

## Electronic Supplementary Information

### Convenient One-Pot Multicomponent Strategy for the Synthesis of 6-Pyrrolylpyrimidines†

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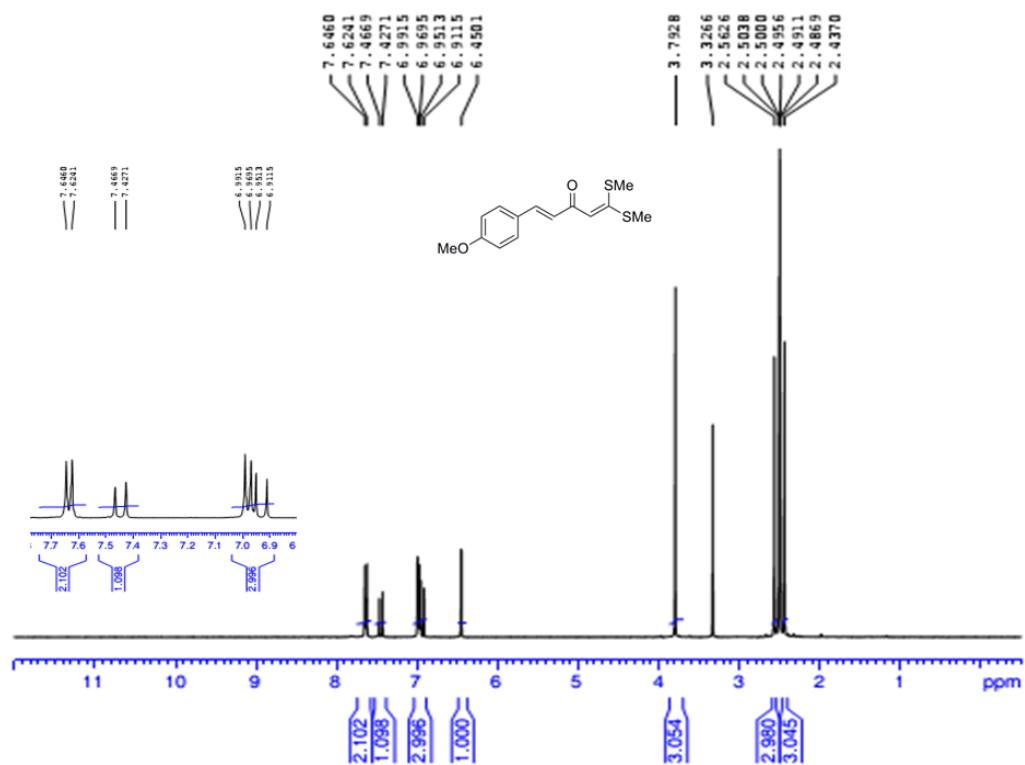
[shivazzen@mkuniversity.org](mailto:shivazzen@mkuniversity.org)

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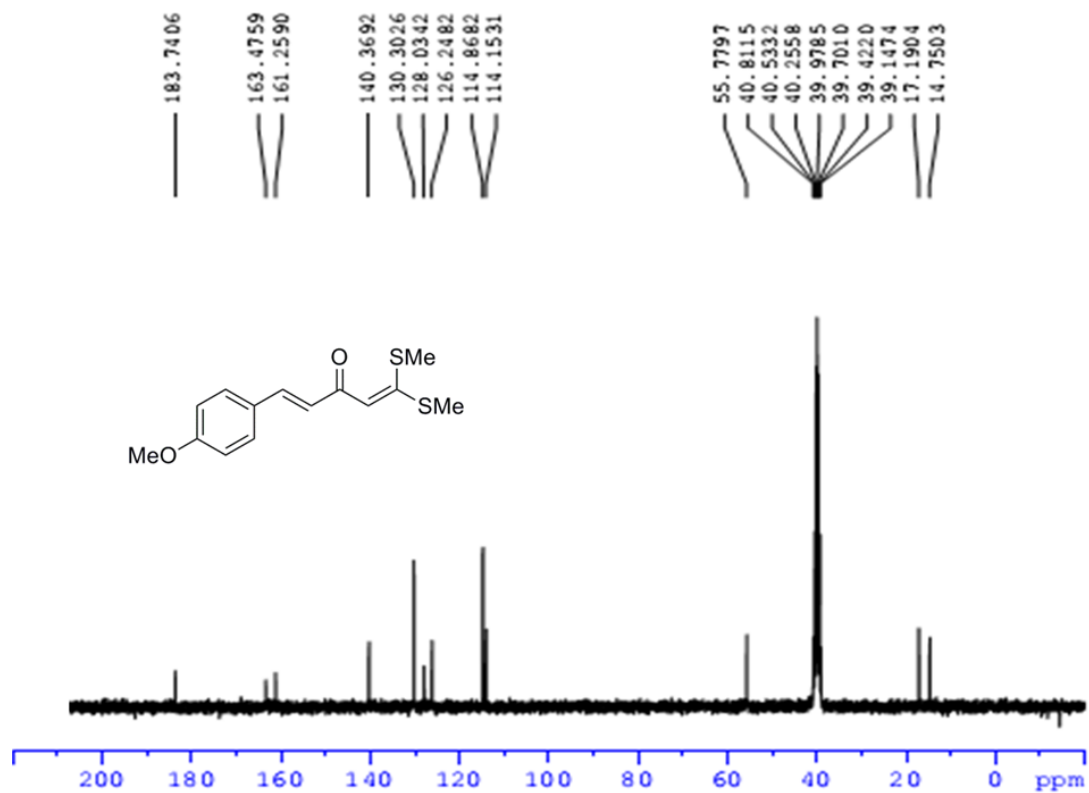
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**I General Experimental information:**

Melting points were determined on melting point apparatus equipped with a thermometer and were uncorrected. Unless stated otherwise, solvents and chemicals were obtained from commercial sources and used without further purification. The  $^1\text{H}$  and  $^{13}\text{C}$ NMR spectra of the new compounds were measured at 400MHz, 300MHz and 100MHz, 75MHz respectively using Bruker NMR instrument in DMSO- $d_6$  or  $\text{CDCl}_3$  and the chemical shifts are reported as  $\delta$  values (ppm) relative to tetramethylsilane. IR values were measured by Thermo Nicolet 6700 FT IR Spectrometer using ATR (attenuated total reflection) KBr Cell. Mass analysis was done in Agilent LC-MS instruments and spectra were recorded in positive and negative mode. Elemental analysis recorded on Thermofinnigan flash 2000 organic elemental CHNS analyser. Petroleum ether employed in column chromatographic purification refers to the fraction which boils at 40-60 °C.



**Figure S1a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2a



**Figure S1b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2a

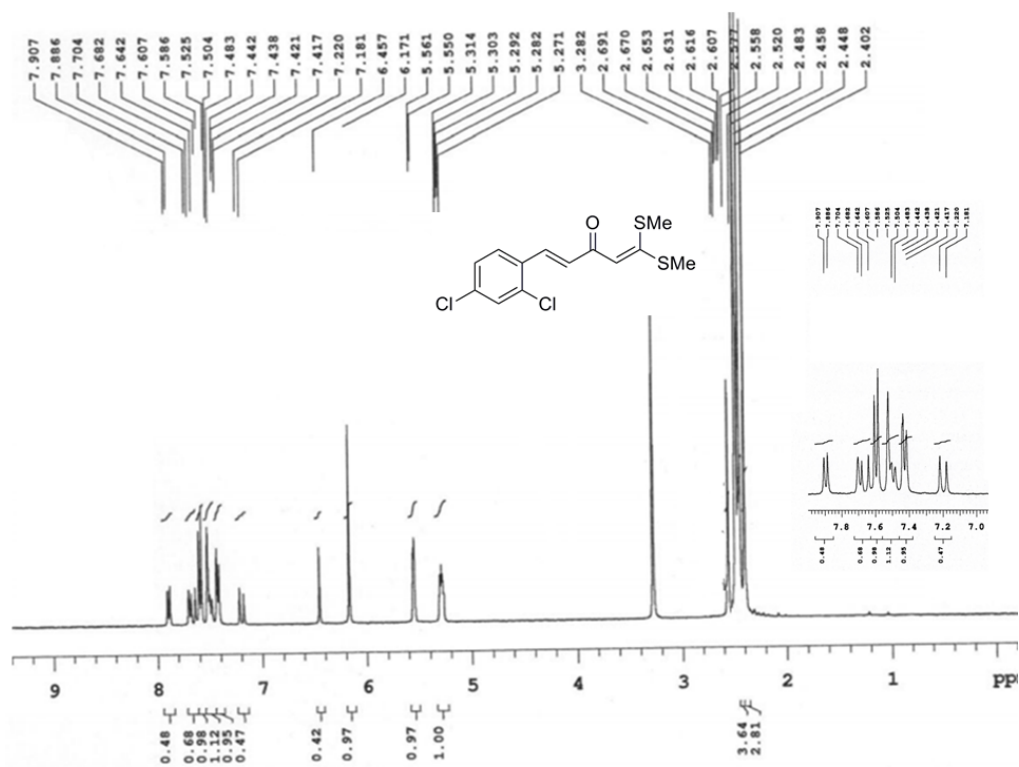


Figure S2a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2b

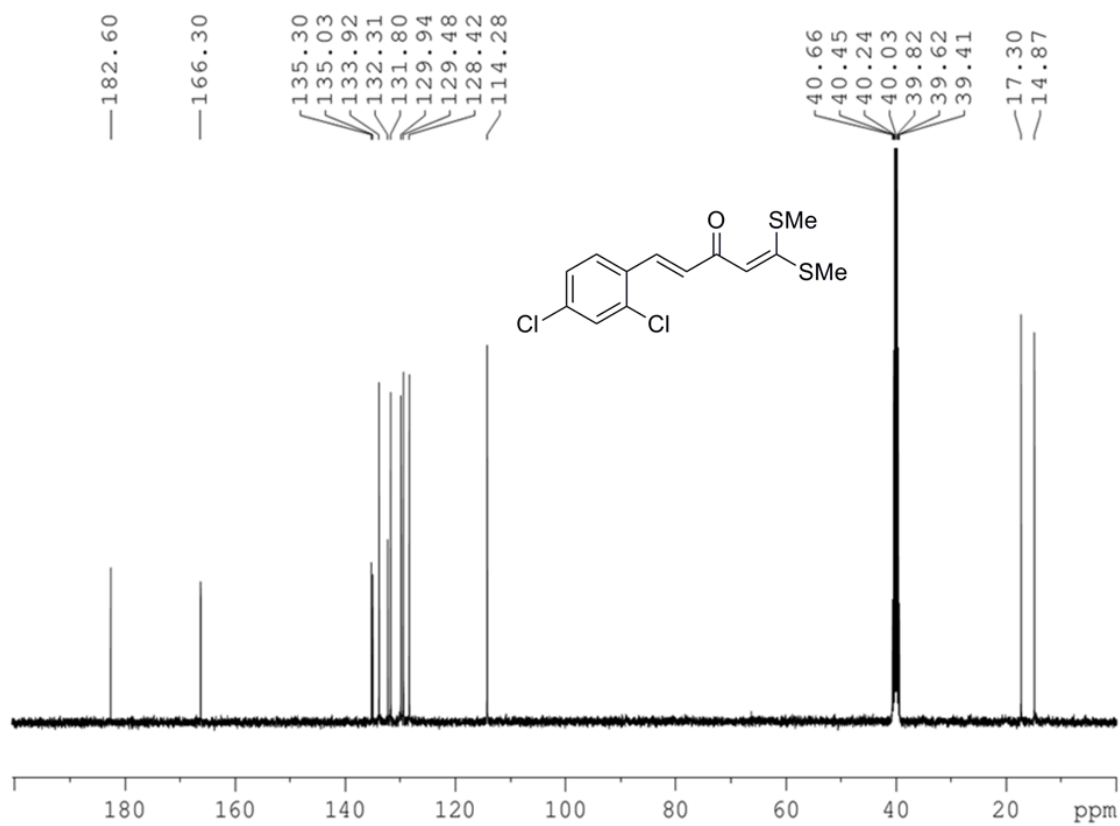
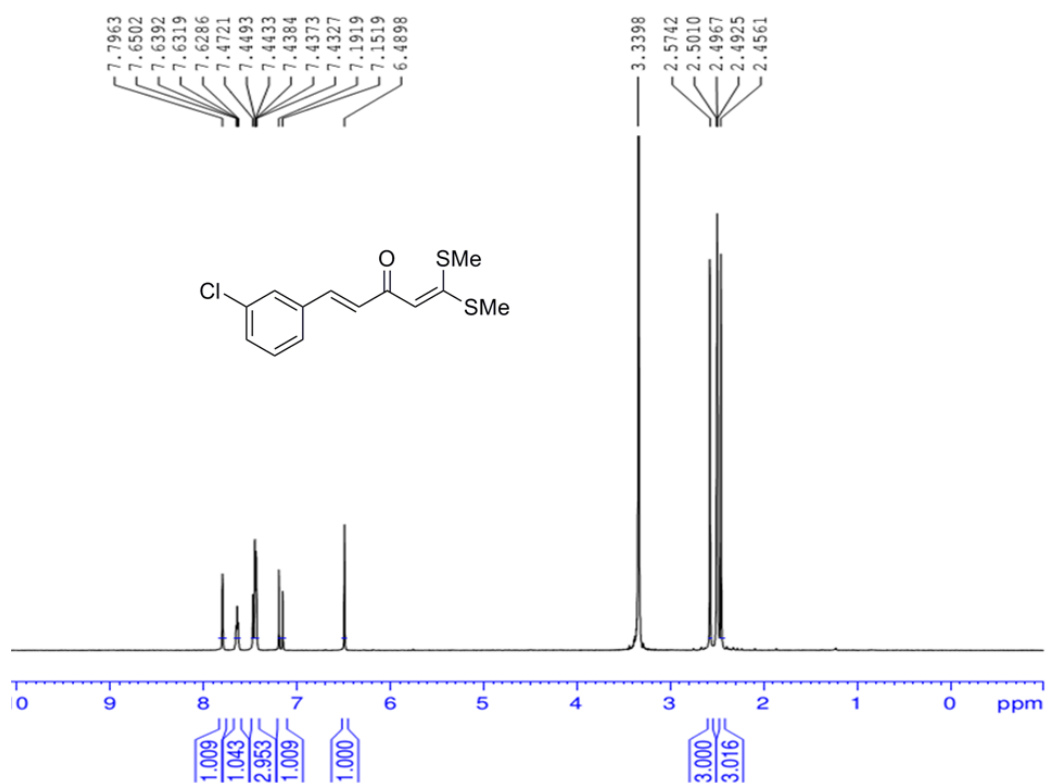
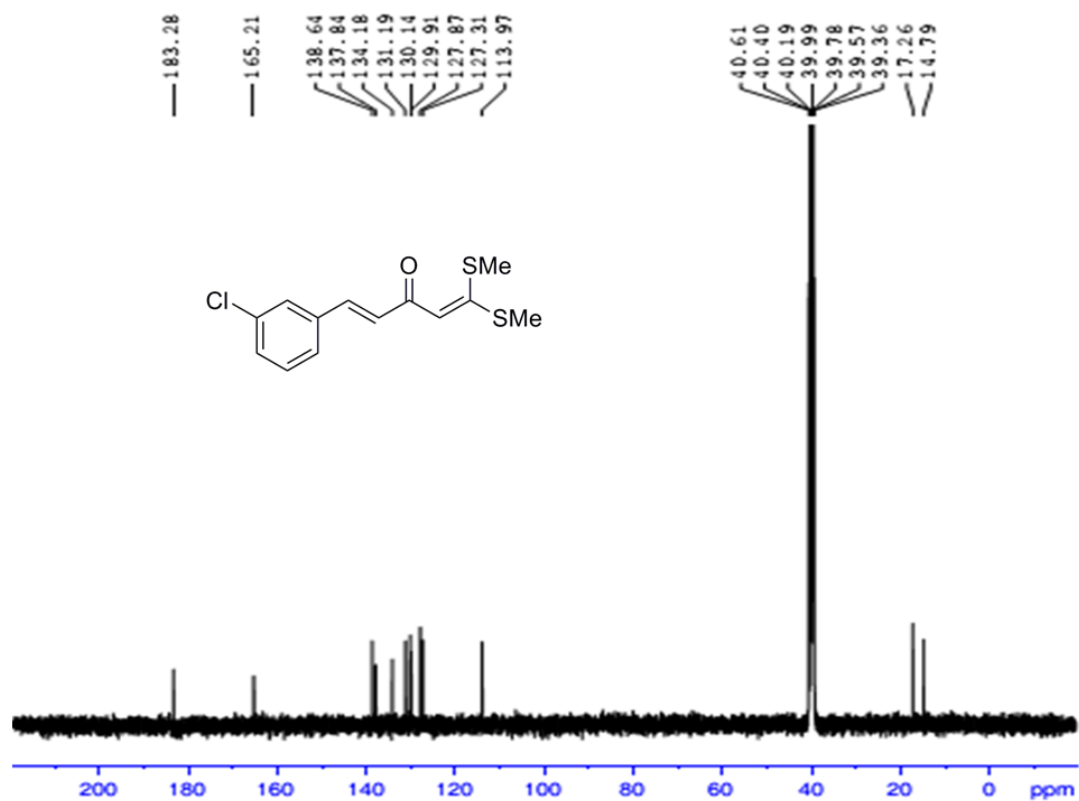


Figure S2b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2b



**Figure S3a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2c



**Figure S3b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2c

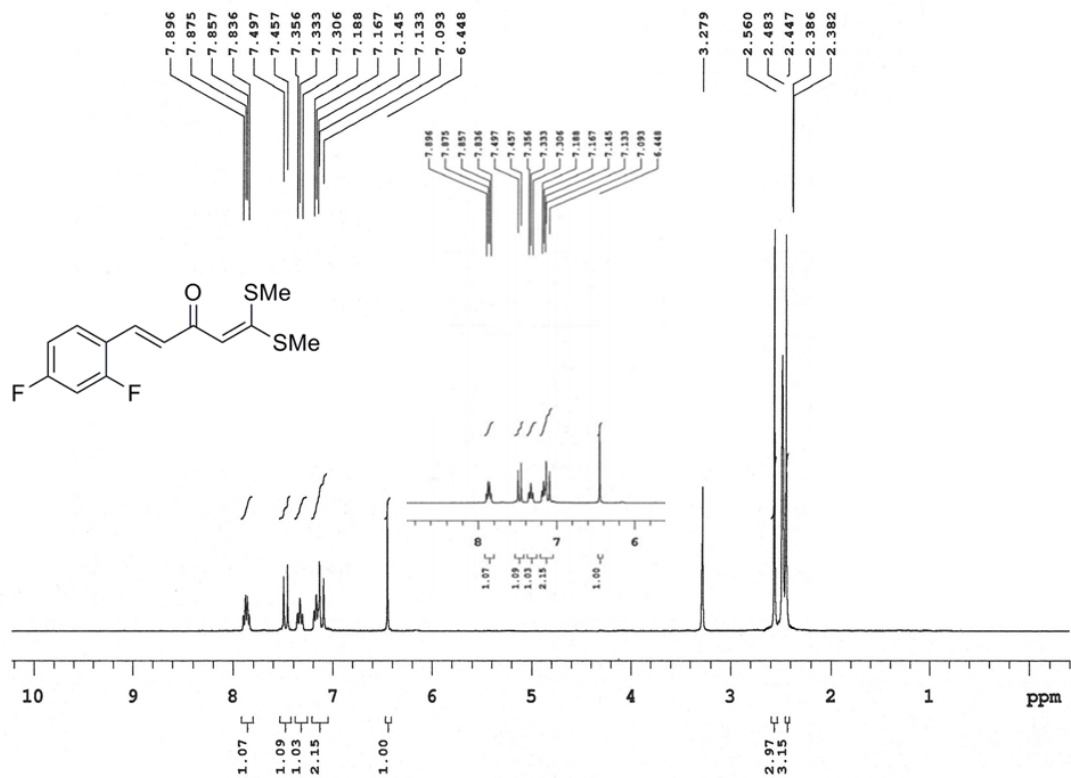


Figure S4a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2e

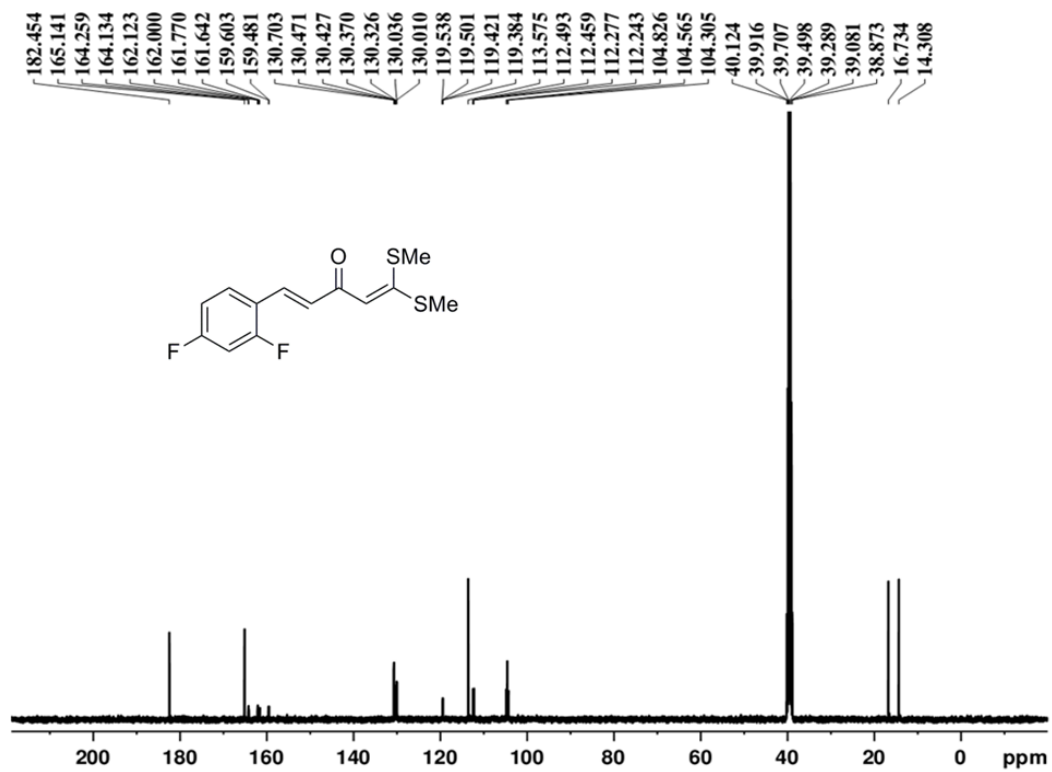
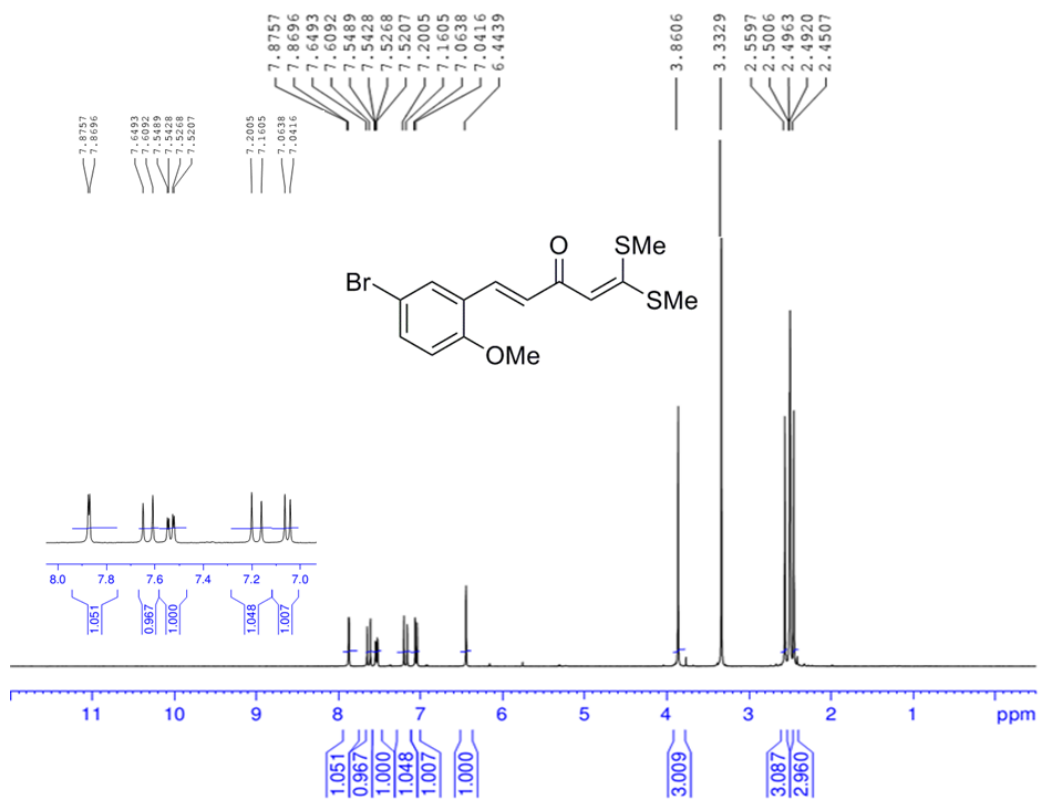
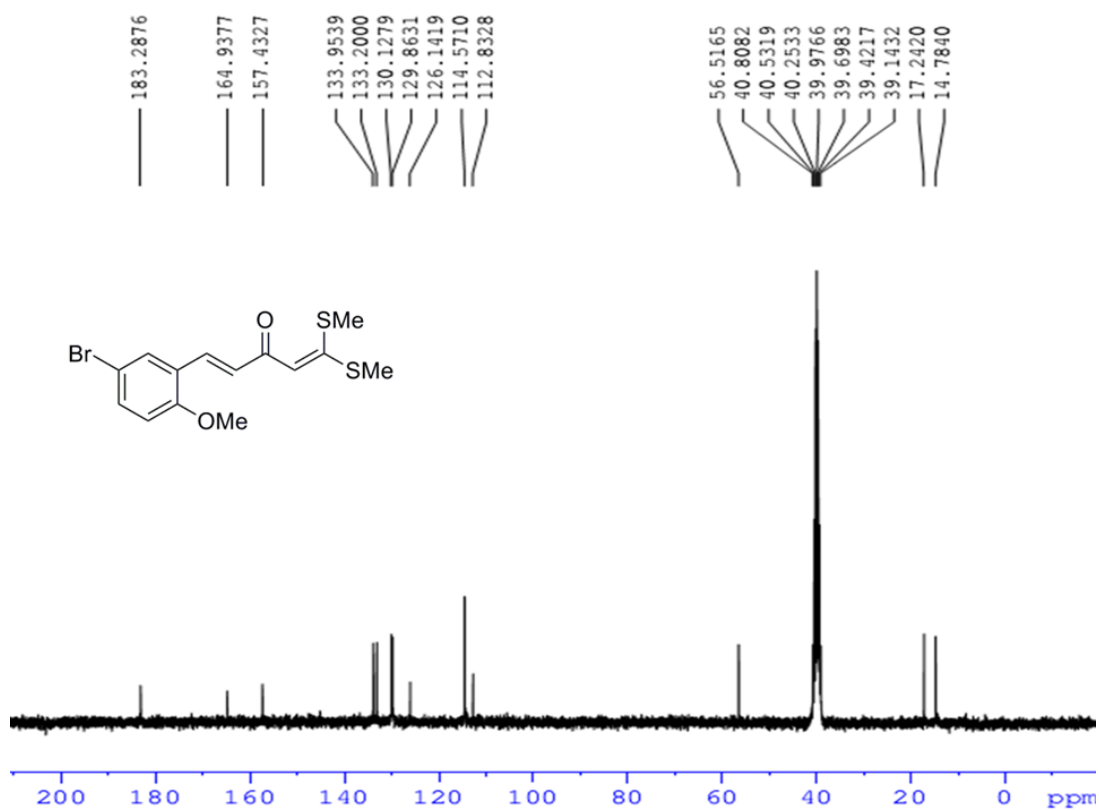


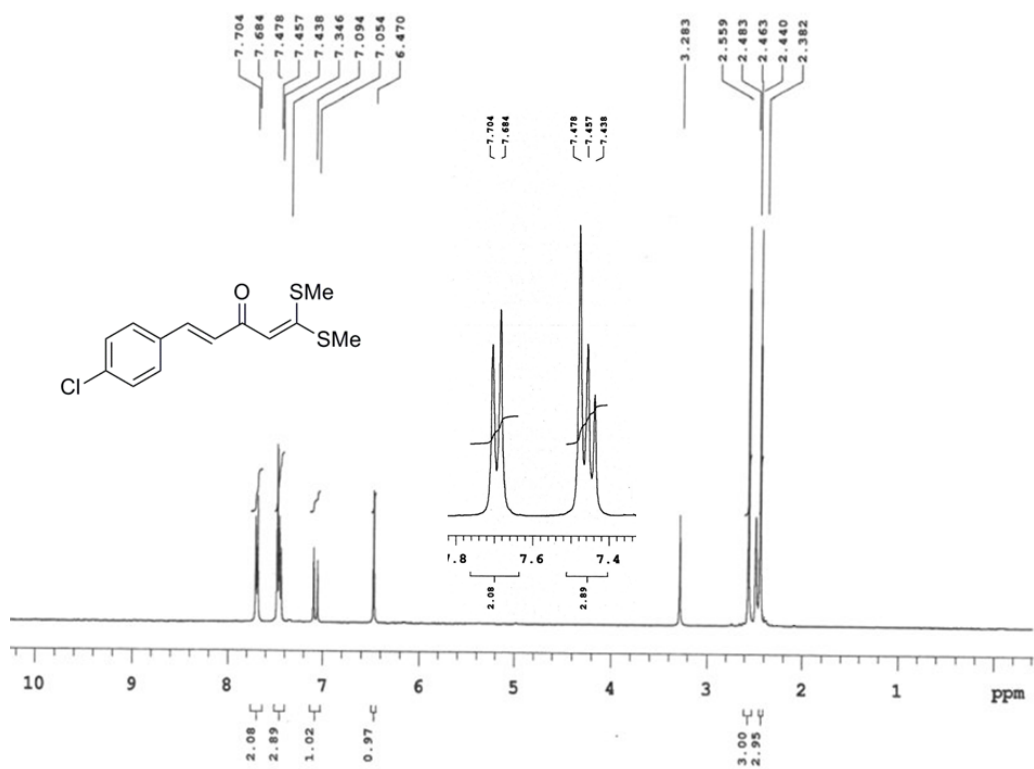
Figure S4b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2e



