SUPPORTING INFORMATION

In vitro Antimycobacterial Activity and Physicochemical Characterization of Diaryl Ether Triclosan Analogues as Potential InhA Reductase Inhibitors

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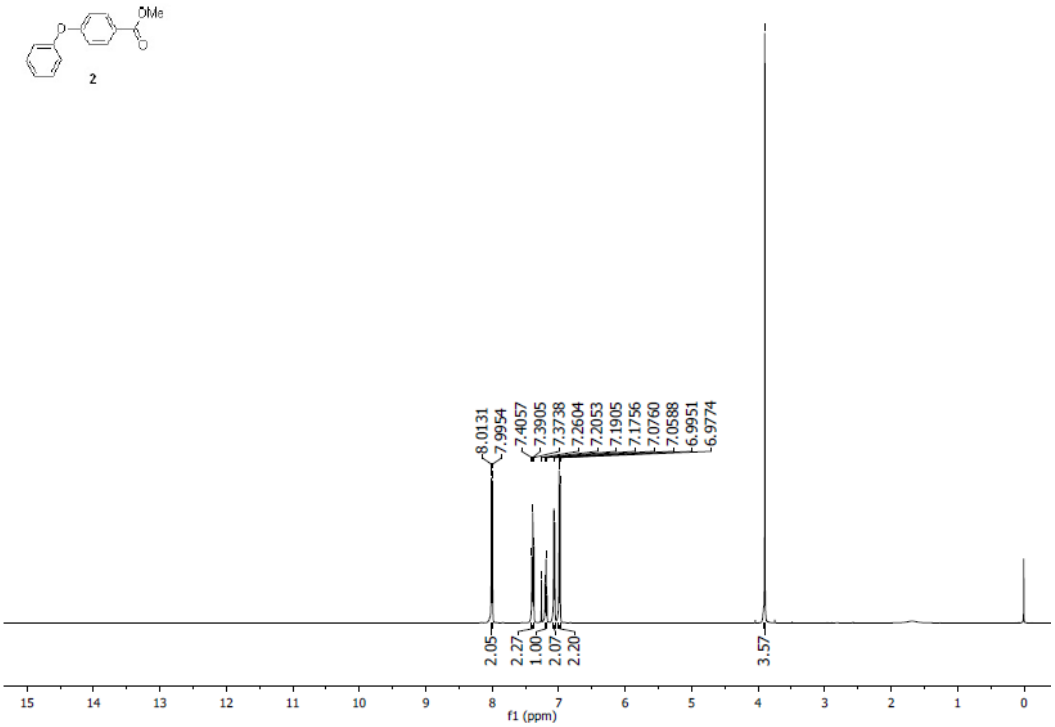
Docking methodology

Discovery Studio 2.5 software (Accelrys Inc., San Diego, CA, USA) was used for docking analysis. Fully automated docking tool using “Dock ligands (CDOCKER)” protocol running on Intel (R) core (TM) i32370 CPU @ 2.4 GHz 2.4 GHz, RAM Memory 2 GB under the Windows 7.0 system. The crystal structure of InhA reductase enzyme (PDB code: 3FNH) was downloaded from protein data bank [32-34]. The docked compounds were built using Chem. 3D ultra 12.0 software [Chemical Structure Drawing Standard; Cambridge Soft corporation, USA (2010)], and copied to Discovery Studio 2.5 software. Automatic protein preparation module was used applying CHARMm force field. The binding site sphere has been defined automatically by the software. Herein, the prepared receptor is given as input for “input receptor molecule” parameter in the CDOCKER protocol parameter explorer. Force fields are applied on compounds Triclosan**, 3**, **8b** and **8g** to get the minimum lowest energy structure. The obtained poses those have displayed the best ligand–InhA reductase enzyme interactions were selected and used for CDOCKER energy (protein-ligand interaction energies) calculations. Receptor–ligand interactions of the complexes were examined in 2D and 3D styles.

^{1}H NMR for compound 2



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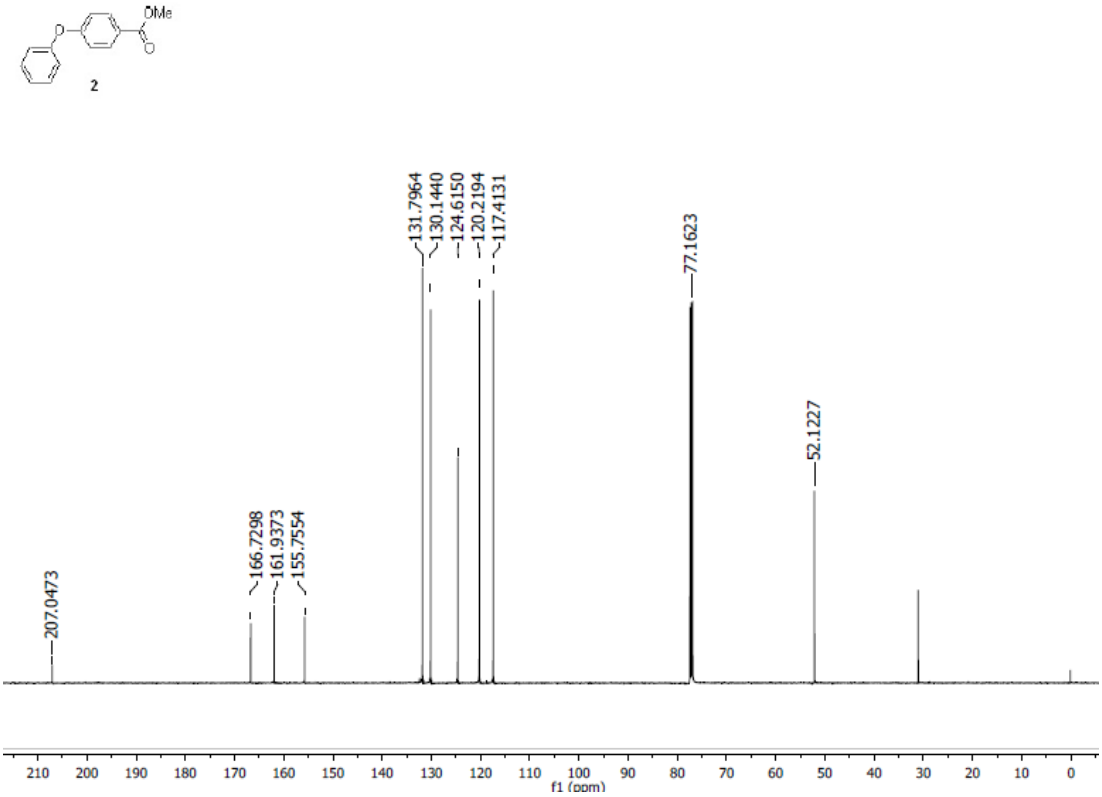

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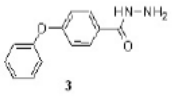

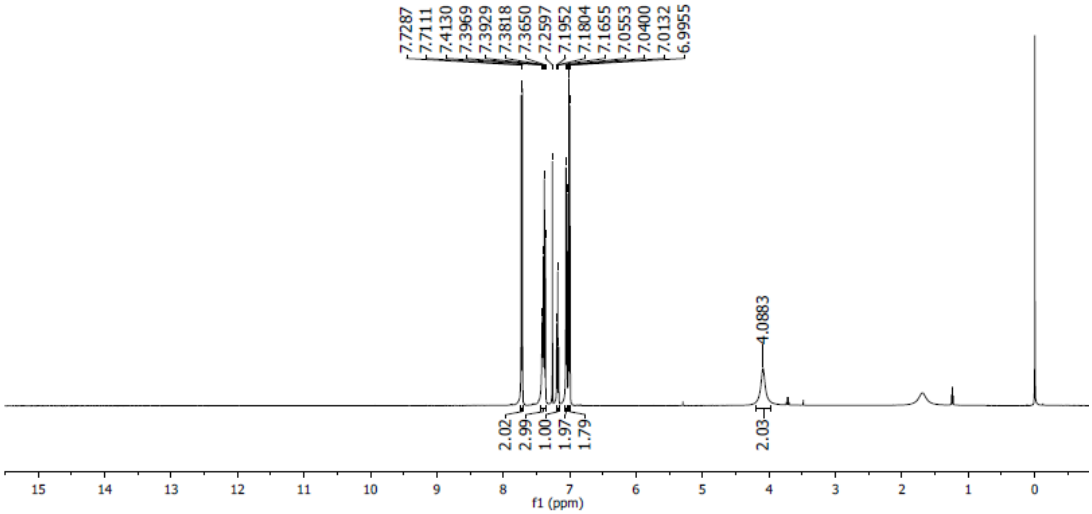

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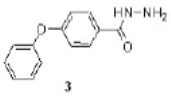

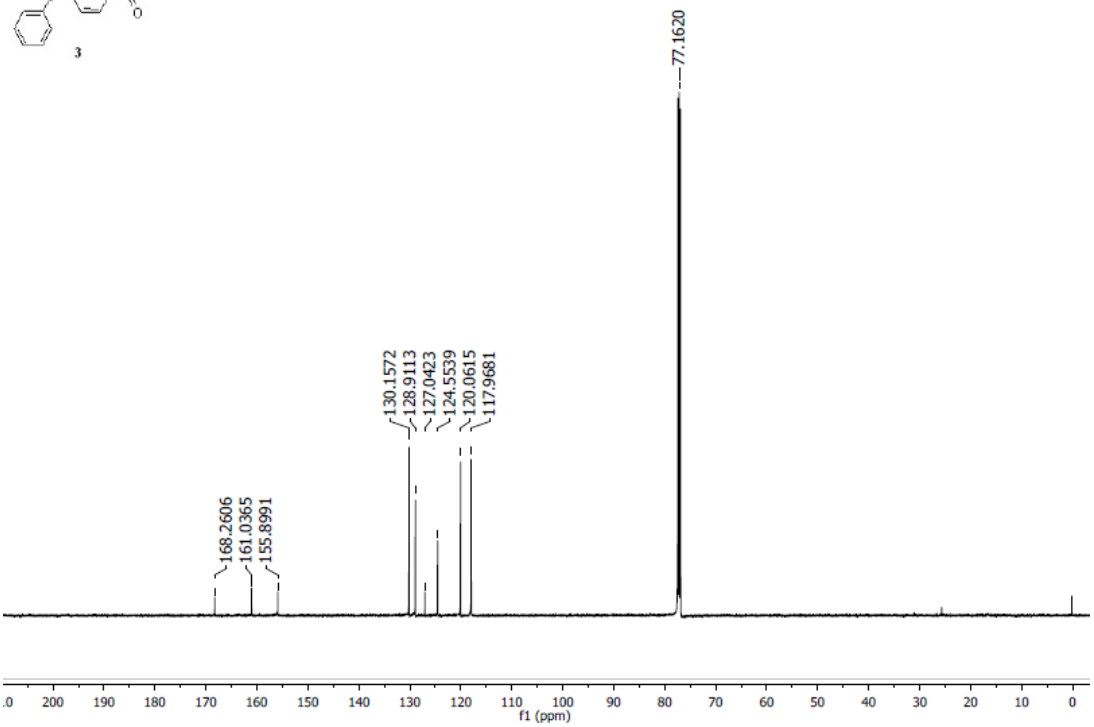

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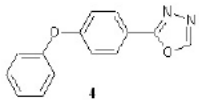

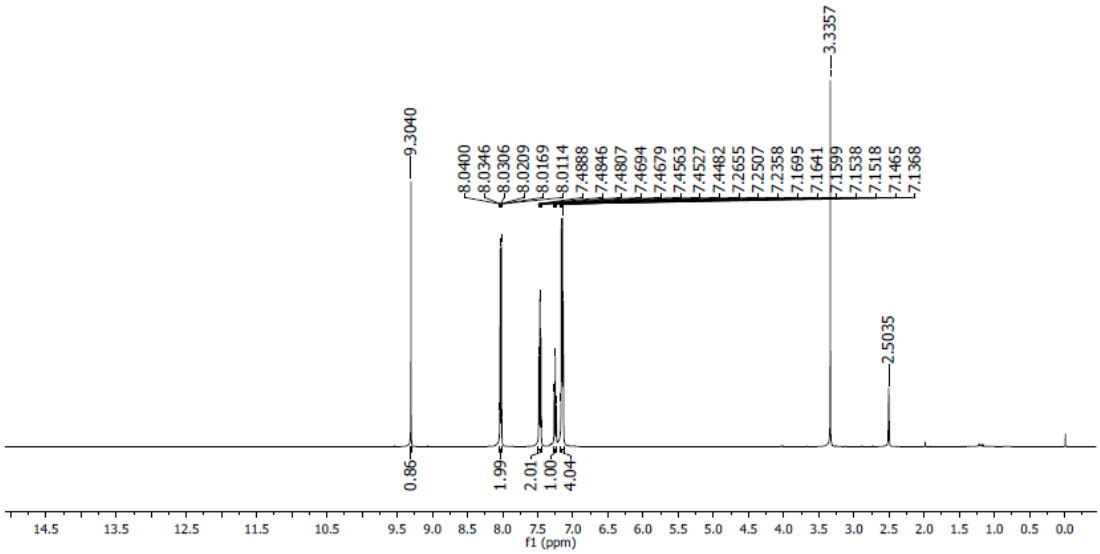

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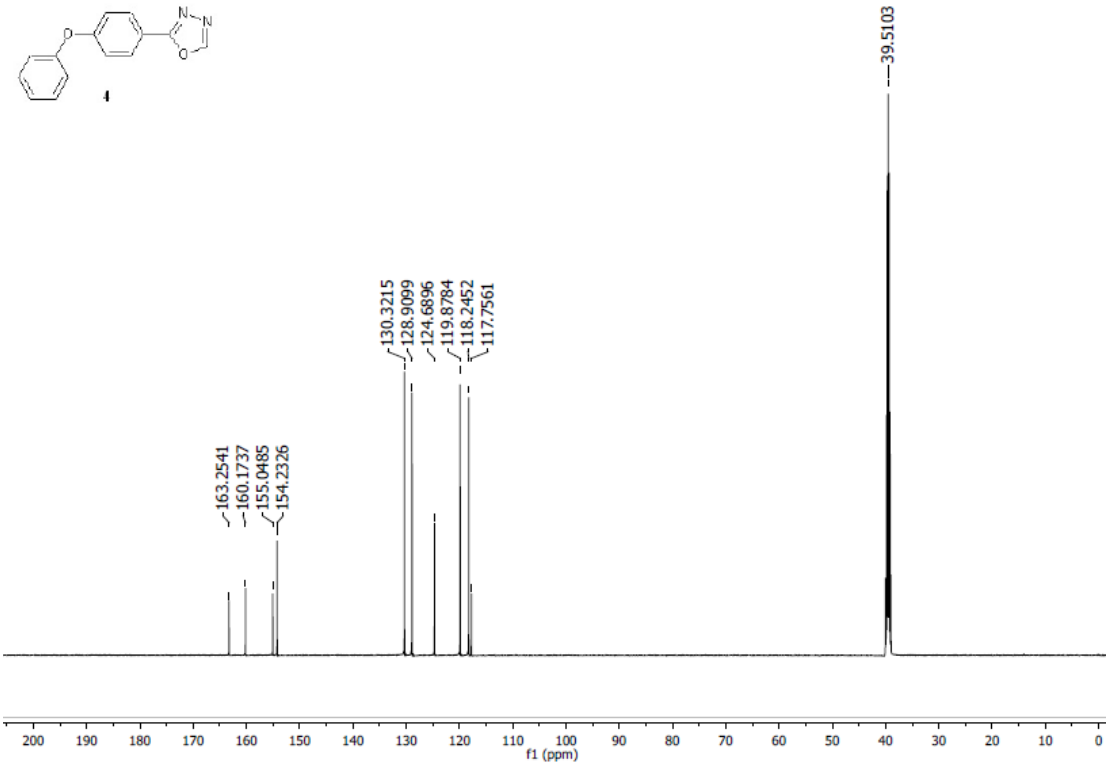

