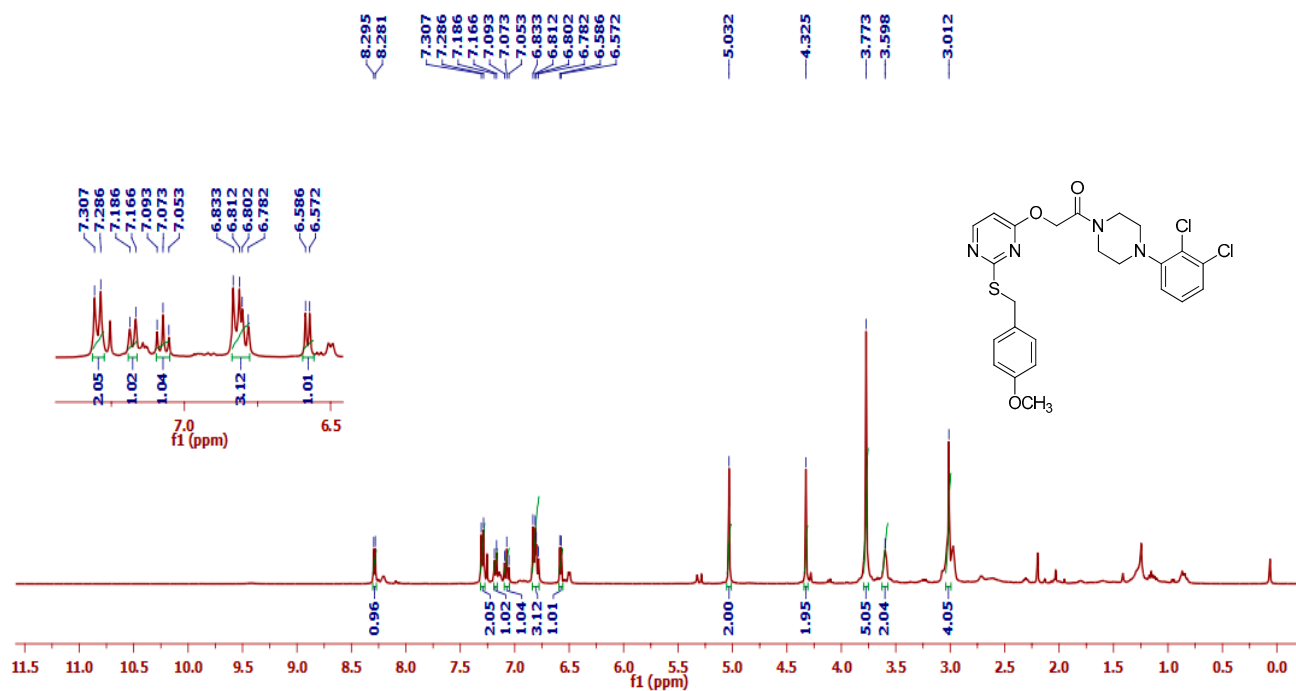


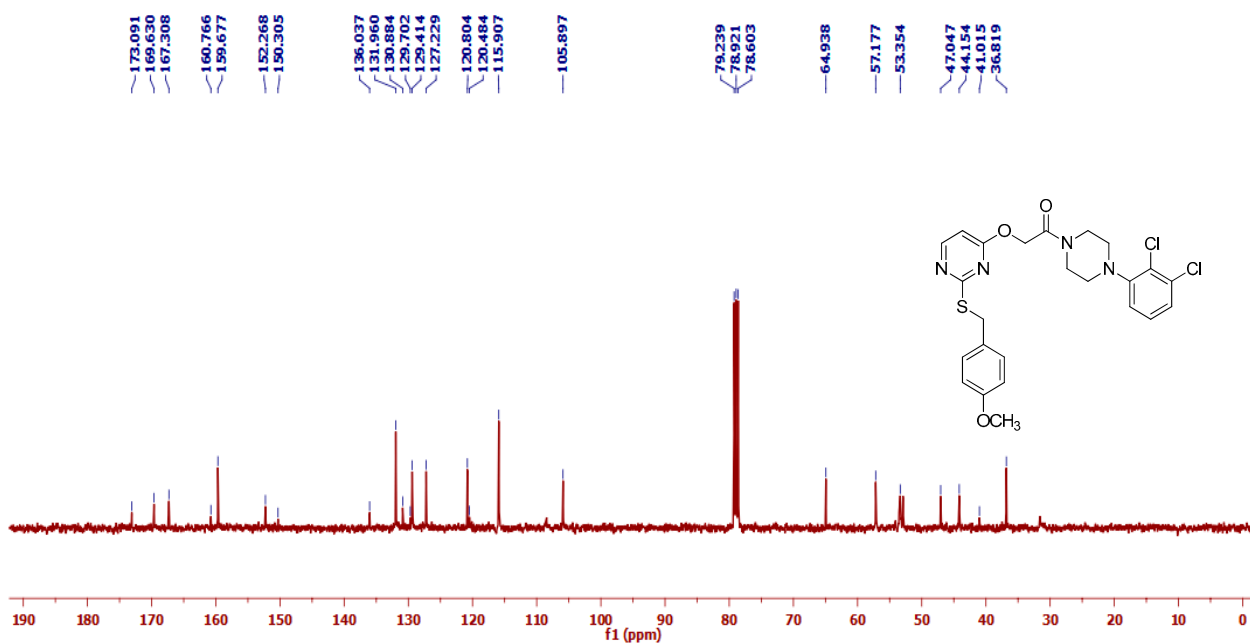
Development of 1-(4-(substituted)piperazin-1-yl)-2-((2-((4-methoxybenzyl)thio)pyrimidin-4-yl)oxy)ethanones that target Poly(ADP -Ribose)Polymerase in human breast cancer cells

Suresha N Deveshegowda, Prashant K Metri, Rashmi Shivakumar, Ji-Rui Yang, Shobith Rangappa, Ananda Swamynayaka, Muthu K Shanmugam, Omantheswara Nagaraja, Mahendra Madegowda, Priya Babu Shubha, Arunachalam Chinnathambi, Sulaiman Ali Alharbi, Vijay Pandey, Kwang Seok Ahn, Peter E. Lobie and Basappa Basappa

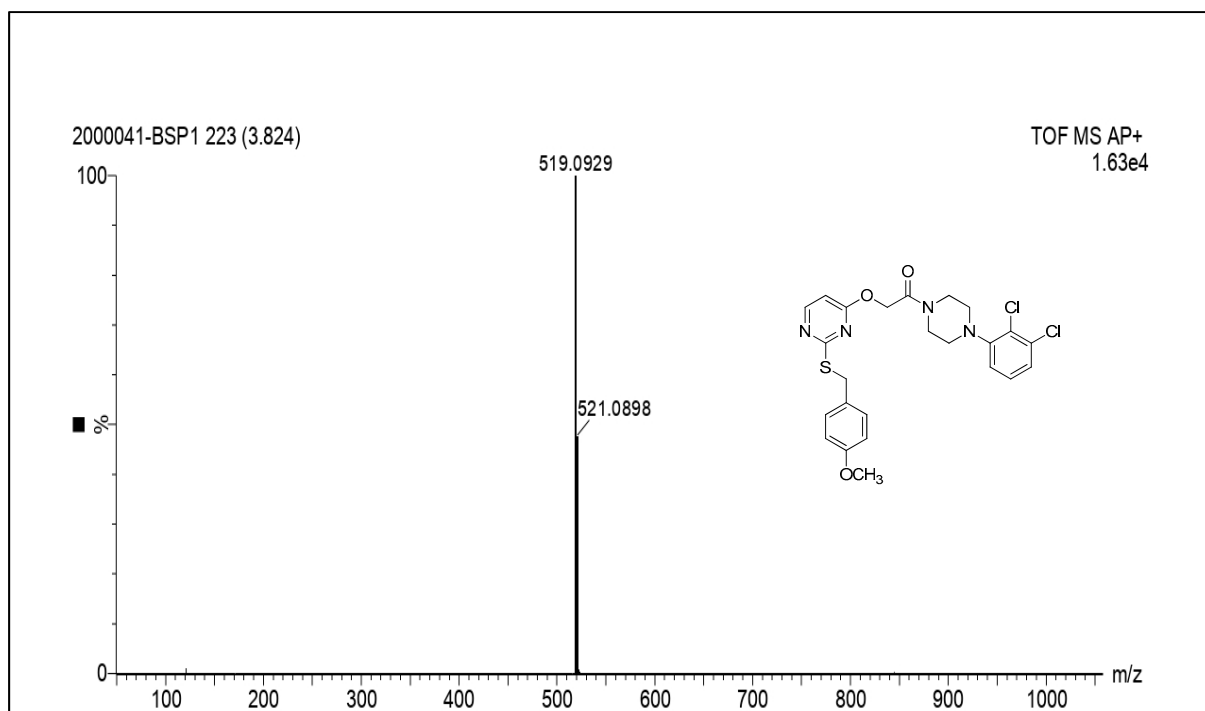
Supplementary data for newly synthesized molecules and their IC₅₀ values determined against human breast cancer cells



