Electrochemical Synthesis of New Isoxazoles and Triazoles Tethered with Thiouracil Base as Inhibitors of Histone Deacetylases in Human Breast Cancer Cells

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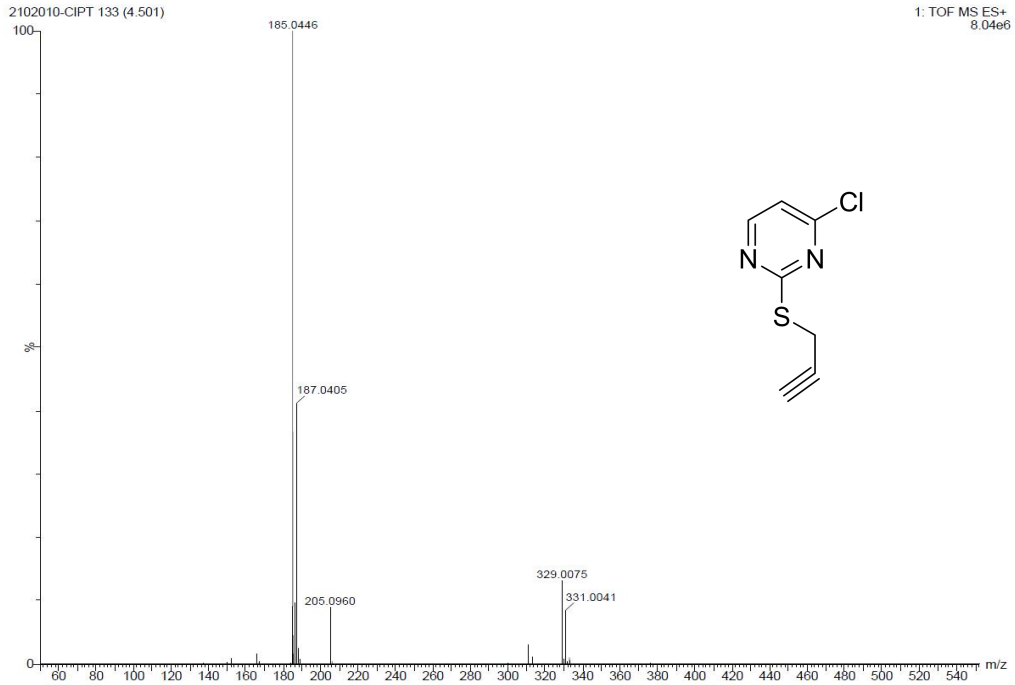
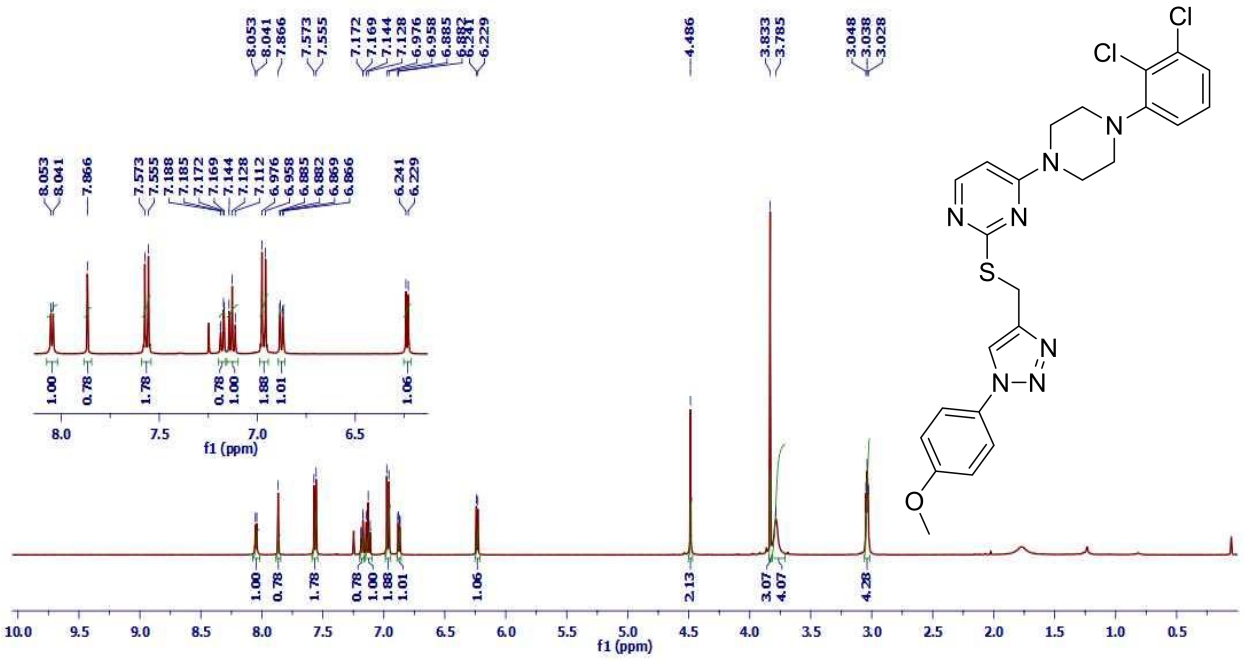
Supplementary data

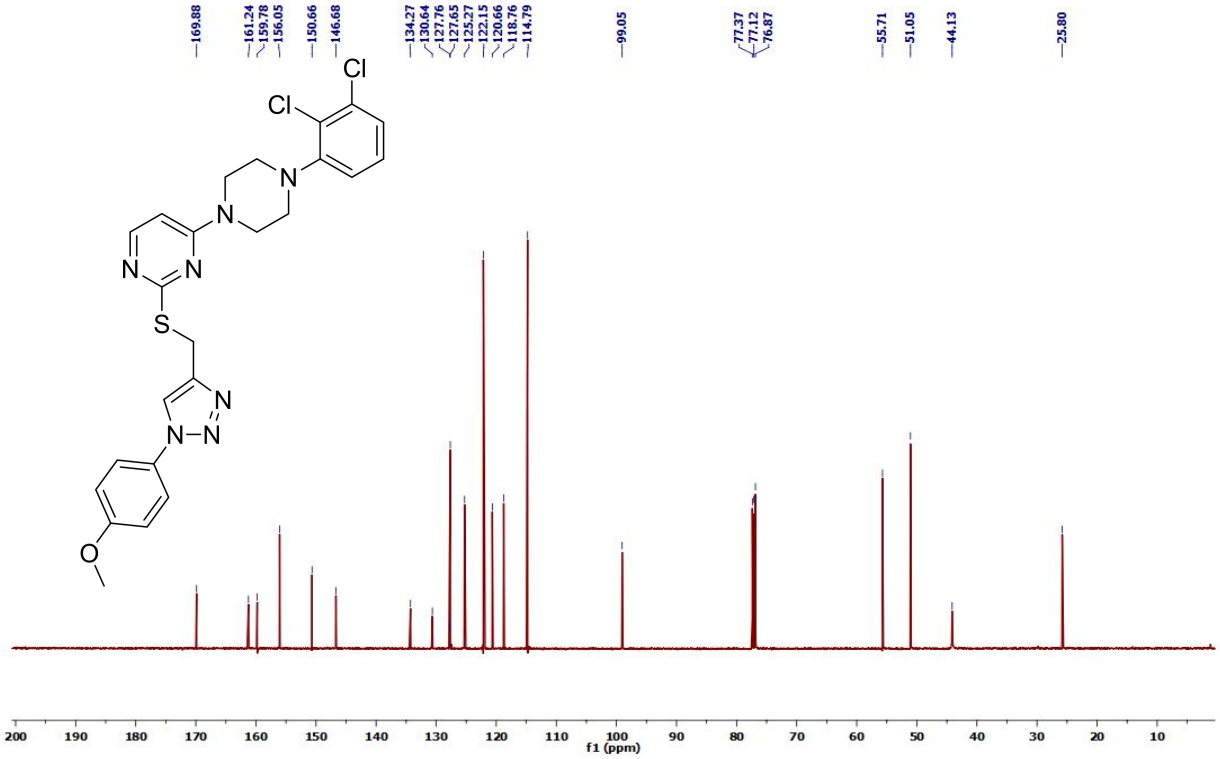
Spectroscopic data (Mass, ^{1}H, and ^{13}C NMR) of synthesized compounds



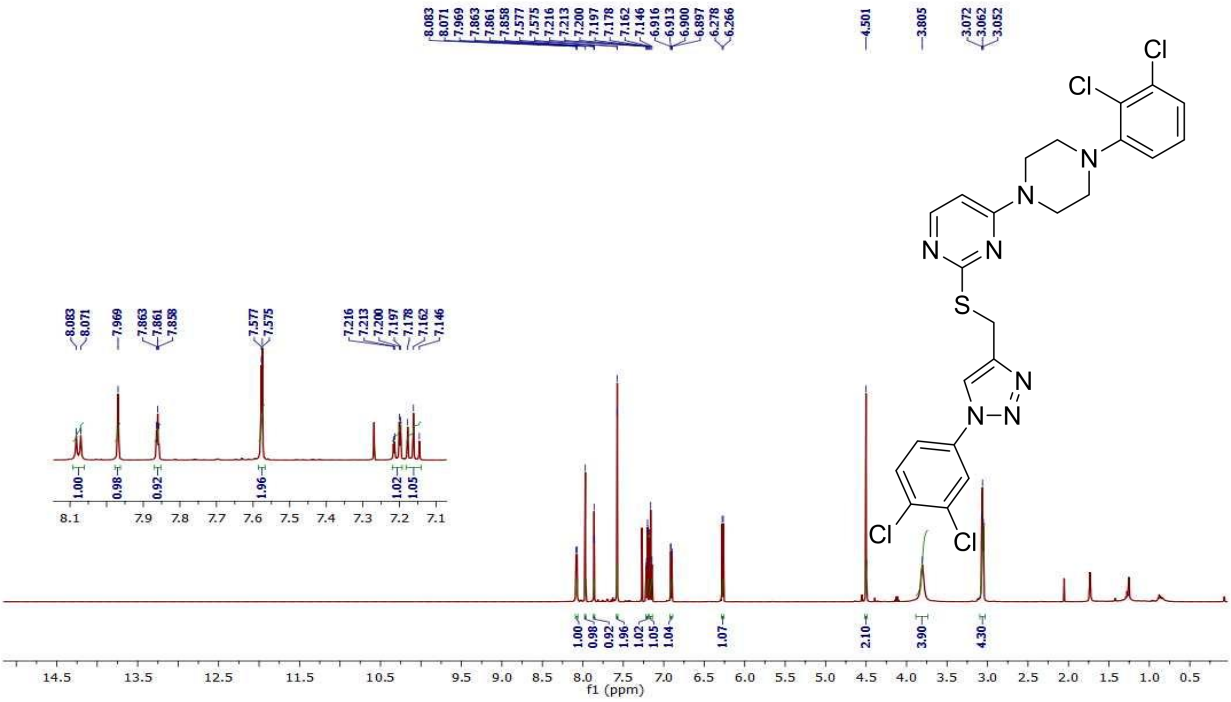
Mass spectrum of 3



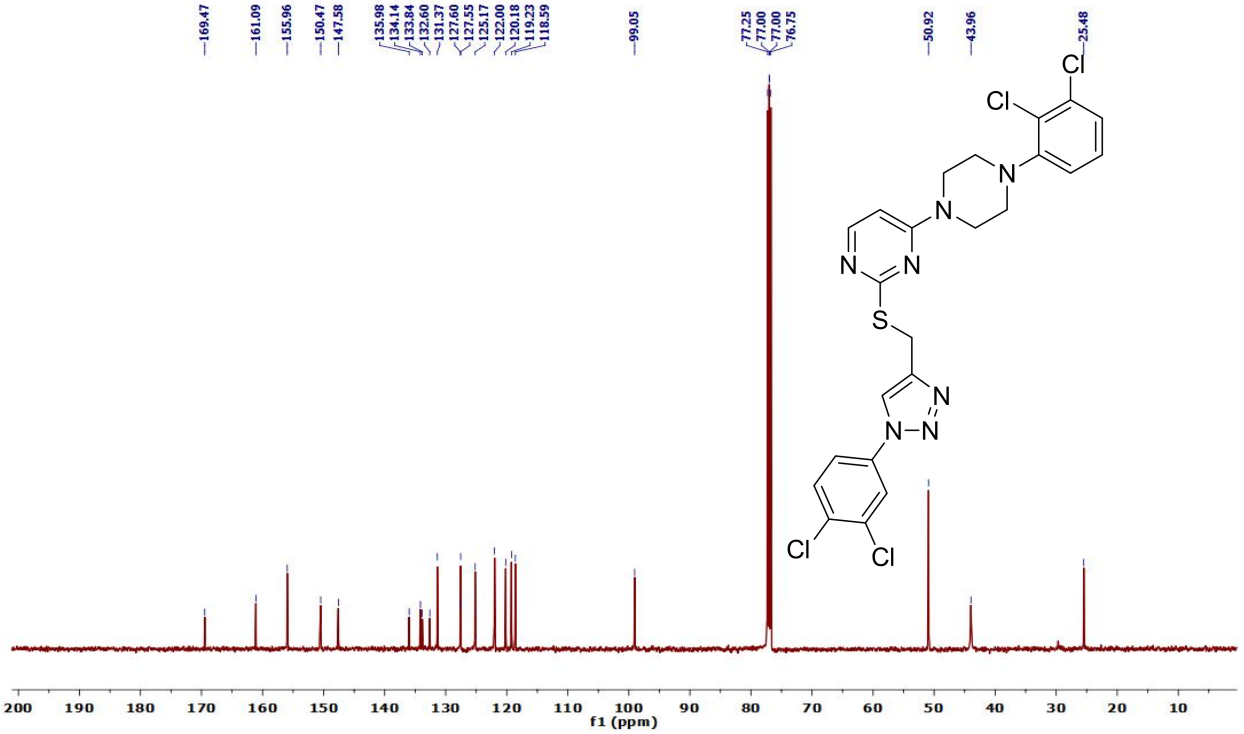
^{1}H NMR of 5a



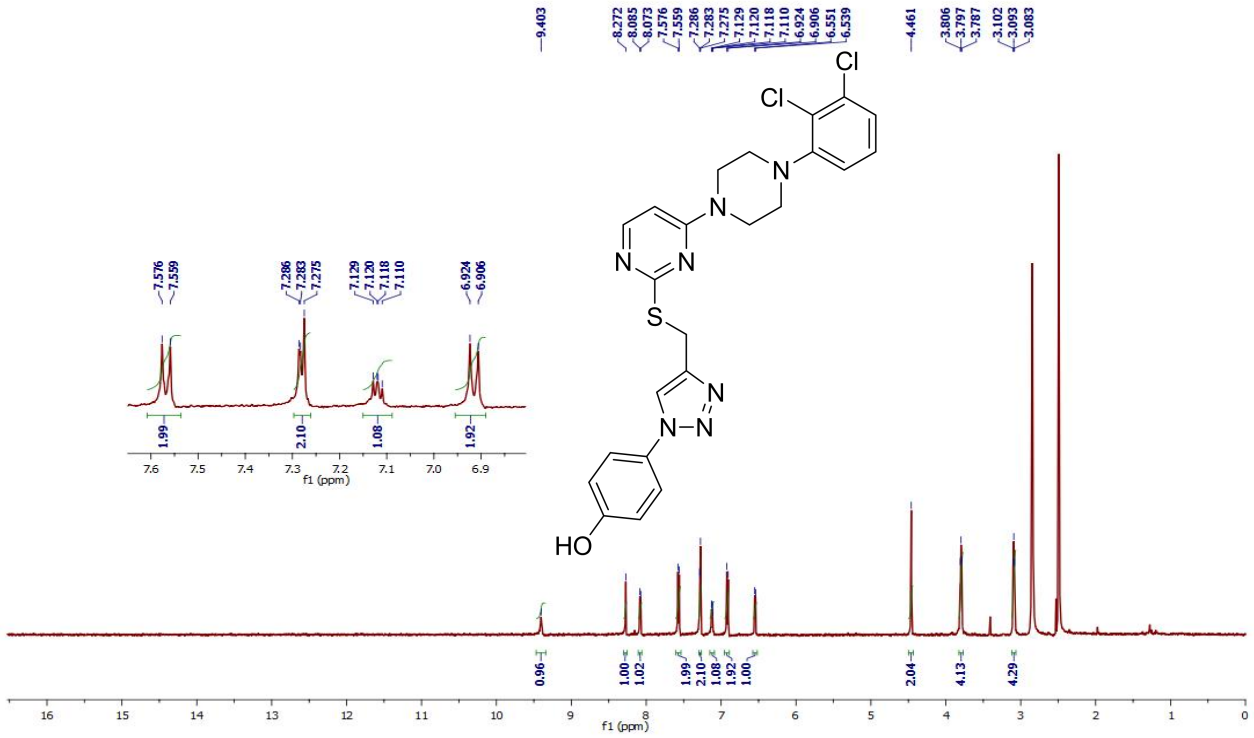
^{13}C NMR of 5a



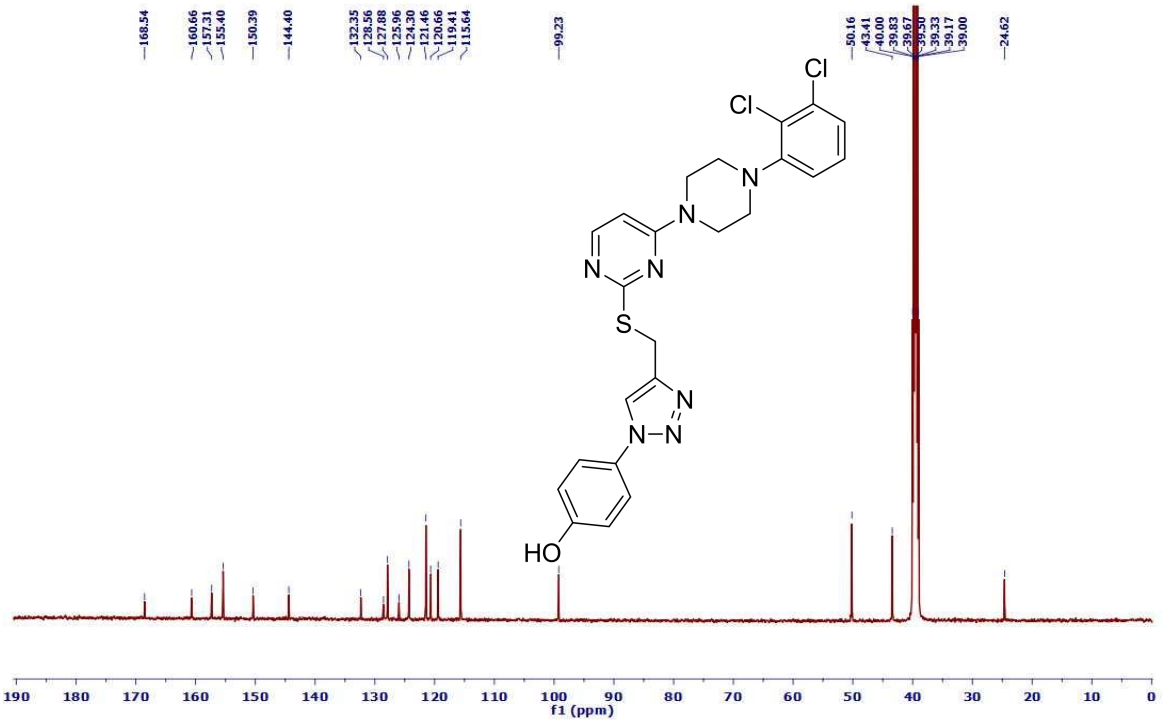
^{1}H NMR of 5b



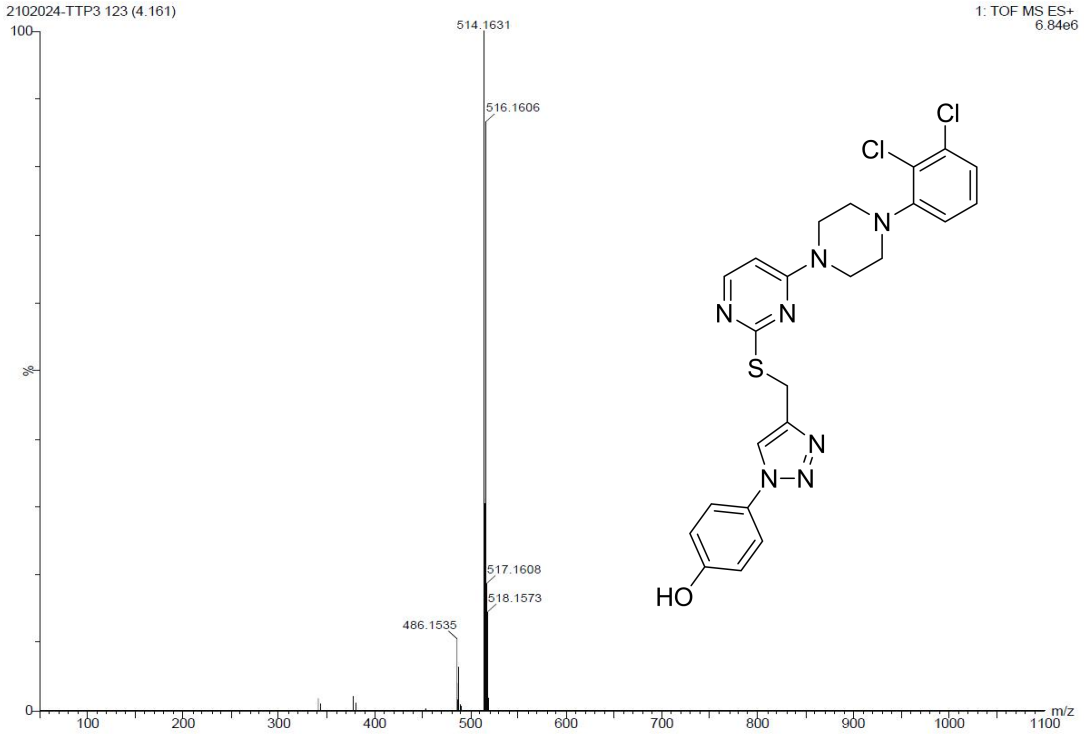
^{13}C NMR of 5b



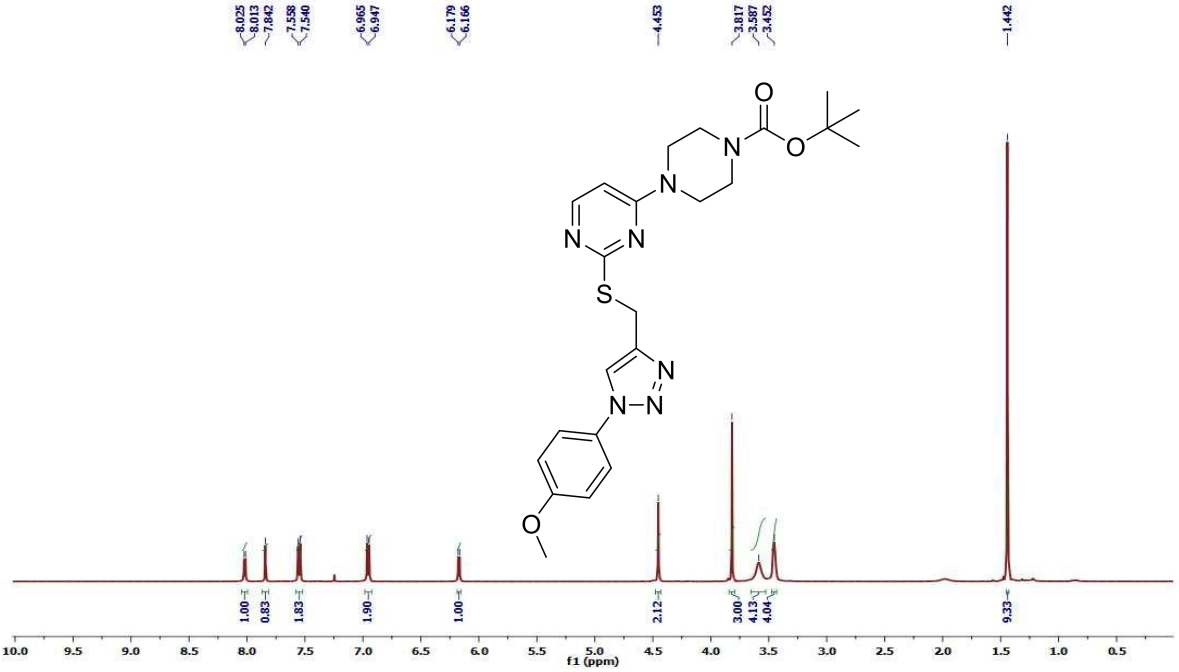
^{1}H NMR of 5c



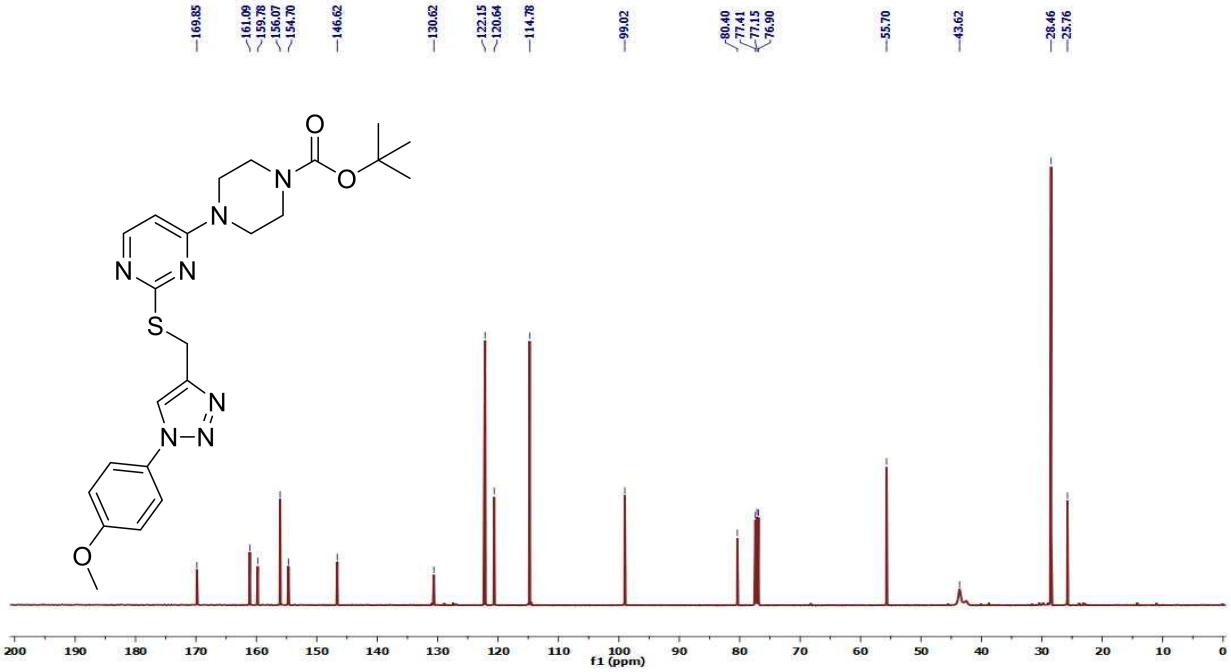
^{13}C NMR of 5c



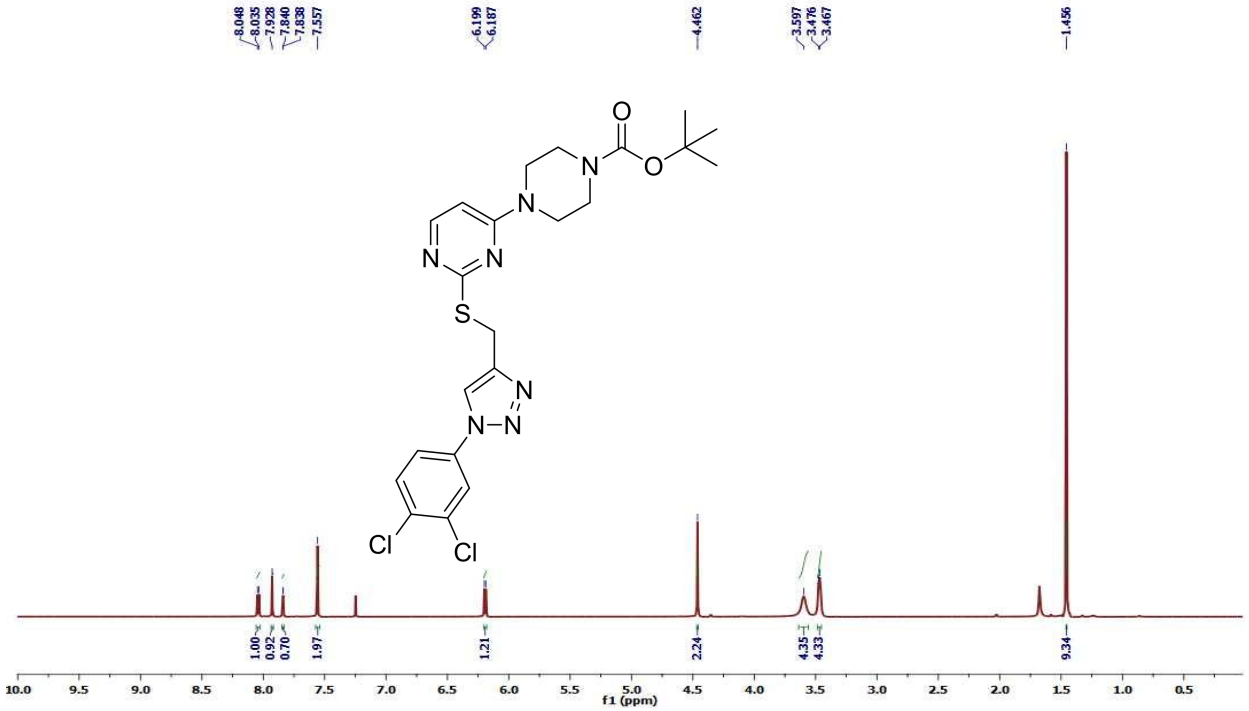
Mass spectrum of 5c



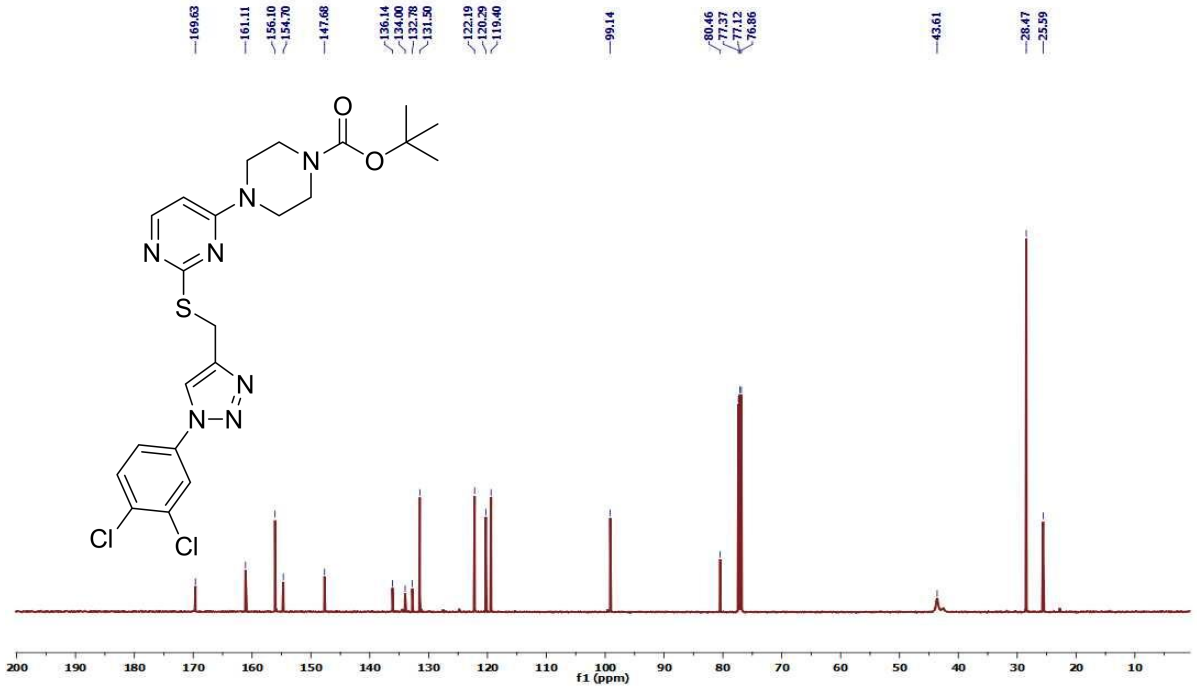
^{1}H NMR of 5d



^{13}C NMR of 5d



^{1}H NMR of 5e



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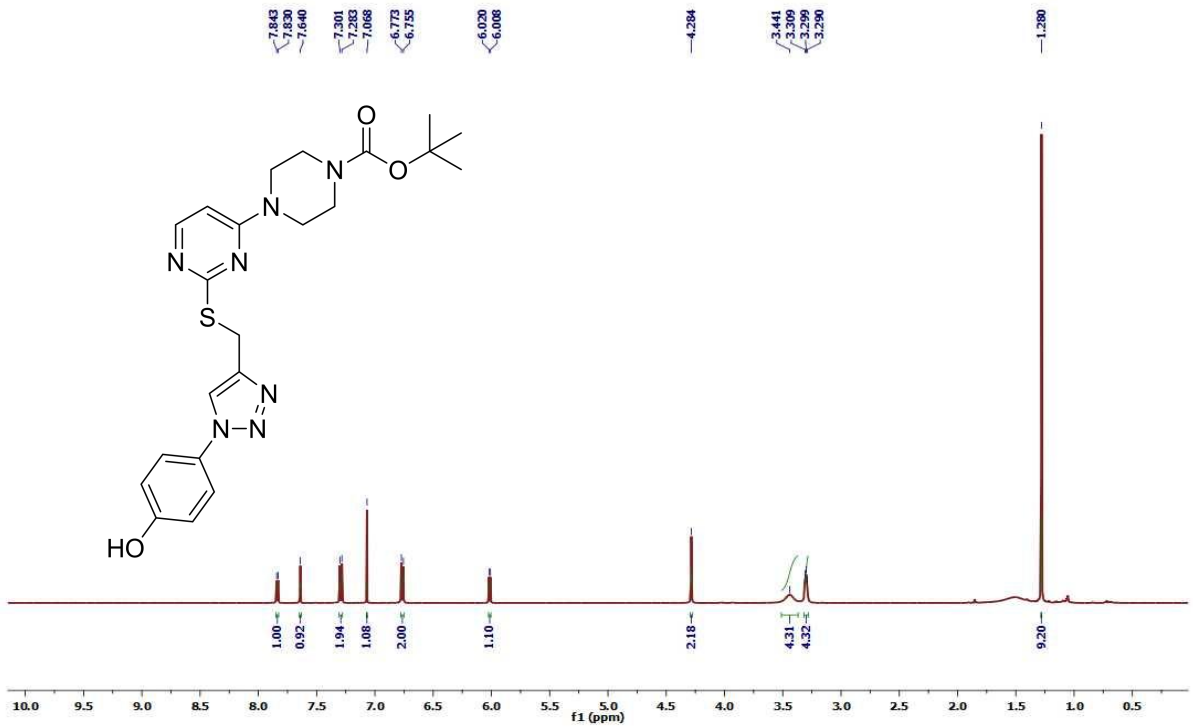
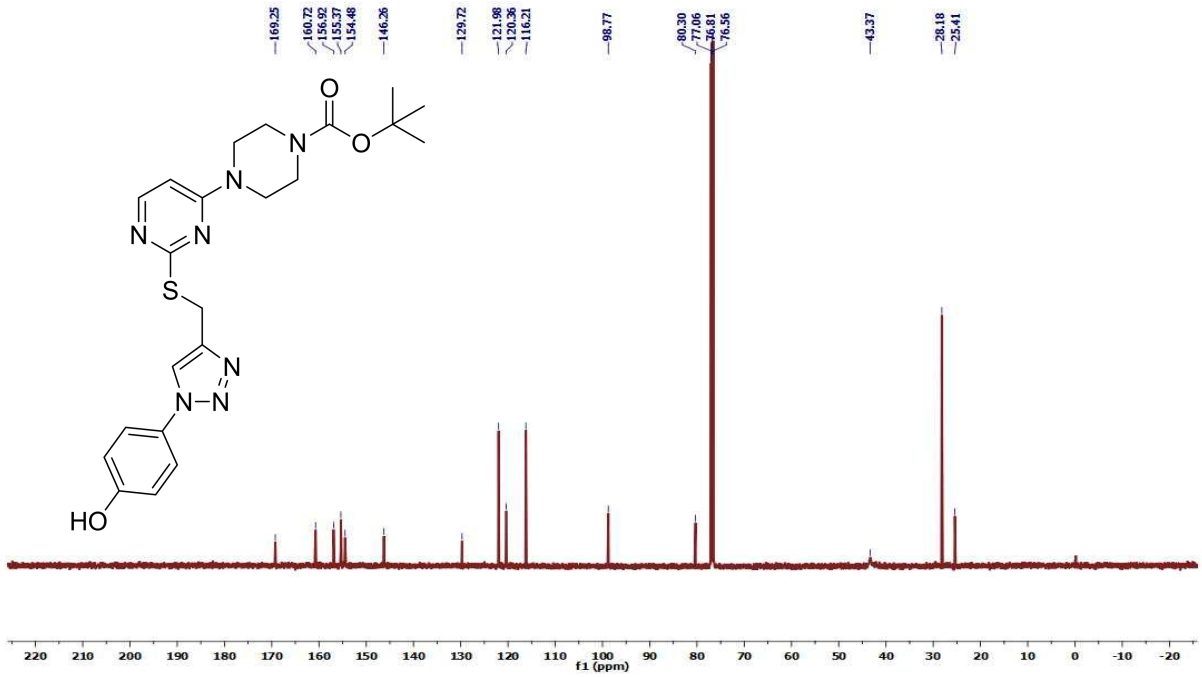


