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Supporting Information

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Supporting Information

for

Palladium-Catalyzed Intermolecular Aerobic Oxidative Amination of Terminal Alkenes: Efficient Synthesis of Linear Allylamine Derivatives

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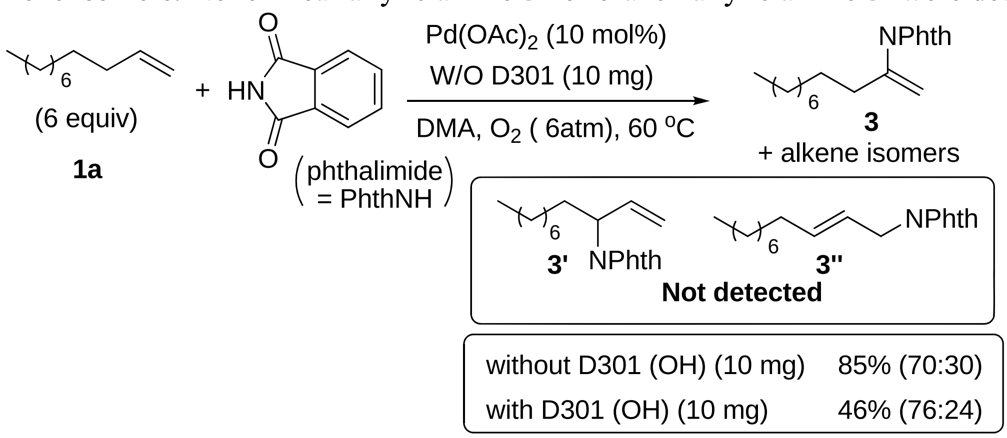
General procedure and new compound's characterization

General Considerations.

All commercially available compounds were used as received, and all were purchased from Aldrich. ^{1}H and ^{13}C spectra were recorded on a Varian Mercury-300 MHz or a Varian Unity-500 MHz spectrometer, and $CDCl_3$ was purchased from Aldrich. The chemical shifts (δ) are given in parts per million relative to internal standard TMS (0 ppm for ^{1}H), $CDCl_3$ (77.0 ppm for ^{13}C) and DMF-d_7 (2.75 ppm for ^{1}H).. Flash column chromatography was performed on silica gel 60 (particle size 200-400 mesh ASTM, purchased from Yantai, China) and eluted with hexanes/ether. Solvents (DMF, DMA and NMP) were dried with CaH_2 at around 100 ^{0}C for 5hrs, distilled under vacuum, and kept with 4Å Molecular Seives.

General procedure for the reaction of 1-undecene with phthalimide.

In a glass tube, 1-undecene (0.6 mmol), saccharin (0.1 mmol), catalyst (0.01 mmol), Maleic anhydride (0.04 mmol), base (10–70 mg, depending on additive), and 4Å molecular sieves (25 mg) were combined in 0.5 mL of solvent. The reaction tubes with different alkene substrates were placed into a 12-well parallel reactor mounted in a 300 mL Parr bomb and sealed. The whole system was purged with molecular oxygen for ca. 10 times. Then the oxygen pressure was increased to 6 atm and the reactor was warmed to 60° C. The reactions were stirred for 8-12 hours. After the reactions were stopped, the reaction mixture was concentrated *in vacuo*. After concentrating, 1,3,5-trimethoxybenzene (1mL of a known concentration solution in $CDCl_3$) was added to the reaction mixture. The oxidative amaintion product was evaluated by 1H NMR spectroscopy relative to an internal standard. The products contained enimide **3** and various alkene isomers. None linear allylic amine **3”** or branch allylic amine **3’** were detected.



General procedure for the reaction condition screening of saccharin.

In a glass tube, 1-undecene (0.6 mmol), phthalimide (0.1 mmol), $Pd(OAc)_2$ (0.01 mmol), with or without base D301 (OH) (10 mg) were combined in 0.5 mL of solvent. The reaction tubes with different alkene substrates were placed into a 12-well parallel reactor mounted in a 300 mL Parr bomb and sealed. The whole system was purged with molecular oxygen for ca. 10 times. Then the oxygen pressure was increased to 6 atm and the reactor was warmed to 60° C. The reactions were stirred for 8-12 hours. After the reactions were stopped, the reaction mixture was concentrated *in vacuo*. After concentrating, 1,3,5-trimethoxybenzene (1mL of a known concentration solution in $CDCl_3$) was added to the reaction mixture. The oxidative amination product was evaluated by ^{1}H NMR spectroscopy relative to an internal standard.

The results were summarized in Table S1. The products contained linear (E)-allylimide and alkene isomers. However, no isomeric imine and branch product were detected.

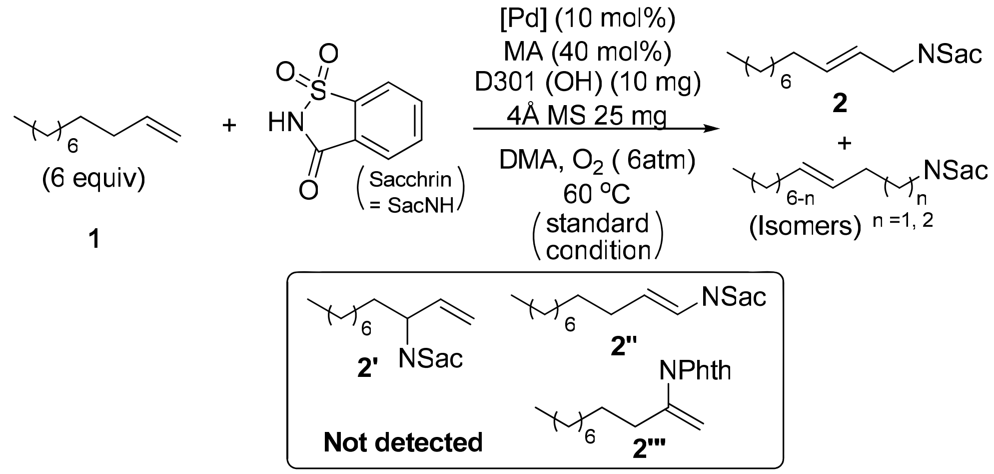


Table S1. Screening results of 1-undecene and saccharin catalyzed by Pd.[a]

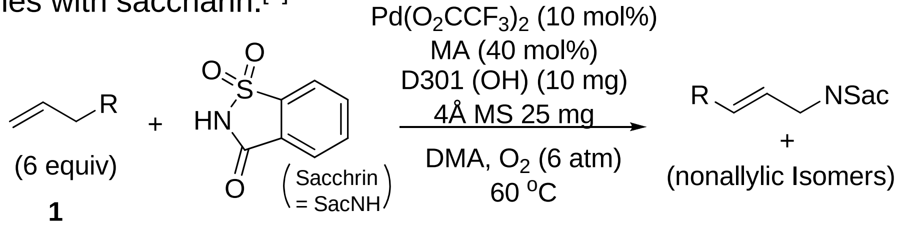
Entry	[Pd]	Additives	Yield[b]
1	$Pd(OAc)_2$	--	trace
2	$Pd(OAc)_2$	NaOAc (20 mol%)	35% (67:33)
3	$Pd(OAc)_2$	Amberlite IRA-400 (OH) (35 mg)	48% (73:27)
4	$Pd(OAc)_2$	D301 (OH) (10 mg)	55% (85:15)
5	$Pd(OAc)_2$	D301 (OH) (10mg) + MA	60% (86:14)
6	$Pd(OAc)_2$	D301 (OH) + MA + 4Å MS	68% (61:39)
7	$Pd(OAc)_2$	D301 (OH) + BQ + 4Å MS	59% (73:27)
8	$PdCl_2$	D301 (OH) + MA + 4Å MS	81% (49:51)
9	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	95% (69:31)
10[c]	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	66% (64:36)
11[d]	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	67% (60:40)
12[e]	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	78% (56:44)
13[e,f]	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	33% (55:45)
14[e,g]	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	20% (71:29)
15[h]	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	10% (77:23)
16[i]	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	77% (66:34)
17[j]	$Pd(O_2CCF_3)_2$	D301 (OH) + MA + 4Å MS	88% (68:32)

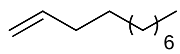
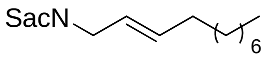
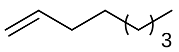
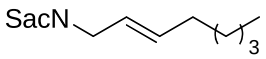
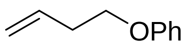
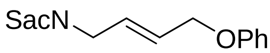
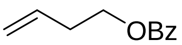
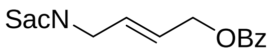
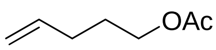
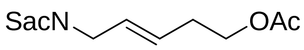
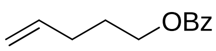
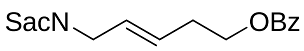
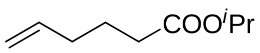
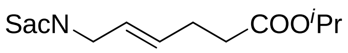
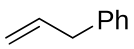
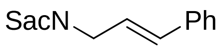
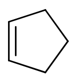
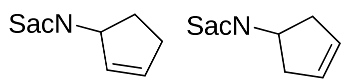
[a] The reaction condition was conducted at 0.1 mmol scale in 0.5 mL DMA; [b] ^{1}HNMR yield with 1,3,5-trimethoxybenzene as internal standard. the data in parentheses is the ratio of allylimide **2** and nonallylic isomers. [c] 5 mol% $Pd(O_2CCF_3)_2$, 20 mol% MA ; [d] **1** (4 equiv); [e] O_2 (1.5 atm) at 0.2 mmol scale in a sealed bottle; [f] **1** (3equiv); [g] **1** (1equiv, 0.2 mmol), saccharin (1.5 equiv, 0.3 mmol); [h] in DMSO; [i] in DMF; [j] in NMP.

General procedure for the reaction of alkenes with saccharin.

In a glass tube, alkenes (1.2 mmol), saccharin (0.2 mmol), catalyst (0.02 mmol), Maleic anhydride (0.04 mmol), D301(OH) (20 mg), and 4Å molecular sieves (50 mg) were combined in 1.0 mL of DMA. The reaction tubes with different alkene substrates were placed into a 9-well parallel reactor mounted in a 300 mL Parr bomb and sealed. The whole system was purged with molecular oxygen for ca. 10 times. Then the oxygen pressure was increased to 6 atm and the reactor was warmed to 60° C. The reactions were stirred for 8-12 hours. After the reactions were stopped, the reaction mixture was concentrated *in vacuo*. The crudes mixture was purified by column chromatography. The results were summarized in Table S2. When alkenes bearing long alkyl chain were treated under standard reaction condition, the reaction afforded the mixture products containing linear allylimides and alkene isomers. And the mixtures can not be separated. In order to characterize the compound, the mixture was hydrogenated by Pd/C under hydrogen (1 atm) to afford simple compound *N*-alkylsaccharin with quantity yield.

Table S2. Palladium-catalyzed oxidative amination of unactivated alkenes with saccharin.[a]

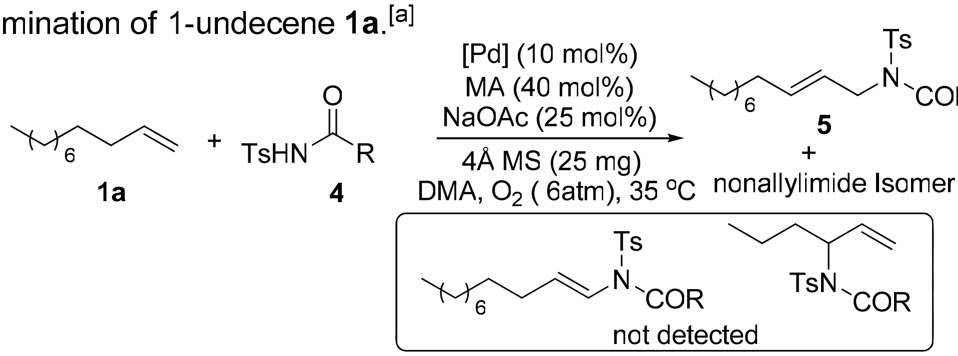


Entry	Alkenes	Products	Yield [b]
1 2[c]			85% (70:30) 76% (56:44)
3			82% (56:44)
4[d]			60%
5[d]			58%
6[d]			73% (77:23)
7[d]			81% (88:12)
8[d]			79% (73:27)
9			73%
10			40%(61:39)

[a] The reaction condition was conducted at 0.1 mmol scale in 0.5 mL DMA; [b] Isolated yield; the data in parentheses is the ratio of allylimide and nonallylic isomers. [c] the reaction conducted under 1.5 atm O_2 atmosphere in sealed bottle; [d]10 mol% $Pd(OAc)_2$;

General procedure for the reaction condition screening of *N*-tosyl carboxamides 4. In a glass tube, 1-undecene **1a** (0.3 mmol), N-tosyl carboxamides **4** (0.1 mmol), catalyst (0.01 mmol), maleic anhydride (0.04 mmol), NaOAc (0.025 mmol,) and 4Å molecular sieves (25 mg) were combined in 0.5 mL of solvent. The reaction tubes with different alkene substrates were placed into a 12-well parallel reactor mounted in a 300 ML Parr bomb and sealed. The whole system was purged with molecular oxygen for ca. 10 times. Then the oxygen pressure was increased to 6 atm and the reactor was warmed to 35° C. The reactions were stirred for 36-48 hours. After the reactions were stopped, the reaction mixture was added diphenyl ether (0.5 mL of a known concentration solution in Dichloroethane). The oxidative amination product was evaluated by GC relative to an internal standard. The results were summarized in Table S3.

Table S3. The screening results of palladium-catalyzed aerobic amination of 1-undecene **1a**.[a]

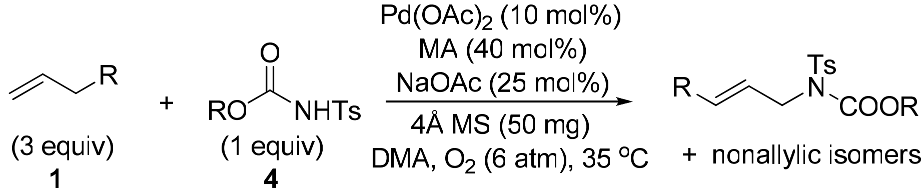


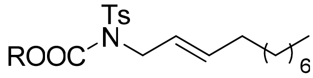
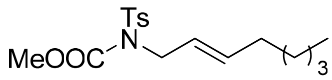
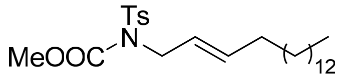
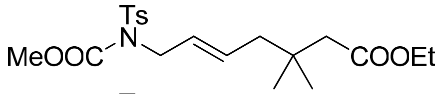
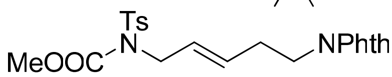
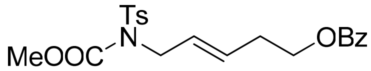
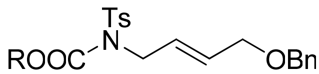
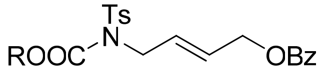
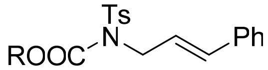
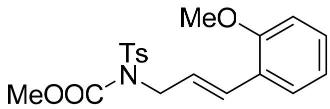
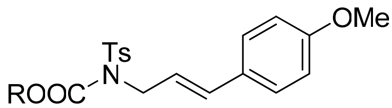
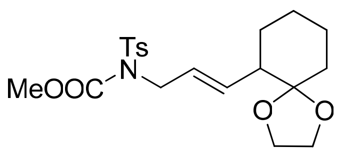
Entry	[Pd]	4	1a:4		Yield [b]
1	$Pd(OAc)_2$	**4a** R= OMe	6:1	**5a**	92% (69:31)
2	$Pd(OAc)_2$	**4a** R= OMe	3:1		88% (64:36)
3[c]	$Pd(OAc)_2$	**4a** R= OMe	1:1.25		52% (65:35)
4[c,d]	$Pd(OAc)_2$	**4a** R= OMe	1:1.25		73% (72:28)
5	$PdCl_2$	**4a** R= OMe	3:1		57% (17:83)
6	$Pd(O_2CCF_3)_2$	**4a** R= OMe	3:1		52% (56:44)
7	$Pd(OAc)_2$	**4b** R= O*t*Bu	3:1	**5b**	74% (73:27)[e]
8	$Pd(OAc)_2$	**4c** R= OBn	3:1	**5c**	67% (65:35)[e]
9	$Pd(OAc)_2$	**4d** R= OCH_2CF_3	3:1	**5d**	32% (62:38)[e]
10	$Pd(OAc)_2$	**4e** R= CH_3	3:1	**5e**	< 5%[e]
11	$Pd(OAc)_2$	**4f** R= Bn	3:1	**5f**	< 5%[e]
12	$Pd(OAc)_2$	**4g**[f]	3:1	**5g**	15%[e]

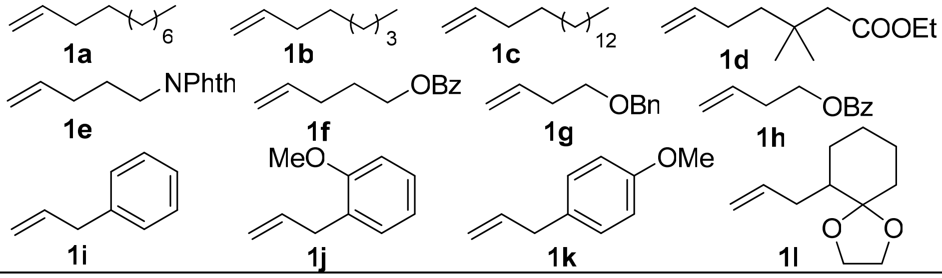
[a] The reaction was conducted at 0.1 mmol scale in 0.5 mL DMA; [b] GC yield, diphenyl ether as internal standard. the data in parentheses is the amount ratio of allylimide and nonallylimide isomers. [c] NaOAc 50 mol%; [d] 20 mol% $Pd(OAc)_2$; [e] ^{1}HNMR yield with 1,3,5-trimethoxybenzene as internal standard; [f] **4g** = $CF_3CH_2OSO_2NHCOOMe$.

General procedure for substrate scope: *N*-tosyl carboxamides 4 as limited reagents. In a glass tube, an alkene **1** (0.6 mmol), *N*-tosyl carboxamides **4** (0.2 mmol), catalyst (0.02 mmol), maleic anhydride (0.08 mmol), NaOAc (0.05 mmol) and 4Å Molecular Seives (50 mg) were combined in 0.8 mL of DMA.
***Alkene* 1 as limited reagent.** Alkenes **1** (0.2 mmol), N-tosyl carboxamides **4** (0.25 mmol), catalyst (0.04 mmol), maleic anhydride (0.08 mmol), NaOAc (0.10 mmol) and 4Å molecular sieves (50 mg) were combined in 0.4 mL of DMA.
The reaction tubes were placed into a 9-well parallel reactor mounted in a 300 ML Parr bomb and sealed. The whole system was purged with molecular oxygen for ca. 10 times. Then the oxygen pressure was increased to 6 atm and the reactor was warmed to 35° C. The reactions were stirred for 36-48 hours. After the reactions were stopped, the reaction mixture was concentrated *in vacuo*. The crude mixture was purified by column chromatography. The results were summarized in Table S4. When alkenes bearing long alkyl chain were treated under standard reaction condition, the reaction afforded the mixture products containing linear allylimides and alkene isomers. And the mixtures can not be separated. In order to characterize the compound, the mixture was hydrogenated by Pd/C under hydrogen (1 atm) to afford a single compound.

Table S4. Palladium-catalyzed oxidative amination of alkenes.[a]



Entry	1	4	Products			Yield [b]
1	1a	4a		5a	R = Me	87% (70:30)
2[c]						65% (71:29)
3		4b		5b	= ^{t}Bu	69% (76:24)
4		4c		5c	= Bn	63% (66:34)
5[c]						61% (74:26)
6	1b	4a		6		75% (69:31)
7	1c	4a		7		74% (57:43)
8	1d	4a		8		63% (84:16)
9[c,d]	1e	4a		9		81% (91:9)
10	1f	4a		10		78% (92:8)
11	1g	4a		11a	R = Me	61%
12		4b		11b	= ^{t}Bu	83%
13[c]						80%
14	1h	4a		12a	R = Me	62%
15		4b		12b	= ^{t}Bu	65%
16	1i	4a		13a	R = Me	70%
17		4b		13b	= ^{t}Bu	62%
18	1j	4a		14		75%
19	1k	4a		15a	R = Me	71%
20		4b		15b	= ^{t}Bu	67%
21		4c		15c	= Bn	80%
22[c]						64%
23[c]	1l	4a		16		53%

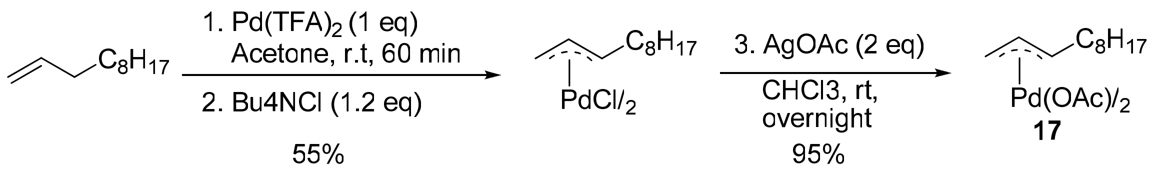


[a] The reaction condition was conducted at 0.2 mmol scale in 0.8 mL DMA; [b] Isolated yield; the data in parentheses is the ratio of allylimide and nonallylimide isomers. [c] Alkene as limited reagent: **1** (0.2 mmol, 1 equivalent), **4** (0.25 mmol, 1.25 equivalent), Pd(OAc)2 (20 mol%), NaOAc (50 mol%), DMA (0.4 mL). [d] PhthN = Phthalimidyl

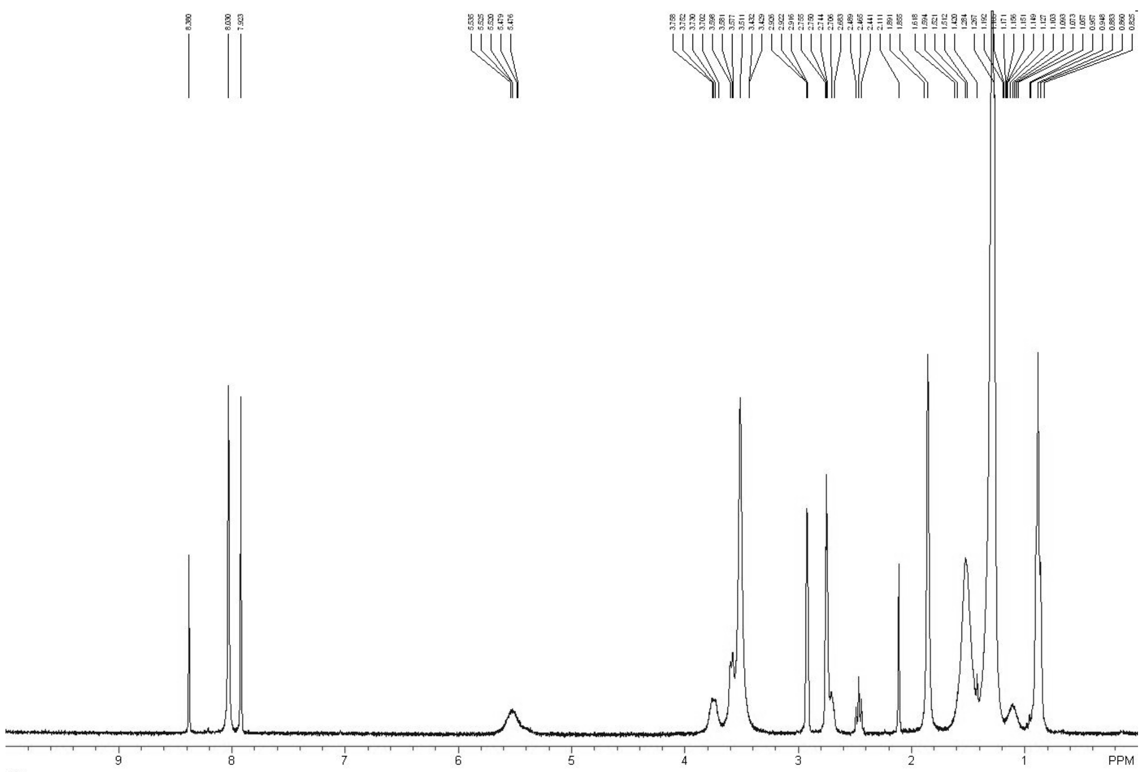
General procedure for Hydrogenation of linear (E)-allylic imides: In a schleck bottle, the mixture of linear (E)-allylic imide and the corresponding alkene isomers (0.1 mmol), and 10% Pd/C (10% w.t) were added to 10 mL methanol. The mixture was stirred for overnight under 1 atm hydrogen atmosphere. The mixture was filtered over a plug of Celite (to remove Pd/C), concentrated and purified *via* fast column chromatography to give the corresponding single akylimide in quantitative yield.