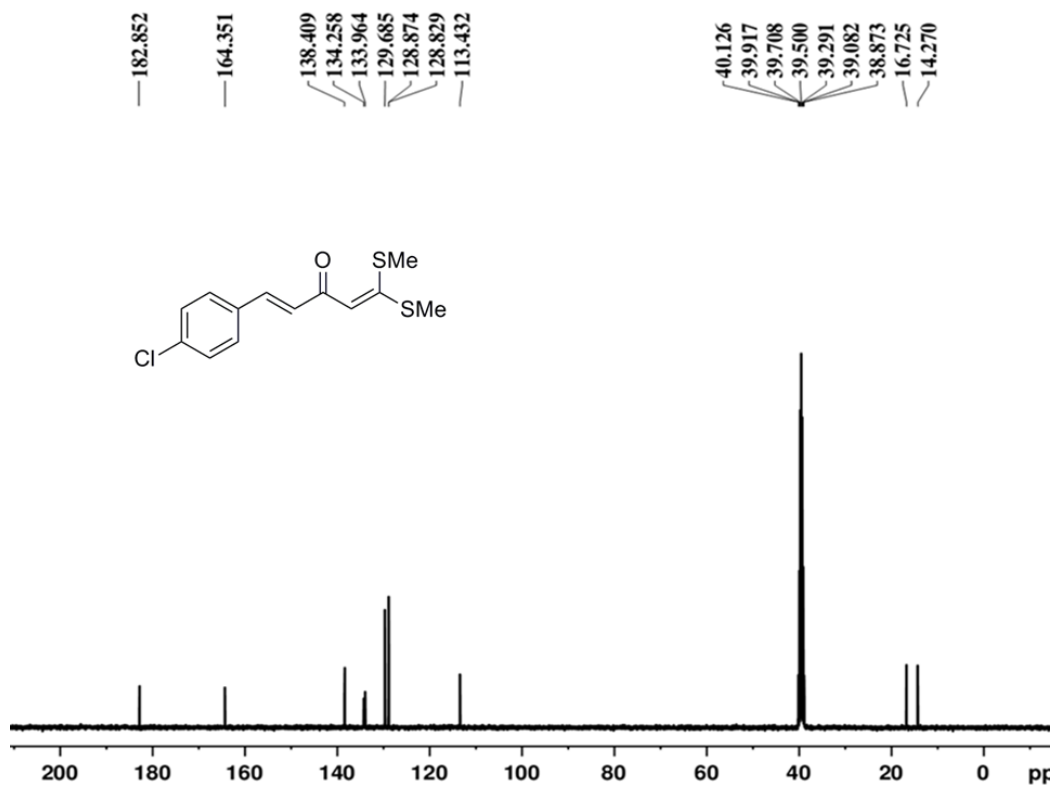
**Figure S5a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **2f**



**Figure S5b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **2f**

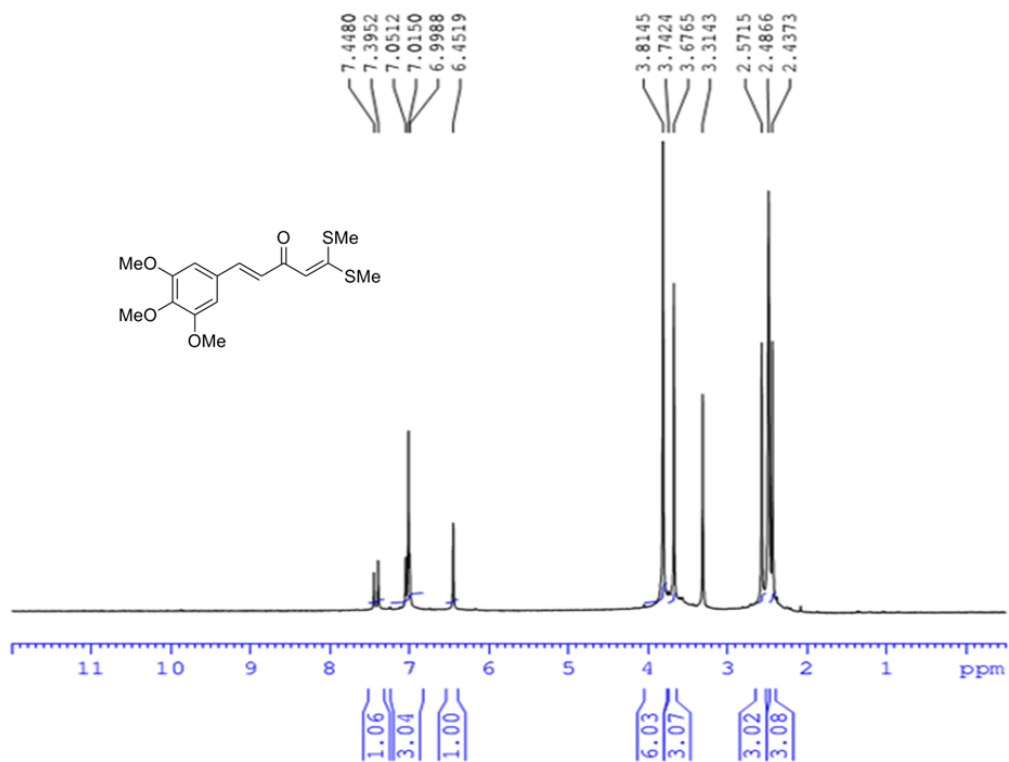


**Figure S6a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2g

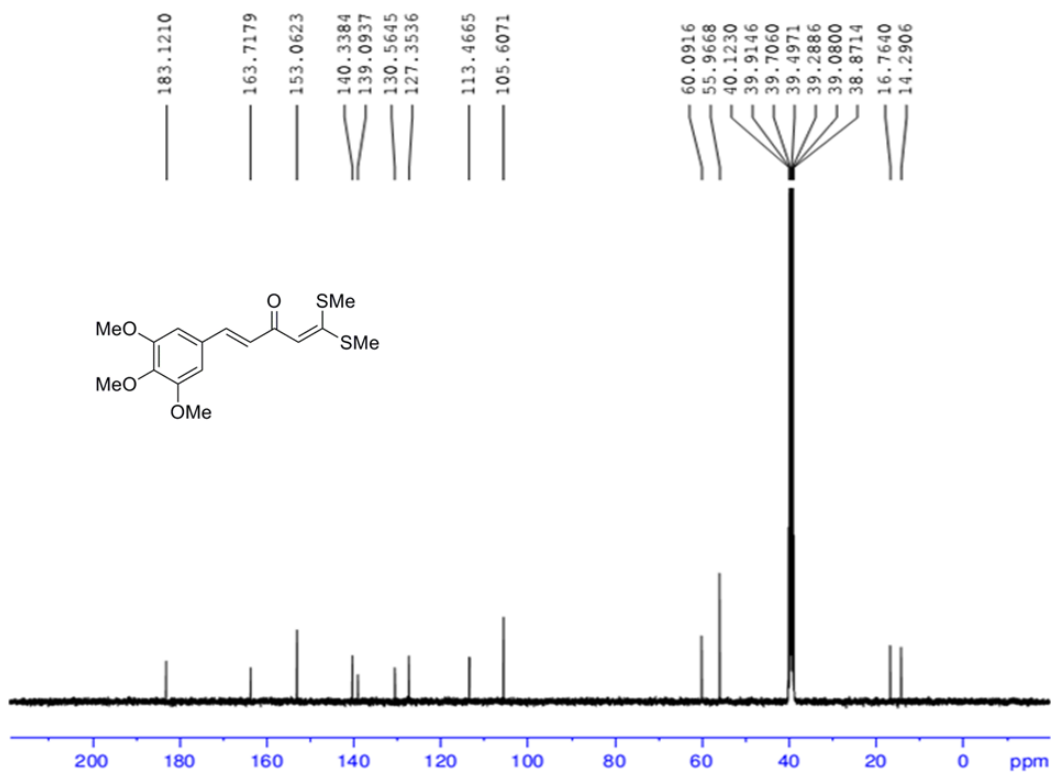


**Figure S6b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2g





**Figure S7a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **2h**



**Figure S7b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **2h**

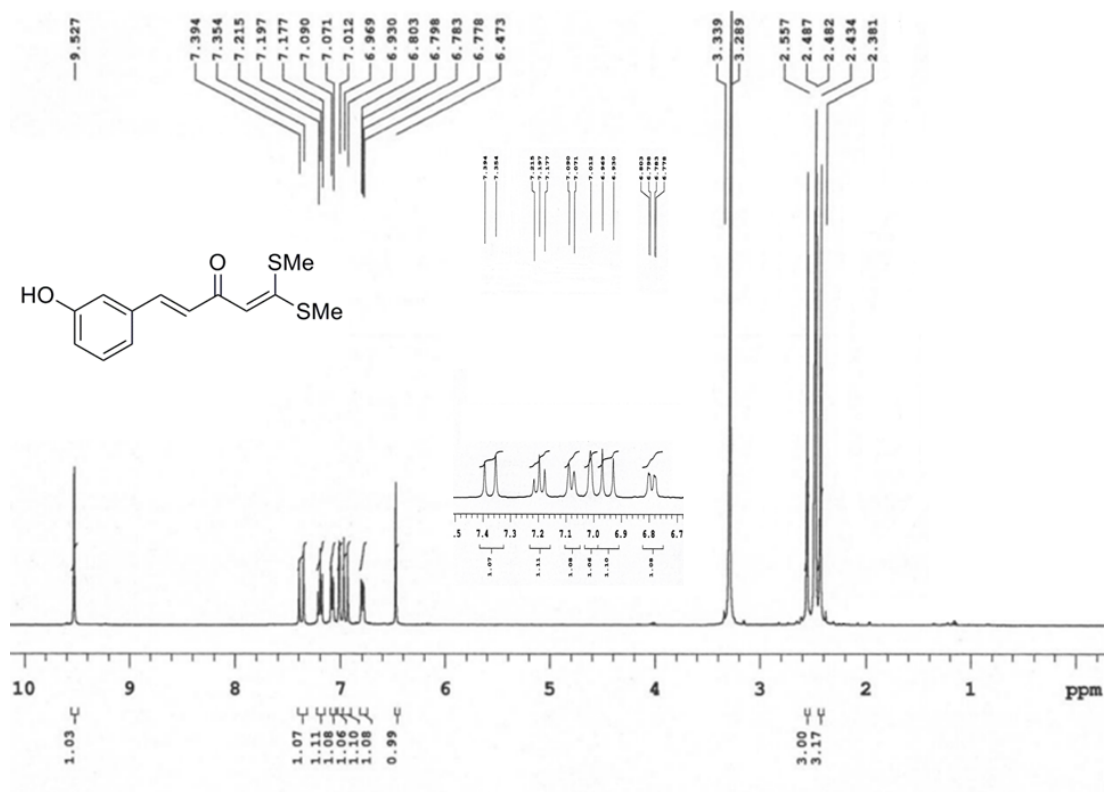


Figure S8a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2i

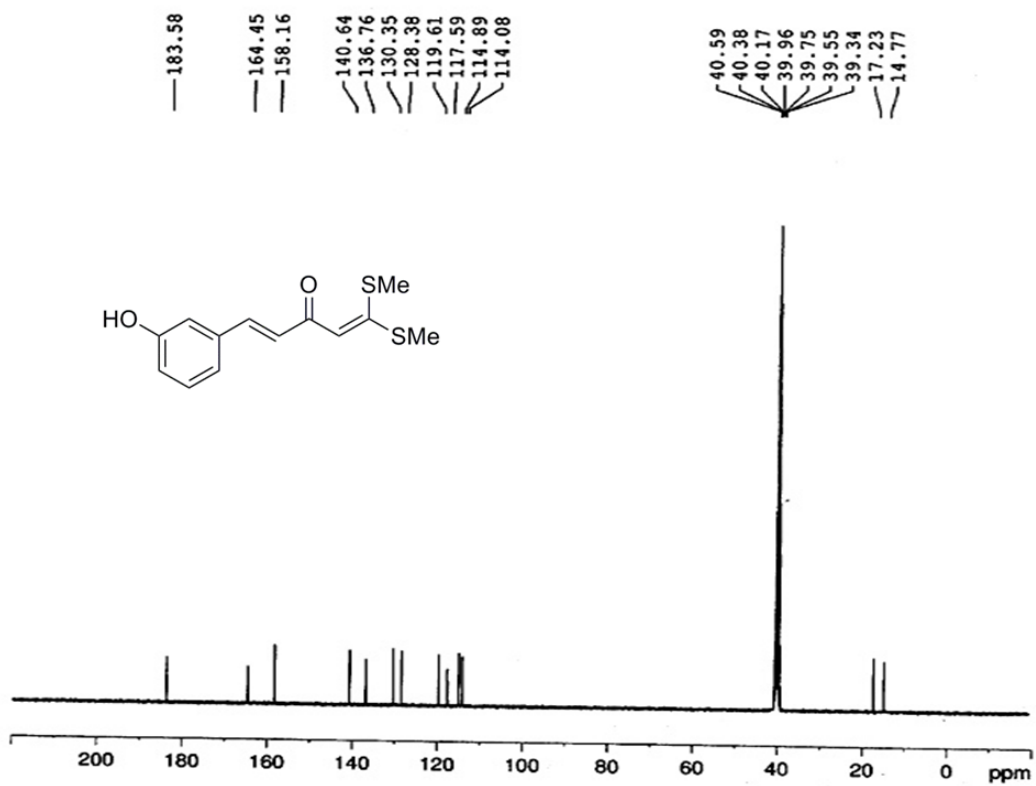
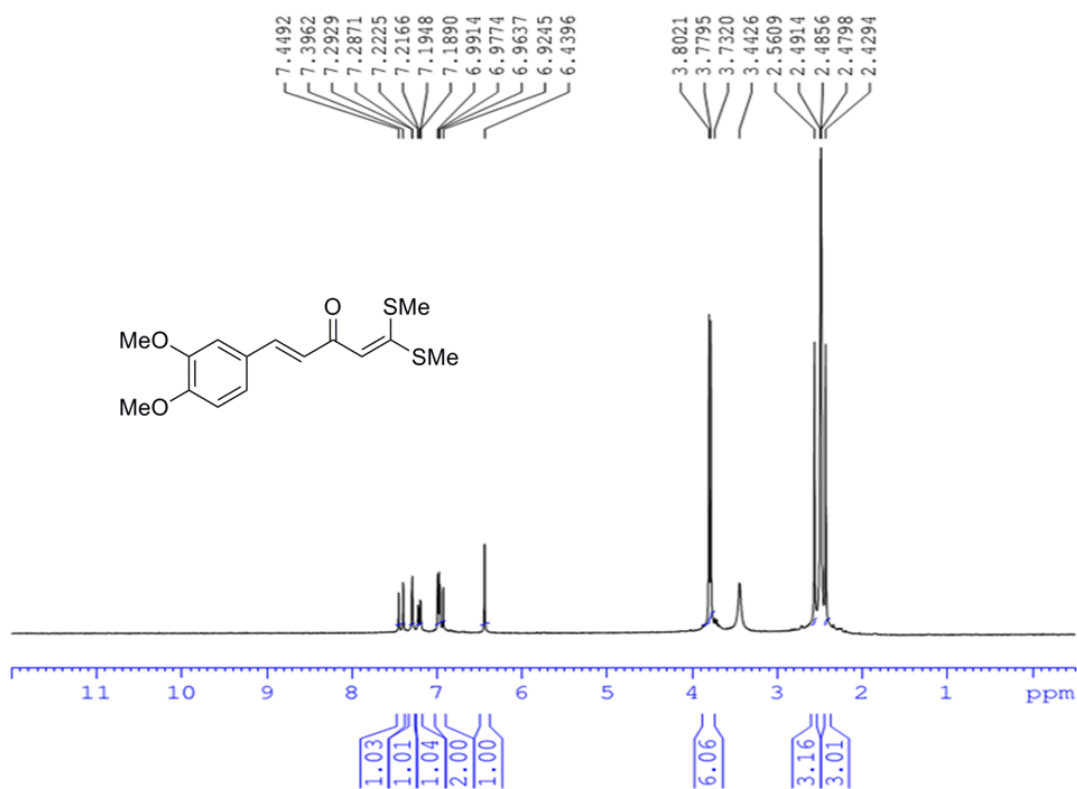
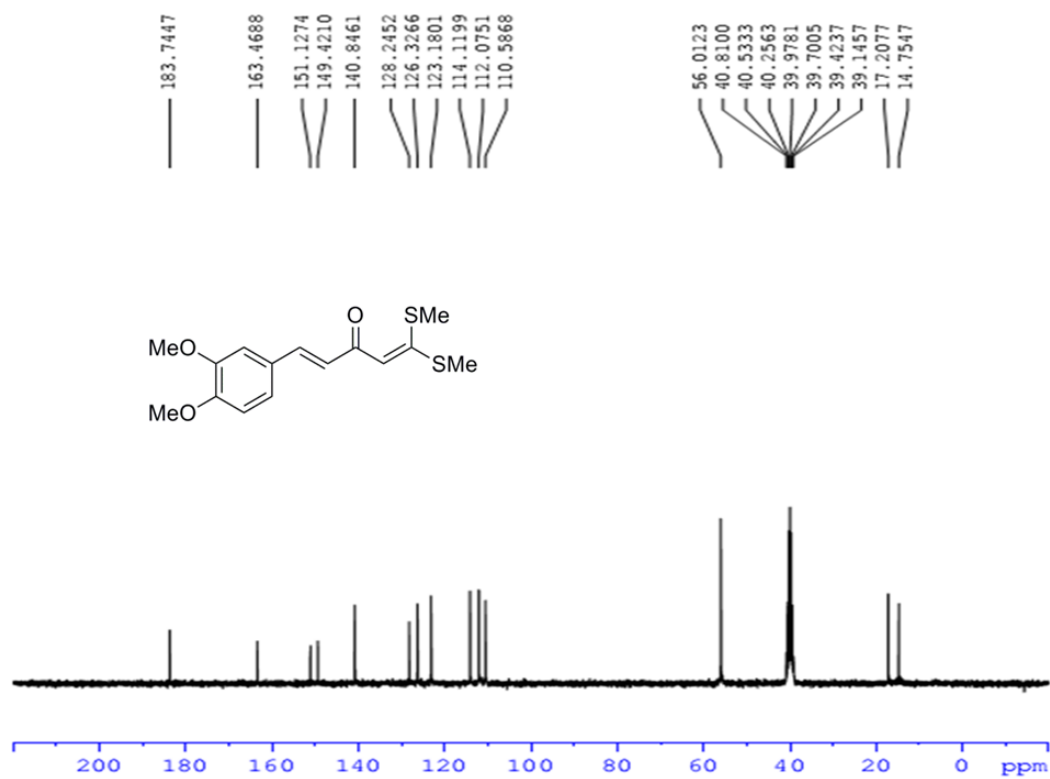


Figure S8b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2i



**Figure S9a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **2j**



**Figure S9b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **2j**

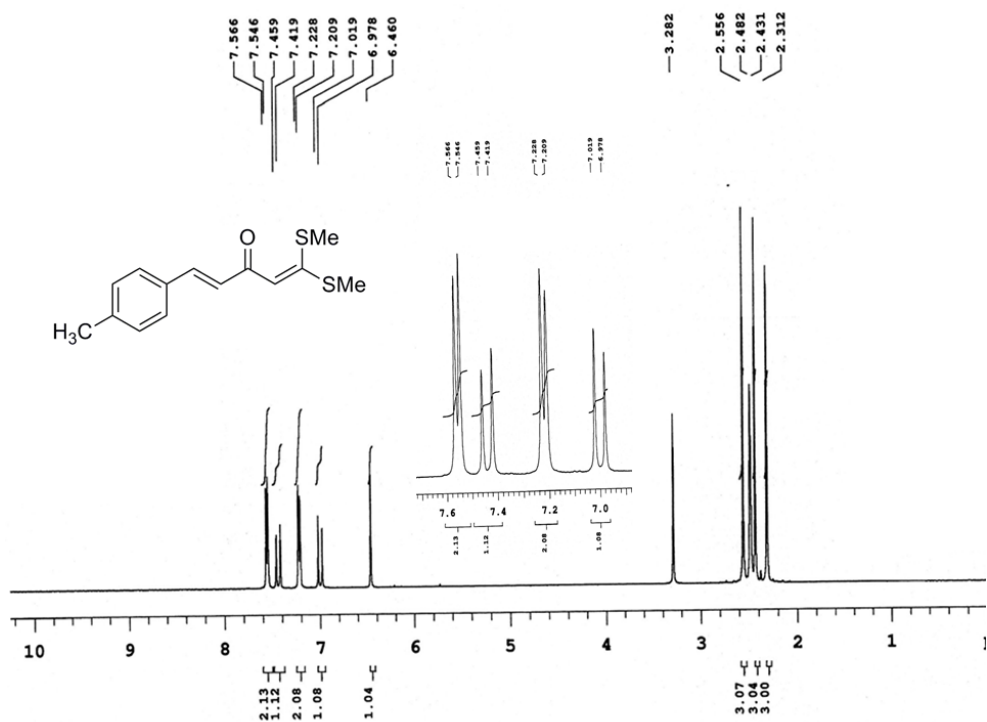


Figure S10a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2k

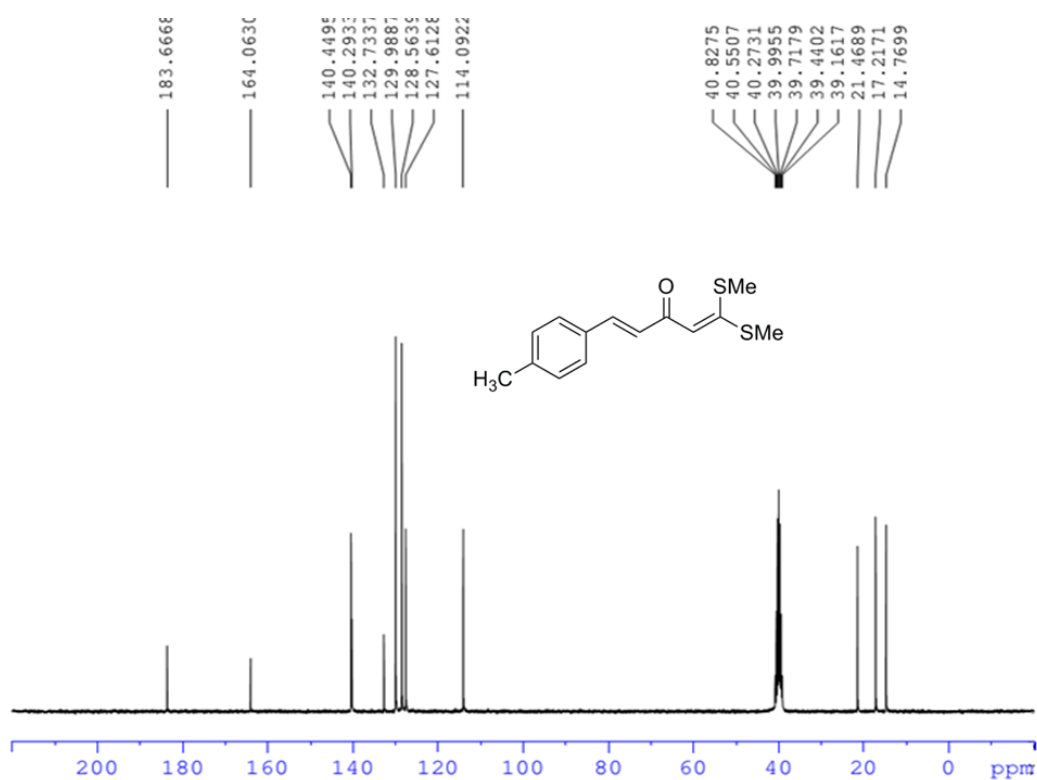
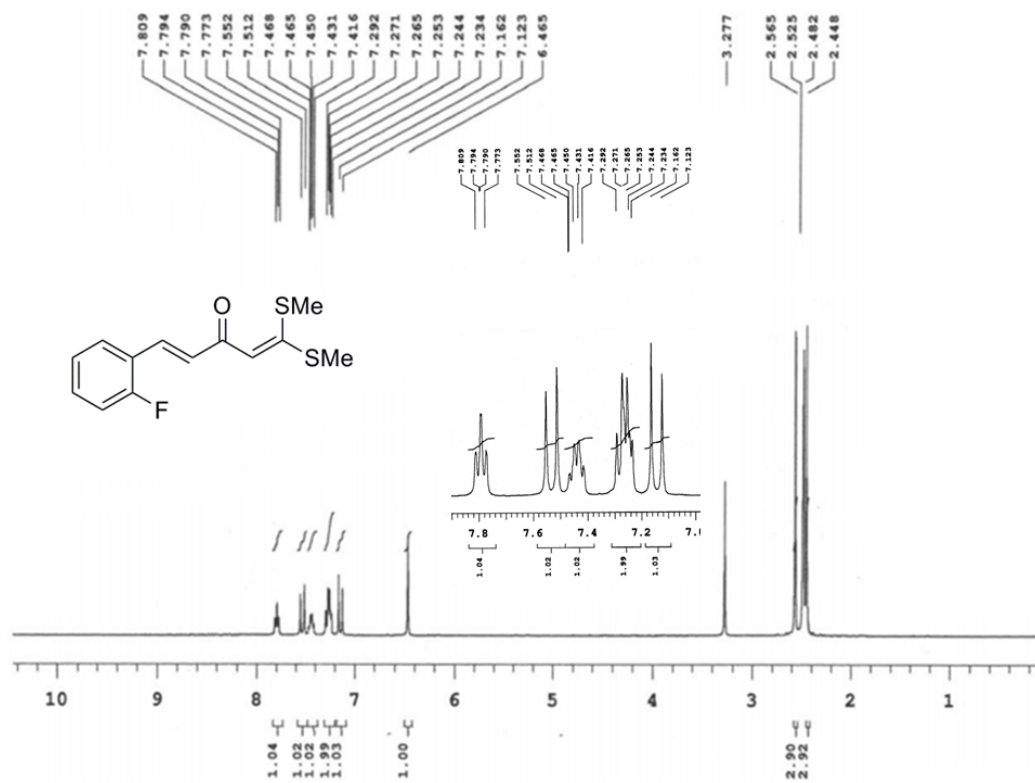
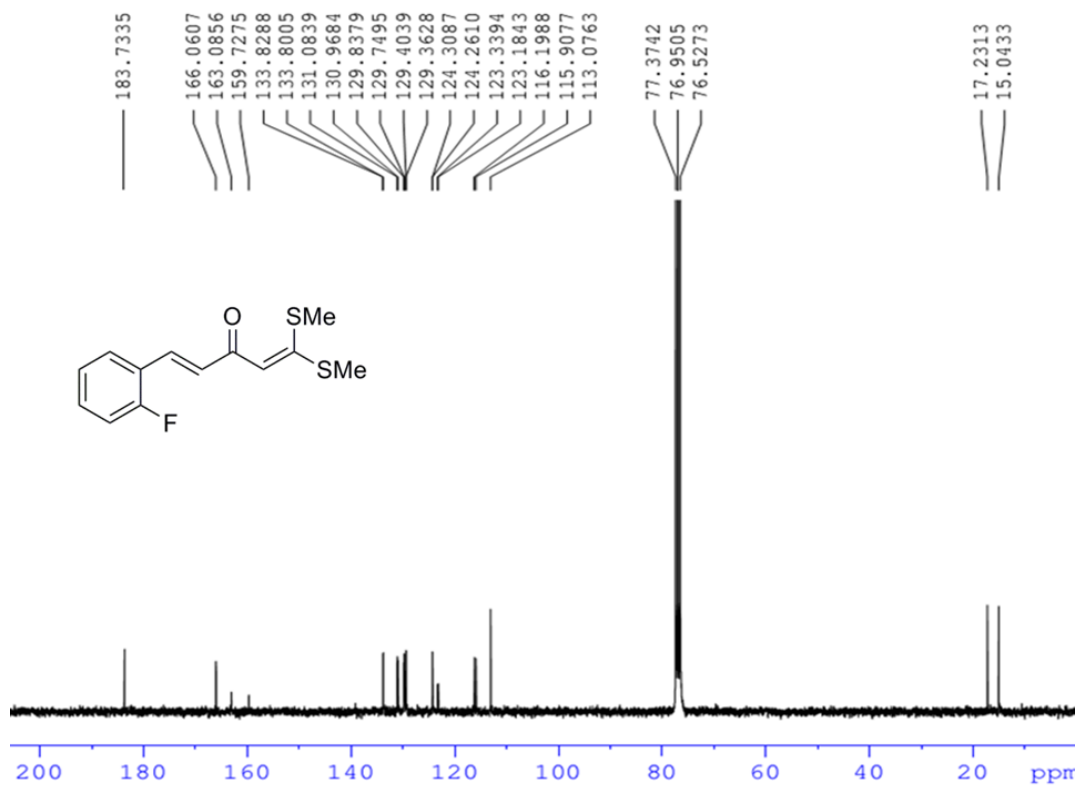


