

Electronic Supplementary Information for New Journal of Chemistry

Synthesis and Antiproliferative efficiency of novel bis(imidazol-1-yl)vinyl-1,2,4-oxadiazoles

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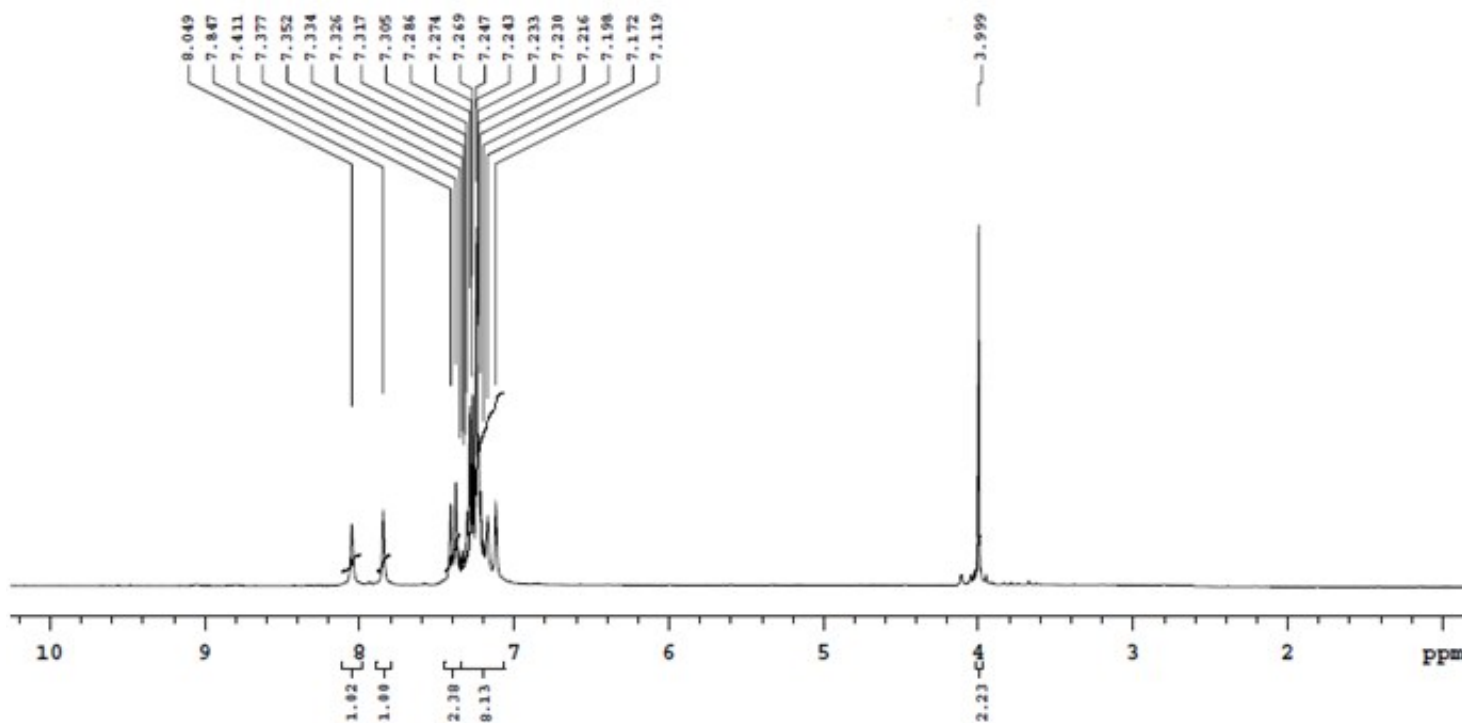
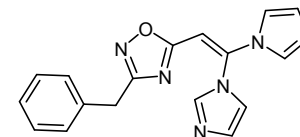
1. General information

Materials and methods: All work relating to analytical thin layer chromatography were performed with E. Merck silica gel 60F₂₅₄ aluminum plates and were visualized with UV light. The following mobile phases were employed for TLC: chloroform, methanol and hexane, and ethyl acetate in different ratios. The instrumental techniques employed for the characterization of the newly synthesized compounds include ¹H and ¹³C NMR and mass spectroscopy. ¹H and ¹³C NMR spectra were recorded on a Agilent WM (400MHz) Fourier transforms spectrophotometer in CDCl₃ or DMSO-d₆ solution using tetramethylsilane (TMS) as internal standard. Chemical shifts were recorded in ppm relative to TMS. Mass and purity were recorded on a LC-MSD-Trap-XCT (Agilent technologies Inc). All the reagents and chemicals used were from sigma Aldrich chemicals.

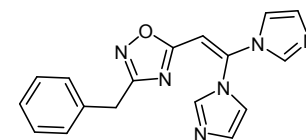
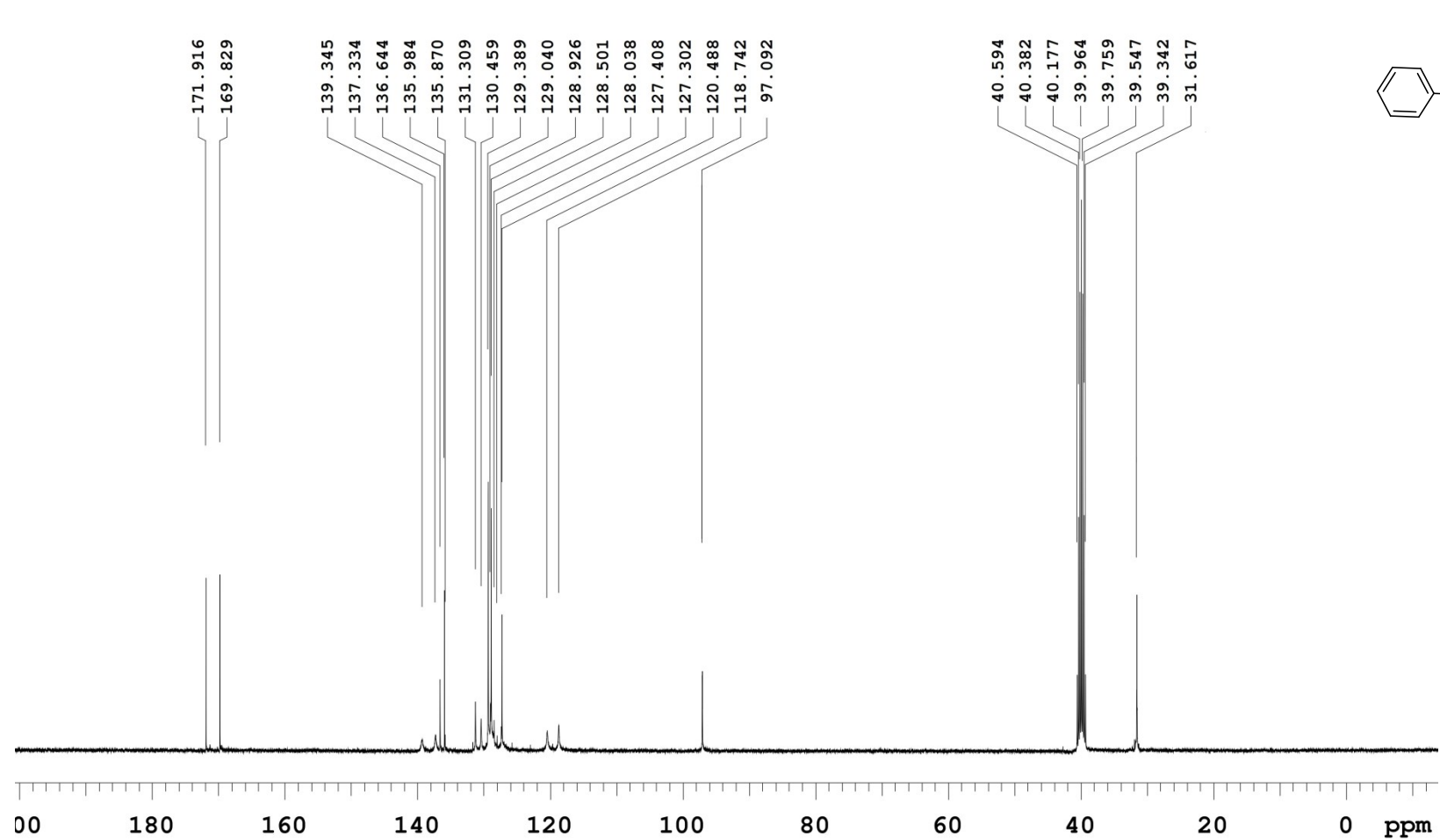
2. General procedure for the synthesis of oxadiazoles: To a solution of 3,3,3-trifluoropropanoic acid (1.2 eq) in DMF (10 v), CDI (2.0 eq) was added and stirred at room temperature for 2 h. After 2 h amidoxime (1.0 eq) was added and heated at 100 °C for 6 h. Reaction was monitored by TLC. After the completion of reaction, reaction mixture was extracted with ethyl acetate, washed with water and then brine, dried over Na₂SO₄. The solvent was removed under reduced pressure. Obtained crude was purified by silica gel column chromatography.

3. ^1H NMR and ^{13}C NMR of compounds 3a-3o

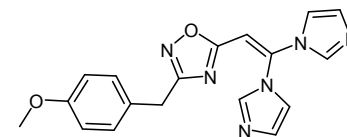
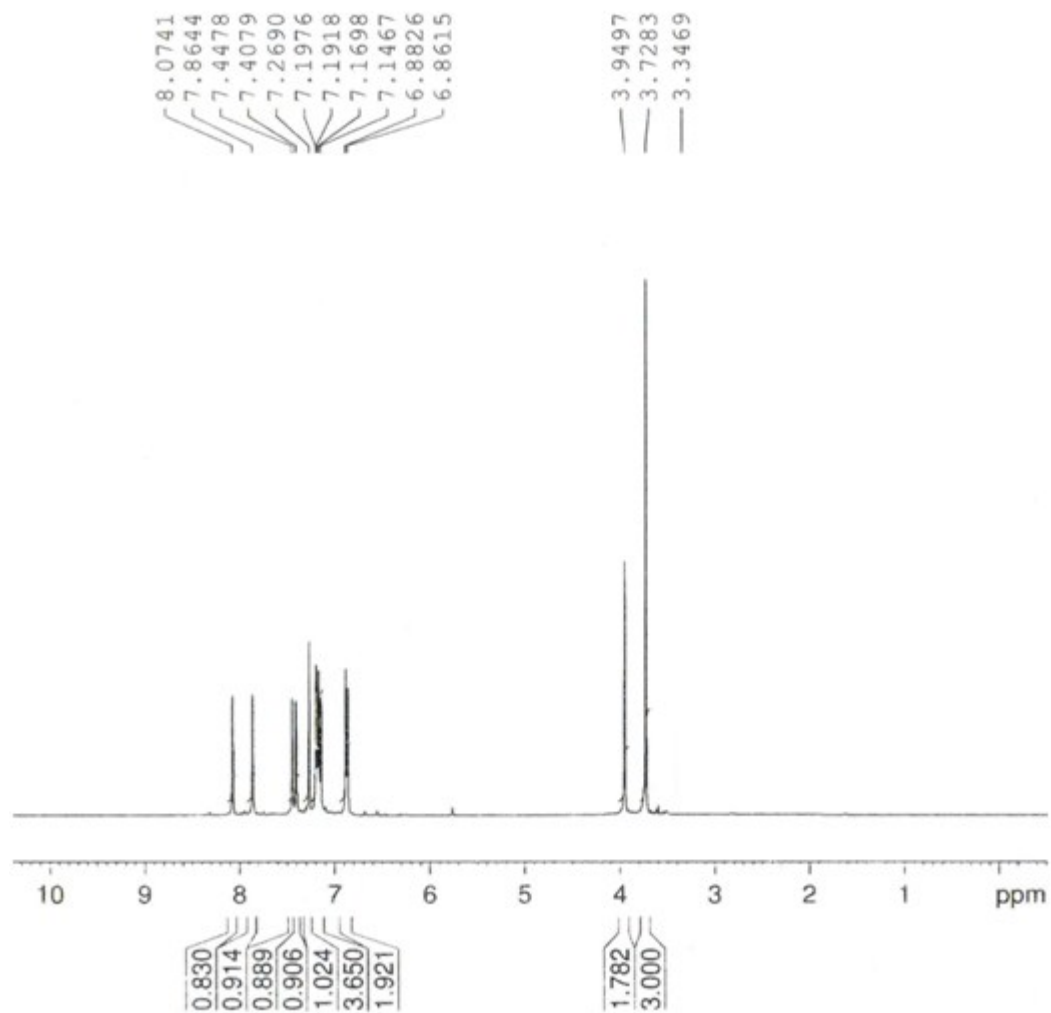
^1H NMR of 3a



