

Supporting Information

Silver-mediated three-component cycloaddition reaction for direct synthesis of 1-N-vinyl-substituted 1,2,3-triazoles

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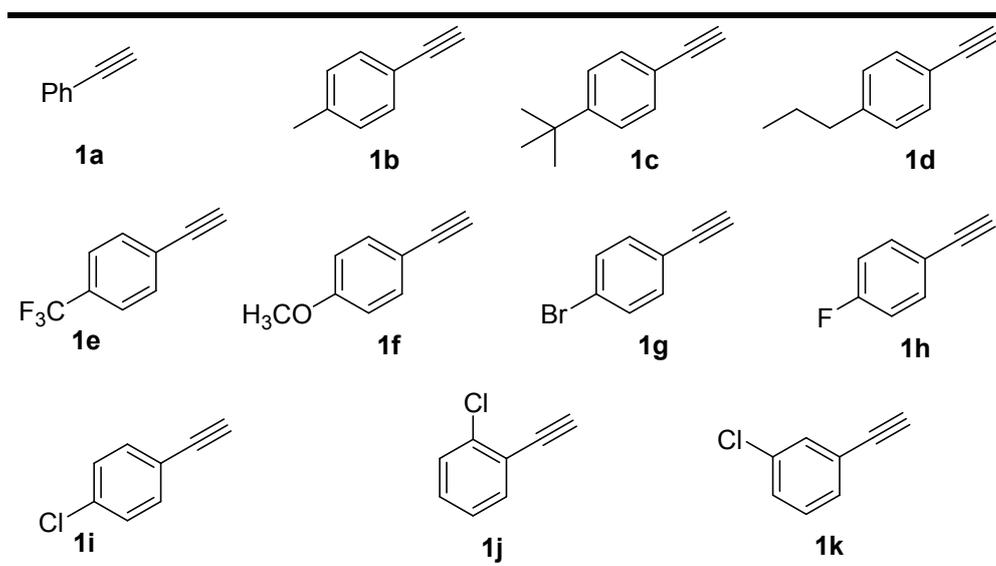
^bSchool of Chemical & Environmental Engineering, Wuyi University, Jiangmen, Guangdong Province

529090, China.

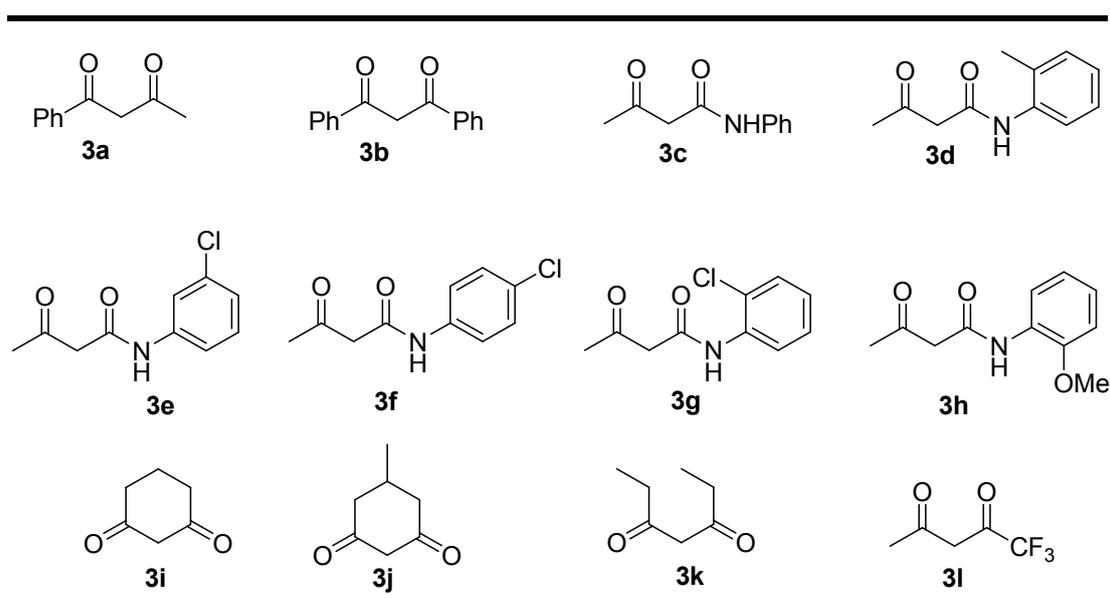
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Substrates employed for the reaction



Scheme S1. Phenylacetylenes employed for the synthesis of 1-N-vinyl-1,2,3-triazoles.



Scheme S2. 1,3-Dicarbonyls employed for the synthesis of 1-N-vinyl-1,2,3-triazoles.

Single Crystal X-ray Diffraction of 4aa'

White block-like single crystals of **4aa'** were grown by layering a dichloromethane solution with n-hexane at ambient temperature. X-Ray diffraction data of one these crystals were collected on a Bruker SMART. The measurements were performed with Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$). Data were collected at 296 (2) K, using the phi and

omega scans to a maximum θ value of 25.027° . The data were refined by full-matrix least-squares techniques on F^2 with SHELXL-2014. And the structures were solved by direct methods SHELXL-2014. All the non-hydrogen atoms were refined anisotropically. The hydrogen atoms were included at geometrically idealized positions. An ORTEP representation of the structure is shown below.

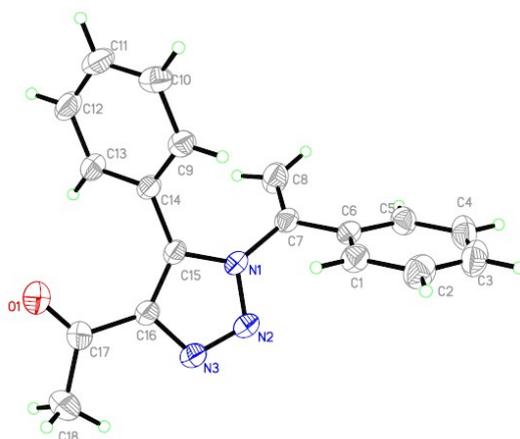


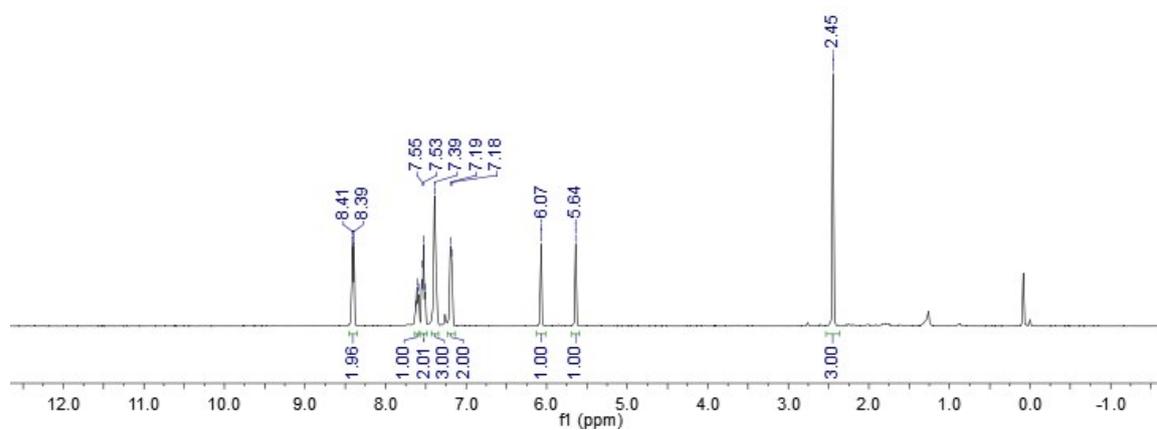
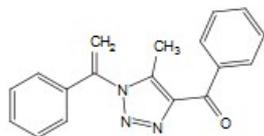
Figure S1. ORTEP drawing of **4aa'** with the numbering scheme

Table S5. Crystal data and structure refinement for **4aa'**

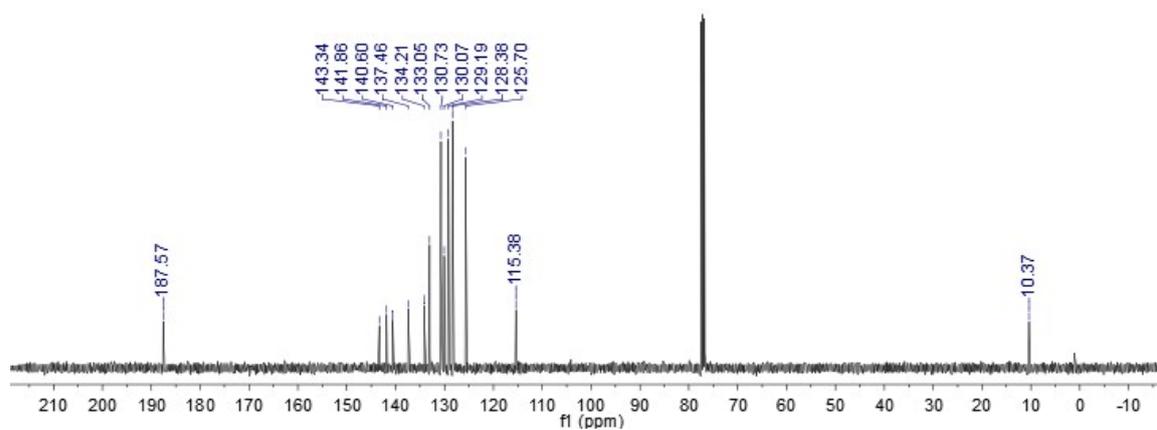
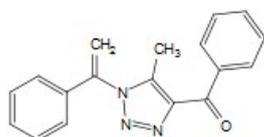
| | | |
|---------------------------------|--|-----------------|
| Identification code | 4aa' | |
| Empirical formula | $C_{18}H_{15}N_3O$ | |
| Formula weight | 289.33 | |
| Temperature | 296 (2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 9.405(7) Å | a = 84.218(8)°. |
| | b = 9.471(7) Å | b = 63.798(7)°. |
| | c = 9.815(7) Å | g = 78.437(8)°. |
| Volume | 768.5(10) Å ³ | |
| Z | 2 | |
| Density (calculated) | 1.250 Mg/m ³ | |
| Absorption coefficient | 0.080 mm ⁻¹ | |
| F(000) | 304 | |
| Crystal size | 0.21 x 0.2 x 0.19 mm ³ | |
| Theta range for data collection | 2.992 to 25.027°. | |
| Index ranges | -11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -11 ≤ l ≤ 11 | |
| Reflections collected | 7291 | |

NMR spectra of the obtained compounds

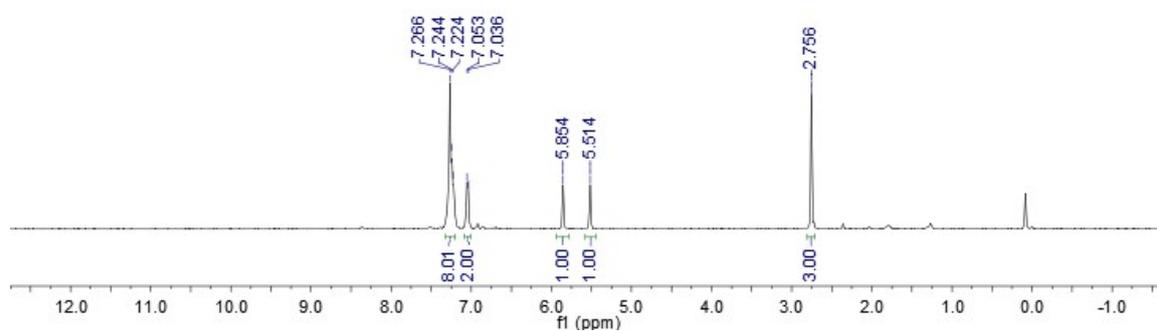
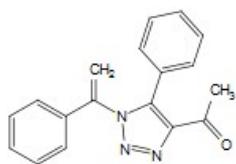
$^1\text{H-NMR}$ spectrum of 4aa



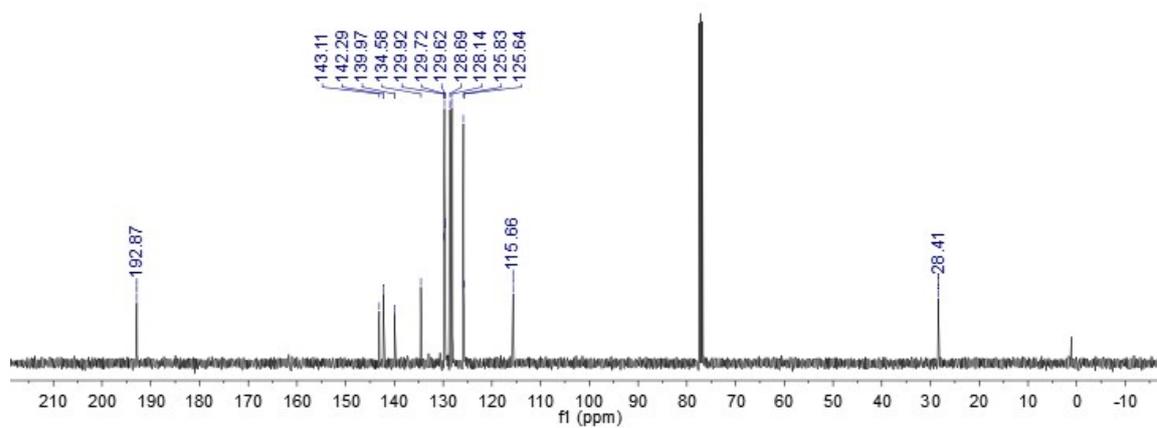
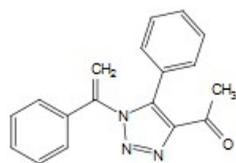
$^{13}\text{C-NMR}$ spectrum of 4aa