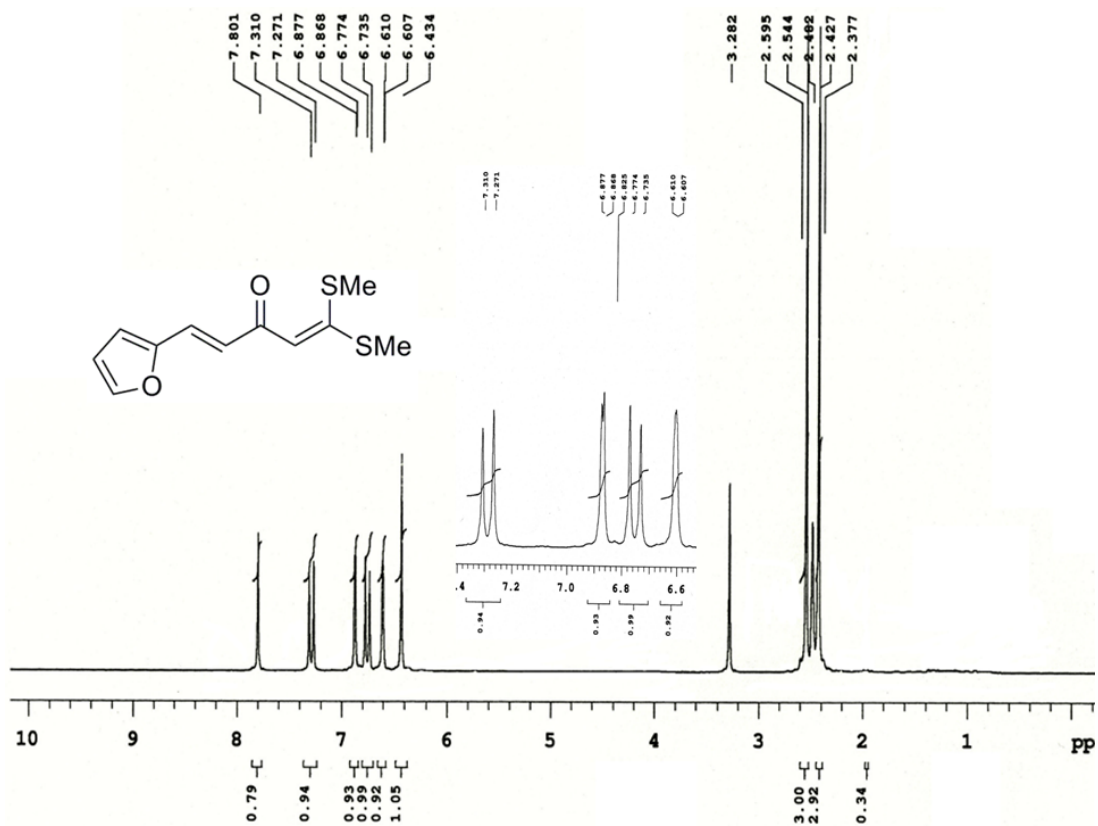
Figure S10b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2k



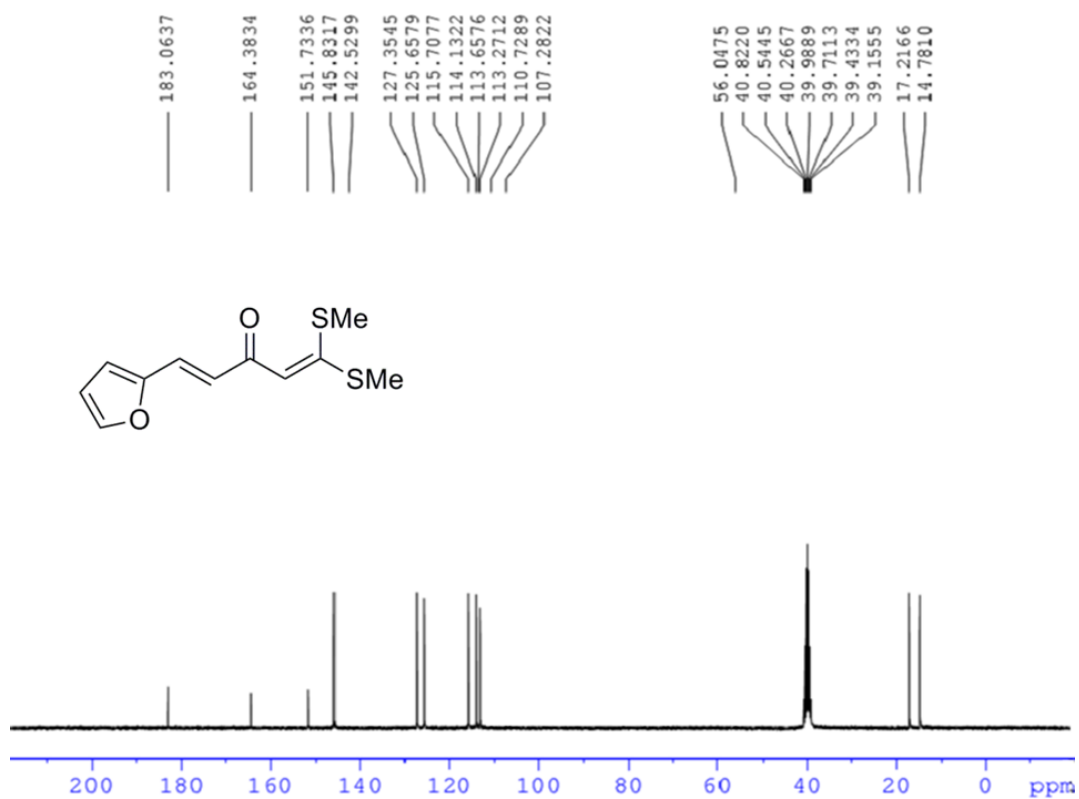
**Figure S11a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **2l**



**Figure S11b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **2l**



**Figure S12a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **2m**



**Figure S12b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **2m**

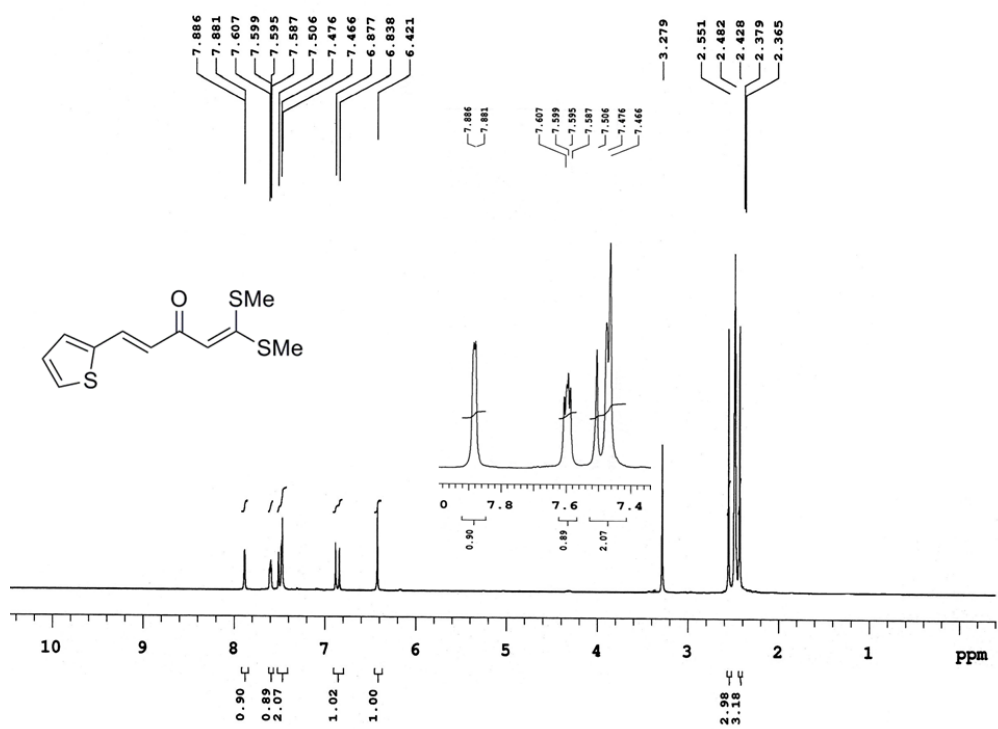


Figure S13a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2n

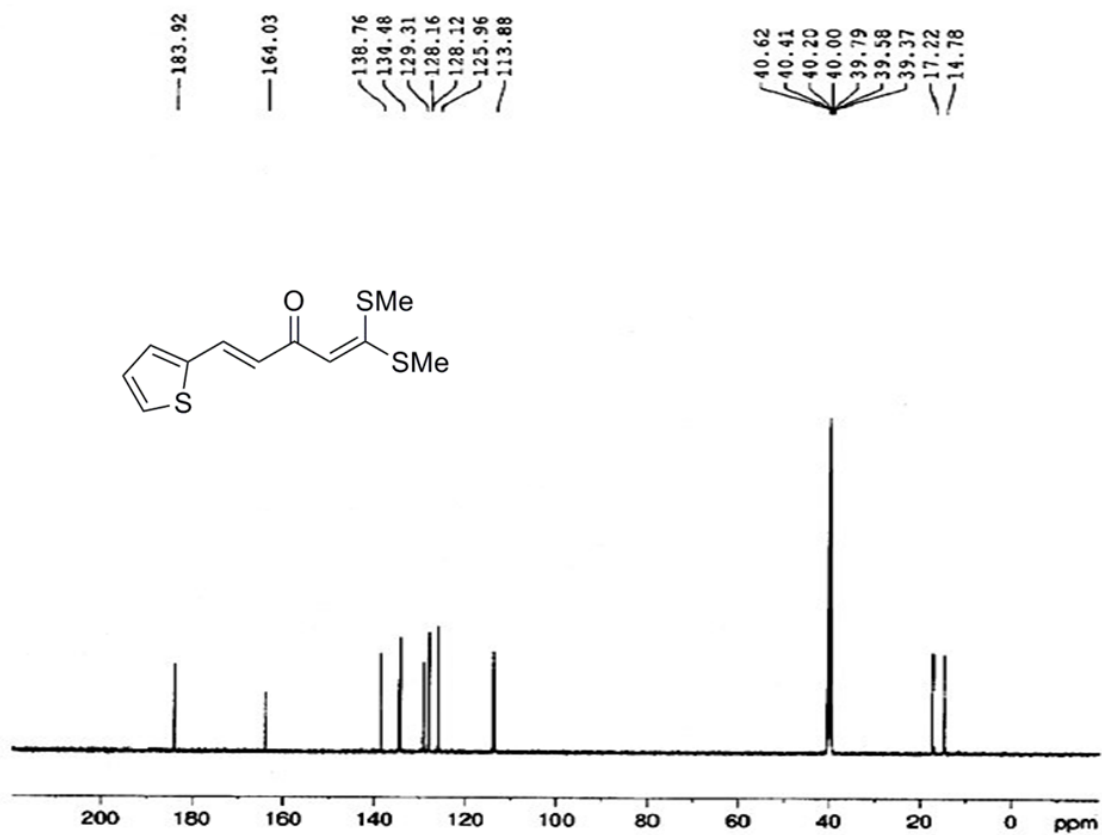


Figure S13b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2n

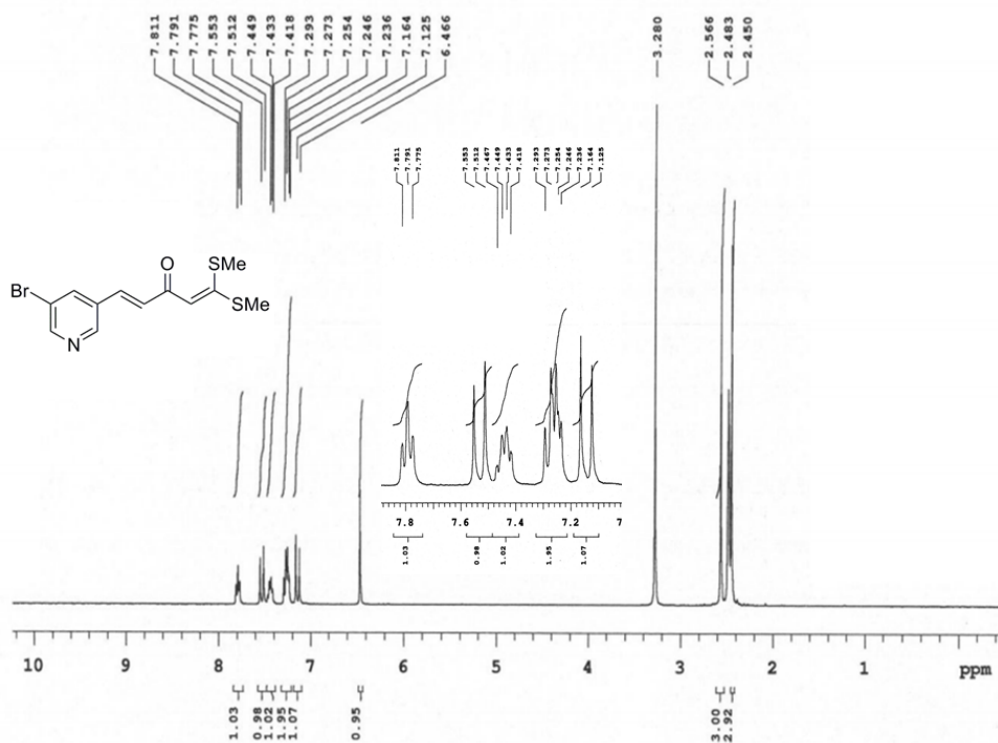


Figure S14a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 2o

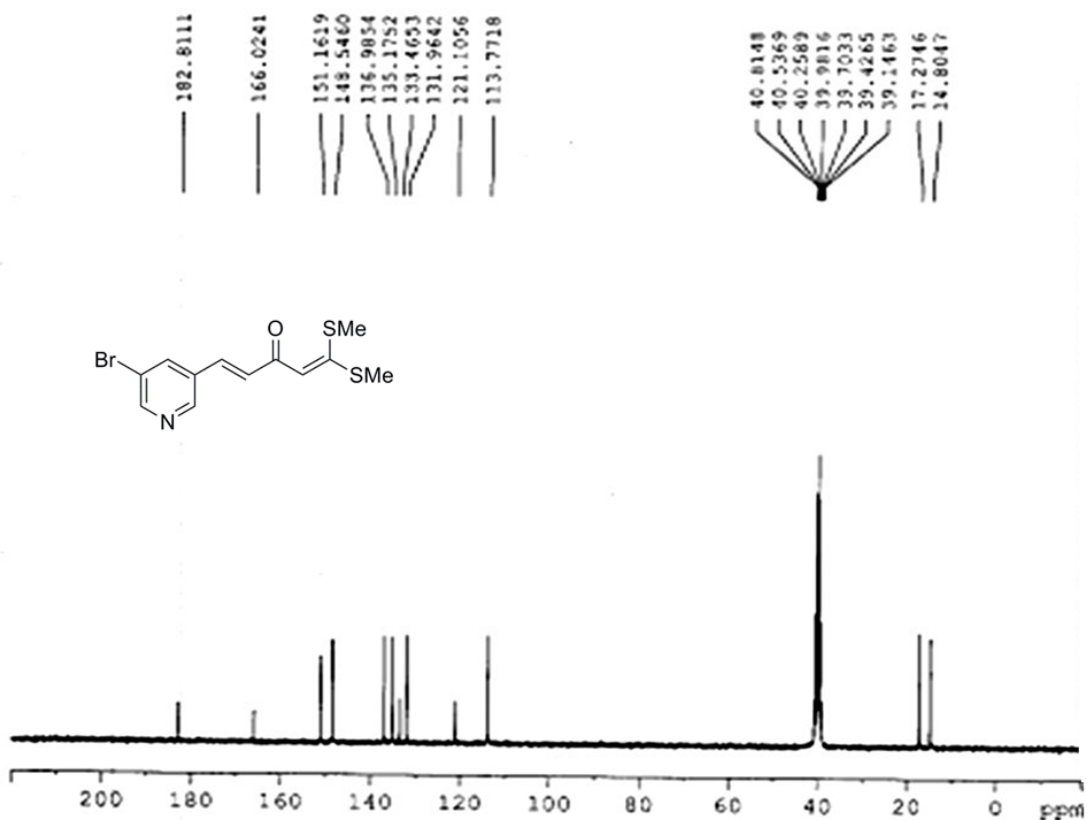
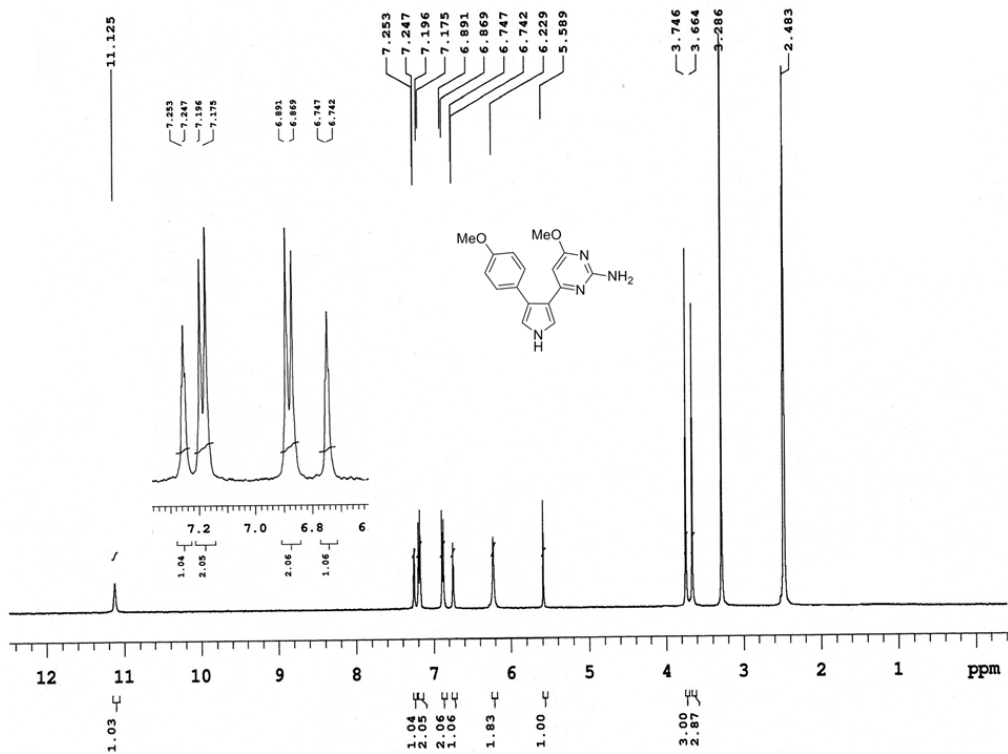
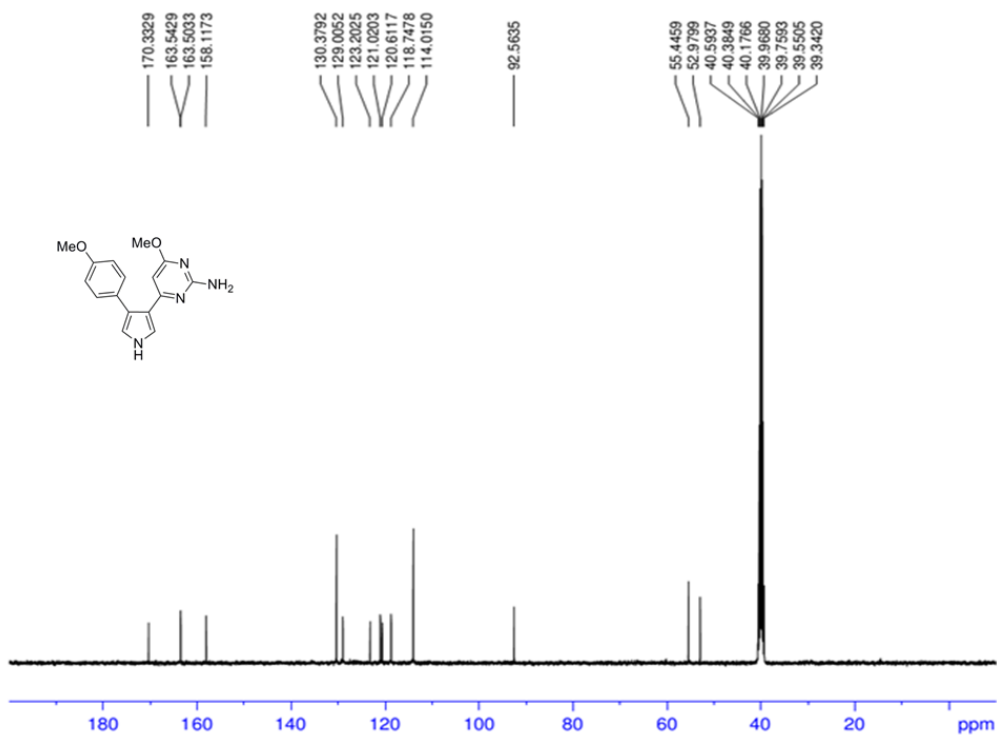


