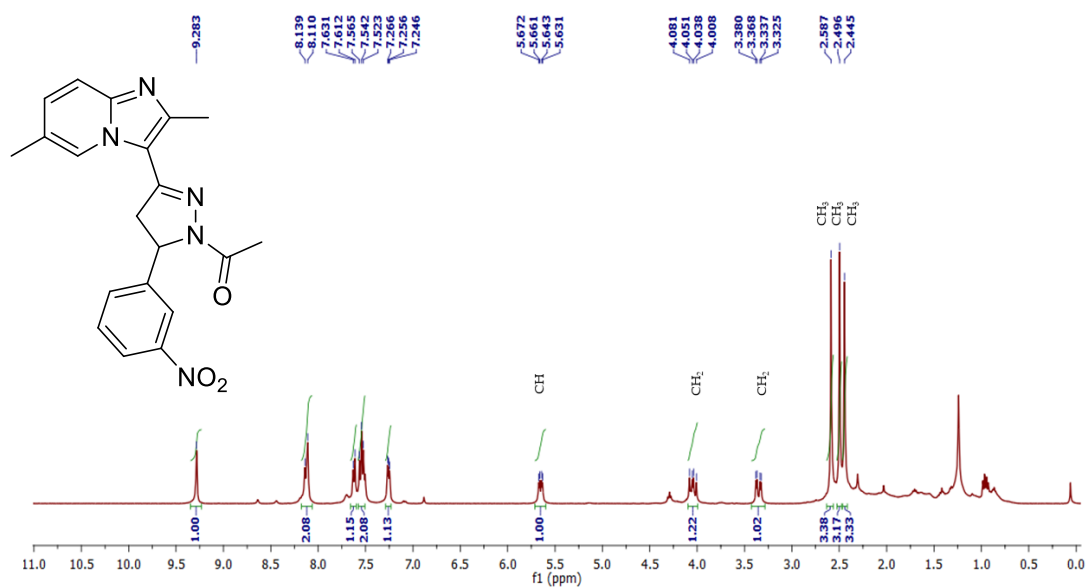


***De novo* drug design of imidazopyridine tethered pyrazoles that Targets
Phosphorylation of STAT3 in Human Breast Cancer Cells**

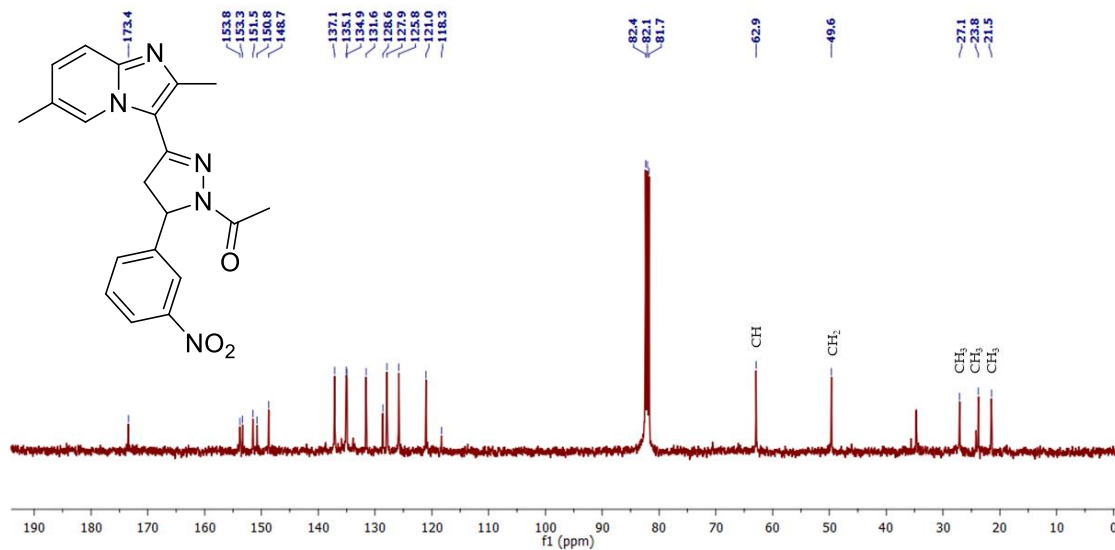
**Akshay Ravish^{1,#}, Rashmi Shivakumar^{1,#}, Zhang Xi^{2,#}, Min Hee Yang³, Ji-Rui Yang⁴,
Ananda Swamynayaka⁵, Omantheswara Nagaraja⁵, Mahendra Madegowda⁵,
Arunachalam Chinnathambi⁶, Sulaiman Ali Alharbi⁶, Vijay Pandey^{4,7}, Gautam
Sethi^{8,*}, Kwang Seok Ahn^{2,9,*}, Peter E. Lobie^{3,4,7,*}, Basappa Basappa^{1*}**

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

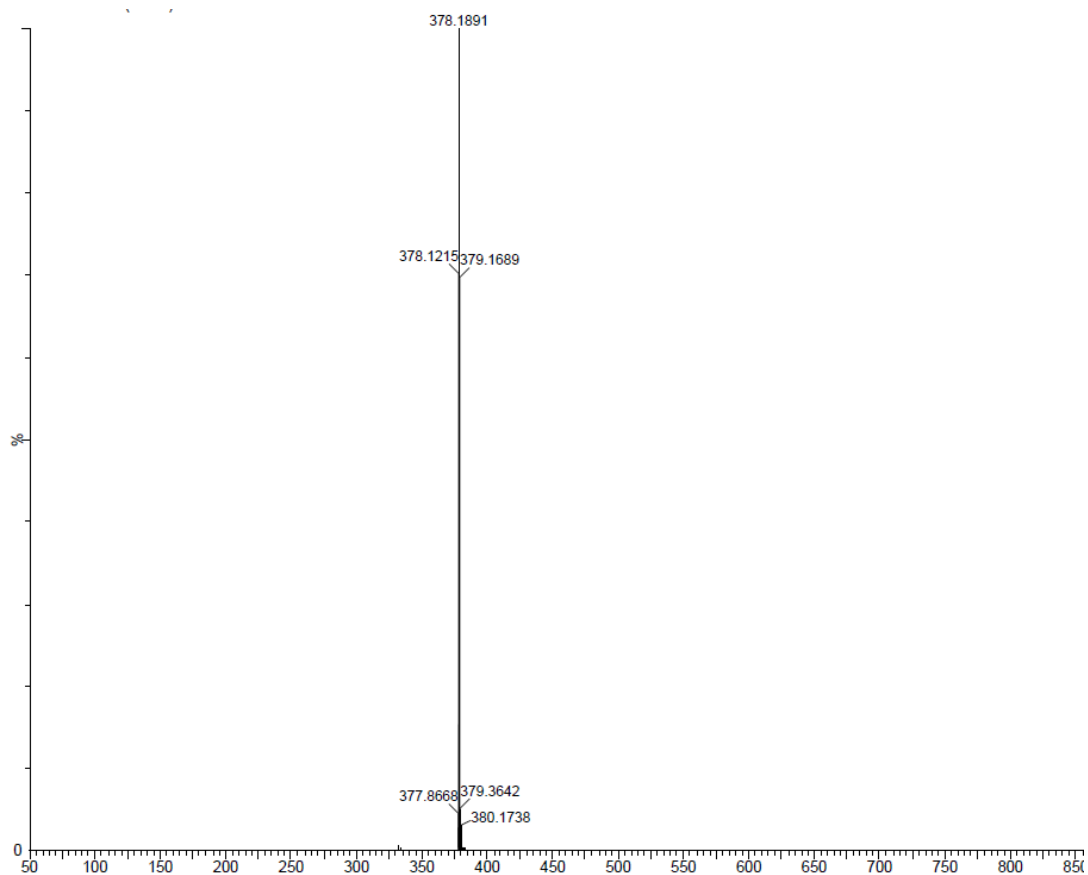
NMR DATA



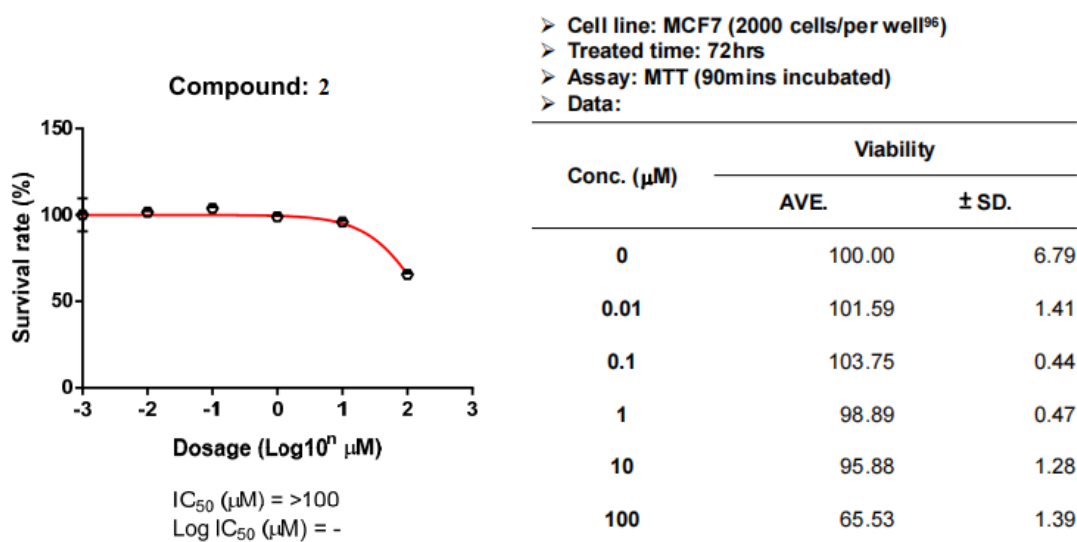
¹H NMR of 2



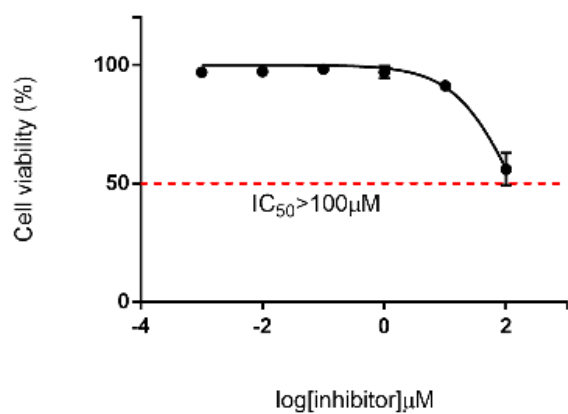
¹³C NMR of 2



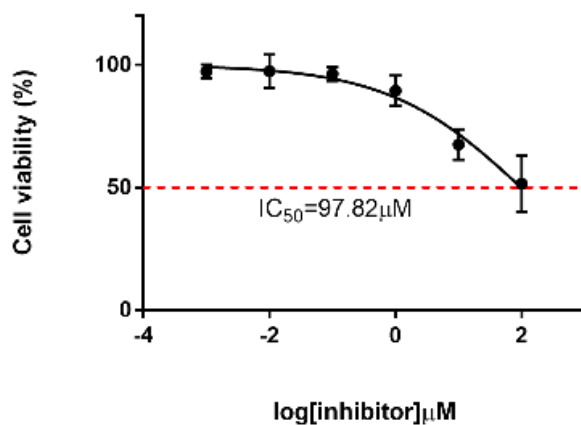
Mass spectra of 2



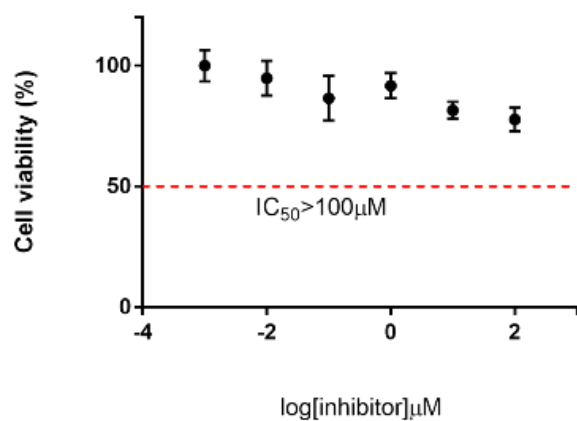
MCF-7 Log curve of 2



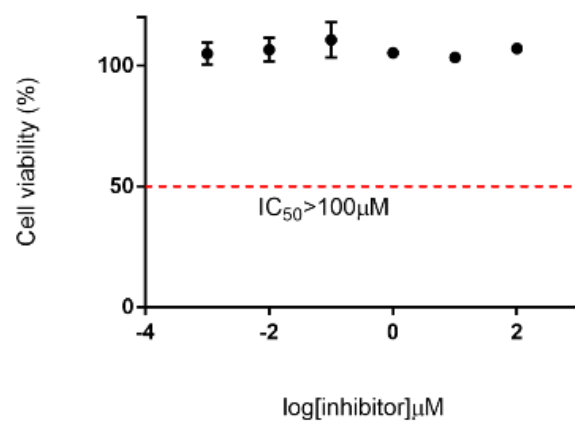
T47D Log curve of 2



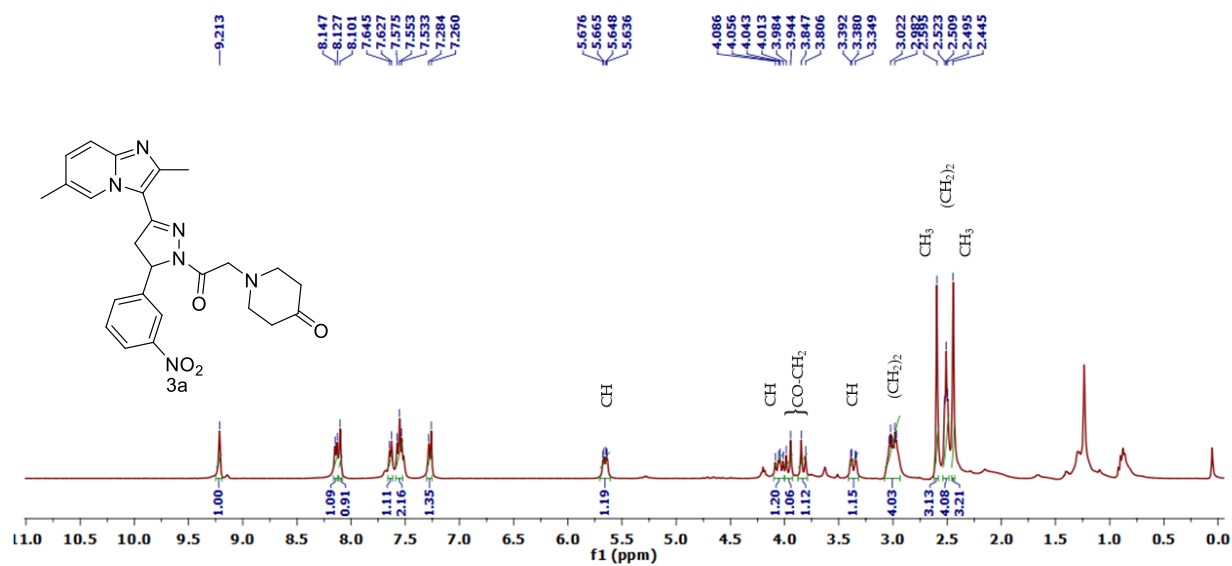
BT474 Log curve of 2



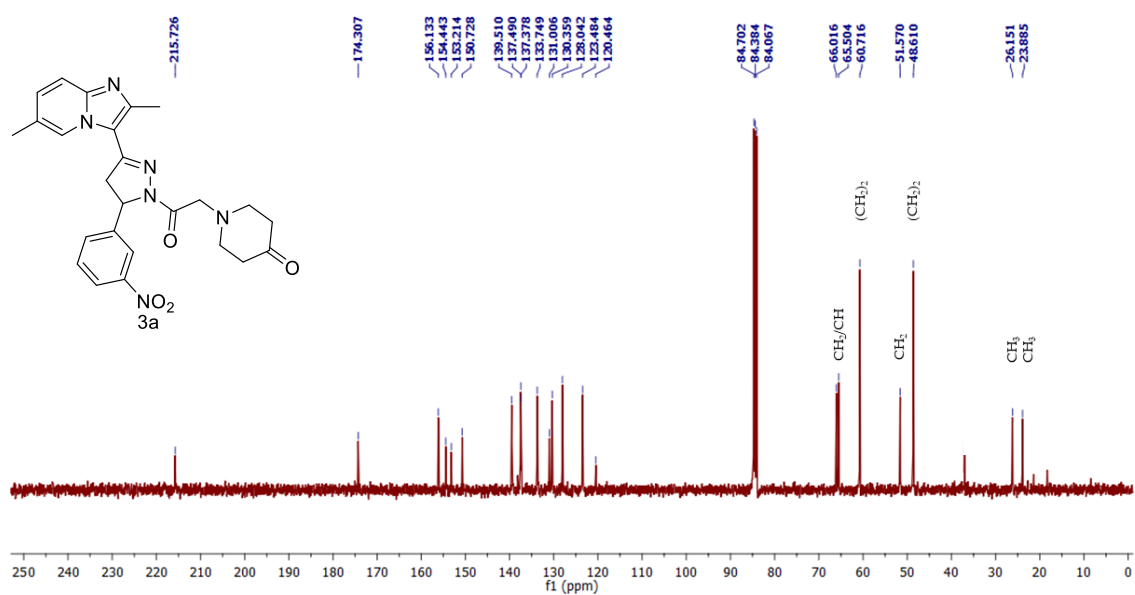
SK-BR-3 log curve of 2



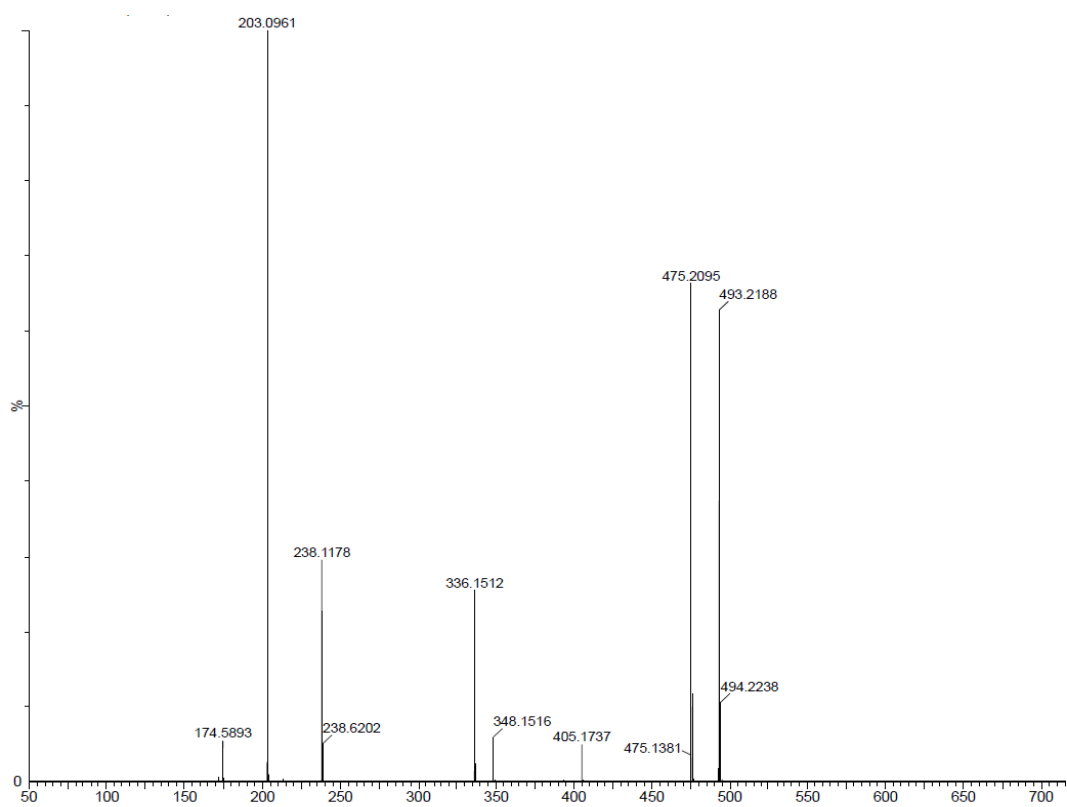
MCF-10A log curve of 2



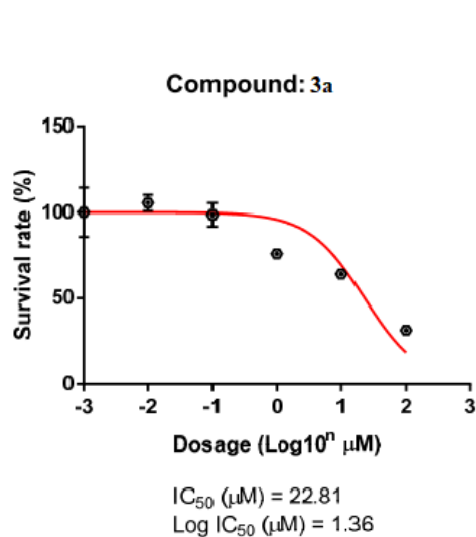
^1H NMR of 3a



^{13}H NMR of **3a**



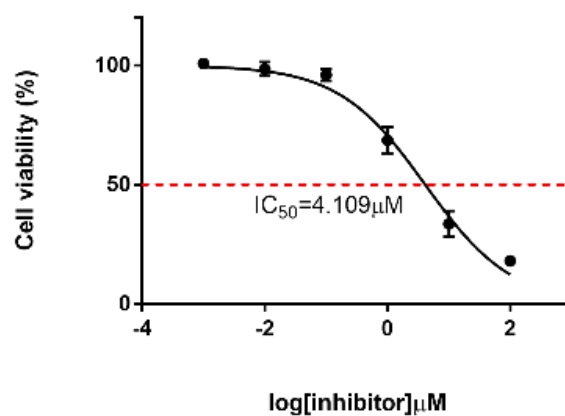
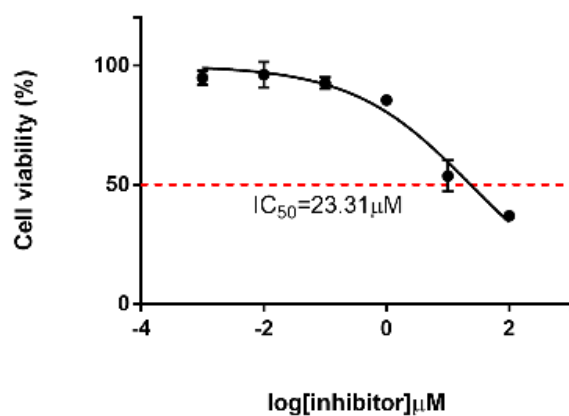
Mass spectra of **3a**



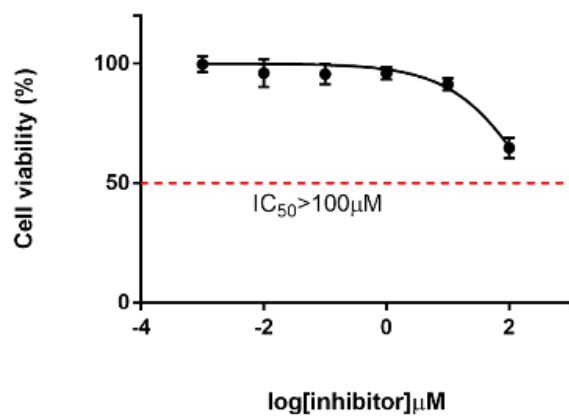
- Cell line: MCF7 (2000 cells/per well⁹⁶)
- Treated time: 72hrs
- Assay: MTT (90mins incubated)
- Data: 3a

Conc. (μM)	Viability	
	AVE.	\pm SD.
0	100.00	10.10
0.01	105.50	4.69
0.1	98.61	6.78
1	75.99	1.24
10	64.01	0.42
100	31.59	0.04