^{1}H NMR of 5f



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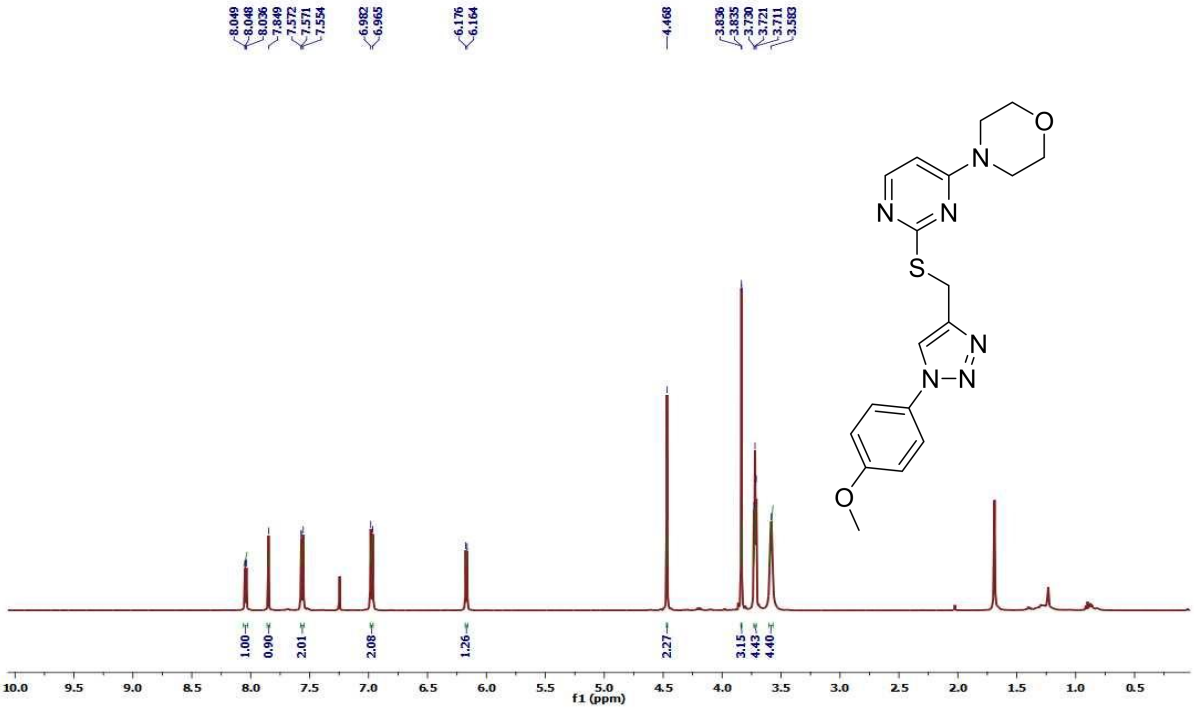
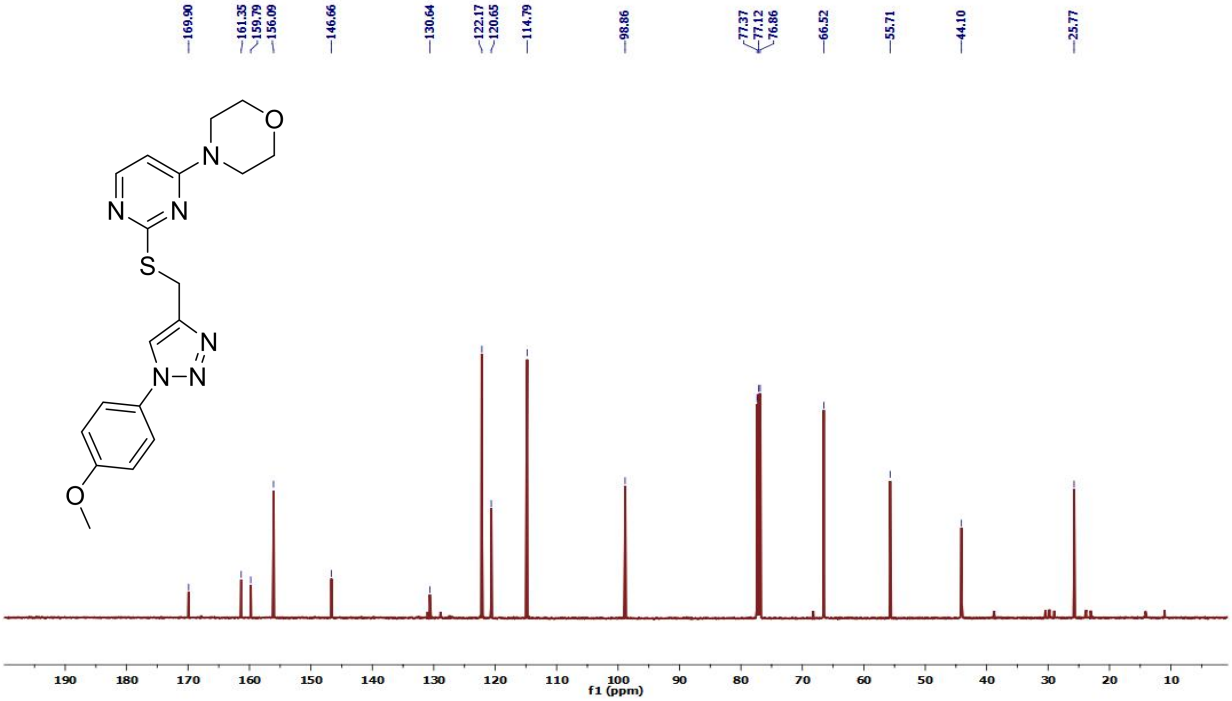


^{1}H NMR of 5g



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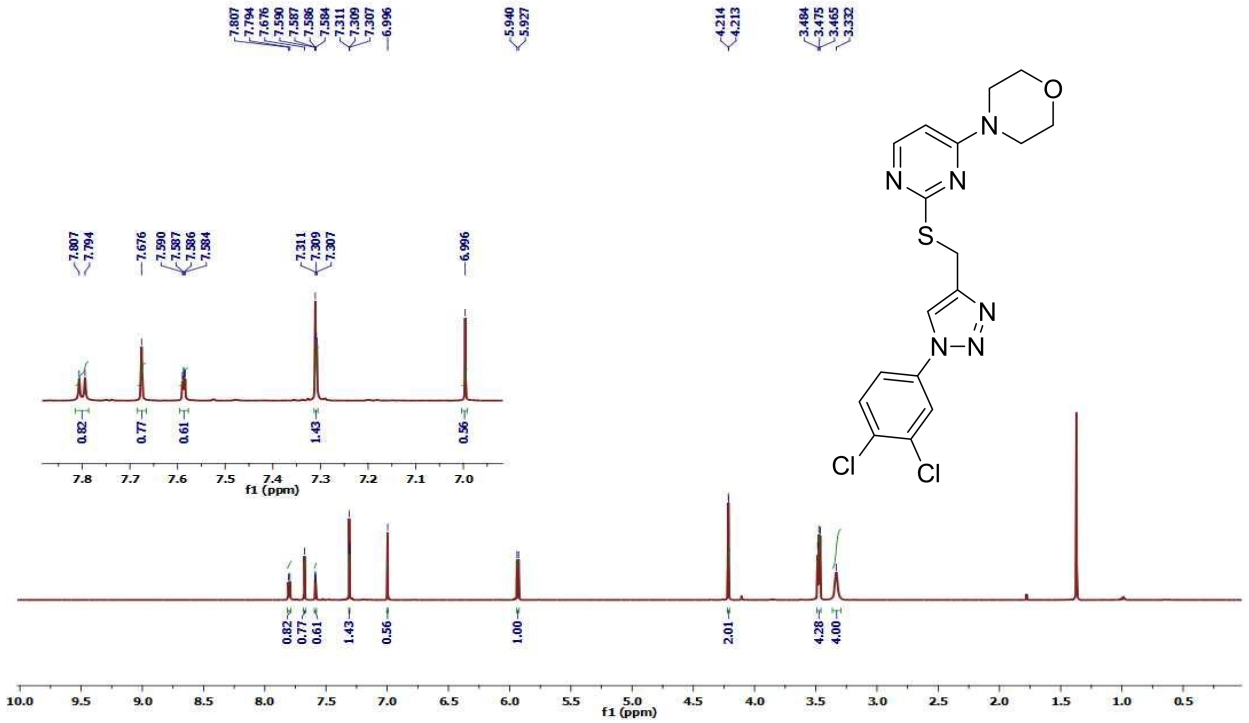

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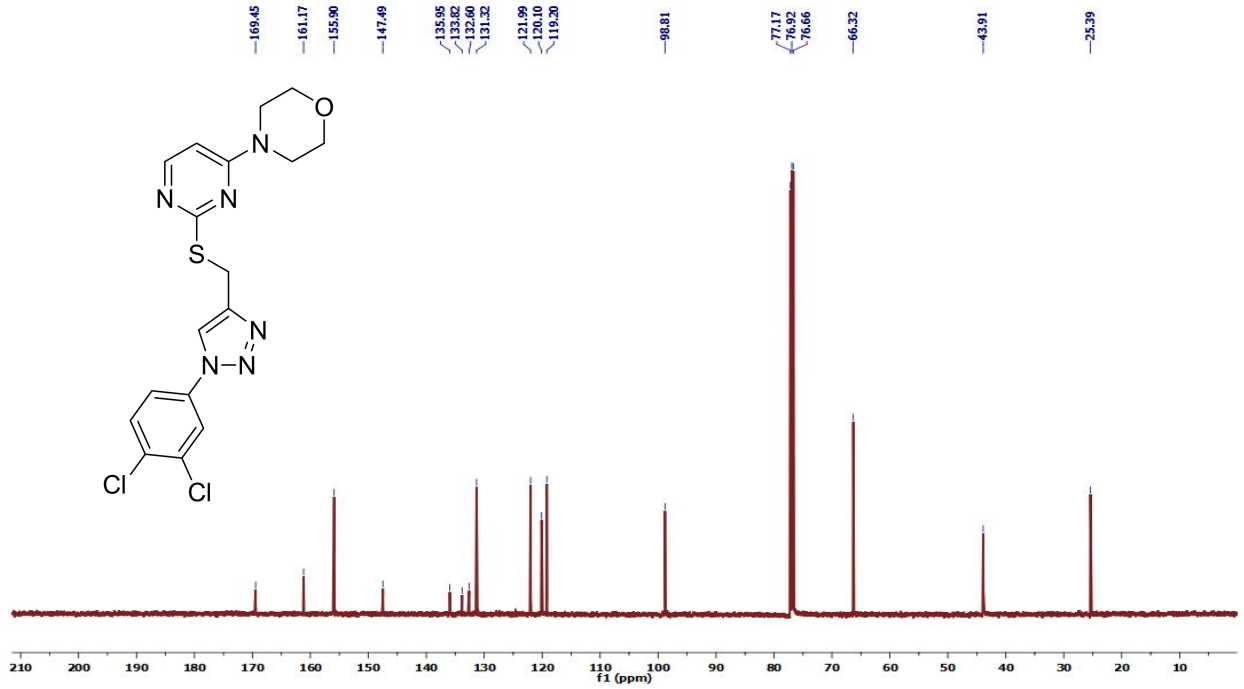

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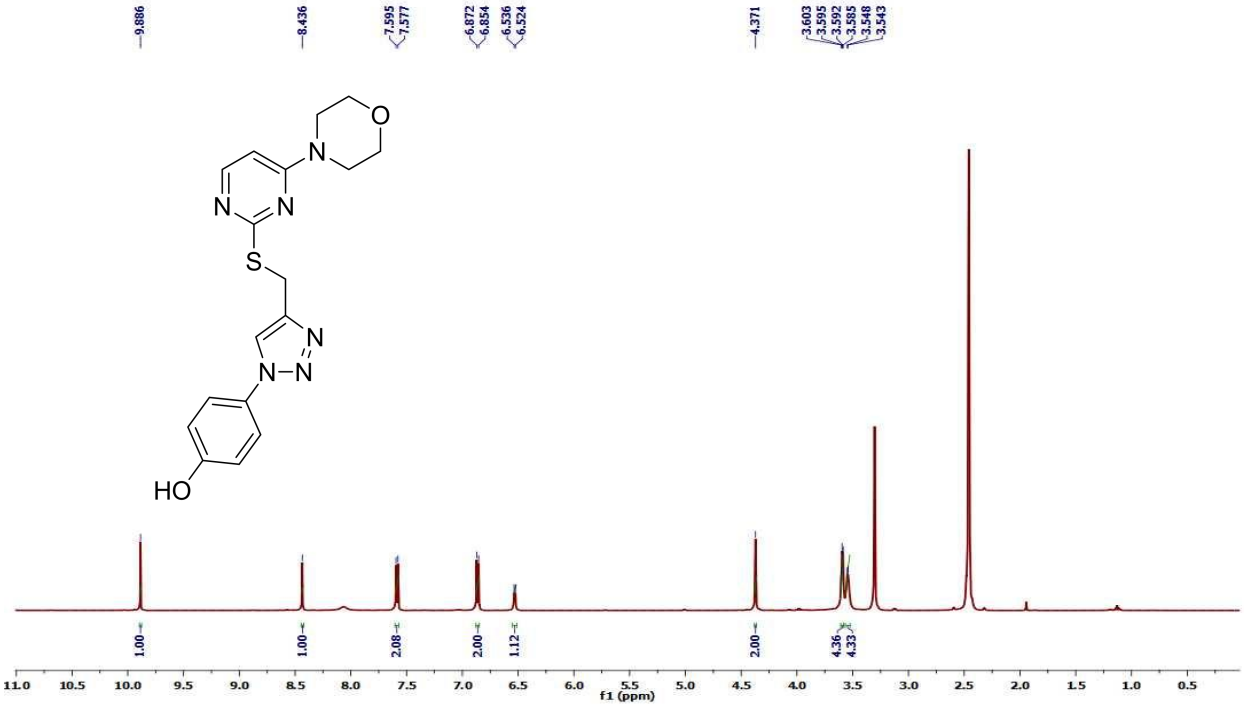
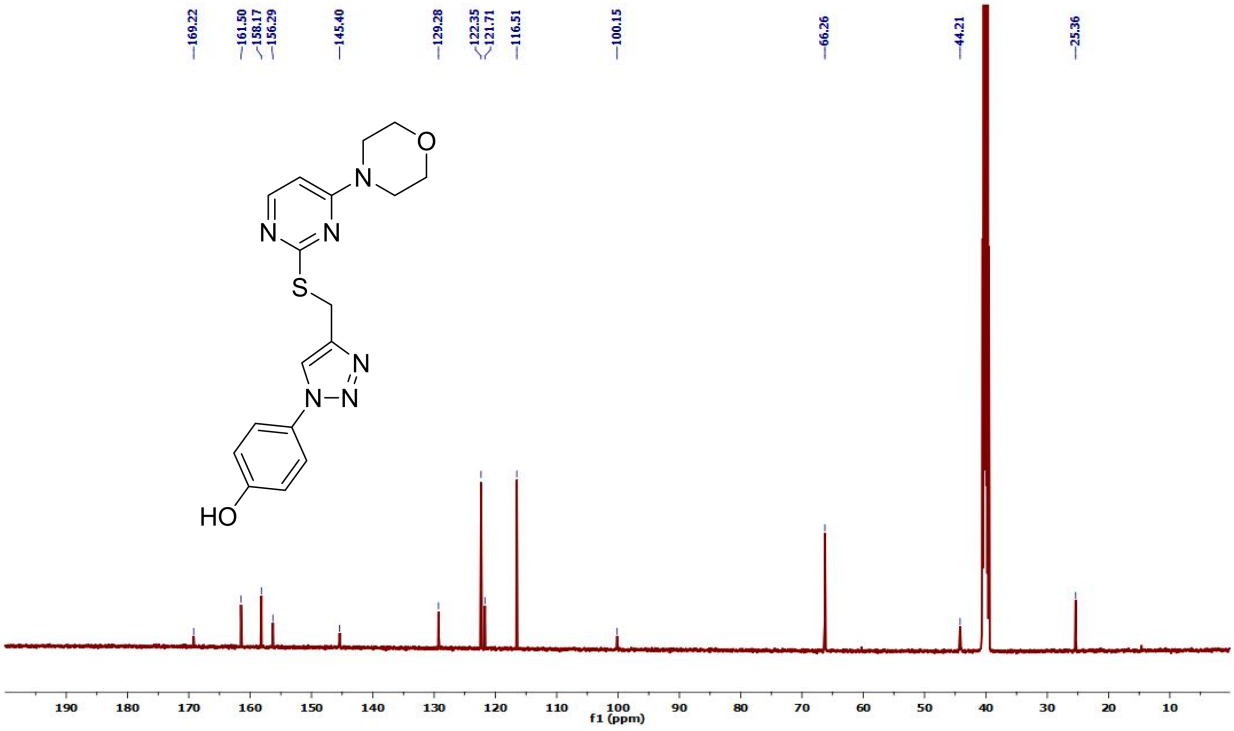


^{1}H NMR of 5i



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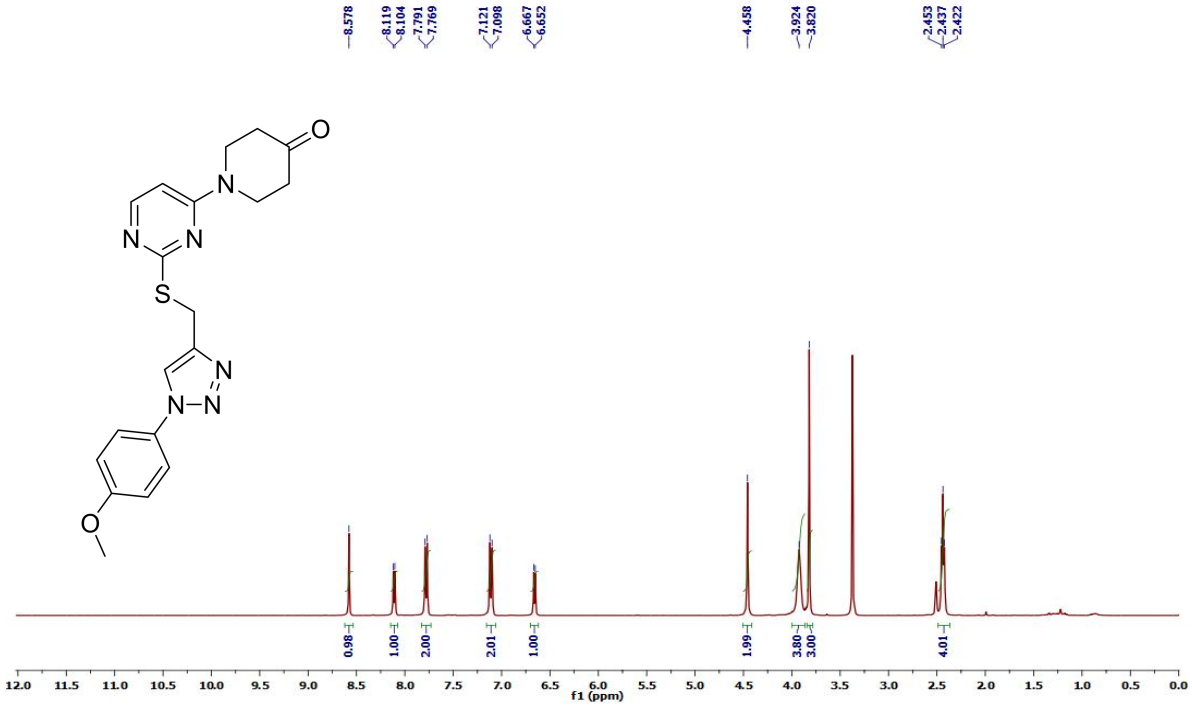

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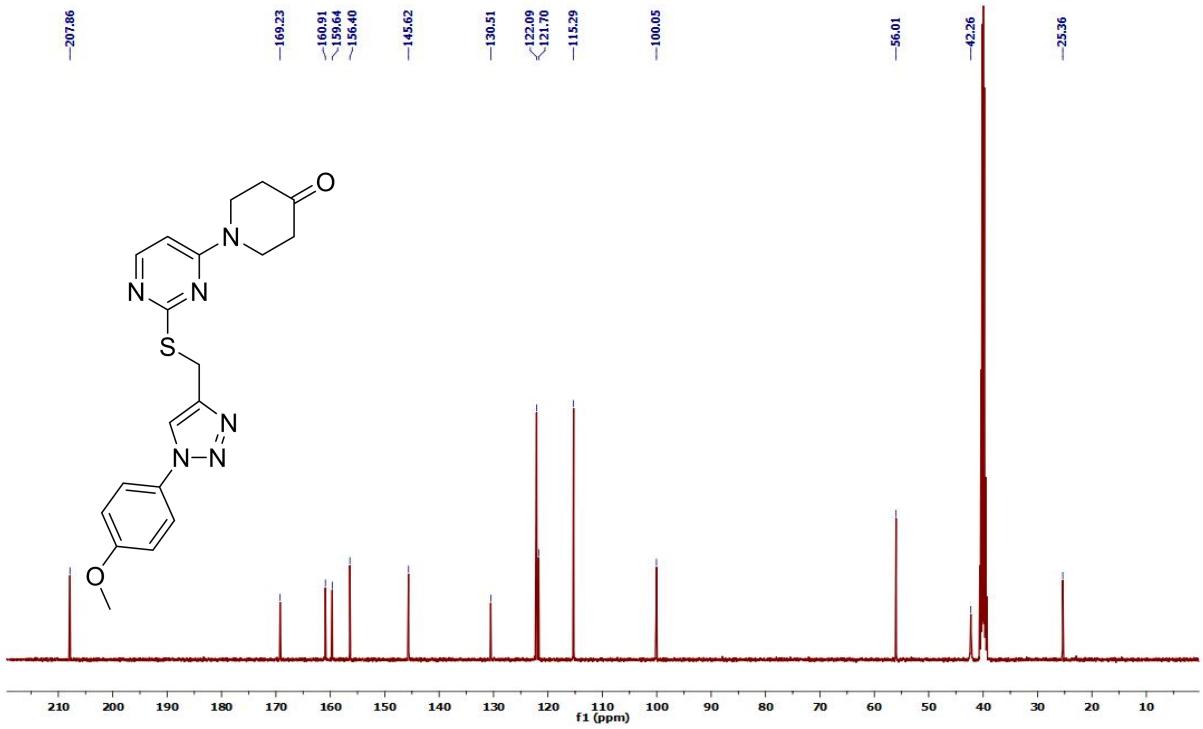

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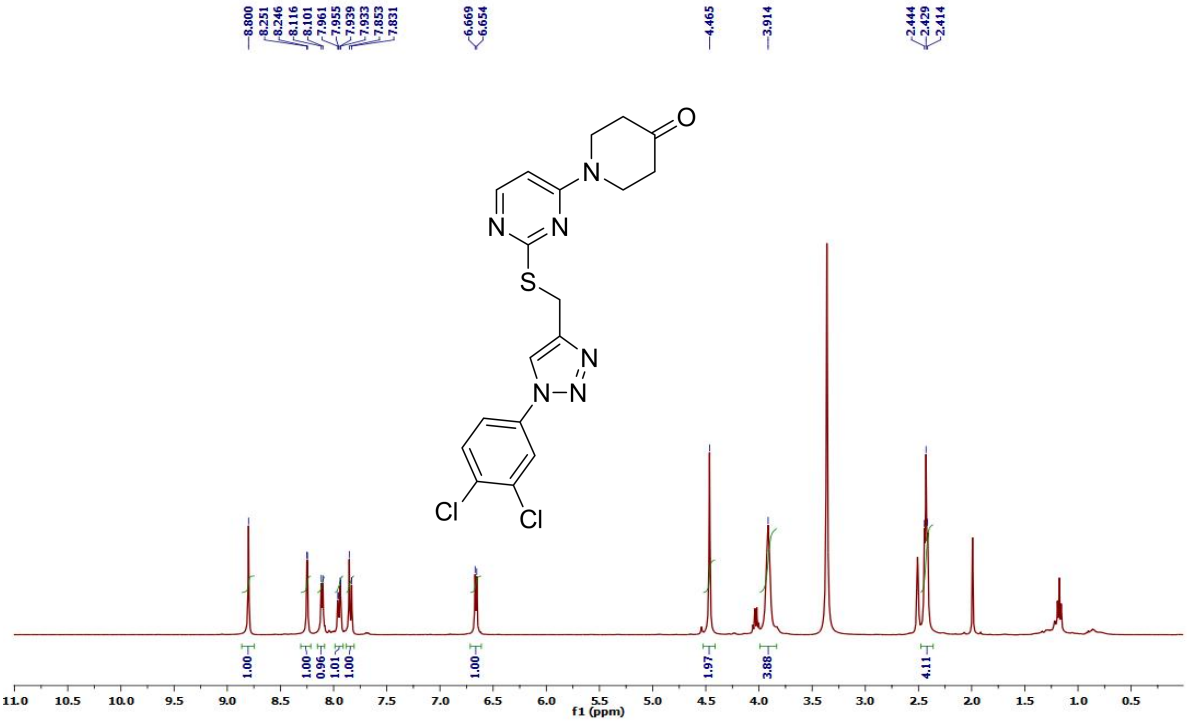

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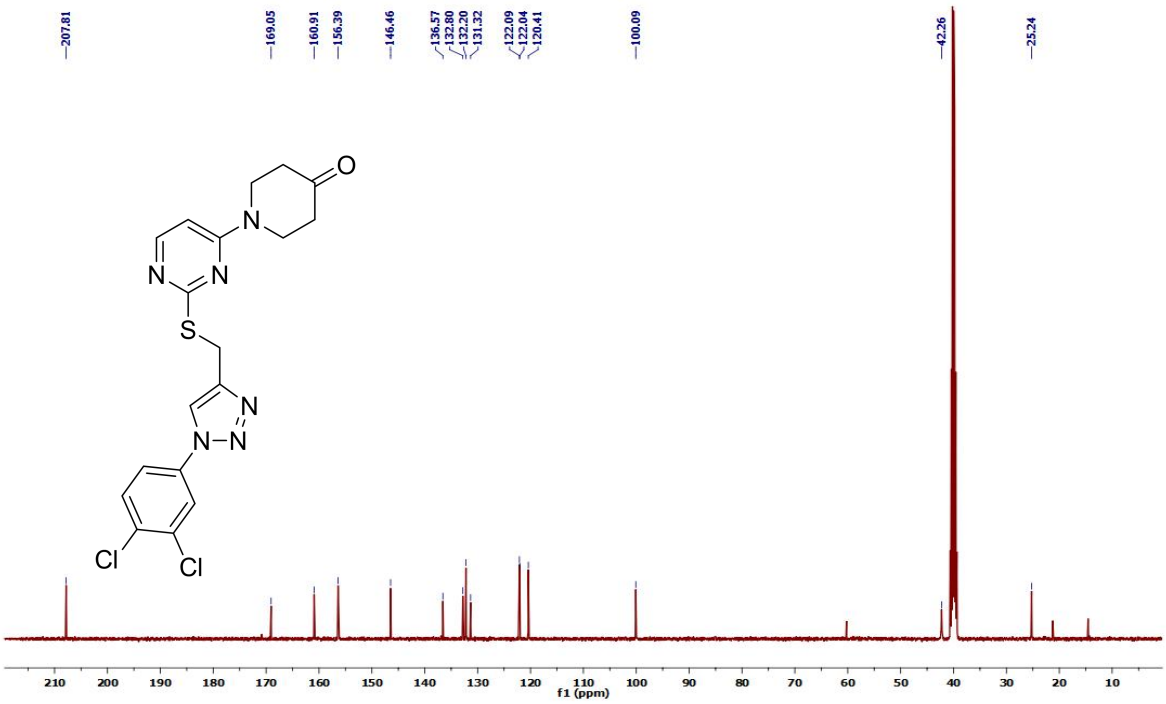

