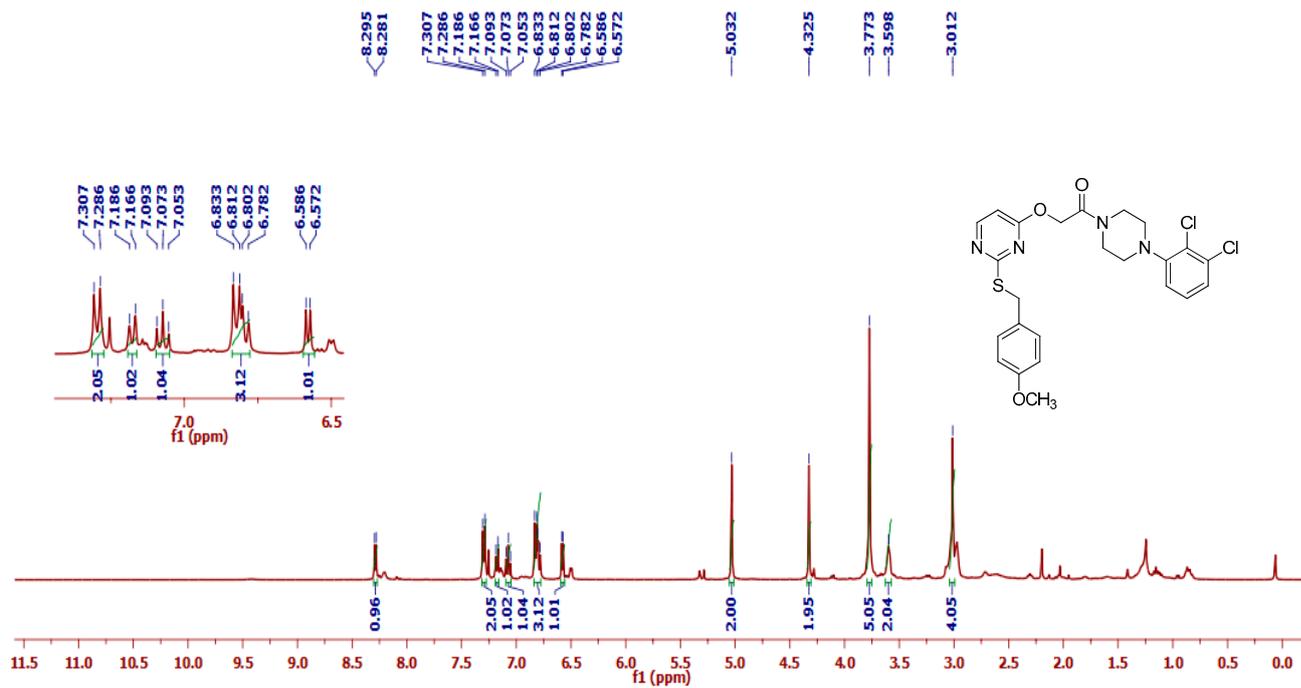


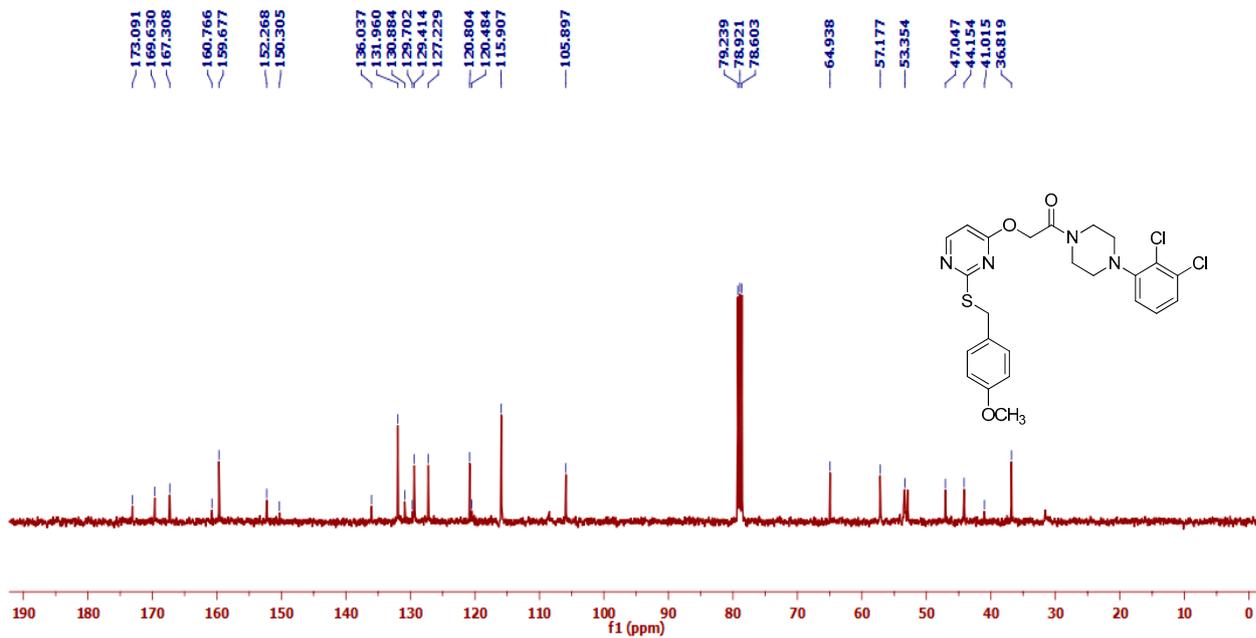
# **Development of 1-(4-(substituted)piperazin-1-yl)-2-((2-((4-methoxybenzyl)thio)pyrimidin-4-yl)oxy)ethanones that target Poly(ADP -Ribose)Polymerase in human breast cancer cells**

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

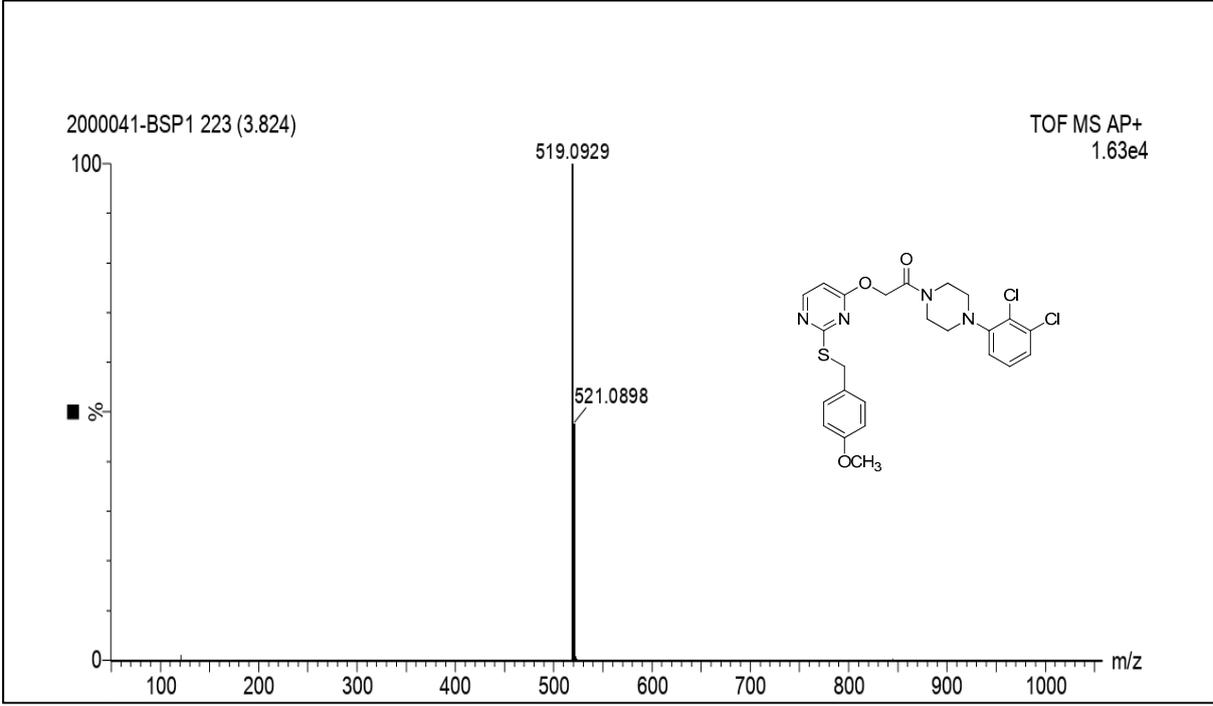
**Supplementary data for newly synthesized molecules and their IC50 values determined against human breast cancer cells**