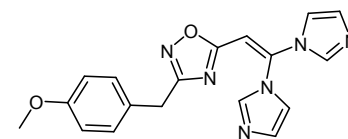
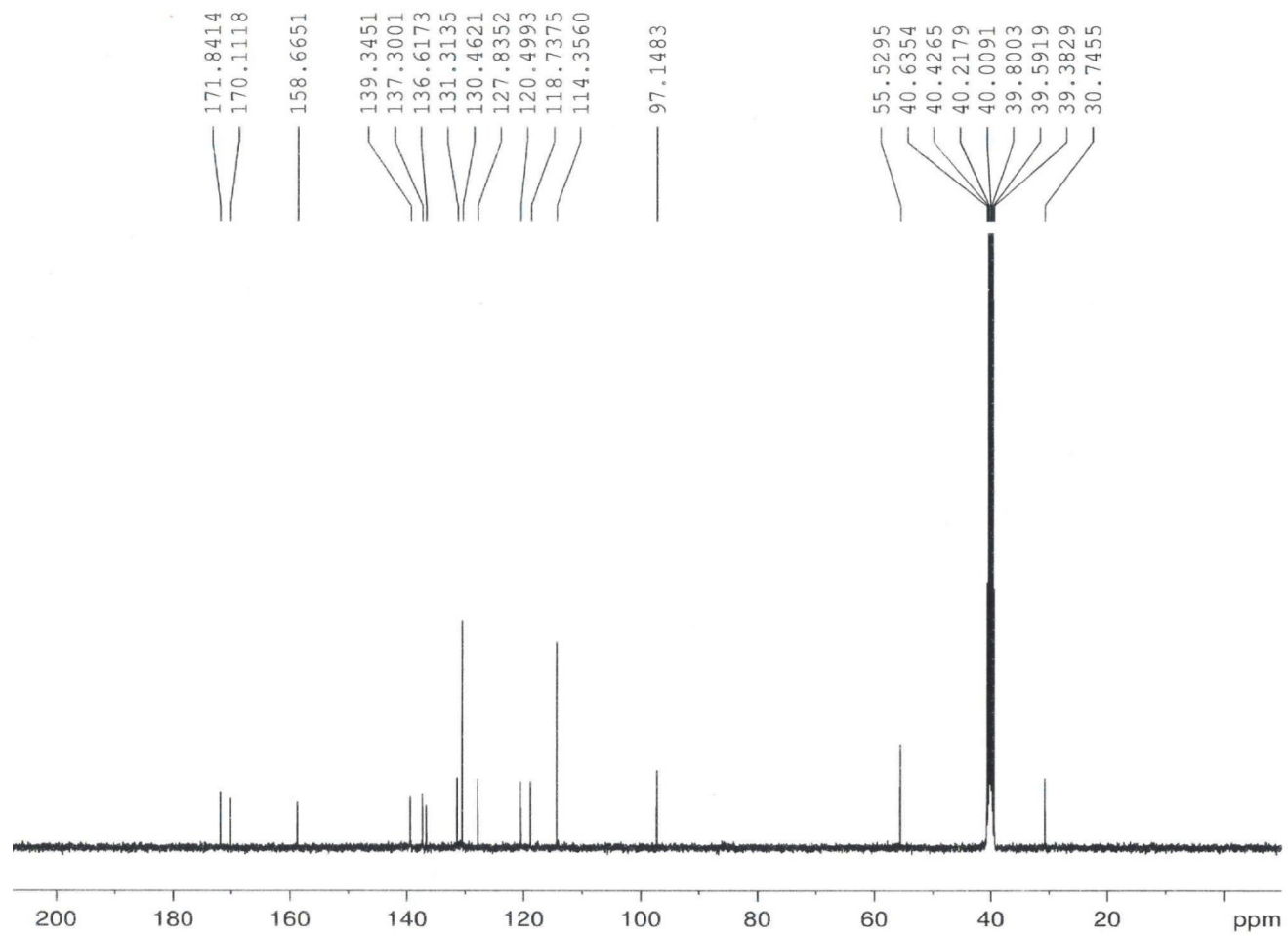
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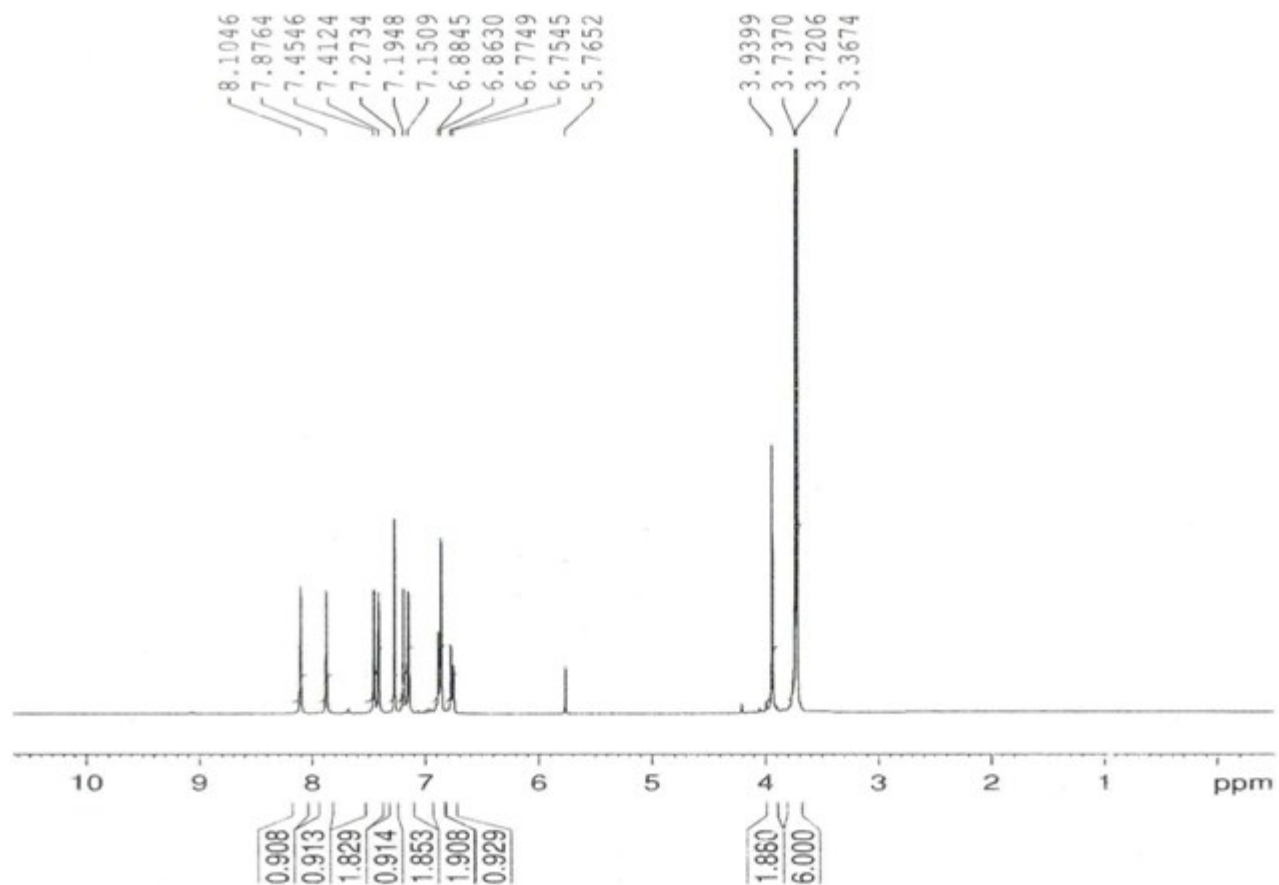
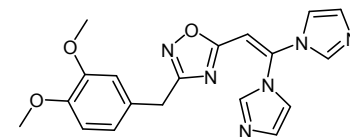
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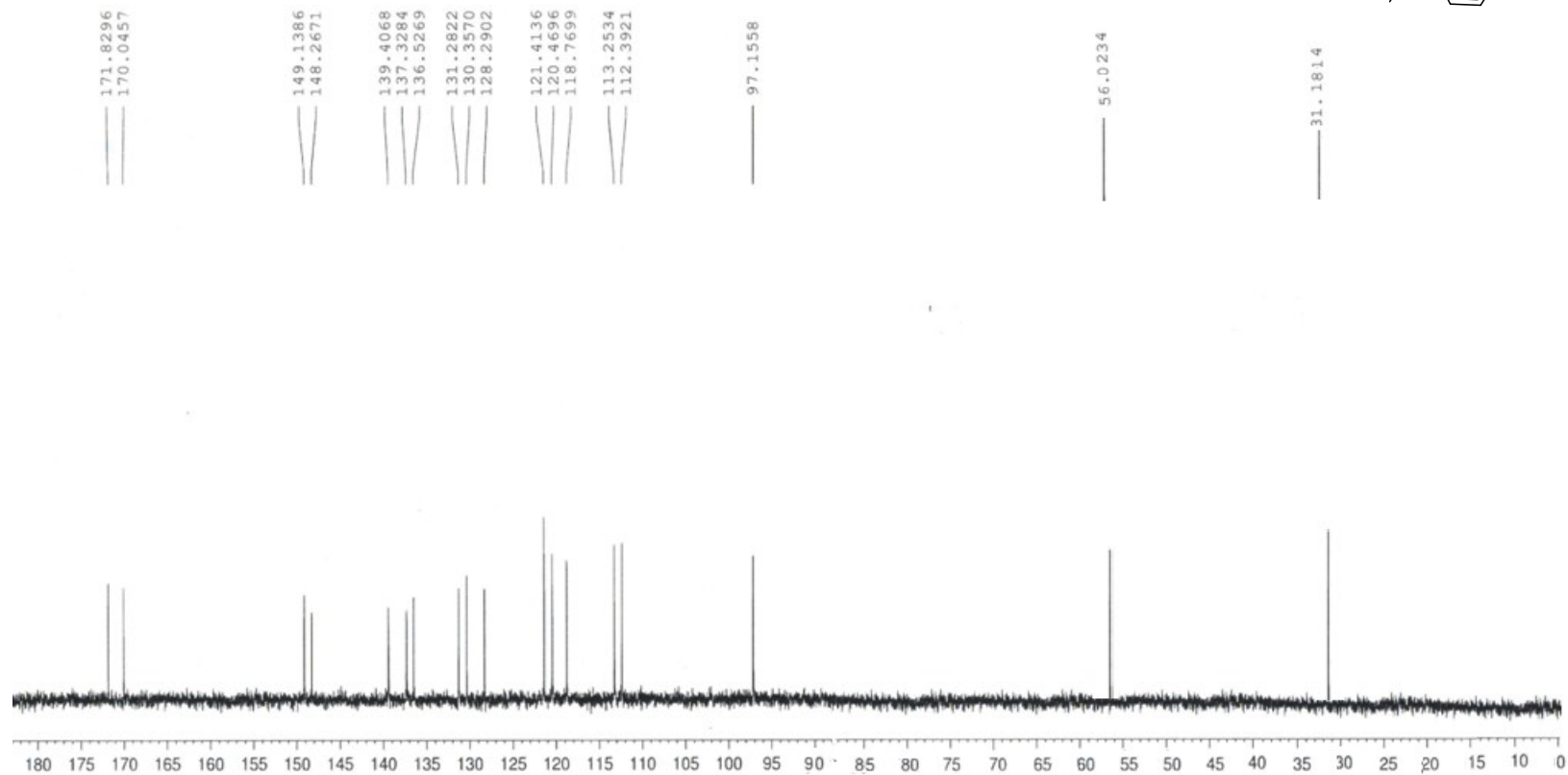
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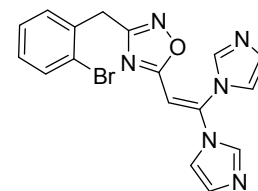