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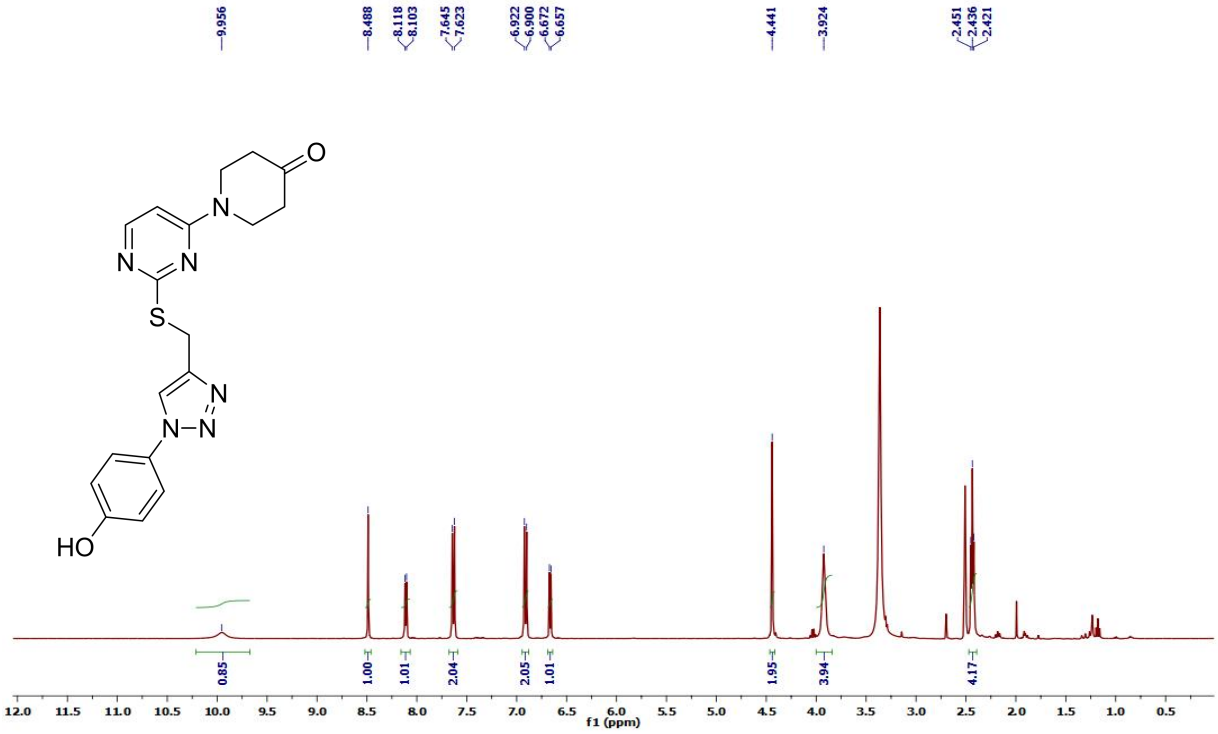

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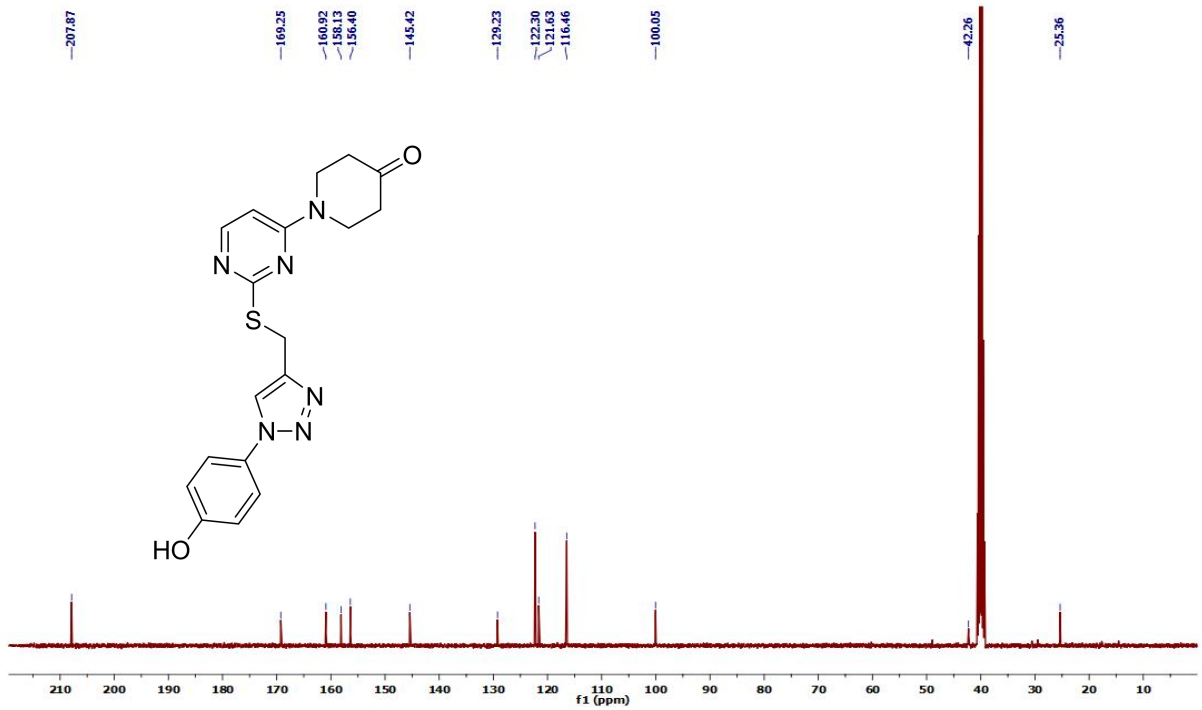

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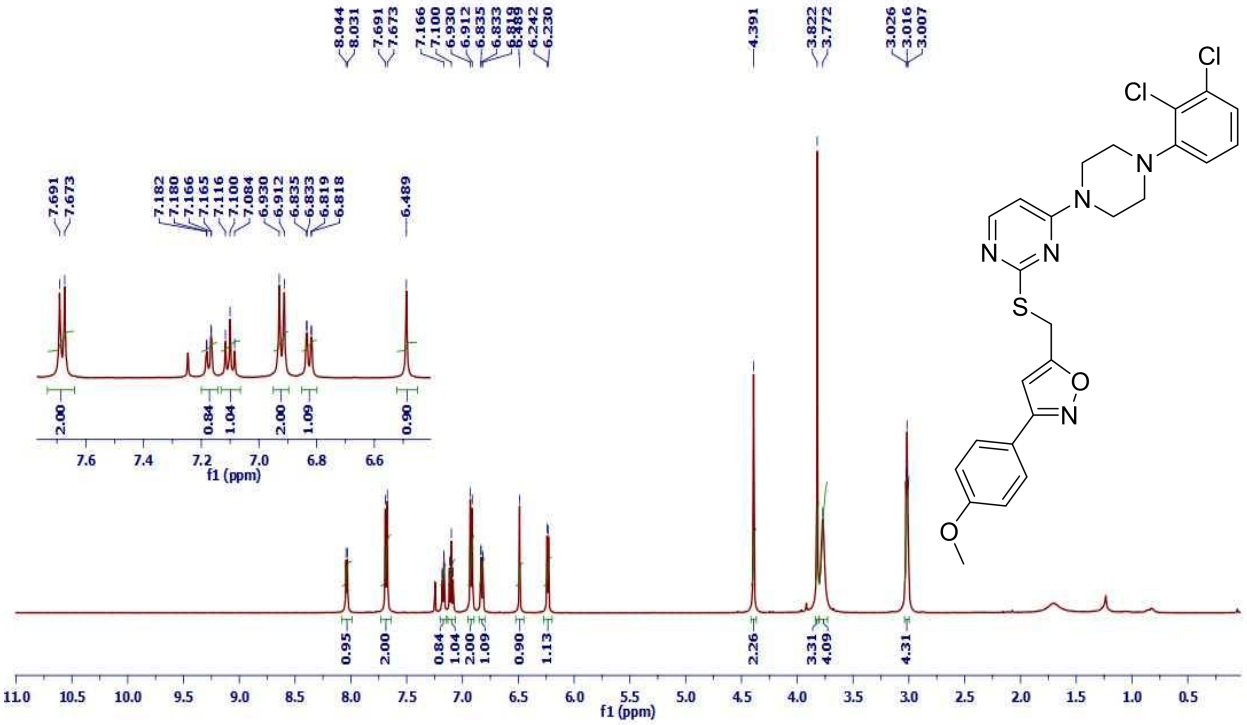
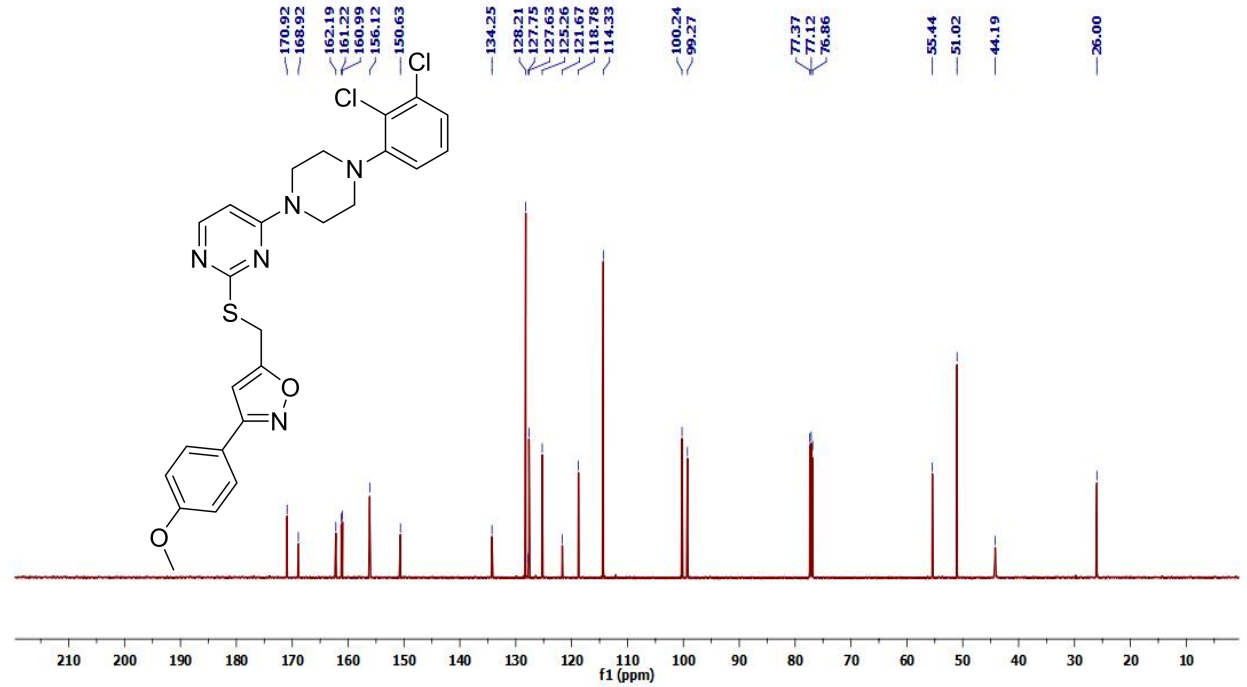


^{1}H NMR of 6a



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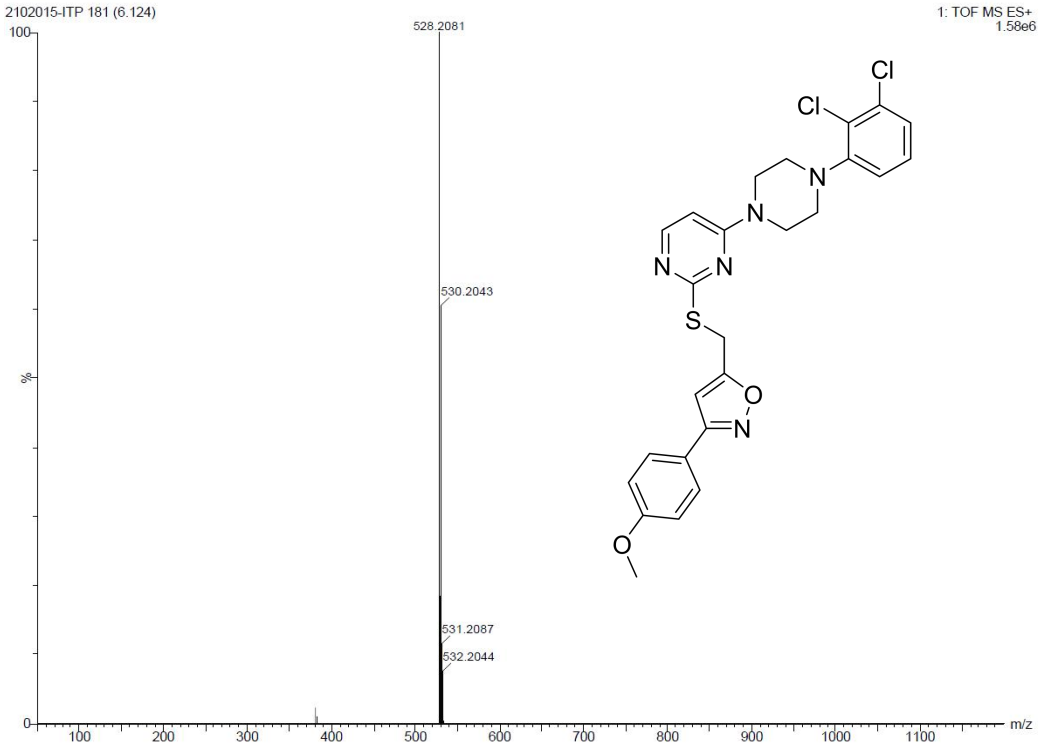
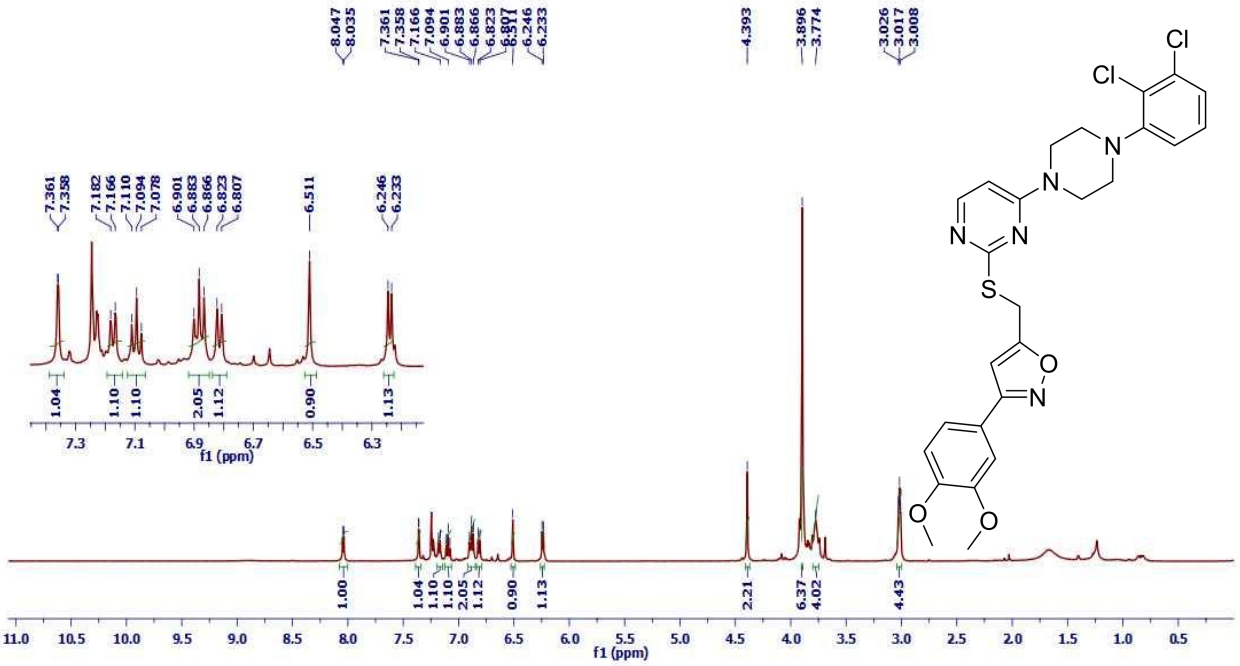


Mass spectrum of 6a



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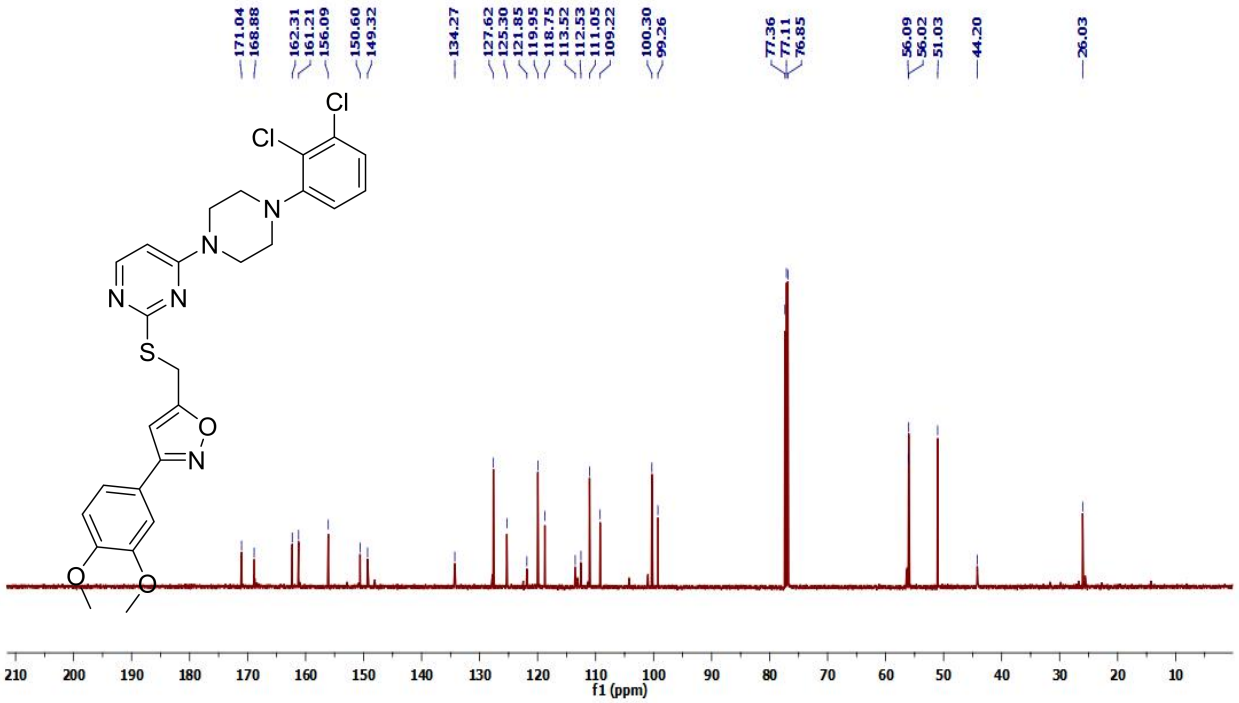

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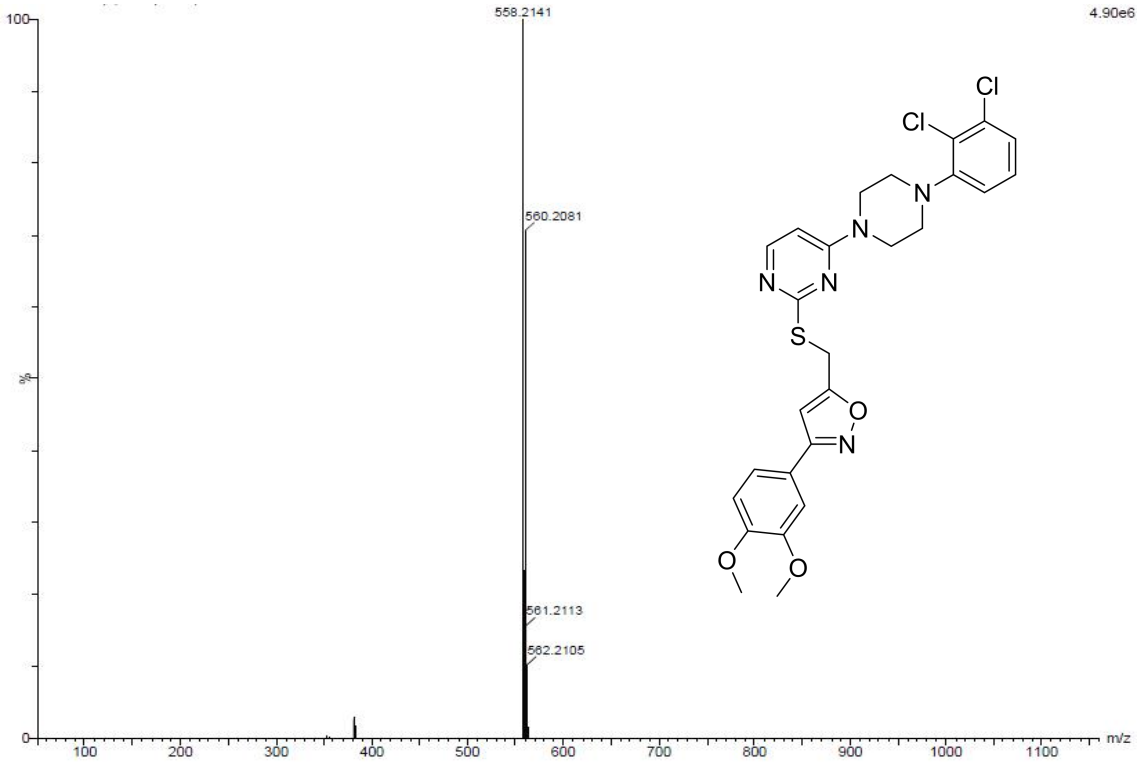
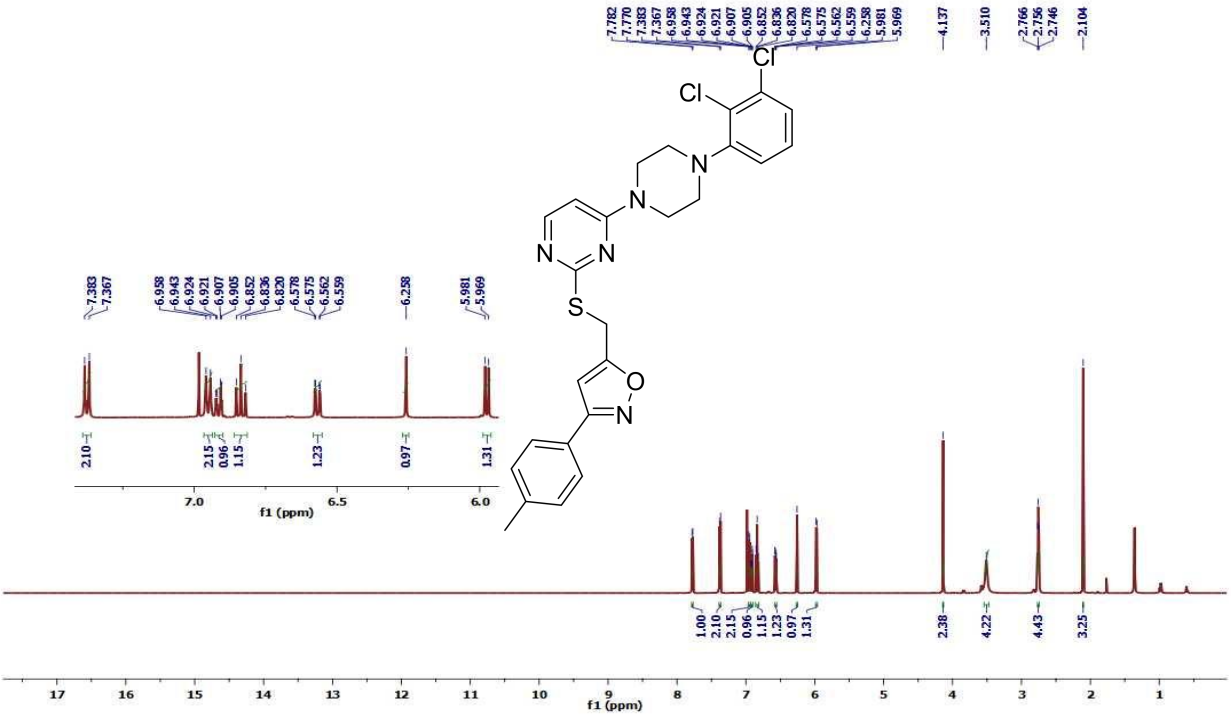


Mass spectrum of 6b



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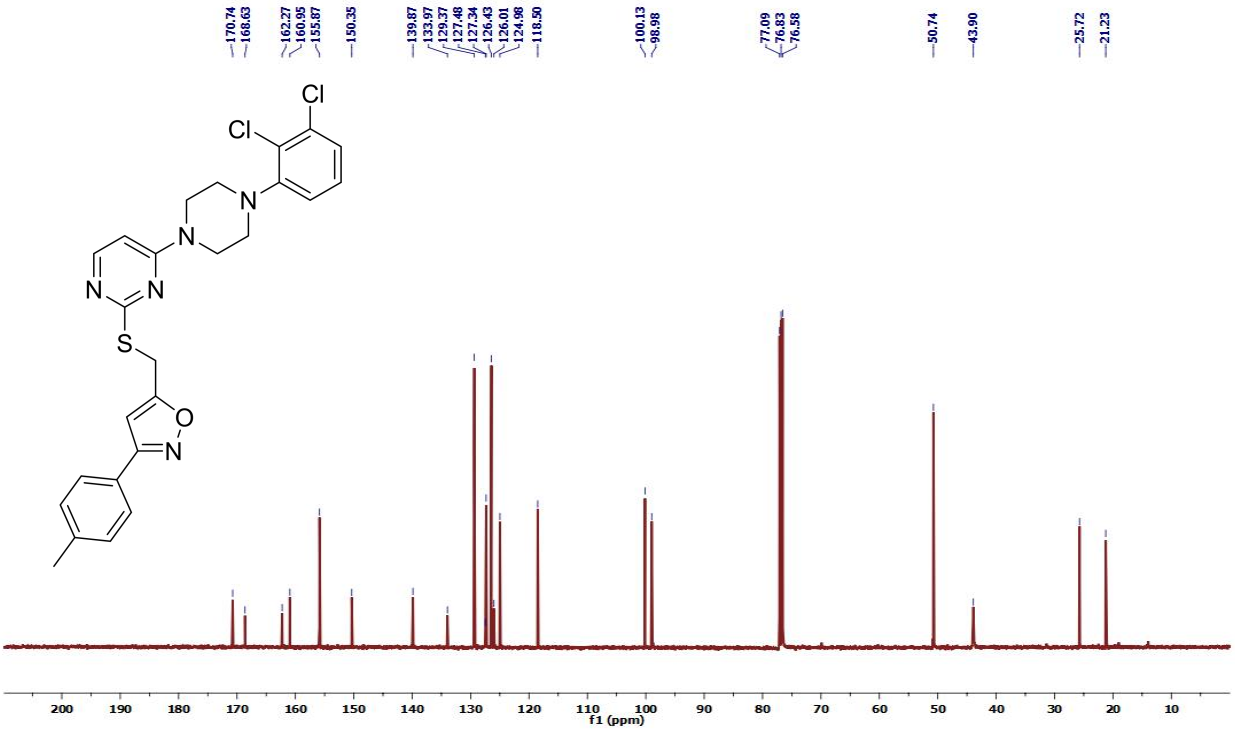

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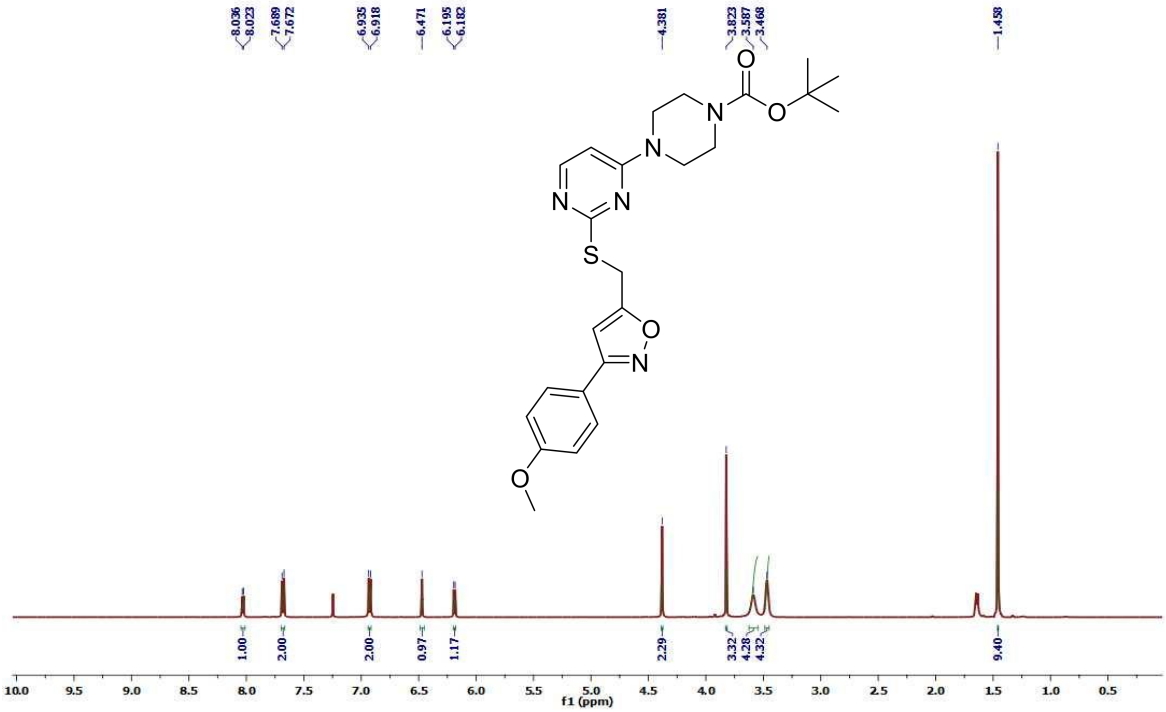

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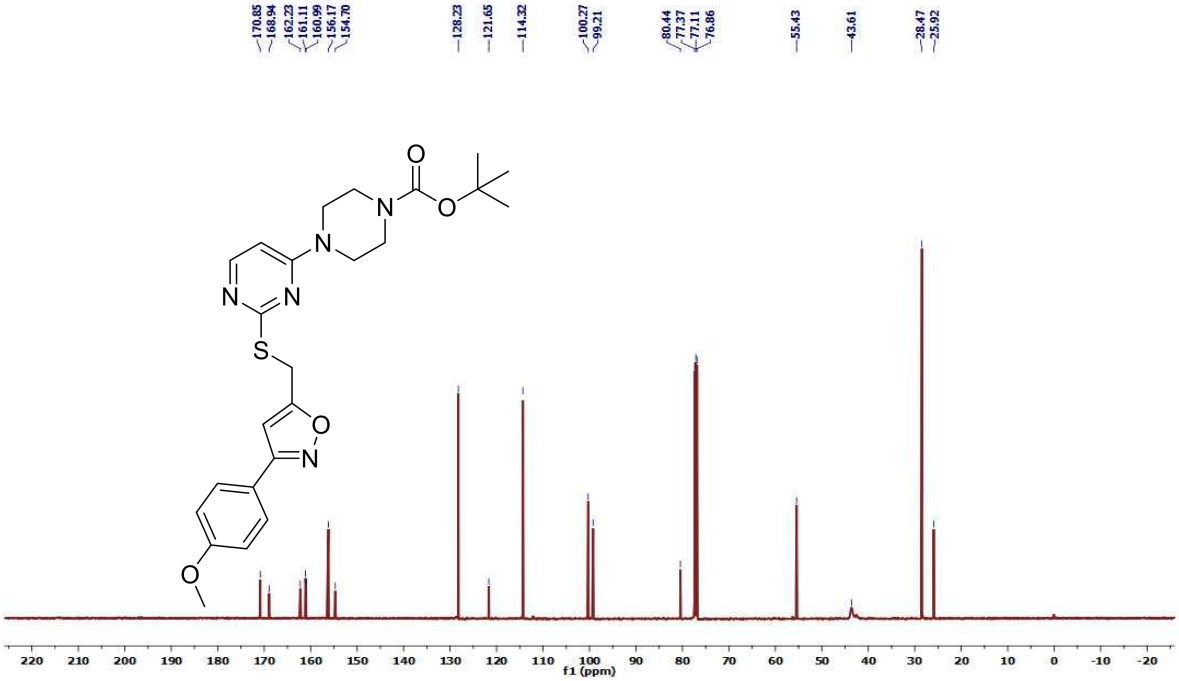

