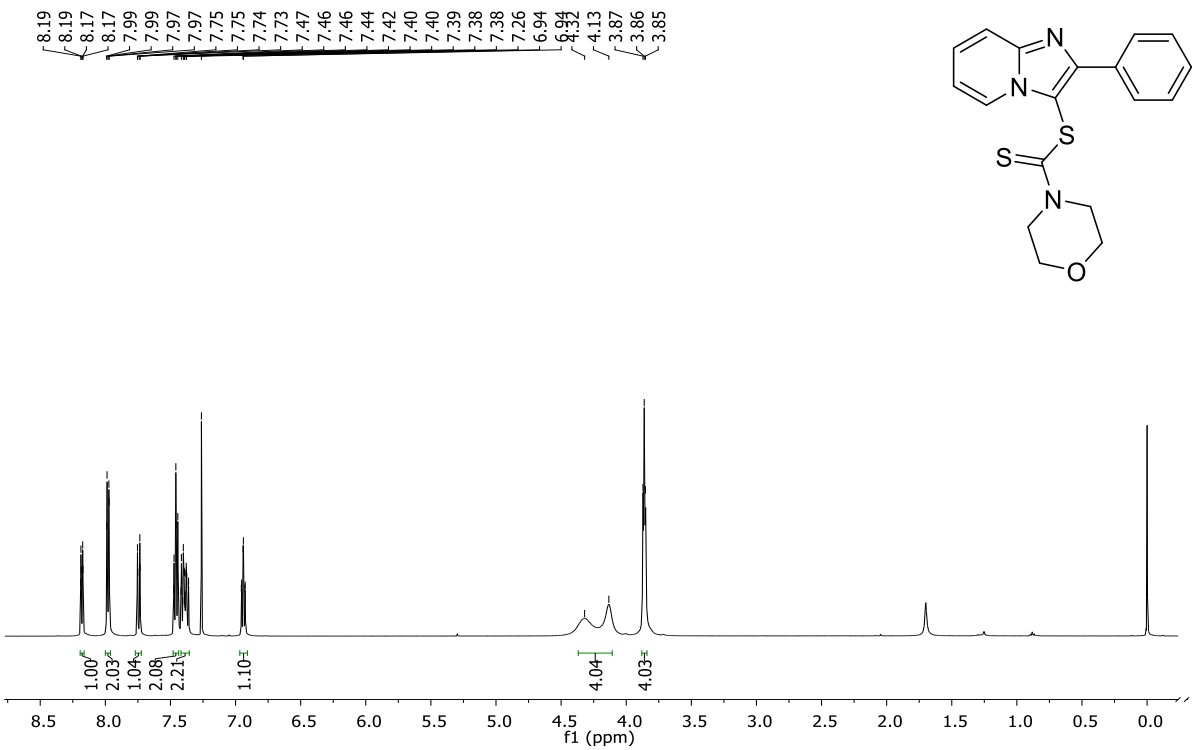
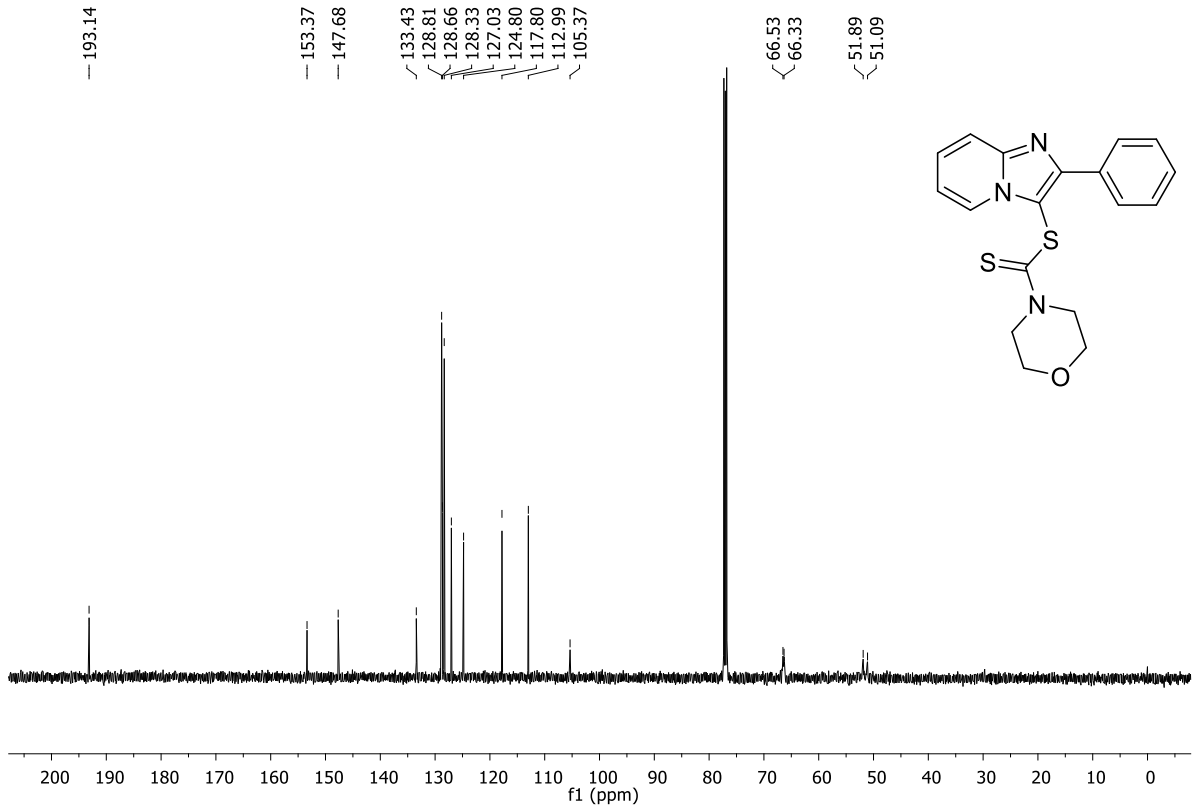
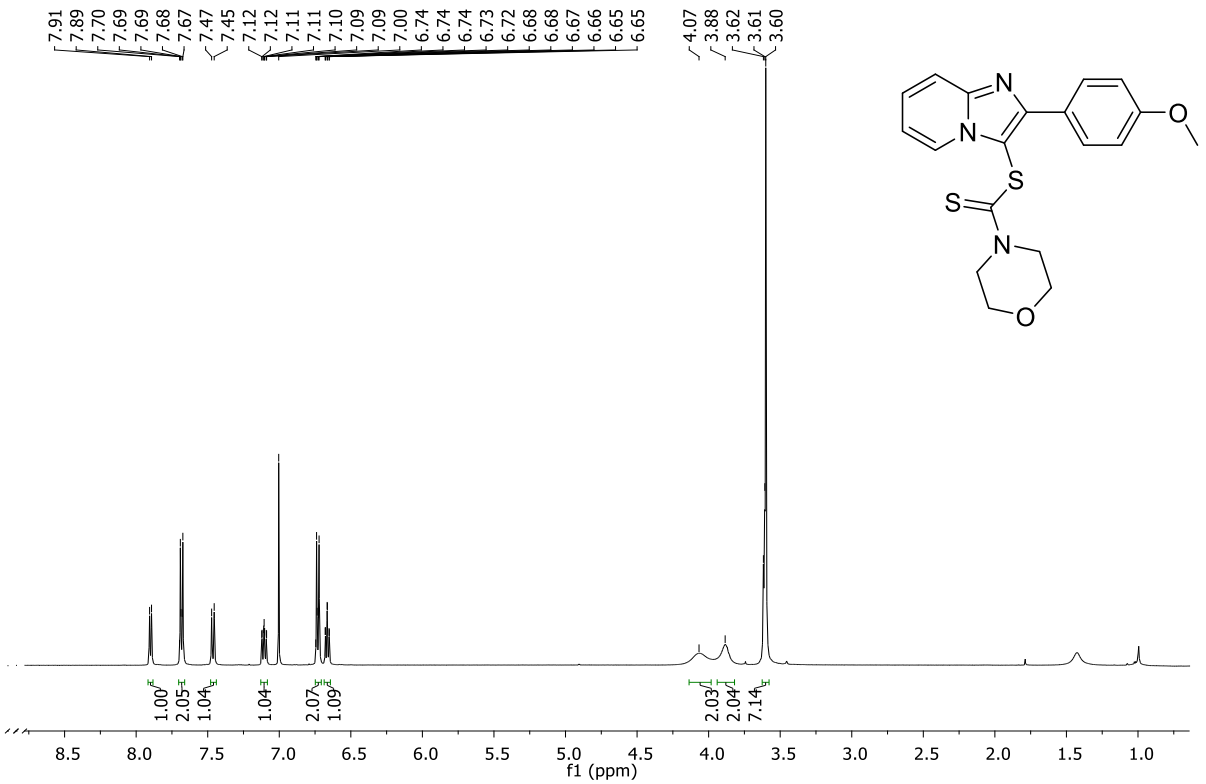


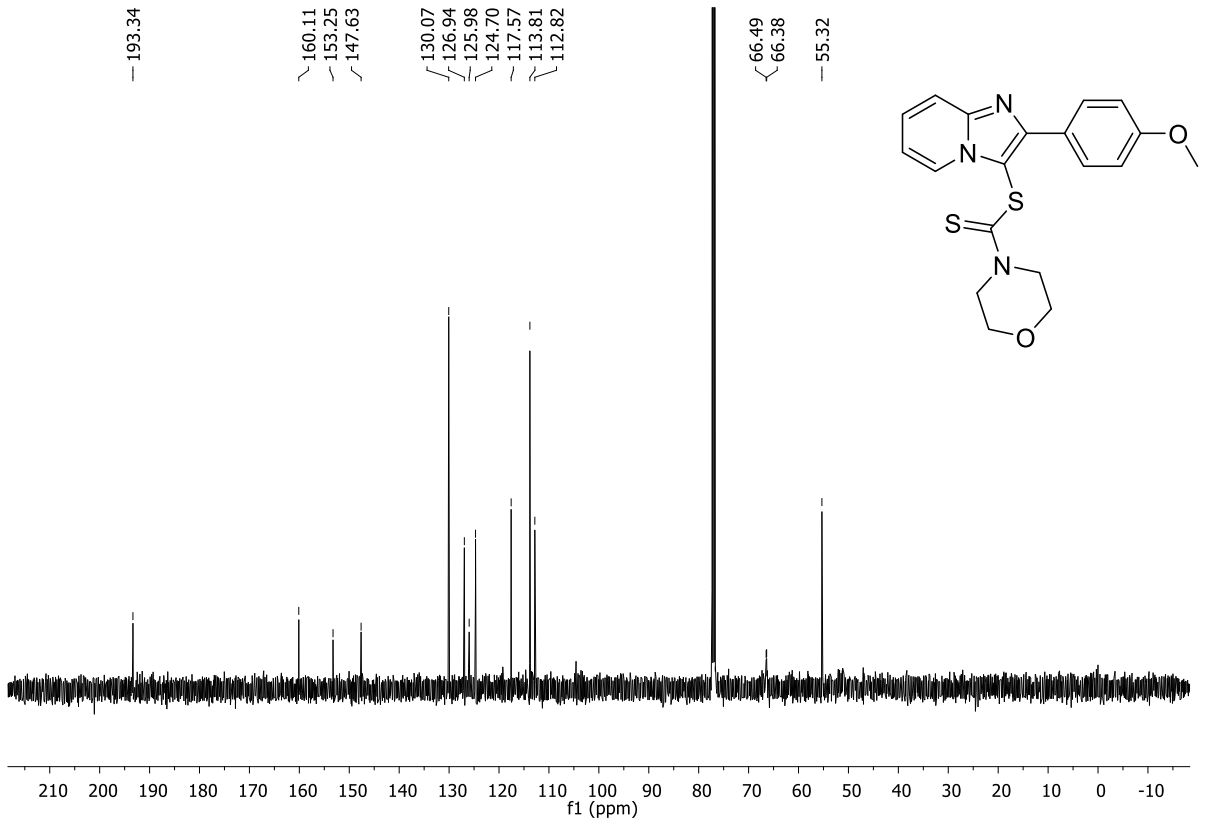
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3aa**



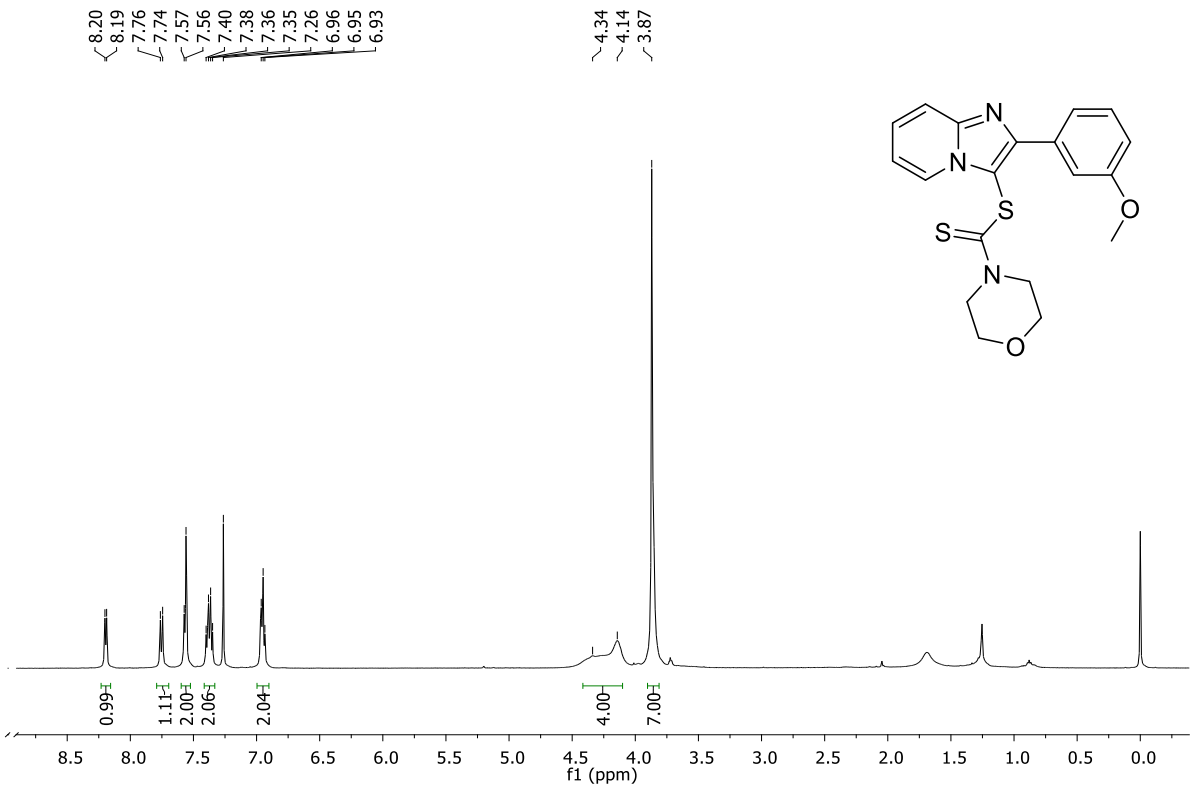
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3aa**



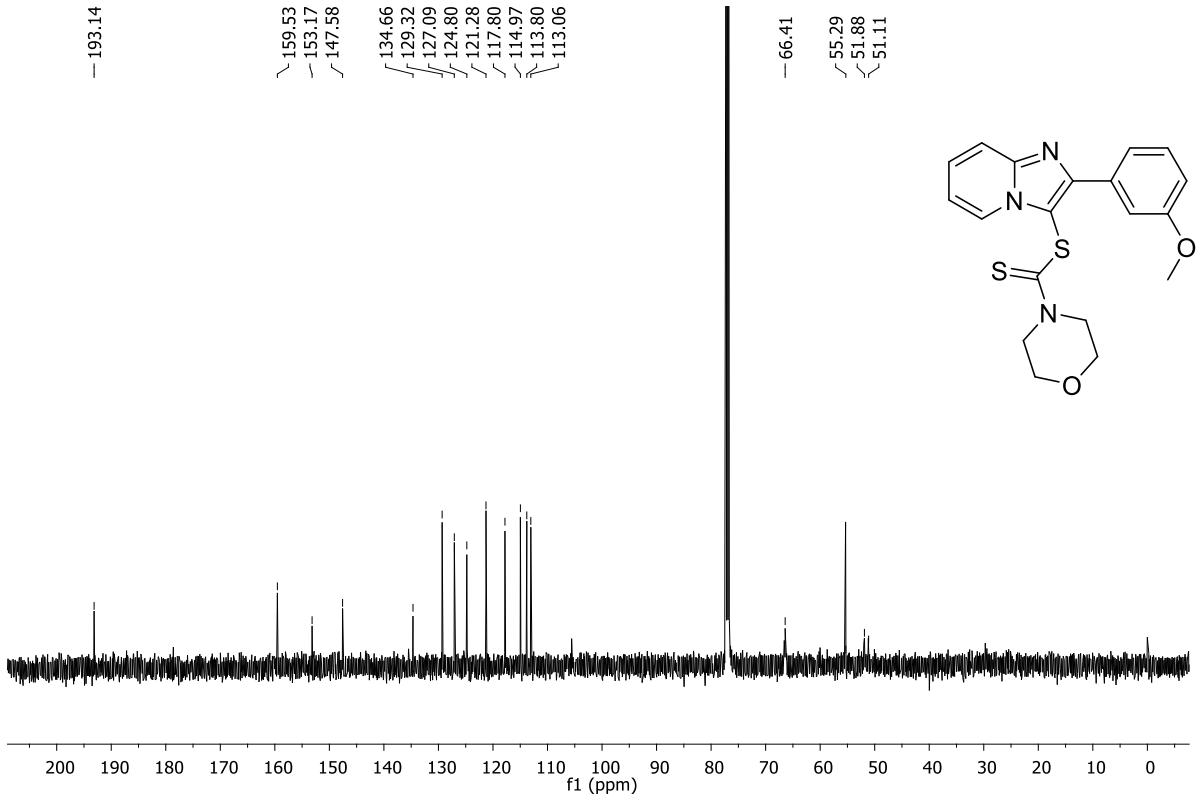
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ba**



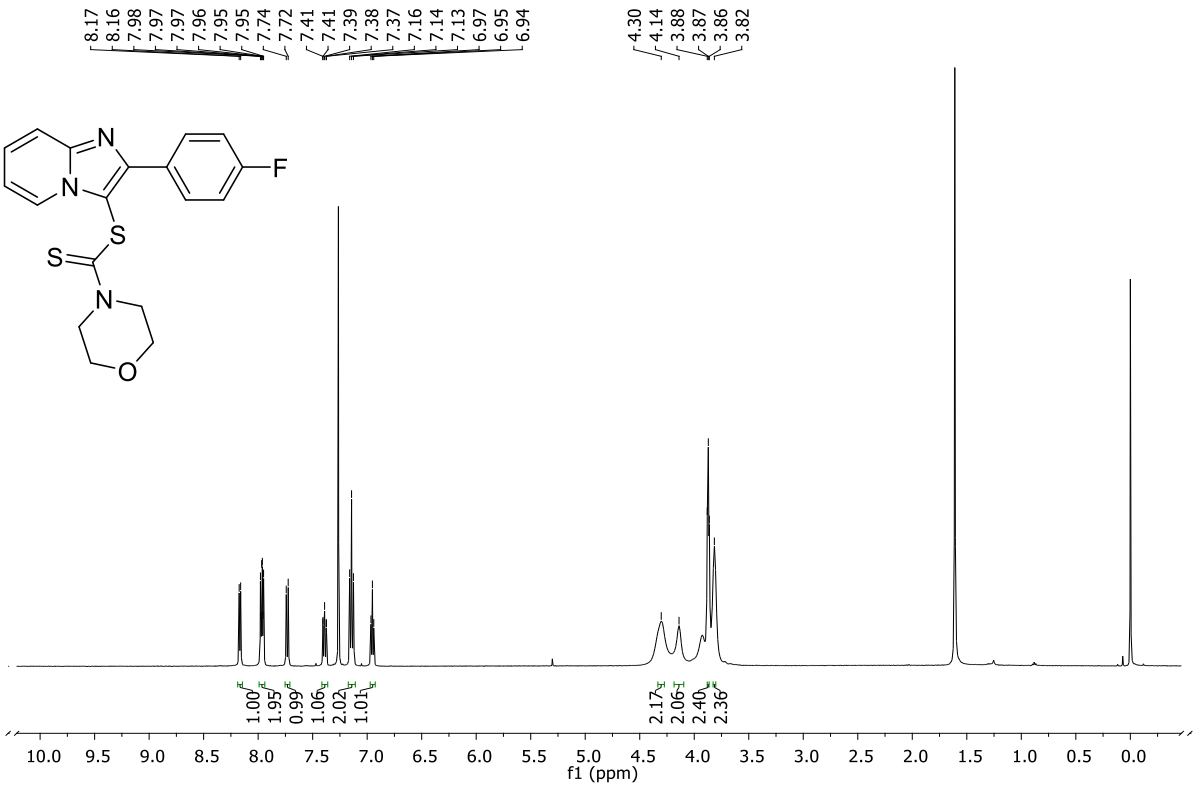
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ba**