¹H NMR of 3c

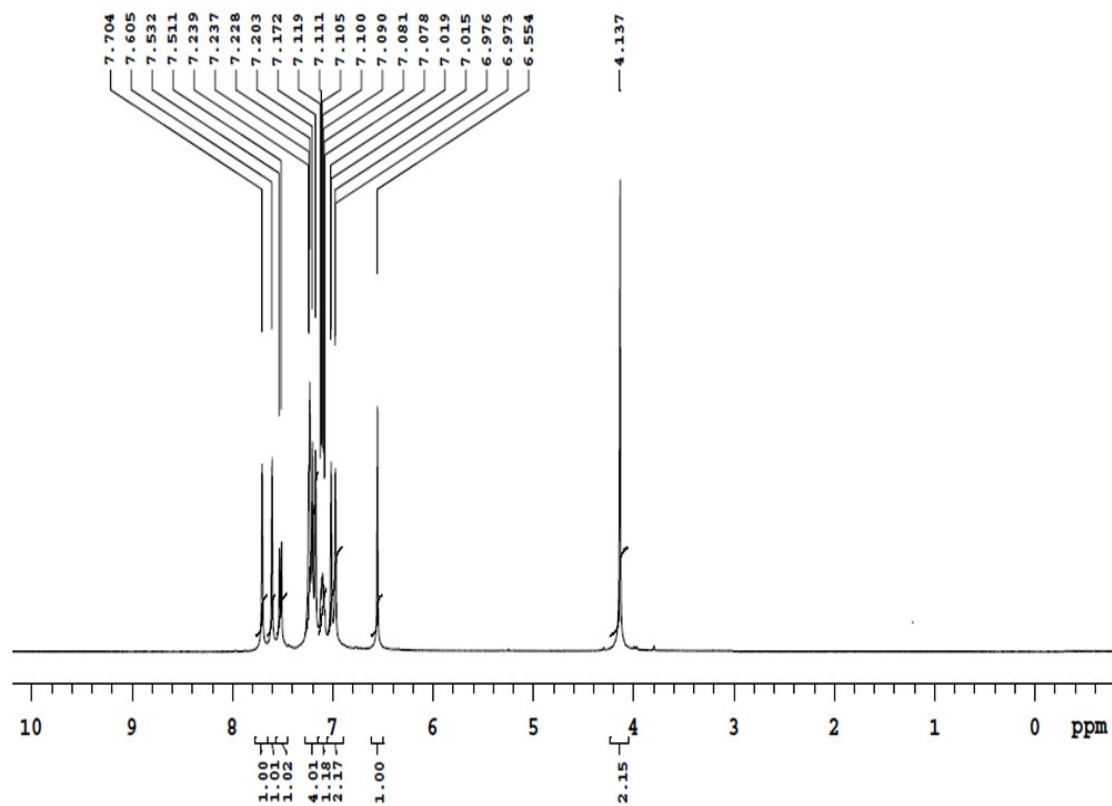


¹³C NMR of 3c

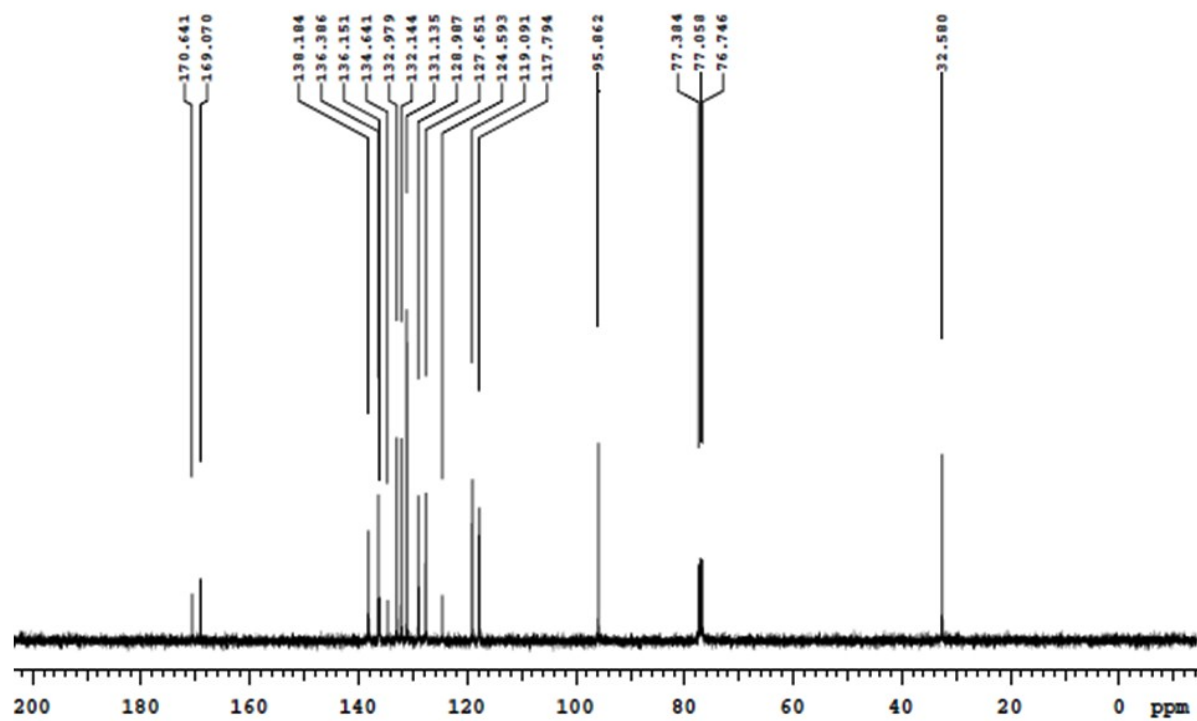
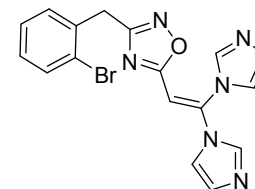




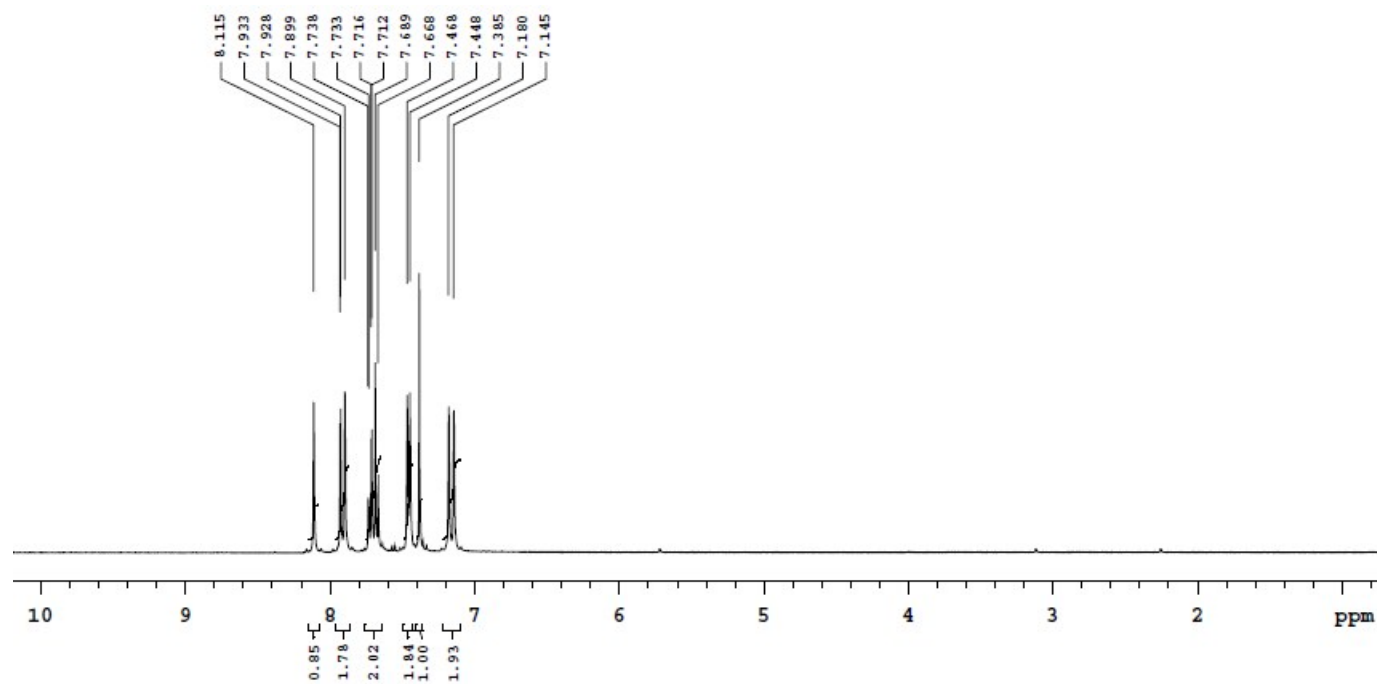
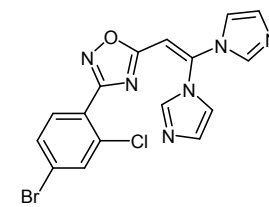
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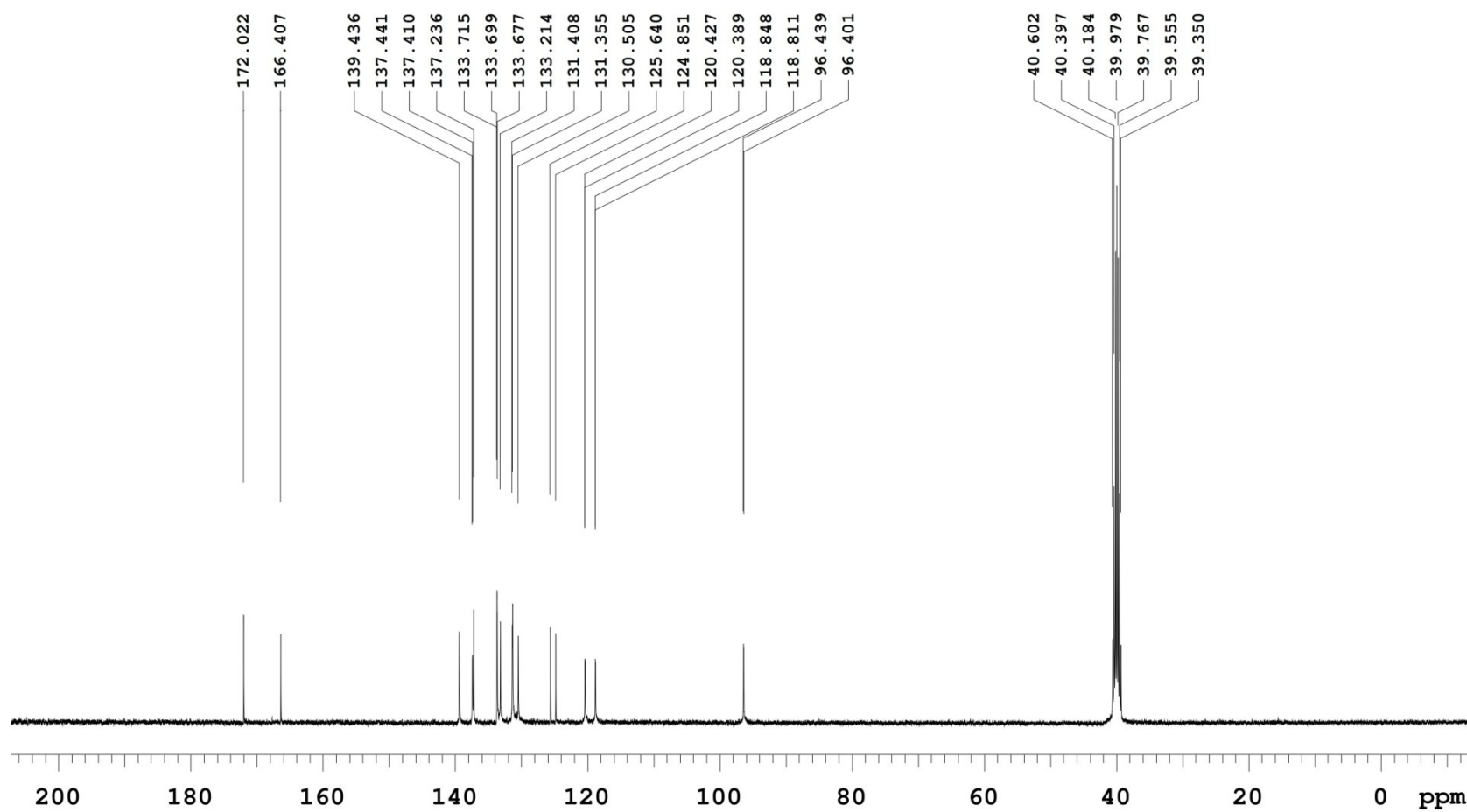
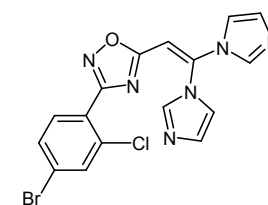
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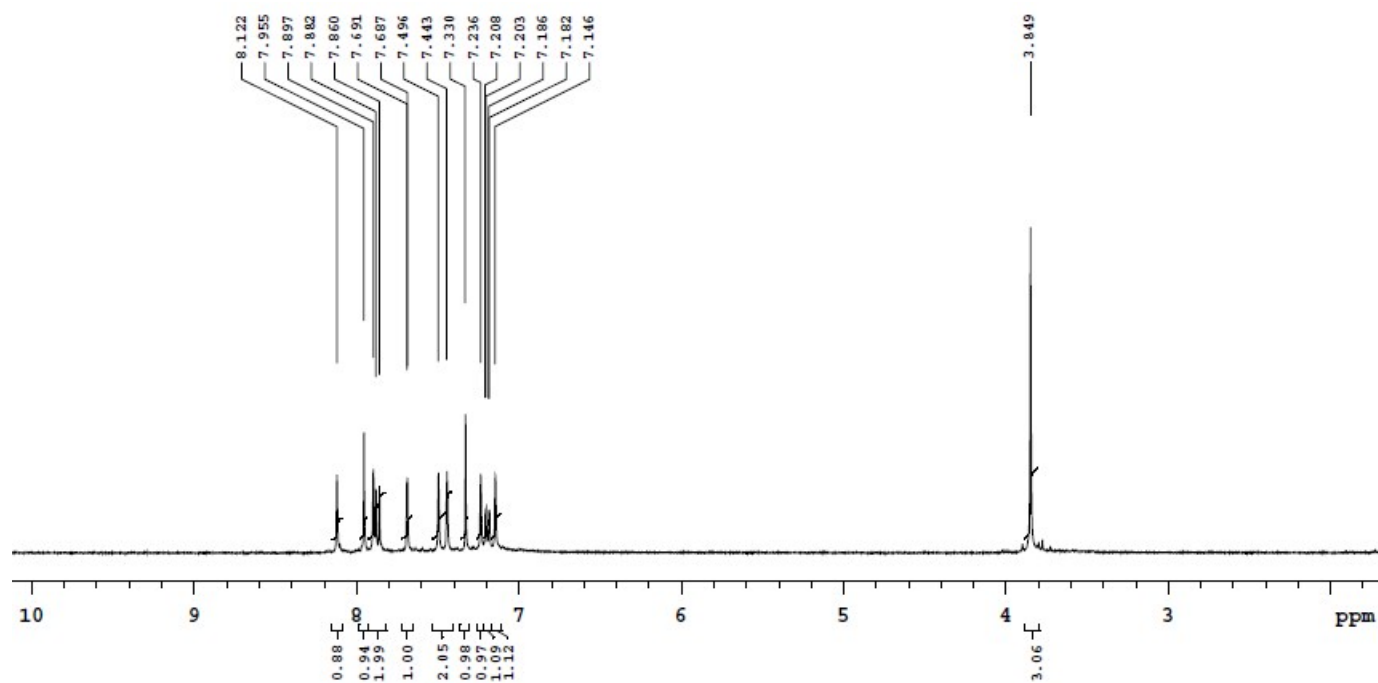
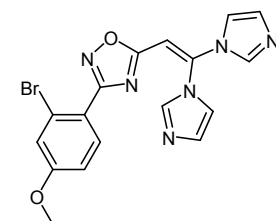
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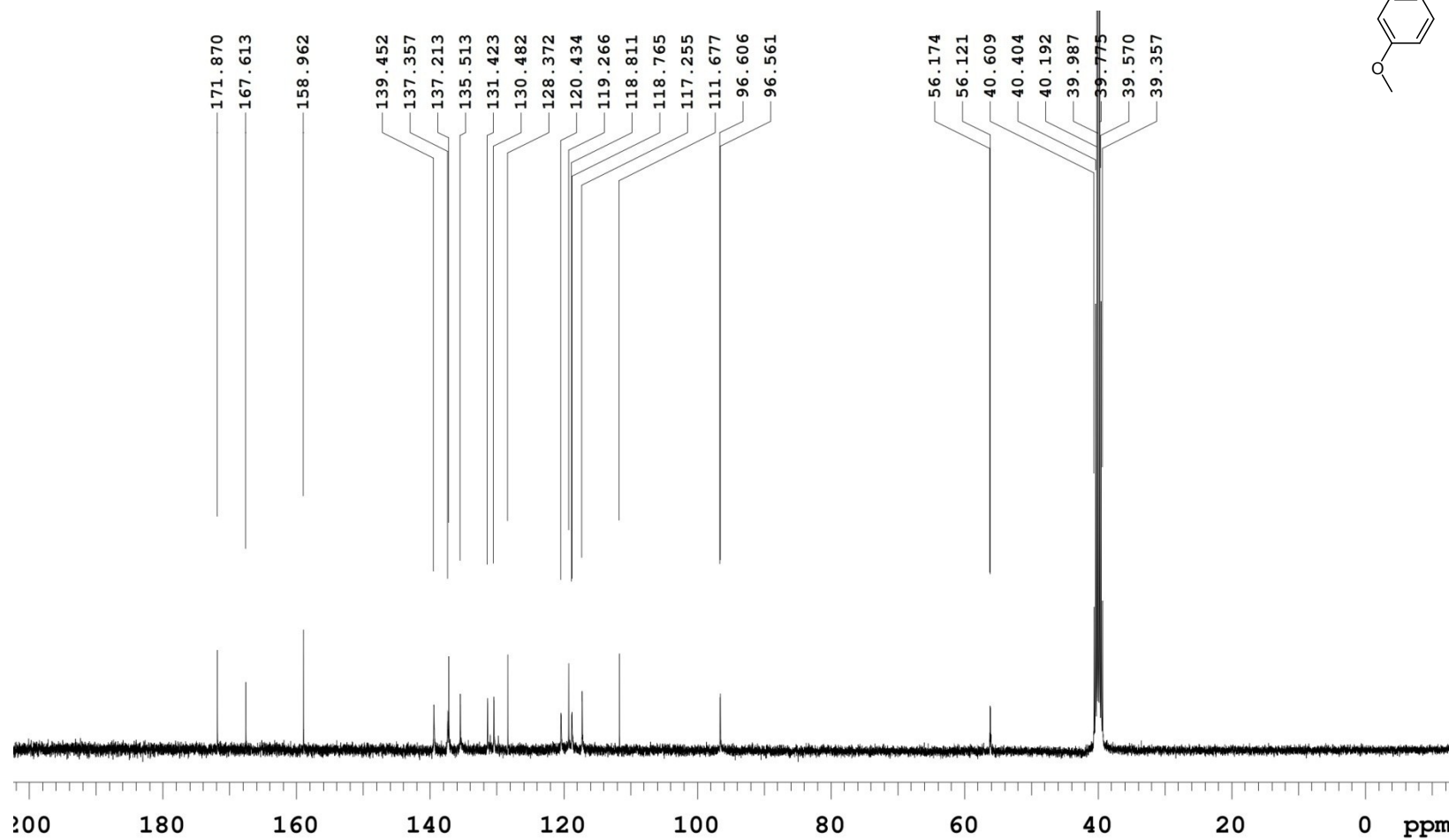
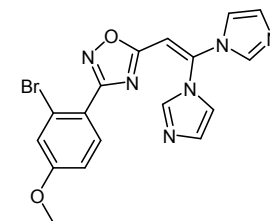
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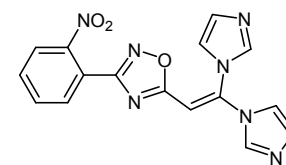


