Supporting Information

Stereoselective Synthesis of Backbone Extended π-Conjugated Amino Esters

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1) ORTEP Diagrams:

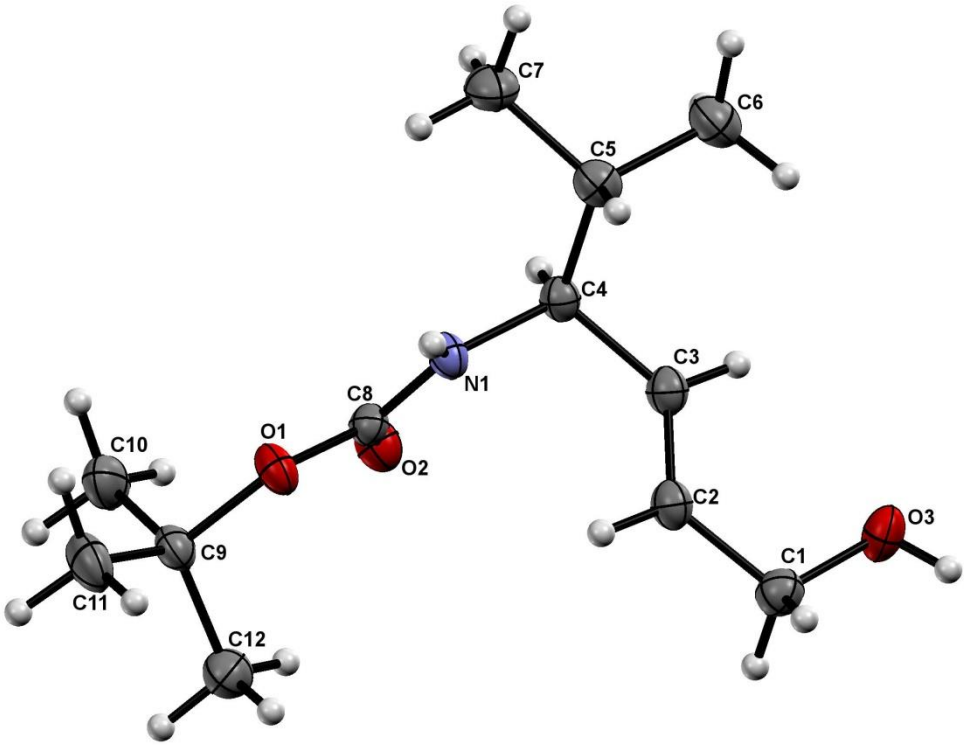


Figure S1: ORTEP diagram of compound **2a**. All H-atoms are not labeled for clarity. Ellipsoids are drawn at 50% probability. (CCDC no 2213473)

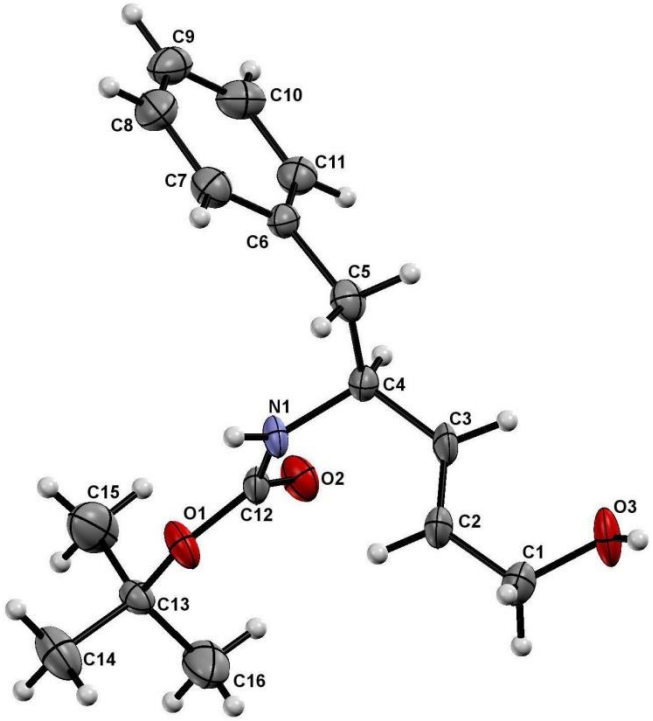


Figure S2: ORTEP diagram of compound **2b**. All H-atoms are not labeled for clarity. Ellipsoids are drawn at 50% probability. (CCDC no 2213474)

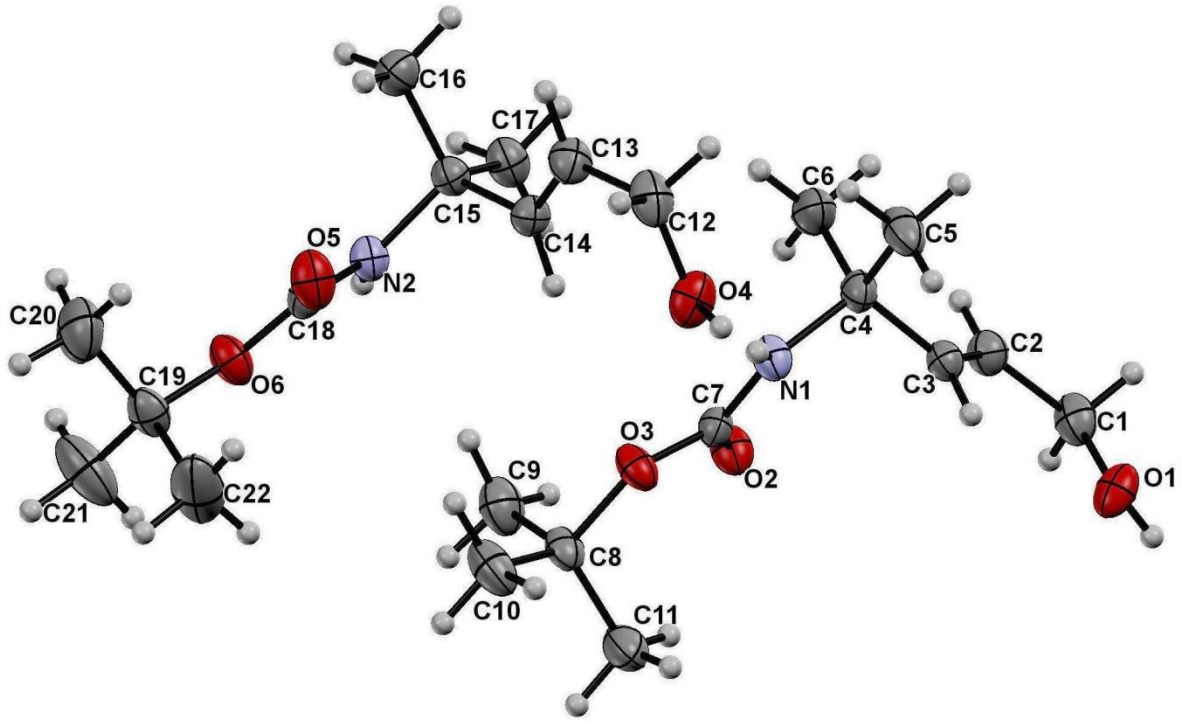


Figure S3: ORTEP diagram of compound **2c**. All H-atoms are not labeled for clarity. Two molecules appeared in the asymmetric unit. Ellipsoids are drawn at 50% probability. (CCDC no 2213475)

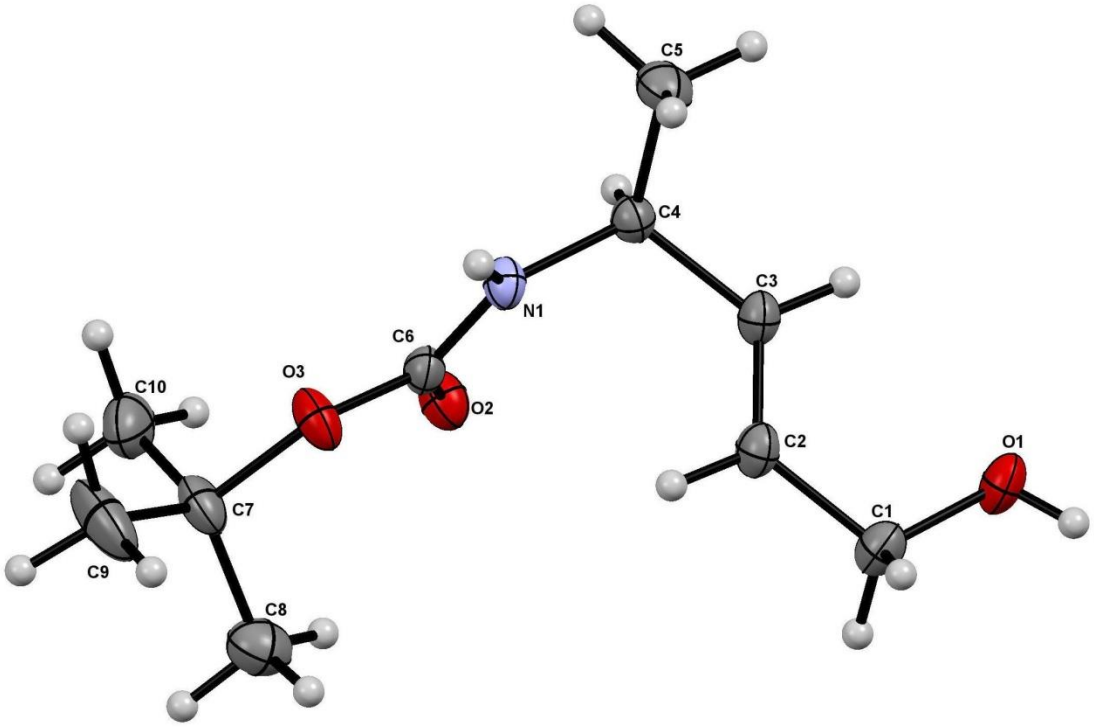


Figure S4: ORTEP diagram of compound 2**d**. All H-atoms are not labeled for clarity. Ellipsoids are drawn at 50% probability. (CCDC no 2213476)

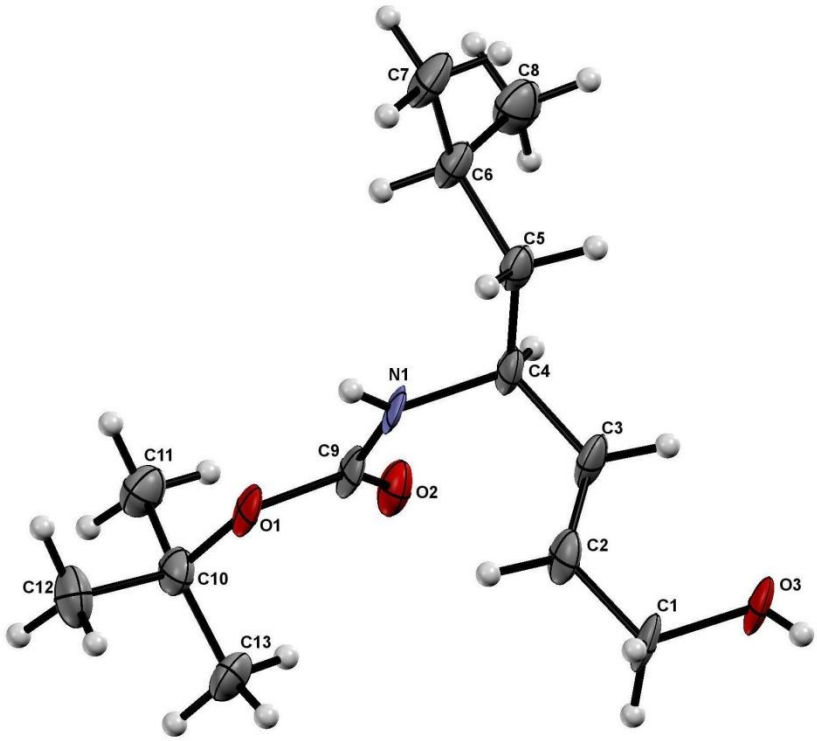


Figure S5: ORTEP diagram of compound **2e**. All H-atoms are not labeled for clarity. Ellipsoids are drawn at 50% probability. (CCDC no 2213477)

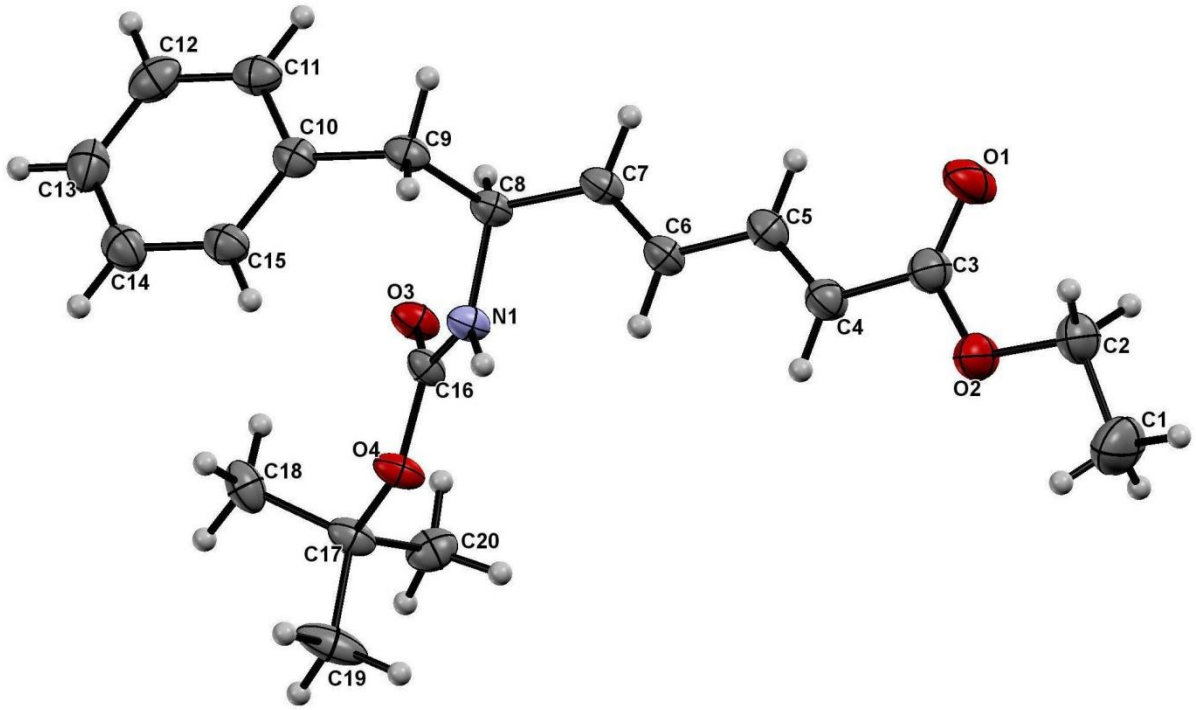


Figure S6: ORTEP diagram of compound **4b**. All H-atoms are not labeled for clarity. Ellipsoids are drawn at 50% probability. (CCDC no 2213478)

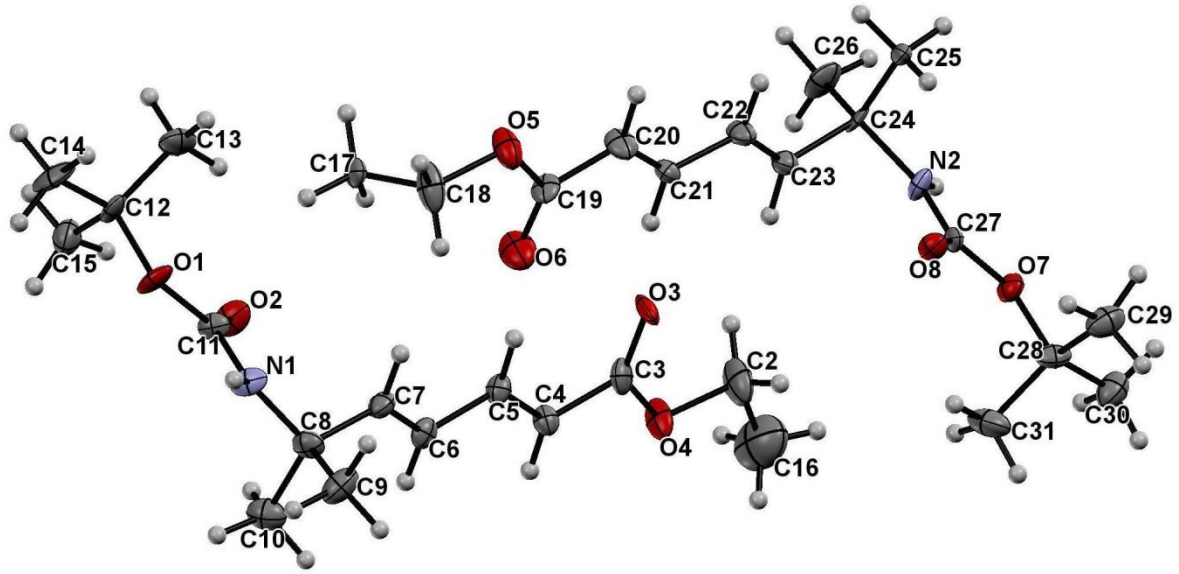


Figure S7: ORTEP diagram of compound **4c**. All H-atoms are not labeled for clarity. Two molecules appeared in the asymmetric unit. Ellipsoids are drawn at 50% probability. (CCDC no 2213479)

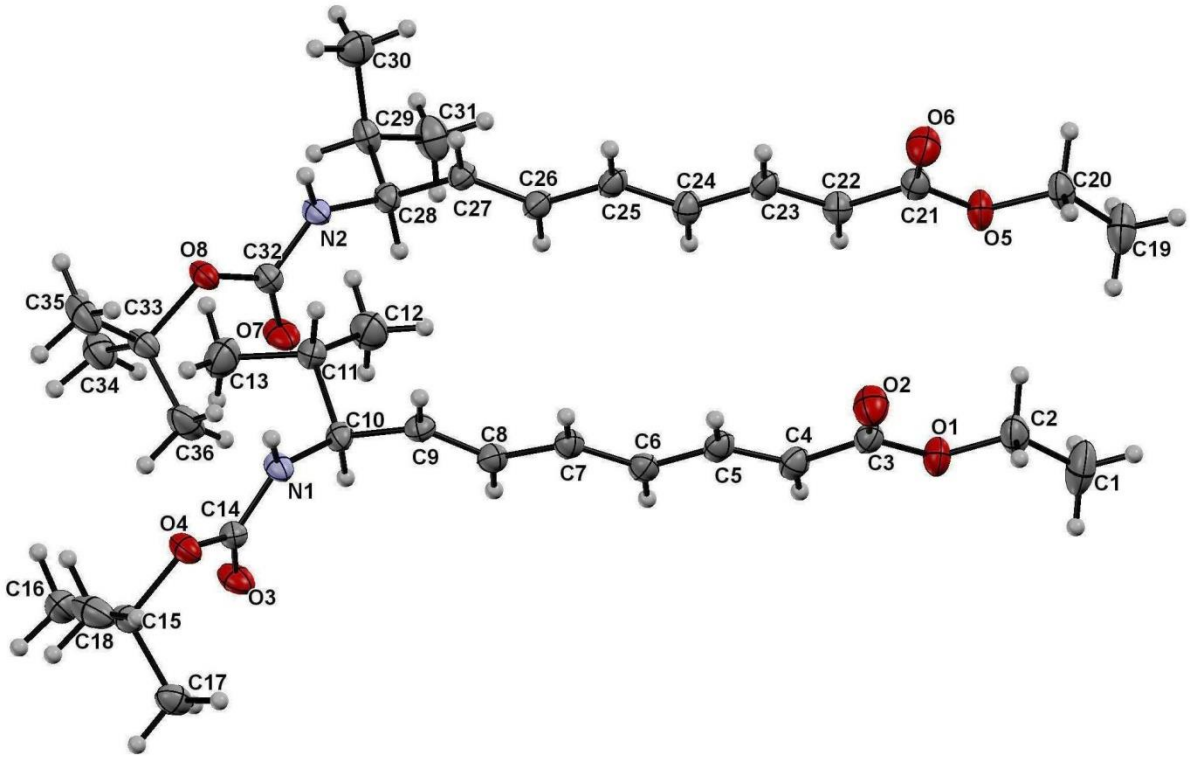


Figure S8: ORTEP diagram of compound **7a**. All H-atoms are not labeled for clarity. Two molecules appeared in the asymmetric unit. Ellipsoids are drawn at 50% probability. (CCDC no 2213480)

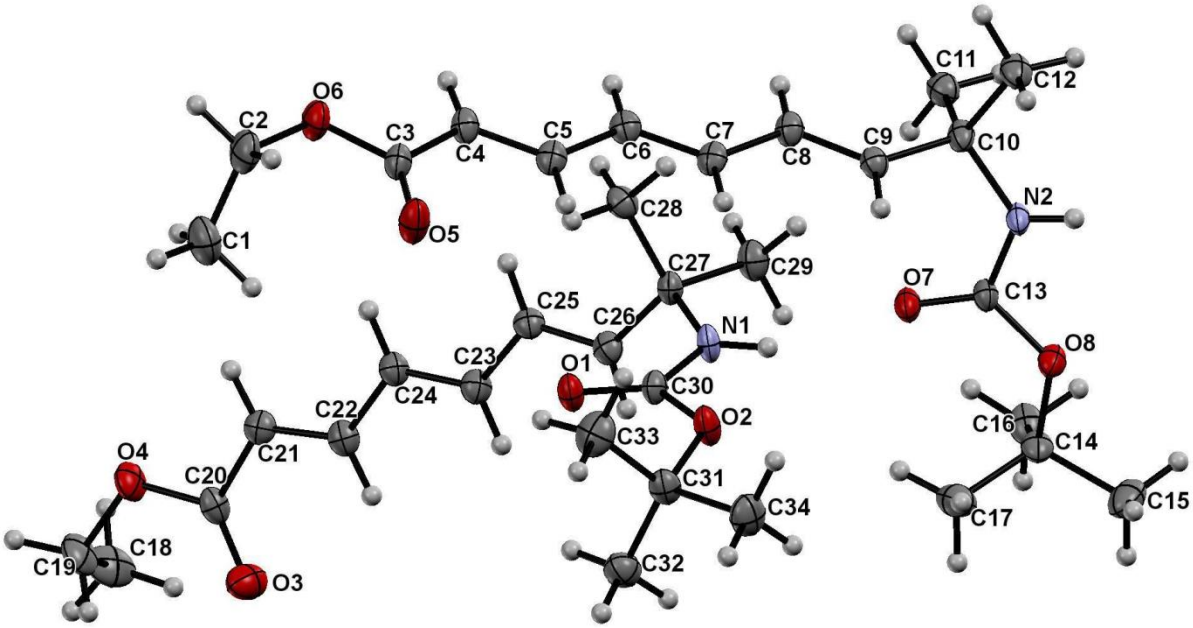


Figure S9: ORTEP diagram of compound **7c**. All H-atoms are not labeled for clarity. Two molecules appeared in the asymmetric unit. Ellipsoids are drawn at 50% probability. (CCDC no 2213481)

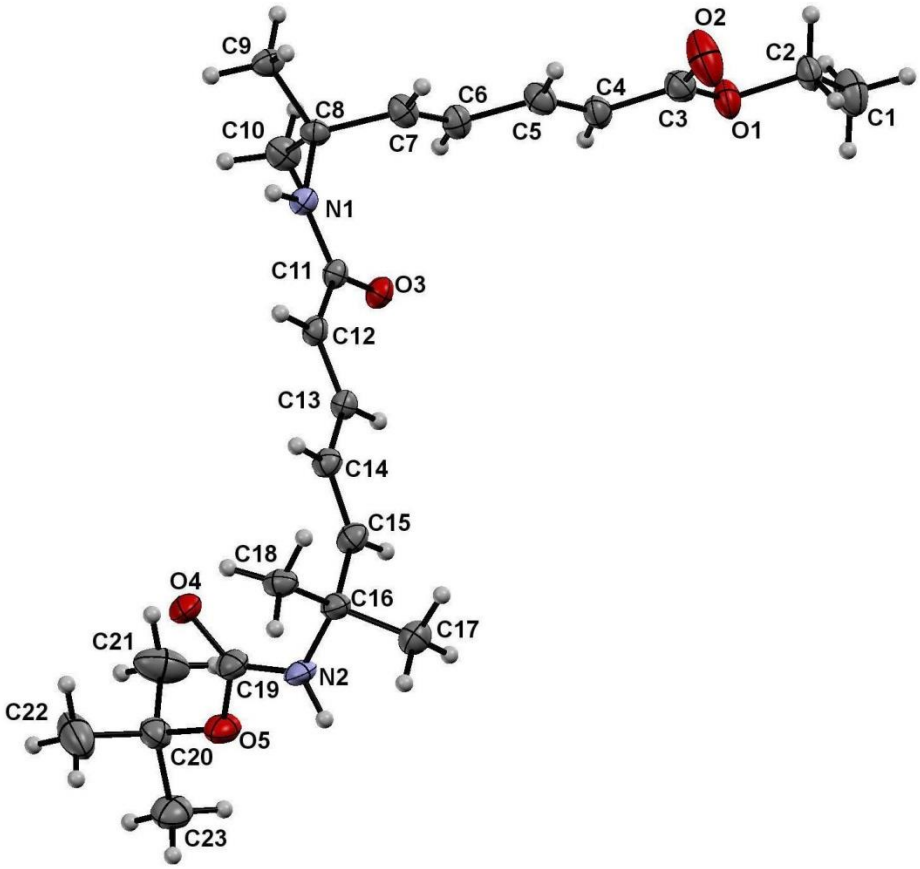


Figure S10: ORTEP diagram of compound **8a**. All H-atoms are not labeled for clarity. Ellipsoids are drawnat 50% probability. (CCDC no 2213482)

2) Crystallographic Information:

Compound 2a: Colourless needle shape Crystals of 2a were grown by slow evaporation from a solution of dichloromethane and n-heptane. A good quality single crystal (0.3 × 0.05 × 0.05 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 149.64), for a total of 12047 independent reflections. Space group P 21 21 21, a = 6.3864(10), b = 10.5866(17), c = 19.684(3), β = 90, V = 1330.8(4) Å^3, Orthorhombic, Z = 4 for chemical formula C_{12} H_{23} N O_3, with one molecule in asymmetric unit; ρ calcd = 1.145 gcm^{-3}, μ = 0.655 mm^{-1}, F (000) = 504.0, Rint= 0.0499. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0416 (wR2 = 0.0791) 2590 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 152 variables, S = 1.062. The largest difference peak and hole were 0.195 and -0.167 eÅ^3, respectively.

