

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;

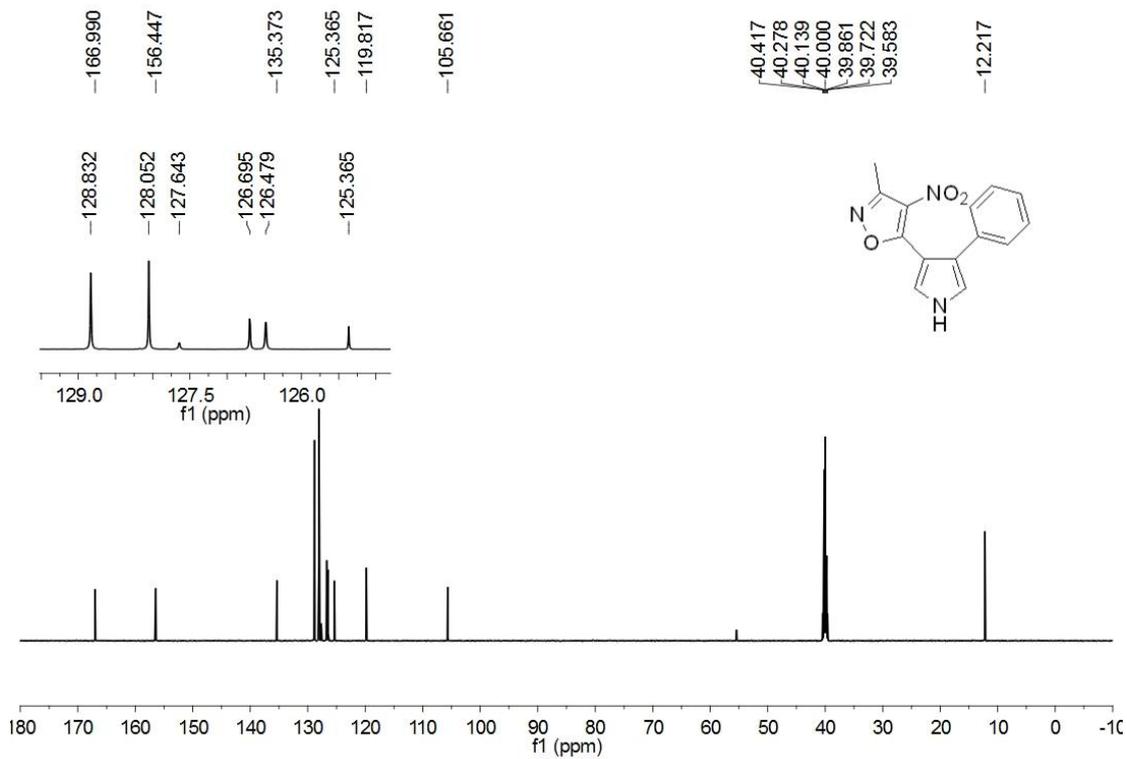
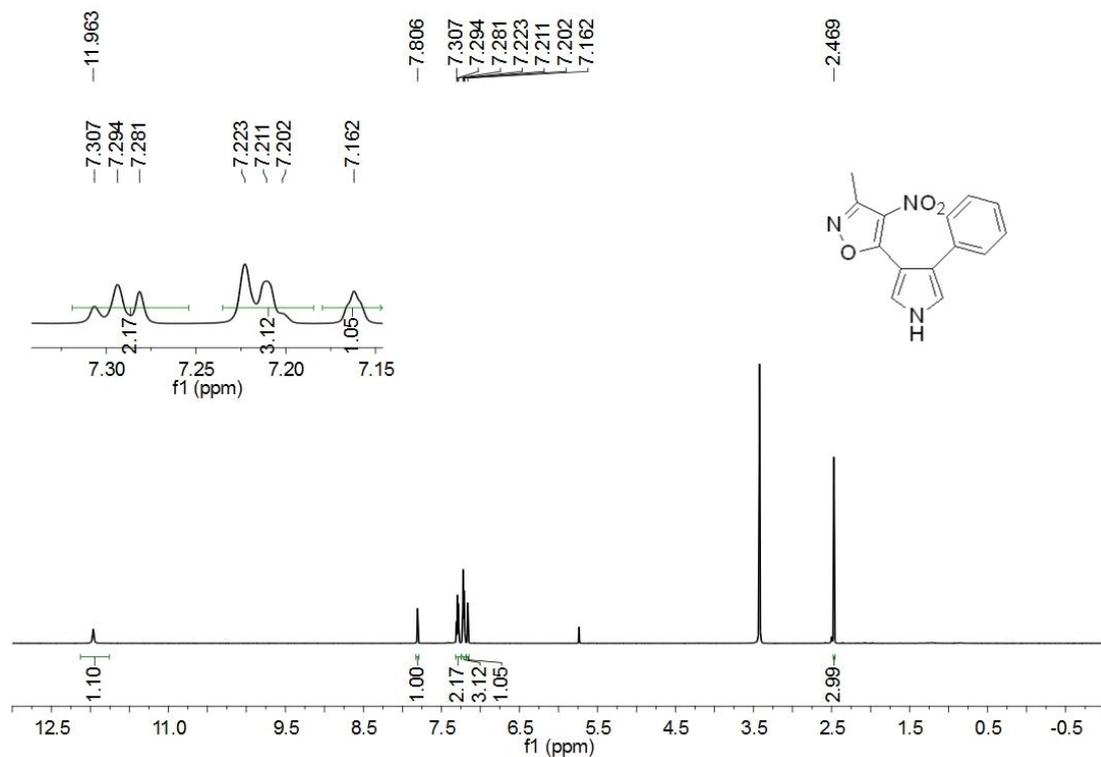
* Correspondence: z_dw@jlu.edu.cn; Tel.: +86-431-878-36471

Contents

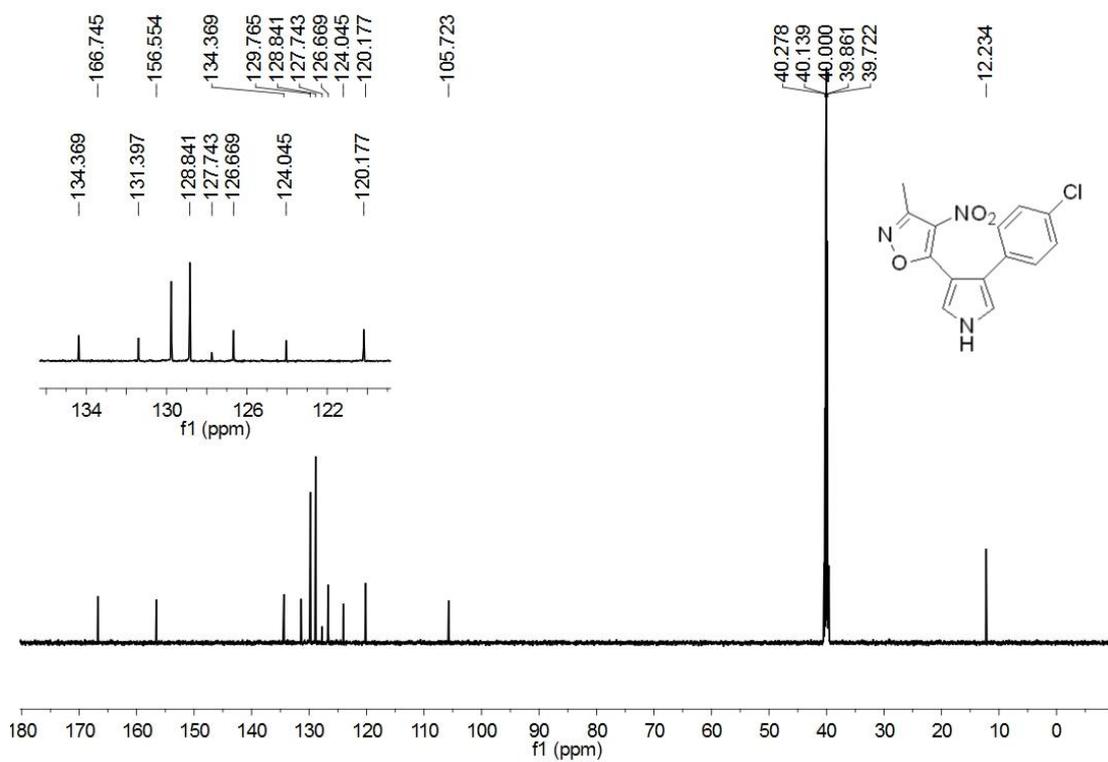
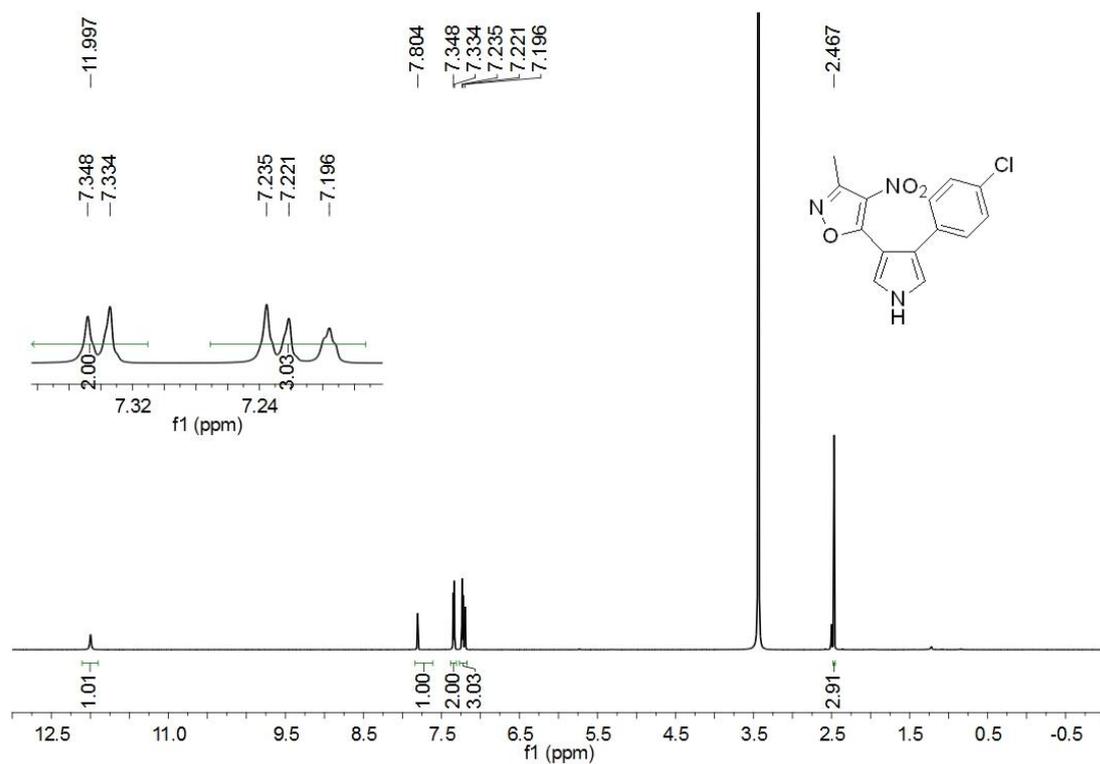
I. Copies of ¹ H NMR and ¹³ C NMR spectra of compounds 3aa-3fb	S2
II. Copies of NOE-NMR spectra of compounds 3aq	S24
III. Crystal data and structural refinement for 3ac	S25

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

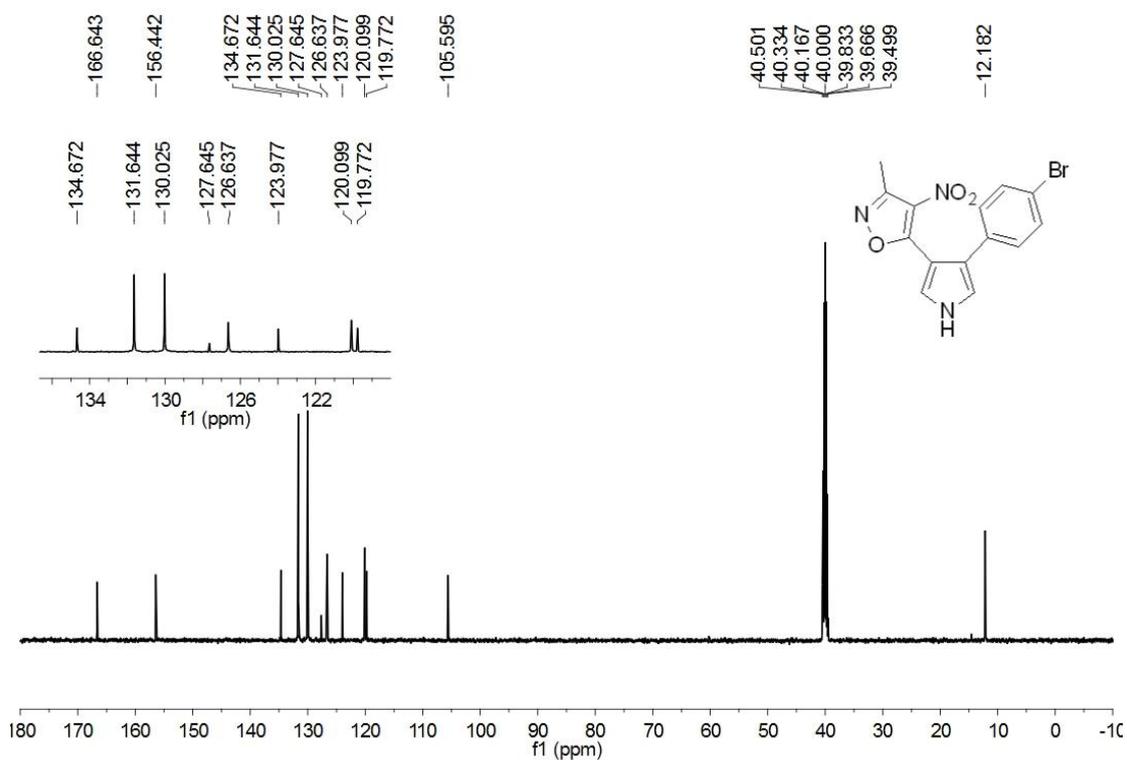
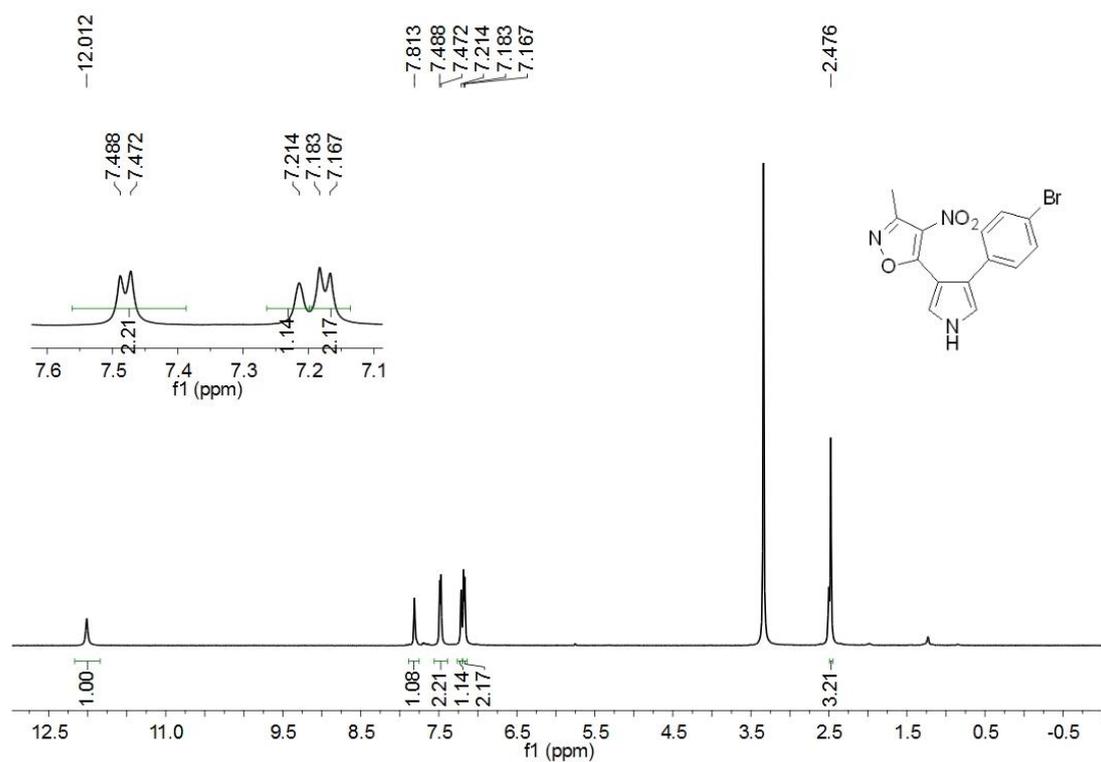
^1H NMR and ^{13}C NMR of **3aa**



