

## **Supporting Information**

### **Solvent-free Synthesis, Molecular simulation and Cytotoxicity of 1,4-benzodiazepine-2,5-diones**

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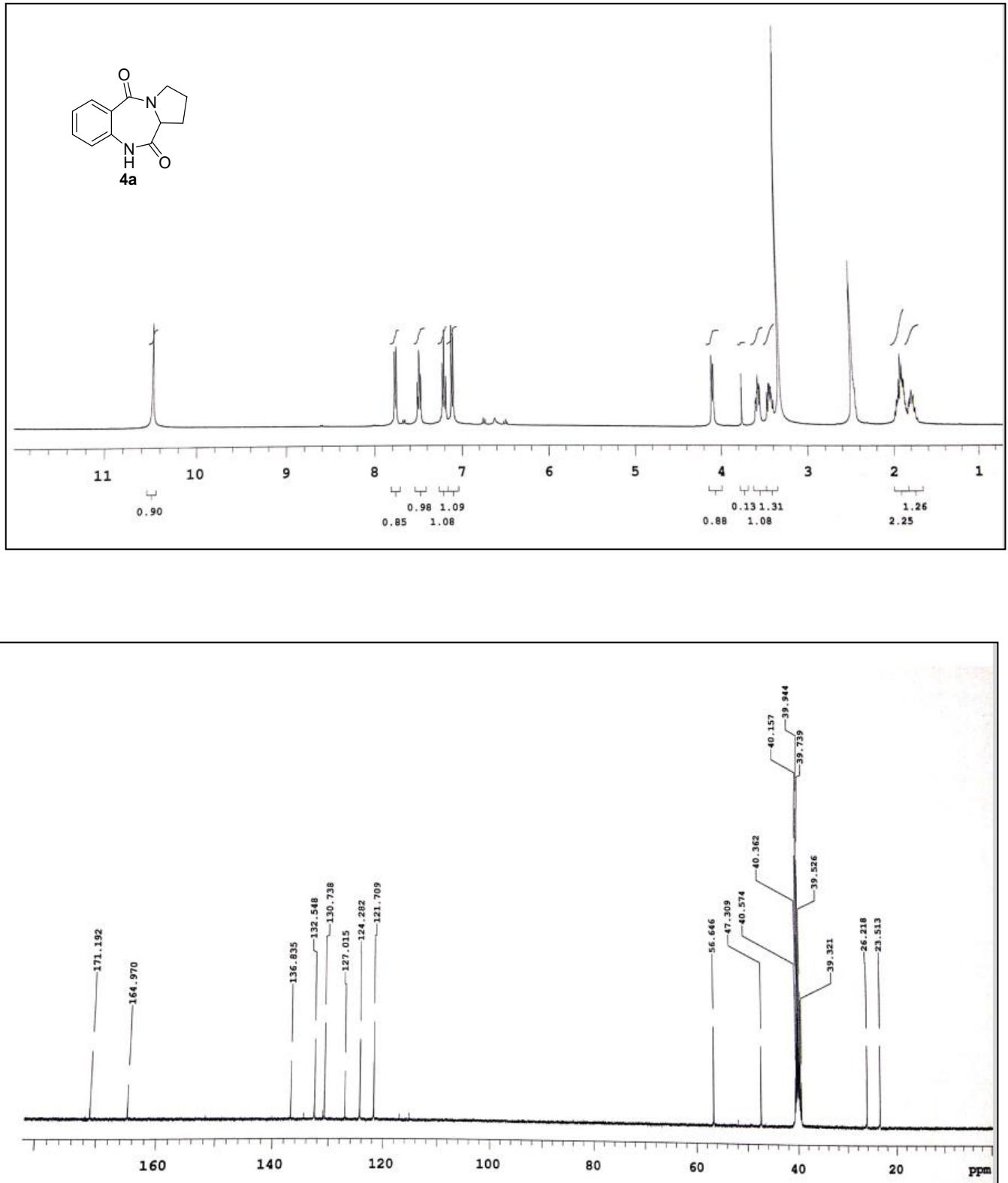