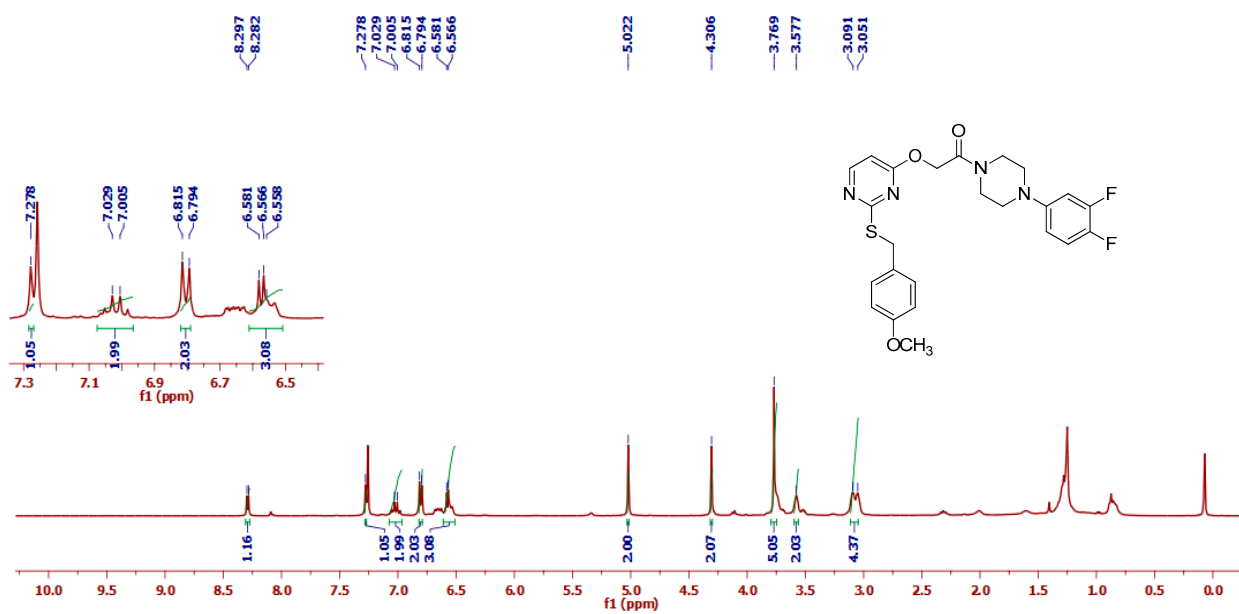
¹H NMR of compound 5a



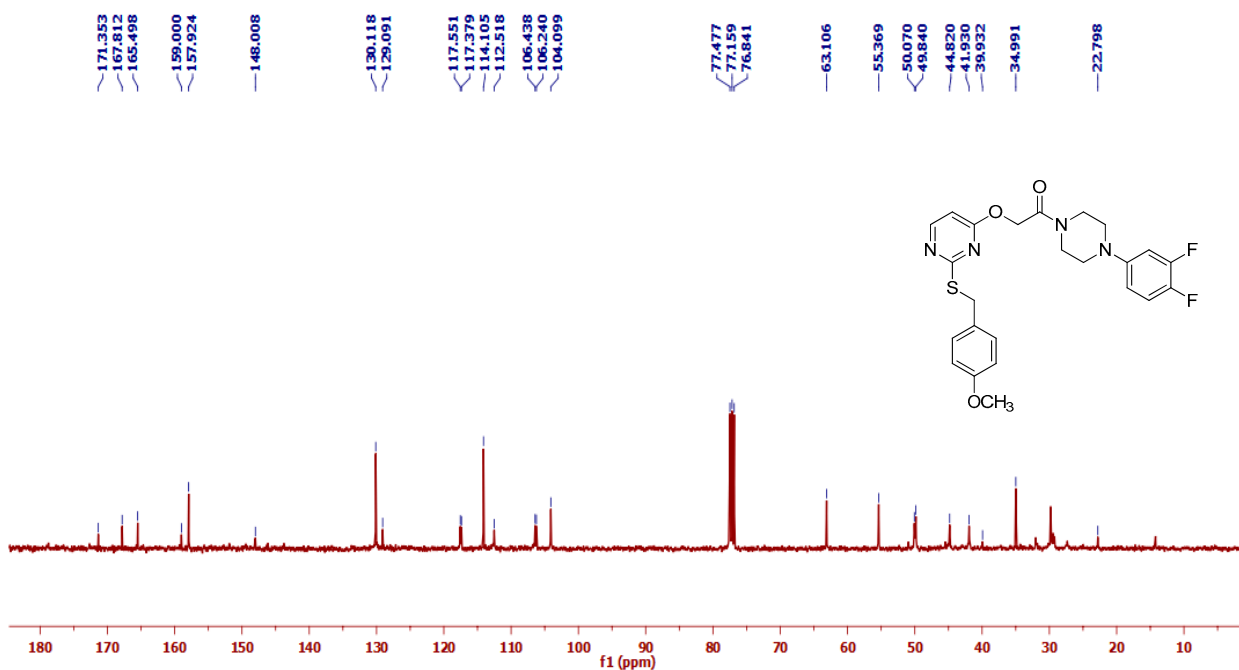
¹³C NMR of compound 5a



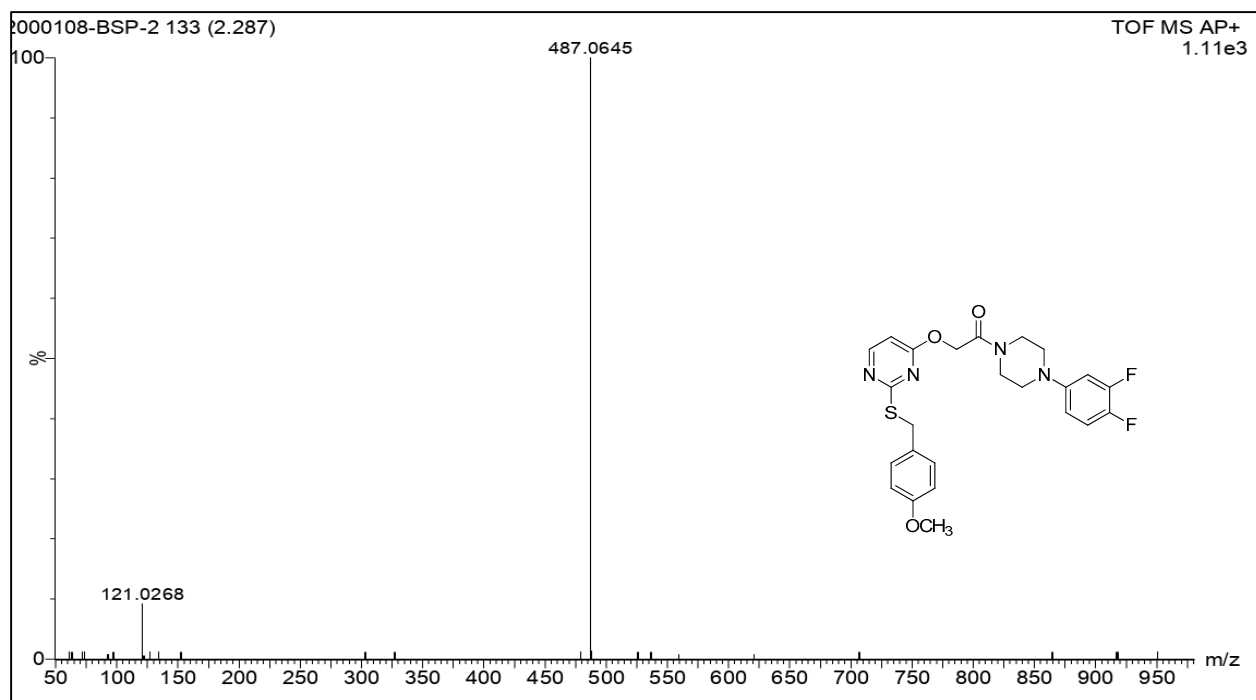
Mass spectra of **5a**



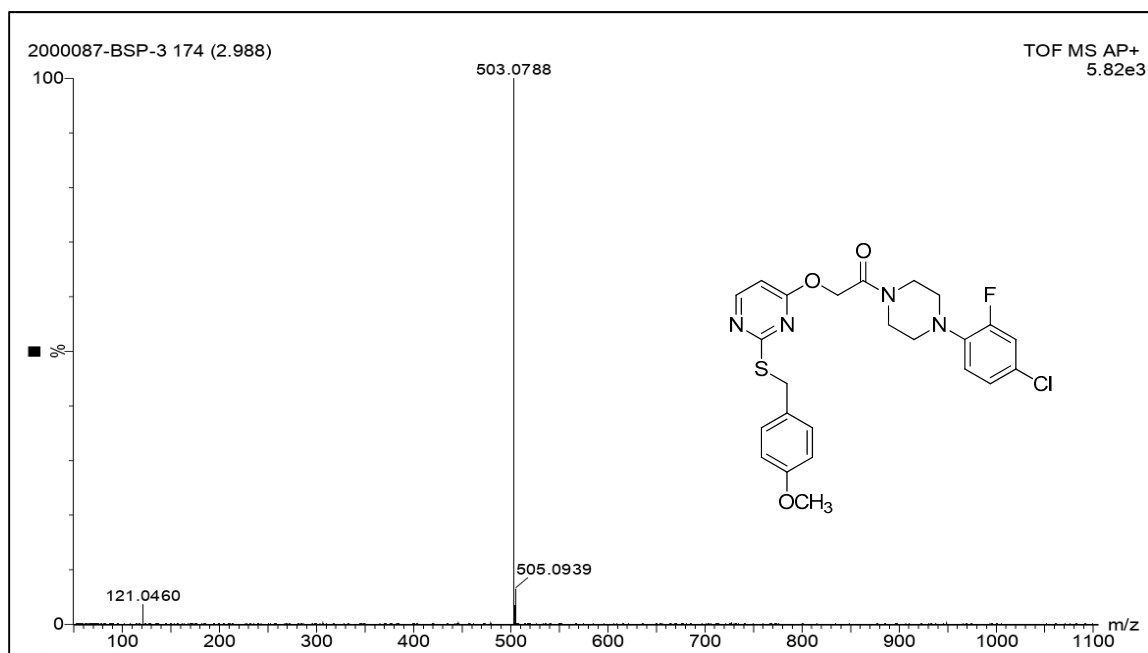
¹H NMR of compound 5b



