

# Highly regioselective 1,3-dipolar cycloaddition of nitrilimines and thioaurones towards spiro-2-pyrazolines: Synthesis, characterization, and mechanistic study

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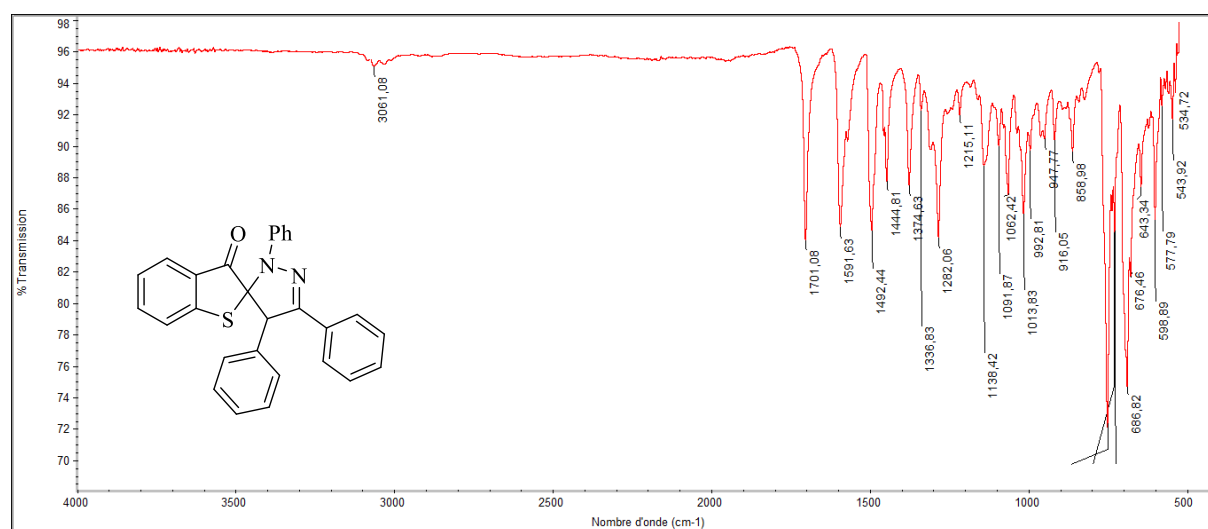
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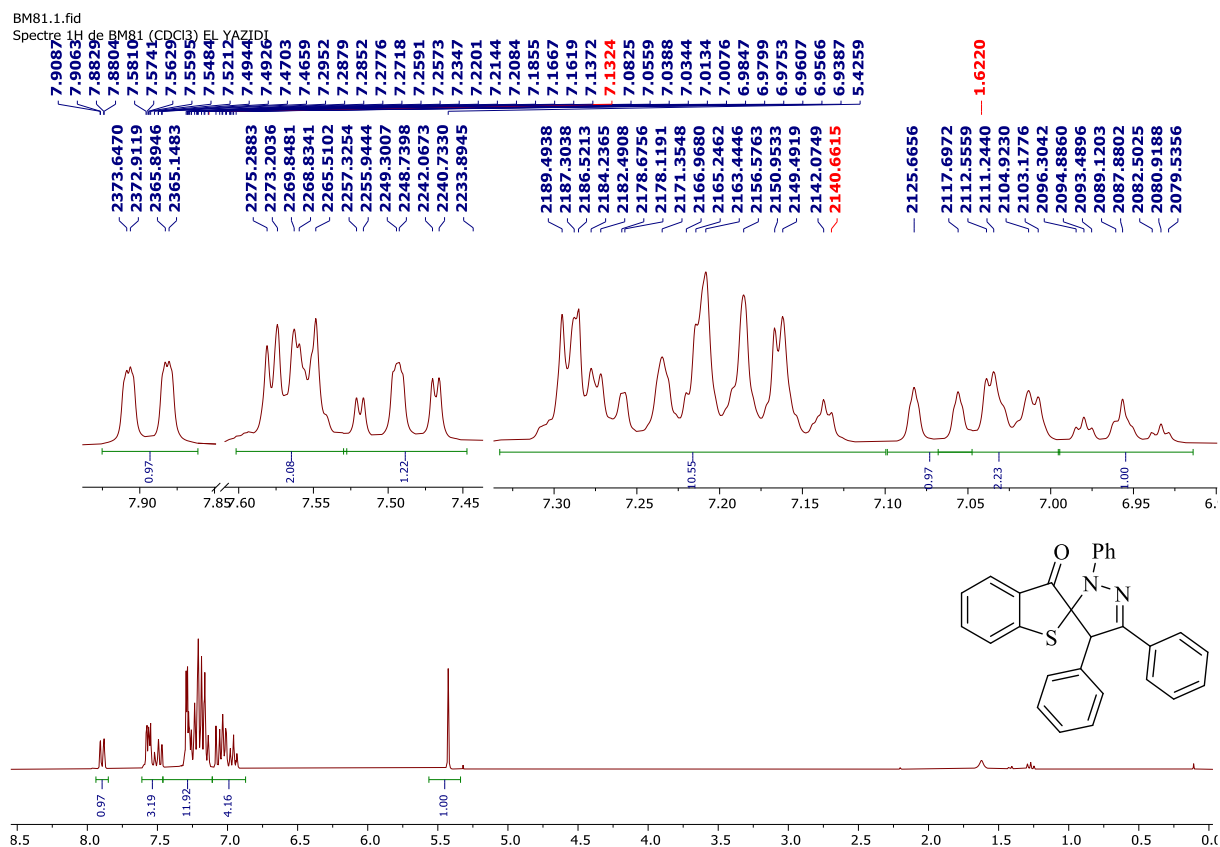
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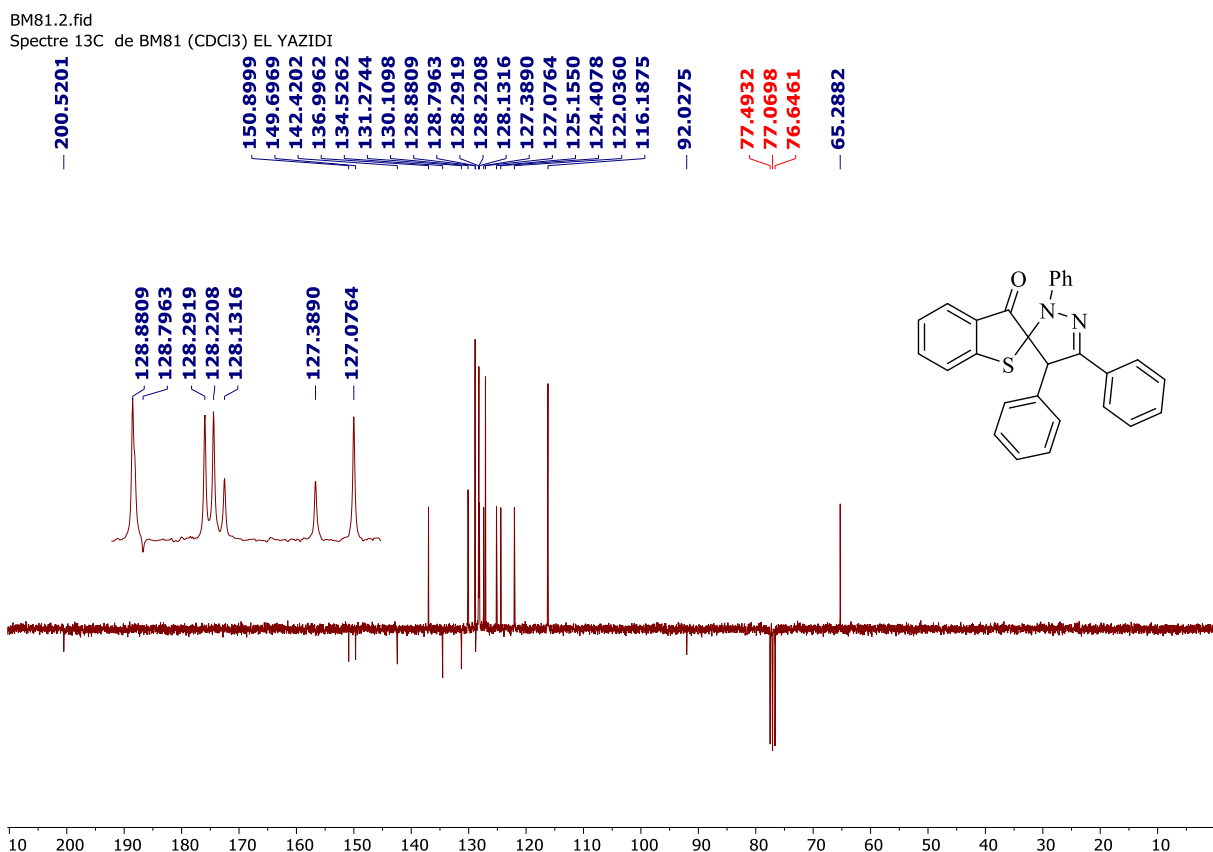
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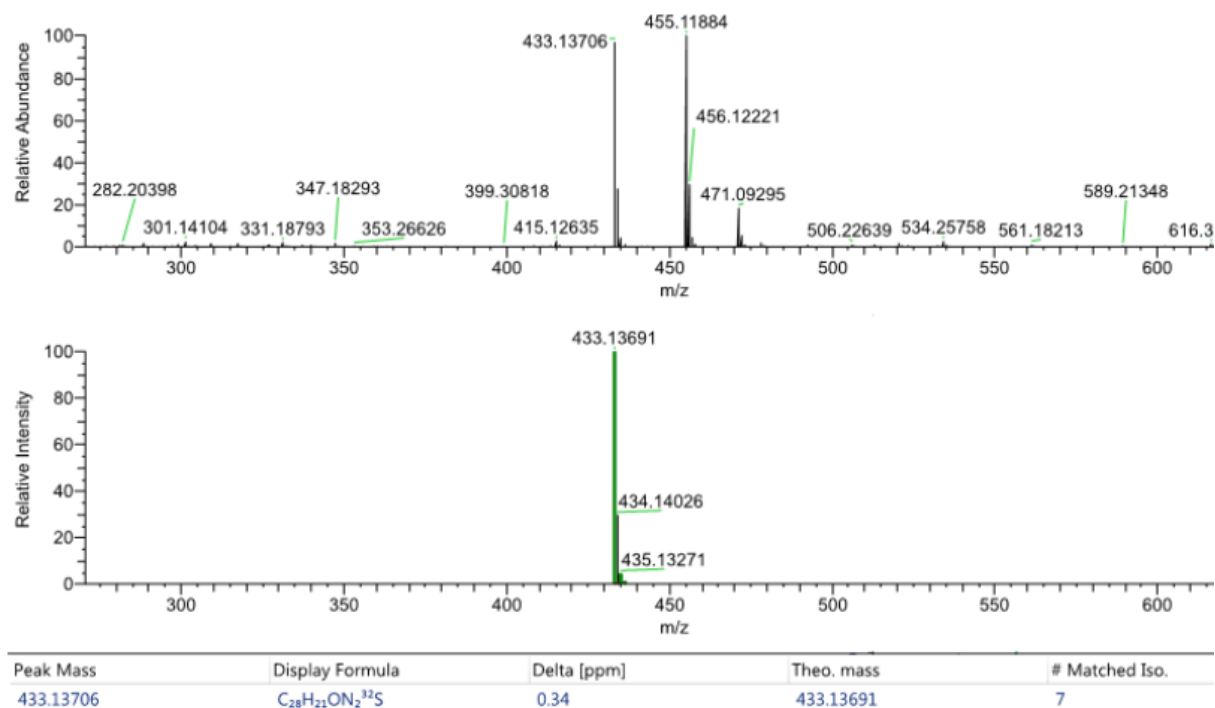
**Figure S1.** ATR-IR spectrum of spiro-pyrazoline **3aa**.