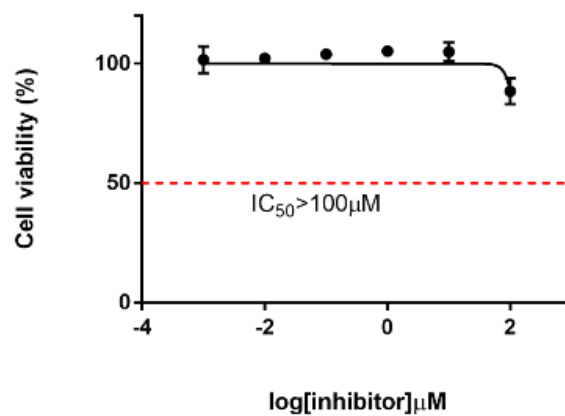
MCF-7 Log curve of 3a



T47D Log curve of 3a

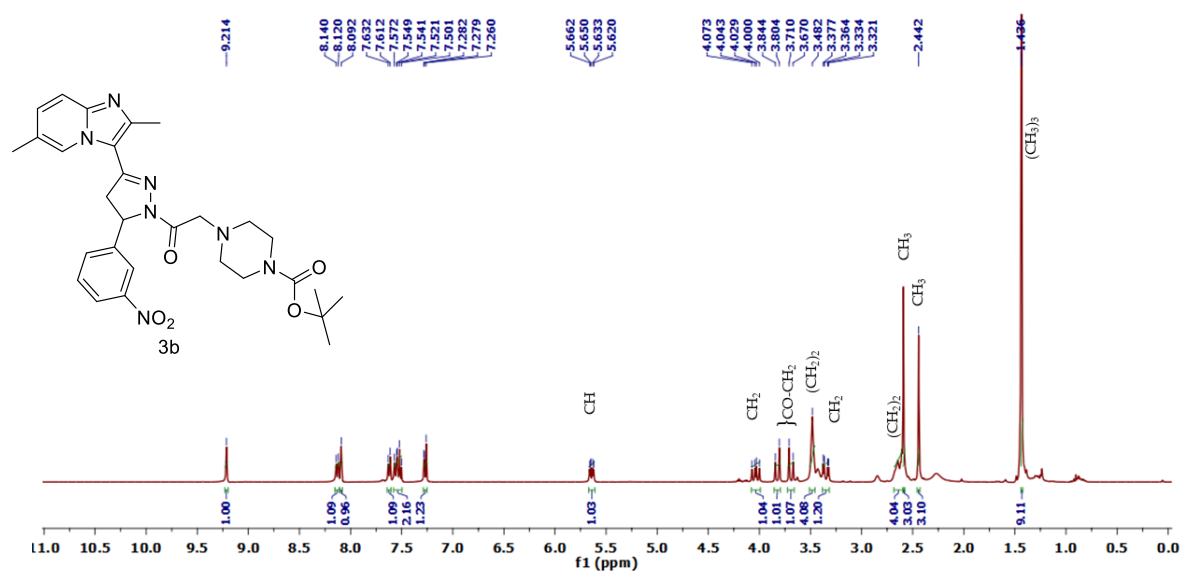


BT474 Log curve of 3a

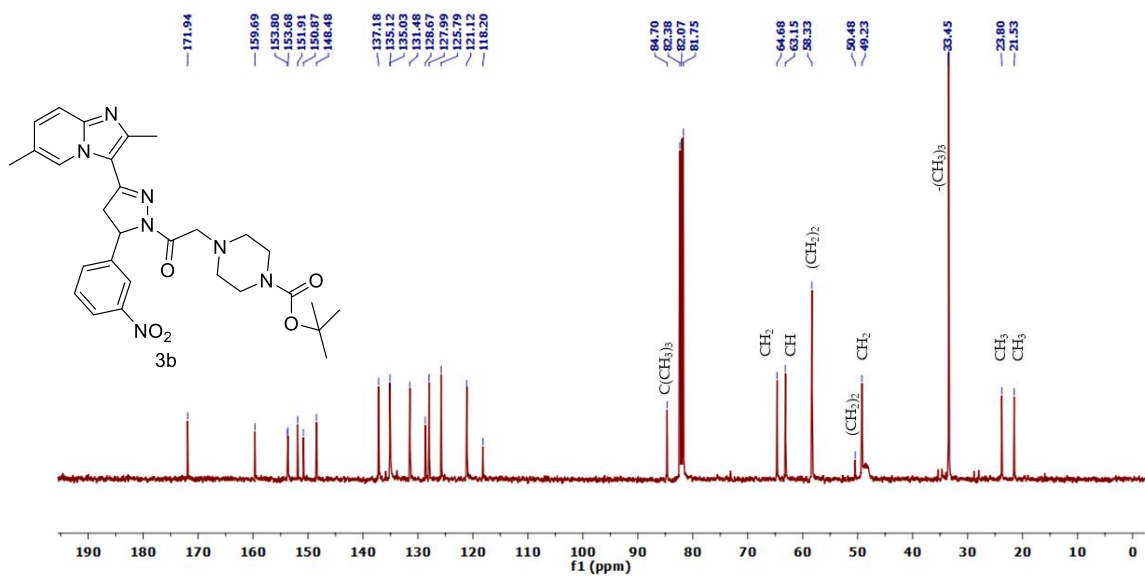


SK-BR-3 log curve of 3a

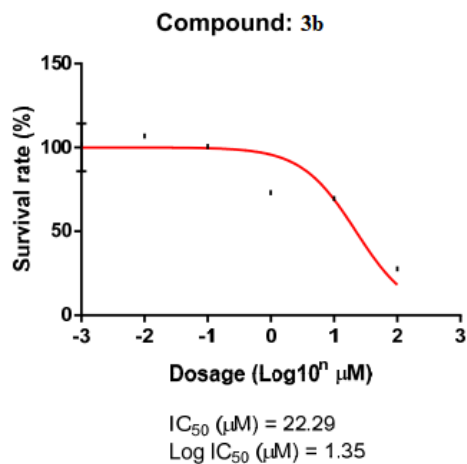
MCF-10A log curve of 3a



¹H NMR of **3b**



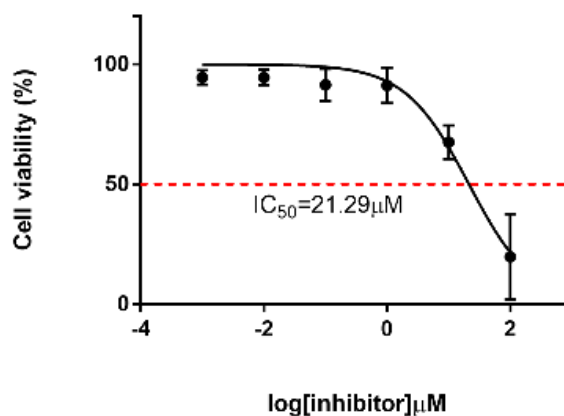
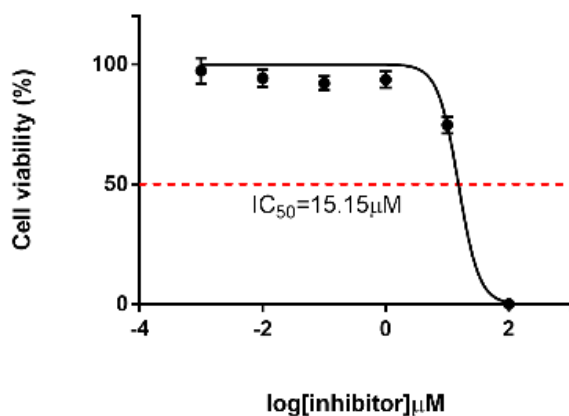
¹³C NMR of **3b**



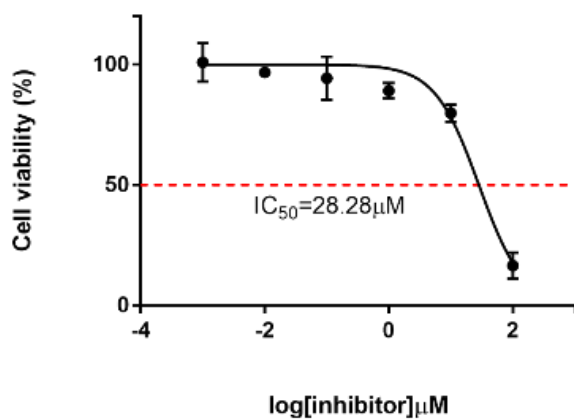
- Cell line: MCF7 (2000 cells/per well⁹⁶)
- Treated time: 72hrs
- Assay: MTT (90mins incubated)
- Data: 3b

Conc. (μM)	Viability	
	AVE.	\pm SD.
0	100.00	10.10
0.01	105.31	0.45
0.1	99.02	0.39
1	71.53	1.51
10	68.11	2.70
100	26.22	0.70

