

Supporting Information

[3+2] Cycloaddition of Tosylmethyl Isocyanide with Styrylisoxazoles: Facile Access to Polysubstituted 3-(Isoxazol-5-yl)pyrroles

Xueming Zhang¹, Xianxiu Xu² and Dawei Zhang^{1,*}

¹ College of Chemistry, Jilin University, Changchun 130012, China;

² College of Chemistry, Chemical Engineering and Materials Science, Key Laboratory of
Molecular and Nano Probes, Ministry of Education, Shandong Normal University, Jinan
250014, China;

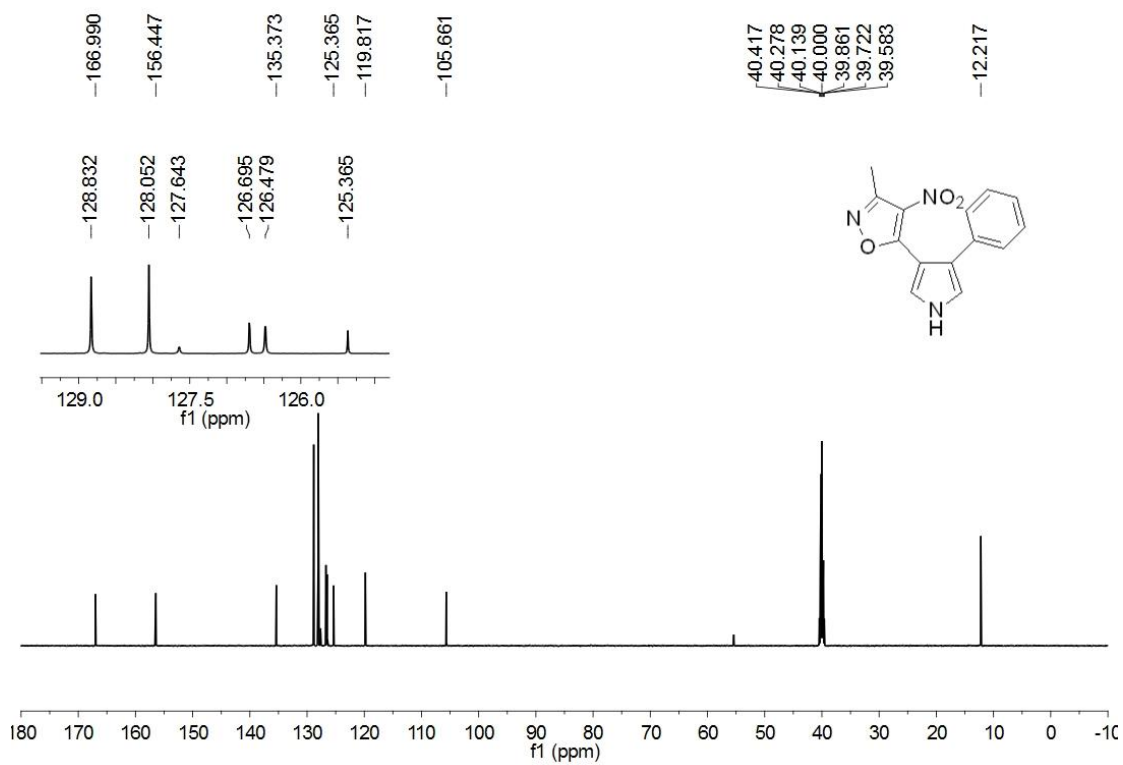
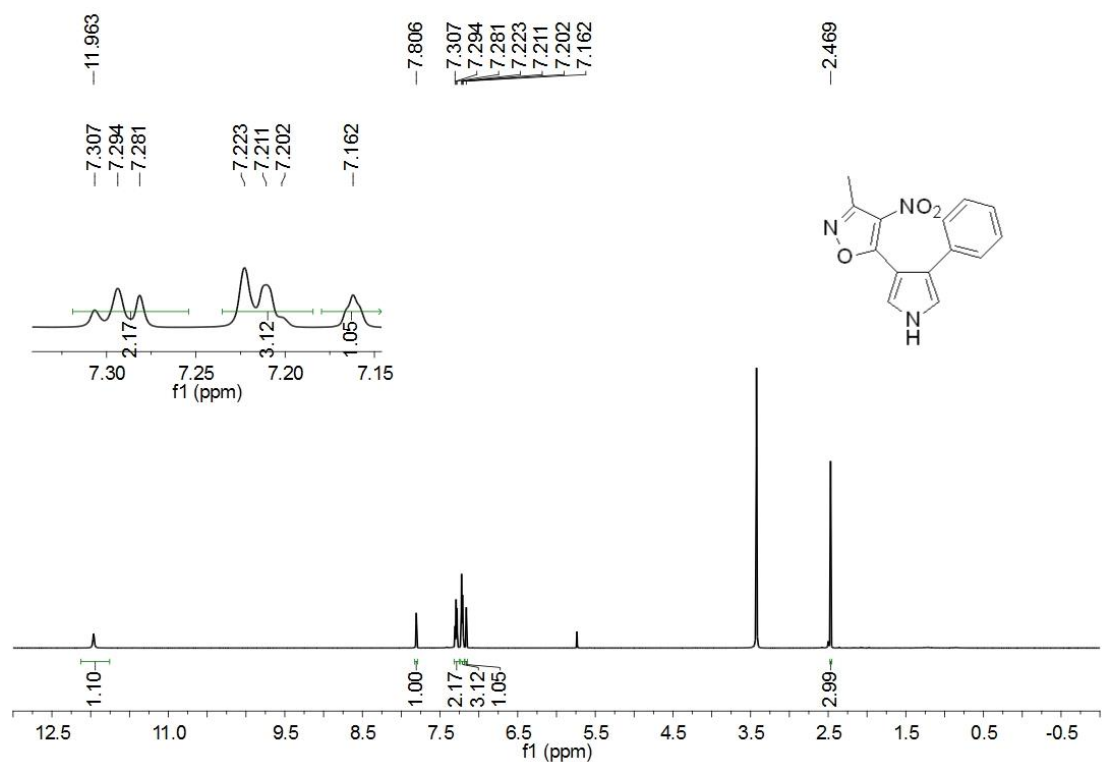
* Correspondence: z_dw@jlu.edu.cn; Tel.: +86-431-878-36471

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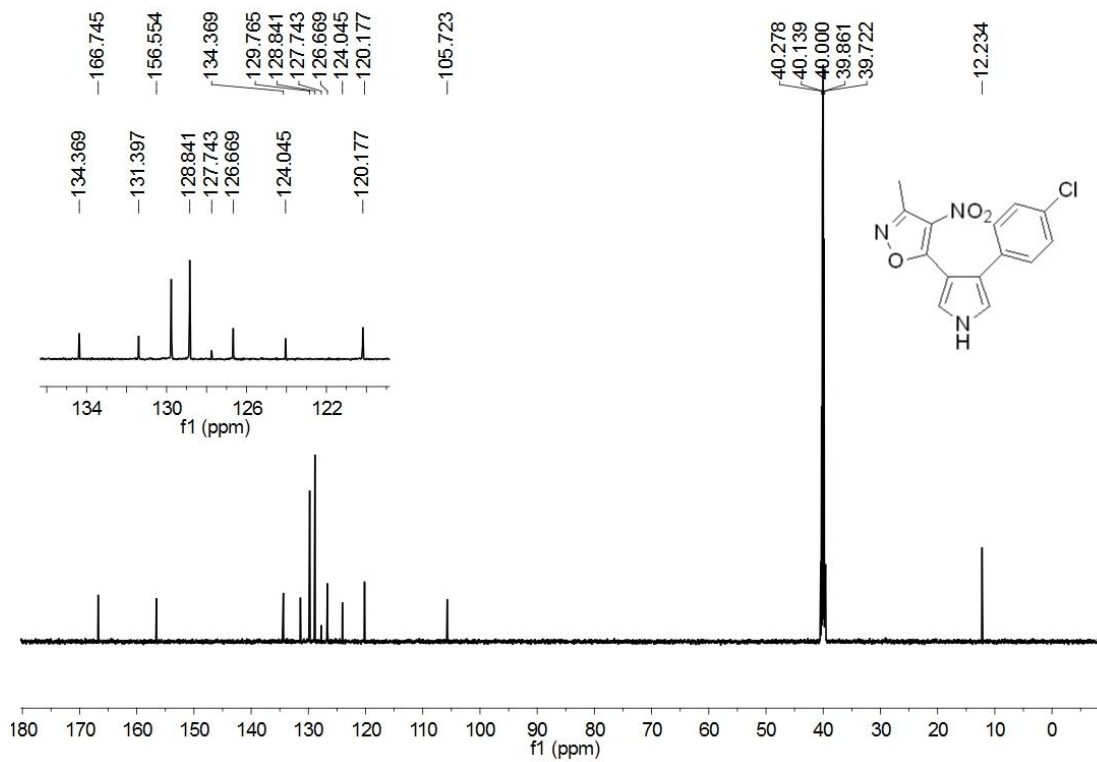
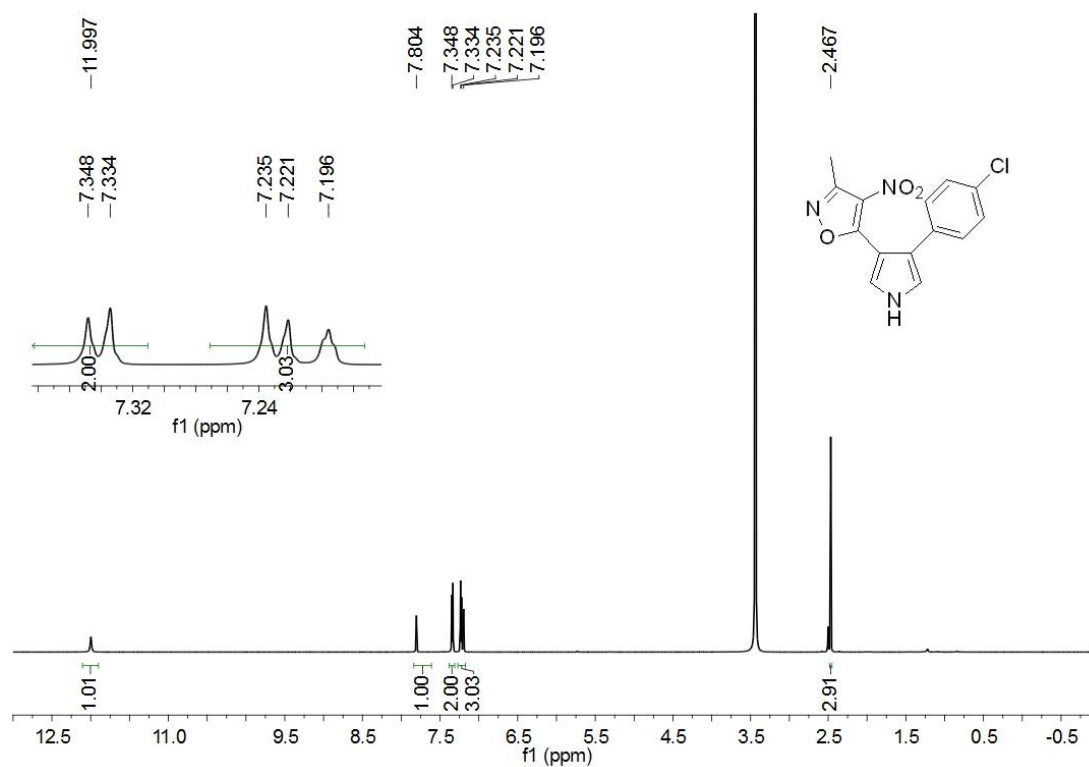
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I. Copies of ^1H NMR and ^{13}C NMR spectra of compounds **3aa-3fb**

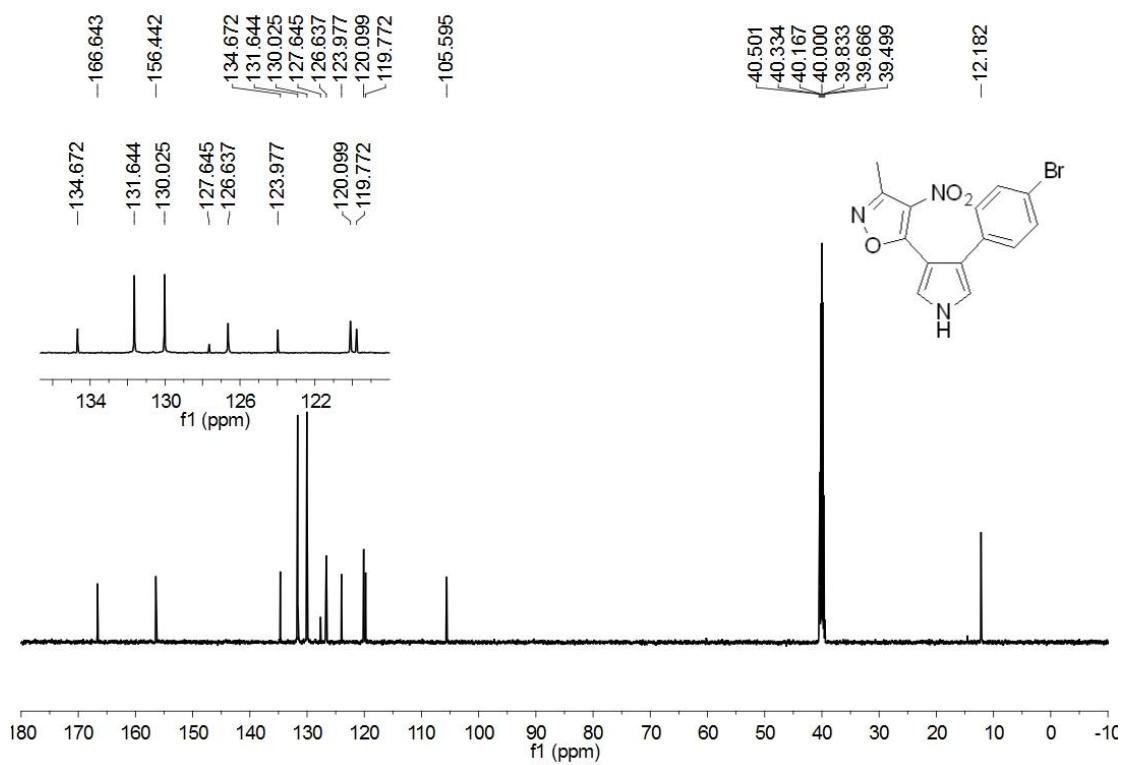
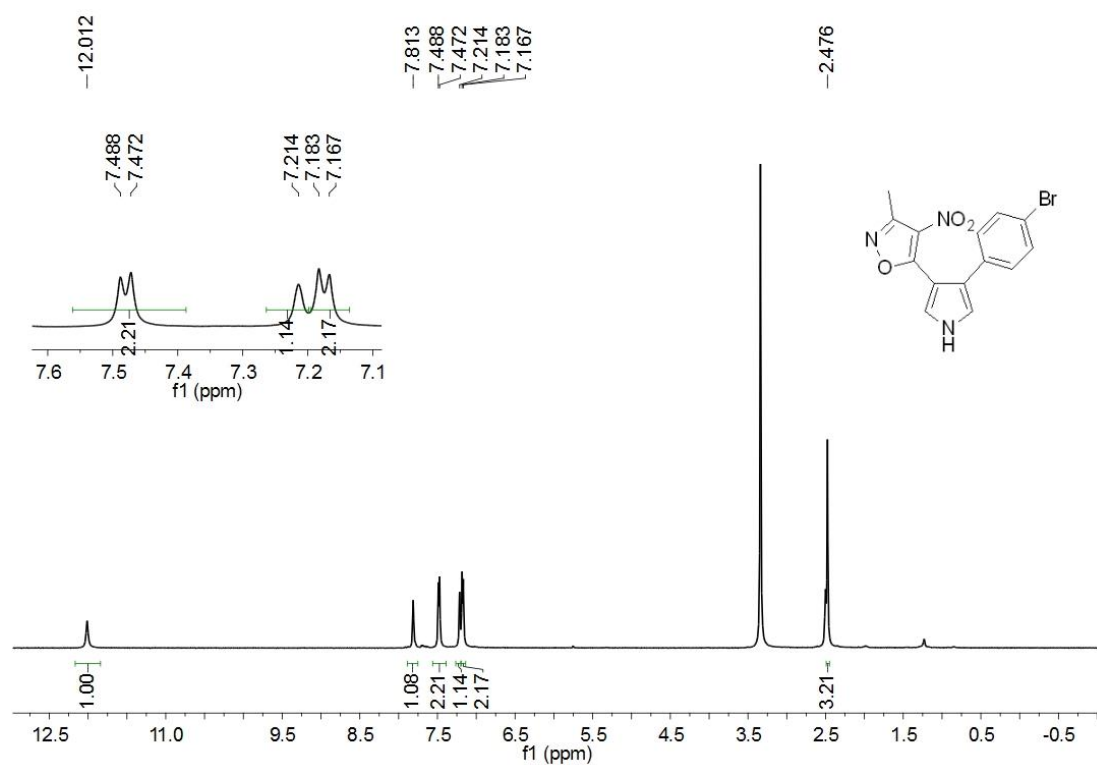
^1H NMR and ^{13}C NMR of **3aa**



