

Supporting Information

Synthesis and Biological Evaluation of Novel 2-Substituted Quinazolin-4(3H)-ones with Antiproliferative Activities

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Cpd Name	Kinases											
	CAMK4A	CDC42BPAA	CDK2A	CDKL1A	CHEK2A	CLK1A	CLK3A	DYRK2A	CSNK1EA	EPHA4A	FECHHSF	HIPK2HSF
17	-0.3	-1.3	0.8	0.4	1.4	4.6	-0.1	2.3	1.2	0.3	0.2	1.1
21	-0.4	-0.8	1.2	0.5	1.2	3.9	0.8	2.5	1.4	-0.1	-2.4	0.8
19	0.7	-0.5	1.4	0.7	1.7	3.1	1.6	1.4	0.7	0.1	0.8	1.2
34	-0.5	-1.2	0.5	0.1	0.6	3.2	0.1	1.6	1.3	-0.2	2.1	0.7
20	-0.4	-0.7	0.0	0.3	0.5	2.1	-0.1	1.1	0.6	-0.1	2.4	0.5
35	-0.5	-0.9	0.3	0.4	0.4	2.4	0.0	1.4	1.4	0.1	6.3	0.6
18	-0.4	-0.7	0.2	0.5	1.4	3.4	0.0	1.5	1.3	0.4	4.0	0.6
33	-0.3	-0.7	0.5	0.4	0.3	2.1	0.4	1.1	1.2	0.0	4.5	0.6
30	0.2	-0.4	0.9	0.3	2.6	4.6	1.5	3.7	2.1	0.3	3.1	2.0
32	-0.5	-1.2	0.5	0.2	0.4	2.5	0.0	1.1	1.1	-0.4	0.2	0.5
31	-0.7	-0.2	0.2	0.6	0.5	2.5	0.5	1.0	0.5	-0.4	1.5	0.5
25	-0.6	-0.5	0.6	0.5	0.9	4.2	1.3	3.8	2.2	0.0	2.1	2.3
37	0.0	-0.3	0.6	0.7	0.0	0.0	-0.3	0.3	0.9	0.1	0.8	0.6
36	-0.3	-0.9	0.4	0.3	-0.1	0.3	-0.4	0.4	1.0	0.0	-0.9	0.3
Staurosporine	7.1	2.6	15.2	4.2	16.5	11.9	5.3	7.0	3.1	5.6	2.1	4.6

Table S1: DFS results

Cpd Name	Kinases										
	MSSK1A	NQO2A	DAPK1A	DCAMKL1A	DMPK1A	EPHA5A	EPHA7A	EPHB3A	FGFR1B	FGFR2A	GAKA
17	1.0	-0.1	1.3	-0.7	-0.2	0.3	-3.2	1.0	0.2	0.0	4.7
21	0.2	0.2	0.4	-1.4	-0.4	0.1	-2.7	0.3	0.3	0.1	3.9
19	0.3	0.4	0.8	-1.1	-0.5	0.3	-2.3	1.1	0.5	0.4	2.4
34	0.2	-0.5	-0.1	-1.5	-0.4	-0.7	-3.9	0.5	0.1	0.0	2.0
20	0.1	0.2	0.0	0.3	-0.3	-0.3	-3.4	1.0	0.1	-0.3	1.0
35	0.0	0.0	0.2	-0.7	0.1	-0.1	-3.0	1.0	0.3	0.1	1.4
18	0.5	0.0	0.8	0.2	0.5	-0.1	-3.0	1.3	0.2	-0.1	2.0
33	0.1	0.4	0.9	-0.4	1.6	0.2	-2.3	0.5	0.3	-0.1	1.3
30	0.4	-0.1	0.8	0.2	0.6	0.4	-2.7	0.6	0.1	-0.4	2.8
32	0.1	-0.2	-0.2	-1.3	-0.6	-0.3	-3.8	0.2	0.2	-0.2	1.5
31	0.0	0.3	0.1	0.0	-0.2	-0.5	-2.5	-0.4	-0.2	-0.4	0.6
25	0.0	-0.4	1.0	-0.5	0.1	-0.5	-2.7	0.6	0.0	-0.4	2.8
37	0.0	0.0	-0.4	-2.0	-0.1	-0.3	-2.3	0.6	0.0	-0.1	-0.2
36	0.3	0.3	-0.5	-2.5	-0.9	-0.4	-4.0	3.1	0.2	-0.1	0.3
Staurosporine	3.7	-0.2	9.0	11.8	8.2	7.7	9.5	5.5	6.4	8.4	8.9

Table S2: DFS results

Cpd Name	Kinases										
	DAPK3A	DYRK1AA	FESA	GSG2A	TTKA	EPHA2A	MAPK1A	MERTKA	MST3A	MST4A	GPRK5A
17	2.0	4.0	0.1	2.6	0.2	1.1	-0.1	-0.7	0.6	0.3	1.0
21	2.1	3.2	0.2	1.5	-0.2	0.8	-0.2	-0.6	0.7	0.3	1.5
19	4.1	5.0	0.9	0.8	0.3	0.8	-0.4	-0.5	3.0	1.1	1.2
34	1.4	2.7	0.0	3.1	-0.3	0.7	-0.4	-1.1	0.4	0.3	0.5
20	0.9	2.2	0.0	-0.4	-0.2	0.5	-0.5	-0.8	0.3	0.0	0.3
35	1.2	2.4	-0.1	0.4	-0.4	0.6	-0.3	-0.8	0.2	0.0	0.7
18	1.3	2.3	0.5	-0.1	-1.2	0.7	-0.2	-0.6	-0.1	-0.2	0.4
33	2.0	2.0	0.1	0.3	-0.1	0.7	-0.3	-0.3	0.4	0.1	0.5
30	2.1	2.8	0.0	3.1	0.2	0.8	-0.2	0.0	0.8	0.3	0.7
32	1.6	2.0	-0.2	3.0	-0.4	0.6	-0.3	-1.0	0.0	-0.2	0.3
31	0.5	1.4	-0.3	0.3	-2.0	0.2	-0.3	-0.7	0.1	0.1	-0.2
25	1.7	5.3	0.0	2.9	-0.1	0.7	-0.2	-0.5	0.2	0.2	0.7
37	0.4	-0.4	-0.1	0.5	-0.6	0.6	-0.4	-1.0	0.3	0.1	0.3
36	0.2	1.2	0.0	0.8	-0.2	0.5	-0.2	-1.5	-0.1	0.5	-0.1
Staurosporine	16.3	12.8	7.7	2.3	8.4	7.4	1.3	5.7	9.1	7.8	8.0

Table S3: DFS results

Cpd Name	Kinases										
	GSK3BB	MAP2K4A	MAP2K6A	MAP3K5A	MAPK10A	MAPK13A	MAPK14A	MAPK8B	MAPK9A	MAP2K7A	TLK1A
17	5.1	1.0	0.2	2.7	-1.2	0.7	-0.2	1.5	0.8	-0.8	-1.7
21	4.7	2.0	0.3	1.7	-0.2	0.4	0.1	2.5	1.2	-0.7	-1.0
19	2.4	2.3	0.7	2.0	-2.1	0.5	0.4	1.1	-0.5	0.9	-0.4
34	2.4	0.8	0.2	0.3	-3.9	0.4	-0.4	-0.8	-0.5	-1.0	-2.1
20	4.1	0.9	0.2	0.3	-3.3	0.5	-0.5	-0.8	-0.4	-0.2	-1.7
35	2.6	0.9	0.2	0.2	-3.1	0.4	-0.3	-0.4	-0.3	-0.3	-1.8
18	3.9	0.8	0.3	0.7	-1.1	0.8	-0.3	0.9	0.2	0.1	-1.7
33	2.1	0.6	0.2	0.3	-2.5	0.5	0.0	0.0	-0.4	-0.1	-1.6
30	3.0	1.1	0.2	5.1	-0.6	0.4	0.1	1.8	-0.2	0.1	-1.1
32	1.5	1.3	0.0	0.3	-3.9	0.3	-0.5	-0.4	-0.5	-0.4	-2.0
31	0.8	0.2	0.1	0.8	-2.3	0.3	-0.4	0.6	-0.5	-0.8	-1.8
25	3.7	1.2	0.3	1.9	-1.2	0.5	-0.1	1.6	0.4	-0.6	-1.3
37	0.9	0.6	0.1	0.0	-2.8	0.4	-0.3	-0.6	-0.9	-0.7	-1.6
36	0.5	0.4	0.0	-0.2	-4.9	0.4	-0.6	-1.3	-0.7	-1.5	-1.7
Staurosporine	11.2	11.5	11.8	16.9	4.7	6.5	0.9	8.0	3.2	8.3	8.5

Table S4: DFS results

Cpd Name	Kinases										
	MARK3A	MARK4A	MELKA	NEK1A	NEK2A	NEK7A_2	OSR1A	PAK1A	PIM3A	FLT1A	PCTK1A
17	-1.0	-0.6	1.8	0.1	0.4	-2.6	-0.2	-0.1	3.2	2.3	1.0
21	-0.6	-0.3	0.9	-0.5	1.1	-1.2	0.2	1.2	6.5	1.3	1.2
19	0.3	-0.4	1.4	0.5	1.7	0.3	1.0	1.2	3.0	1.3	0.2
34	-0.3	-0.5	1.6	0.1	0.5	-2.2	-0.4	0.3	2.5	1.4	0.4
20	-1.1	-1.1	0.9	0.0	0.4	-1.8	-0.2	0.4	1.0	1.3	0.1
35	-0.8	-0.6	0.8	0.2	0.6	-1.4	-0.4	0.4	3.5	1.2	0.4
18	-0.8	-1.0	0.7	0.5	0.8	-1.4	-0.1	0.6	1.2	1.4	0.6
33	-0.7	-0.9	1.0	-0.5	0.4	-1.8	-0.1	0.4	2.9	1.2	0.4
30	-0.4	0.0	1.7	0.2	0.8	-0.5	0.3	0.4	3.0	2.5	0.6
32	-1.6	-0.8	1.0	-0.1	1.5	-2.0	-0.6	0.1	1.9	1.5	0.2
31	-0.3	-0.7	0.4	-0.2	0.5	-1.1	-0.2	0.1	1.2	1.1	-0.1
25	-0.7	-0.2	1.0	0.0	0.6	-0.6	-0.1	0.3	2.7	1.0	0.6
37	-0.9	-1.0	0.1	-0.1	1.1	-1.2	-0.1	1.1	2.7	0.2	0.4
36	-0.7	-0.6	-0.1	-0.1	0.5	-2.2	-0.6	0.1	2.8	0.5	0.4
Staurosporine	18.1	15.8	12.8	-0.2	4.6	1.4	6.1	7.8	19.6	13.5	9.3

Table S5: DFS results

Cpd Name	Kinases											
	PKMYT1A	PLK4A	RPS6KA5A	SLKA	SRCA	SRPK1A	PAK4A	PHKG2A	PIM1A	RPS6KA1A	STK10A	MAPK7
17	-0.3	1.8	0.6	-1.2	0.2	0.3	-0.2	2.3	2.6	1.3	-1.0	-0.2
21	0.6	1.3	0.3	-0.3	0.5	0.3	-0.3	1.0	5.4	0.6	-0.2	-0.2
19	0.2	0.9	3.4	1.1	0.4	0.8	-0.3	1.4	2.2	0.3	1.2	-0.2
34	0.1	1.3	2.2	-1.3	0.2	0.0	-0.5	1.1	1.3	0.5	-0.9	0.0
20	-0.9	1.1	1.0	-1.0	-0.4	-0.1	-1.1	0.1	1.0	-0.2	-1.2	-0.1
35	0.0	1.1	3.0	-1.2	0.0	0.0	-0.9	0.3	1.6	0.3	-0.9	-0.2
18	-0.3	1.0	-1.0	-1.2	0.0	0.3	-0.8	0.2	1.1	0.7	-0.8	-0.4
33	-0.2	0.5	2.7	-0.7	-0.1	0.2	-0.3	0.5	1.4	0.2	-0.9	0.1
30	-0.1	2.5	2.5	-0.4	0.3	0.5	-0.1	2.5	3.6	2.2	-0.6	0.0
32	0.0	0.8	1.4	-1.3	0.1	0.0	-0.5	0.9	1.6	0.3	-1.2	0.2
31	-1.1	0.5	0.7	-1.1	-0.3	-0.1	-0.5	0.3	1.3	0.3	-0.9	0.2
25	-0.1	1.6	4.1	-0.8	0.1	0.2	-0.2	1.3	2.8	1.3	-1.2	-0.1
37	0.1	0.2	-0.4	-0.5	0.1	0.2	-0.4	0.2	1.3	0.1	-0.5	-0.2
36	0.1	0.2	-0.2	-1.3	0.3	-0.2	-0.1	-0.3	1.3	-0.1	-1.2	0.3
Staurosporine	0.5	21.5	15.3	15.3	5.4	6.7	11.3	22.0	12.3	3.2	22.7	

Table S6: DFS results

Cpd Name	Kinases											
	AKT3A	BMP2KA	BMPR2A	CAMK1DA	CAMK1GA	STK17AA	STK17BA	STK38LA	STK39A	BRD4A	STK3A	MEK5
17	0.1	9.0	3.2	-2.2	-0.1	3.2	-2.2	-0.3	-0.8	-1.3	0.8	5.3
21	0.2	7.0	2.6	-2.4	0.2	2.2	-1.2	0.0	-0.2	-1.0	1.4	2.8
19	0.4	3.3	1.8	-1.5	1.1	1.4	-0.7	0.3	0.5	-0.4	2.1	5.2
34	0.2	4.5	1.4	-2.4	-0.3	1.6	-2.8	-0.4	-0.8	-0.9	0.5	3.3
20	-0.1	1.3	1.5	-1.8	-0.3	0.1	-3.2	-0.2	-0.6	-1.9	0.0	1.5
35	0.0	2.5	0.9	-2.2	0.4	1.1	-2.8	-0.3	-0.6	-1.0	1.0	2.2
18	0.3	4.8	2.1	-2.0	0.1	0.8	-2.1	-0.4	-0.9	-1.2	0.5	2.8
33	0.2	1.8	0.4	-2.1	0.3	1.8	-1.7	-0.3	-0.9	-1.3	0.4	1.7
30	0.0	7.0	2.8	-1.9	0.1	3.8	-0.6	-0.1	-0.7	-2.5	0.2	6.1
32	0.2	2.8	0.6	-2.6	0.0	1.5	-3.2	-0.2	-0.9	-0.6	0.0	2.2
31	0.0	1.3	0.8	-1.9	-0.3	0.7	-0.6	0.1	-0.6	-1.1	-1.6	2.5
25	0.0	5.0	2.8	-1.8	-0.1	2.6	0.1	-0.1	-0.8	-0.7	1.0	6.5
37	0.3	0.0	0.2	-1.0	-0.8	-0.4	-2.6	-0.1	-0.9	-0.7	0.0	1.5
36	0.2	0.8	0.3	-3.4	-1.1	-0.5	-4.1	-0.2	-0.7	-1.2	-0.7	0.6
Staurosporine	6.8	18.3	2.5	9.2	10.7	12.3	11.1	0.3	8.7	0.5	16.1	