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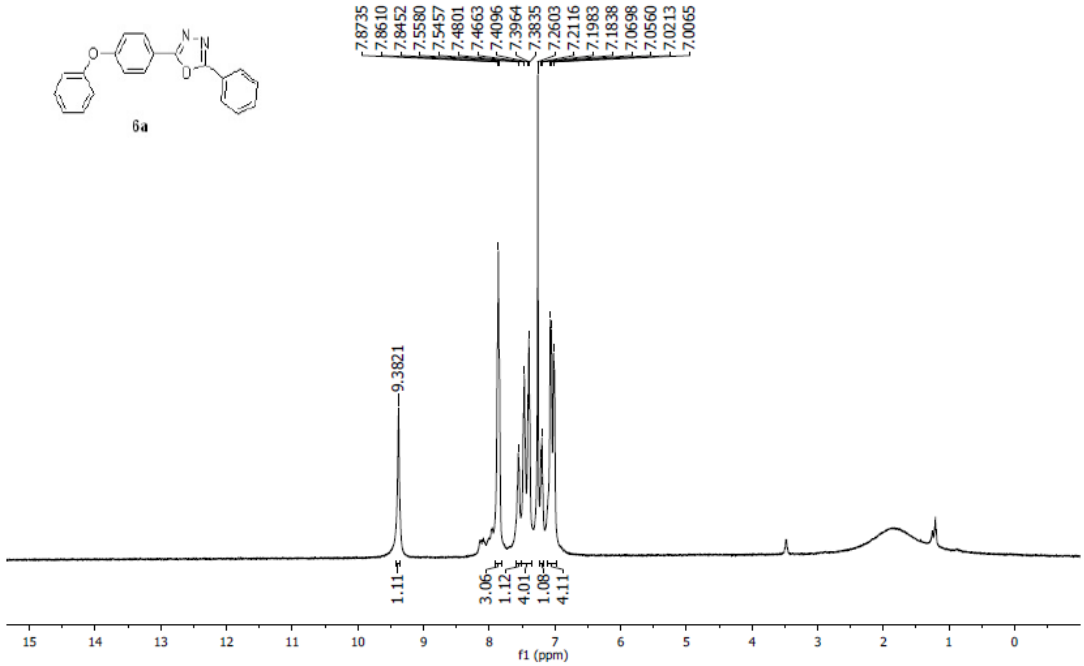

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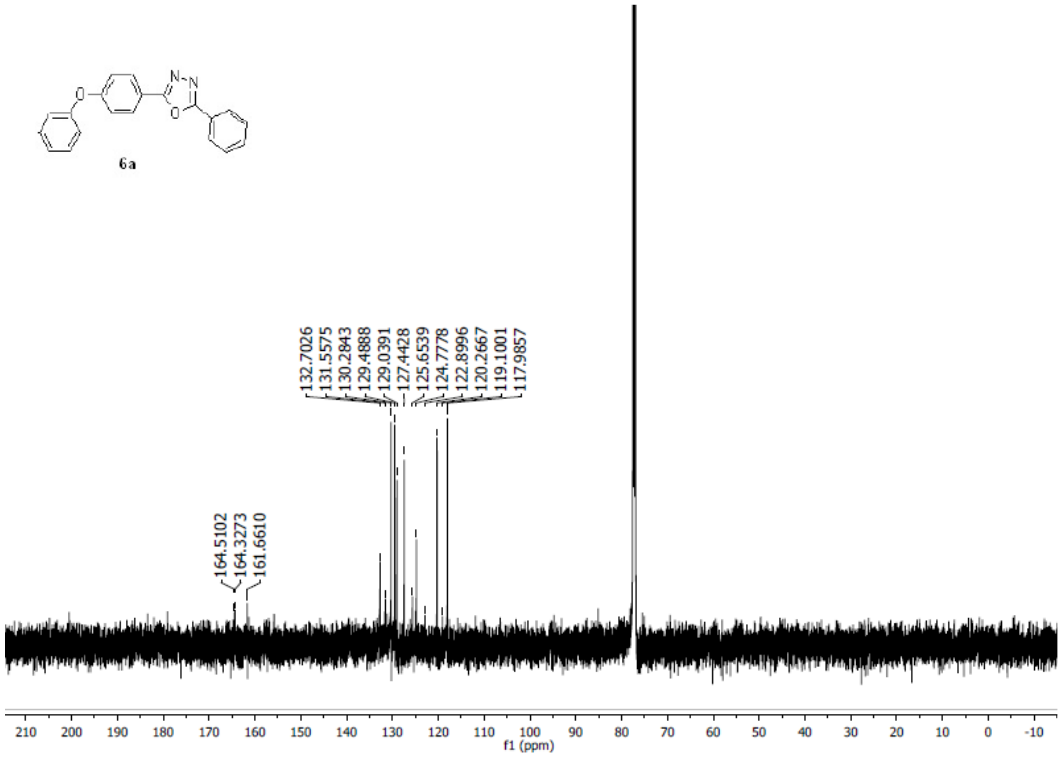

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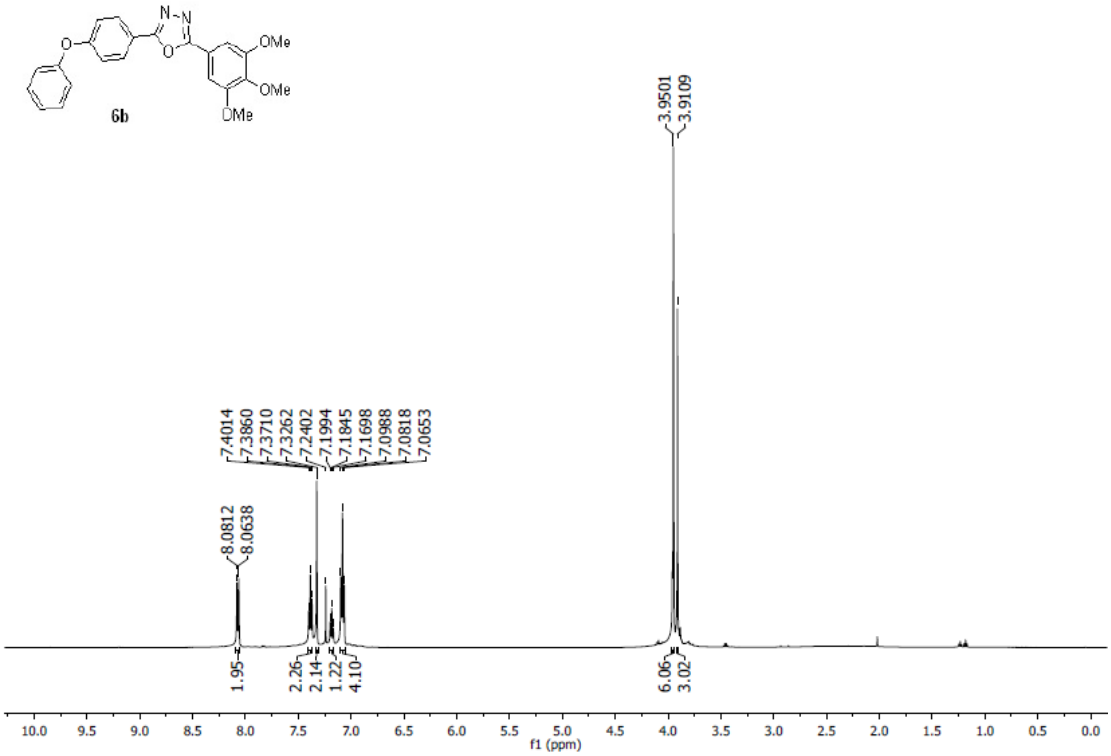

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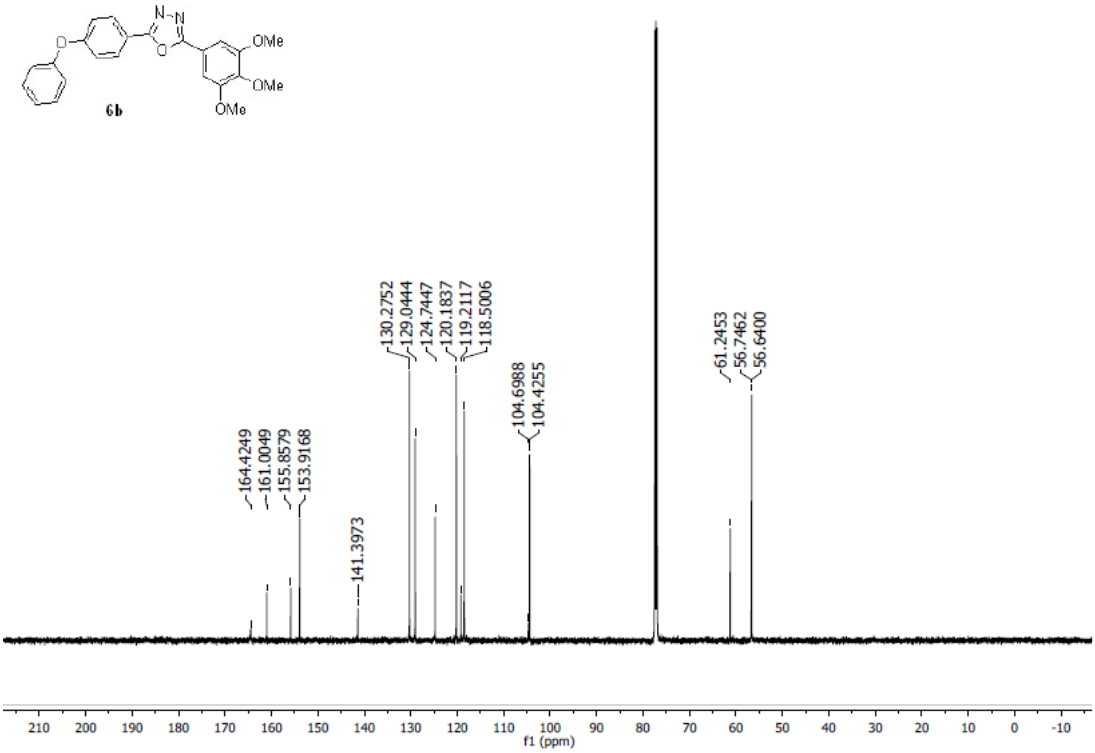

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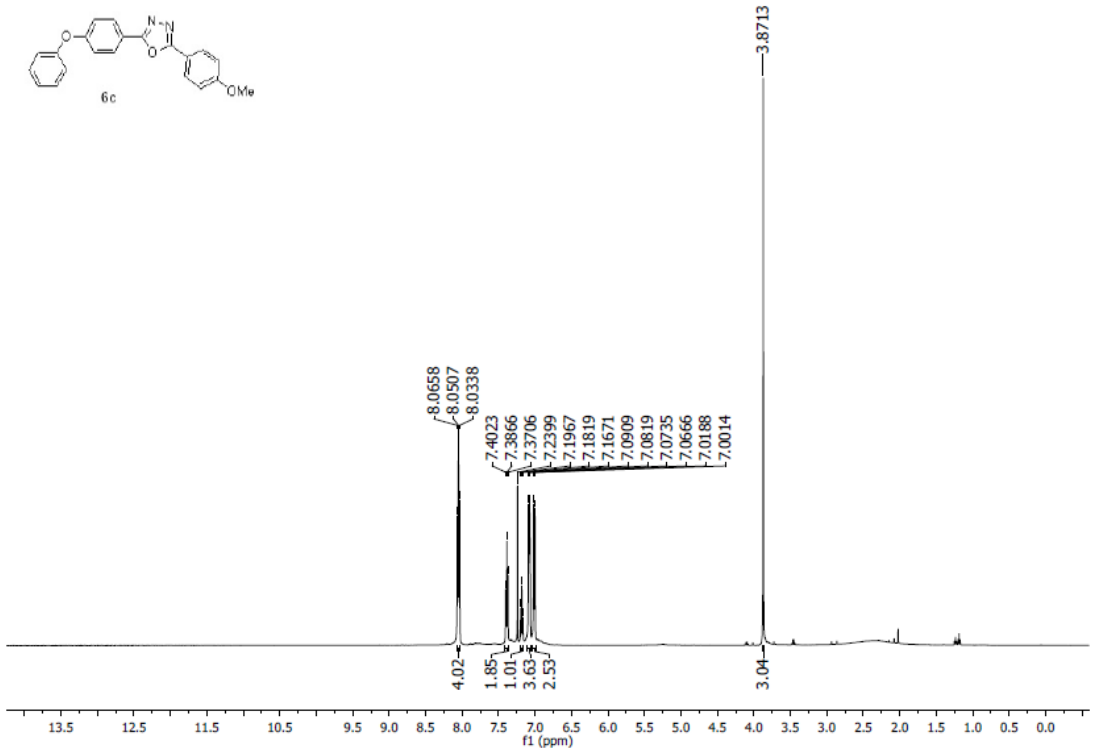

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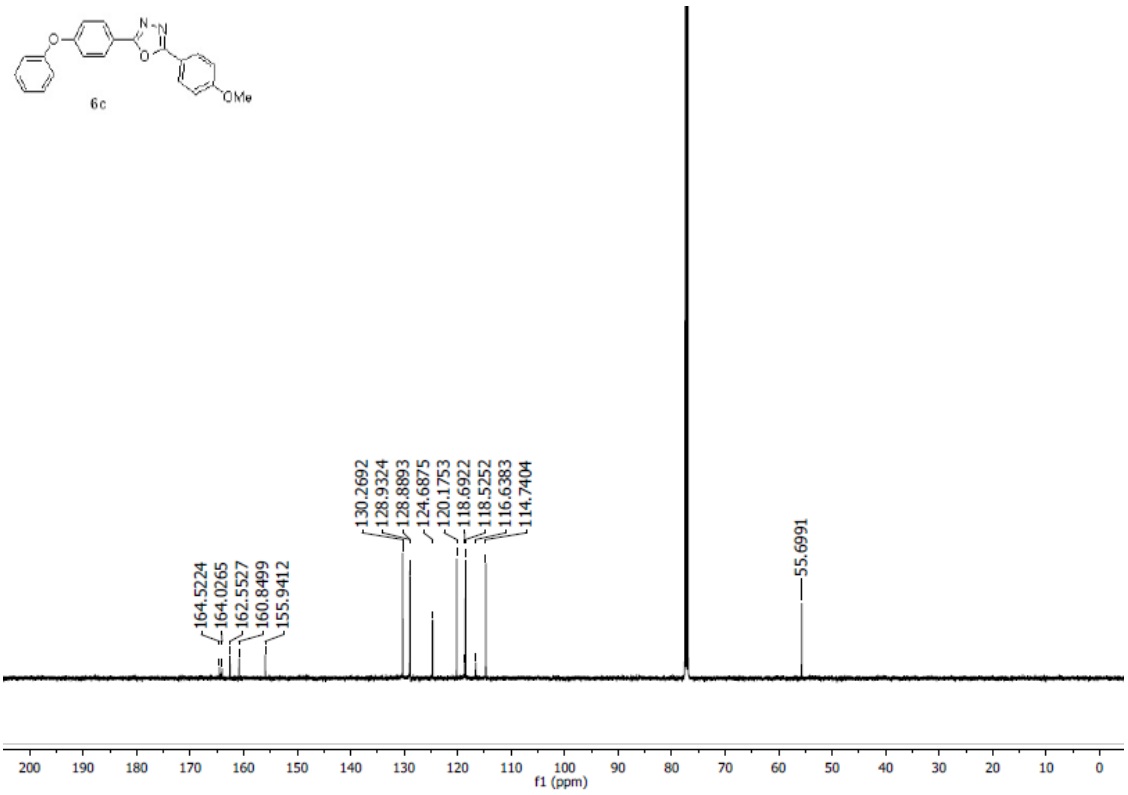