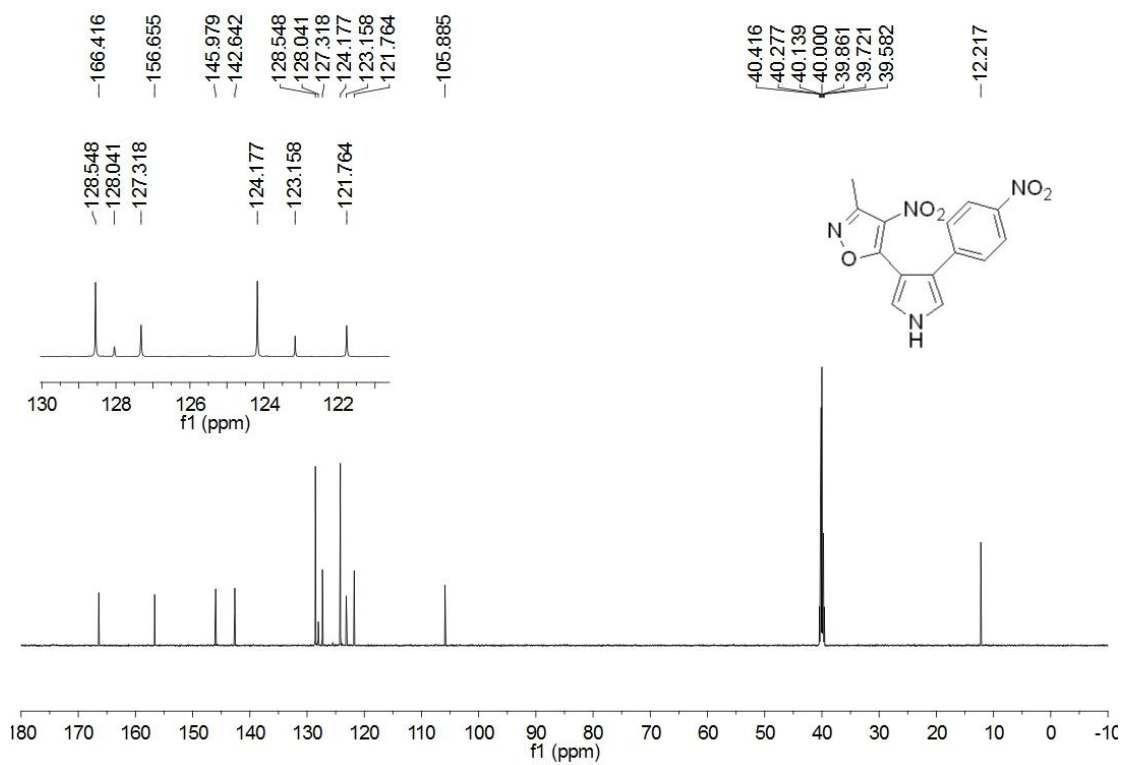
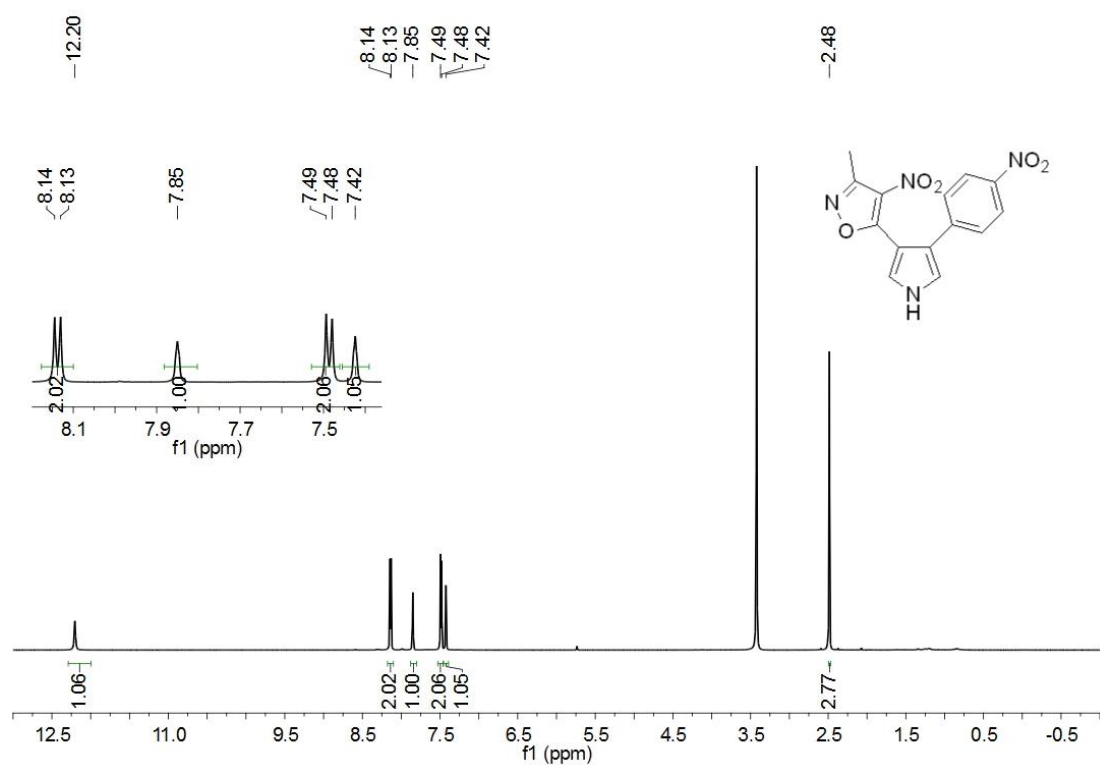
^1H NMR and ^{13}C NMR of **3ab**



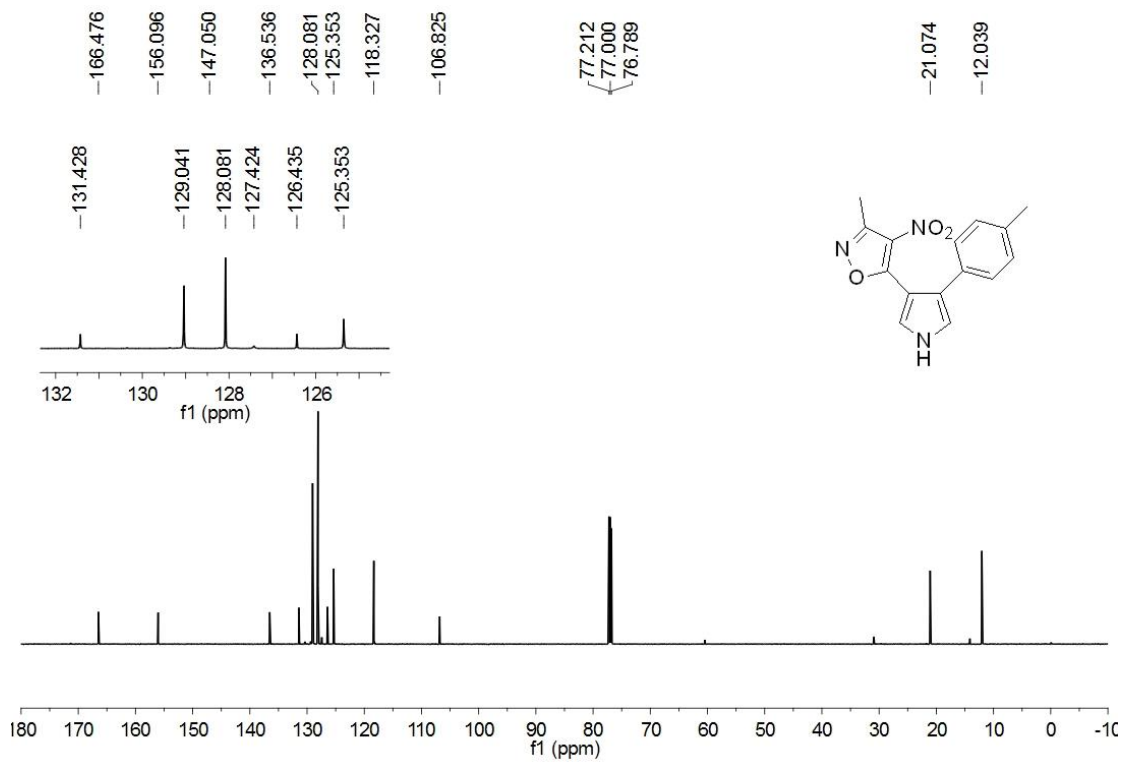
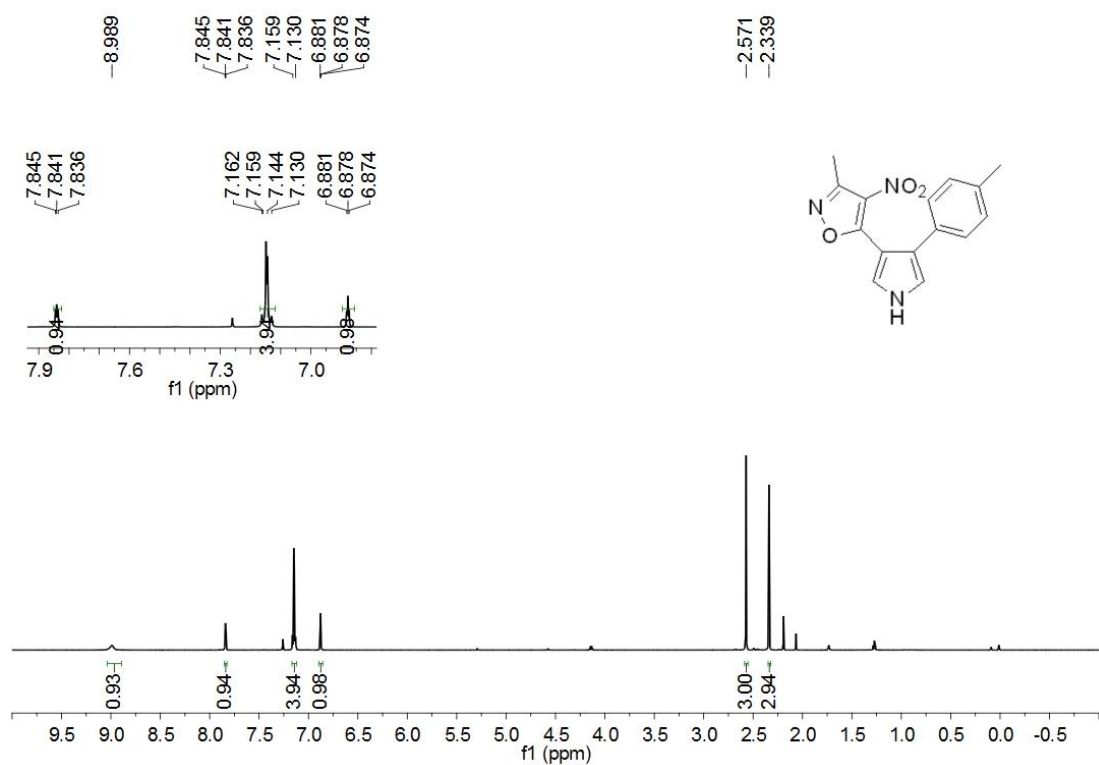
^1H NMR and ^{13}C NMR of **3ac**



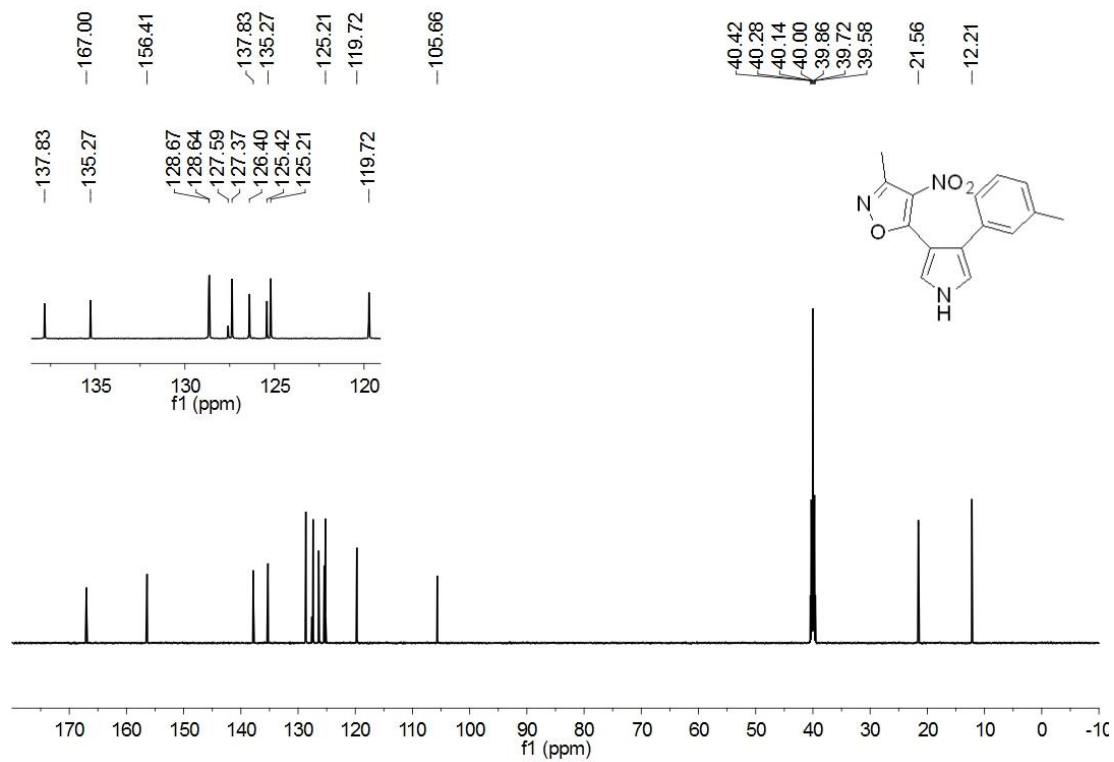
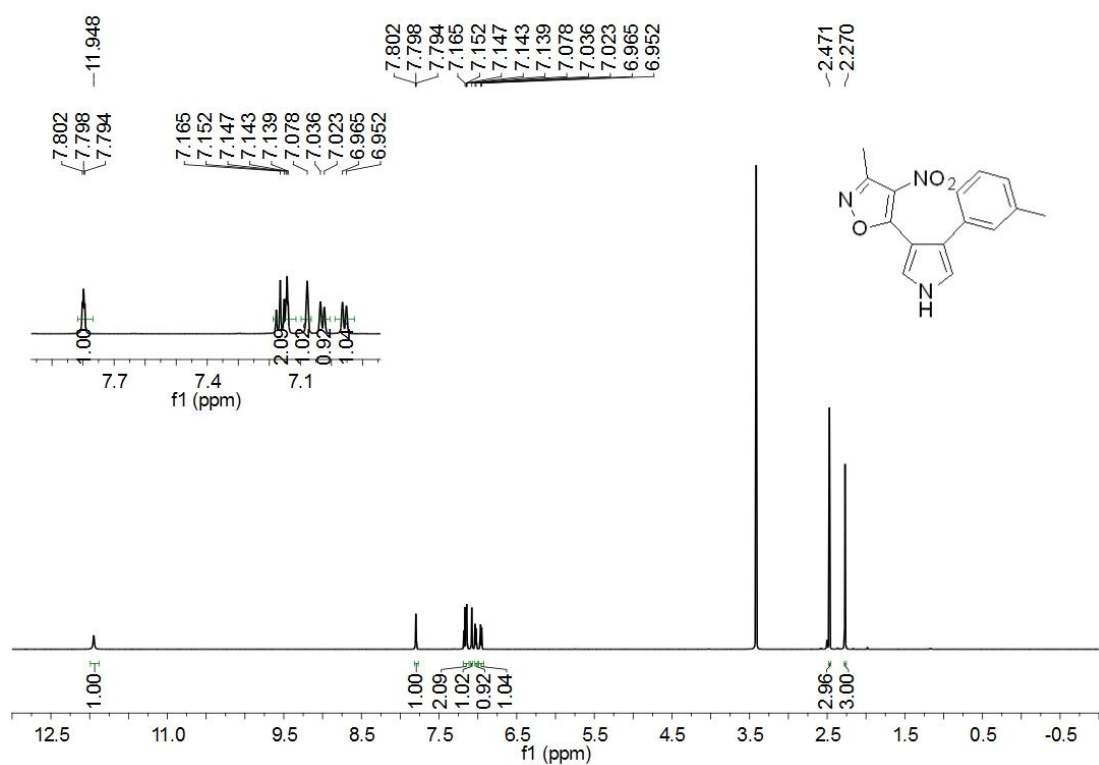
^1H NMR and ^{13}C NMR of **3ad**