Figure S14b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 2o





**Figure S15a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8a**



**Figure S15b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8a**

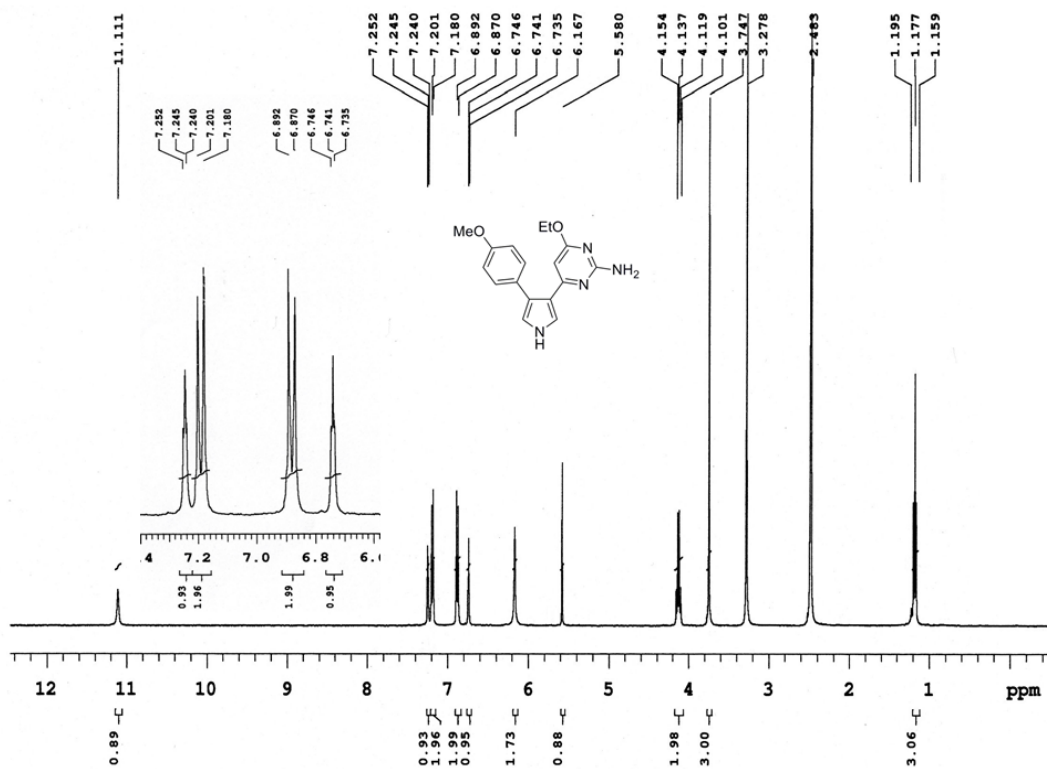


Figure S16a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8b**

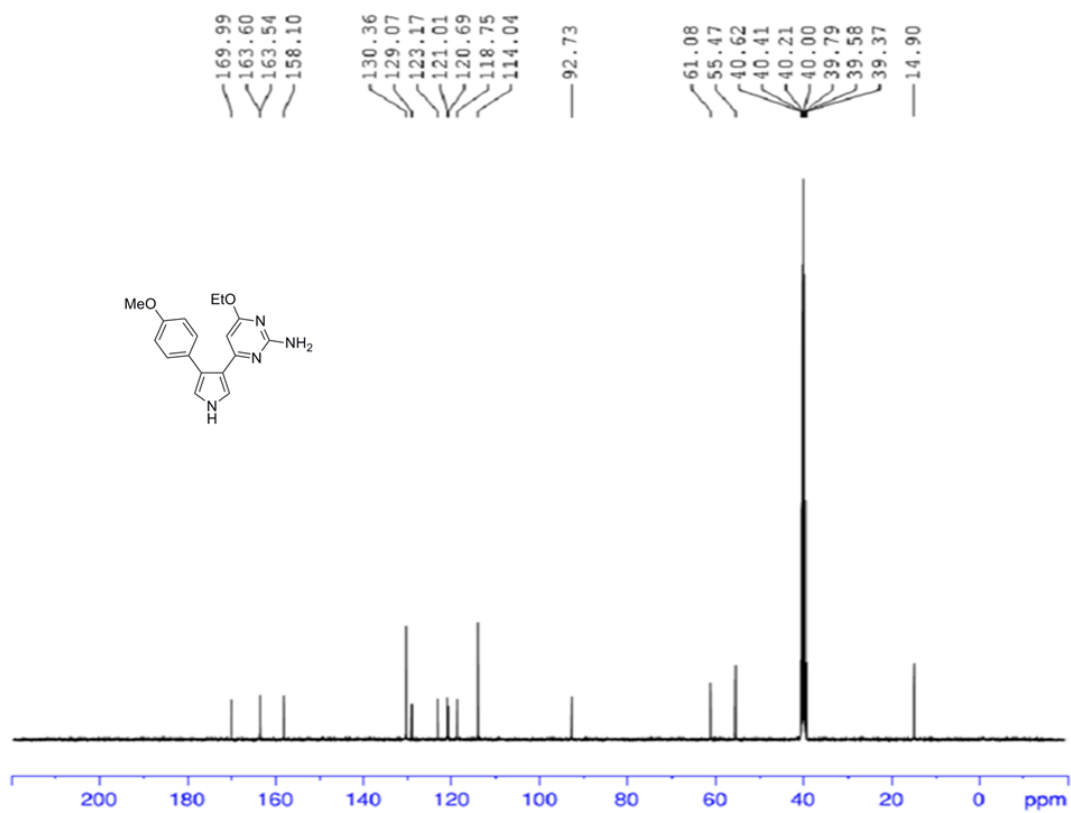


Figure S16b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8b**

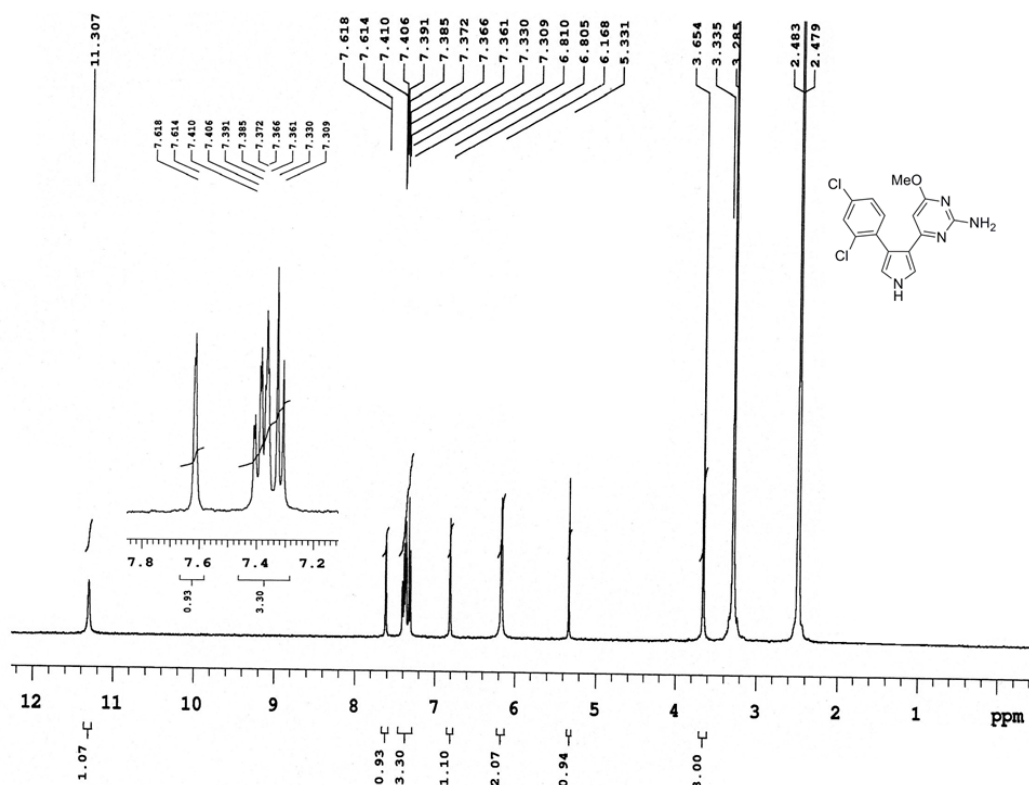


Figure S17a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8C**

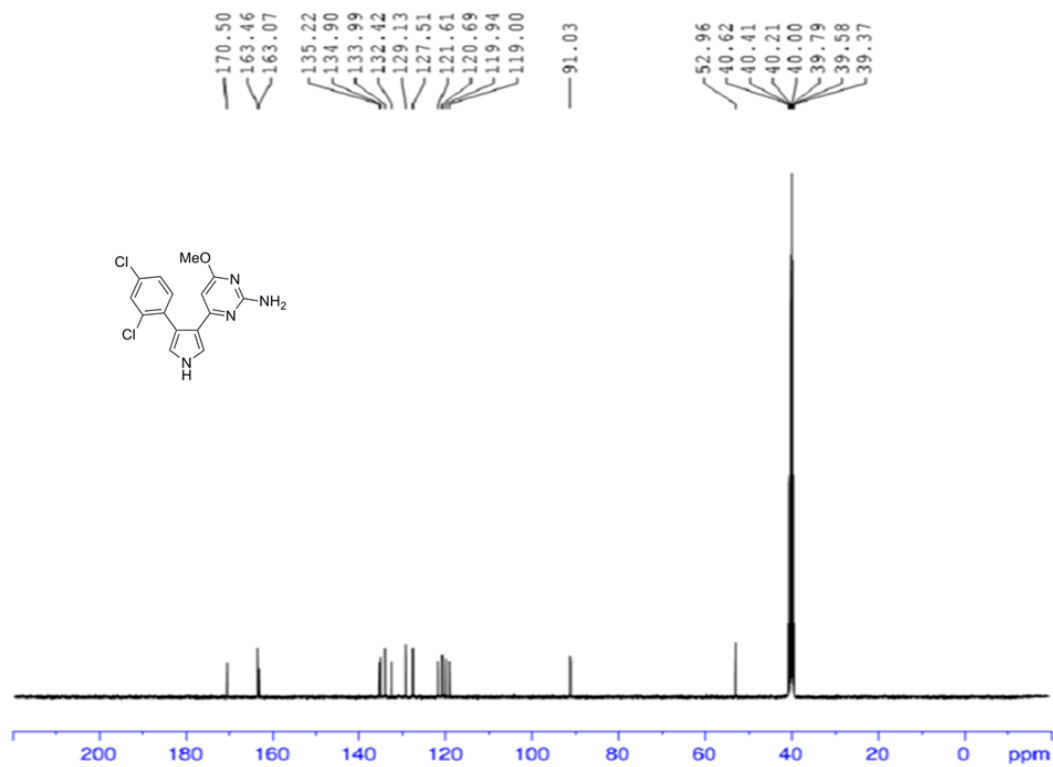


Figure S17b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8C**

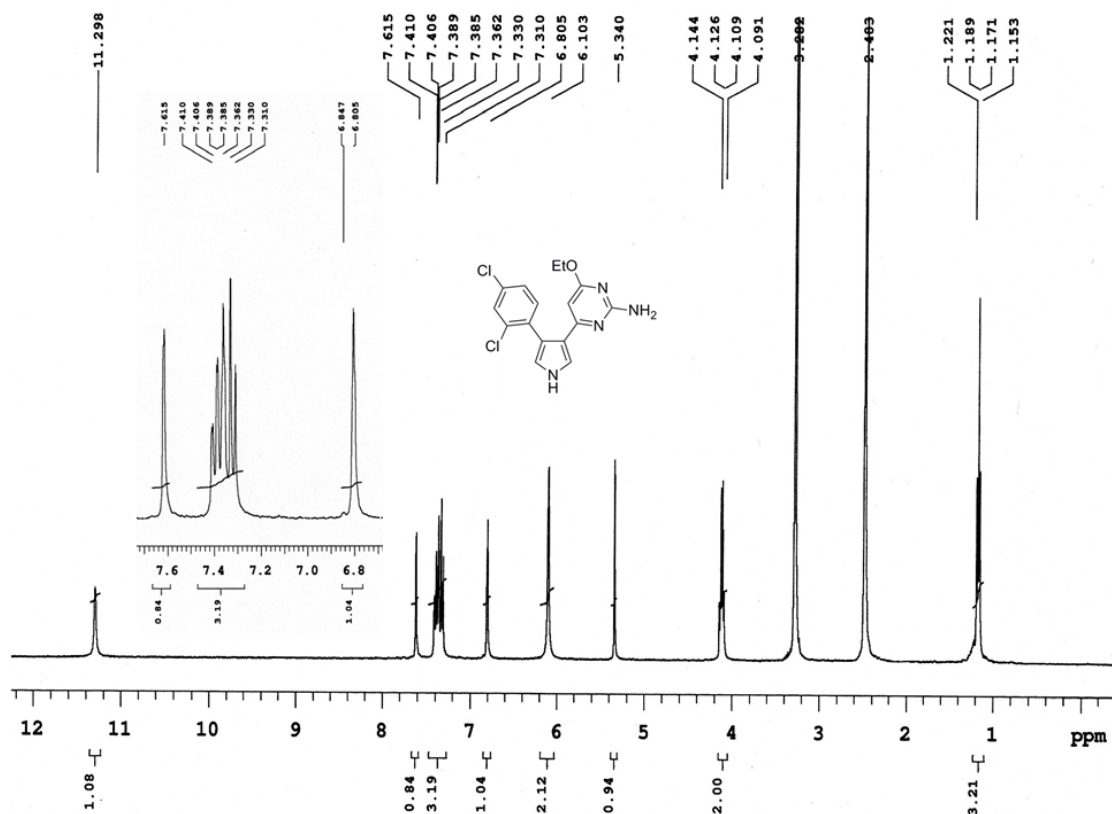


Figure S18a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8d**

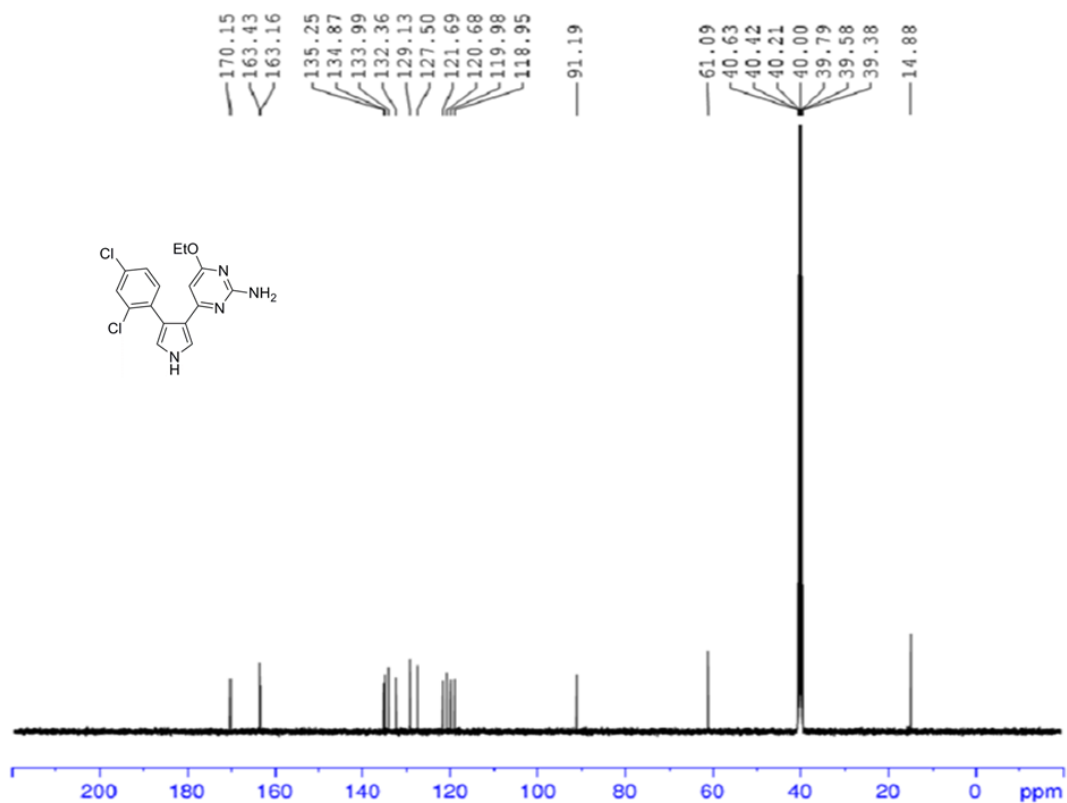


Figure S18b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8d**

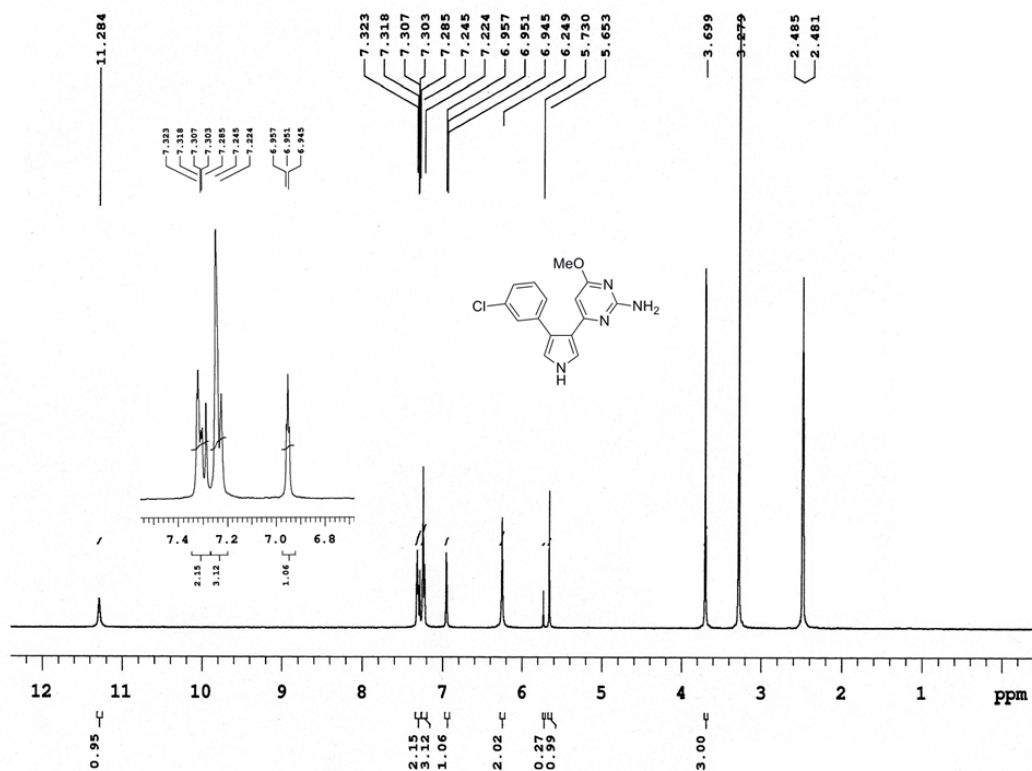


Figure S19a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8e**

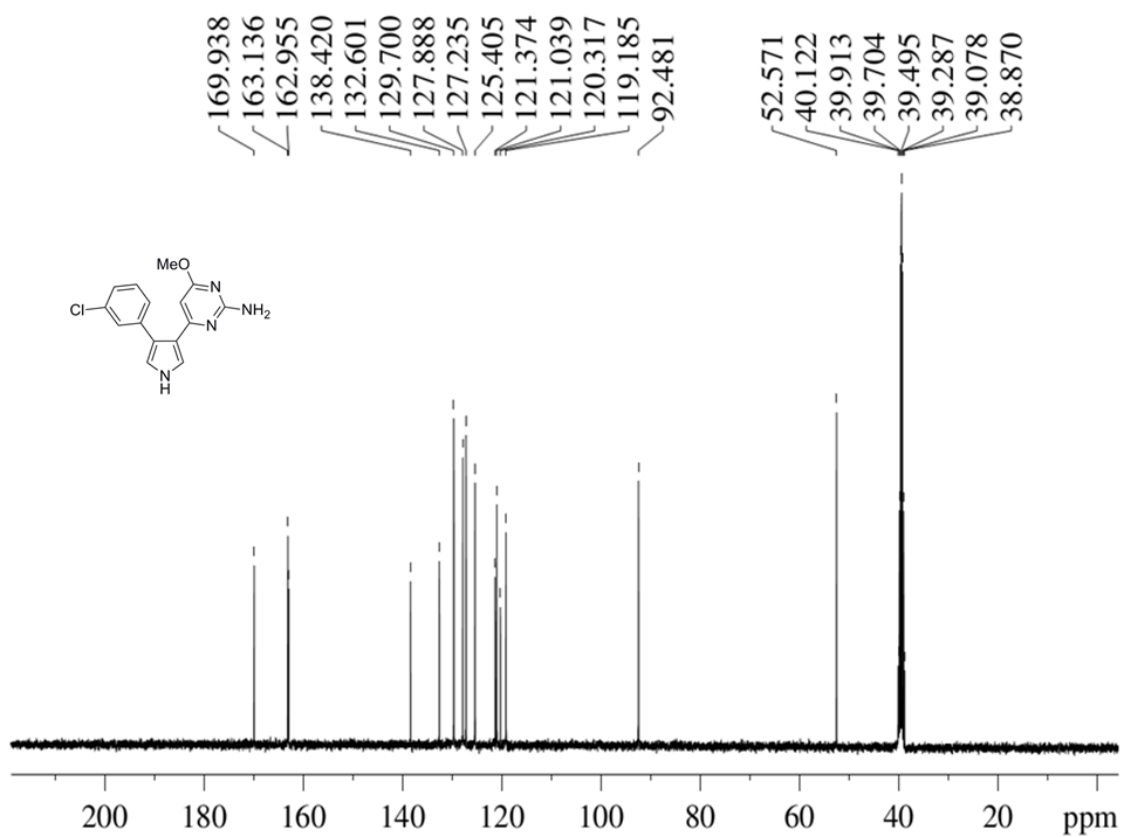
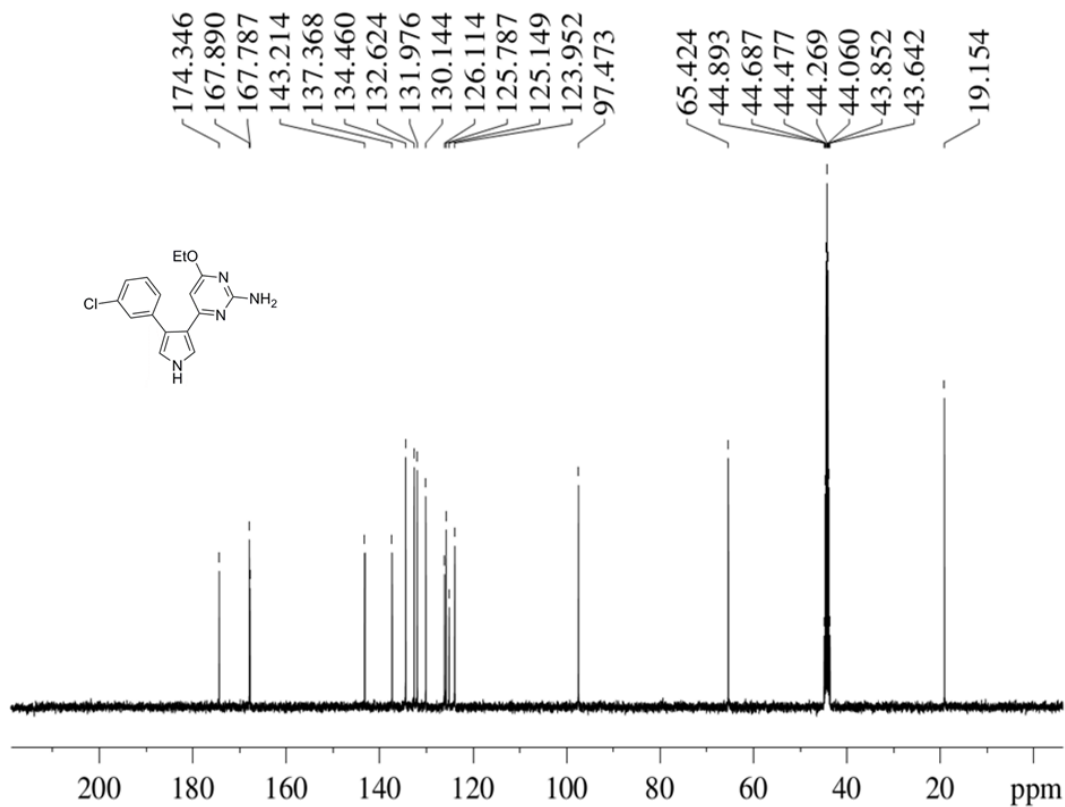
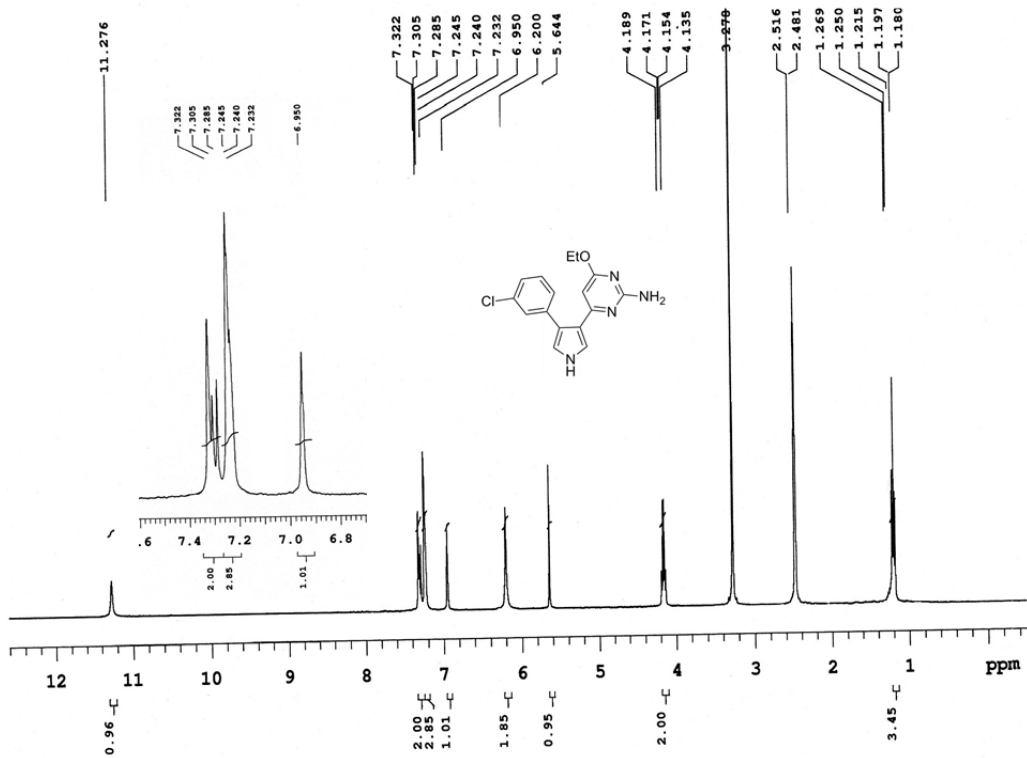