¹³C NMR of 3f

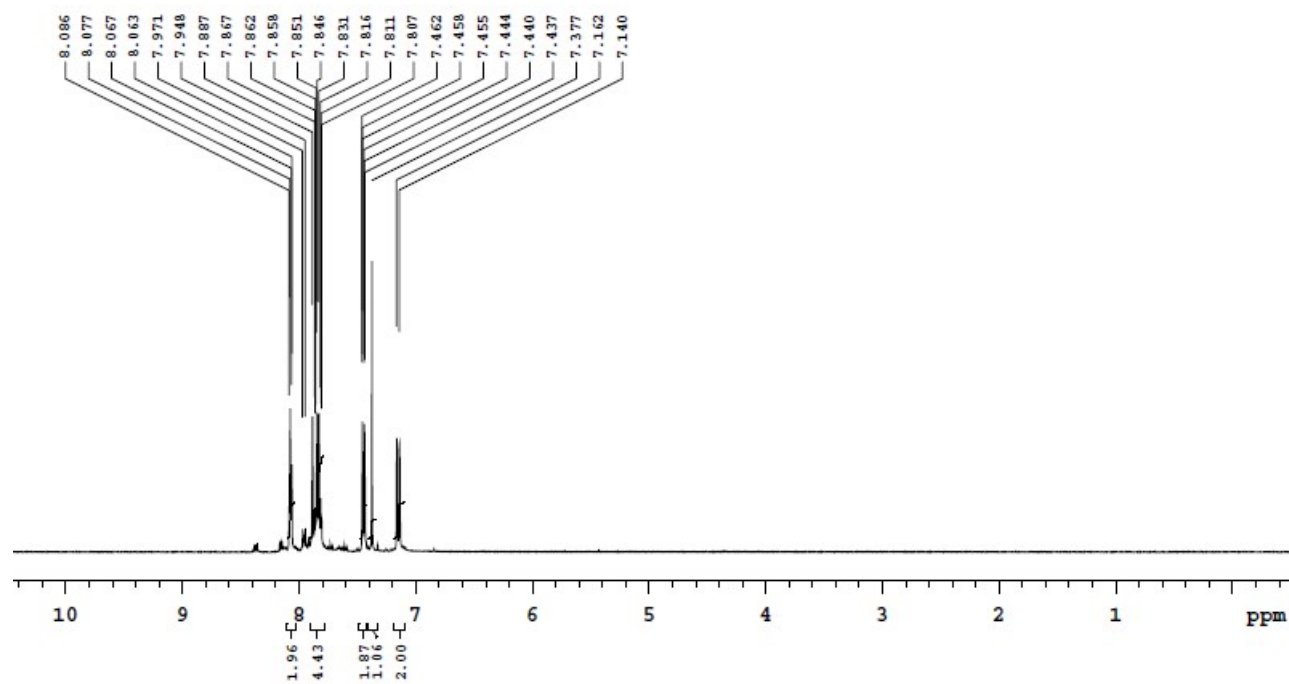


¹³C NMR of 3f

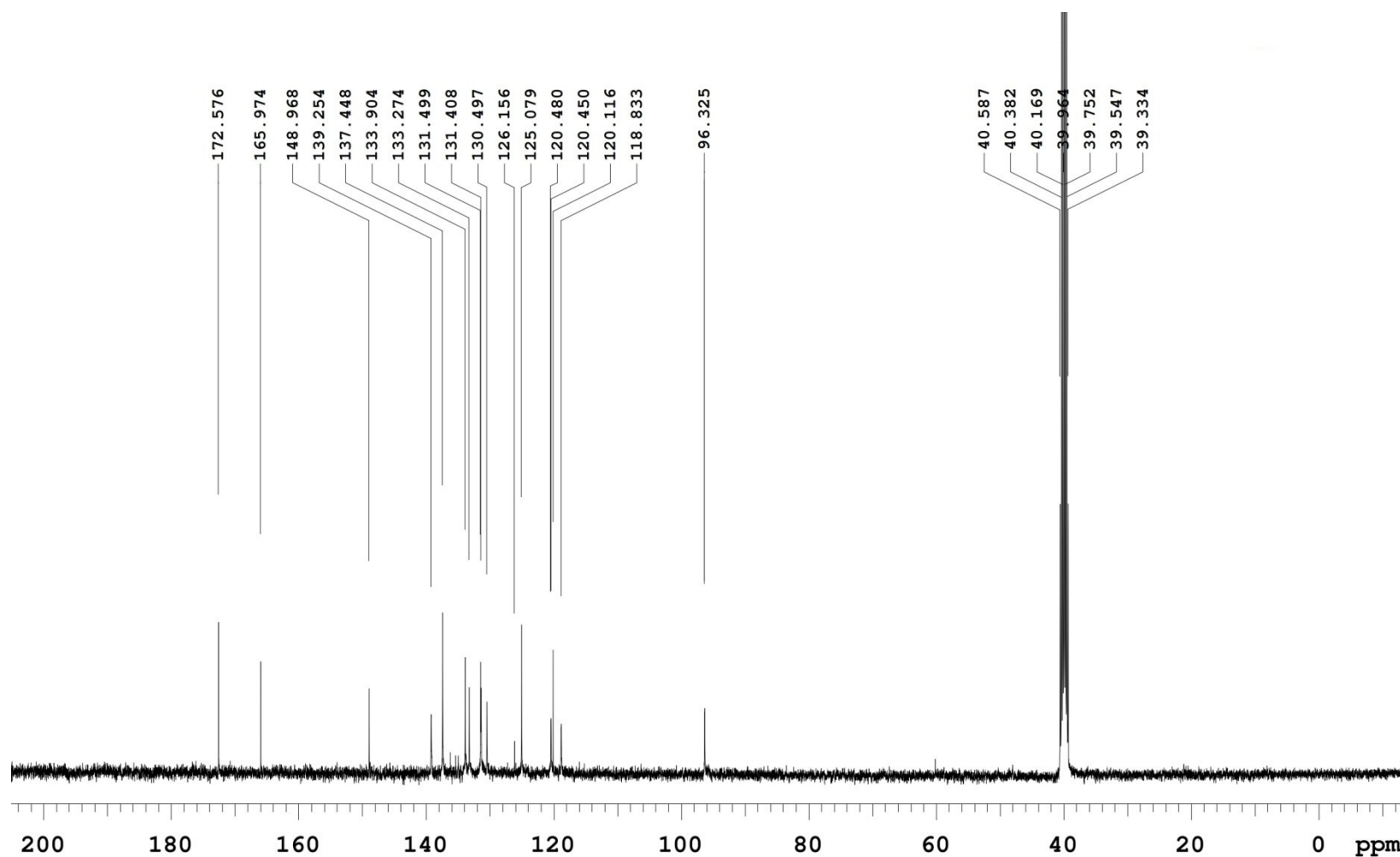
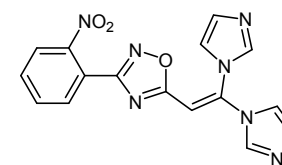




