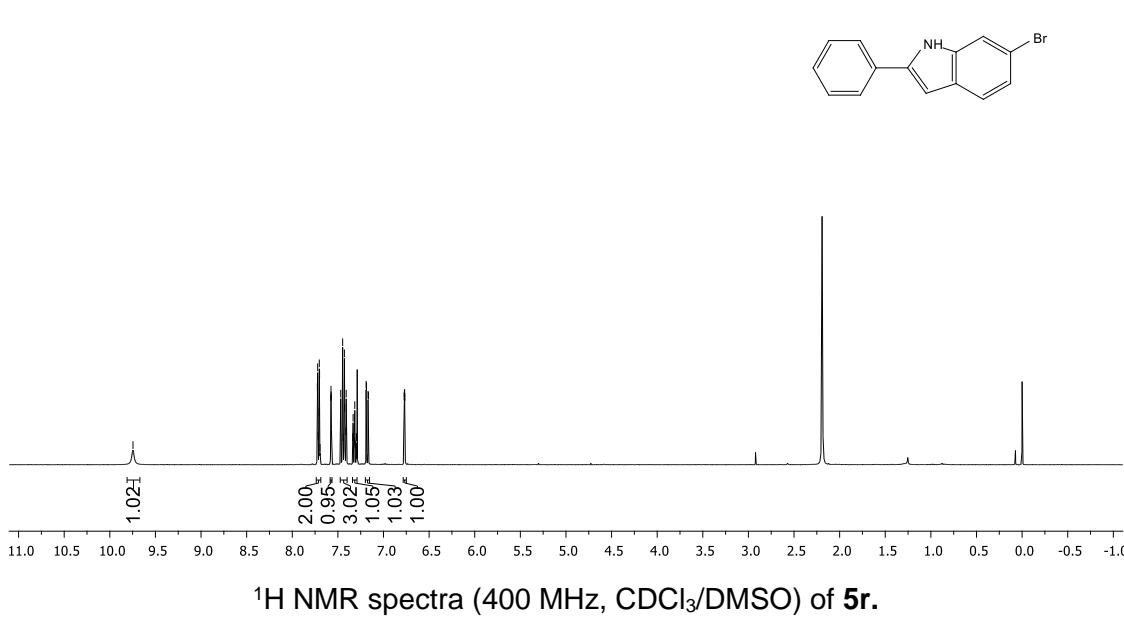


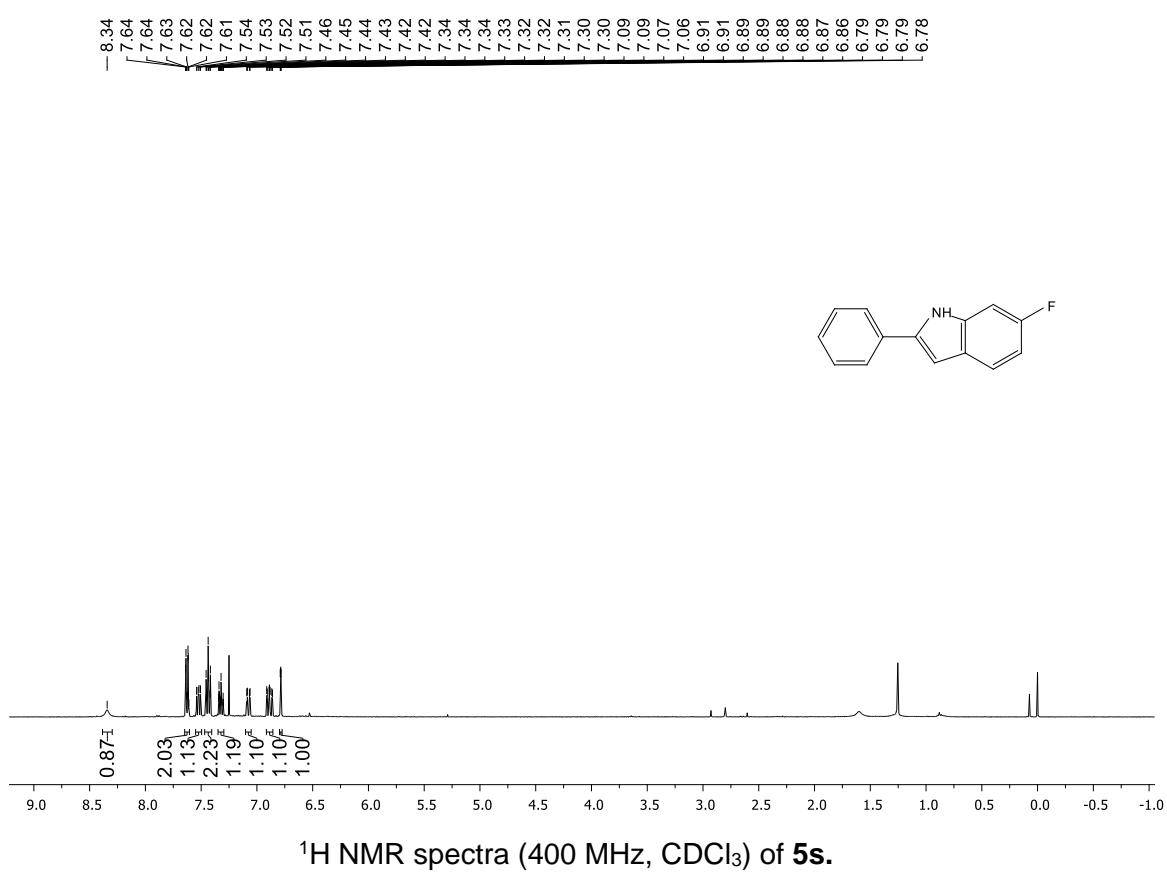