Figure S19b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8e**



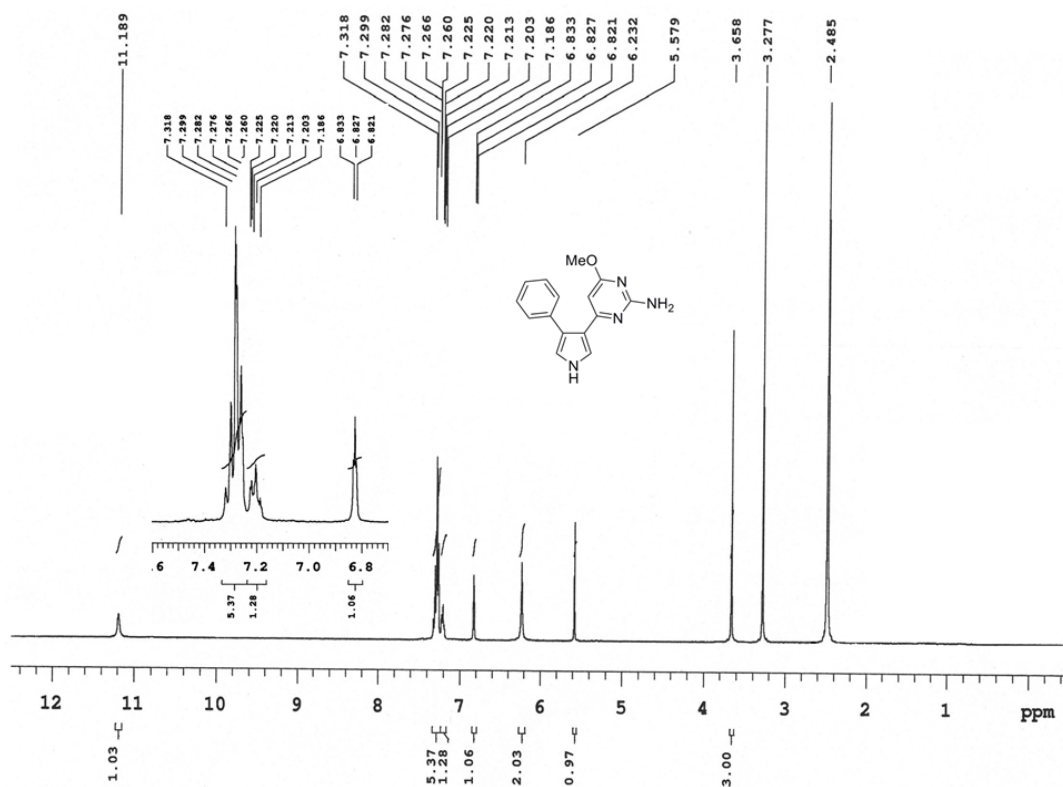


Figure S21a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8g**

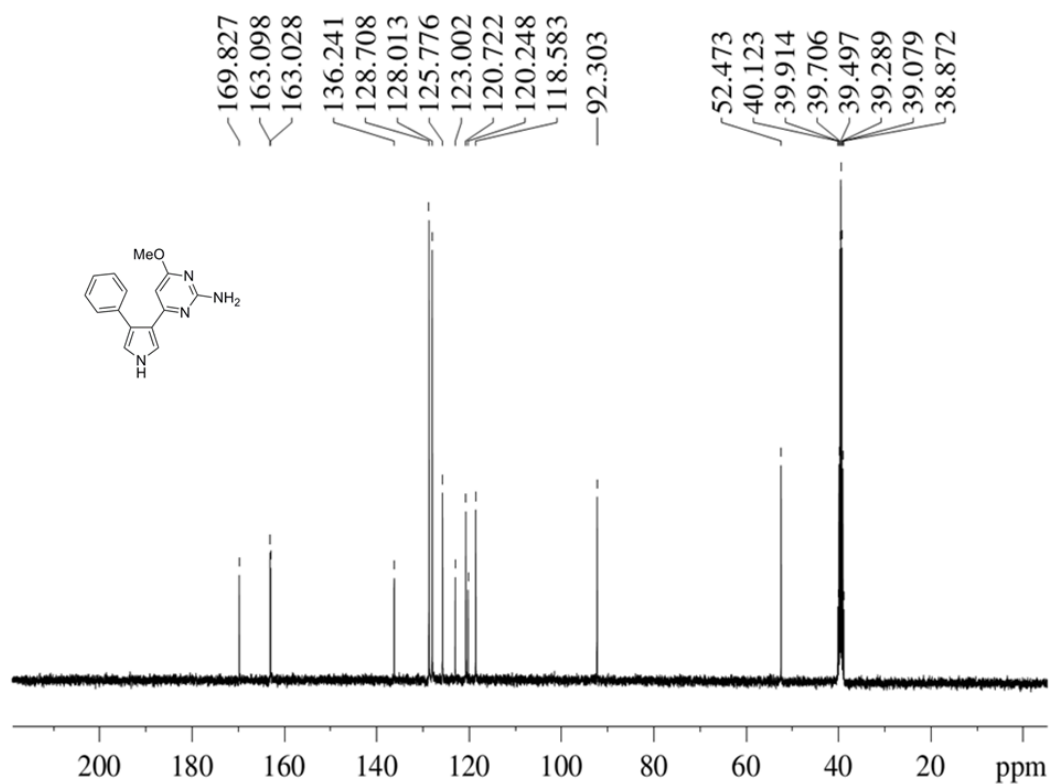


Figure S21b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8g**

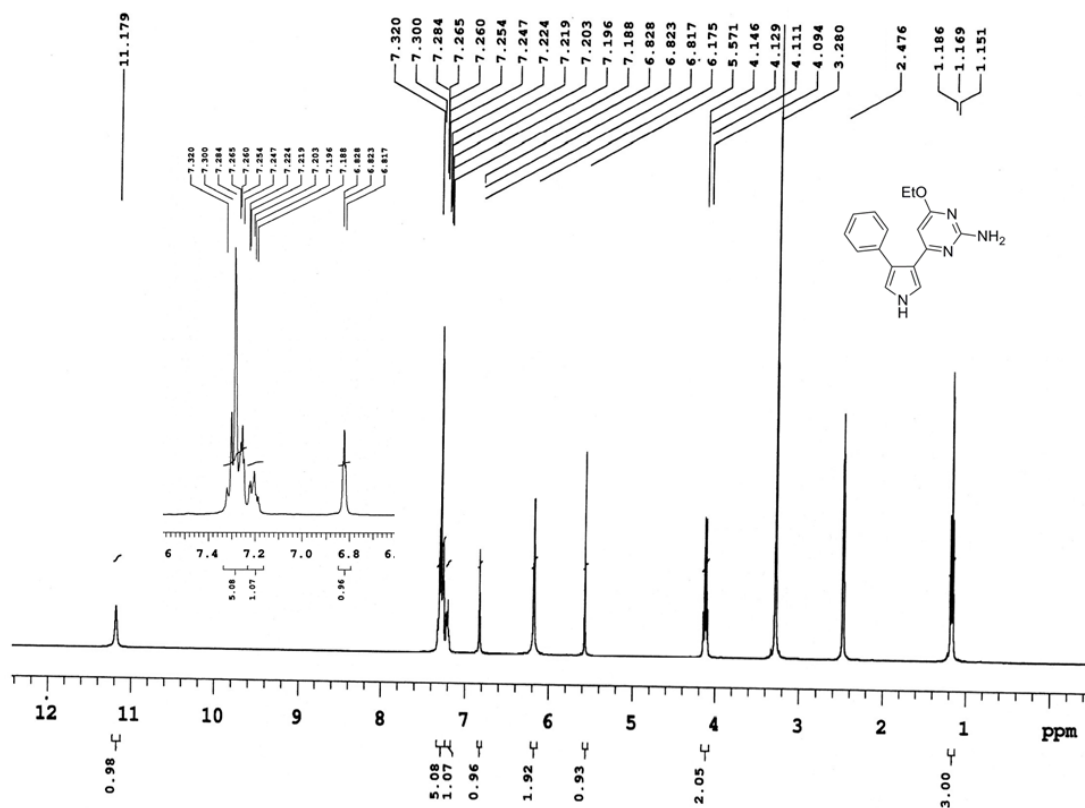


Figure S22a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 8h

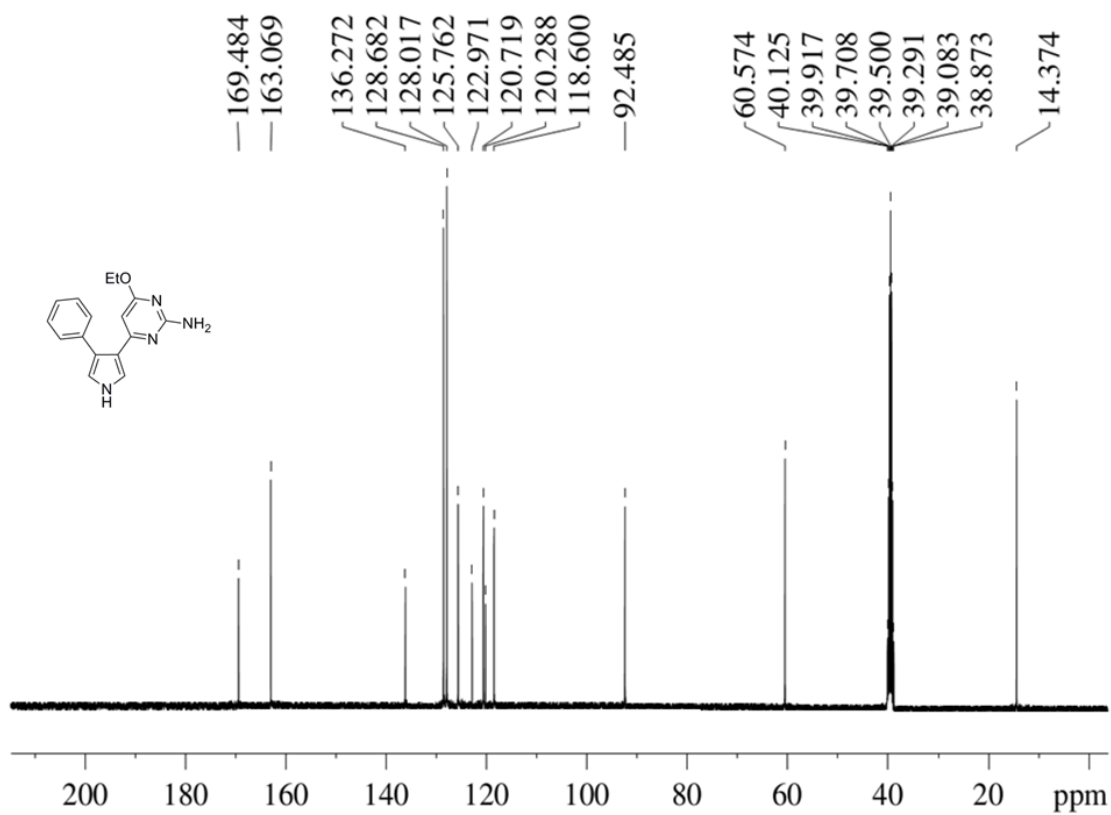


Figure S22b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 8h



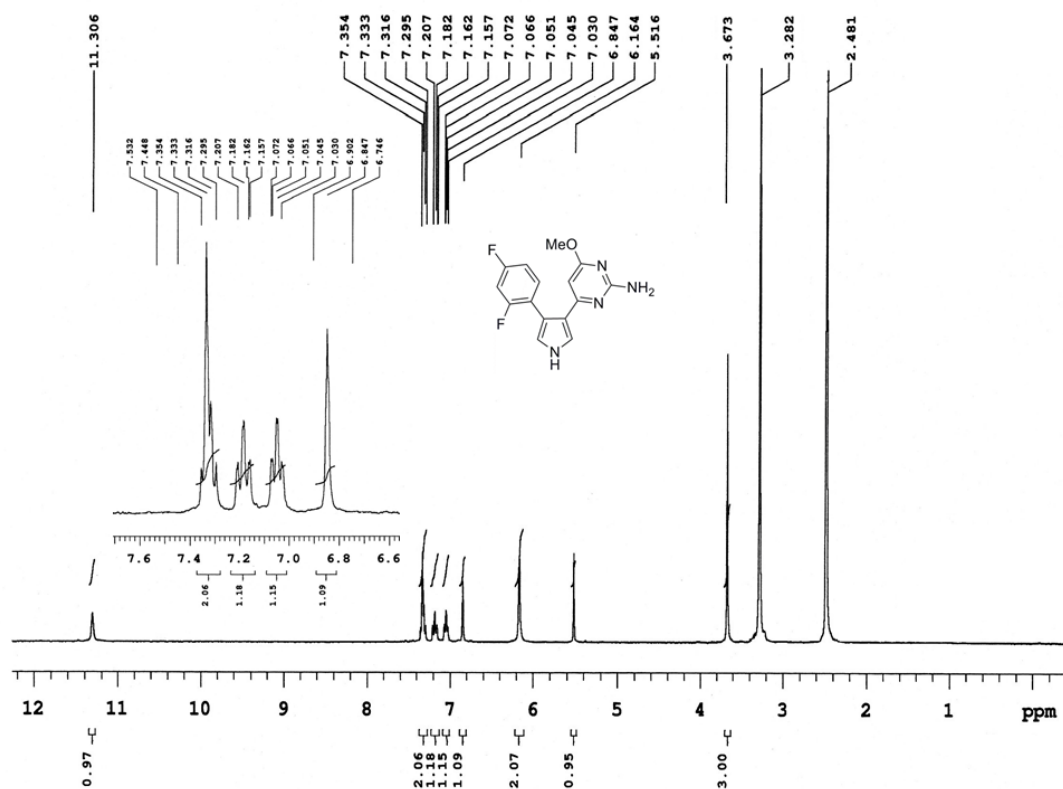


Figure S23a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8i**

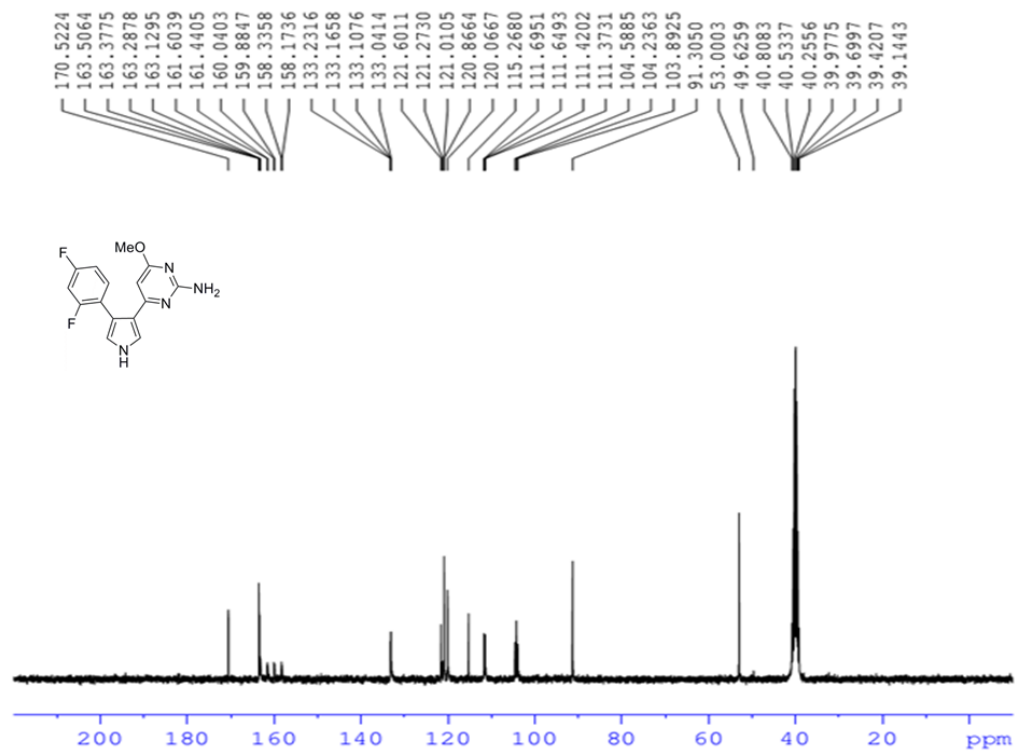


Figure S23b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8i**

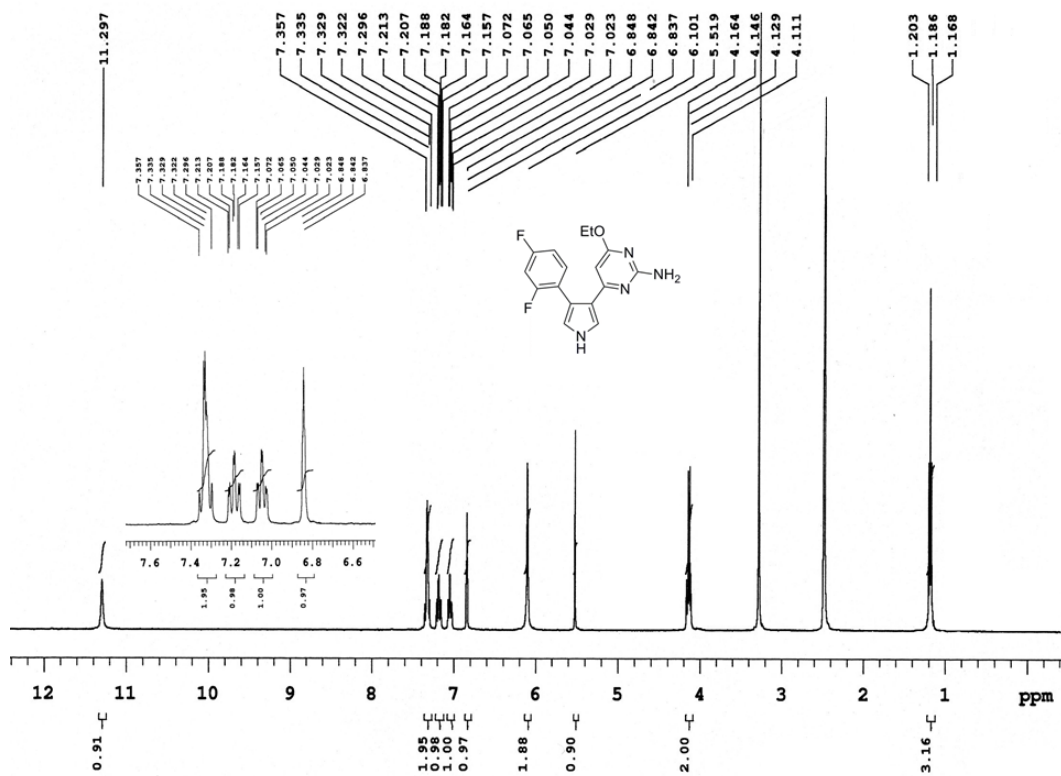


Figure S24a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8j**

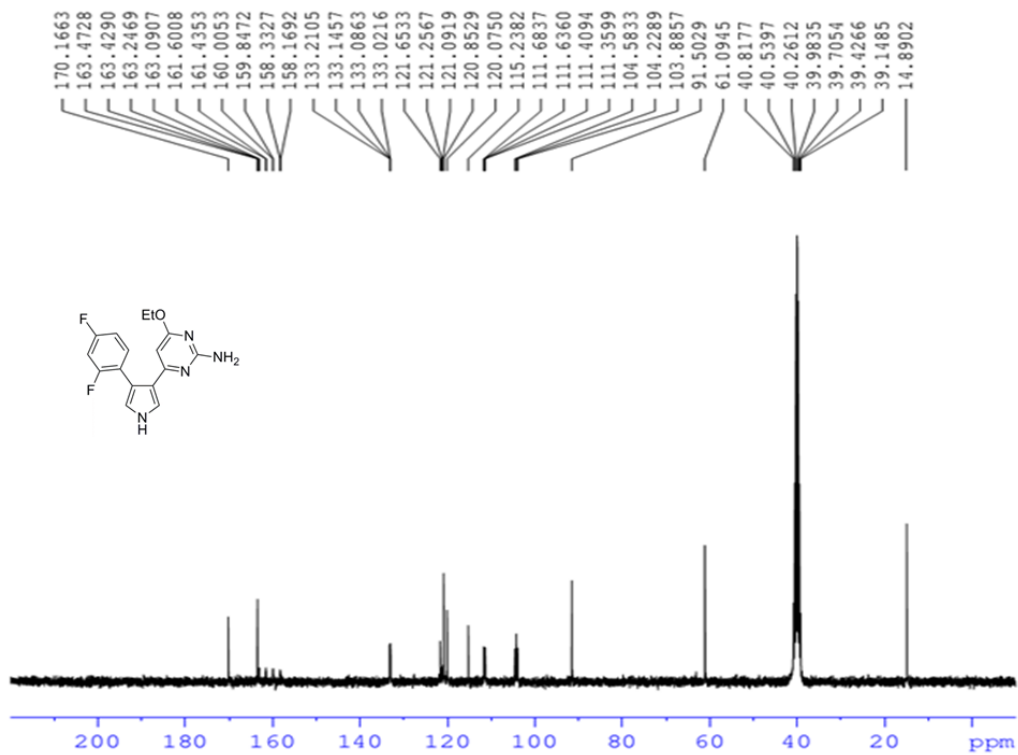


Figure S24b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8j**

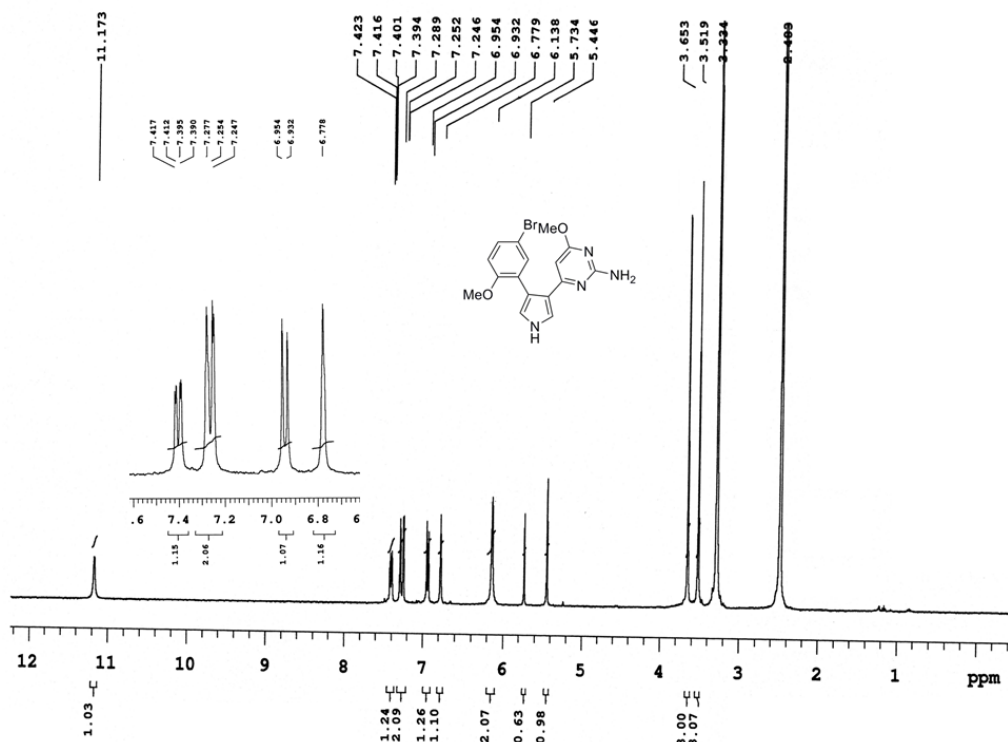


Figure S25a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8k**

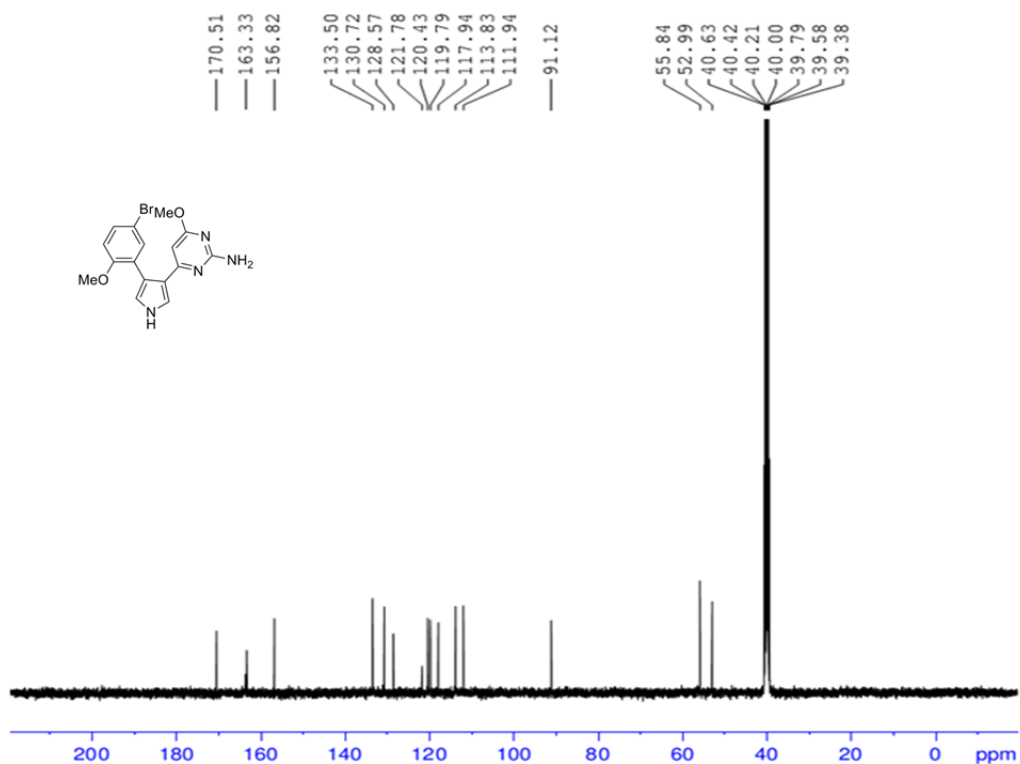
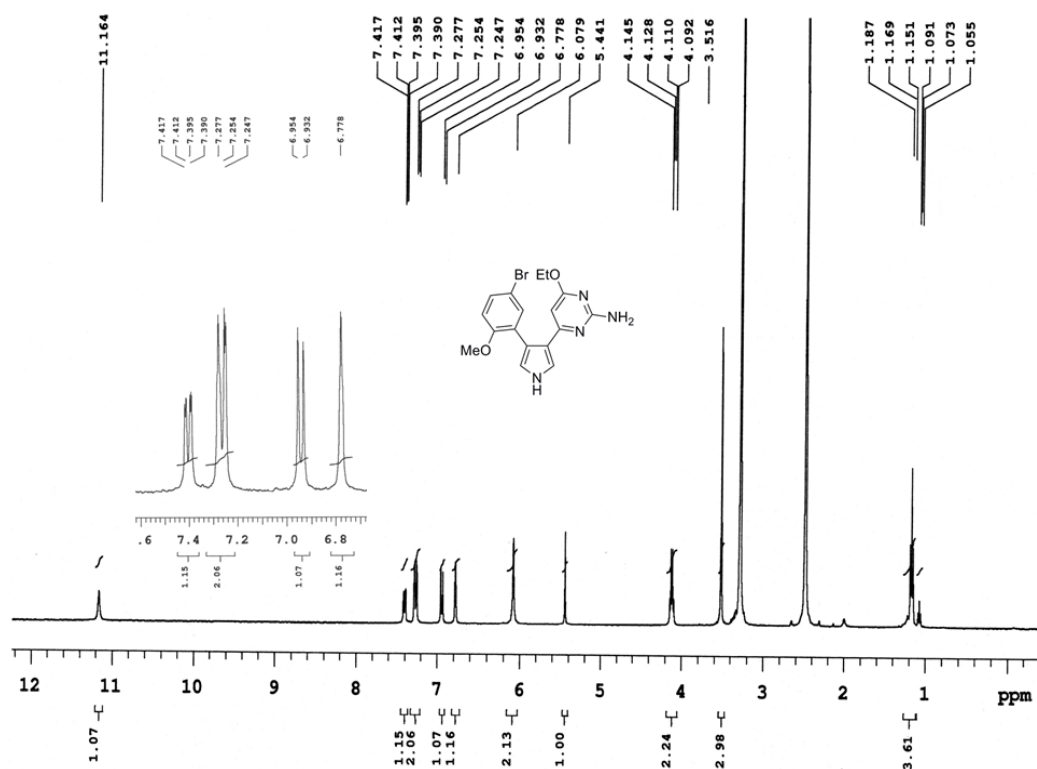
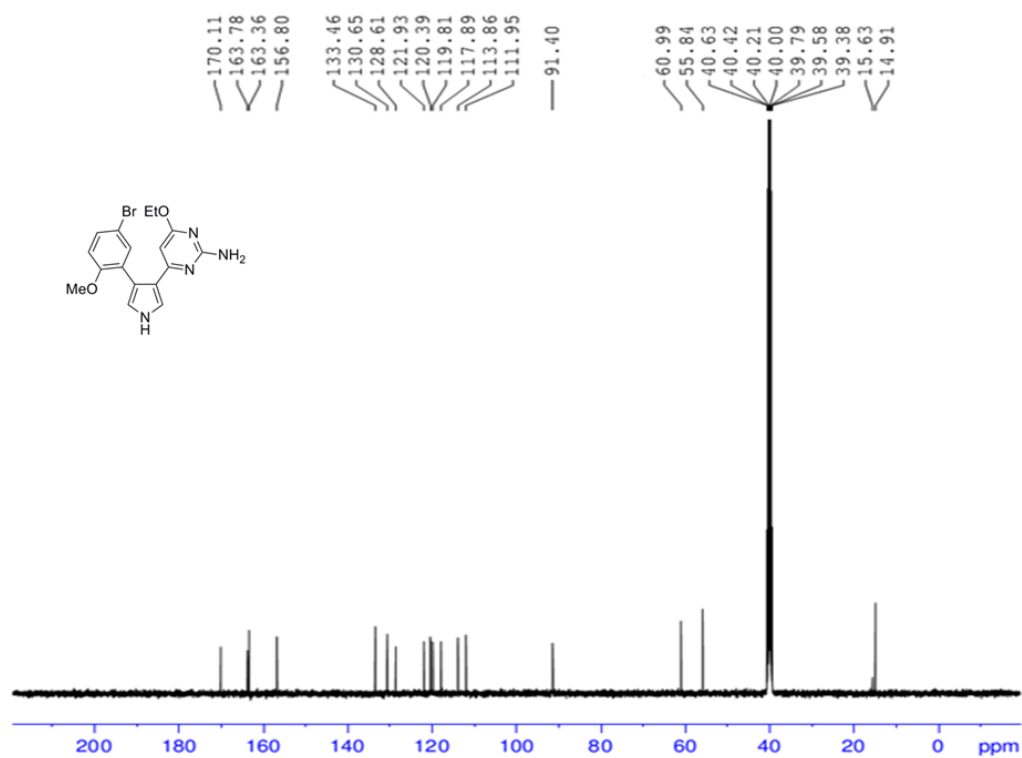


Figure S25b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8k**



**Figure S26a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8l**



**Figure S26b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8l**

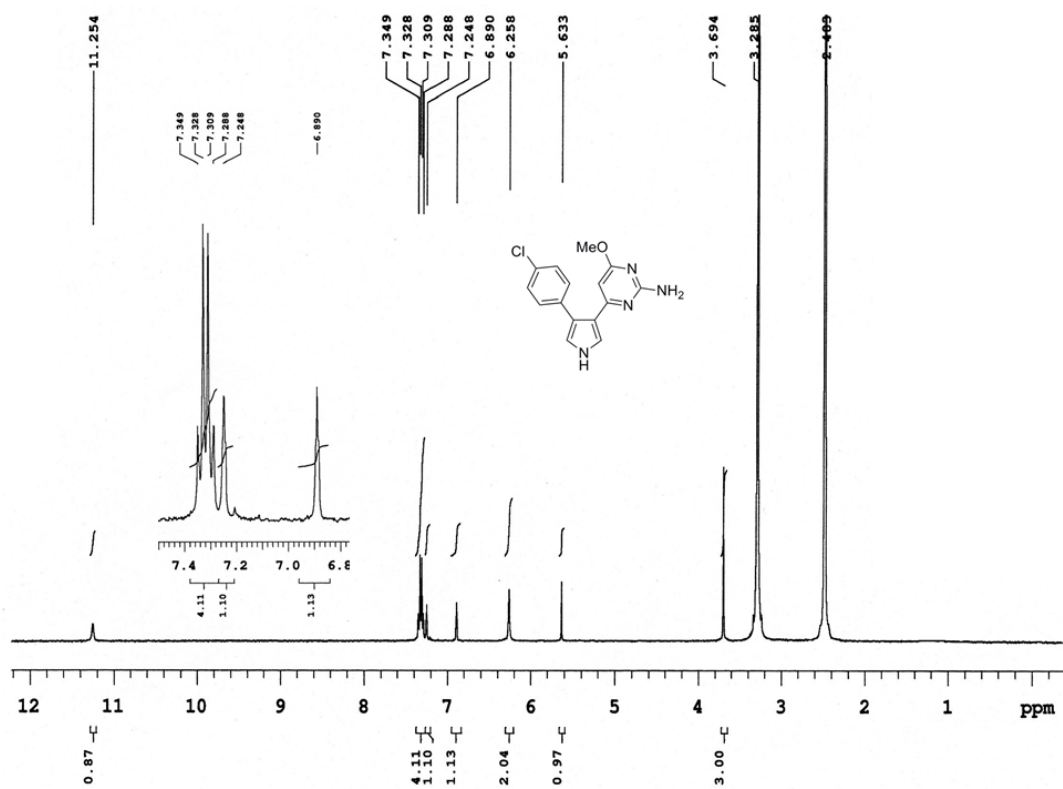


Figure S27a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8m**

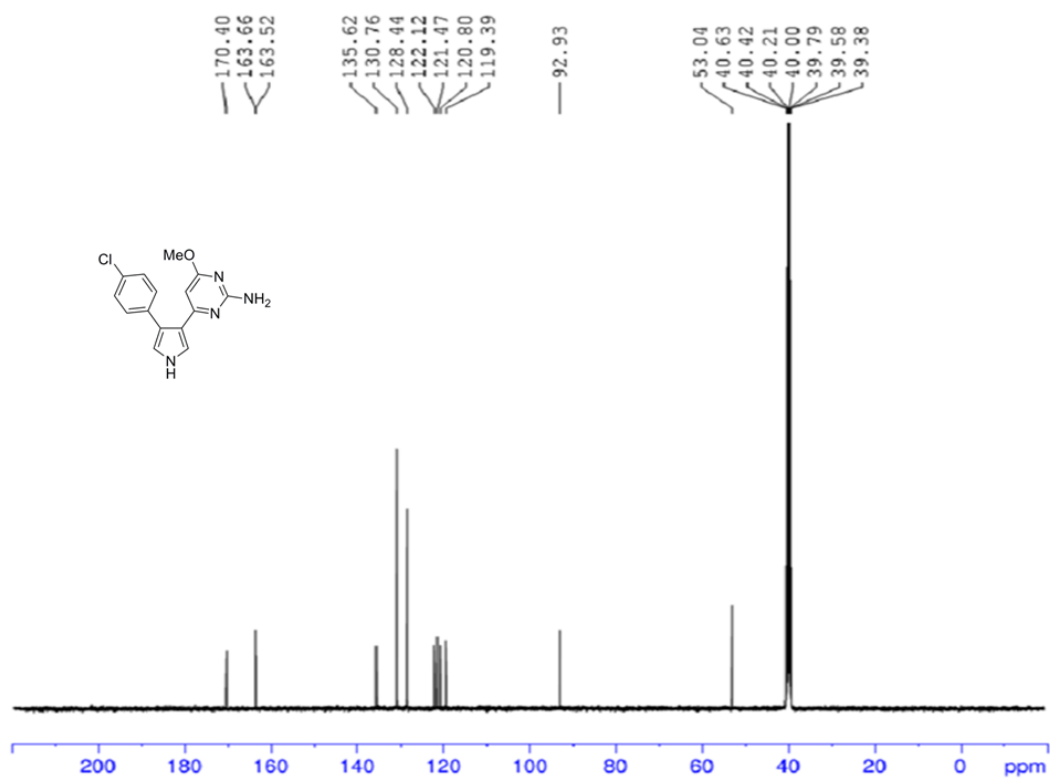


Figure S27b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8m**

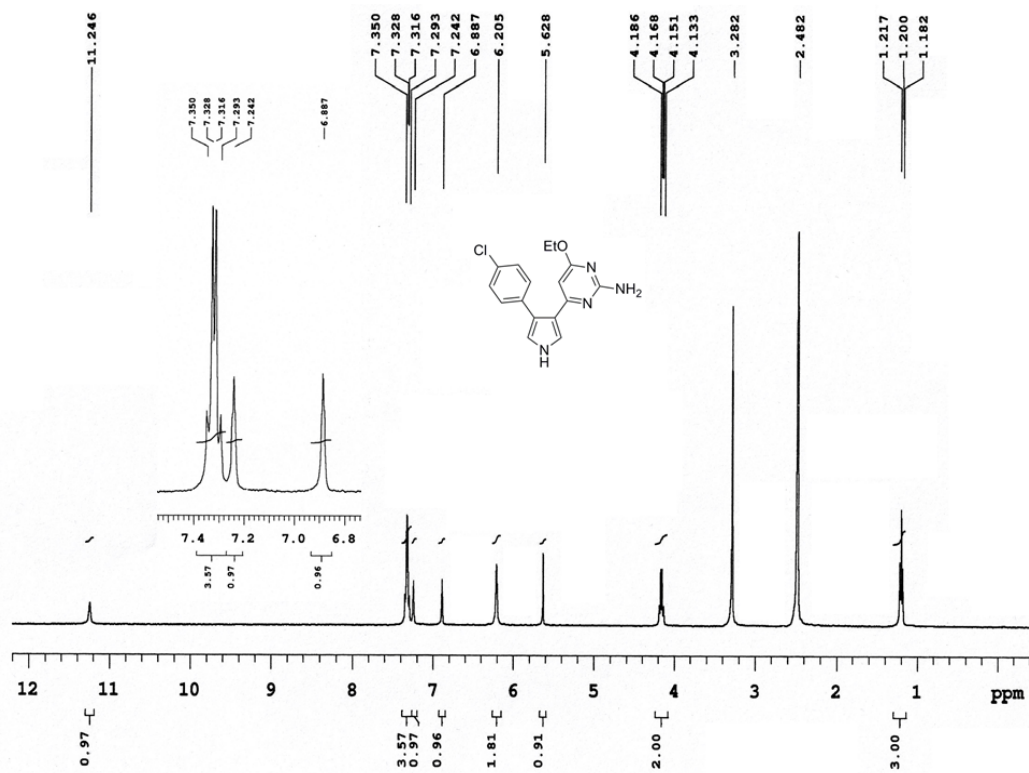


Figure S28a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 8n

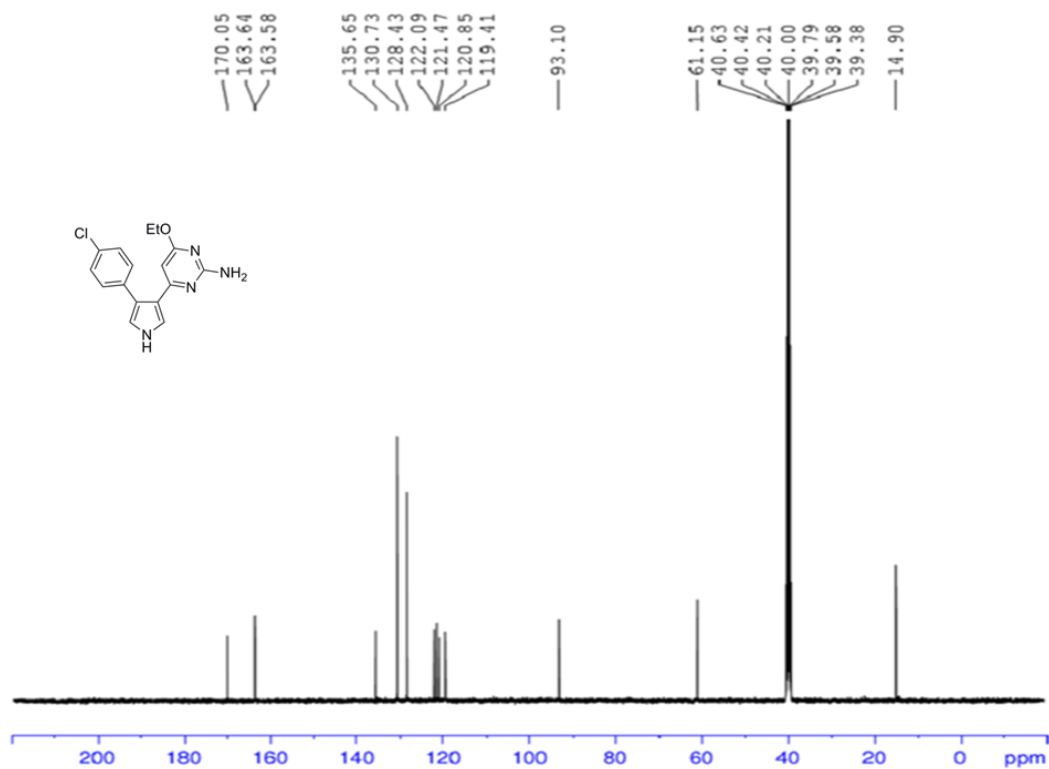
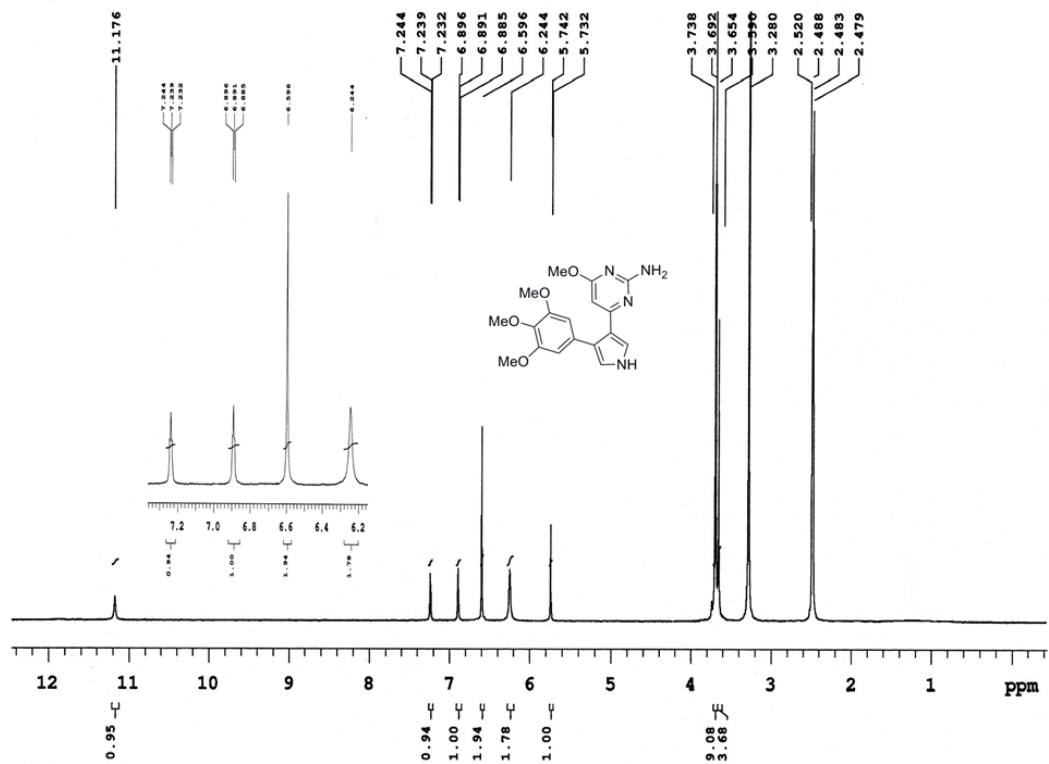
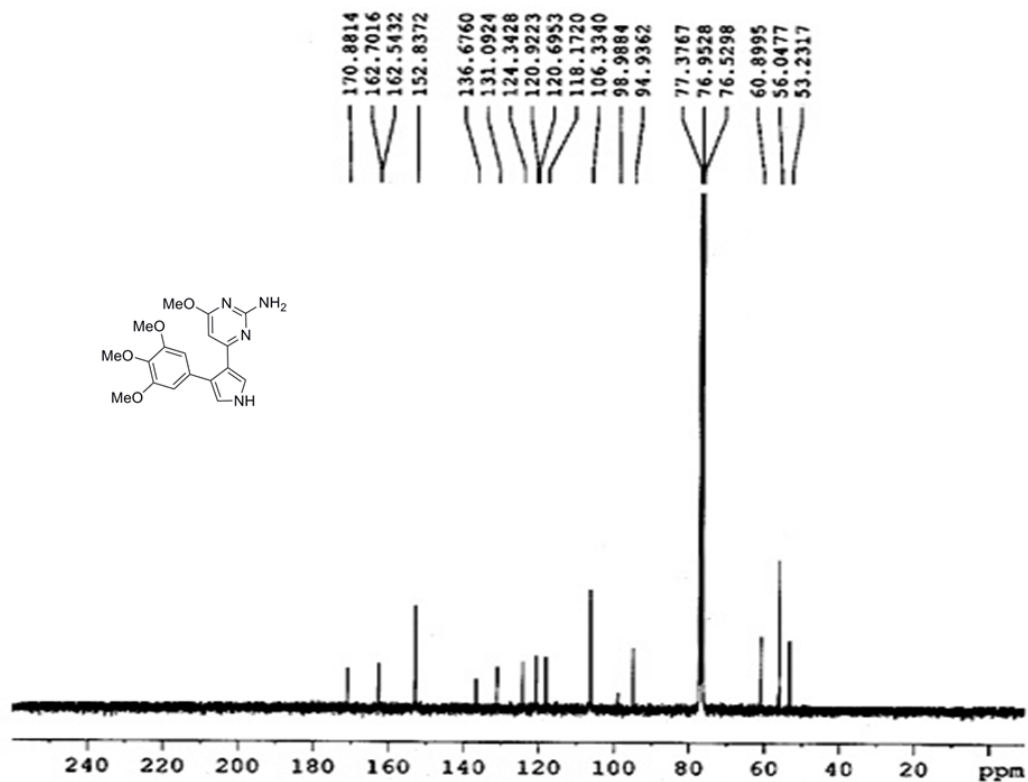