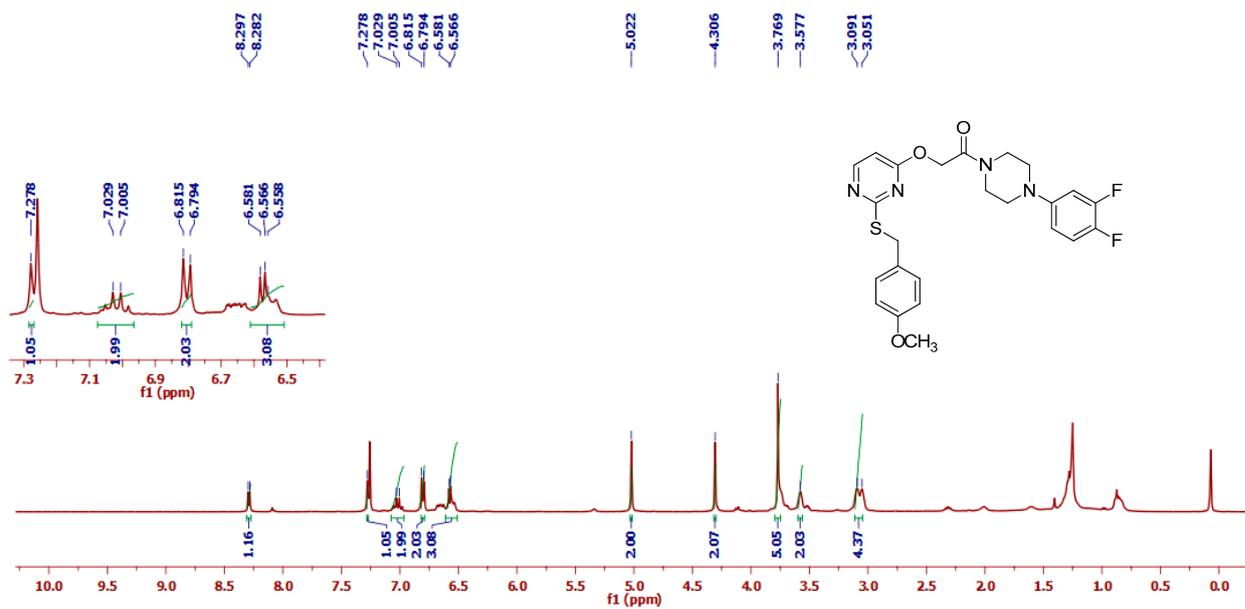
<sup>1</sup>H NMR of compound 5a



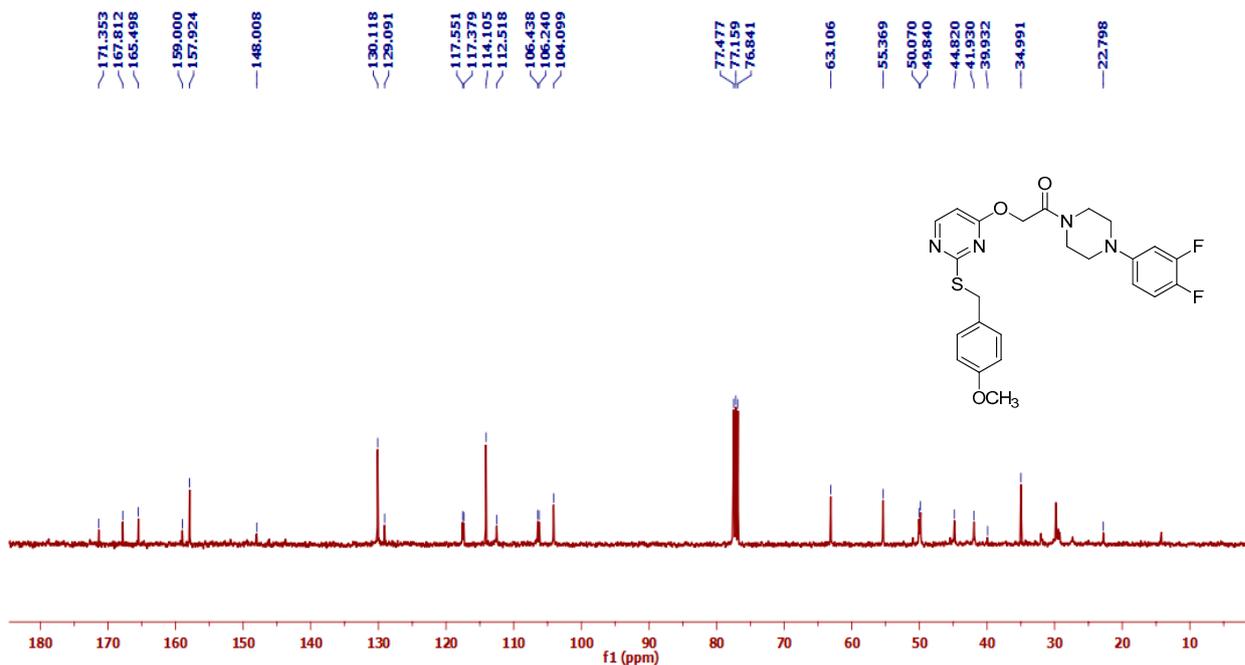
<sup>13</sup>C NMR of compound 5a



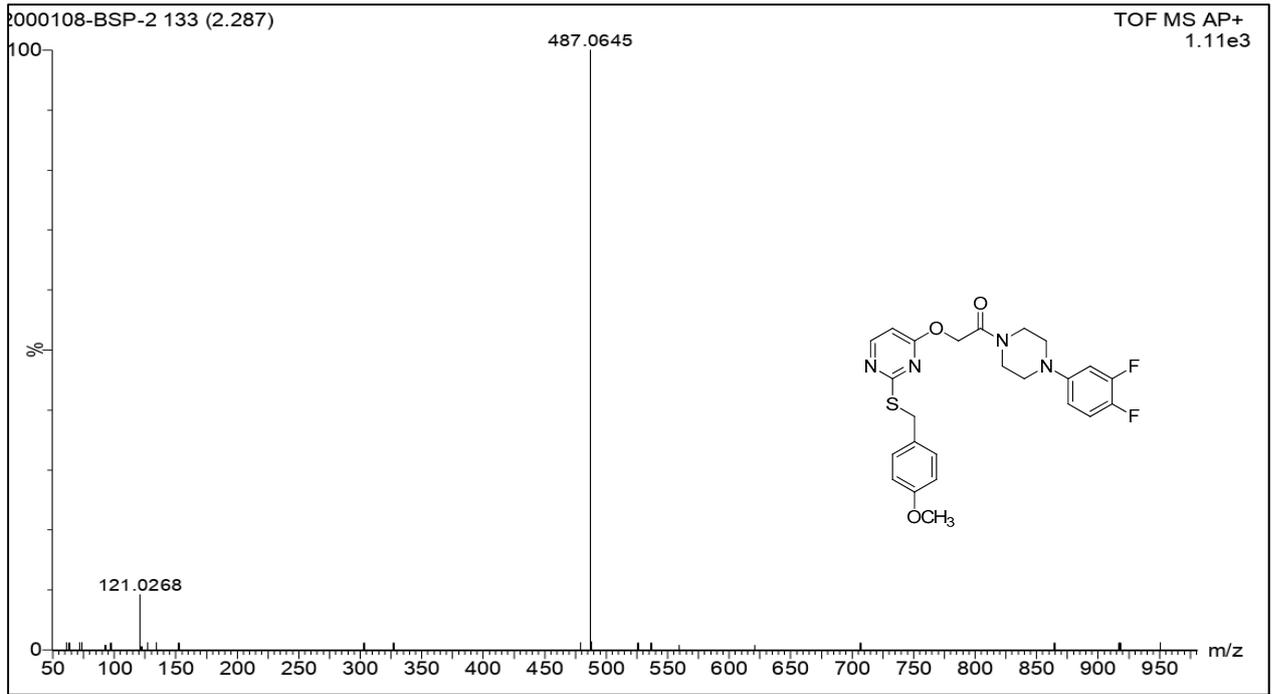
Mass spectra of **5a**



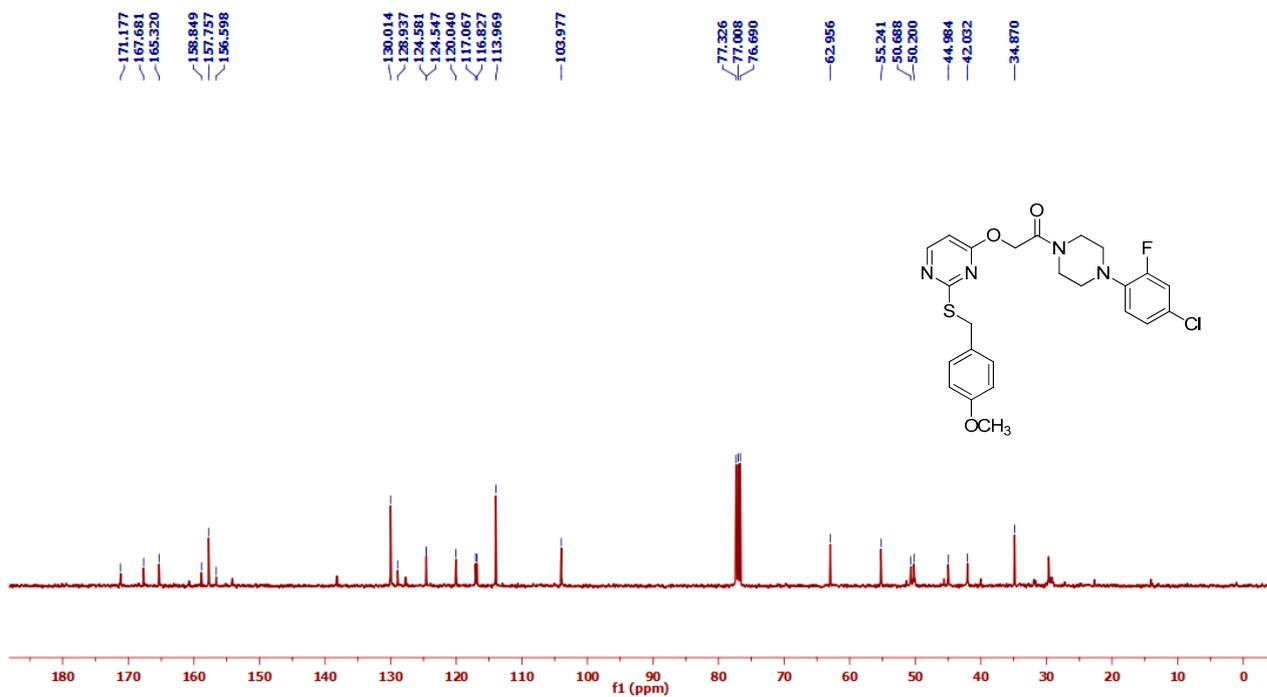
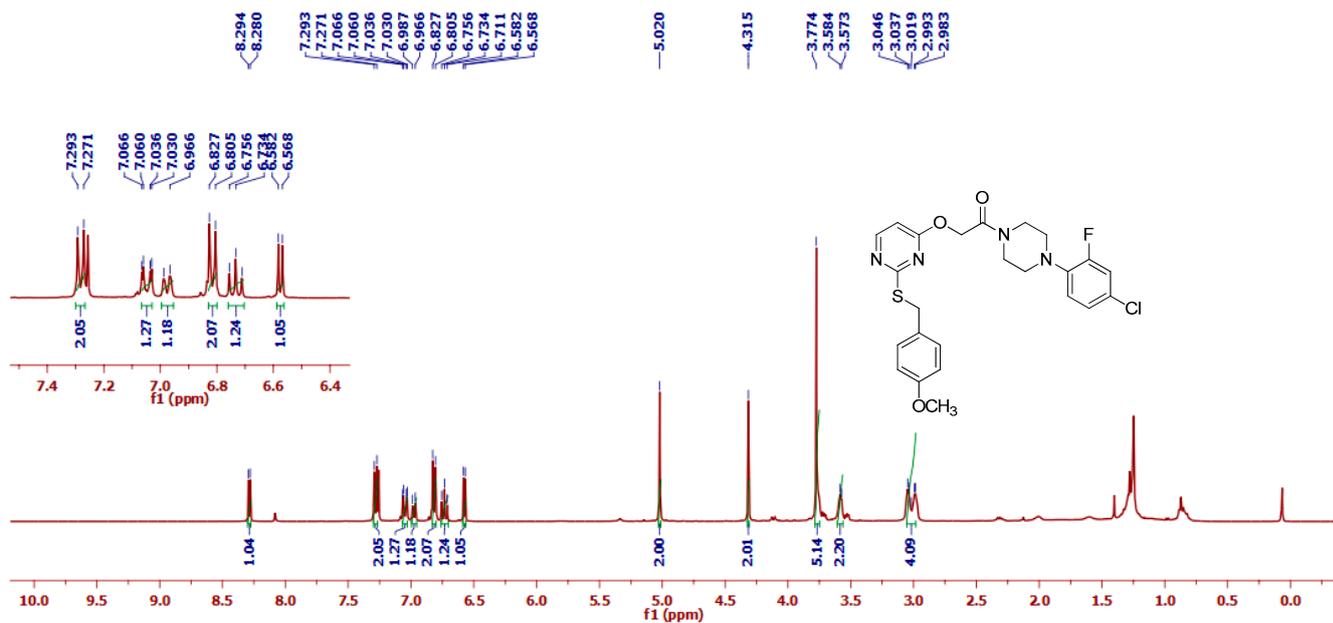
<sup>1</sup>H NMR of compound 5b