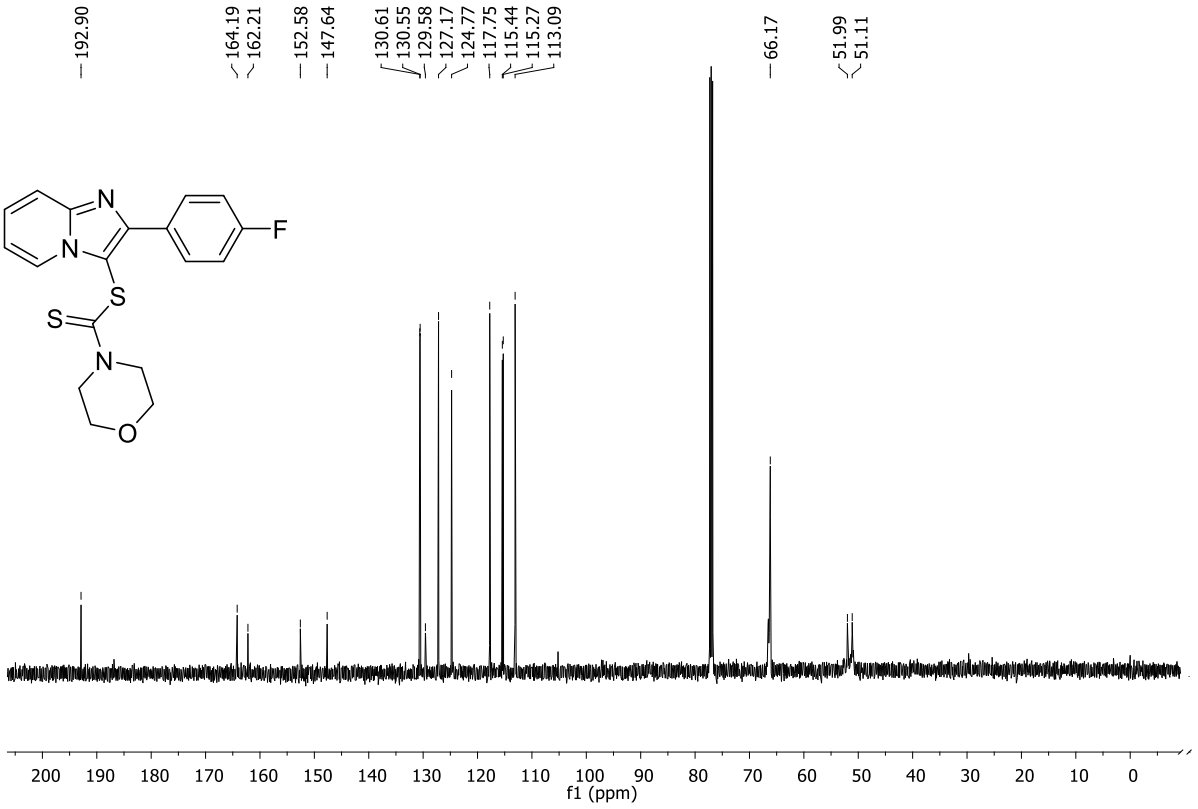
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ca**



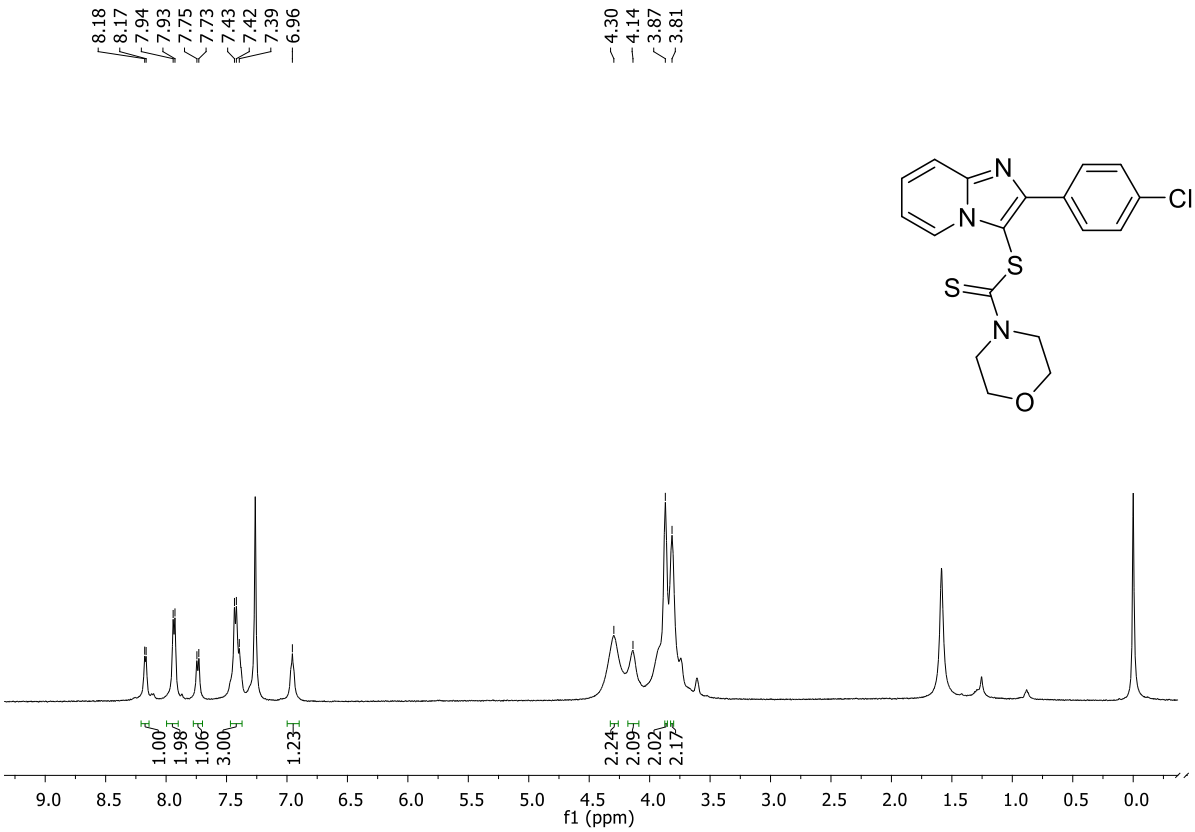
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ca**



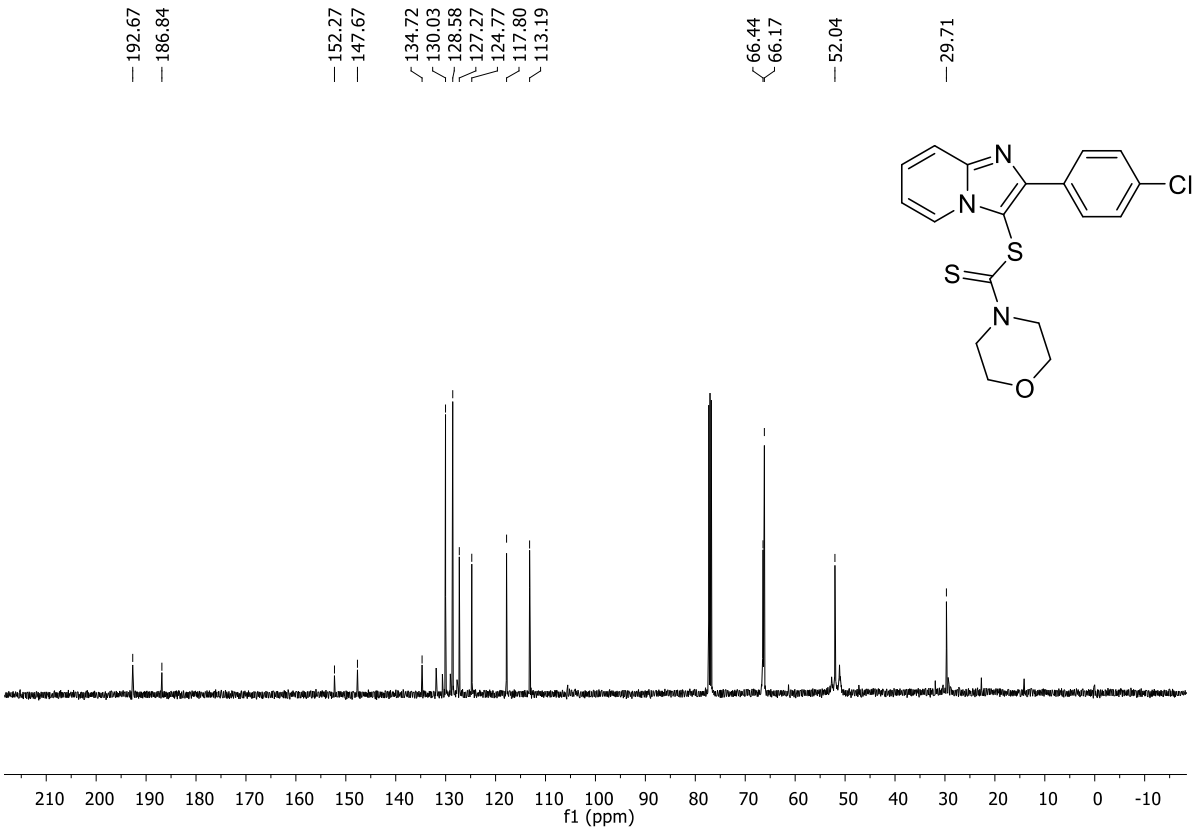
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3da**



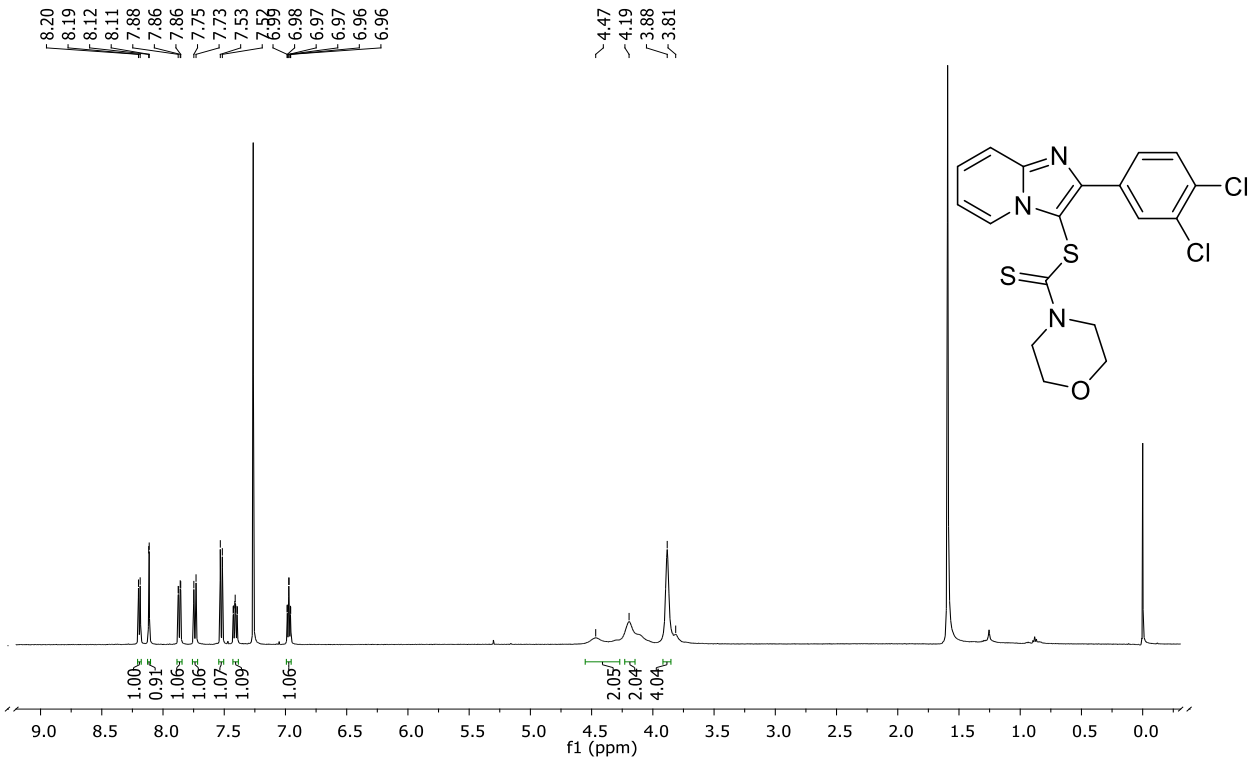
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3da**



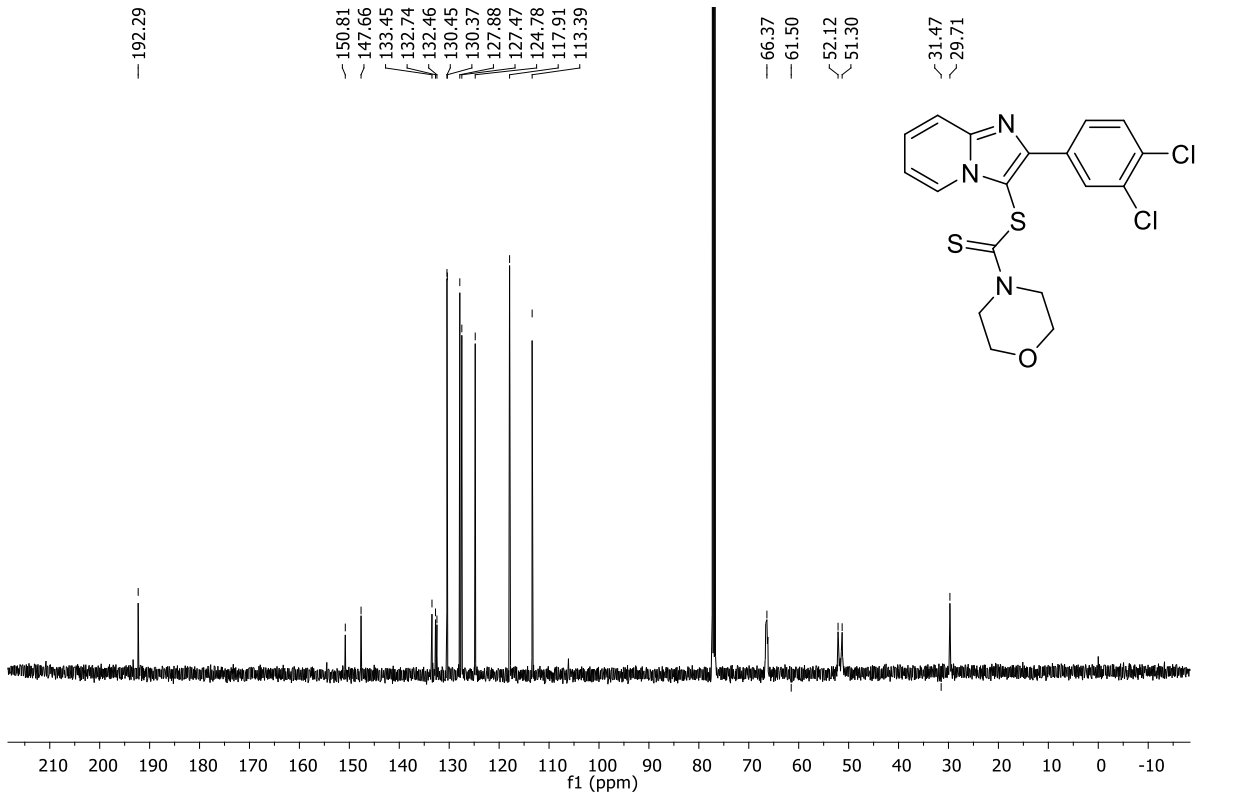
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ea**



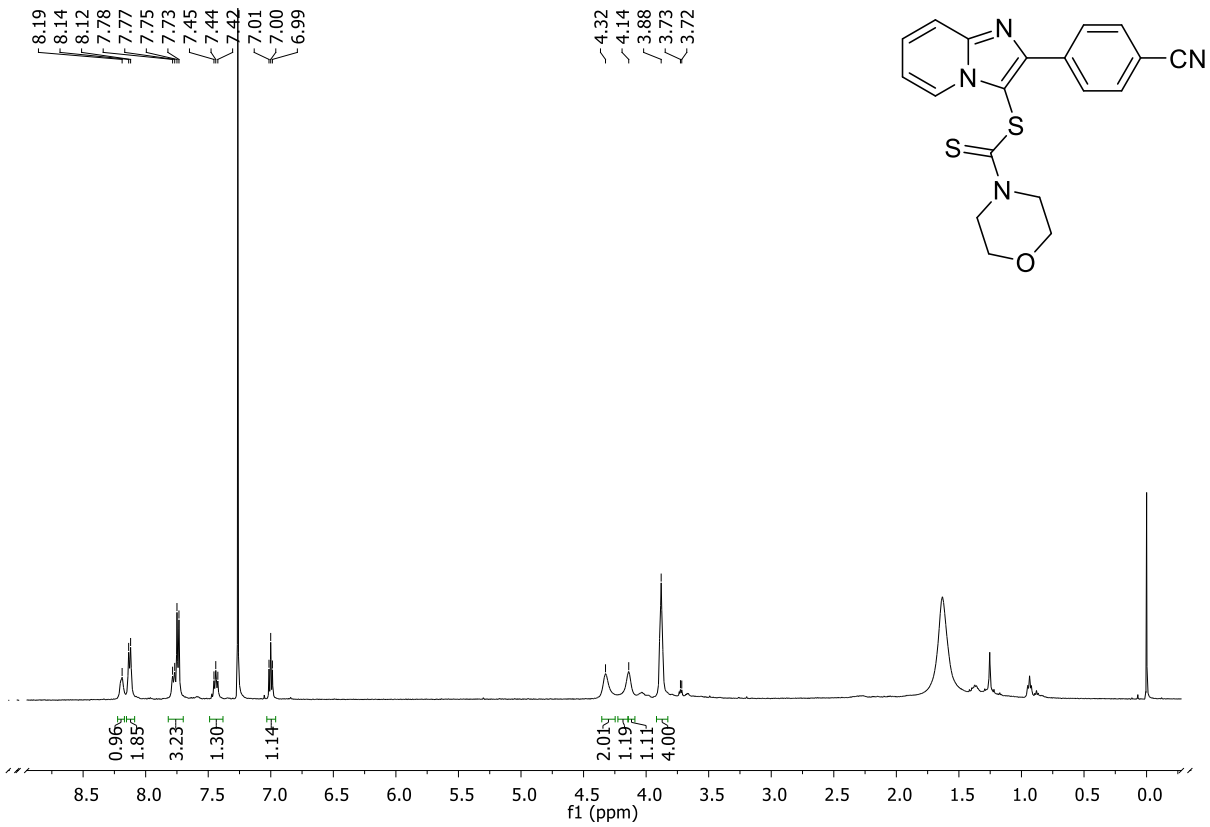
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ea**



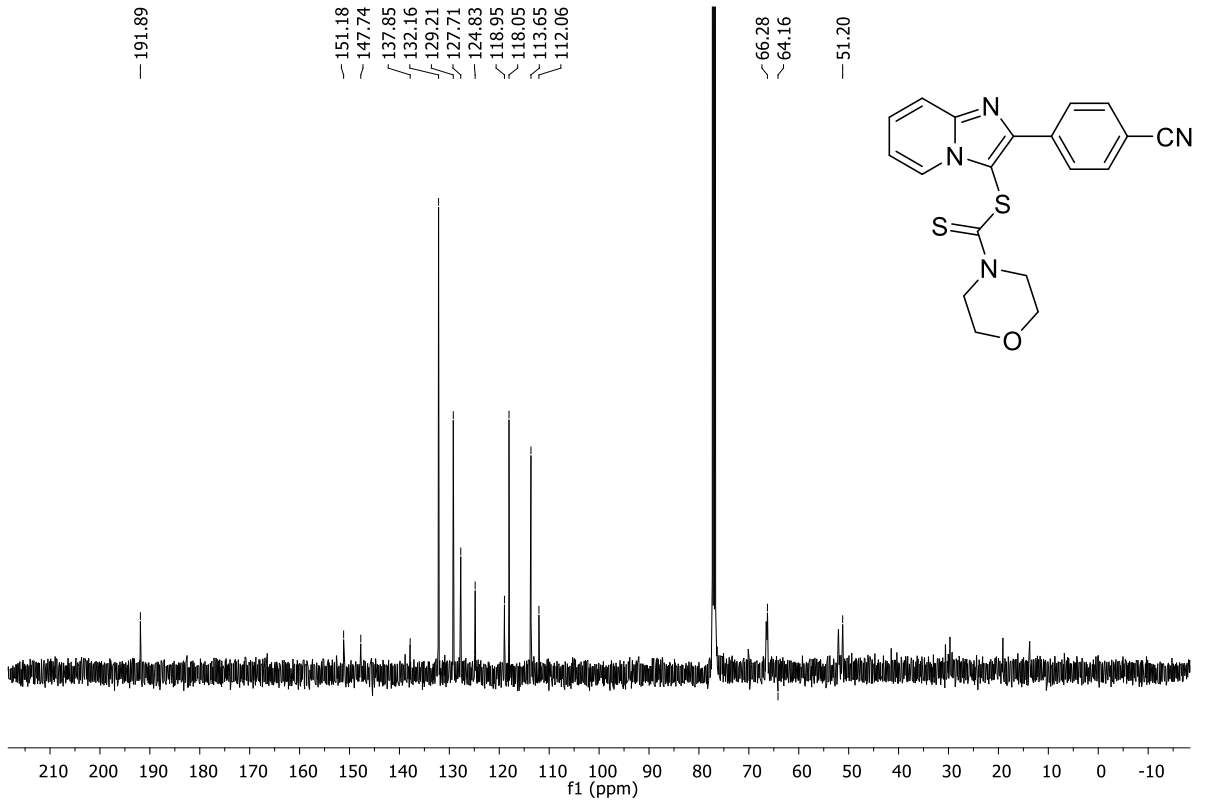
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3fa**



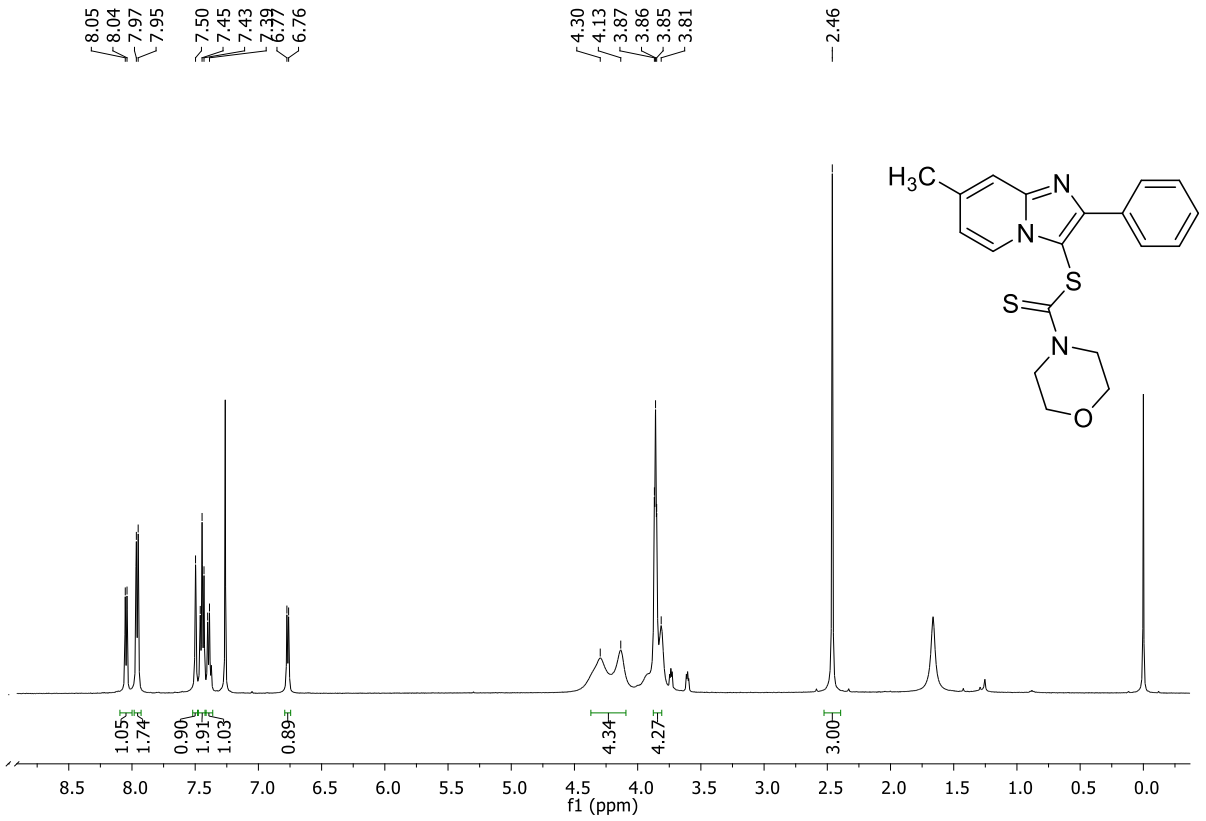
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3fa**



