Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

$AlCl_3$-Catalyzed Regioselective Intermolecular α or γ Mono- or α,γ Bis-Hydroalkoxylation of Allenamides with Alcohols

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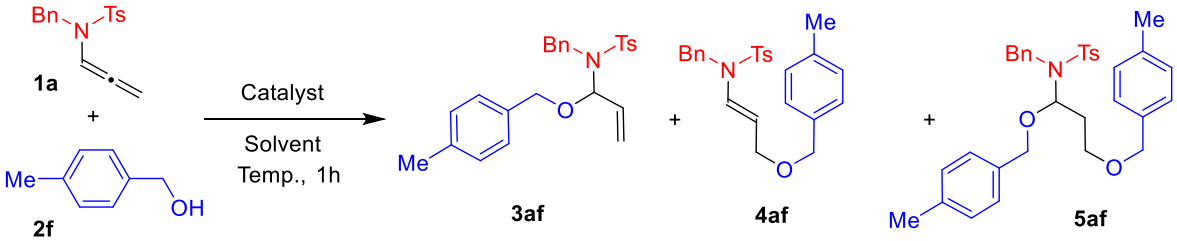
Contents

1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ on JEOL ECS 400 MHz and/or JEOL ECA 500 MHz NMR spectrometers. Chemical shifts (δ) and coupling constants (*J*) are given in parts per million (ppm) and in hertz (Hz), respectively. The following abbreviations were used to designate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, sextet = sx, dd = doublet of doublets, dt = doublet of triplets, tt = triplet of triplets, m = multiplet. High-resolution mass spectrometry data were recorded on a Synapt G2 HDMS (q-TOF with ion mobility). Reactions were monitored by thin-layer chromatography (TLC) carried out on silica gel plates (60 F254) using UV light as the visualizing agent. Purifications by flash column chromatography were carried out the using SiliaFlash® P60 silica gel with a hexane−ethyl acetate solvent mixture with 1% triethylamine. As observed in ^{1}H and ^{13}C NMR spectra, some of the products contain amides (generated from the hydrolysis/decomposition of products during reaction and/or purification) and α,γ bis-hydroalkoxylation products (**5**) as minor impurities. When impurities were detected by ^{1}H NMR, the purity of the compounds were calculated and provided with each compound. Allenamides **1** were prepared according to the literature procedure.[1] $AlCl_3$ (99.999%) and $AlCl_3$ (98.5%) was purchased form Acros Organics. Unless otherwise noted, all reagents were purchased from commercial sources and used without further purification.

2. Optimization of reaction conditions

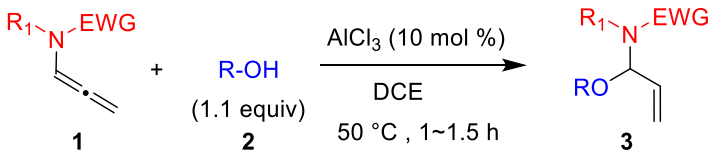


Entry	Catalyst (mol %)	Solvent	Temp	Yield (%)[b]		
				3af	4af	5af
1[c]	$(PPh_3)AuCl/AgSbF_6$ (10)	Toluene	rt	-	-	-
2[d]	$CeCl_3$ (10)	Toluene	rt	trace	-	-
3[d]	$ZnCl_2$ (10)	Toluene	rt	trace	-	-
4[c]	$FeCl_3$ (10)	Toluene	rt	-	-	-
5[e]	$AlCl_3$ (10)	Toluene	rt	42	33	-

6[d,f]	$AlCl_3$ (10)	Toluene	rt	trace	-	-
7[f,g,h]	$AlCl_3$ (10)	Toluene	50	42(75)	3(9)	-
8[f,i]	$AlCl_3$ (10)	Toluene	50	-	5	65
9[f]	$AlCl_3$ (10)	DCE	50	78	13	-
10[f]	$AlCl_3$ (10)	EtOAc	50	48	22	-
11[f,g]	$AlCl_3$ (10)	Dioxane	50	20	-	-
12[f]	$AlCl_3$ (10)	MeCN	50	36	42	-
13[f]	$AlCl_3$ (10)	THF	50	34	15	-
14[f,i]	$AlCl_3$ (10)	DCE	50	-	trace	81
15[f,g]	$AlCl_3$ (5)	DCE	50	16	-	-
16[f]	$AlCl_3$ (20)	DCE	50	55	24	-
17[j]	-	DCE	50	18	-	-
18[f]	$AlCl_3$ (10)	DCE	80	trace	73	-

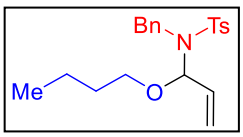
[a] Conditions (unless otherwise noted): reactions were carried out with substrate **1a** (0.1 mmol), *p*-methylbenzyl alcohol **2f** (0.11 mmol) in appropriate solvent (0.2 M) for 1 h. [b] ^{1}H NMR yield using dibromomethane as internal standard. [c] decomposition. [d] >90% of starting material recovered. [e] 98.5% pure $AlCl_3$ was used. [f] 99.999% pure $AlCl_3$ was used. [g] full conversion was not achieved within 1 h. [h] yield after 2 h shown in parenthesis. [i] 3 equiv. of **2f**. [j] 66% of starting material **1a** remained after 1 h.

3. *α*-Hydroalkoxylation of allenamide: General procedure

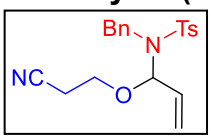


In a screw cap 7 mL vial, allenamide **1** (0.2 mmol), aluminum chloride (2.6 mg, 0.02 mmol) was taken and dichloroethane (1 mL, 0.2 M) followed by alcohol **2** (0.22 mmol) was added to it. The mixture was stirred at 50 °C and the reaction progress was monitored by TLC and/or ^{1}H NMR analysis. After completion (approx. 1~1.5 h), the reaction mixture was cool down to room temperature and a drop of Et_3N was added as stabilizer to prevent isomerization. The solvent was concentrated under reduced pressure and the crude

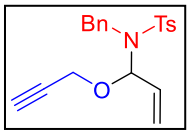
mixture was subjected to silica gel column chromatography. The product was isolated using ethyl acetate-hexane with 1% triethylamine as eluent.

***N*-benzyl-*N*-(1-butoxyallyl)-4-methylbenzenesulfonamide (3aa).** According to general procedure, **3aa** was obtained in 45% (33.6 mg) yield as colorless oil; 

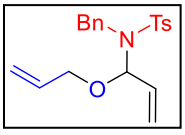
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 6.7 Hz, 2H), 7.25 – 7.18 (m, 5H), 5.55 (d, *J* = 3.9 Hz, 1H), 5.50 – 5.31 (m, 2H), 5.17 (d, *J* = 9.9 Hz, 1H), 4.40 (d, *J* = 15.6 Hz, 1H), 4.18 (d, *J* = 15.6 Hz, 1H), 3.38 – 3.22 (m, 2H), 2.39 (s, 3H), 1.35 – 1.14 (m, 4H), 0.81 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.1, 138.0, 137.6, 134.1, 129.4, 128.7, 127.9, 127.0, 118.6, 87.1, 67.6, 46.6, 31.0, 21.4, 19.1, 13.8; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{21}H_{28}NO_3S$ 374.1784, found 374.1779.

***N*-benzyl-*N*-(1-(2-cyanoethoxy)allyl)-4-methylbenzenesulfonamide (3ab).** According to general procedure, **3ab** (purity >96%) was obtained in 48% (35.5 mg) yield as colorless oil; 

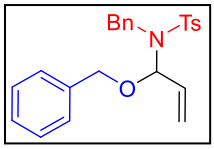
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.30 (m, 2H), 7.30 – 7.23 (m, 5H), 5.63 – 5.56 (m, 1H), 5.48 – 5.21 (m, 3H), 4.54 (d, *J* = 15.4 Hz, 1H), 4.08 (d, *J* = 15.4 Hz, 1H), 3.52 (dd, *J* = 7.1, 5.5 Hz, 2H), 2.42 (s, 3H), 2.14 (dt, *J* = 16.9, 5.4 Hz, 1H), 1.96 (dt, *J* = 16.9, 7.2 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.6, 137.7, 137.5, 132.5, 129.8, 128.8, 128.1, 127.4, 126.8, 119.9, 117.5, 86.7, 61.5, 46.8, 21.5, 17.8; **HRMS** (ESI-TOF) m/z: [M+ Na]$^+$ calcd. for $C_{20}H_{22}N_2NaO_3S$ 393.1243, found 393.1229.

***N*-benzyl-4-methyl-*N*-(1-(prop-2-yn-1-yloxy)allyl)benzenesulfonamide (3ac).** 

According to general procedure, **3ac** (purity >90%) was obtained in 51% (36.2 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.34 – 7.27 (m, 2H), 7.26 – 7.20 (m, 5H), 5.77 (d, *J* = 3.6 Hz, 1H), 5.53 – 5.34 (m, 2H), 5.23 (d, *J* = 10.1 Hz, 1H), 4.43 (d, *J* = 15.6 Hz, 1H), 4.19 (d, *J* = 15.6 Hz, 1H), 4.03 – 3.87 (m, 2H), 2.40 (s, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.5, 137.7, 137.5, 133.2, 129.7, 128.8, 128.2, 127.4, 127.3, 119.8, 86.1, 79.0, 74.7, 54.7, 47.0, 21.6; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{20}H_{22}NO_3S$ 356.1314, found 356.1306.

***N*-(1-(allyloxy)allyl)-*N*-benzyl-4-methylbenzenesulfonamide (3ad).** According to general procedure, **3ad** was obtained in 71% (37.0 mg) yield as colorless oil; 

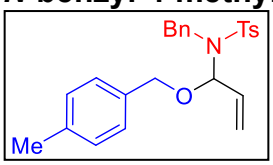
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.29 (m, 2H), 7.26 – 7.18 (m, 5H), 5.71 – 5.55 (m, 2H), 5.52 – 5.33 (m, 2H), 5.25 – 5.03 (m, 3H), 4.44 (d, *J* = 15.6 Hz, 1H), 4.19 (d, *J* = 15.6 Hz, 1H), 3.85 (d, *J* = 5.5 Hz, 2H), 2.40 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.2, 137.8, 137.6, 133.6, 133.4, 129.5, 128.7, 128.0, 127.1, 127.0, 119.0, 117.1, 86.4, 68.1, 46.7, 21.4; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{20}H_{24}NO_3S$ 358.1471, found 358.1465.

***N*-benzyl-*N*-(1-(benzyloxy)allyl)-4-methylbenzenesulfonamide (3ae).** According to general procedure, **3ae** (purity >95%) was obtained in 56% (45.6 mg) yield as colorless oil; 

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.31 (m, 2H), 7.29 – 7.17 (m, 8H), 7.11 – 7.04 (m, 2H), 5.68 (d, *J* = 2.7 Hz, 1H), 5.53 – 5.37 (m, 2H), 5.22 (d, *J* = 9.2 Hz, 1H), 4.50 (d,

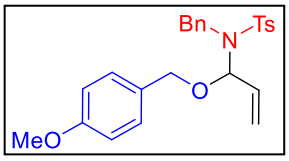
J = 15.6 Hz, 1H), 4.43 – 4.33 (m, 2H), 4.23 (d, J = 15.6 Hz, 1H), 2.40 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.4, 138.0, 137.7, 137.4, 133.8, 129.7, 128.9, 128.3, 128.2, 127.8, 127.6, 127.3, 127.2, 119.3, 86.9, 69.5, 47.0, 21.6; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{24}H_{26}NO_3S$ 408.1628, found 408.1618.

***N*-benzyl-4-methyl-*N*-(1-((4-methylbenzyl)oxy)allyl)benzenesulfonamide (3af).**



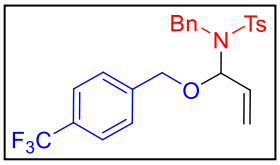
According to general procedure, **3af** was obtained in 66% (55.6 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.2 Hz, 2H), 7.38 – 7.32 (m, 2H), 7.23 (t, J = 6.7 Hz, 5H), 7.08 (d, J = 7.9 Hz, 2H), 6.98 (d, J = 7.9 Hz, 2H), 5.67 (d, J = 2.9 Hz, 1H), 5.53 – 5.37 (m, 2H), 5.21 (d, J = 9.5 Hz, 1H), 4.49 (d, J = 15.6 Hz, 1H), 4.40 – 4.29 (m, 2H), 4.23 (d, J = 15.7 Hz, 1H), 2.40 (s, 3H), 2.32 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.4, 138.0, 137.8, 137.4, 134.4, 134.0, 129.6, 129.0, 128.9, 128.2, 128.0, 127.3, 127.2, 86.7, 69.4, 47.0, 21.6, 21.3; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{25}H_{28}NO_3S$ 422.1784, found 422.1775.

***N*-benzyl-*N*-(1-((4-methoxybenzyl)oxy)allyl)-4-methylbenzenesulfonamide (3ag).**



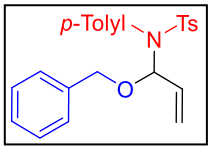
According to general procedure, **3ag** was obtained in 63% (55.2 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.2 Hz, 2H), 7.38 – 7.32 (m, 2H), 7.26 – 7.19 (m, 5H), 7.01 (d, J = 8.5 Hz, 2H), 6.80 (d, J = 8.5 Hz, 2H), 5.66 (d, J = 3.3 Hz, 1H), 5.51 – 5.34 (m, 2H), 5.20 (d, J = 9.6 Hz, 1H), 4.48 (d, J = 15.6 Hz, 1H), 4.32 (d, J = 2.2 Hz, 2H), 4.21 (d, J = 15.6 Hz, 1H), 3.78 (s, 3H), 2.40 (s, 3H); **^{13}C NMR** (101 MHz $CDCl_3$) δ 159.0, 143.2, 137.8, 137.7, 133.8, 129.5, 129.4, 129.4, 128.8, 128.1, 127.1, 127.0, 119.1, 113.5, 86.5, 69.0, 55.2, 46.8, 21.5; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{25}H_{28}NO_4S$ 438.1733, found 438.1728.

***N*-benzyl-4-methyl-*N*-(1-((4-(trifluoromethyl)benzyl)oxy)allyl)benzenesulfonamide (3ah).**

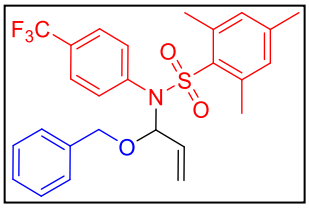


According to general procedure, **3ah** (purity >93%) was obtained in 59% (56.1 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (d, J = 8.2 Hz, 2H), 7.49 (d, J = 8.1 Hz, 2H), 7.37 – 7.32 (m, 2H), 7.22 (m, 5H), 7.11 (d, J = 8.0 Hz, 2H), 5.71 – 5.63 (m, 1H), 5.44 (m, 2H), 5.30 – 5.21 (m, 1H), 4.53 (d, J = 15.5 Hz, 1H), 4.44 (s, 2H), 4.17 (d, J = 15.5 Hz, 1H), 2.40 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.6, 141.5 (q, J_{C-F} = 1.2 Hz), 137.9, 137.6, 133.4, 129.8, 129.6 (q, J_{C-F} = 32.3 Hz), 128.9, 128.3, 127.6, 127.4, 127.0, 125.1 (q, J_{C-F} = 3.8 Hz), 124.2 (q, J_{C-F} = 272.0 Hz), 119.6, 86.9, 68.4, 47.0, 21.6; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ calcd. for $C_{25}H_{24}F_3NNaO_3S$ 498.1321, found 498.1294.

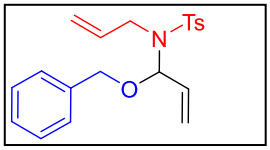
***N*-(1-(benzyloxy)allyl)-4-methyl-*N*-(p-tolyl)benzenesulfonamide (3be).** According to general procedure, **3be** was obtained in 70% (57.0 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 (d, J = 8.1 Hz, 2H), 7.37 – 7.26 (m, 5H), 7.16 (d, J = 7.8 Hz, 2H), 7.05 (d, J = 8.0 Hz, 2H), 6.97 – 6.90 (m, 2H), 6.01 (d, J = 5.8 Hz, 1H), 5.49 (ddd, J = 16.1, 10.3, 5.8 Hz, 1H), 5.31 (d, J = 17.2 Hz, 1H), 5.12 (d, J = 10.4 Hz, 1H), 4.80 (d, J = 11.8 Hz, 1H), 4.66 (d, J = 11.9 Hz, 1H), 2.39 (s, 3H), 2.31 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.3, 138.7, 137.6, 137.4, 133.9, 132.3, 131.8, 129.4, 129.3, 128.4, 127.8, 127.7, 127.6, 118.7,



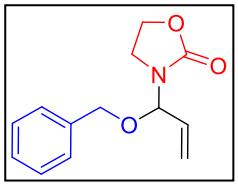
88.3, 69.7, 21.6, 21.3; **HRMS** (ESI-TOF) m/z: [M + H]$^+$ calcd. for $C_{24}H_{26}NO_3S$ 408.1628, found 408.1617.

***N*-(1-(benzyloxy)allyl)-2,4,6-trimethyl-*N*-(4-(trifluoromethyl)phenyl)benzene-sulfonamide (3ce).** 

According to general procedure, **3ce** was obtained in 73% (71.5 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.4 Hz, 2H), 7.44 – 7.27 (m, 5H), 7.13 (d, *J* = 8.3 Hz, 2H), 6.88 (s, 2H), 6.11 (d, *J* = 5.3 Hz, 1H), 5.53 (ddd, *J* = 16.4, 10.3, 5.4 Hz, 1H), 5.37 (d, *J* = 17.1 Hz, 1H), 5.16 (d, *J* = 10.3 Hz, 1H), 5.06 (d, *J* = 11.9 Hz, 1H), 4.79 (d, *J* = 11.9 Hz, 1H), 2.35 (s, 6H), 2.30 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.2, 140.4, 138.4 (q, J_{C-F} = 1.5 Hz), 137.5, 133.4, 133.0, 132.5, 131.9, 130.6 (q, J_{C-F} = 32.9 Hz), 128.5, 127.8, 127.8, 125.6 (q, J_{C-F} = 3.8 Hz), 123.8 (q, J_{C-F} = 272.4 Hz),119.3, 87.2, 70.2, 22.8, 21.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.53; **HRMS** (ESI-TOF) m/z: [M + Na]$^+$ calcd. for $C_{26}H_{26}F_3NNaO_3S$ 512.1478, found 512.1456.

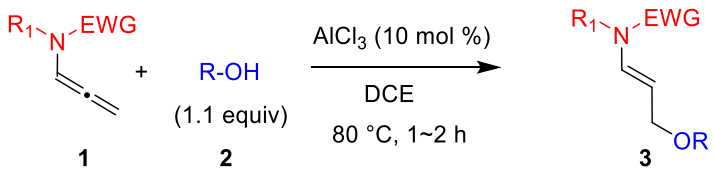
***N*-allyl-*N*-(1-(benzyloxy)allyl)-4-methylbenzenesulfonamide (3de).** 

According to general procedure, **3de** was obtained in 64% (45.7 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.39 – 7.20 (m, 7H), 5.84 – 5.70 (m, 1H), 5.67 (d, *J* = 4.0 Hz, 1H), 5.57 (ddd, *J* = 17.1, 10.4, 4.1 Hz, 1H), 5.40 (d, *J* = 17.1 Hz, 1H), 5.22 (d, *J* = 10.4 Hz, 1H), 5.15 (d, *J* = 17.1 Hz, 1H), 5.04 (d, *J* = 10.1 Hz, 1H), 4.64 (d, *J* = 11.9 Hz, 1H), 4.50 (d, *J* = 11.9 Hz, 1H), 3.94 – 3.67 (m, 2H), 2.41 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.4, 137.9, 137.6, 135.2, 134.0, 129.6, 128.4, 127.8, 127.7, 127.3, 119.0, 117.5, 86.5, 69.4, 45.7, 21.6; **HRMS** (ESI-TOF) m/z: [M + Na]$^+$ calcd. for $C_{20}H_{23}NNaO_3S$ 380.1291, found 380.1278.

3-(1-(benzyloxy)allyl)oxazolidin-2-one (3ee). 

According to general procedure, **3ee** (purity >94%) was obtained in 54% (24.2 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.25 (m, 5H), 5.79 (ddd, *J* = 17.2, 10.6, 4.2 Hz, 1H), 5.66 (d, *J* = 4.0 Hz, 1H), 5.51 (d, *J* = 17.3 Hz, 1H), 5.35 (d, *J* = 10.6 Hz, 1H), 4.59 (q, *J* = 12.1 Hz, 2H), 4.27 (q, *J* = 8.3 Hz, 1H), 4.15 (q, *J* = 8.5 Hz, 1H), 3.49 – 3.41 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.1, 137.6, 133.1, 128.5, 127.9, 127.7, 119.1, 82.5, 70.4, 62.5, 39.2; **HRMS** (ESI-TOF) m/z: [M + Na]$^+$ calcd. for $C_{13}H_{15}NNaO_3$ 256.0944, found 256.0937.

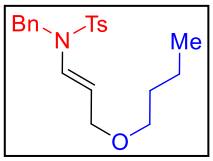
4. *γ*-Hydroalkoxylation of allenamide: General procedure



1 **2** **3**

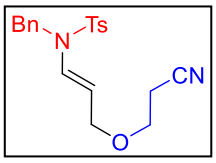
In a screw cap 7 mL vial, allenamide **1** (0.2 mmol), aluminum chloride (2.6 mg, 0.02 mmol) was taken and dichloroethane (1 mL, 0.2 M) followed by alcohol **2** (0.22 mmol) was added to it. The mixture was stirred at 80 °C and the reaction progress was monitored by TLC and/or ^{1}H NMR analysis. After completion (approx. 1~2 h), the reaction mixture was cool down to room temperature. The solvent was concentrated under reduced pressure and the crude mixture was subjected to silica gel column chromatography. The product was isolated using ethyl acetate-hexane with 1 % Et_3N as eluent.

(*E*)-*N*-benzyl-*N*-(3-butoxyprop-1-en-1-yl)-4-methylbenzenesulfonamide (4aa).



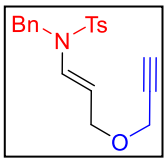
According to general procedure, **4aa** (purity >87%) was obtained in 46% (34.4 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.32 – 7.23 (m, 7H), 6.92 (d, *J* = 14.1 Hz, 1H), 4.80 – 4.69 (m, 1H), 4.51 (s, 2H), 3.86 – 3.76 (m, 2H), 3.21 (t, *J* = 6.7 Hz, 2H), 2.42 (s, 3H), 1.48 – 1.37 (m, 2H), 1.29 – 1.19 (m, 2H), 0.84 (t, *J* = 5.1 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.1, 136.0, 135.3, 129.9, 129.6, 128.6, 127.5, 127.0, 126.9, 107.8, 69.6, 69.4, 49.5, 31.7, 21.6, 19.4, 14.0; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{21}H_{28}NO_3S$ 374.1784, found 374.1774.

(*E*)-*N*-benzyl-*N*-(3-(2-cyanoethoxy)prop-1-en-1-yl)-4-methylbenzenesulfonamide



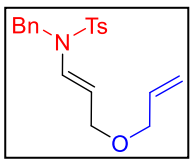
(4ab). According to general procedure, **4ab** was obtained in 58% (43.0 mg) yield as colorless oil**; ^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.1 Hz, 2H), 7.35 – 7.21 (m, 7H), 6.94 (d, *J* = 14.2 Hz, 1H), 4.70 (dt, *J* = 14.0, 6.9 Hz, 1H), 4.52 (s, 2H), 3.89 (d, *J* = 6.9 Hz, 2H), 3.38 (t, *J* = 6.5 Hz, 2H), 2.42 (s, 3H), 2.41 (t, *J* = 6.5 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.3, 135.8, 135.1, 130.5, 130.1, 128.7, 127.6, 127.0, 127.0, 117.8, 106.6, 70.2, 63.6, 49.5, 21.7, 18.8; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{20}H_{22}N_2NaO_3S$ 393.1243, found 393.1228.

(*E*)-*N*-benzyl-4-methyl-*N*-(3-(prop-2-yn-1-yloxy)prop-1-en-1-yl)benzenesulfonamide



(4ac). According to general procedure, **4ac** was obtained in 42% (29.8 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.33 – 7.21 (m, 7H), 7.00 (d, *J* = 14.2 Hz, 1H), 4.70 (dd, *J* = 14.2, 7.1 Hz, 1H), 4.51 (s, 2H), 4.00 – 3.86 (m, 4H), 2.42 (s, 3H), 2.39 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.1, 135.8, 135.0, 130.8, 129.9, 128.6, 127.5, 126.9, 126.8, 106.1, 79.4, 74.5, 68.3, 55.9, 49.4, 21.5; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{20}H_{22}NO_3S$ 356.1315, found 356.1305.

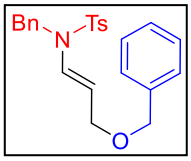
(*E*)-*N*-(3-(allyloxy)prop-1-en-1-yl)-*N*-benzyl-4-methylbenzenesulfonamide (4ad).



According to general procedure, **4ad** was obtained in 56% (40.0 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.32 – 7.23 (m, 7H), 6.94 (d, *J* = 14.2 Hz, 1H), 5.87 – 5.70 (m, 1H), 5.23 – 5.06 (m, 2H), 4.75 (dt, *J* = 14.0, 6.9 Hz, 1H), 4.52 (s, 2H), 3.84 (d, *J* = 6.8 Hz, 2H), 3.77 (d, *J* = 5.7 Hz, 2H), 2.42 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.1, 136.0, 135.3, 134.7, 130.0, 129.9, 128.7, 127.5, 127.0, 126.9, 117.3, 107.4, 70.4,

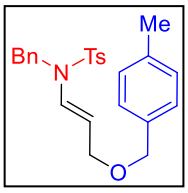
69.0, 49.5, 21.6; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{20}H_{24}NO_3S$ 358.1471, found 358.1462.

(*E*)-*N*-benzyl-*N*-(3-(benzyloxy)prop-1-en-1-yl)-4-methylbenzenesulfonamide (4ae).



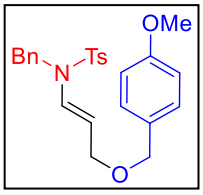
According to general procedure, **4ae** (purity >90%) was obtained in 70% (57.0 mg) yield as colorless oil**; ^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.34 – 7.18 (m, 12H), 6.96 (d, *J* = 14.2 Hz, 1H), 4.80 (dt, *J* = 14.0, 6.9 Hz, 1H), 4.54 (s, 2H), 4.30 (s, 2H), 3.90 (d, *J* = 6.9 Hz, 2H), 2.42 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.0, 138.0, 135.8, 135.2, 129.8, 128.5, 128.3, 127.8, 127.5, 127.4, 126.9, 126.8, 107.4, 71.2, 68.9, 49.4, 21.5; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{24}H_{26}NO_3S$ 408.1628, found 408.1617.

(*E*)-*N*-benzyl-4-methyl-*N*-(3-((4-methylbenzyl)oxy)prop-1-en-1-yl)benzene-sulfonamide (4af).



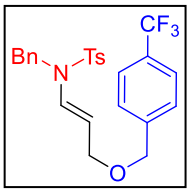
According to general procedure, **4af** was obtained in 60% (50.5 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.32 – 7.22 (m, 8H), 7.13 – 7.04 (m, 4H), 6.93 (d, *J* = 14.2 Hz, 1H), 4.77 (dt, *J* = 14.0, 6.9 Hz, 1H), 4.52 (s, 2H), 4.25 (s, 2H), 3.86 (d, *J* = 6.9 Hz, 2H), 2.42 (s, 3H), 2.32 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.1, 137.4, 136.0, 135.3, 135.0, 130.0, 130.0, 129.1, 128.7, 128.1, 127.6, 127.0, 126.9, 107.6, 71.2, 68.9, 49.5, 21.7, 21.2; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{25}H_{28}NO_3S$ 422.1784, found 422.1773.

(*E*)-*N*-benzyl-*N*-(3-((4-methoxybenzyl)oxy)prop-1-en-1-yl)-4-methylbenzene-sulfonamide (4ag).



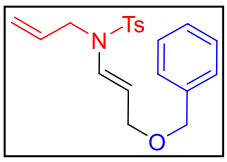
According to general procedure, **4ag** (purity >94%) was obtained in 73% (63.9 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.33 – 7.20 (m, 7H), 7.11 (d, *J* = 8.5 Hz, 2H), 6.94 (d, *J* = 14.2 Hz, 1H), 6.83 (d, *J* = 8.6 Hz, 2H), 4.77 (dt, *J* = 14.0, 6.9 Hz, 1H), 4.52 (s, 2H), 4.21 (s, 2H), 3.86 (d, *J* = 6.9 Hz, 2H), 3.78 (s, 3H), 2.42 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.2, 144.1, 136.0, 135.3, 130.2, 130.0, 129.9, 129.6, 128.7, 127.5, 127.0, 126.9, 113.8, 107.6, 71.0, 68.8, 55.3, 49.5, 21.6; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ calcd. for $C_{25}H_{27}NNaO_4S$ 460.1553, found 460.1534.

(*E*)-*N*-benzyl-4-methyl-*N*-(3-((4-(trifluoromethyl)benzyl)oxy)prop-1-en-1-yl)benzenesulfonamide (4ah).



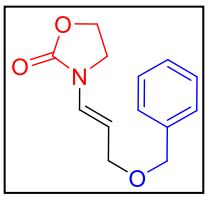
According to general procedure, **4ah** (purity >94%) was obtained in 64% (60.9 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.33 – 7.23 (m, 9H), 6.96 (d, *J* = 14.2 Hz, 1H), 4.77 (dt, *J* = 14.0, 6.9 Hz, 1H), 4.53 (s, 2H), 4.31 (s, 2H), 3.92 (d, *J* = 6.9 Hz, 2H), 2.42 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 144.2, 142.3, 135.9, 135.2, 130.3, 130.0, 139.7 (q, J_{C-F} = 32.9 Hz) 128.7, 127.8, 127.6, 127.0, 126.9, 125.3 (q, J_{C-F} = 3.8 Hz), 124.2 (q, J_{C-F} = 272.2 Hz), 107.1, 70.4, 69.4, 49.5, 21.6; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{25}H_{25}F_3NO_3S$ 476.1517, found 476.1487.

(*E*)-*N*-allyl-*N*-(3-(benzyloxy)prop-1-en-1-yl)-4-methylbenzenesulfonamide (4de).



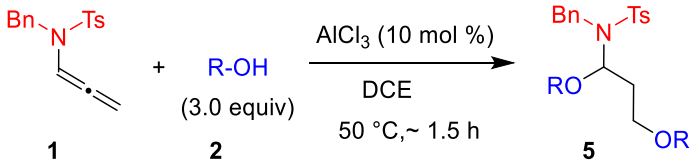
According to general procedure, **4de** was obtained in 57% (40.7 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.2 Hz, 2H), 7.37 – 7.25 (m, 7H), 6.91 (d, *J* = 14.2 Hz, 1H), 5.68 – 5.55 (m, 1H), 5.23 – 5.10 (m, 2H), 4.92 (dt, *J* = 14.1, 7.0 Hz, 1H), 4.44 (s, 2H), 4.05 – 3.94 (m, 4H), 2.40 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.9, 138.1, 136.1, 131.4, 129.9, 129.8, 128.4, 127.8(2C), 127.6, 126.9, 117.9, 106.2, 71.5, 69.1, 48.1, 21.5; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ calcd. for $C_{20}H_{23}NNaO_3S$ 380.1291, found 380.1276.

(*E*)-3-(3-(benzyloxy)prop-1-en-1-yl)oxazolidin-2-one (4ee).



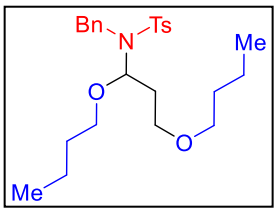
According to general procedure, **4ee** was obtained in 41% (19.2 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 – 7.28 (m, 5H), 6.90 (d, *J* = 14.3 Hz, 1H), 4.97 (dt, *J* = 14.1, 7.0 Hz, 1H), 4.50 (s, 2H), 4.47 – 4.39 (m, 2H), 4.04 (d, *J* = 7.5 Hz, 2H), 3.75 – 3.66 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ13C NMR (101 MHz, Chloroform-d) δ 155.4, 138.1, 128.5, 127.9, 127.8, 106.5, 72.0, 68.8, 62.3, 42.4; **HRMS** (ESI-TOF) m/z: $[M + Na]^+$ calcd. for $C_{13}H_{15}NNaO_3$ 256.0944, found 256.0937.

5. α,γ-*bis*-Hydroalkoxylation of allenamide: General procedure



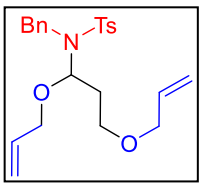
In a screw cap 7 mL vial, allenamide **1** (0.2 mmol), aluminum chloride (2.6 mg, 0.02 mmol) was taken and dichloroethane (1 mL, 0.2 M) followed by alcohol **2** (0.6 mmol) was added to it. The mixture was stirred at 50 °C and the reaction progress was monitored by TLC and/or ^{1}H NMR analysis. After completion (approx. 1 h), the reaction mixture was cool down to room temperature, solvent was concentrated under reduced pressure and the crude mixture was subjected to silica gel column chromatography. The product **5** was isolated using ethyl acetate-hexane.