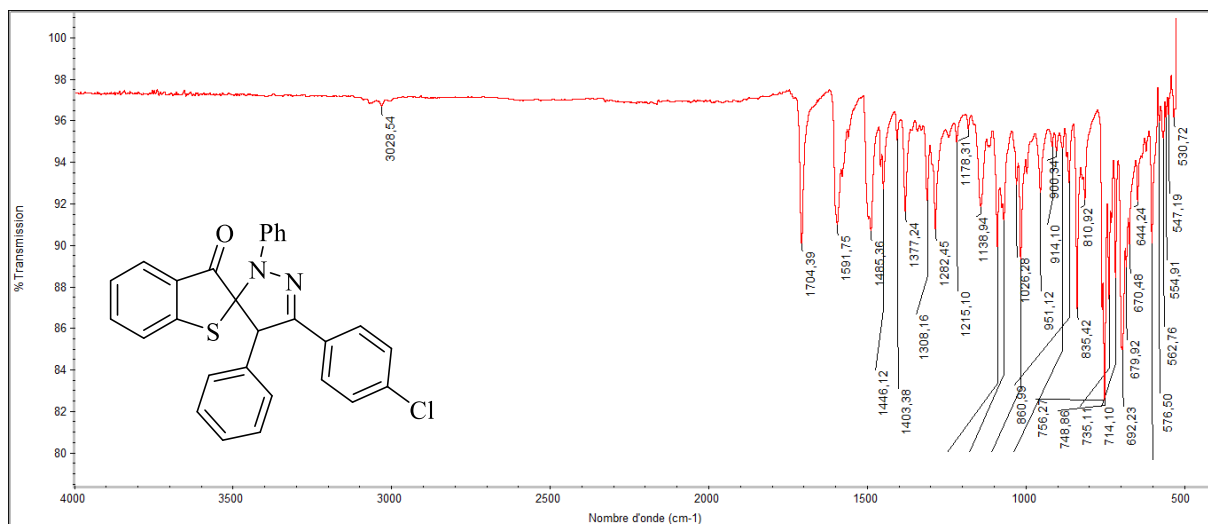
**Figure S2.** <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of spiropyrazoline **3aa**.