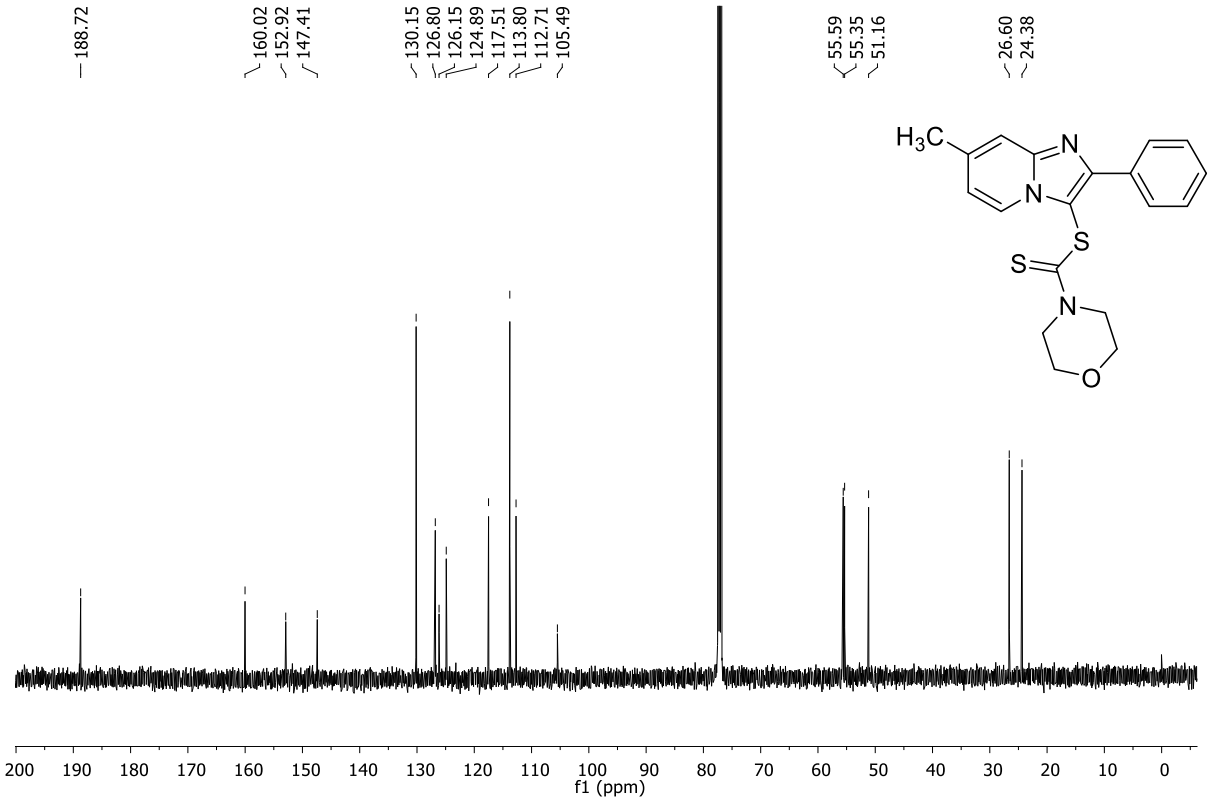
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ga**



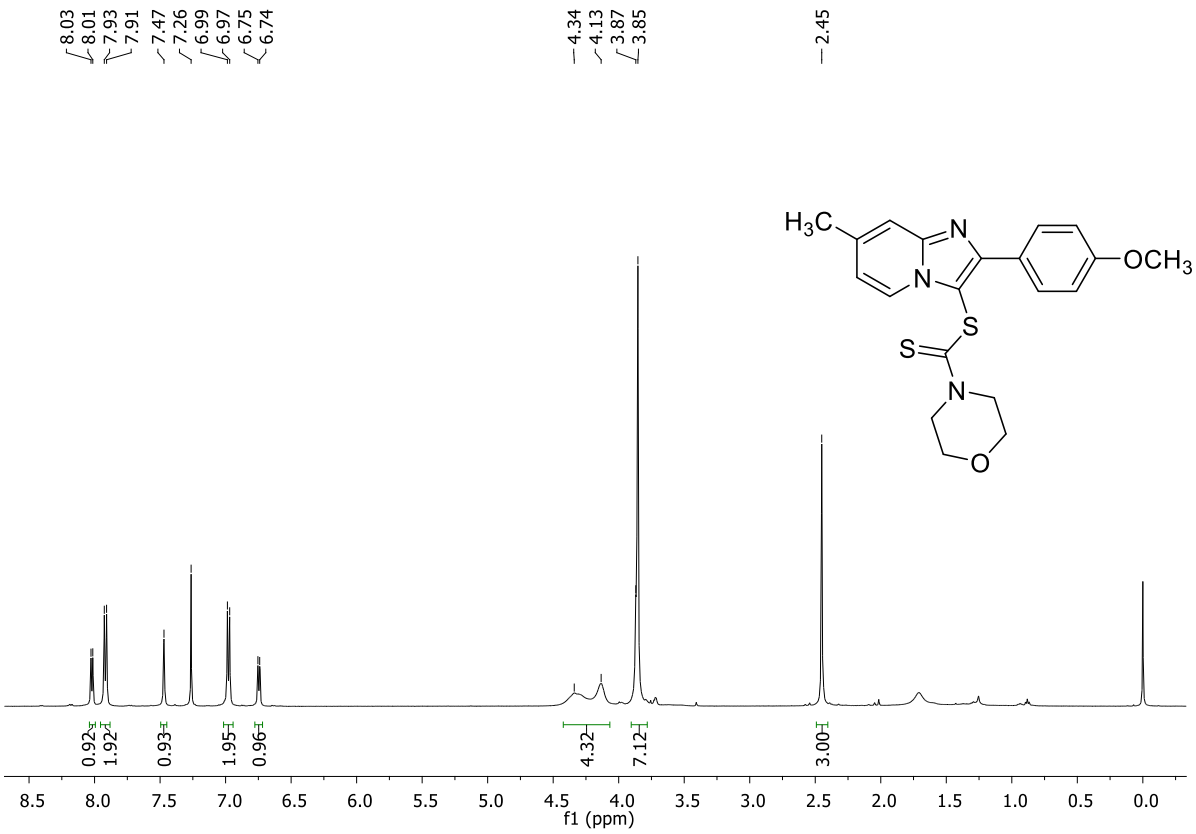
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ga**



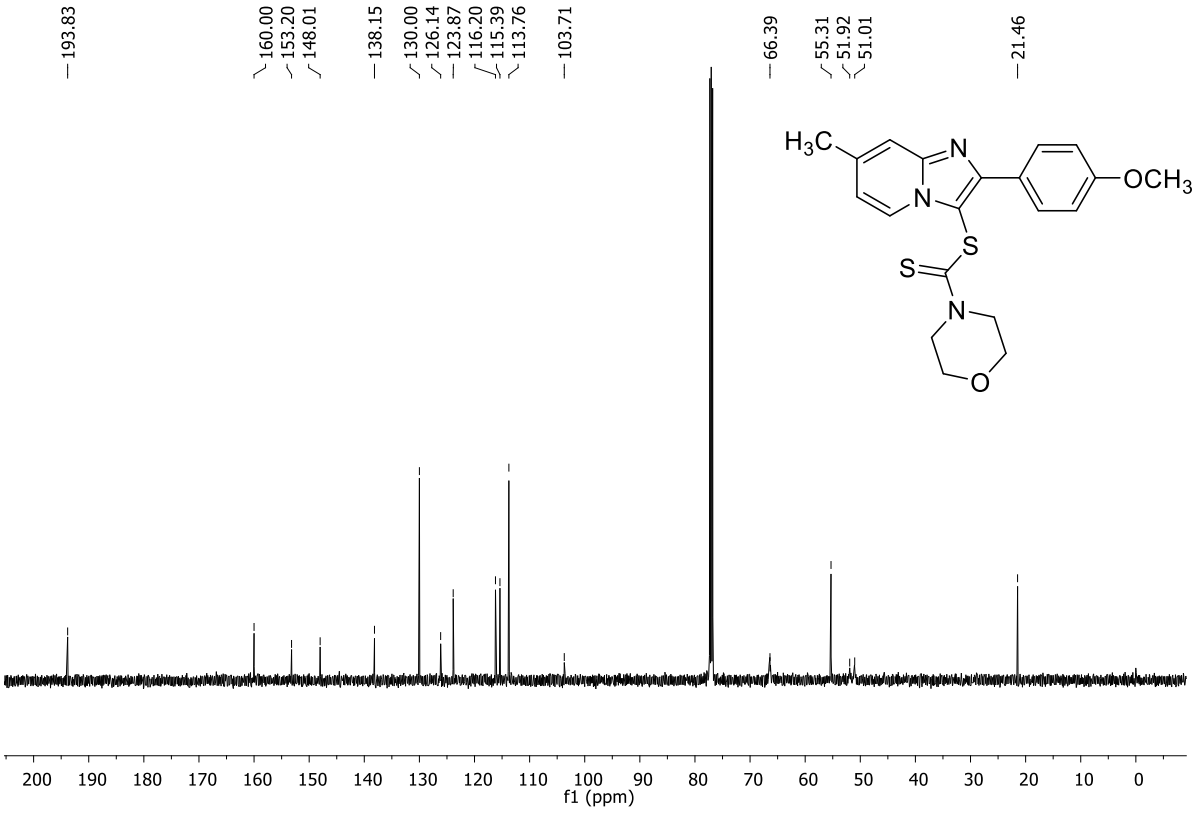
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ha**



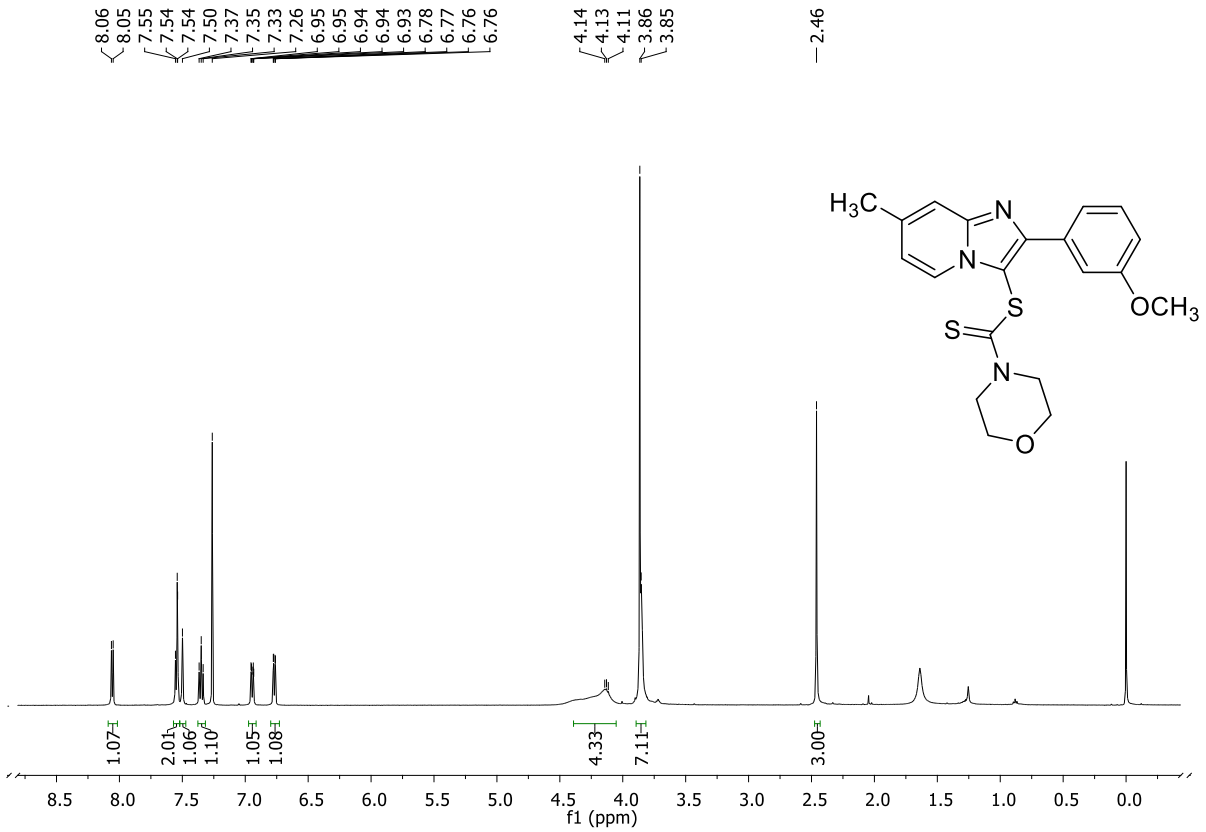
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ha**



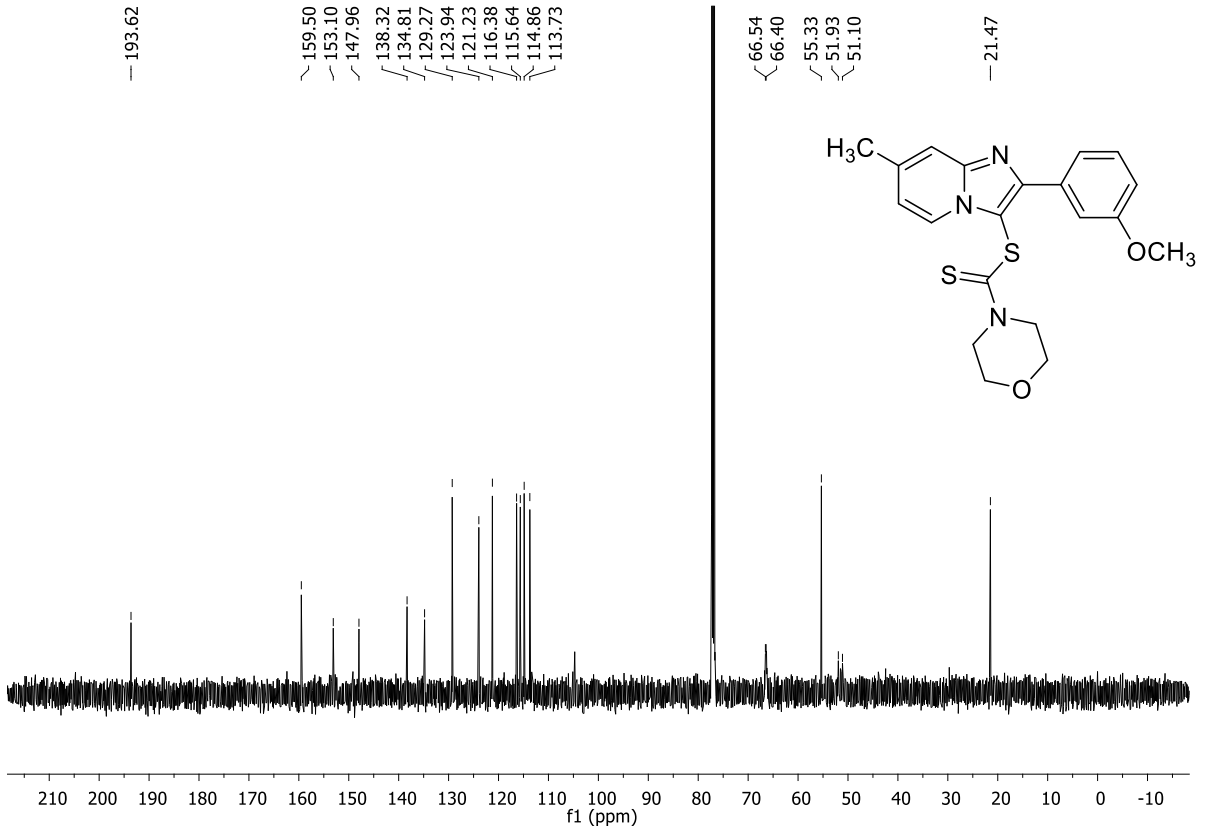
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ia**



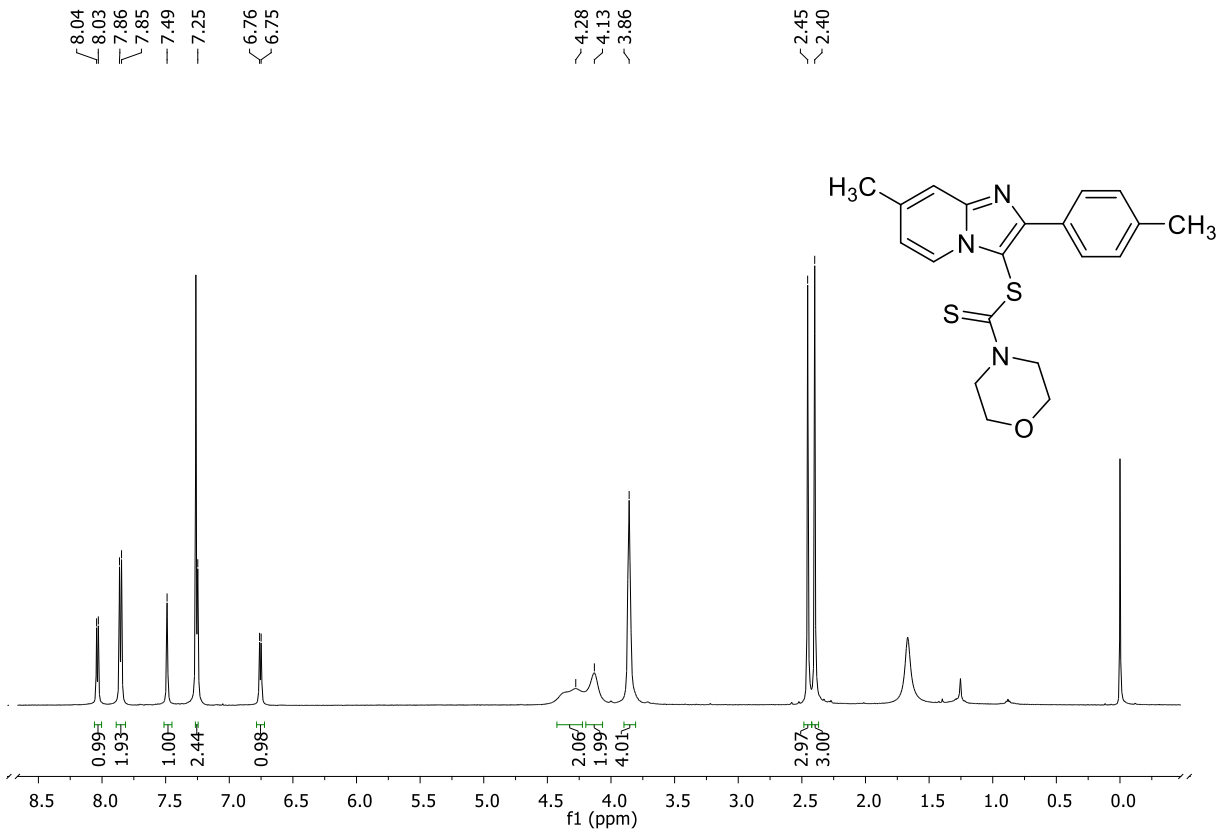
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ia**



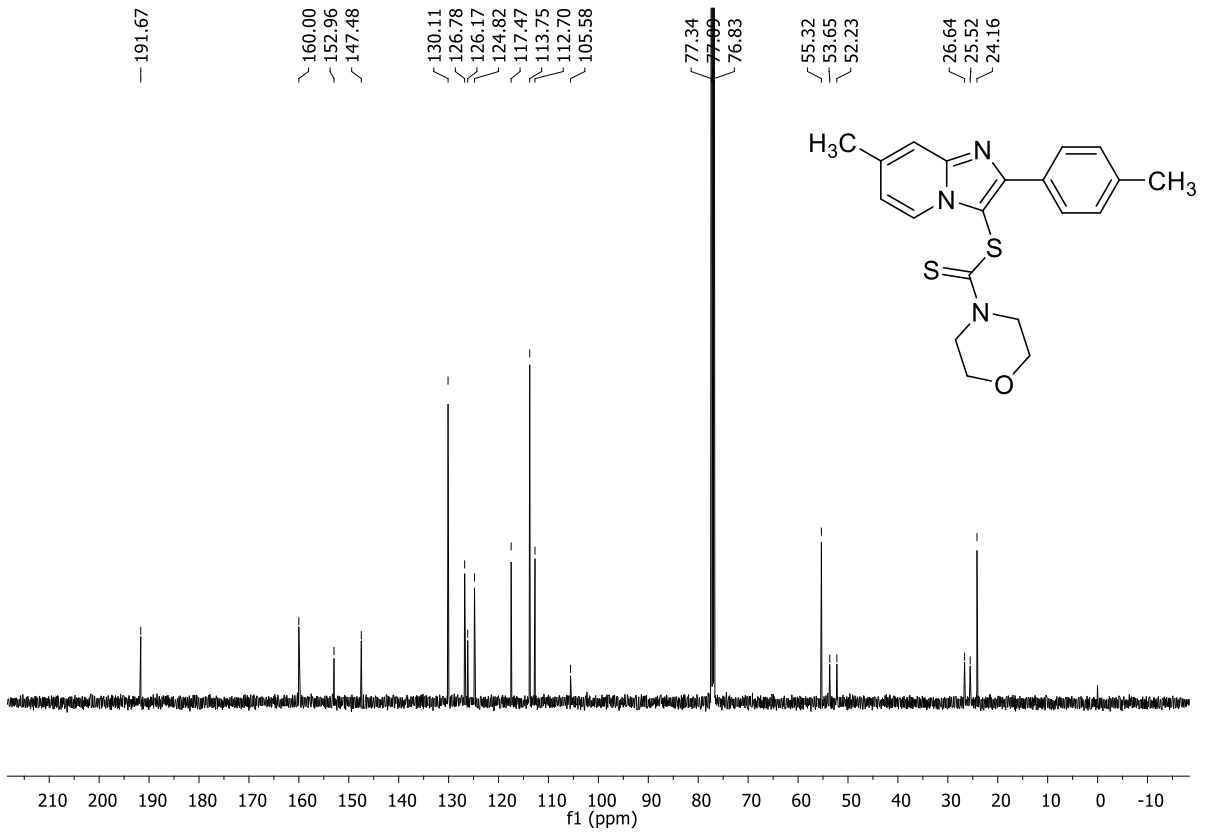
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ja**