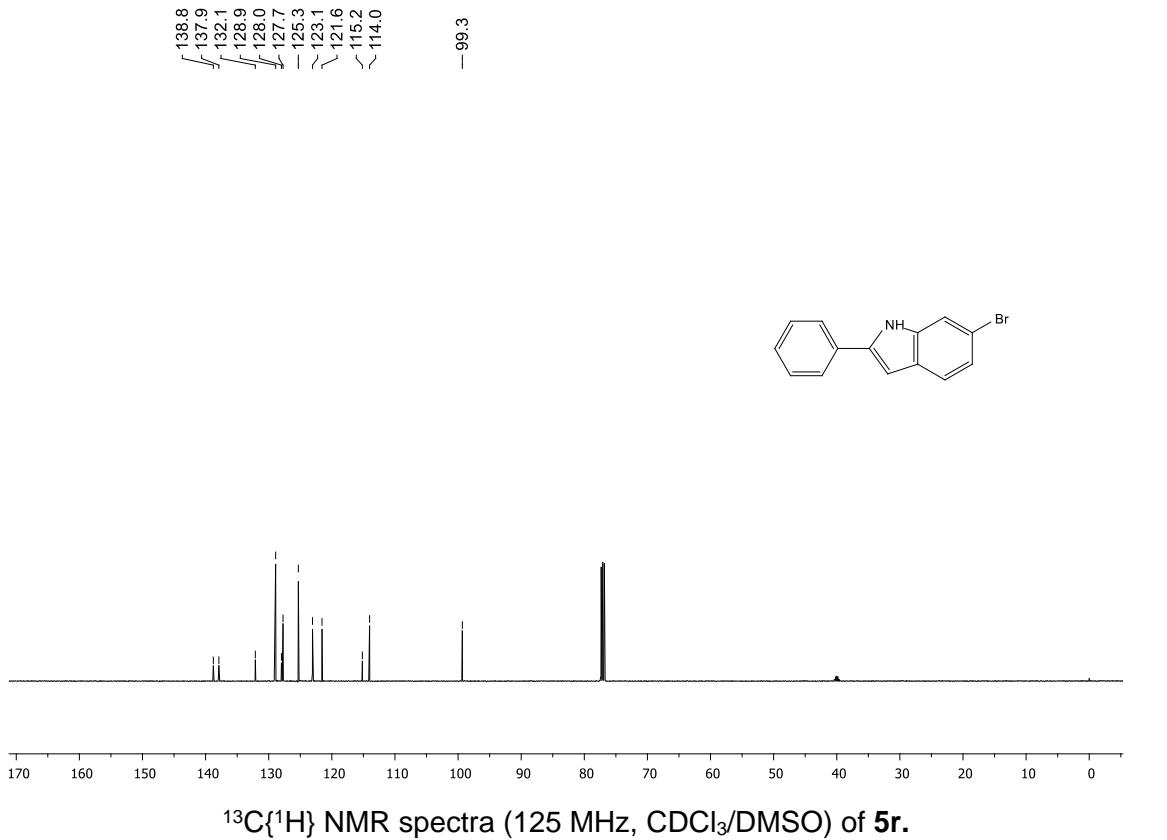


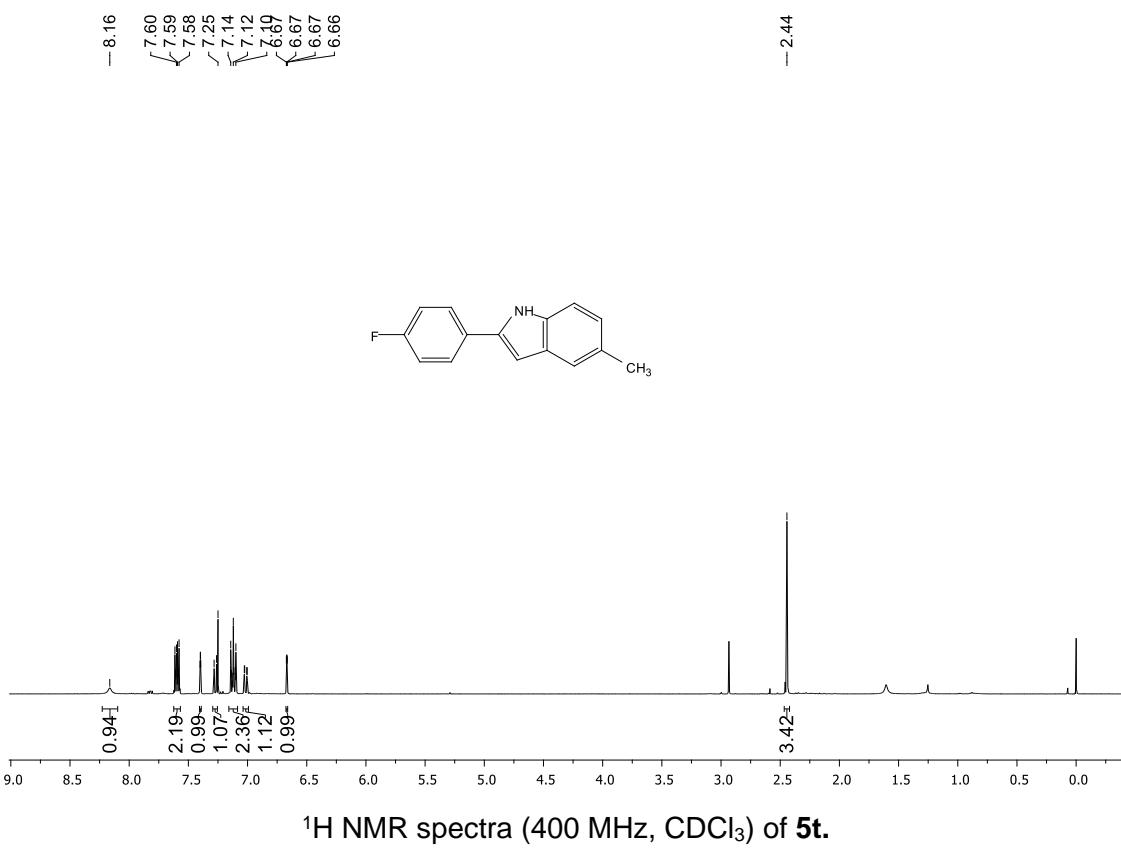