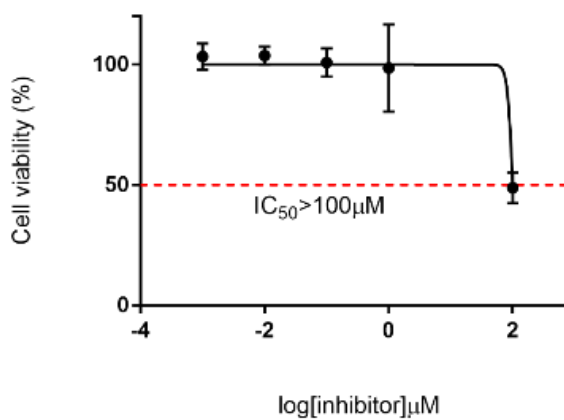
MCF-7 Log curve of 3b



T47D Log curve of 3b

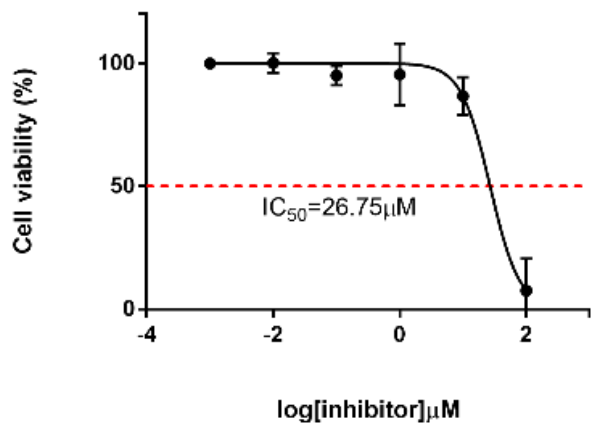


BT474 Log curve of 3b

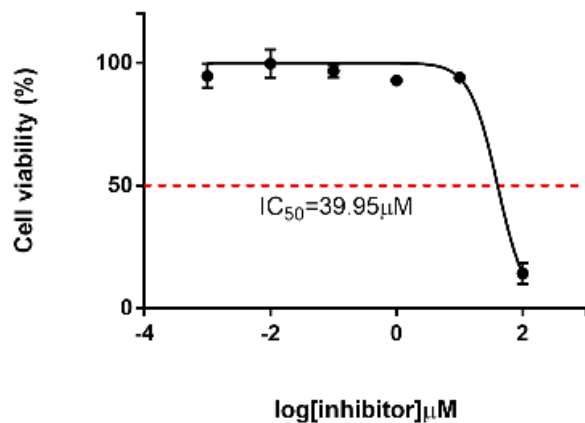


SK-BR-3 log curve of 3b

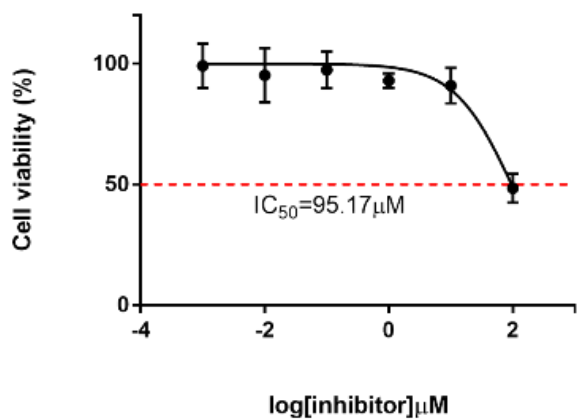
MCF-10A log curve of 3b



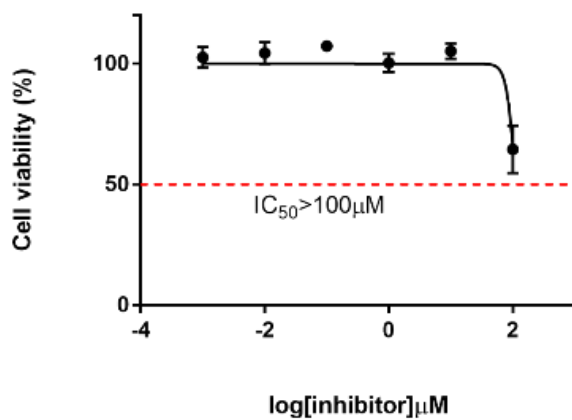
T47D Log curve of 3c



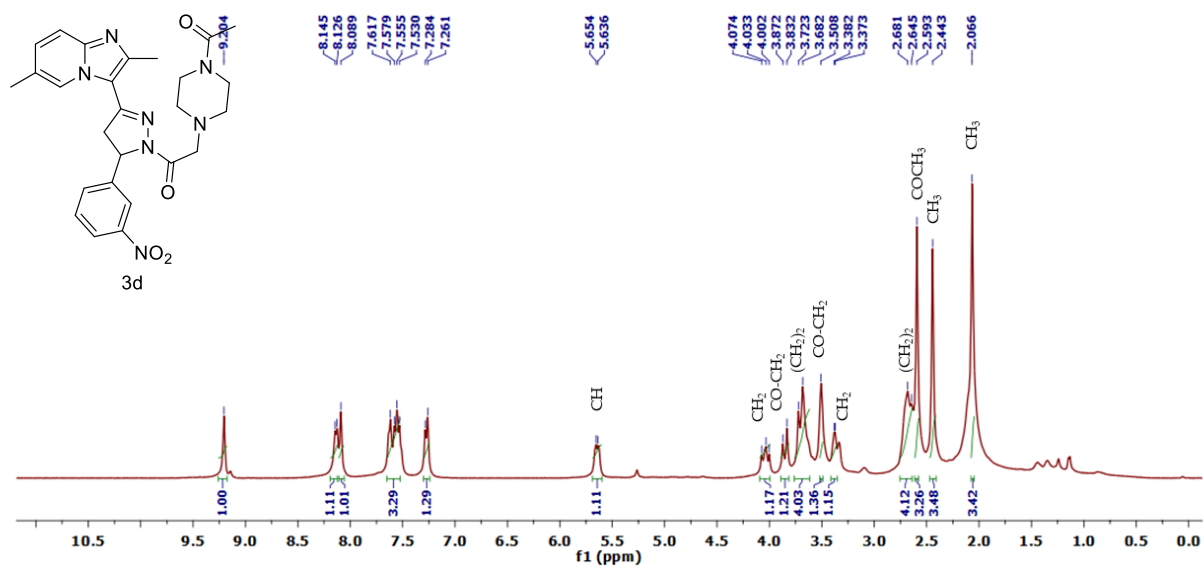
BT474 Log curve of 3c



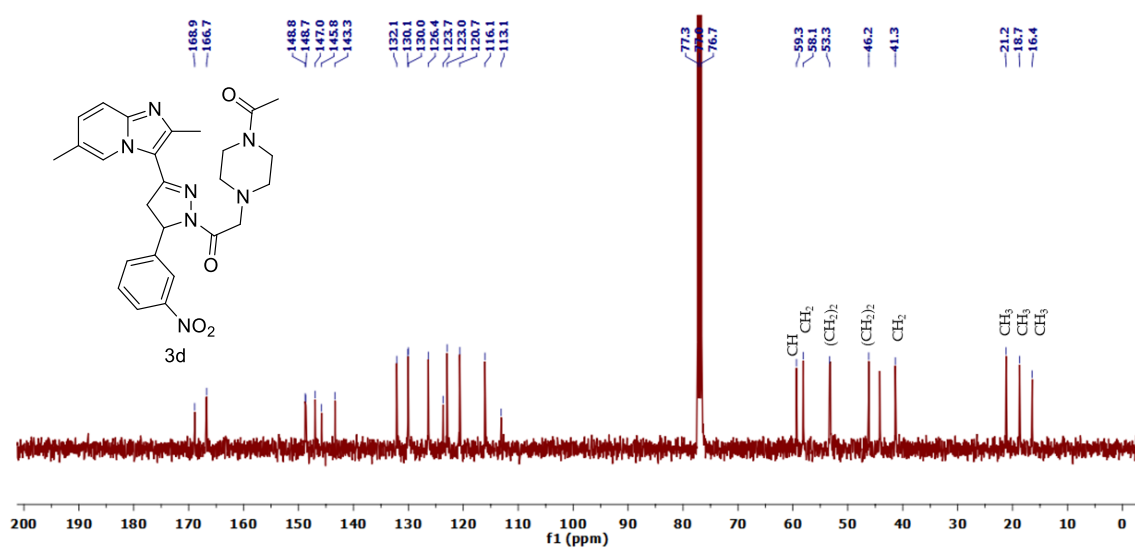
SK-BR-3 log curve of 3c



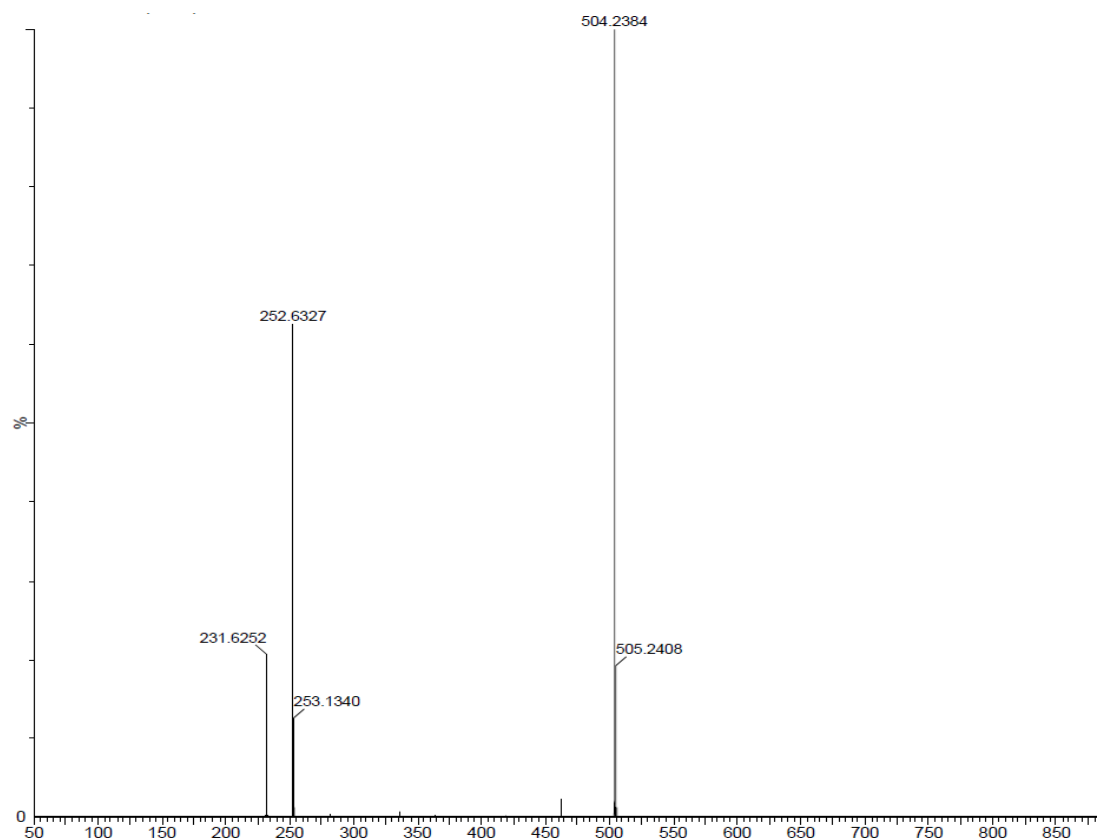
MCF-10A log curve of 3c



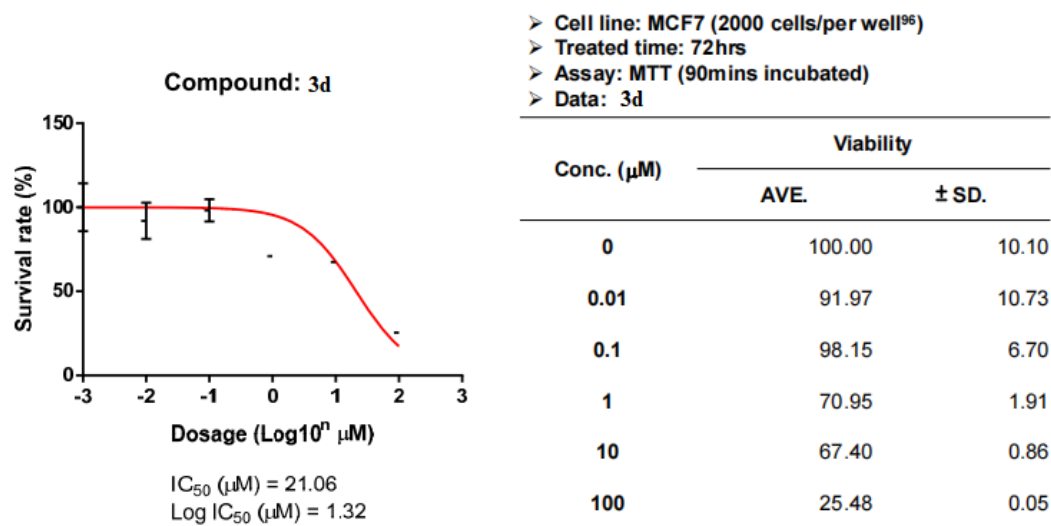
^1H NMR of **3d**



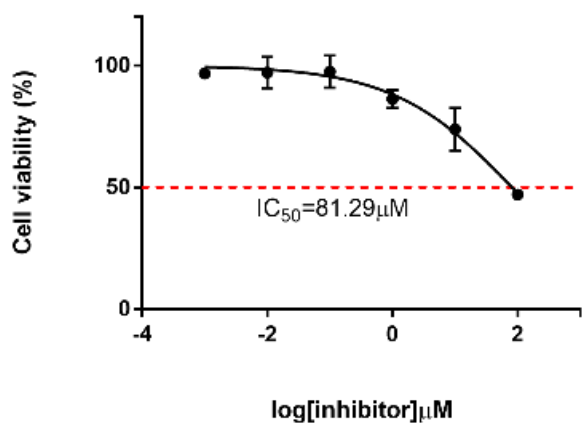
^{13}C NMR of **3d**



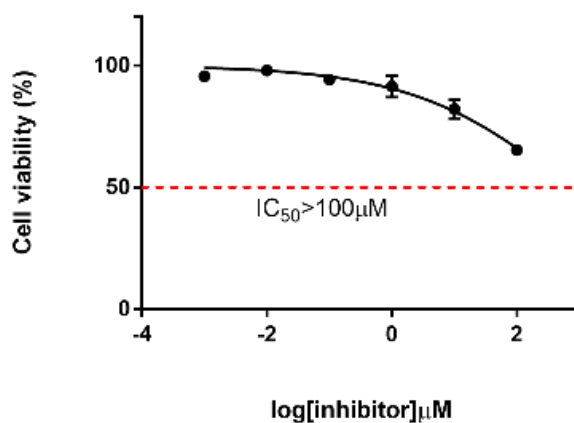
Mass spectra of **3d**



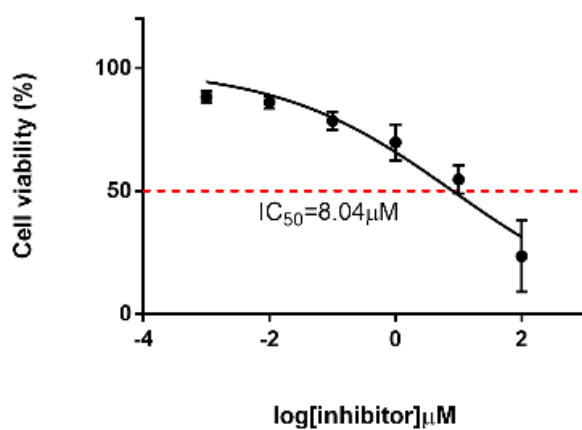
MCF-7 Log curve of **3d**



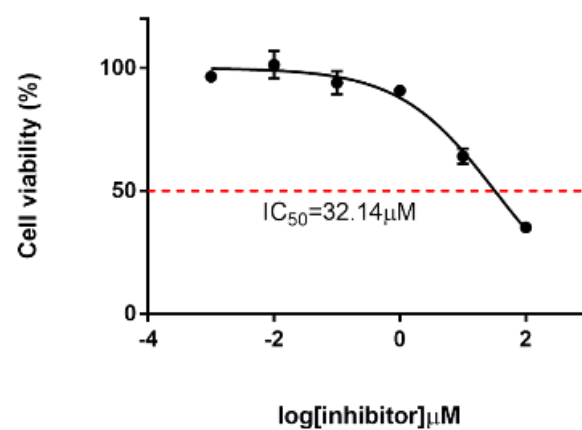
T47D Log curve of 3d



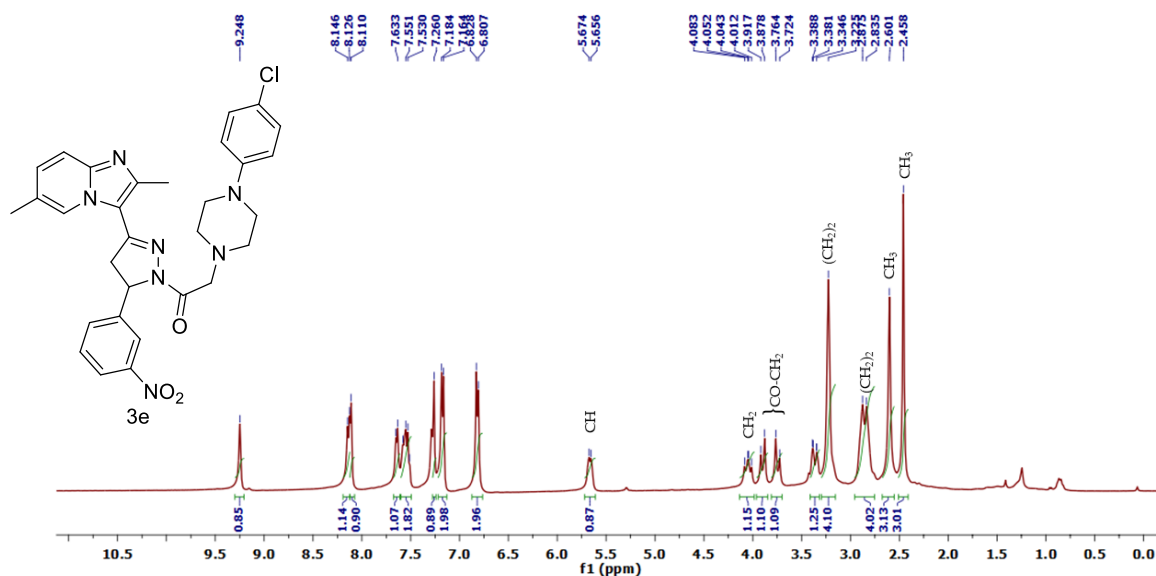
BT474 Log curve of 3d



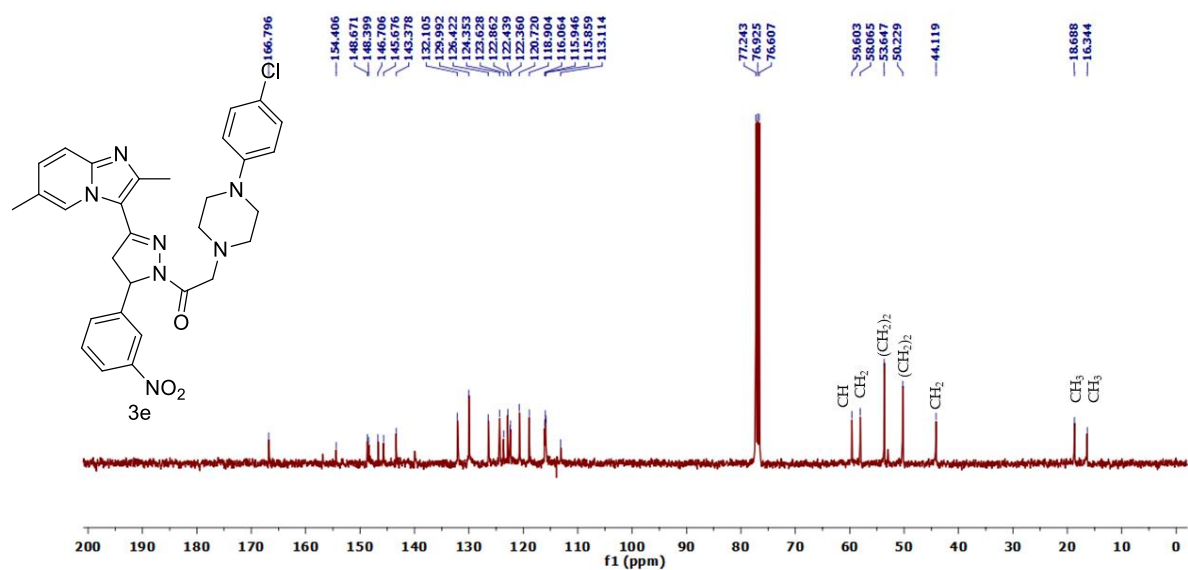
SK-BR-3 log curve of 3d



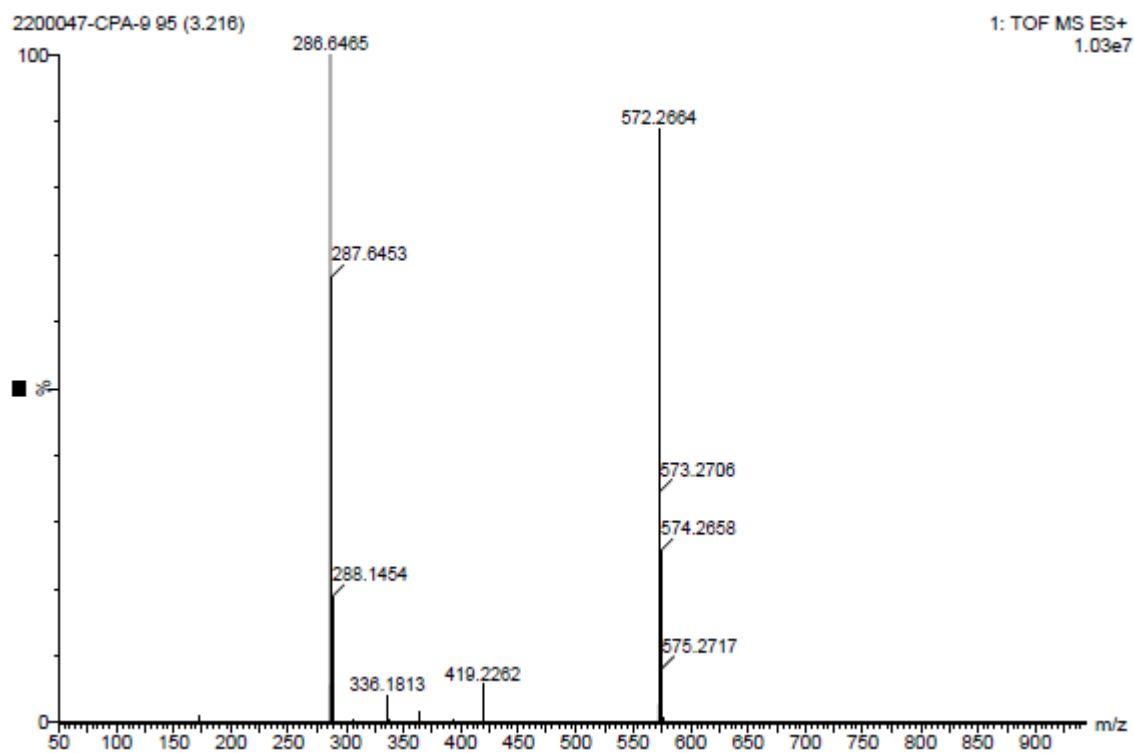
MCF-10A log curve of 3d



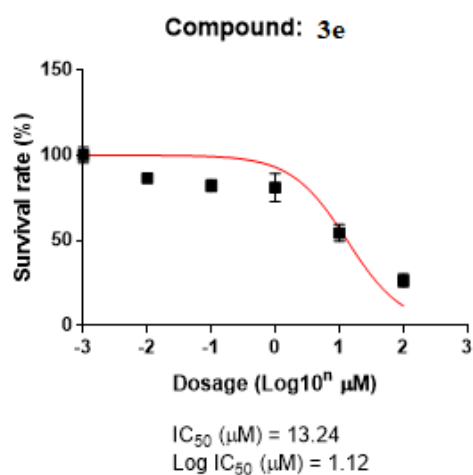
1H NMR of 3e



¹³C NMR of 3e



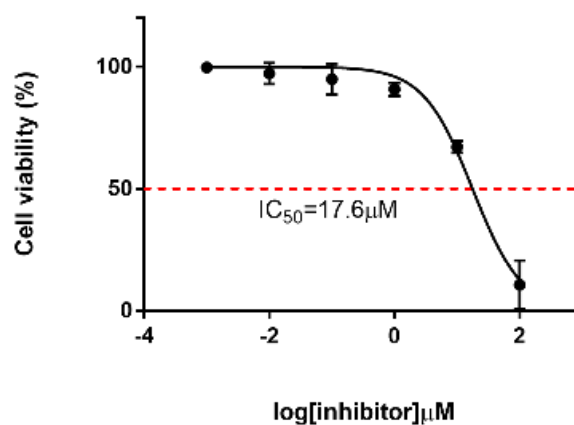
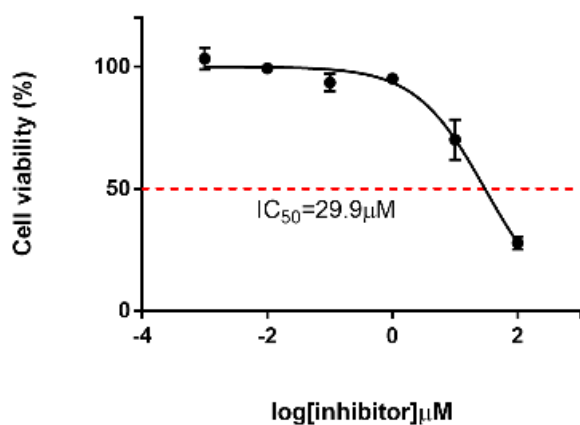
Mass spectra of compound 3e



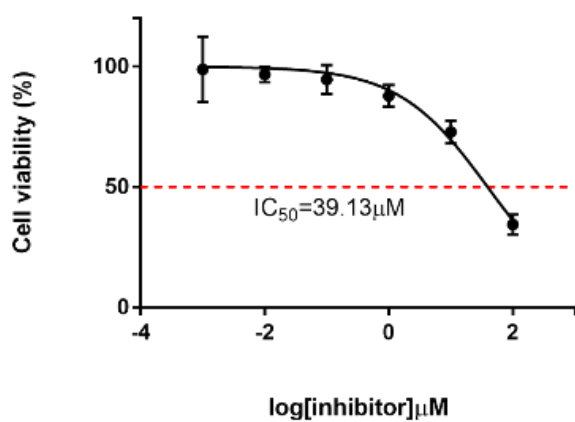
> Cell line: MCF7 (2000 cells/per well⁹⁶)
 > Treated time: 72hrs
 > Assay: alamarBlue (4hrs incubated)
 > Data: 3e

Conc. (μM)	Viability	
	AVE.	\pm SD.
0	100.00	4.64
0.01	86.60	1.67
0.1	82.25	3.61
1	81.12	8.26
10	54.43	4.91
100	26.54	3.76

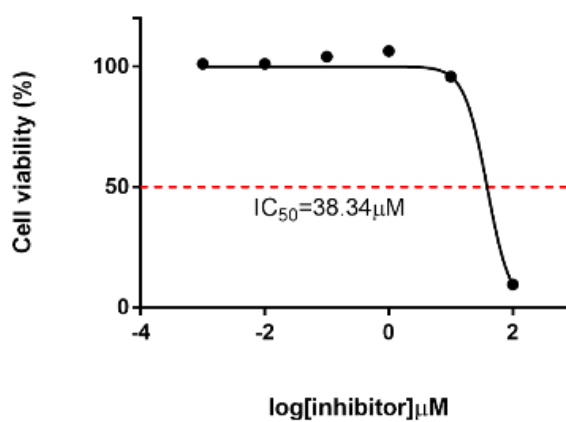
MCF-7 Log curve of 3e



T47D Log curve of 3e

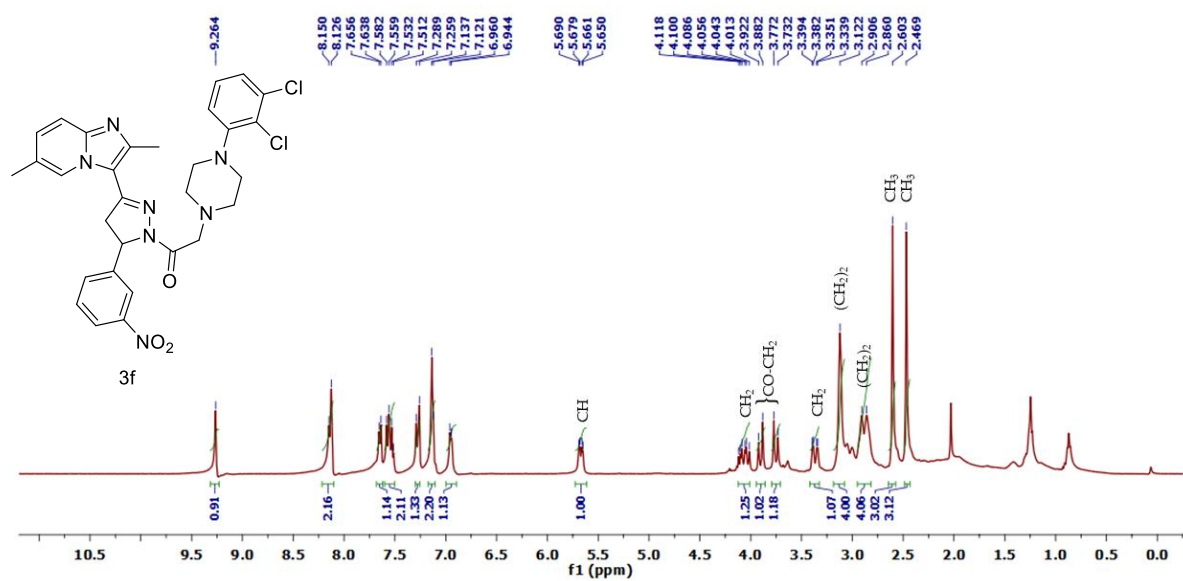


BT474 Log curve of 3e

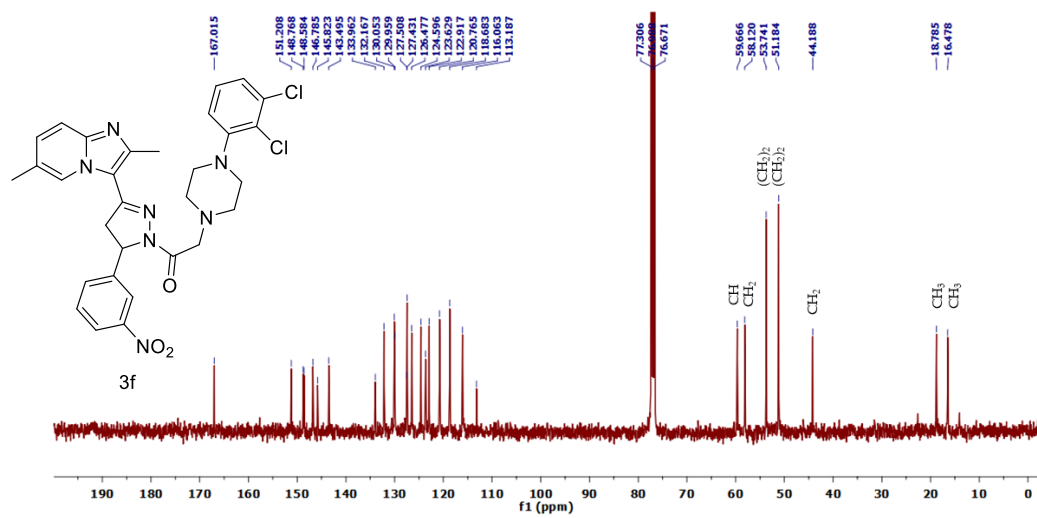


SK-BR-3 log curve of 3e

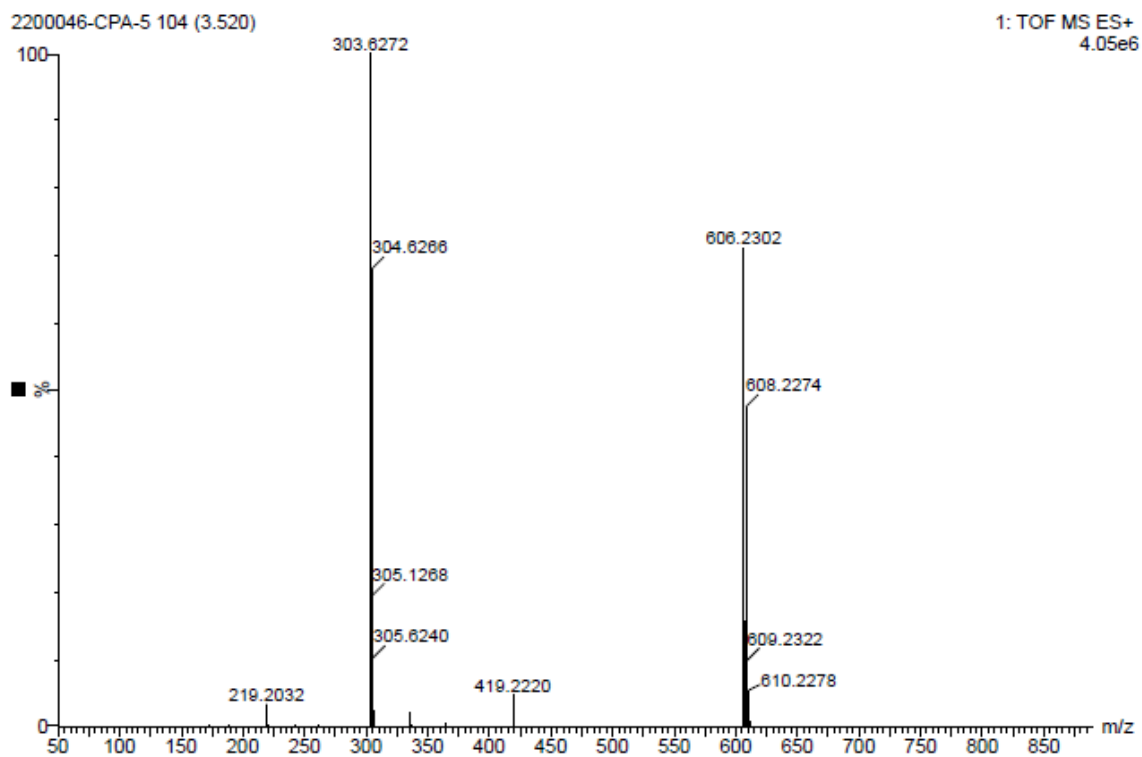
MCF-10A log curve of 3e



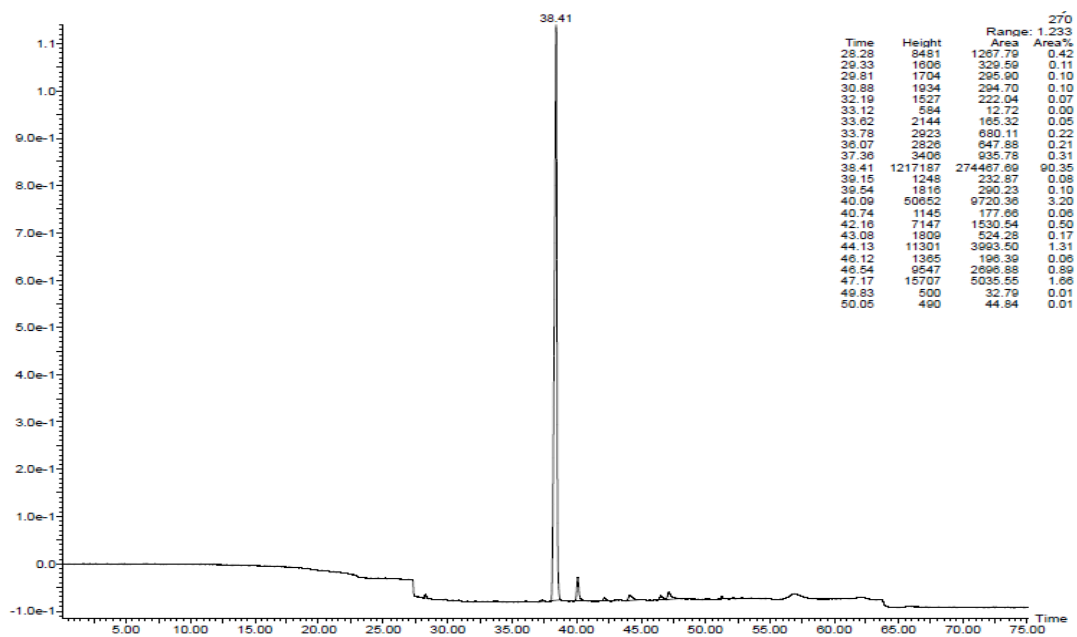
¹H NMR of 3f



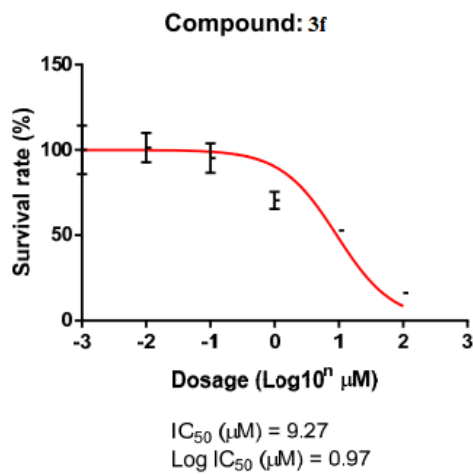
¹³C NMR of 3f



Mass spectra of **3f**



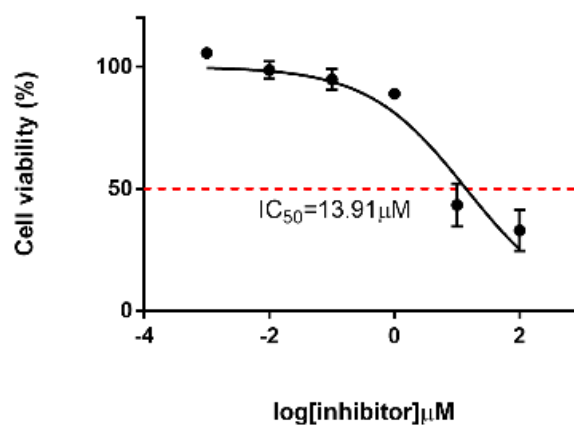
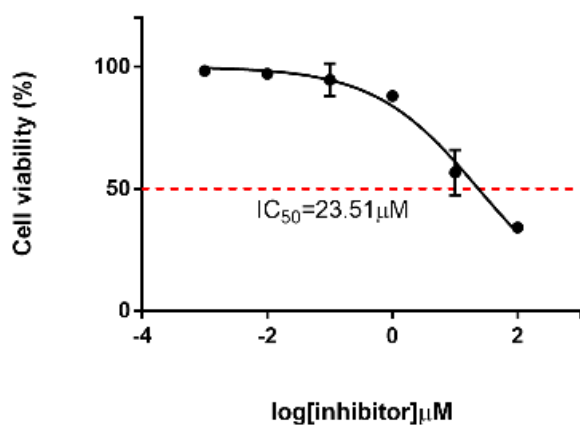
HPLC of **3f**