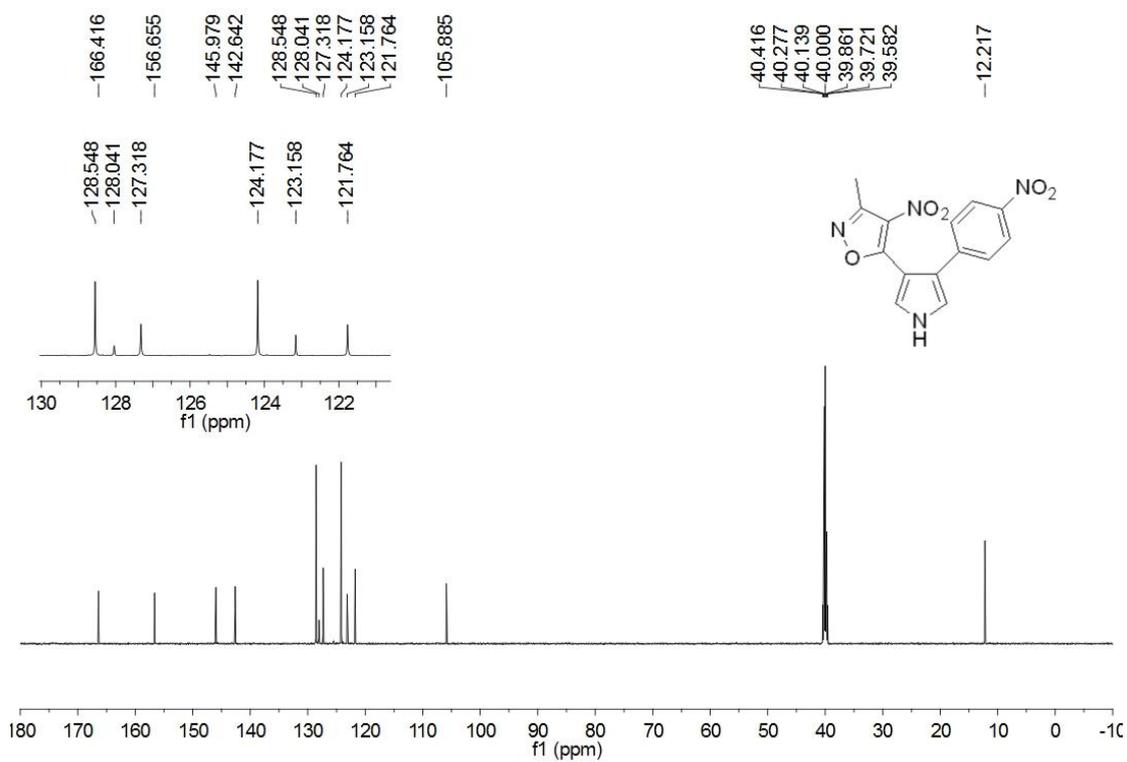
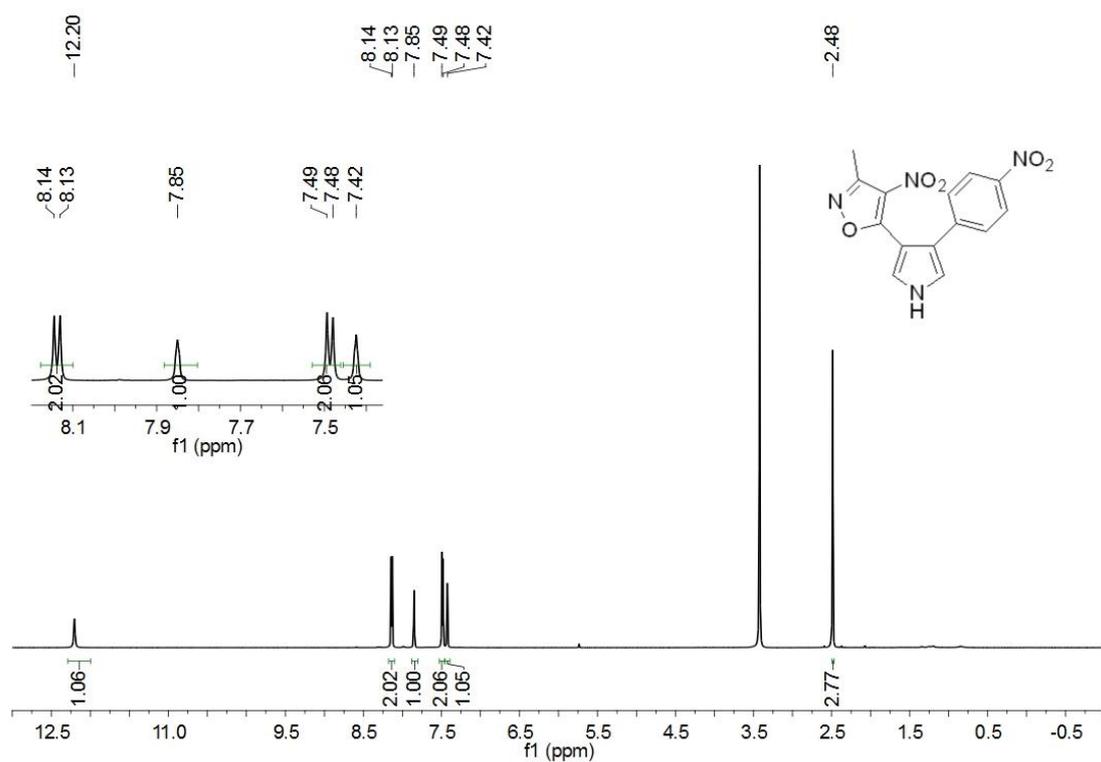
^1H NMR and ^{13}C NMR of **3ab**



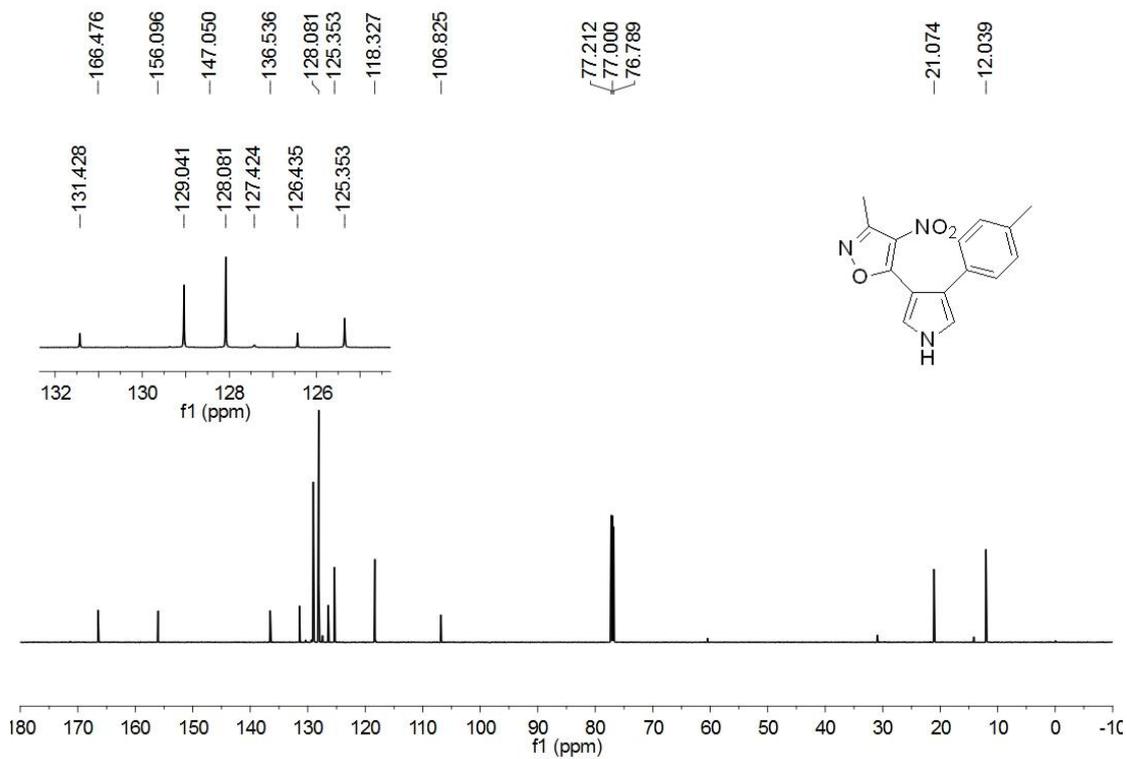
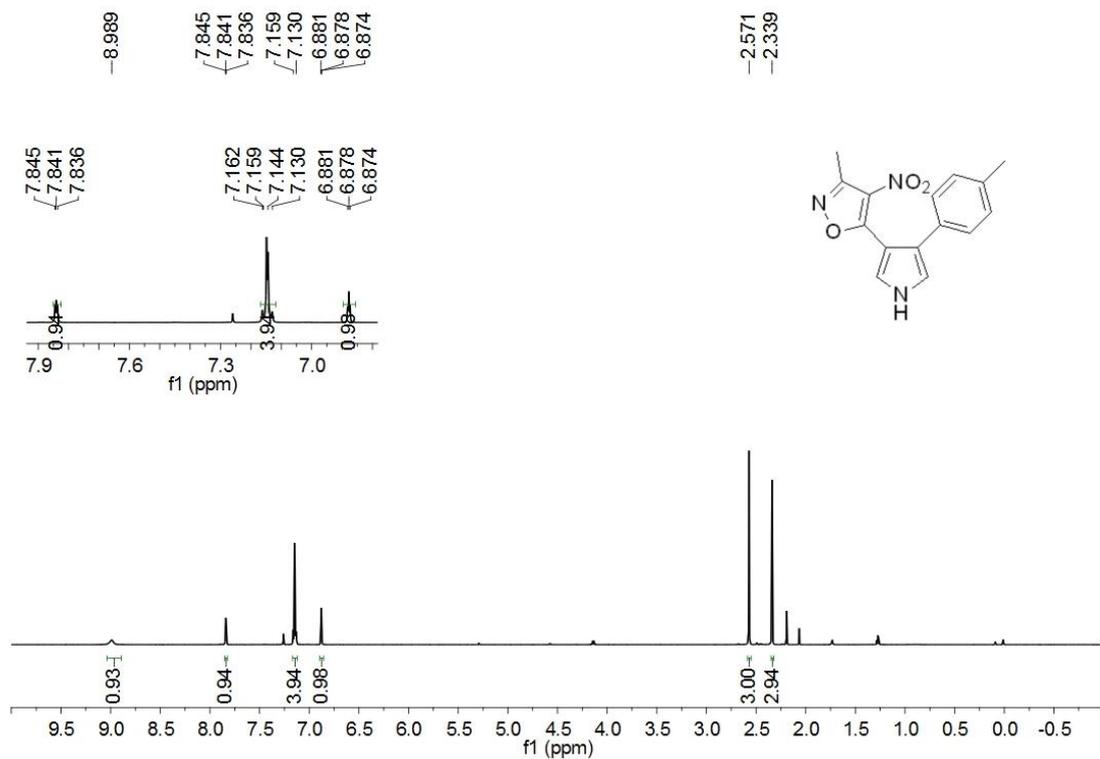
^1H NMR and ^{13}C NMR of **3ac**