Synthesis of complex 17:

Scheme S1

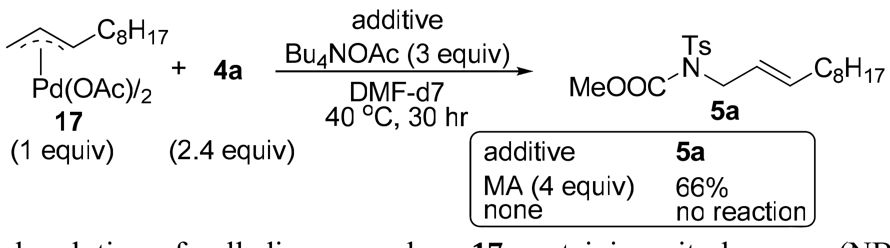


bis[acetate(1,2,3-trihapto-1-undecene)palladium(II)] 17, was synthesized using a literature procedure[s1] with 52% yield (two step). The final products contain 20% of 2-undecanone. This compound ^{1}H NMR (in $CDCl_3$) spectroscopy is consistent with the literature. The ^{1}H NMR (300 MHz, DMF-d_7) δ 5.52 (bs, 2H), 3.74 (bs, 2H), 3.57 (bd, J = 5.7Hz, 2H), 2.69 (bs, 2H), 1.86 (bs, 4H), 1.42 (bs, 8H), 1.28 (bs, 16H), 0.86 (bs, 6H).



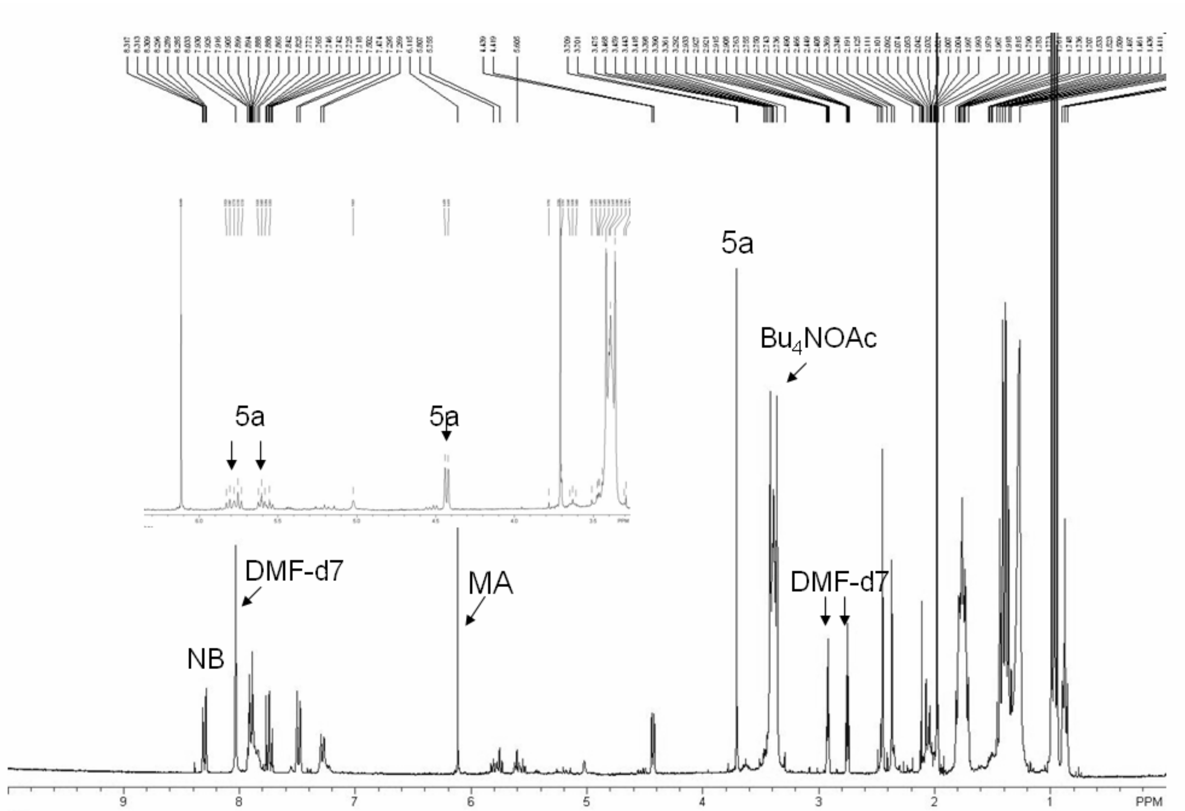
Reation of complexe 17 with imide 4a in DMF-d7 (with MA).

Scheme S2

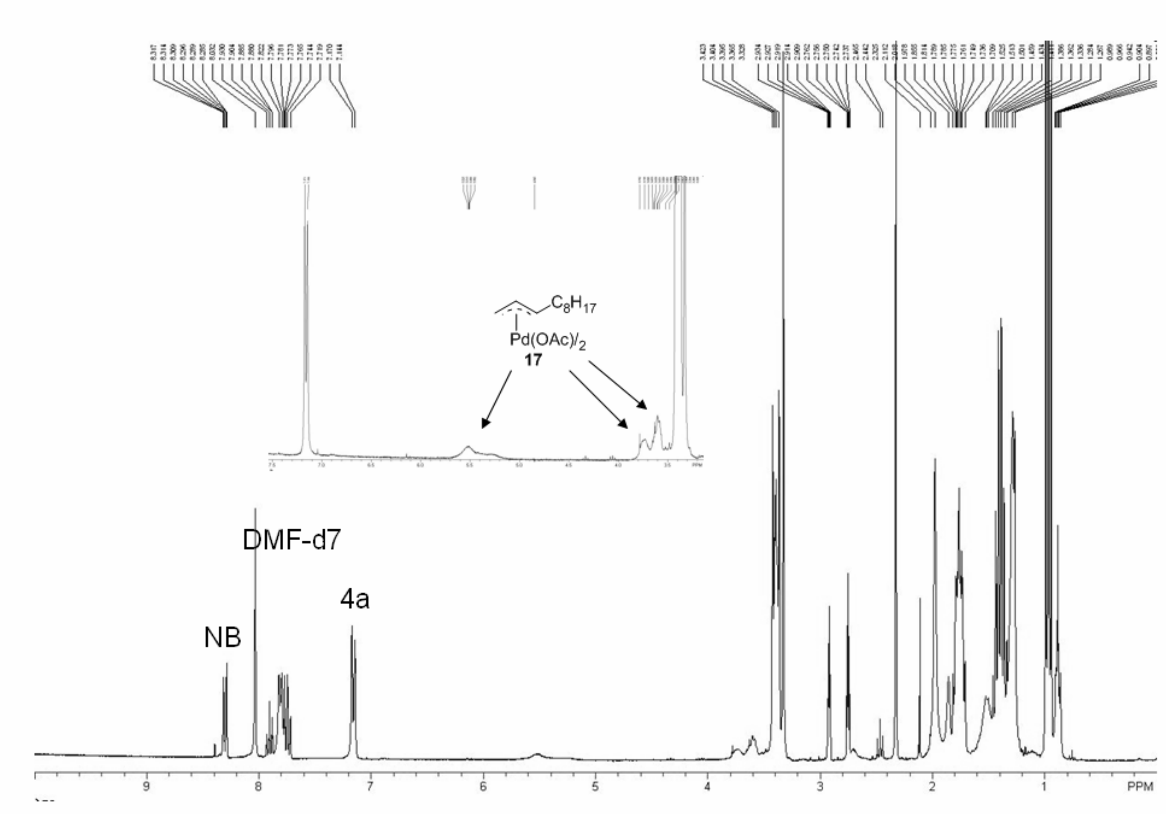


A 20 mM stock solution of palladium complexe **17** containing nitrobenzene (NB, internal standard, 25 mM) in DMF-d_7 (0.5 mL) was added to NMR tube which have imide **4a** (5.6 mg, 0.024 mmol),

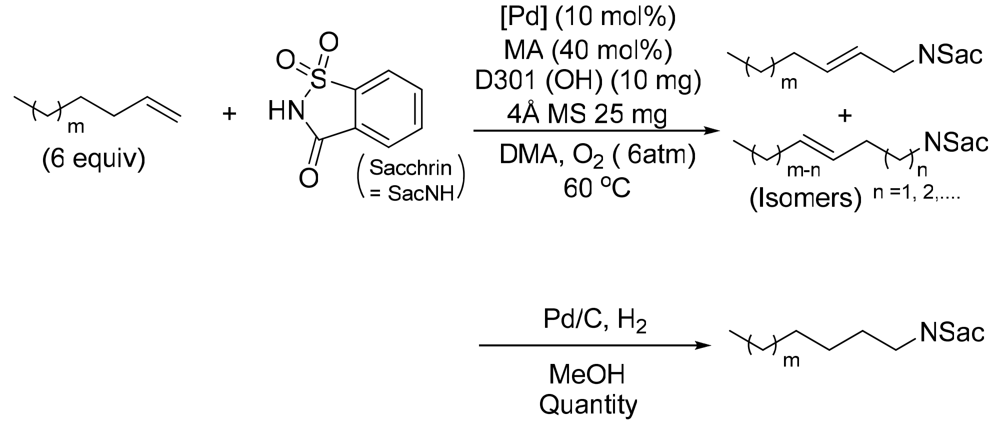
Bu_4NOAc (9.0 mg, 0.03 mmol), and maleic anhydride (MA, 4.4 mg, 0.045 mmol). The mixture was heated in an oil bath (40 ^{0}C) and monitored by ^{1}H NMR. The reaction afforded linear (*E*)-allylimide **5a** in 66% yield. No nonallylic isomers and branch allylimide were observed.

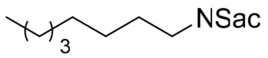


Reation of complexe 17 with imide 4a in DMF-d7 (with MA). The reaction condition was the same as above except that no maleic was absent. No amination product was observed.

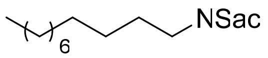


New compounds characterization:

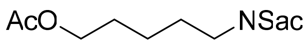




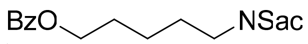
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dt, *J* = 6.8, 0.6 Hz, 1H), 7.94-7.80 (m, 3H), 3.77 (t, *J* = 7.5 Hz, 2H), 1.85 (m, 2H), 1.45-1.20 (m, 10H), 0.88 (t, *J* = 6.0 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 158.9, 137.6, 134.6, 134.2, 127.4, 125.0, 120.8, 39.4, 31.7, 29.1, 29.0, 28.4, 26.7, 22.6, 14.0. HRMS: m/z (EI) calculated $[M]^+$ 295.1242, measured 295.1246.



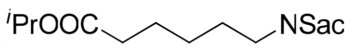
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dt, *J* = 6.6, 0.6 Hz, 1H), 7.93-7.79 (m, 3H), 3.77 (t, *J* = 7.5 Hz, 2H), 1.85 (m, 2H), 1.45-1.20 (m, 16H), 0.88 (t, *J* = 6.0 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 158.9, 137.6, 134.6, 134.2, 127.4, 125.0, 120.8, 39.4, 31.8, 29.52, 29.51, 29.41, 29.27, 29.0, 28.4, 26.7, 22.6, 14.1. HRMS: m/z (ESI) calculated $[M+Na]^+$ 338.1783, measured 338.1784.



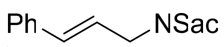
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dt, *J* = 6.8, 0.6 Hz, 1H), 7.95-7.81 (m, 3H), 4.07 (t, *J* = 6.6 Hz, 2H), 3.79 (t, *J* = 7.5 Hz, 2H), 2.05 (s, 3H), 1.92 (m, 2H), 1.71 (m, 2H), 1.51 (m, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 171.2, 158.9, 137.5, 134.7, 134.3, 127.3, 125.1, 120.9, 64.1, 39.1, 28.0, 27.9, 23.2, 21.0. HRMS: m/z (ESI) calculated $[M+H]^+$ 312.0900, measured 312.0900.



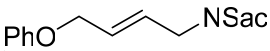
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (m, 3H), 7.95-7.81 (m, 3H), 7.55 (m, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 4.34 (t, *J* = 6.3Hz, 2H), 3.82 (t, *J* = 7.5 Hz, 2H), 1.99-1.81 (m, 4H), 1.61 (m, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 166.6, 158.9, 137.6, 134.7, 134.3, 132.8, 130.3, 129.5, 128.3, 127.3, 125.1, 120.9, 64.6, 39.1, 28.2, 28.1, 23.3. HRMS: m/z (ESI) calculated $[M+H]^+$ 374.1062, measured 374.1057.



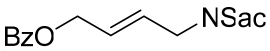
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dt, *J* = 6.8, 0.6 Hz, 1H), 7.95-7.81 (m, 3H), 5.00 (m, 1H), 3.78 (t, *J* = 7.5 Hz, 2H), 2.29 (t, *J* = 7.5 Hz, 2H), 1.86 (m, 2H), 1.69 (m, 2H), 1.45 (m, 2H). 1.23 (d, *J* = 6.3 Hz, 6H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 172.9, 158.8, 137.5, 134.6, 134.2, 127.3, 125.0, 120.8, 67.4, 39.1, 34.3, 28.0, 26.1, 24.3, 21.7. HRMS: m/z (ESI) calculated $[M+Na]^+$ 362.1032, measured 362.1033.



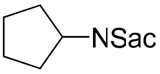
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 6.6, 1.8 Hz, 1H), 7.95-7.81 (m, 3H), 7.41-7.24 (m, 5H), 6.79 (d, *J* = 15.9 Hz, 1H), 6.33 (dt, *J* = 6.6, 15.9 Hz, 1H), 4.54 (d, *J* = 6.6 Hz, 2H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 158.6, 137.7, 135.9, 135.2, 134.8, 134.3, 128.5, 128.1, 127.3, 126.7, 125.2, 121.4, 120.9, 41.0. HRMS: m/z (EI) calculated $[M]^+$ 299.0616, measured 299.0622.



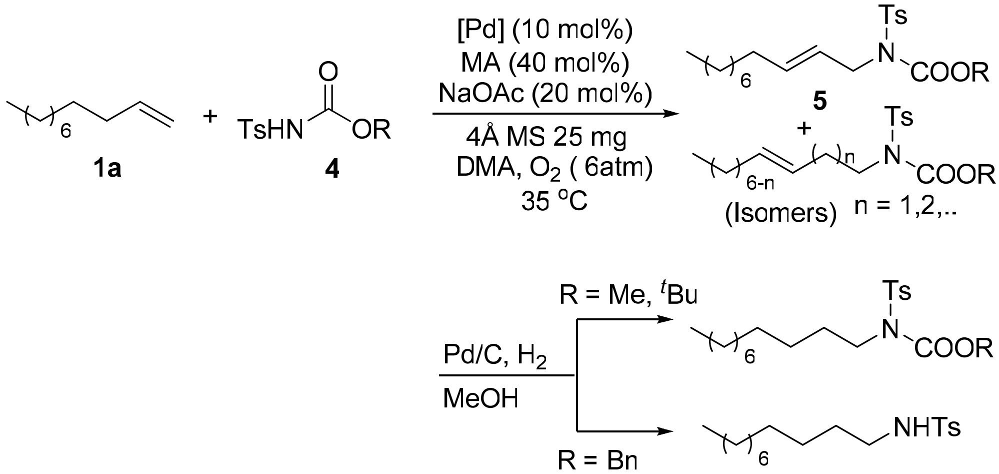
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 6.6, 1.8 Hz, 1H), 7.95-7.81 (m, 3H), 7.27 (m, 2H), 6.91 (m, 3H), 6.13 (dt, *J* = 15.6, 4.8 Hz, 1H), 6.01 (dt, *J* = 15.6, 6.0 Hz, 1H), 4.55 (d, *J* = 4.8 Hz, 2H). 4.42 (d, *J* = 6.0 Hz, 2H). $^{13}C\{1H\}$ NMR (75 MHz, $CDCl_3$) δ 158.6, 158.3, 137.7, 134.8, 134.3, 130.8, 129.4, 127.2, 125.2, 125.1, 120.9, 120.8, 114.6, 67.2, 40.1. HRMS: m/z (ESI) calculated $[M+Na]^+$ 352.0614, measured 352.0614.

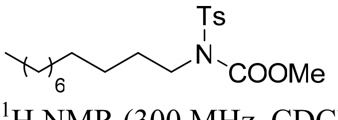


^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (m, 3H), 7.95-7.80 (m, 3H), 7.61-7.41 (m, 3H), 6.13 (dt, *J* = 15.3, 5.1Hz, 1H), 6.01 (dt, *J* = 15.6, 6.0 Hz, 1H), 4.85 (d, *J* = 4.8 Hz, 2H). 4.43 (d, *J* = 6.0 Hz, 2H). $^{13}C\{1H\}$ NMR (75 MHz, $CDCl_3$) δ166.1, 158.5, 137.6, 134.8, 134.3, 133.0, 129.8, 129.6, 129.5, 128.4, 128.3, 126.1, 125.2, 120.9, 64.0, 40.0.
HRMS: m/z (ESI) calculated $[M+Na]^+$ 380.0574, measured 380.0563.

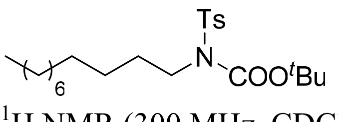


^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.4 Hz, 1H), 7.91-7.78 (m, 3H), 4.67 (quant, *J* = 8.7 Hz, 1H), 2.29-2.11 (m, 4H). 1.95 (m, 2H), 1.67 (m, 2H). $^{13}C\{1H\}$ NMR (75 MHz, $CDCl_3$) δ159.0, 137.7, 134.5, 134.1, 127.4, 124.8, 120.6, 54.5, 29.4, 24.0. HRMS: m/z (ESI) calculated $[M+Na]^+$ 274.0503, measured 274.0508.

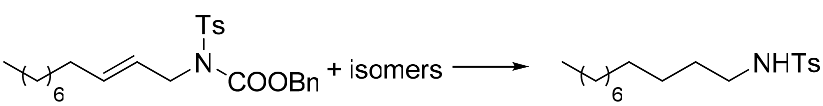




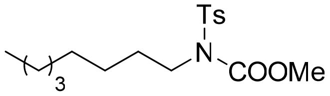
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 3.81 (t, *J* = 7.5 Hz, 2H), 3.69 (s, 3H), 2.44 (s, 3H), 1.73 (m, 2H), 1.30 (m, 16H), 0.88 (t, *J* = 6.0 Hz, 3H). $^{13}C\{1H\}$ NMR (75 MHz, $CDCl_3$) δ 152.9, 144.4, 136.6, 129.3, 128.3, 53.7, 47.5, 31.9, 30.1, 29.6, 29.5, 29.3, 29.2, 26.6, 22.7, 21.6, 14.2. HRMS: m/z (ESI) calculated $[M+Na]^+$ 406.2039, measured 406.2023.



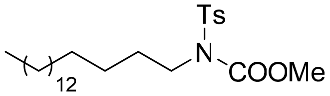
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 3.73 (t, *J* = 7.5 Hz, 2H), 2.36 (s, 3H), 1.67 (m, 2H), 1.26 (m, 25H), 0.81 (t, *J* = 6.3 Hz, 3H). $^{13}C\{1H\}$ NMR (75 MHz, $CDCl_3$) δ 150.9, 143.9, 137.5, 129.1, 127.7, 83.9, 47.2, 31.8, 30.1, 29.5, 29.4, 29.3, 29.2, 27.8, 26.6, 22.6, 21.5, 14.1. HRMS: m/z (ESI) calculated $[M+Na]^+$ 448.2491, measured 448.2492.



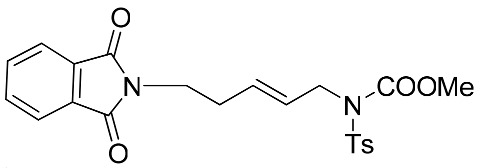
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 4.78 (br s, 1H), 2.90 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.44 (m, 2H), 1.24 (m, 16H), 0.88 (t, *J* = 6.0 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ143.2, 136.9, 129.6, 127.1, 43.2, 31.9, 29.5, 29.4, 29.38, 29.25, 29.0, 26.4, 22.6, 21.5, 14.1. HRMS: m/z (EI) calculated $[M]^+$ 325.2076, measured 325.2070.



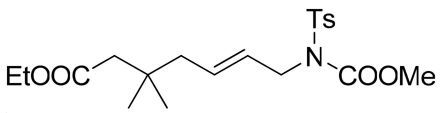
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 3.81 (t, *J* = 7.5 Hz, 2H), 3.69 (s, 3H), 2.44 (s, 3H), 1.73 (m, 2H), 1.30 (m, 10H), 0.88 (t, *J* = 6.0 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 152.9, 144.4, 136.6, 129.3, 128.3, 53.7, 47.5, 31.8, 30.0, 29.2, 29.1, 26.5, 22.6, 21.6, 14.1. HRMS: m/z (ESI) calculated $[M+Na]^+$ 364.1549, measured 364.1553.



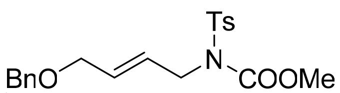
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 3.81 (t, *J* = 7.5 Hz, 2H), 3.69 (s, 3H), 2.44 (s, 3H), 1.73 (m, 2H), 1.30 (m, 28H), 0.88 (t, *J* = 6.0 Hz, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 152.9, 144.5, 136.6, 129.3, 128.3, 53.7, 47.5, 31.9, 30.1, 29.7, 29.65, 29.56, 29.51, 29.3, 29.2 26.6, 22.7, 21.6, 14.1. HRMS: m/z (ESI) calculated $[M+Na]^+$ 490.2965, measured 490.2962.