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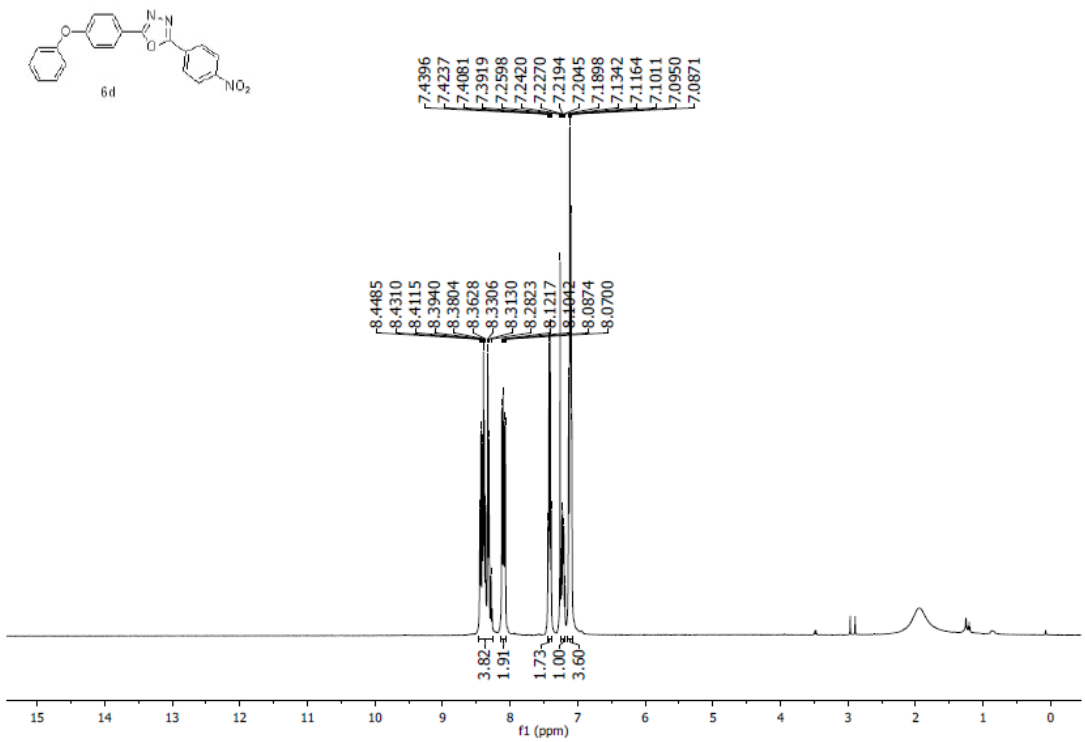

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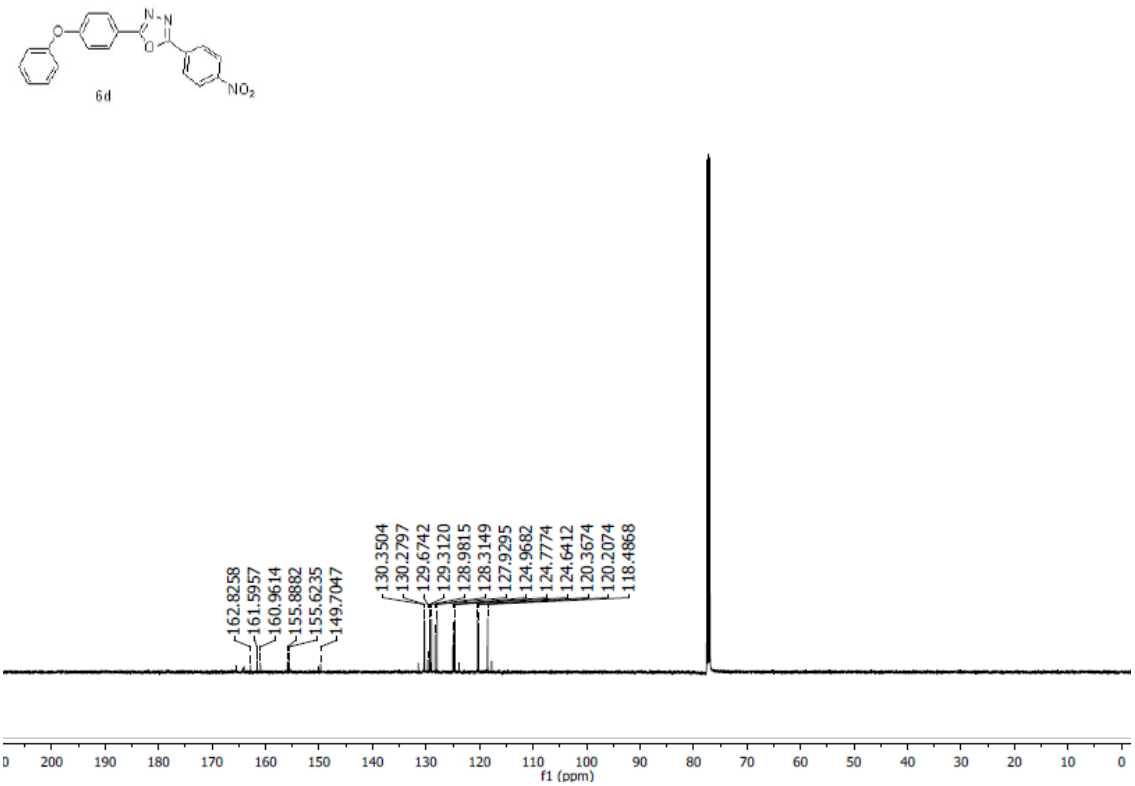

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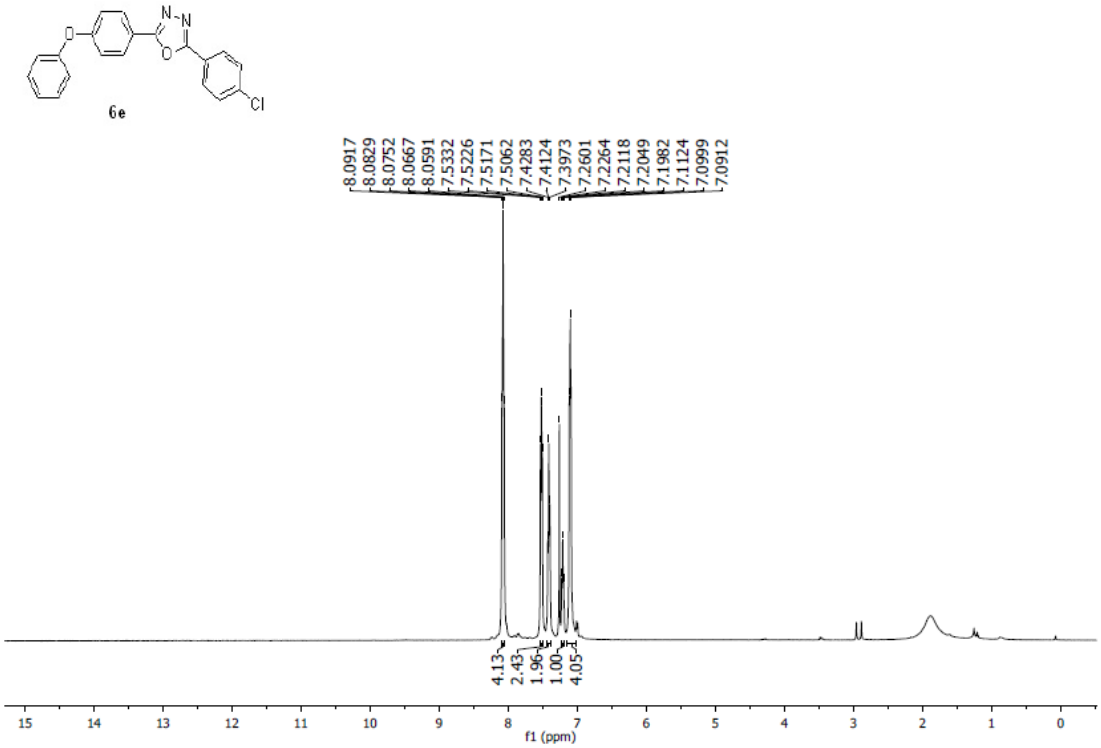

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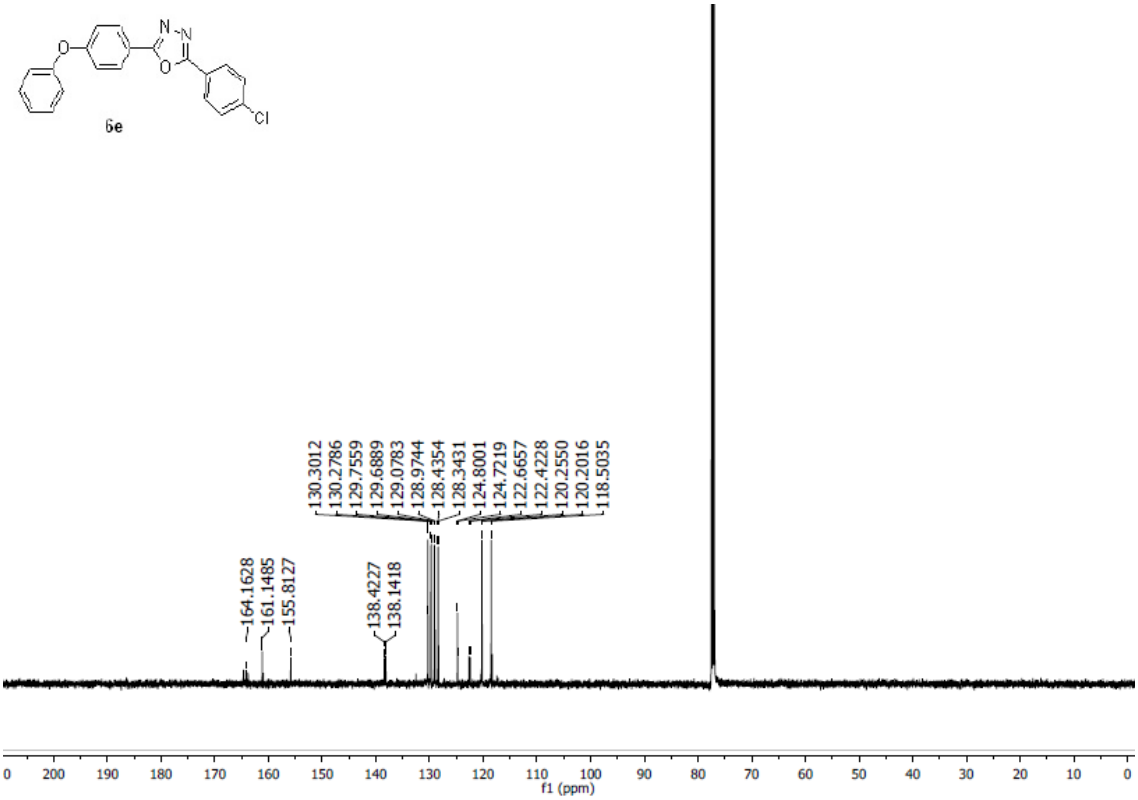

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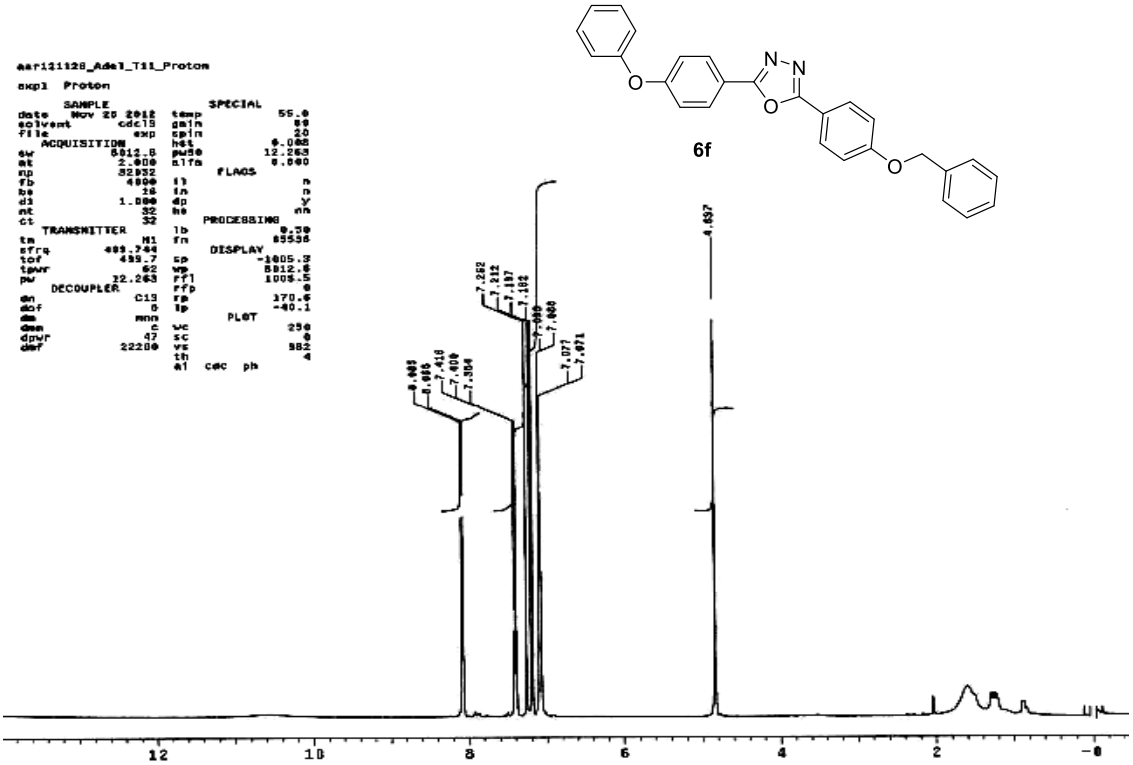

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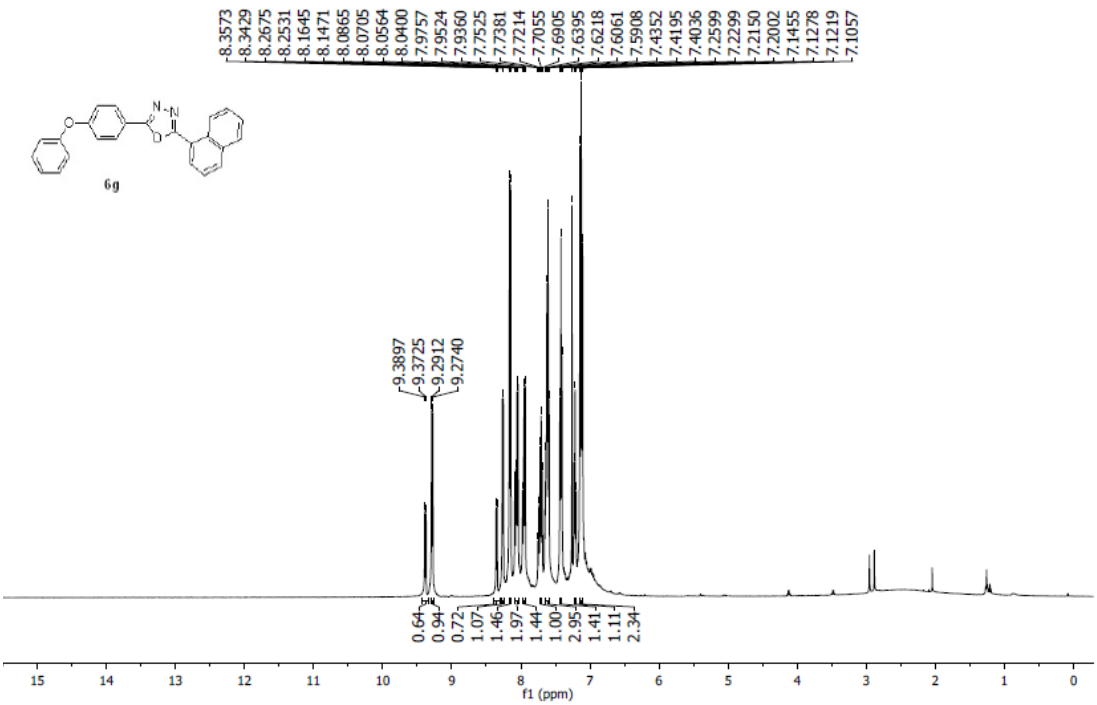