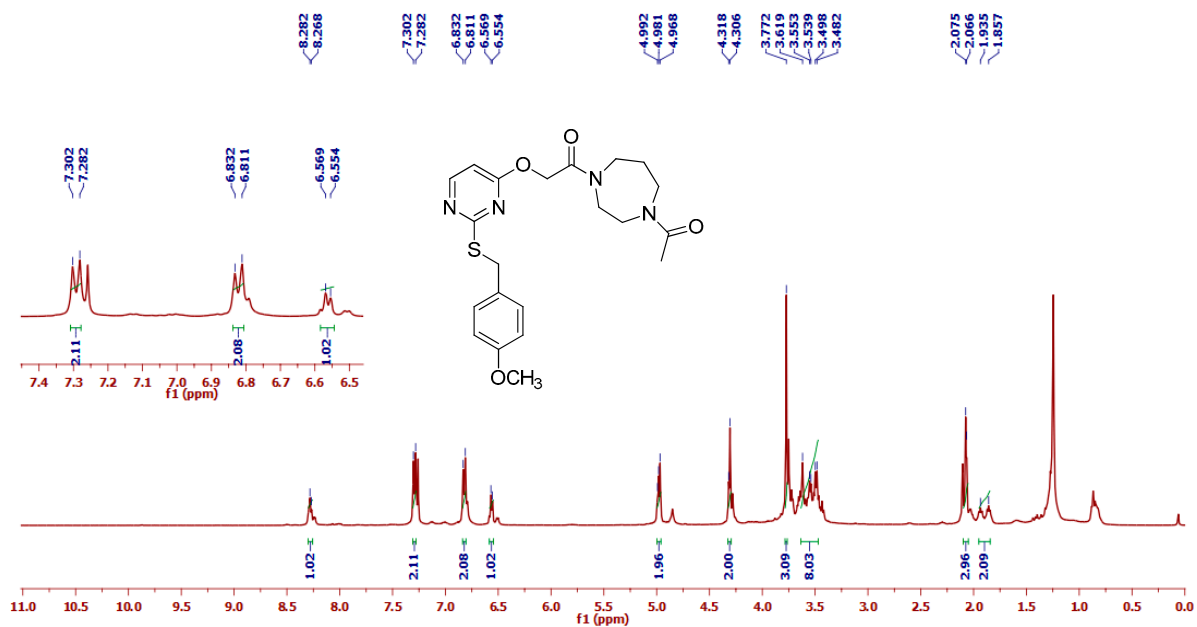
¹³C NMR of compound 5b



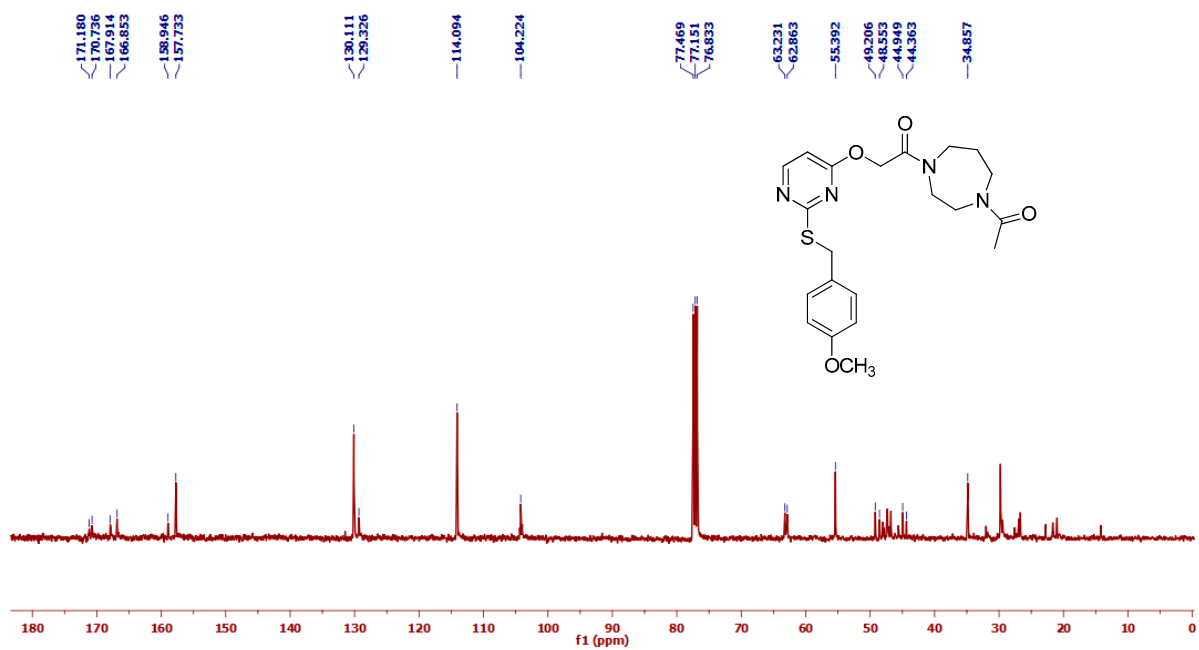
Mass spectra of **5b**



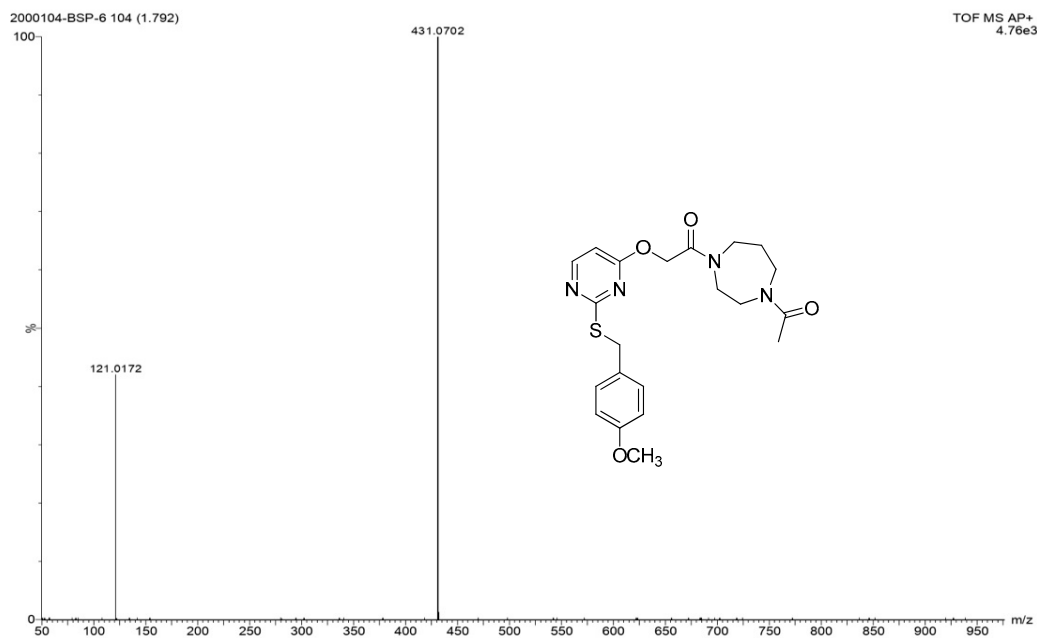
Mass spectra of 5c



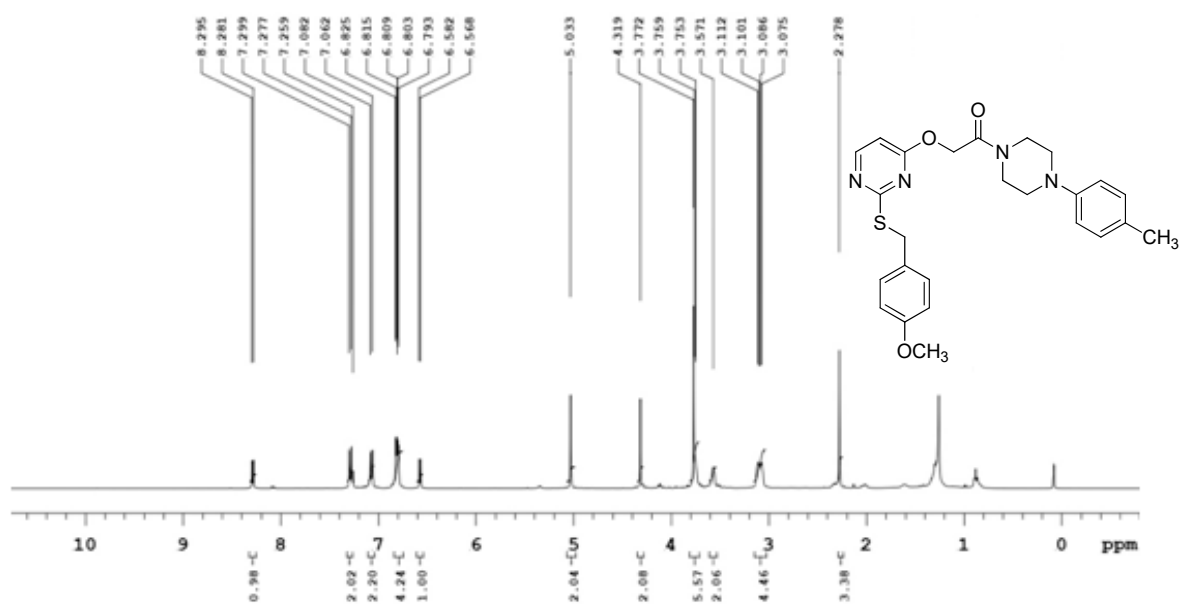
¹H NMR of compound 5d



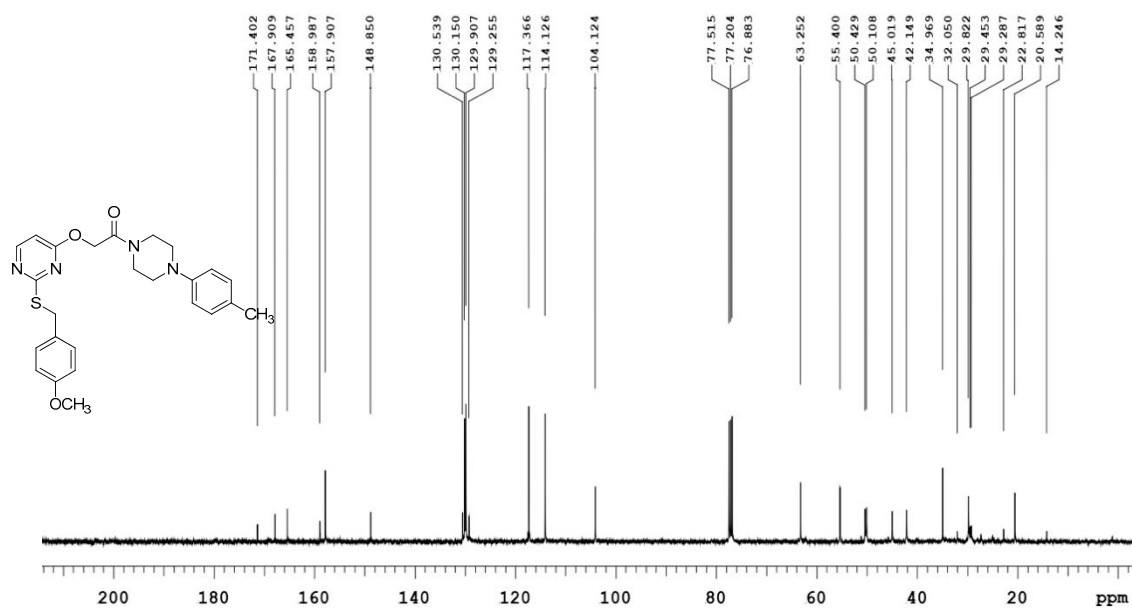
