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Supplementary Material

Competitive 1,3-dipolar cycloaddition reactions of an azomethine ylide with aromatic and carbonyl groups of nitro-substituted isatoic anhydrides

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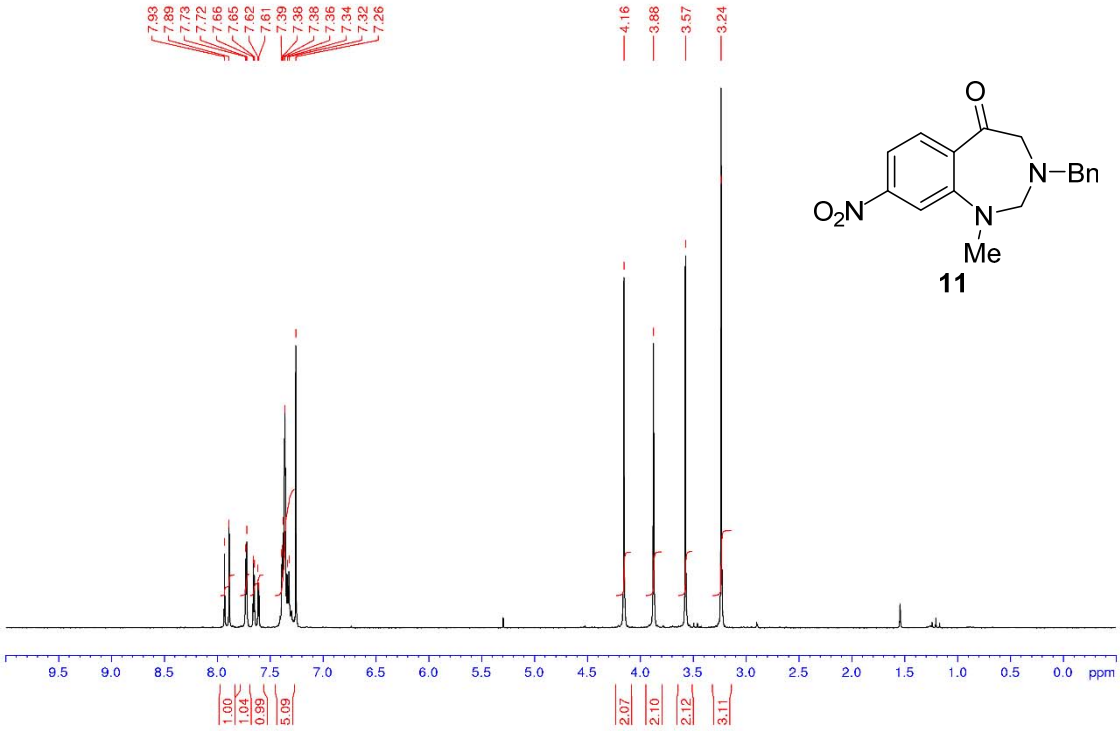
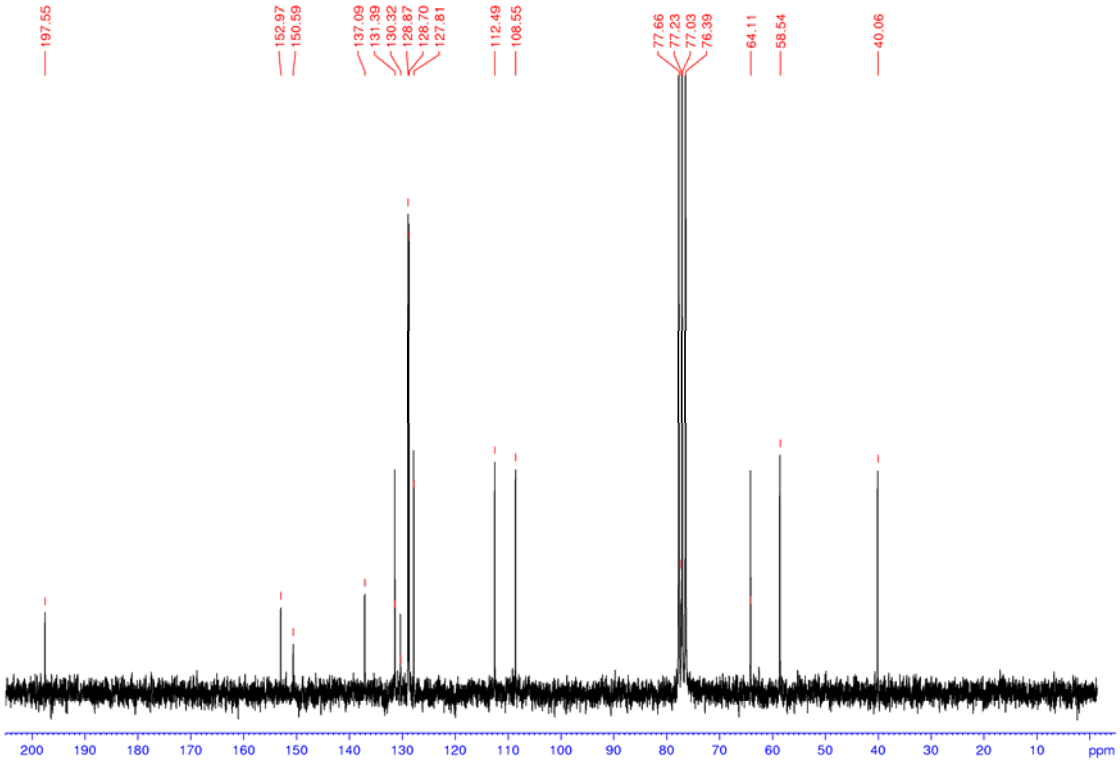
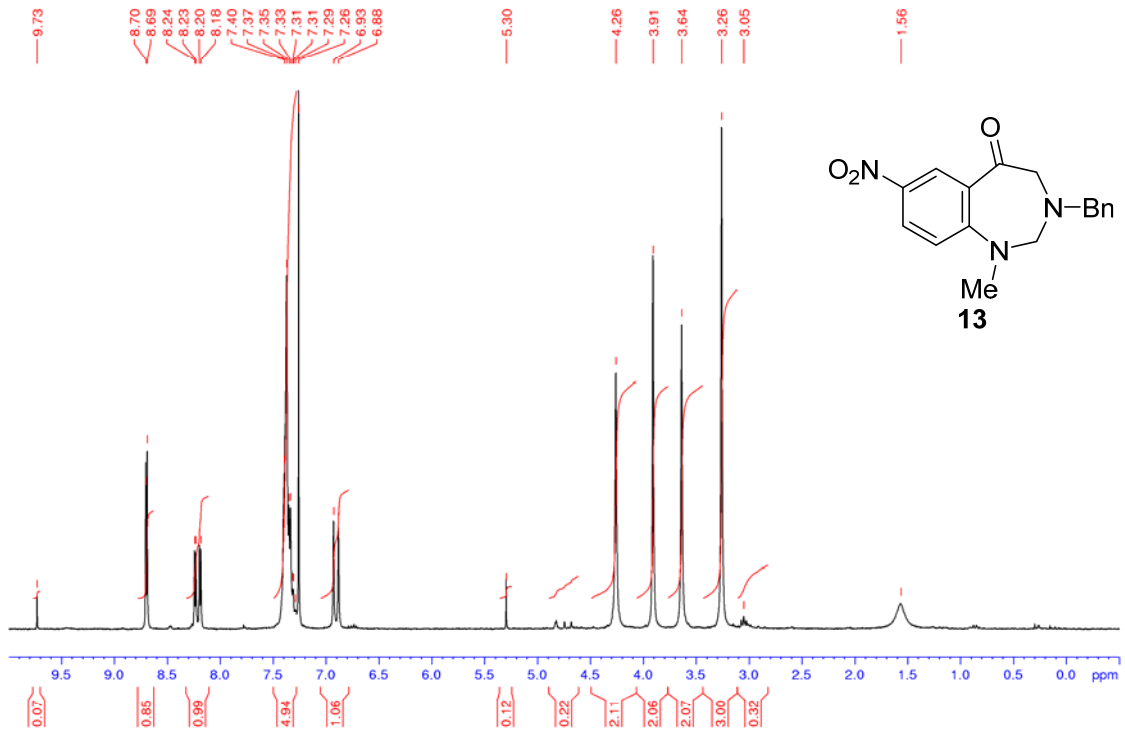
1. Copies of ^{1}H and ^{13}C NMR spectra for new compounds.



