

## Supporting Information

### **A Highly Green Approach towards Aromatic Nitro Group Substitutions: Catalyst Free Reactions of Nitroimidazoles with Carbon Nucleophiles in Water**

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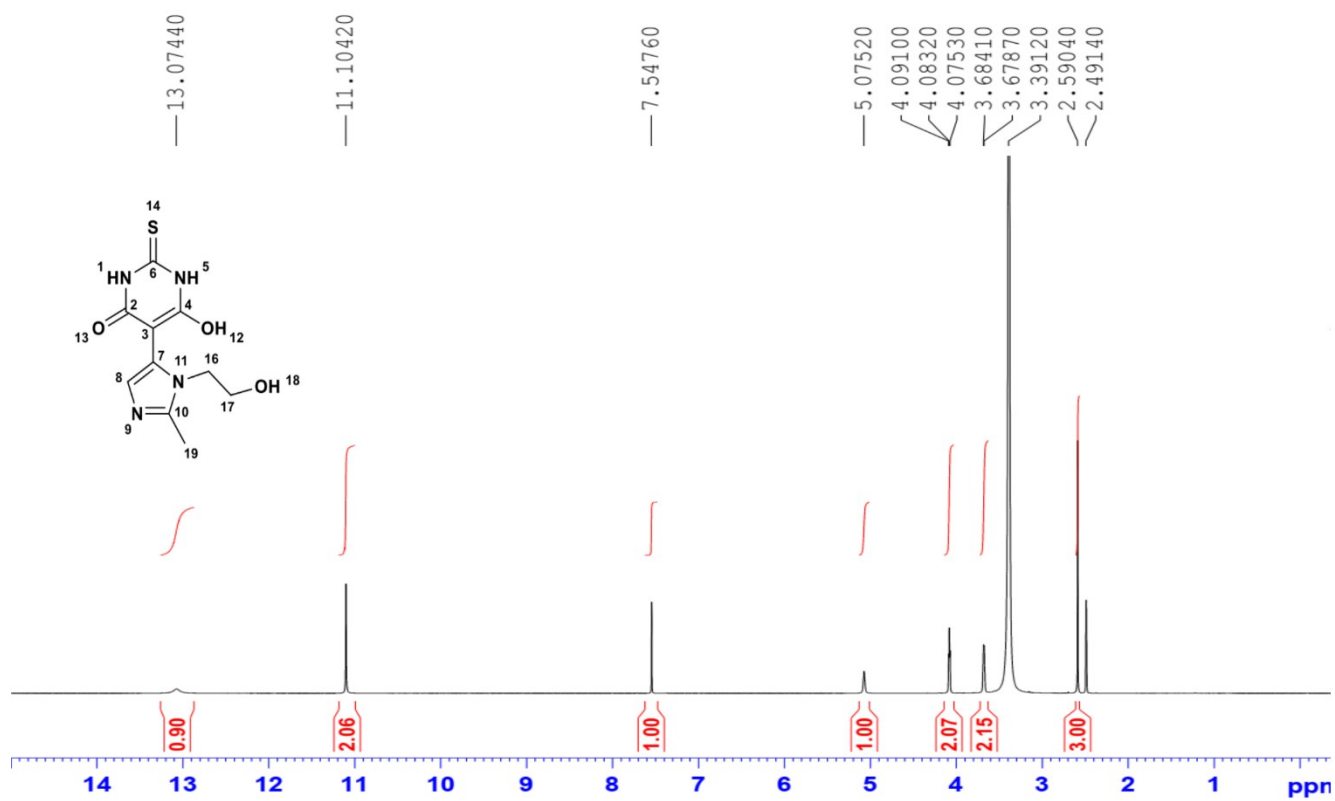


Figure S1. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 1.

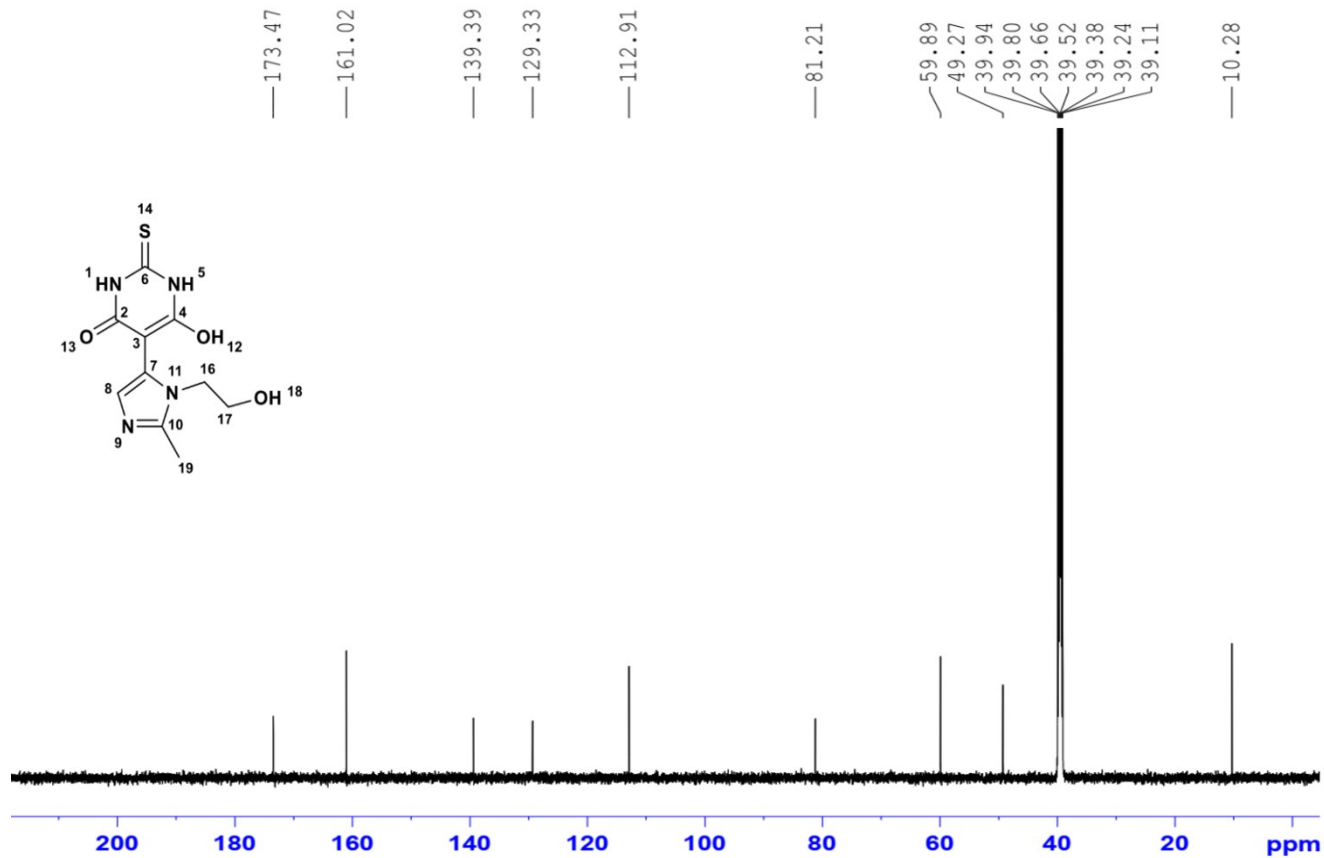


Figure S2. <sup>13</sup>C NMR spectrum (151 MHz, DMSO-*d*<sub>6</sub>) of Compound 1.

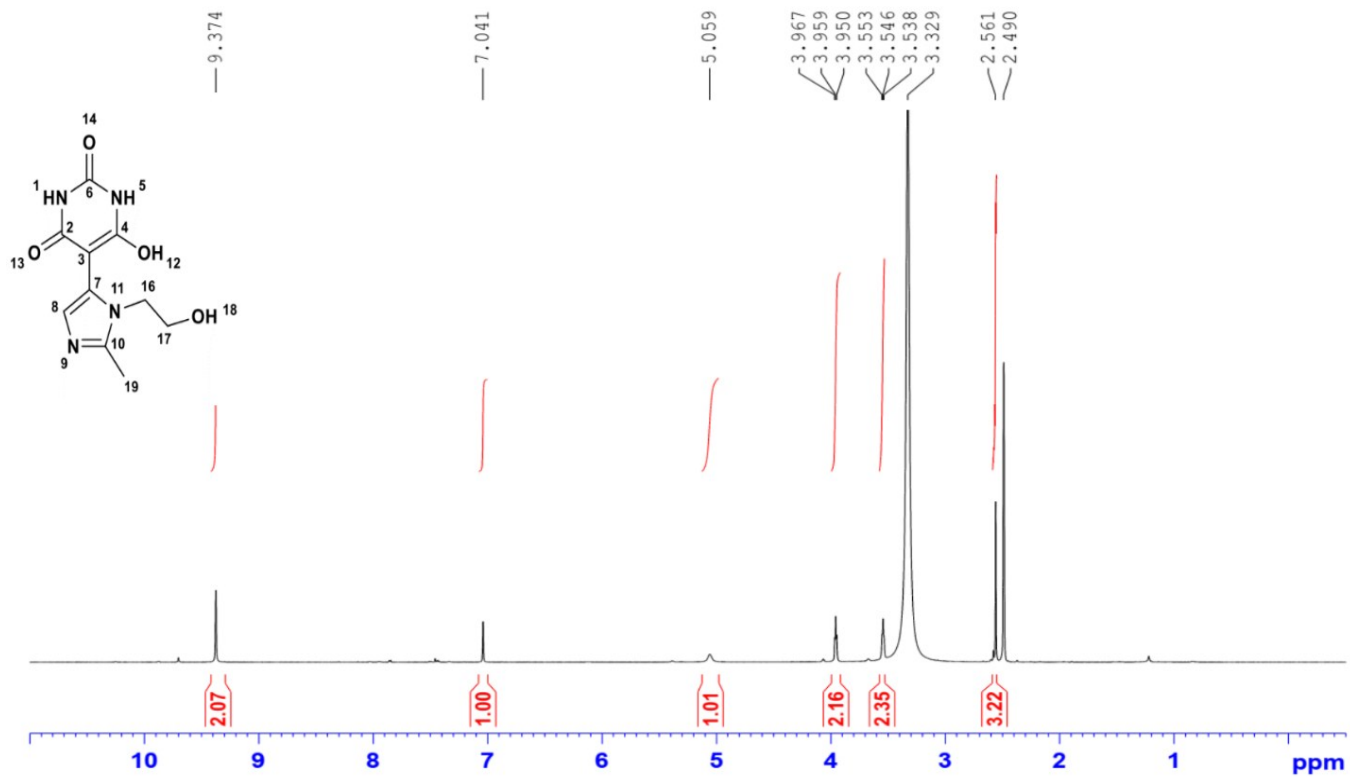


Figure S3. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 2.