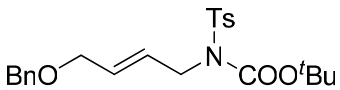
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (m, 4H), 7.71 (dd, *J* = 7.2, 5.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 5.76 (dt, *J* = 15.3, 6.6 Hz, 1H), 5.63 (dt, *J* = 15.3, 6.0 Hz, 1H), 4.37 (d, *J* = 6.0 Hz, 2H), 3.76 (t, *J* = 6.9 Hz, 2H), 3.67 (s, 3H), 2.47 (m, 2H), 2.43 (s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 168.2, 152.5, 144.5, 136.3, 133.9, 131.9, 130.8, 129.2, 128.4, 127.4, 123.2, 53.7, 48.3, 37.1, 31.3, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 465.1089, measured 465.1091.



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 7H), 5.82 (dt, *J* = 15.3, 7.5 Hz, 1H), 5.57 (dt, *J* = 15.3, 6.0 Hz, 1H), 4.43 (d, *J* = 6.0 Hz, 2H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.69 (s, 3H), 2.43 (s, 3H), 2.17 (s, 2H), 2.09 (d, *J* = 7.5 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H), 0.99 (s, 6H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 172.1, 152.6, 144.4, 131.5, 129.3, 129.2, 128.3, 127.5, 59.9, 53.7, 48.5, 45.6, 44.5, 33.6, 27.0, 21.6, 14.2. HRMS: m/z (ESI) calculated $[M+Na]^+$ 434.1610, measured 434.1608.

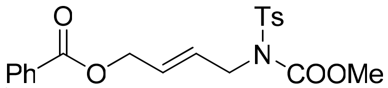


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.37-7.24 (m, 7H), 5.89 (m, 2H), 4.52 (s, 2H), 4.47 (d, *J* = 5.4 Hz, 2H), 4.03 (d, *J* = 5.4 Hz, 2H), 3.69 (s, 3H), 2.41 (s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 152.6, 144.6, 138.1, 136.3, 130.9, 129.3, 128.5, 128.4, 127.7, 127.6, 127.3, 72.2, 69.7, 53.8, 48.0, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 412.1205, measured 412.1189.

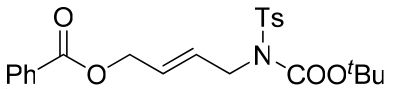


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.35-7.24 (m, 7H), 5.87 (m, 2H), 4.52 (s, 2H), 4.46 (d, *J* = 4.8 Hz, 2H), 4.05 (d, *J* = 4.2 Hz, 2H), 2.41 (s, 3H), 1.34 (s, 9H). ^{13}C{1H} NMR (75 MHz,

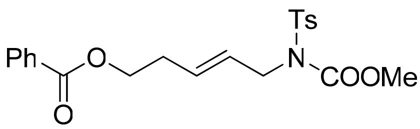
$CDCl_3$) δ 150.7, 144.1, 138.2, 137.1, 130.6, 129.1, 128.3, 128.0, 127.9, 127.7, 127.6, 84.2, 72.0, 69.7, 47.8, 27.8, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 454.1669, measured 454.1659.



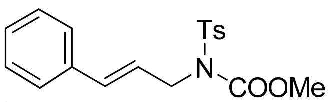
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.4 Hz, 2H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 5.97 (m, 2H), 4.84 (d, *J* = 4.8 Hz, 2H), 4.51 (d, *J* = 5.1 Hz, 2H), 3.70 (s, 3H), 2.40 (s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 166.1, 152.5, 144.7, 136.2, 133.0, 129.9, 129.6, 129.3, 128.7, 128.5, 128.4, 128.3, 64.2, 53.9, 47.8, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 426.0980, measured 426.0982.



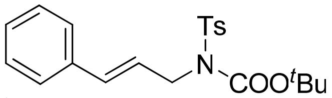
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.8 Hz, 2H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 5.97 (m, 2H), 4.85 (d, *J* = 3.6 Hz, 2H), 4.49 (d, *J* = 3.6 Hz, 2H), 2.40 (s, 3H), 1.34 (s, 9H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 166.1, 150.6, 144.2, 136.9, 133.0, 130.0, 129.6, 129.3, 129.2, 128.4, 128.1, 128.0, 84.4, 64.4, 47.5, 27.8, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 468.1458, measured 468.1451.



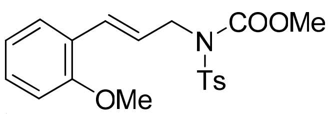
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.5 Hz, 2H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 5.85 (dt, *J* = 15.3, 6.3Hz, 1H), 5.71 (dt, *J* = 15.3, 6.3 Hz, 1H), 4.44 (d, *J* = 5.7 Hz, 2H), 4.36 (t, *J* = 6.6 Hz, 2H), 3.66 (s, 3H), 2.53 (q, *J* = 6.6 Hz, 2H), 2.41 (s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 166.4, 152.5, 144.5, 136.3, 132.8, 130.5, 130.1, 129.4, 129.2, 128.3, 128.2, 127.3, 63.7, 53.7, 48.3, 31.5, 21.5. HRMS: m/z (ESI) calculated $[M+Na]^+$ 440.1137, measured 440.1138.



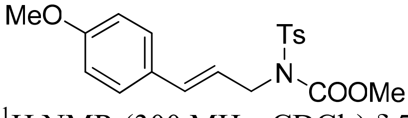
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.4 Hz, 2H), 7.40-7.24 (m, 7H), 6.68 (d, *J* = 15.9 Hz, 1H), 6.25 (dt, *J* = 15.9, 6.6 Hz, 1H), 4.63 (d, *J* = 6.6 Hz, 2H), 3.72 (s, 3H), 2.41 (s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 152.6, 144.6, 136.2, 136.1, 134.0, 129.3, 128.5, 128.45, 127.9, 126.5, 123.7, 53.8, 48.7, 21.5. HRMS: m/z (ESI) calculated $[M+Na]^+$ 368.0925, measured 368.0927.



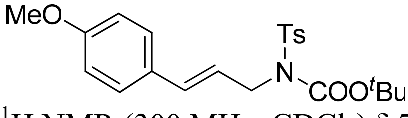
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.4 Hz, 2H), 7.40-7.24 (m, 7H), 6.67 (d, *J* = 15.6 Hz, 1H), 6.28 (dt, *J* = 15.6, 6.3 Hz, 1H), 4.60 (d, *J* = 6.3 Hz, 2H), 2.42 (s, 3H), 1.36 (s, 9H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 150.8, 144.1, 137.2, 136.4, 133.9, 129.2, 128.6, 128.1, 127.9, 126.6, 124.2, 84.3, 48.5, 27.9, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 410.1413, measured 410.1397.



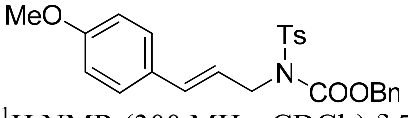
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.01 (d, *J* = 15.9 Hz, 1H), 6.90 (m, 2H), 6.24 (dt, *J* = 15.9, 6.6 Hz, 1H), 4.63 (d, *J* = 6.6 Hz, 2H), 3.85 (s, 3H), 3.71 (s, 3H), 2.40 (s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 156.8, 152.7, 144.4, 136.4, 129.3, 129.2, 129.0, 128.6, 127.0, 125.2, 124.2, 120.5, 110.8, 55.4, 53.8, 49.2, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 398.1033, measured 398.1032.



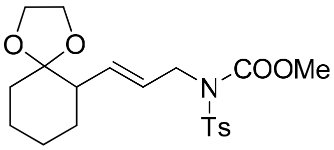
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.7 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.63 (d, *J* = 15.9 Hz, 1H), 6.10 (dt, *J* = 15.9, 6.6 Hz, 1H), 4.60 (d, *J* = 6.6 Hz, 2H), 3.82 (s, 3H), 3.71 (s, 3H), 2.41 (s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 159.5, 152.7, 144.5, 136.4, 133.7, 129.3, 129.0, 128.6, 127.8, 121.4, 114.0, 55.3, 53.9, 48.9, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 398.1033, measured 398.1033.



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.7 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.62 (d, *J* = 15.6 Hz, 1H), 6.15 (dt, *J* = 15.6, 6.6 Hz, 1H), 4.57 (d, *J* = 6.6 Hz, 2H), 3.82 (s, 3H), 2.41 (s, 3H), 1.35 (s, 9H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 159.4, 150.8, 144.0, 137.2, 133.5, 130.3, 129.1, 128.0, 127.7, 121.9, 113.9, 84.2, 55.2, 48.6, 27.9, 21.5. HRMS: m/z (ESI) calculated $[M+Na]^+$ 440.1498, measured 440.1502.

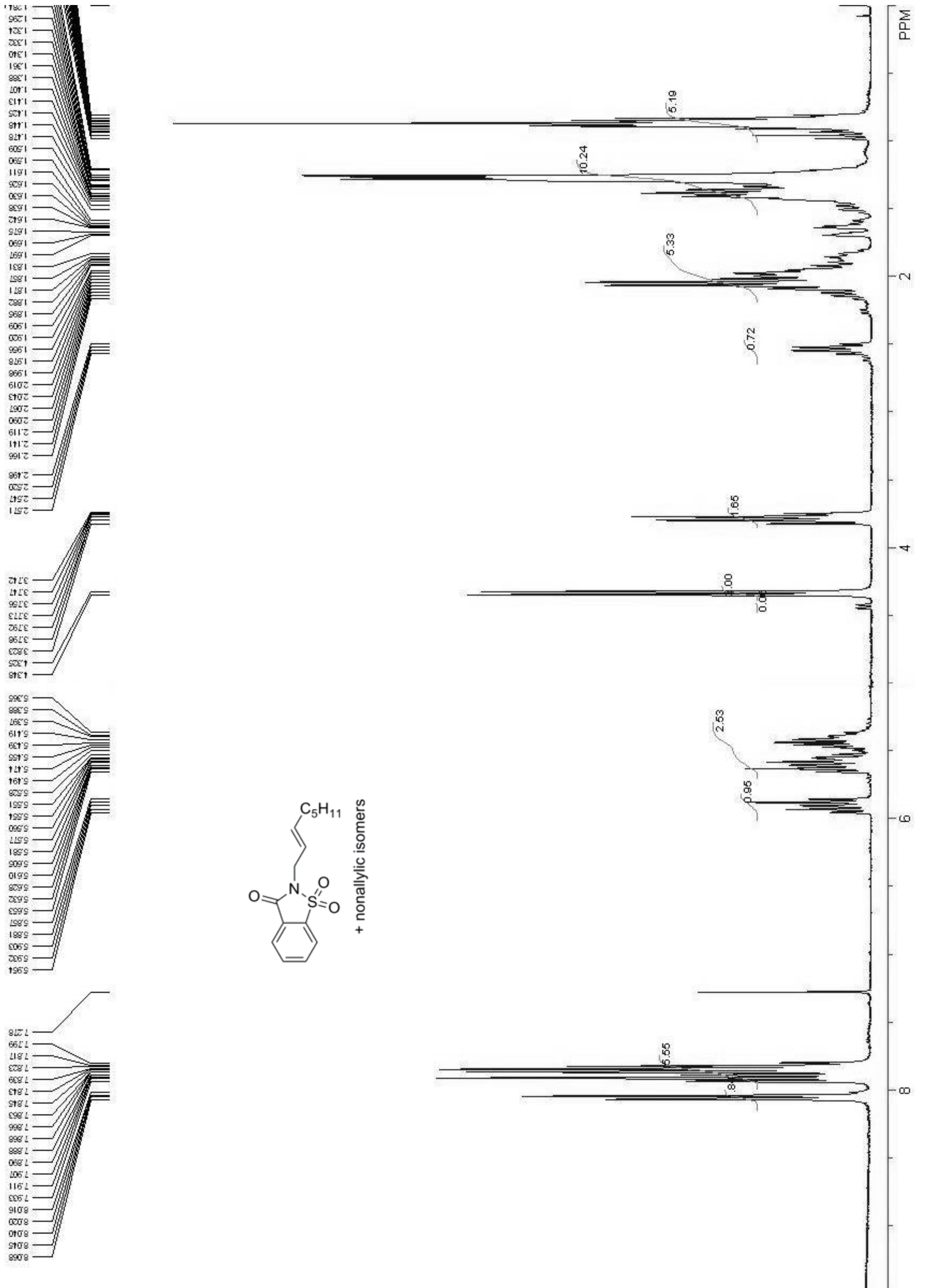


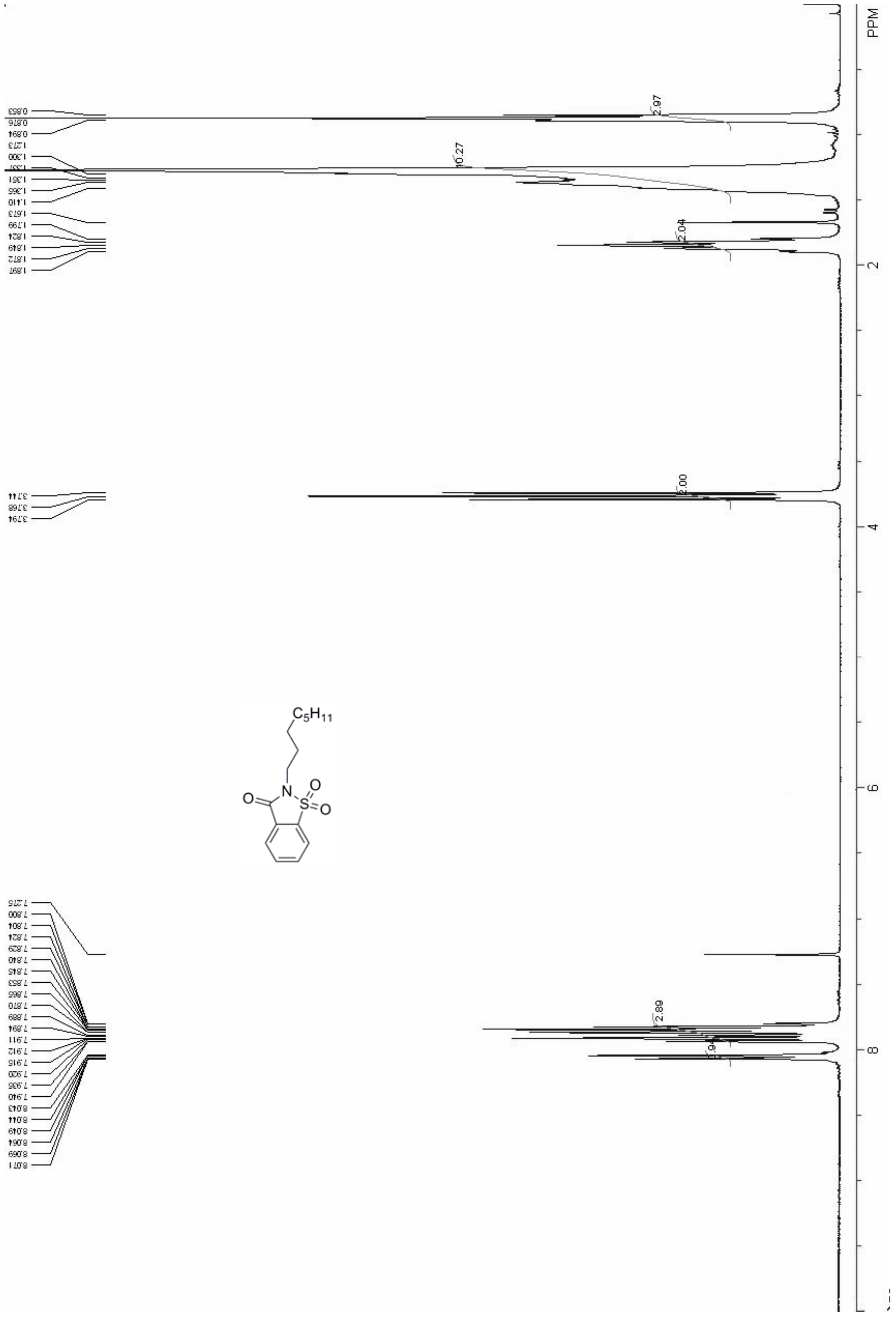
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.34-7.14 (m, 9H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.58 (d, *J* = 15.9 Hz, 1H), 6.11 (dt, *J* = 15.9, 6.9 Hz, 1H), 5.10 (s, 2H), 4.61 (d, *J* = 6.9 Hz, 2H), 3.82 (s, 3H), 2.38 (s, 3H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 159.4, 152.1, 144.4, 136.3, 134.5, 133.8, 129.2, 128.9, 128.5, 128.4, 128.3, 127.8, 121.3, 113.9, 68.9, 55.2, 48.9, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 474.1351, measured 474.1346.

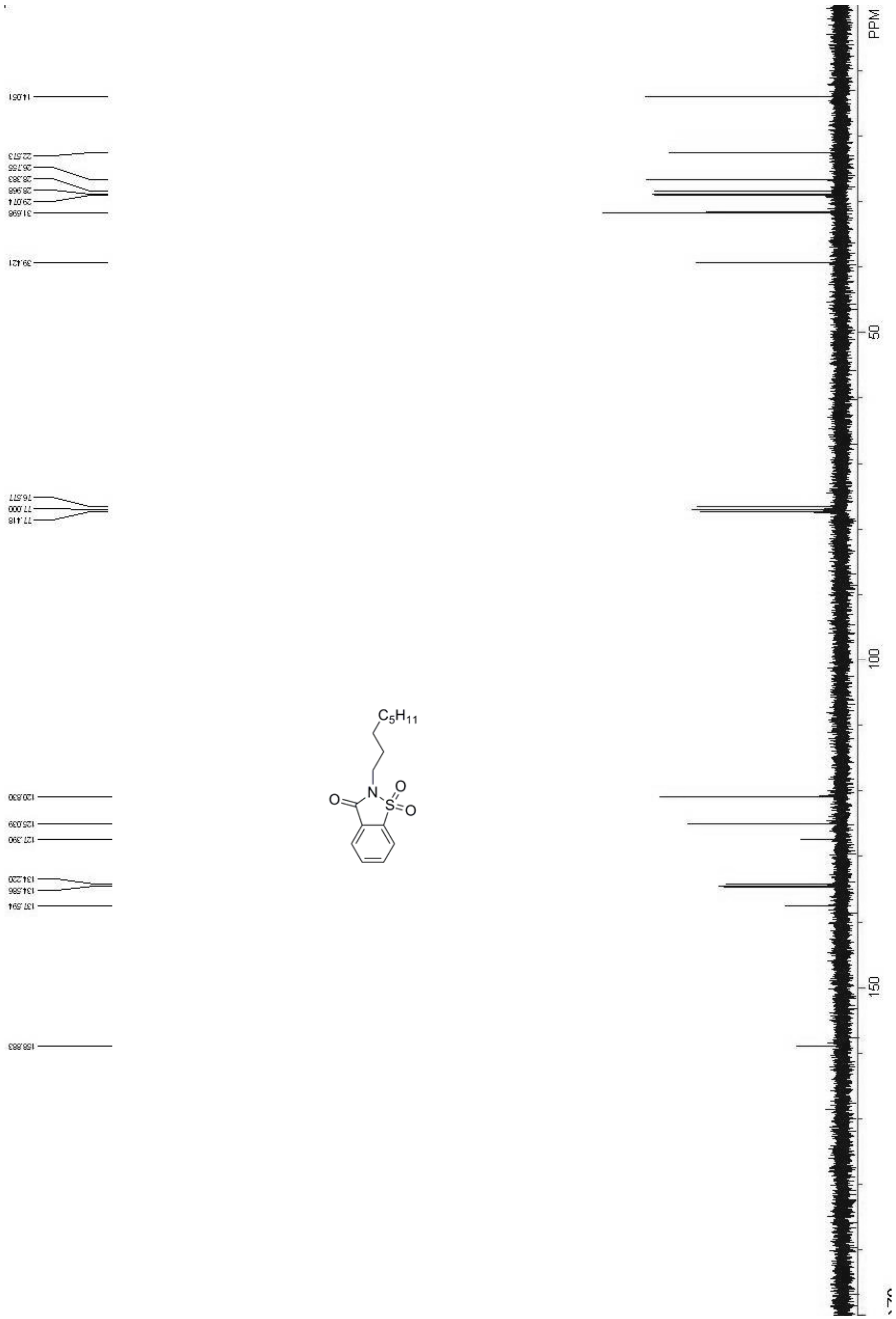


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 5.82 (dd, *J* = 15.6, 7.8 Hz, 1H), 5.50 (dt, *J* = 15.6, 6.3 Hz, 1H), 4.37 (d, *J* = 6.3 Hz, 2H), 3.87 (m, 4H), 3.61 (s, 3H), 2.37 (s, 3H), 2.25 (m, 1H), 1.72-1.20 (m, 8H). ^{13}C{1H} NMR (75 MHz, $CDCl_3$) δ 152.6, 144.4, 136.5, 135.1, 129.2, 128.5, 125.4, 109.8, 65.1, 64.9, 53.7, 48.8, 48.3, 35.3, 30.0, 24.4, 23.8, 21.6. HRMS: m/z (ESI) calculated $[M+Na]^+$ 432.1459, measured 432.1451.

[S1] B. M. Trost, P. J. Metzner, *J. Am. Chem. Soc.* **1980**, *102*, 3572-3577.


