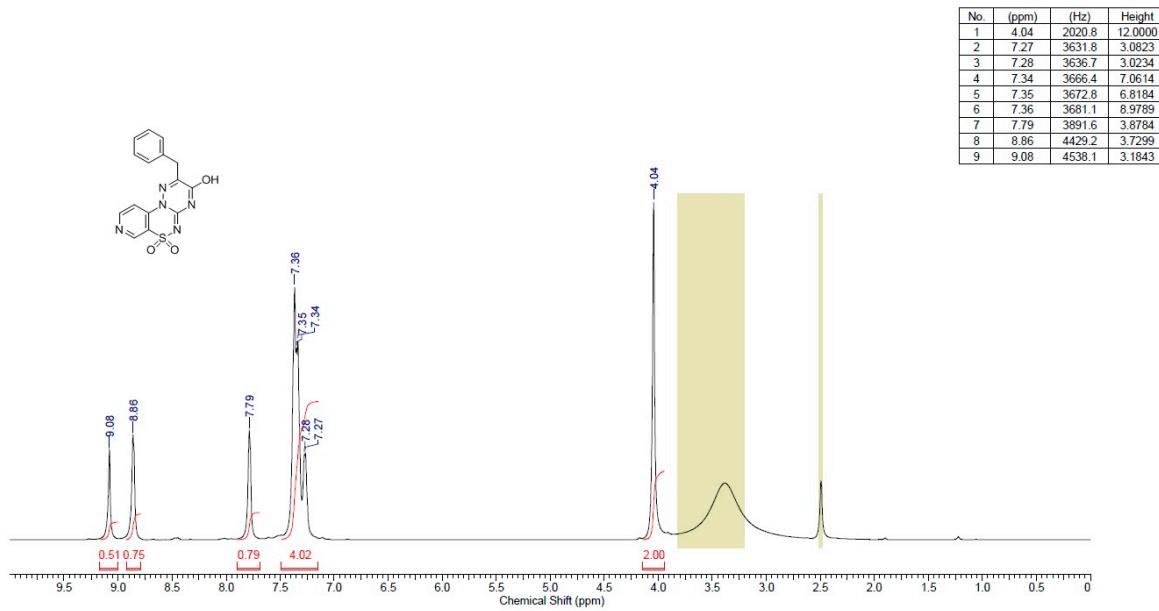
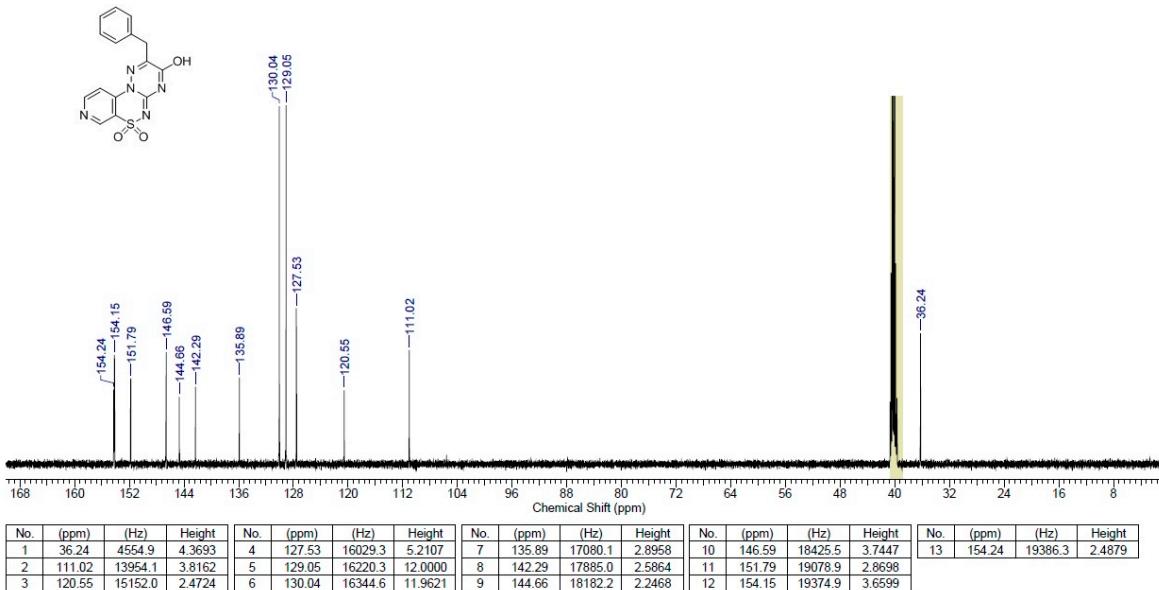


# Supplementary Materials: Synthesis of Novel Pyrido[4,3-*e*][1,2,4]triazino[3,2-*c*][1,2,4]thiadiazine 6,6-Dioxide Derivatives with Potential Anticancer Activity

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Compound	Page
Compound <b>5</b> <sup>1</sup> H-NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> )	S2
Compound <b>5</b> <sup>13</sup> C-NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> )	S2
Compound <b>5</b> IR	S3
Compound <b>6</b> <sup>1</sup> H-NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> )	S3
Compound <b>6</b> <sup>13</sup> C-NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> )	S4
Compound <b>6</b> IR	S4
Compound <b>8</b> <sup>1</sup> H-NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> )	S5
Compound <b>8</b> <sup>13</sup> C-NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> )	S5
Compound <b>8</b> IR	S6
Compound <b>17</b> <sup>1</sup> H-NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> )	S6
Compound <b>17</b> <sup>13</sup> C-NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> )	S7
Compound <b>17</b> IR	S7
Compound <b>19</b> <sup>1</sup> H-NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> )	S8
Compound <b>19</b> <sup>13</sup> C-NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> )	S8
Compound <b>19</b> IR	S9
Compound <b>22</b> <sup>1</sup> H-NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> )	S9
Compound <b>22</b> <sup>13</sup> C-NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> )	S10
Compound <b>22</b> IR	S10
Compound <b>26</b> <sup>1</sup> H-NMR (500 MHz, DMSO- <i>d</i> <sub>6</sub> )	S11
Compound <b>26</b> <sup>13</sup> C-NMR (125 MHz, DMSO- <i>d</i> <sub>6</sub> )	S11
Compound <b>26</b> IR	S12
Compound <b>7</b> COSY	S12
Compound <b>7</b> ROESY	S13
Compound <b>7</b> HMBC	S13
Compound <b>7</b> LC-MS	S14
Compound <b>25</b> COSY	S14
Compound <b>25</b> ROESY	S15
Compound <b>25</b> HMBC	S15

**Figure S1.**  $^1\text{H}$ -NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound 5.**Figure S2.**  $^{13}\text{C}$ -NMR (125 MHz, DMSO- $d_6$ ) spectrum of compound 5.