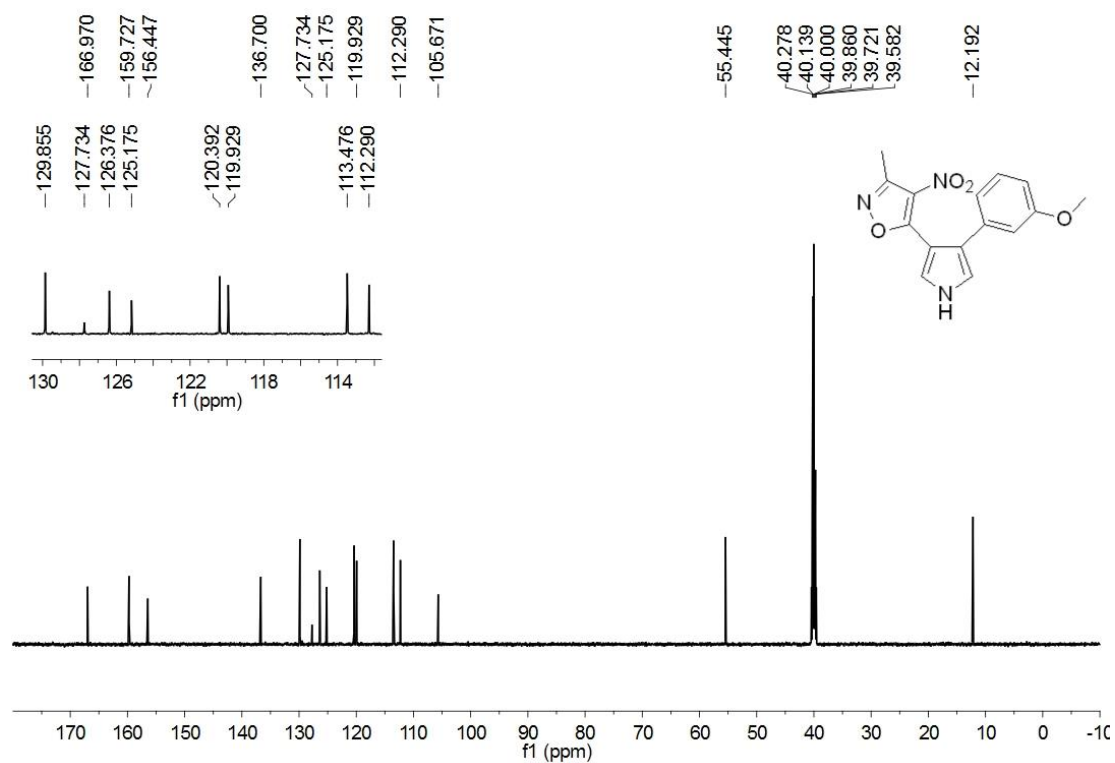
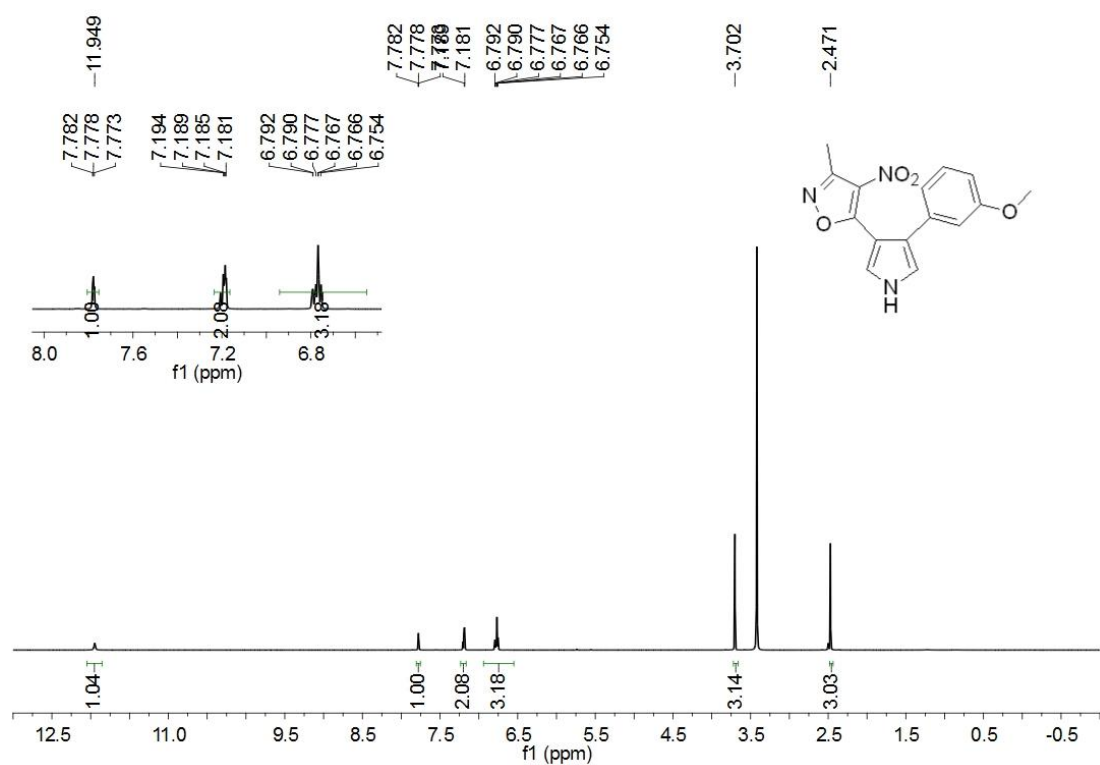
^1H NMR and ^{13}C NMR of **3ae**



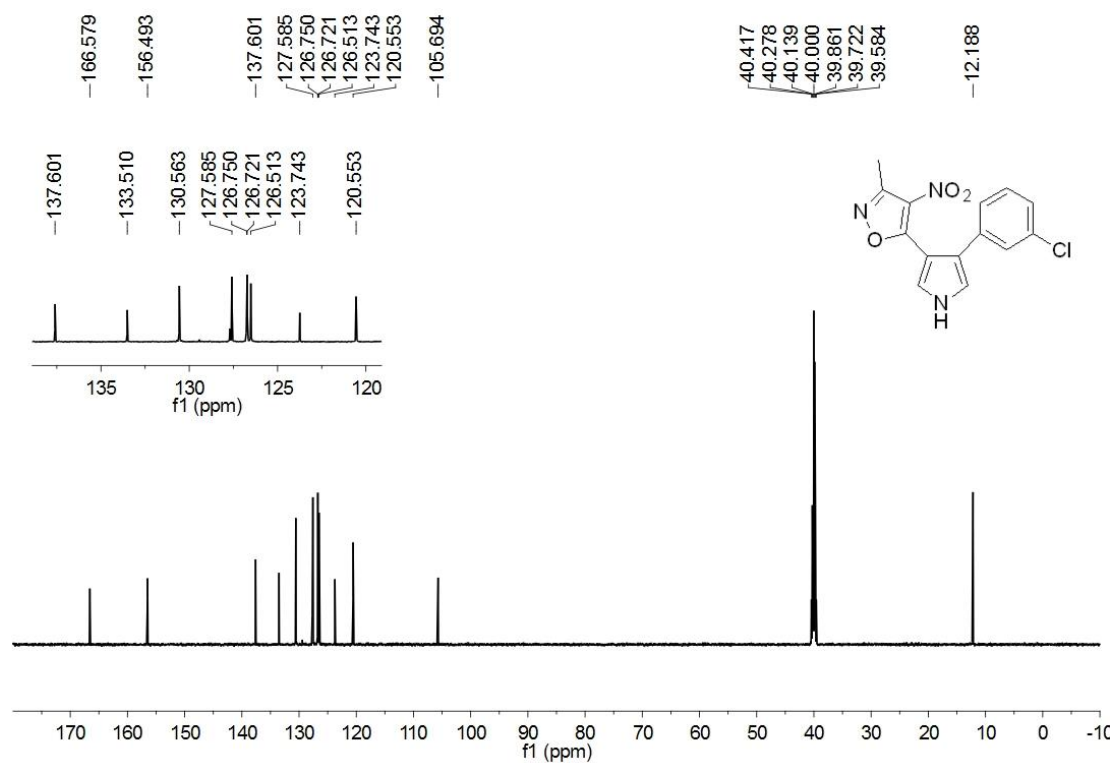
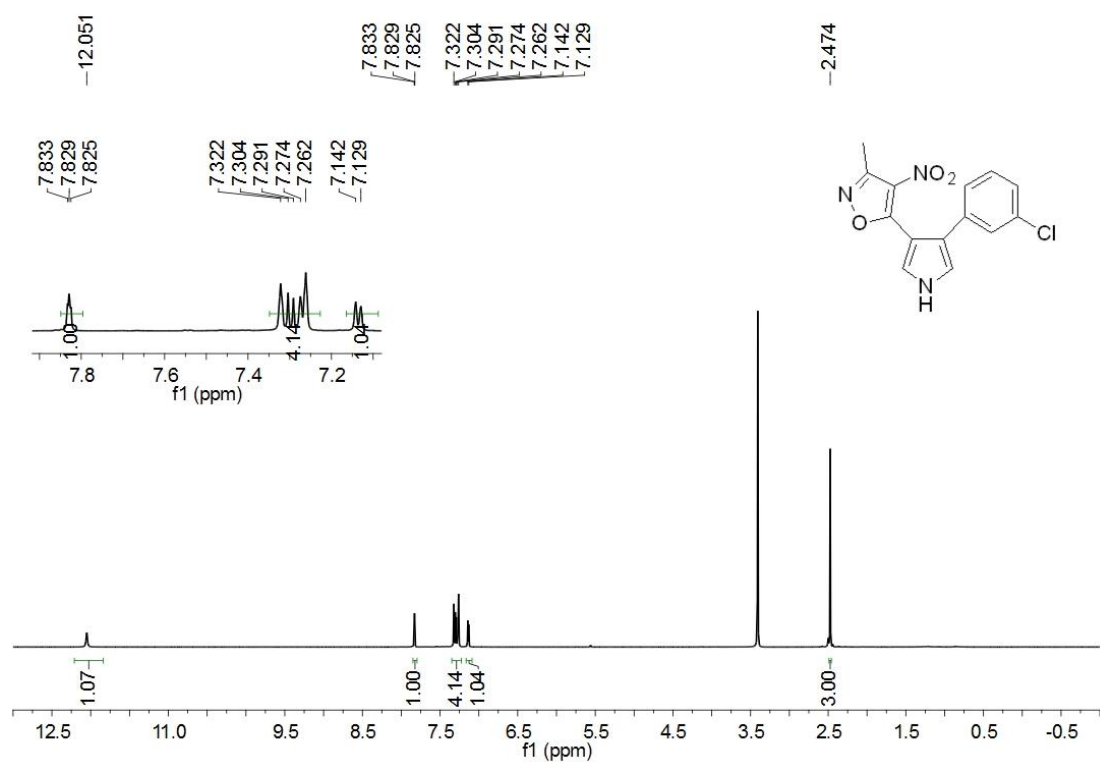
^1H NMR and ^{13}C NMR of **3af**