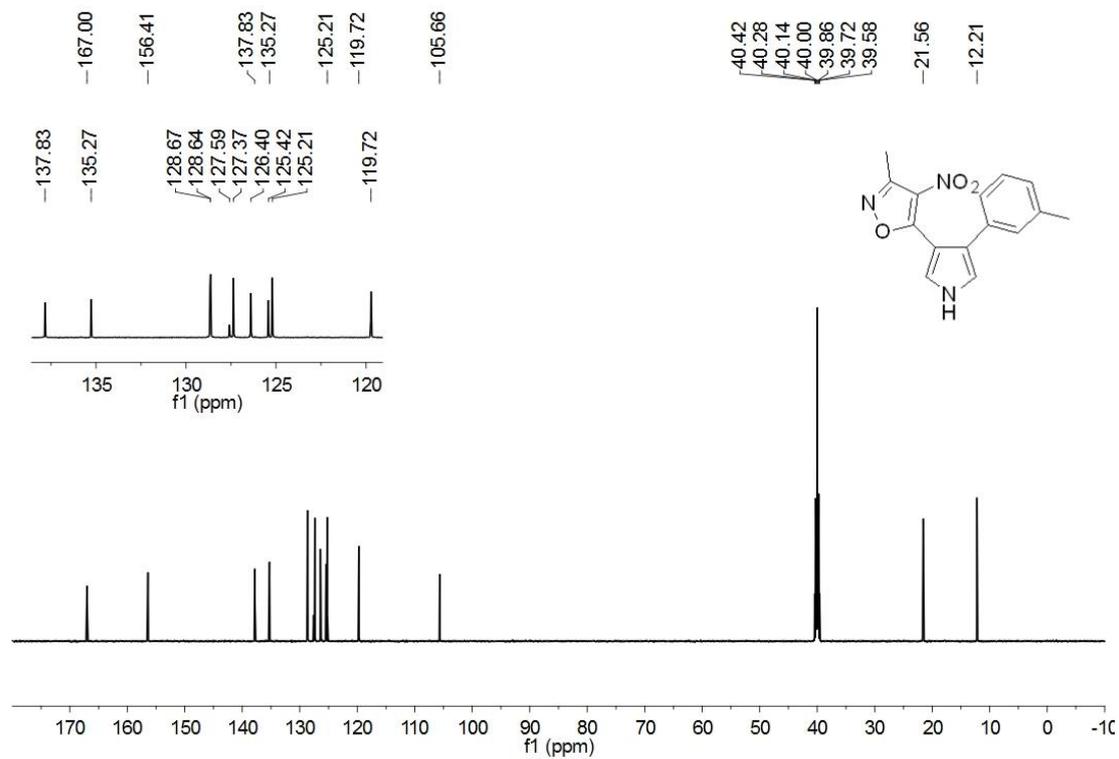
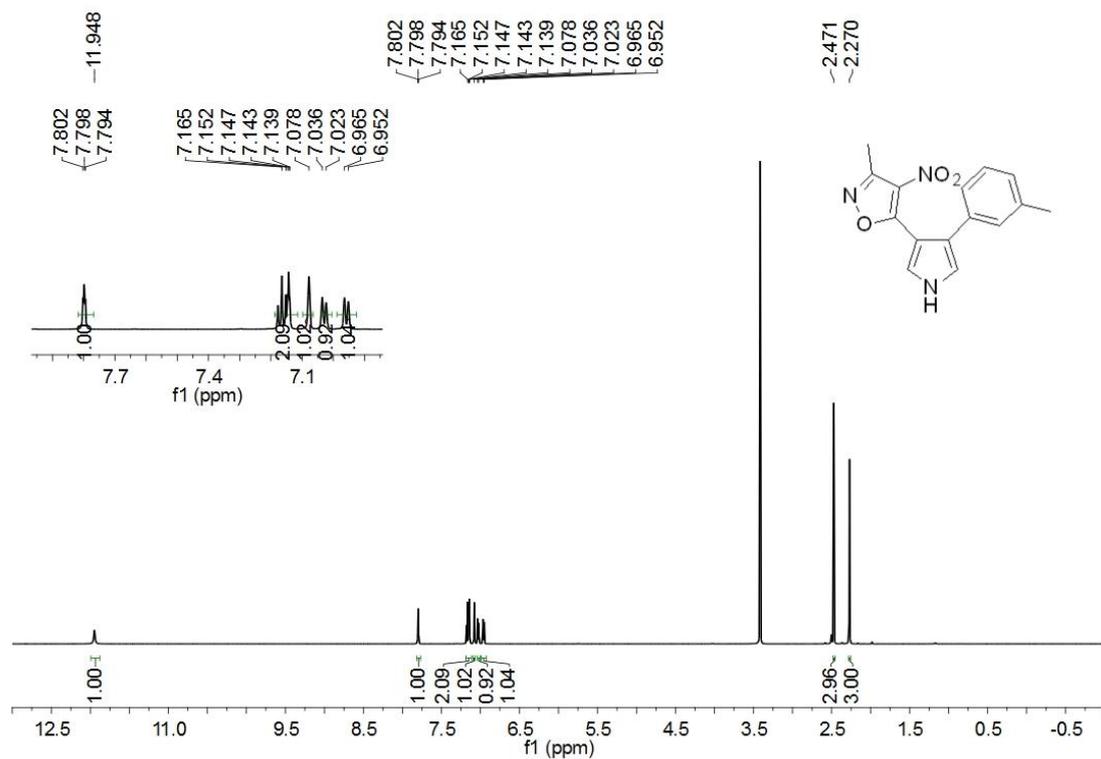
^1H NMR and ^{13}C NMR of **3ad**



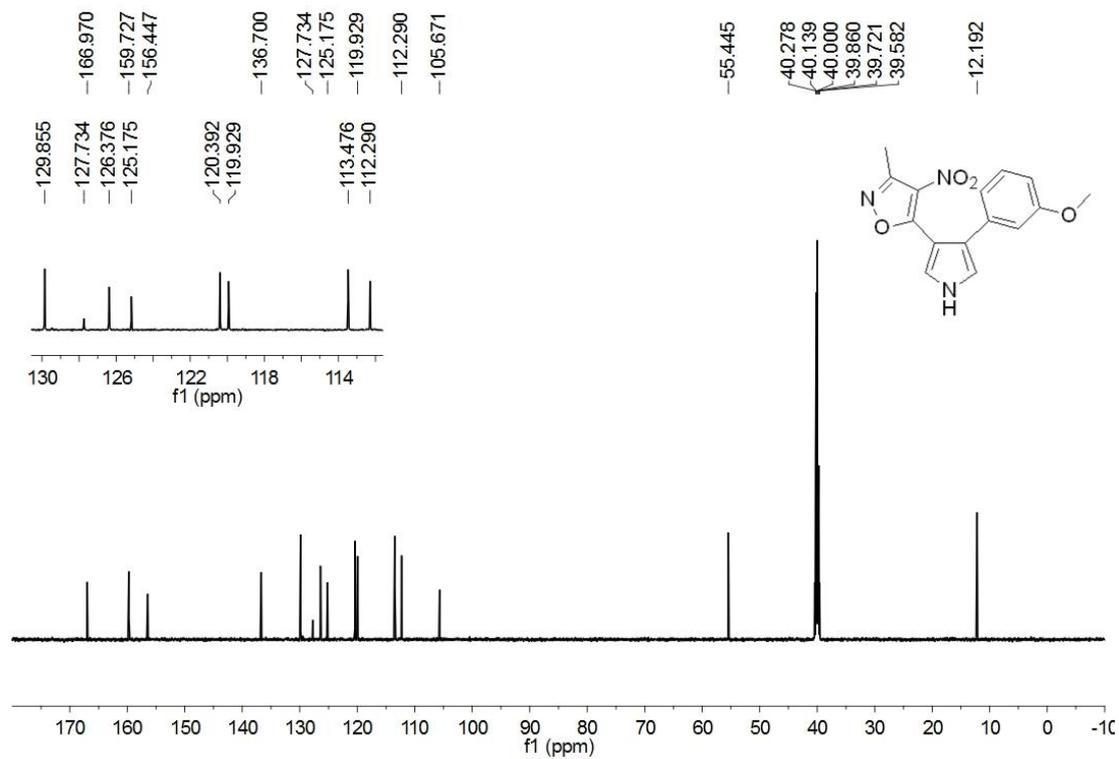
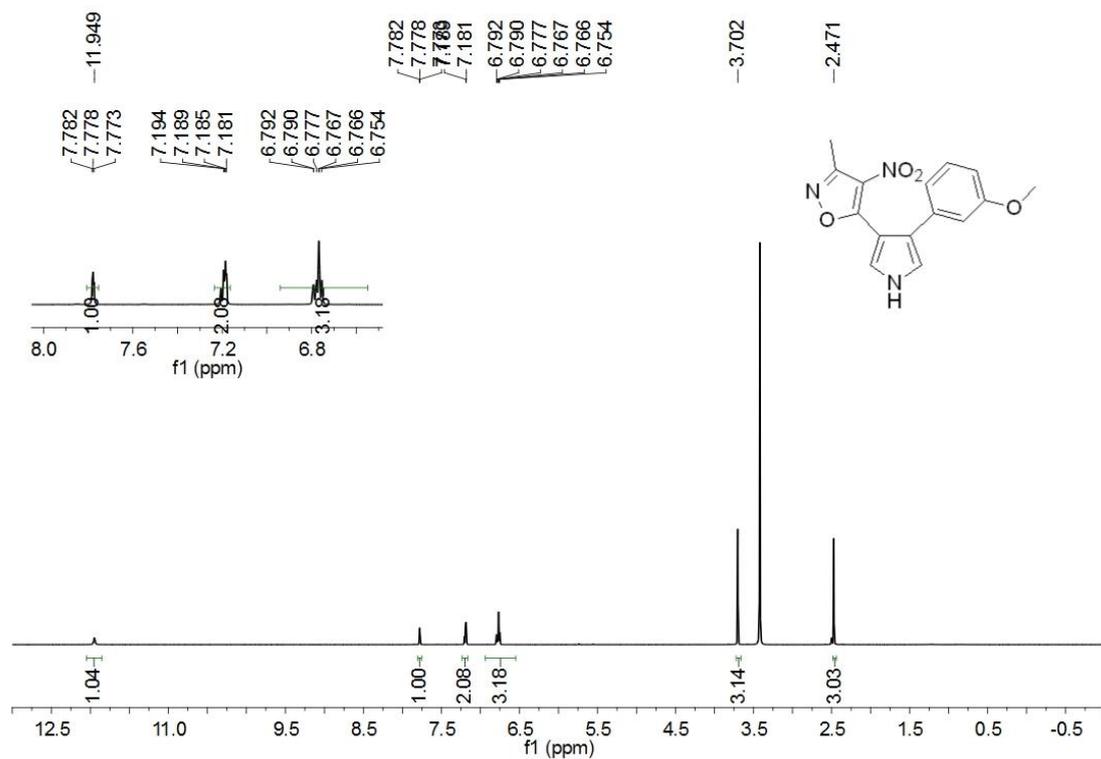
^1H NMR and ^{13}C NMR of **3ae**



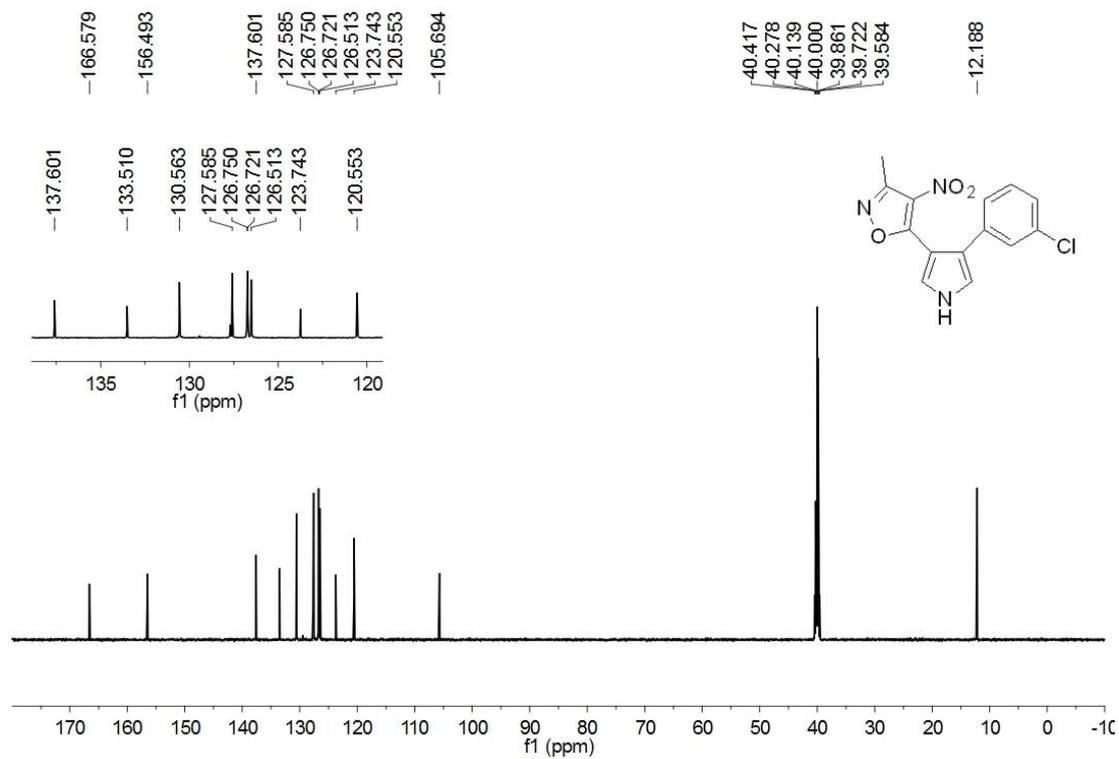
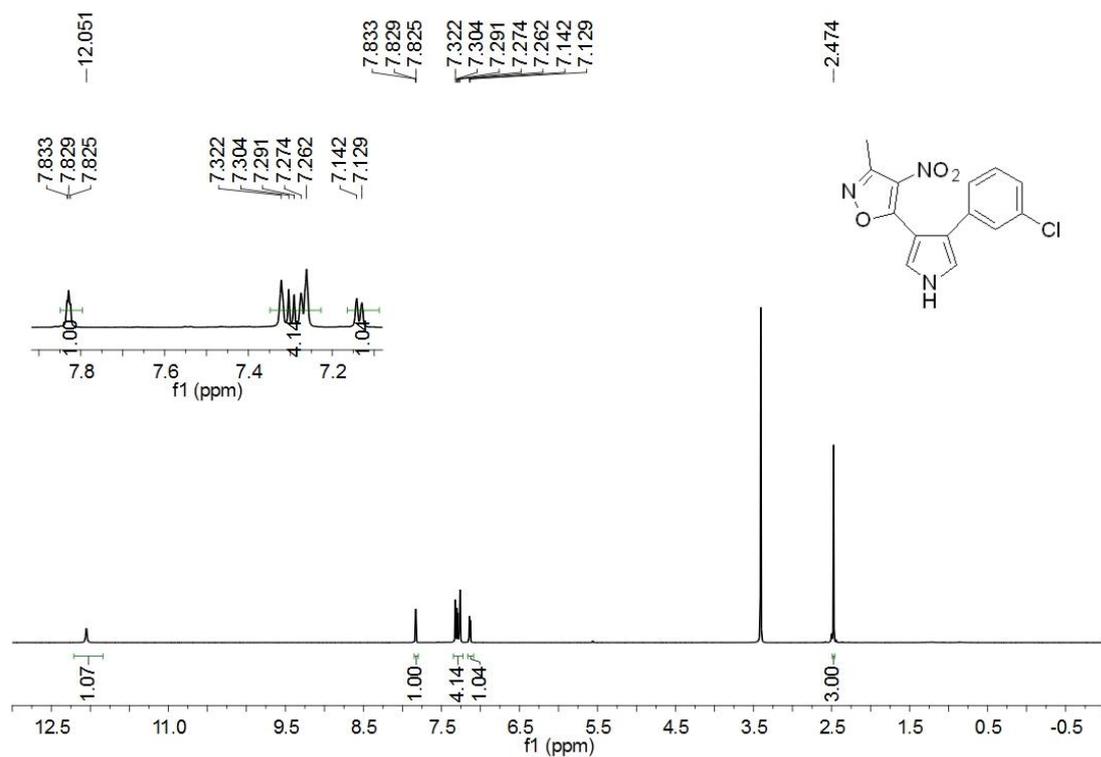
^1H NMR and ^{13}C NMR of **3af**