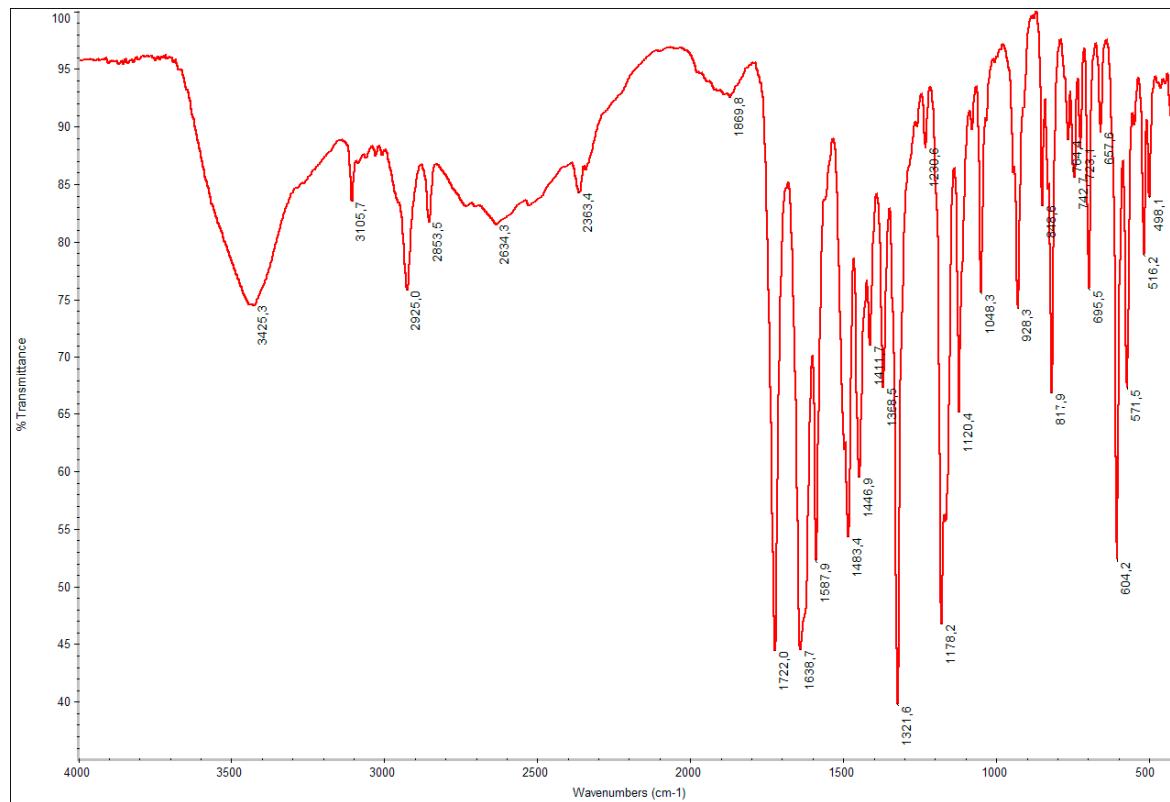
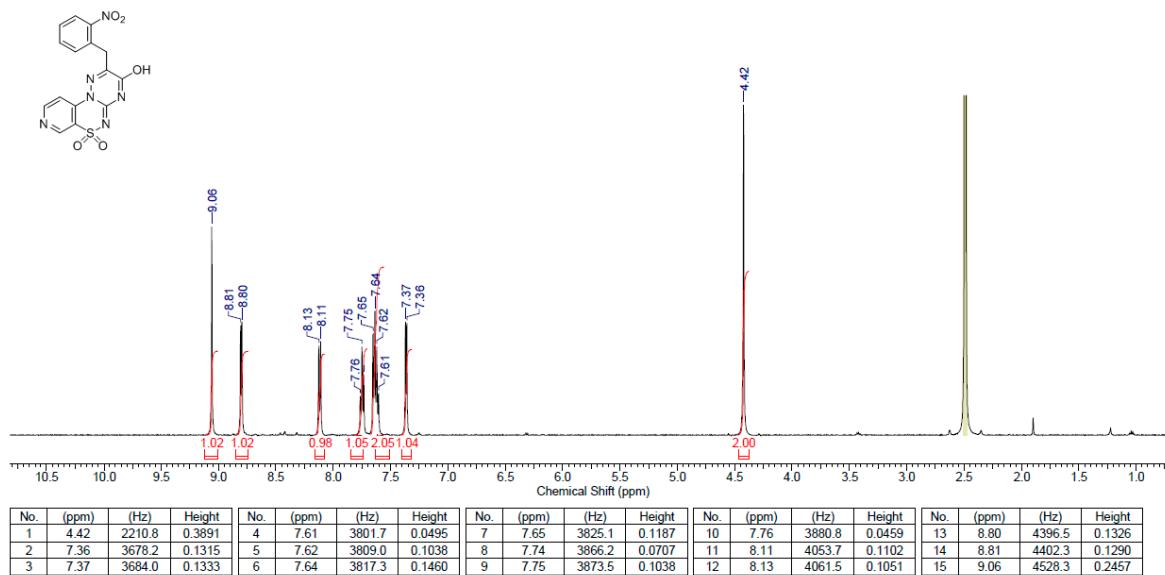
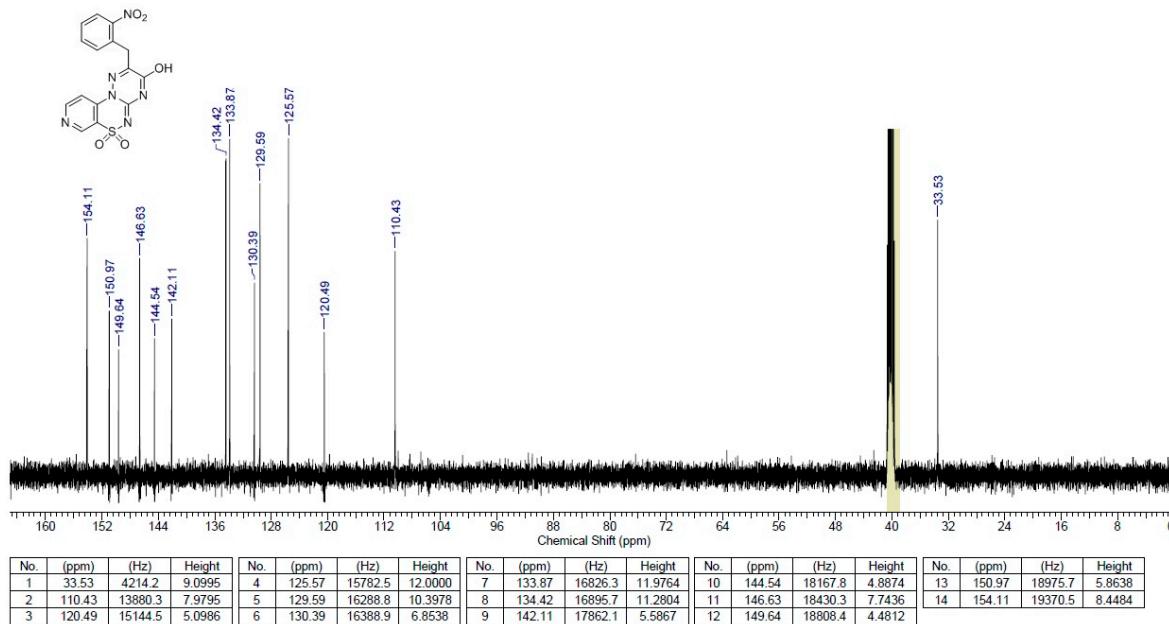
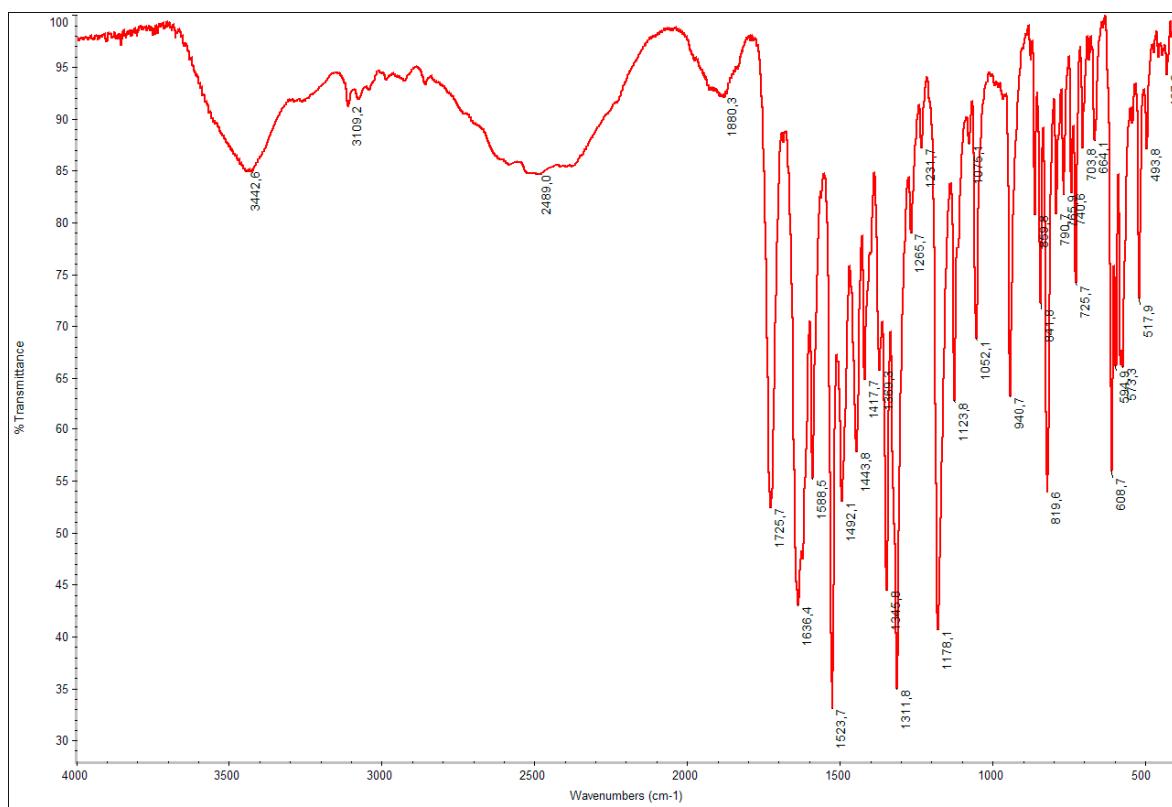


Figure S3. IR spectrum of compound 5.