+ nonallylic isomers
PPM
2
4
6
8
5.19
10.24
5.33
0.72
1.65
2.53
0.95
5.55




PPM
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100
150
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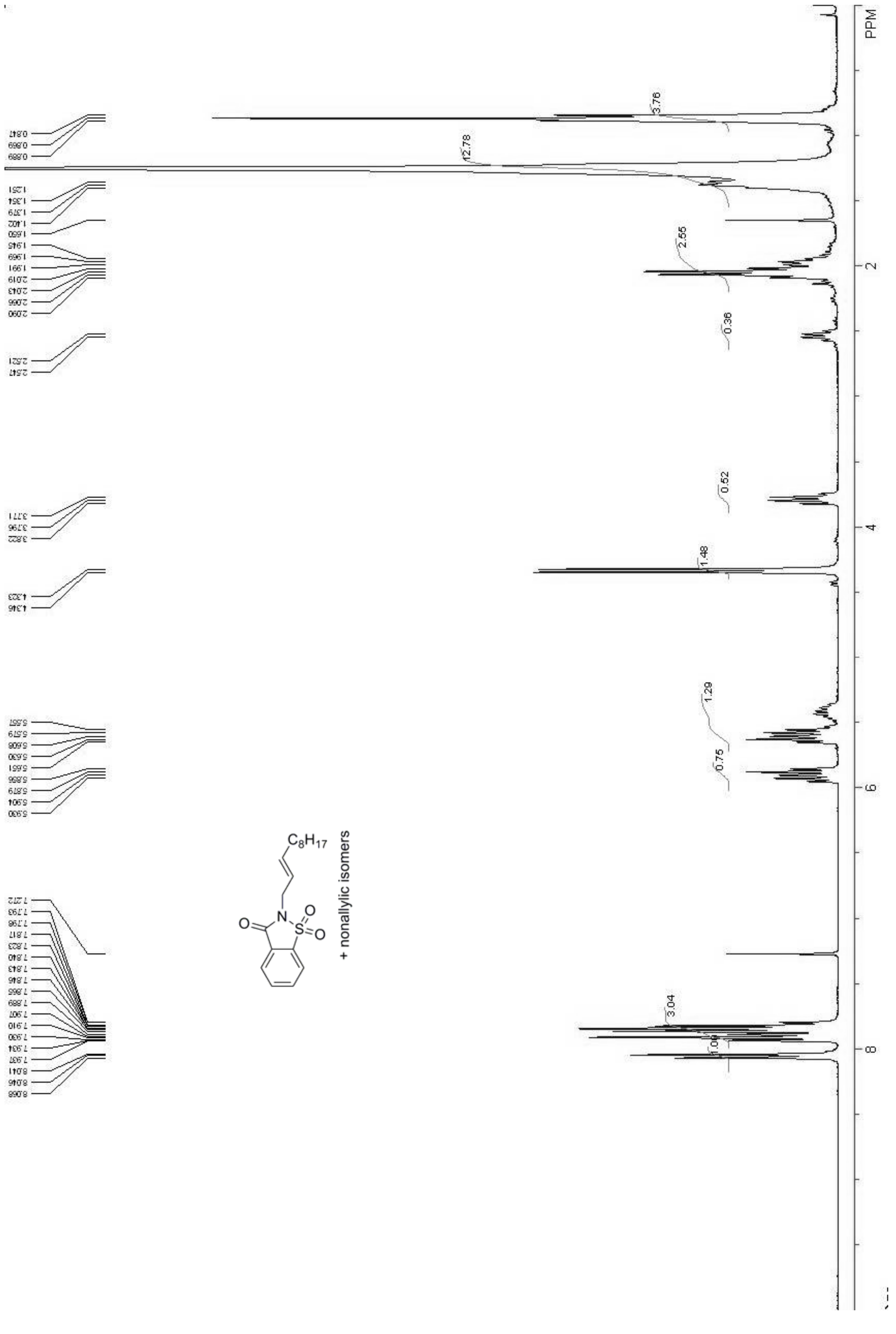
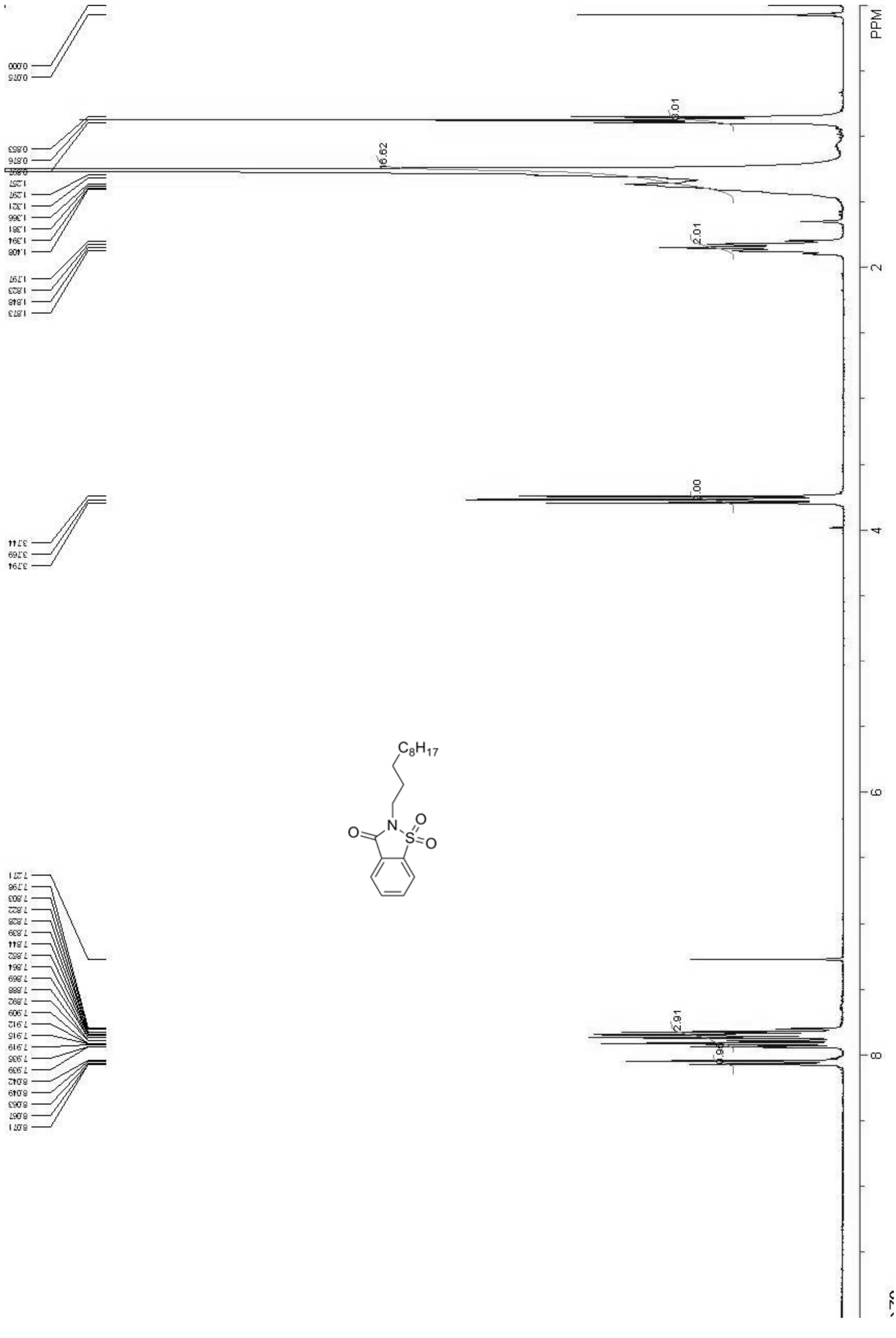
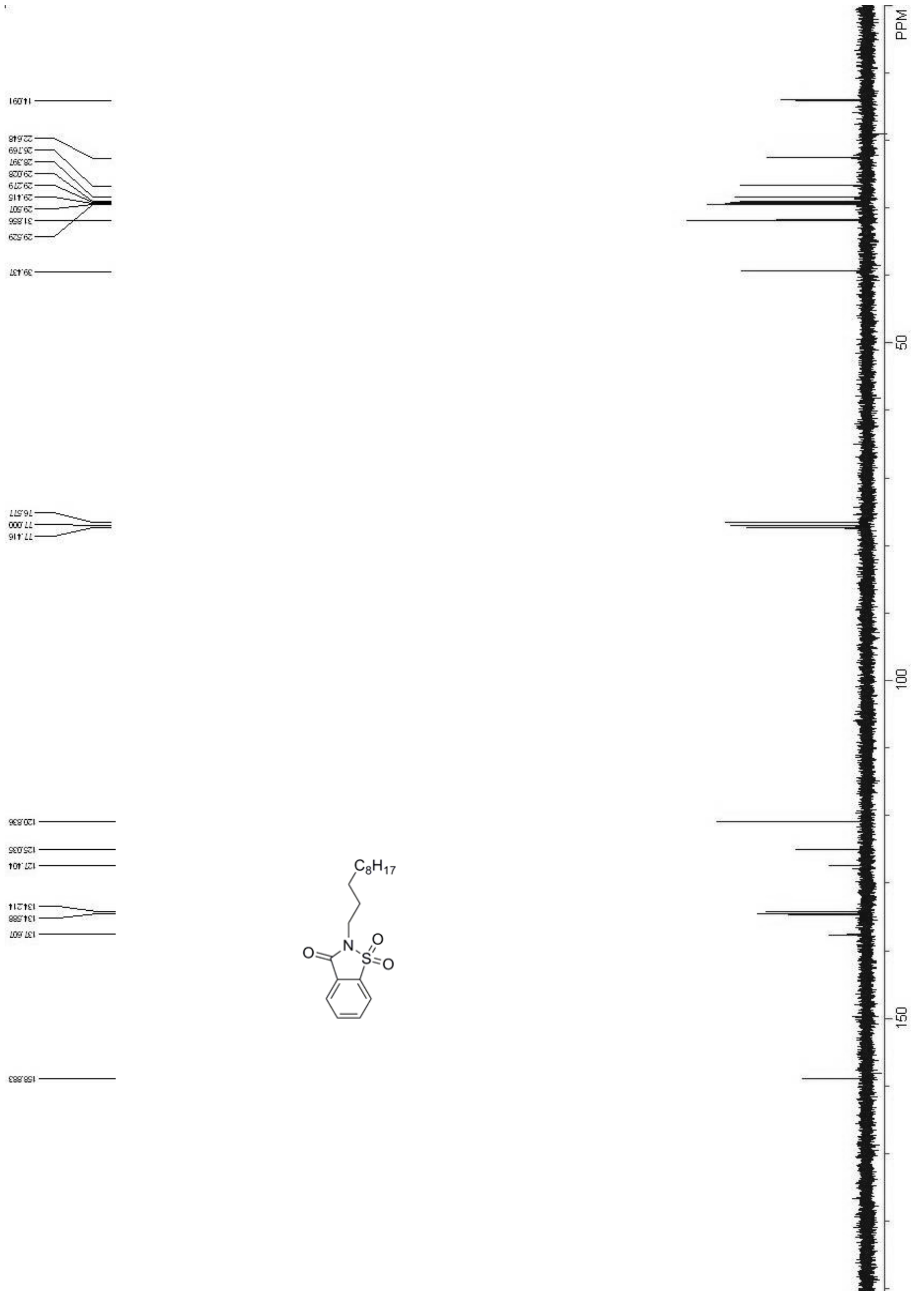
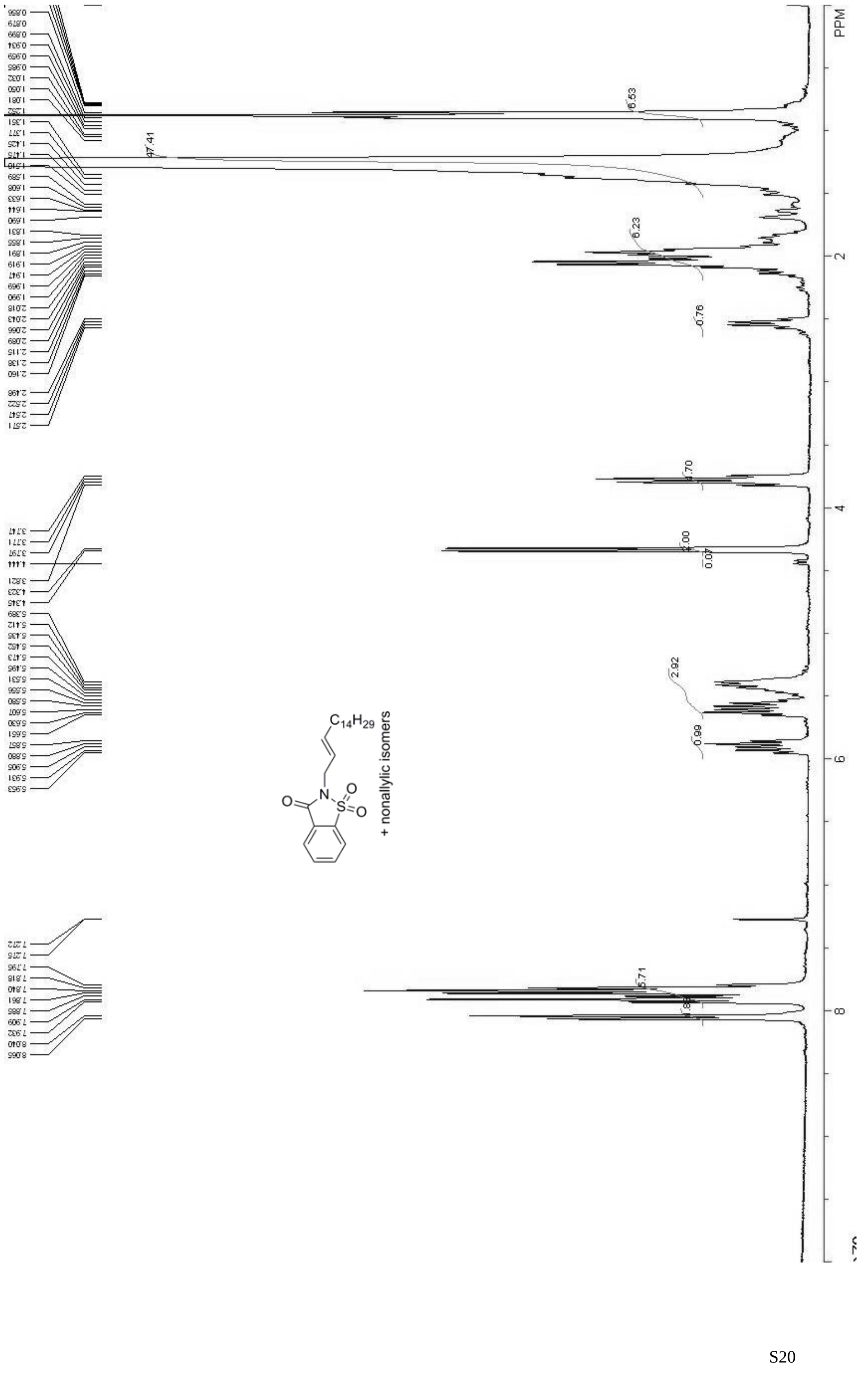
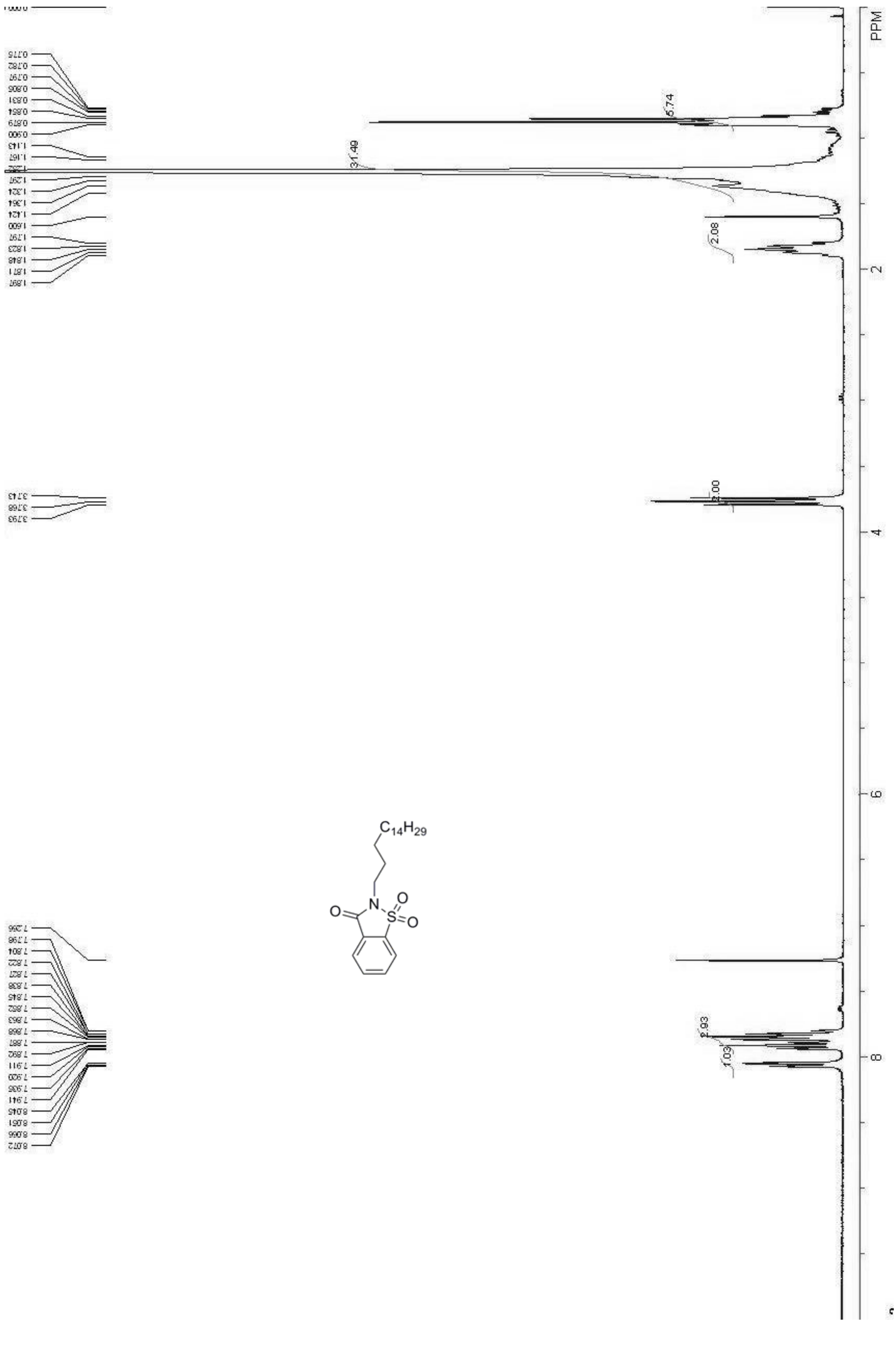
22.573
26.755
28.383
28.968
29.014
31.698
39.121
76.577
77.000
77.418
120.830
125.039
127.390
134.220
134.586
137.594
158.863
C5H11
O
N
S
O
O