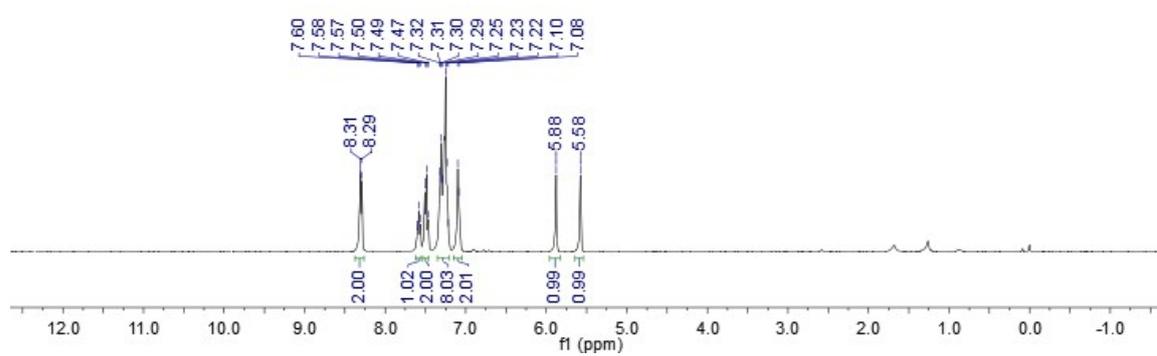
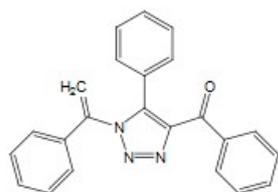
¹H-NMR spectrum of 4aa'



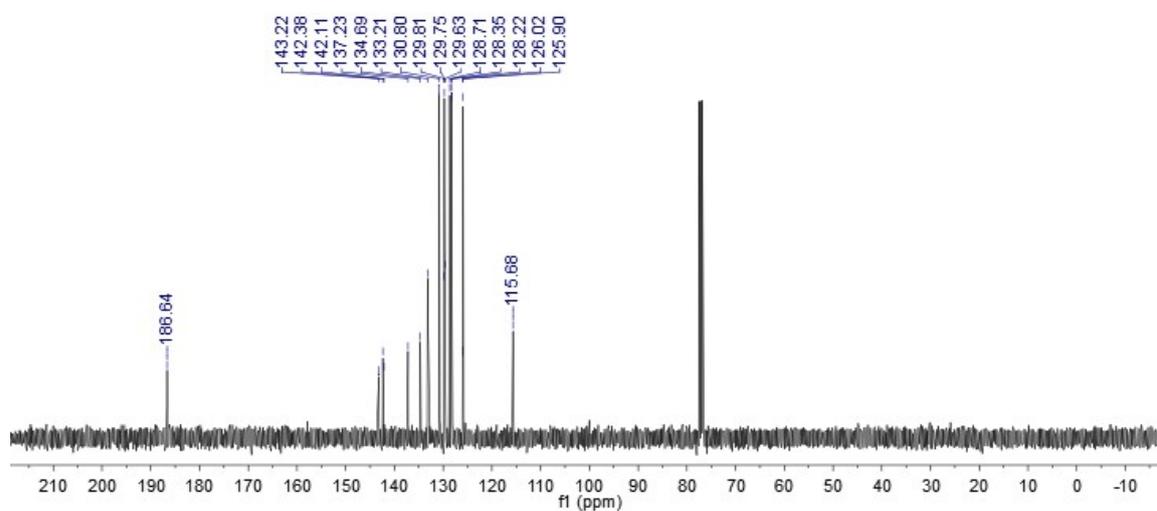
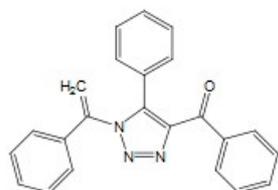
¹³C-NMR spectrum of 4aa'