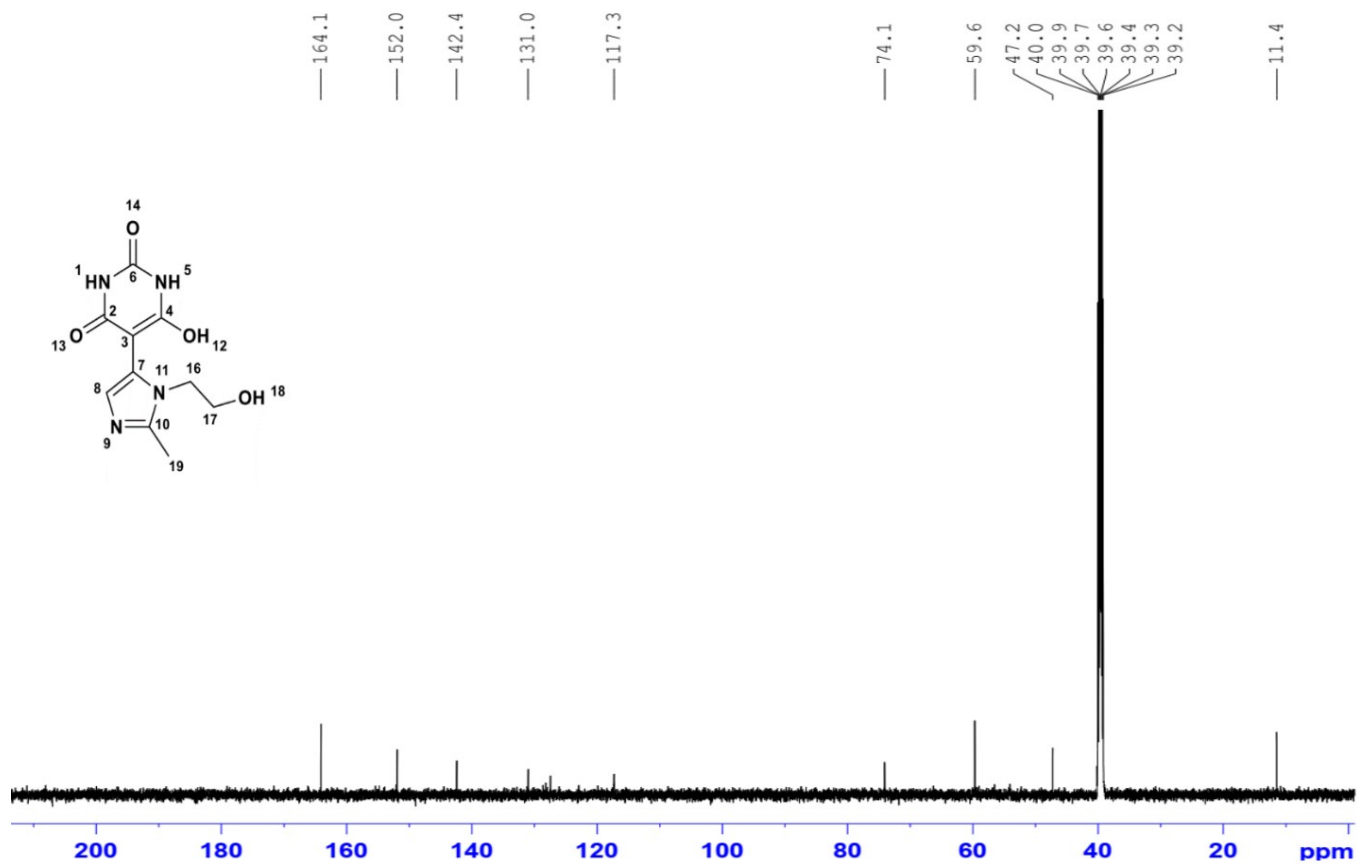


Figure S4. <sup>13</sup>C NMR Spectrum (151 MHz, DMSO-*d*<sub>6</sub>) compound of 2.

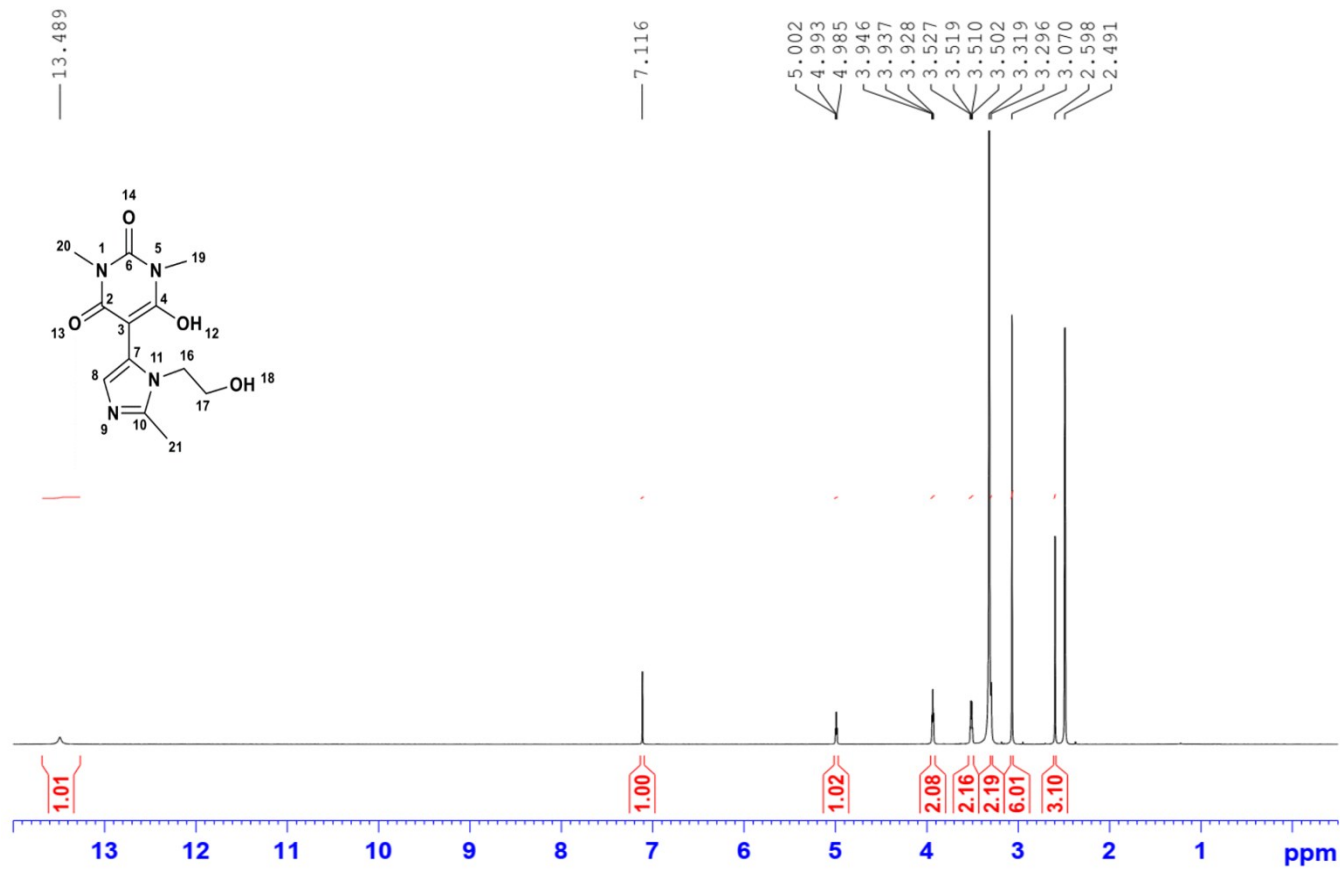


Figure S5. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 3.

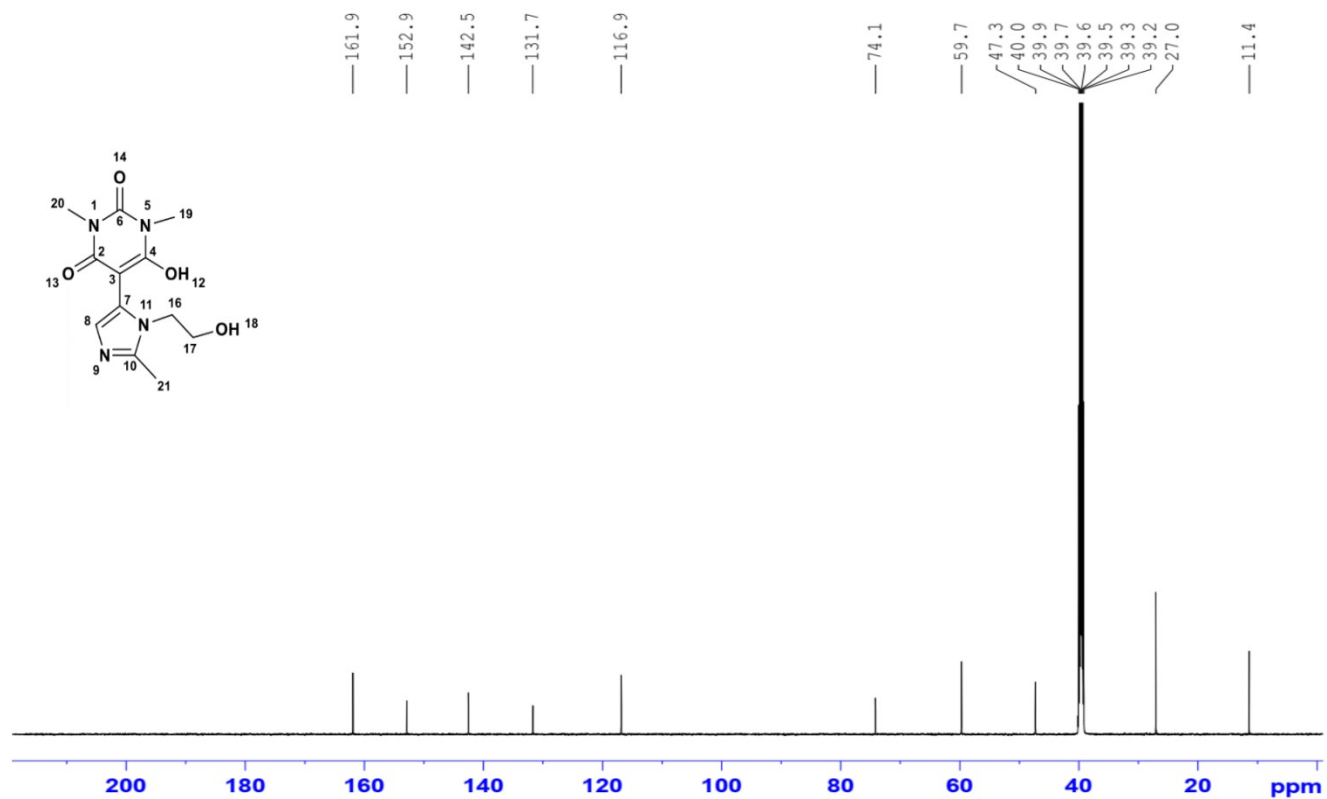


Figure S6. <sup>13</sup>C NMR Spectrum (151 MHz, DMSO-*d*<sub>6</sub>) of compound 3.