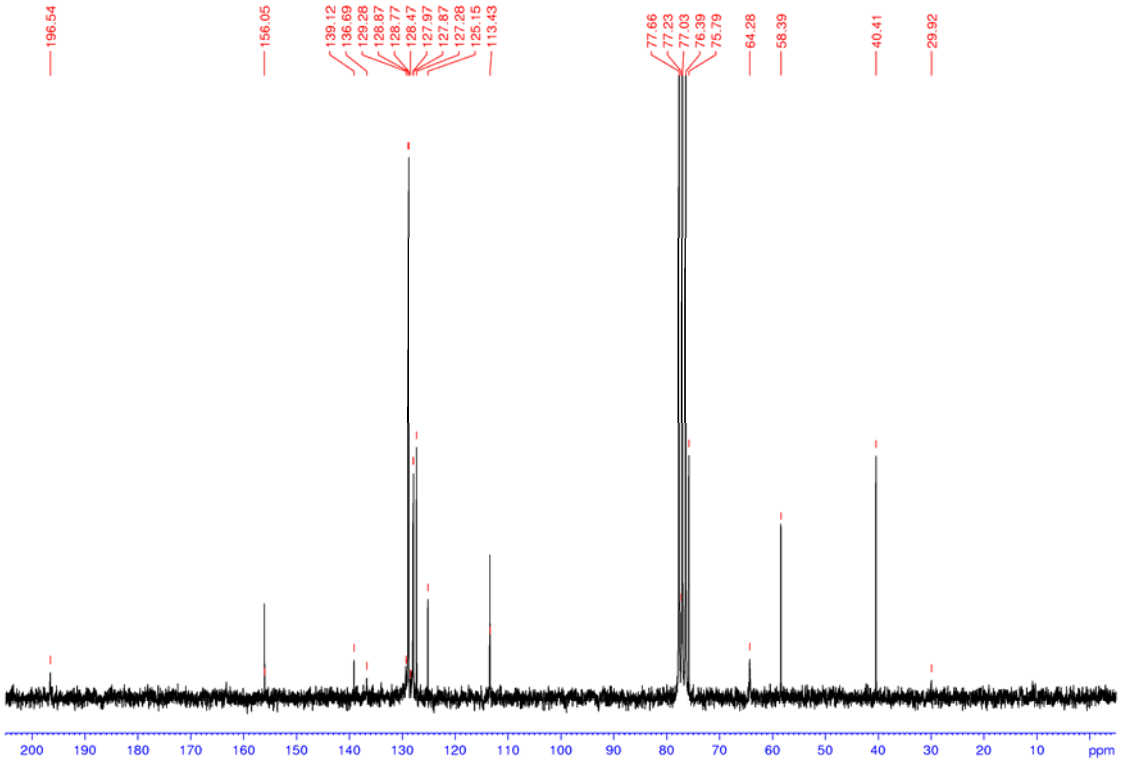
^{1}H NMR spectrum of **11** (200 MHz, $CDCl_3$)