Table S7: DFS results

Cpd Name	Kinases											
	STK4A	STK6A	ULK3A	VRK1A	WNK1A	BRPF1B	EPHB1A	MAPK15HS	MAPKAPK2A	TAF1A	CSNK1G2	MEK1
17	1.4	1.6	4.2	0.8	-0.5	-1.2	0.7	2.3	0.1	0.2	1.8	0.2
21	1.4	0.8	1.8	0.7	-0.8	-0.7	0.3	1.4	0.1	0.3	1.8	0.1
19	1.7	1.6	3.0	1.1	0.4	-0.2	0.7	0.7	0.6	0.5	1.1	0.1
34	0.3	0.0	2.1	0.5	-0.6	-1.3	0.1	1.0	-0.2	0.1	1.4	0.0
20	-0.3	0.3	1.3	0.5	-0.3	-1.7	0.9	-0.4	-0.2	0.0	0.8	-0.1
35	0.3	0.0	1.5	0.4	-0.4	-1.0	0.6	-0.2	-0.2	0.3	0.7	0.2
18	0.5	0.7	1.5	0.4	-0.1	-1.3	1.0	0.0	0.0	0.2	1.0	-0.3
33	0.0	0.3	1.6	0.6	-0.4	-1.2	0.5	0.6	-0.1	0.0	0.9	0.1
30	1.5	1.6	5.4	0.8	-0.4	-1.2	0.3	2.1	0.4	0.3	2.5	0.3
32	0.2	-0.4	1.7	0.4	-0.6	-1.3	0.1	1.0	-0.2	0.0	0.9	-0.2
31	-0.5	-0.1	1.7	0.3	-0.4	-1.8	-0.4	0.1	-0.2	-1.1	0.7	0.3
25	1.3	1.0	4.1	0.7	-0.5	-1.5	0.4	1.7	0.0	0.2	2.2	0.2
37	0.4	-0.3	0.9	-0.2	-0.3	-1.1	-0.1	-0.4	-0.1	-0.1	0.6	0.2
36	-0.2	-0.5	0.8	0.2	-0.4	-0.8	0.1	0.2	-0.3	0.2	0.9	0.3
Staurosporine	15.7	16.9	19.0	3.2	1.2	0.0	6.2	14.2	3.5	0.0	2.0	