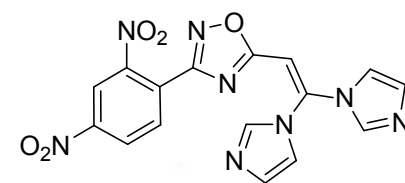
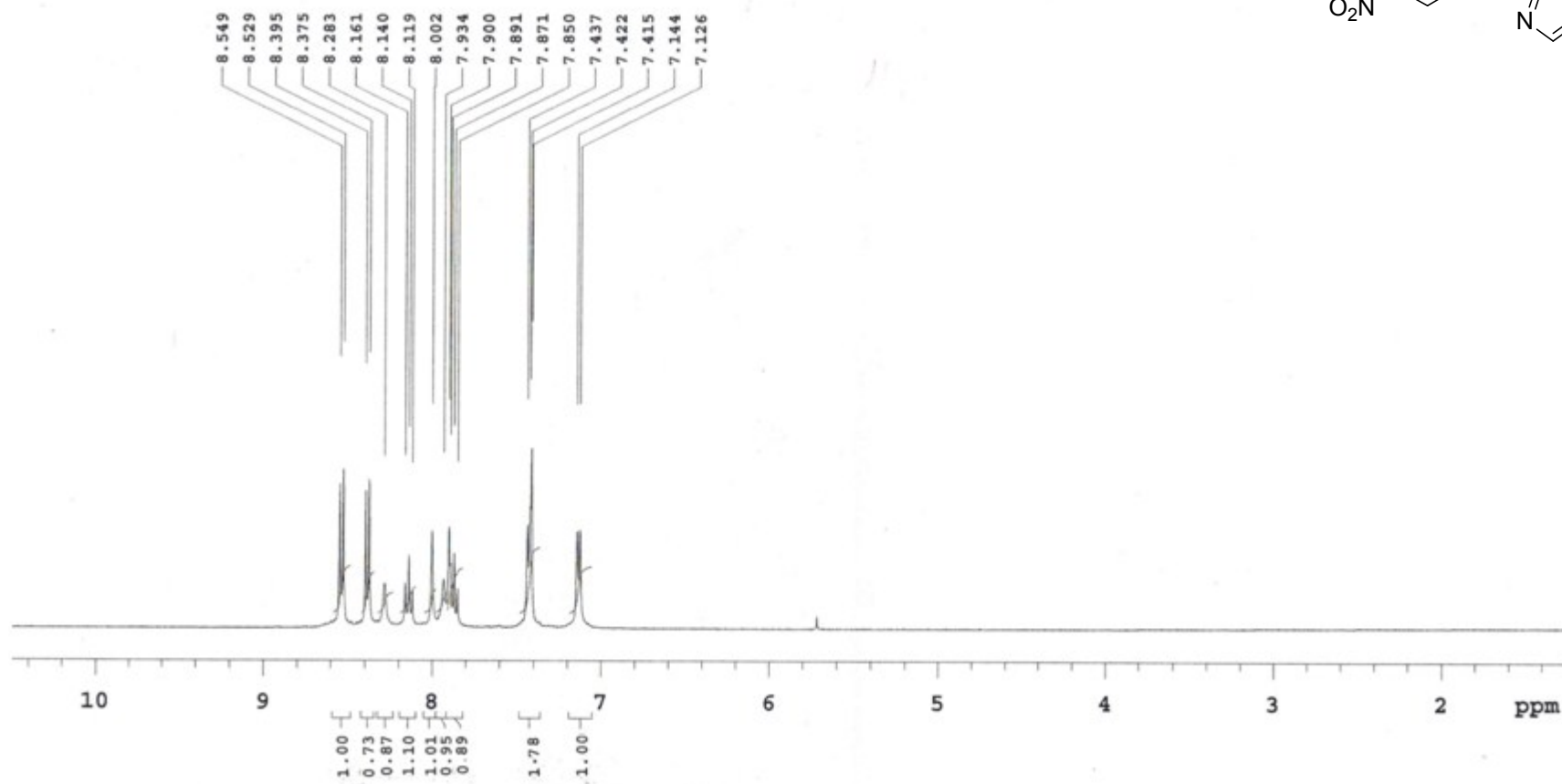
^1H NMR of 3g



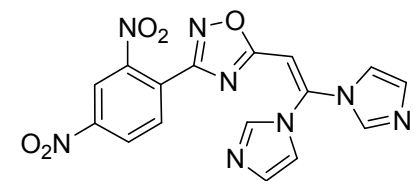
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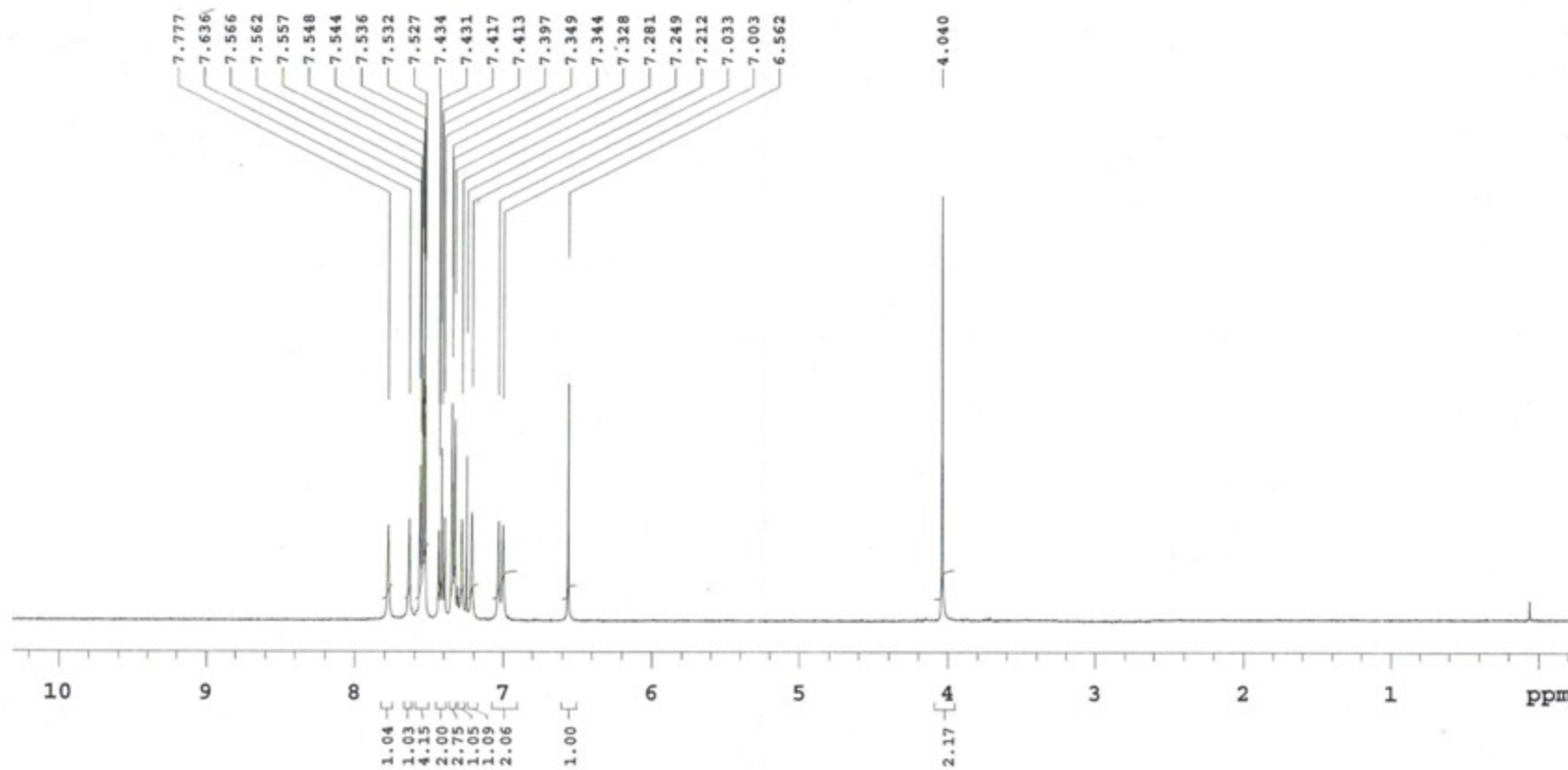
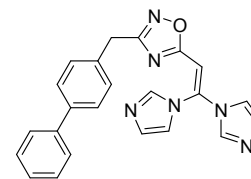
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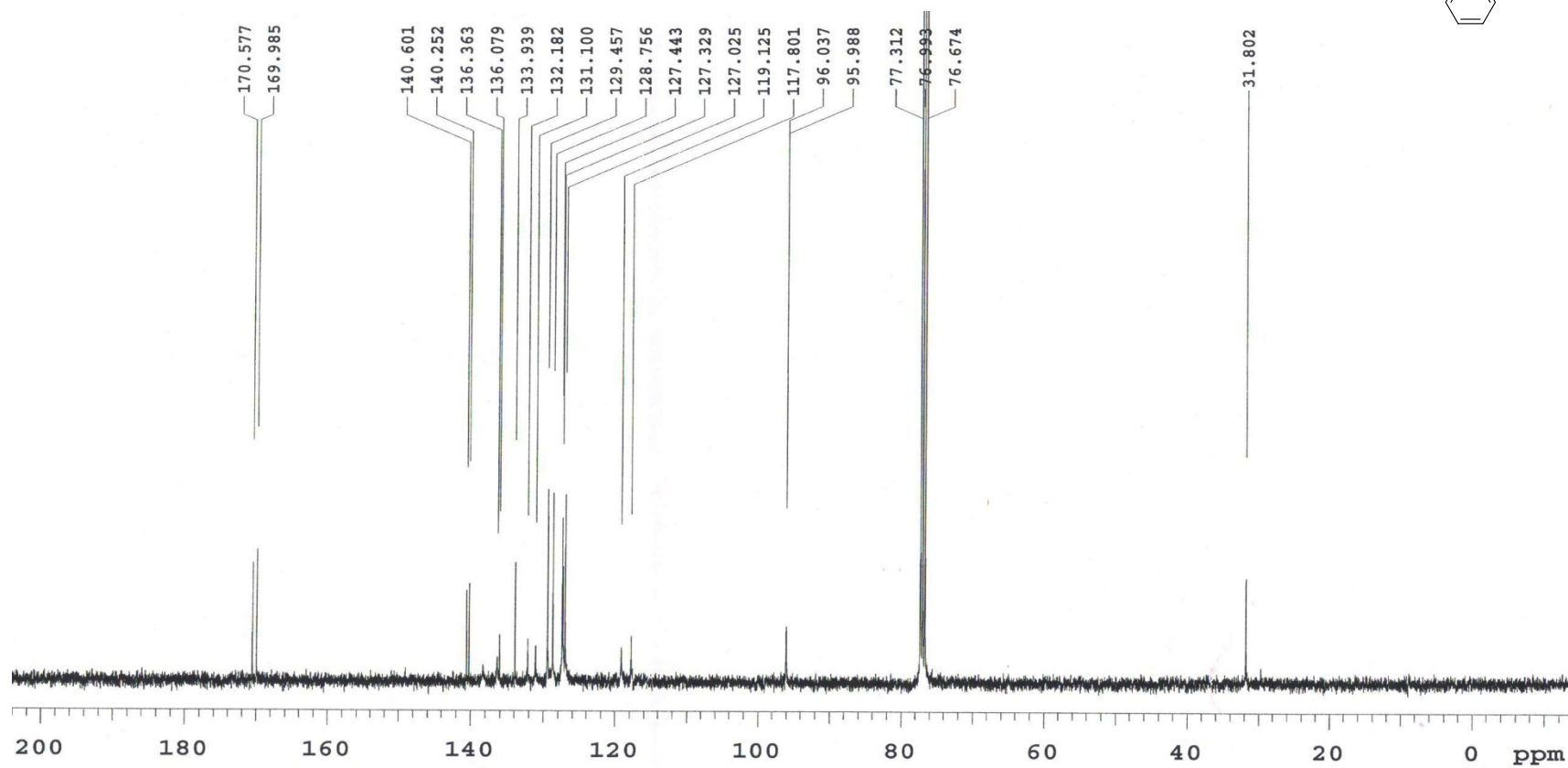
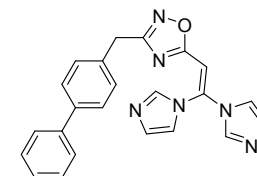
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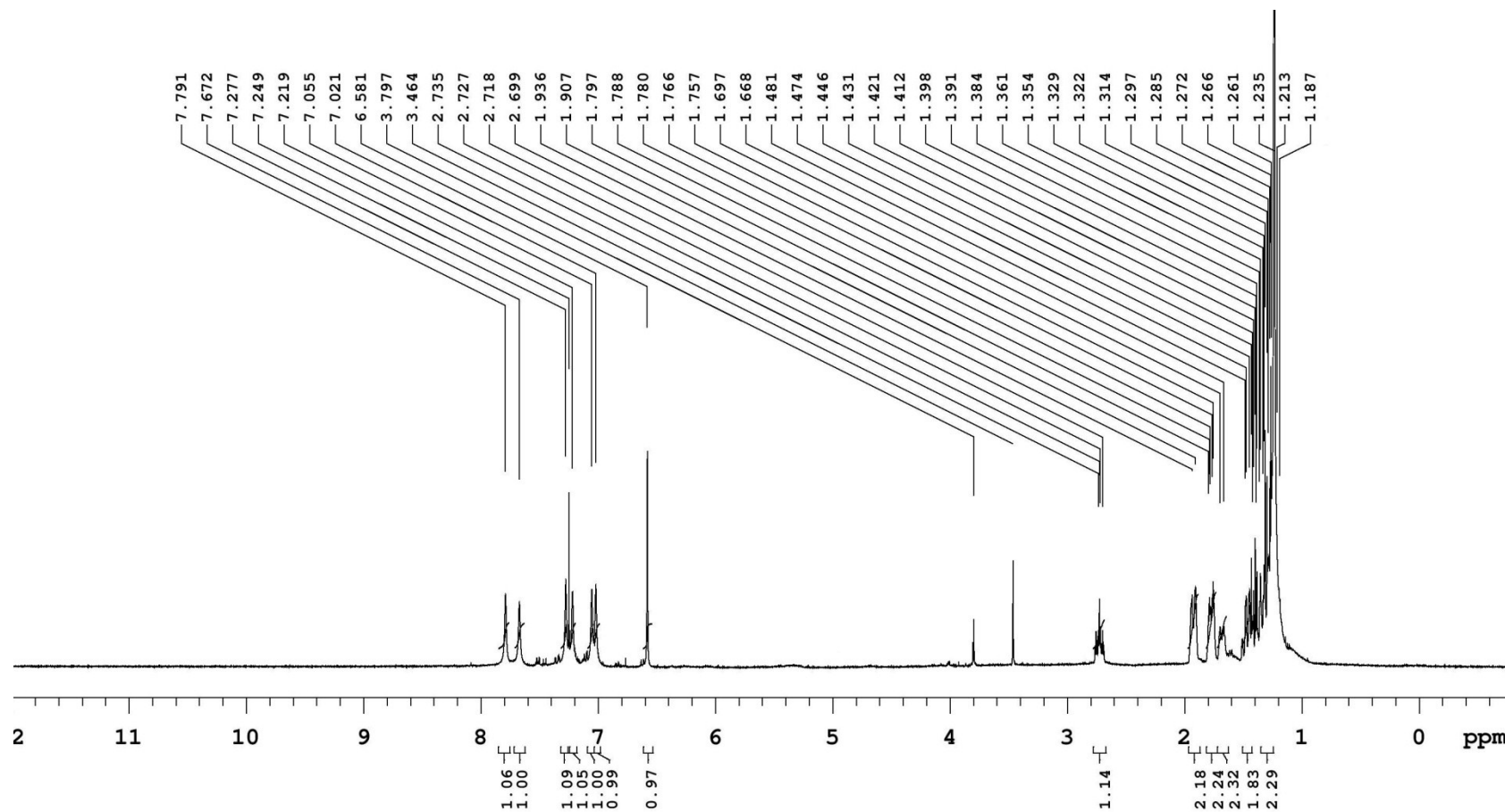
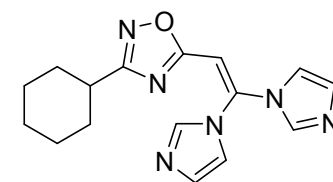
¹H NMR of 3i



