Direct Transformation of N-protected α,β-Unsaturated γ-Amino Amides into γ-Lactams through a Base Mediated Molecular Rearrangement

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1. ORTEP diagrams:

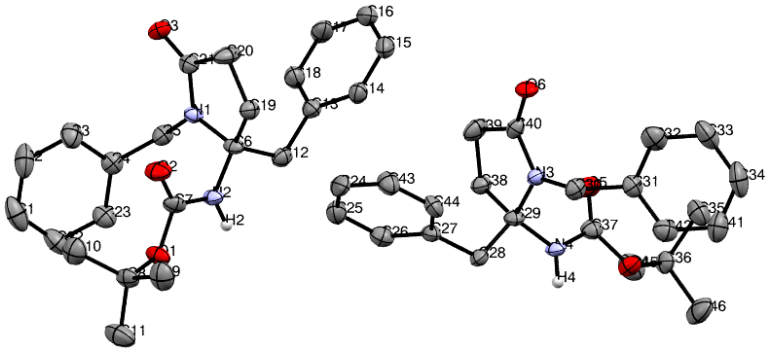


Fig. S1: ORTEP diagram of compound **2a.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 1498002).

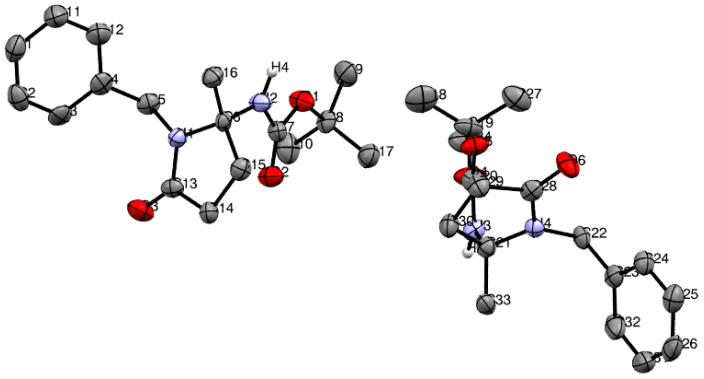


Fig. S2: ORTEP diagram of compound **2b.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 1498003)

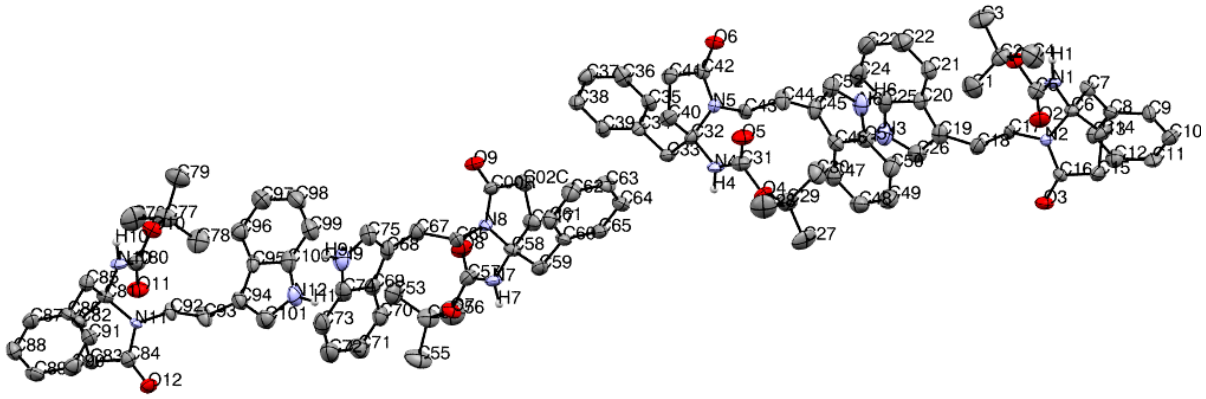


Fig S3: ORTEP diagram of compound **2e.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 1498004).

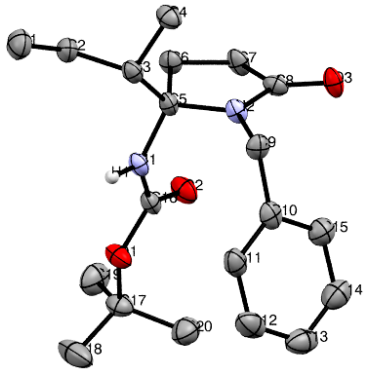


Fig S4: ORTEP diagram of compound **2f.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 1498005).

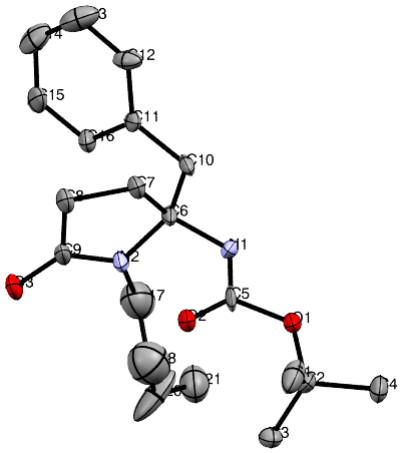


Fig S5: ORTEP diagram of compound **2h.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 1498006).

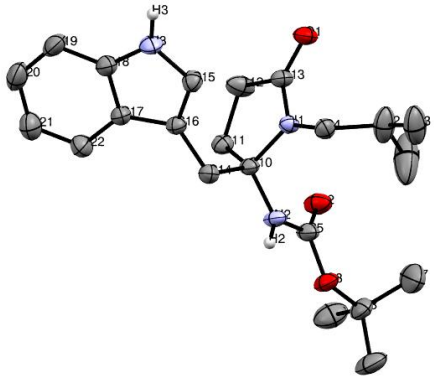


Fig S6: ORTEP diagram of compound **2i.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 1498007).

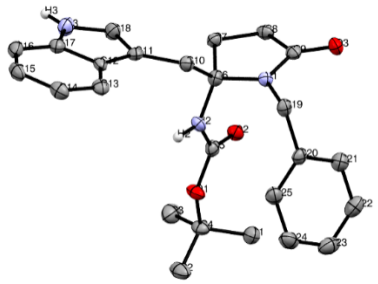


Fig S7: ORTEP diagram of compound **2j.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 1498008).

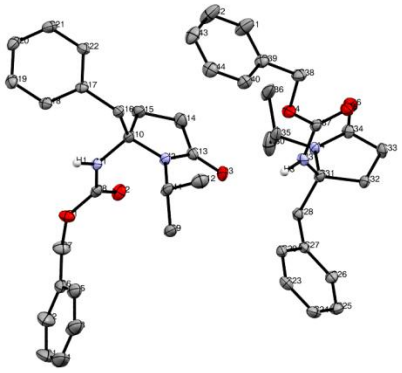


Fig S8: ORTEP diagram of compound **2m.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 1498009).

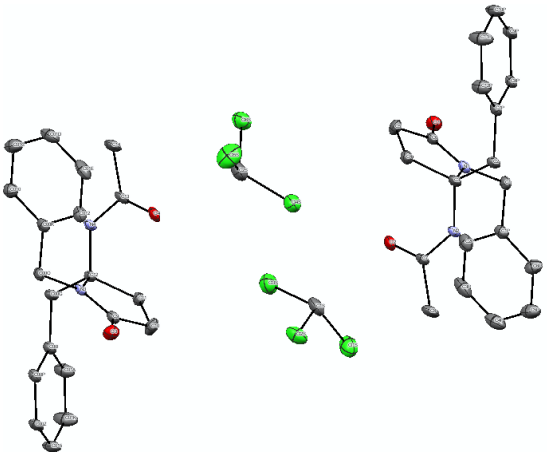


Fig S9: ORTEP diagram of compound **5c.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no1871180).

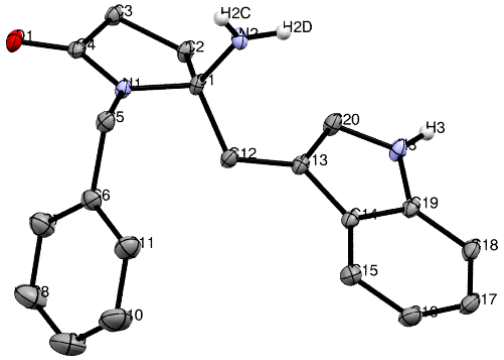


Fig S10: ORTEP diagram of compound **3j.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 14980010).

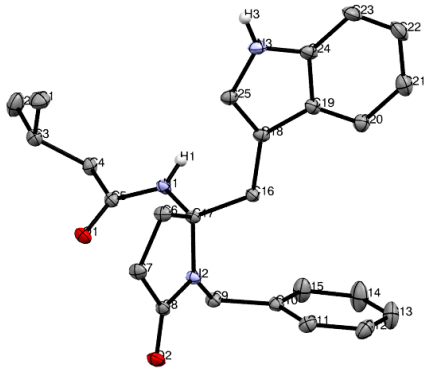


Fig S11: ORTEP diagram of compound **4j.** H-atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (CCDC no 14980011).

2. Crystallographic Information:

Compound 2a: Crystals of **2a** were grown by slow evaporation from a solution of EtOAc. A single crystal (0.2 × 0.1 × 0.08 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 57.04), for a total of 12065 independent reflections. Space group P12(1)1, a = 6.639 (3), b = 8.413 (3), c = 36.816 (16), β = 90.173 (10), V = 2065.3 (16) $Å^3$, Monoclinic, Z = 4 for chemical formula C23 H28 N2 O3, with two molecules in asymmetric unit; ρ calcd = 1.229 gcm^{-3}, μ = 0.081 mm^{-1}, F (000) = 816, R_{int}= 0.0529. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0620 (wR2 = 0.1167) 8305 observed reflections ($F_0 \geq 4\sigma$ (|F_0|)) and 511 variables, S = 0.973.

Compound 2b: Crystals of **2b** were grown by slow evaporation from a solution of EtOAc. A single crystal (0.15 × 0.1 × 0.05 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 66.65), for a total of 20711

independent reflections. Space group C 2, a = 14.9637(5), b = 11.3042(4), c = 21.2771(9), β = 110.4360(10), V = 3372.6 (2) Å^3, Monoclinic, Z = 8 for chemical formula C17 H24 N2 O3, with two molecule in asymmetric unit; ρcalcd = 1.199 gcm^{-3}, μ = 0.665 mm^{-1}, F (000) = 1312, R_{int}= 0.0243. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.055 (wR2 = 0.2125) 5783 observed reflections ($F_0 \geq 4\sigma$ (|F_0|)) and 405 variables, S = 2.070.

Compound 2e: Crystals of **2e** were grown by slow evaporation from a solution of EtOAc. A single crystal (0.1 × 0.05 × 0.03 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 66.39), for a total of 9955 independent reflections. Space group P1, a = 6.8272 (3), b = 8.0949 (3), c = 42.0284 (15), β = 89.977 (2), V = 2322.72(16) Å^3, triclinic, Z = 4 for chemical formula C26 H31 N3 O3, with four molecule in asymmetric unit; ρcalcd = 1.240 gcm^{-3}, μ = 0.652 mm^{-1}, F (000) = 1012, R_{int}= 0.0950. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0664 (wR2 = 0.1056) 14782 observed reflections ($F_0 \geq 4\sigma$ (|F_0|)) and 1165 variables, S = 1.263.

Compound 2f: Crystals of **2f** were grown by slow evaporation from a solution of aqueous methanol. A single crystal (0.15 × 0.1 × 0.05 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 50.48), for a total of 15144 independent reflections. Space group P21, a = 6.696(2), b = 13.783(4), c = 10.694(4), β = 102.690(8), V = 962.8(5) Å^3, monoclinic, Z = 2 for chemical formula C20 H30 N2 O3, with one molecule in asymmetric unit; ρcalcd = 1.195 gcm^{-3}, μ = 0.080 mm^{-1}, F (000) = 376, R_{int}= 0.0551. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0599 (wR2 = 0.1470) 4750 observed reflections ($F_0 \geq 4\sigma$ (|F_0|)) and 231 variables, S = 1.026.

Compound 2h: Crystals of **2h**were grown by slow evaporation from a solution of EtOAc. A single crystal (0.1 × 0.07 × 0.05 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 57.358), for a total of 34755 independent reflections. Space group C 2/c, a = 28.90(4), b = 10.508(13), c = 13.397(17), β = 106.42(3), V = 3902(9) $Å^3$, monoclinic, Z = 8 for chemical formula C20 H29 N2 O3, with one molecule in asymmetric unit; ρcalcd = 1.176 gcm^{-3}, μ = 0.079 mm^{-1}, F (000) = 1480, R_{int}= 0.0719. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.1511 (wR2 = 0.3044) 4863 observed reflections ($F_0 \geq 4\sigma$ ($|F_0|$)) and 230 variables, S = 1.308. Author comment on check CIF: The investigated single crystal was a small-sized,brittle and poorly diffracting. Numerous datasets were collected on singlecrystals from different batches, whereof the one of the highest quality is reported herein.

Compound 2i: Crystals of **2i**were grown by slow evaporation from a solution of EtOAc. A single crystal (0.15 × 0.1 × 0.05 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 50.48), for a total of 52510 independent reflections. Space group P -1, a = 6.8063(18), b = 13.002(4), c = 13.629(4), β = 92.523(7), V = 1106.6(5) $Å^3$, triclinic, Z = 2 for chemical formula C22 H30 N3 O3, with one molecule in asymmetric unit; ρcalcd = 1.154 gcm^{-3}, μ = 0.077 mm^{-1}, F (000) = 484, R_{int}= 0.2621. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0841 (wR2 = 0.1747) 5554 observed reflections ($F_0 \geq 4\sigma$ ($|F_0|$)) and 257 variables, S = 1.017. Author comment on check CIF: The investigated single crystal was a small-sized, brittle and poorly diffracting.

Numerous datasets were collected on single crystals from different batches, whereof the one of the highest quality is reported herein.

Compound 2j: Crystals of **2j**were grown by slow evaporation from a solution of aqueous methanol. A single crystal (0.15 × 0.1 × 0.05 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Cu K_α radiation (λ = 1.54178 Å), ω-scans (2θ = 66.765), for a total of 34755 independent reflections. Space group P 21/n, a = 6.7044(10), b = 28.659(4), c = 11.4082(18), β = 91.966(9), V = 2190.7(6) Å^3, monoclinic, Z = 4 for chemical formula C25 H29 N3 O3, with one molecule in asymmetric unit; ρ calcd = 1.272 gcm^{-3}, μ = 0.675 mm^{-1}, F (000) = 816, R_{int}= 0.0721. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0712 (wR2 = 0.1771) 3756 observed reflections ($F_0 \geq 4\sigma$ (|F_0|)) and 283 variables, S = 1.090.

Compound 2m: Crystals of **2m** were grown by slow evaporation from a solution of EtOAc. A single crystal (0.12 × 0.1 × 0.06 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 50.48), for a total of 47013 independent reflections. Space group P 21/c, a = 12.367(5), b = 16.811(7), c = 19.201(8), β = 90.00, V = 3992(3) Å^3, monoclinic, Z = 8 for chemical formula C22 H26 N2 O3, with two molecule in asymmetric unit; ρ calcd = 1.219 gcm^{-3}, μ = 0.081 mm^{-1}, F (000) = 1706, R_{int}= 0.077. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0407 (wR2 = 0.1008) 6229 observed reflections ($F_0 \geq 4\sigma$ (|F_0|)) and 491 variables, S = 0.665.

Compound 5c: Crystals of **5c** were grown by slow evaporation from a solution of EtOAc. A single crystal (0.13 × 0.1 × 0.05 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 57.172), for a total of 11092independent reflections. Space group P-1, a=6.6014(15), b = 9.469(2), c= 35.287(8) α = 93.454(5) β=93.826(5) γ=98.649(5), V = 2170.3(8) $Å^3$, monoclinic, Z = 2 for chemical formula C_{20} H_{22} N_2 O_2, C H Cl_3, with two molecule in asymmetric unit; ρ calcd = 1.352 gcm^{-3}, μ = 0.442 mm^{-1}, F (000) = 918.0, The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0913, wR2 =0.3006 (11029) observed reflections ($F_0 \geq 4\sigma$ ($|F_0|$)) and 507 variables, S = 0.781.

Compound 3j: Crystals of **3j**were grown by slow evaporation from a solution of EtOAc. A single crystal (0.2 × 0.1 × 0.08 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 50.48), for a total of 15583 independent reflections. Space group P -1, a = 6.5787(11), b = 9.2449(14), c = 14.324(2), β = 77.982(4), V = 822.4(2) $Å^3$, triclinic, Z = 4 for chemical formula C20 H21 N3 O, with one molecule in asymmetric unit; ρ calcd = 1.290 gcm^{-3}, μ = 0.081 mm^{-1}, F (000) = 364, R_{int}= 0.0273. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0523 (wR2 = 0.1857) 4106 observed reflections ($F_0 \geq 4\sigma$ ($|F_0|$)) and 217 variables, S = 1.563. Author comment on check CIF: It is possible that shorter D-H..H-D distances are an artifact of refinement.

Compound 4j: Crystals of **4j** were grown by slow evaporation from a solution of EtOAc. A single crystal (0.18 × 0.1 × 0.06 mm) was mounted on loop with a small amount of the paraffin oil. The X-ray data were collected at 100K temperature on a Bruker APEX(II) DUO CCD diffractometer using Mo K_α radiation (λ = 0.71073 Å), ω-scans (2θ = 50.48), for a total of 34755 independent

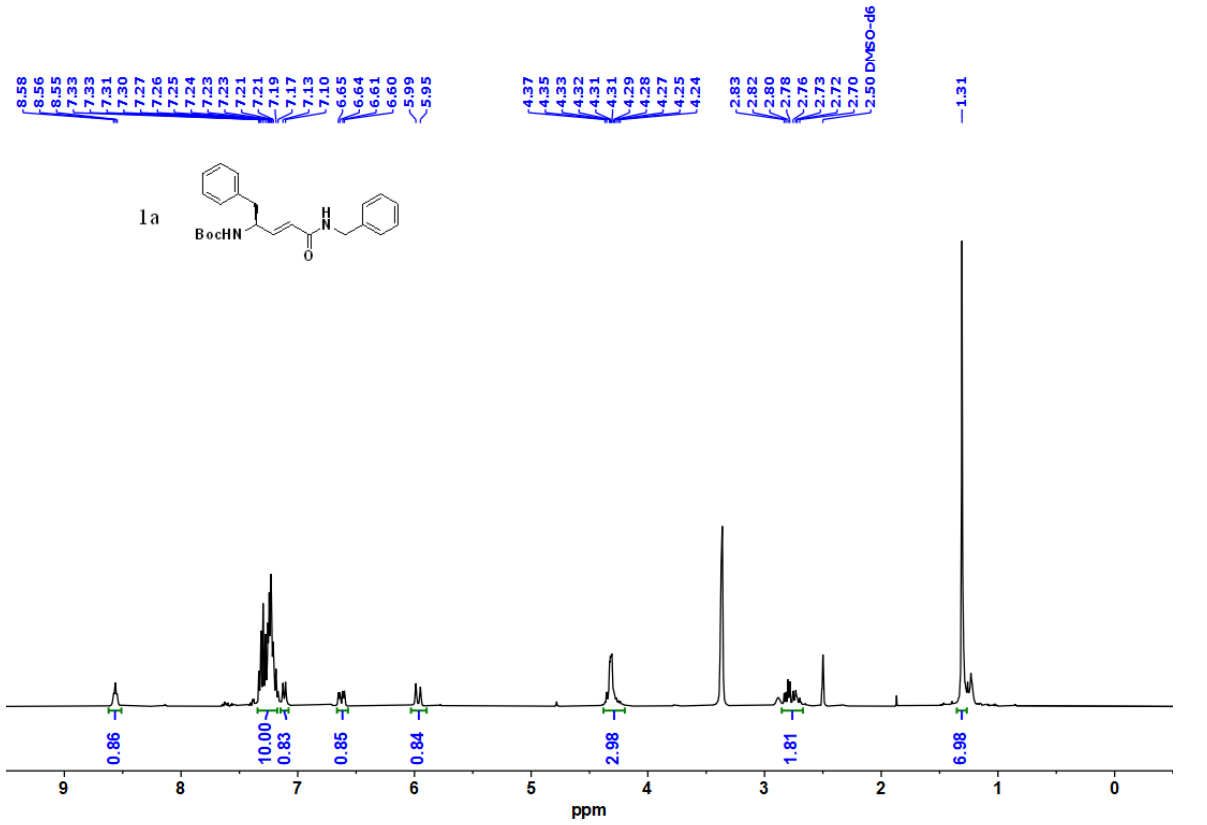
reflections. Space group Cc, a = 6.9007(11), b = 25.211(4), c = 13.042(2), β = 101.886(4), V = 2220.2(6) Å^3, monoclinic, Z = 4 for chemical formula C25 H29 N3 O2, with one molecule in asymmetric unit; ρ calcd = 1.207 gcm^{-3}, μ = 0.077 mm^{-1}, F (000) = 968, R_{int}= 0.0412. The structure was obtained by intrinsic methods using SHELXS-97.The final R value was 0.0361 (wR2 = 0.0975) 11452 observed reflections ($F_0 \geq 4\sigma$ (|F_0|)) and 635 variables, S = 0.761.

3) List of organic and inorganic bases used for the rearrangement

Table **S1**: List of organic and inorganic bases used for the rearrangement

Base	Solvent	Conversion	Time
LiOH (1*N*)	THF	-	2 d
NaOH (1*N*)	THF	40 %	2 d
CsOH (1*N*)	THF/DMF	50%	2 d
DBU(up to 3.0 equvi)	THF/DCM	-	2d
n-BuLi (1.0 equvi)	THF	-	1 d
KO^{t}Bu (up to 3.0 equvi)	THF	100%	8 h