Table S8: DFS results

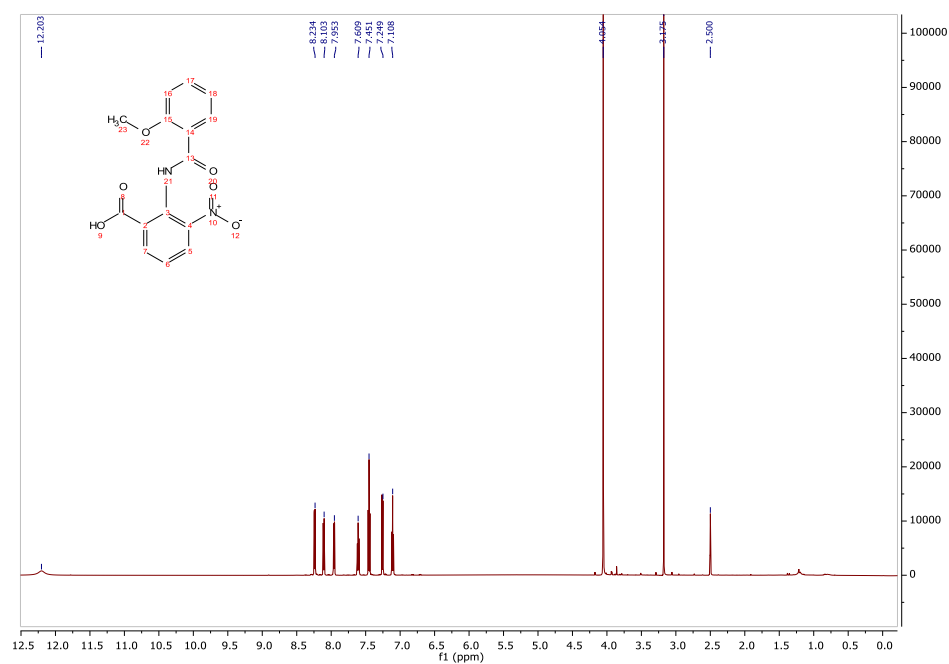


Figure S1: ¹H NMR spectrum of 3

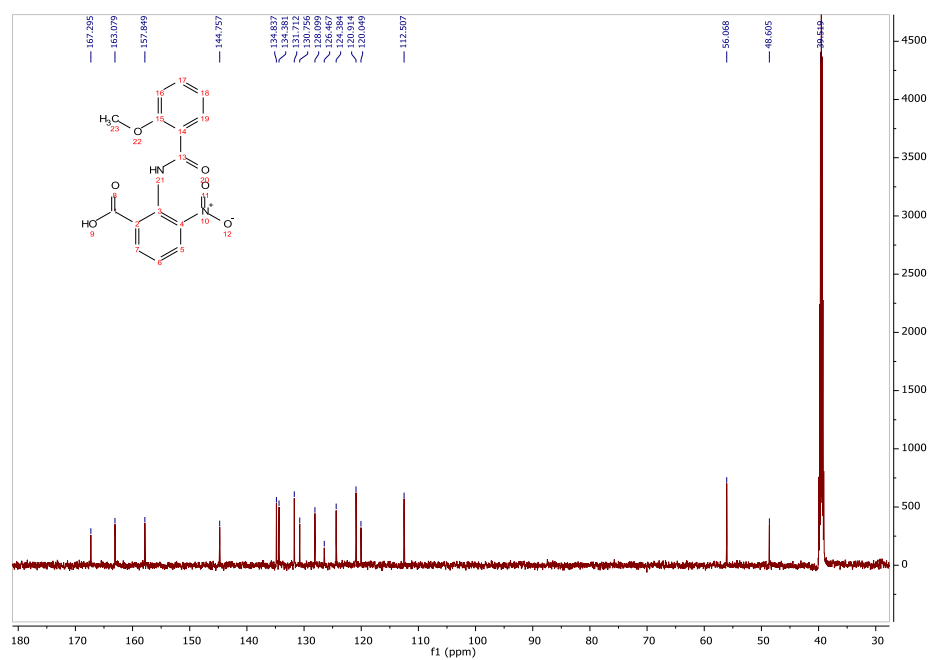


Figure S2: ¹³C NMR spectrum of 3

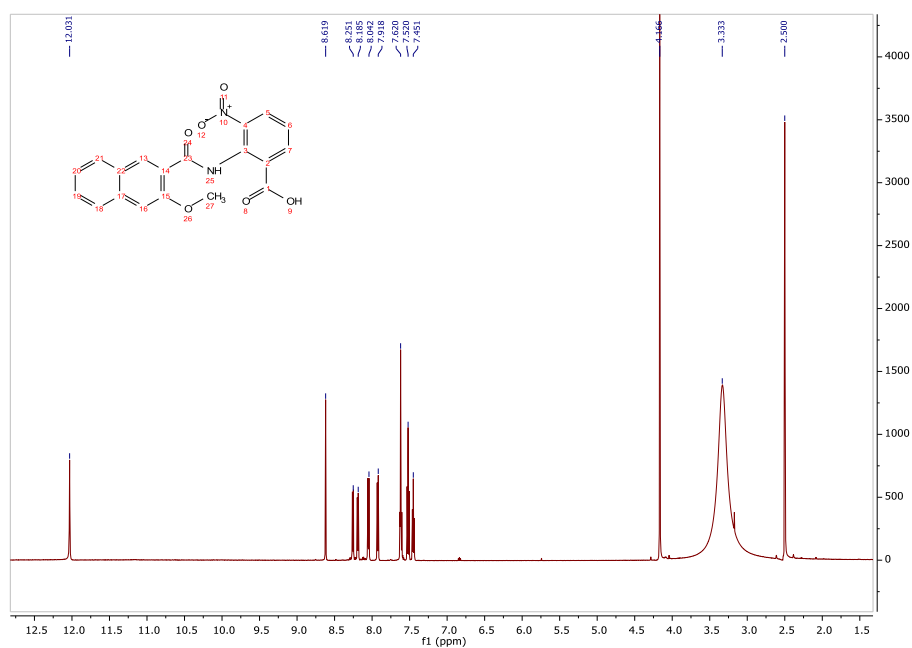


Figure S3: ¹H NMR spectrum of 4

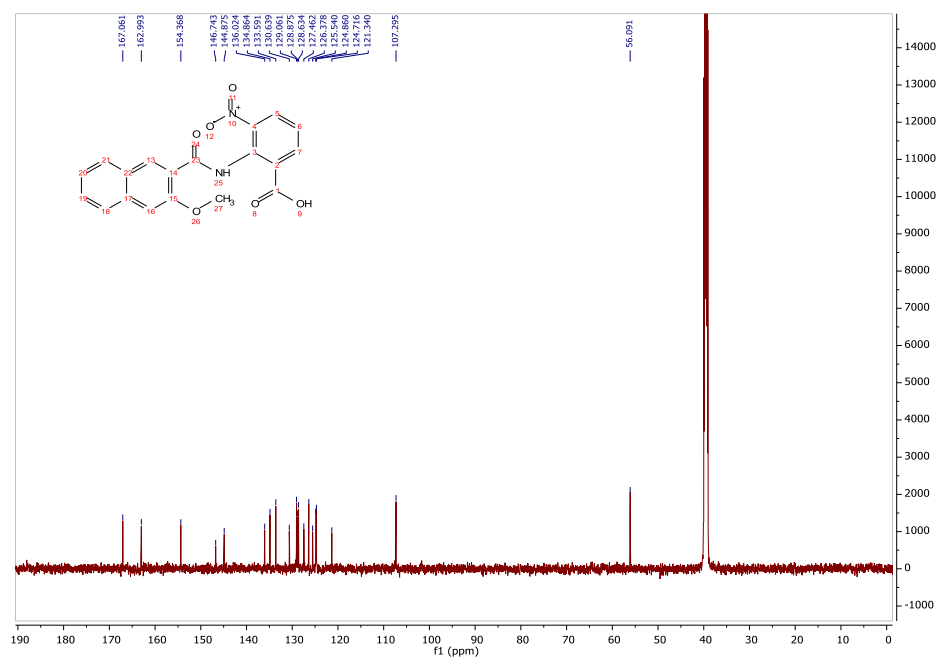


Figure S4: ¹³C NMR spectrum of 4

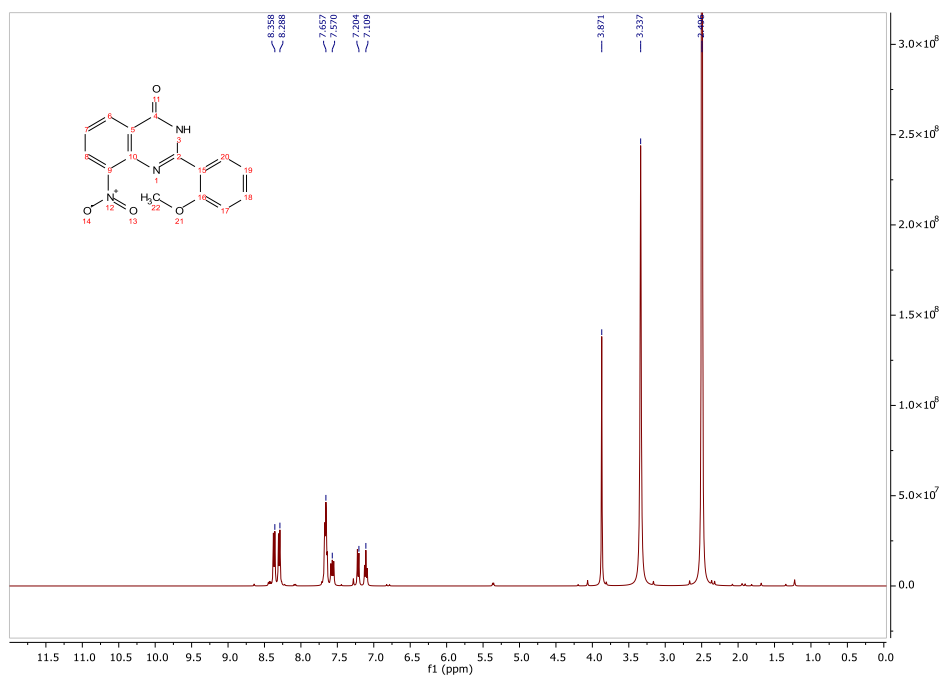


Figure S5: ^1H NMR spectrum of 9

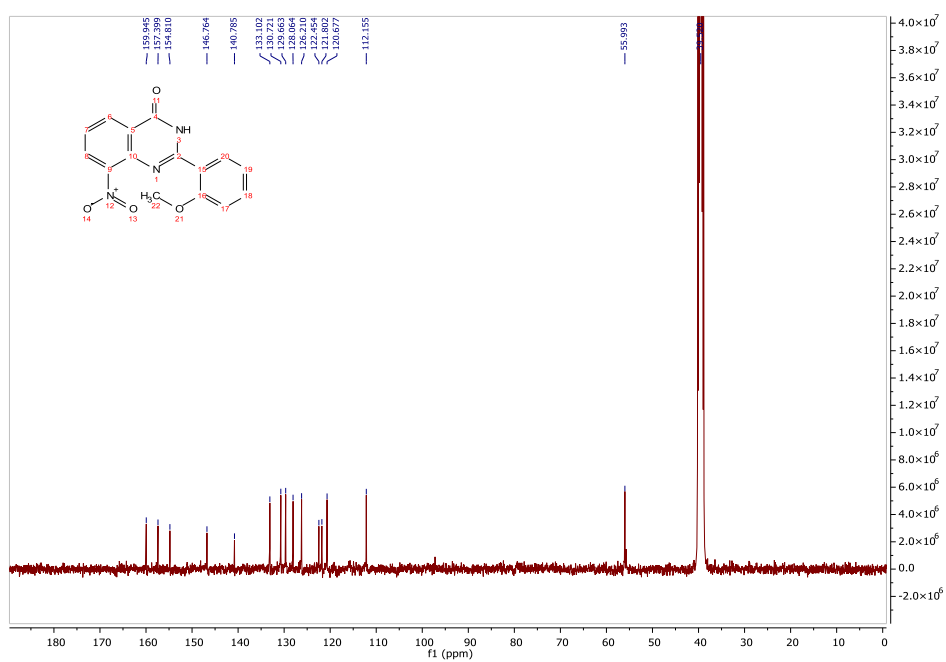


Figure S6: ^{13}C NMR spectrum of 9

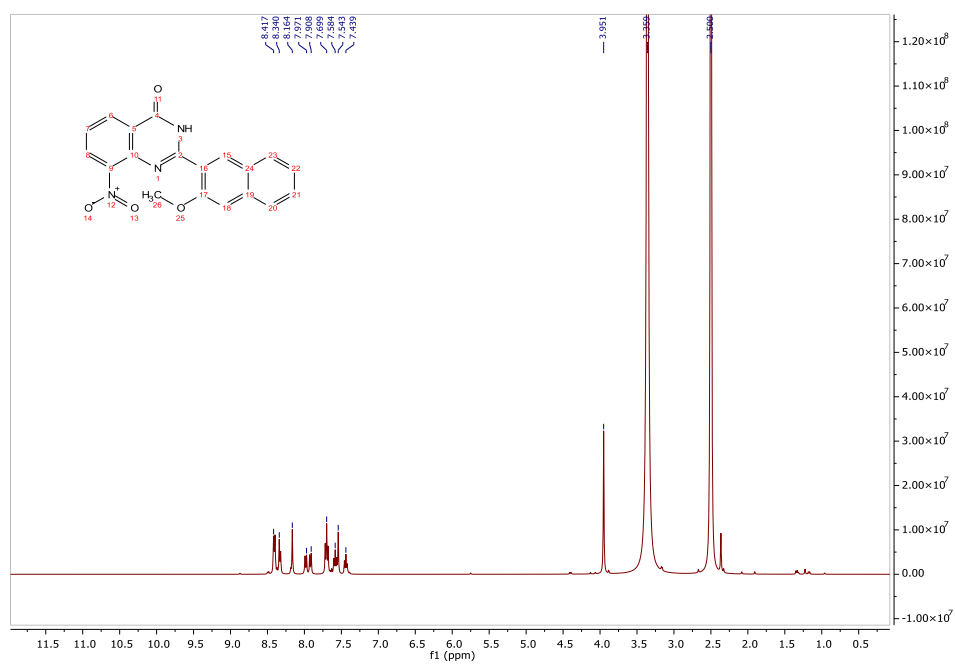


Figure S7: ^1H NMR spectrum of 10

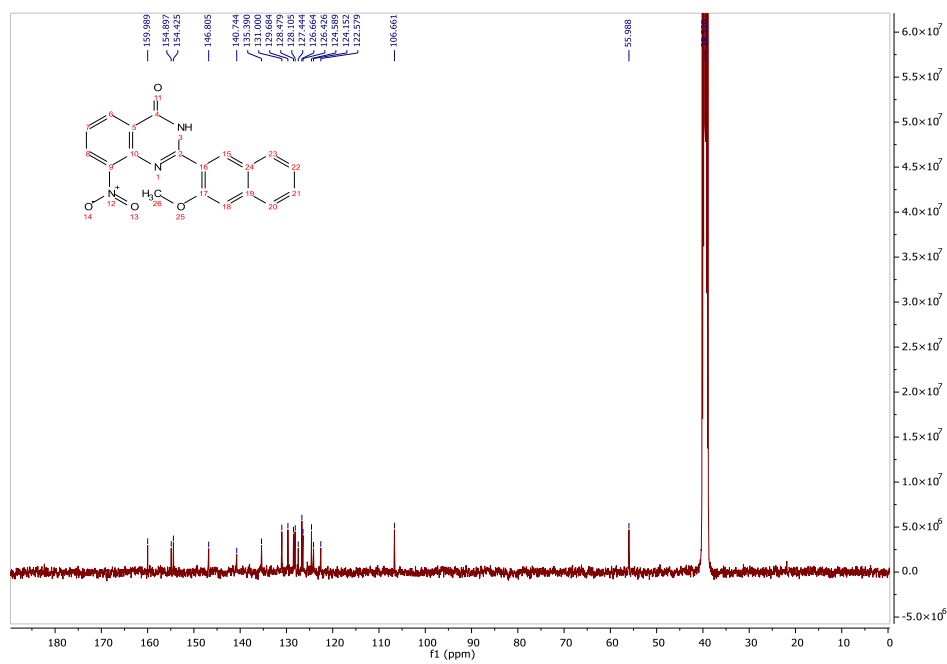


Figure S8: ^{13}C NMR spectrum of 10

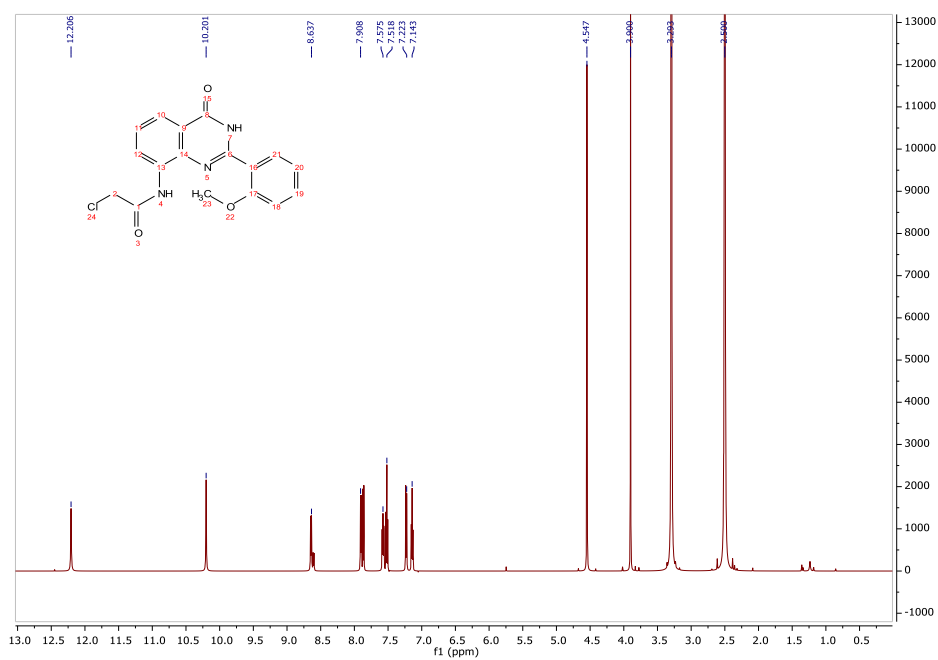


