Supporting Information

Exploring the Ring-Closing Metathesis for the Construction of the Solomonamide Macrocyclic Core: Identification of Bioactive Precursors

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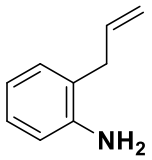
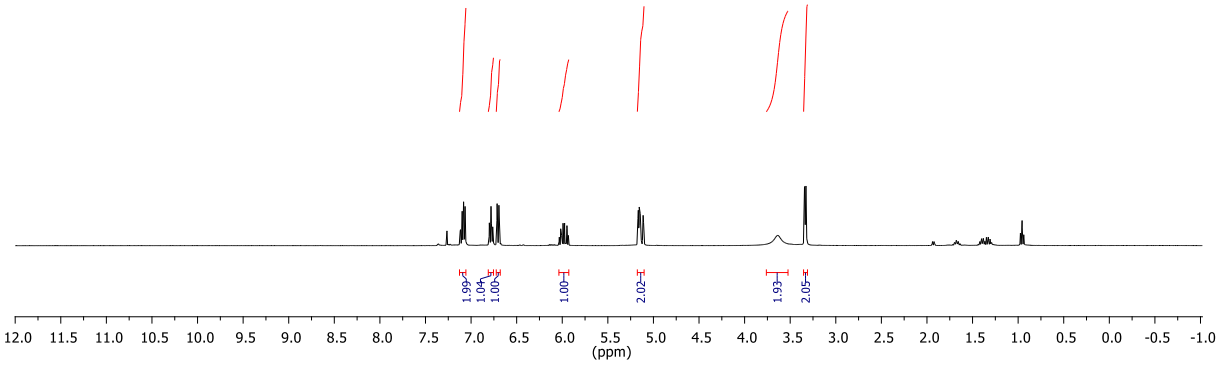
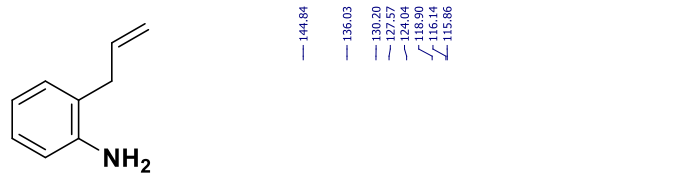
1. ^{1}H and ^{13}C NMR Spectra



19

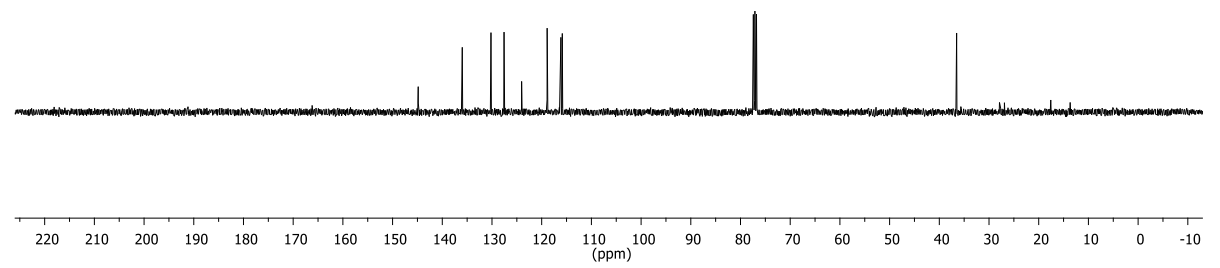
^{1}H NMR (400 MHz, $CDCl_3$)

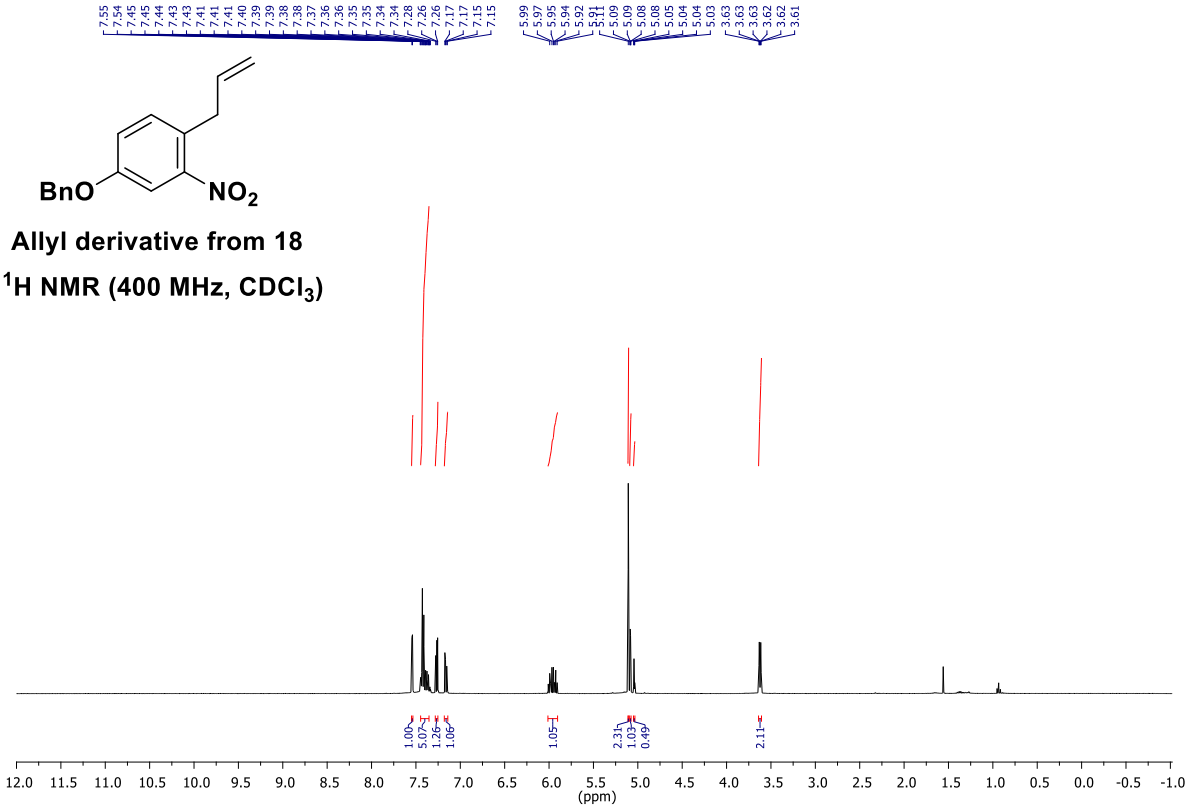




19

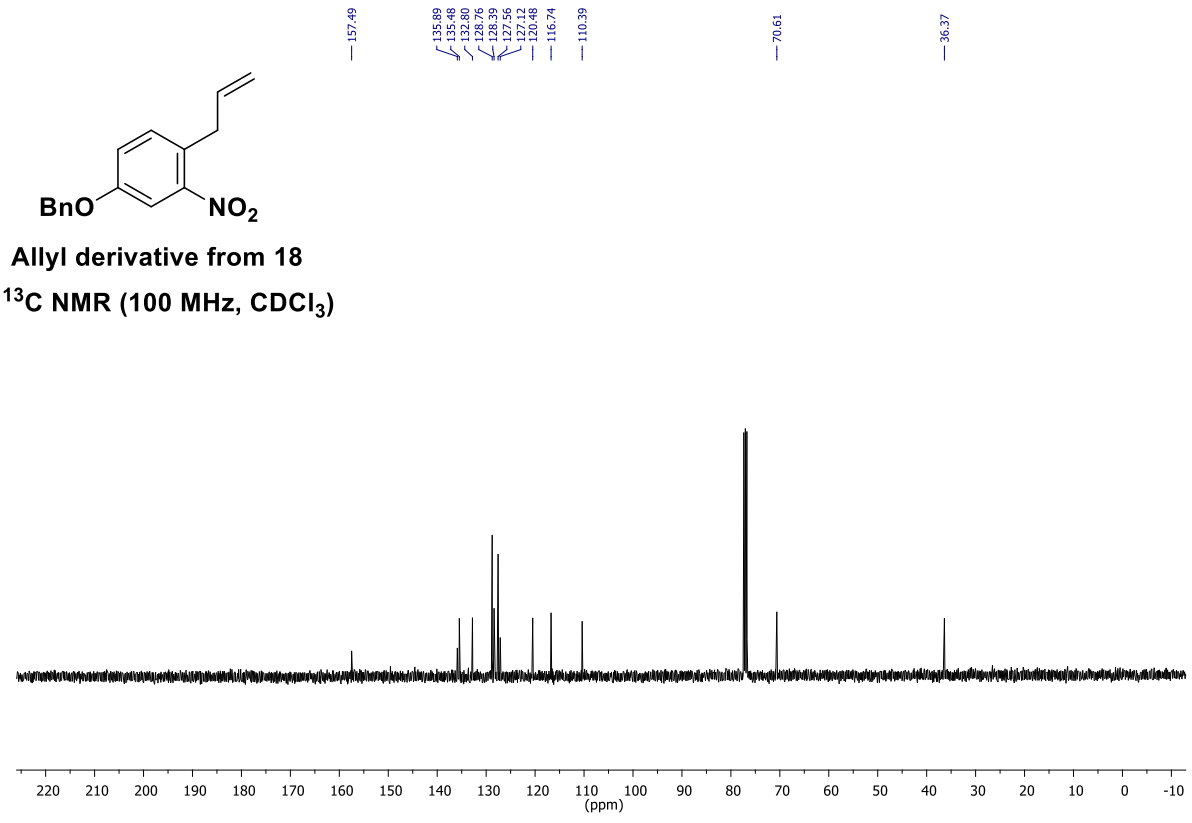
^{13}C NMR (100 MHz, $CDCl_3$)





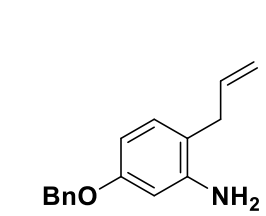
Allyl derivative from 18

^{1}H NMR (400 MHz, $CDCl_3$)



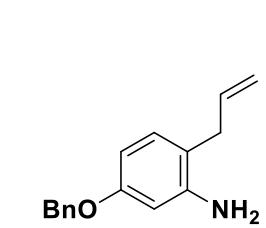
Allyl derivative from 18

^{13}C NMR (100 MHz, $CDCl_3$)



20

^{1}H NMR (400 MHz, $CDCl_3$)



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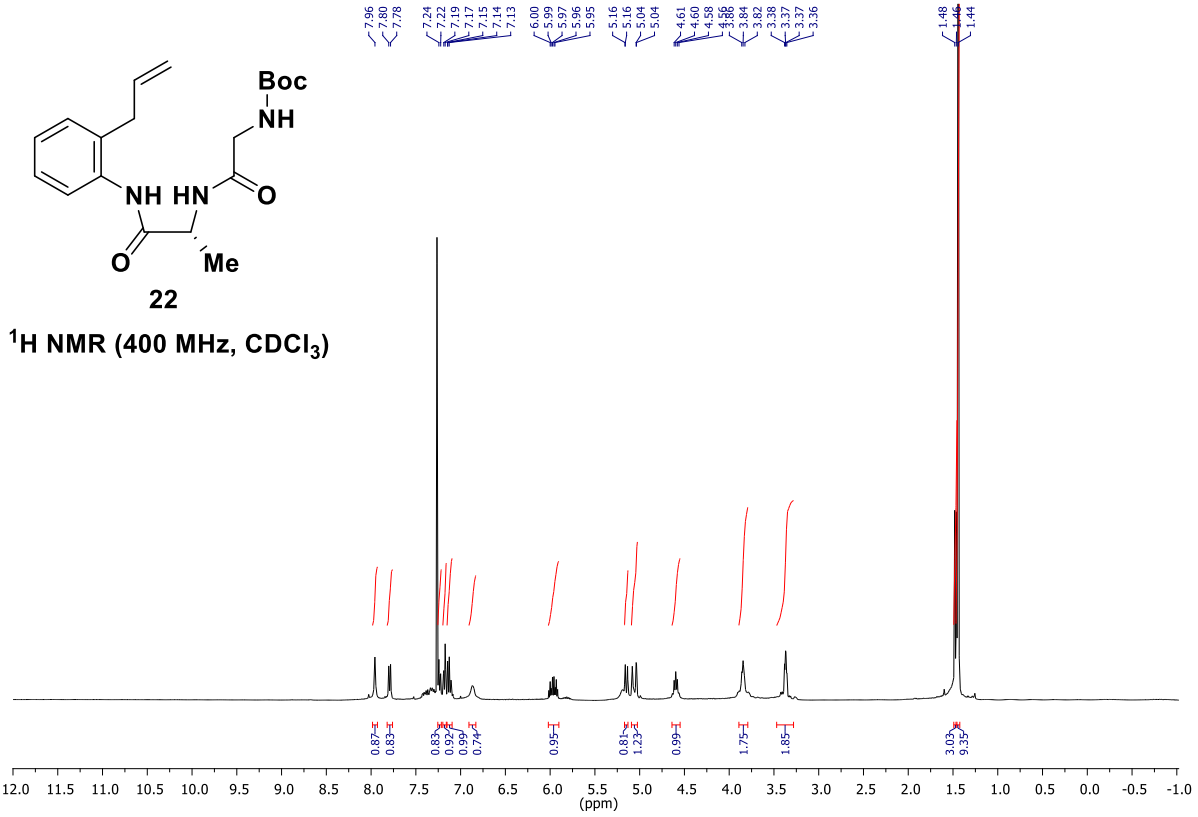
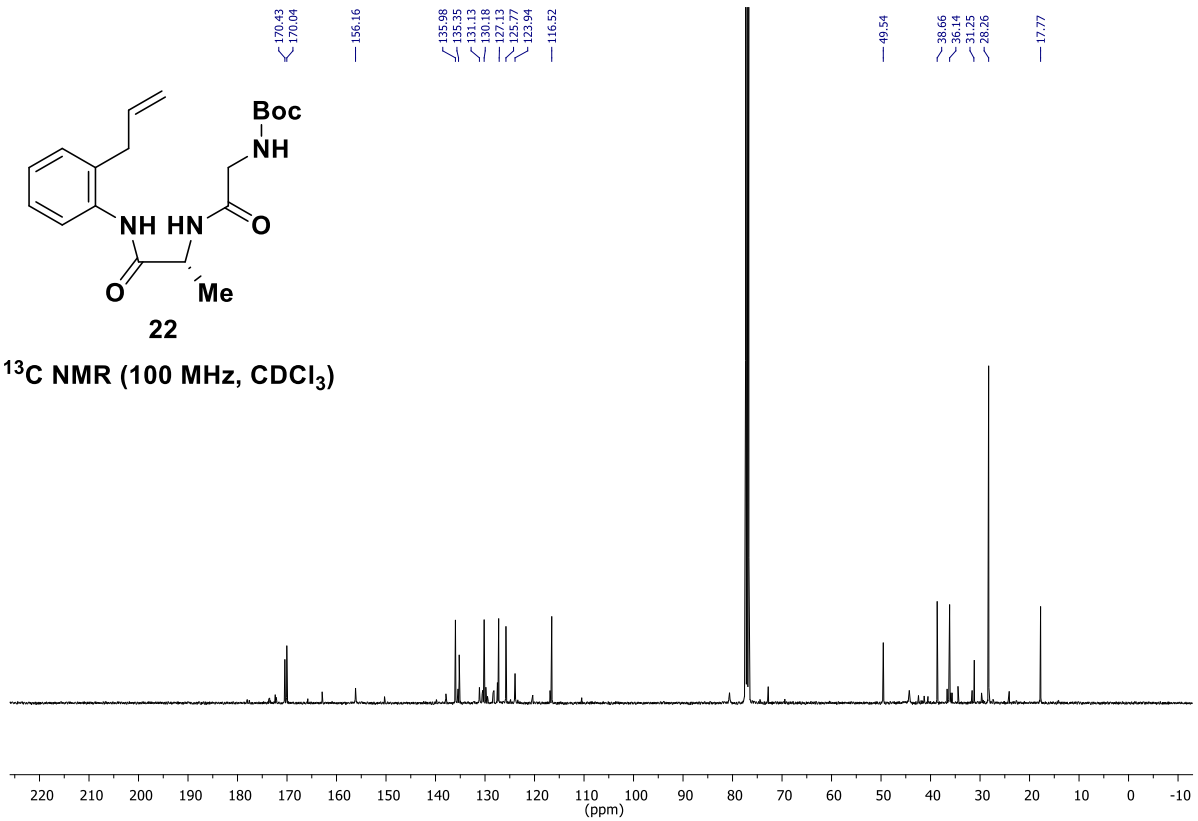
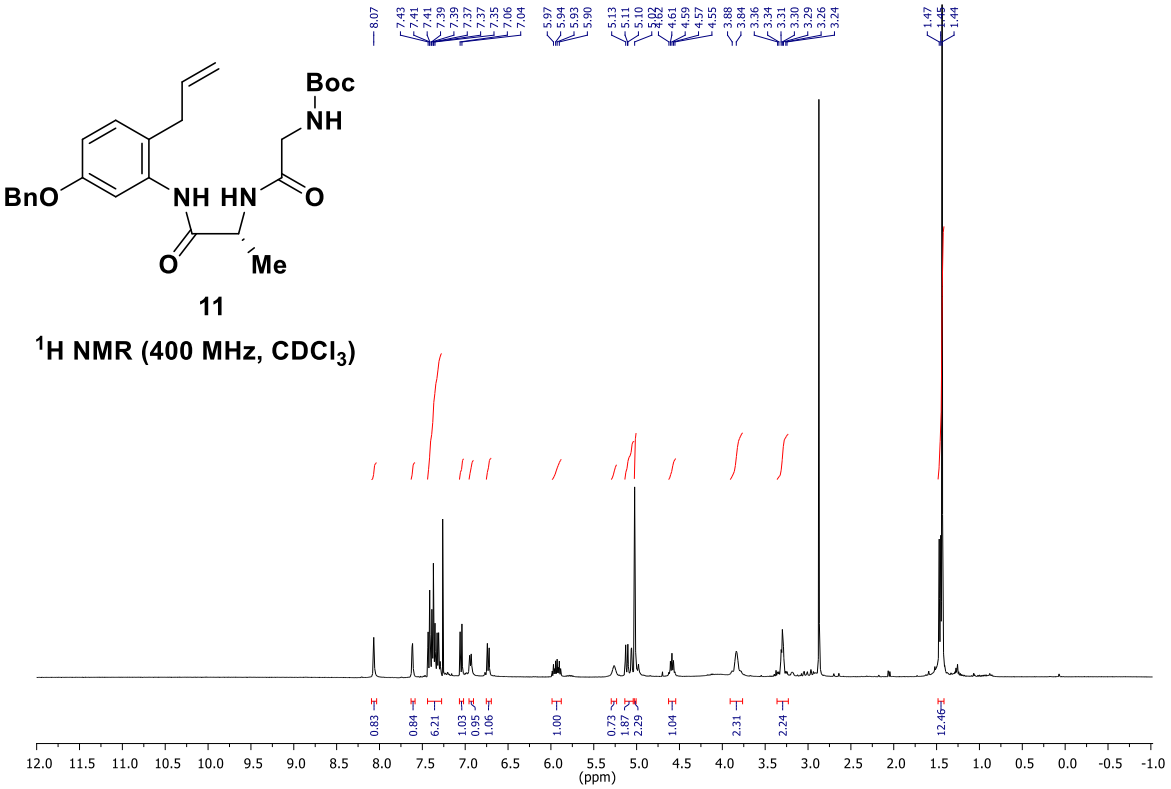
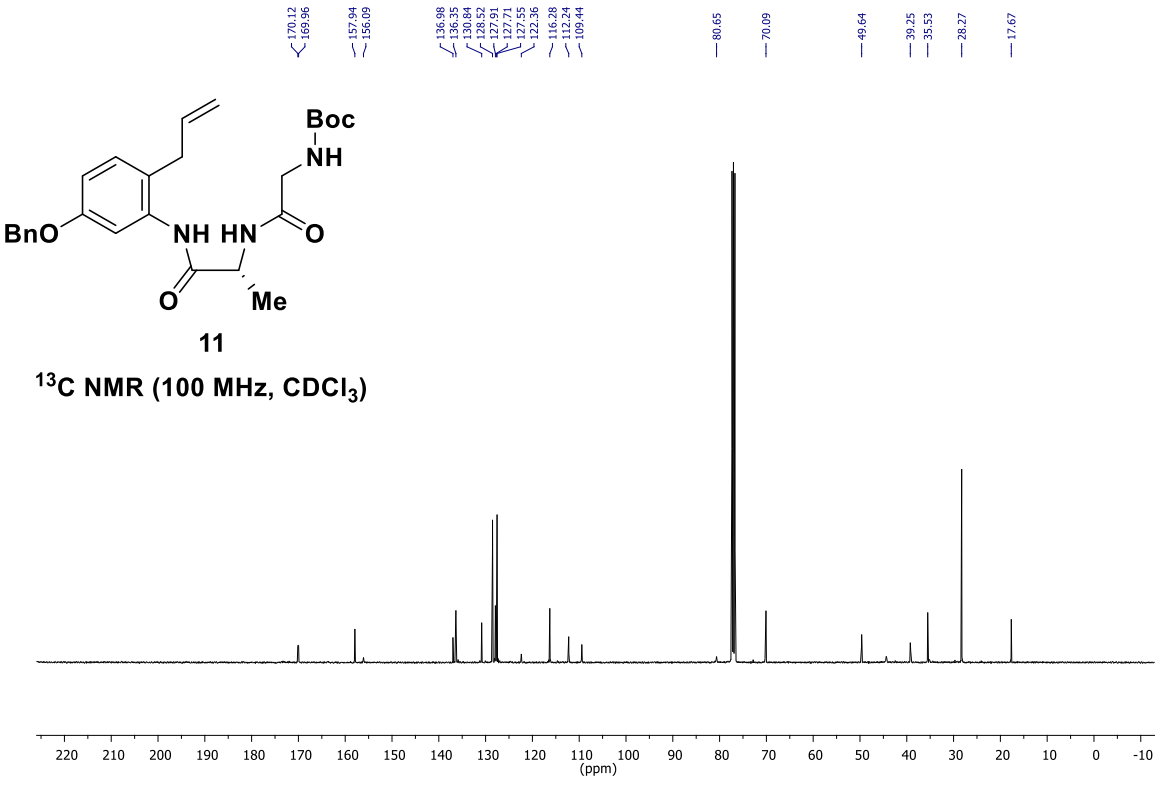
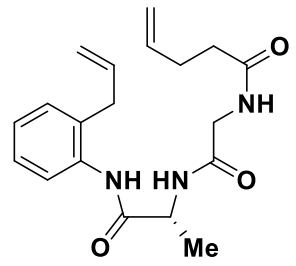

Boc
NH
NH HN
O
O
Me
22
^{1}H NMR (400 MHz, CDCl$_3$)
(ppm)


Boc
NH
NH HN
O
O
Me
22
^{13}C NMR (100 MHz, CDCl$_3$)
(ppm)

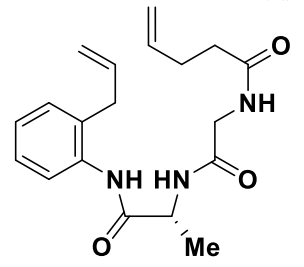

Boc
NH
BnO
NH HN
O
O
Me
11
^{1}H NMR (400 MHz, $CDCl_3$)
(ppm)


Boc
NH
BnO
NH HN
O
O
Me
11
^{13}C NMR (100 MHz, $CDCl_3$)
(ppm)



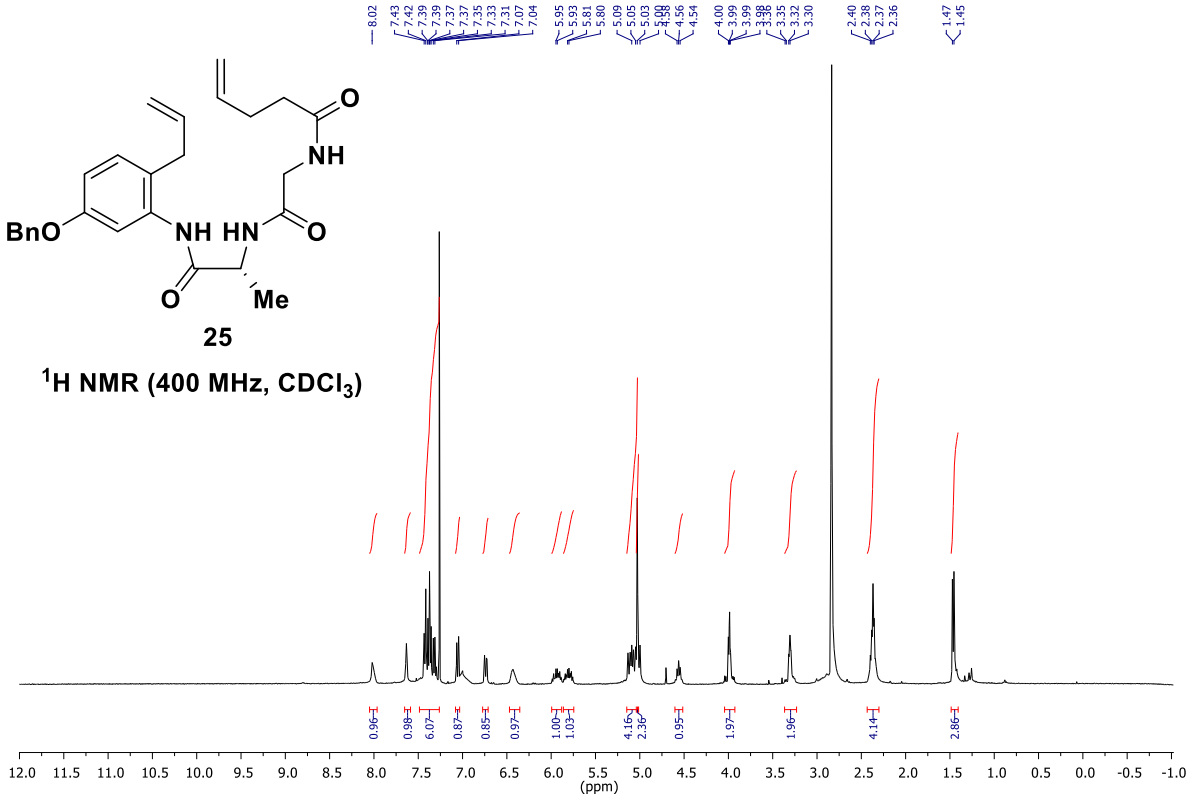
24

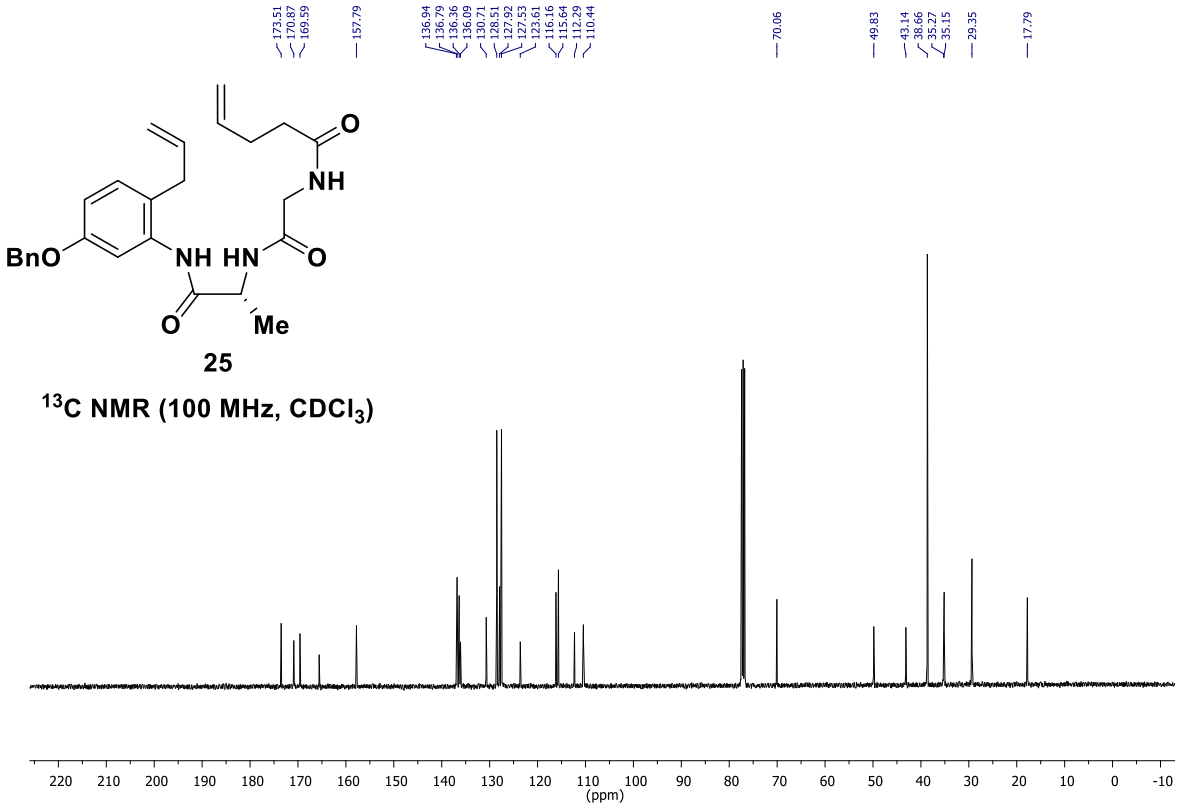
^{1}H NMR (400 MHz, $CDCl_3$)

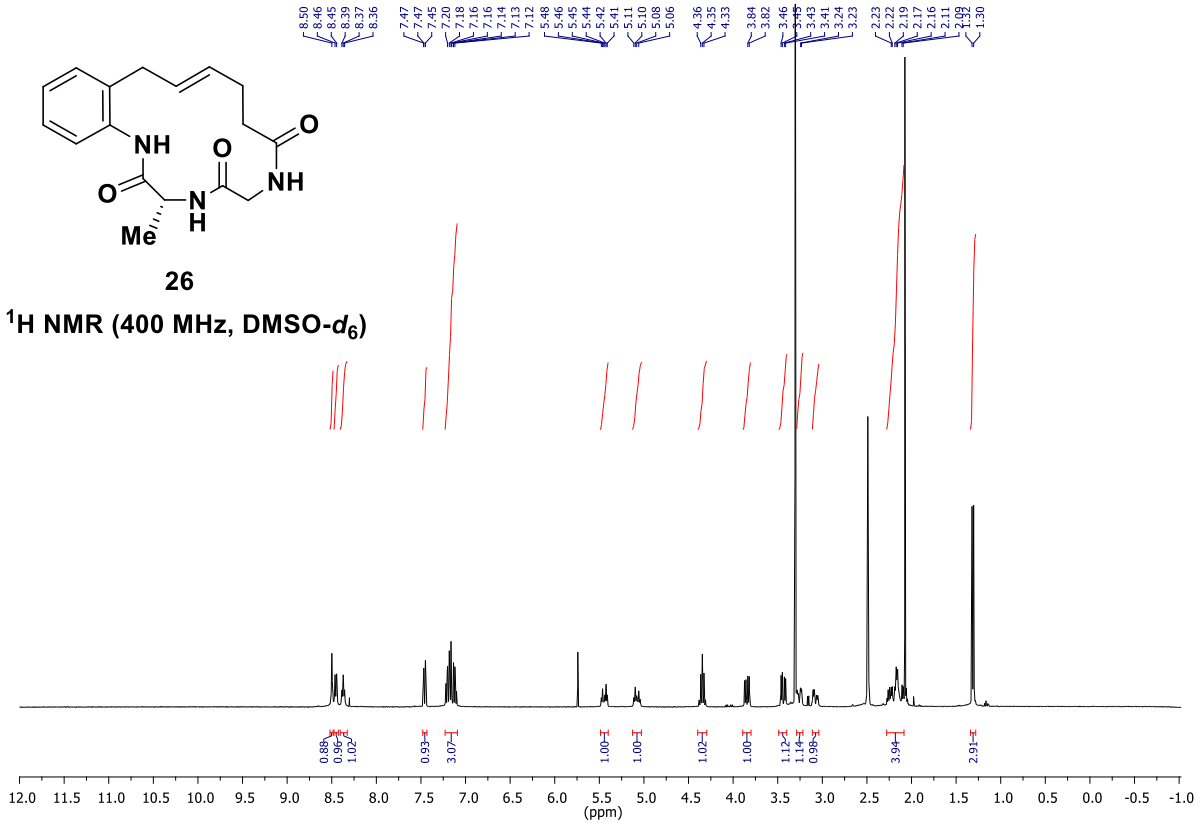


24

^{13}C NMR (100 MHz, $CDCl_3$)

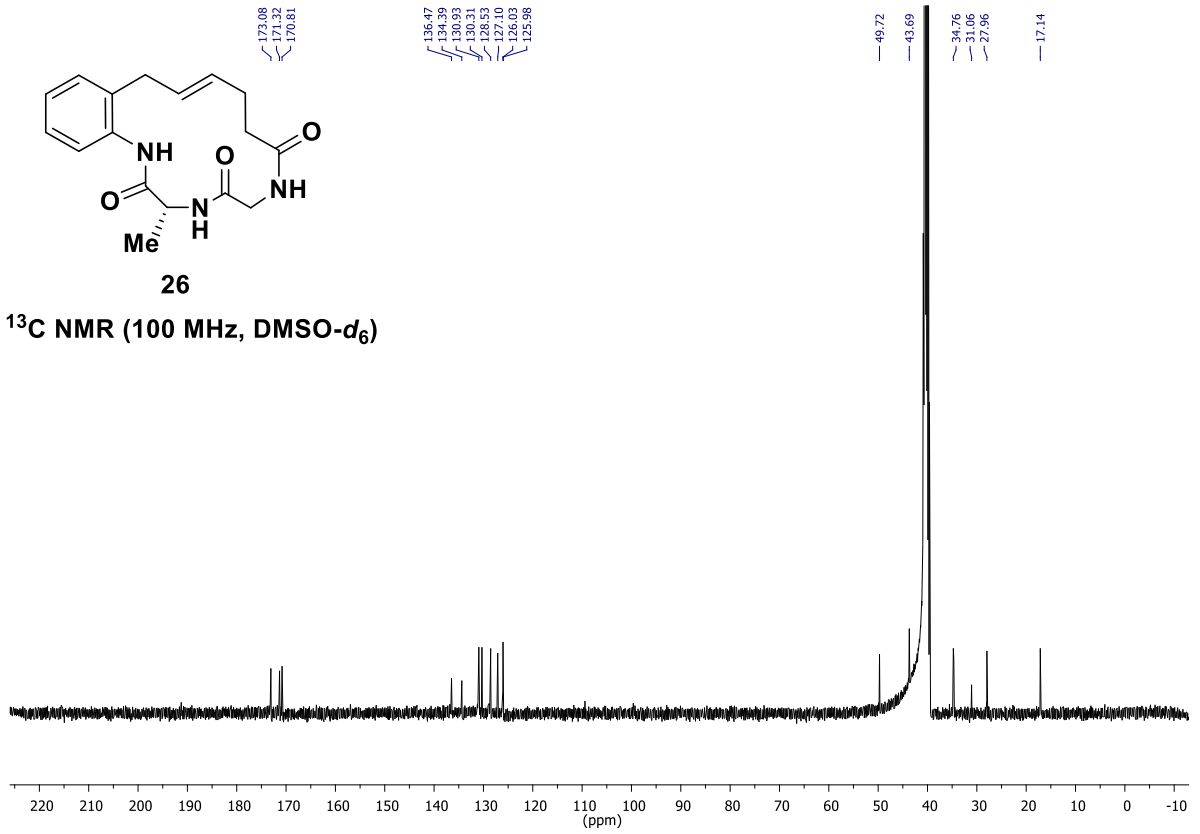

BnO
NH HN
NH
O
O
O
O
Me
25
^{1}H NMR (400 MHz, $CDCl_3$)
(ppm)


BnO
NH HN
NH
O
O
O
O
Me
25
^{13}C NMR (100 MHz, $CDCl_3$)
(ppm)



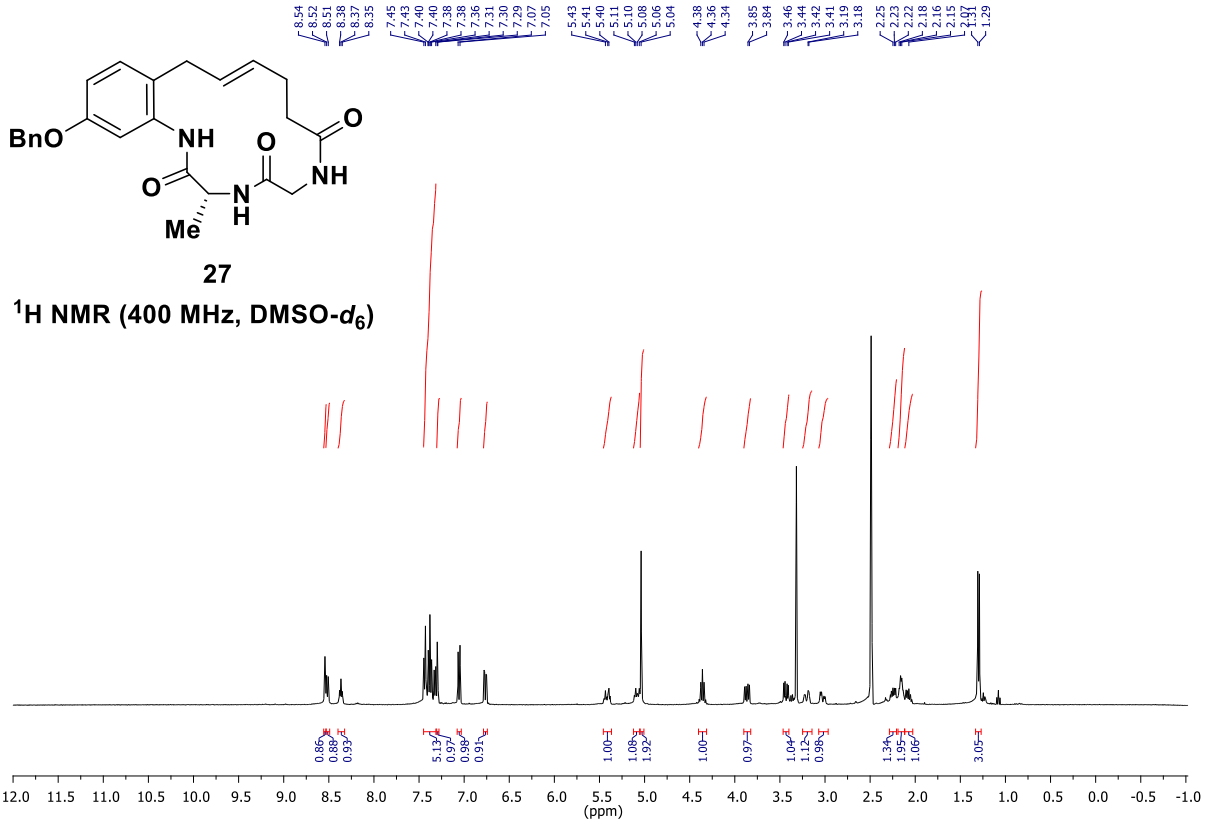
26

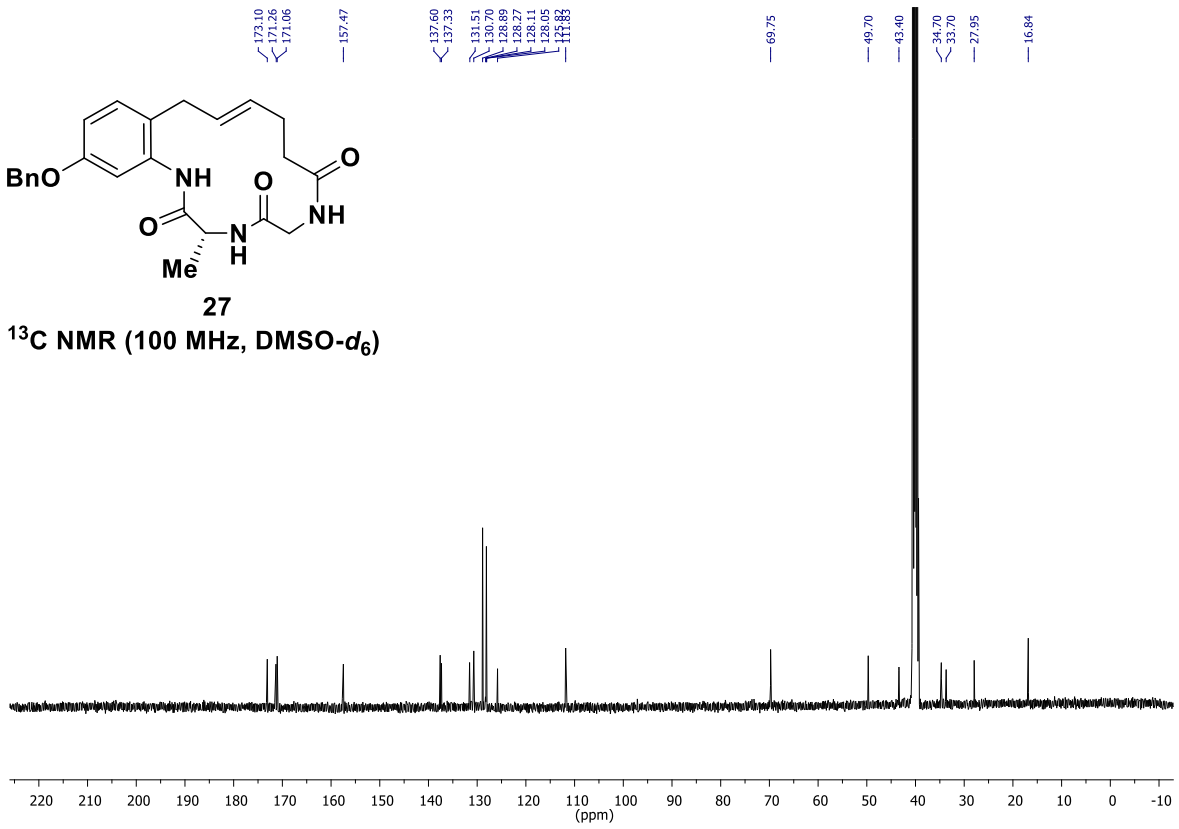
^{1}H NMR (400 MHz, DMSO-d_6)