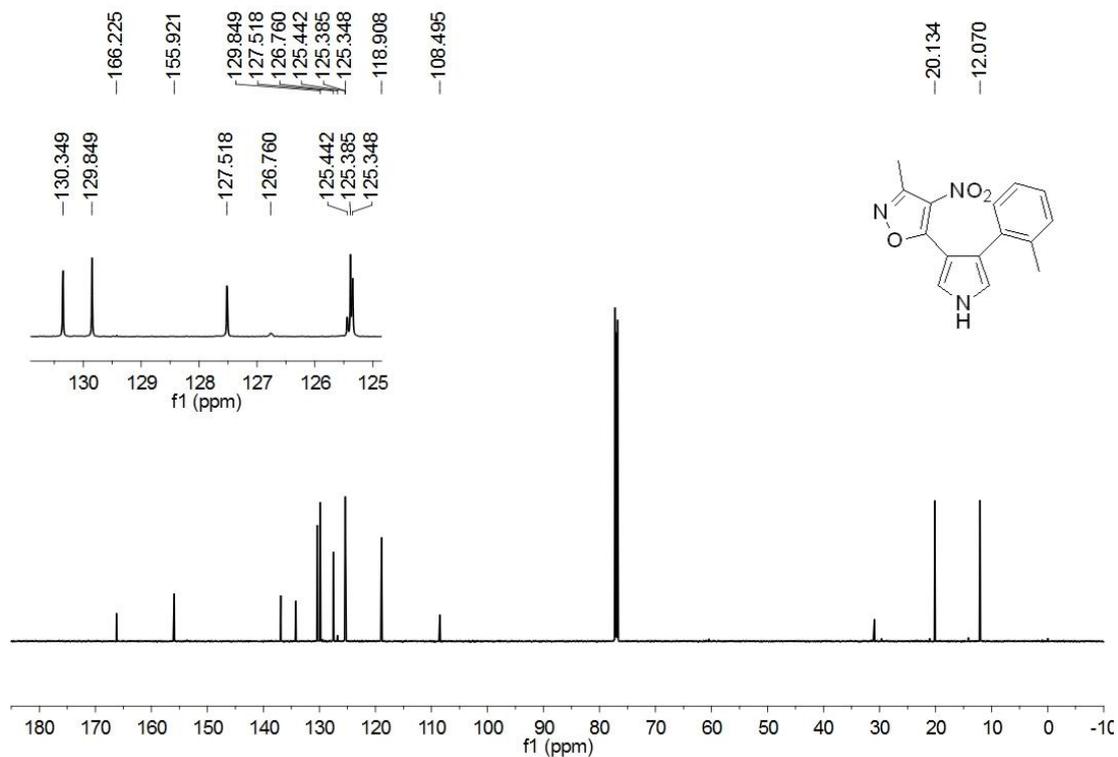
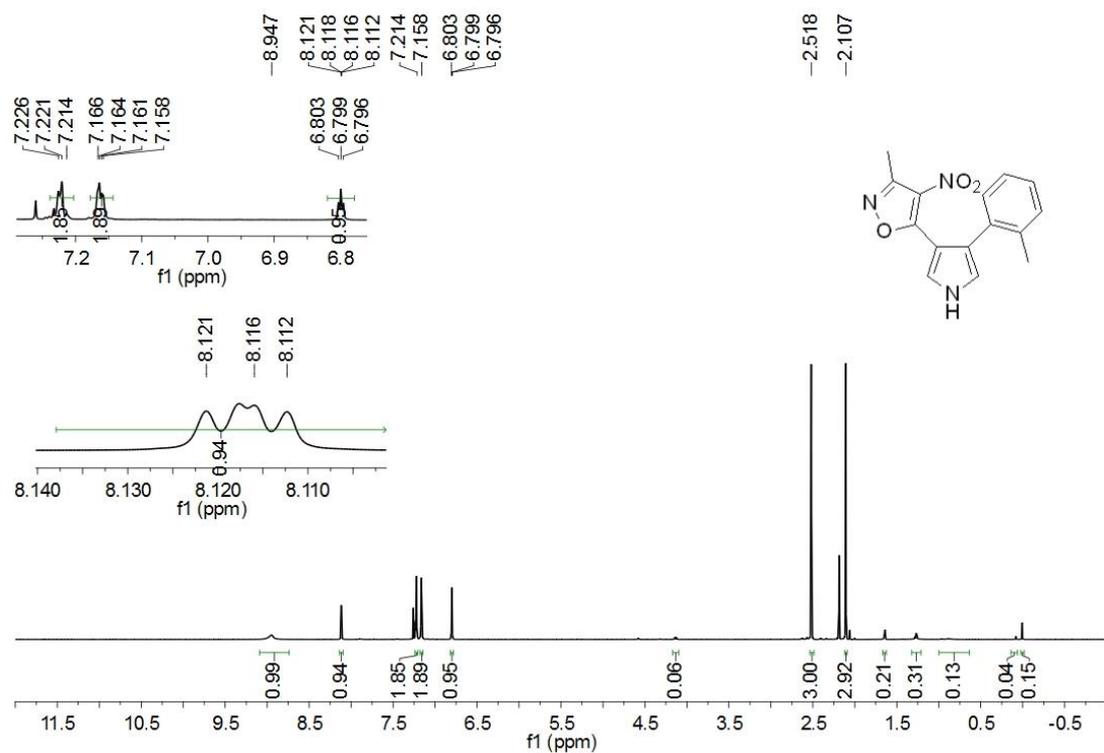
^1H NMR and ^{13}C NMR of **3ag**



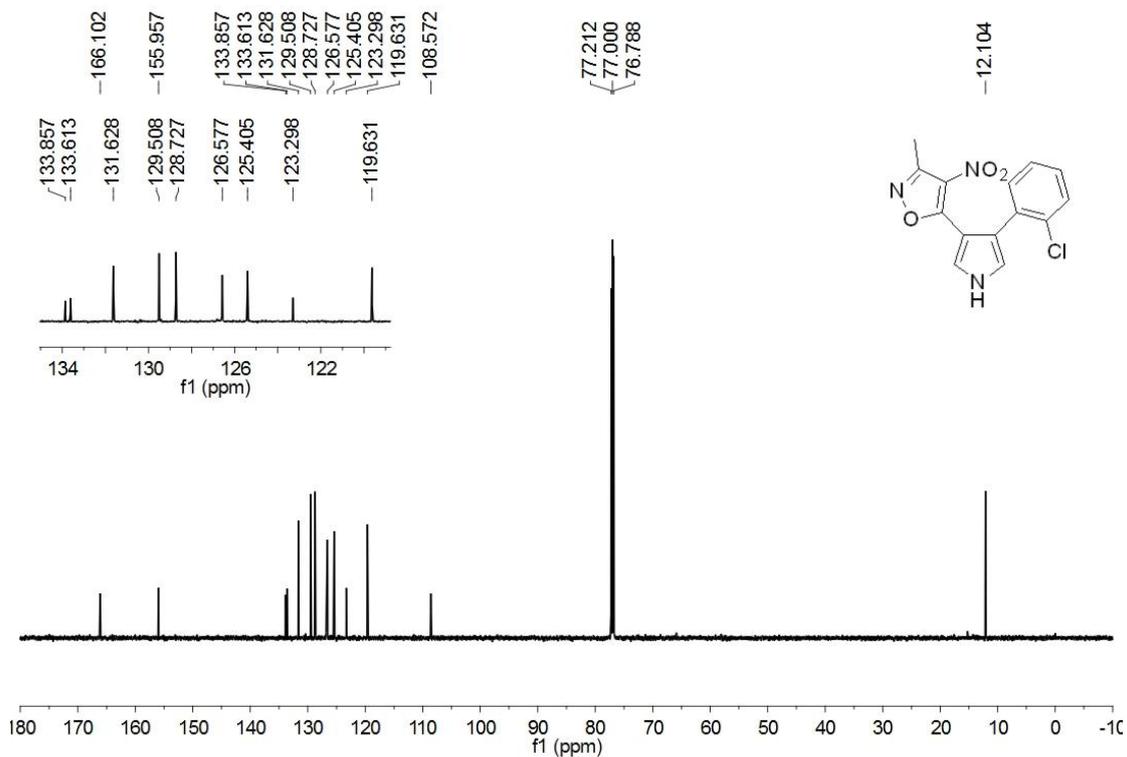
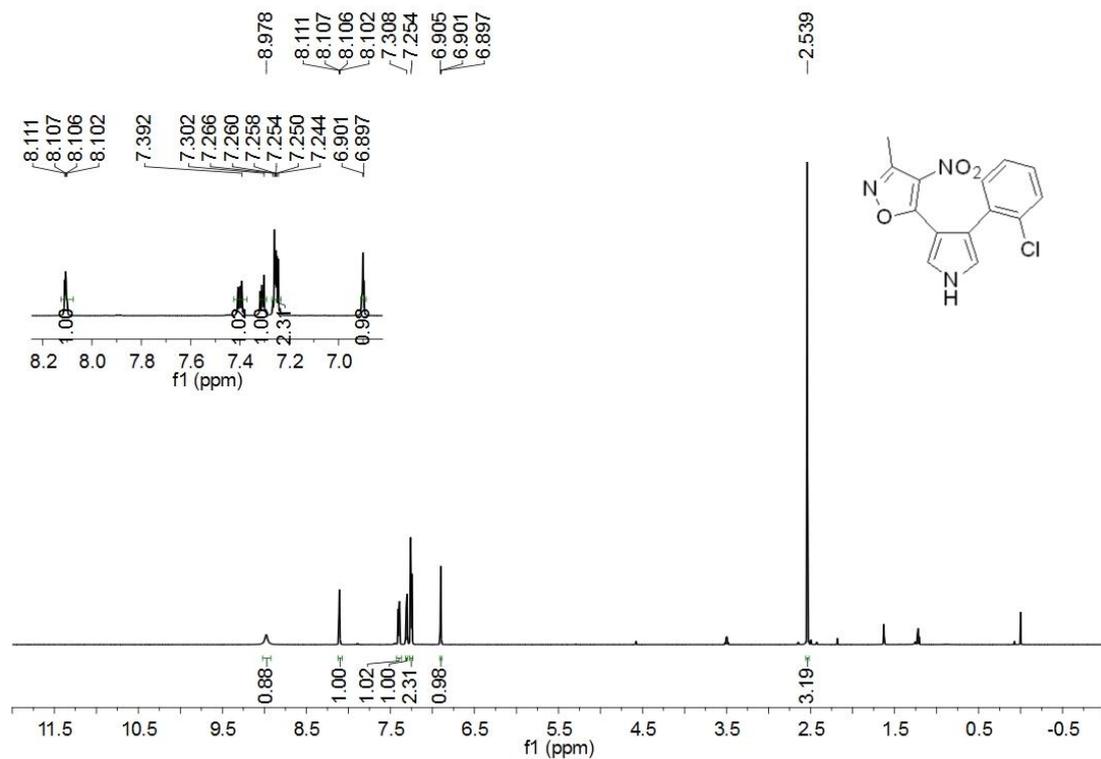
^1H NMR and ^{13}C NMR of **3ah**



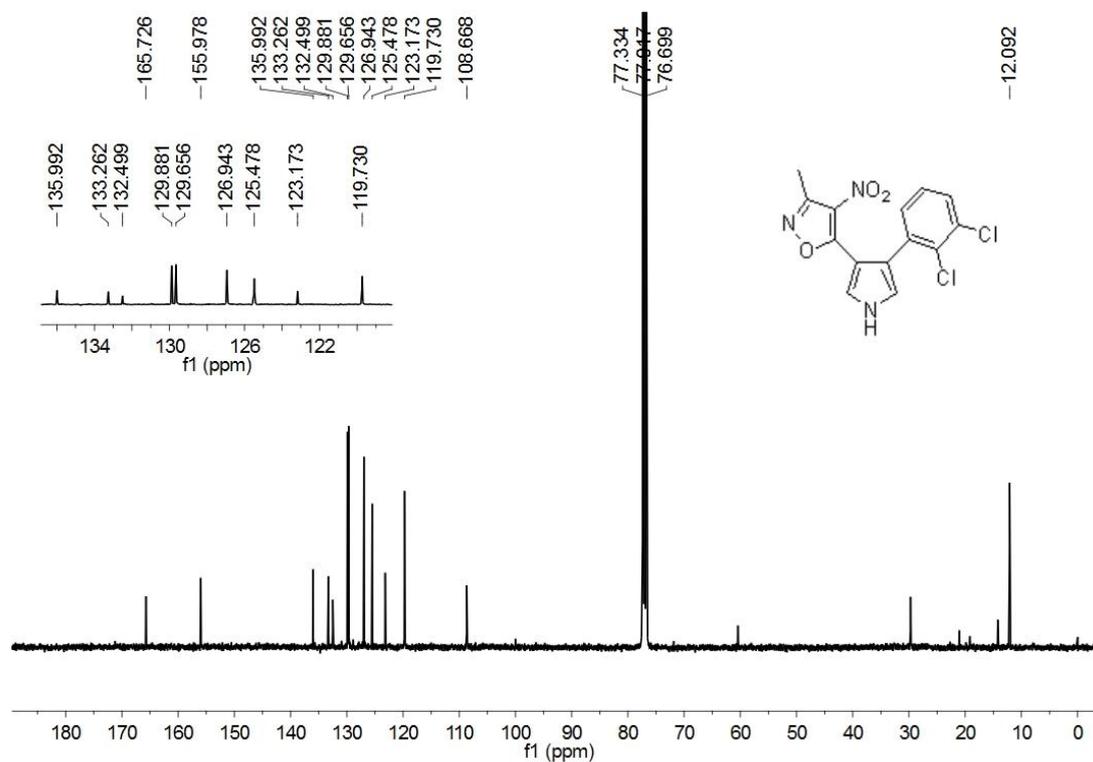
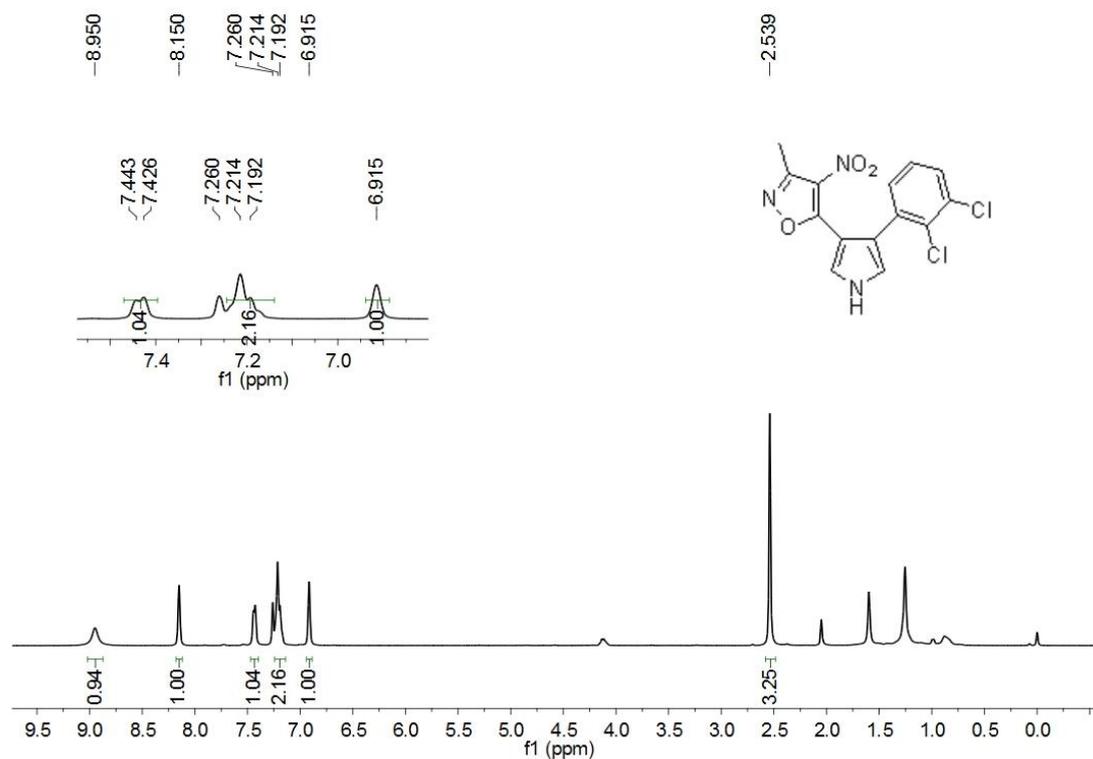
^1H NMR and ^{13}C NMR of **3ai**