+ nonallylic isomers
PPM




PPM
50
100
150
C8H17
N
S
O
O
O


+ nonallylic isomers
PPM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6
8
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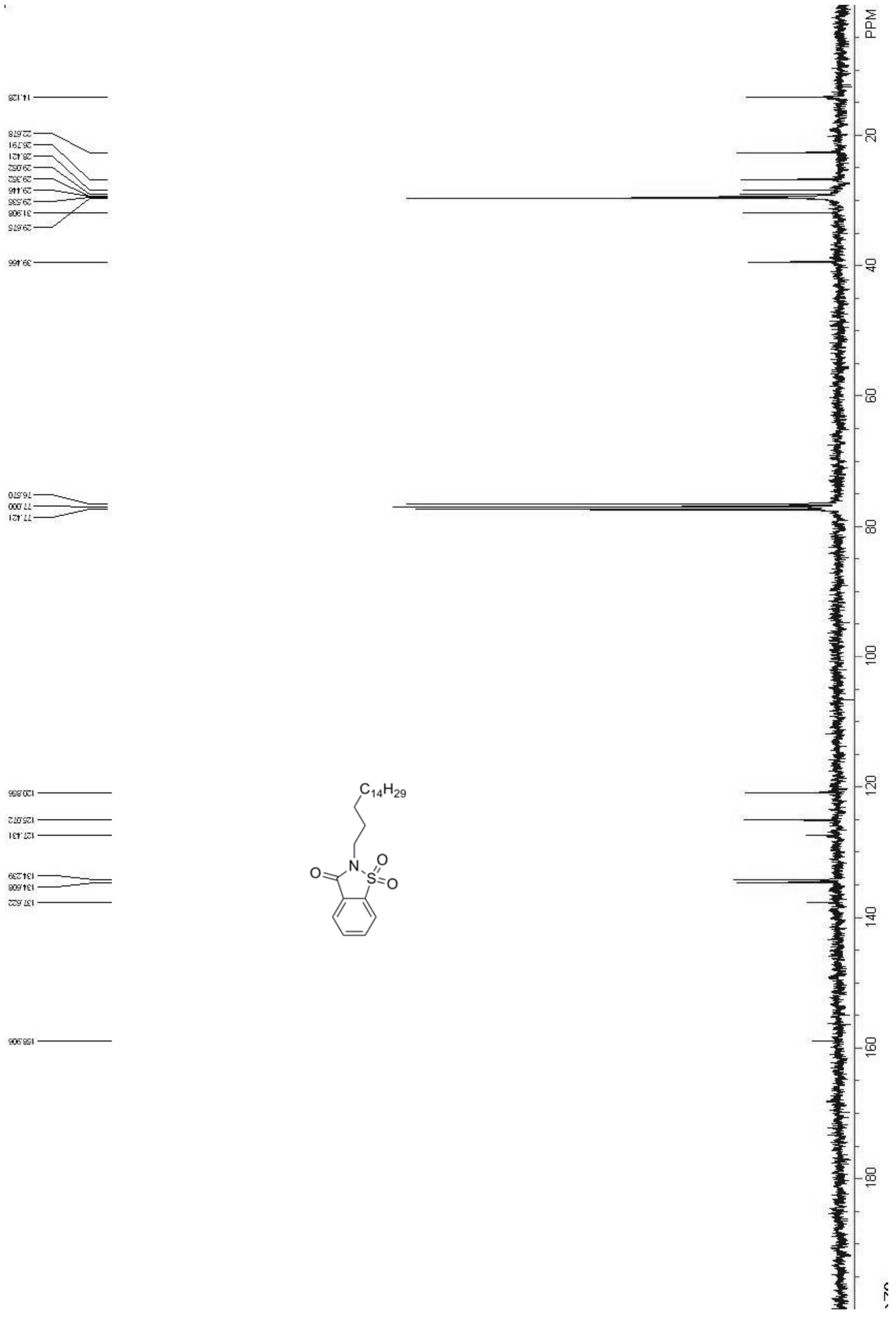
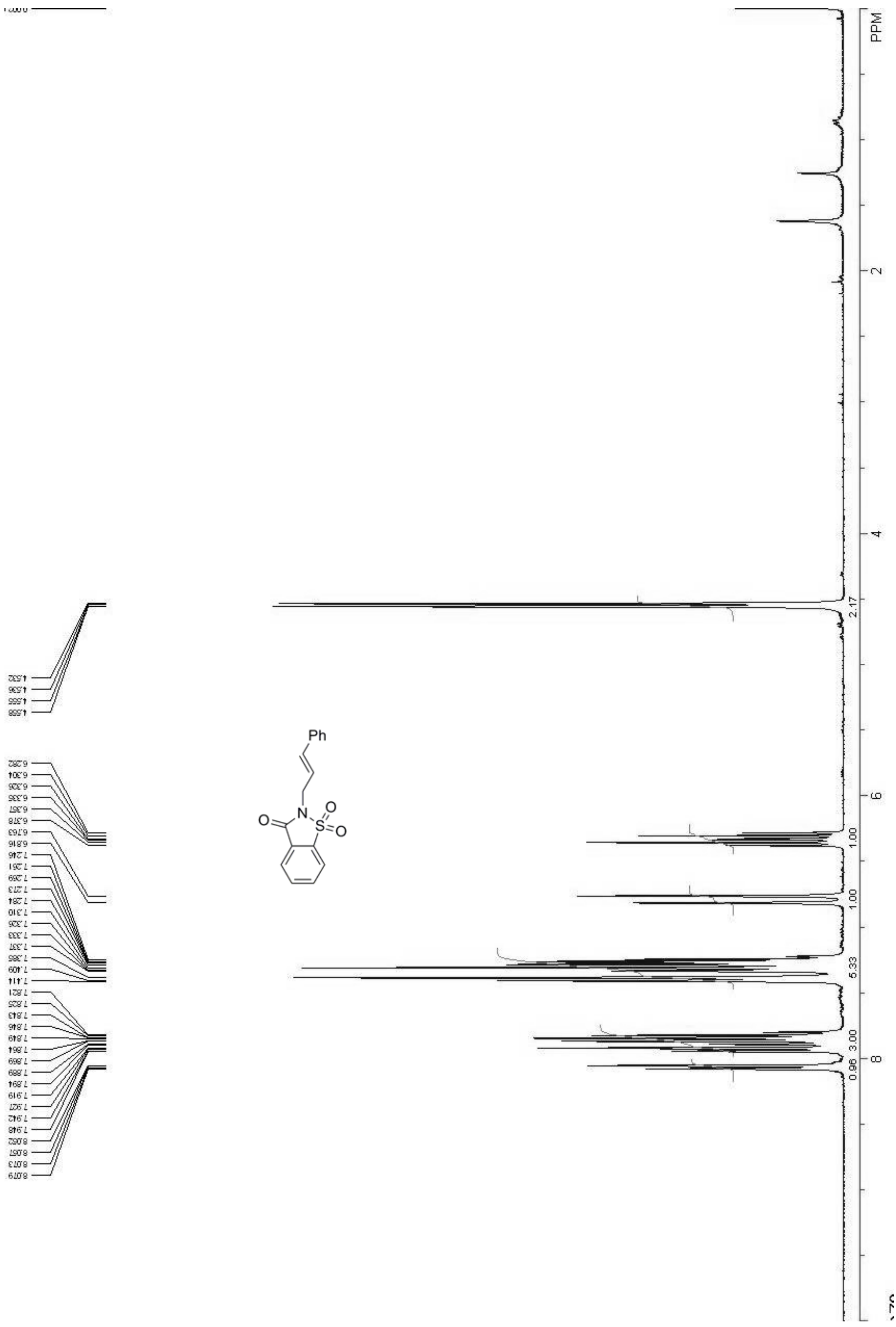
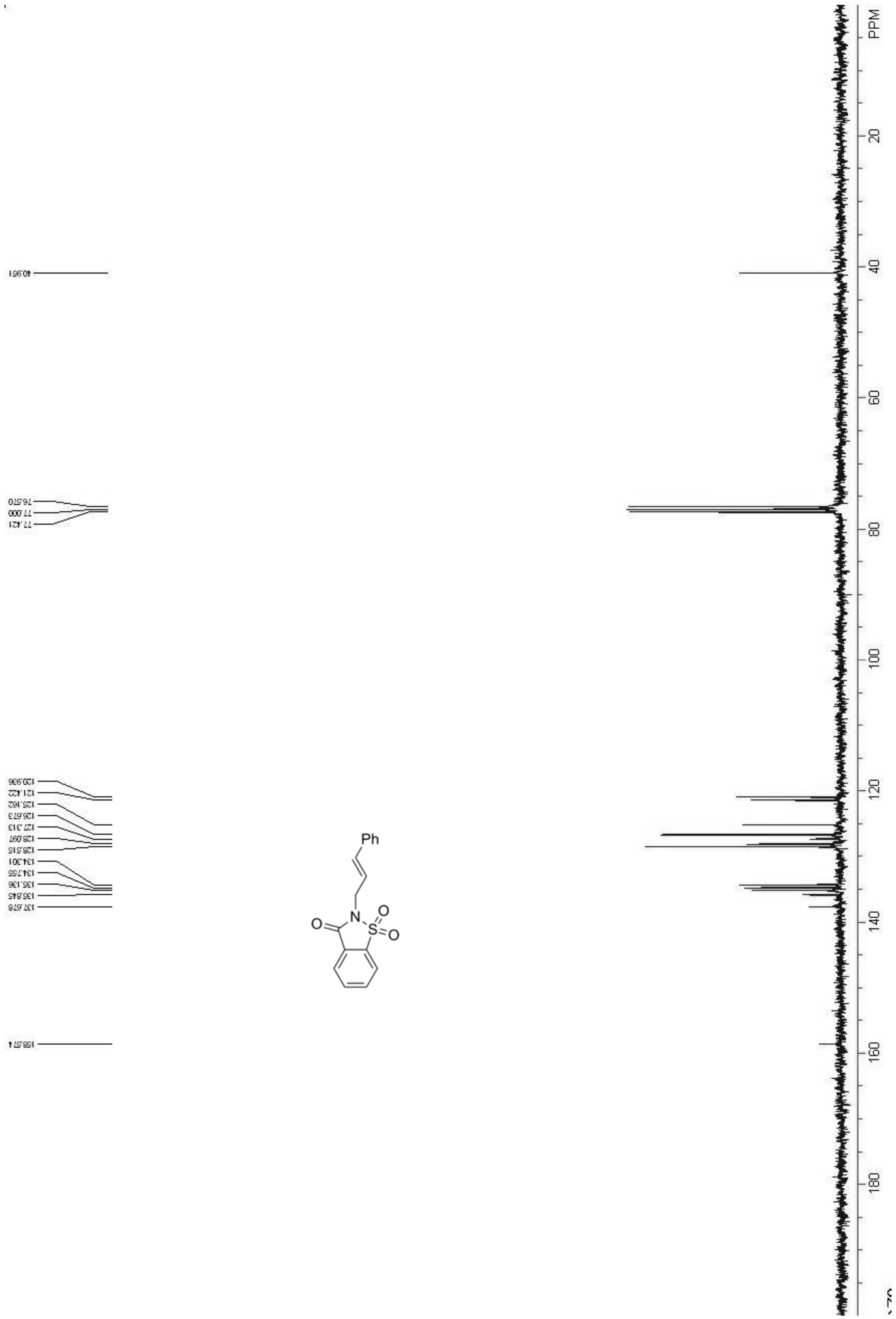
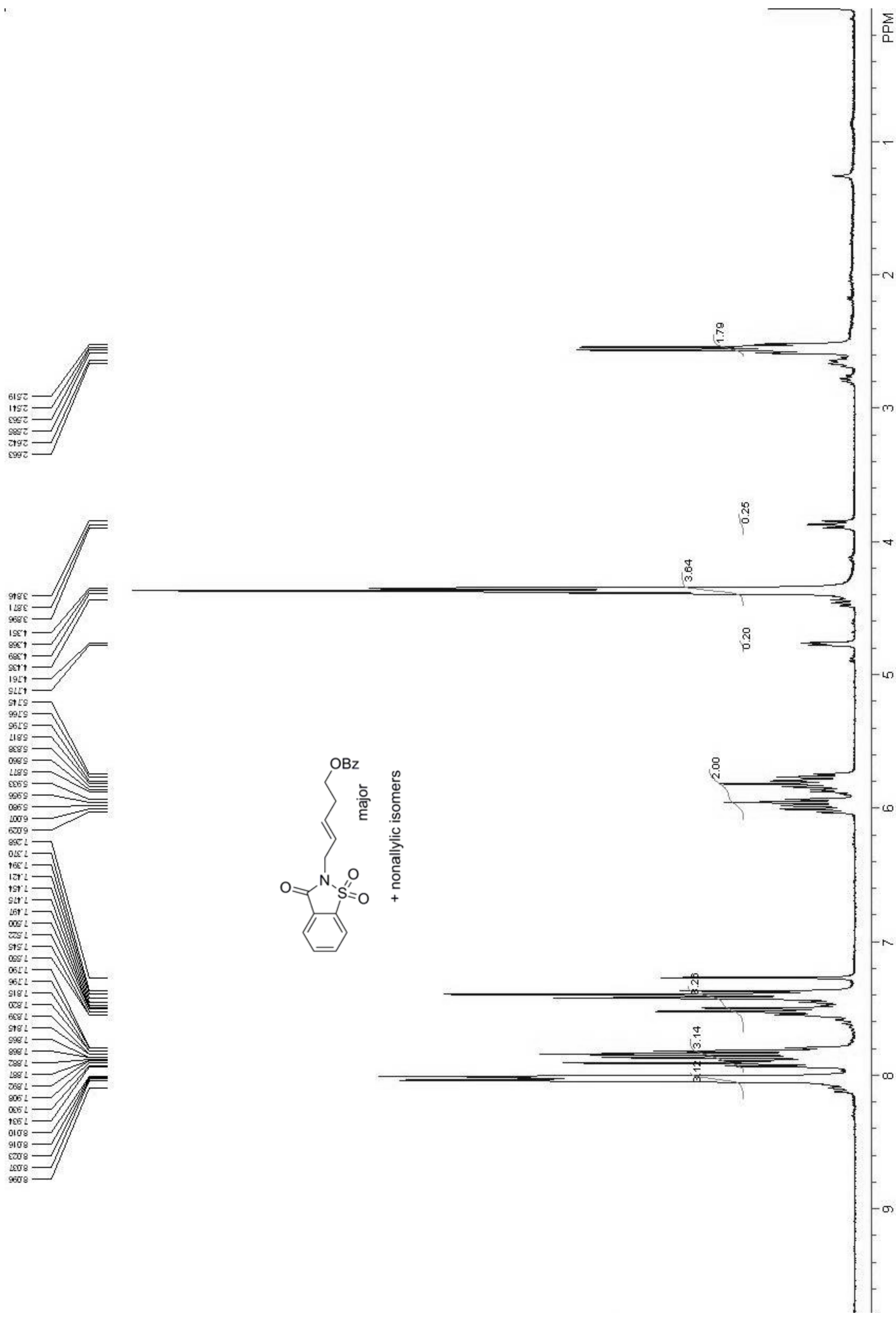
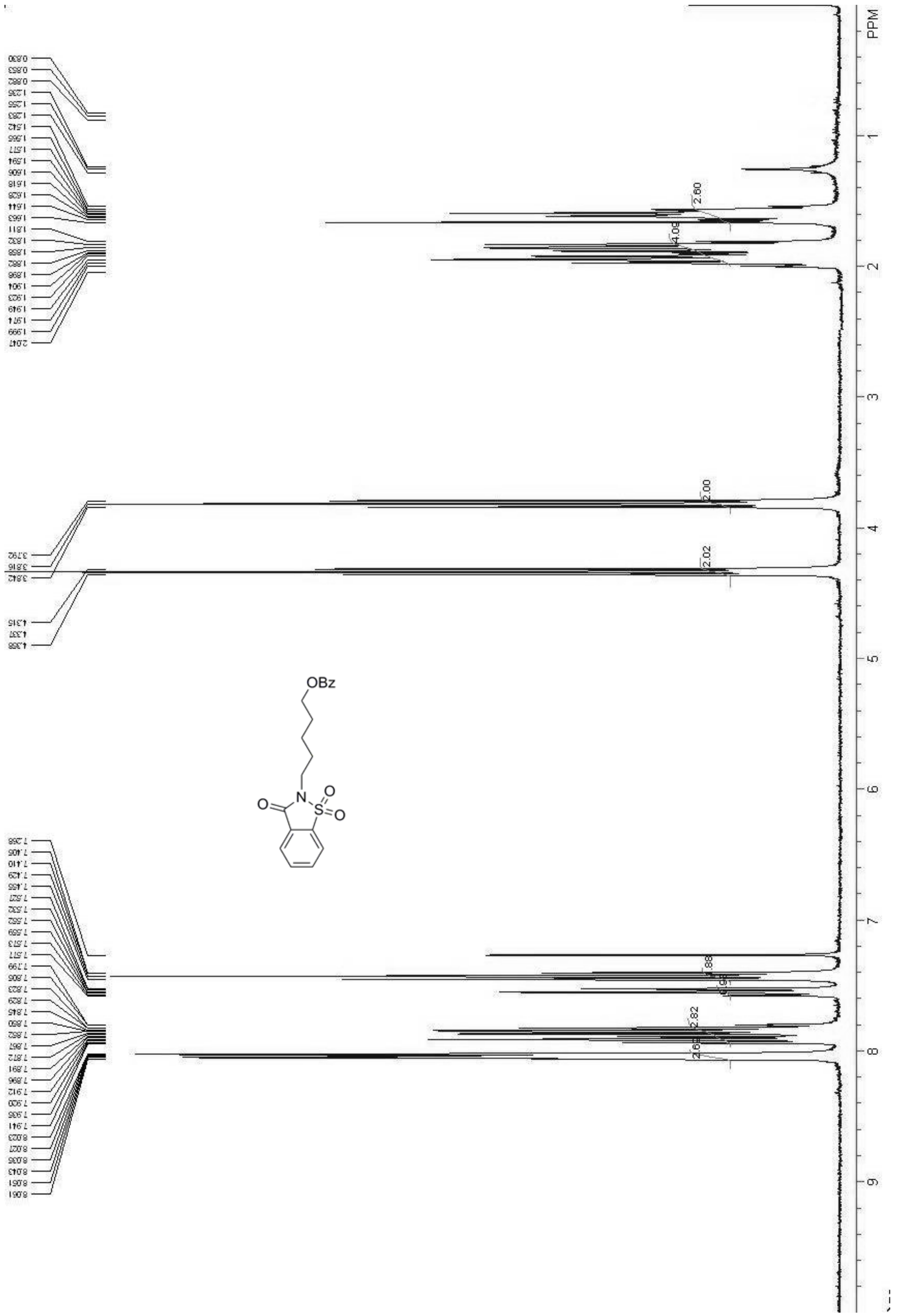
31.49
2.08
2.00
2.93
1.03
C14H29
N
S
O