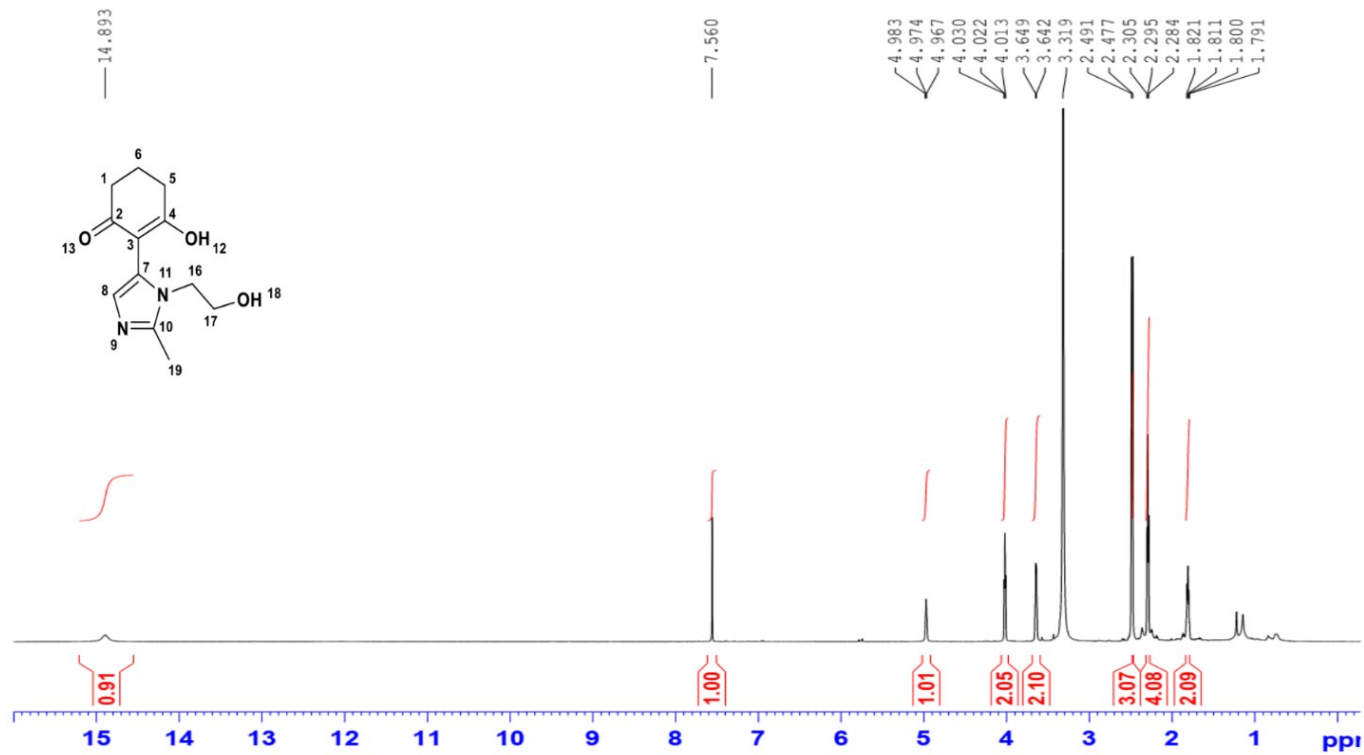


Figure S7. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 4.



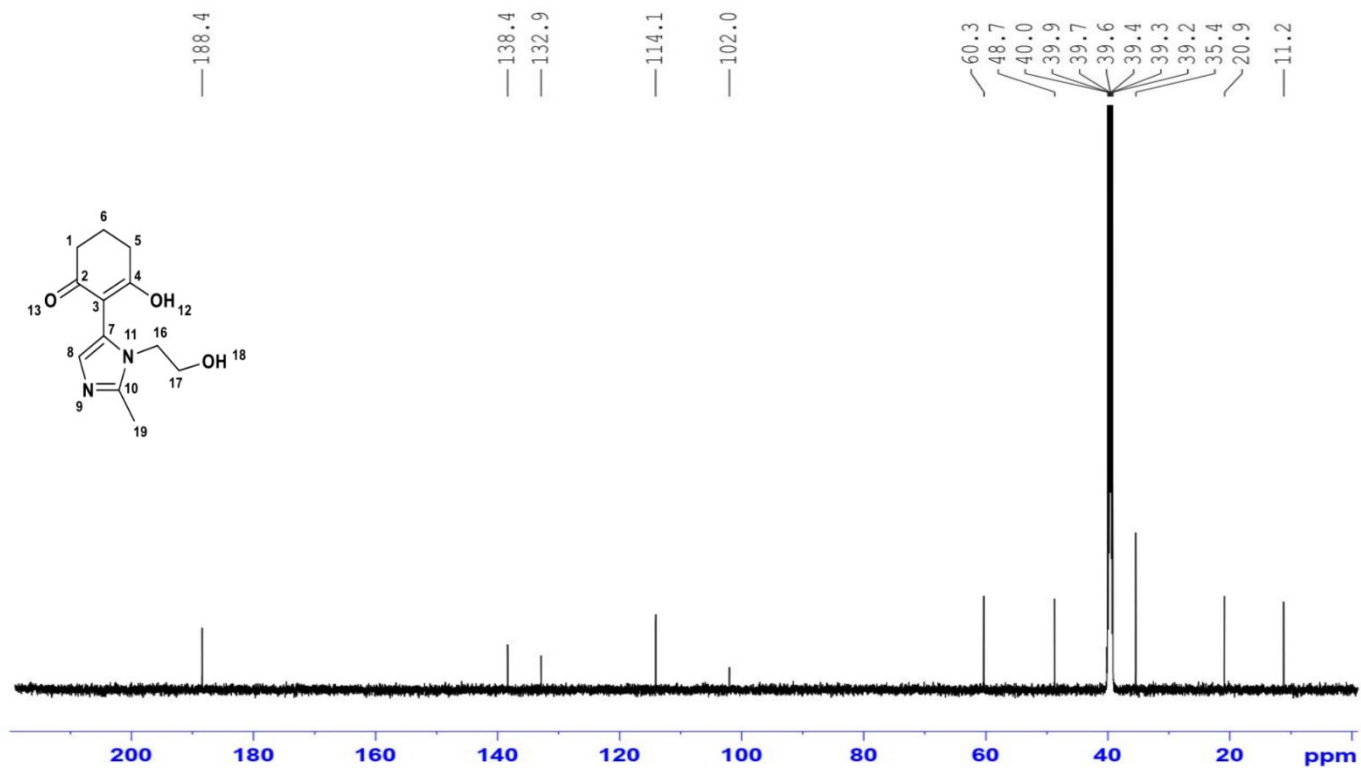


Figure S8.  $^{13}\text{C}$  NMR Spectrum (151 MHz,  $\text{DMSO-}d_6$ ) of compound 4.

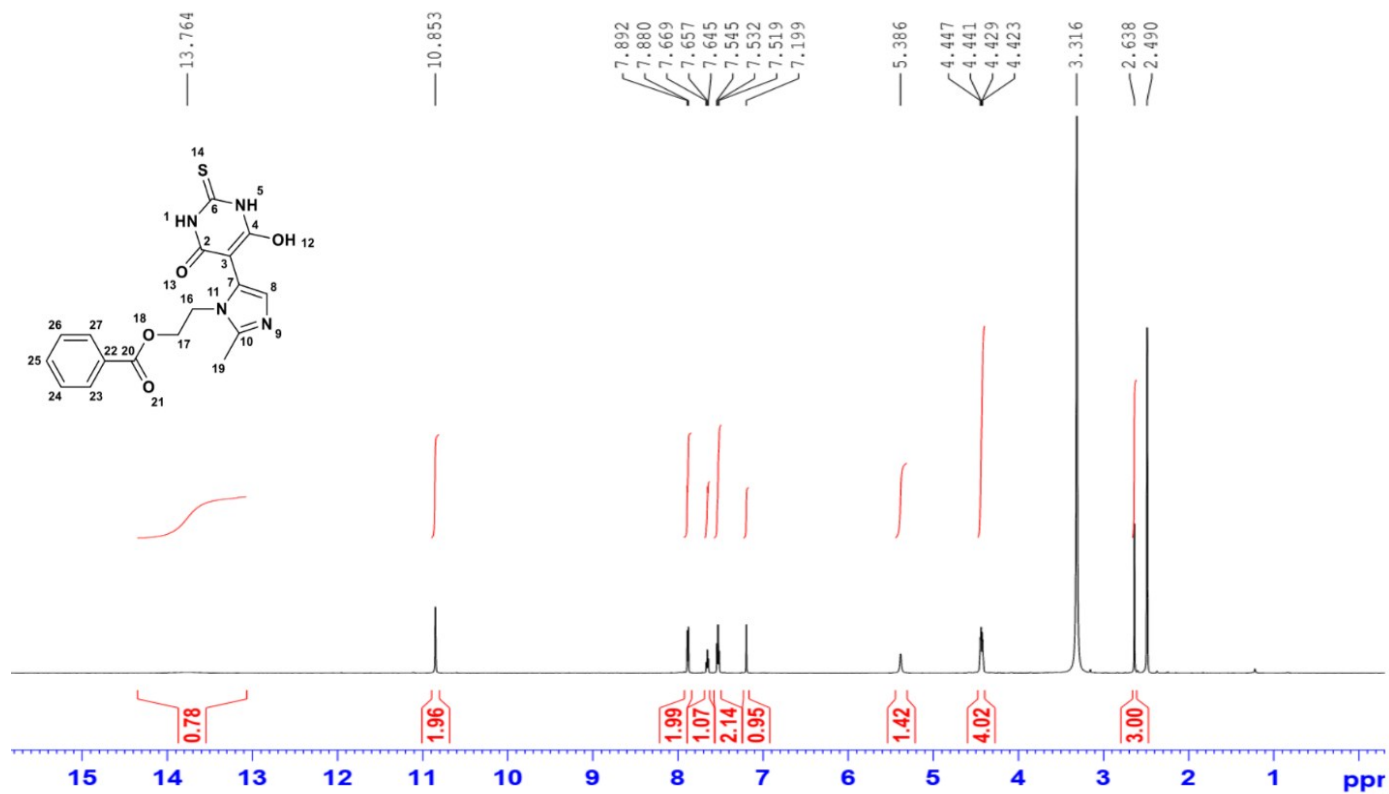


Figure S9. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 5.

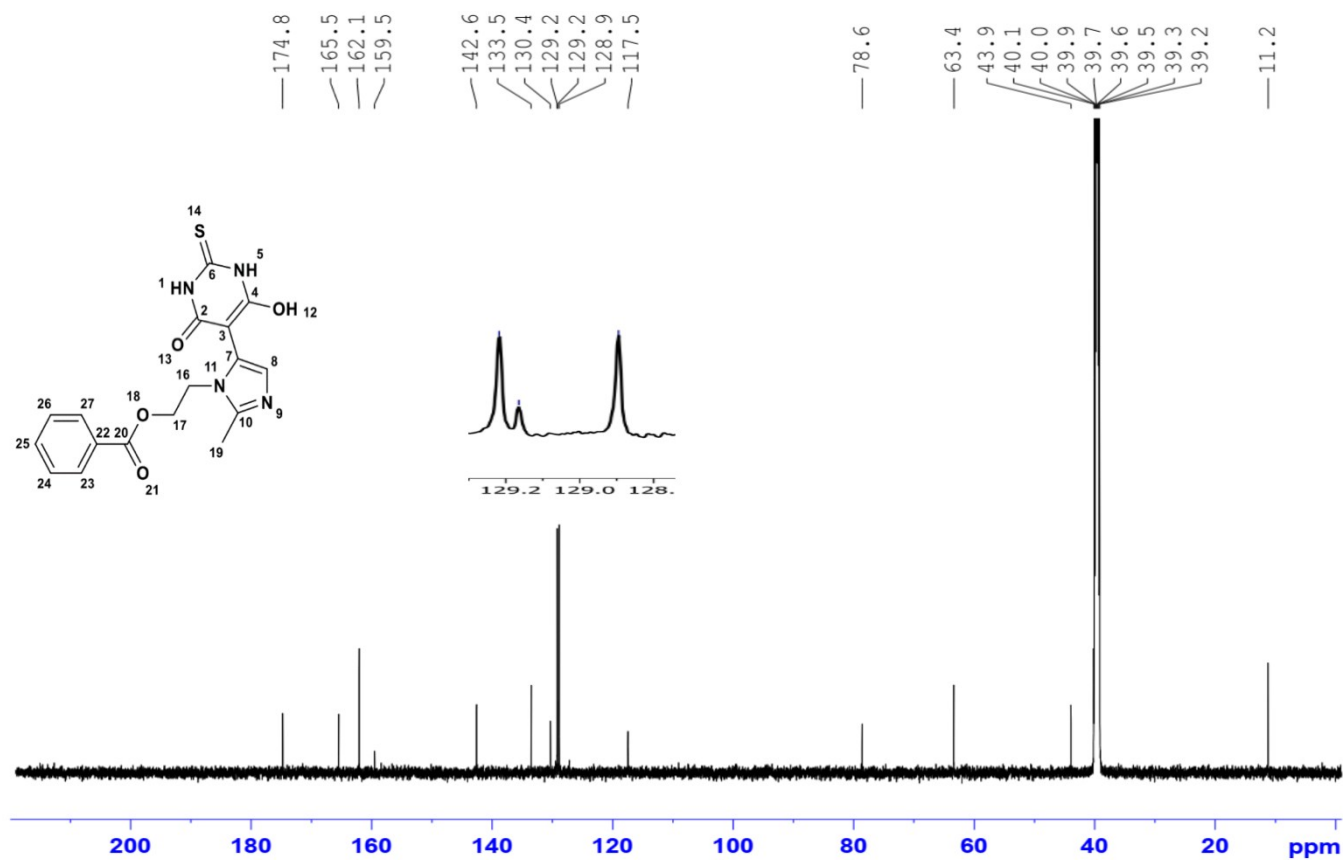


Figure S10.  $^{13}\text{C}$  NMR Spectrum (151 MHz,  $\text{DMSO-}d_6$ ) of compound 5.