Figure S9: ¹H NMR spectrum of 13

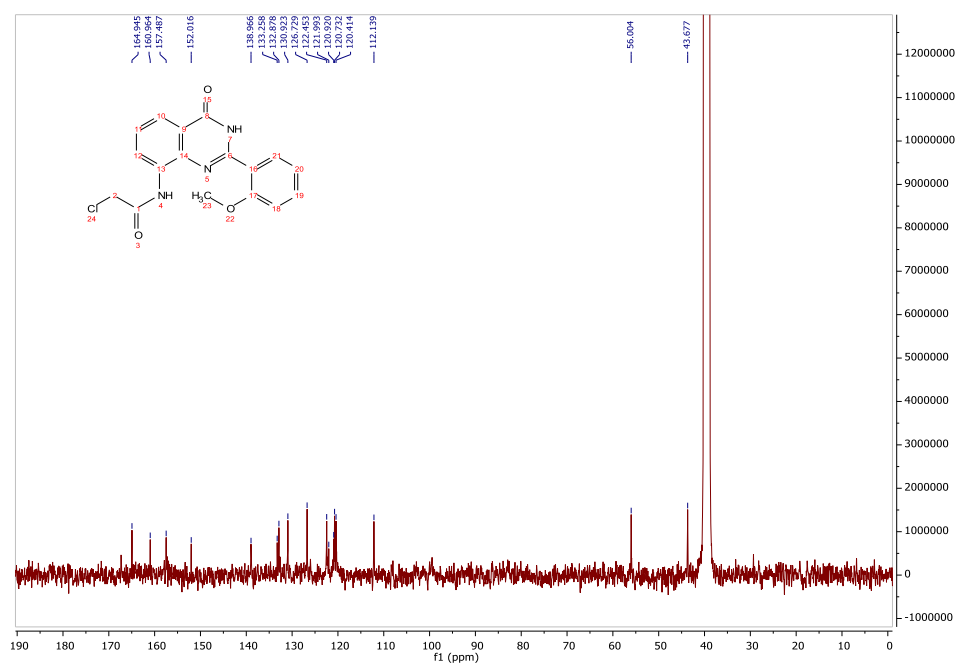


Figure S10: ¹³C NMR spectrum of 13

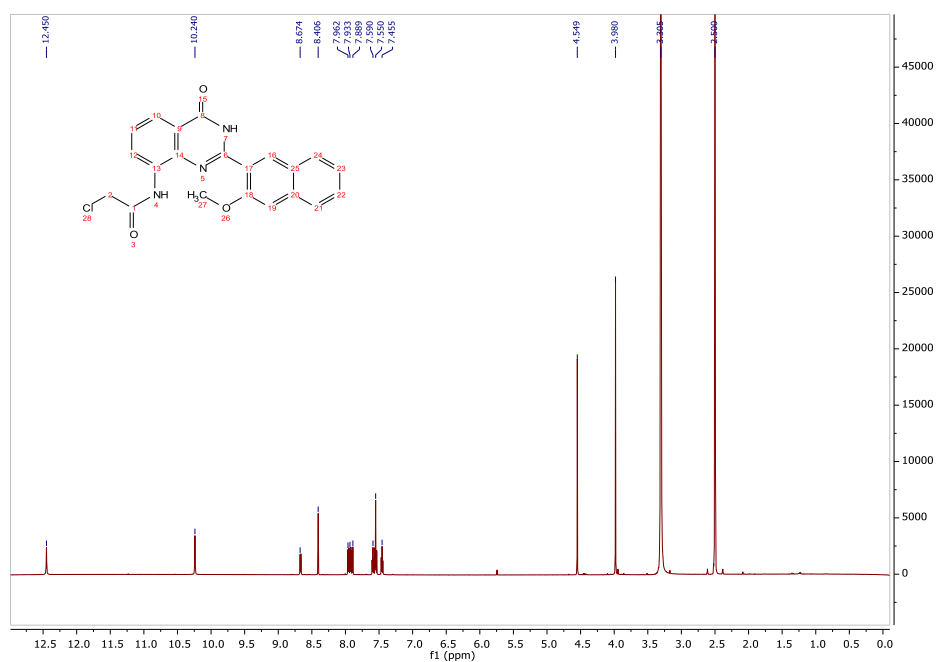


Figure S11: ¹H NMR spectrum of 14

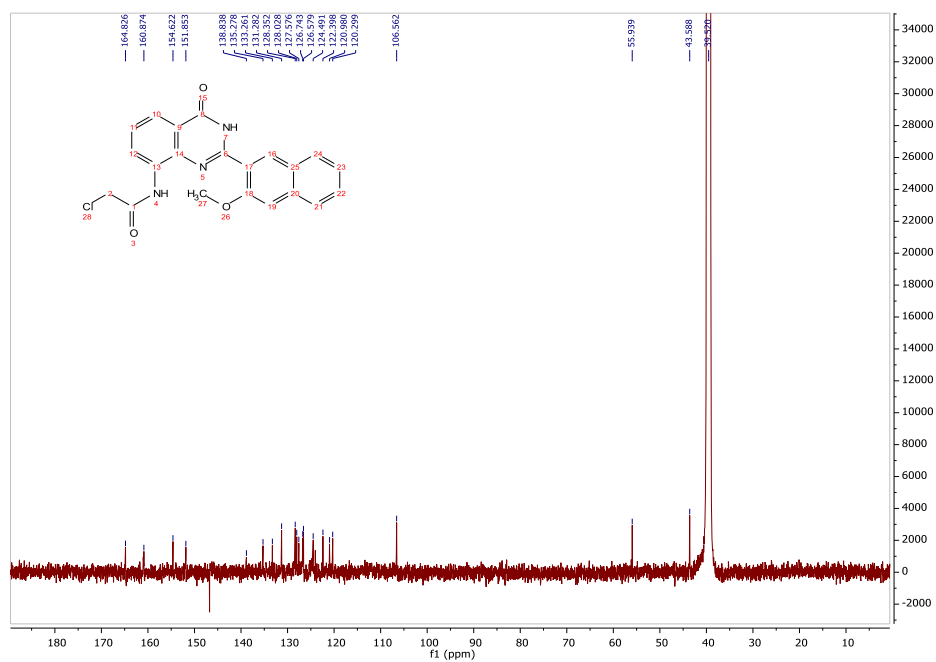


Figure S12: ¹³C NMR spectrum of 14

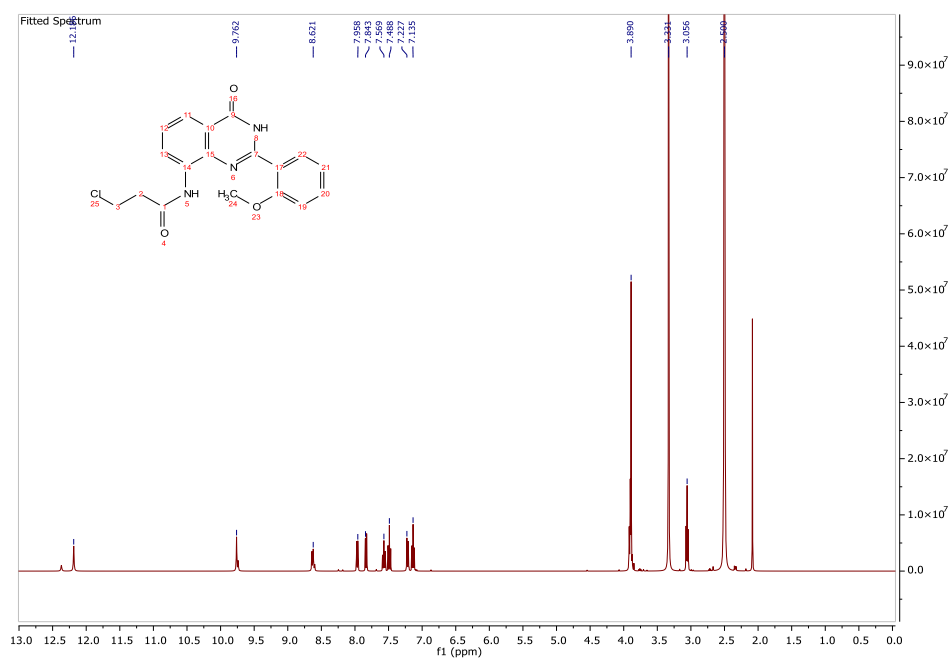


Figure S13: ^1H NMR spectrum of 15

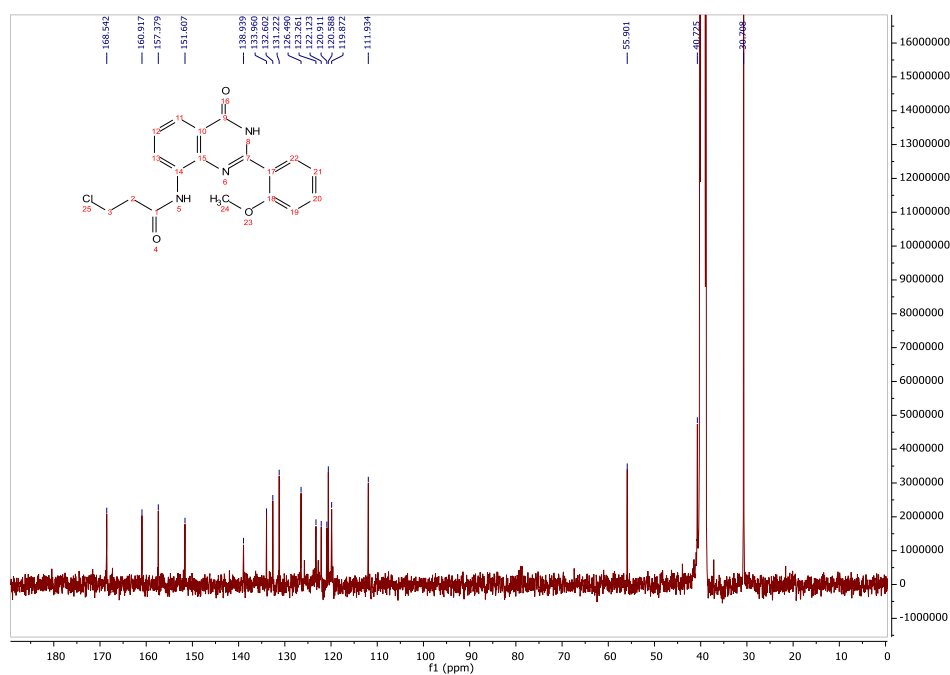


Figure S14: ^{13}C NMR spectrum of 15

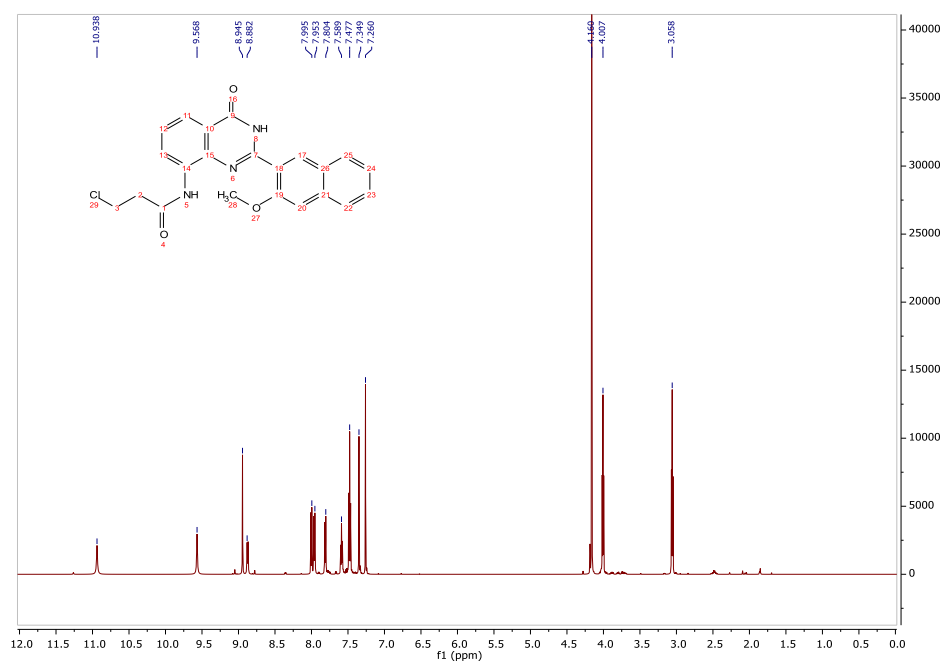


Figure S15: ¹H NMR spectrum of 16

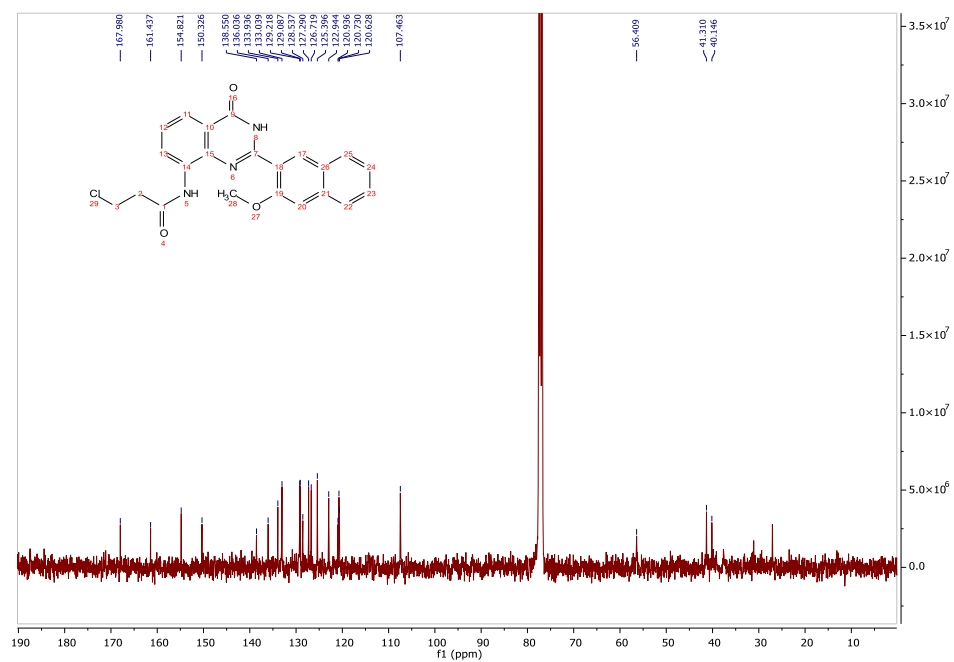


Figure S16: ¹³C NMR spectrum of 16

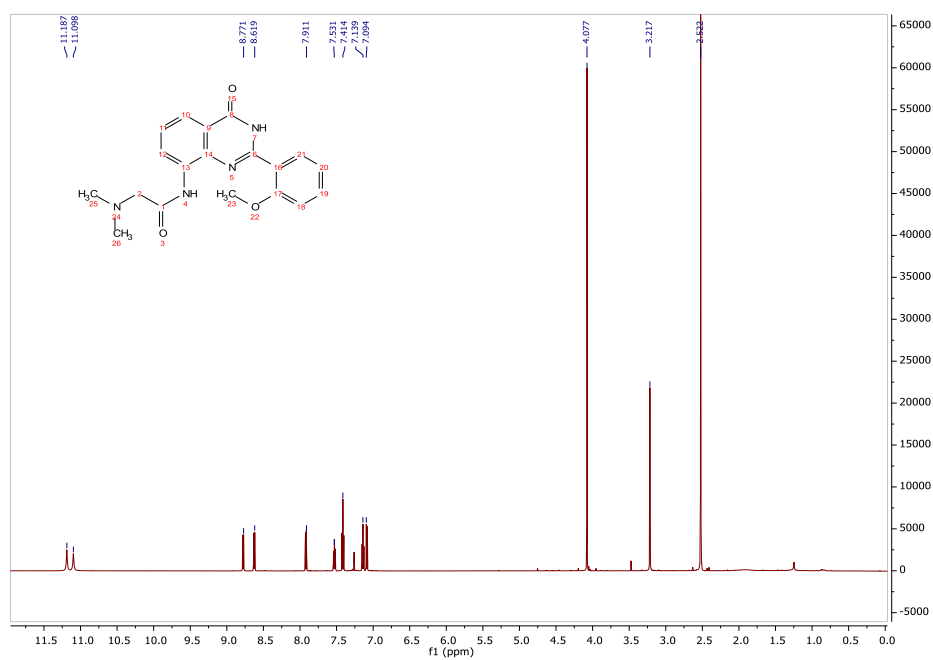


Figure S17: ^1H NMR spectrum of 17

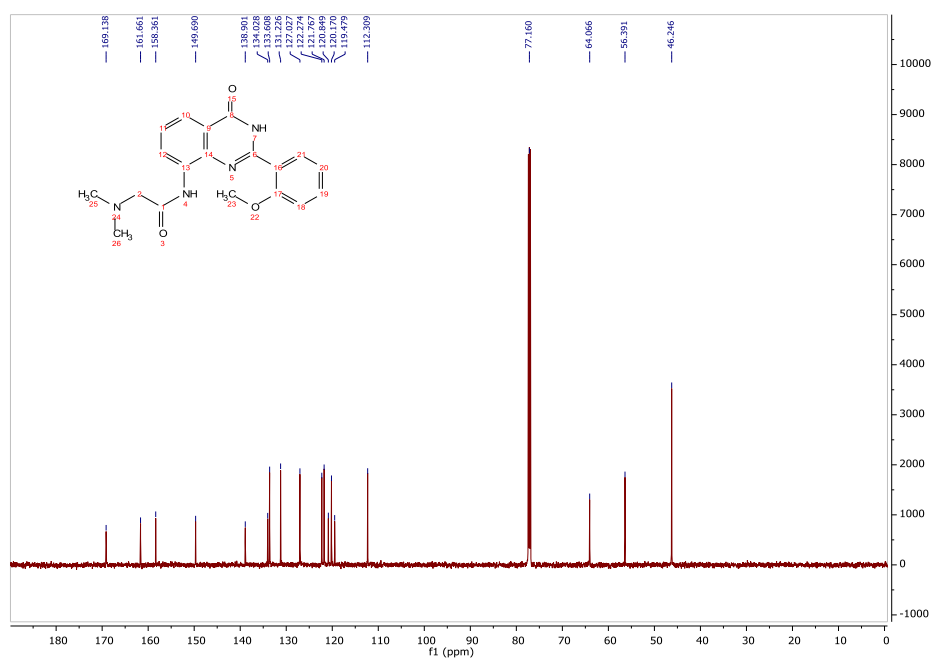