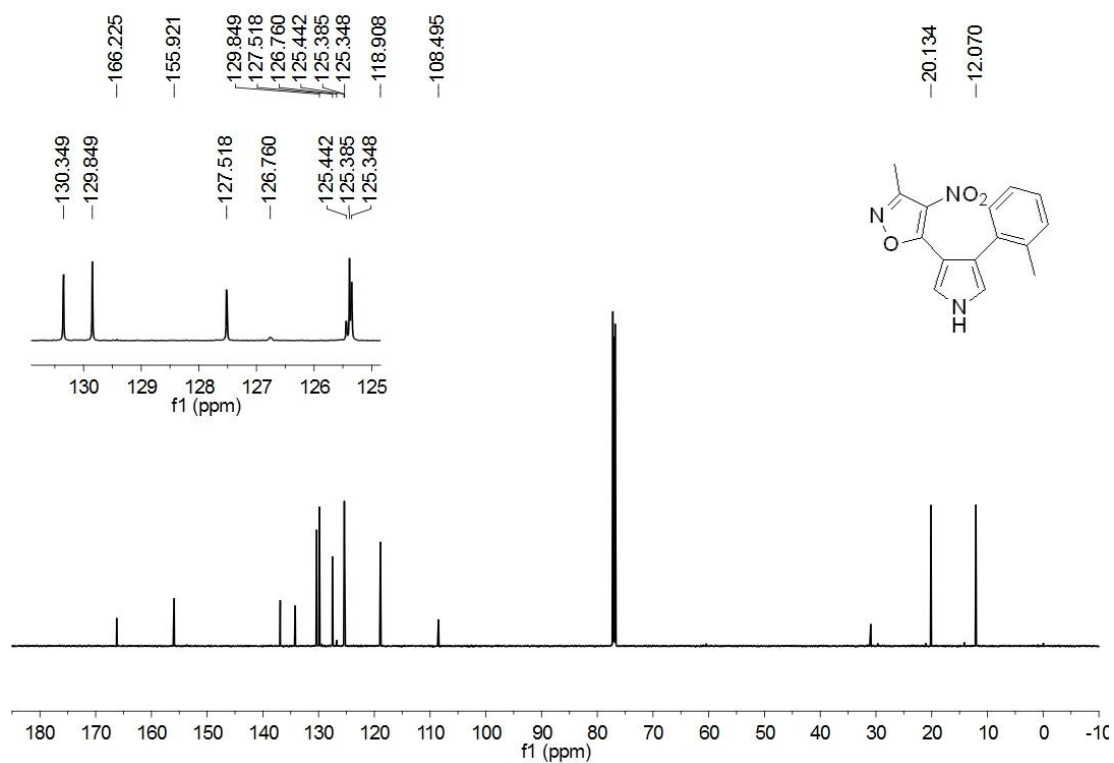
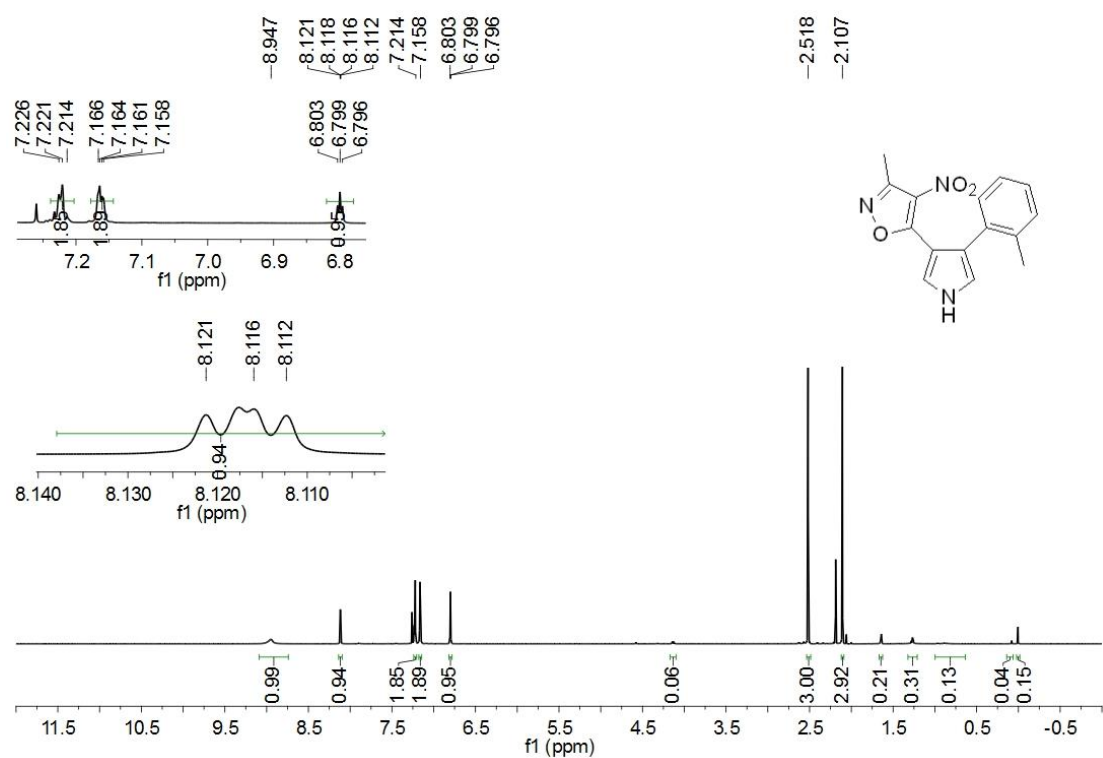
^1H NMR and ^{13}C NMR of **3ag**



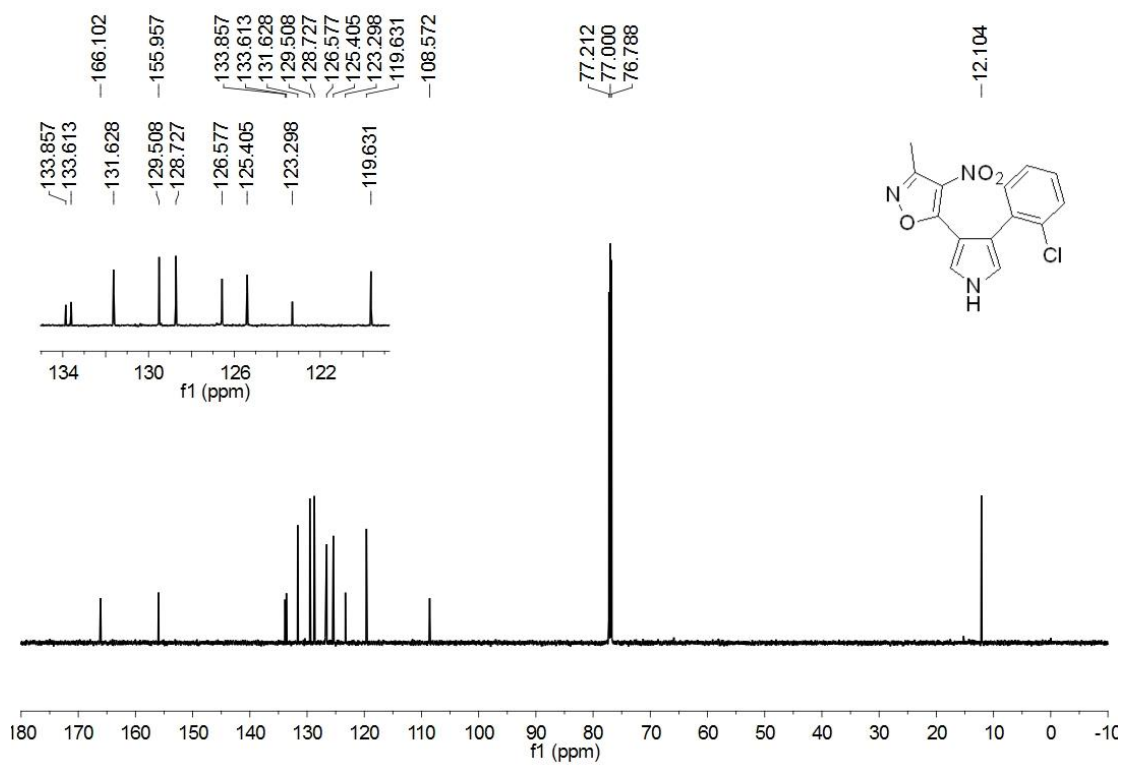
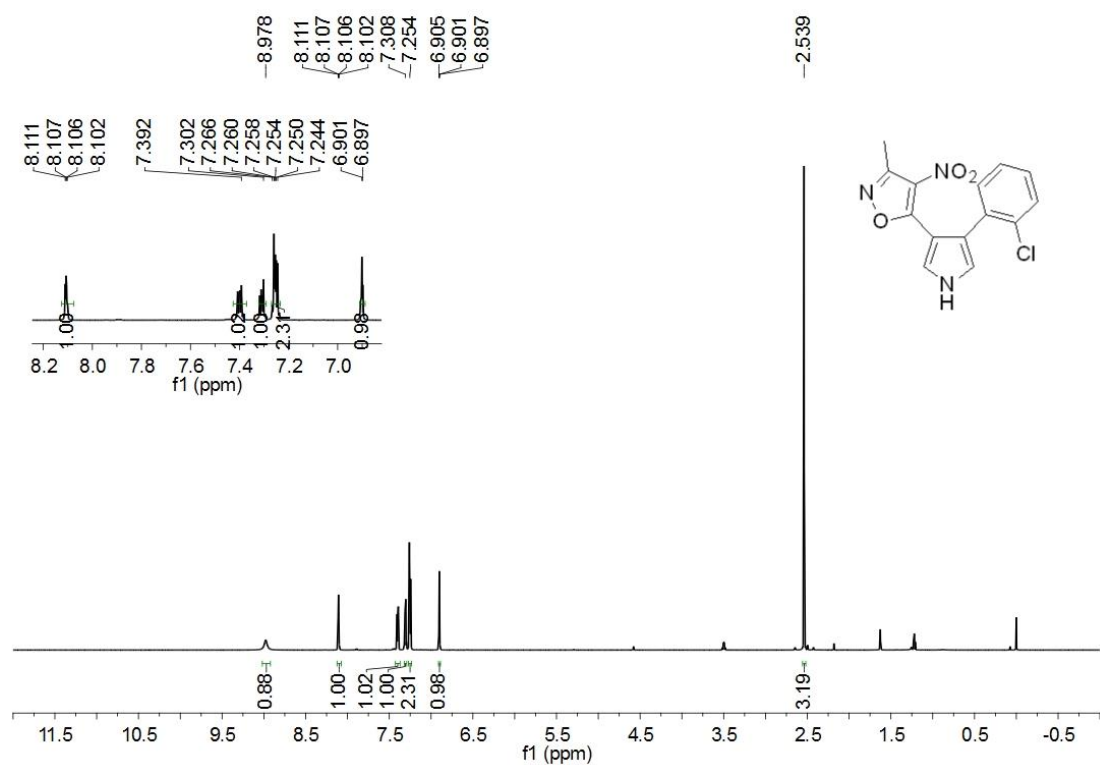
^1H NMR and ^{13}C NMR of **3ah**



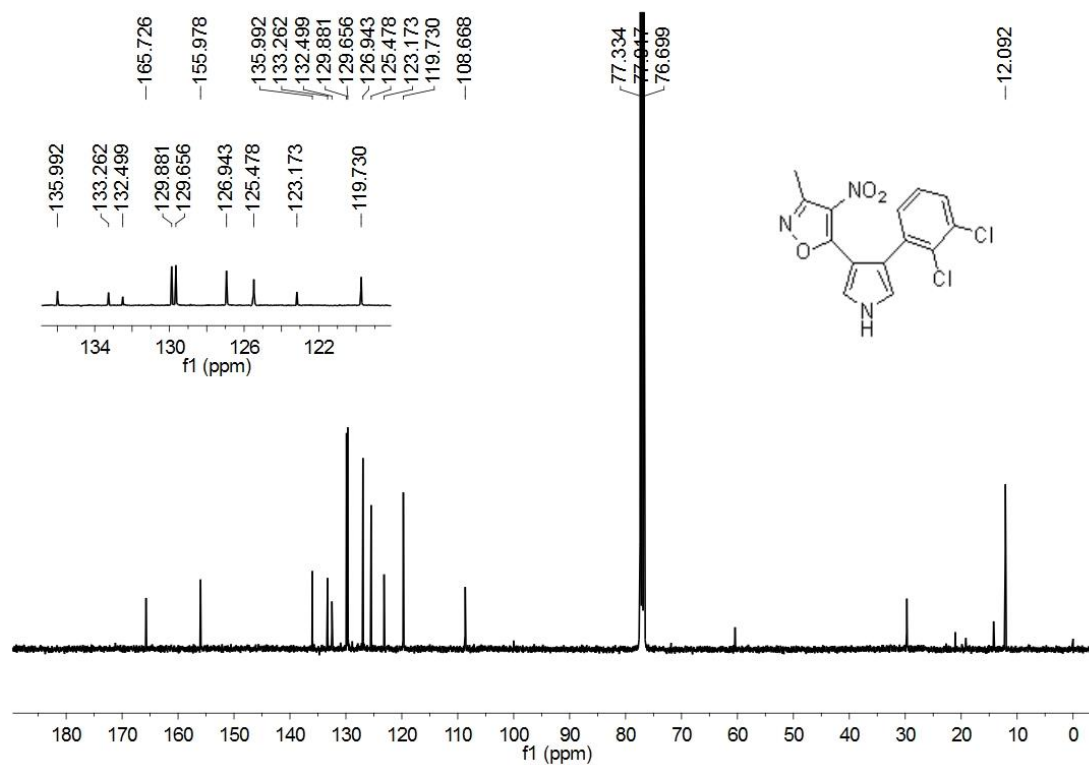
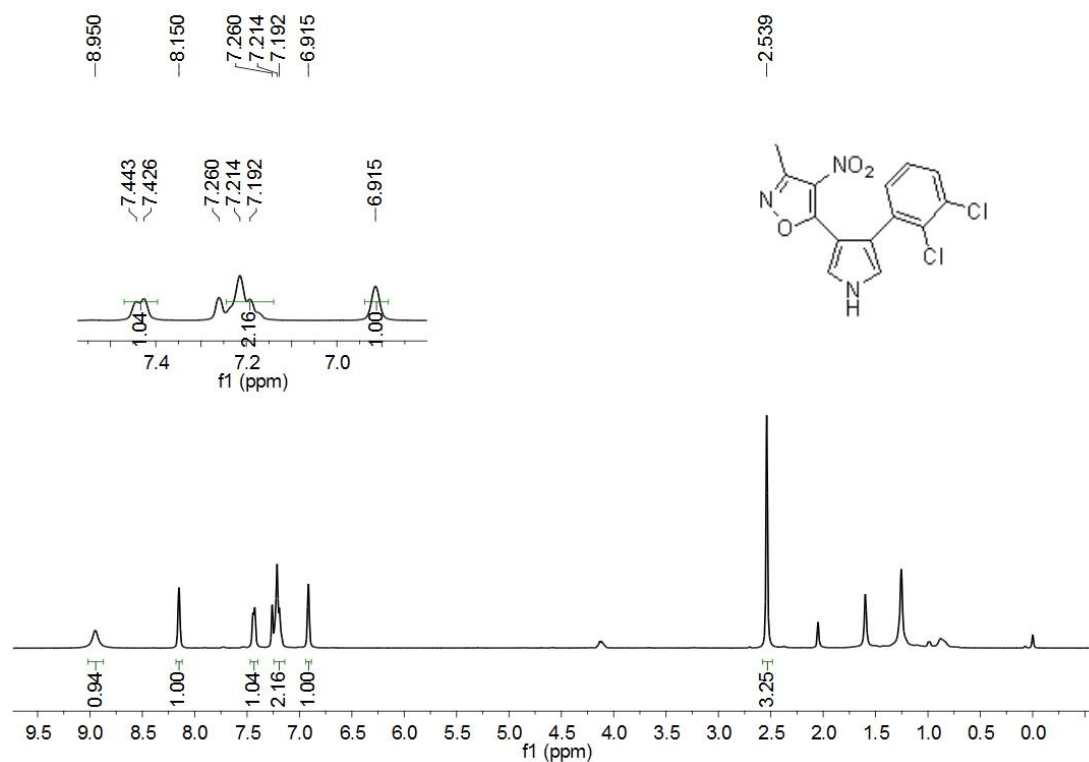
^1H NMR and ^{13}C NMR of **3ai**