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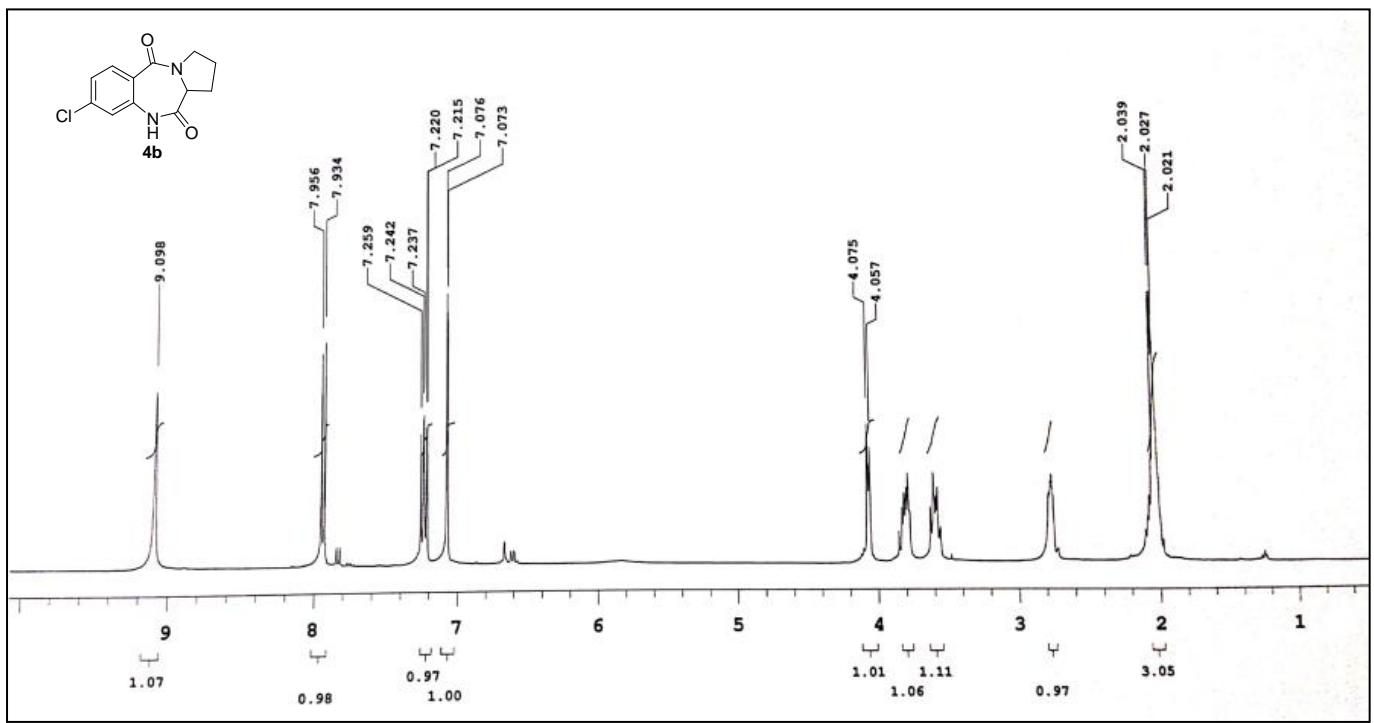
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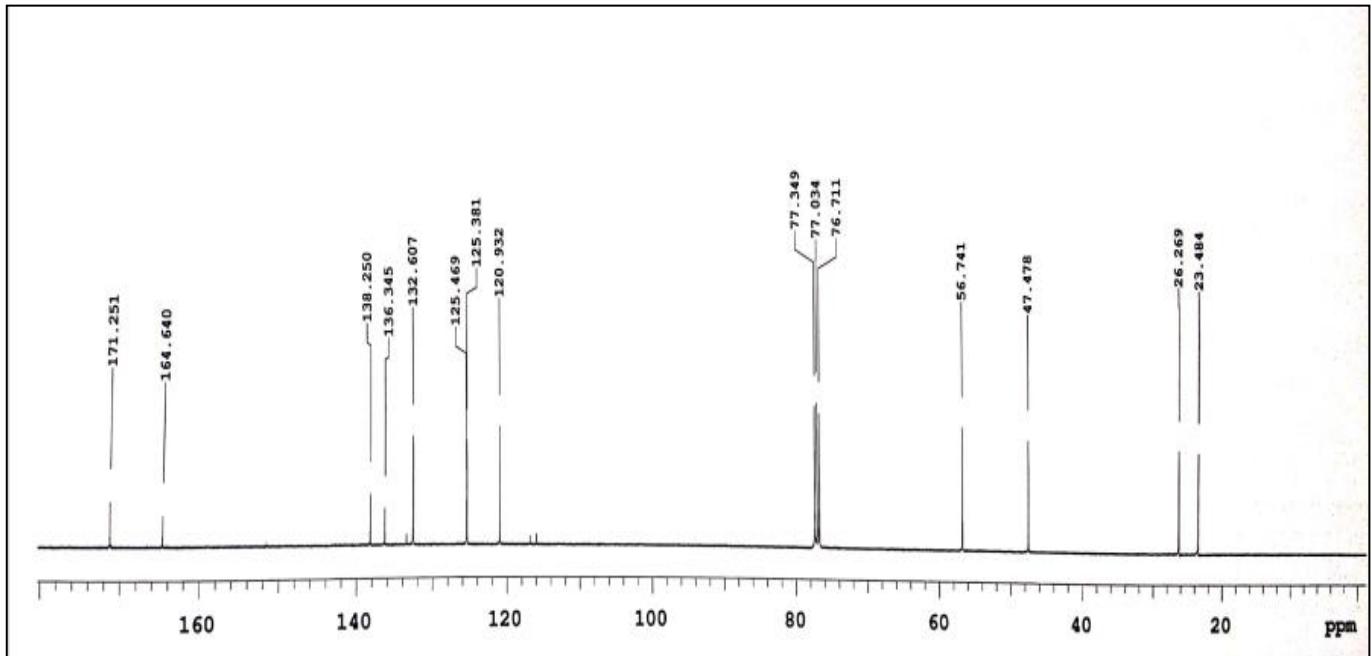