Figure S18: ^{13}C NMR spectrum of 17

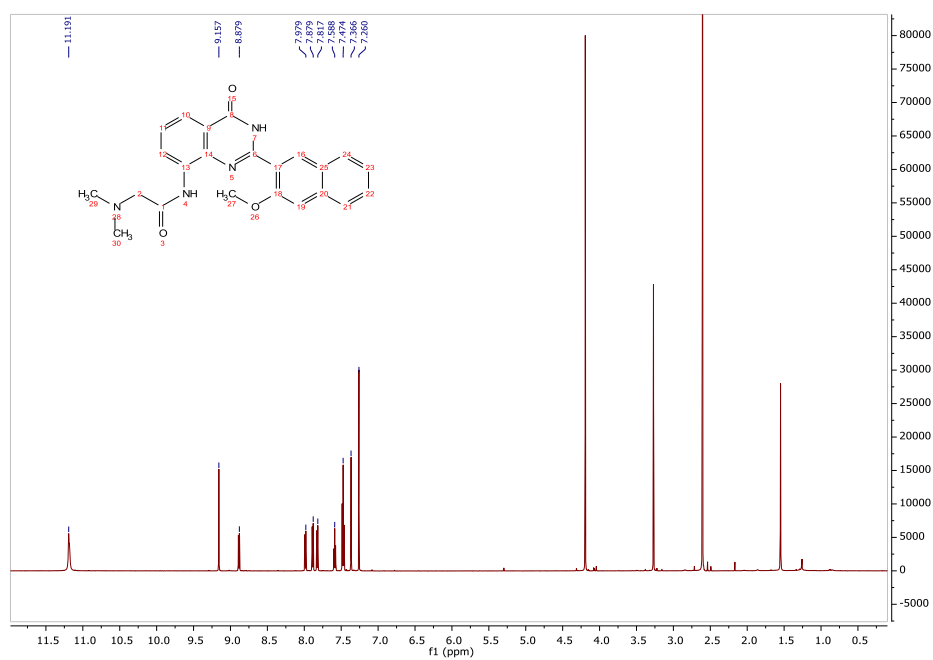


Figure S19: ^1H NMR spectrum of 18

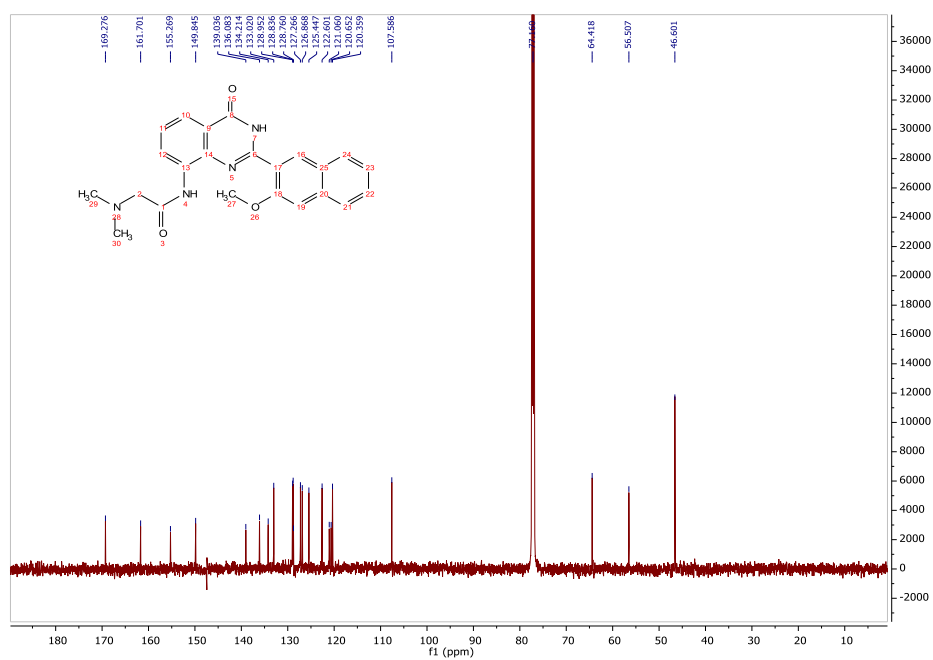


Figure S20: ^{13}C NMR spectrum of 18

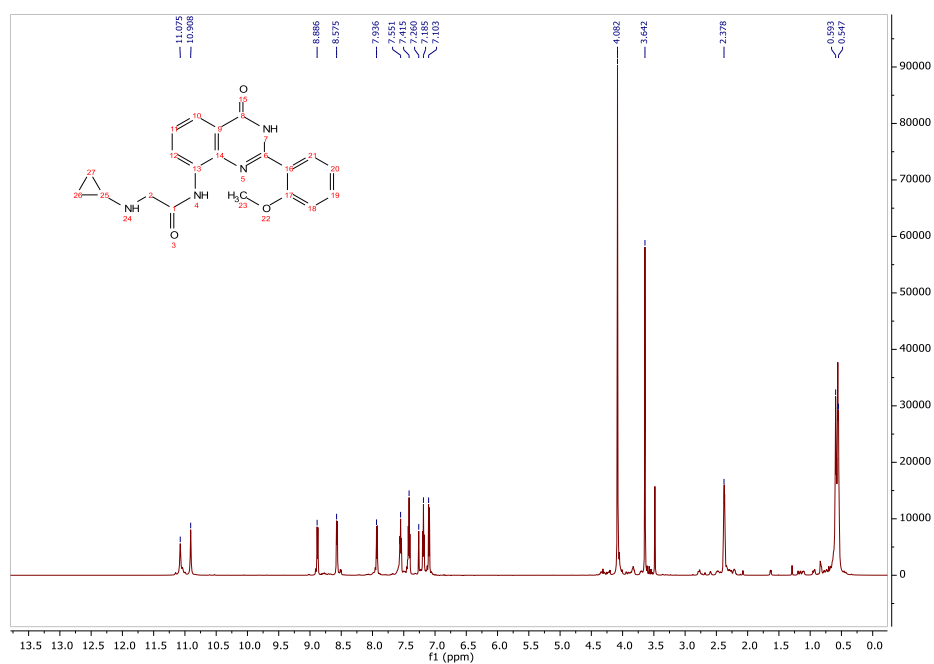


Figure S21: ¹H NMR spectrum of 19

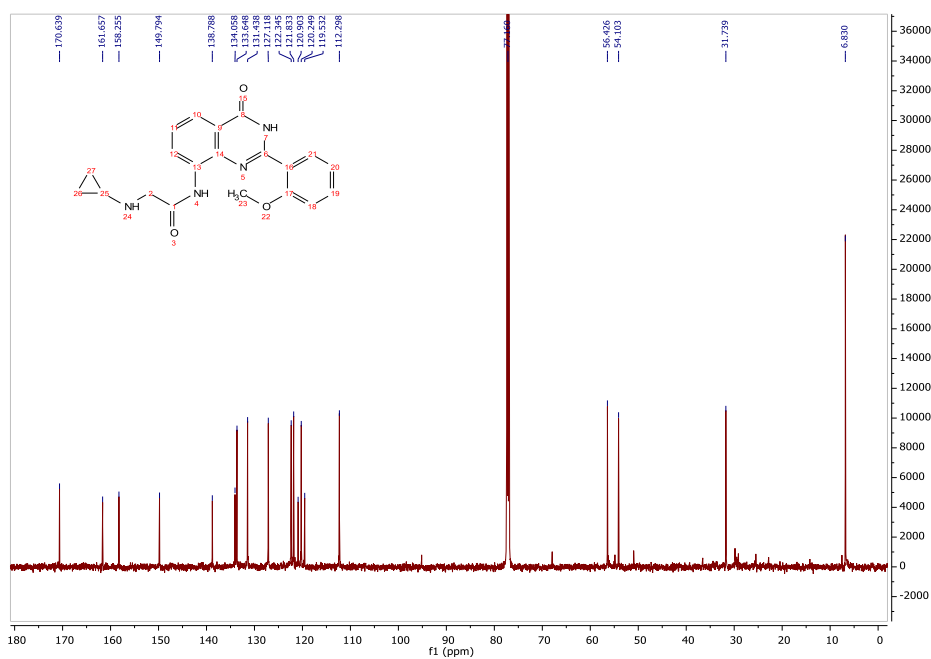


Figure S22: ¹³C NMR spectrum of 19

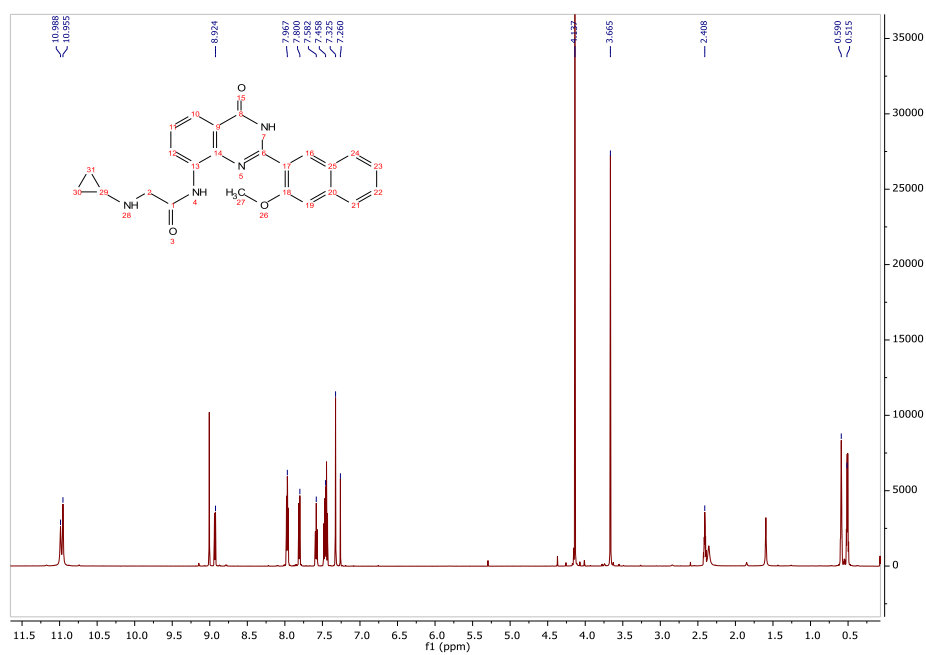


Figure S23: ¹H NMR spectrum of 20

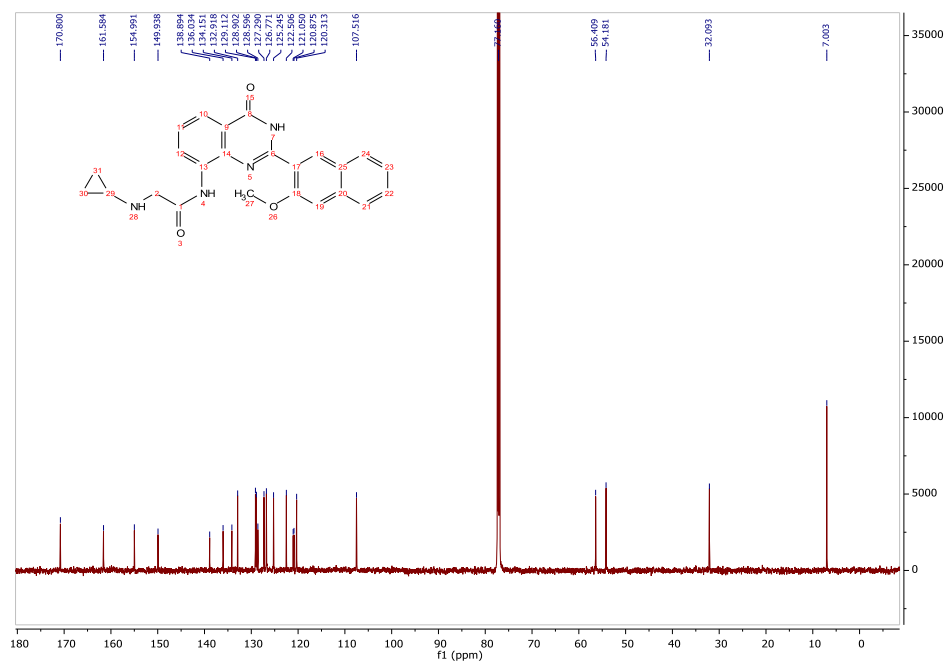


Figure S24: ¹³C NMR spectrum of 20

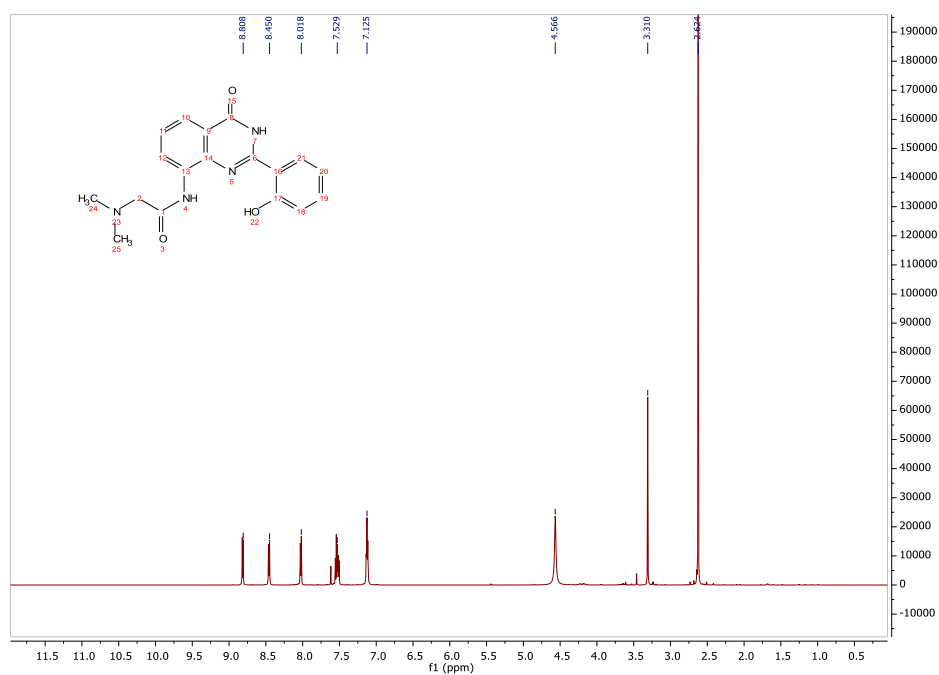


Figure S25: ^1H NMR spectrum of 21

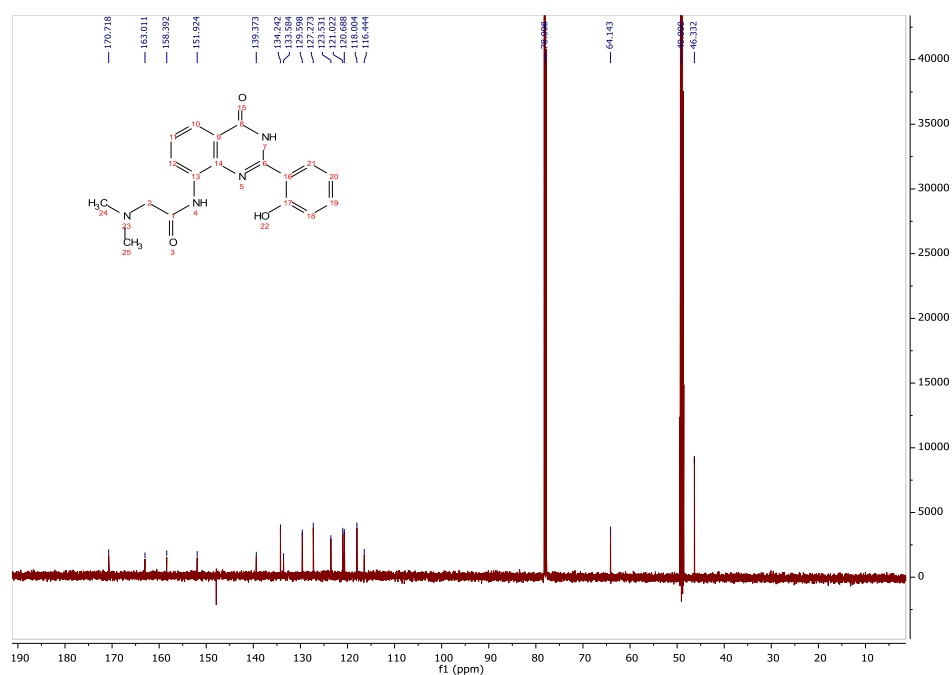


Figure S26: ^{13}C NMR spectrum of 21