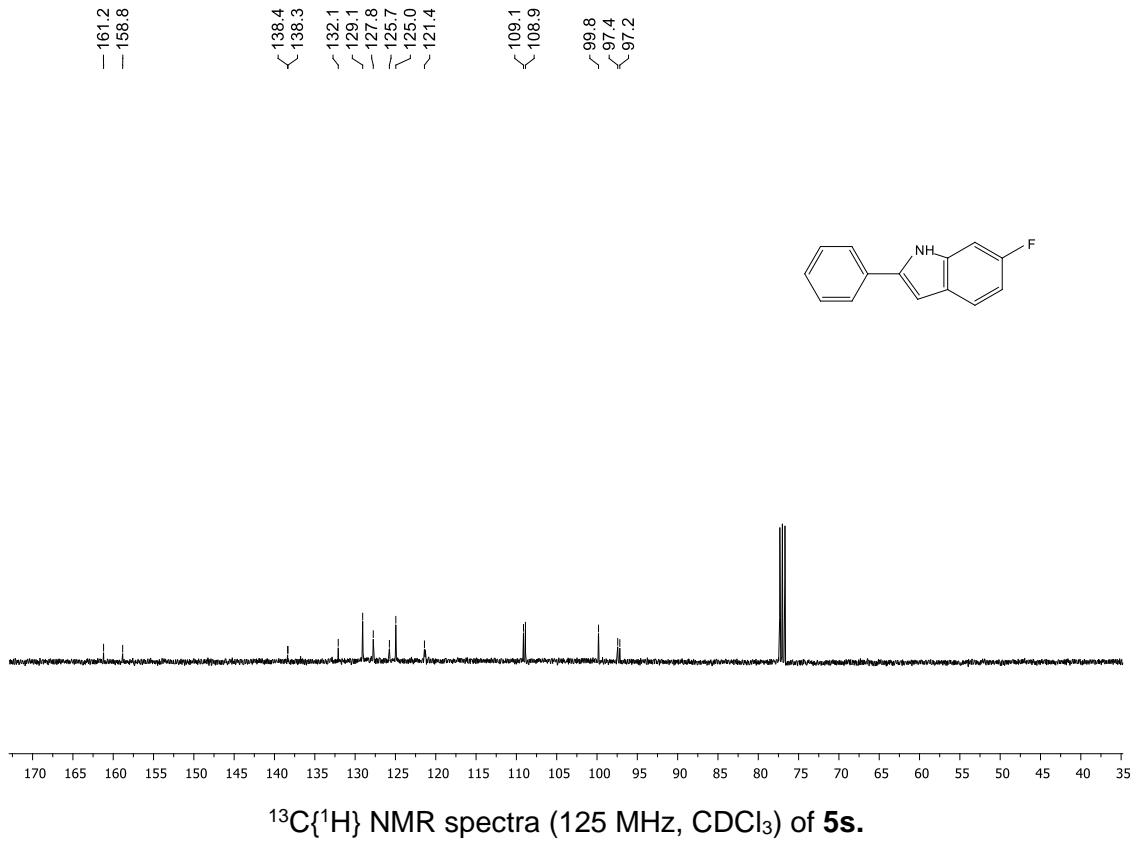


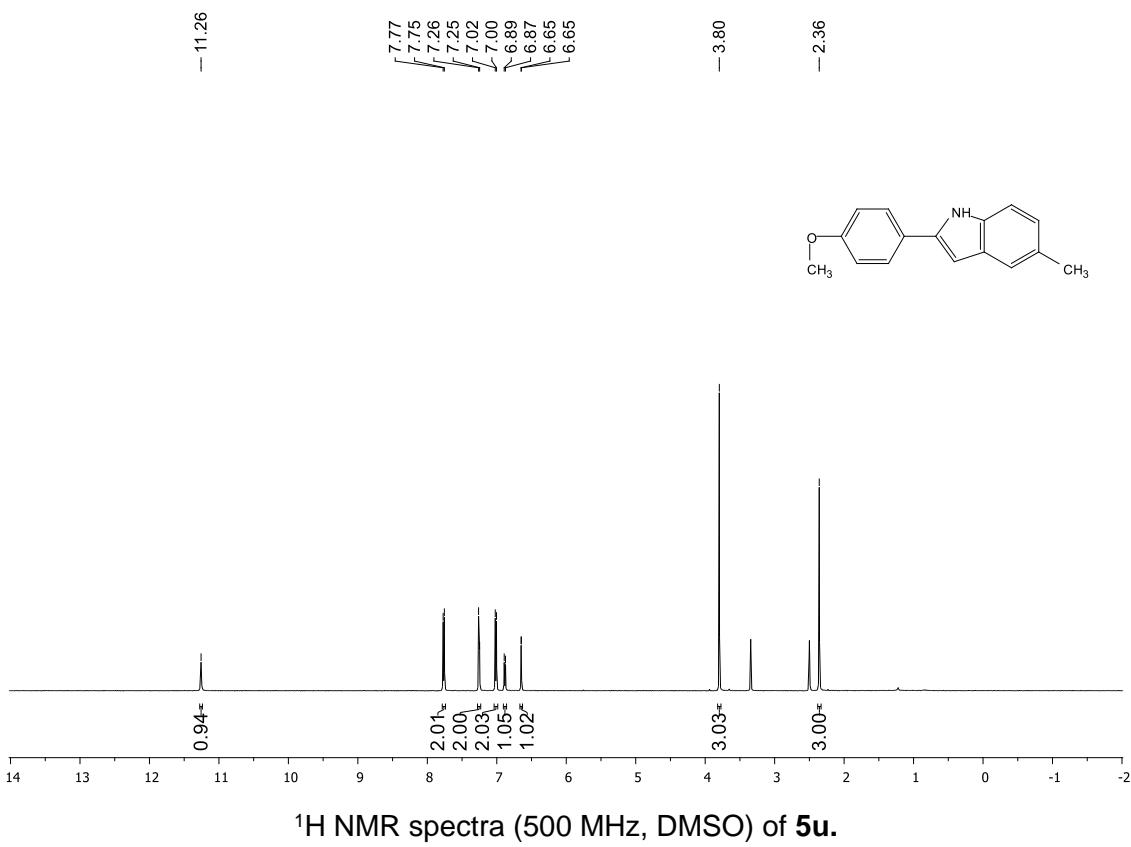