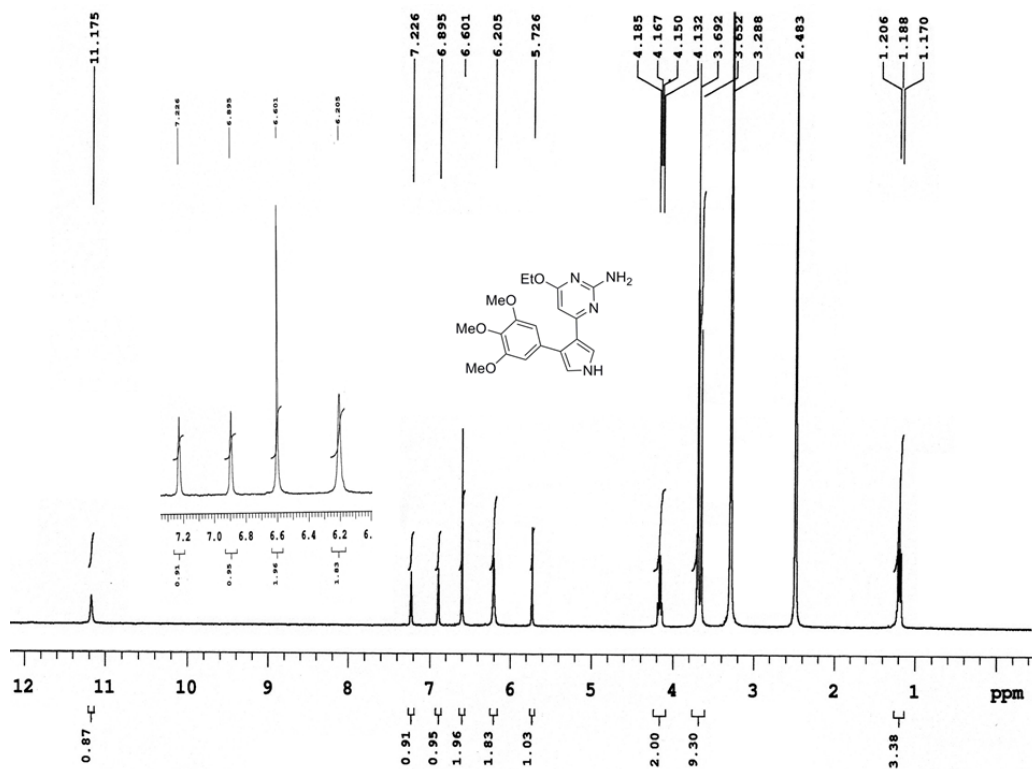
Figure S28b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 8n



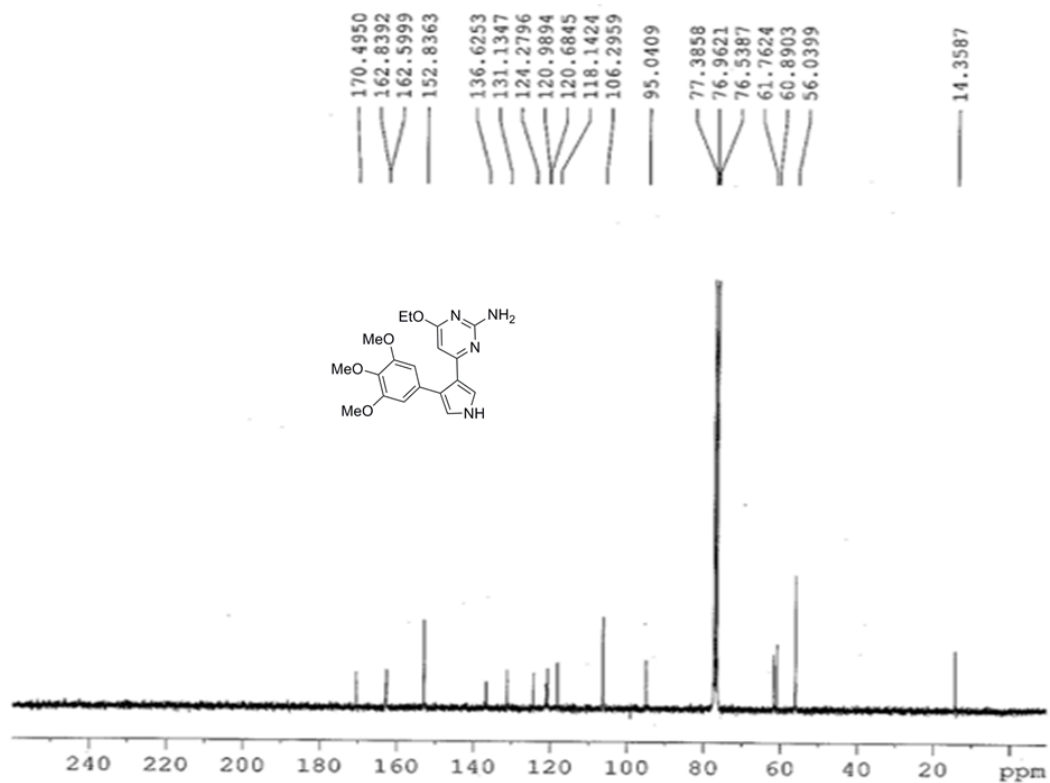
**Figure S29a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 8o**