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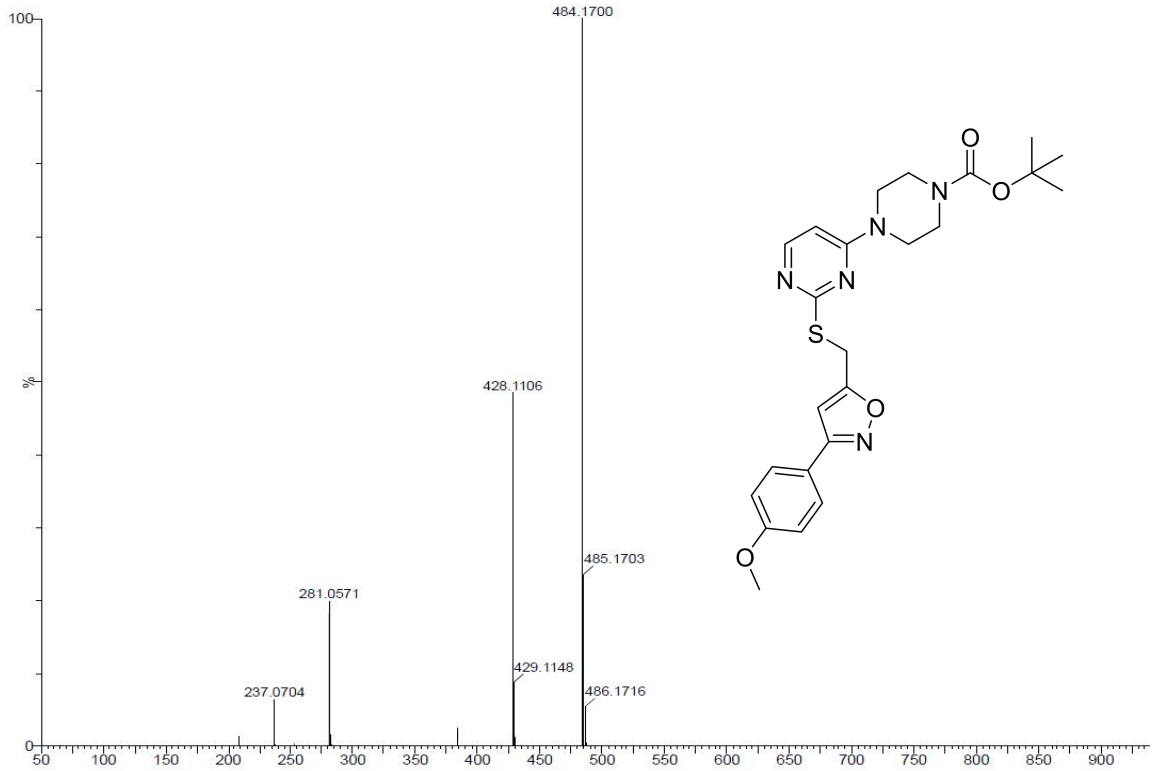
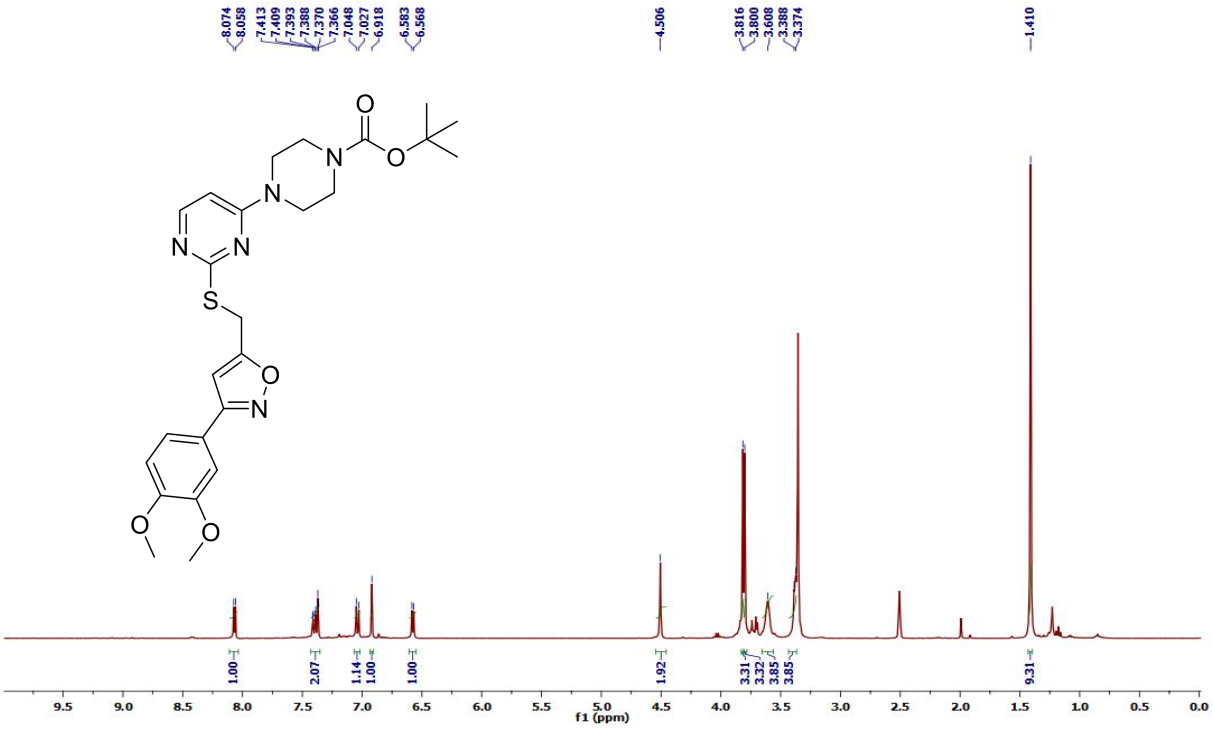


Mass spectrum of 6d



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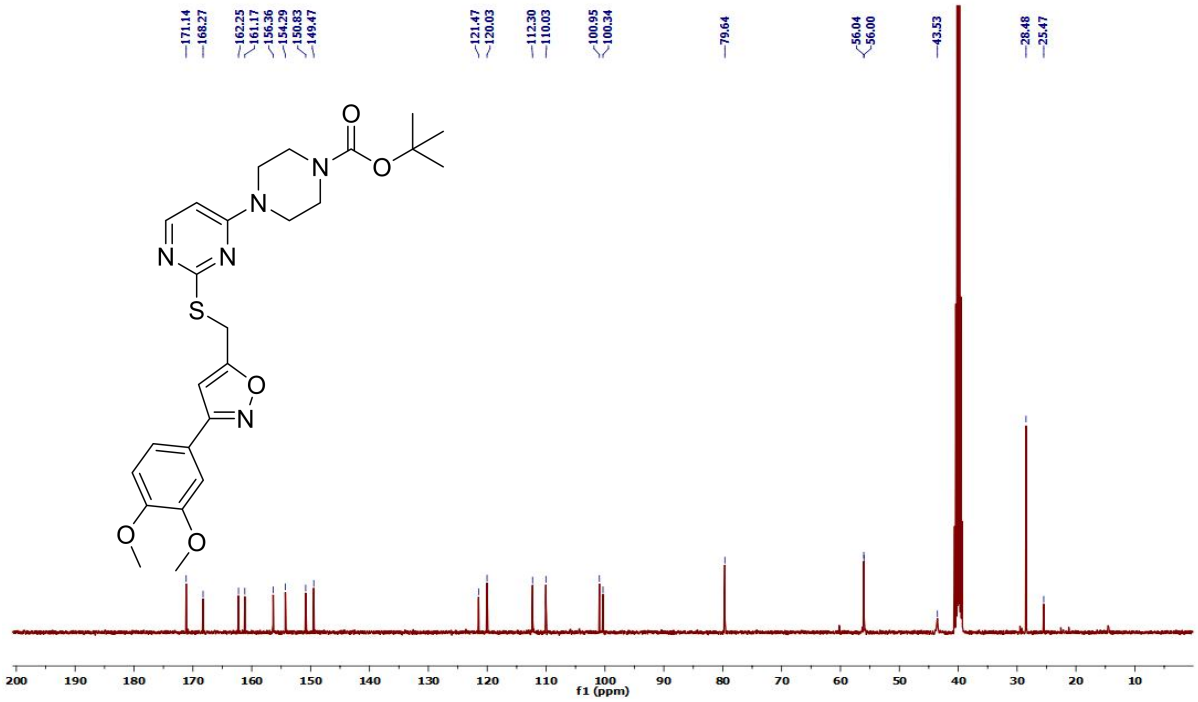

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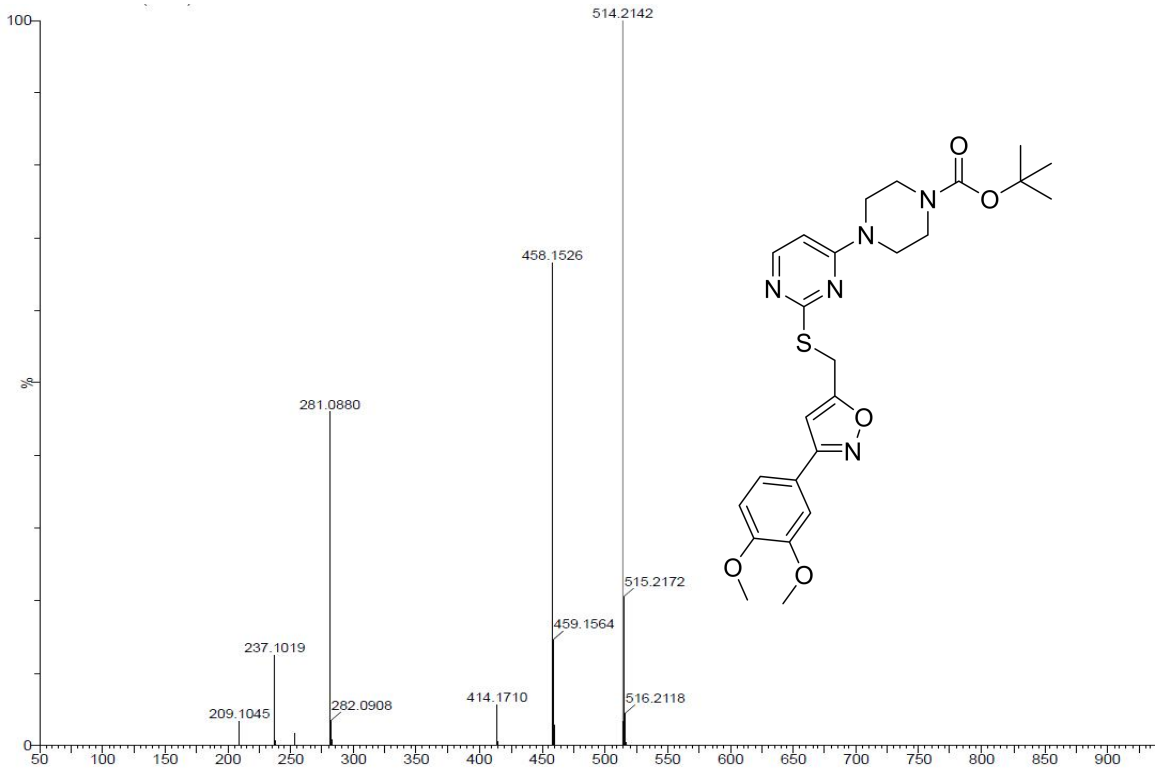
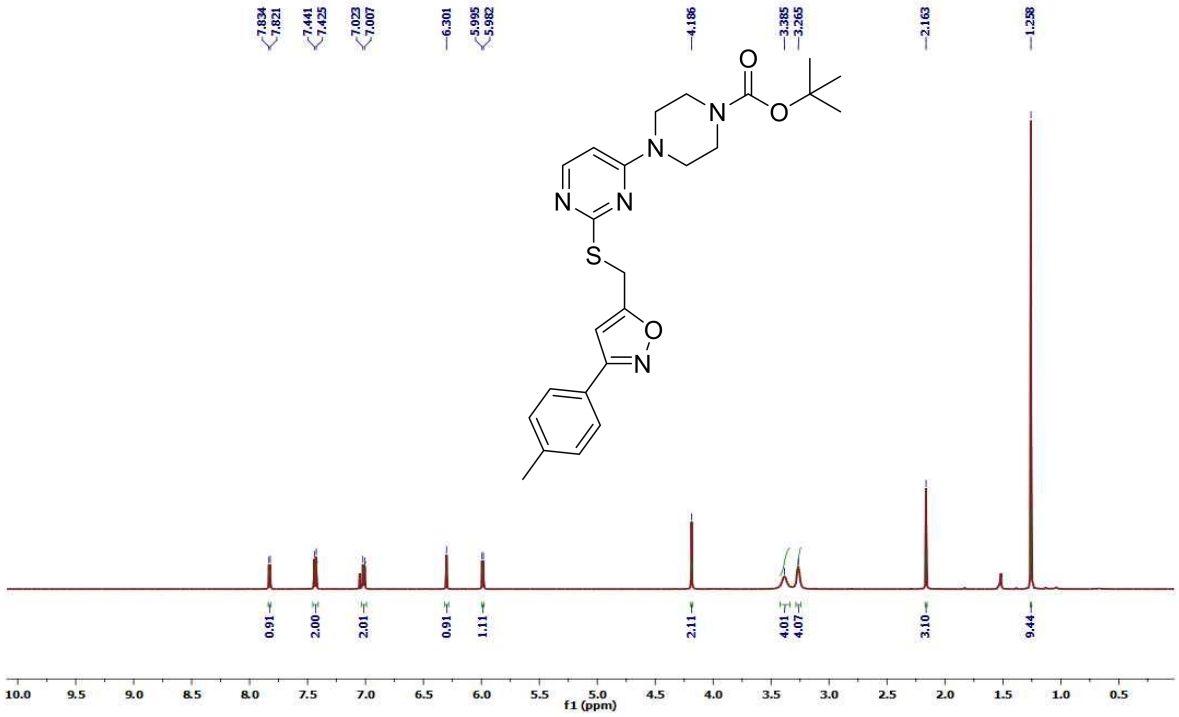
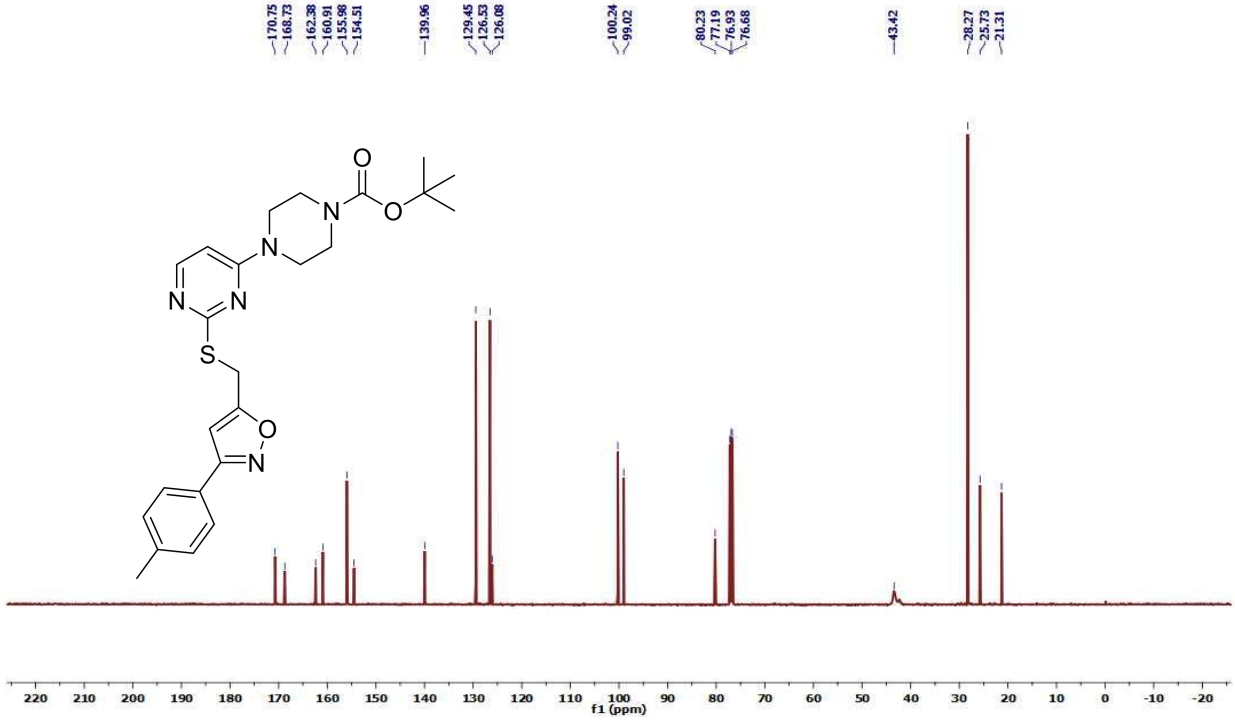


Mass spectrum of 6e



^{1}H NMR of 6f



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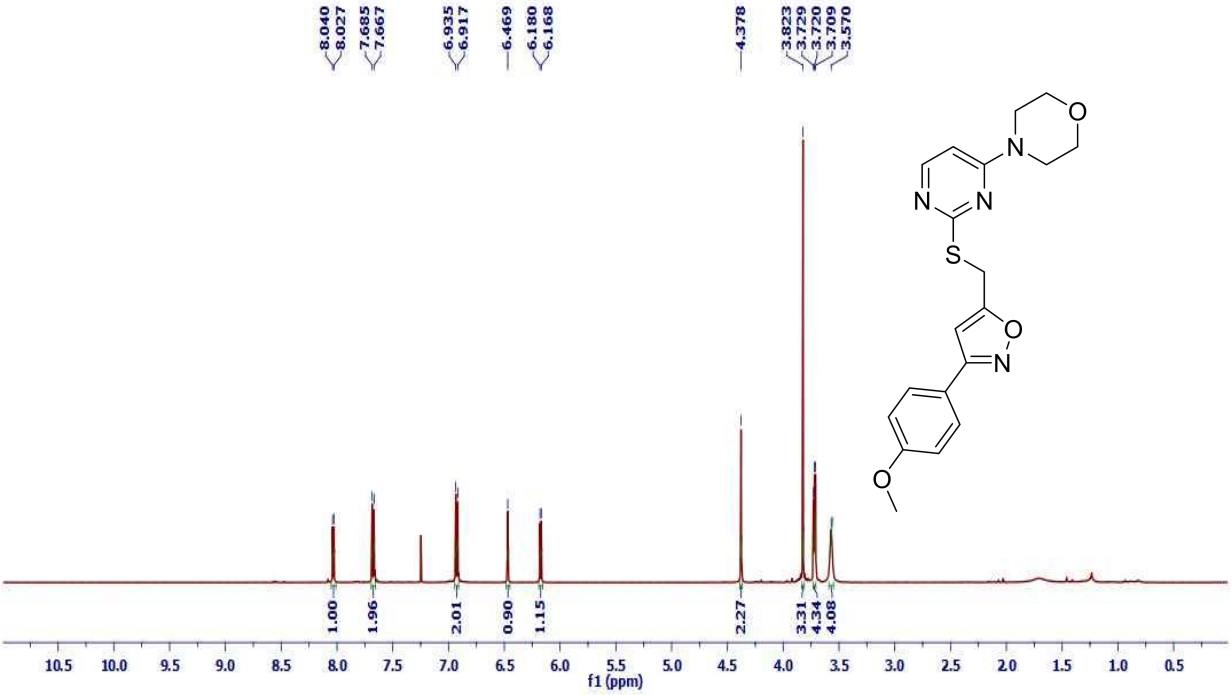

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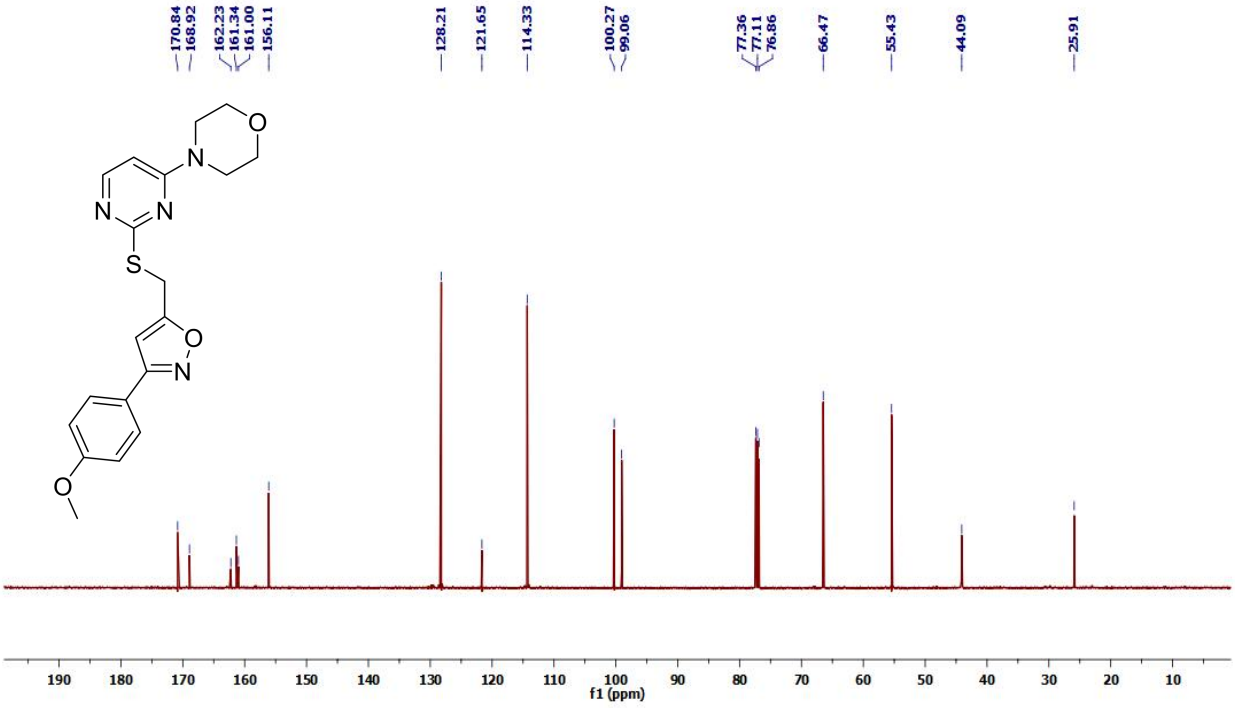

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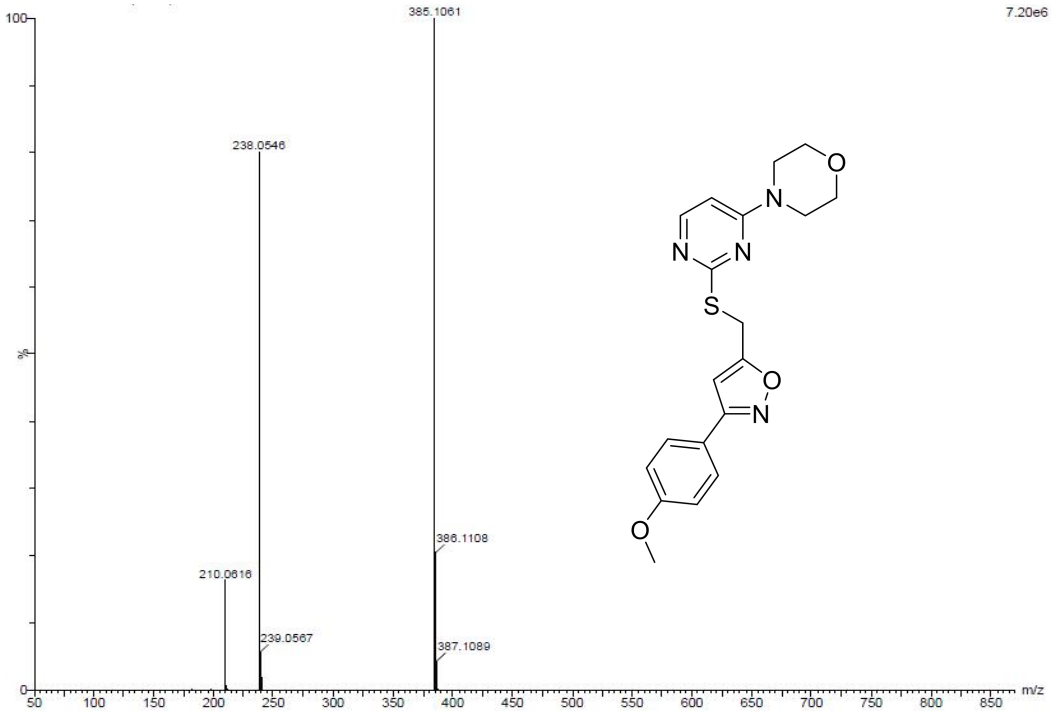
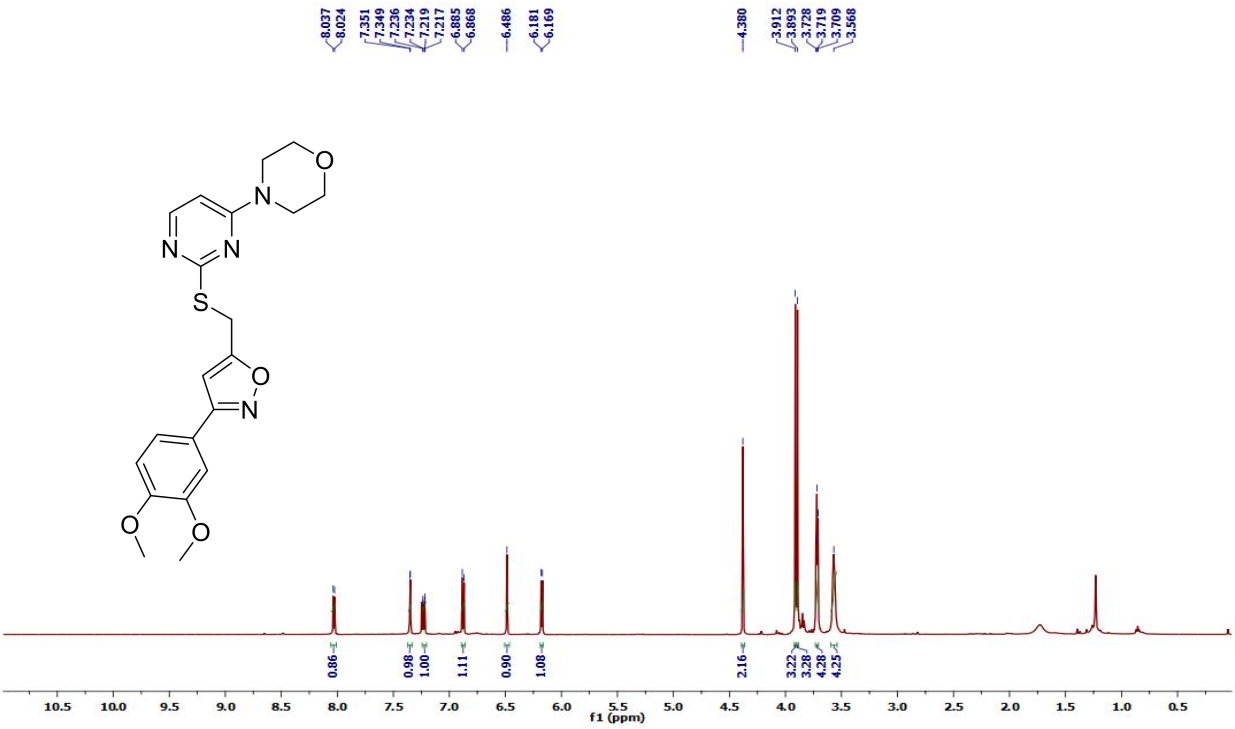


Mass spectrum of 6g



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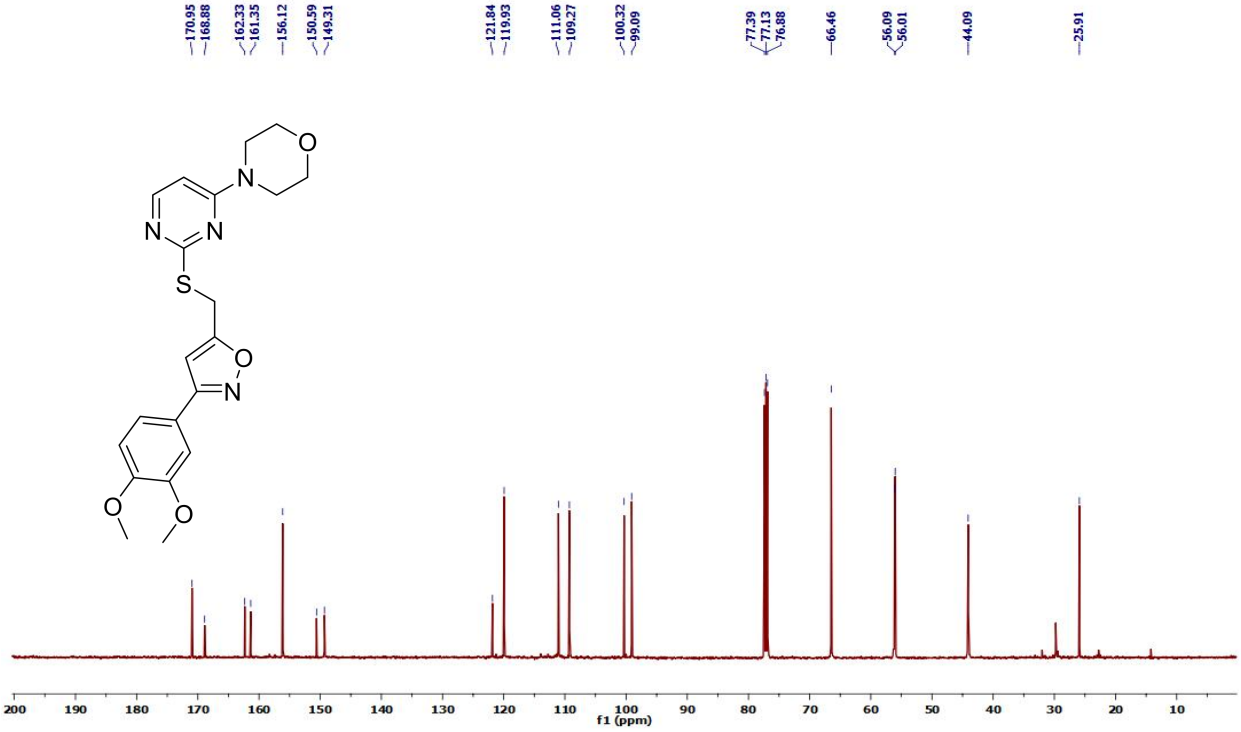