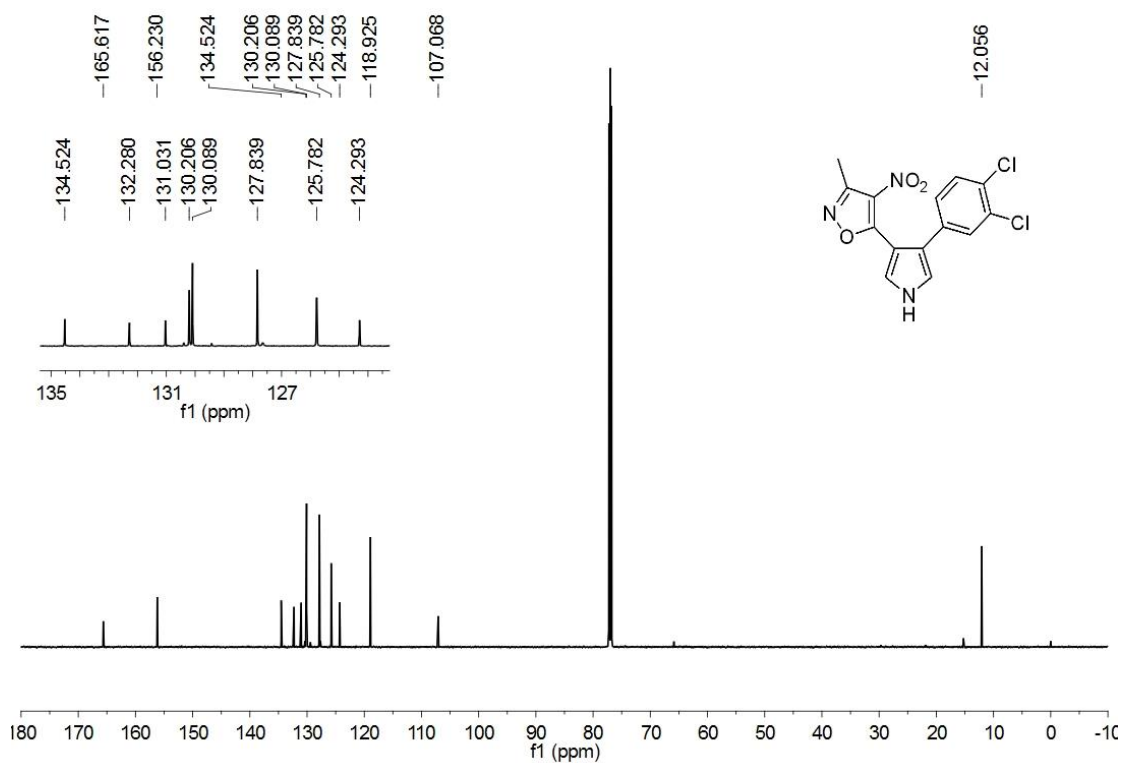
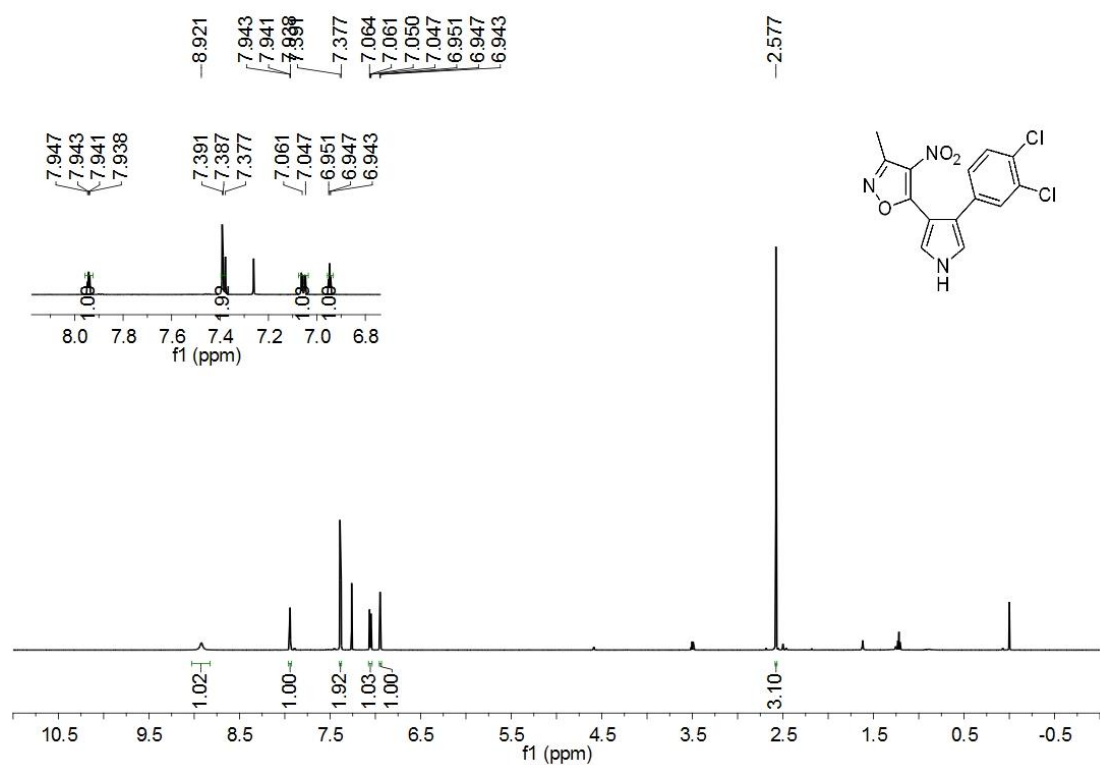
^1H NMR and ^{13}C NMR of **3aj**



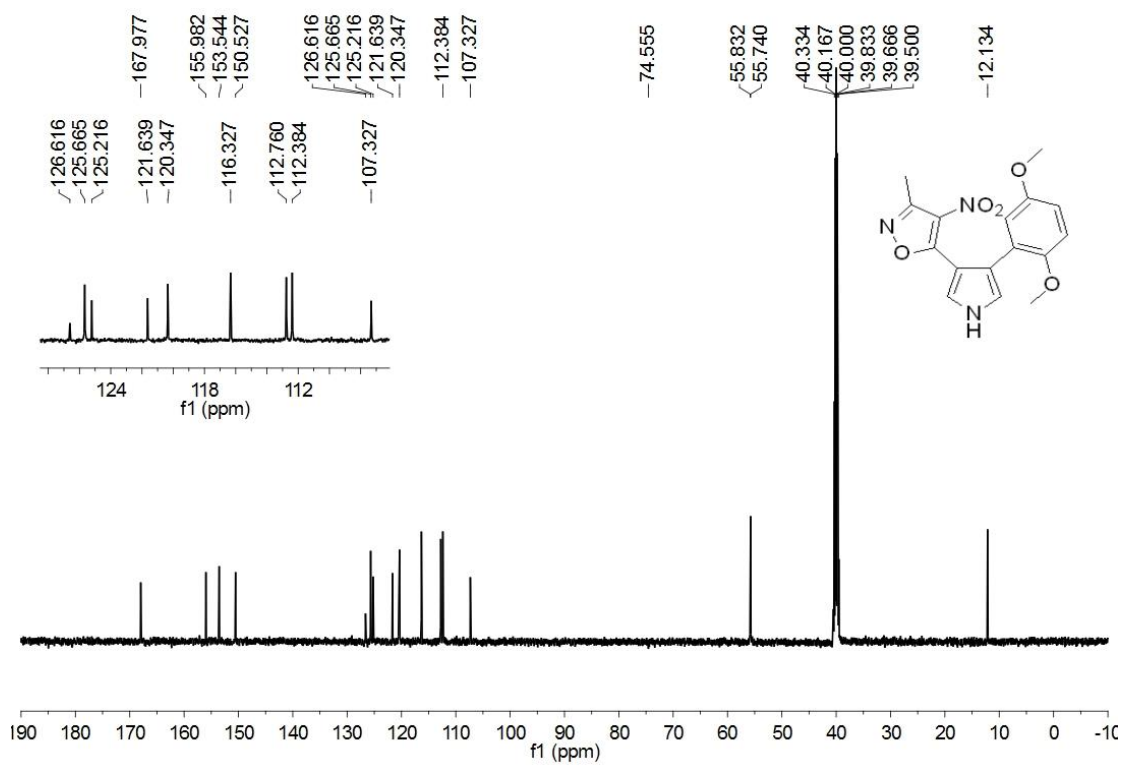
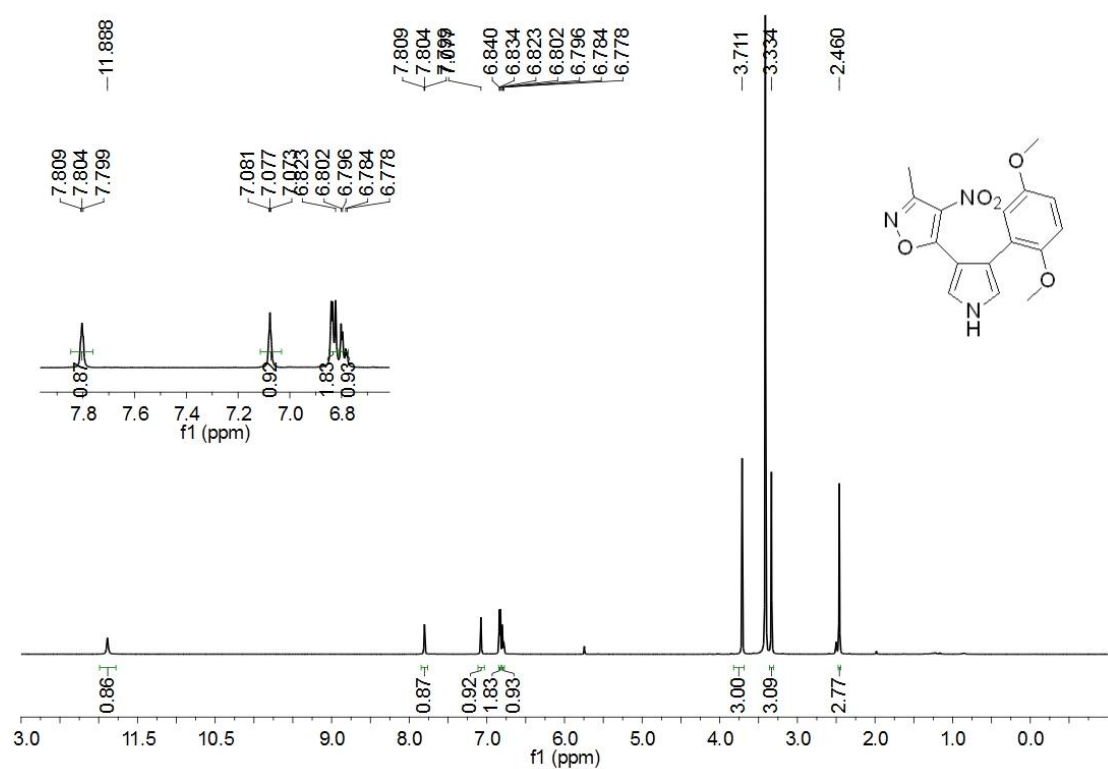
^1H NMR and ^{13}C NMR of **3ak**



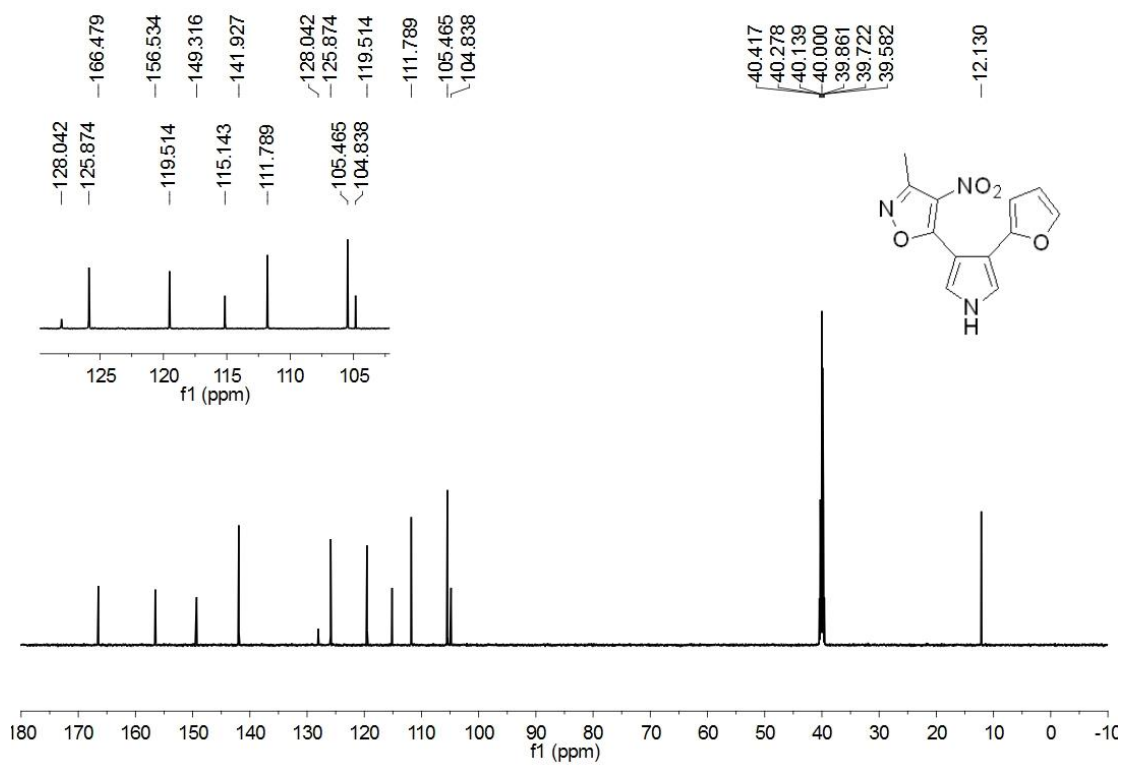
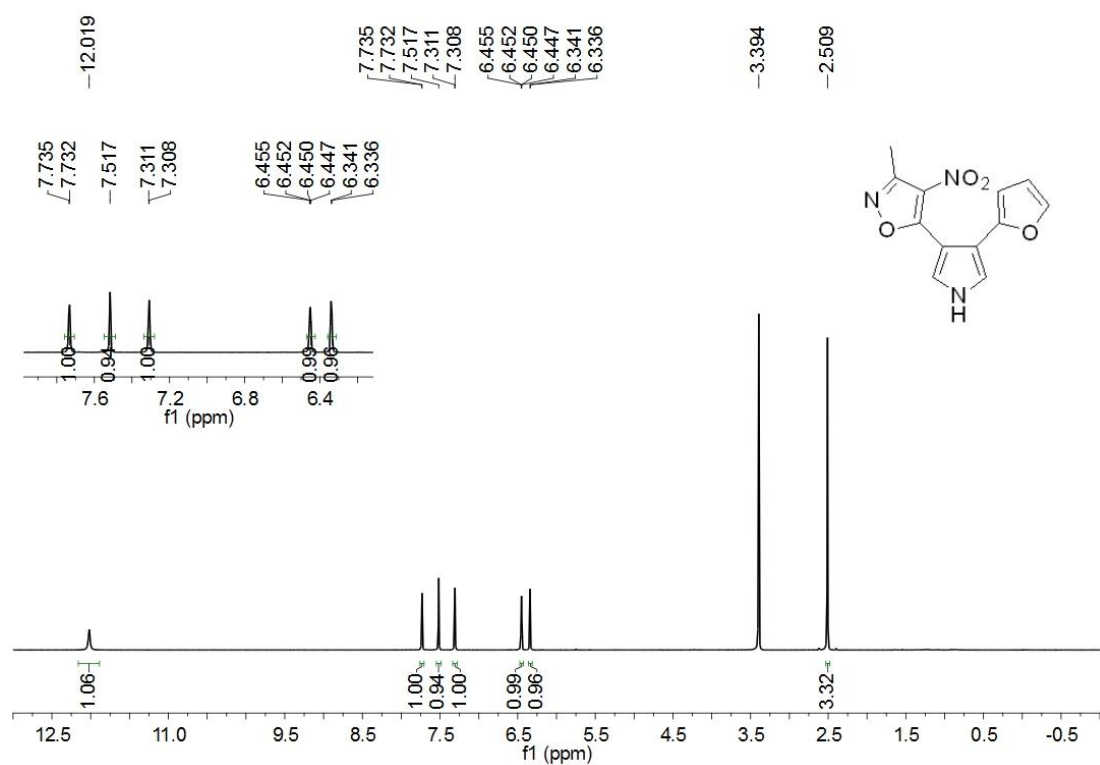
^1H NMR and ^{13}C NMR of **3al**



