

## Article

# Straightforward One-pot Synthesis of New 4-Phenyl-1,2,5,6-tetraazafluoranthene-3(2H)-one Derivatives: X-Ray Single Crystal Structure and Hirshfeld Analyses

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## Supporting Materials

### X-Ray structure determinations

The crystal of nd29 and nd5 were immersed in cryo-oil, mounted in a loop, and measured at a temperature of 120 K. The X-ray diffraction data was collected on a Rigaku Oxford Diffraction Supernova diffractometer using Cu K $\alpha$  radiation. The *CrysAlisPro*<sup>1</sup> software package was used for cell refinement and data reduction. An analytical or multi-scan absorption correction (*CrysAlisPro*<sup>1</sup>) was applied to the intensities before structure solution for nd29 and nd5 respectively. Structures were solved by intrinsic phasing (*SHELXT*<sup>2</sup>) method. Structural refinements were carried out using *SHELXL*<sup>3</sup> software with *SHELXLE*<sup>4</sup> graphical user interface. The NH hydrogen atom was located from the difference Fourier map and refined isotropically. All other hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C-H = 0.95 – 0.99 Å and U<sub>iso</sub> = 1.2–1.5·U<sub>eq</sub>(parent atom).

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## NMR Spectra

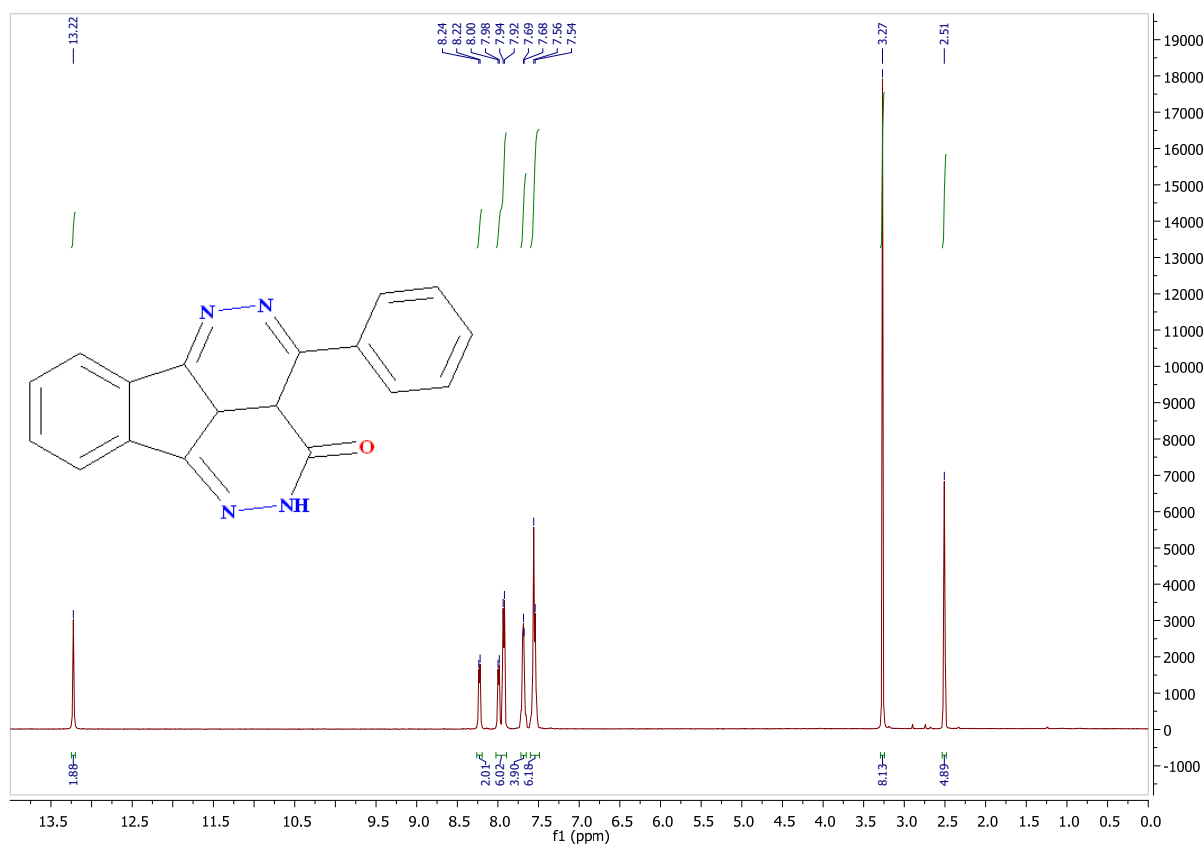