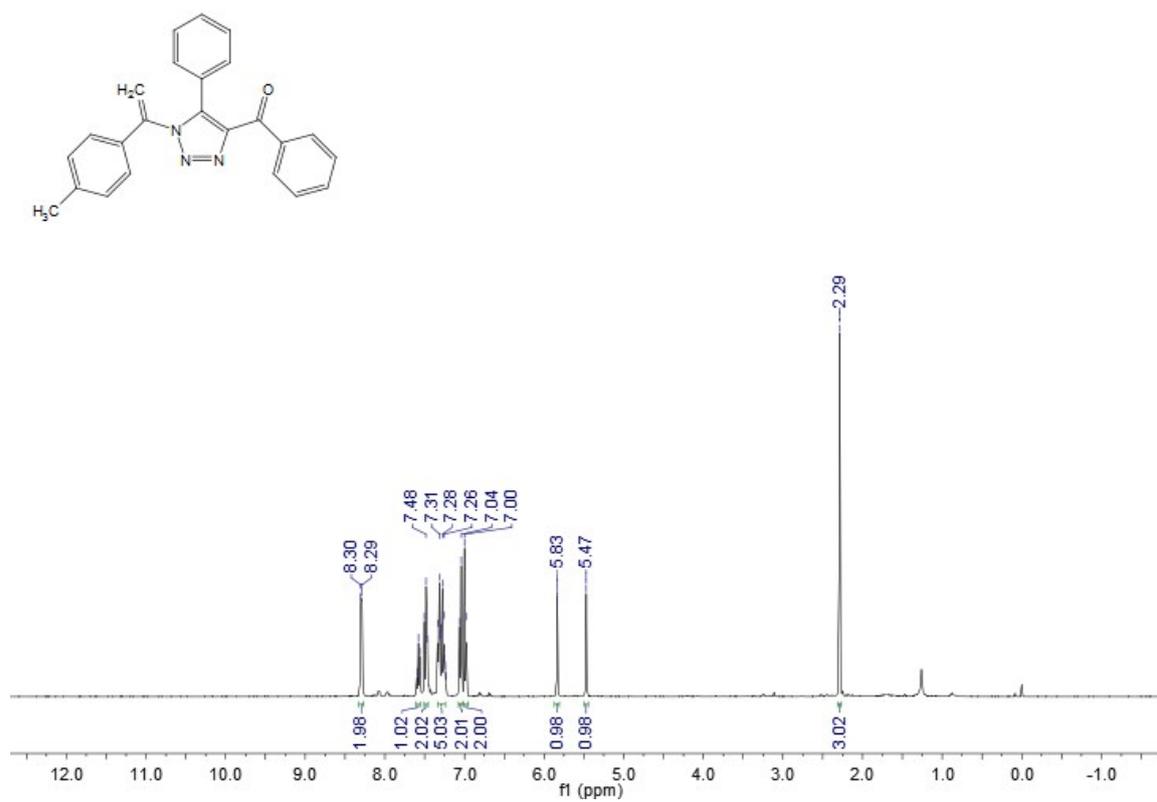
¹H-NMR spectrum of 4ab



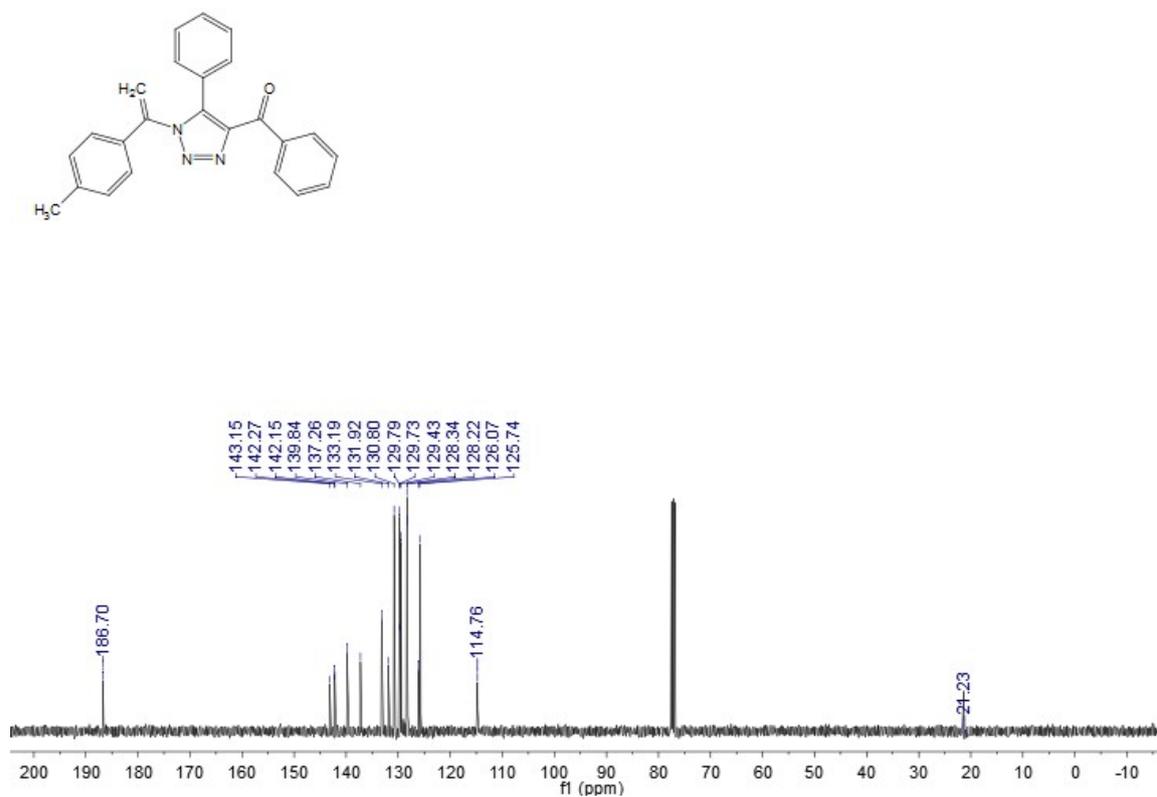
¹³C-NMR spectrum of 4ab



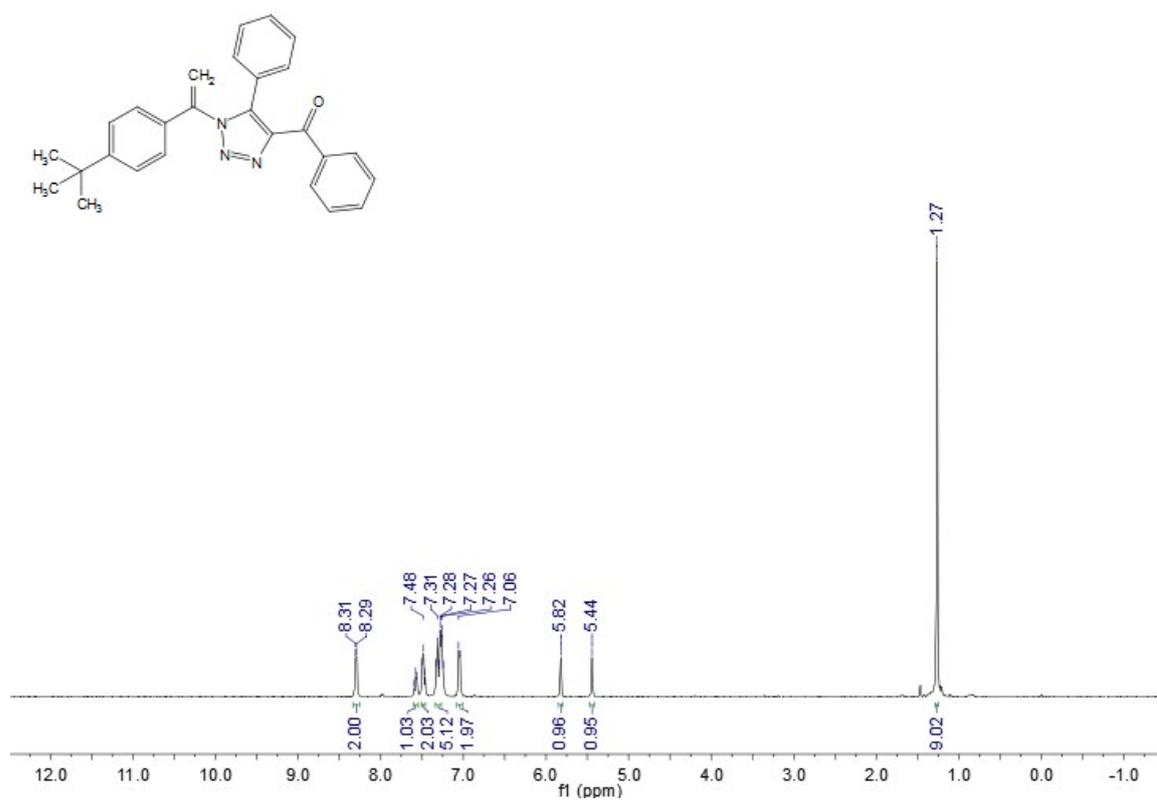
¹H-NMR spectrum of 4bb



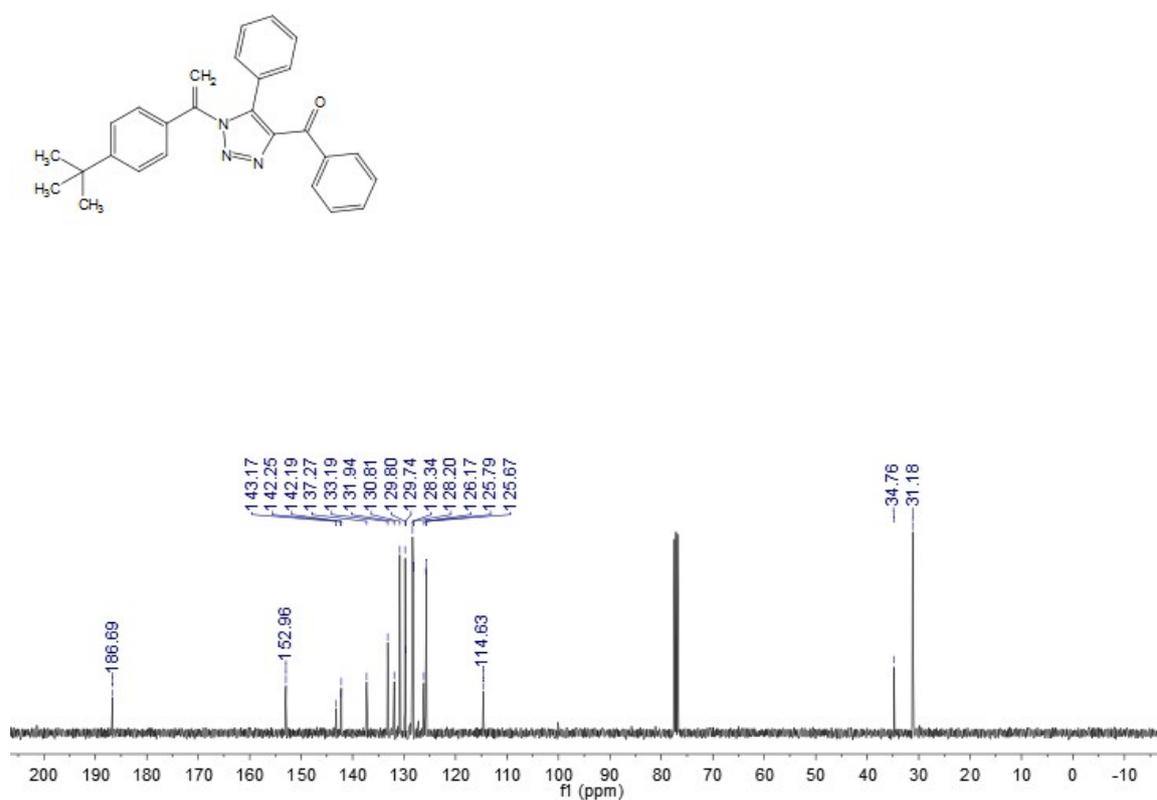
¹³C-NMR spectrum of 4bb



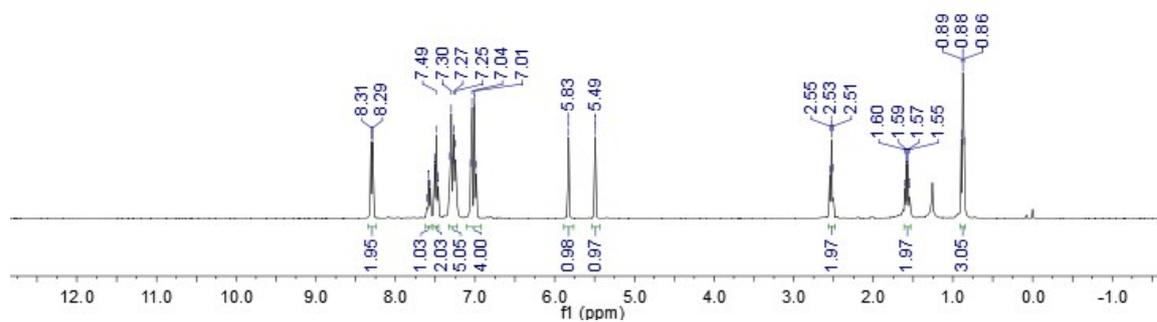
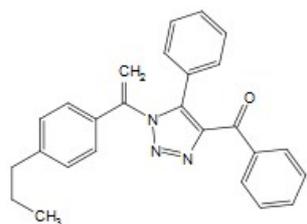
¹H-NMR spectrum of 4cb



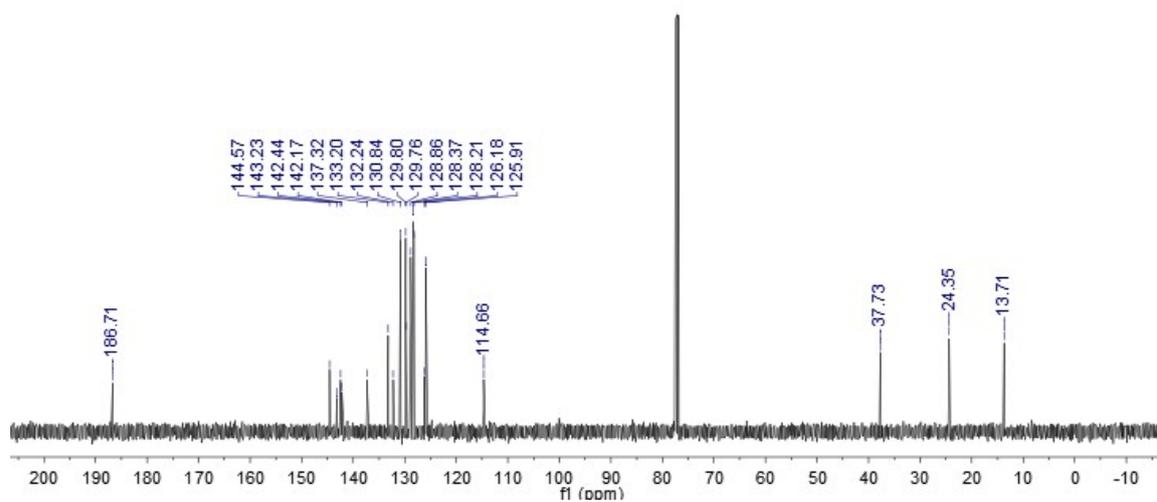
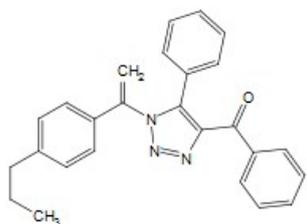
¹³C-NMR spectrum of 4cb



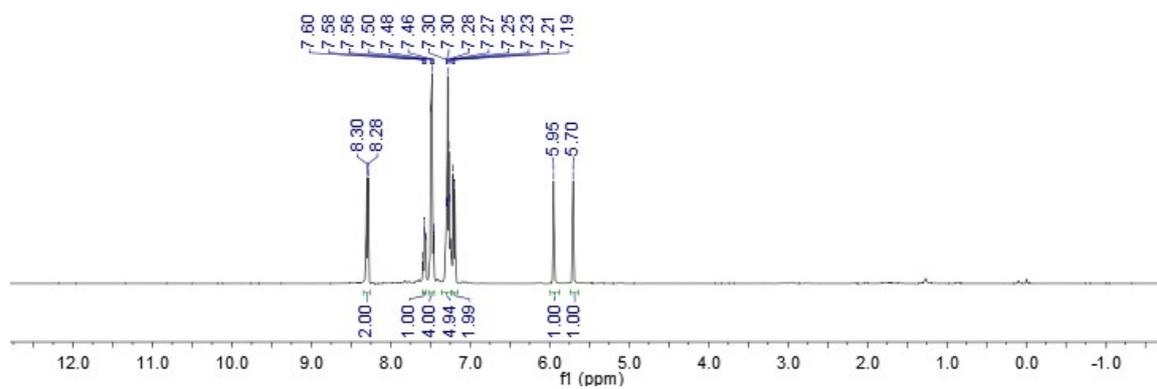
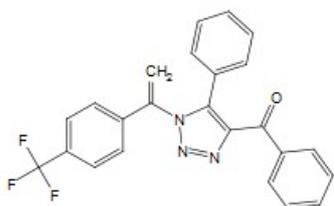
¹H-NMR spectrum of 4db



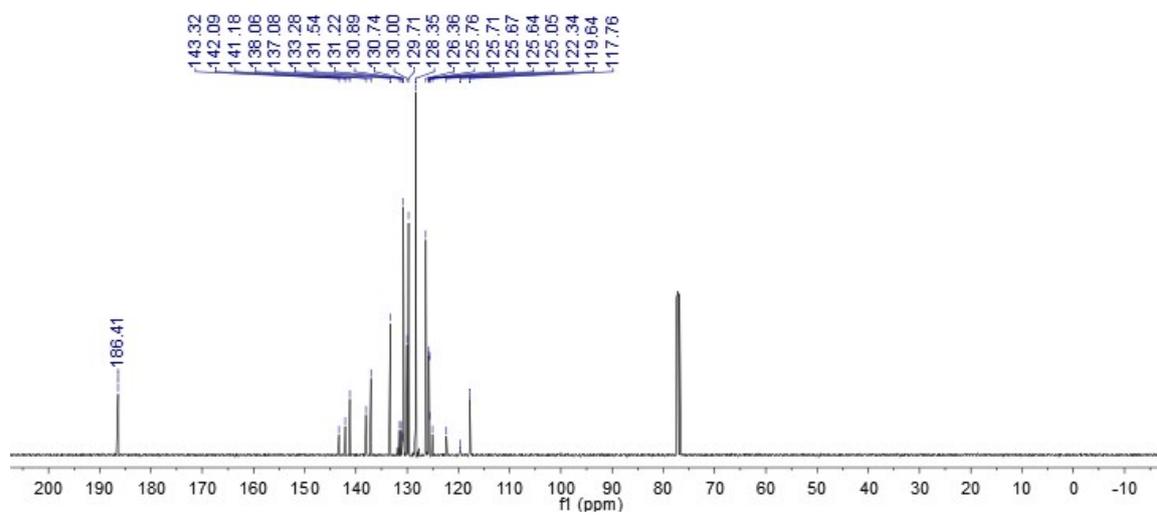
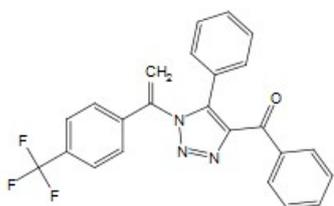
¹³C-NMR spectrum of 4db