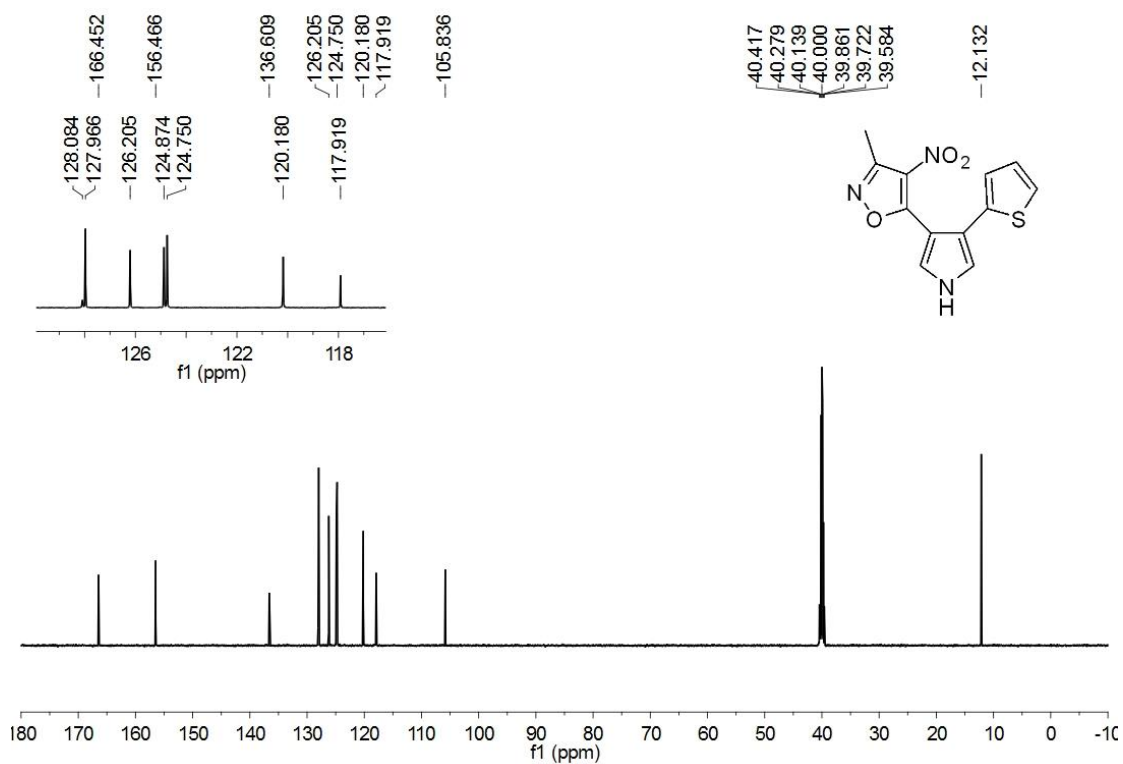
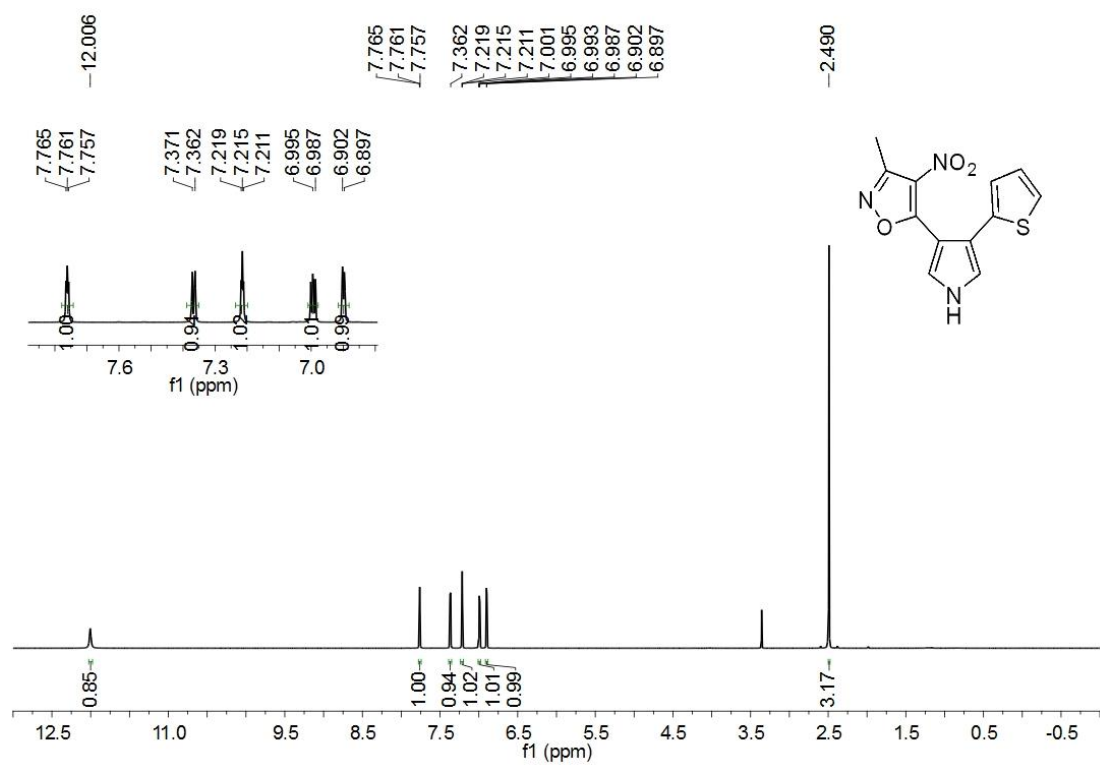
^1H NMR and ^{13}C NMR of **3am**



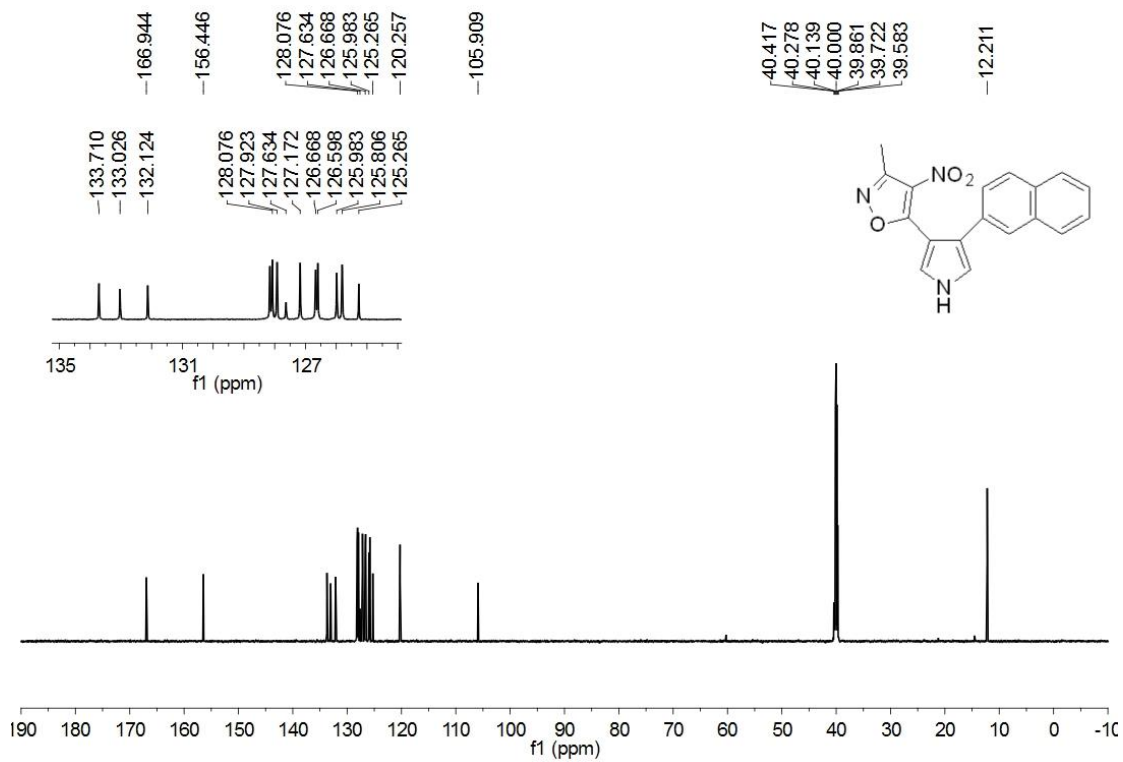
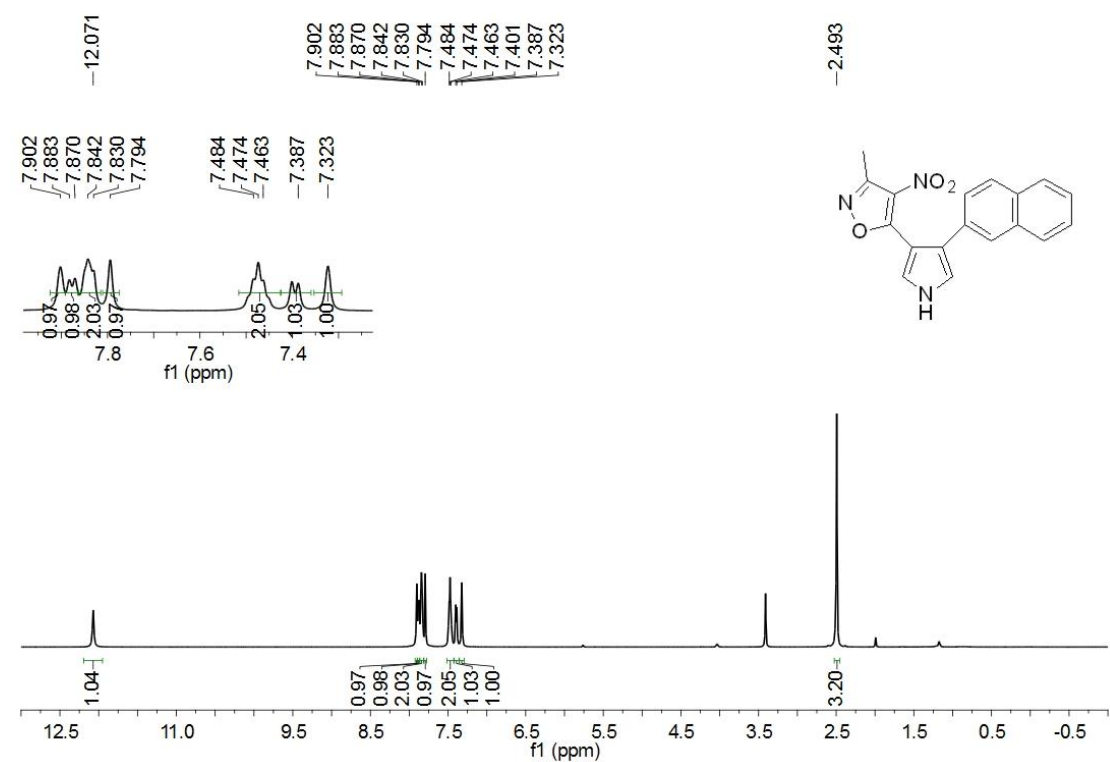
^1H NMR and ^{13}C NMR of **3an**



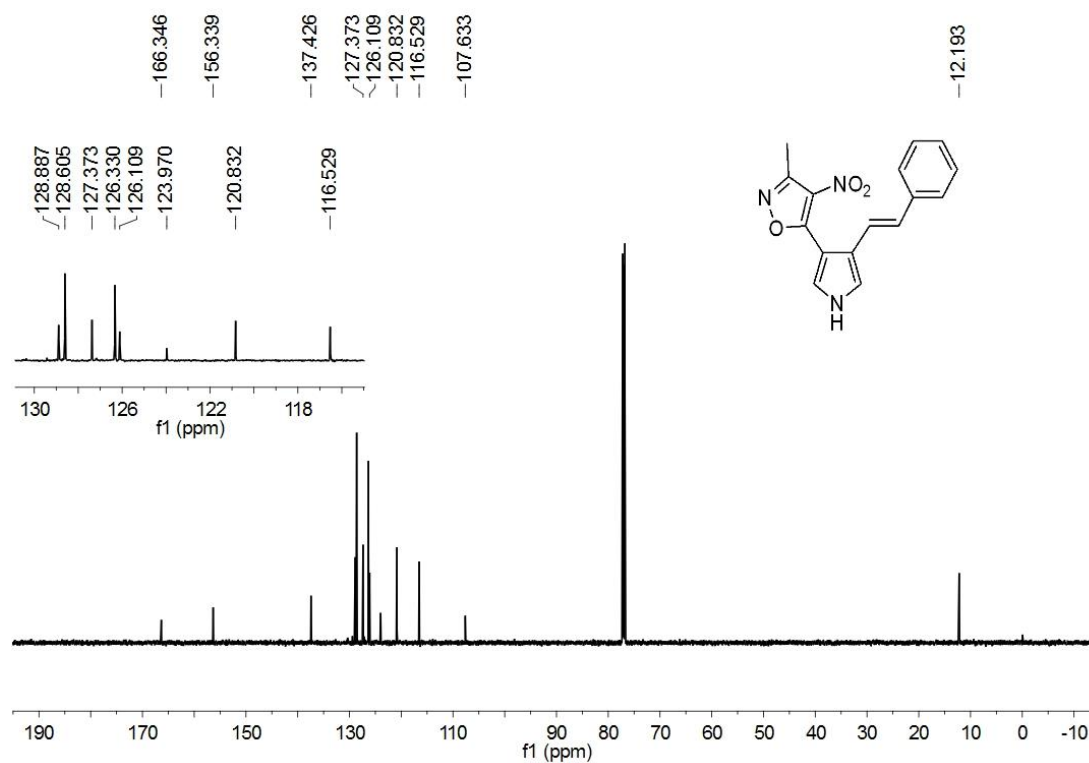
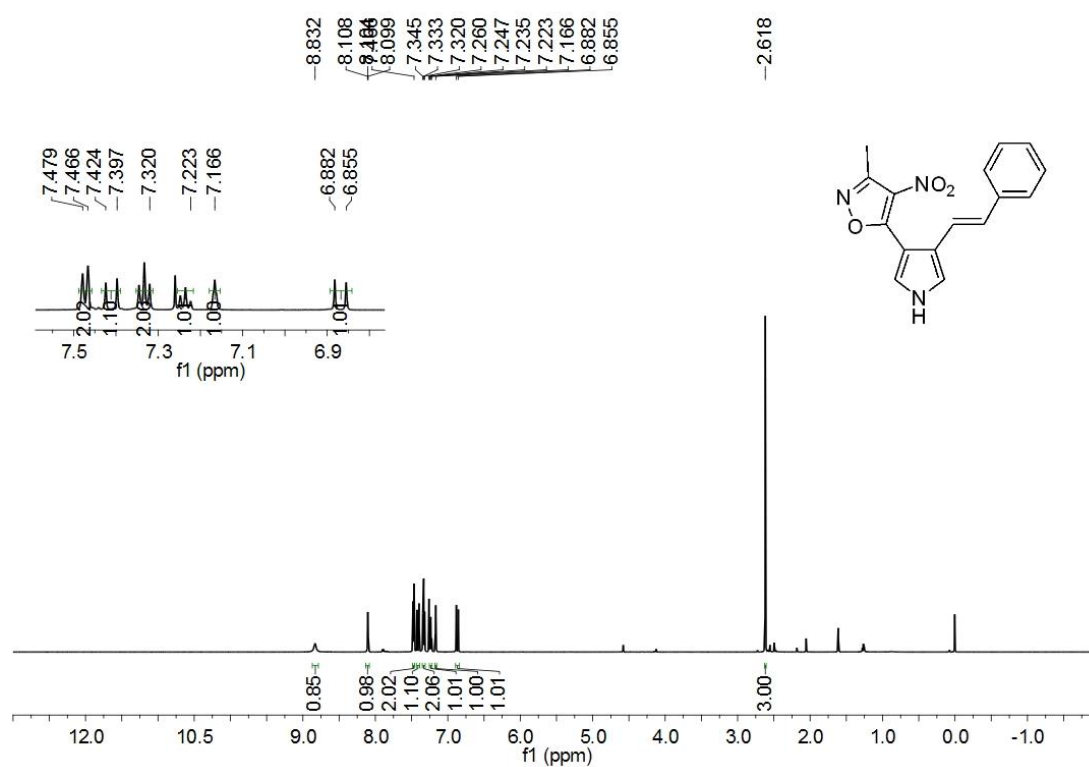
^1H NMR and ^{13}C NMR of **3ao**