¹³C NMR of compound **5d**



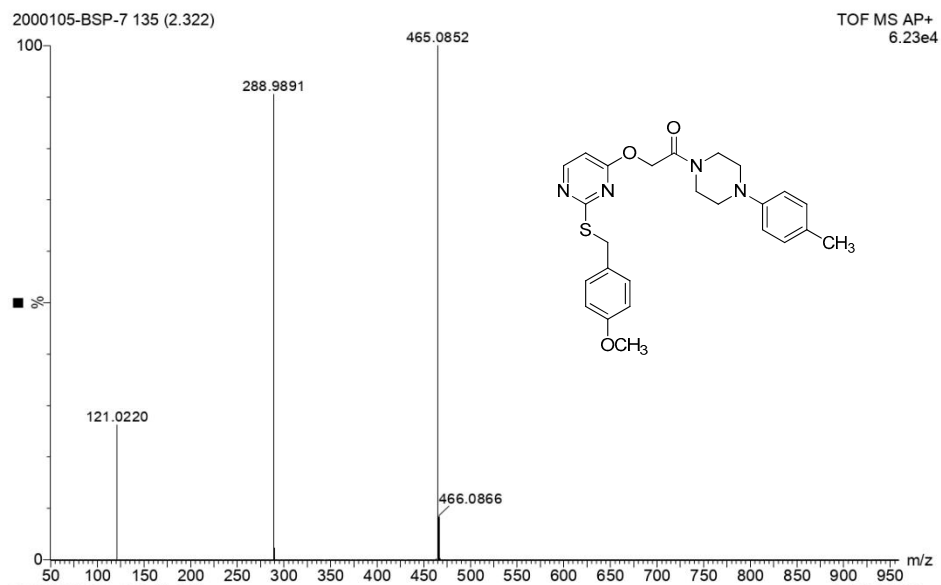
Mass spectra of **5d**



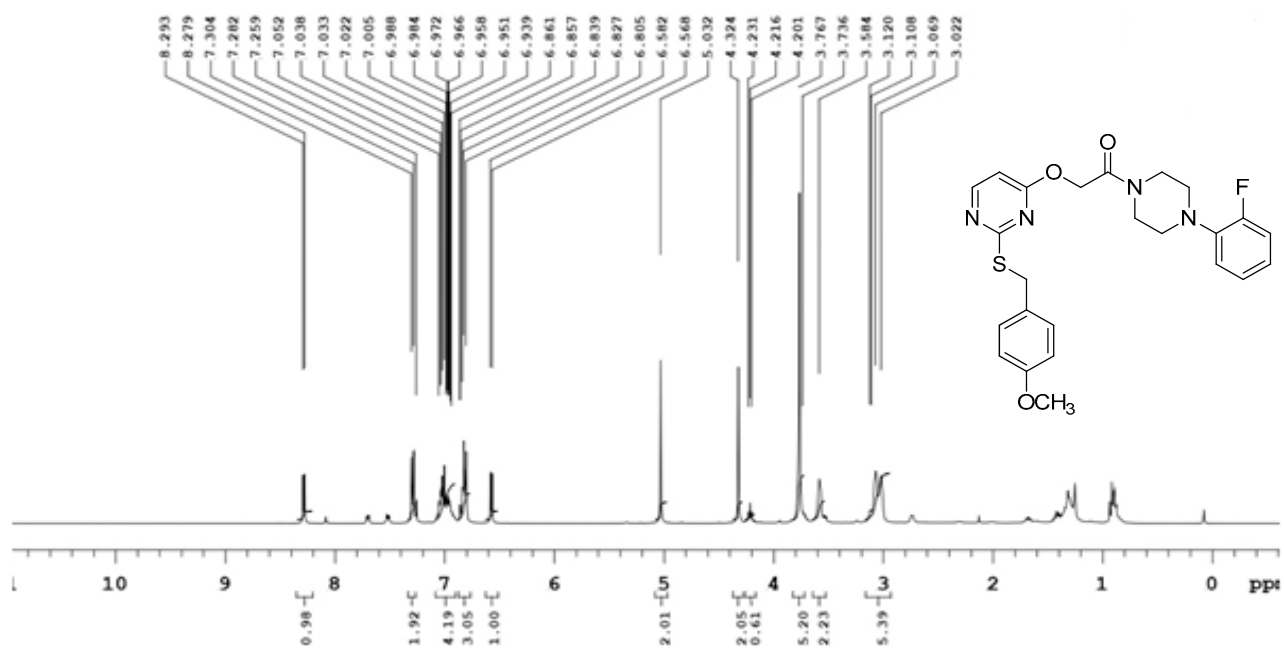
¹H NMR of compound **5e**



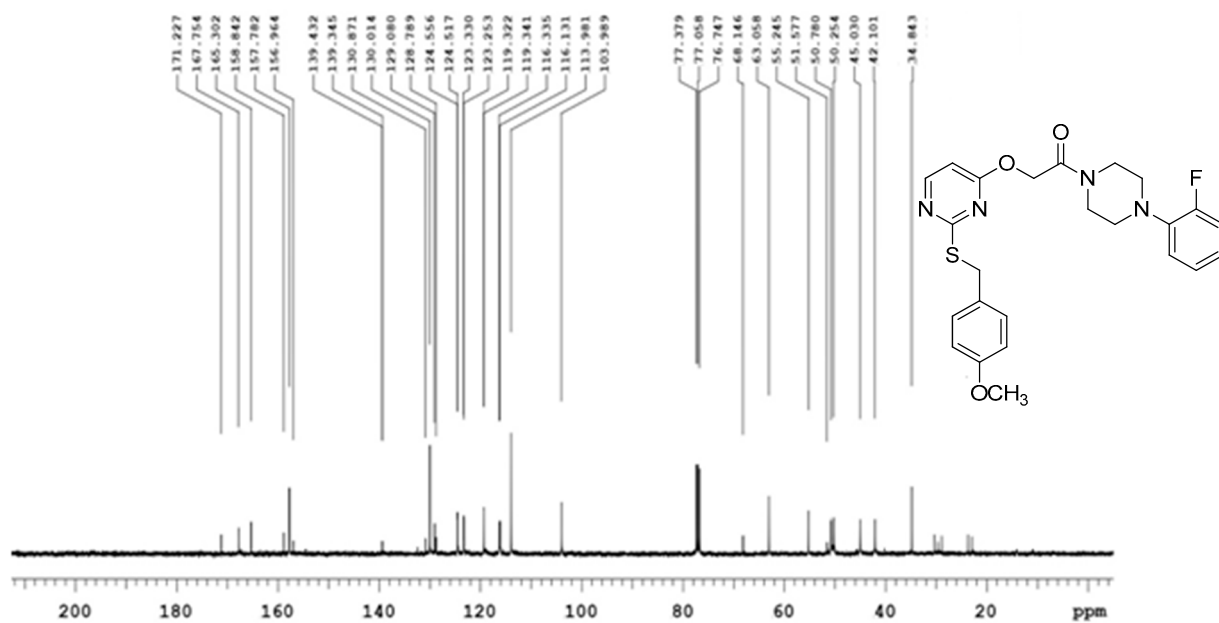
¹³C NMR of compound **5e**



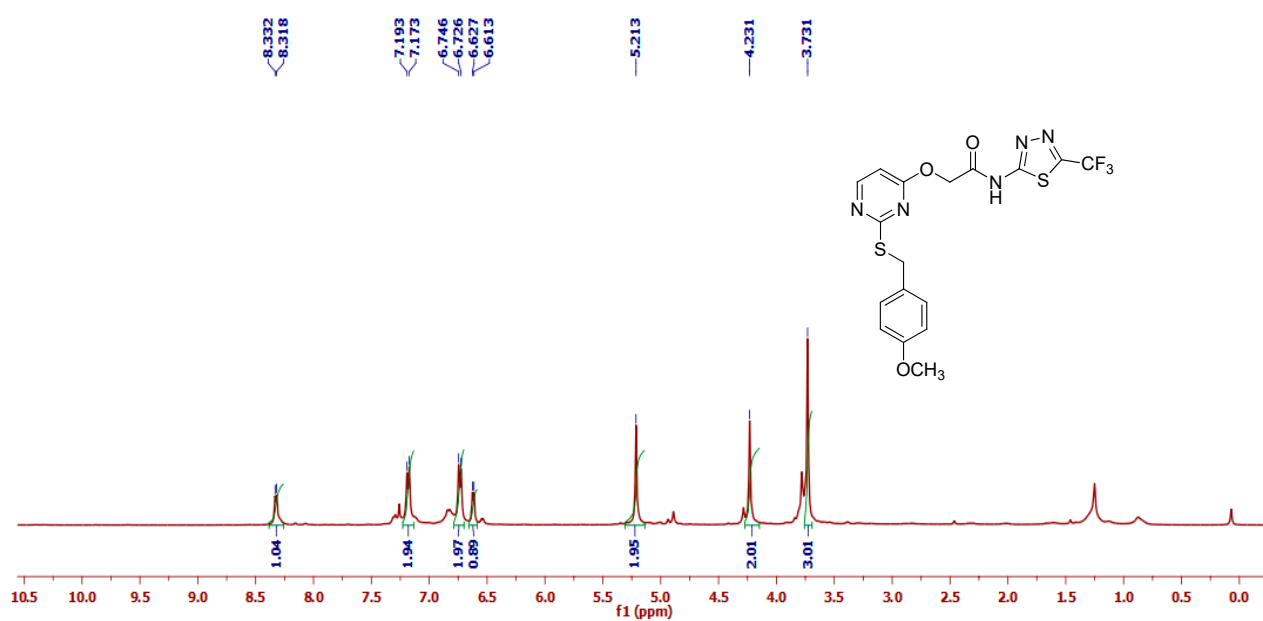