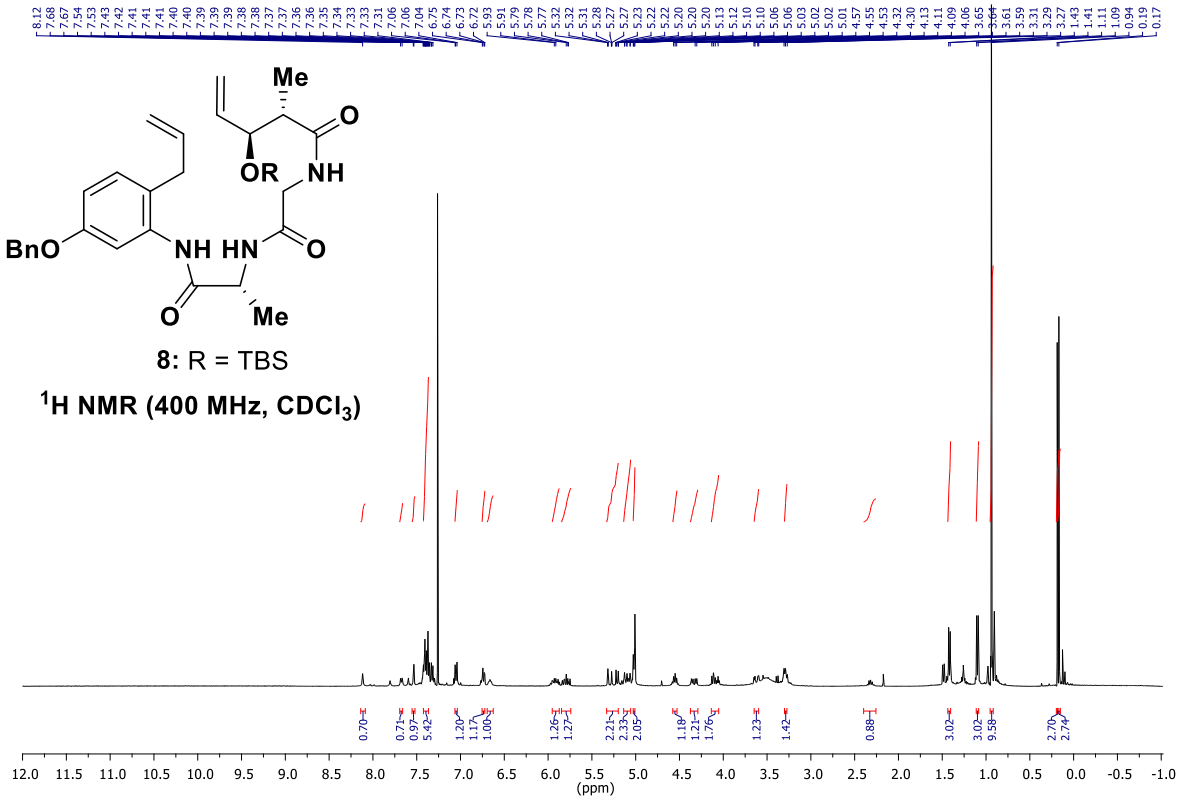


26

^{13}C NMR (100 MHz, DMSO-d_6)

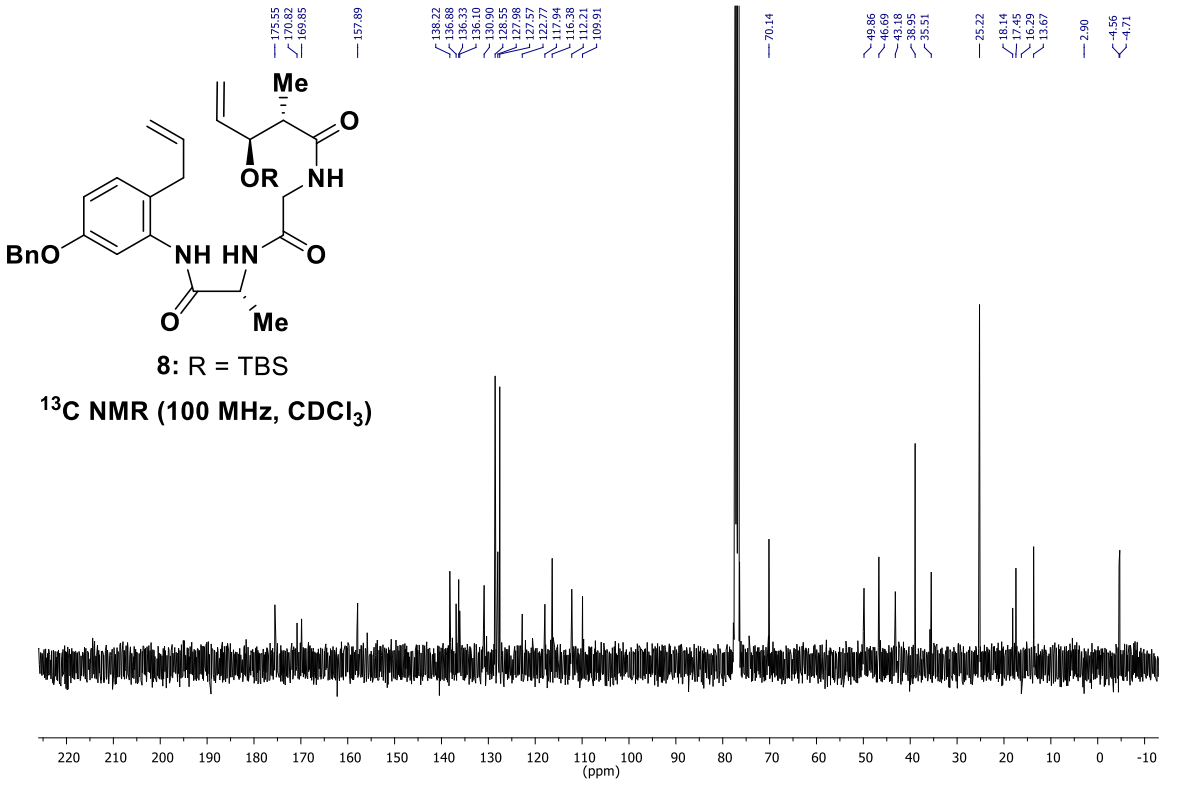

BnO
NH
O
O
NH
O
N
H
Me
NH
O
27
1H NMR (400 MHz, DMSO-d6)
(ppm)


BnO
NH
O
O
NH
O
N
H
Me
NH
O
27
13C NMR (100 MHz, DMSO-d6)
(ppm)



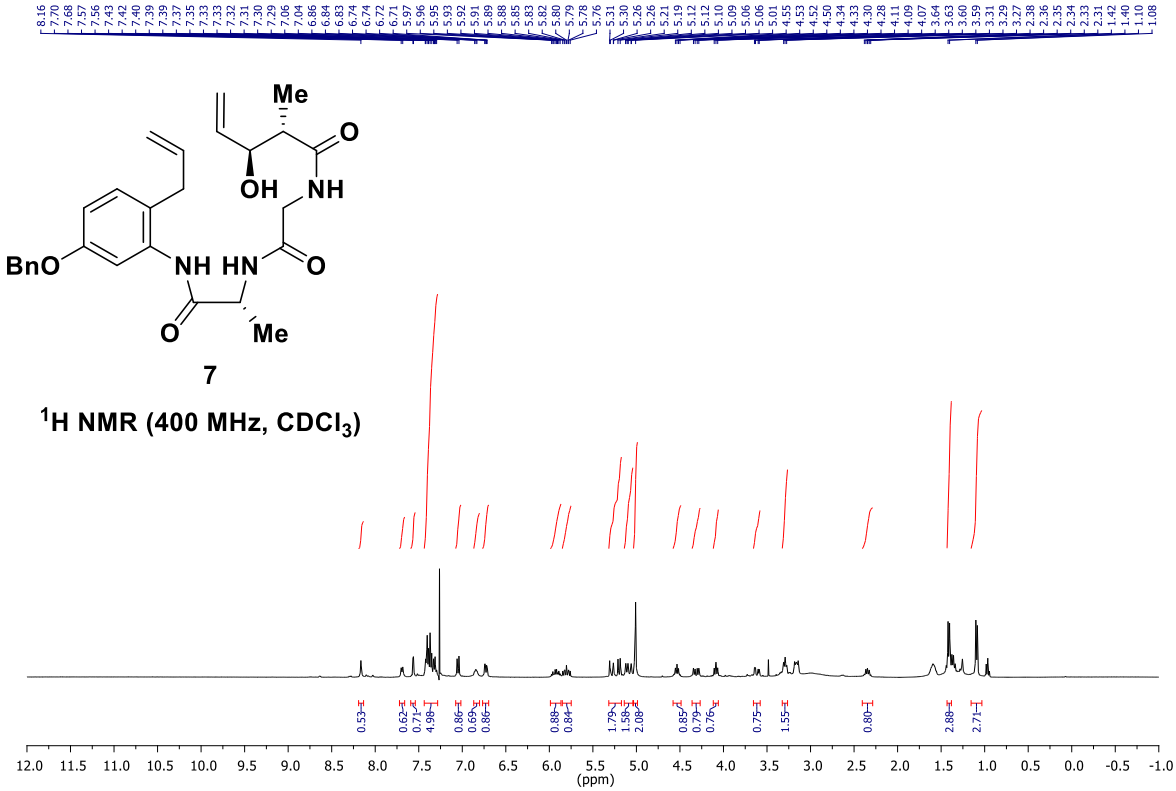
8: R = TBS

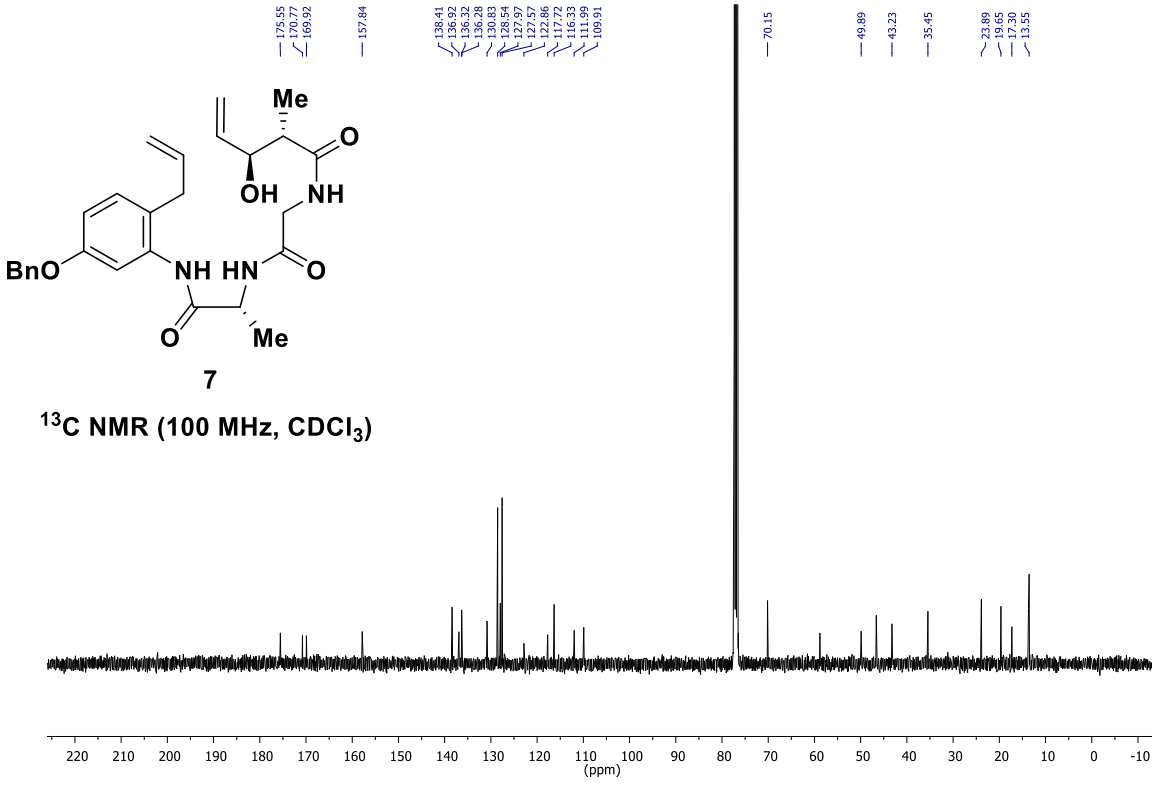
^{1}H NMR (400 MHz, $CDCl_3$)

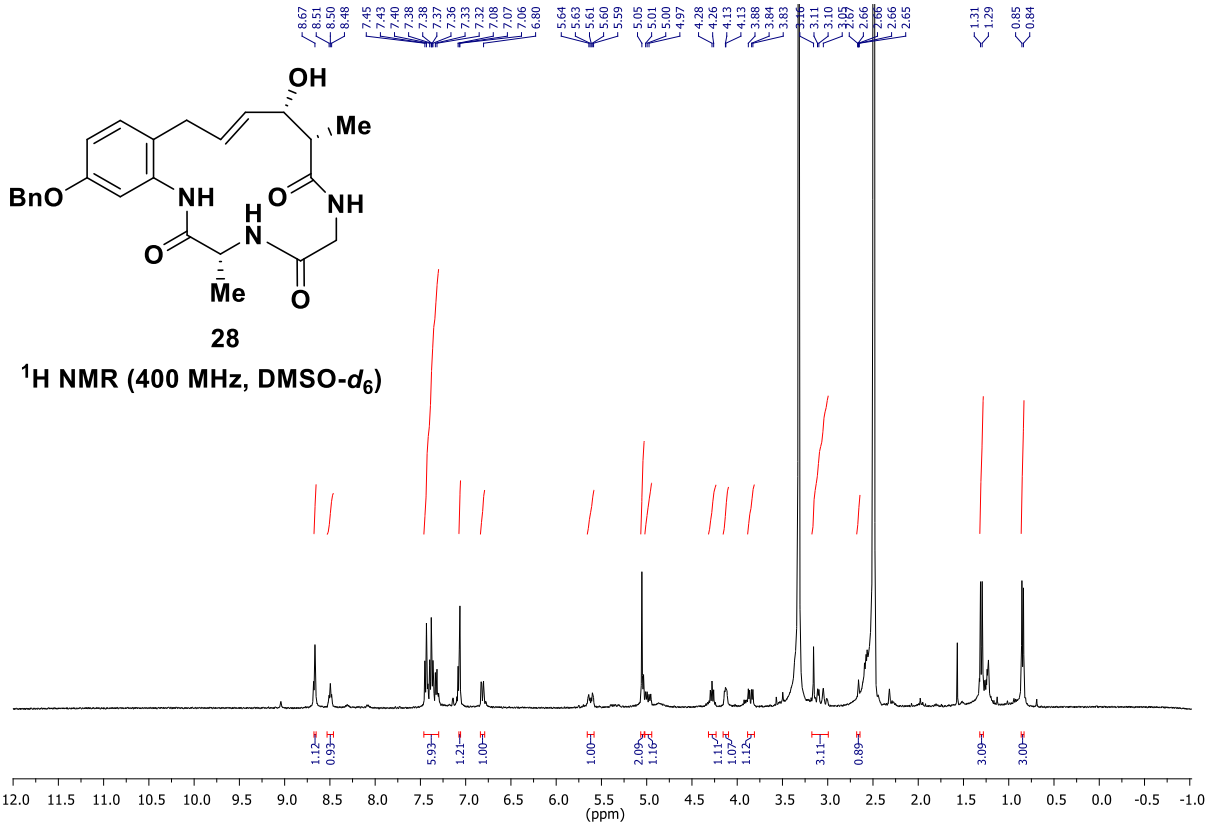


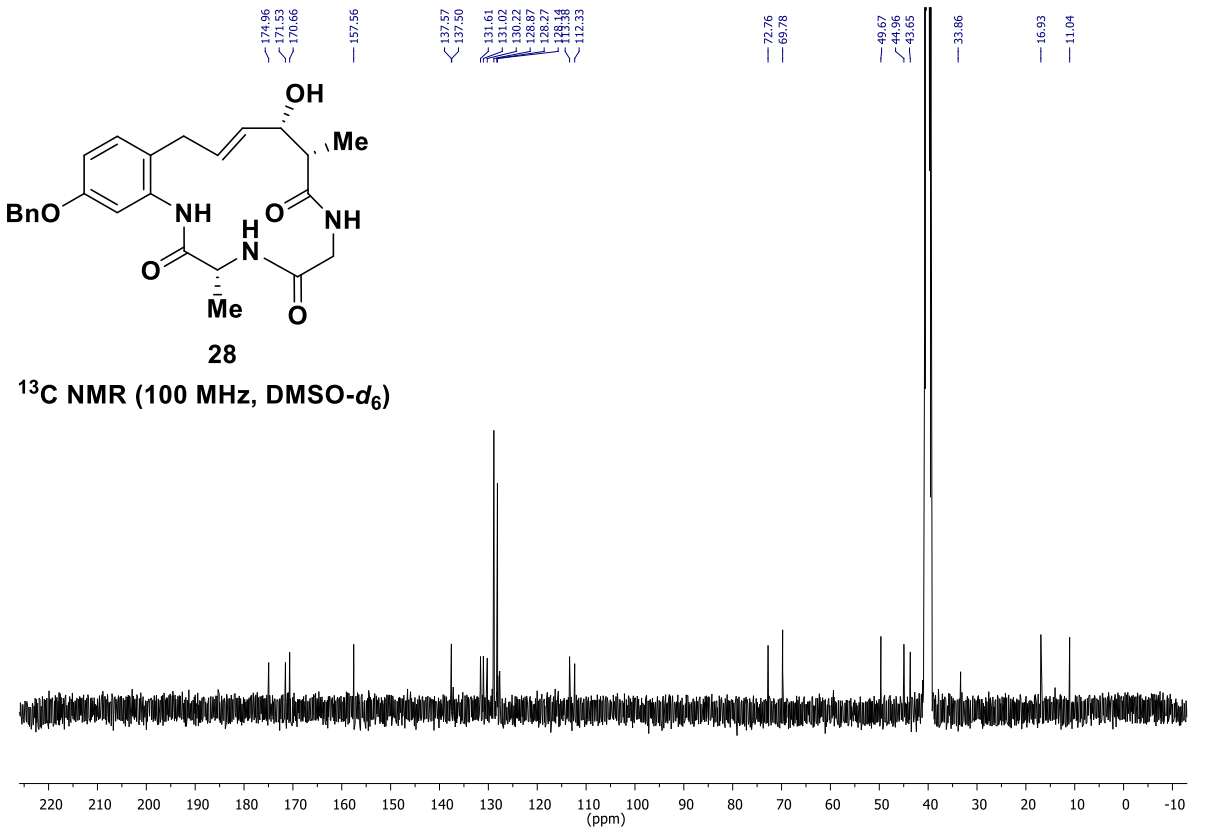
8: R = TBS

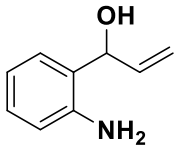
^{13}C NMR (100 MHz, $CDCl_3$)


Me
O
OH
NH
BnO
NH HN
O
O
Me
7
1H NMR (400 MHz, CDCl3)
(ppm)


Me
O
OH
NH
BnO
NH HN
O
O
Me
7
13C NMR (100 MHz, CDCl3)
(ppm)

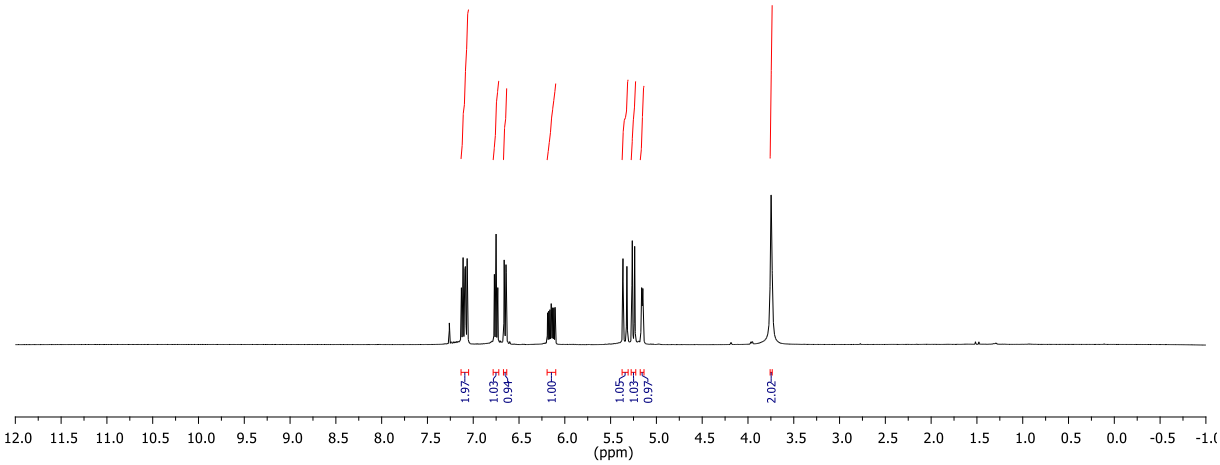

OH
Me
BnO
NH
O
NH
H
N
O
Me
O
28
1H NMR (400 MHz, DMSO-d6)
(ppm)

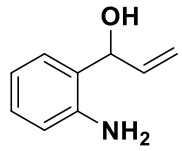

OH
Me
BnO
NH
O
NH
H
N
O
Me
O
28
13C NMR (100 MHz, DMSO-d6)
(ppm)



30

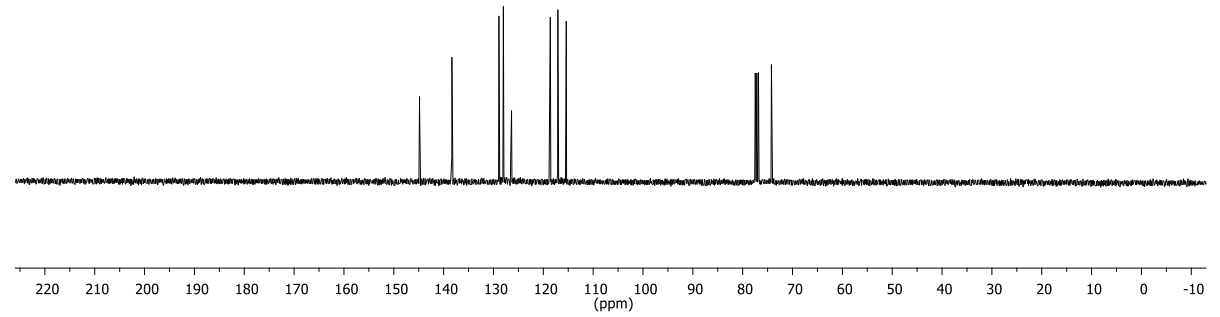
^{1}H NMR (400 MHz, $CDCl_3$)

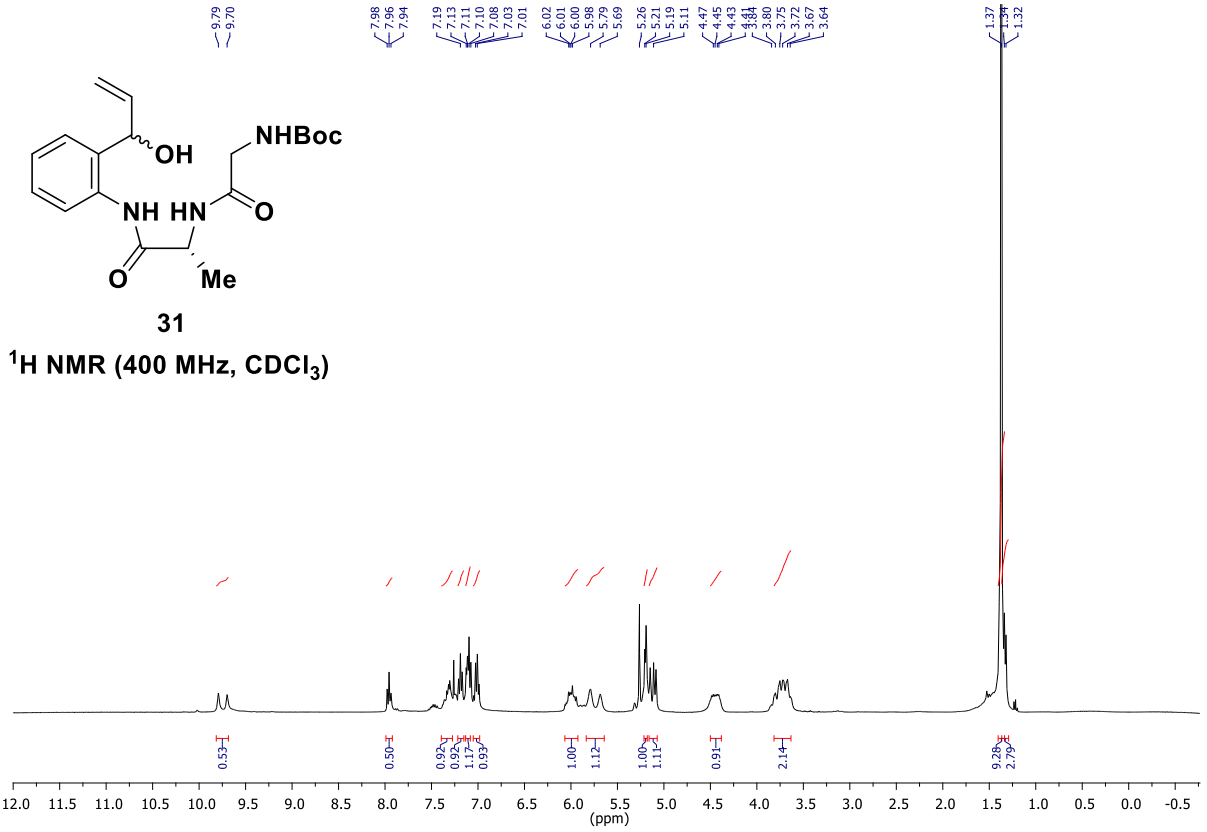




30

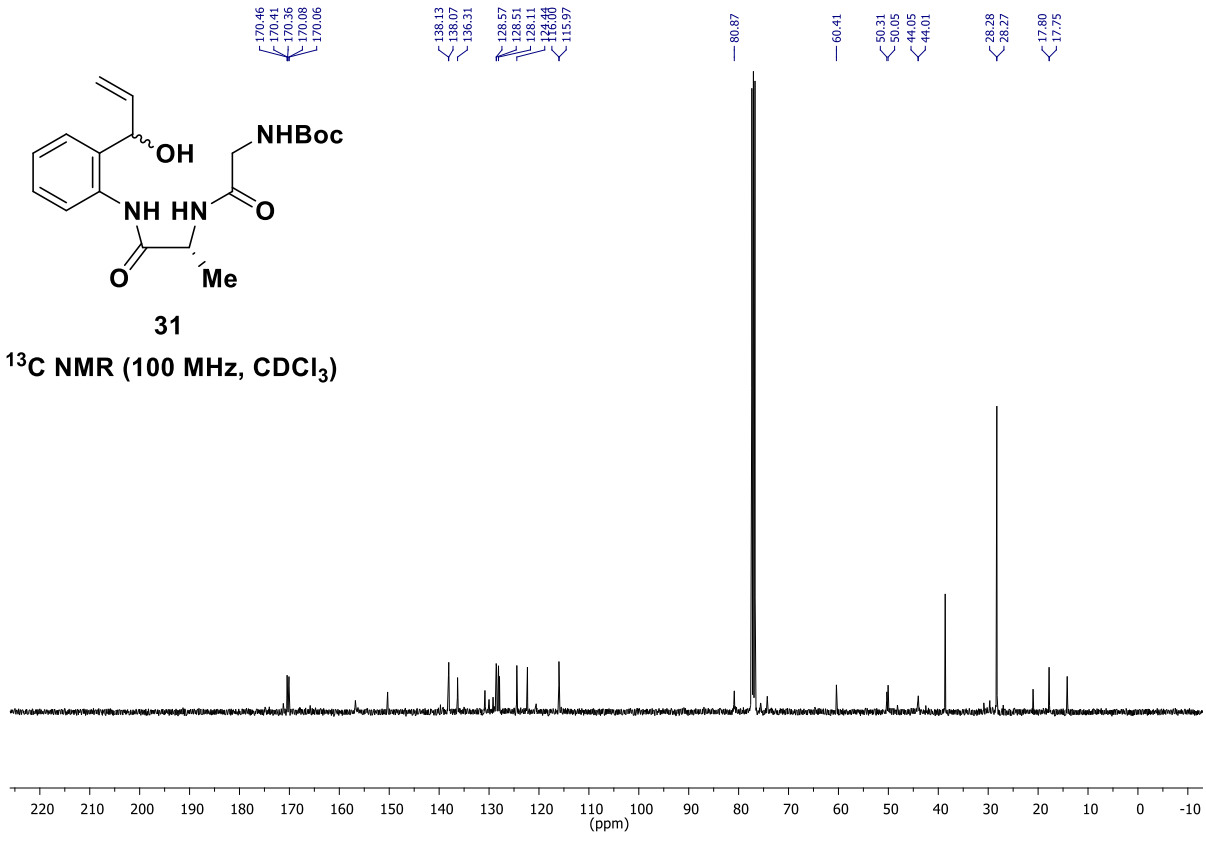
^{13}C NMR (100 MHz, $CDCl_3$)





31

^{1}H NMR (400 MHz, $CDCl_3$)



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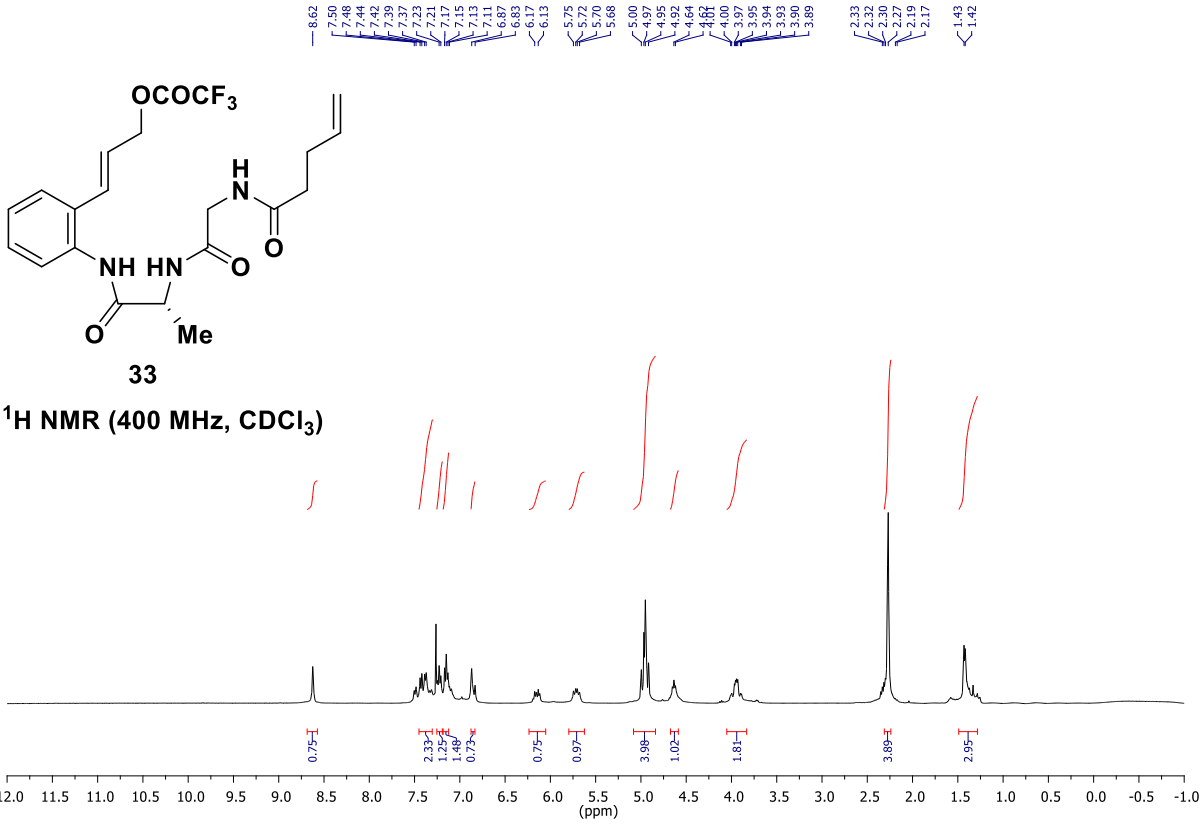
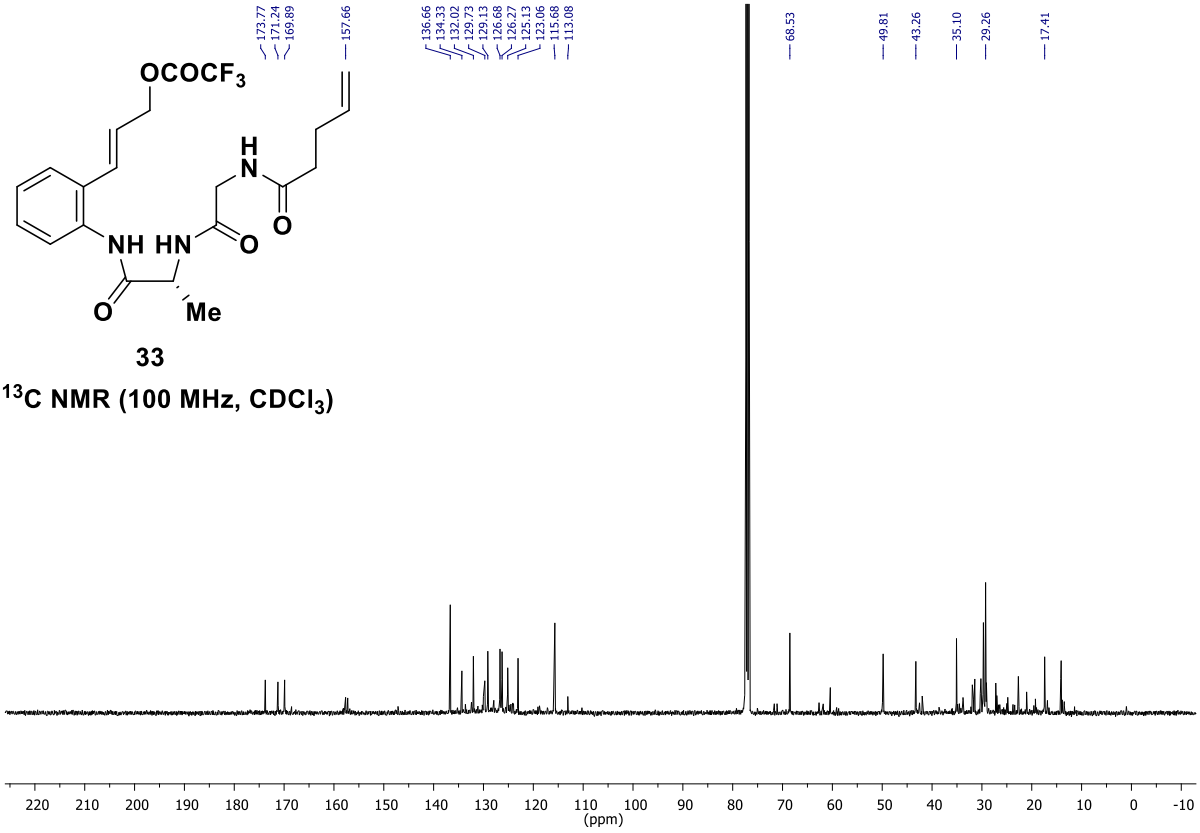
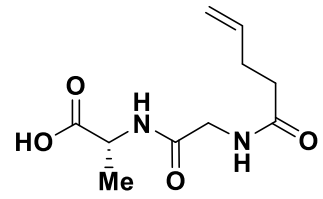
^{13}C NMR (100 MHz, $CDCl_3$)

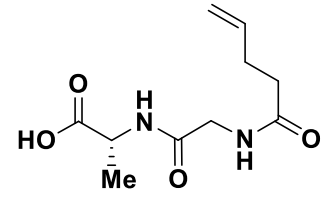

OCOCF3
H
N
O
NH HN
O
O
Me
33
1H NMR (400 MHz, CDCl3)
(ppm)


OCOCF3
H
N
O
NH HN
O
O
Me
33
13C NMR (100 MHz, CDCl3)
(ppm)



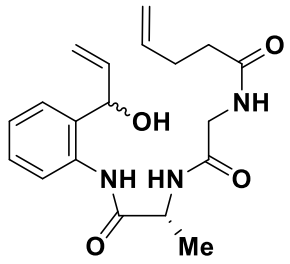
36

^{1}H NMR (400 MHz, $CDCl_3$)



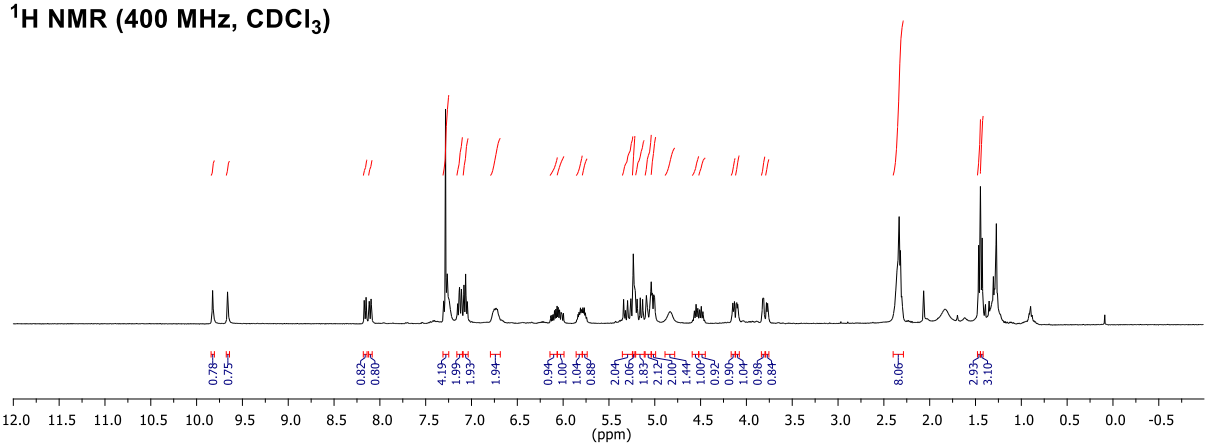
36

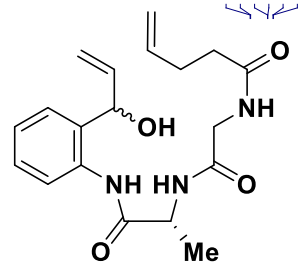
^{13}C NMR (100 MHz, $CDCl_3$)