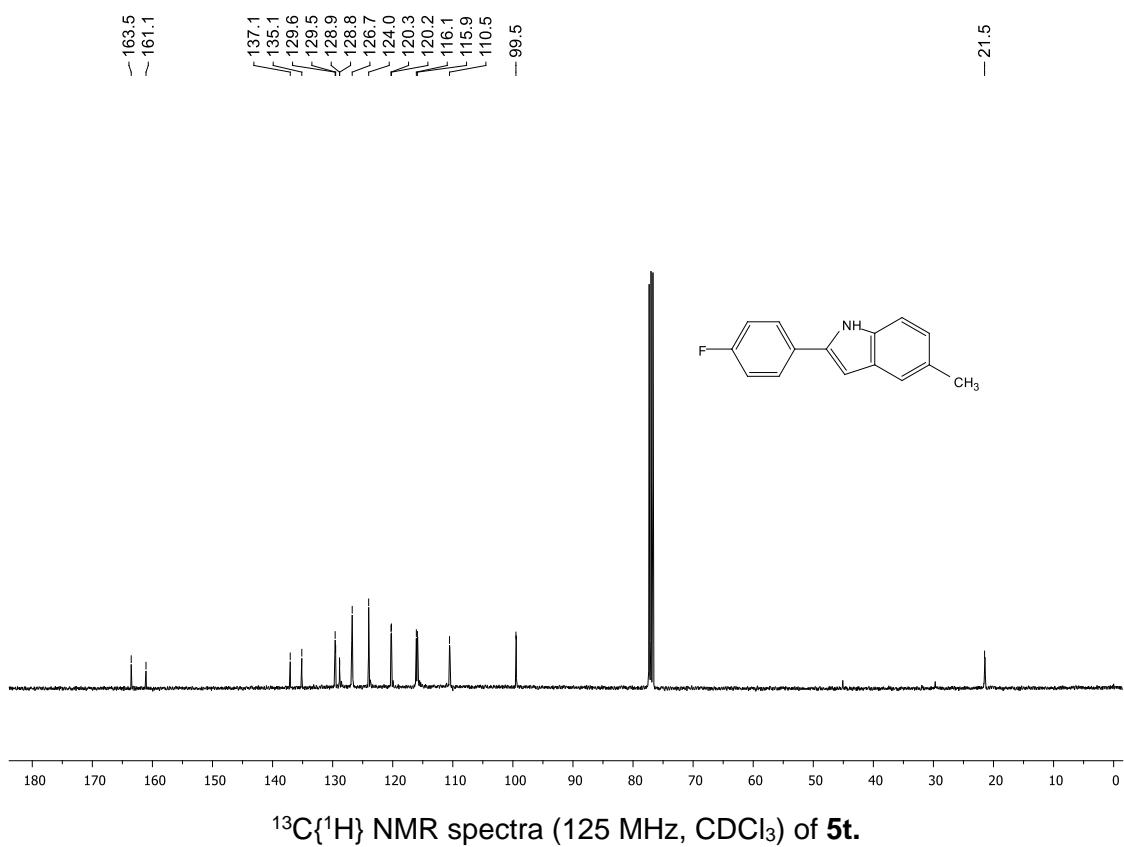


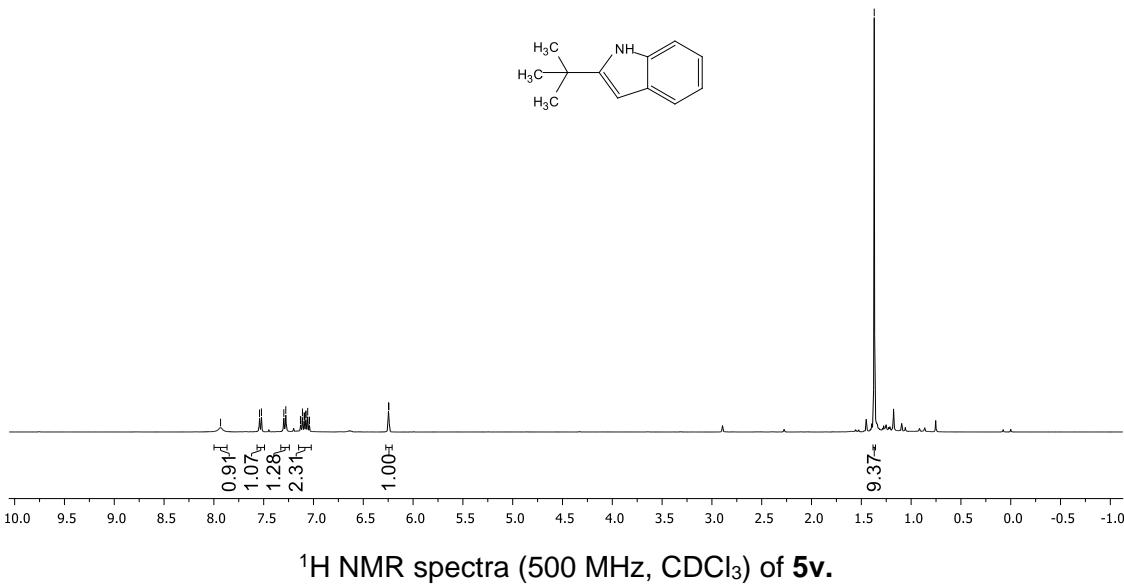