4) ^{1}H and ^{13}C NMR of all compounds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8.55
7.33
7.33
7.31
7.30
7.27
7.26
7.25
7.24
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7.21
7.21
7.19
7.17
7.13
7.10
6.65
6.64
6.61
6.60
5.99
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2.76
2.73
2.72
2.70
2.50 DMSO-d6
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0.84
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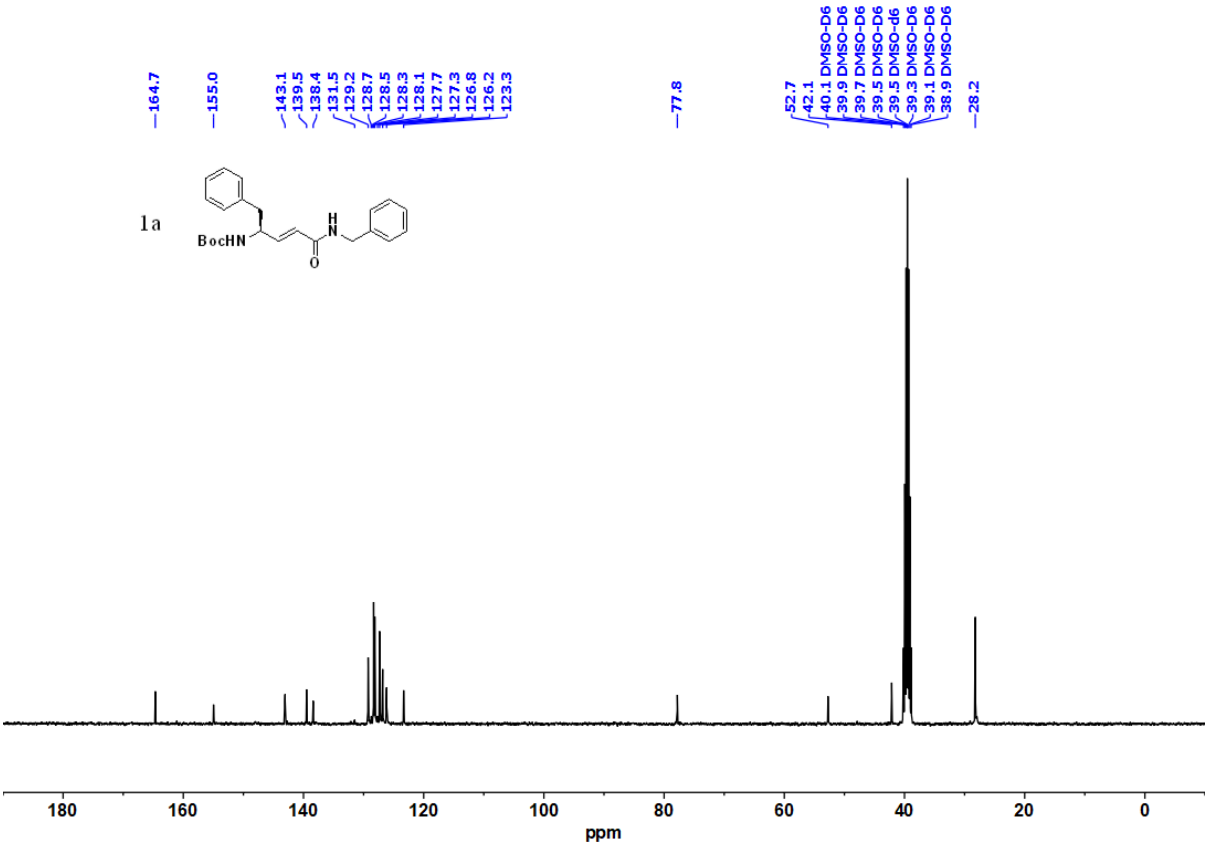
1.81
6.98
ppm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128.5
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128.1
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126.8
126.2
123.3
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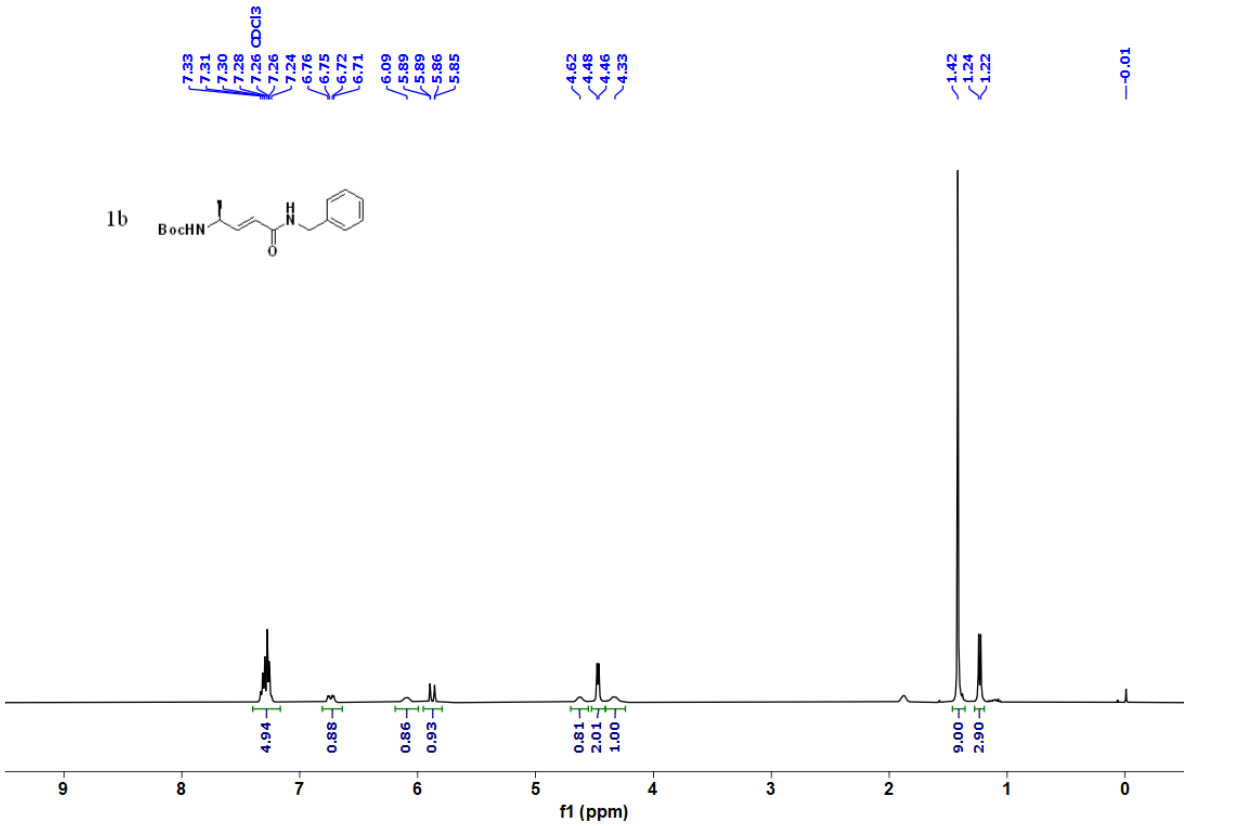
38.9 DMSO-D6
28.2
1a
BocHN
ppm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7.26 CDCl3
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4.48
4.46
4.33
1.42
1.24
1.22
0.01
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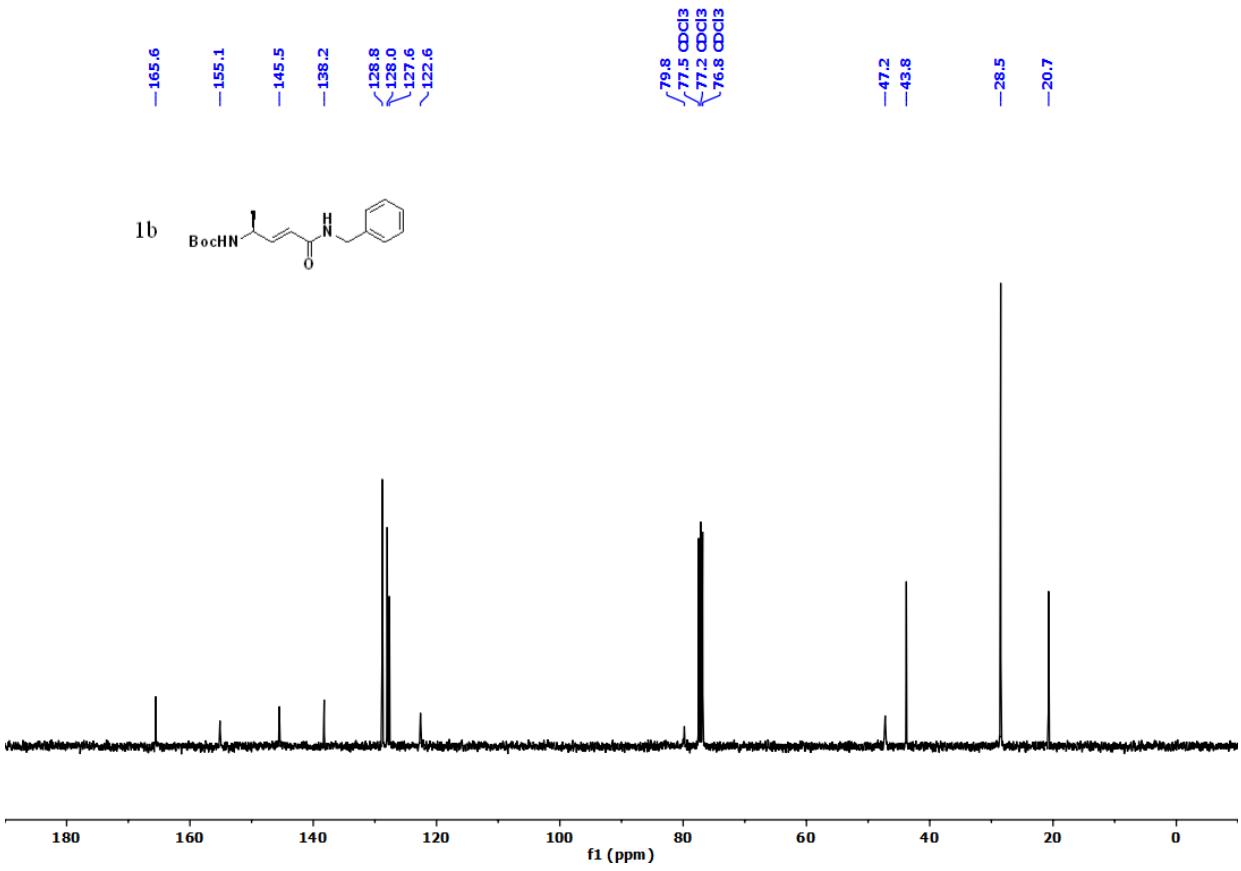
1.00
9.00
2.90
f1 (ppm)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128.0
127.6
122.6
79.8
77.5 CDCl3
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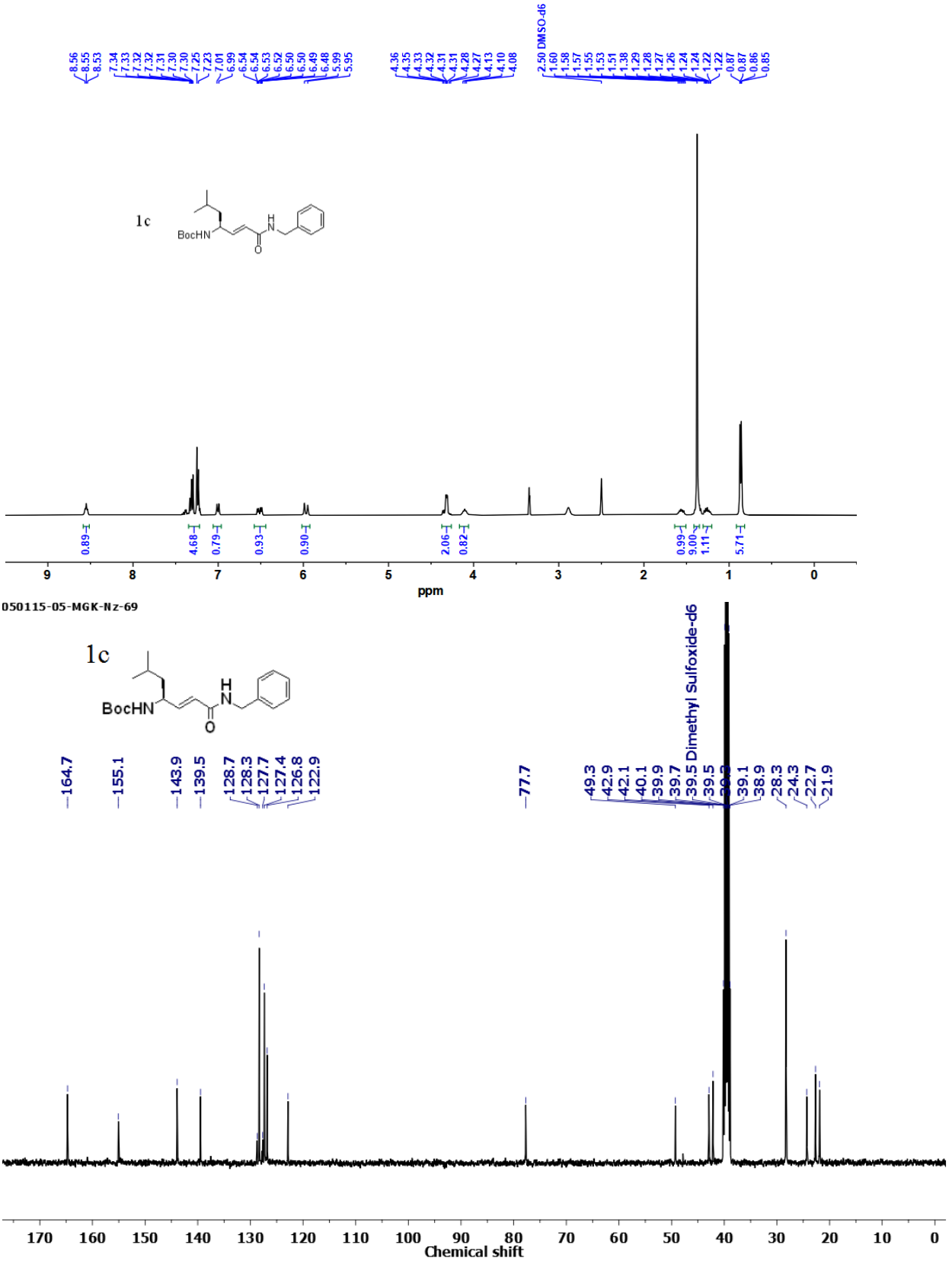
47.2
43.8
28.5
20.7
1b
BocHN
f1 (ppm)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ppm
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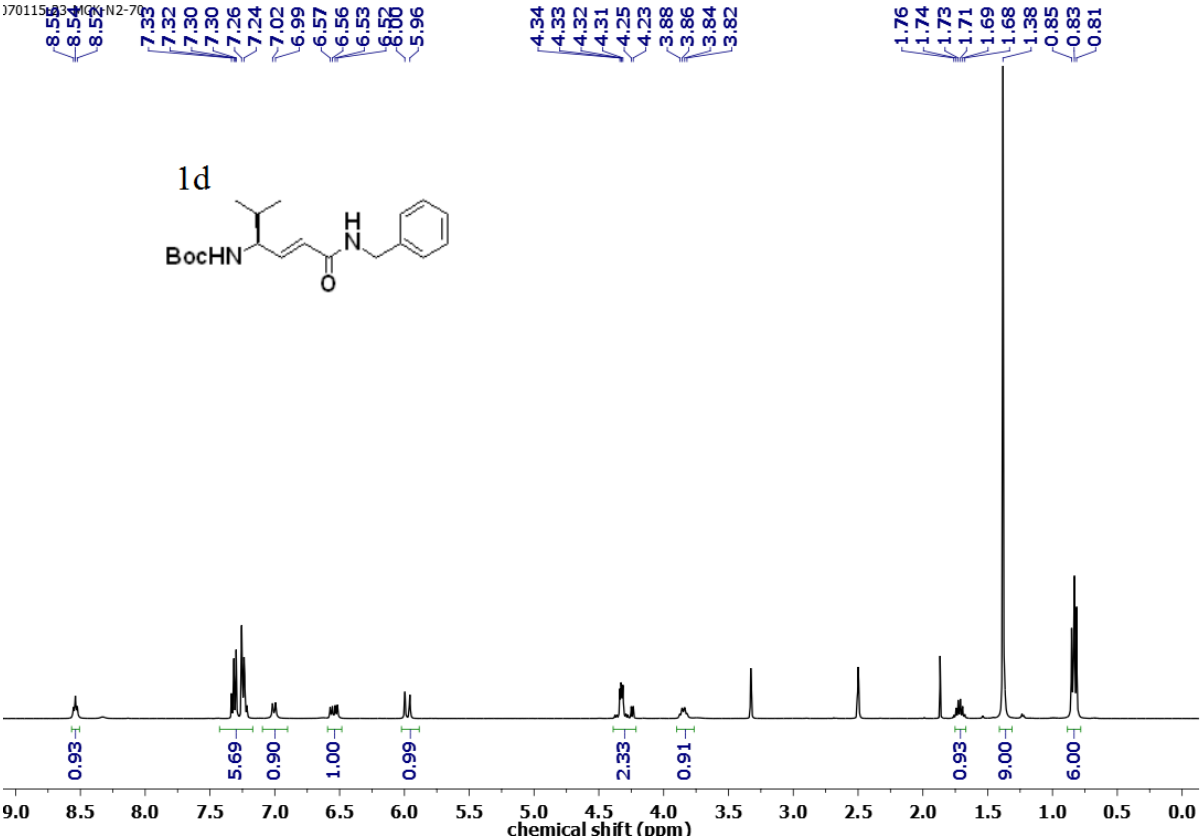
Chemical shift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BocHN
H
N
O
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6.57
6.56
6.53
6.52
6.00
5.96
4.34
4.33
4.32
4.31
4.25
4.23
3.88
3.86
3.84
3.82
1.76
1.74
1.73
1.71
1.69
1.68
1.38
0.85
0.83
0.81
0.93
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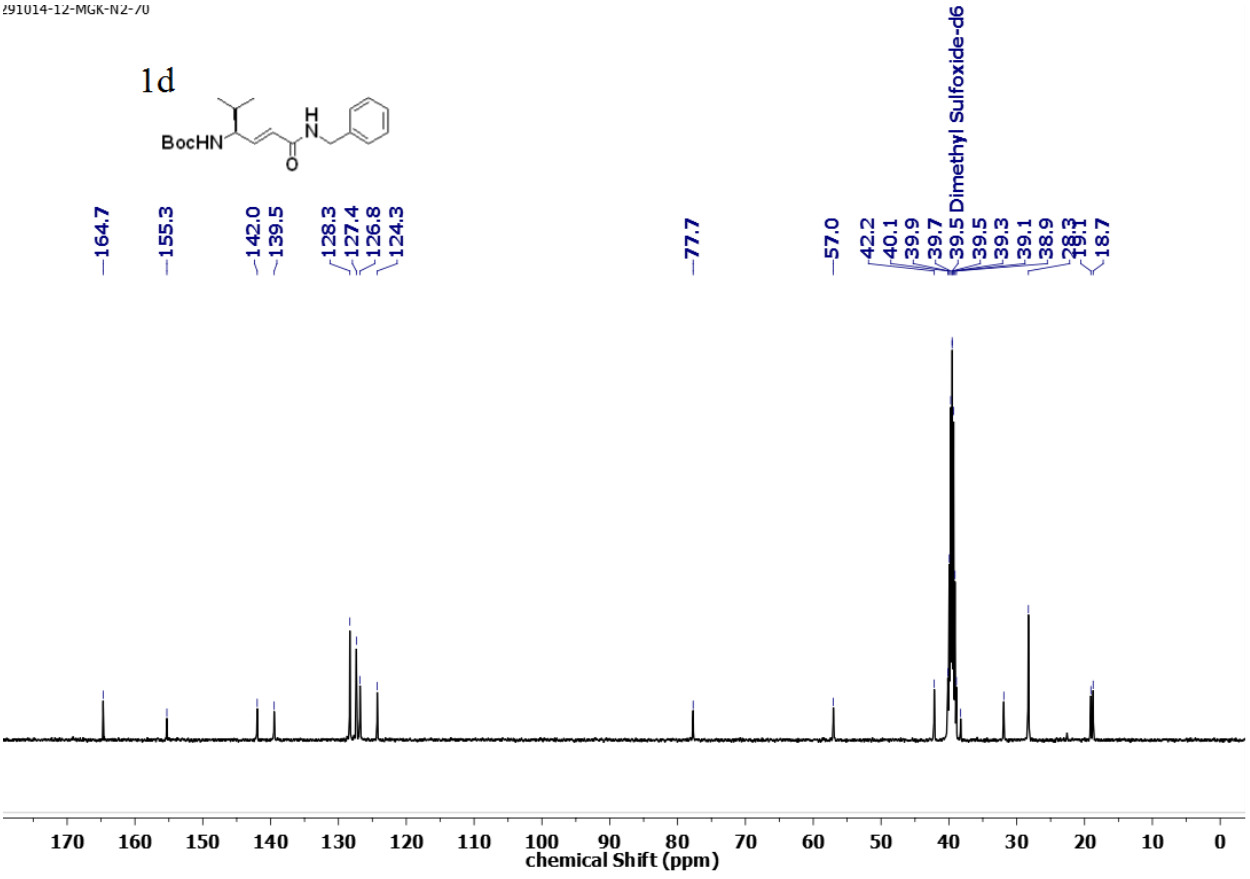
0.90
1.00
0.99
2.33
0.91
0.93
9.00
6.00
chemical shift (ppm)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77.7
57.0
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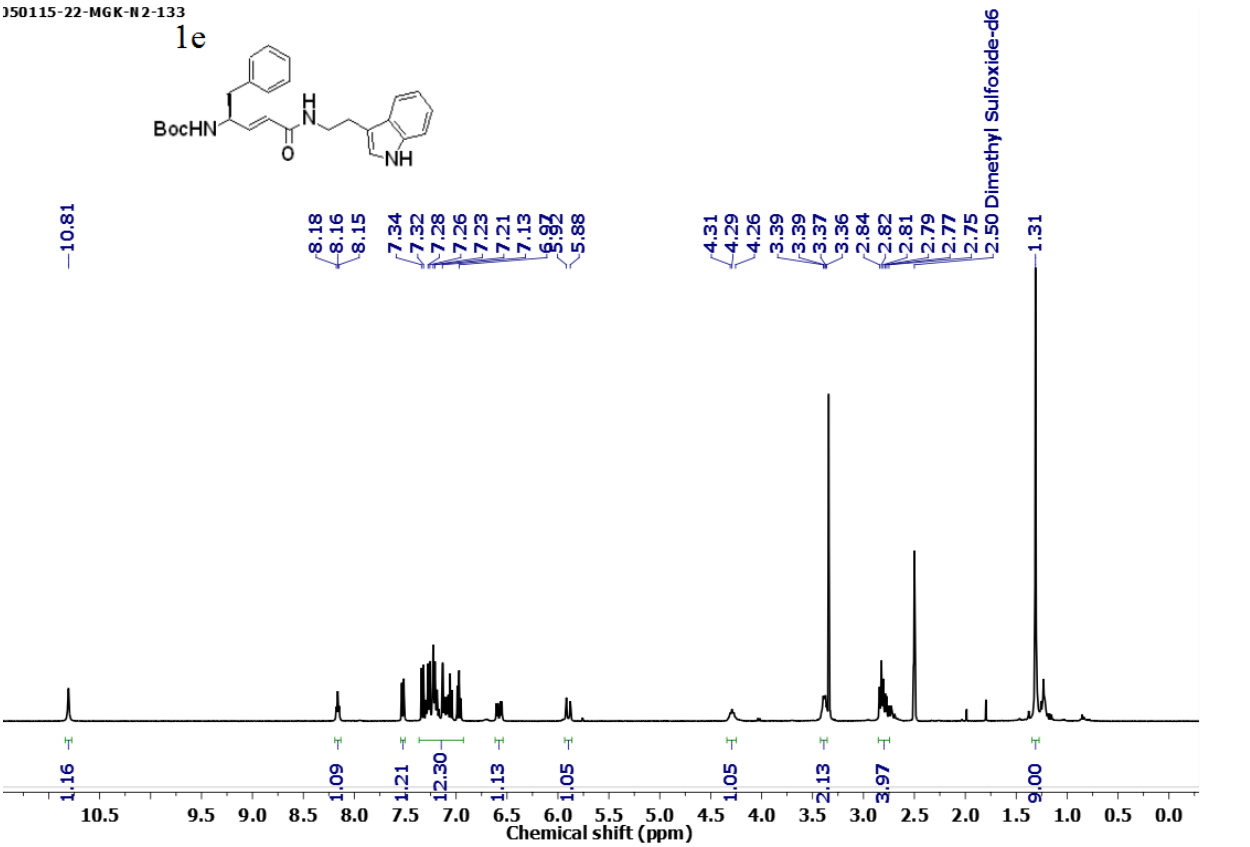
39.3
39.1
38.9
28.3
18.7
chemical Shift (ppm)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BocHN
H
N
O
NH
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8.16
8.15
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7.23
7.21
7.13
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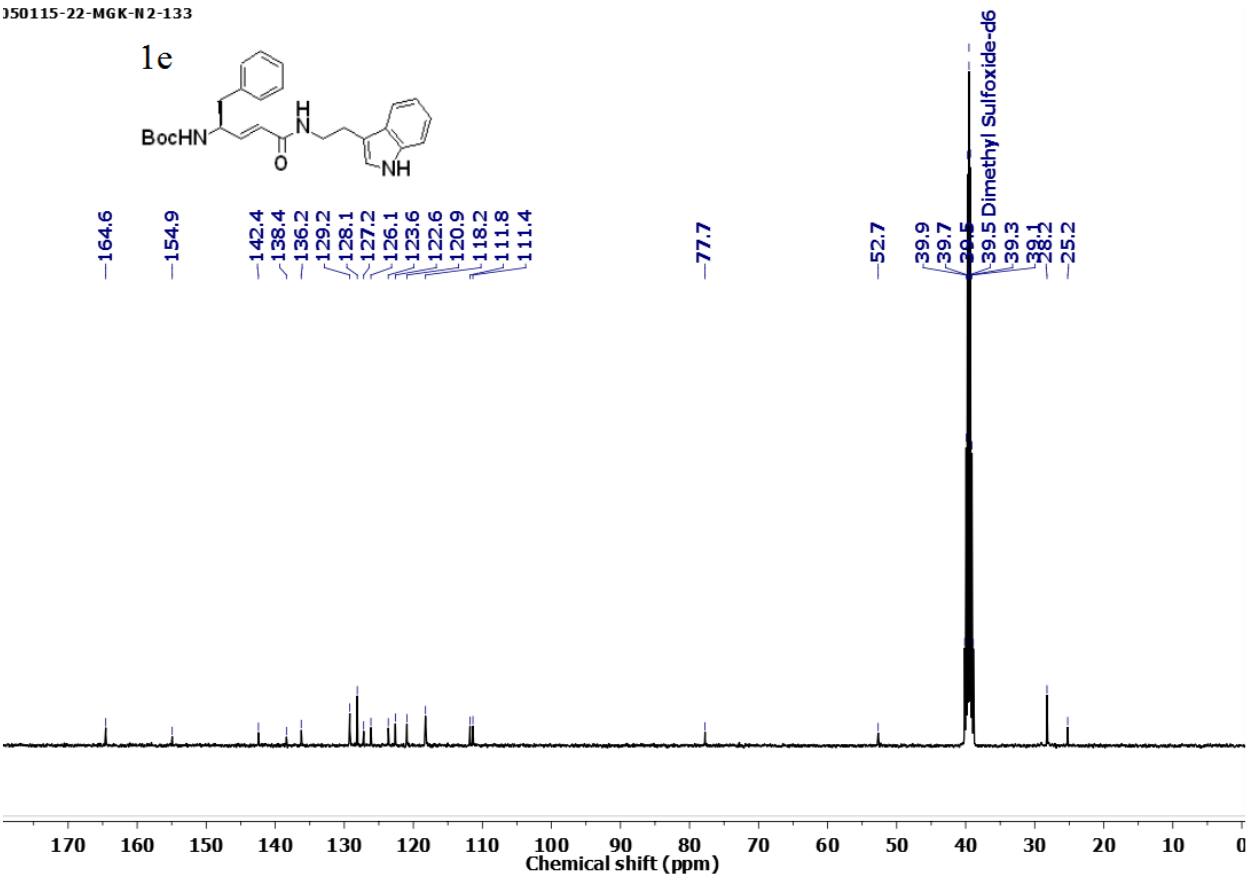
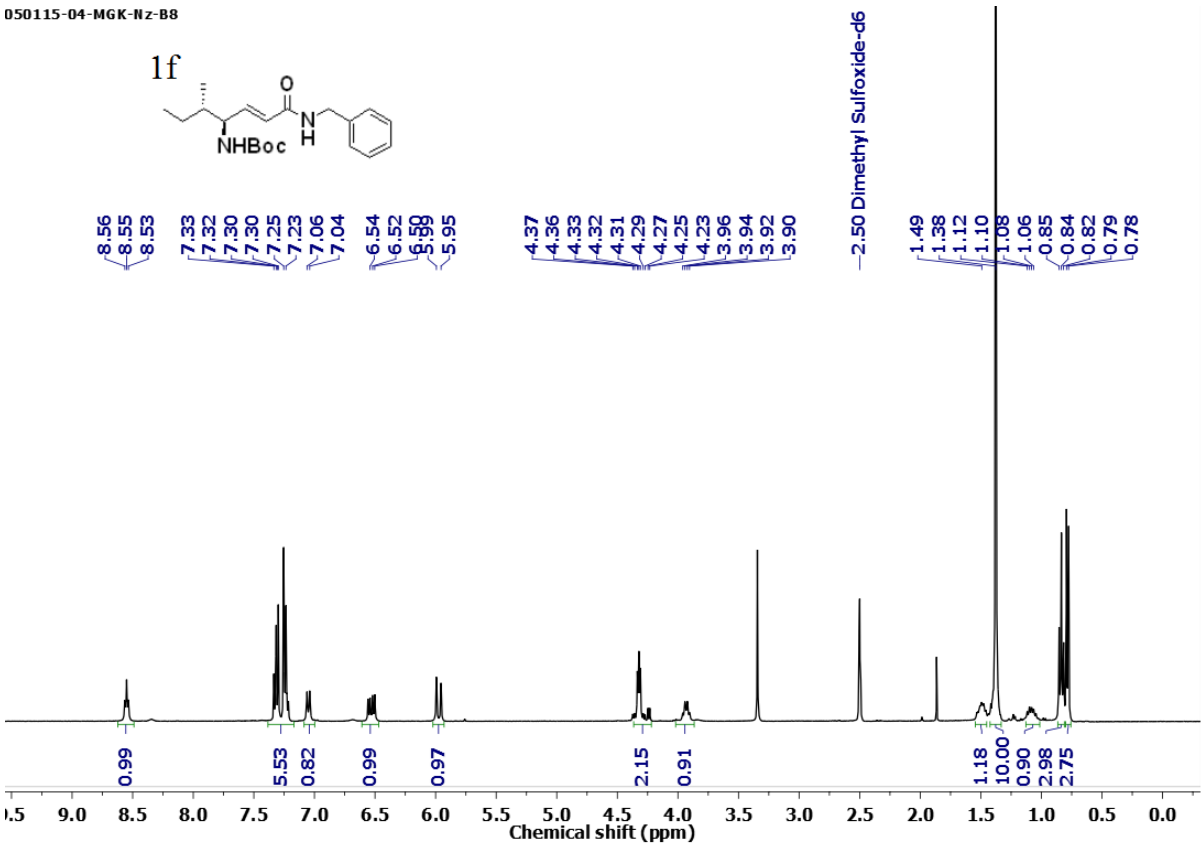
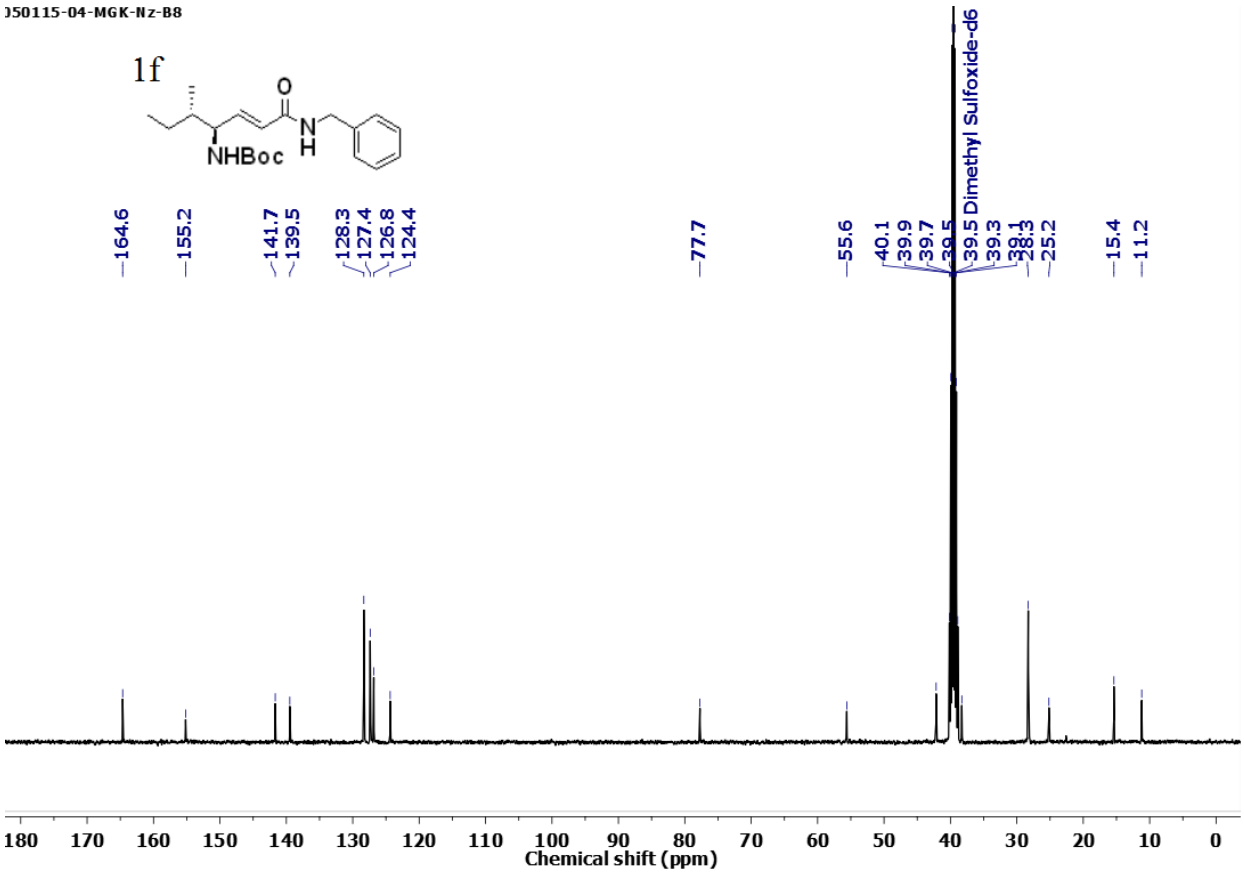
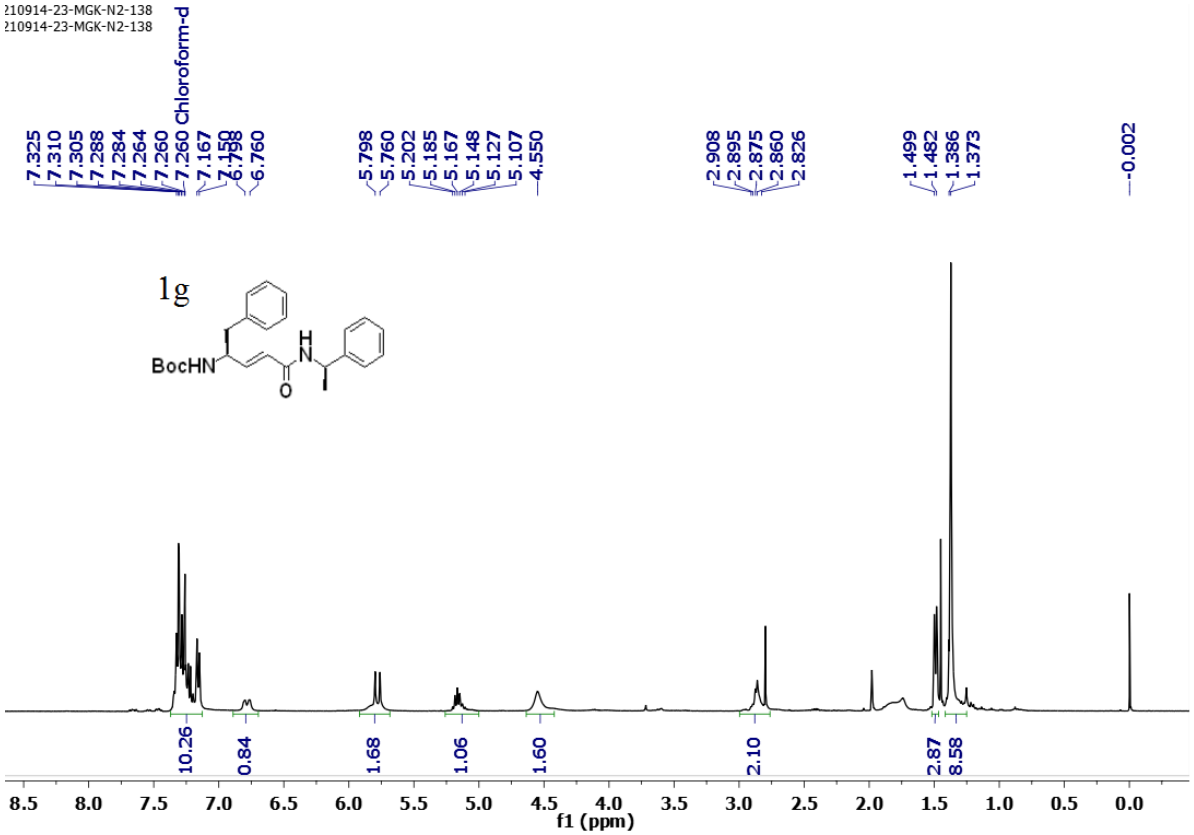
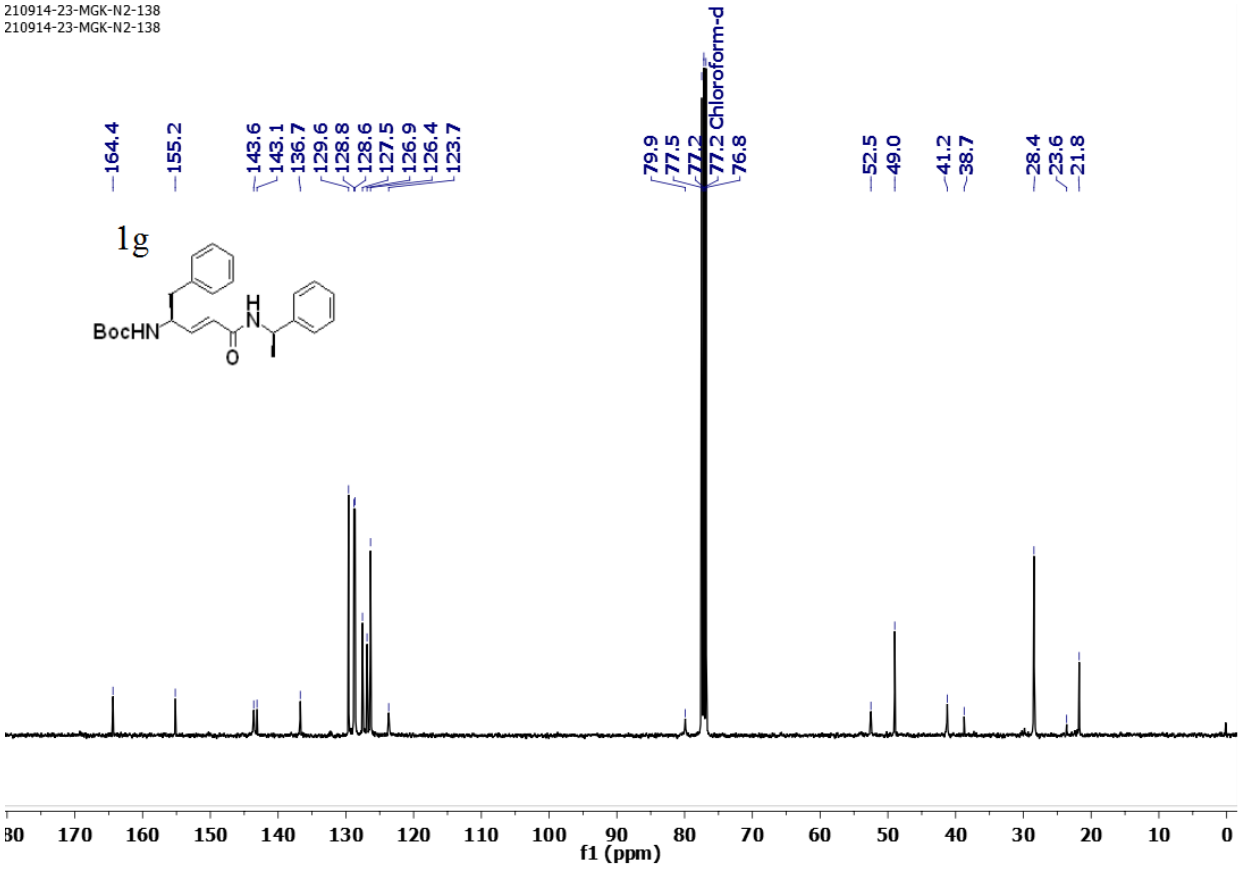
1.31
1.16
1.09
1.21
12.30
1.13
1.05
1.05
2.13
3.97
9.00
Chemical shift (ppm)

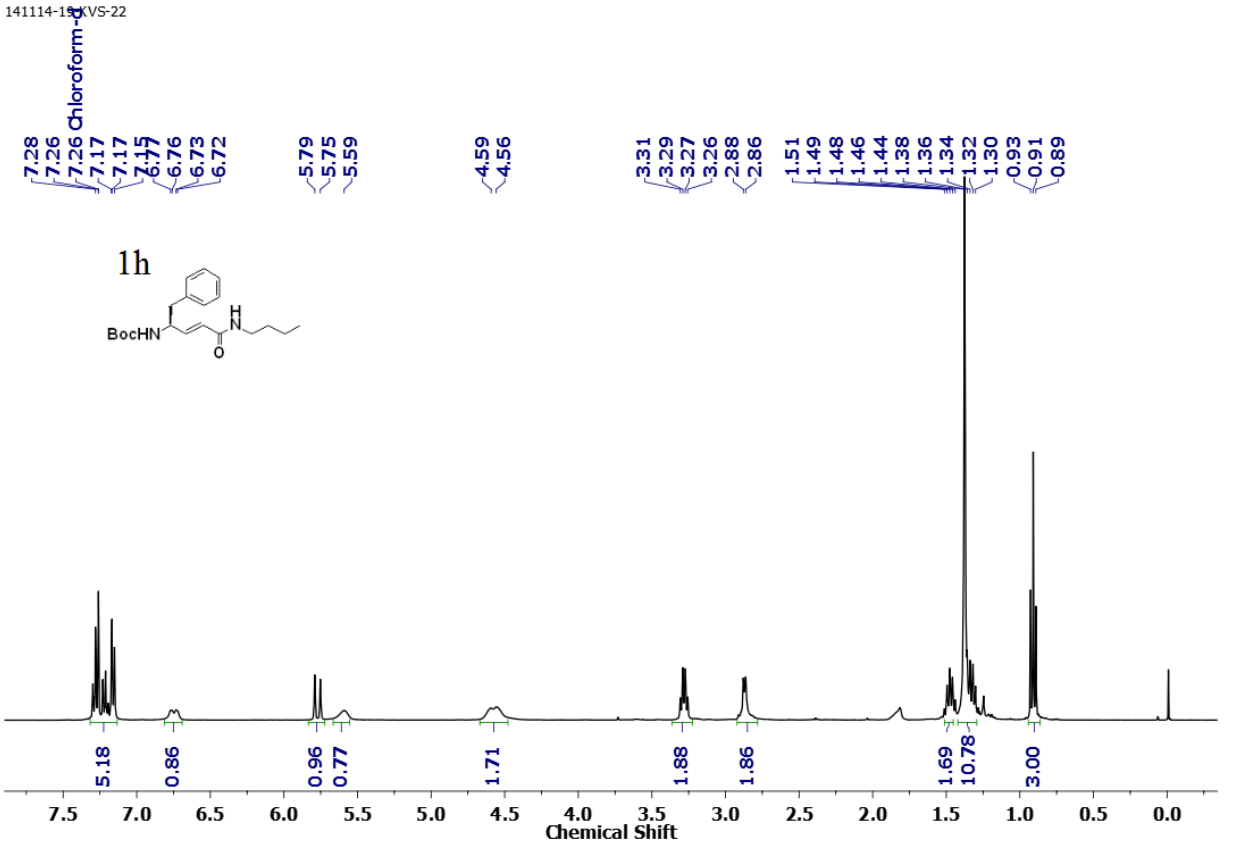

J50115-22-MGK-N2-133
1e
BocHN
H
N
O
NH
164.6
154.9
142.4
138.4
136.2
129.2
128.1
127.2
126.1
123.6
122.6
120.9
118.2
111.8
111.4
77.7
52.7
39.9
39.7
39.5 Dimethyl Sulfoxide-d6
39.3
28.1
28.2
25.2
Chemical shift (ppm)

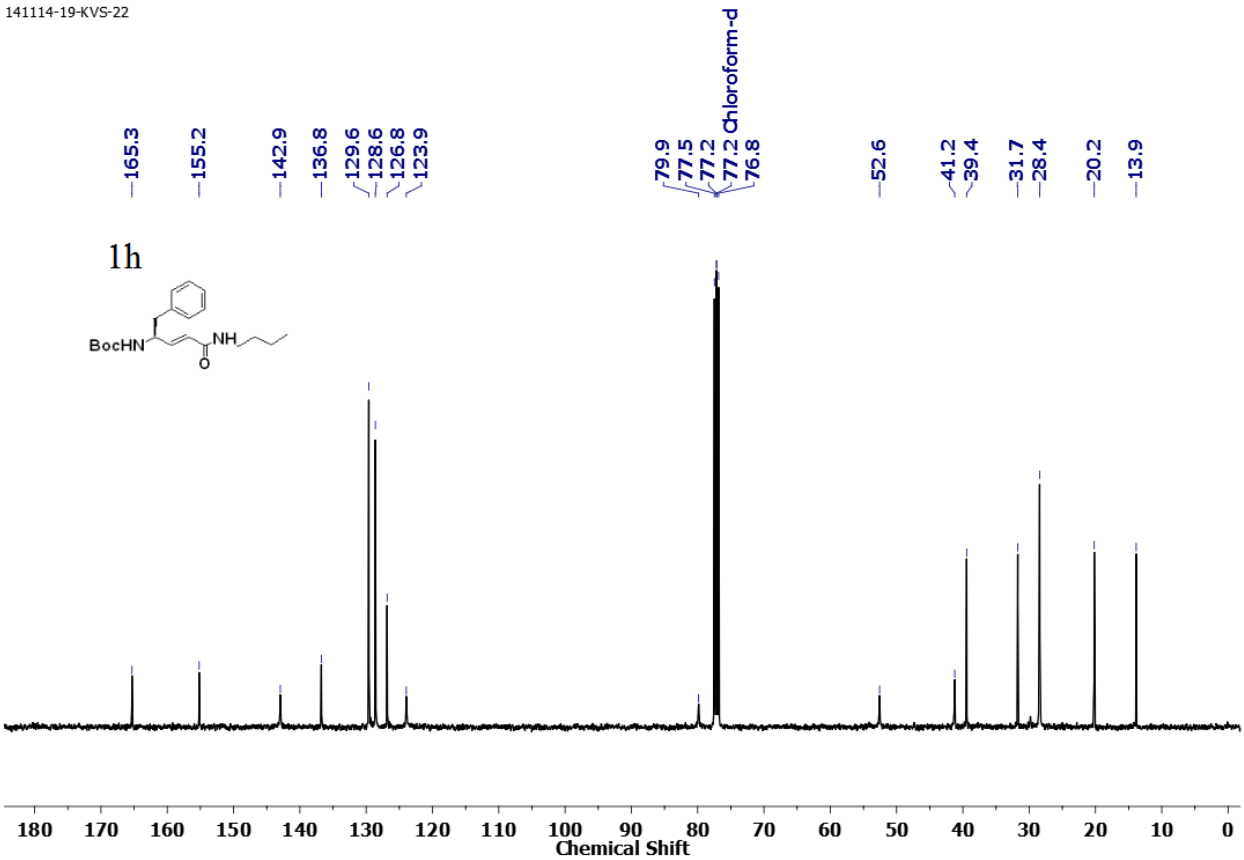

050115-04-MGK-Nz-B8
1f
NHBoc
2.50 Dimethyl Sulfoxide-d6
Chemical shift (ppm)

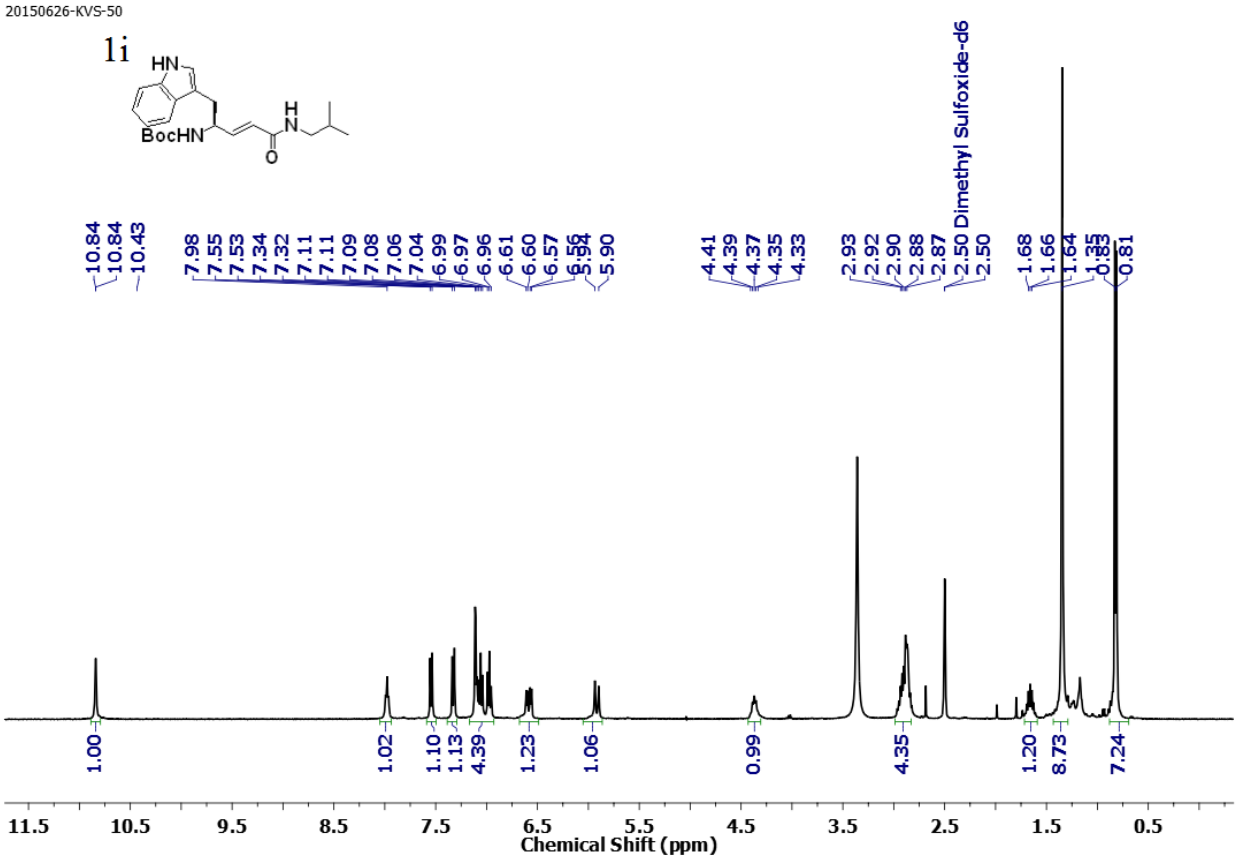

050115-04-MGK-Nz-B8
1f
NHBoc
39.5 Dimethyl Sulfoxide-d6
Chemical shift (ppm)