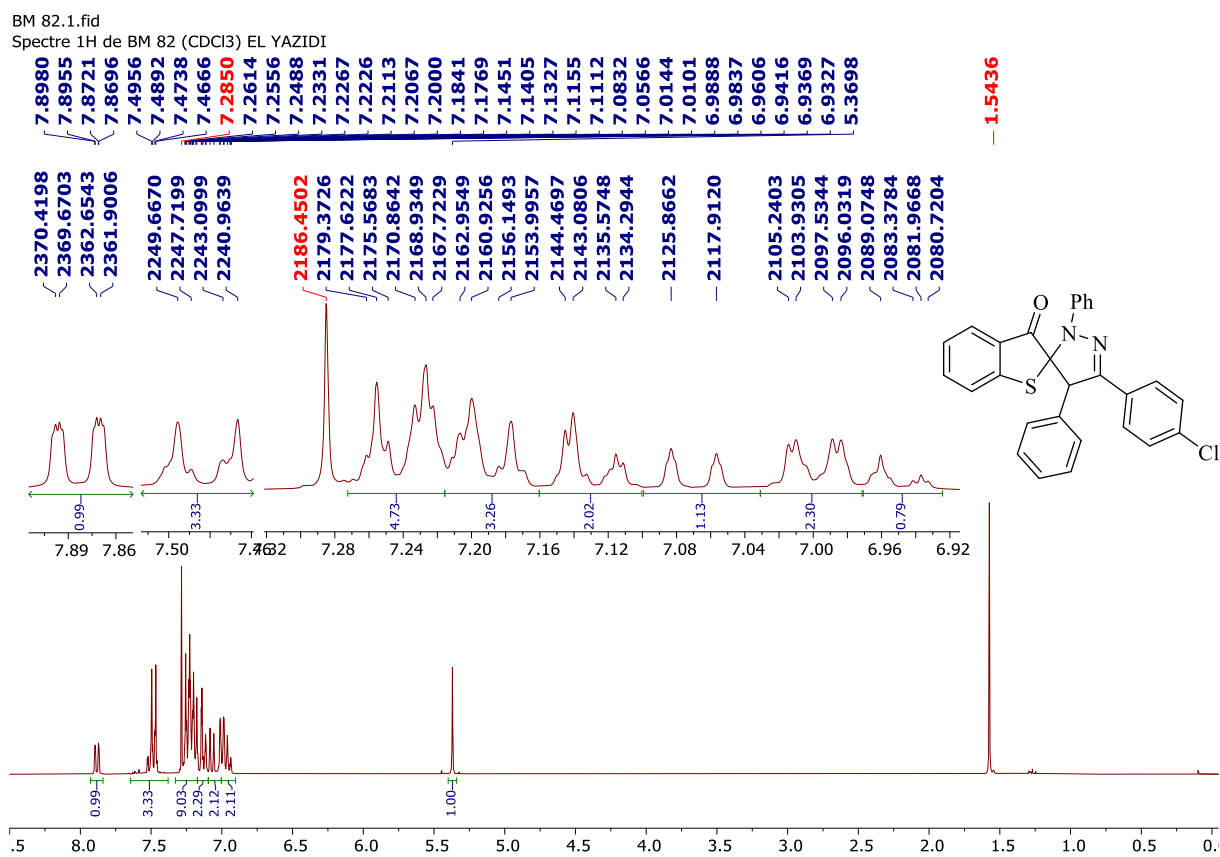
**Figure S3.** <sup>13</sup>C-APT NMR (75 MHz, CDCl<sub>3</sub>) spectrum of spiropyrazoline **3aa**.