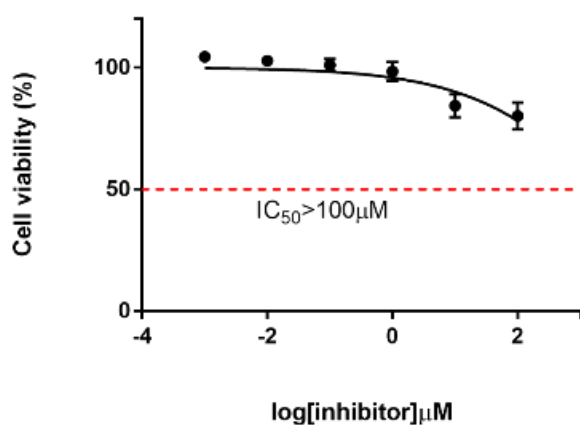
- Cell line: MCF7 (2000 cells/per well⁹⁶)
- Treated time: 72hrs
- Assay: MTT (90mins incubated)
- Data: 3f

Conc. (μM)	Viability	
	AVE.	\pm SD.
0	100.00	10.10
0.01	101.30	8.59
0.1	95.19	8.64
1	70.46	5.03
10	52.84	1.47
100	16.14	0.59

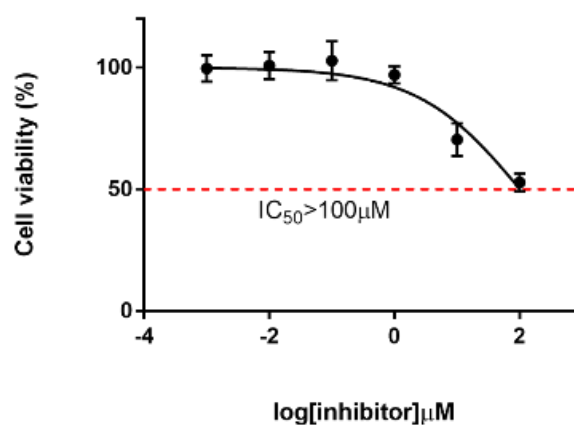
MCF-7 Log curve of 3f



T47D Log curve of 3f

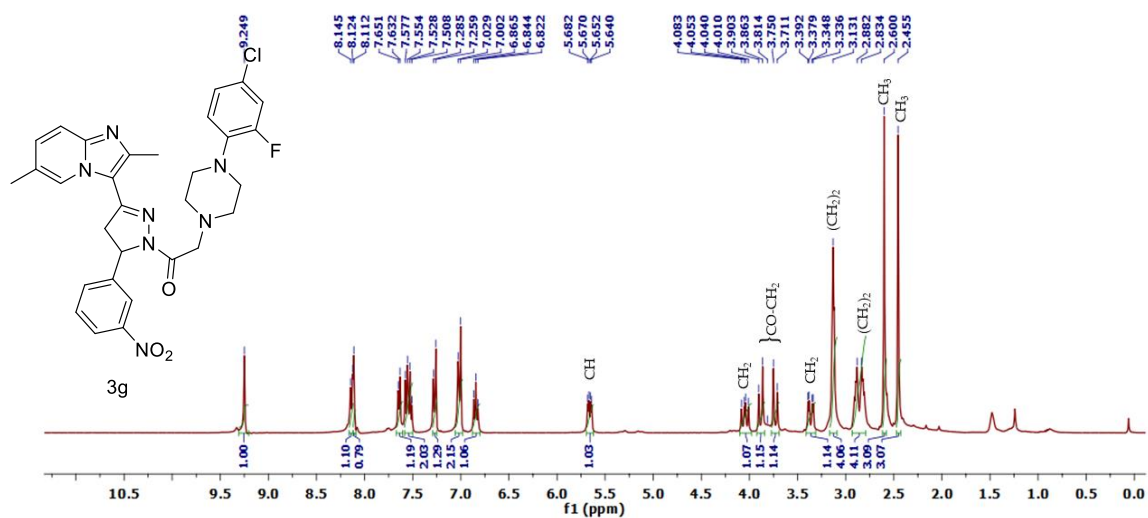


BT474 Log curve of 3f

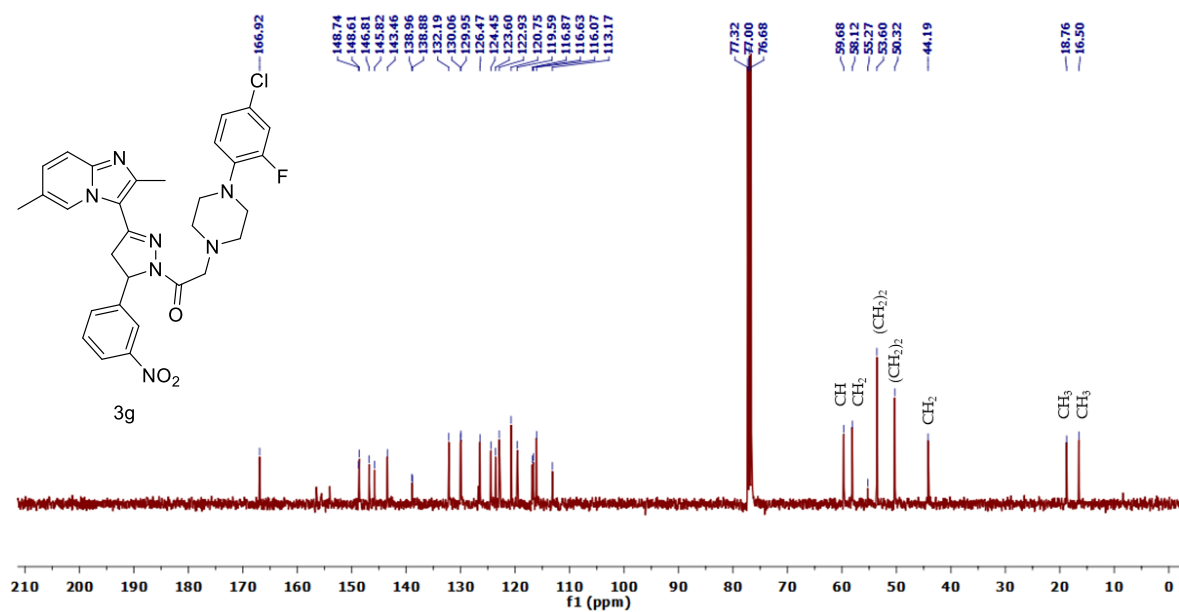


SK-BR-3 log curve of 3f

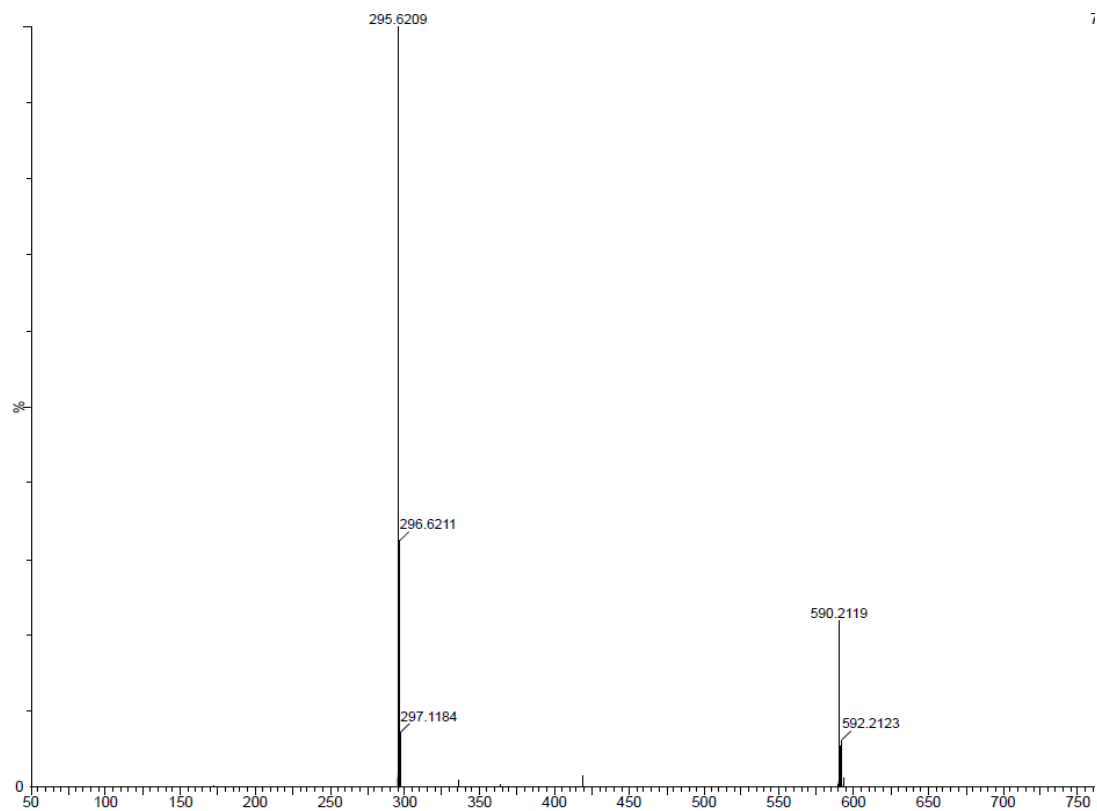
MCF-10A log curve of 3f



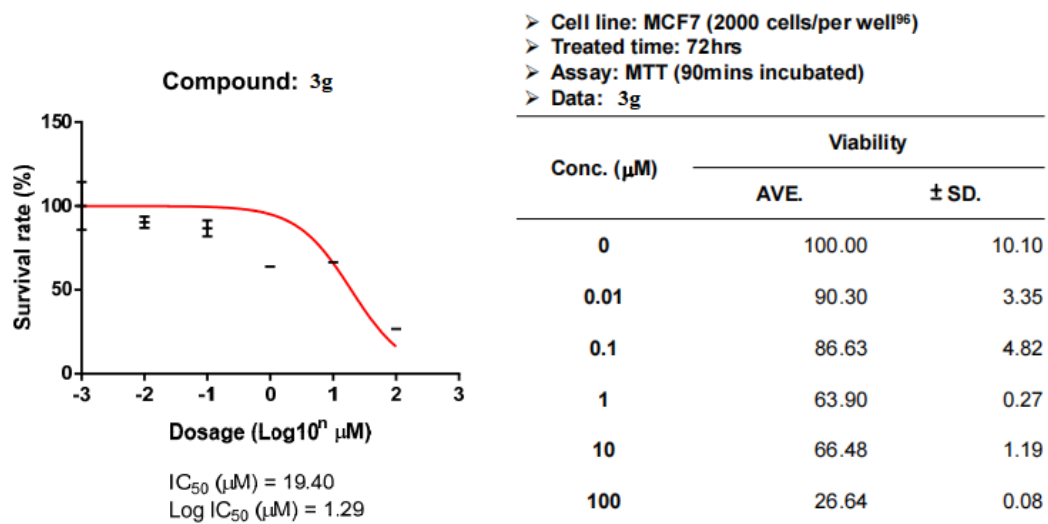
¹H NMR of 3g



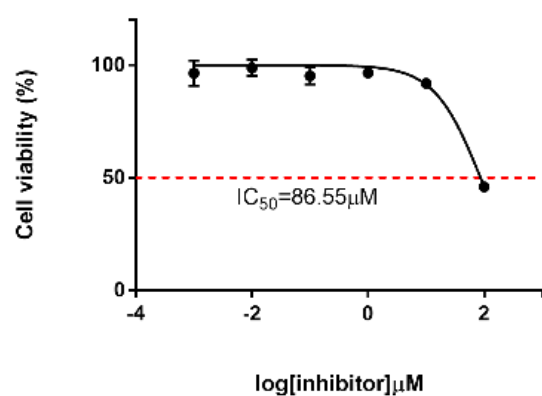
¹³C NMR of 3g



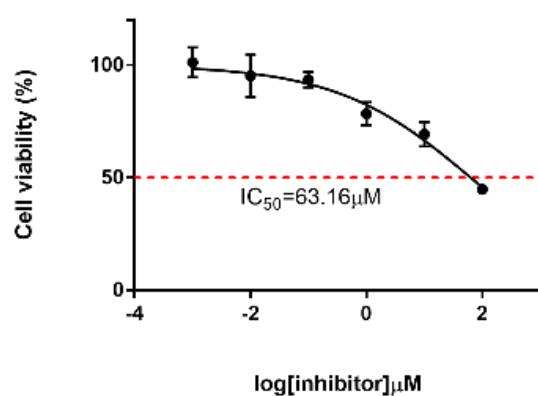
Mass spectra of 3g



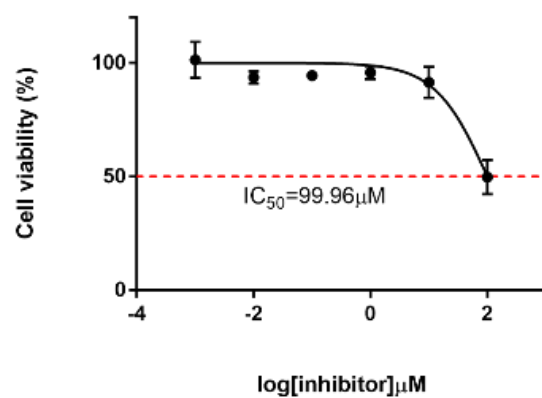
MCF-7 Log curve of 3g



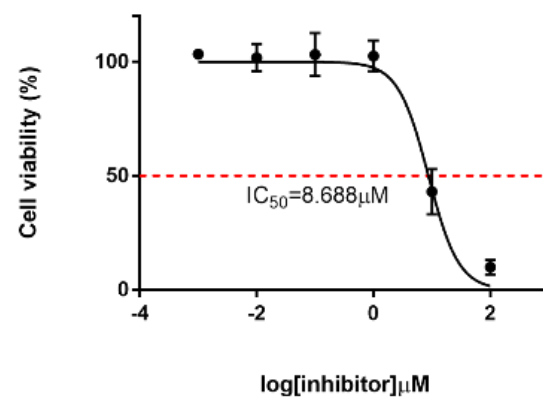
T47D Log curve of 3g



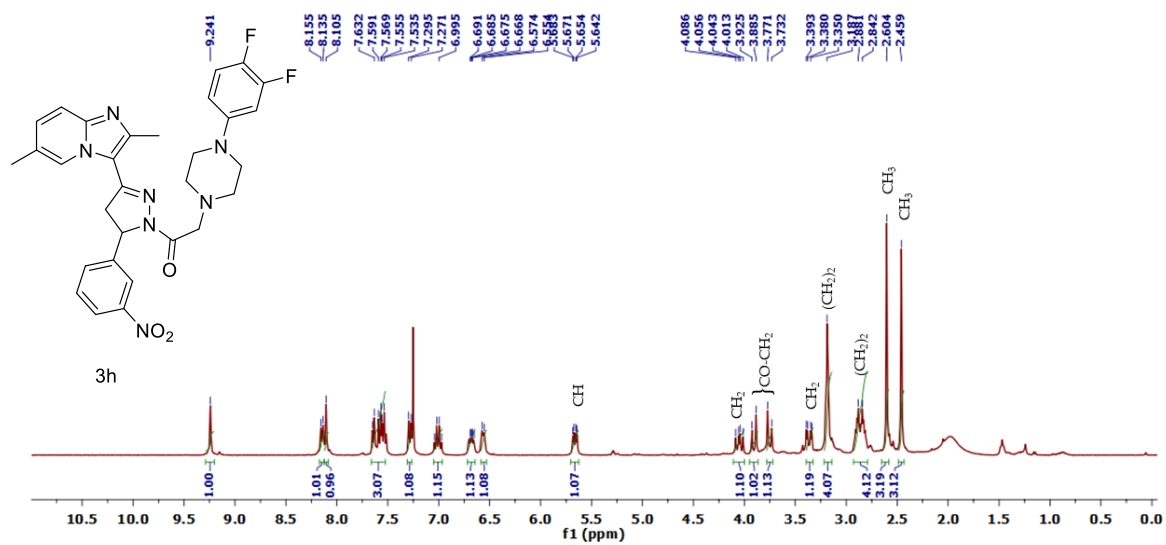
BT474 Log curve of 3g



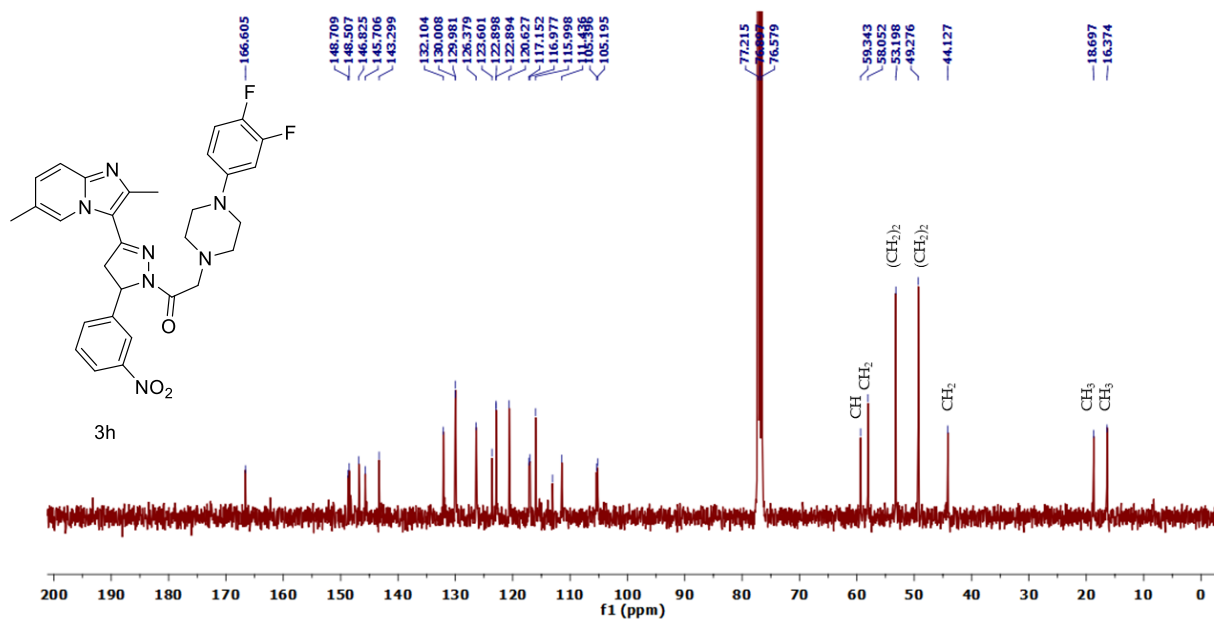
SK-BR-3 log curve of 3g



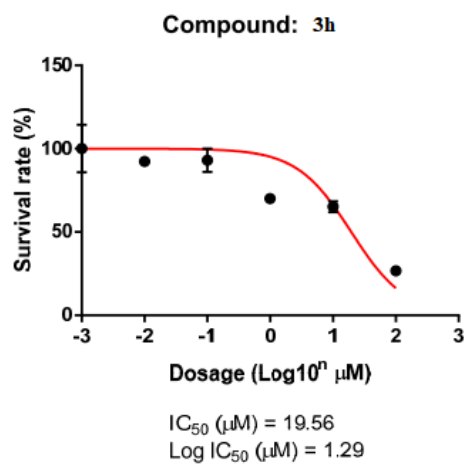
MCF-10A log curve of 3g



¹H NMR of 3h



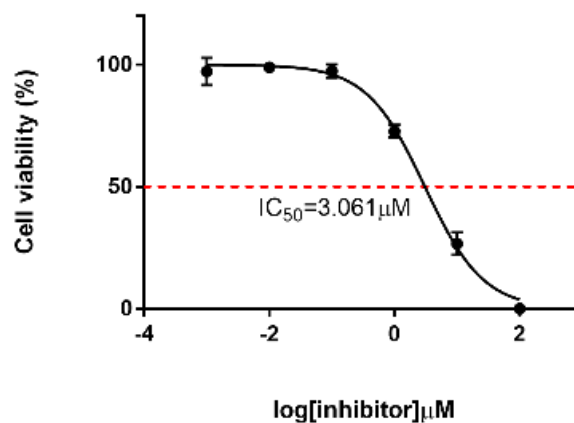
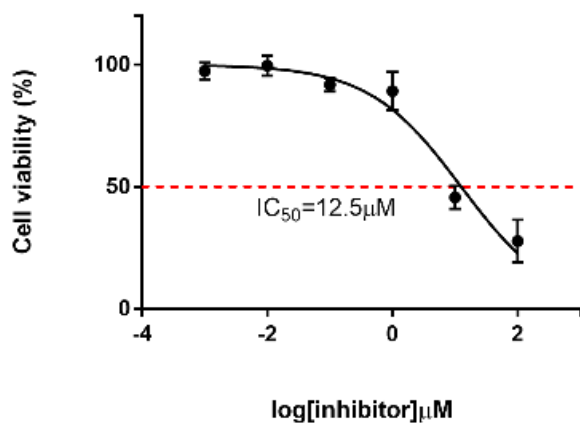
¹³C NMR of 3h



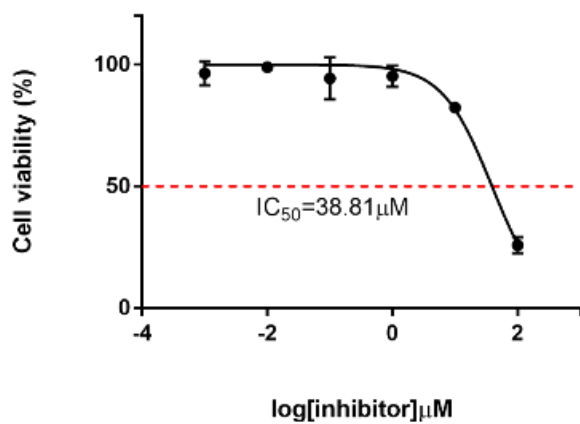
➤ Cell line: MCF7 (2000 cells/per well⁹⁶)
 ➤ Treated time: 72hrs
 ➤ Assay: MTT (90mins incubated)
 ➤ Data: 3h

Conc. (μM)	Viability	
	AVE.	\pm SD.
0	100.00	10.10
0.01	92.34	0.73
0.1	93.00	7.07
1	70.06	1.19
10	65.18	3.20
100	26.74	1.54

