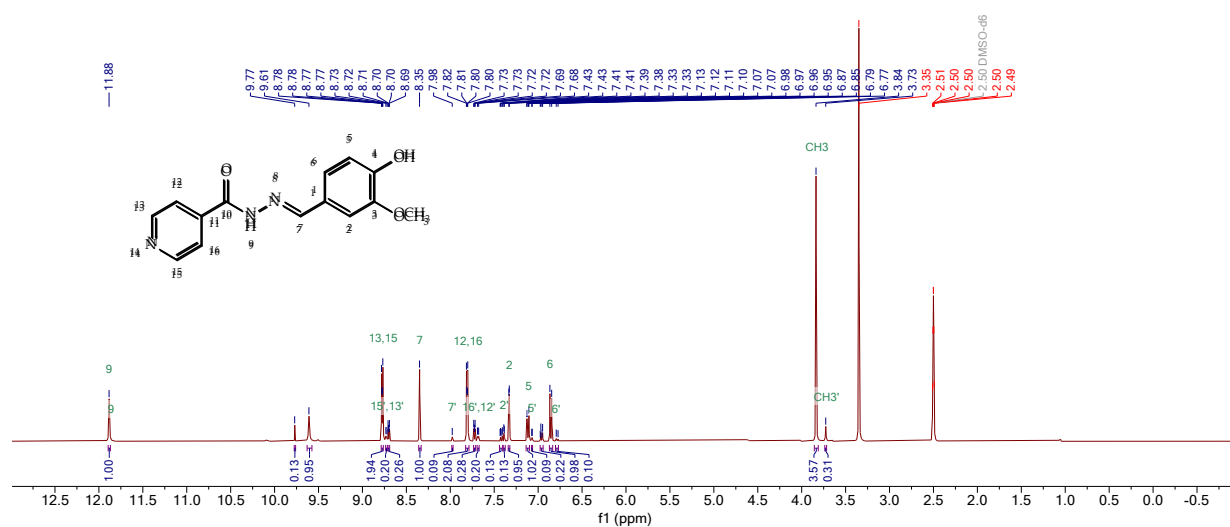
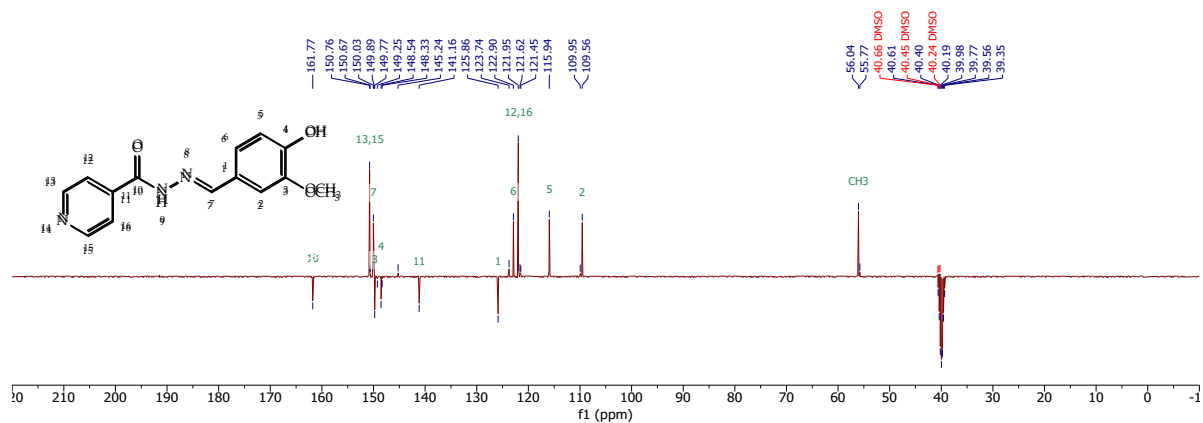


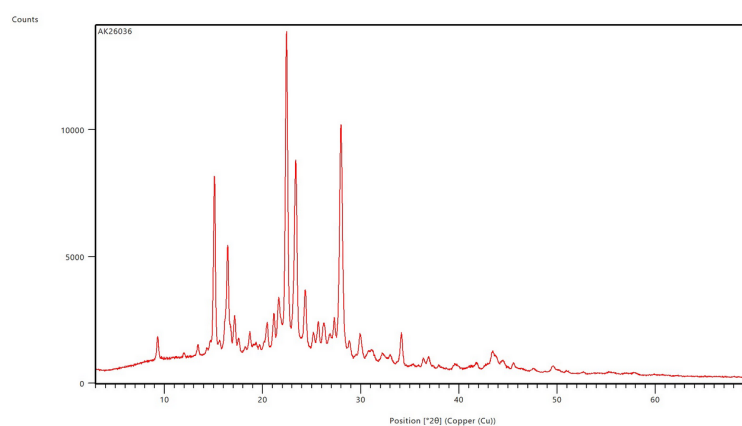
## Supplementary Materials



**Figure S1:**  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ , 298 K) of compound **1**



**Figure S2:**  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 298 K) of compound **1**



**Figure S3:** Powder XRD of compound **1**

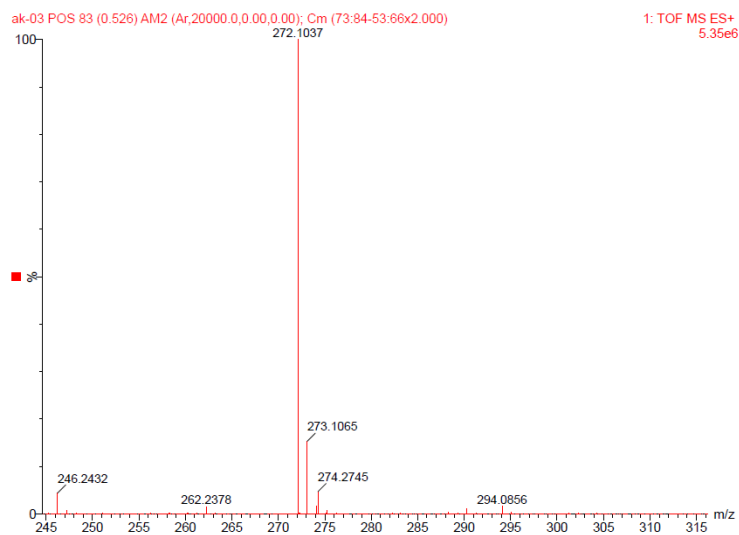


Figure S4: HRMS of compound 1

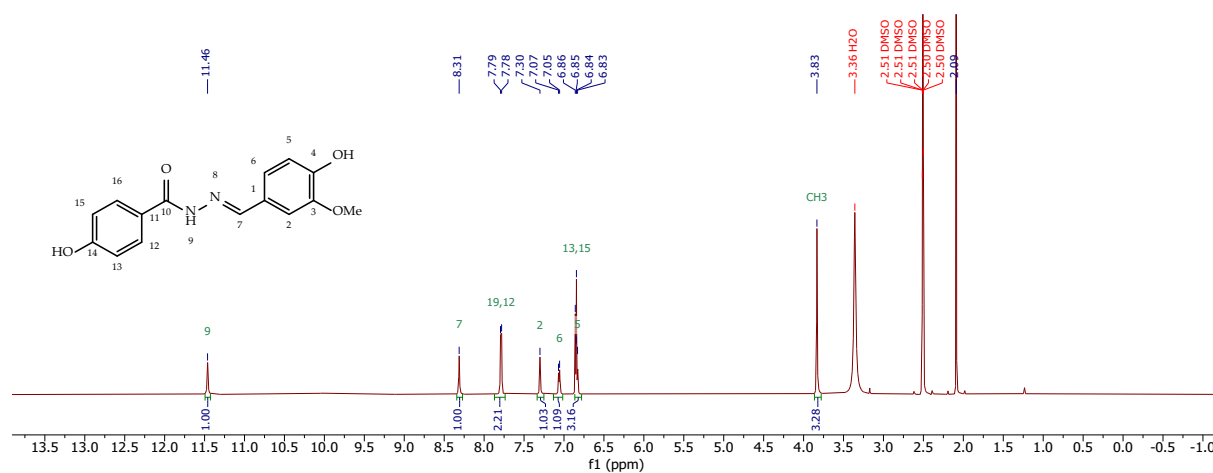


Figure S5: <sup>1</sup>H NMR (600 MHz, DMSO-d<sub>6</sub>, 298 K) of compound 2

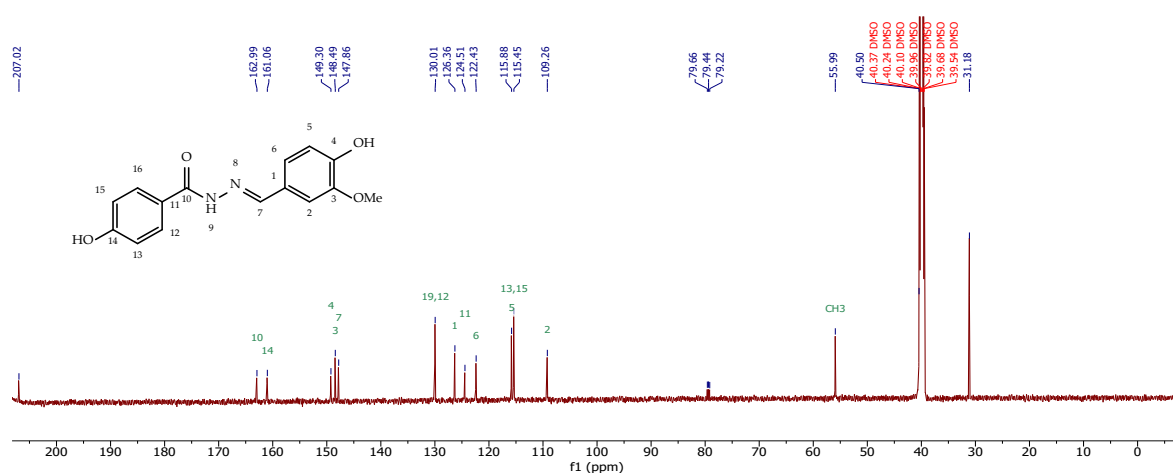
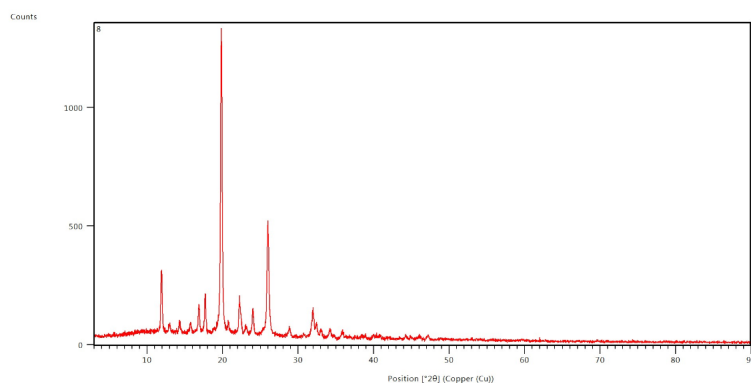


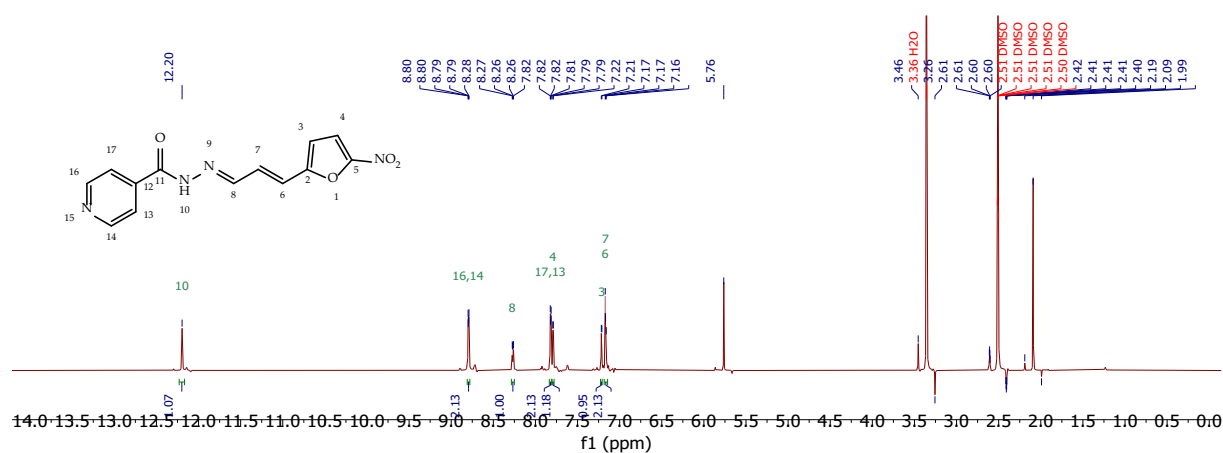
Figure S6: <sup>13</sup>C NMR (150 MHz, DMSO-d<sub>6</sub>, 298 K) of compound 2



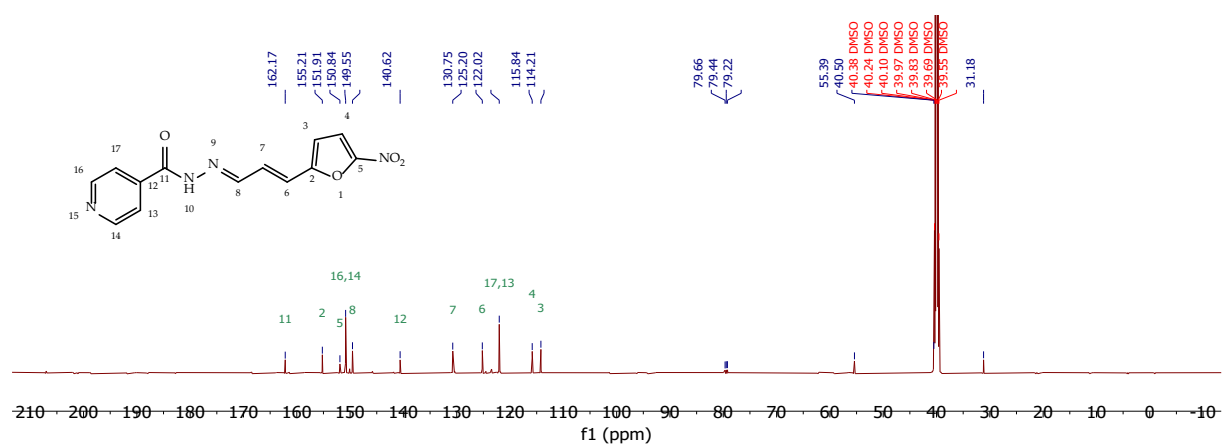
**Figure S7:** Powder XRD of compound **2**



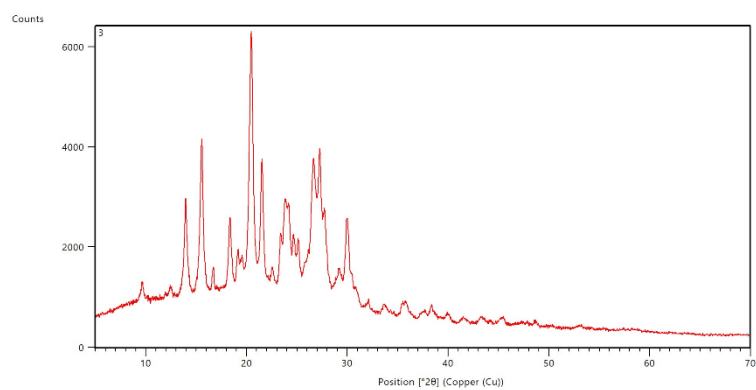
**Figure S8:** HRMS of compound **2**



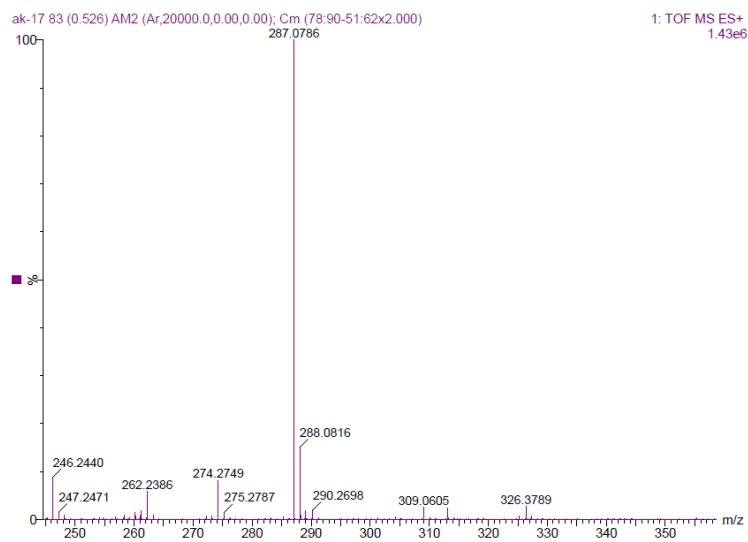
**Figure S9:**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound **3**