***N*-benzyl-*N*-(1-butoxyallyl)-4-methylbenzenesulfonamide (5aa).**

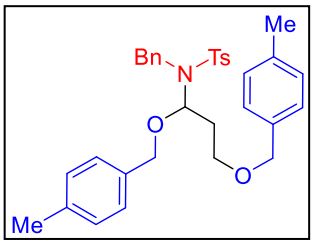


According to general procedure, **5aa** was obtained in 63% (56.4 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 6.6 Hz, 2H), 7.28 – 7.17 (m, 5H), 5.24 (dd, *J* = 8.9, 3.8 Hz, 1H), 4.44 – 4.22 (m, 2H), 3.40 – 3.09 (m, 6H), 2.39 (s, 3H), 1.76 (td, *J* = 8.9, 4.5 Hz, 1H), 1.59 – 1.47 (m, 3H), 1.40 – 1.14 (m, 6H), 0.92 (t, *J* = 7.3 Hz, 3H), 0.81 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.1, 138.2, 137.9, 129.5, 128.6, 128.2, 127.2, 127.2, 85.8, 70.7, 68.1, 66.7, 46.1, 35.1, 31.9,

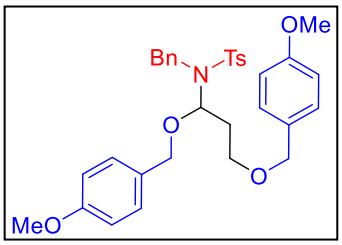
31.2, 21.5, 19.4, 19.2, 14.1, 13.9; **HRMS** (ESI-TOF) m/z: [M + Na]$^+$ calcd. for $C_{25}H_{37}NNaO_4S$ 470.2336, found 470.2313.

***N*-(1-(allyloxy)allyl)-*N*-benzyl-4-methylbenzenesulfonamide (5ad).** 

According to general procedure, **5ad** (purity >92%) was obtained in 66% (54.9 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 6.4 Hz, 2H), 7.23 (dt, *J* = 8.0, 3.4 Hz, 5H), 5.86 (ddd, *J* = 16.1, 10.6, 5.3 Hz, 1H), 5.61 (ddd, *J* = 16.2, 10.8, 5.5 Hz, 1H), 5.32 (dd, *J* = 8.8, 3.8 Hz, 1H), 5.28 – 5.03 (m, 4H), 4.48 – 4.21 (m, 2H), 3.95 – 3.71 (m, 4H), 3.36 (t, *J* = 5.9 Hz, 2H), 2.39 (s, 3H), 1.85 (ddt, *J* = 13.8, 9.5, 5.0 Hz, 1H), 1.58 (dtd, *J* = 14.0, 7.3, 4.0 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.3, 138.1, 137.8, 134.8, 133.7, 129.6, 128.7, 128.3, 127.3, 127.2, 117.5, 116.8, 85.3, 71.8, 68.8, 66.2, 46.3, 34.8, 21.6; **HRMS** (ESI-TOF) m/z: [M + Na]$^+$ calcd. for $C_{23}H_{29}NNaO_4S$ 438.1710, found 438.1690.

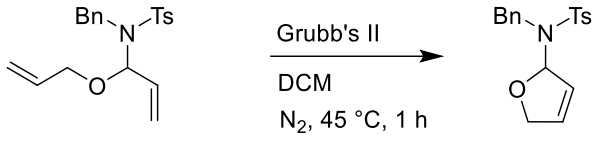
***N*-benzyl-4-methyl-*N*-(1-((4-methylbenzyl)oxy)allyl)benzenesulfonamide (5af).** 

According to general procedure, **5af** (purity >92%) was obtained in 70% (76.2 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.1 Hz, 2H), 7.41 – 7.34 (m, 2H), 7.25 (d, *J* = 6.4 Hz, 3H), 7.18 (d, *J* = 8.8 Hz, 6H), 7.08 (d, *J* = 7.8 Hz, 2H), 6.96 (d, *J* = 7.8 Hz, 2H), 5.44 (dd, *J* = 9.0, 3.3 Hz, 1H), 4.51 (d, *J* = 15.6 Hz, 1H), 4.39 – 4.19 (m, 5H), 3.36 (dt, *J* = 8.9, 5.0 Hz, 2H), 2.39 (s, 3H), 2.36 (s, 3H), 2.31 (s, 3H), 1.88 (td, *J* = 9.1, 4.5 Hz, 1H), 1.58 (ddd, *J* = 14.1, 9.6, 4.5 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.1, 137.8, 137.8, 137.2, 137.1, 135.2, 134.3, 129.4, 128.9, 128.8, 128.6, 128.2, 128.1, 127.7, 127.2, 127.1, 85.2, 72.6, 69.7, 65.9, 46.2, 34.8, 21.4, 21.1, 21.1; **HRMS** (ESI-TOF) m/z: [M + Na]$^+$ calcd. for $C_{33}H_{37}NNaO_4S$ 566.2312, found 566.2336.

***N*-benzyl-*N*-(1,3-bis((4-methylbenzyl)oxy)propyl)-4-methylbenzenesulfonamide (5ag).** 

According to general procedure, **5ag** was obtained in 60% (69.0 mg) yield as colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.37 – 7.31 (m, 2H), 7.24 (d, *J* = 7.1 Hz, 3H), 7.17 (t, *J* = 8.3 Hz, 4H), 6.98 (d, *J* = 8.5 Hz, 2H), 6.87 (d, *J* = 8.5 Hz, 2H), 6.78 (d, *J* = 8.5 Hz, 2H), 5.40 (dd, *J* = 9.0, 3.3 Hz, 1H), 4.54 – 4.42 (m, 1H), 4.33 – 4.25 (m, 2H), 4.23 – 4.14 (m, 3H), 3.79 (s, 3H), 3.75 (s, 3H), 3.32 (ddt, *J* = 18.2, 9.2, 4.5 Hz, 2H), 2.37 (s, 3H), 1.85 (td, *J* = 9.5, 9.1, 5.0 Hz, 1H), 1.53 (dq, *J* = 8.3, 4.4, 3.4 Hz, 1H); **^{13}C NMR** (101 MHz $CDCl_3$) δ 159.0, 143.1, 137.8, 130.4, 129.7, 129.5, 129.2, 128.6, 128.2, 127.2, 127.1, 113.6, 113.5, 85.1, 72.4, 69.5, 65.8, 55.2, 55.2, 46.2, 34.8, 21.5; **HRMS** (ESI-TOF) m/z: [M + Na]$^+$ calcd. for $C_{33}H_{37}NNaO_6S$ 598.2210, found 598.2234.

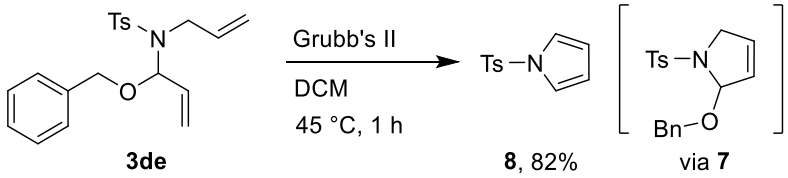
6. Ring closing metathesis of 3ad



3ad **6**, 88%

In a screw cap 7 mL vial, Grubb's 2nd generation catalyst (4.2 mg, 0.005 mmol) was placed, and dichloromethane (2.0 mL) was added to it. A solution of **3ad** (35.7 mg, 0.1 mmol) in dichloromethane (1.0 mL) were added and the resulting mixture was stirred at 45 °C for 1 h under nitrogen atmosphere. After completion, the reaction mixture was concentrated in vacuo, the resulting crude product was purified by a rapid filtration using short plug of silica gel, giving product **6** (31.4 mg) in 88% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 393.5, 8.2 Hz, 2H), 7.27 (s, 4H), 7.26 – 7.16 (m, 3H), 6.74 (bd, 1H), 5.97 – 5.90 (m, 1H), 5.42 – 5.34 (m, 1H), 4.61 – 4.44 (m, 2H), 4.30 (d, *J* = 16.4 Hz, 1H), 3.89 (d, *J* = 16.4 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR** (101 MHz $CDCl_3$) δ 143.4, 138.2, 137.0, 130.9, 129.5, 128.2, 127.9, 127.7, 127.1, 126.0, 94.5, 75.6, 46.1, 21.6; **HRMS** (ESI-TOF) m/z: $[M + H]^+$ calcd. for $C_{18}H_{20}NO_3S$ 330.1171, found 330.1152.

7. Ring closing metathesis of 3de



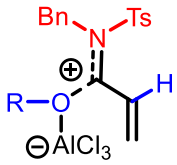
3de **8**, 82% via **7**

In a screw cap 7 mL vial, Grubb's 2nd generation catalyst (4.2 mg, 0.005 mmol) was placed, and dichloromethane (2.0 mL) was added to it. A solution of **3de** (35.7 mg, 0.1 mmol) in dichloromethane (1.0 mL) were added and the resulting mixture was stirred at 45 °C for 2 h under nitrogen atmosphere. After completion, the reaction mixture was concentrated in vacuo, the resulting crude product was purified by silica gel column chromatography eluting with ethyl acetate-hexane (1: 9 to 1: 5) giving product **8** (18.1 mg) in 82% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 3H), 7.14 (s, 2H), 6.27 (s, 2H), 2.38 (s, 3H). Spectral data was in agreement with literature values.[2]

8. Computational Details

The Gaussian 09 computational program[3] was used in the present mechanistic study. Geometrical optimizations in the gas phase were performed by the wB97XD density functional method[4] and the 6-311++G** basis set was used for all elements. For all calculations implicit solvation was introduced using the PCM model with dichloroethane as the solvent. Frequency calculations were analyzed to characterize the nature of the stationary point as minima (no imaginary frequency) or transition state (one imaginary frequency).

Optimized Geometries and Electronic Energies



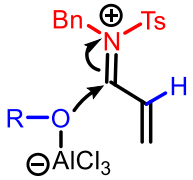
Optimized Geometry:

C	2.22254	-0.56202	0.80172
N	1.37886	0.17263	-0.14146
C	3.71996	-0.35307	0.66709
C	4.55709	-1.11458	1.48242
H	4.12810	-1.83921	2.16828
C	5.93554	-0.95524	1.42359
H	6.57480	-1.55583	2.06080
C	6.49264	-0.02925	0.54621
H	7.56822	0.09648	0.49601
C	5.66234	0.73092	-0.26792
H	6.08653	1.45172	-0.95769
C	4.28172	0.56896	-0.20792
H	3.64735	1.16062	-0.85698
S	1.08499	-0.56737	-1.63652

O	2.34802	-1.09791	-2.10960
O	0.36133	0.42161	-2.41416
C	0.02055	-1.94037	-1.29790
C	-1.35401	-1.75393	-1.36060
H	-1.76946	-0.78042	-1.58330
C	-2.18638	-2.84088	-1.15175
H	-3.26010	-2.70047	-1.20427
C	-1.66522	-4.10283	-0.86330
C	-2.57576	-5.26398	-0.58048
C	-0.27885	-4.26000	-0.80790
H	0.14314	-5.23747	-0.60103
C	0.57295	-3.18950	-1.03349
H	1.64719	-3.32888	-1.02968
C	0.88993	1.48252	0.07254
C	1.68778	2.29313	1.06118
C	1.43439	3.57326	1.29821
H	1.99528	-1.62643	0.70102
H	1.91266	-0.30088	1.81544
H	-2.71204	-5.37749	0.49992
H	-2.15684	-6.19821	-0.95947
H	-3.56060	-5.11545	-1.02595
C	-1.63899	-0.32090	1.87061
C	-1.01471	-1.55173	2.07074
H	0.06308	-1.60529	2.16896
C	-1.76507	-2.71492	2.17554
H	-1.26814	-3.66483	2.33482
C	-3.14980	-2.65967	2.06656

H	-3.73722	-3.56755	2.14539
C	-3.78109	-1.43908	1.85760
H	-4.86069	-1.38961	1.77623
C	-3.02956	-0.27411	1.77271
H	-3.53274	0.67894	1.64793
C	-0.83953	0.94754	1.85953
O	-0.57698	1.46705	0.49820
H	-1.35546	1.74672	2.38852
H	0.13016	0.81167	2.33140
Al	-1.86705	2.53918	-0.40472
Cl	-3.25917	1.31708	-1.44905
Cl	-0.78806	3.82963	-1.71467
Cl	-2.81593	3.62997	1.16947
H	2.51688	1.81065	1.56288
H	0.62730	4.11006	0.81086
H	2.04131	4.13079	2.00128
H	0.81514	1.99988	-0.87870

Electronic Energy: -3231.3882945 Hartree



Optimized Geometry:

C	-2.49785	-0.89448	-0.40370
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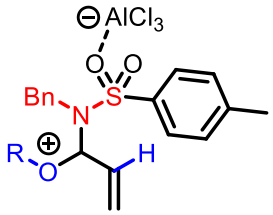
C	-4.58036	-0.70339	-1.77312

H	-3.98686	-0.97639	-2.64012
C	-5.94265	-0.46694	-1.91635
H	-6.40503	-0.55996	-2.89214
C	-6.70533	-0.10388	-0.81216
H	-7.76642	0.08686	-0.92370
C	-6.10113	0.01804	0.43449
H	-6.68960	0.30235	1.29918
C	-4.74114	-0.22675	0.58057
H	-4.28597	-0.13307	1.55989
S	-1.26997	-0.75043	2.11887
O	-2.23727	-1.80173	2.32199
O	-1.17125	0.37997	3.00803
C	0.31254	-1.41445	1.78016
C	1.43599	-0.67464	2.13702
H	1.33295	0.30560	2.58475
C	2.68324	-1.22618	1.91005
H	3.56785	-0.66051	2.17898
C	2.81926	-2.48868	1.32676
C	4.18405	-3.07718	1.11487
C	1.67060	-3.19737	0.96875
H	1.76400	-4.17089	0.50283
C	0.40972	-2.67293	1.19390
H	-0.47609	-3.24013	0.93649
C	-1.57728	1.23833	0.37368
C	-2.02123	1.98742	-0.76398
C	-1.74676	3.29801	-0.80380
H	-2.34711	-1.92361	-0.07952

H	-1.99603	-0.78050	-1.36386
H	4.15312	-3.91033	0.41193
H	4.58666	-3.44533	2.06345
H	4.87670	-2.32383	0.73347
C	1.39181	-0.92036	-2.07315
C	0.59659	-2.00179	-2.44313
H	-0.46751	-1.85968	-2.60466
C	1.14968	-3.26616	-2.63054
H	0.51319	-4.09650	-2.91658
C	2.51362	-3.45912	-2.45582
H	2.95051	-4.44051	-2.60419
C	3.31825	-2.38280	-2.09071
H	4.38441	-2.52531	-1.95467
C	2.76049	-1.12735	-1.89469
H	3.39420	-0.29675	-1.60201
C	0.80290	0.46383	-1.91551
O	0.96941	0.99082	-0.62229
H	1.25027	1.12590	-2.67030
H	-0.26847	0.42234	-2.15245
Al	1.95470	2.34658	-0.14060
Cl	4.04244	1.86321	0.14683
Cl	1.15253	3.07265	1.74396
Cl	1.79835	3.92282	-1.62325
H	-2.57038	1.50126	-1.55982
H	-1.19800	3.78615	-0.00472
H	-2.06252	3.91033	-1.63961
H	-1.05246	1.76070	1.16972

Electronic Energy: -3231.39604117 Hartree



Optimized Geometry:

C	-0.36774	1.62859	-0.81683
N	-0.11902	1.31585	0.59815
C	-1.82139	1.86361	-1.17545
C	-2.15178	1.96438	-2.52617
H	-1.38123	1.83791	-3.28084
C	-3.46006	2.22092	-2.91411
H	-3.70381	2.29449	-3.96799
C	-4.45500	2.37476	-1.95322
H	-5.47883	2.56587	-2.25376
C	-4.13054	2.26952	-0.60691
H	-4.90009	2.37297	0.14944
C	-2.81789	2.01906	-0.21953
H	-2.58111	1.92370	0.83399
S	-0.22018	-0.25035	1.06253
O	-1.42380	-0.73560	0.31223
O	-0.24541	-0.31714	2.50097
C	1.10014	-1.21671	0.41689
C	2.27548	-1.28079	1.15741
H	2.37745	-0.73438	2.08621
C	3.31200	-2.06262	0.67974

H	4.23509	-2.11850	1.24415
C	3.19664	-2.75776	-0.52499
C	4.32938	-3.60100	-1.03608
C	2.00728	-2.65997	-1.25009
H	1.90407	-3.19218	-2.18908
C	0.94929	-1.89527	-0.78874
H	0.02284	-1.84368	-1.34611
C	0.60966	2.23506	1.49829
C	0.09116	3.63852	1.28775
C	0.78992	4.73638	1.53860
H	0.05674	0.84748	-1.45559
H	0.19555	2.53581	-1.03883
H	4.48927	-3.43087	-2.10321
H	4.10487	-4.66307	-0.90099
H	5.25741	-3.38030	-0.50710
C	3.68965	1.55341	-0.19712
C	3.44426	0.92822	-1.41742
H	2.54238	1.16548	-1.97298
C	4.35281	0.01332	-1.93834
H	4.15039	-0.46734	-2.88889
C	5.51574	-0.28639	-1.23942
H	6.22617	-0.99769	-1.64539
C	5.76243	0.32300	-0.01302
H	6.66777	0.09037	0.53662
C	4.85533	1.23982	0.50228
H	5.05647	1.72604	1.45162
C	2.74360	2.58992	0.34479

O	2.00060	2.07581	1.46300
H	3.31232	3.45467	0.69625
H	2.07679	2.93912	-0.44326
Al	-2.96730	-1.72947	0.37069
Cl	-2.34090	-3.68964	0.94997
Cl	-3.68884	-1.65997	-1.63014
Cl	-4.25382	-0.82175	1.80605
H	-0.94904	3.71168	0.98557
H	1.82194	4.70205	1.86895
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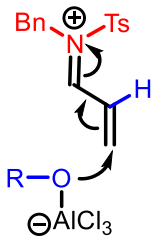
H	0.33893	1.92474	2.50822

Electronic Energy: -3231.39454831 Hartree



Optimized Geometry:

C	-1.35650	-1.22128	-0.50286
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C	-3.49686	-1.58655	-1.69903
H	-2.91884	-1.56927	-2.61770
C	-4.87619	-1.72209	-1.75628
H	-5.36776	-1.81369	-2.71792
C	-5.62395	-1.74625	-0.58216

H	-6.70156	-1.85435	-0.62520
C	-4.98038	-1.64267	0.64330
H	-5.55166	-1.67135	1.56399
C	-3.59630	-1.50259	0.70052
H	-3.11958	-1.43066	1.67102
S	0.15489	-2.97168	1.05790
O	-0.70378	-3.93061	0.41258
O	0.40262	-2.98808	2.47843
C	1.64133	-2.74345	0.16025
C	2.71278	-2.11863	0.79351
H	2.64855	-1.81804	1.83116
C	3.86234	-1.88546	0.06332
H	4.70241	-1.39455	0.54133
C	3.95076	-2.25616	-1.28218
C	5.19166	-1.94357	-2.06757
C	2.86339	-2.89547	-1.88092
H	2.92507	-3.20117	-2.91897
C	1.69980	-3.14392	-1.17079
H	0.86185	-3.64743	-1.63709
C	-0.61643	-0.50062	1.71585
C	-1.24069	0.77817	1.64545
C	-1.02483	1.64381	2.64607
H	-0.87895	-1.88925	-1.21956
H	-1.13381	-0.20463	-0.83453
H	5.19571	-2.45401	-3.03118
H	6.08769	-2.23233	-1.51377
H	5.25340	-0.86686	-2.25096

C	-1.41416	3.45177	-0.62376
C	-1.61541	2.52686	-1.64840
H	-0.81298	2.32575	-2.35018
C	-2.82298	1.84710	-1.76551
H	-2.96338	1.12676	-2.56352
C	-3.84797	2.07809	-0.85282
H	-4.77857	1.52632	-0.93068
C	-3.66986	3.02350	0.15318
H	-4.46835	3.22350	0.85918
C	-2.46296	3.70915	0.25868
H	-2.32833	4.44597	1.04530
C	-0.06160	4.09853	-0.42125
O	0.71625	3.35525	0.48742
H	-0.19779	5.10858	-0.01778
H	0.44028	4.20193	-1.39325
Al	2.00851	2.23250	0.20558
Cl	3.78362	3.21236	-0.56591
Cl	1.46653	0.68643	-1.22844
Cl	2.48675	1.27656	2.09509
H	-1.45710	2.63551	2.61858
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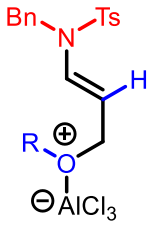
Electronic Energy: -3231.39435188 Hartree



Optimized Geometry:

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C	3.32096	-1.67516	1.13931
C	4.67839	-1.89765	0.93425
C	5.09773	-2.78549	-0.04917
C	4.15212	-3.44849	-0.82685
C	2.79641	-3.22802	-0.61812
S	-1.23979	-3.04434	-0.75484
O	-0.90119	-4.28077	-0.07853
O	-1.58196	-3.04091	-2.16397
C	-2.53186	-2.22950	0.14262
C	-3.38932	-1.37434	-0.53625
C	-4.35350	-0.68367	0.18264
C	-4.46530	-0.83135	1.56479
C	-5.47817	-0.03905	2.34335
C	-3.59585	-1.70910	2.21840
C	-2.62660	-2.40981	1.51920
C	0.16179	-0.90243	-1.38244
C	1.01219	0.11152	-1.19877
C	0.94974	1.32138	-2.05177
C	2.52387	2.82250	0.08961

C	2.20615	2.69751	1.44250
C	3.10685	2.11204	2.32201
C	4.33526	1.65192	1.85653
C	4.66115	1.77799	0.51175
C	3.75801	2.36320	-0.36811
C	1.54009	3.43346	-0.86380
O	0.48283	2.48710	-1.25275
Al	-1.25654	2.47831	-0.51006
Cl	-1.66810	4.53315	-0.10234
Cl	-1.26395	1.32149	1.27840
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H	5.40708	-1.36658	1.53636
H	6.15545	-2.95664	-0.21457
H	4.47201	-4.14032	-1.59806
H	2.06174	-3.74013	-1.23029
H	-3.30612	-1.24977	-1.60809
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H	-3.68132	-1.84826	3.29060
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H	-5.01660	0.87208	2.73670
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H	2.85394	2.01833	3.37180

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H	5.61567	1.41862	0.14546
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H	2.01172	3.76078	-1.79047
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H	0.24037	1.22623	-2.87242
H	1.91811	1.61825	-2.45138

Electronic Energy: -3231.40720993 Hartree

9. References

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4. J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys.,* 2008, **10**, 6615.

10. ^{1}H and ^{13}C NMR spectra

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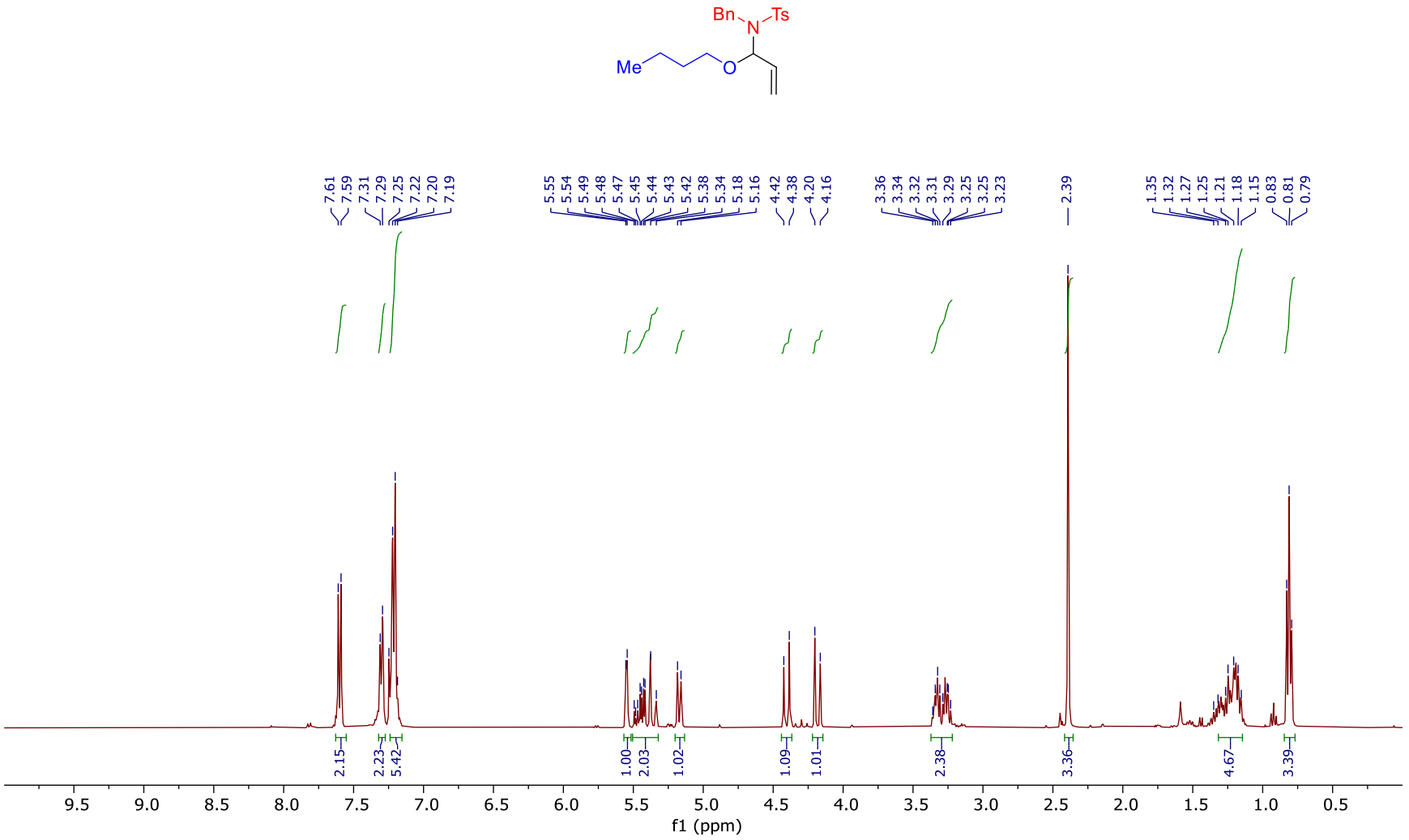

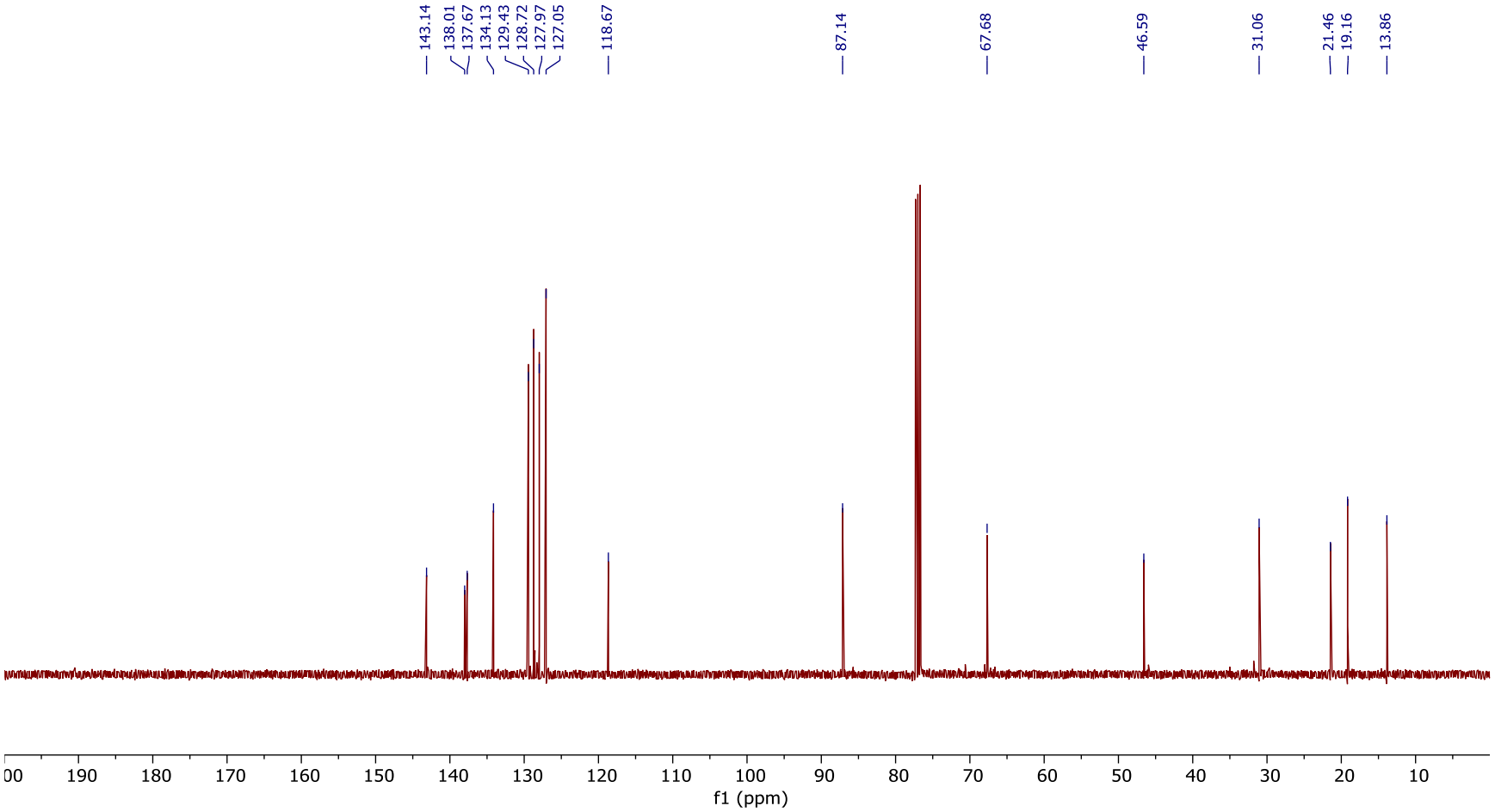
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f1 (ppm)