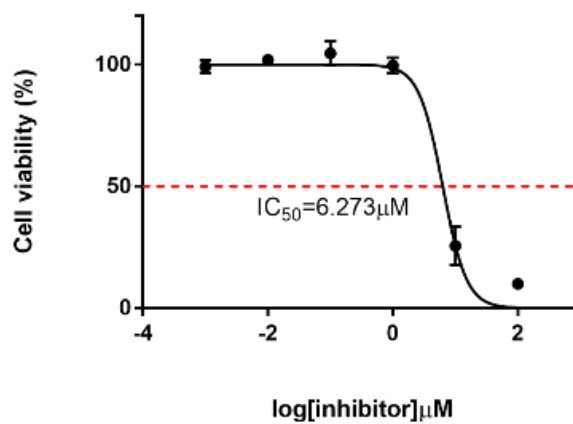
MCF-7 Log curve of 3h



T47D Log curve of 3h

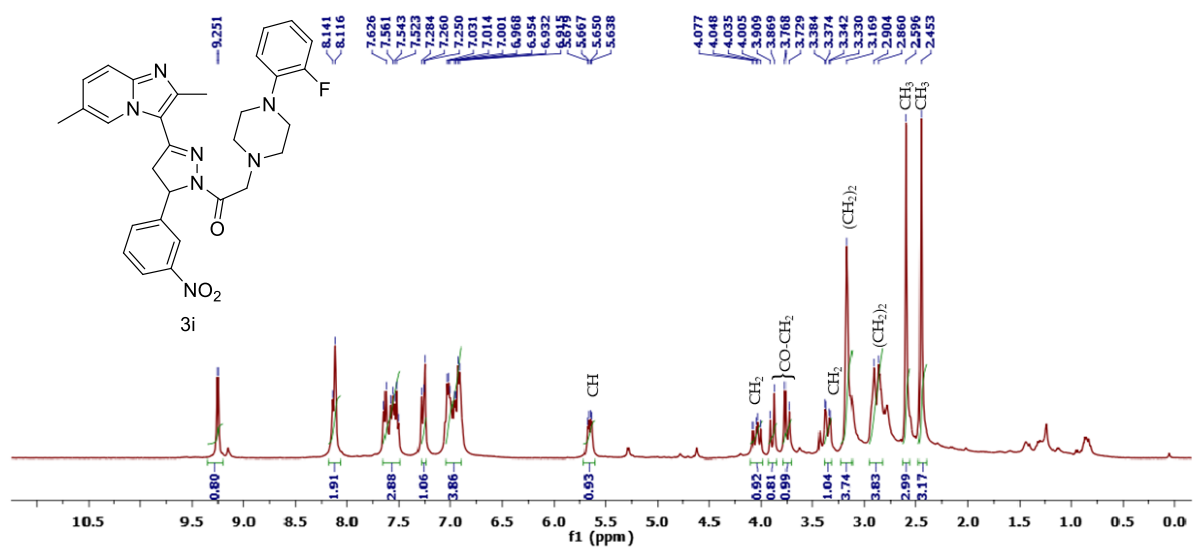


BT474 Log curve of 3h

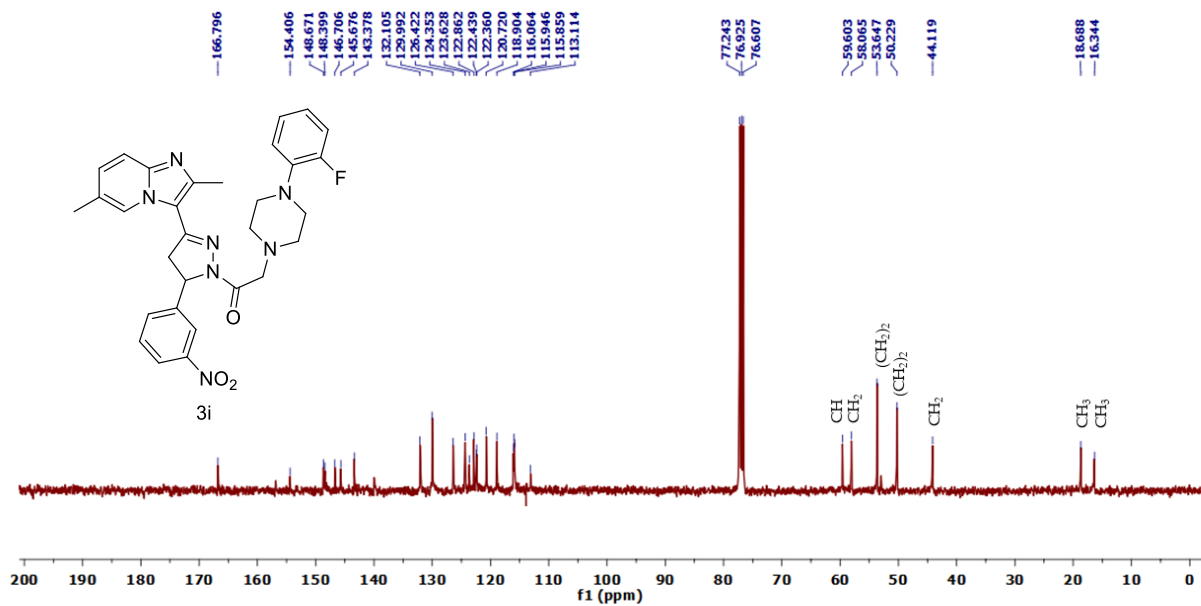


SK-BR-3 log curve of 3h

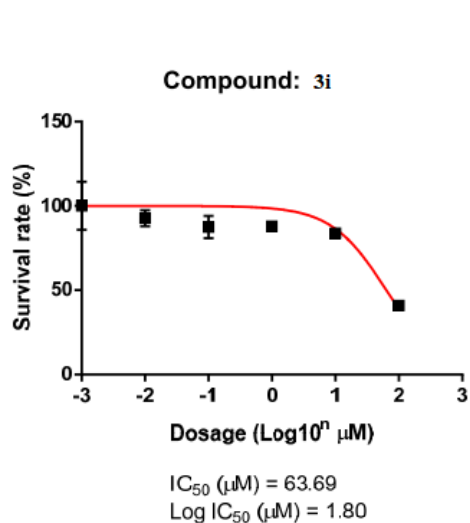
MCF-10A log curve of 3h



¹H NMR of 3i



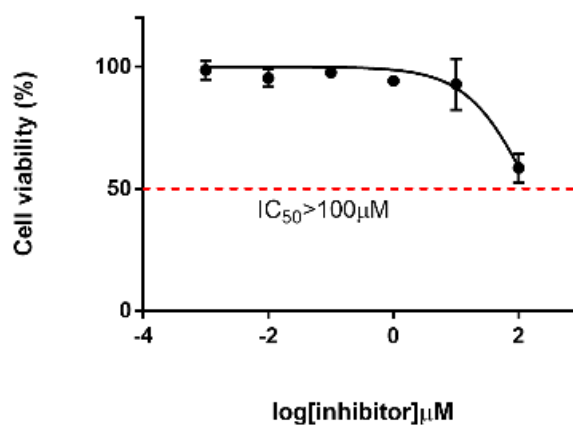
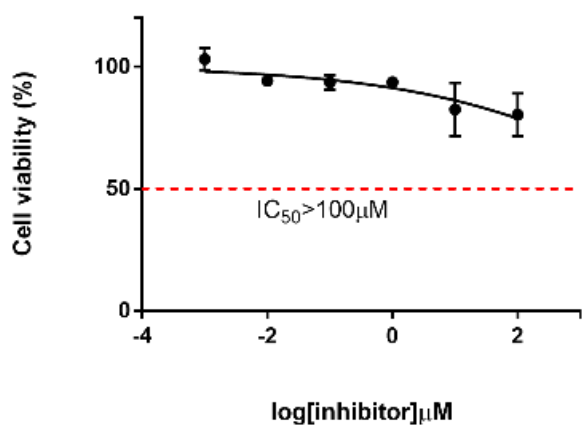
¹³C NMR of 3i



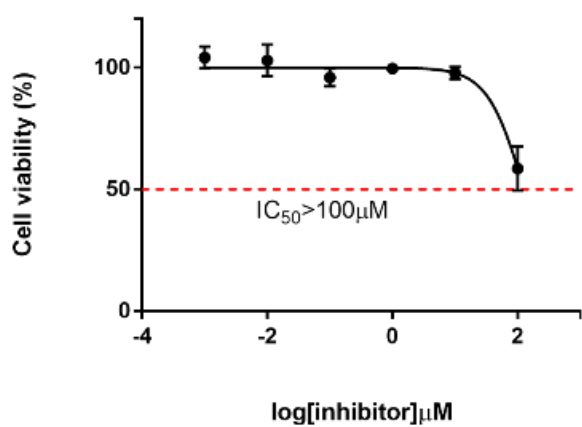
- Cell line: MCF7 (2000 cells/per well⁹⁶)
- Treated time: 72hrs
- Assay: MTT (90mins incubated)
- Data: 3i

Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	10.10
0.01	92.65	4.79
0.1	87.45	6.60
1	87.89	1.99
10	83.77	1.75
100	40.98	0.58