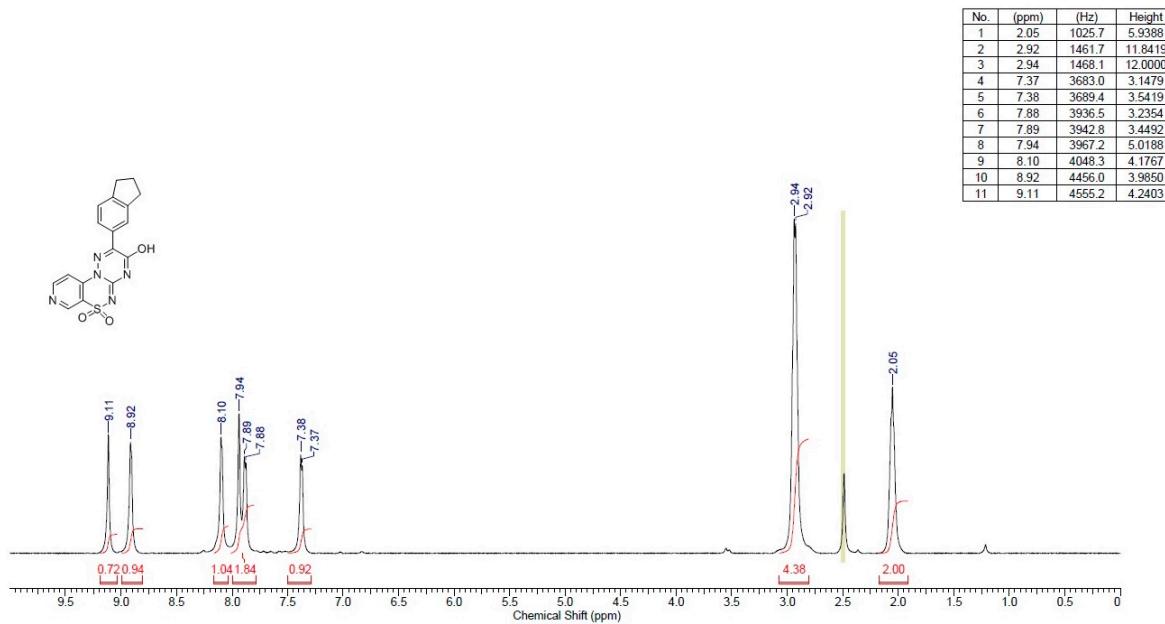
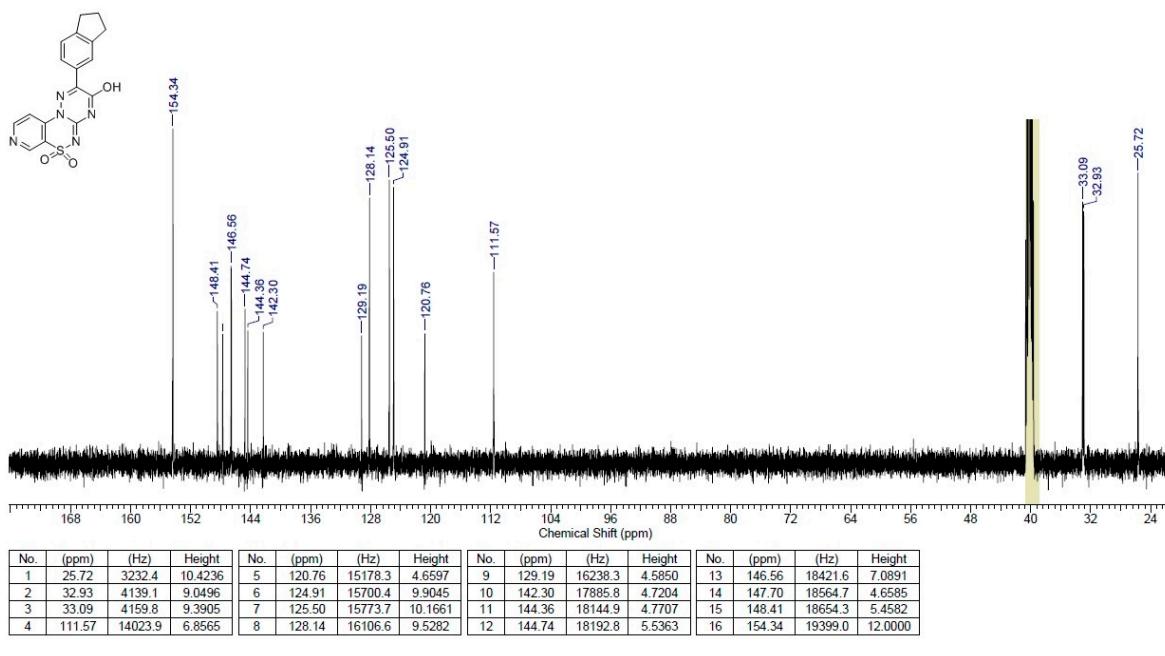
Figure S4. <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 6.

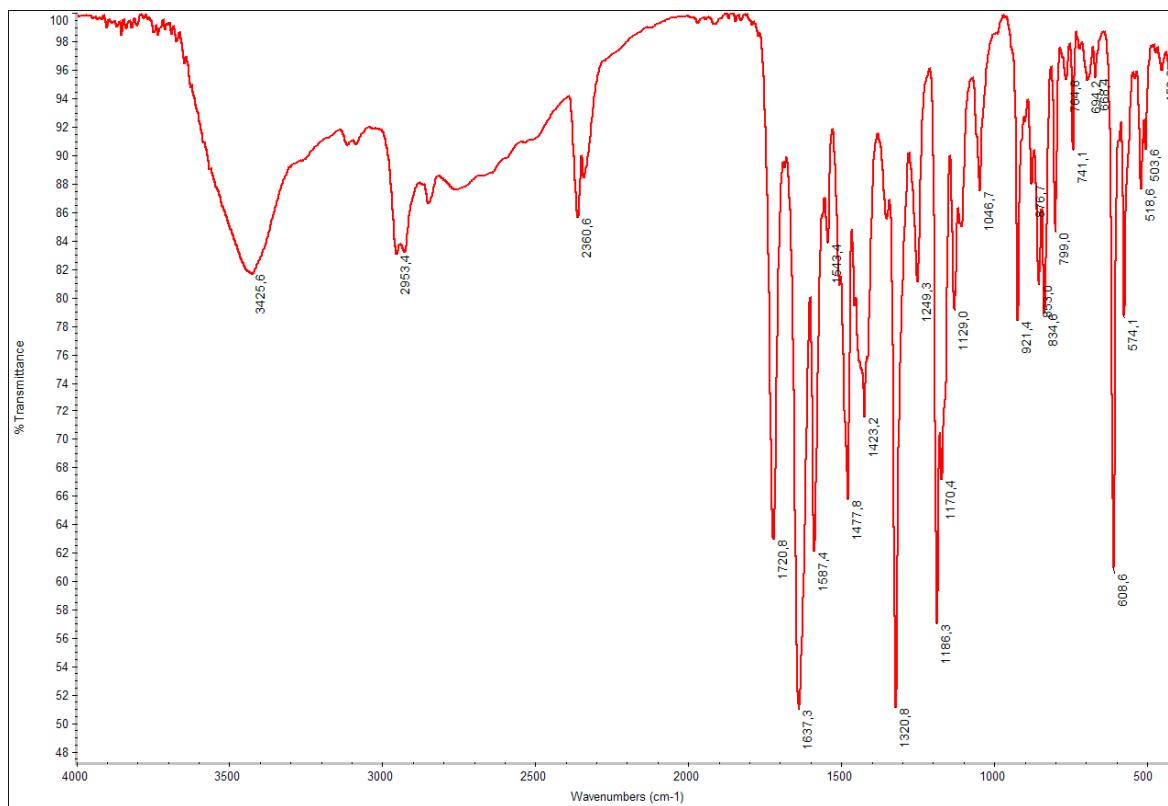


**Figure S5.** <sup>13</sup>C-NMR (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 6.



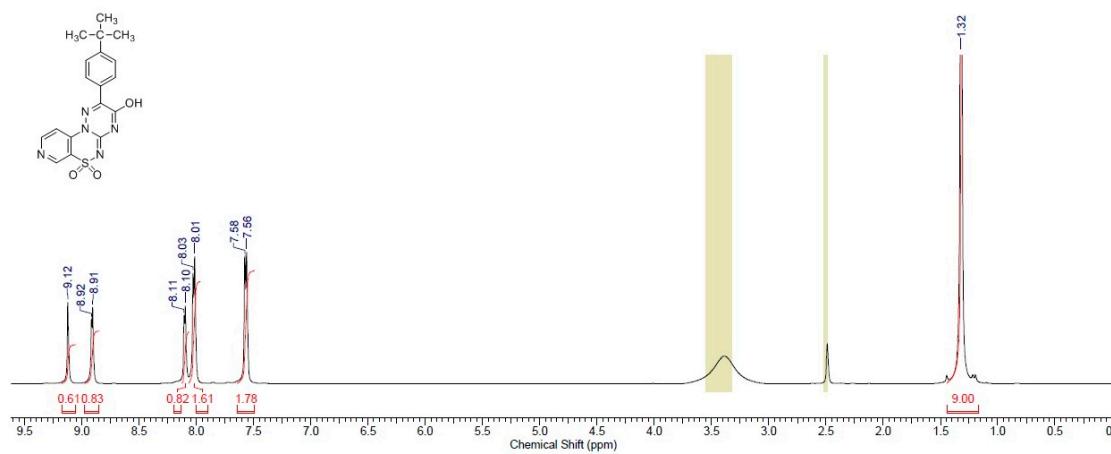
**Figure S6.** IR spectrum of compound 6.

**Figure S7.**  $^1\text{H}$ -NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound 8.**Figure S8.**  $^{13}\text{C}$ -NMR (125 MHz, DMSO- $d_6$ ) spectrum of compound 8.