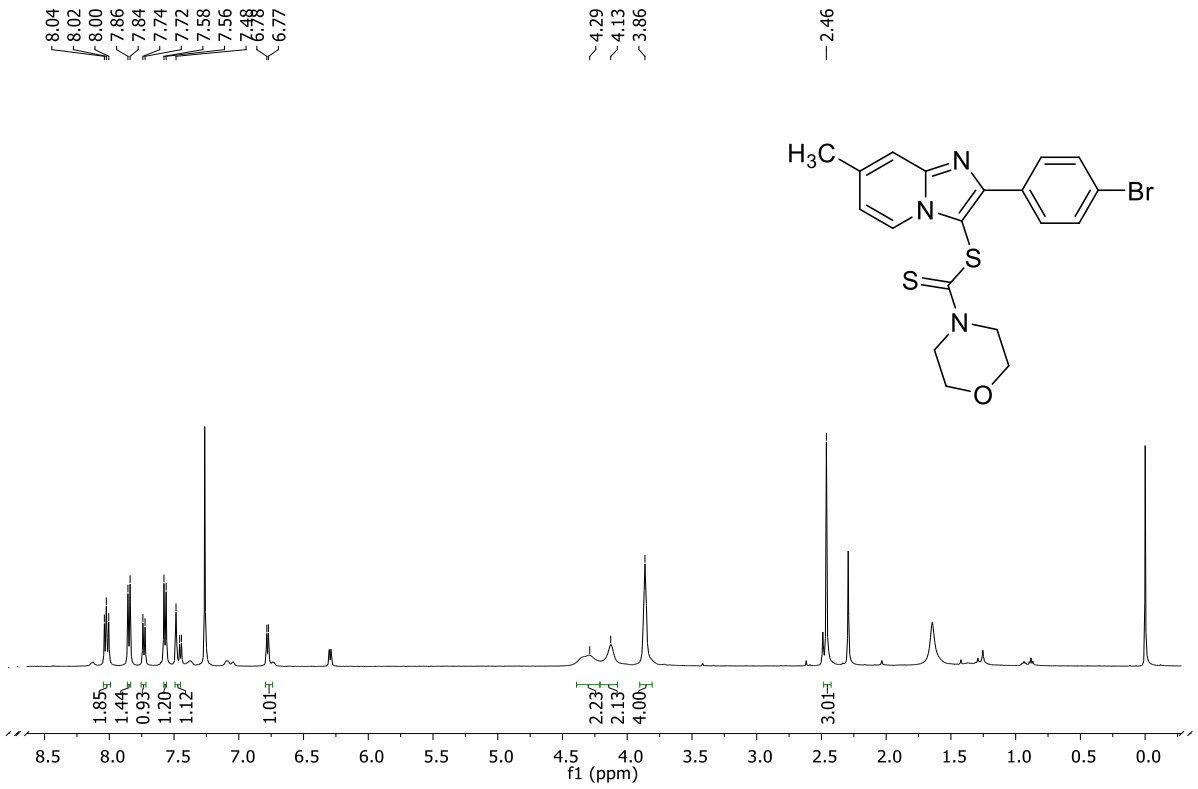
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ja**



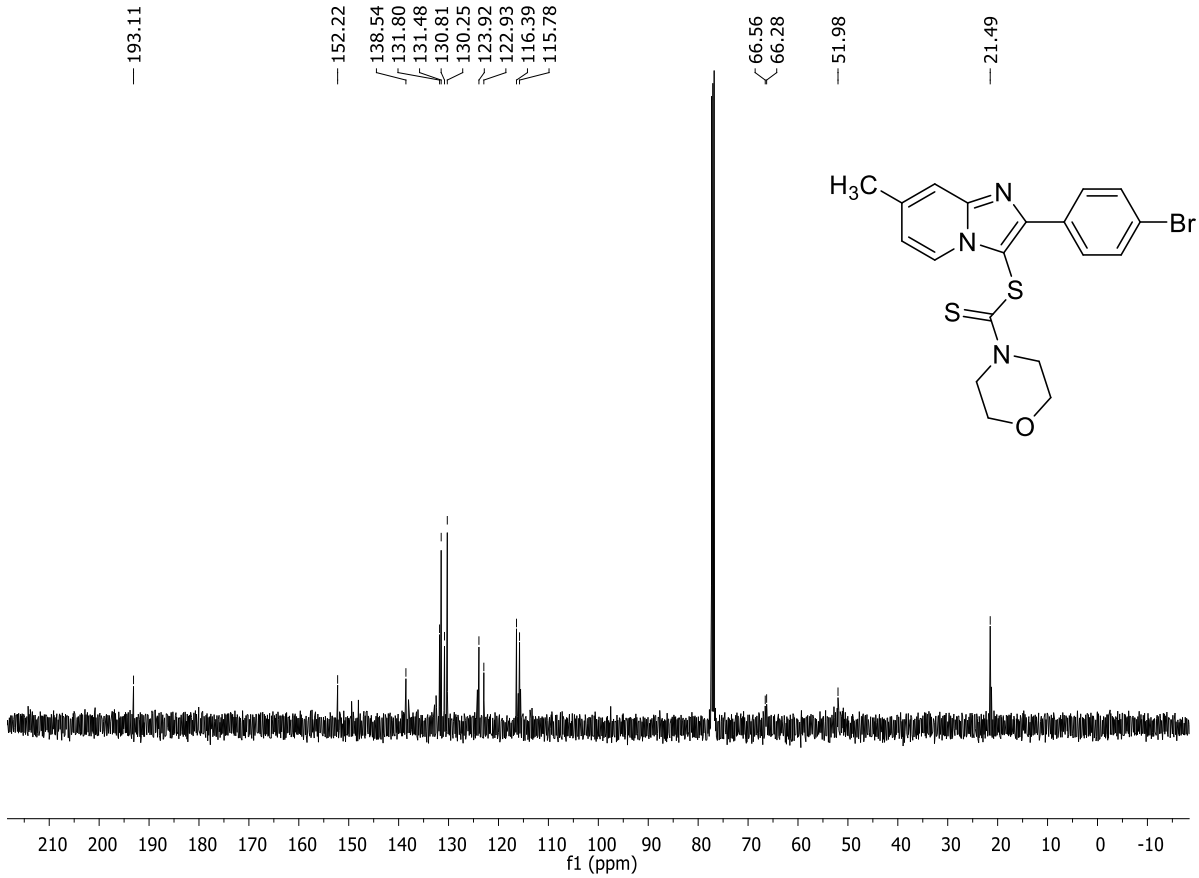
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ka**



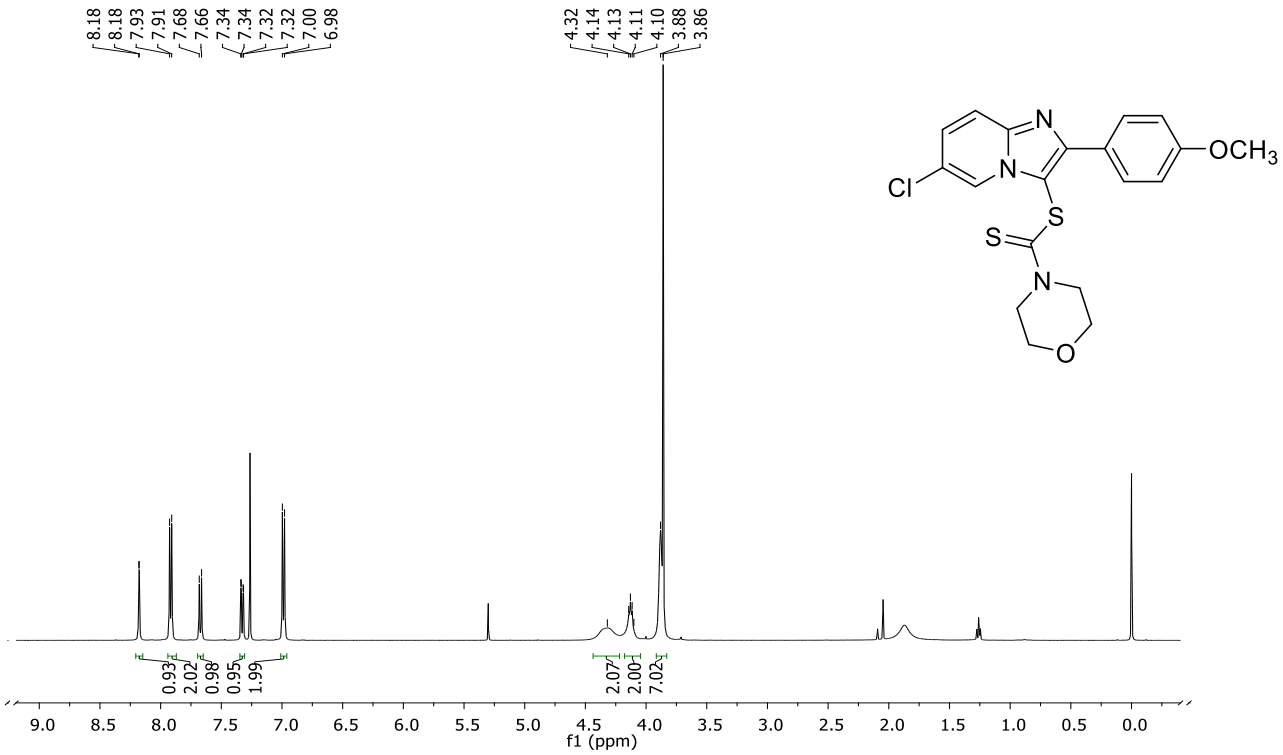
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ka**



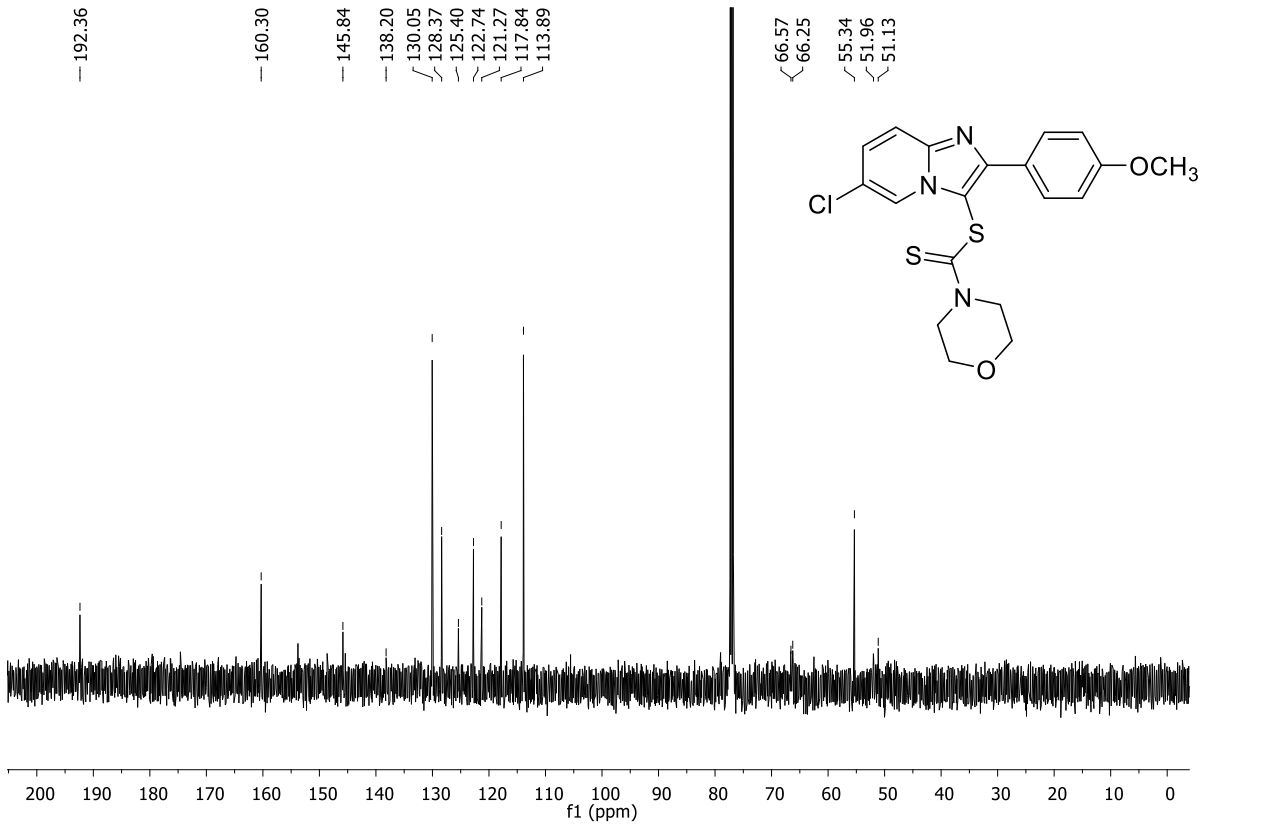
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3la**



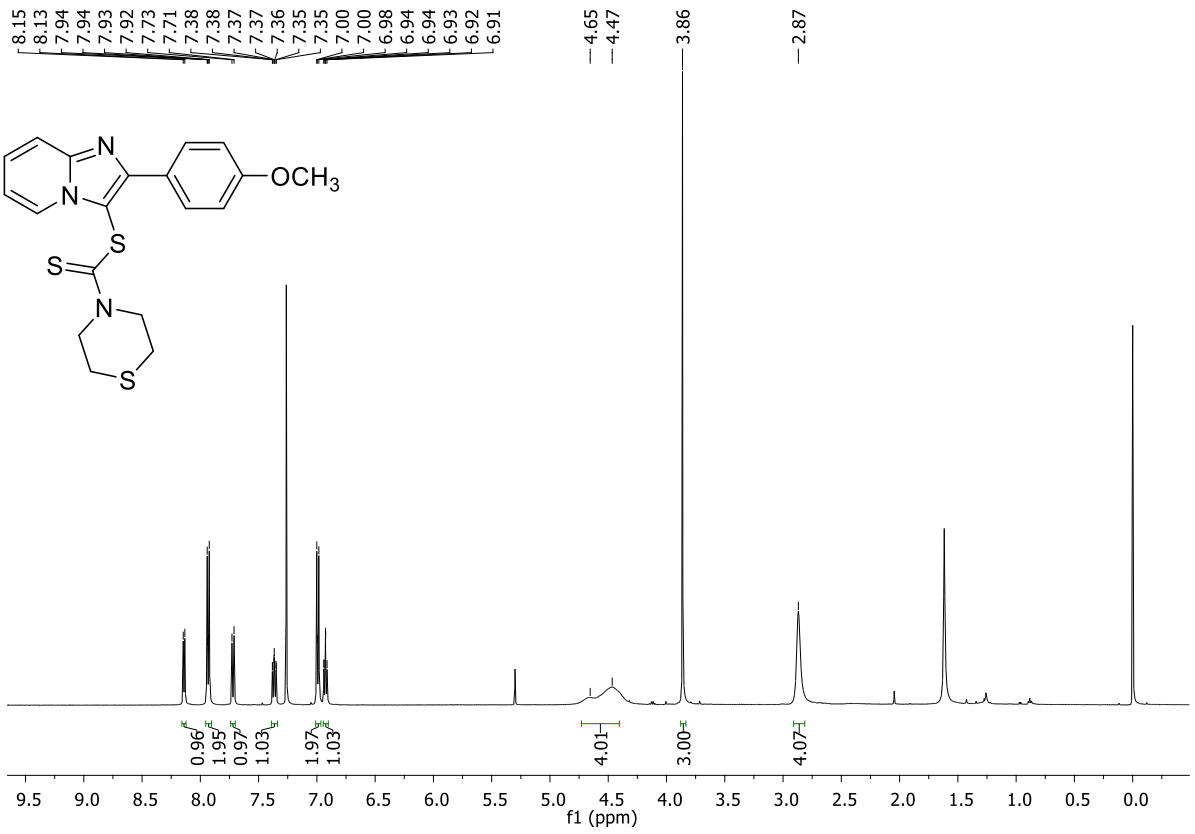
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3la**



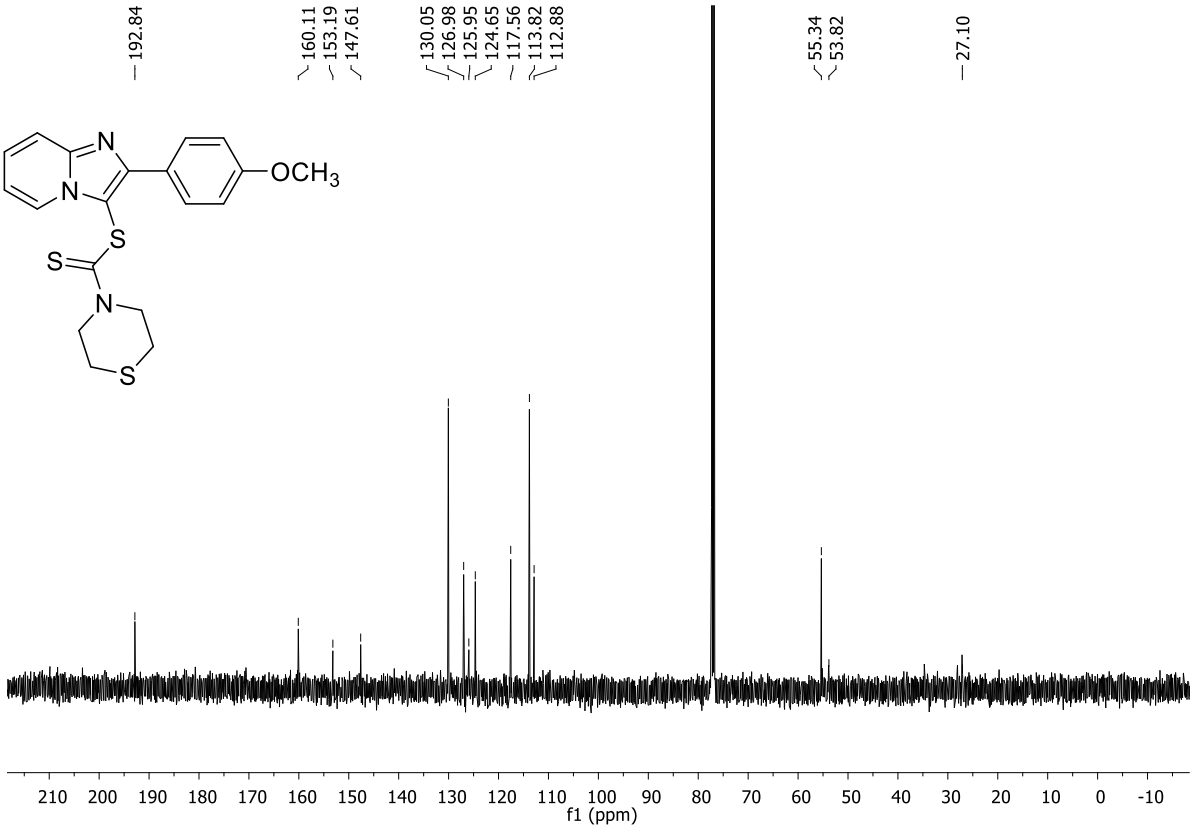
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3ma**



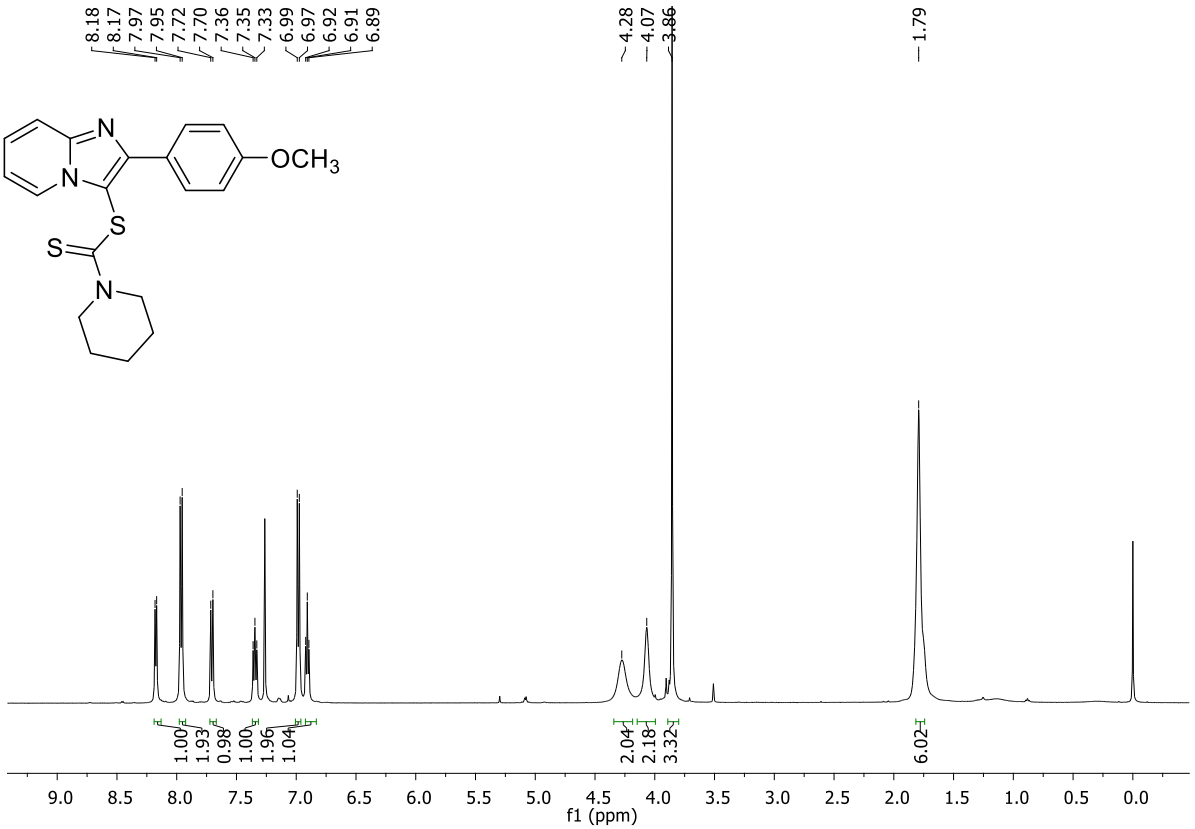
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3ma**