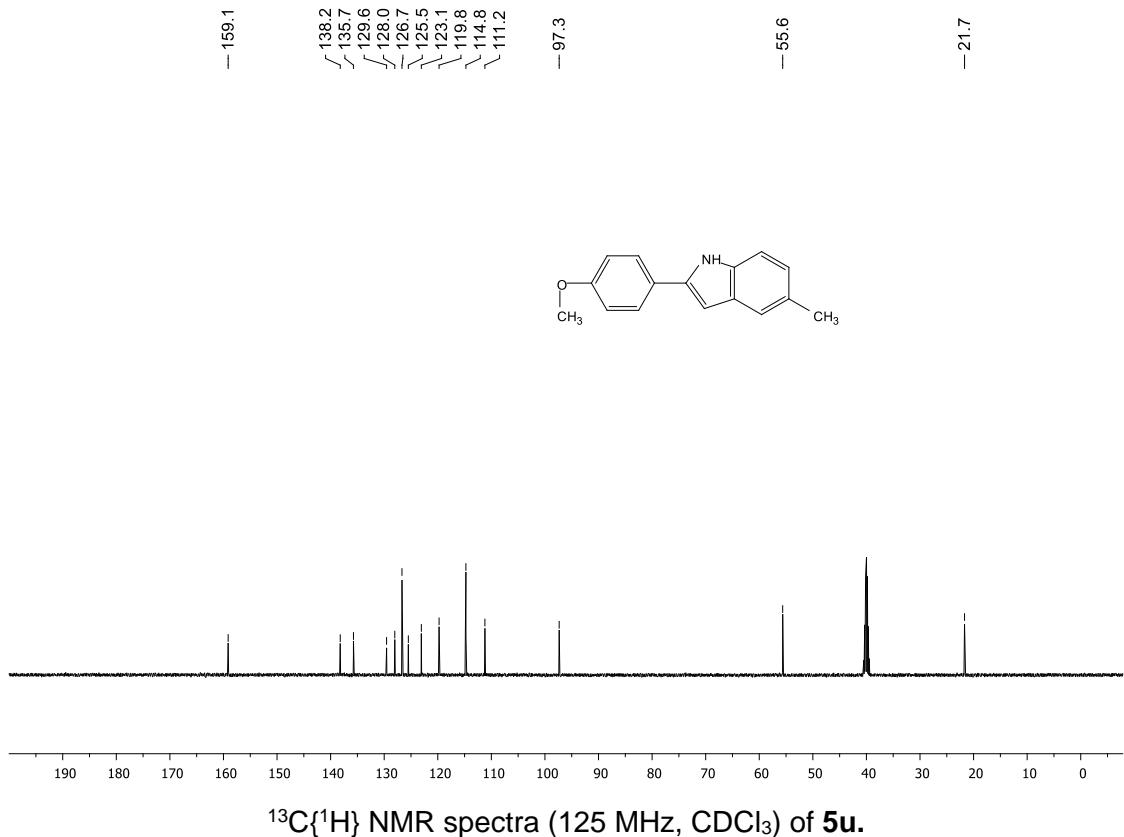
^1H NMR spectra (400 MHz, $\text{CDCl}_3/\text{DMSO}$) of **5r**.