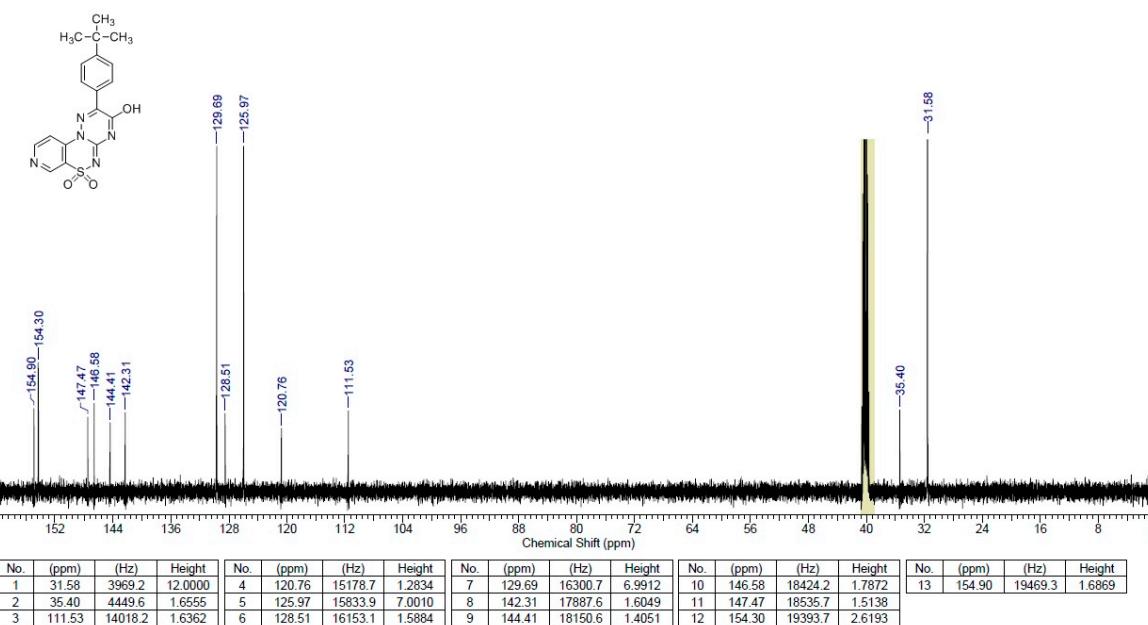


**Figure S9.** IR spectrum of compound 8.

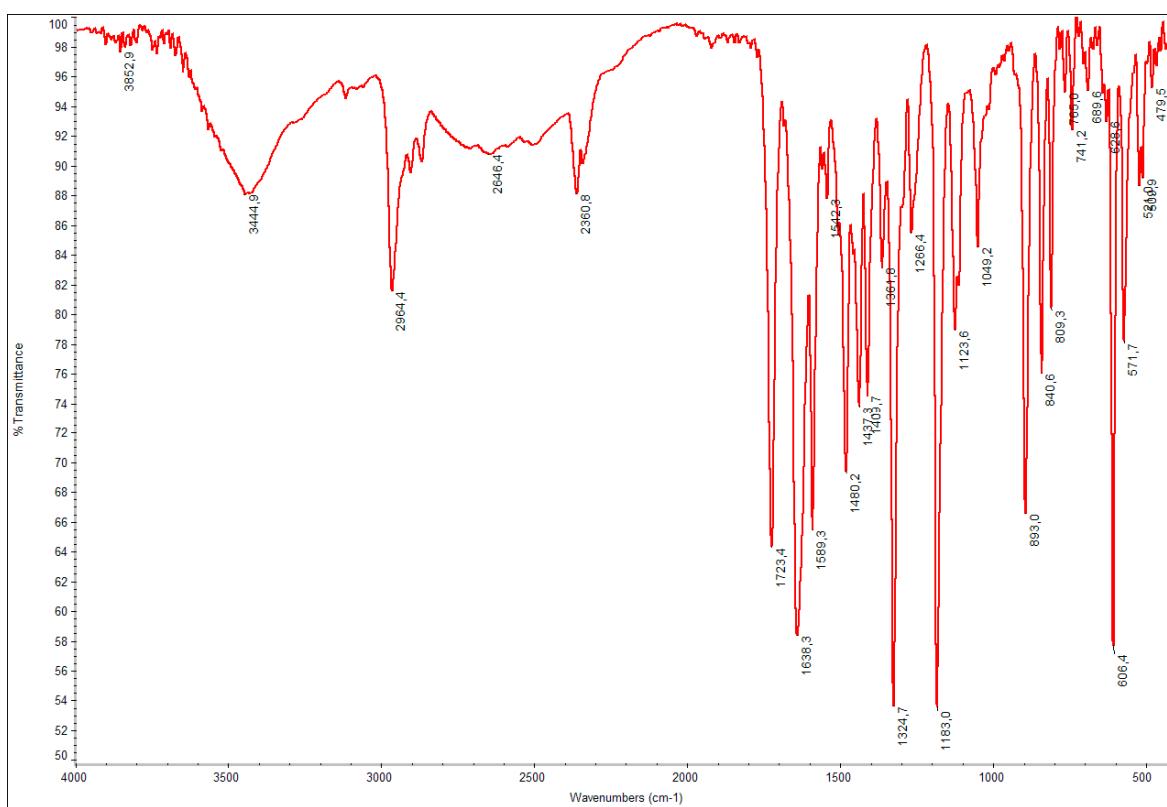
No.	(ppm)	(Hz)	Height
1	1.32	660.9	1.0000
2	7.56	3779.2	1.3736
3	7.58	3786.6	1.3280
4	8.01	4005.3	1.3279
5	8.03	4012.7	1.1563
6	8.10	4045.8	0.8155
7	8.11	4052.2	0.7716
8	8.91	4451.2	0.7960
9	8.92	4456.5	0.6663
10	9.12	4560.1	0.5186



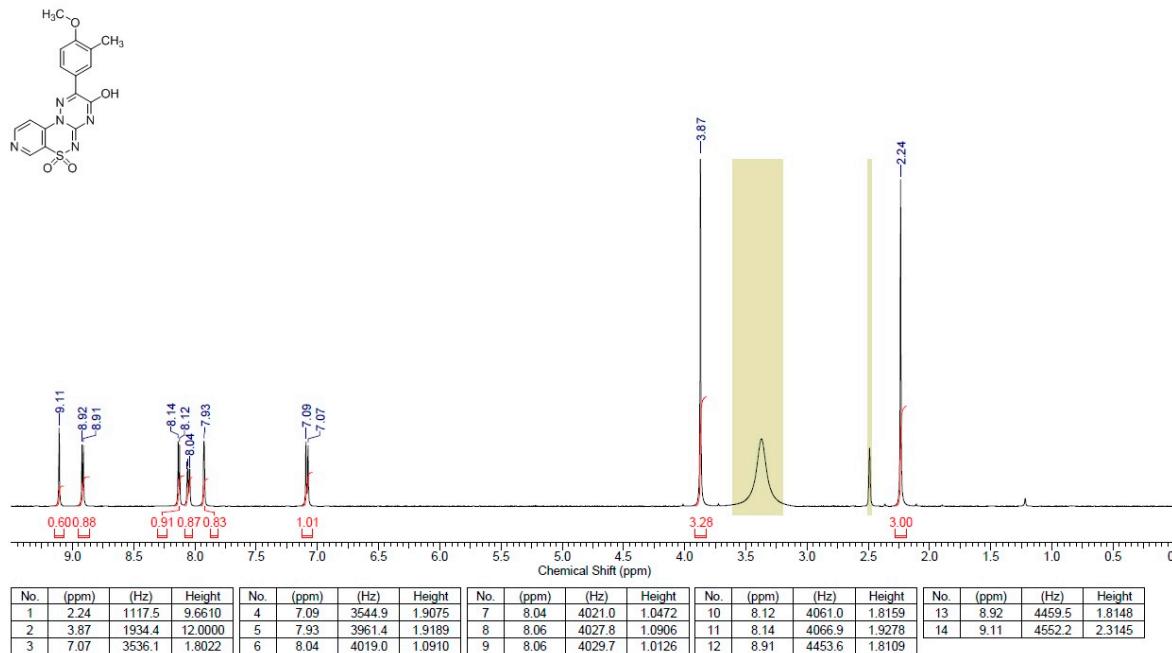
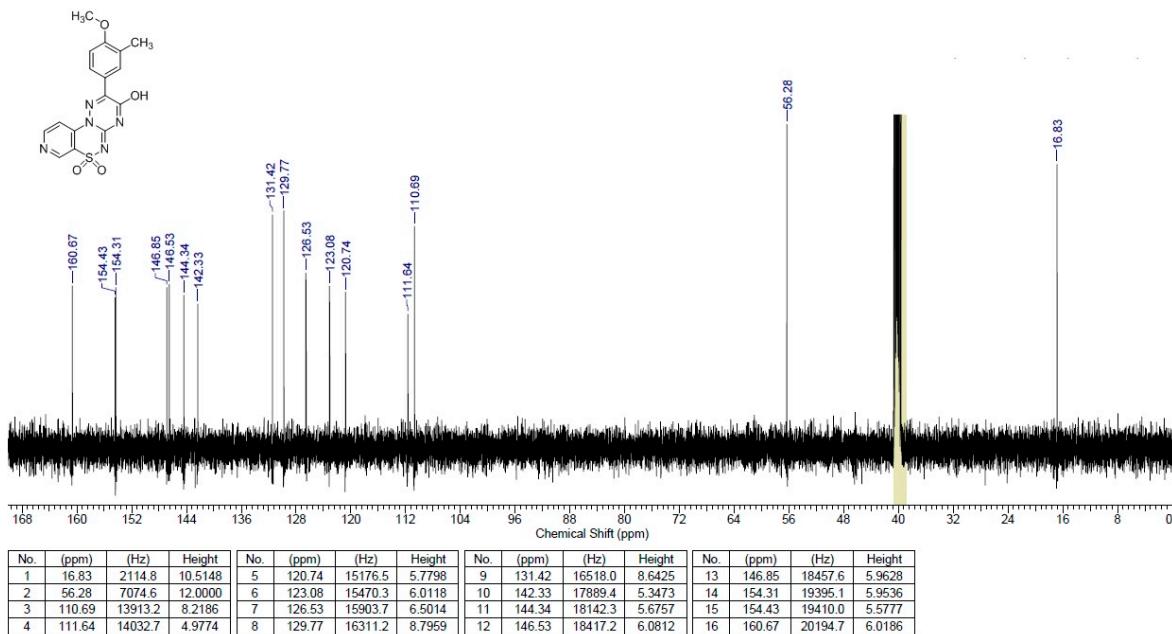
**Figure S10.**  $^1\text{H}$ -NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound 17.