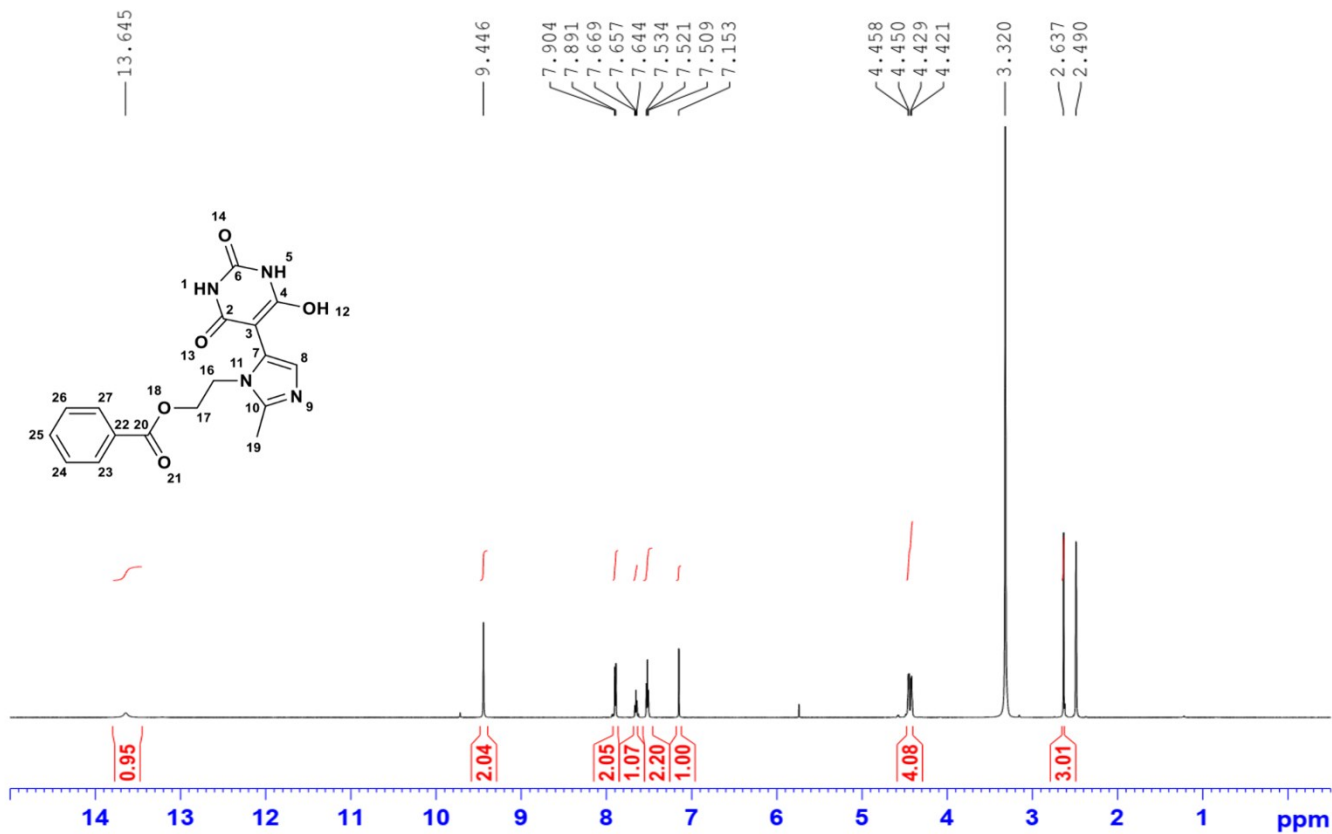


Figure S11. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound **6**.

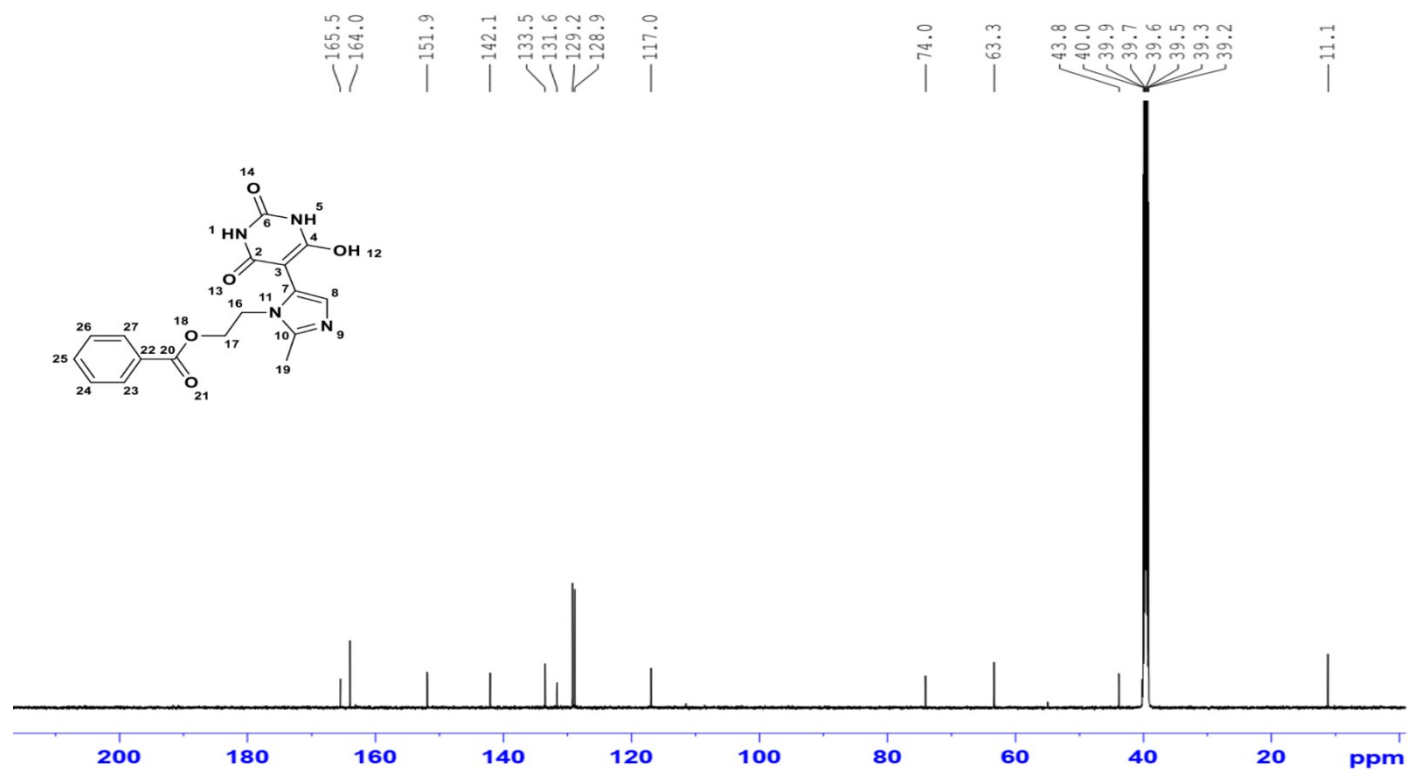


Figure S12.  $^{13}\text{C}$  NMR Spectrum (151 MHz,  $\text{DMSO-}d_6$ ) of compound of compound **6**.