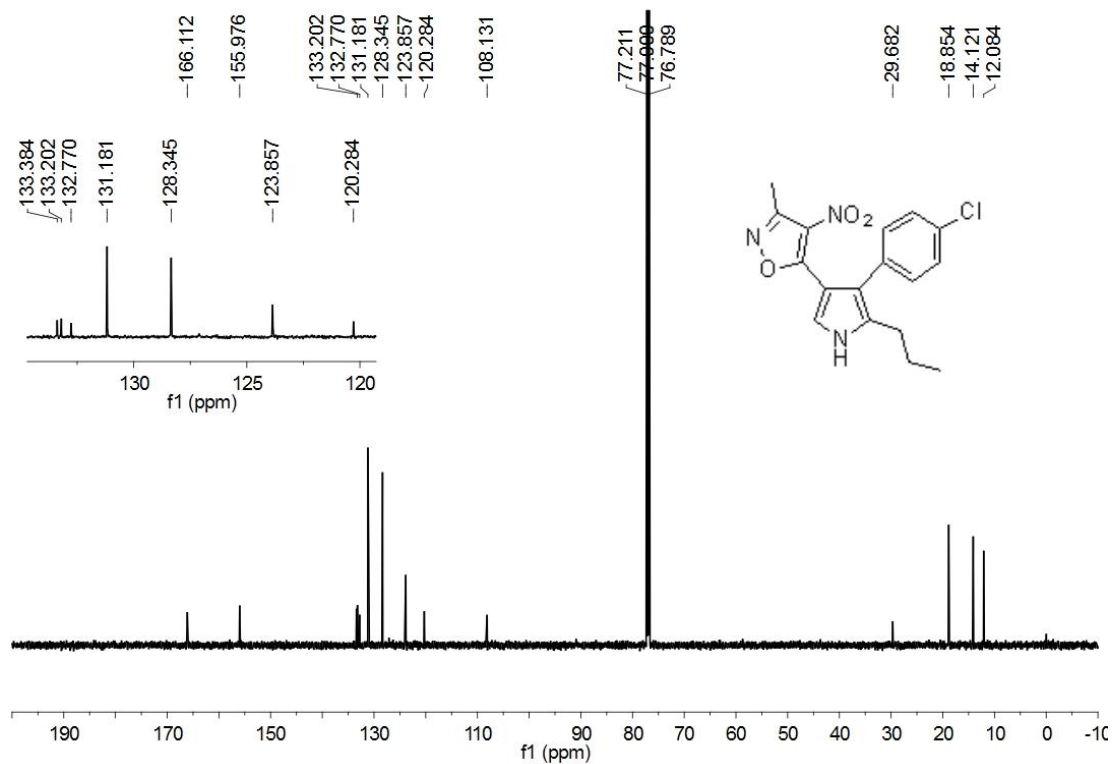
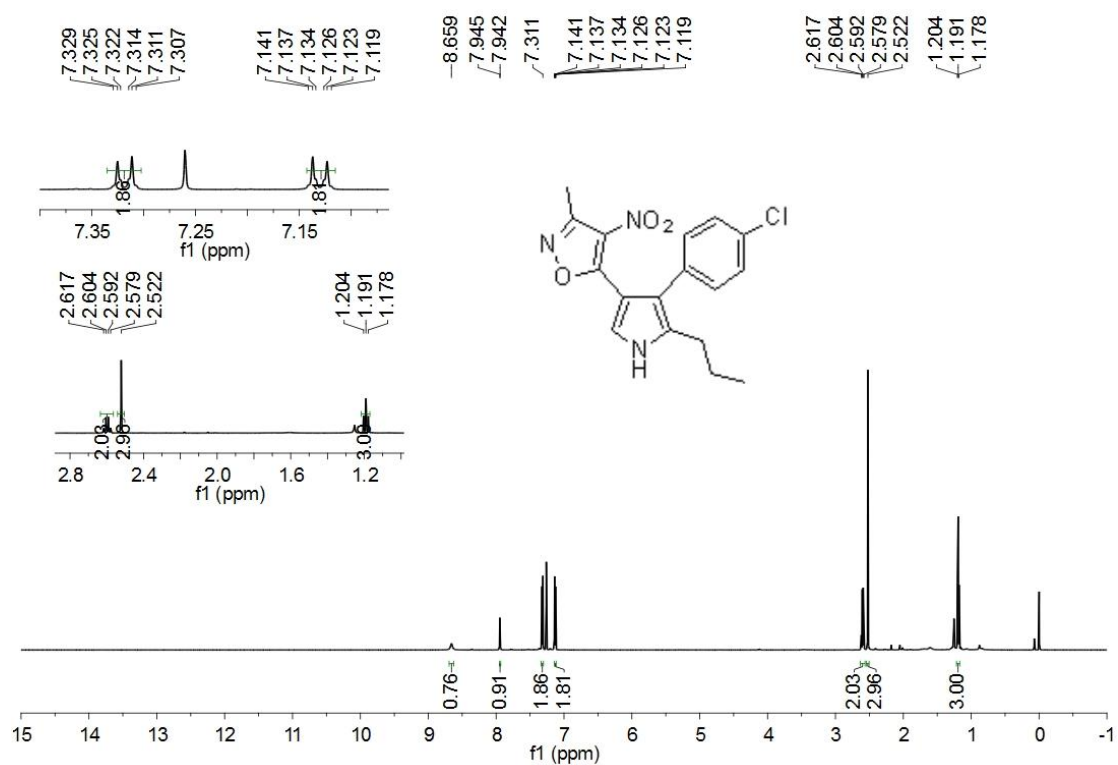
^1H NMR and ^{13}C NMR of **3ap**



^1H NMR and ^{13}C NMR of **3aq**



^1H NMR and ^{13}C NMR of **3bb**

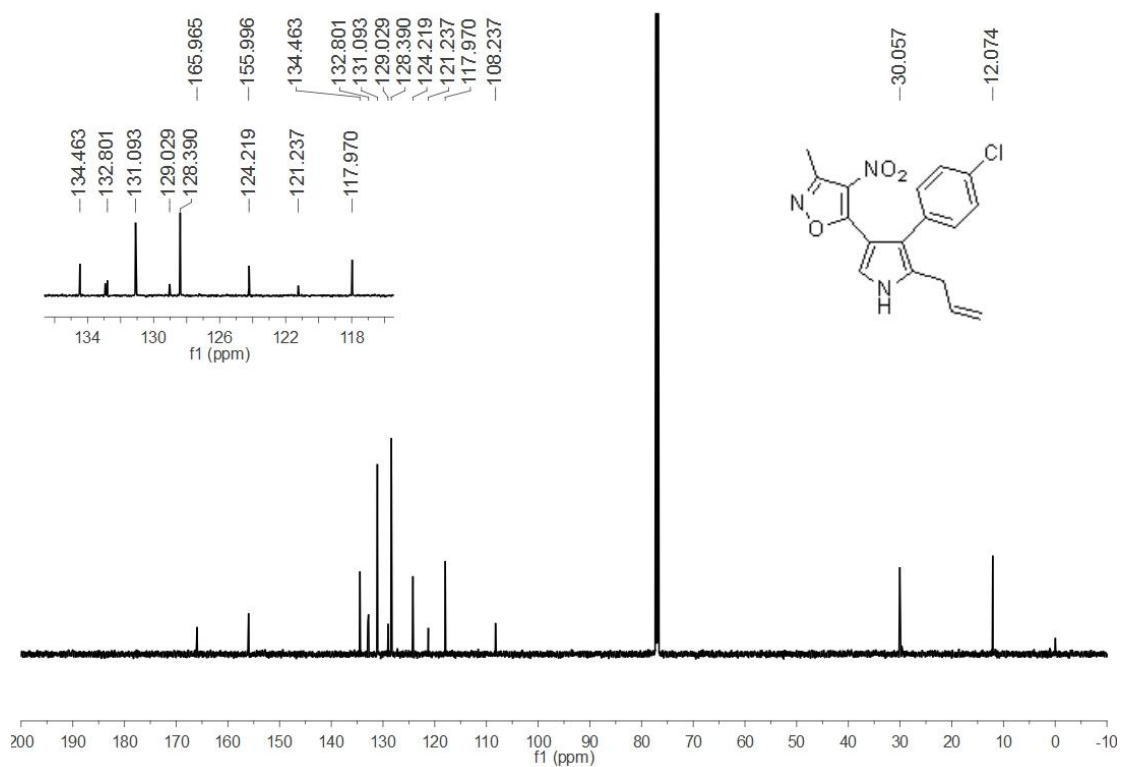


Chemical structure of compound 10: C=CCc1c[nH]c2c1c3c(c[nO3]C=C2[N+](=O)[O-])C4=CC=C(C=C4)Cl

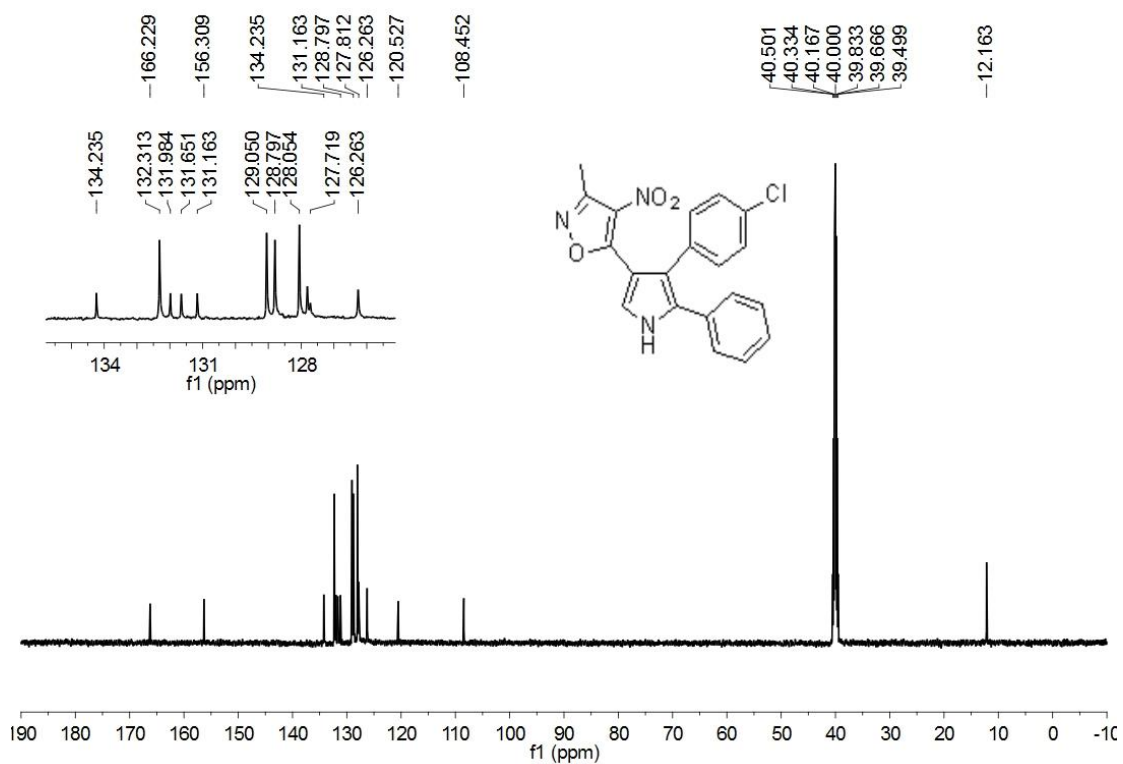
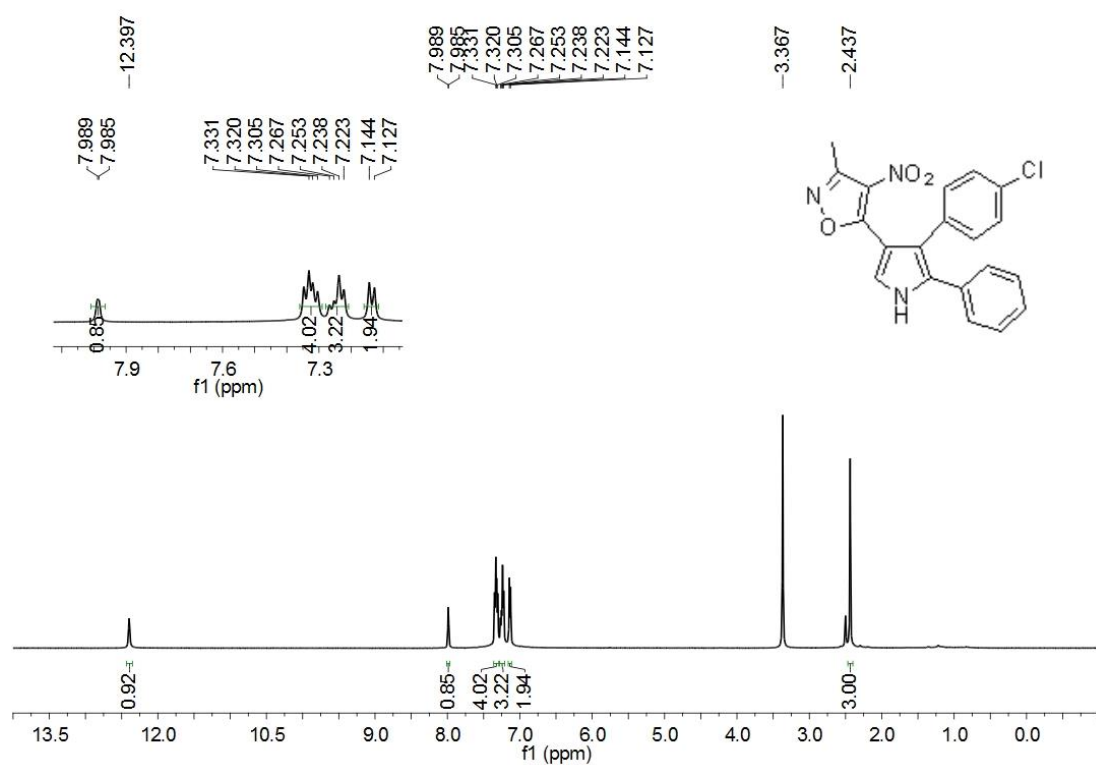
¹H NMR spectrum (CDCl₃) of compound 10. The spectrum shows peaks from 10.5 to -0.5 ppm. Integration values are provided below the peaks.

Chemical shift (ppm): 10.513, 10.139, 10.125, 8.581, 7.953, 7.948, 7.327, 7.313, 7.139, 7.125, 5.915, 5.886, 5.876, 5.869, 5.859, 5.207, 5.190, 5.173, 5.147, 5.175, 5.173, 5.147, 5.144, 3.334, 3.324, -2.526.