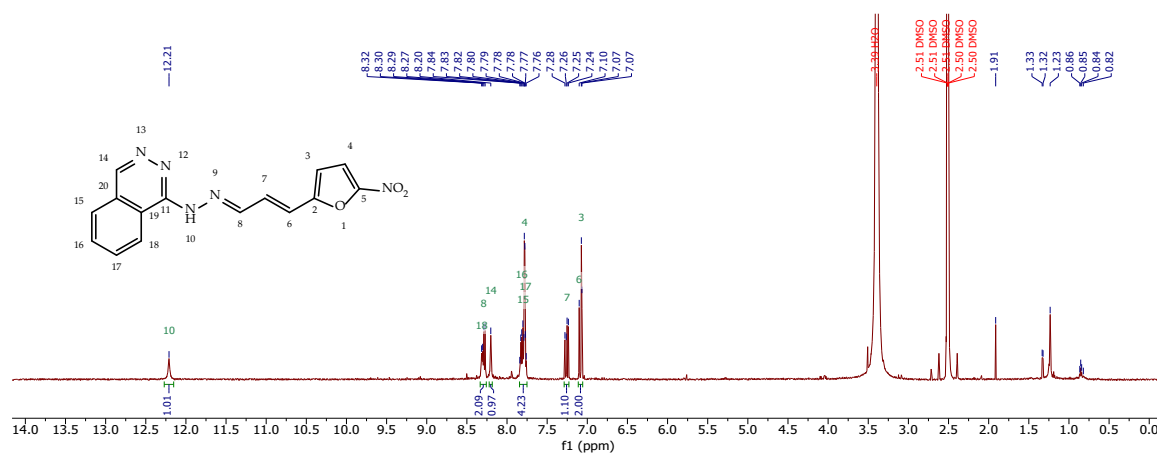
**Figure S10:** <sup>13</sup>C NMR (150 MHz, DMSO-d<sub>6</sub>, 298 K) of compound **3**



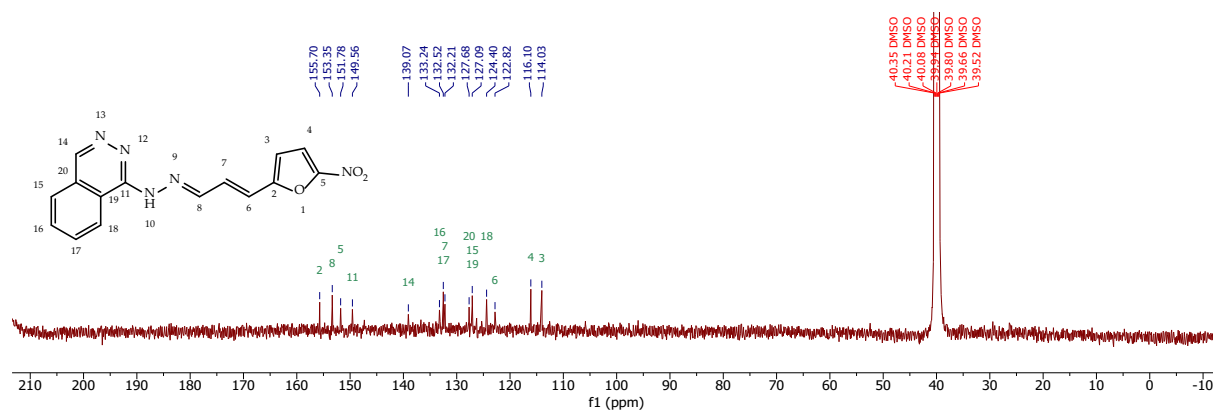
**Figure S11:** Powder XRD of compound **3**



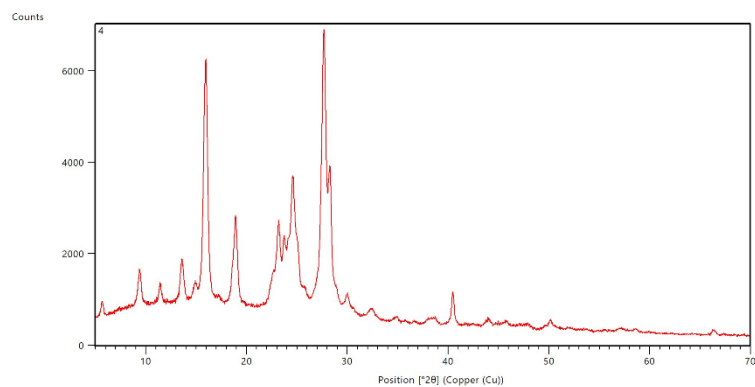
**Figure S12:** HRMS of compound **3**



**Figure S13:**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound 4



**Figure S14:**  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ , 298 K) of compound 4



**Figure S15:** Powder XRD of compound 4

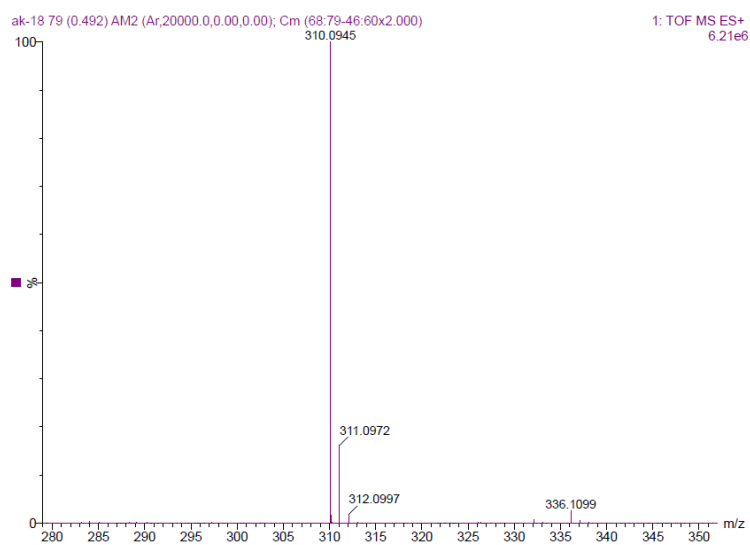


Figure S16: HRMS of compound 4

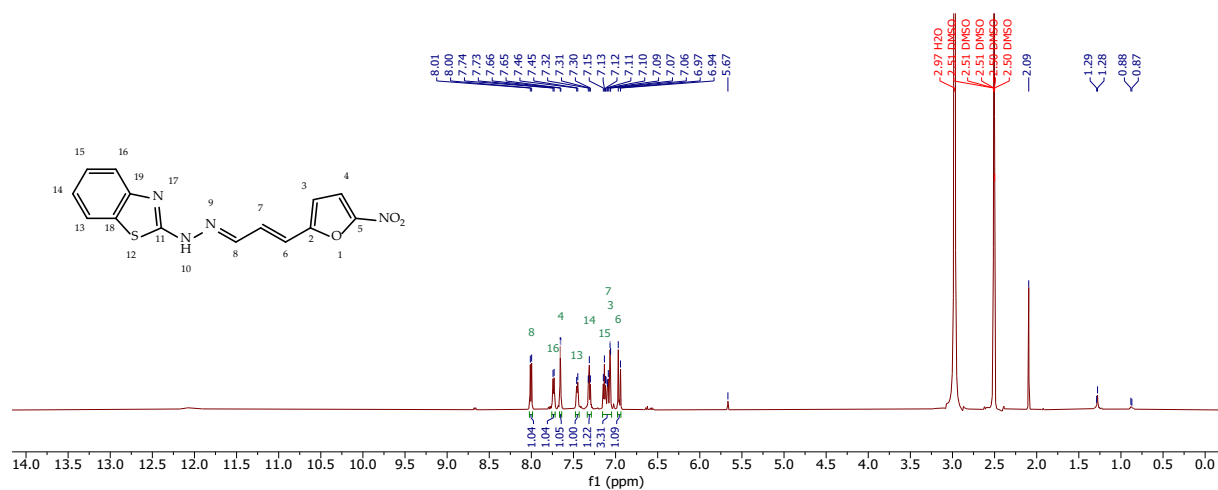


Figure S17:  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 378 K) of compound 5

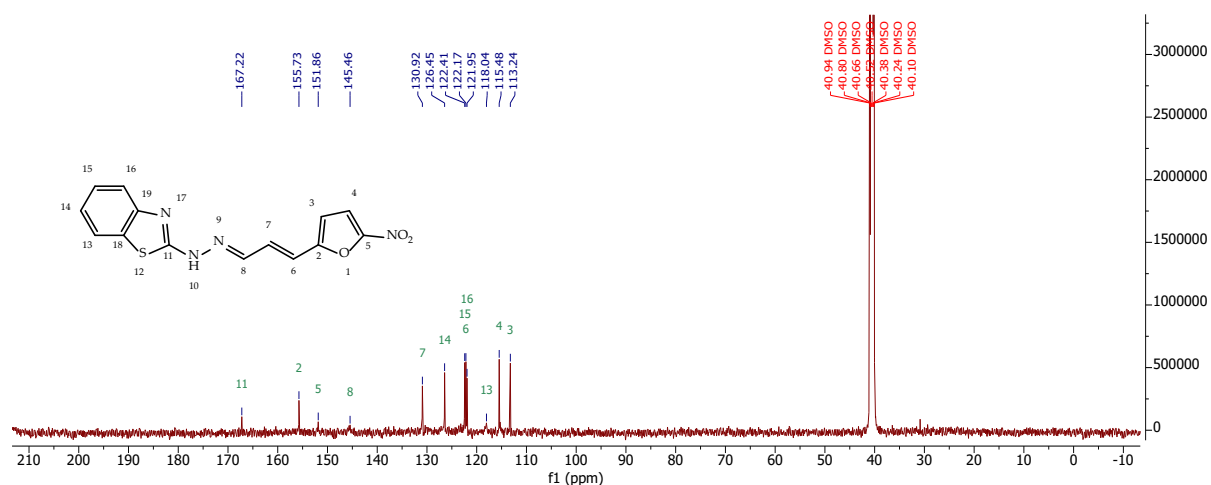
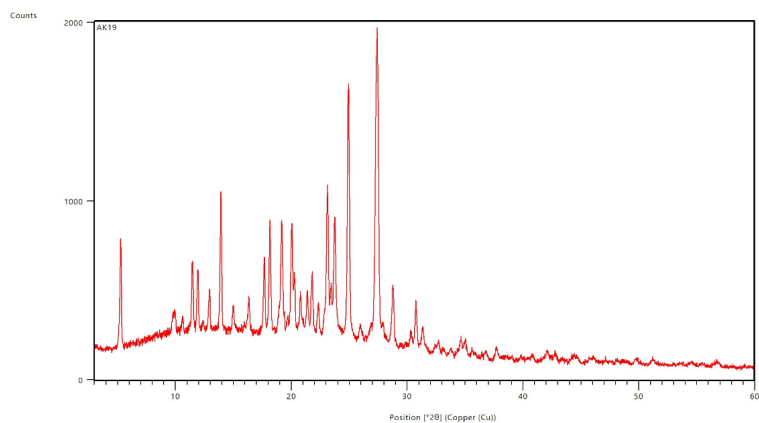
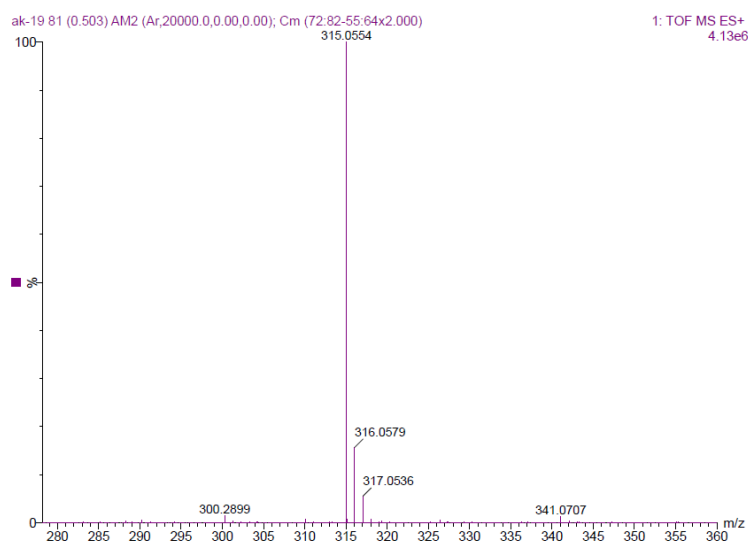


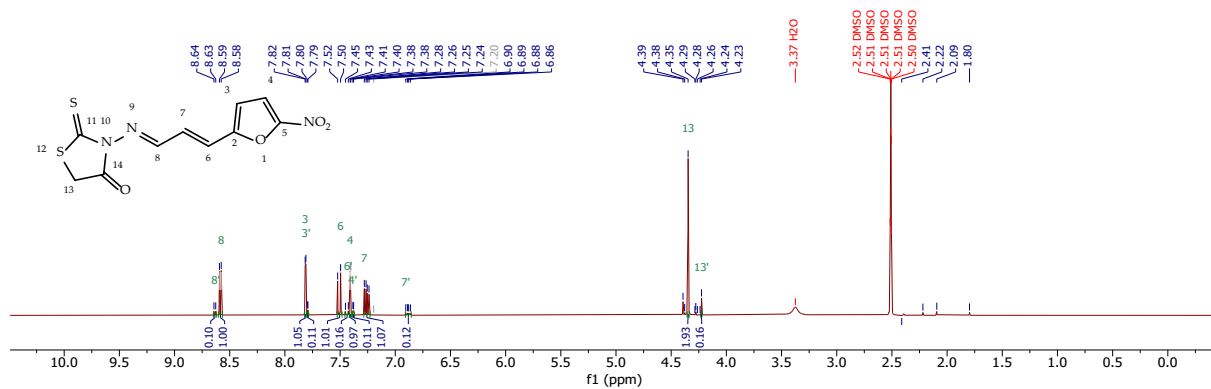
Figure S18:  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ , 378 K) of compound 5



**Figure S19:** Powder XRD of compound 5



**Figure S20:** HRMS of compound 5



**Figure S21:**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound 6

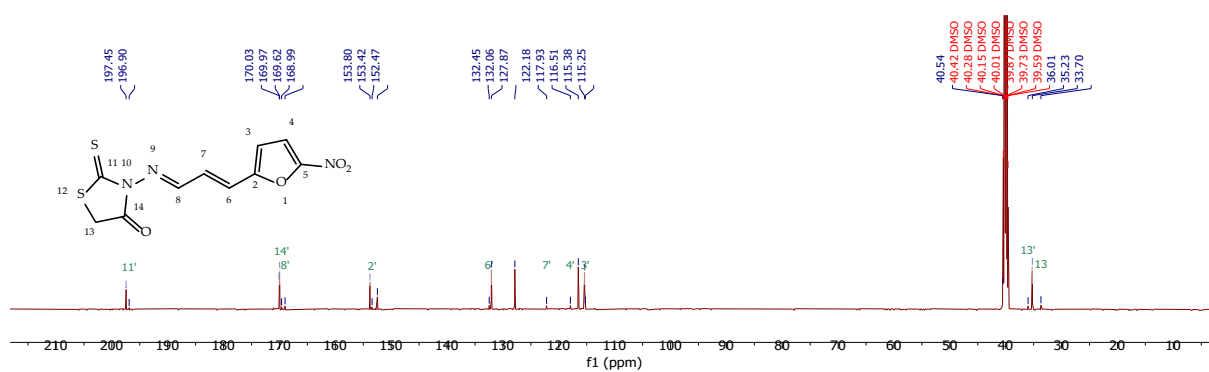


Figure S22: <sup>13</sup>C NMR (150 MHz, DMSO-d<sub>6</sub>, 298 K) of compound 6