32

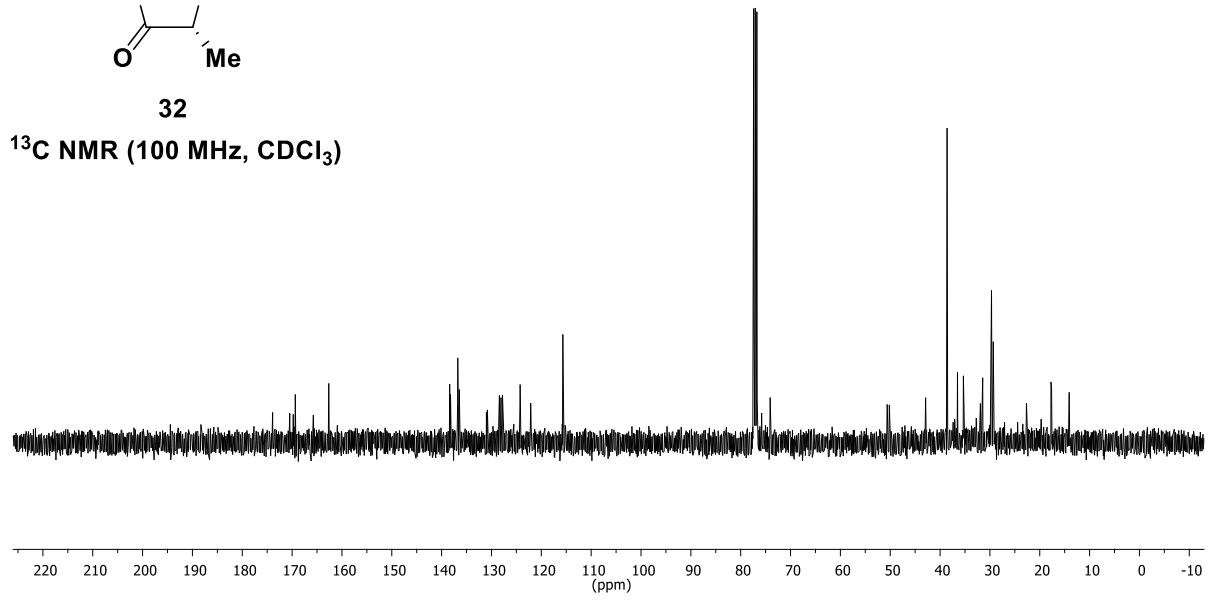
^{1}H NMR (400 MHz, $CDCl_3$)

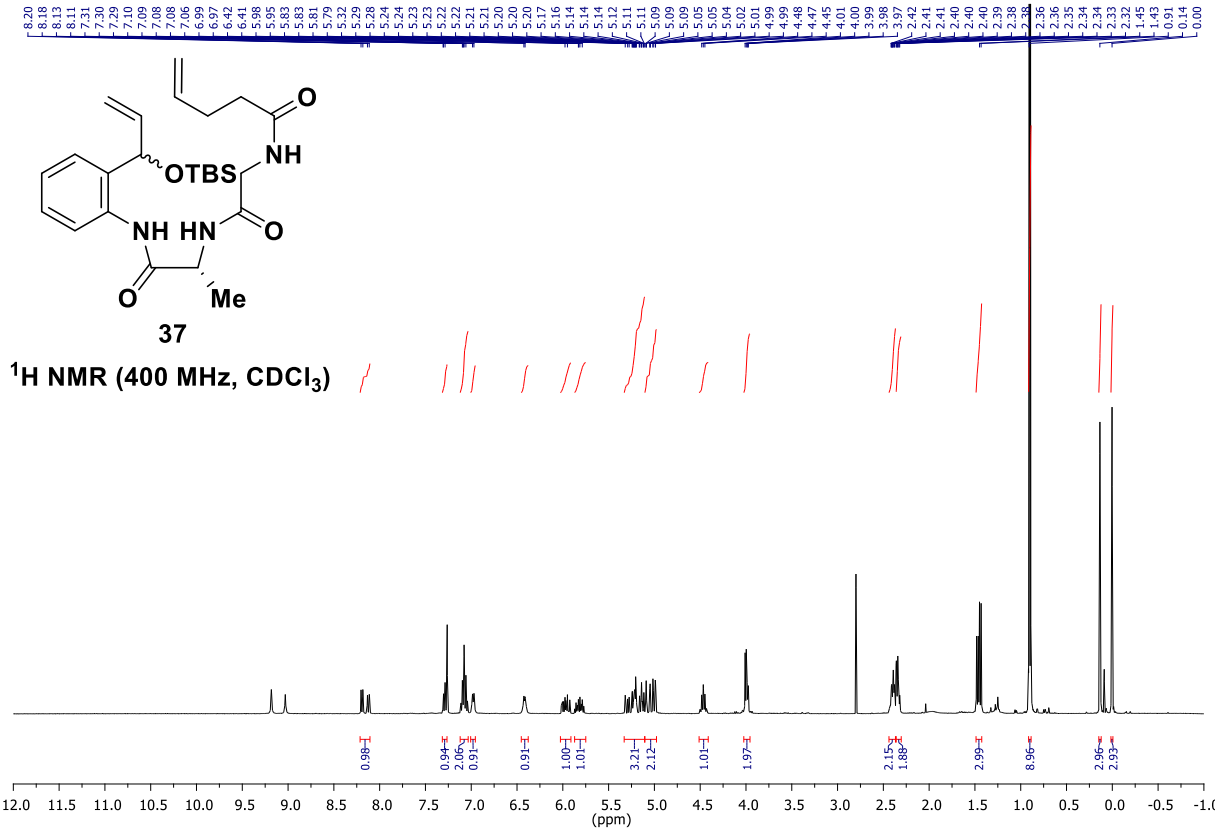




32

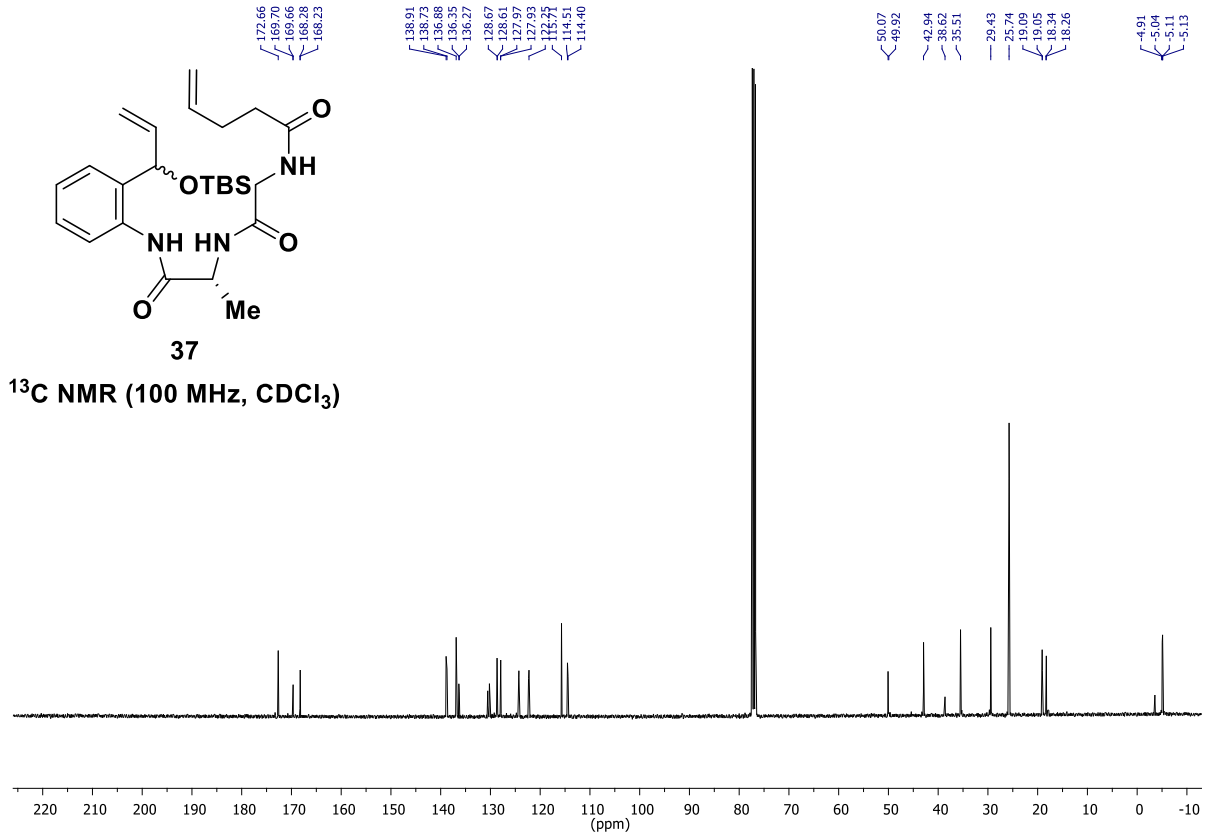
^{13}C NMR (100 MHz, $CDCl_3$)





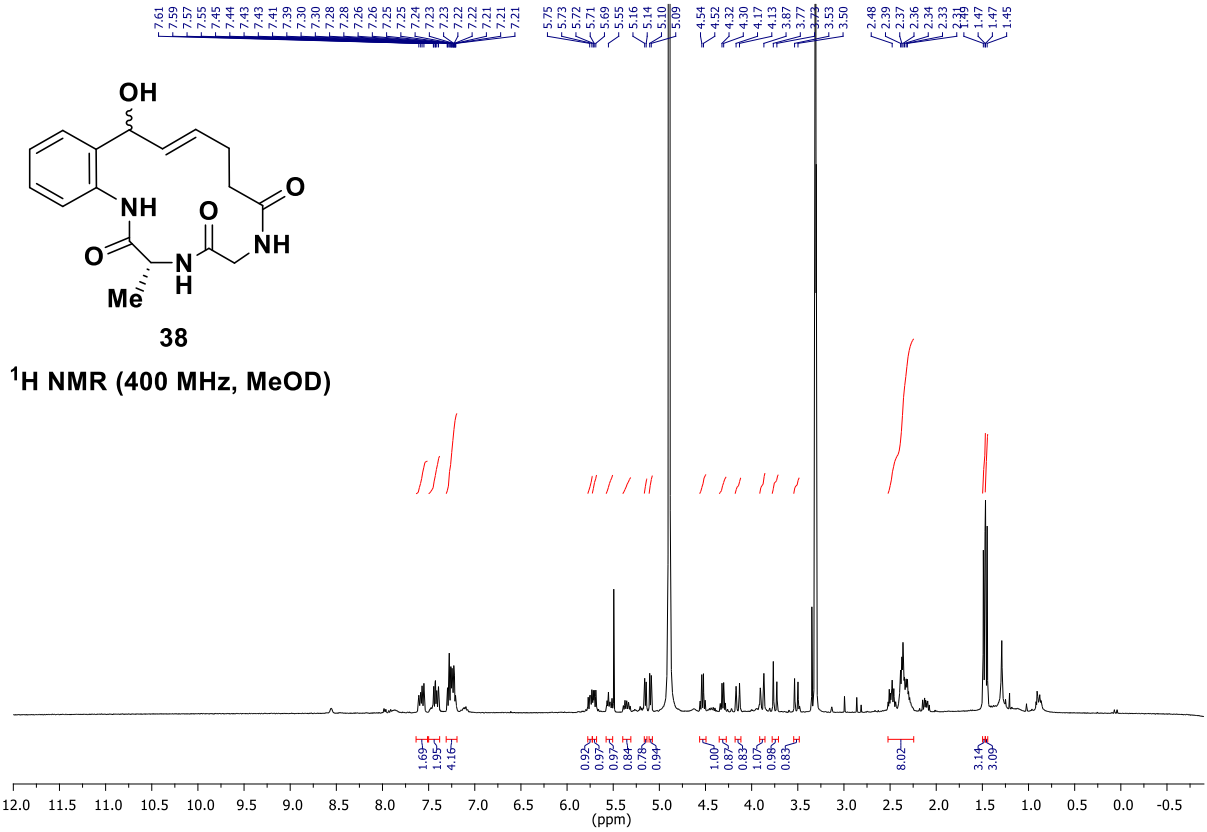
37

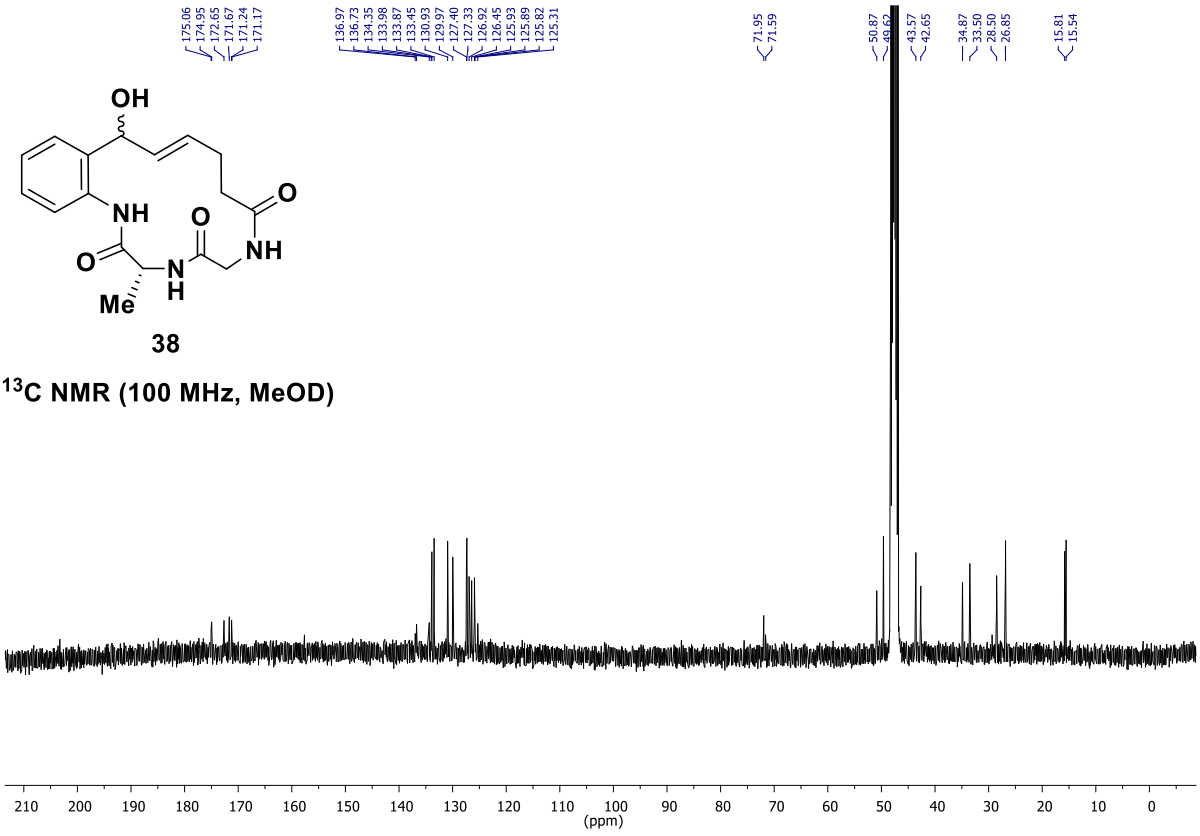
^{1}H NMR (400 MHz, $CDCl_3$)

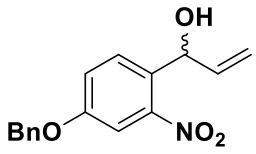


37

^{13}C NMR (100 MHz, $CDCl_3$)

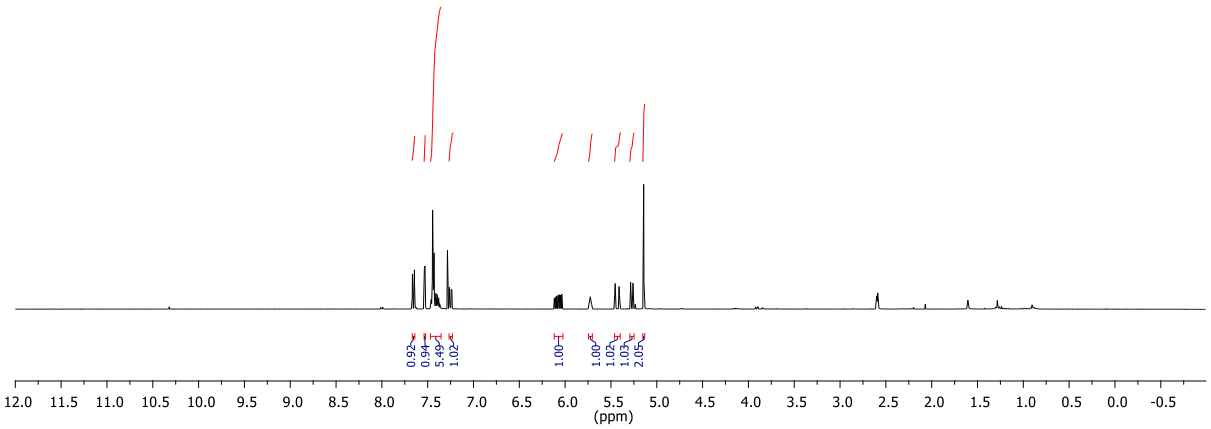

OH
NH
O
O
NH
O
N
H
Me
38
1H NMR (400 MHz, MeOD)
(ppm)

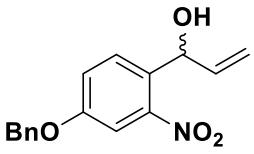

OH
NH
O
O
NH
O
N
H
Me
38
13C NMR (100 MHz, MeOD)
(ppm)



41

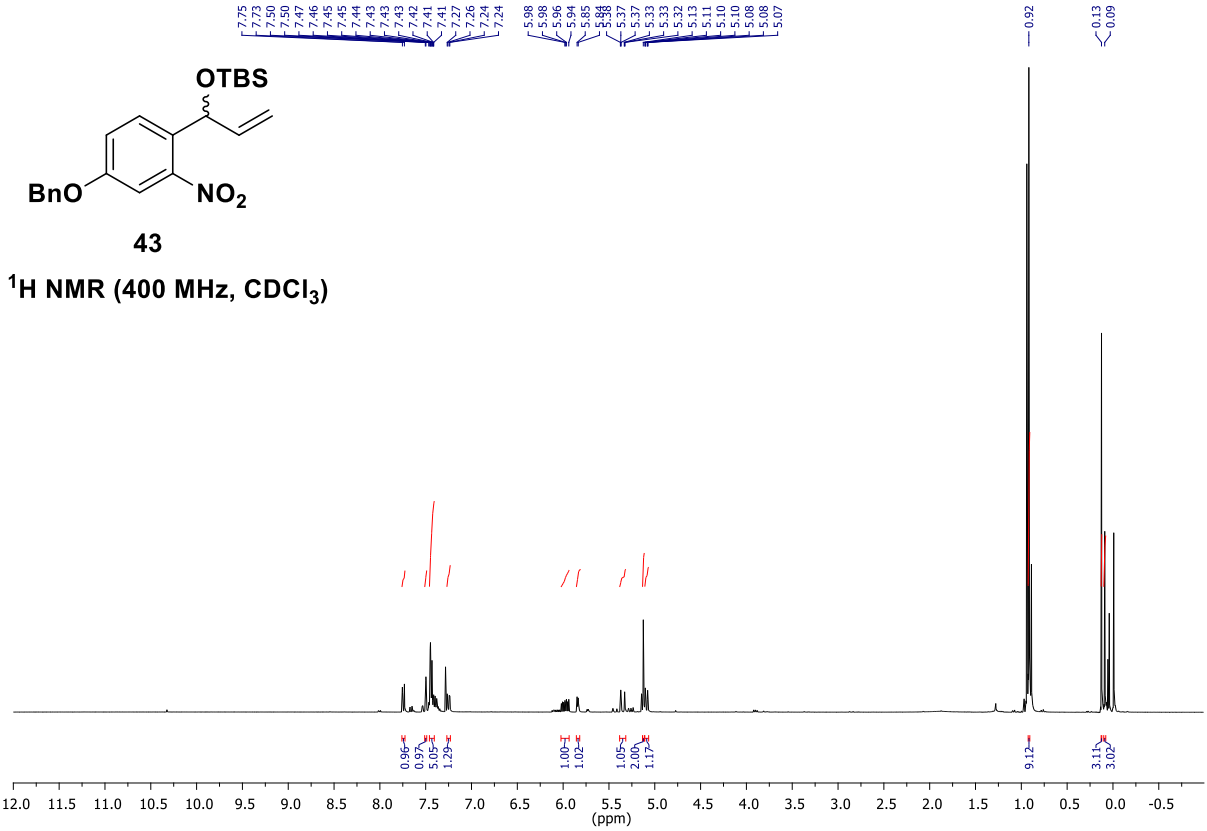
^{1}H NMR (400 MHz, $CDCl_3$)

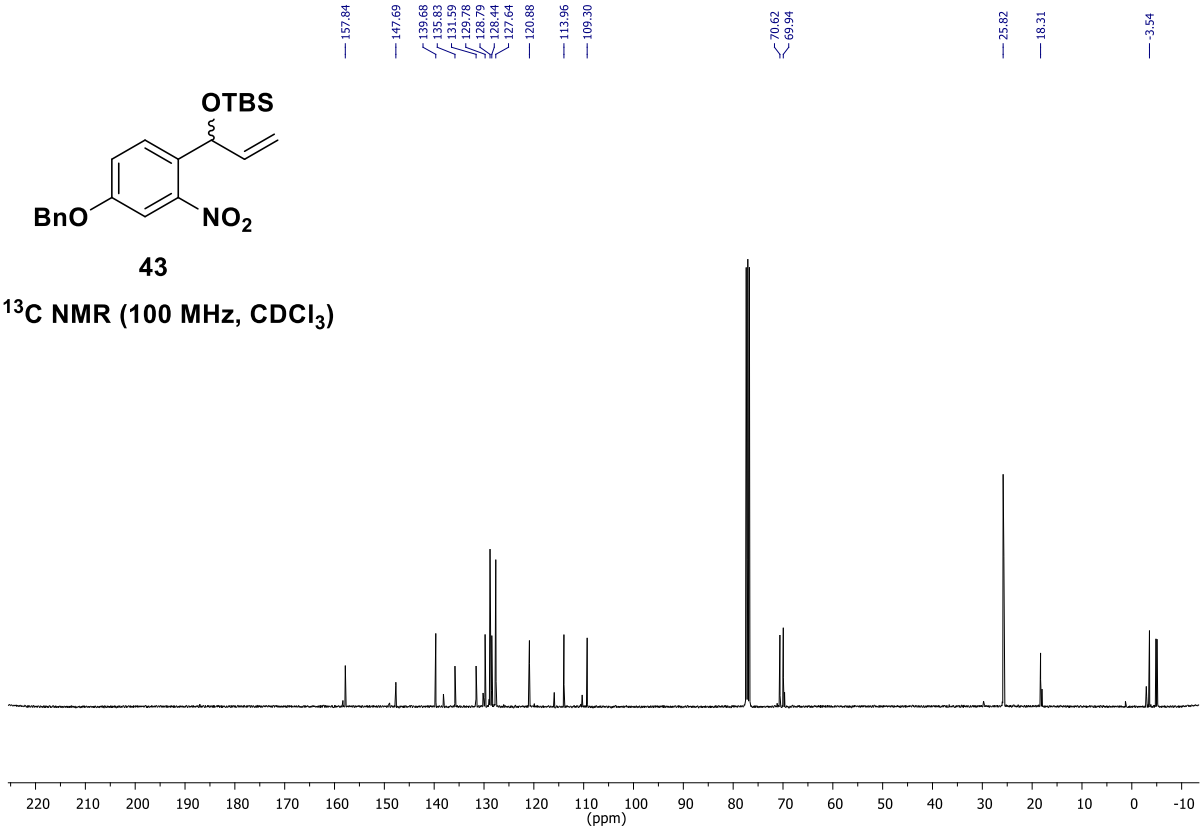


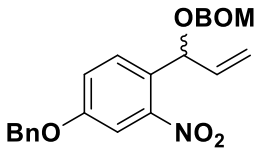


41

^{13}C NMR (100 MHz, $CDCl_3$)

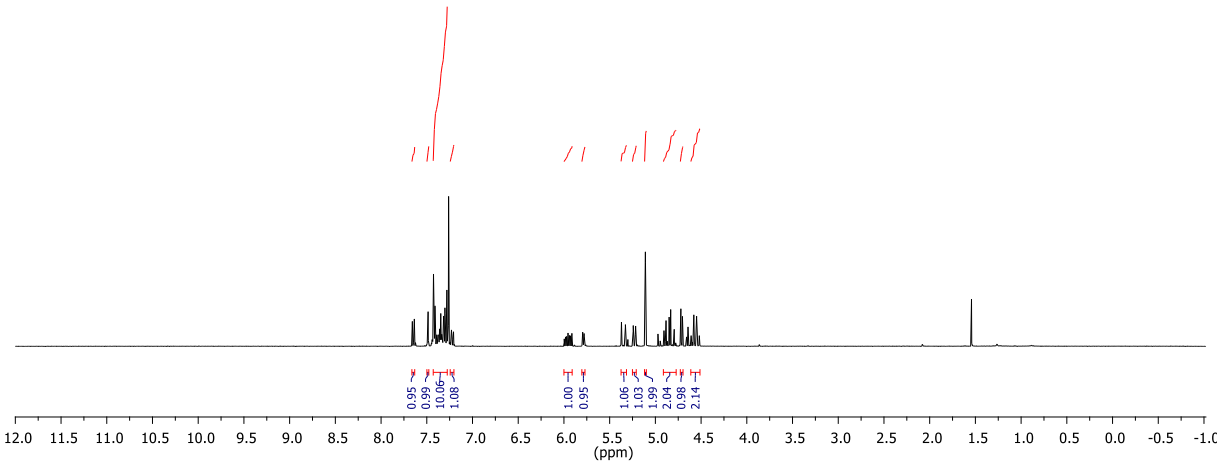

OTBS
BnO
NO2
43
1H NMR (400 MHz, CDCl3)
(ppm)

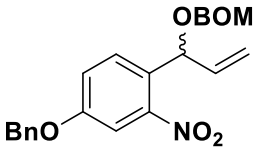

OTBS
BnO
NO2
43
13C NMR (100 MHz, CDCl3)
(ppm)



45

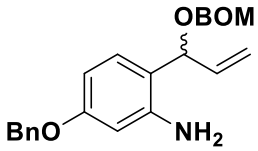
^{1}H NMR (400 MHz, $CDCl_3$)





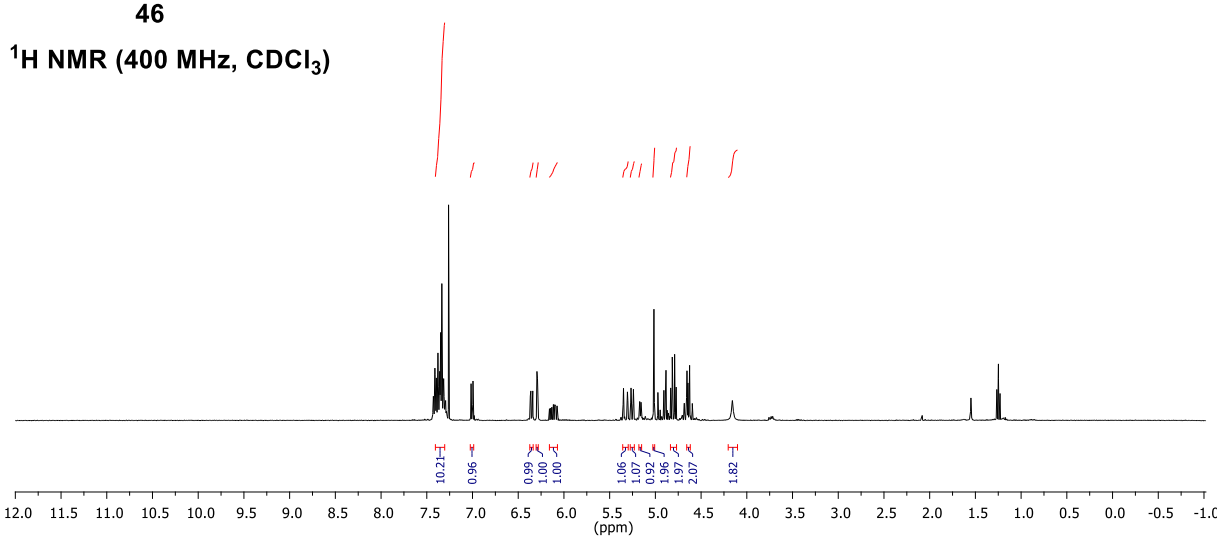
45

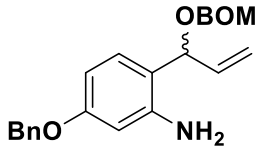
^{13}C NMR (100 MHz, $CDCl_3$)



46

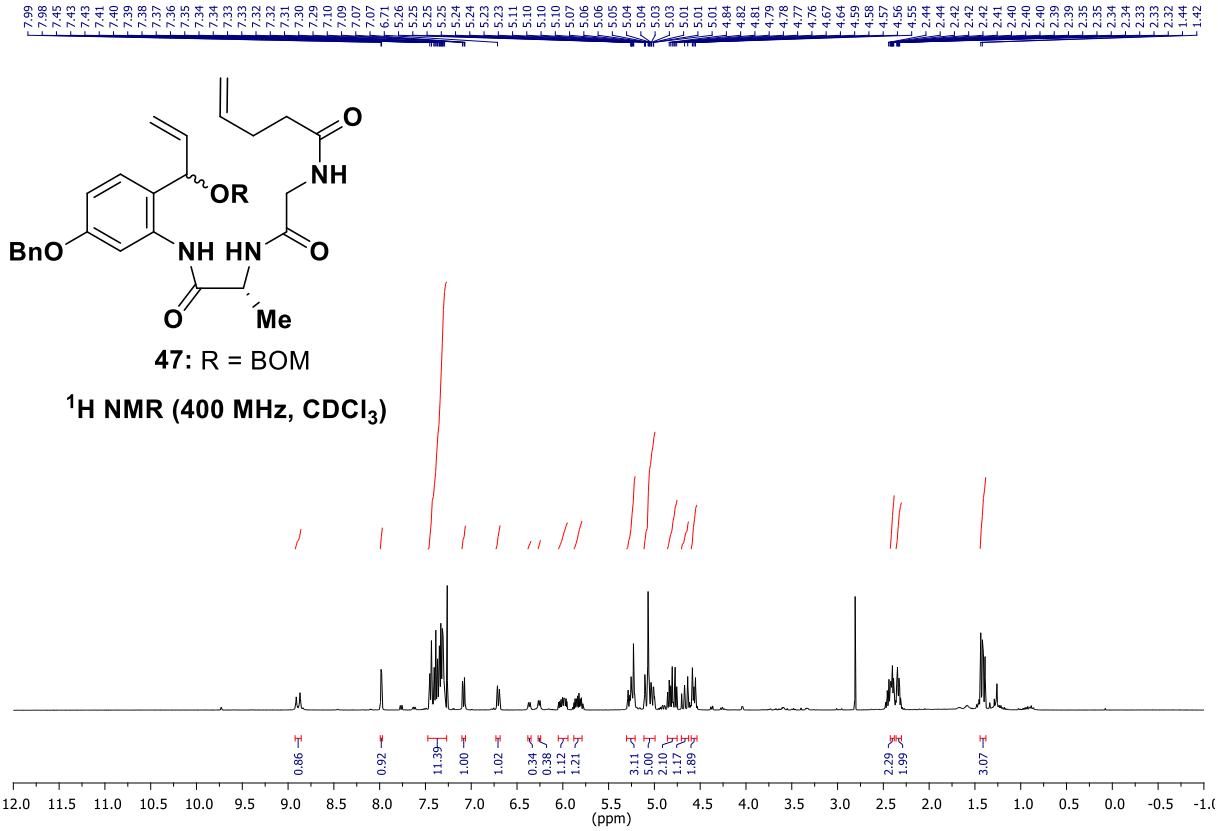
^{1}H NMR (400 MHz, $CDCl_3$)





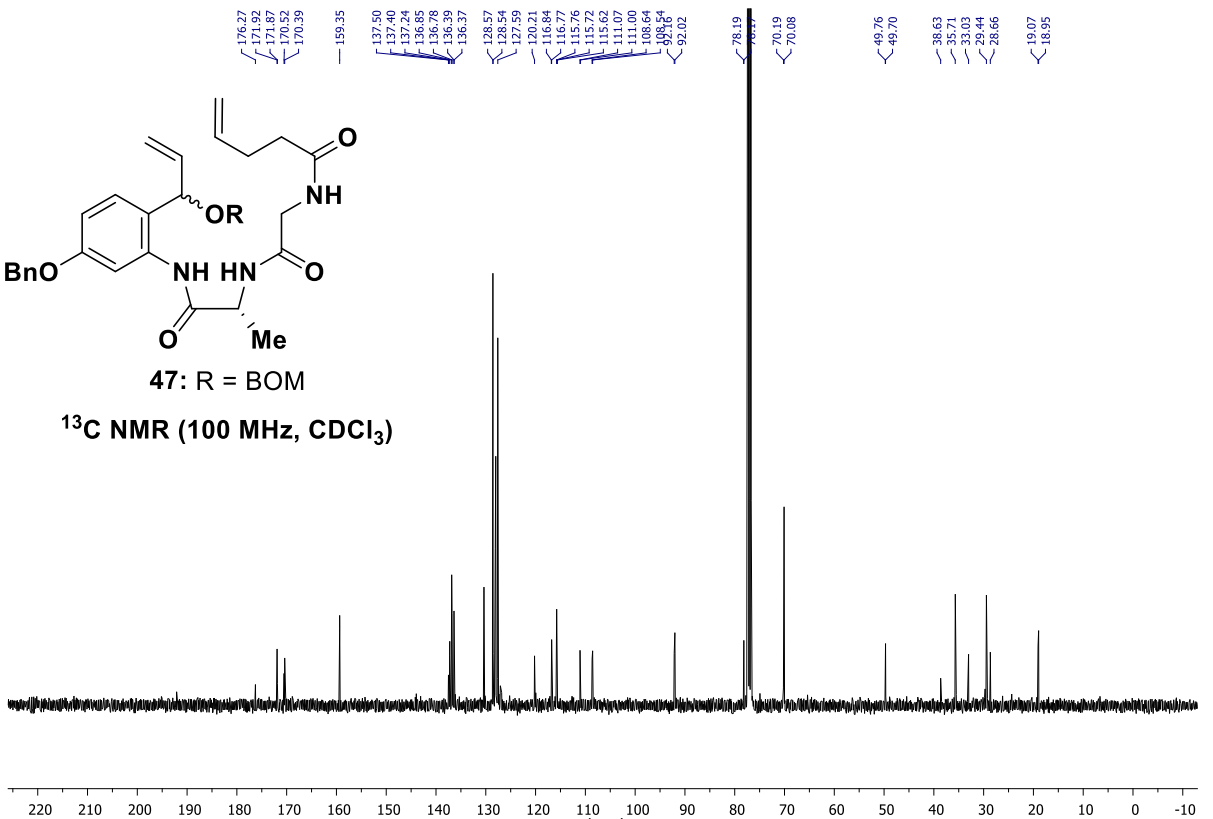
46

^{13}C NMR (100 MHz, $CDCl_3$)



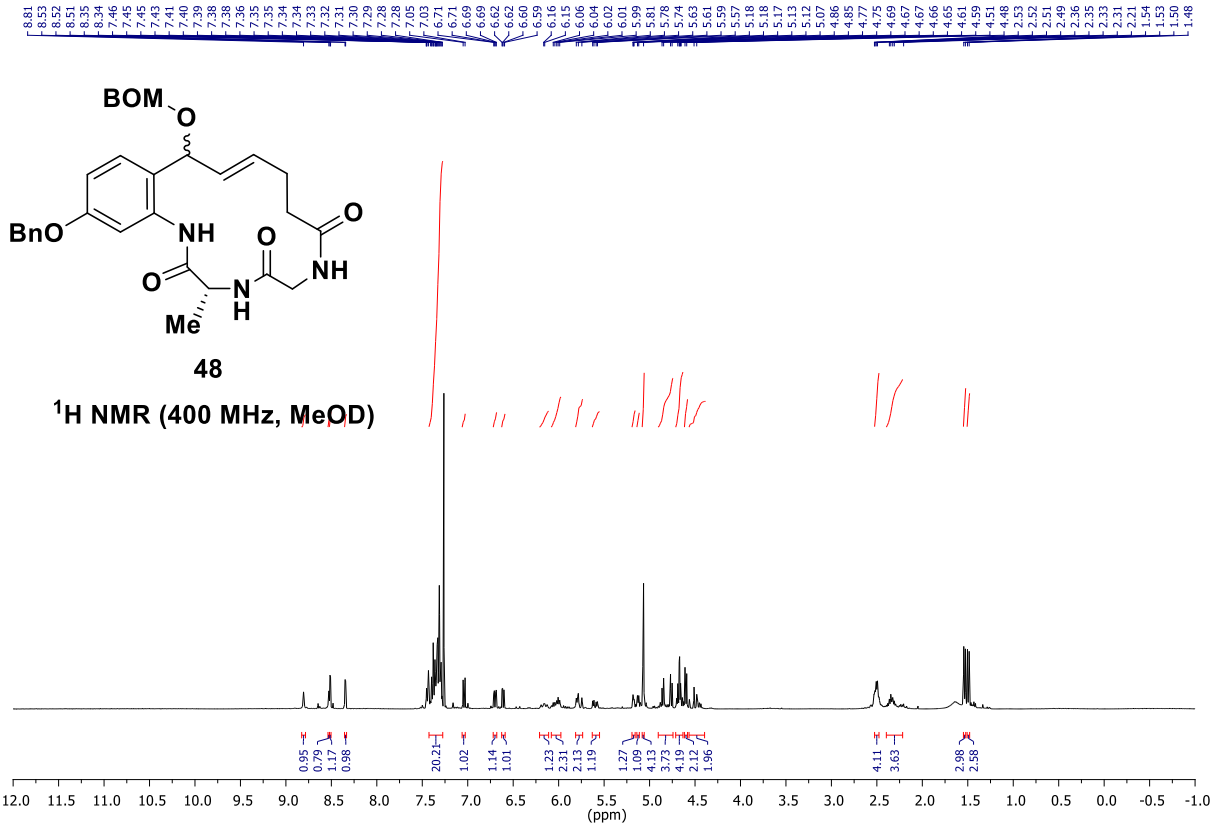
47: R = BOM

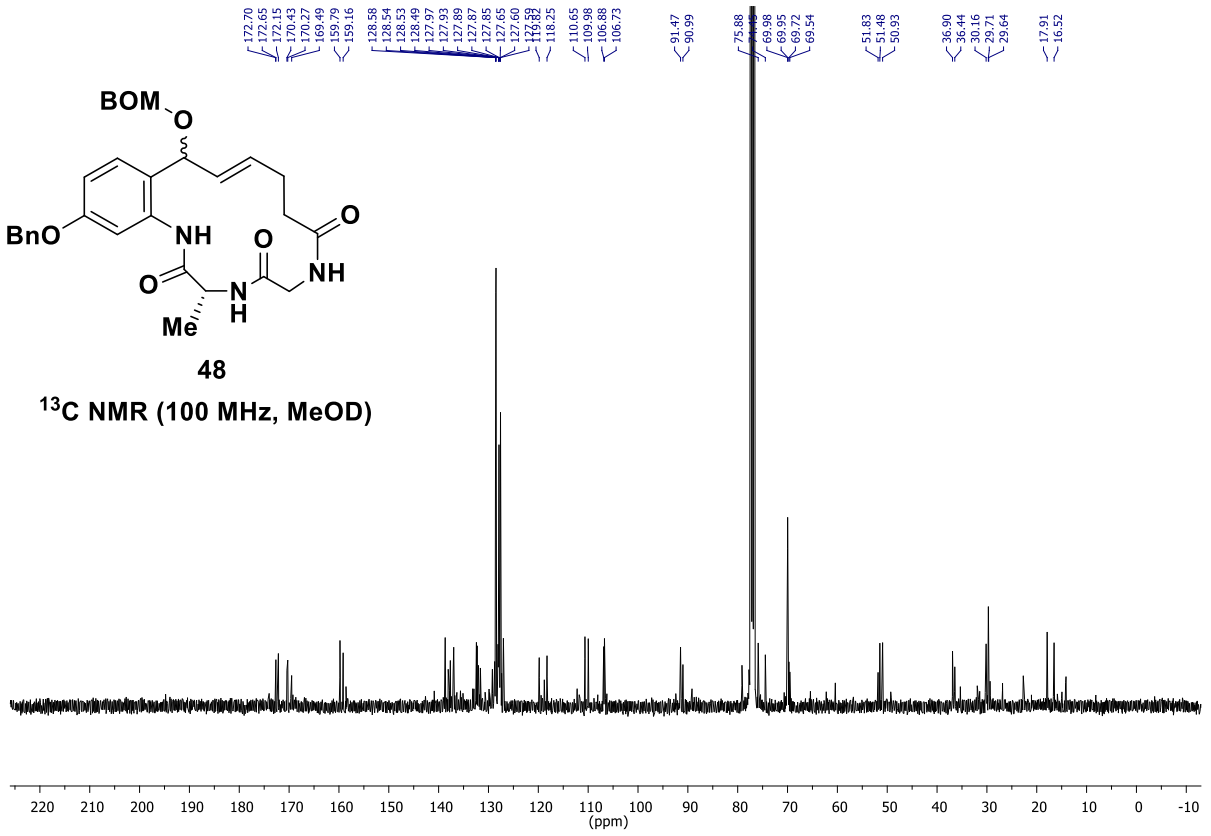
^{1}H NMR (400 MHz, $CDCl_3$)