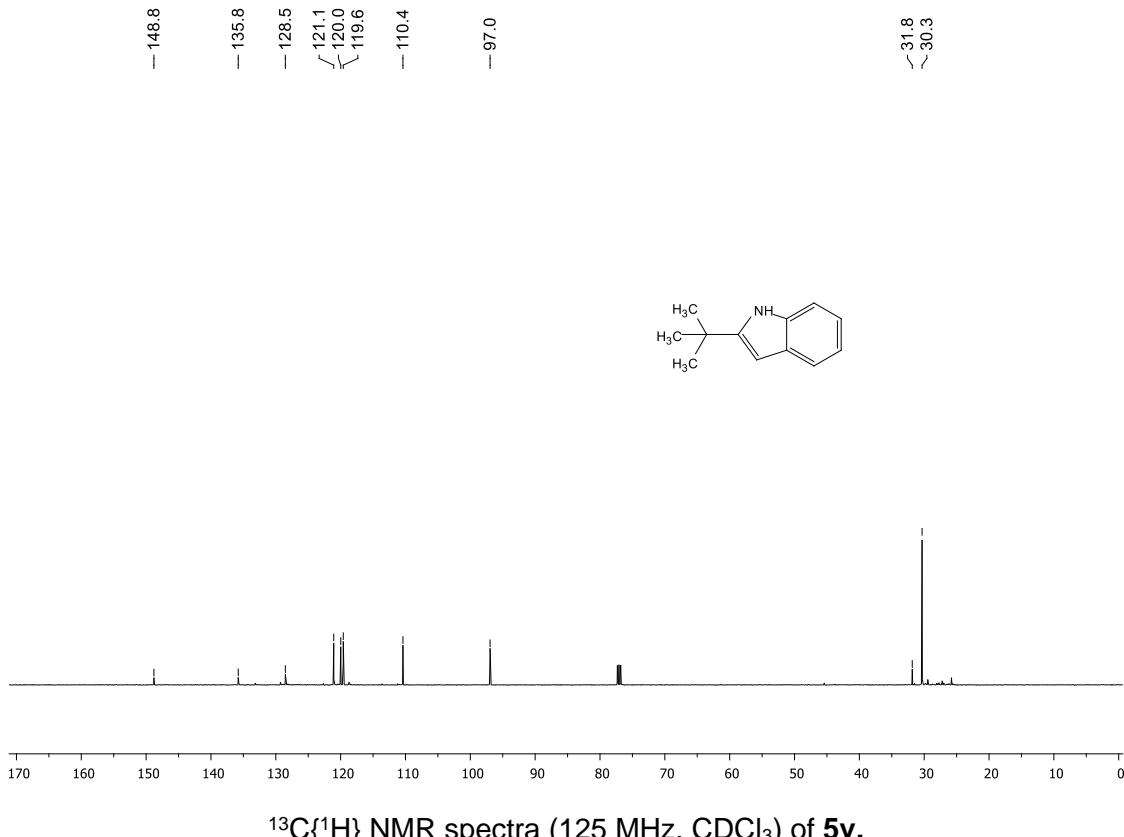


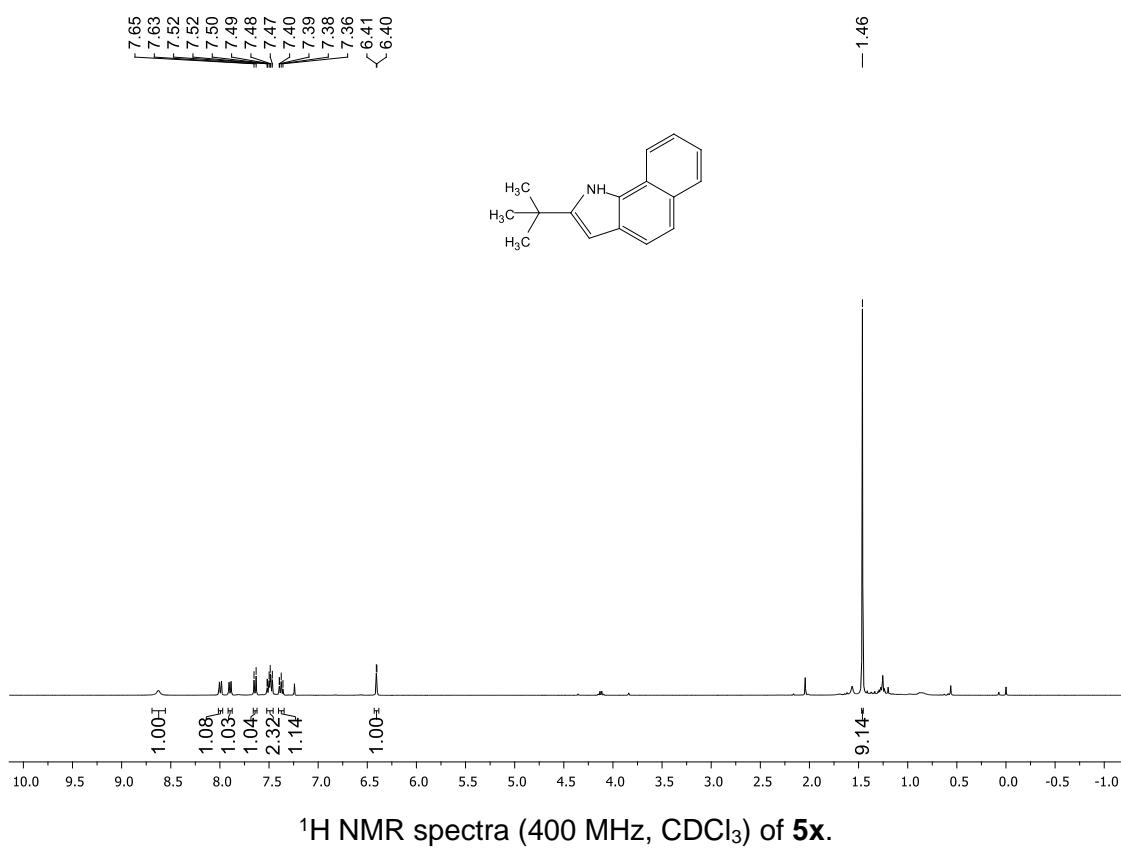