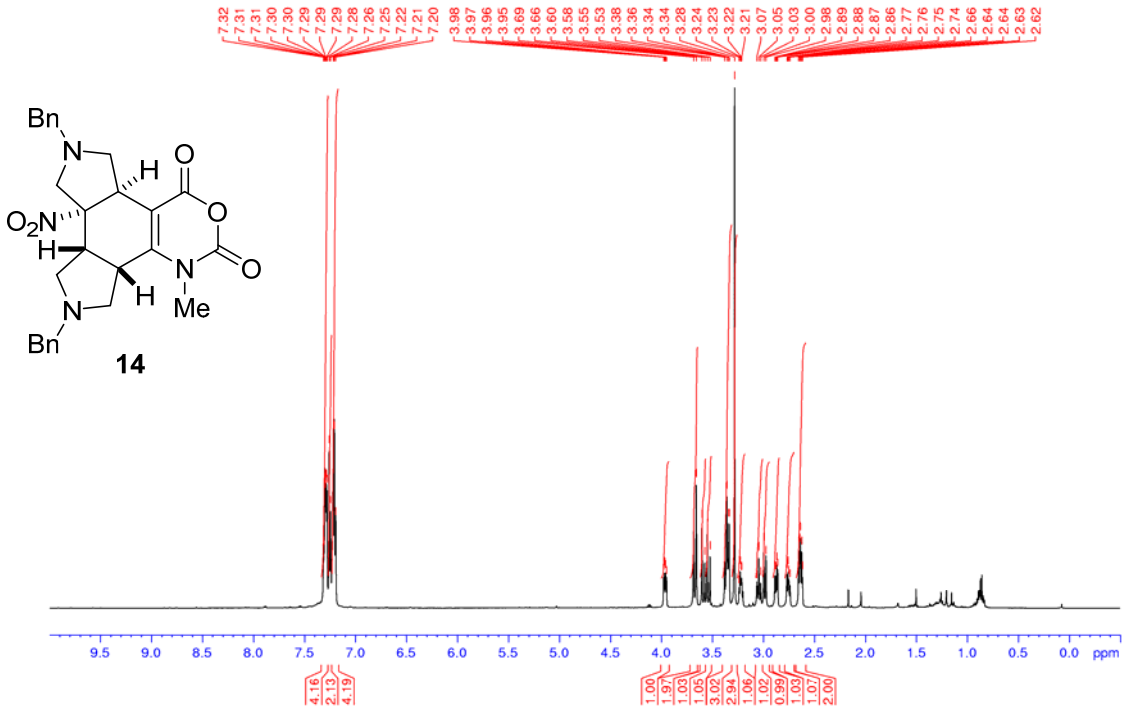
$^{13}C\{^{1}H\}$ NMR spectrum of **11** (50 MHz, $CDCl_3$)



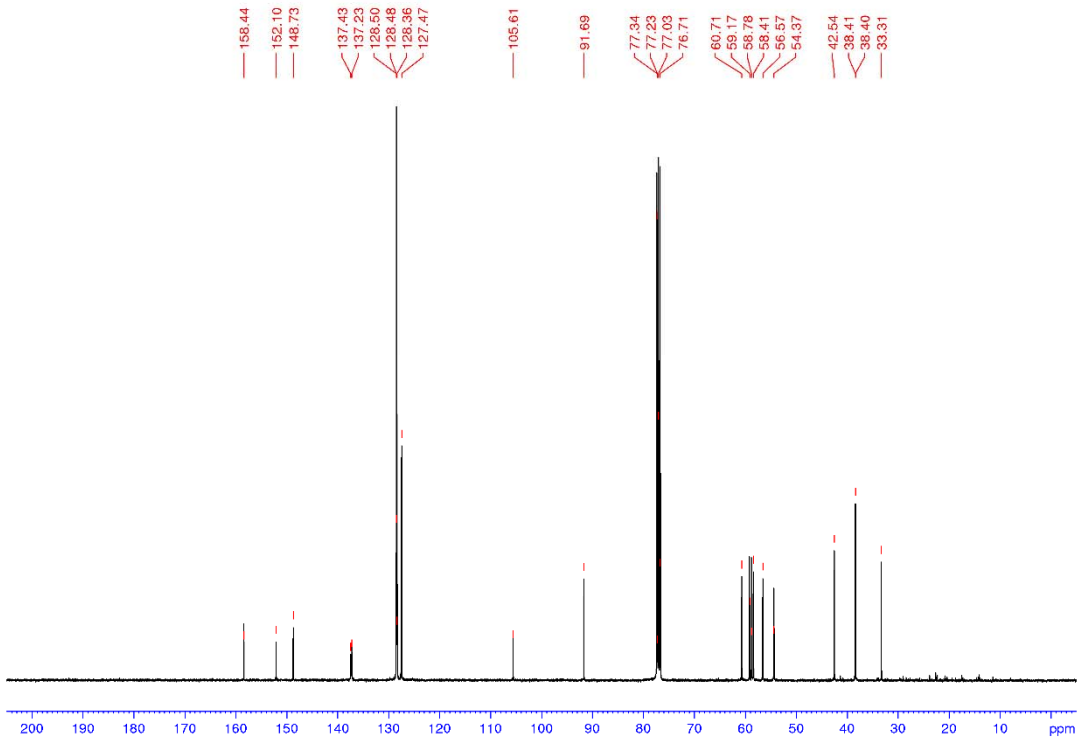
^{1}H NMR spectrum of **13** (200 MHz, $CDCl_3$)