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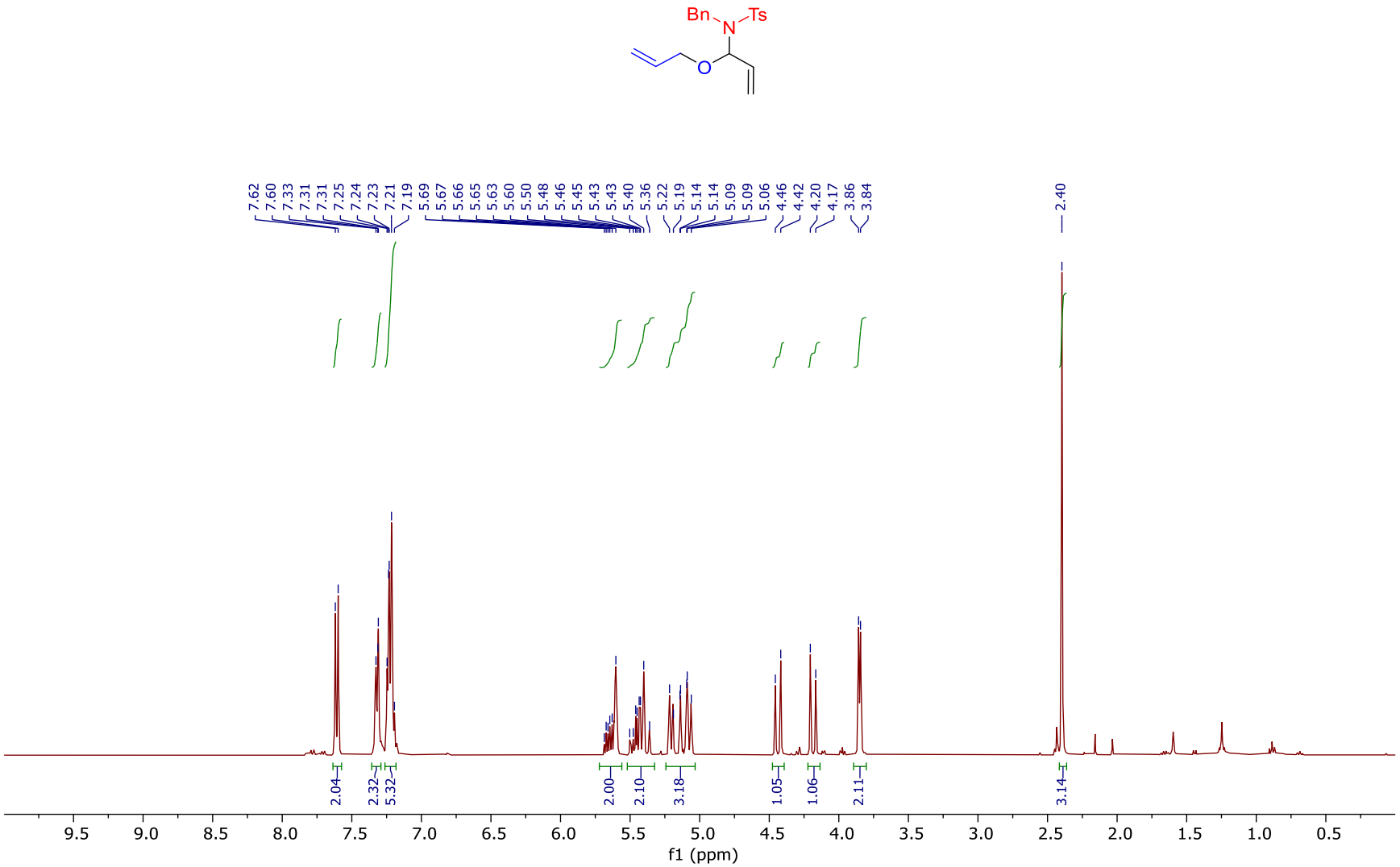
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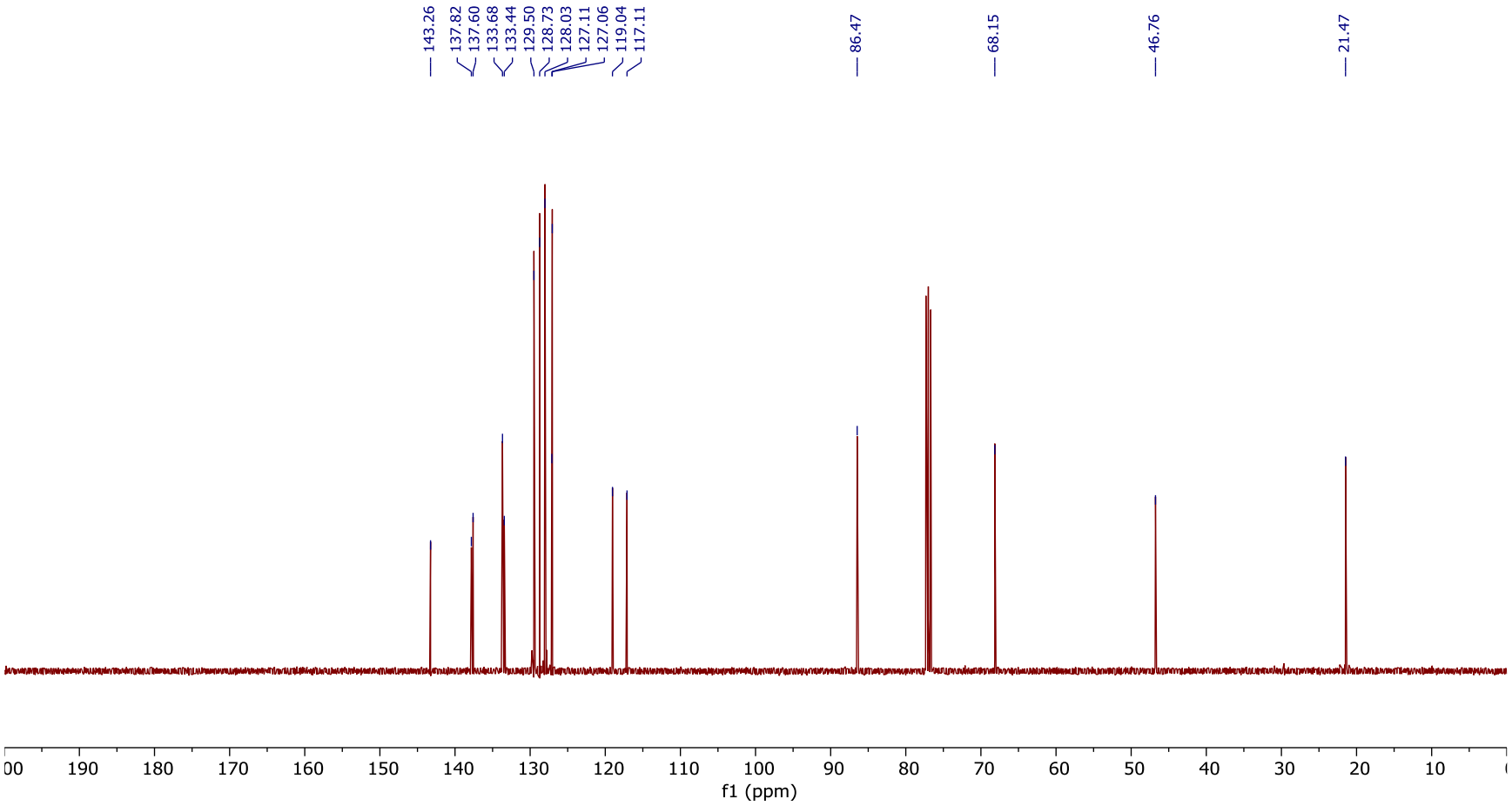
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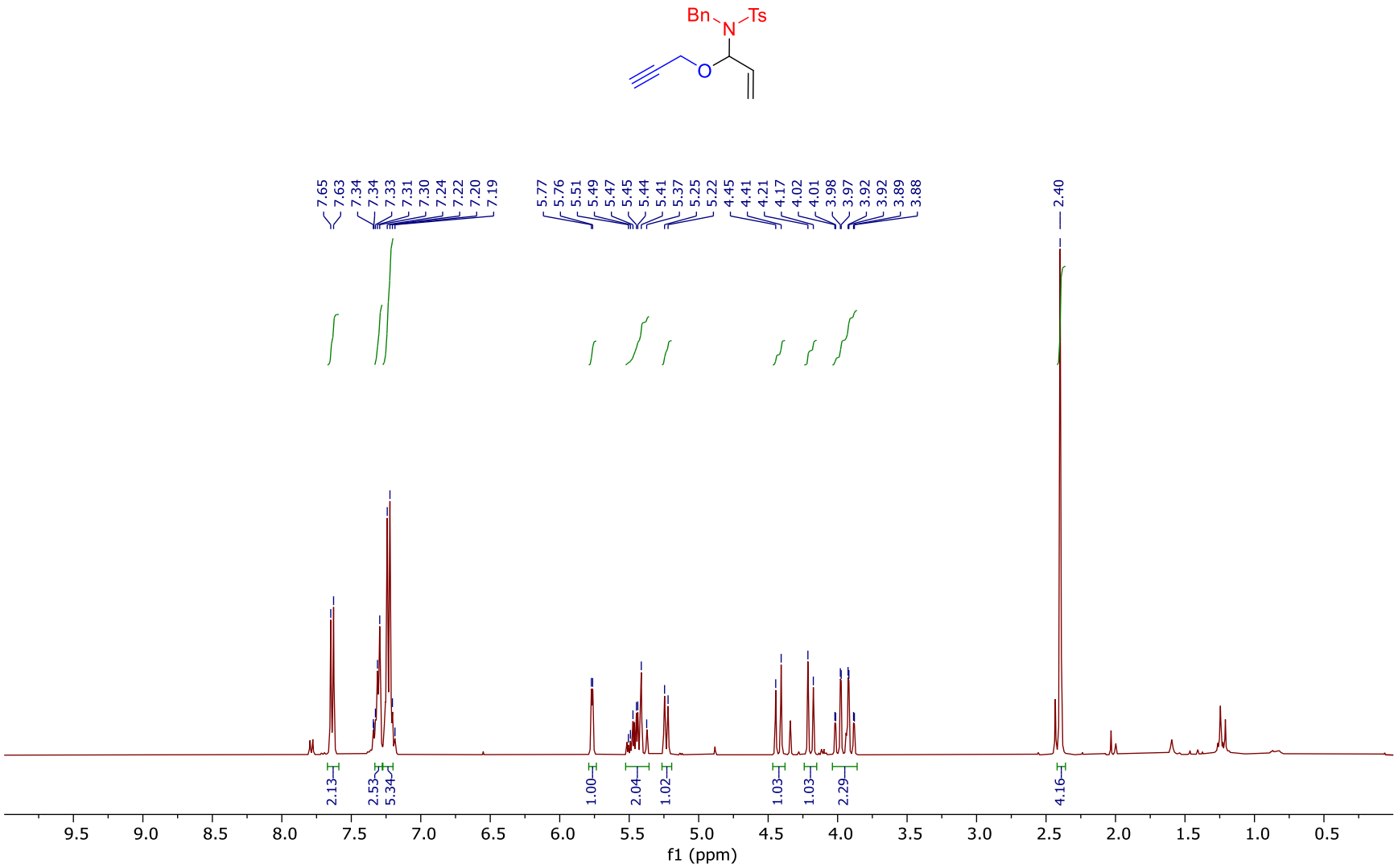
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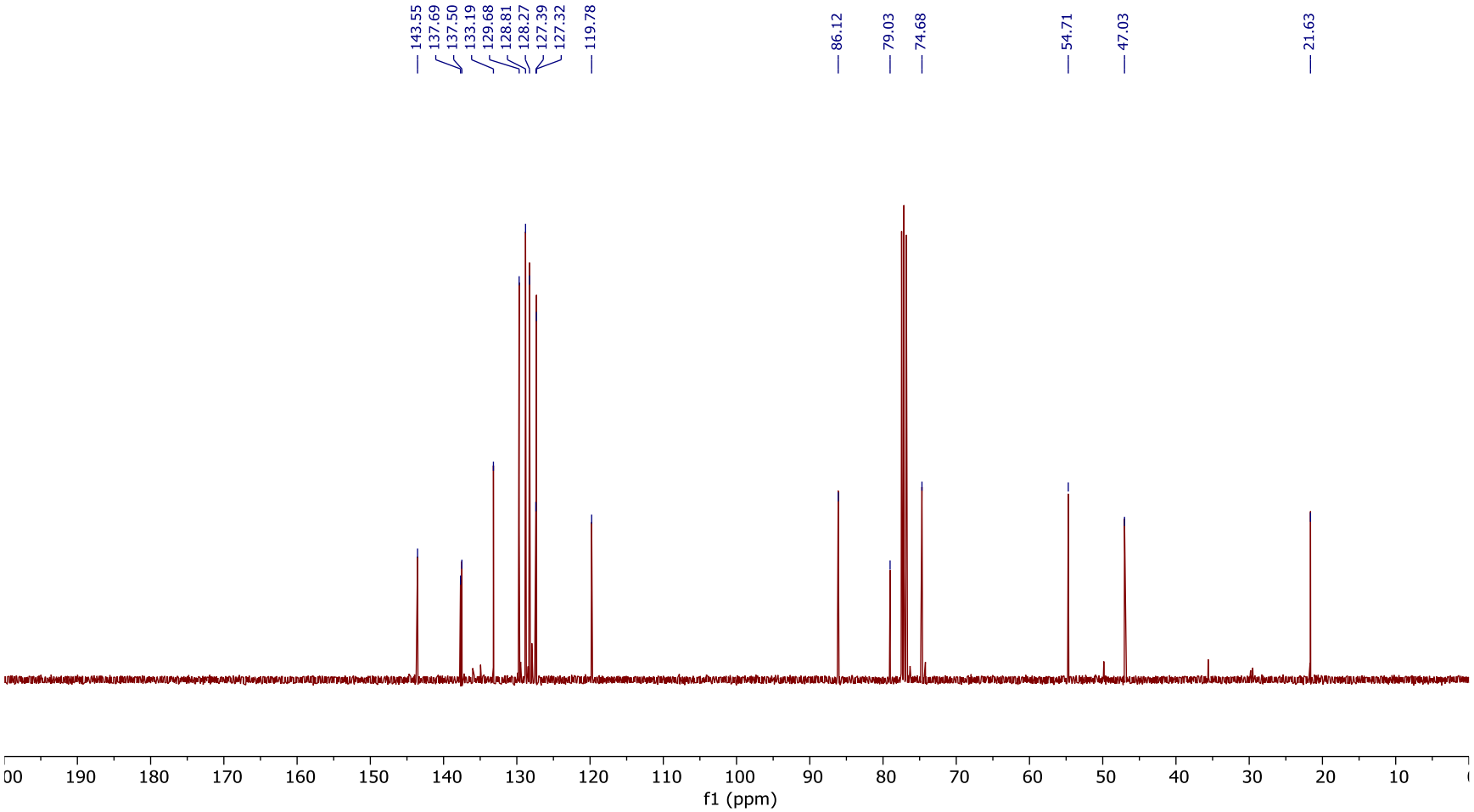
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f1 (ppm)