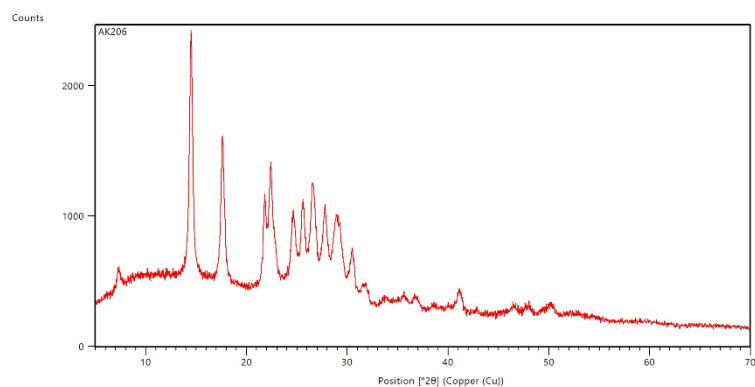


Figure S23: Powder XRD of compound 6

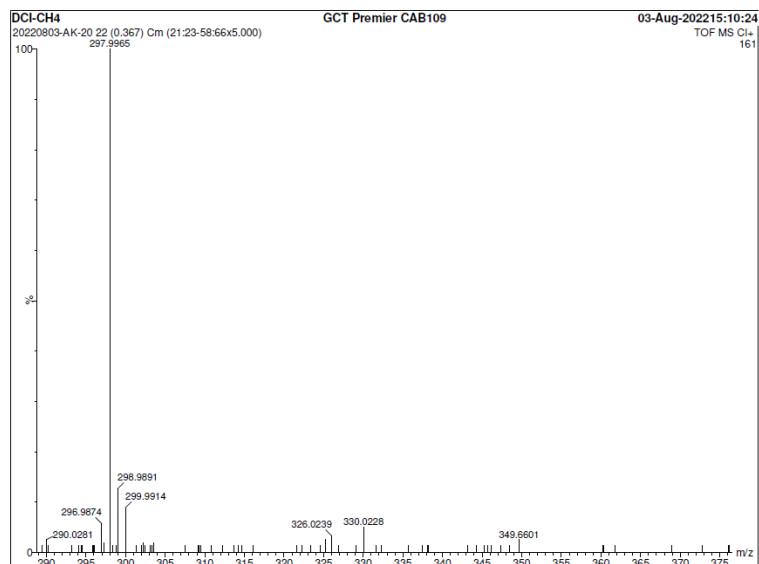


Figure S24: HRMS of compound 6



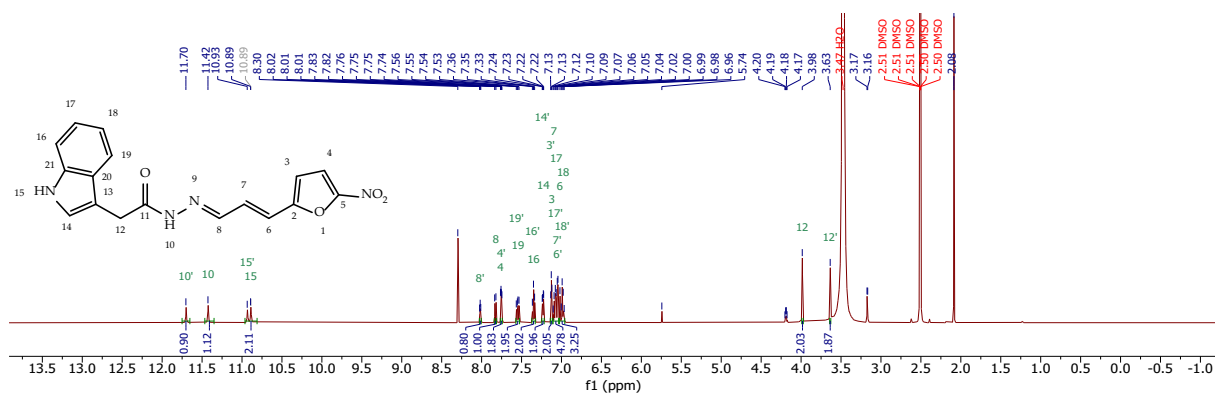


Figure S25:  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound 7

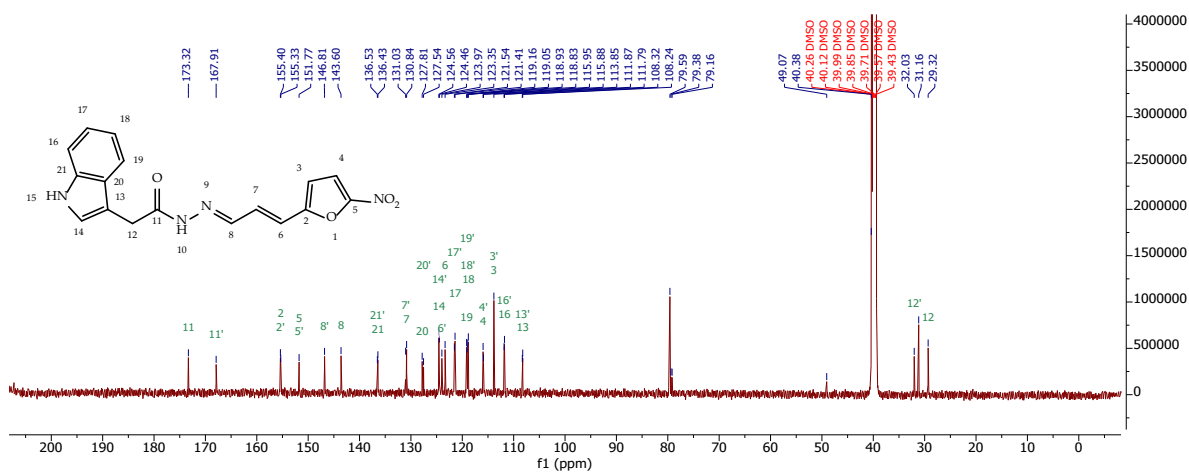


Figure S26:  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ , 298 K) of compound 7

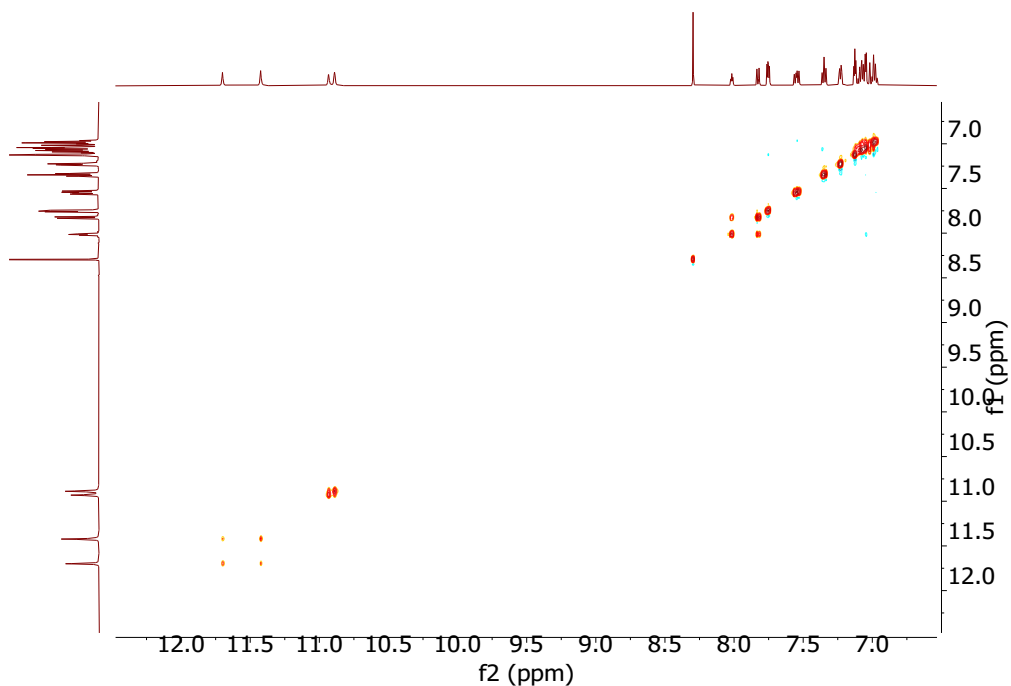
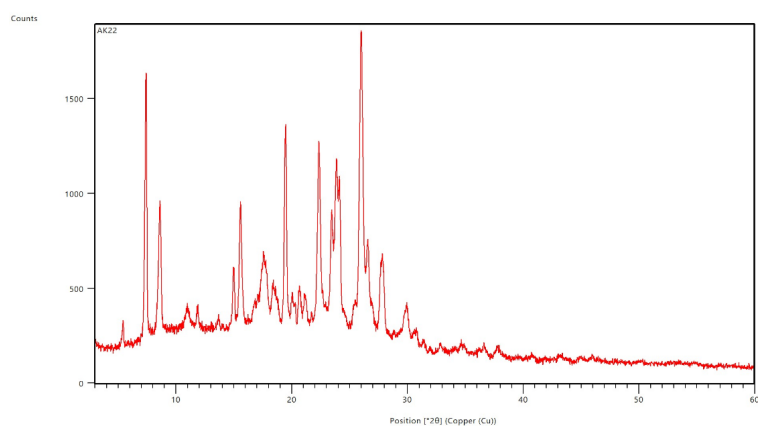


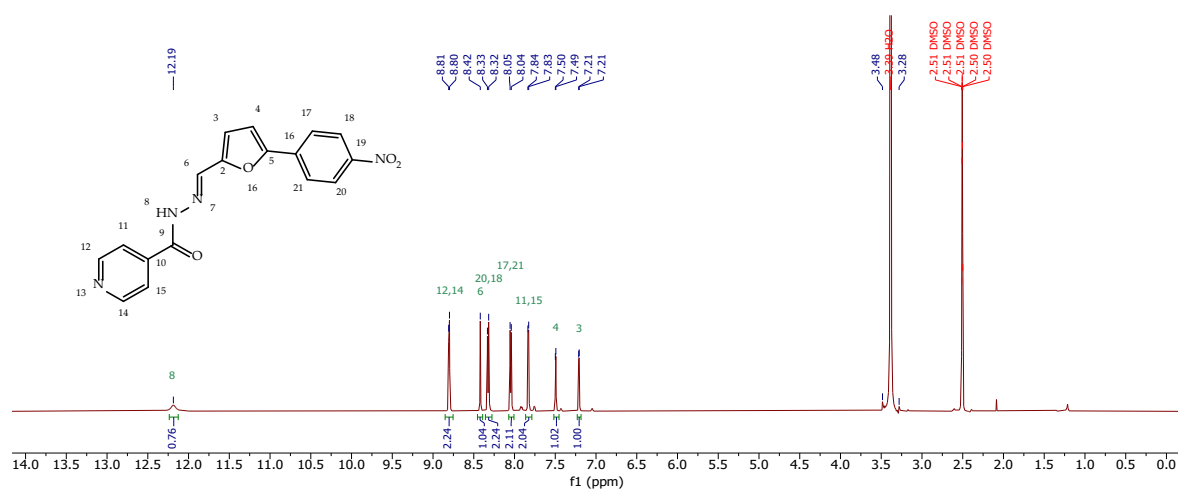
Figure S27: ROESY NMR (DMSO- $d_6$ , 298 K) of compound 7



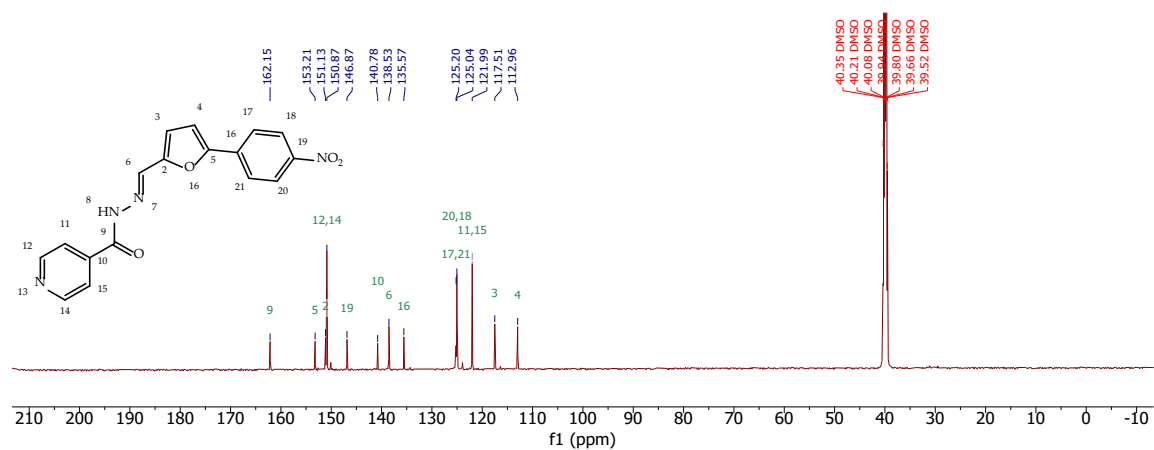
**Figure S28:** Powder XRD of compound **7**