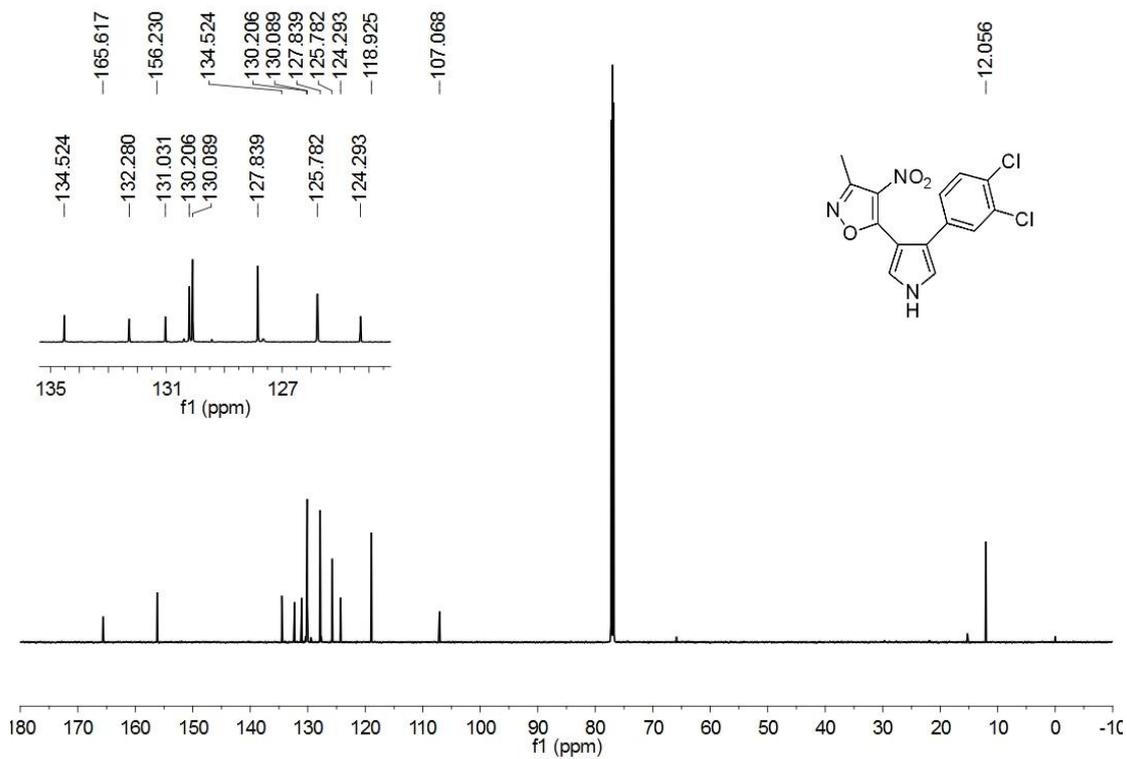
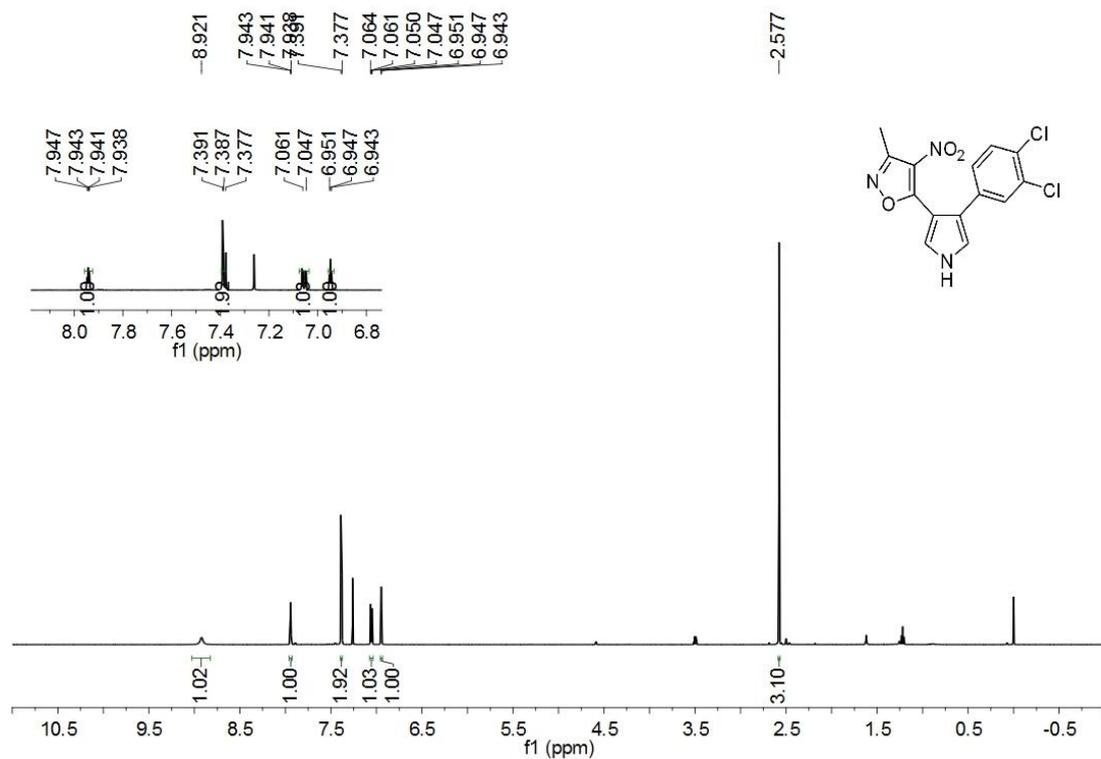
^1H NMR and ^{13}C NMR of **3aj**



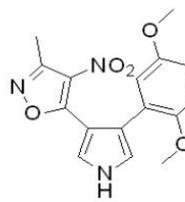
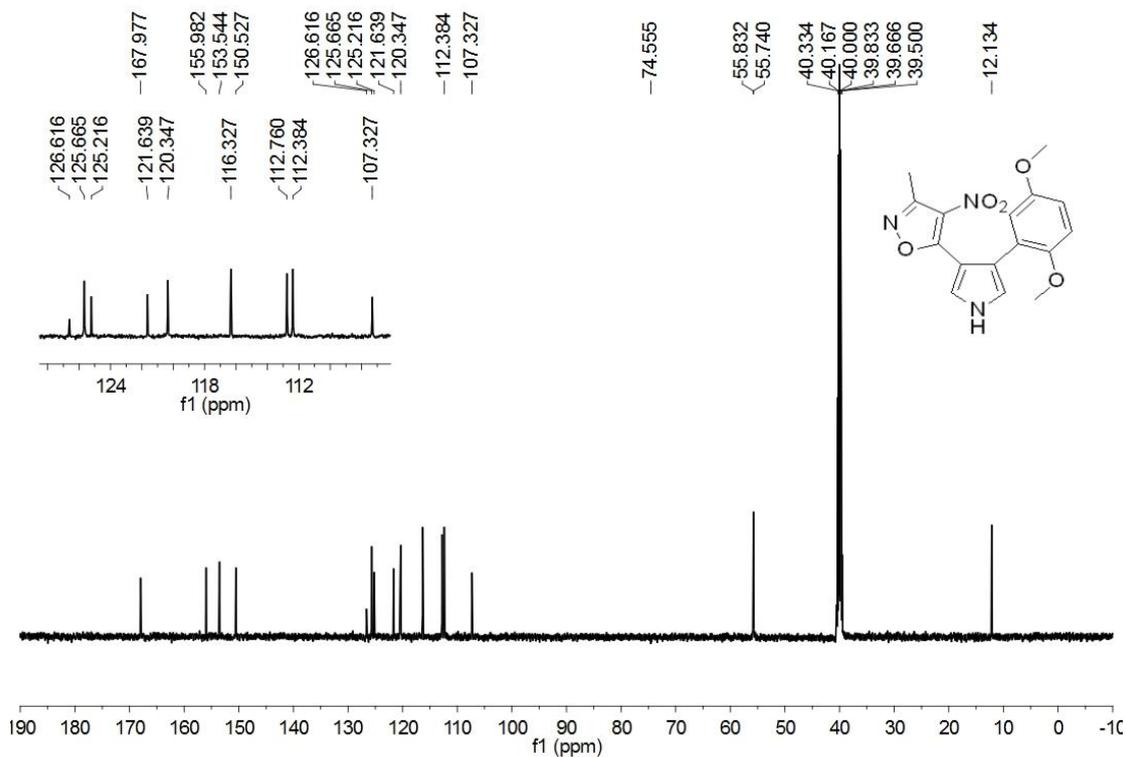
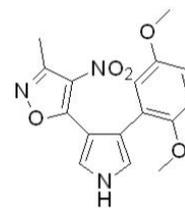
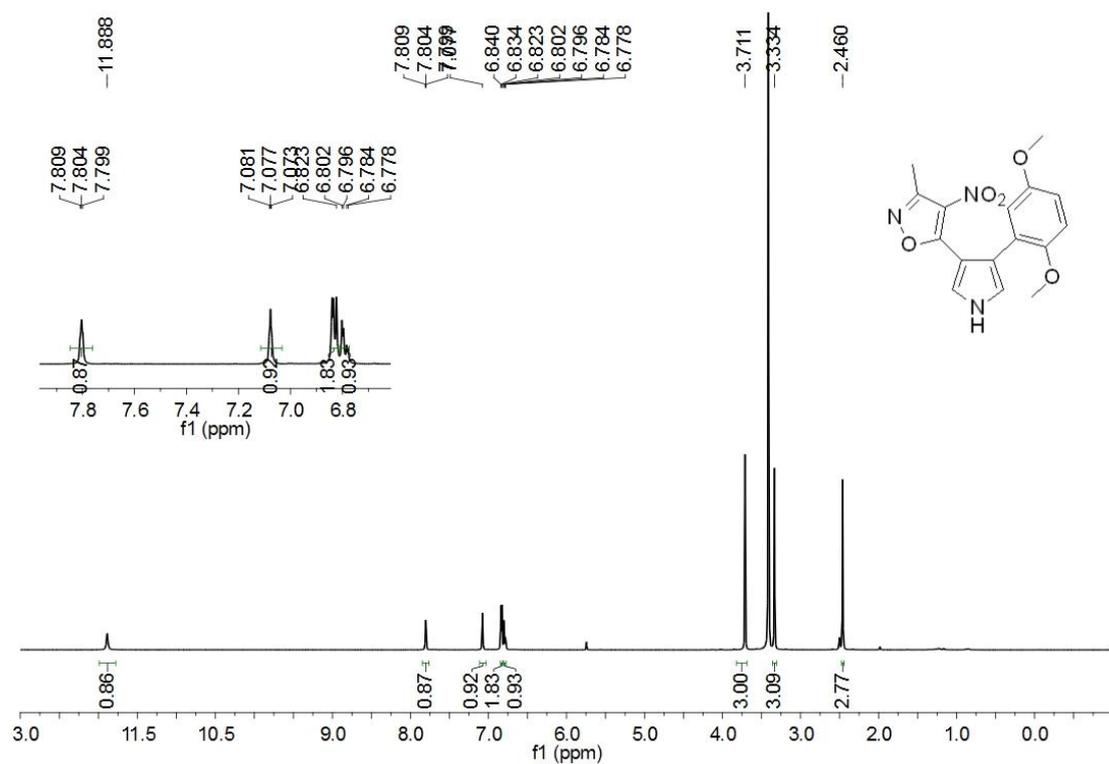
^1H NMR and ^{13}C NMR of **3ak**



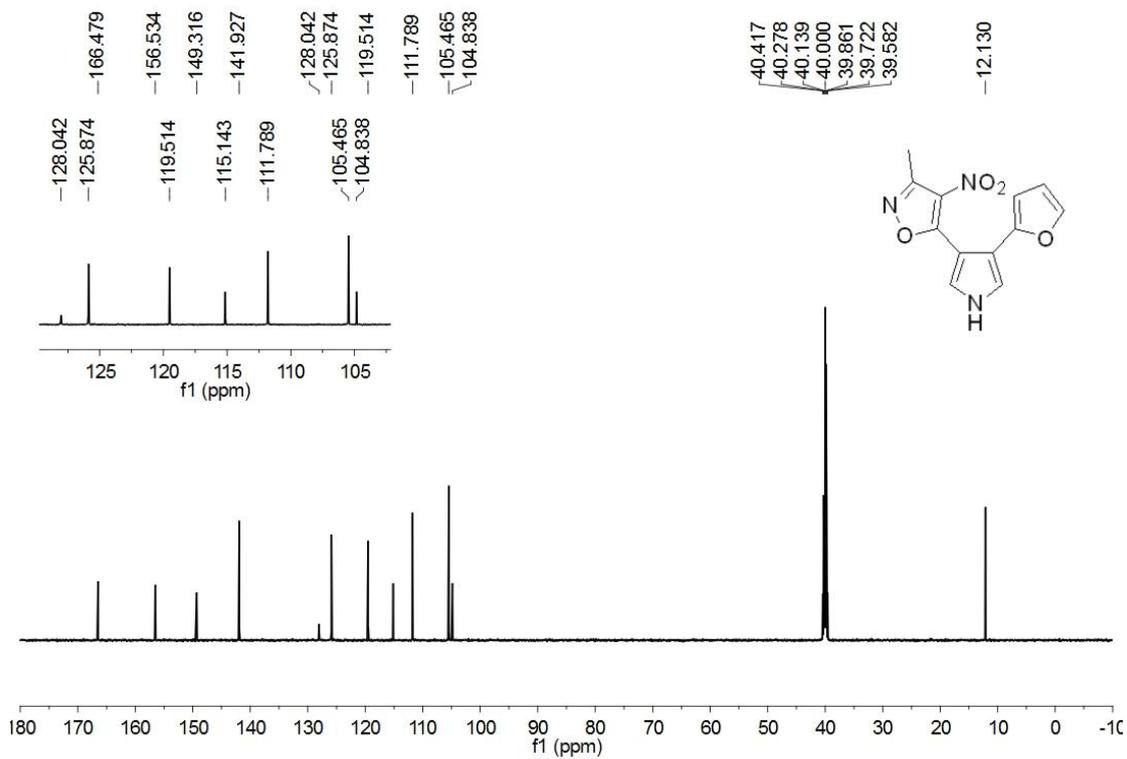
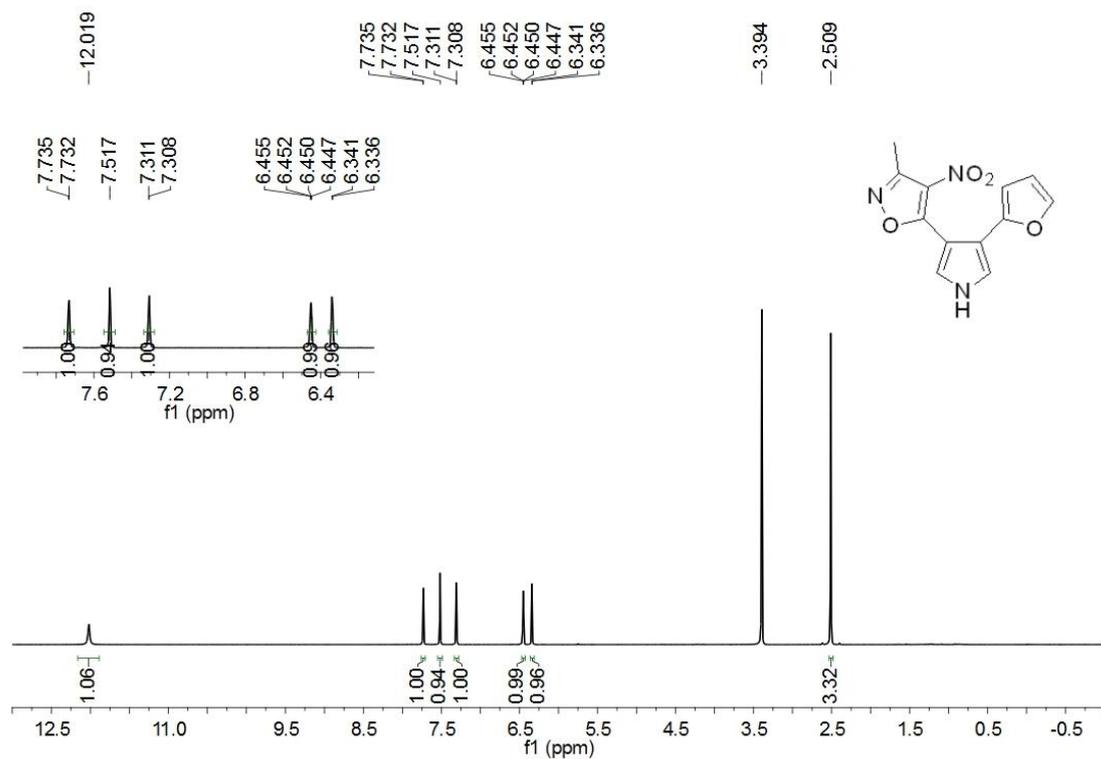
^1H NMR and ^{13}C NMR of **3al**