Compound 2b: Colourless rod shape Crystals of 2b were grown by slow evaporation from a solution of ethyl acetate and n-hexane. A good quality single crystal (0.2 × 0.1 × 0.1 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 56.824), for a total of 68381 independent reflections. Space group P 21 21 21, a = 6.061(2), b = 12.023(4), c = 21.699(7), β = 90, V = 1581.3(8) Å^3, Orthorhombic, Z = 4 for chemical formula C_{16} H_{23} N O_3, with one molecule in asymmetric unit; ρ calcd = 1.165 gcm^{-3}, μ = 0.080 mm^{-1}, F (000) = 600.0, Rint= 0.1671. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0865 (wR2 = 0.0657) 3927 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 185 variables, S = 1.940. The largest difference in peak and hole were 0.223 and -0.218 eÅ^3, respectively.

Compound 2c: Colourless plate shape Crystals of 2c were grown by slow evaporation from a solution of dichloromethane and n-heptane. A good quality single crystal (0.52 × 0.41 × 0.31 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 52.698), for a total of 35186 independent reflections. Space group P -1, a = 9.165(2), b = 10.586(3), c = 13.936(3), β = 108.378(7), V = 1282.1(5) Å^3, Triclinic, Z = 4 for chemical formula C_{11} H_{21} N O_3, with two molecules in asymmetric unit; ρ calcd = 1.115 gcm^{-3}, μ = 0.080 mm^{-1}, F (000) = 472.0, Rint= 0.0765. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0941 (wR2 = 0.1383) 5120 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 284 variables, S = 1.152. The largest difference peak and hole were 0.251 and -0.250 eÅ^3, respectively.

Compound 2d: Colourless Plate shape Crystals of 2d were grown by slow evaporation from a solution of dichloromethane and n-heptane. A good quality single crystal (0.7 × 0.6 × 0.5 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 56.688), for a total of 17718 independent reflections. Space group P 21 21 21, a = 6.5455(12), b = 9.445(2), c = 19.264(4), β = 90, V = 1191.0(4) Å^3, Orthorhombic, Z = 4 for chemical formula C_{10} H_{19} N O_3, with one molecule in asymmetric unit; ρ calcd = 1.122 gcm^{-3}, μ = 0.082 mm^{-1}, F (000) = 440.0, Rint= 0.0488. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0352 (wR2 = 0.0781) 2966 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 133 variables, S = 0.995. The largest difference peak and hole were 0.175 and -0.186 eÅ^3, respectively.

Compound 2e: Colourless plate shape Crystals of 2e were grown by slow evaporation from a solution of ethyl acetate and n-hexane. A good quality single crystal (0.4 × 0.3 × 0.2 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 48.998), for a total of 15175 independent reflections. Space group P 21 21 2, a = 11.178(7), b = 21.505(13), c = 6.138(4), β = 90, V = 1475.4(15) Å^3, Orthorhombic, Z = 4 for chemical formula C_{13} H_{25} N O_3, with one molecule in asymmetric unit; ρ calcd = 1.095 gcm^{-3}, μ = 0.077 mm^{-1}, F (000) = 536.0, Rint= 0.1319. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0942 (wR2 = 0.2125) 2434 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 149 variables, S = 1.021. The largest difference peak and hole were 0.484 and -0.311 eÅ^3, respectively.

Compound 4b: Colourless plate shape Crystals of 4b were grown by slow evaporation from a solution of dichloromethane and n-heptane. A good quality single crystal (0.33 × 0.25 × 0.17 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 56.702), for a total of 27968 independent reflections. Space group C 2, a = 35.93(5), b = 5.117(8), c = 10.707(16), β = 92.39(3), V = 1967(5) Å^3, Monoclinic, Z = 4 for chemical formula C_{20} H_{27} N O_4, with one molecule in asymmetric unit; ρ calcd = 1.166 gcm^{-3}, μ = 0.081 mm^{-1}, F (000) = 744.0, Rint= 0.0730. The structure was obtained by direct methods using SHELXL-

97.[4] The final R value was 0.0522 (wR2 = 0.1352) 4866 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 231 variables, S = 0.679. The largest difference peak and hole were 0.278 and -0.242 eÅ^3, respectively.

Compound 4c: Colourless plate shape Crystals of 4c were grown by slow evaporation from a solution of dichloromethane and n-heptane. A good quality single crystal (0.42 × 0.30 × 0.22 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 56.844), for a total of 63821 independent reflections. Space group P c, a = 9.1906(18), b = 18.987(4), c = 9.7142(16), β = 100.338(6), V = 1667.6(5) Å^3, Monoclinic, Z = 4 for chemical formula C_{15} H_{25} N O_4, with two molecules in asymmetric unit; ρ calcd = 1.129 gcm^{-3}, μ = 0.081 mm^{-1}, F (000) = 616.0, Rint= 0.1210. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0866 (wR2 = 0.1342) 8309 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 374 variables, S = 0.997. The largest difference peak and hole were 0.749 and -0.406 eÅ^3, respectively.

Compound 7a: Colourless plate shape Crystals of 7a were grown by slow evaporation from a solution of dichloromethane and n-heptane. A good quality single crystal (0.28 × 0.21 × 0.17 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 57.14), for a total of 25003 independent reflections. Space group P -1, a = 10.171(4), b = 11.307(4), c = 18.203(6), β = 78.945(8), V = 1922.9(12) Å^3, Triclinic, Z = 4 for chemical formula C_{18} H_{29} N O_4, with two molecules in asymmetric unit; ρ calcd = 1.117 gcm^{-3}, μ = 0.078 mm^{-1}, F (000) = 704.0, Rint= 0.0976. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0681 (wR2 = 0.1411) 9658 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 428 variables, S = 0.919. The largest difference peak and hole were 0.324 and -0.253 eÅ^3, respectively.

Compound 7c: Colourless rod shape Crystals of 7c were grown by slow evaporation from a solution of dichloromethane and n-heptane. A good quality single crystal (0.38 × 0.15 × 0.14

mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 56.844), for a total of 78922 independent reflections. Space group P 21/c, a = 9.880(3), b = 20.895(7), c = 18.293(6), β = 105.188(10), V = 3645(2) Å^3, Monoclinic, Z = 8 for chemical formula C_{17} H_{27} N O_4, with two molecules in asymmetric unit; ρ calcd = 1.128 gcm^{-3}, μ = 0.079 mm^{-1}, F (000) = 1344.0, Rint= 0.1187. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0619 (wR2 = 0.1811) 9130 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 410 variables, S = 0.726. The largest difference peak and hole were 0.339 and -0.311 eÅ^3, respectively.

Compound 8a: Colourless plate shape Crystals of 8a were grown by slow evaporation from a solution of methanol and water. A good quality single crystal (0.2× 0.09 × 0.05 mm) was mounted on the head of a goniometer using a loop with a small amount of paraffin oil. The X-ray diffraction data of a single crystal 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 = 57.312), for a total of 33779 independent reflections. Space group P n a 21, a = 9.447(4), b = 7.160(3), c = 36.118(16), β = 90, V = 2443.1(19) Å^3, Orthorhombic, Z = 4 for chemical formula C_{23} H_{36} N_2 O_5, with one molecule in asymmetric unit; ρ calcd = 1.143 gcm^{-3}, μ = 0.080 mm^{-1}, F (000) = 912, Rint= 0.0837. The structure was obtained by direct methods using SHELXL-97.[4] The final R value was 0.0652 (wR2 = 0.1504) 6159 observed reflections ($F0 \geq 4\sigma$ (|F0|)) and 280 variables, S = 1.041. The largest difference peak and hole were 0.477 and -0.238 eÅ^3, respectively.

3) Chiral HPLC Trace of Compounds 2a, 4a, 5a, 7a, 2e and 4e :

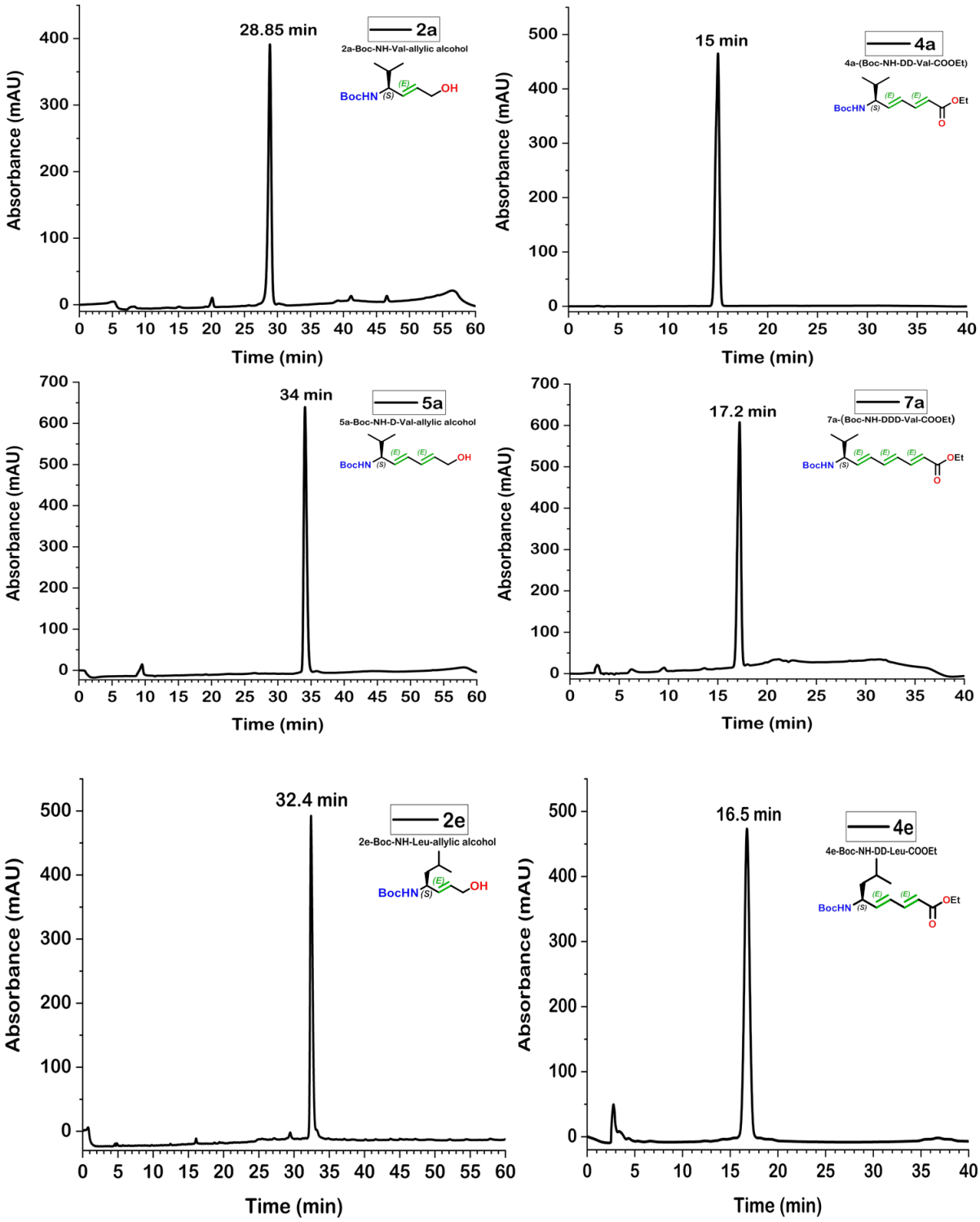
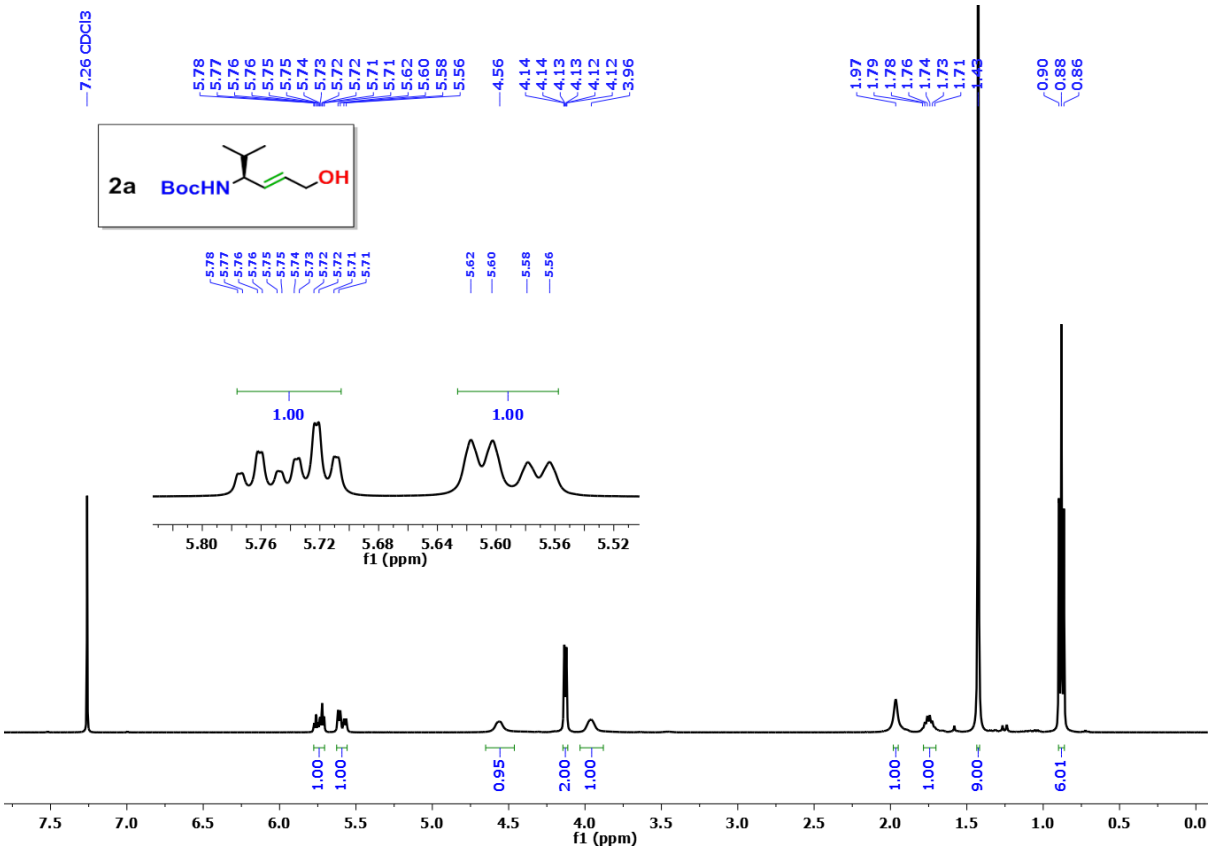
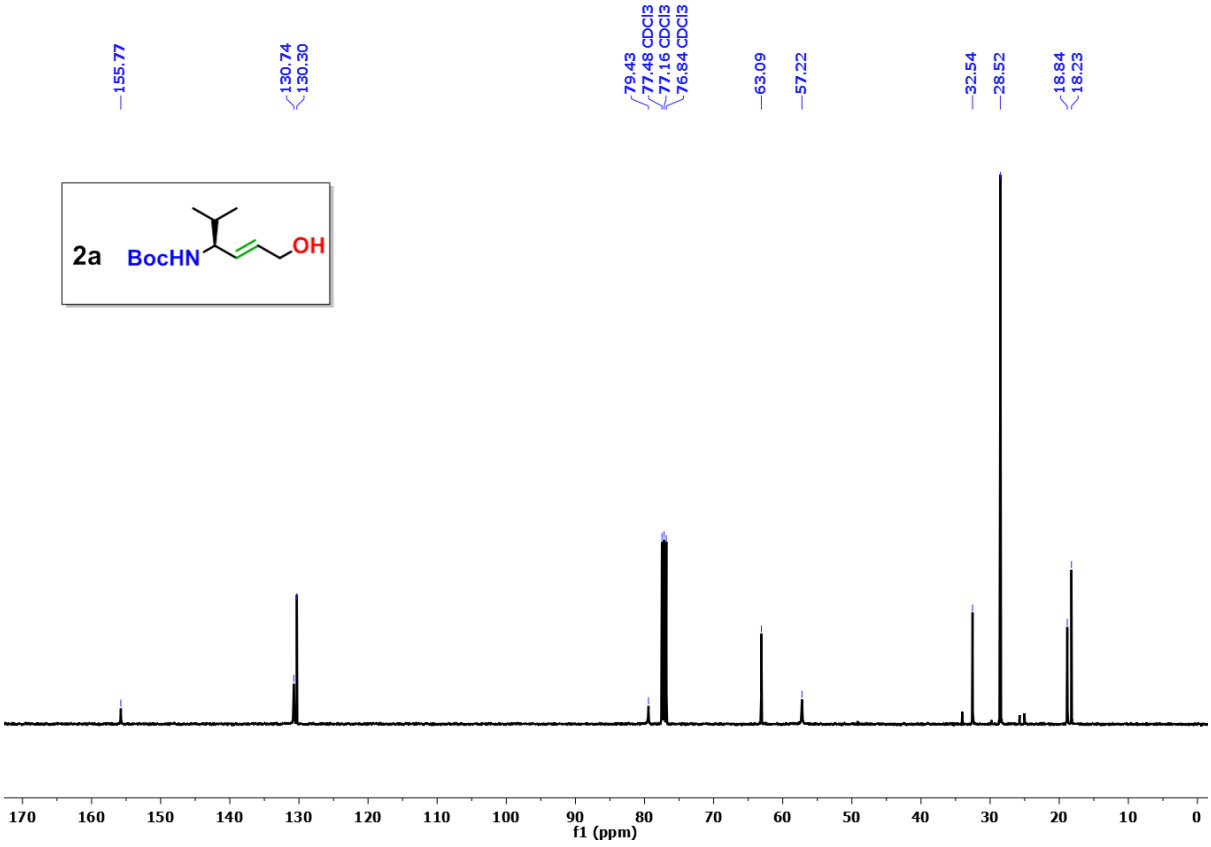
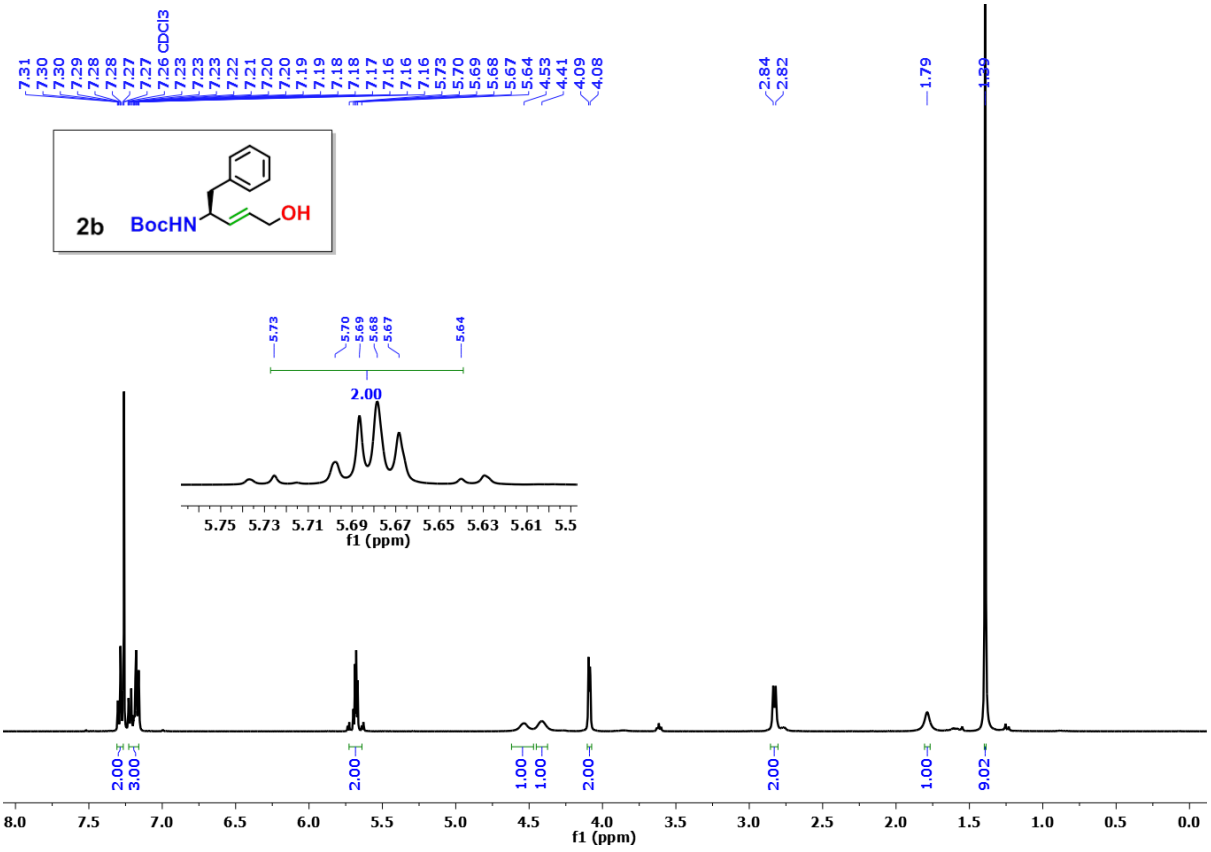


Figure S11: Chiral HPLC trace of Compounds **2a, 4a, 5a, 7a, 2e** and **4e**. The HPLC was performed on the DAICEL CHIRALPAK-IC column using an n-hexane/isopropanol (95/5) solvent system at isocratic mode with a flow rate of 1 mL/min.