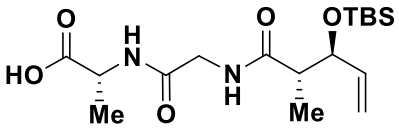


47: R = BOM

^{13}C NMR (100 MHz, $CDCl_3$)

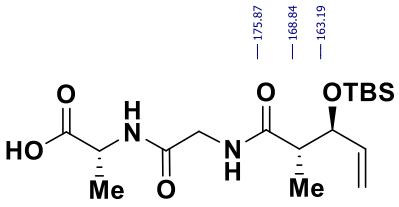

BOM
O
BnO
NH
O
O
NH
O
N
H
Me
48
1H NMR (400 MHz, MeOD)
(ppm)


BOM
O
BnO
NH
O
O
NH
O
N
H
Me
48
13C NMR (100 MHz, MeOD)
(ppm)



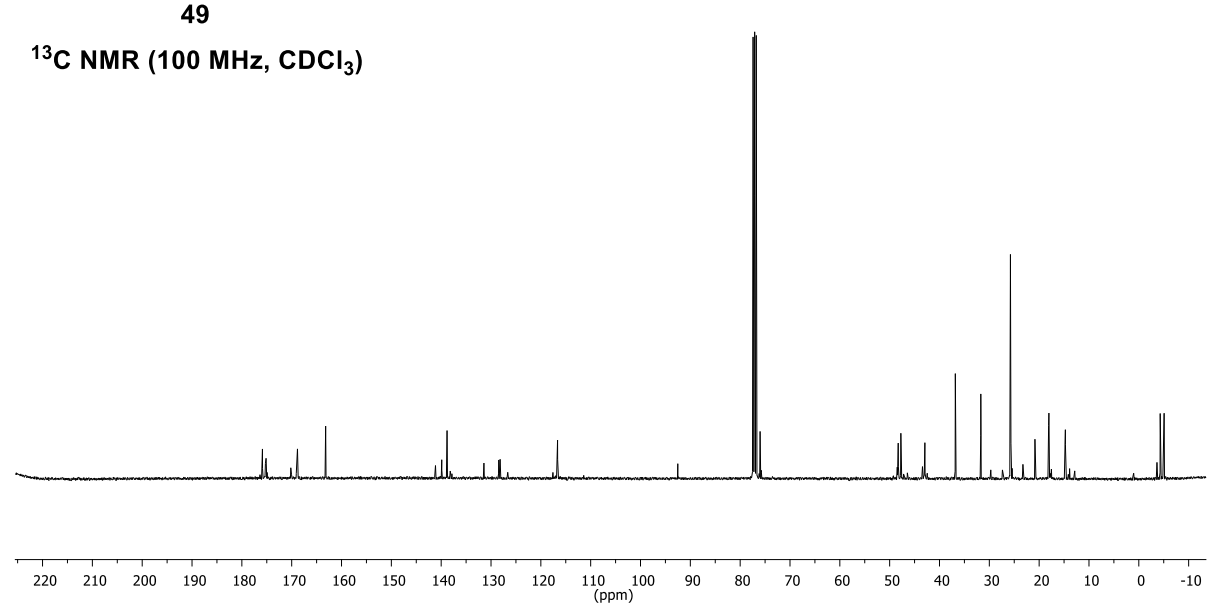
49

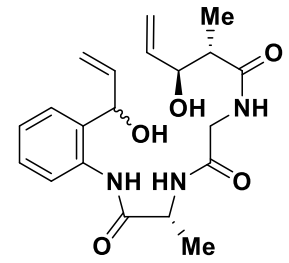
^{1}H NMR (400 MHz, $CDCl_3$)



49

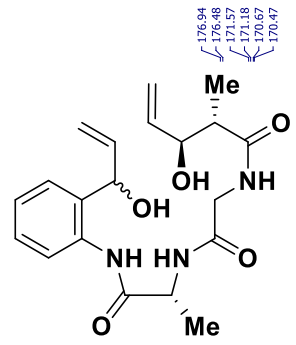
^{13}C NMR (100 MHz, $CDCl_3$)





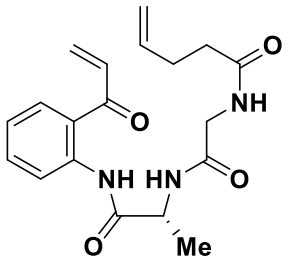
51

^{1}H NMR (400 MHz, $CDCl_3$)



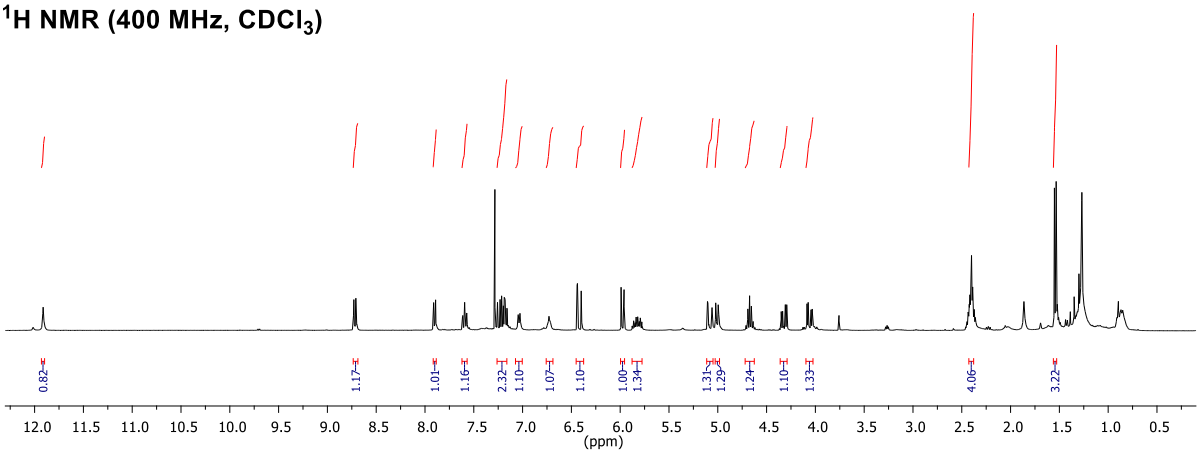
51

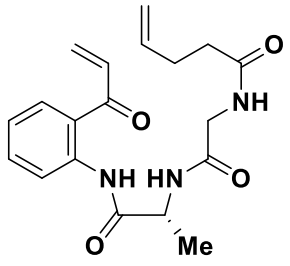
^{13}C NMR (100 MHz, $CDCl_3$)



53

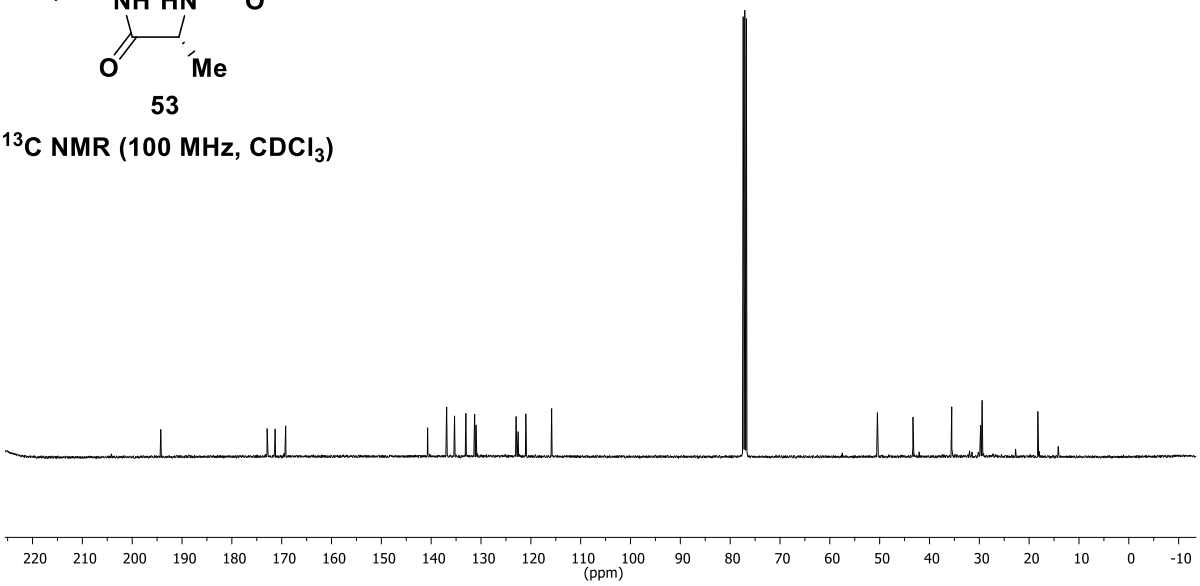
^{1}H NMR (400 MHz, $CDCl_3$)

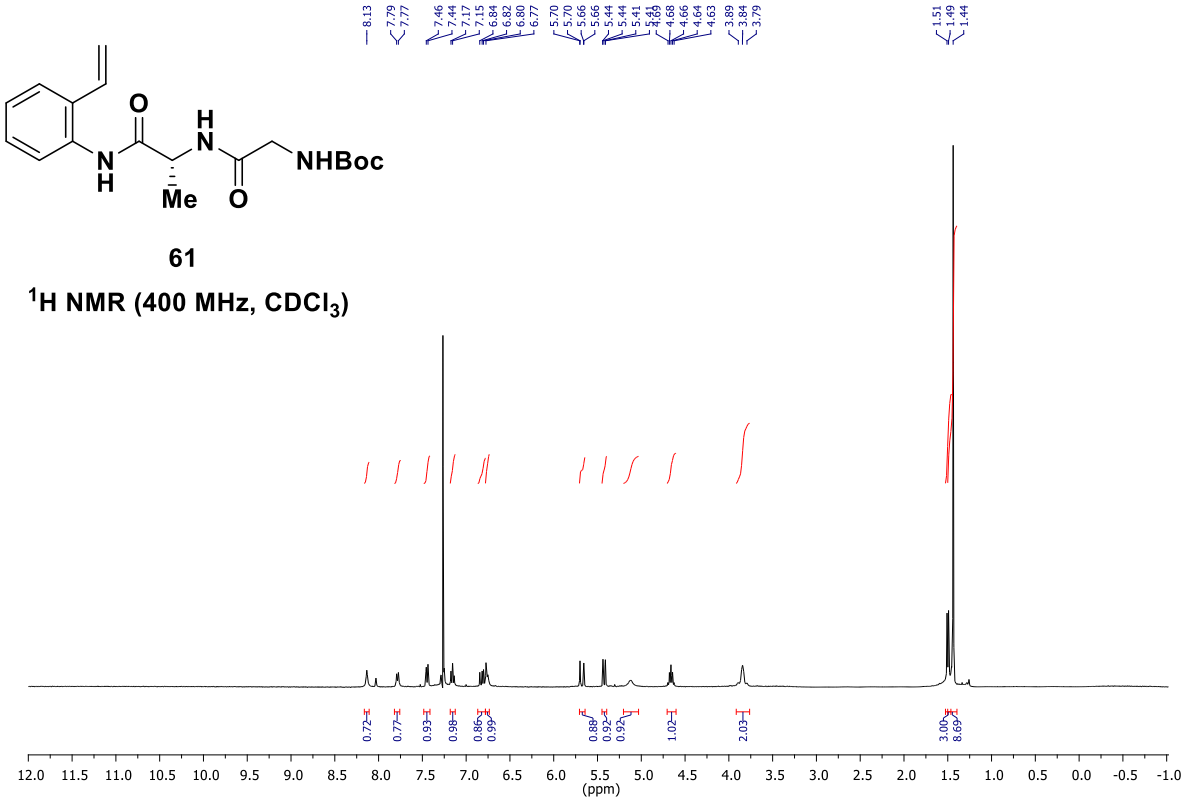




53

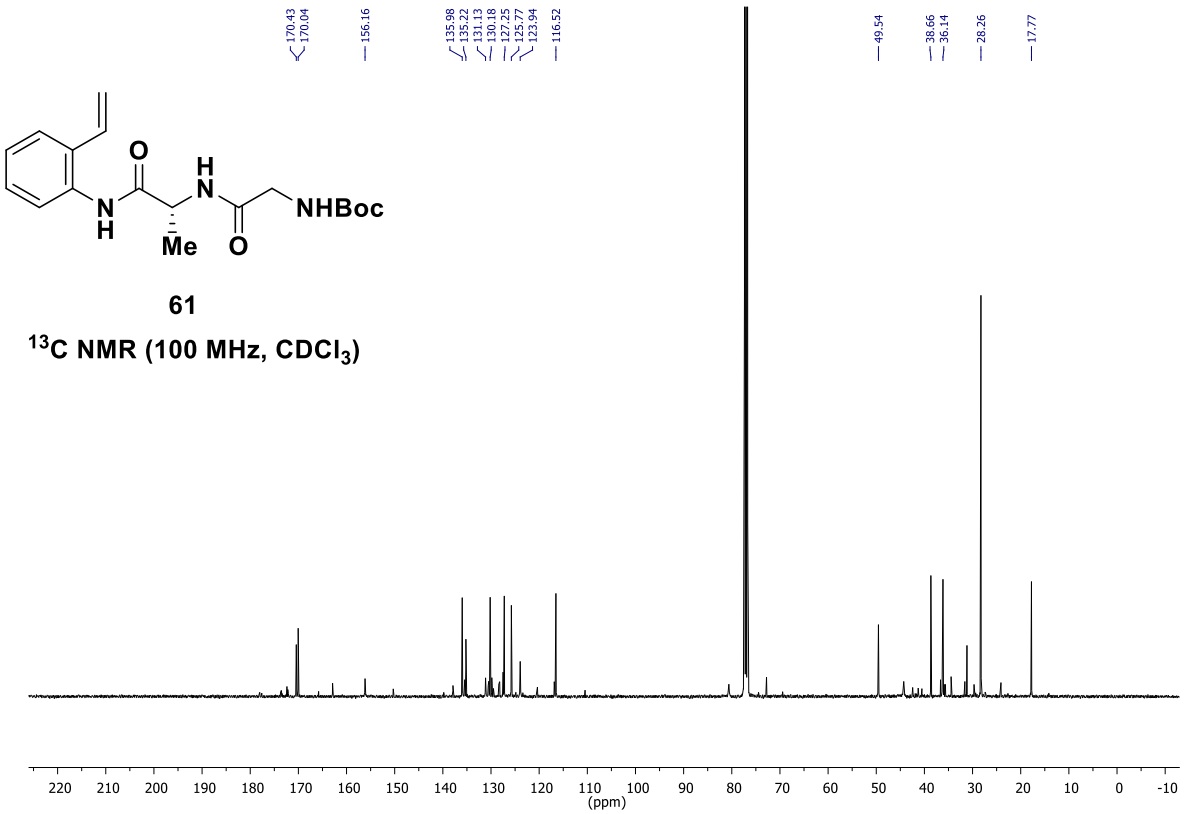
^{13}C NMR (100 MHz, $CDCl_3$)





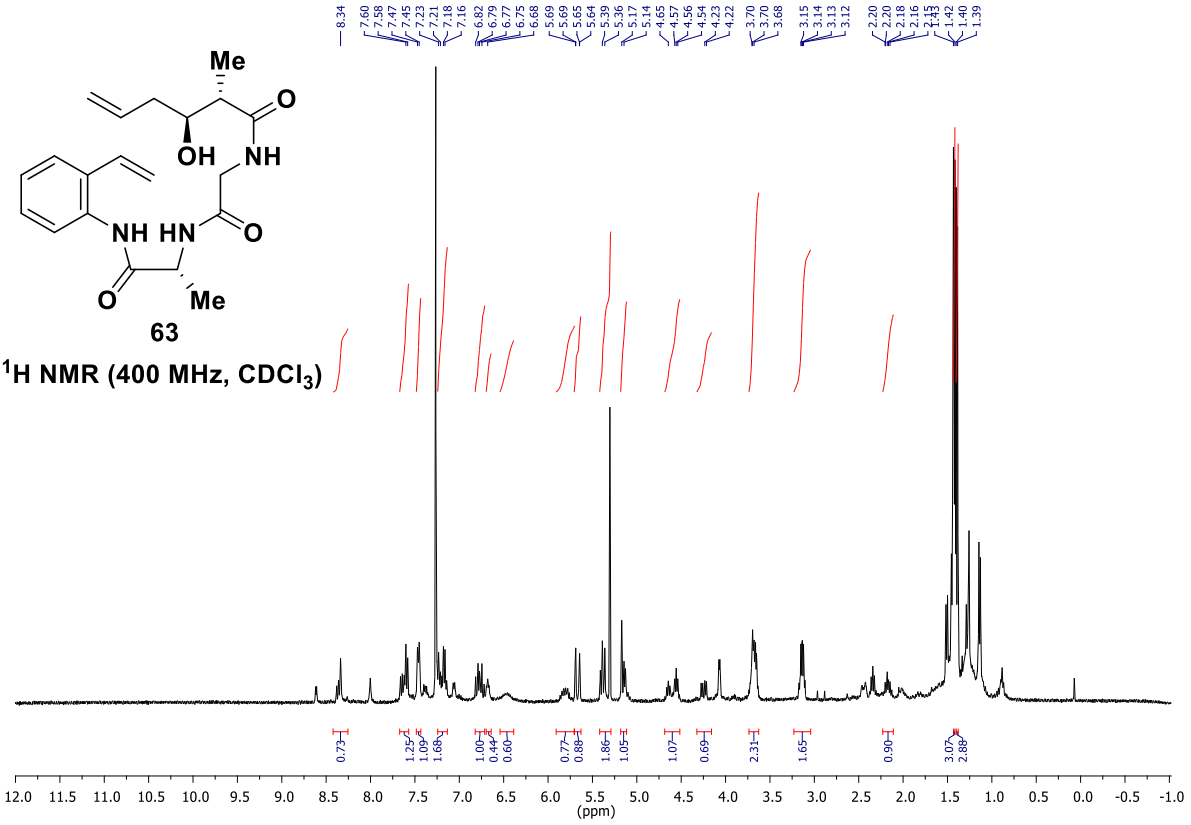
61

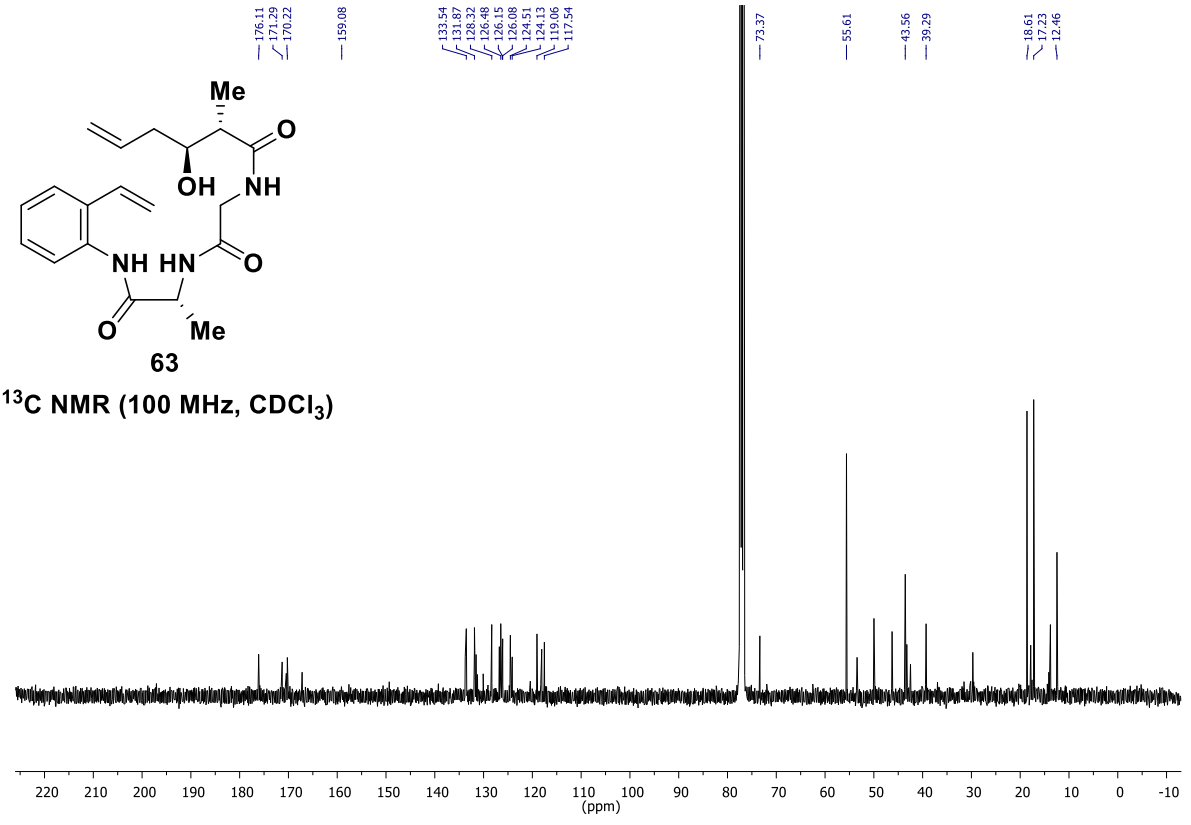
^{1}H NMR (400 MHz, $CDCl_3$)

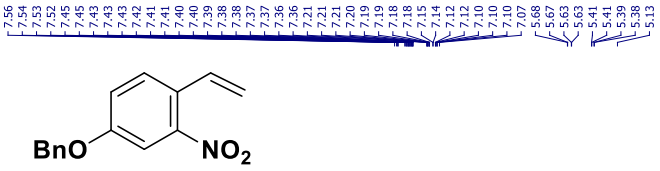


61

^{13}C NMR (100 MHz, $CDCl_3$)

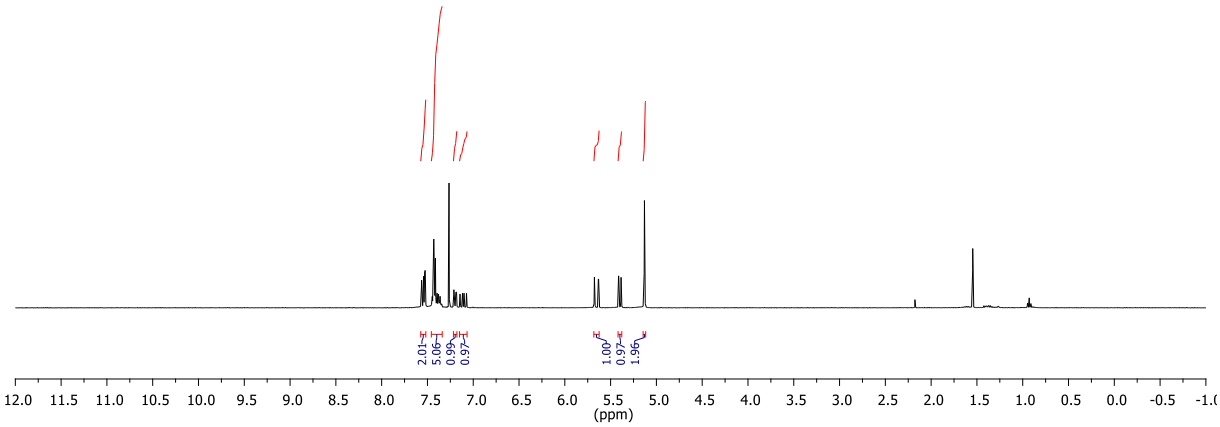

Me
O
OH
NH
NH
HN
O
O
Me
63
^{1}H NMR (400 MHz, CDCl$_3$)
(ppm)

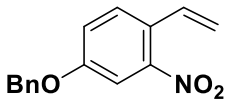

Me
O
OH
NH
NH
HN
O
O
Me
63
^{13}C NMR (100 MHz, CDCl$_3$)
(ppm)



65

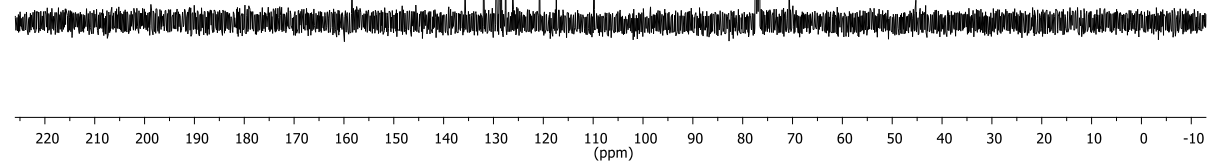
^{1}H NMR (400 MHz, $CDCl_3$)

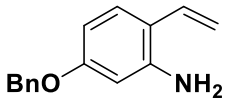




65

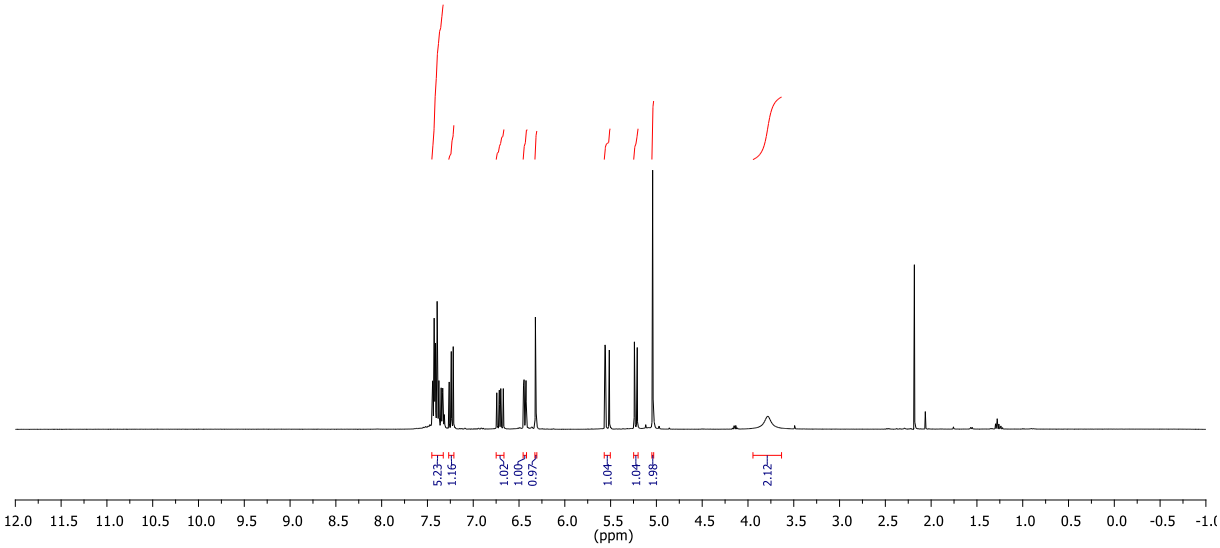
^{13}C NMR (100 MHz, $CDCl_3$)

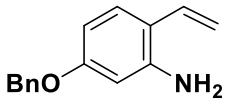




66

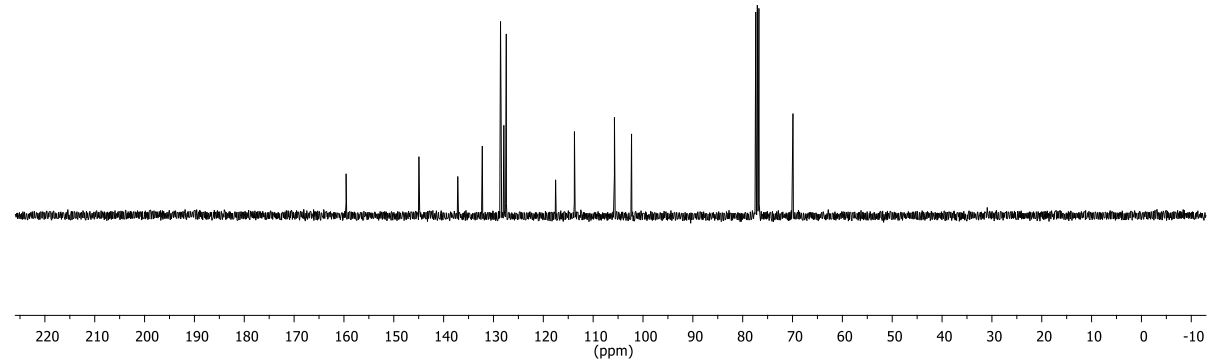
^{1}H NMR (400 MHz, $CDCl_3$)

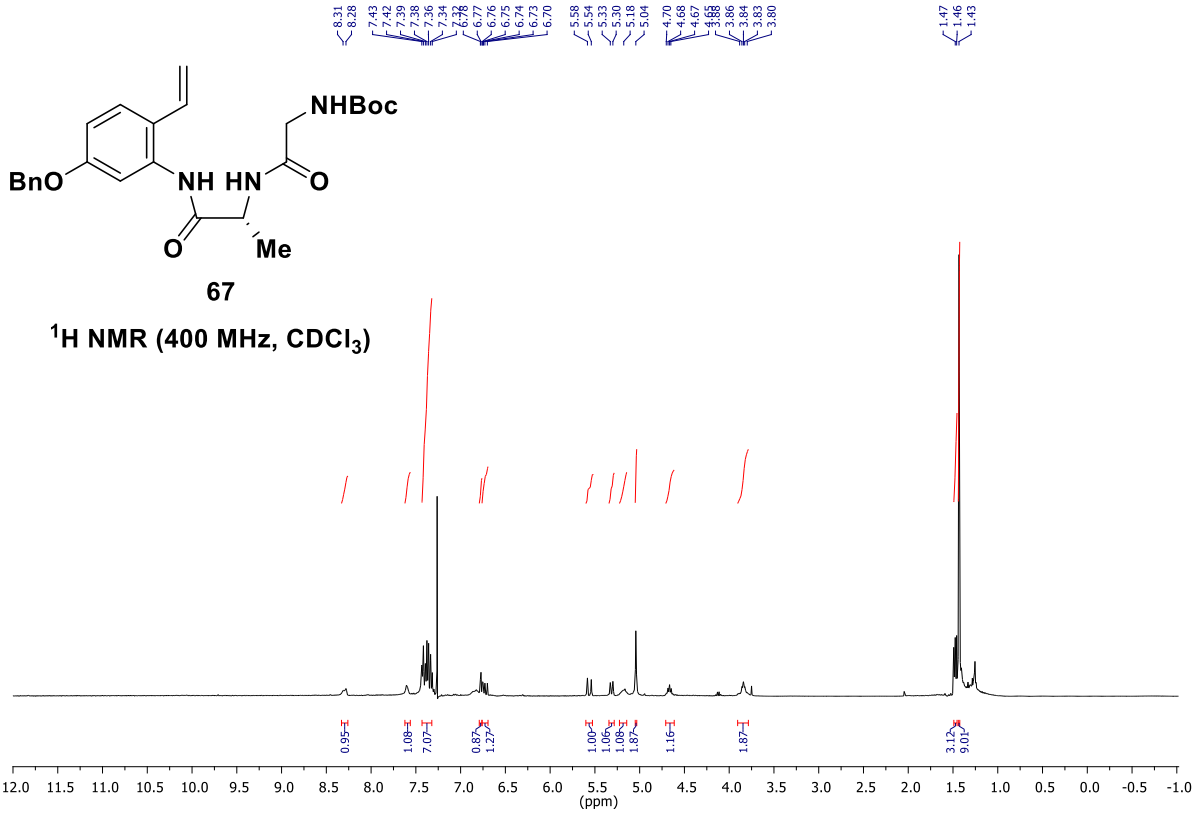


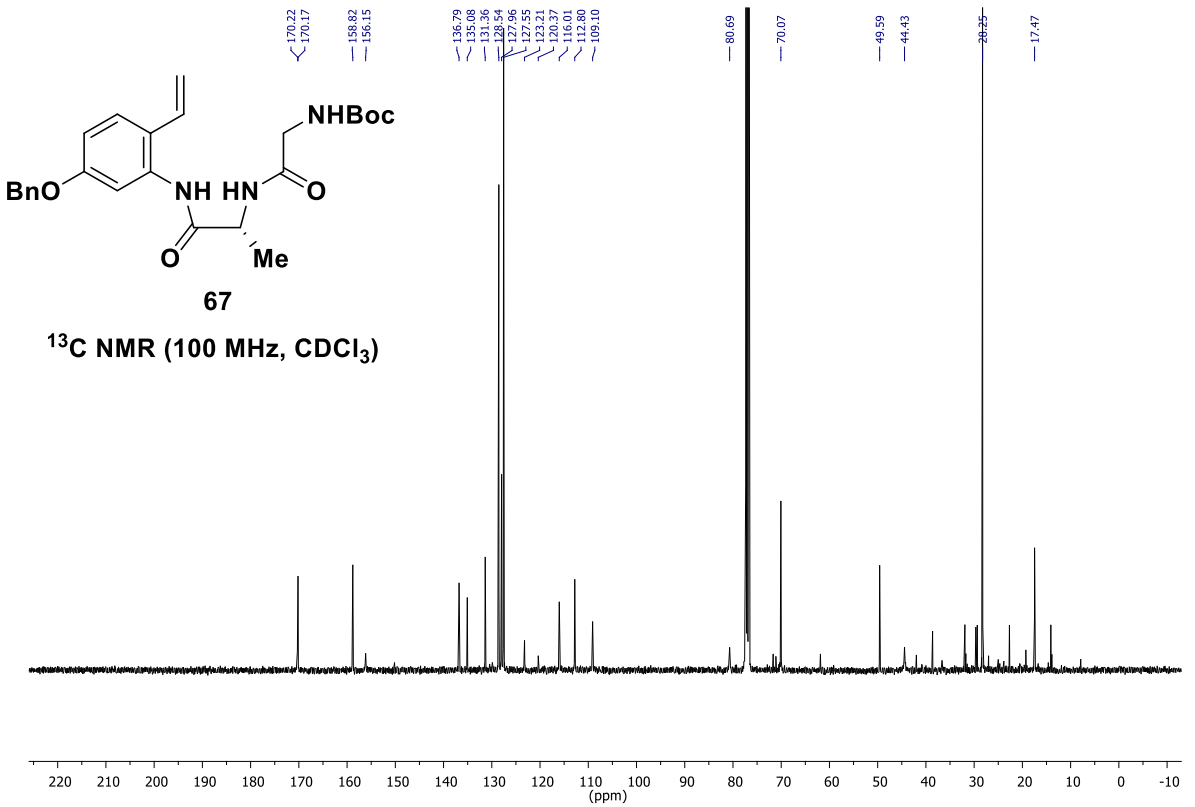


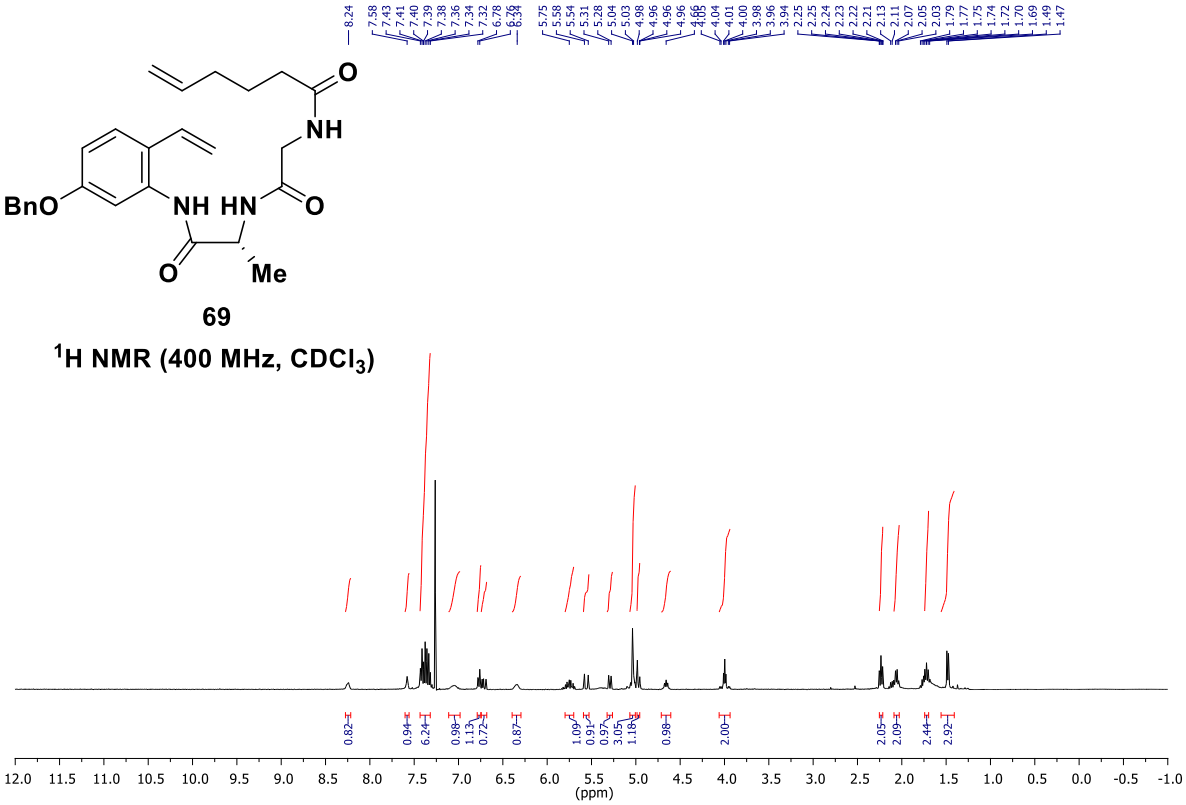
66

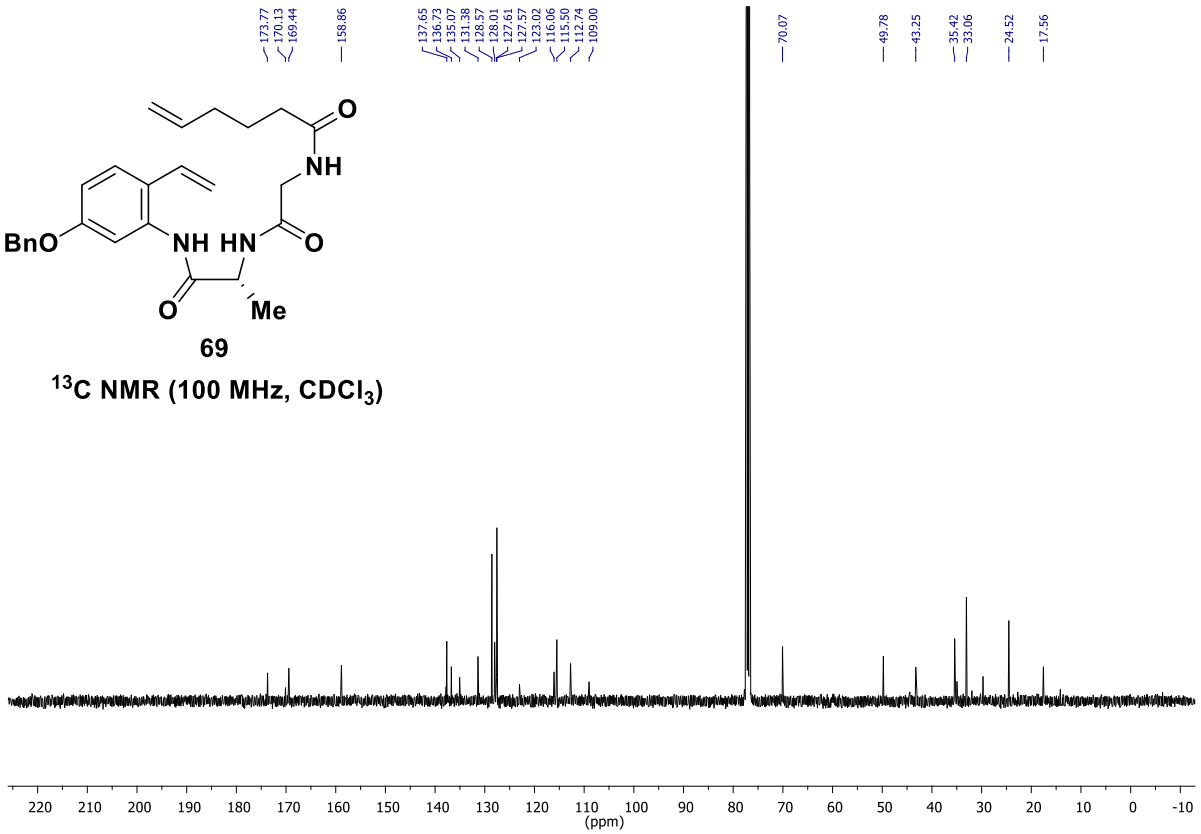
^{13}C NMR (100 MHz, $CDCl_3$)