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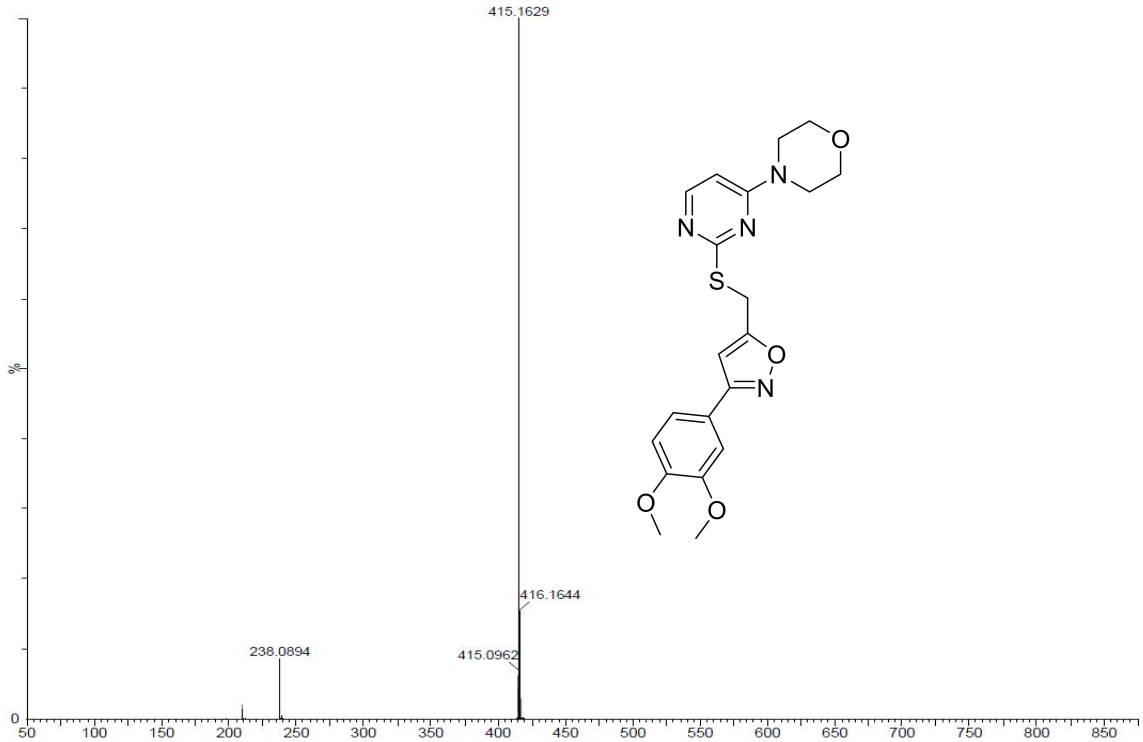
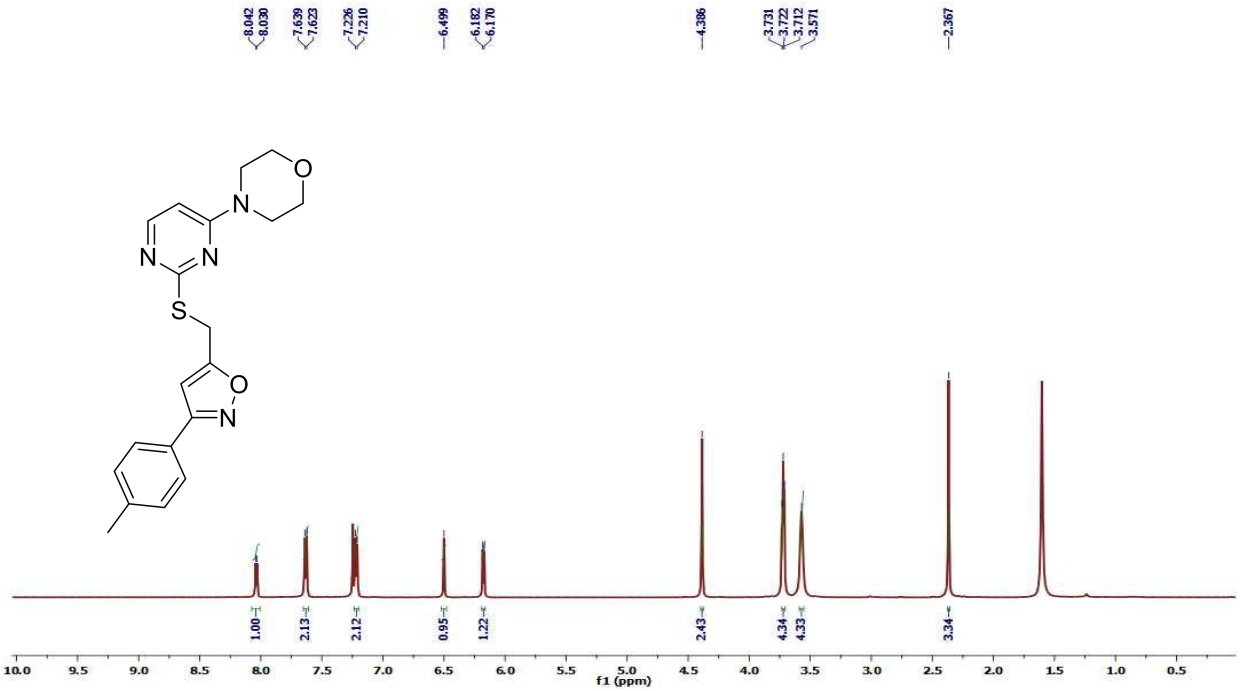
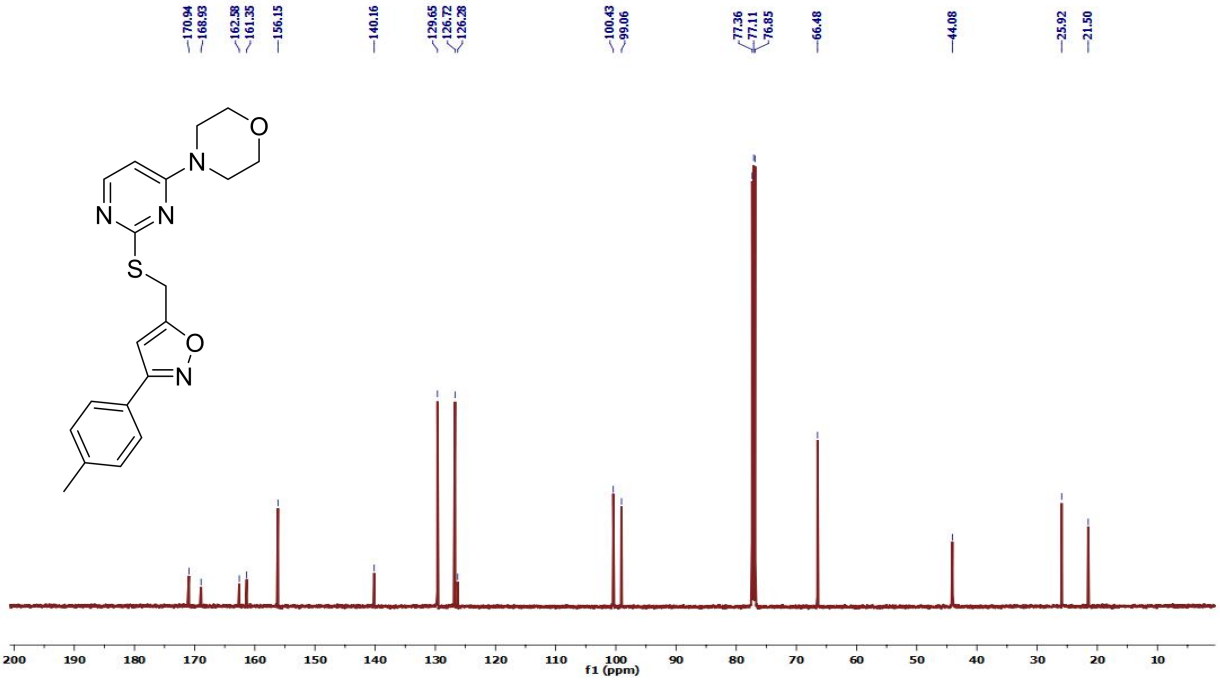


Mass spectrum of 6h



^{1}H NMR of 6i



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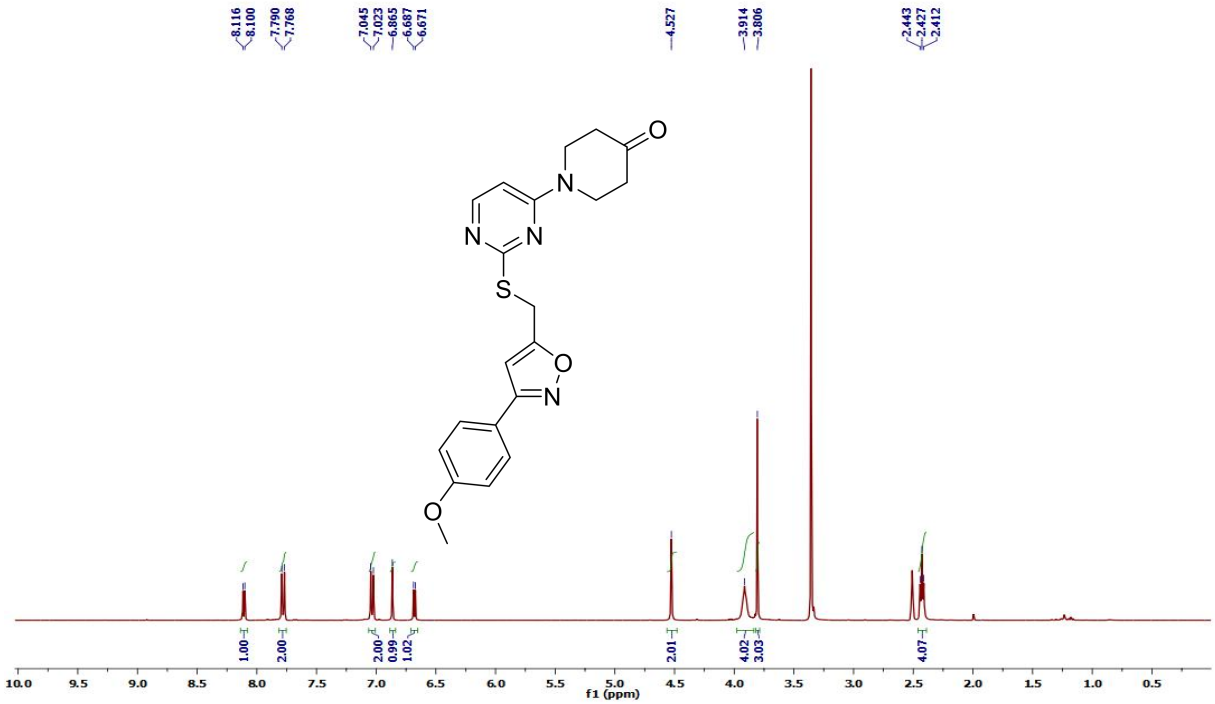

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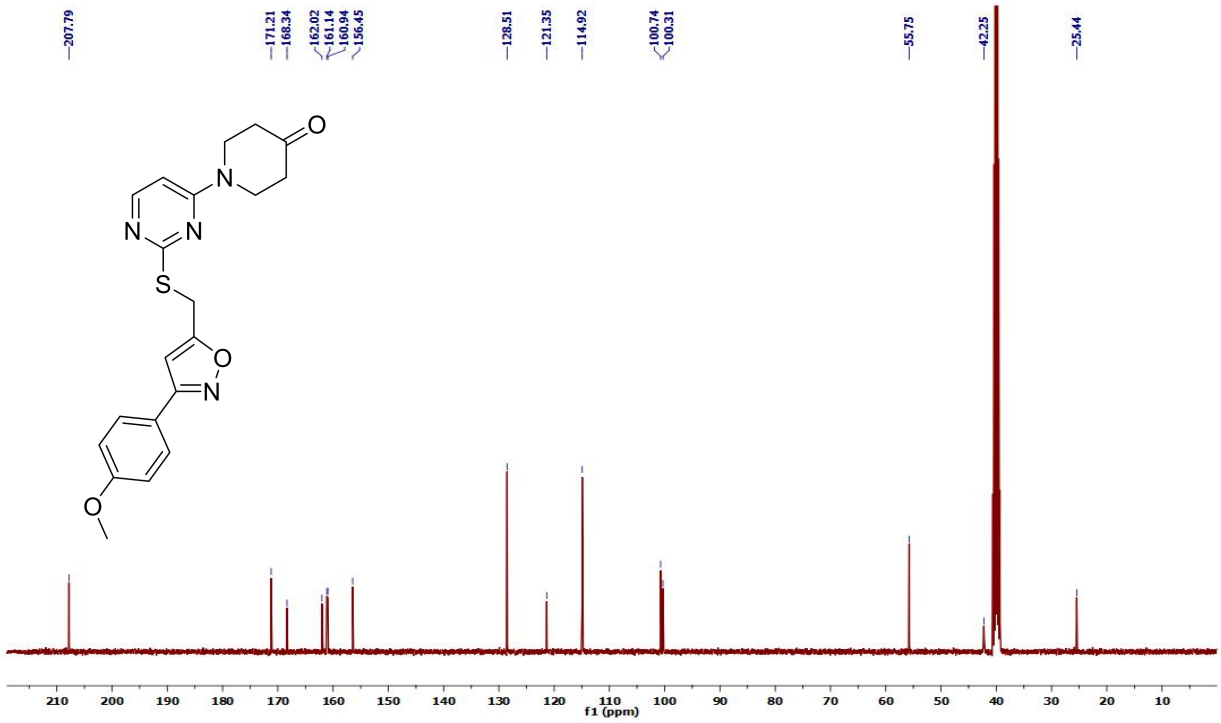

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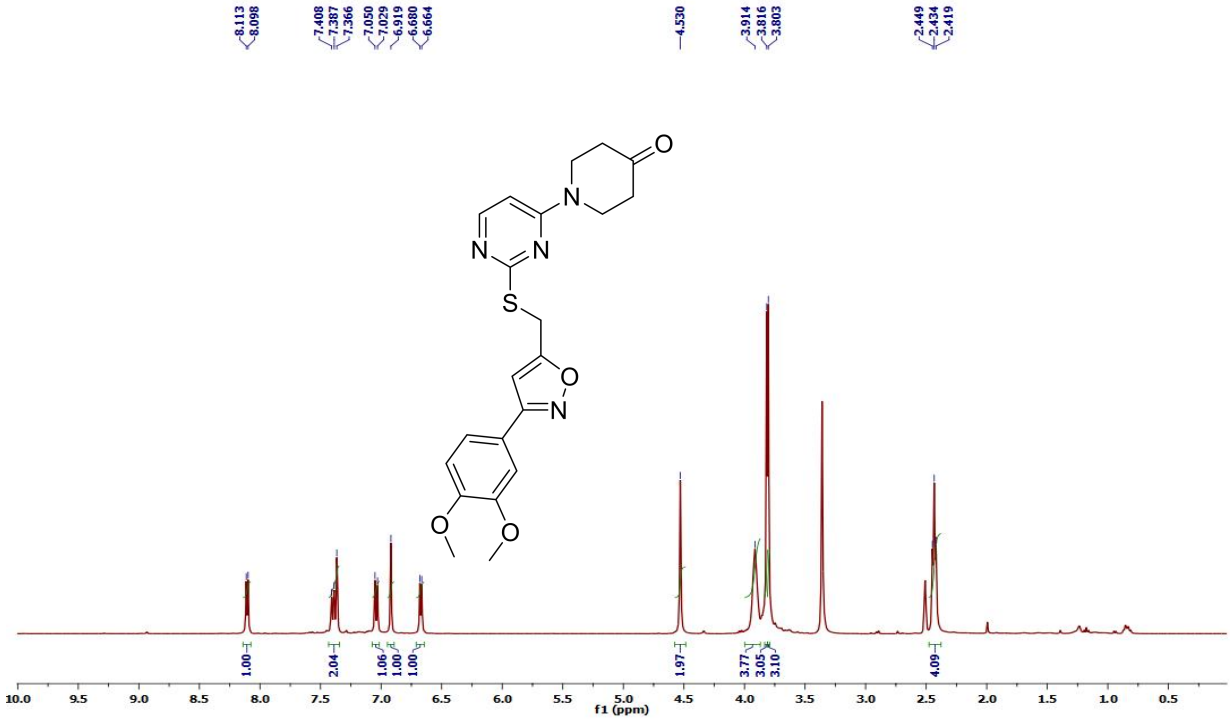

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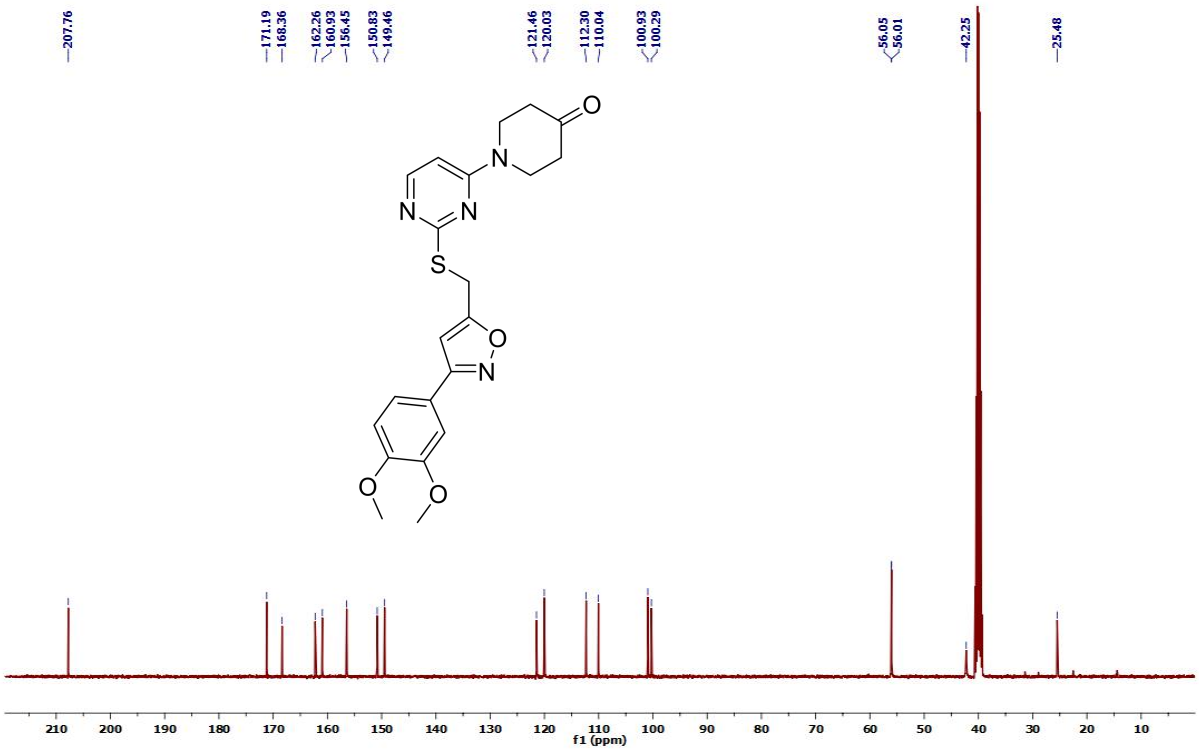

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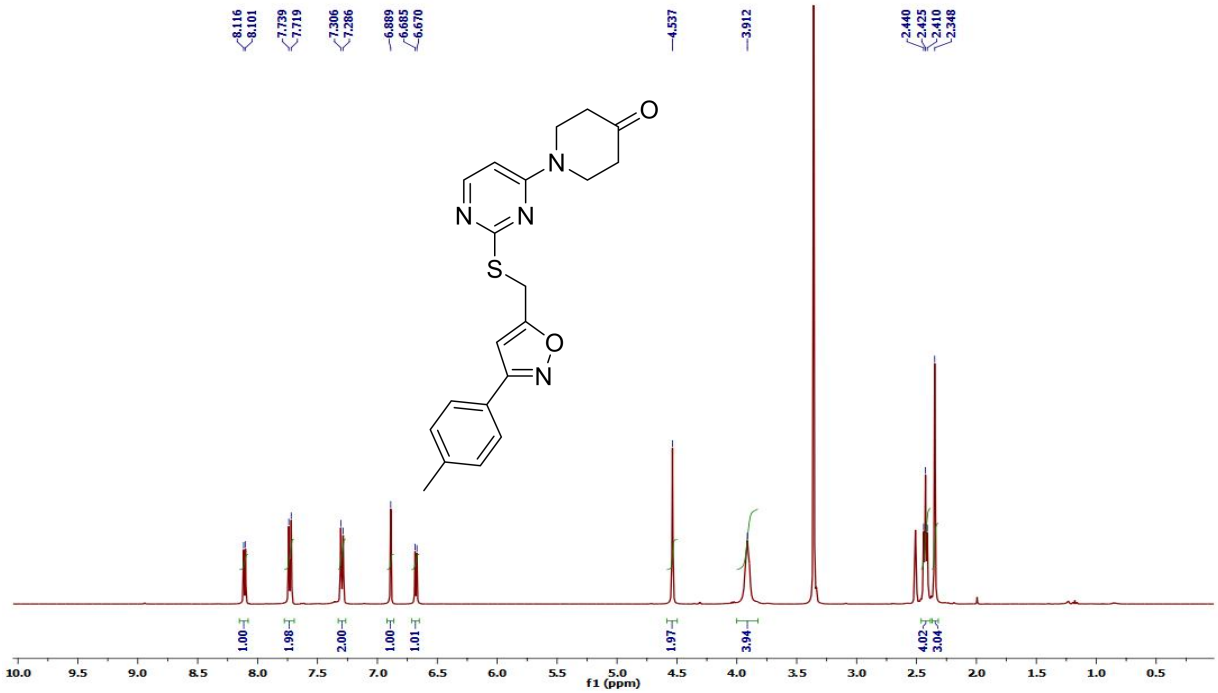

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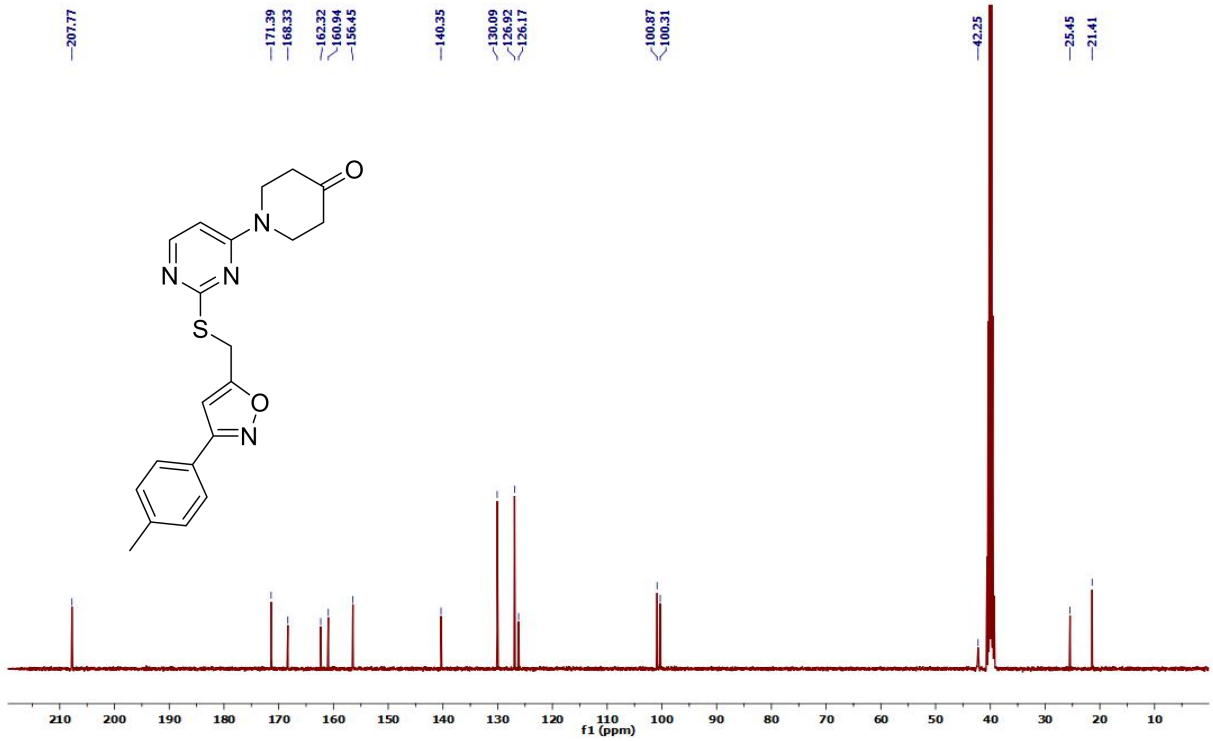

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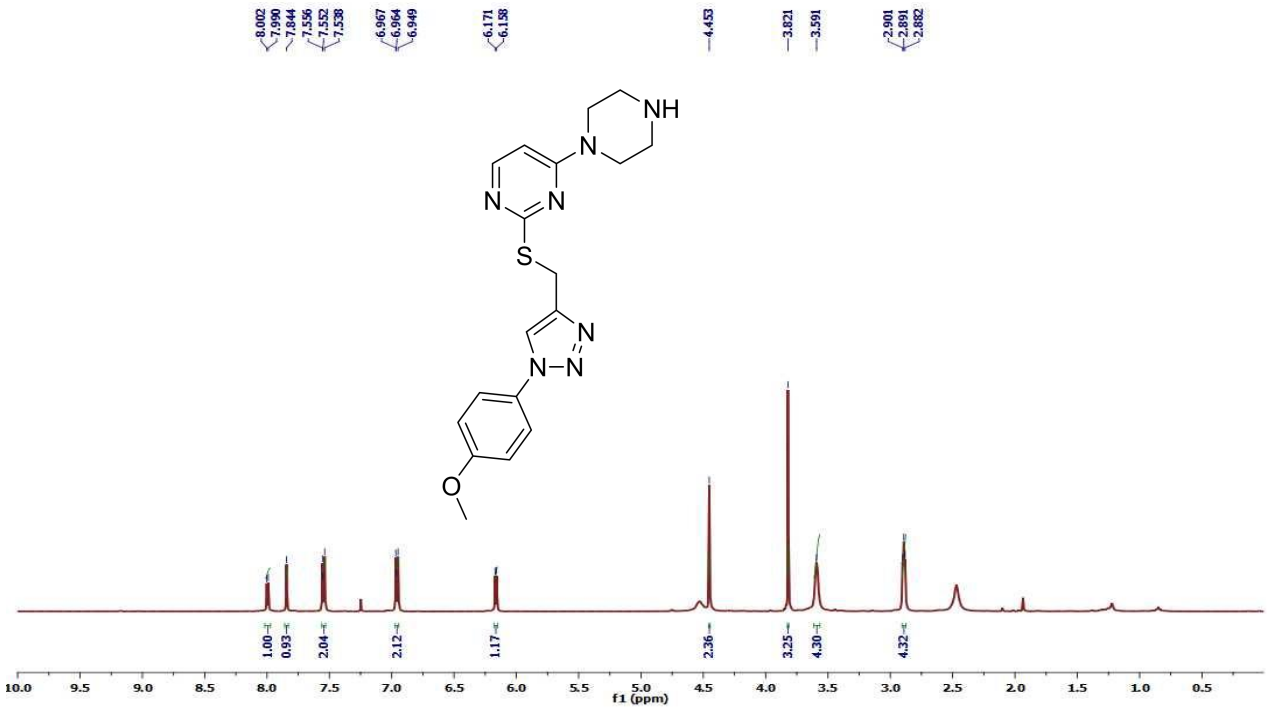
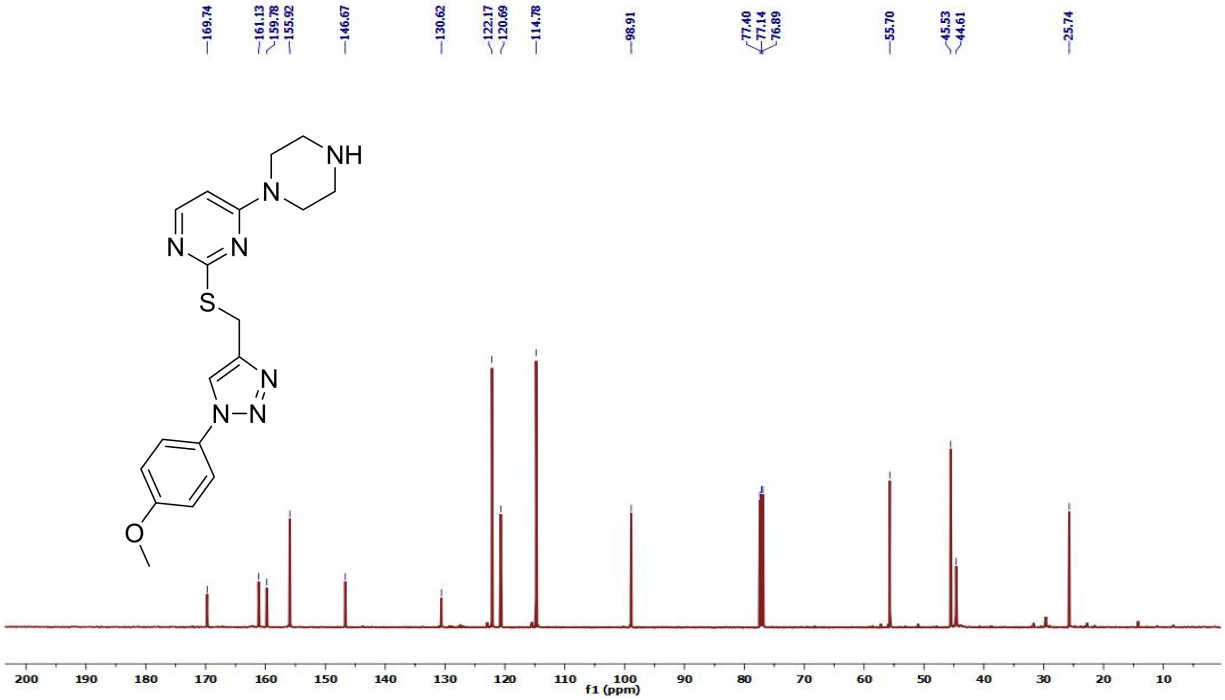
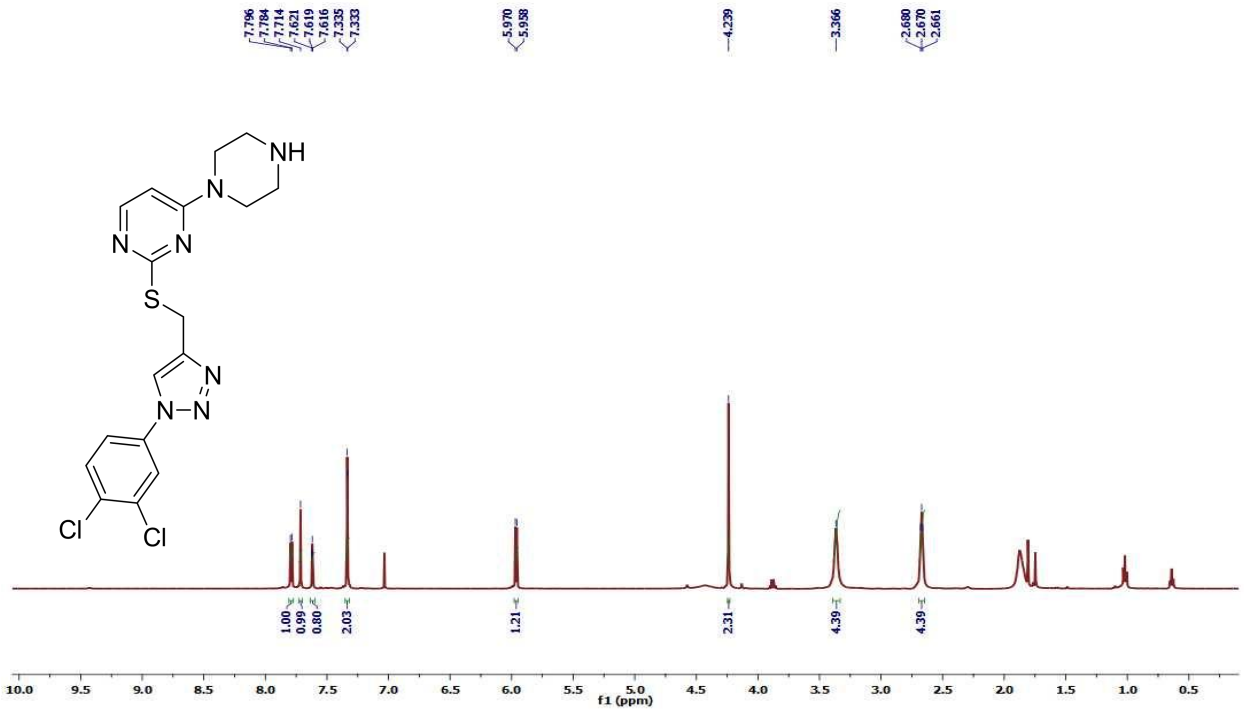