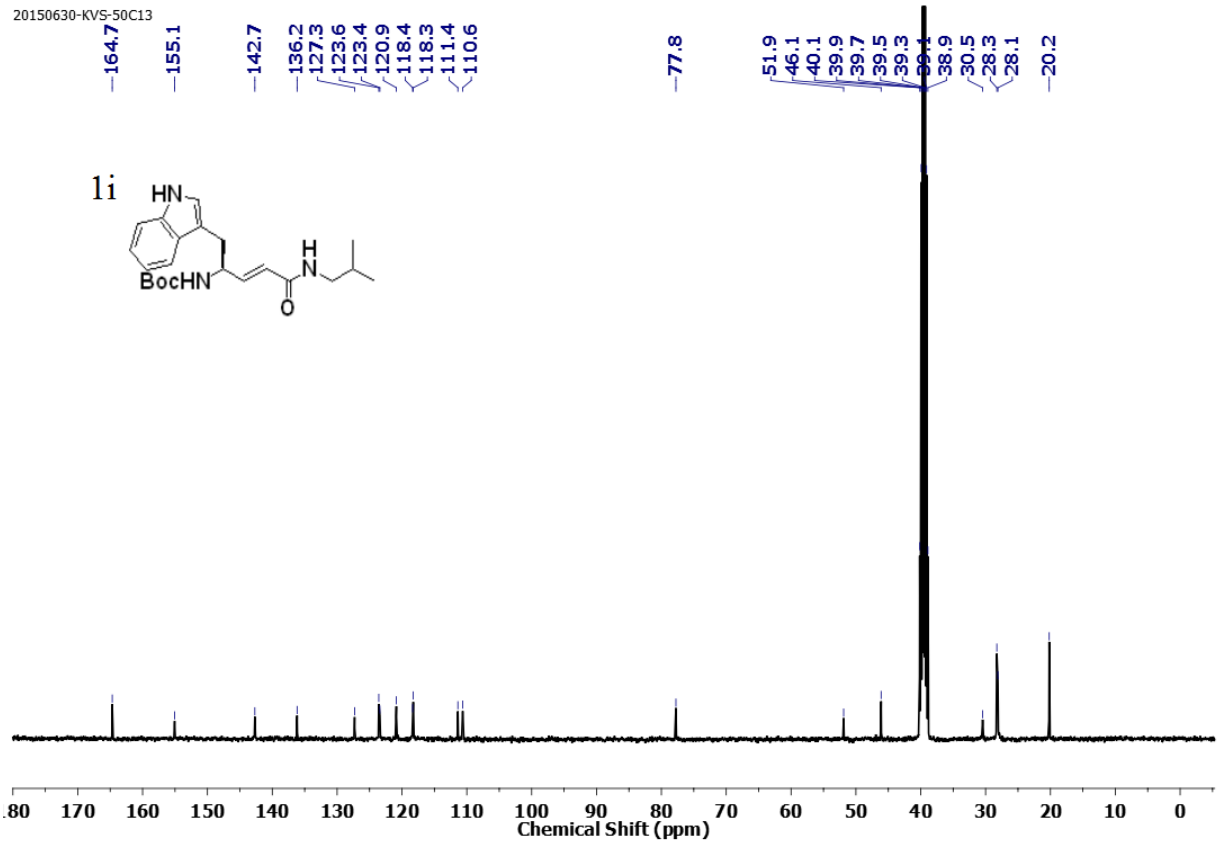

210914-23-MGK-N2-138
210914-23-MGK-N2-138
7.325
7.310
7.305
7.288
7.284
7.264
7.260
7.260 Chloroform-d
7.167
6.798
6.760
5.798
5.760
5.202
5.185
5.167
5.148
5.127
5.107
4.550
2.908
2.895
2.875
2.860
2.826
1.499
1.482
1.386
1.373
-0.002
1g
BocHN
H
N
O
10.26
0.84
1.68
1.06
1.60
2.10
2.87
8.58
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

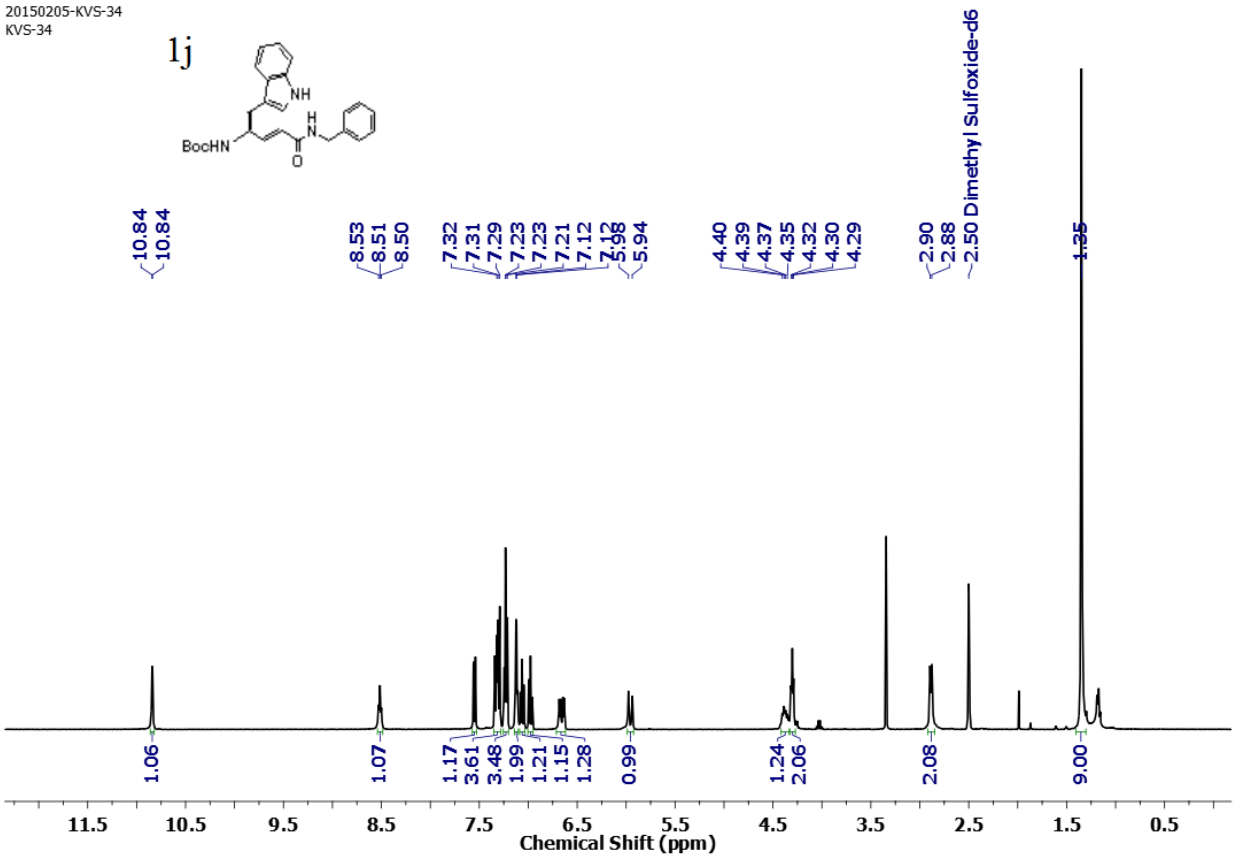

210914-23-MGK-N2-138
210914-23-MGK-N2-138
164.4
155.2
143.6
143.1
136.7
129.6
128.8
128.6
127.5
126.9
126.4
123.7
79.9
77.5
77.2 Chloroform-d
76.8
52.5
49.0
41.2
38.7
28.4
23.6
21.8
1g
BocHN
H
N
O
30 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

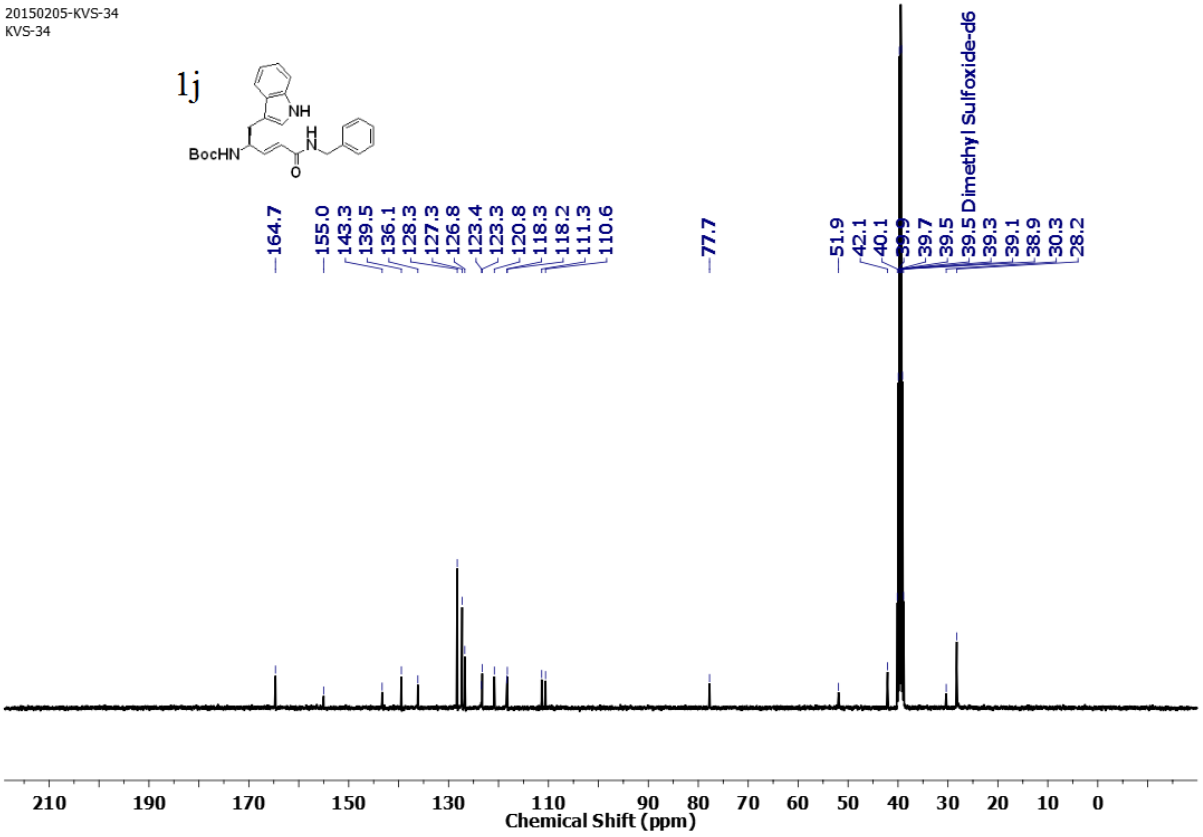

141114-19-KVS-22
Chloroform-d
7.28
7.26
7.26
7.17
7.17
7.15
6.77
6.76
6.73
6.72
5.79
5.75
5.59
4.59
4.56
3.31
3.29
3.27
3.26
2.88
2.86
1.51
1.49
1.48
1.46
1.44
1.38
1.36
1.34
1.32
1.30
0.93
0.91
0.89
1h
BocHN
H
N
O
5.18
0.86
0.96
0.77
1.71
1.88
1.86
1.69
10.78
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical Shift

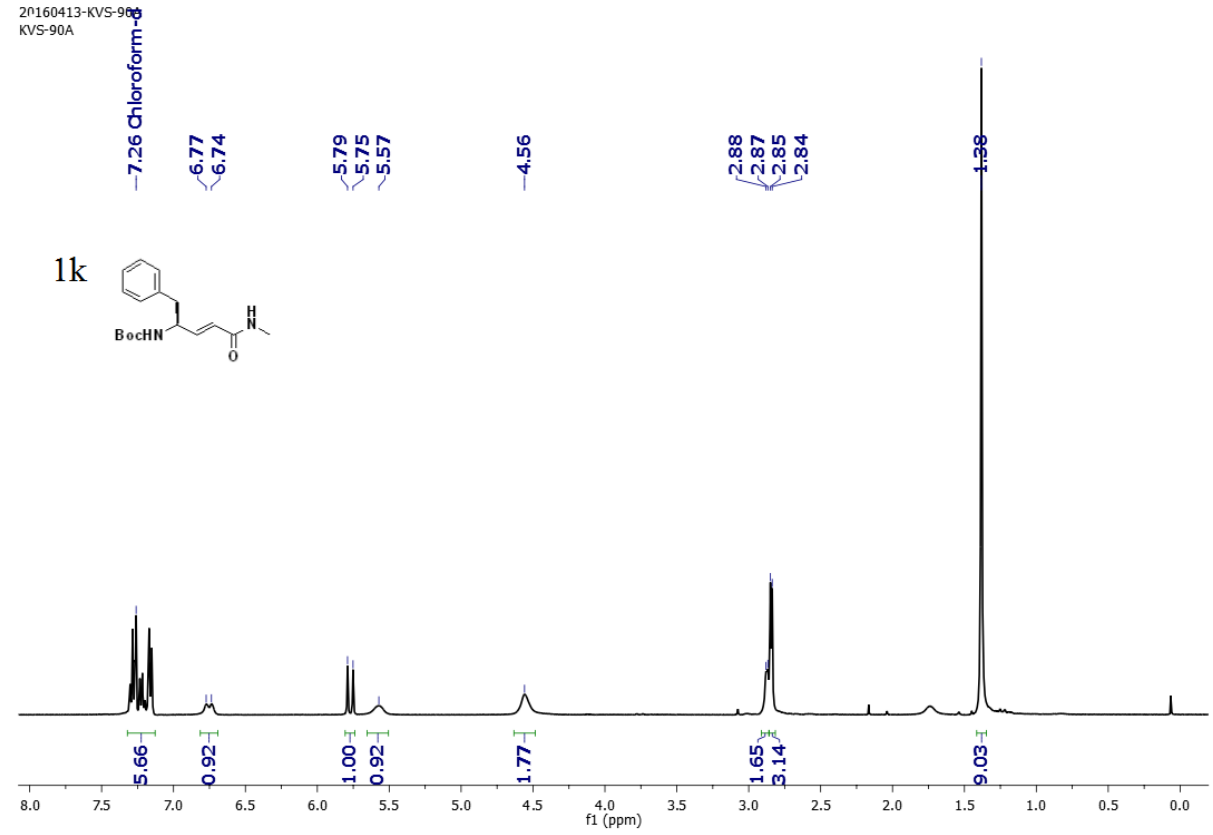

141114-19-KVS-22
165.3
155.2
142.9
136.8
129.6
128.6
126.8
123.9
79.9
77.5
77.2
77.2
Chloroform-d
76.8
52.6
41.2
39.4
31.7
28.4
20.2
13.9
1h
BocHN
NH
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift

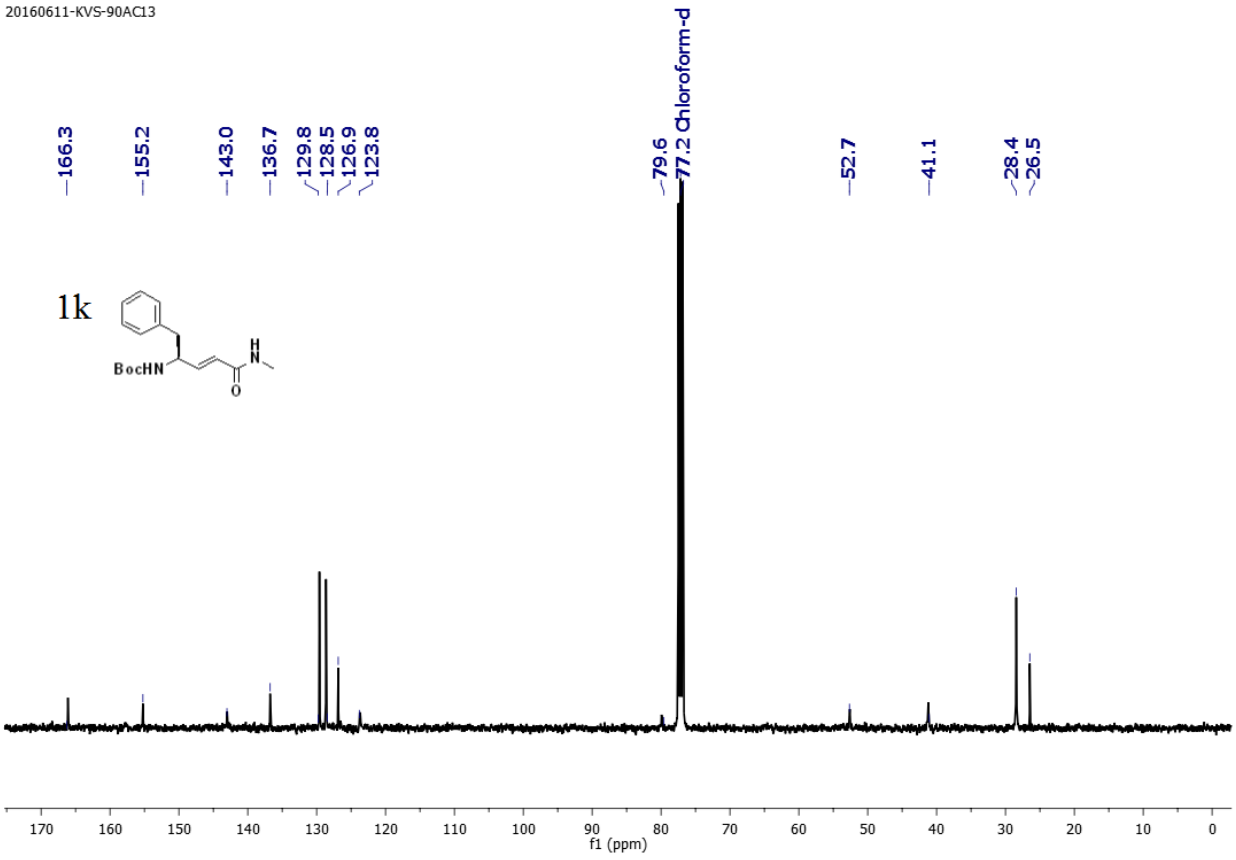

20150626-KVS-50
1i
HN
BocHN
H
N
O
Dimethyl Sulfoxide-d6
10.84
10.84
10.43
7.98
7.55
7.53
7.34
7.32
7.11
7.11
7.09
7.08
7.06
7.04
6.99
6.97
6.96
6.61
6.60
6.57
5.90
4.41
4.39
4.37
4.35
4.33
2.93
2.92
2.90
2.88
2.87
2.50
2.50
1.68
1.66
1.64
0.83
0.81
1.00
1.02
1.10
1.13
4.39
1.23
1.06
0.99
4.35
1.20
8.73
7.24
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
Chemical Shift (ppm)

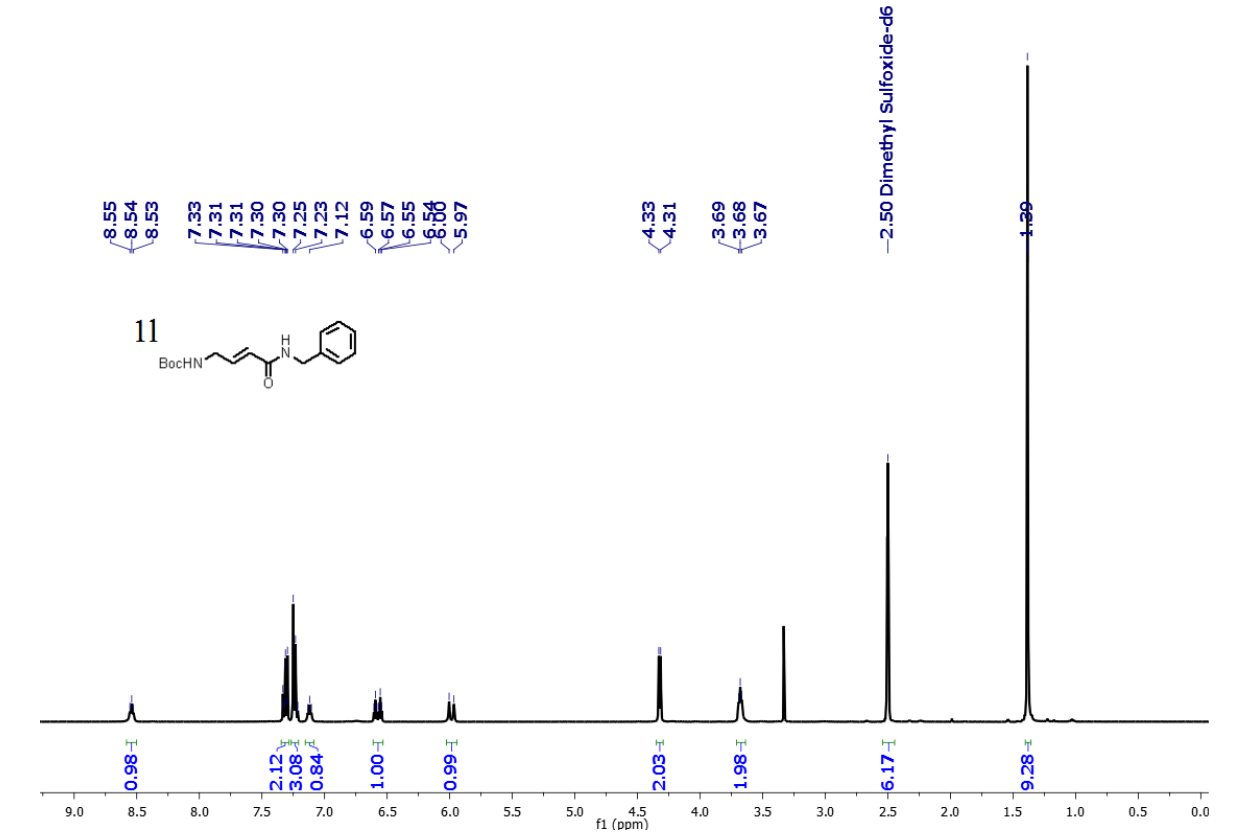

20150630-KVS-50C13
164.7
155.1
142.7
136.2
127.3
123.6
123.4
120.9
118.4
118.3
111.4
110.6
77.8
51.9
46.1
40.1
39.9
39.7
39.5
39.3
38.9
30.5
28.3
28.1
20.2
1i
HN
BocHN
H
N
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

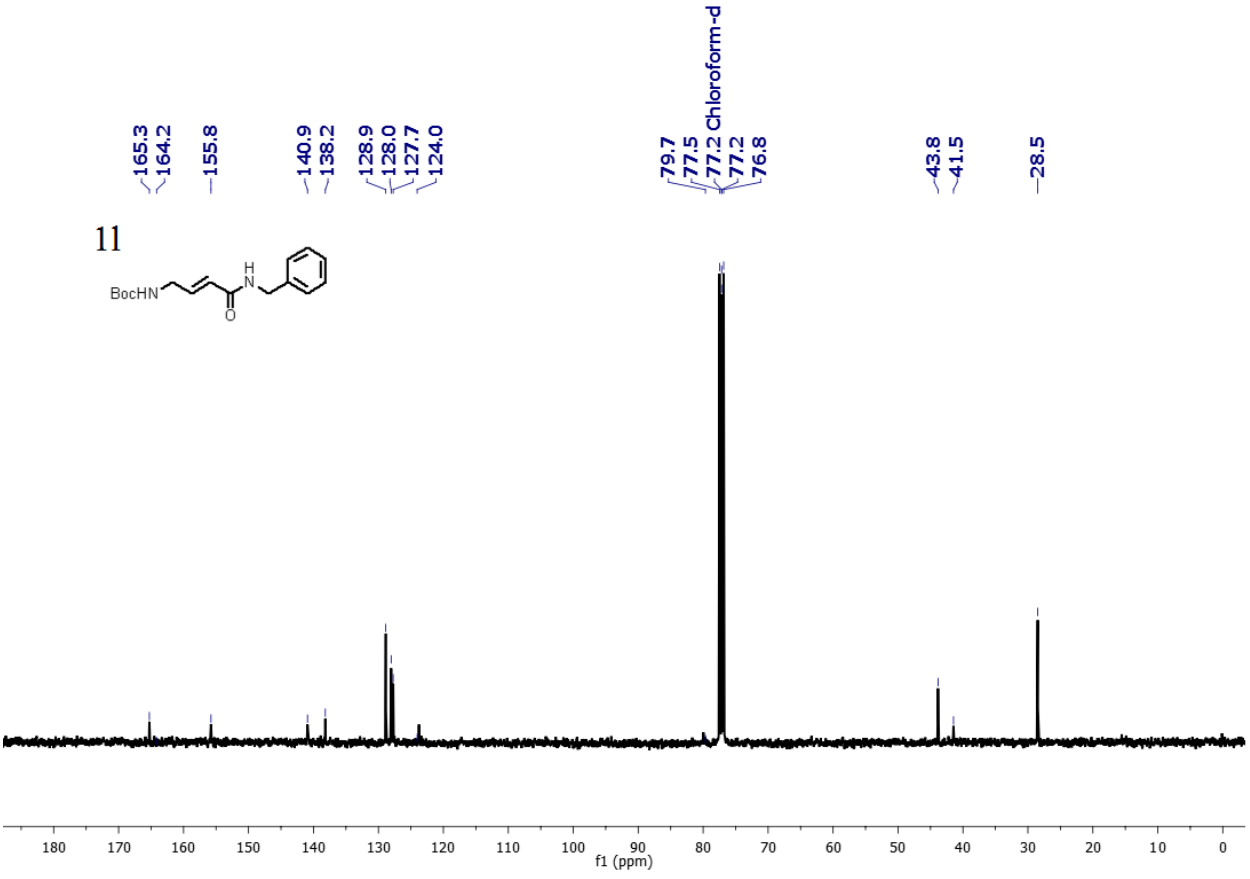

20150205-KVS-34
KVS-34
1j
BocHN
NH
H
N
O
10.84
10.84
8.53
8.51
8.50
7.32
7.31
7.29
7.23
7.23
7.21
7.12
5.98
5.94
4.40
4.39
4.37
4.35
4.32
4.30
4.29
2.90
2.88
2.50 Dimethyl Sulfoxide-d6
1.35
1.06
1.07
1.17
3.61
3.48
1.99
1.21
1.15
1.28
0.99
1.24
2.06
2.08
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
Chemical Shift (ppm)

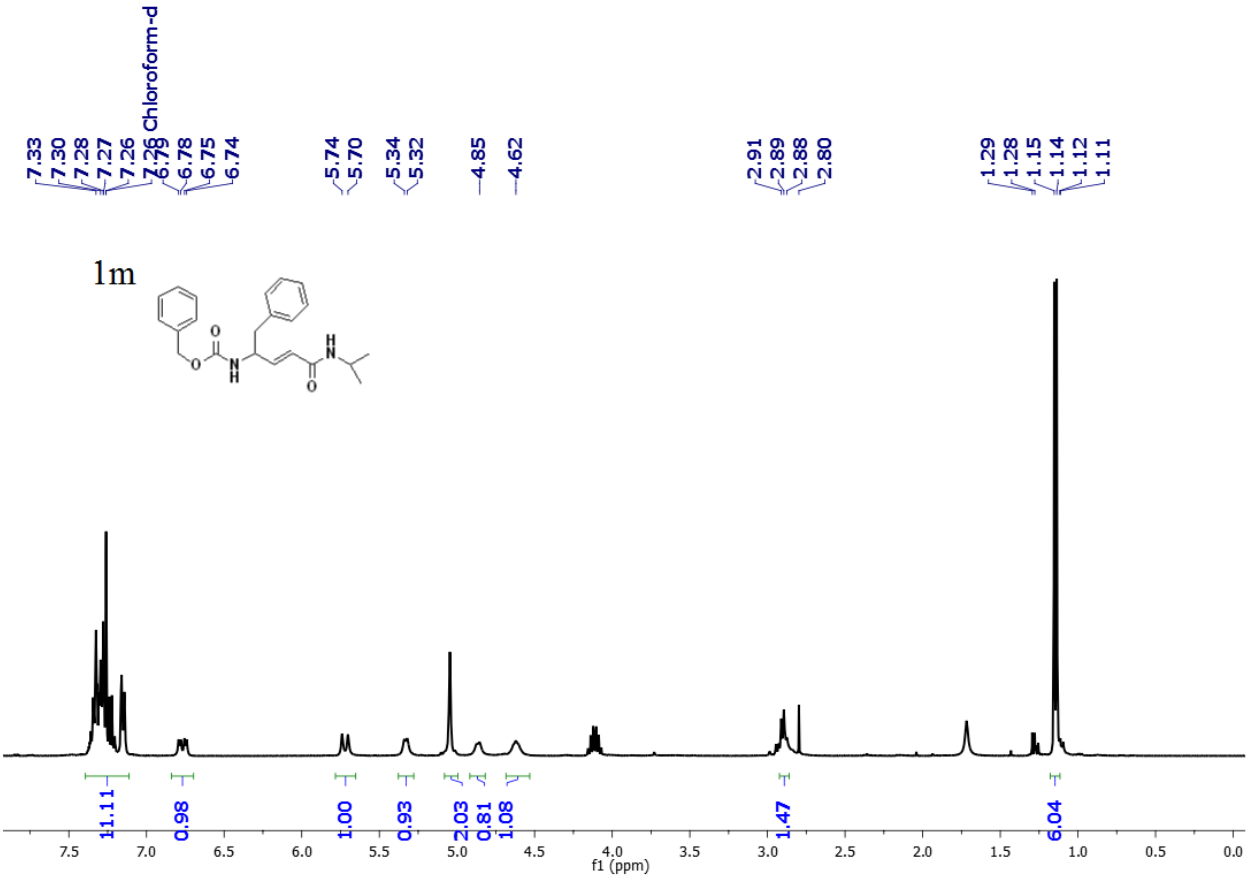

20150205-KVS-34
KVS-34
1j
BocHN
NH
H
N
O
164.7
155.0
143.3
139.5
136.1
128.3
127.3
126.8
123.4
123.3
120.8
118.3
118.2
111.3
110.6
77.7
51.9
42.1
40.1
39.9
39.7
39.5
39.5 Dimethyl Sulfoxide-d6
39.3
39.1
38.9
30.3
28.2
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

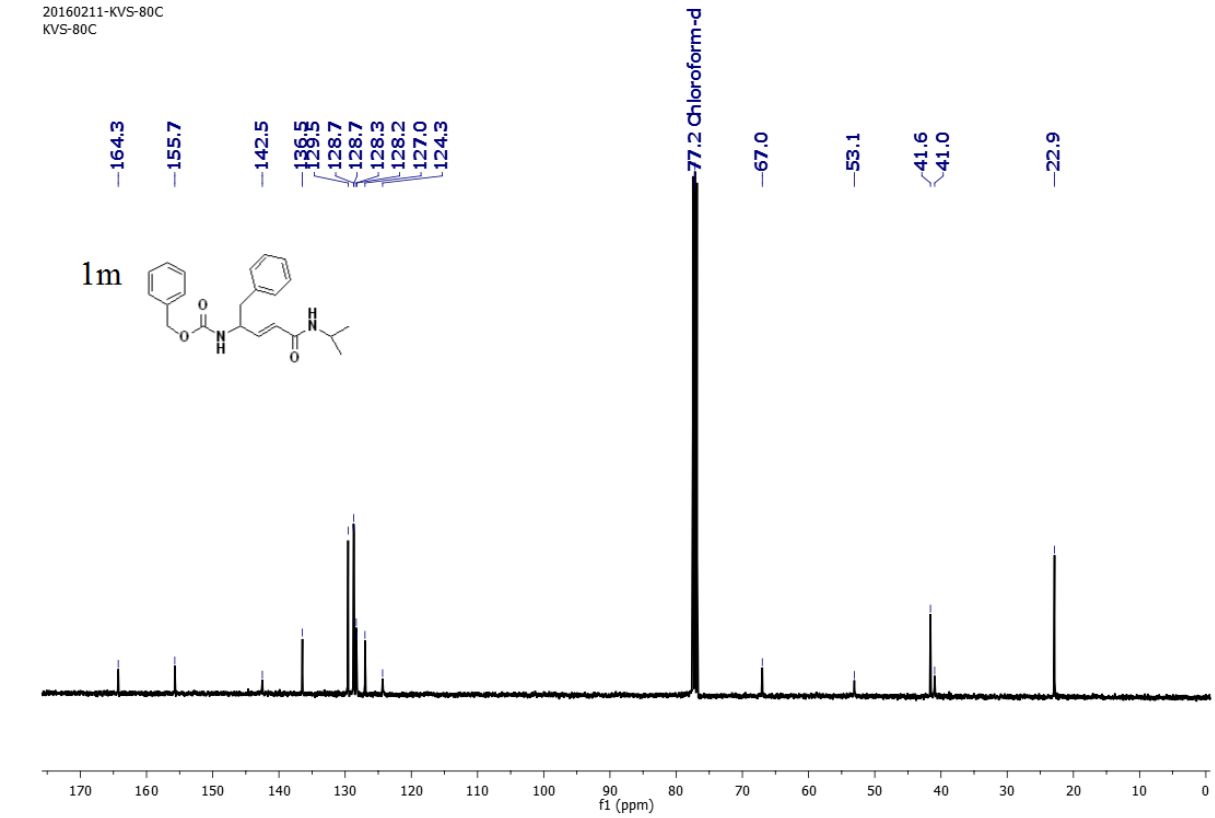

20160413-KVS-90A
7.26 Chloroform-d
6.77
6.74
5.79
5.75
5.57
4.56
2.88
2.87
2.85
2.84
1.38
1k
BocHN
5.66
0.92
1.00
0.92
1.77
1.65
3.14
9.03
f1 (ppm)

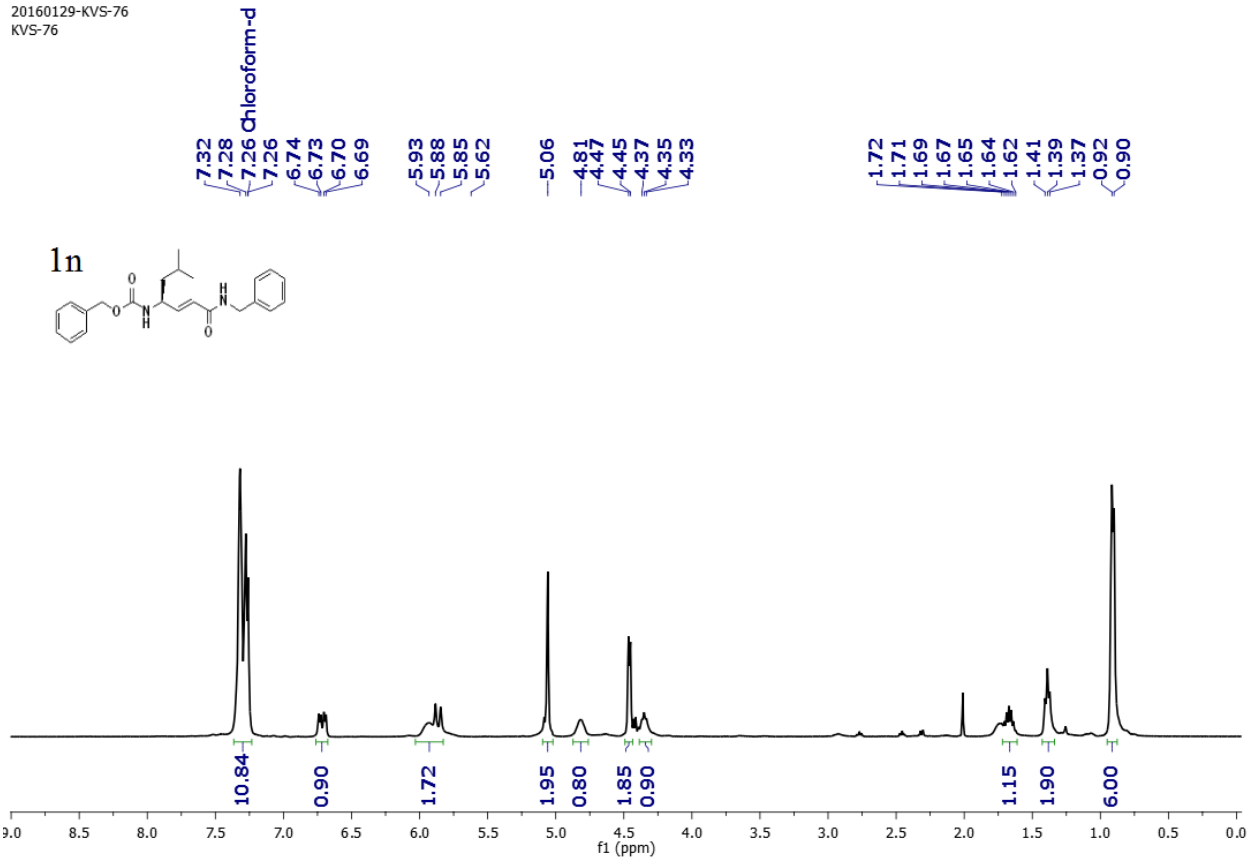

20160611-KVS-90AC13
166.3
155.2
143.0
136.7
129.8
128.5
126.9
123.8
79.6
77.2 Chloroform-d
52.7
41.1
28.4
26.5
1k
BocHN
f1 (ppm)

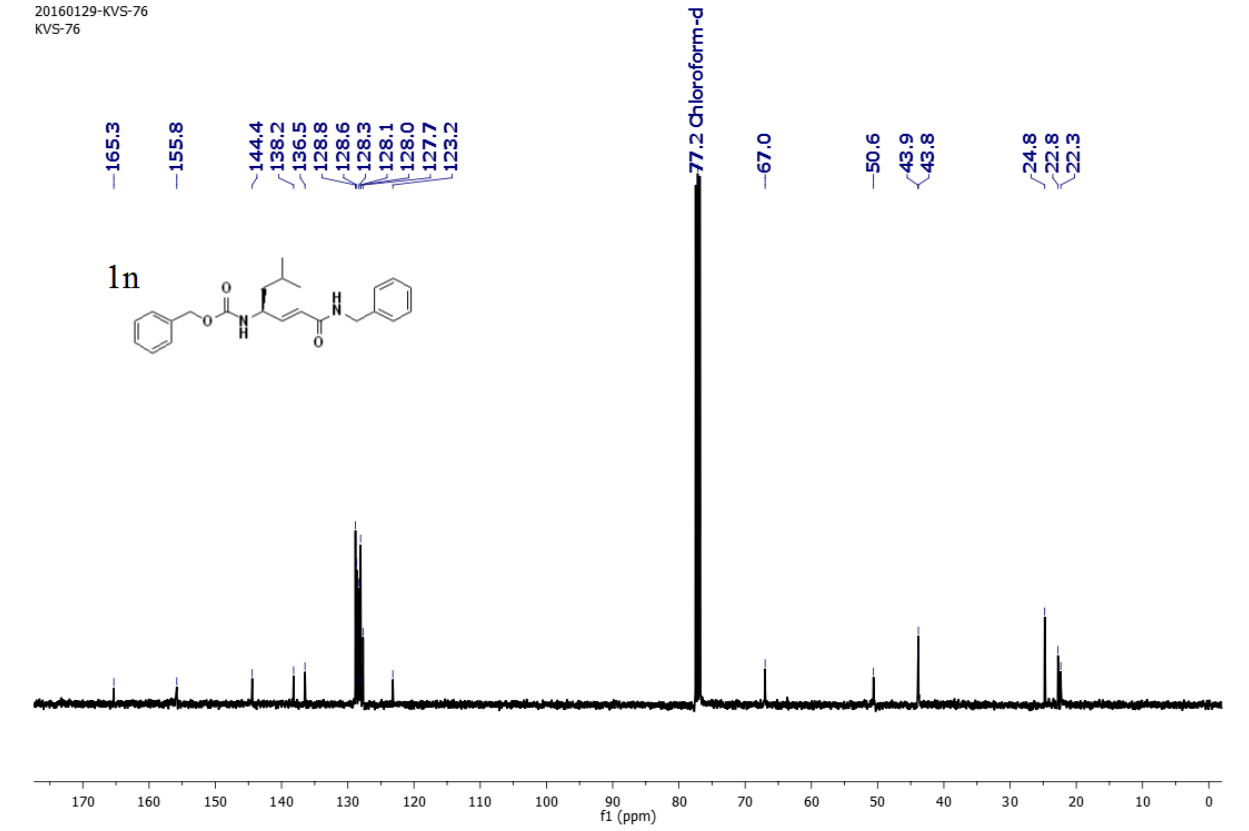

8.55
8.54
8.53
7.33
7.31
7.31
7.30
7.30
7.25
7.23
7.12
6.59
6.57
6.55
6.54
6.00
5.97
4.33
4.31
3.69
3.68
3.67
2.50 Dimethyl Sulfoxide-d6
1.39
11
BocHN
0.98
2.12
3.08
0.84
1.00
0.99
2.03
1.98
6.17
9.28
f1 (ppm)