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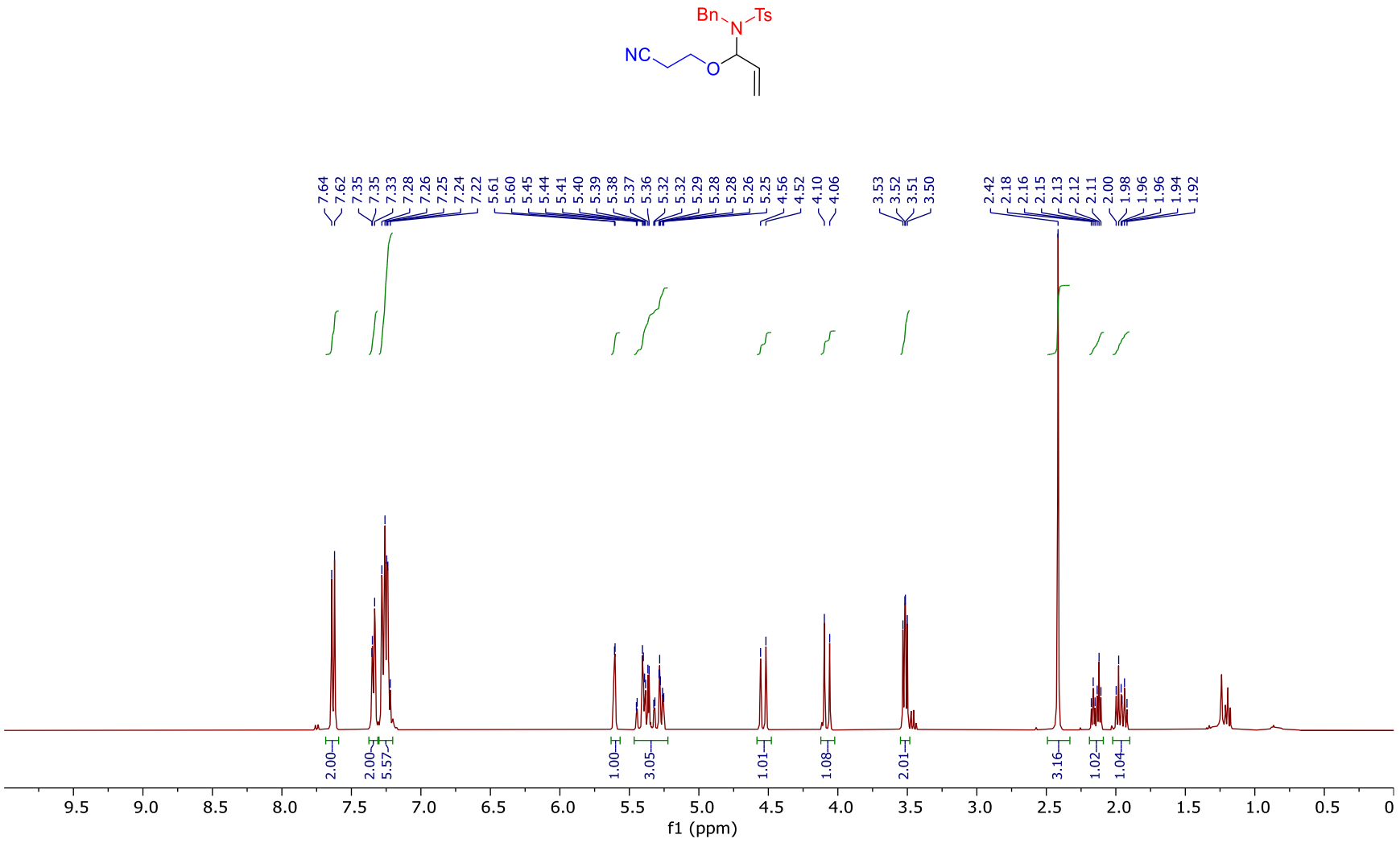
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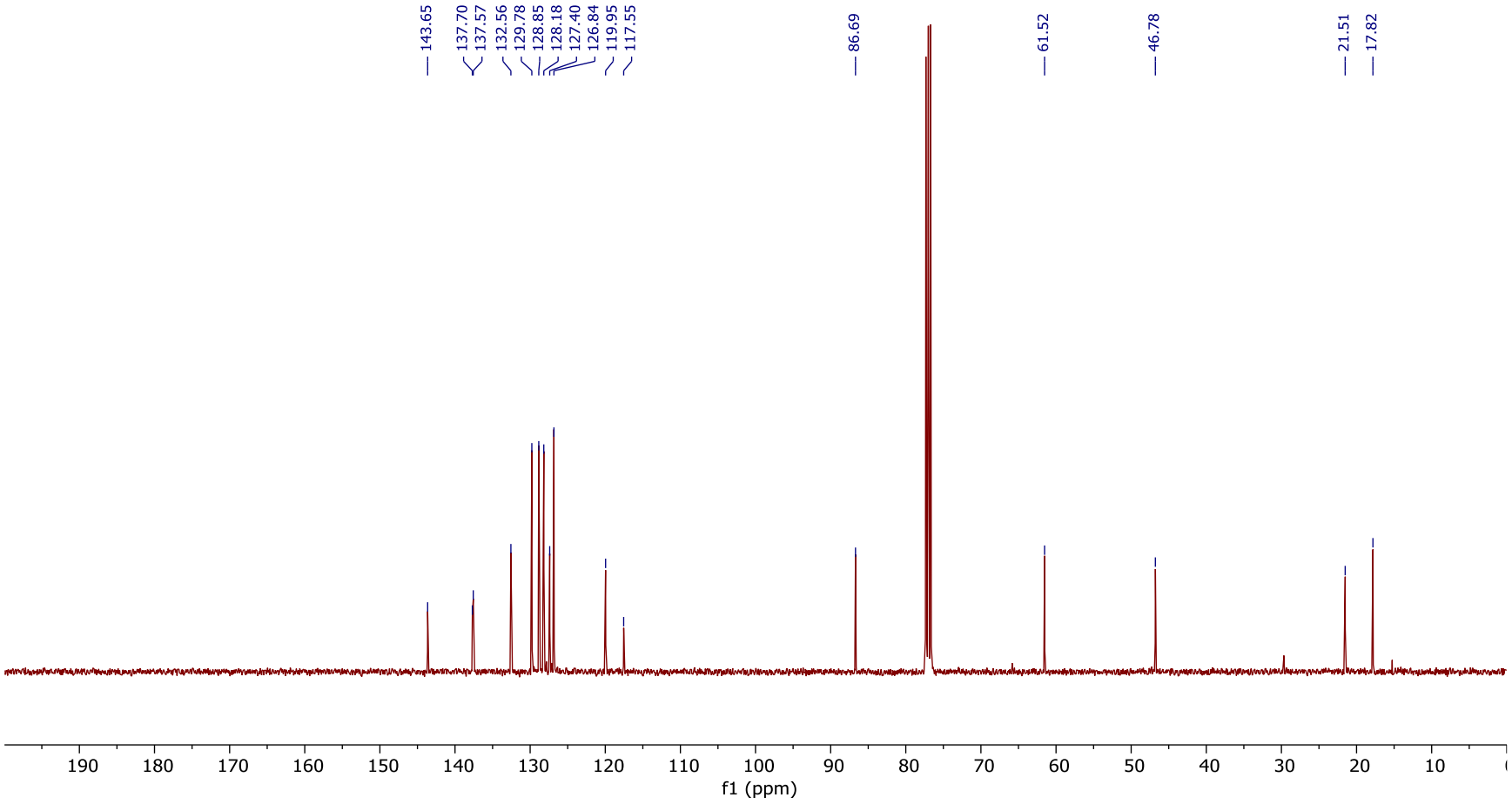
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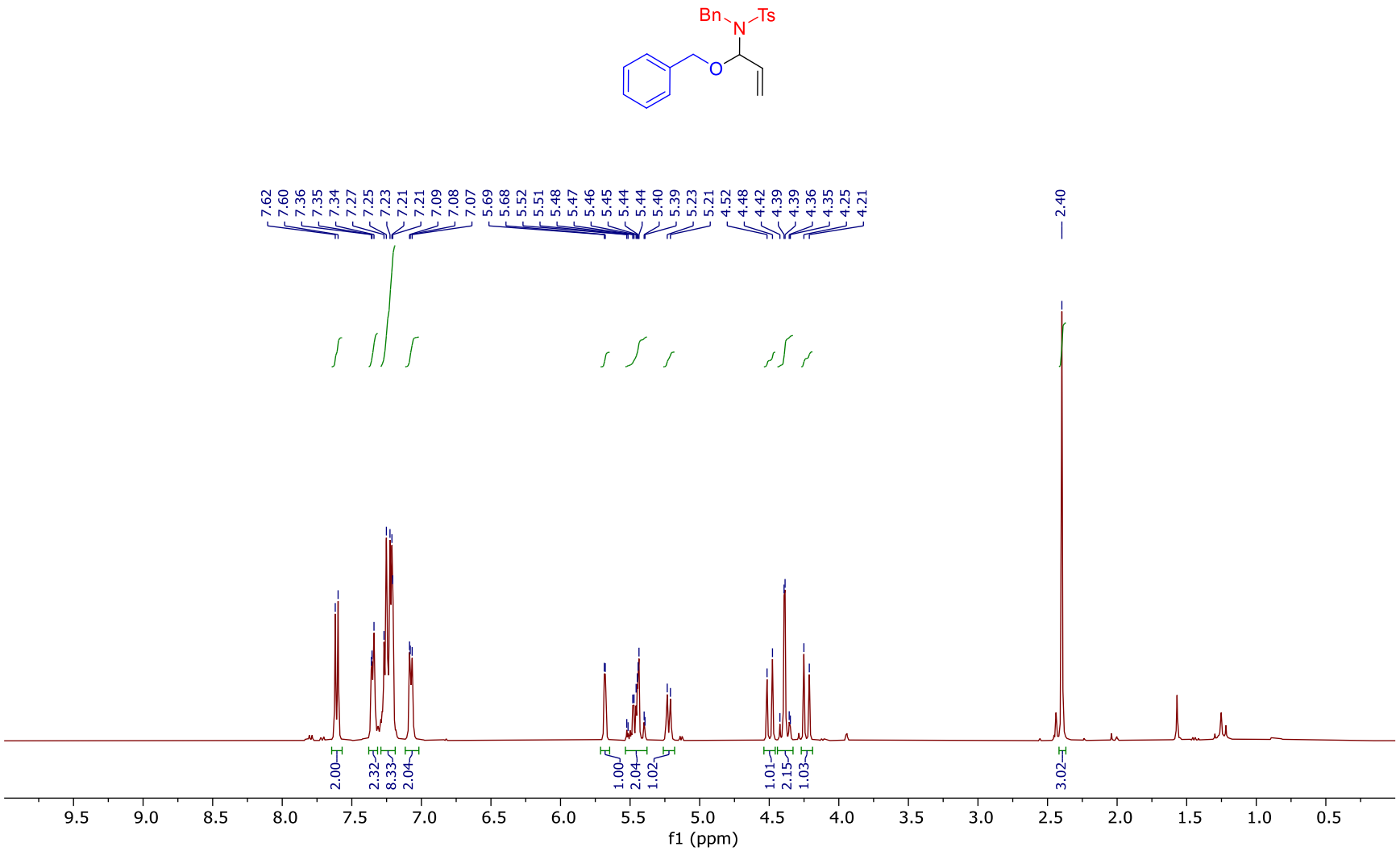
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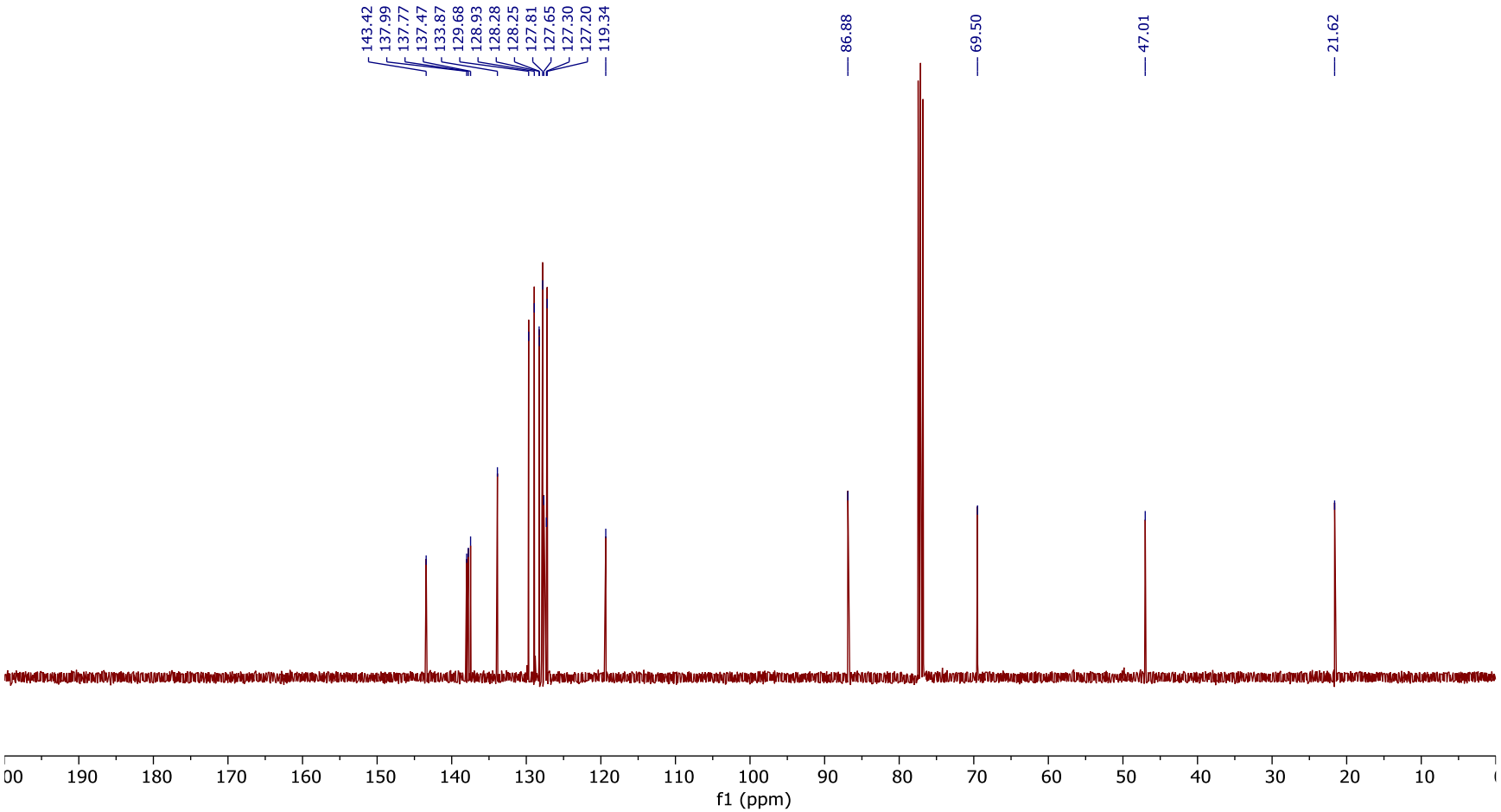
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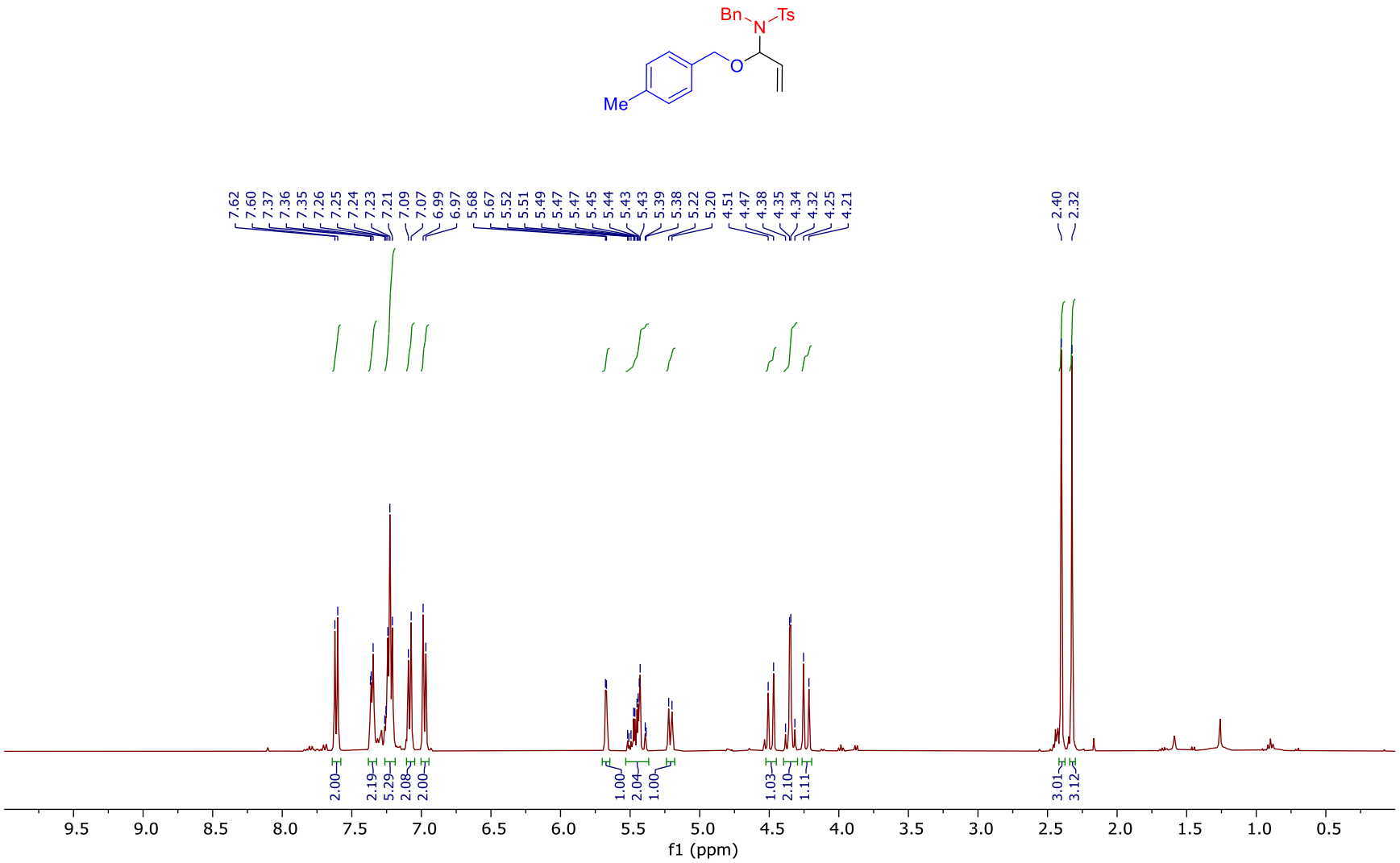
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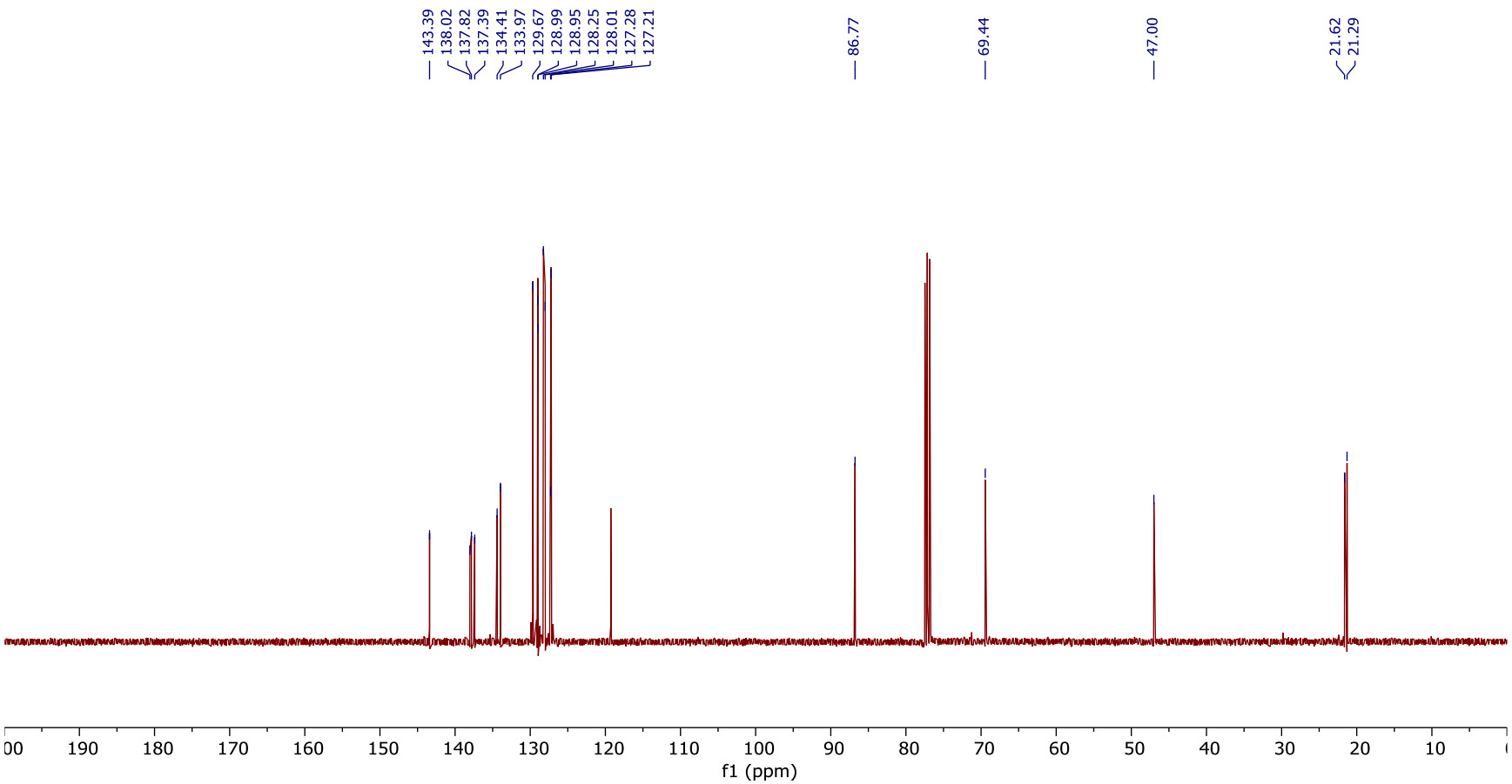
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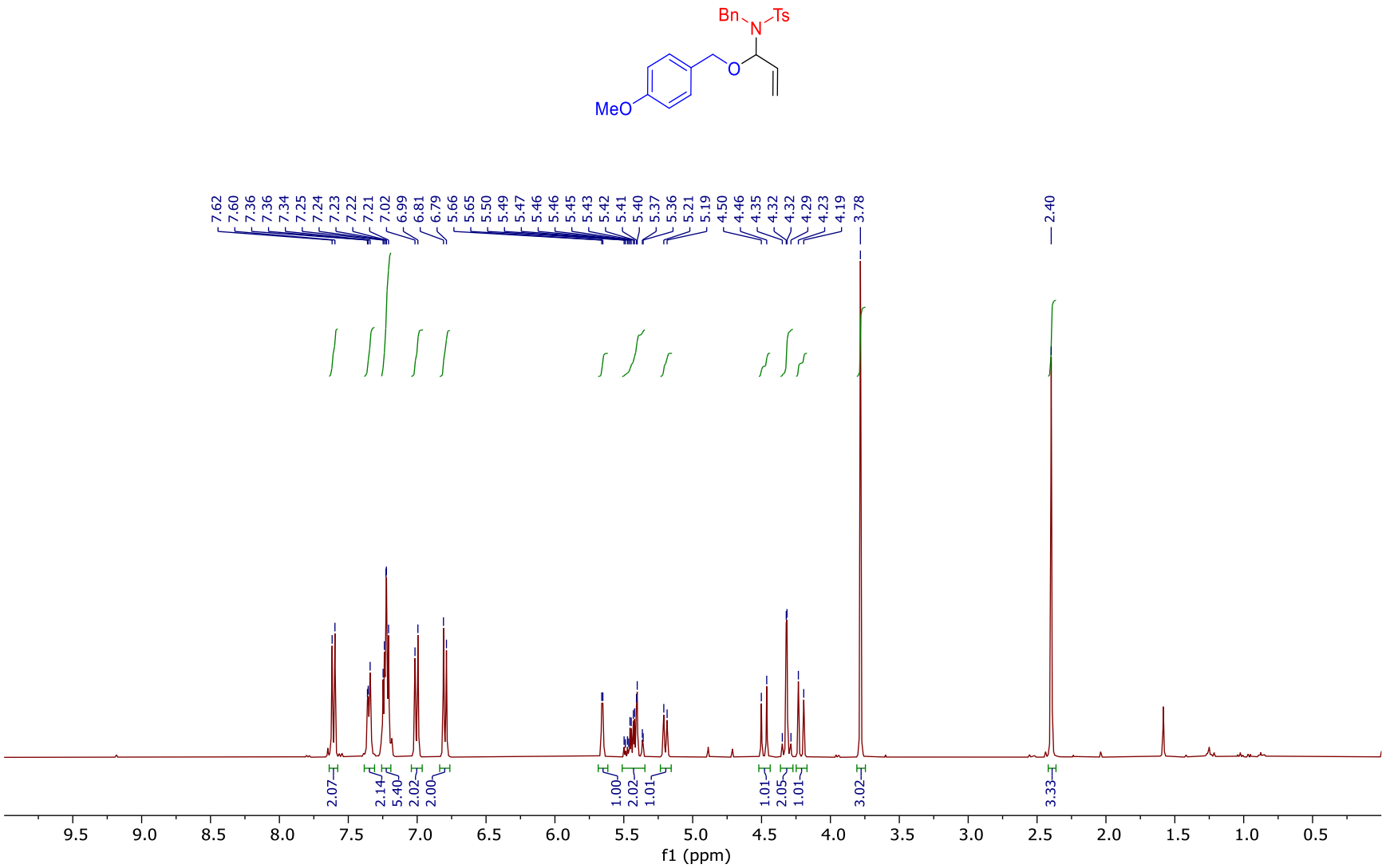
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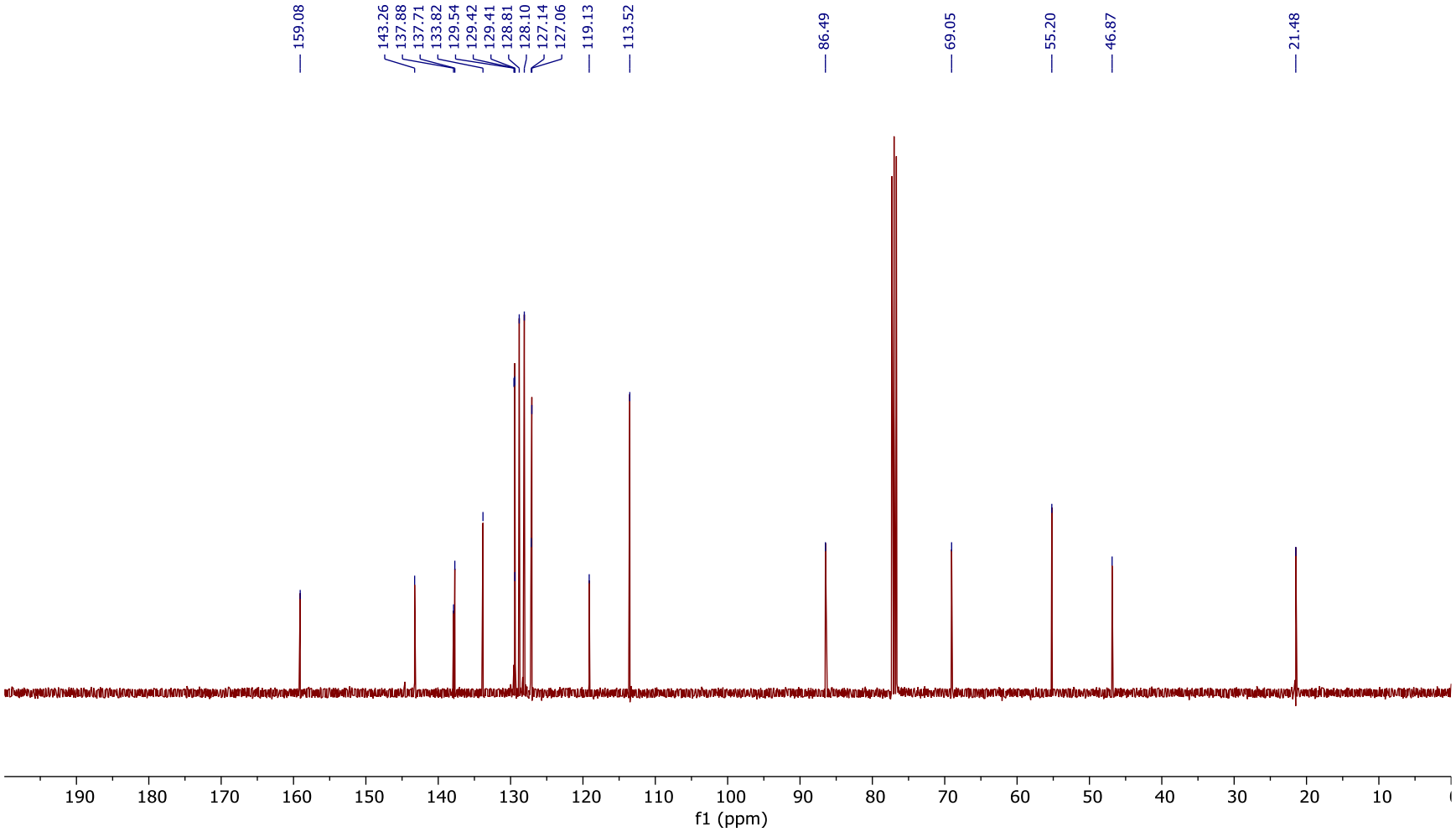
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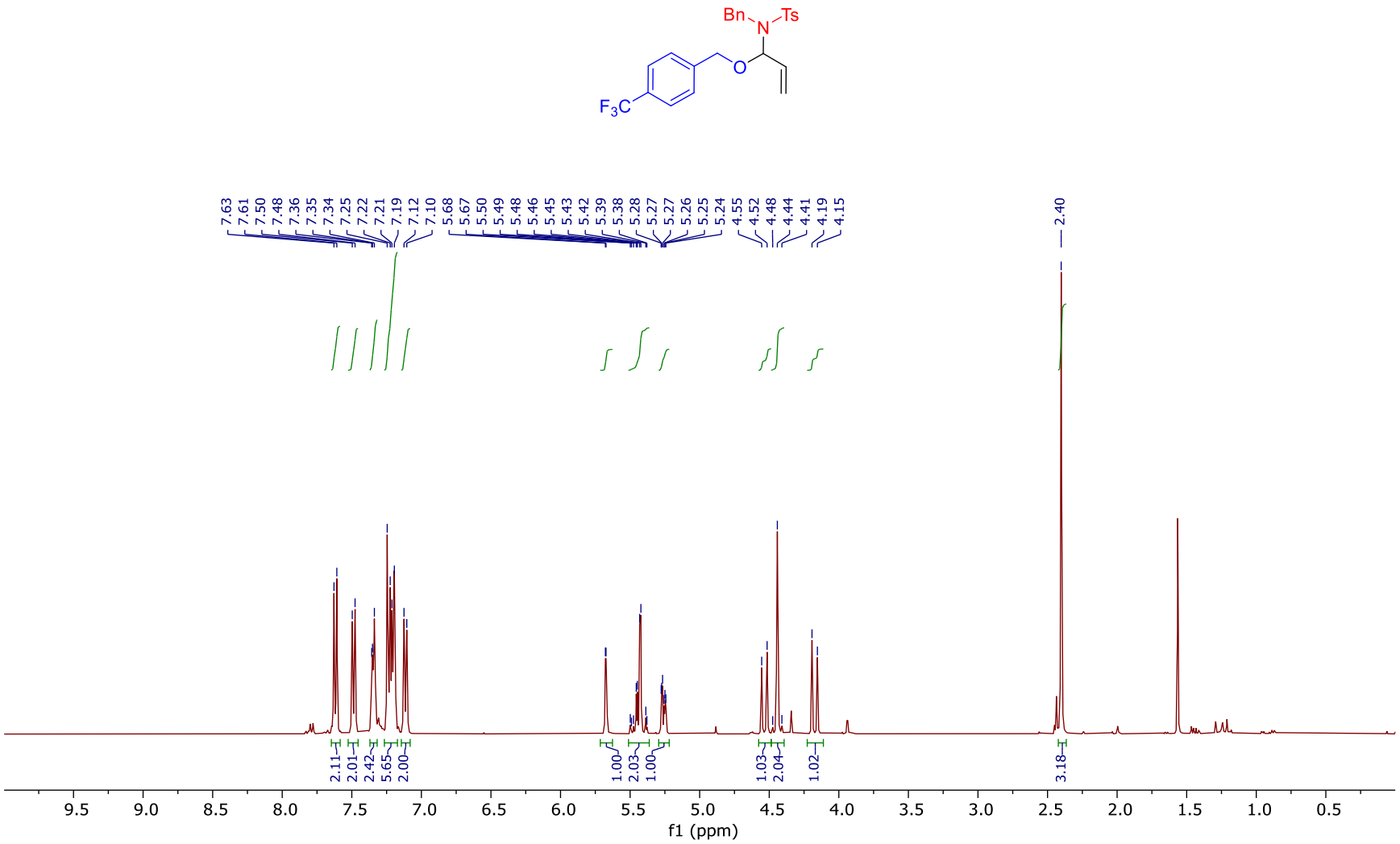
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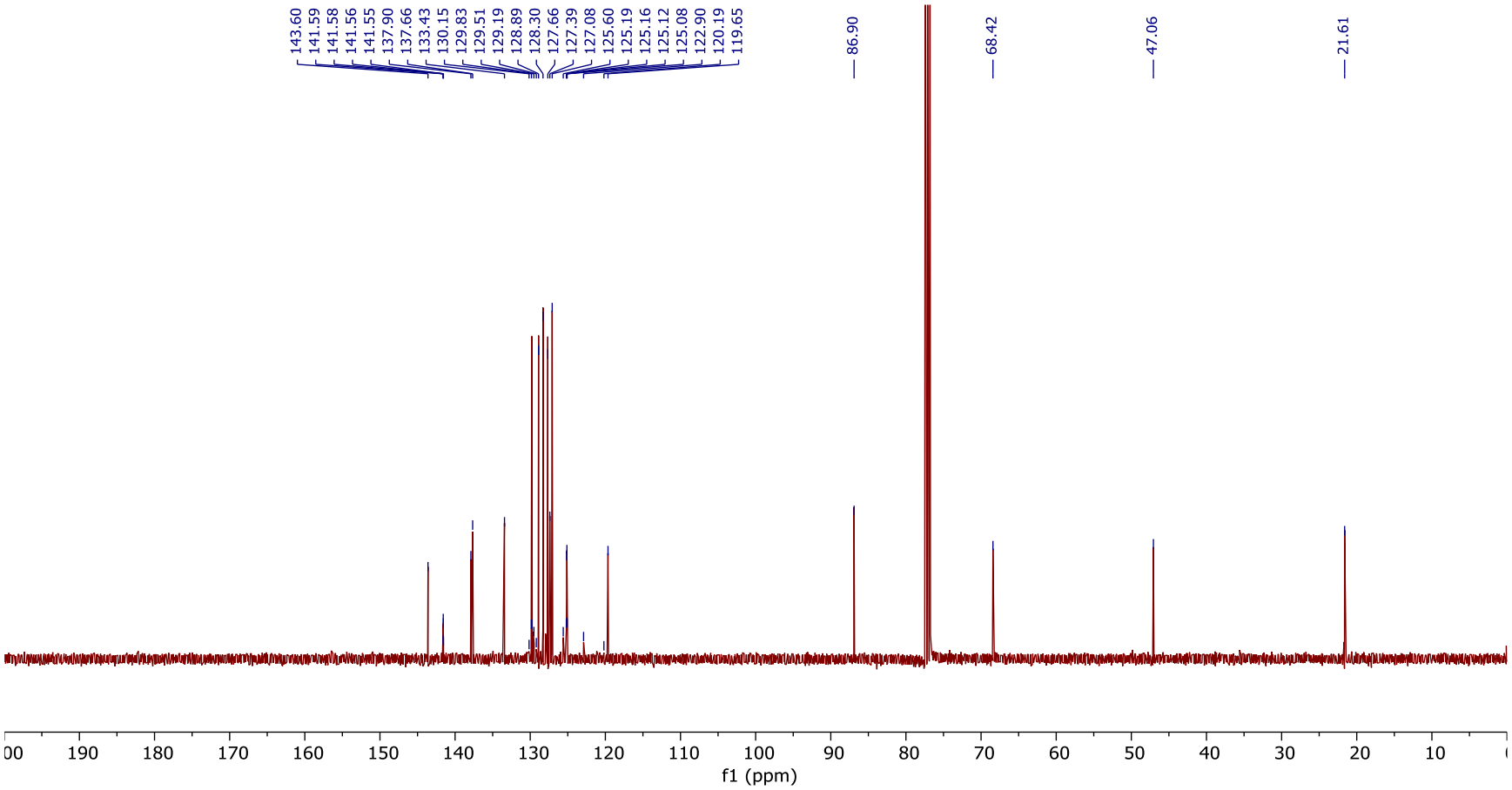
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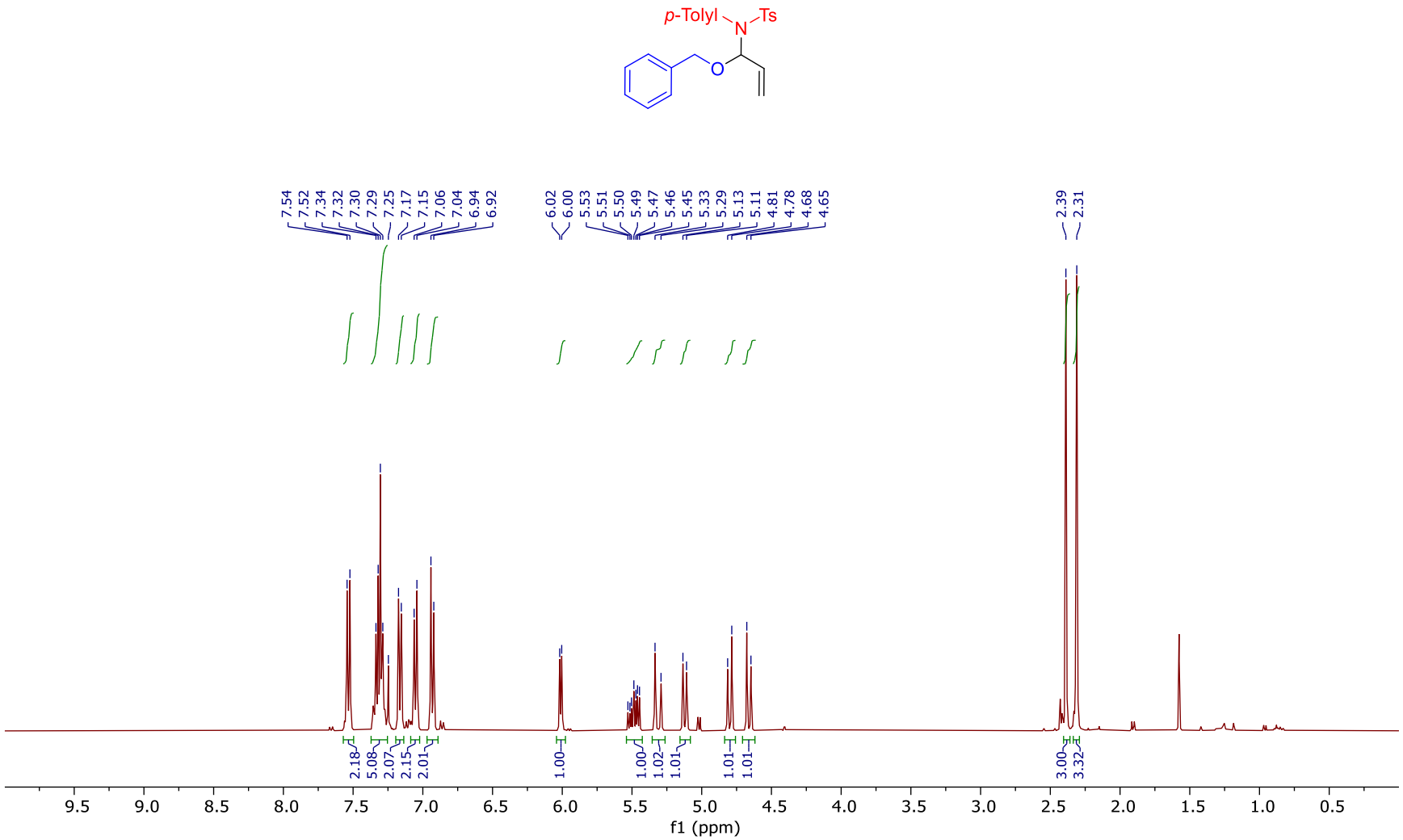
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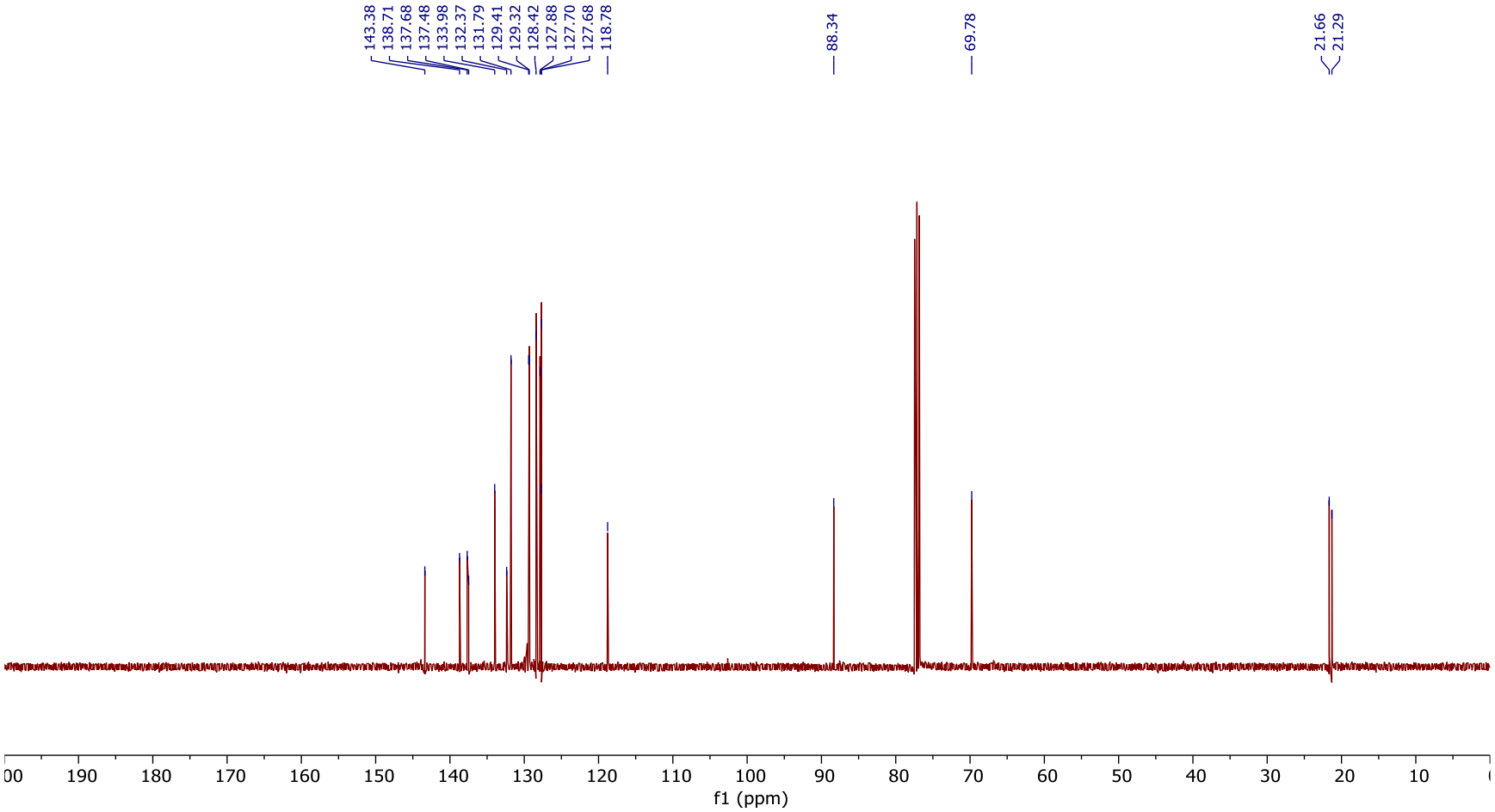
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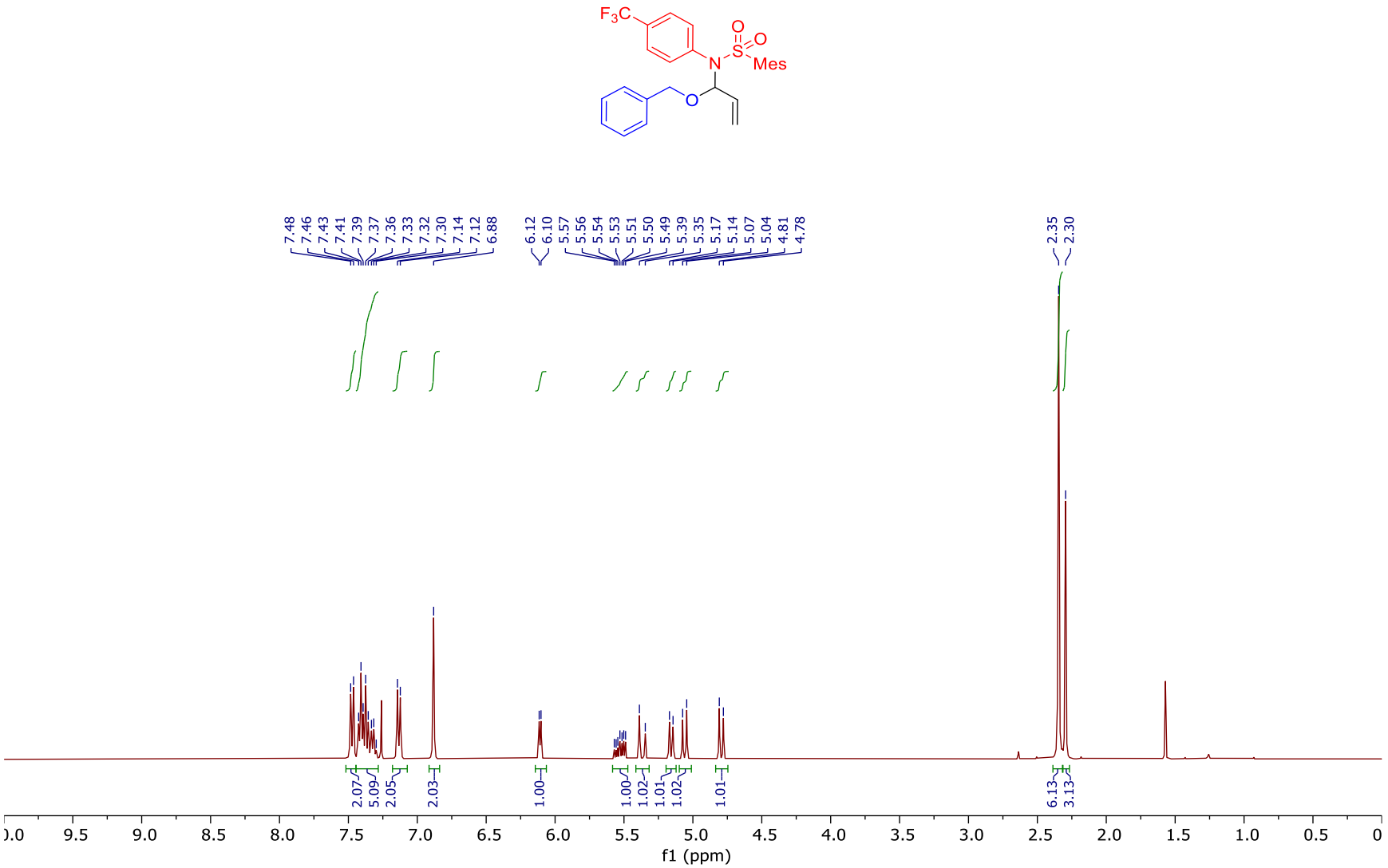
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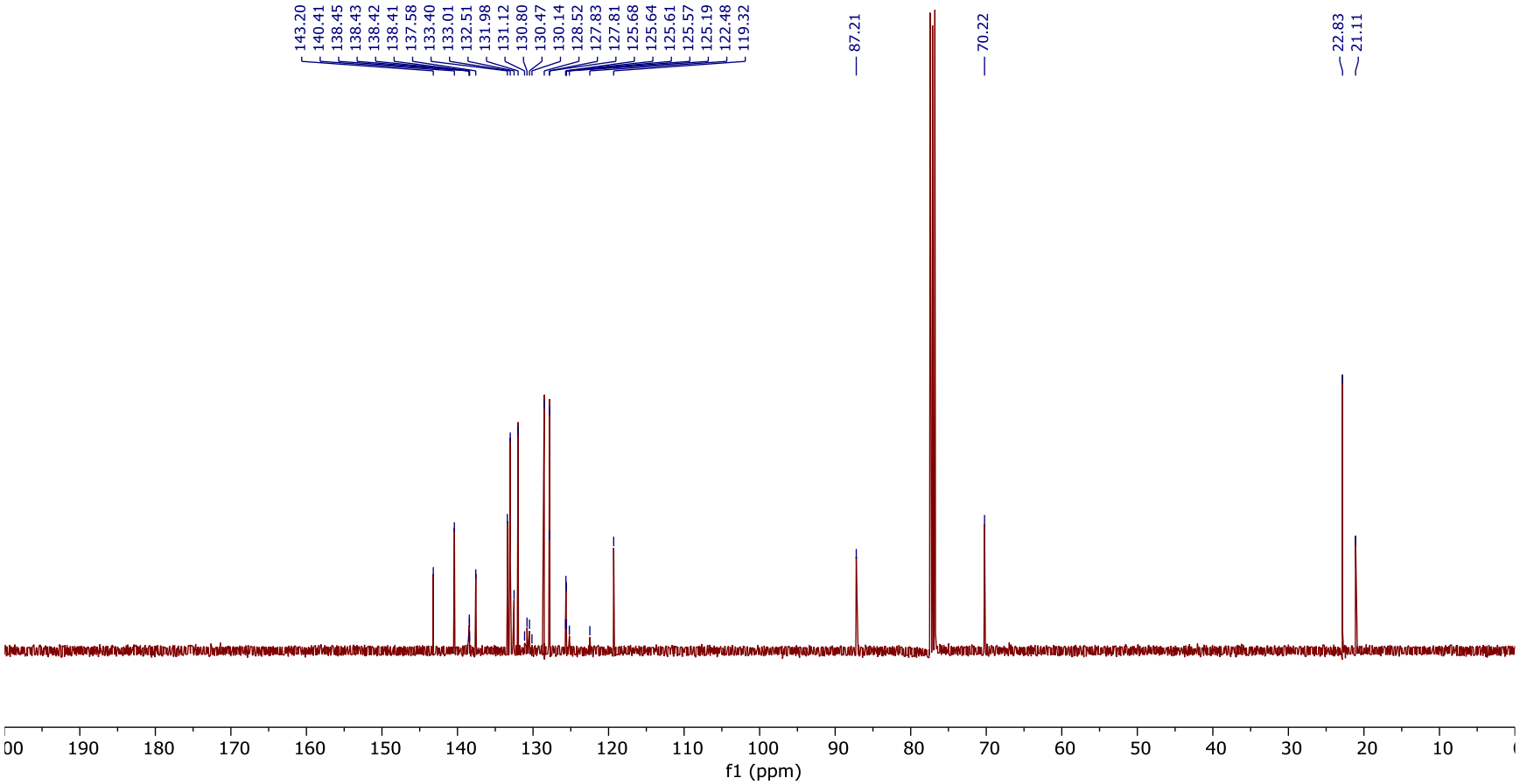
3.13
f1 (ppm)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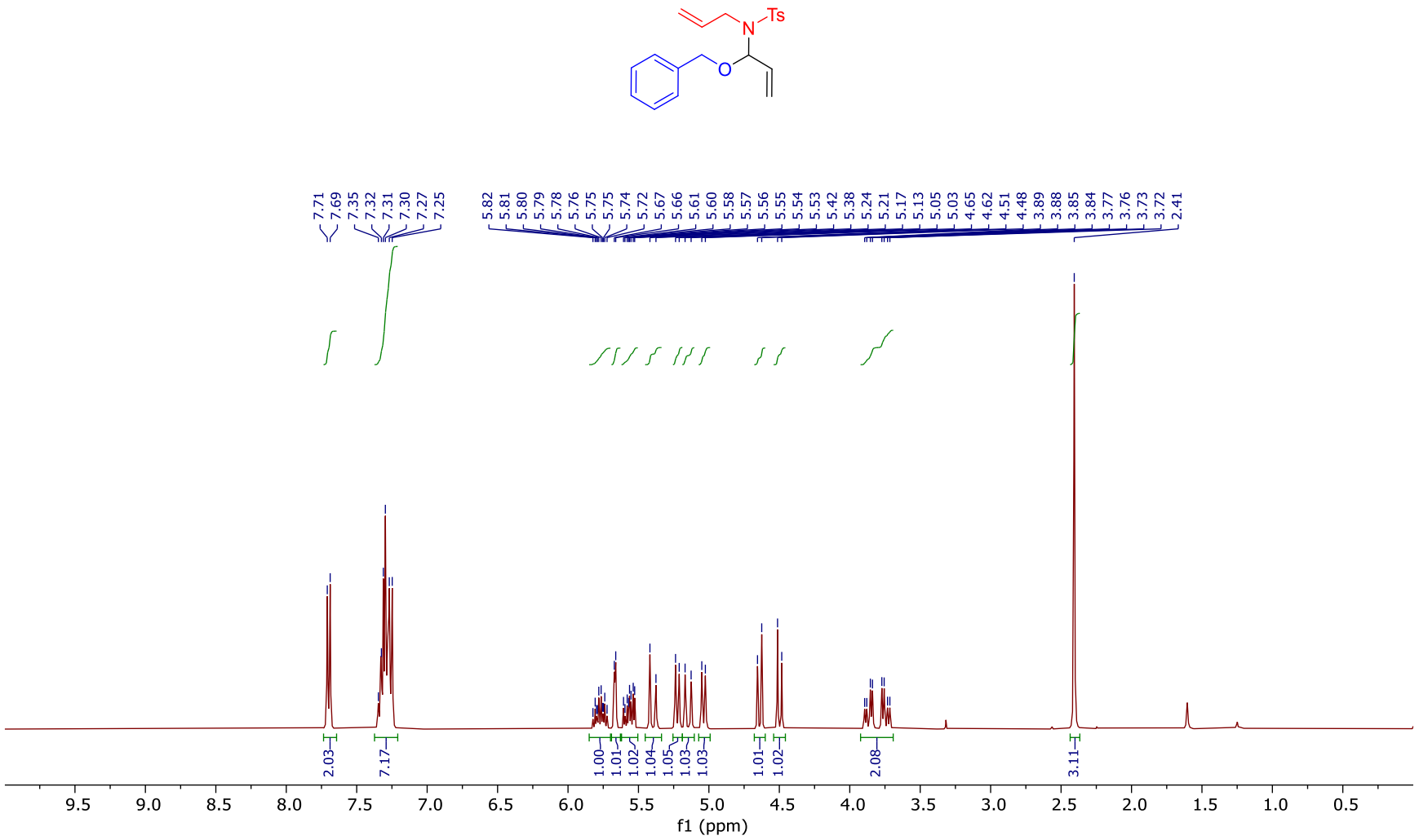
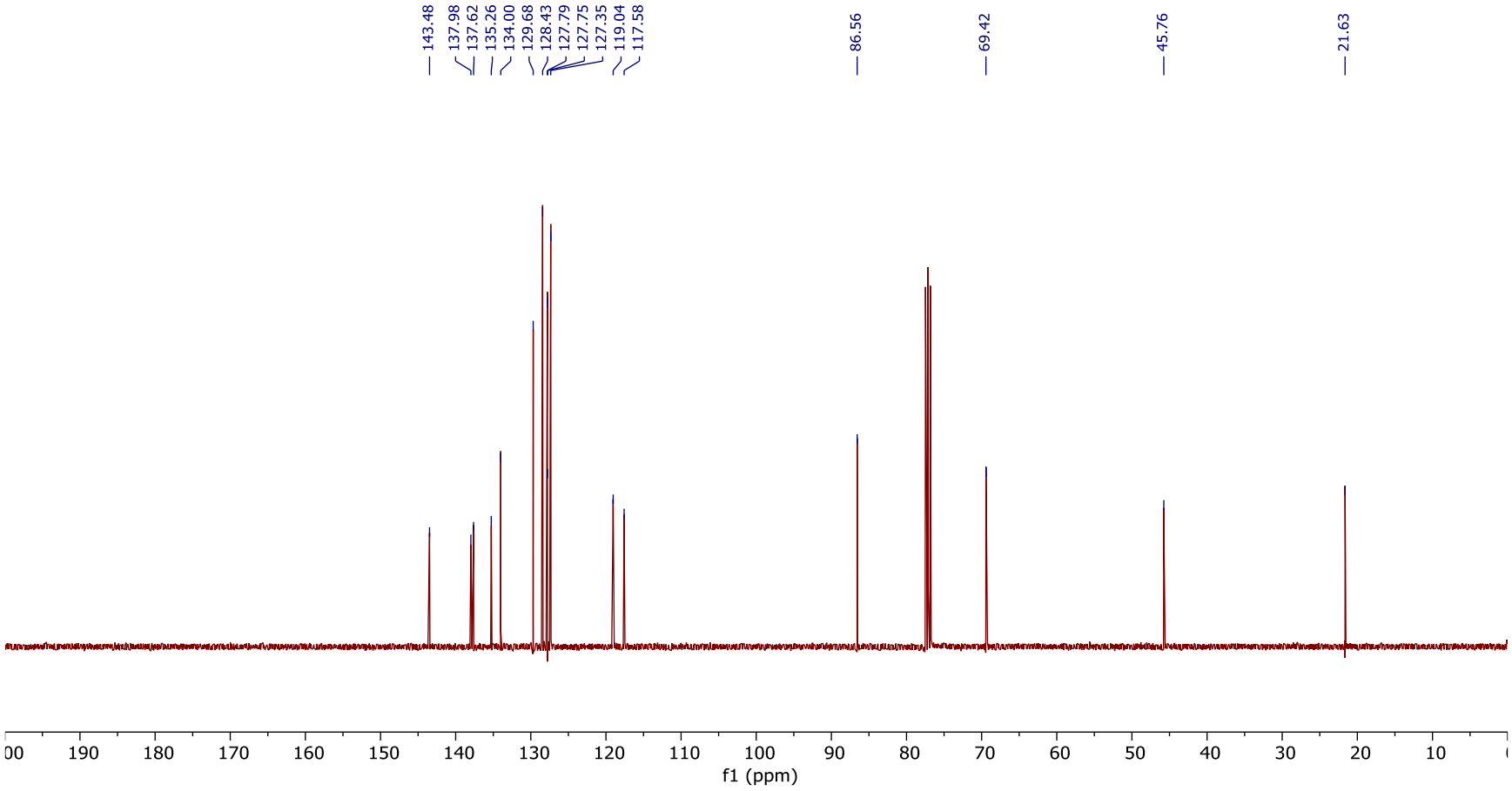
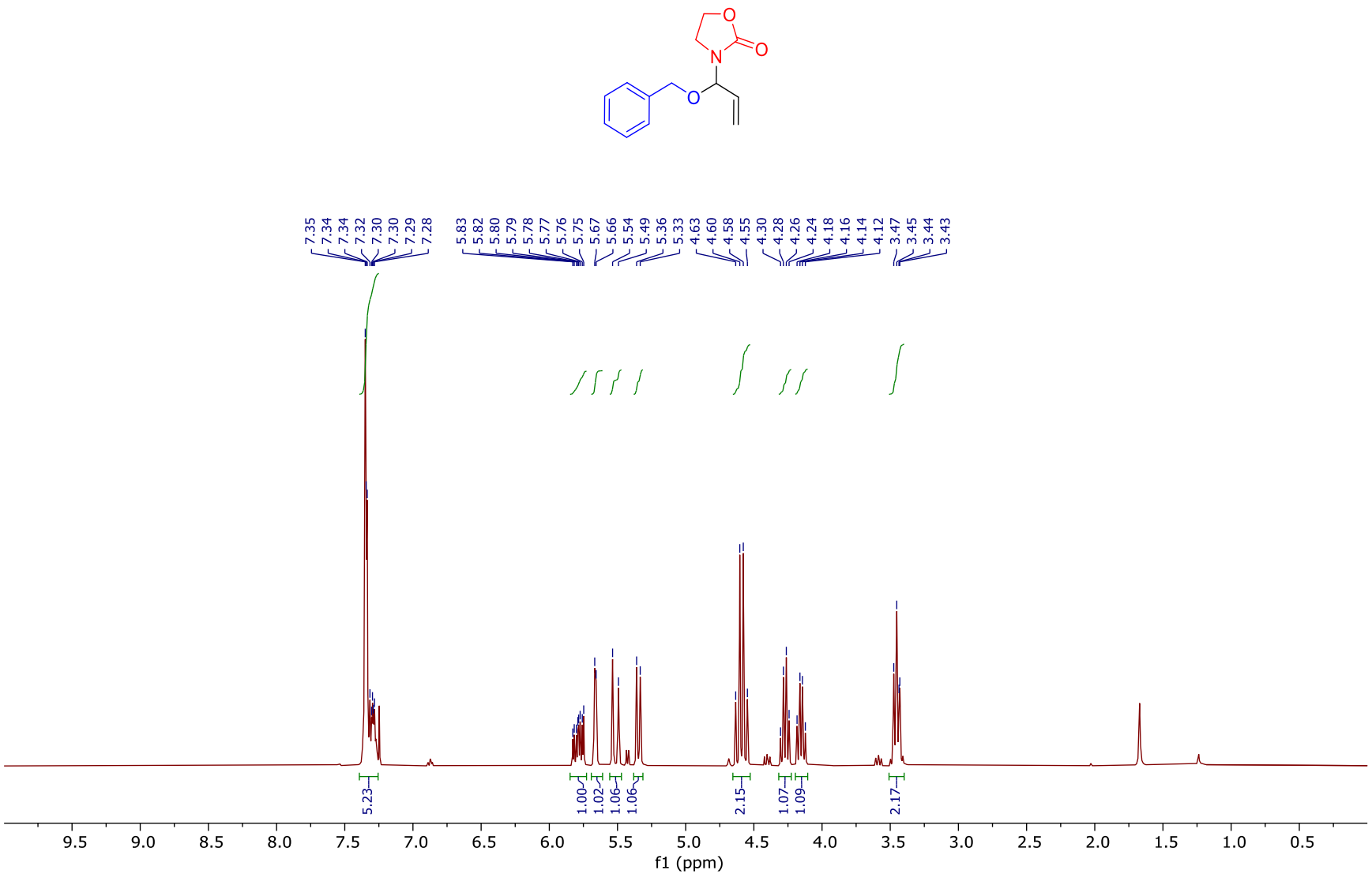
140.41
138.45
138.43
138.42
138.41
137.58
133.40
133.01
132.51
131.98
131.12
130.80
130.47
130.14
128.52
127.83
127.81
125.68
125.64
125.61
125.57
125.19
122.48
119.32
87.21
70.22
22.83
21.11
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