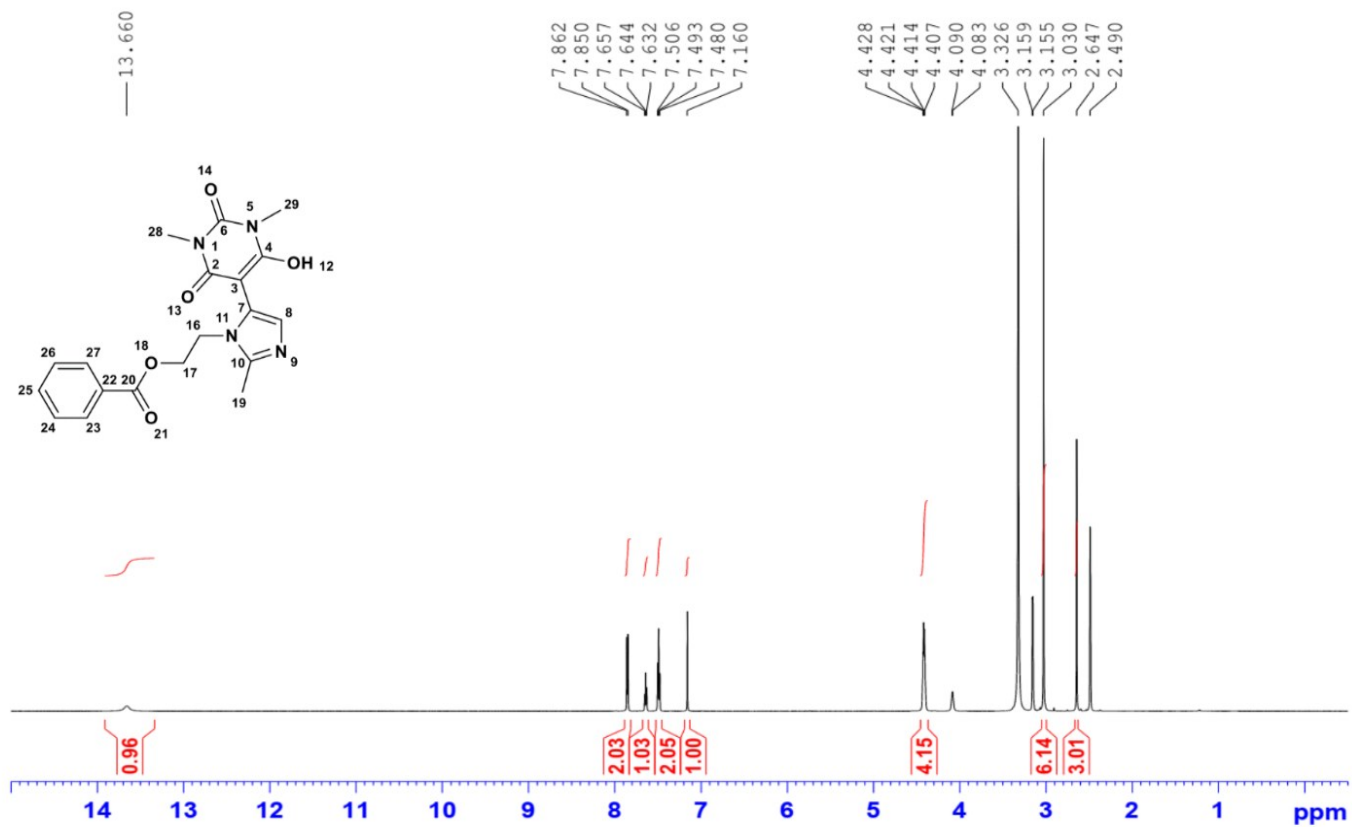


Figure S13. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 7

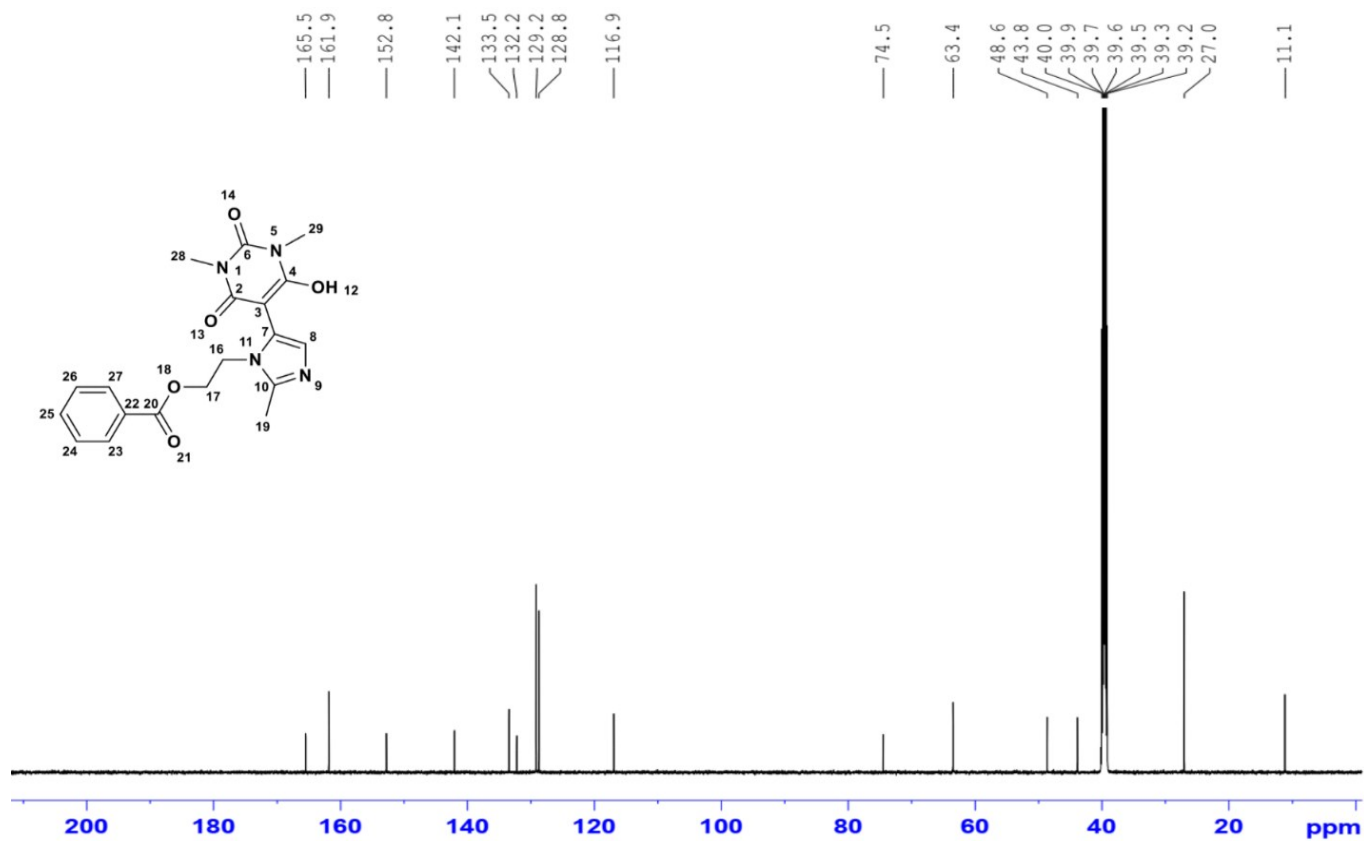


Figure S14. <sup>13</sup>C NMR Spectrum (151 MHz, DMSO-*d*<sub>6</sub>) of compound 7.

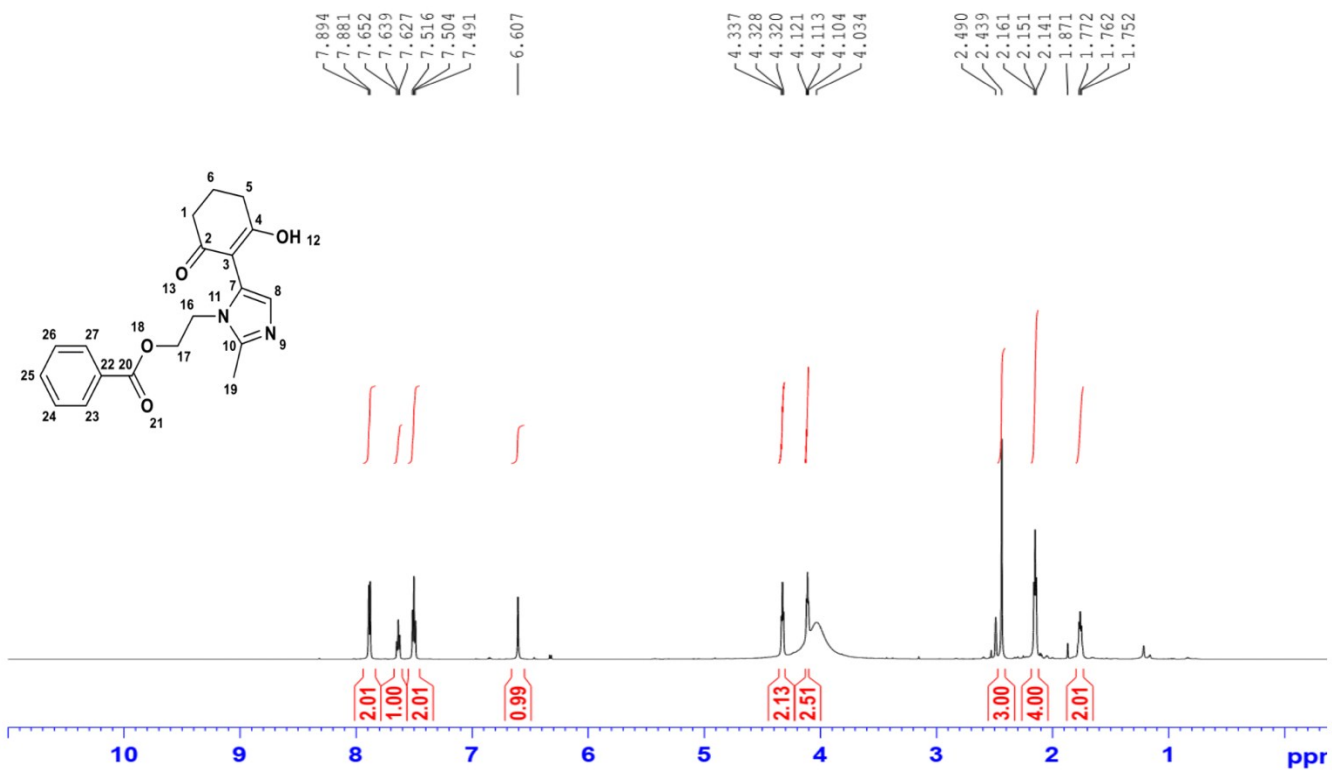


Figure S15. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound **8**.



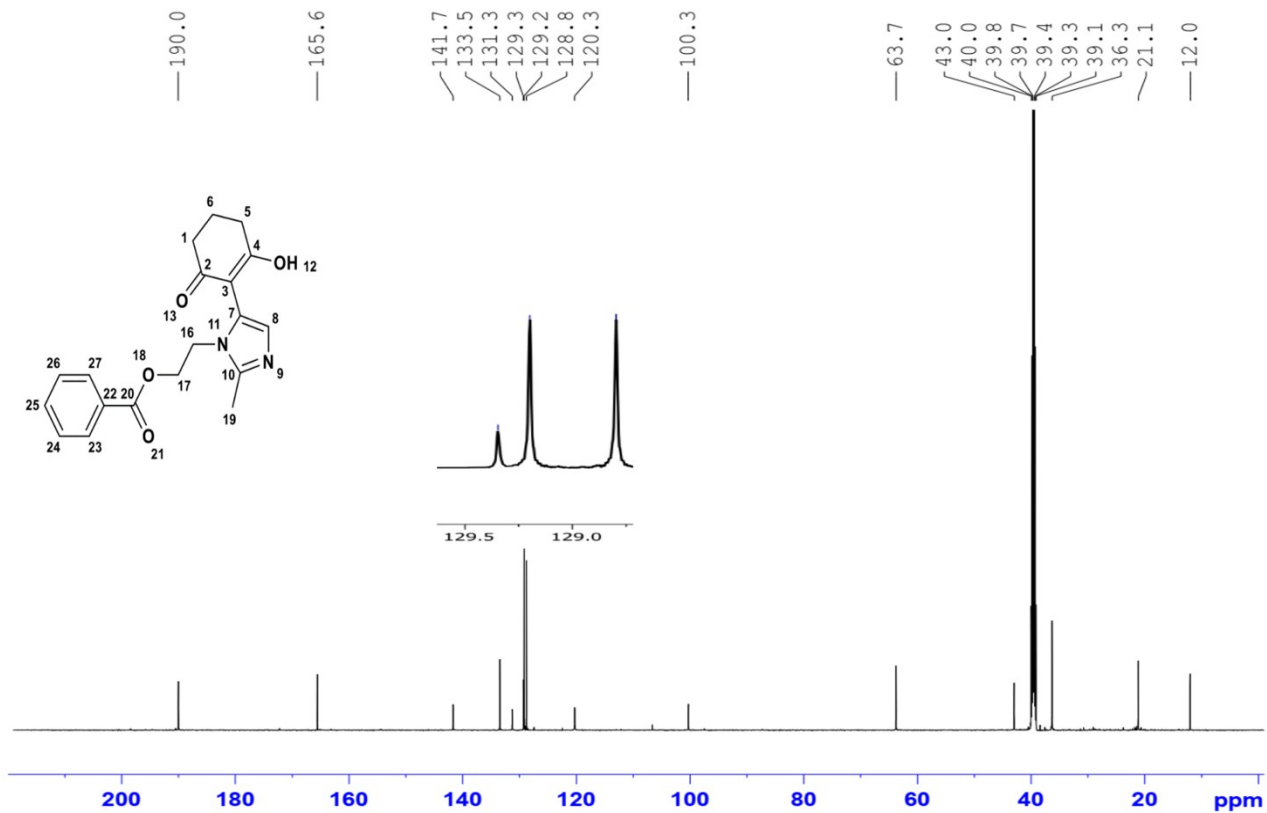


Figure S16. <sup>13</sup>C NMR Spectrum (151 MHz, DMSO-*d*<sub>6</sub>) of compound **8**.