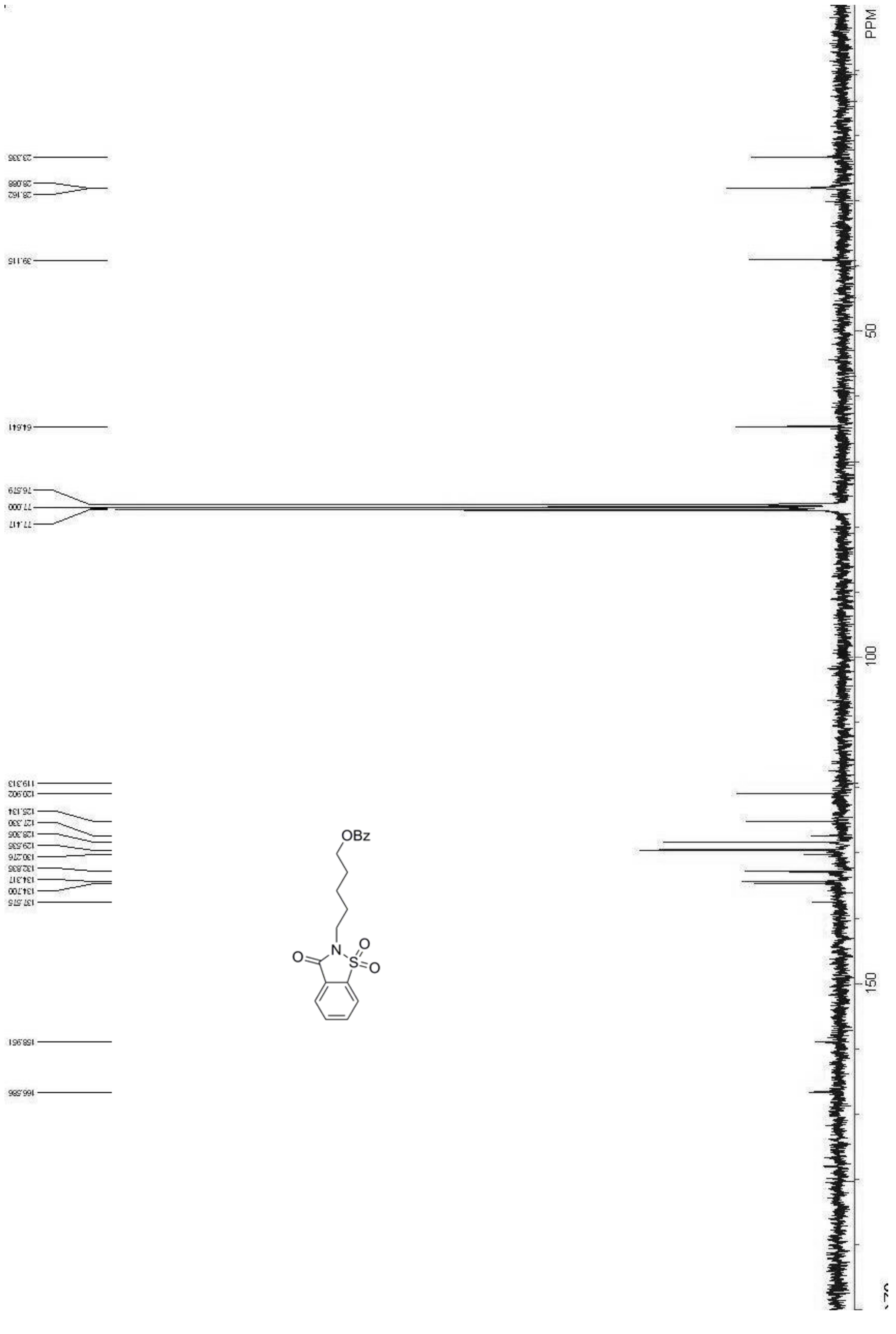



Ph
N
S
O
PPM
2
4
6
8
2.17
1.00
1.00
5.33
3.00
0.96




OBz
major
+ nonallylic isomers
PPM
1.79
0.25
3.64
0.20
2.00
3.14
3.12


OBz
PPM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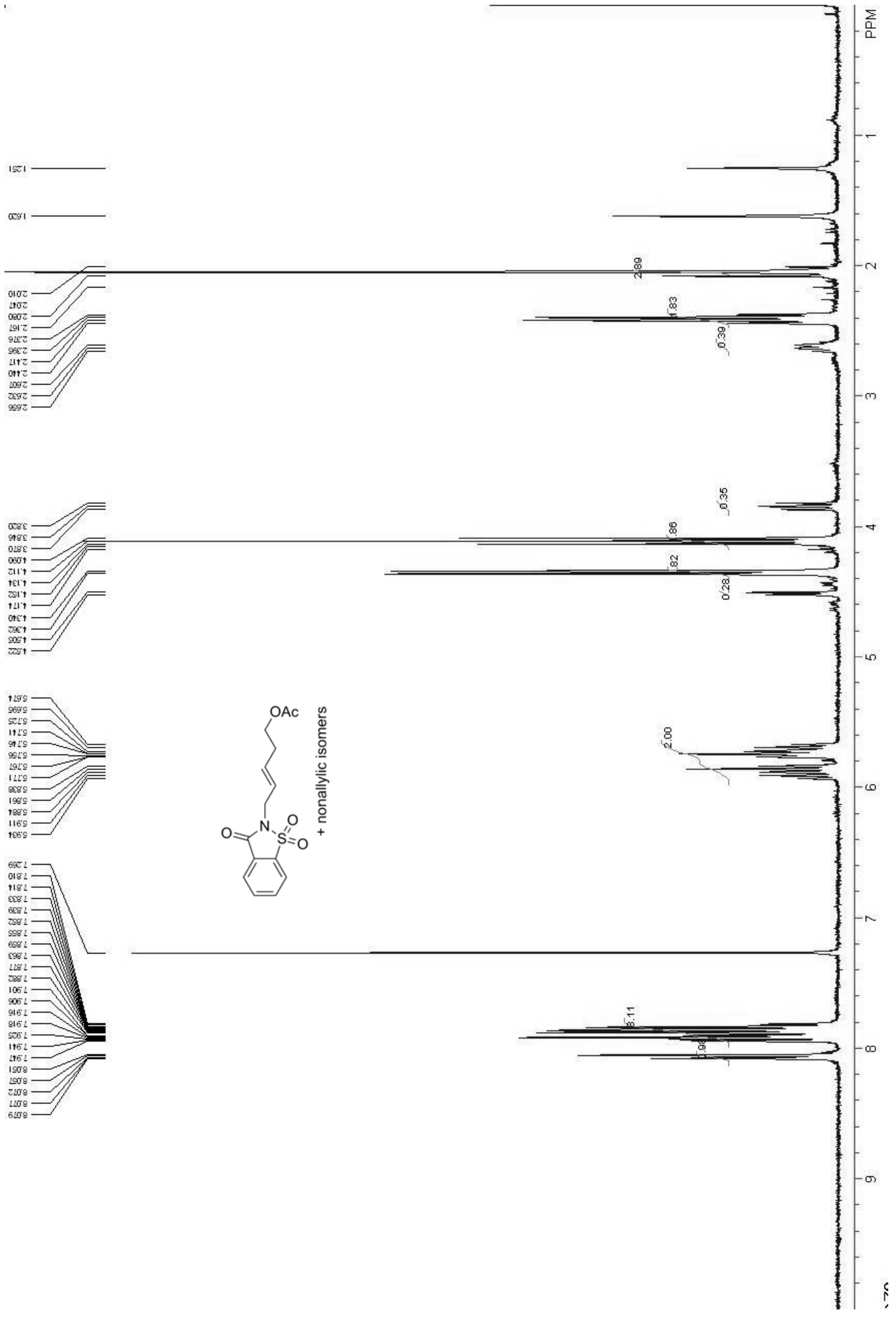
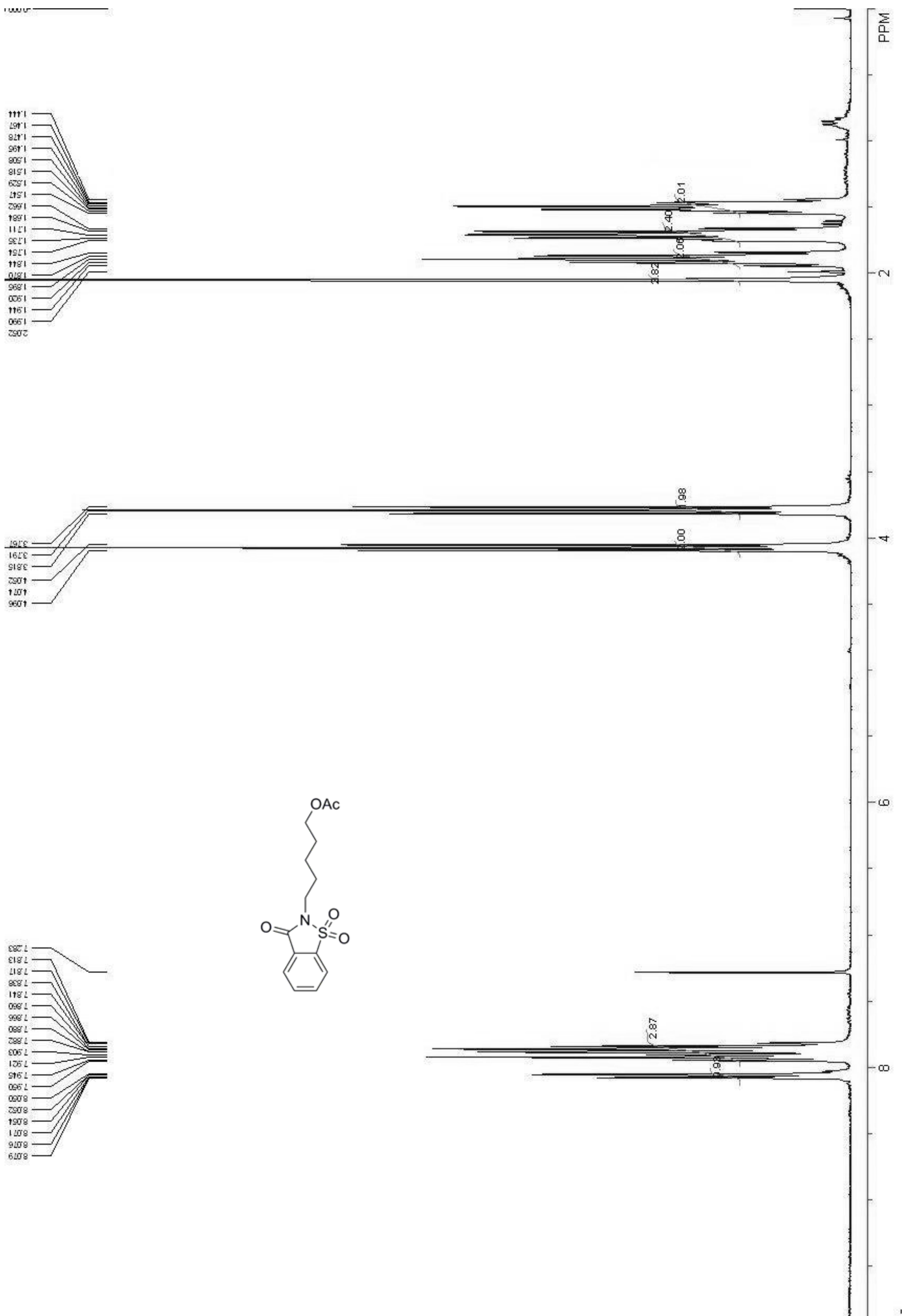
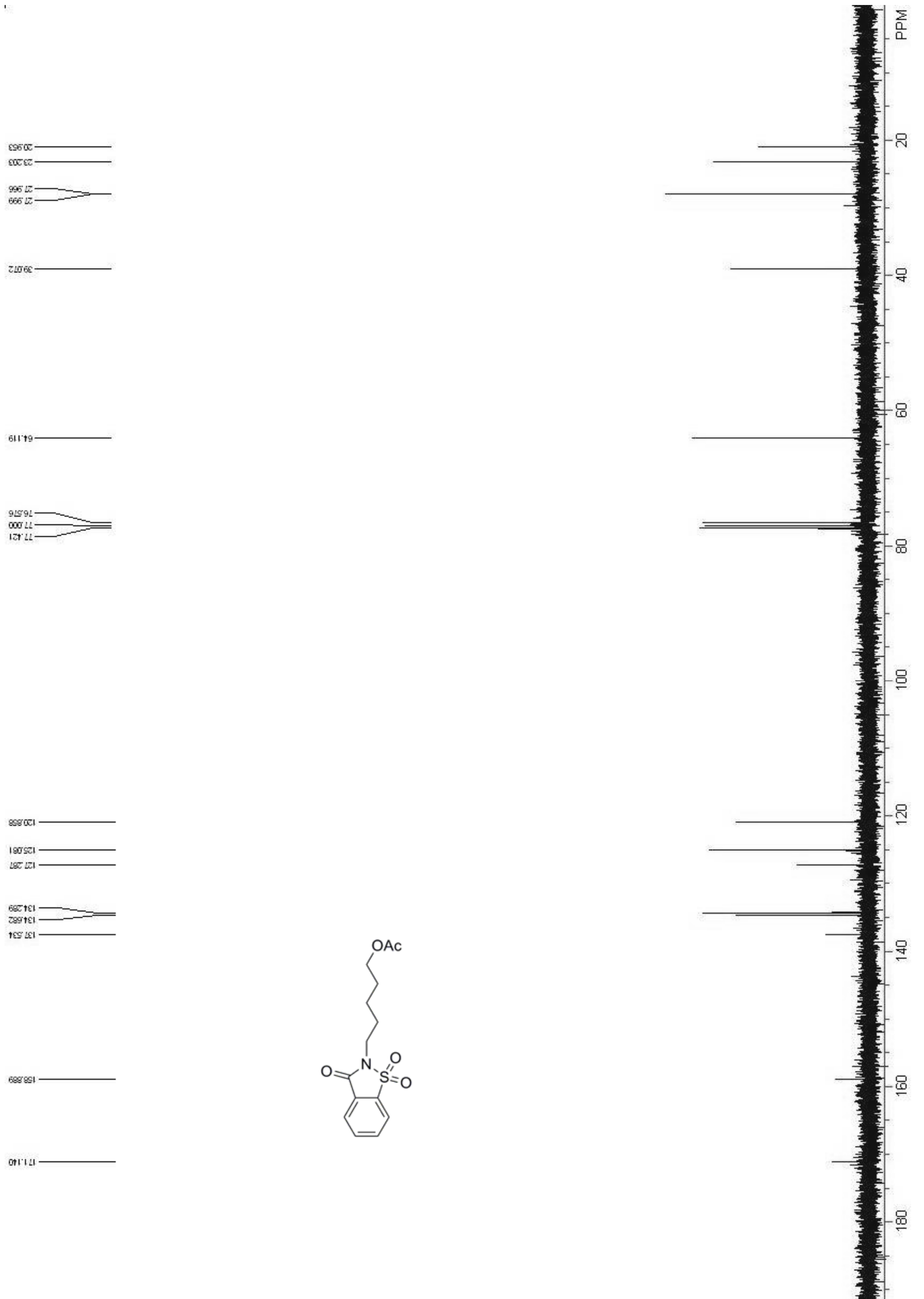
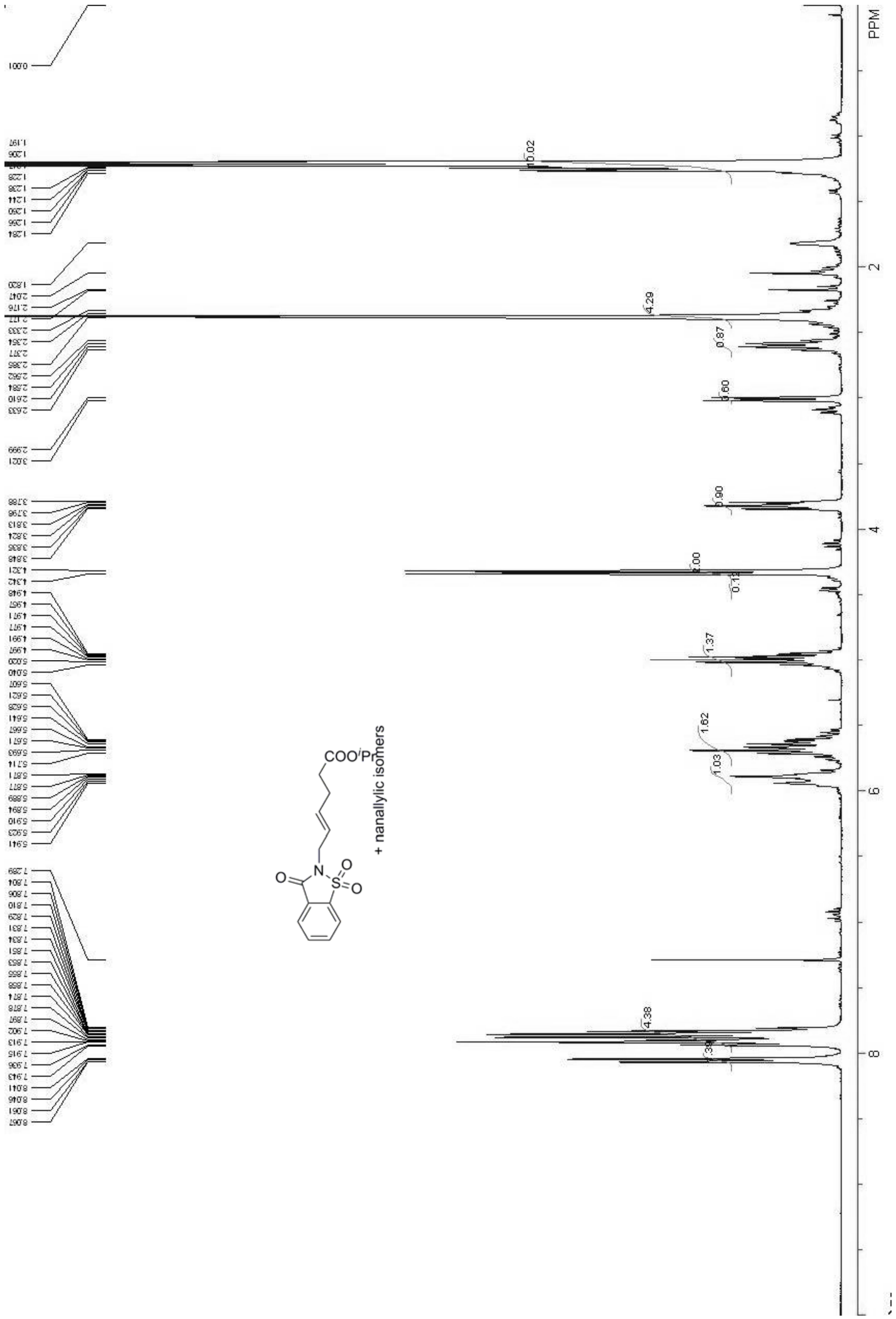
28.088
28.162
39.115
61.641
76.579
77.000
77.417
119.313
120.902
125.134
127.330
128.305
129.535
130.276
132.835
134.317
134.700
137.575
158.961
166.586
OBz
PPM
50
100
150

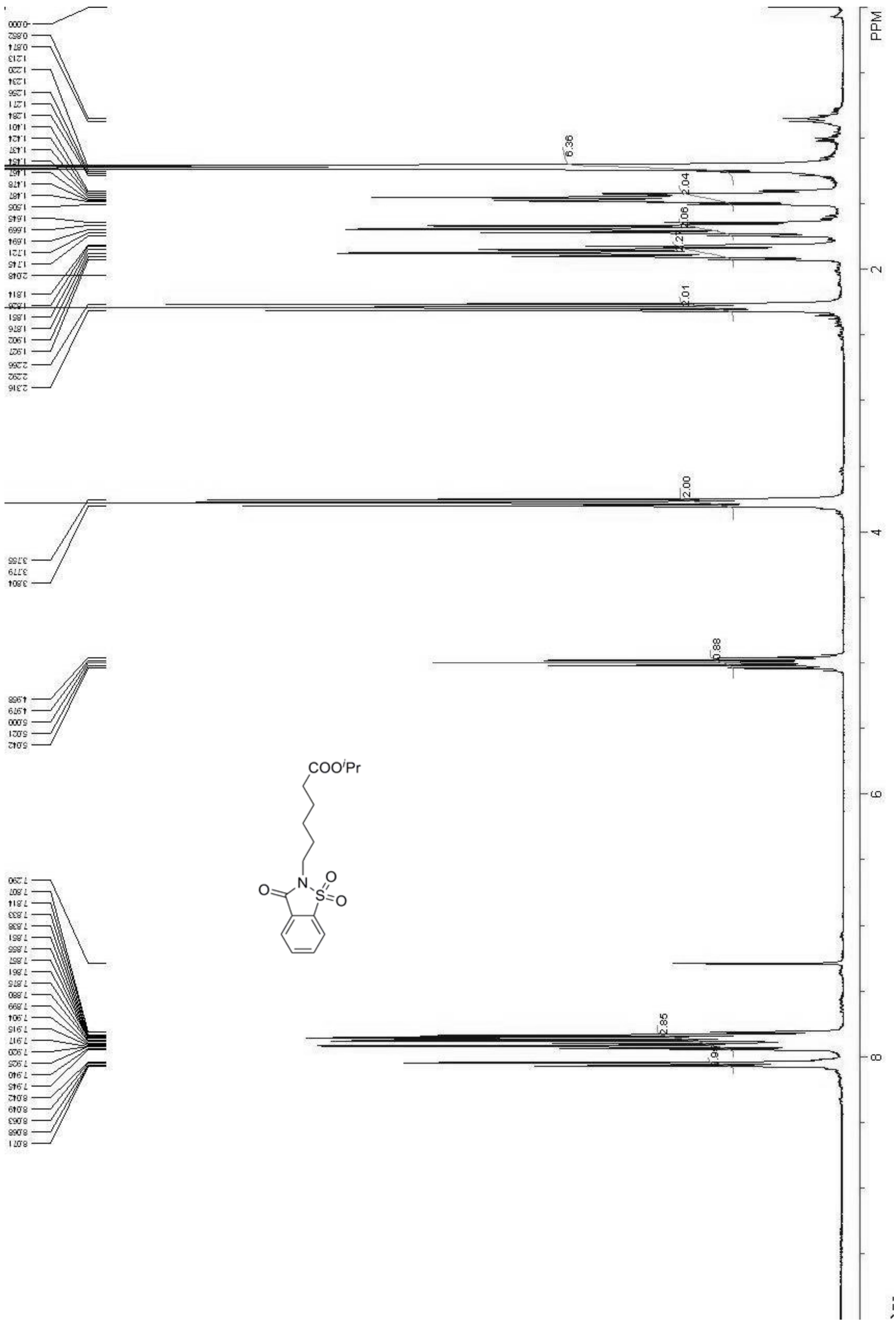

OAc
+ nonallylic isomers
PPM



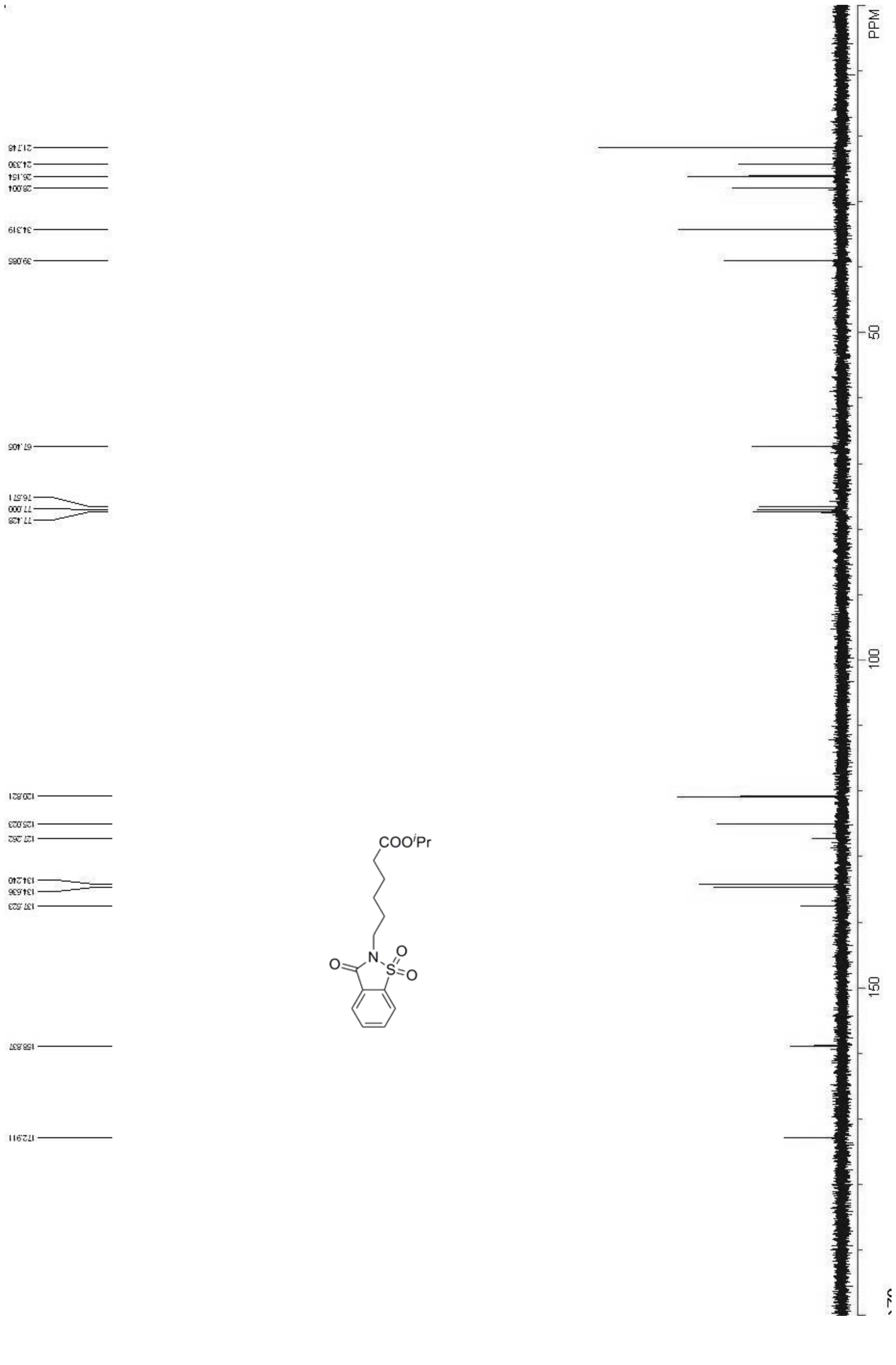
OAc
N
S
O
PPM

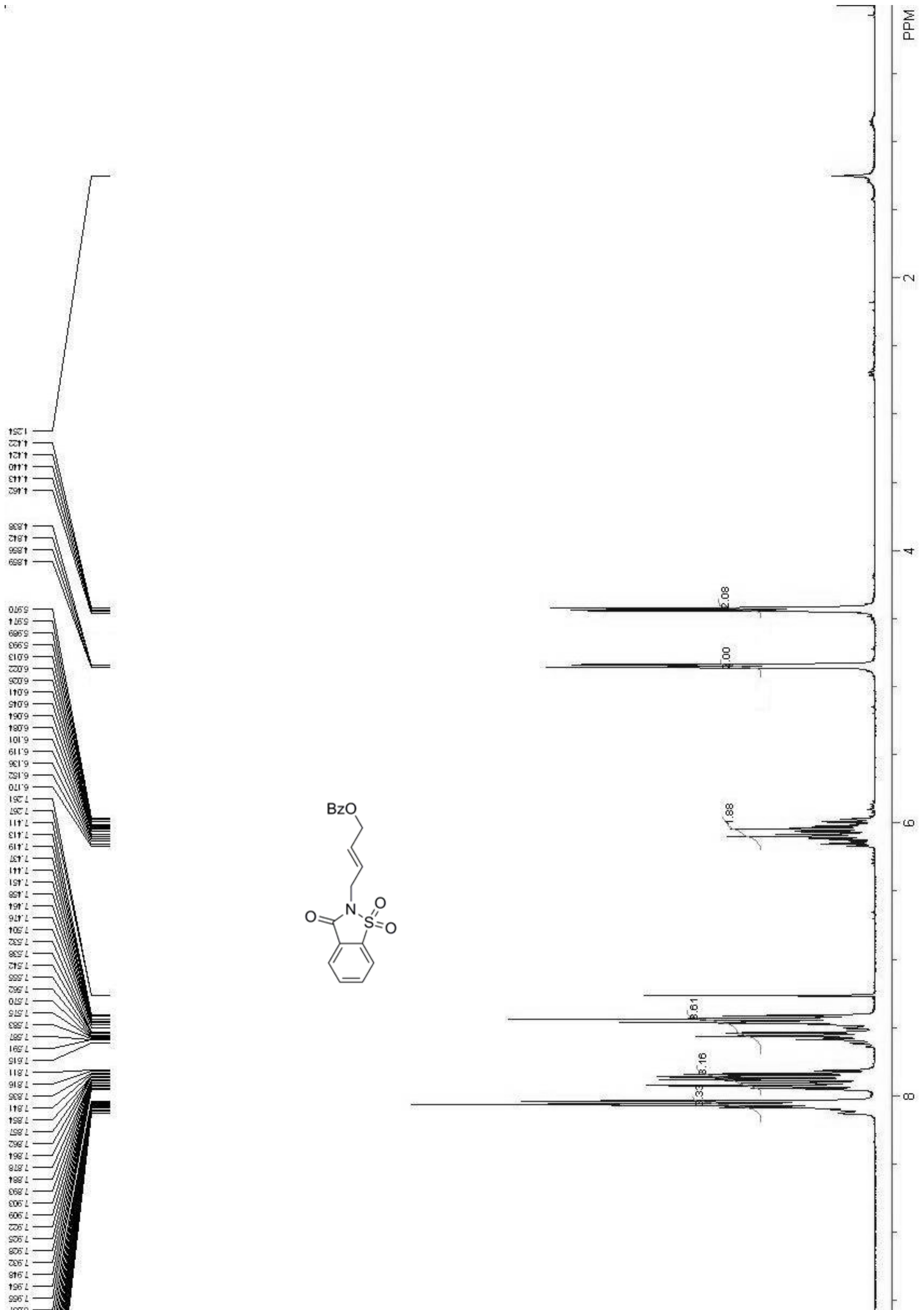

20.963
23.203
27.966
27.999
39.072
64.119
76.576
77.000
77.421
120.888
125.081
127.287
134.289
134.682
137.534
158.889
171.140
OAc
N
S
O
PPM
20
40
60
80
100
120
140
160
180