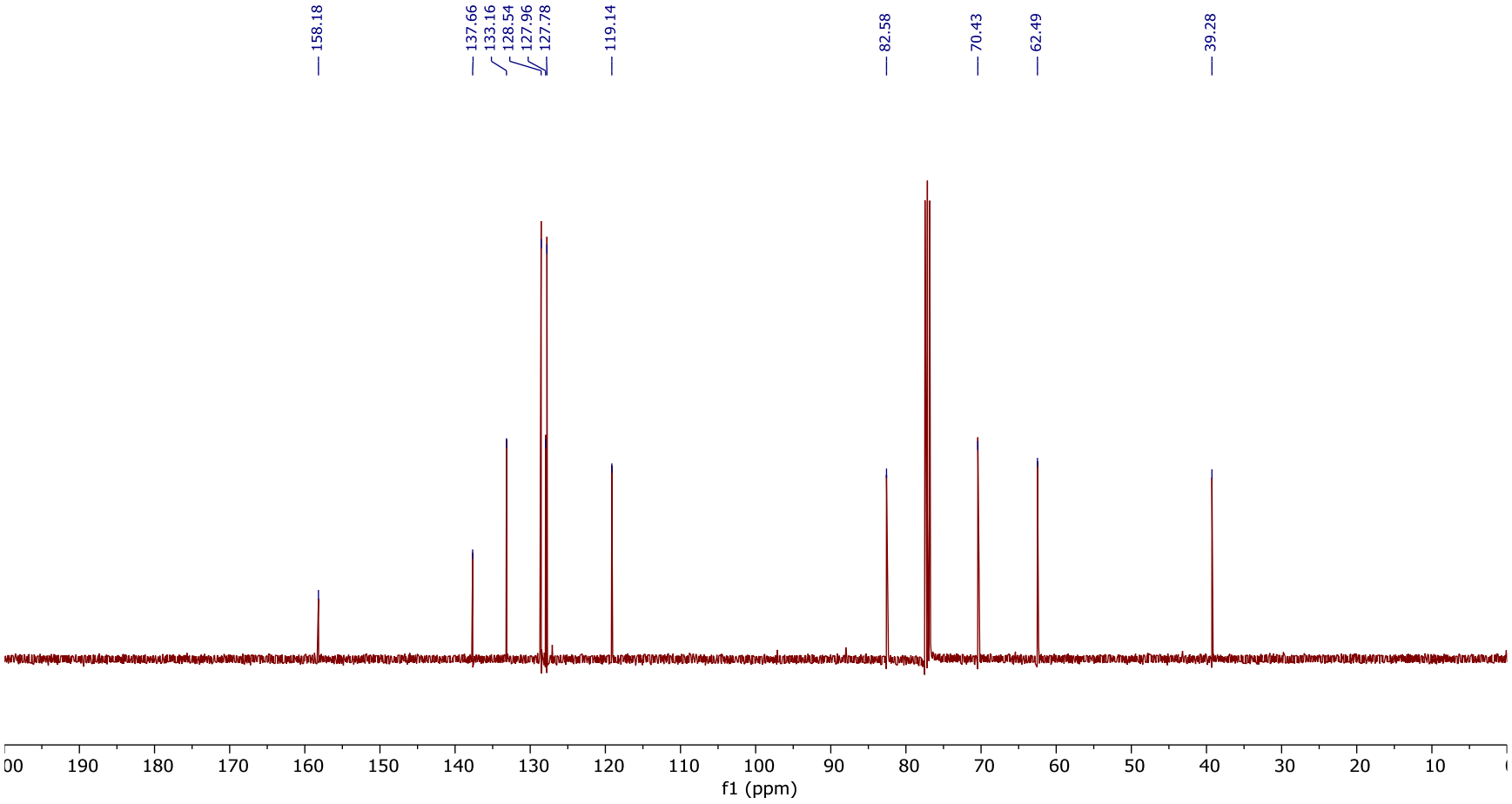
3de


Ts
N
O
7.71
7.69
7.35
7.32
7.31
7.30
7.27
7.25
5.82
5.81
5.80
5.79
5.78
5.76
5.75
5.75
5.74
5.72
5.67
5.66
5.61
5.60
5.58
5.57
5.56
5.55
5.54
5.53
5.42
5.38
5.24
5.21
5.17
5.13
5.05
5.03
4.65
4.62
4.51
4.48
3.89
3.88
3.85
3.84
3.77
3.76
3.73
3.72
2.41
2.03
7.17
1.00
1.01
1.02
1.04
1.05
1.03
1.03
1.01
1.02
2.08
3.11
9.5
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
f1 (ppm)

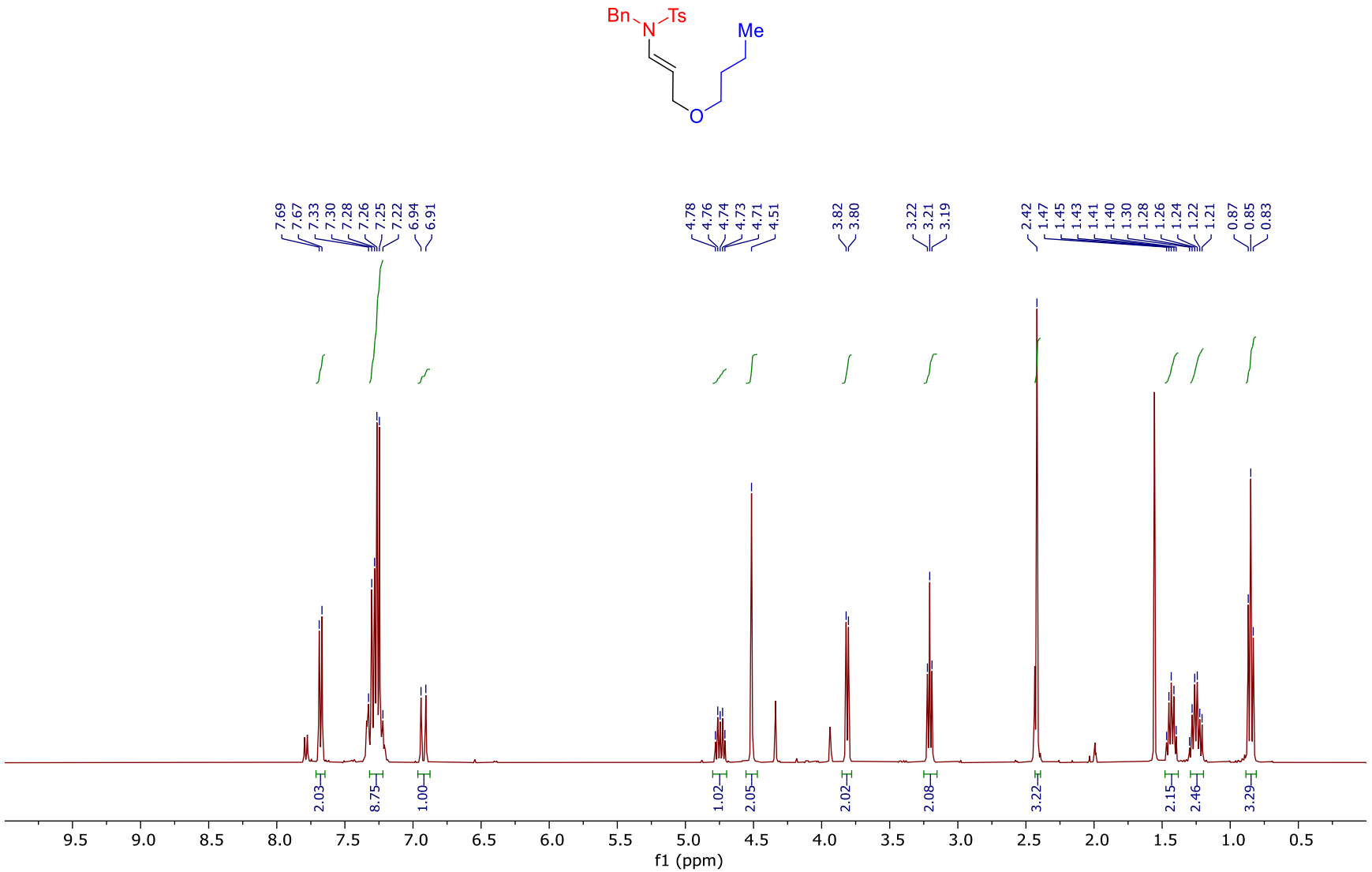

143.48
137.98
137.62
135.26
134.00
129.68
128.43
127.79
127.75
127.35
119.04
117.58
86.56
69.42
45.76
21.63
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

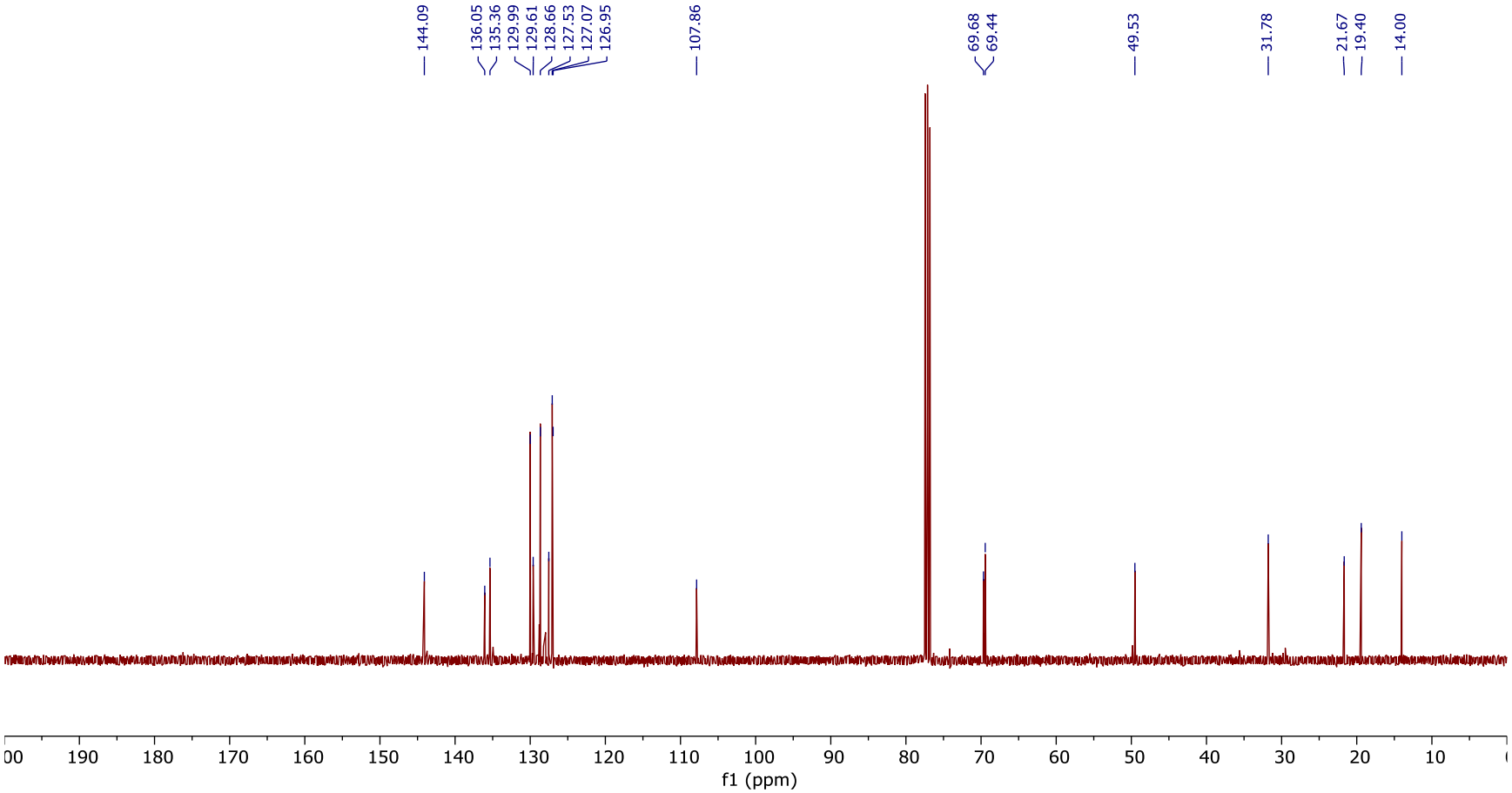
3ee


7.35
7.34
7.34
7.32
7.30
7.30
7.29
7.28
5.83
5.82
5.80
5.79
5.78
5.77
5.76
5.75
5.67
5.66
5.54
5.49
5.36
5.33
4.63
4.60
4.58
4.55
4.30
4.28
4.26
4.24
4.18
4.16
4.14
4.12
3.47
3.45
3.44
3.43
5.23
1.00
1.02
1.06
1.06
2.15
1.07
1.09
2.17
9.5
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
f1 (ppm)

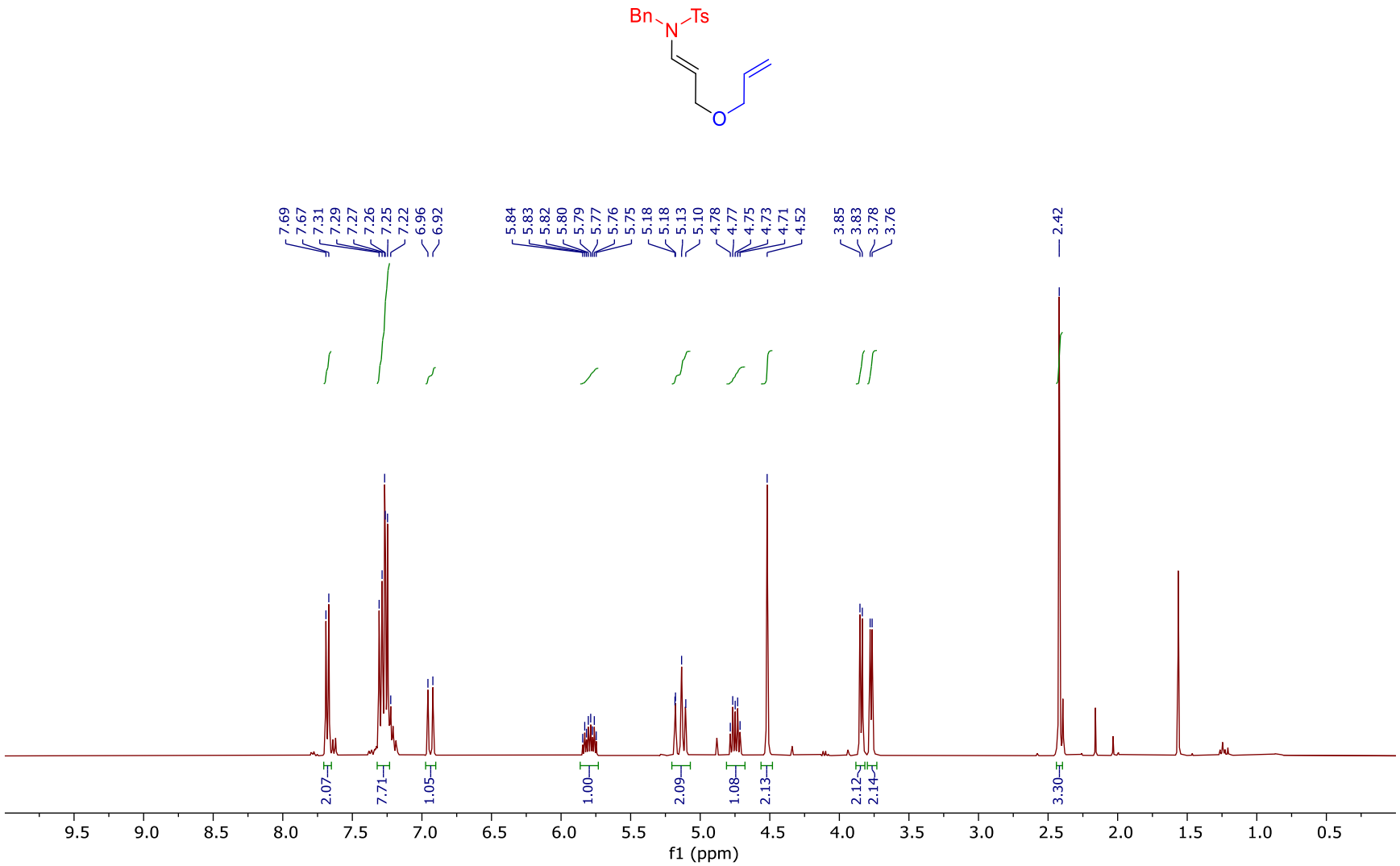

158.18
137.66
133.16
128.54
127.96
127.78
119.14
82.58
70.43
62.49
39.28
f1 (ppm)

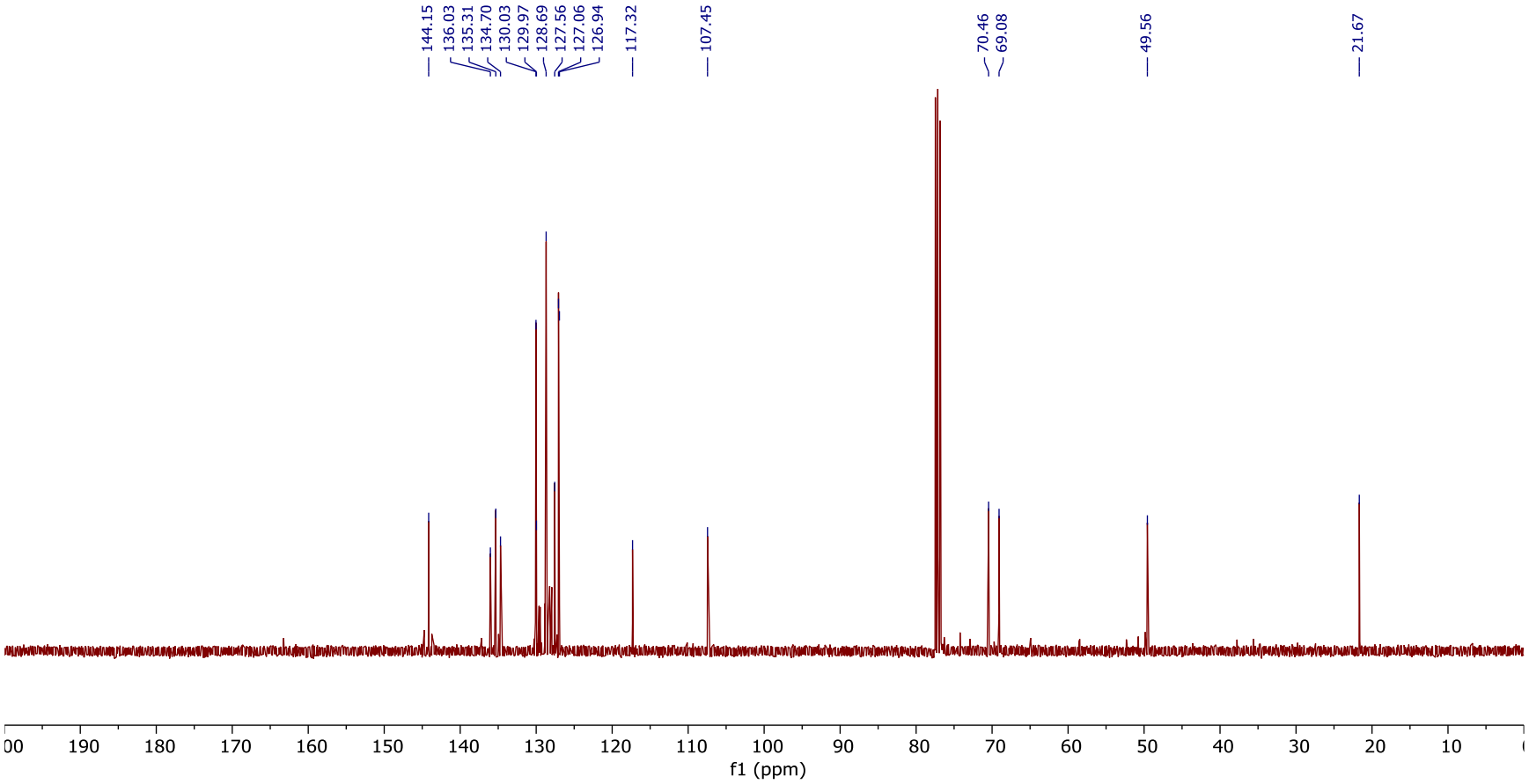
4aa


Bn
N
Ts
Me
O
7.69
7.67
7.33
7.30
7.28
7.26
7.25
7.22
6.94
6.91
4.78
4.76
4.74
4.73
4.71
4.51
3.82
3.80
3.22
3.21
3.19
2.42
1.47
1.45
1.43
1.41
1.40
1.30
1.28
1.26
1.24
1.22
1.21
0.87
0.85
0.83
2.03
8.75
1.00
1.02
2.05
2.02
2.08
3.22
2.15
2.46
3.29
f1 (ppm)

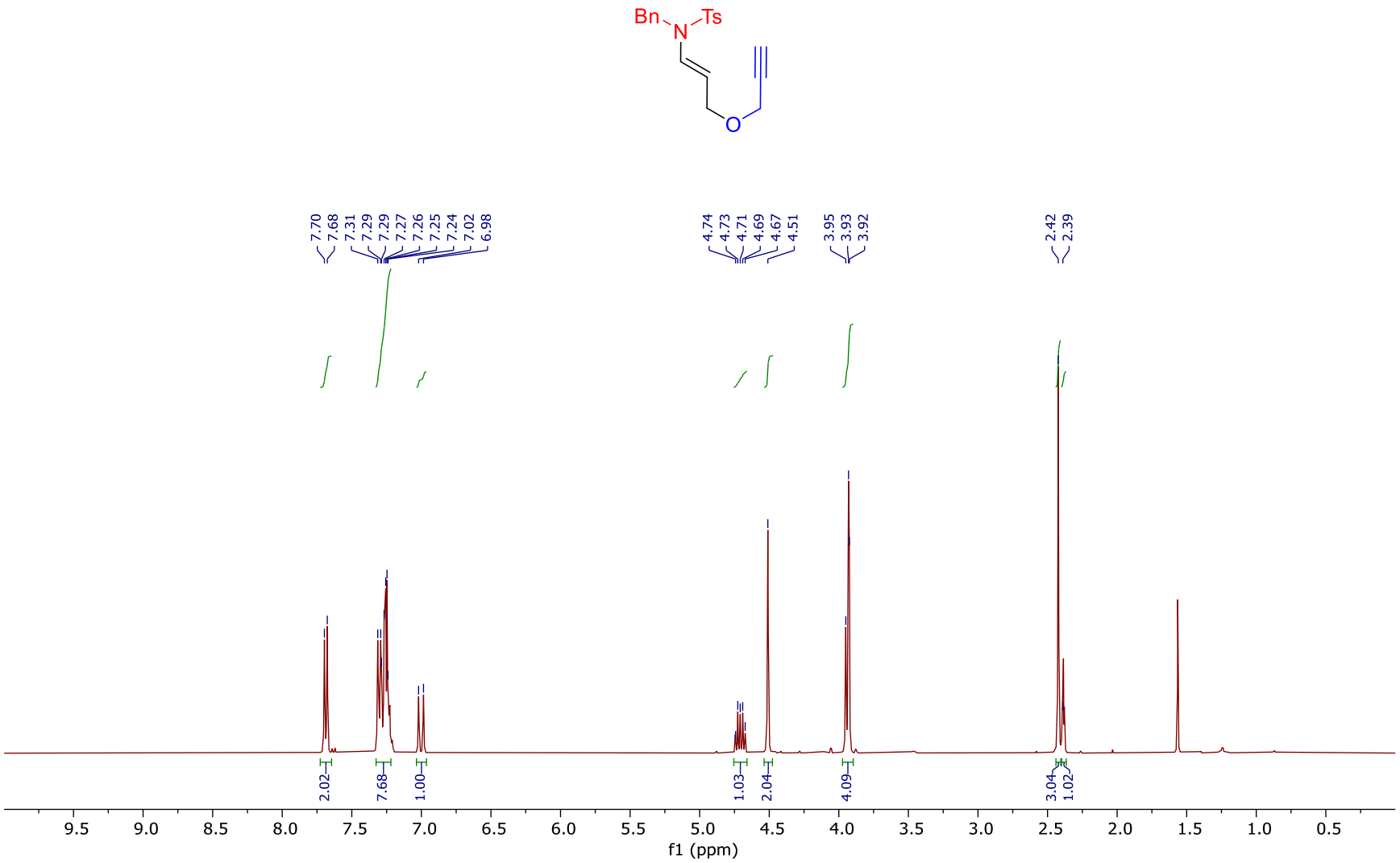

144.09
136.05
135.36
129.99
129.61
128.66
127.53
127.07
126.95
107.86
69.68
69.44
49.53
31.78
21.67
19.40
14.00
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

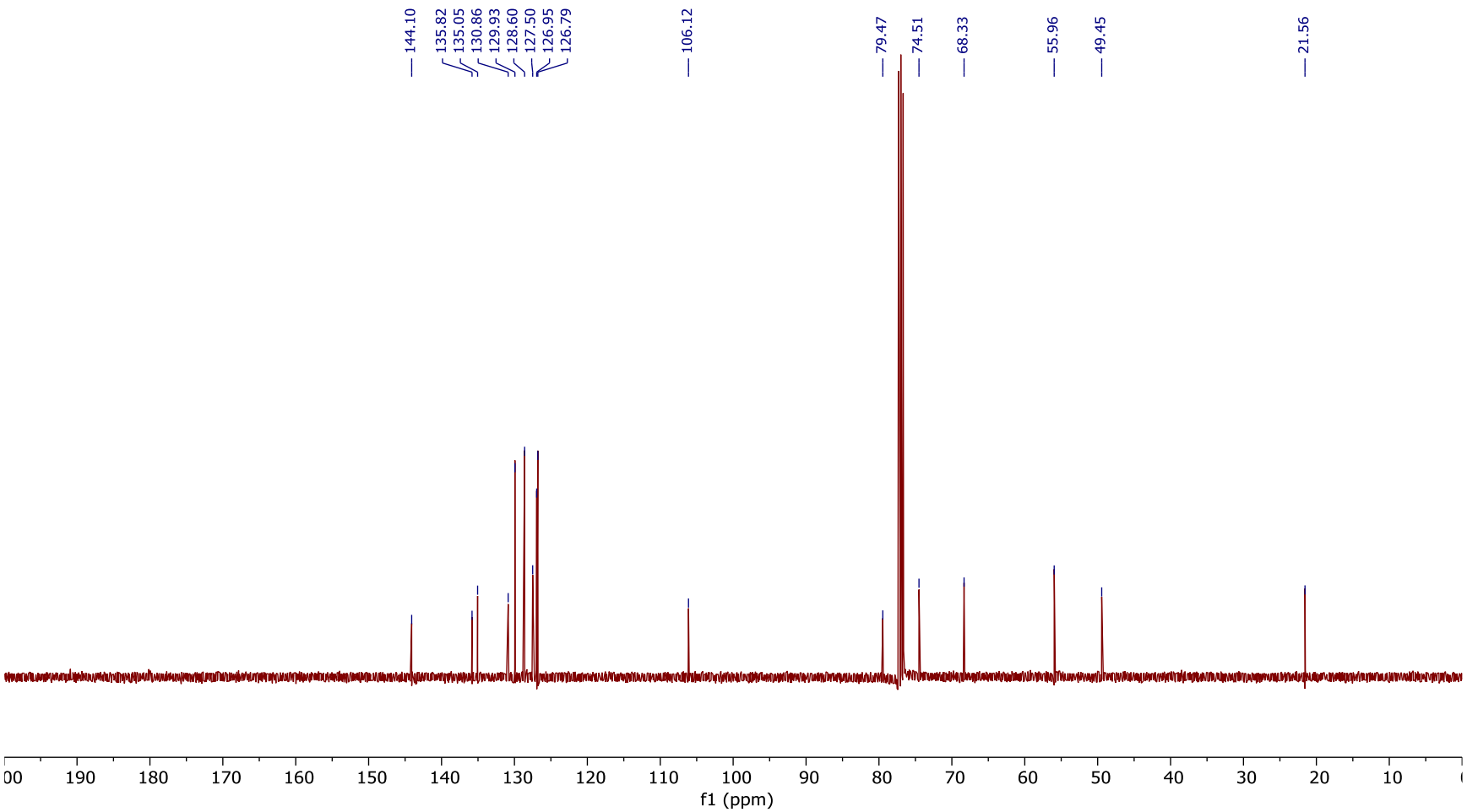
4ad


Bn
N
Ts
O
7.69
7.67
7.31
7.29
7.27
7.26
7.25
7.22
6.96
6.92
5.84
5.83
5.82
5.80
5.79
5.77
5.76
5.75
5.18
5.18
5.13
5.10
4.78
4.77
4.75
4.73
4.71
4.52
3.85
3.83
3.78
3.76
2.42
2.07
7.71
1.05
1.00
2.09
1.08
2.13
2.12
2.14
3.30
9.5
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
f1 (ppm)