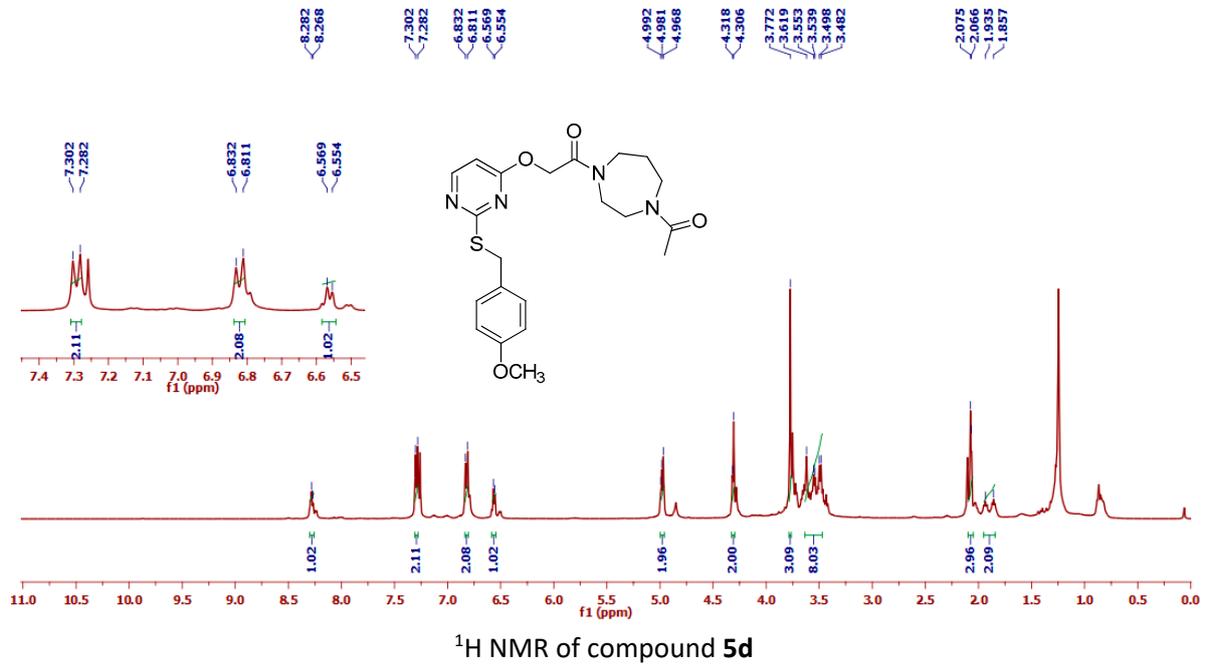
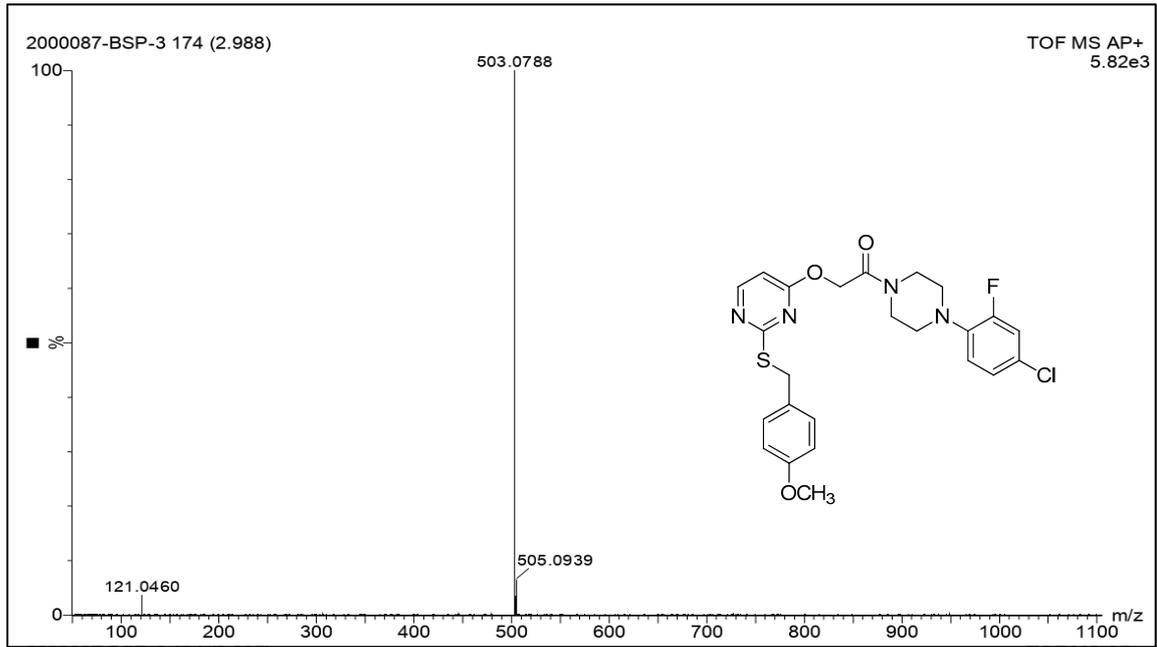