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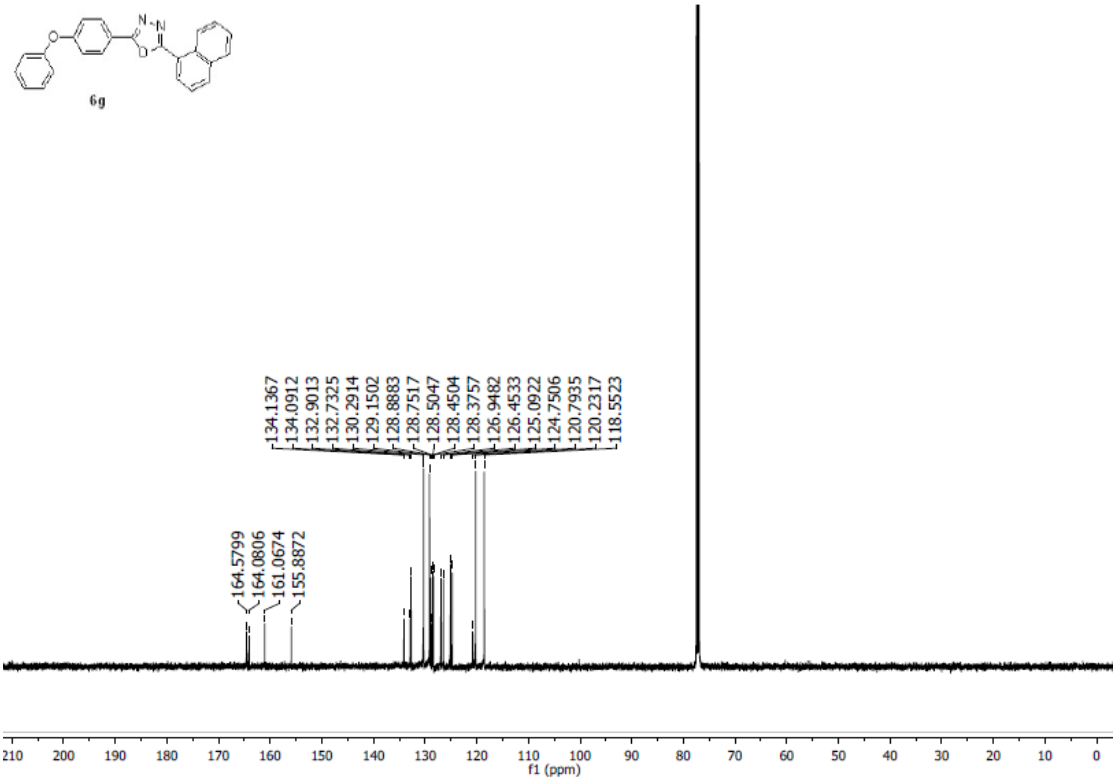

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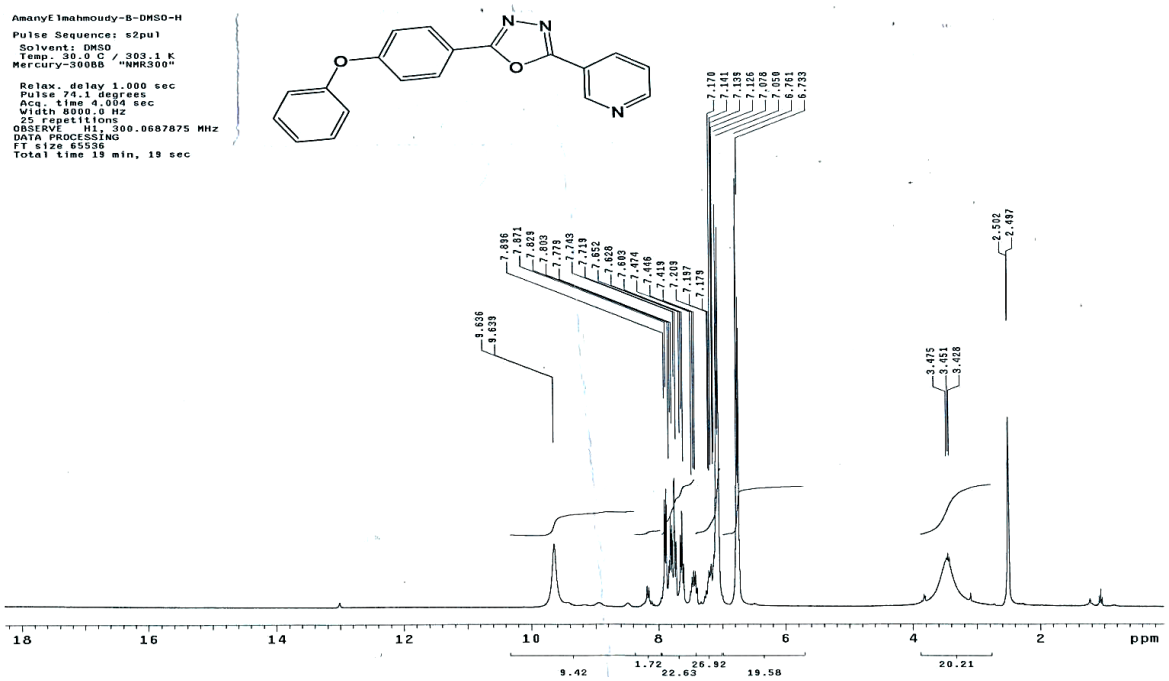

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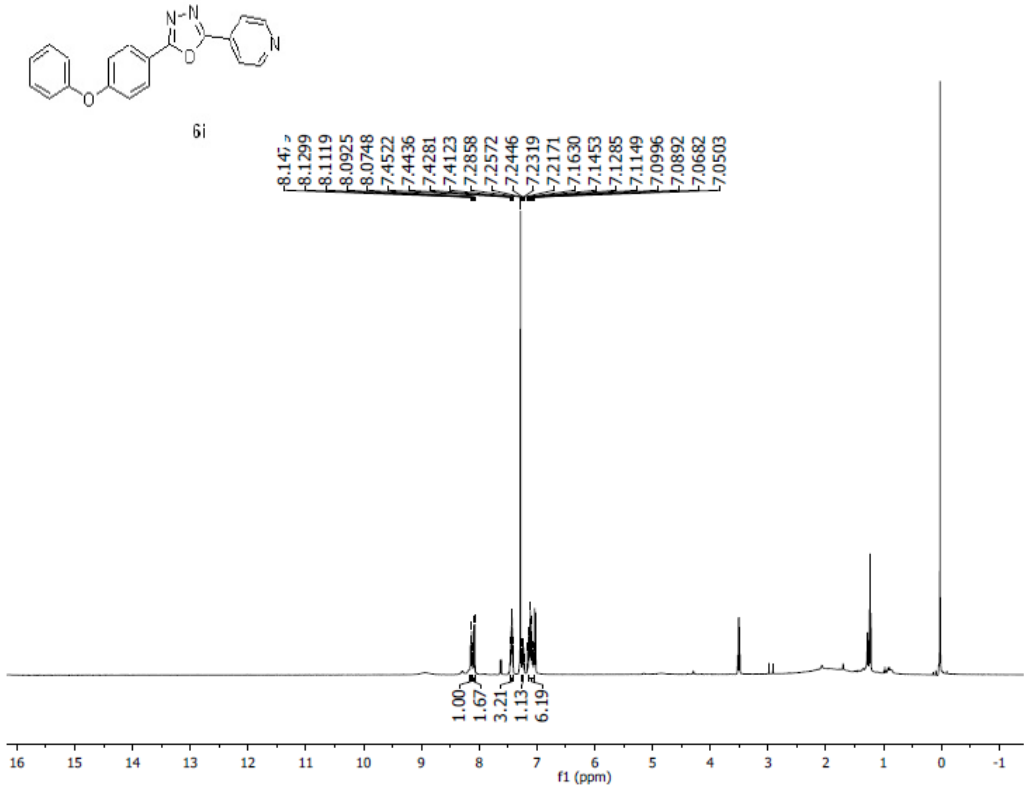

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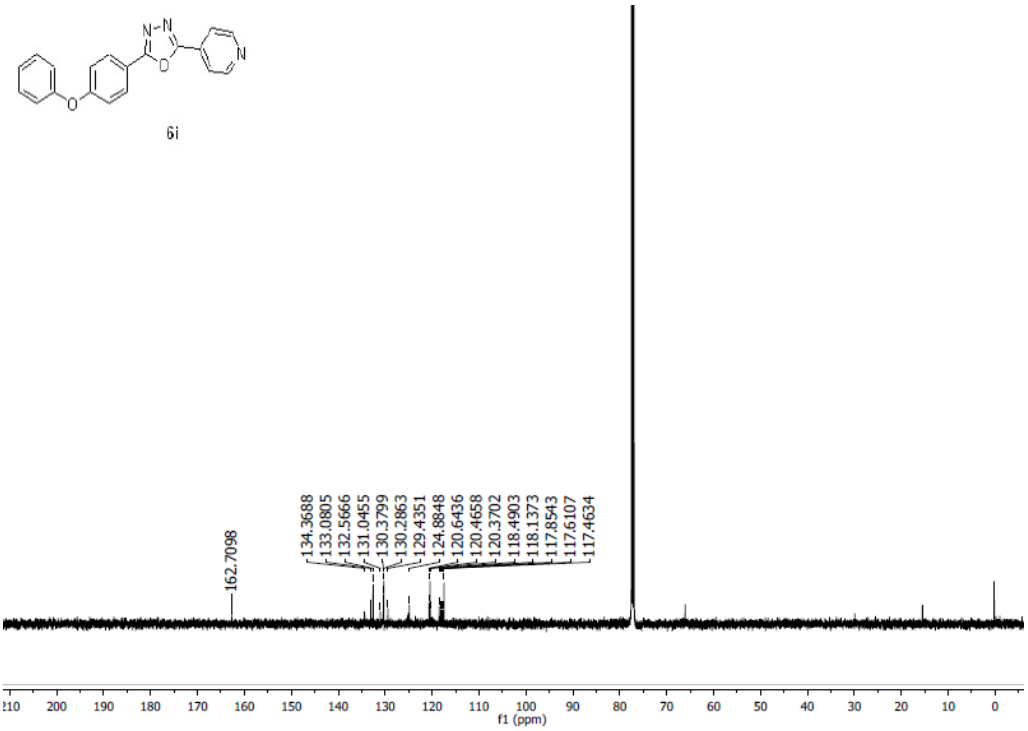

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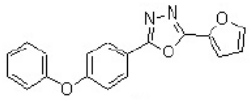

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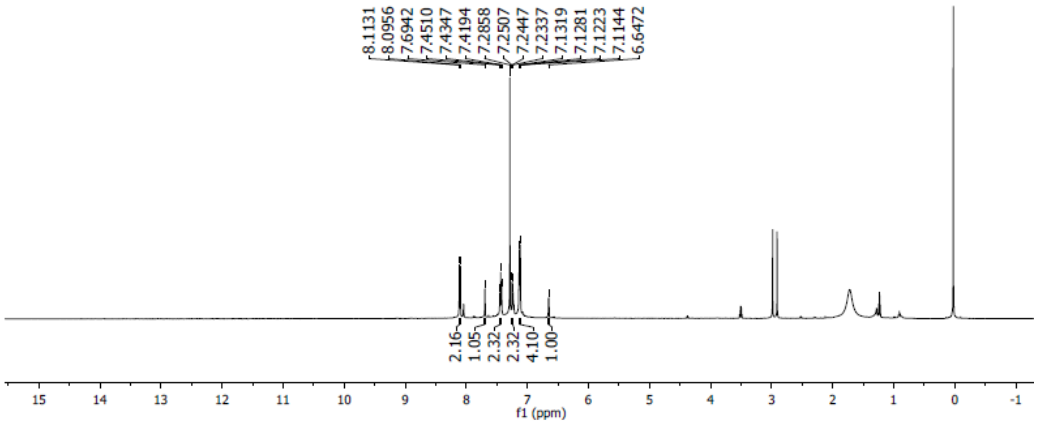

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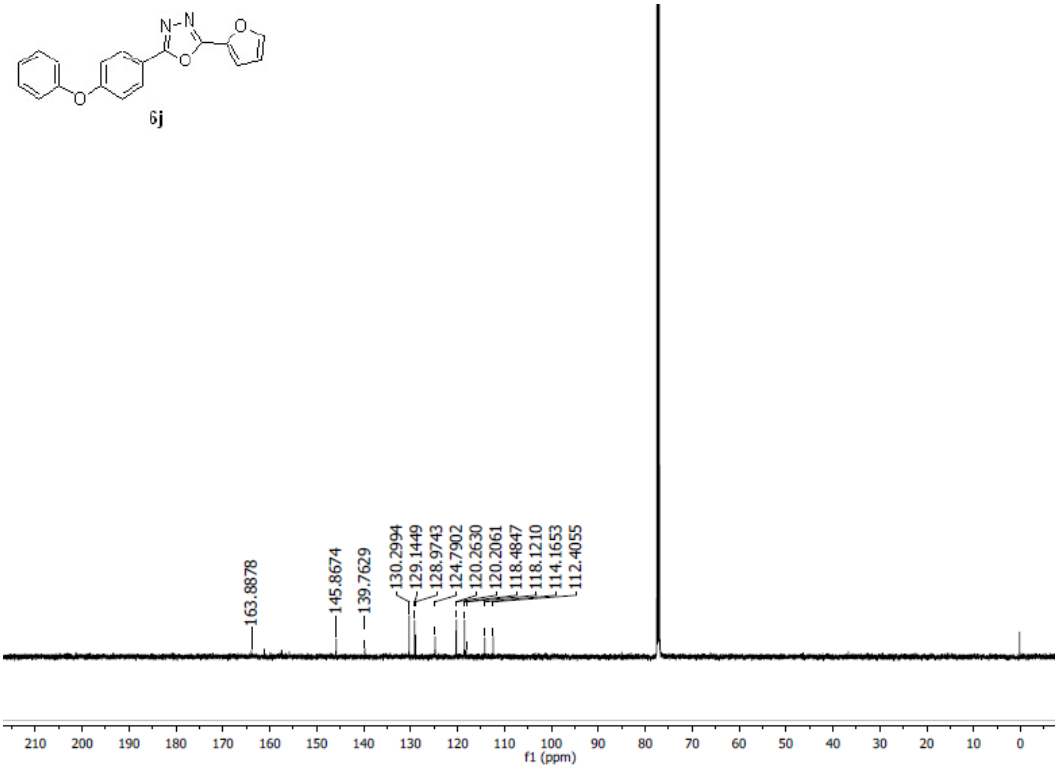

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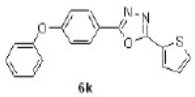

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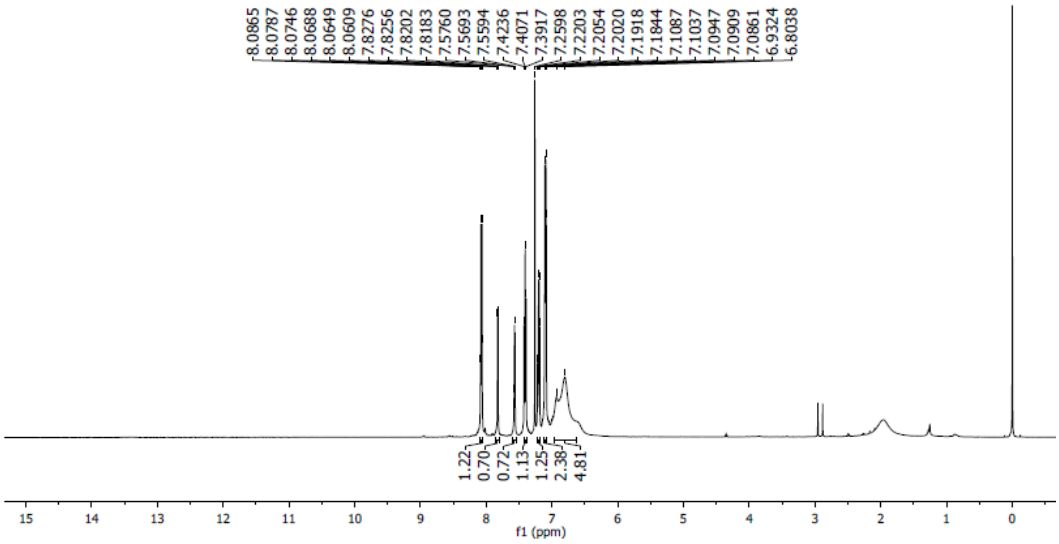
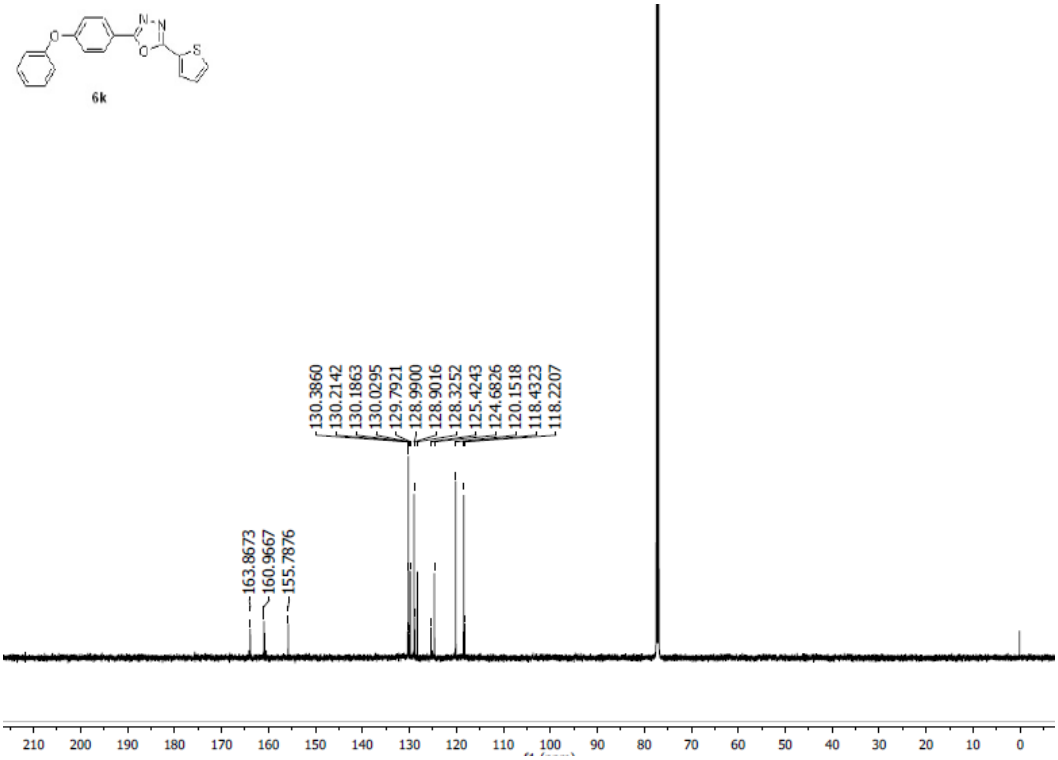