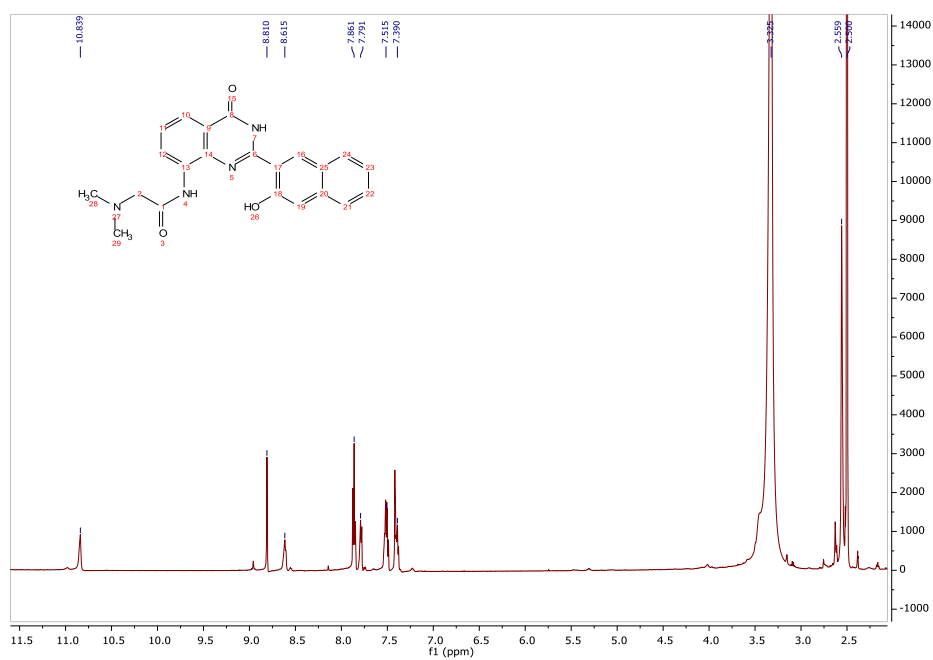


Figure S27: ^1H NMR spectrum of 22

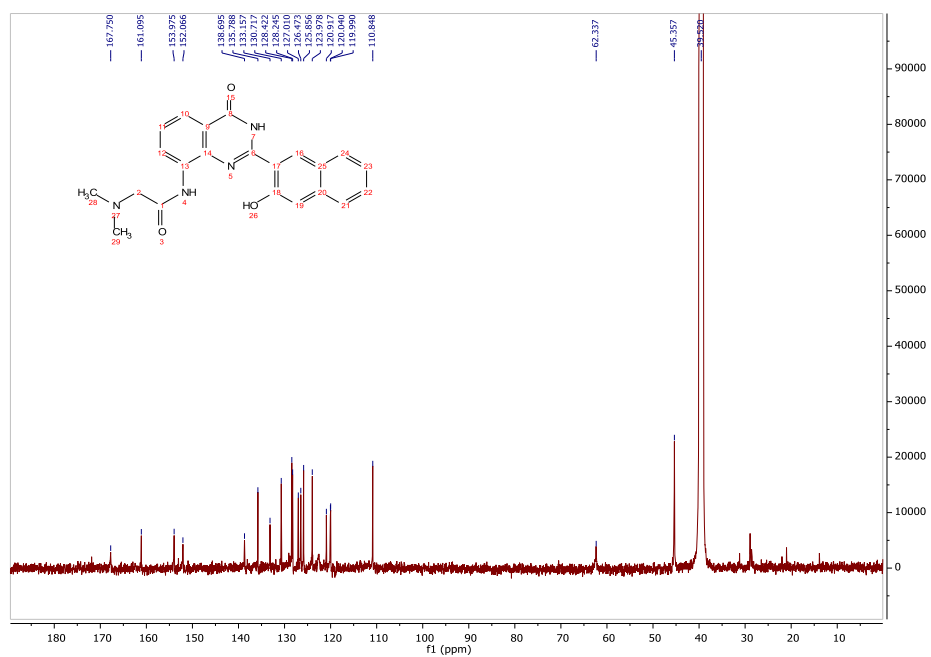


Figure S28: ^{13}C NMR spectrum of 22

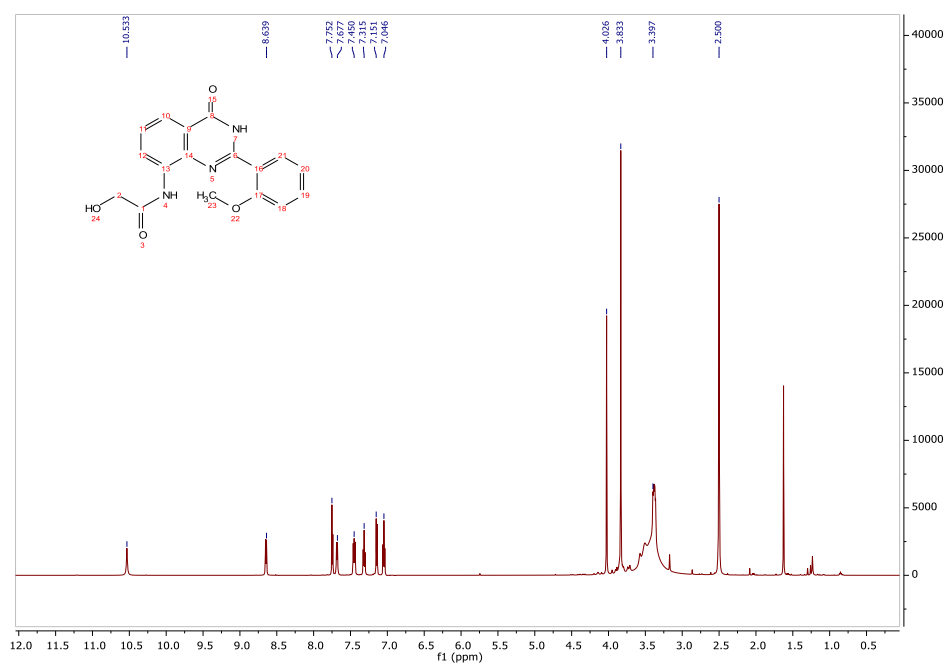


Figure S29: ¹H NMR spectrum of 25

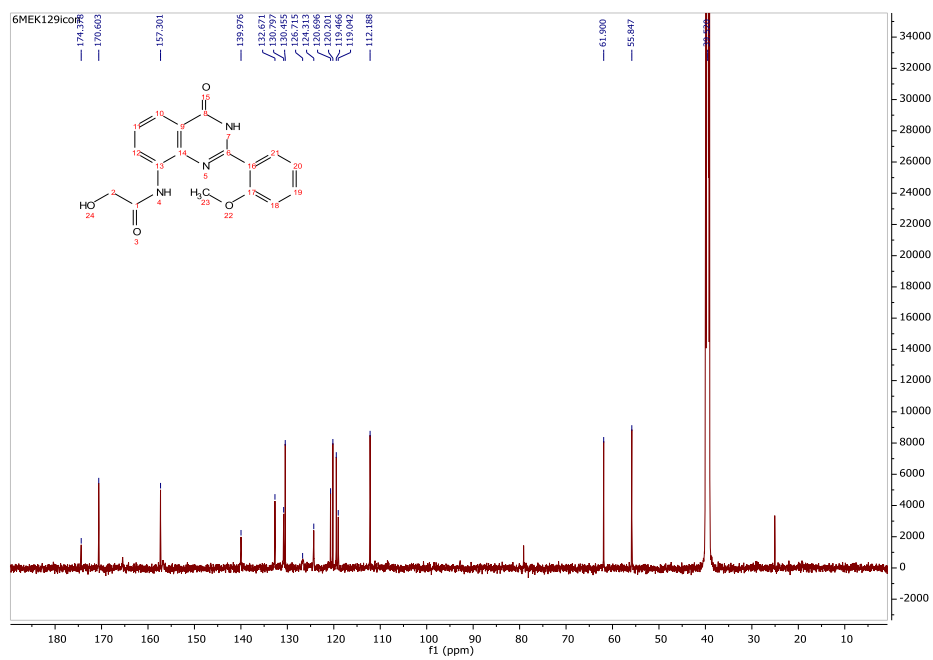


Figure S30: ¹³C NMR spectrum of 25

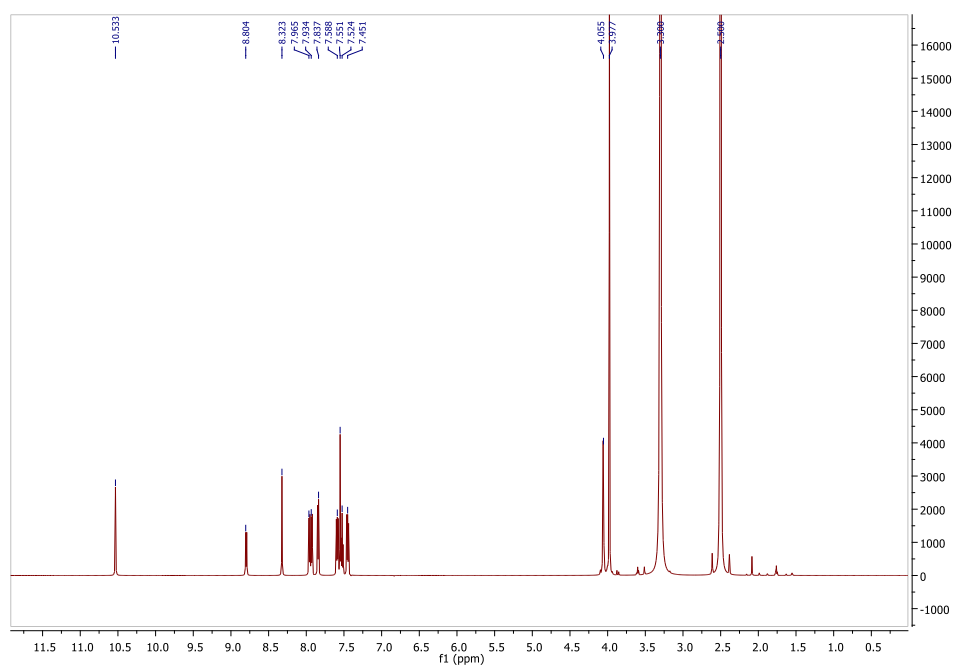


Figure S31: ^1H NMR spectrum of 26

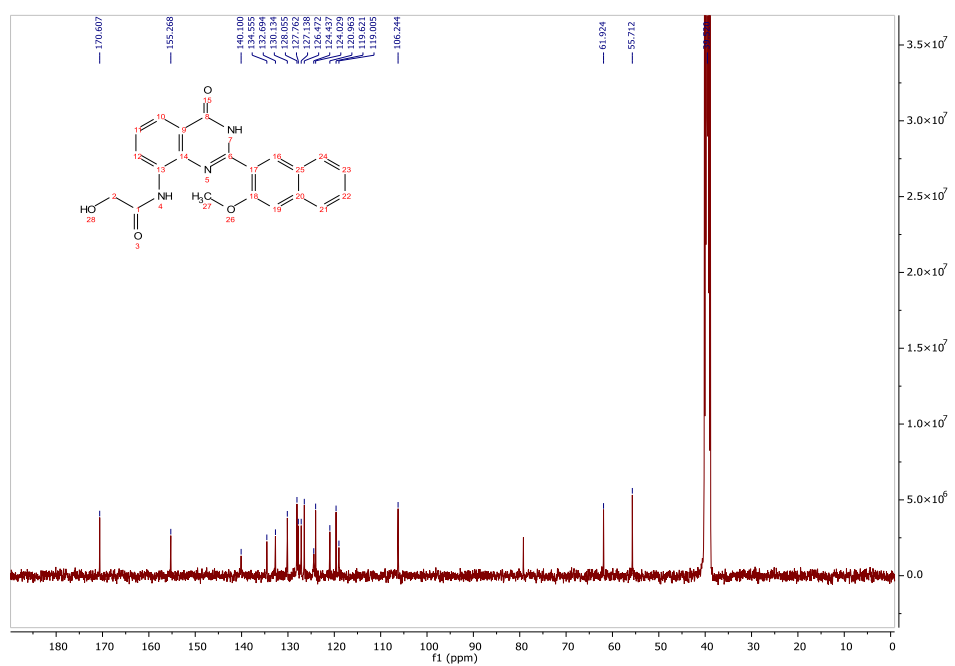


Figure S32: ^{13}C NMR spectrum of 26

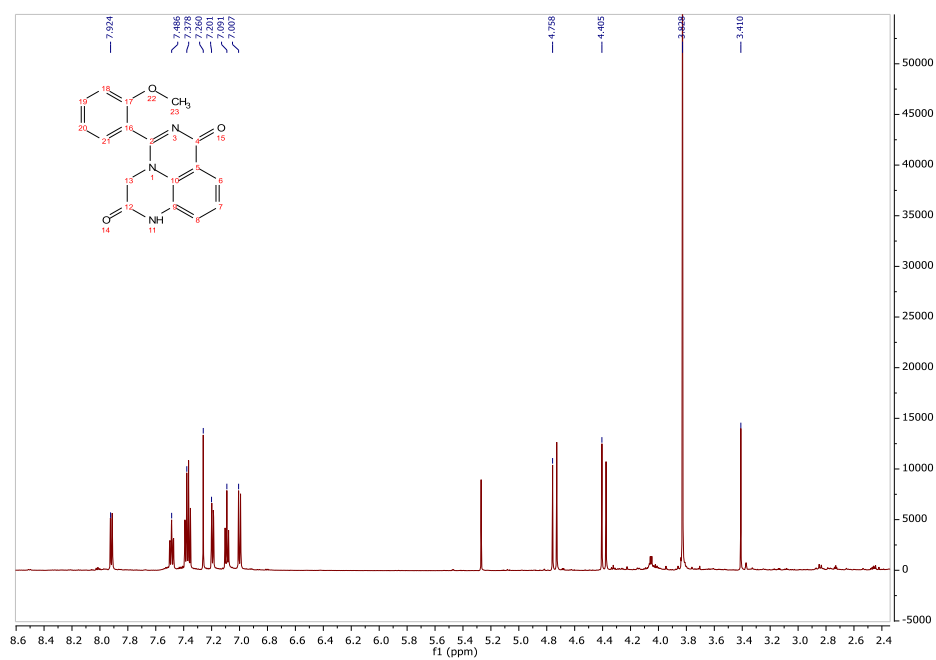


Figure S33: ^1H NMR spectrum of 27

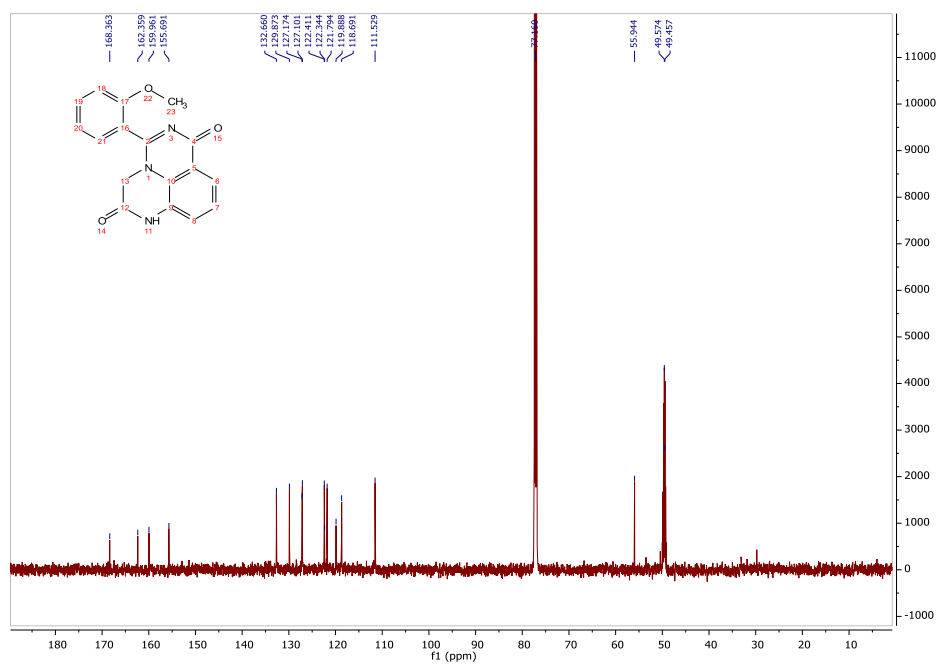


Figure S34: ^{13}C NMR spectrum of 27

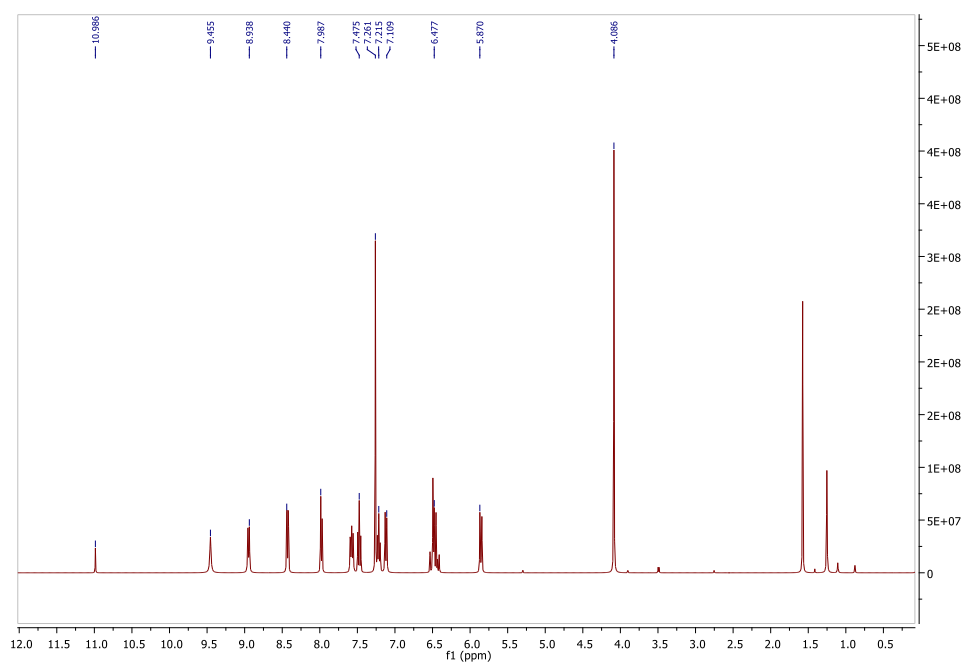