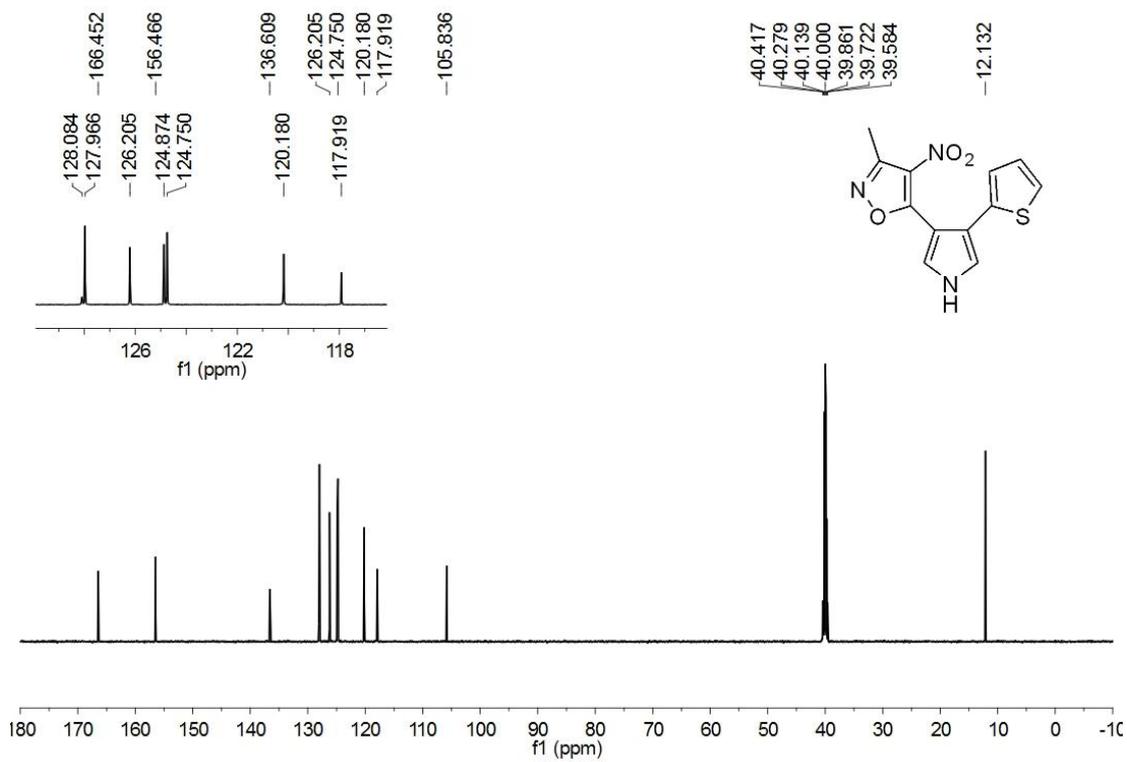
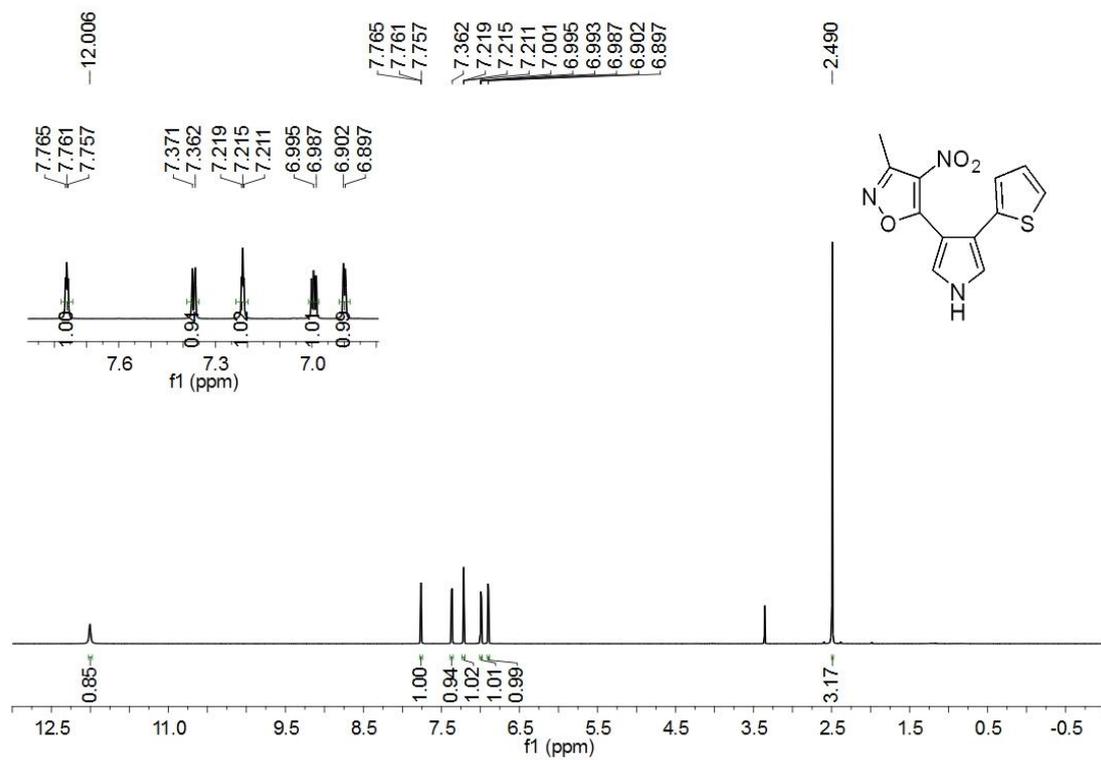
^1H NMR and ^{13}C NMR of **3am**



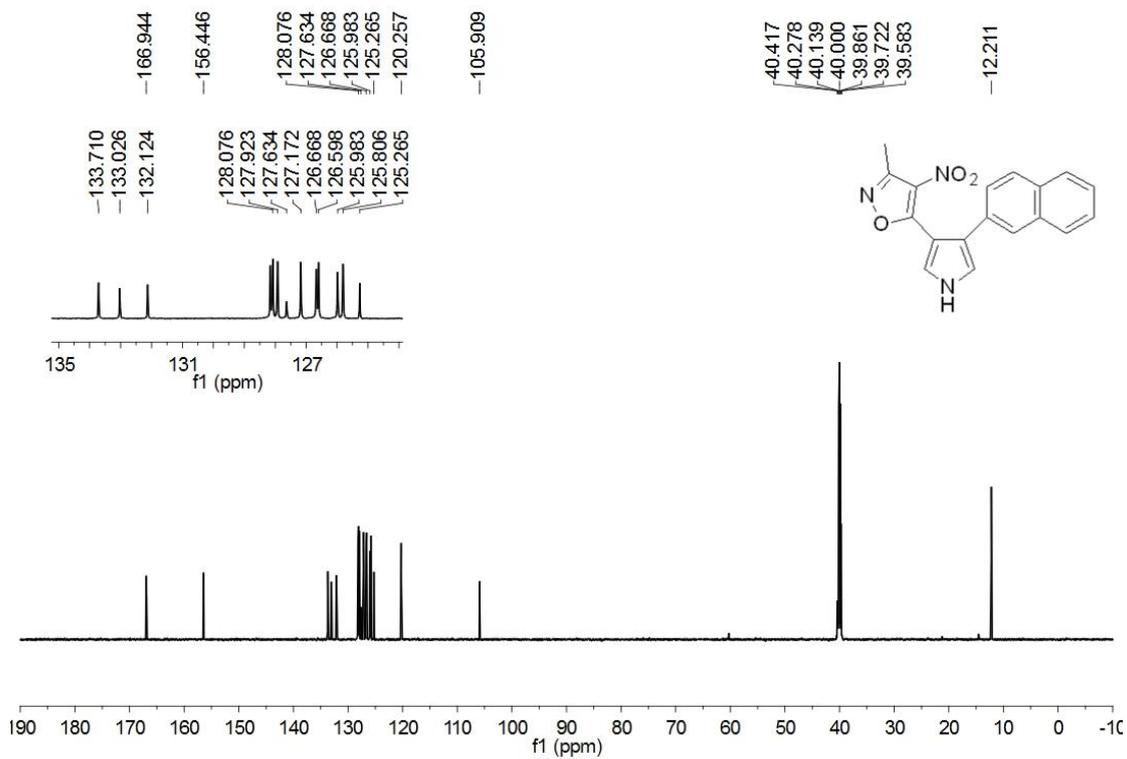
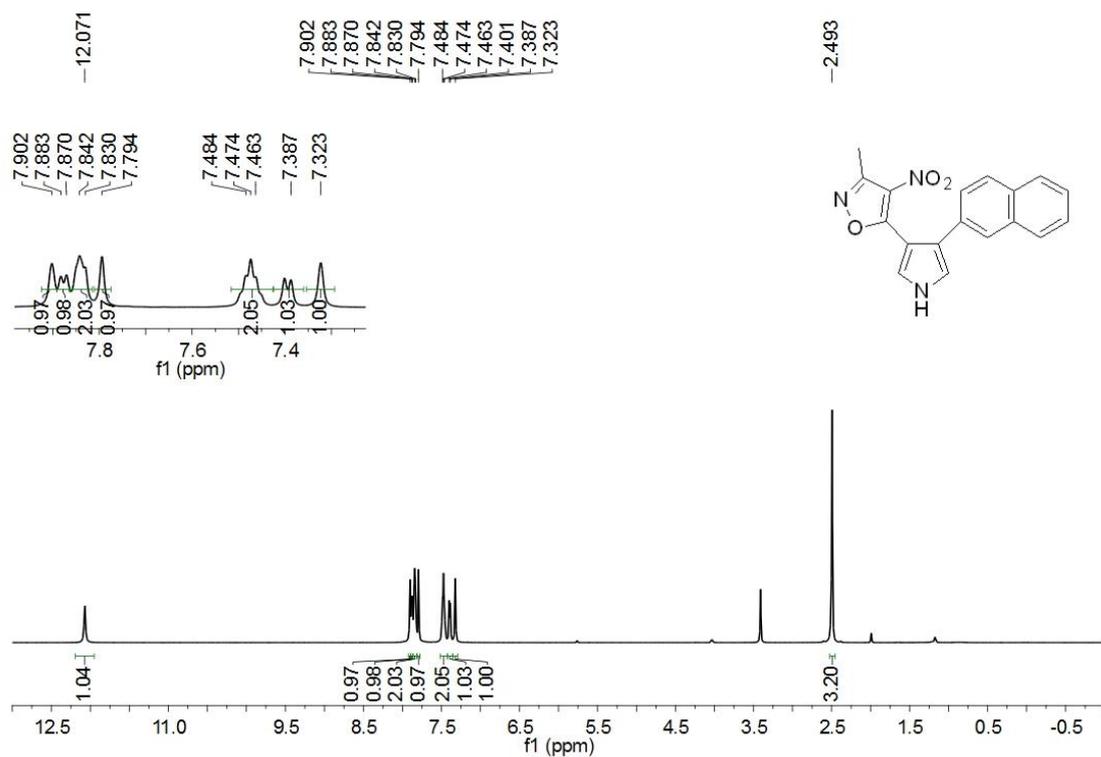
^1H NMR and ^{13}C NMR of **3an**