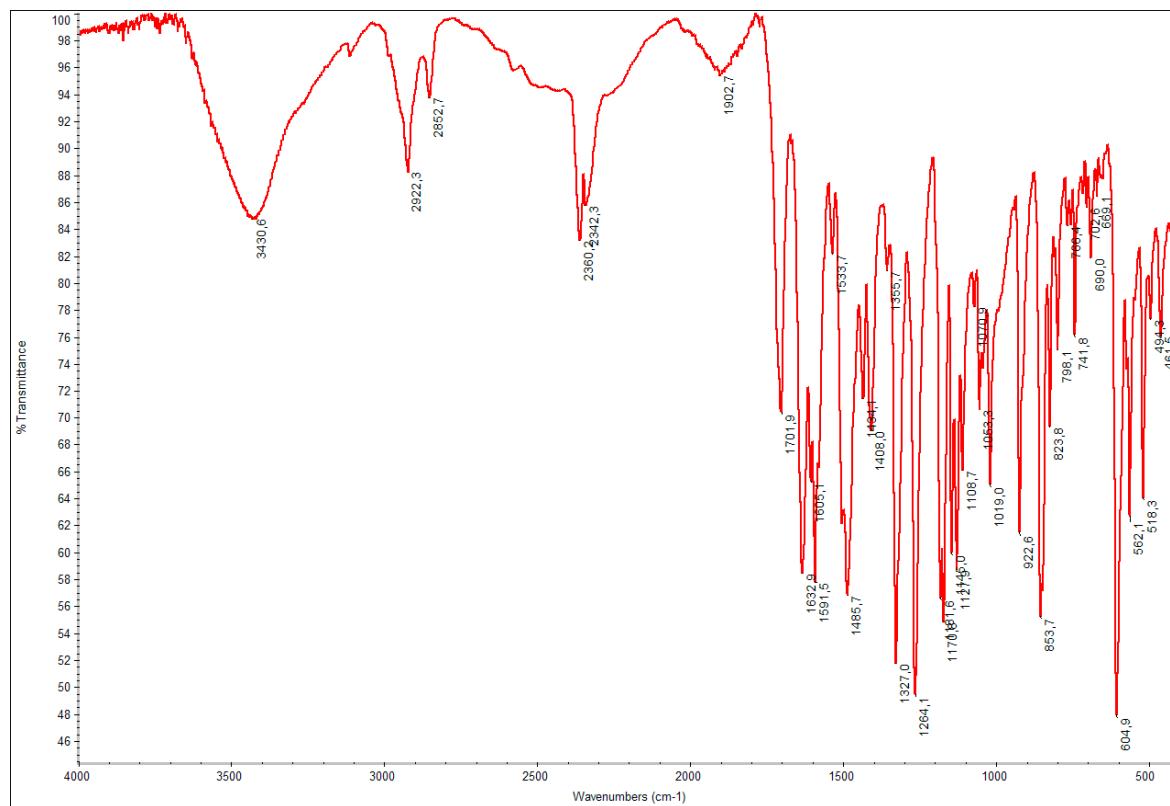


**Figure S11.**  $^{13}\text{C}$ -NMR (125 MHz, DMSO- $d_6$ ) spectrum of compound **17**.

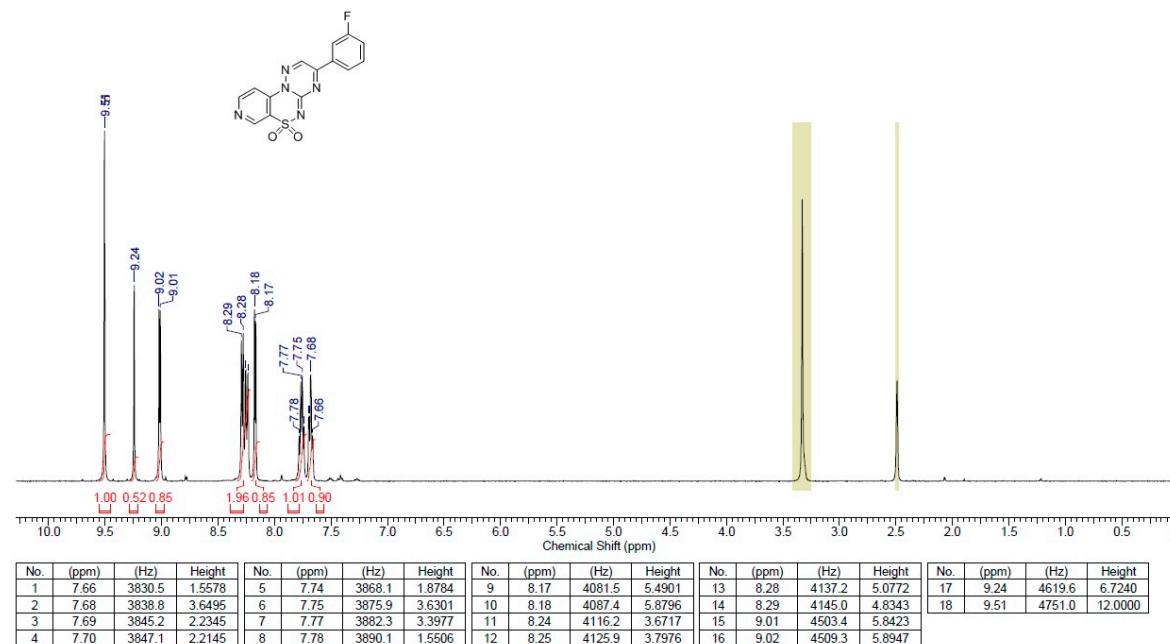


**Figure S12.** IR spectrum of compound 17.

**Figure S13.** <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 19.**Figure S14.** <sup>13</sup>C-NMR (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 19.