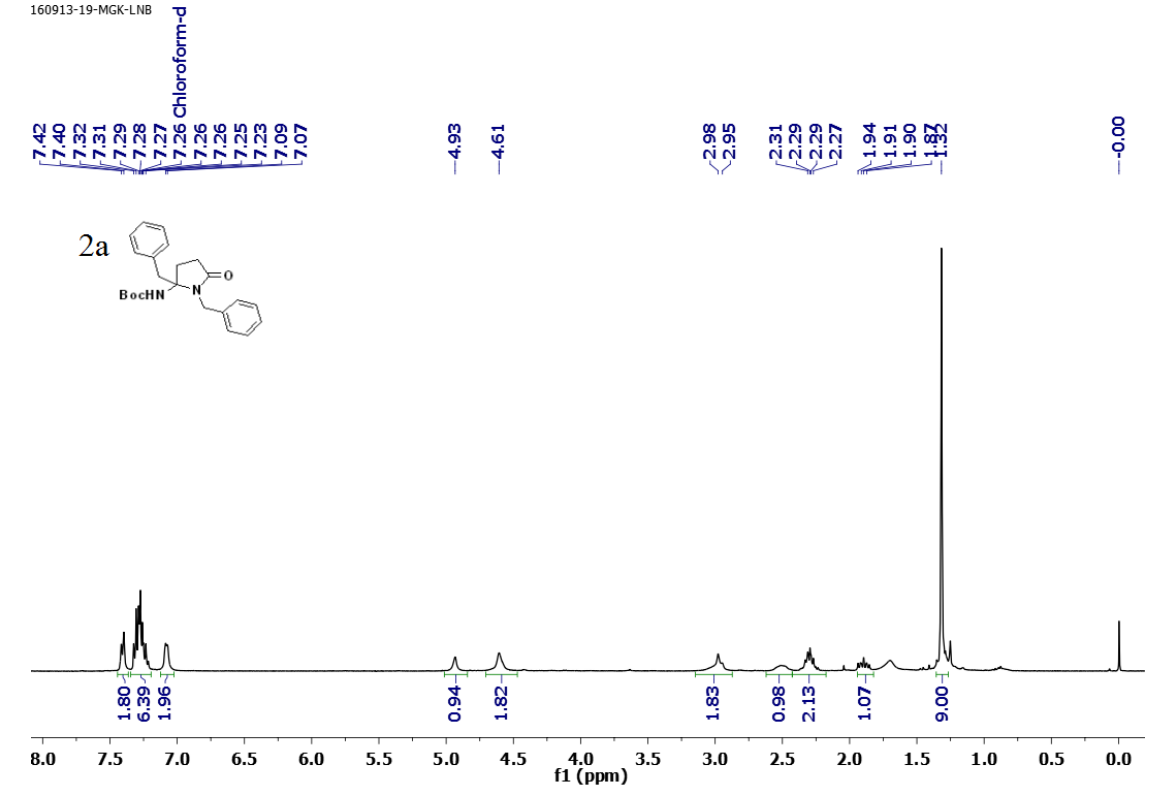

165.3
164.2
155.8
140.9
138.2
128.9
128.0
127.7
124.0
79.7
77.5
77.2 Chloroform-d
77.2
76.8
43.8
41.5
28.5
11
BocHN
f1 (ppm)

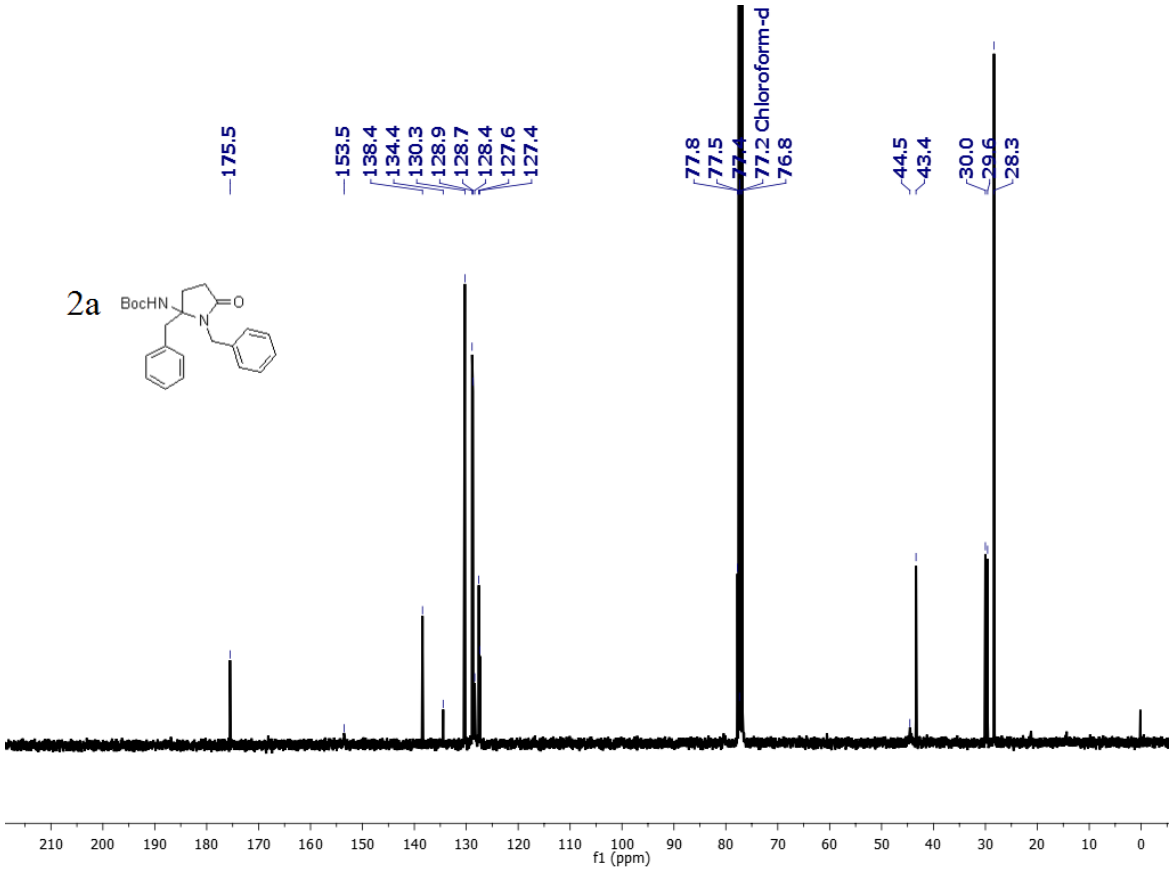

7.33
7.30
7.28
7.27
7.26
Chloroform-d
6.79
6.78
6.75
6.74
5.74
5.70
5.34
5.32
4.85
4.62
2.91
2.89
2.88
2.80
1.29
1.28
1.15
1.14
1.12
1.11
1m
11.11
0.98
1.00
0.93
2.03
0.81
1.08
1.47
6.04
f1 (ppm)

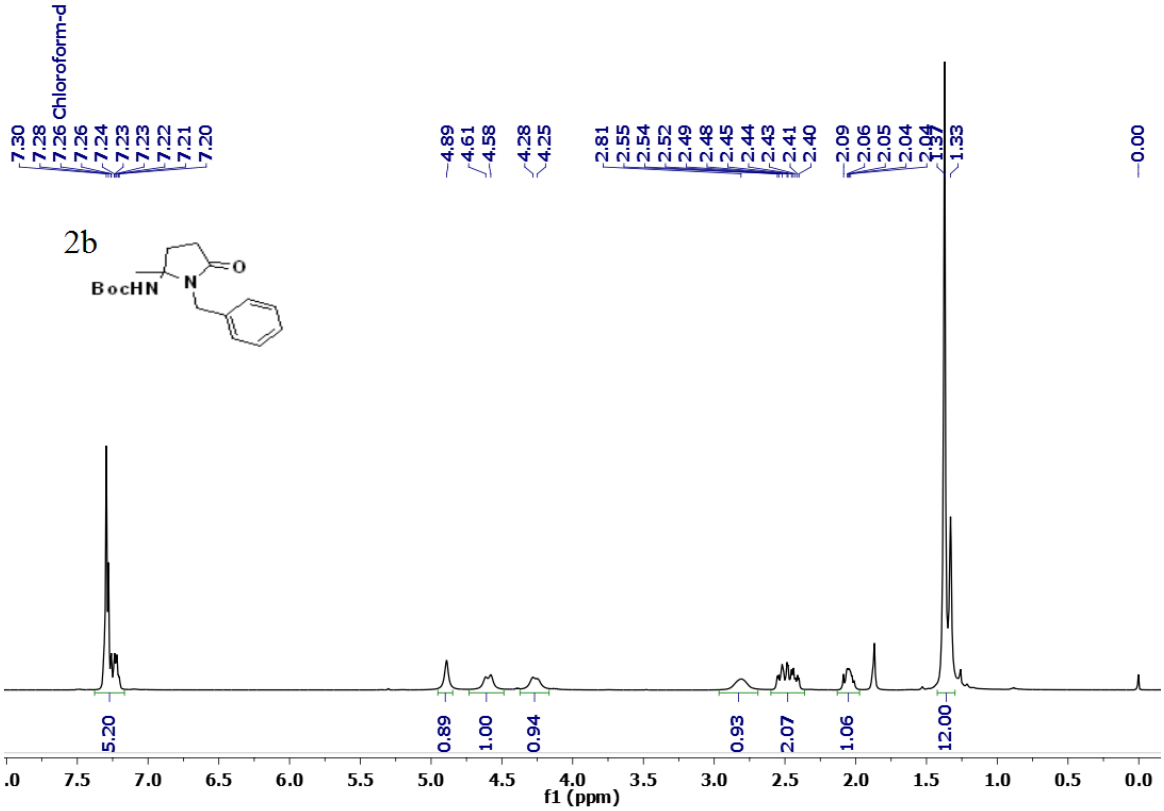

20160211-KVS-80C
KVS-80C
164.3
155.7
142.5
136.5
129.5
128.7
128.7
128.3
128.2
127.0
124.3
77.2 Chloroform-d
67.0
53.1
41.6
41.0
22.9
1m
f1 (ppm)

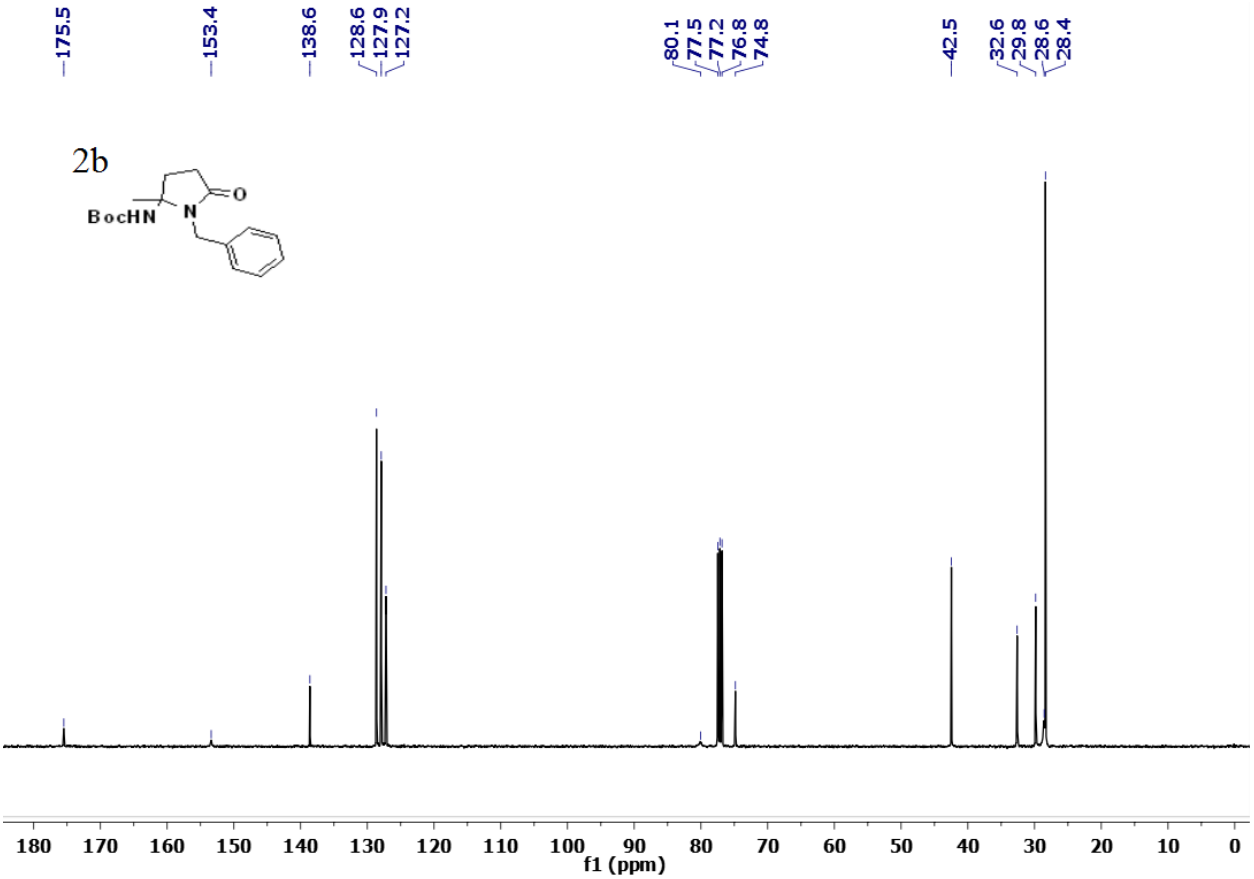

20160129-KVS-76
KVS-76
7.32
7.28
7.26 Chloroform-d
7.26
6.74
6.73
6.70
6.69
5.93
5.88
5.85
5.62
5.06
4.81
4.47
4.45
4.37
4.35
4.33
1.72
1.71
1.69
1.67
1.65
1.64
1.62
1.41
1.39
1.37
0.92
0.90
1n
10.84
0.90
1.72
1.95
0.80
1.85
0.90
1.15
1.90
6.00
f1 (ppm)

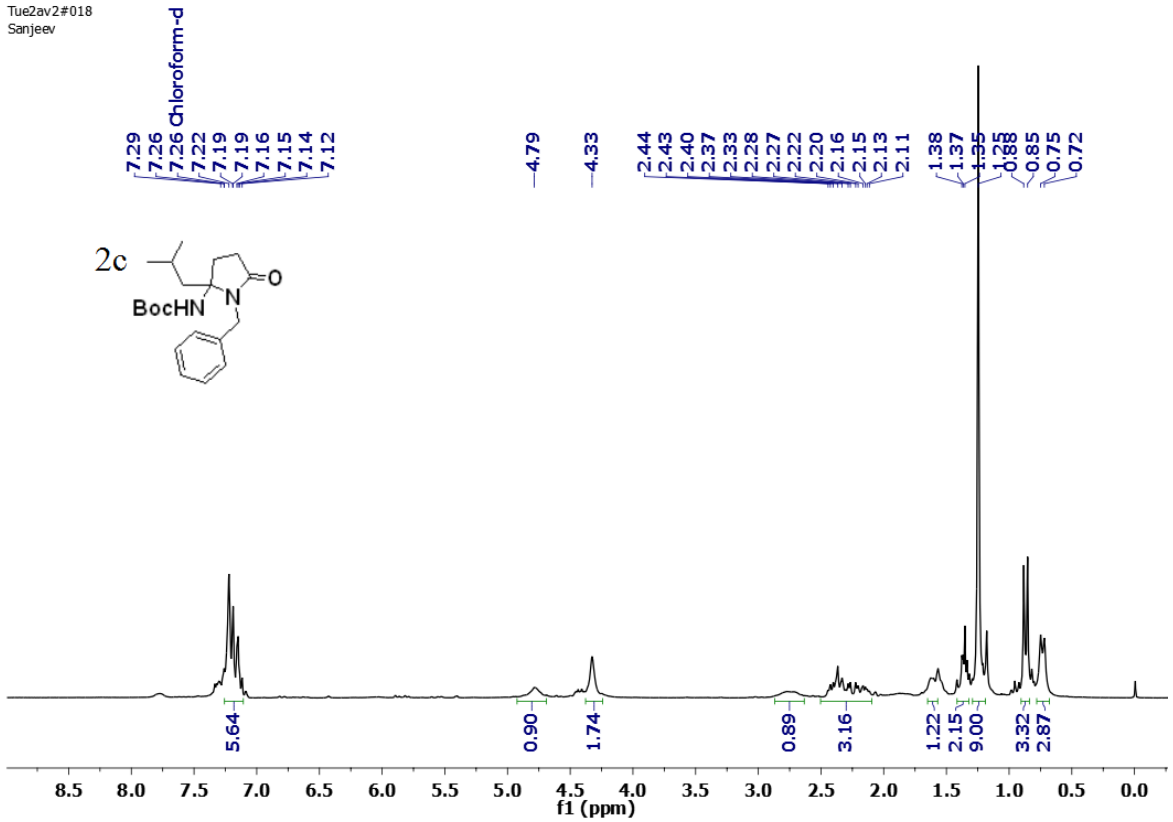

20160129-KVS-76
KVS-76
165.3
155.8
144.4
138.2
136.5
128.8
128.6
128.3
128.1
128.0
127.7
123.2
77.2 Chloroform-d
67.0
50.6
43.9
43.8
24.8
22.8
22.3
1n
f1 (ppm)

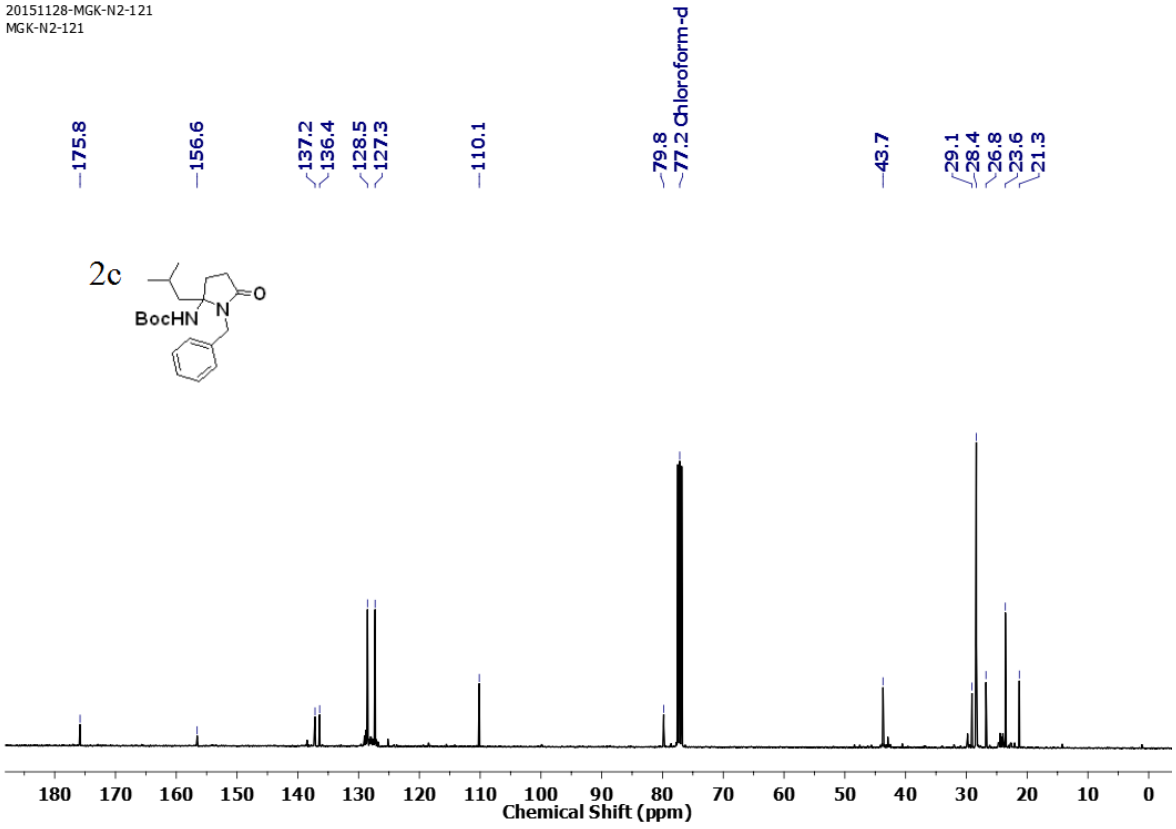

160913-19-MGK-LNB
Chloroform-d
7.42
7.40
7.32
7.31
7.29
7.28
7.27
7.26
7.26
7.26
7.25
7.23
7.09
7.07
4.93
4.61
2.98
2.95
2.31
2.29
2.29
2.27
1.94
1.91
1.90
1.87
1.82
0.00
2a
BocHN
O
N
1.80
6.39
1.96
0.94
1.82
1.83
0.98
2.13
1.07
9.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

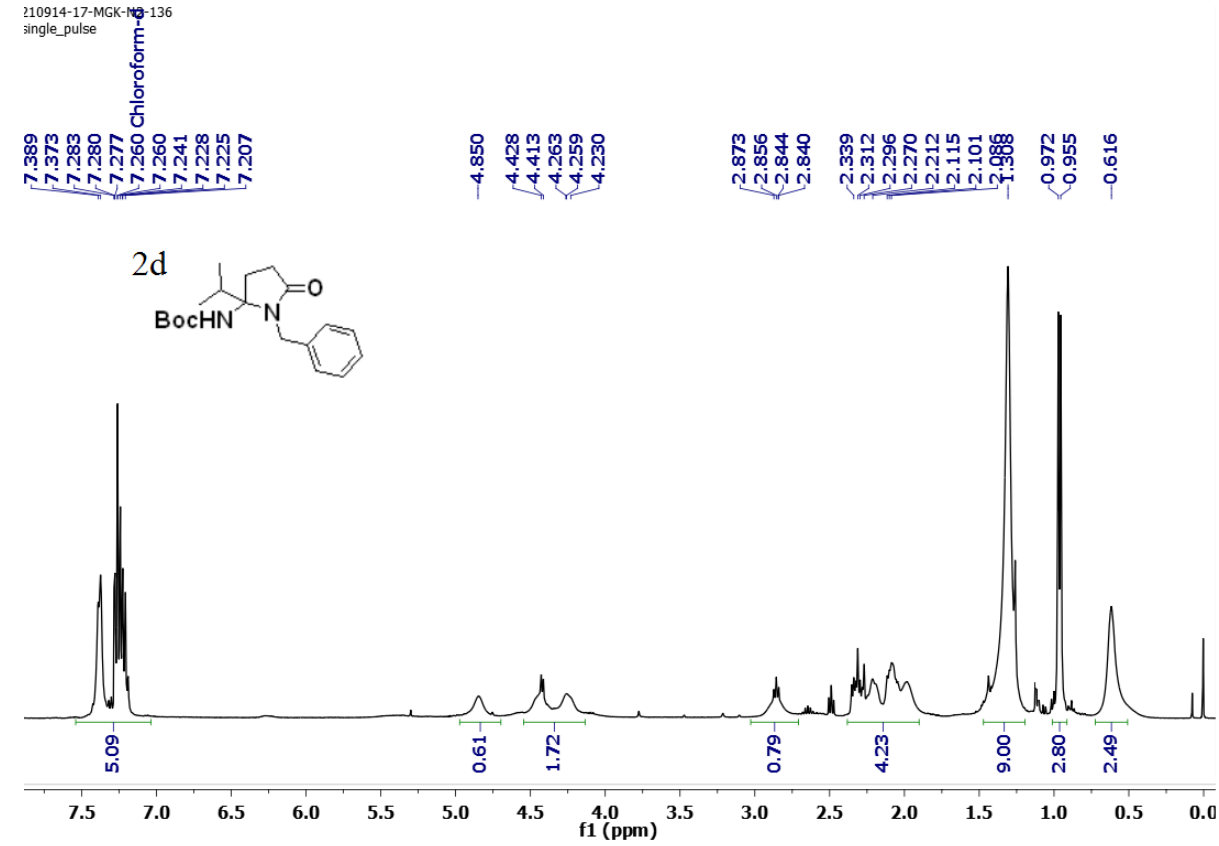

175.5
153.5
138.4
134.4
130.3
128.9
128.7
128.4
127.6
127.4
77.8
77.5
77.4
77.2 Chloroform-d
76.8
44.5
43.4
30.0
29.6
28.3
2a
BocHN
O
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

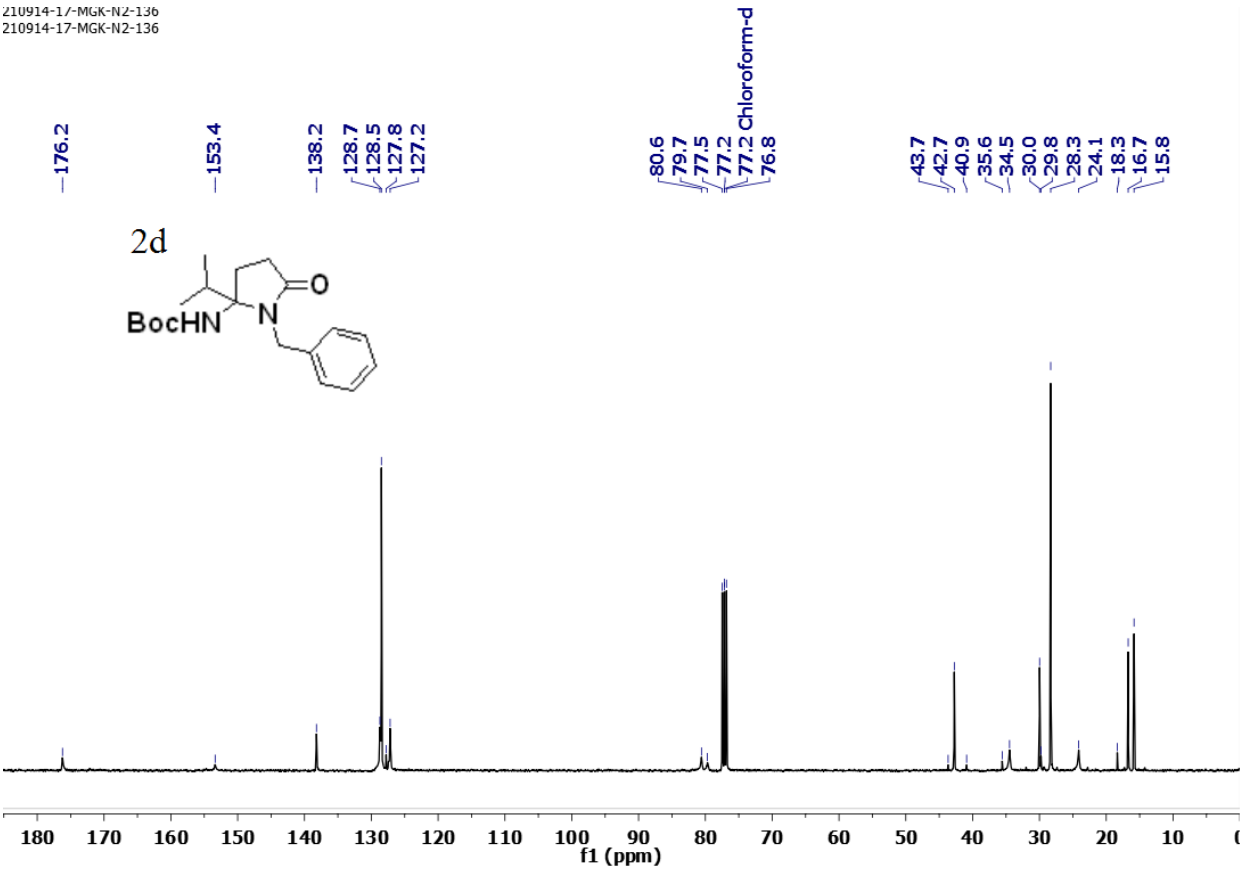

7.30
7.28
7.26 Chloroform-d
7.26
7.24
7.23
7.23
7.22
7.21
7.20
4.89
4.61
4.58
4.28
4.25
2.81
2.55
2.54
2.52
2.49
2.48
2.45
2.44
2.43
2.41
2.40
2.09
2.06
2.05
2.04
1.37
1.33
0.00
2b
BocHN
O
N
5.20
0.89
1.00
0.94
0.93
2.07
1.06
12.00
f1 (ppm)

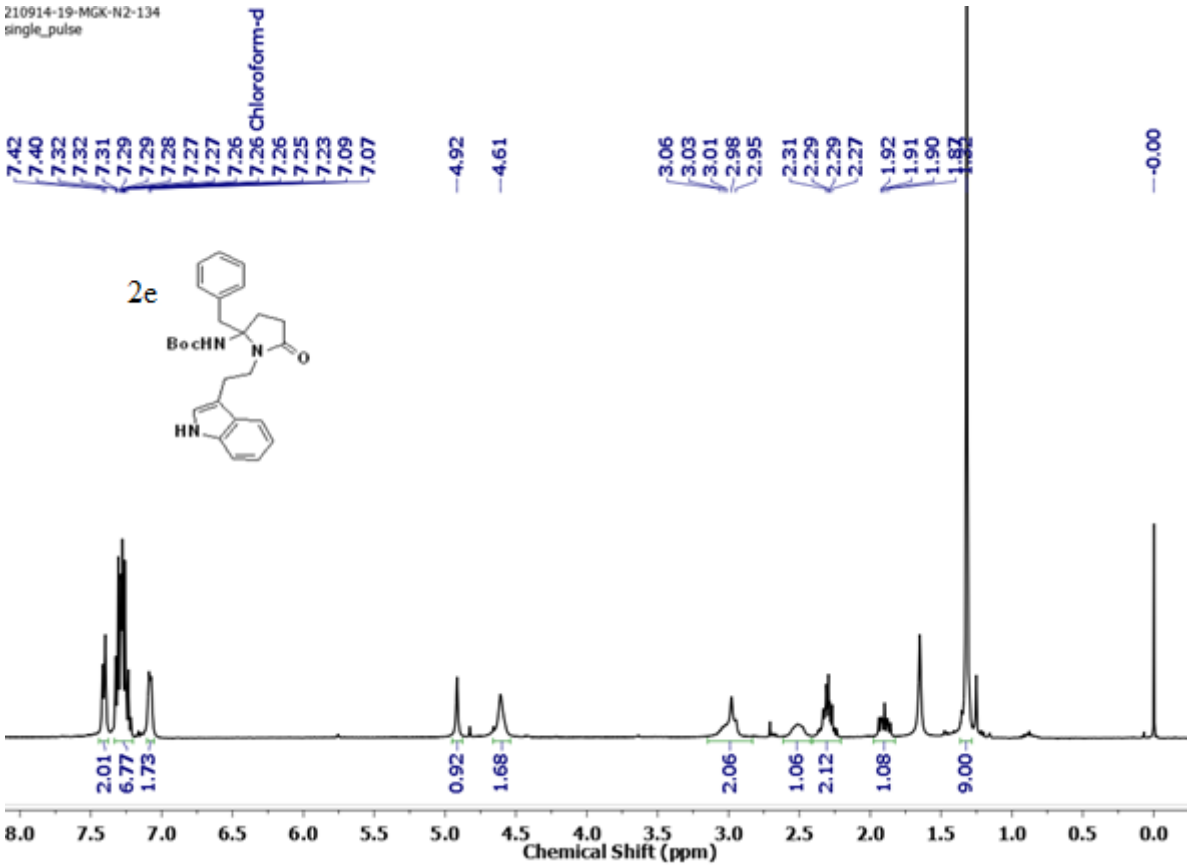

175.5
153.4
138.6
128.6
127.9
127.2
80.1
77.5
77.2
76.8
74.8
42.5
32.6
29.8
28.6
28.4
2b
BocHN
O
N
f1 (ppm)

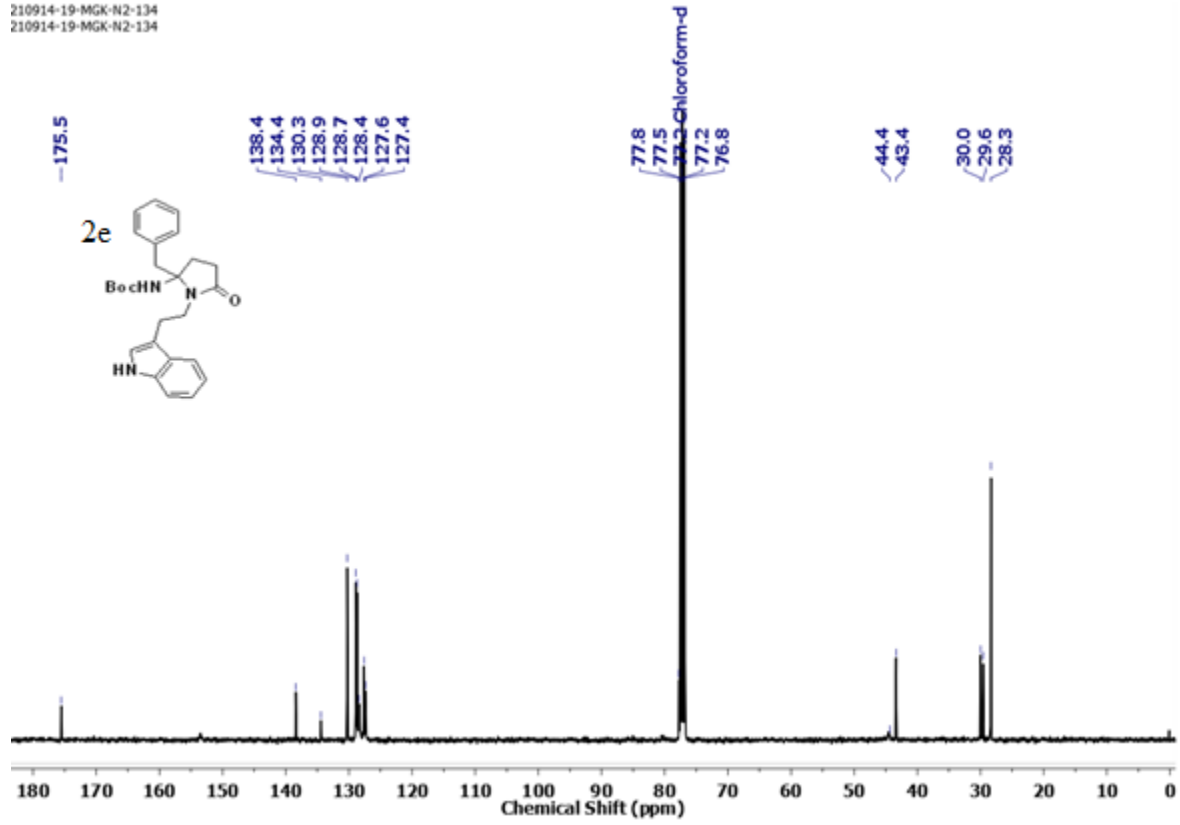

Tue2av2#018
Sanjeev
Chloroform-d
7.29
7.26
7.26
7.22
7.19
7.19
7.16
7.15
7.14
7.12
4.79
4.33
2.44
2.43
2.40
2.37
2.33
2.28
2.27
2.22
2.20
2.16
2.15
2.13
2.11
1.38
1.37
1.35
1.25
0.88
0.85
0.75
0.72
2c
BocHN
O
N
5.64
0.90
1.74
0.89
3.16
1.22
2.15
9.00
3.32
2.87
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