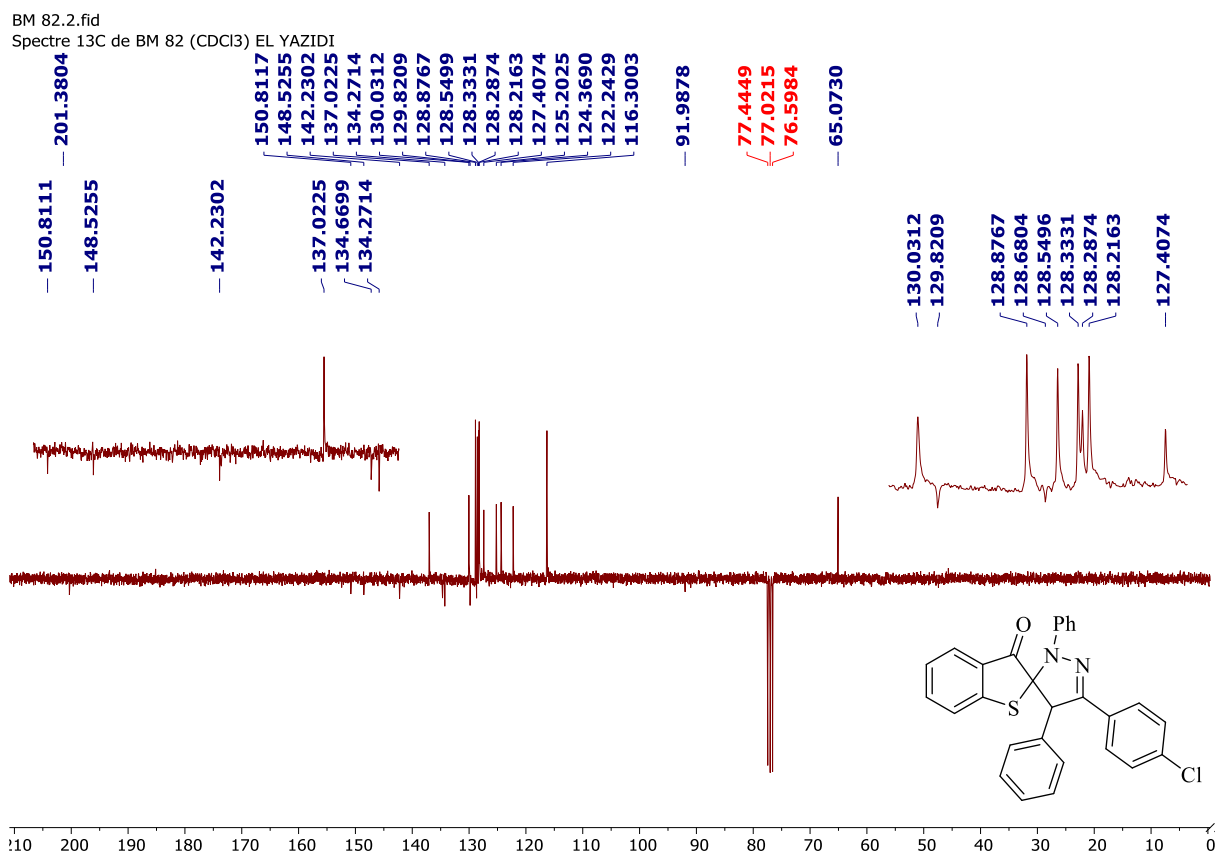
**Figure S4.** ESI+ spectrum of spiropyrazoline **3aa**.



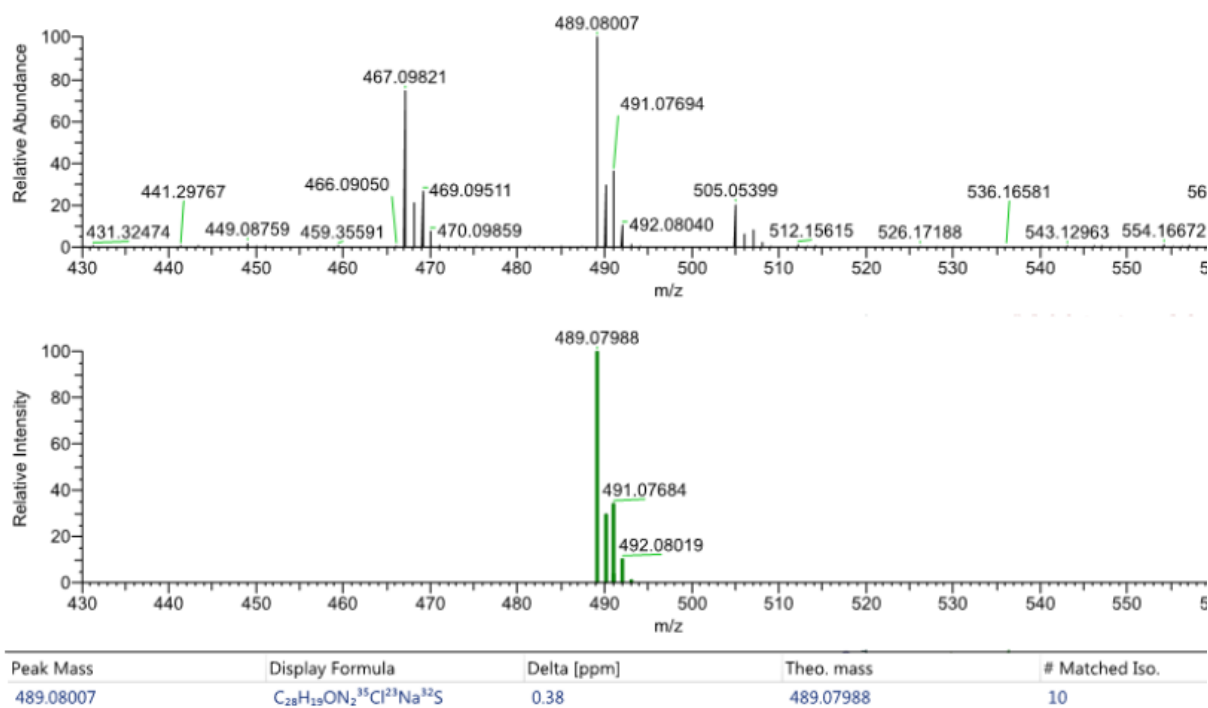
**Figure S5.** ATR-IR spectrum of spiropyrazoline **3ab**.