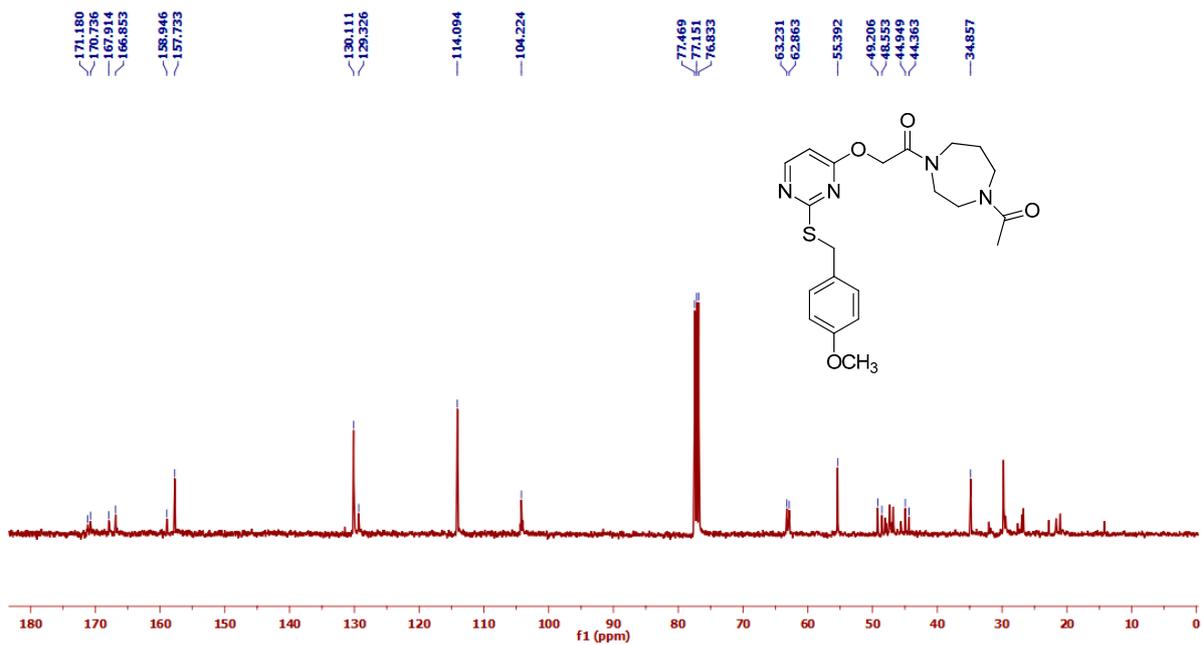
<sup>13</sup>C NMR of compound 5b



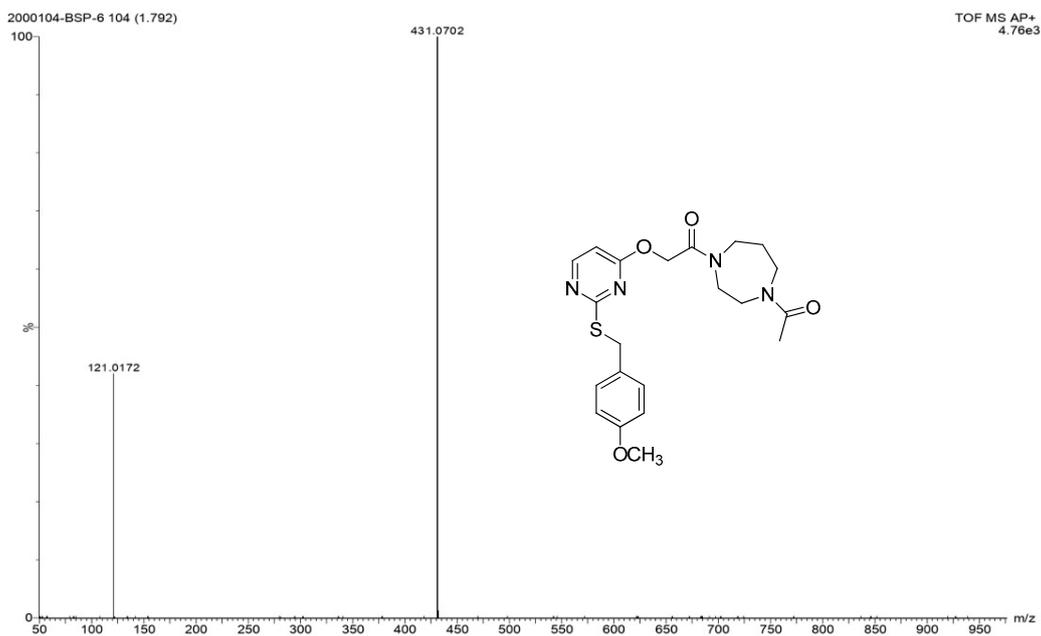
Mass spectra of **5b**



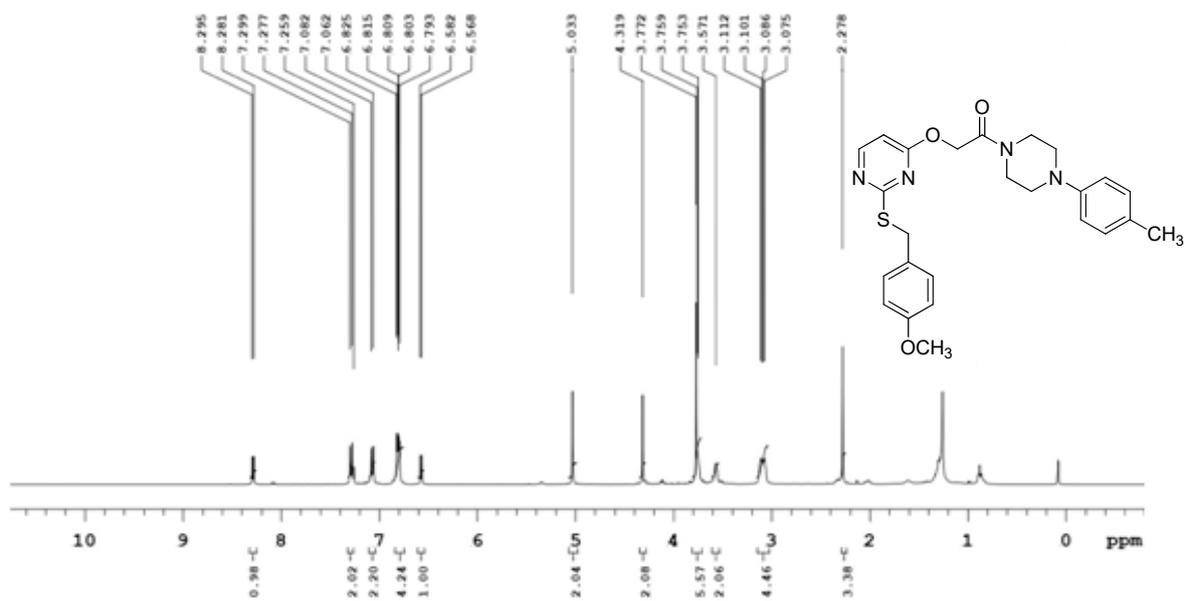




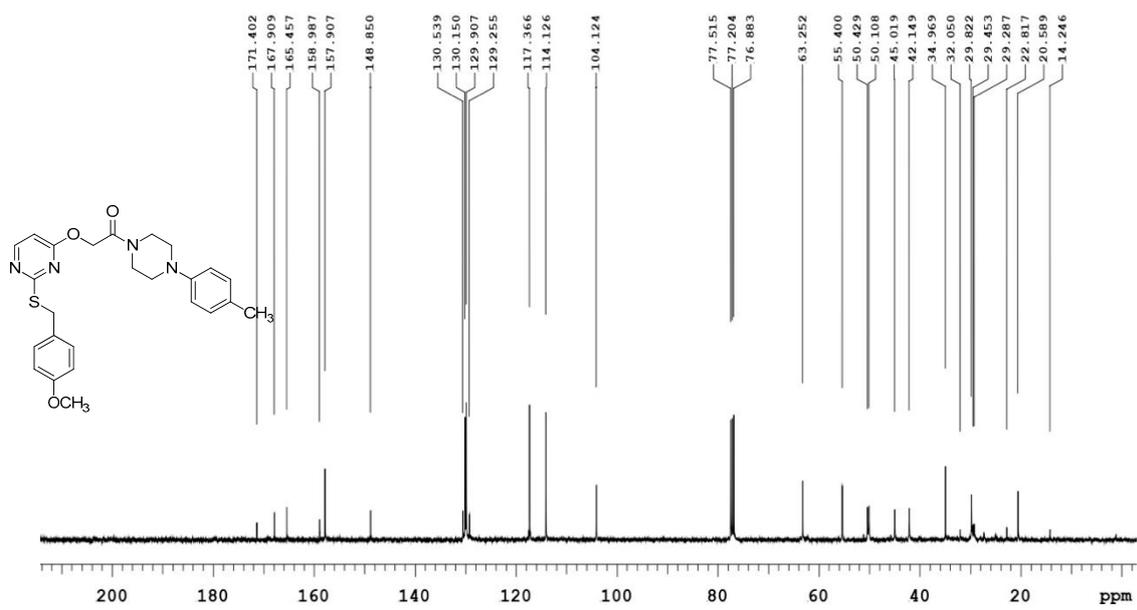
$^{13}\text{C}$  NMR of compound 5d



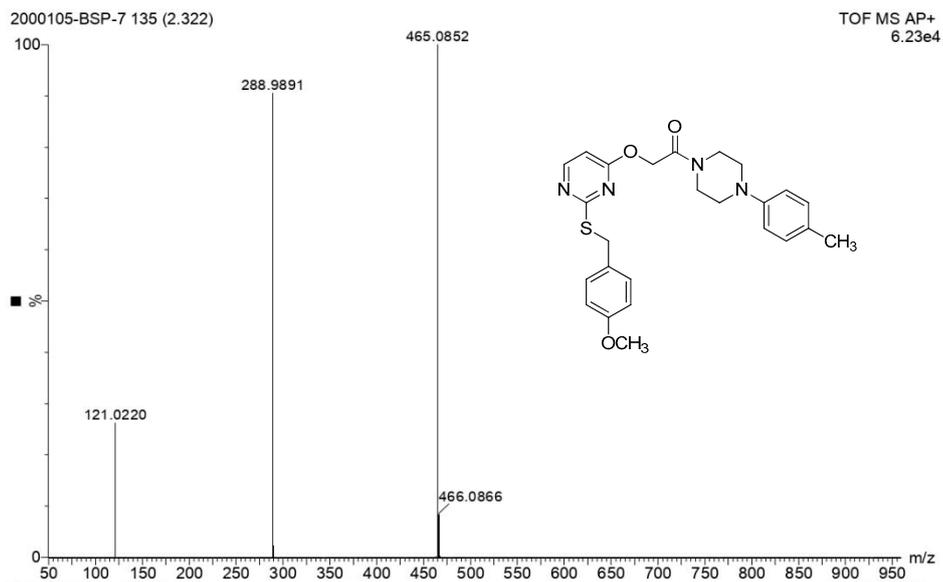
Mass spectra of 5d



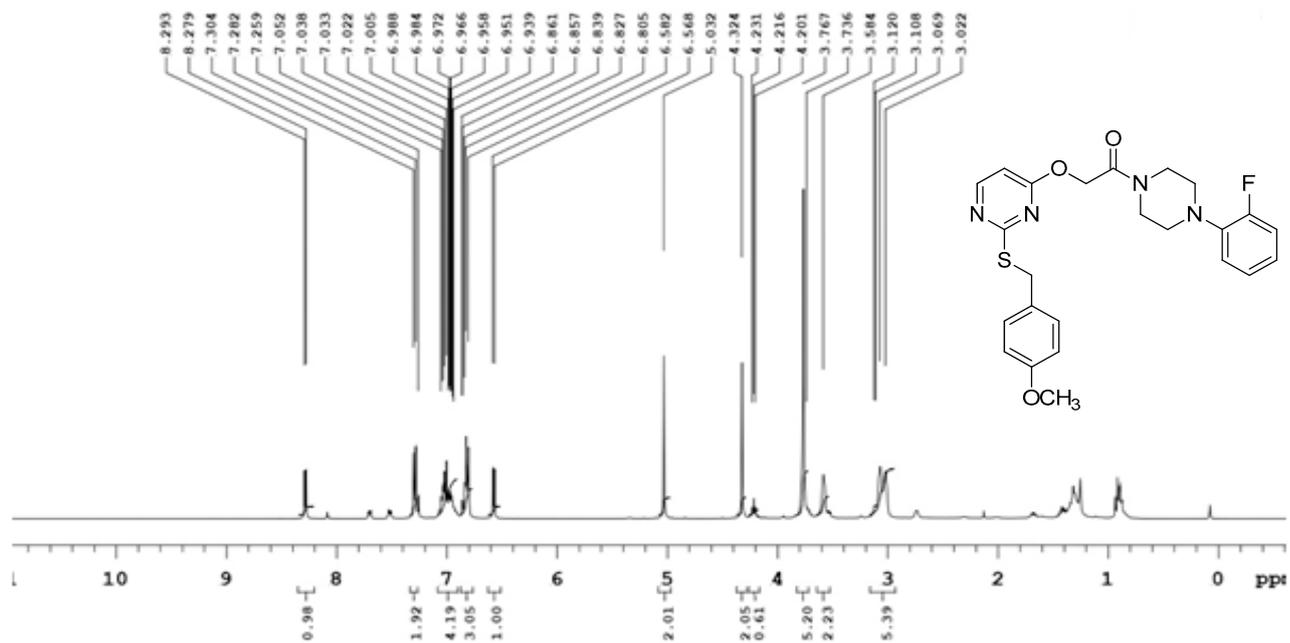
<sup>1</sup>H NMR of compound 5e



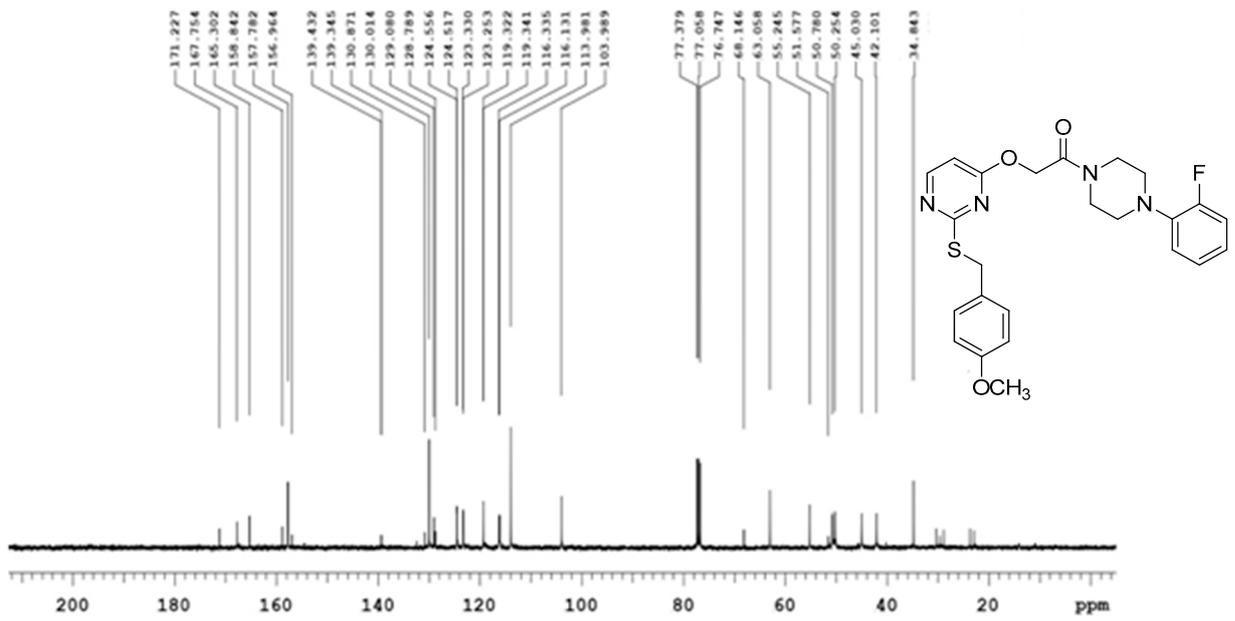