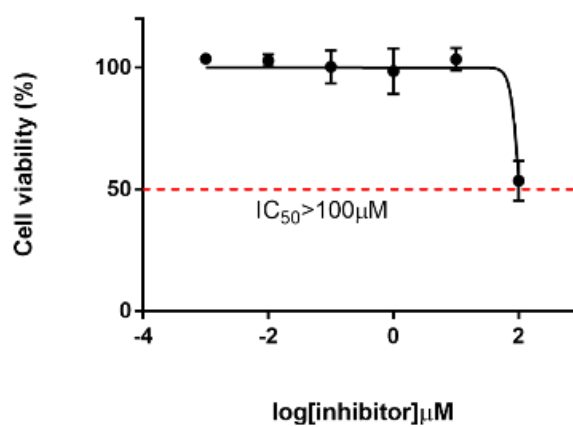
MCF-7 Log curve of 3i



T47D Log curve of 3i

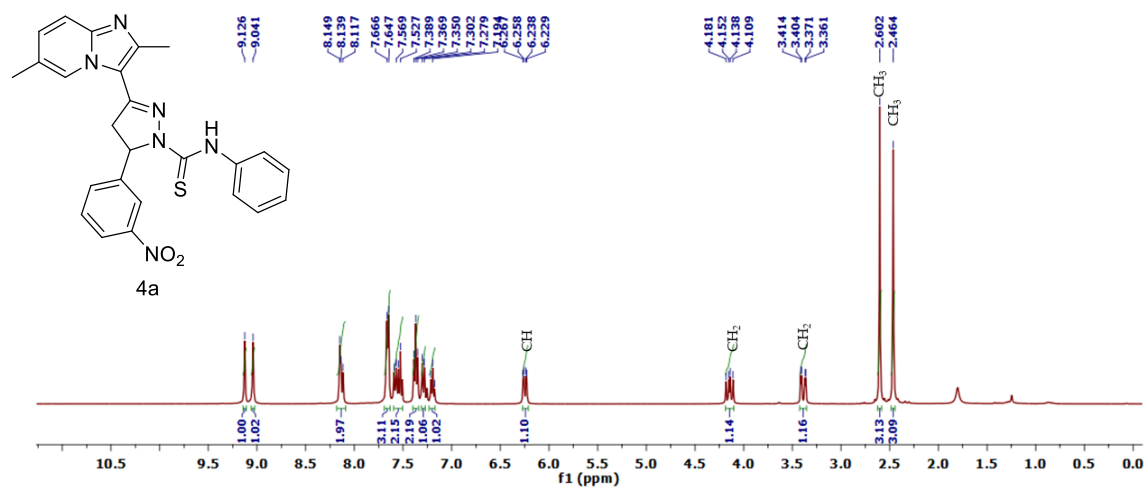


BT474 Log curve of 3i

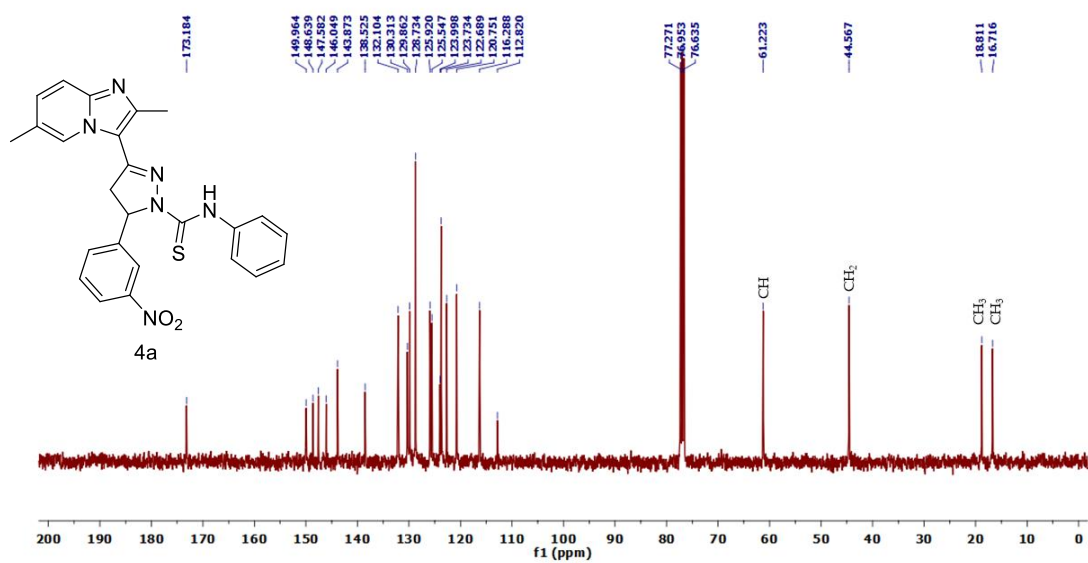


SK-BR-3 log curve of 3i

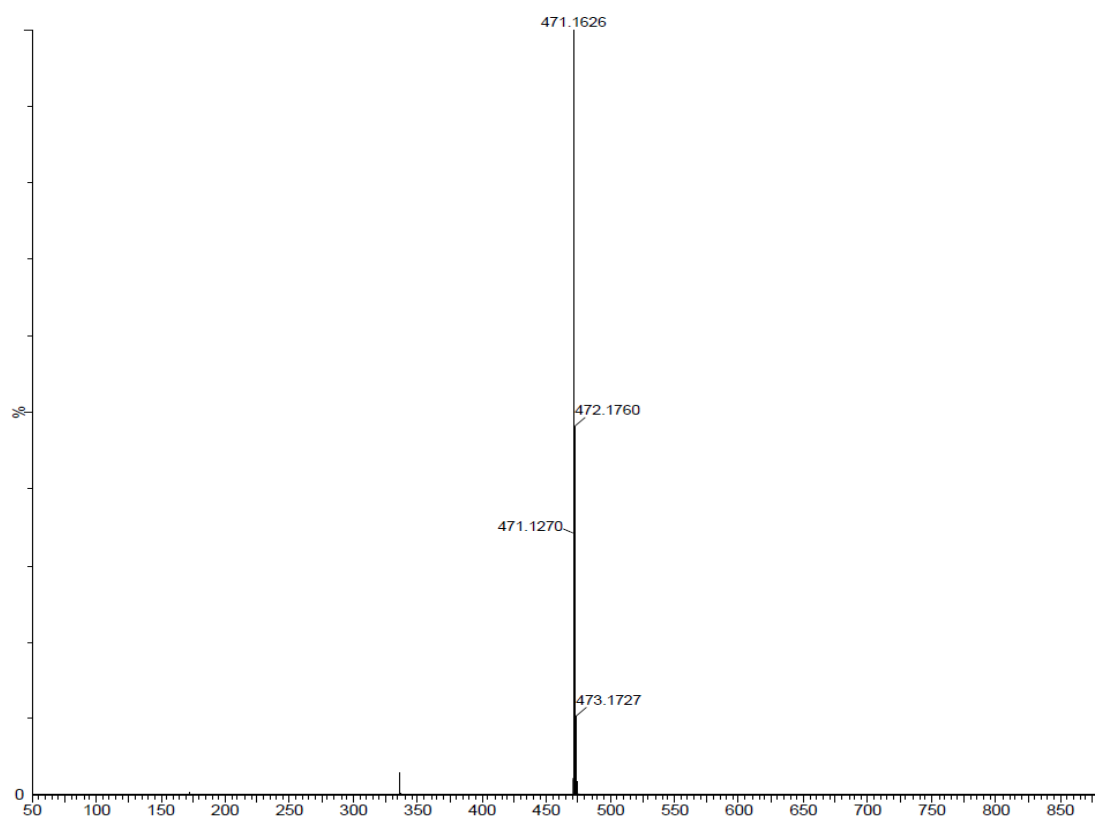
MCF-10A log curve of 3i



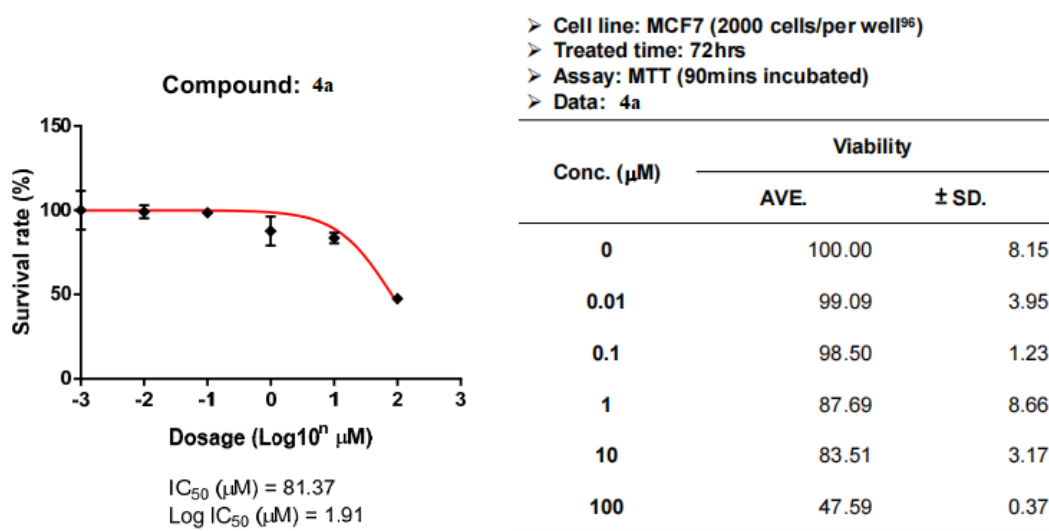
^1H NMR of **4a**



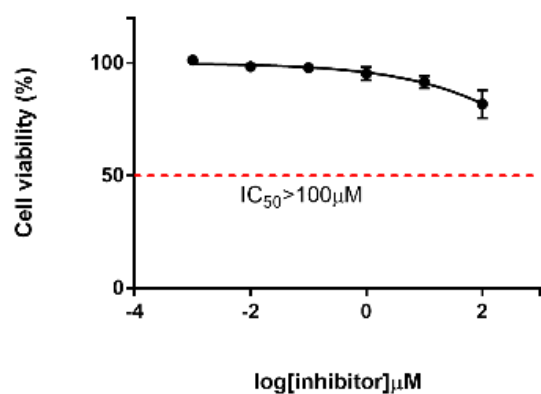
^{13}C NMR of **4a**



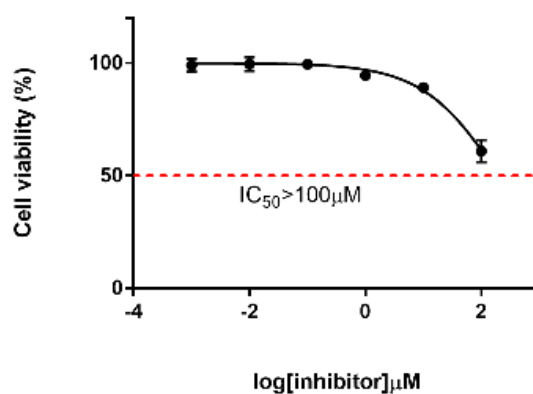
Mass spectra of **4a**



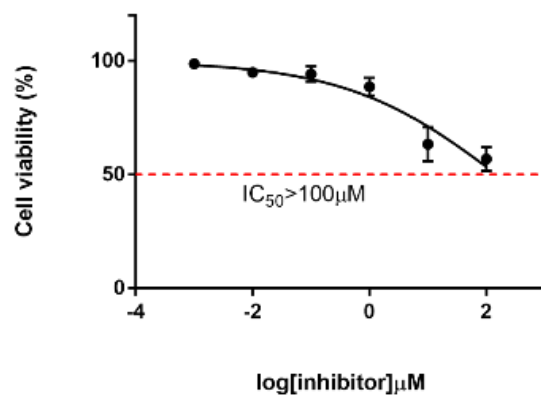
MCF-7 Log curve of **4a**



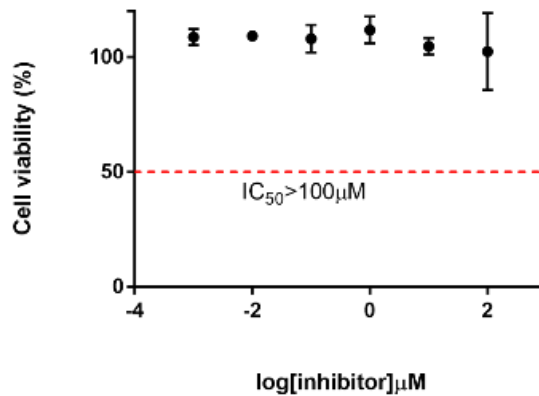
T47D Log curve of 4a



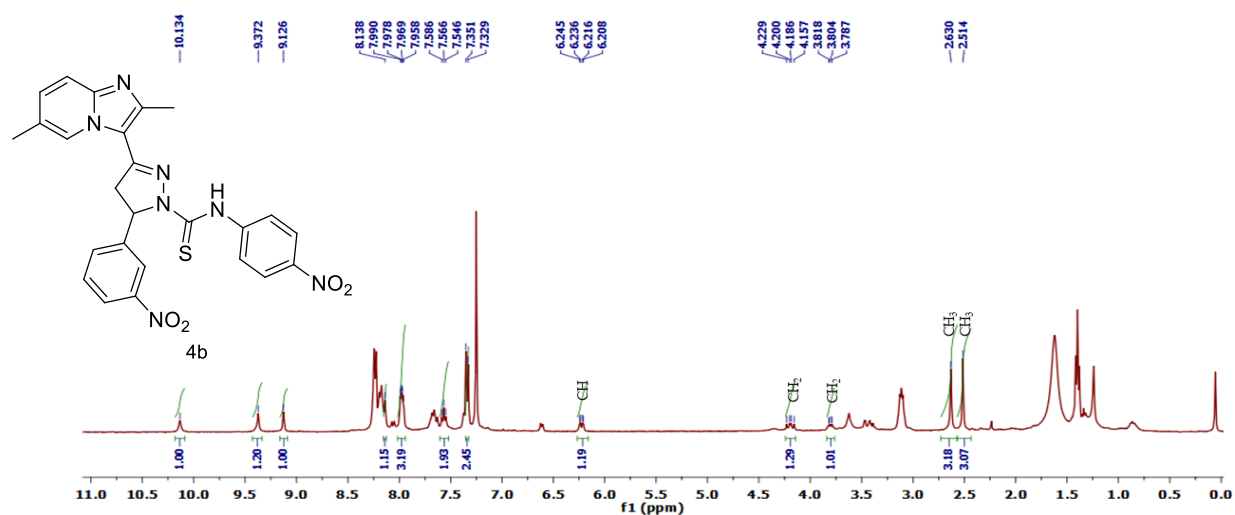
BT474 Log curve of 4a



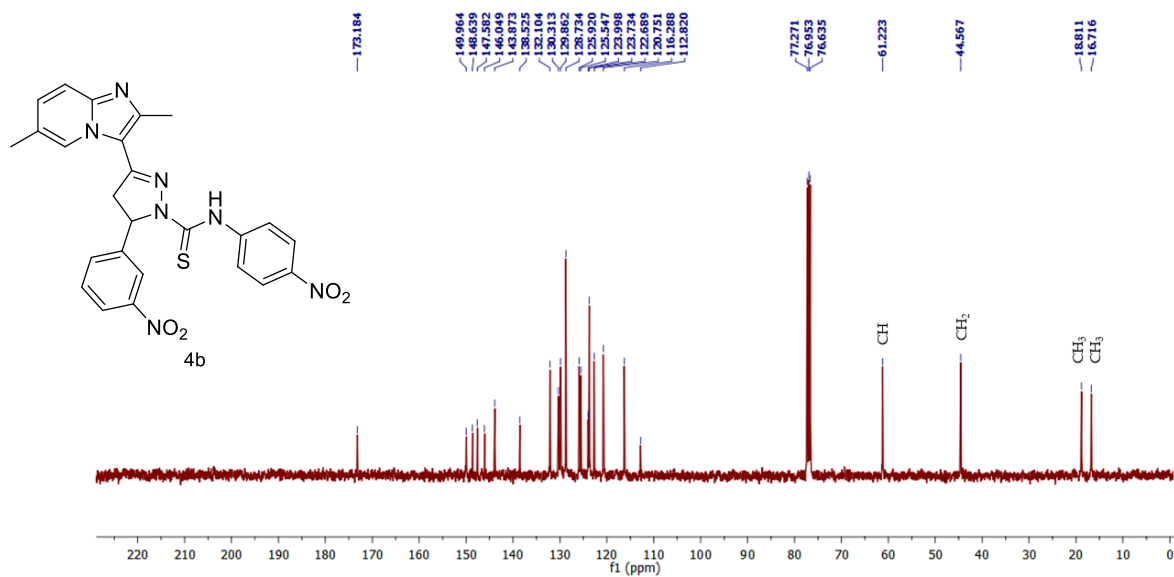
SK-BR-3 log curve of 4a



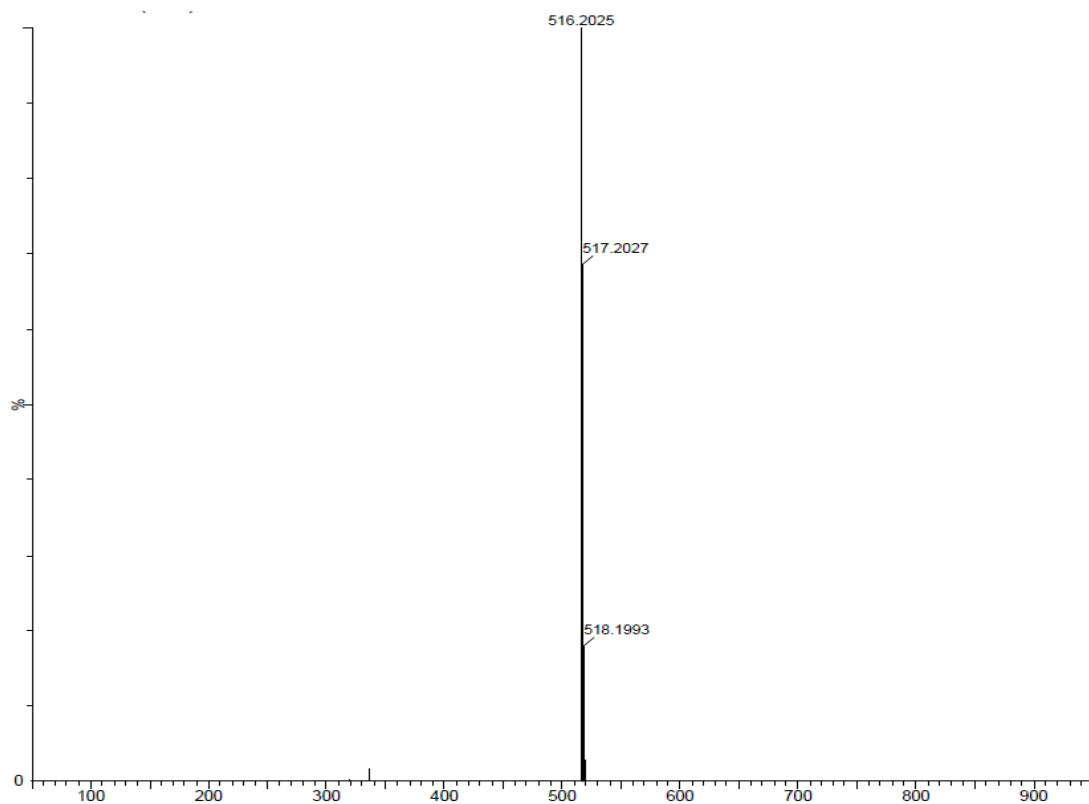
MCF-10A log curve of 4a



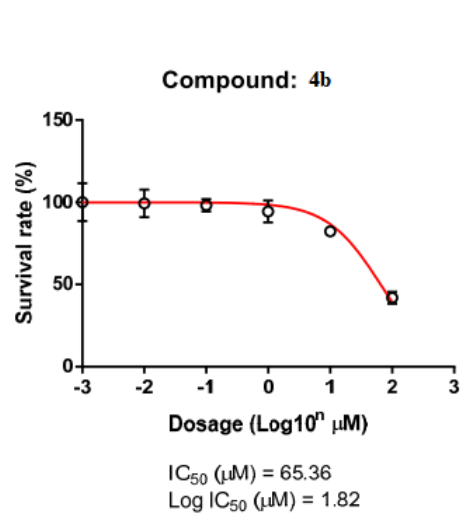
1H NMR of 4b



^{13}C NMR of **4b**



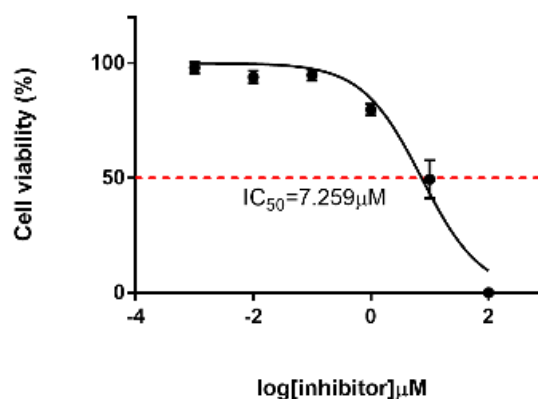
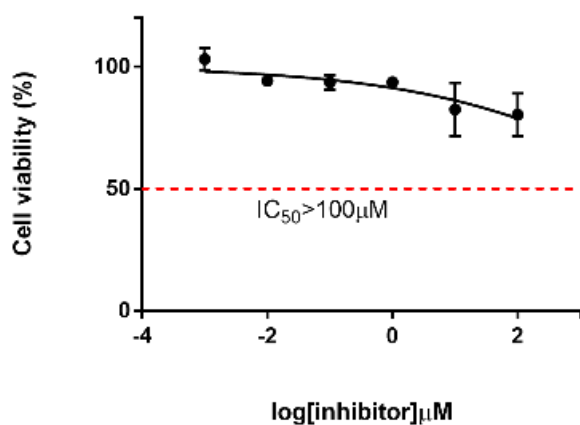
Mass spectra of **4b**



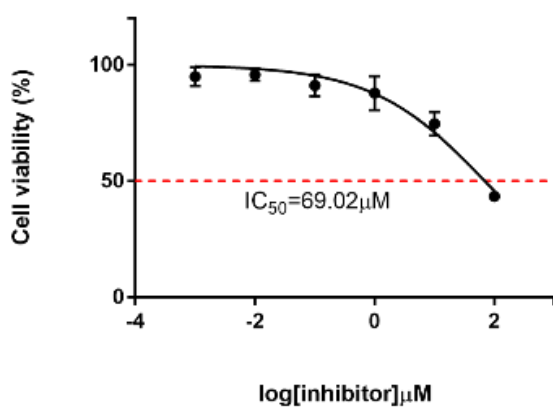
- Cell line: MCF7 (2000 cells/per well⁹⁶)
- Treated time: 72hrs
- Assay: MTT (90mins incubated)
- Data: 4b

Conc. (μM)	Viability	
	AVE.	\pm SD.
0	100.00	8.15
0.01	99.30	8.37
0.1	98.13	3.79
1	94.47	6.67
10	82.35	0.89
100	41.89	3.66

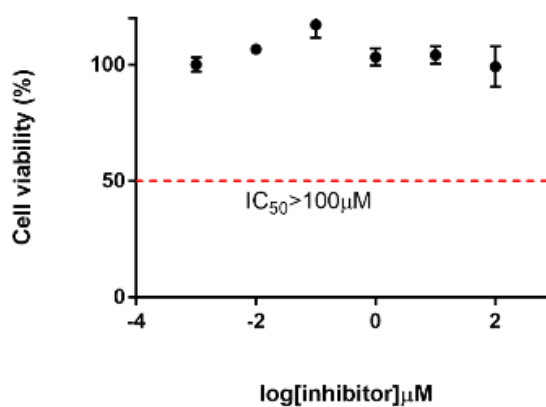
MCF-7 Log curve of 4b



T47D Log curve of 4b

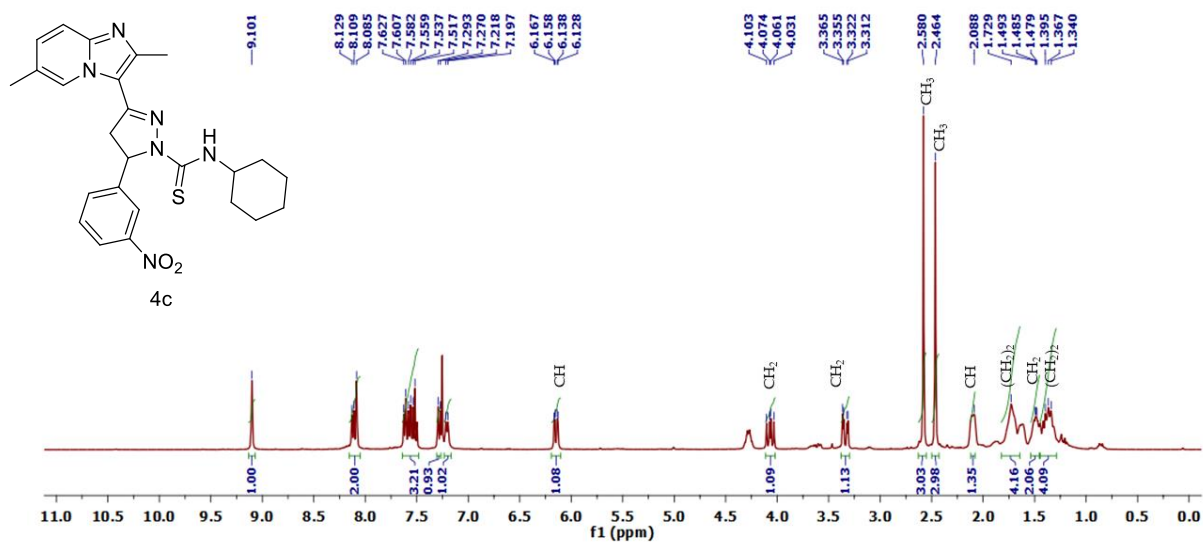


BT474 Log curve of 4b

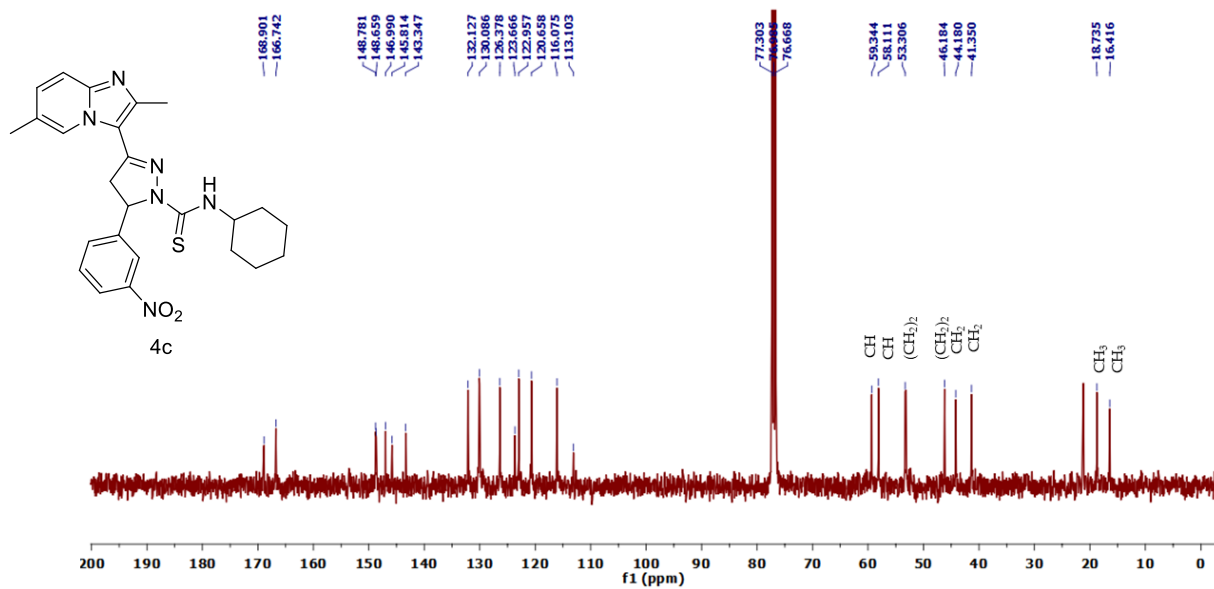


SK-BR-3 log curve of 4b

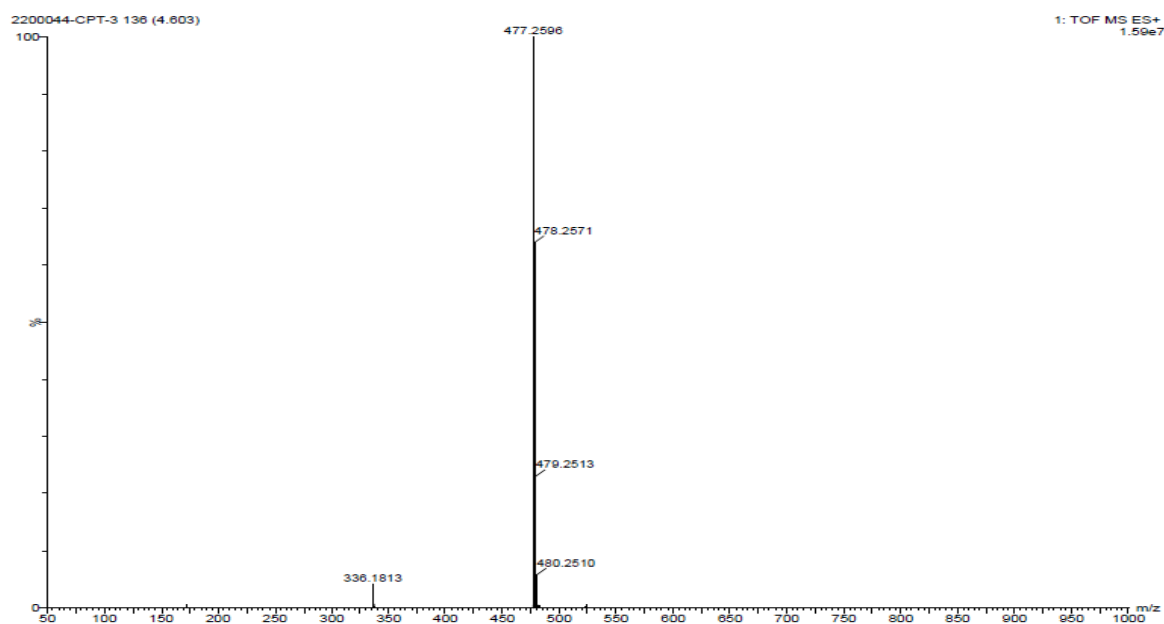
MCF-10A log curve of 4b



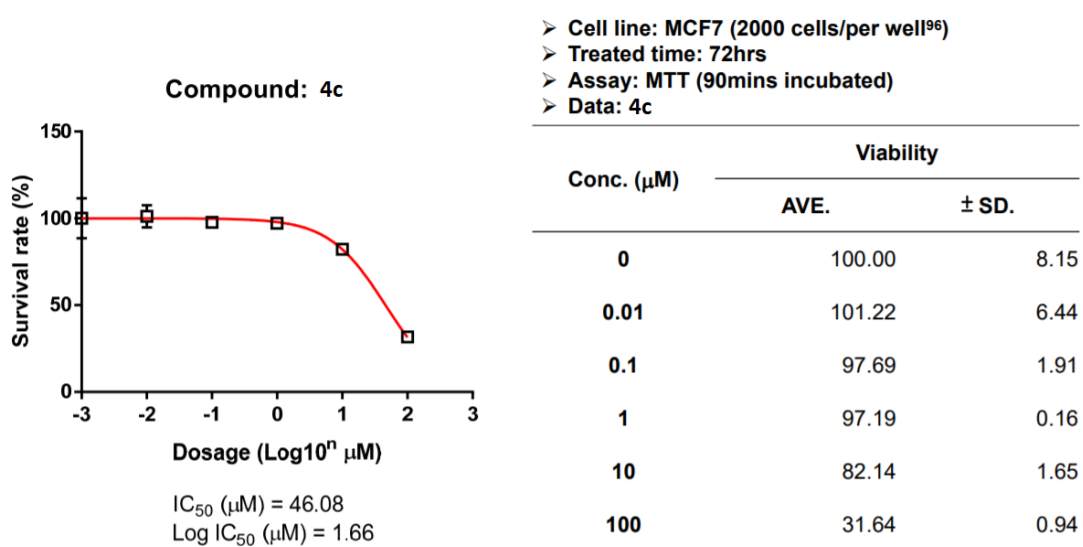
^1H NMR of 4c



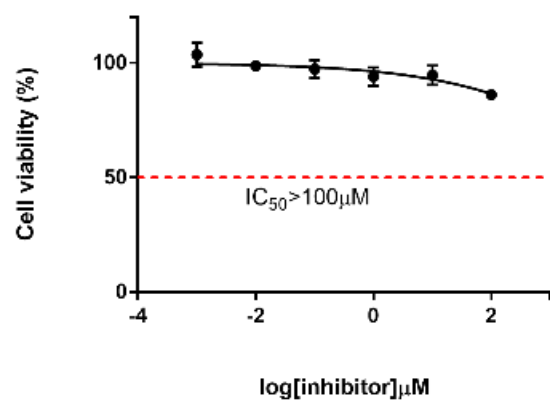
^{13}C NMR of 4c



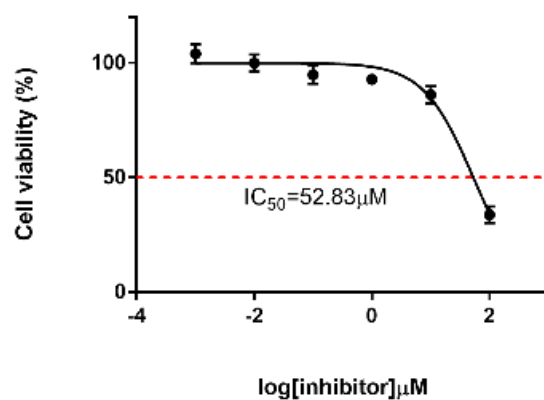
Mass spectra of compound 4c



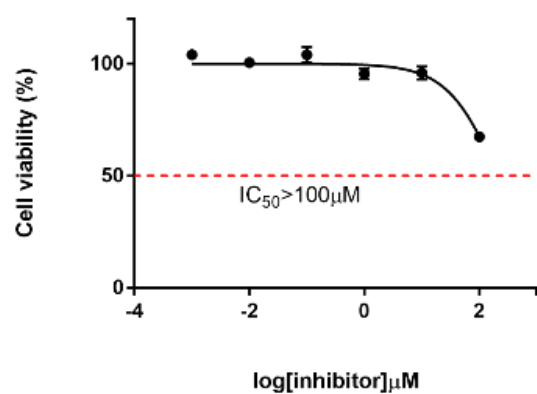
MCF-7 Log curve of 4c



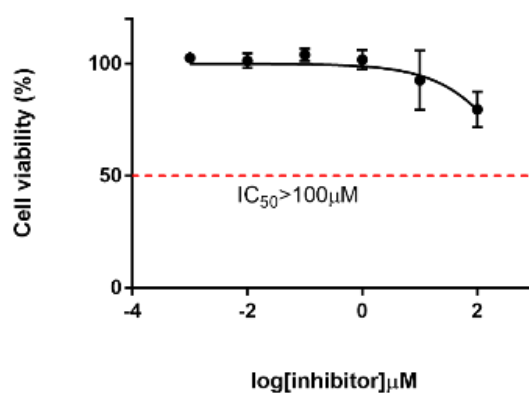
T47D Log curve of 4c



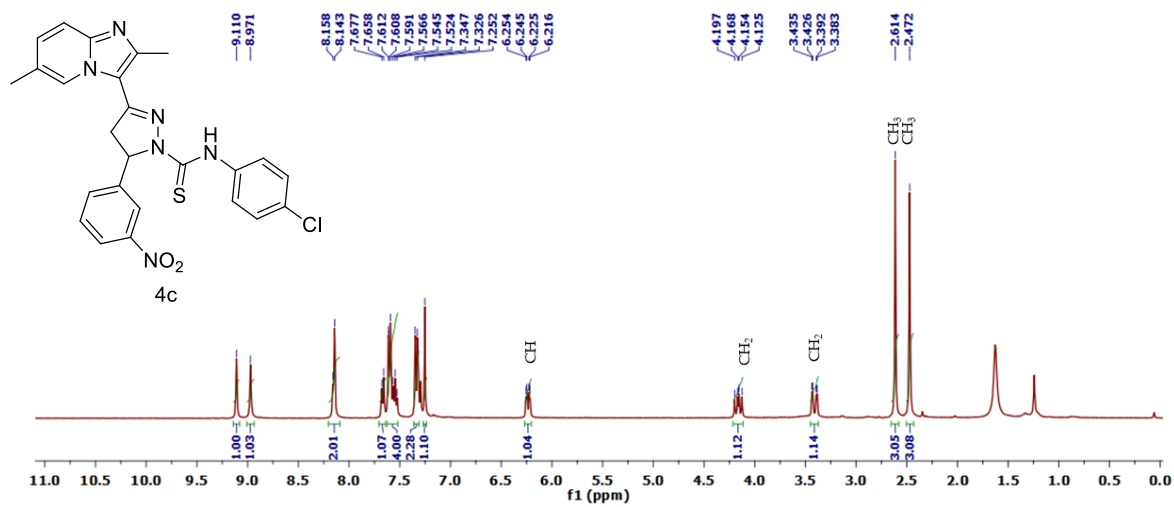
BT474 Log curve of 4c



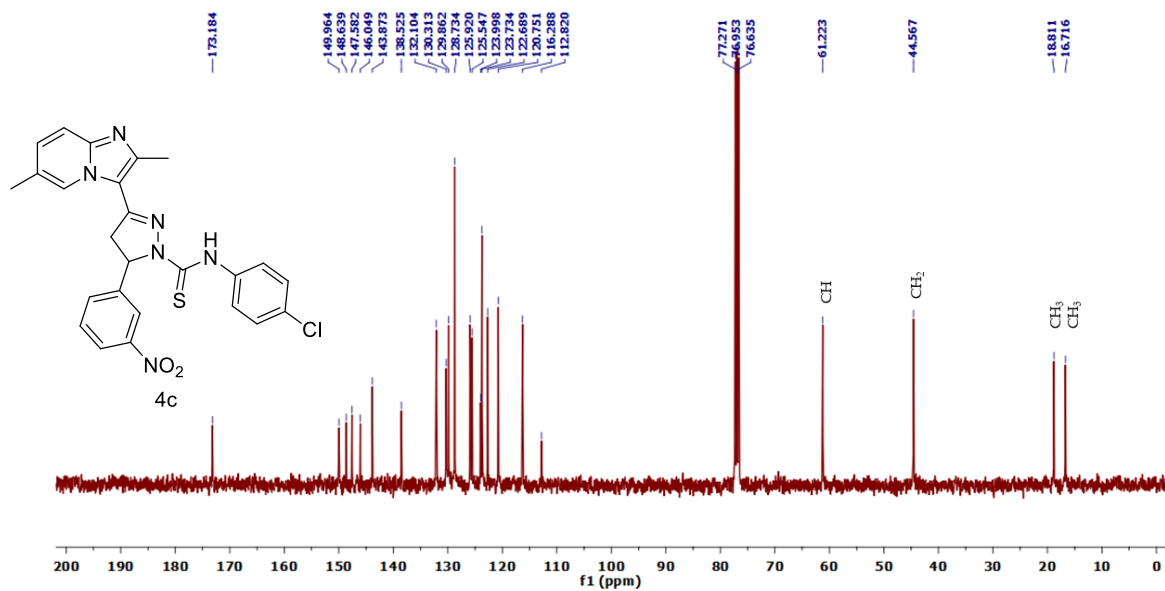
SK-BR-3 log curve of 4c



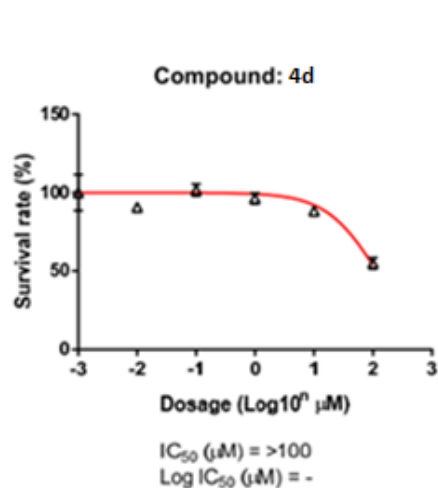
MCF-10A log curve of 4c



^1H NMR of 4d



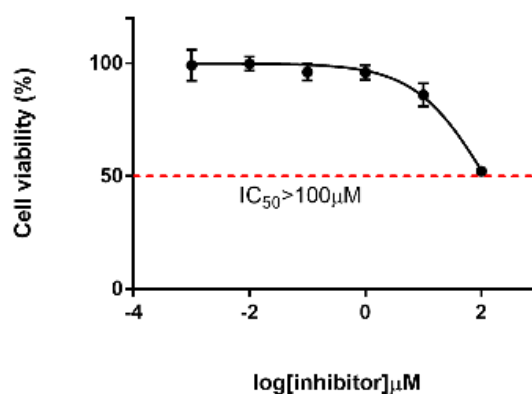
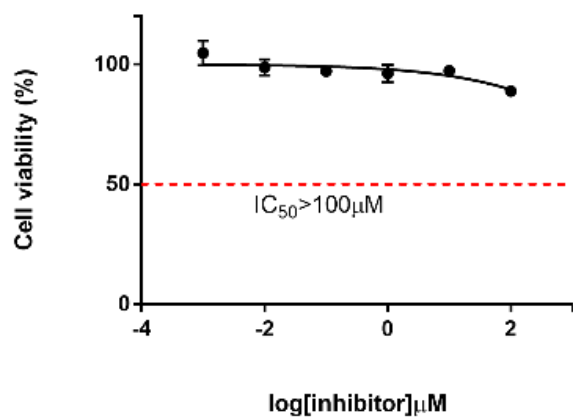
^{13}C NMR of 4d