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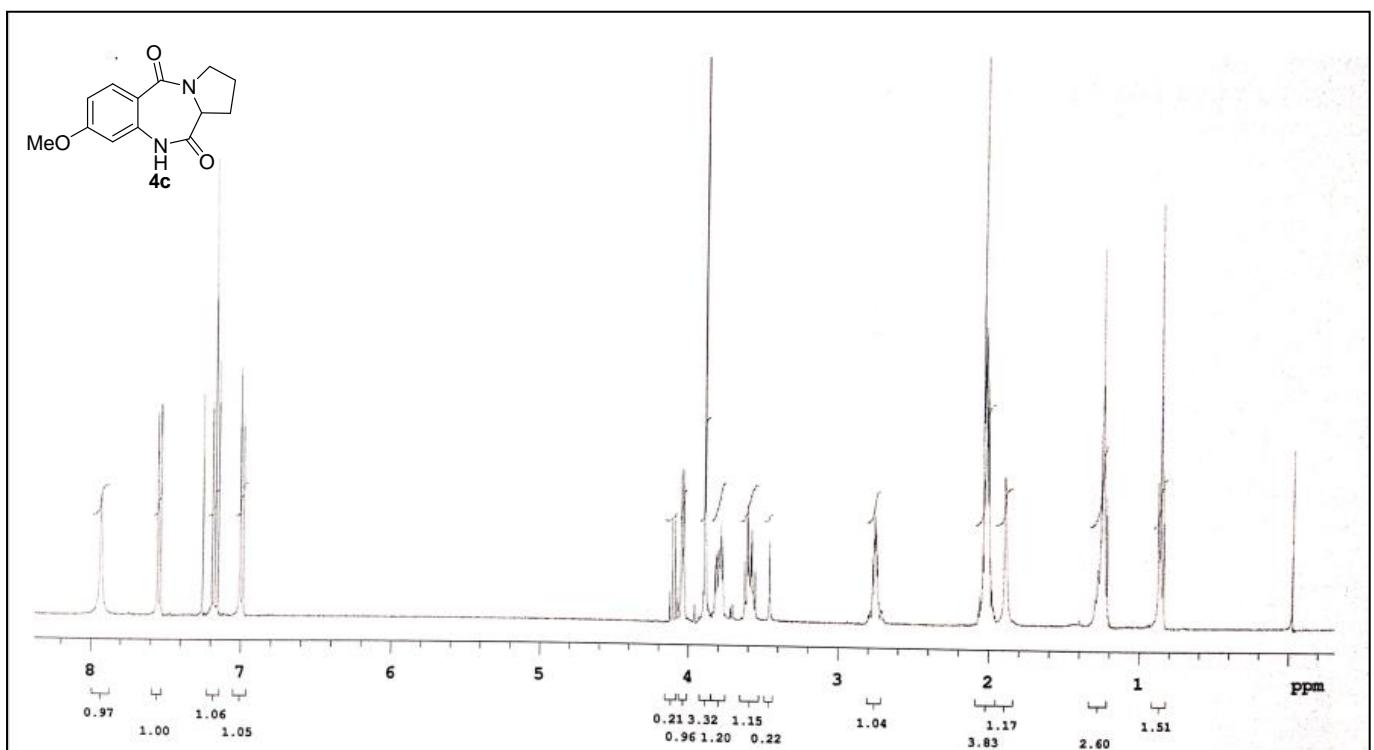
**Figure S2:**  $^{13}\text{C}$ -NMR (100 MHz, DMSO- $\text{d}_6$ ), Spectrum of Compound 4a



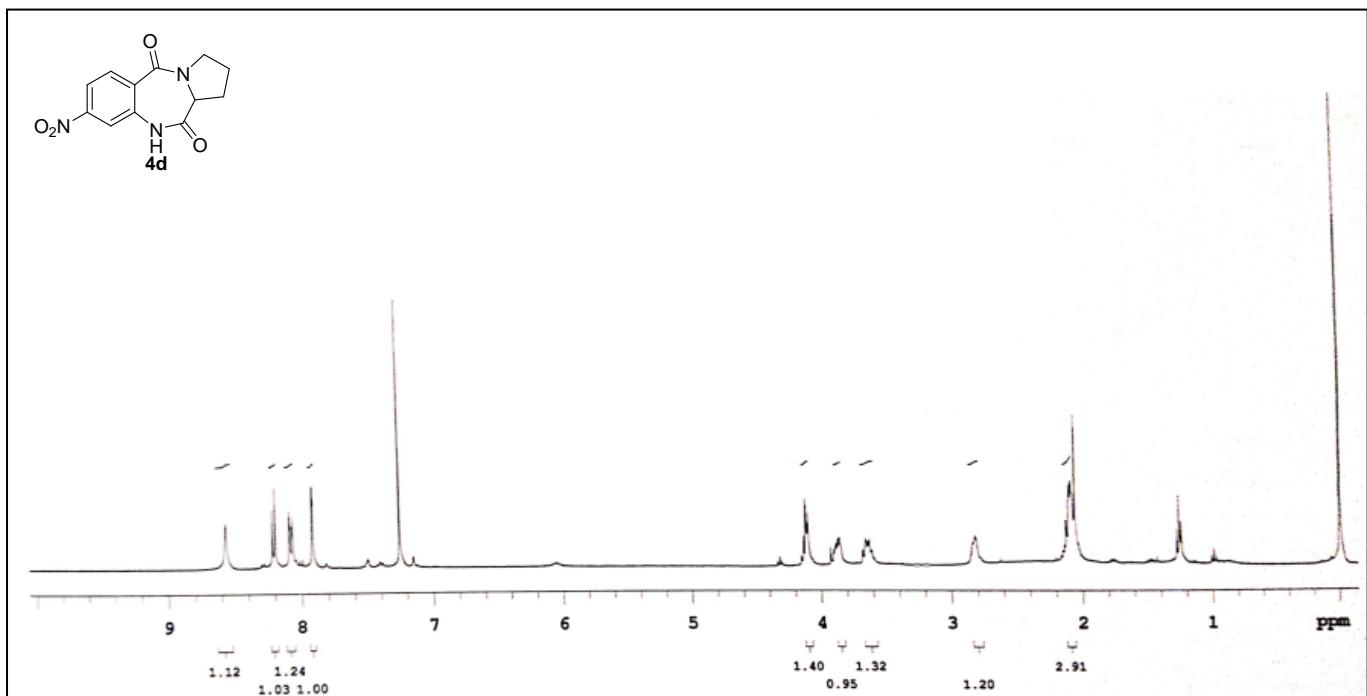