<sup>13</sup>C NMR of compound 5e



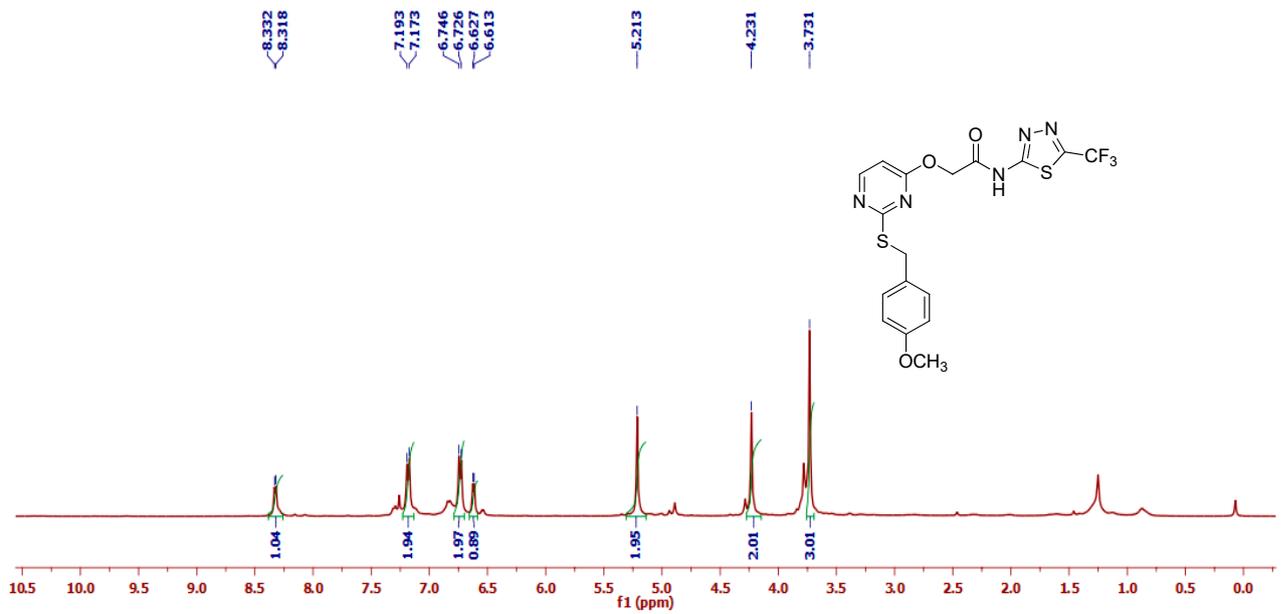
Mass spectra of 5e



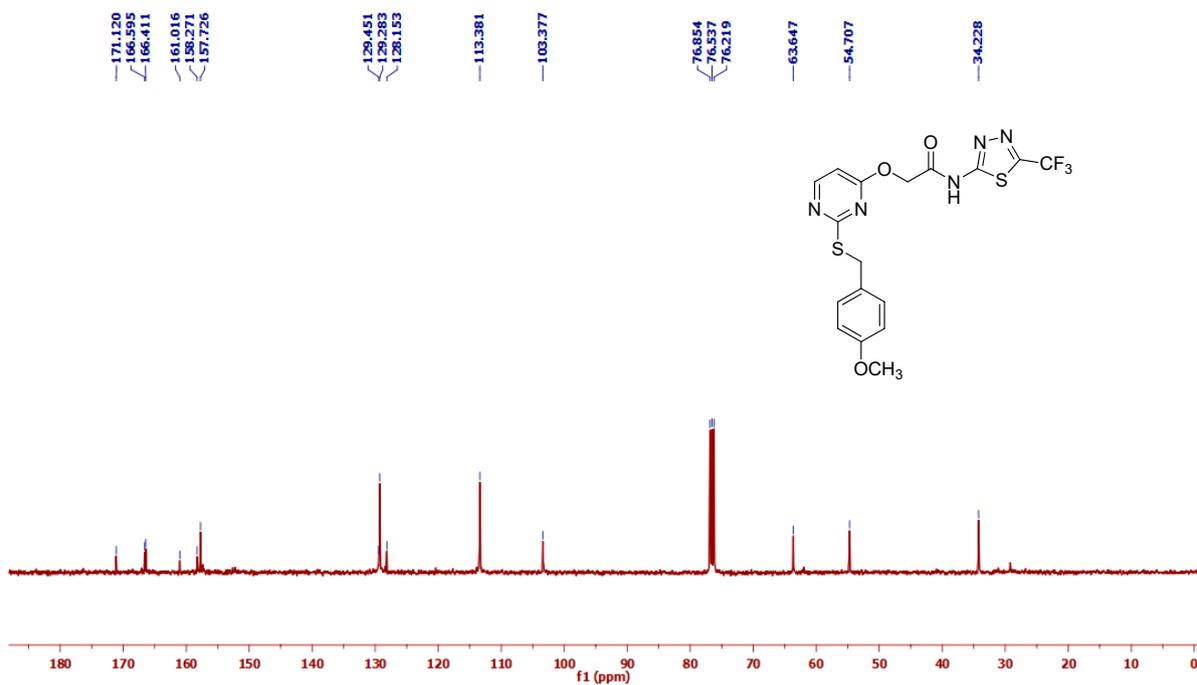
<sup>1</sup>H NMR of compound 5f



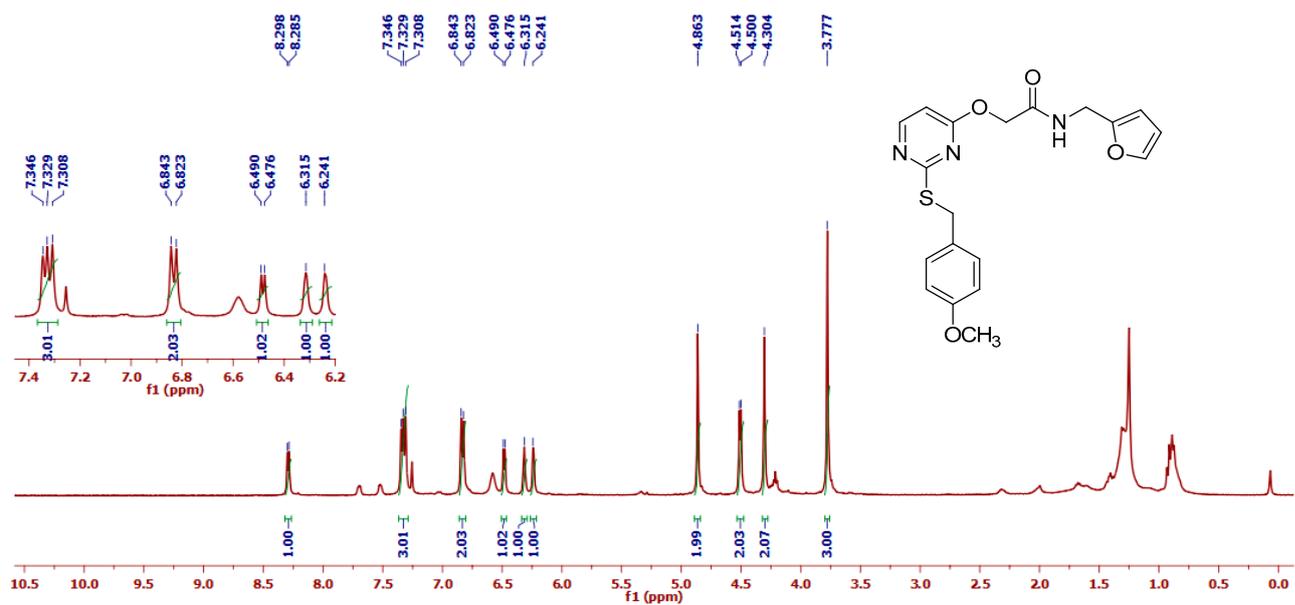
<sup>13</sup>C NMR of compound 5f



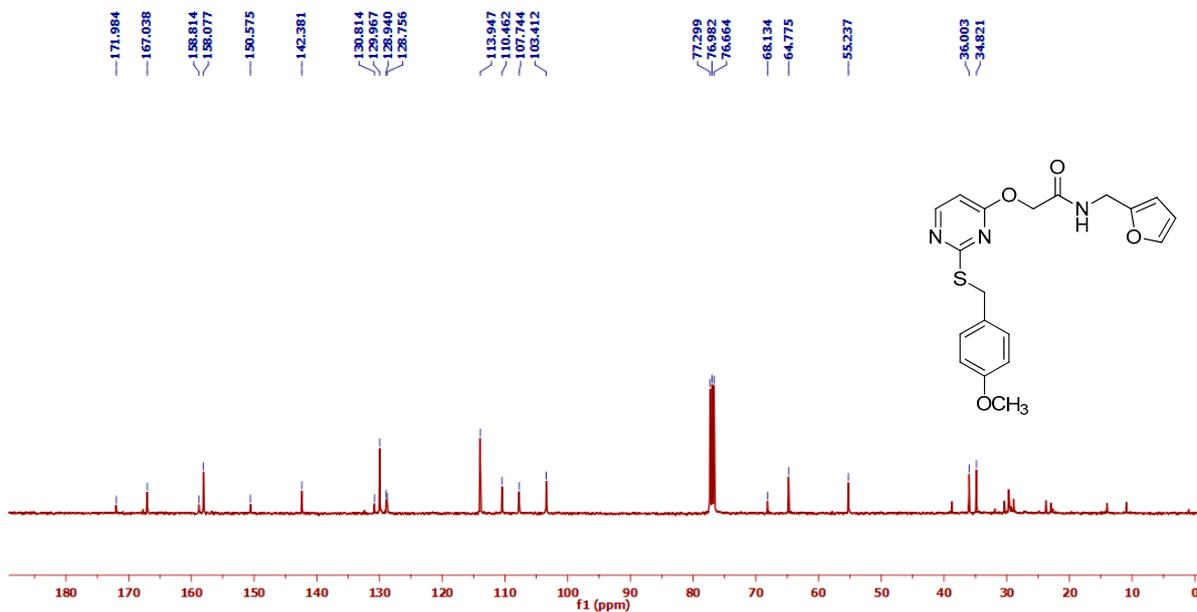
<sup>1</sup>H NMR of compound 5g



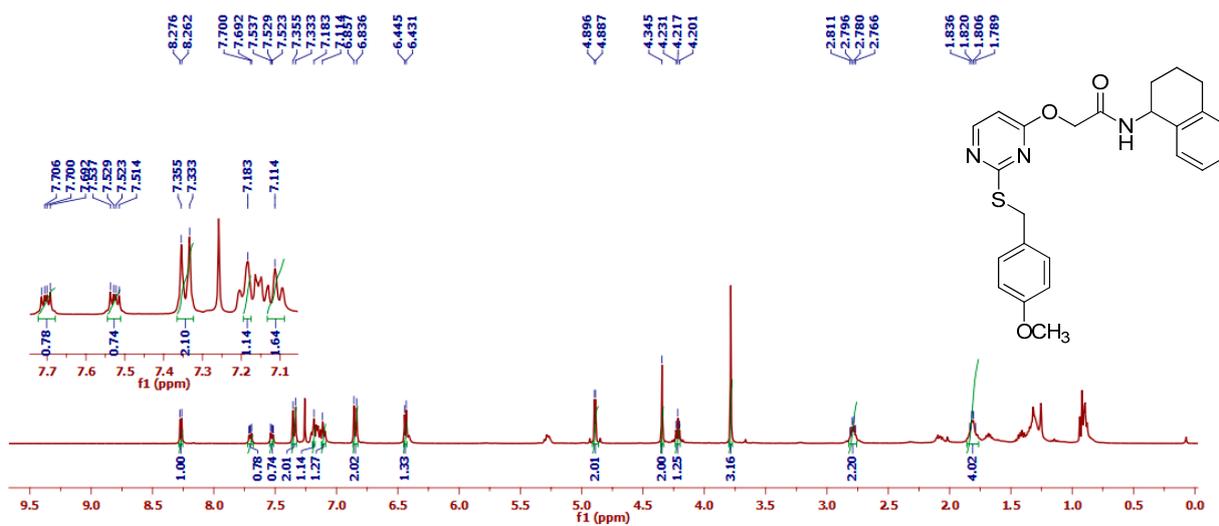
<sup>13</sup>C NMR of compound 5g



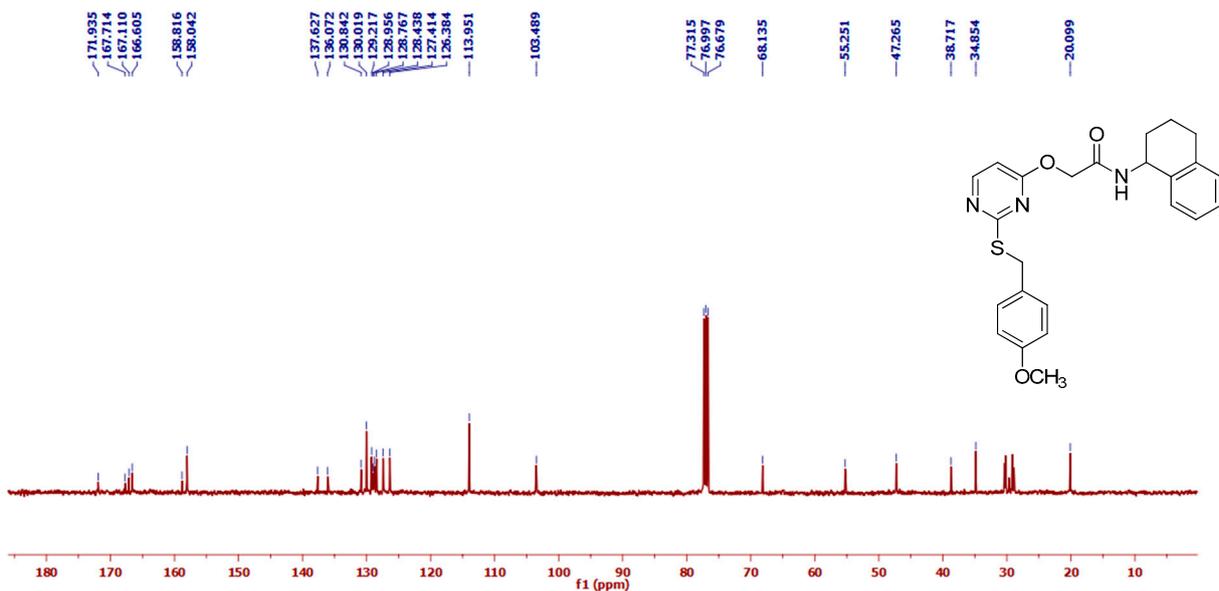