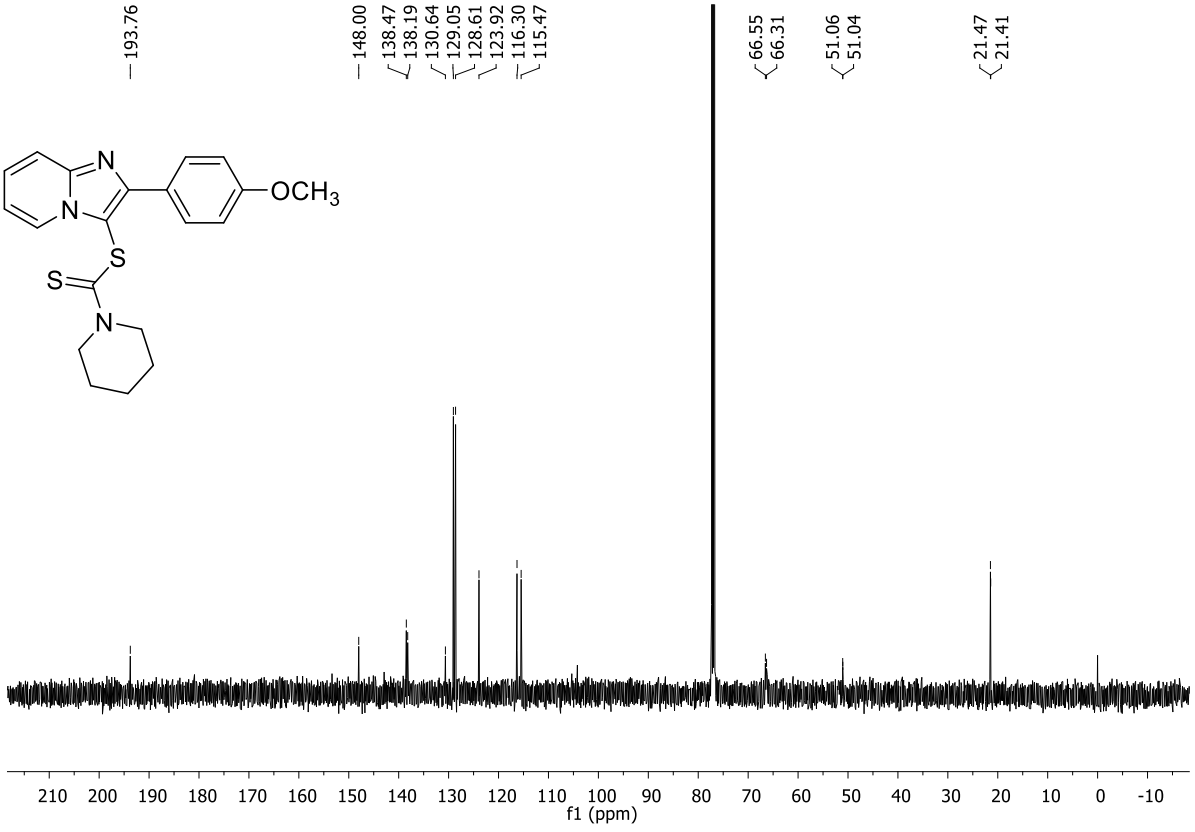
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3bb**



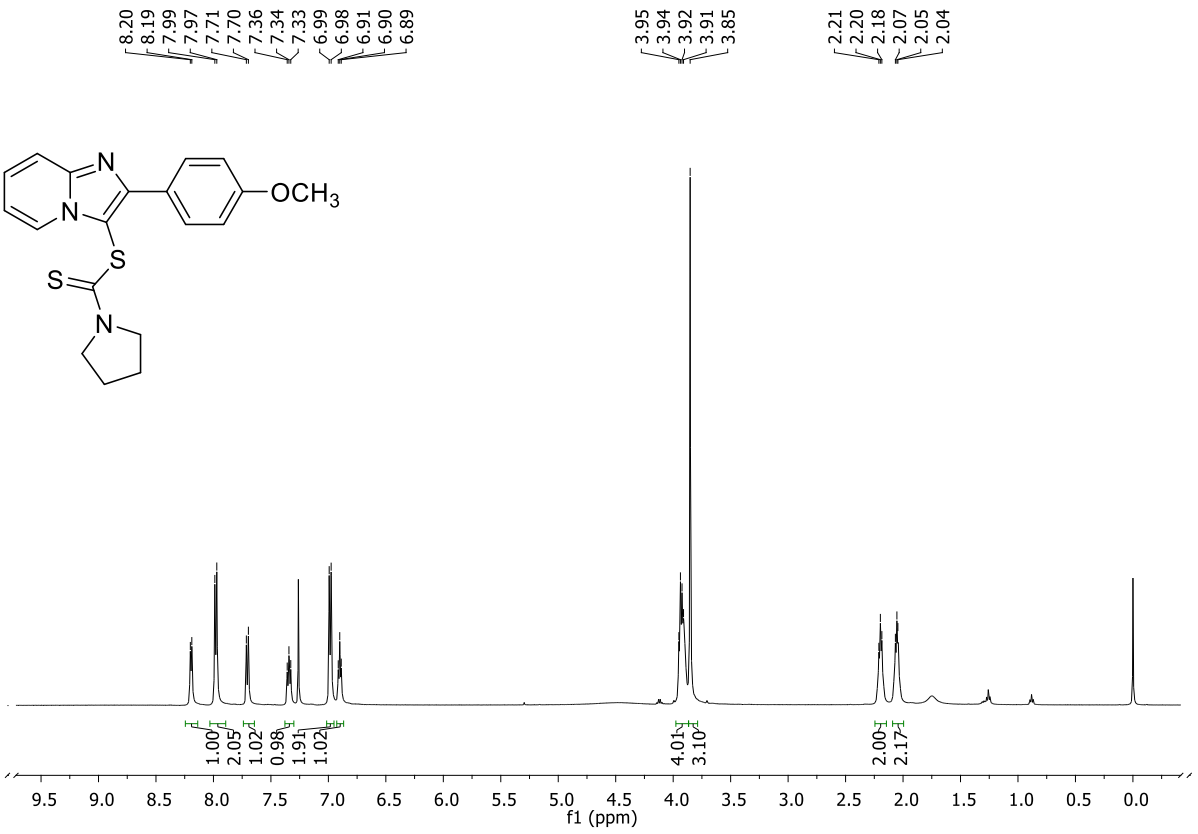
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3bb**



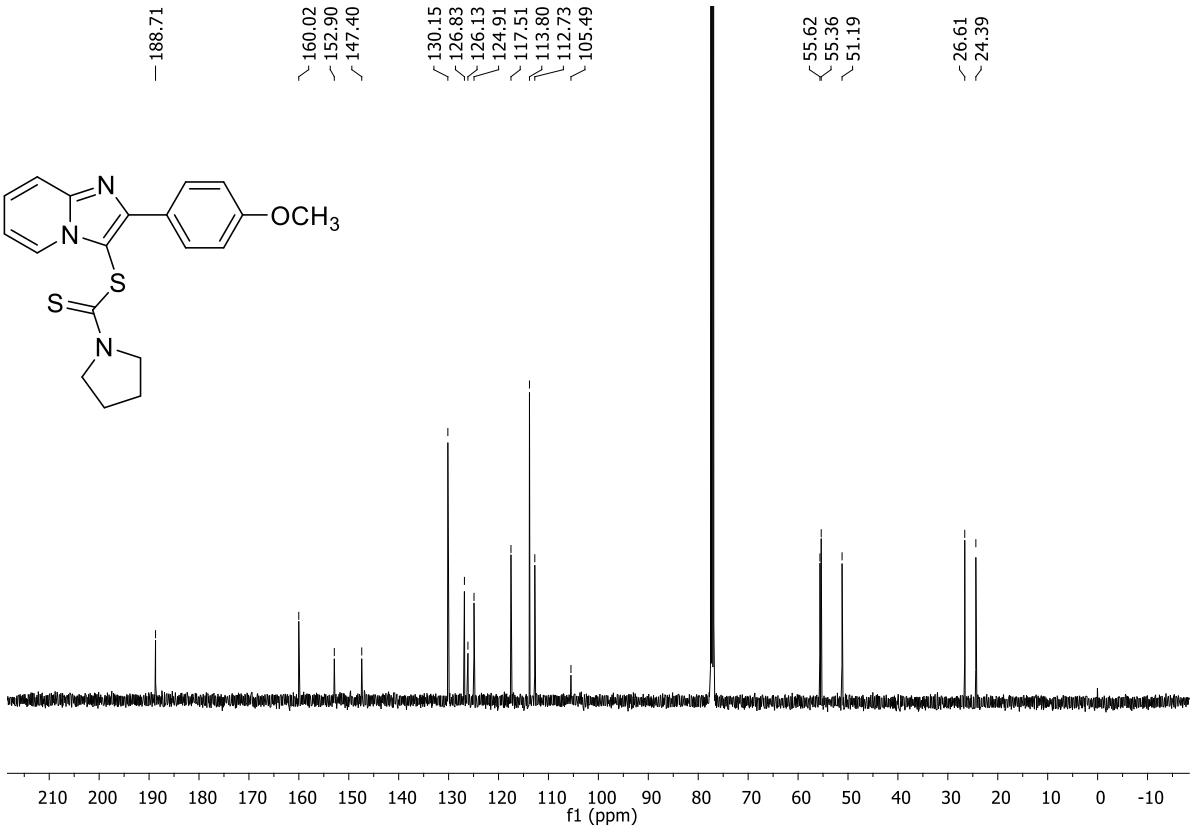
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3bc**



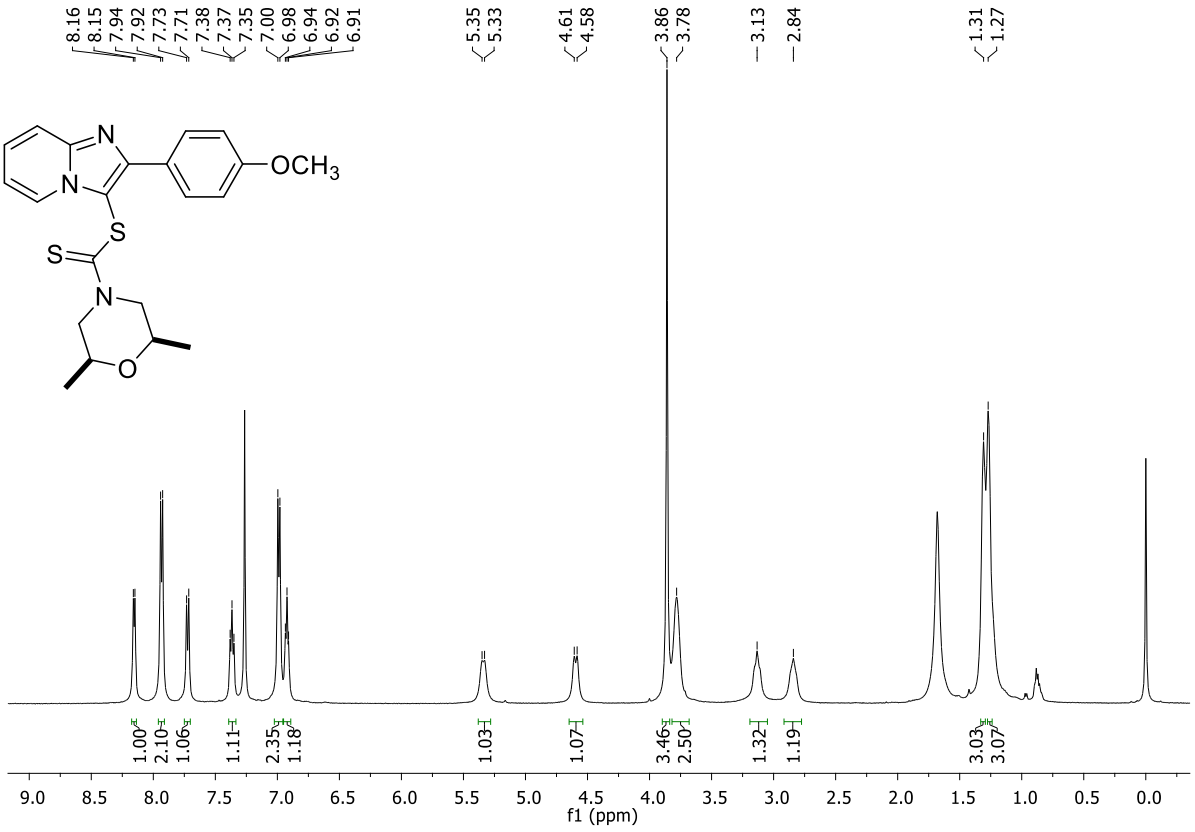
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3bc**



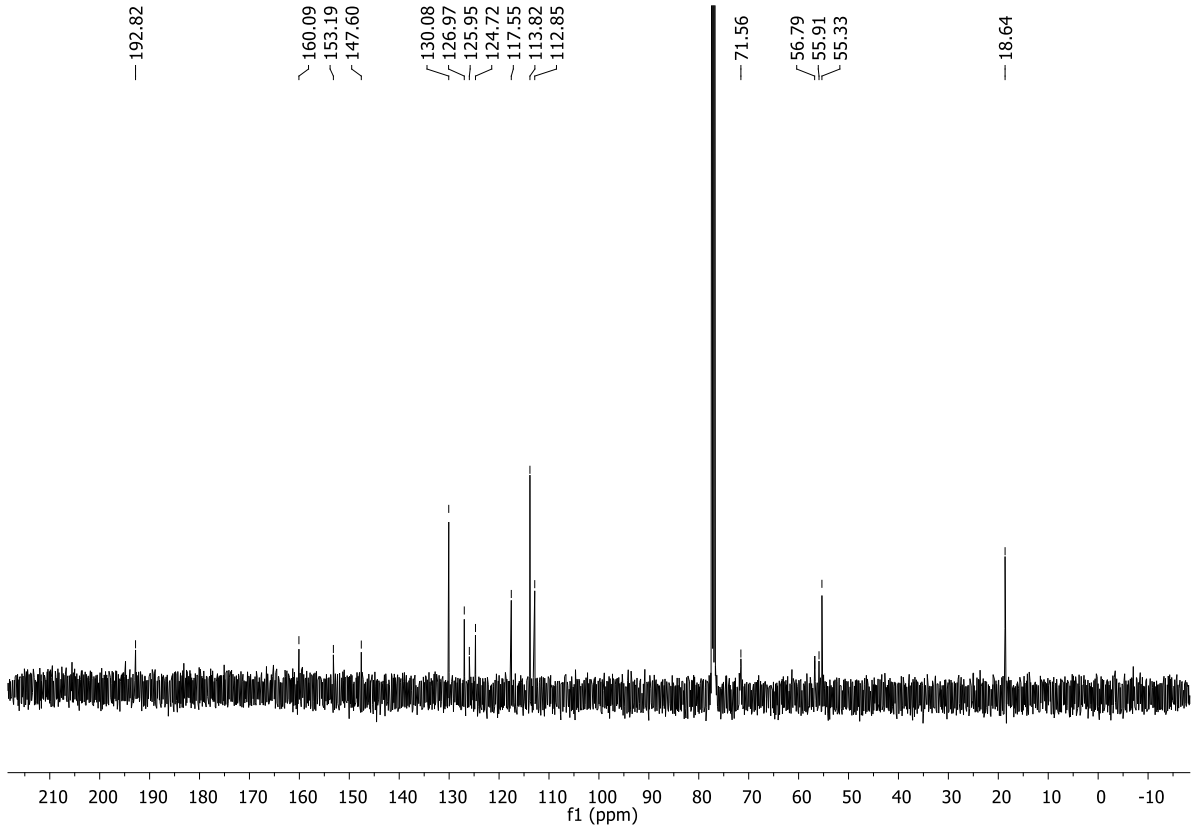
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3bd**



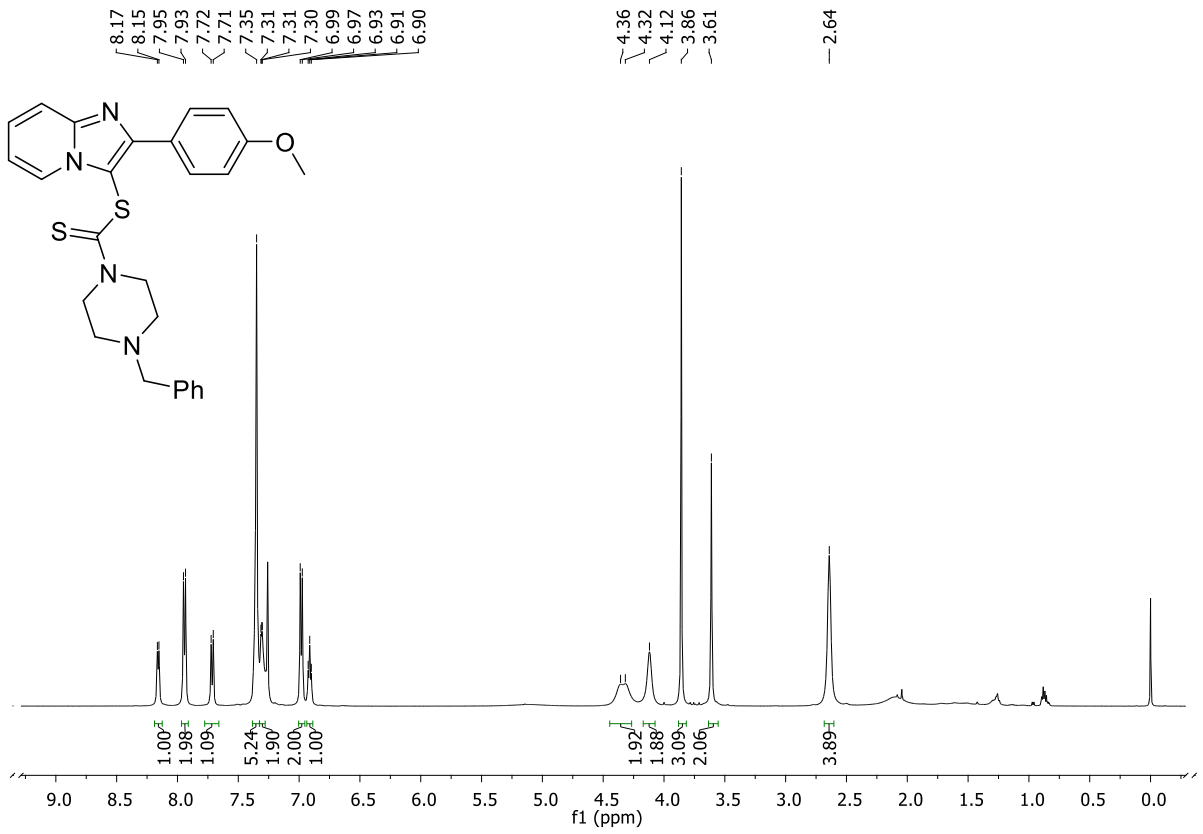
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3bd**



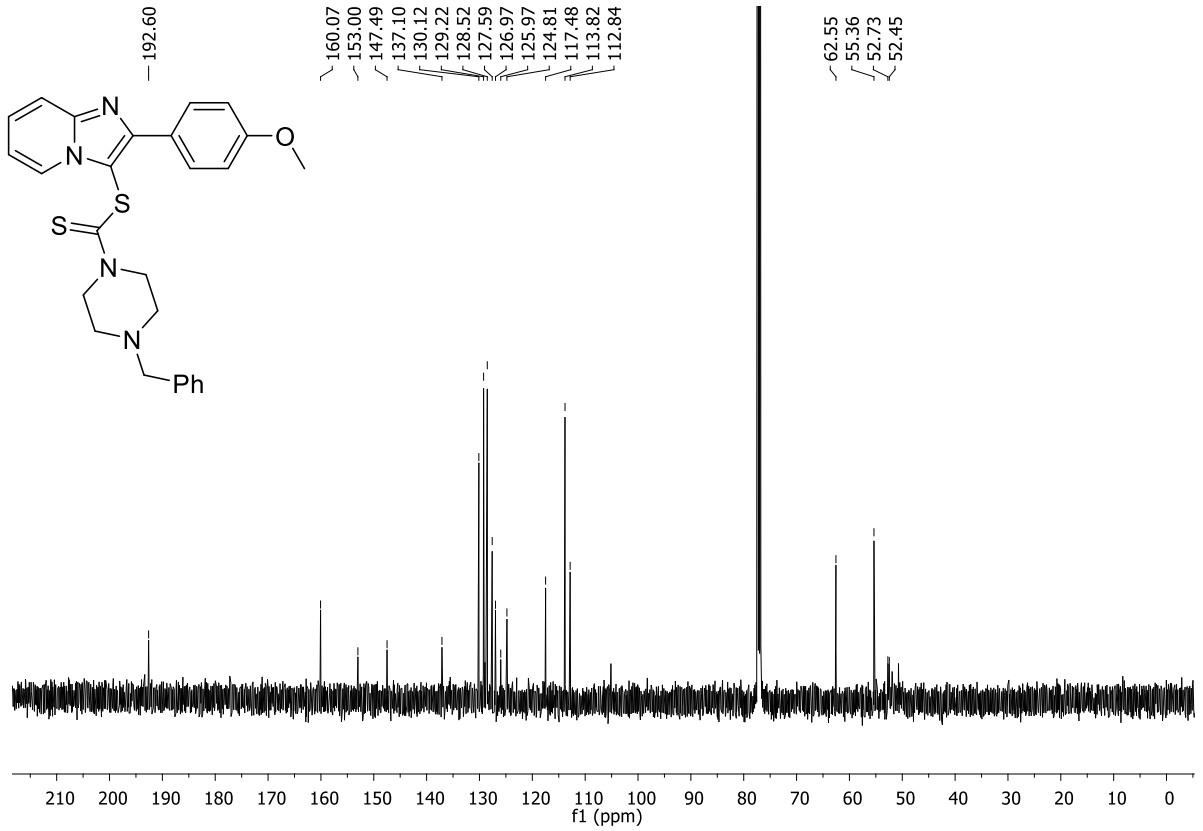
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3be**