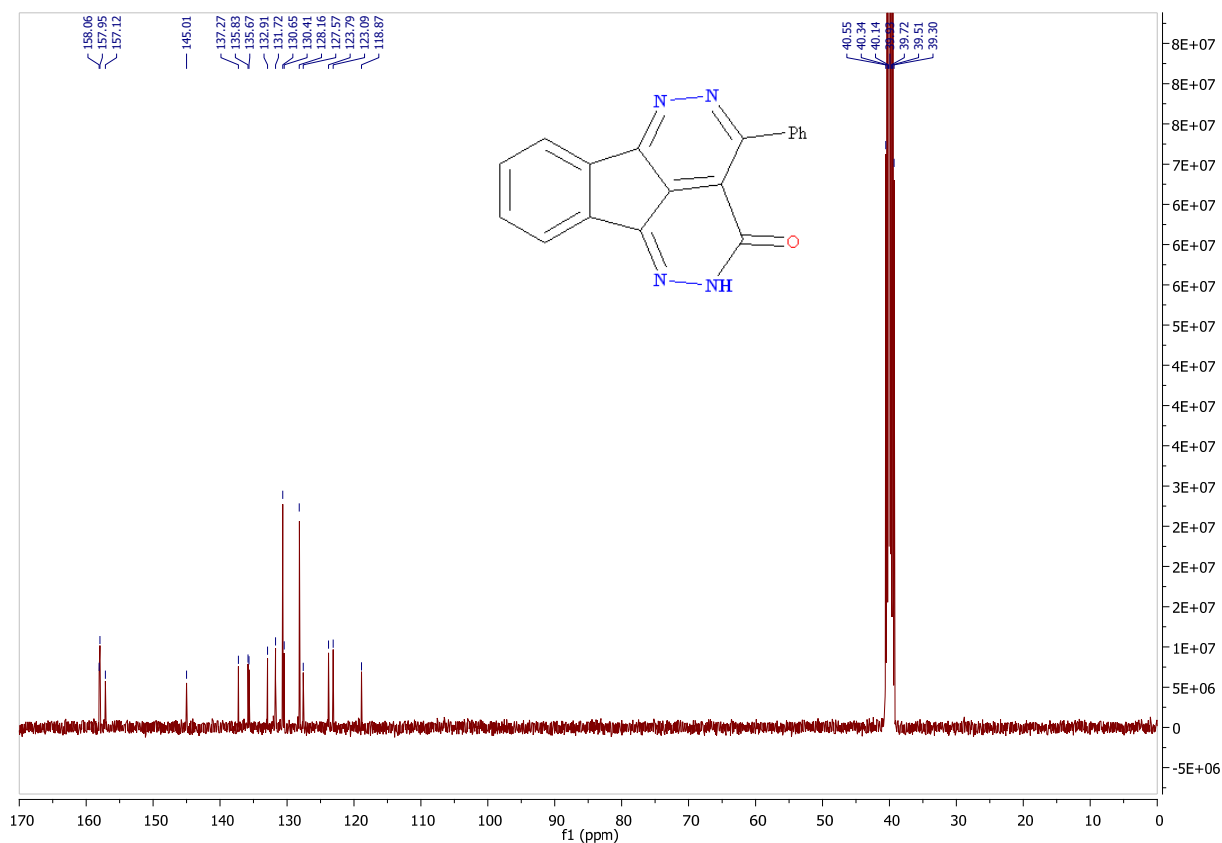
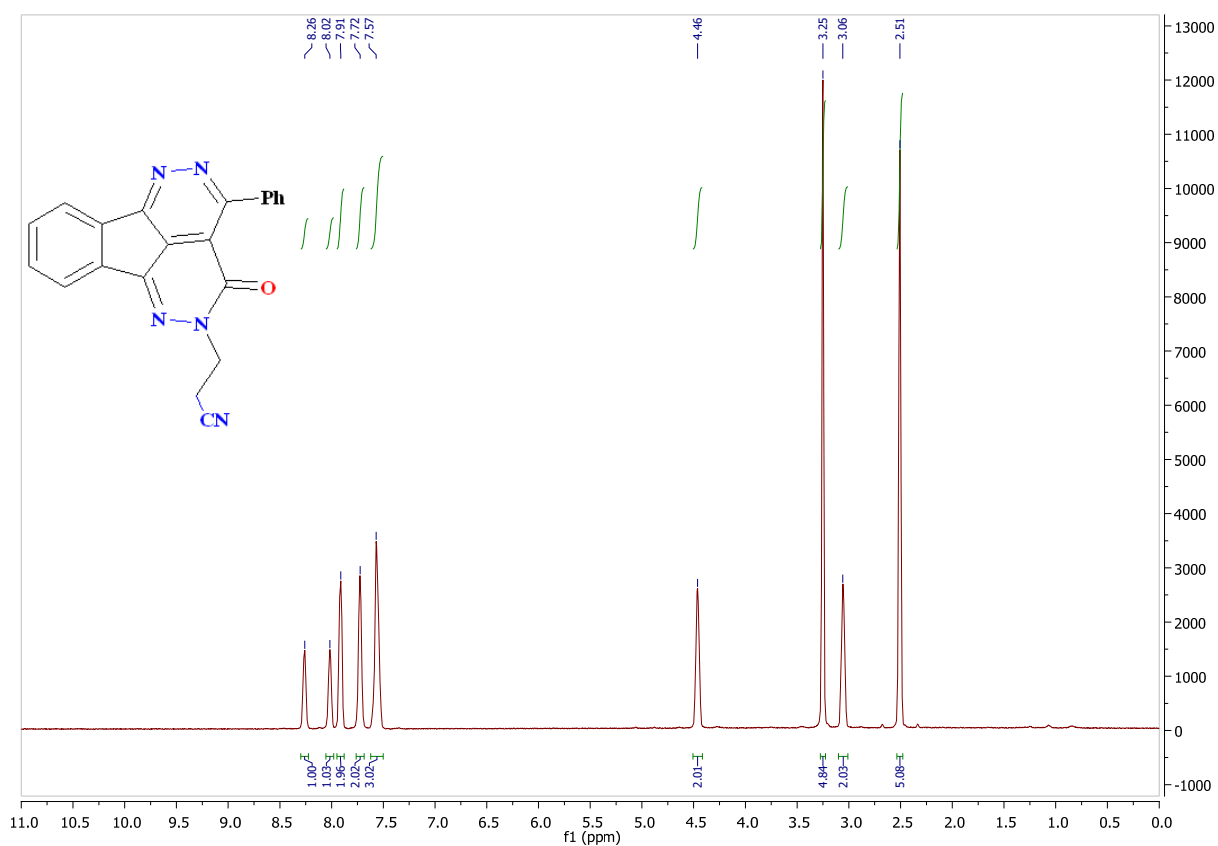
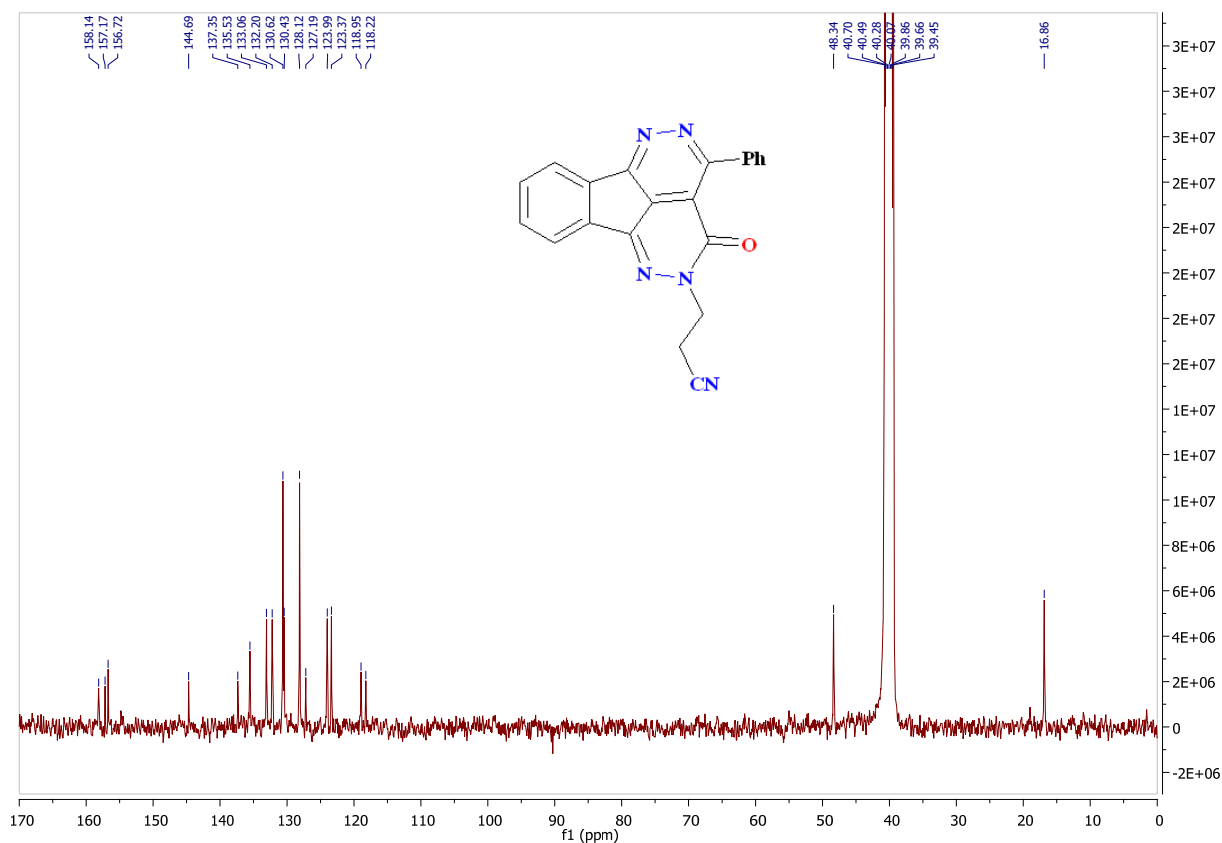
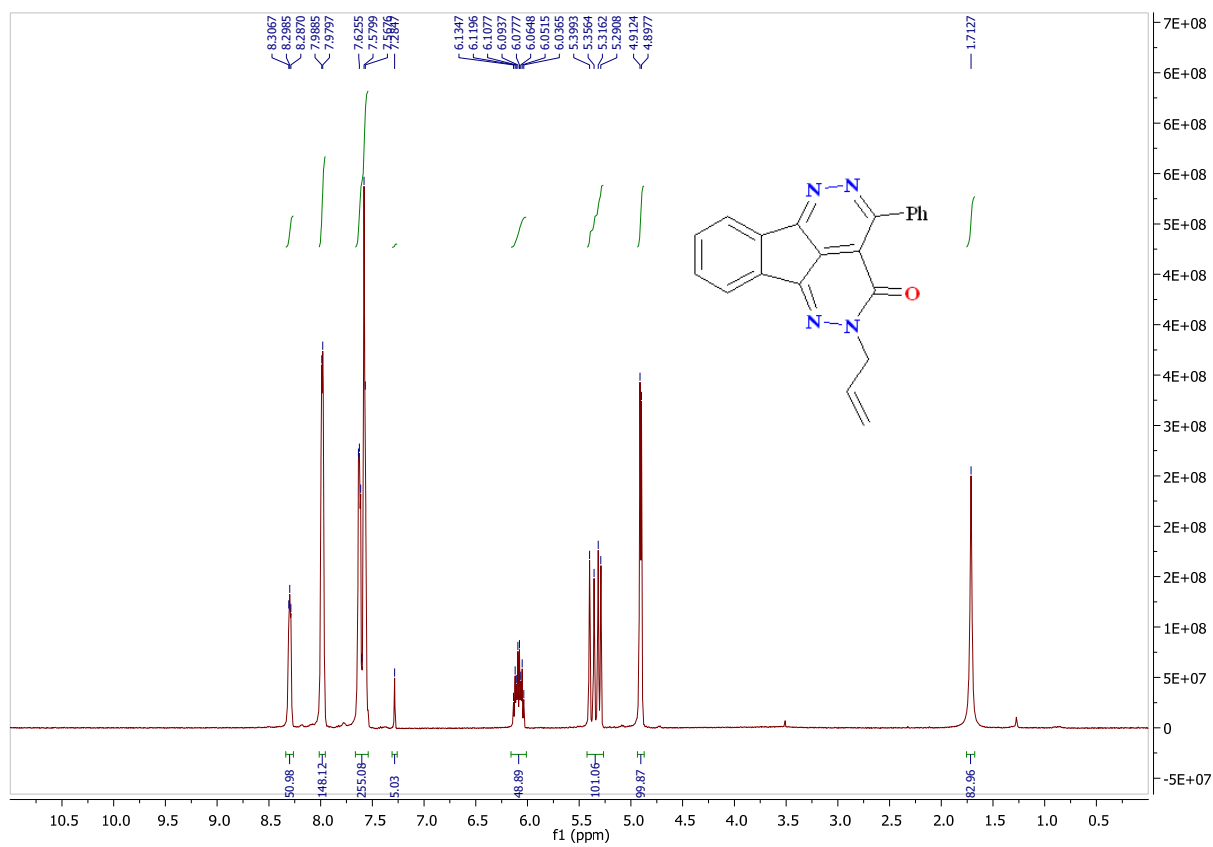
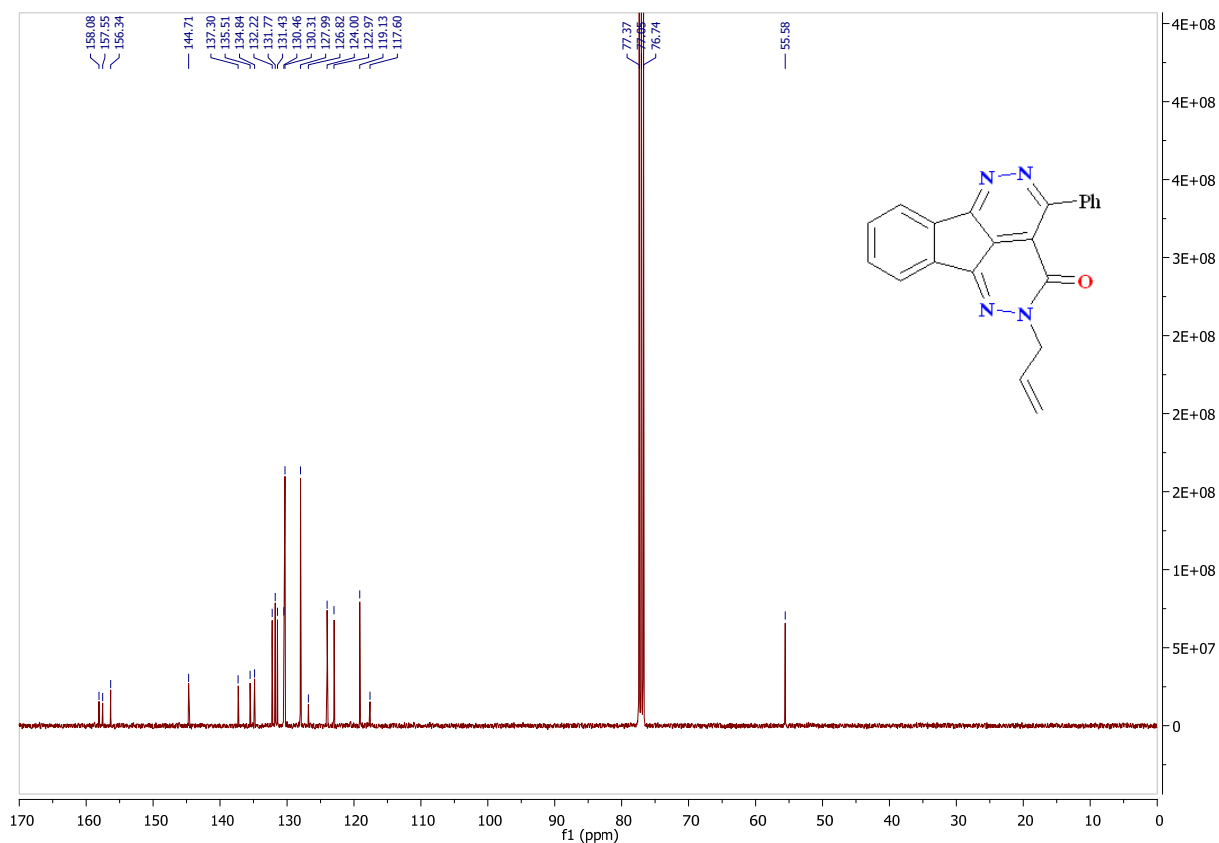
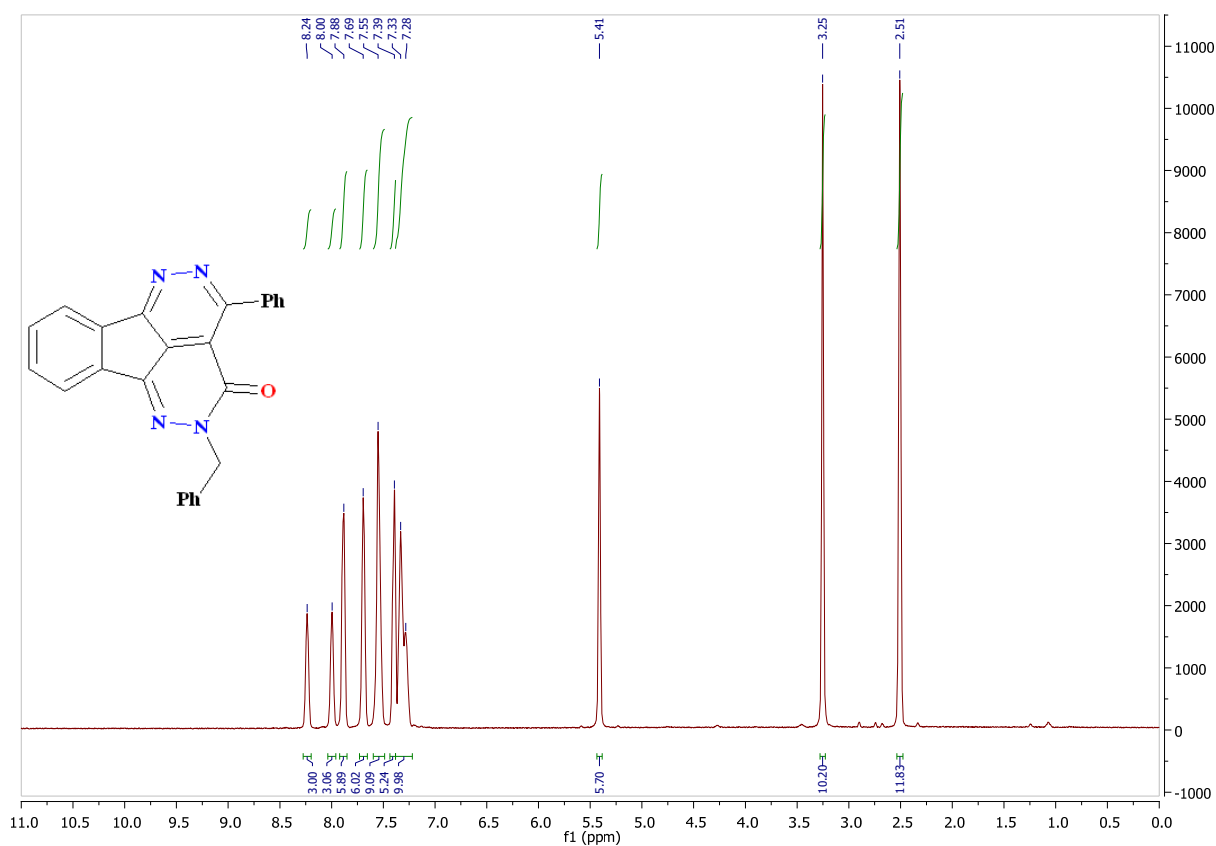
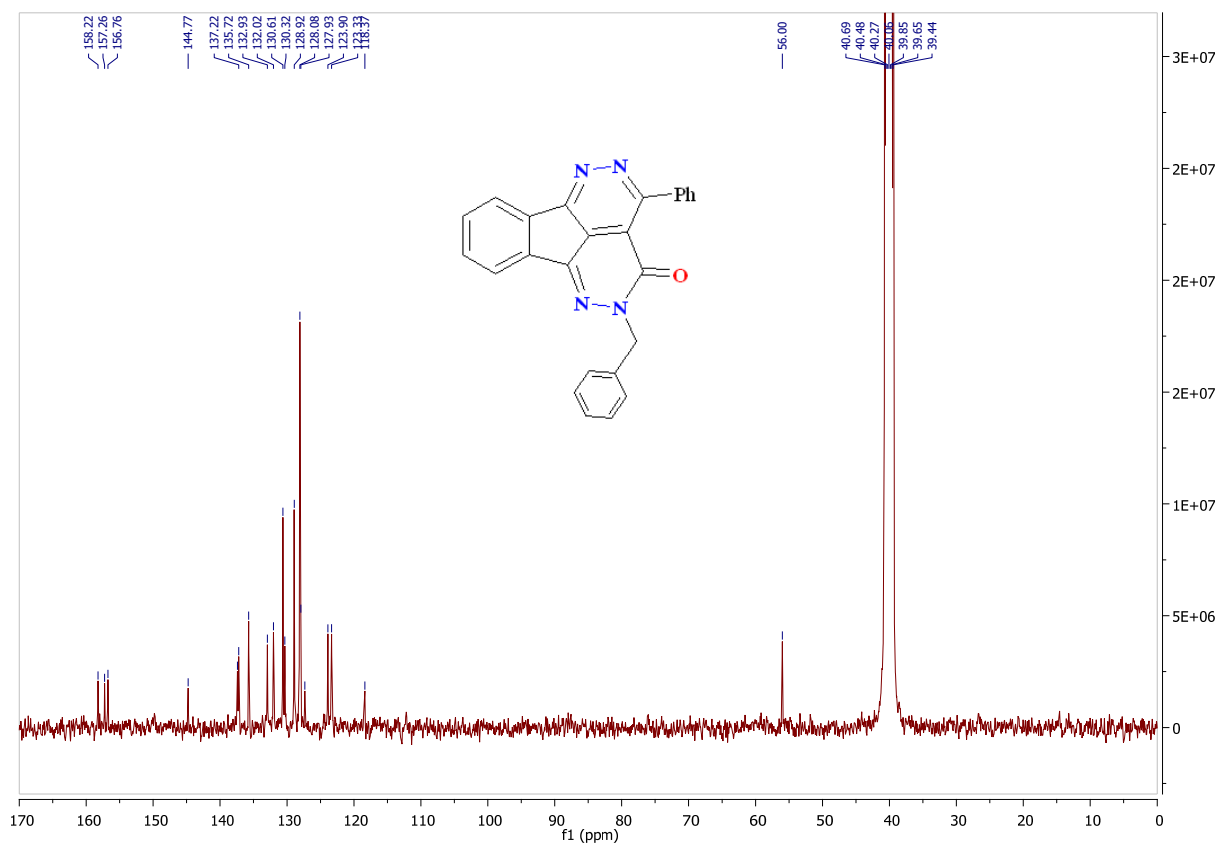
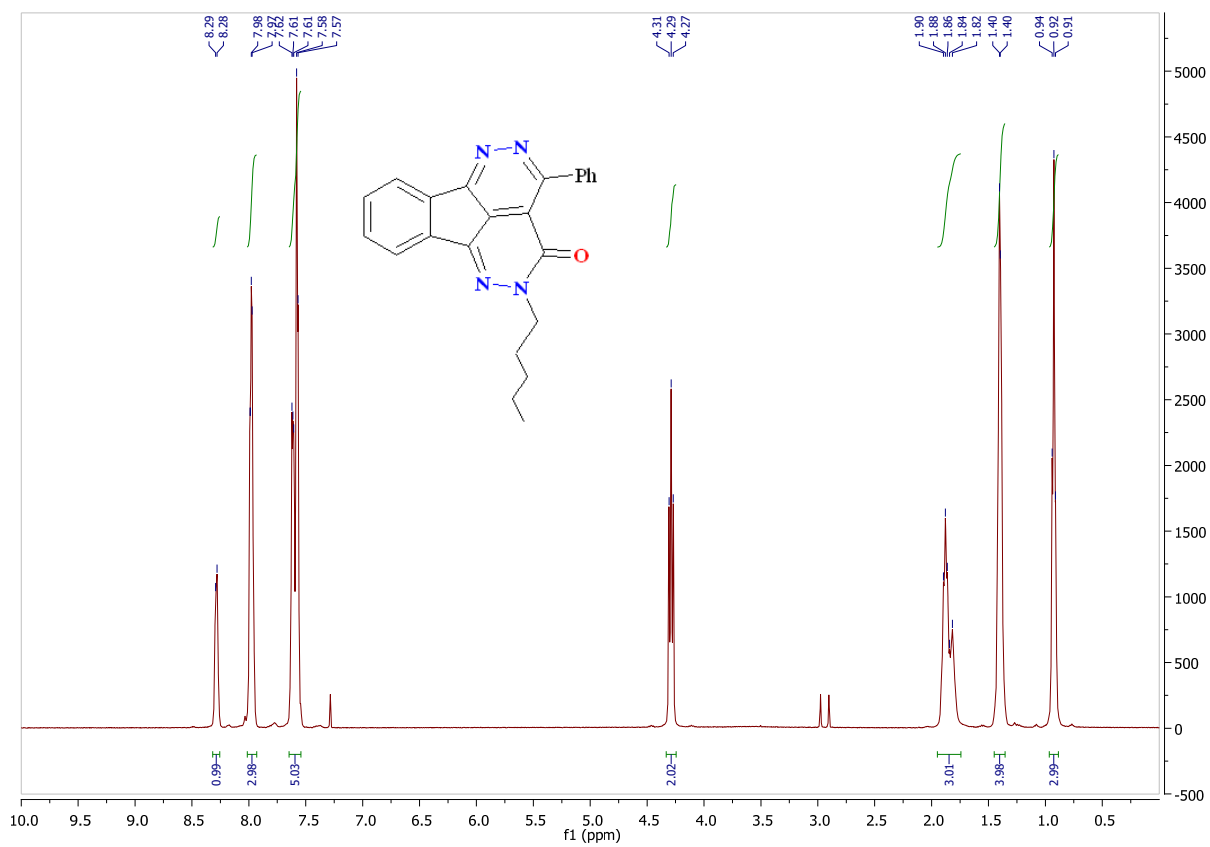