4) ^{1}H and ^{13}C NMR Spectra of all Compounds



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2.84 2.82
1.79
1.39
2b
BocHN
OH
5.73 5.70 5.69 5.68 5.67 5.64
2.00
5.75 5.73 5.71 5.69 5.67 5.65 5.63 5.61 5.5
f1 (ppm)
2.00 3.00 2.00 1.00 1.00 2.00 2.00 1.00 9.02
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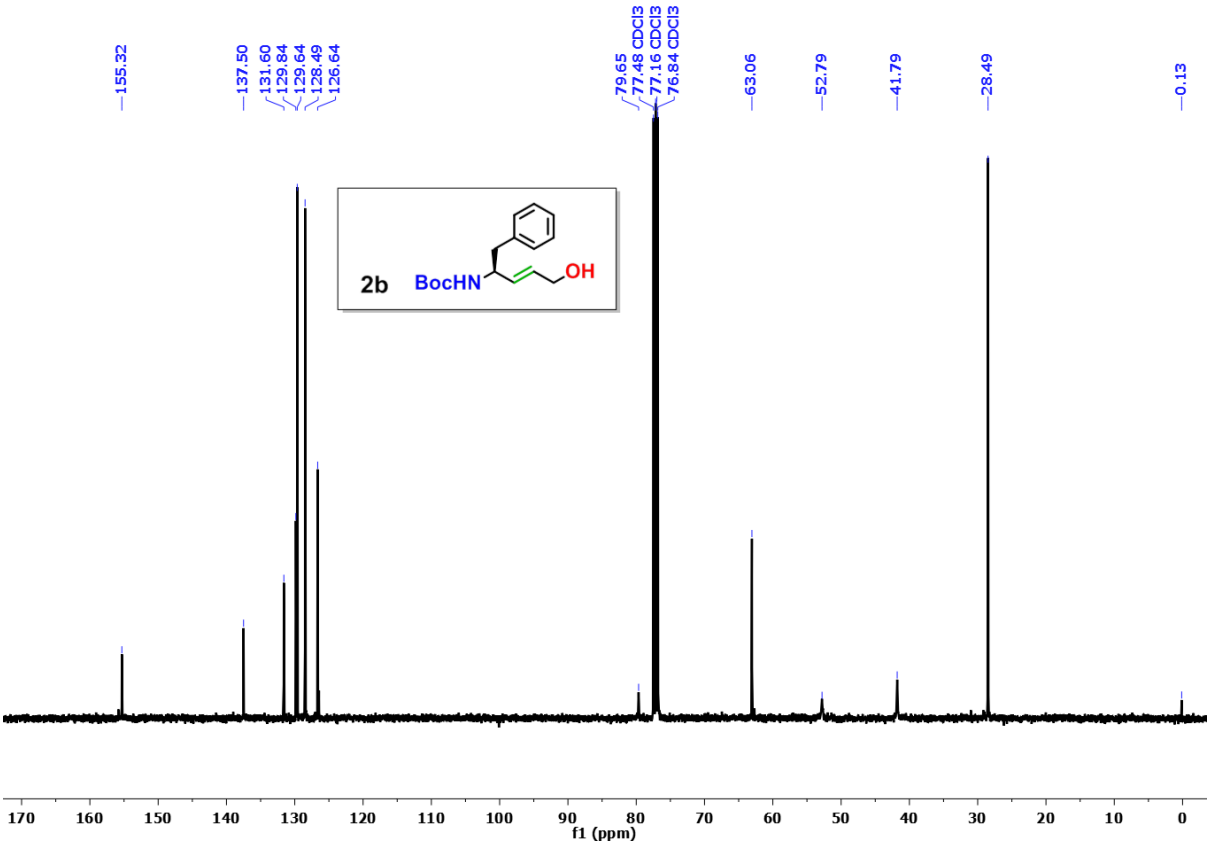
f1 (ppm)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63.06
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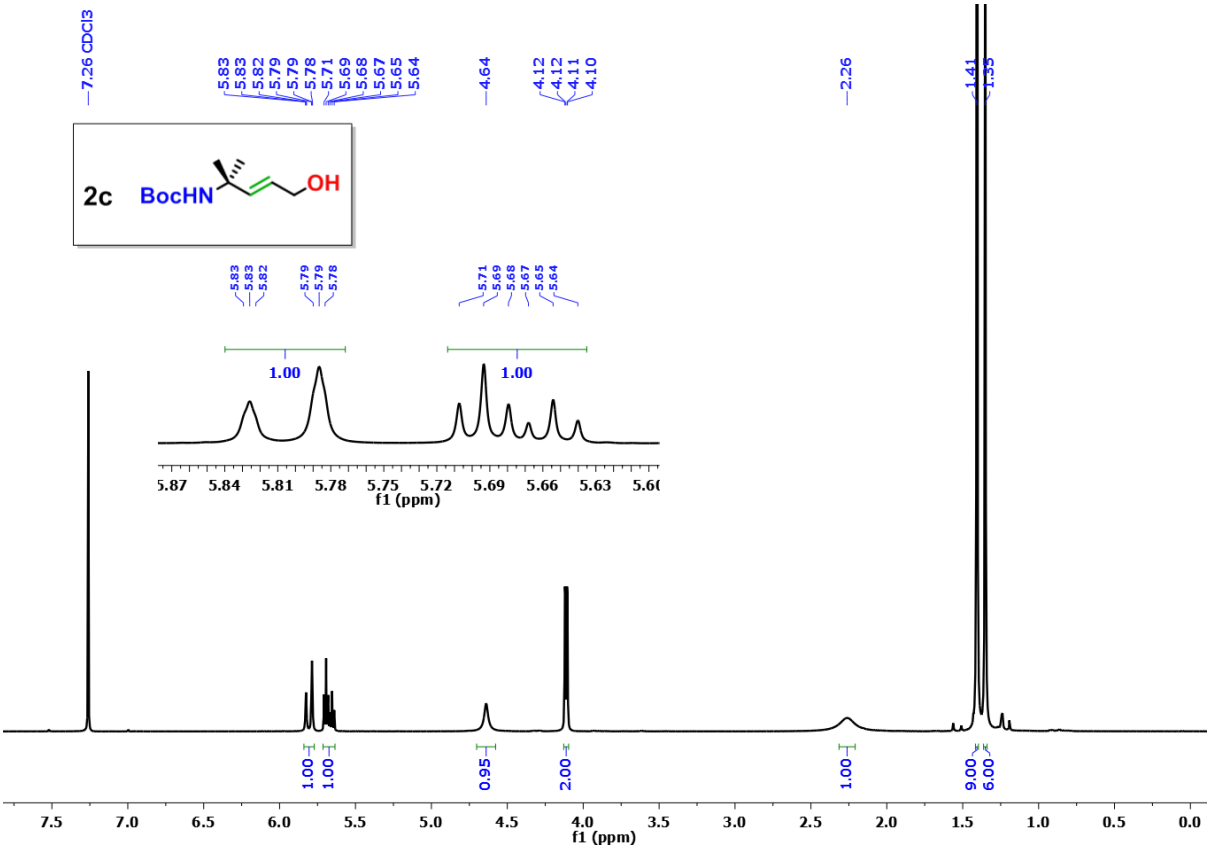
28.49
0.13
2b
BocHN
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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4.10
2.26
1.41
1.35
2c
BocHN
OH
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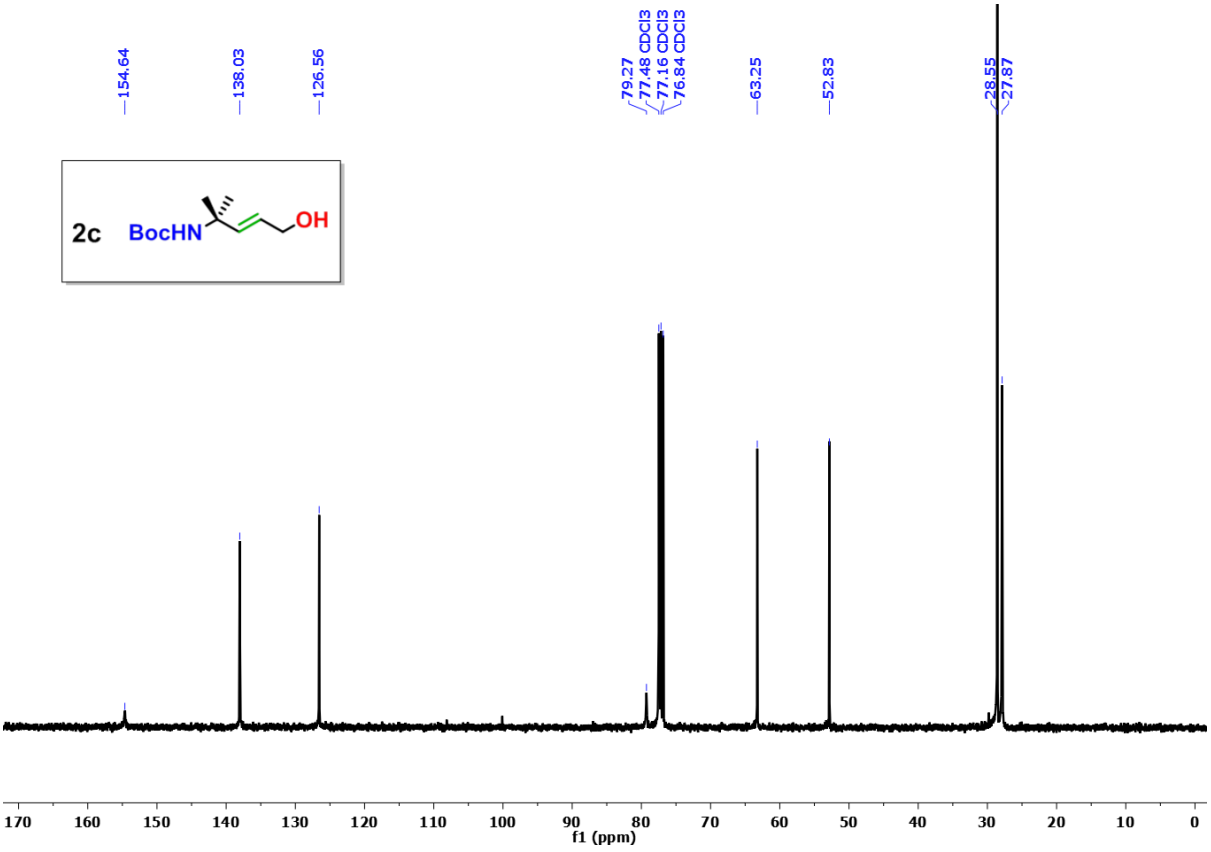
6.00
f1 (ppm)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63.25
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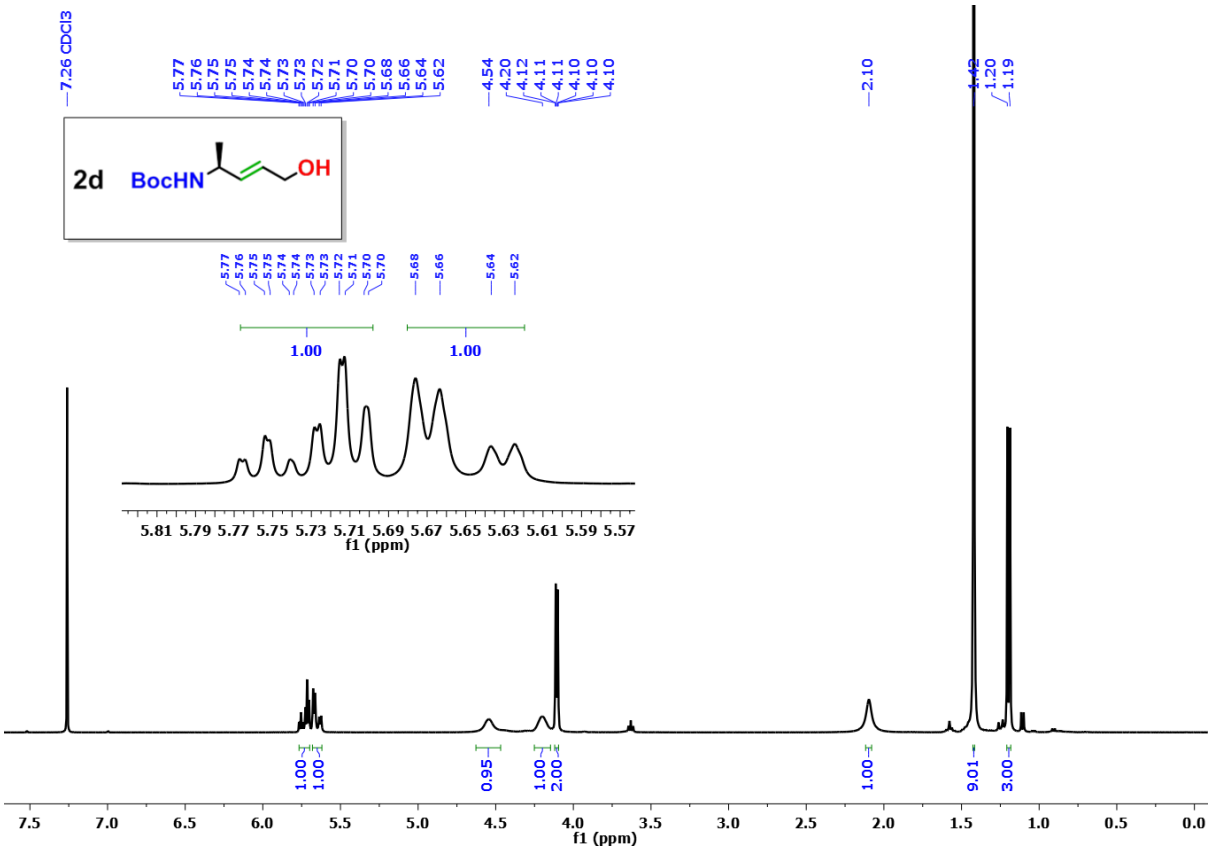
BocHN
OH
f1 (ppm)
f1 (ppm)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4.54 4.20 4.12 4.11 4.11 4.10 4.10 4.10
2.10
1.42 1.20 1.19
2d BocHN OH
1.00 1.00
5.81 5.79 5.77 5.75 5.73 5.71 5.69 5.67 5.65 5.63 5.61 5.59 5.57
f1 (ppm)
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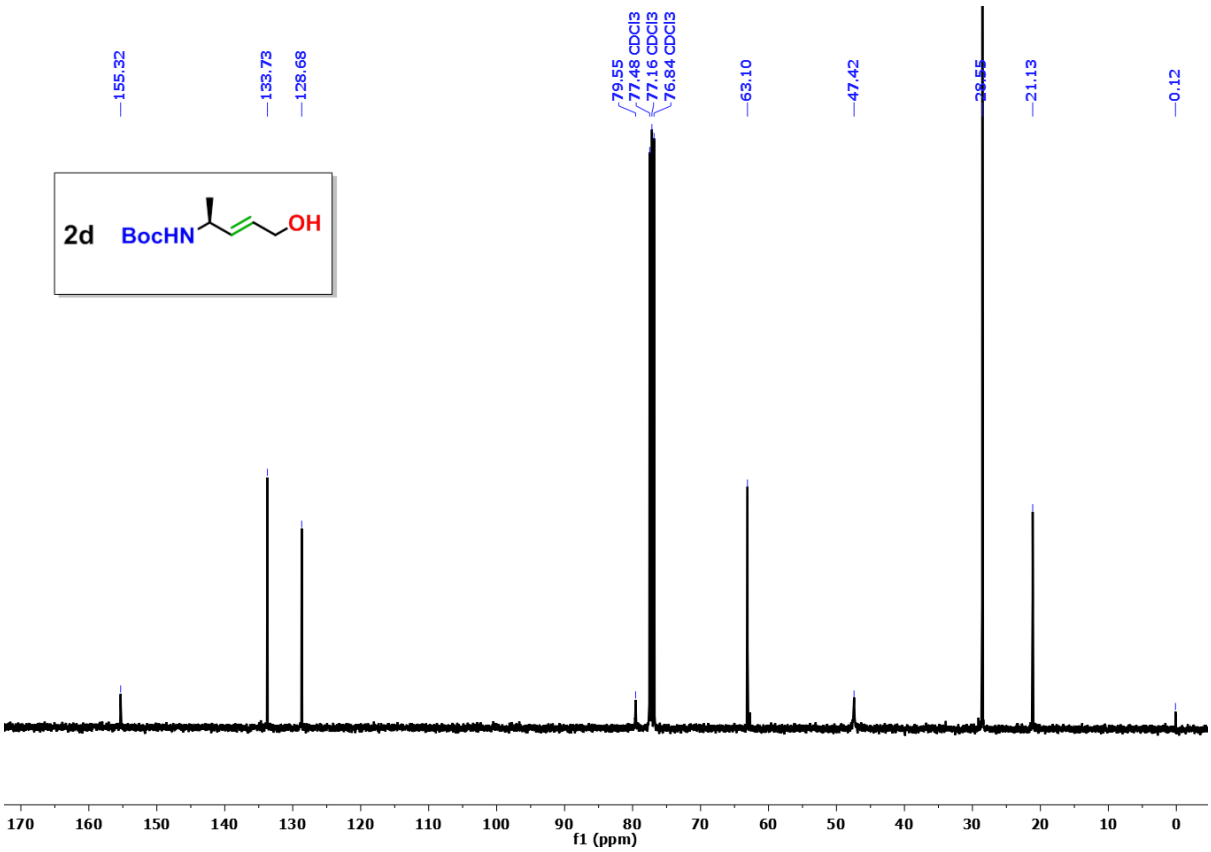
f1 (ppm)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128.68
79.55
77.48 CDCl3
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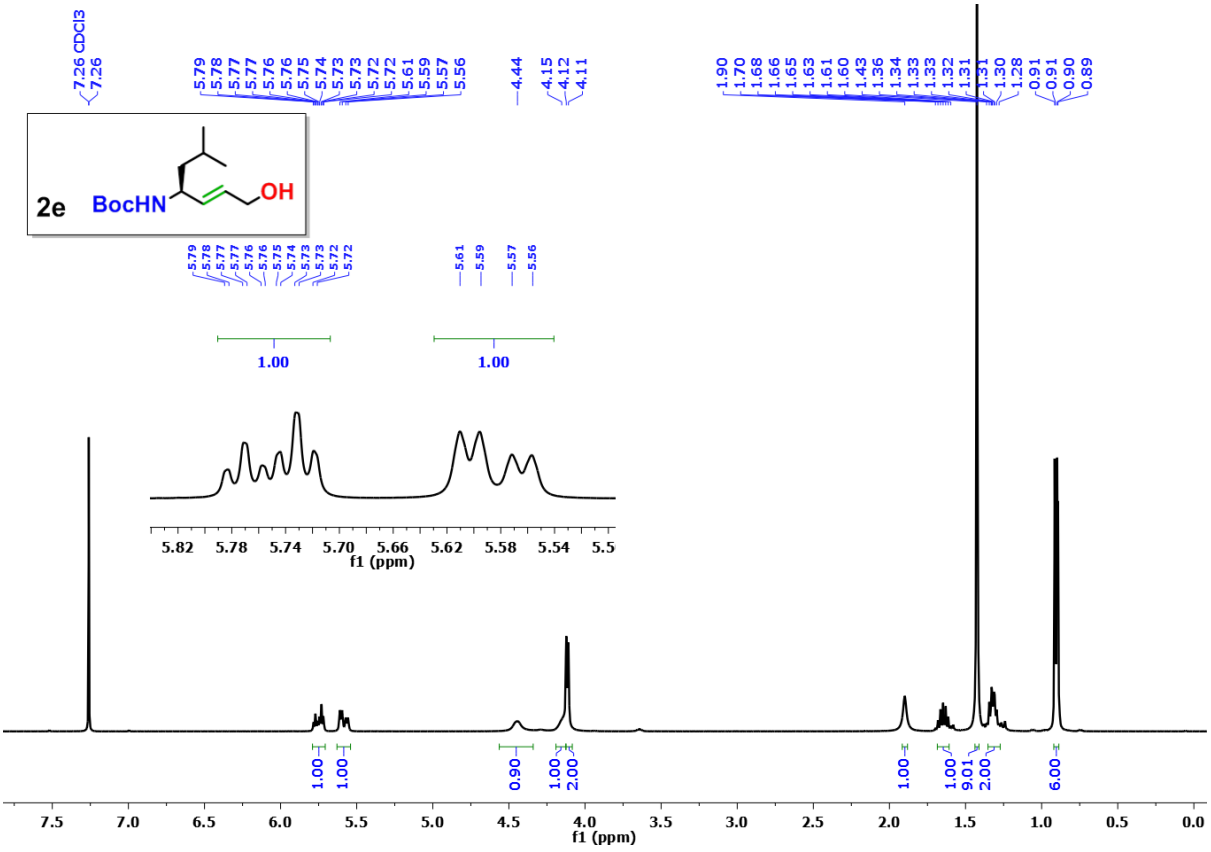
f1 (ppm)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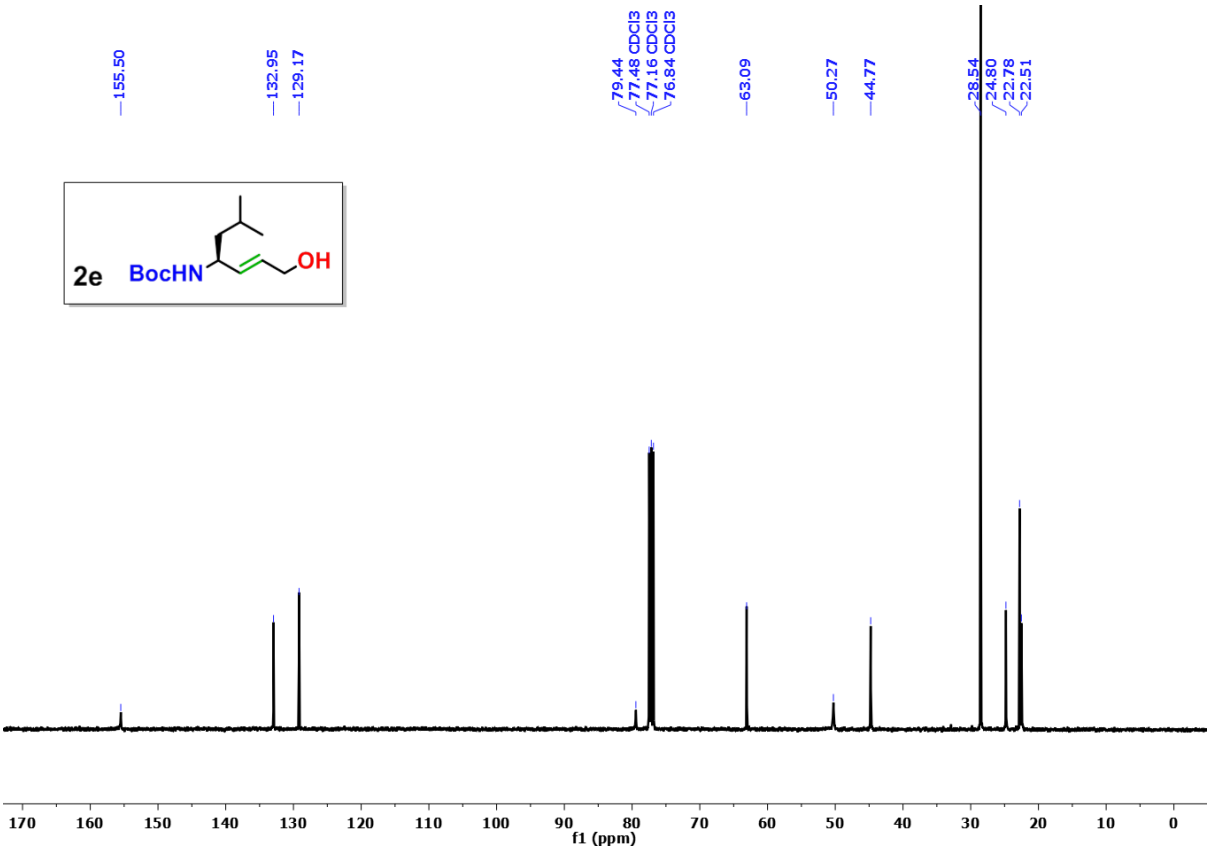
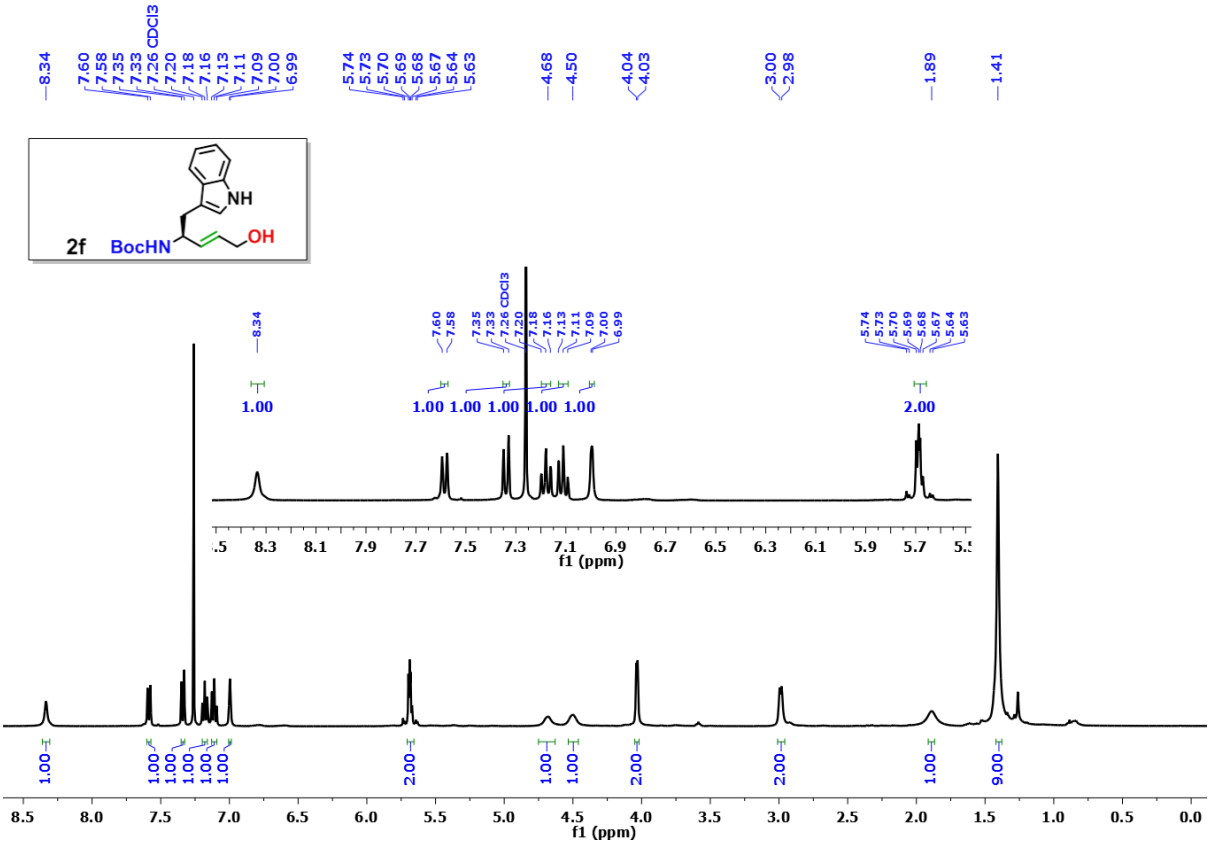
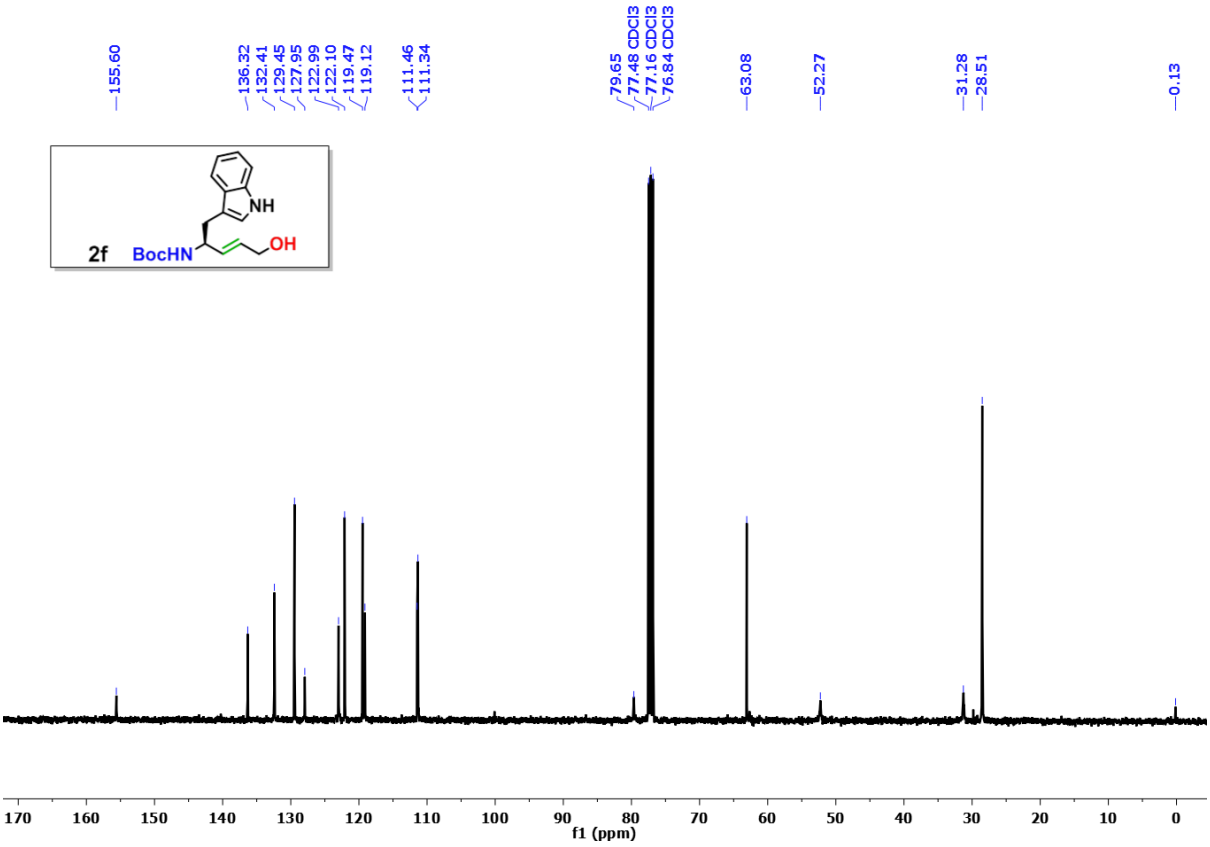
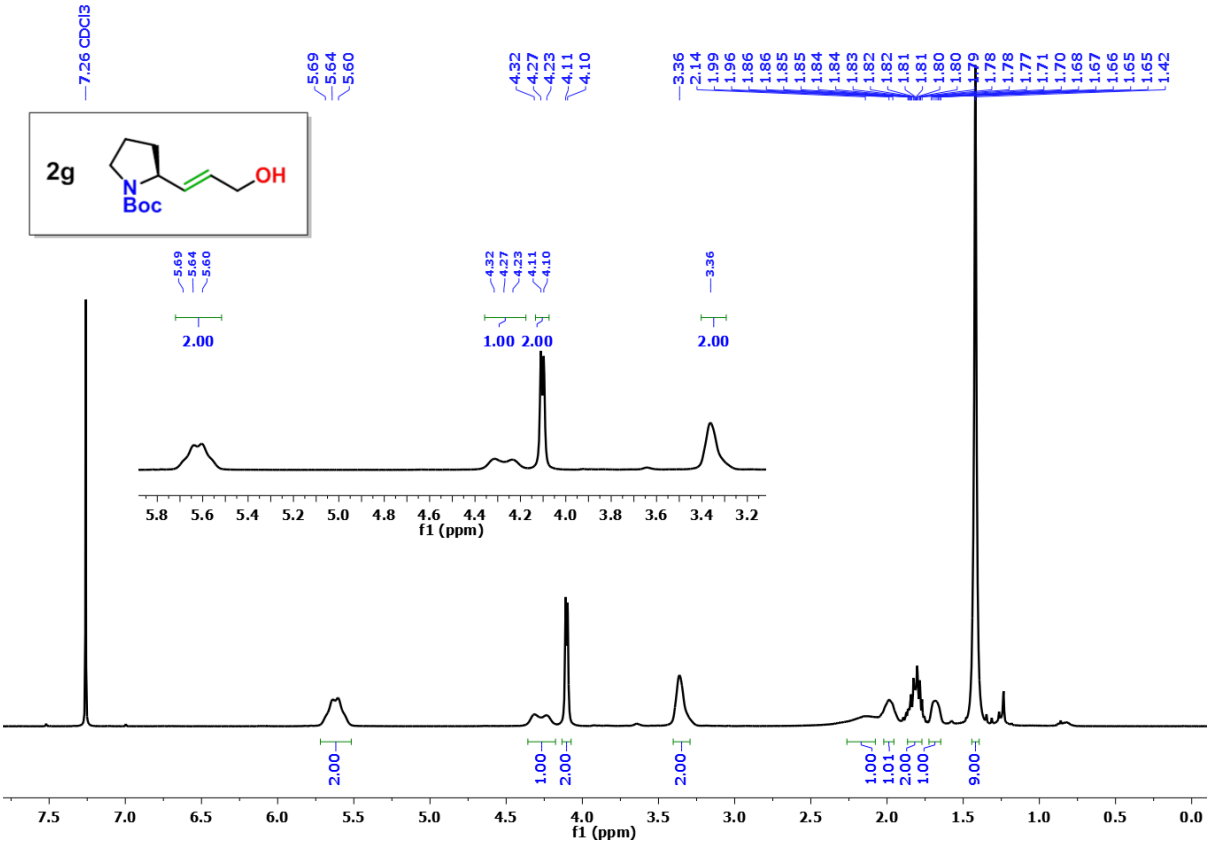
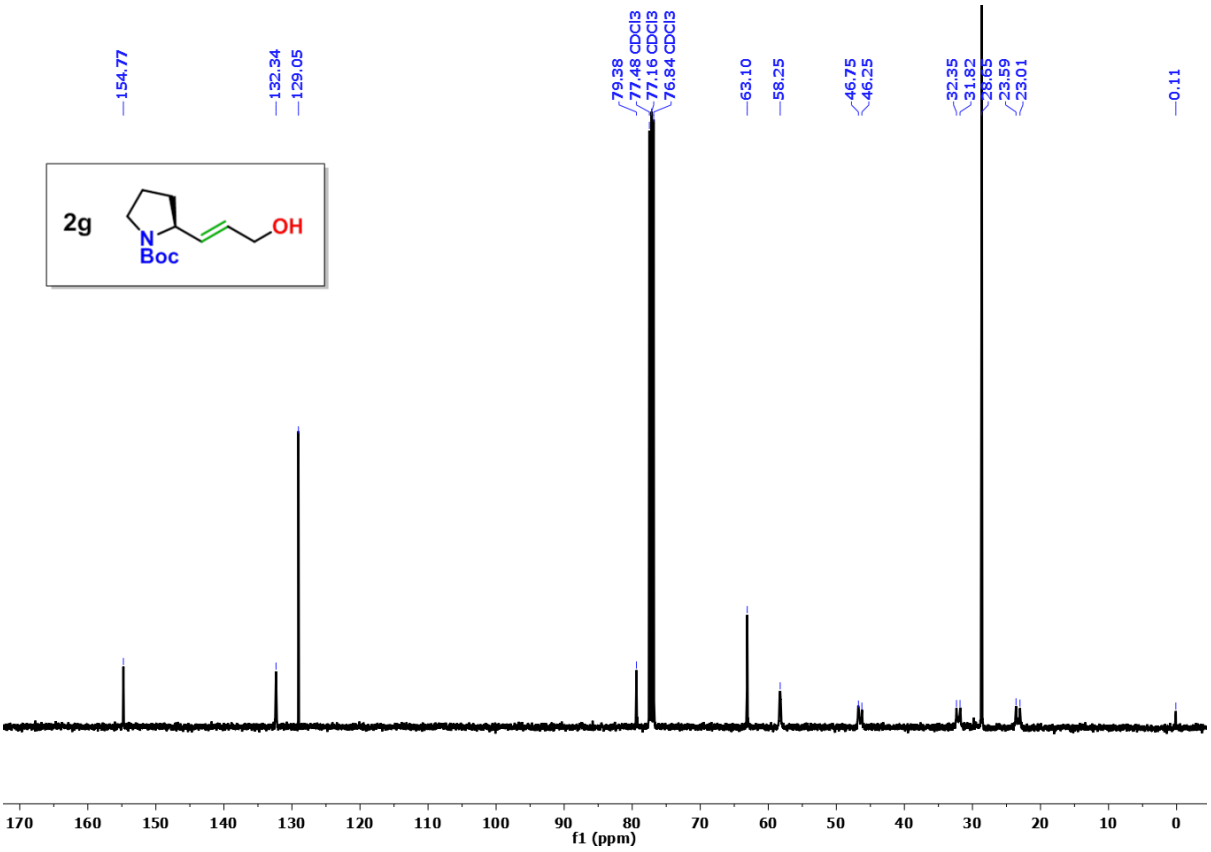
0.90
0.89
2e
BocHN
OH
1.00
1.00
5.82
5.78
5.74
5.70
5.66
5.62
5.58
5.54
5.5
f1 (ppm)
1.00
1.00
0.90
1.00
2.00
1.00
1.00
9.01
2.00
6.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