Mass spectra of **5e**



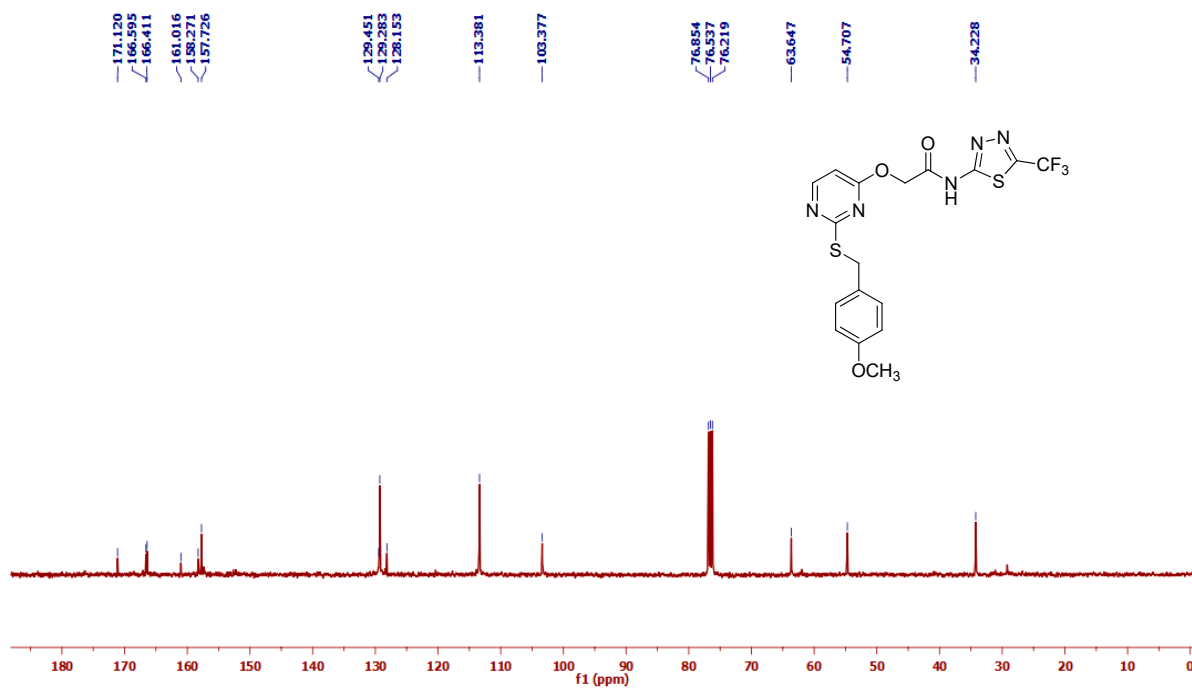
^1H NMR of compound **5f**



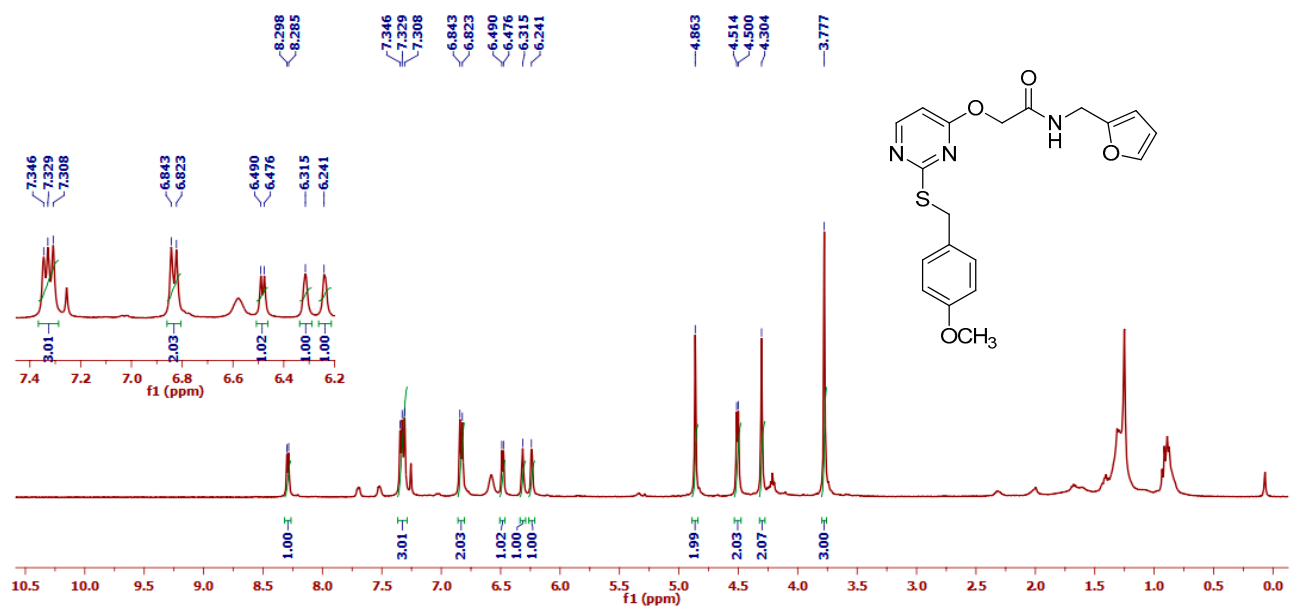
¹³C NMR of compound **5f**



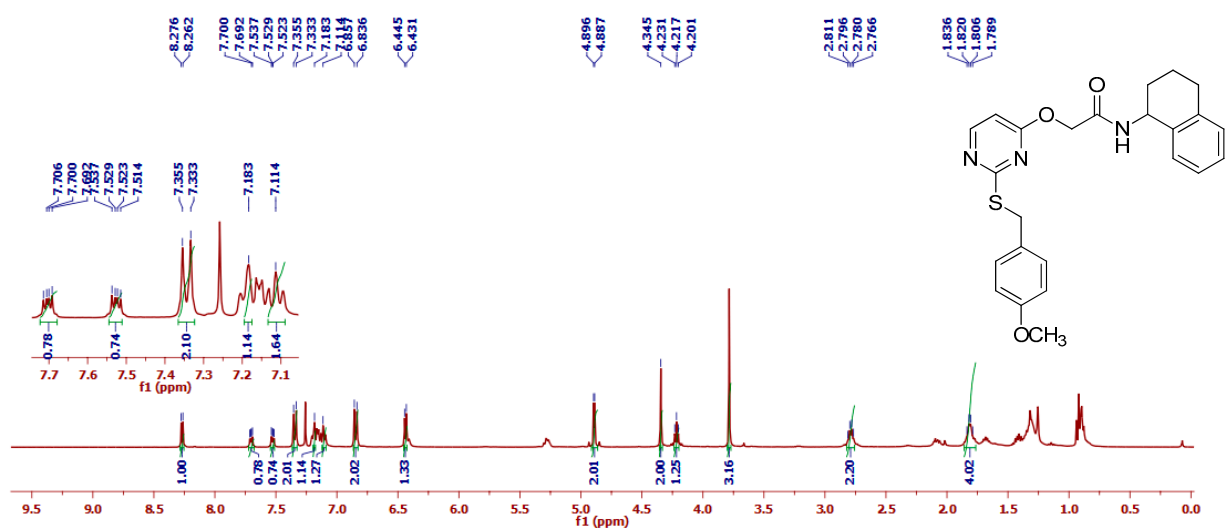
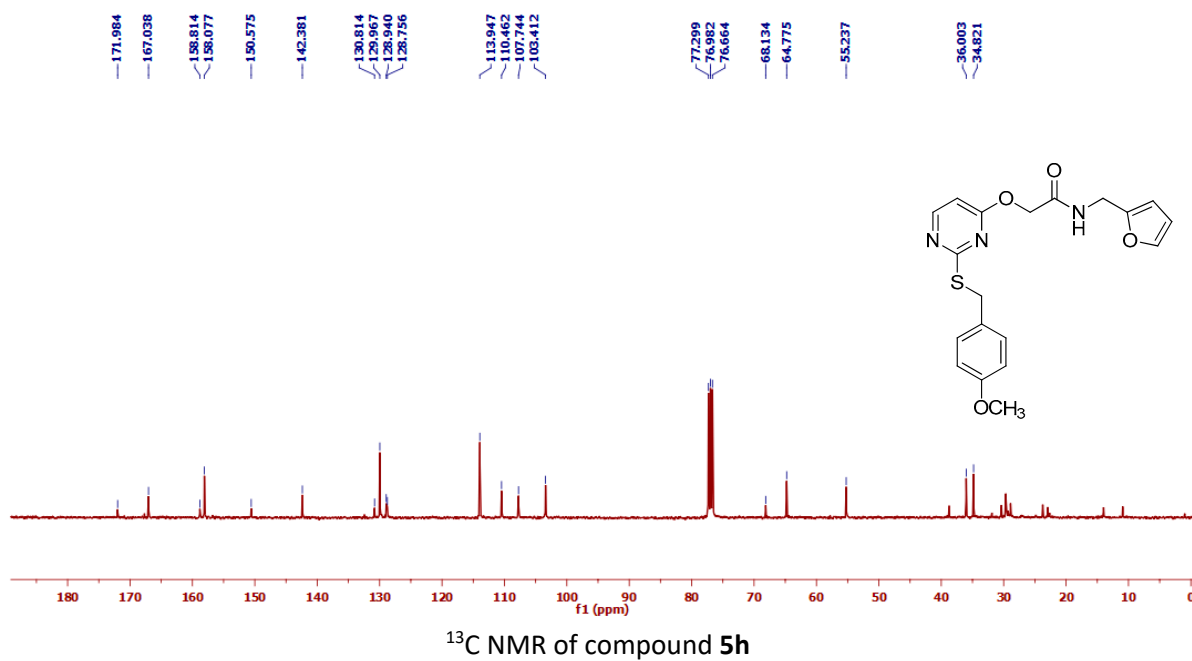
¹H NMR of compound **5g**