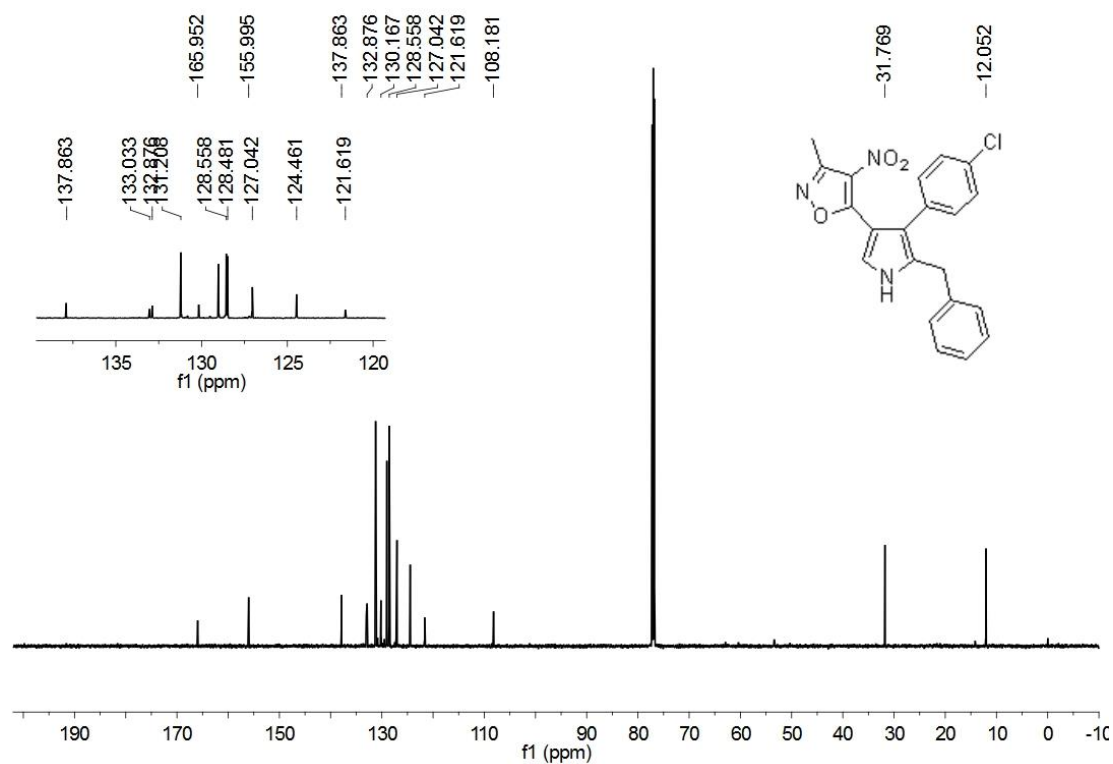
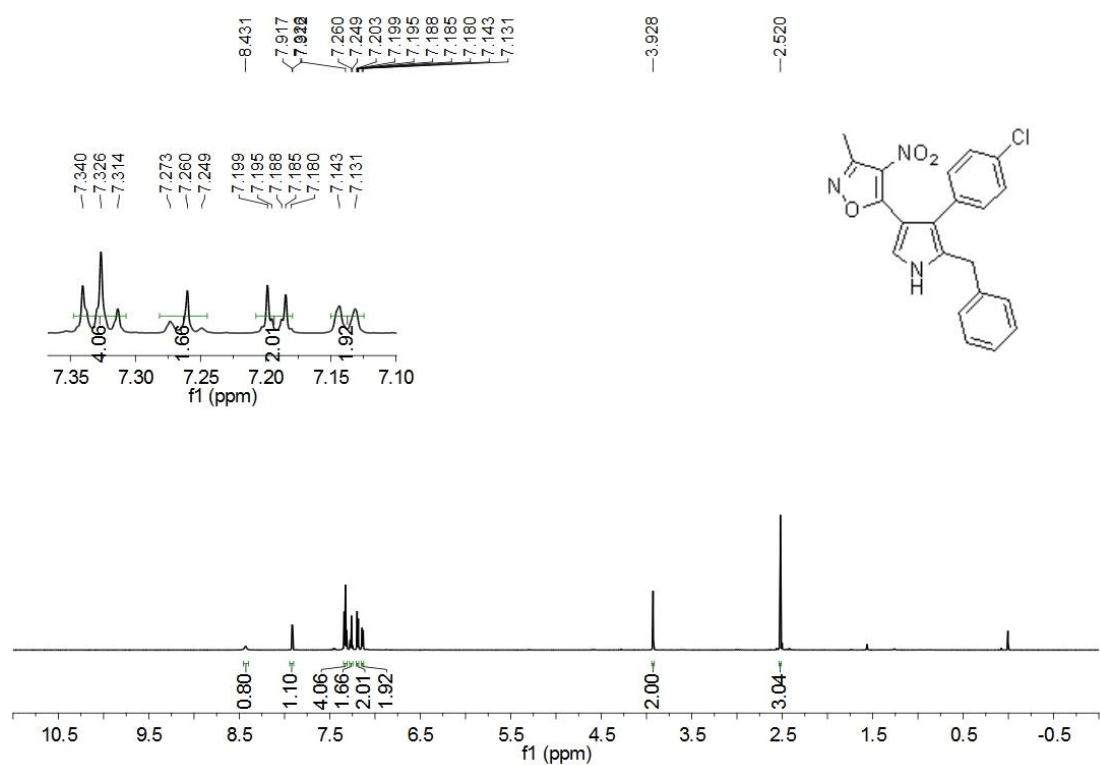
Integration values: 1.96, 1.85, 0.96, 1.98, 0.87, 0.86, 1.90, 1.85, 0.96, 1.98, 1.99, 3.00.



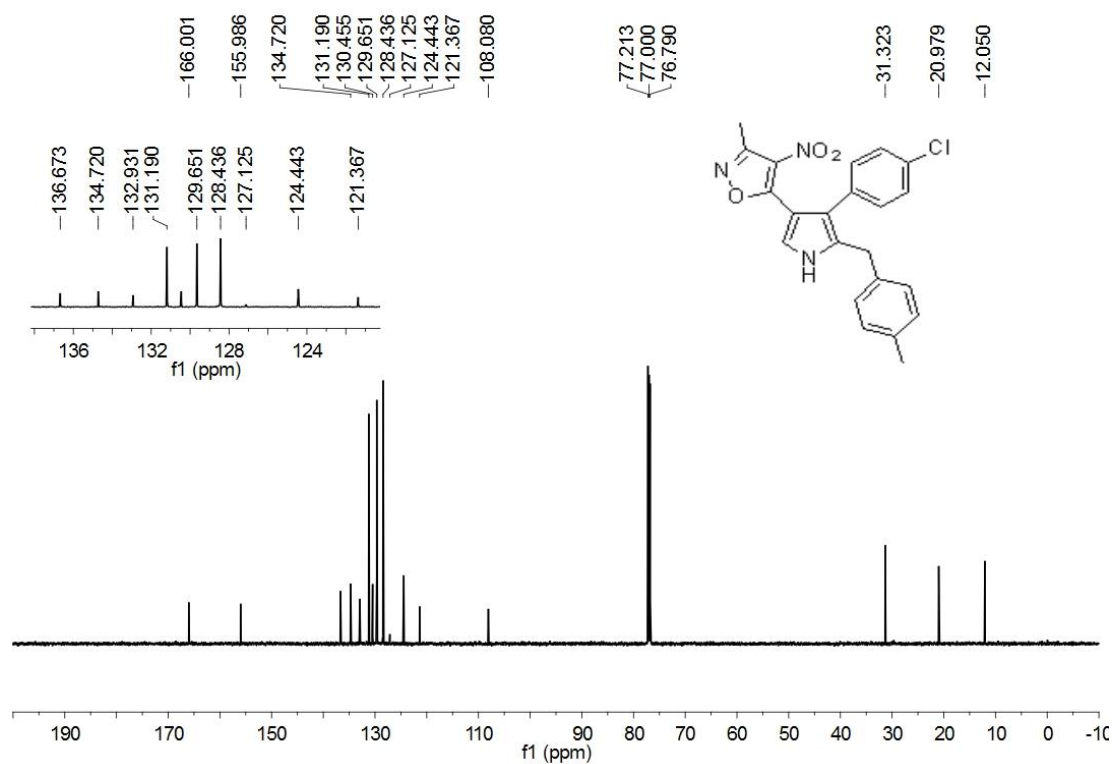
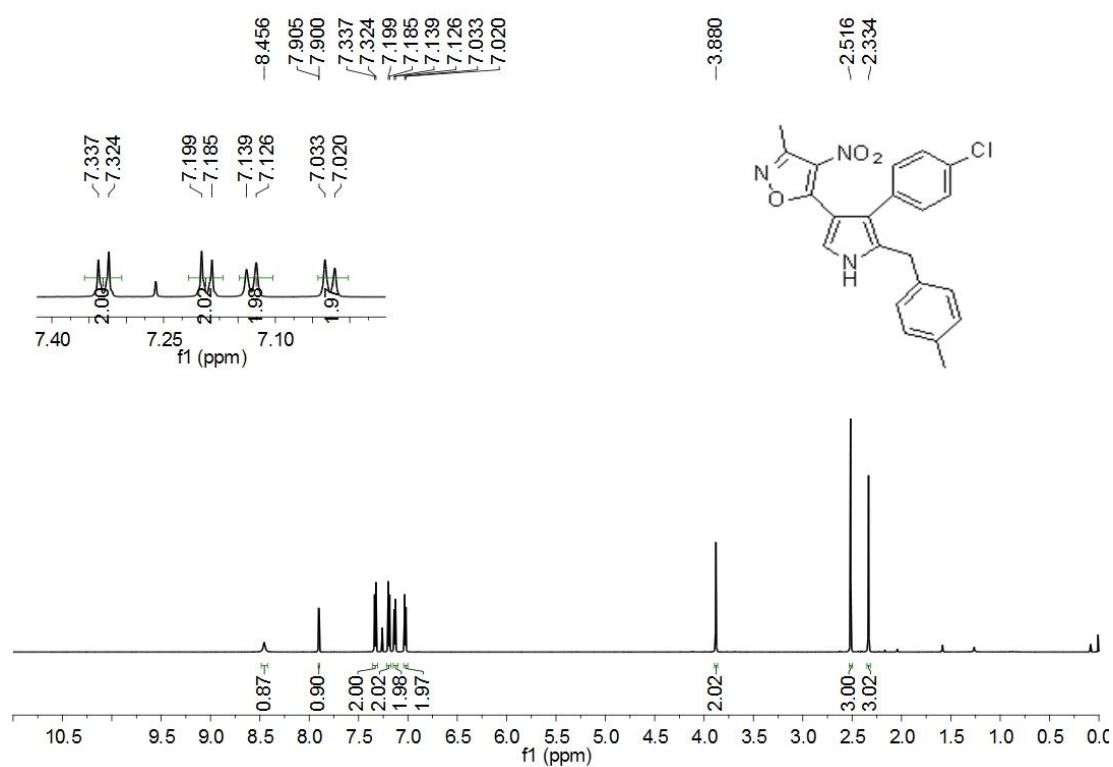
^1H NMR and ^{13}C NMR of **3db**



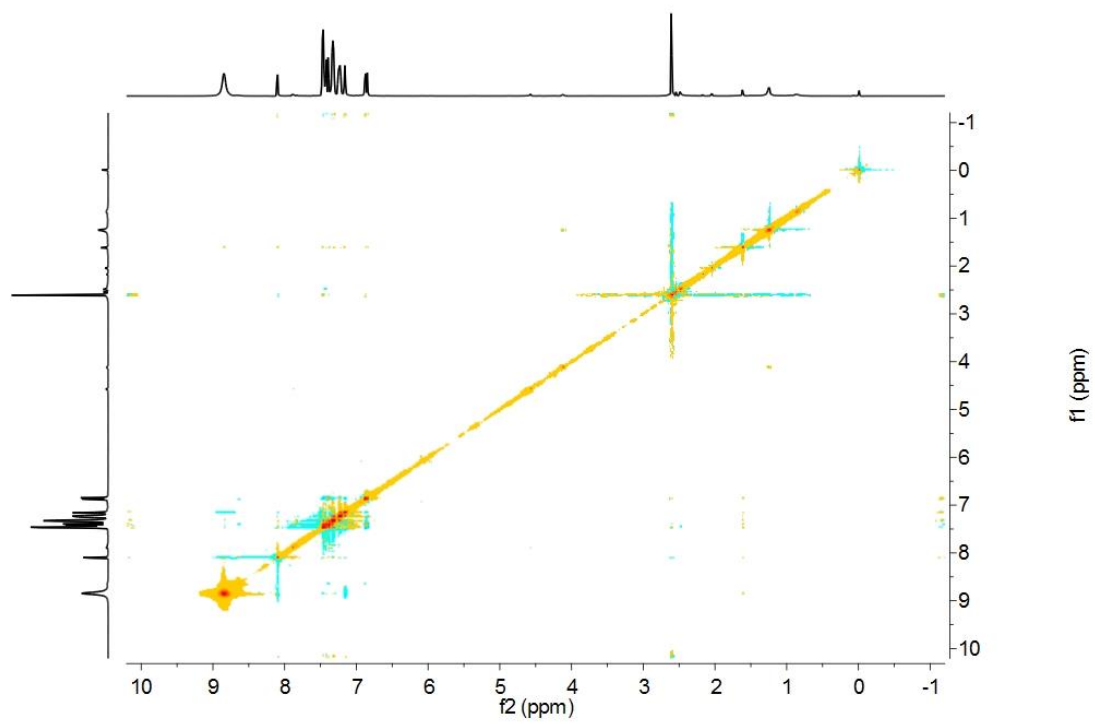
^1H NMR and ^{13}C NMR of **3eb**



^1H NMR and ^{13}C NMR of **3fb**

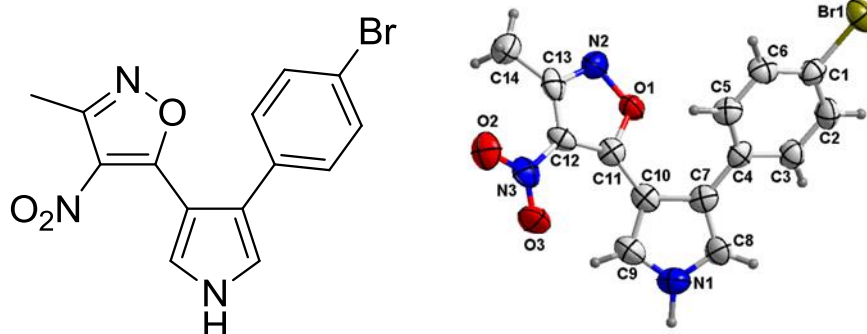


II. Copies of NOE-NMR spectra of compounds **3aq**



III. Crystal data and structural refinement for **3ac**

1. ORTEP drawing of compound **3ac**.



2. Crystal data for **3ac**

$C_{14}H_{10}BrN_3O_3$, Green solid, $M_r = 348.15$, monoclinic, space group $C2/c$, $a = 7.6080(11)$, $b = 7.7910(11)$, $c = 23.078(3)$ Å, $\alpha = 90.000$, $\beta = 90.000$, $\gamma = 90.000^\circ$, $V = 1367.9(3)$ Å³, $Z = 4$, calcd = 1.691, $T = 293(2)$ K, 3166 reflections (2578 unique), 253 refined parameters, $R = 0.0653$ (2578 data with $I > 2\sigma(I)$), $wR2 = 0.1516$. The hydrogen atoms were refined as rigid groups.

Crystallographic data for the structures **3ac** have been deposited in the Cambridge Crystallography Data Centre (CCDC No. 1552332).