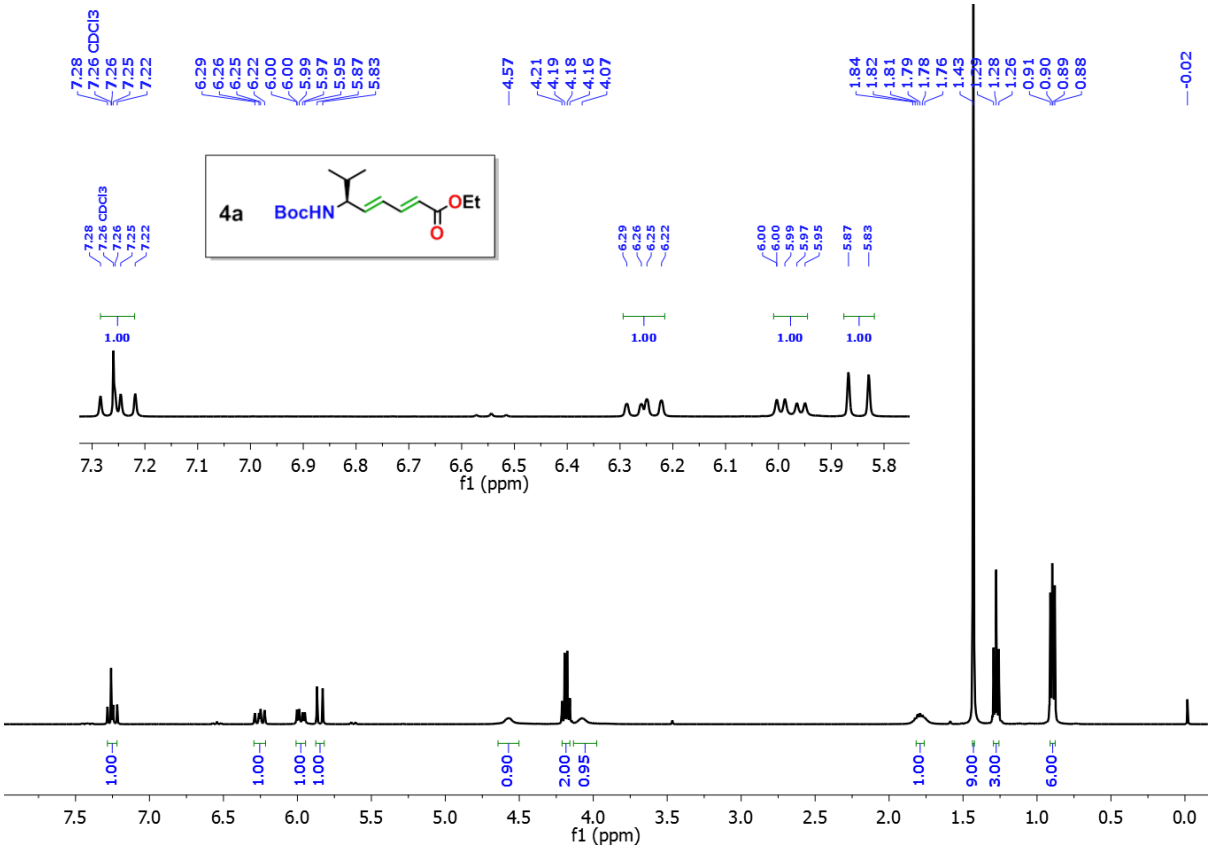

155.50
132.95
129.17
79.44
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
63.09
50.27
44.77
28.54
24.80
22.78
22.51
2e
BocHN
OH
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

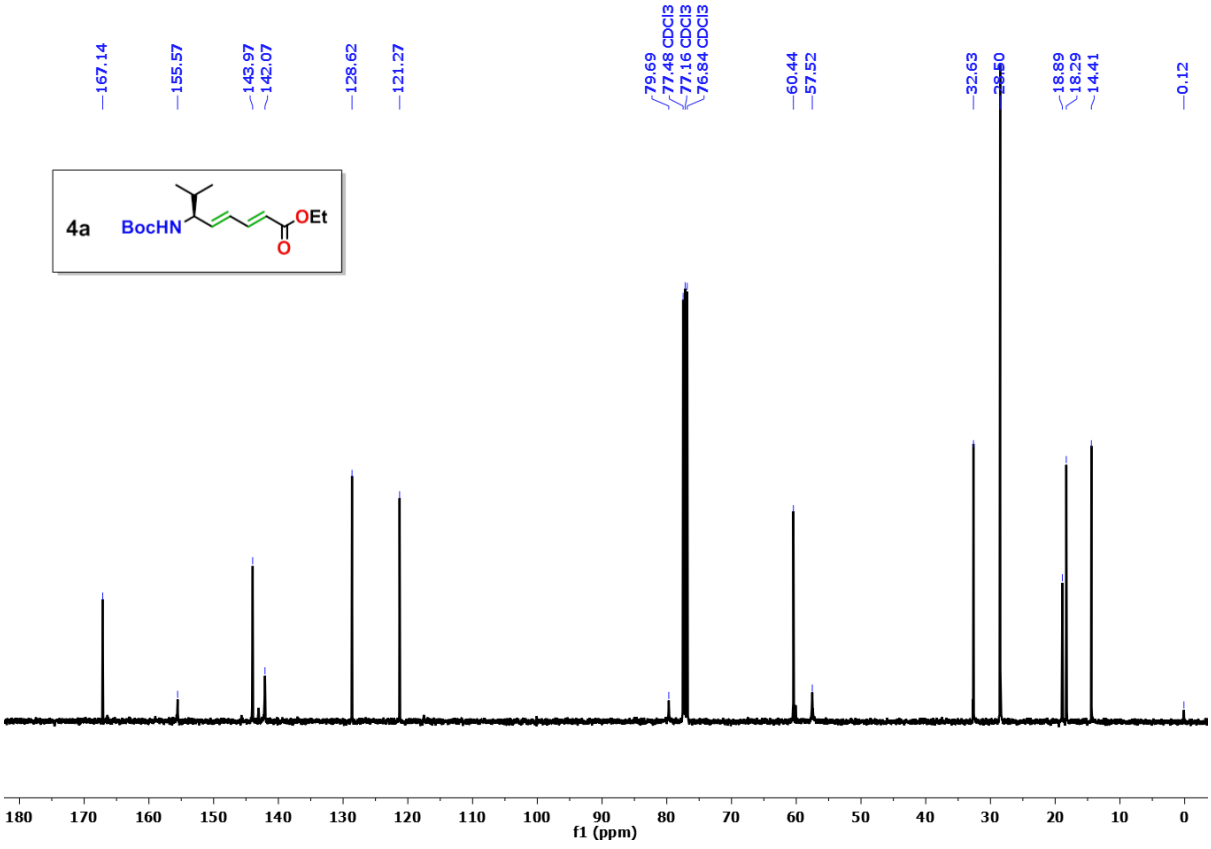

8.34
7.60
7.58
7.35
7.33
7.26 CDCl3
7.20
7.18
7.16
7.13
7.11
7.09
7.00
6.99
5.74
5.73
5.70
5.69
5.68
5.67
5.64
5.63
4.68
4.50
4.04
4.03
3.00
2.98
1.89
1.41
NH
2f BocHN OH
1.00 1.00 1.00 1.00 1.00 1.00 2.00
f1 (ppm)
1.00 1.00 1.00 1.00 1.00 2.00 1.00 1.00 2.00 2.00 1.00 9.00
f1 (ppm)

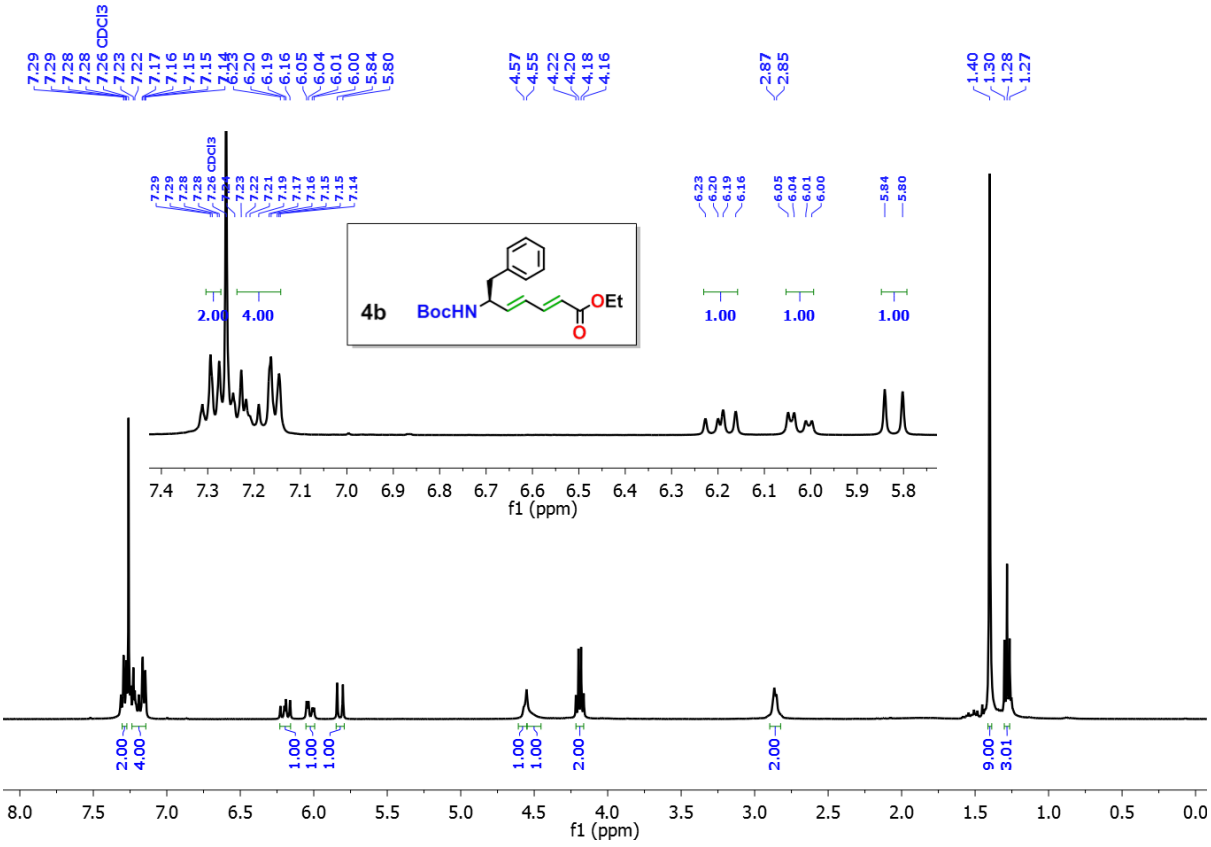

155.60
136.32
132.41
129.45
127.95
122.99
122.10
119.47
119.12
111.46
111.34
79.65
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
63.08
52.27
31.28
28.51
0.13
NH
2f BocHN OH
f1 (ppm)