^{13}C NMR for compound 6k

6k



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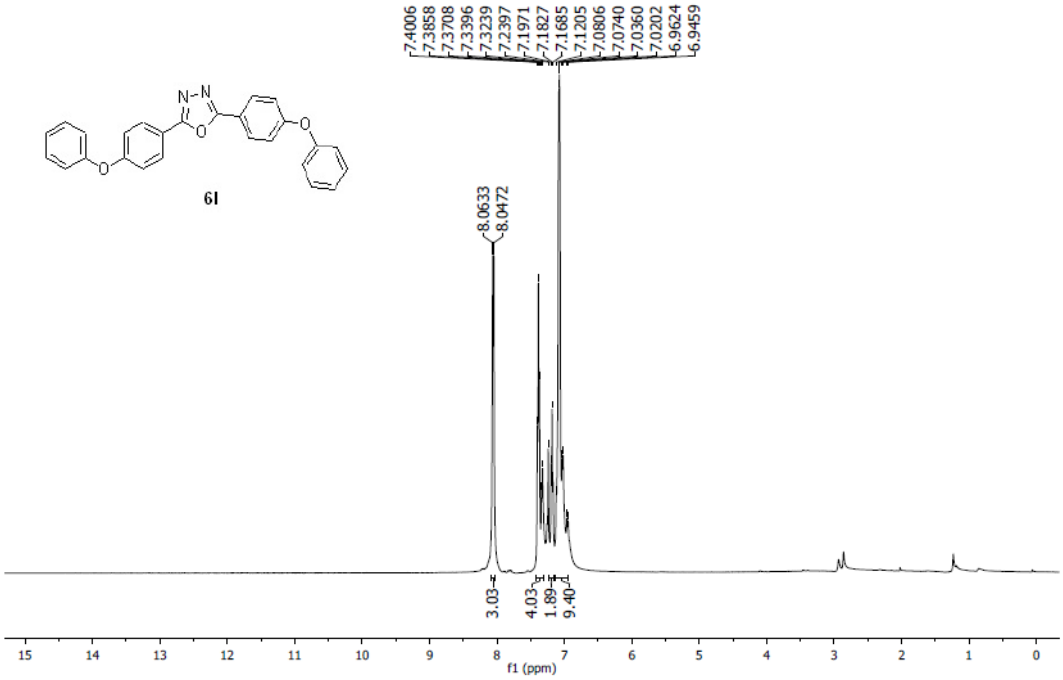

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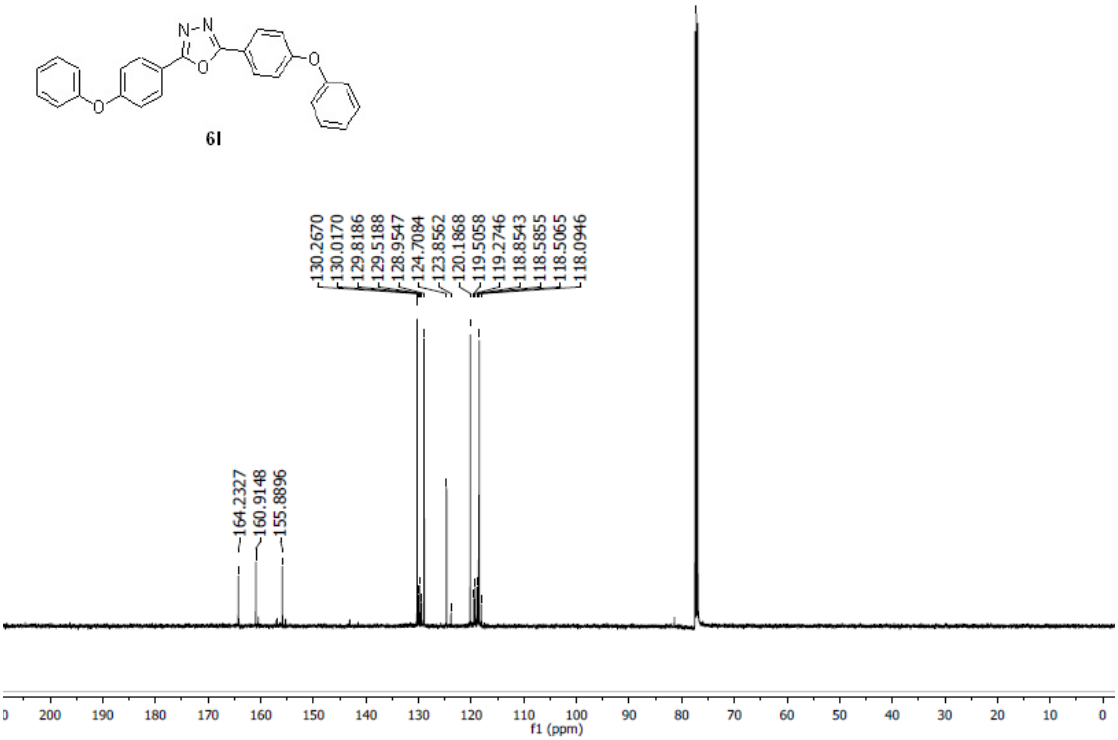

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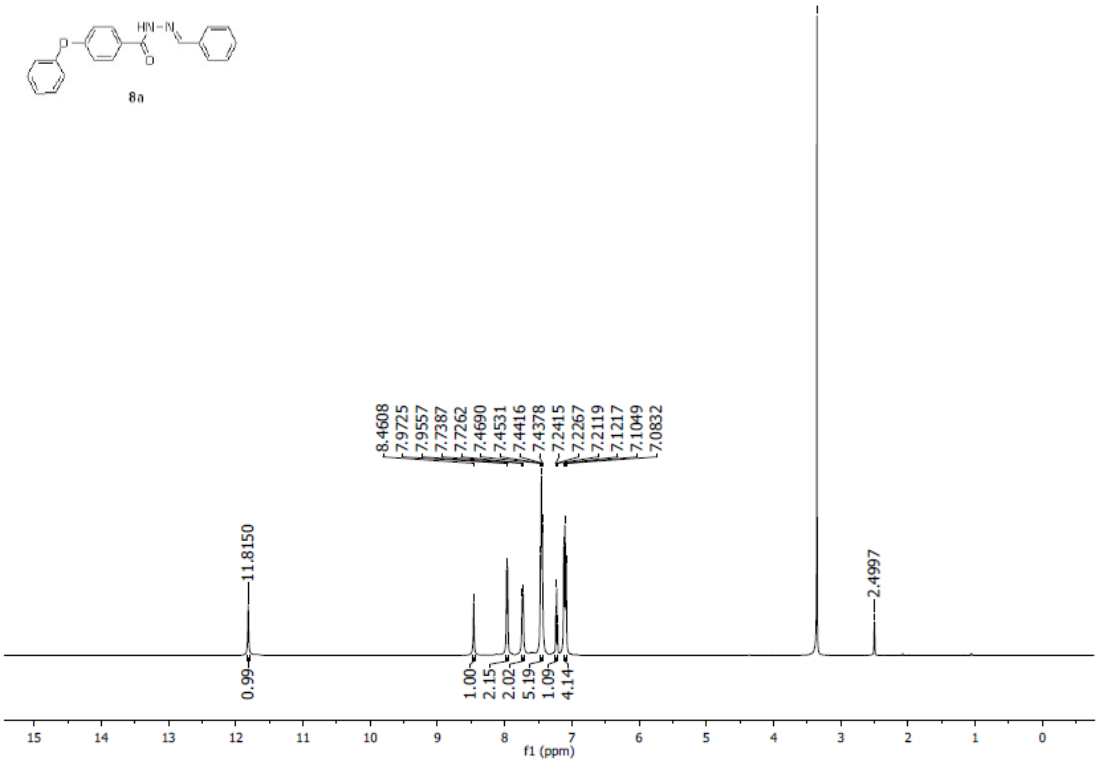

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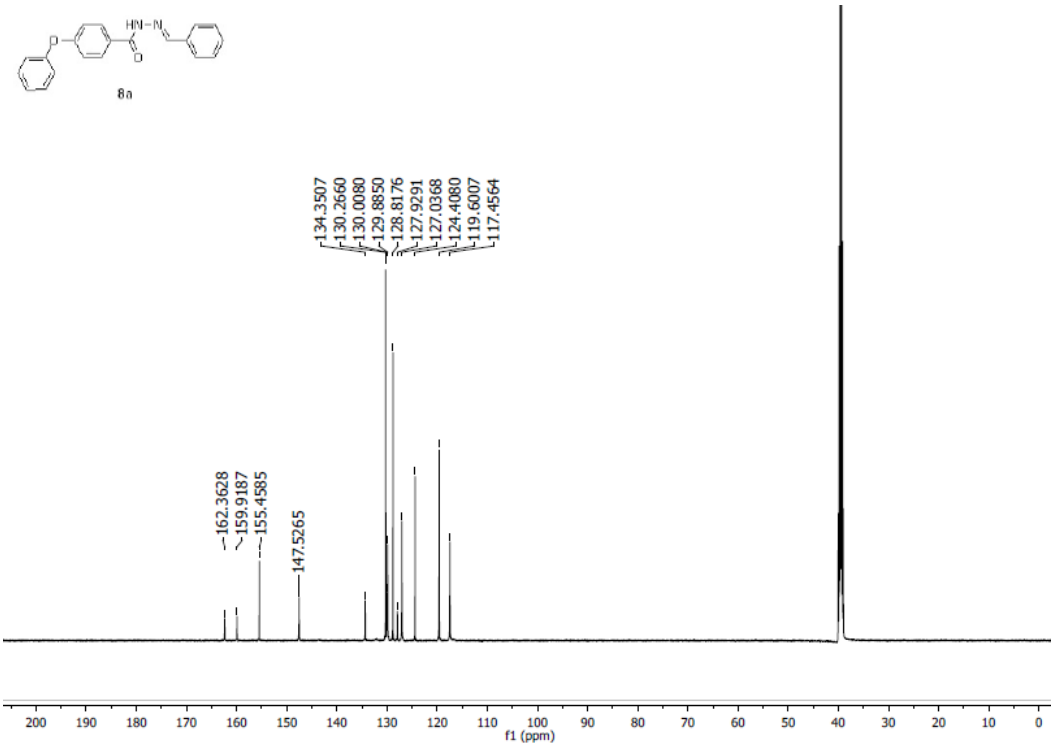

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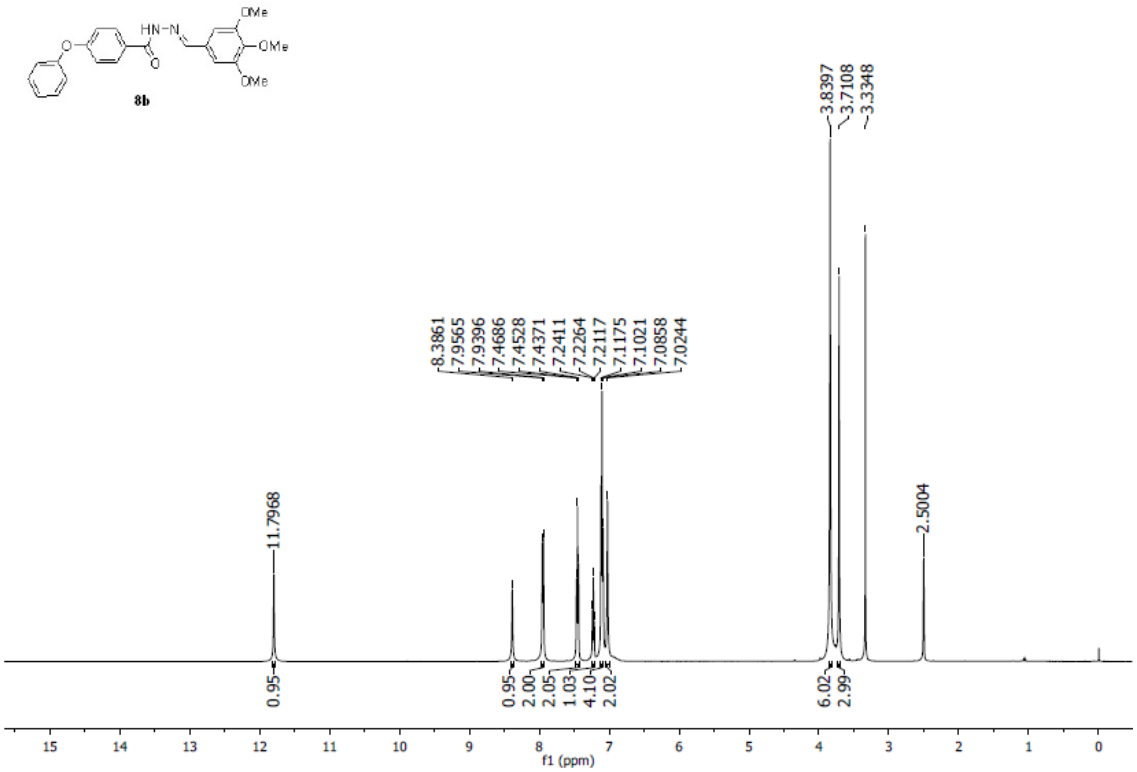

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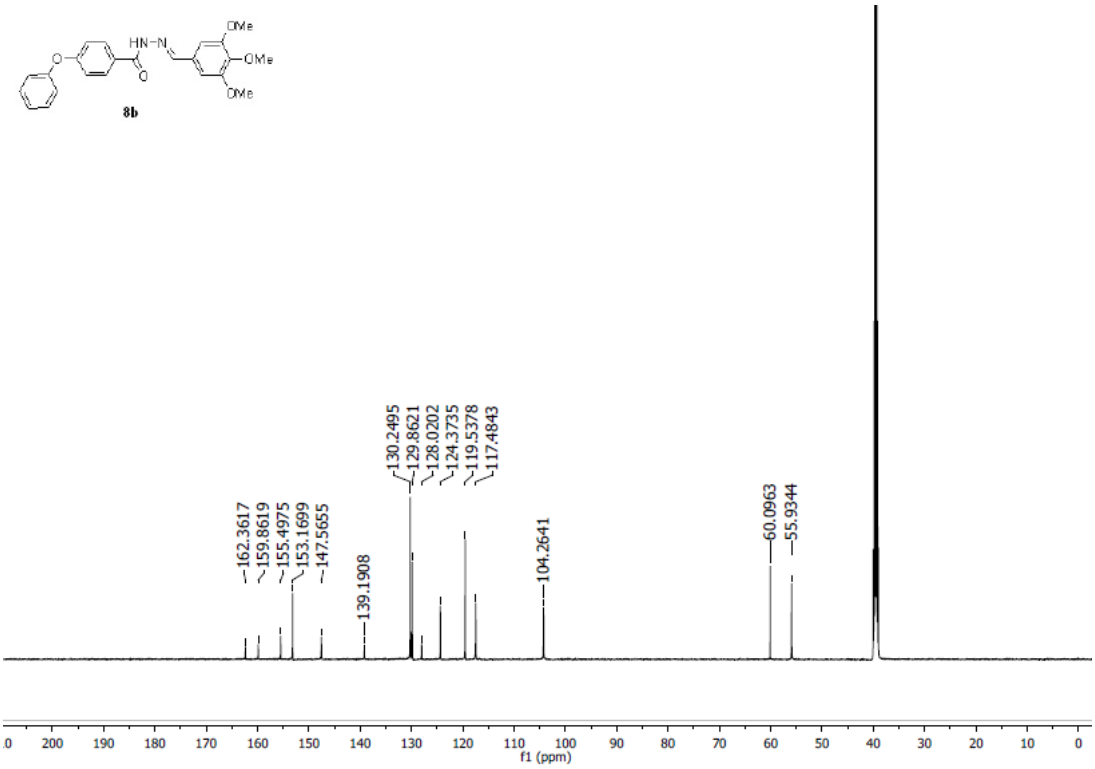