**Figure S29:** HRMS of compound **7**



**Figure S30:** <sup>1</sup>H NMR (600 MHz, DMSO-d<sub>6</sub>, 298 K) of compound 8



**Figure S31:** <sup>13</sup>C NMR (150 MHz, DMSO-d<sub>6</sub>, 298 K) of compound 8

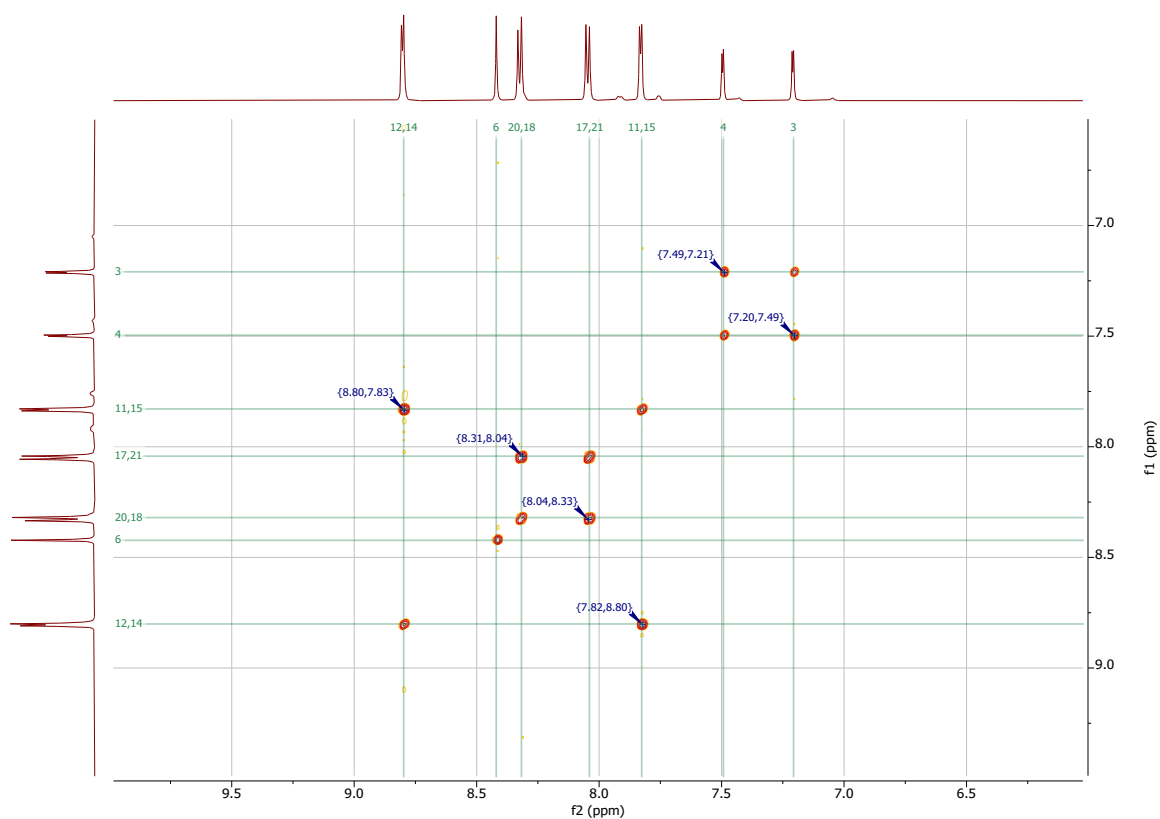


Figure S32: COSY NMR (DMSO-d<sub>6</sub>, 298 K) of compound 8

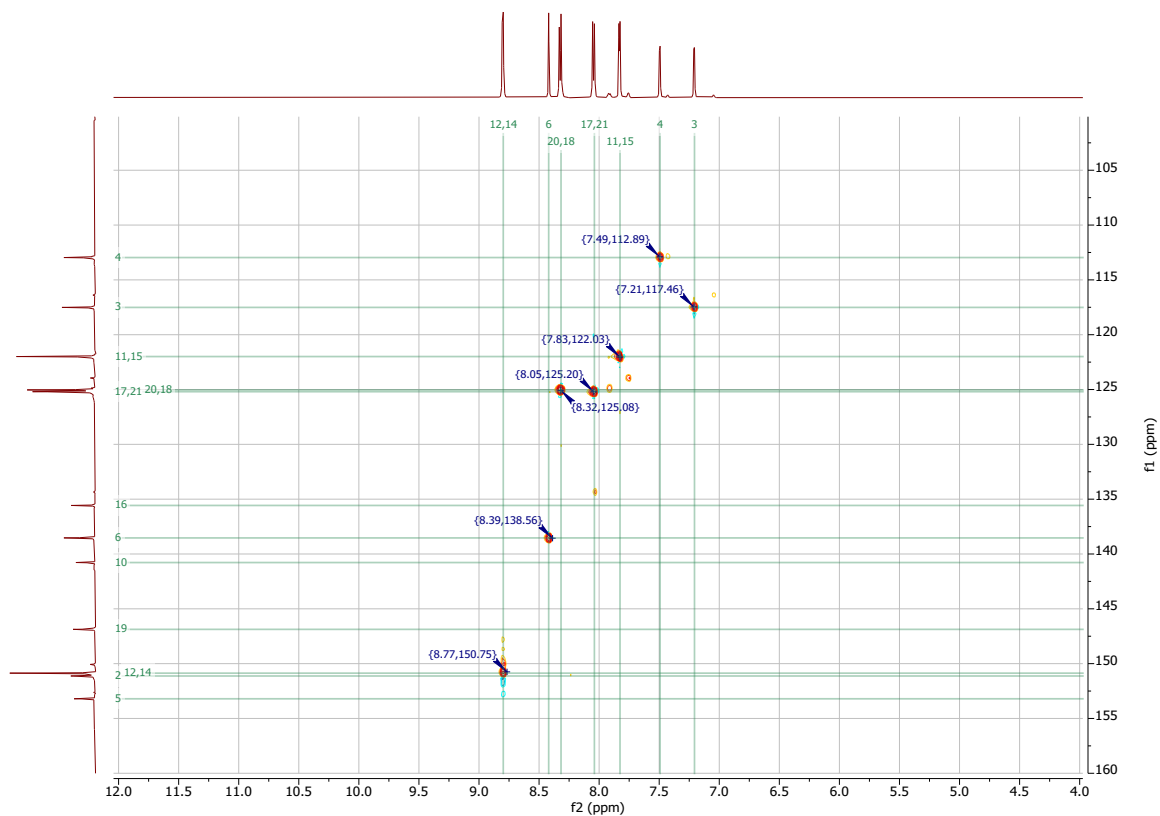


Figure S33: HSQS NMR (DMSO-d<sub>6</sub>, 298 K) of compound 8

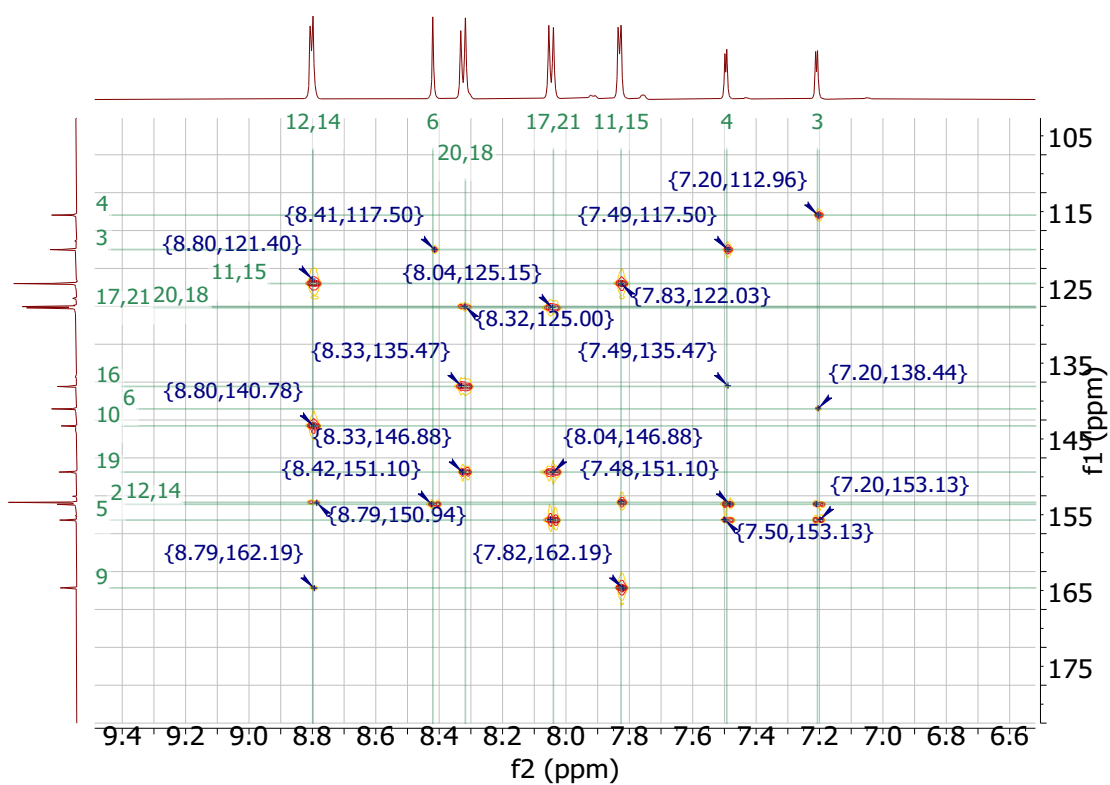


Figure S34: HMBC NMR (DMSO-d<sub>6</sub>, 298 K) of compound 8

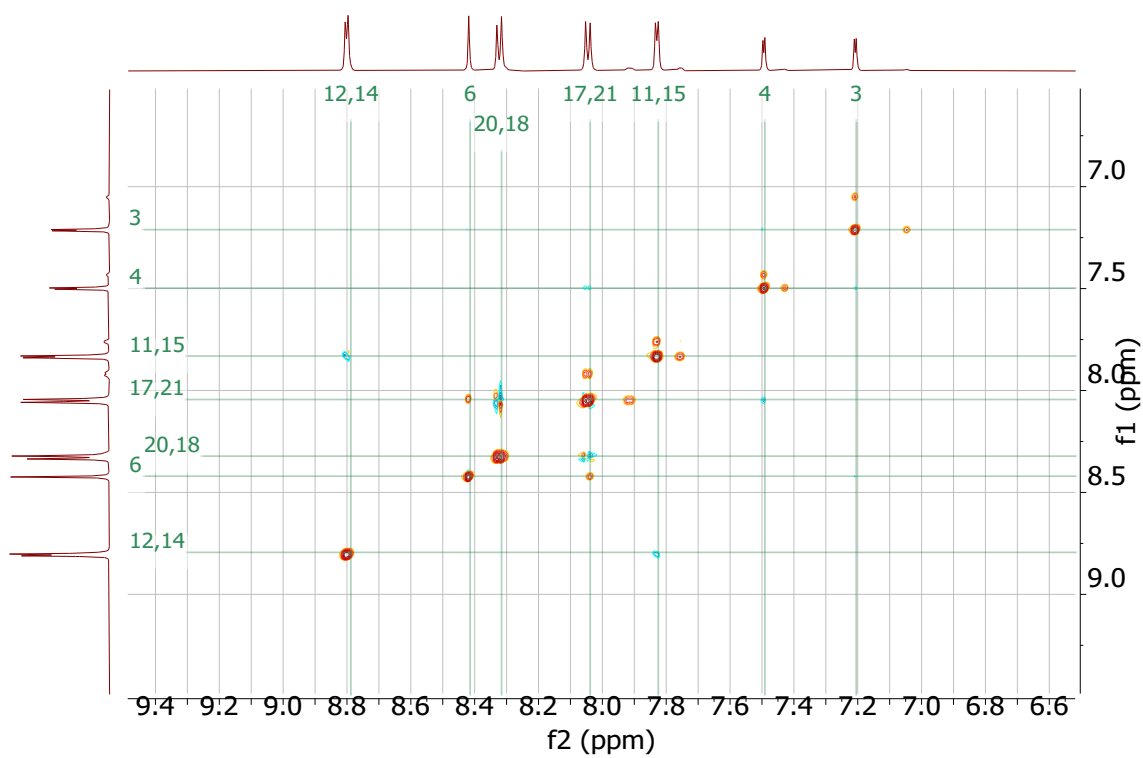
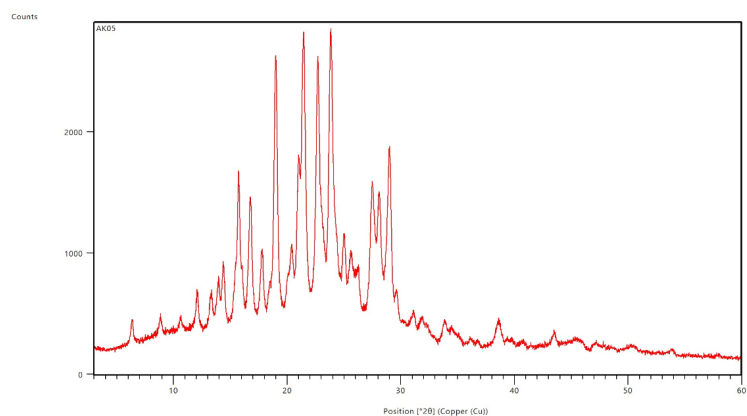
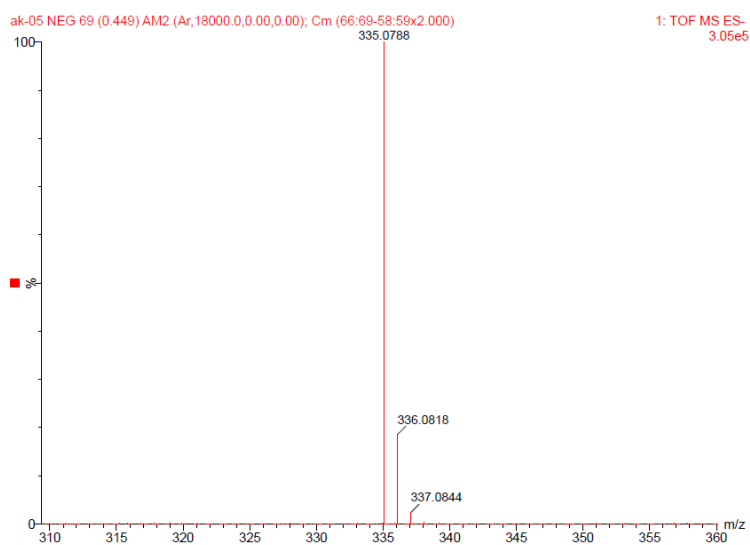


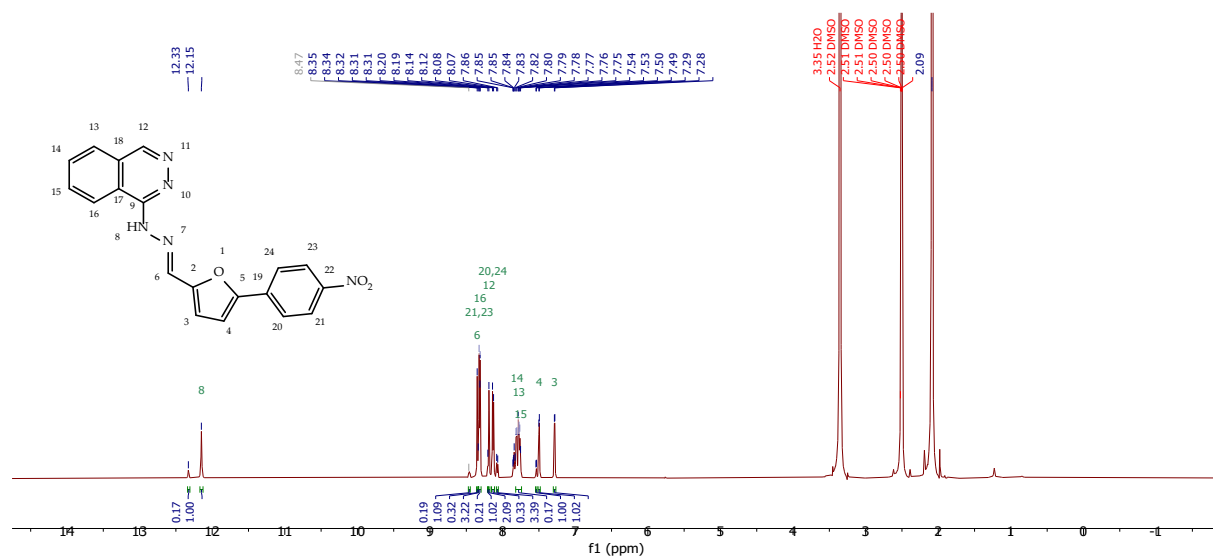
Figure S35: ROESY NMR (DMSO-d<sub>6</sub>, 298 K) of compound 8



**Figure S36:** Powder XRD of compound **8**



**Figure S37:** HRMS of compound **8**



**Figure S38:**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound **9**

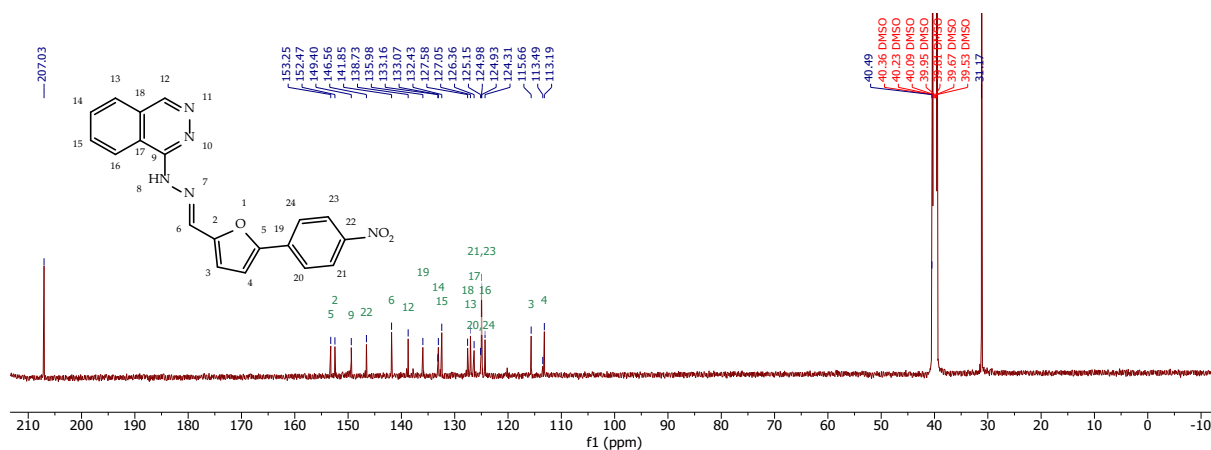


Figure S39:  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ , 298 K) of compound 9