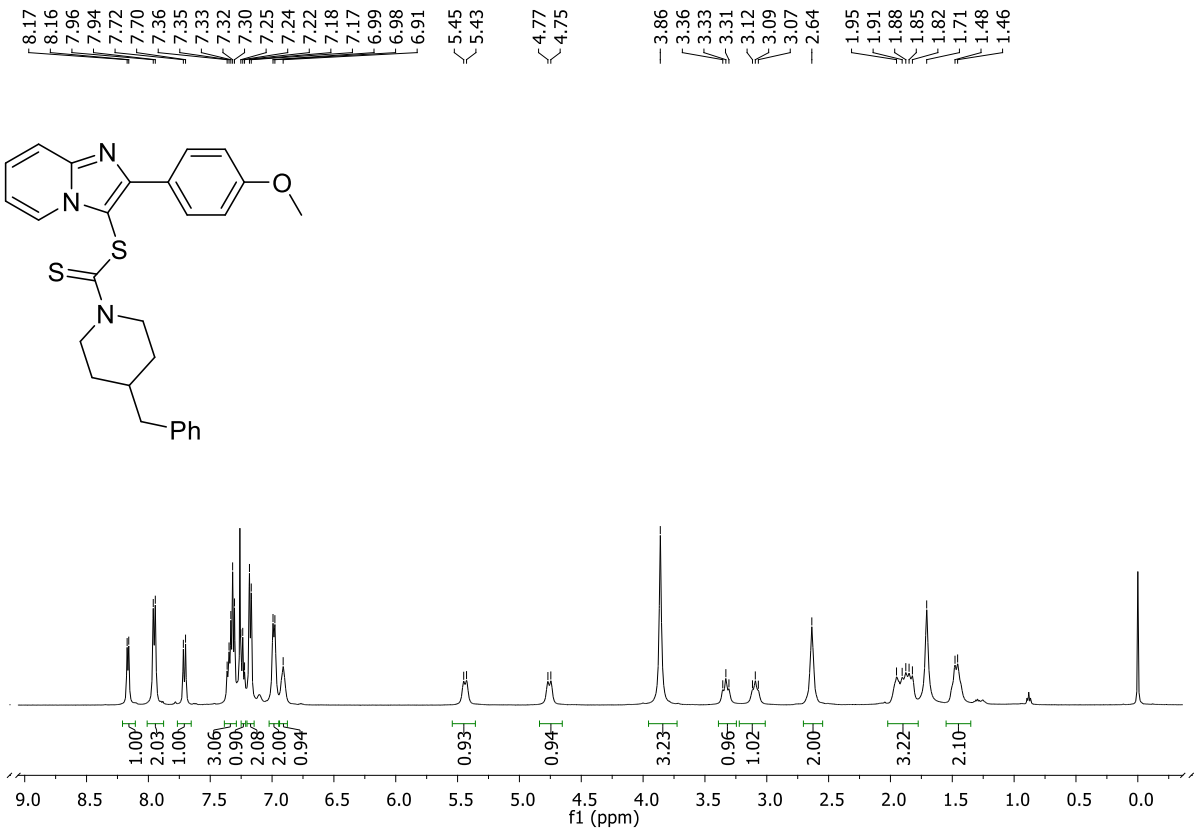
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3be**



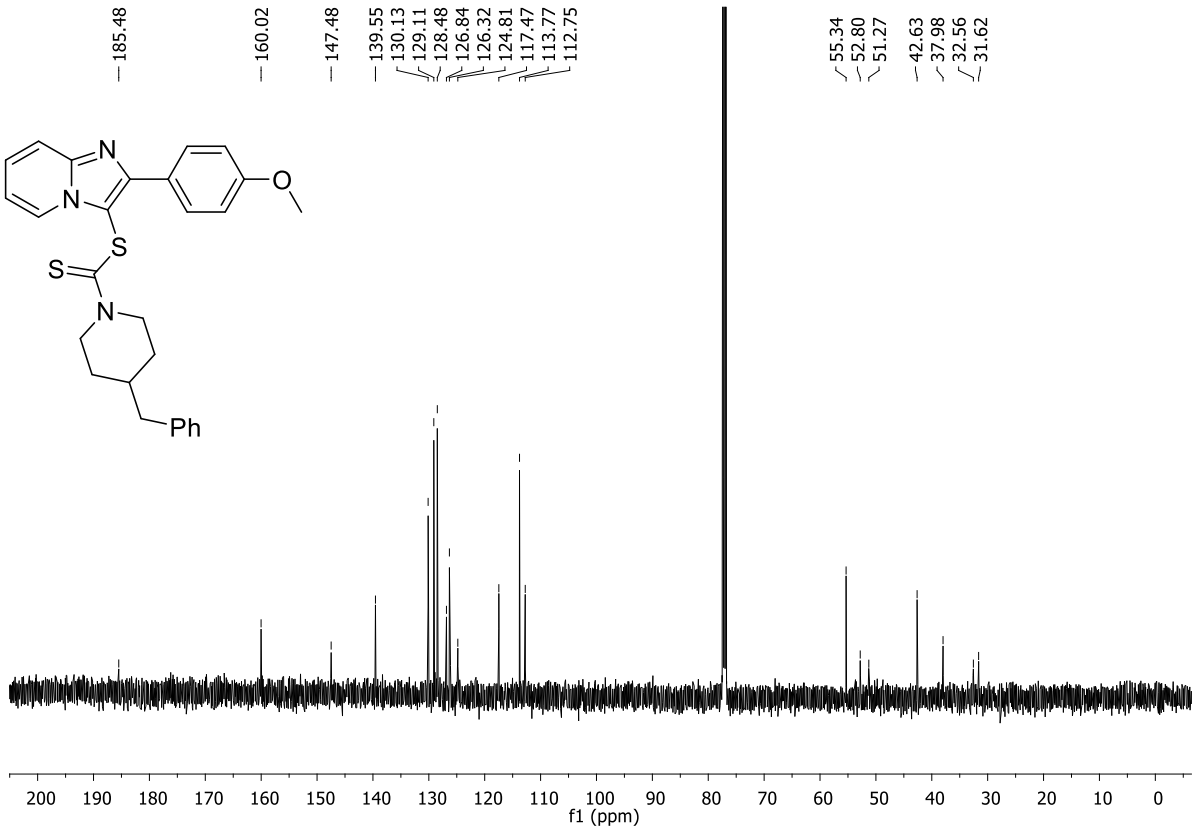
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3bf**



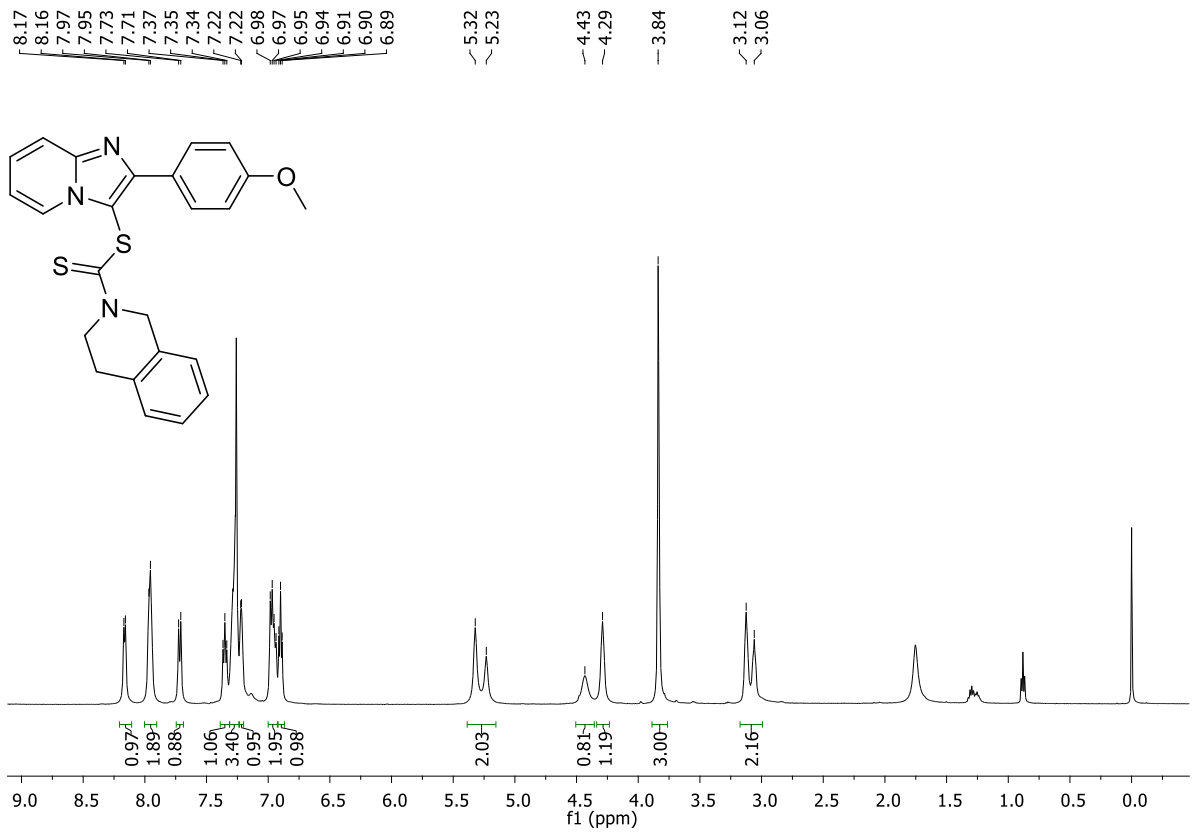
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3bf**



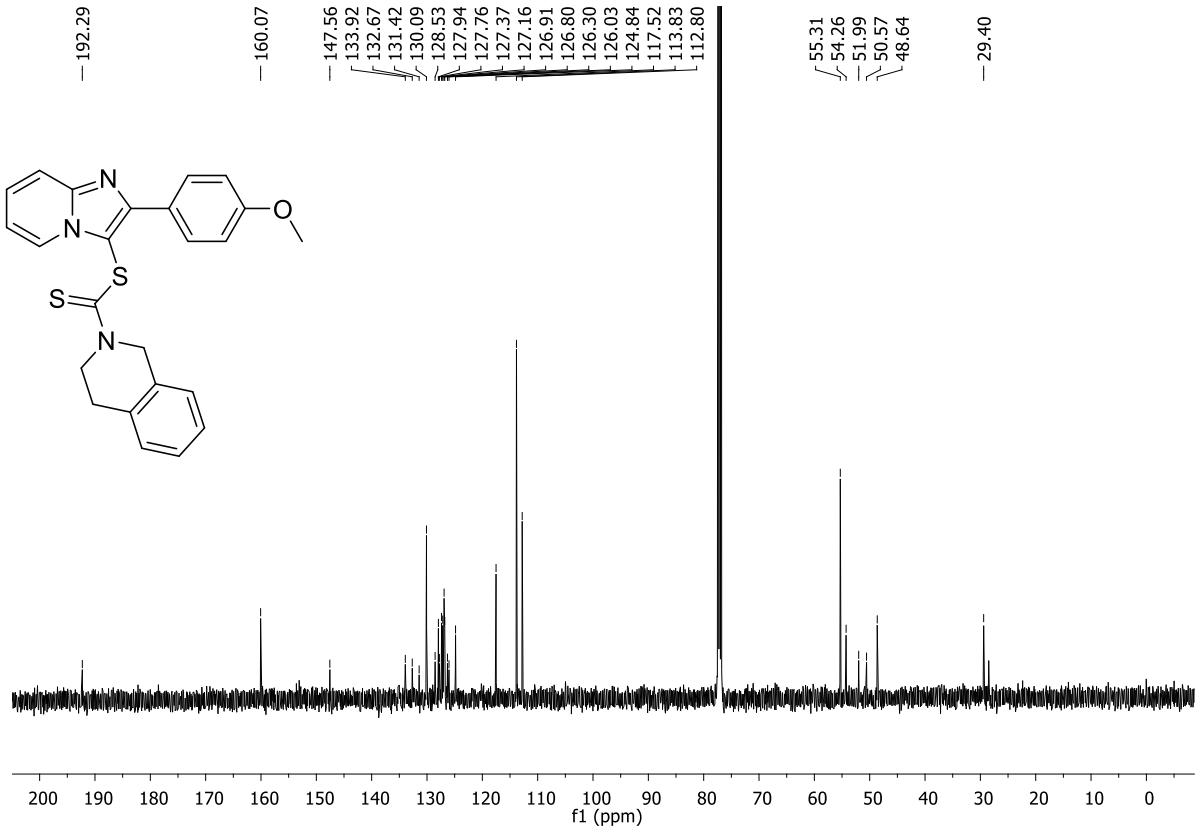
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3bg**



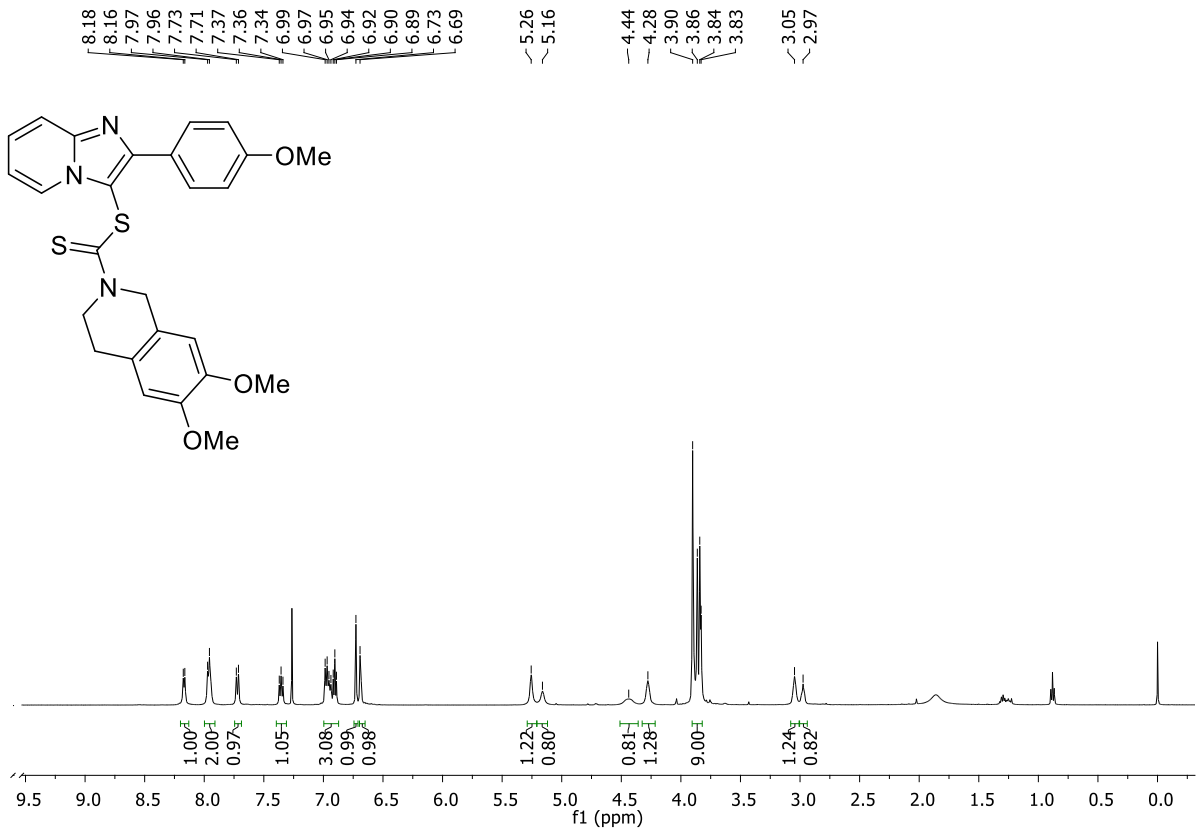
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3g**



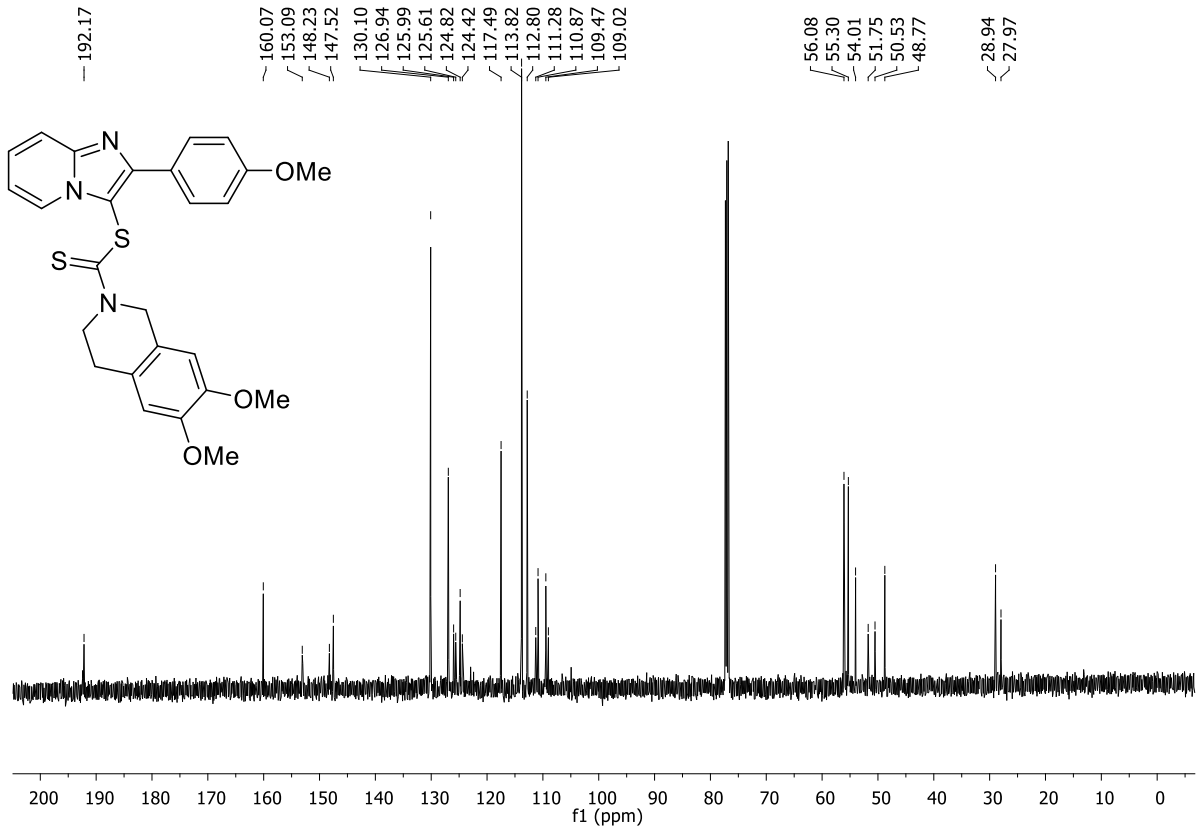
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3bh**



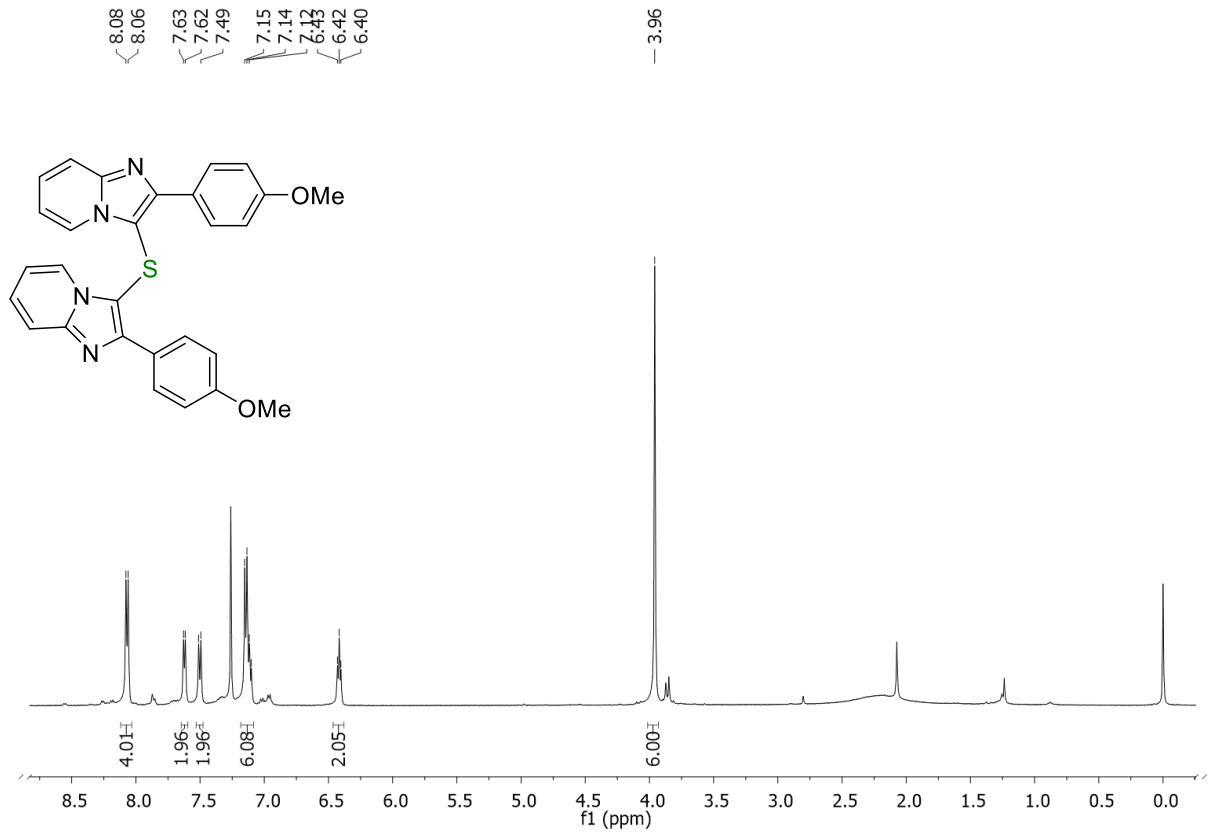
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3bh**