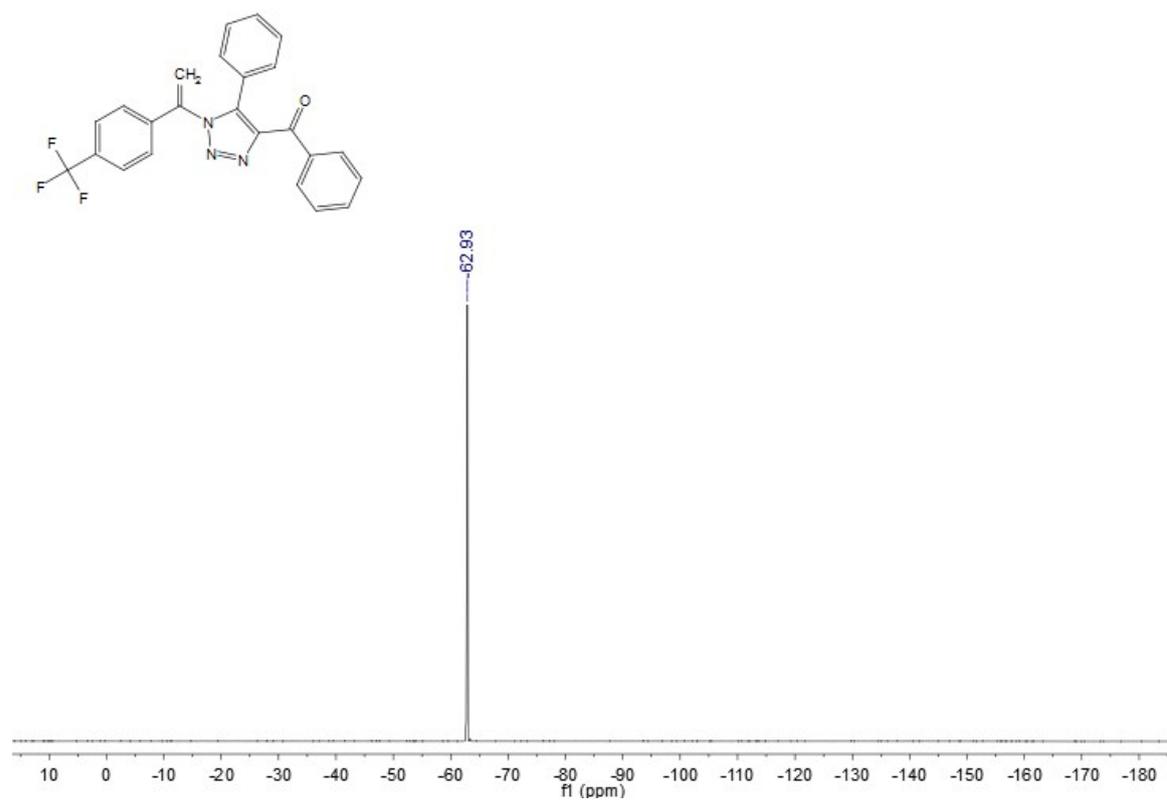
¹H-NMR spectrum of 4eb



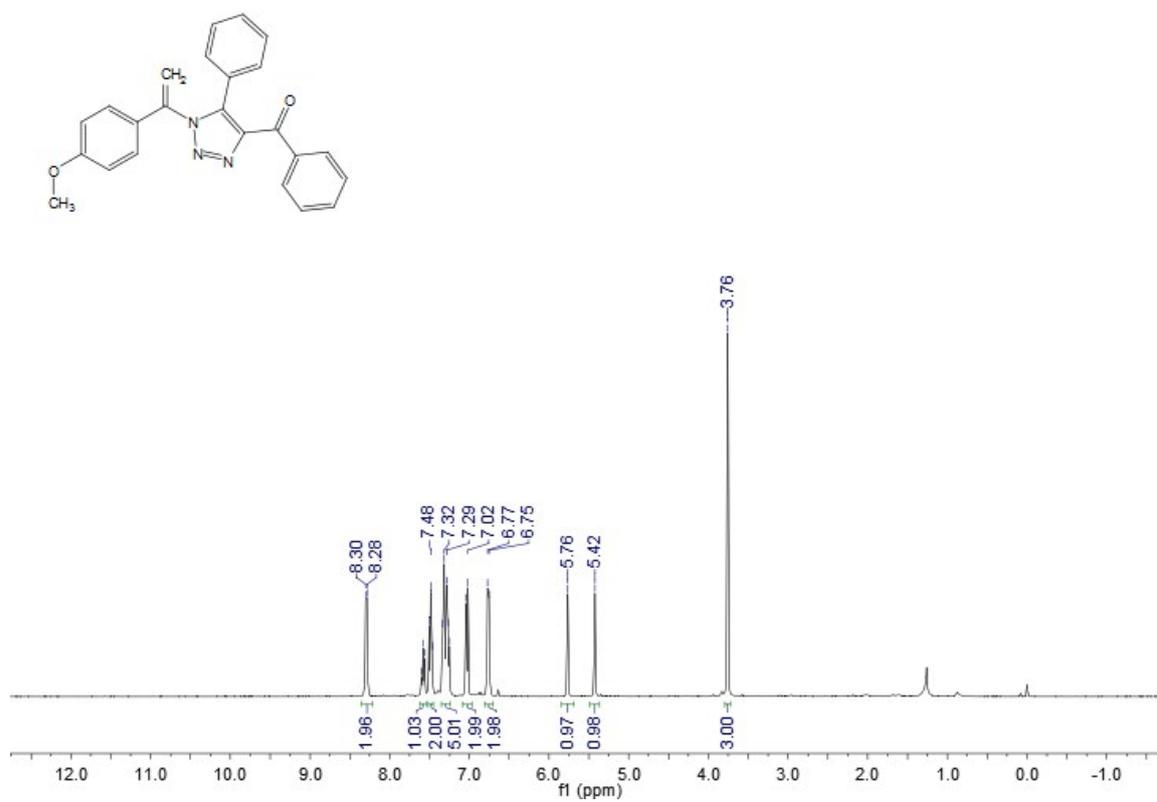
¹³C-NMR spectrum of 4eb



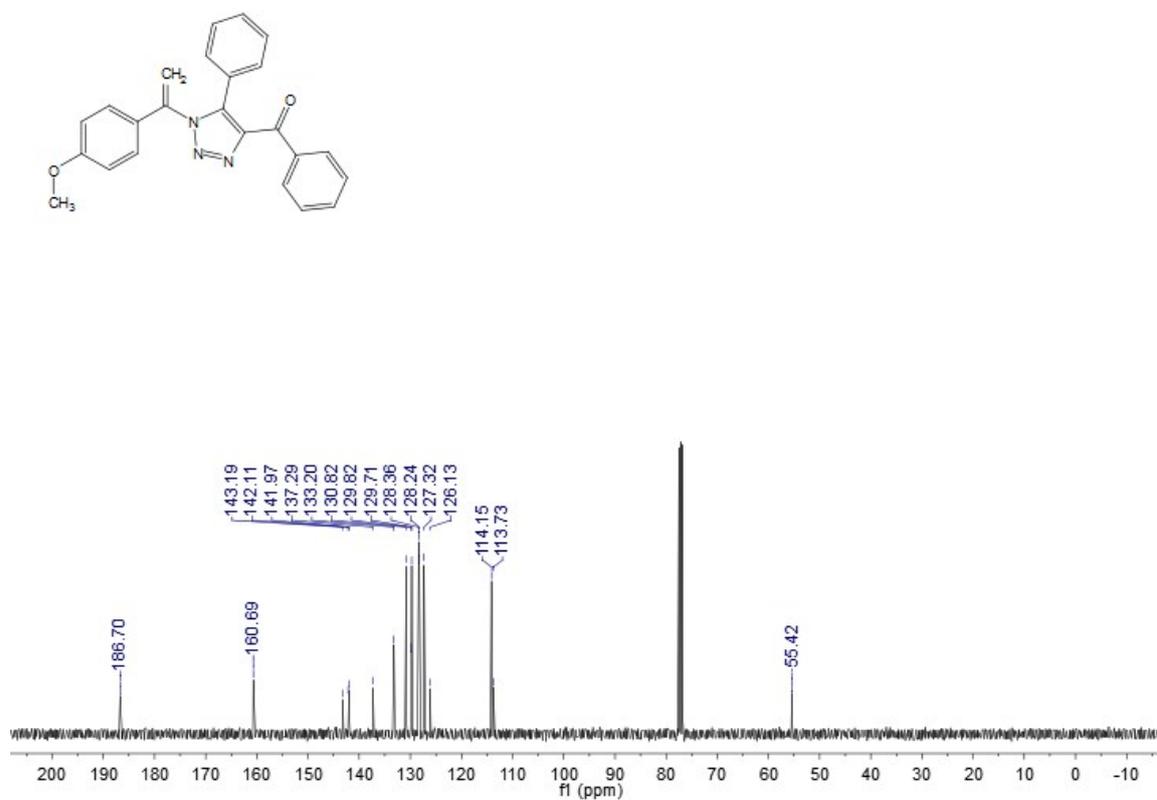
¹⁹F-NMR spectrum of 4eb



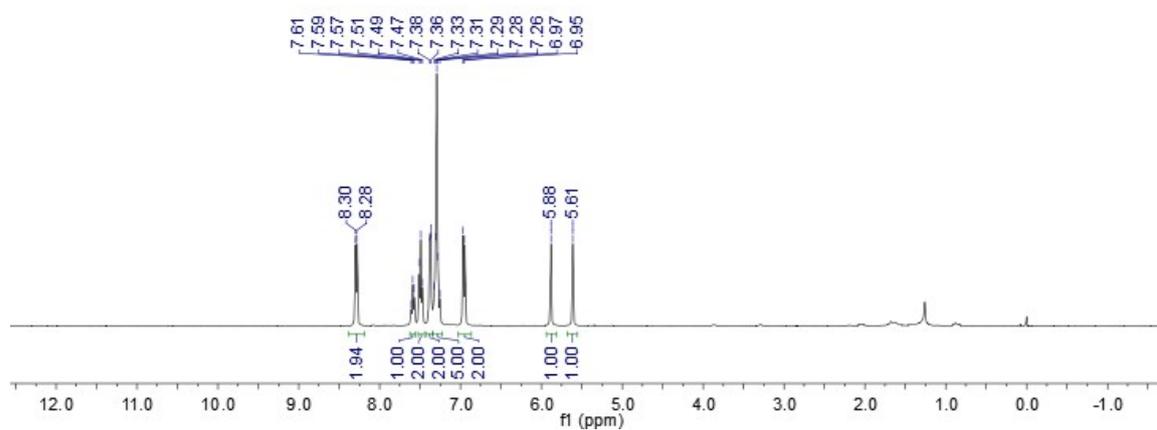
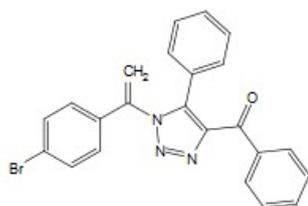
¹H-NMR spectrum of 4fb



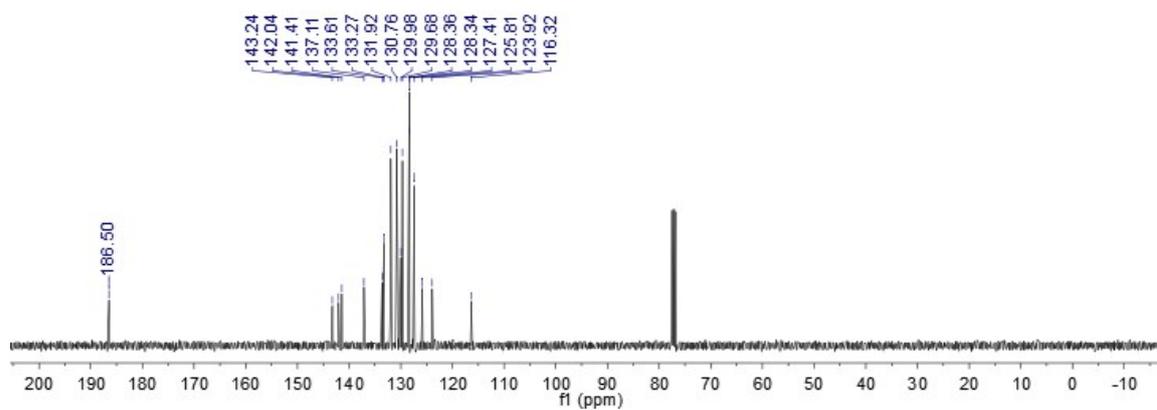
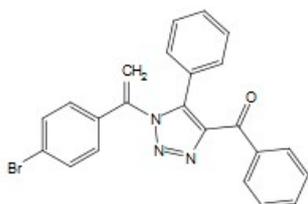
¹³C-NMR spectrum of 4fb



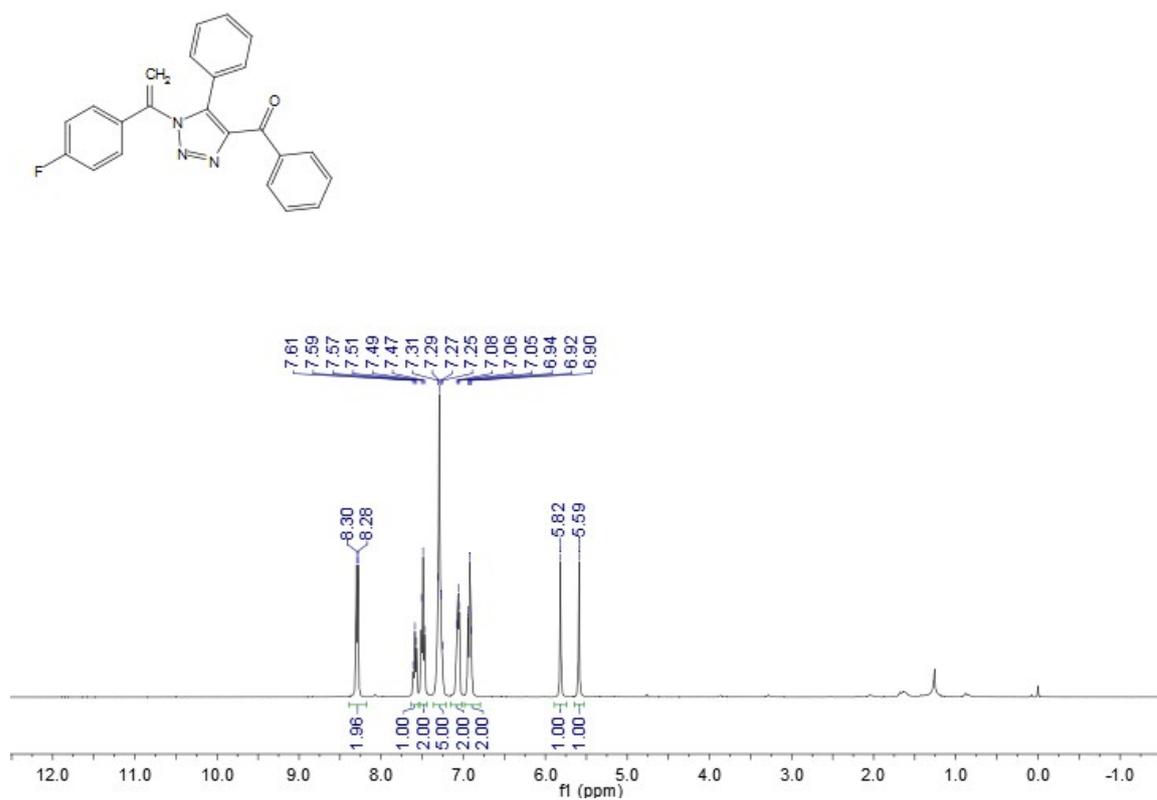
¹H-NMR spectrum of 4gb



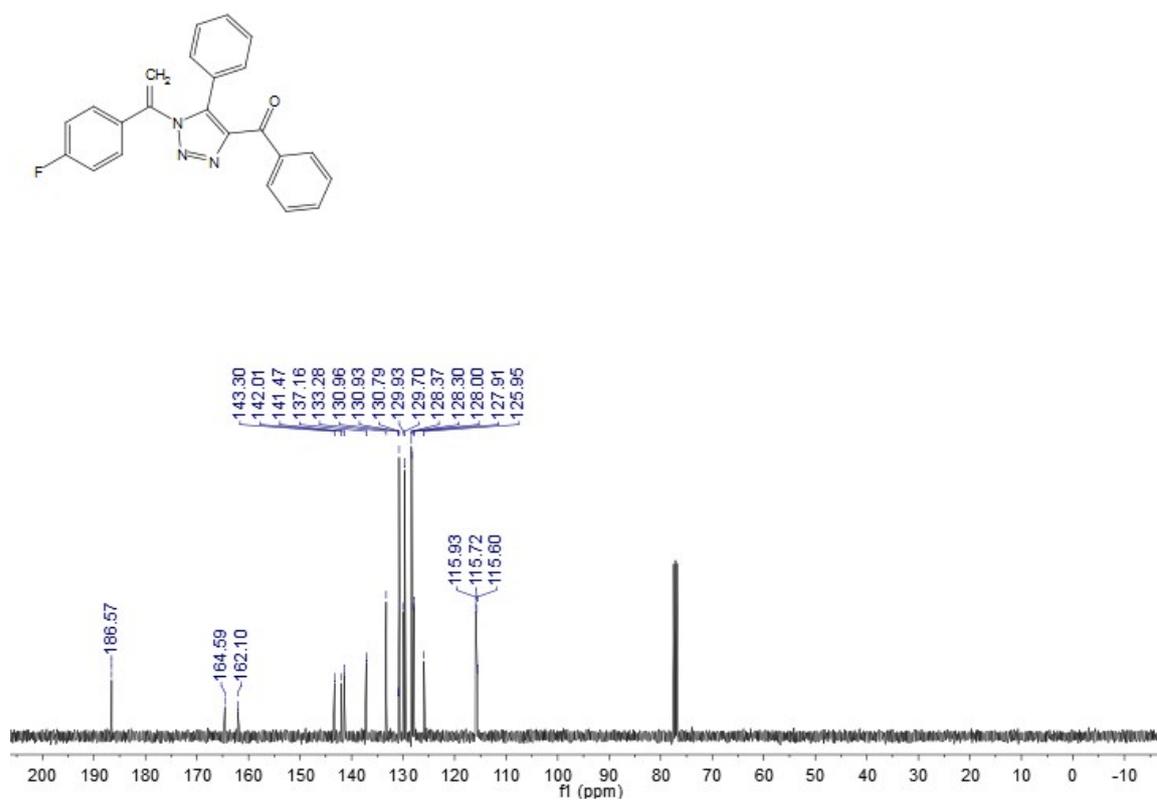
¹³C-NMR spectrum of 4gb



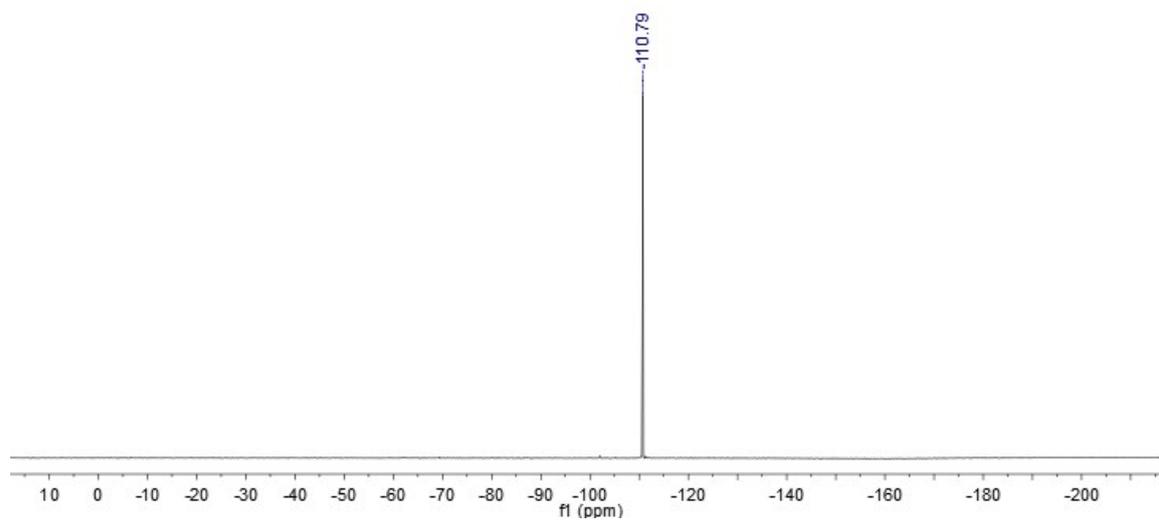
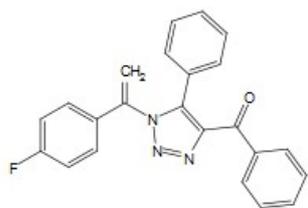
¹H-NMR spectrum of 4hb