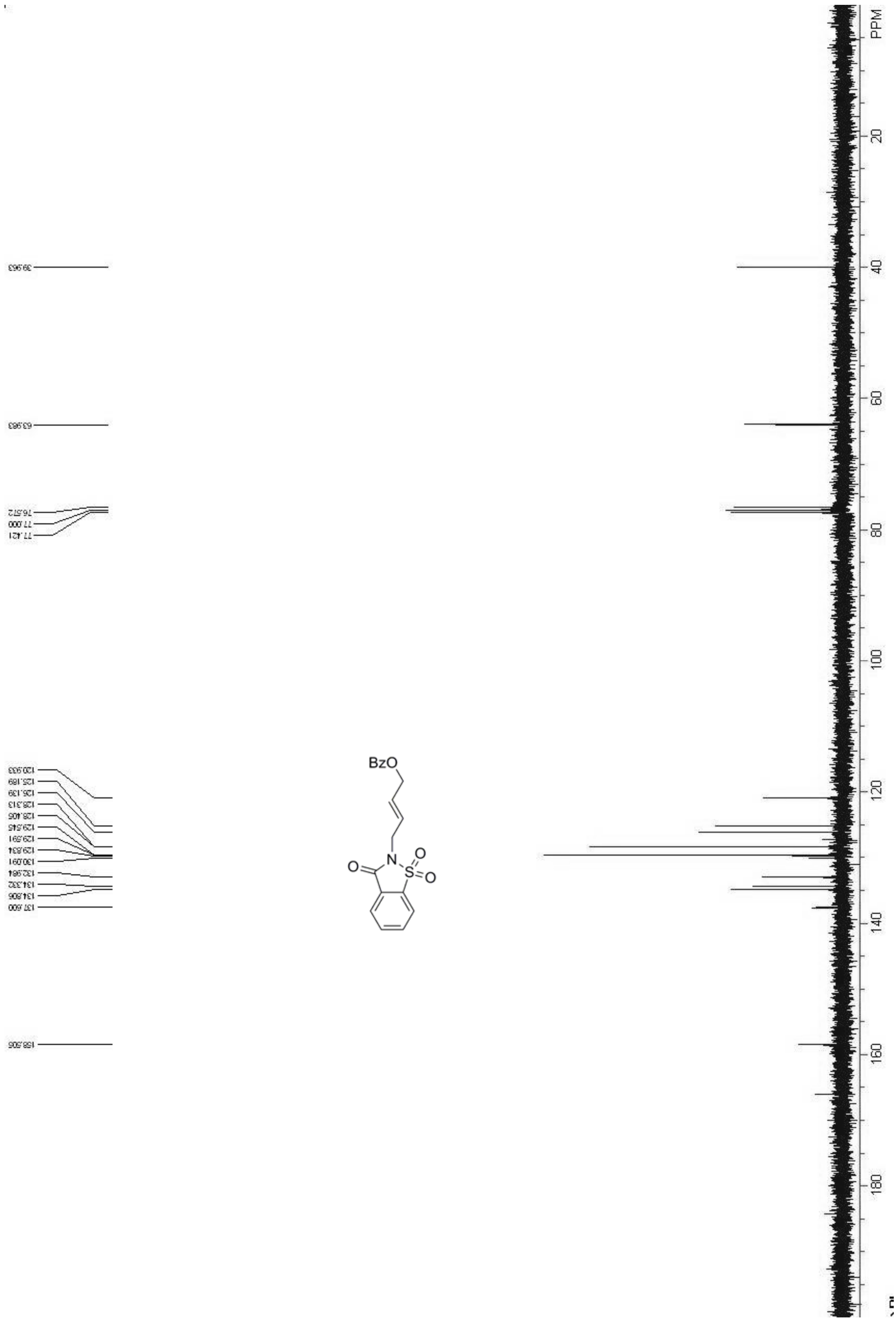

PPM
+ nanallylic isomers



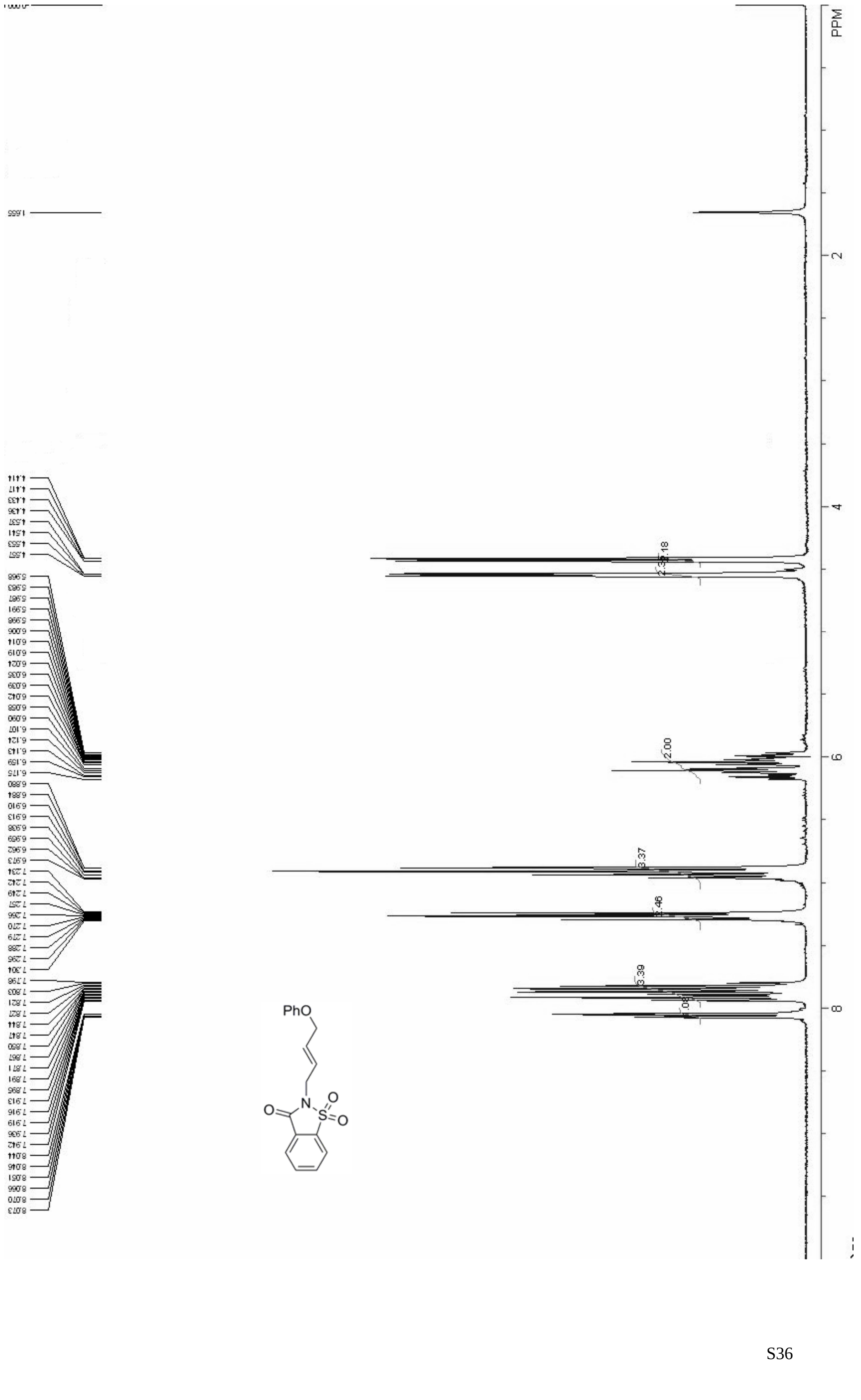
COO^iPr
PPM
2
4
6
8
6.36
2.04
2.06
2.01
2.00
0.88
2.85

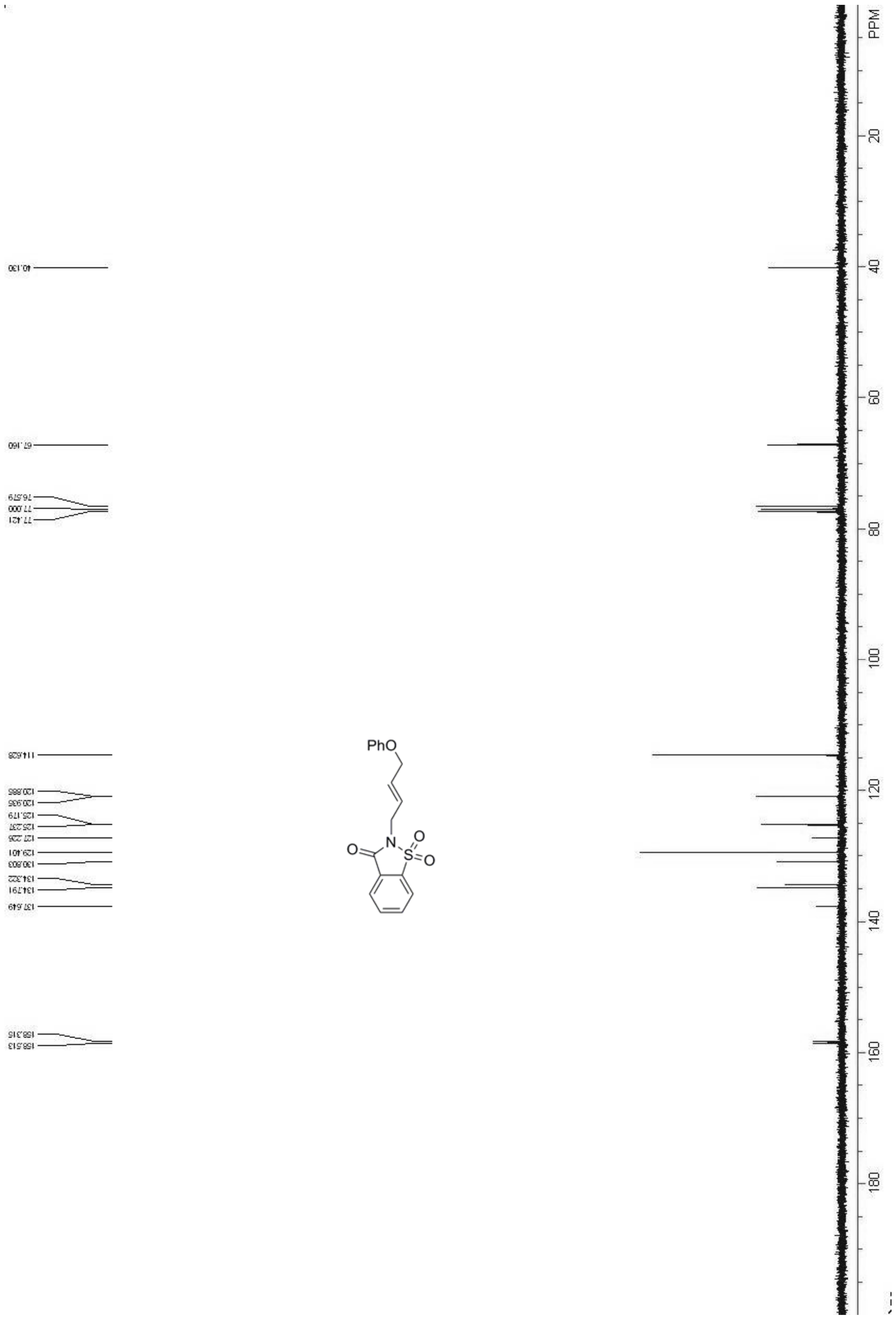




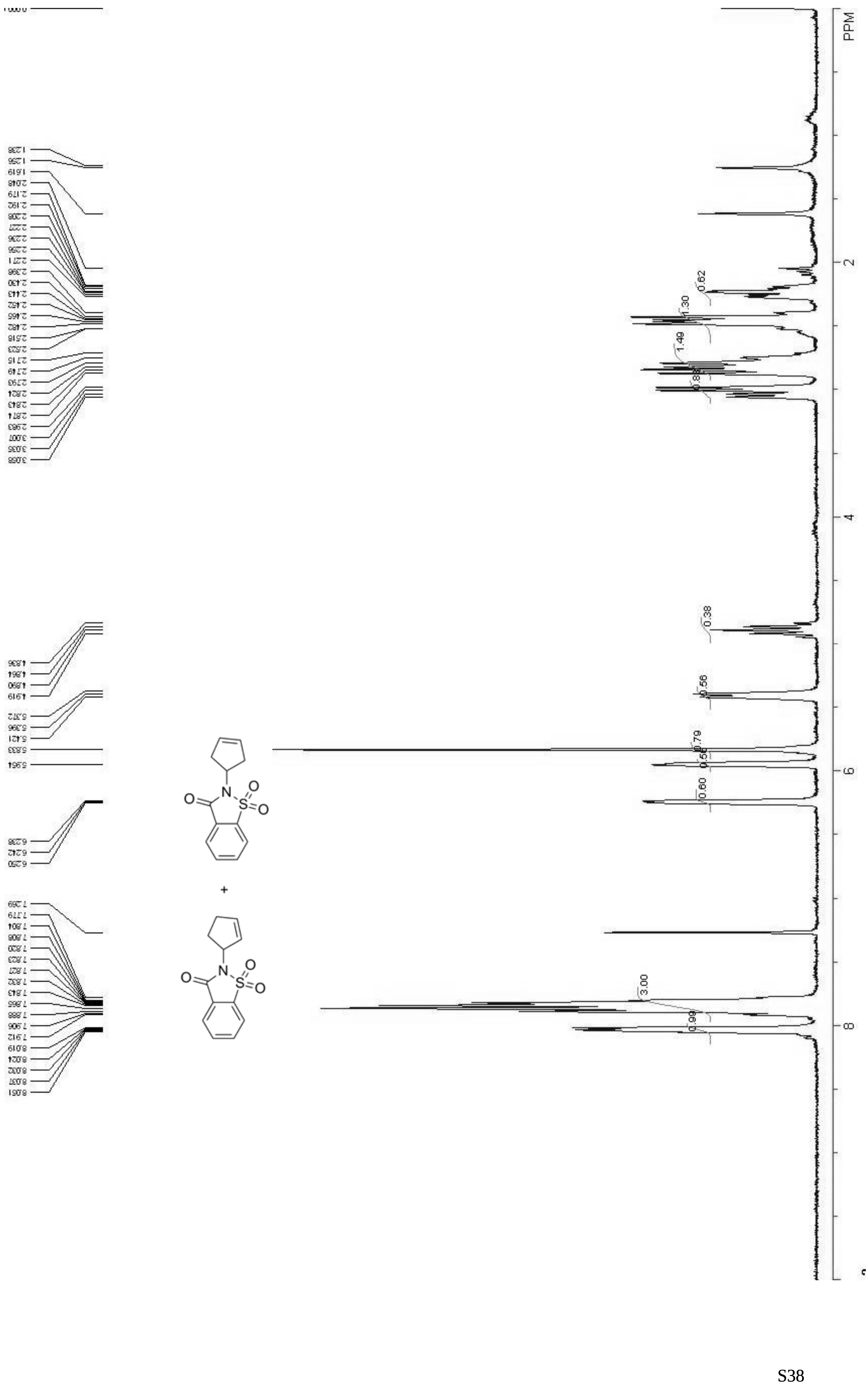


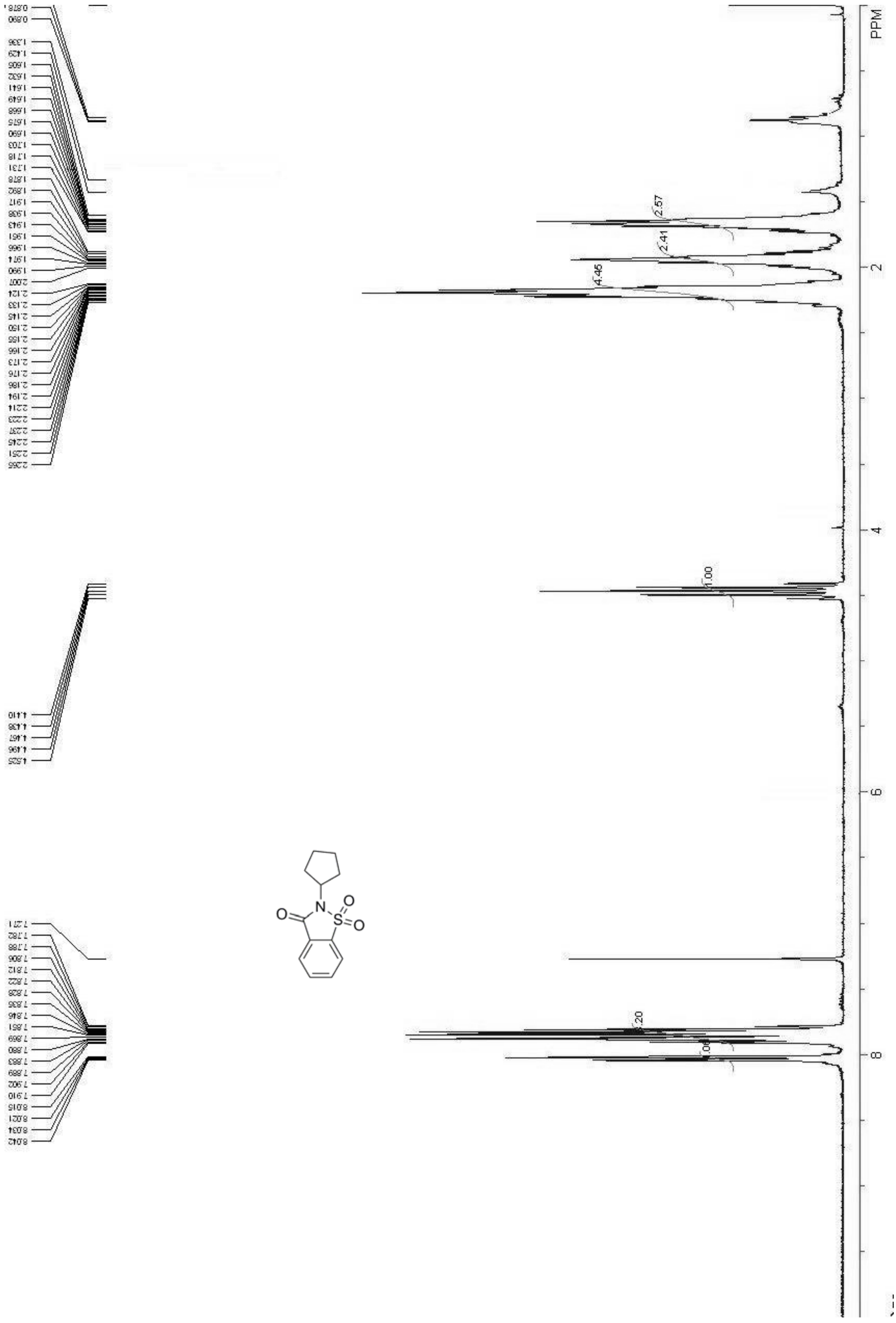
39.963
63.983
76.572
77.000
77.421
120.933
125.189
126.139
128.313
128.405
129.515
129.791
129.831
130.091
132.981
134.332
134.806
137.600
158.905
BzO
PPM
20
40
60
80
100
120
140
160
180


PPM
PhO
N
S
O
O
O



40.130
67.160
76.579
77.000
77.421
114.628
120.885
120.935
125.179
125.237
127.226
129.401
130.803
134.322
134.791
137.619
158.316
158.513
PhO
N
S
O
PPM
20
40
60
80
100
120
140
160
180




PPM
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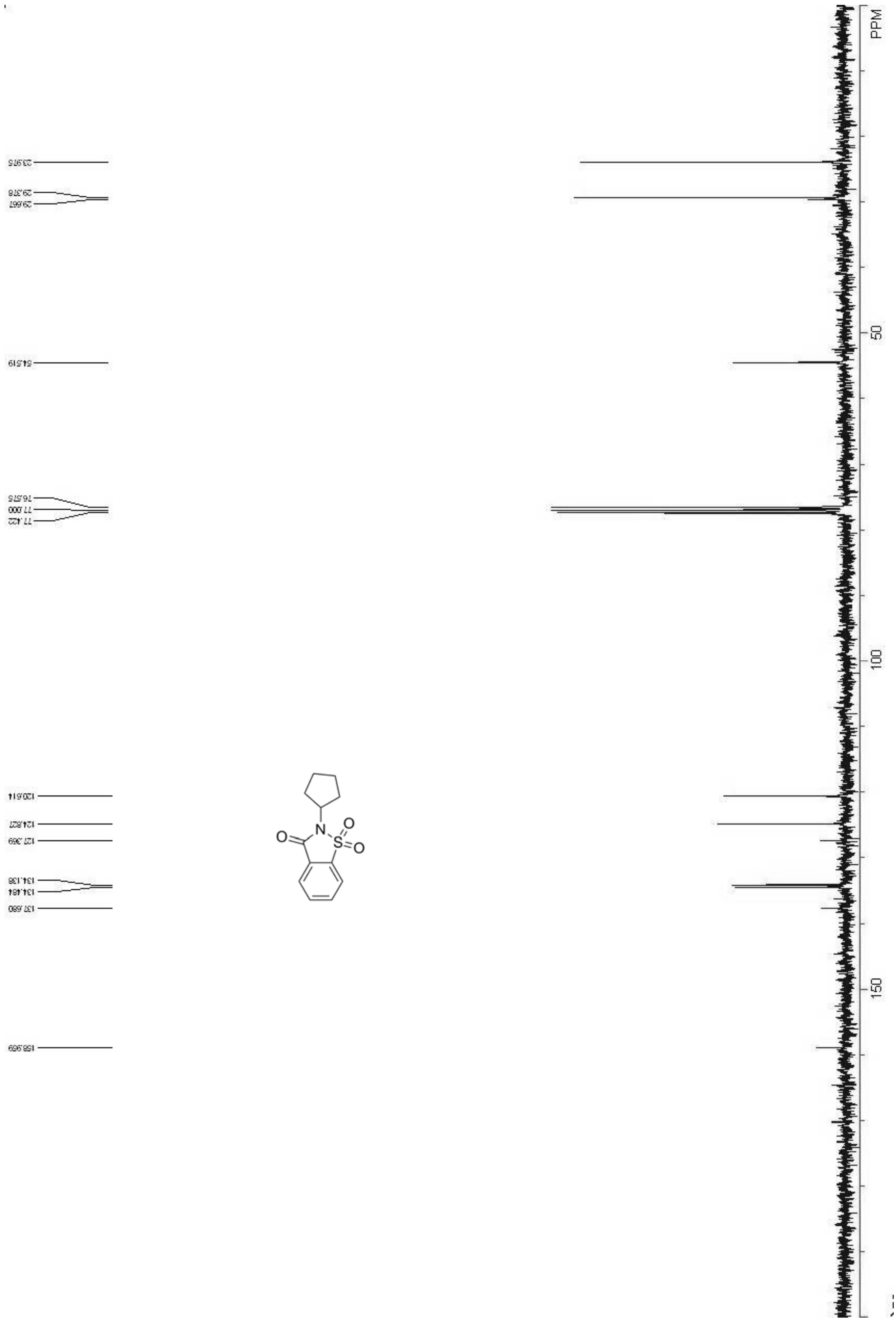
4
6
8
2.57
2.41
4.45
1.00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29.661
51.519
76.575
77.000
77.422
120.614
124.827
127.369
134.136
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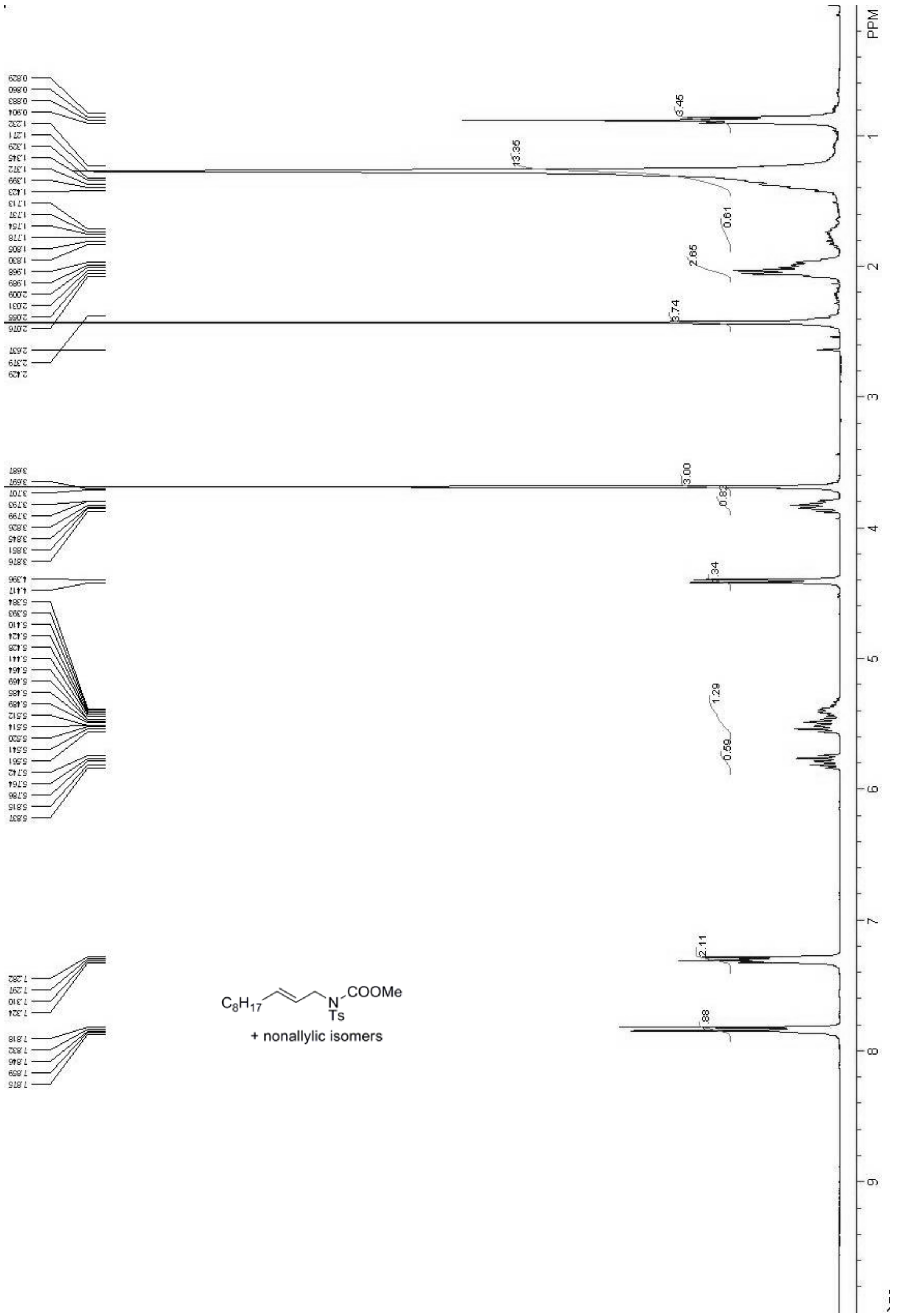
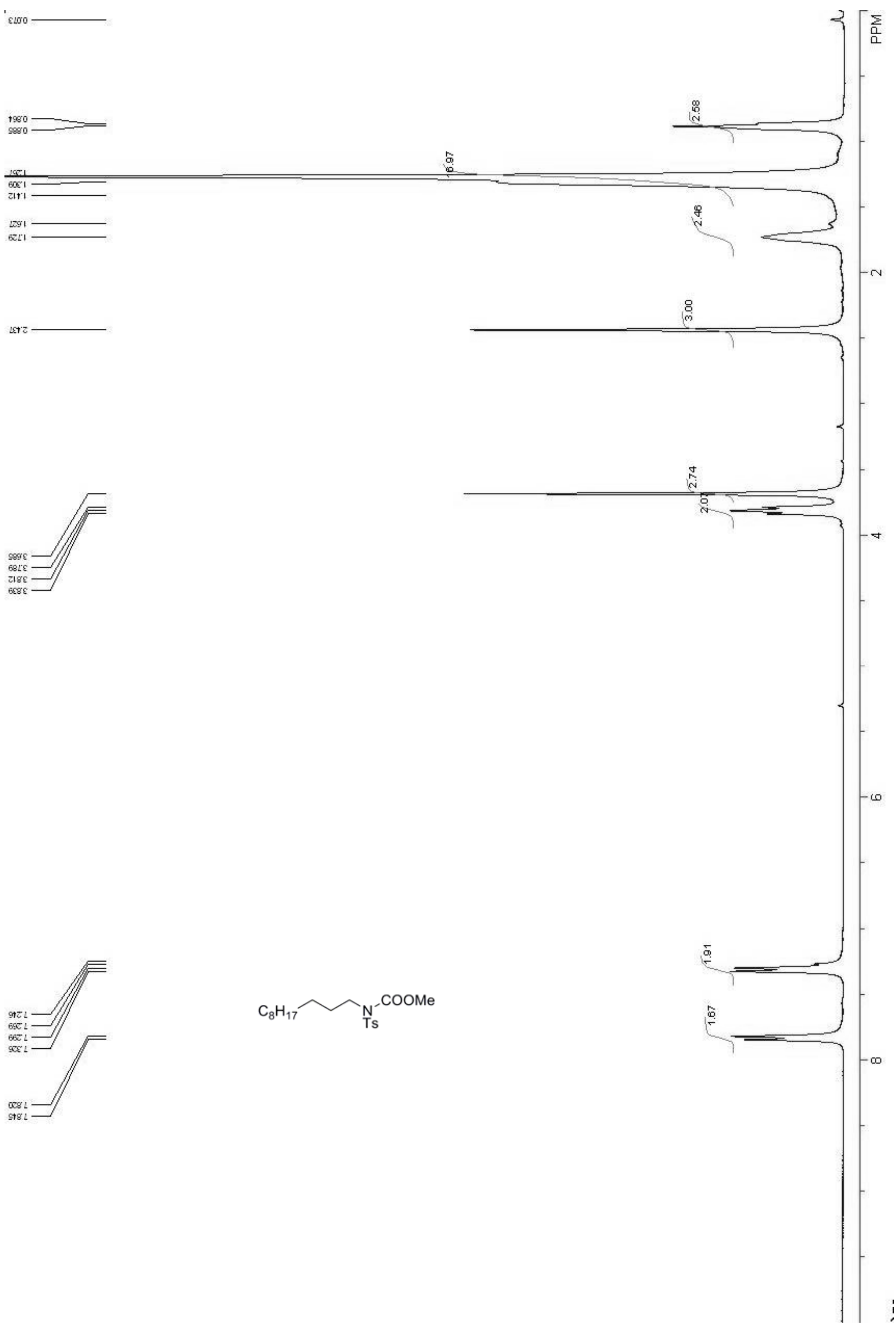
PPM
50
100
150