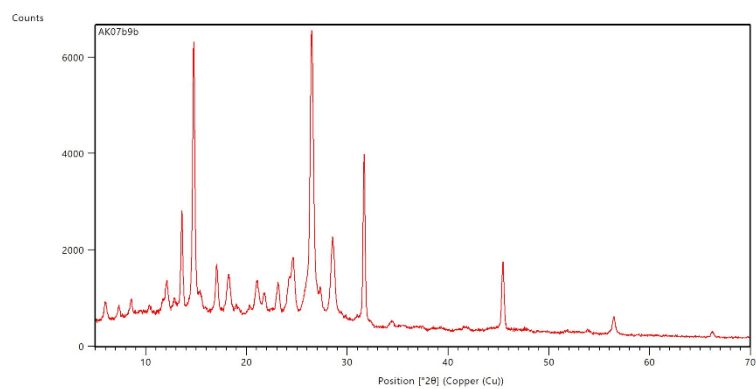


Figure S40: Powder XRD of compound 9

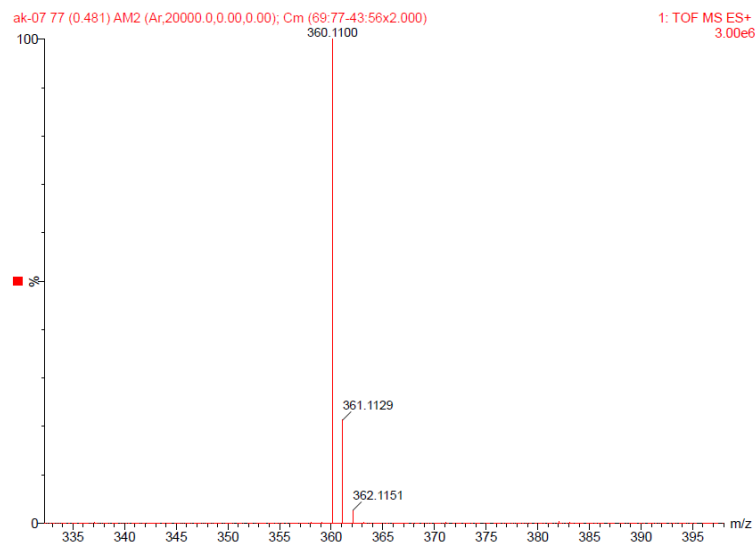
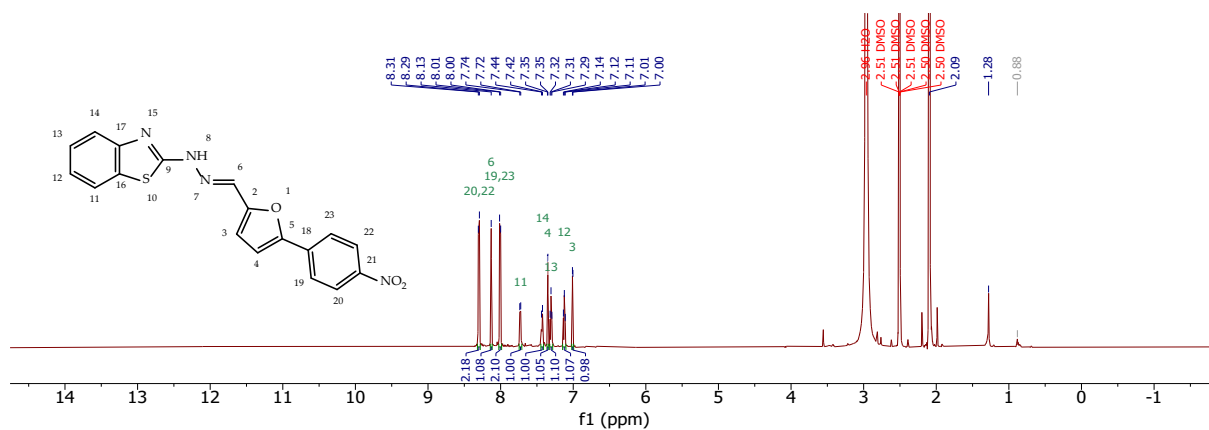
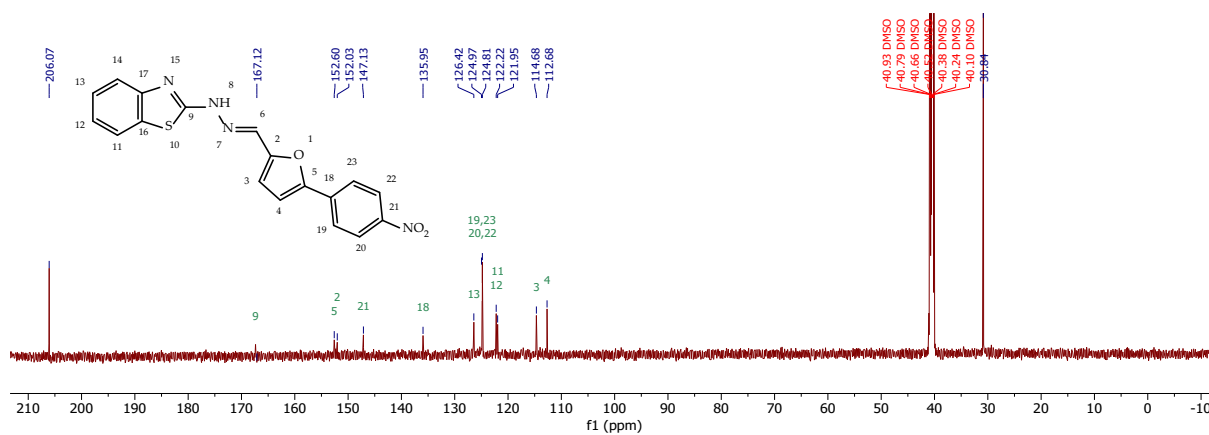


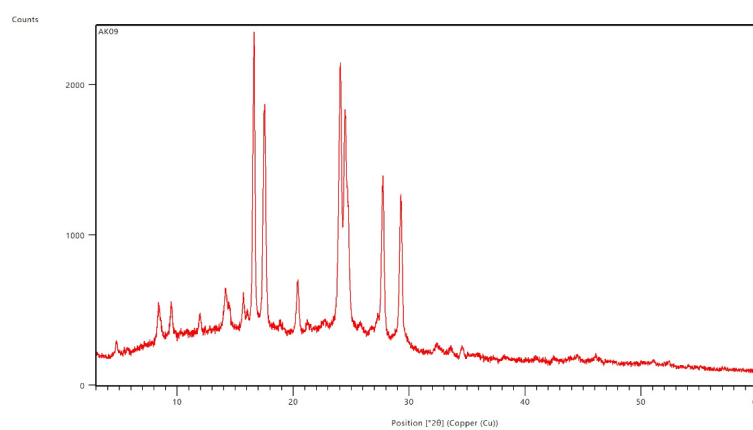
Figure S41: HRMS of compound 9



**Figure S42:** <sup>1</sup>H NMR (600 MHz, DMSO-d<sub>6</sub>, 383 K) of compound **10**



**Figure S43:** <sup>13</sup>C NMR (150 MHz, DMSO-d<sub>6</sub>, 383 K) of compound **10**



**Figure S44:** Powder XRD of compound **10**



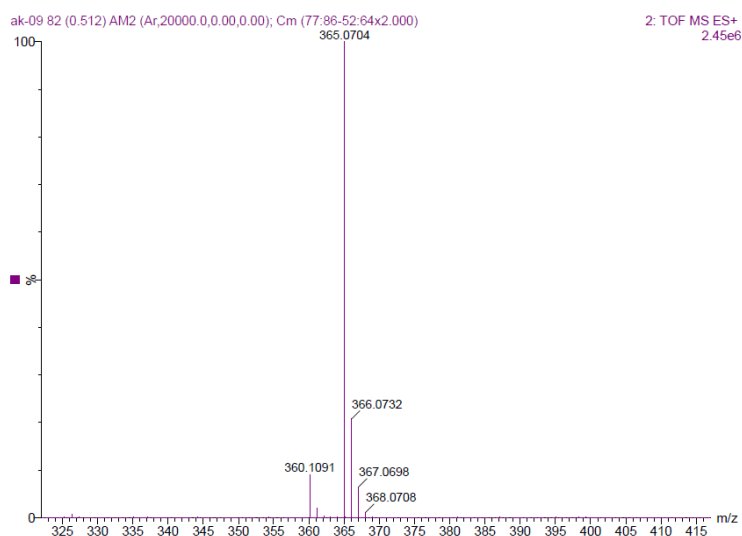


Figure S45: HRMS of compound 10

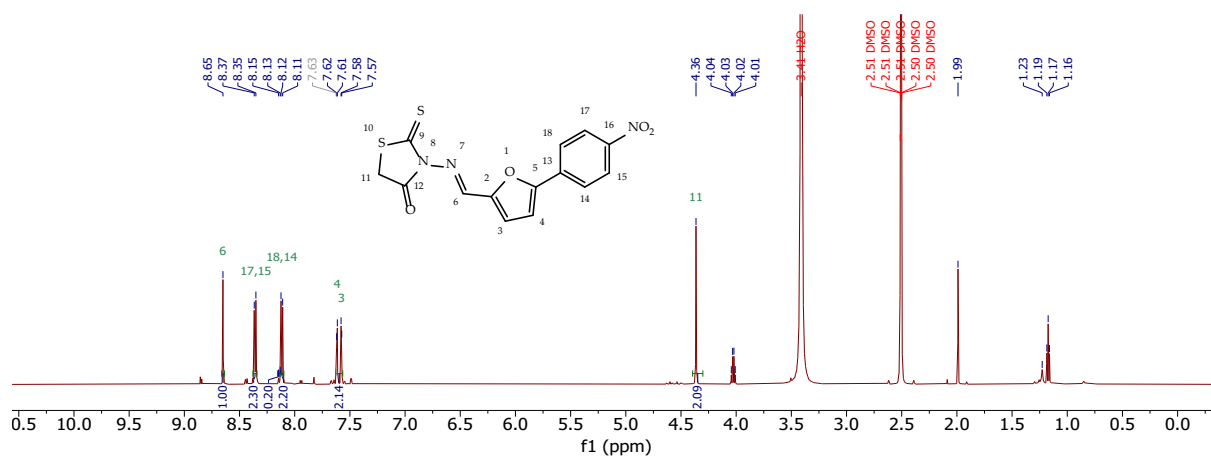


Figure S46:  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound 11

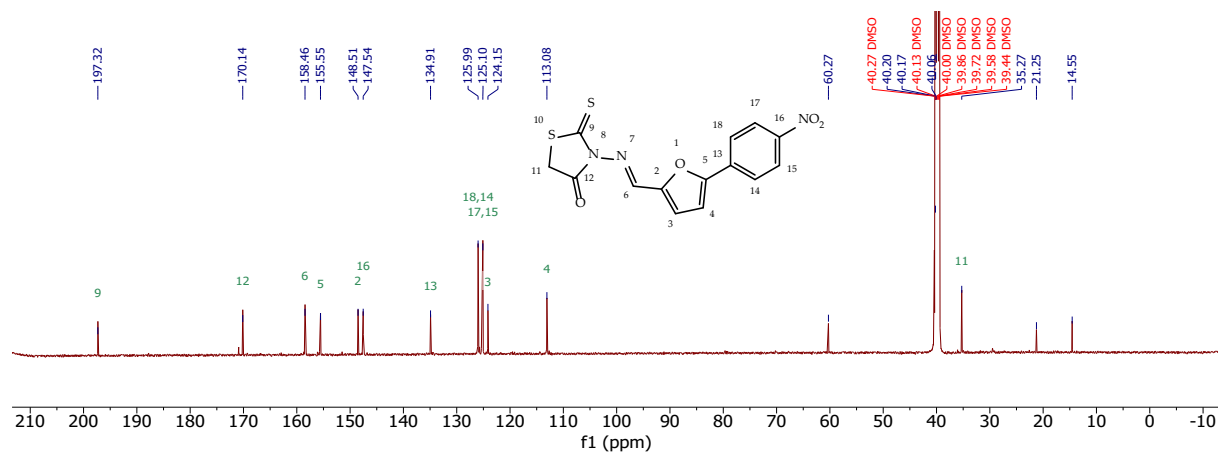


Figure S47:  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ , 298 K) of compound 11

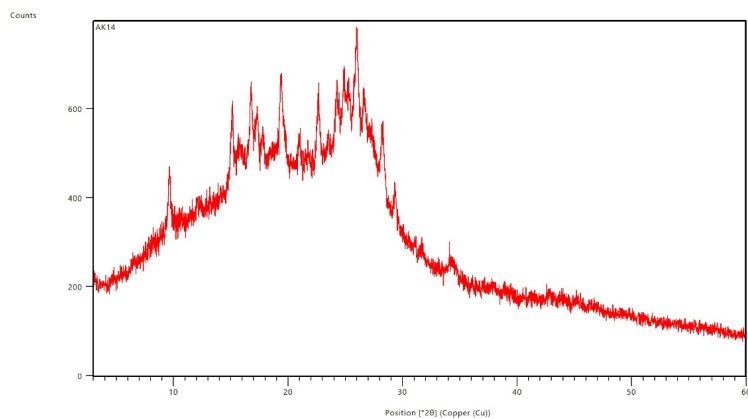


Figure S48: Powder XRD of compound 11

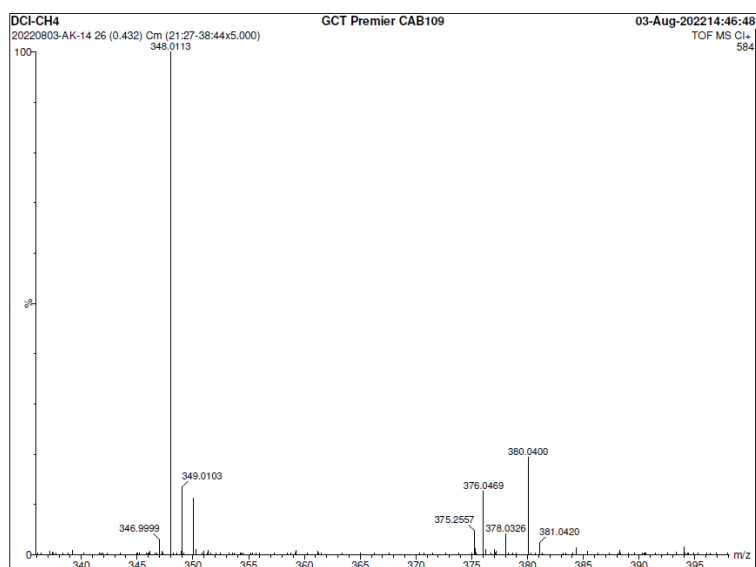


Figure S49: HRMS of compound 11

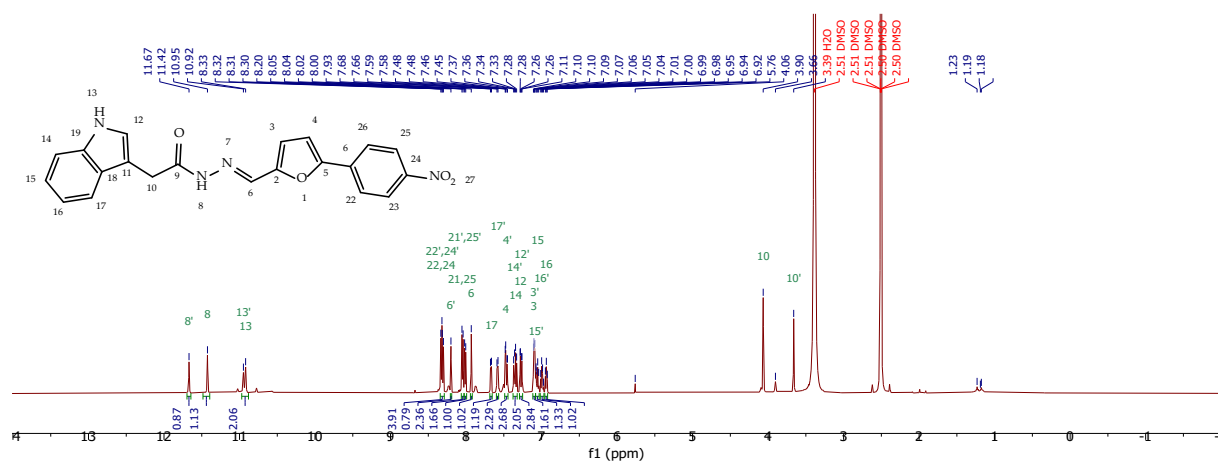


Figure S50: <sup>1</sup>H NMR (600 MHz, DMSO-d<sub>6</sub>, 298 K) of compound 12

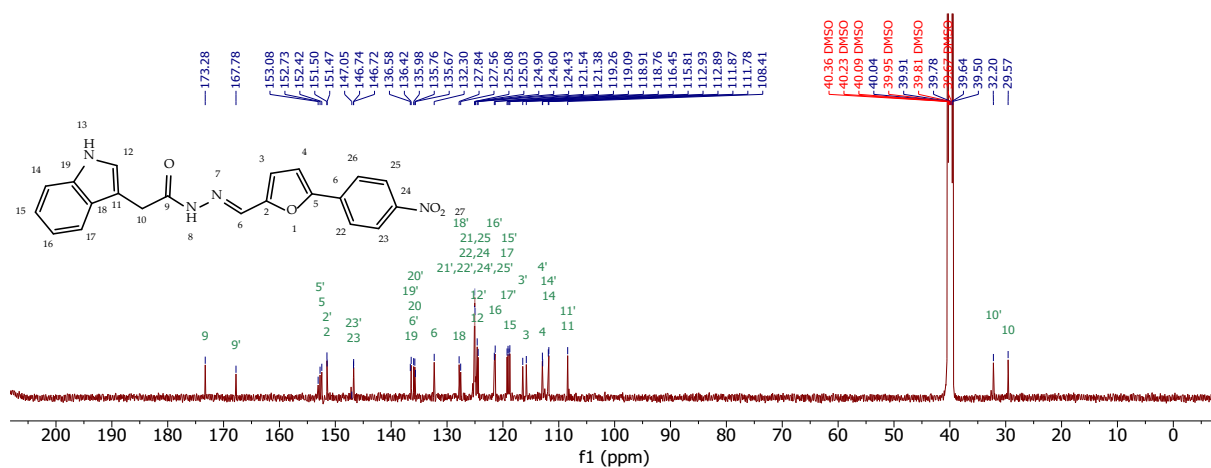


Figure S51:  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ , 298 K) of compound 12