**Figure S29b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 8o**



**Figure S30a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8p**



**Figure S30b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8p**



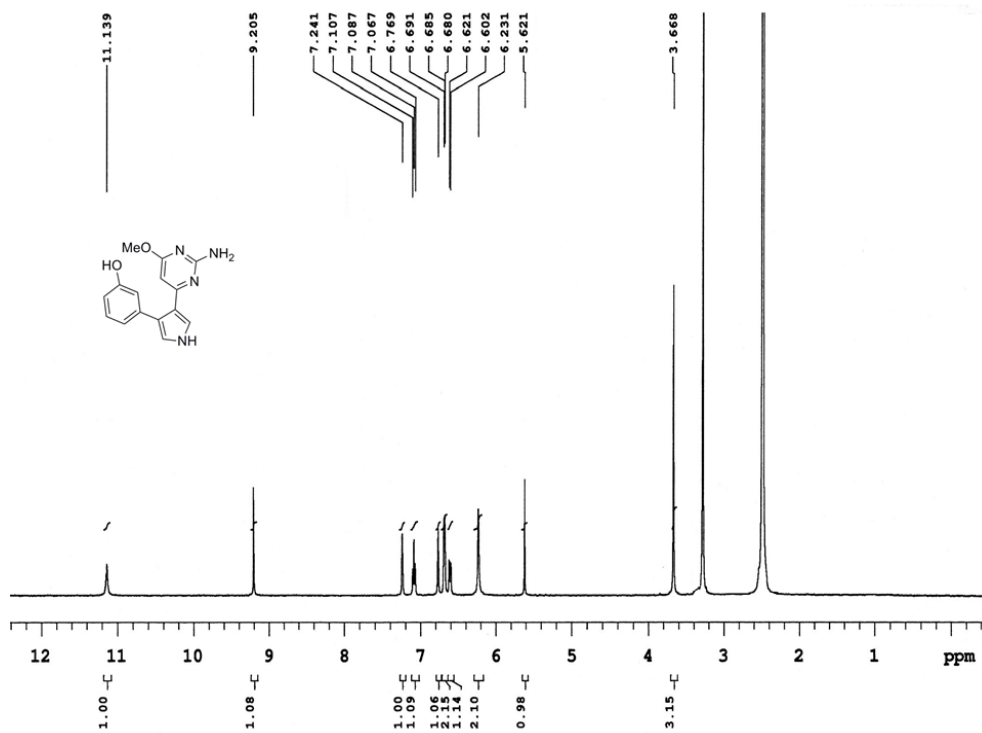


Figure S31a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8q**

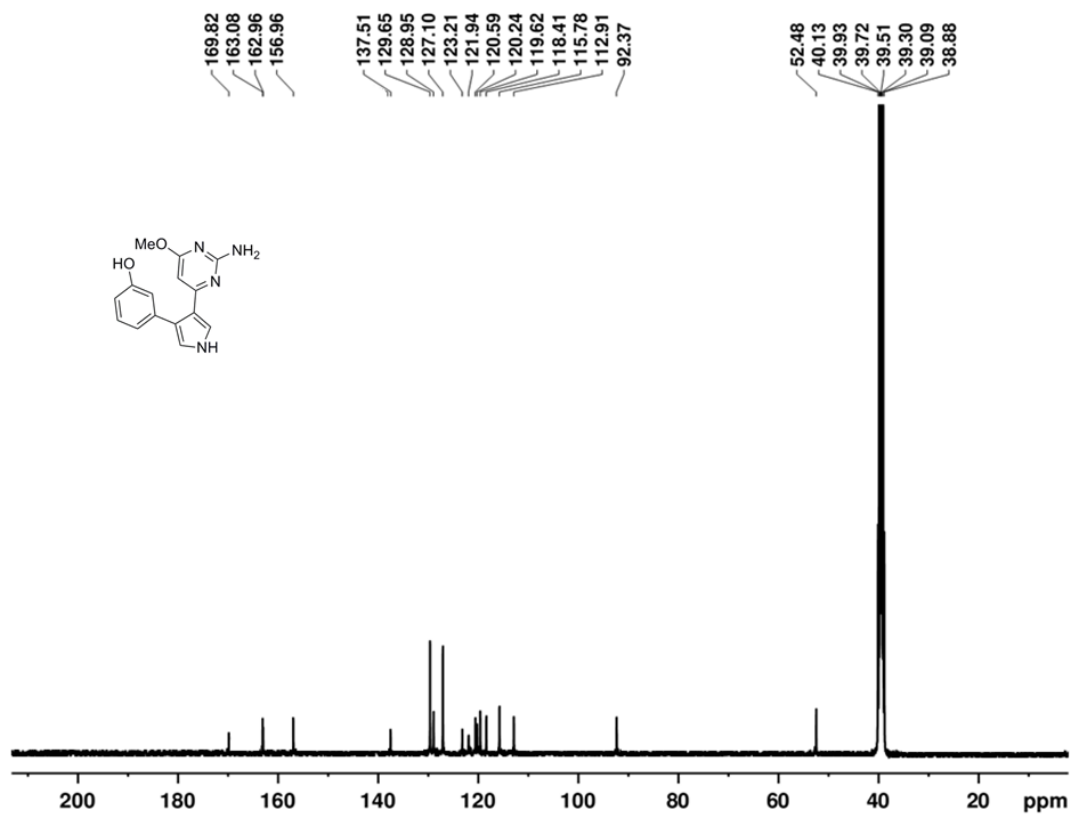


Figure S31b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8q**

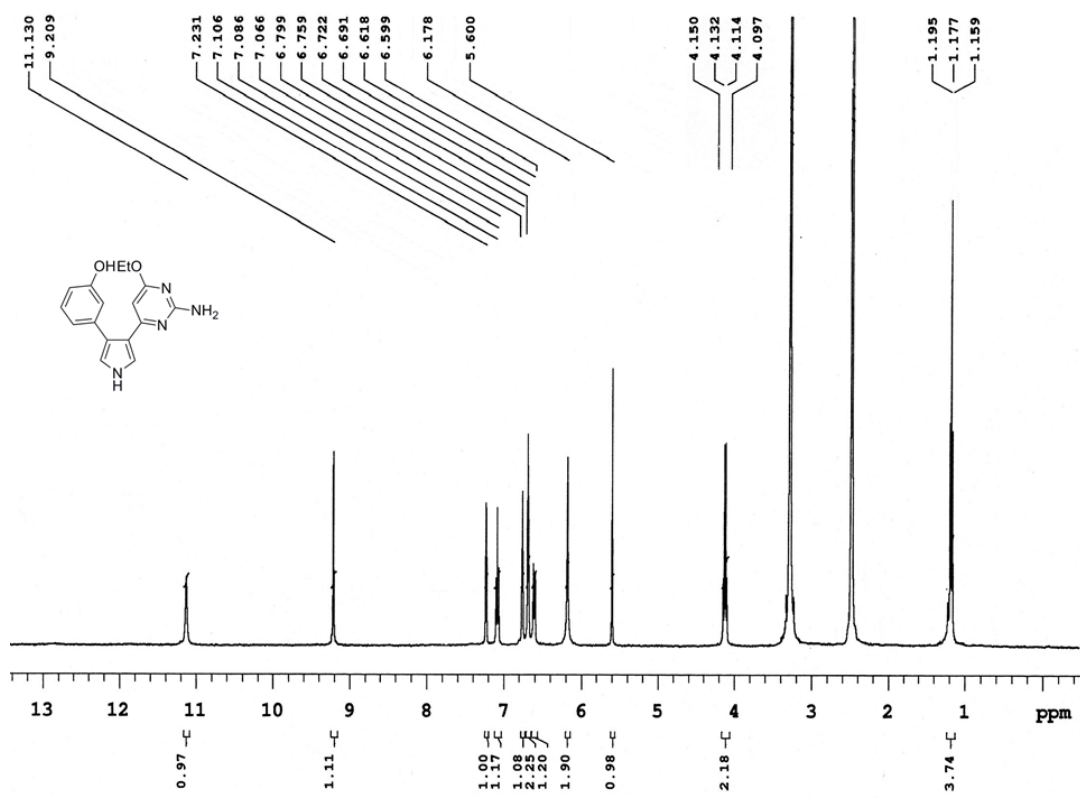


Figure S32a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8r**

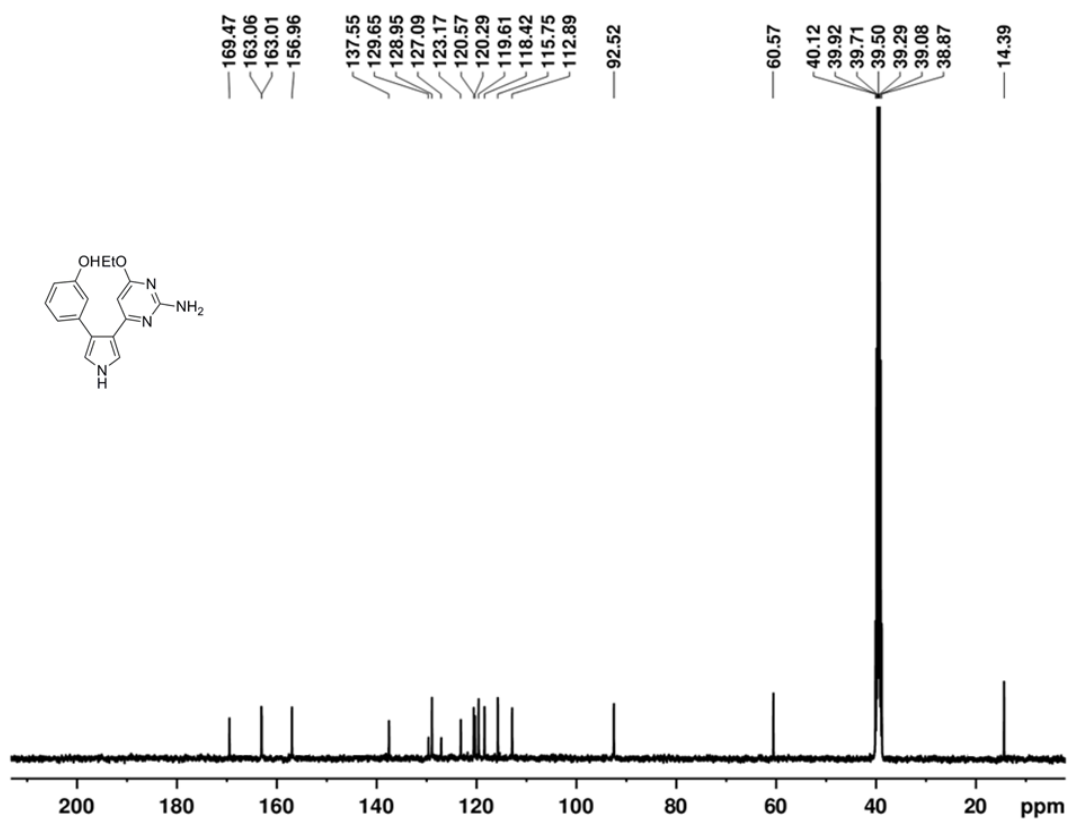


Figure S32b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8r**

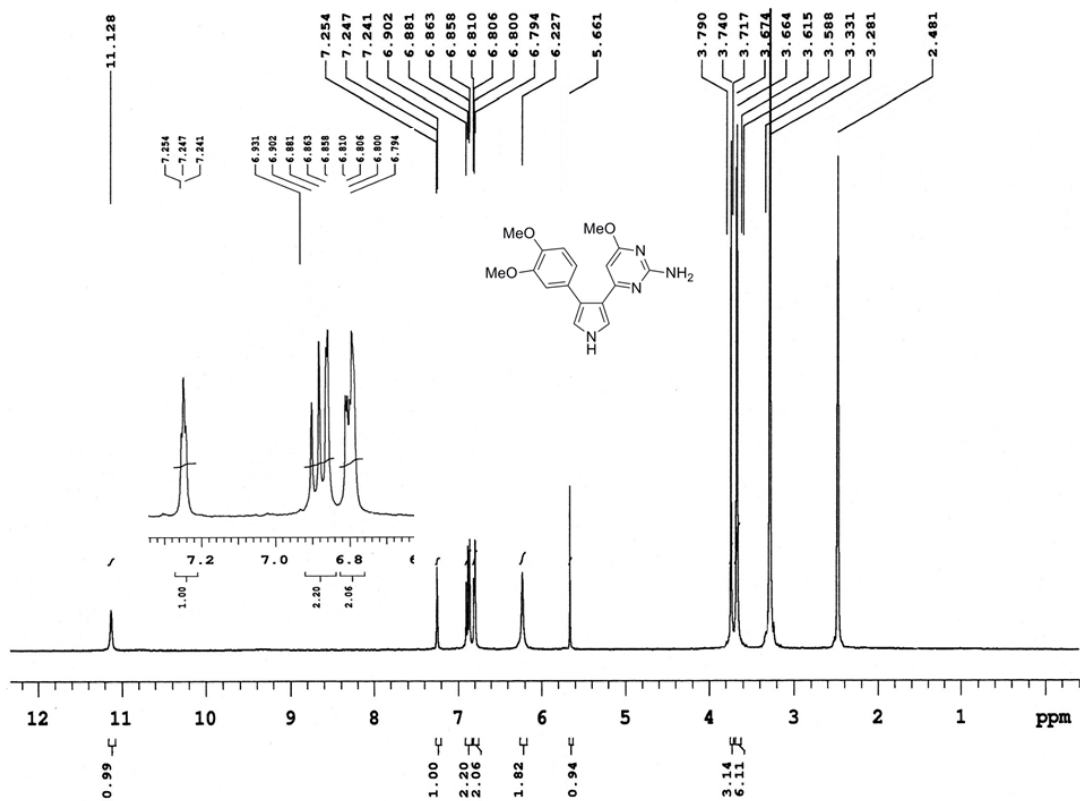


Figure S33a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8s**

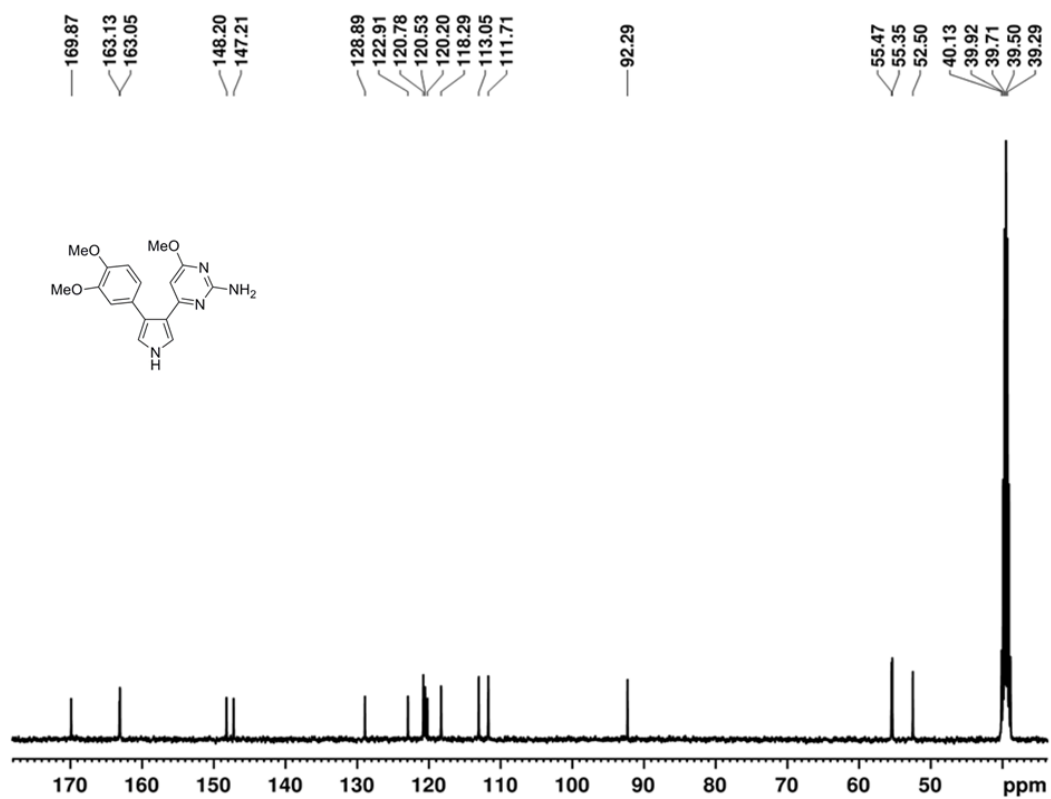


Figure S33b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8s**

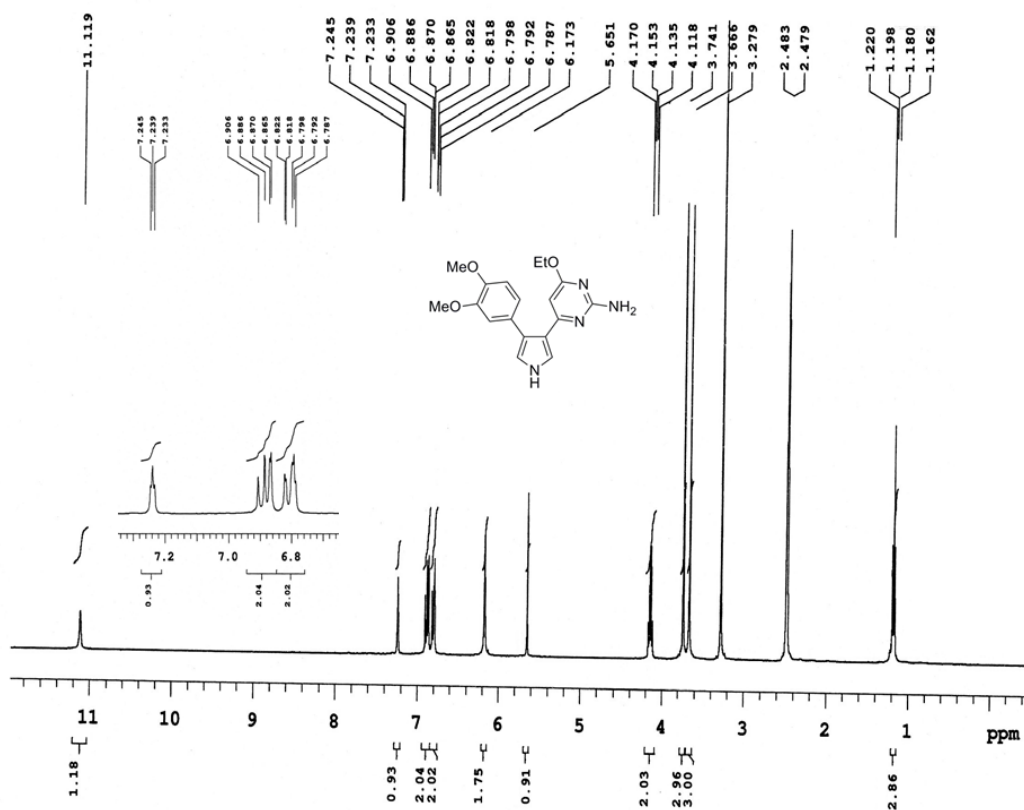


Figure S34a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8t**

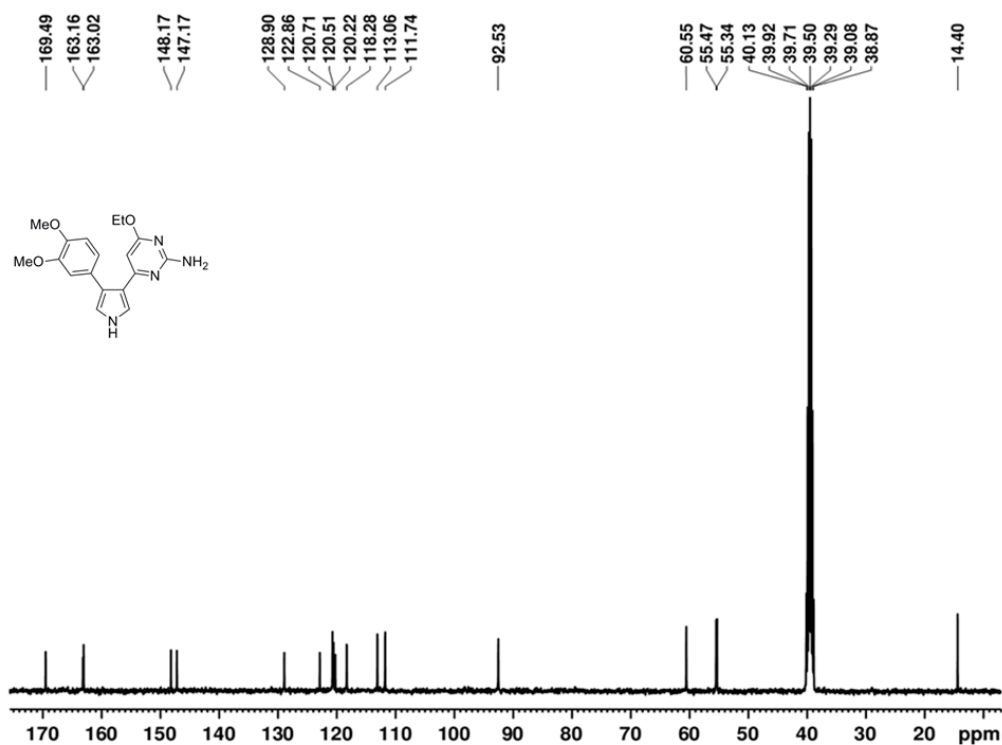


Figure: S34b (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8t**

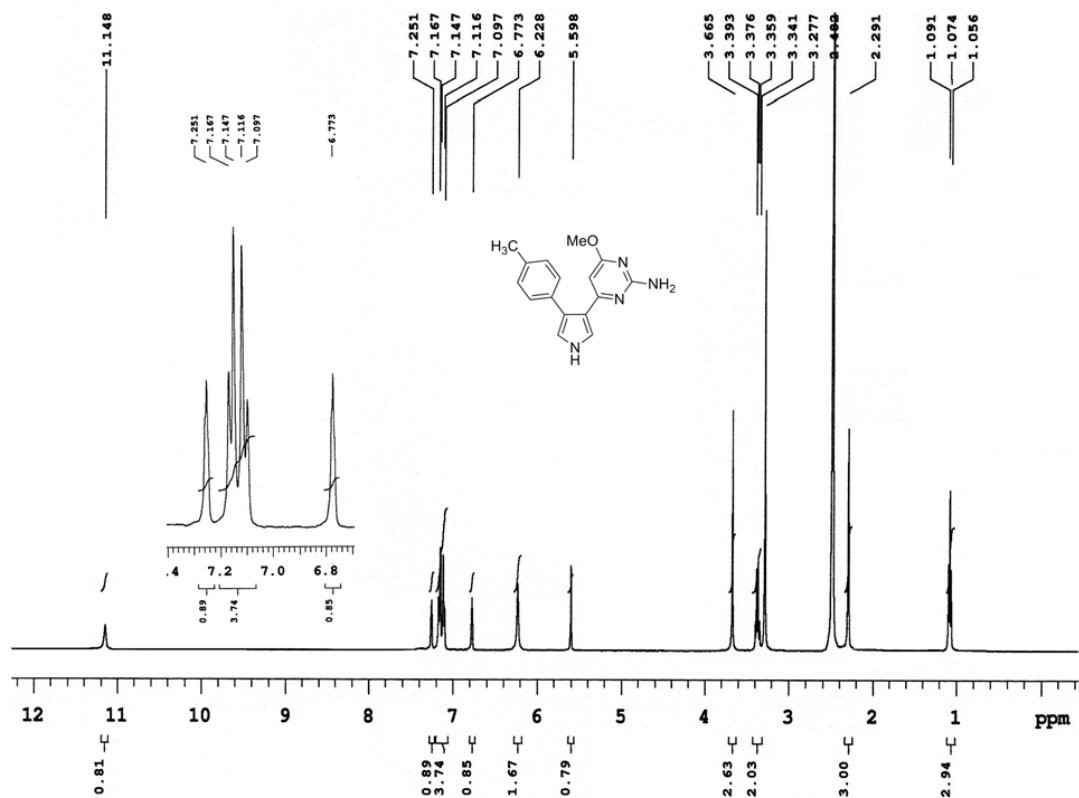


Figure S35a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8u**

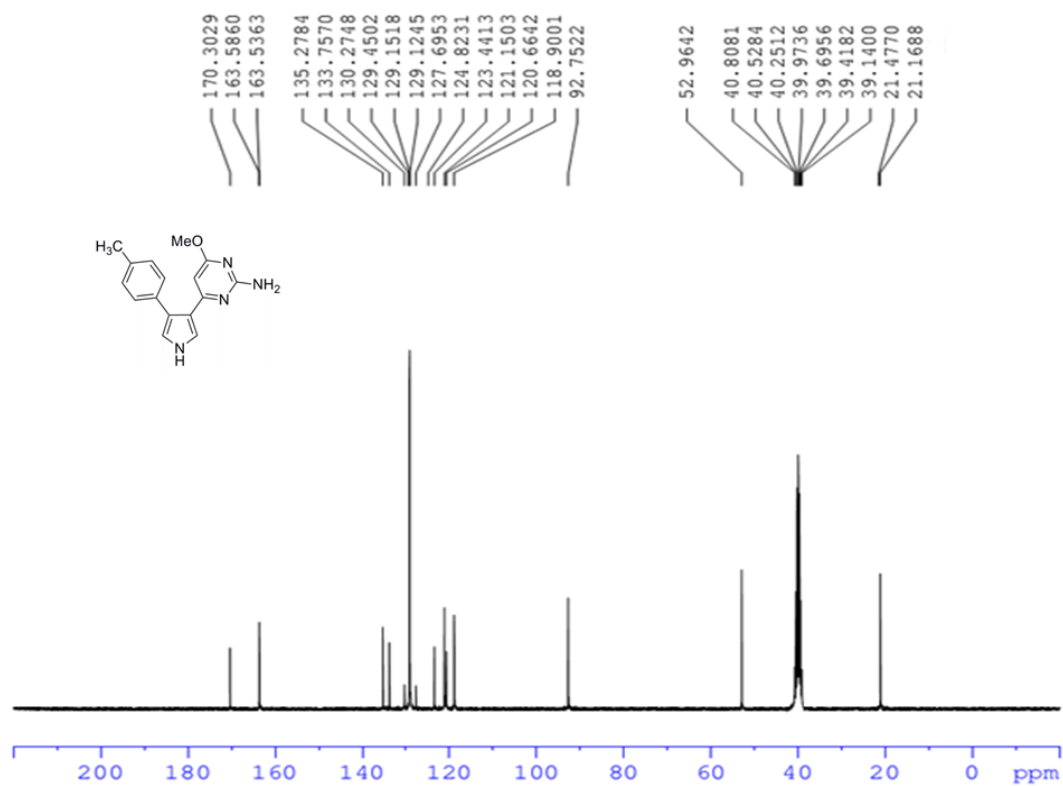


Figure S35b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8u**

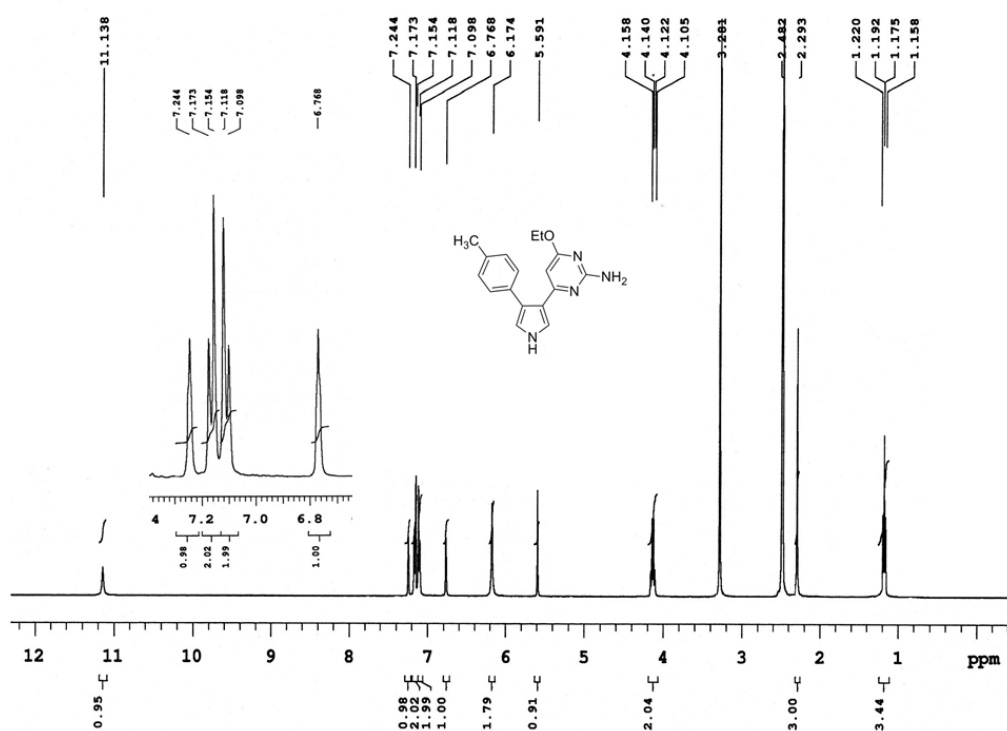


Figure S36a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8v**

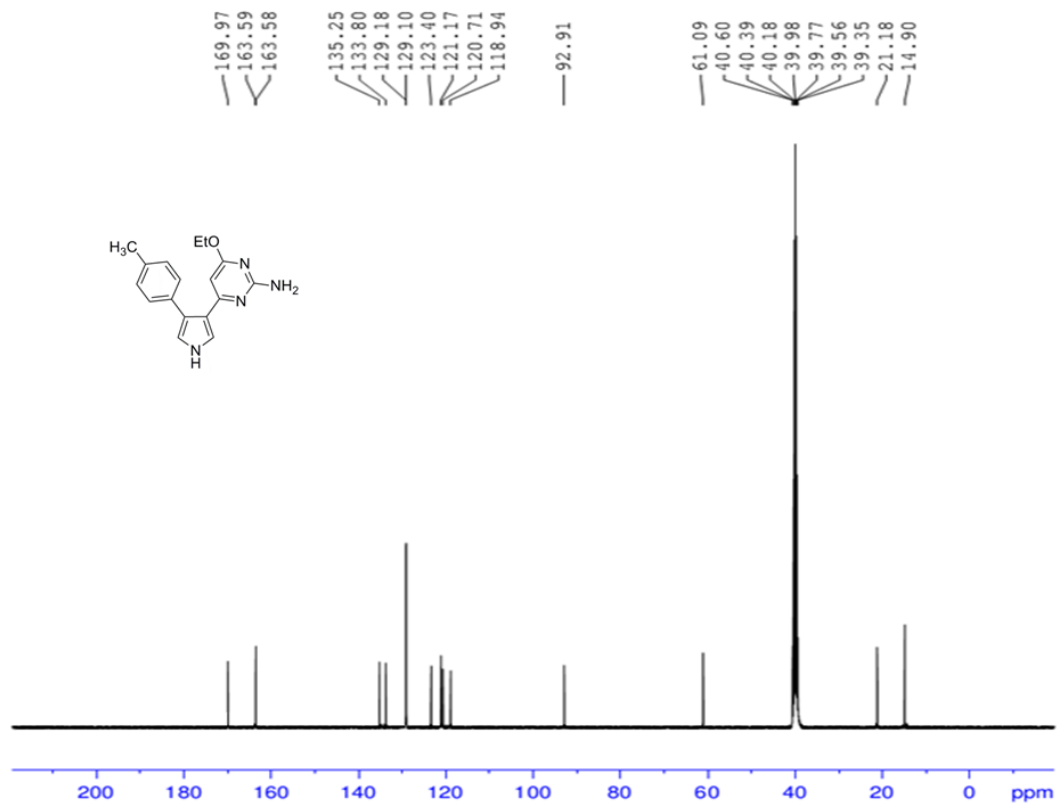
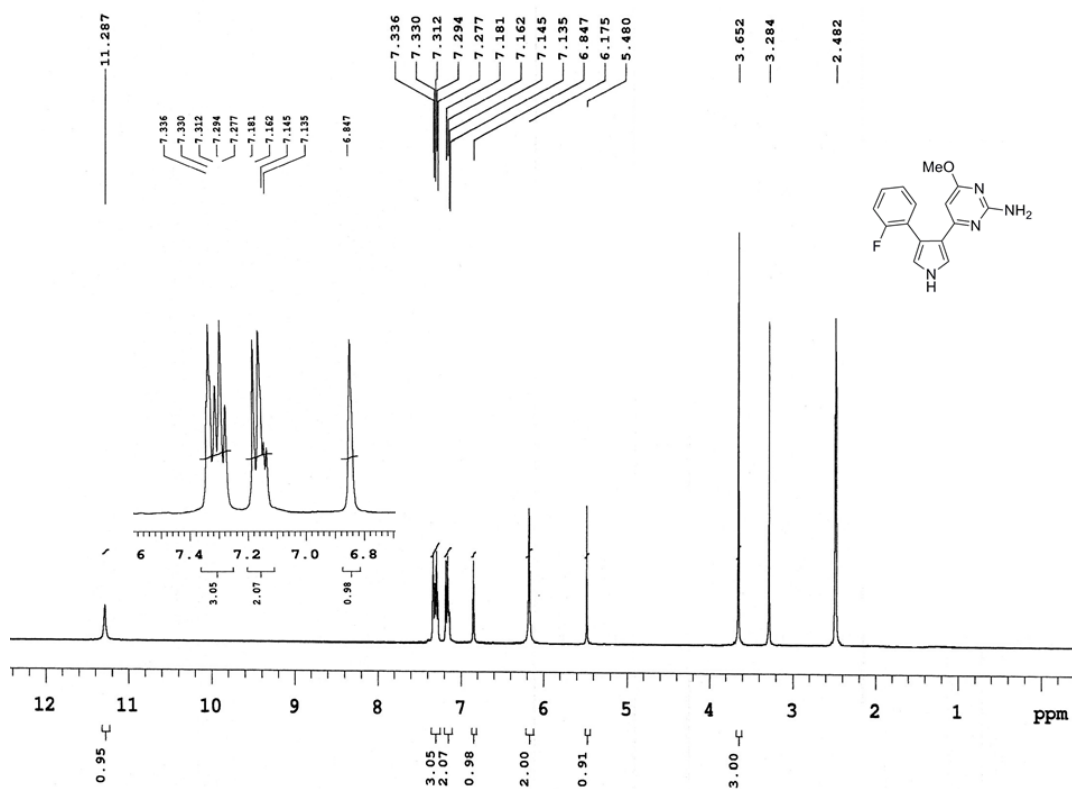
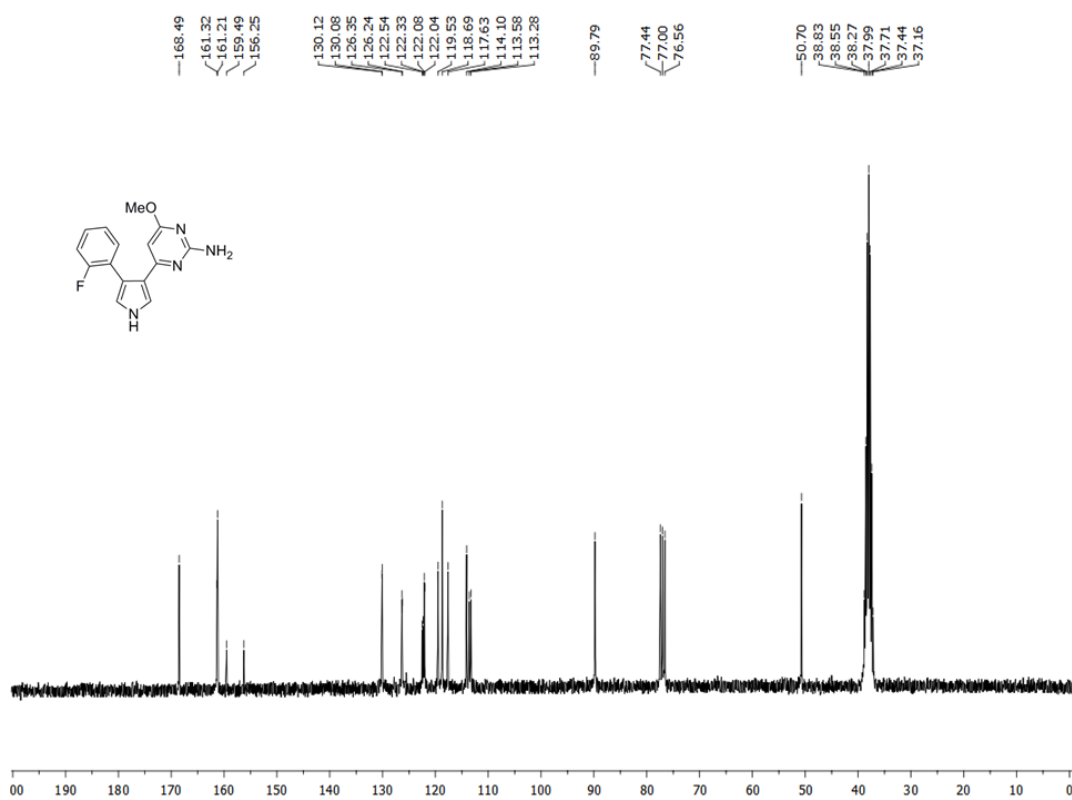


Figure S36b: (75MHz, CDCl<sub>3</sub>) <sup>13</sup>C NMR spectrum of compound **8v**



**Figure S37a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8w**



**Figure S37b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8w**

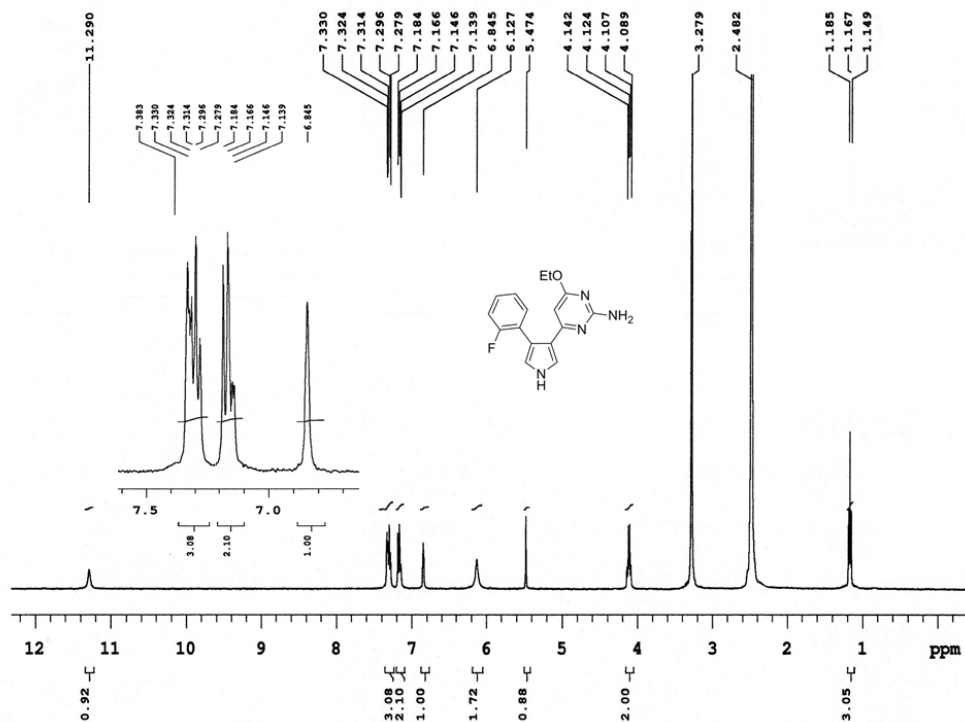


Figure S38a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8x**

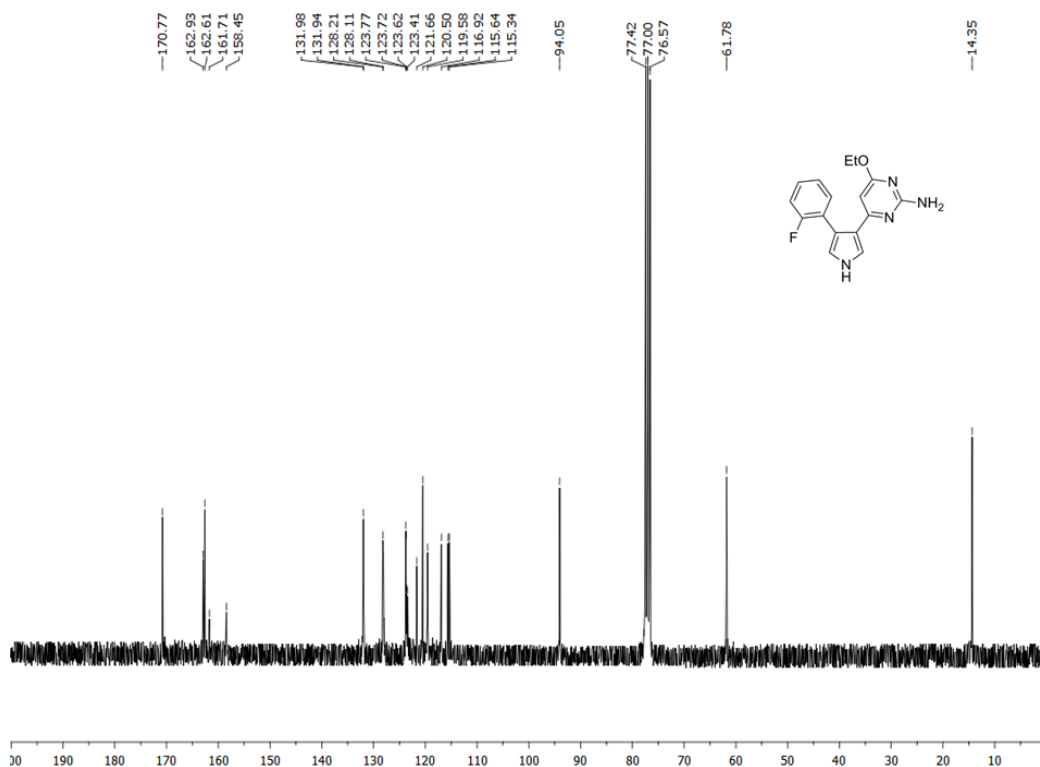


Figure S38b: (75MHz, CDCl<sub>3</sub>) <sup>13</sup>C NMR spectrum of compound **8x**



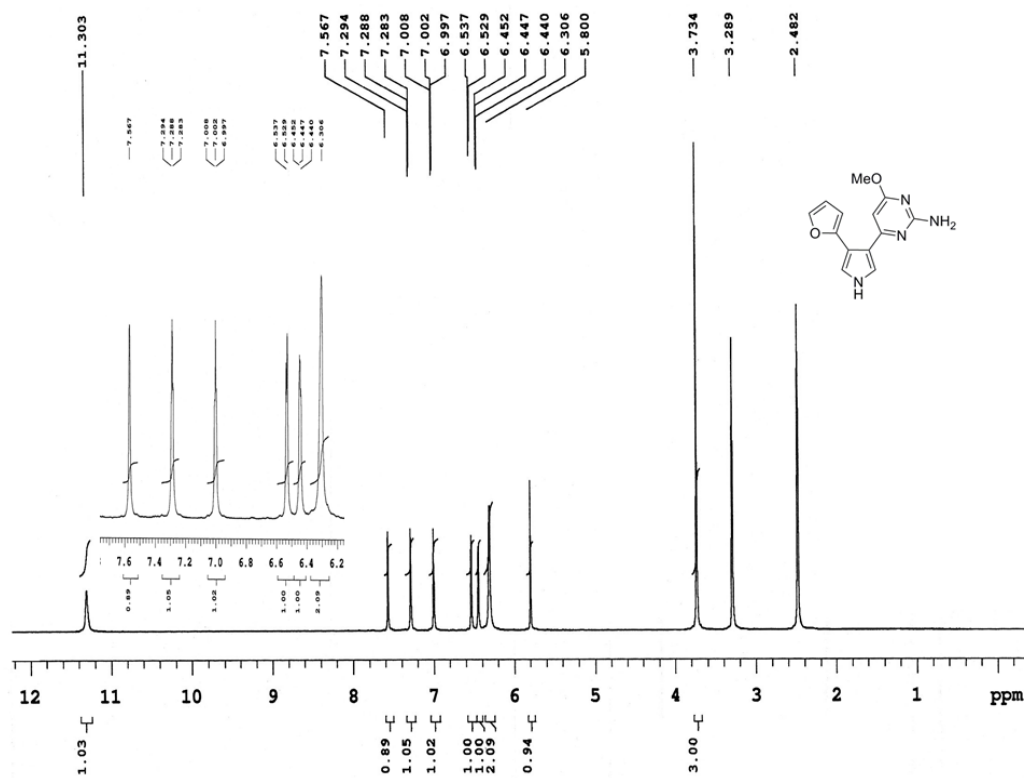


Figure S39a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 8y

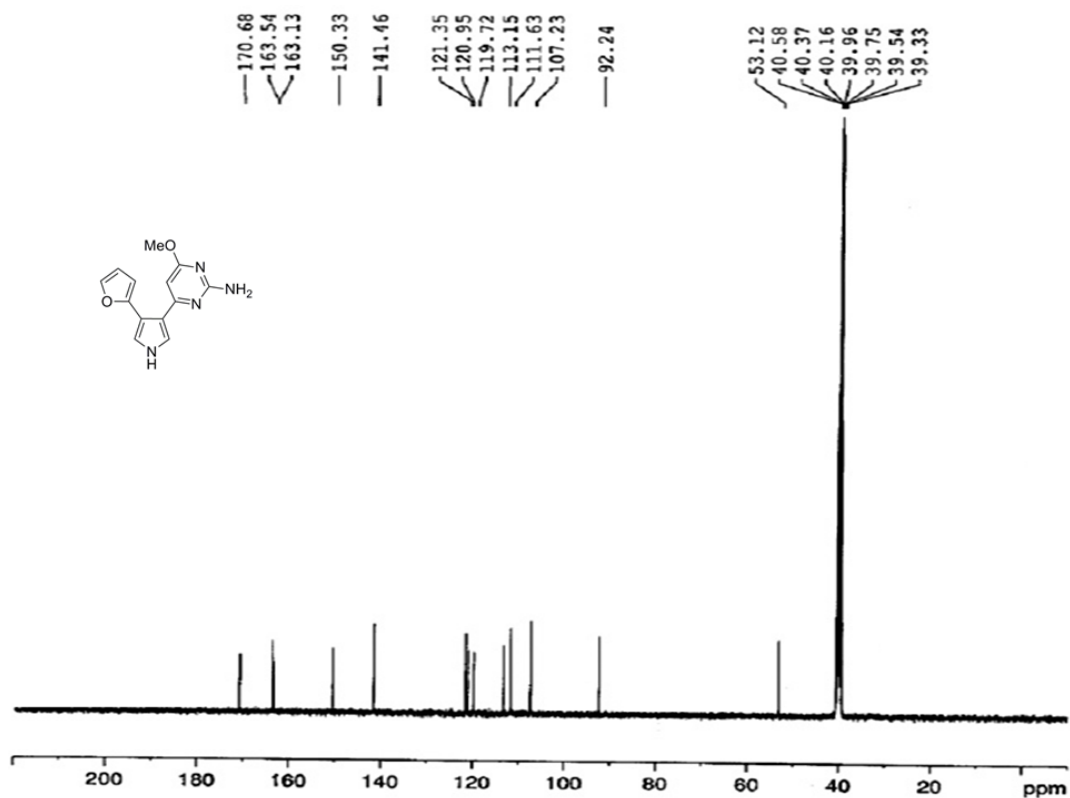
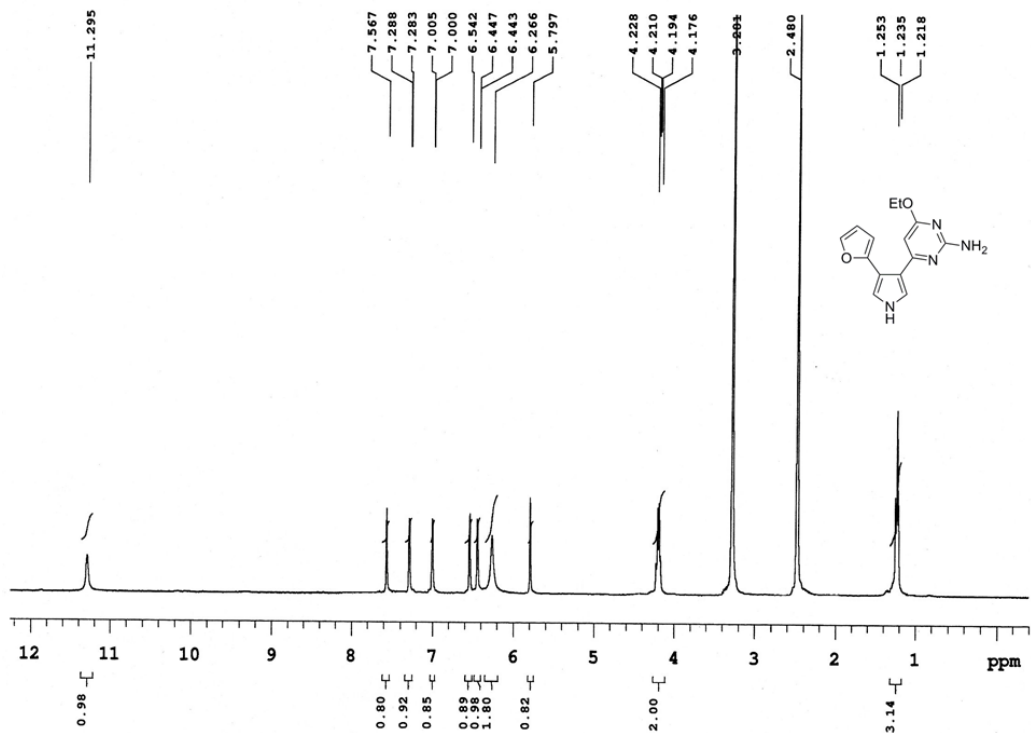
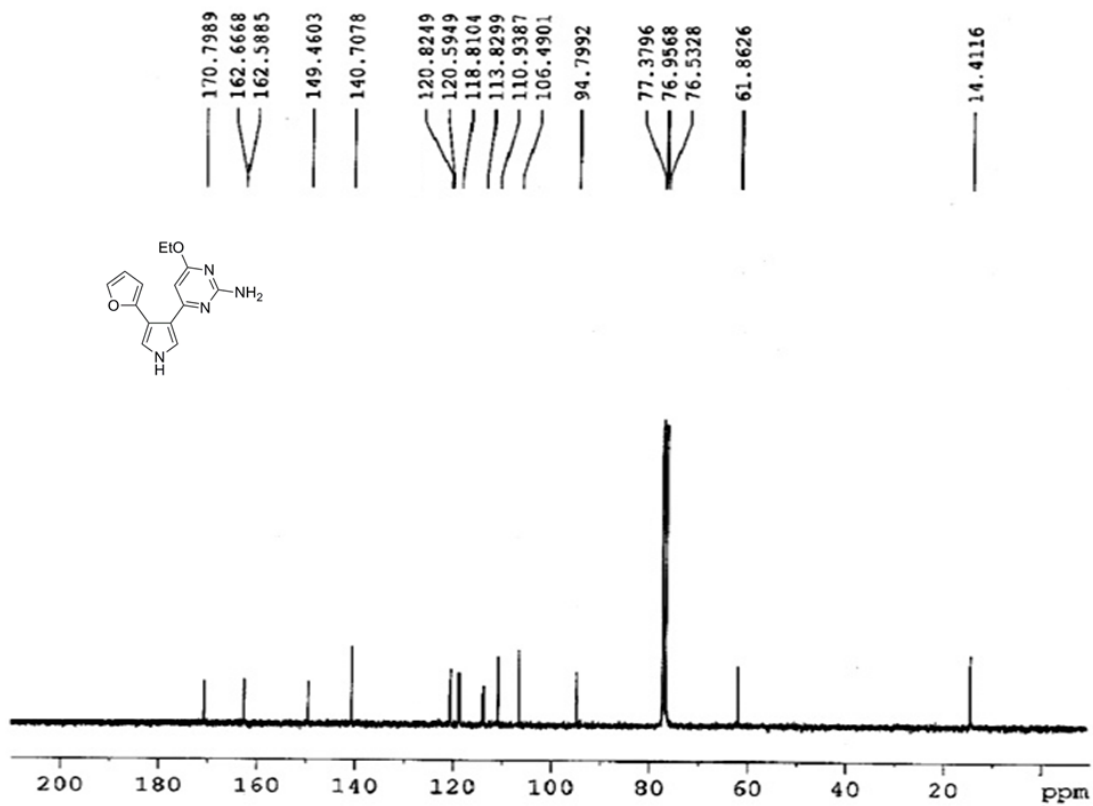