**Figure S3:**  $^1\text{H}$ -NMR (400 MHz,  $\text{CDCl}_3$ ), Spectrum of Compound 4b



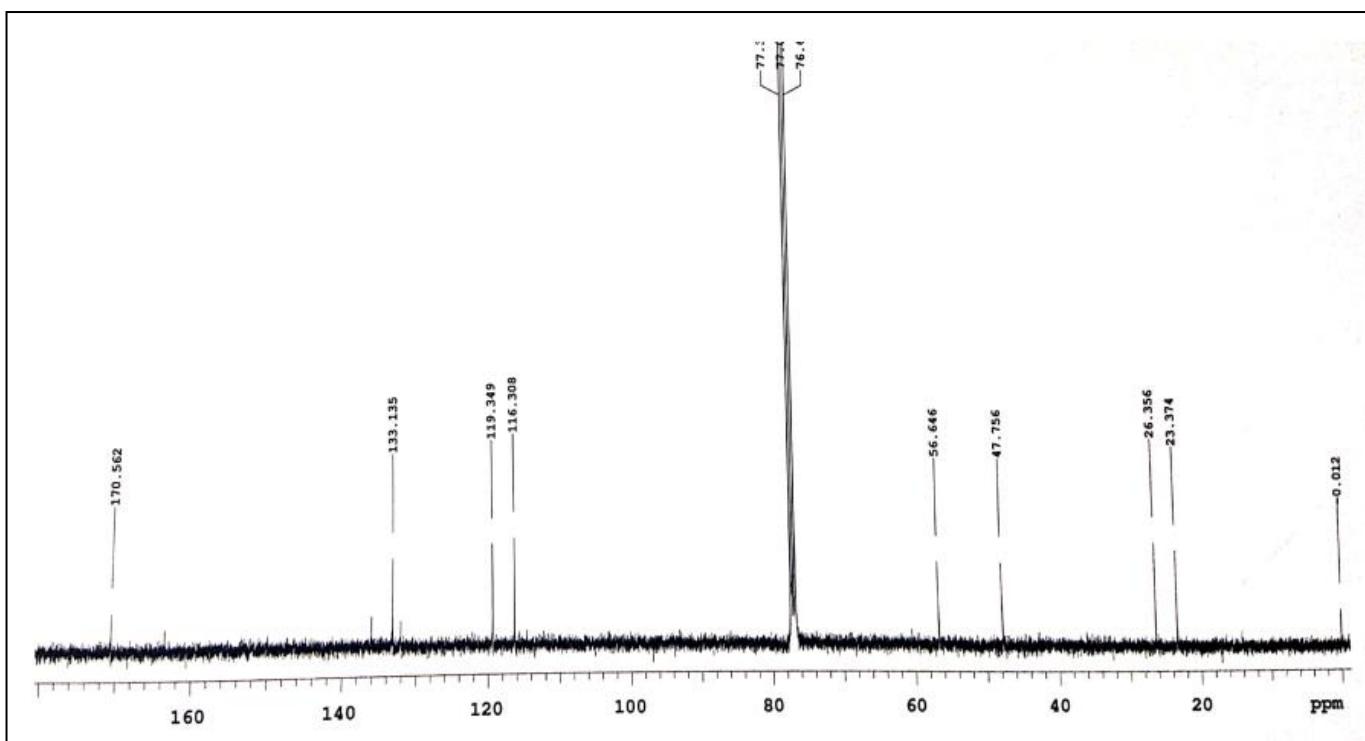
**Figure S4:**  $^{13}\text{C}$ -NMR (100 MHz,  $\text{CDCl}_3$ ), Spectrum of Compound 4b