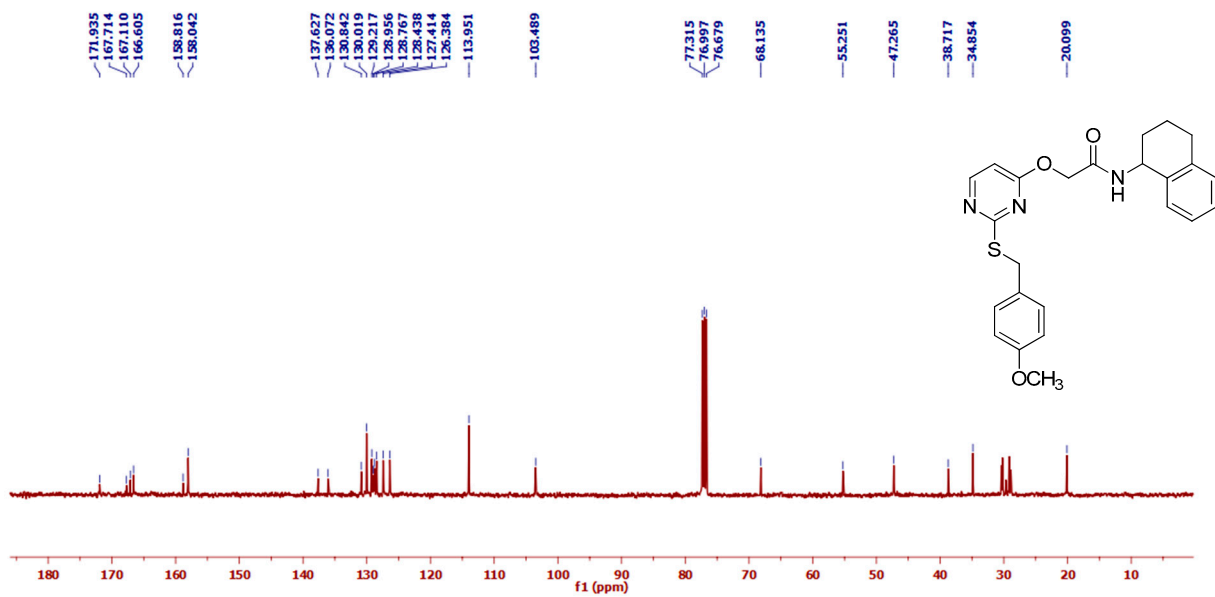


¹³C NMR of compound 5g

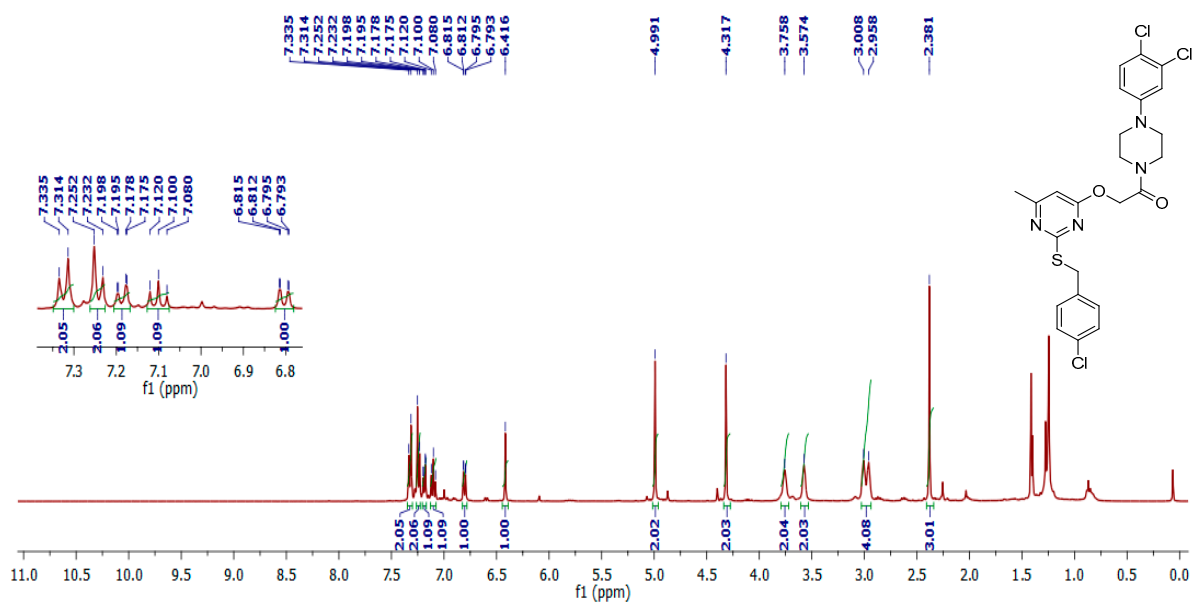


¹H NMR of compound 5h

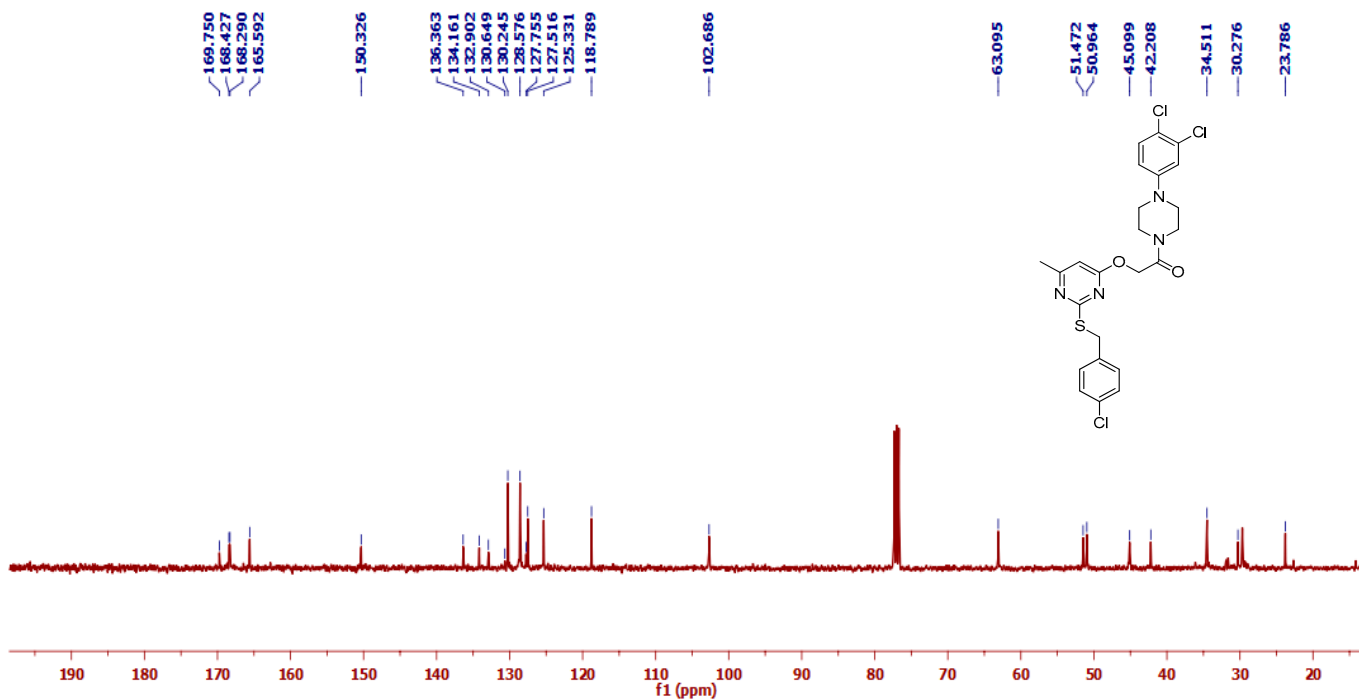




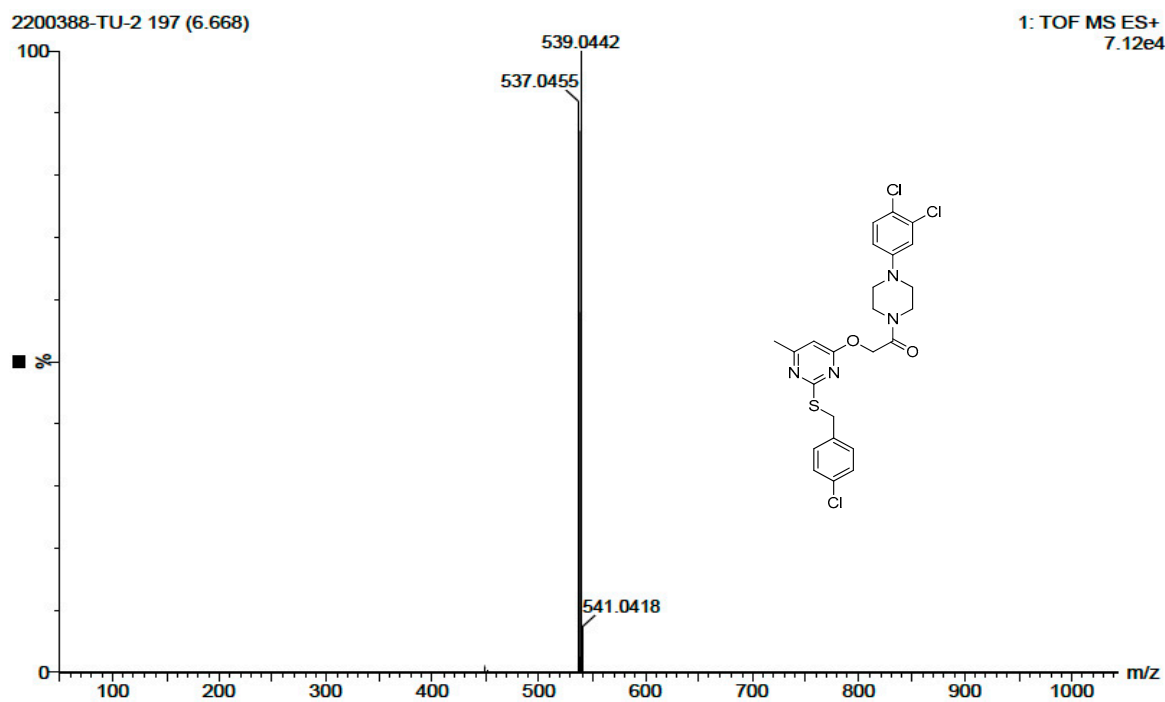
¹³C NMR of compound 5i



¹H NMR of compound 5j

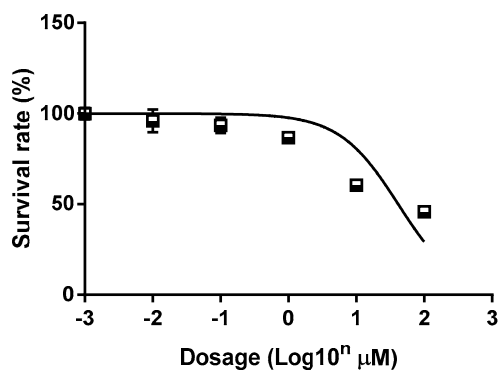


¹³C NMR of compound 5j



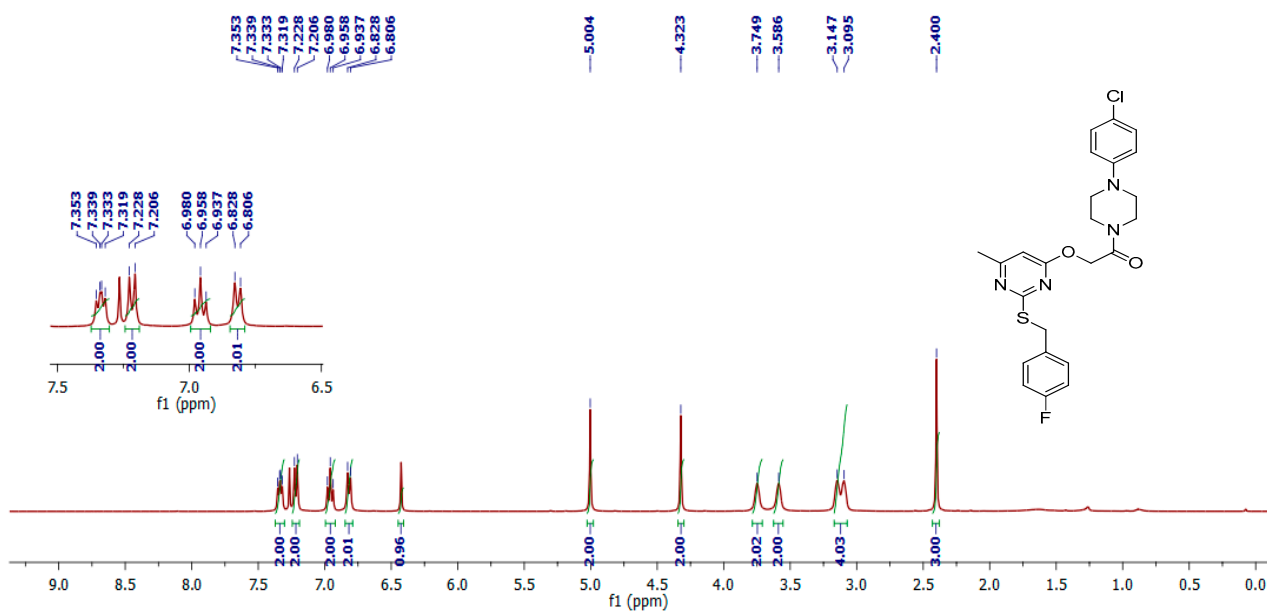