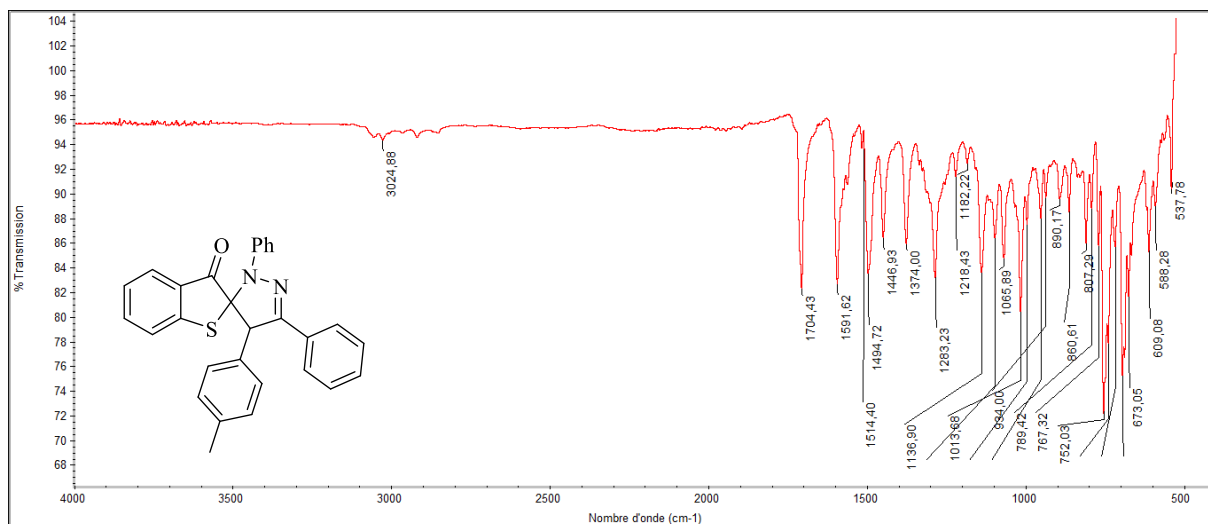
**Figure S2.** <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of spiropyrazoline **3ab**.



**Figure S7.** <sup>13</sup>C-APT NMR (75 MHz, CDCl<sub>3</sub>) spectrum of spiropyrazoline **3ab**.



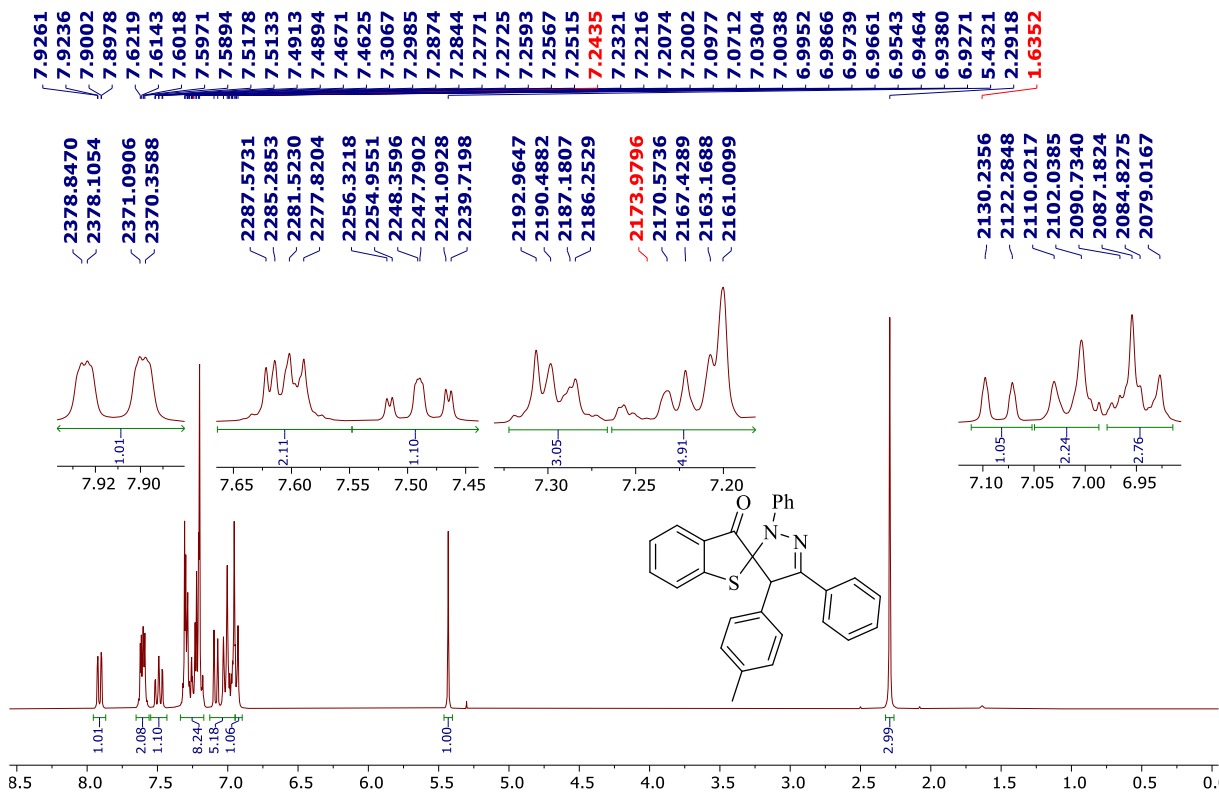
**Figure S8.** ESI+ spectrum of spiropyrazoline **3ab**.