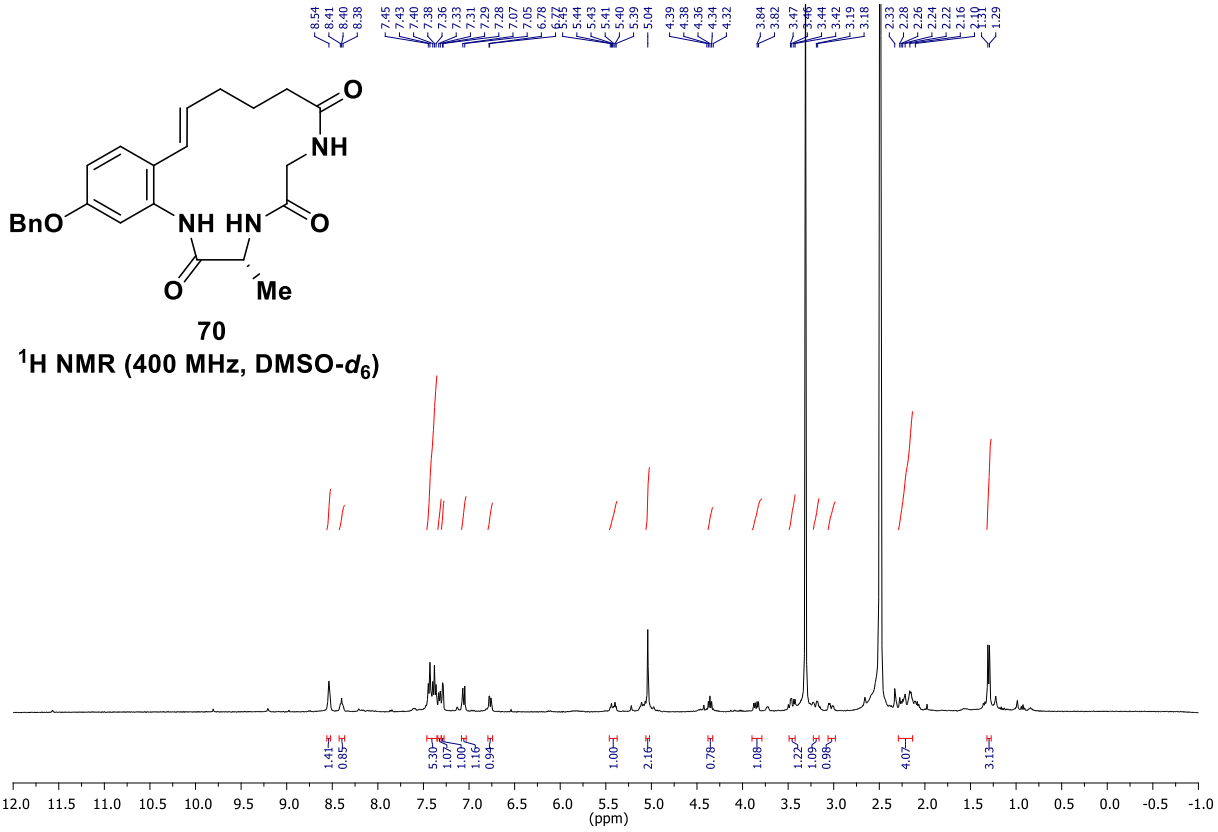



NHBoc
BnO
NH HN
O
O
Me
67
1H NMR (400 MHz, CDCl3)
(ppm)


NHBoc
BnO
NH HN
O
O
Me
67
13C NMR (100 MHz, CDCl3)
(ppm)

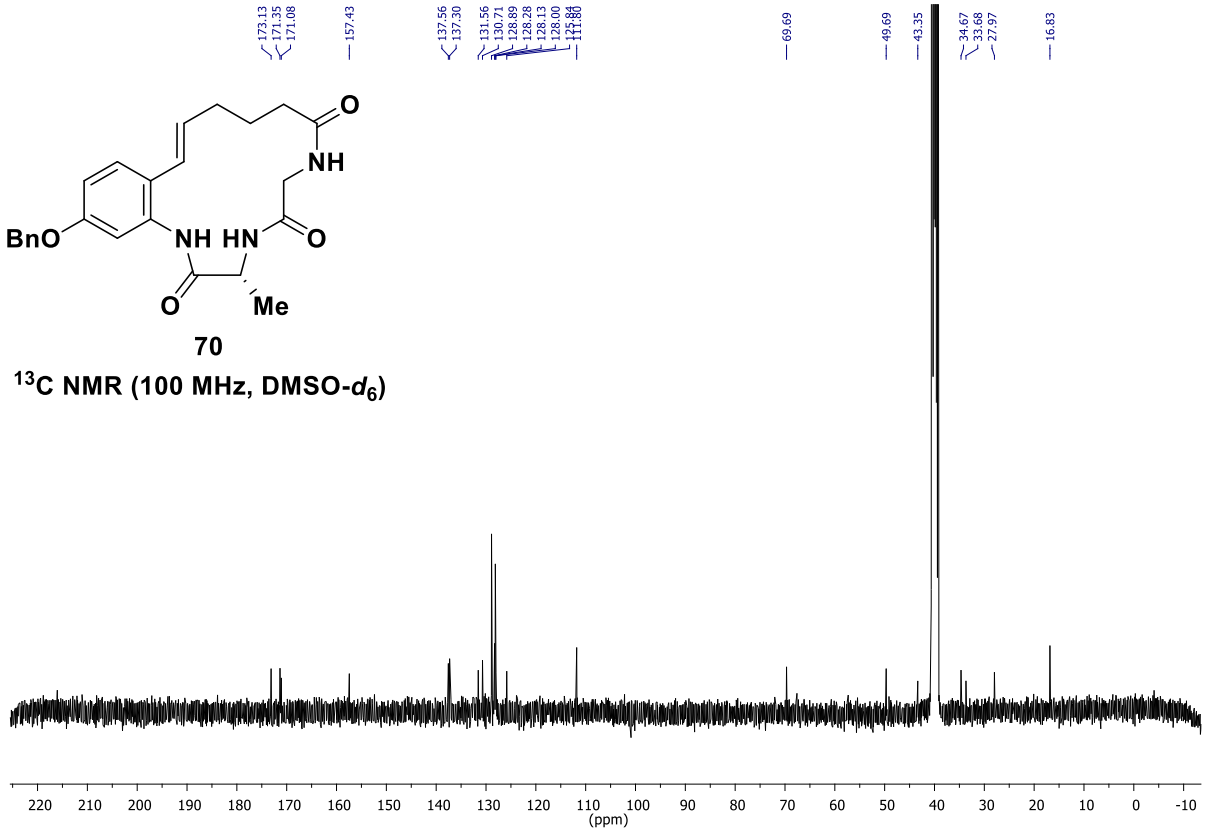

BnO
NH
NH HN
O
O
O
Me
69
1H NMR (400 MHz, CDCl3)
(ppm)


BnO
NH
NH HN
O
O
O
Me
69
13C NMR (100 MHz, CDCl3)
(ppm)



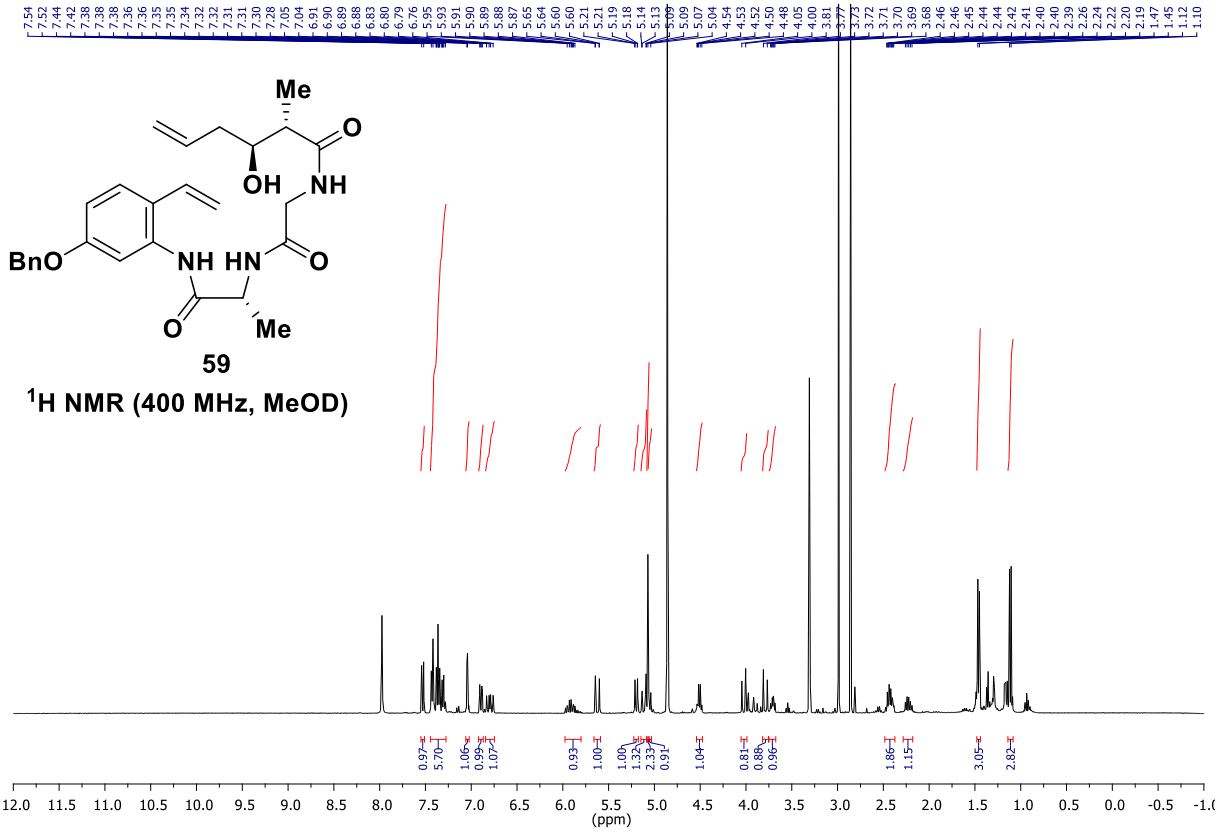
70

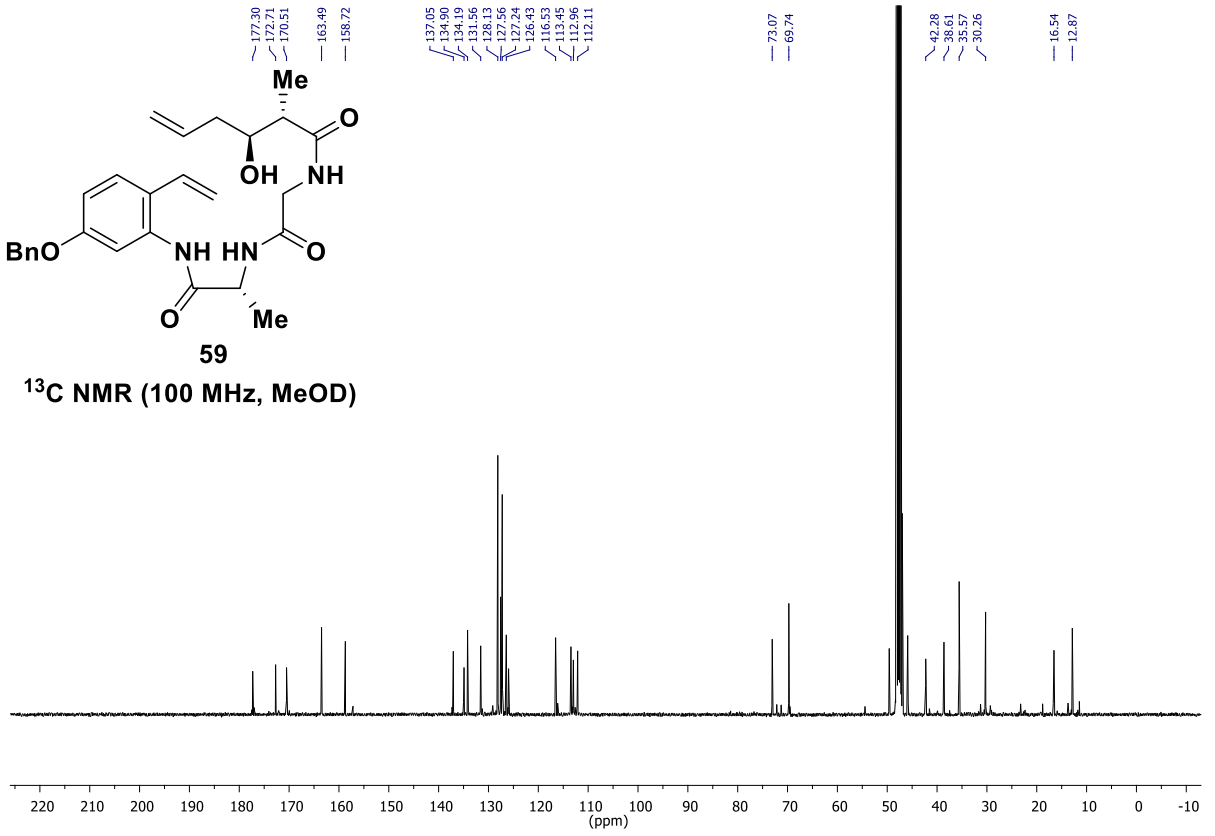
^{1}H NMR (400 MHz, DMSO-d_6)

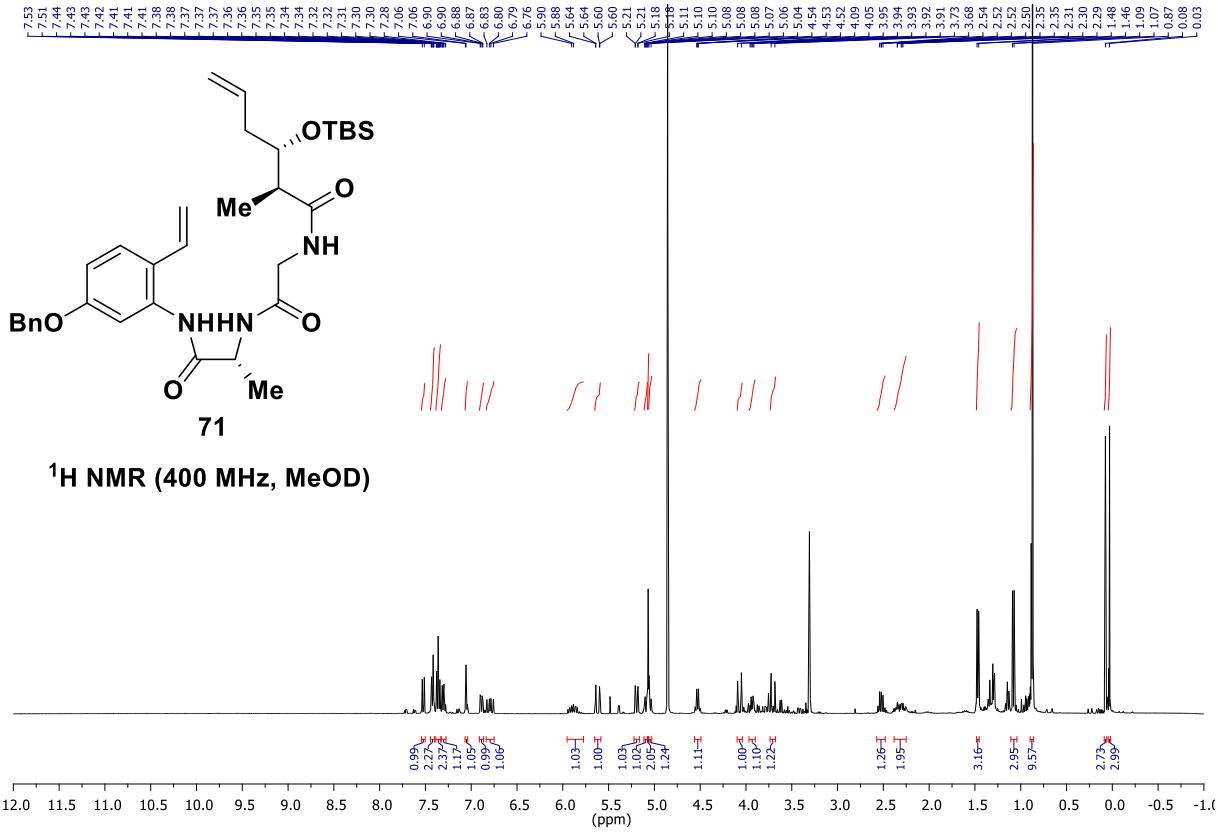


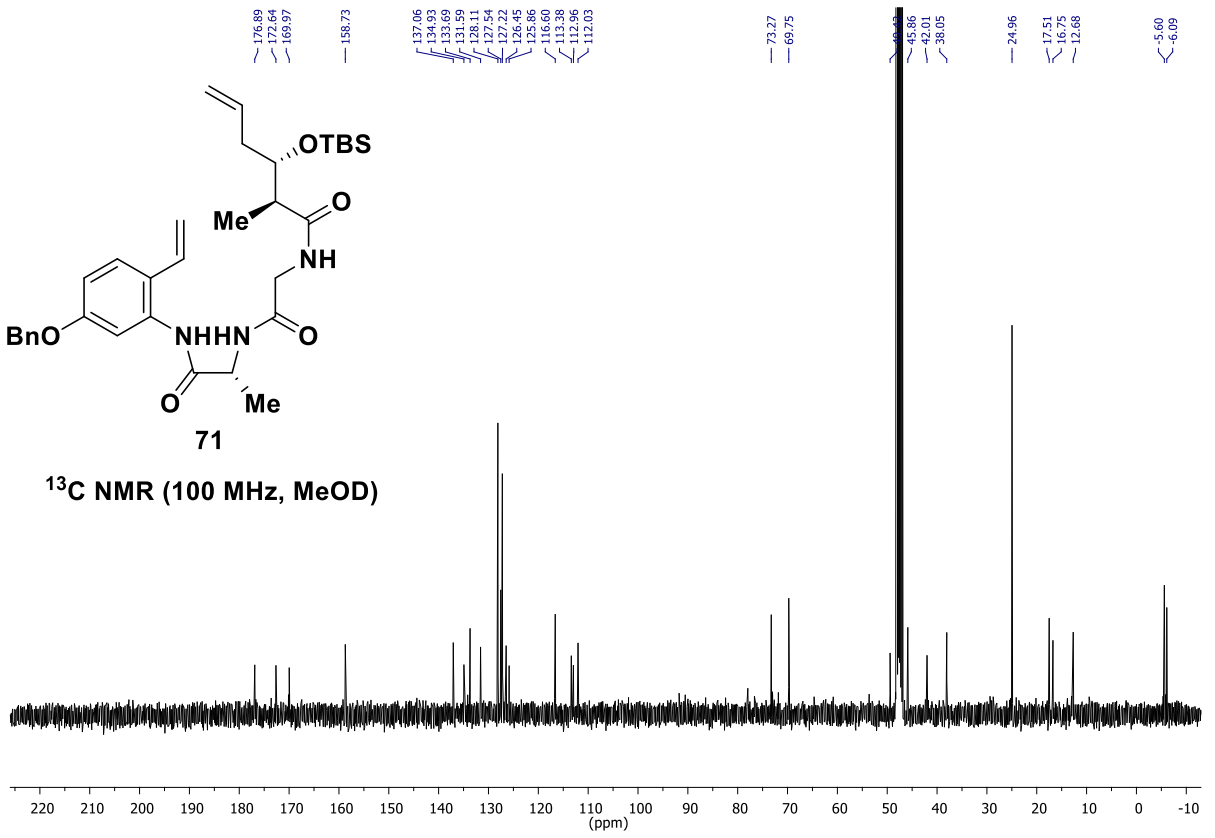
70

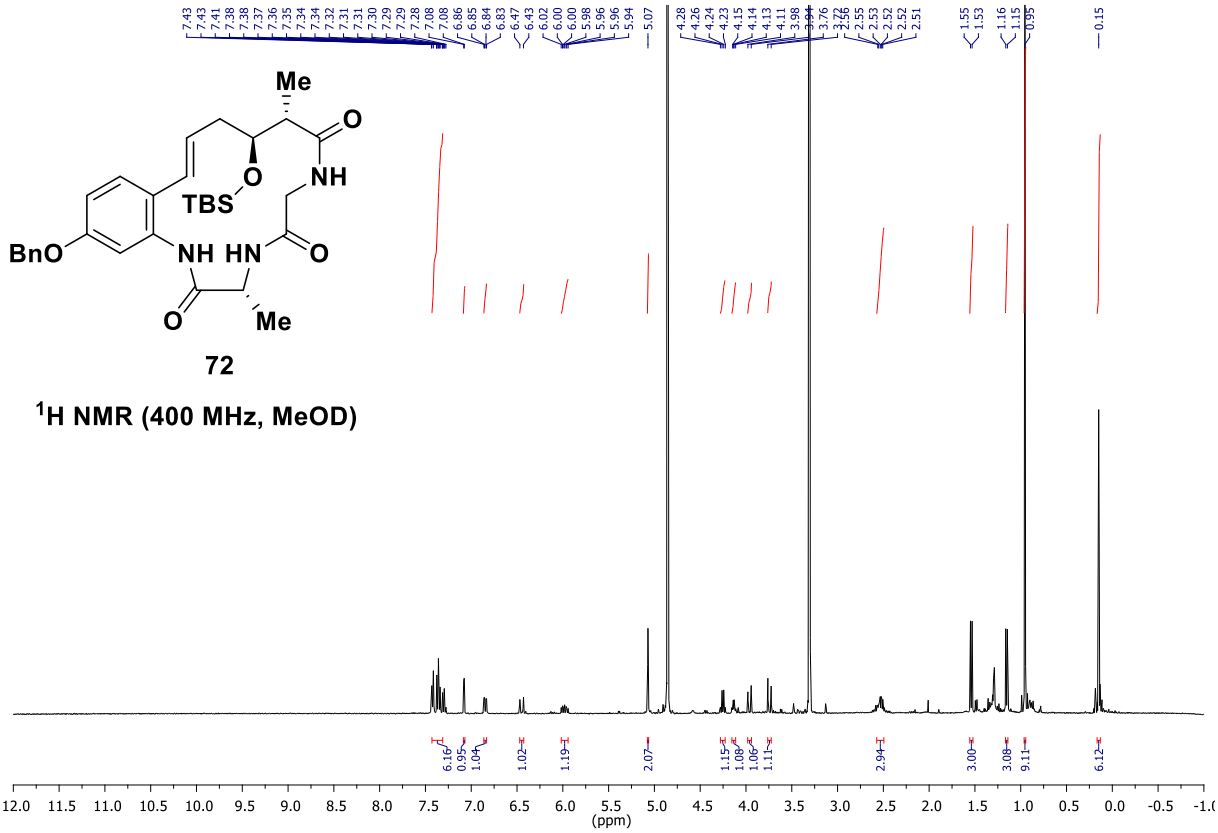
^{13}C NMR (100 MHz, DMSO-d_6)


Me
O
OH
NH
BnO
NH
HN
O
O
Me
59
1H NMR (400 MHz, MeOD)
(ppm)


Me
O
OH
NH
BnO
NH
HN
O
O
Me
59
13C NMR (100 MHz, MeOD)
(ppm)

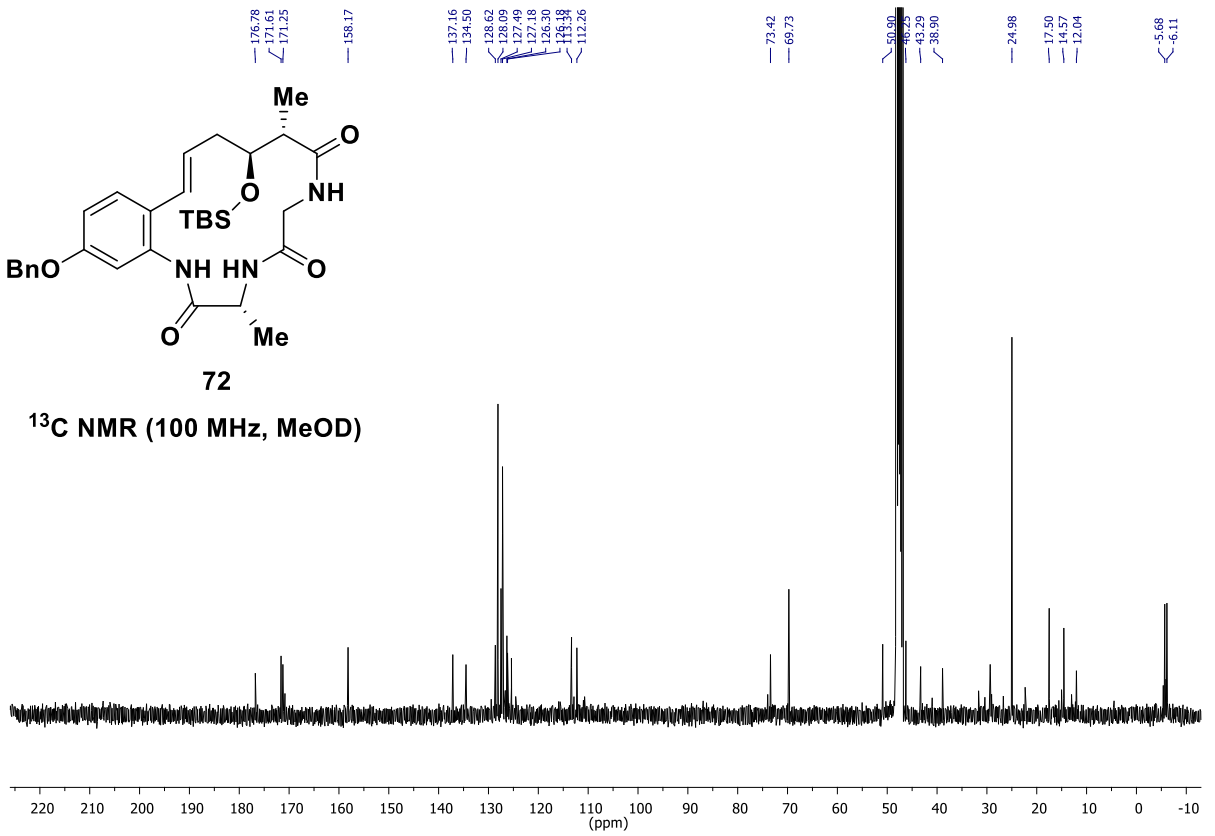

OTBS
Me
O
NH
BnO
NHHN
O
O
Me
71
1H NMR (400 MHz, MeOD)
(ppm)


OTBS
Me
O
NH
BnO
NHHN
O
O
Me
71
13C NMR (100 MHz, MeOD)
(ppm)



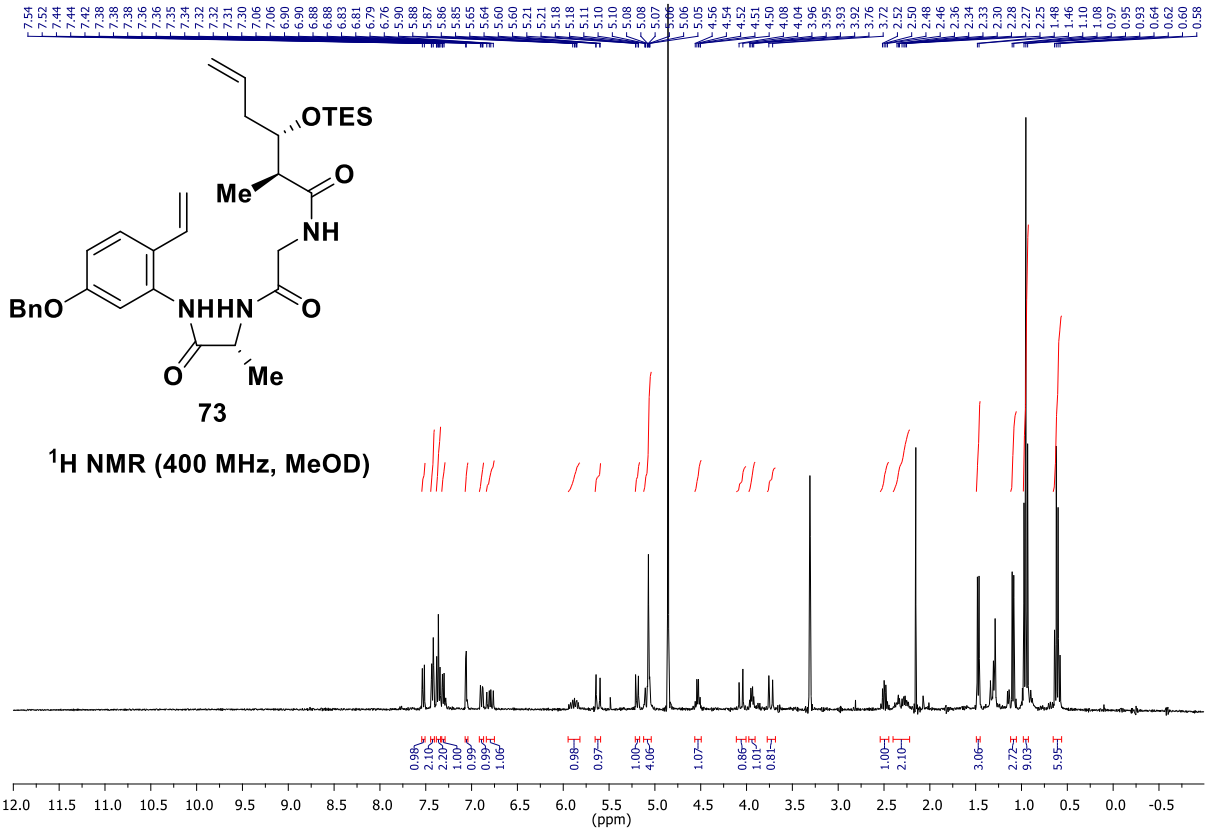
72

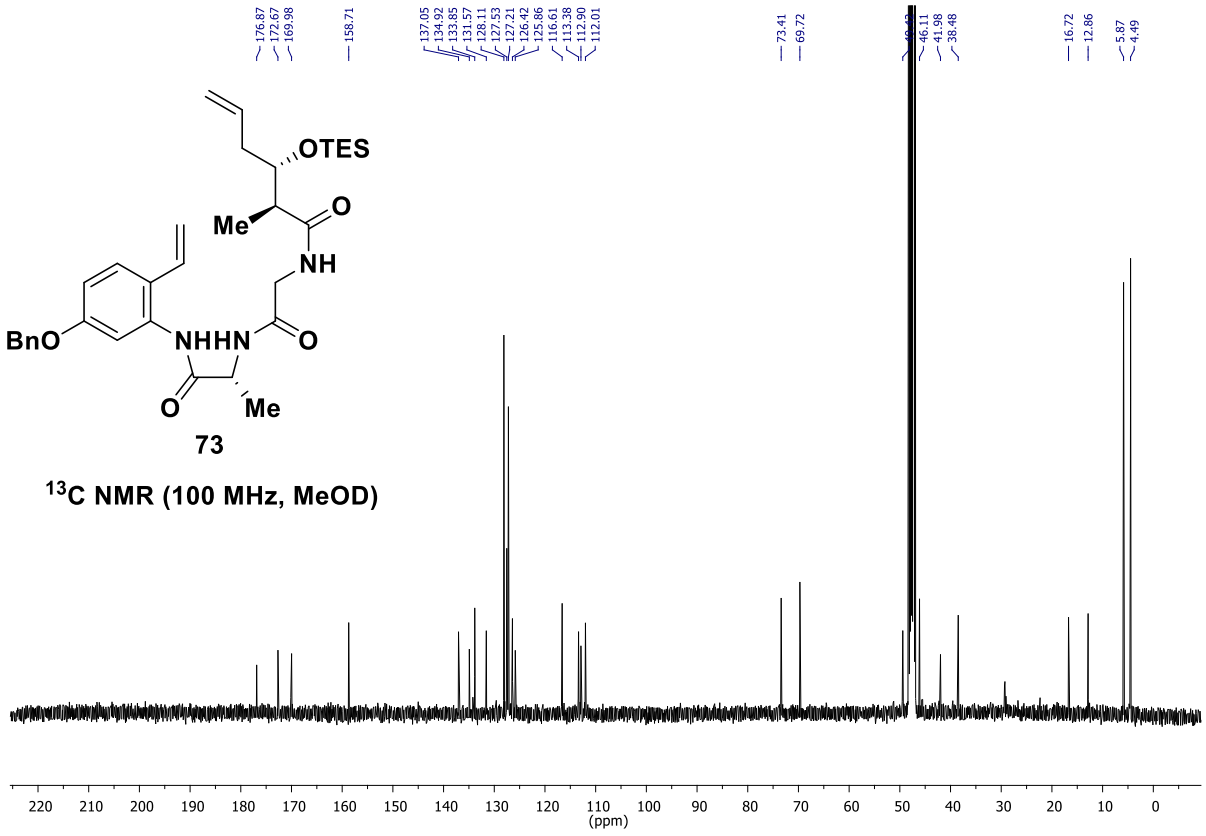
^{1}H NMR (400 MHz, MeOD)

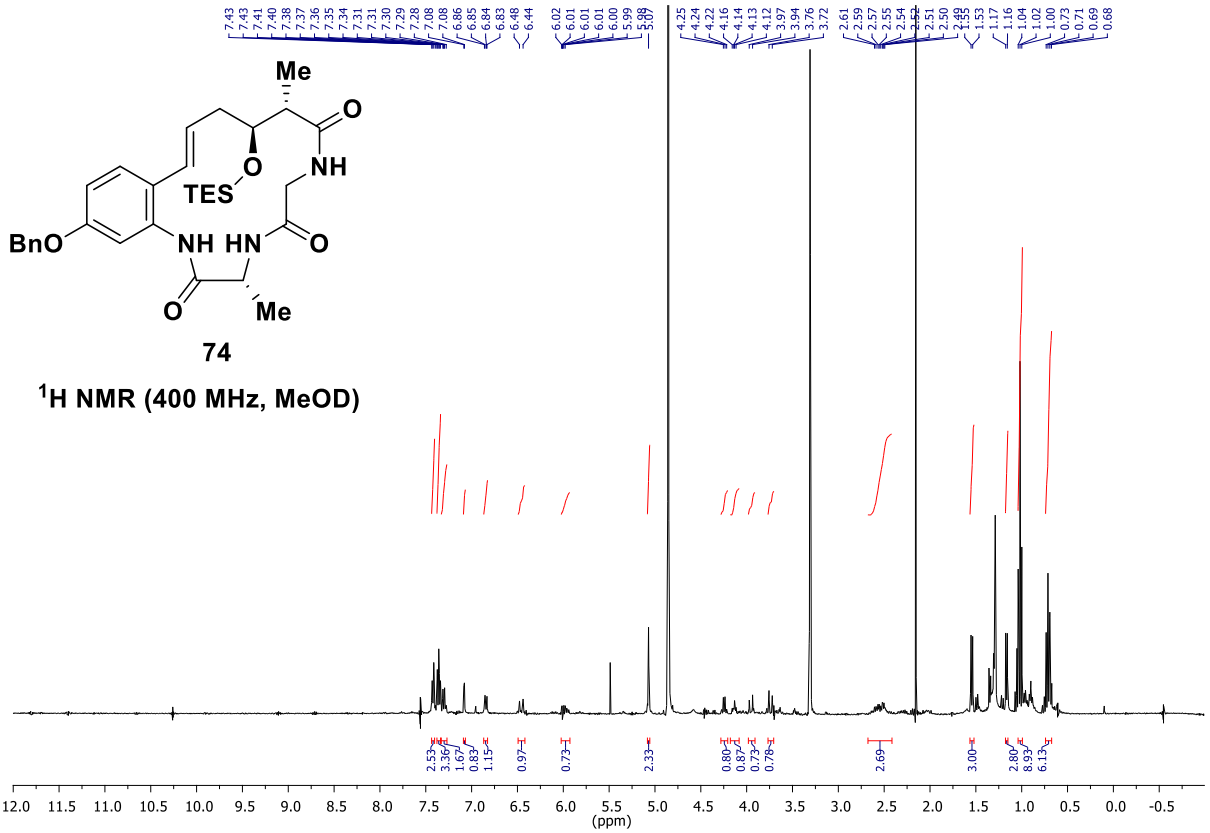


72

^{13}C NMR (100 MHz, MeOD)

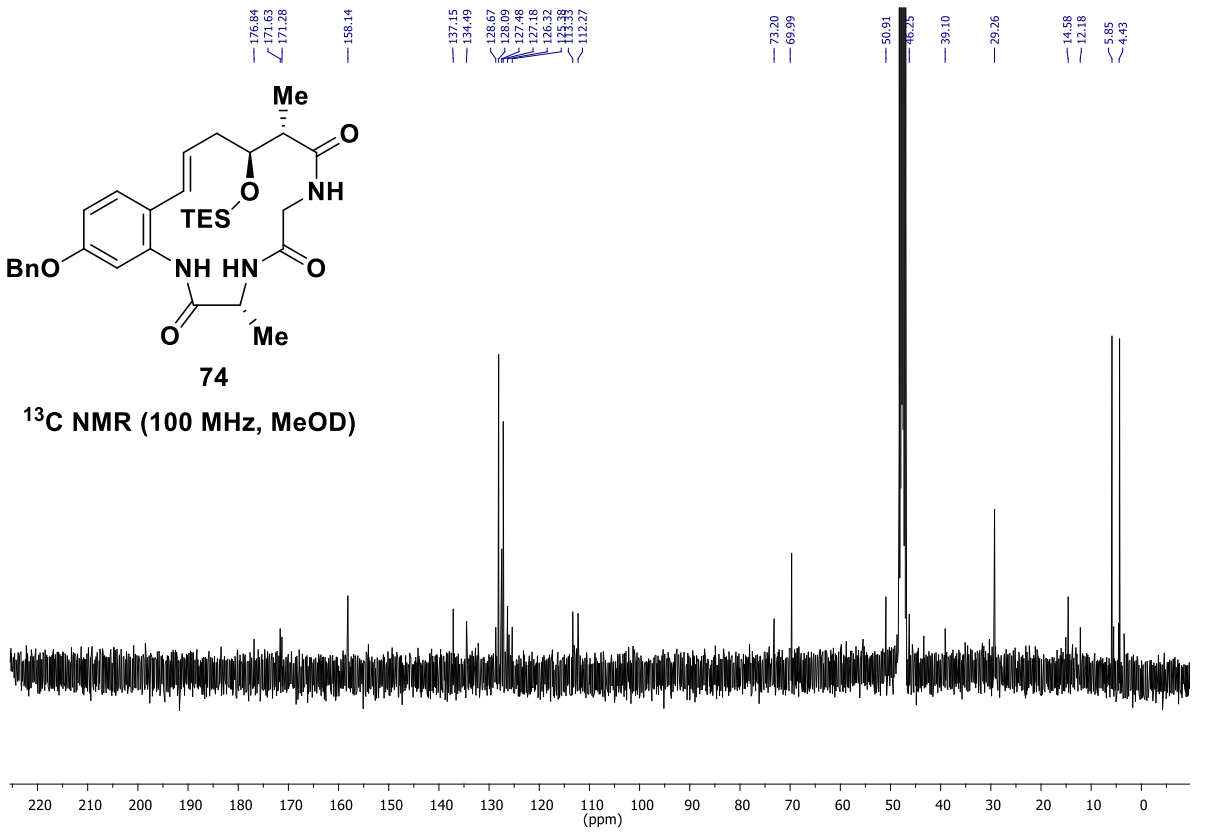

OTES
Me
O
NH
BnO
NHHN
O
O
Me
73
1H NMR (400 MHz, MeOD)
(ppm)