Figure S39b: (100MHz, CDCl<sub>3</sub>) <sup>13</sup>C NMR spectrum of compound 8y



**Figure S40a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8z**



**Figure S40b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8z**

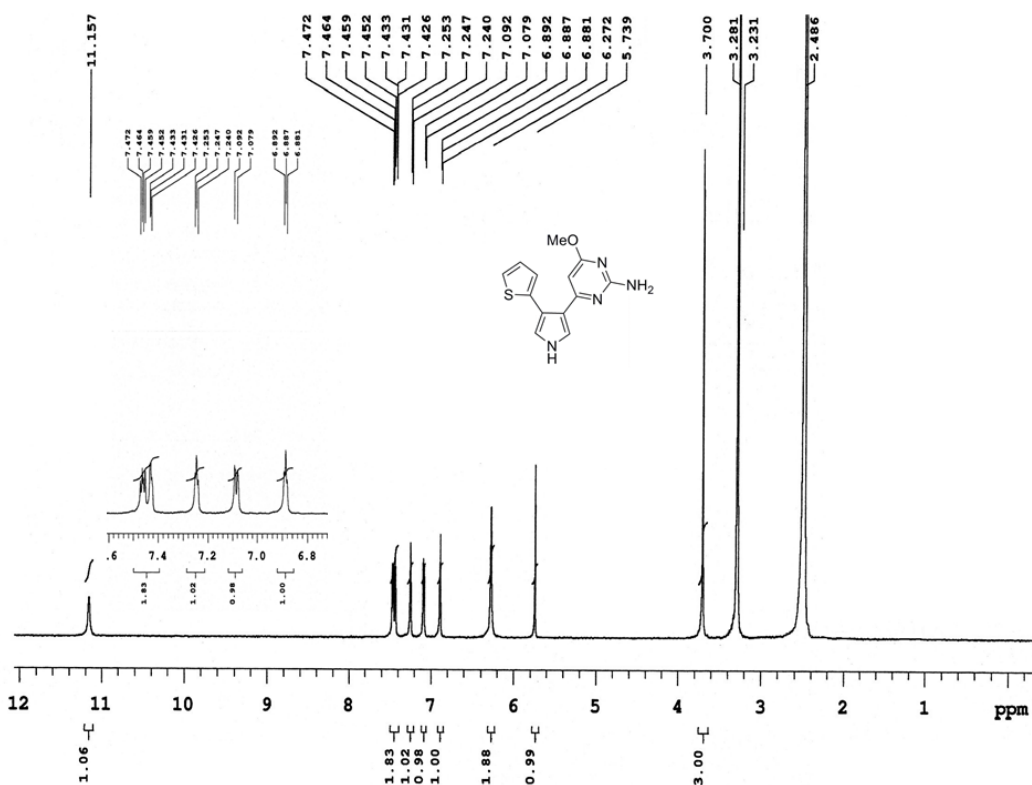


Figure S41a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8aa**

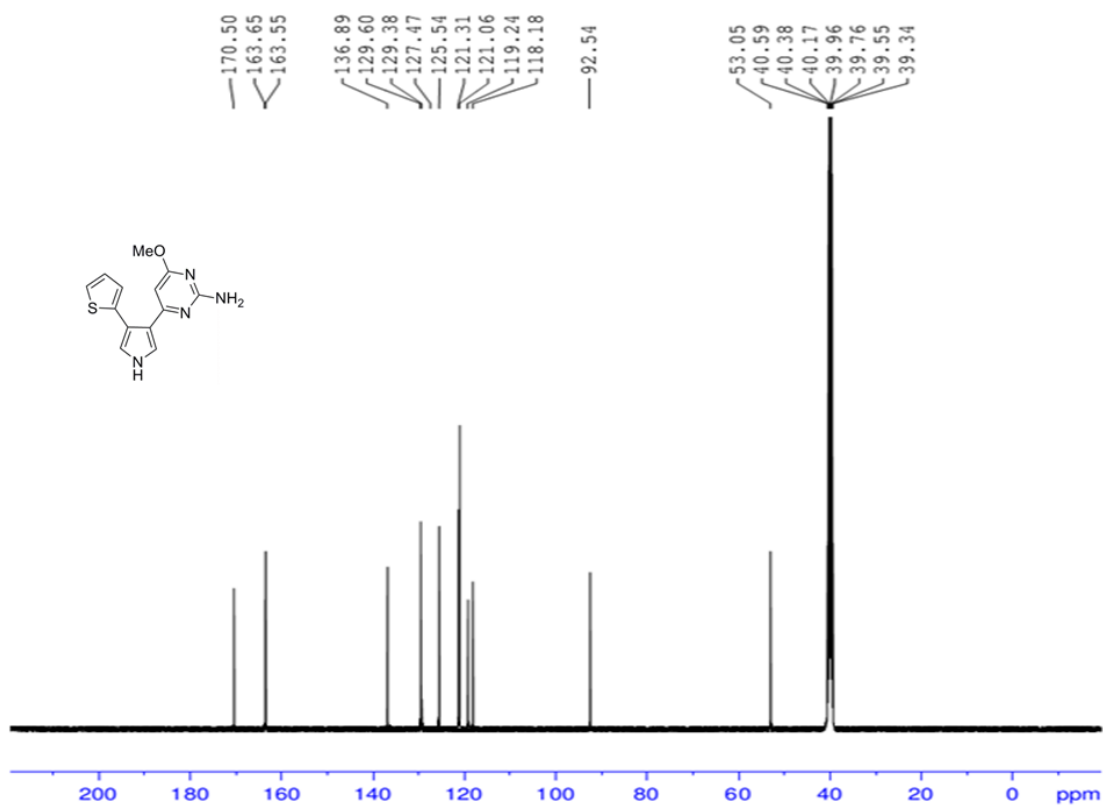


Figure S41b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8aa**

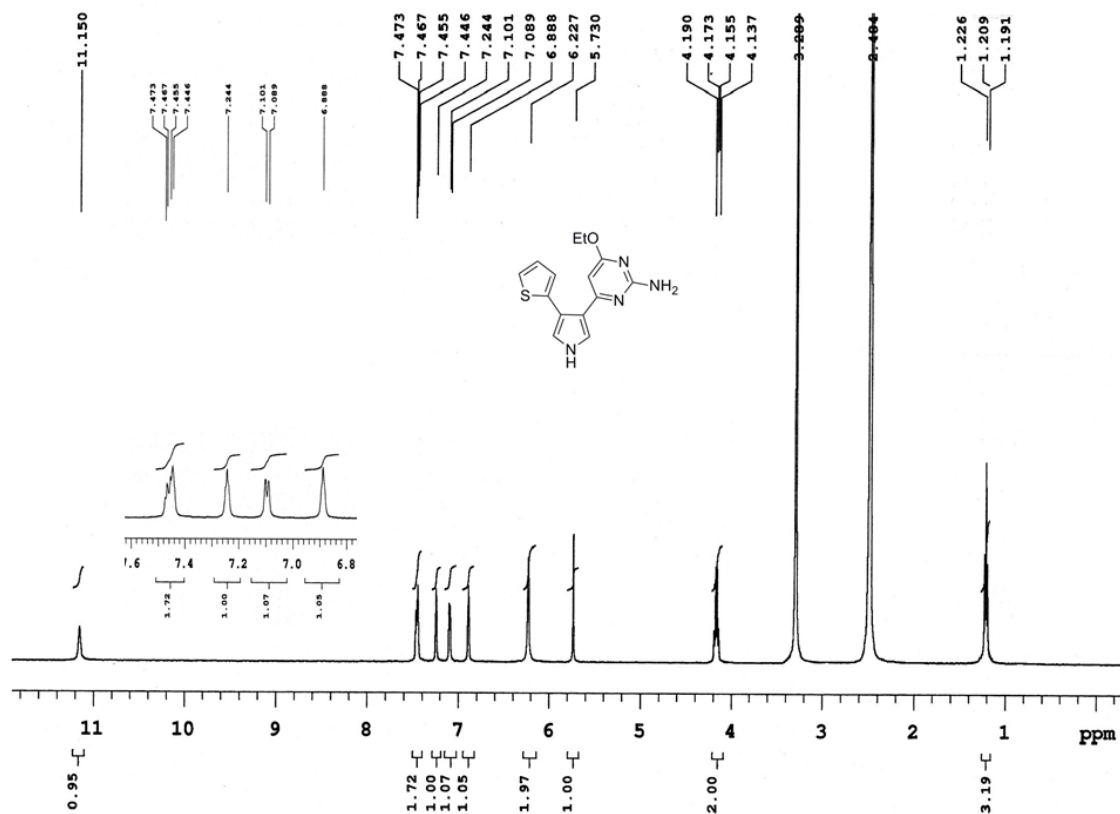


Figure S42a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8ab**

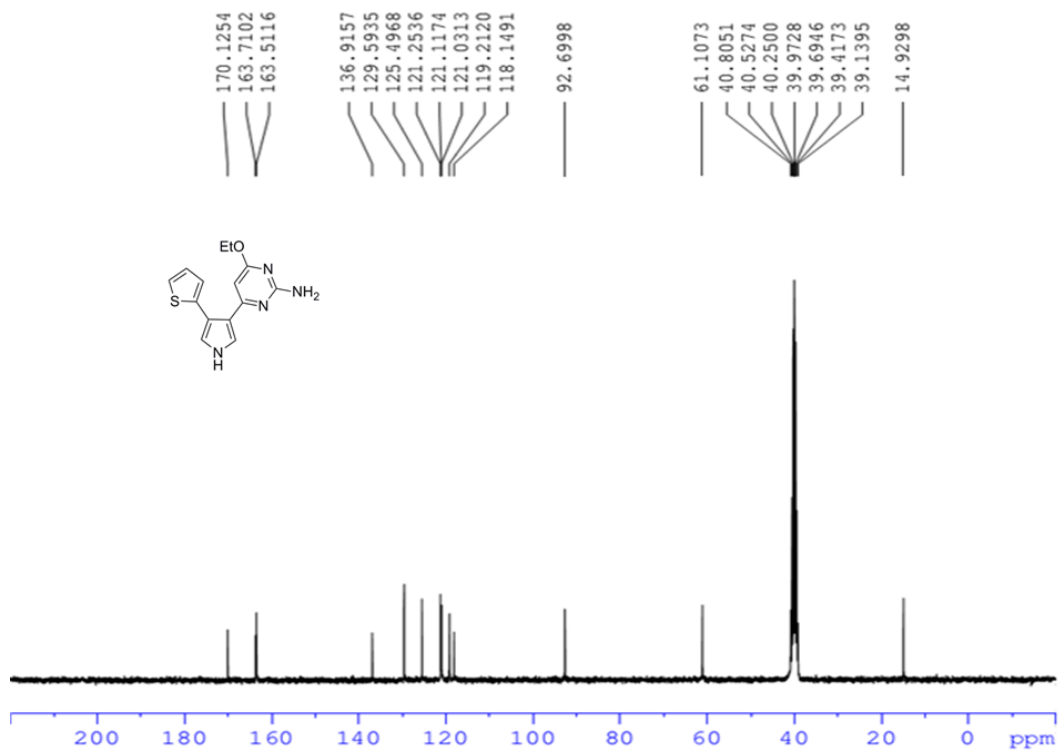
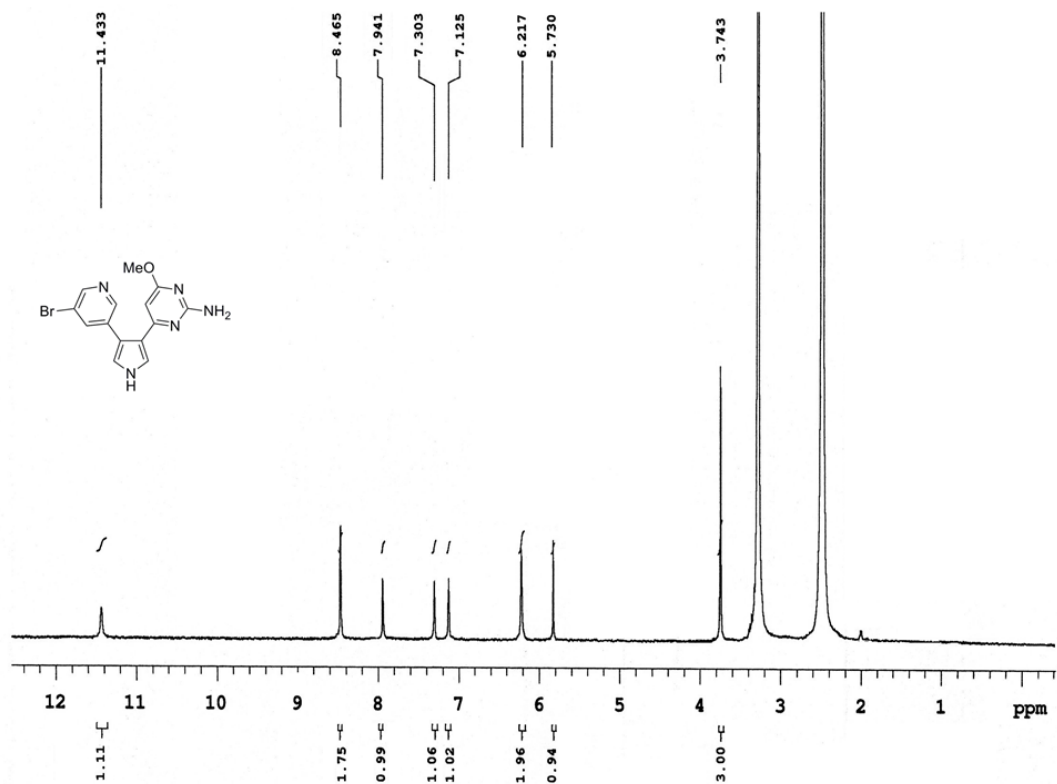
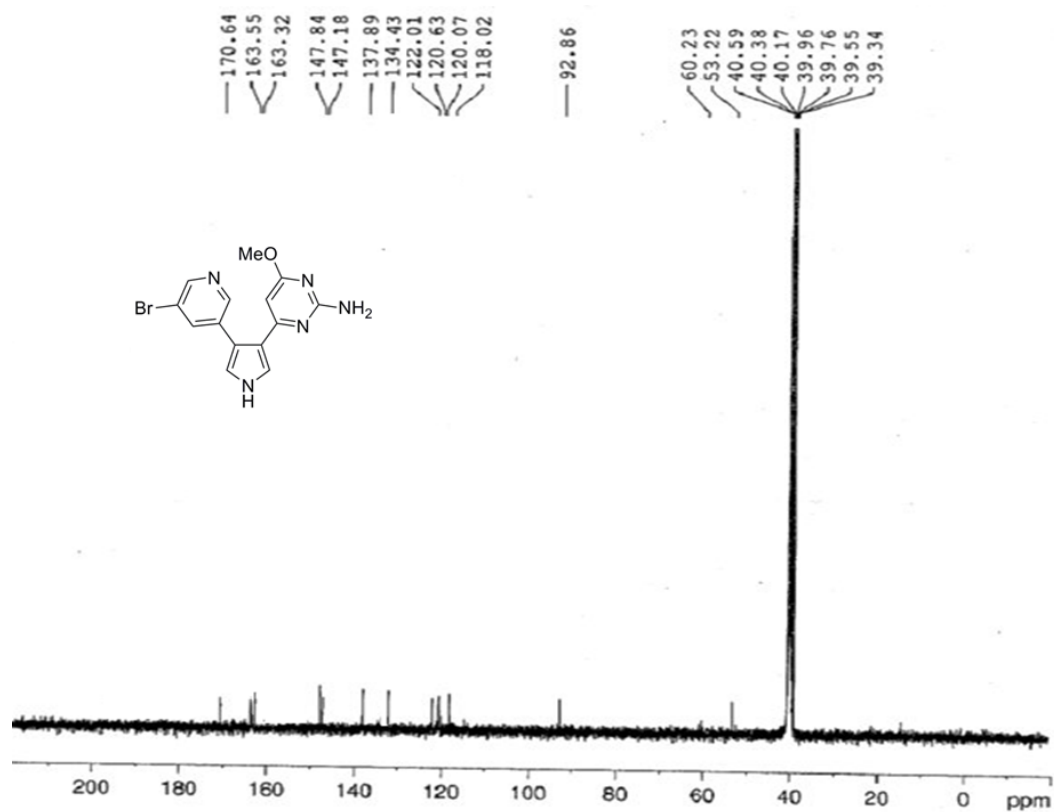


Figure S42b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8ab**



**Figure S43a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8ac**



**Figure S43b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8ac**

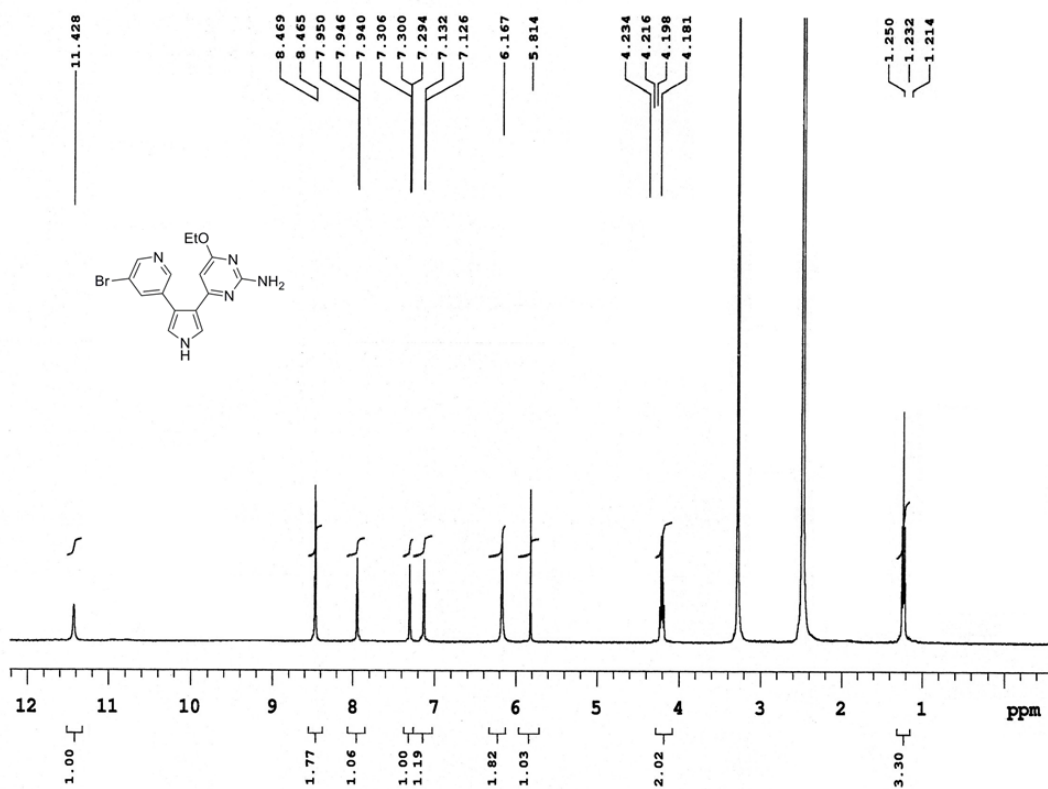


Figure S44a: (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound **8ad**

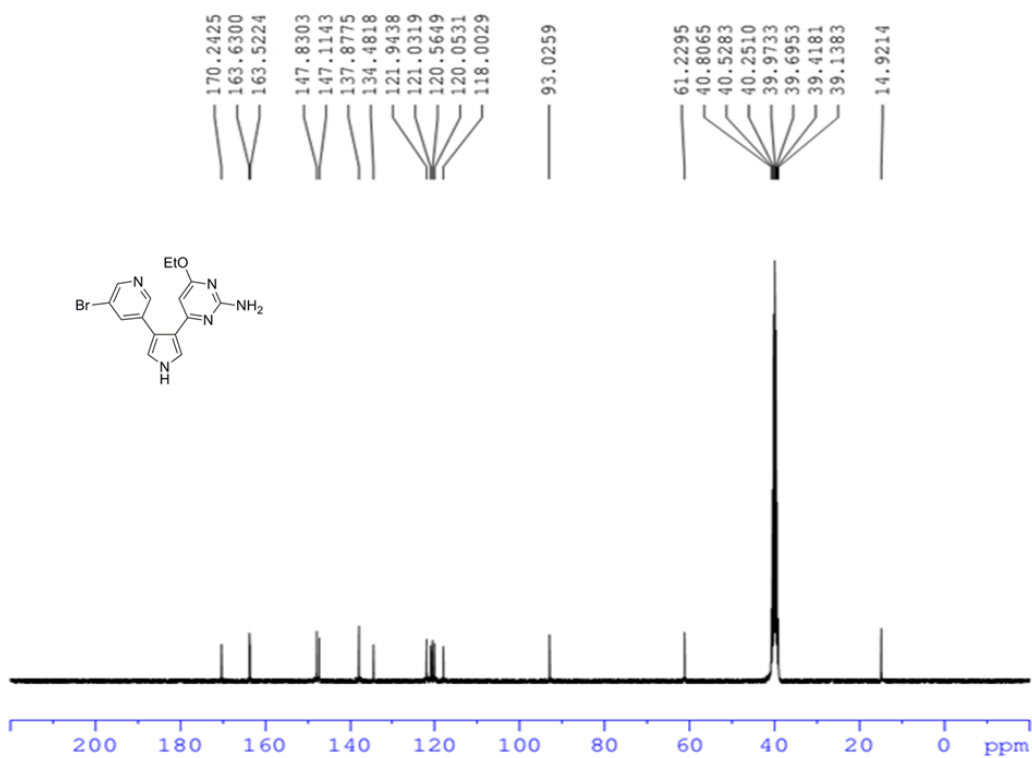
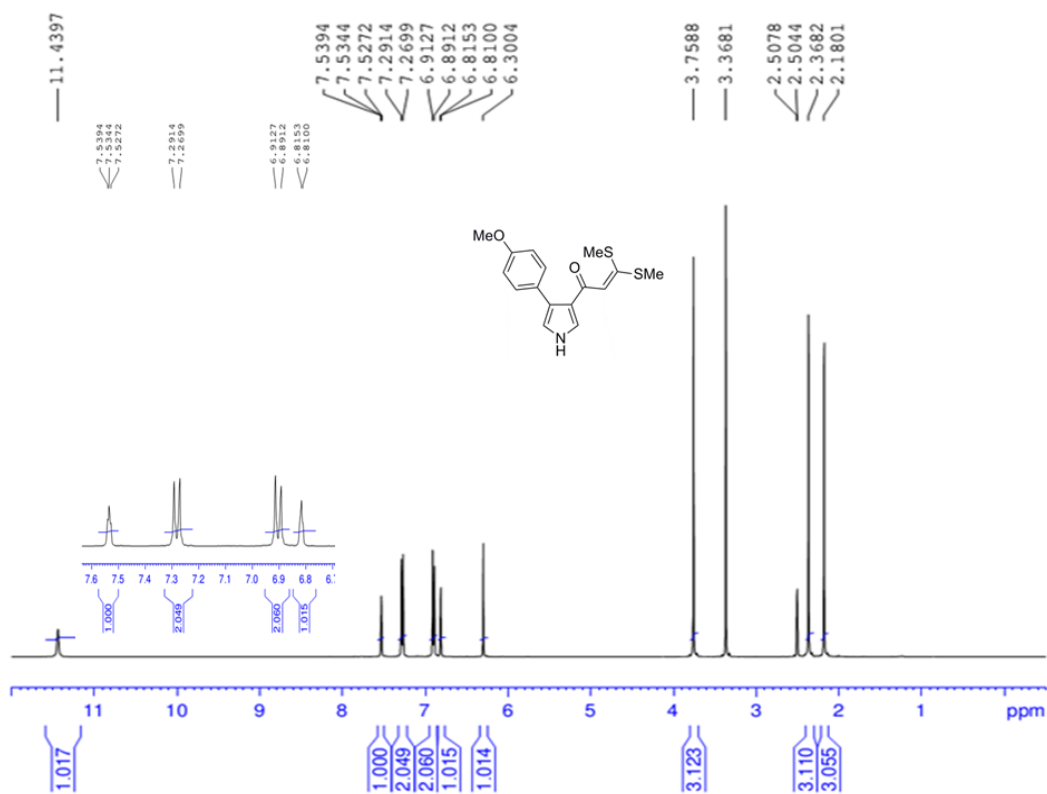
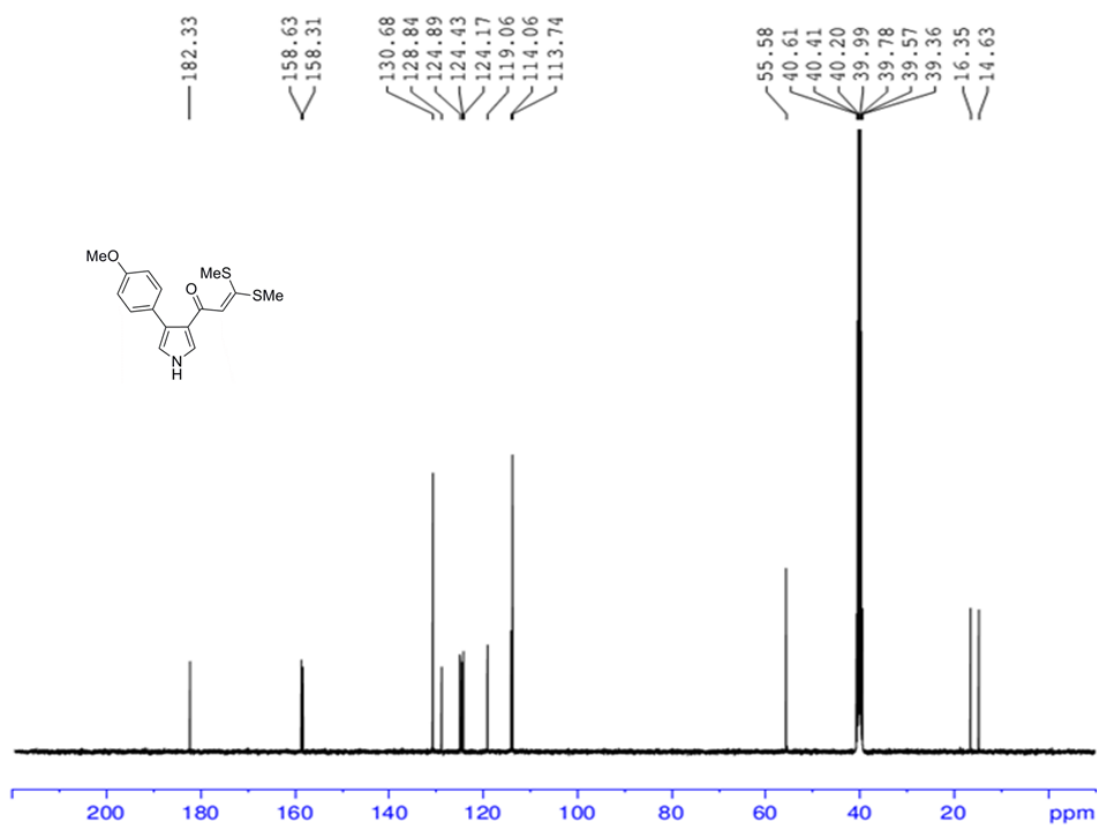


Figure S44b: (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound **8ad**



**Figure S45a:** (400MHz, DMSO-d<sub>6</sub>) <sup>1</sup>H NMR spectrum of compound 4a



**Figure S45b:** (100MHz, DMSO-d<sub>6</sub>) <sup>13</sup>C NMR spectrum of compound 4a

## II X-ray crystal structure of 8e