Figure S35: ^1H NMR spectrum of 28

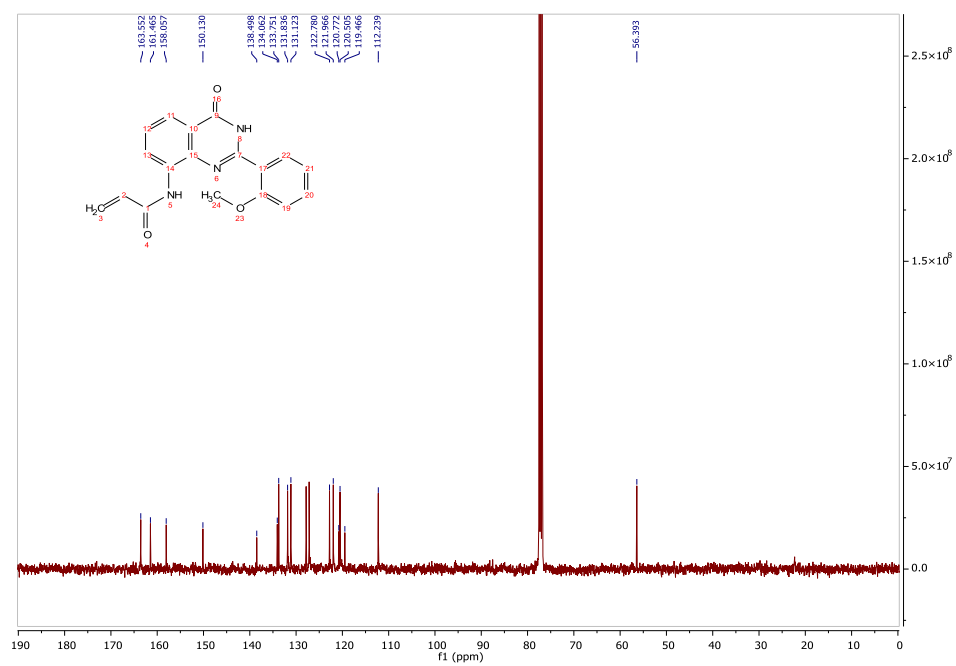


Figure S36: ^{13}C NMR spectrum of 28

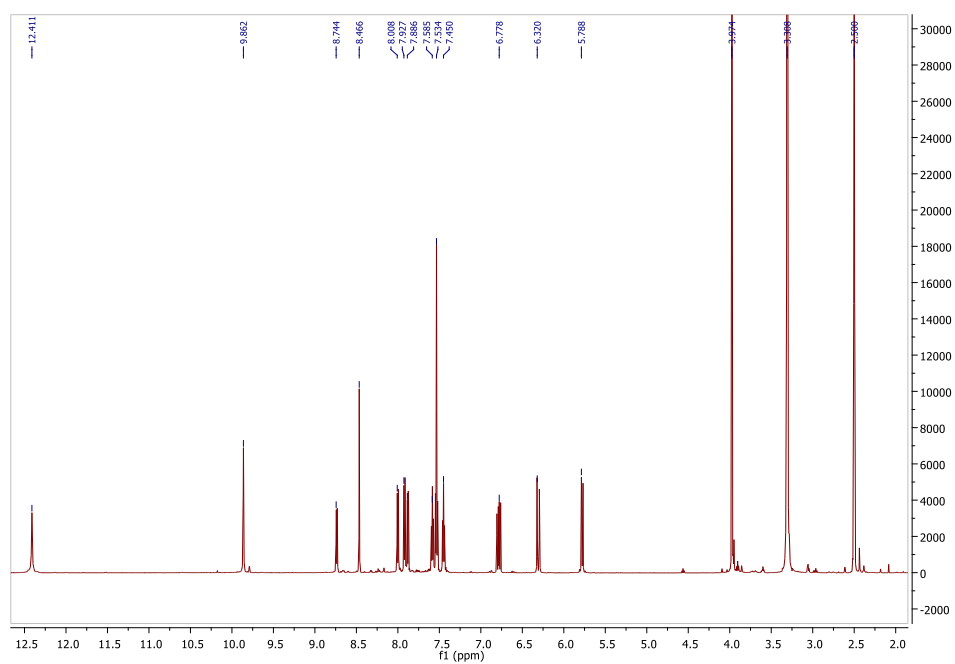


Figure S37: ^1H NMR spectrum of 29

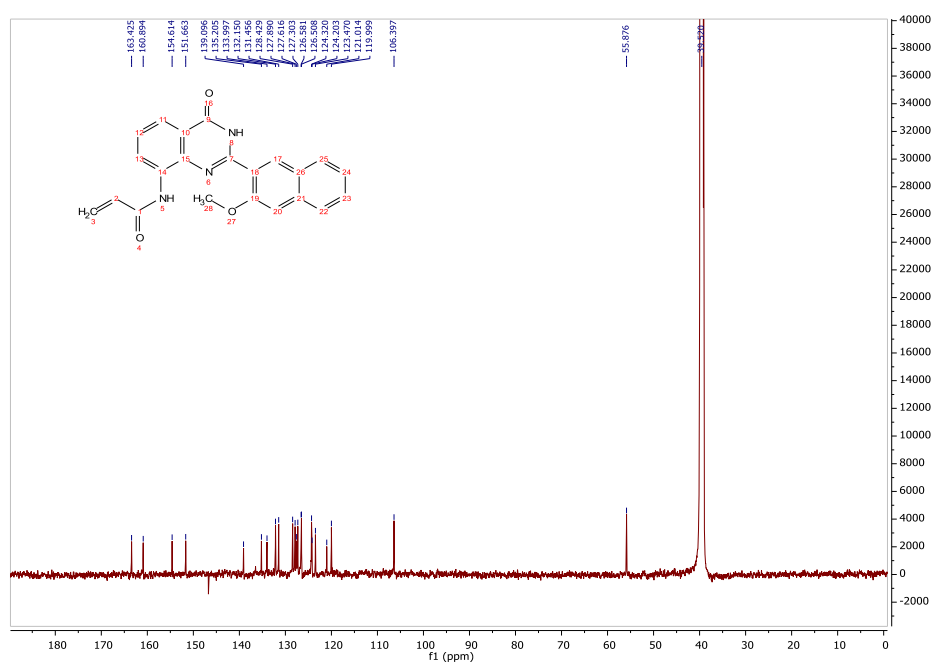


Figure S38: ^{13}C NMR spectrum of 29

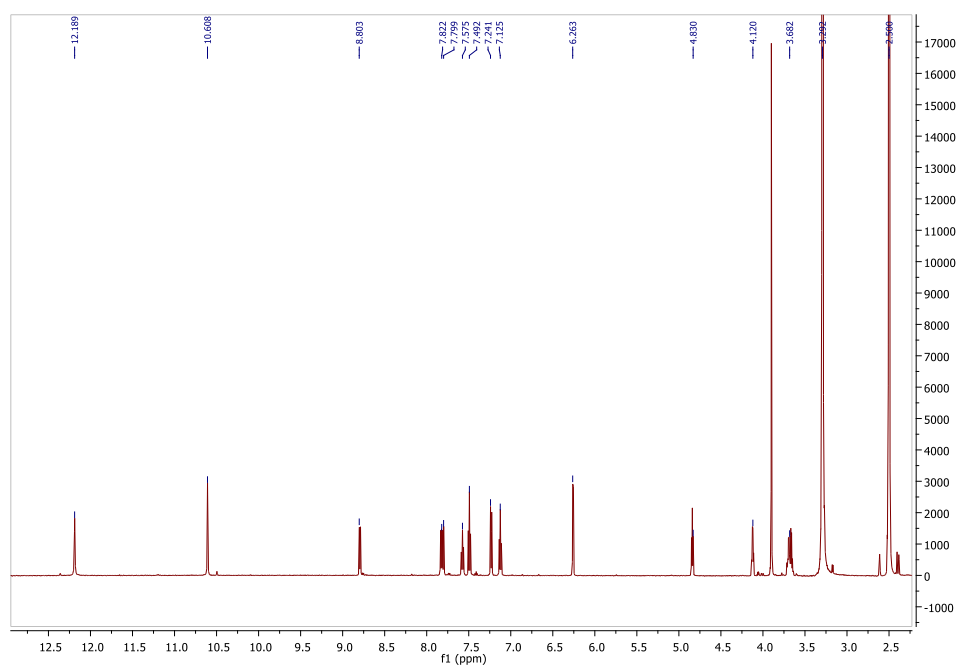


Figure S39: ^1H NMR spectrum of 30

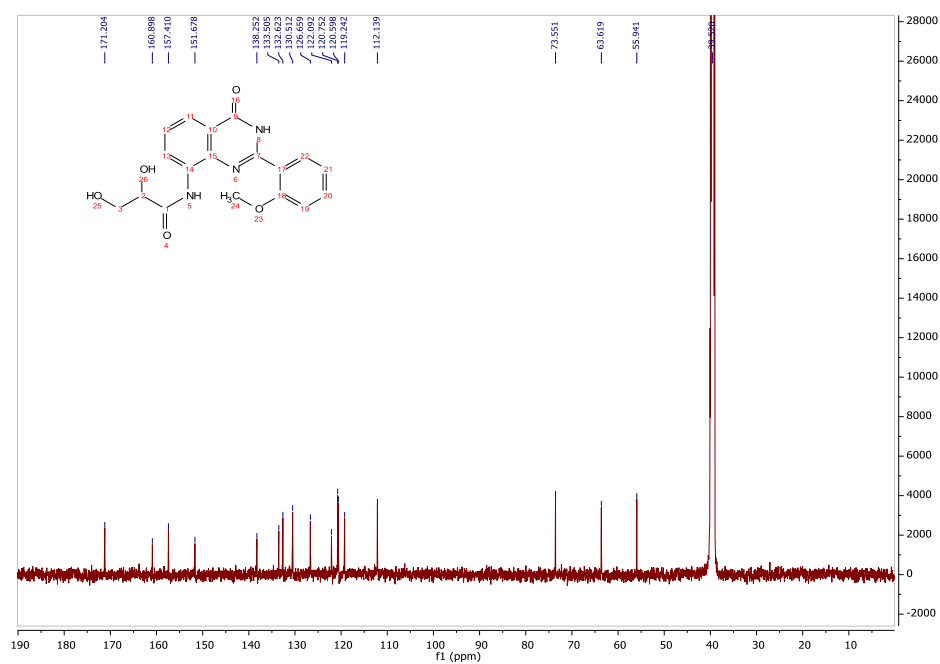


Figure S40: ^{13}C NMR spectrum of 30

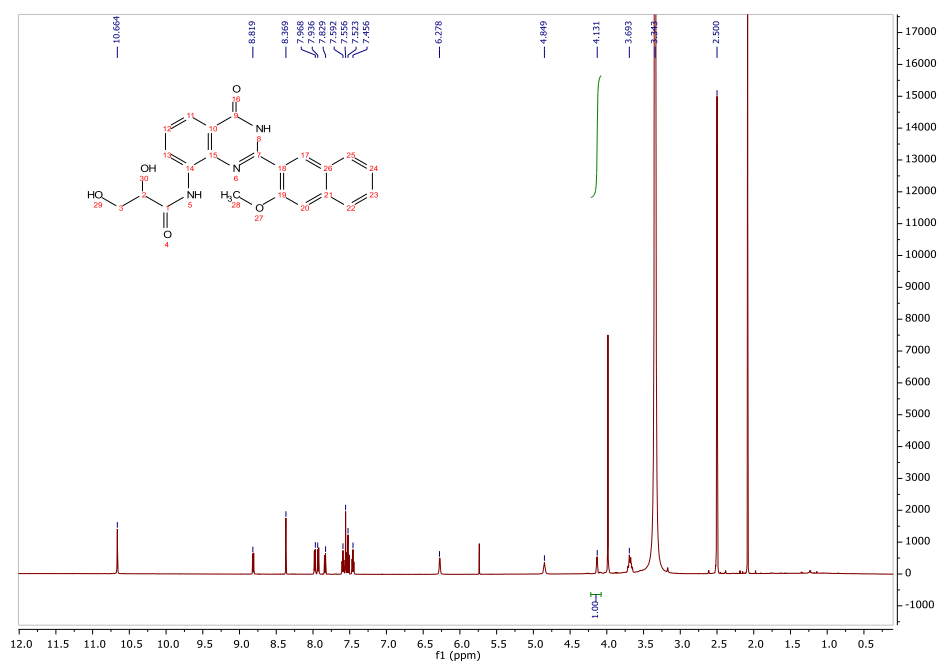


Figure S41: ¹H NMR spectrum of 31

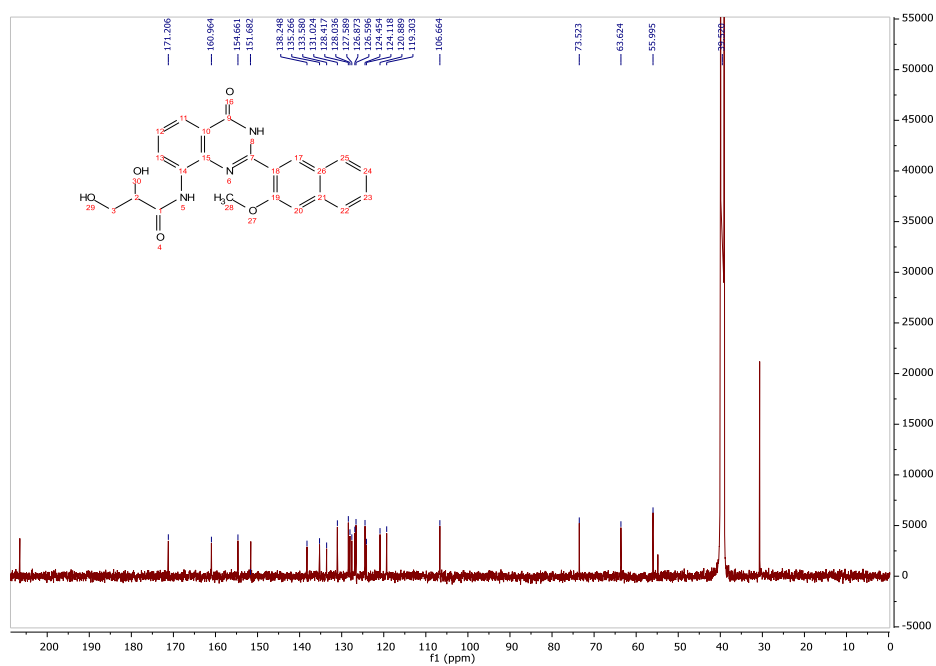


Figure S42: ¹³C NMR spectrum of 31

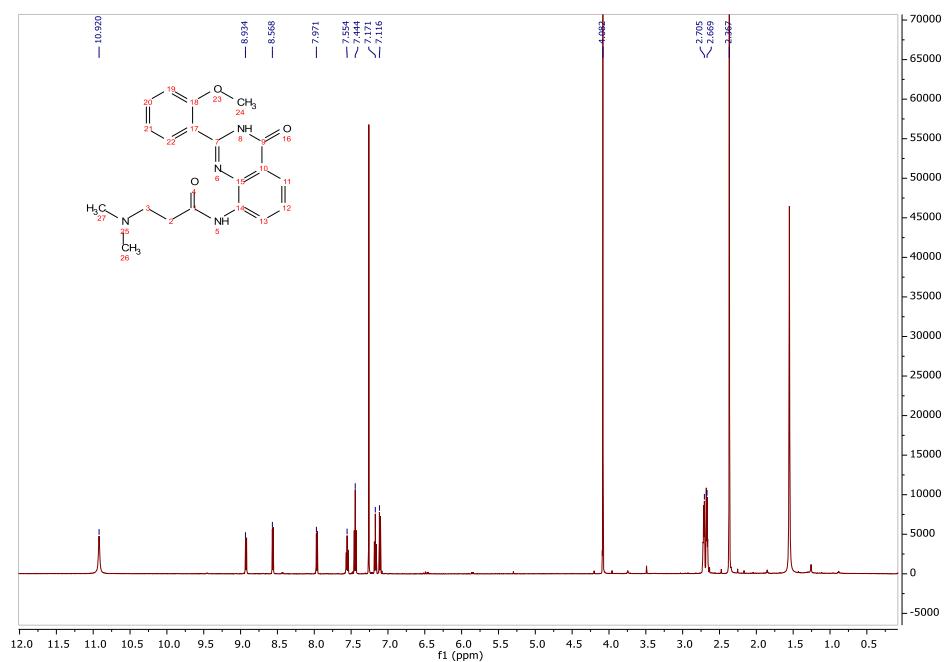


Figure S43: ^1H NMR spectrum of 32

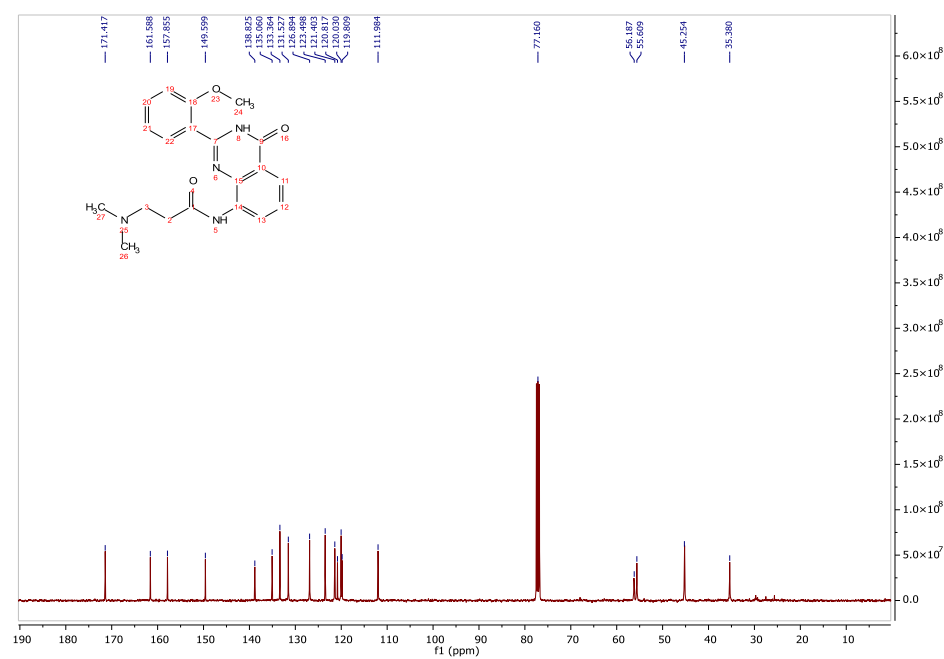