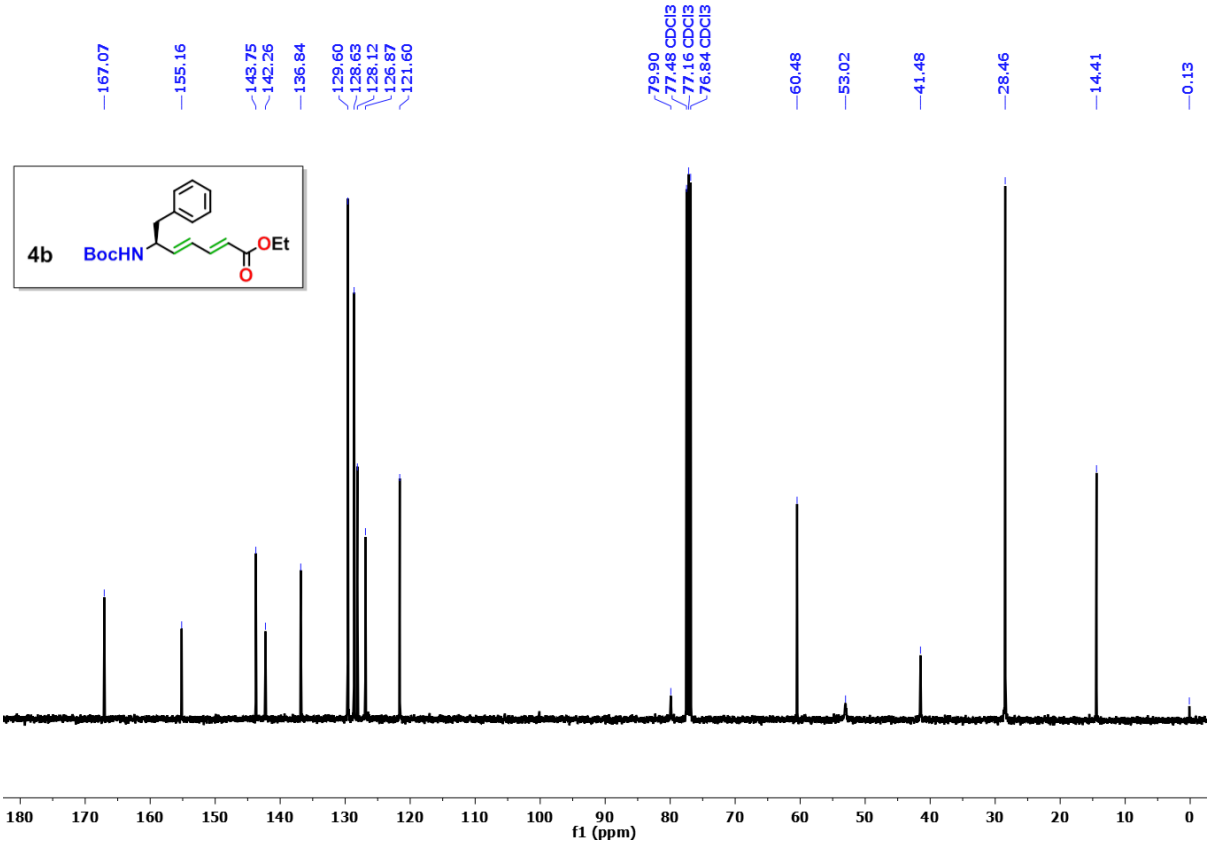

7.26 CDCl3
5.69
5.64
5.60
4.32
4.27
4.23
4.11
4.10
3.36
2.14
1.99
1.96
1.86
1.85
1.85
1.84
1.84
1.83
1.82
1.82
1.81
1.81
1.80
1.80
1.79
1.78
1.78
1.77
1.71
1.70
1.68
1.67
1.66
1.65
1.65
1.42
2g
N
Boc
OH
2.00
1.00
2.00
2.00
f1 (ppm)
2.00
1.00
2.00
2.00
1.00
1.01
2.00
1.00
9.00
f1 (ppm)

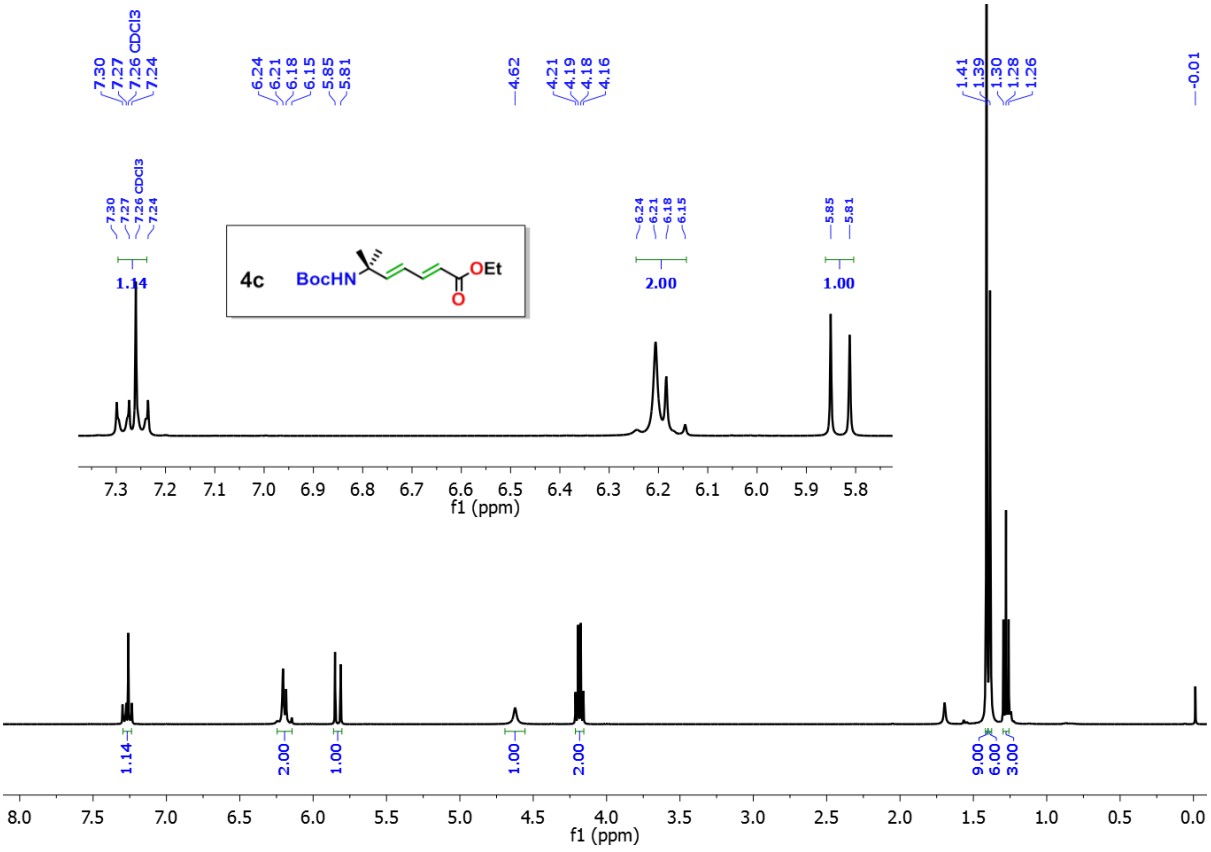

154.77
132.34
129.05
79.38
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
63.10
58.25
46.75
46.25
32.35
31.82
28.65
23.59
23.01
0.11
2g
N
Boc
OH
f1 (ppm)

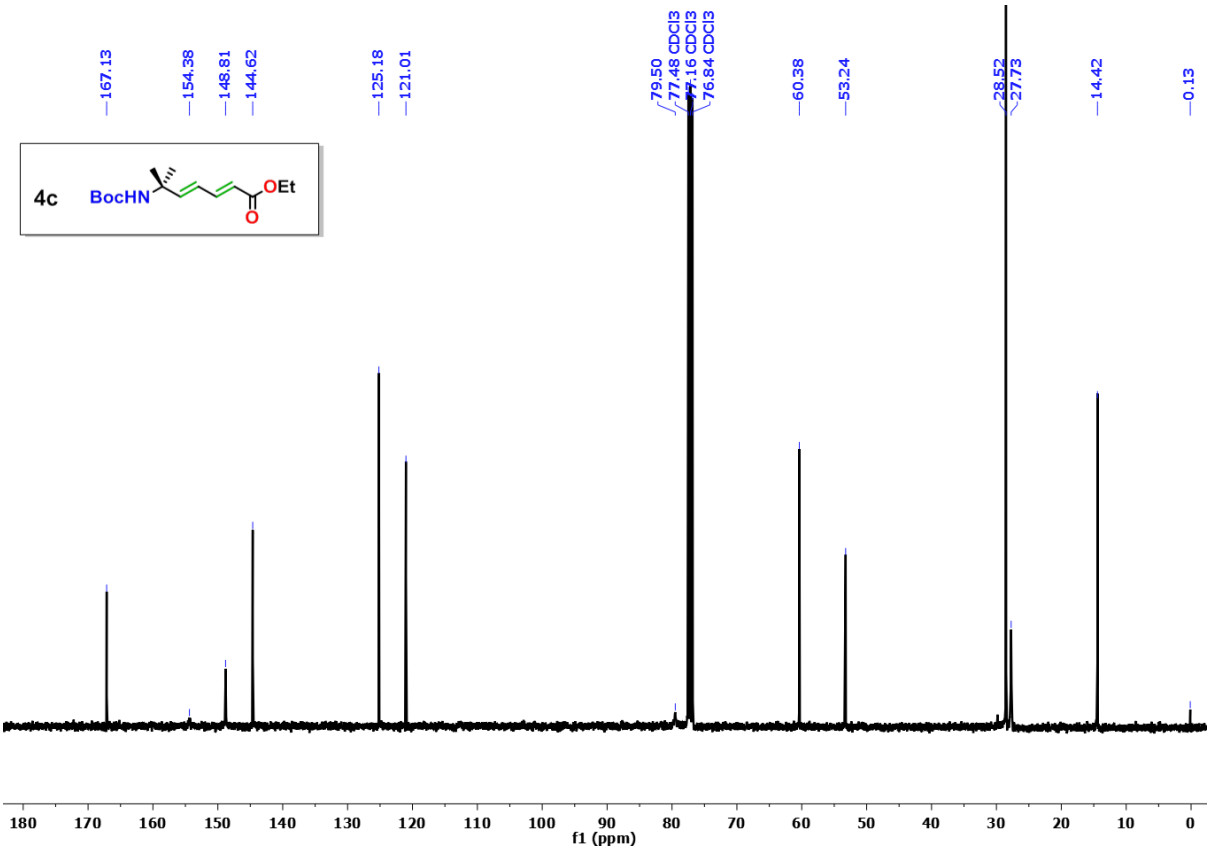

4a
BocHN
OEt
O
f1 (ppm)

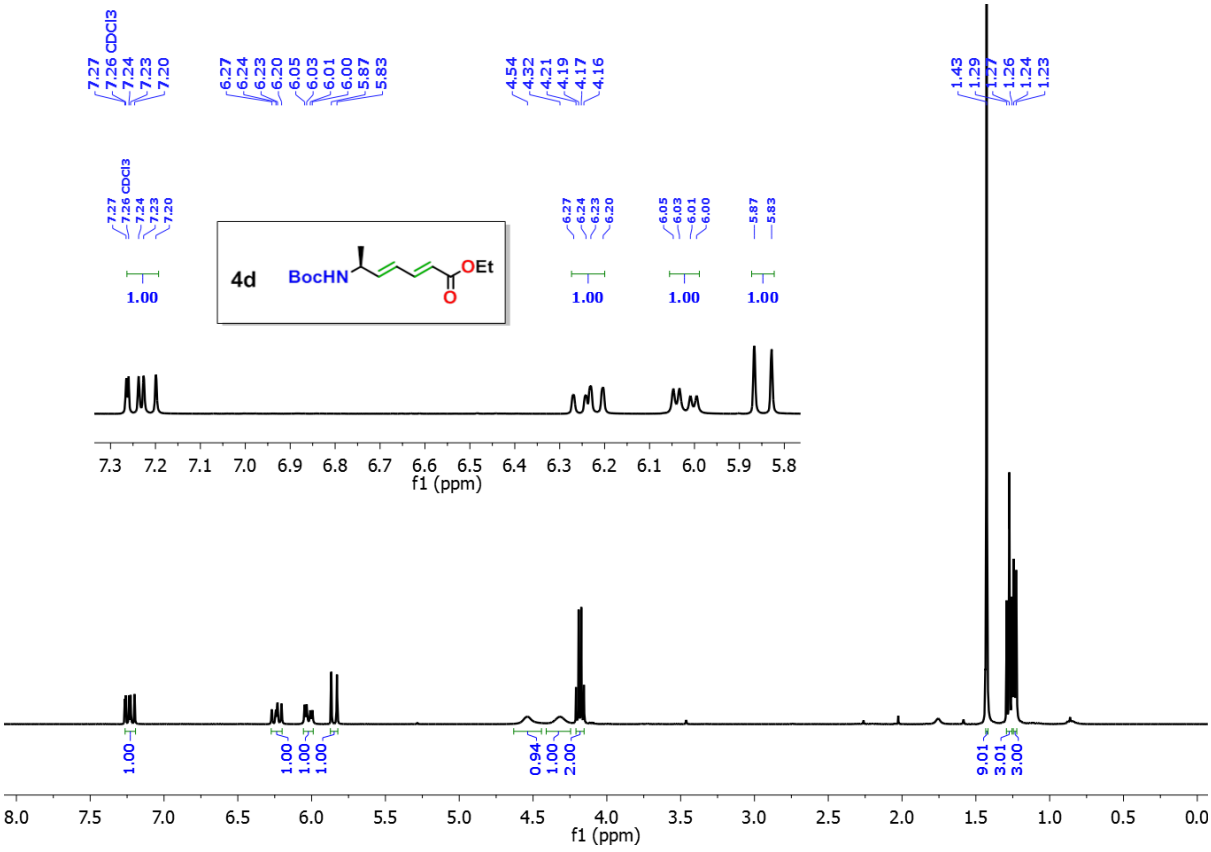

4a
BocHN
OEt
O
f1 (ppm)

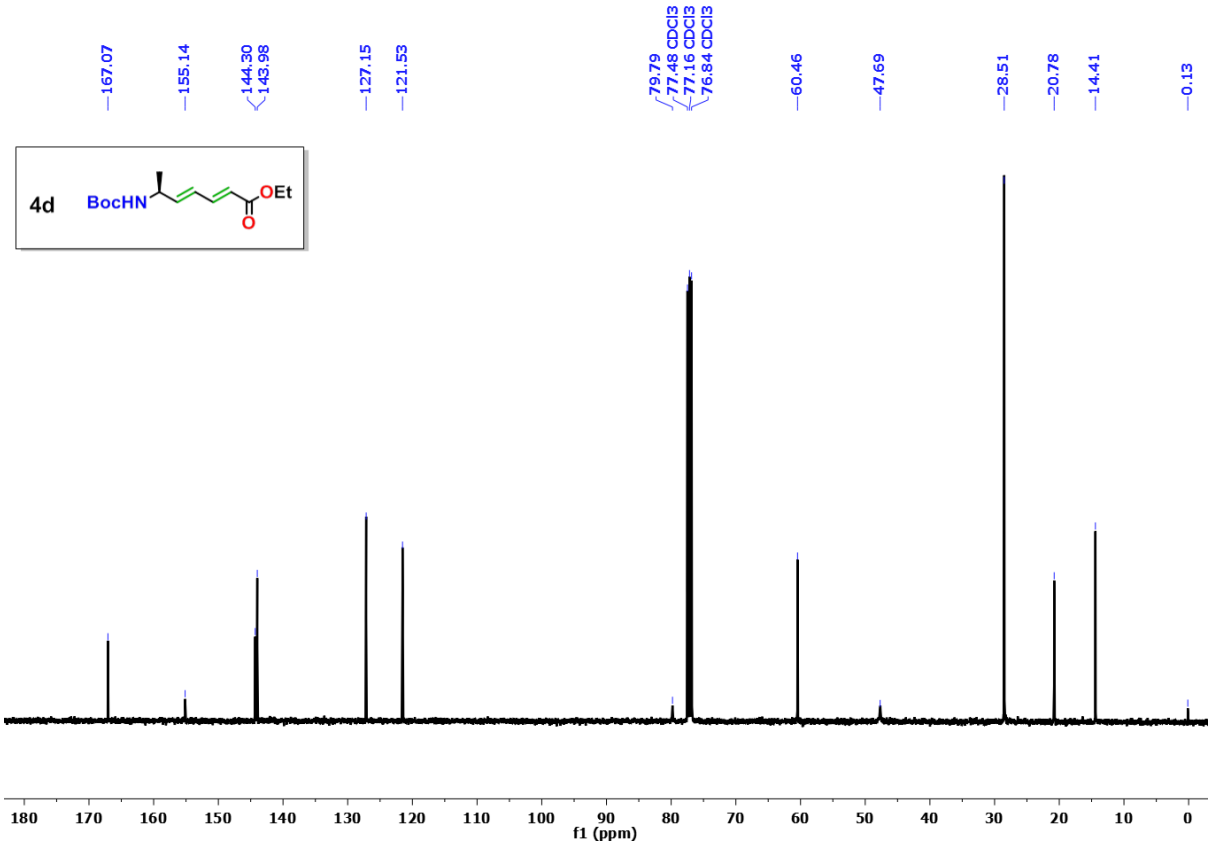

4b
BocHN
OEt
O
f1 (ppm)

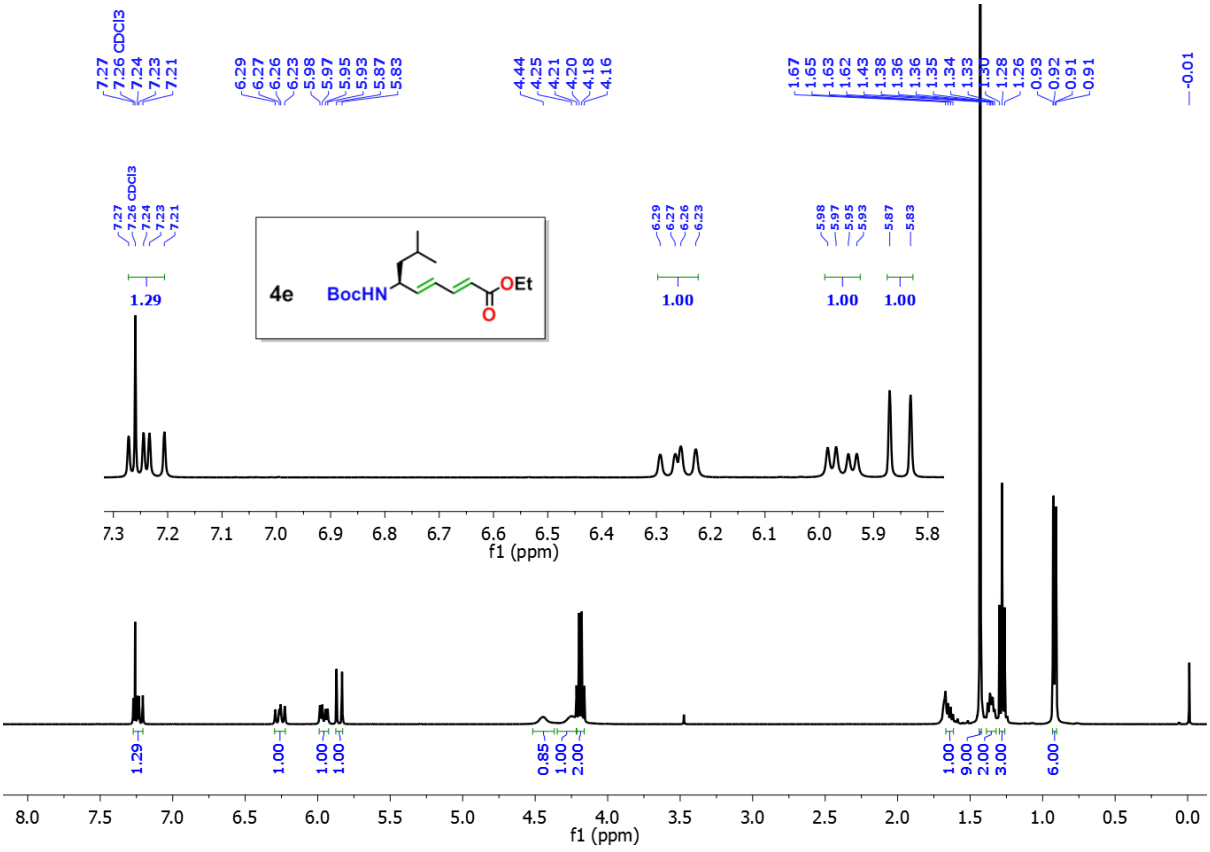

4b
BocHN
OEt
O
f1 (ppm)

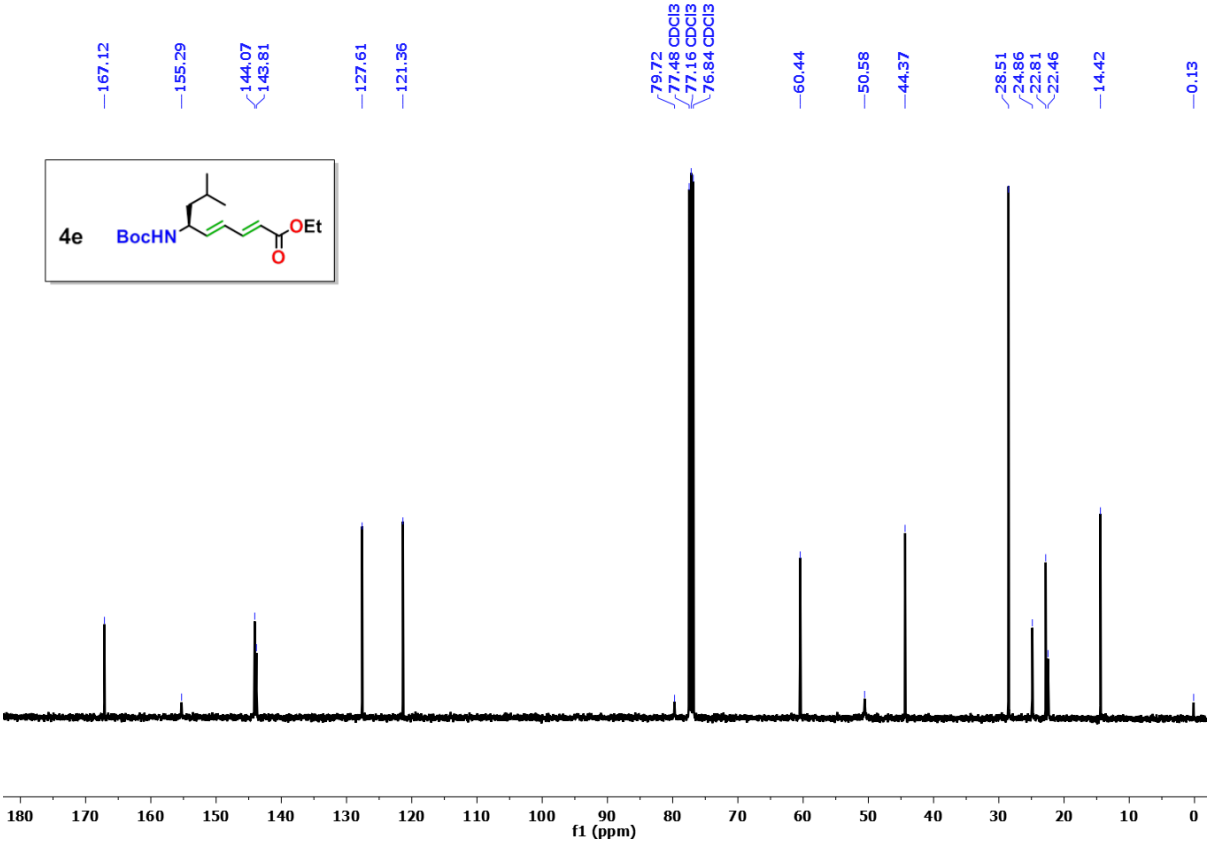

7.30
7.27
7.26 CDCl3
7.24
6.24
6.21
6.18
6.15
5.85
5.81
4.62
4.21
4.19
4.18
4.16
1.41
1.39
1.30
1.28
1.26
-0.01
4c
BocHN
OEt
O
1.14
2.00
1.00
f1 (ppm)

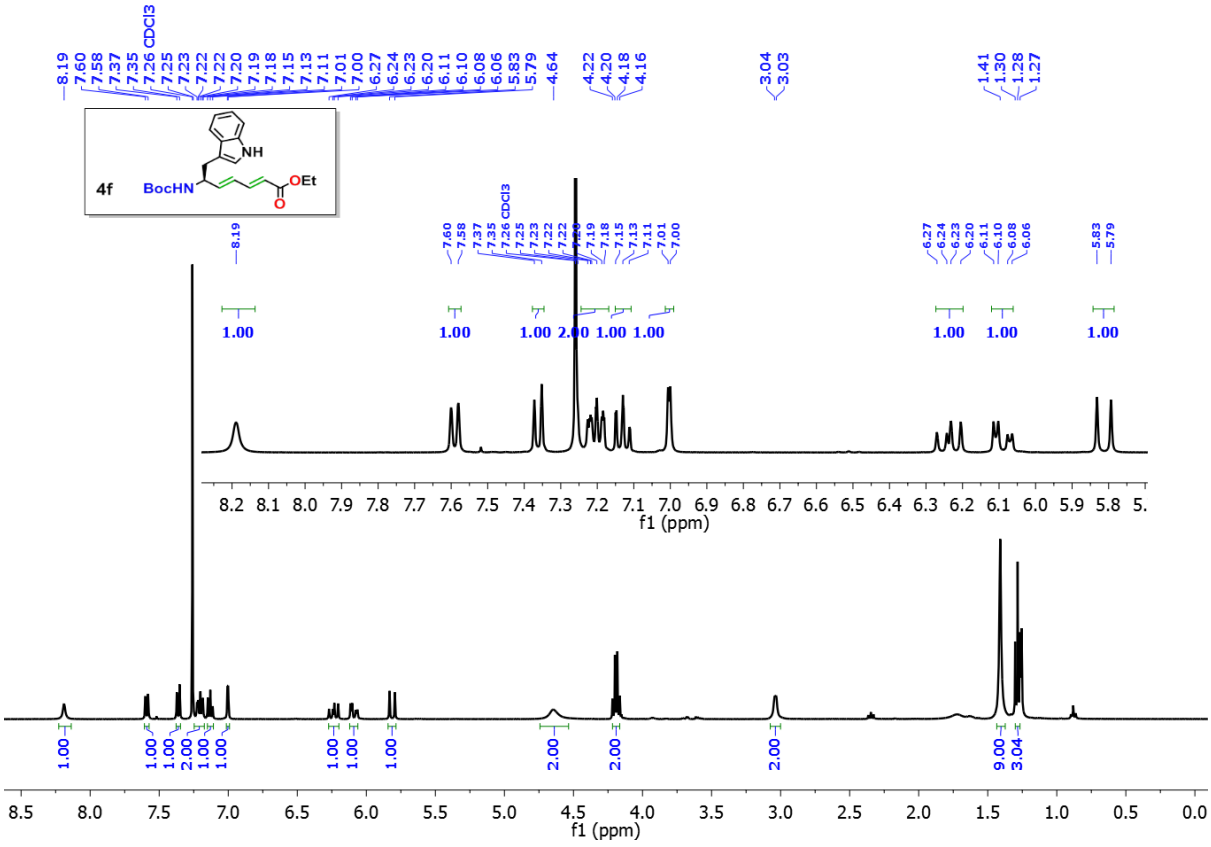

167.13
154.38
148.81
144.62
125.18
121.01
79.50
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
60.38
53.24
28.52
27.73
14.42
-0.13
4c
BocHN
OEt
O
f1 (ppm)