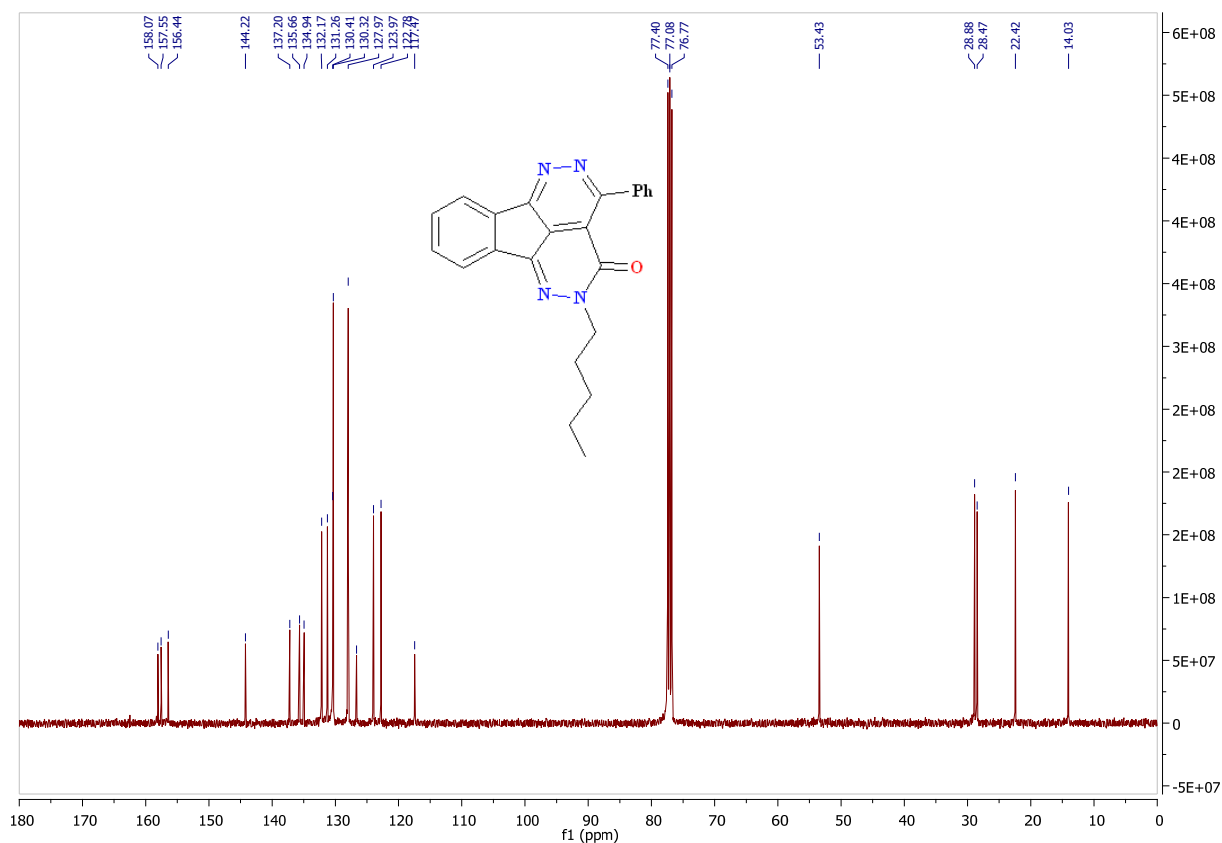
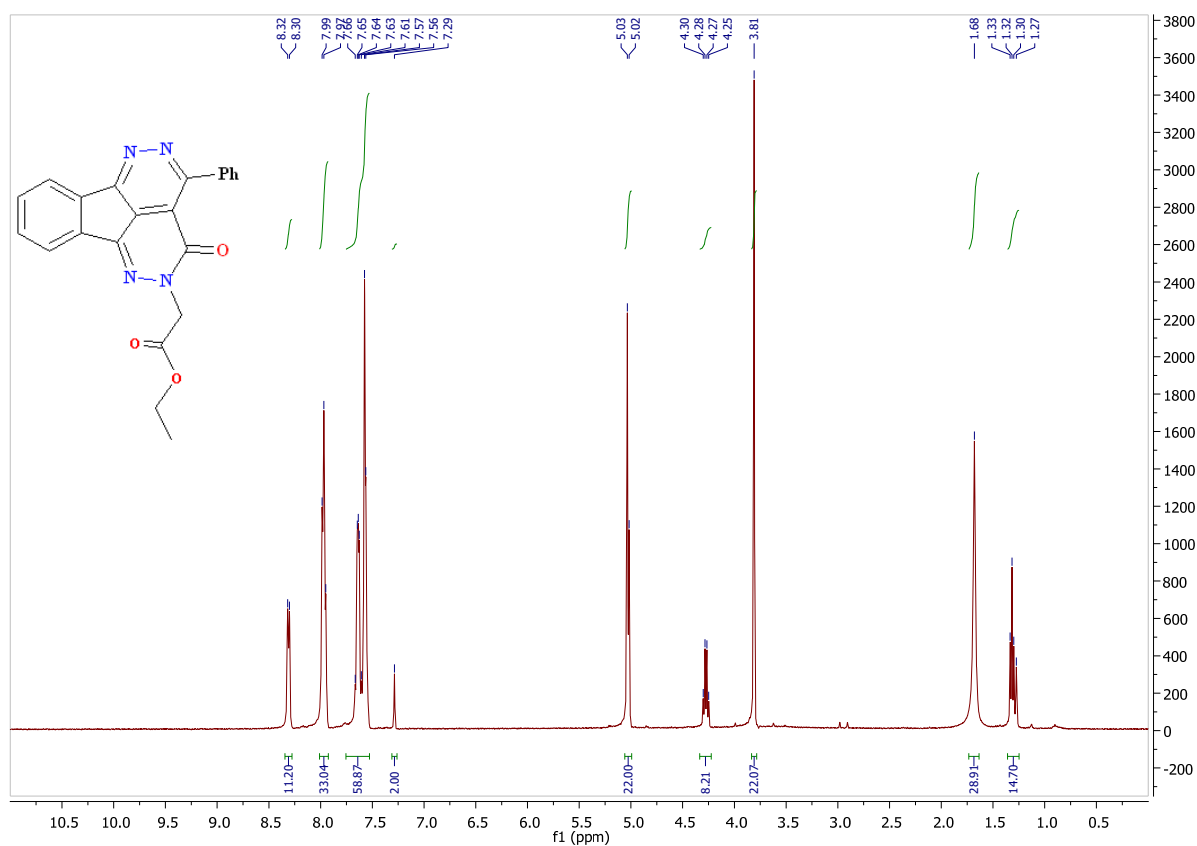
Figure S1. <sup>1</sup>H NMR of 2