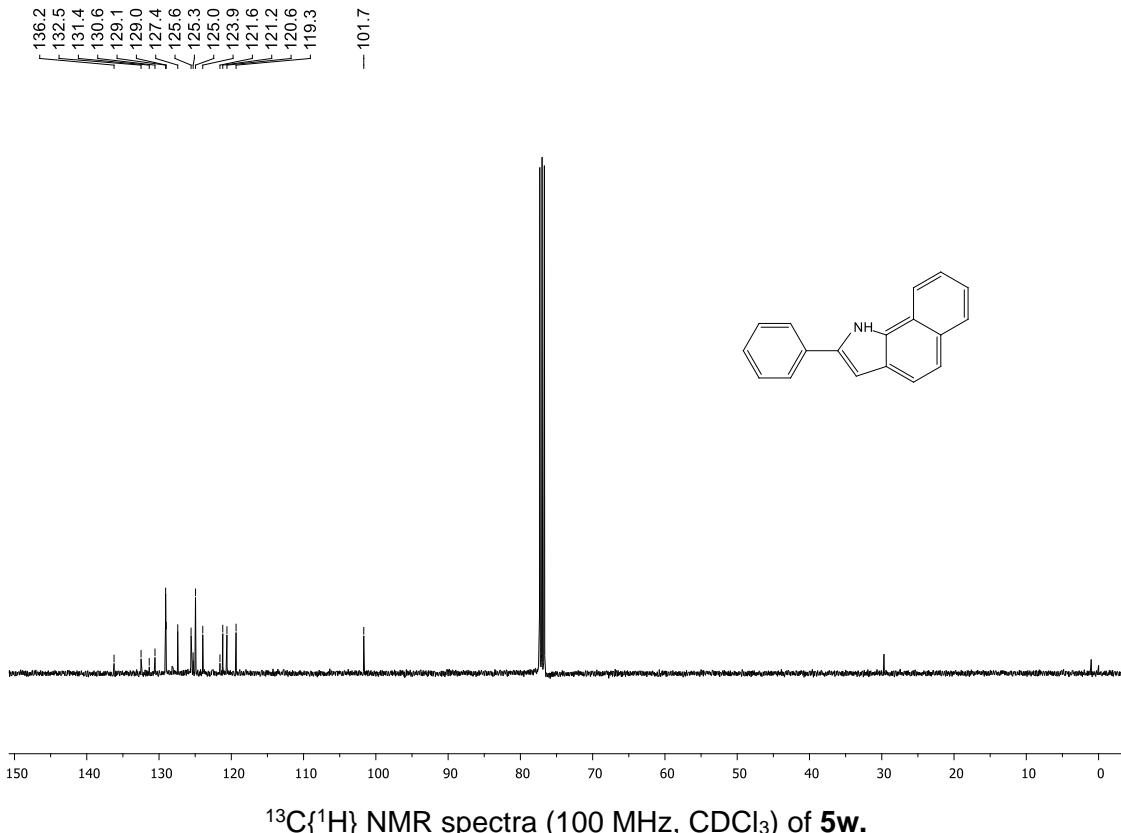


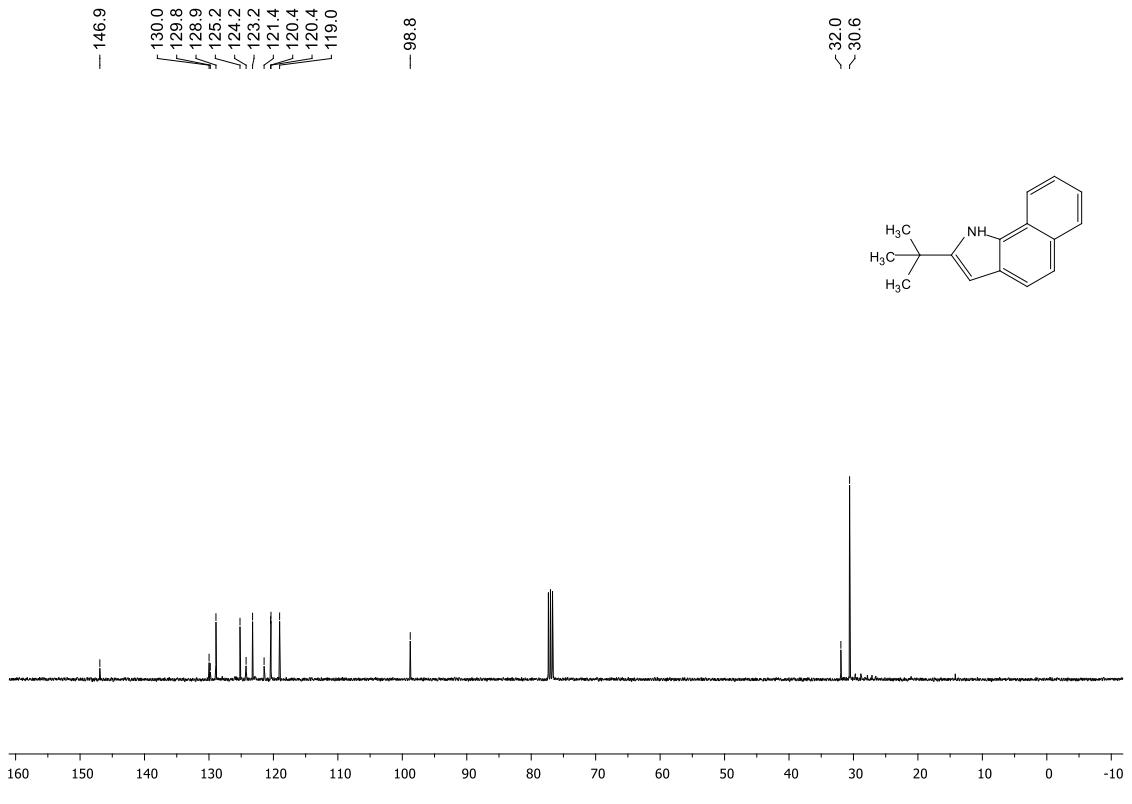




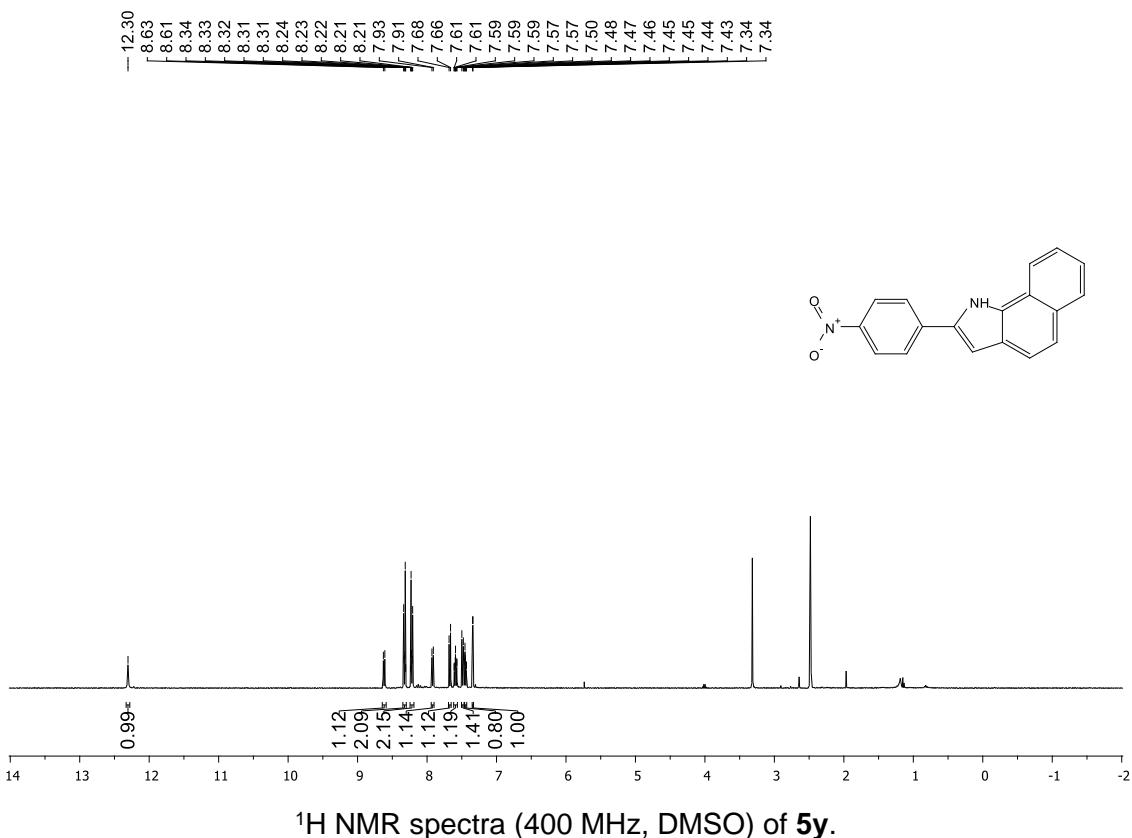








¹³C{¹H} NMR spectra (100 MHz, CDCl₃) of **5x**.



¹H NMR spectra (400 MHz, DMSO) of **5y**.