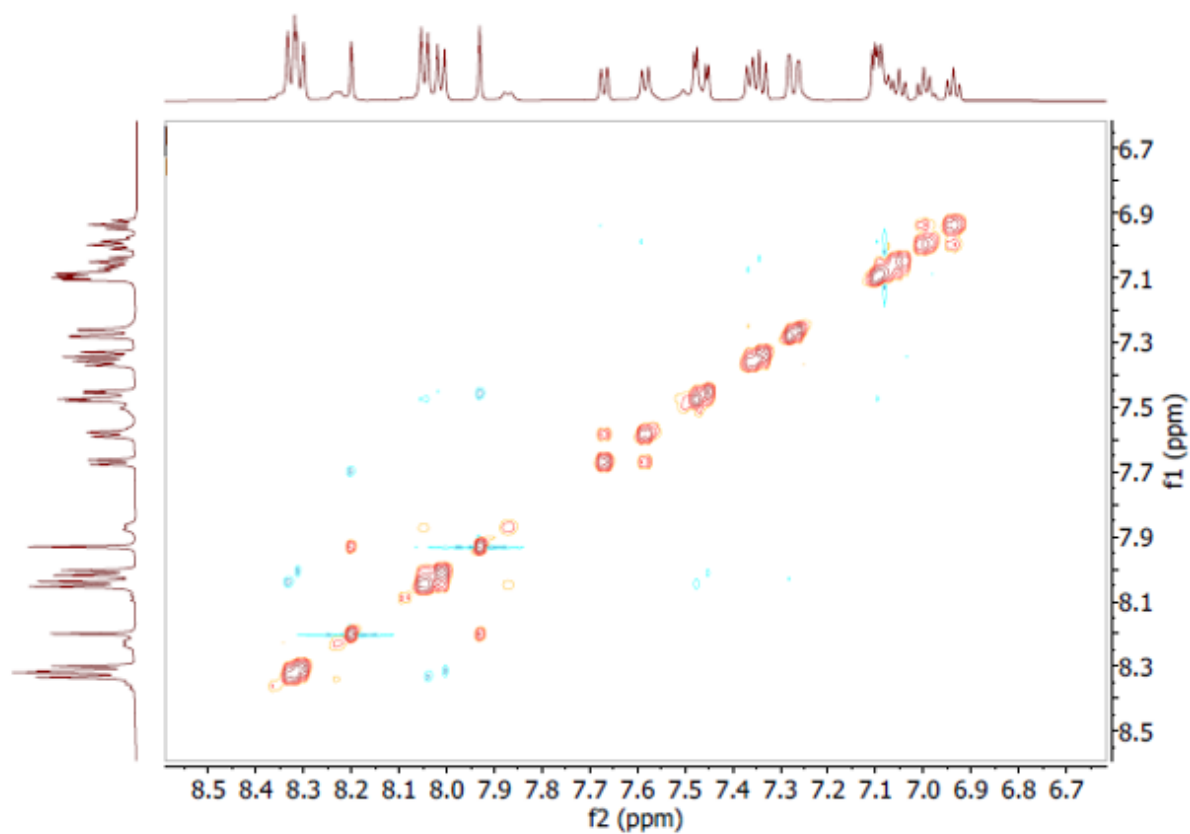
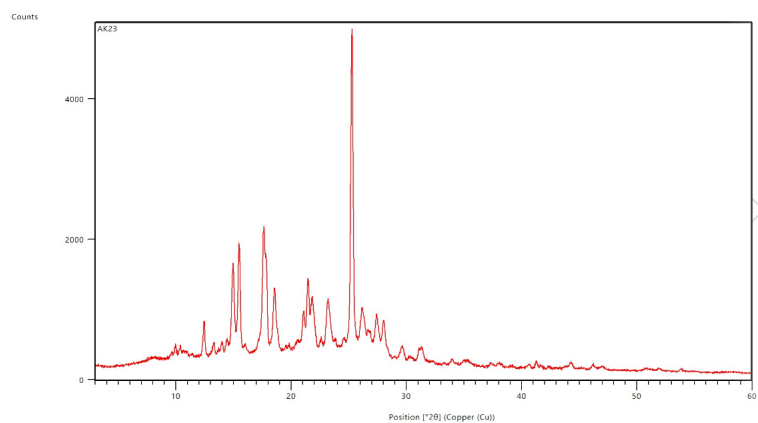
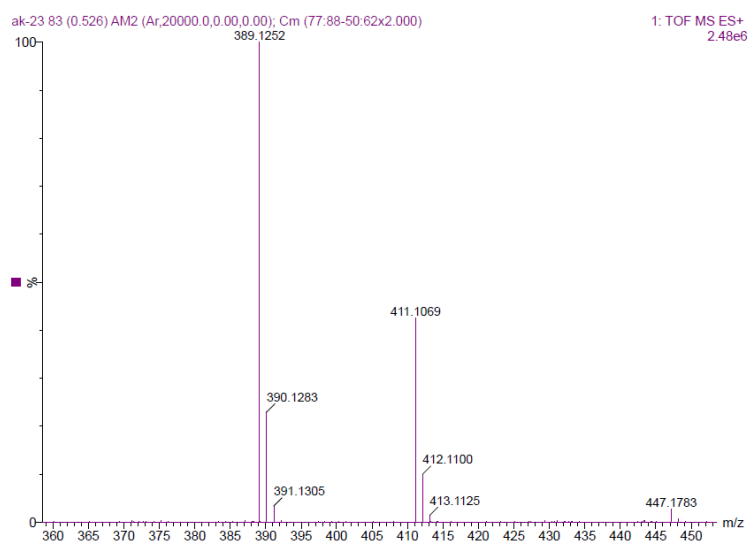


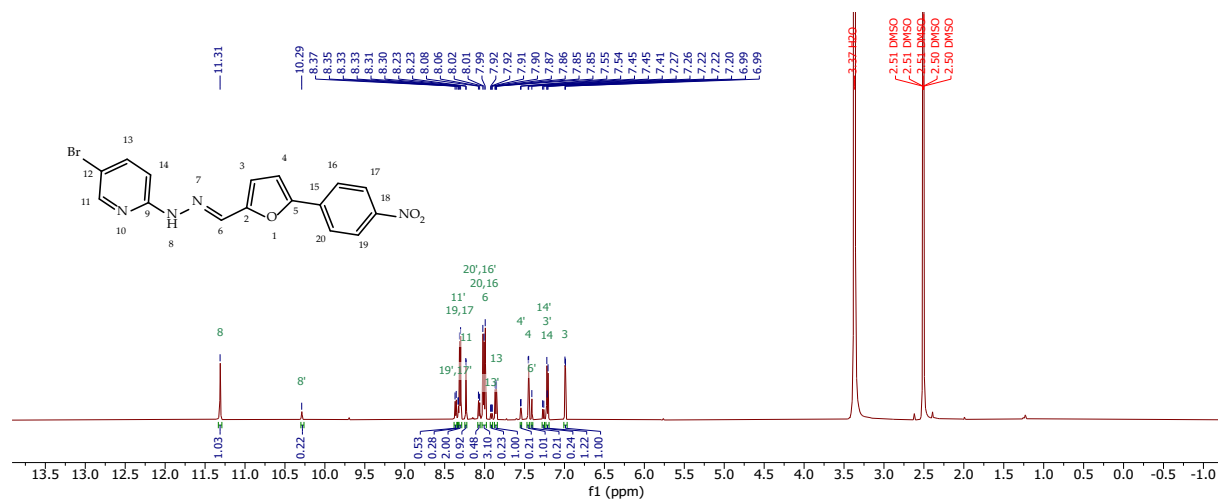
Figure S52: ROESY NMR (DMSO- $d_6$ , 298 K) of compound 12



**Figure S53:** Powder XRD of compound **12**



**Figure S54:** HRMS of compound **12**



**Figure S55:**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound **13**

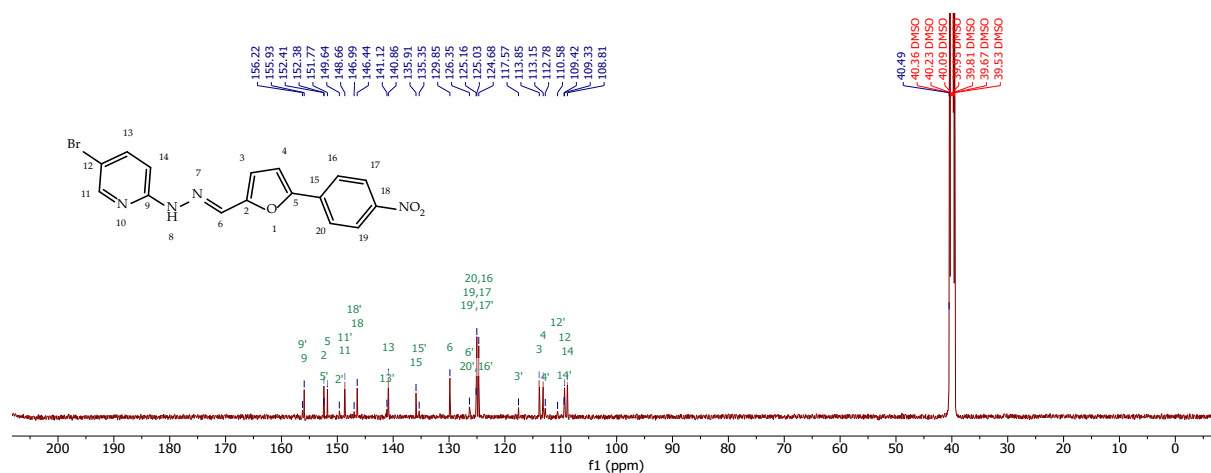


Figure S56: <sup>13</sup>C NMR (150 MHz, DMSO-d<sub>6</sub>, 298 K) of compound 13

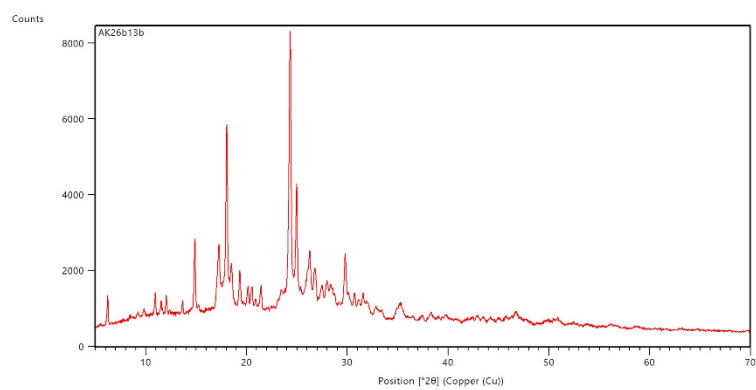


Figure S57: Powder XRD of compound 13

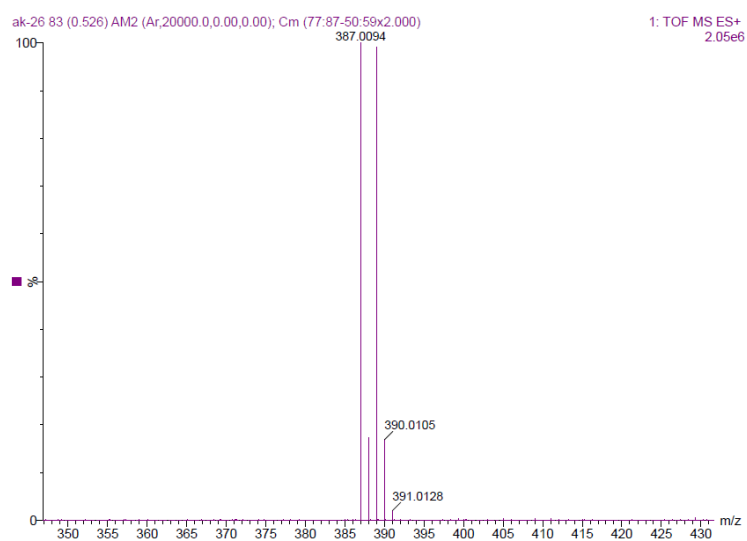


Figure S58: HRMS of compound 13

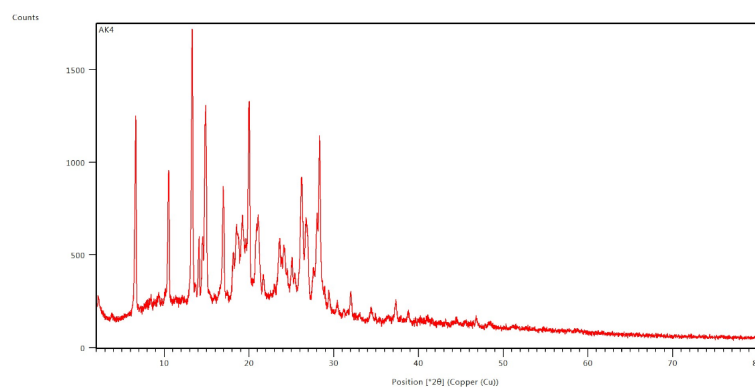
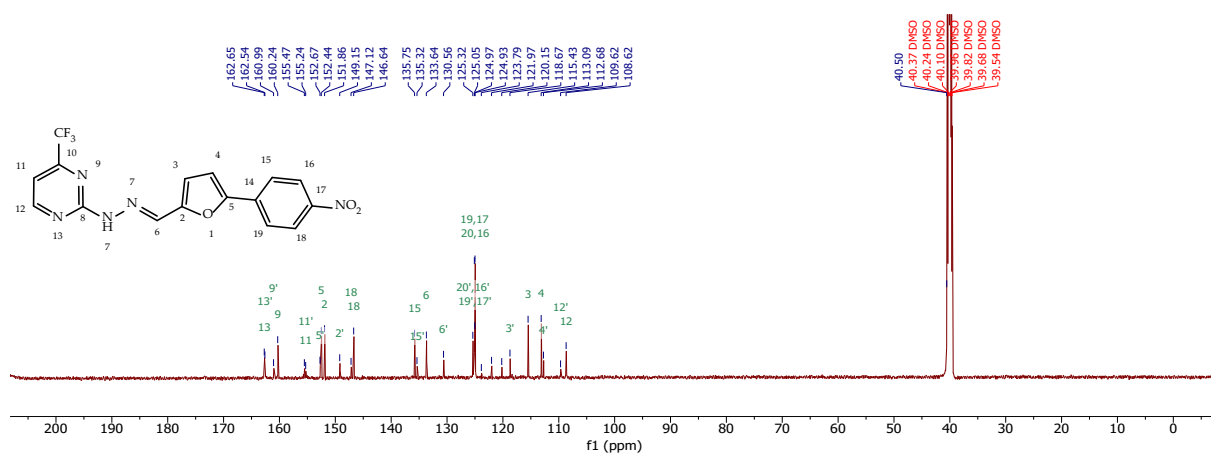
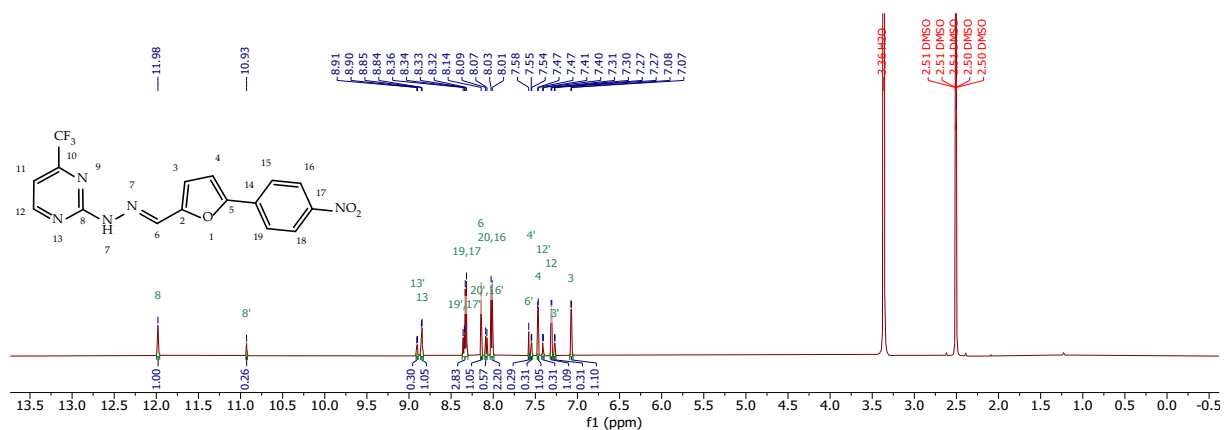