<sup>1</sup>H NMR of compound 5h



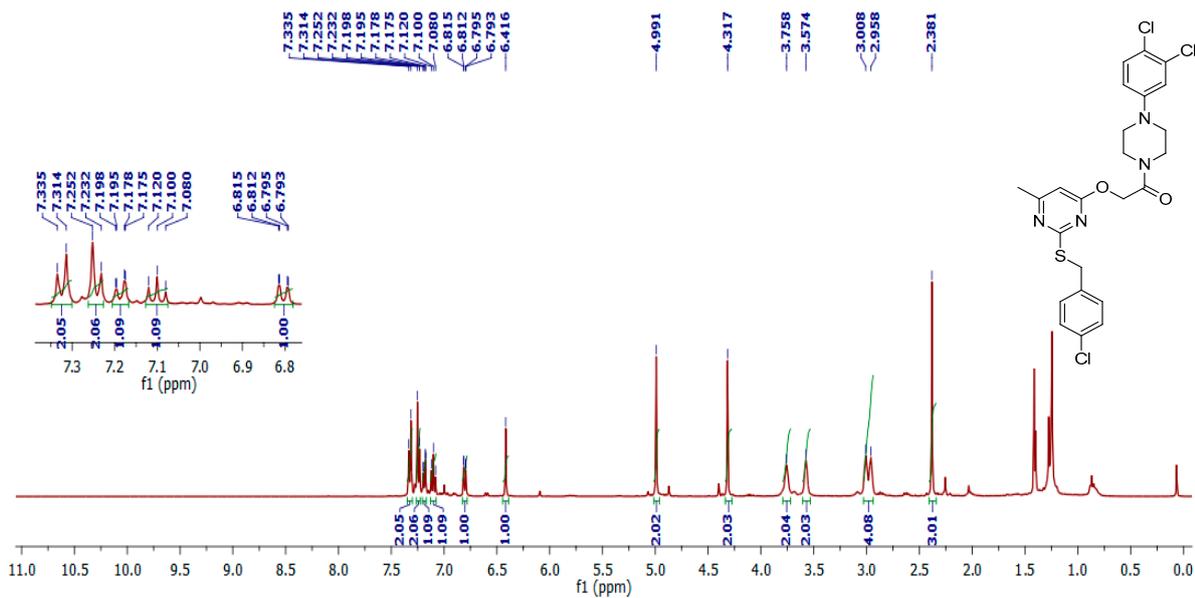
<sup>13</sup>C NMR of compound 5h



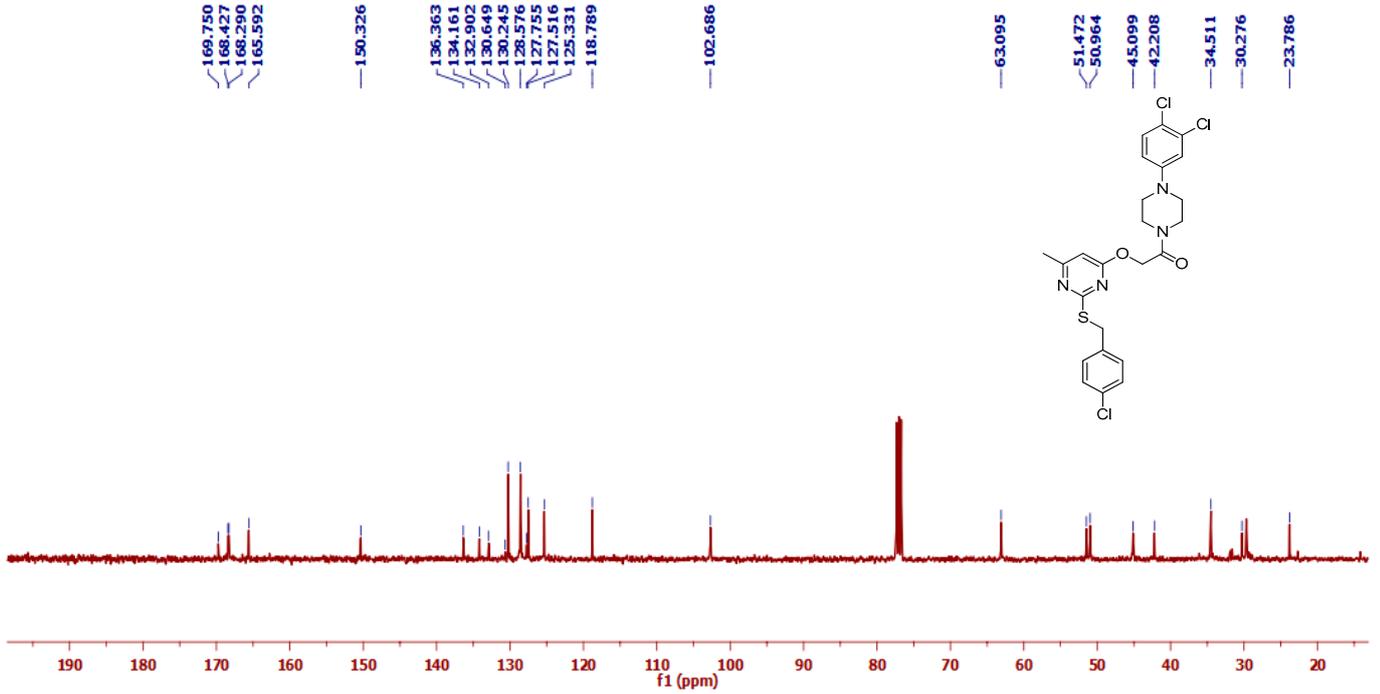
<sup>1</sup>H NMR of compound 5i



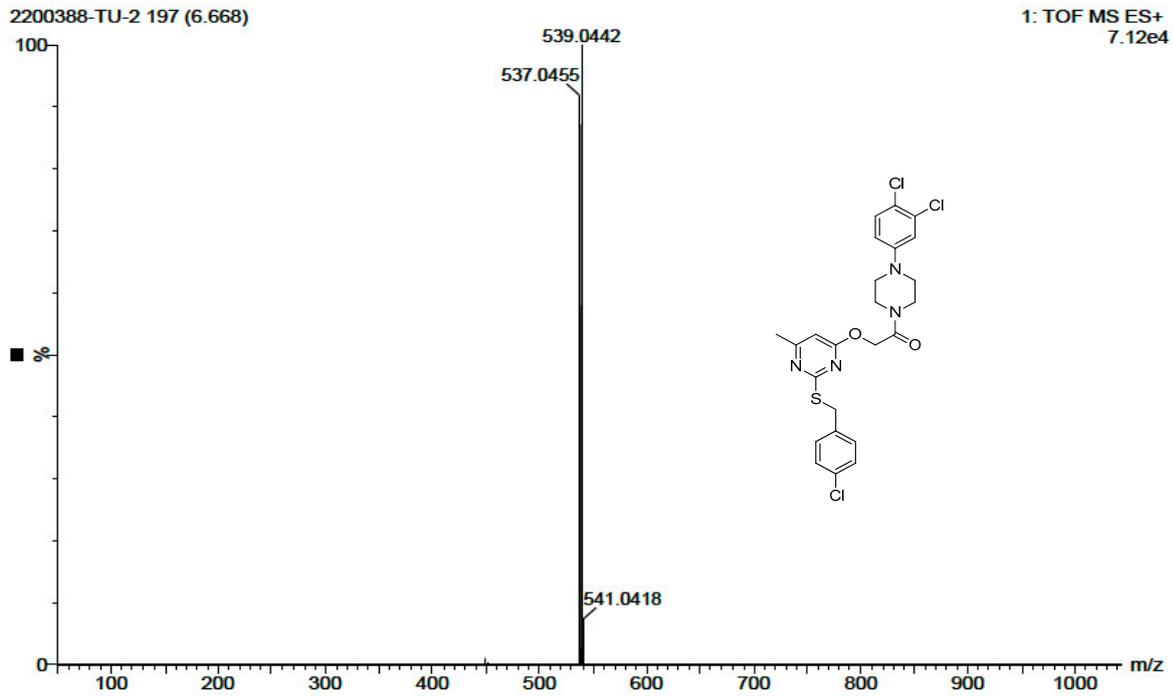
<sup>13</sup>C NMR of compound 5i



<sup>1</sup>H NMR of compound 5j

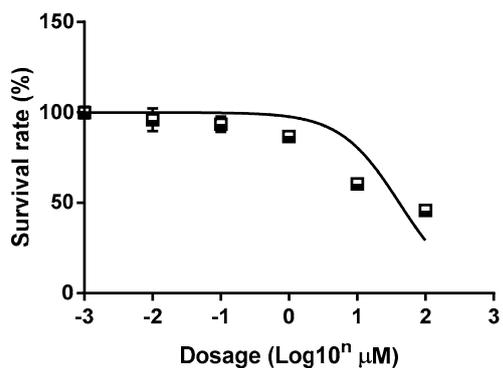


$^{13}\text{C}$  NMR of compound 5j



Mass spectra of 5j