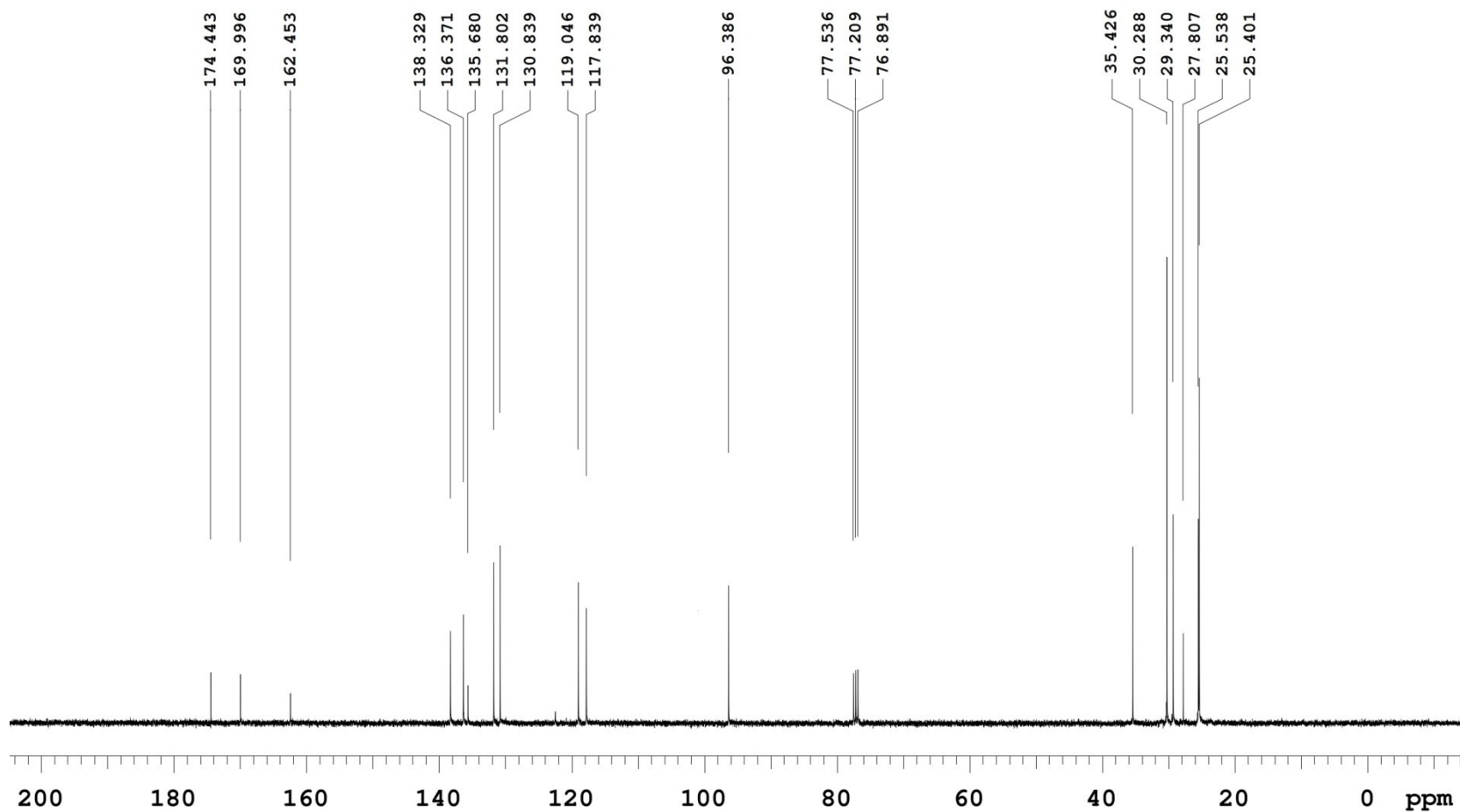
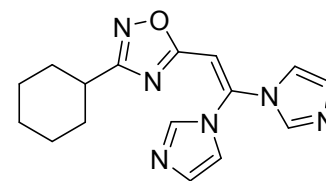
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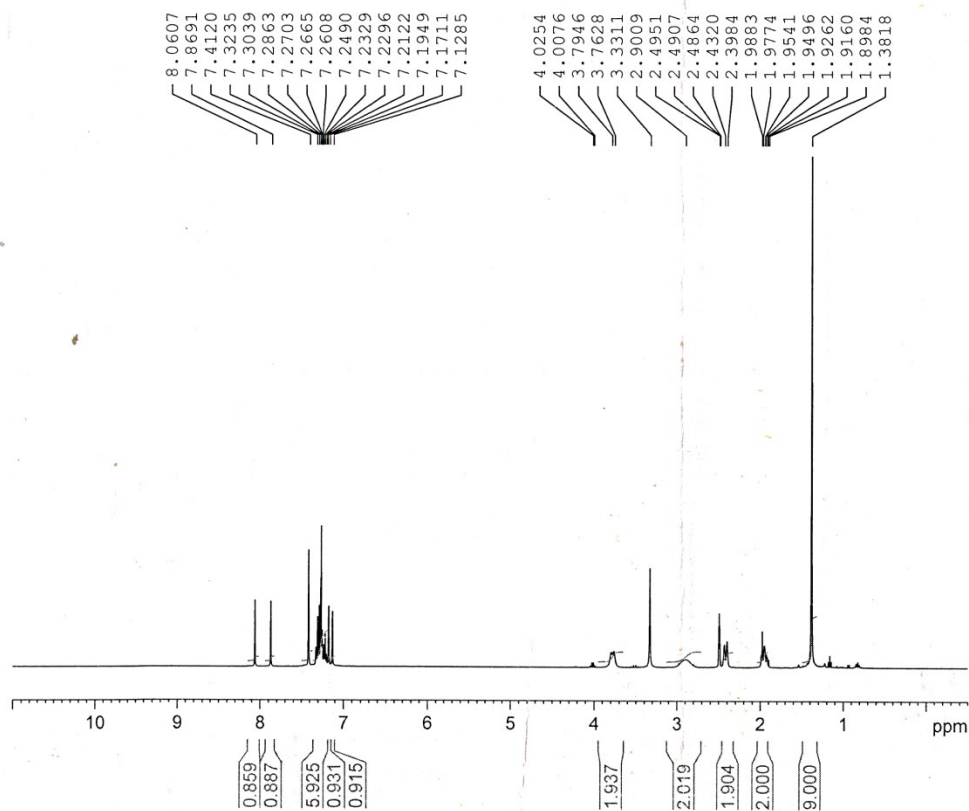
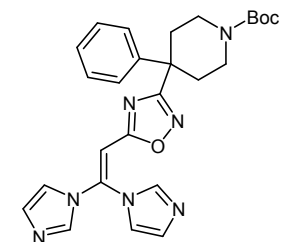
¹H NMR of 3j



¹³C NMR of 3j



¹H NMR of 3k



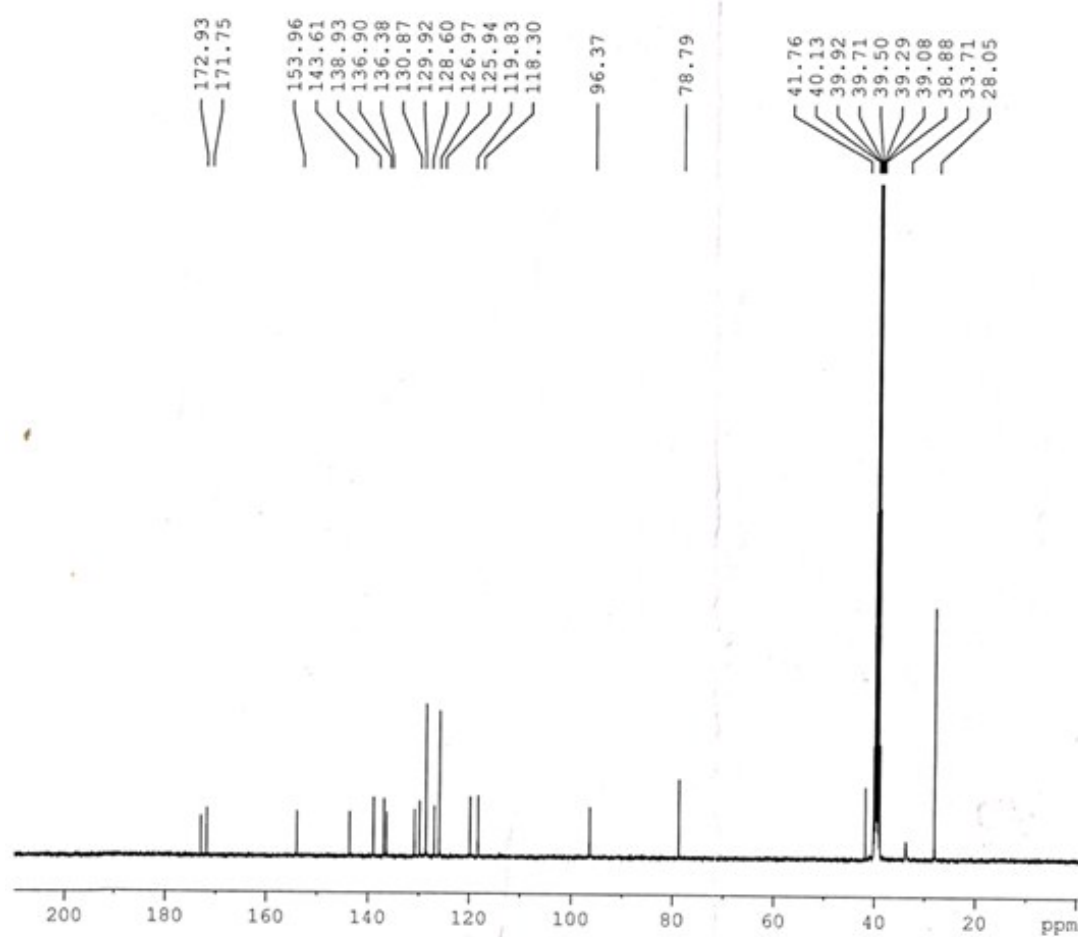
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¹³C NMR of 3k