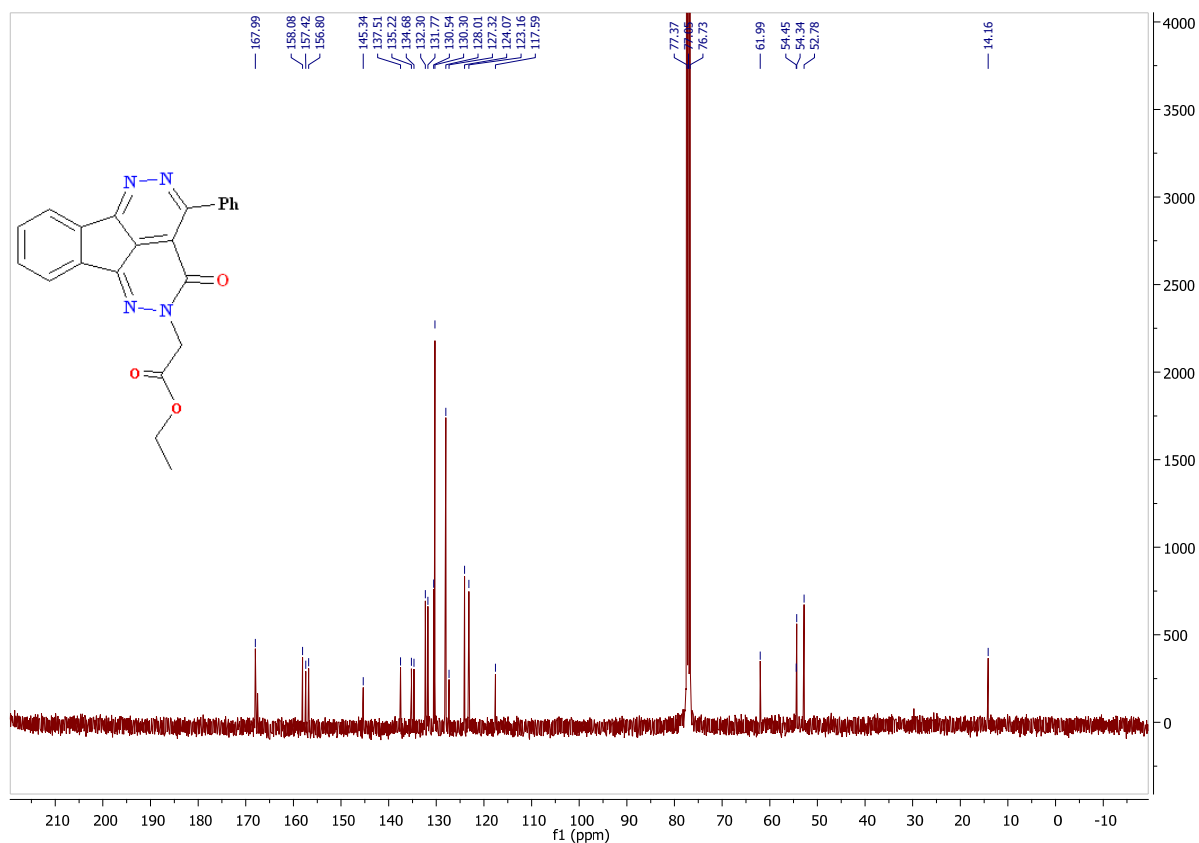
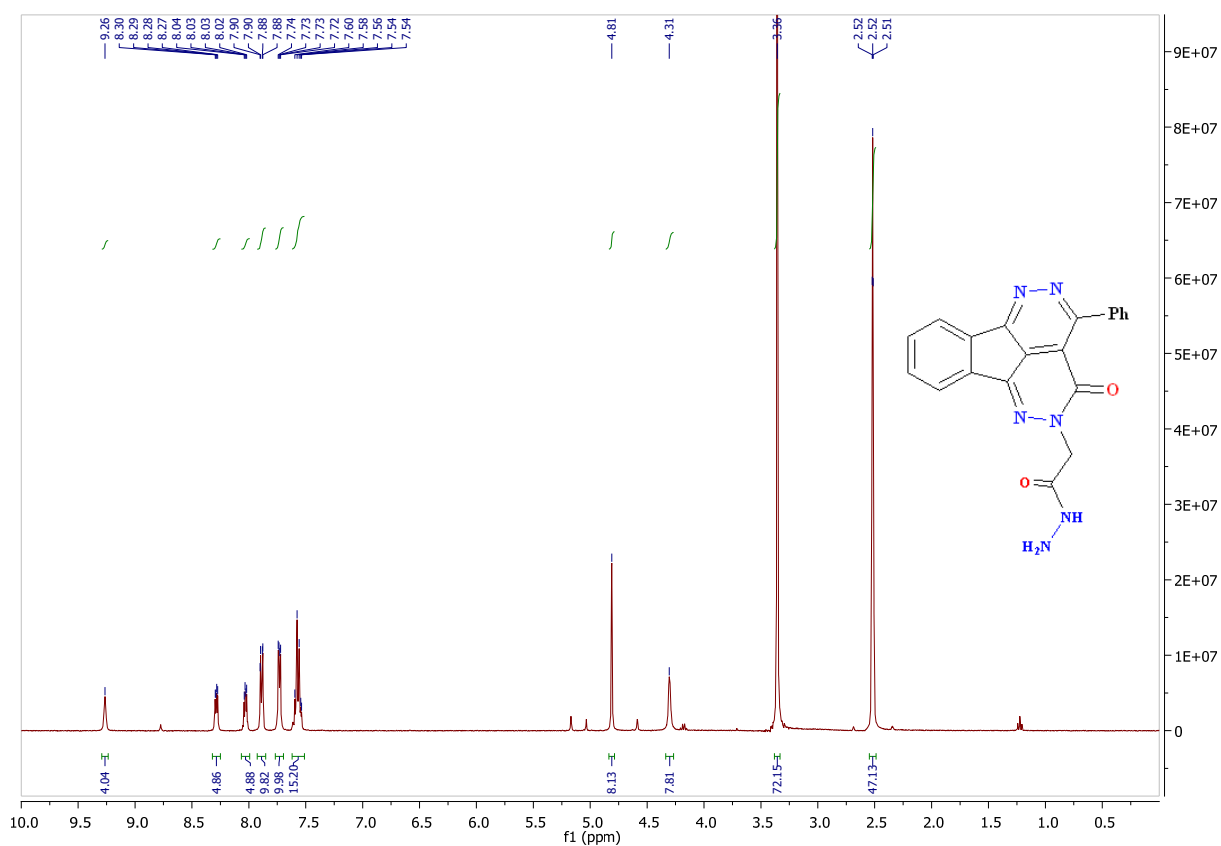
Figure S2. <sup>13</sup>C NMR of 2Figure S3. <sup>1</sup>H NMR of 3