Figure S62: HRMS of compound 14

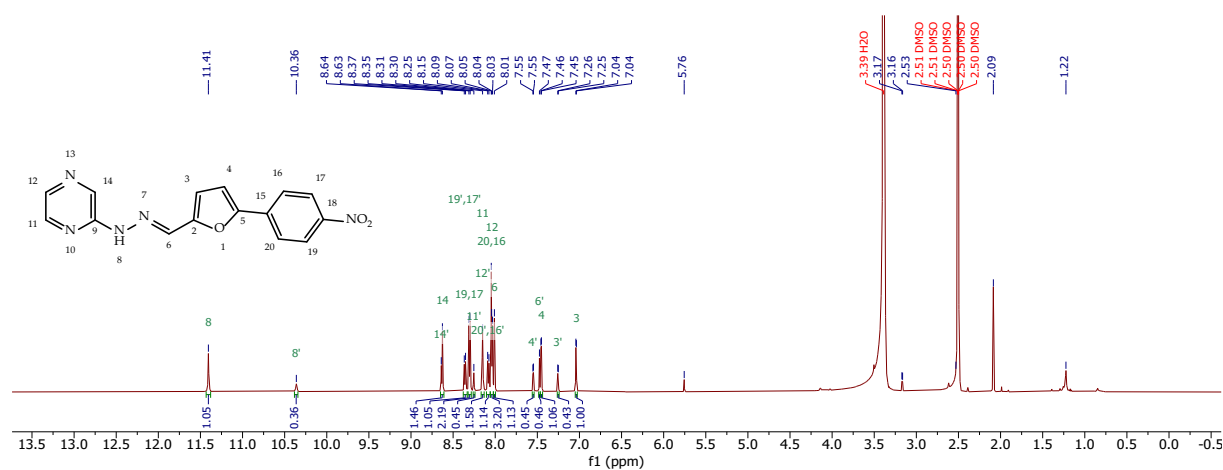


Figure S63:  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound 15

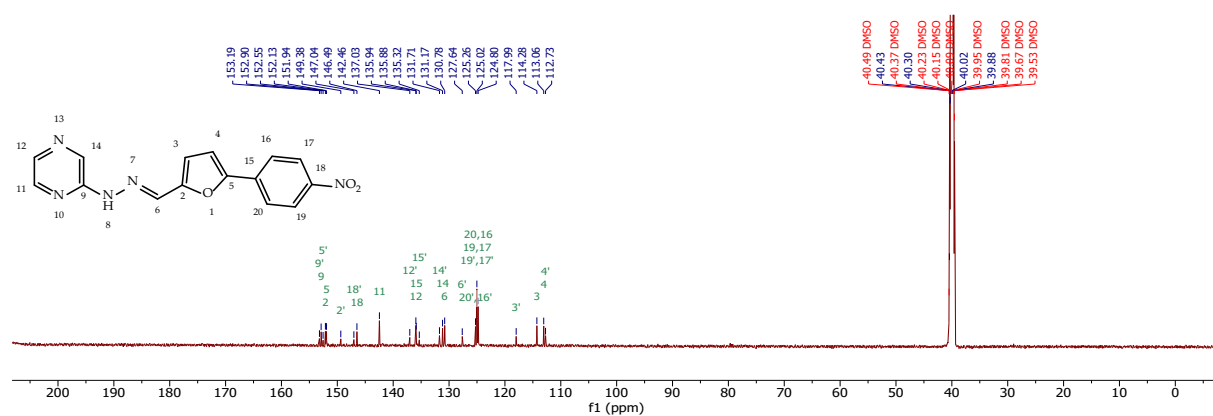
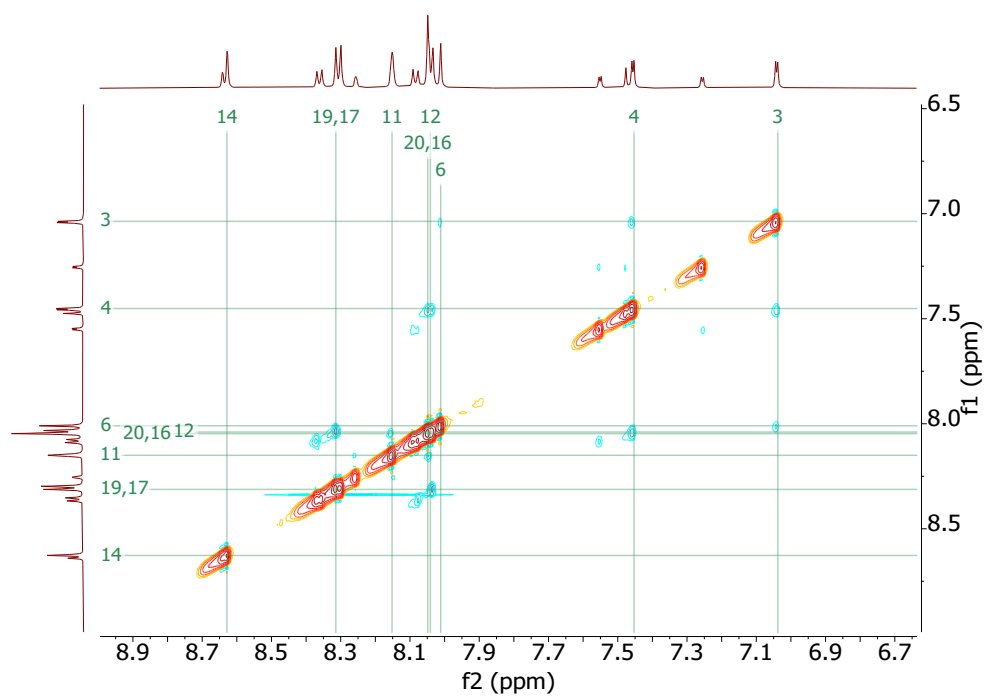
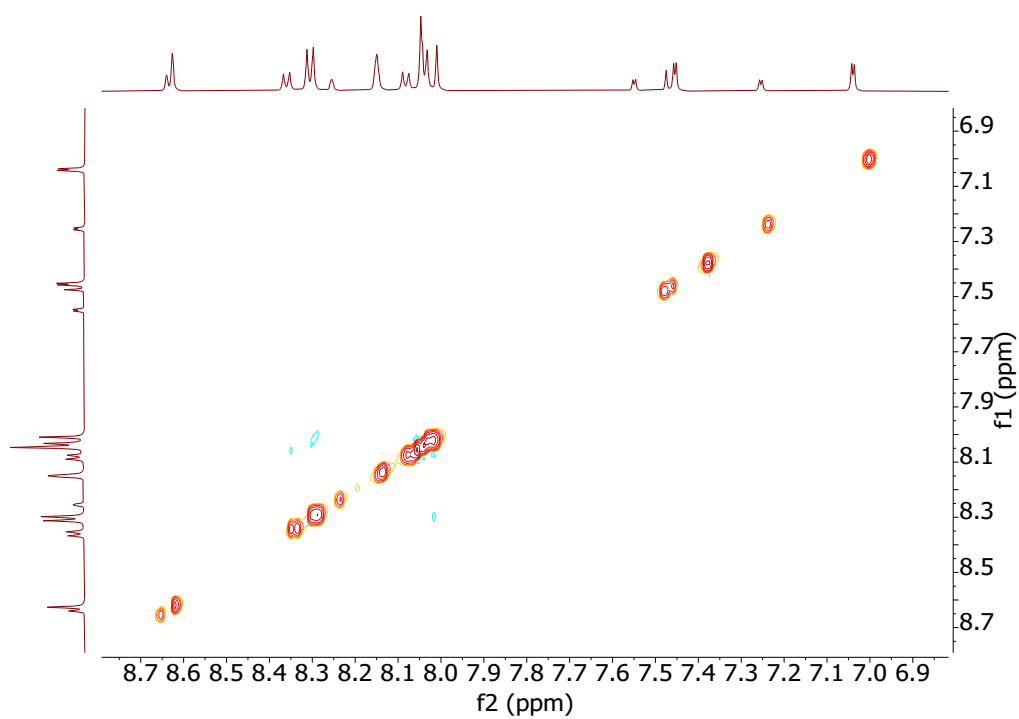


Figure S64:  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ , 298 K) of compound 15

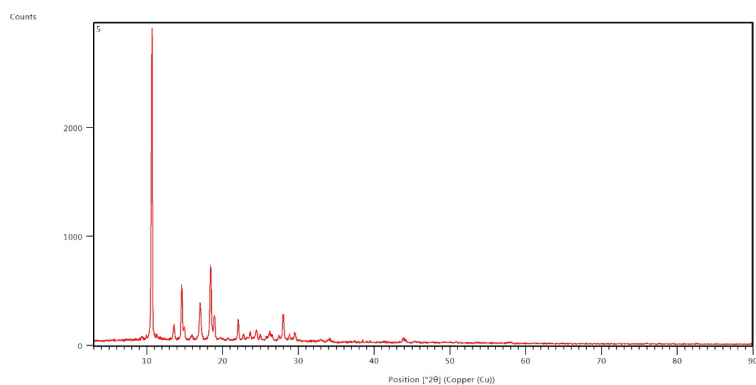


**Figure S65a:** ROESY NMR (DMSO-d<sub>6</sub>, 298 K) of compound 15

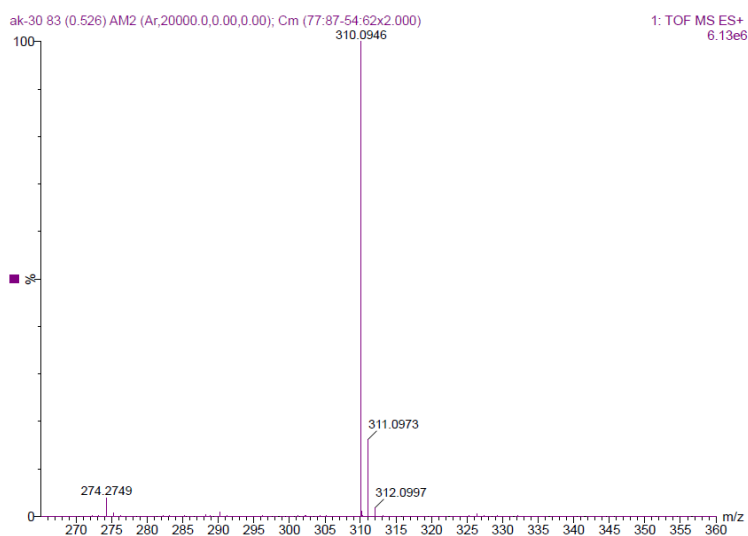


**Figure S65b:** ROESY NMR (DMSO-d<sub>6</sub>, 348 K) of compound 15

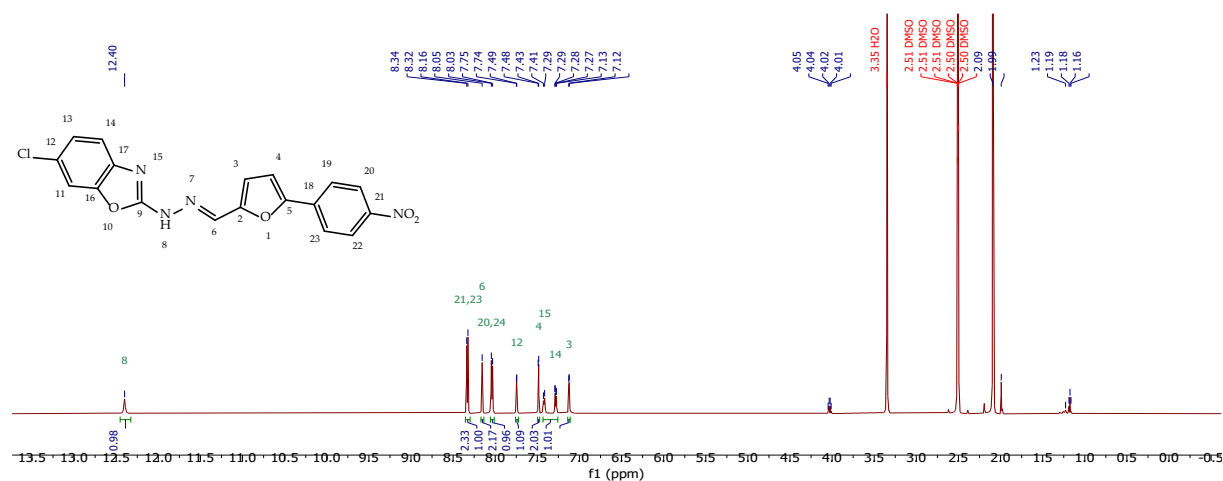




**Figure S66:** Powder XRD of compound **15**



**Figure S67:** HRMS of compound **15**



**Figure S68:**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound **16**

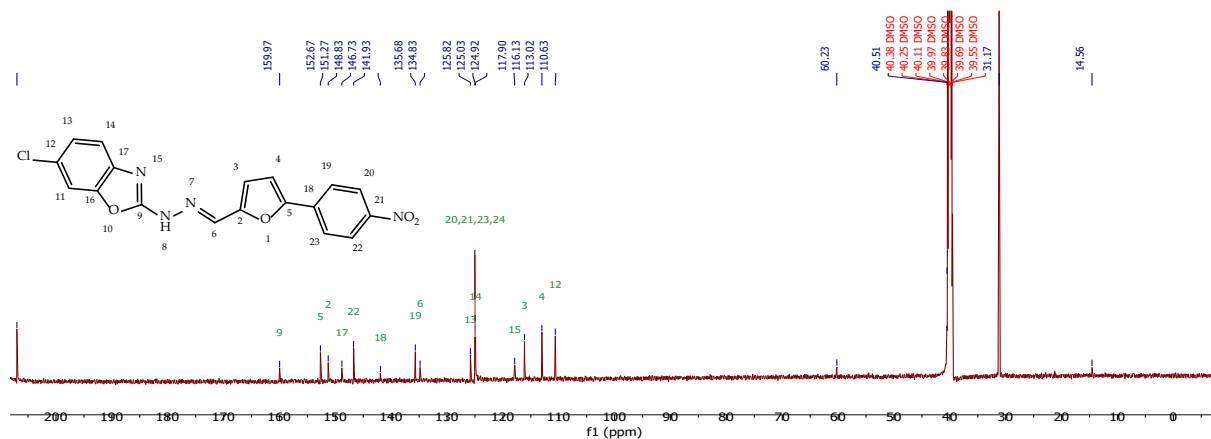


Figure S69:  $^{13}\text{C}$  NMR (150 MHz, DMSO-d<sub>6</sub>, 298 K) of compound 16