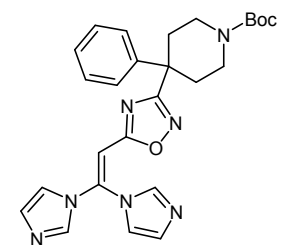
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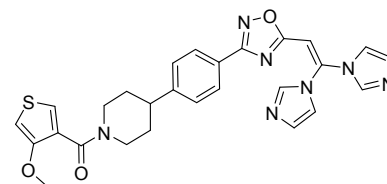
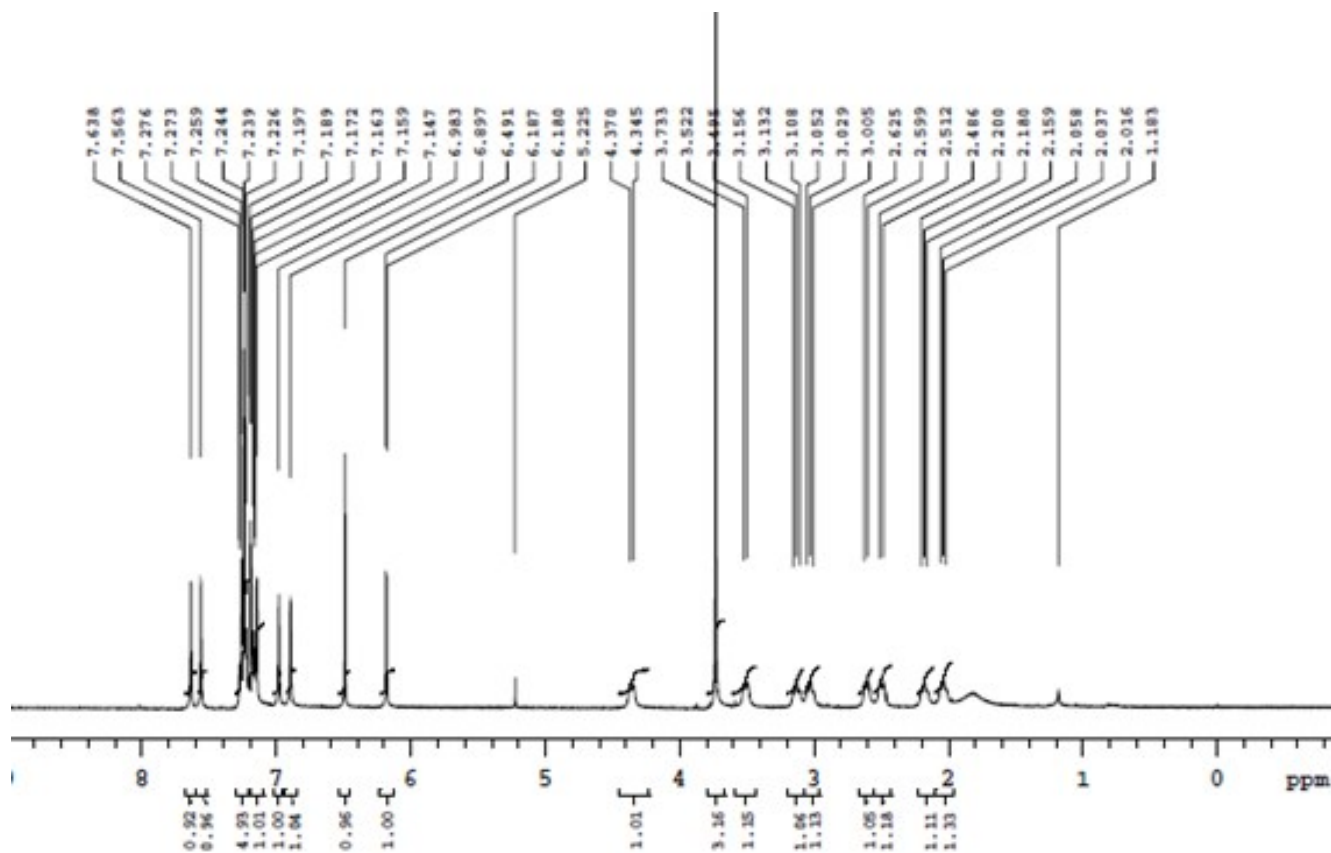
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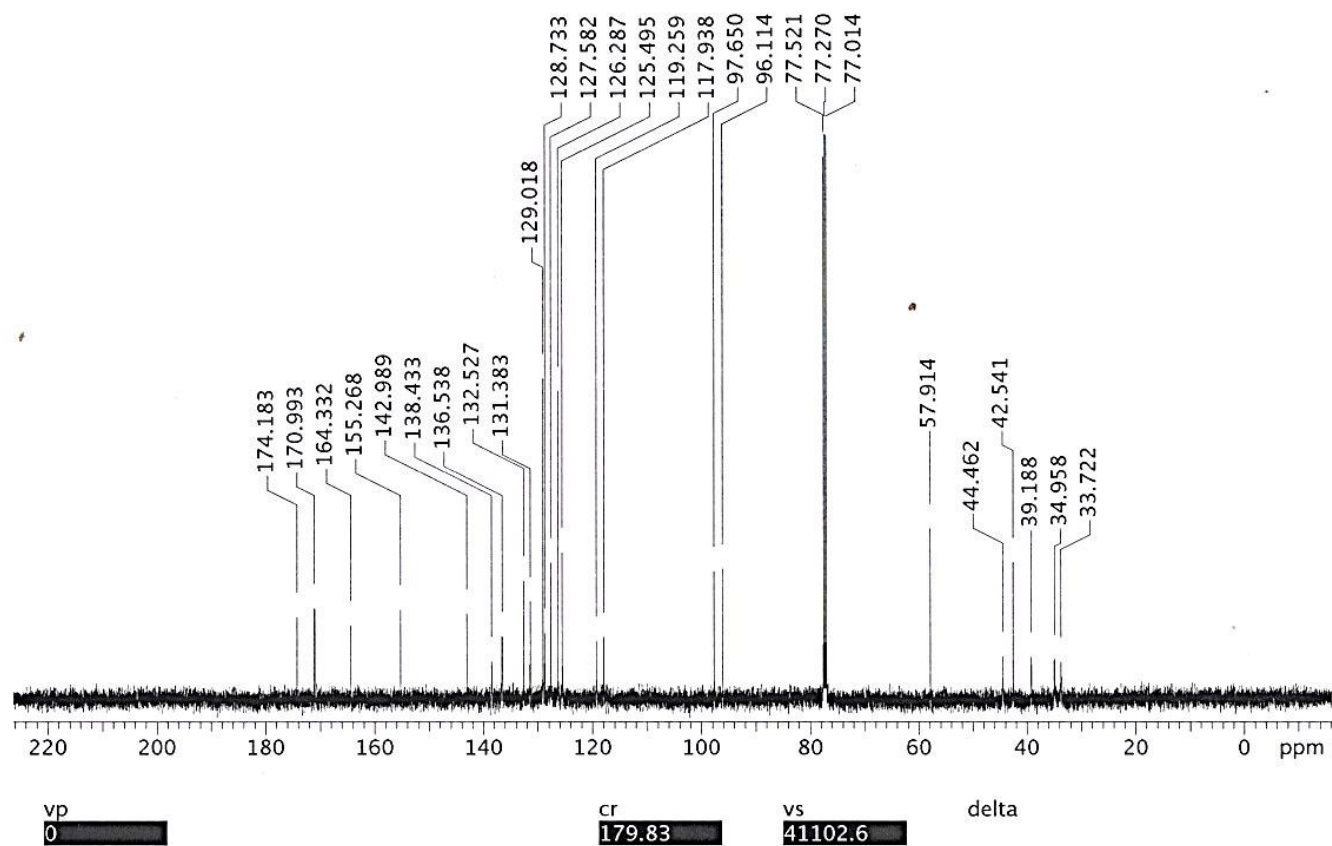
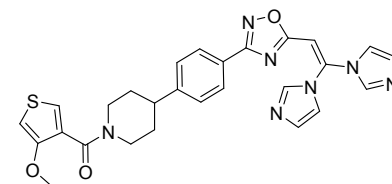
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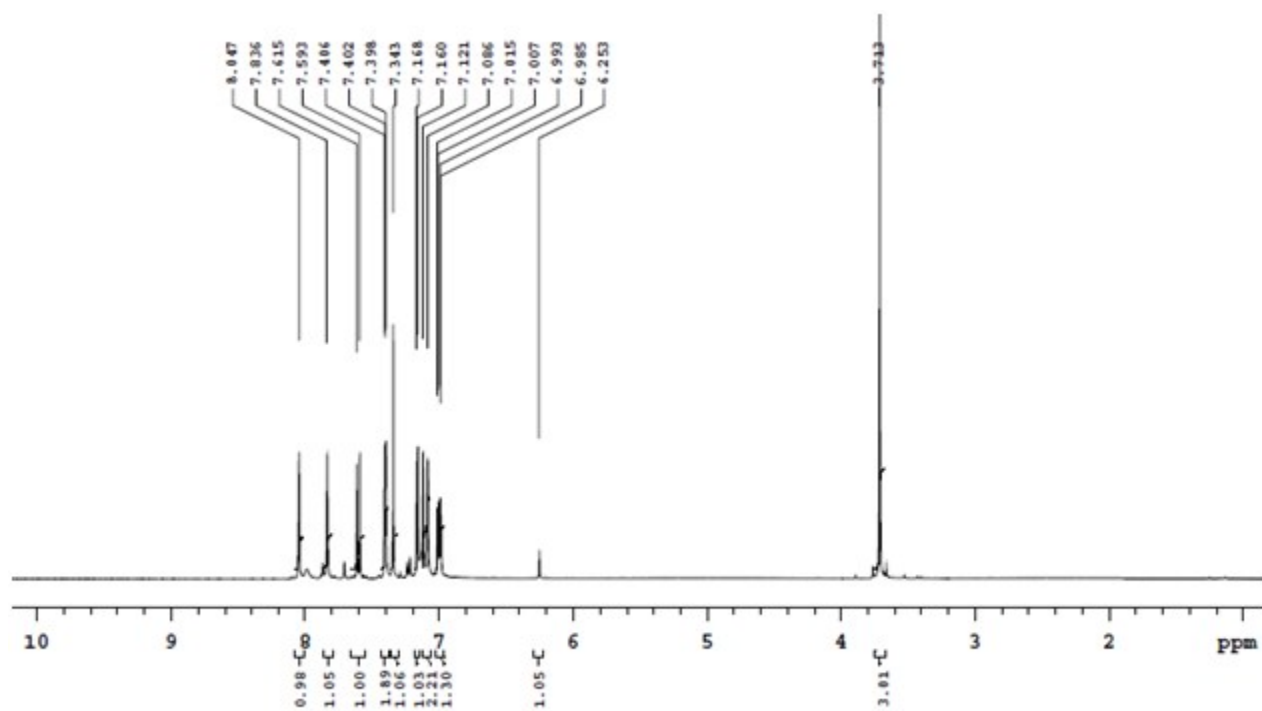
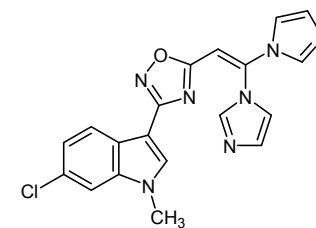
¹H NMR of 3l