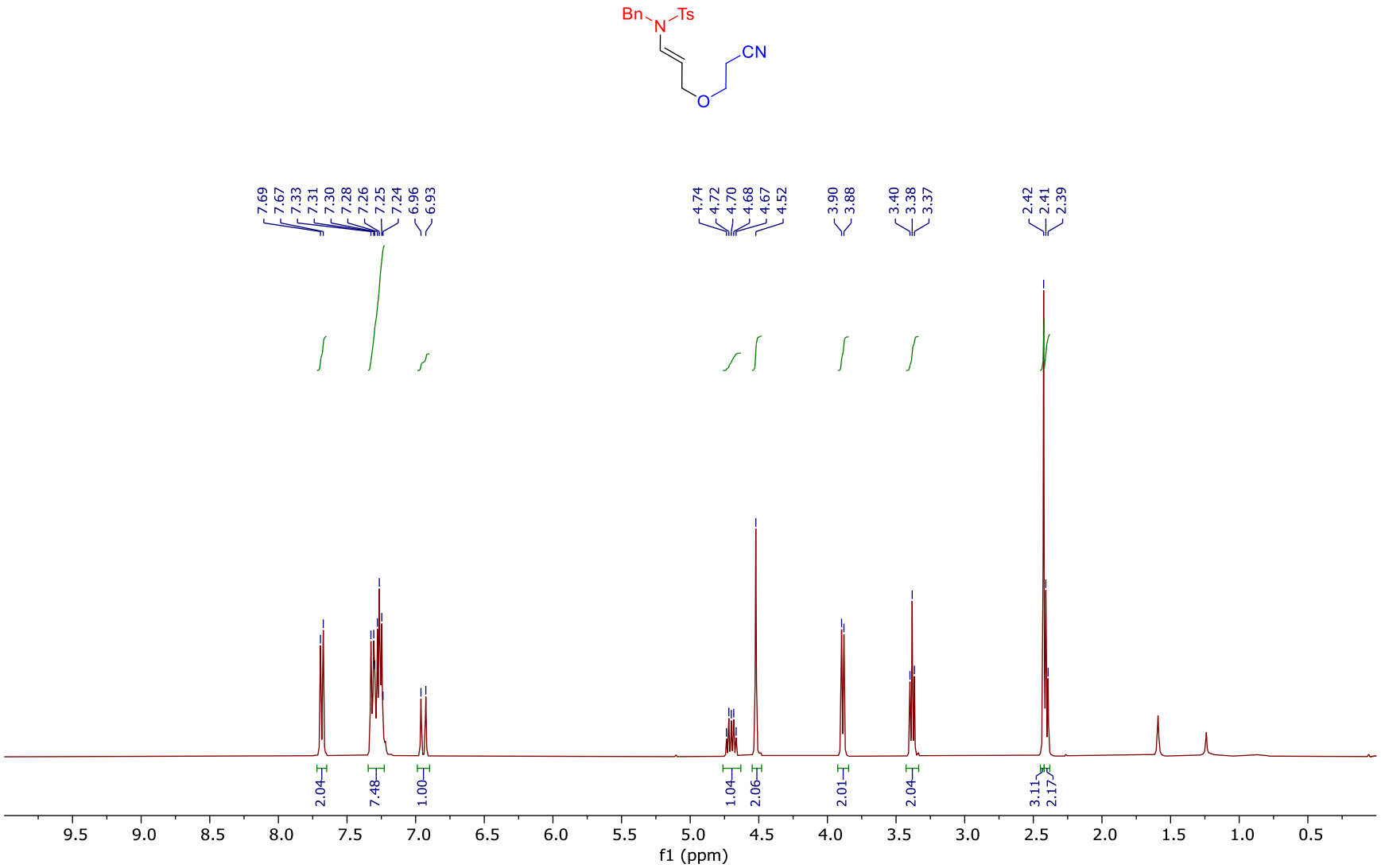

144.15
136.03
135.31
134.70
130.03
129.97
128.69
127.56
127.06
126.94
117.32
107.45
70.46
69.08
49.56
21.67
f1 (ppm)

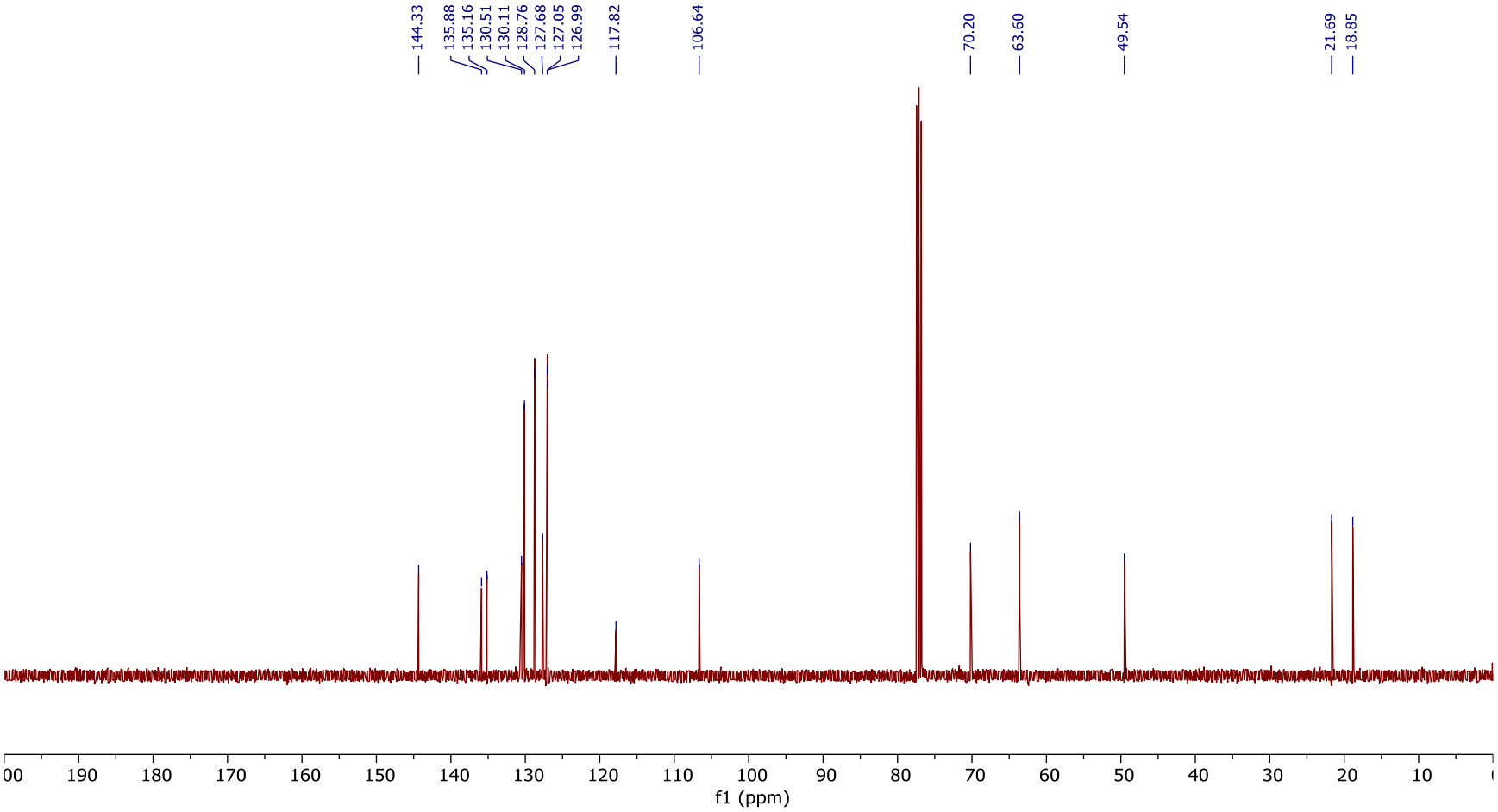
4ac


Bn
N
Ts
O
7.70
7.68
7.31
7.29
7.29
7.27
7.26
7.25
7.24
7.02
6.98
4.74
4.73
4.71
4.69
4.67
4.51
3.95
3.93
3.92
2.42
2.39
2.02
7.68
1.00
1.03
2.04
4.09
3.04
1.02
9.5
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
f1 (ppm)

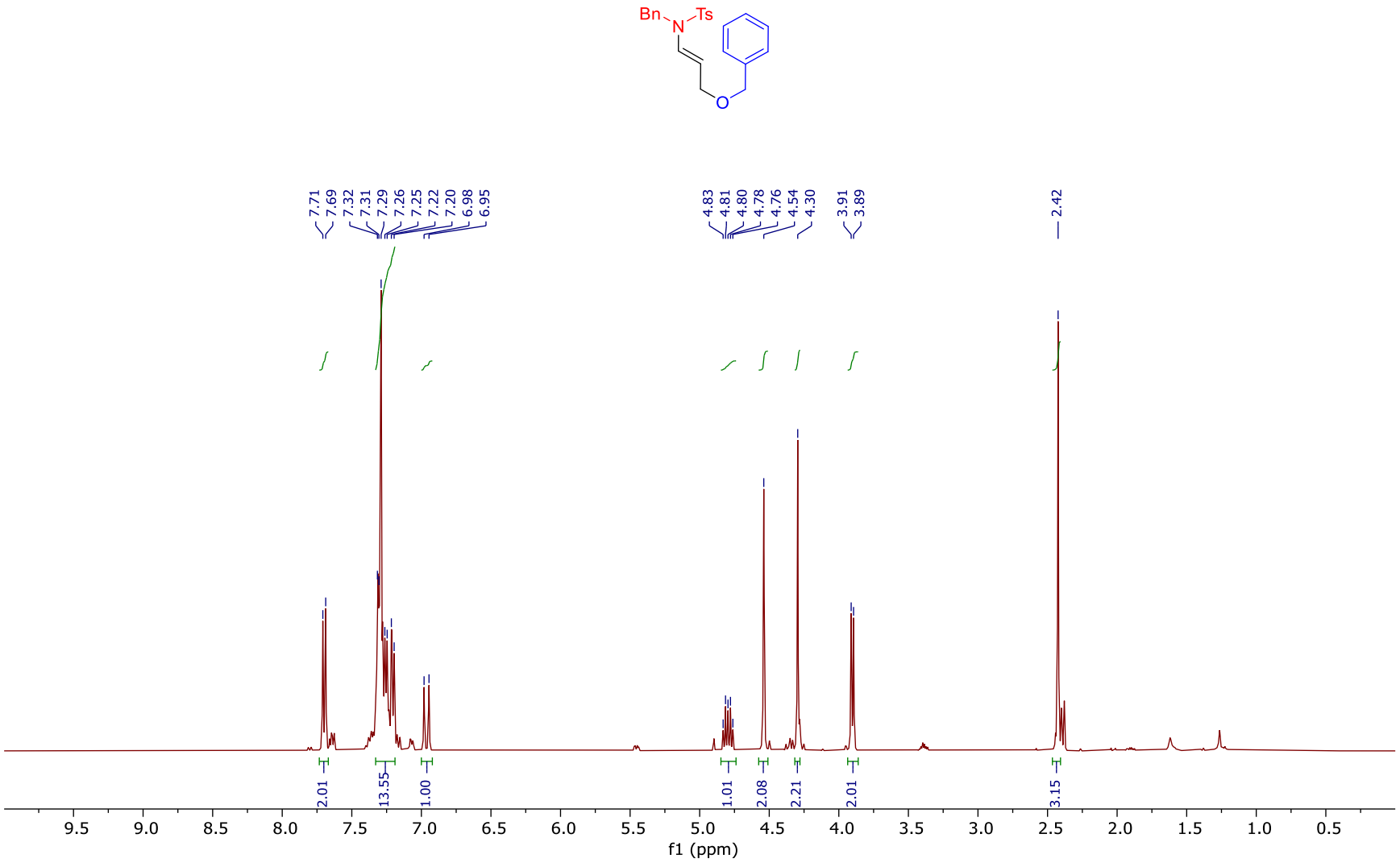

144.10
135.82
135.05
130.86
129.93
128.60
127.50
126.95
126.79
106.12
79.47
74.51
68.33
55.96
49.45
21.56
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

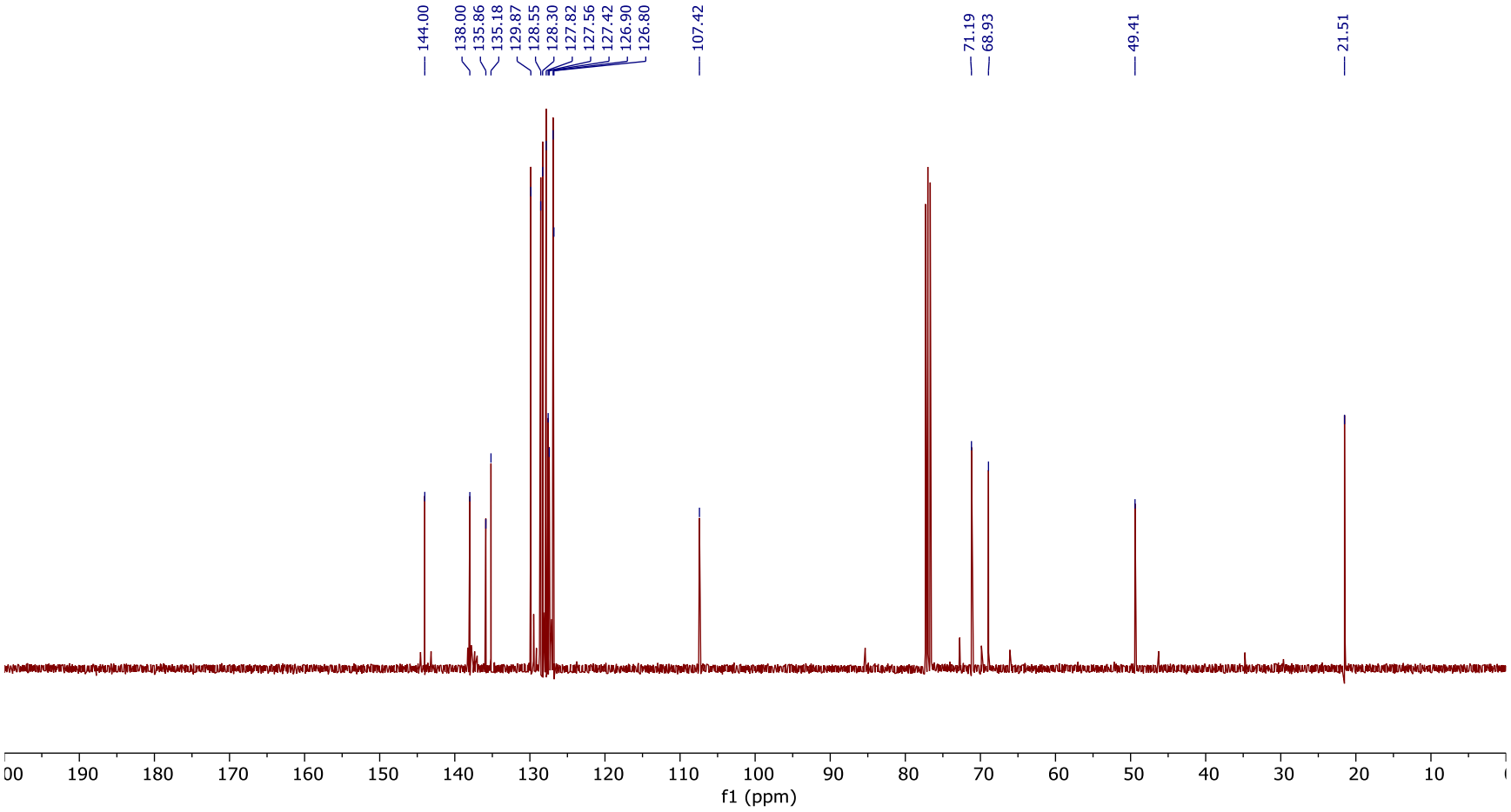
4ab


Bn
N
Ts
CN
O
7.69
7.67
7.33
7.31
7.30
7.28
7.26
7.25
7.24
6.96
6.93
4.74
4.72
4.70
4.68
4.67
4.52
3.90
3.88
3.40
3.38
3.37
2.42
2.41
2.39
2.04
7.48
1.00
1.04
2.06
2.01
2.04
3.11
2.17
9.5
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
f1 (ppm)

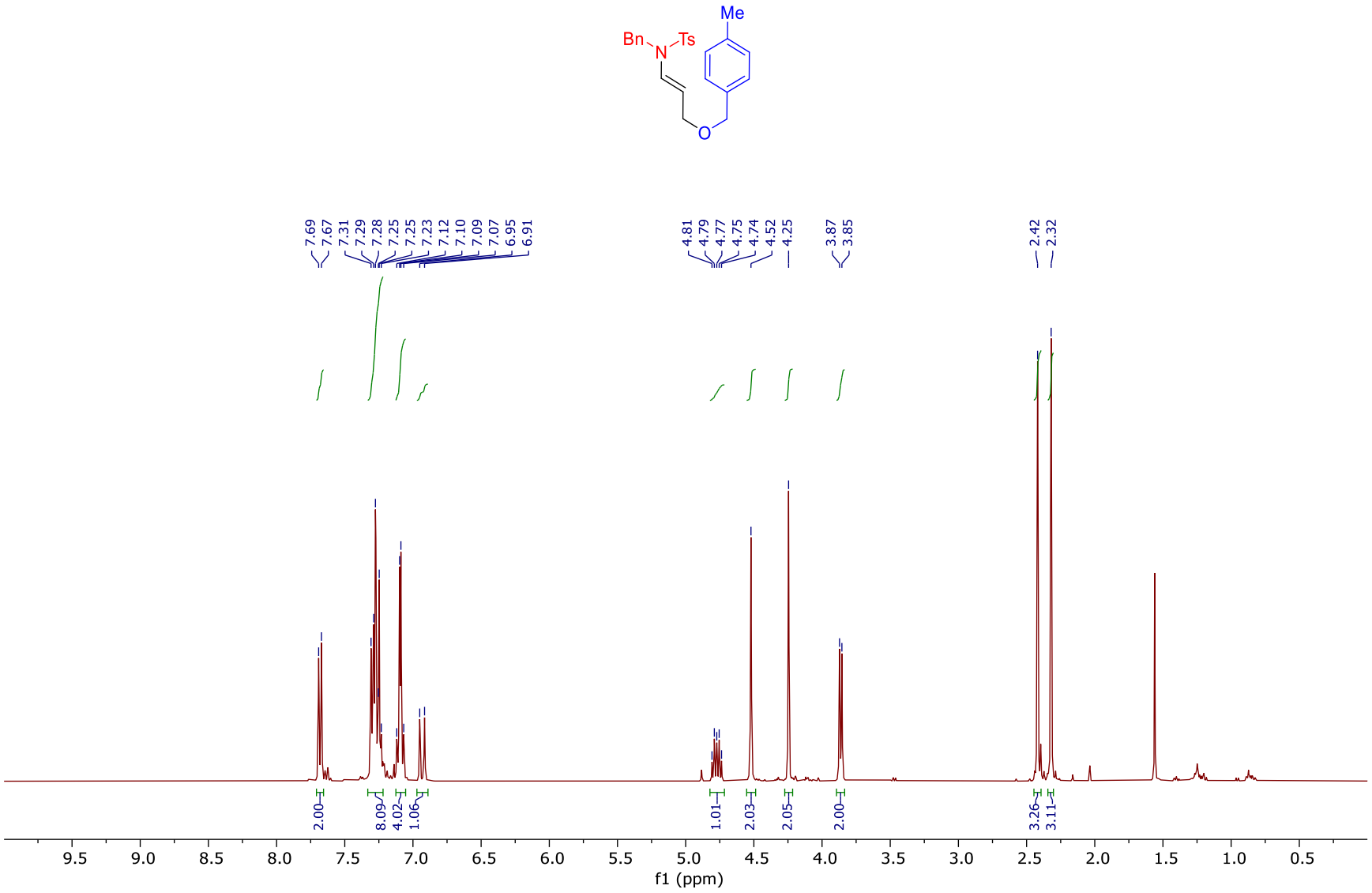

144.33
135.88
135.16
130.51
130.11
128.76
127.68
127.05
126.99
117.82
106.64
70.20
63.60
49.54
21.69
18.85
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

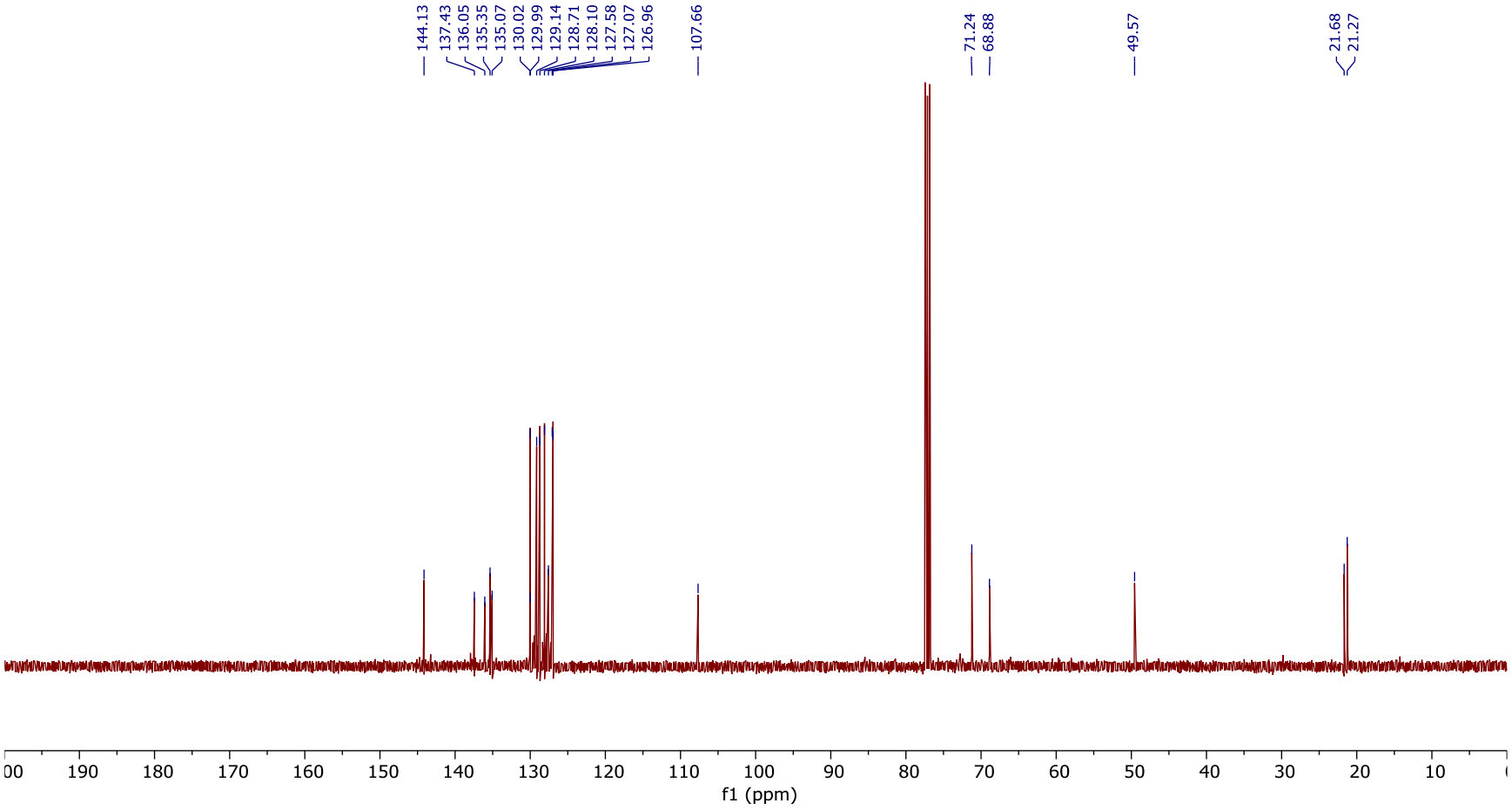
4ae


Bn
N
Ts
O
7.71
7.69
7.32
7.31
7.29
7.26
7.25
7.22
7.20
6.98
6.95
4.83
4.81
4.80
4.78
4.76
4.54
4.30
3.91
3.89
2.42
2.01
13.55
1.00
1.01
2.08
2.21
2.01
3.15
9.5
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
f1 (ppm)

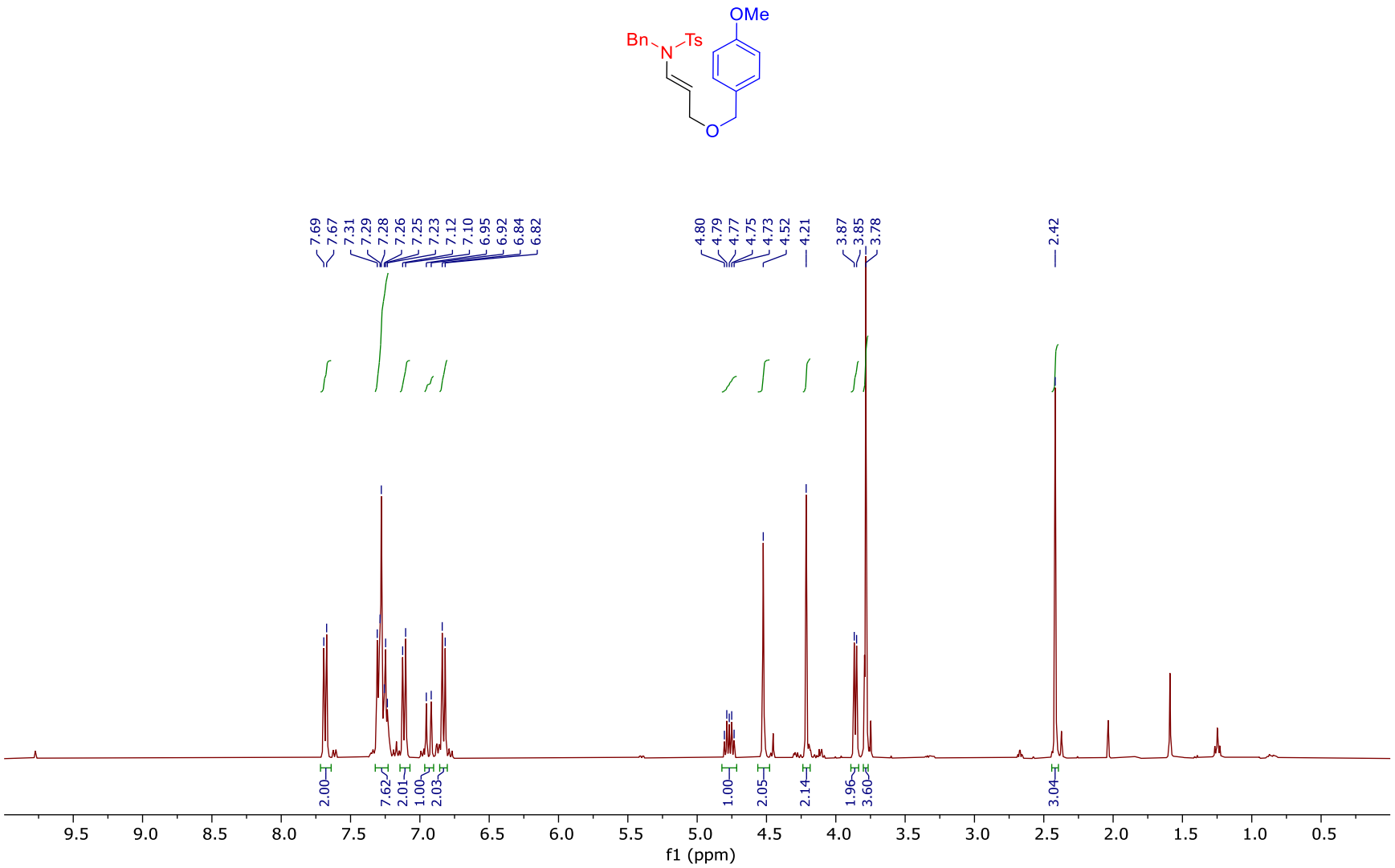

144.00
138.00
135.86
135.18
129.87
128.55
128.30
127.82
127.56
127.42
126.90
126.80
107.42
71.19
68.93
49.41
21.51
f1 (ppm)

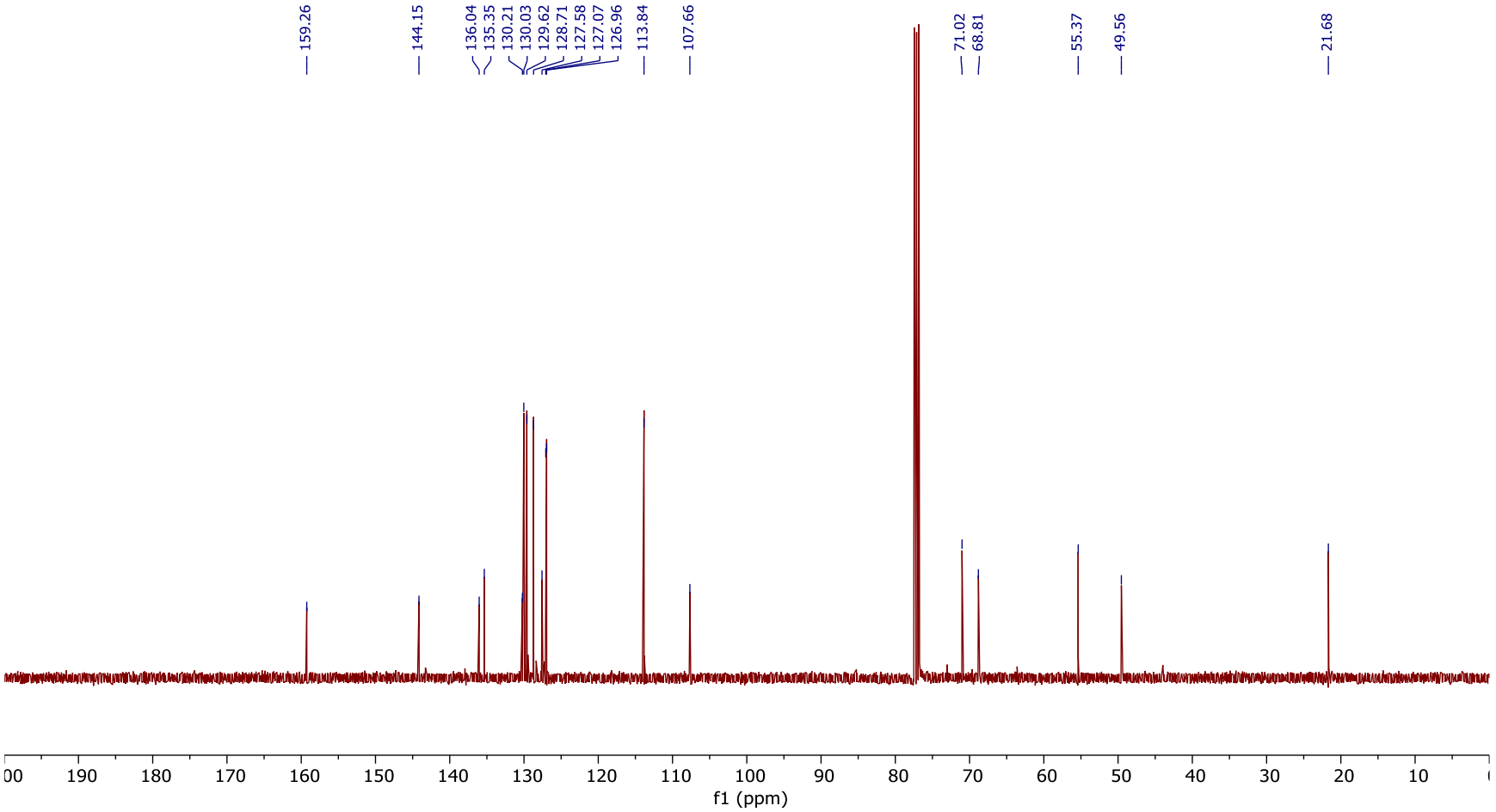
4af


Me
Bn
N
Ts
O
7.69
7.67
7.31
7.29
7.28
7.25
7.25
7.23
7.12
7.10
7.09
7.07
6.95
6.91
4.81
4.79
4.77
4.75
4.74
4.52
4.25
3.87
3.85
2.42
2.32
2.00
8.09
4.02
1.06
1.01
2.03
2.05
2.00
3.26
3.11
9.5
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
f1 (ppm)