Mass spectra of 5j

Compound: 5j

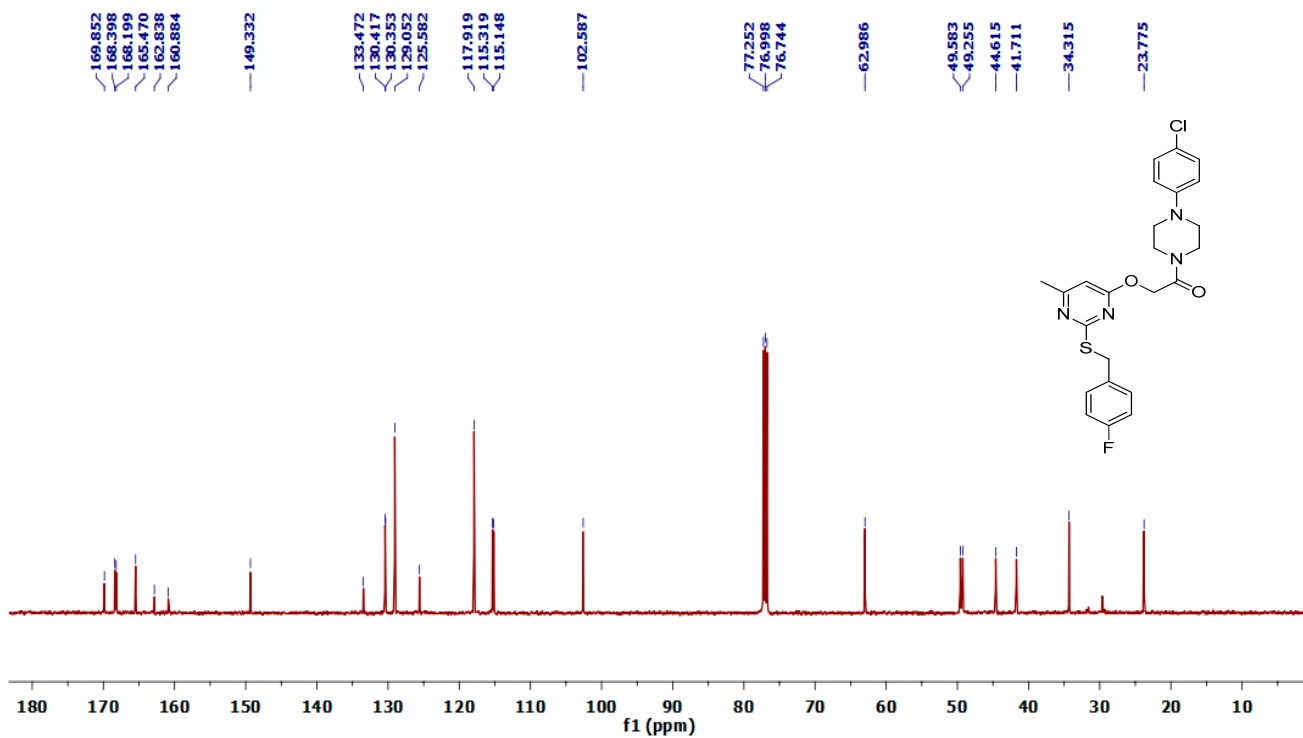


- Cell line: MCF7 (2000 cells/per well⁹⁶)
- Treated time: 72hrs
- Assay: alamarBlue (4hrs incubated)
- Data: 5j

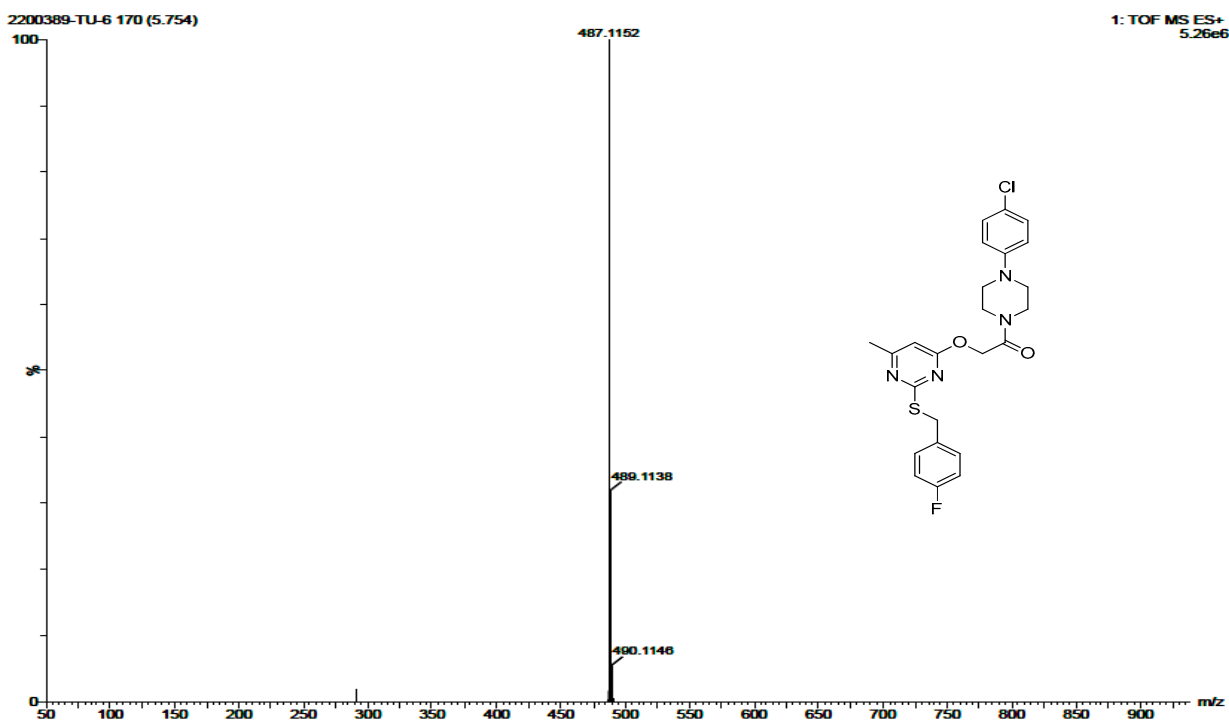
Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	3.13
0.01	95.89	6.24
0.1	93.43	4.27
1	86.66	0.58
10	60.45	2.92
100	45.78	1.83