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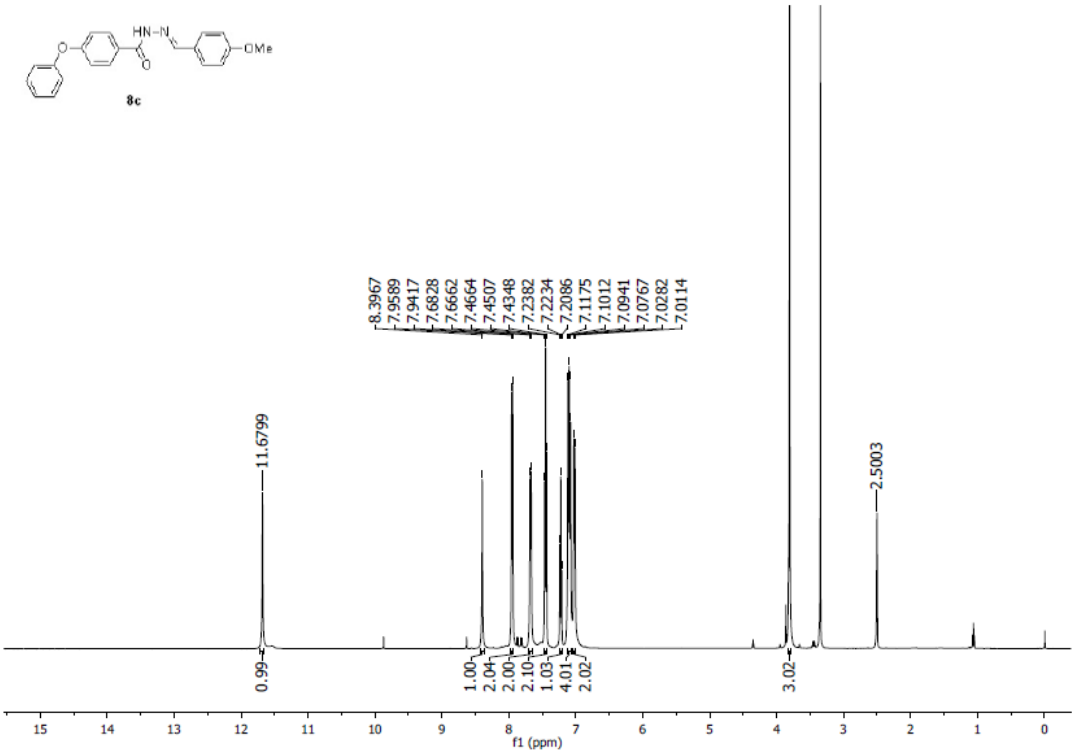

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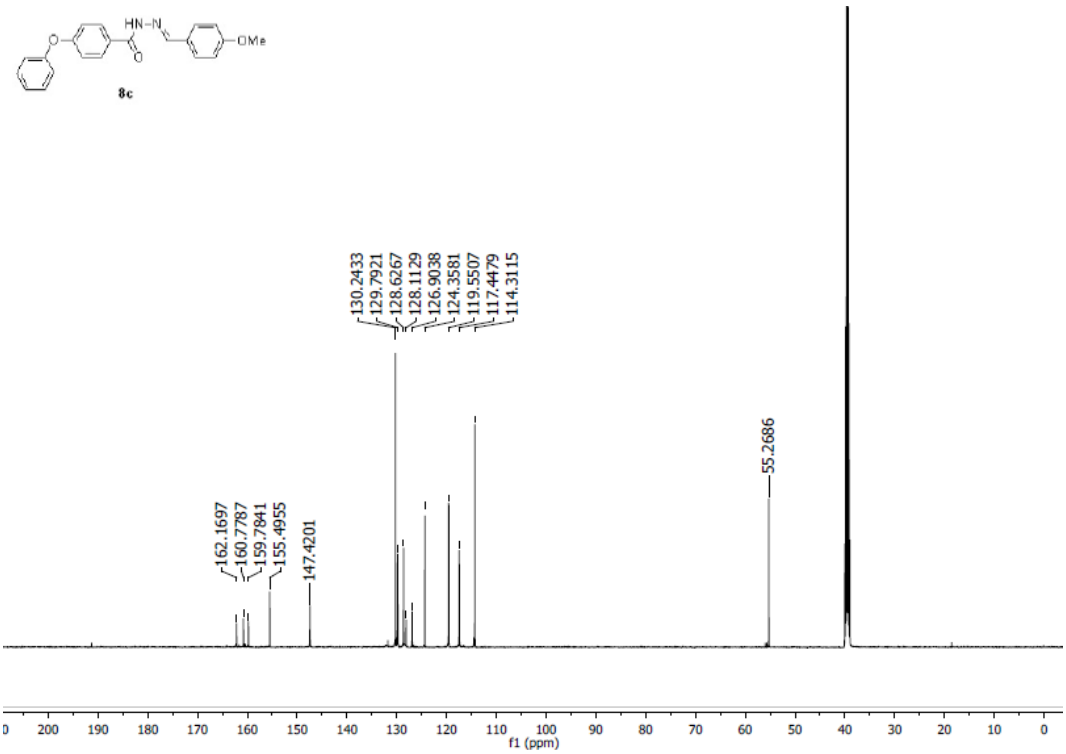

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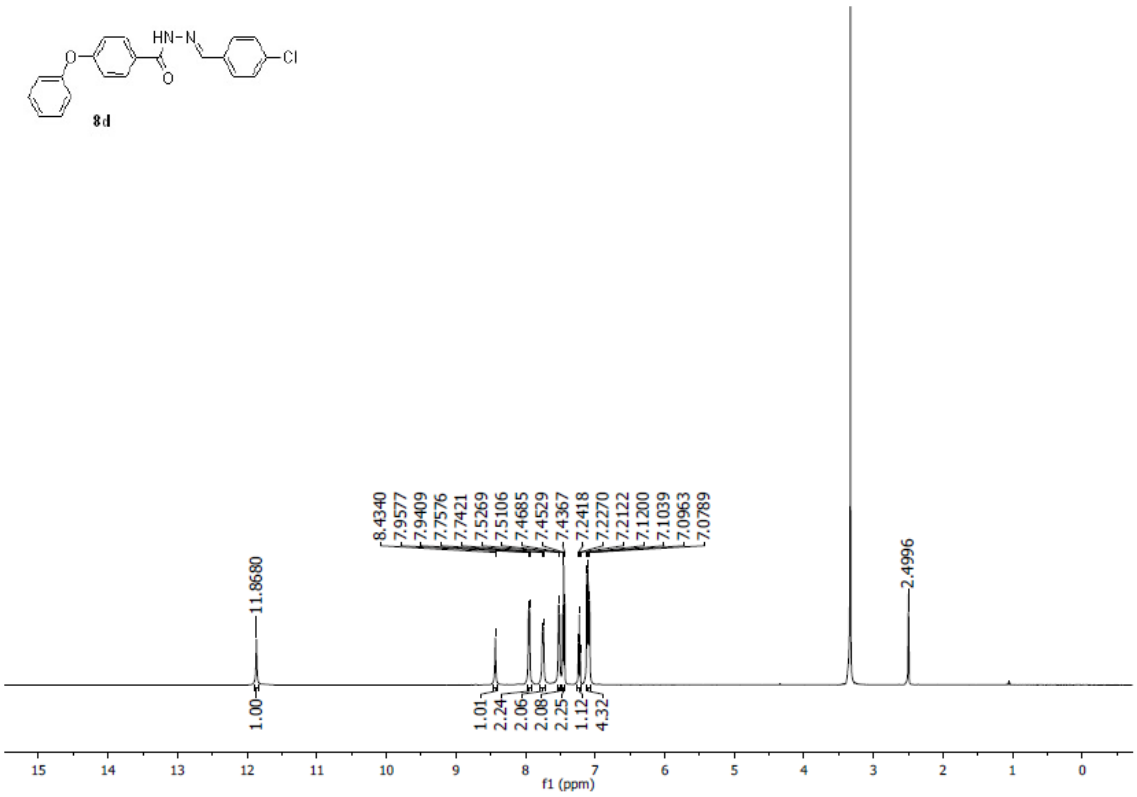

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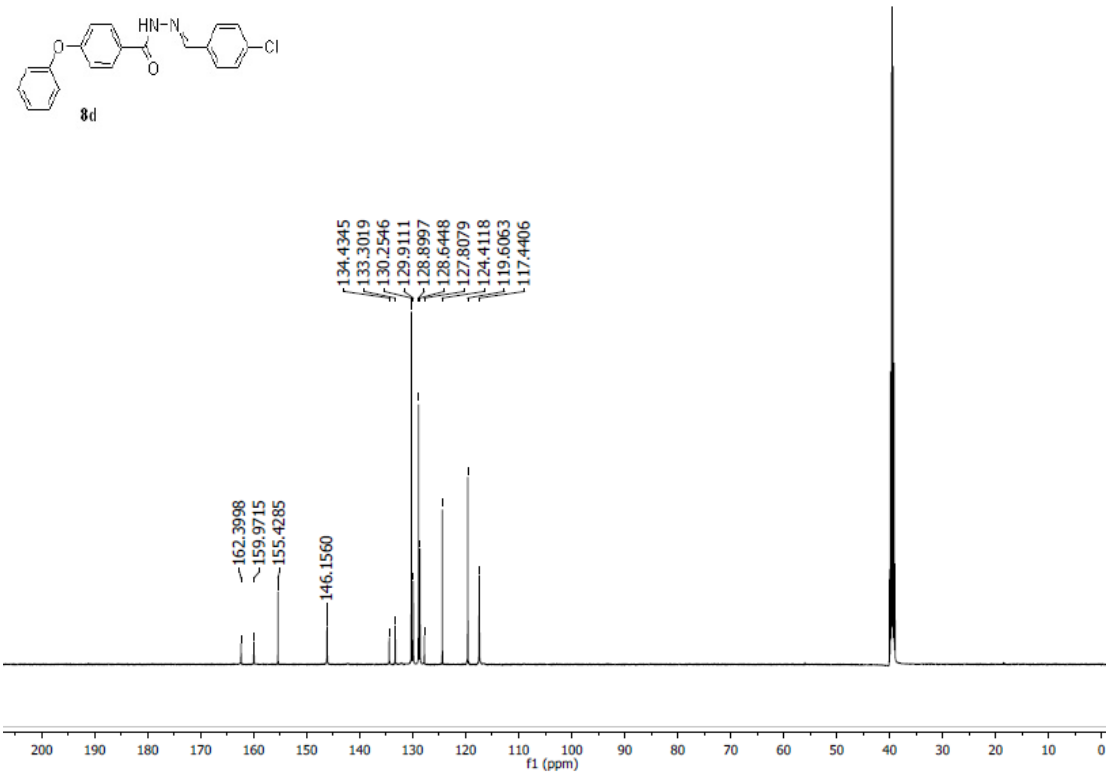

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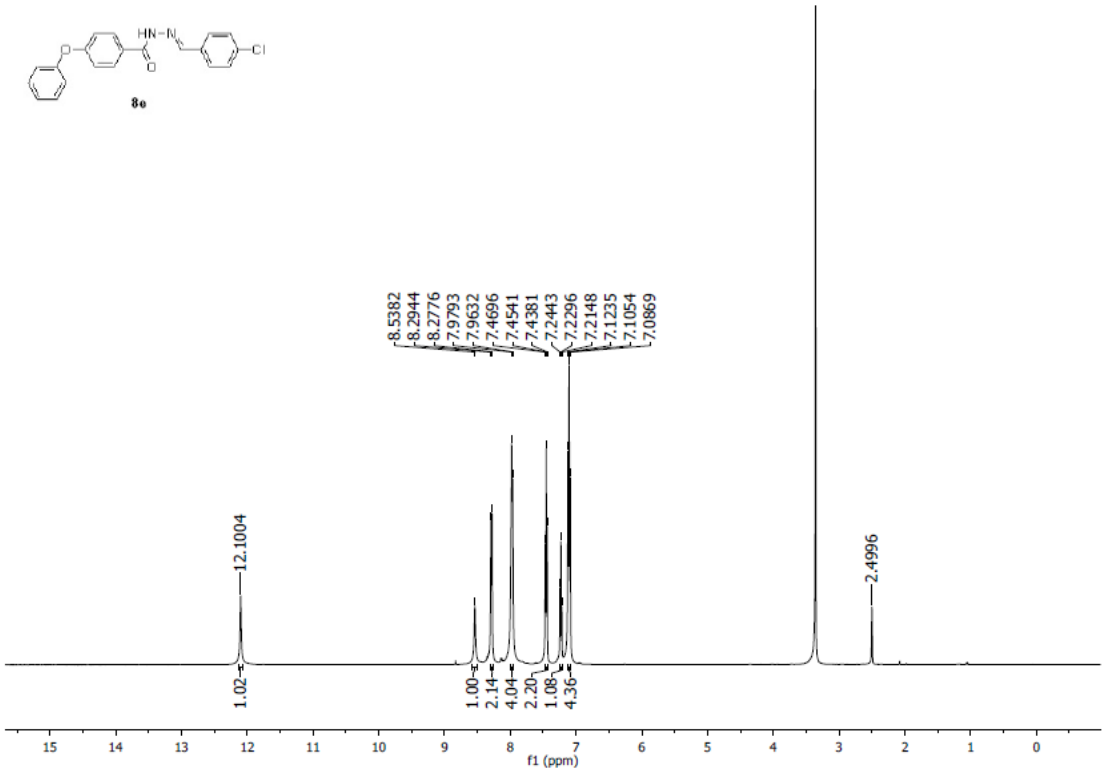

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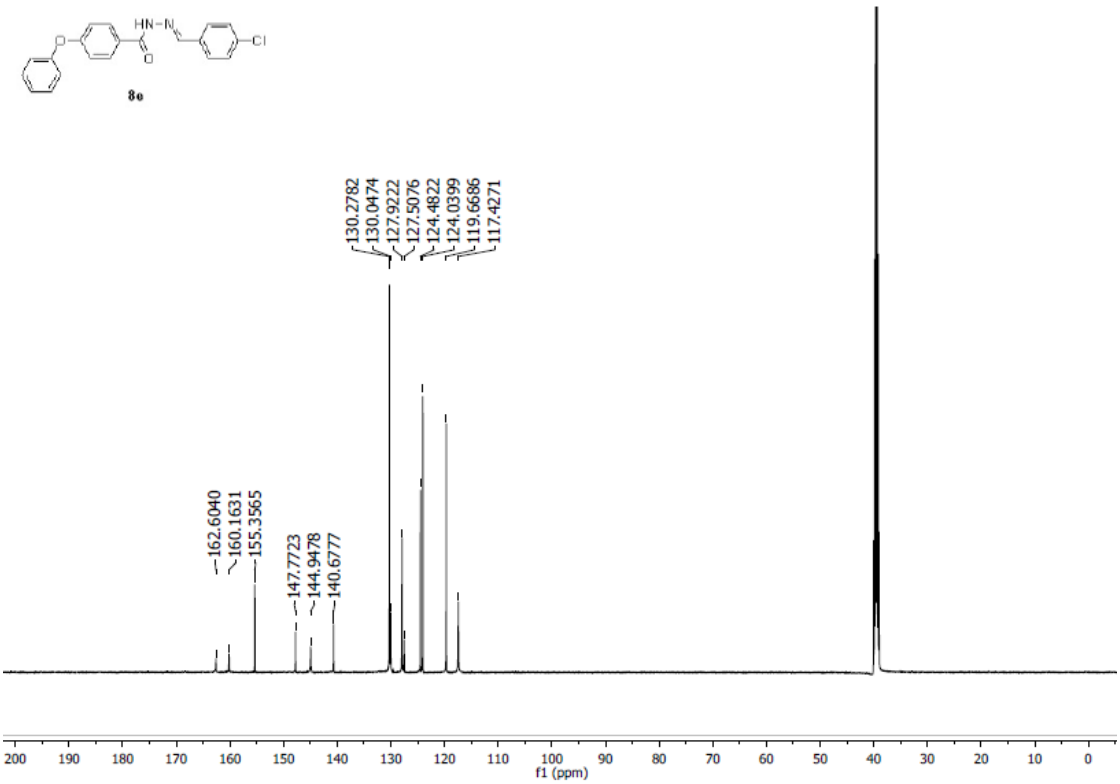