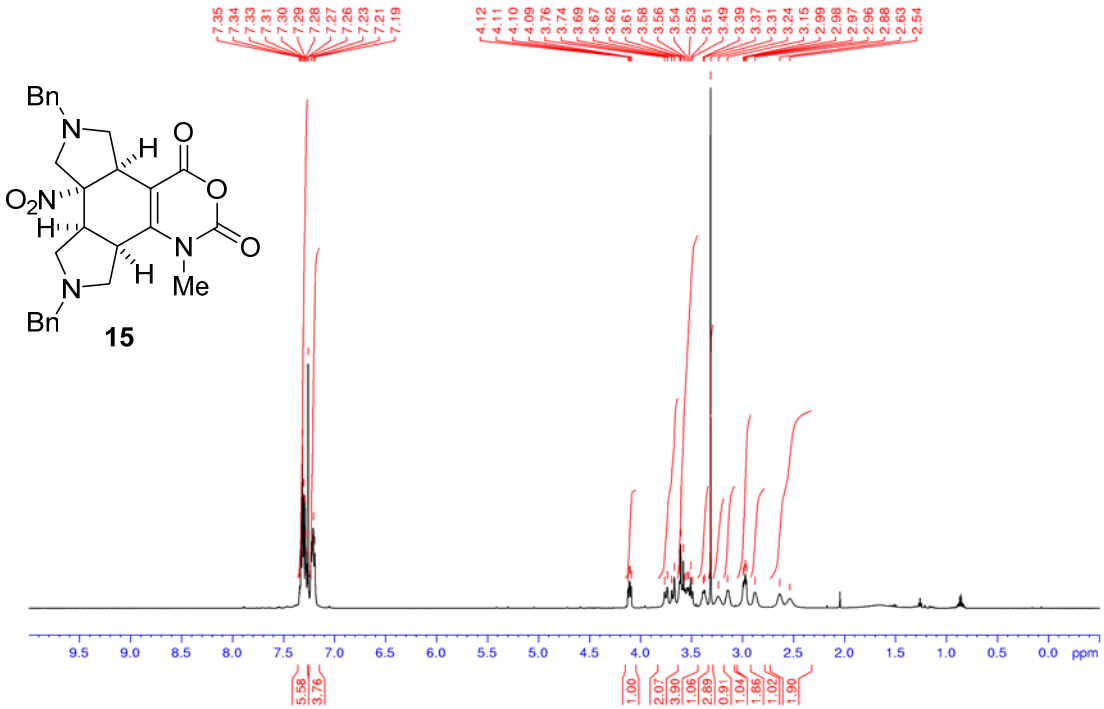
$^{13}C\{^{1}H\}$ NMR spectrum of **13** (50 MHz, $CDCl_3$)