**Figure S15.** IR spectrum of compound **19**.



**Figure S16.**  $^1\text{H}$ -NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound 22.

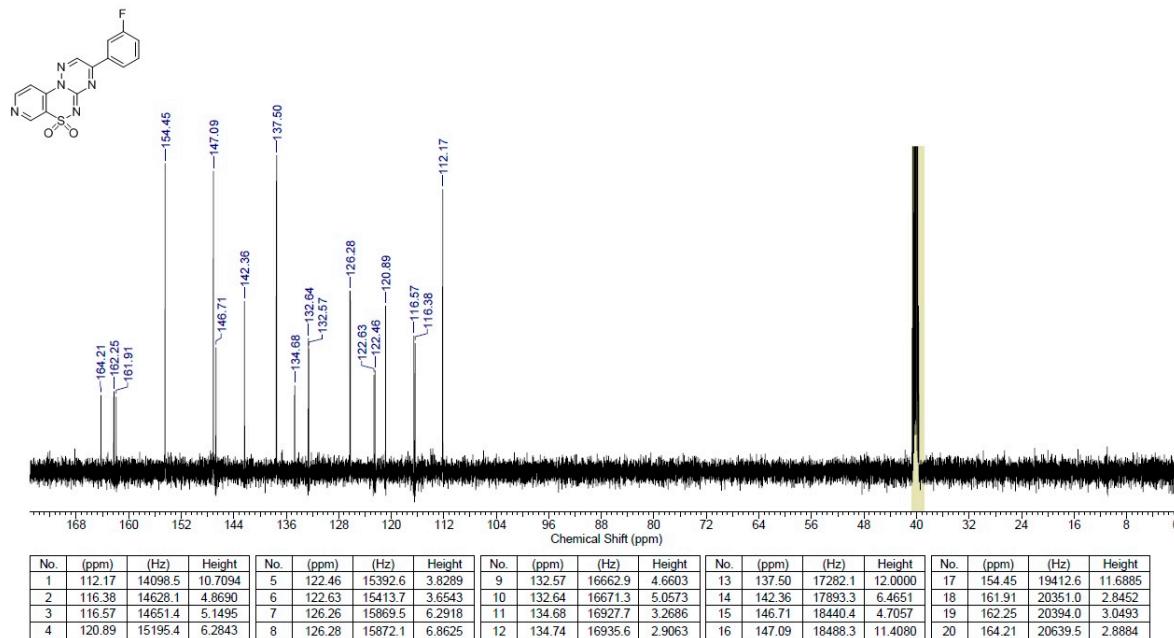
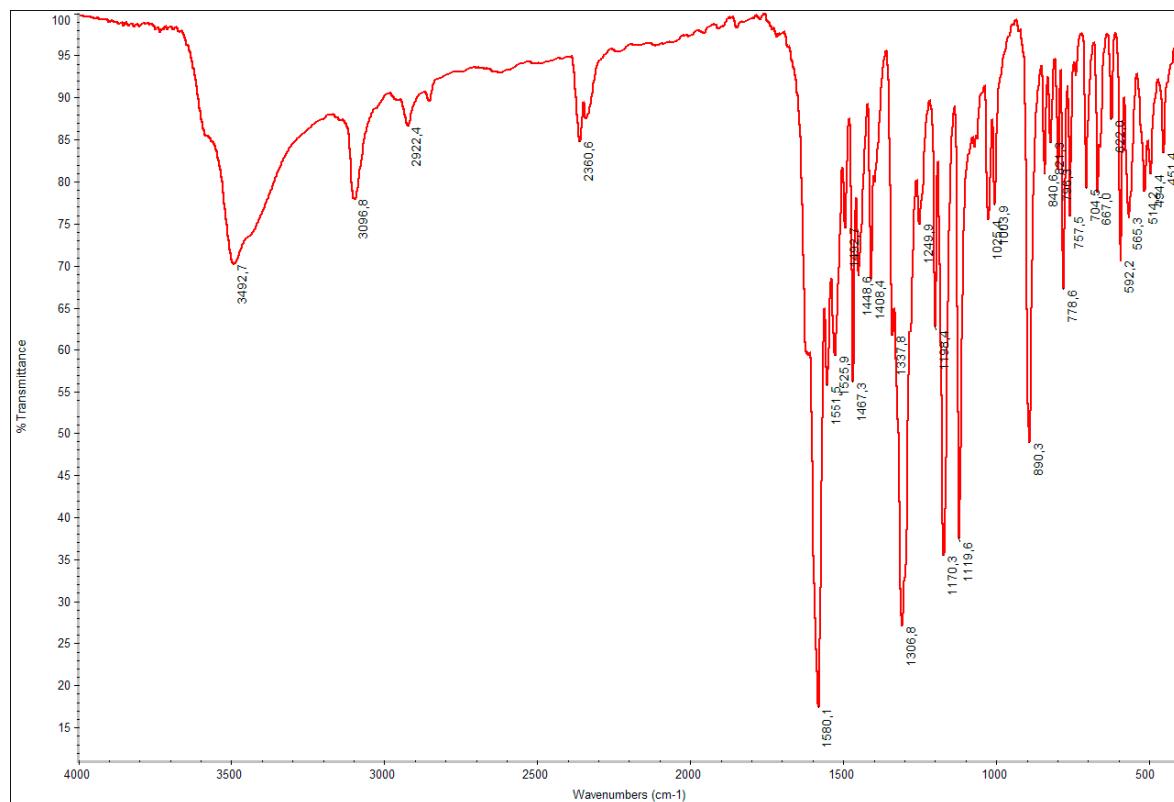
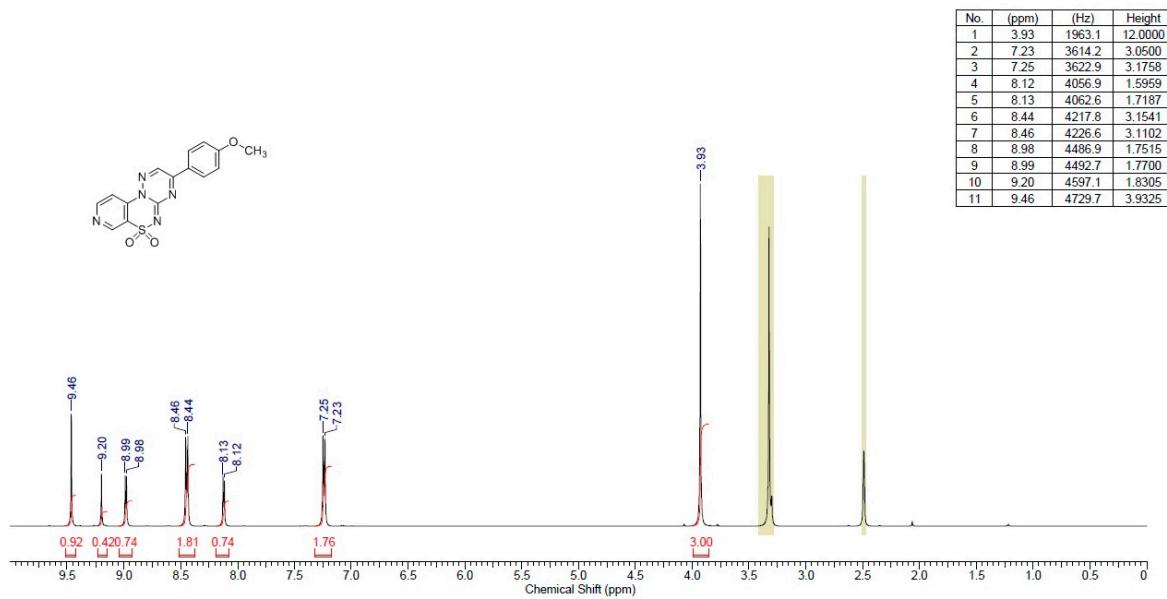
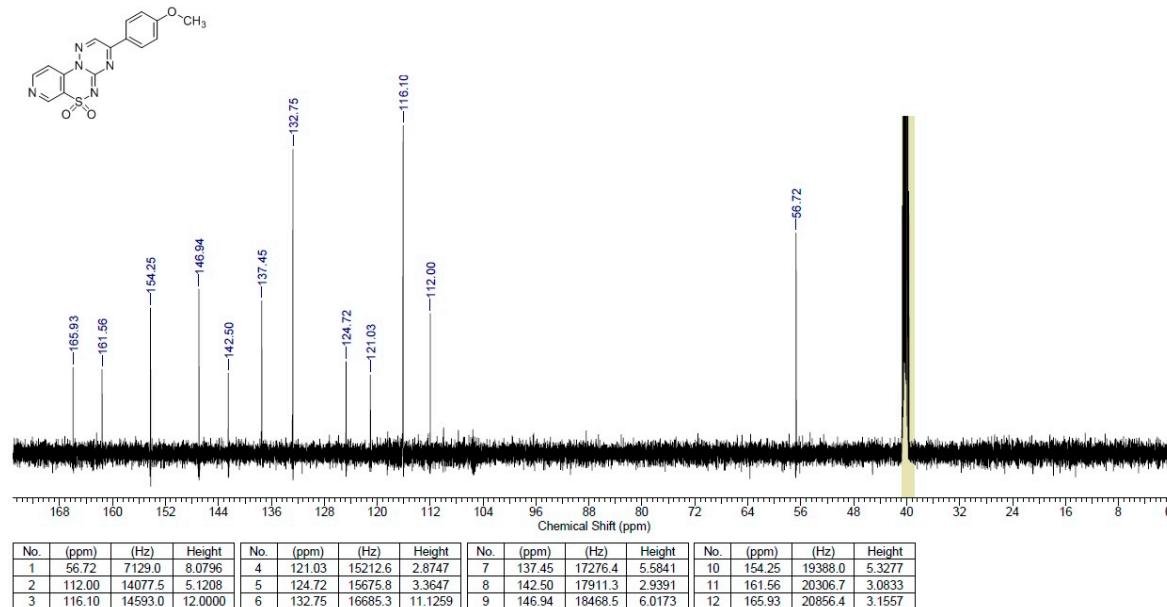
Figure S17.  $^{13}\text{C}$ -NMR (125 MHz, DMSO- $d_6$ ) spectrum of compound 22.

Figure S18. IR spectrum of compound 22.

**Figure S19.** <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 26.**Figure S20.** <sup>13</sup>C-NMR (125 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 26.