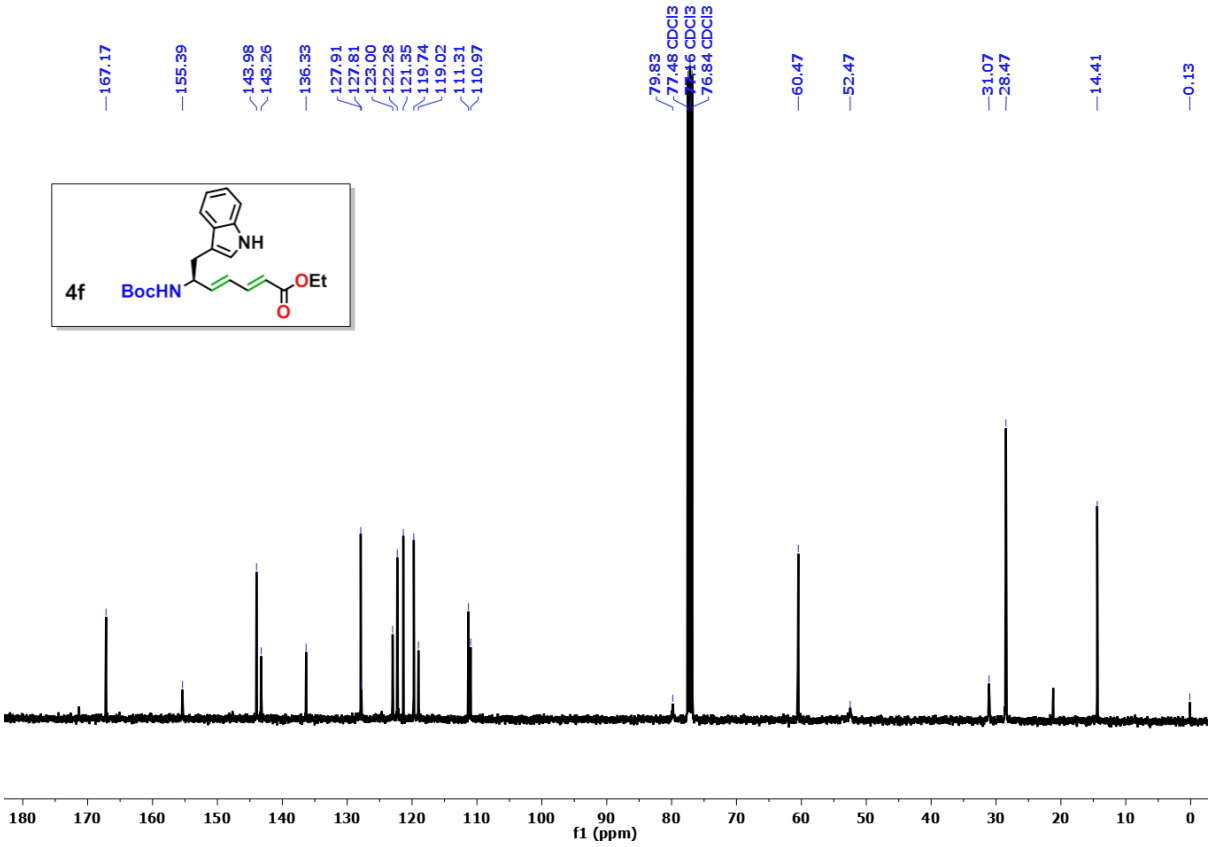

7.27
7.26 CDCl3
7.24
7.23
7.20
6.27
6.24
6.23
6.20
6.05
6.03
6.01
6.00
5.87
5.83
4.54
4.32
4.21
4.19
4.17
4.16
1.43
1.29
1.27
1.26
1.24
1.23
4d
BocHN
OEt
O
1.00
f1 (ppm)
0.94
2.00
9.01
3.01
3.00

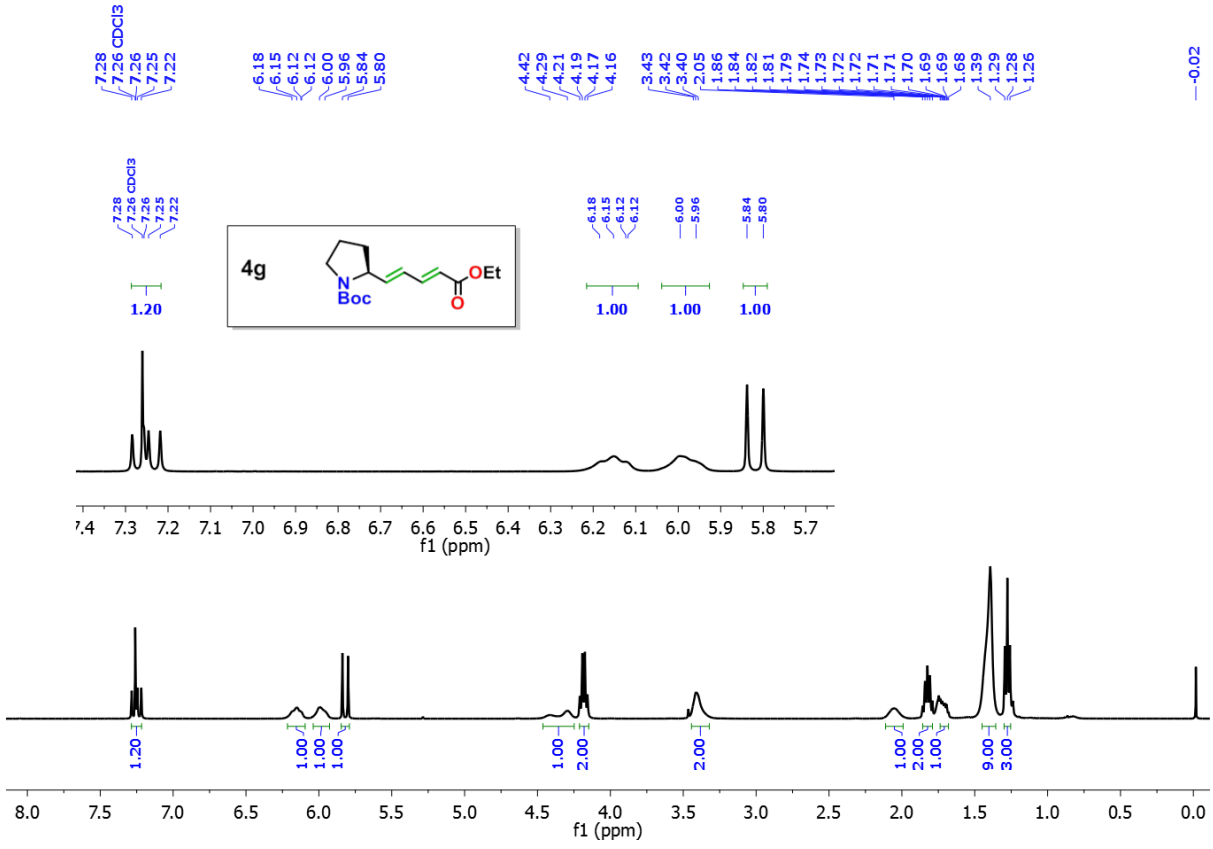

167.07
155.14
144.30
143.98
127.15
121.53
79.79
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
60.46
47.69
28.51
20.78
14.41
0.13
4d
BocHN
OEt
O
f1 (ppm)

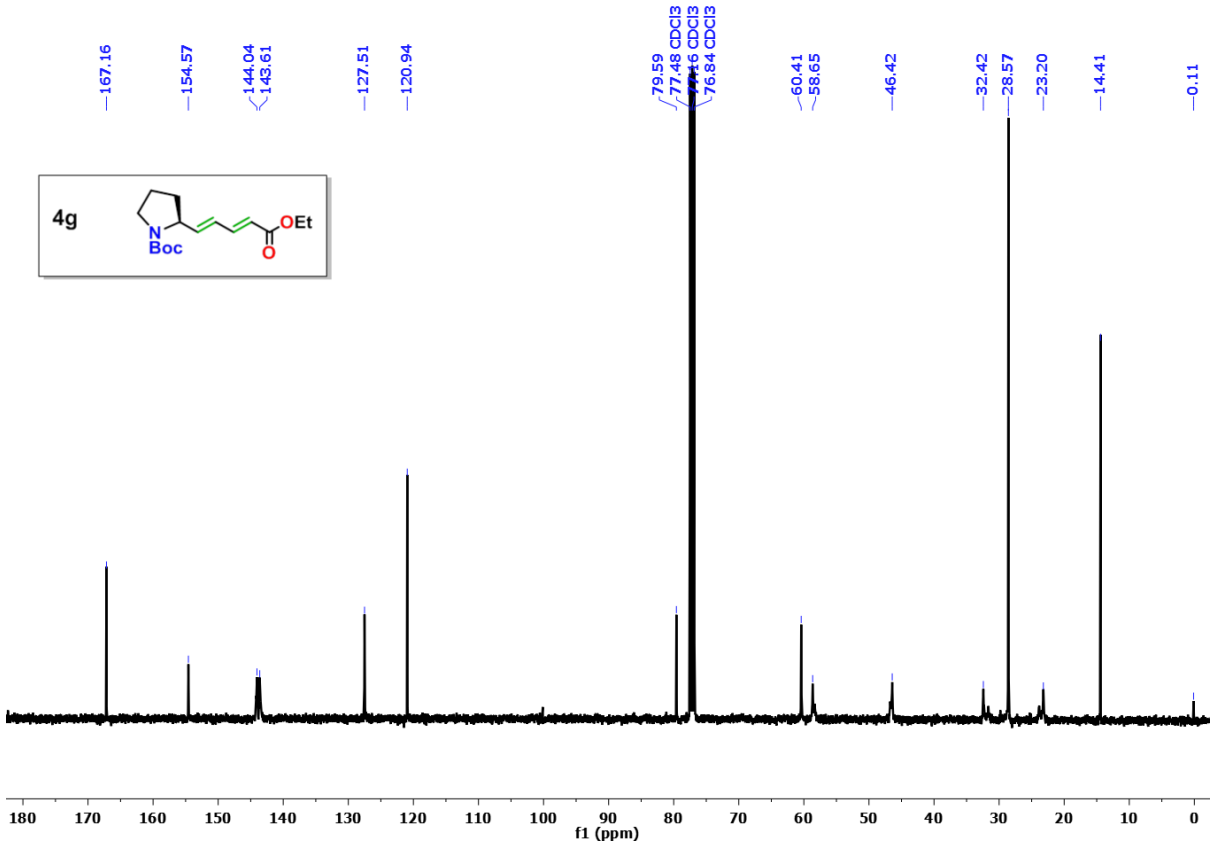

4e
BocHN
OEt
O
f1 (ppm)

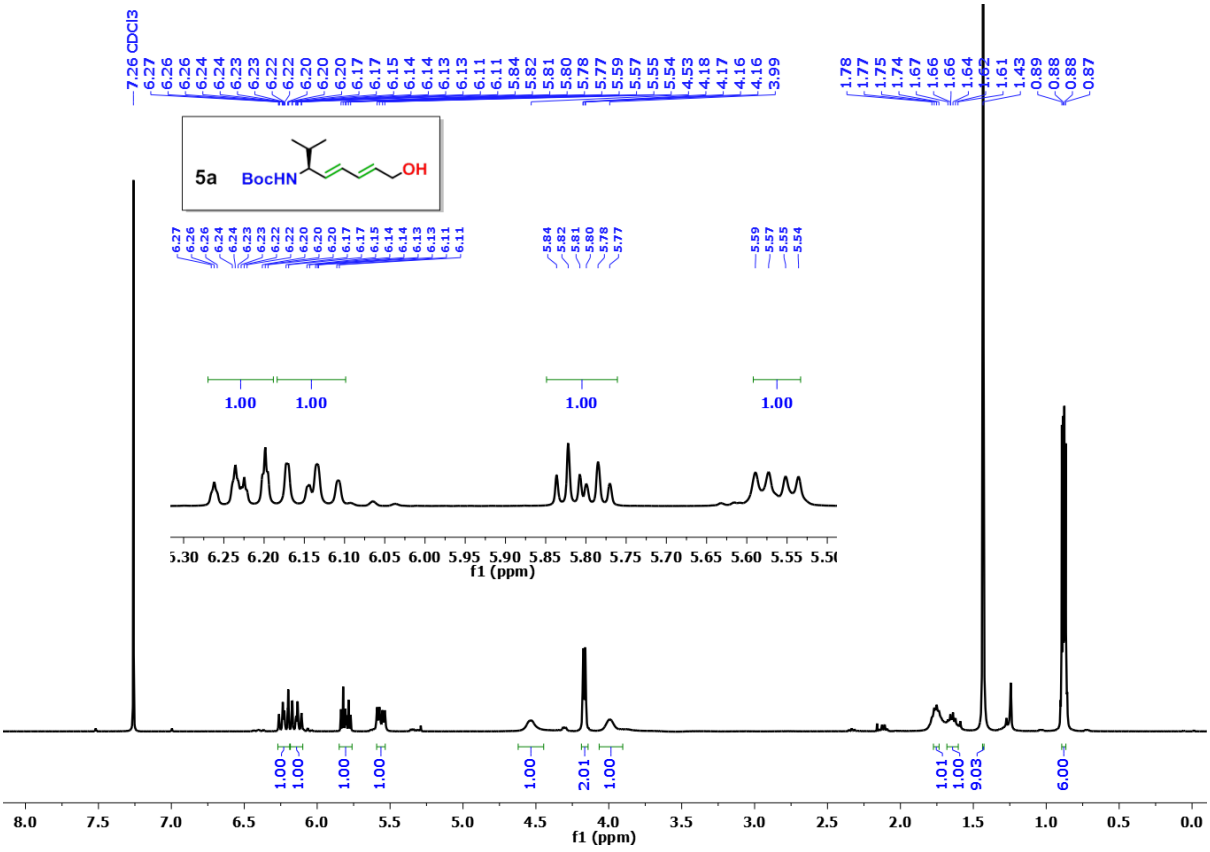

4e
BocHN
OEt
O
f1 (ppm)

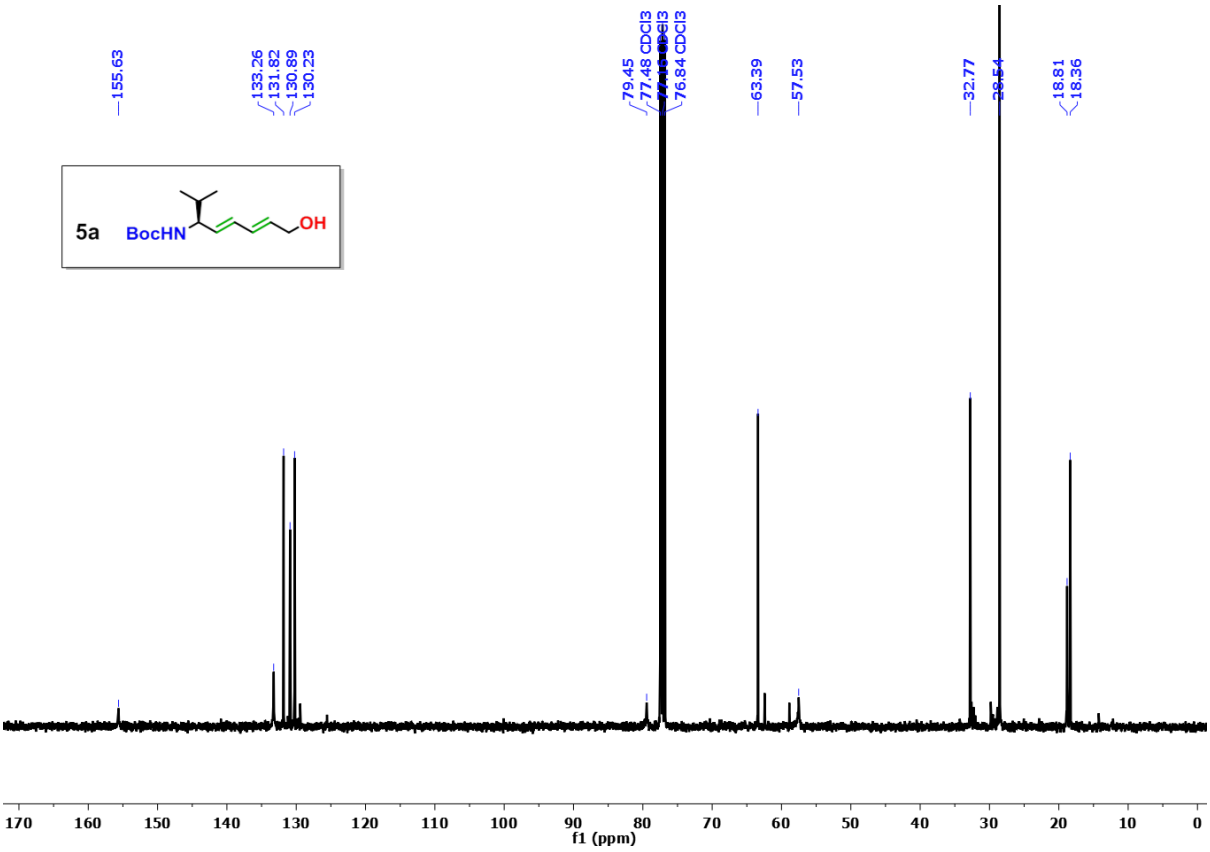

4f
BocHN
NH
OEt
O
f1 (ppm)

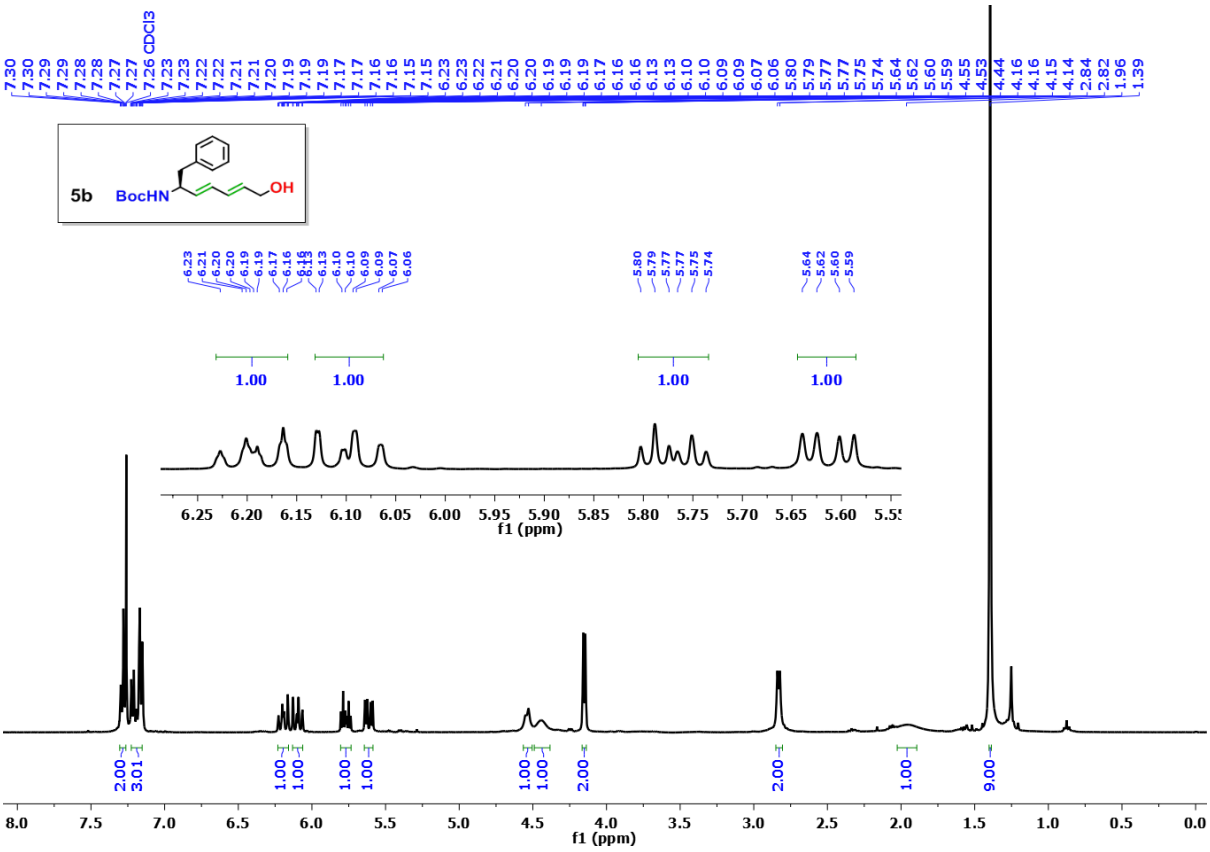

4f
BocHN
NH
OEt
O
f1 (ppm)

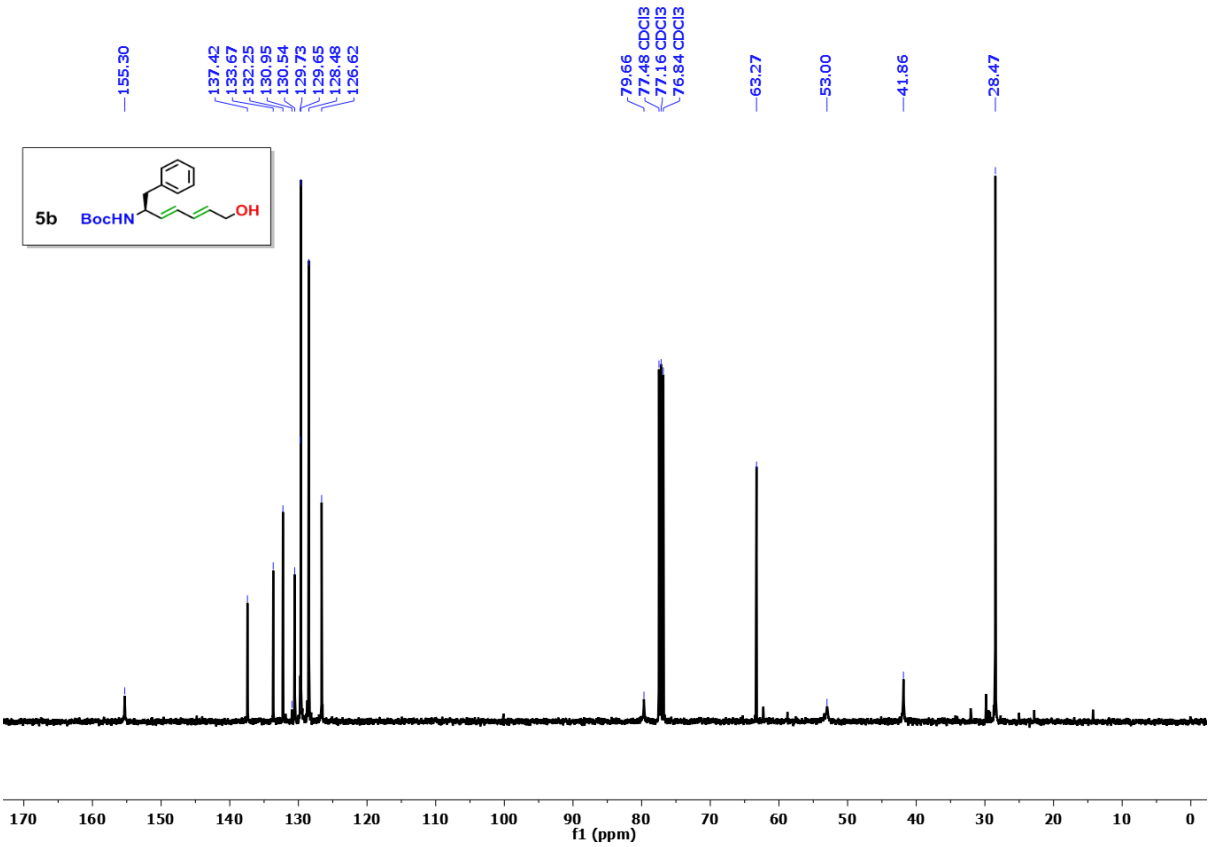

4g
OEt
Boc
O
f1 (ppm)