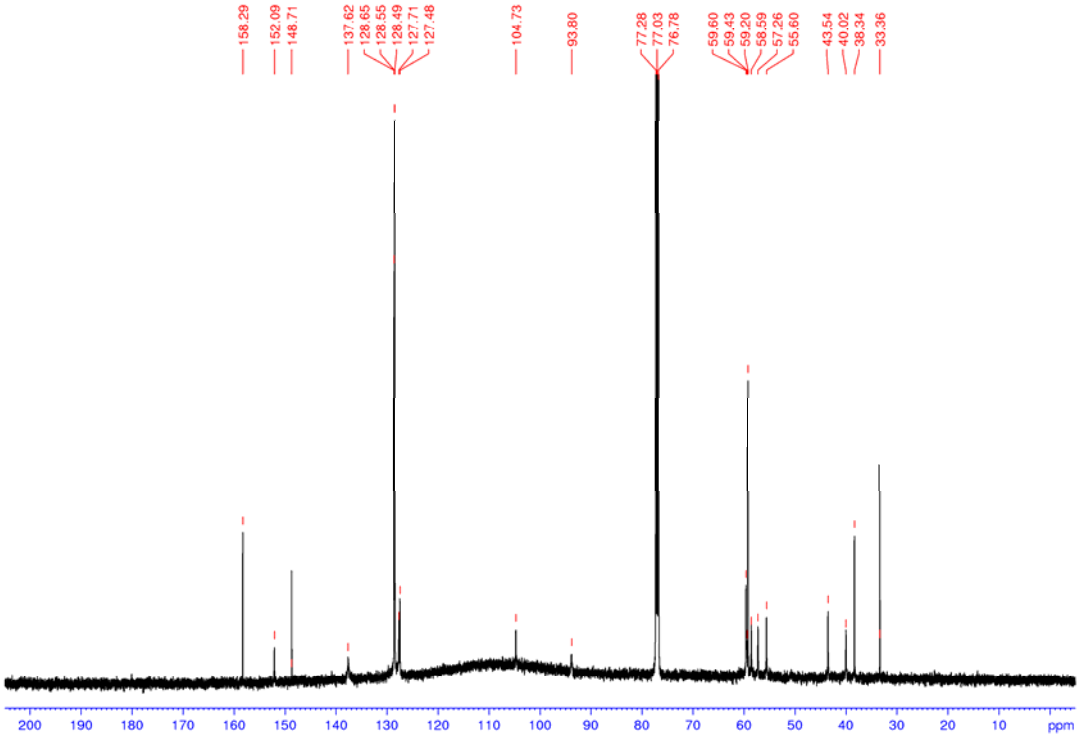
^{1}H NMR spectrum of **14** (500 MHz, $CDCl_3$)