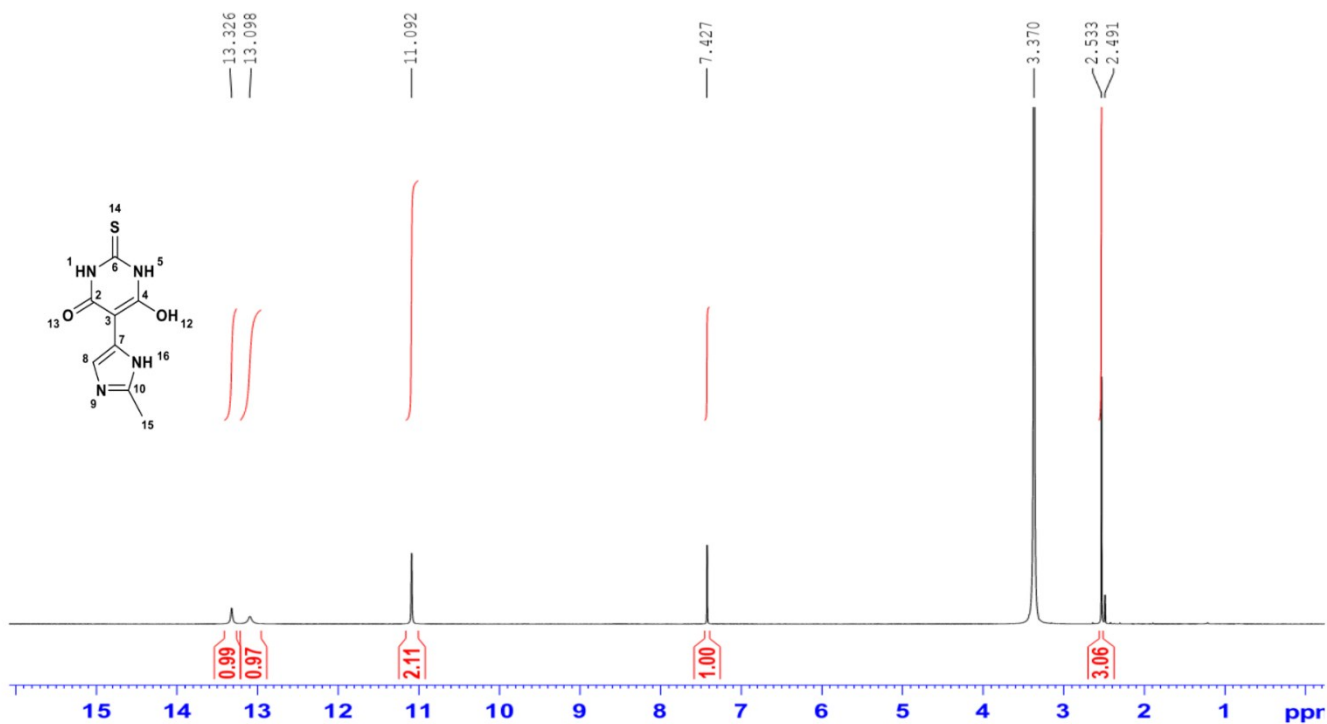


Figure: S17. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 9.

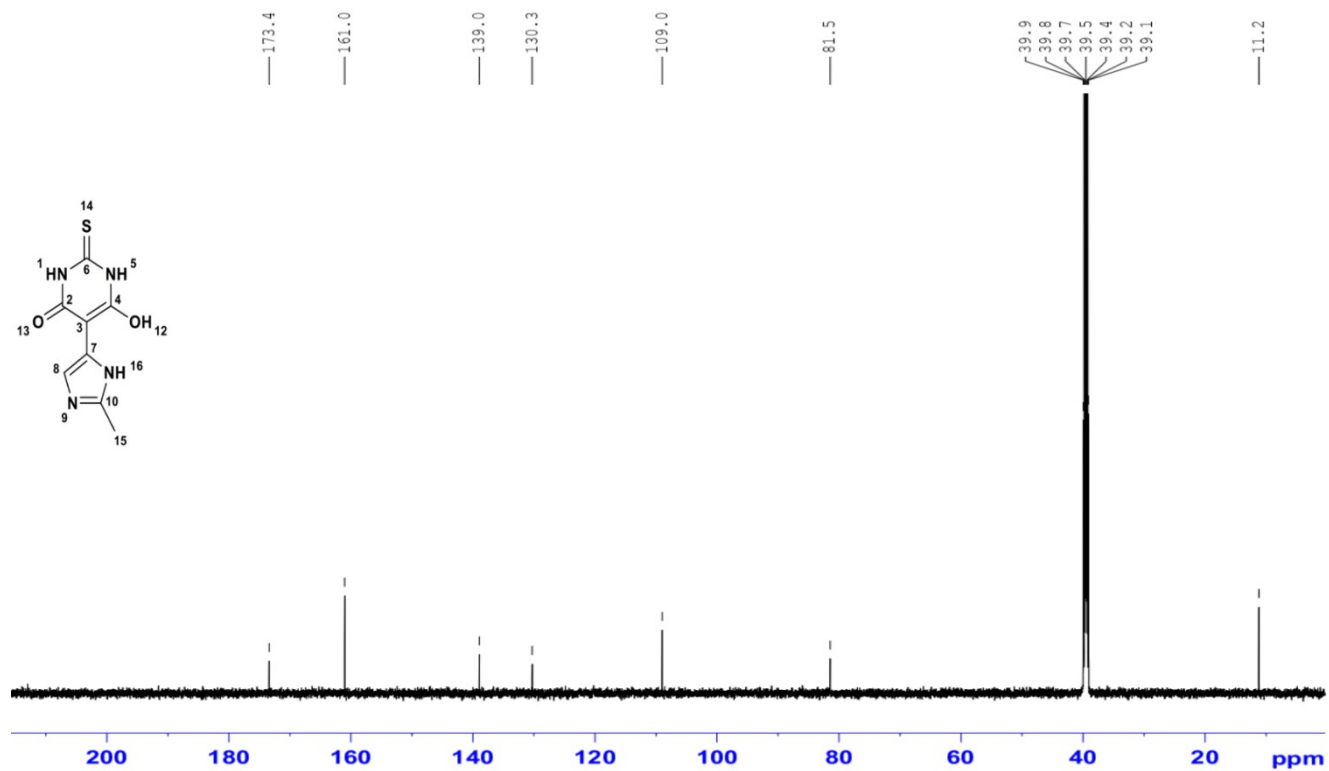


Figure S18.  $^{13}\text{C}$  NMR Spectrum (151 MHz,  $\text{DMSO-}d_6$ ) of compound 9.

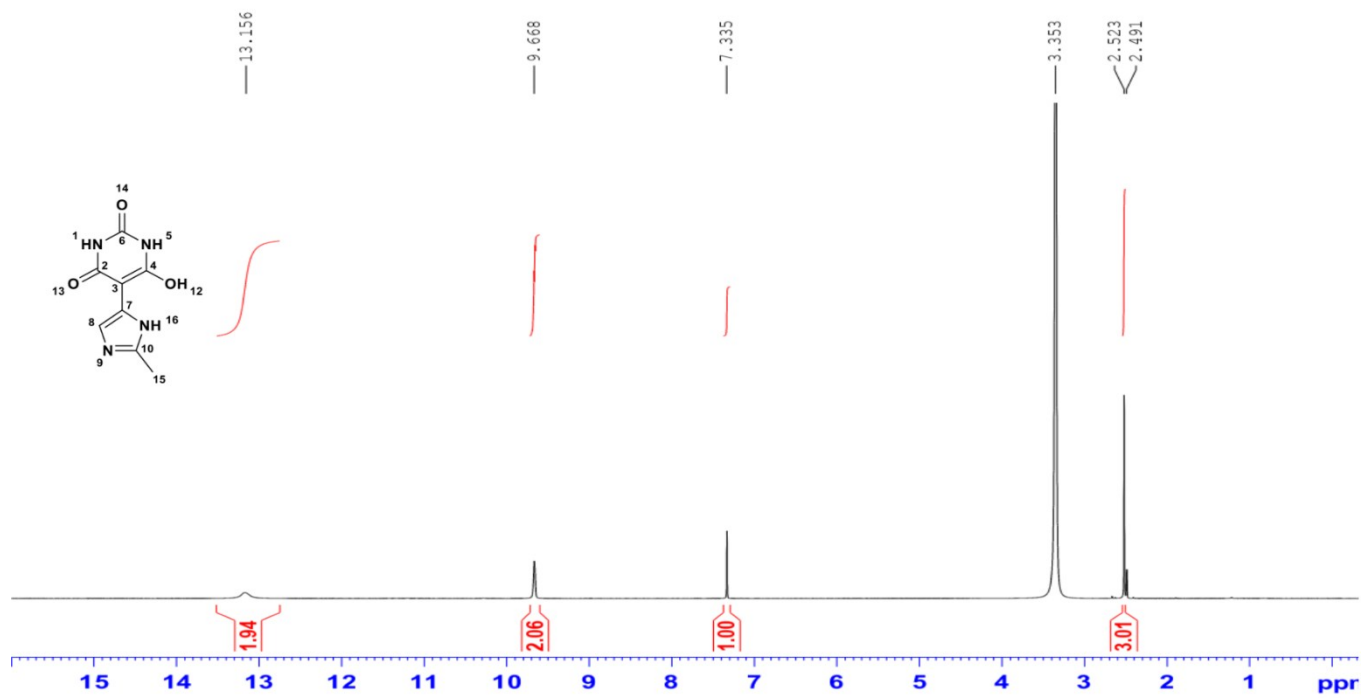


Figure S19. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound **10**.

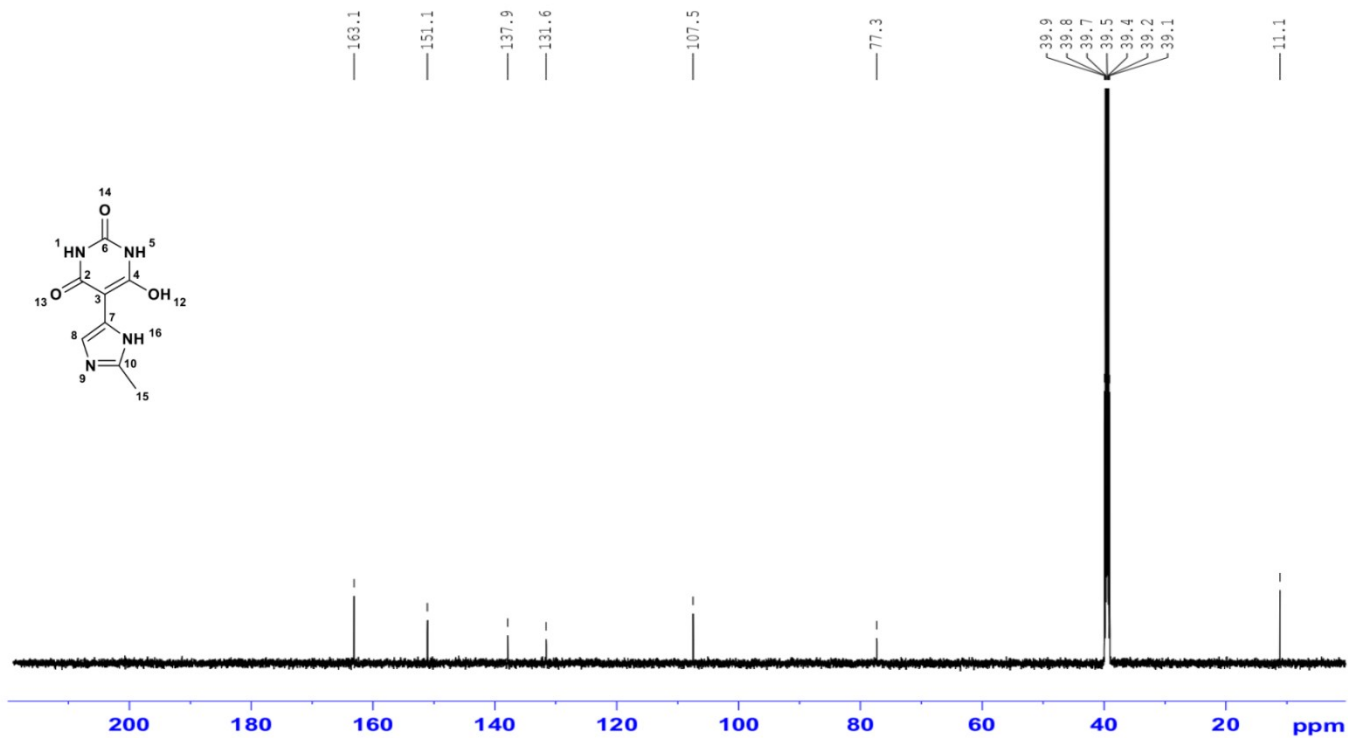


Figure S20. <sup>13</sup>C NMR Spectrum (151 MHz, DMSO-*d*<sub>6</sub>) of compound 10.