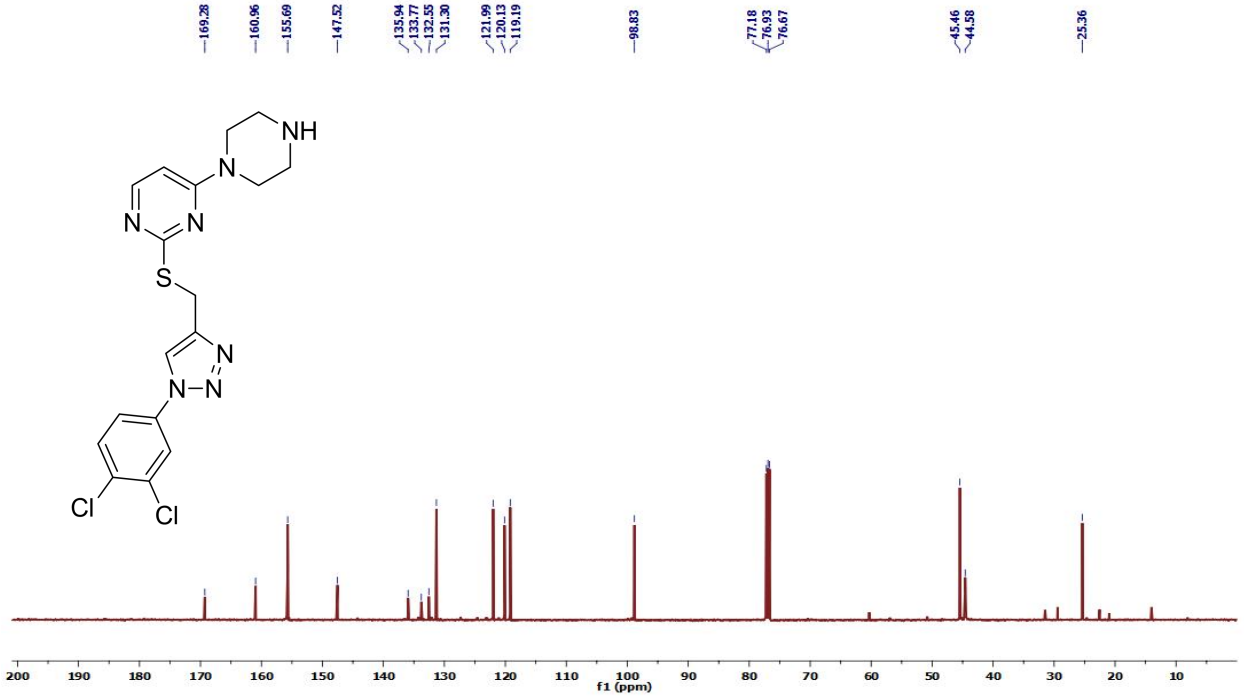
^{1}H NMR of 7a



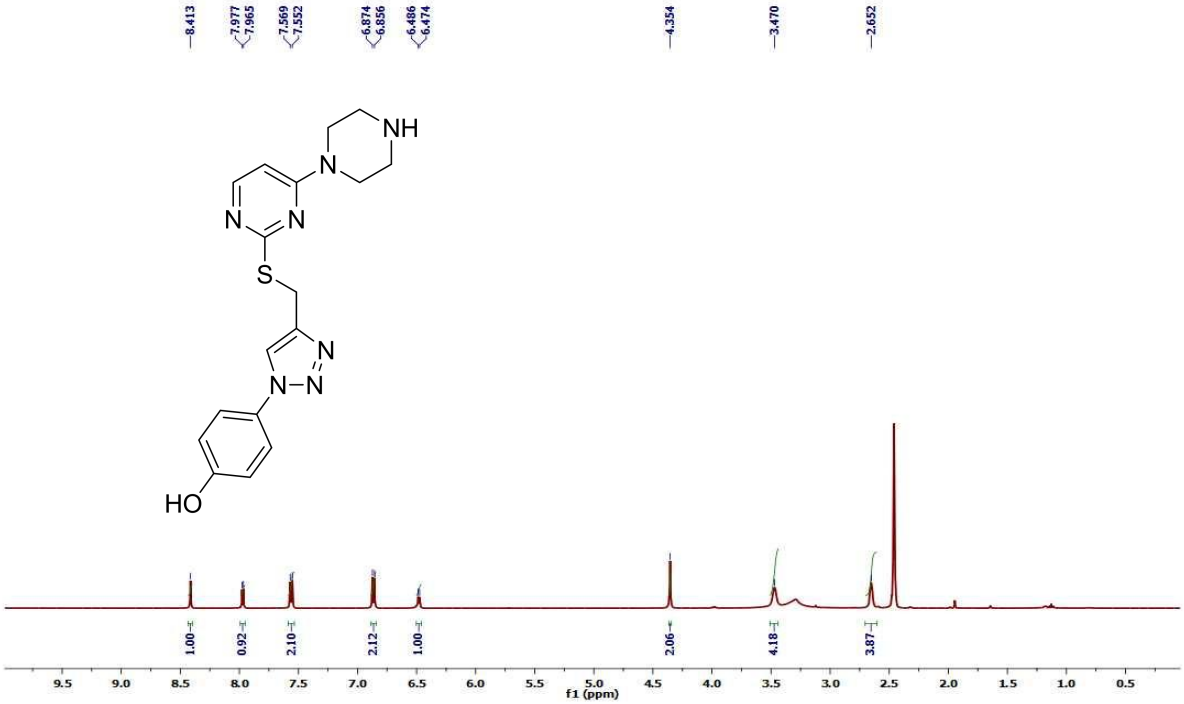
^{13}C NMR of 7a



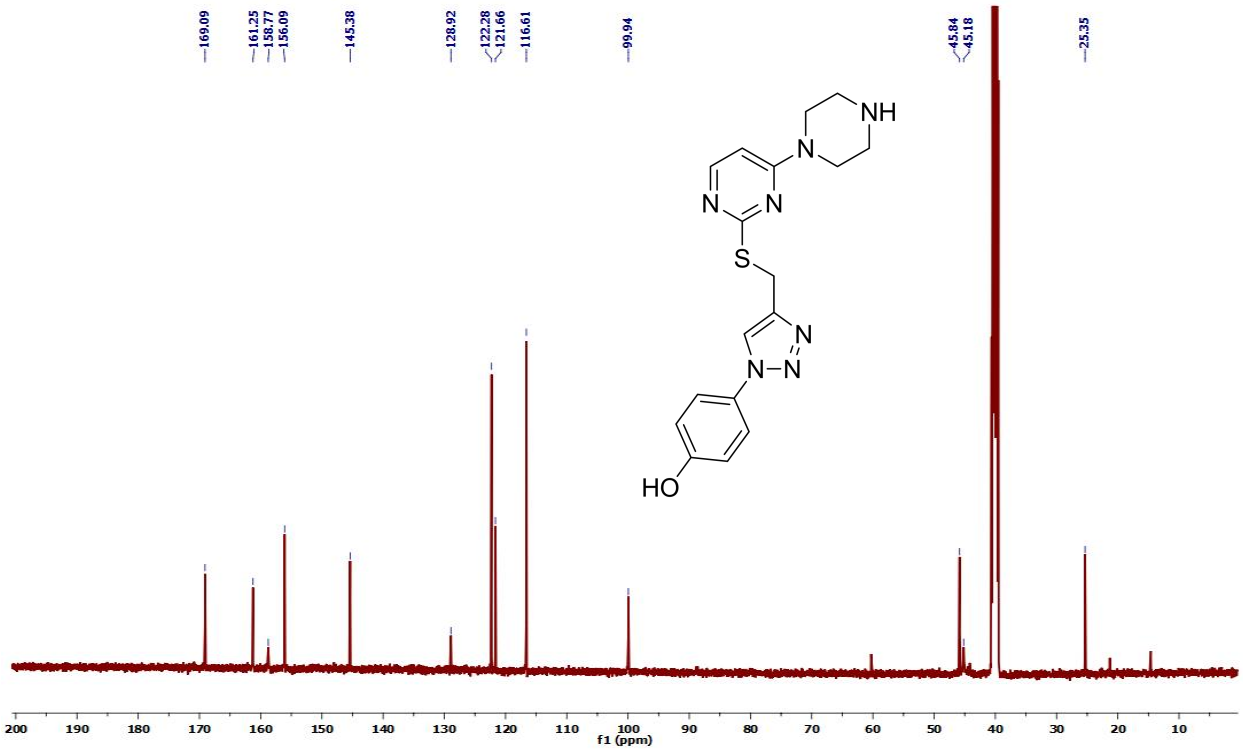
^{1}H NMR of 7b



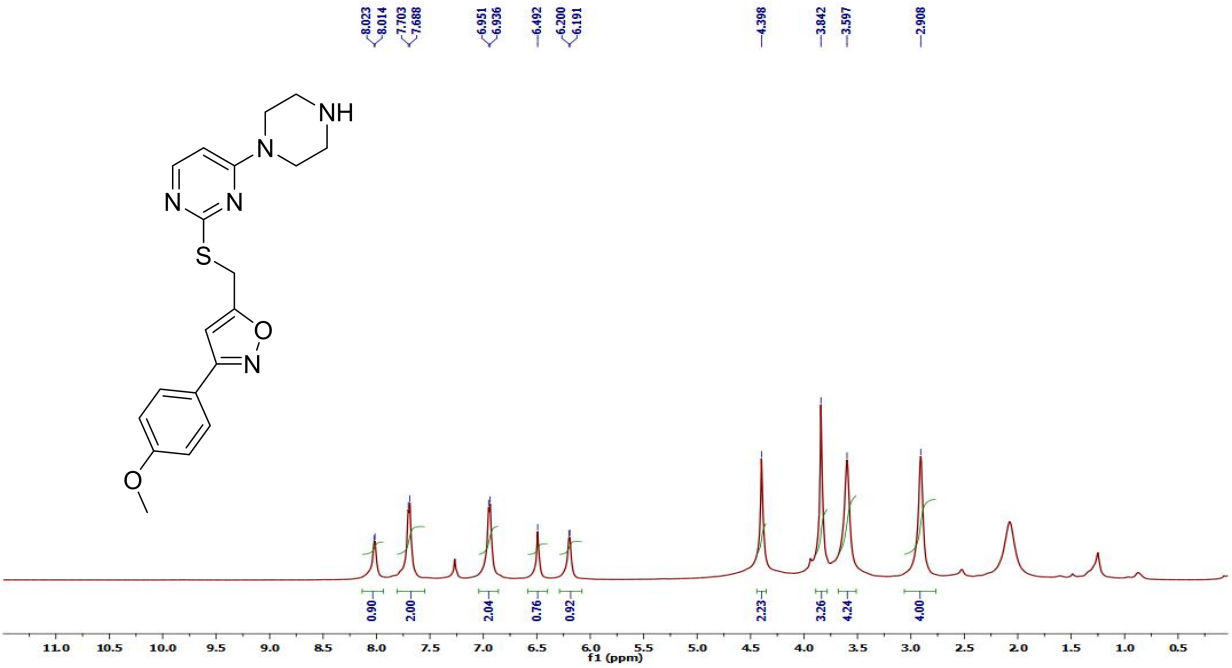
^{13}C NMR of 7b



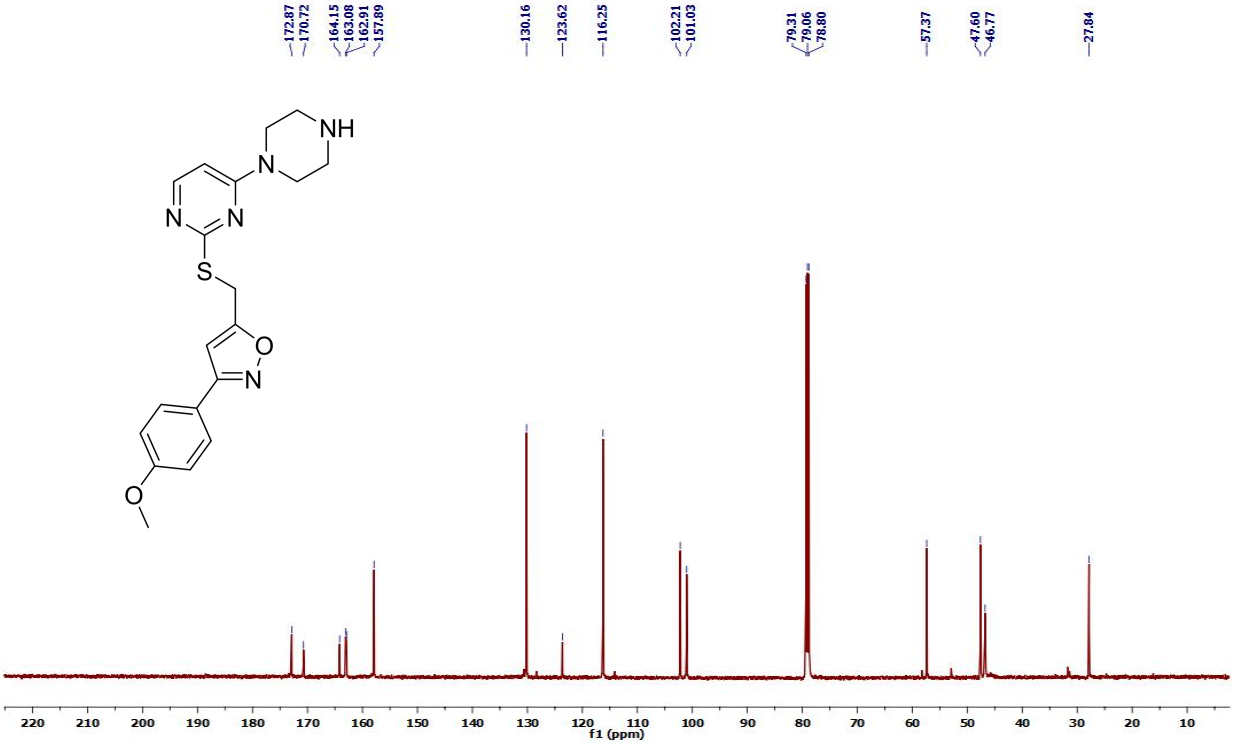
^{1}H NMR of 7c



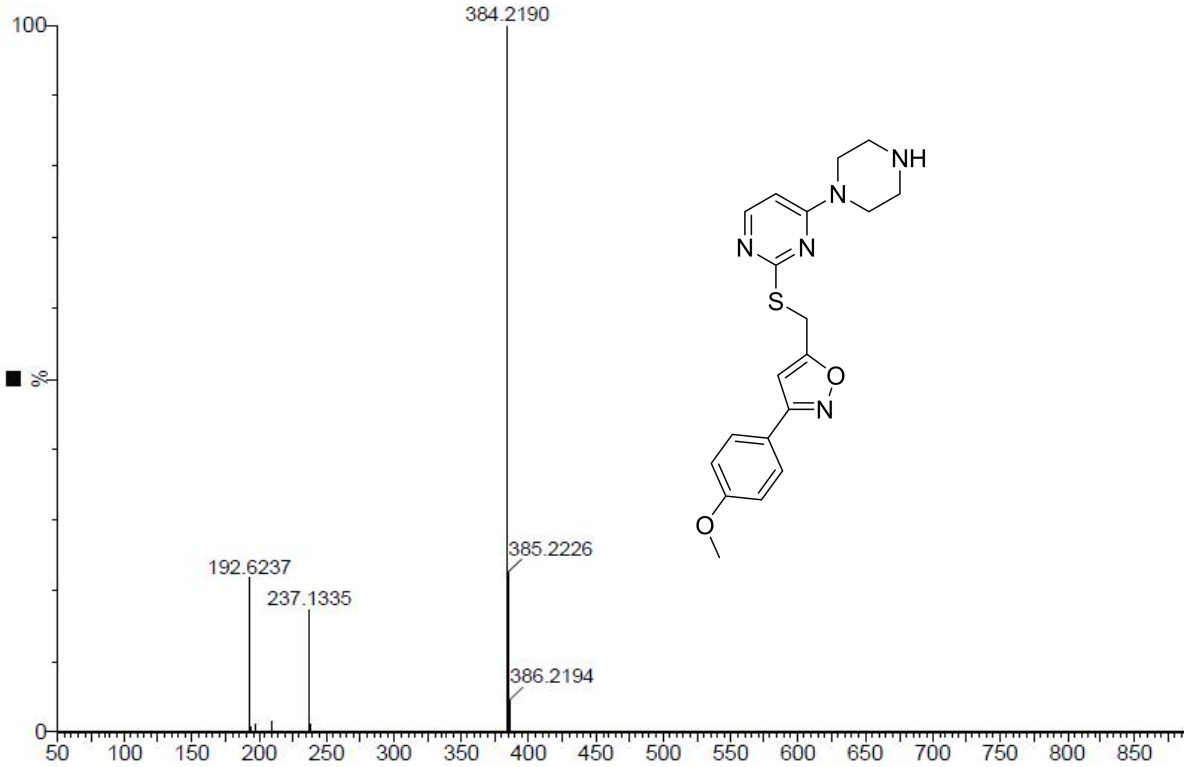
^{13}C NMR of 7c



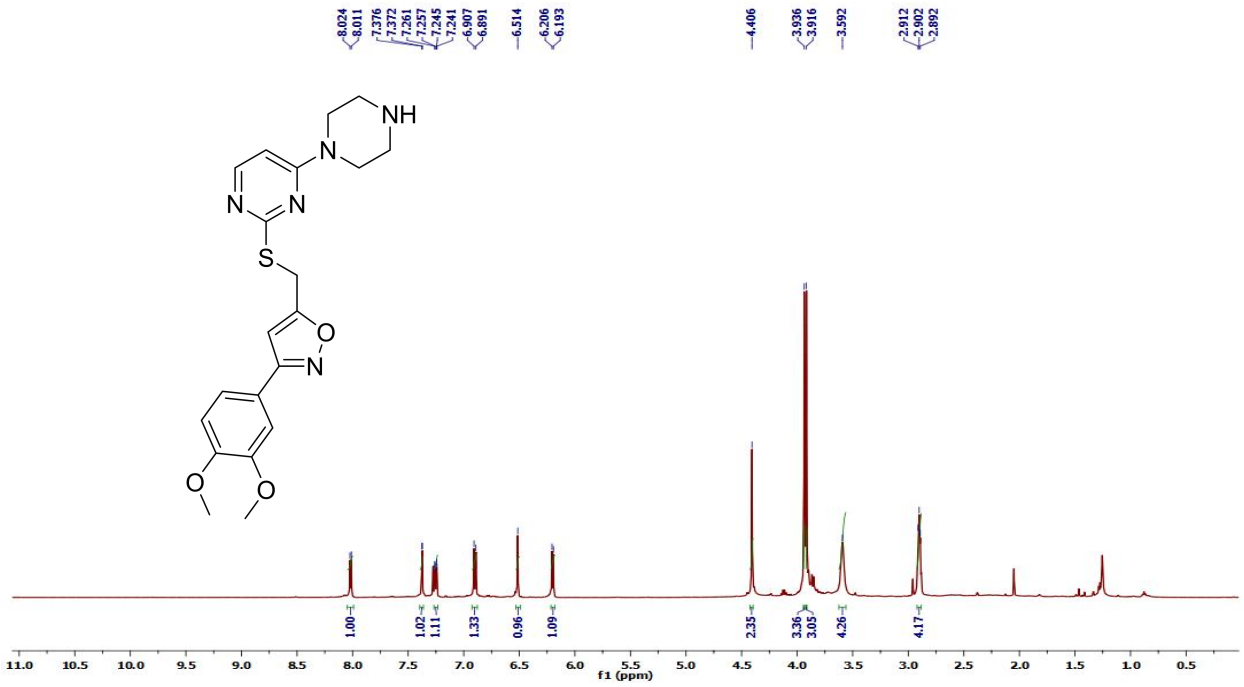
^{1}H NMR of 7d



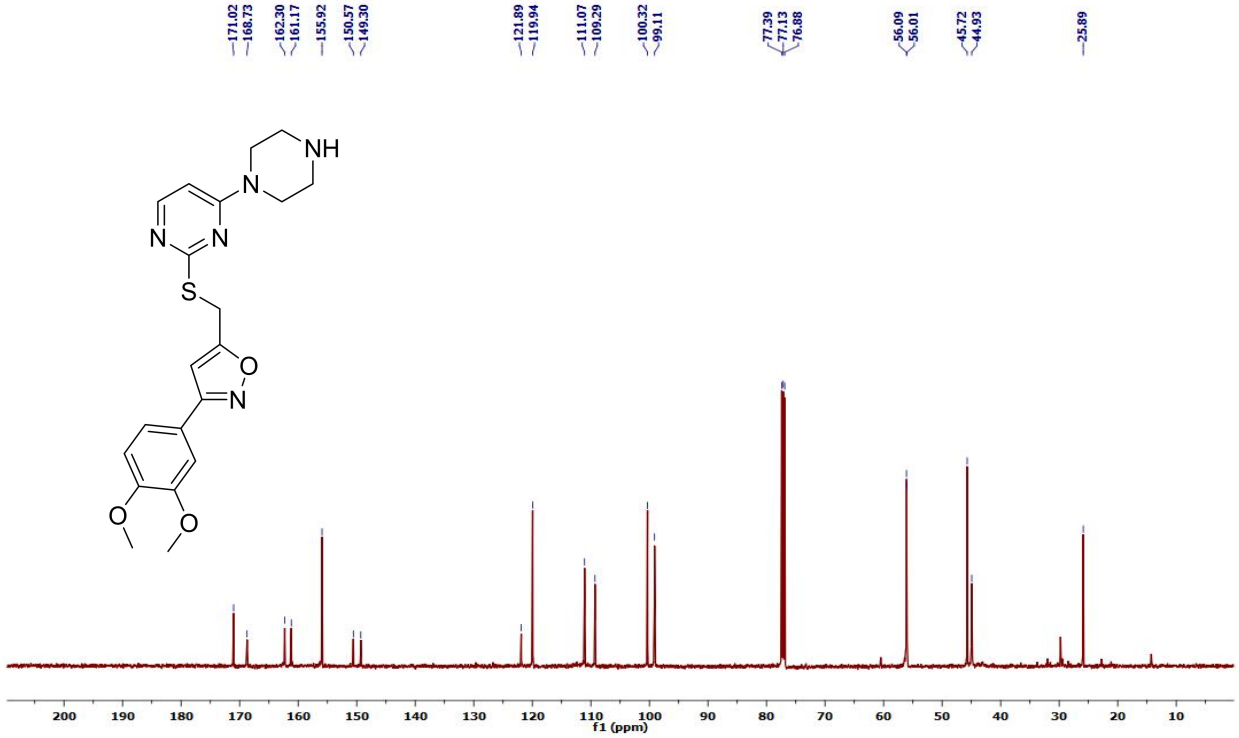
^{13}C NMR of 7d



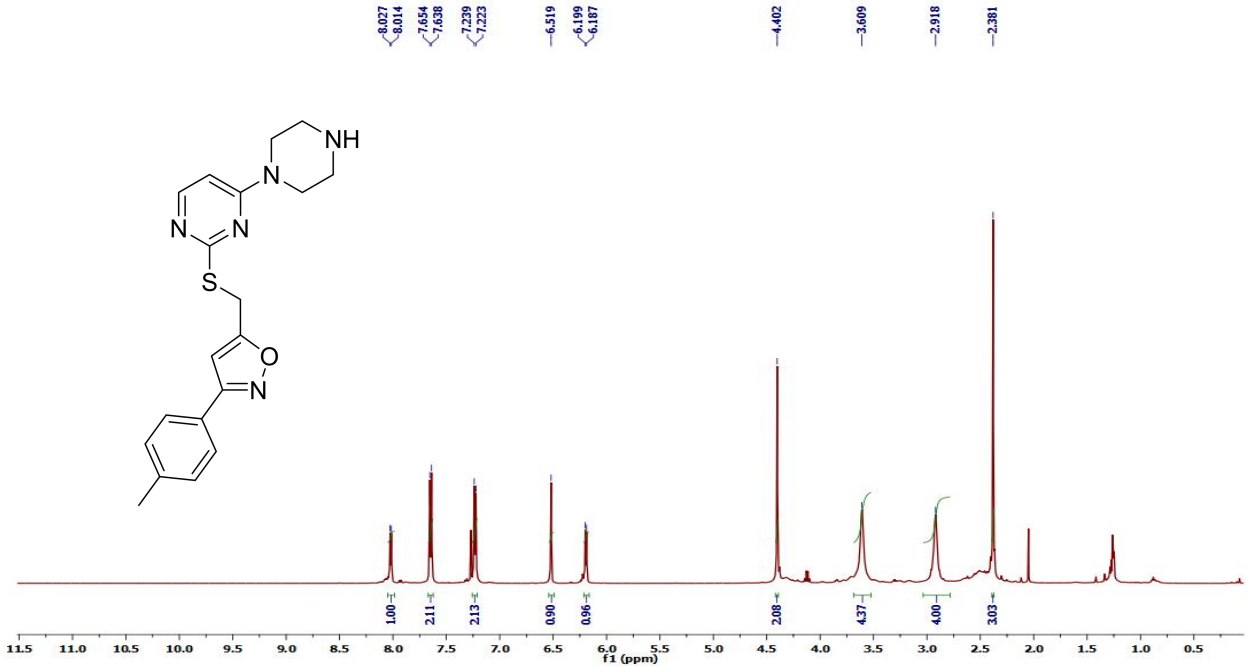
Mass spectrum of 7d



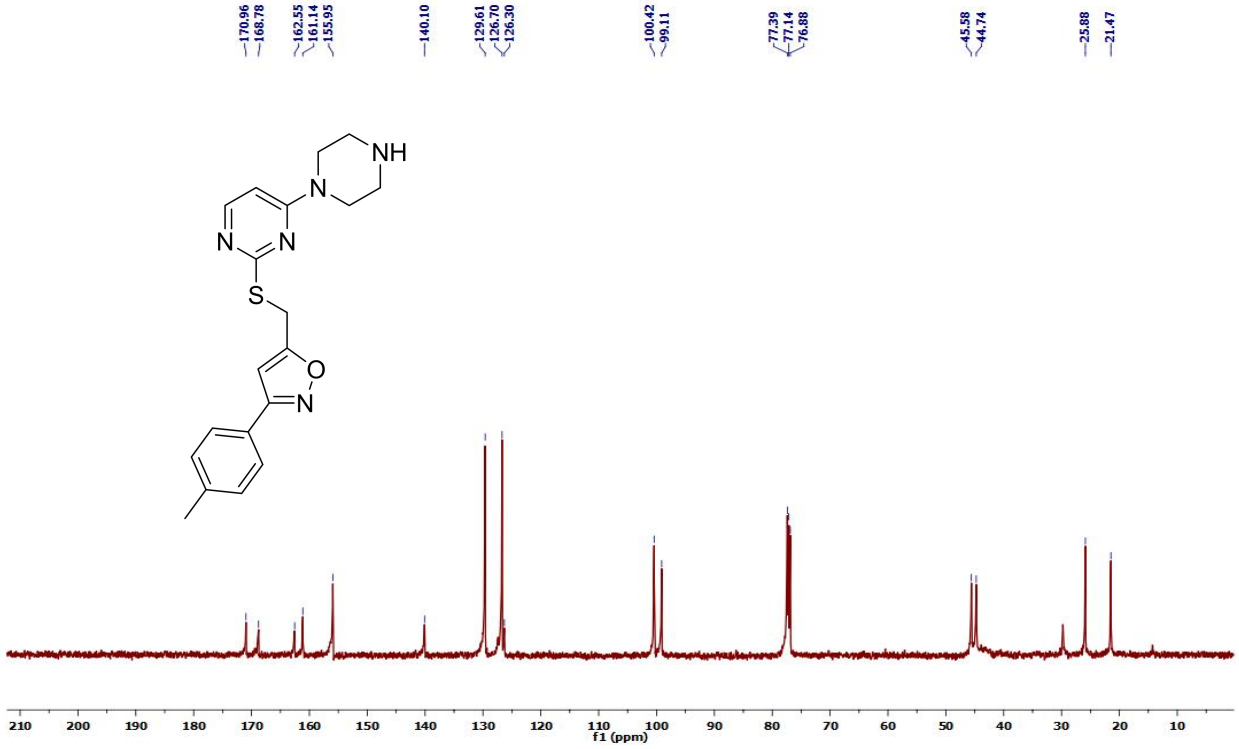
^{1}H NMR of 7e



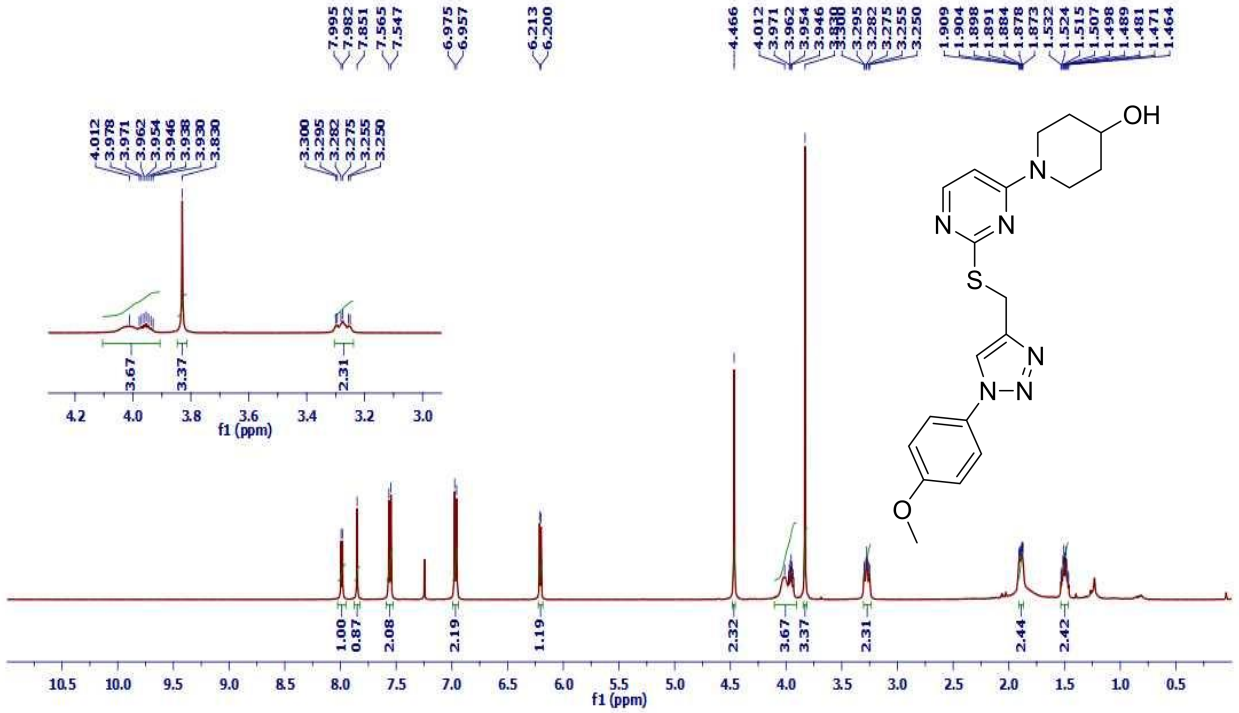
^{13}C NMR of 7e



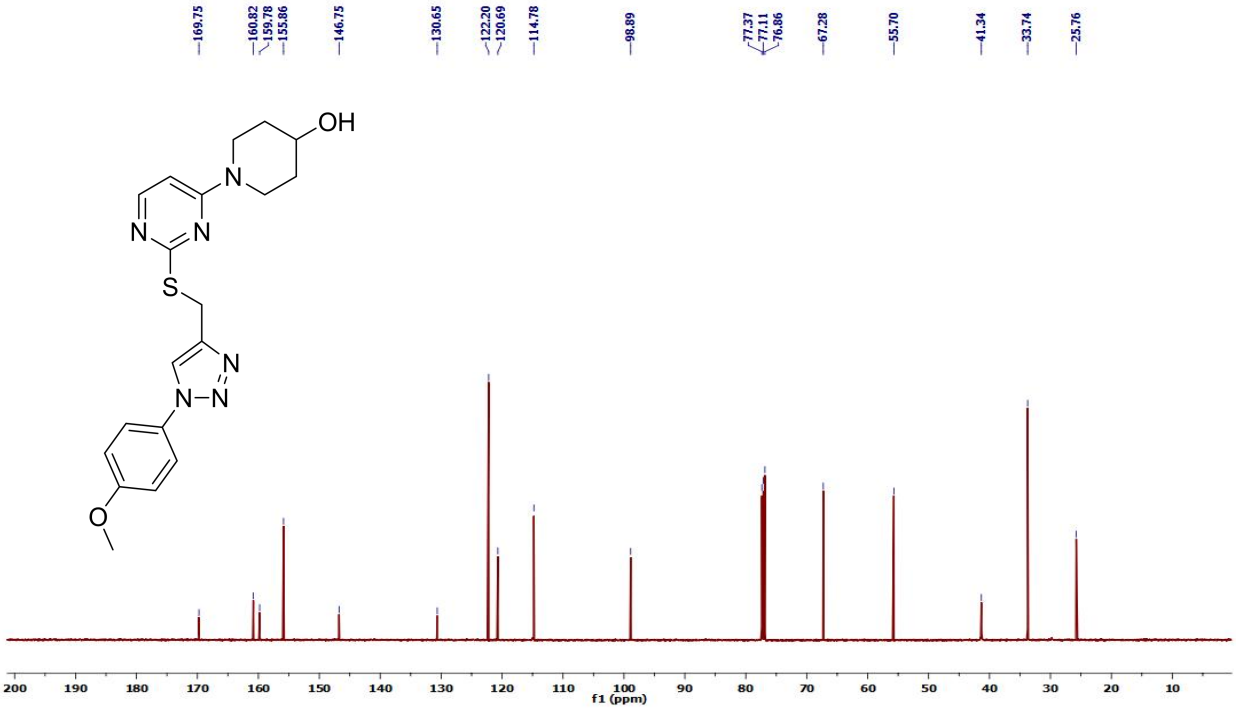
^{1}H NMR of 7f



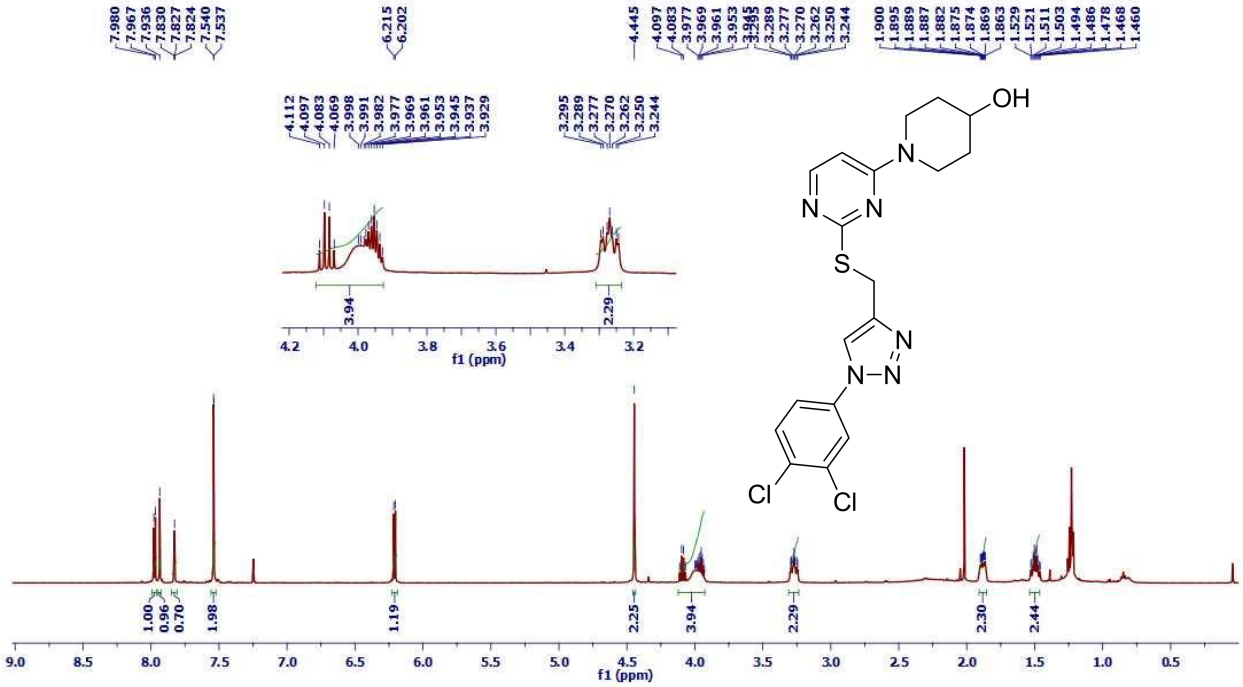
^{13}C NMR of 7f



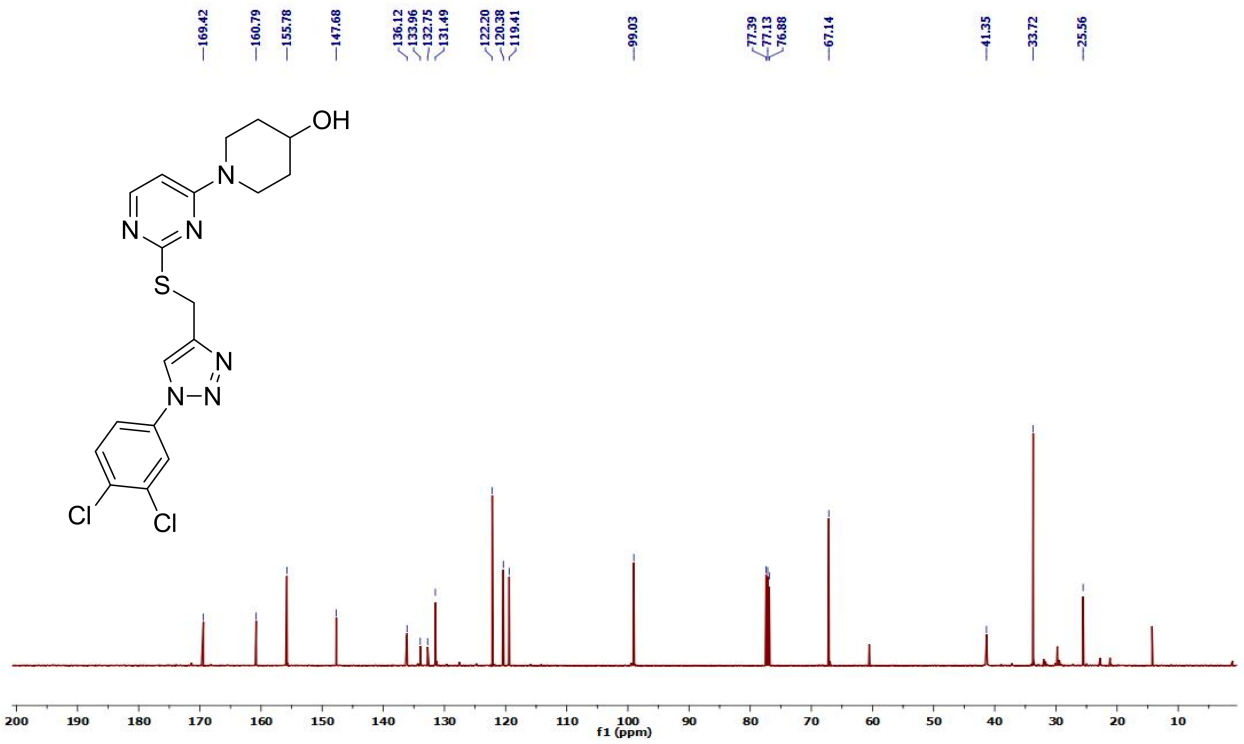