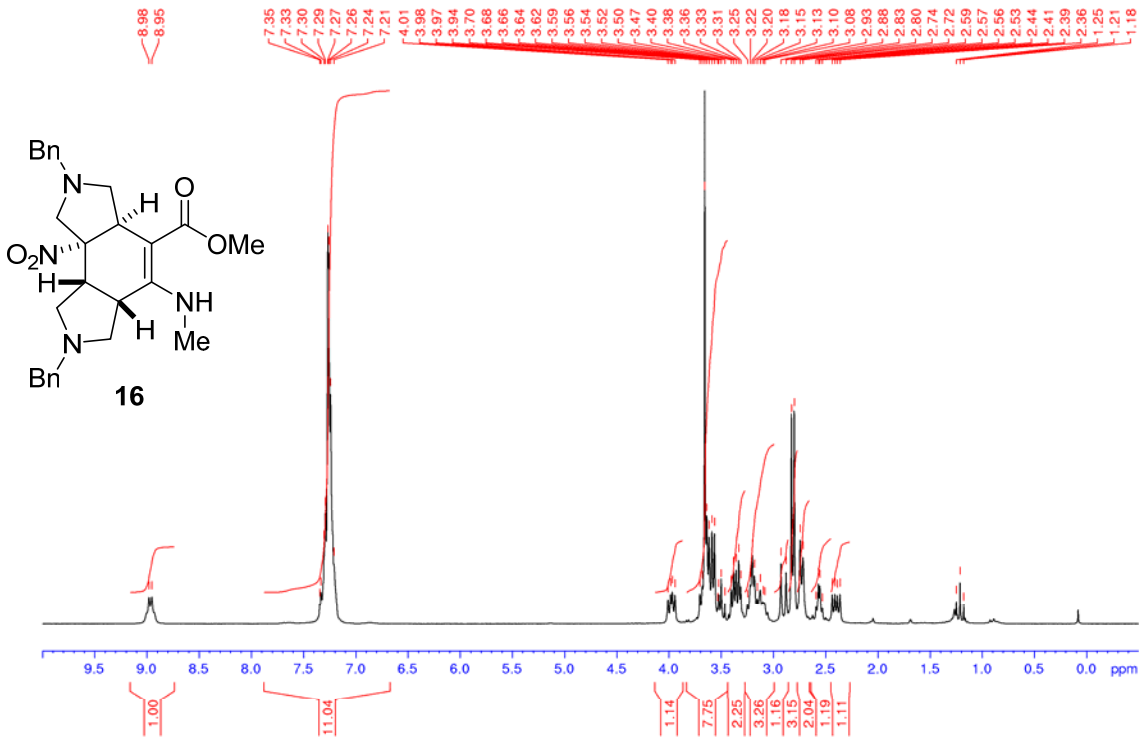
$^{13}C\{^{1}H\}$ NMR spectrum of **14** (100 MHz, $CDCl_3$)



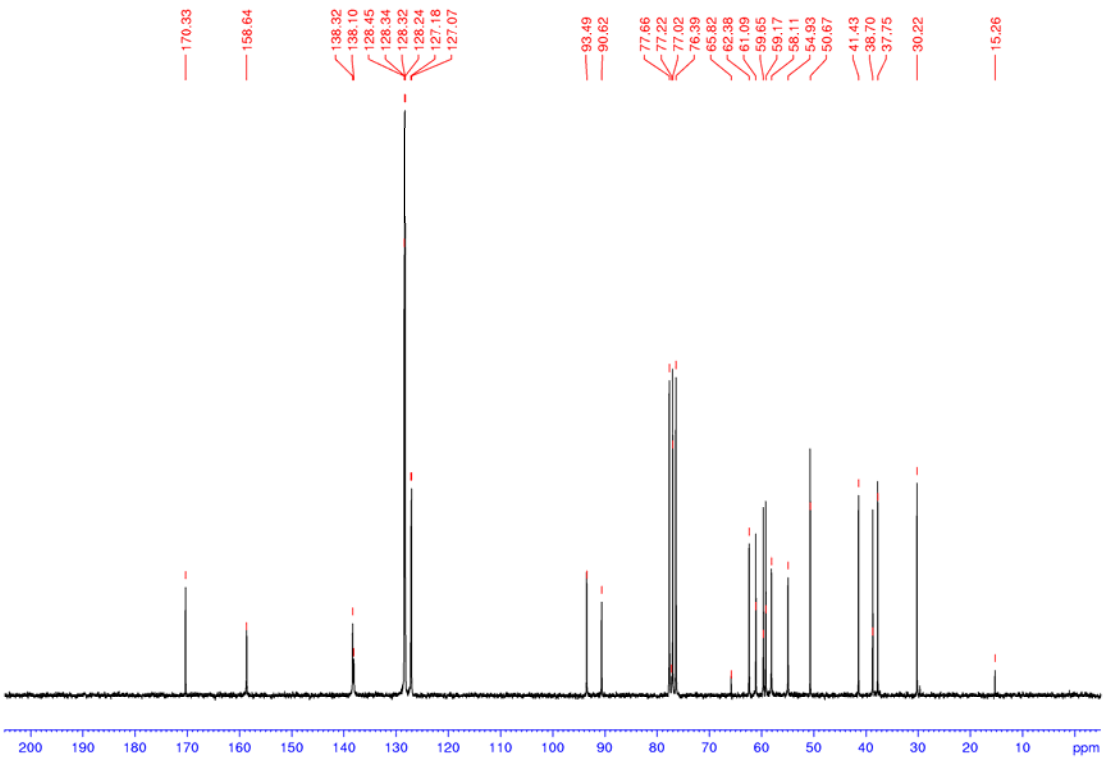
^{1}H NMR spectrum of **15** (500 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR spectrum of **15** (126 MHz, $CDCl_3$)