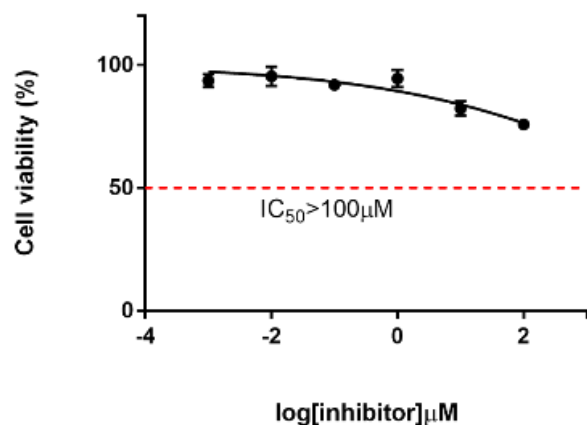
> Cell line: MCF7 (2000 cells/per wellTM)
 > Treated time: 72hrs
 > Assay: MTT (90mins incubated)
 > Data: 4d

Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	8.15
0.01	90.64	0.94
0.1	101.68	3.79
1	96.32	3.43
10	88.34	1.94
100	54.96	3.56

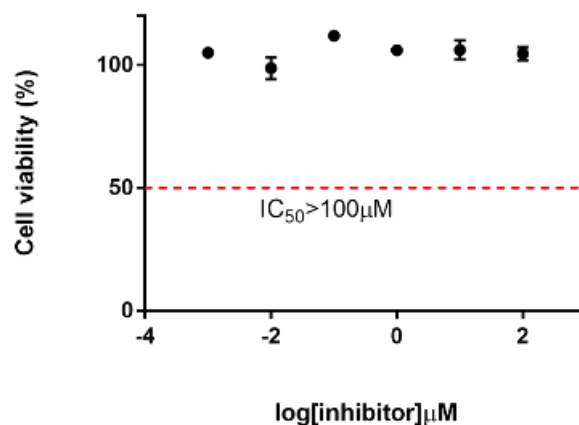
MCF-7 Log curve of 4d



T47D Log curve of 4d

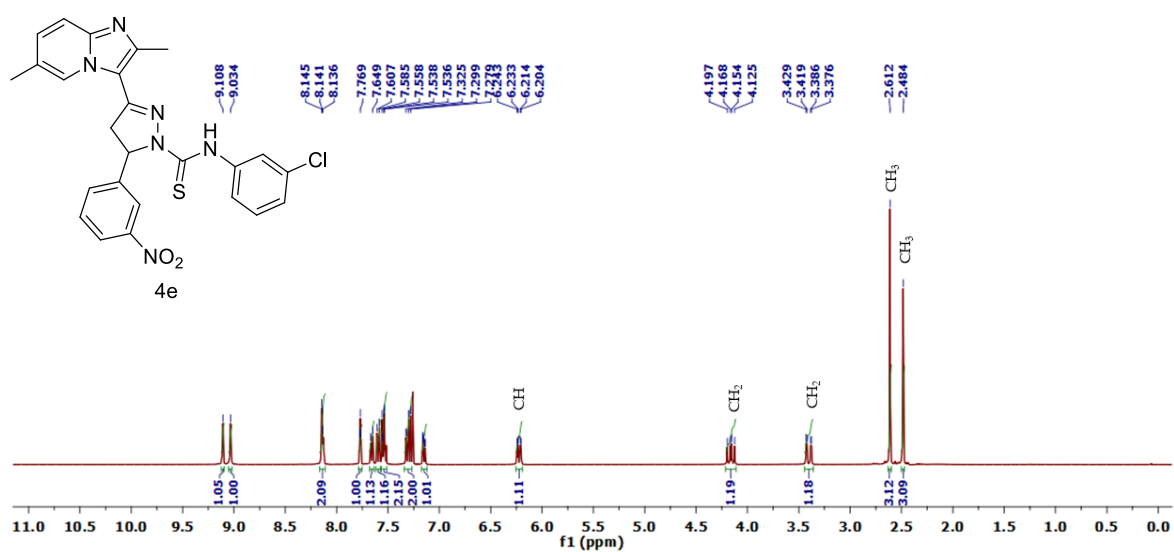


BT474 Log curve of 4d

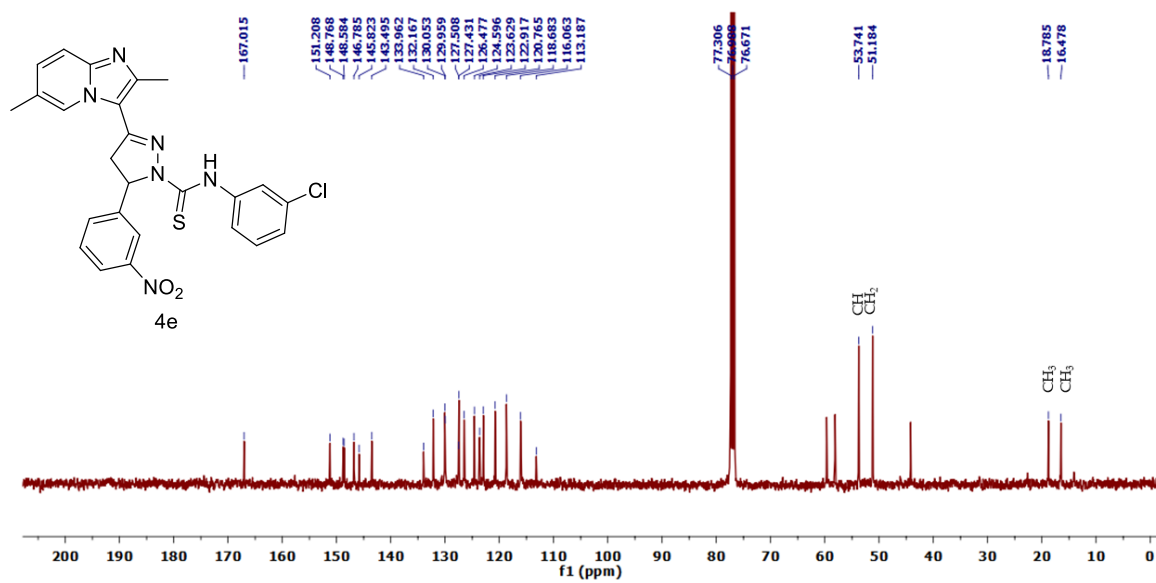


SK-BR-3 log curve of 4d

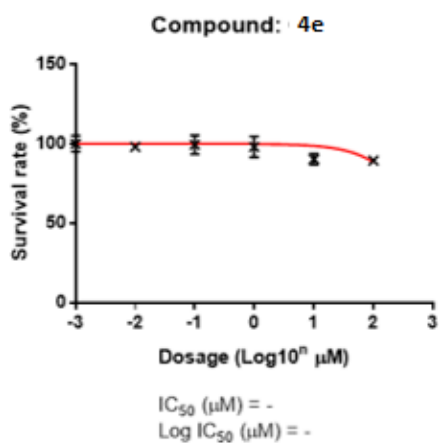
MCF-10A log curve of 4d



^1H NMR of 4e



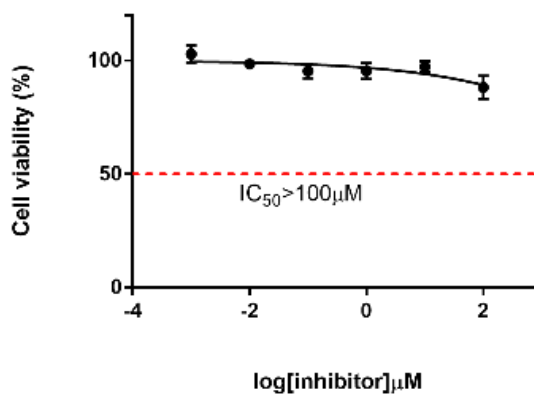
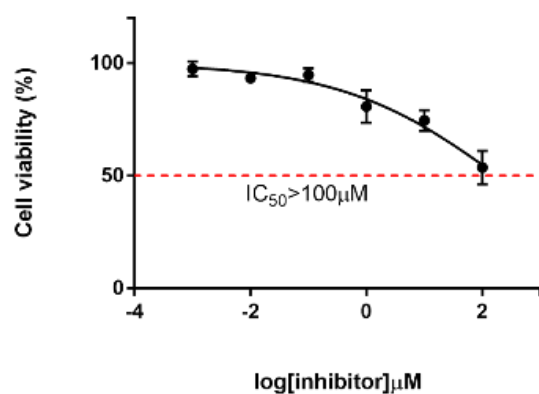
^{13}C NMR of 4e



> Cell line: MCF7 (2000 cells/per well⁸⁹)
 > Treated time: 72hrs
 > Assay: alamarBlue (4hrs incubated)
 > Data: 4e

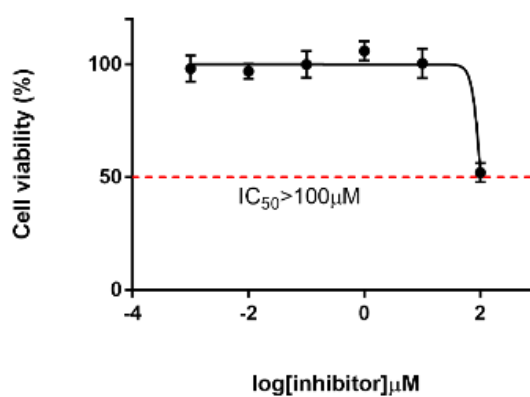
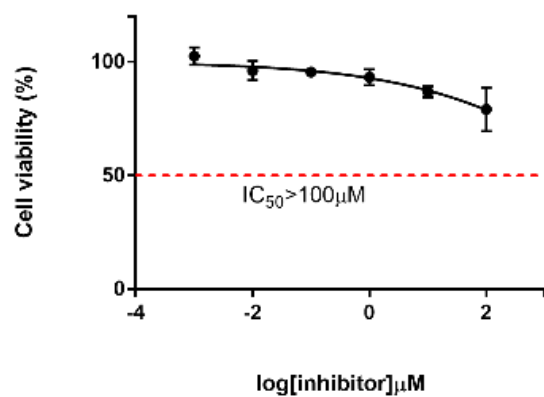
Conc. (μM)	Viability	
	AVE.	\pm SD.
0	100.00	5.15
0.01	98.04	0.80
0.1	99.43	5.84
1	98.11	6.52
10	90.29	3.55
100	89.47	2.21