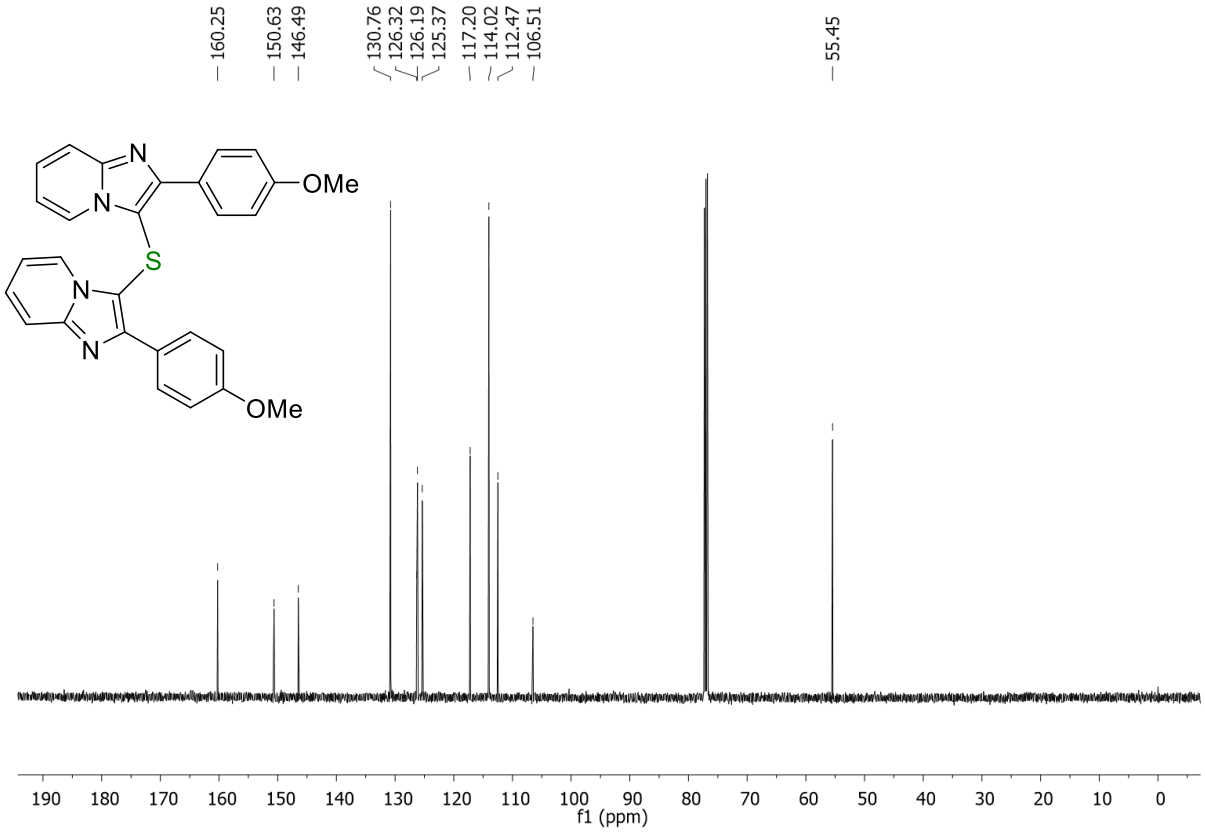
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3bi**



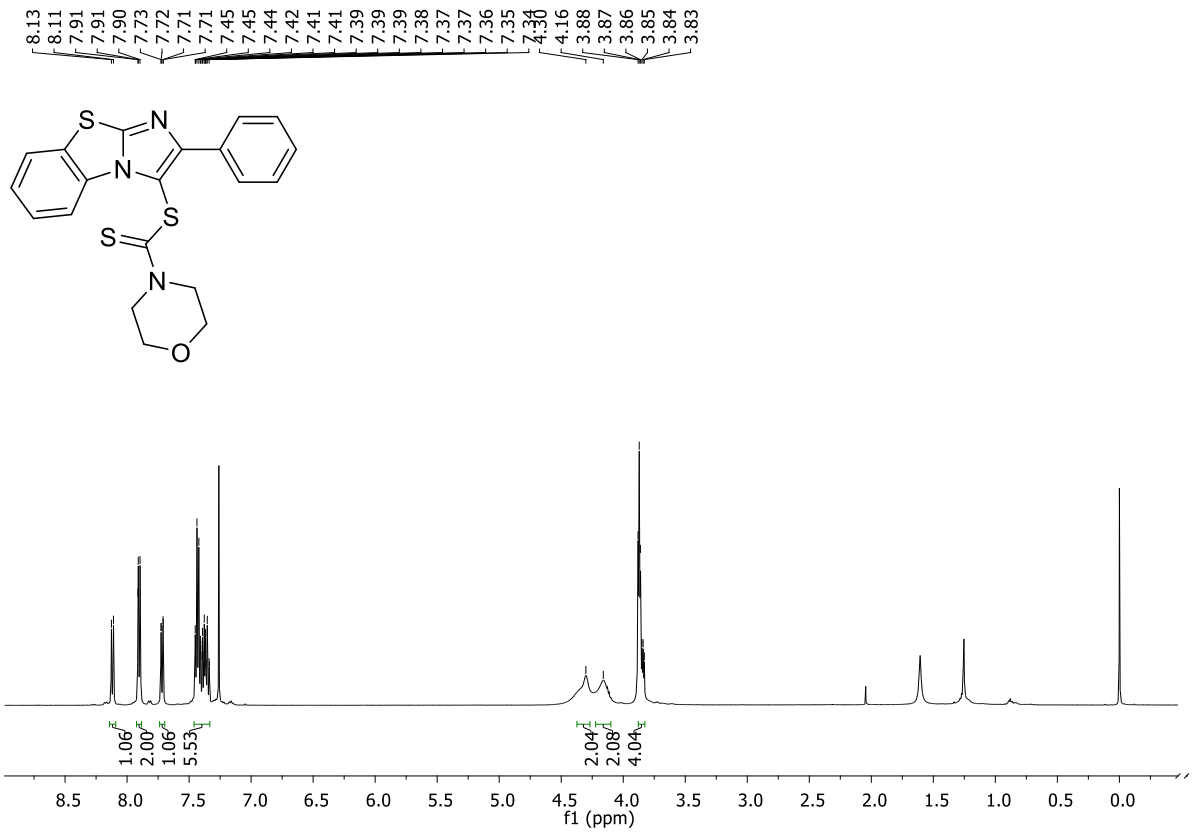
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3bi**



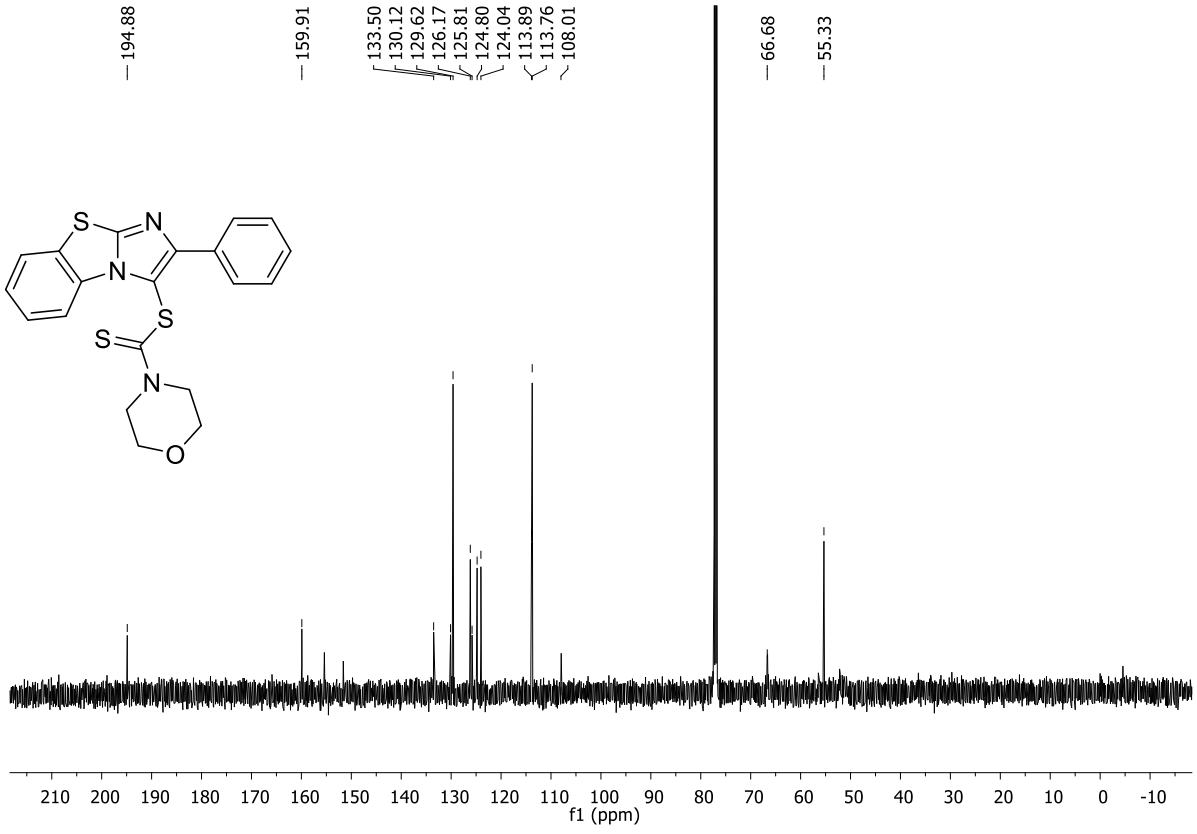
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **3bj'**



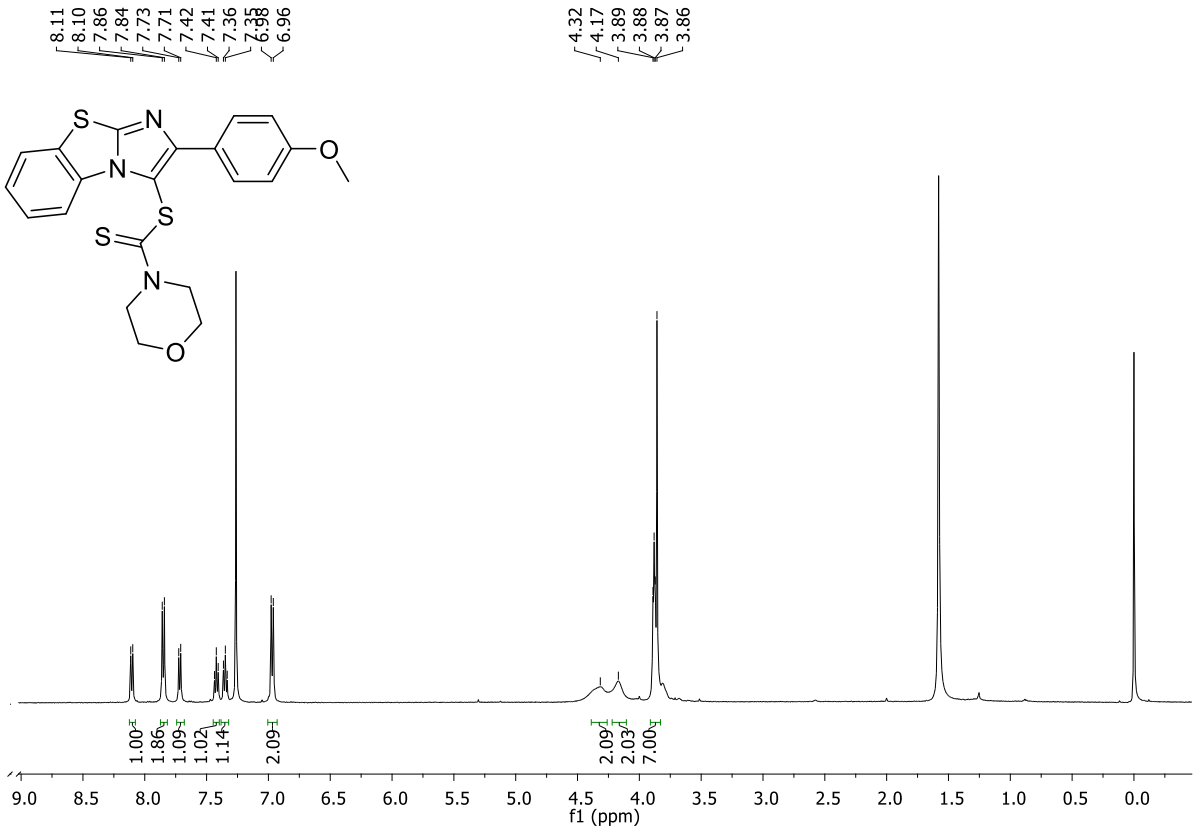
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **3bj'**



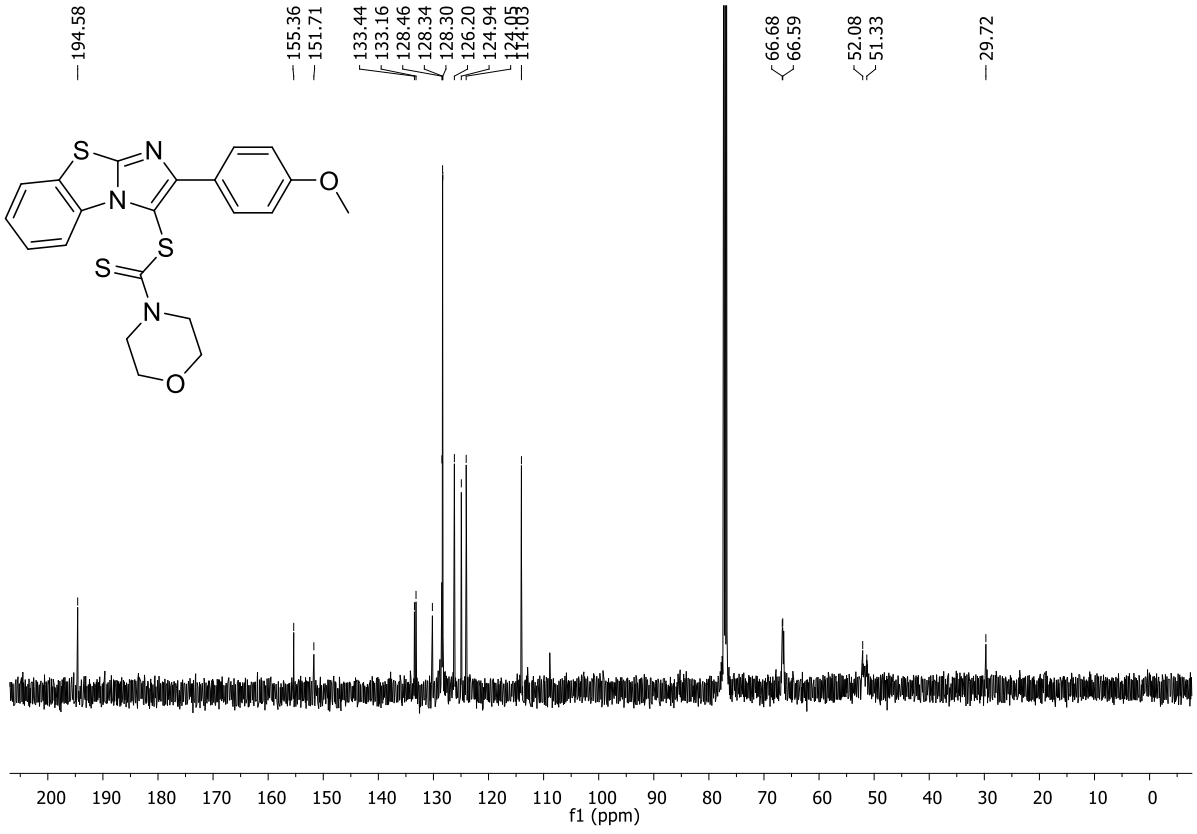
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **5a**



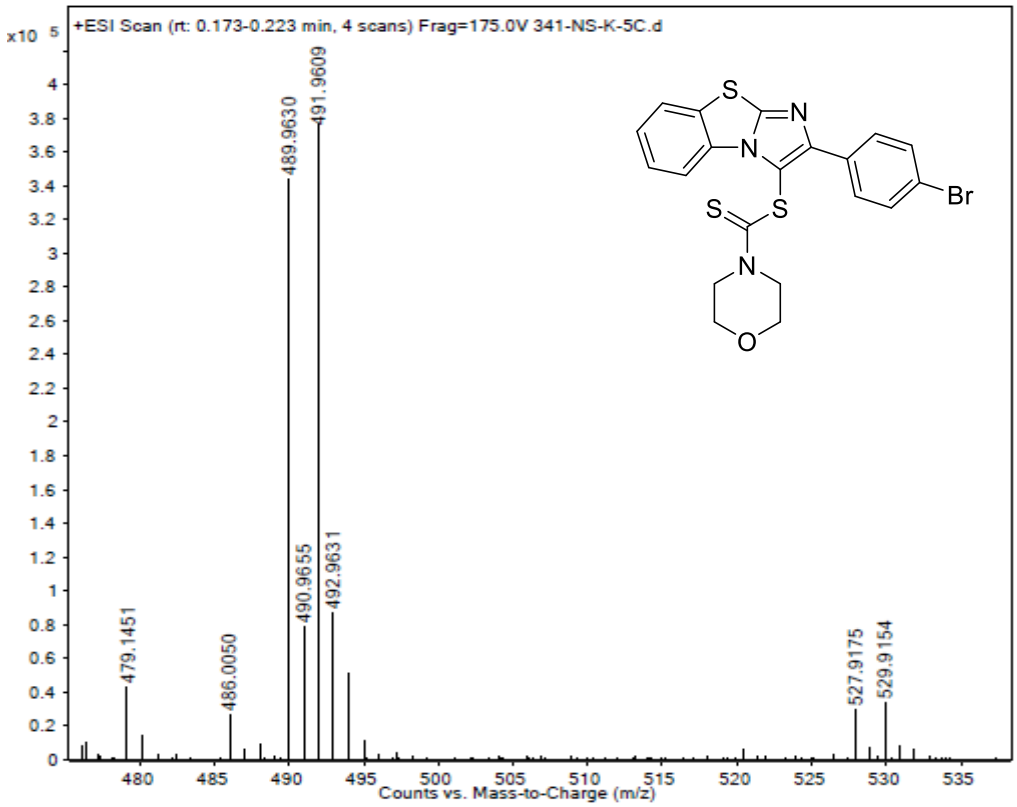
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **5a**



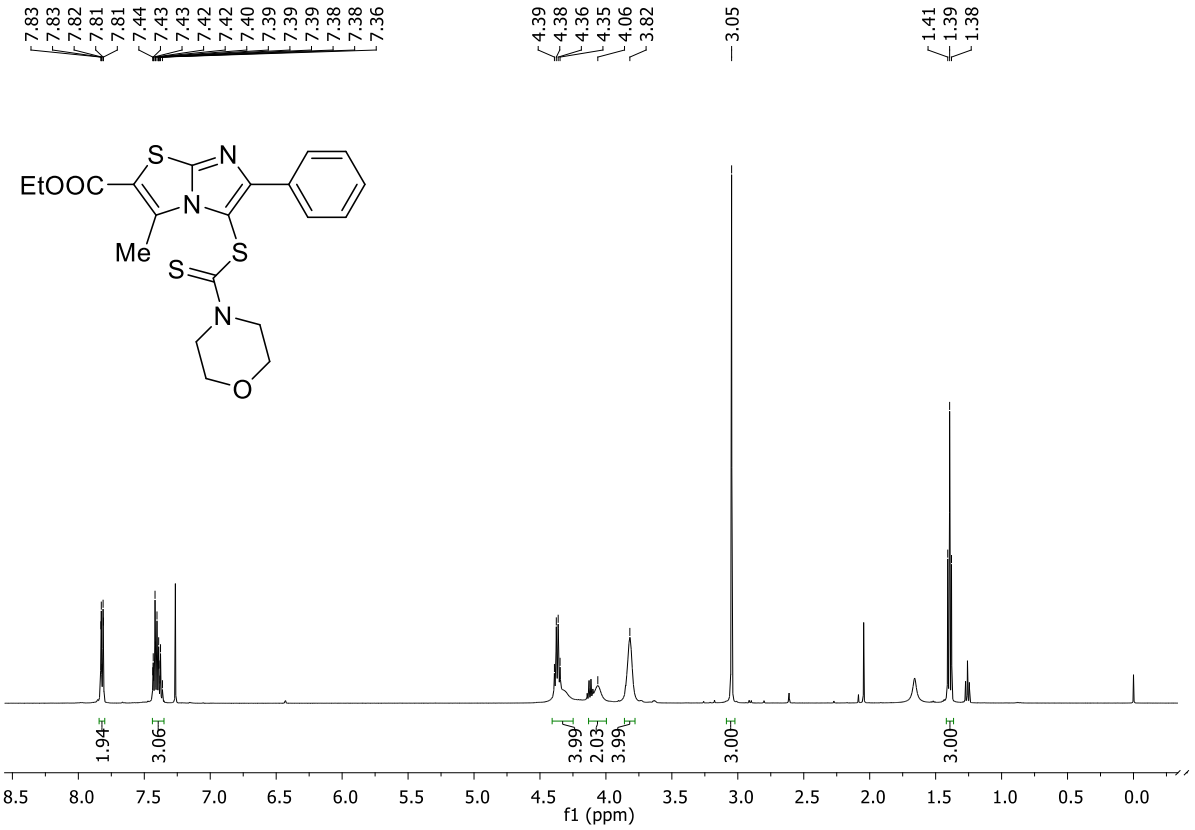
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **5b**