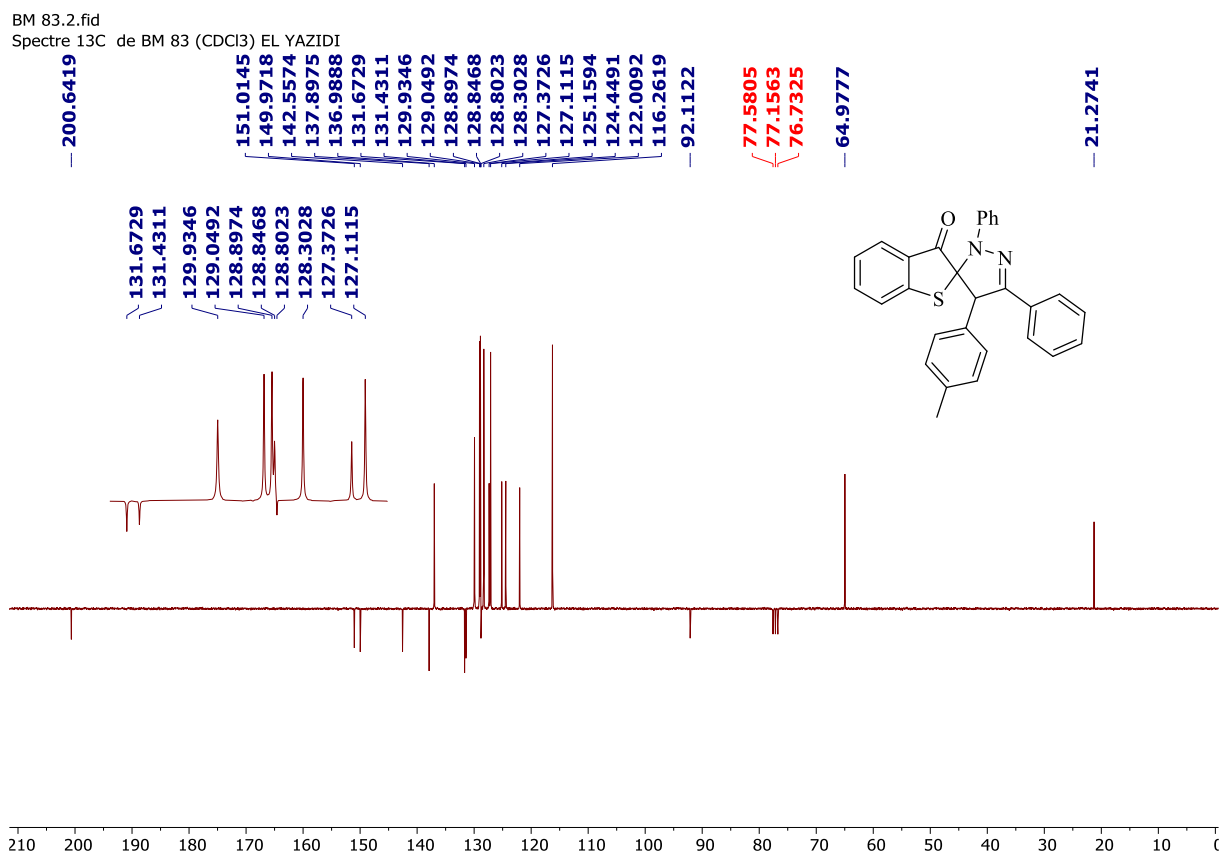
**Figure S9.** ATR-IR spectrum of spiropyrazoline **3ba**.

BM 83.1.fid

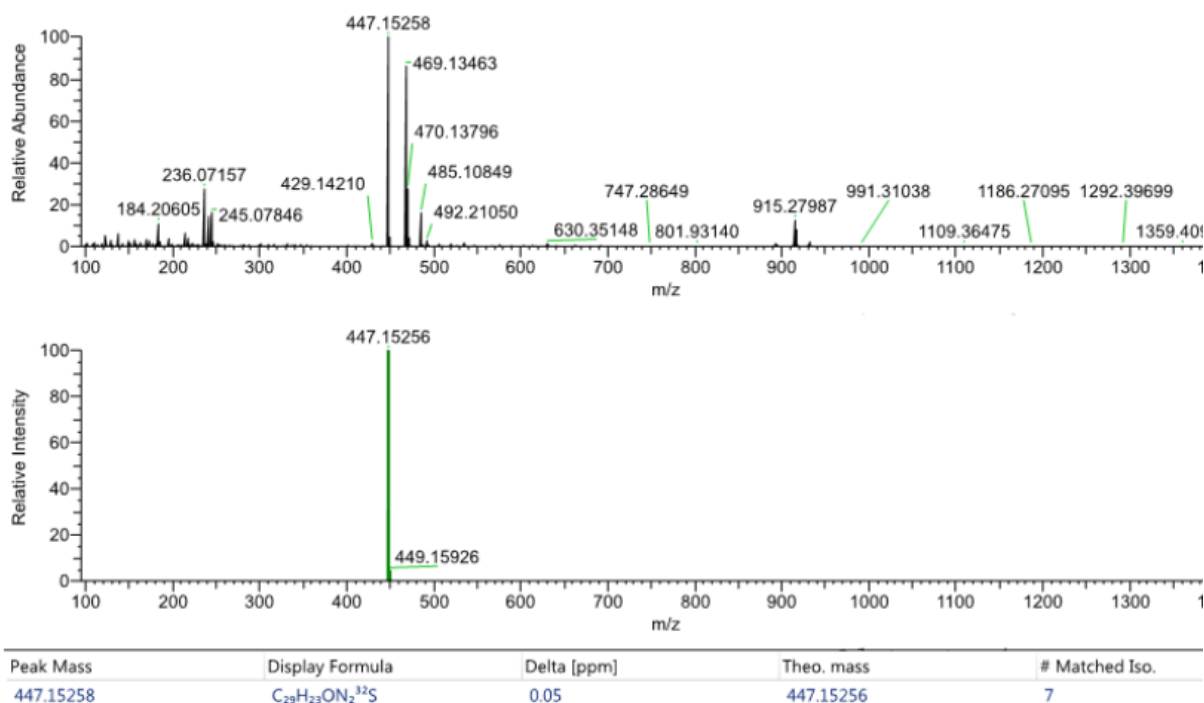
Spectre 1H de BM 83 (CDCl<sub>3</sub>) EL YAZIDI



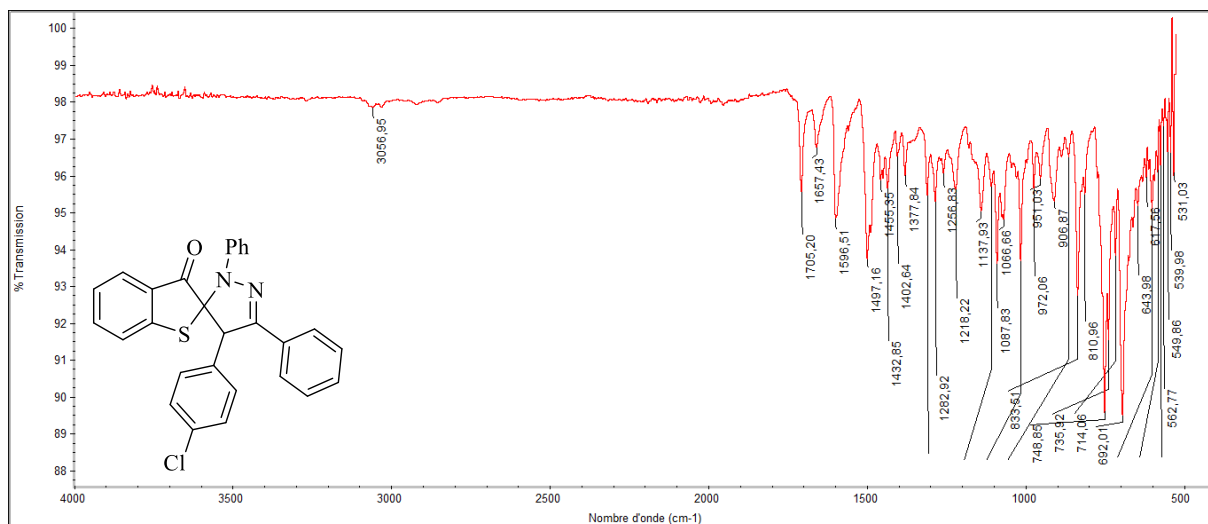
**Figure S10.** <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of spiropyrazoline **3ba**.