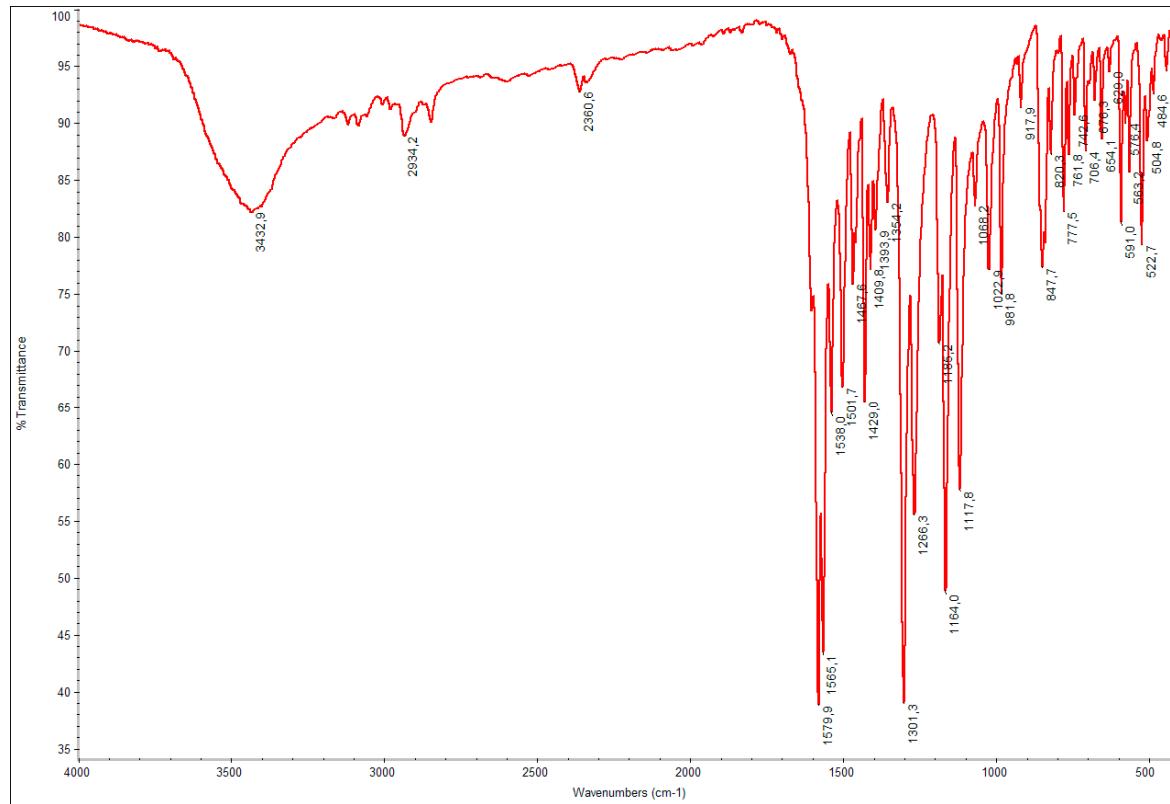


Figure S21. IR spectrum of compound 26.

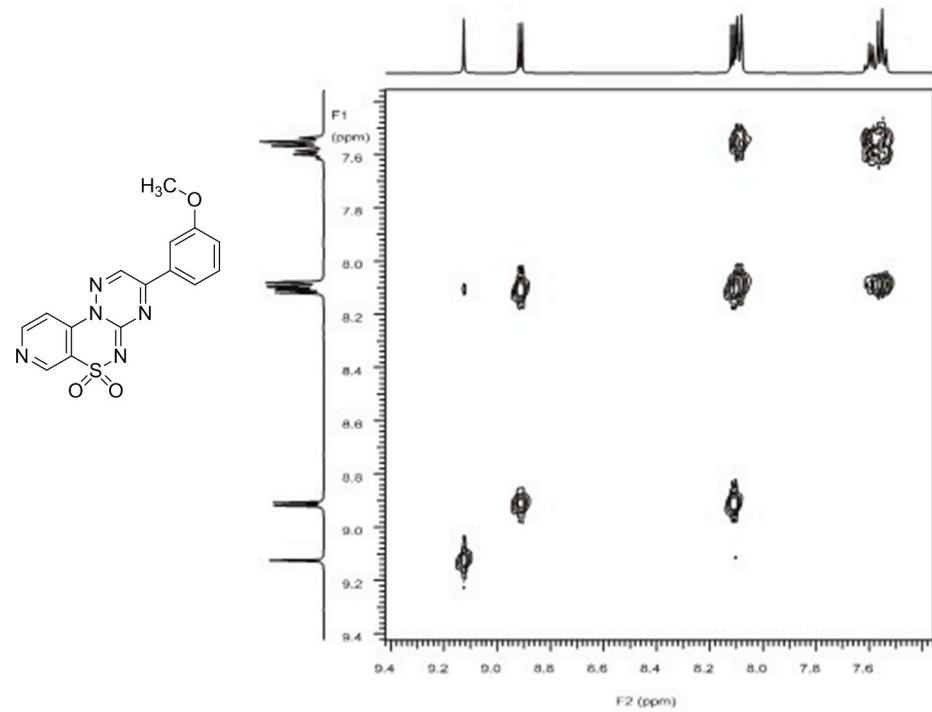
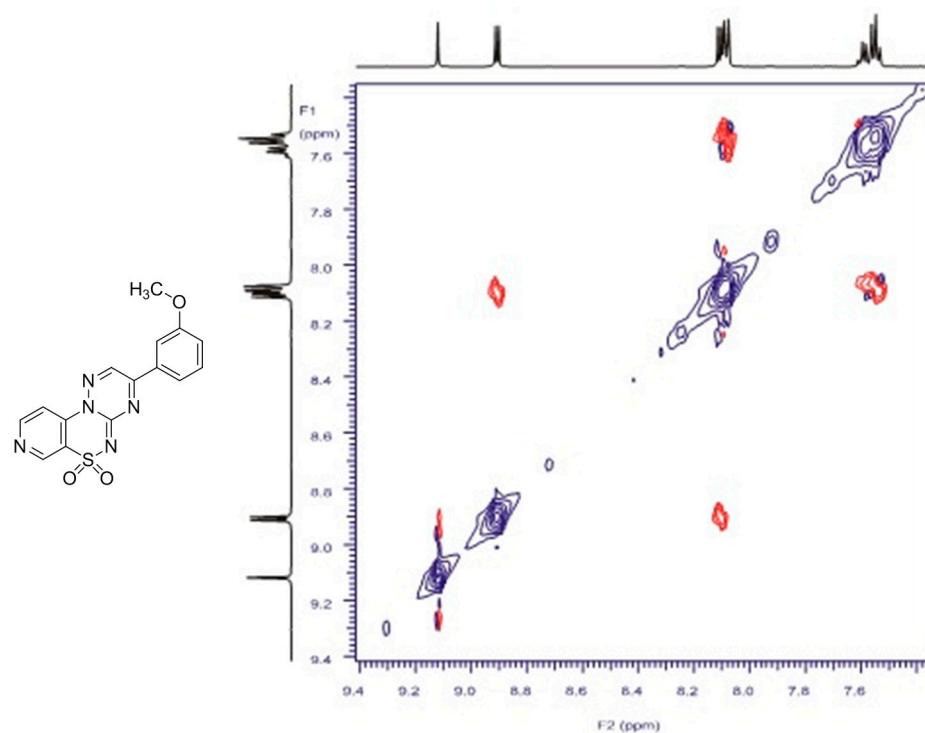
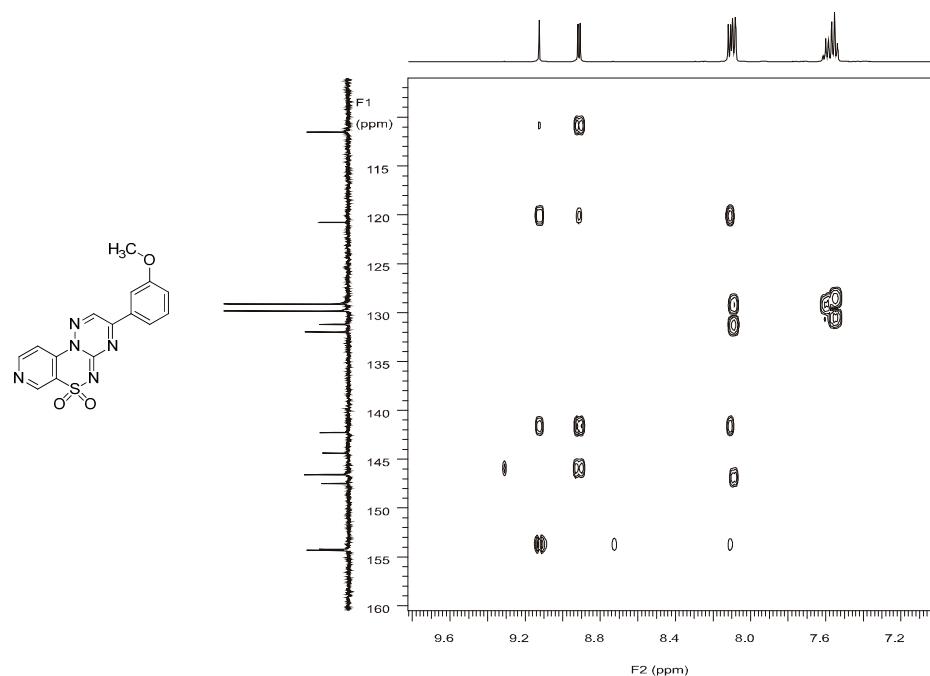
<sup>2</sup>D-NMR Spectra of Compound 7

Figure S22. COSY spectrum of compound 7.