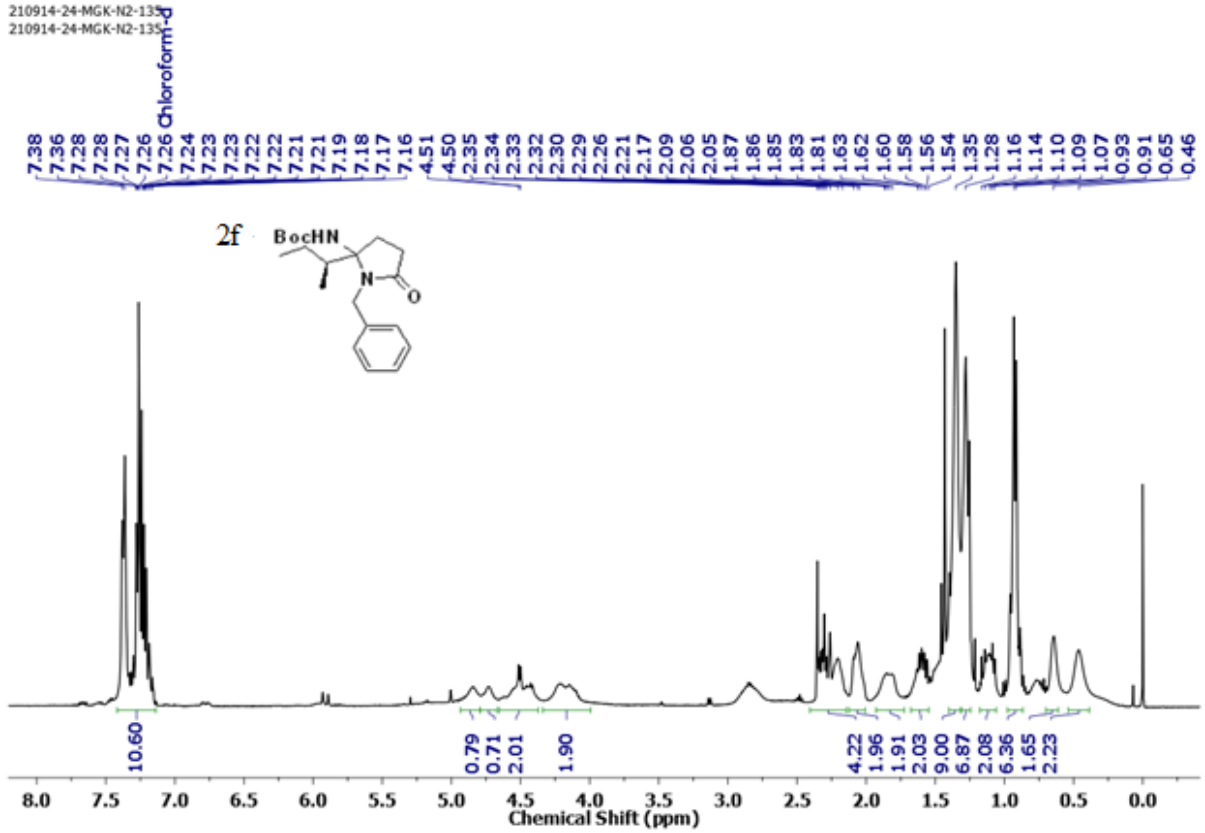

20151128-MGK-N2-121
MGK-N2-121
175.8
156.6
137.2
136.4
128.5
127.3
110.1
79.8
77.2 Chloroform-d
43.7
29.1
28.4
26.8
23.6
21.3
2c
BocHN
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

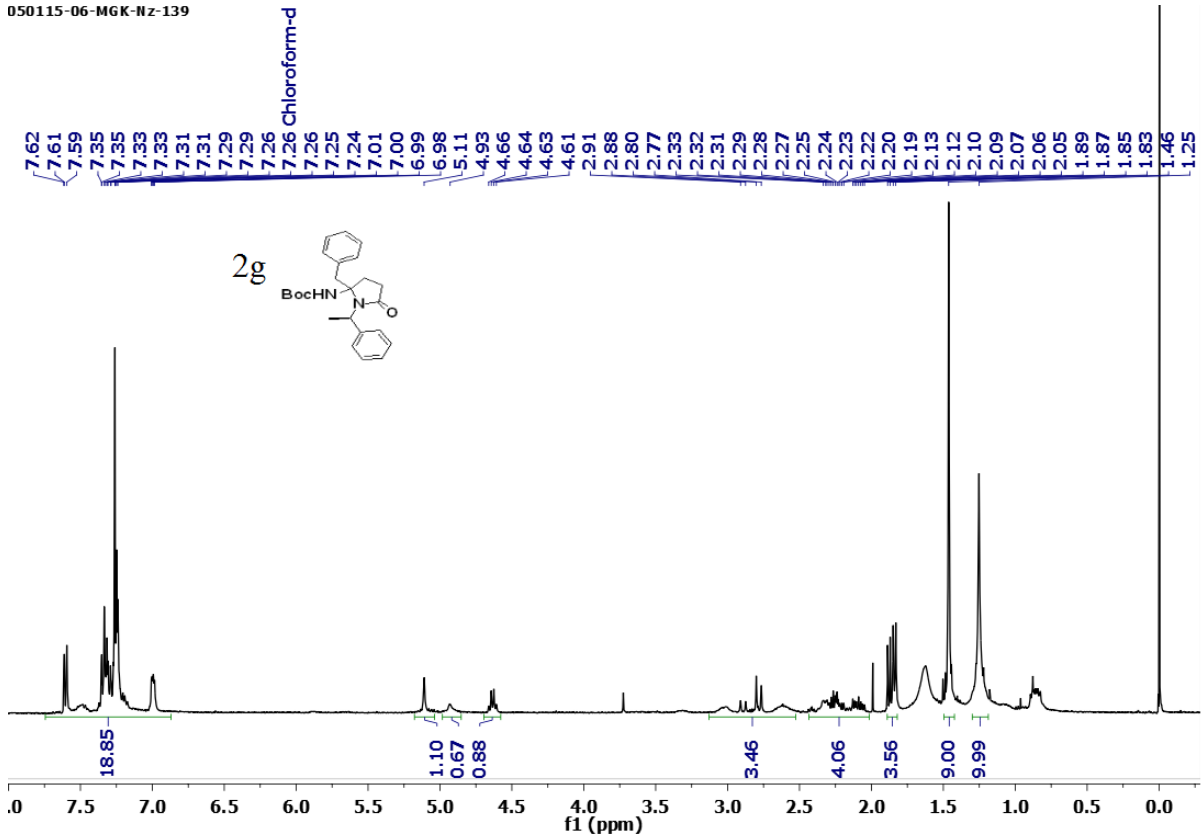

210914-17-MGK-N2-136
single_pulse
Chloroform-d
7.389
7.373
7.283
7.280
7.277
7.260
7.260
7.241
7.228
7.225
7.207
4.850
4.428
4.413
4.263
4.259
4.230
2.873
2.856
2.844
2.840
2.339
2.312
2.296
2.270
2.212
2.115
2.101
2.086
1.388
0.972
0.955
0.616
2d
BocHN
O
N
5.09
0.61
1.72
0.79
4.23
9.00
2.80
2.49
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

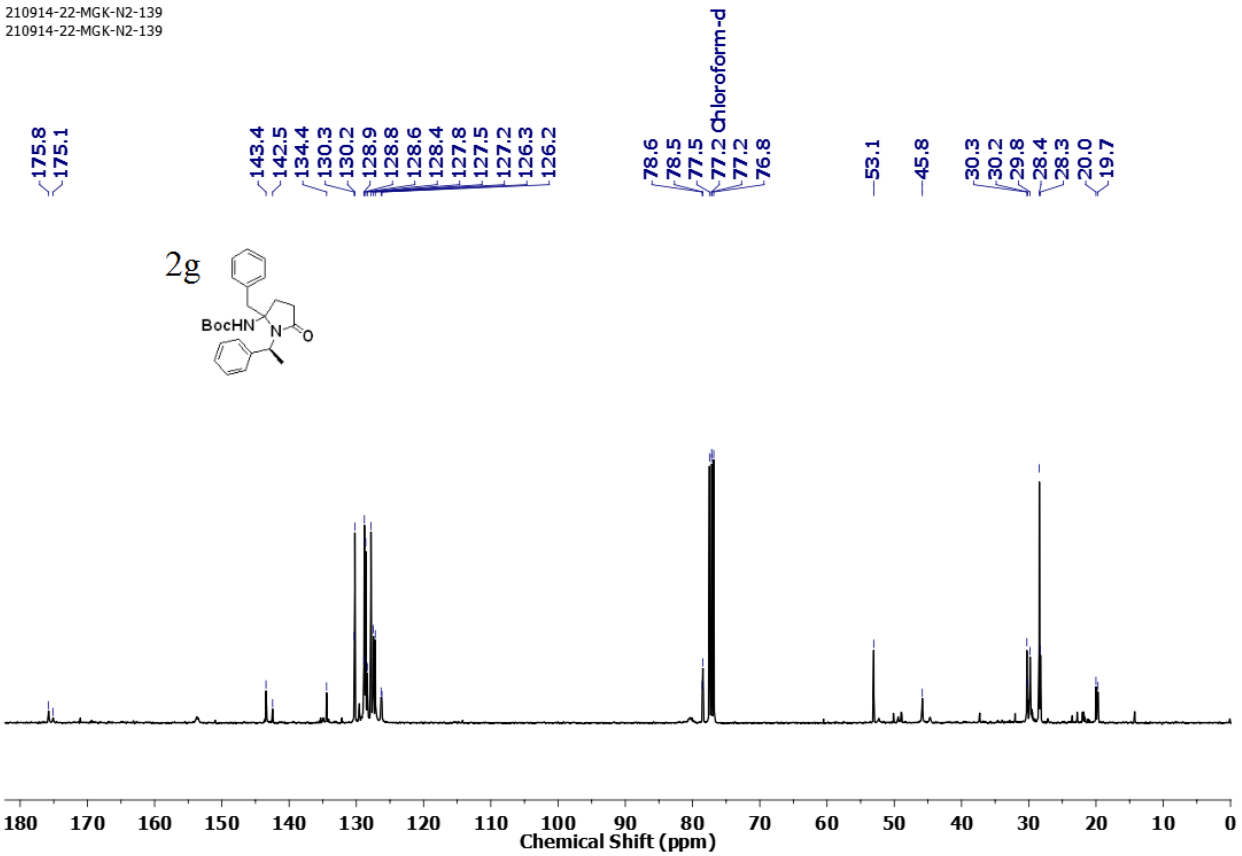

210914-17-MGK-N2-136
210914-17-MGK-N2-136
Chloroform-d
176.2
153.4
138.2
128.7
128.5
127.8
127.2
80.6
79.7
77.5
77.2
77.2
76.8
43.7
42.7
40.9
35.6
34.5
30.0
29.8
28.3
24.1
18.3
16.7
15.8
2d
BocHN
O
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

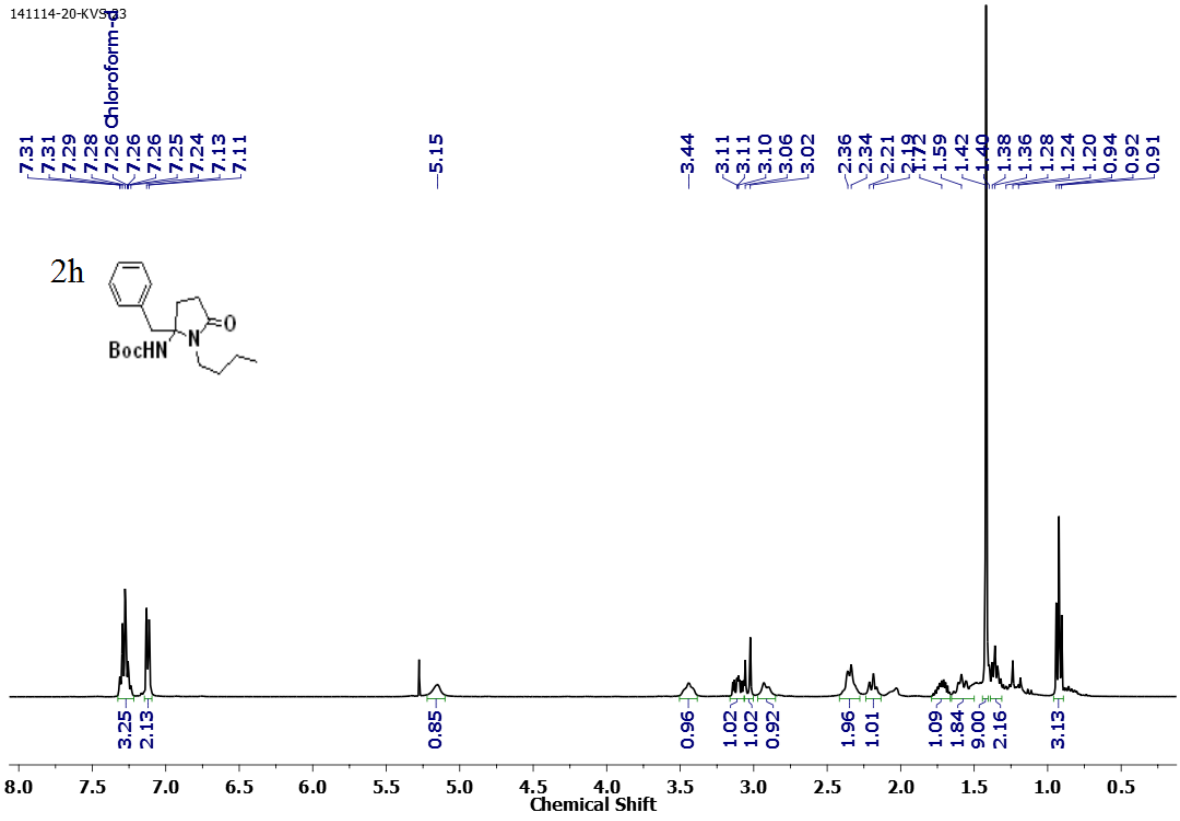

210914-19-MGK-N2-134
single_pulse
Chloroform-d
2e
BocHN
HN
Chemical Shift (ppm)

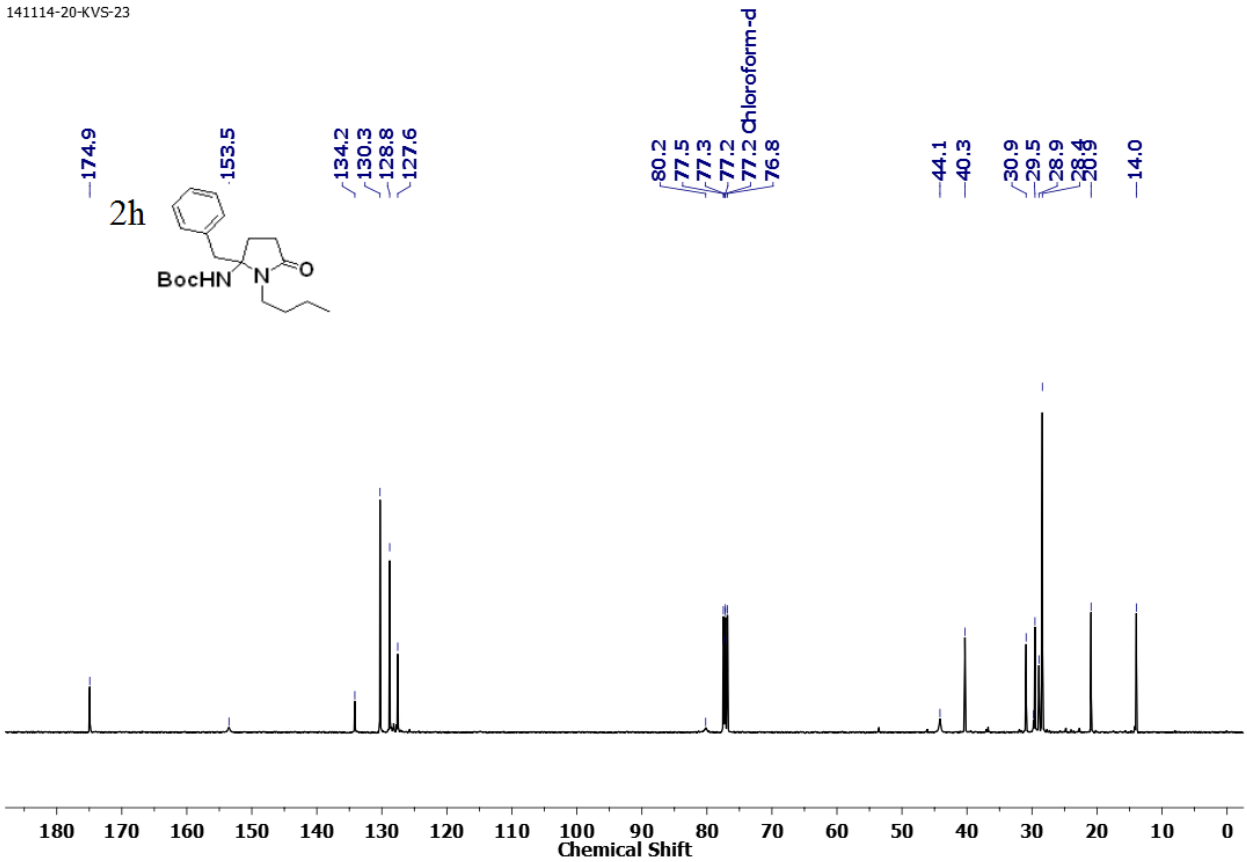

210914-19-MGK-N2-134
210914-19-MGK-N2-134
Chloroform-d
2e
BocHN
HN
Chemical Shift (ppm)

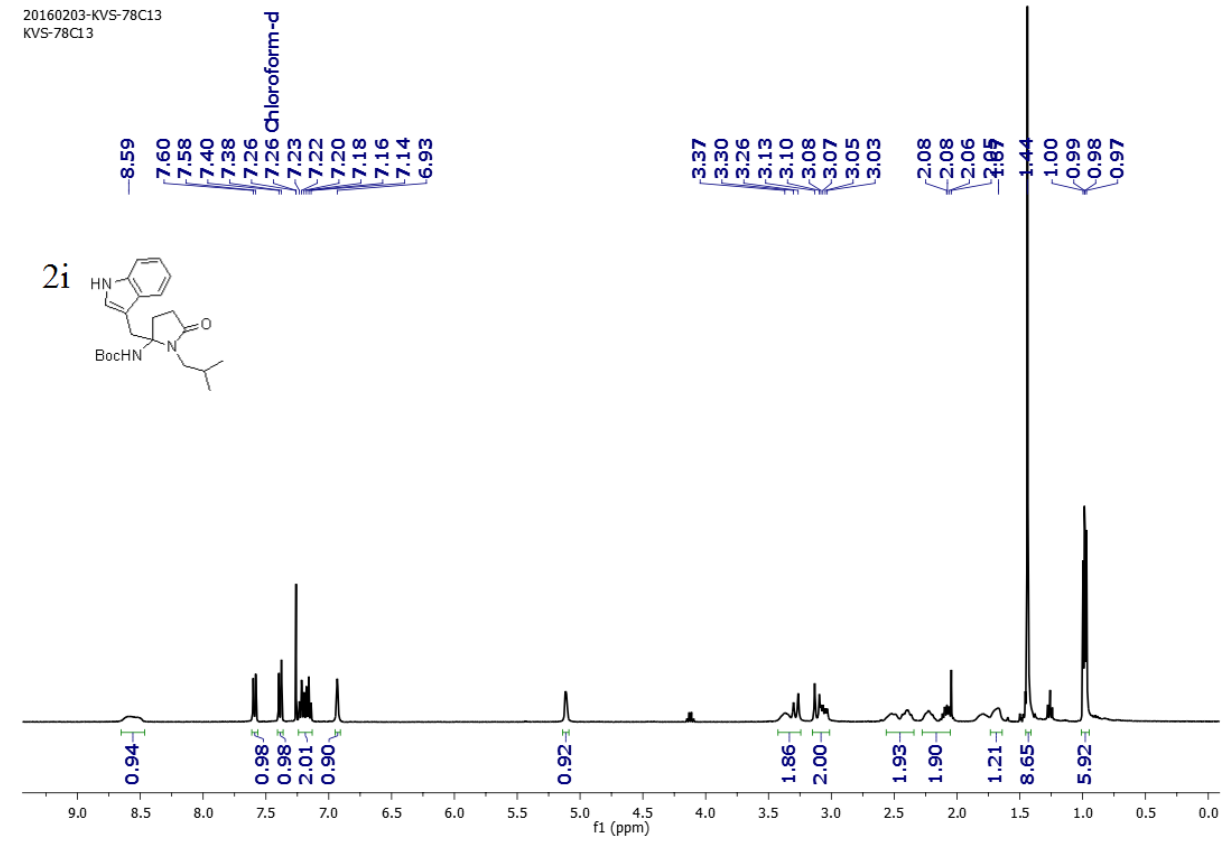

210914-24-MGK-N2-135
210914-24-MGK-N2-135
Chloroform-d
2f
BocHN
N
O
10.60
0.79
0.71
2.01
1.90
4.22
1.96
1.91
2.03
9.00
6.87
2.08
6.36
1.65
2.23
Chemical Shift (ppm)

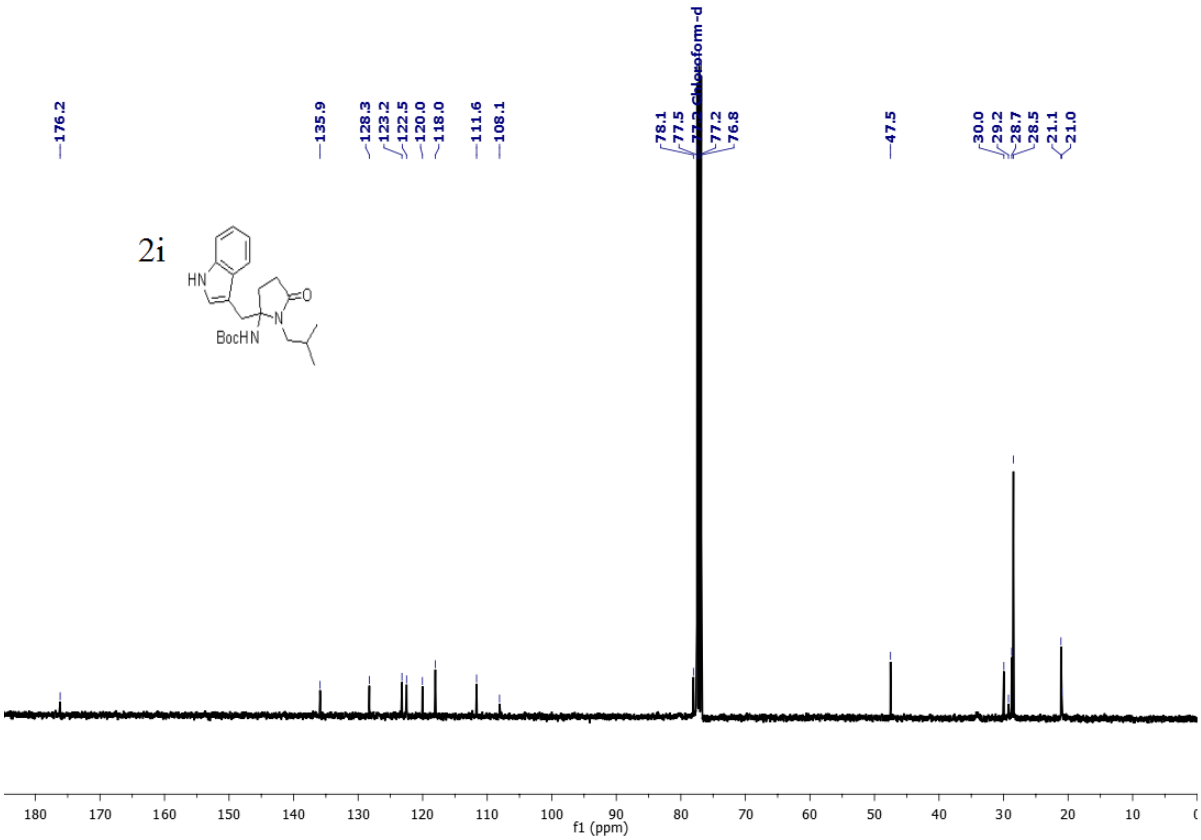

050115-06-MGK-Nz-139
Chloroform-d
2g
BocHN
N
O
18.85
1.10
0.67
0.88
3.46
4.06
3.56
9.00
9.99
f1 (ppm)

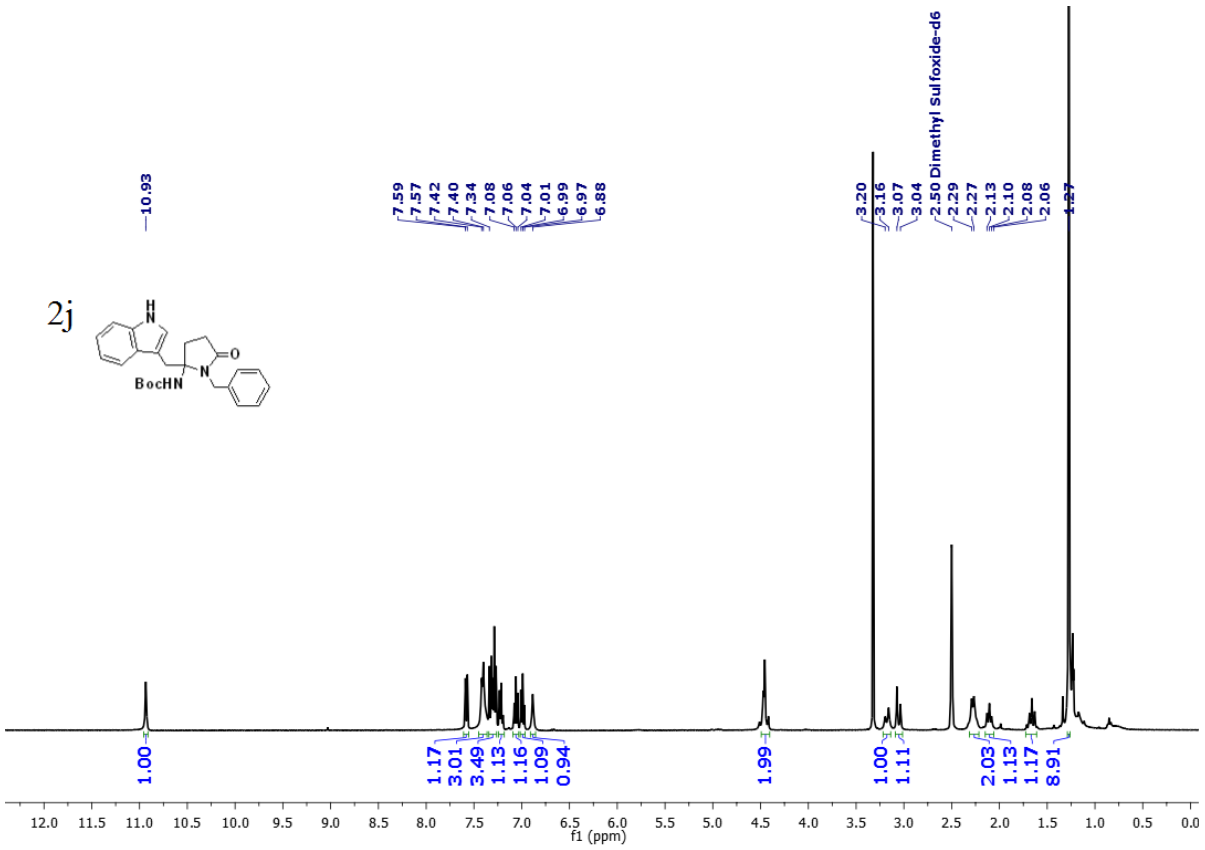

210914-22-MGK-N2-139
210914-22-MGK-N2-139
175.8
175.1
143.4
142.5
134.4
130.3
130.2
128.9
128.8
128.6
128.4
127.8
127.5
127.2
126.3
126.2
78.6
78.5
77.5
77.2 Chloroform-d
77.2
76.8
53.1
45.8
30.3
30.2
29.8
28.4
28.3
20.0
19.7
2g
BocHN
N
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

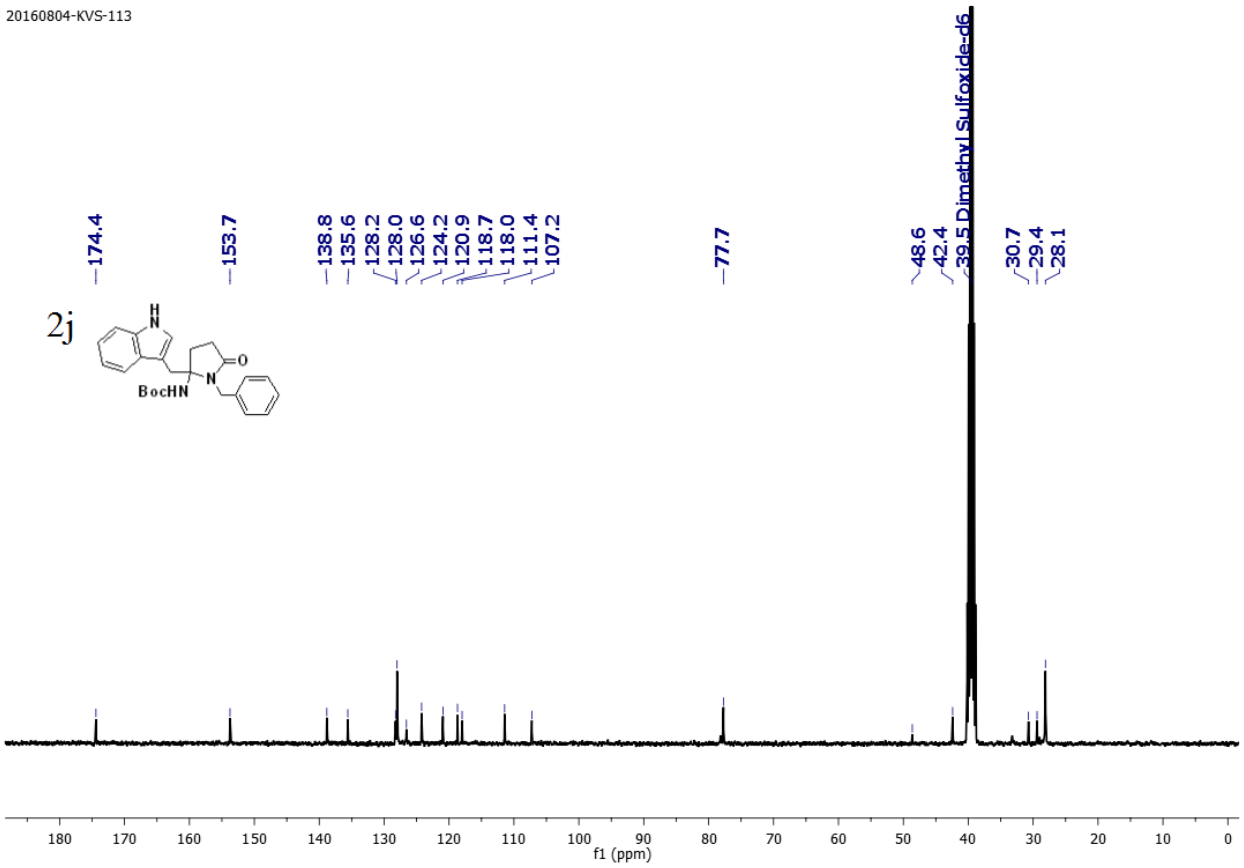

141114-20-KVS-33
7.31
7.31
7.29
7.28
7.26 Chloroform-d
7.26
7.26
7.25
7.24
7.13
7.11
5.15
3.44
3.11
3.11
3.10
3.06
3.02
2.36
2.34
2.21
2.19
1.72
1.59
1.42
1.40
1.38
1.36
1.28
1.24
1.20
0.94
0.92
0.91
2h
BocHN
N
O
3.25
2.13
0.85
0.96
1.02
1.02
0.92
1.96
1.01
1.09
1.84
9.00
2.16
3.13
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
Chemical Shift

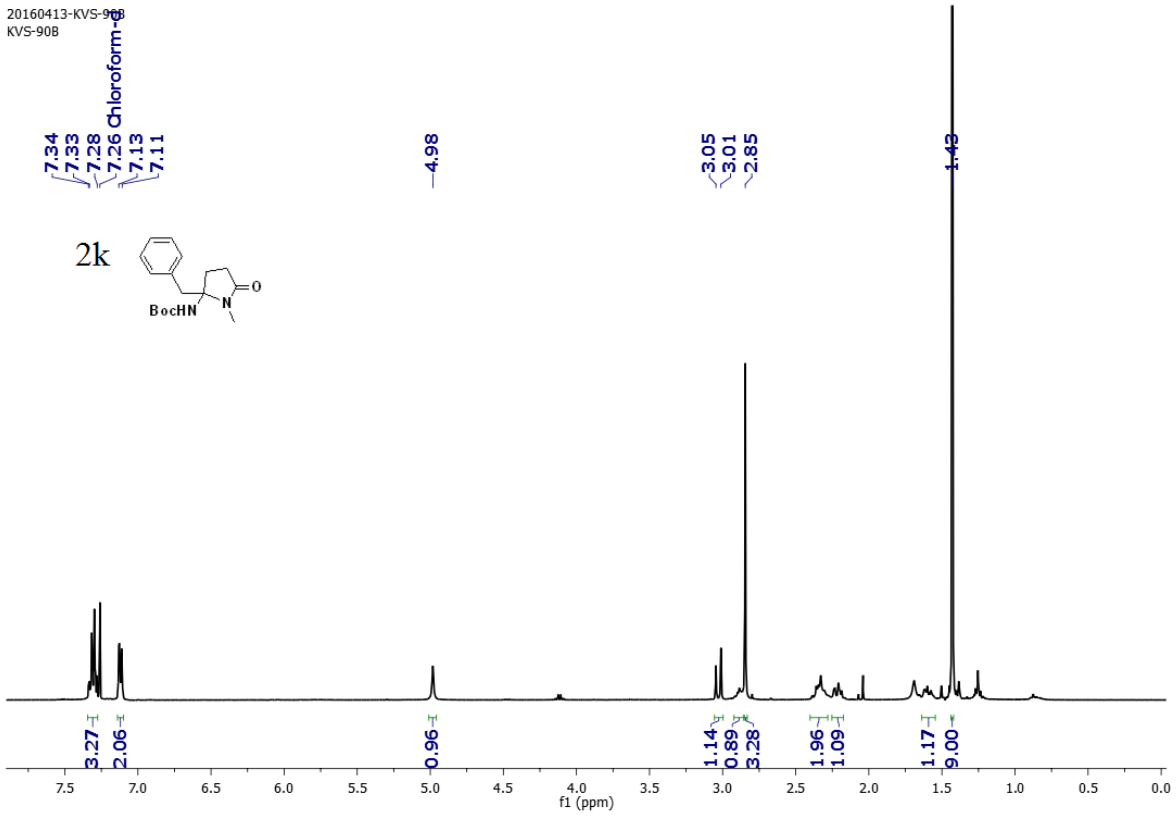

141114-20-KVS-23
174.9
153.5
134.2
130.3
128.8
127.6
80.2
77.5
77.3
77.2
77.2 Chloroform-d
76.8
44.1
40.3
30.9
29.5
28.9
28.4
20.9
14.0
2h
BocHN
N
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift

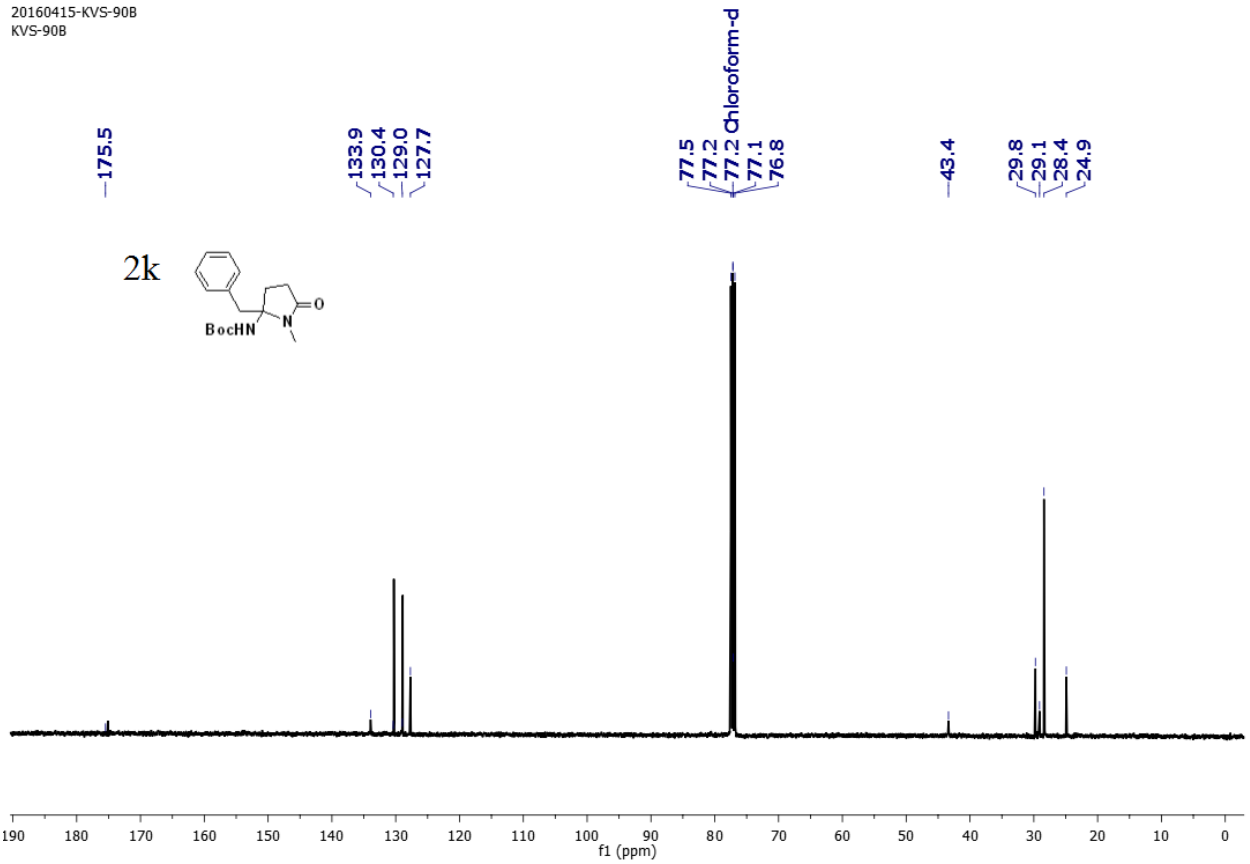

20160203-KVS-78C13
KVS-78C13
8.59
7.60
7.58
7.40
7.38
7.26
7.26 Chloroform-d
7.23
7.22
7.20
7.18
7.16
7.14
6.93
3.37
3.30
3.26
3.13
3.10
3.08
3.07
3.05
3.03
2.08
2.08
2.06
1.44
1.00
0.99
0.98
0.97
2i
HN
BocHN
N
O
0.94
0.98
0.98
2.01
0.90
0.92
1.86
2.00
1.93
1.90
1.21
8.65
5.92
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