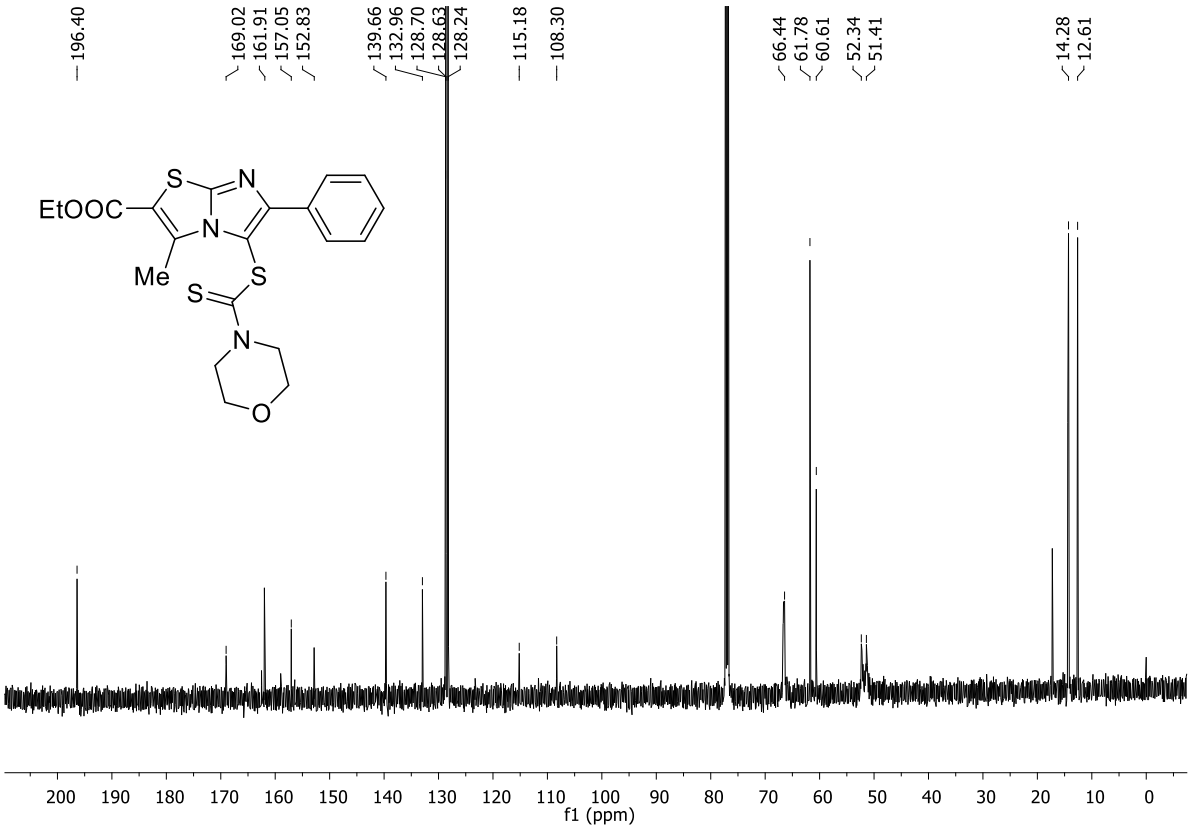
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **5b**



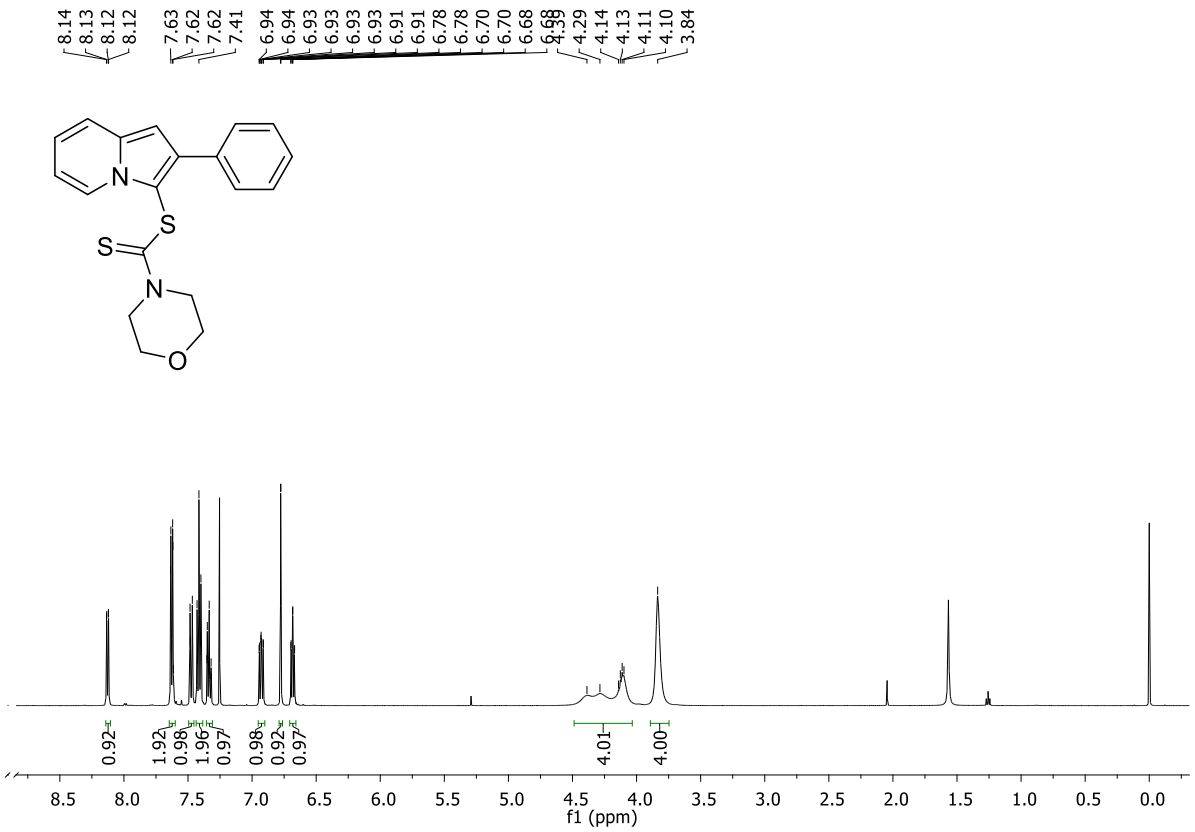
HR-MS of compound 5c



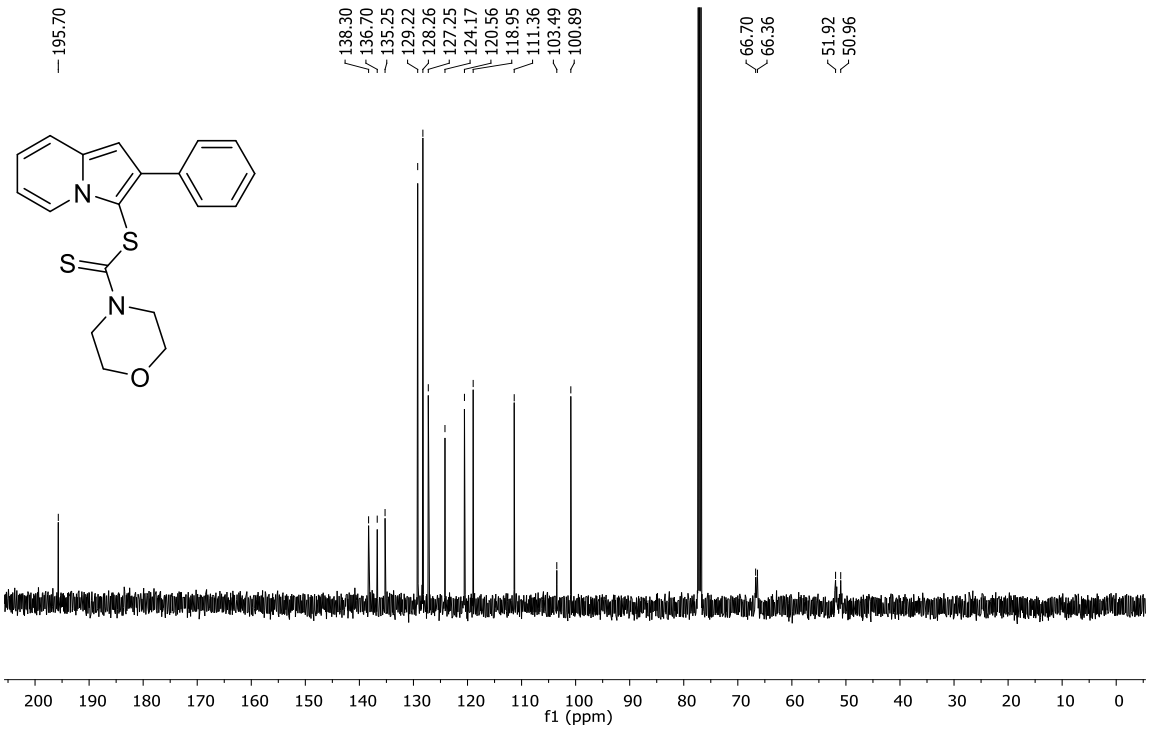
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **5d**



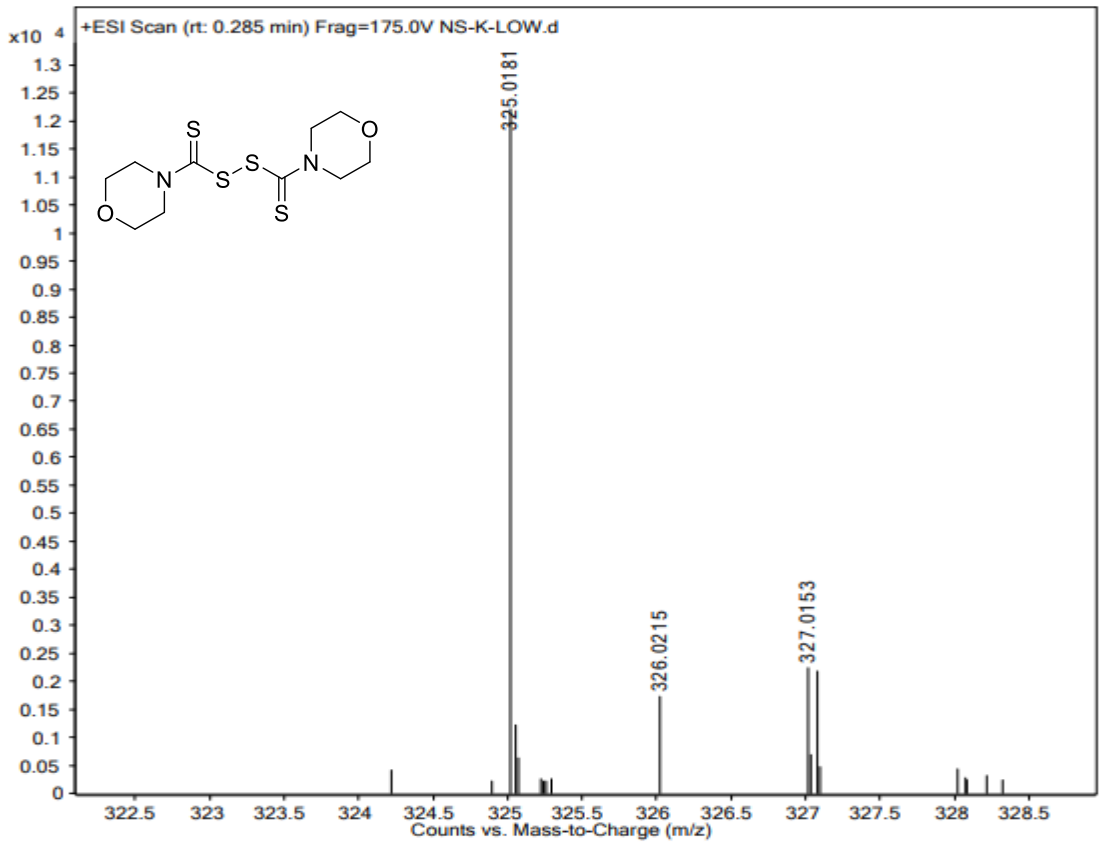
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **5d**



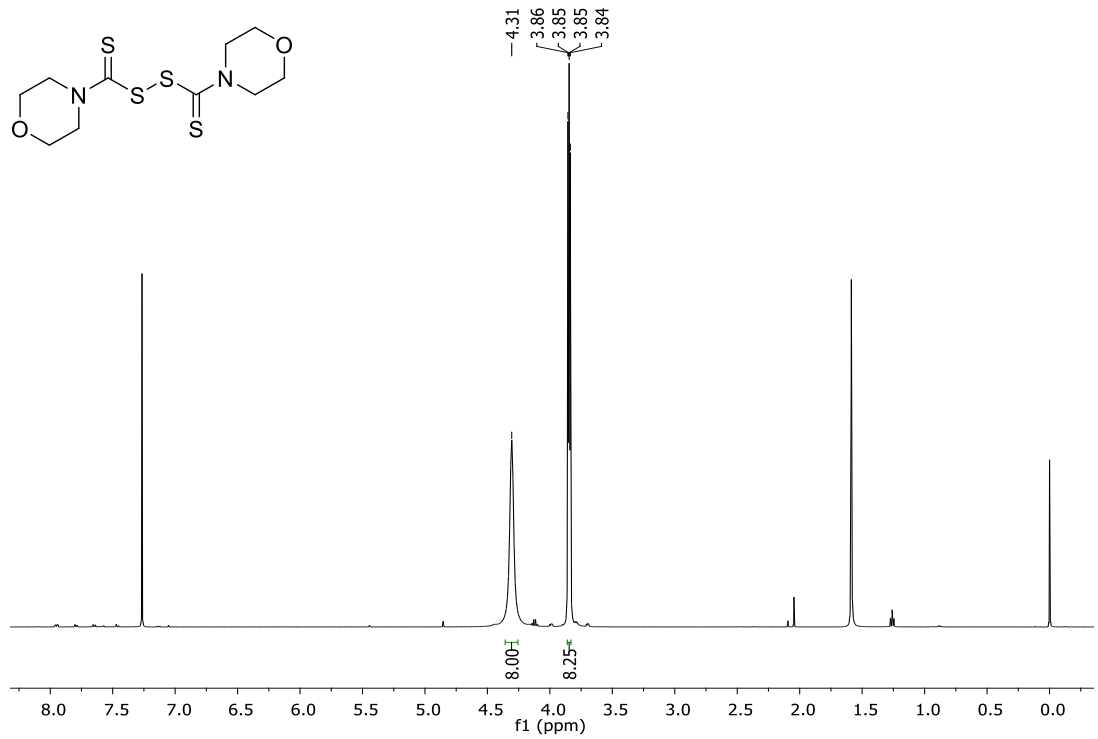
^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **5e**



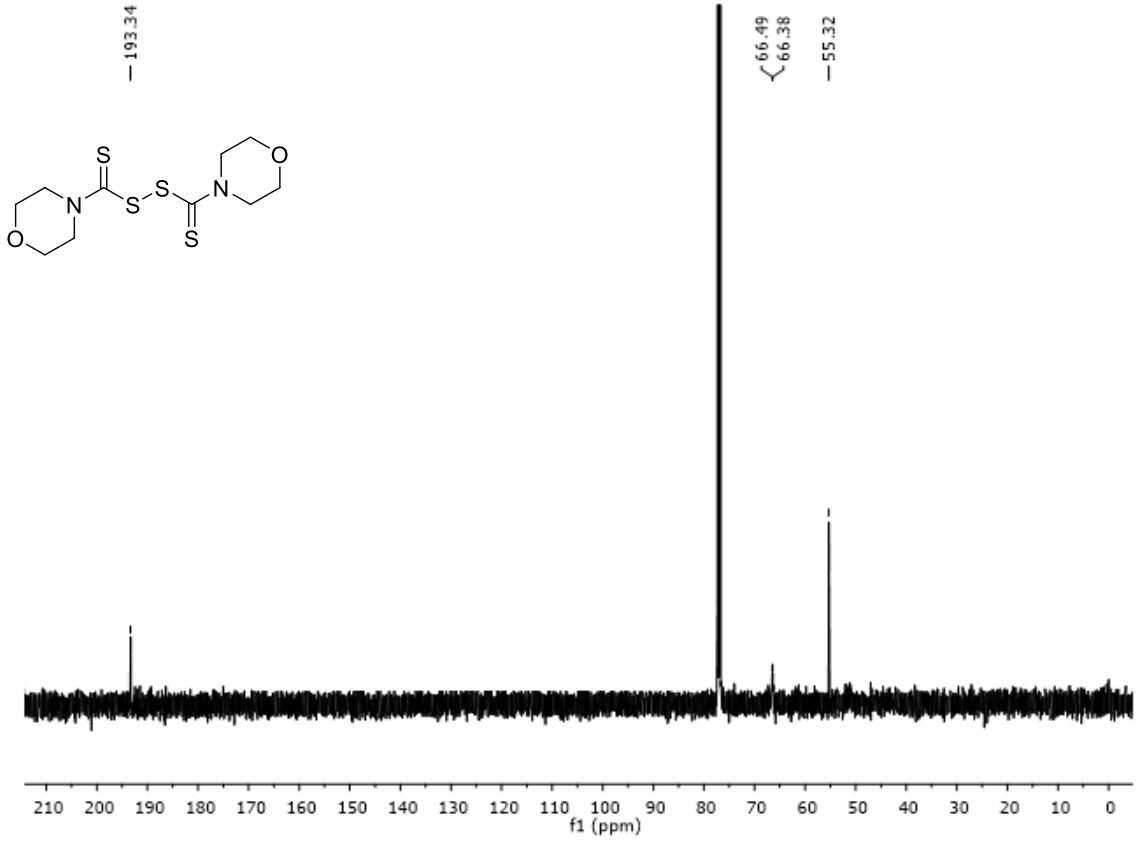
^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **5e**



HR-MS of compound 6



^{1}H NMR (500 MHz, DMSO–d_6) spectrum of compound **6**



^{13}C NMR (125 MHz, DMSO–d_6) spectrum of compound **6**

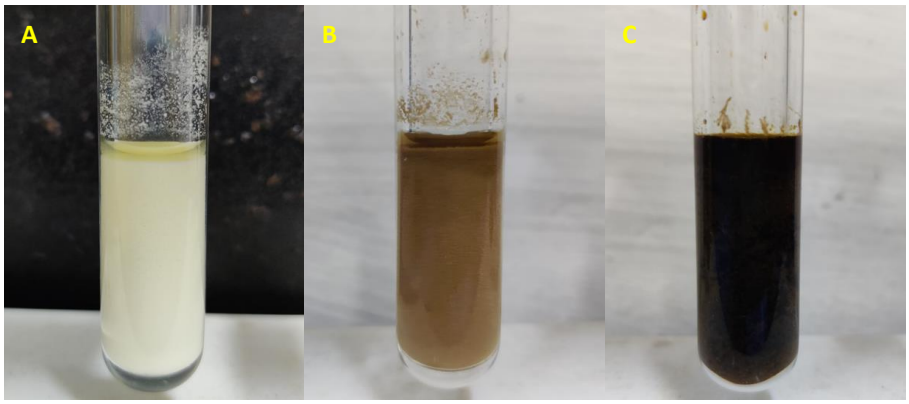


Figure S1. **A**) Imidazopyridines, secondary amine, and CS_2; **B**) After addition of water-soluble copper(I) catalyst and O_2 purging; **C**) Reaction mixture after microwave-irradiation.

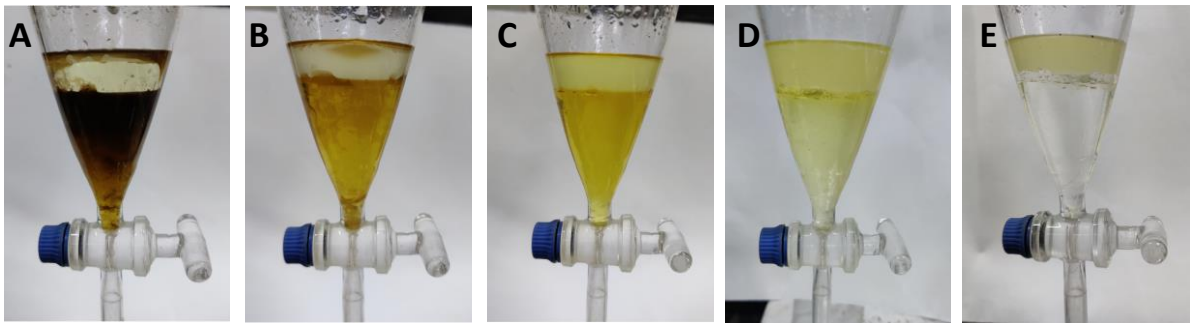


Figure S2. A-E suggests the change in the colour of organic layer of CH_2Cl_2 (below) and aqueous layer (above) due to decreased catalyst loading during recyclability of catalyst in each cycle.

Table S1. Percentage inhibition of compounds **3aa**–**3na**, **3bb**–**3bi** and **5a**–**5e**[a]

Compound	Percentage Inhibition % (50 µM)	
	HCT-116[b]	**MCF-7**[c]
3aa	<50	<50
3ba	<50	<50
3ca	<50	<50
3da	<50	<50
3ea	<50	65.84
3fa	<50	<50
3ga	<50	<50
3ha	<50	<50
3ia	<50	>50
3ja	<50	<50
3ka	<50	<50
3la	<50	<50
3ma	<50	>50
3na	<50	57.17
3bb	<50	**90.17**
3bc	<50	83.40
3bd	<50	<50

3be	52.67	**91.10**
3bf	<50	55.78
3bg	<50	<50
3bh	<50	80.42
3bi	<50	<50
5a	<50	50.42
5b	<50	<50
5d	<50	<50
5e	<50	<50
5-FU[d]	75.82	70.35

[a]Percentage inhibition on HCT-116 and MCF-7 cancer cell lines at 50 μM concentration after 48 h. [b] Human colon cancer cell line. [c] Human breast cancer cell line. [d] Standard drug 5-fluorouracil.

Table S2. Cytotoxic activity (IC_{50} in μM)[a] of most active analogues.

Compound	**IC_{50} value (μM)**		
	HCT-116[b]	**MCF-7**[c]	**BEAS-2B**[d]
3bb	–	10.20±2.10	>50
3be	–	7.28±2.31	>50
Standard[e]	16.58±2.23	24.78±0.08	–

[a] 50% inhibitory concentration after 48 h of compound treatment. [b] Human colon cancer cell line. [c] Human breast cancer cell line. [d] Normal human lung epithelial cells. [e] 5- Fluorouracil (5-FU).