Figure S44: ^{13}C NMR spectrum of 32

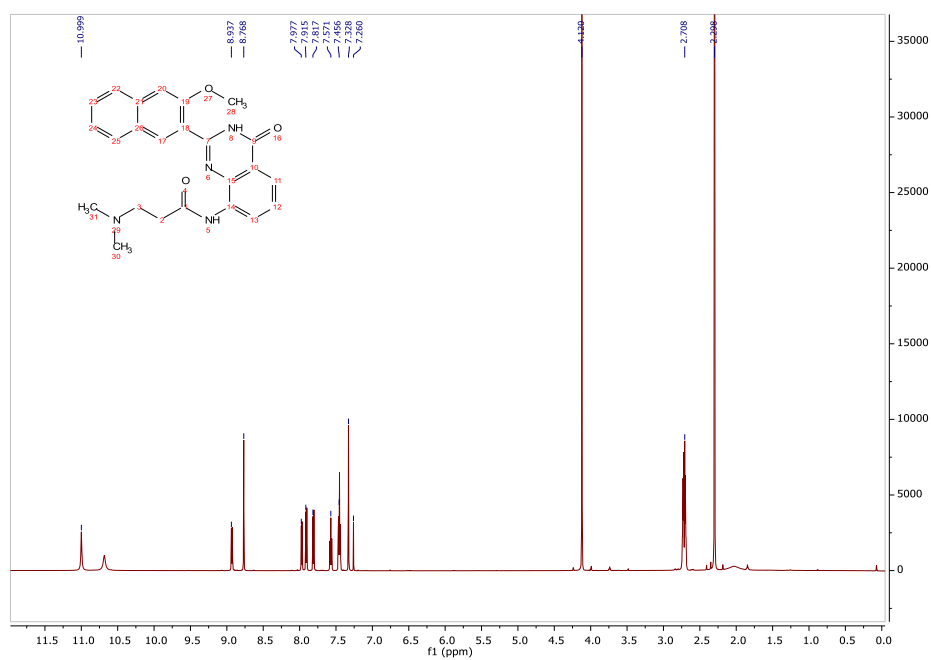


Figure S45: ¹H NMR spectrum of 33

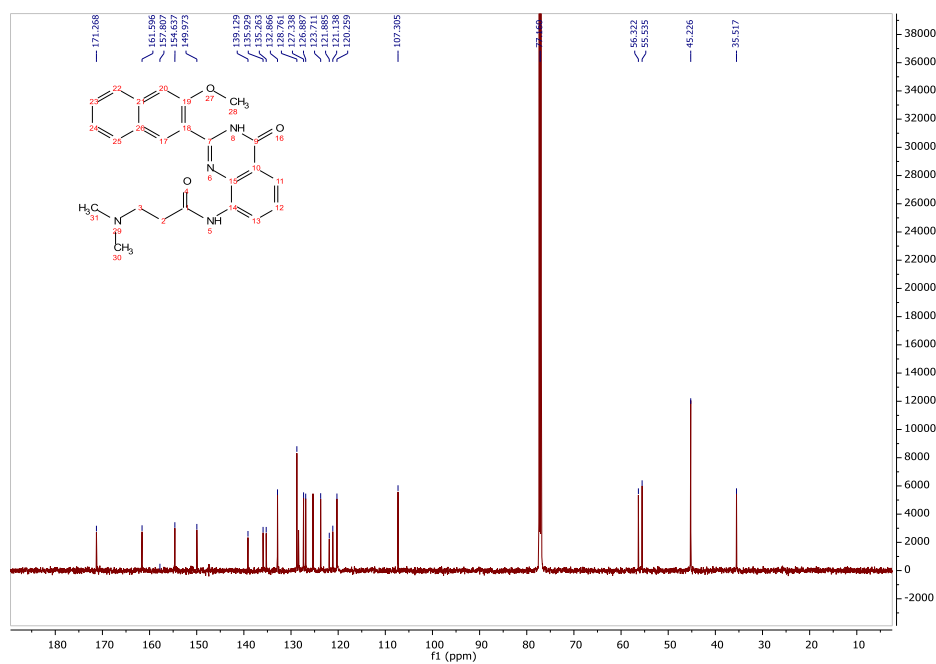


Figure S46: ¹³C NMR spectrum of 33

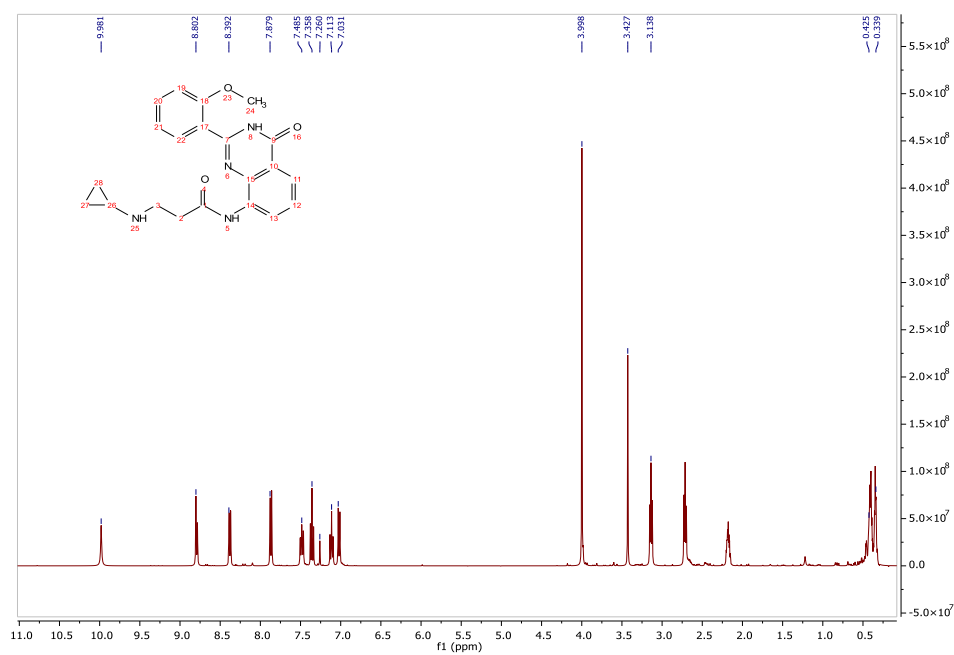


Figure S47: ^1H NMR spectrum of 34

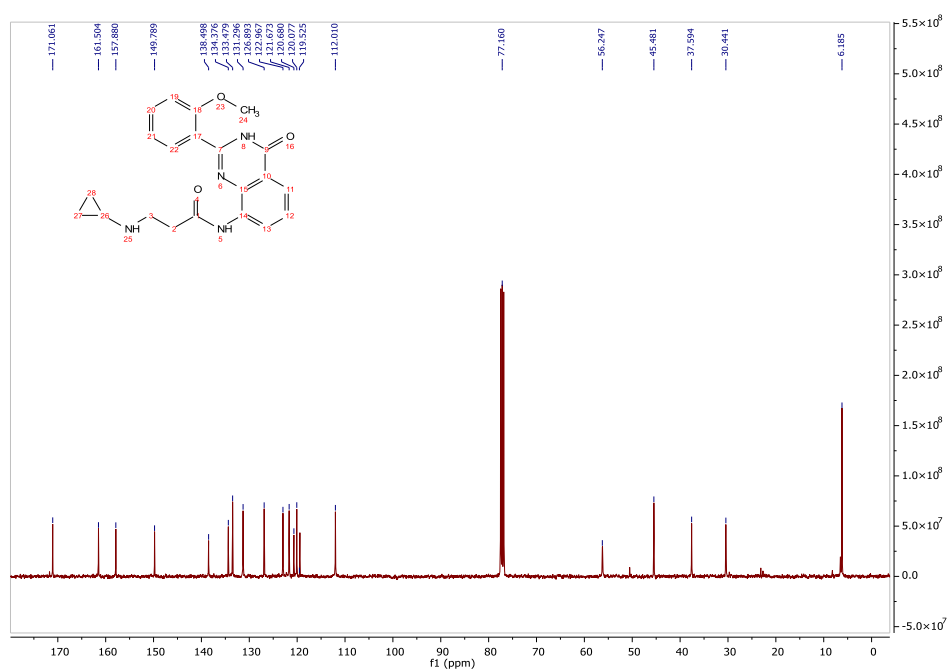


Figure S48: ^{13}C NMR spectrum of 34

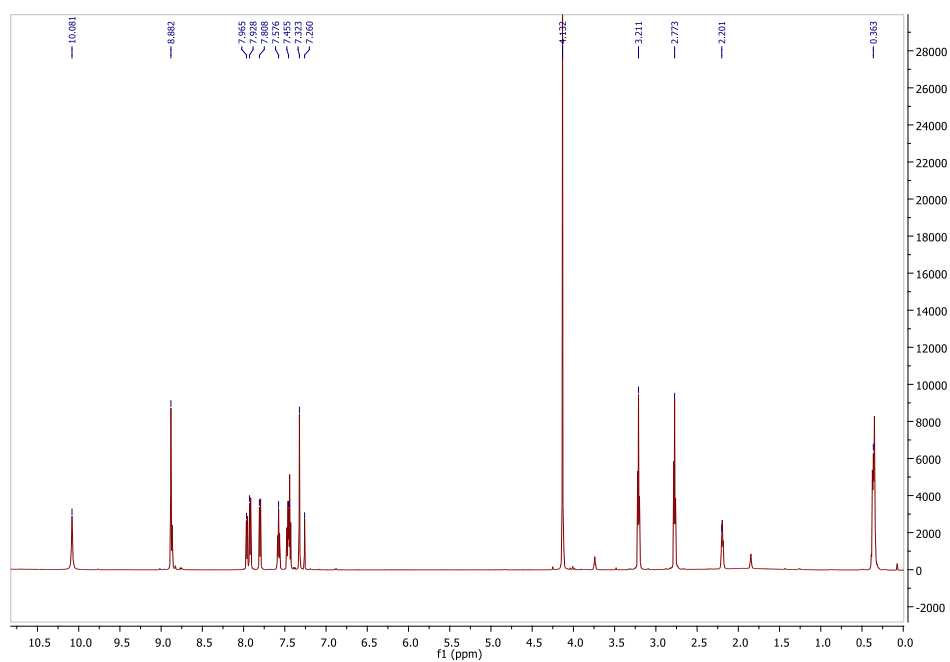


Figure S49: ^1H NMR spectrum of 35

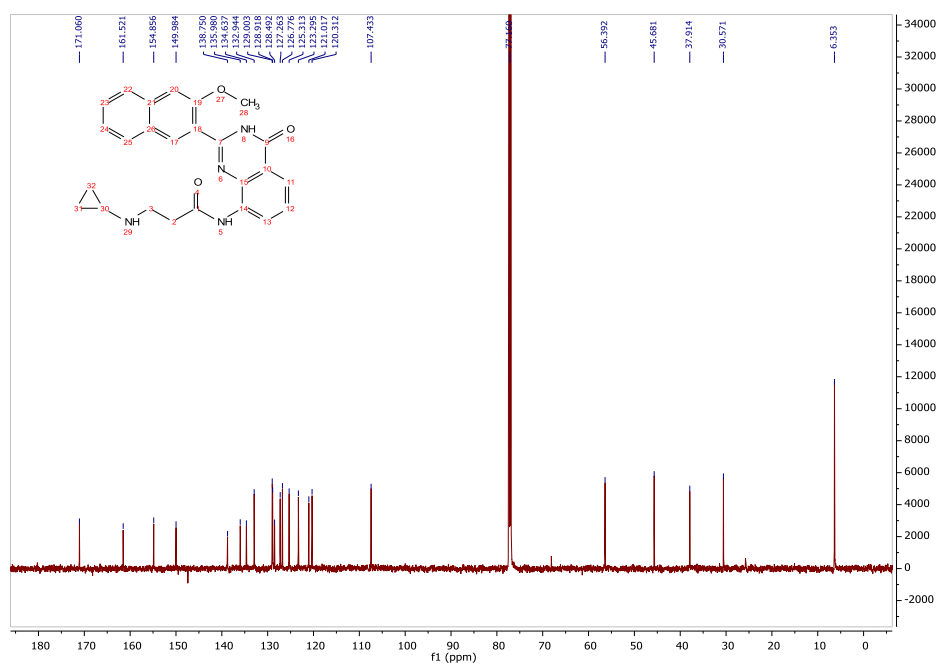


Figure S50: ^{13}C NMR spectrum of 35

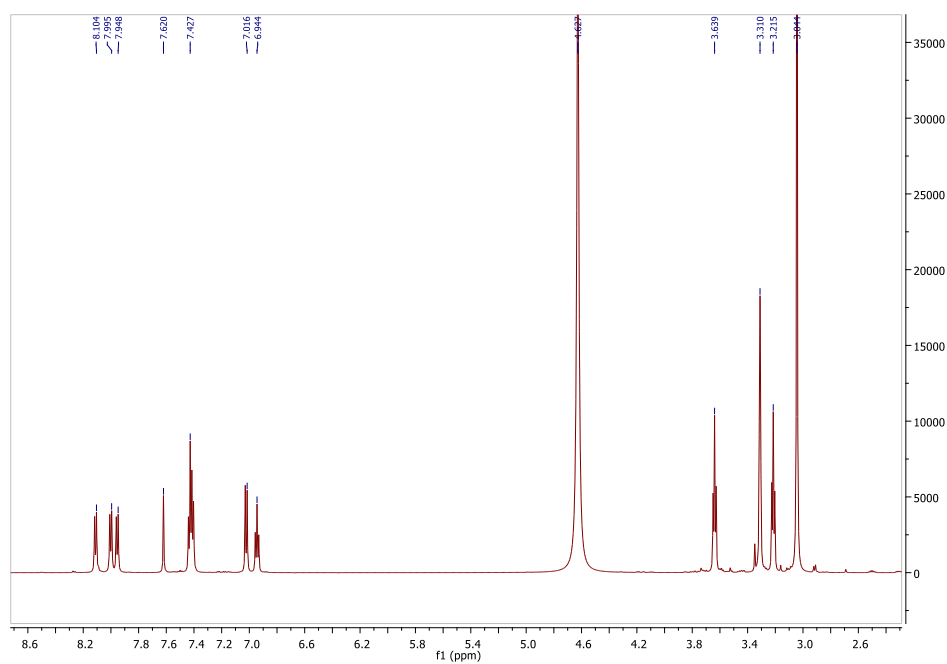


Figure S51: ^1H NMR spectrum of 36

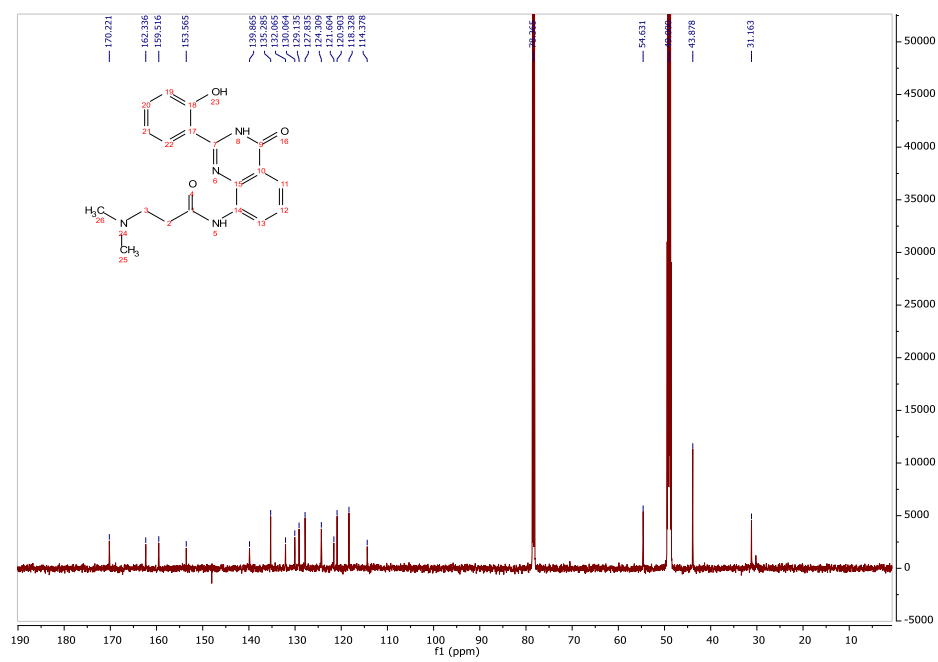


Figure S52: ^{13}C NMR spectrum of 36