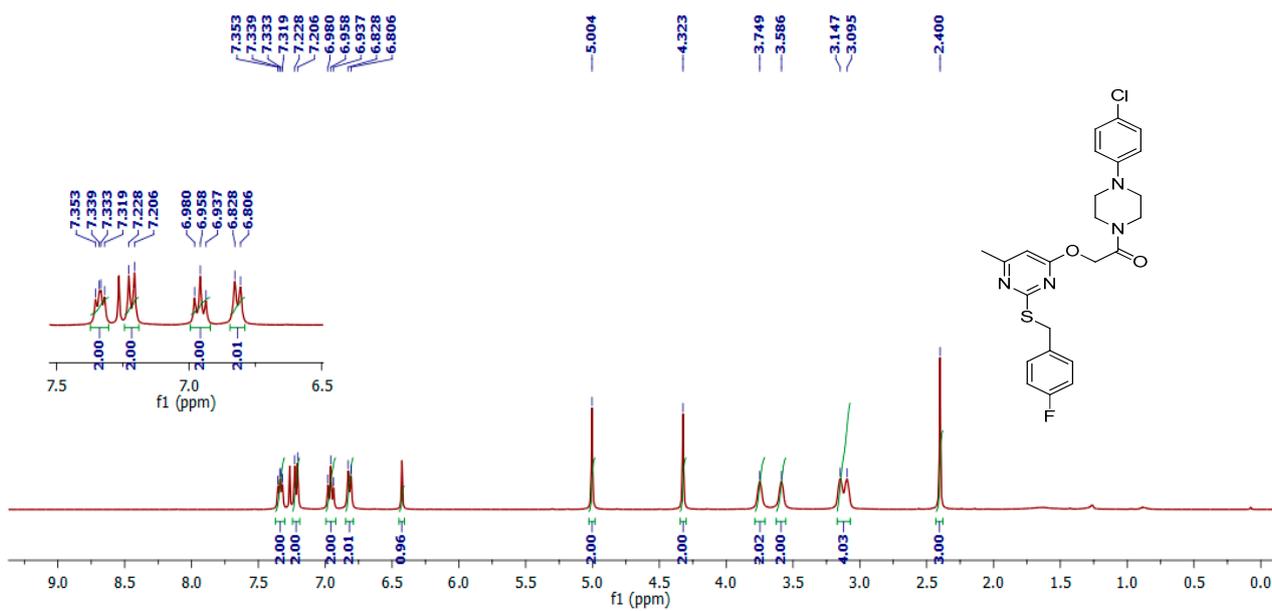
### Compound: 5j

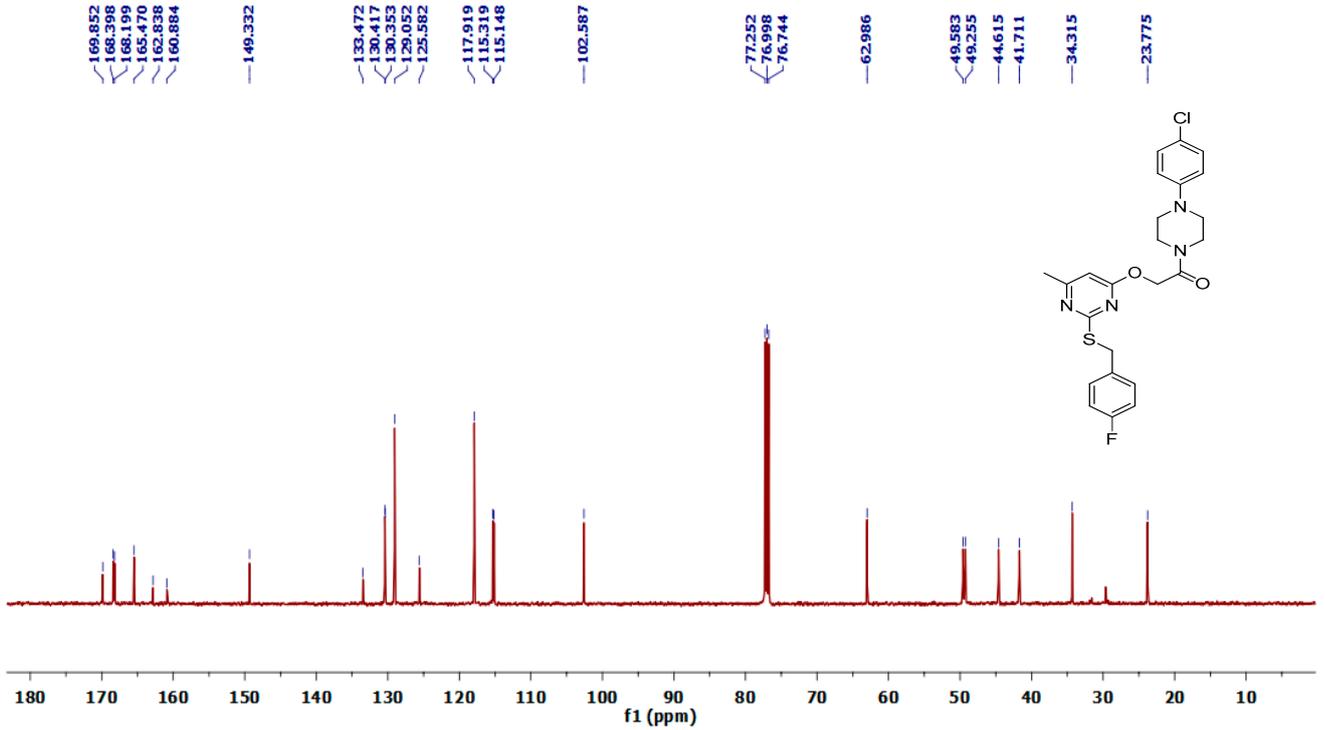


$\text{IC}_{50} (\mu\text{M}) = 41.38$   
 $\text{Log IC}_{50} (\mu\text{M}) = 1.62$

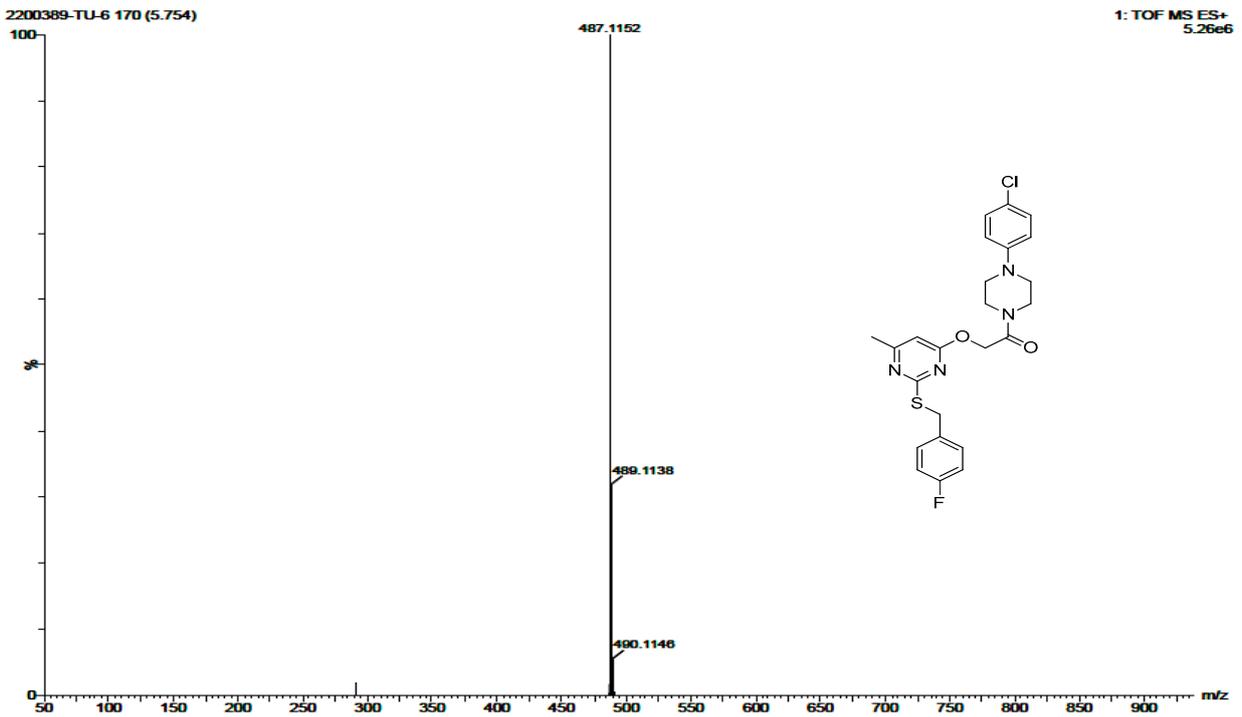
- Cell line: MCF7 (2000 cells/per well<sup>96</sup>)
- Treated time: 72hrs
- Assay: alamarBlue (4hrs incubated)
- Data: 5j

Conc. ( $\mu\text{M}$ )	Viability	
	AVE.	$\pm$ 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