Figure S4. <sup>13</sup>C NMR of 3Figure S5. <sup>1</sup>H NMR of 4

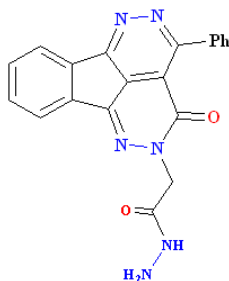
Figure S6. <sup>13</sup>C NMR of 4Figure S7. <sup>1</sup>H NMR of 5

Figure S8. <sup>13</sup>C NMR of **5**Figure S9. <sup>1</sup>H NMR of **6**

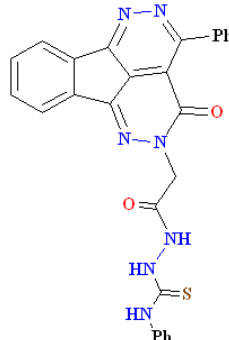
Figure S10. <sup>13</sup>C NMR of 6Figure S11. <sup>1</sup>H NMR of 7

Figure S12. <sup>13</sup>C NMR of 7Figure S13. <sup>1</sup>H NMR of 8





**Figure S14.**  $^{13}\text{C}$  NMR of **8**



**Figure S15.**  $^1\text{H}$  NMR of **9**

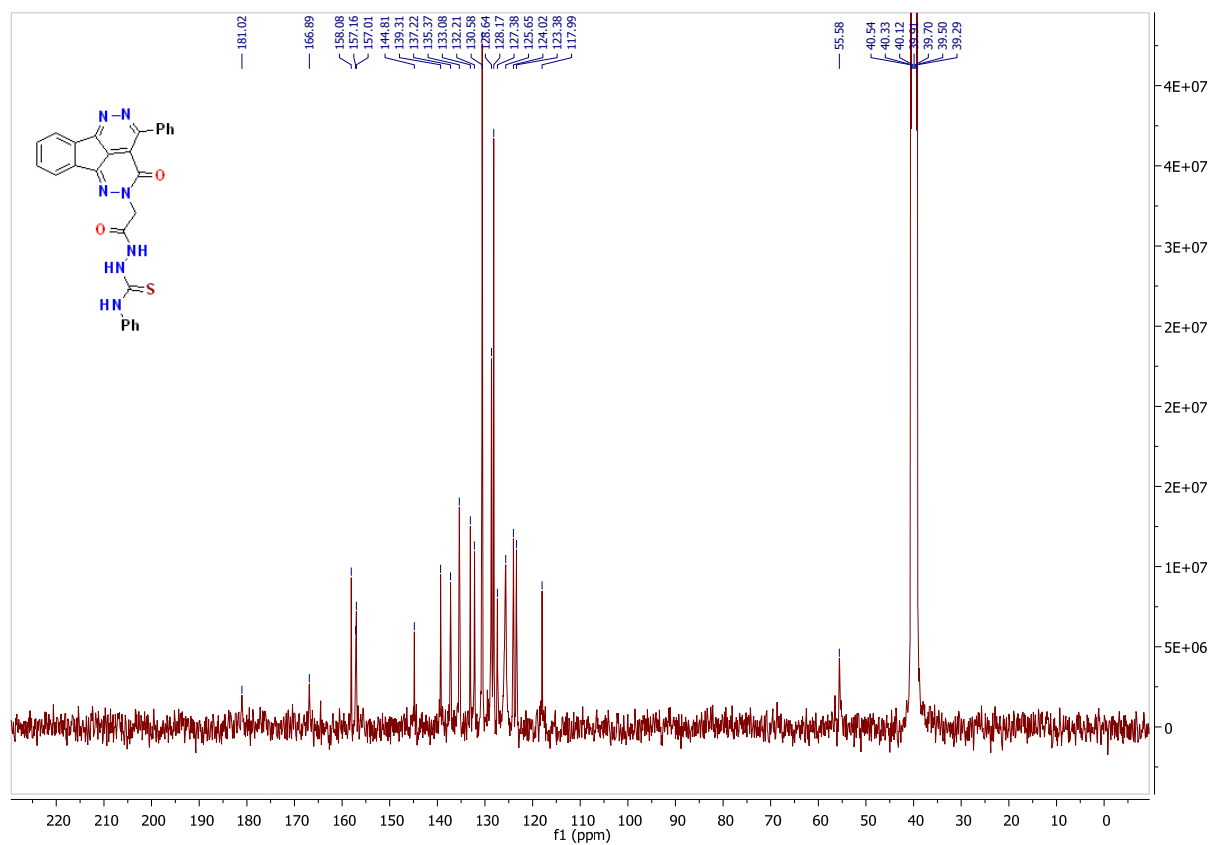


Figure S16. <sup>13</sup>C NMR of 9