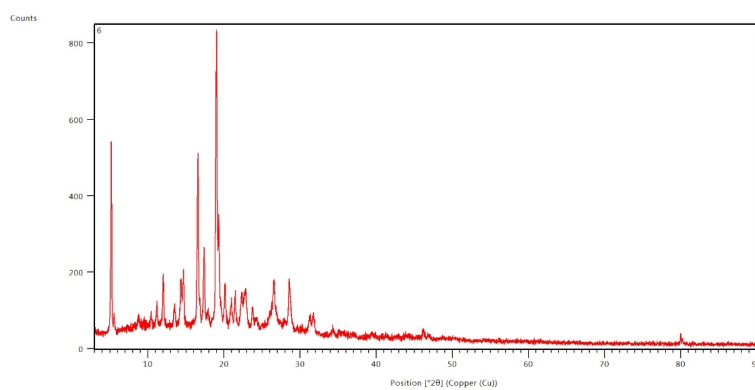


Figure S70: Powder XRD of compound 16

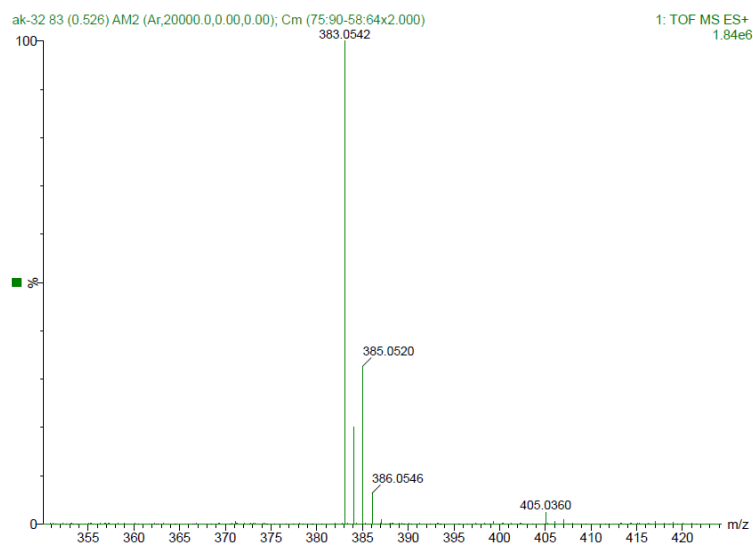
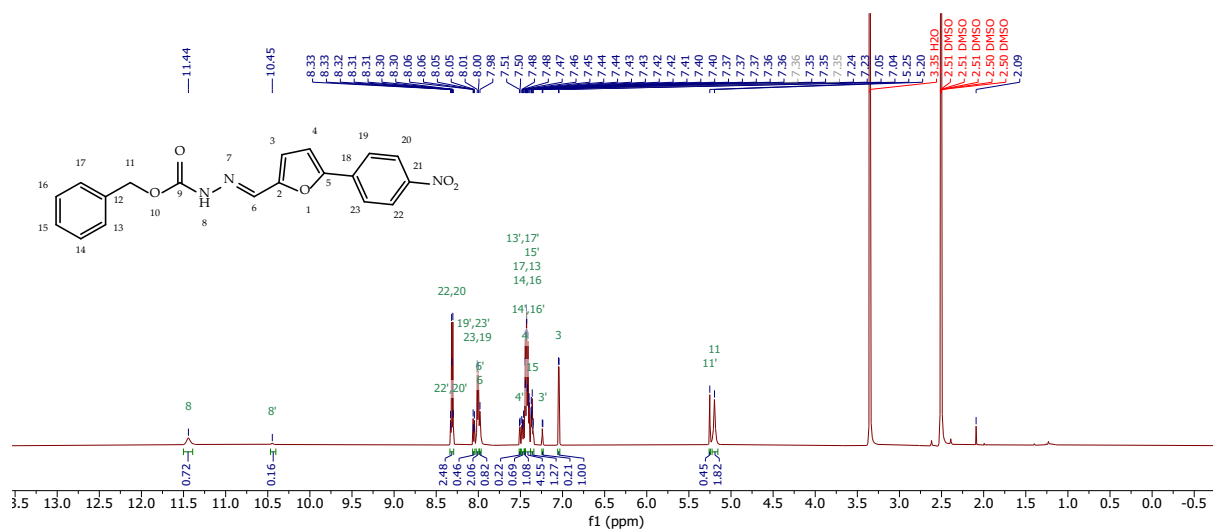
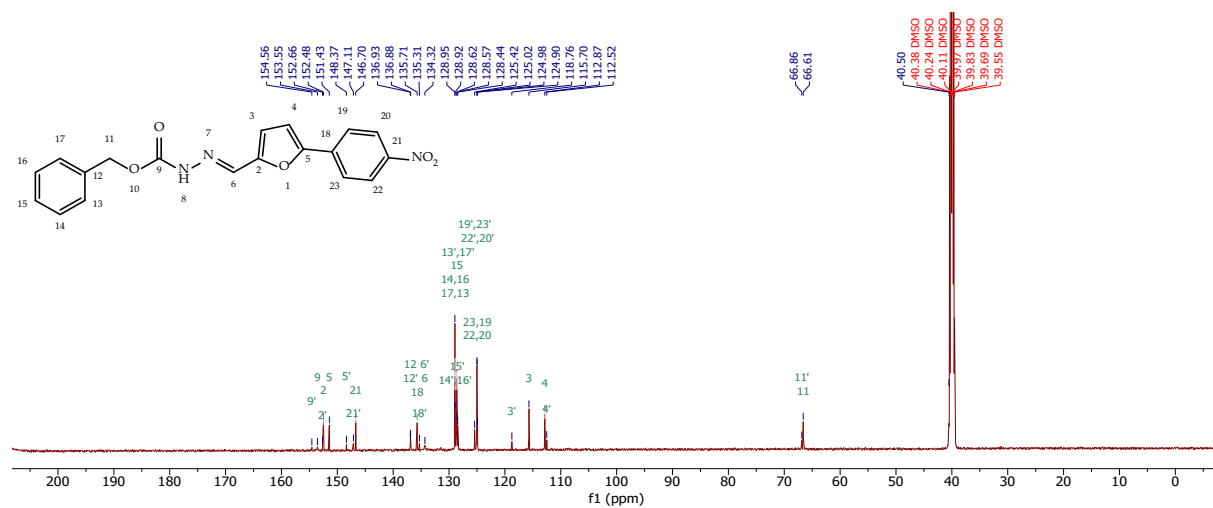


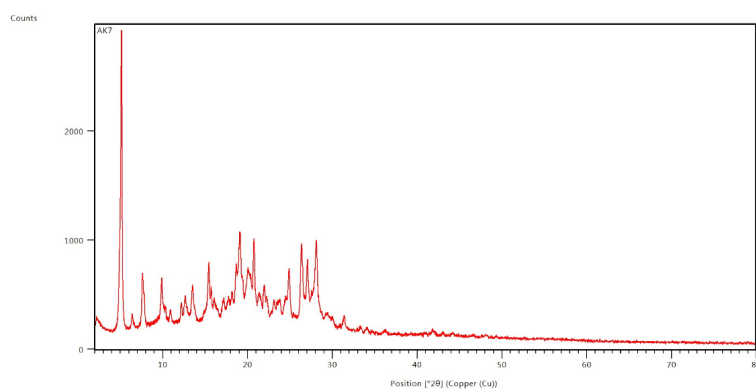
Figure S71: HRMS of compound 16



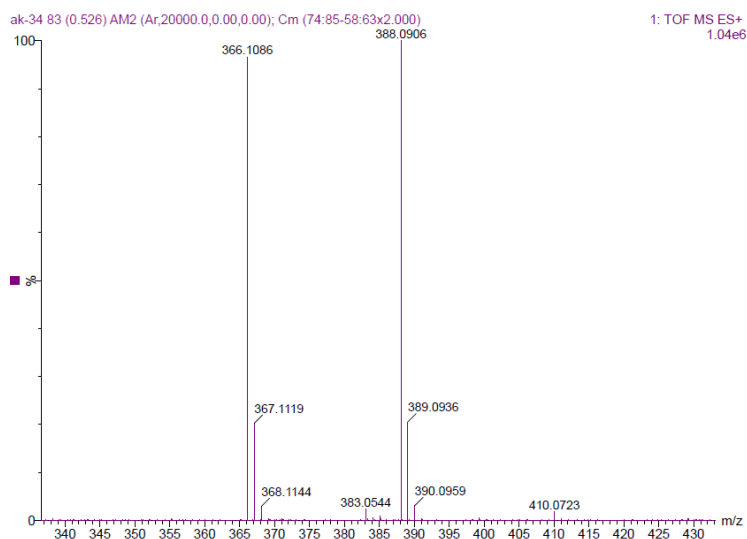
**Figure S72:**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ , 298 K) of compound **17**



**Figure S73:**  $^{13}\text{C}$  NMR (150 MHz, DMSO- $d_6$ , 298 K) of compound **17**



**Figure S74:** Powder XRD of compound **17**



**Figure S75:** HRMS of compound **17**

**Table S1a.**  $^1\text{H}$  NMR Spectroscopic Data of **1–7** in DMSO- $d_6$  ( $\delta$  in ppm, J in Hz)

No.	1	1'	2	3	4	5	6	6'	7	7'
CH <sub>3</sub>	3.84, s	3.73, s								
2	7.33, d (1.9)	7.39, d (1.9)	7.30, s							
3				7.21, d (4.0)	7.07, d (4)	7.06, d (3.9)	7.81, d (3.9)	7.79, d (3.9)	7.12, t (4.3)	7.12, t (4.3)
4				7.79, d (4.0)	7.84 – 7.75, m	7.65, d (3.9)	7.41, d (4.0)	7.38, d (4.0)	7.76, d (4.0)	7.75, d (4.0)
5	7.12, dd (8.2) (1.9)	7.07, d (1.9)	6.84, m							
6	6.86, d (8.1)	6.78, d (8.1)	7.06, d (8.2)	7.18 – 7.15, m	7.10, s	6.95, d (16.0)	7.51, d (16.0)	7.44, d (15.5)	7.02 – 6.96, m	7.11 – 7.03, m
7	8.35, s	7.98, s	8.31, s	7.18 – 7.15, m	7.26, dd (16.0) (9.7)	7.12 – 7.08, m	7.26, dd (16.0) (9.6)	6.88, dd (15.5) (9.7)	7.11 – 7.03, m	7.11 – 7.03, m
8	11.88, s	9.77, s		8.27, dd (6.9) (1.9)	8.28, d (9.7)	8.00, d (9.3)	8.59, d (9.6)	8.63, d (9.7)	7.83, d (9.3)	8.03 – 8.00, m
9			11.46, s							
10				12.20, s	12.21, s				11.70, s	11.42, s
12	7.84 – 7.78, m	7.68, m	7.79, d (8.3)						3.98, s	3.63, s
13	8.81 – 8.75, m	8.73, m	6.84, m	7.85 – 7.80, m		7.46, d (8.0)	4.35, s	4.23, s		
14				8.81 – 8.77, m	8.20, s	7.31, t (7.6)			7.22, d (2.4)	7.24, d (2.4)
15	8.81 – 8.75, m	8.73, m	6.84, m		7.84 – 7.75, m	7.13, t (7.6)			10.93, s	10.89, s
16	7.84 – 7.78, m	7.68, m		8.81 – 8.77, m	7.84 – 7.75, m	7.74, d (7.8)			7.35, t (8.3)	7.35, t (8.3)
17				7.85 – 7.80, m	7.84 – 7.75, m				7.11 – 7.03, m	7.11 – 7.03, m
18					8.31, d (7.9)				7.02 – 6.96, m	7.02 – 6.96, m
19			7.79, d (8.3)						7.54, d (7.9)	7.56, d (7.9)

**Table S1b.**  $^1\text{H}$  NMR Spectroscopic Data of **8–17** in DMSO- $d_6$  ( $\delta$  in ppm, J in Hz)

No.	8	9	10	11	12	12'	13	13'	14	14'	15	15'	16	17	17'
3	7.21, d (3.6)	7.28, d (3.7)	7.01, d (3.7)	7.58, d (3.8)	7.12 – 7.07, m	7.12 – 7.07, m	6.99, d (3.6)	7.23 – 7.19, m	7.07, d (3.7)	7.27, d (3.7)	7.04, d (3.6)	7.25, d (3.8)	7.12, d (3.7)	7.04, d (3.7)	7.24, d (3.8)

4	7.50, d (3.7)	7.50, d (3.7)	7.35, d (3.7)	7.62, d (3.7)	7.48, d (3.7)	7.45, d (3.6)	7.45, d (3.6)	7.55, d (3.8)	7.47, d (3.7)	7.55, d (3.7)	7.45, d (3.6)	7.55, d (3.7)	7.49, d (3.7)	7.46 – 7.39, m	7.51, d (3.7)
6	8.42, s	8.35, s	8.13, s	8.65, s	7.93, s	8.20, s	7.99, s	7.41, s	8.14, s	7.58, s	8.01, s	7.47, s	8.16, s	7.98, s	7.98, s
8	12.19, s	12.15, s			11.42, s	11.67, s	11.31, s	10.29, s	11.98, s	10.93, s	11.41, s	10.36, s	12.40, s	11.44, s	10.45, s
10					4.06, s	3.66, s									
11	7.83, d (5.8)		7.73, d (7.8)	4.36, s			8.23, d (2.4)	8.33, d (2.4)			8.16 – 8.14, m	8.25, s		5.20, s	5.25, s
12	8.80, d (5.8)	8.19, s	7.12, t (5.1)		7.28, d (2.4)	7.26, d (2.4)			7.31, d (4.9)	7.41, d (4.9)	8.05 – 8.03, m	8.16 – 8.14, m	7.75, d (2.1)		
13		7.74- 7.79, m	7.31, t (7.1)		10.92, s	10.95, s	7.86, dd (9.0) (2.5)	7.91, dd (8.9) (2.5)	8.85, d (4.9)	8.90, d (4.9)				7.46 – 7.39, m	7.49 – 7.46, m
14	8.80, d (5.8)	7.81, d (7.3)	7.43, d (7.9)	8.12, d (8.9)	7.34, d (8.3)	7.36, d (7.4)	7.23 – 7.19, m	7.27, d (8.9)			8.63, s	8.64, s	7.28, dd (8.4) (2.0)	7.46 – 7.39, m	7.46 – 7.39, m
15	7.83, d (5.8)	7.79- 7.74, m		8.36, d (8.9)	7.05, t (7.5)	7.12 – 7.07, m							7.42, d (8.3)	7.38 – 7.34, m	7.38 – 7.34, m
16		8.33 – 8.30, m			6.94, t (7.5)	7.00, t (7.3)	8.01, d (9.0)	8.07, d (8.7)	8.02, d (8.9)	8.08, d (8.9)	8.05 – 8.03, m	8.08, d (8.9)		7.46 – 7.39, m	7.46 – 7.39, m
17	8.05, d (8.8)			8.36, d (8.9)	7.67, d (7.9)	7.58, d (8.0)	8.31, d (8.9)	8.36, d (8.9)	8.32, d (9.0)	8.35, d (8.9)	8.31, d (8.8)	8.36, d (9.0)		7.46 – 7.39, m	7.49 – 7.46, m
18	8.32, d (8.9)			8.12, d (8.9)											
19			8.01, d (9.0)				8.31, d (8.9)	8.36, d (8.9)	8.32, d (9.0)	8.35, d (8.9)	8.31, d (8.8)	8.36, d (9.0)		8.01, d (8.5)	8.08 – 8.03, m
20	8.32, d (8.9)	8.13, d (8.5)	8.30, d (8.9)				8.01, d (9.0)	8.07, d (8.7)	8.02, d (8.9)	8.08, d (8.9)	8.05 – 8.03, m	8.08, d (8.9)	8.04, d (8.8)	8.35 – 8.28, m	8.35 – 8.28, m
21	8.05, d (8.8)	8.33 – 8.30, m			8.05, d (8.9)	8.01, d (8.8)							8.33, d, (8.9)		
22			8.30, d (8.9)		8.33, d (8.9)	8.31, d (8.9)								8.35 – 8.28, m	8.35 – 8.28, m
23		8.33 – 8.30, m	8.01, d (9.0)										8.33, d (8.9)	8.01, d (8.5)	8.08 – 8.03, m
24		8.13, d (8.5)			8.33, d (8.9)	8.31, d (8.9)							8.04, d (8.8)		
25					8.05, d (8.9)	8.01, d (8.8)									

**Table S2a.** <sup>13</sup>C NMR Spectroscopic Data of **1–7** in DMSO-d<sub>6</sub> (δ in ppm)

No.	1	2	3	4	5	6	6'	7	7'
CH <sub>3</sub>	56.04, CH <sub>3</sub>	55.99, CH <sub>3</sub>							
1	125.86 (1C)	126.36, C							
2	109.56, CH	109.26, CH	155.21, C	155.70, C	155.73, C	153.80, C	153.42, C	155.33, C	155.40, C
3	149.77, C	148.49, C	114.21, CH	114.03, CH	113.24, CH	115.38, CH	115.25, CH	113.85, CH	113.85, CH
4	148.54, C	149.30, C	115.84, CH	116.10, CH	115.48, CH	116.51, CH	117.93, CH	115.88, CH	115.95, CH
5	115.94, CH	115.88, CH	151.91, C	151.78, C	151.86, C	152.47, C	152.77, C	151.77, C	151.77, C
6	122.90, CH	122.43, CH	125.20, CH	122.82, CH	122.17, CH	132.06, CH	132.45, CH	123.35, CH	123.97, CH
7	150.03, CH	147.86, CH	130.75, CH	132.21, CH	130.92, CH	127.87, CH	122.18, CH	130.84, CH	131.03, CH
8			149.55, C	153.35, CH	145.46, CH	169.97, CH	168.99, CH	143.60, CH	146.81, CH
10	161.77, C=O	162.99, C=O							
11	141.16, C	124.51, C	162.17, C=O	149.56, C	167.22, C	197.45, C=S	196.90, C=S	173.32, C=O	167.91, C=O
12	121.95, CH	130.01, CH	140.62, C					29.32, CH <sub>2</sub>	31.16, CH <sub>2</sub>
13	150.76, CH	115.45, CH	122.02, CH		118.04, CH	35.23, CH <sub>2</sub>	36.01, CH <sub>2</sub>	108.24, C	108.32, C
14		161.06, C	150.84, CH	139.07, CH	126.45, CH	170.03, C=O	169.62, C=O	124.56, CH	124.46, CH