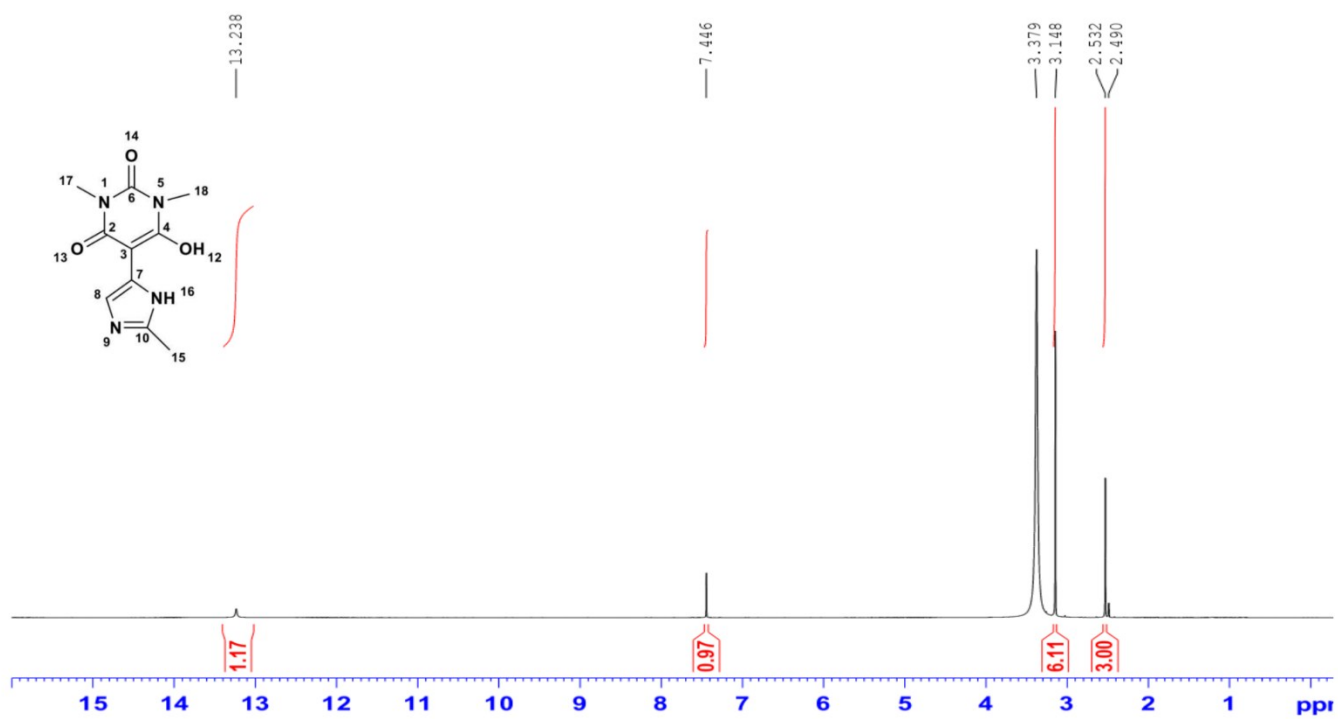


Figure S21. <sup>1</sup>H NMR Spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 11.

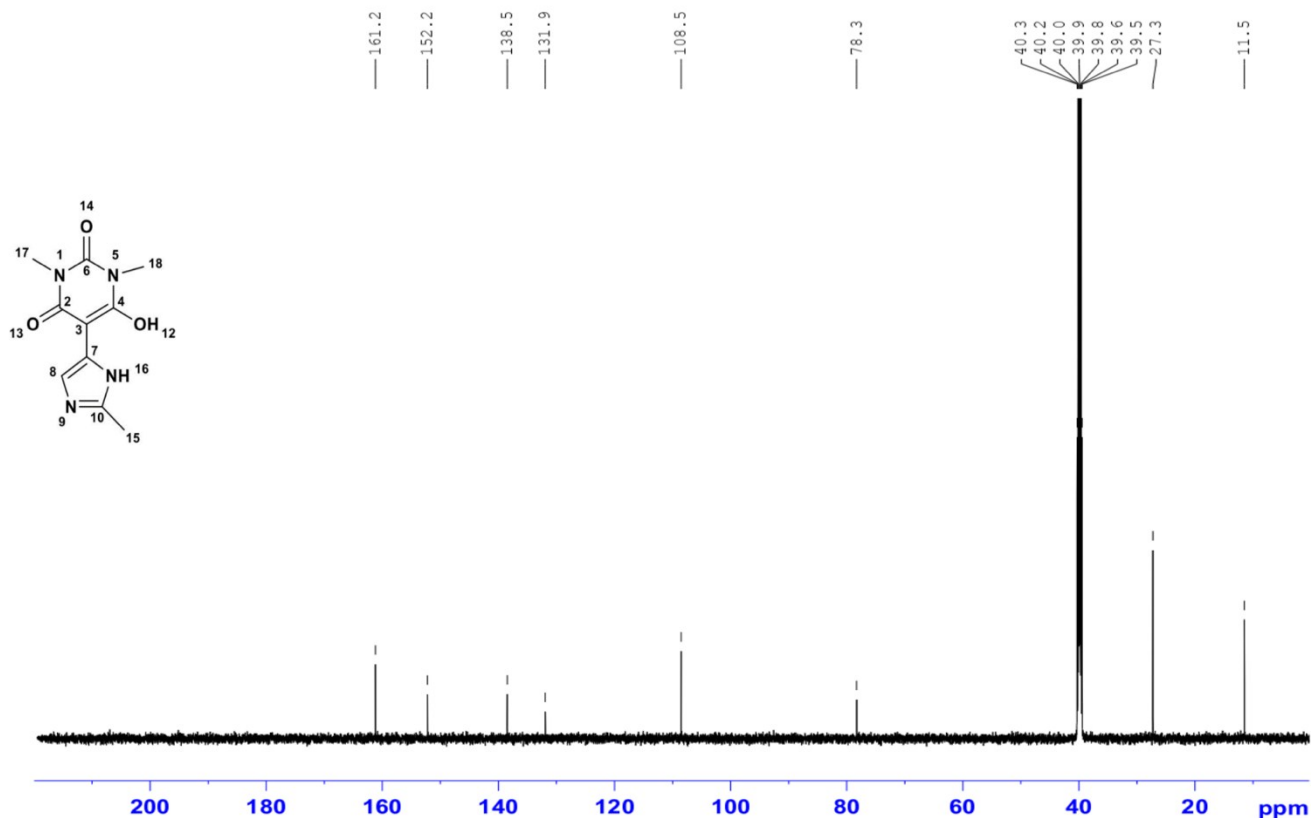


Figure S22. <sup>13</sup>C NMR Spectrum (151 MHz, DMSO-*d*<sub>6</sub>) of compound **11**.

### Structural Analysis with X-Ray

For X-ray measurements, Single crystals of **1**, **3** and **7** were mounted on a MiTeGen loop with grease and examined on a Bruker D8 Venture APEX diffractometer equipped with Photon 100 CCD area detector at 296 (2) K using graphite-monochromated Mo-K<sub>α</sub> radiation ( $\lambda = 0.71073\text{\AA}$ ). Data were collected using the APEX-II software,<sup>1</sup> integrated using SAINT<sup>2</sup> and corrected for absorption using a multi-scan approach (SADABS).<sup>3</sup> Final cell constants were determined from full least squares refinement of all observed reflections. The structure was solved using intrinsic phasing (SHELXT).<sup>4</sup> All non-H atoms were located in subsequent difference maps and refined anisotropically with SHELXL-2014/7.<sup>5</sup> H-atoms were added at calculated positions and refined with a riding model. The structures of **1**, **3** and **7** have been deposited with the CCDC (CCDC deposition numbers 1995006–1995008).

(1) APEX-II, Bruker AXS, Madison, WI, USA.

- (2) SAINT, Bruker AXS, Madison, WI, USA.
- (3) SADABS, Bruker AXS, Madison, WI, USA.
- (4) G. M. Sheldrick, Acta Crystallogr., Sect. A: Found. Adv., 2015, 71, 3.
- (5) SHELXTL, Bruker AXS, Madison, Wisconsin, USA, 2015.

### Crystal Structures of the Representative Compounds

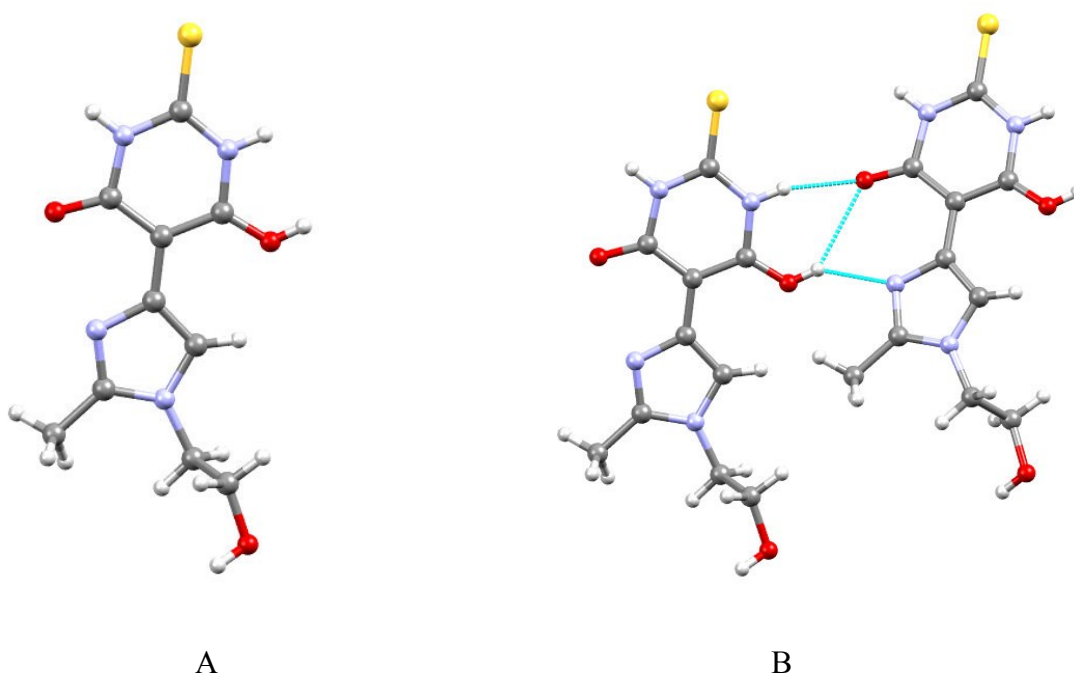


Figure S23: (A) Crystal Structure of compound 1 (B) hydrogen bonding in compound 1, H-bonds are shown in blue.