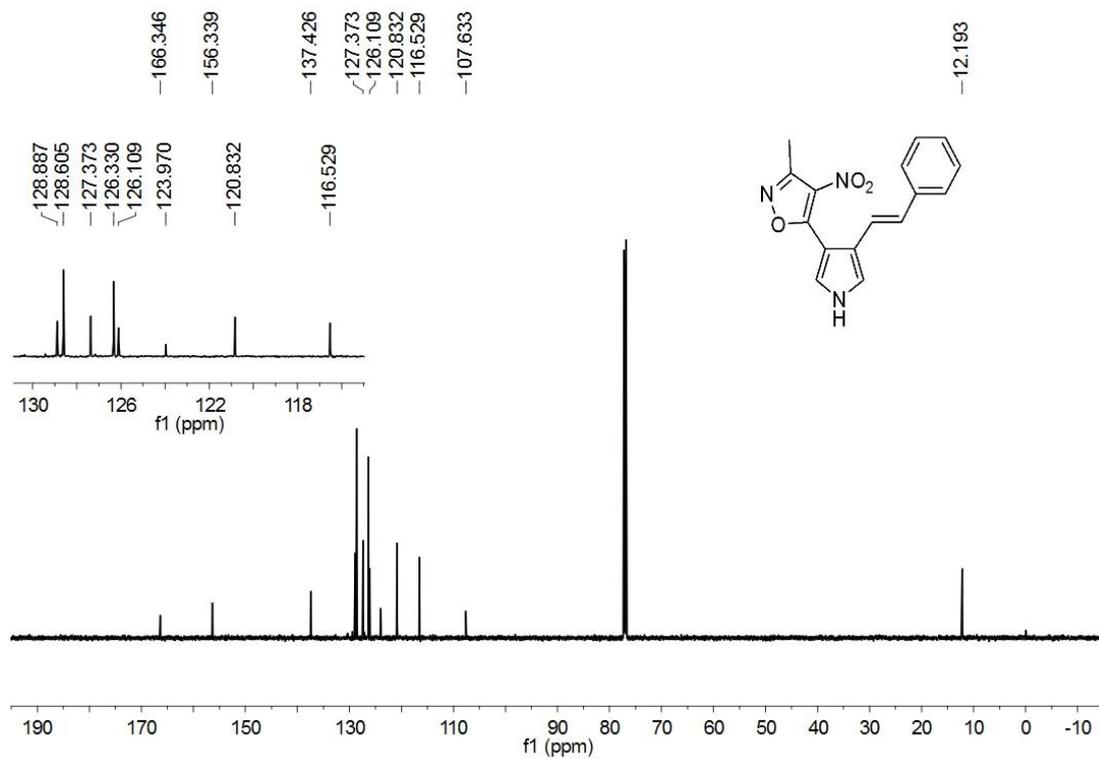
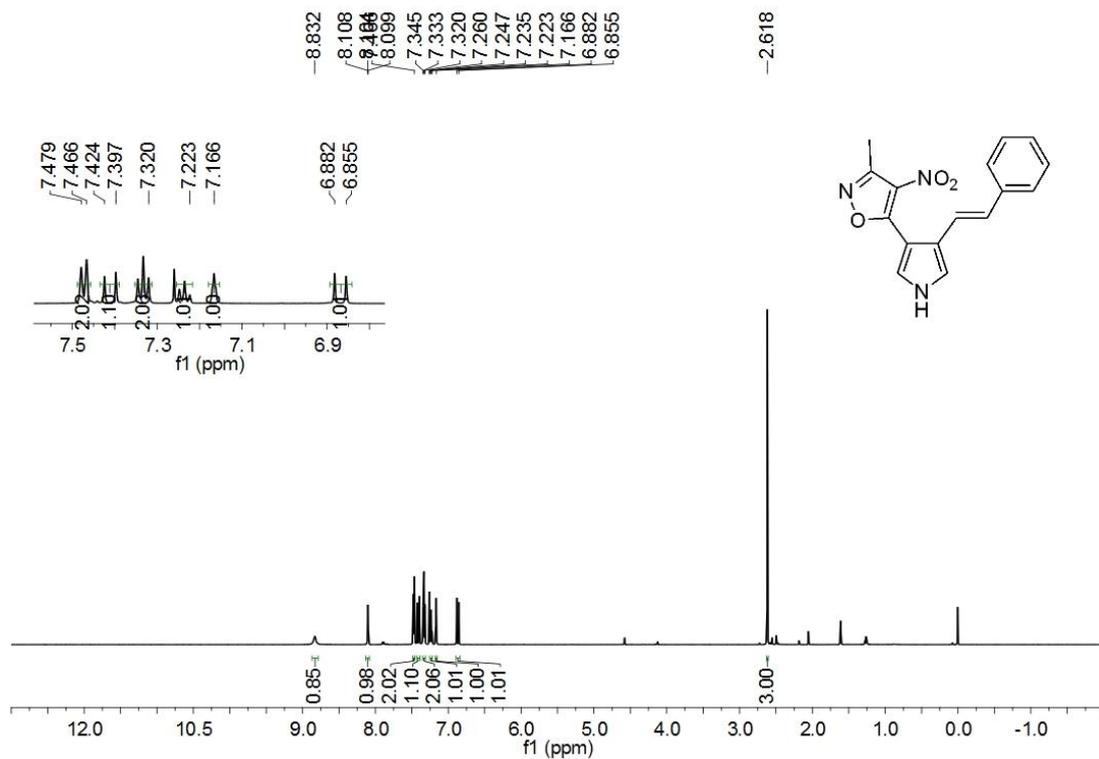
^1H NMR and ^{13}C NMR of **3ao**



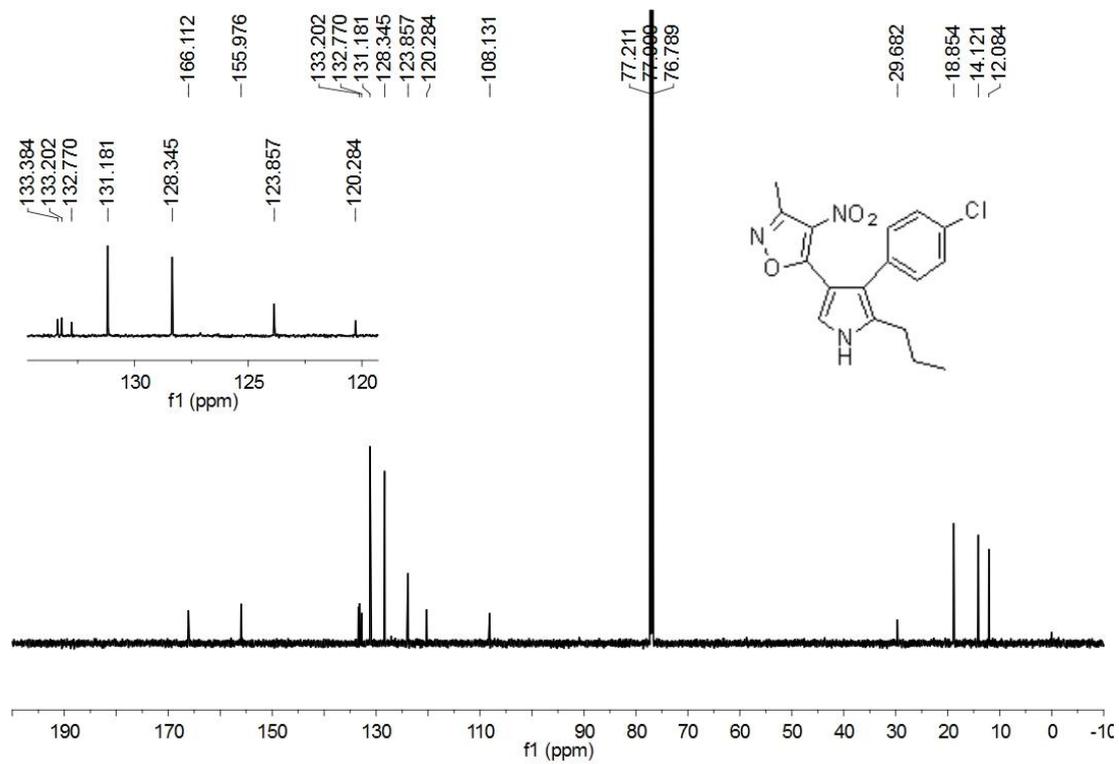
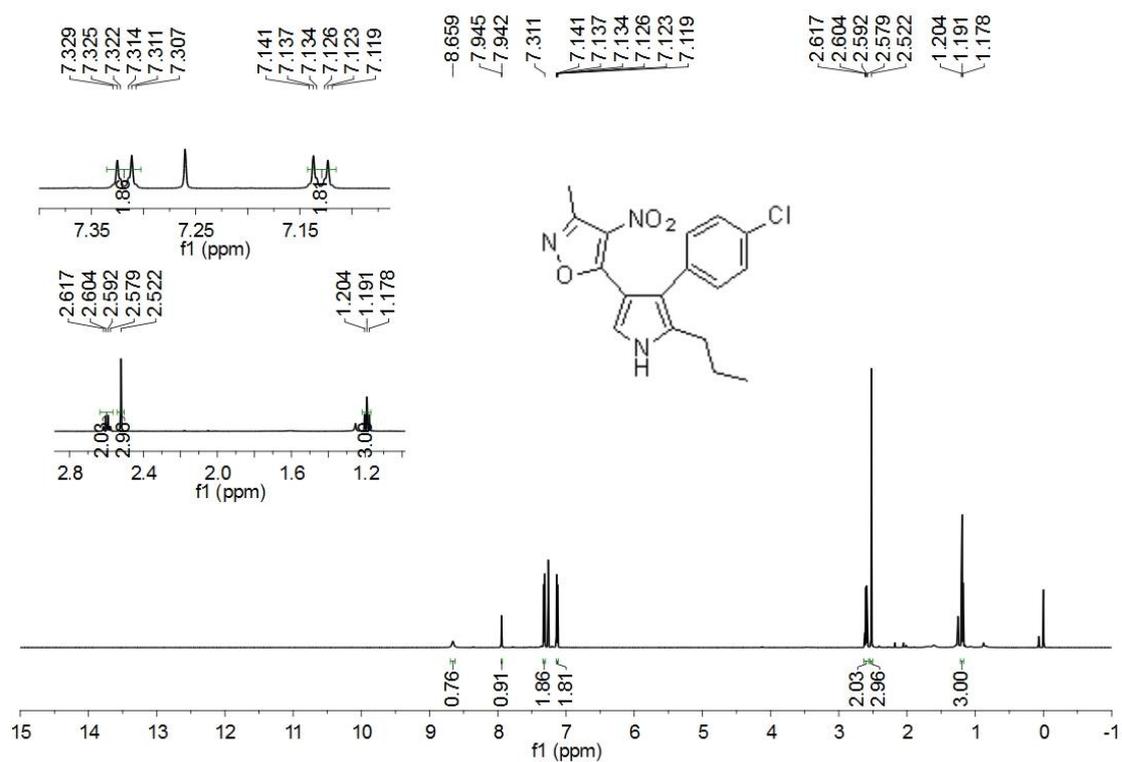
^1H NMR and ^{13}C NMR of **3ap**



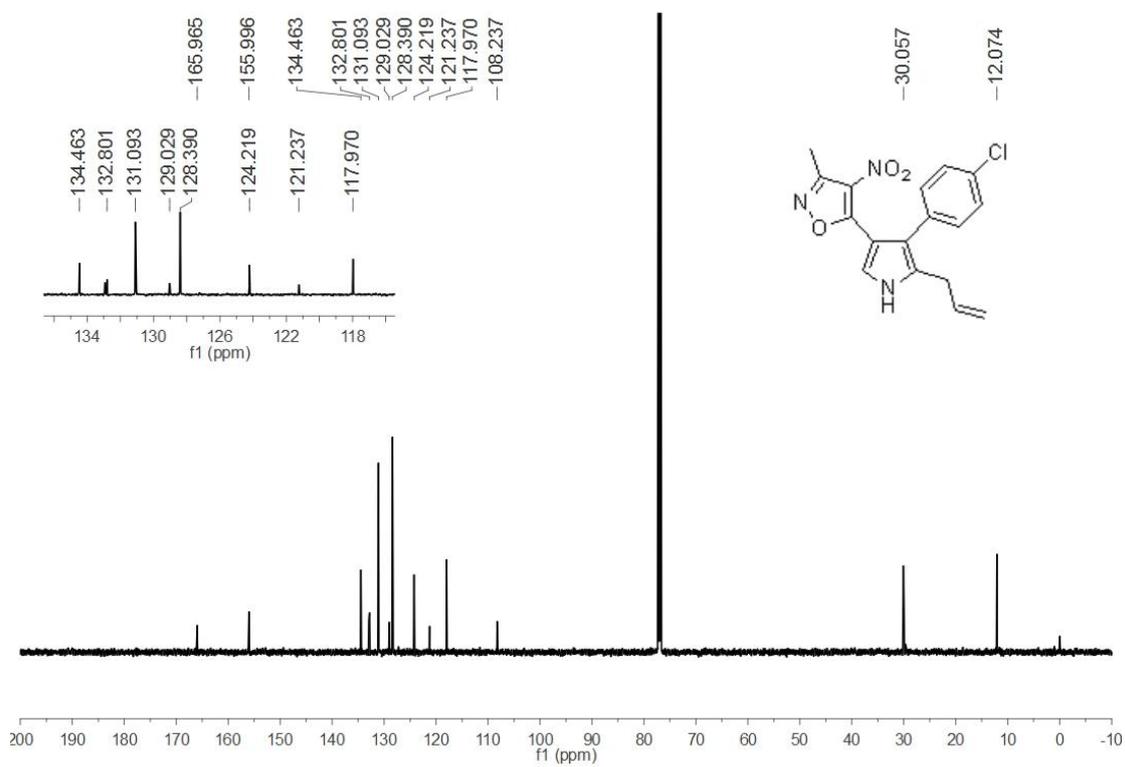
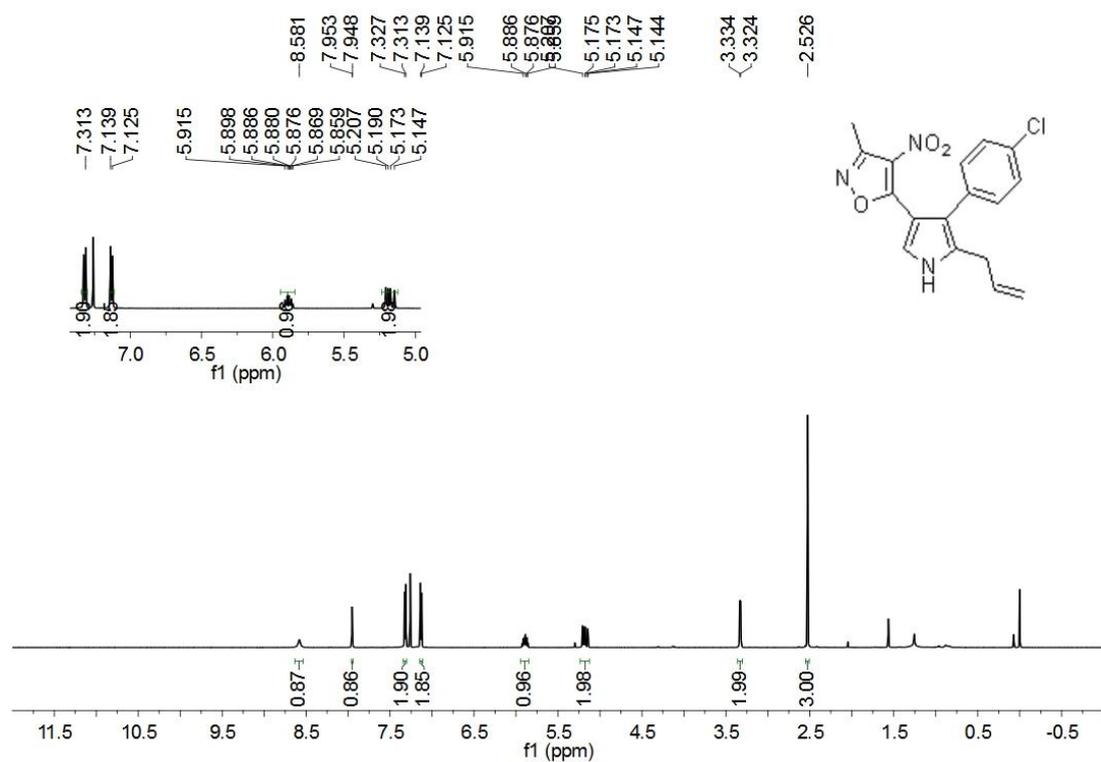
^1H NMR and ^{13}C NMR of **3aq**