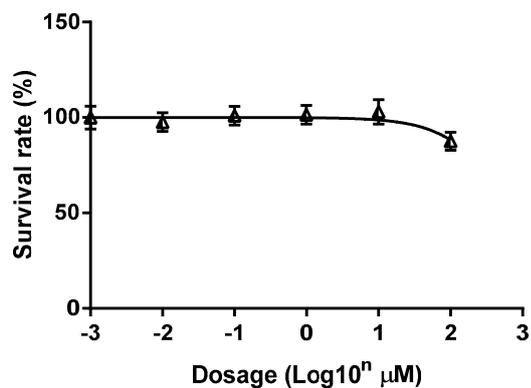


<sup>13</sup>C NMR of compound 5k



Mass spectra of 5k

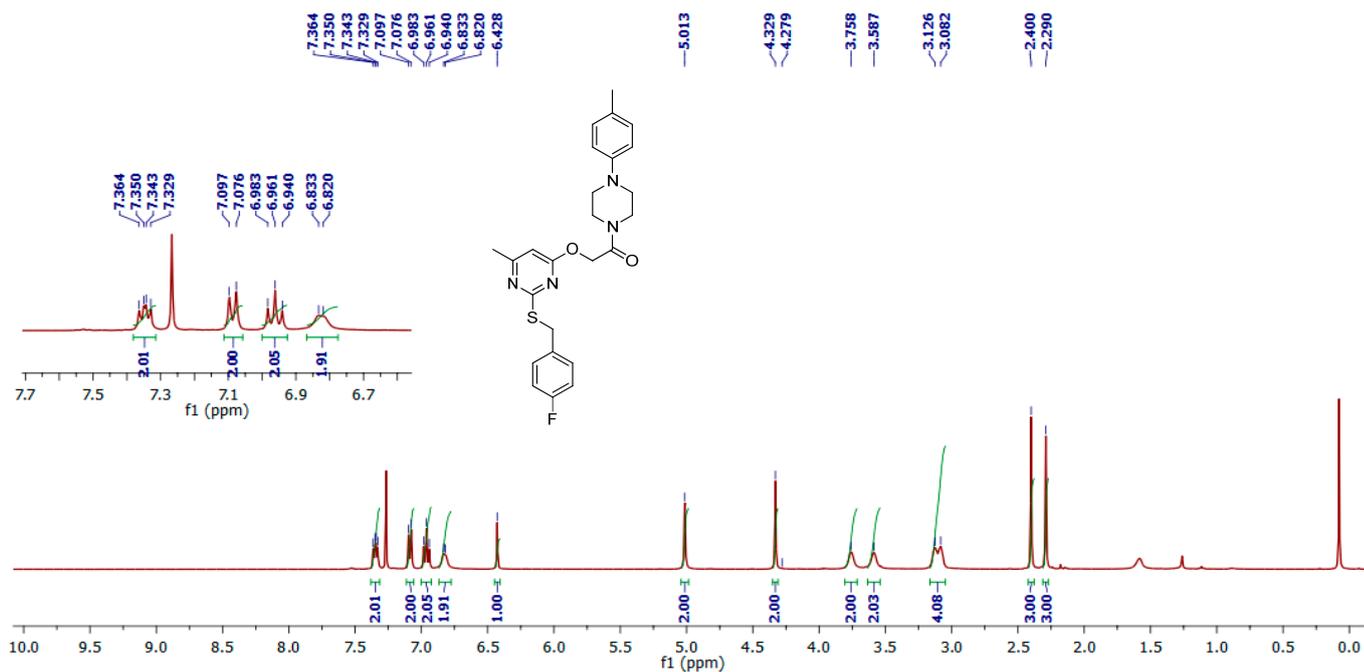
### Compound: 5k



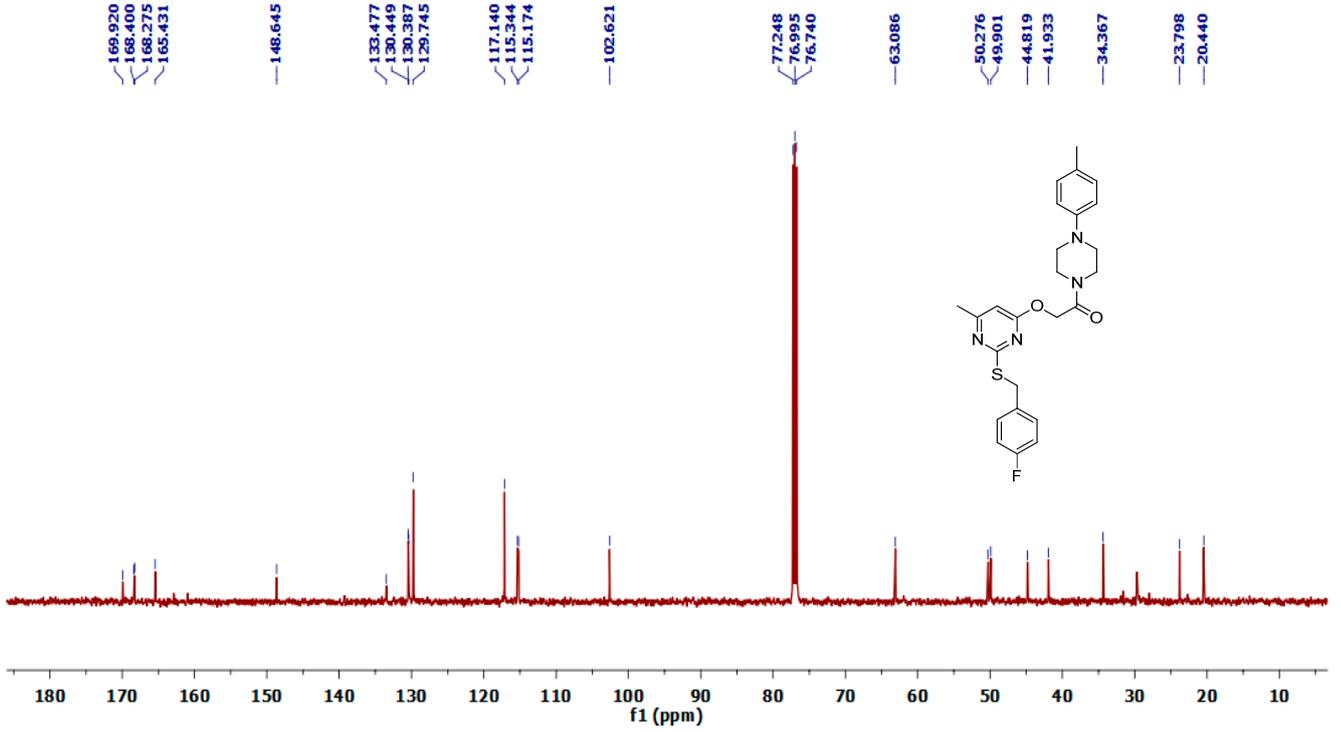
IC<sub>50</sub> (μM) = -  
Log IC<sub>50</sub> (μM) = -

- Cell line: MCF7 (2000 cells/per well<sup>96</sup>)
- Treated time: 72hrs
- Assay: alamarBlue (4hrs incubated)
- Data: 5k

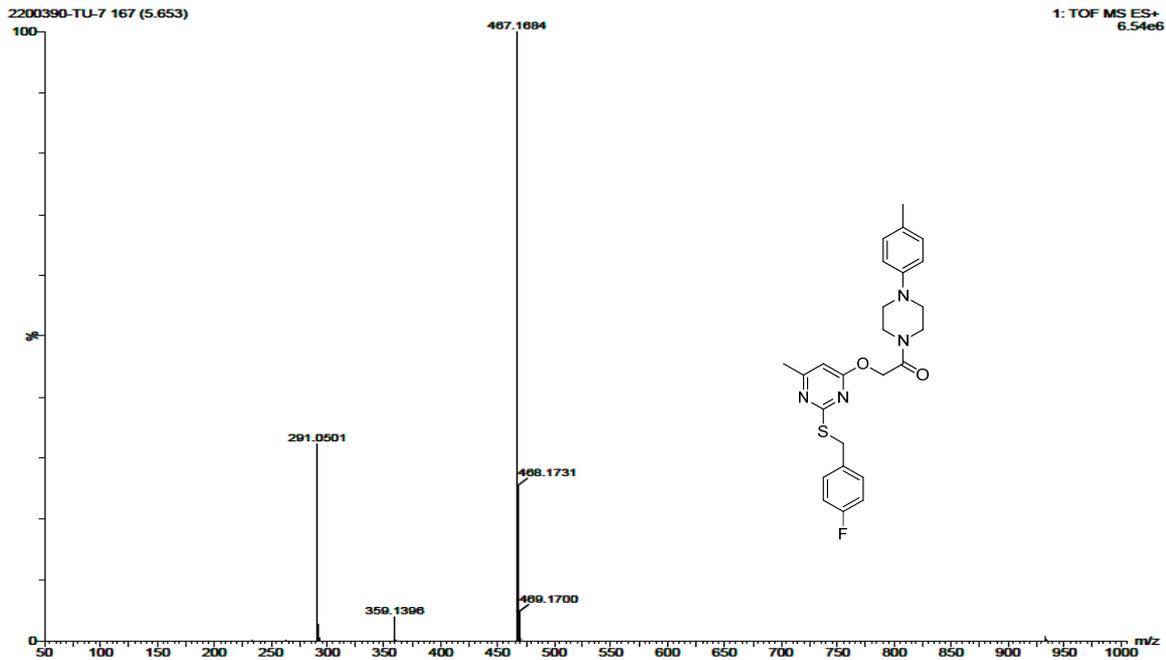
Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	6.07
0.01	97.52	4.94
0.1	100.92	4.88
1	101.38	4.88
10	102.91	6.46
100	87.62	4.75



<sup>1</sup>H NMR of compound 5I

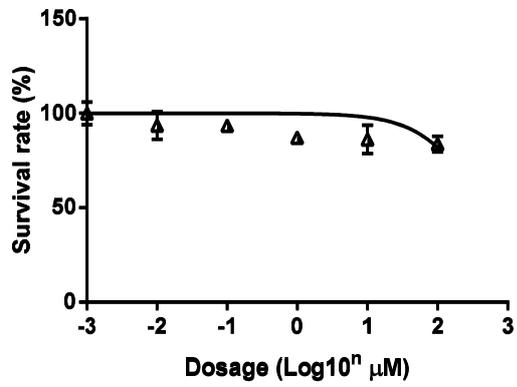


$^{13}\text{C}$  NMR of compound 5I



Mass spectra of 5I

**Compound: 5I**

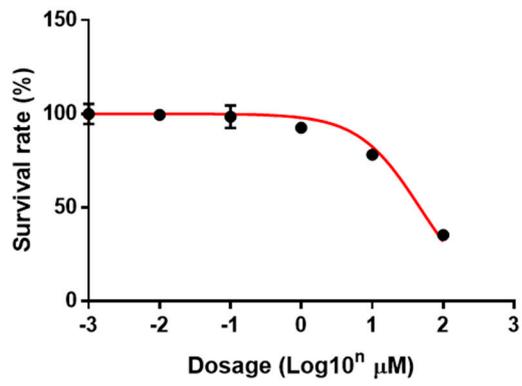


IC<sub>50</sub> (μM) = -  
Log IC<sub>50</sub> (μM) = -

- Cell line: MCF7 (2000 cells/per well<sup>96</sup>)
- Treated time: 72hrs
- Assay: alamarBlue (4hrs incubated)
- Data: 5I

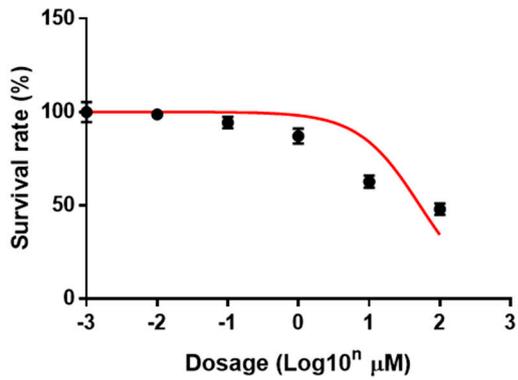
Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	6.07
0.01	93.61	7.43
0.1	93.47	2.24
1	87.02	2.06
10	86.20	7.47
100	83.71	4.17

- Assay: alamarBlue
- Cell line: MCF-10A, 2000 cells/per well<sup>96</sup>
- Compound: 5a
- Treatment: 72hrs, 2% serum



IC<sub>50</sub> (μM) = 46.95  
 Log IC<sub>50</sub> (μM) = 1.67

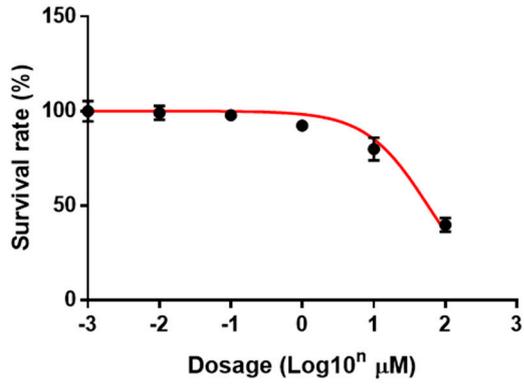
Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	5.42
0.01	99.06	3.68
0.1	97.86	1.61
1	92.36	2.10
10	79.89	6.06
100	39.78	3.66



- Assay: alamarBlue
- Cell line: MCF-10A, 2000 cells/per well<sup>96</sup>
- 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

- Assay: alamarBlue
- Cell line: MCF-10A, 2000 cells/per well<sup>96</sup>
- Compound: **Olaparib**
- Treatment: 72hrs, 2% serum



$\text{IC}_{50} (\mu\text{M}) = 57.36$   
 $\text{Log IC}_{50} (\mu\text{M}) = 1.76$

Conc. ( $\mu\text{M}$ )	Viability	
	AVE.	$\pm$ 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