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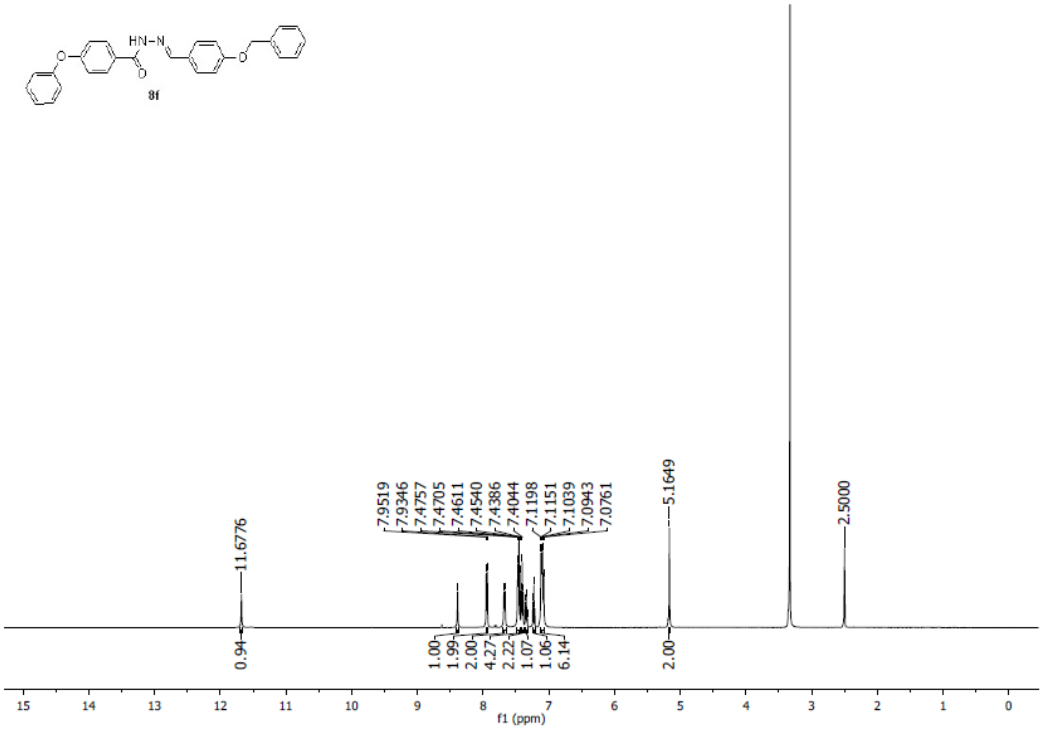

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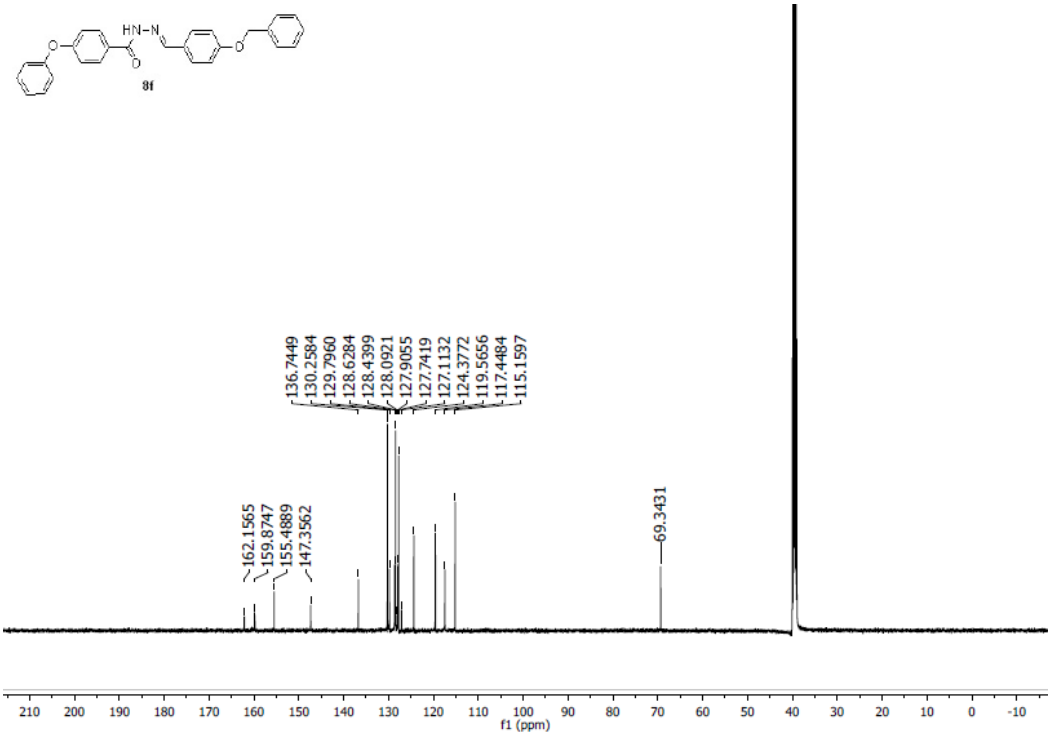

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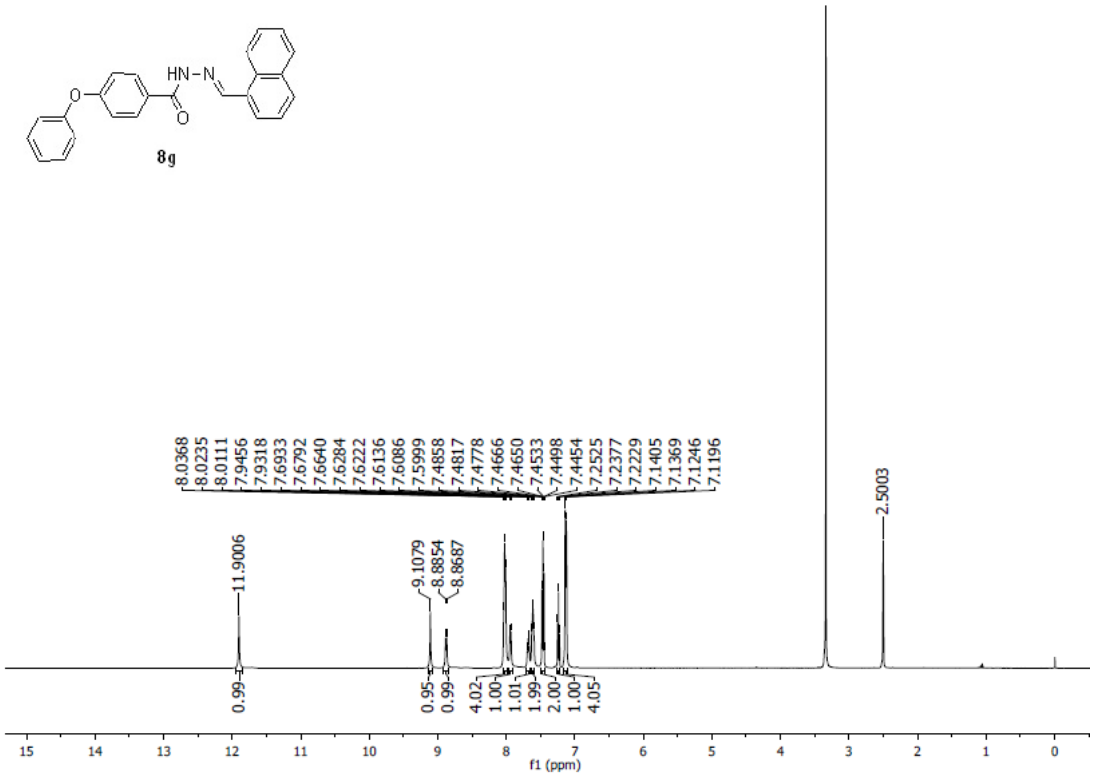

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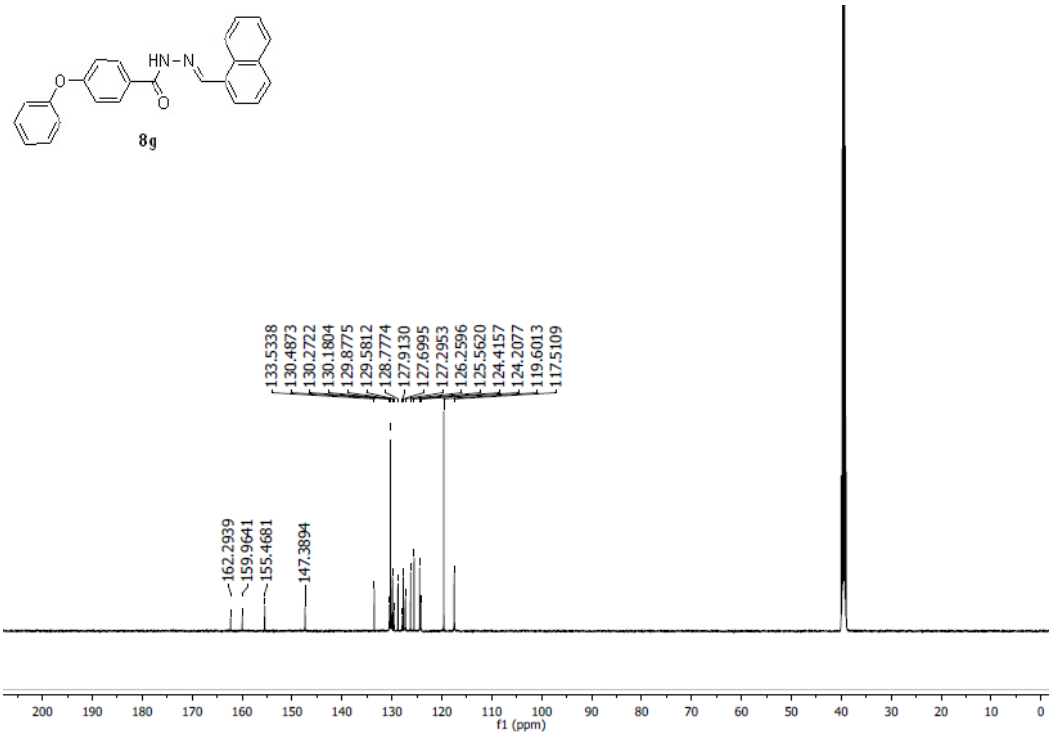

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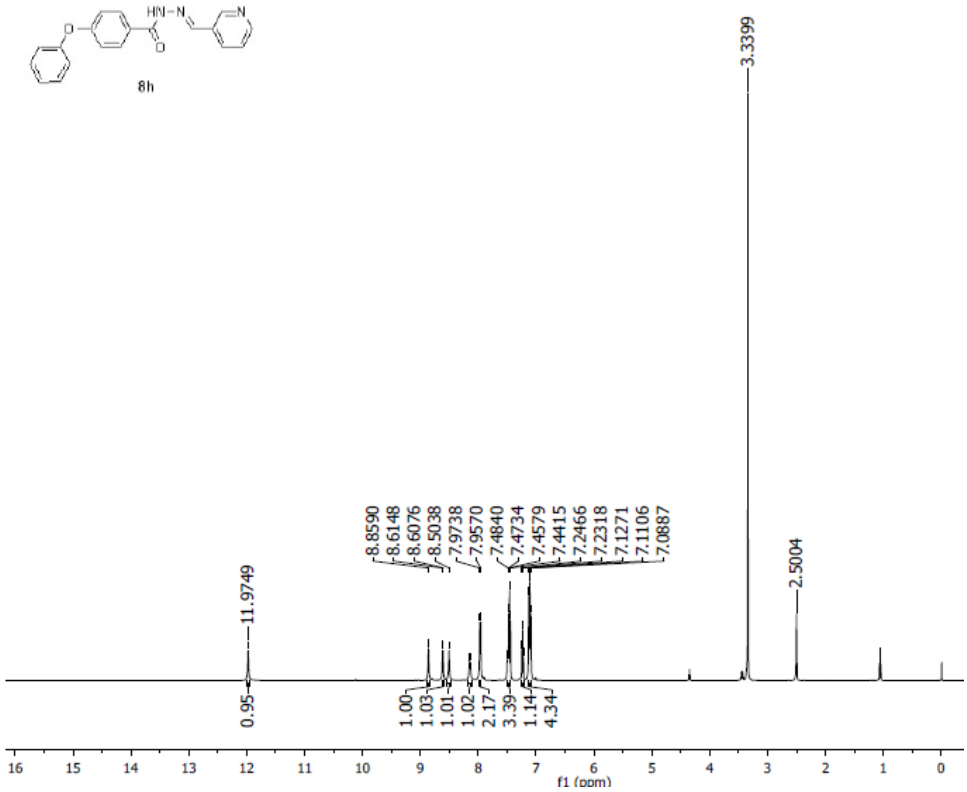