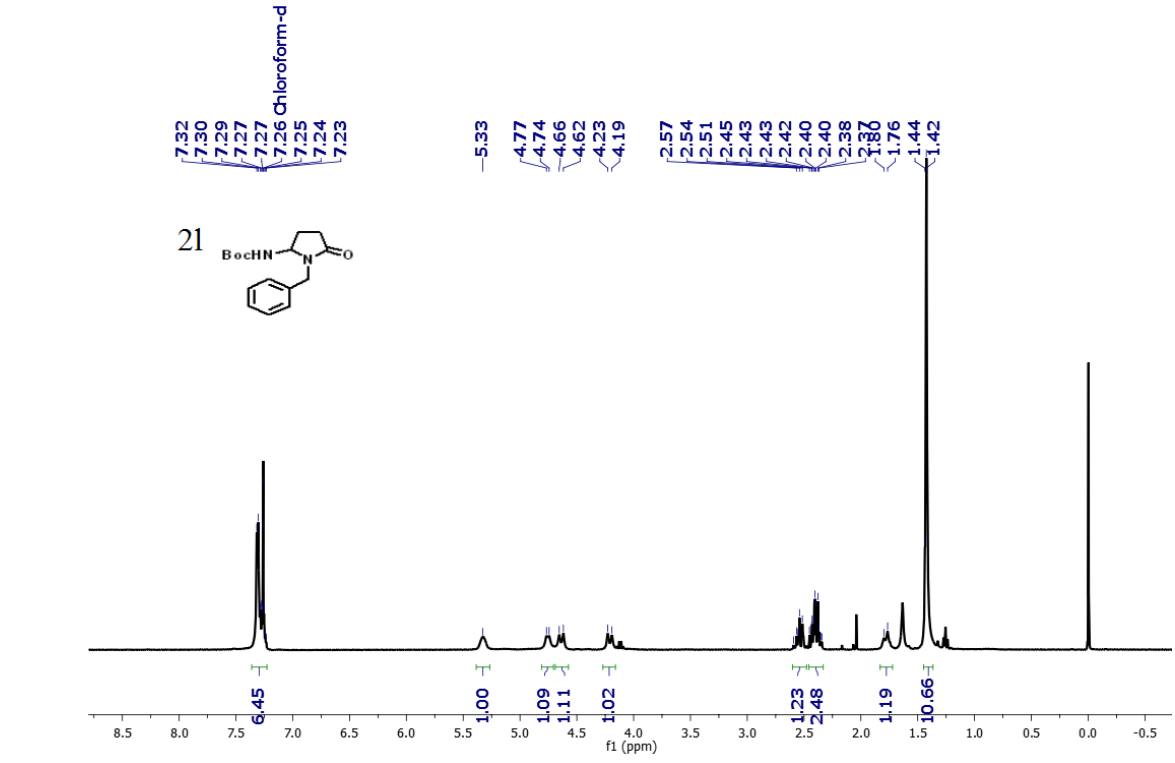

176.2
135.9
128.3
123.2
122.5
120.0
118.0
111.6
108.1
78.1
77.5
77.2
76.8
47.5
30.0
29.2
28.7
28.5
21.1
21.0
2i
HN
BocHN
f1 (ppm)

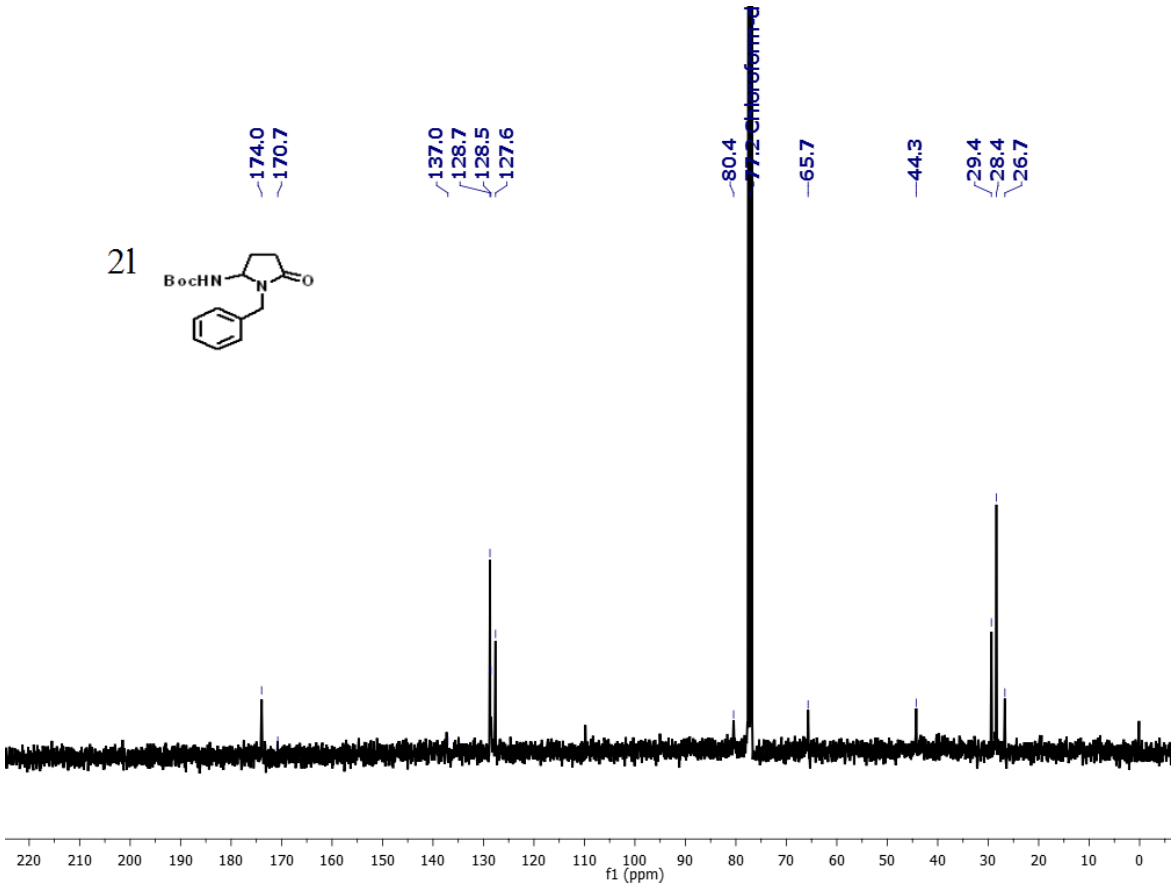

10.93
7.59
7.57
7.42
7.40
7.34
7.08
7.06
7.04
7.01
6.99
6.97
6.88
3.20
3.16
3.07
3.04
2.50 Dimethyl Sulfoxide-d6
2.29
2.27
2.13
2.10
2.08
2.06
1.27
2j
BocHN
1.00
1.17
3.01
3.49
1.13
1.16
1.09
0.94
1.99
1.00
1.11
2.03
1.13
1.17
8.91
f1 (ppm)

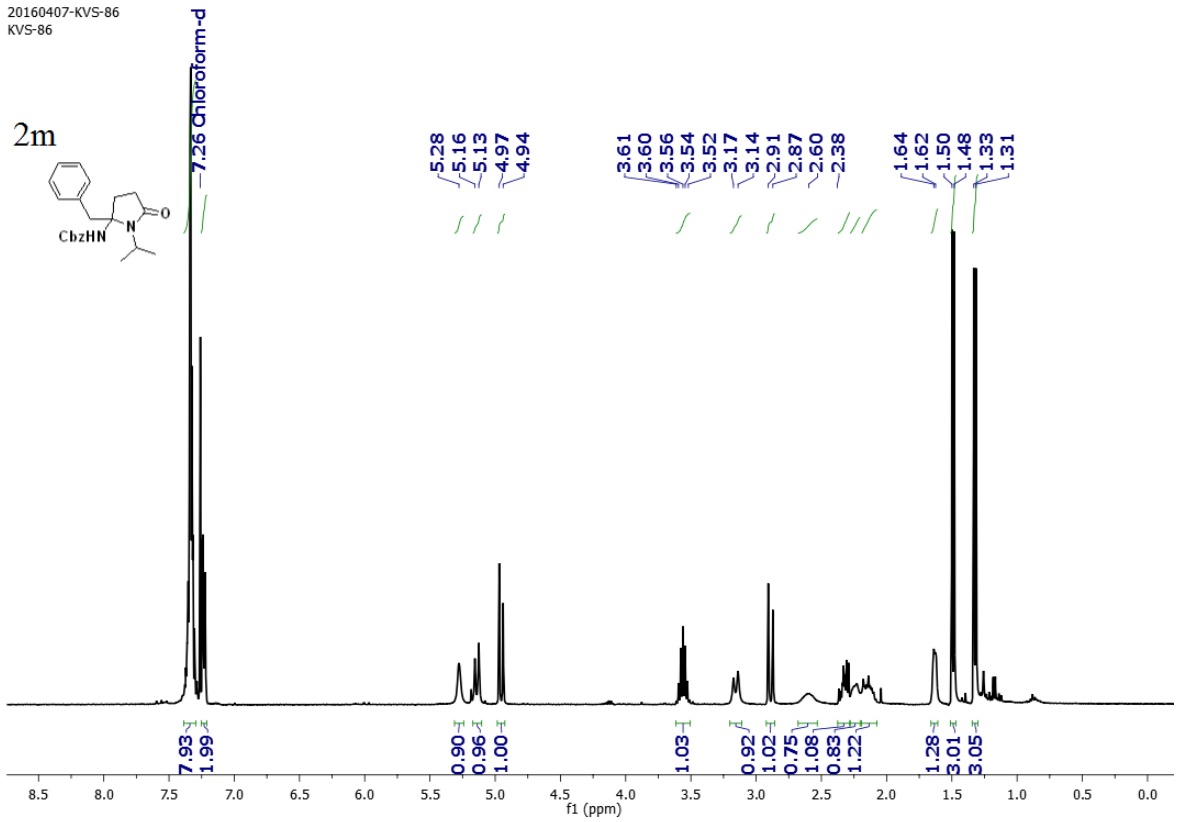

20160804-KVS-113
174.4
153.7
138.8
135.6
128.2
128.0
126.6
124.2
120.9
118.7
118.0
111.4
107.2
77.7
48.6
42.4
39.5 Dimethyl Sulfoxide-d6
30.7
29.4
28.1
2j
BocHN
f1 (ppm)

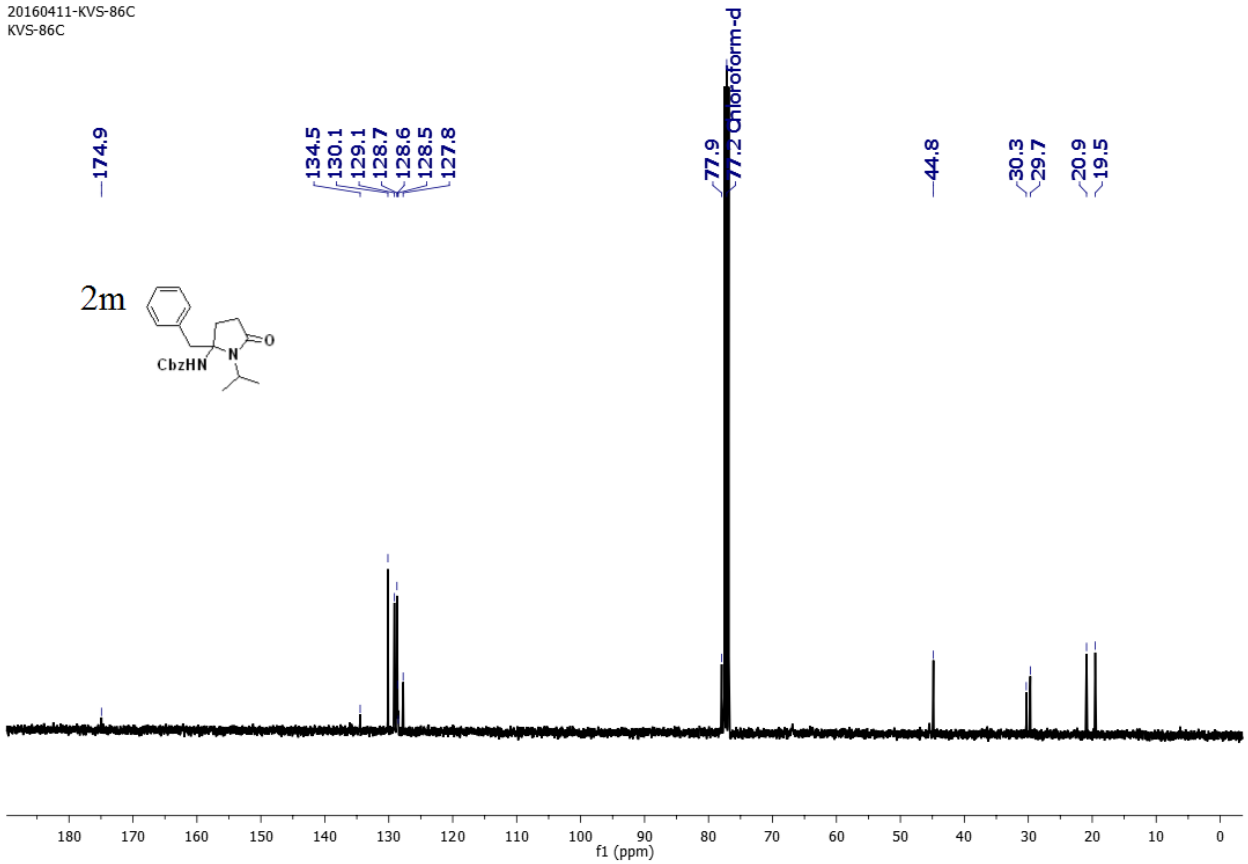

20160413-KVS-90B
KVS-90B
7.34
7.33
7.28
7.26 Chloroform-d
7.13
7.11
4.98
3.05
3.01
2.85
1.43
2k
BocHN
3.27
2.06
0.96
1.14
0.89
3.28
1.96
1.09
1.17
9.00
f1 (ppm)

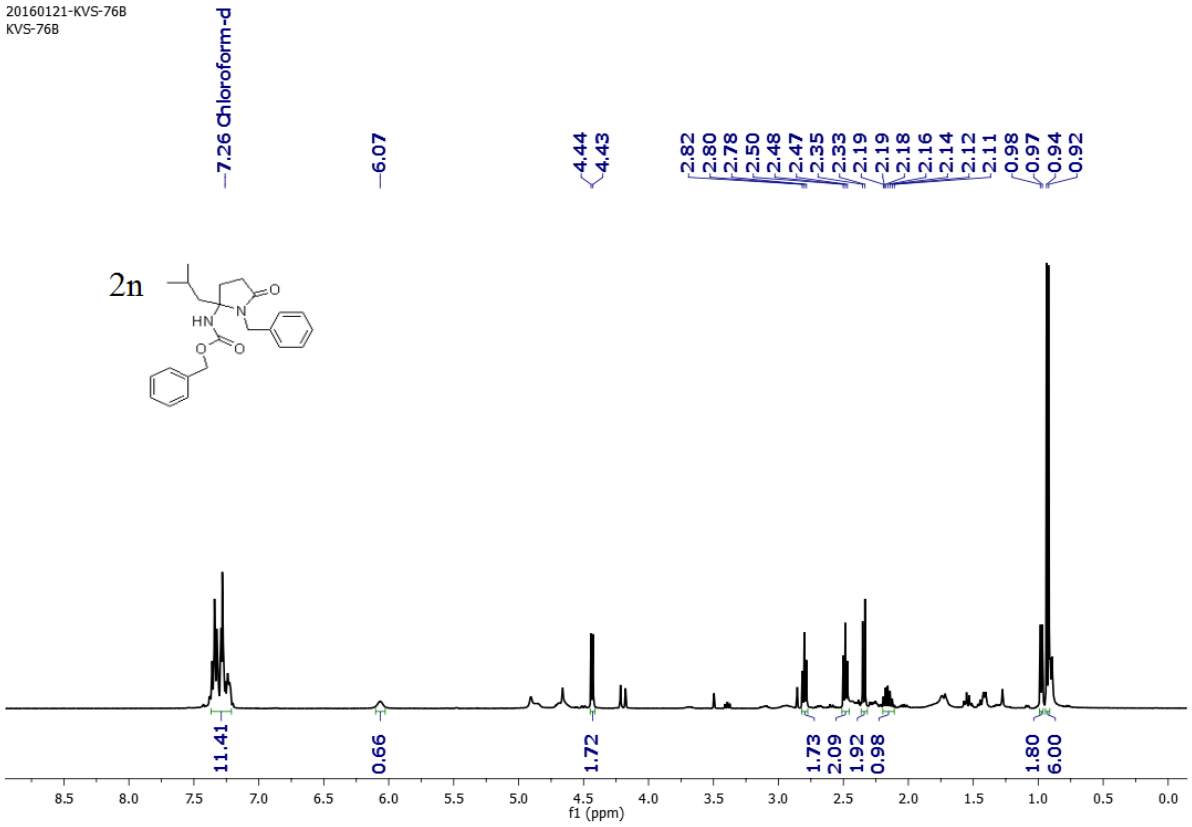

20160415-KVS-90B
KVS-90B
175.5
133.9
130.4
129.0
127.7
77.5
77.2
77.2 Chloroform-d
77.1
76.8
43.4
29.8
29.1
28.4
24.9
2k
BocHN
f1 (ppm)

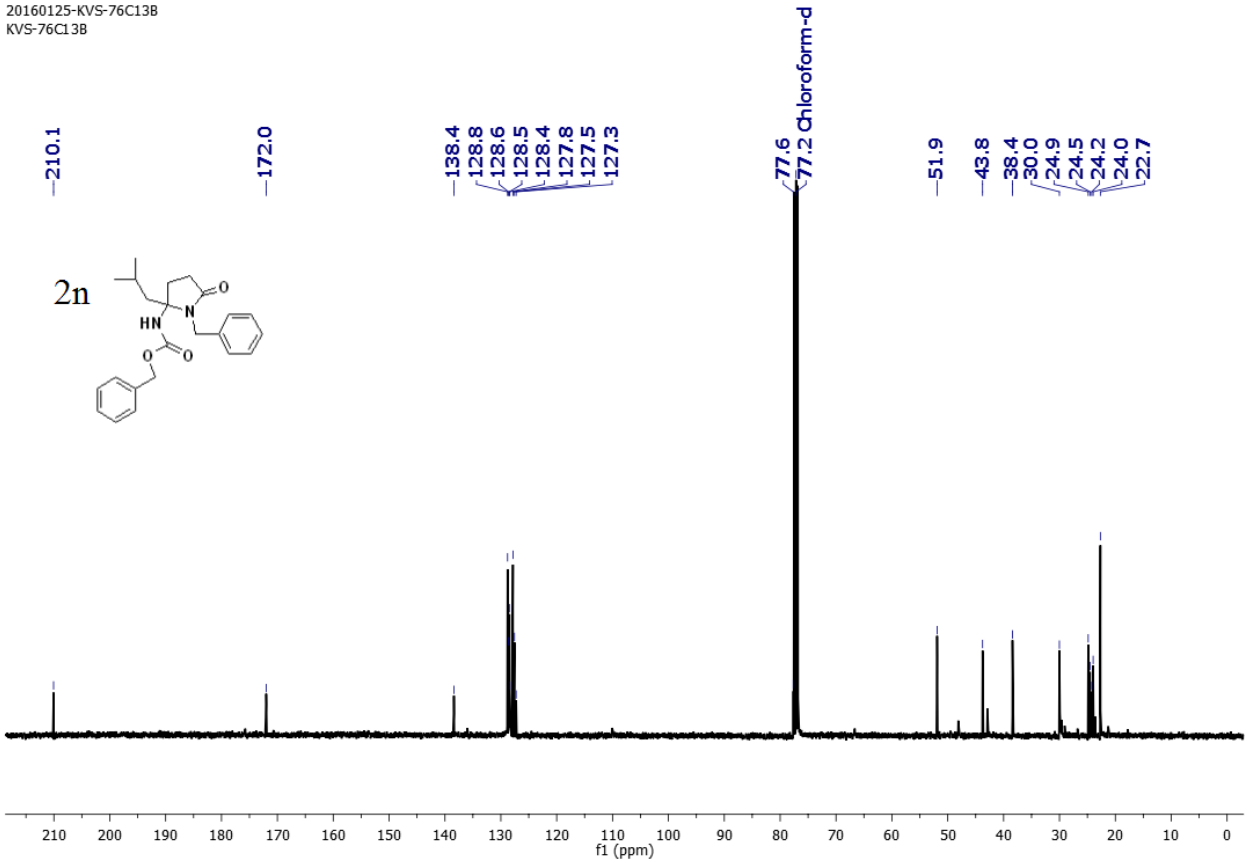

7.32
7.30
7.29
7.27
7.27
7.26 Chloroform-d
7.25
7.24
7.23
5.33
4.77
4.74
4.66
4.62
4.23
4.19
2.57
2.54
2.51
2.45
2.43
2.42
2.40
2.40
2.38
1.80
1.76
1.44
1.42
21
BocHN
6.45
1.00
1.09
1.11
1.02
1.23
2.48
1.19
10.66
f1 (ppm)

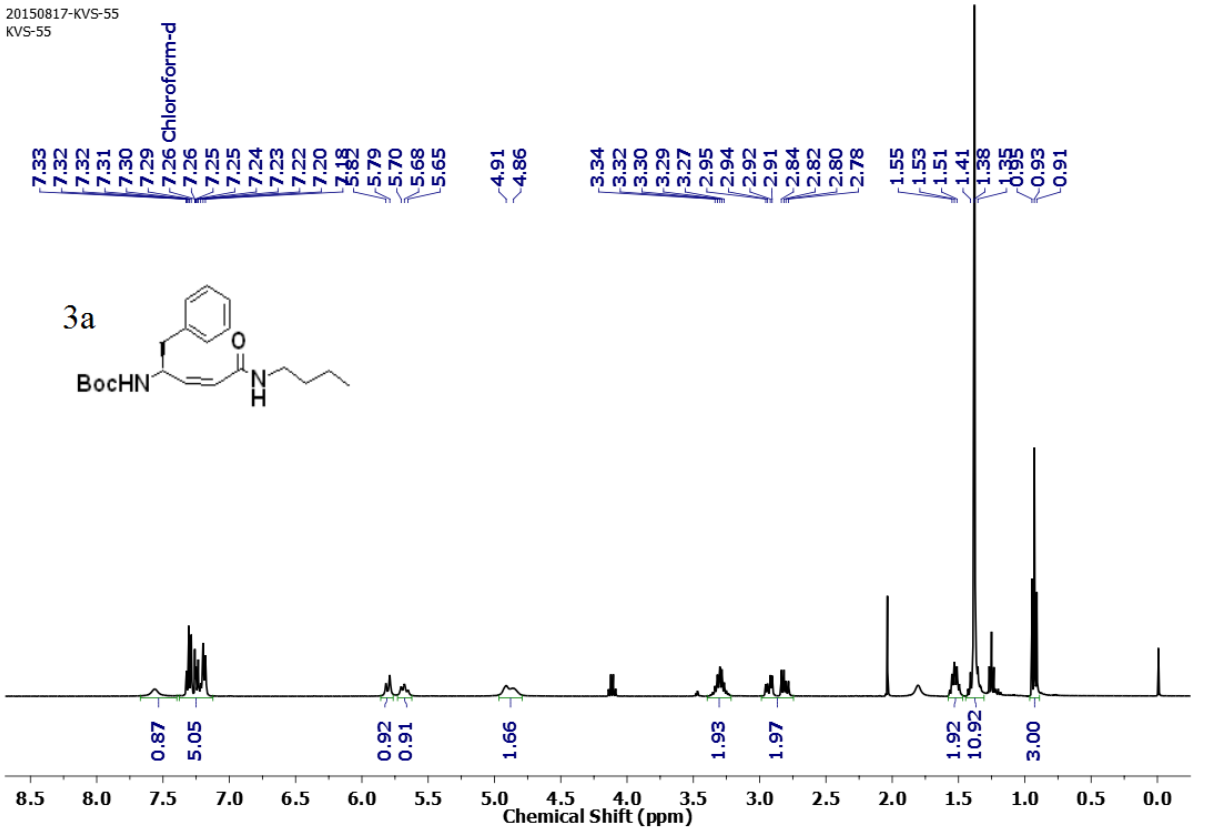

174.0
170.7
137.0
128.7
128.5
127.6
80.4
77.2 Chloroform-d
65.7
44.3
29.4
28.4
26.7
21
BocHN
N
O
f1 (ppm)

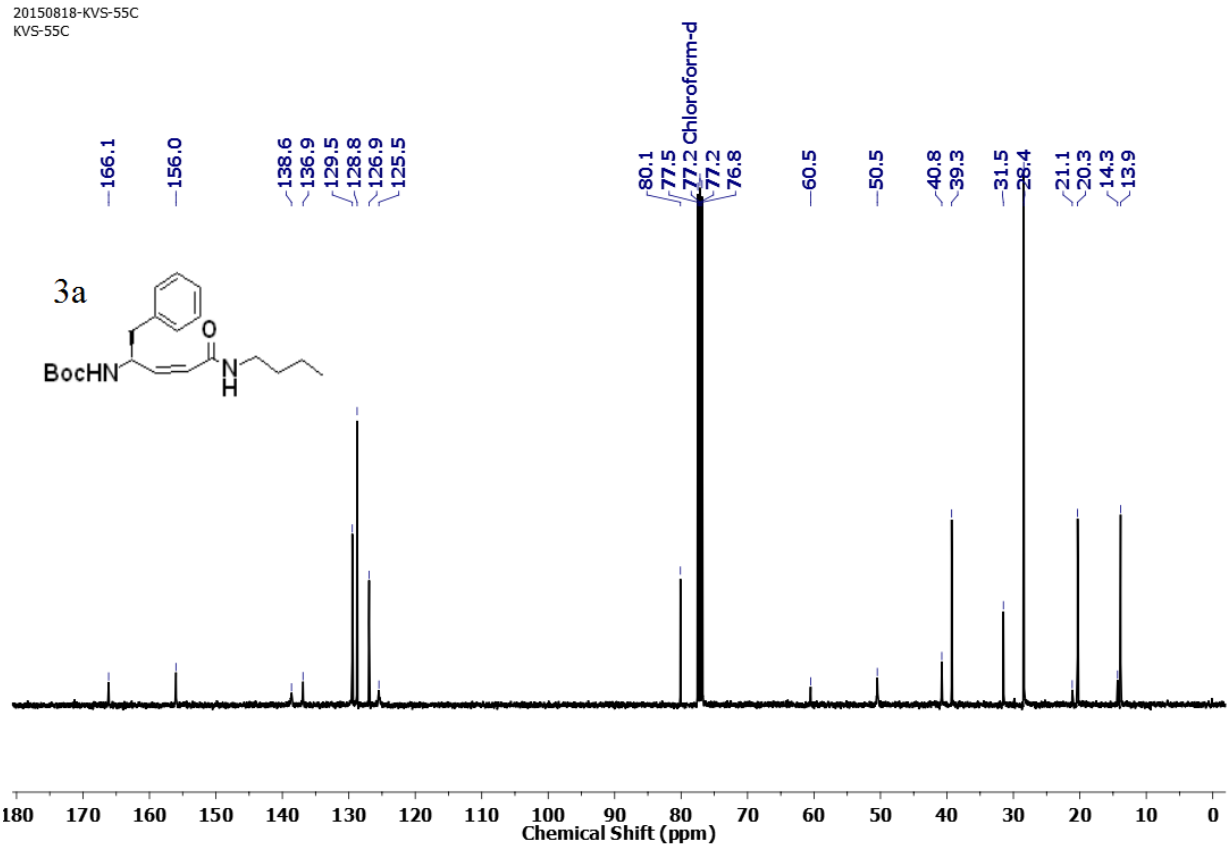

20160407-KVS-86
KVS-86
7.26 Chloroform-d
5.28
5.16
5.13
4.97
4.94
3.61
3.60
3.56
3.54
3.52
3.17
3.14
2.91
2.87
2.60
2.38
1.64
1.62
1.50
1.48
1.33
1.31
2m
CbzHN
N
O
7.93
1.99
0.90
0.96
1.00
1.03
0.92
1.02
0.75
1.08
0.83
1.22
1.28
3.01
3.05
f1 (ppm)

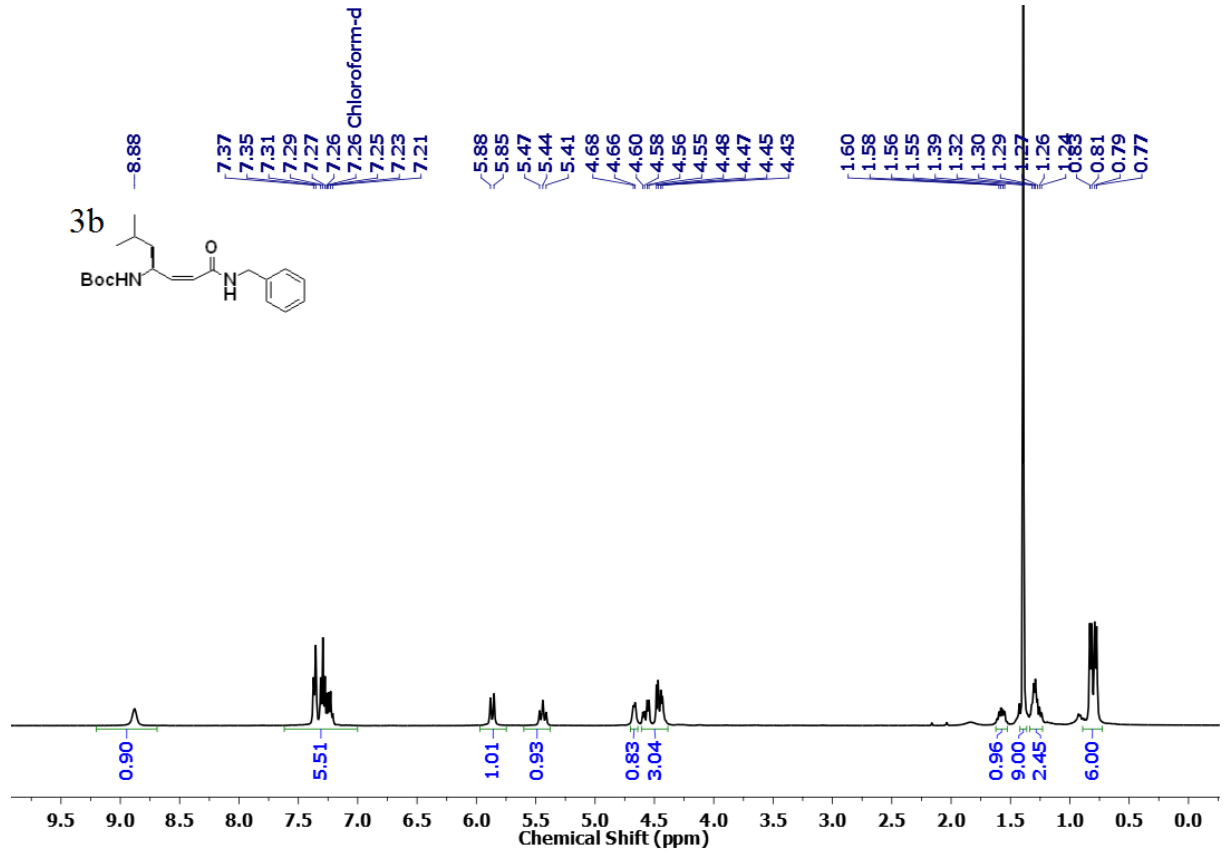

20160411-KVS-86C
KVS-86C
174.9
134.5
130.1
129.1
128.7
128.6
128.5
127.8
77.9
77.2 Chloroform-d
44.8
30.3
29.7
20.9
19.5
2m
CbzHN
f1 (ppm)

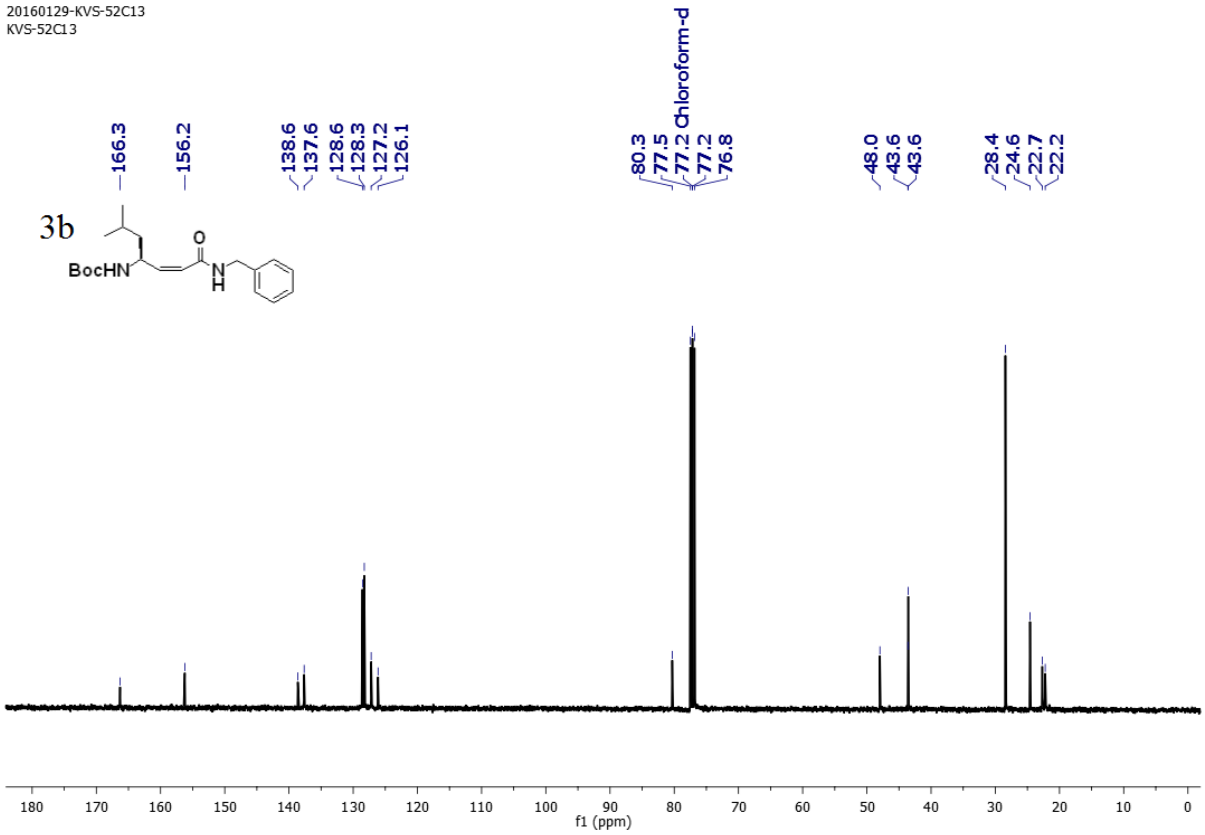

20160121-KVS-76B
KVS-76B
7.26 Chloroform-d
6.07
4.44
4.43
2.82
2.80
2.78
2.50
2.48
2.47
2.35
2.33
2.19
2.19
2.18
2.16
2.14
2.12
2.11
0.98
0.97
0.94
0.92
2n
11.41
0.66
1.72
1.73
2.09
1.92
0.98
1.80
6.00
f1 (ppm)

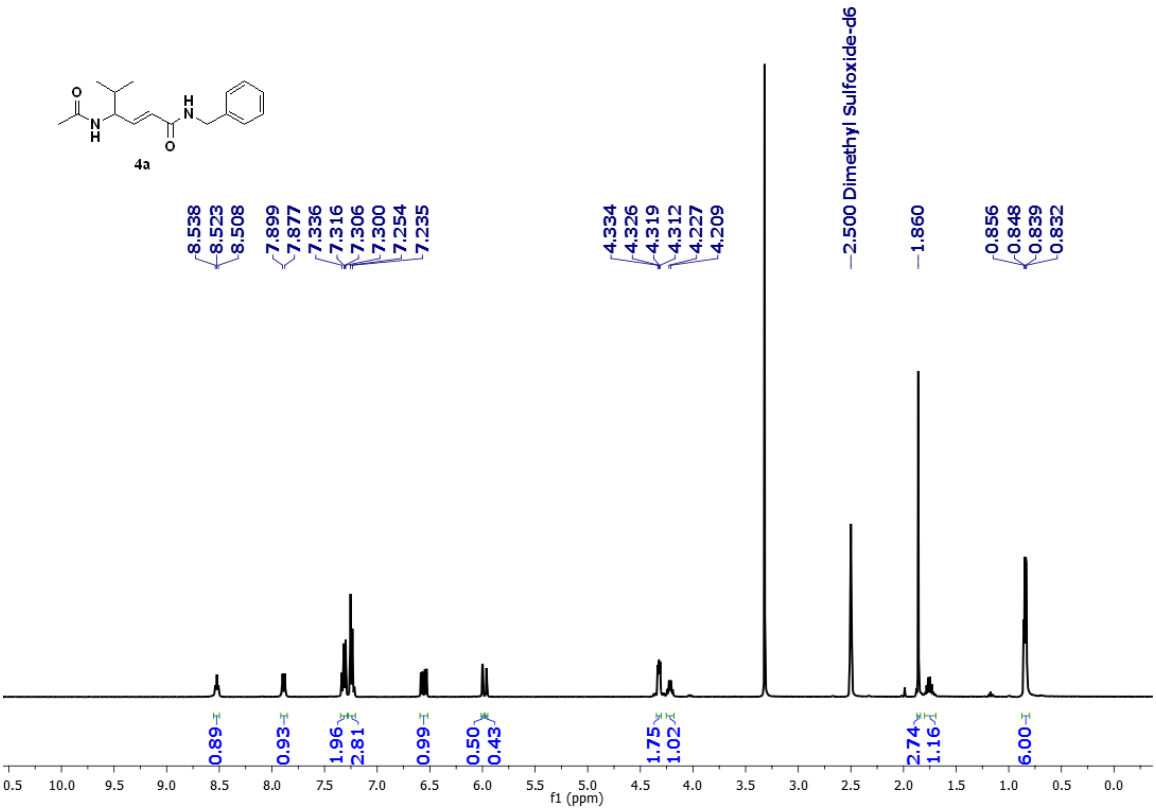

20160125-KVS-76C13B
KVS-76C13B
210.1
172.0
138.4
128.8
128.6
128.5
128.4
127.8
127.5
127.3
77.6
77.2 Chloroform-d
51.9
43.8
38.4
30.0
24.9
24.5
24.2
24.0
22.7
2n
f1 (ppm)