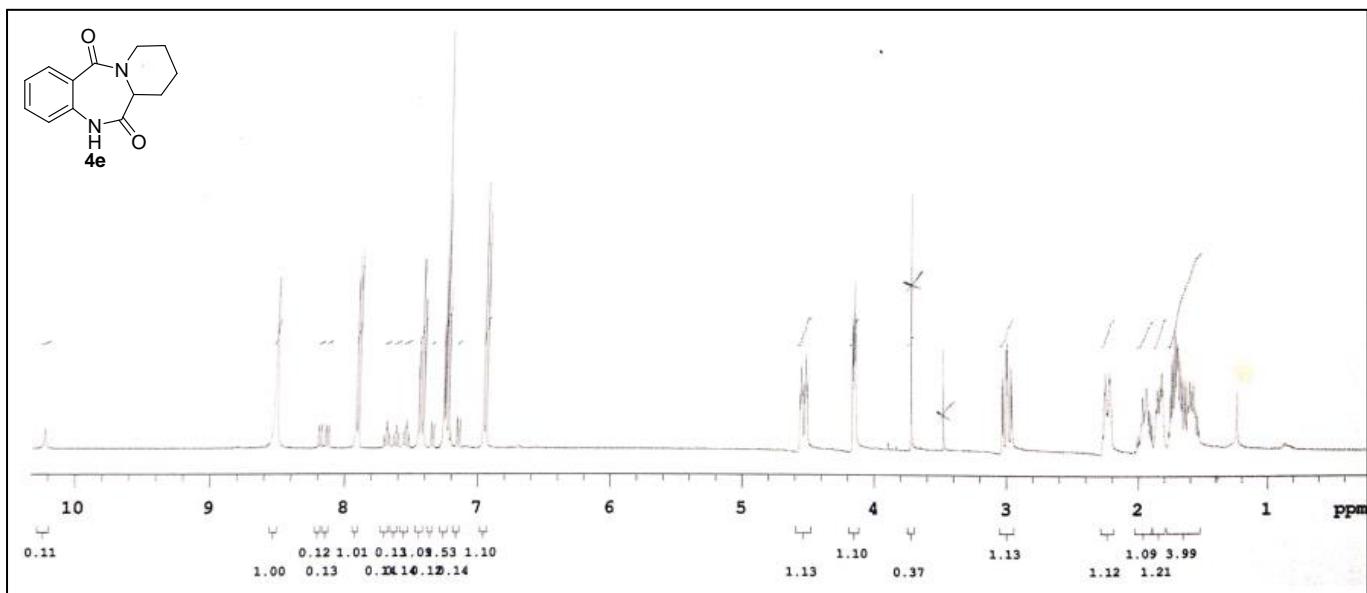
**Figure S5:** <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>), Spectrum of Compound 4c



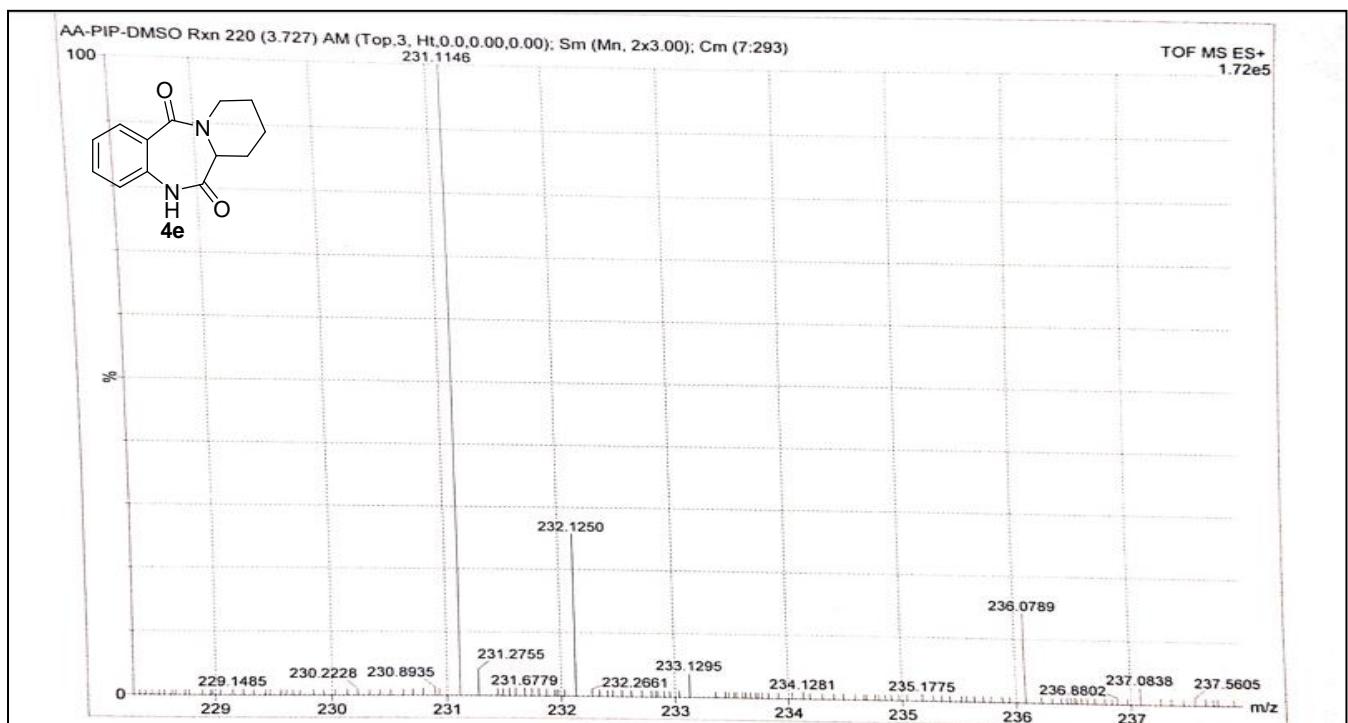
**Figure S6:** <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