OTES
Me
O
NH
BnO
NHHN
O
O
Me
73
13C NMR (100 MHz, MeOD)
(ppm)



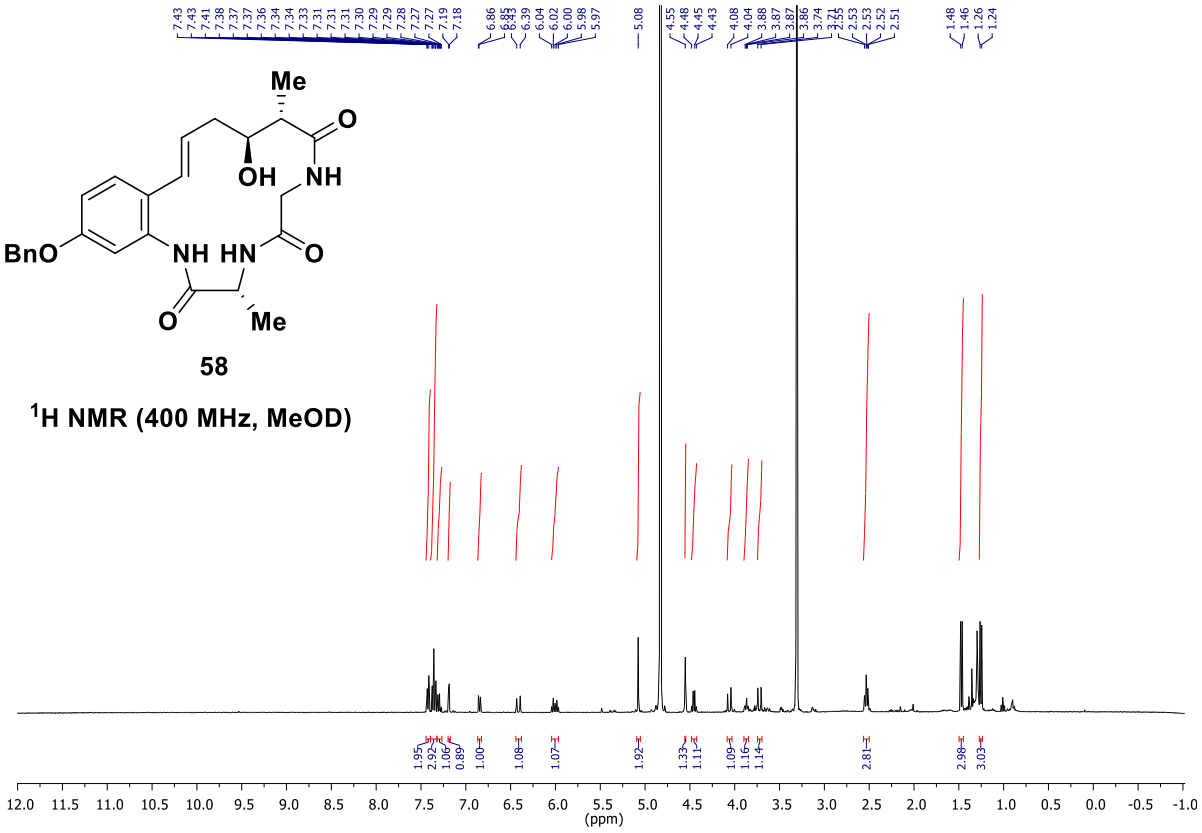
74

^{1}H NMR (400 MHz, MeOD)



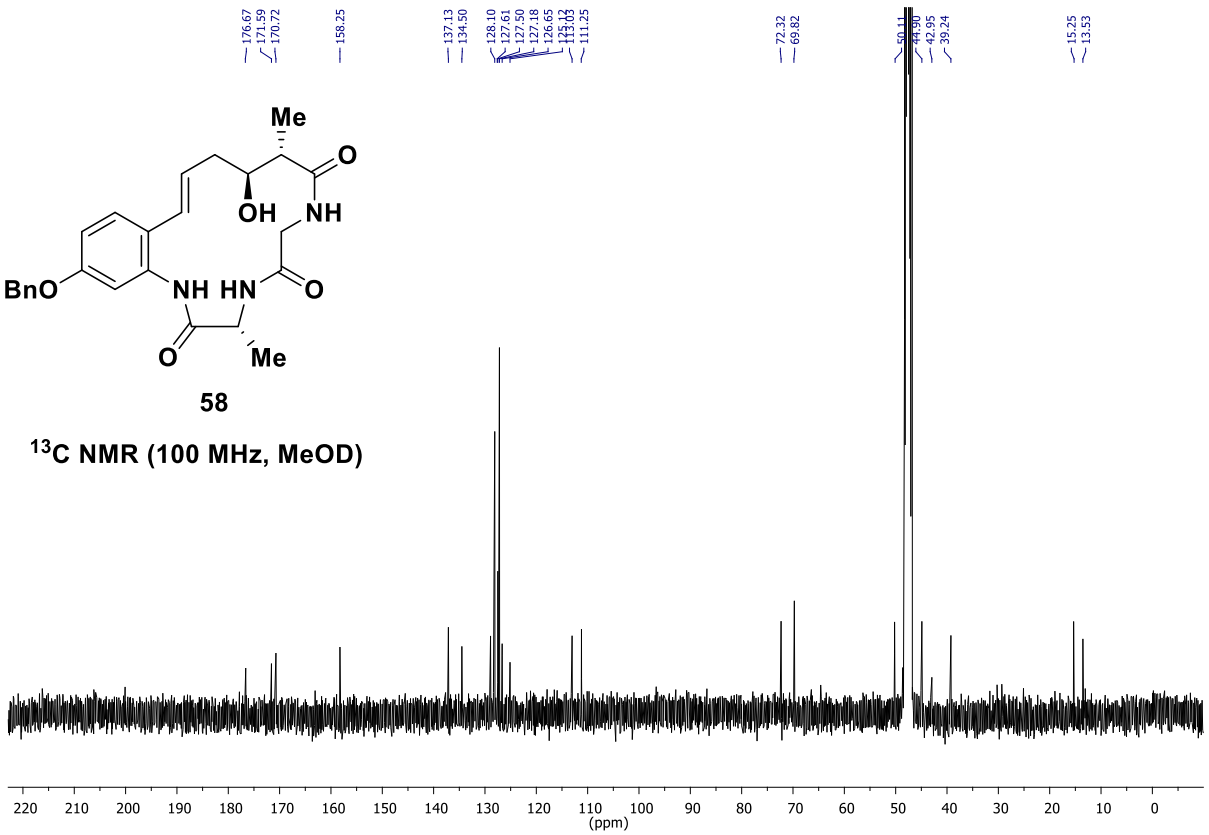
74

^{13}C NMR (100 MHz, MeOD)



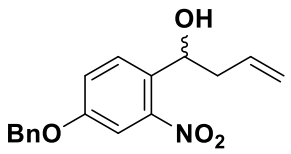
58

^{1}H NMR (400 MHz, MeOD)



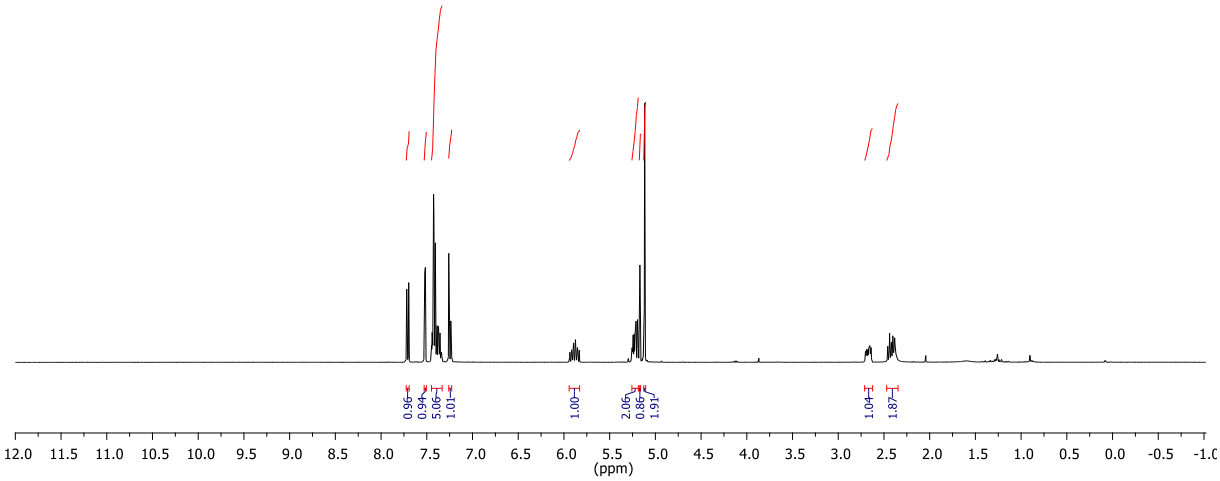
58

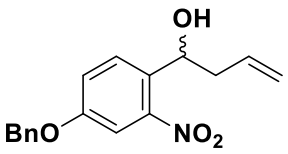
^{13}C NMR (100 MHz, MeOD)



77

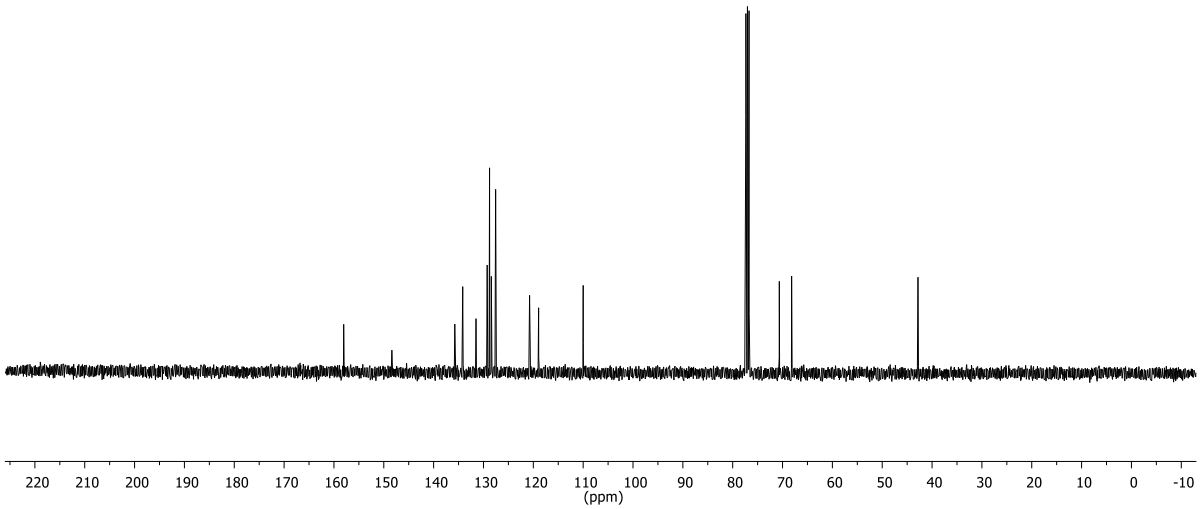
^{1}H NMR (400 MHz, $CDCl_3$)

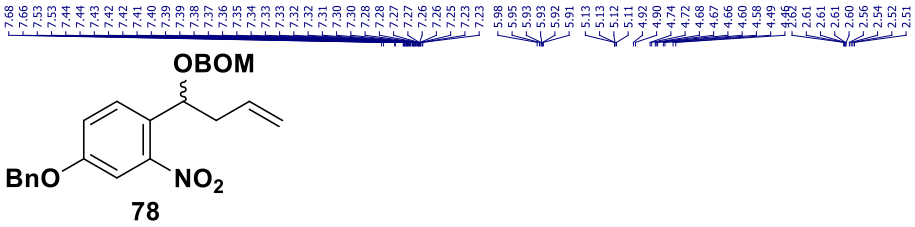




77

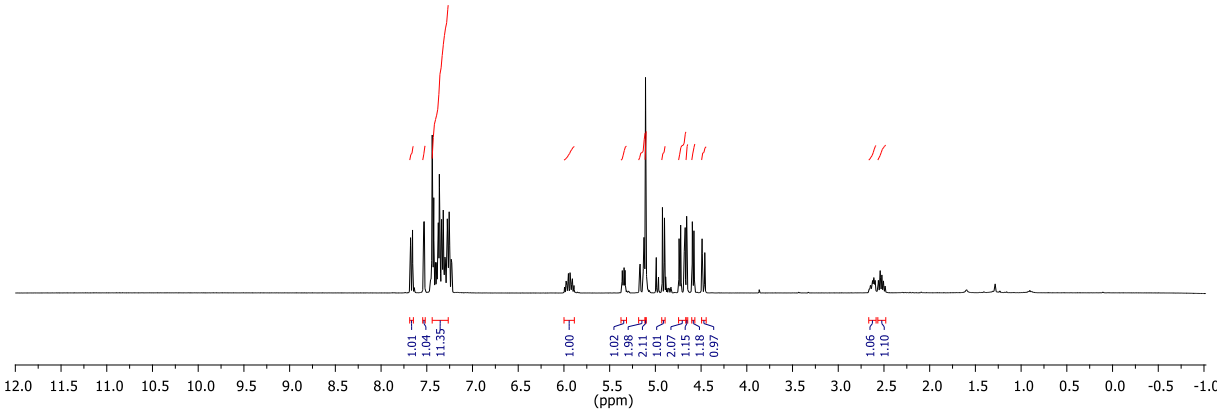
^{13}C NMR (100 MHz, $CDCl_3$)

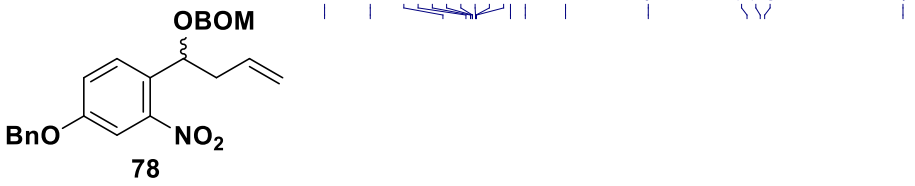




78

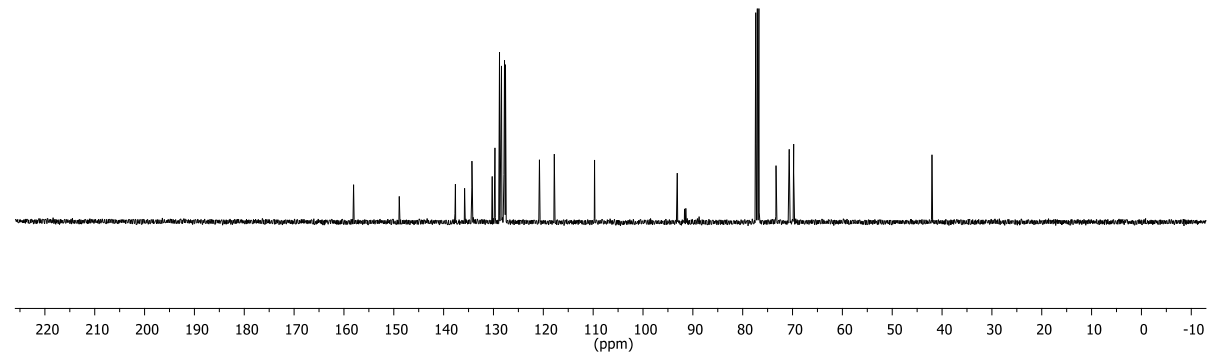
^{1}H NMR (400 MHz, $CDCl_3$)

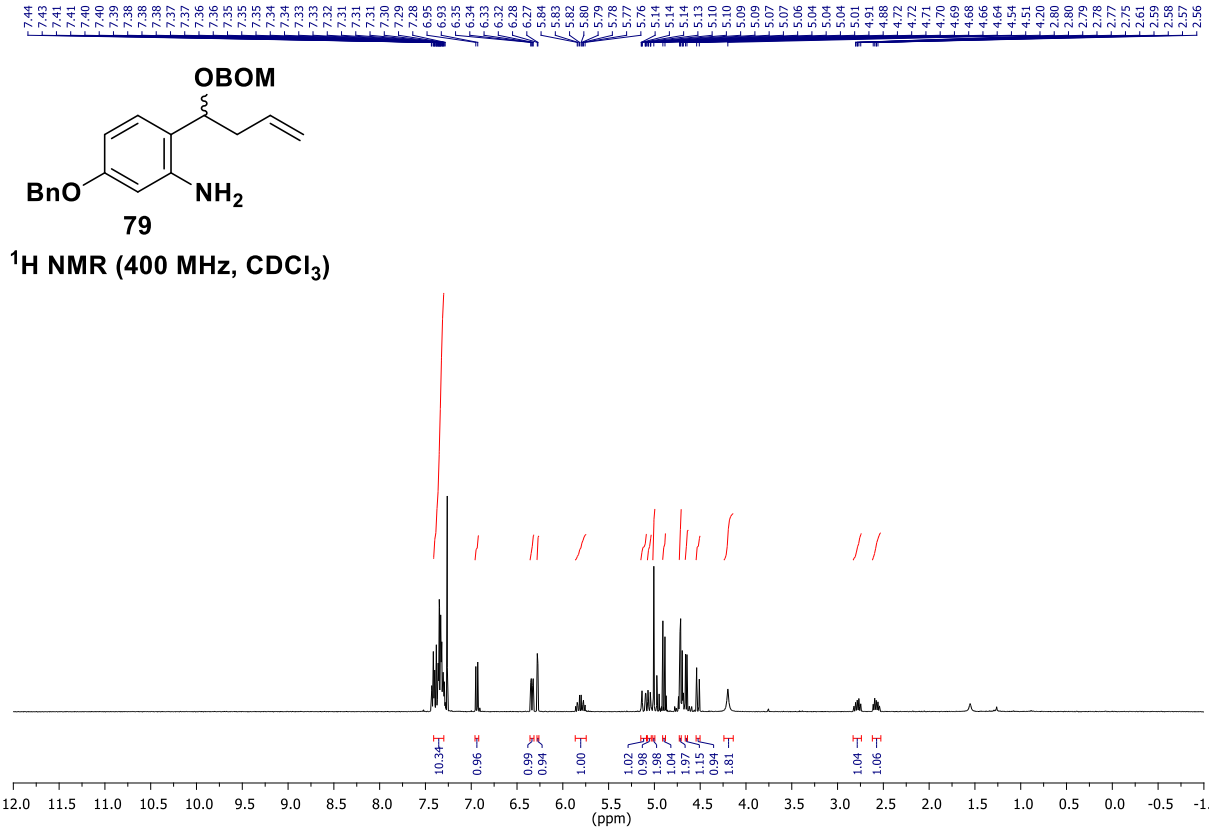


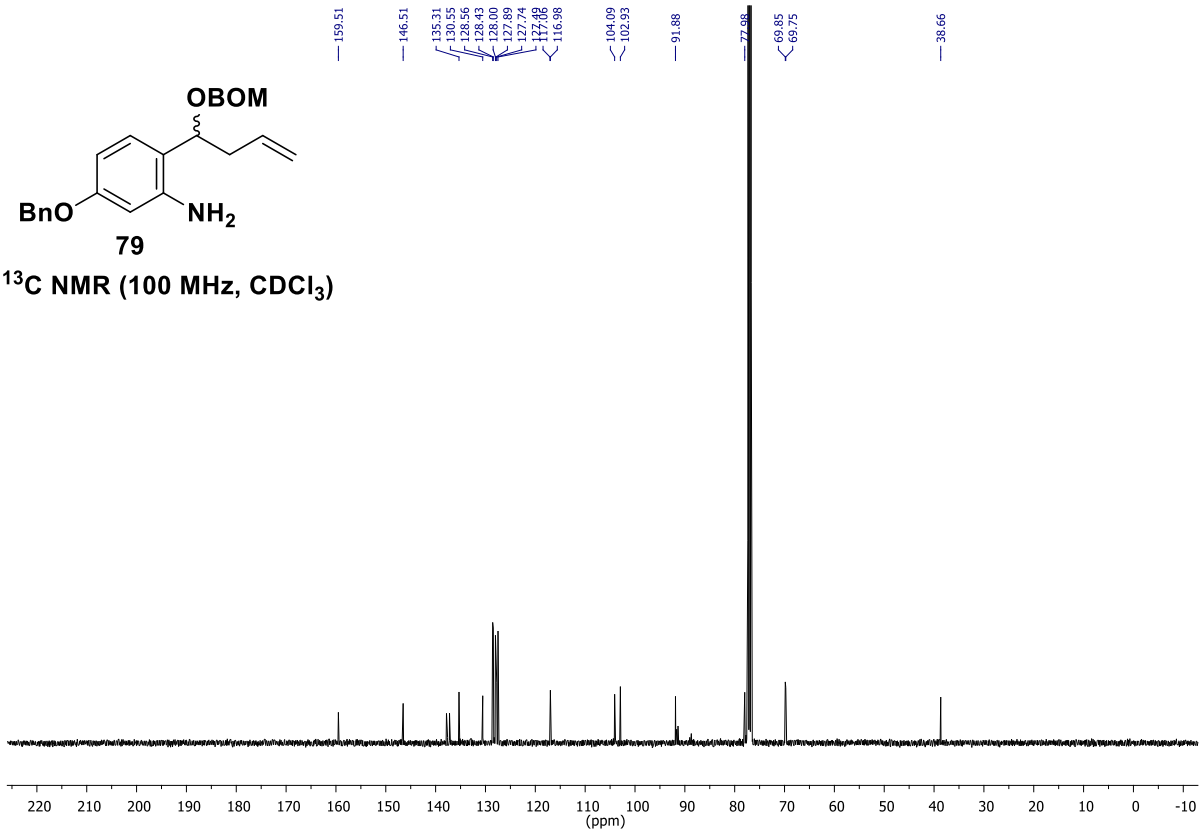


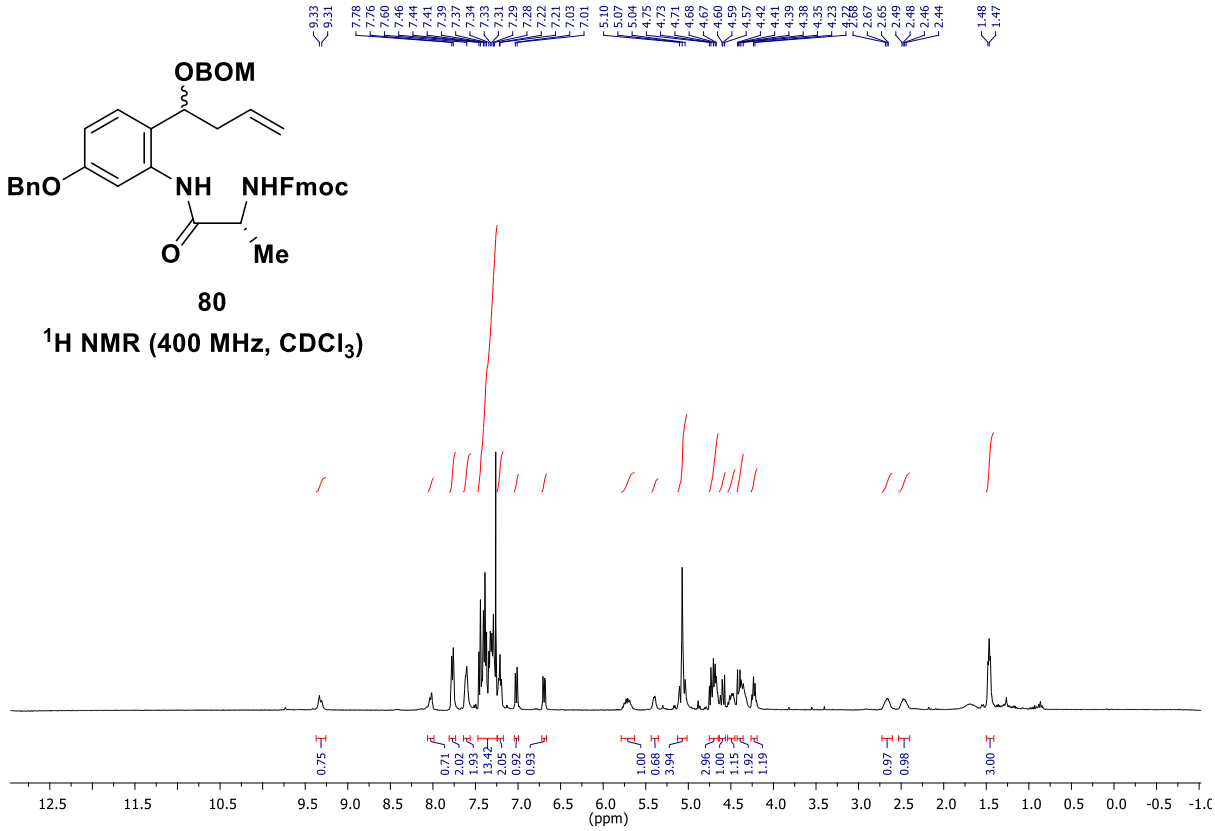
78

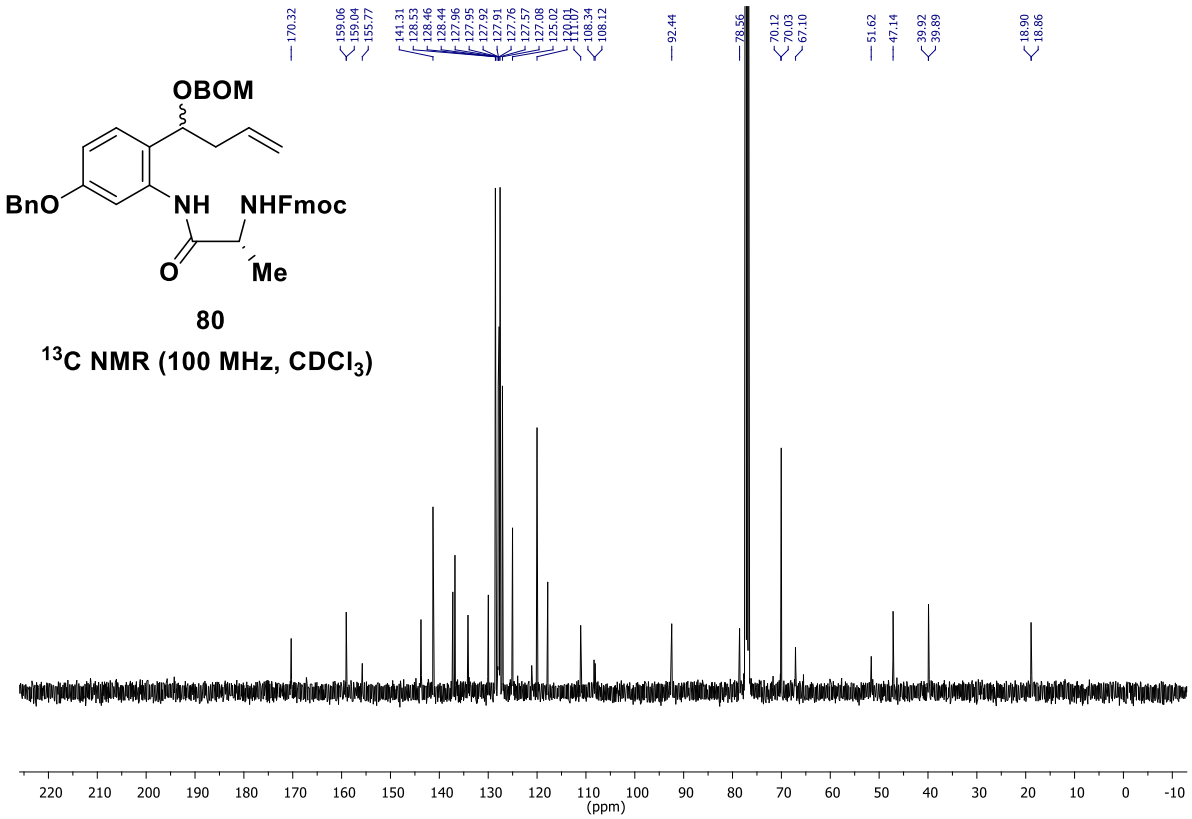
^{13}C NMR (100 MHz, $CDCl_3$)

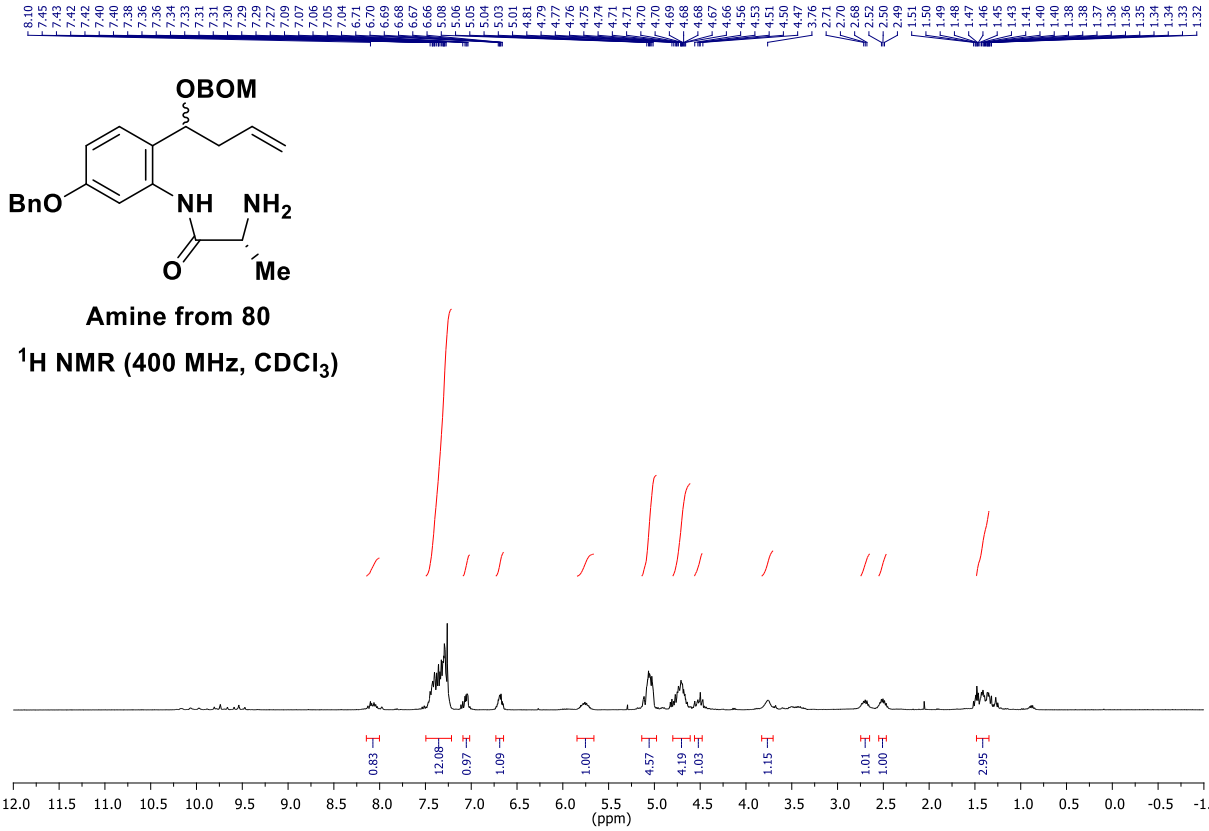


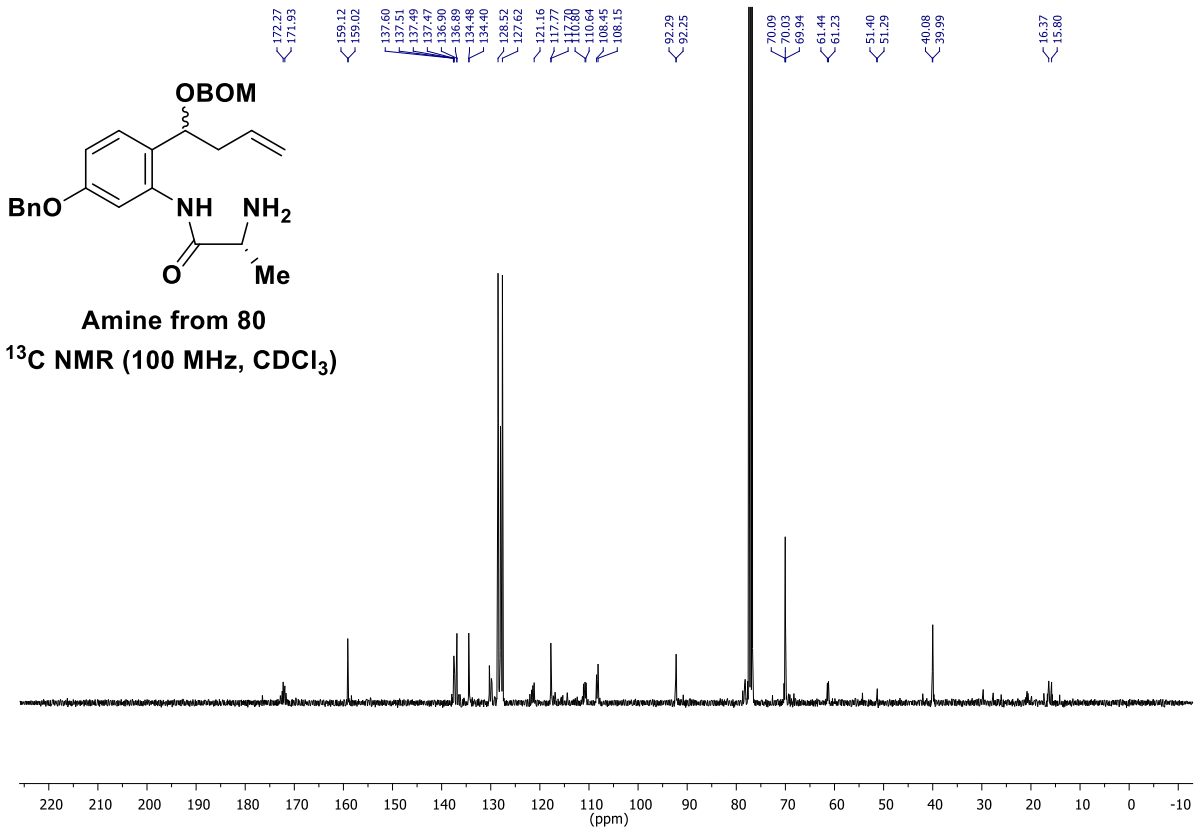

OBOM
BnO
NH2
79
1H NMR (400 MHz, CDCl3)
(ppm)

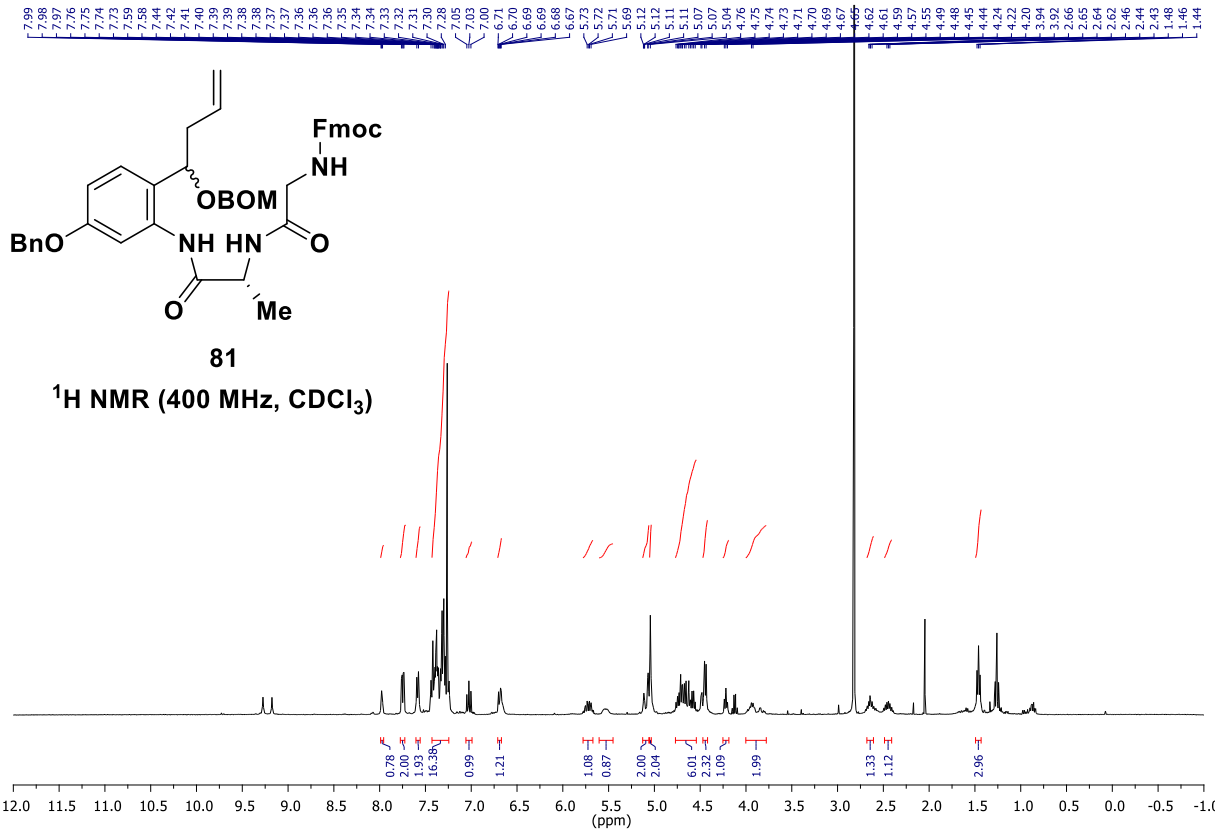

OBOM
BnO
NH2
79
13C NMR (100 MHz, CDCl3)
(ppm)

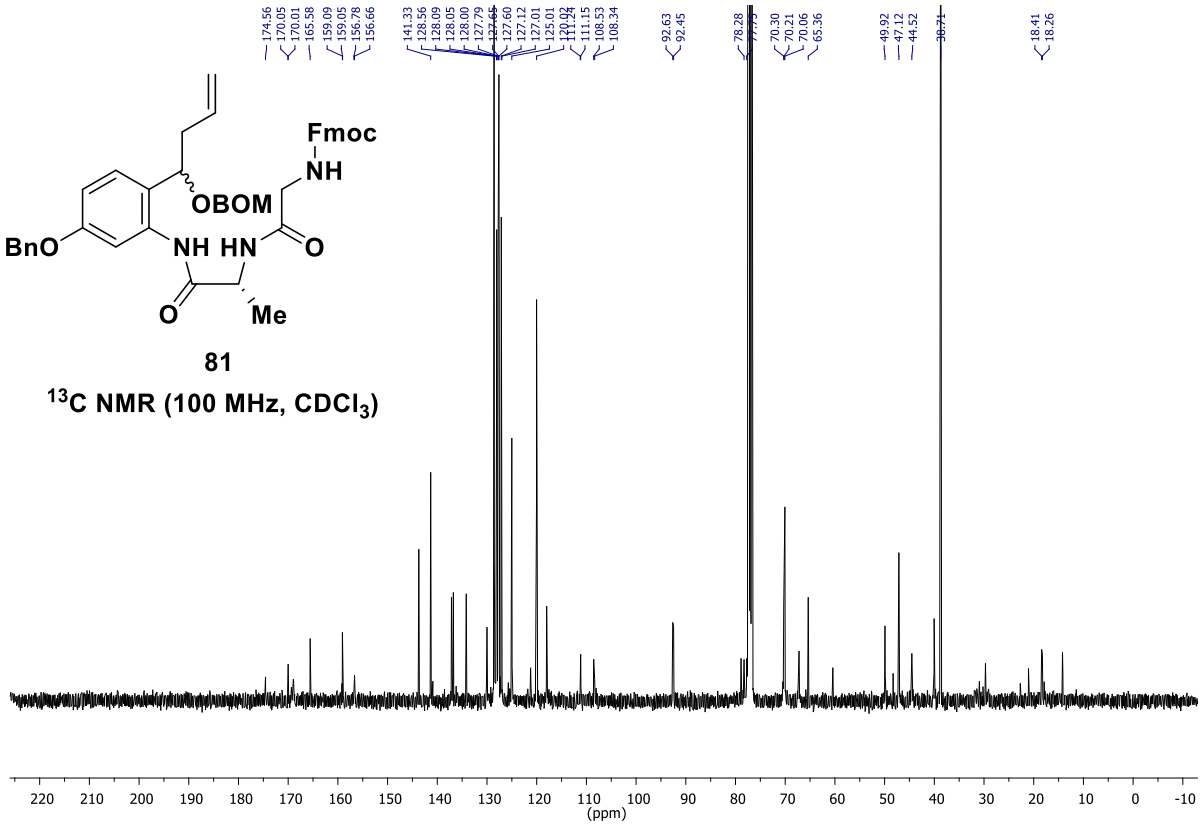

OBOM
BnO
NH
NHFmoc
O
Me
80
1H NMR (400 MHz, CDCl3)
(ppm)