**Figure S23.** ROESY spectrum of compound 7.



**Figure S24.** HMBC spectrum of compound 7.

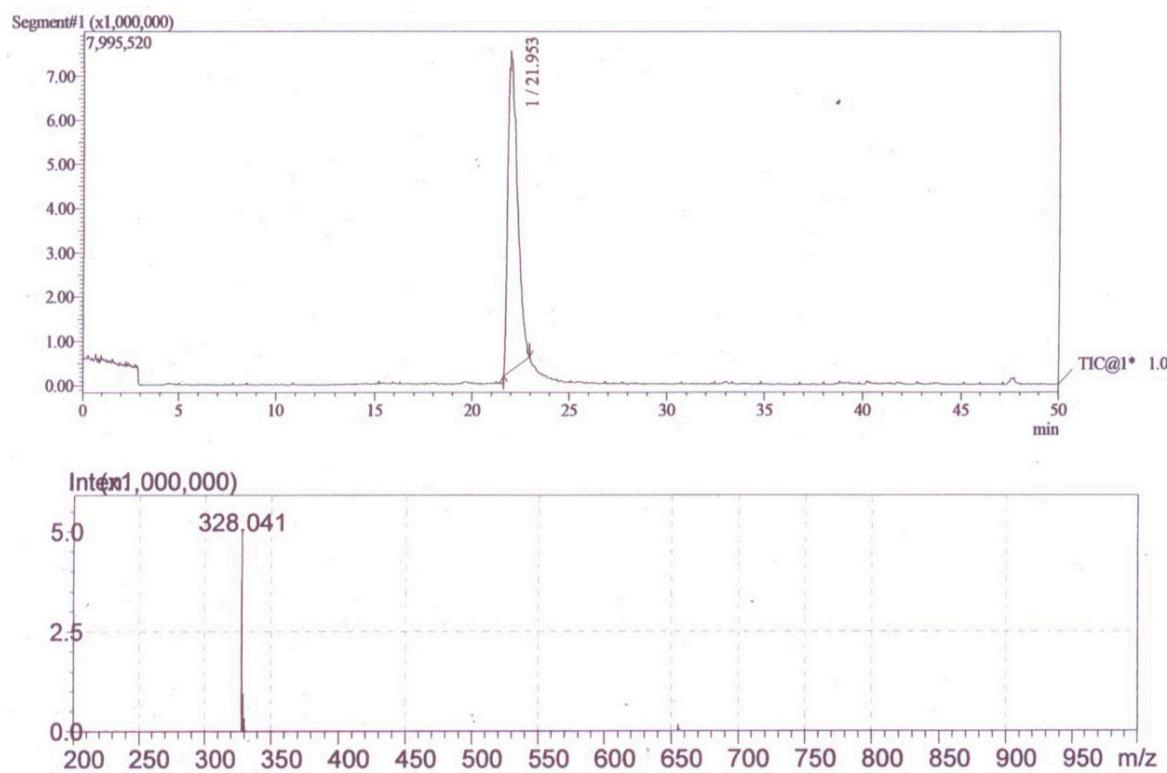


Figure S25. LC-MS spectrum of compound 7.

### 2D-NMR Spectra of Compound 25

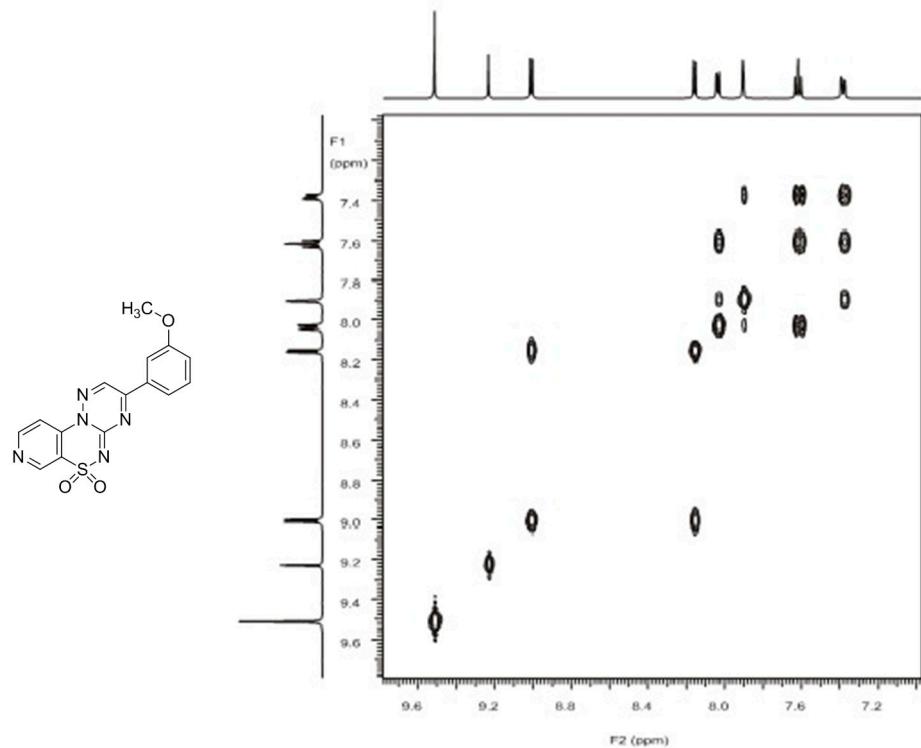
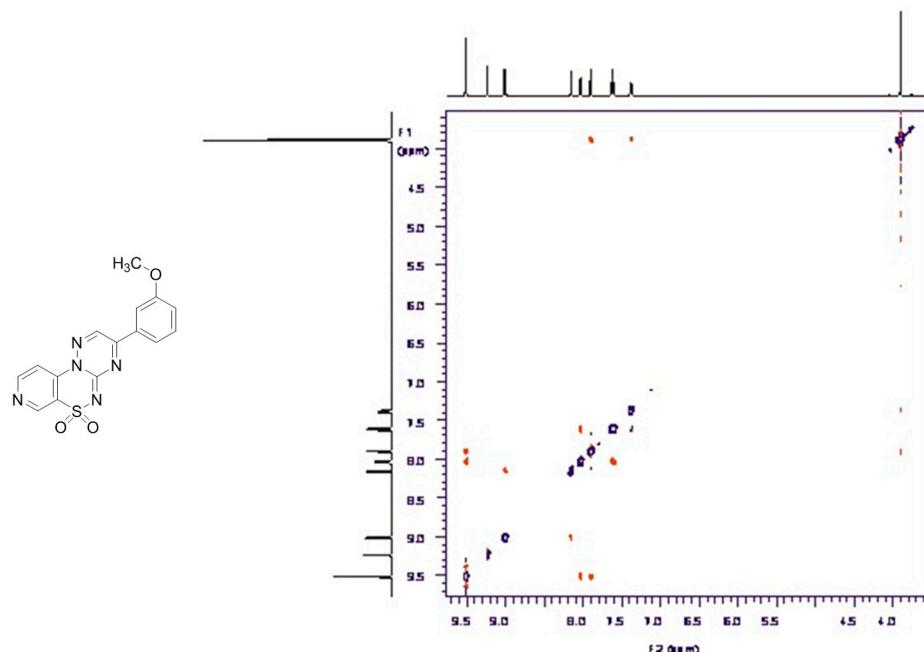
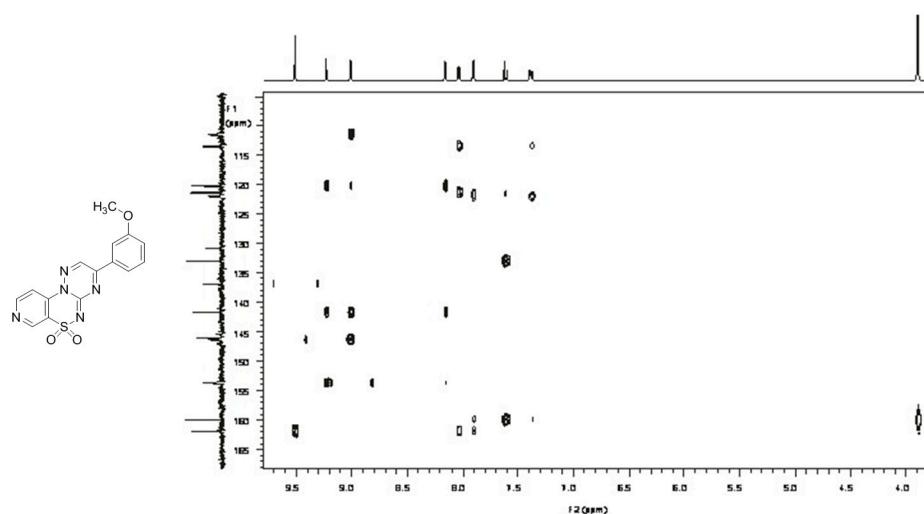


Figure S26. COSY spectrum of compound 25.



**Figure S27.** ROESY spectrum of compound 25.



**Figure S28.** HMBC spectrum of compound 25.