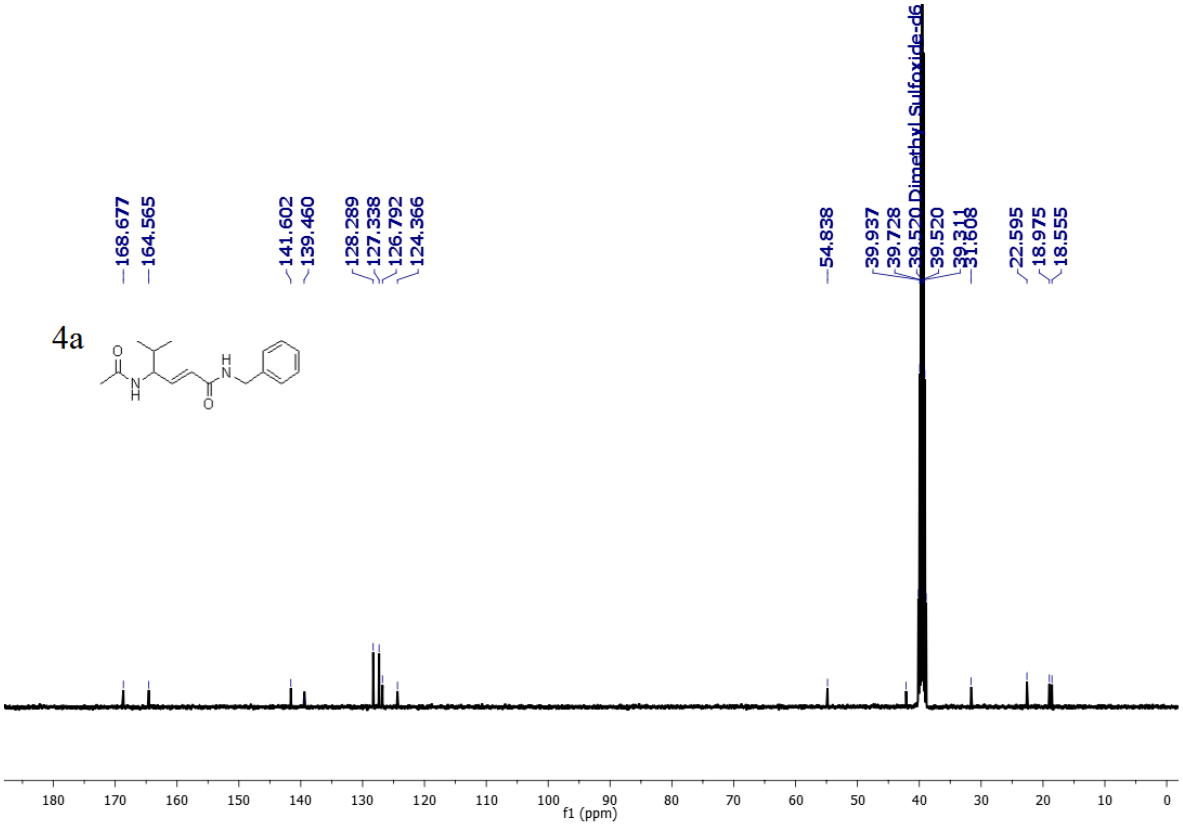

20150817-KVS-55
KVS-55
7.33
7.32
7.32
7.31
7.30
7.29
7.26 Chloroform-d
7.26
7.25
7.25
7.24
7.23
7.22
7.20
5.79
5.70
5.68
5.65
4.91
4.86
3.34
3.32
3.30
3.29
3.27
2.95
2.94
2.92
2.91
2.84
2.82
2.80
2.78
1.55
1.53
1.51
1.41
1.38
0.93
0.91
3a
BocHN
0.87
5.05
0.92
0.91
1.66
1.93
1.97
1.92
10.92
3.00
Chemical Shift (ppm)

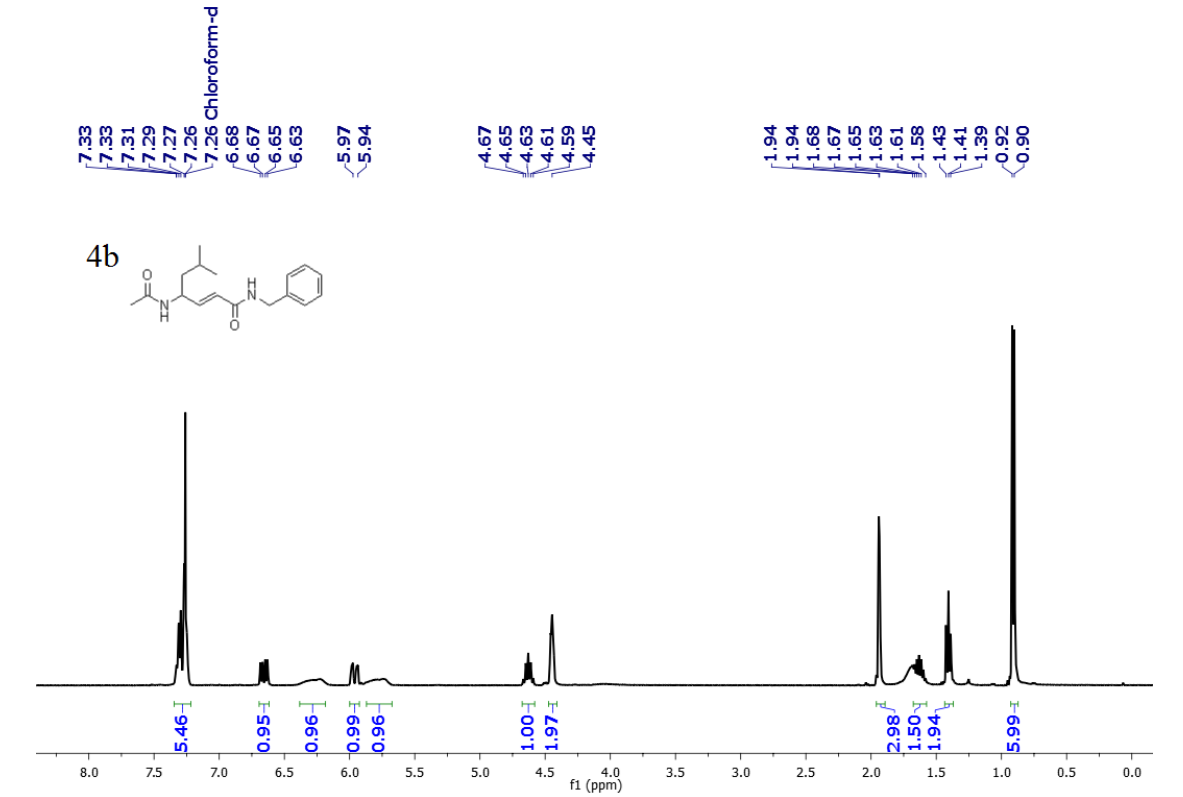

20150818-KVS-55C
KVS-55C
166.1
156.0
138.6
136.9
129.5
128.8
126.9
125.5
80.1
77.5
77.2 Chloroform-d
77.2
76.8
60.5
50.5
40.8
39.3
31.5
28.4
21.1
20.3
14.3
13.9
3a
BocHN
O
N
H
Chemical Shift (ppm)

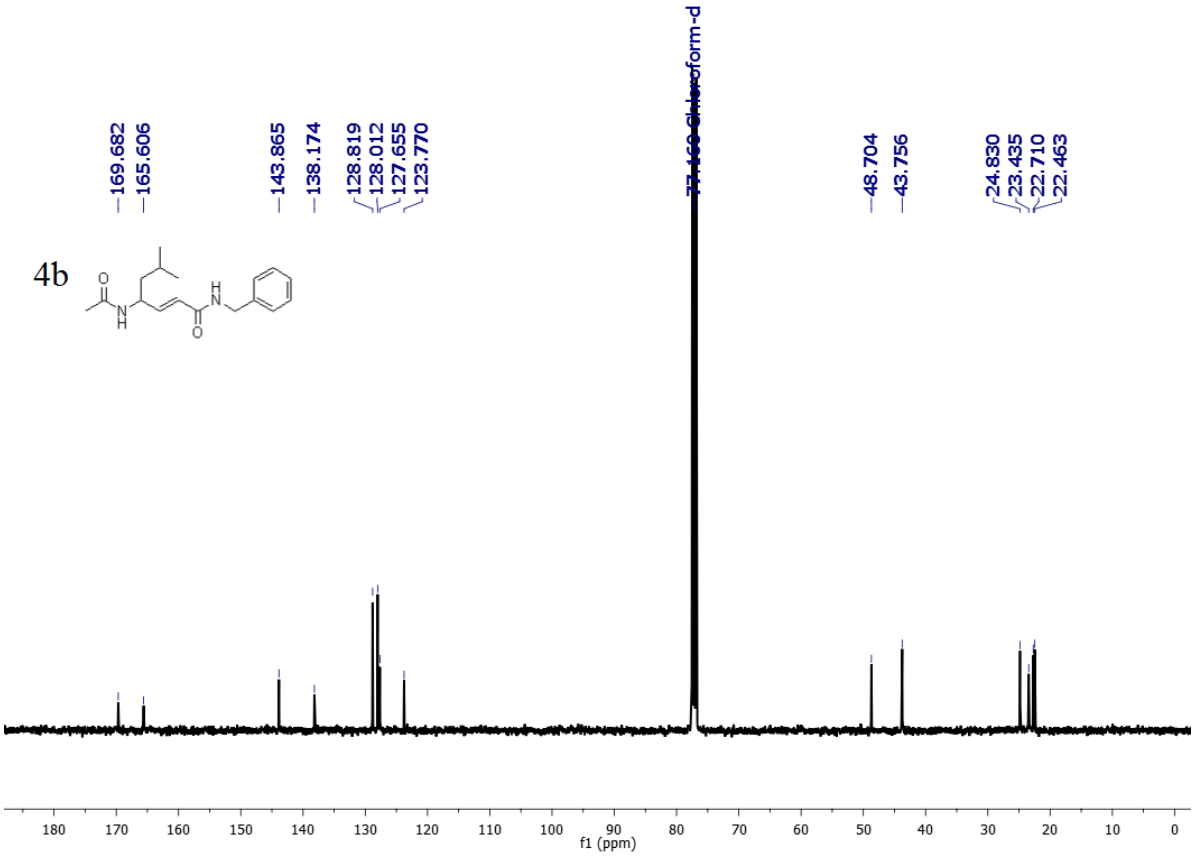

8.88
7.37
7.35
7.31
7.29
7.27
7.26
7.26 Chloroform-d
7.25
7.23
7.21
5.88
5.85
5.47
5.44
5.41
4.68
4.66
4.60
4.58
4.56
4.55
4.48
4.47
4.45
4.43
1.60
1.58
1.56
1.55
1.39
1.32
1.30
1.29
1.27
1.26
0.83
0.81
0.79
0.77
3b
BocHN
O
N
H
0.90
5.51
1.01
0.93
0.83
3.04
0.96
9.00
2.45
6.00
Chemical Shift (ppm)

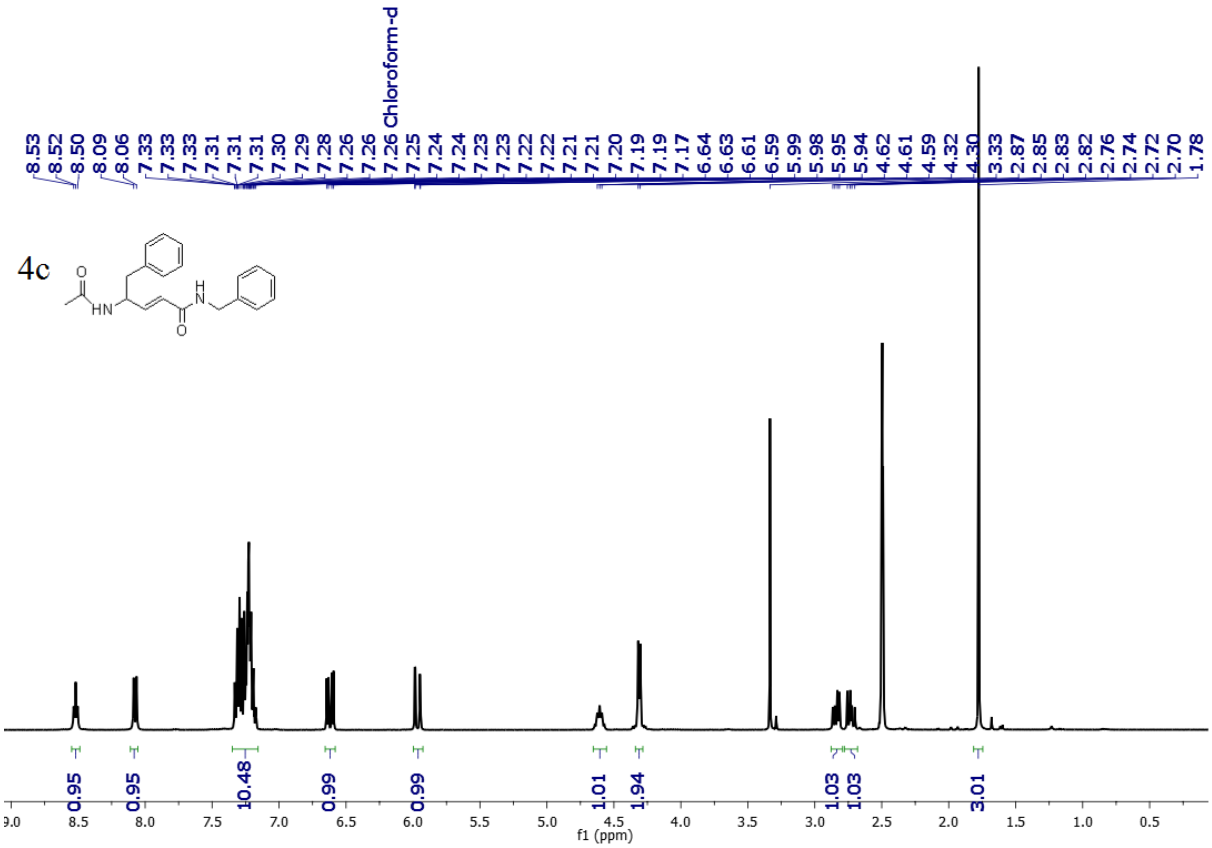

20160129-KVS-52C13
KVS-52C13
166.3
156.2
138.6
137.6
128.6
128.3
127.2
126.1
80.3
77.5
77.2 Chloroform-d
77.2
76.8
48.0
43.6
43.6
28.4
24.6
22.7
22.2
3b
BocHN
O
N
H
f1 (ppm)

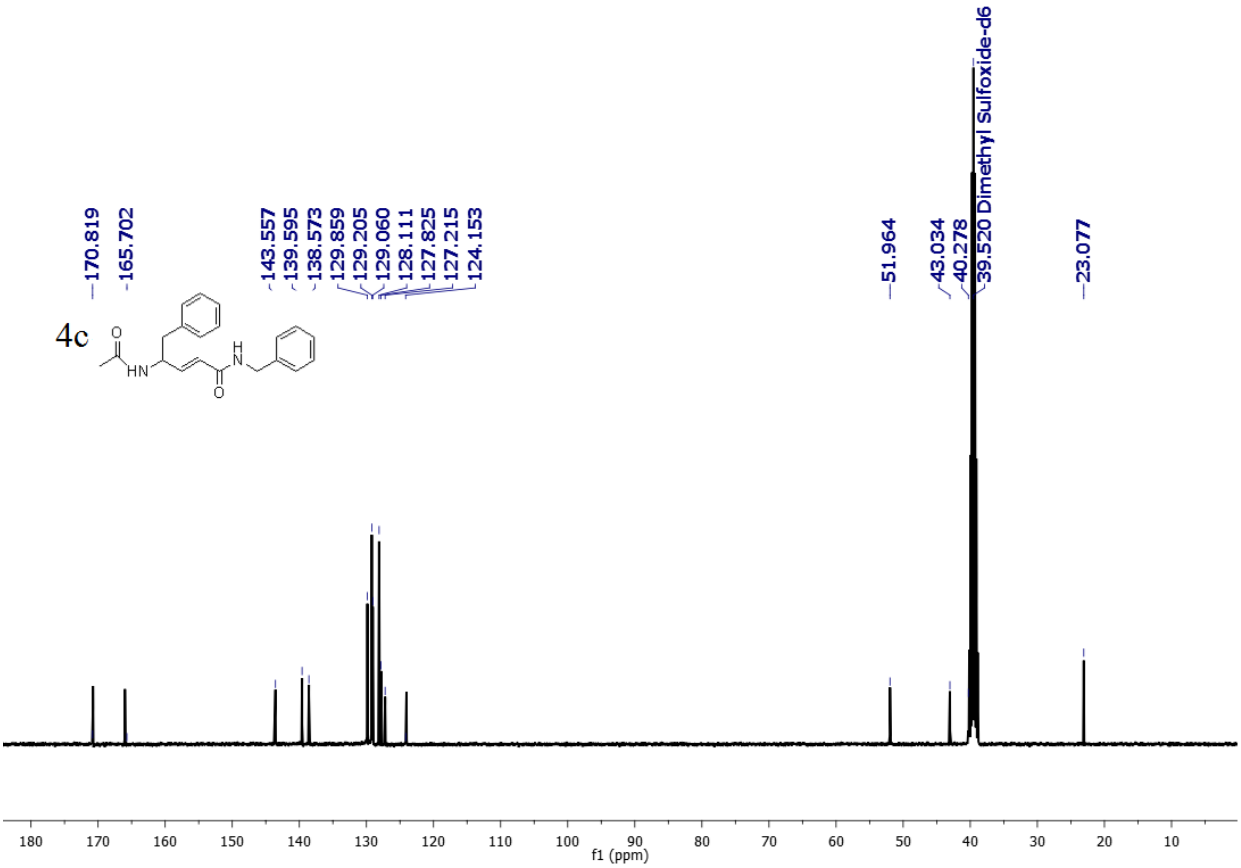

4a
8.538
8.523
8.508
7.899
7.877
7.336
7.316
7.306
7.300
7.254
7.235
4.334
4.326
4.319
4.312
4.227
4.209
2.500 Dimethyl Sulfoxide-d6
1.860
0.856
0.848
0.839
0.832
0.89
0.93
1.96
2.81
0.99
0.50
0.43
1.75
1.02
2.74
1.16
6.00
f1 (ppm)

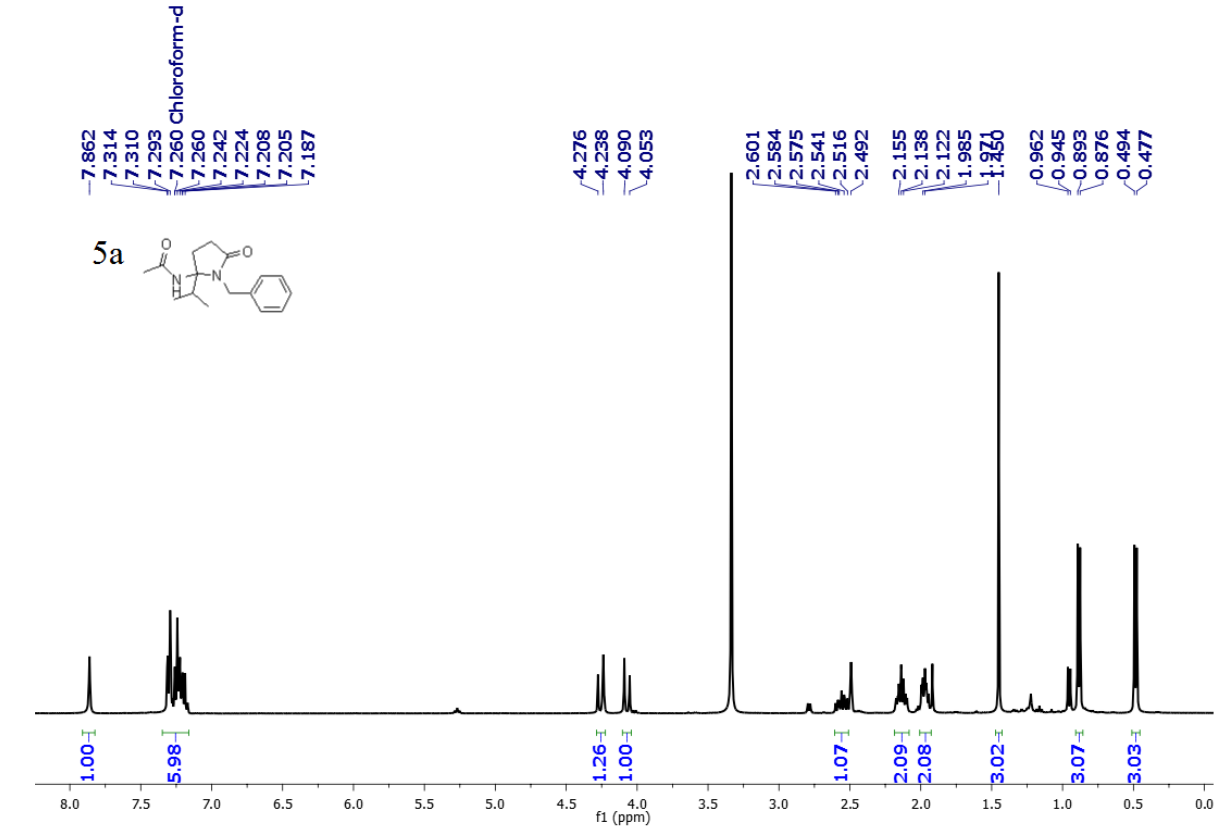

168.677
164.565
141.602
139.460
128.289
127.338
126.792
124.366
54.838
39.937
39.728
39.520 Dimethyl Sulfoxide-d6
39.520
39.311
31.808
22.595
18.975
18.555
4a
f1 (ppm)

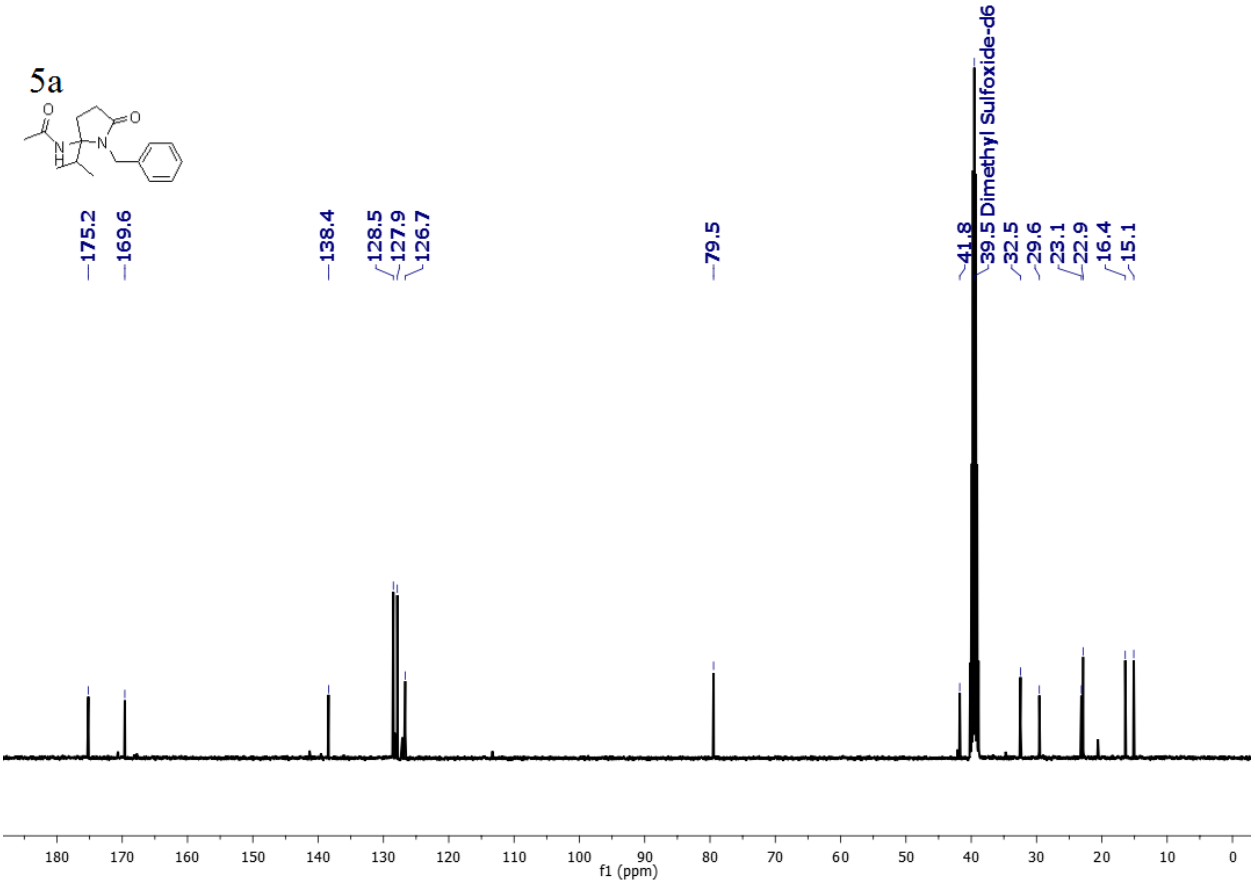

7.33
7.33
7.31
7.29
7.27
7.26
7.26 Chloroform-d
6.68
6.67
6.65
6.63
5.97
5.94
4.67
4.65
4.63
4.61
4.59
4.45
1.94
1.94
1.68
1.67
1.65
1.63
1.61
1.58
1.43
1.41
1.39
0.92
0.90
4b
5.46
0.95
0.96
0.99
0.96
1.00
1.97
2.98
1.50
1.94
5.99
f1 (ppm)

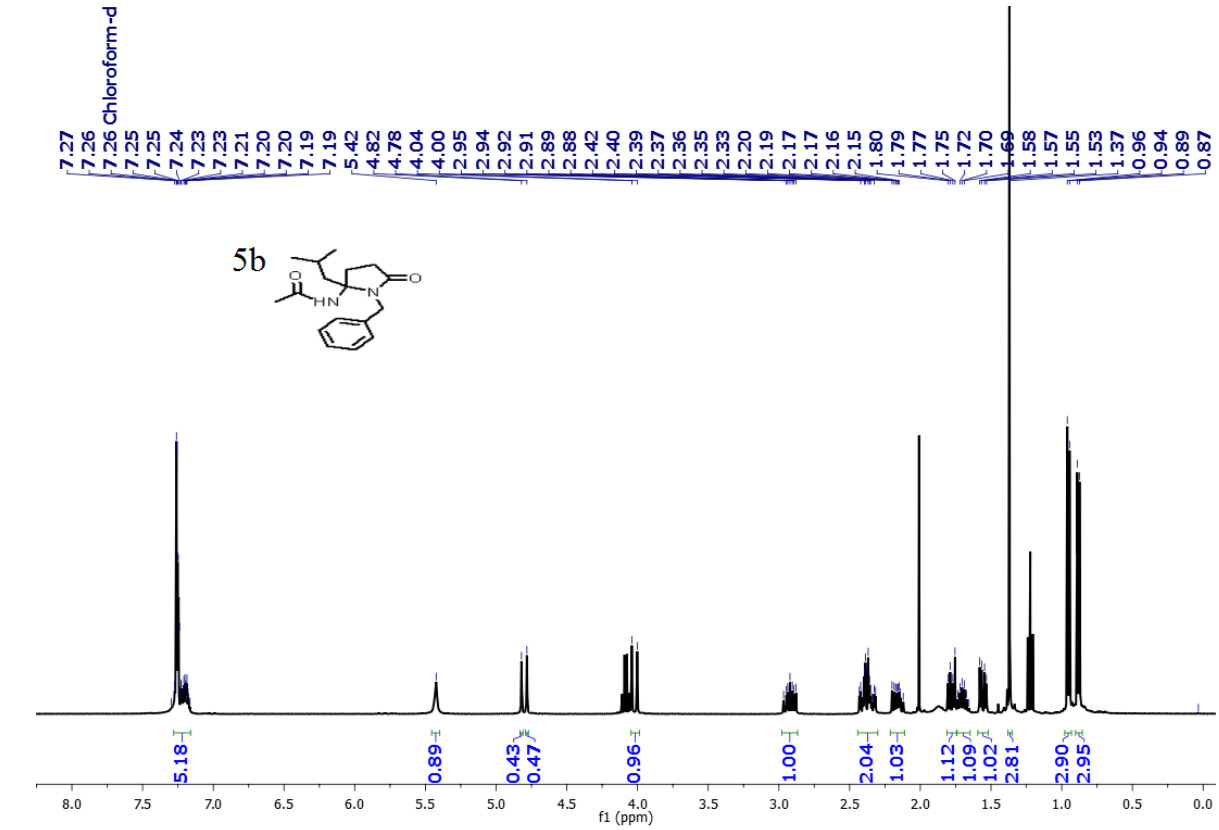

169.682
165.606
143.865
138.174
128.819
128.012
127.655
123.770
77.160 Chloroform-d
48.704
43.756
24.830
23.435
22.710
22.463
4b
f1 (ppm)

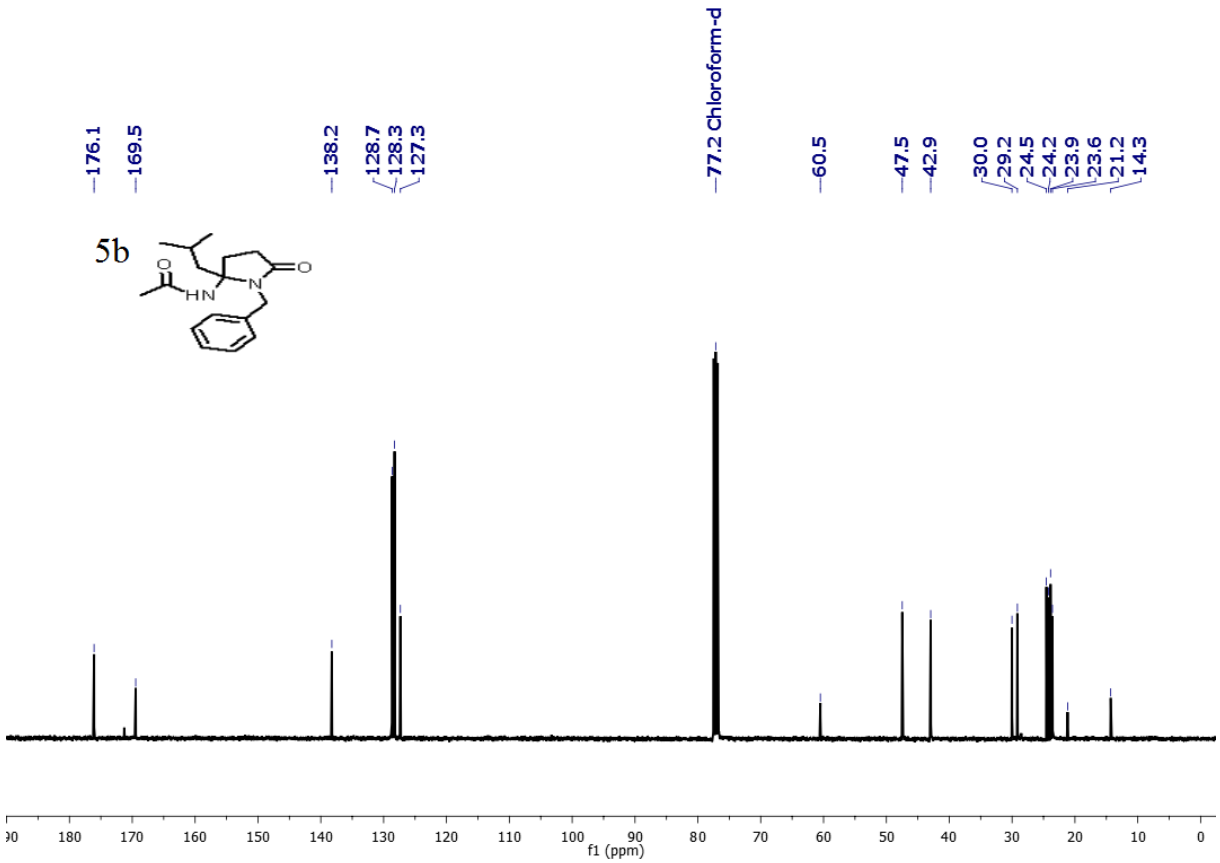

Chloroform-d
4c
0.95
0.95
10.48
0.99
0.99
1.01
1.94
1.03
1.03
3.01
f1 (ppm)

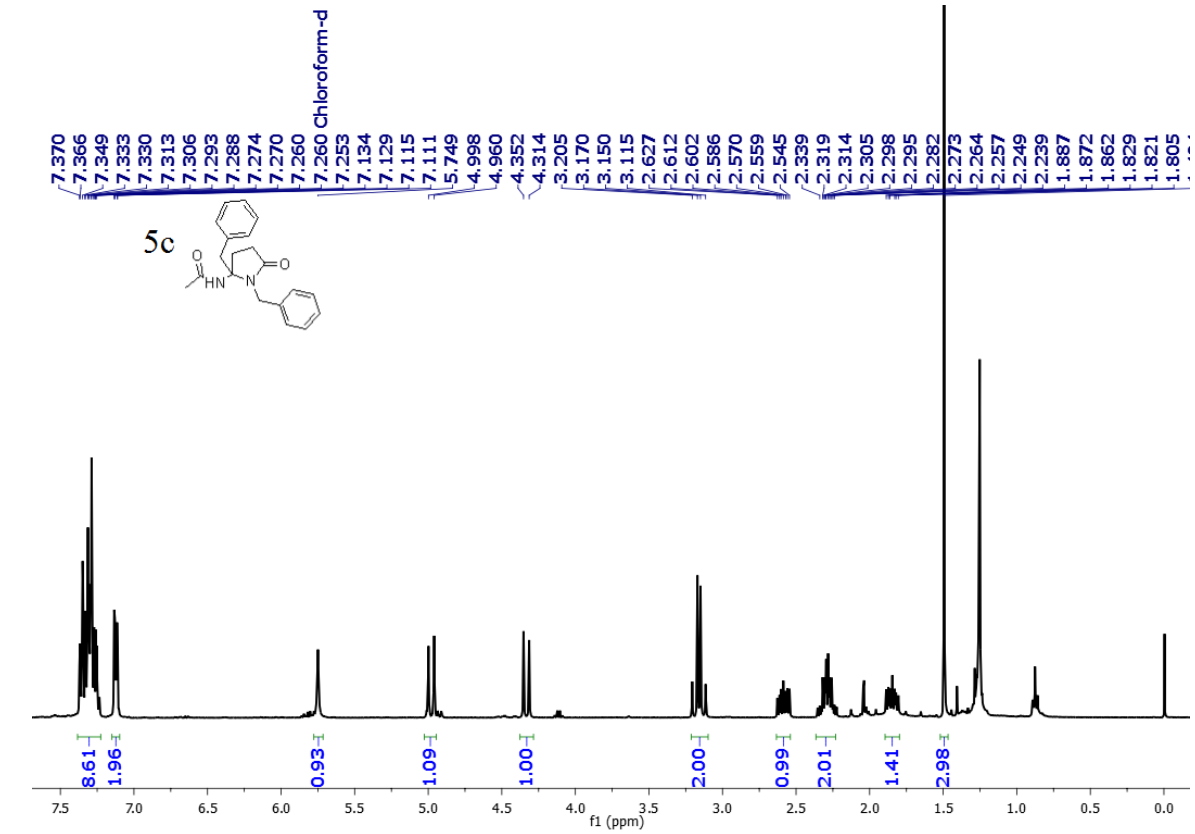

170.819
165.702
143.557
139.595
138.573
129.859
129.205
129.060
128.111
127.825
127.215
124.153
51.964
43.034
40.278
39.520 Dimethyl Sulfoxide-d6
23.077
4c
f1 (ppm)