>), Spectrum of Compound 4d



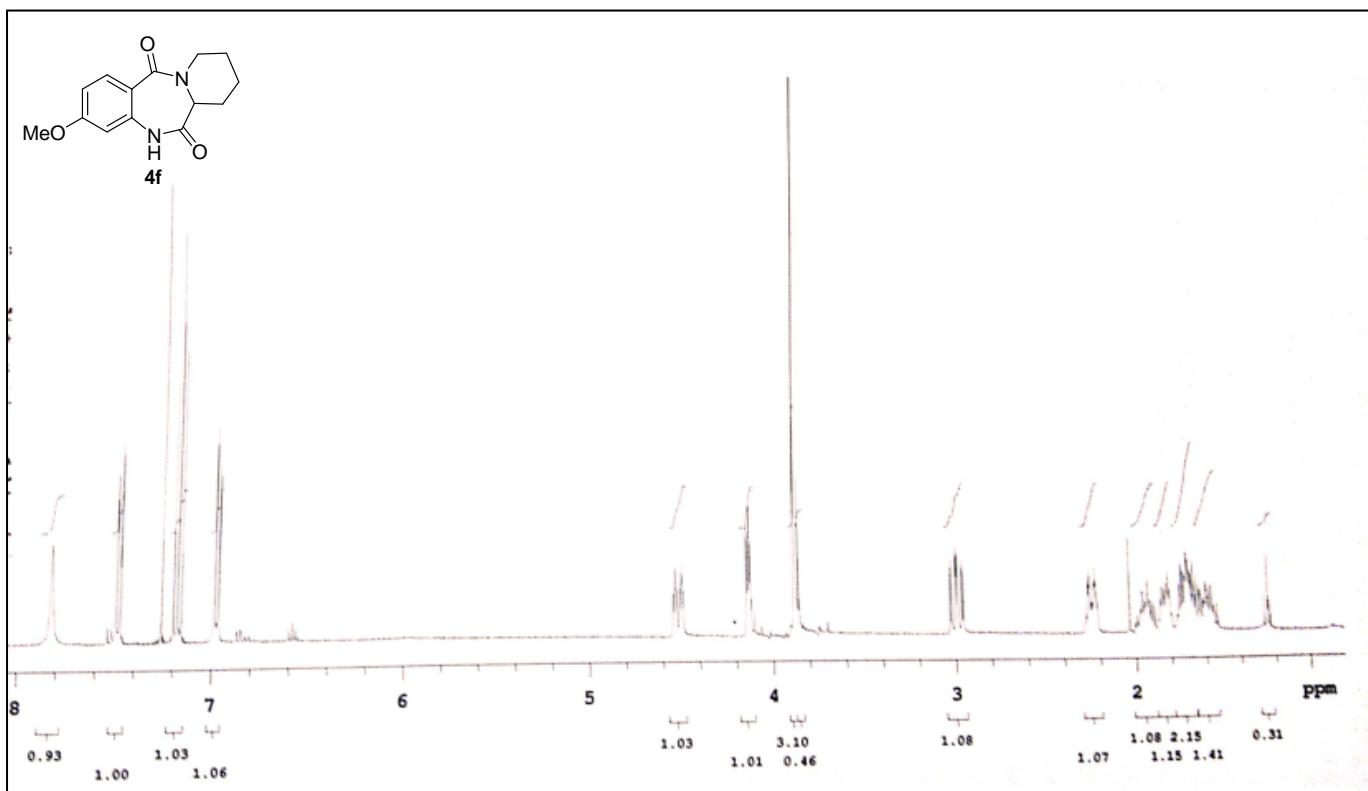
**Figure S7:** <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>), Spectrum of Compound 4d



**Figure S8:** <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>), Spectrum of Compound 4e



**Figure S8:** Mass Spectrum of Compound 4e



**Figure S9:** <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>), Spectrum of Compound 4f