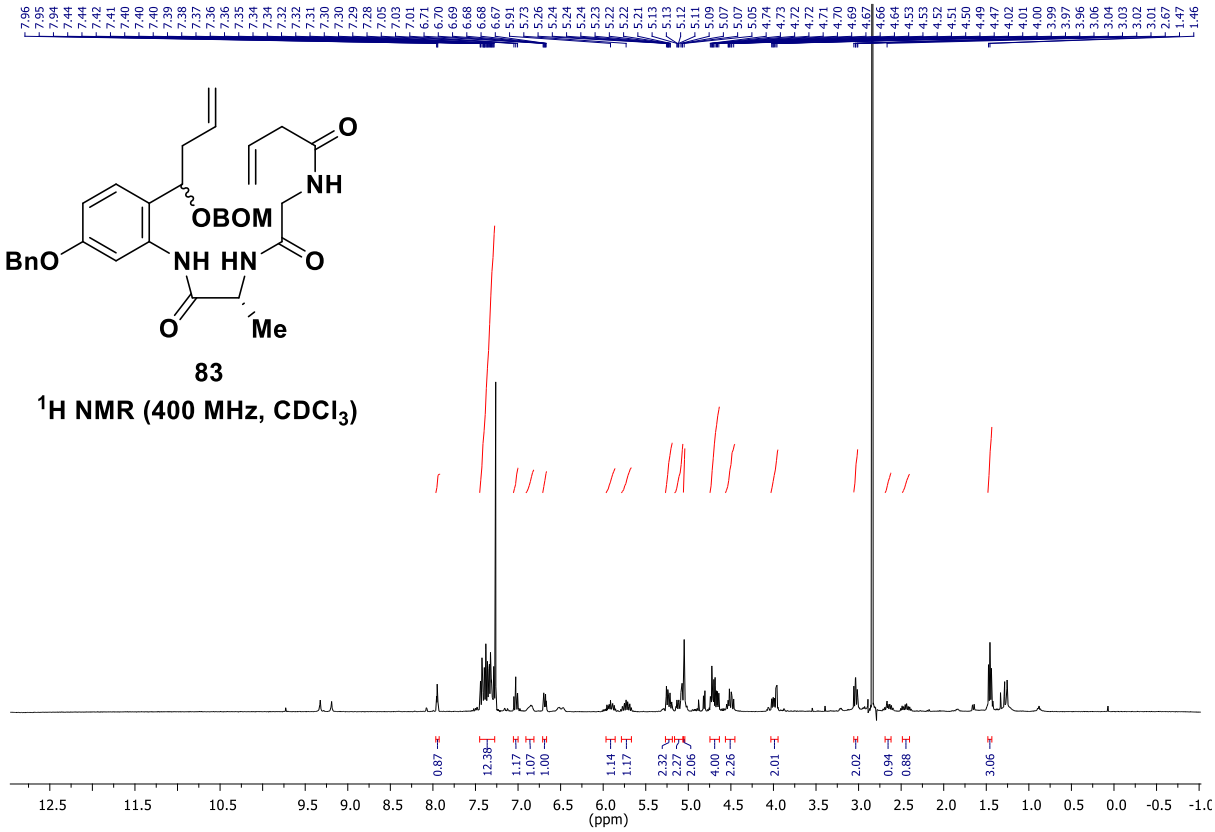

OBOM
BnO
NH
NHFmoc
O
Me
80
13C NMR (100 MHz, CDCl3)
(ppm)


OBOM
BnO
NH
NH2
O
Me
Amine from 80
1H NMR (400 MHz, CDCl3)
(ppm)


OBOM
BnO
NH
NH2
O
Me
Amine from 80
13C NMR (100 MHz, CDCl3)
(ppm)

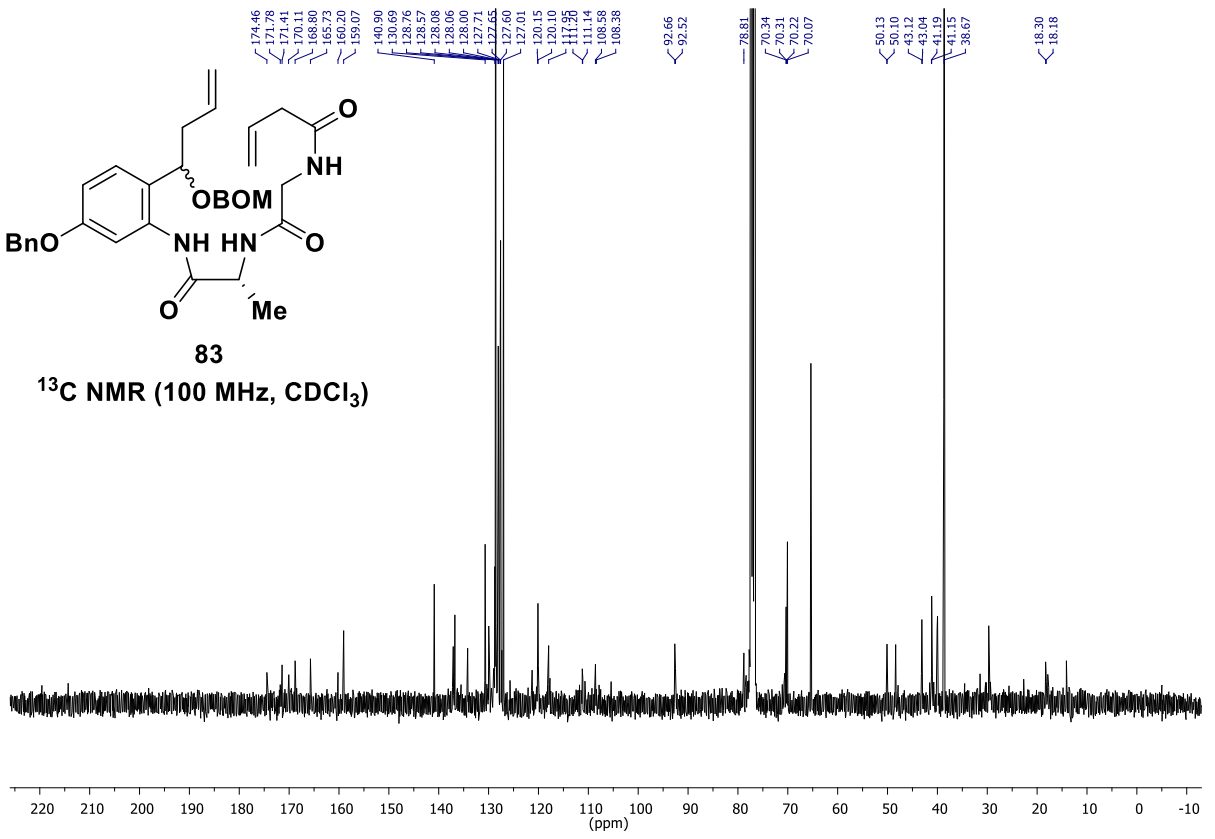

Fmoc
NH
OBOM
BnO
NH HN
O
O
Me
81
1H NMR (400 MHz, CDCl3)
(ppm)


Fmoc
NH
OBOM
BnO
NH HN
O
O
Me
81
13C NMR (100 MHz, CDCl3)
(ppm)



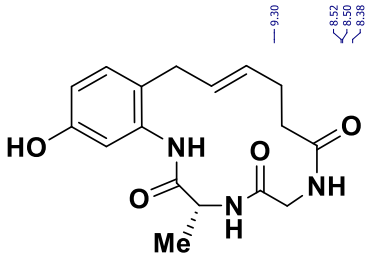
83

^{1}H NMR (400 MHz, $CDCl_3$)



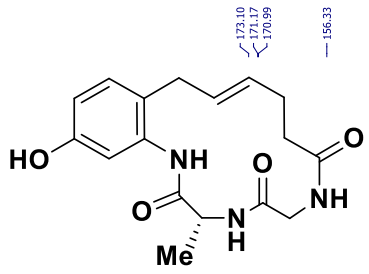
83

^{13}C NMR (100 MHz, $CDCl_3$)



85

^{1}H NMR (400 MHz, DMSO-d_6)



85

^{13}C NMR (100 MHz, DMSO-d_6)

2. Dose-dependent effect on the vitro growth of tumor and endotelial-cells by the tested compounds

2.1. Human promyelocytic leukemia (HL60)

Table S1. Dose-Dependent Effect of Compounds on the in vitro growth of HL60 cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100	100	100	100	100	94,95603157	74,40811725	57,72266065		>50
27	100	100	100	100	100	100	100	100	94,9267193	55,69334837		>50
28	100	100	100	100	100	100	89,61748634	59,92125984	38,66141732	23,54330709		17,2 ± 6,6
70	100	100	100	100	100	100	85,03937008	60,5511811	33,85826772	16,2992126		20,5 ± 5,2
85	100	100	100	100	100	100,6765068	100	96,43245541	86,29023318	61,75887805		>50
38	100	100	100	100	100	100	100	100	96,46081868	62,54797758		>50
74	100,6629271	100	100	100	100	100	100	100	100	99,35251799		>50
58	100	100	100	100	100	100	89,30117502	64,31663575	1,298701299	0,865800866		14,7 ± 4,4

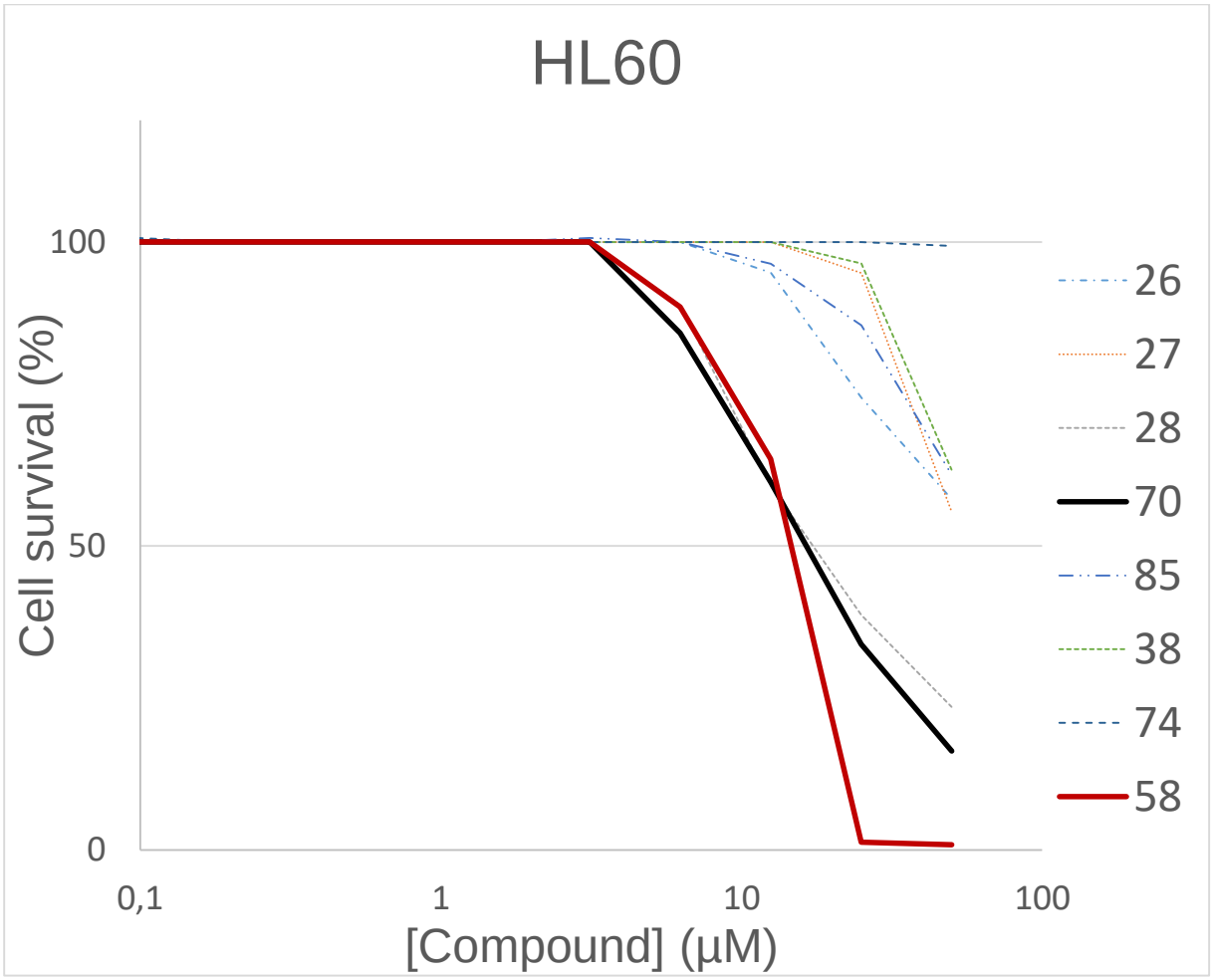


Figure S1. Dose-Response Plots of Compounds against HL60

2.2. Chronic Myelogenous leukemia (KU812F)

Table S2. Dose-Dependent Effect of Compounds on the in vitro growth of KU812F cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100	100	100	100	100	99,1463415	90,3658537	86,95121951		>50
27												
28												
70	100	100	100	100	100	100	100	96,3099631	92,496925	80,81180812		>50
85	100	100	100	100	100	100,644382	100	94,8339483	87,8228782	58,30258303		>50
38	100	100	100	100	100	100	100	93,409379	80,2281369	69,0747782		>50
74	100	100	100,462963	100	100	100	100	97,6851852	82,4074074	89,35185185		>50
58	100	100	100	100	99,006458	95,6284153	89,0710383	33,8301043	-1,3412817	0,049677099		14,03 ± 3,05

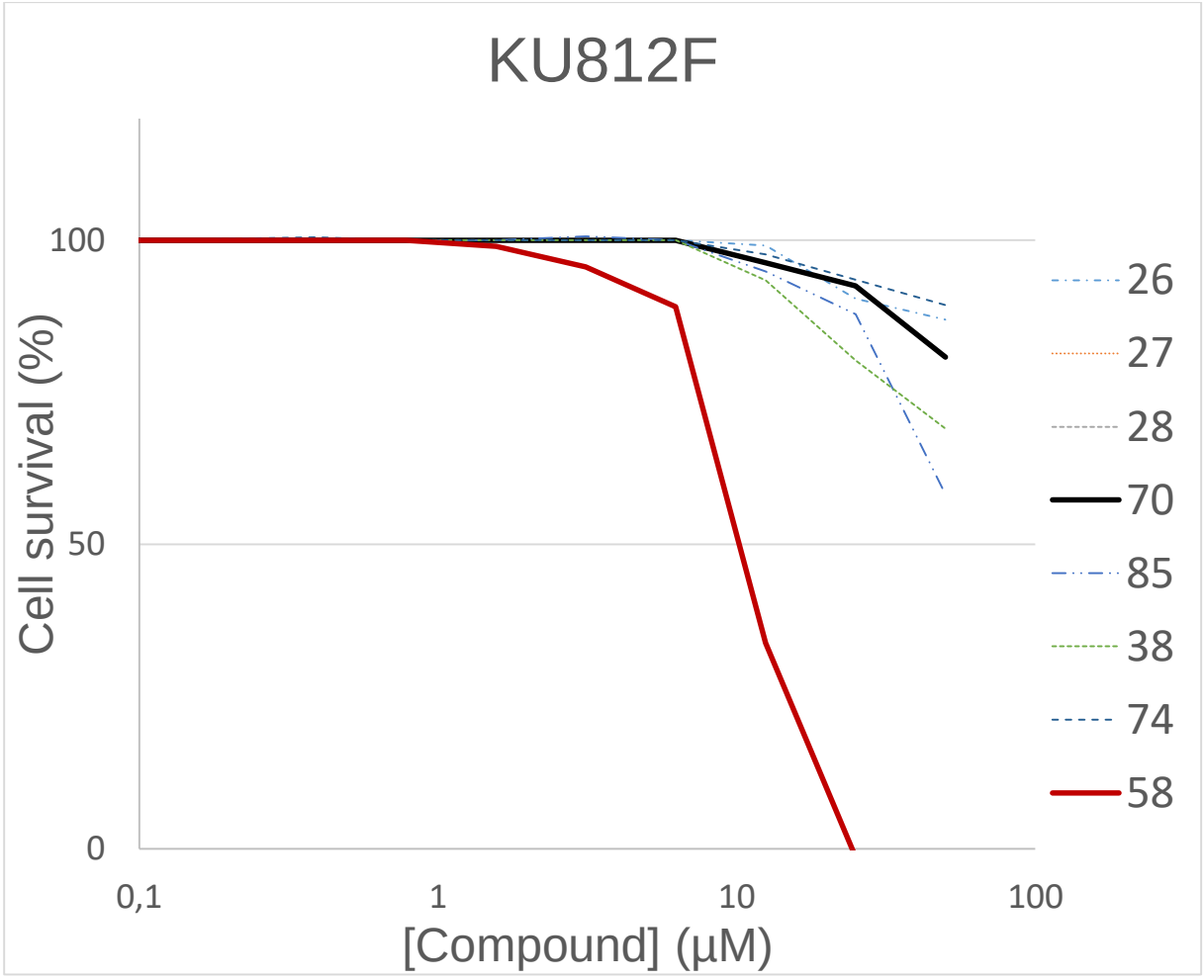


Figure S2. Dose-Response Plots of Compounds against KU812F

2.3. Histiocytic lymphoma (U937)

Table S3. Dose-Dependent Effect of Compounds on the in vitro growth of U937 cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100,37037	100	100	100	100	96,0185185	92,0740741	85,92592593		>50
27												
28												
70	100	100	100	100	100	100	96,6315789	91,1902834	80,3076923	56,92307692		>50
85	100	100	100	100	100	100	100	100	97,1039182	93,3560477		>50
38	100	100	100	100	100	100	96,3894967	94,4201313	86,761488	72,21006565		>50
74	100	100	100	100	100	100	94,9317739	87,8167641	82,4561404	77,68031189		>50
58	100	100	100,229314	96,8660424	93,1970189	85,8589719	63,3862029	11,7141219	0	0,401299446		7,02 ± 2,32

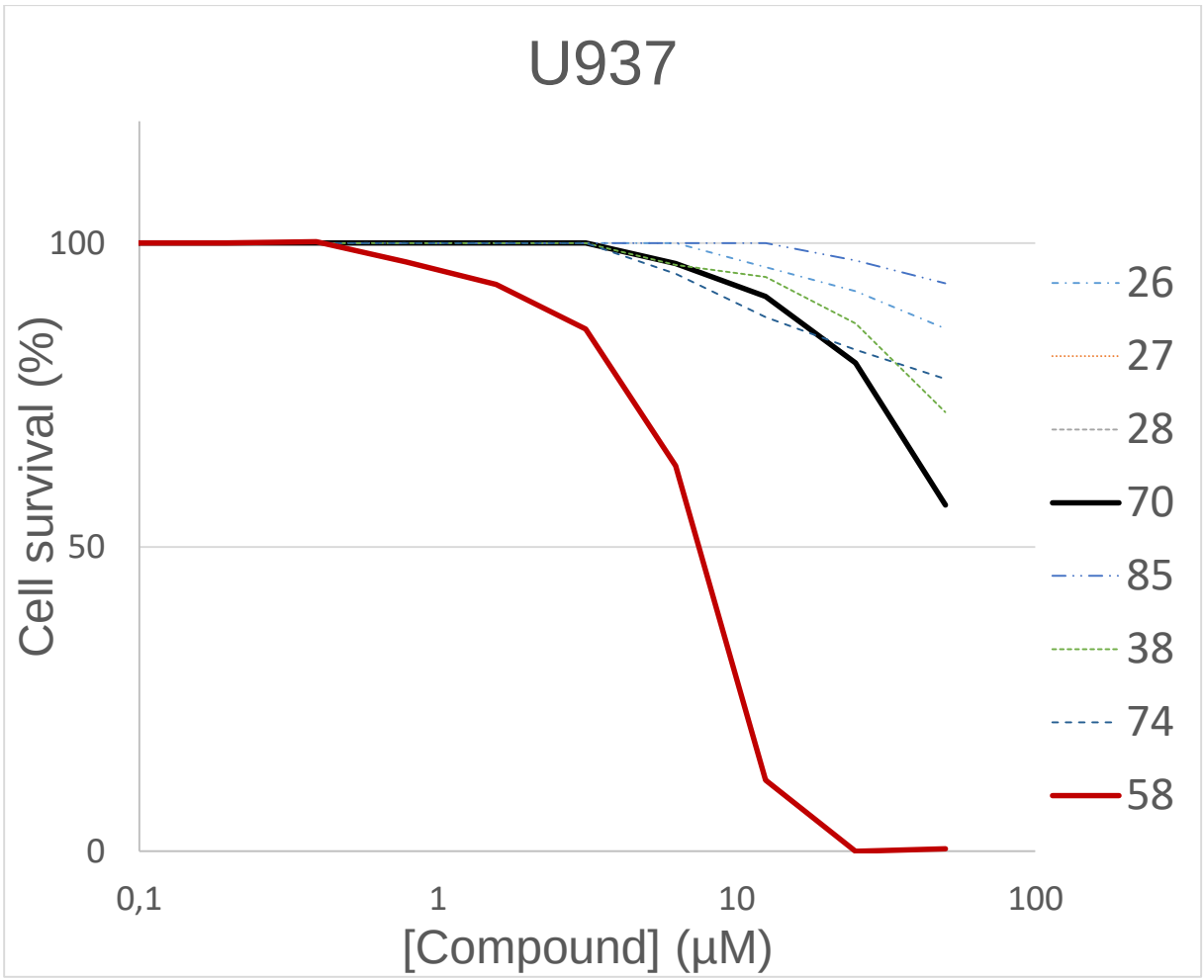


Figure S3. Dose-Response Plots of Compounds against U937

2.4. Human fibrosarcoma (HT1080)

Table S4. Dose-Dependent Effect of Compounds on the in vitro growth of HT1080 cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100	100	100	100	100	100	99,26956522	92,24347826	78,4695652	>100
27	100	100	100	100	100	100	100	100	91,7333333	80,32463768	53,4724638	>100
28	99,01046895	99,35465366	100	100,7887566	100	100	98,32209953	83,35006453	76,92528324	65,56718772		>50
70	99,2695652	100	100	100	100	100	94,8869565	83,2	63,6521739	44,52173913	6,4	31,1 ± 2,8
85	100	100	100	100	100	100	100	100	100	99,21596579	82,1097648	>100
38	100	100	100	100	100	100	100	96,0085531	87,59800428	74,83962937	54,88239487	>100
74	100	100	100	100	100	100,701199	100	93,9154038	83,6914725	81,7914499	72,019905	>100
58	100	100	100	100	100	100	90,7763259	71,2528824	0,92236741	-3,84319754	-3,5357417	16,33 ± 2,95

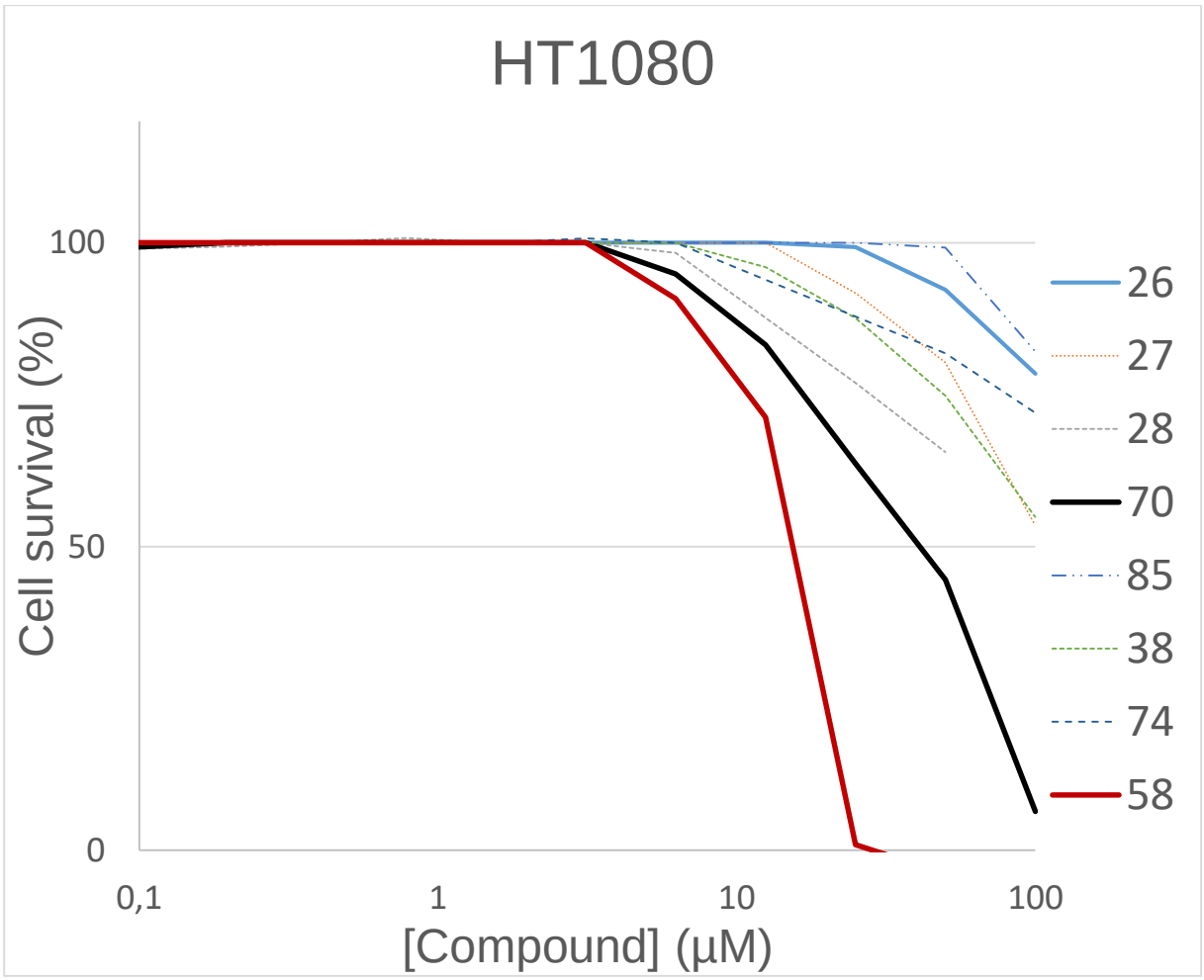


Figure S4. Dose-Response Plots of Compounds against HT1080

2.5. Human breast adenocarcinoma (MDA-MB-231)

Table S5. Dose-Dependent Effect of Compounds on the in vitro growth of MDA-MB-231 cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100	100	100	100	100	100	100	98,24561404	83,891547	>100
27	100	100	100	100	100	100	100	87,0288537	78,5027294	77,98284377	68,0010398	>100
28												
70	100	100,194553	100	100	100	100	100	99,0272374	92,4124514	87,93774319	76,459144	>100
85	100	100	100	100	100	100	100	100	100	87,93774319	76,459144	>100
38	100	100	100	99,9498244	100	100	100,351229	100	100	86,40240843	71,8514802	>100
74	100	100	100	100	100	100	100	100	96,8810916	88,49902534	69,005848	>100
58	100	100	100	100	100	98,5280865	94,7431661	81,4058276	17,3225193	-0,760989286	-0,3003905	16,45 ± 1,01

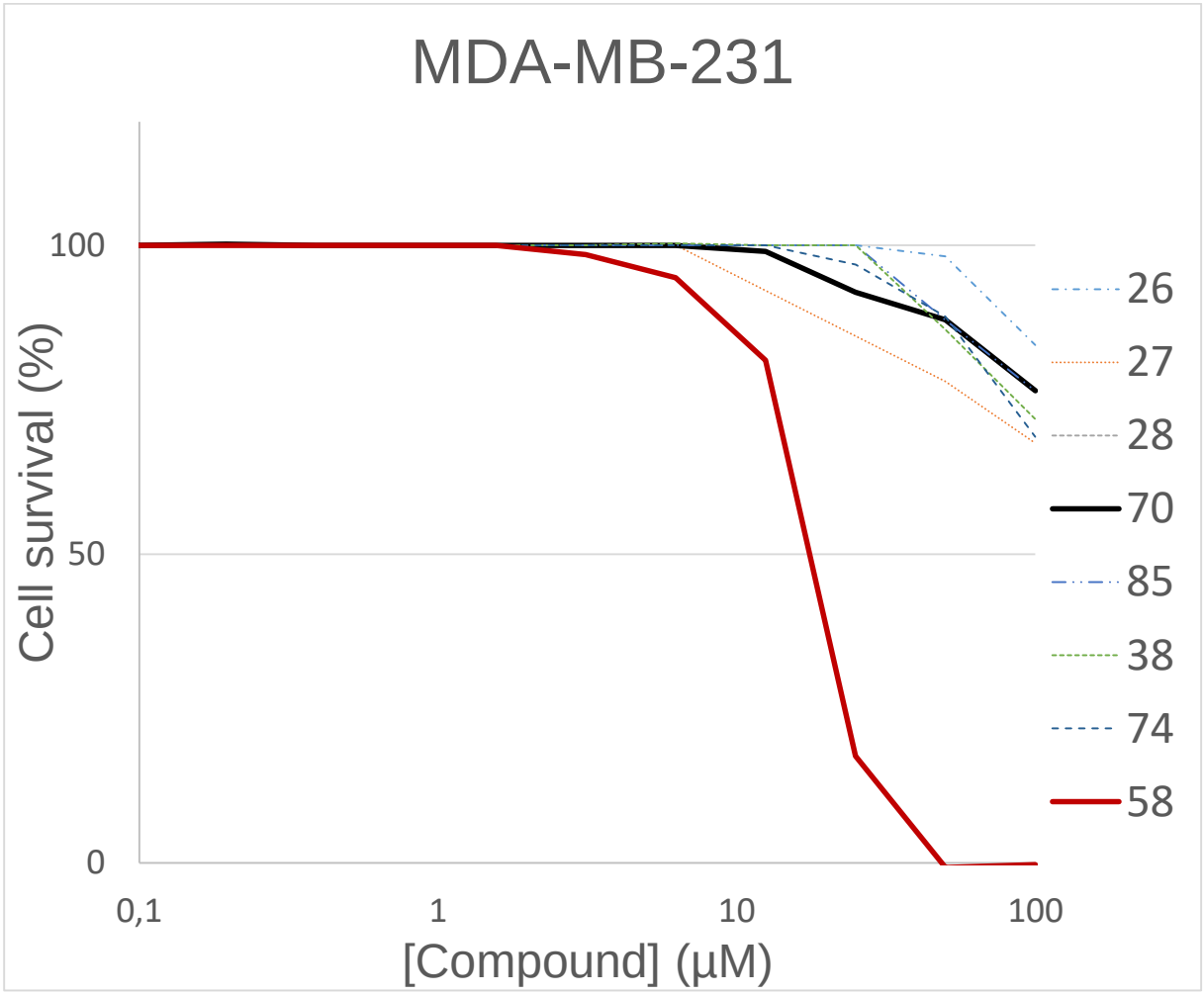


Figure S5. Dose-Response Plots of Compounds against MDA-MB-231

2.6. Gioblastoma (U87MG)

Table S6. Dose-Dependent Effect of Compounds on the in vitro growth of U87MG cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100	100	100	100	99,7582949	100	98,3520105	95,71522742	90,3537684	>100
27	100,00	100	100	100	100	98,676386	100	96,9457262	81,2129202	70,05053834	60,3823336	>100
28												
70	100	99,9033816	100	100	100	100	95,8031202	83,6739178	71,1052516	55,1087673	50,8020215	>100
85	100	100	99,3318486	99,4209354	100	100	100	100	87,3942094	78,21826281	64,4988864	>100
38	100	100	100,311943	100	100	100	100	100	100	93,40463458	70,5882353	>100
74	100	100	100	100	99,5479204	100	100	100	100	99,27667269	99,2766727	>100
58	100	100	100	100	100	100	100	94,2940039	66,827853	0	2,51450677	34,78 ± 5,05

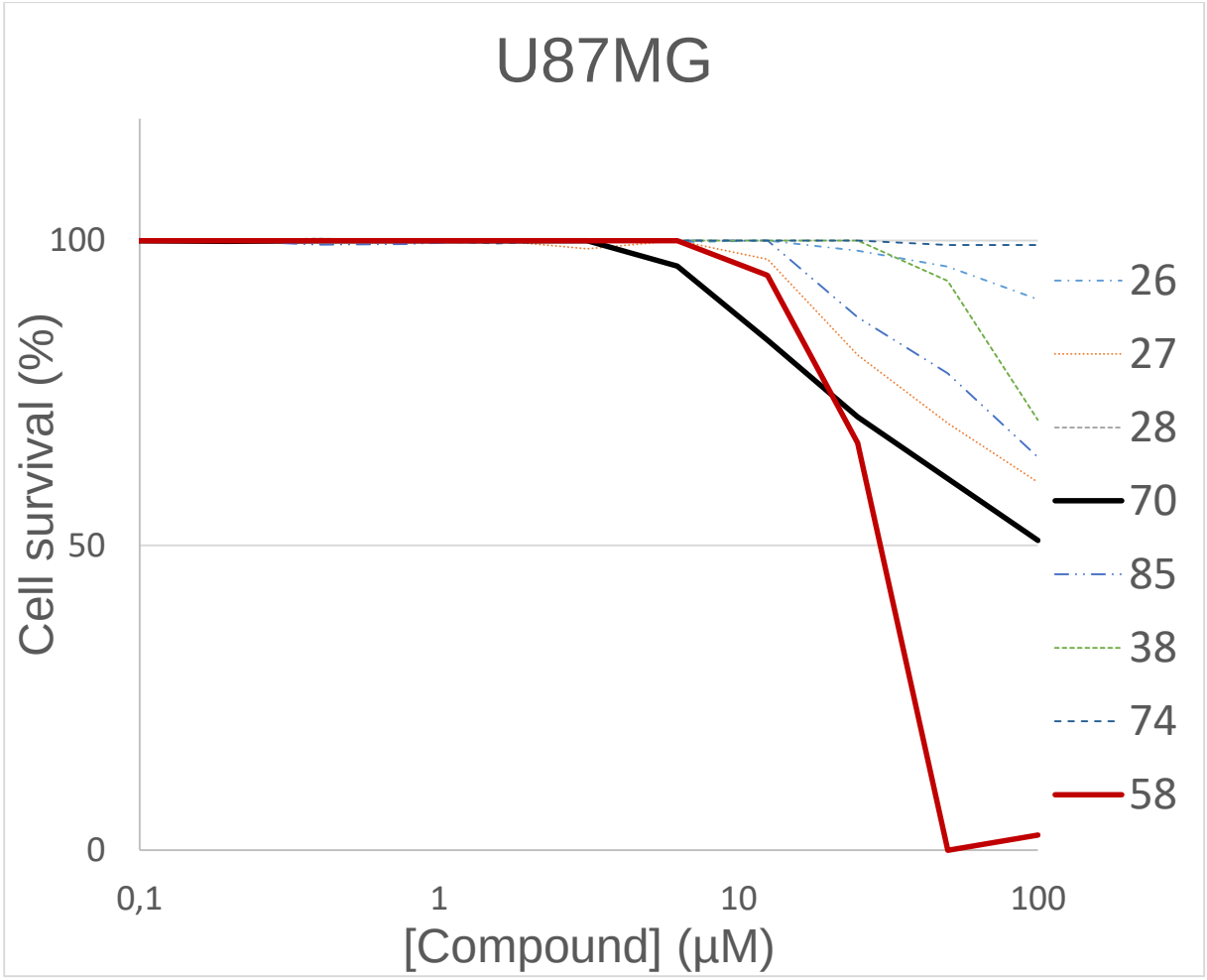


Figure S6. Dose-Response Plots of Compounds against U87MG

2.7. Hepatocellular carcinoma (HepG2)

Table S7. Dose-Dependent Effect of Compounds on the in vitro growth of HepG2 cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100	100	100	100	100	90,2874903	82,7505828	75,05827506	66,045066	>100
27	100	100	100	100	100	100	100	93,26788219	85,8345021	79,66339411	72,3702665	>100
28												
70	100	100	100	100	100	100	89,5380435	78,125	68,2065217	58,9673913	52,7173913	>100
85	100	100	100	100	100	100	100	100	95,9883297	90,59080963	86,7250182	>100
38	100	100	100	99,7361478	100	100	100	100	100	100	100	>100
74	100	100	100	100	100	100	100	100	100	100	100	>100
58	100	100	100	100	100	100	98,31081081	89,07657658	22,63513514	4,954954955	11,26126126	18,96 ±1,51

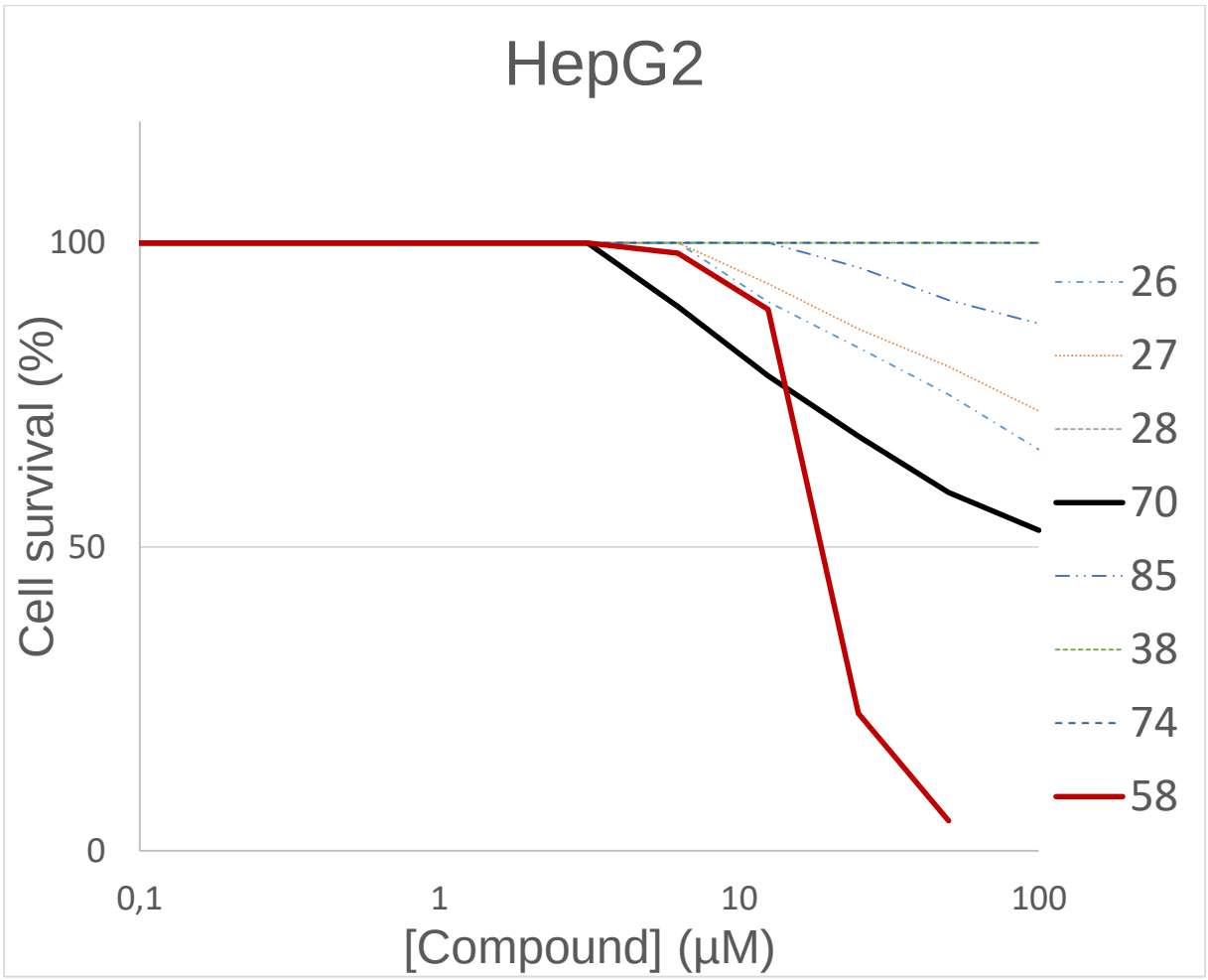


Figure S7. Dose-Response Plots of Compounds against HepG2

2.8. Colorectal adenocarcinoma (HT-29)

Table S8. Dose-Dependent Effect of Compounds on the in vitro growth of HT-29 cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100	100	100	100	100	100	100	100	95,4700855	>100
27	100	100	100	100	100	100	100	100	100	96,520251	64,346834	>100
28												
70	100	100	100	100	100	100	100	100	99,5415473	95,07163324	61,7765043	>100
85	100	100	100	100	100	100	100	100	100,083822	97,82062028	82,9840738	>100
38	100	100	100	100	100	100	100	100	100	96,05700713	73,0166271	>100
74	100	100	100	100	100	100	100	100	100	100	94,0695297	>100
58	100	100	100	100	95,9193471	92,1267403	78,6845895	45,8953433	2,59241479	2,400384061	6,24099856	13,35 ± 0,59