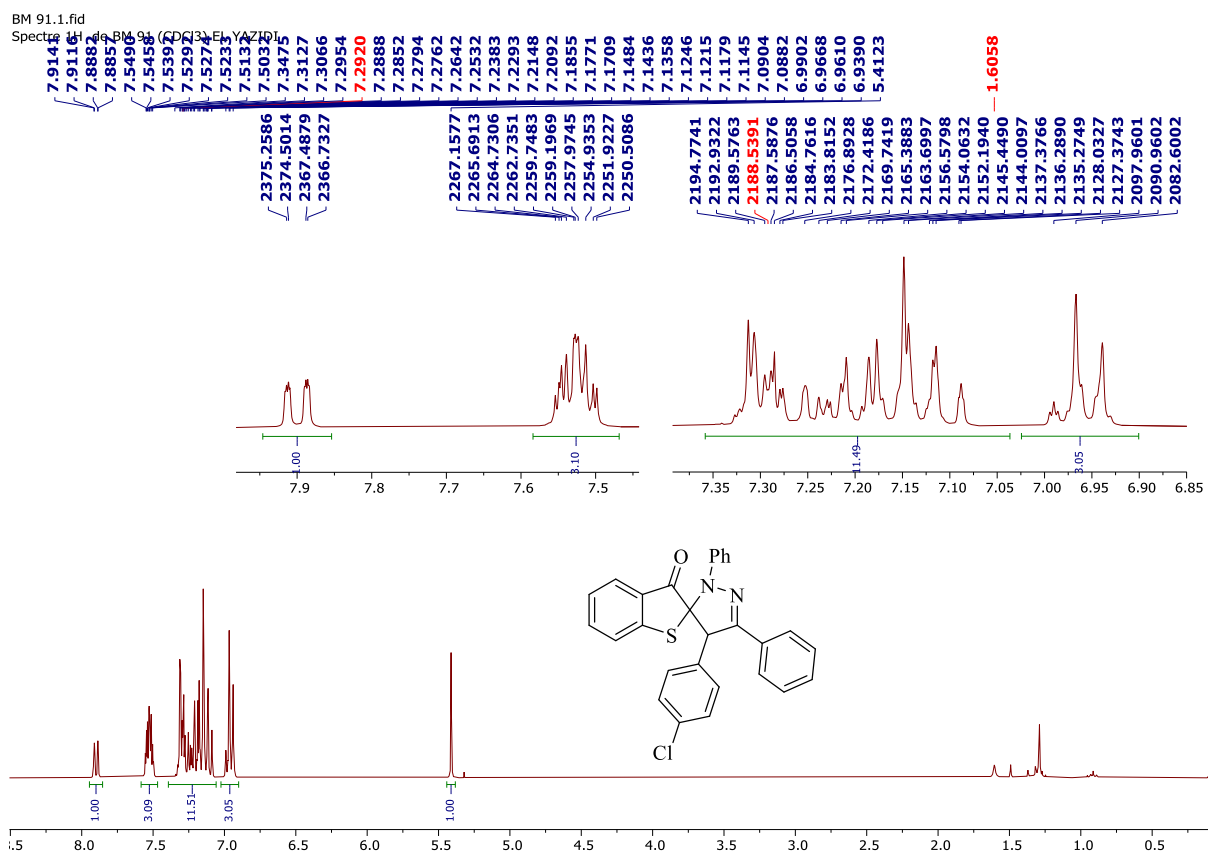
**Figure S3.** <sup>13</sup>C-APT NMR (75 MHz, CDCl<sub>3</sub>) spectrum of spiropyrazoline **3ba**.