^{1}H NMR of 8a



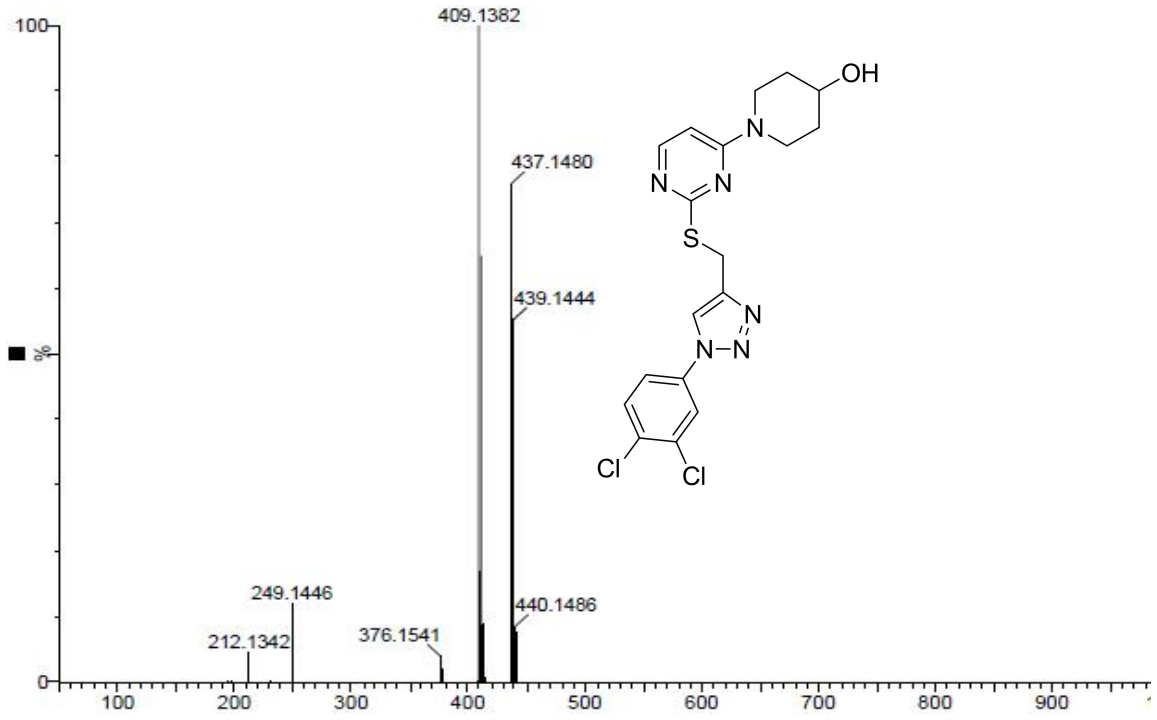
^{13}C NMR of 8a



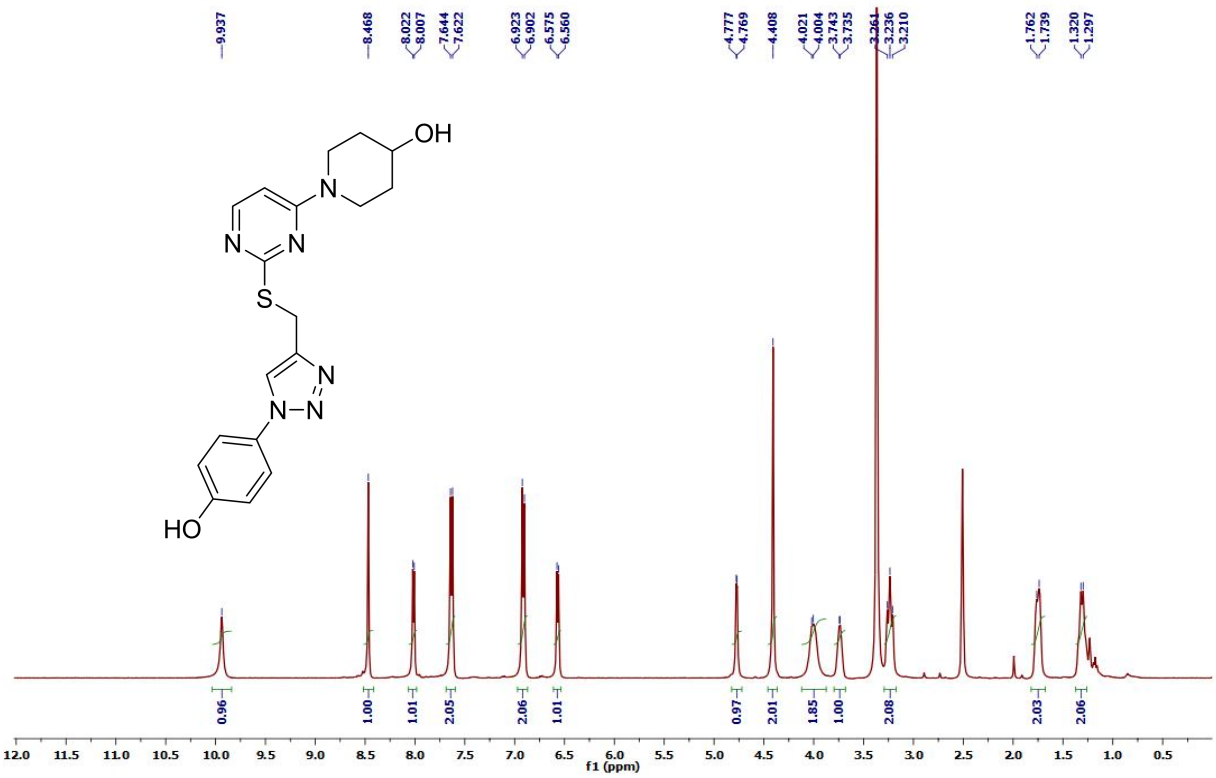
^{1}H NMR of 8b



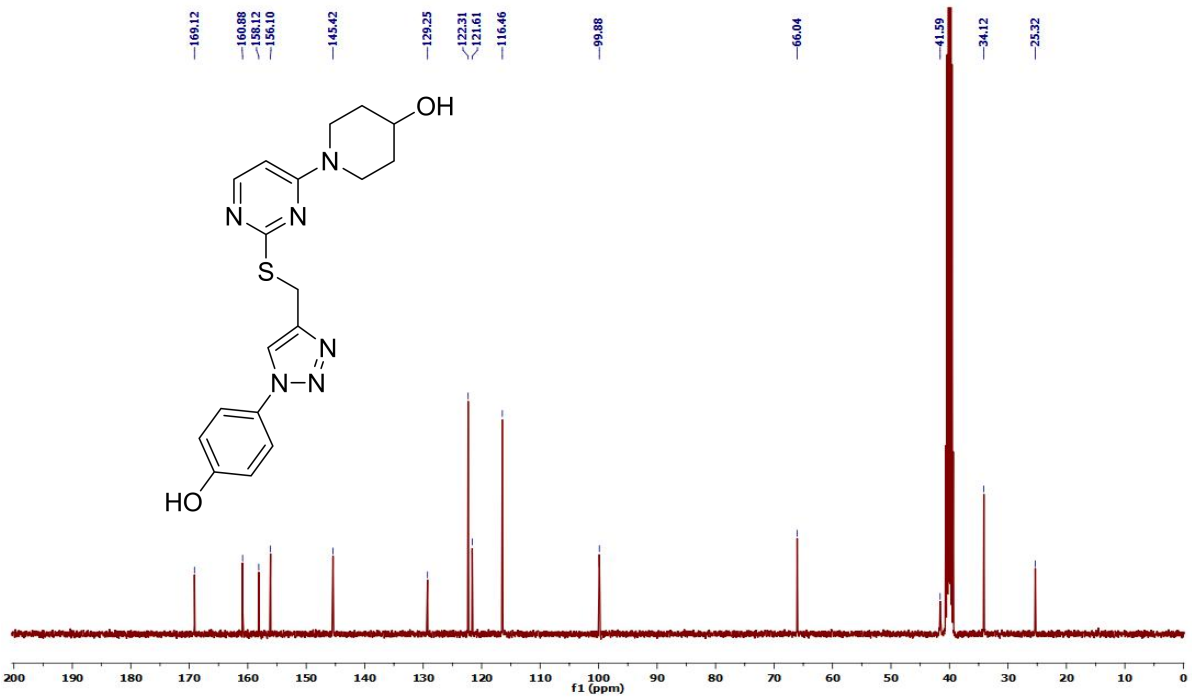
^{13}C NMR of 8b



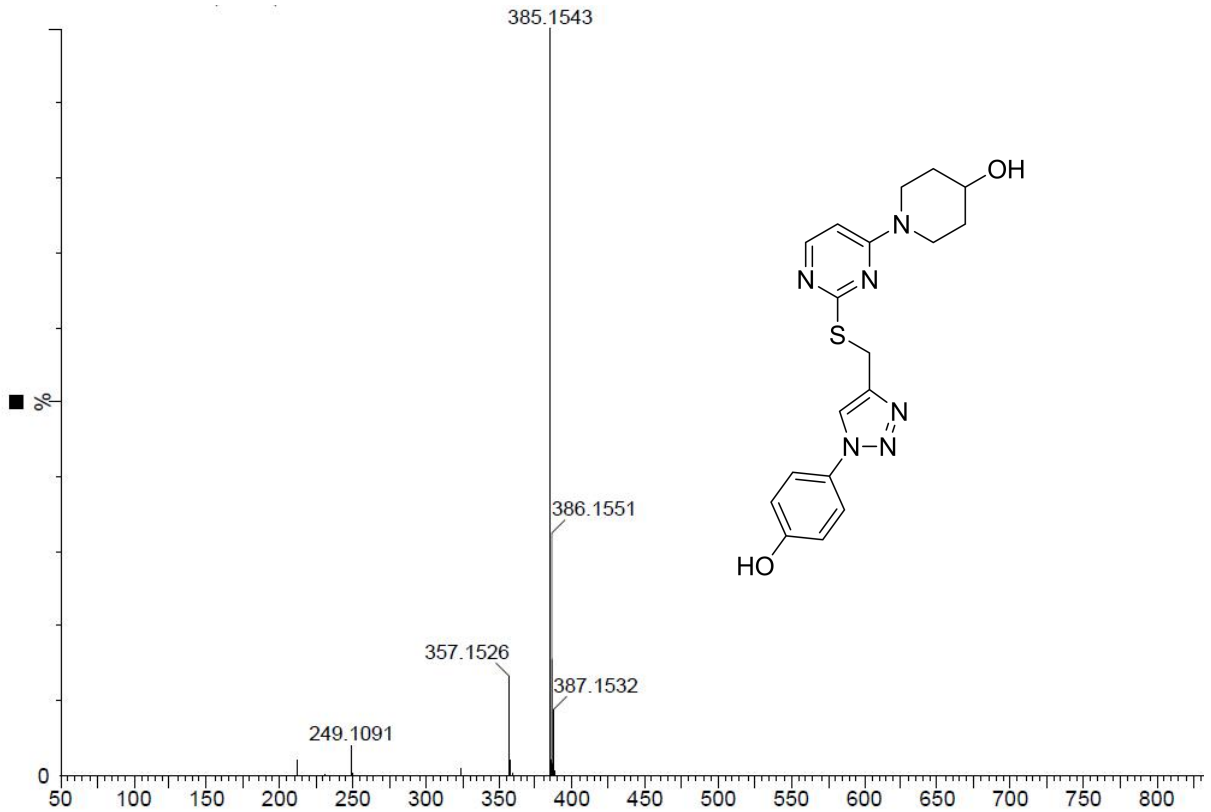
Mass spectrum of 8b



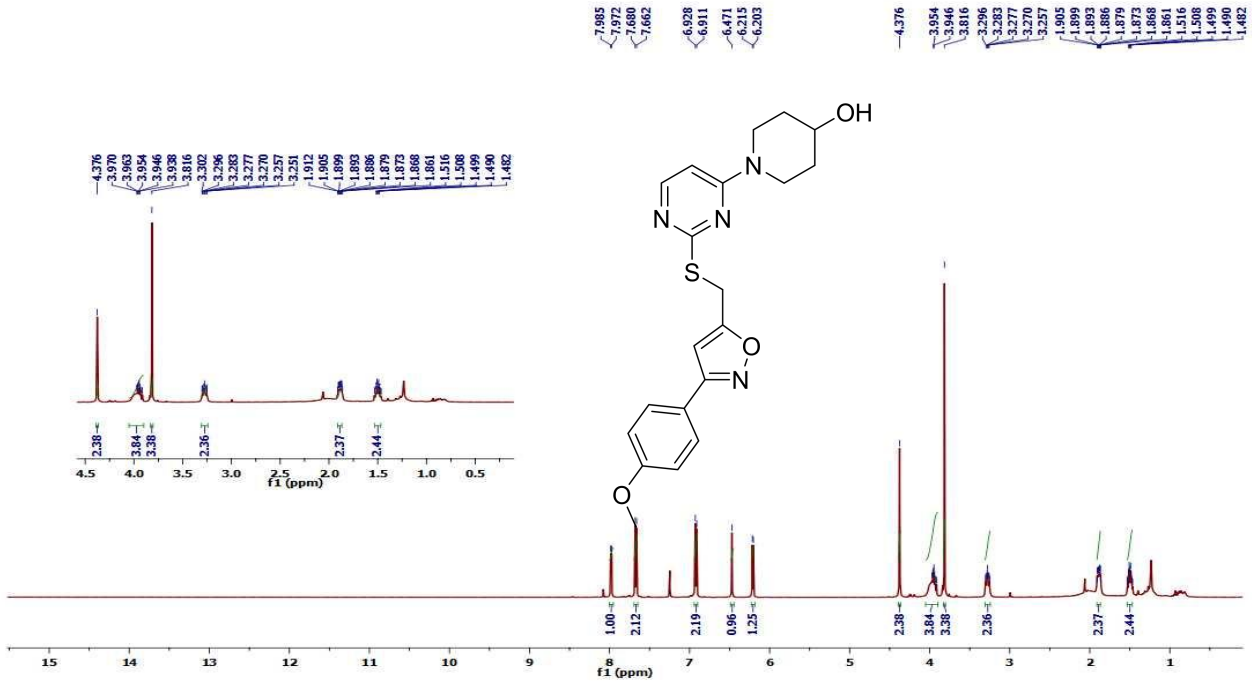
^{1}H NMR of 8c



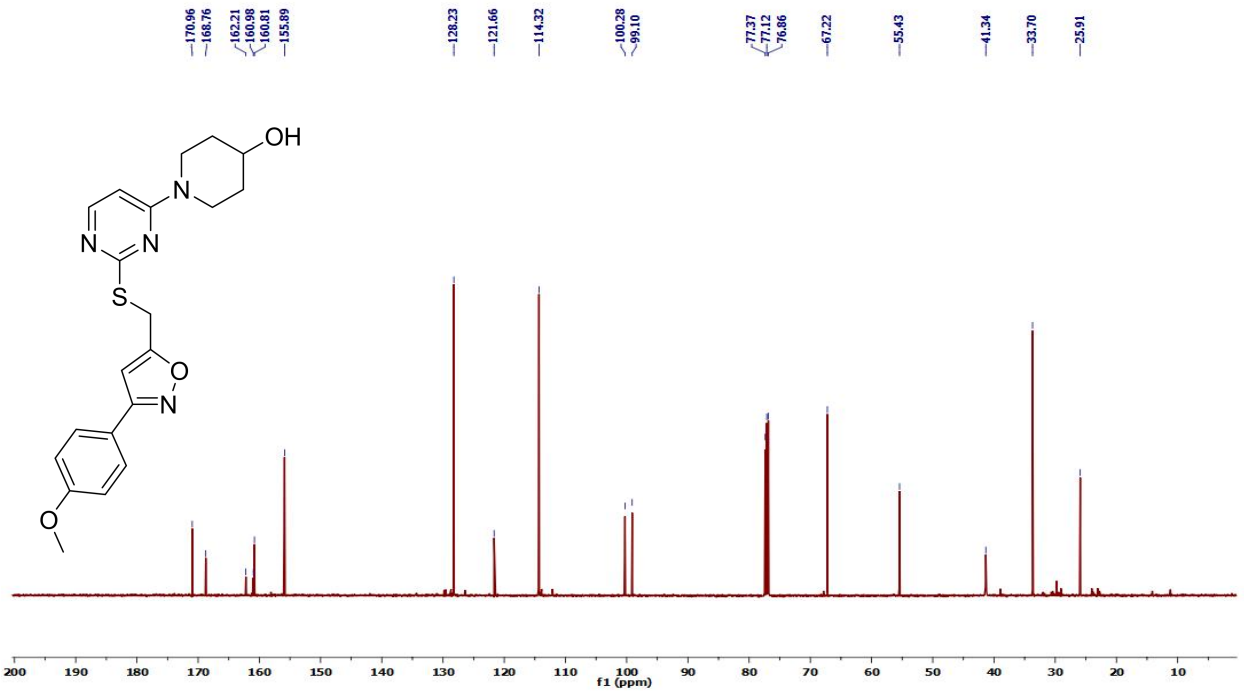
^{13}C NMR of 8c



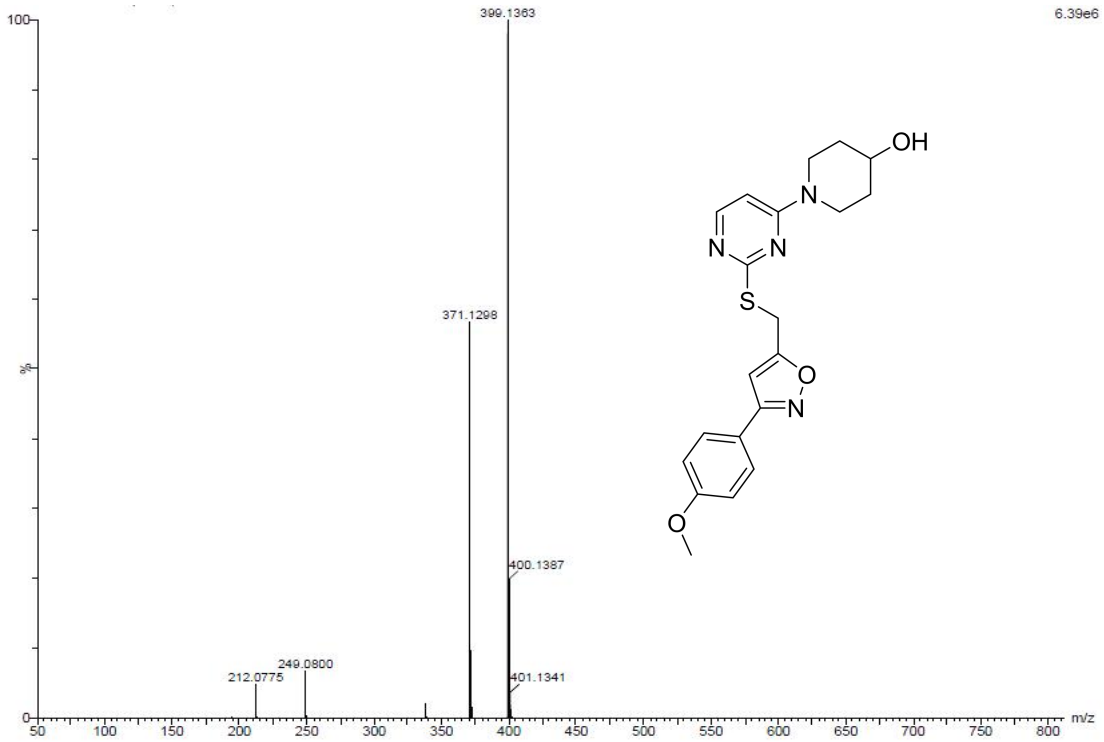
Mass spectrum of 8c



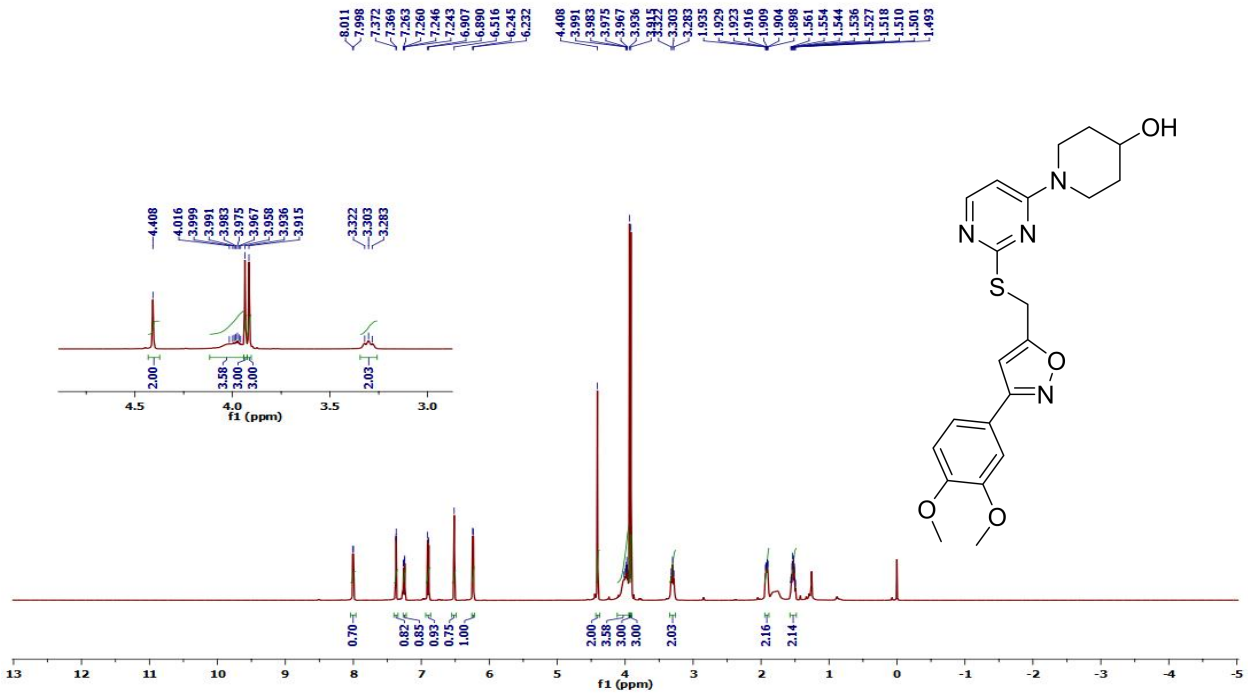
^{1}H NMR of 8d



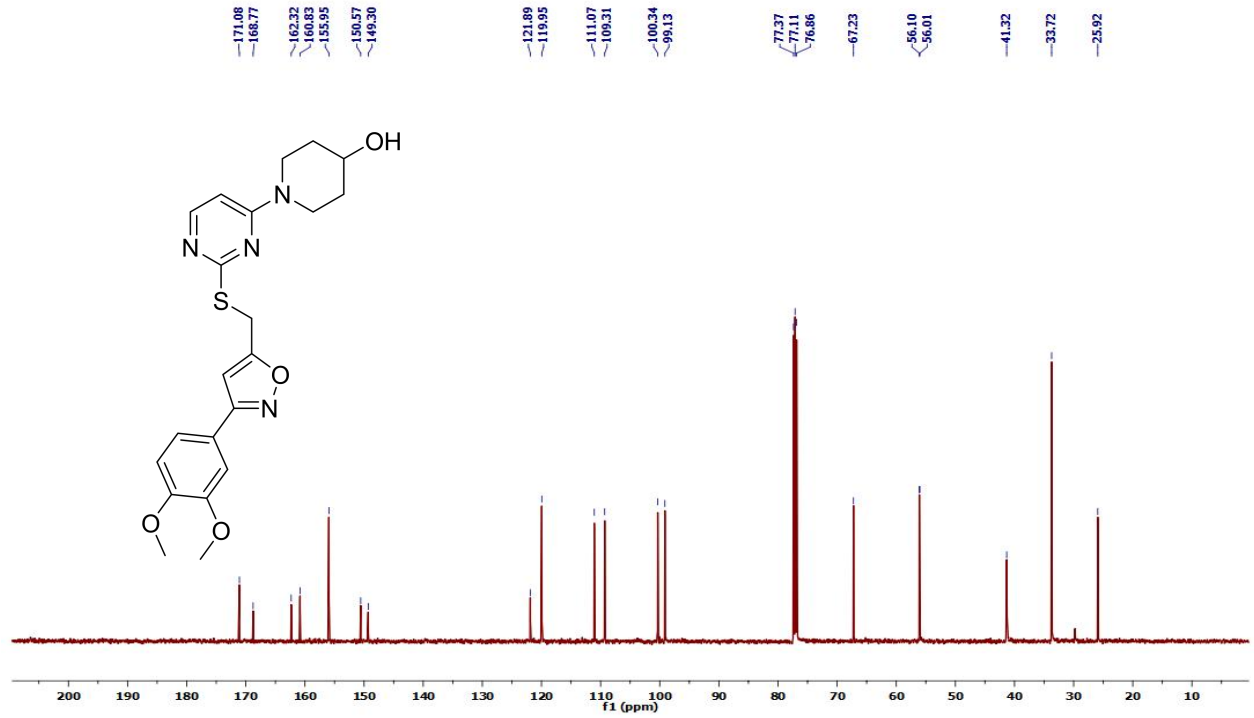
^{13}C NMR of 8d



Mass spectrum of 8d



^{1}H NMR of 8e



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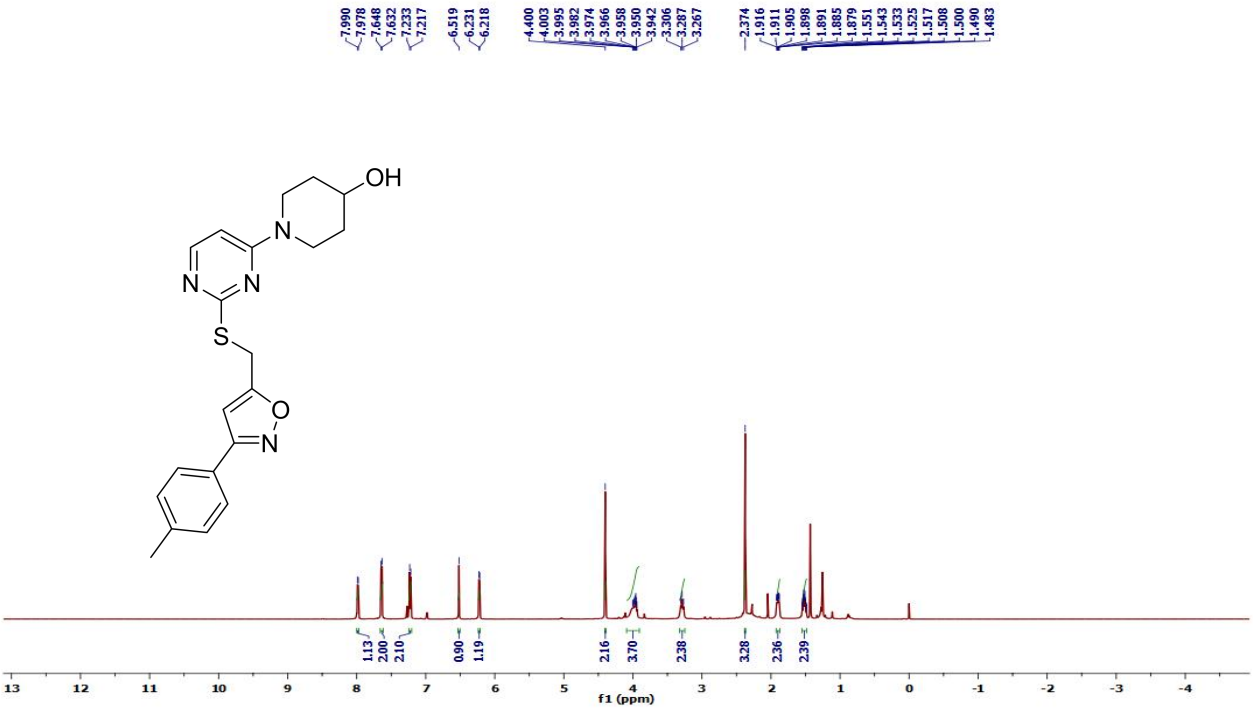
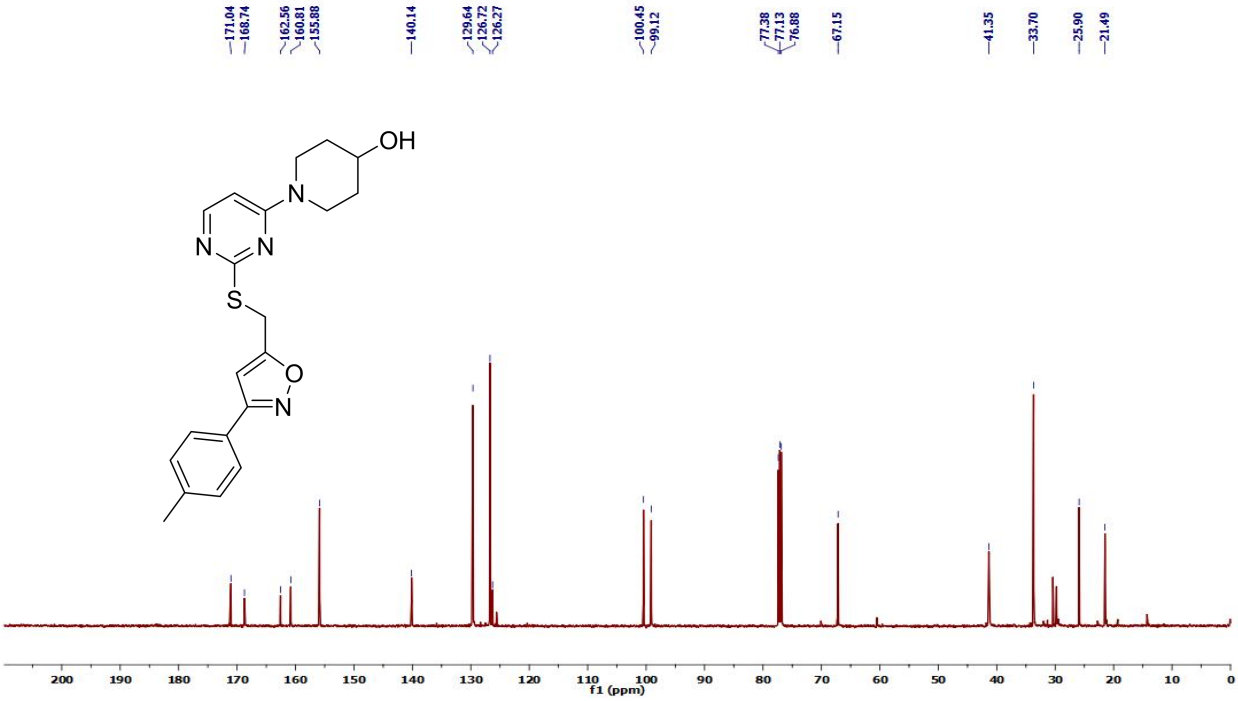
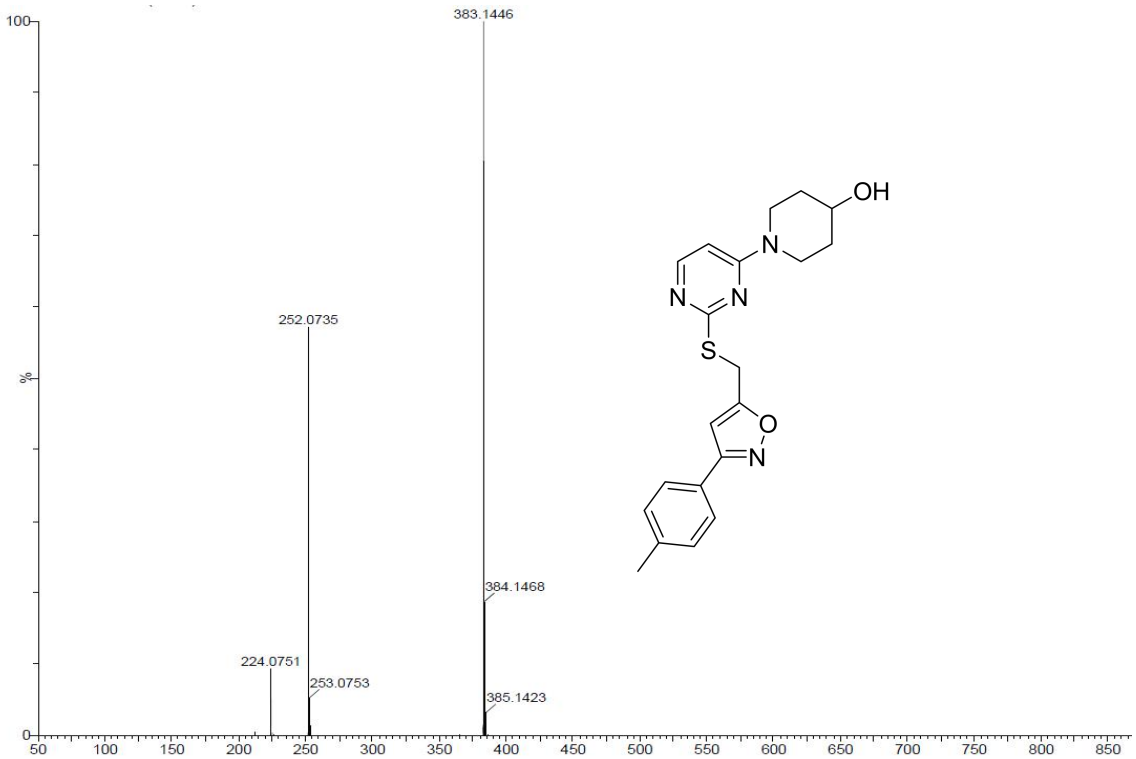