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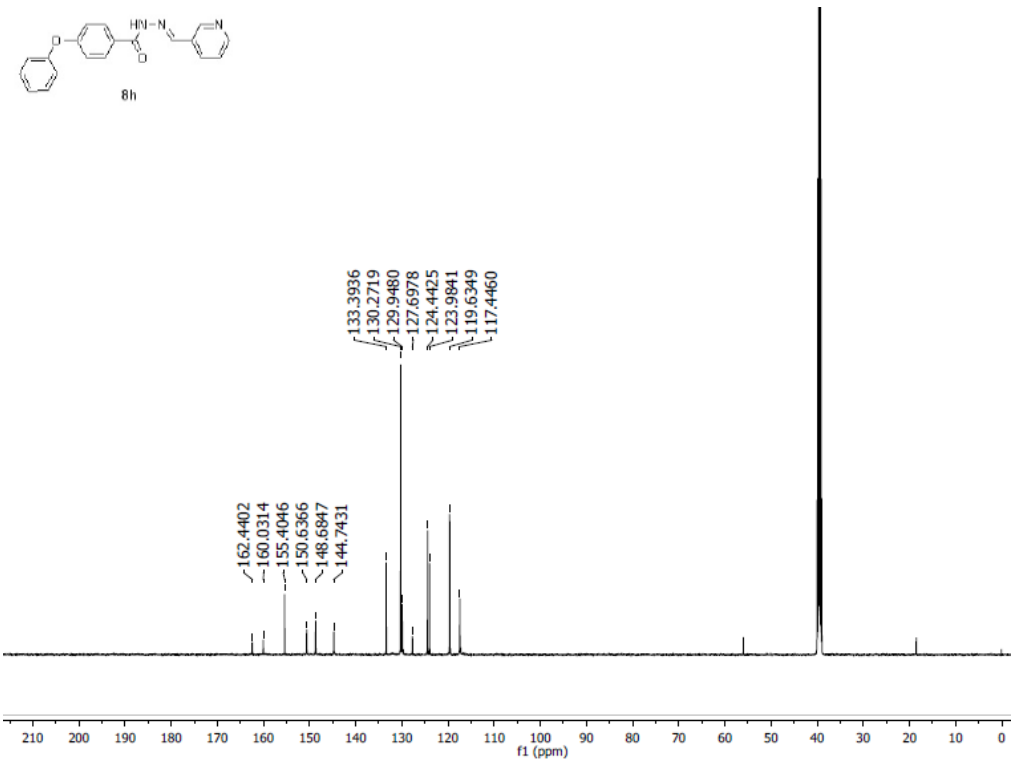
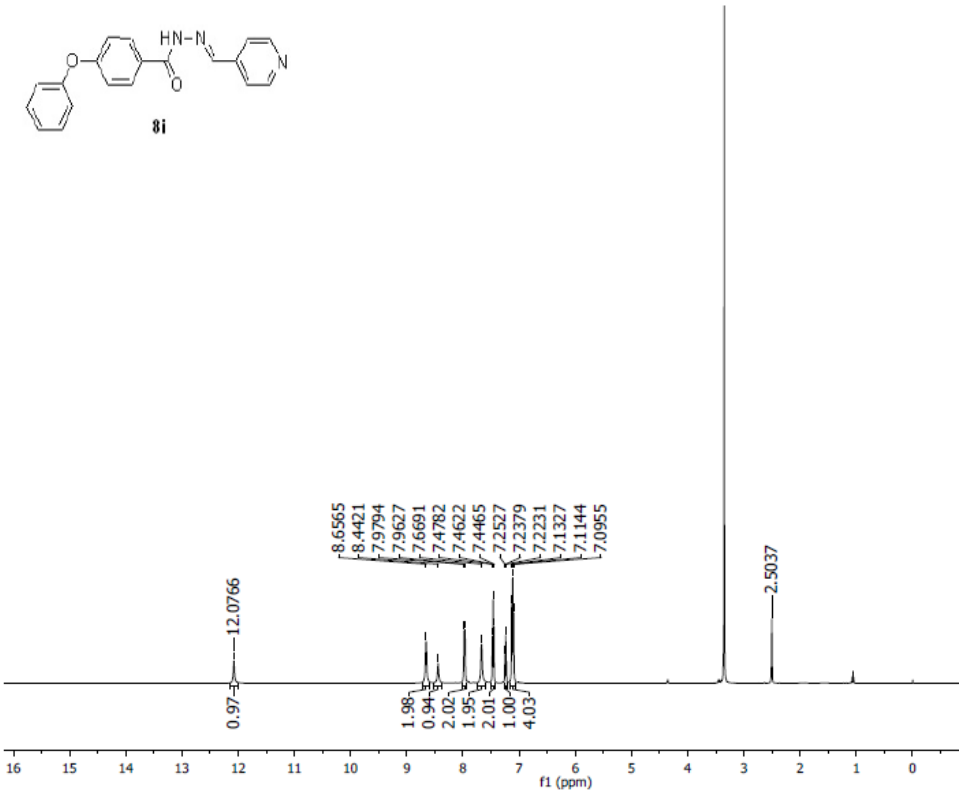
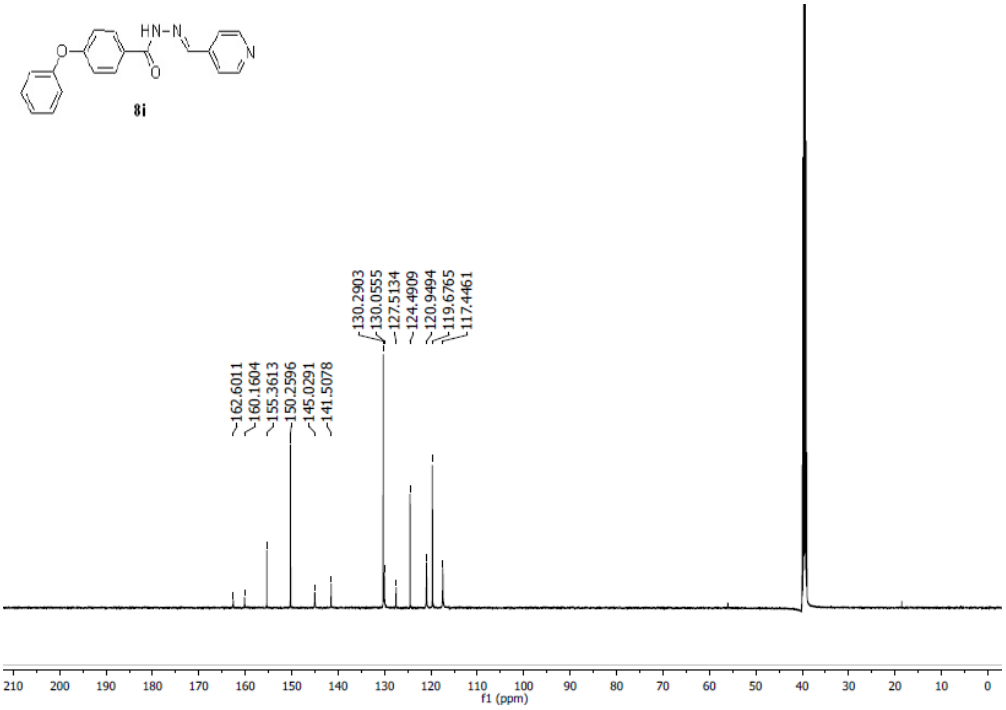


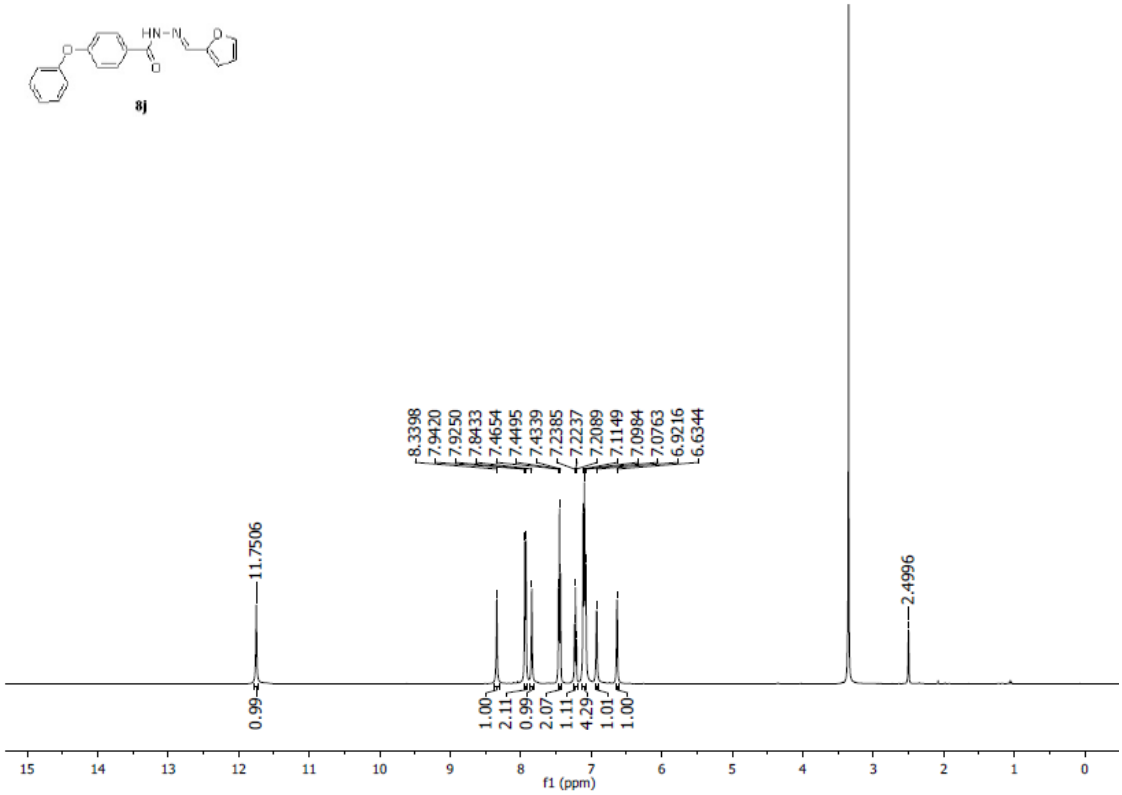
^{1}H NMR for compound 8i



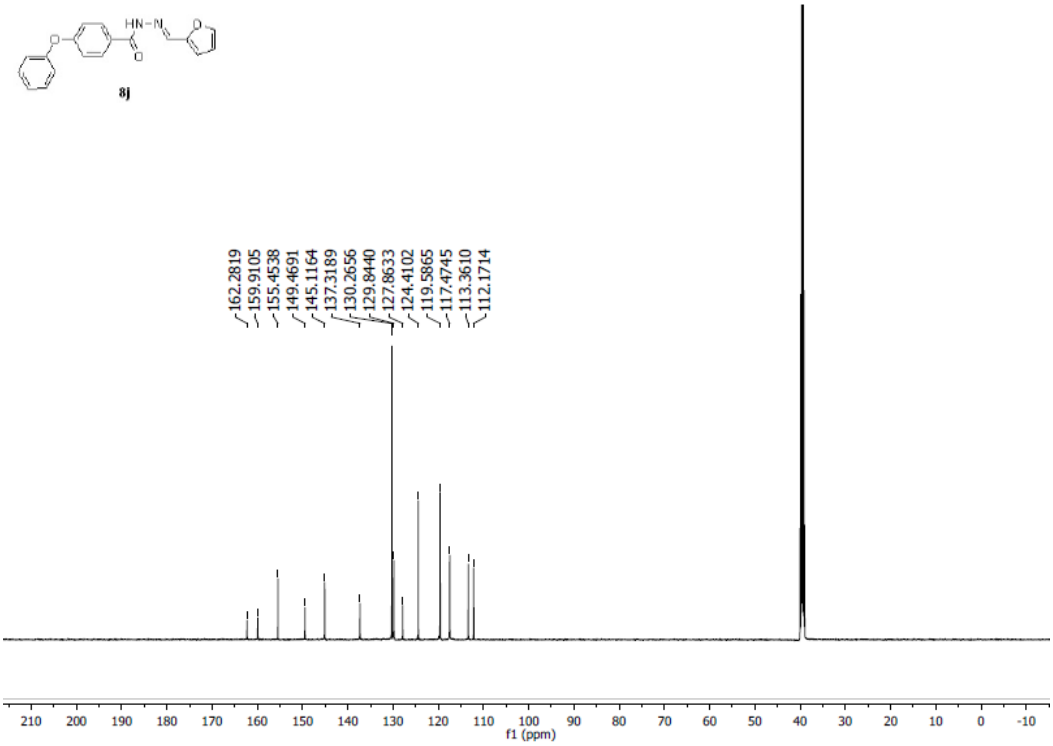
^{13}C NMR for compound 8i



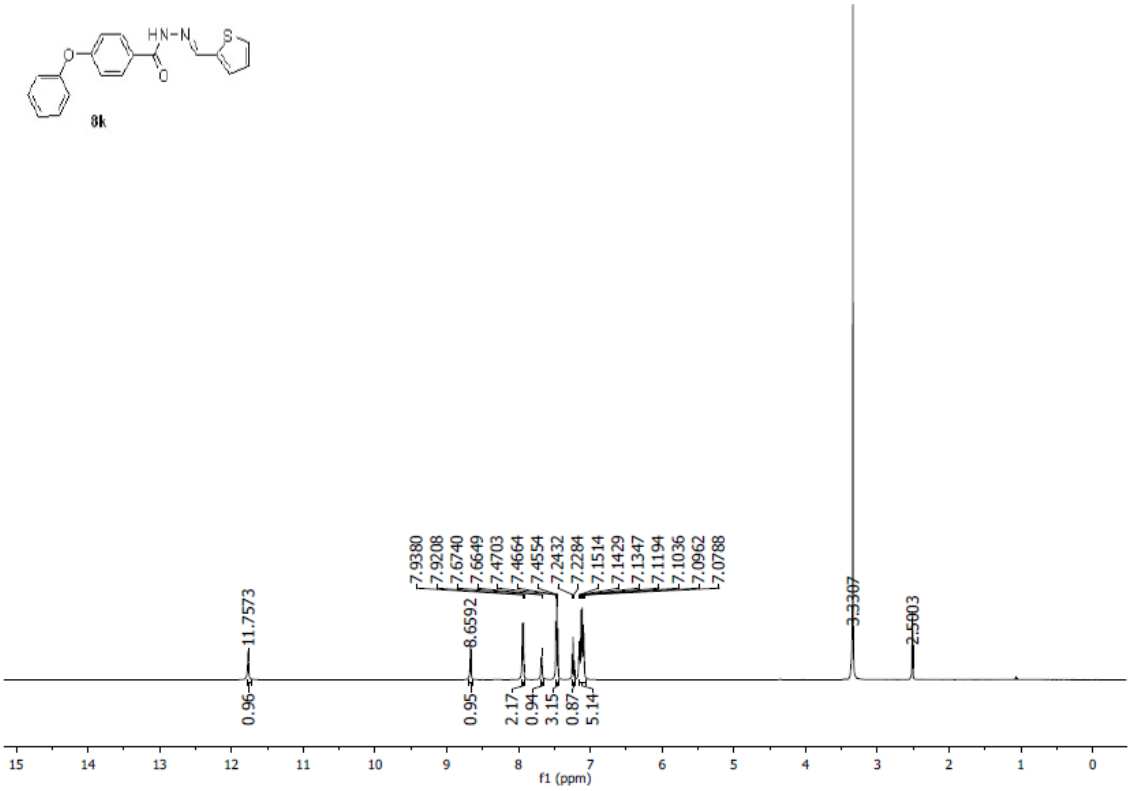
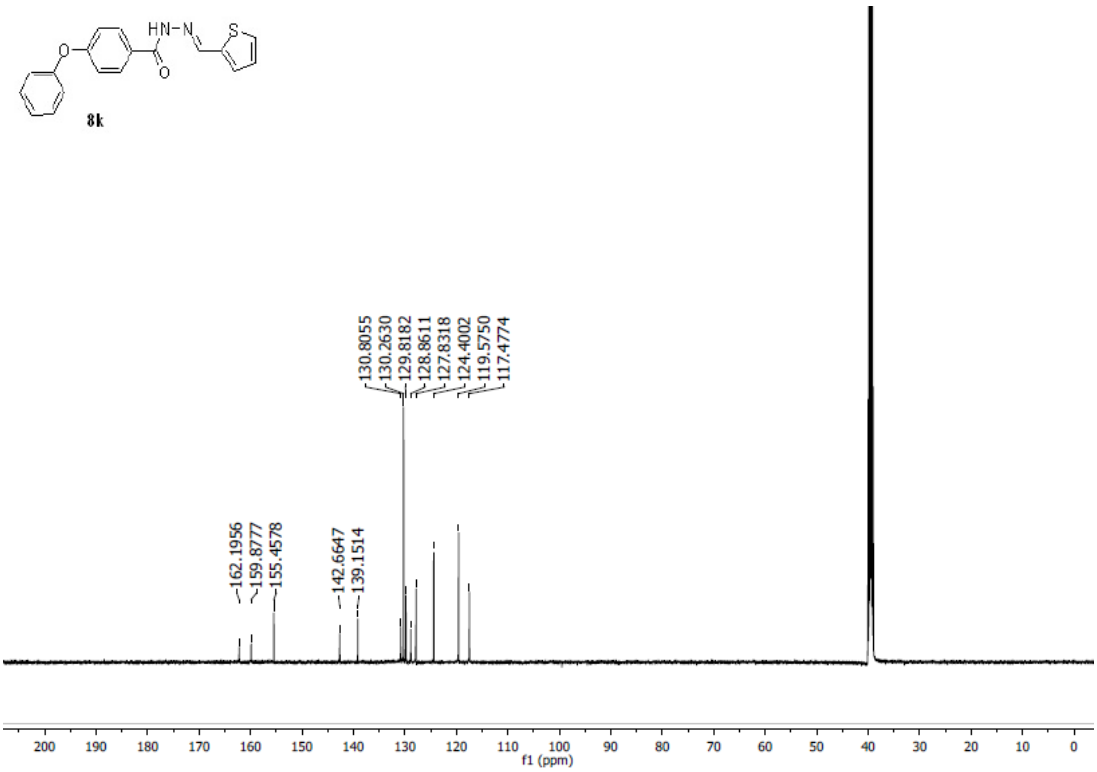
^{1}H NMR for compound 8j



^{13}C NMR for compound 8j



^{1}H NMR for compound 8k



^{13}C NMR for compound 8k