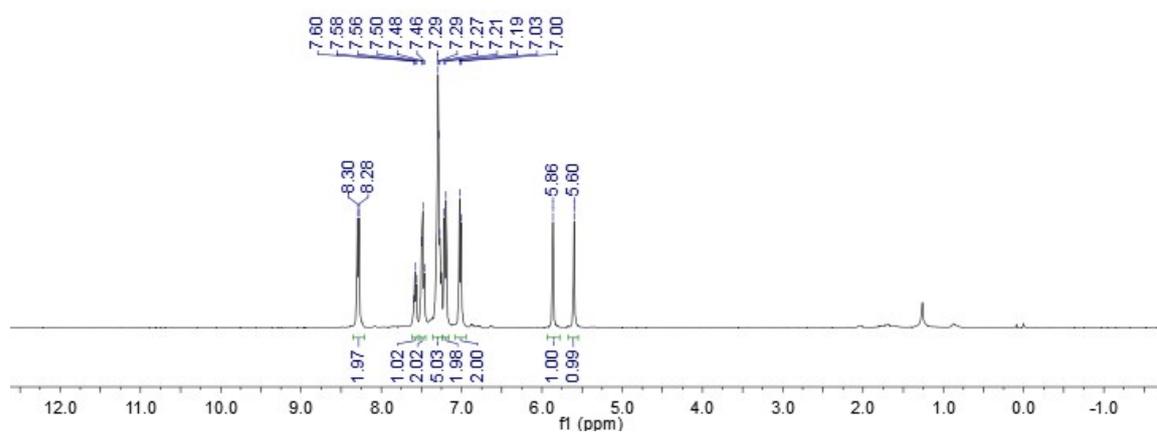
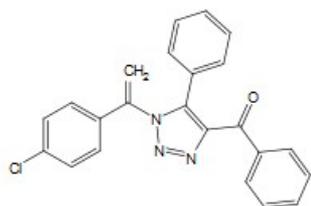
¹³C-NMR spectrum of 4hb



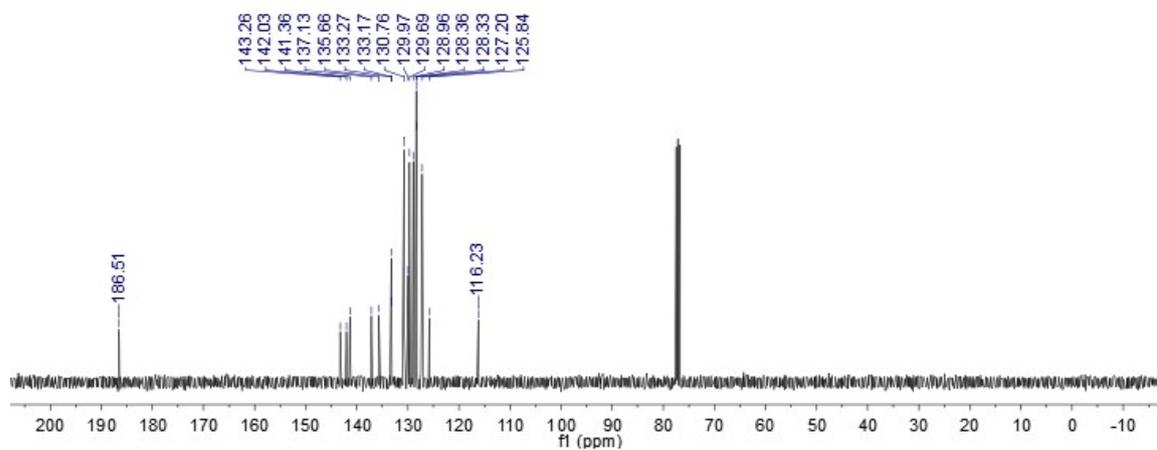
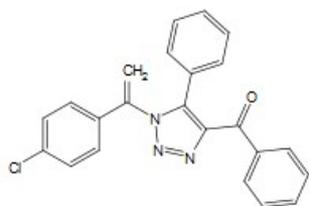
^{19}F -NMR spectrum of 4hb



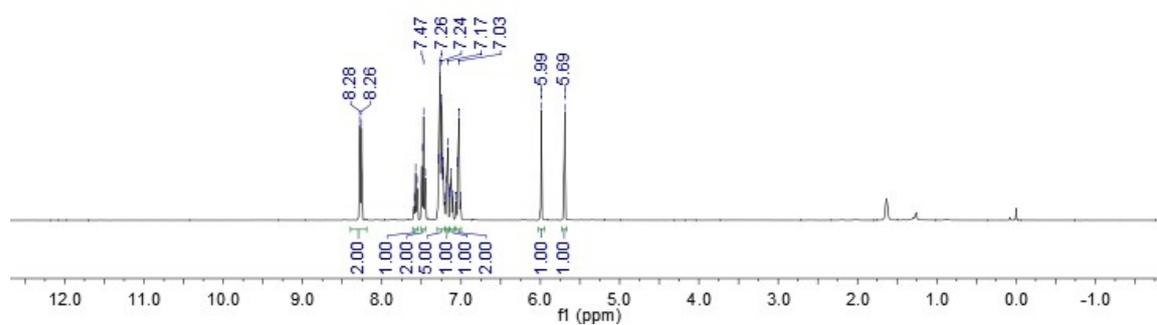
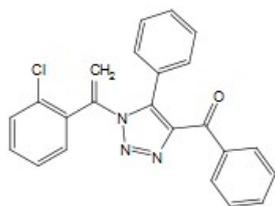
¹H-NMR spectrum of 4ib



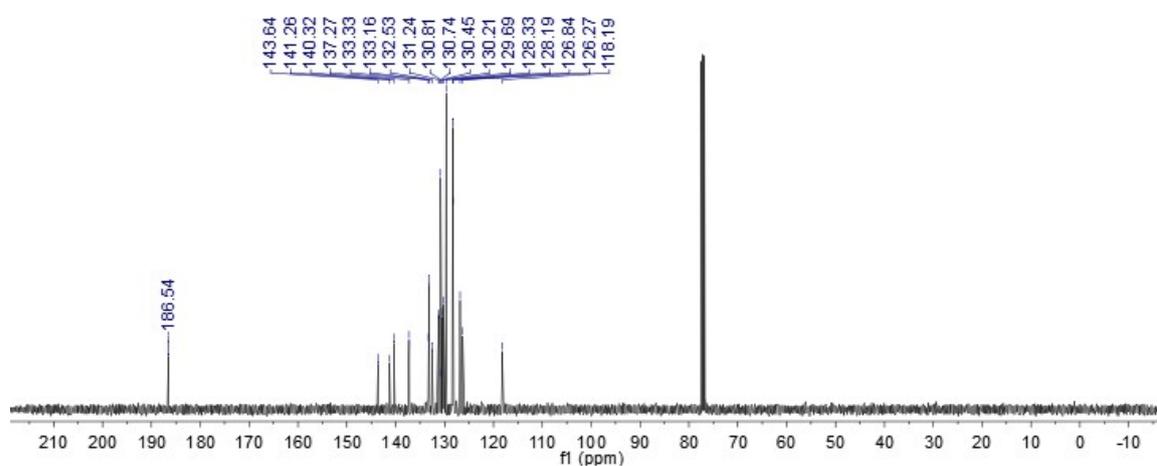
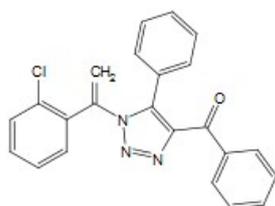
¹³C-NMR spectrum of 4ib