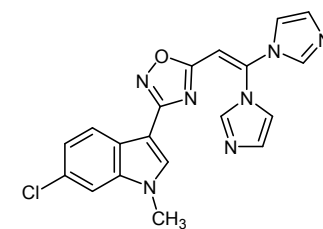


¹³C NMR of 3I

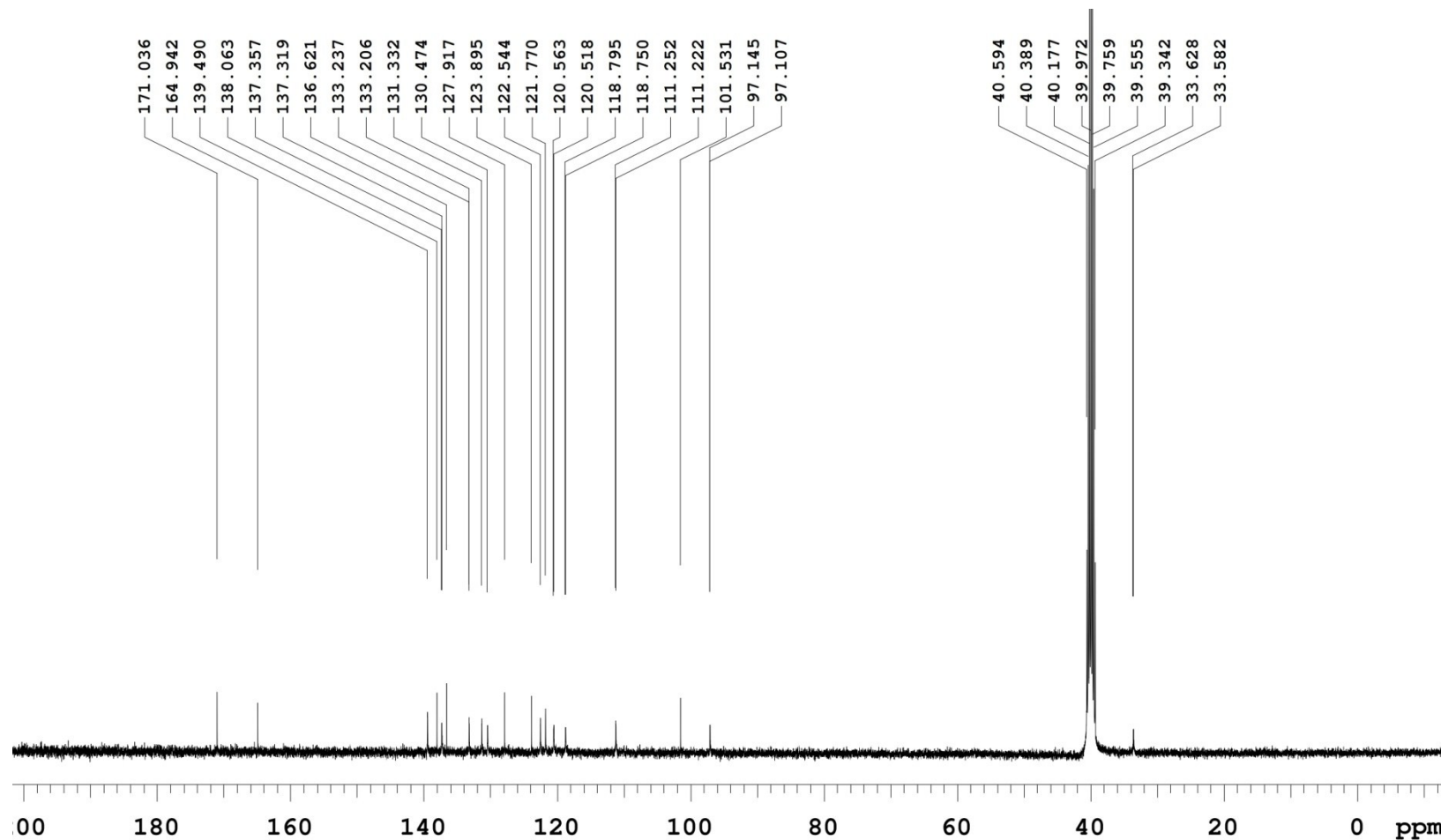


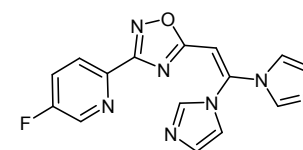
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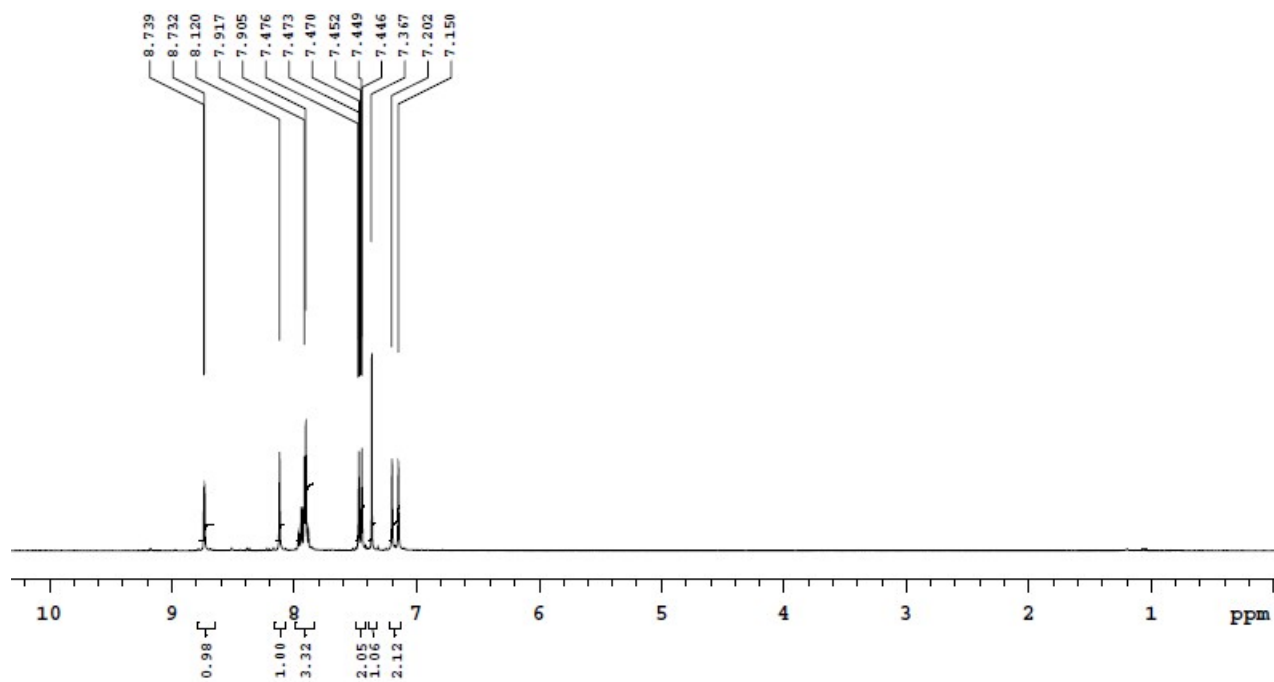


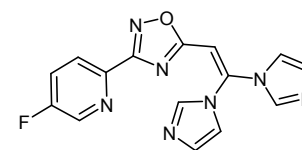
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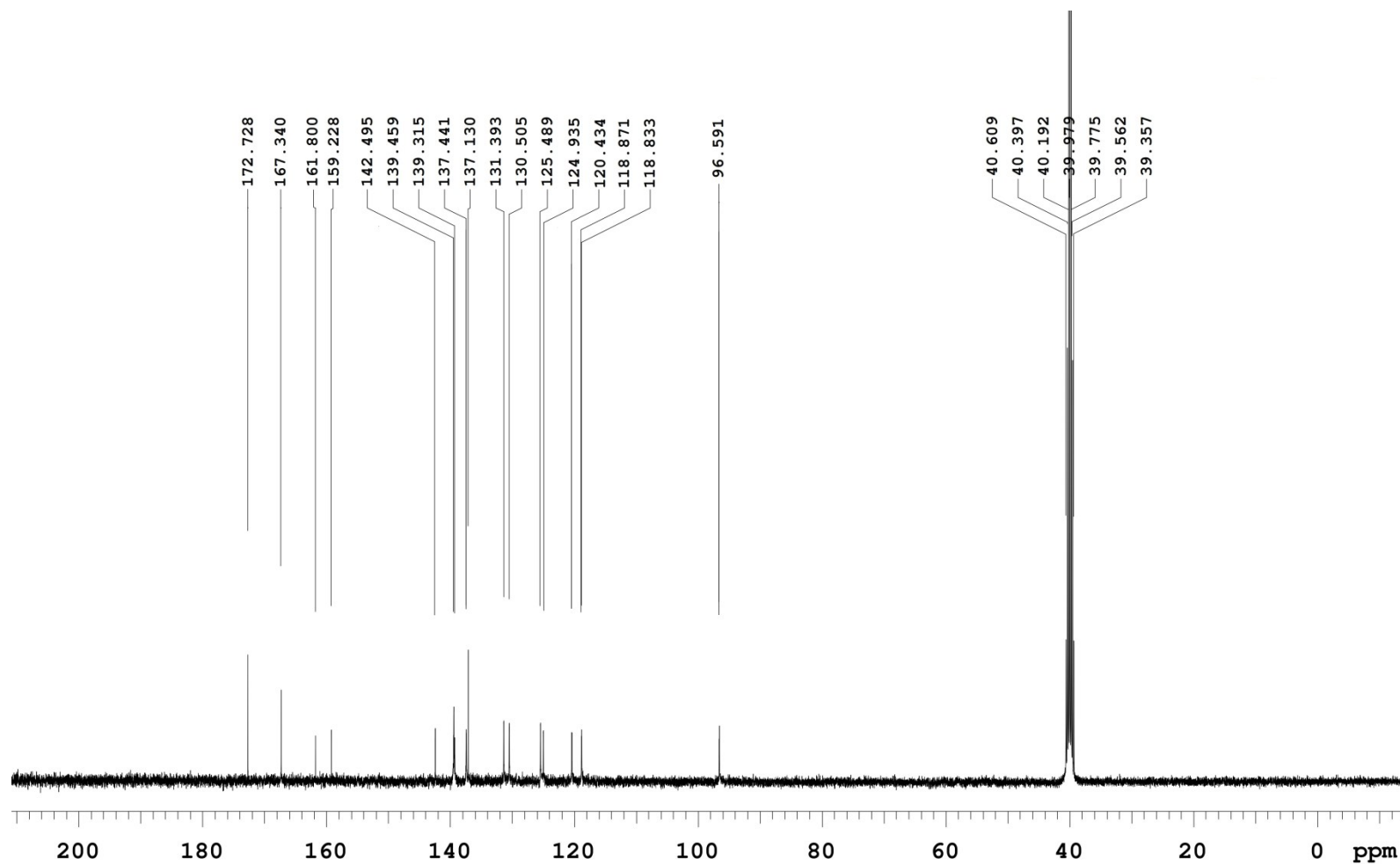


^1H NMR of 3n

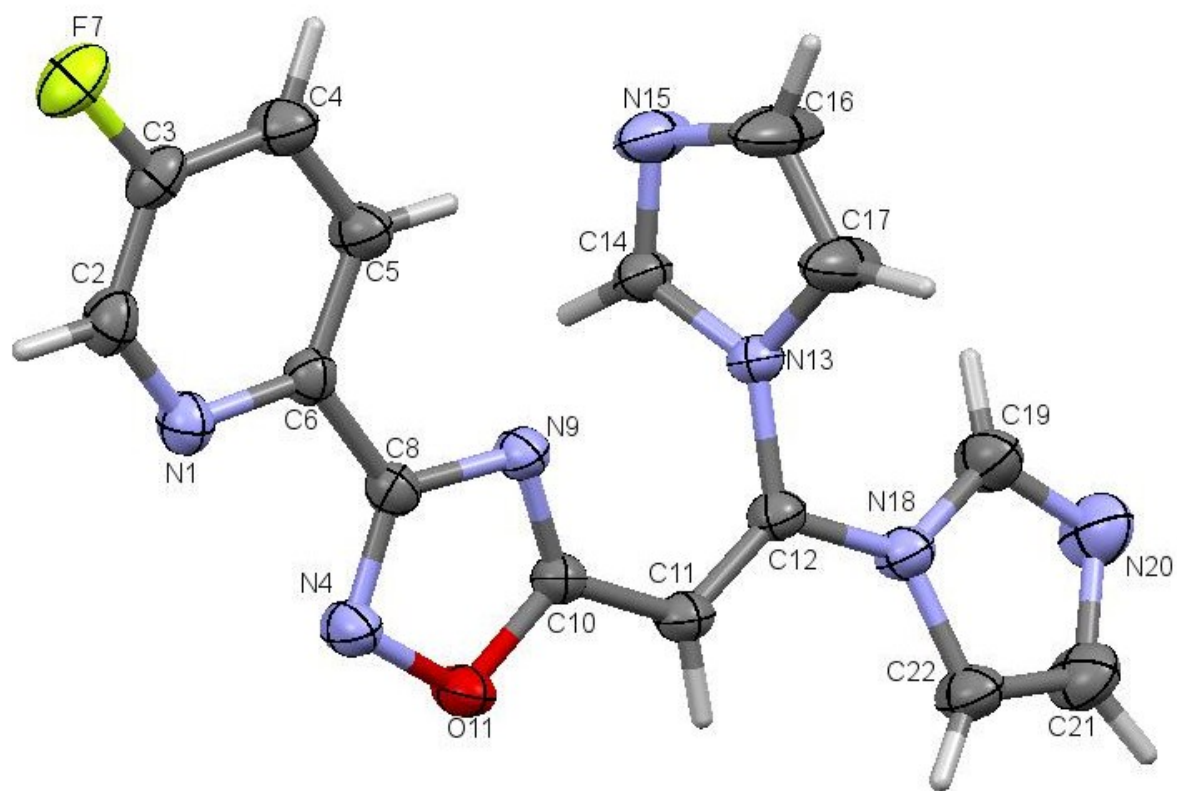




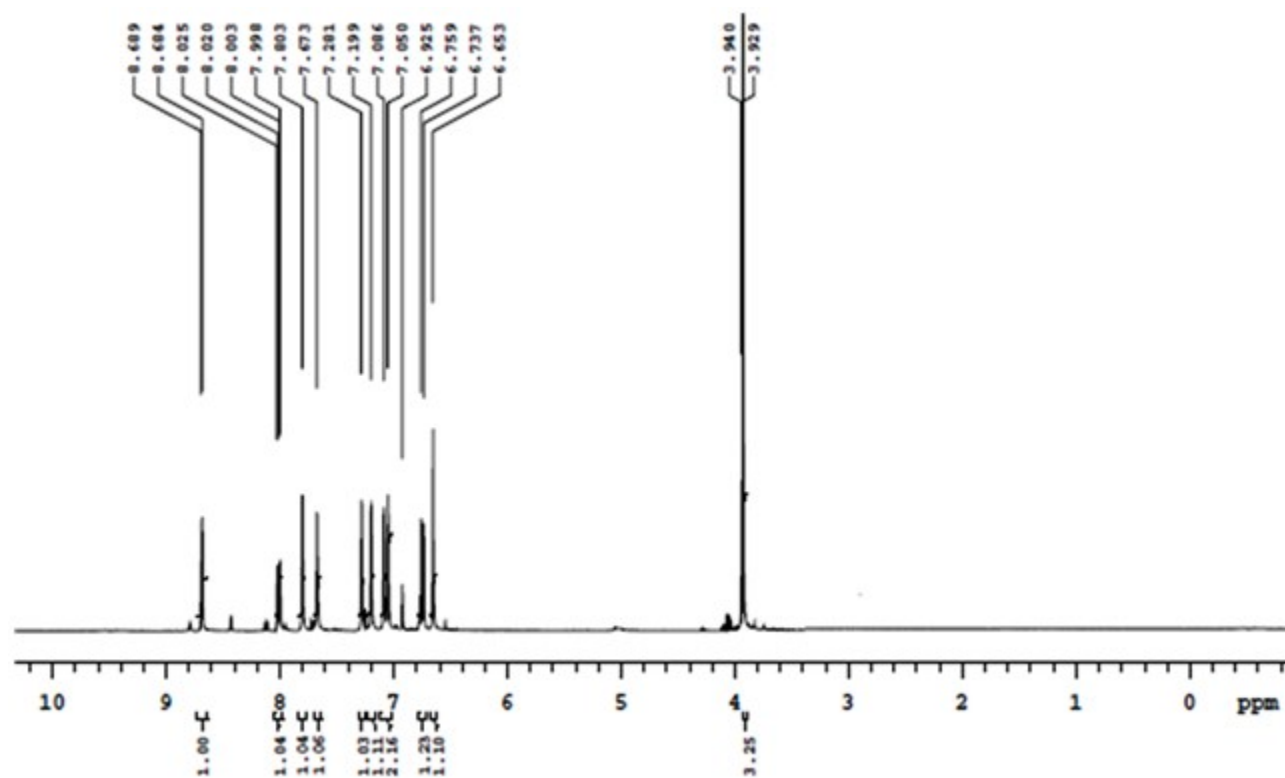
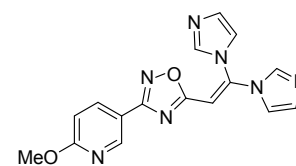
¹³C NMR of 3n

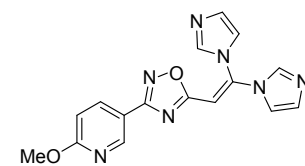


4. ORTEP of 3n



^1H NMR of 3o





^{13}C NMR of 3o