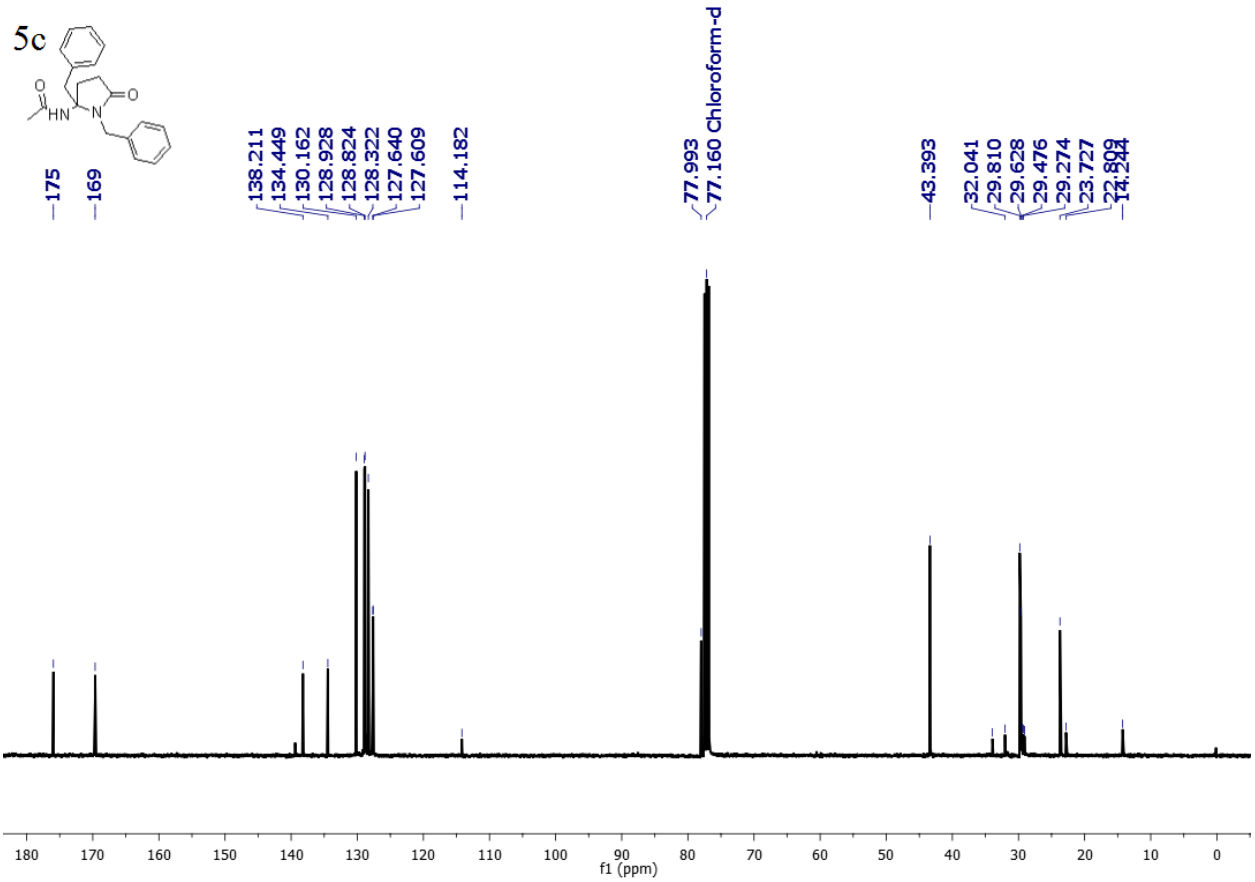

7.862
7.314
7.310
7.293
7.260 Chloroform-d
7.260
7.242
7.224
7.208
7.205
7.187
4.276
4.238
4.090
4.053
2.601
2.584
2.575
2.541
2.516
2.492
2.155
2.138
2.122
1.985
1.971
1.450
0.962
0.945
0.893
0.876
0.494
0.477
5a
1.00
5.98
1.26
1.00
1.07
2.09
2.08
3.02
3.07
3.03
f1 (ppm)

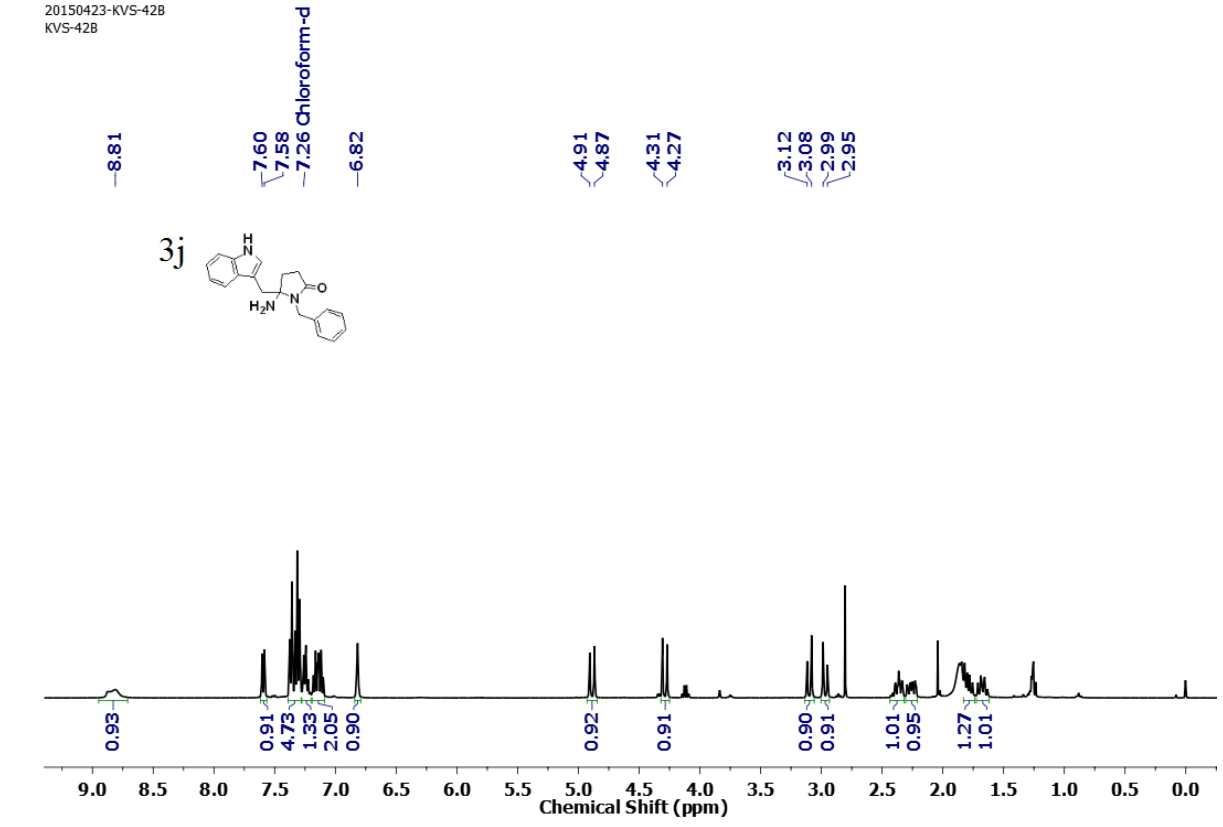

5a
175.2
169.6
138.4
128.5
127.9
126.7
79.5
41.8
39.5 Dimethyl Sulfoxide-d6
32.5
29.6
23.1
22.9
16.4
15.1
f1 (ppm)

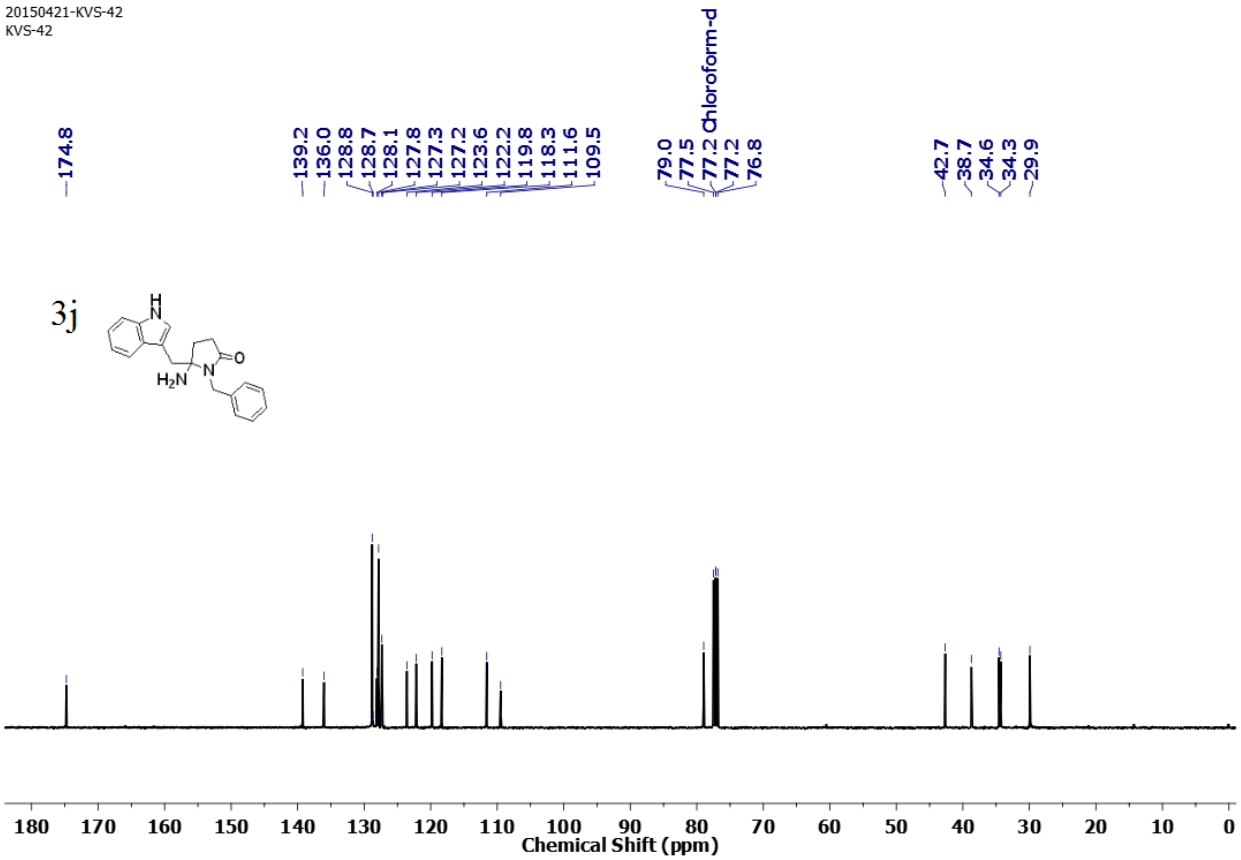

7.27
7.26 Chloroform-d
7.26
7.25
7.25
7.24
7.23
7.23
7.21
7.20
7.20
7.19
7.19
5.42
4.82
4.78
4.04
4.00
2.95
2.94
2.92
2.91
2.89
2.88
2.42
2.40
2.39
2.37
2.36
2.35
2.33
2.20
2.19
2.17
2.17
2.16
2.15
1.80
1.79
1.77
1.75
1.72
1.70
1.69
1.58
1.57
1.55
1.53
1.37
0.96
0.94
0.89
0.87
5b
5.18
0.89
0.43
0.47
0.96
1.00
2.04
1.03
1.12
1.09
1.02
2.81
2.90
2.95
f1 (ppm)

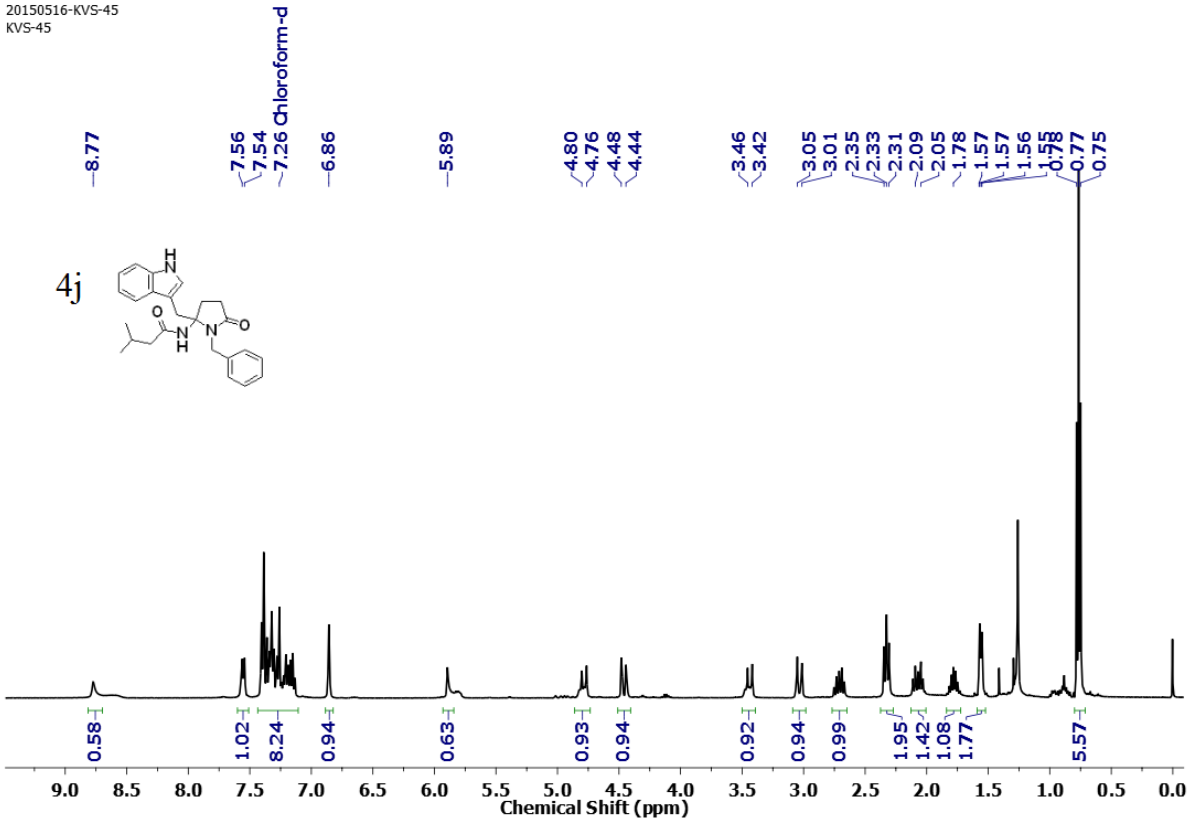

176.1
169.5
138.2
128.7
128.3
127.3
77.2 Chloroform-d
60.5
47.5
42.9
30.0
29.2
24.5
24.2
23.9
23.6
21.2
14.3
5b
f1 (ppm)

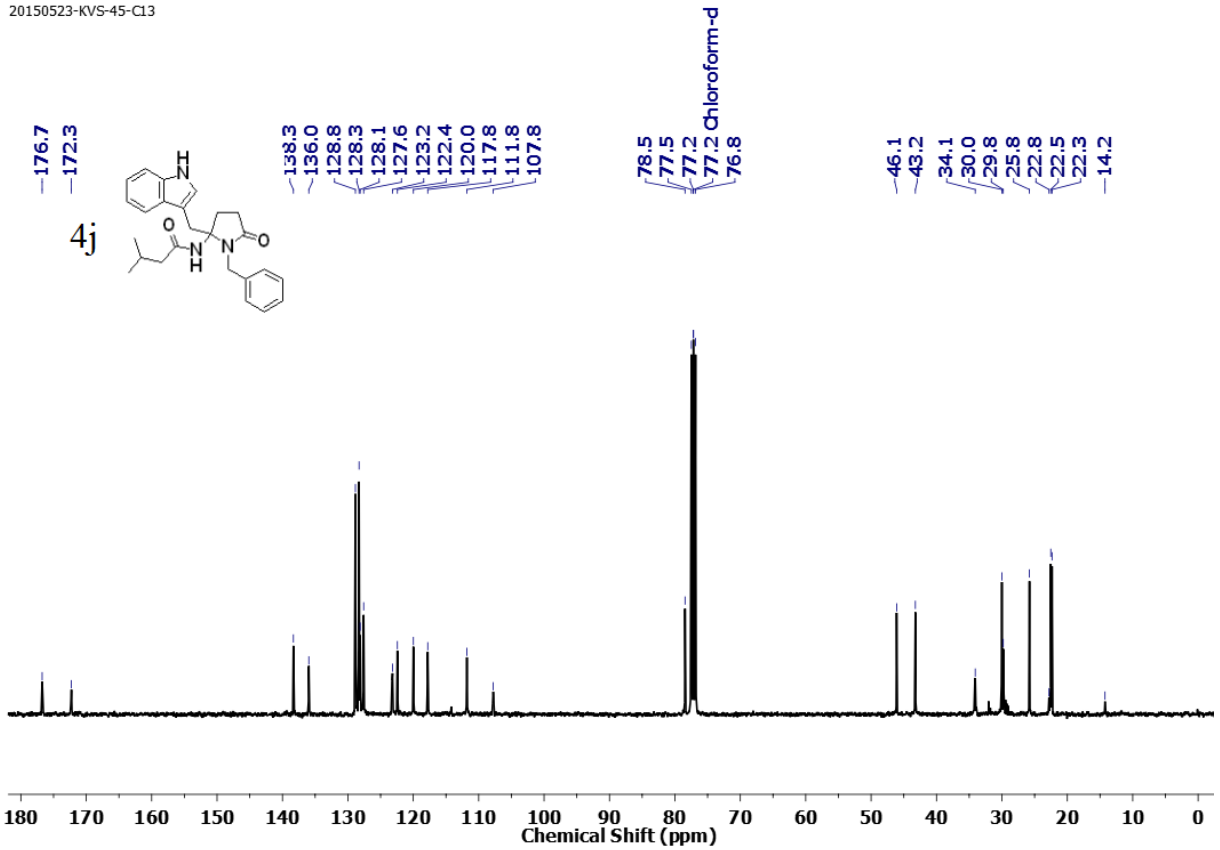

7.260 Chloroform-d
5c
8.61
1.96
0.93
1.09
1.00
2.00
0.99
2.01
1.41
2.98
f1 (ppm)

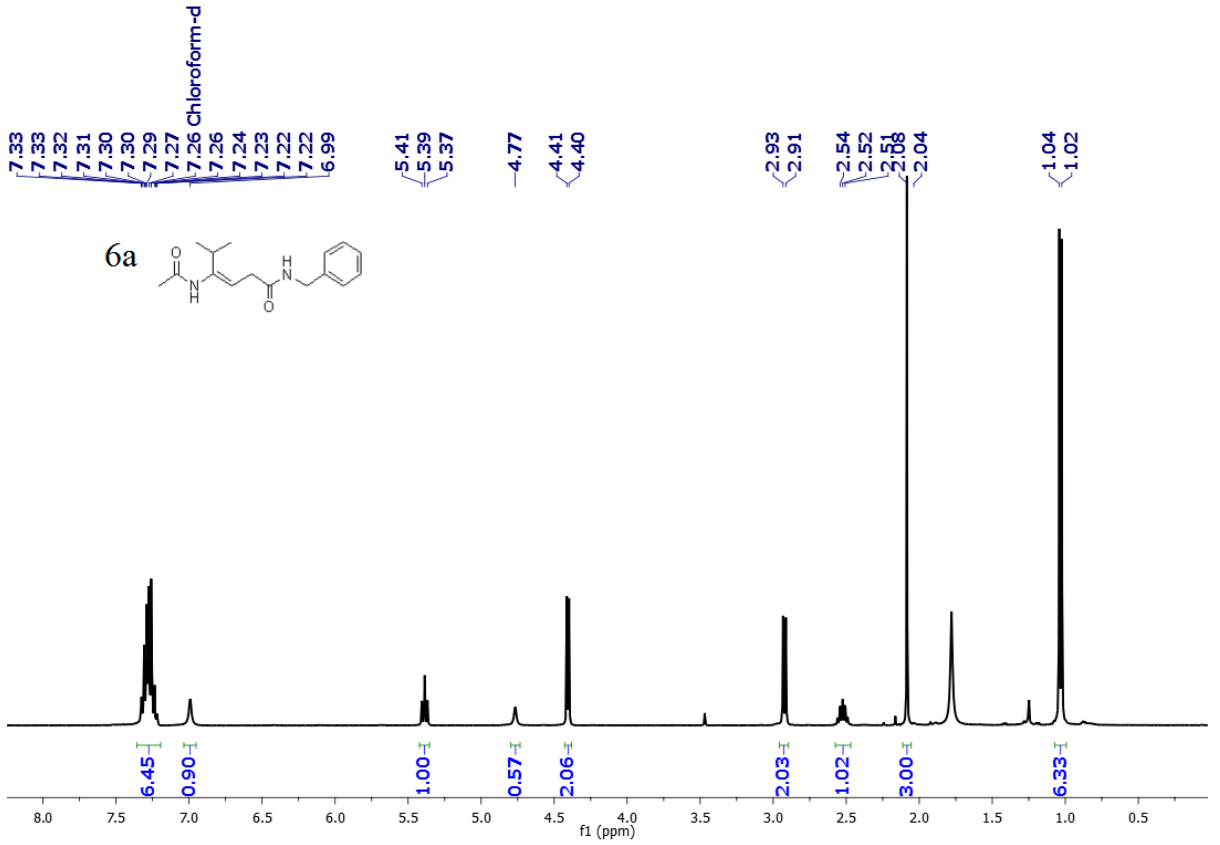

5c
175
169
138.211
134.449
130.162
128.928
128.824
128.322
127.640
127.609
114.182
77.993
77.160 Chloroform-d
43.393
32.041
29.810
29.628
29.476
29.274
23.727
22.809
14.244
f1 (ppm)

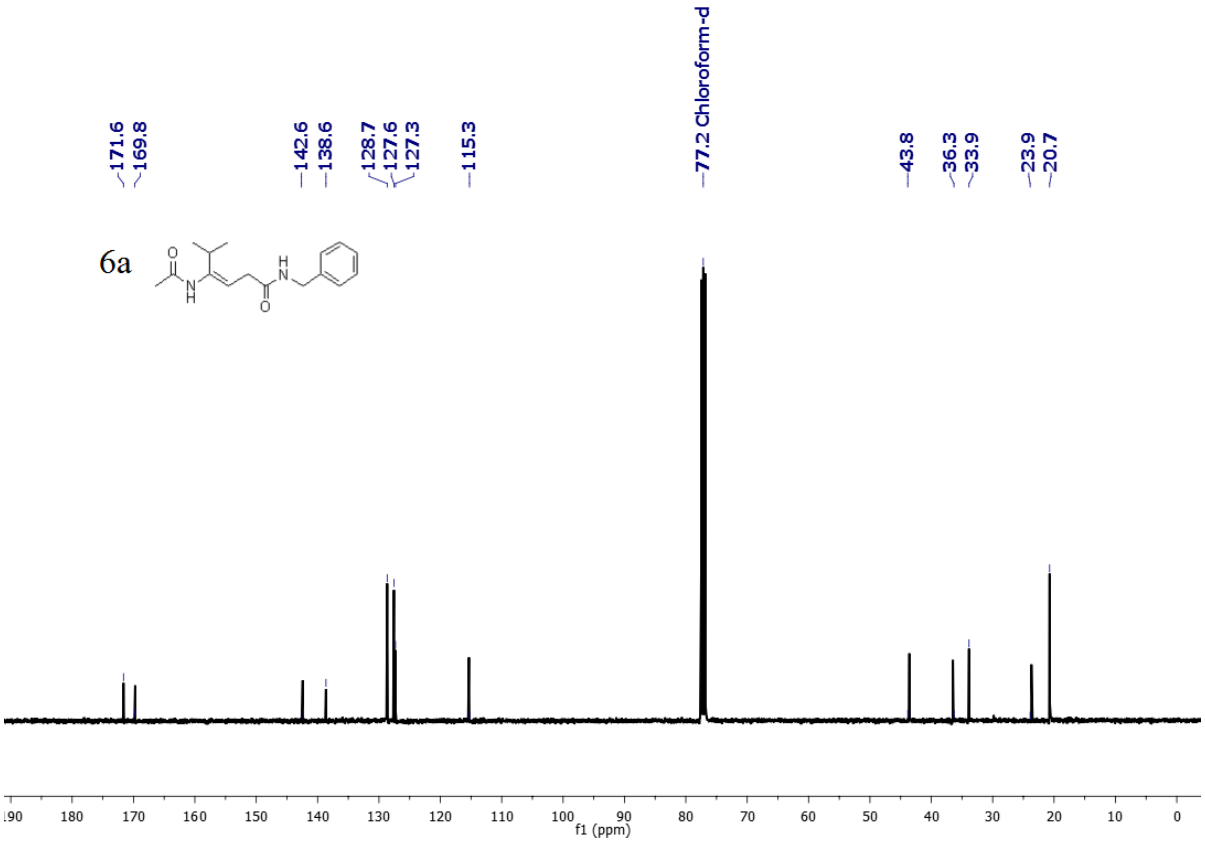

20150423-KVS-42B
KVS-42B
8.81
7.60
7.58
7.26 Chloroform-d
6.82
4.91
4.87
4.31
4.27
3.12
3.08
2.99
2.95
3j
0.93
0.91
4.73
1.33
2.05
0.90
0.92
0.91
0.90
0.91
1.01
0.95
1.27
1.01
Chemical Shift (ppm)

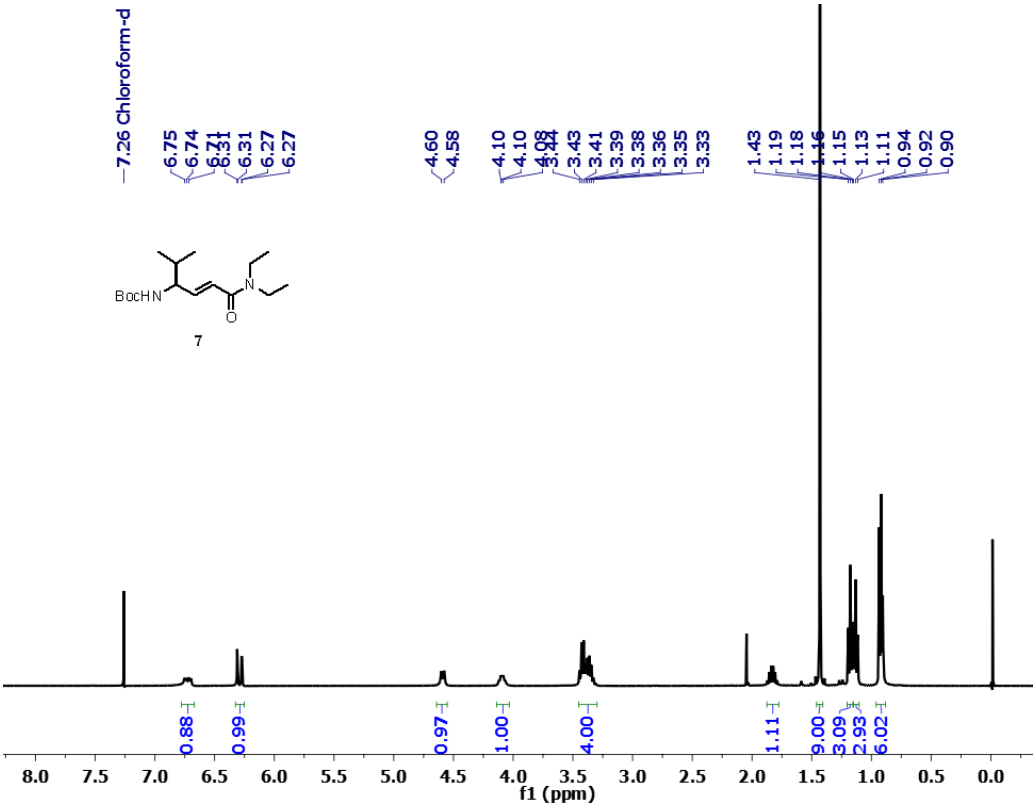

20150421-KVS-42
KVS-42
174.8
139.2
136.0
128.8
128.7
128.1
127.8
127.3
127.2
123.6
122.2
119.8
118.3
111.6
109.5
79.0
77.5
77.2 Chloroform-d
77.2
76.8
42.7
38.7
34.6
34.3
29.9
3j
Chemical Shift (ppm)

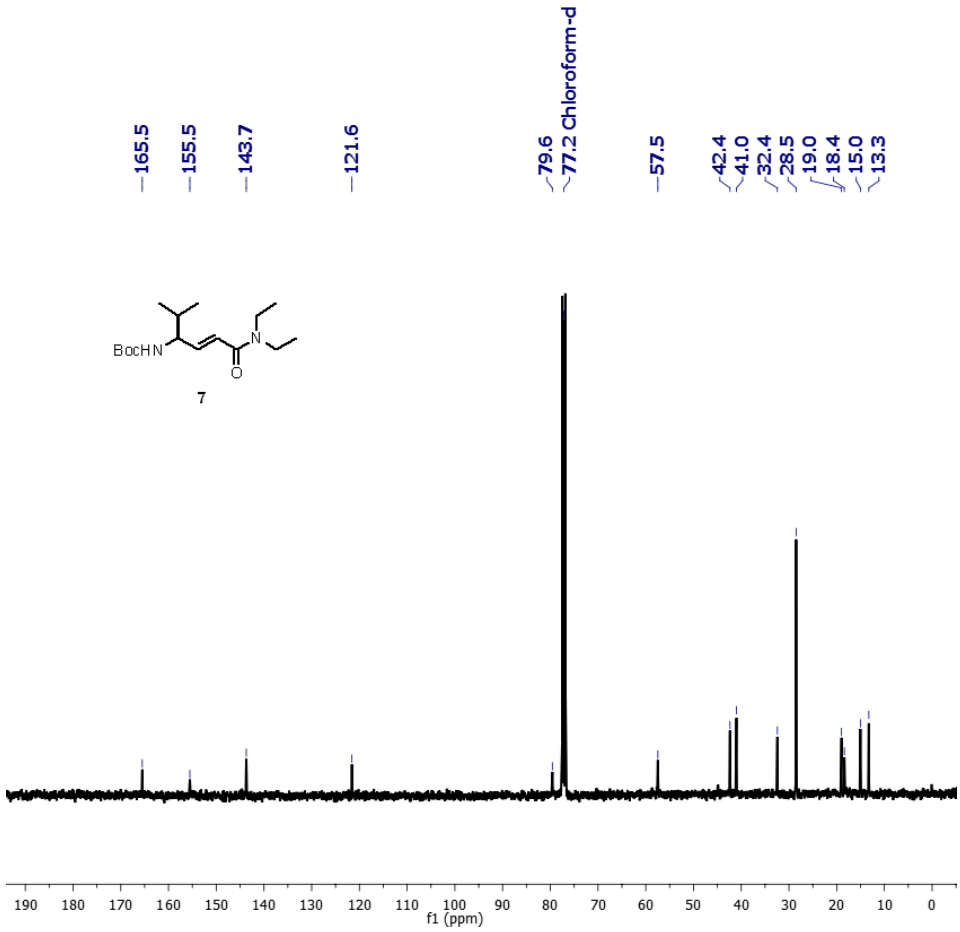

20150516-KVS-45
KVS-45
8.77
7.56
7.54
7.26 Chloroform-d
6.86
5.89
4.80
4.76
4.48
4.44
3.46
3.42
3.05
3.01
2.35
2.33
2.31
2.09
2.05
1.78
1.57
1.57
1.56
1.55
0.78
0.77
0.75
4j
0.58
1.02
8.24
0.94
0.63
0.93
0.94
0.92
0.94
0.99
1.95
1.42
1.08
1.77
5.57
Chemical Shift (ppm)

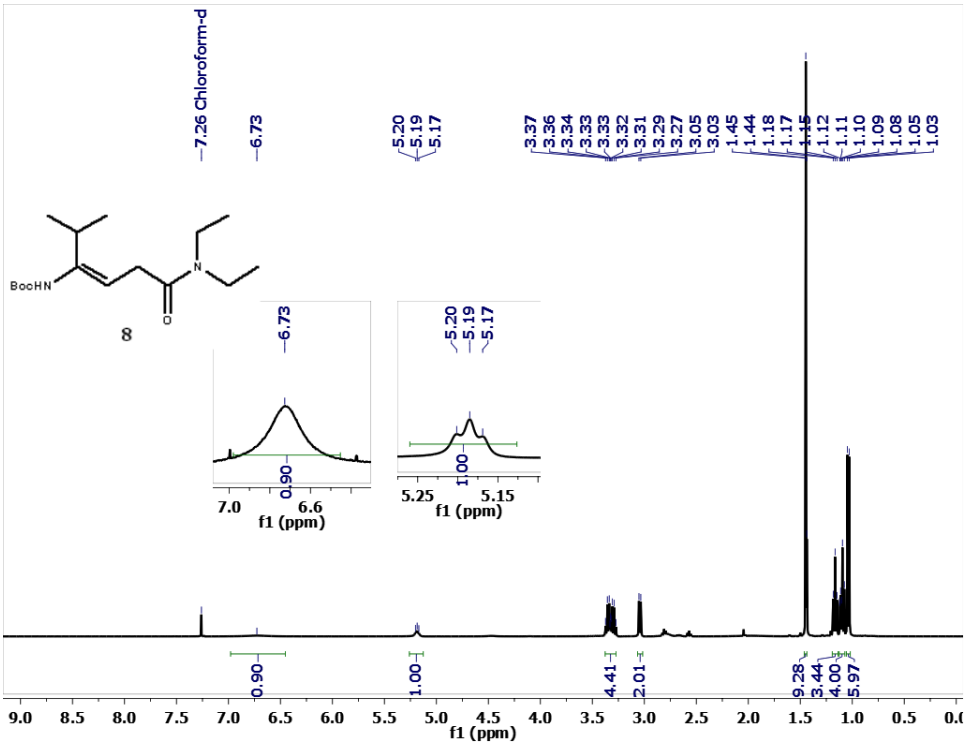

20150523-KVS-45-C13
176.7
172.3
138.3
136.0
128.8
128.3
128.1
127.6
123.2
122.4
120.0
117.8
111.8
107.8
78.5
77.5
77.2
77.2 Chloroform-d
76.8
46.1
43.2
34.1
30.0
29.8
25.8
22.8
22.5
22.3
14.2
4j
Chemical Shift (ppm)

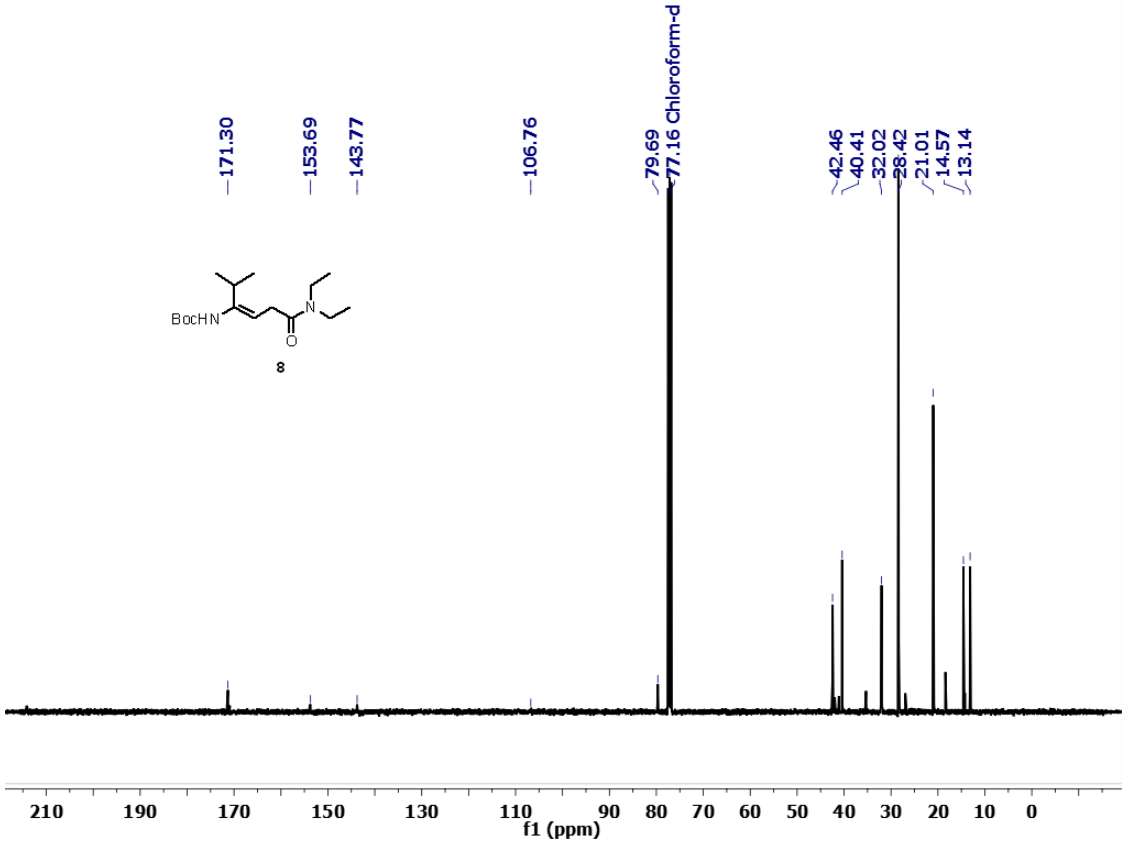

7.33
7.33
7.32
7.31
7.30
7.30
7.29
7.27
7.26 Chloroform-d
7.26
7.24
7.23
7.22
7.22
6.99
5.41
5.39
5.37
4.77
4.41
4.40
2.93
2.91
2.54
2.52
2.08
2.04
1.04
1.02
6a
6.45
0.90
1.00
0.57
2.06
2.03
1.02
3.00
6.33
f1 (ppm)


171.6
169.8
142.6
138.6
128.7
127.6
127.3
115.3
77.2 Chloroform-d
43.8
36.3
33.9
23.9
20.7
6a
f1 (ppm)


7.26 Chloroform-d
6.75
6.74
6.31
6.27
4.60
4.58
4.10
3.43
3.41
3.39
3.38
3.36
3.35
3.33
1.43
1.19
1.18
1.15
1.13
1.11
0.94
0.92
0.90
BocHN
7
0.88
0.99
0.97
1.00
4.00
1.11
9.00
3.09
2.93
6.02
f1 (ppm)


165.5
155.5
143.7
121.6
79.6
77.2 Chloroform-d
57.5
42.4
41.0
32.4
28.5
19.0
18.4
15.0
13.3
BocHN
N
O
7
f1 (ppm)


7.26 Chloroform-d
6.73
5.20
5.19
5.17
3.37
3.36
3.34
3.33
3.33
3.32
3.31
3.29
3.27
3.05
3.03
1.45
1.44
1.18
1.17
1.15
1.12
1.11
1.10
1.09
1.08
1.05
1.03
BocHN
N
O
8
0.90
1.00
4.41
2.01
9.28
3.44
4.00
5.97
f1 (ppm)


171.30
153.69
143.77
106.76
79.69
77.16 Chloroform-d
42.46
40.41
32.02
28.42
21.01
14.57
13.14
BocHN
N
O
8
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)