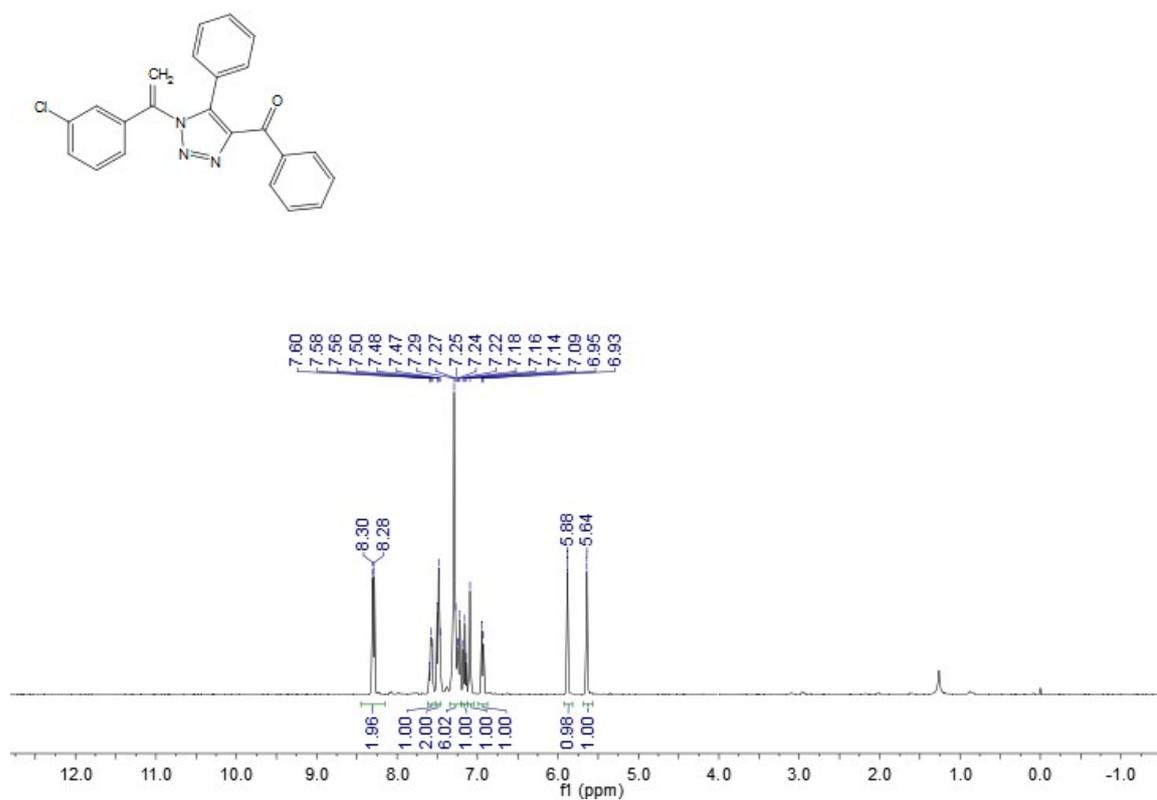
¹H-NMR spectrum of 4jb



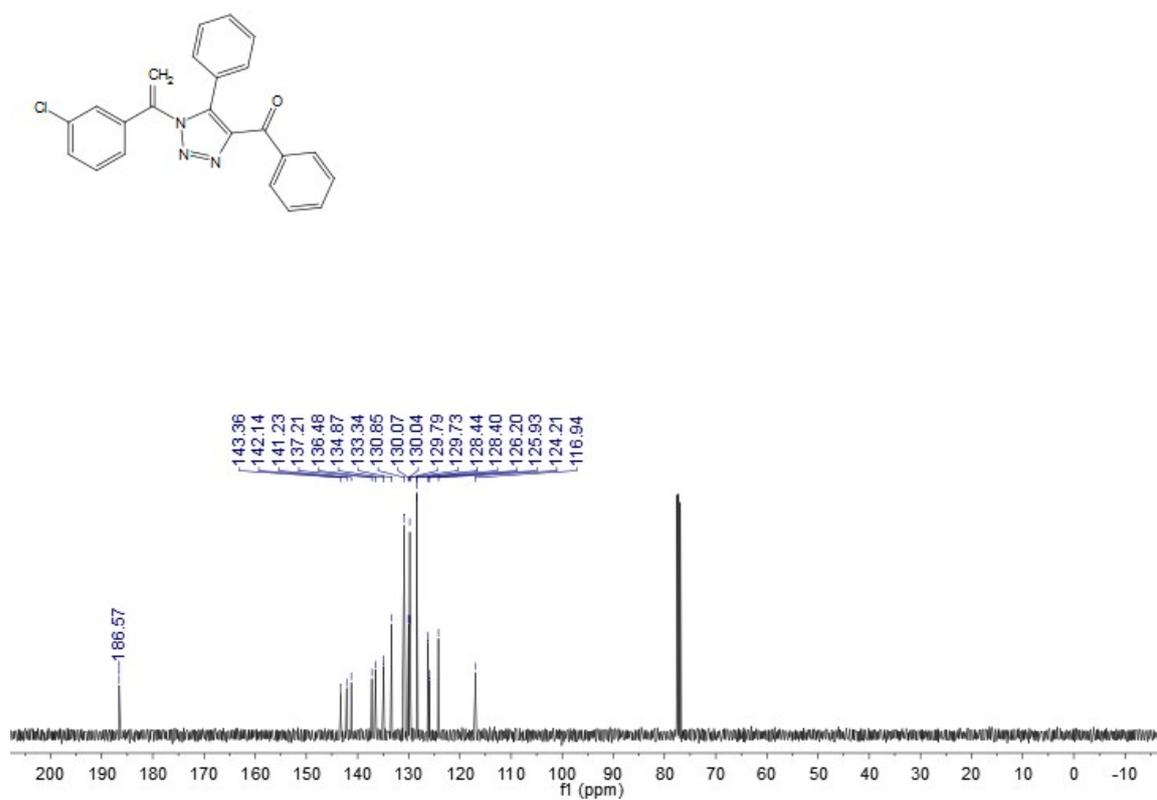
¹³C-NMR spectrum of 4jb



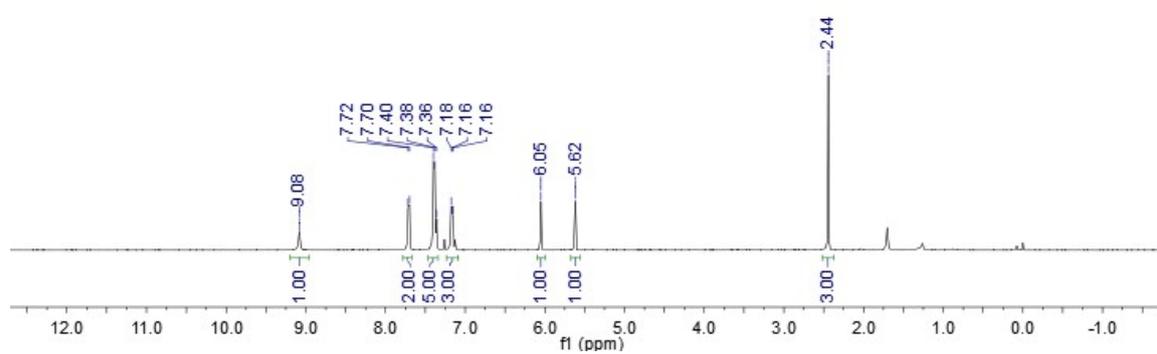
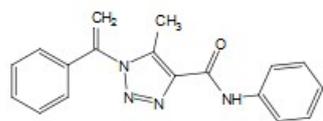
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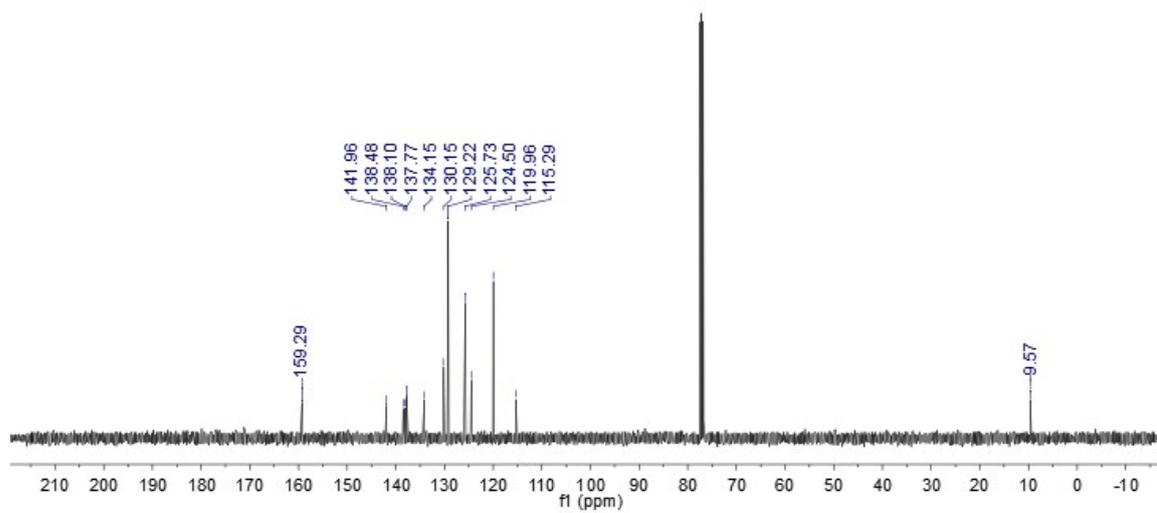
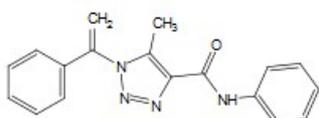
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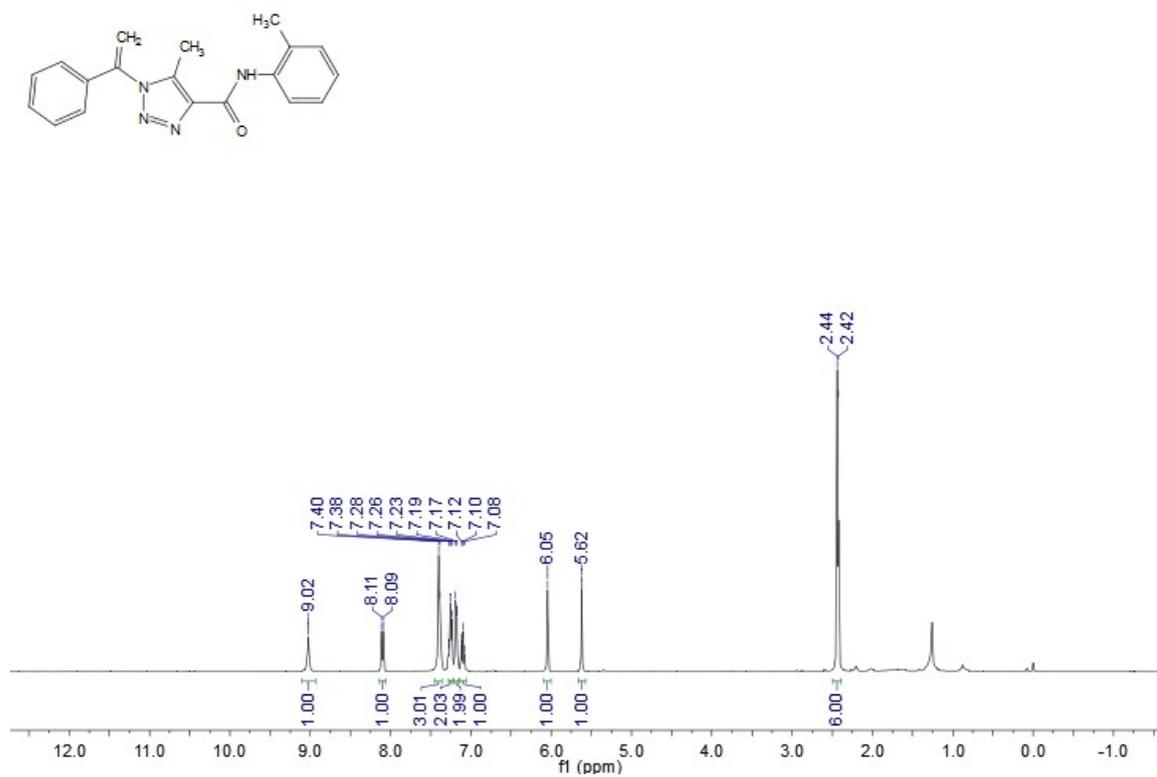
¹H-NMR spectrum of 4ac



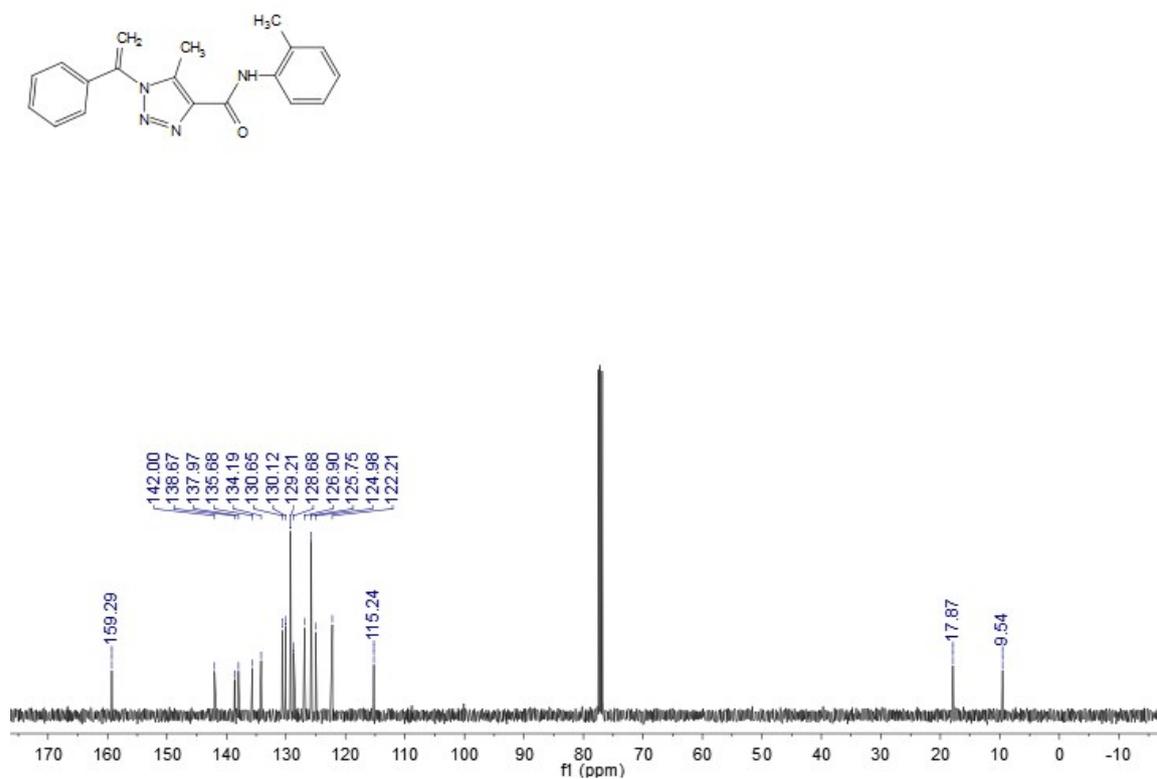
¹³C-NMR spectrum of 4ac



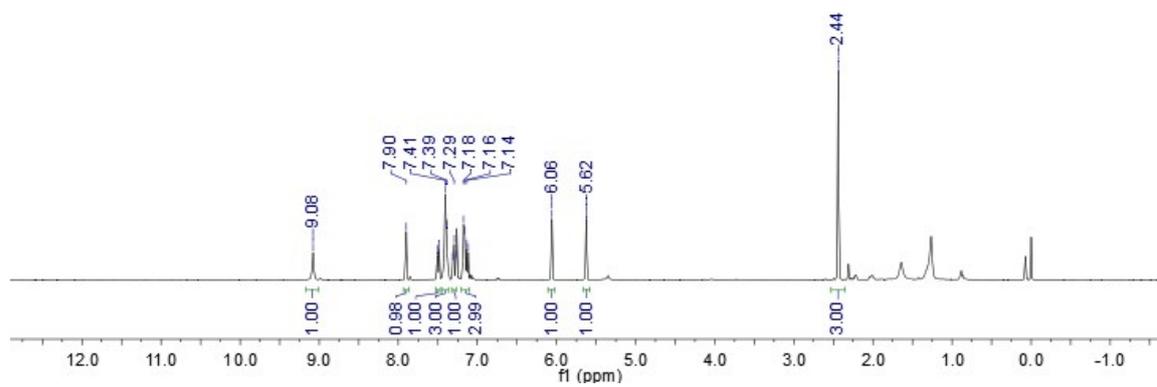
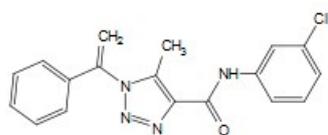
¹H-NMR spectrum of 4ad



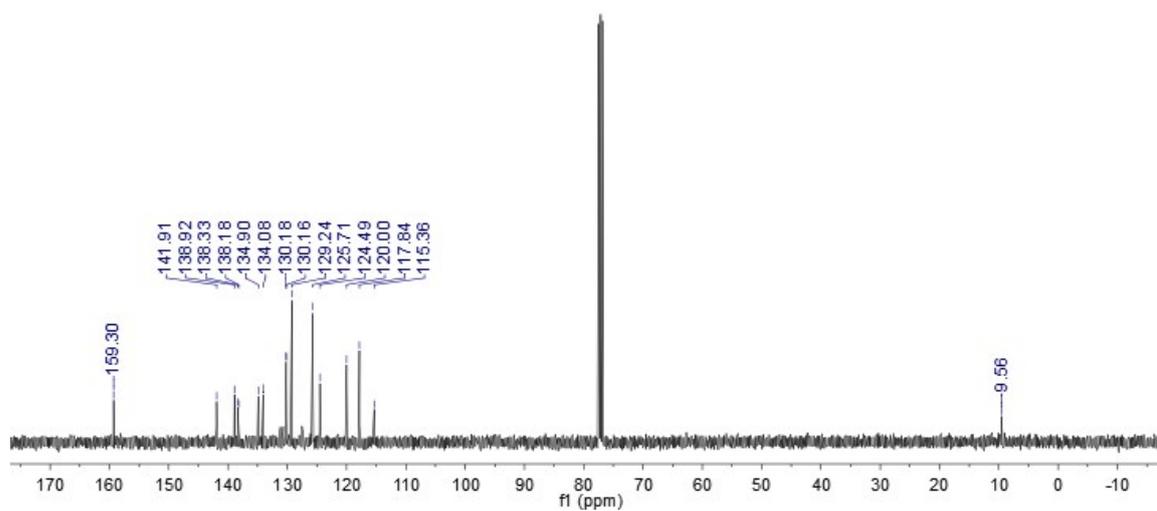
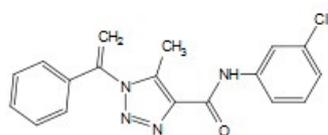
¹³C-NMR spectrum of 4ad