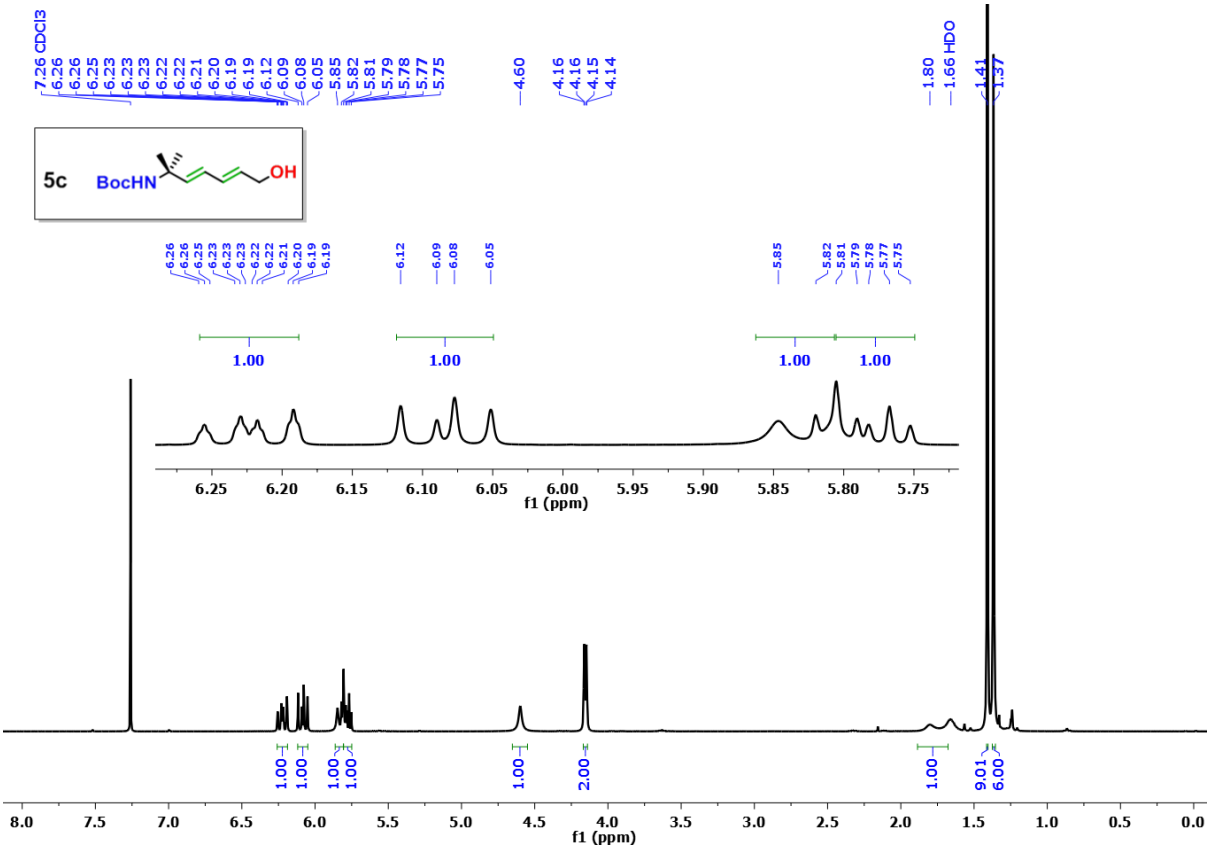

4g
OEt
Boc
O
f1 (ppm)

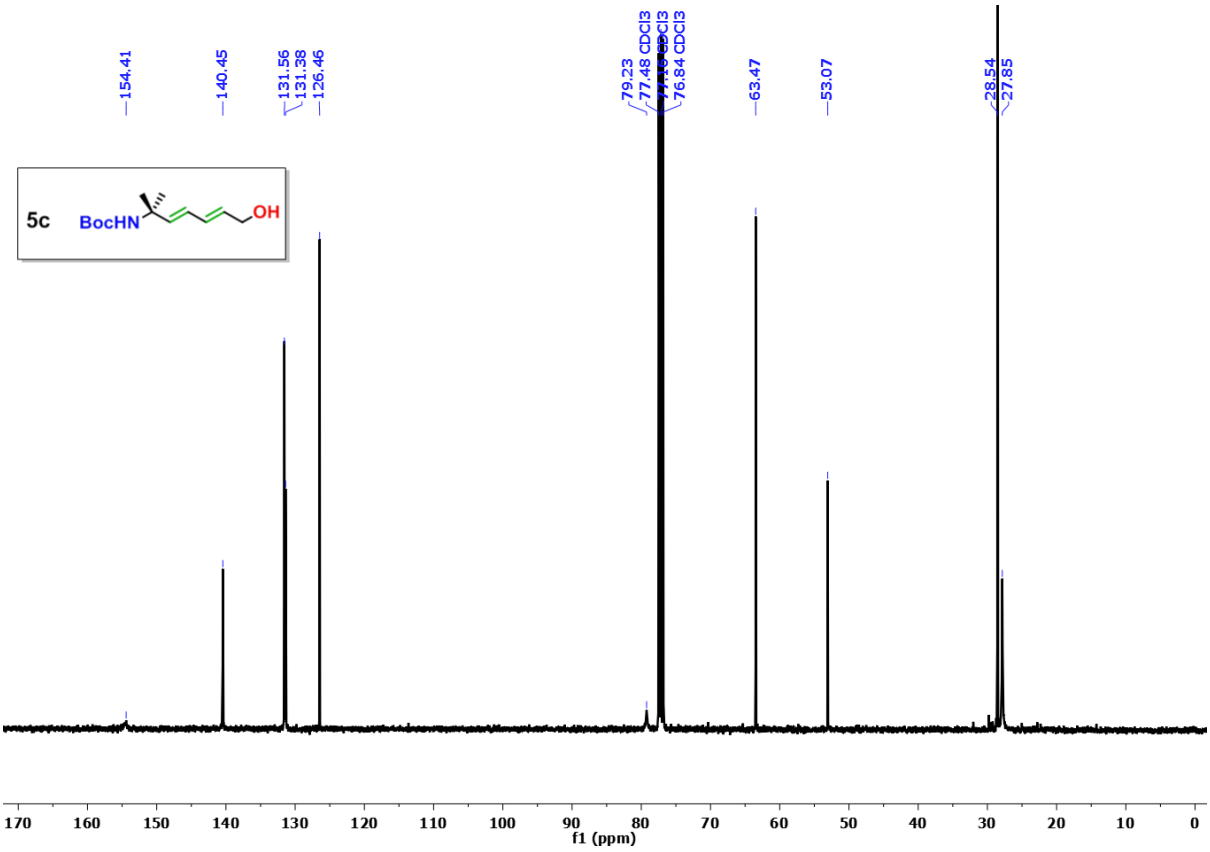

7.26 CDCl3
5a
BocHN
OH
1.00
1.00
1.00
1.00
f1 (ppm)

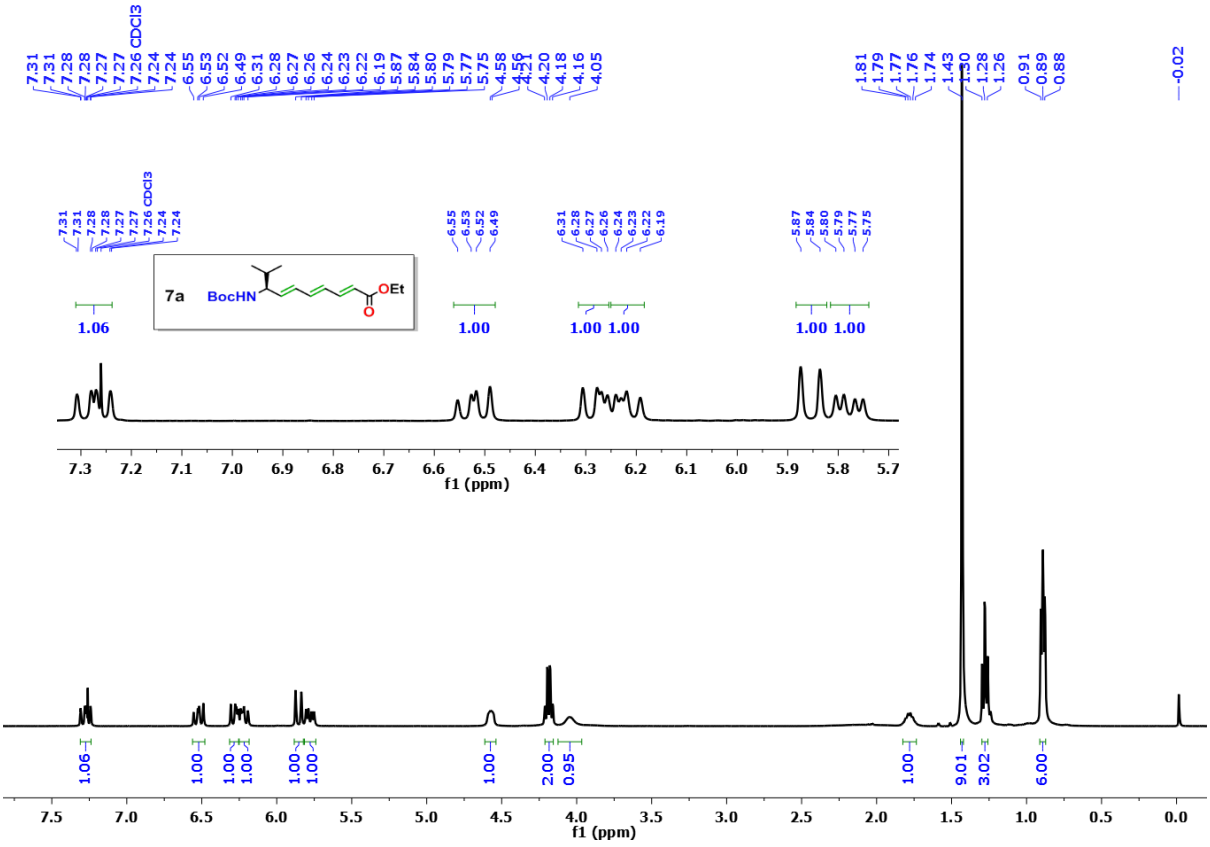

155.63
133.26
131.82
130.89
130.23
79.45
77.48 CDCl3
76.84 CDCl3
63.39
57.53
32.77
28.54
18.81
18.36
5a
BocHN
OH
f1 (ppm)

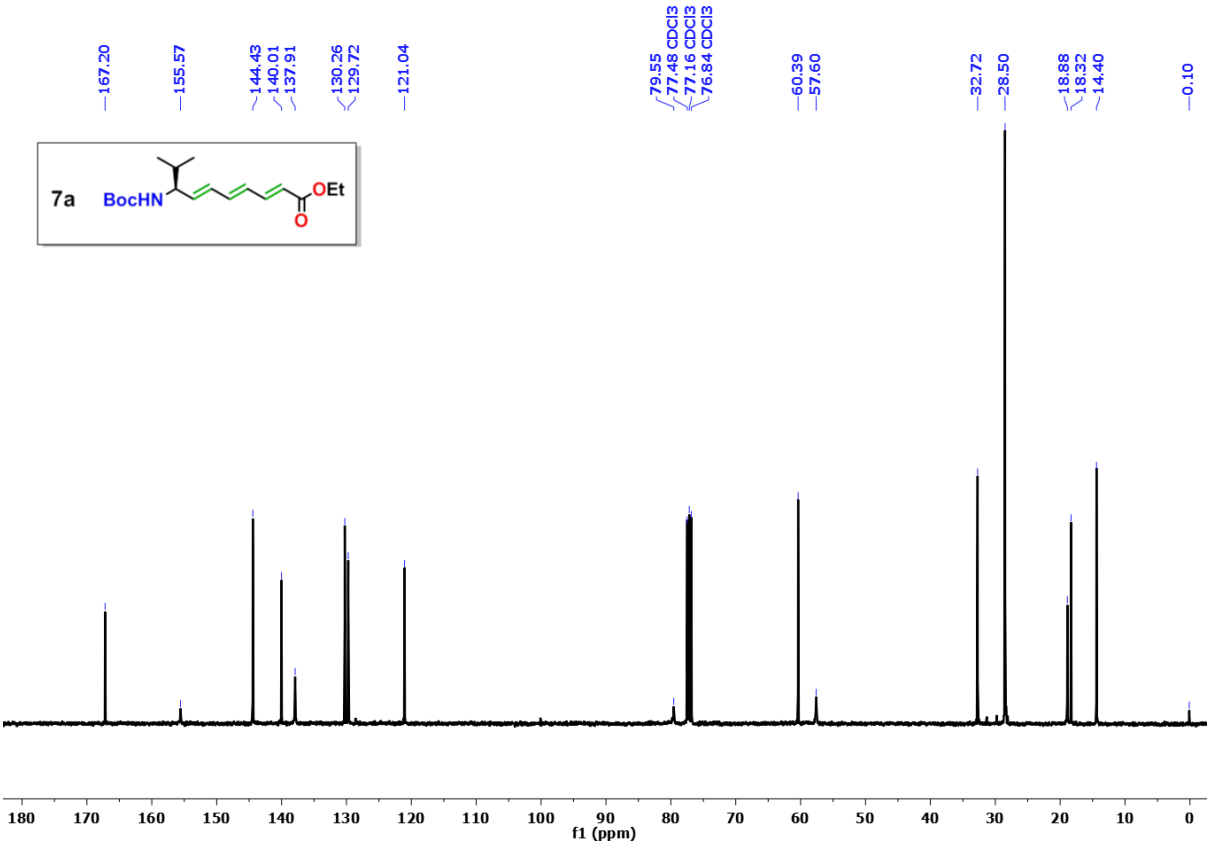

5b
BocHN
OH
f1 (ppm)

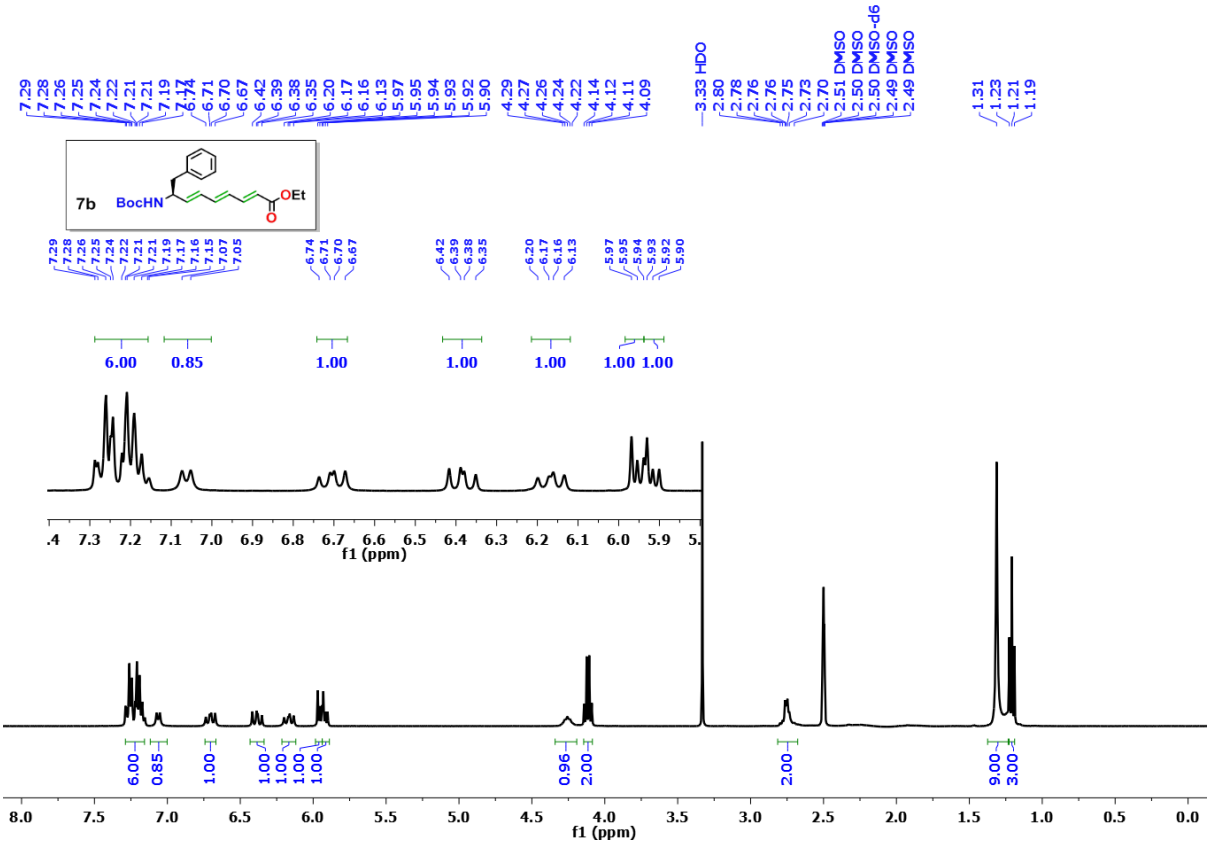

5b
BocHN
OH
f1 (ppm)

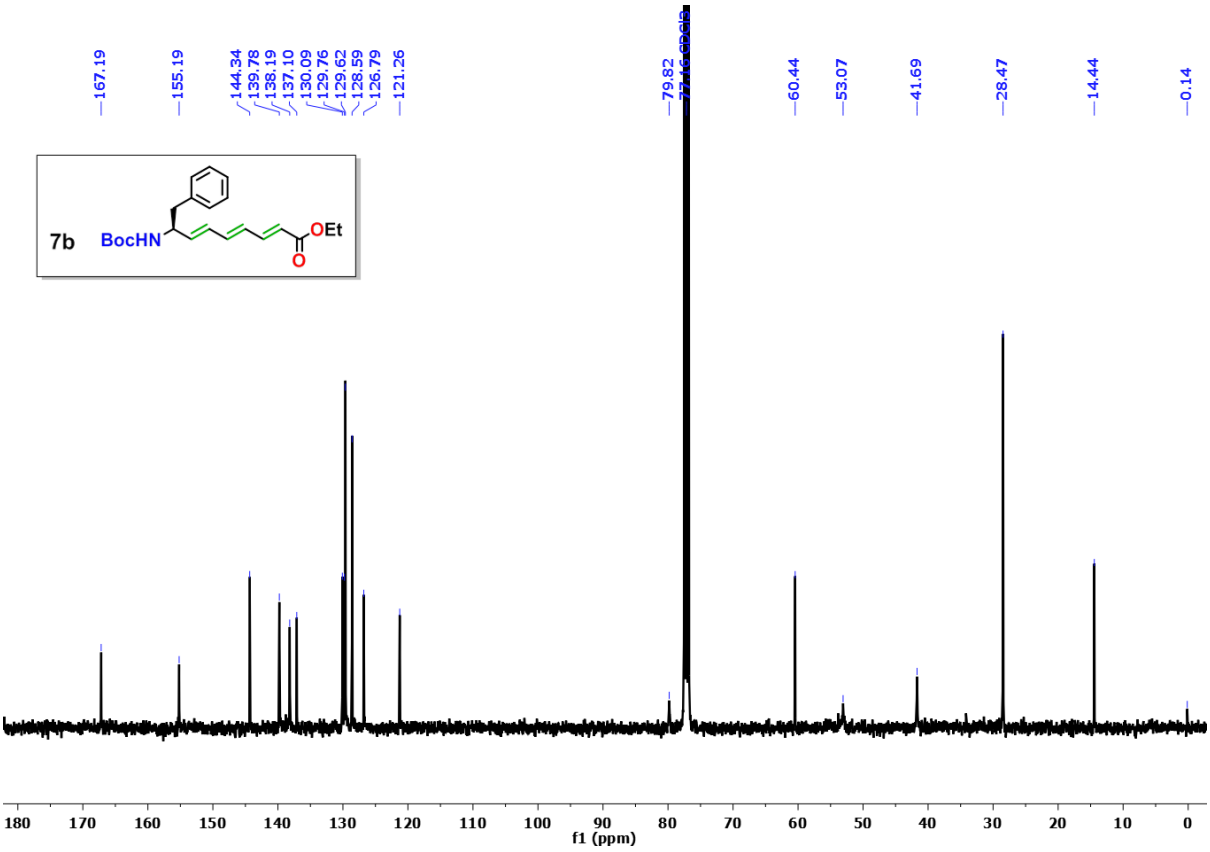

7.26 CDCl3
6.26
6.25
6.23
6.22
6.21
6.20
6.19
6.12
6.09
6.08
6.05
5.85
5.82
5.81
5.79
5.78
5.77
5.75
4.60
4.16
4.15
4.14
1.80
1.66 HDO
1.41
1.37
5c
BocHN
OH
1.00
1.00
1.00
1.00
f1 (ppm)
f1 (ppm)

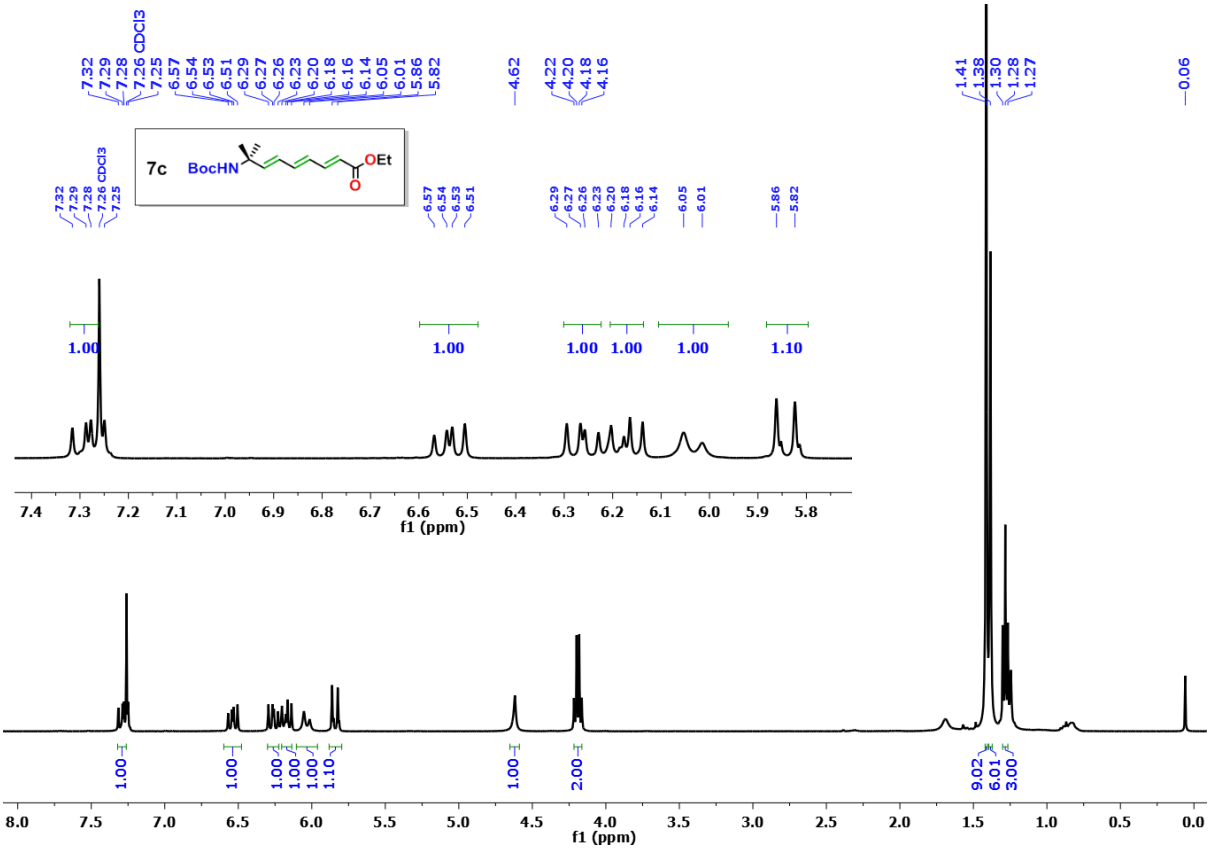

154.41
140.45
131.56
131.38
126.46
79.23
77.48 CDCl3
76.84 CDCl3
63.47
53.07
28.54
27.85
5c
BocHN
OH
f1 (ppm)