^{1}H NMR of 8f

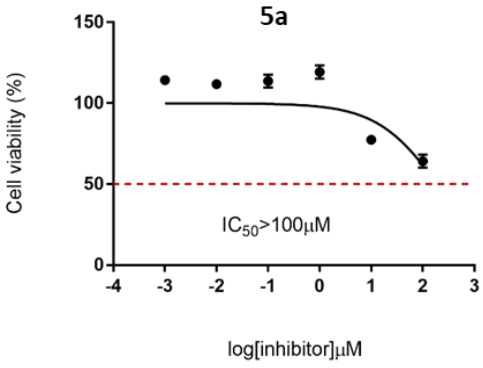


^{13}C NMR of 8f

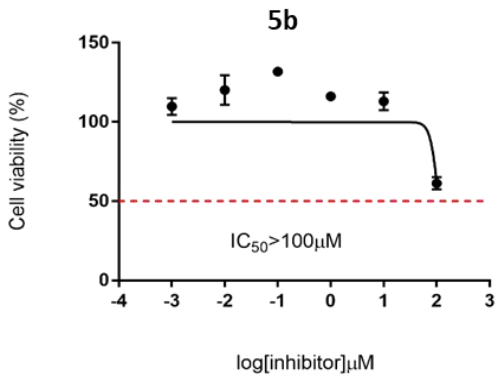


Mass spectrum of 8f

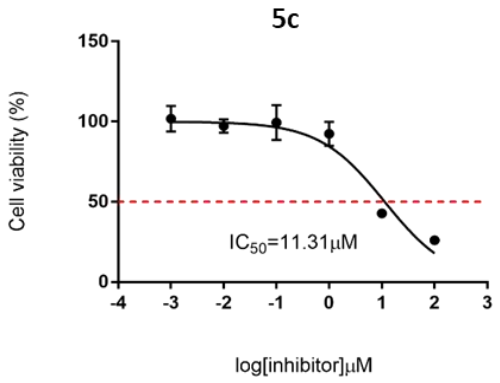
Log curves of synthesized compounds on MCF-7 cells



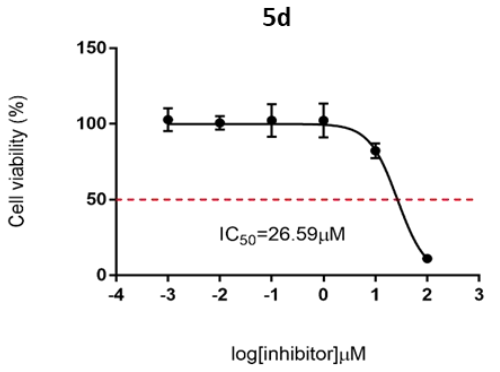
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	2.5
0.01	111.8	0.8
0.1	113.6	4.0
1	119.4	4.1
10	77.5	1.4
100	64.2	4.1



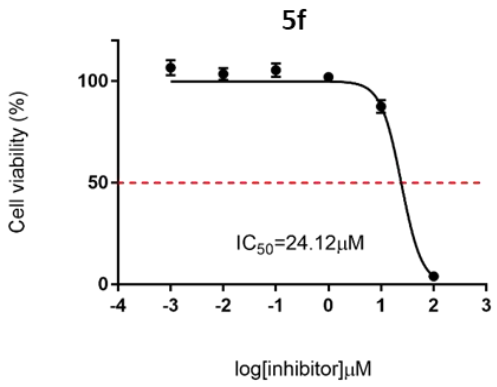
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	5.3
0.01	120.2	9.2
0.1	131.8	0.2
1	116.2	1.3
10	113.0	5.7
100	61.3	3.7



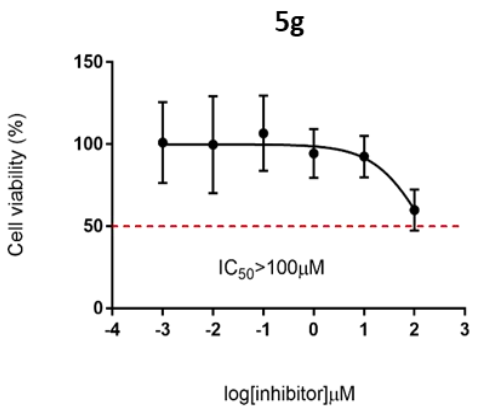
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	8.0
0.01	97.3	4.2
0.1	99.4	10.9
1	92.4	7.5
10	42.8	2.1
100	26.1	2.6



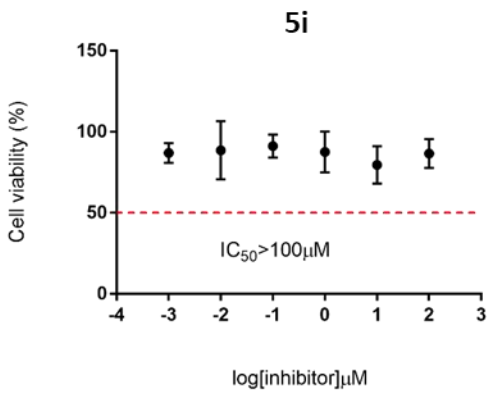
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	7.5
0.01	100.7	4.4
0.1	102.4	10.9
1	102.4	11.2
10	82.3	4.9
100	11.0	1.4



Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	3.8
0.01	103.6	2.9
0.1	105.6	3.3
1	102.2	1.2
10	87.7	3.2
100	4.1	0.9



Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	24.7
0.01	99.8	29.5
0.1	106.7	22.8
1	94.4	14.9
10	92.5	12.6
100	60.0	12.5



Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	6.2
0.01	88.5	18.0
0.1	91.2	7.2
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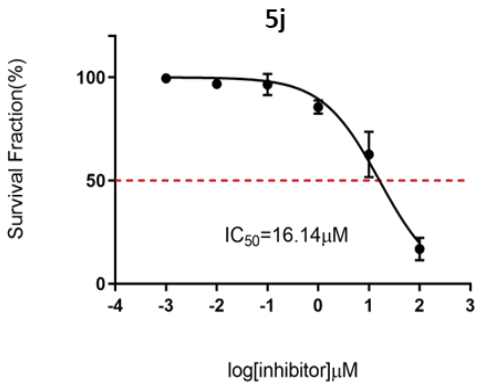
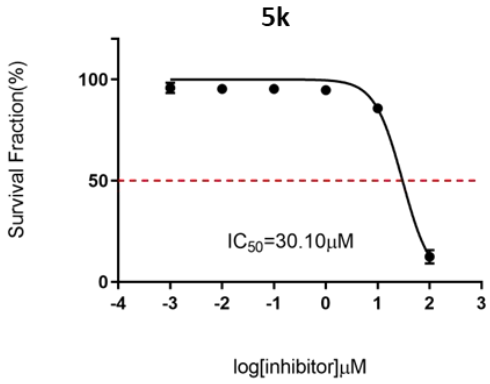
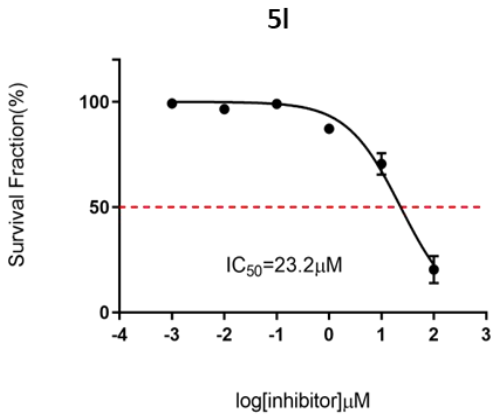
10	79.6	11.5
100	86.6	8.9



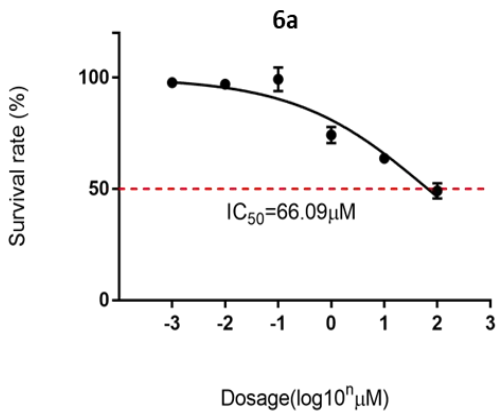
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	0.68
0.01	96.88	1.51
0.1	96.57	5.14
1	85.70	3.22
10	62.63	11.00
100	16.82	5.43



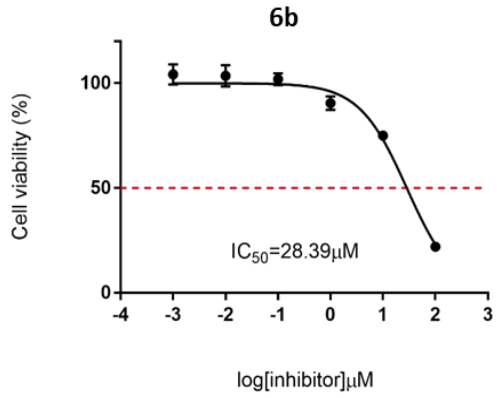
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	2.48
0.01	95.36	1.08
0.1	95.32	2.32
1	94.80	2.21
10	85.77	2.25
100	12.40	3.38



Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	0.64
0.01	96.60	1.56
0.1	99.00	1.06
1	87.20	2.16
10	70.57	5.11
100	20.33	6.40



Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	2.01
0.01	97.00	1.17
0.1	99.28	5.36
1	74.21	3.65
10	63.73	0.37
100	49.14	3.41



Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	4.8
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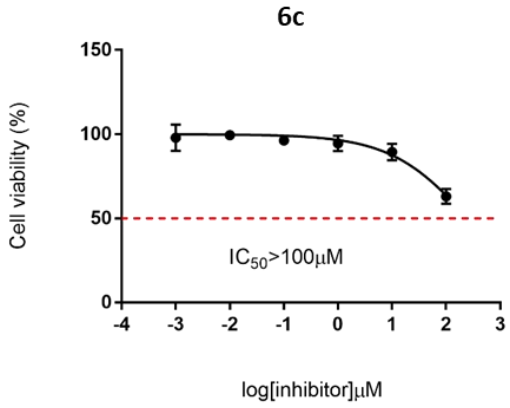
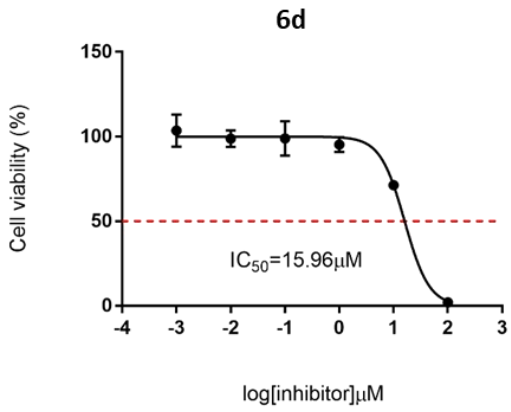
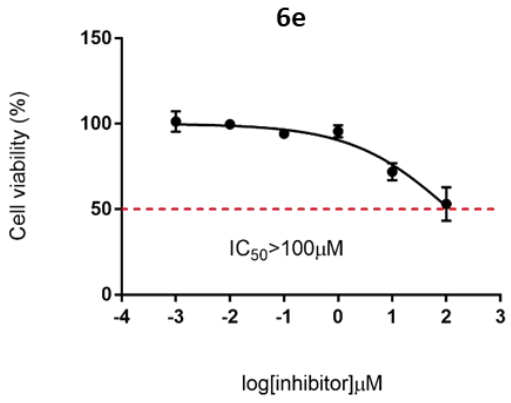
0.1	102.0	2.9
1	90.5	3.2
10	75.0	1.5
100	22.0	1.4



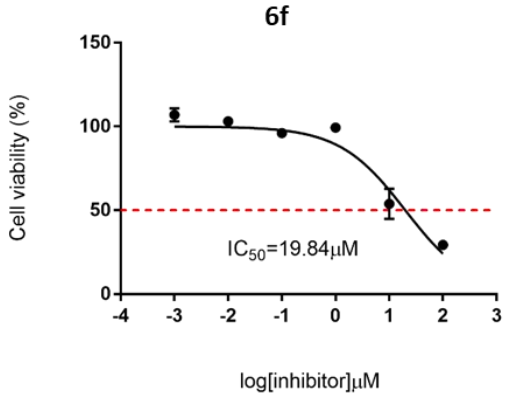
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	7.7
0.01	99.5	1.9
0.1	96.3	1.3
1	94.6	4.5
10	89.4	4.9
100	63.1	4.5



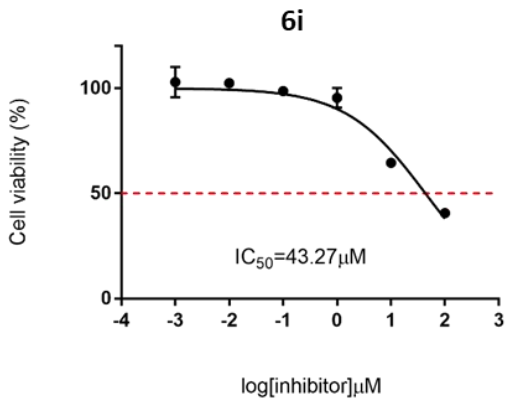
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	9.5
0.01	98.8	4.9
0.1	98.9	10.1
1	95.3	4.4
10	71.4	0.5
100	2.1	0.5



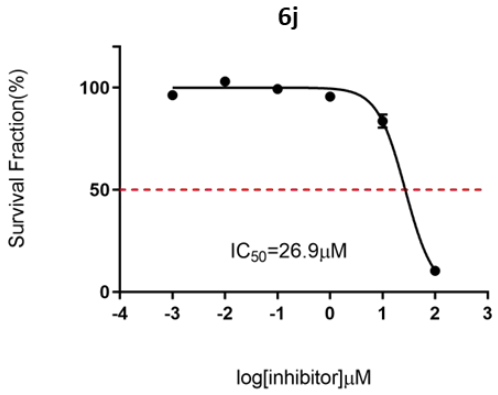
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	6.0
0.01	99.7	2.6
0.1	94.1	1.0
1	95.6	3.5
10	72.0	5.1
100	53.1	9.7



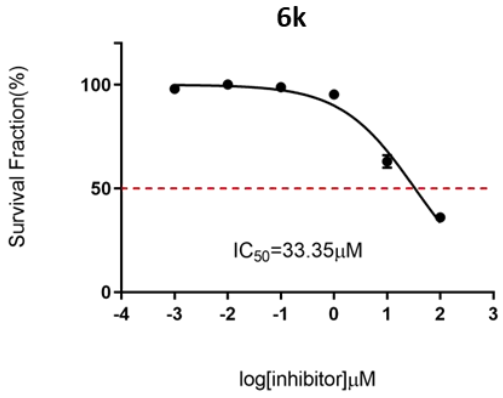
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	4.0
0.01	103.1	2.8
0.1	96.1	2.7
1	99.3	2.0
10	53.8	9.0
100	29.3	1.9



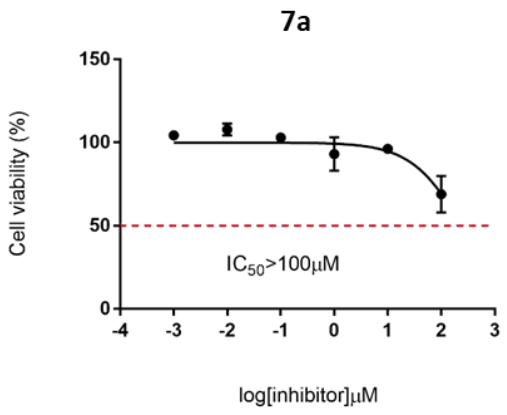
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	7.2
0.01	102.4	1.5
0.1	98.7	1.0
1	95.5	4.8
10	64.6	1.0
100	40.7	0.8



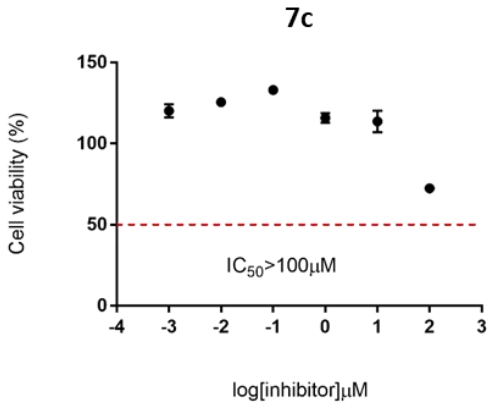
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	1.53
0.01	103.00	1.00
0.1	99.33	0.58
1	95.67	0.58
10	83.67	3.21
100	10.34	0.15



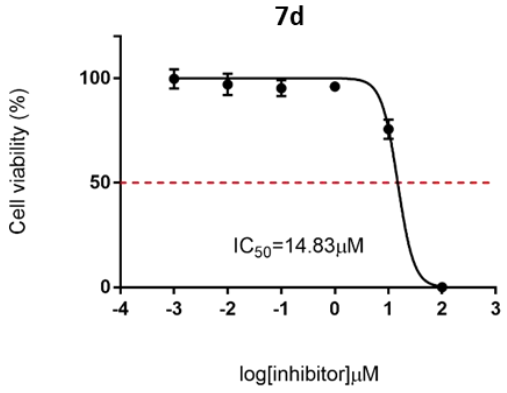
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	2.00
0.01	100.17	0.15
0.1	98.83	0.68
1	95.33	0.58
10	63.00	3.00
100	36.00	2.00



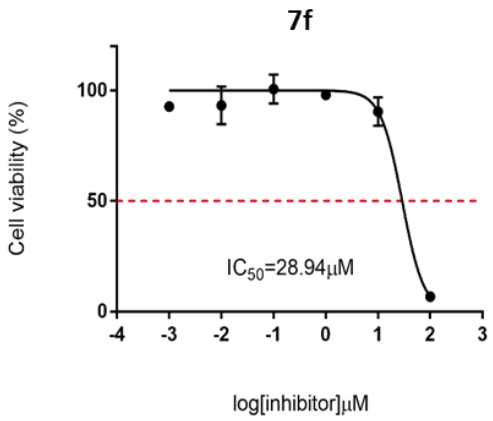
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	2.4
0.01	107.9	3.6
0.1	103.0	1.7
1	93.0	10.0
10	96.2	1.5
100	68.9	11.0



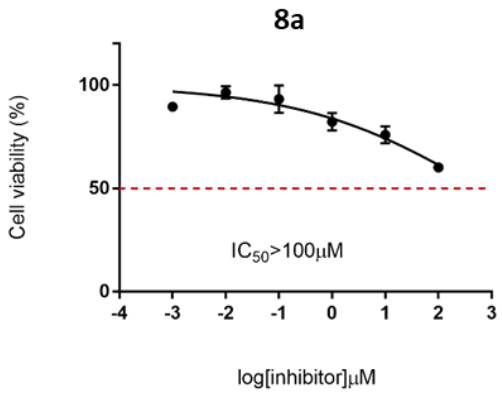
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	4.0
0.01	125.6	1.1
0.1	133.1	1.2
1	115.9	3.0
10	113.7	6.7
100	72.4	2.5



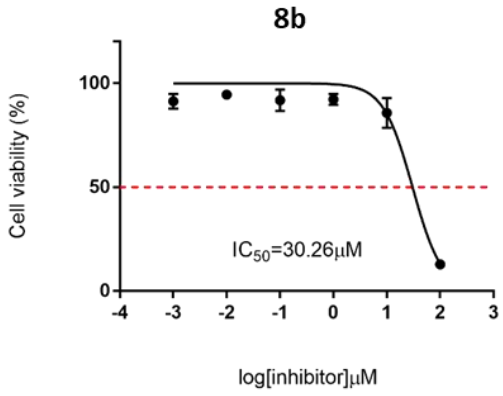
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	4.7
0.01	97.1	5.1
0.1	95.2	3.9
1	96.0	1.7
10	75.7	4.6
100	0.0	0.0



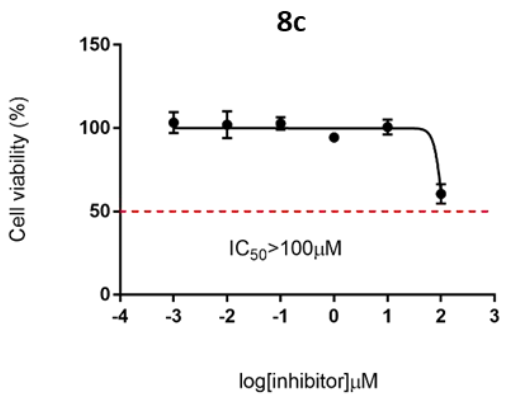
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	2.2
0.01	93.3	8.5
0.1	100.6	6.5
1	98.1	1.9
10	90.4	6.4
100	6.8	1.0



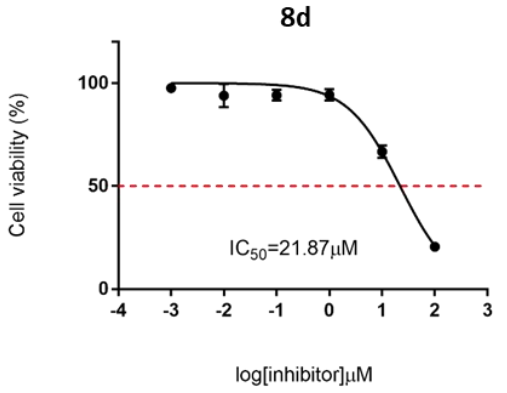
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	1.3
0.01	96.5	3.0
0.1	93.2	6.6
1	82.3	4.2
10	76.0	4.2
100	60.2	1.8



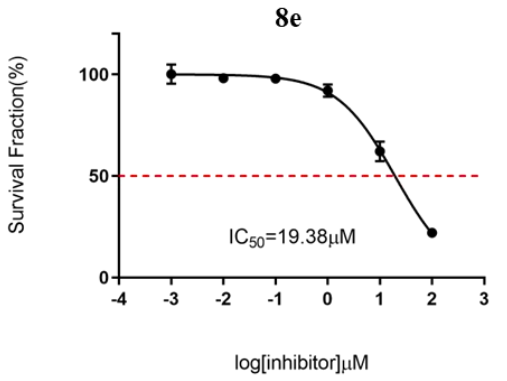
Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	3.5
0.01	94.6	0.8
0.1	91.9	5.1
1	92.2	2.6
10	85.7	7.2
100	12.8	0.8



Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	6.3
0.01	102.1	8.1
0.1	102.8	3.8
1	94.4	2.9
10	100.7	4.5
100	60.6	5.8

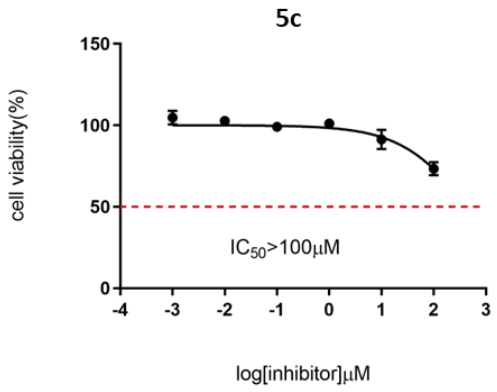


Conc.(μM)	Viability (%)	
	AVE.	±SD
0	100.0	2.3
0.01	93.9	5.7
0.1	94.1	2.6
1	94.4	2.7
10	66.8	3.0
100	20.5	2.3

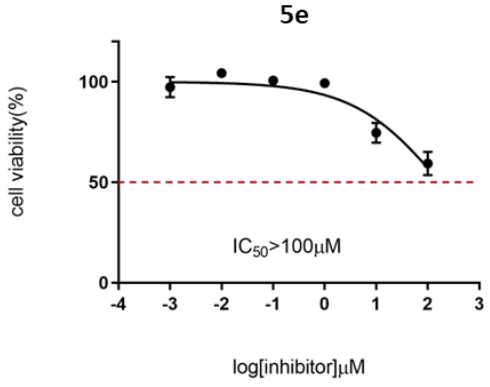


Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	4.71
0.01	98.20	2.39
0.1	97.93	2.08
1	92.07	3.06
10	62.13	4.79
100	22.00	1.00

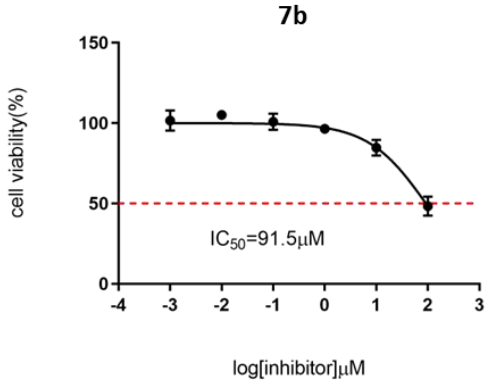
Log curves of active compounds on MCF-10A cells



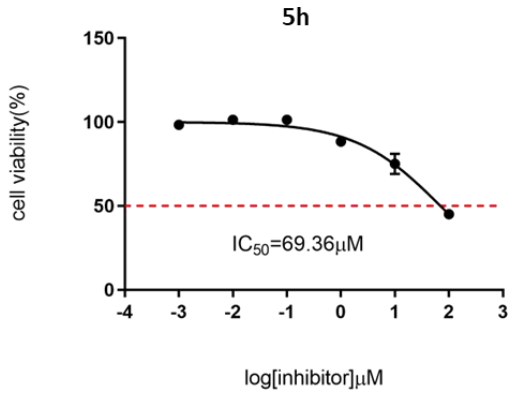
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	4.16
0.01	102.67	2.52
0.1	99.00	1.00
1	101.00	2.65
10	91.33	5.86
100	73.33	4.04



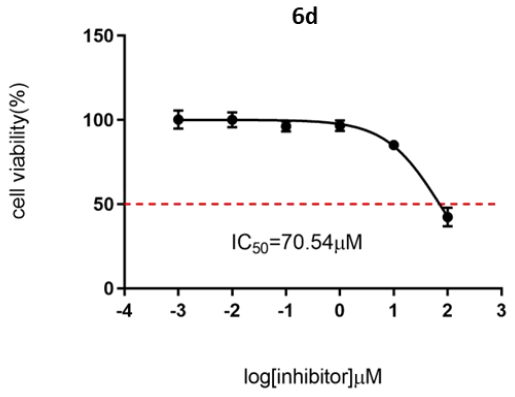
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	5.03
0.01	104.33	2.08
0.1	100.67	1.15
1	99.32	0.78
10	74.67	4.93
100	59.33	5.77



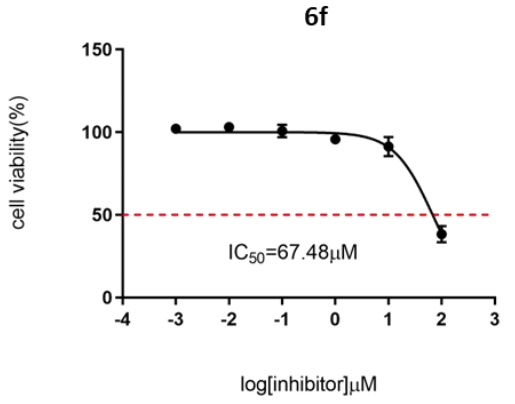
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	6.33
0.01	105.12	2.90
0.1	100.80	5.00
1	96.42	1.66
10	84.67	4.93
100	48.33	5.86



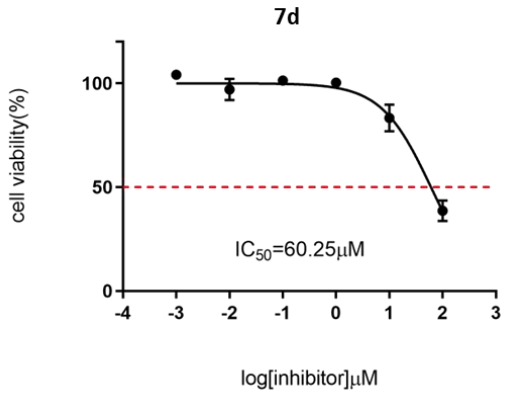
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	1.08
0.01	101.31	1.14
0.1	101.33	0.58
1	88.33	1.15
10	75.00	6.08
100	45.00	1.00



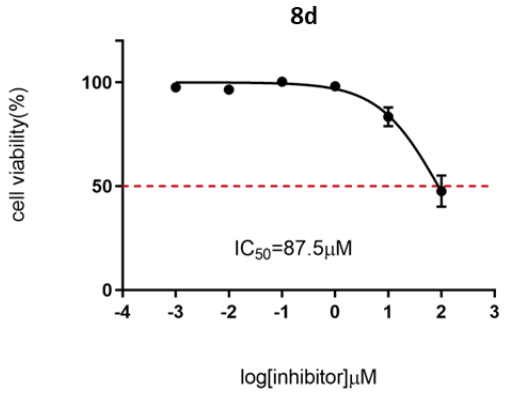
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	5.41
0.01	100.10	4.46
0.1	96.23	3.06
1	96.50	3.13
10	85.00	1.00
100	42.33	5.51



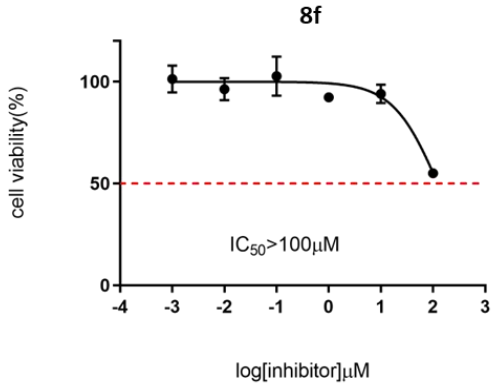
Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	2.65
0.01	103.07	2.79
0.1	100.67	3.79
1	95.67	1.15
10	91.33	5.77
100	38.33	4.93



Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	1.06
0.01	97.08	5.09
0.1	101.33	1.15
1	100.33	1.53
10	83.33	6.43
100	38.67	4.93



Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	2.34
0.01	96.59	1.51
0.1	100.33	1.53
1	98.19	1.72
10	83.47	4.52
100	47.60	7.51



Conc.(μM)	Viability	
	AVE.	±SD
0	100.00	6.63
0.01	96.34	5.39
0.1	102.74	9.63
1	92.36	1.92
10	94.00	4.58
100	55.00	1.00