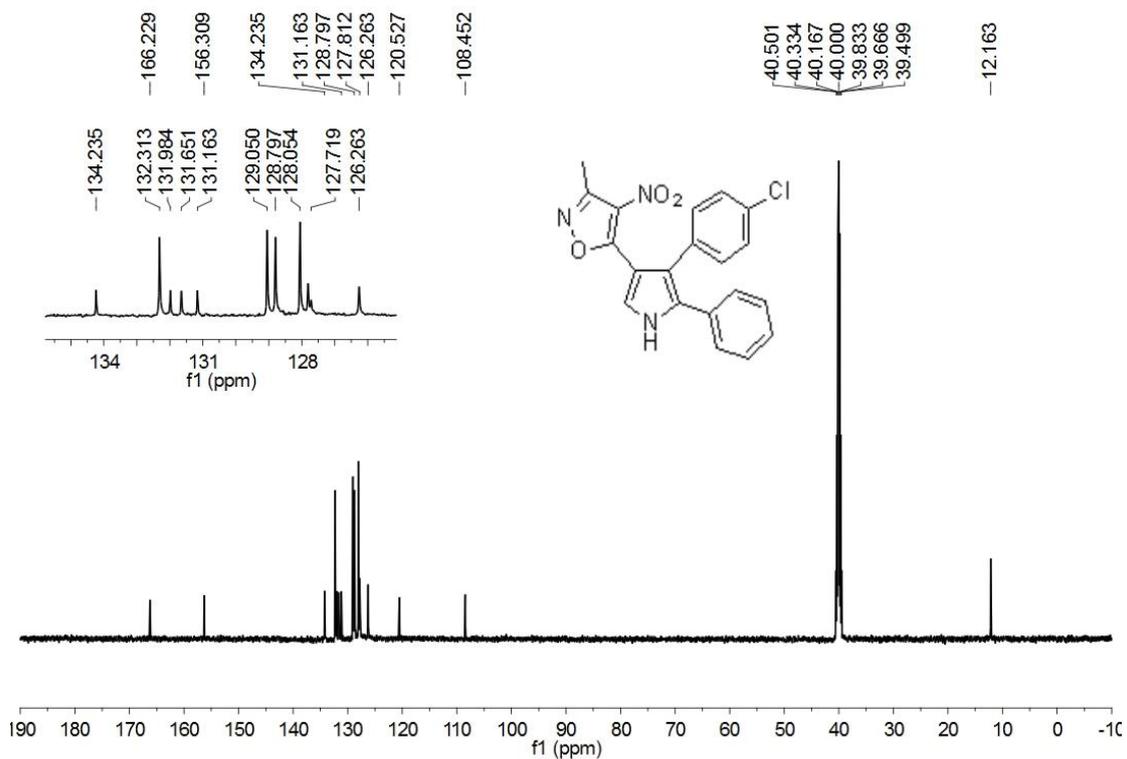
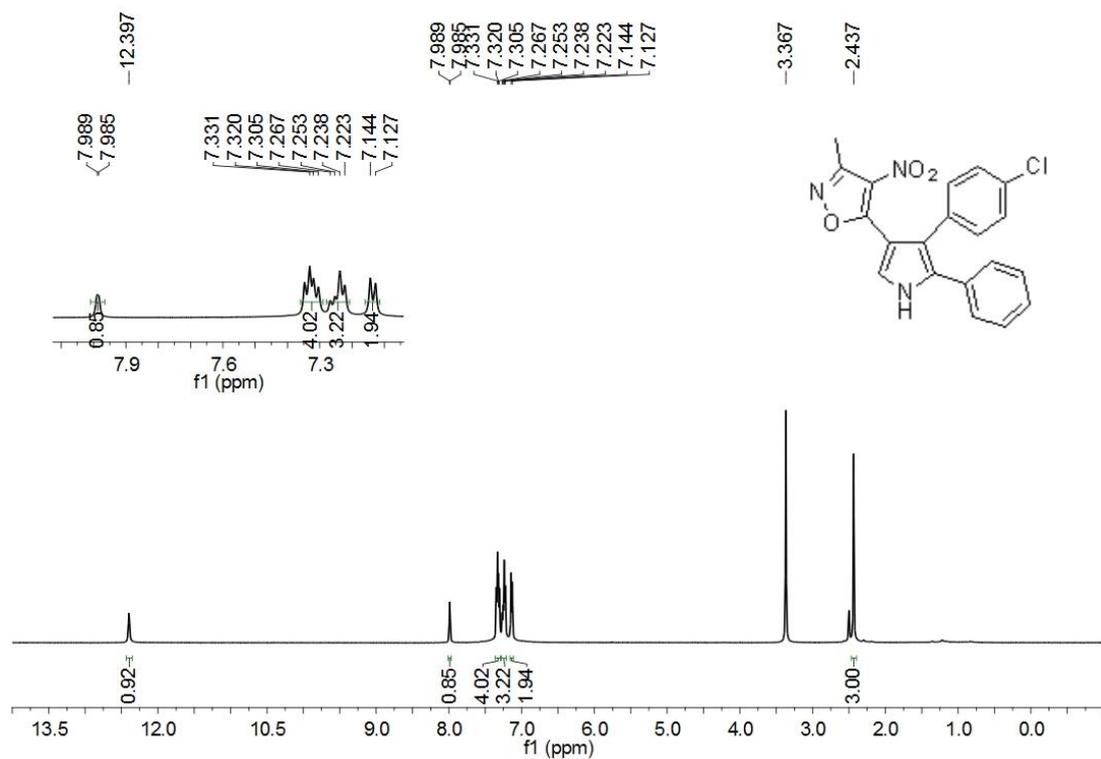
¹H NMR and ¹³C NMR of **3bb**



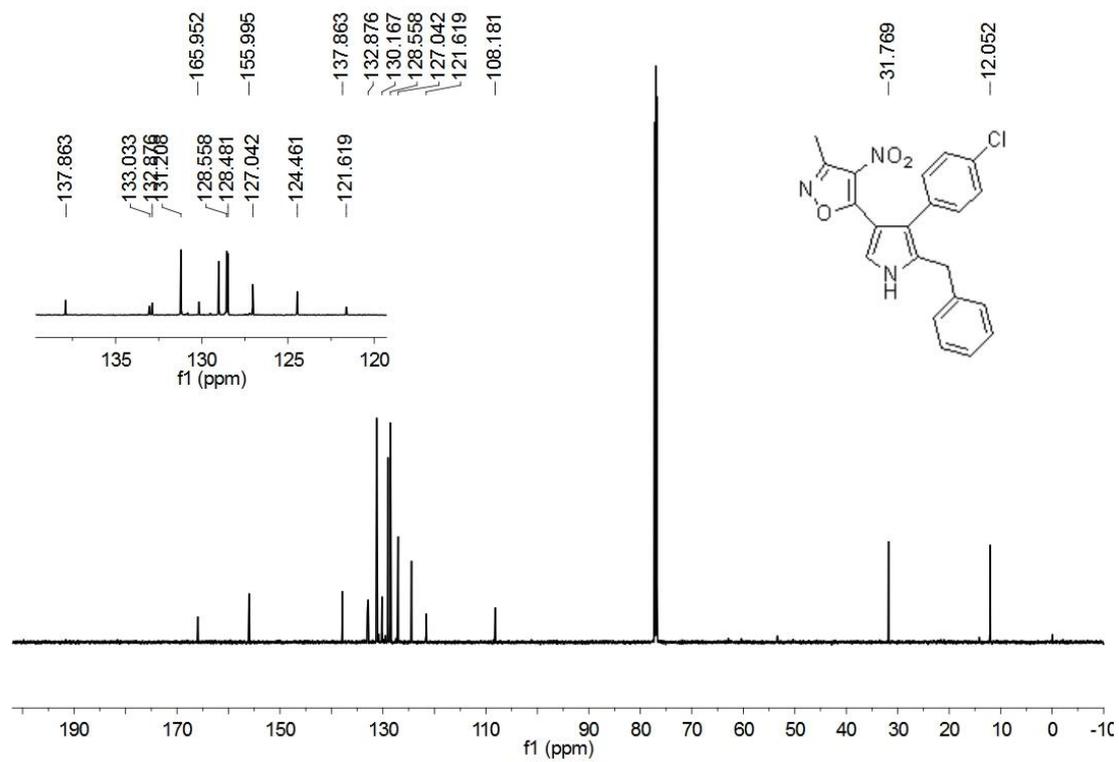
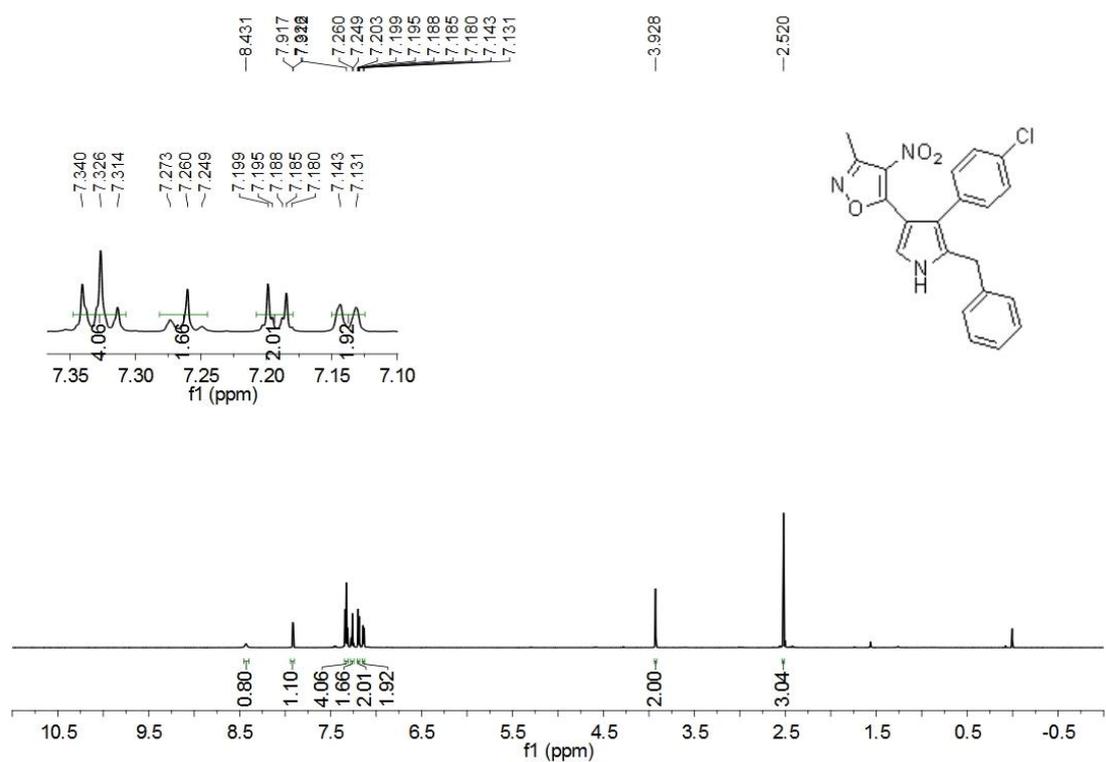
^1H NMR and ^{13}C NMR of **3cb**



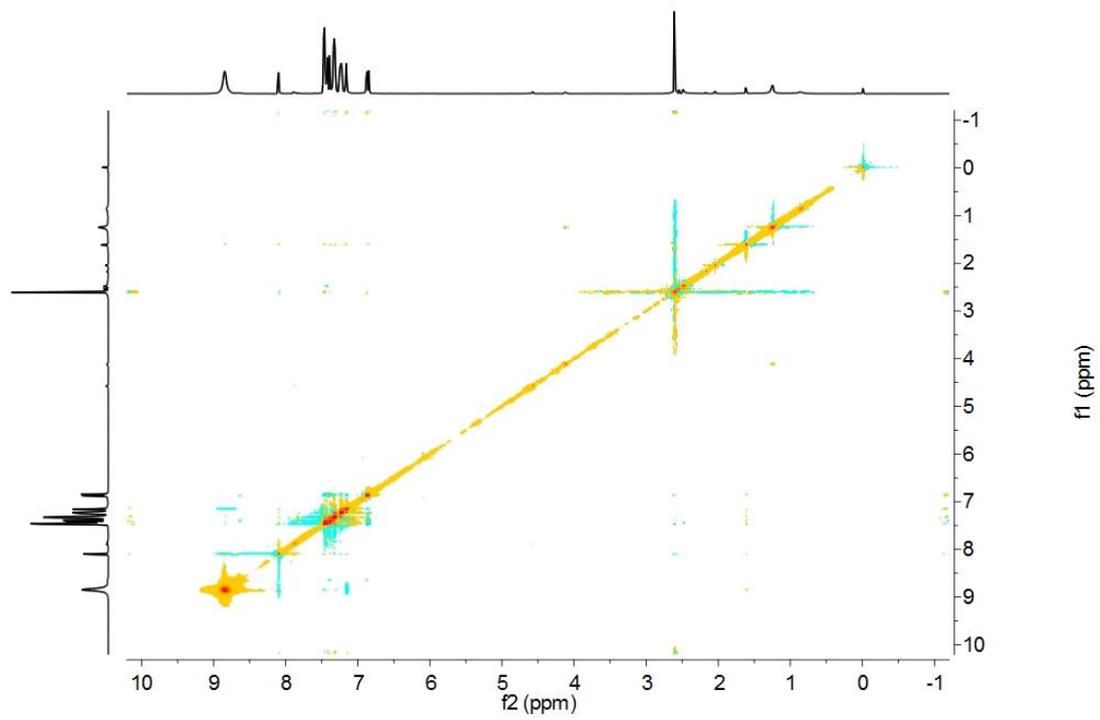
^1H NMR and ^{13}C NMR of **3db**



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

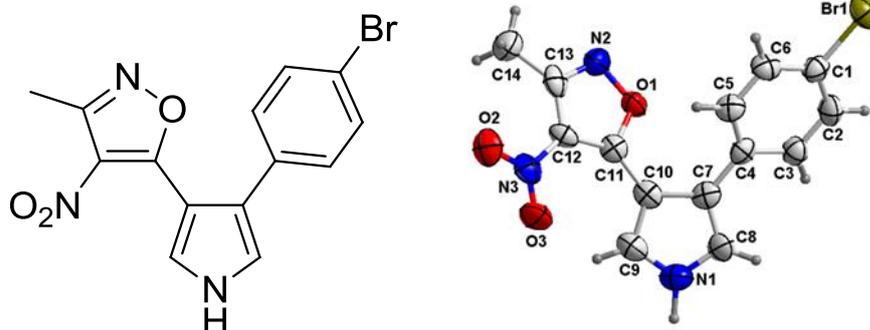


II. Copies of NOE-NMR spectra of compounds **3aq**



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

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



2. Crystal data for **3ac**

C₁₄H₁₀BrN₃O₃, Green solid, Mr = 348.15, monoclinic, space group C2/c, a = 7.6080(11), b = 7.7910(11), c = 23.078(3) Å, α = 90.000, β = 90.000, γ = 90.000 °, 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 > 2σ(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).