**Figure S12.** ESI+ spectrum of spiropyrazoline **3ba**.

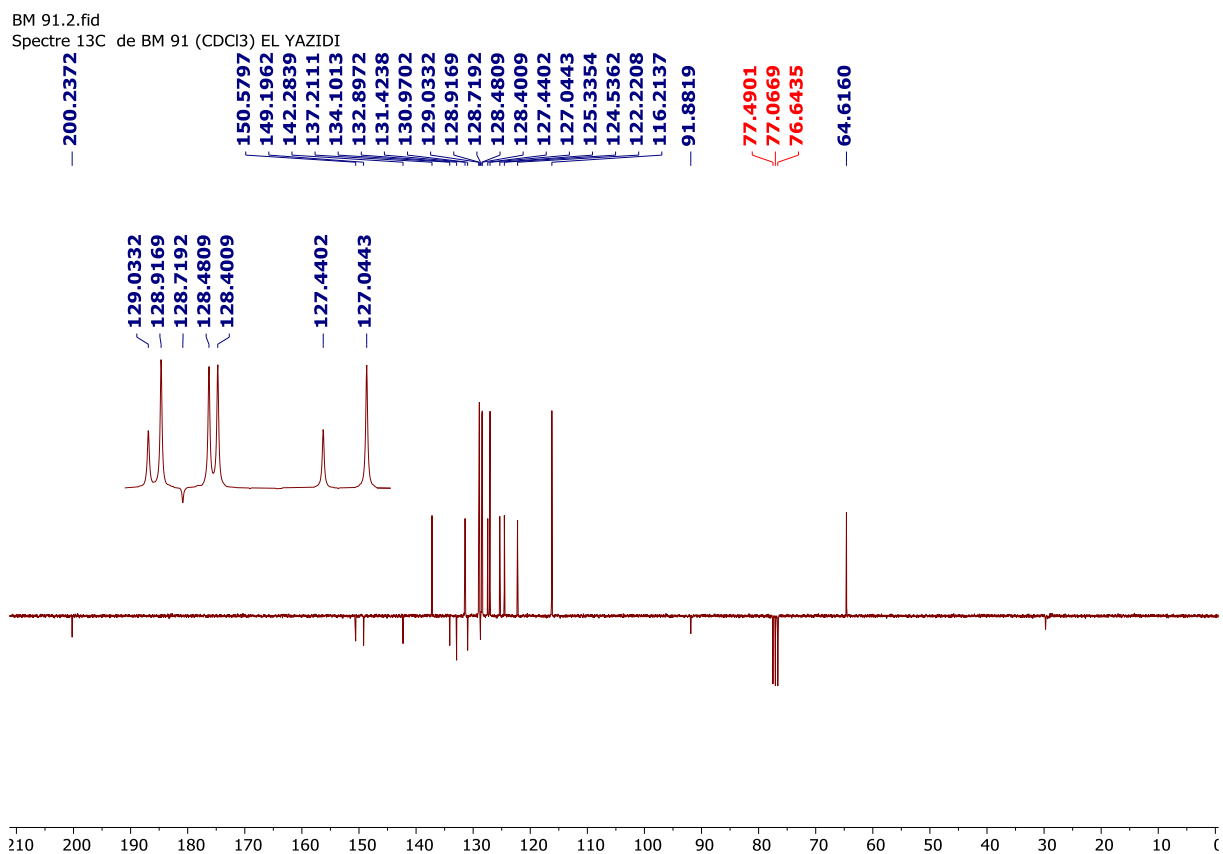


**Figure S13.** ATR-IR spectrum of spiropyrazoline **3ca**.



**Figure S14.** <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of spiropyrazoline **3ac**.

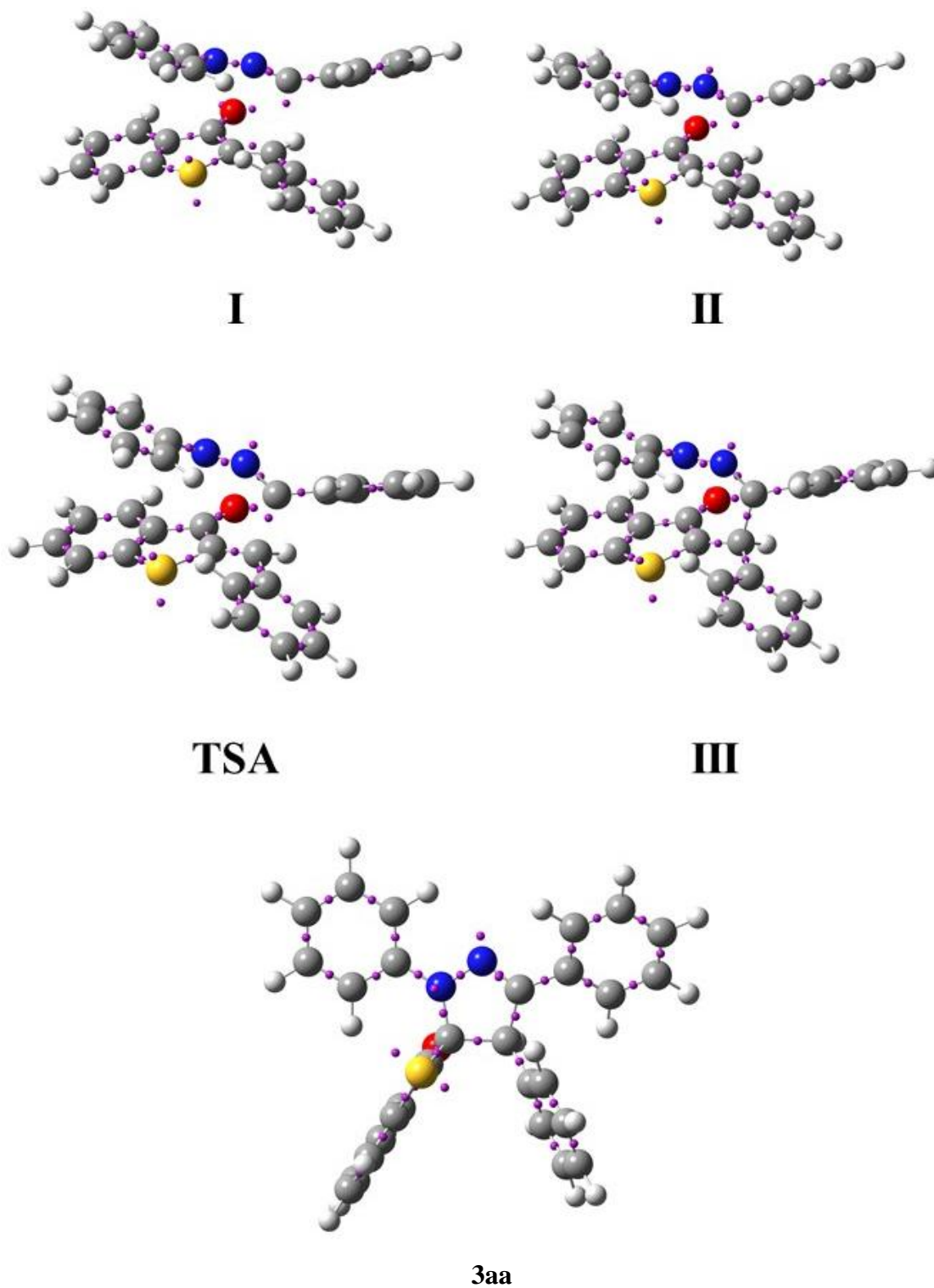




**Figure S15.**  $^{13}\text{C}$ -APT NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of spiropyrazoline **3ca**.

## Theoretical calculations

### ELF basin attractor positions



**Figure S46.** ELF basin attractor positions of all intermediates in the 1,3-DC reaction between **1a** and **2a**.