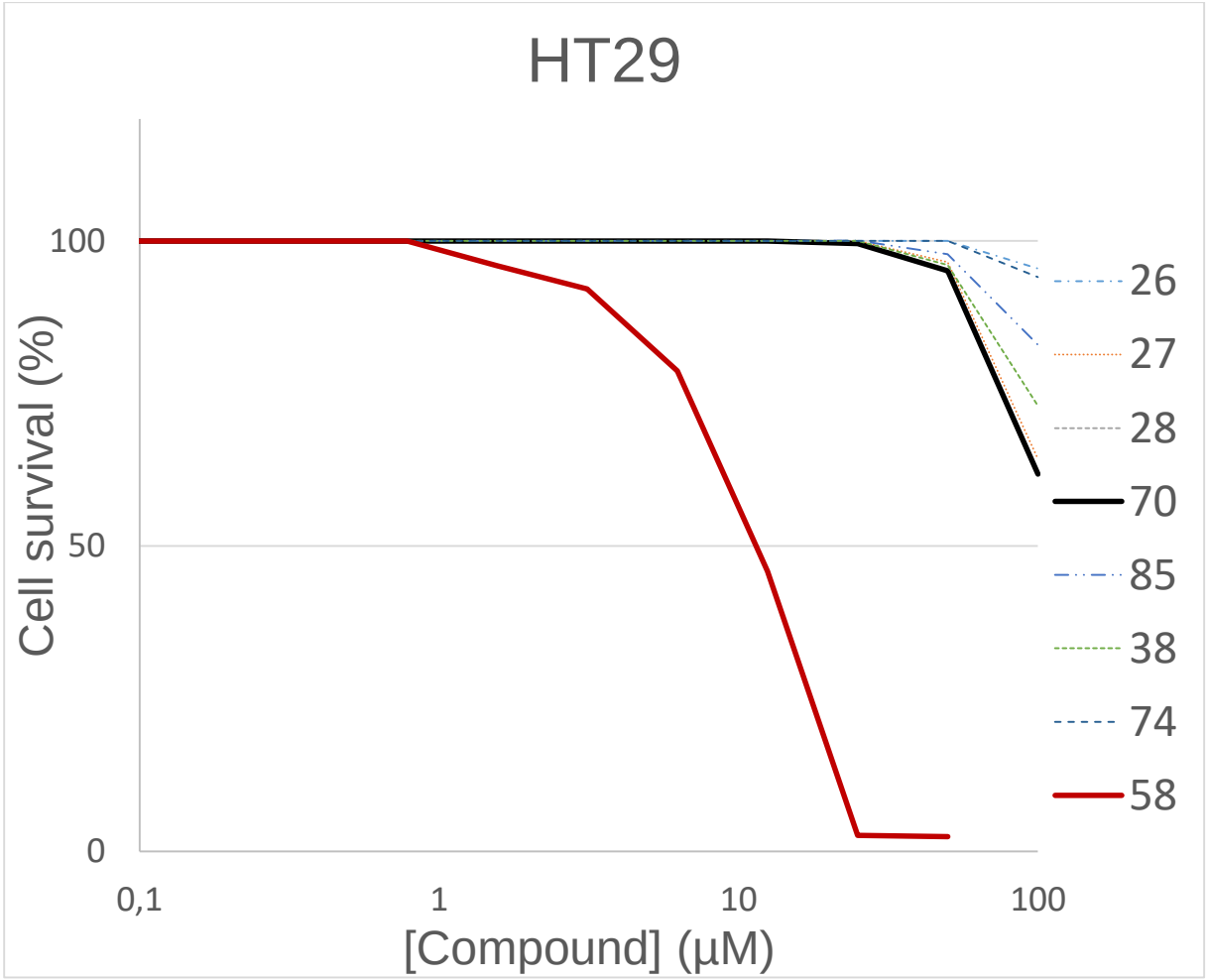


Figure S8. Dose-Response Plots of Compounds against HT-29

2.9. Osteosarcoma (U2OS)

Table S9. Dose-Dependent Effect of Compounds on the in vitro growth of U2OS cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100	100	100	100	99,8296422	100	100	100	93,6967632	>100
27	100	100	100	100	100	100	100	100	100	100	100	>100
28												
70	100	100	100	100	100	100	100	90,4214559	79,3867121	74,61669506	61,3287905	>100
85	100	100	100	100	100	100	100	100	100	100	97,4820144	>100
38	100	100	100,656455	100	100,875274	100,547046	100	96,3894967	94,4201313	86,76148796	72,2100656	>100
74	100	100	99,5618839	100	100	100	99,890471	100	100	100	91,6666667	>100
58	100	100	100	100	100	100	87,6033058	68,1818182	0		7,02479339	12,94 ± 3,11

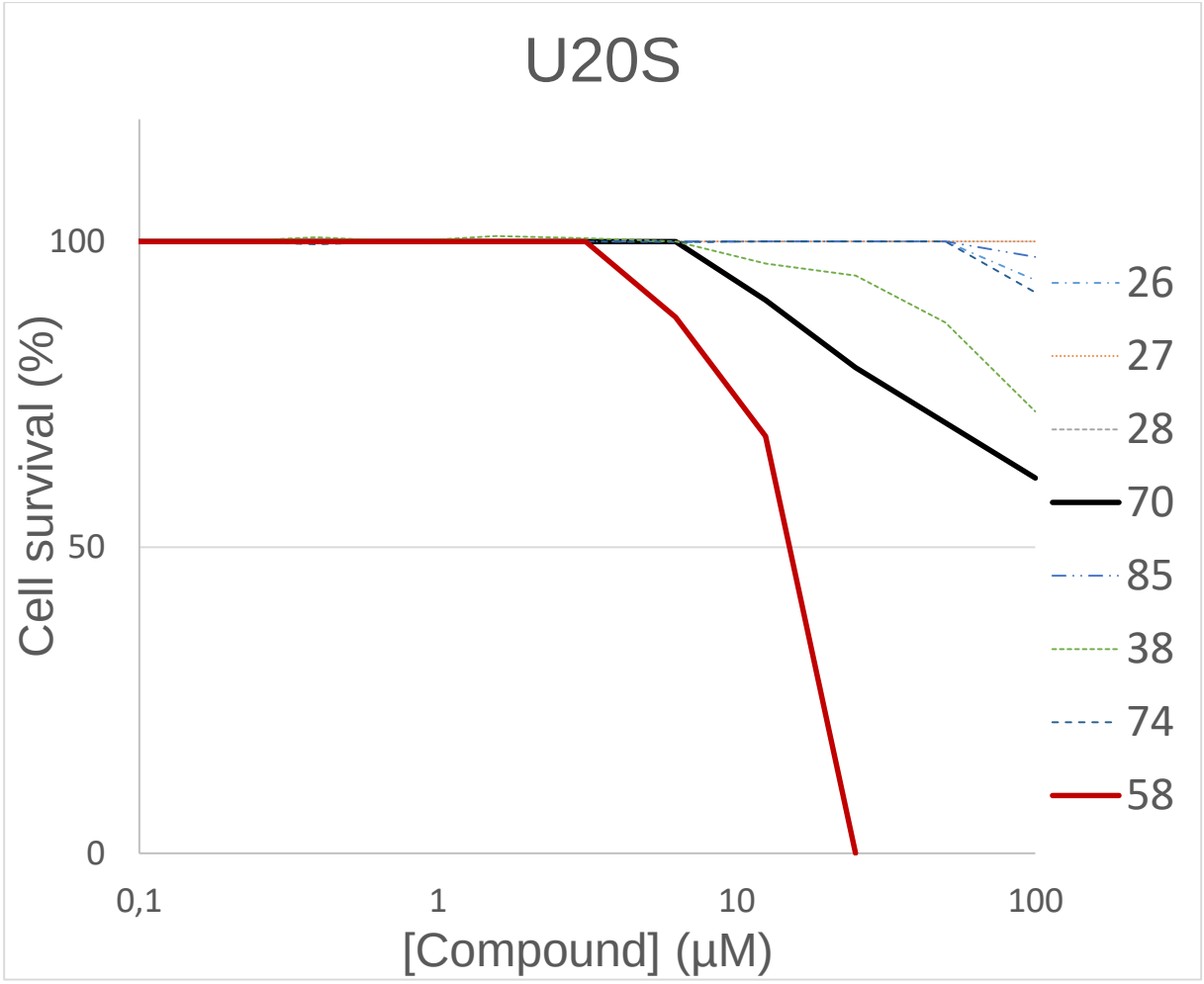


Figure S9. Dose-Response Plots of Compounds against U2OS

2.10. Non-transformed bovine aortic endothelial cells (BAEC)

Table S10. Dose-Dependent Effect of Compounds on the in vitro growth of BAEC cells

	0,09765625	0,1953125	0,390625	0,78125	1,5625	3,125	6,25	12,5	25	50	100	ic50
26	100	100	100,00	100,00	100,00	95,39828626	84,18491484	80,03808315	74,86512218	66,75129588	60,58394161	>100
27	100	100,00	100,00	100,00	100,00	100,00	89,81	74,42145351	63,21802602	46,6201206	36,36940654	43,8 ± 1,2
28	100	100	100	100	100	100	93,0649427	84,01586835	77,0790479	66,61416397	50,39670879	>100
70	100	100	100	100	100	96,70878636	88,06935057	79,07728475	72,61240082	60,15280635	35,3217749	69,12 ± 12,5
85	100,00	100	100,492611	100	100	100	100	100	94,13434248	82,25953958	63,10312204	>100
38	98,90829694	100	100	100	100	100	100	100	96,55620533	90,64327485	85,93957115	>100
74	100	100	100	100	100	100	100	94,6410516	87,6980115	70,98078868	57,16211662	>100
58	100	100	100	100	100	95,44994944	87,61375126	67,64408493	9,757330637	0,000000000	1,971688574	18,1 ± 2,2

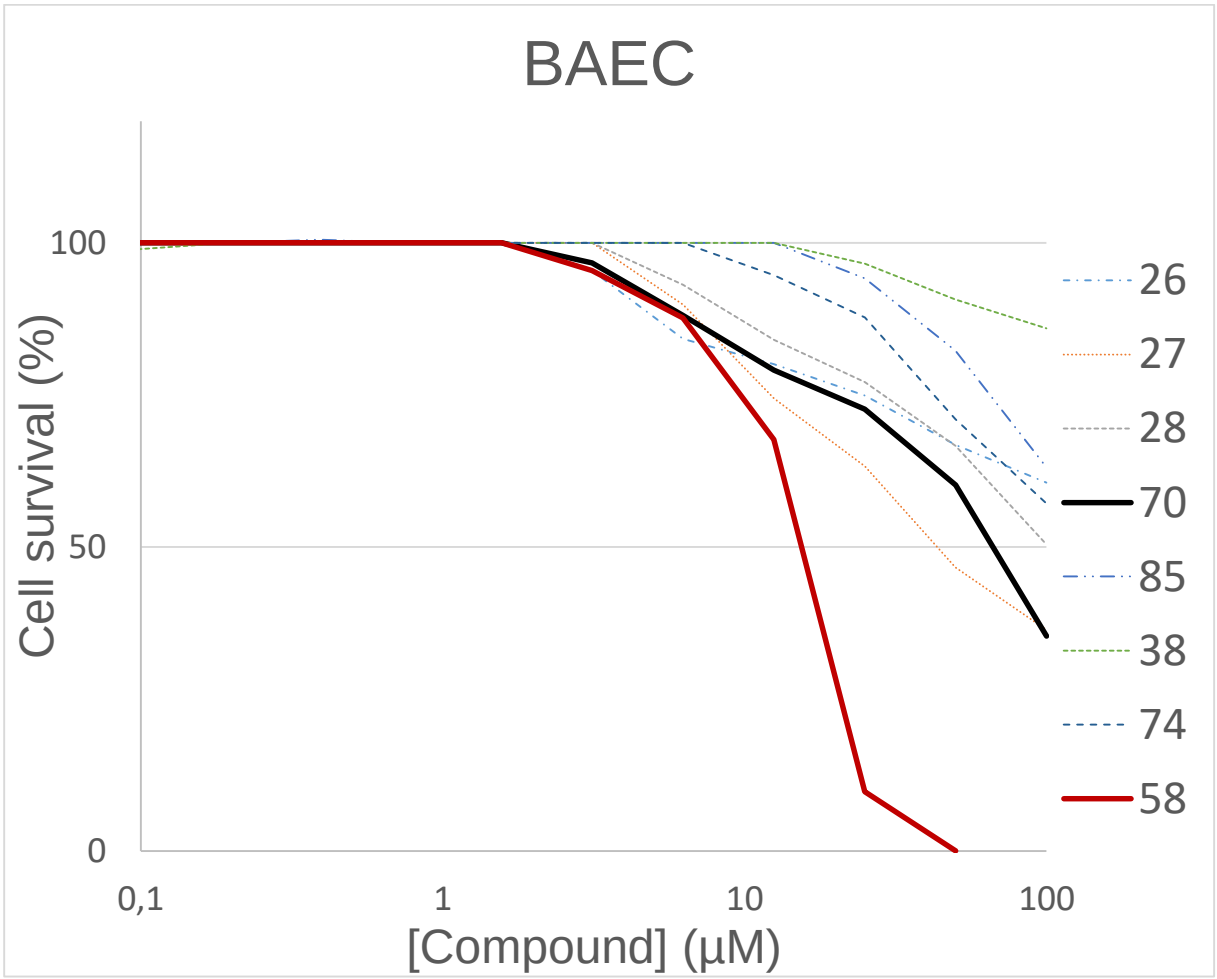


Figure S10. Dose-Response Plots of Compounds against BAEC

3. Theoretical Calculations

Minimum energy conformations were calculated in vacuo using the PM3 method found in HyperChem 5.0 software. Optimization was performed using Polak-Ribiere algorithm until the RMS gradient reached a value below 0.001 kcal/(Å·mol).

The resulting minimum-energy conformations for compounds **27**, **28**, **58** and **70** are contained in the following .mol files:

Compound 27:

Table S11. Optimized Coordinates for **27**

```
 58 60  0  0  0  0  0  0  0  0999 V2000
  -0.8613    1.8384    1.0385 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.1404    1.6973    0.5259 C   0  0  0  0  0  0  0  0  0  0  0  0
  -2.6545    0.3990    0.3587 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.8962   -0.7217    0.6968 C   0  0  0  0  0  0  0  0  0  0  0  0
  -0.5795   -0.5720    1.1861 C   0  0  0  0  0  0  0  0  0  0  0  0
  -0.0604    0.7376    1.3738 C   0  0  0  0  0  0  0  0  0  0  0  0
  -3.9373    0.3464   -0.1478 O   0  0  0  0  0  0  0  0  0  0  0  0
  -4.4524   -0.9376   -0.5140 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.0056   -1.6929    0.6490 C   0  0  0  0  0  0  0  0  0  0  0  0
  -4.5813   -2.9996    0.9133 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.1452   -3.7154    1.9690 C   0  0  0  0  0  0  0  0  0  0  0  0
  -6.1252   -3.1292    2.7697 C   0  0  0  0  0  0  0  0  0  0  0  0
  -6.5412   -1.8220    2.5162 C   0  0  0  0  0  0  0  0  0  0  0  0
  -5.9848   -1.1058    1.4580 C   0  0  0  0  0  0  0  0  0  0  0  0
   1.2792    1.0313    1.9588 C   0  0  0  0  0  0  0  0  0  0  0  0
   2.3733    1.2797    0.9872 C   0  0  0  0  0  0  0  0  0  0  0  0
   2.2484    1.4062   -0.3376 C   0  0  0  0  0  0  0  0  0  0  0  0
   0.2122   -1.6961    1.4842 N   0  0  0  0  0  0  0  0  0  0  0  0
  -0.0402   -3.0147    1.1455 C   0  0  0  0  0  0  0  0  0  0  0  0
  -1.0646   -3.4122    0.5644 O   0  0  0  0  0  0  0  0  0  0  0  0
   1.0894   -4.0270    1.5163 C   0  0  0  0  0  0  0  0  0  0  0  0
   2.2999   -3.7326    0.7887 N   0  0  0  0  0  0  0  0  0  0  0  0
   0.5739   -5.4402    1.2628 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.1866   -2.7756    1.2326 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.1171   -2.3000    2.3838 O   0  0  0  0  0  0  0  0  0  0  0  0
   4.2354   -2.2661    0.2336 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.6151   -1.3107   -0.6458 N   0  0  0  0  0  0  0  0  0  0  0  0
   3.3945    1.7042   -1.2339 C   0  0  0  0  0  0  0  0  0  0  0  0
   3.6872    0.5928   -2.2247 C   0  0  0  0  0  0  0  0  0  0  0  0
   4.3666   -0.5972   -1.5711 C   0  0  0  0  0  0  0  0  0  0  0  0
   5.5185   -0.9542   -1.8786 O   0  0  0  0  0  0  0  0  0  0  0  0
  -0.4546    2.8522    1.1873 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.7537    2.5685    0.2603 H   0  0  0  0  0  0  0  0  0  0  0  0
  -2.3421   -1.7250    0.5974 H   0  0  0  0  0  0  0  0  0  0  0  0
  -5.2862   -0.6640   -1.2224 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.6759   -1.5322   -1.0634 H   0  0  0  0  0  0  0  0  0  0  0  0
  -3.7904   -3.4611    0.2990 H   0  0  0  0  0  0  0  0  0  0  0  0
  -4.8108   -4.7434    2.1715 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.5674   -3.6957    3.6023 H   0  0  0  0  0  0  0  0  0  0  0  0
  -7.3085   -1.3551    3.1508 H   0  0  0  0  0  0  0  0  0  0  0  0
  -6.3031   -0.0719    1.2553 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.6122    0.2232    2.6681 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.1872    1.9609    2.5957 H   0  0  0  0  0  0  0  0  0  0  0  0
   3.3642    1.3850    1.4669 H   0  0  0  0  0  0  0  0  0  0  0  0
   1.0390   -1.5203    2.0192 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  1.3078   -3.9125    2.6230 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.3450   -4.0333   -0.1574 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.3133   -5.5862    0.1869 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.3402   -6.1934    1.5637 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.3521   -5.5948    1.8679 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.6708   -3.1053   -0.3785 H   0  0  0  0  0  0  0  0  0  0  0  0
  5.0760   -1.8014    0.8265 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.7980   -0.8584   -0.2922 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.3215    1.9214   -0.6375 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.1519    2.6361   -1.8166 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.3819    0.9763   -3.0191 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.7412    0.2568   -2.7247 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.2673    1.3100   -0.8330 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  4  0  0  0  0
 1  6  4  0  0  0  0
 1 32  1  0  0  0  0
 2  3  4  0  0  0  0
 2 33  1  0  0  0  0
 3  4  4  0  0  0  0
 3  7  1  0  0  0  0
 4  5  4  0  0  0  0
 4 34  1  0  0  0  0
 5  6  4  0  0  0  0
 5 18  1  0  0  0  0
 6 15  1  0  0  0  0
 7  8  1  0  0  0  0
 8  9  1  0  0  0  0
 8 35  1  0  0  0  0
 8 36  1  0  0  0  0
 9 10  4  0  0  0  0
 9 14  4  0  0  0  0
10 11  4  0  0  0  0
10 37  1  0  0  0  0
11 12  4  0  0  0  0
11 38  1  0  0  0  0
12 13  4  0  0  0  0
12 39  1  0  0  0  0
13 14  4  0  0  0  0
13 40  1  0  0  0  0
14 41  1  0  0  0  0
15 16  1  0  0  0  0
15 42  1  0  0  0  0
15 43  1  0  0  0  0
16 17  2  0  0  0  0
16 44  1  0  0  0  0
17 28  1  0  0  0  0
17 58  1  0  0  0  0
18 19  1  0  0  0  0
18 45  1  0  0  0  0
19 20  2  0  0  0  0
19 21  1  0  0  0  0
21 22  1  0  0  0  0
21 23  1  0  0  0  0
21 46  1  0  0  0  0
22 24  1  0  0  0  0
22 47  1  0  0  0  0
23 48  1  0  0  0  0
23 49  1  0  0  0  0
23 50  1  0  0  0  0
24 25  2  0  0  0  0
24 26  1  0  0  0  0
26 27  1  0  0  0  0
26 51  1  0  0  0  0
```

```
 26 52  1  0  0  0  0
 27 30  1  0  0  0  0
 27 53  1  0  0  0  0
 28 29  1  0  0  0  0
 28 54  1  0  0  0  0
 28 55  1  0  0  0  0
 29 30  1  0  0  0  0
 29 56  1  0  0  0  0
 29 57  1  0  0  0  0
 30 31  2  0  0  0  0
M  END
```

Compound 28:

Table S12. Optimized Coordinates for **28**

```
 62 64  0  0  0  0  0  0  0  0999 V2000
   -1.5482    2.2310    1.1603 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7819    1.9721    0.5861 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1469    0.6330    0.3587 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2897   -0.4123    0.7024 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.0199   -0.1399    1.2577 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6497    1.2103    1.5012 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.3936    0.4616   -0.2077 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7425   -0.8536   -0.6520 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.2581   -1.7191    0.4498 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.7079   -2.9860    0.6727 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.2336   -3.8088    1.6683 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.3014   -3.3691    2.4505 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.8439   -2.1014    2.2386 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.3256   -1.2789    1.2401 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.6296    1.6202    2.1474 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7335    1.9889    1.2256 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.6259    2.2299   -0.0840 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1297   -1.1835    1.5688 N   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2021   -2.5008    1.1481 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.1308   -2.9761    0.4727 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.0115   -3.3958    1.5529 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.2263   -2.9185    0.9377 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.6895   -4.8412    1.1871 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.9514   -1.8845    1.4890 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7391   -1.4781    2.6492 O   0  0  0  0  0  0  0  0  0  0  0  0
    4.0011   -1.2050    0.5984 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.3390   -0.3209   -0.3225 N   0  0  0  0  0  0  0  0  0  0  0  0
    2.7873    2.6590   -0.9269 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.2844    1.5872   -1.9123 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.0598    0.5022   -1.1736 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.2794    0.3304   -1.3521 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.2593    3.2768    1.3552 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.4728    2.7819    0.3162 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6193   -1.4541    0.5539 H   0  0  0  0  0  0  0  0  0  0  0  0
   -5.5690   -0.6420   -1.3895 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8790   -1.3314   -1.1853 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.8493   -3.3309    0.0731 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8002   -4.8053    1.8381 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7133   -4.0198    3.2356 H   0  0  0  0  0  0  0  0  0  0  0  0
   -7.6813   -1.7499    2.8588 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7442   -0.2751    1.0705 H   0  0  0  0  0  0  0  0  0  0  0  0
    1.0079    0.8353    2.8600 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.4255    2.5270    2.7912 H   0  0  0  0  0  0  0  0  0  0  0  0
    2.7114    2.0864    1.7338 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.6249   -0.9478    2.1816 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
  1.1353   -3.3234    2.6776 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.3837   -3.1696   -0.0108 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.5249   -4.9508    0.0880 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.5177   -5.5171    1.5068 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.2515   -5.1390    1.7099 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.6054   -1.9604    0.0208 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.7103   -0.6418    1.2723 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.4168   -0.0284   -0.0804 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.6535    2.9663   -0.2689 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.4261    3.7720   -1.7429 O   0  0  0  0  0  0  0  0  0  0  0  0
  4.0258    2.0962   -2.5973 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.1709    1.0149   -2.7571 C   0  0  0  0  0  0  0  0  0  0  0  0
  0.6627    2.1526   -0.6159 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.0175    4.4240   -1.1615 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.6804    1.8457   -3.3228 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.3938    0.5114   -2.1333 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.5803    0.2737   -3.4850 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  4  0  0  0  0
 1  6  4  0  0  0  0
 1 32  1  0  0  0  0
 2  3  4  0  0  0  0
 2 33  1  0  0  0  0
 3  4  4  0  0  0  0
 3  7  1  0  0  0  0
 4  5  4  0  0  0  0
 4 34  1  0  0  0  0
 5  6  4  0  0  0  0
 5 18  1  0  0  0  0
 6 15  1  0  0  0  0
 7  8  1  0  0  0  0
 8  9  1  0  0  0  0
 8 35  1  0  0  0  0
 8 36  1  0  0  0  0
 9 10  4  0  0  0  0
 9 14  4  0  0  0  0
10 11  4  0  0  0  0
10 37  1  0  0  0  0
11 12  4  0  0  0  0
11 38  1  0  0  0  0
12 13  4  0  0  0  0
12 39  1  0  0  0  0
13 14  4  0  0  0  0
13 40  1  0  0  0  0
14 41  1  0  0  0  0
15 16  1  0  0  0  0
15 42  1  0  0  0  0
15 43  1  0  0  0  0
16 17  2  0  0  0  0
16 44  1  0  0  0  0
17 28  1  0  0  0  0
17 58  1  0  0  0  0
18 19  1  0  0  0  0
18 45  1  0  0  0  0
19 20  2  0  0  0  0
19 21  1  0  0  0  0
21 22  1  0  0  0  0
21 23  1  0  0  0  0
21 46  1  0  0  0  0
22 24  1  0  0  0  0
22 47  1  0  0  0  0
23 48  1  0  0  0  0
23 49  1  0  0  0  0
23 50  1  0  0  0  0
```

```
 24 25  2  0  0  0  0
 24 26  1  0  0  0  0
 26 27  1  0  0  0  0
 26 51  1  0  0  0  0
 26 52  1  0  0  0  0
 27 30  1  0  0  0  0
 27 53  1  0  0  0  0
 28 29  1  0  0  0  0
 28 54  1  0  0  0  0
 28 55  1  0  0  0  0
 29 30  1  0  0  0  0
 29 56  1  0  0  0  0
 29 57  1  0  0  0  0
 30 31  2  0  0  0  0
 55 59  1  0  0  0  0
 57 60  1  0  0  0  0
 57 61  1  0  0  0  0
 57 62  1  0  0  0  0
M  END
```

Compound 70:

Table S13. Optimized Coordinates for **70**

```
 58 60  0  0  0  0  0  0  0  0999 V2000
   -1.2823    1.1922    1.1258 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.5345    0.8480    1.6112 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0193   -0.4521    1.3771 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.2490   -1.4001    0.6997 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9692   -1.0466    0.2246 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4950    0.2800    0.4127 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.2817   -0.6905    1.8815 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8265   -1.9926    1.6153 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.2065   -2.0328    2.1833 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7194   -3.2572    2.6283 C   0  0  0  0  0  0  0  0  0  0  0  0
   -8.0187   -3.3294    3.1264 C   0  0  0  0  0  0  0  0  0  0  0  0
   -8.8094   -2.1816    3.1905 C   0  0  0  0  0  0  0  0  0  0  0  0
   -8.2981   -0.9599    2.7539 C   0  0  0  0  0  0  0  0  0  0  0  0
   -7.0004   -0.8839    2.2490 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7621    0.7141   -0.1786 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7010    1.4289    0.4533 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.9375    1.8924   -0.2241 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.1291   -1.9932   -0.3921 N   0  0  0  0  0  0  0  0  0  0  0  0
   -0.5424   -3.0788   -1.1383 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7390   -3.3396   -1.3591 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.5699   -4.0293   -1.6672 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.6631   -3.3462   -2.3150 N   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0820   -5.0702   -2.5759 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7530   -2.8862   -1.6122 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7893   -2.9641   -0.3645 O   0  0  0  0  0  0  0  0  0  0  0  0
    3.9343   -2.3043   -2.4088 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.7086   -1.3675   -1.6493 N   0  0  0  0  0  0  0  0  0  0  0  0
    4.1623    1.1301    0.2566 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1777    0.9417   -0.8538 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.6421   -0.0009   -1.9159 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.1989    0.4184   -3.0020 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.8978    2.2120    1.2870 H   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1529    1.5680    2.1642 H   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6327   -2.4163    0.5194 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8605   -2.1607    0.5039 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1717   -2.7689    2.0954 H   0  0  0  0  0  0  0  0  0  0  0  0
```

```
 -6.0963   -4.1627    2.5841 H   0  0  0  0  0  0  0  0  0  0  0  0
 -8.4195   -4.2935    3.4721 H   0  0  0  0  0  0  0  0  0  0  0  0
 -9.8336   -2.2407    3.5862 H   0  0  0  0  0  0  0  0  0  0  0  0
 -8.9181   -0.0530    2.8064 H   0  0  0  0  0  0  0  0  0  0  0  0
 -6.5898    0.0791    1.9079 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.5990    1.7088    1.5138 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.8490   -1.8564   -0.2413 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.9828   -4.5524   -0.7473 H   0  0  0  0  0  0  0  0  0  0  0  0
  1.6090   -3.2157   -3.2966 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.5430   -4.5886   -3.4714 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.6690   -5.8260   -2.9070 H   0  0  0  0  0  0  0  0  0  0  0  0
 -0.8930   -5.5844   -2.0045 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.5784   -1.8123   -3.3594 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.5945   -3.1801   -2.6782 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.8851   -1.6364   -0.7041 H   0  0  0  0  0  0  0  0  0  0  0  0
  4.6489    1.6929    1.0961 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.8588    0.1302    0.6657 H   0  0  0  0  0  0  0  0  0  0  0  0
  6.1388    0.5487   -0.4310 H   0  0  0  0  0  0  0  0  0  0  0  0
  5.3942    1.9249   -1.3496 H   0  0  0  0  0  0  0  0  0  0  0  0
  3.0777    2.9889   -0.0239 H   0  0  0  0  0  0  0  0  0  0  0  0
  2.8361    1.7766   -1.3393 H   0  0  0  0  0  0  0  0  0  0  0  0
  0.8937    0.4376   -1.2414 H   0  0  0  0  0  0  0  0  0  0  0  0
 1  2  4  0  0  0  0
 1  6  4  0  0  0  0
 1 32  1  0  0  0  0
 2  3  4  0  0  0  0
 2 33  1  0  0  0  0
 3  4  4  0  0  0  0
 3  7  1  0  0  0  0
 4  5  4  0  0  0  0
 4 34  1  0  0  0  0
 5  6  4  0  0  0  0
 5 18  1  0  0  0  0
 6 15  1  0  0  0  0
 7  8  1  0  0  0  0
 8  9  1  0  0  0  0
 8 35  1  0  0  0  0
 8 36  1  0  0  0  0
 9 10  4  0  0  0  0
 9 14  4  0  0  0  0
10 11  4  0  0  0  0
10 37  1  0  0  0  0
11 12  4  0  0  0  0
11 38  1  0  0  0  0
12 13  4  0  0  0  0
12 39  1  0  0  0  0
13 14  4  0  0  0  0
13 40  1  0  0  0  0
14 41  1  0  0  0  0
15 16  2  0  0  0  0
15 58  1  0  0  0  0
16 17  1  0  0  0  0
16 42  1  0  0  0  0
17 28  1  0  0  0  0
17 56  1  0  0  0  0
17 57  1  0  0  0  0
18 19  1  0  0  0  0
18 43  1  0  0  0  0
19 20  2  0  0  0  0
19 21  1  0  0  0  0
21 22  1  0  0  0  0
21 23  1  0  0  0  0
21 44  1  0  0  0  0
```

```
 22 24  1  0  0  0  0
 22 45  1  0  0  0  0
 23 46  1  0  0  0  0
 23 47  1  0  0  0  0
 23 48  1  0  0  0  0
 24 25  2  0  0  0  0
 24 26  1  0  0  0  0
 26 27  1  0  0  0  0
 26 49  1  0  0  0  0
 26 50  1  0  0  0  0
 27 30  1  0  0  0  0
 27 51  1  0  0  0  0
 28 29  1  0  0  0  0
 28 52  1  0  0  0  0
 28 53  1  0  0  0  0
 29 30  1  0  0  0  0
 29 54  1  0  0  0  0
 29 55  1  0  0  0  0
 30 31  2  0  0  0  0
M  END
```

Compound 58:

Table S14. Optimized Coordinates for **58**

```
 62 64  0  0  0  0  0  0  0  0999 V2000
   -4.2131    1.0331   -0.6592 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4161    0.5634   -0.1572 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4591   -0.7327    0.3903 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.3230   -1.5435    0.4160 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.1018   -1.0645   -0.1022 C   0  0  0  0  0  0  0  0  0  0  0  0
   -3.0480    0.2566   -0.6283 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.7011   -1.1178    0.8509 O   0  0  0  0  0  0  0  0  0  0  0  0
   -6.8115   -2.3820    1.5124 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.3031   -2.3501    2.9155 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.2552   -3.1851    3.3169 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.8239   -3.1740    4.6436 C   0  0  0  0  0  0  0  0  0  0  0  0
   -5.4301   -2.3280    5.5715 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.4695   -1.4872    5.1721 C   0  0  0  0  0  0  0  0  0  0  0  0
   -6.9056   -1.4984    3.8489 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.8168    0.8388   -1.1479 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.6776    0.9161   -0.4478 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.5821    1.4549   -1.0123 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.9490   -1.8665   -0.1499 N   0  0  0  0  0  0  0  0  0  0  0  0
   -1.7480   -3.0966    0.4490 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6096   -3.7010    1.1118 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.3781   -3.7925    0.2137 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.7622   -2.9290    0.3890 N   0  0  0  0  0  0  0  0  0  0  0  0
   -0.4410   -4.4450   -1.1672 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.6031   -3.0596    1.4774 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.3208   -3.7646    2.4633 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.9511   -2.3170    1.4341 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.8882   -0.9070    1.2156 N   0  0  0  0  0  0  0  0  0  0  0  0
    1.5992    1.8236    0.0689 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.9732    1.1653   -0.1522 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.8390   -0.3499   -0.0478 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.7050   -1.0794   -1.0531 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.1628    2.0482   -1.0843 H   0  0  0  0  0  0  0  0  0  0  0  0
   -6.3255    1.1787   -0.1753 H   0  0  0  0  0  0  0  0  0  0  0  0
   -4.3765   -2.5489    0.8627 H   0  0  0  0  0  0  0  0  0  0  0  0
   -7.9273   -2.5467    1.5108 H   0  0  0  0  0  0  0  0  0  0  0  0
```

-6.3187 -3.1879 0.9083 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.7525 -3.8419 2.5871 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.9973 -3.8309 4.9527 H 0 0 0 0 0 0 0 0 0 0 0 0
-5.0870 -2.3206 6.6163 H 0 0 0 0 0 0 0 0 0 0 0 0
-6.9448 -0.8145 5.9005 H 0 0 0 0 0 0 0 0 0 0 0 0
-7.7199 -0.8326 3.5256 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.6327 0.5568 0.5945 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.1748 -1.4637 -0.6337 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.3338 -4.6072 1.0058 H 0 0 0 0 0 0 0 0 0 0 0 0
1.1094 -2.4625 -0.4218 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.4786 -3.6801 -1.9796 H 0 0 0 0 0 0 0 0 0 0 0 0
0.4511 -5.0961 -1.3300 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.3606 -5.0766 -1.2257 H 0 0 0 0 0 0 0 0 0 0 0 0
3.5645 -2.7950 0.6144 H 0 0 0 0 0 0 0 0 0 0 0 0
3.4521 -2.5085 2.4269 H 0 0 0 0 0 0 0 0 0 0 0 0
2.8447 -0.3163 2.0114 H 0 0 0 0 0 0 0 0 0 0 0 0
1.7575 3.2260 0.1887 O 0 0 0 0 0 0 0 0 0 0 0 0
1.2221 1.5219 1.0910 H 0 0 0 0 0 0 0 0 0 0 0 0
3.6497 1.5439 0.6684 H 0 0 0 0 0 0 0 0 0 0 0 0
3.6045 1.5336 -1.4766 C 0 0 0 0 0 0 0 0 0 0 0 0
0.3677 2.3588 -1.6443 H 0 0 0 0 0 0 0 0 0 0 0 0
1.0242 0.6715 -1.6911 H 0 0 0 0 0 0 0 0 0 0 0 0
1.9879 3.5738 -0.6818 H 0 0 0 0 0 0 0 0 0 0 0 0
2.9884 1.1641 -2.3319 H 0 0 0 0 0 0 0 0 0 0 0 0
3.7114 2.6425 -1.5533 H 0 0 0 0 0 0 0 0 0 0 0 0
4.6183 1.0716 -1.5577 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.8853 1.2427 -2.1733 H 0 0 0 0 0 0 0 0 0 0 0 0
1 2 4 0 0 0 0
1 6 4 0 0 0 0
1 32 1 0 0 0 0
2 3 4 0 0 0 0
2 33 1 0 0 0 0
3 4 4 0 0 0 0
3 7 1 0 0 0 0
4 5 4 0 0 0 0
4 34 1 0 0 0 0
5 6 4 0 0 0 0
5 18 1 0 0 0 0
6 15 1 0 0 0 0
7 8 1 0 0 0 0
8 9 1 0 0 0 0
8 35 1 0 0 0 0
8 36 1 0 0 0 0
9 10 4 0 0 0 0
9 14 4 0 0 0 0
10 11 4 0 0 0 0
10 37 1 0 0 0 0
11 12 4 0 0 0 0
11 38 1 0 0 0 0
12 13 4 0 0 0 0
12 39 1 0 0 0 0
13 14 4 0 0 0 0
13 40 1 0 0 0 0
14 41 1 0 0 0 0
15 16 2 0 0 0 0
15 62 1 0 0 0 0
16 17 1 0 0 0 0
16 42 1 0 0 0 0
17 28 1 0 0 0 0
17 56 1 0 0 0 0
17 57 1 0 0 0 0
18 19 1 0 0 0 0
18 43 1 0 0 0 0

```
 19 20  2  0  0  0  0
 19 21  1  0  0  0  0
 21 22  1  0  0  0  0
 21 23  1  0  0  0  0
 21 44  1  0  0  0  0
 22 24  1  0  0  0  0
 22 45  1  0  0  0  0
 23 46  1  0  0  0  0
 23 47  1  0  0  0  0
 23 48  1  0  0  0  0
 24 25  2  0  0  0  0
 24 26  1  0  0  0  0
 26 27  1  0  0  0  0
 26 49  1  0  0  0  0
 26 50  1  0  0  0  0
 27 30  1  0  0  0  0
 27 51  1  0  0  0  0
 28 29  1  0  0  0  0
 28 52  1  0  0  0  0
 28 53  1  0  0  0  0
 29 30  1  0  0  0  0
 29 54  1  0  0  0  0
 29 55  1  0  0  0  0
 30 31  2  0  0  0  0
 52 58  1  0  0  0  0
 55 59  1  0  0  0  0
 55 60  1  0  0  0  0
 55 61  1  0  0  0  0
M  END
```

Table S15. Energies of Computer-generated Conformations for Compounds **27**, **28**, **70** and **58**.

Compound	Energy (Kcal/mol)
27	-123.301,142
28	-134.282,212
70	-123.304,239
58	-134.288,315