MCF-7 Log curve of 4e



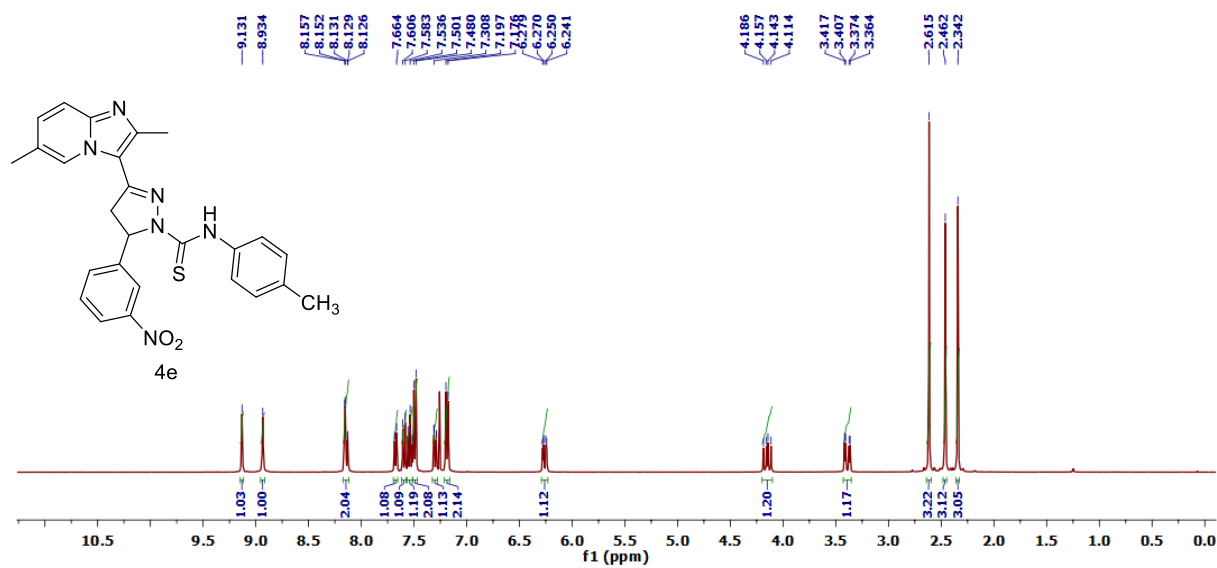
T47D Log curve of 4e

BT474 Log curve of 4e

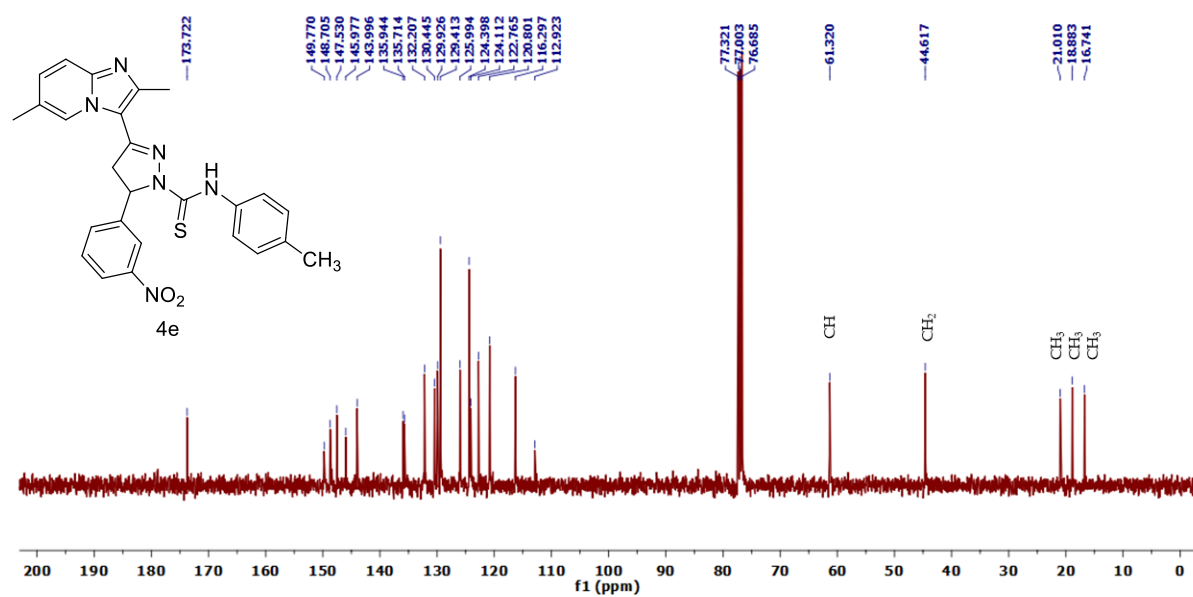


SK-BR-3 log curve of 4e

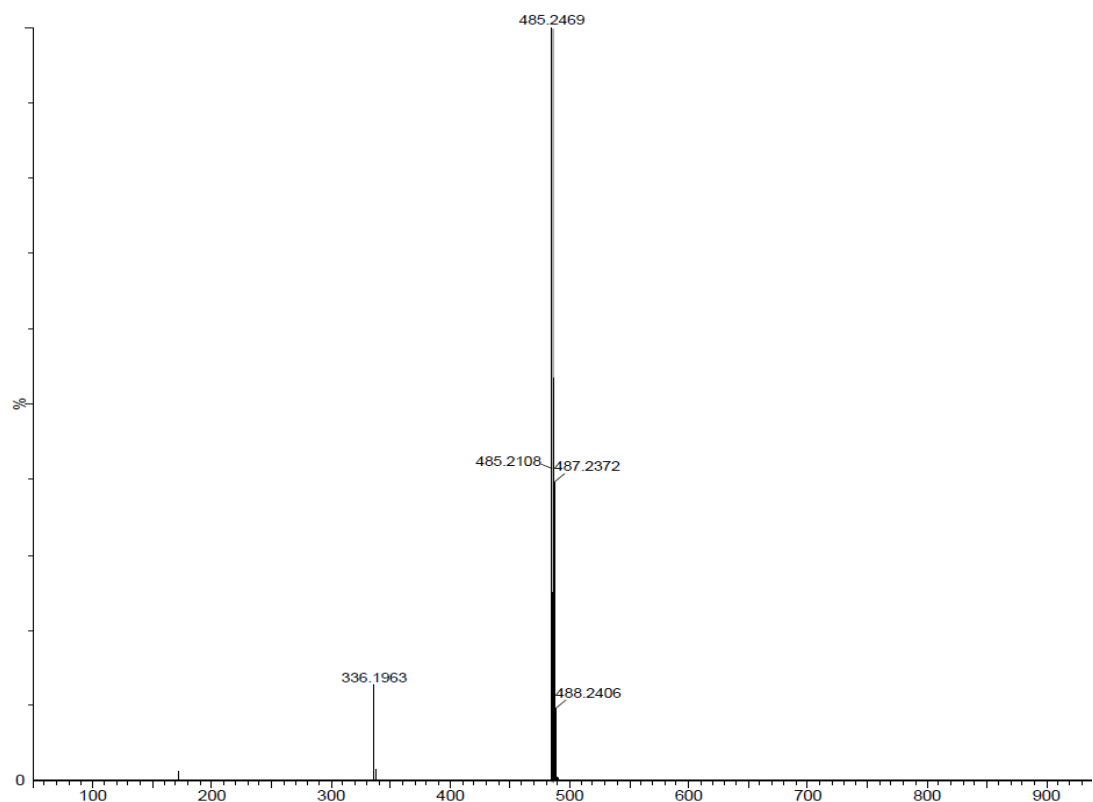
MCF-10A log curve of 4e



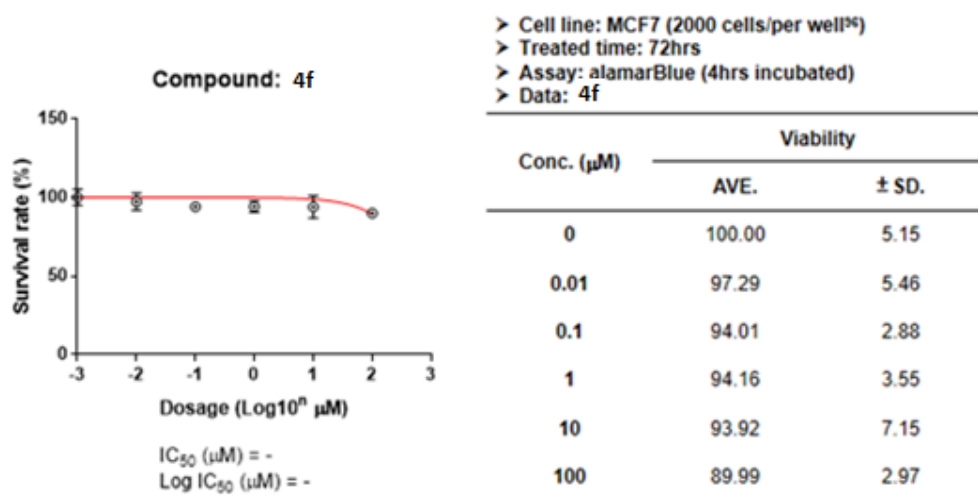
¹H NMR of 4f



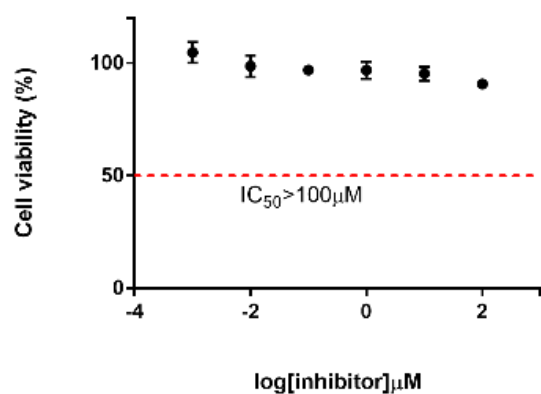
¹³C NMR of 4f



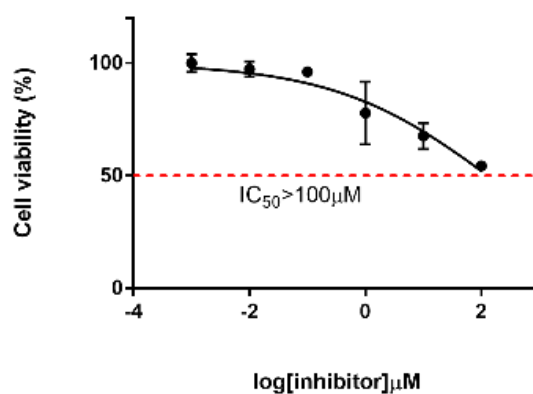
Mass spectra of 4f



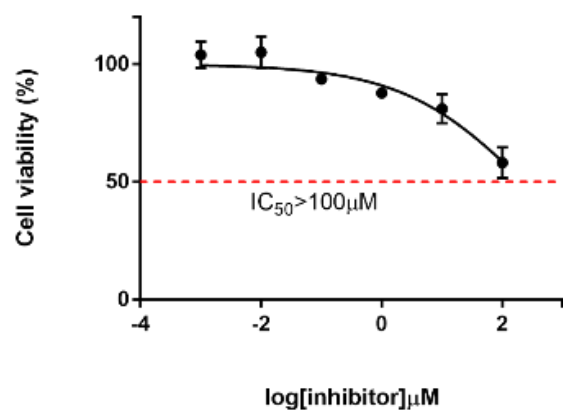
MCF-7 Log curve of 4f



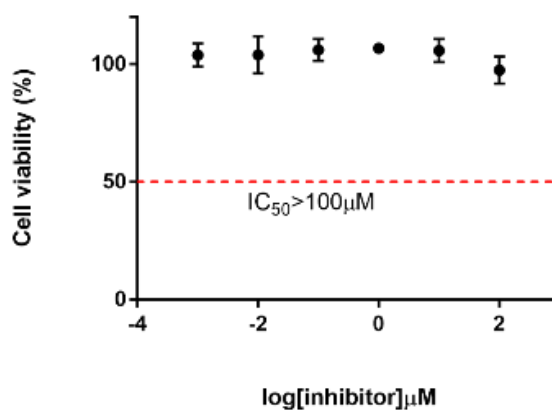
T47D Log curve of 4f



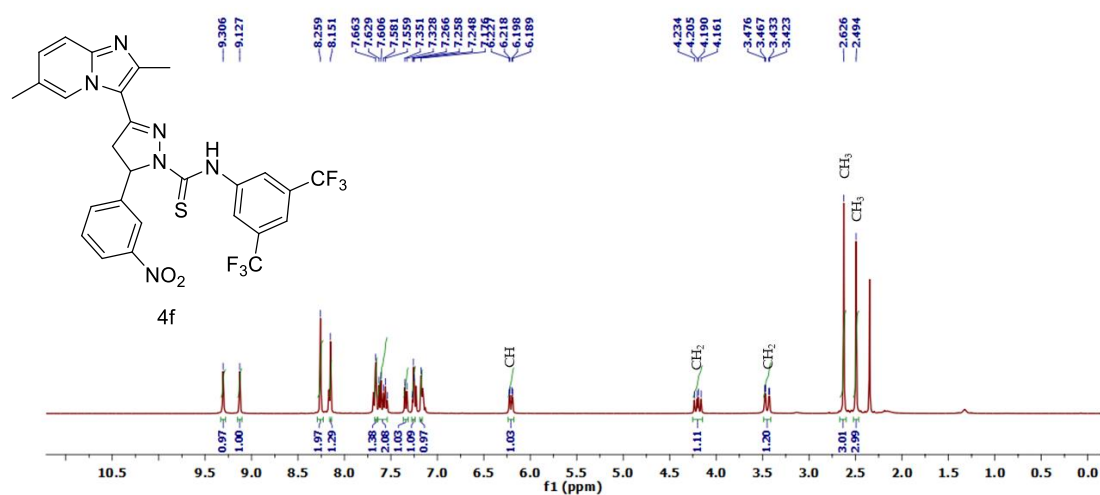
BT474 Log curve of 4f



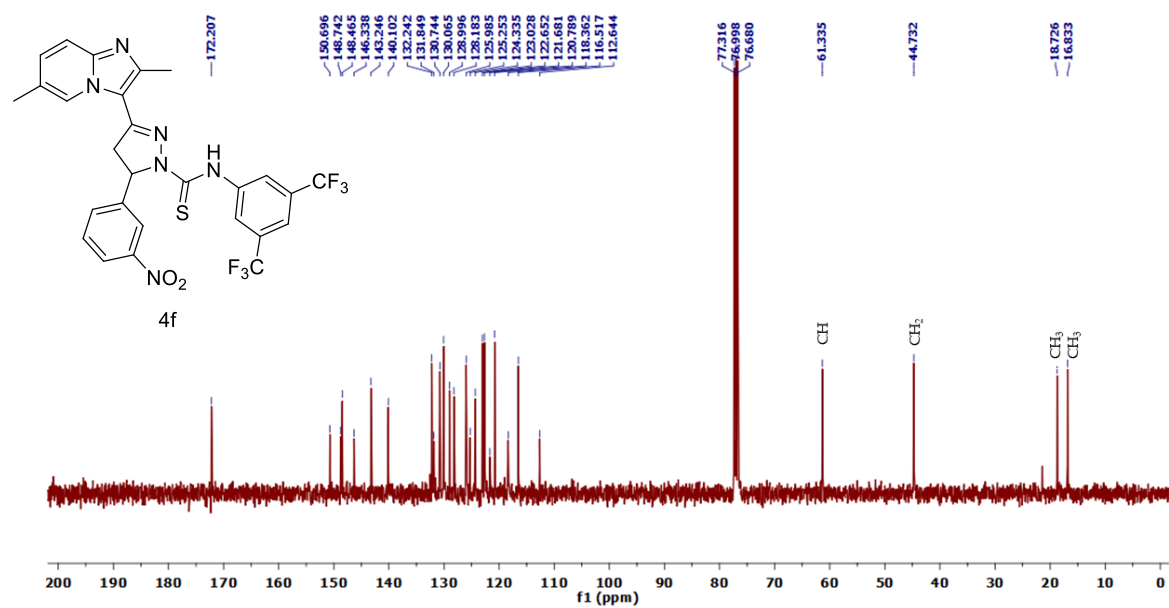
SK-BR-3 log curve of 4f



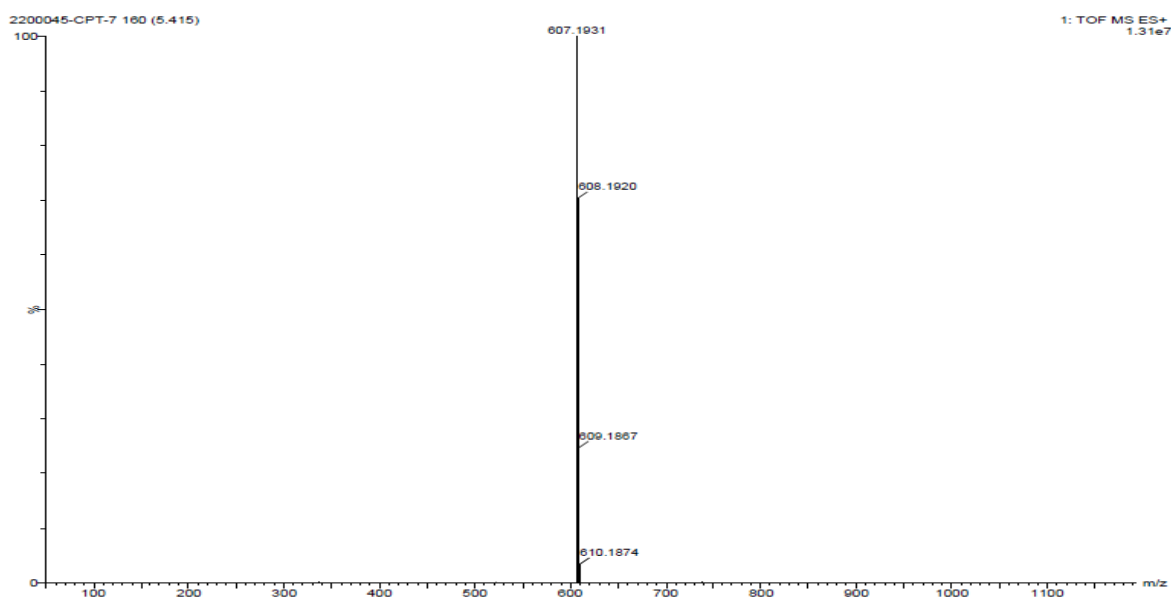
MCF-10A log curve of 4f



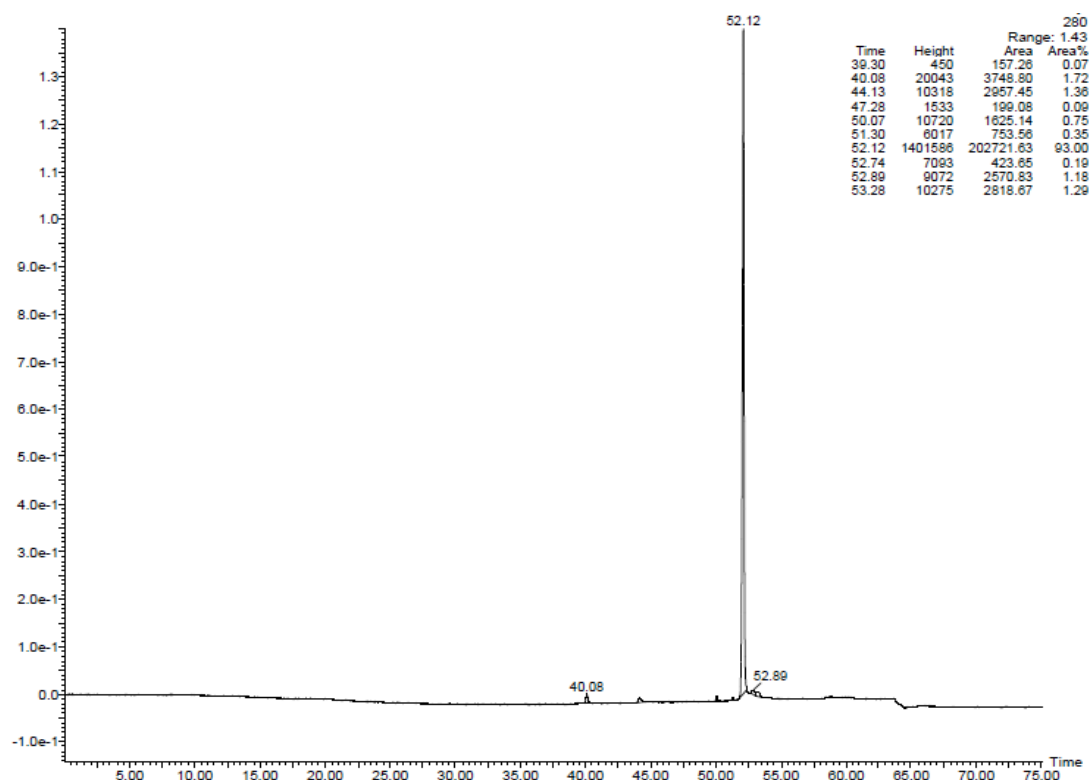
1H NMR of 4g



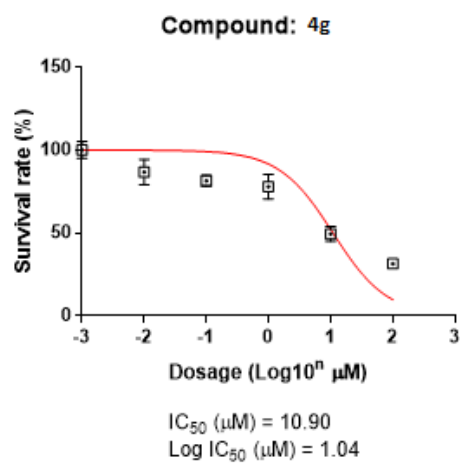
¹³C NMR of **4g**



Mass spectra of compound **4g**

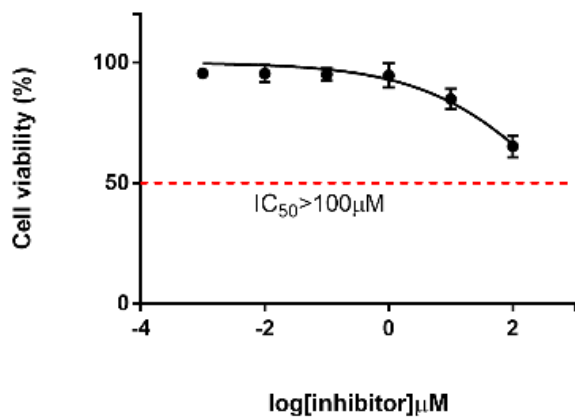


HPLC of 4g

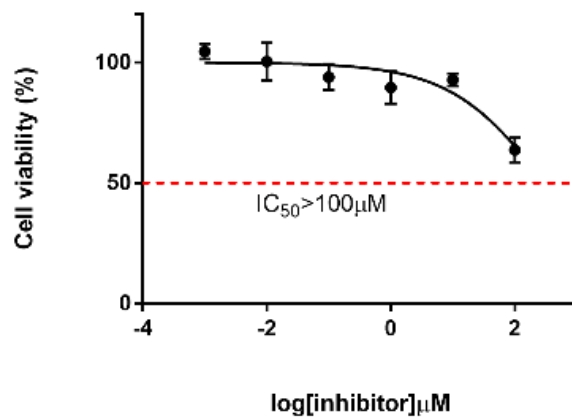


- > Cell line: MCF7 (2000 cells/per well⁹⁶)
- > Treated time: 72hrs
- > Assay: alamarBlue (4hrs incubated)
- > Data: 4g

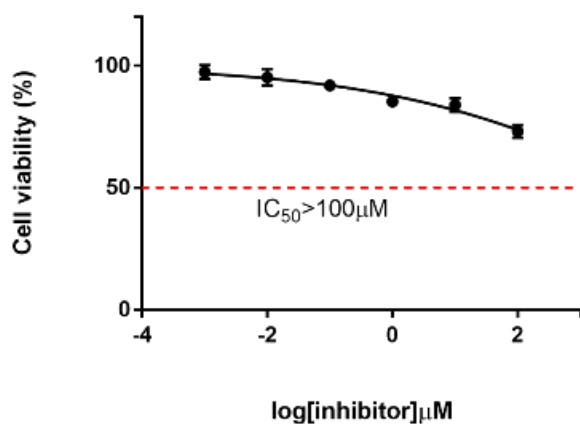
Conc. (μM)	Viability	
	AVE.	± SD.
0	100.00	5.15
0.01	86.63	7.66
0.1	81.43	3.26
1	77.91	7.47
10	49.40	4.47
100	31.40	1.95



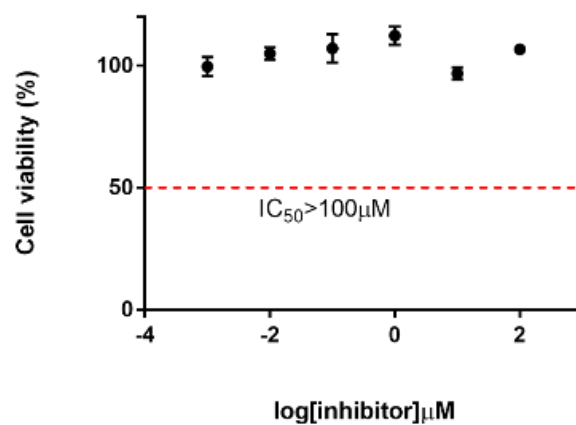
T47D Log curve of 4g



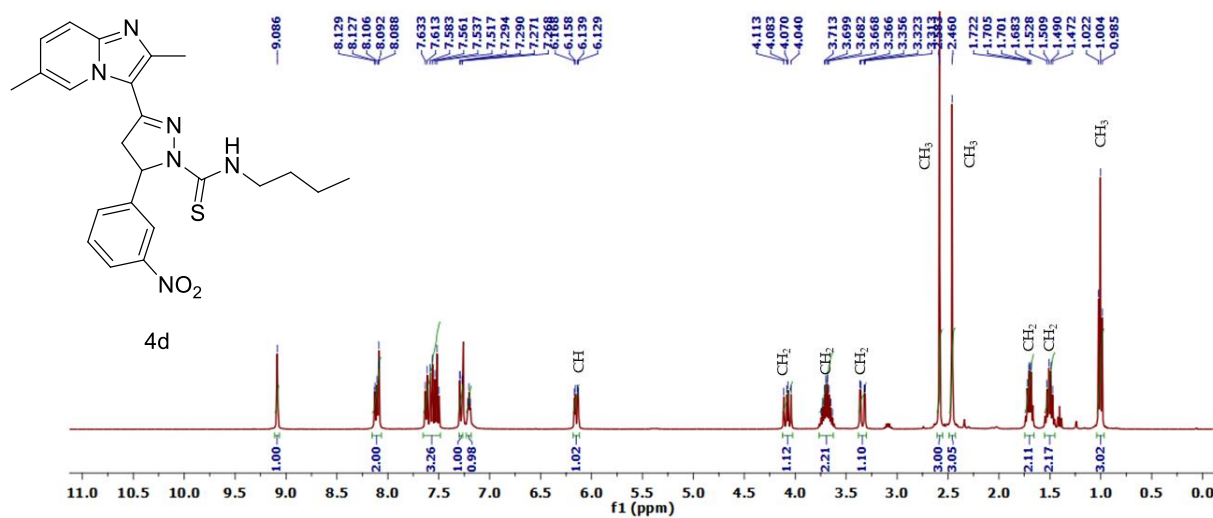
BT474 Log curve of 4g



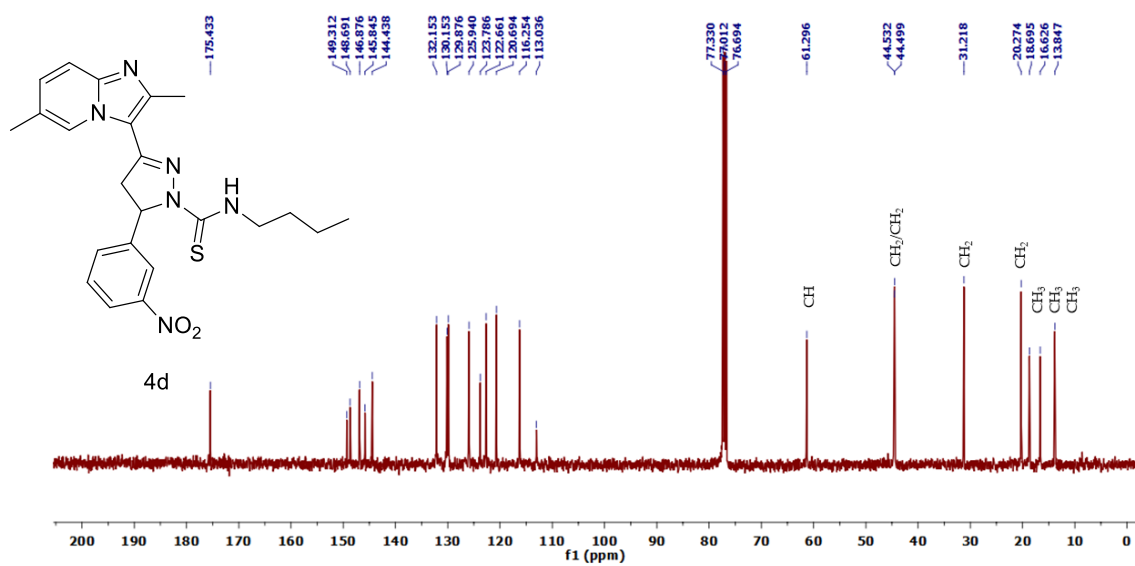
SK-BR-3 log curve of 4g



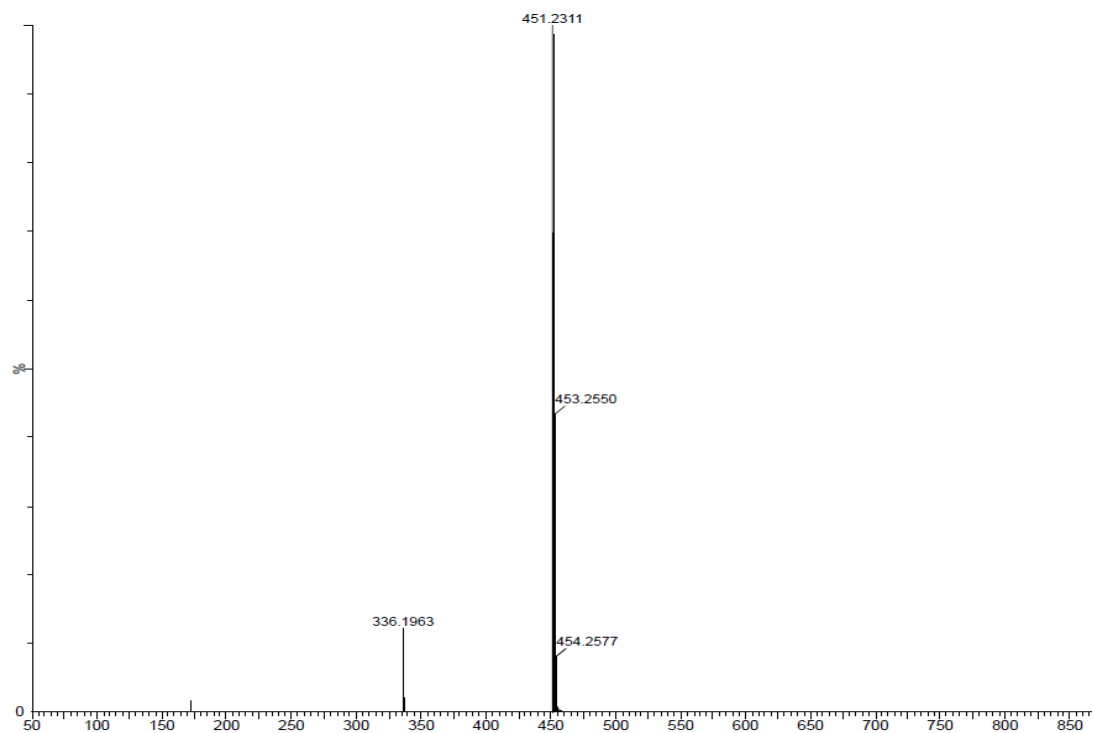
MCF-10A log curve of 4g



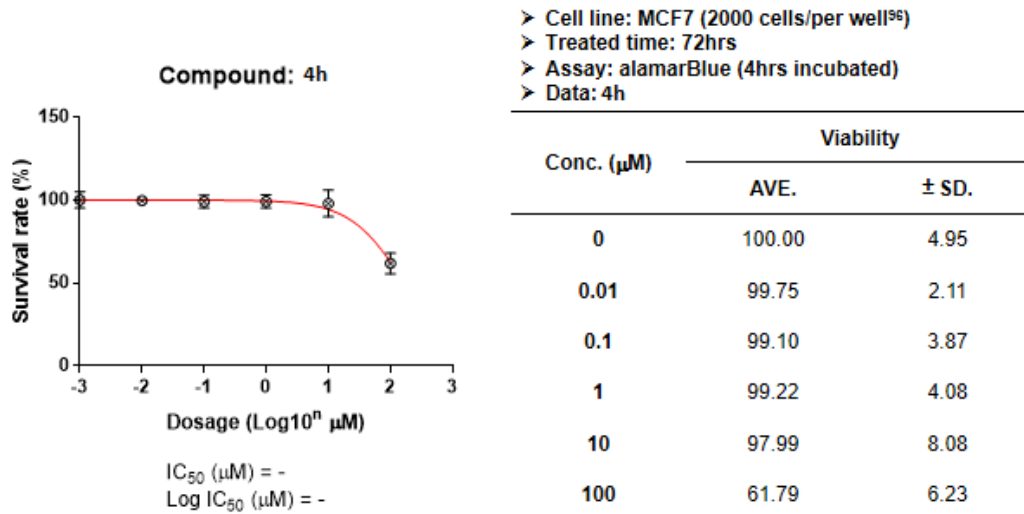
^1H NMR of **4h**



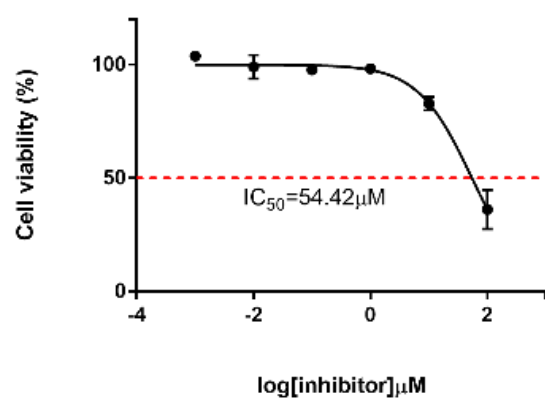
^{13}C NMR of **4h**



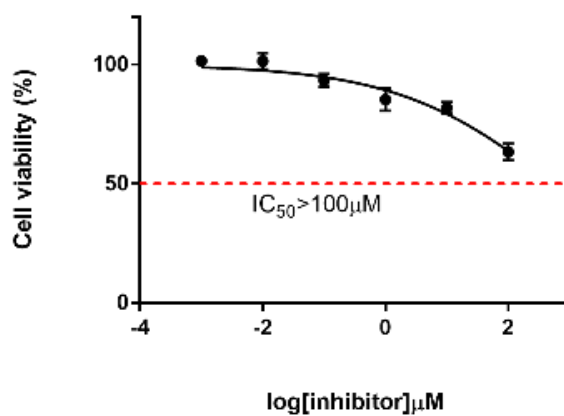
Mass spectra of **4h**



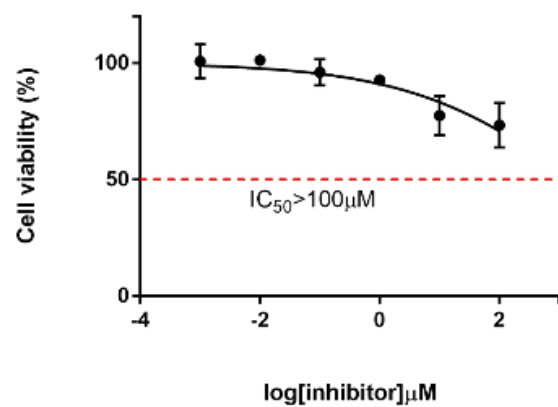
MCF-7 Log curve of **4h**



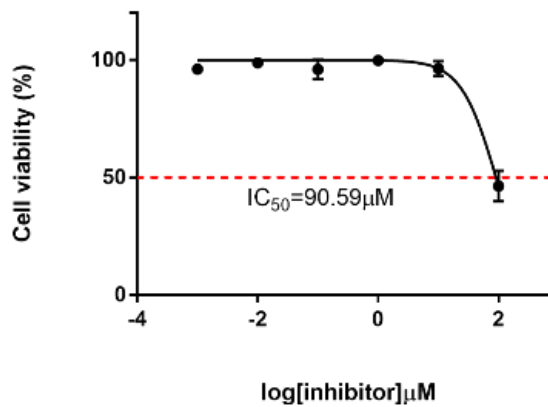
T47D Log curve of 4h



BT474 Log curve of 4h



SK-BR-3 log curve of 4h



MCF-10A log curve of 4h