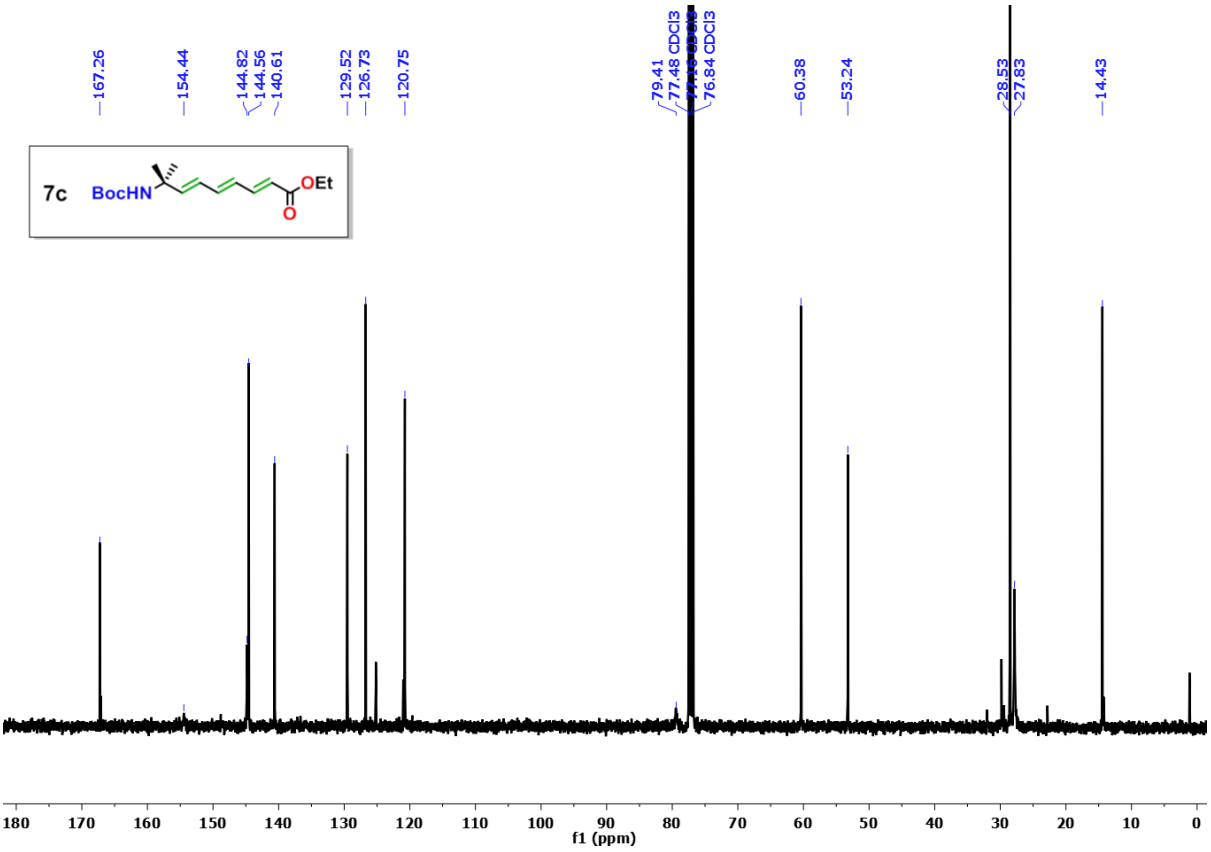

7a
BocHN
OEt
O
1.06
1.00
1.00 1.00
1.00 1.00
f1 (ppm)

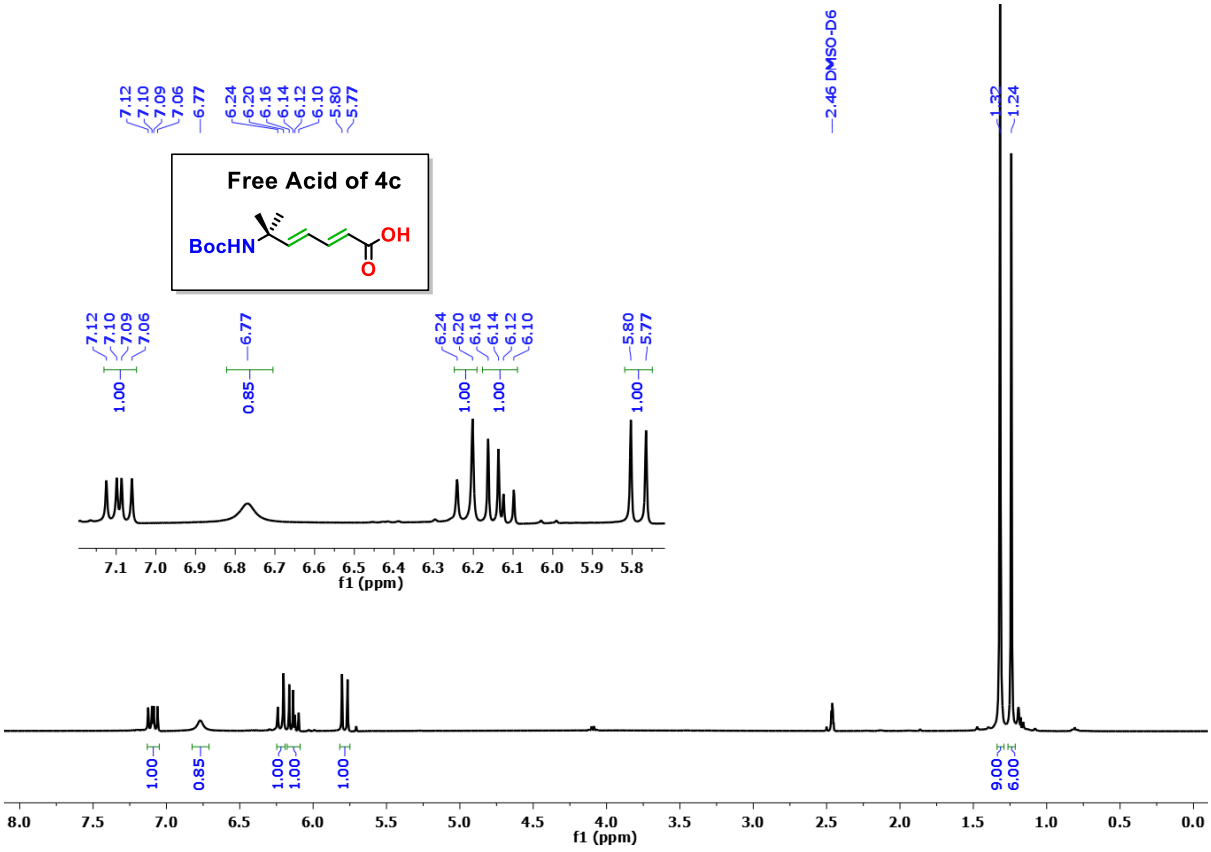

7a
BocHN
OEt
O
f1 (ppm)

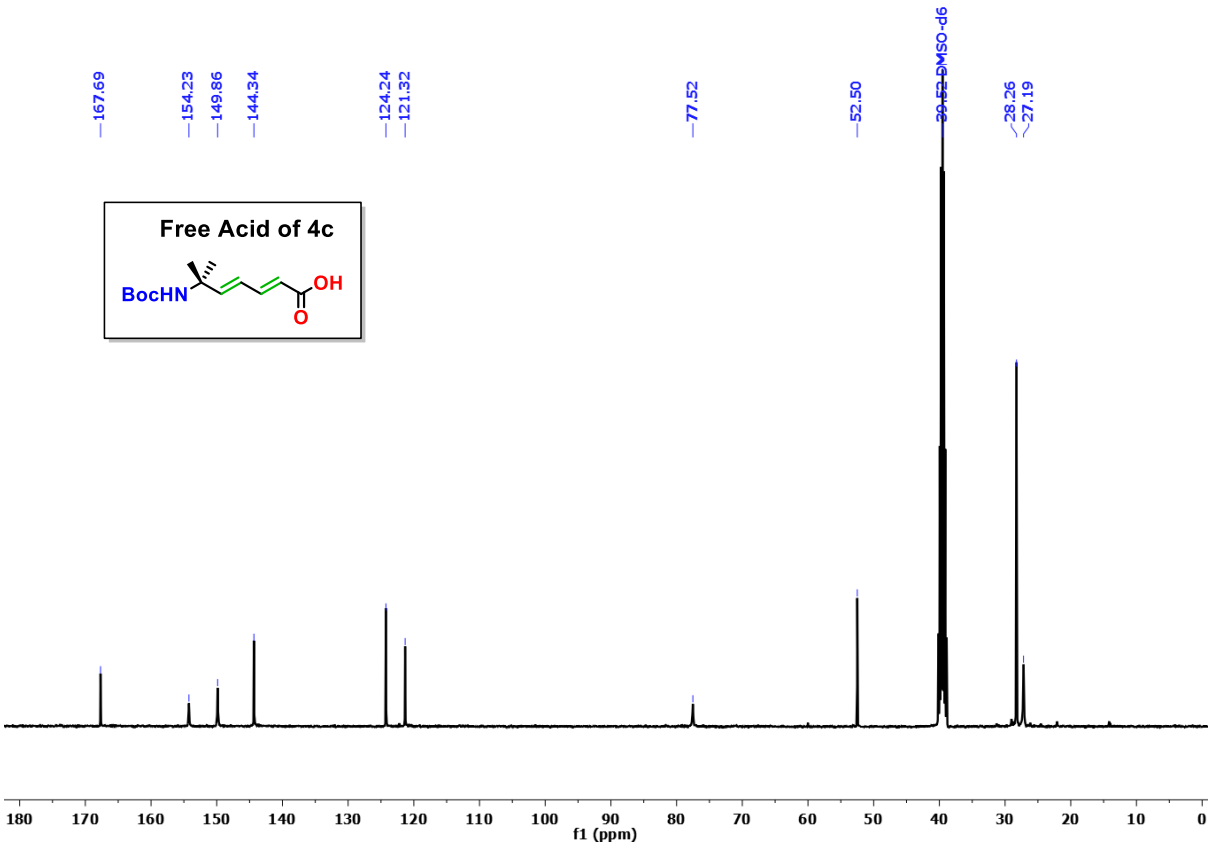

7b
BocHN
OEt
O
f1 (ppm)

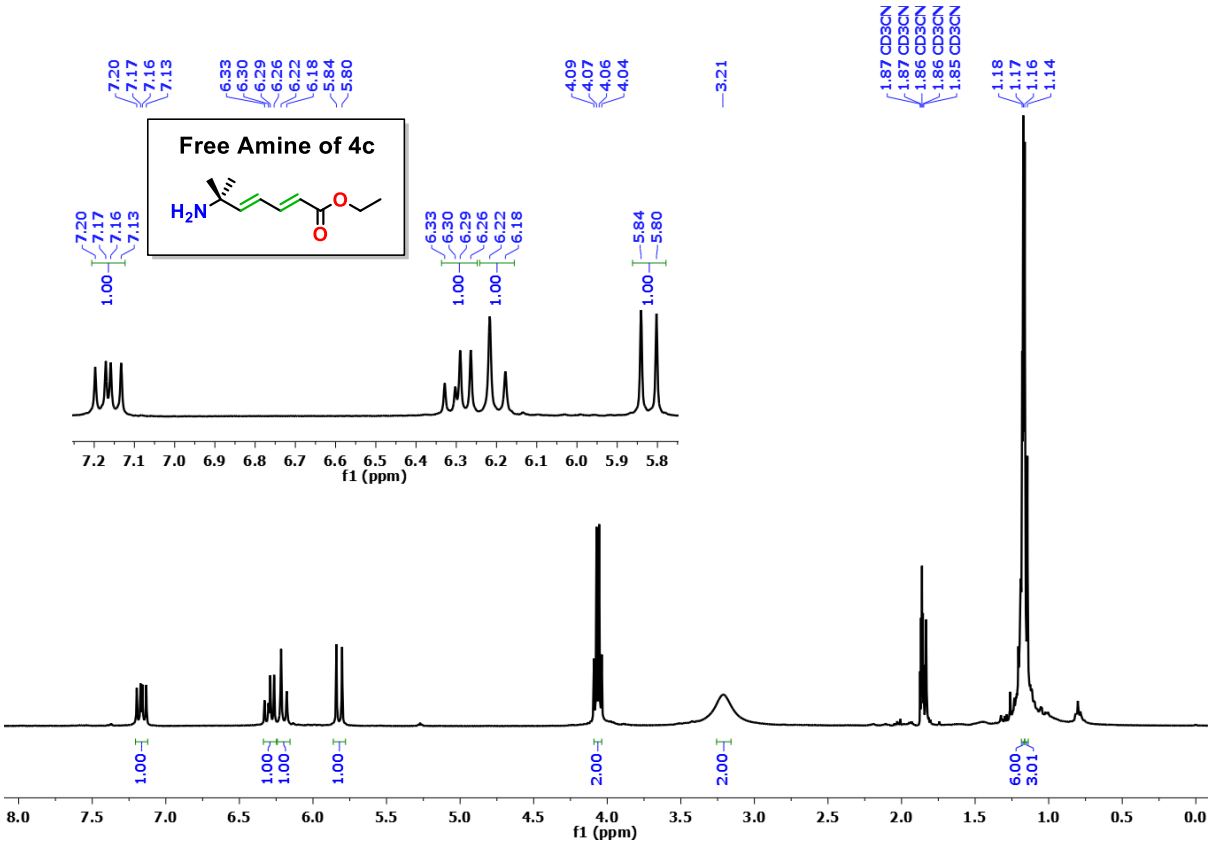

7b
BocHN
OEt
O
f1 (ppm)

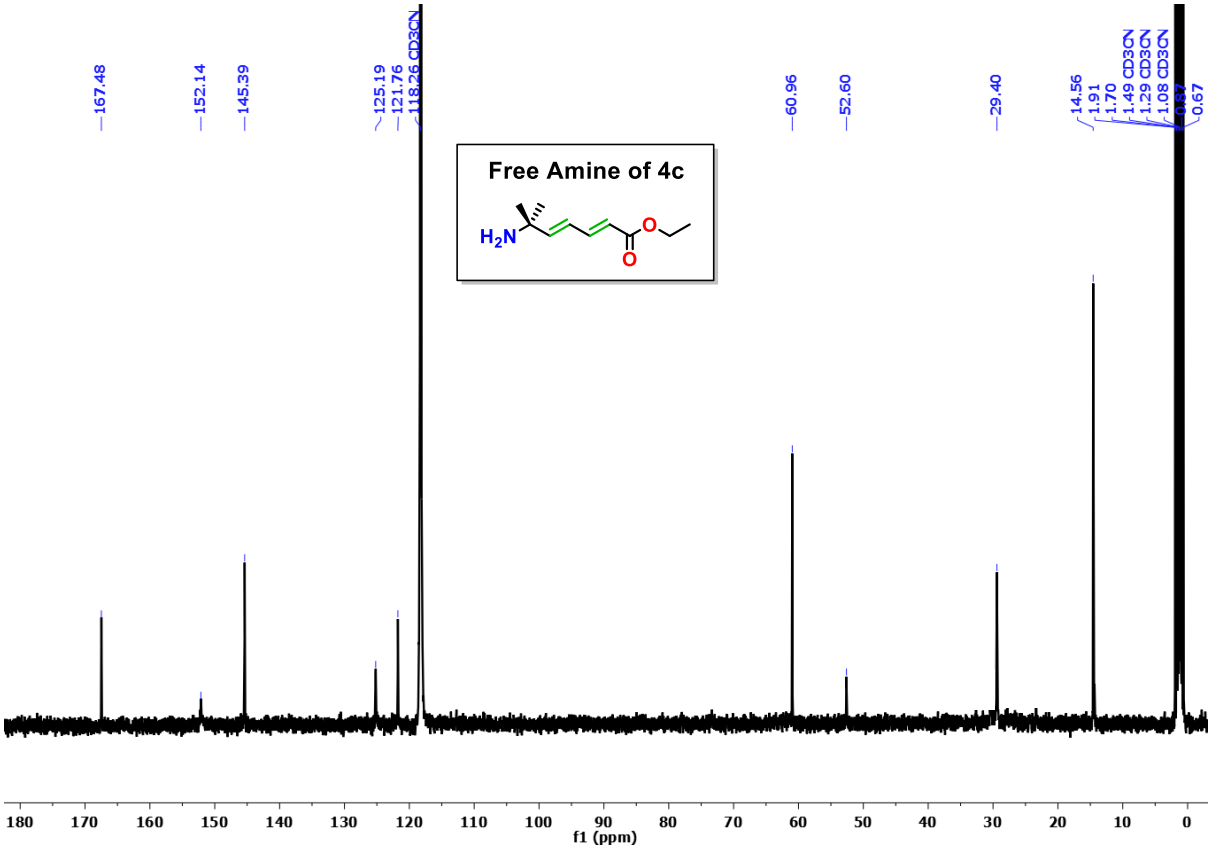

7c
BocHN
OEt
O
f1 (ppm)

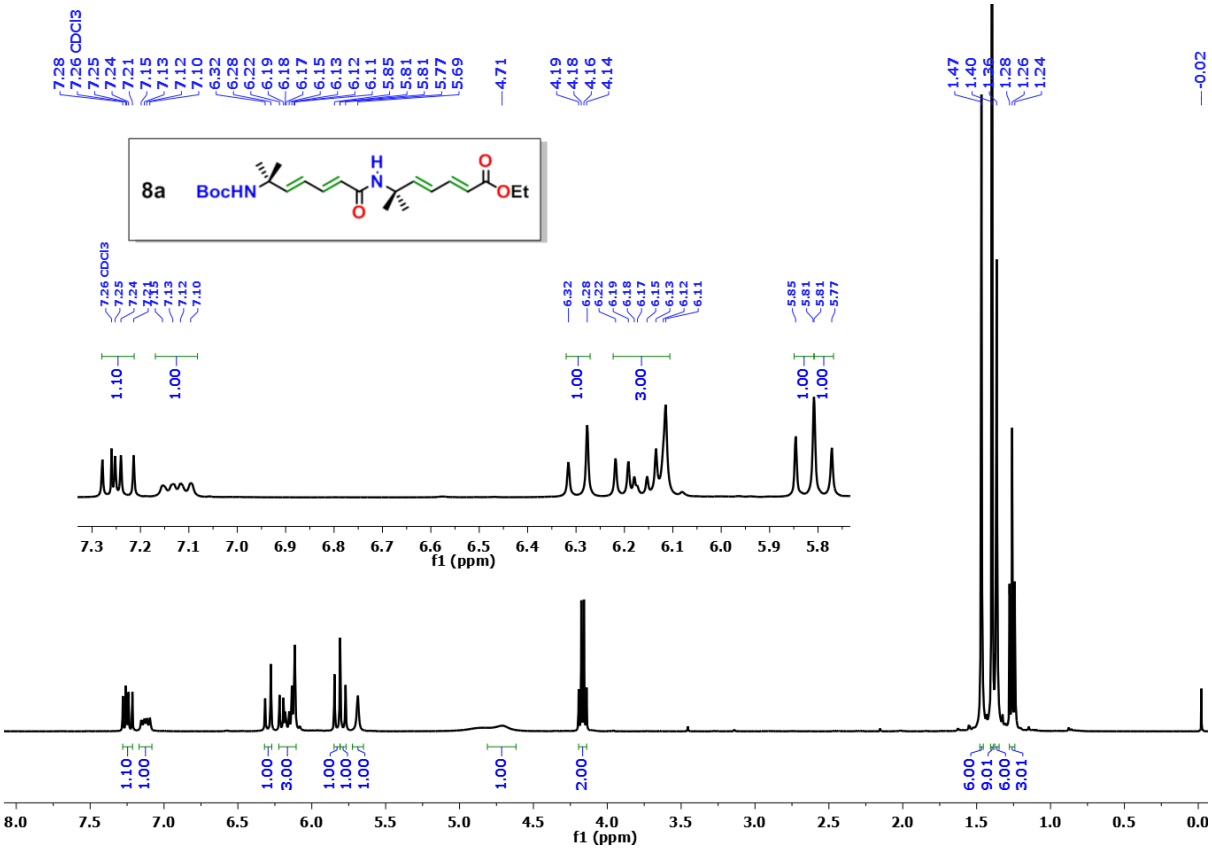

7c
BocHN
OEt
O
f1 (ppm)

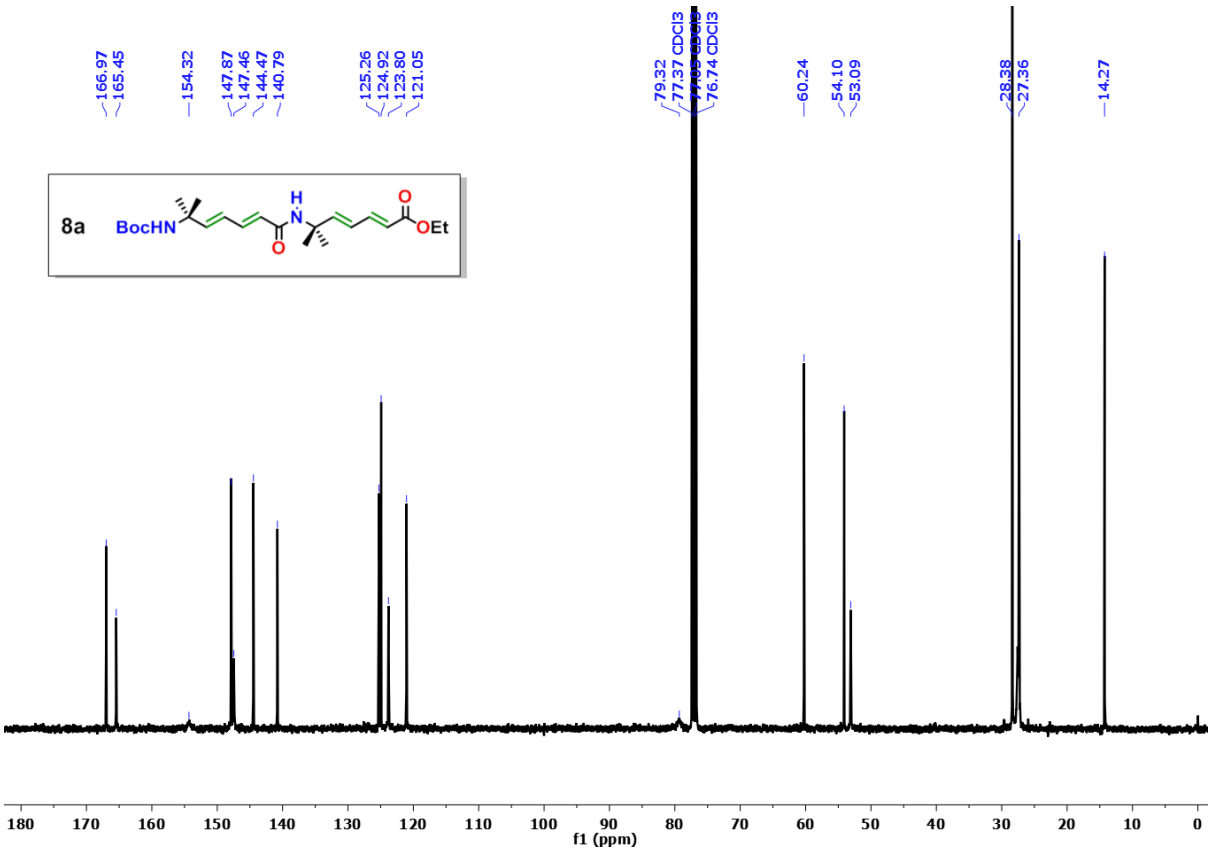

Free Acid of 4c
BocHN
OH
O
f1 (ppm)


Free Acid of 4c
BocHN
OH
O
f1 (ppm)


Free Amine of 4c
f1 (ppm)


Free Amine of 4c
f1 (ppm)


8a
BocHN
OEt
f1 (ppm)


8a
BocHN
OEt
f1 (ppm)