^{1}H NMR spectrum of **16** (200 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR spectrum of **16** (50 MHz, $CDCl_3$)

2. X-ray crystallographic analysis of compound *16*.

Crystallography. Intensity data were collected with an Oxford Diffraction XCalibur CCD diffractometer using Cu- Ka radiation, the temperature during data collection was maintained at 130.0(1) using an Oxford Cryosystems cooling device.

The structure was solved by direct methods and difference Fourier synthesis.[1] Thermal ellipsoid plots were generated using the program ORTEP-3[2] integrated within the WINGX[3] suite of programs.

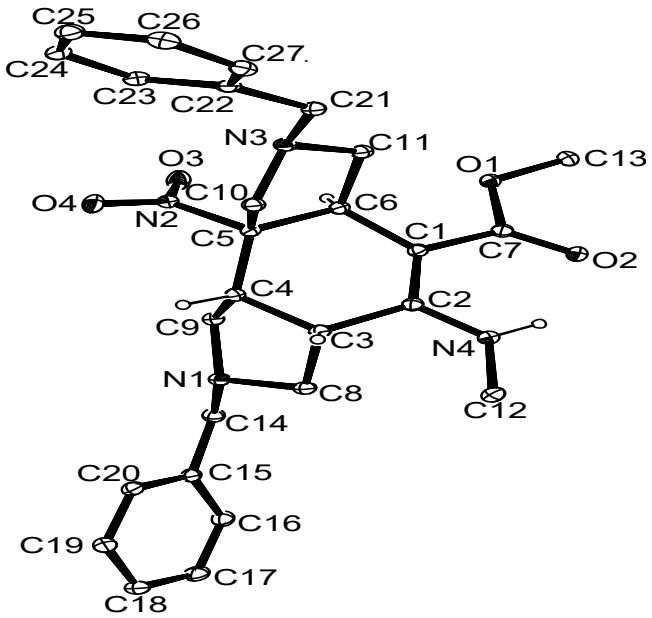


Figure 1. Thermal ellipsoid plot of compound **16**.

Crystal data for **16**. $C_{27}H_{32}N_4O_4$, M = 476.56T = 130.0(2) K, l = 1.54184 Å, Monoclinic, space group $P2_1/c$ a = 17.6227(2), b = 12.02730(10), c = 11.40730(10) Å, V = 2416.41(4) Å^3, Z = 4, D_c = 1.310 Mg M^{-3} m(Cu-Ka) = 0.721 mm^{-1}, *F(000)* = 1016, crystal size 0.39 x 0.37 x 0.17 mm. q_{max} = 73.27°, 11361 reflections measured, 4724 independent reflections (R_{int} = 0.41) the final R = 0.0453 [I > 2s(I), 3801 data] and wR(F^2) = 0.125 (all data) GOOF = 1.049.

References

1. G. Sheldrick, *Acta Crystallogr. Section C*, **2015**, **71**, 3-8.
2. L. J. Farrugia, *J. Appl. Cryst.* **1997**, *30*, 565.
3. L. J. Farrugia, *J. Appl. Cryst.* **1999**, *32*, 837.