¹H NMR of compound 5k

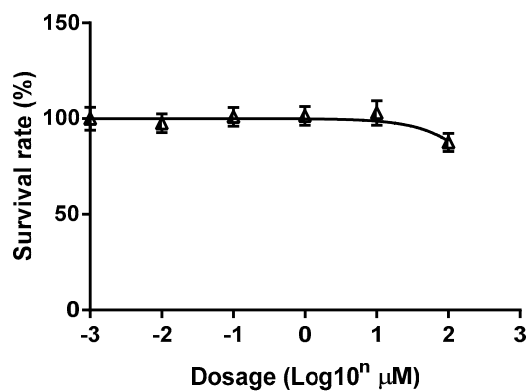


¹³C NMR of compound 5k



Mass spectra of 5k

Compound: 5k

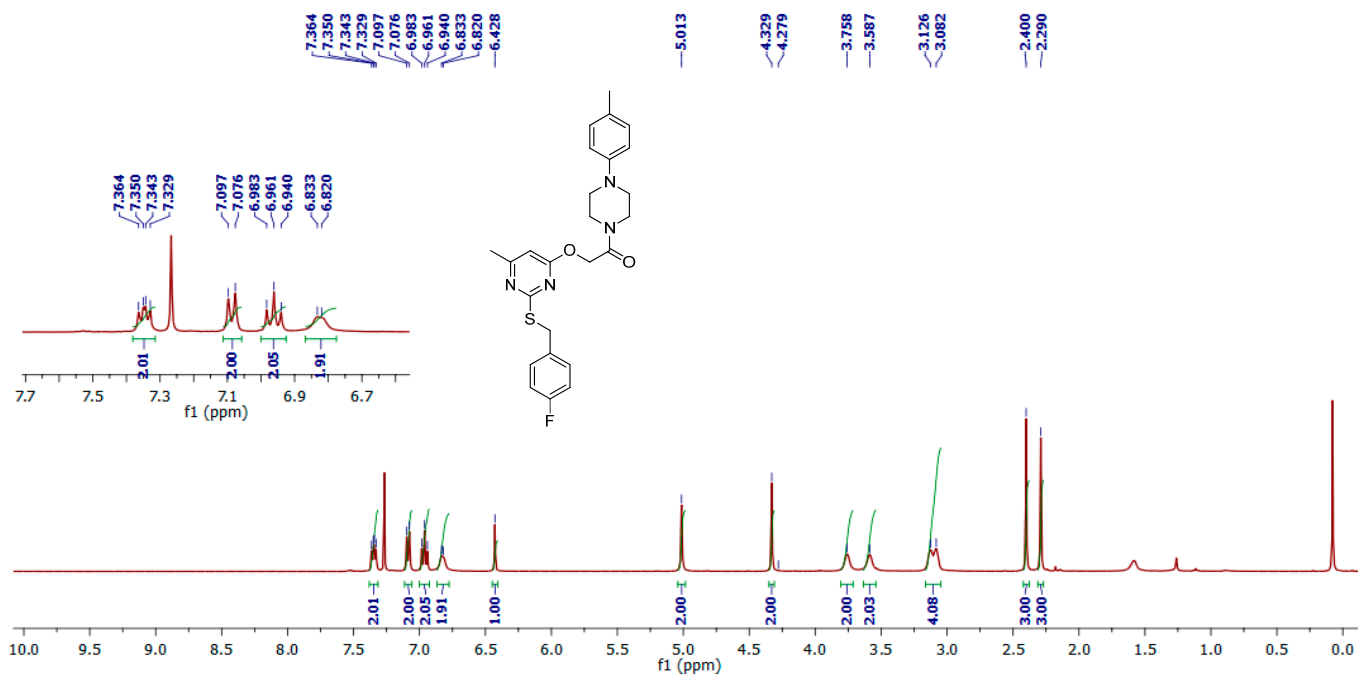


IC₅₀ (μM) = -

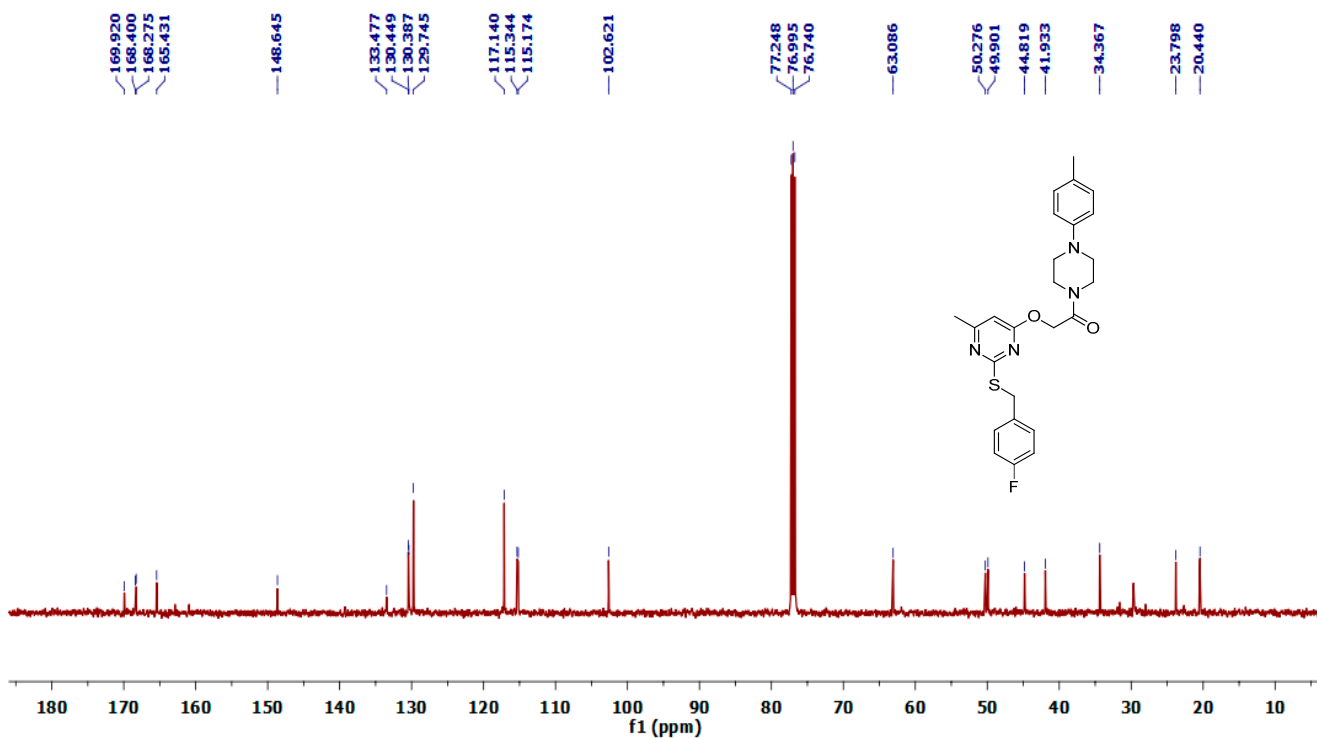
Log IC₅₀ (μM) = -

- Cell line: MCF7 (2000 cells/per well⁹⁶)
- Treated time: 72hrs
- Assay: alamarBlue (4hrs incubated)
- Data: 5k

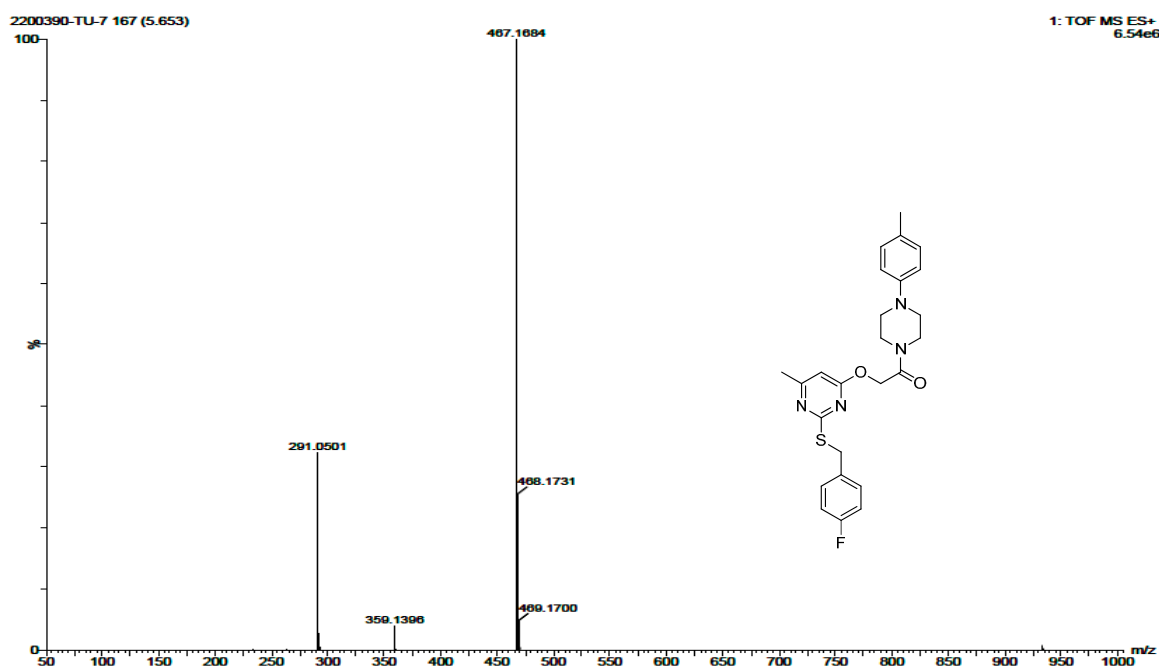
Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	6.07
0.01	97.52	4.94
0.1	100.92	4.88
1	101.38	4.88
10	102.91	6.46
100	87.62	4.75



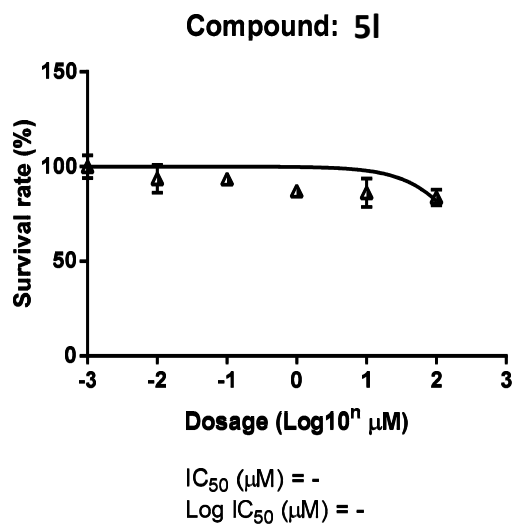
¹H NMR of compound 5I



¹³C NMR of compound 5I

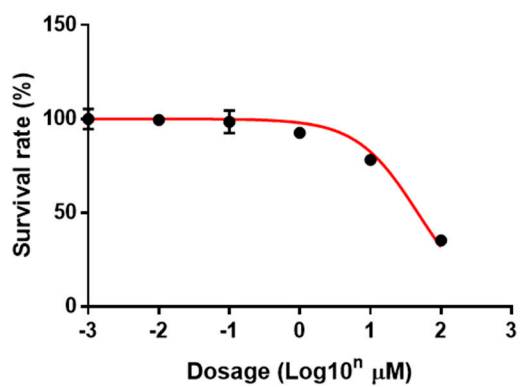


Mass spectra of 5I



- Cell line: MCF7 (2000 cells/per well⁹⁶)
- Treated time: 72hrs
- Assay: alamarBlue (4hrs incubated)
- Data: 5l

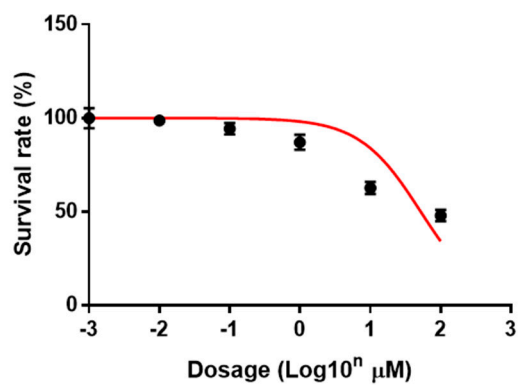
Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	6.07
0.01	93.61	7.43
0.1	93.47	2.24
1	87.02	2.06
10	86.20	7.47
100	83.71	4.17



IC₅₀ (μM) = 46.95
Log IC₅₀ (μM) = 1.67

- Assay: alamarBlue
- Cell line: MCF-10A, 2000 cells/per well⁹⁶
- Compound: 5a
- Treatment: 72hrs, 2% serum

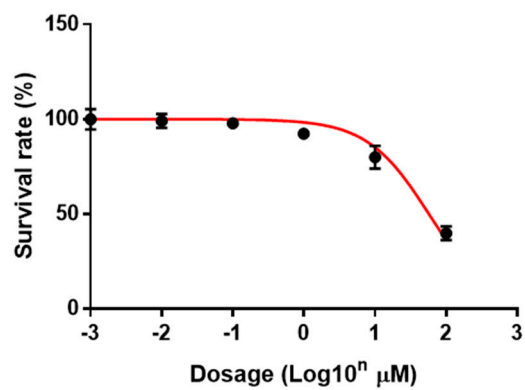
Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	5.42
0.01	99.06	3.68
0.1	97.86	1.61
1	92.36	2.10
10	79.89	6.06
100	39.78	3.66



IC₅₀ (μM) = 52.31
 Log IC₅₀ (μM) = 1.72

- Assay: alamarBlue
- Cell line: MCF-10A, 2000 cells/per well⁹⁶
- Compound: **5e**
- Treatment: 72hrs, 2% serum

Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	5.42
0.01	99.06	3.68
0.1	97.86	1.61
1	92.36	2.10
10	79.89	6.06
100	39.78	3.66



IC₅₀ (μM) = 57.36
 Log IC₅₀ (μM) = 1.76

- **Assay:** alamarBlue
- **Cell line:** MCF-10A, 2000 cells/per well⁹⁶
- **Compound:** Olaparib
- **Treatment:** 72hrs, 2% serum

Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	5.42
0.01	99.06	3.68
0.1	97.86	1.61
1	92.36	2.10
10	79.89	6.06
100	39.78	3.66