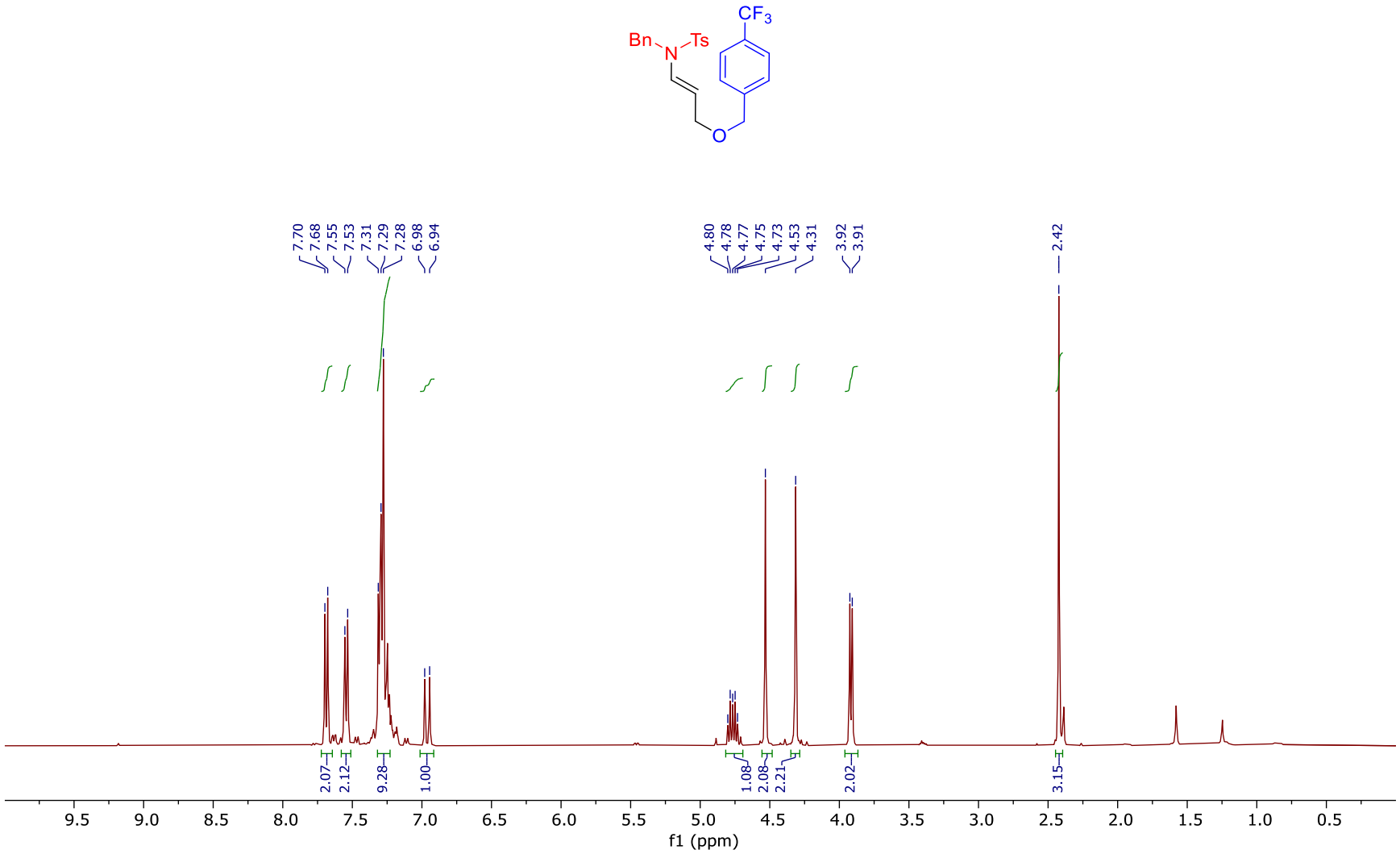

144.13
137.43
136.05
135.35
135.07
130.02
129.99
129.14
128.71
128.10
127.58
127.07
126.96
107.66
71.24
68.88
49.57
21.68
21.27
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

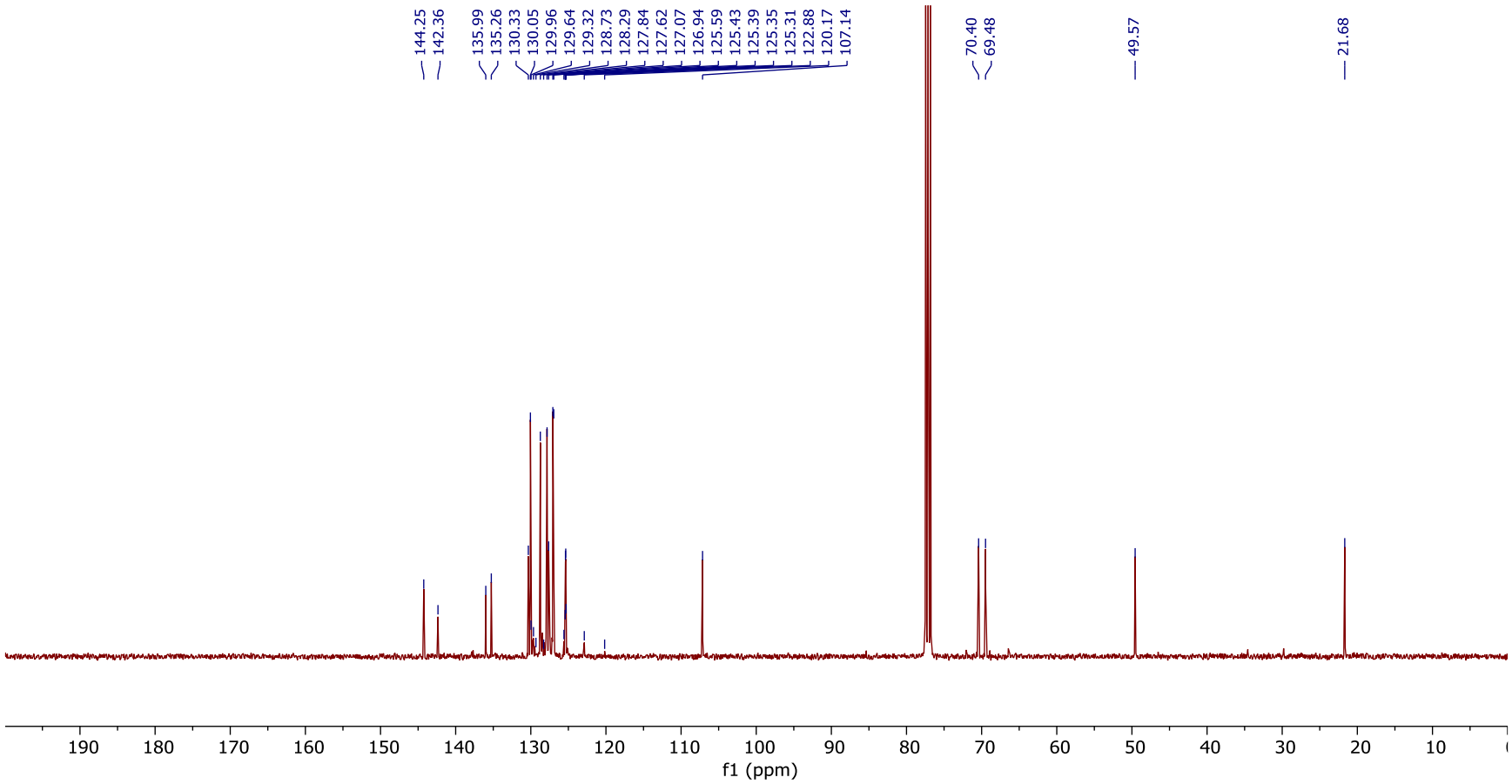
4ag


OMe
Bn
N
Ts
O
7.69
7.67
7.31
7.29
7.28
7.26
7.25
7.23
7.12
7.10
6.95
6.92
6.84
6.82
4.80
4.79
4.77
4.75
4.73
4.52
4.21
3.87
3.85
3.78
2.42
2.00
7.62
2.01
1.00
2.03
1.00
2.05
2.14
1.96
3.60
3.04
9.5
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
f1 (ppm)

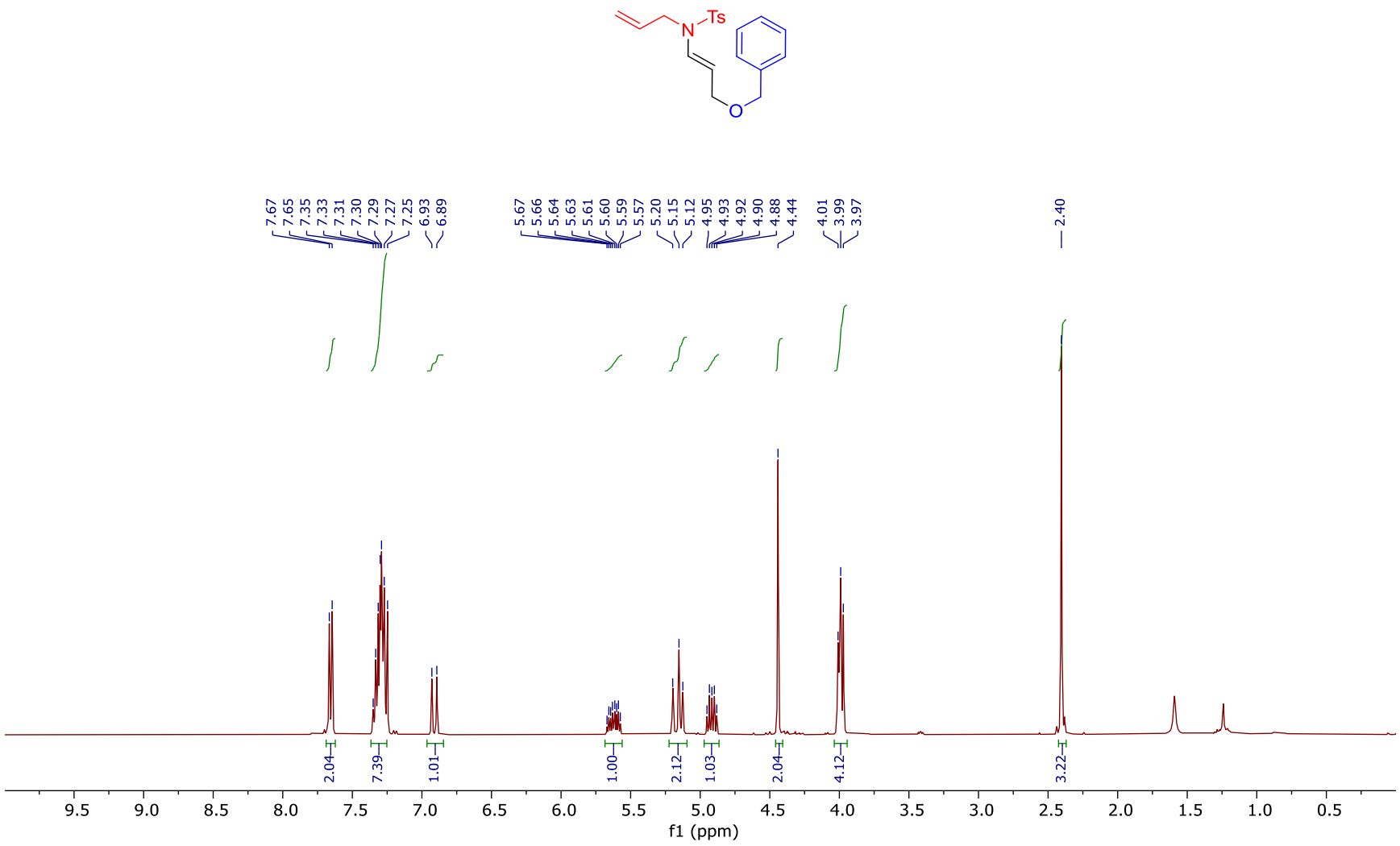

159.26
144.15
136.04
135.35
130.21
130.03
129.62
128.71
127.58
127.07
126.96
113.84
107.66
71.02
68.81
55.37
49.56
21.68
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

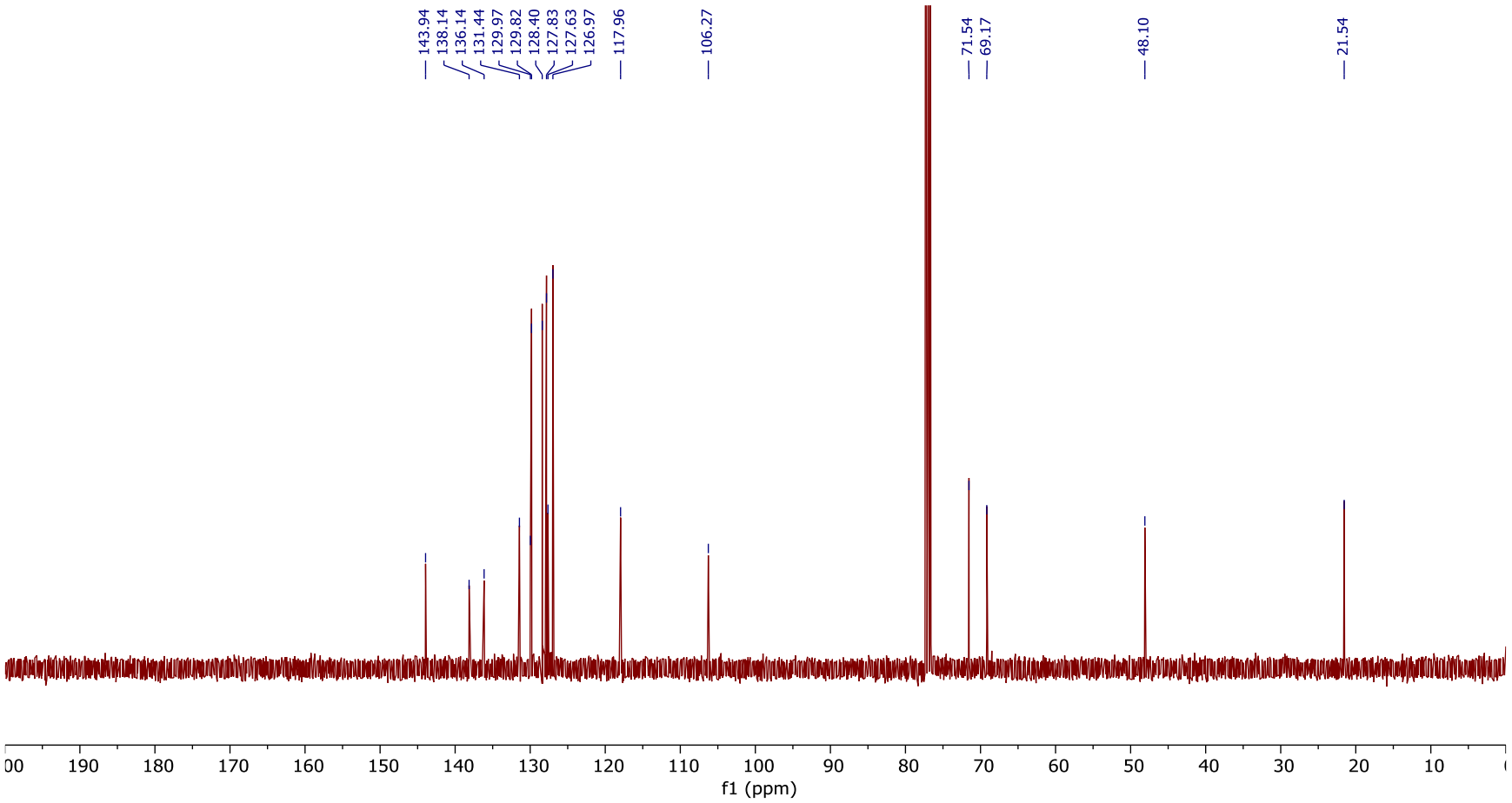
4ah


CF3
Bn
N
Ts
O
7.70
7.68
7.55
7.53
7.31
7.29
7.28
6.98
6.94
4.80
4.78
4.77
4.75
4.73
4.53
4.31
3.92
3.91
2.42
2.07
2.12
9.28
1.00
1.08
2.08
2.21
2.02
3.15
9.5
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
f1 (ppm)

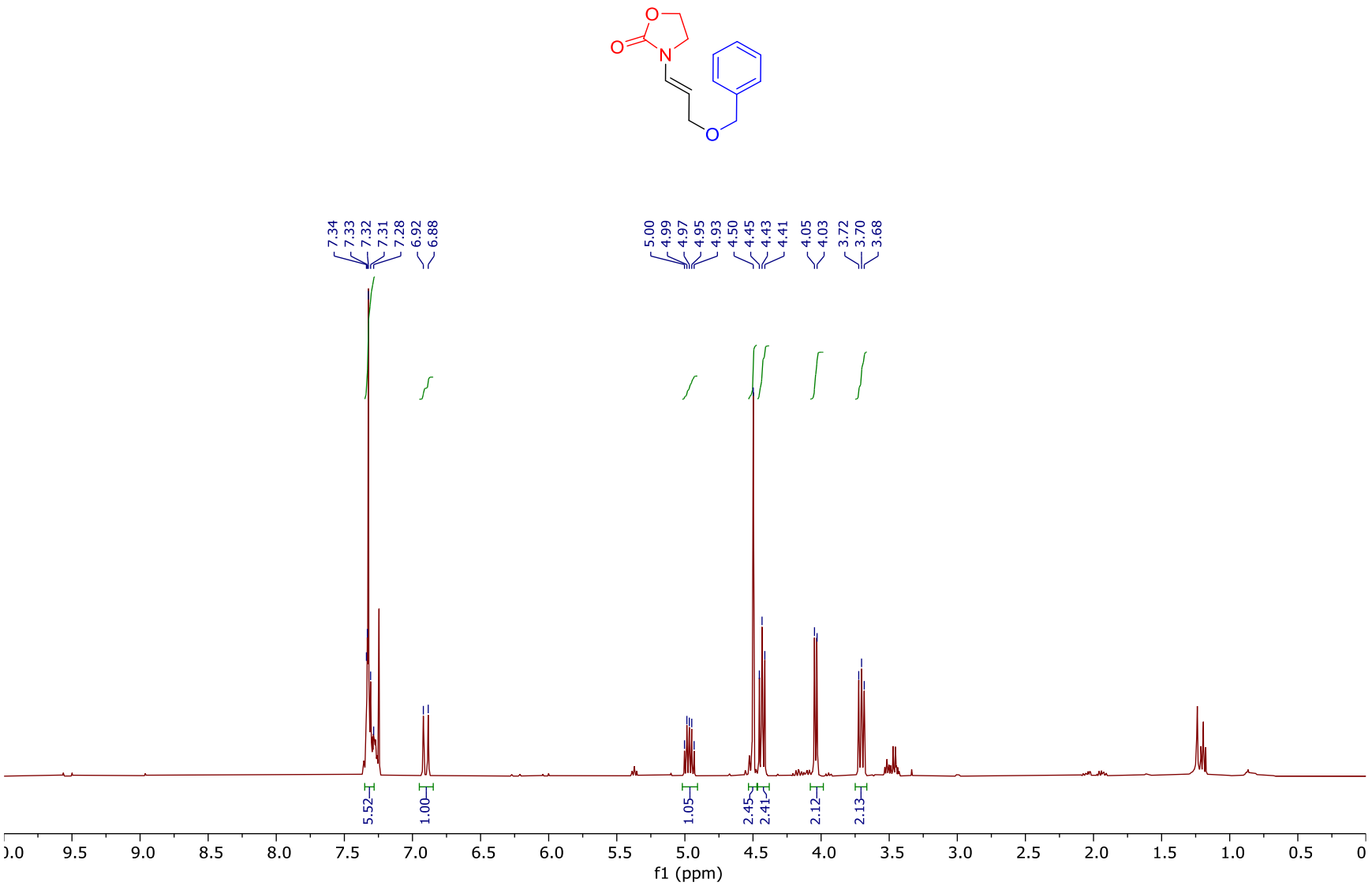

144.25
142.36
135.99
135.26
130.33
130.05
129.96
129.64
129.32
128.73
128.29
127.84
127.62
127.07
126.94
125.59
125.43
125.39
125.35
125.31
122.88
120.17
107.14
70.40
69.48
49.57
21.68
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

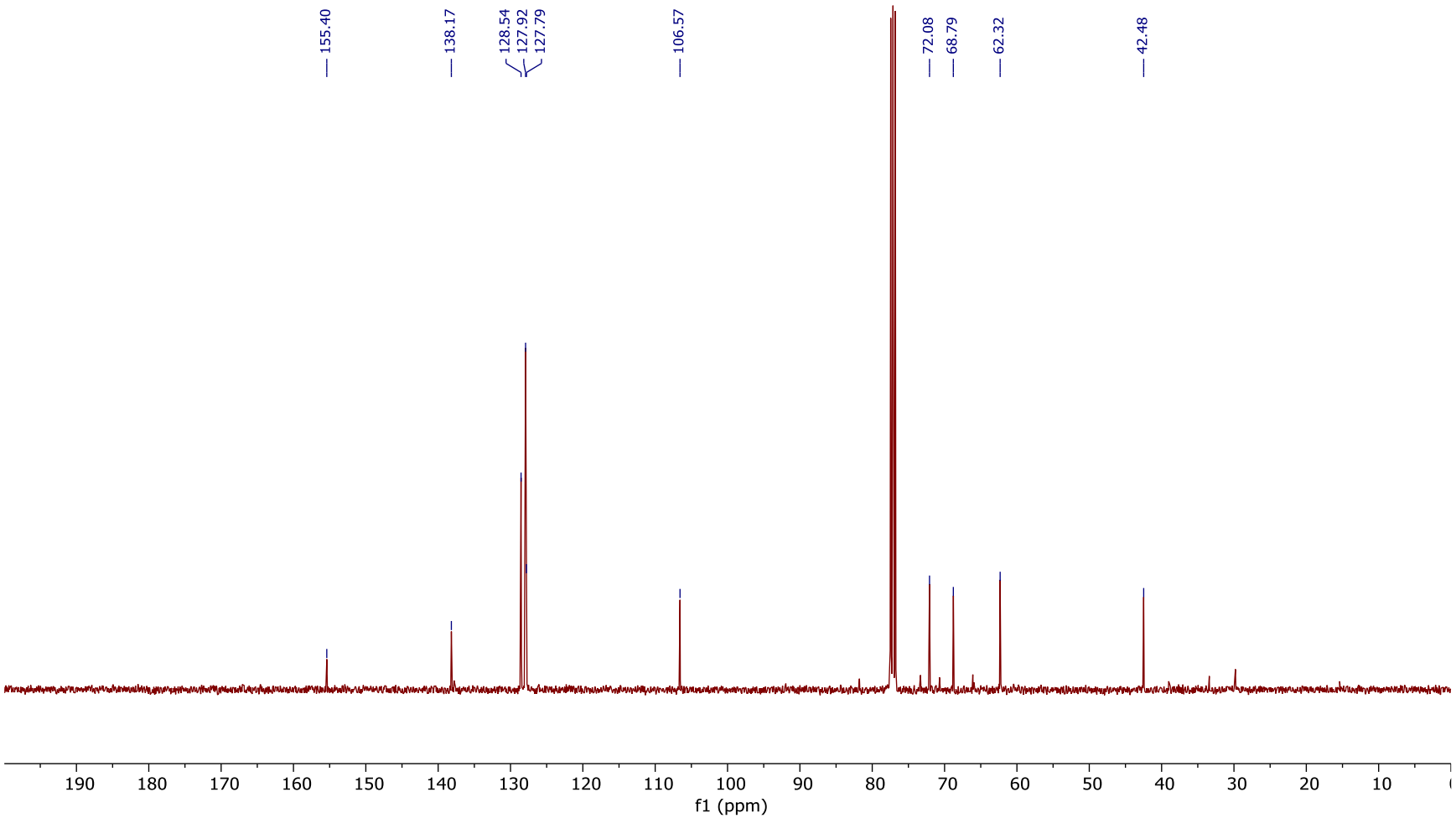
4de


Ts
N
O
7.67
7.65
7.35
7.33
7.31
7.30
7.29
7.27
7.25
6.93
6.89
5.67
5.66
5.64
5.63
5.61
5.60
5.59
5.57
5.20
5.15
5.12
4.95
4.93
4.92
4.90
4.88
4.44
4.01
3.99
3.97
2.40
2.04
7.39
1.01
1.00
2.12
1.03
2.04
4.12
3.22
9.5
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
f1 (ppm)


143.94
138.14
136.14
131.44
129.97
129.82
128.40
127.83
127.63
126.97
117.96
106.27
71.54
69.17
48.10
21.54
f1 (ppm)

4ee


7.34
7.33
7.32
7.31
7.28
6.92
6.88
5.00
4.99
4.97
4.95
4.93
4.50
4.45
4.43
4.41
4.05
4.03
3.72
3.70
3.68
5.52
1.00
1.05
2.45
2.41
2.12
2.13
f1 (ppm)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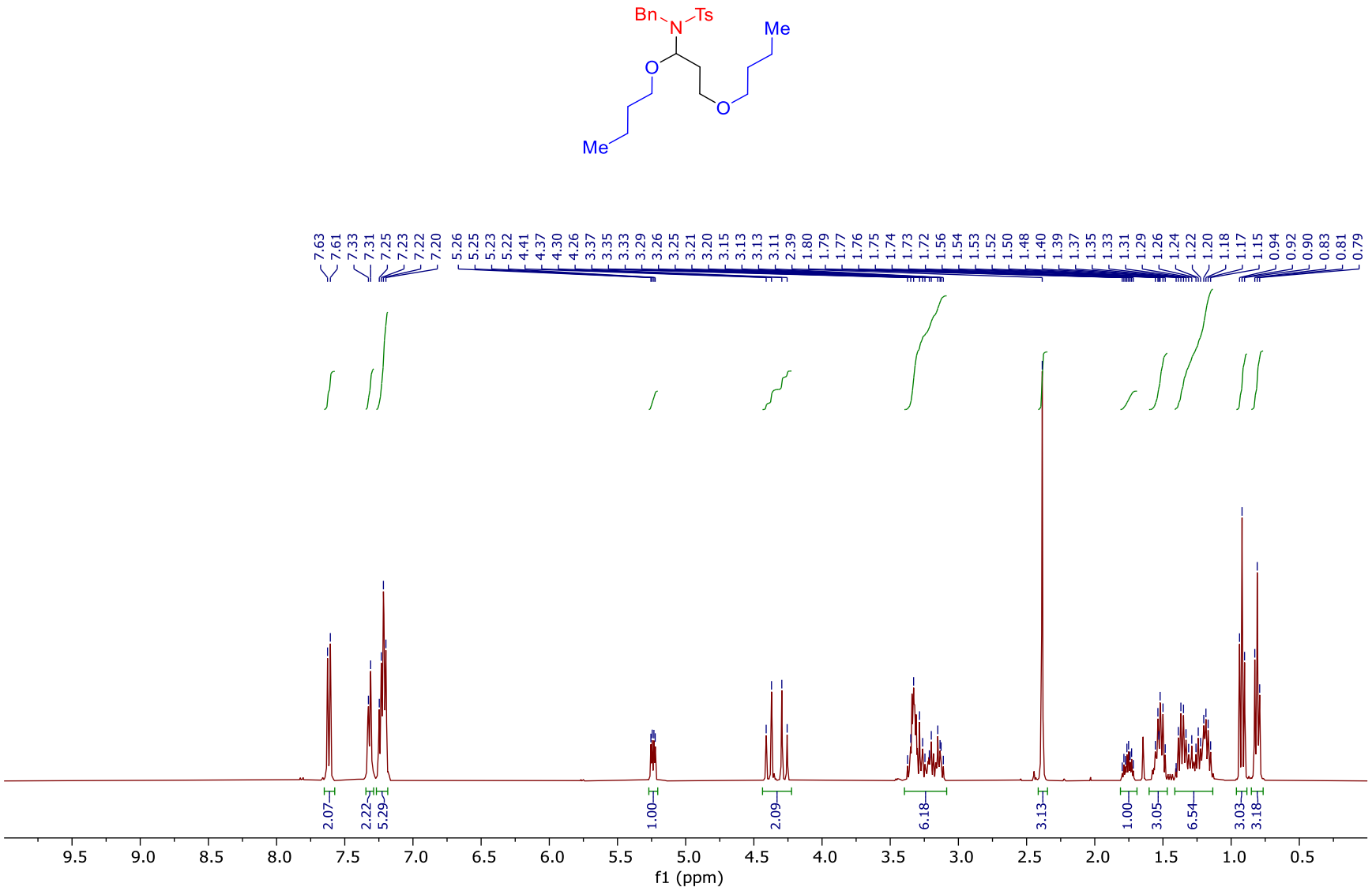
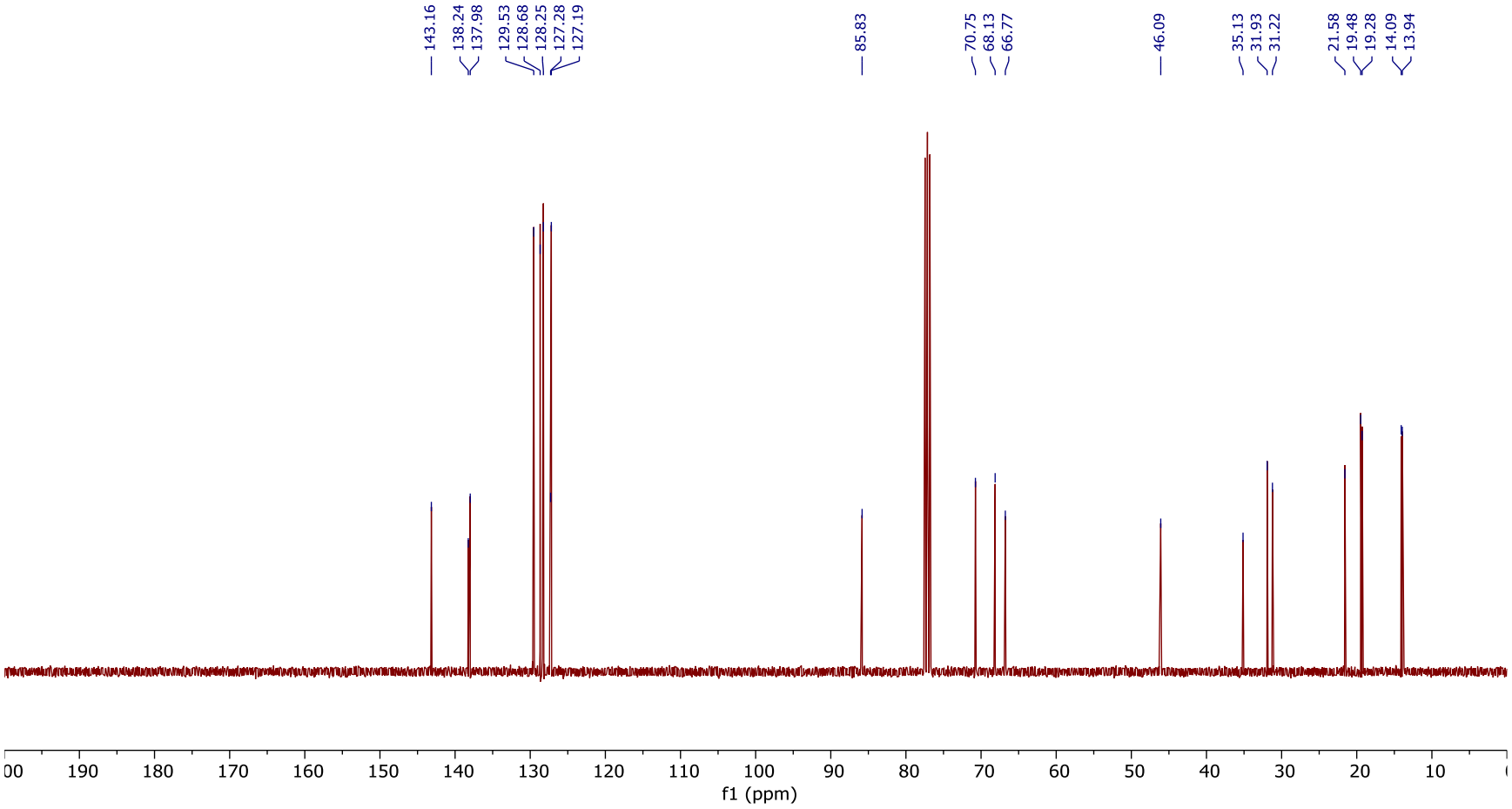
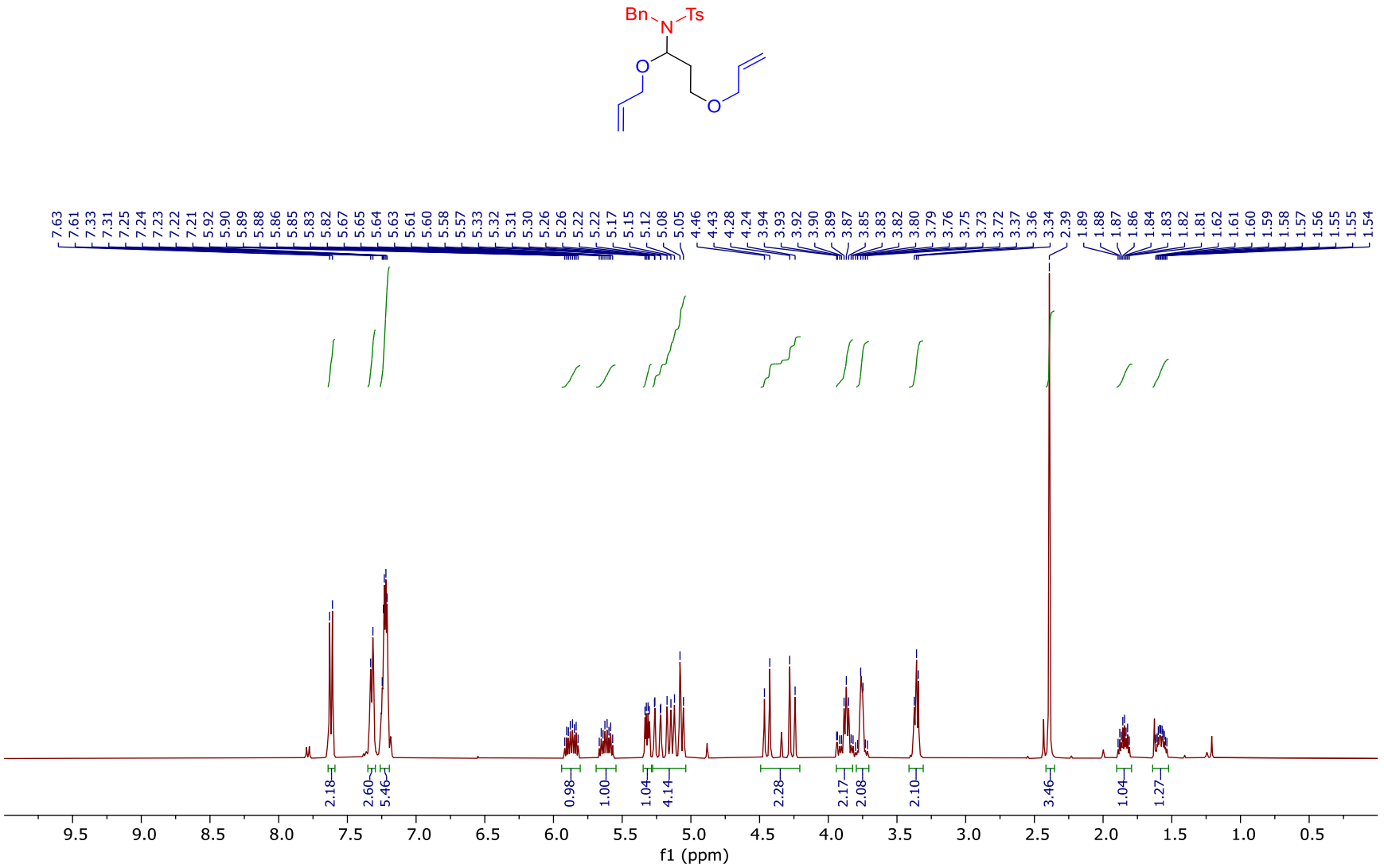
138.17
128.54
127.92
127.79
106.57
72.08
68.79
62.32
42.48
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