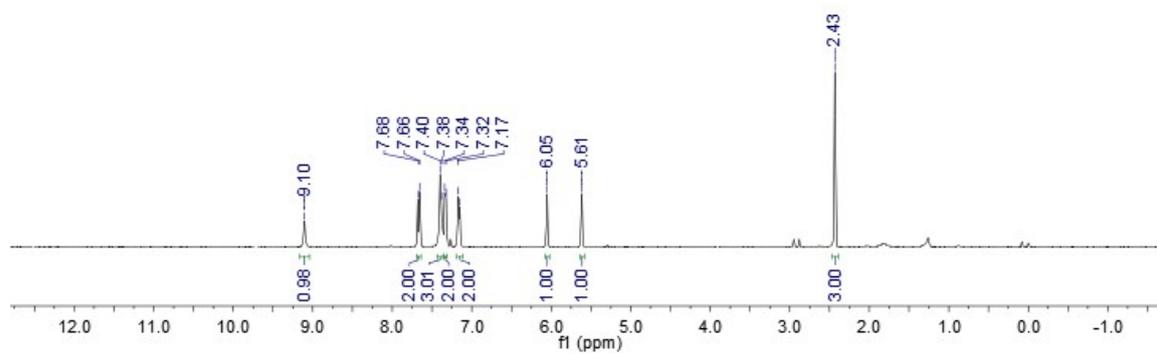
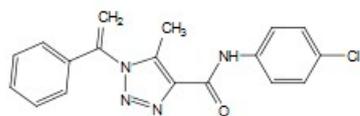
¹H-NMR spectrum of 4ae



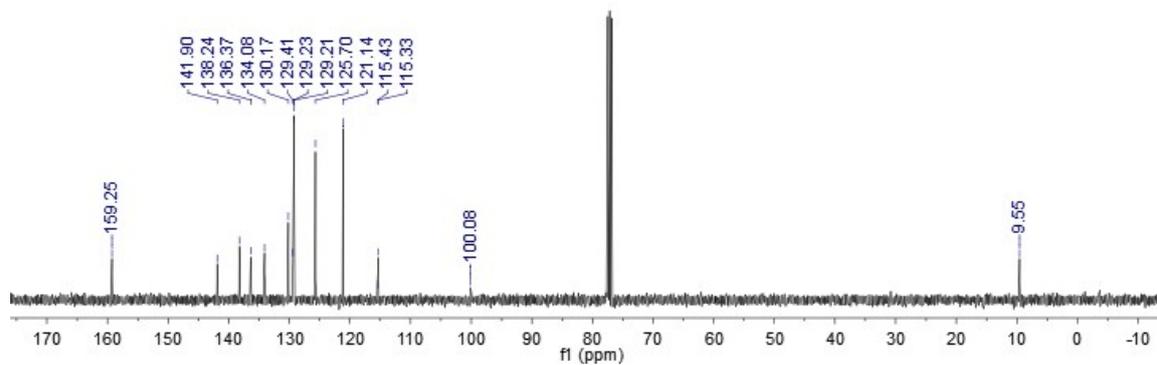
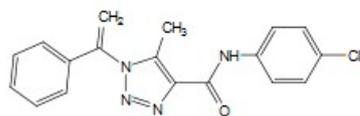
¹³C-NMR spectrum of 4ae



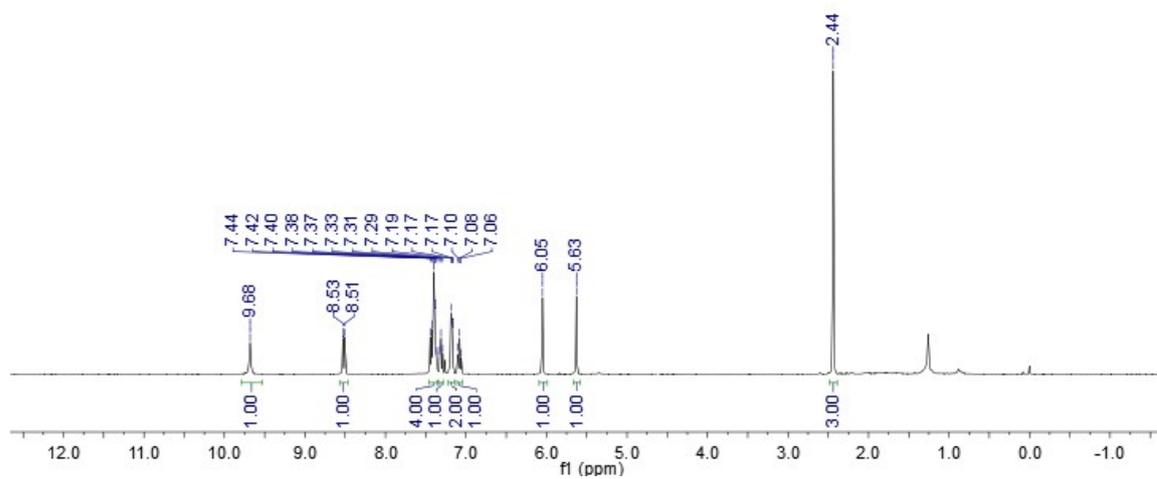
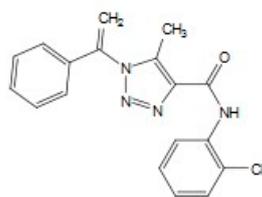
¹H-NMR spectrum of 4af



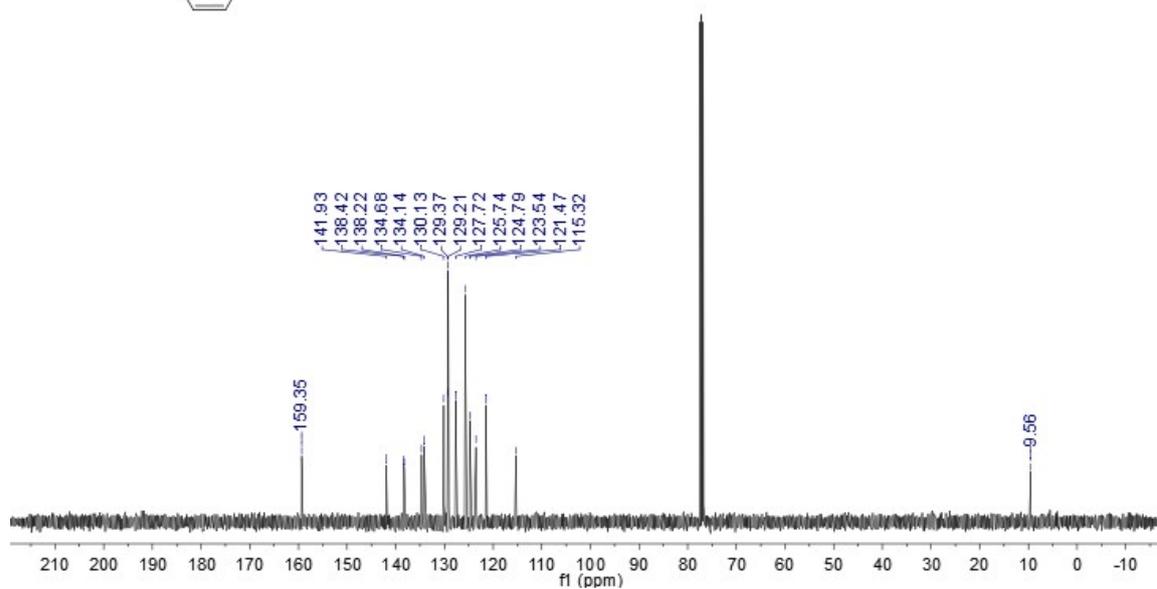
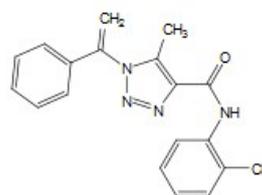
¹³C-NMR spectrum of 4af



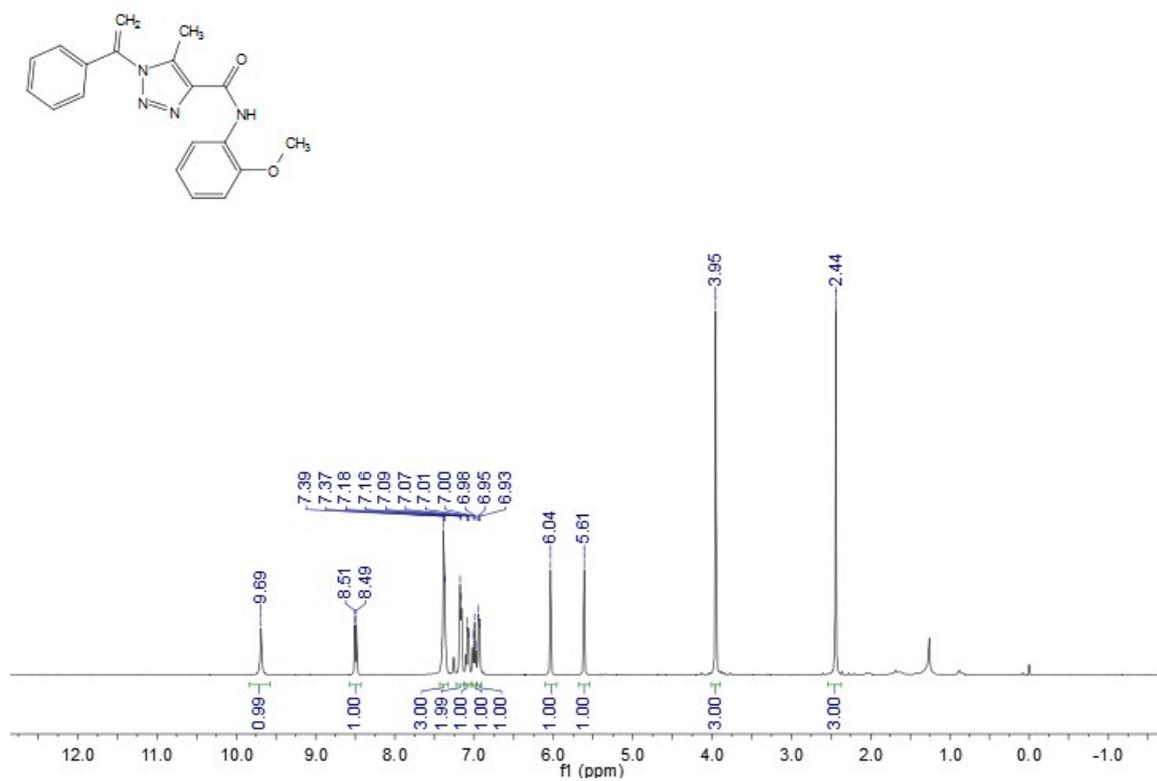
¹H-NMR spectrum of 4ag



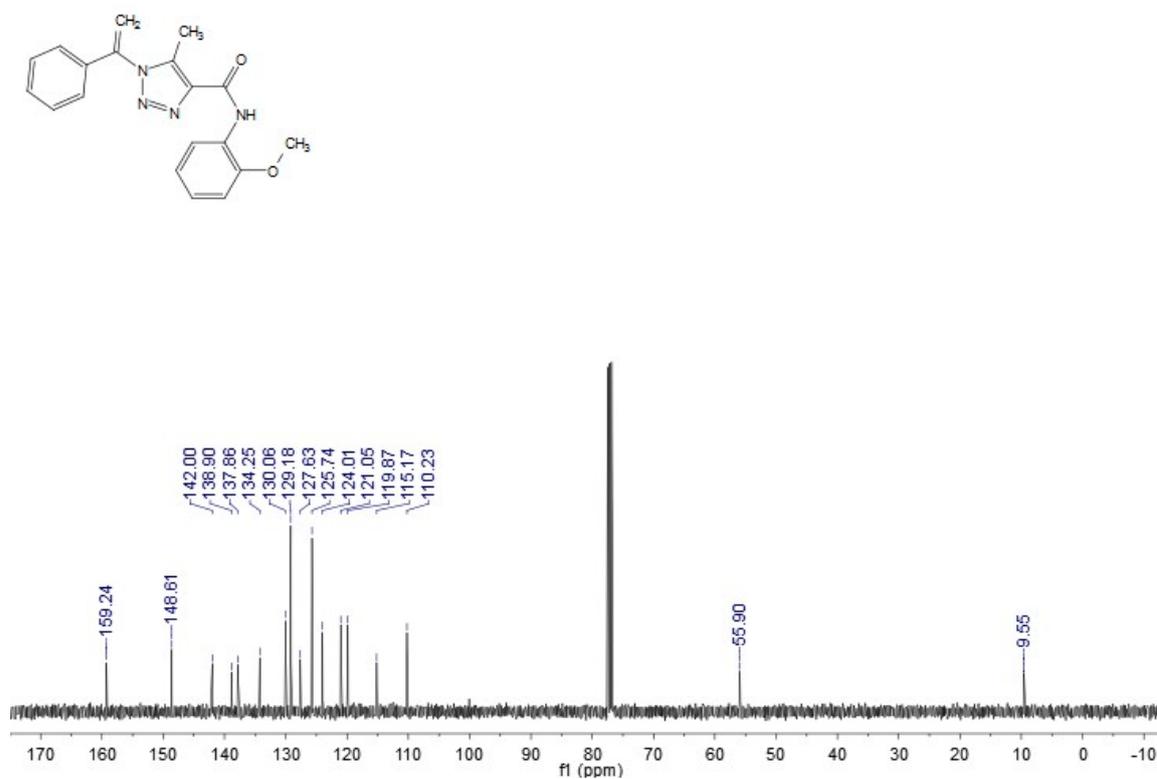
¹³C-NMR spectrum of 4ag



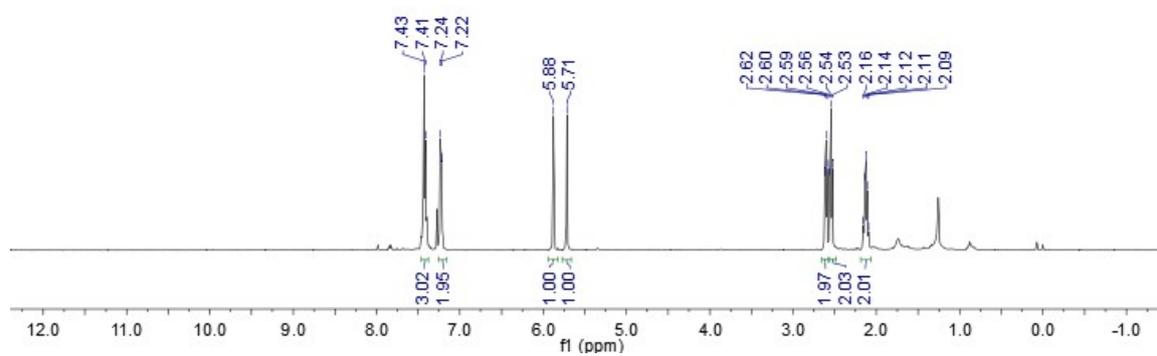
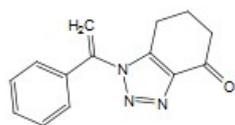
¹H-NMR spectrum of 4ah