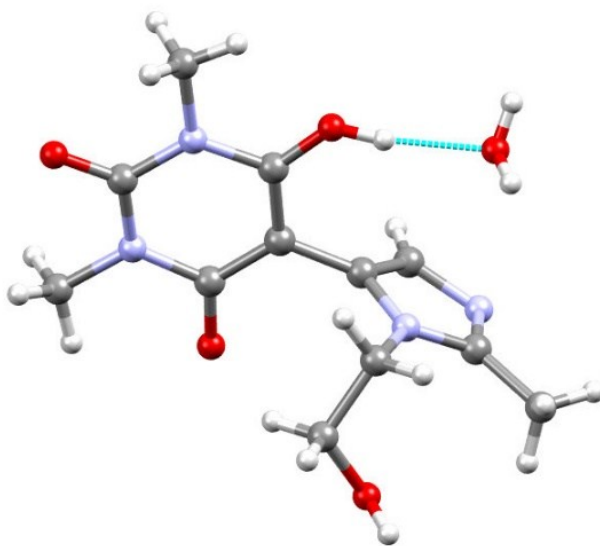


Figure S24. Crystal Structures of Compound 3. H-bond with lattice water molecule is shown in blue.

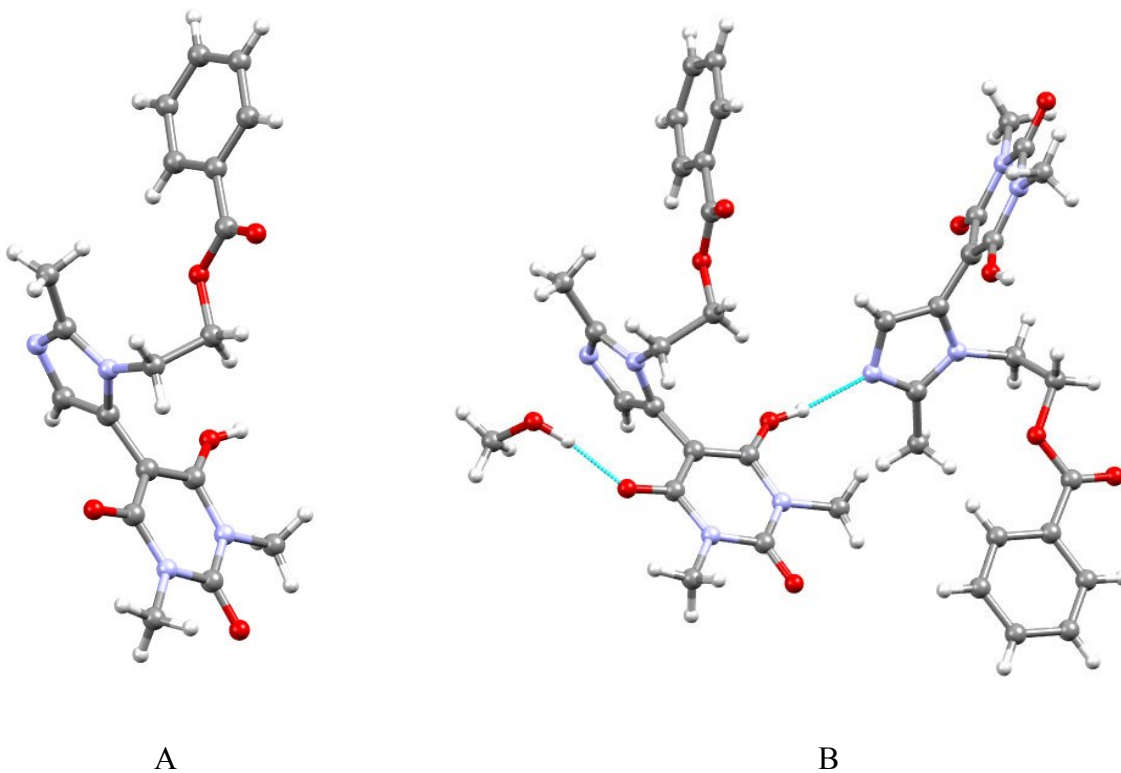


Figure S25. Crystal Structure of compound 5 (B) hydrogen bonding in compound 5, H-bonds are shown in blue.

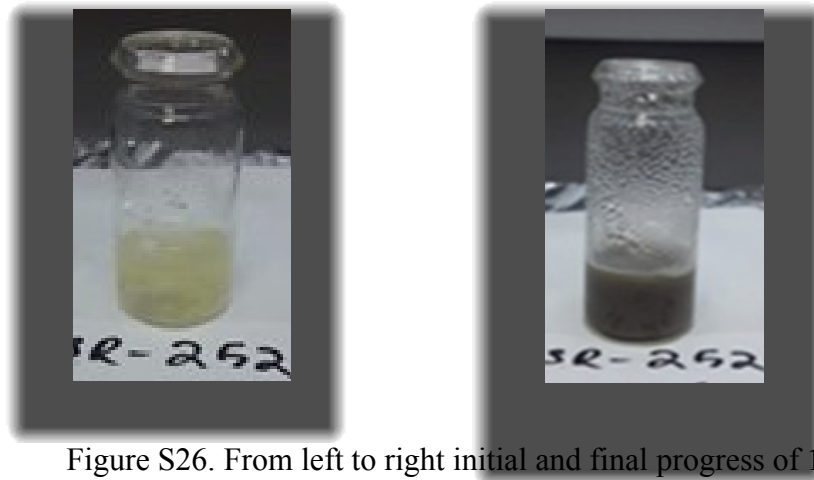


Figure S26. From left to right initial and final progress of 1.

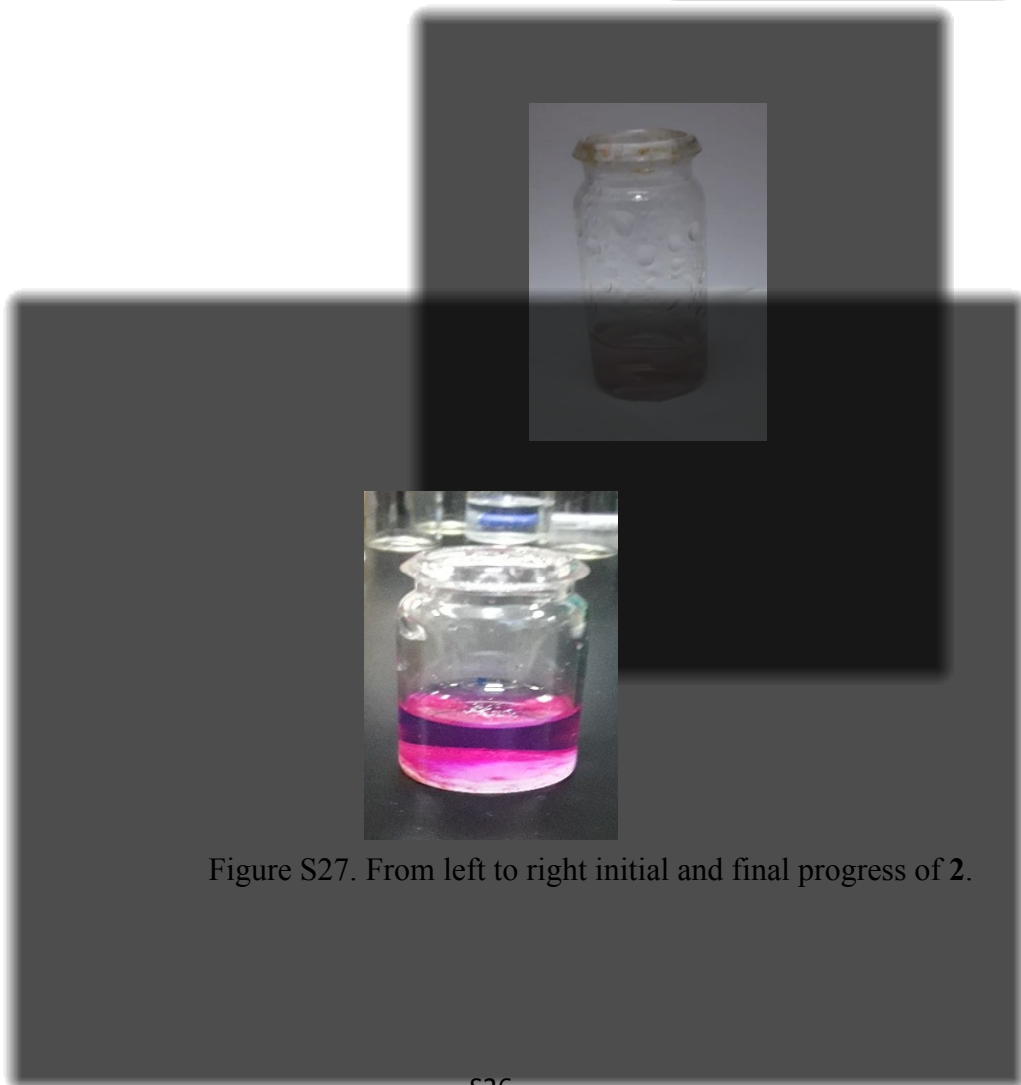


Figure S27. From left to right initial and final progress of 2.



Figure S28. From left to right initial and final progress of **3**.



Figure S29. From left to right initial and final images of **4**.

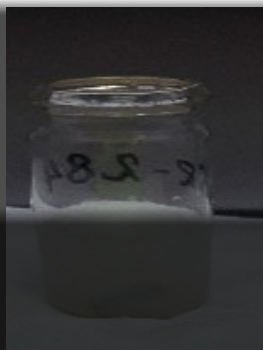


Figure S30. From left to right initial and final images of **5**.

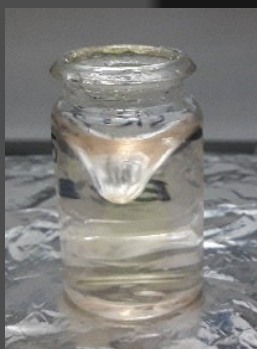
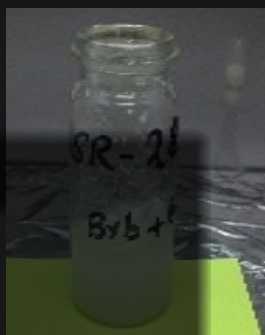


Figure S31. From left to right initial and final images of **6**.

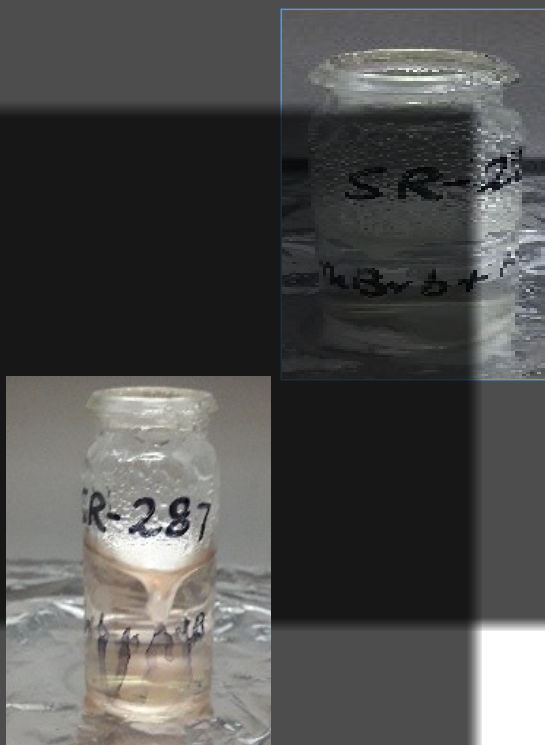


Figure S32. From left to right initial and final images of 7.



Figure S33. From left to right initial and final images of 8.



Figure S34. From left to right initial and final images of **9**.



Figure S35. From left to right initial and final images of **10**.



Figure S36. From left to right initial and final images of **11**.