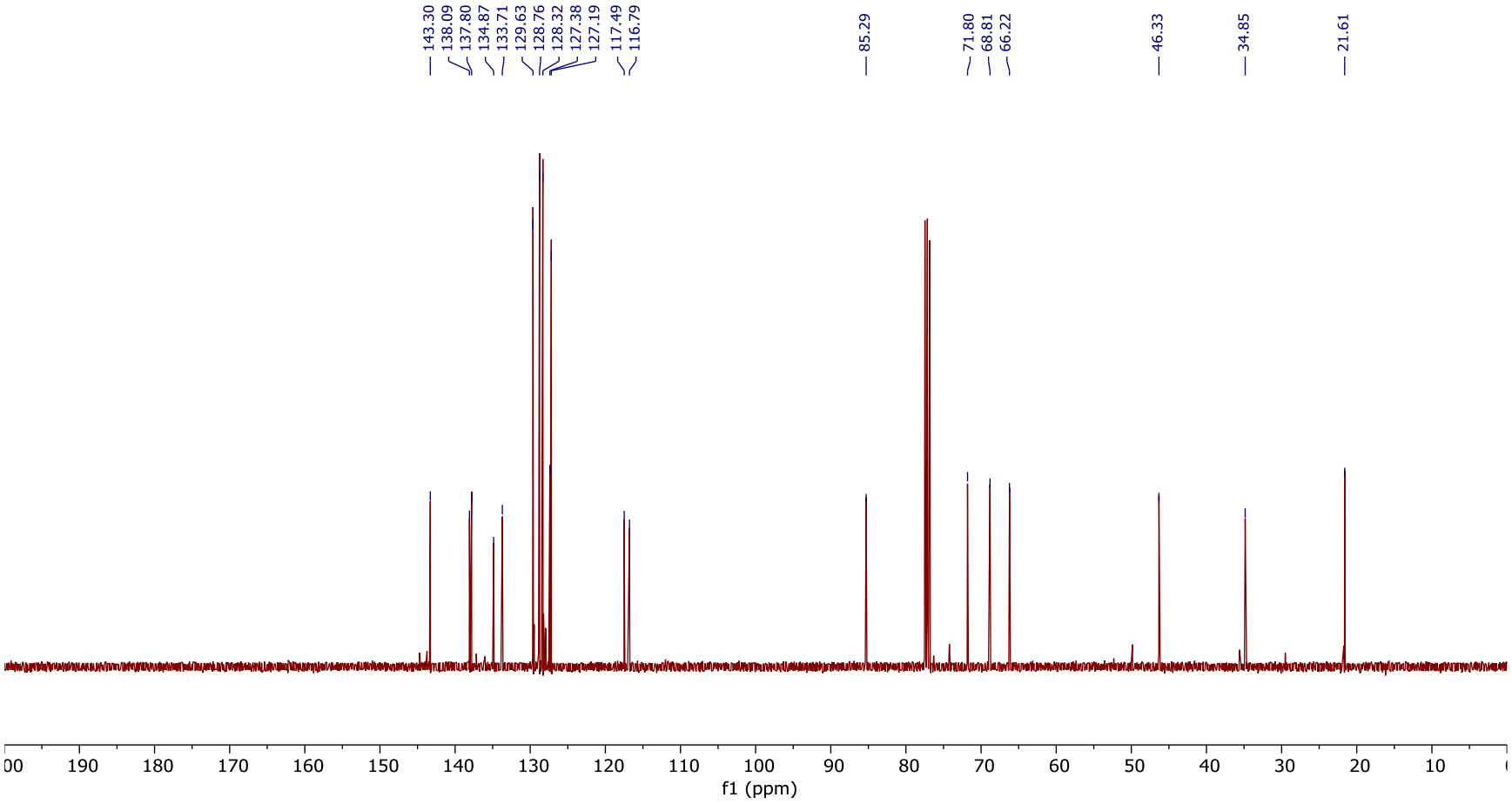
5aa


Bn
N
Ts
Me
O
O
Me
7.63 7.61 7.33 7.31 7.25 7.23 7.22 7.20 5.26 5.25 5.23 5.22 4.41 4.37 4.30 4.26 3.37 3.35 3.33 3.29 3.26 3.25 3.21 3.20 3.15 3.13 3.13 3.11 2.39 1.80 1.79 1.77 1.76 1.75 1.74 1.73 1.72 1.56 1.54 1.53 1.52 1.50 1.48 1.40 1.39 1.37 1.35 1.33 1.31 1.29 1.26 1.24 1.22 1.20 1.18 1.17 1.15 0.94 0.92 0.90 0.83 0.81 0.79
2.07 2.22 5.29 1.00 2.09 6.18 3.13 1.00 3.05 6.54 3.03 3.18
9.5 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
f1 (ppm)

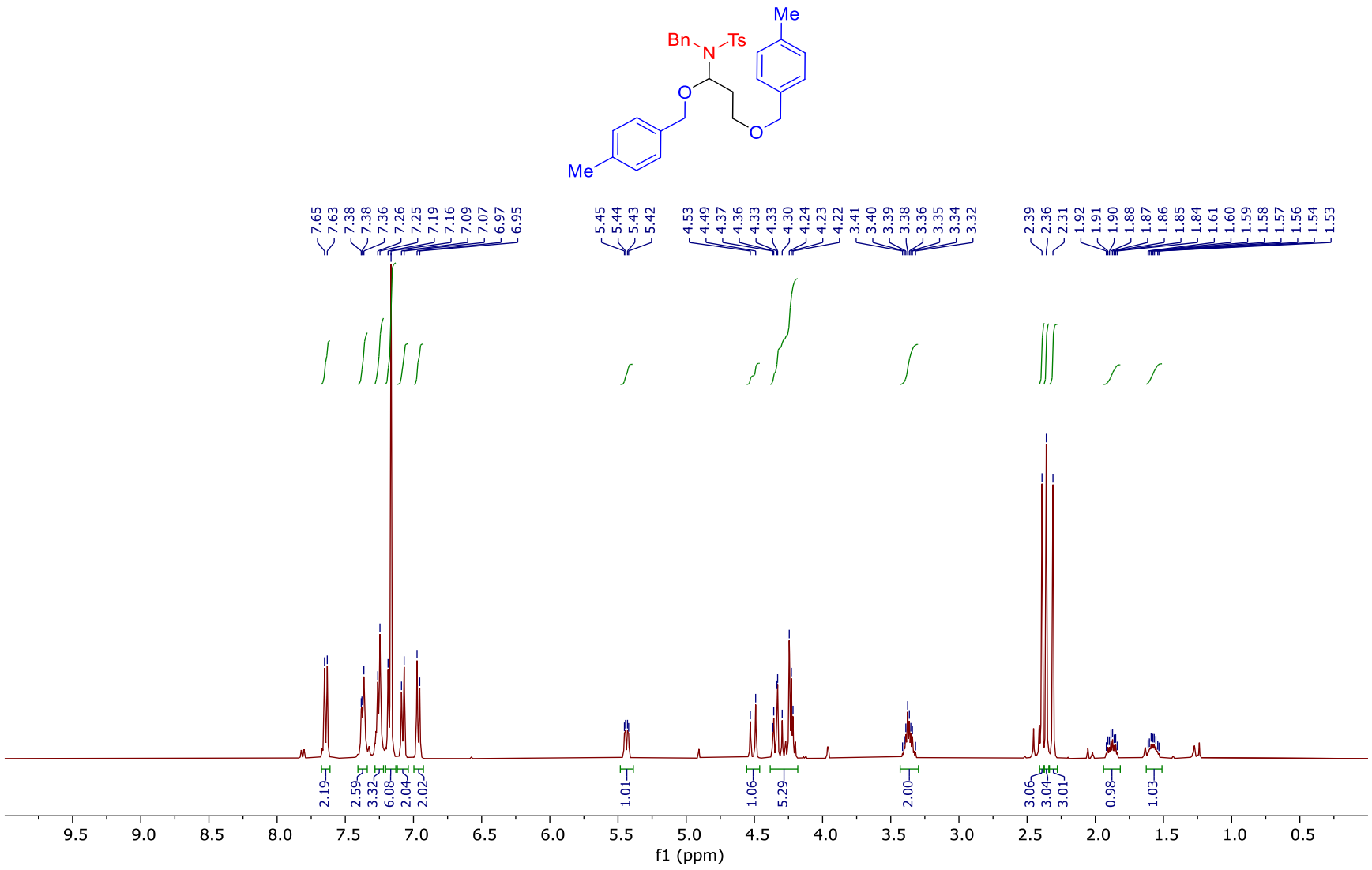

143.16
138.24
137.98
129.53
128.68
128.25
127.28
127.19
85.83
70.75
68.13
66.77
46.09
35.13
31.93
31.22
21.58
19.48
19.28
14.09
13.94
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

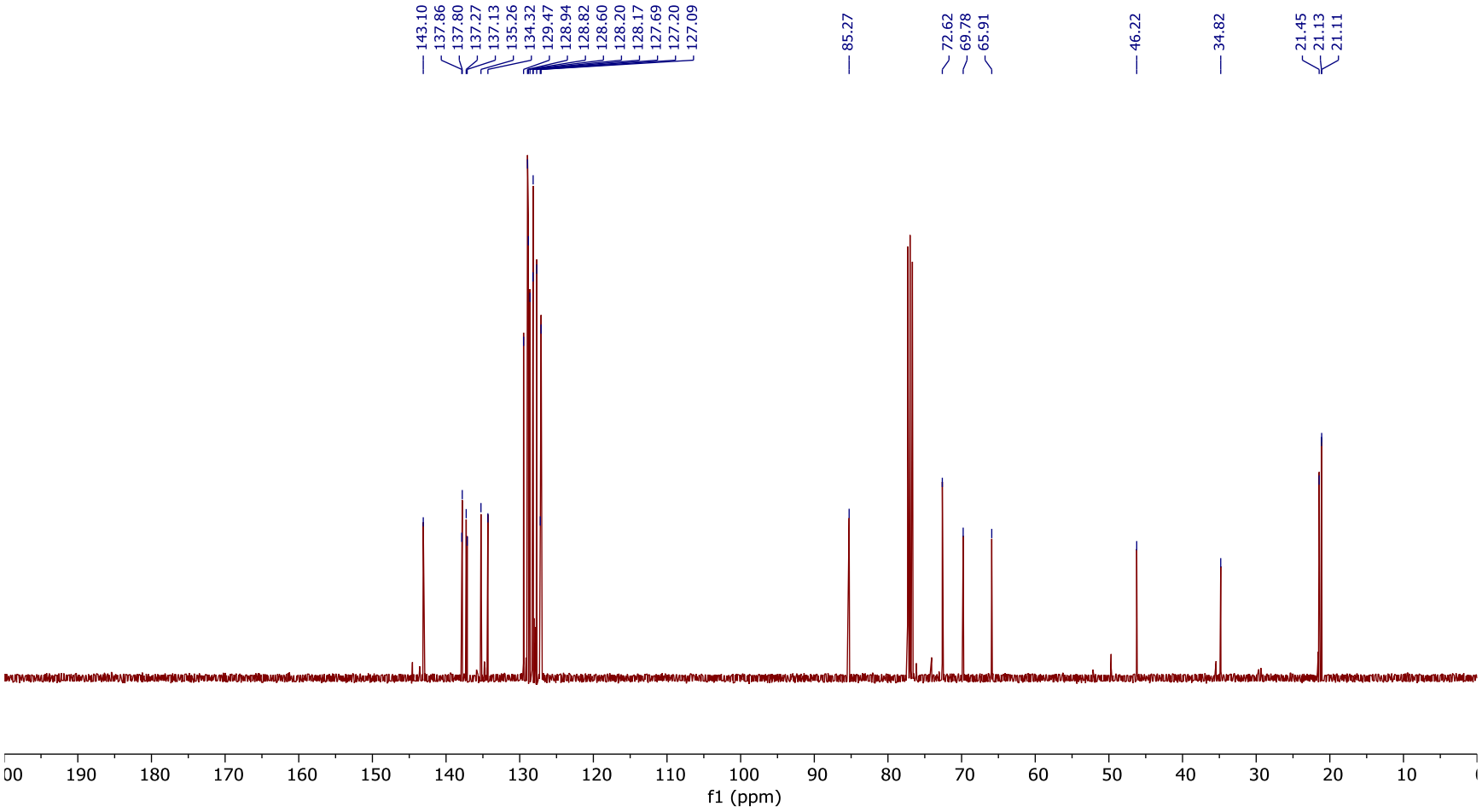
5ad


Bn
N
Ts
O
O
7.63 7.61 7.33 7.31 7.25 7.24 7.23 7.22 7.21 5.92 5.90 5.89 5.88 5.86 5.85 5.83 5.82 5.67 5.65 5.64 5.63 5.61 5.60 5.58 5.57 5.33 5.32 5.31 5.30 5.26 5.26 5.22 5.22 5.17 5.15 5.12 5.08 5.05 4.46 4.43 4.28 4.24 3.94 3.93 3.92 3.90 3.89 3.87 3.85 3.83 3.82 3.80 3.79 3.76 3.75 3.73 3.72 3.37 3.36 3.34 2.39 1.89 1.88 1.87 1.86 1.84 1.83 1.82 1.81 1.62 1.61 1.60 1.59 1.58 1.57 1.56 1.55 1.55 1.54
2.18 2.60 5.46 0.98 1.00 1.04 4.14 2.28 2.17 2.08 2.10 3.46 1.04 1.27
9.5 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
f1 (ppm)

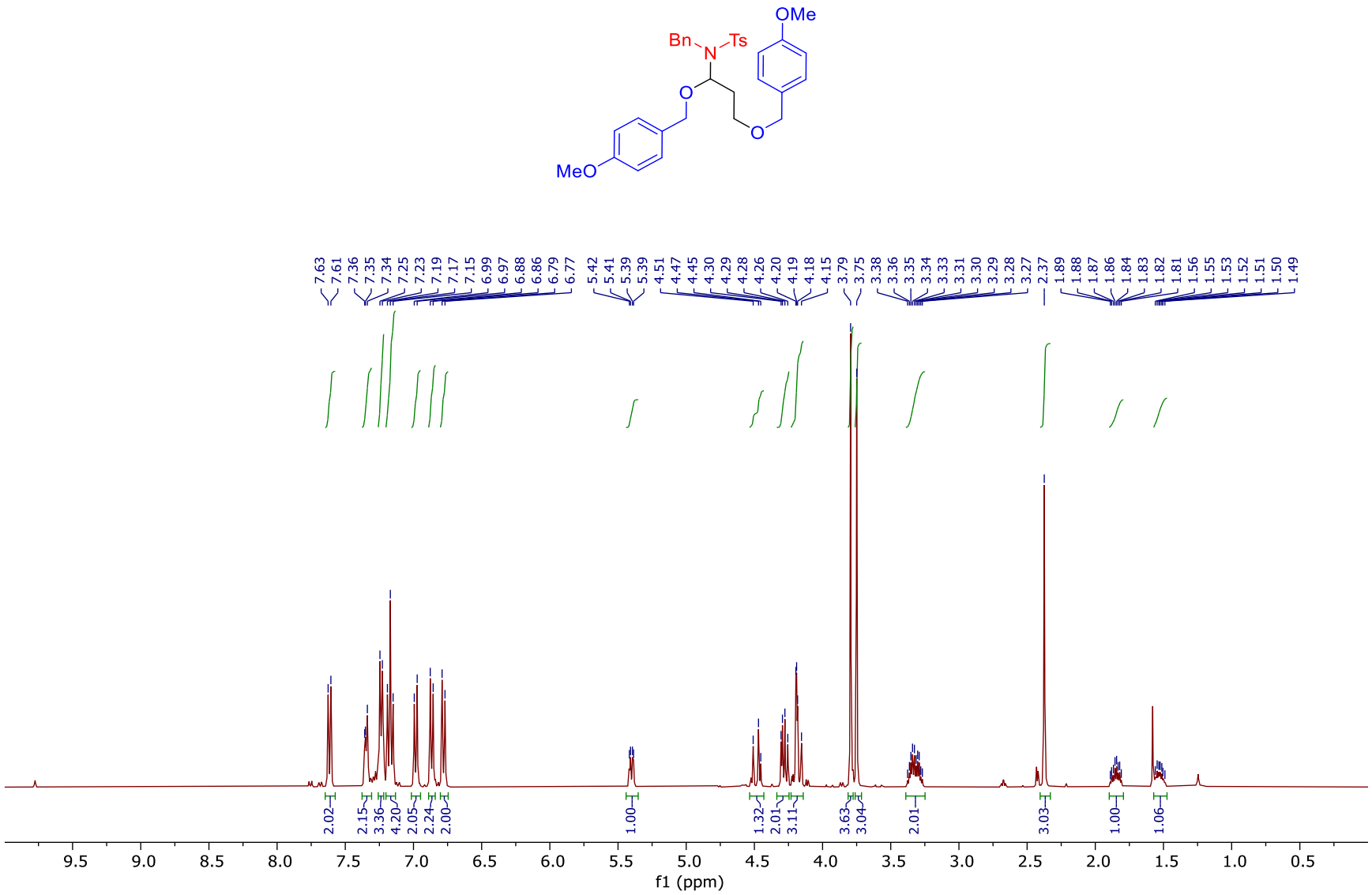

143.30
138.09
137.80
134.87
133.71
129.63
128.76
128.32
127.38
127.19
117.49
116.79
85.29
71.80
68.81
66.22
46.33
34.85
21.61
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

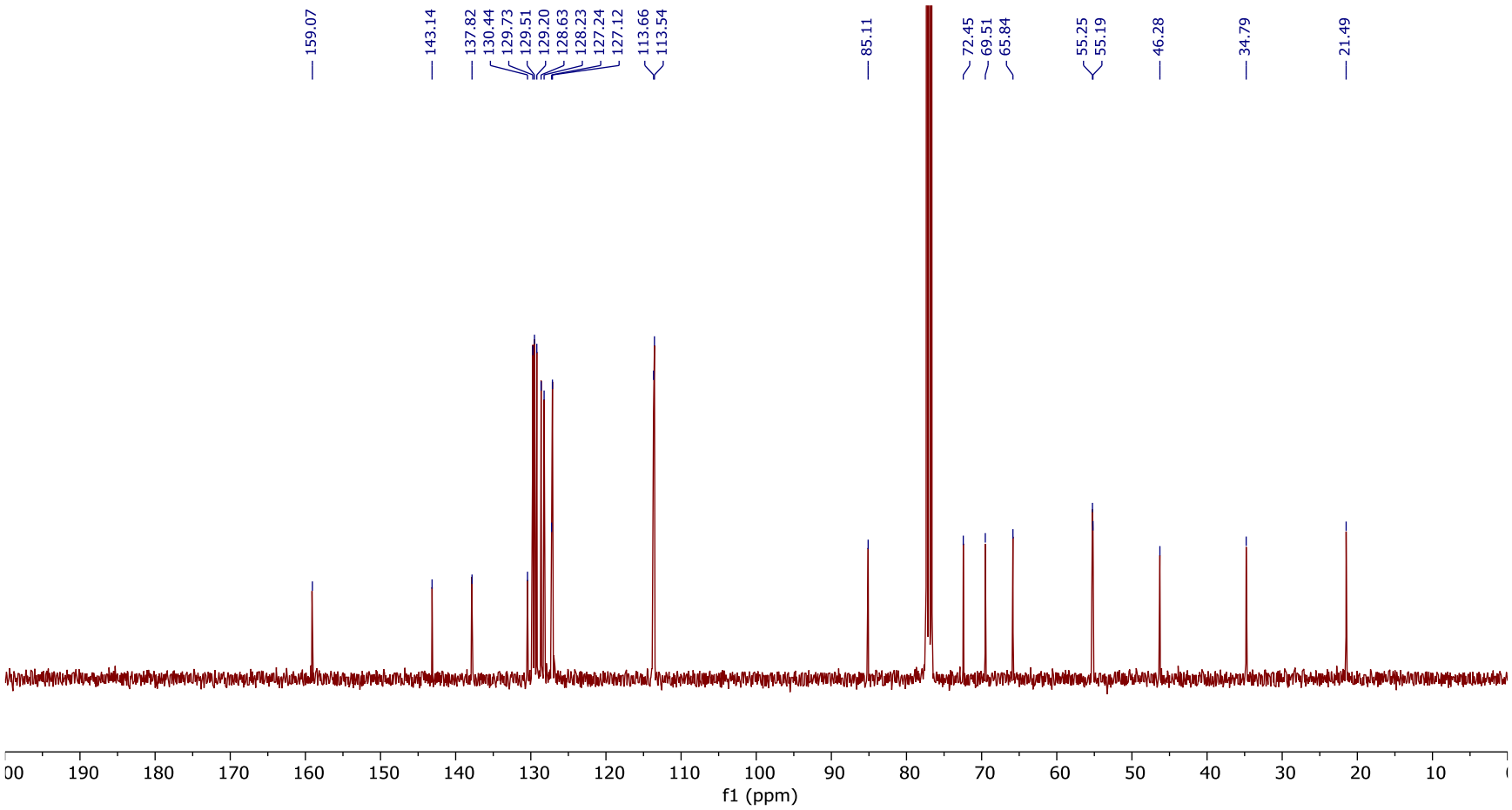
5af


Me
Bn
N
Ts
O
O
Me
7.65 7.63 7.38 7.38 7.36 7.26 7.25 7.19 7.16 7.09 7.07 6.97 6.95
5.45 5.44 5.43 5.42
4.53 4.49 4.37 4.36 4.33 4.33 4.30 4.24 4.23 4.22
3.41 3.40 3.39 3.38 3.36 3.35 3.34 3.32
2.39 2.36 2.31 1.92 1.91 1.90 1.88 1.87 1.86 1.85 1.84 1.61 1.60 1.59 1.58 1.57 1.56 1.54 1.53
2.19 2.59 3.32 6.08 2.04 2.02 1.01 1.06 5.29 2.00 3.06 3.04 3.01 0.98 1.03
9.5 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
f1 (ppm)

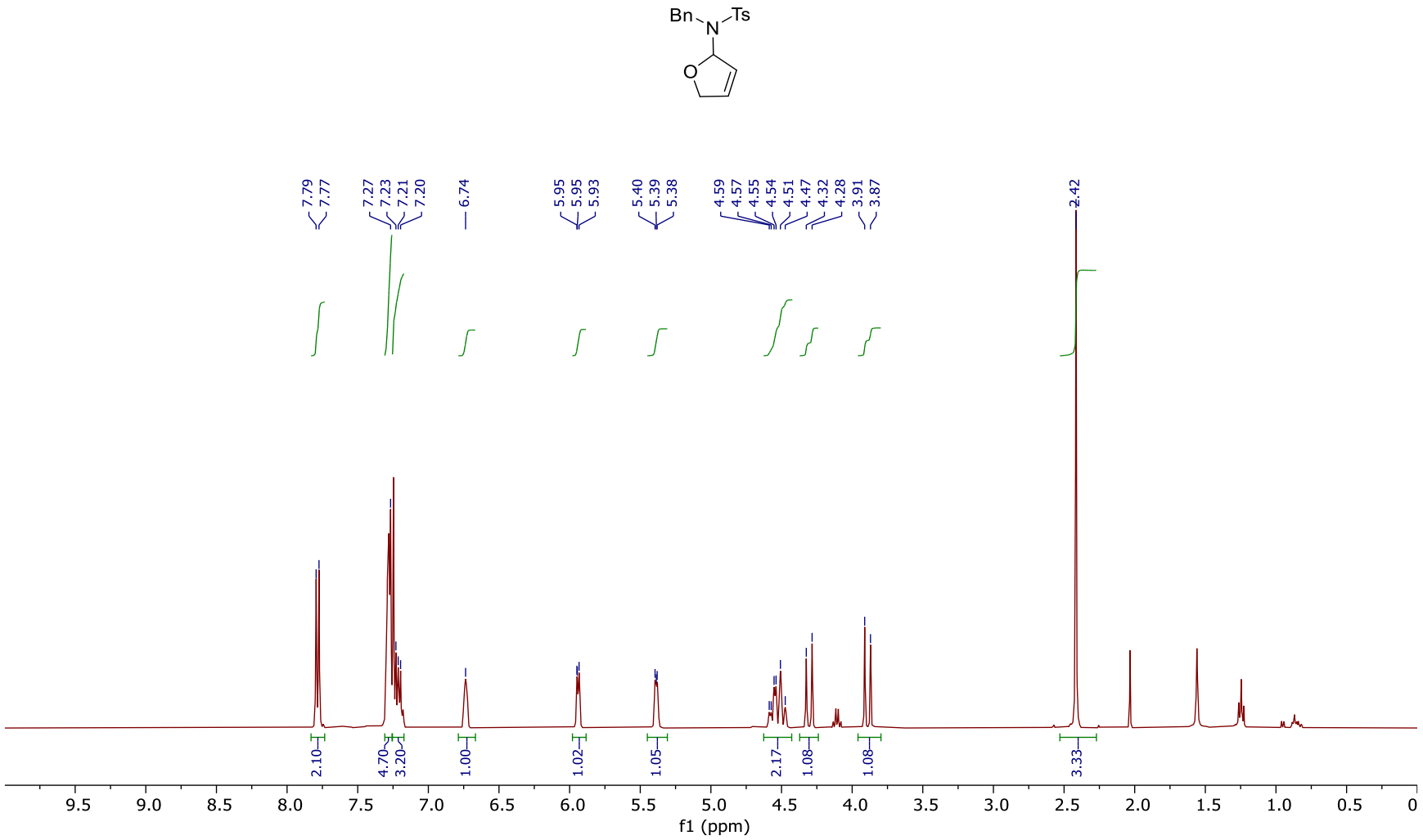

143.10
137.86
137.80
137.27
137.13
135.26
134.32
129.47
128.94
128.82
128.60
128.20
128.17
127.69
127.20
127.09
85.27
72.62
69.78
65.91
46.22
34.82
21.45
21.13
21.11
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

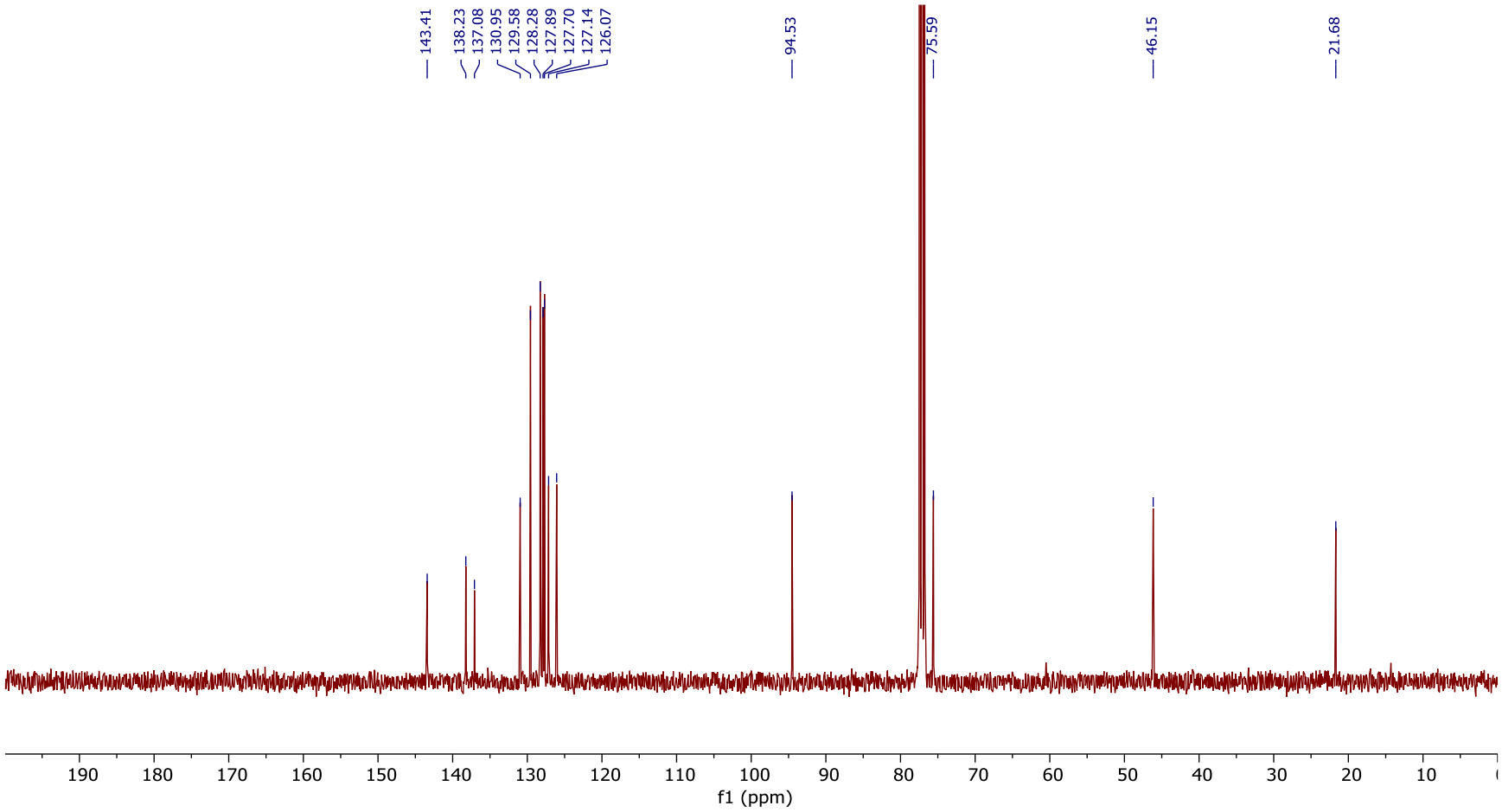
5ag


OMe
Bn
N
Ts
O
O
MeO
7.63
7.61
7.36
7.35
7.34
7.25
7.23
7.19
7.17
7.15
6.99
6.97
6.88
6.86
6.79
6.77
5.42
5.41
5.39
5.39
4.51
4.47
4.45
4.30
4.29
4.28
4.26
4.20
4.19
4.18
4.15
3.79
3.75
3.38
3.36
3.35
3.34
3.33
3.31
3.30
3.29
3.28
3.27
2.37
1.89
1.88
1.87
1.86
1.84
1.83
1.82
1.81
1.56
1.55
1.53
1.52
1.51
1.50
1.49
2.02
2.15
3.36
4.20
2.05
2.24
2.00
1.00
1.32
2.01
3.11
3.63
3.04
2.01
3.03
1.00
1.06
9.5
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
f1 (ppm)


159.07
143.14
137.82
130.44
129.73
129.51
129.20
128.63
128.23
127.24
127.12
113.66
113.54
85.11
72.45
69.51
65.84
55.25
55.19
46.28
34.79
21.49
f1 (ppm)

6


Bn
N
Ts
O
7.79
7.77
7.27
7.23
7.21
7.20
6.74
5.95
5.95
5.93
5.40
5.39
5.38
4.59
4.57
4.55
4.54
4.51
4.47
4.32
4.28
3.91
3.87
2.42
2.10
4.70
3.20
1.00
1.02
1.05
2.17
1.08
1.08
3.33
9.5
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
f1 (ppm)


143.41
138.23
137.08
130.95
129.58
128.28
127.89
127.70
127.14
126.07
94.53
75.59
46.15
21.68
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

8