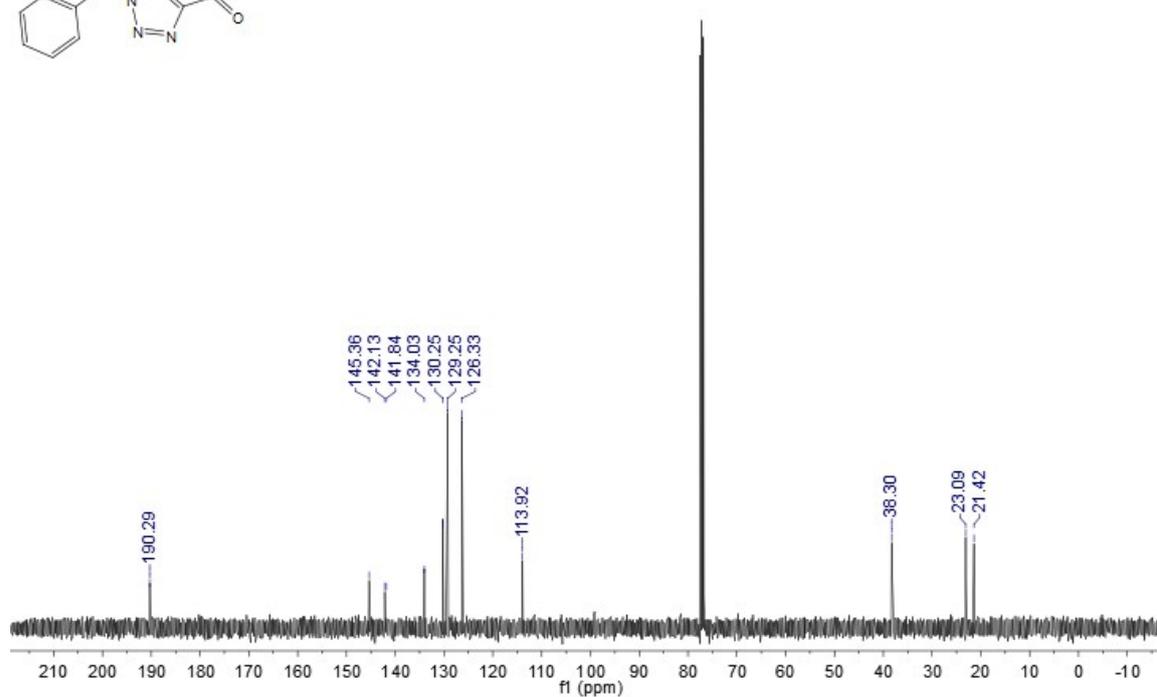
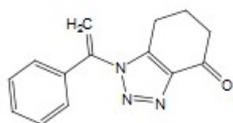
¹³C-NMR spectrum of 4ah



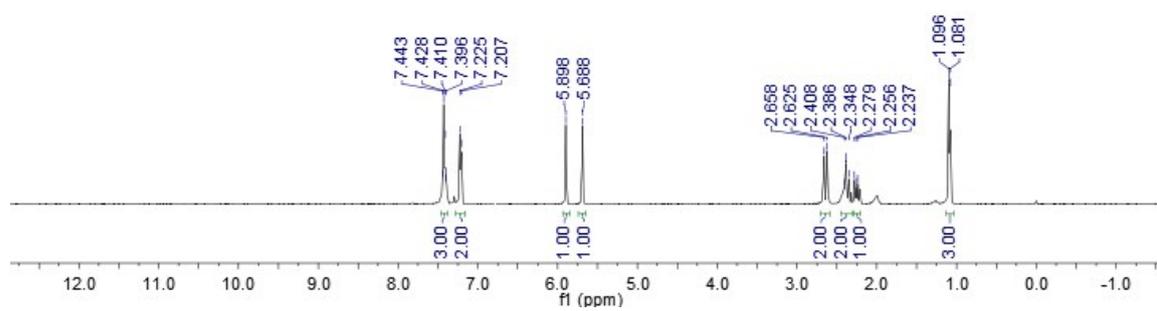
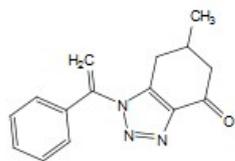
¹H-NMR spectrum of 4ai



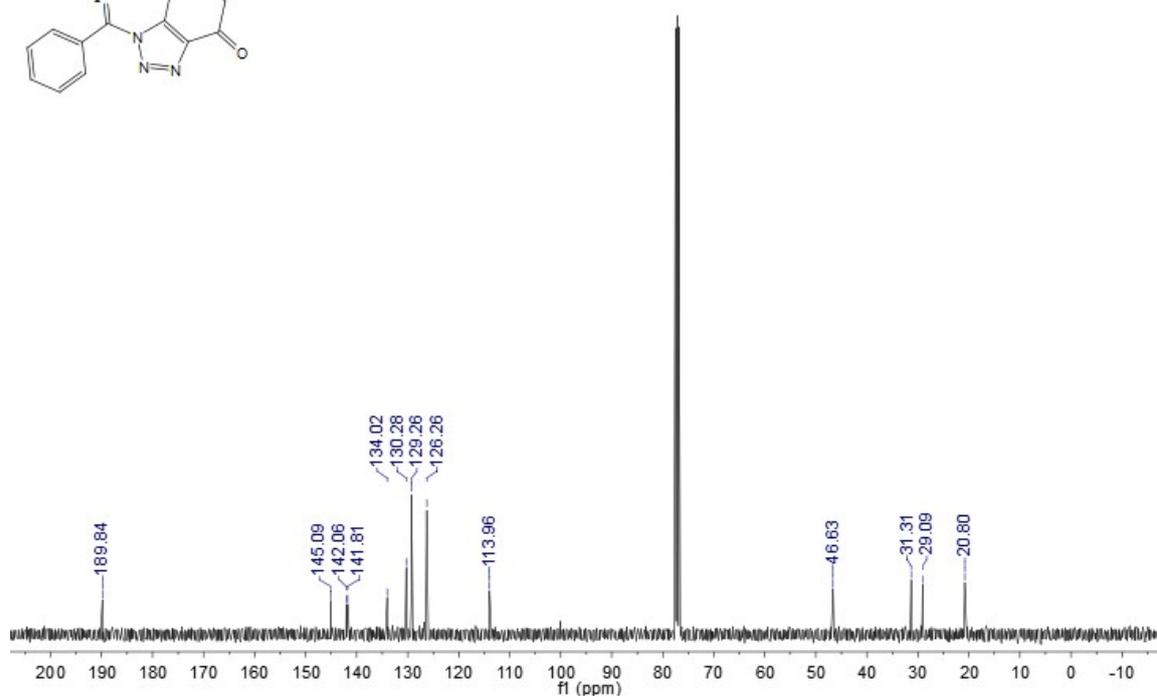
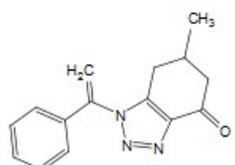
¹³C-NMR spectrum of 4ai



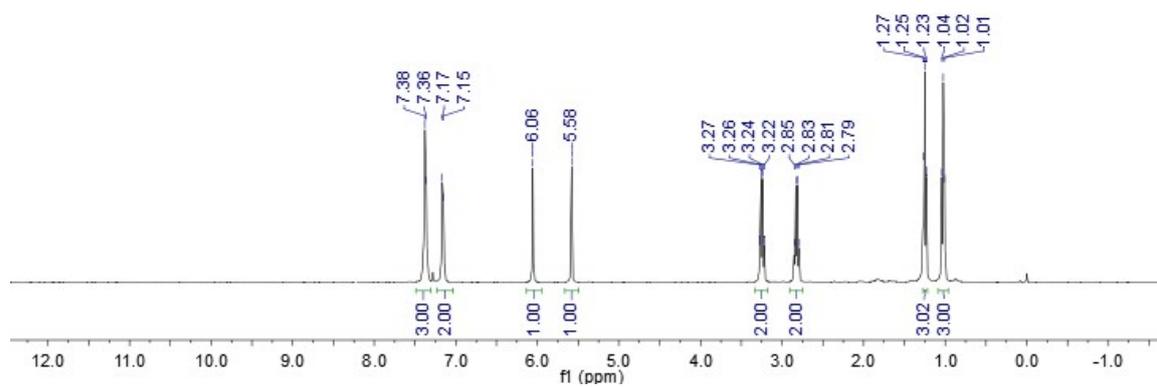
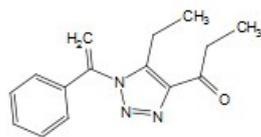
¹H-NMR spectrum of 4aj



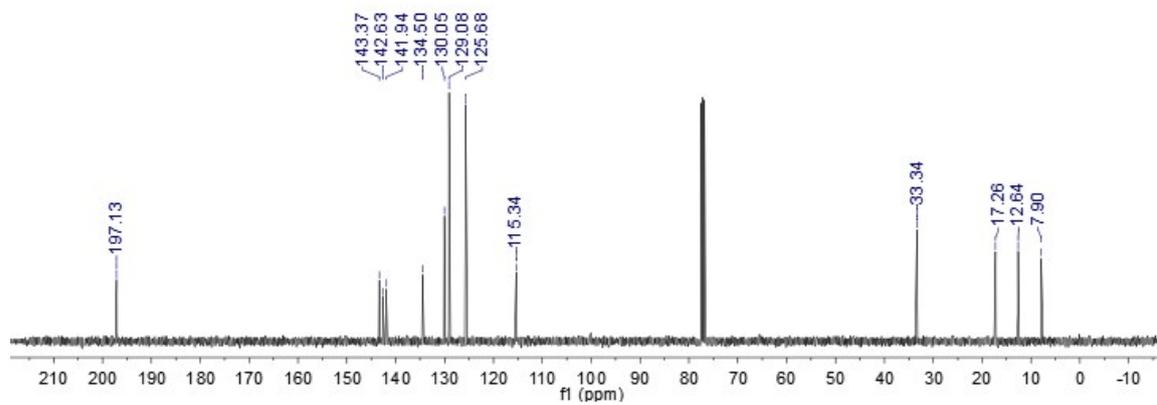
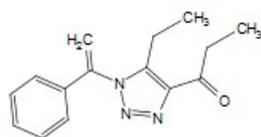
¹³C-NMR spectrum of 4aj



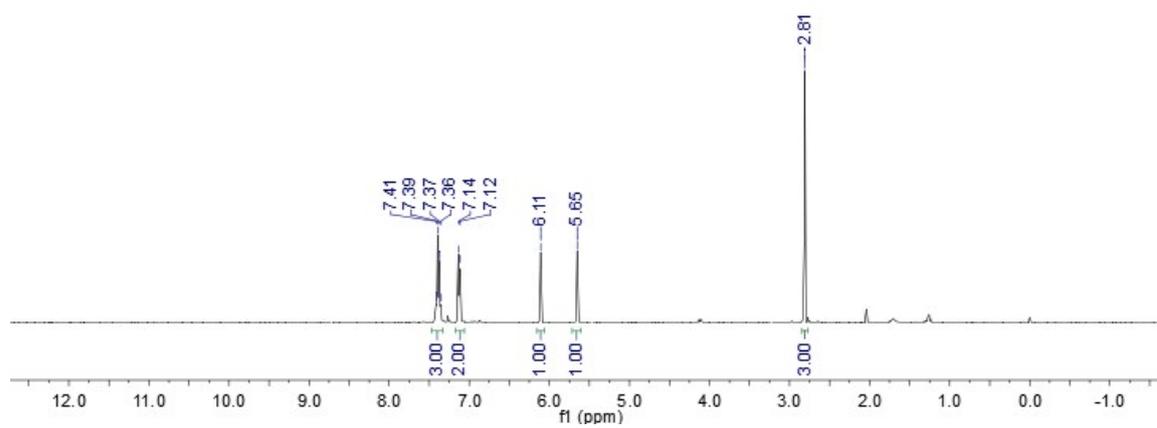
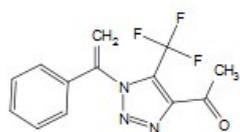
¹H-NMR spectrum of 4ak



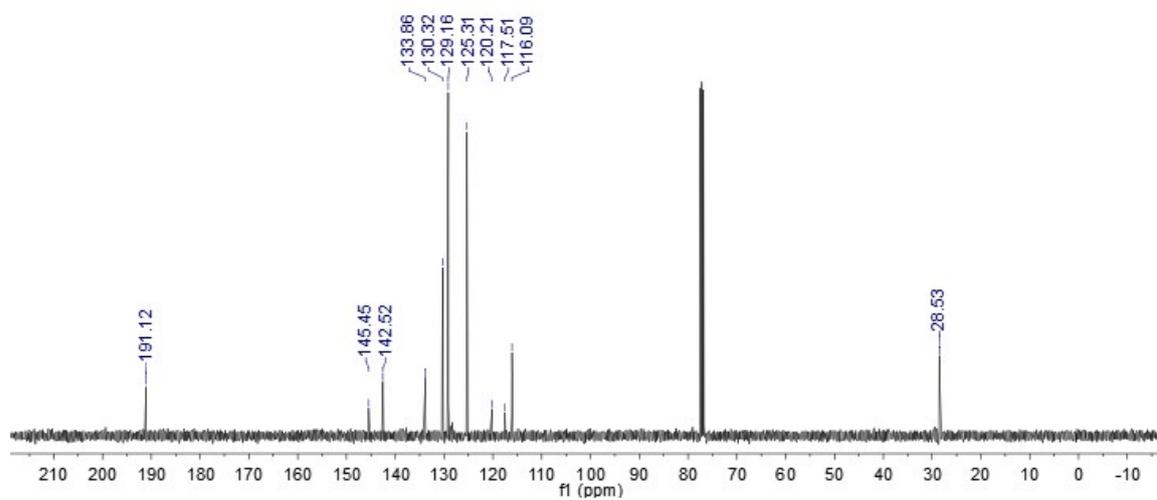
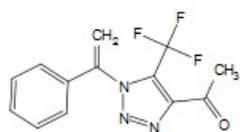
¹³C-NMR spectrum of 4ak



¹H-NMR spectrum of 4al



¹³C-NMR spectrum of 4al



¹⁹F-NMR spectrum of 4al