PPM
+ nonallylic isomers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0.885
1.261
1.309
1.412
1.627
1.729
2.437
3.685
3.789
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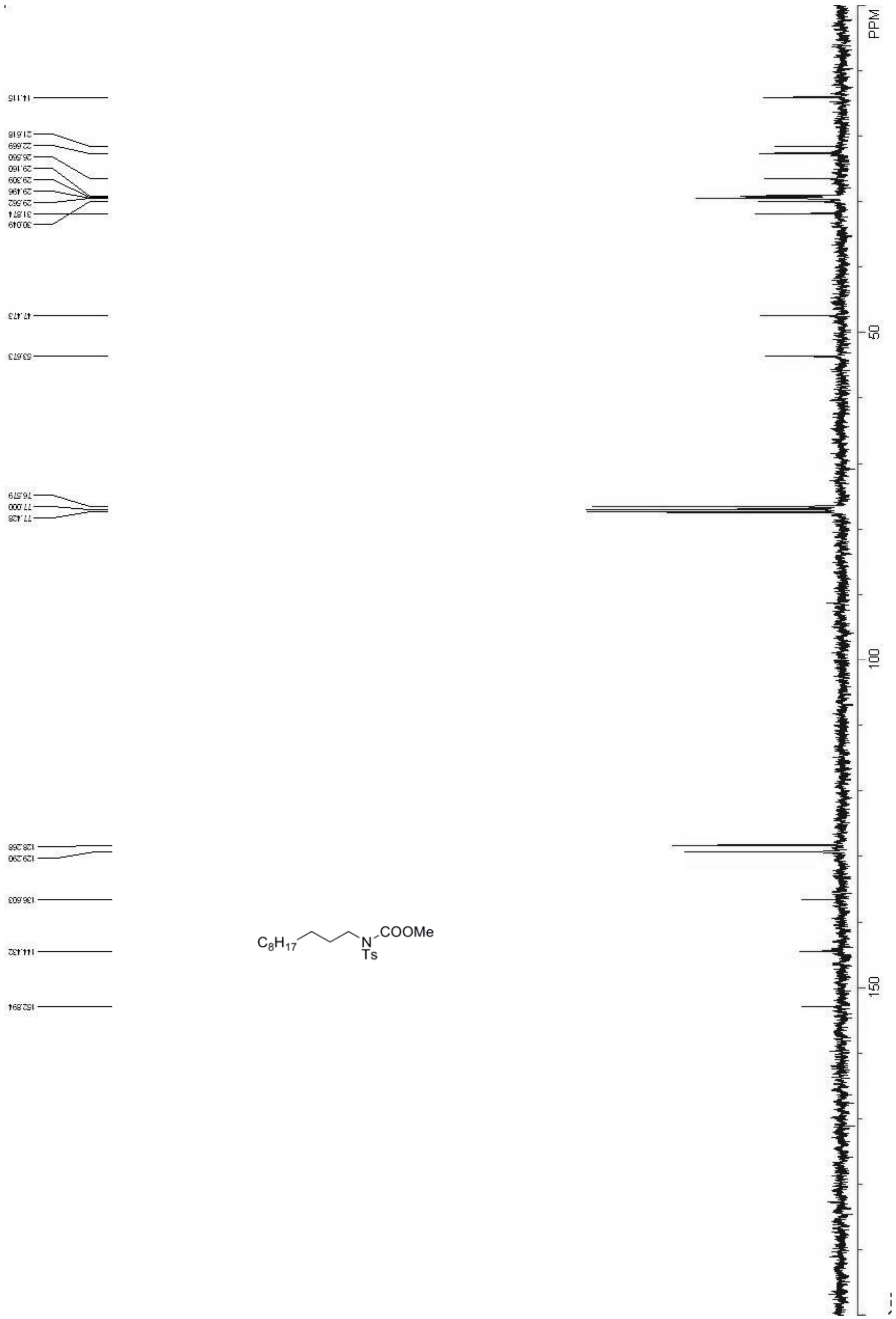
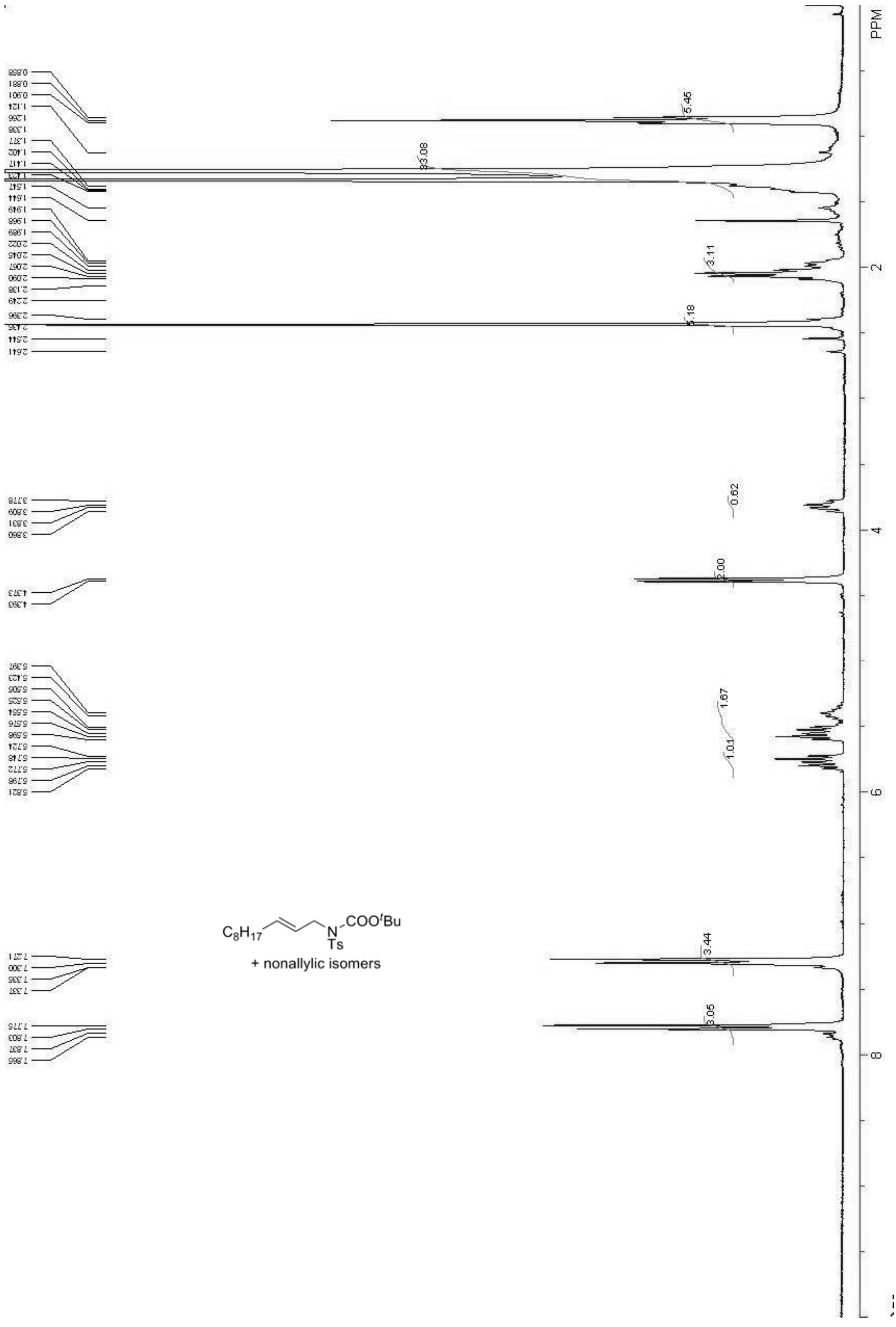
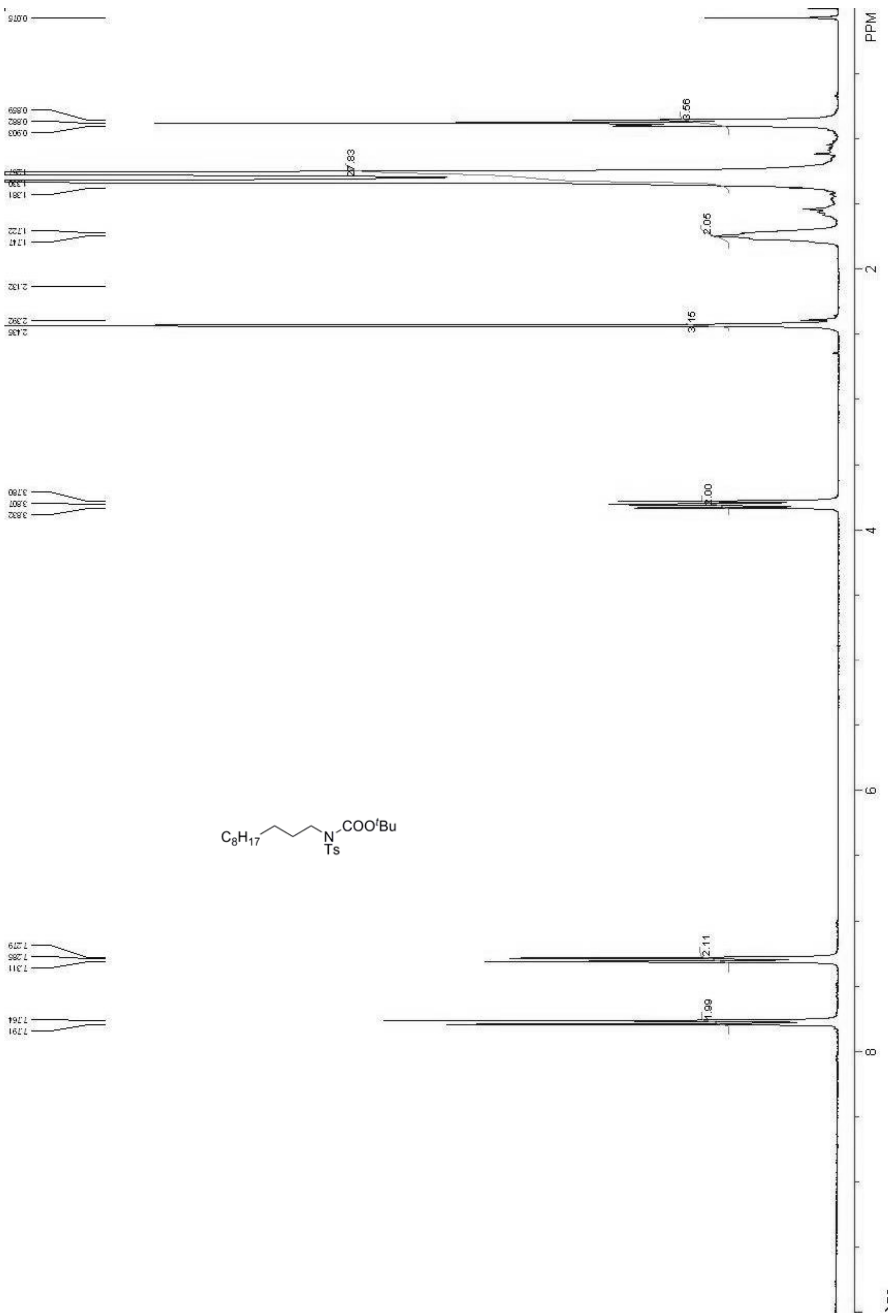
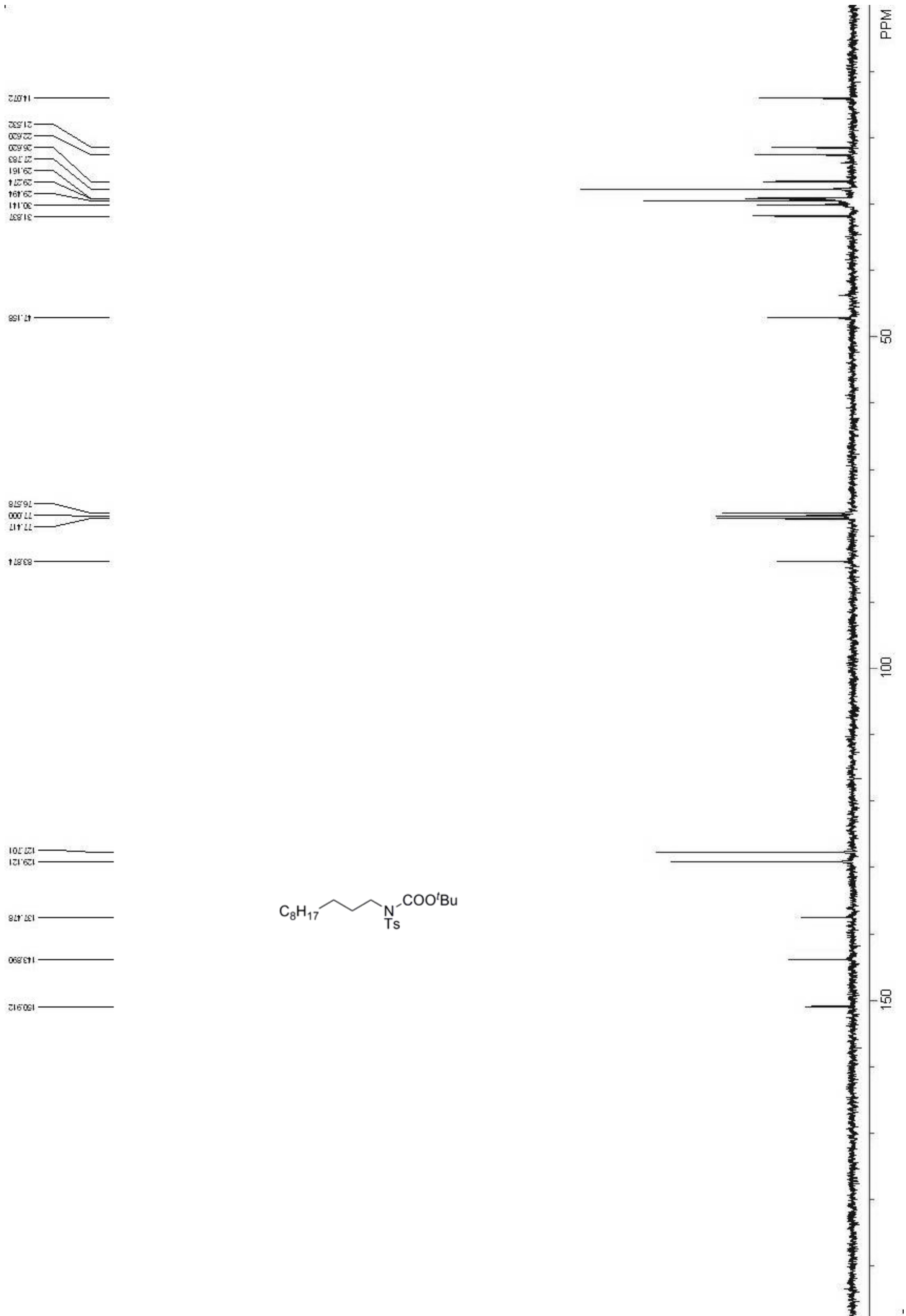
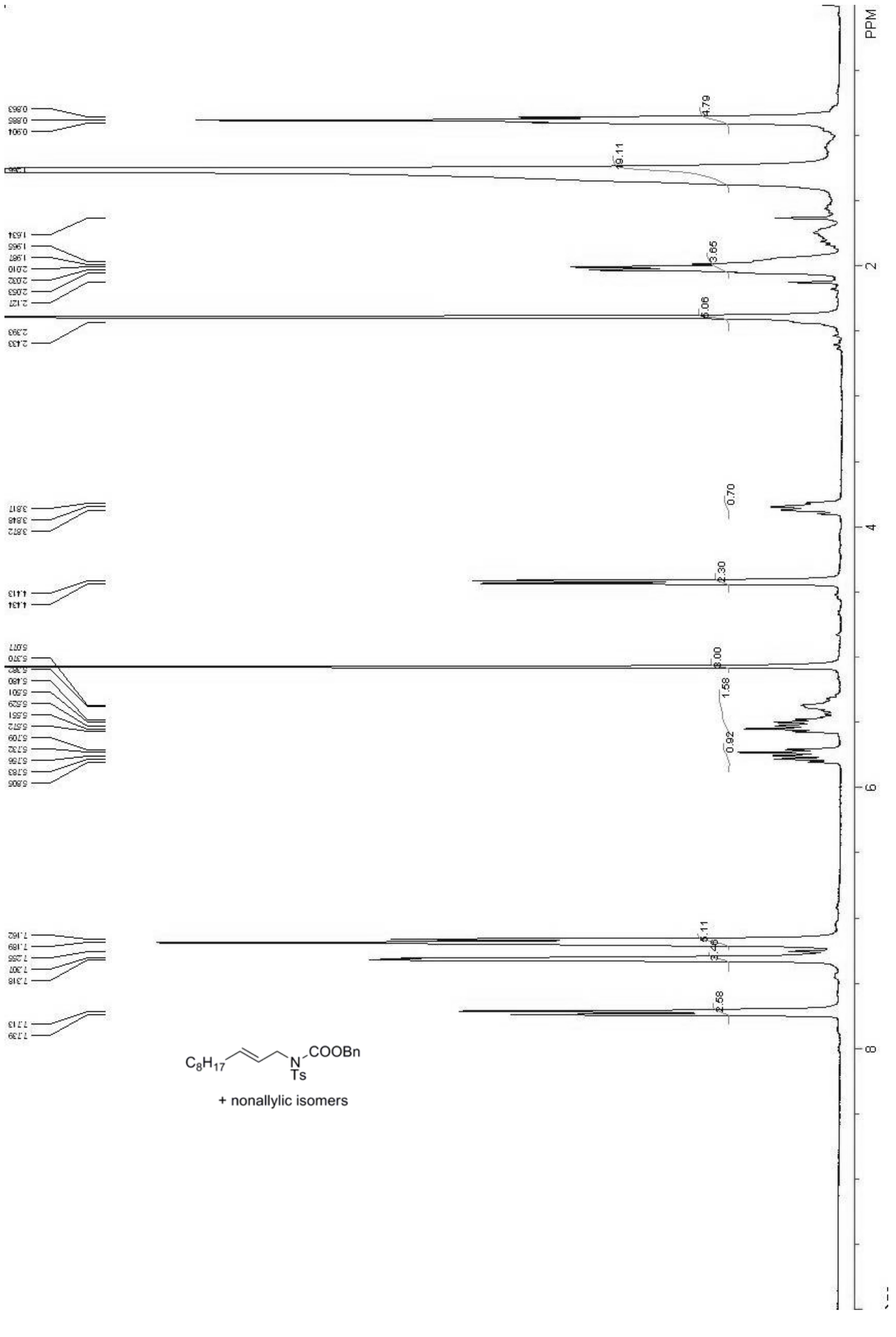
3.839
7.246
7.269
7.299
7.305
7.830
7.845
2.58
6.97
2.46
3.00
2.74
2.07
1.91
1.67
PPM
2
4
6
8
C_8H_{17} N COOMe Ts

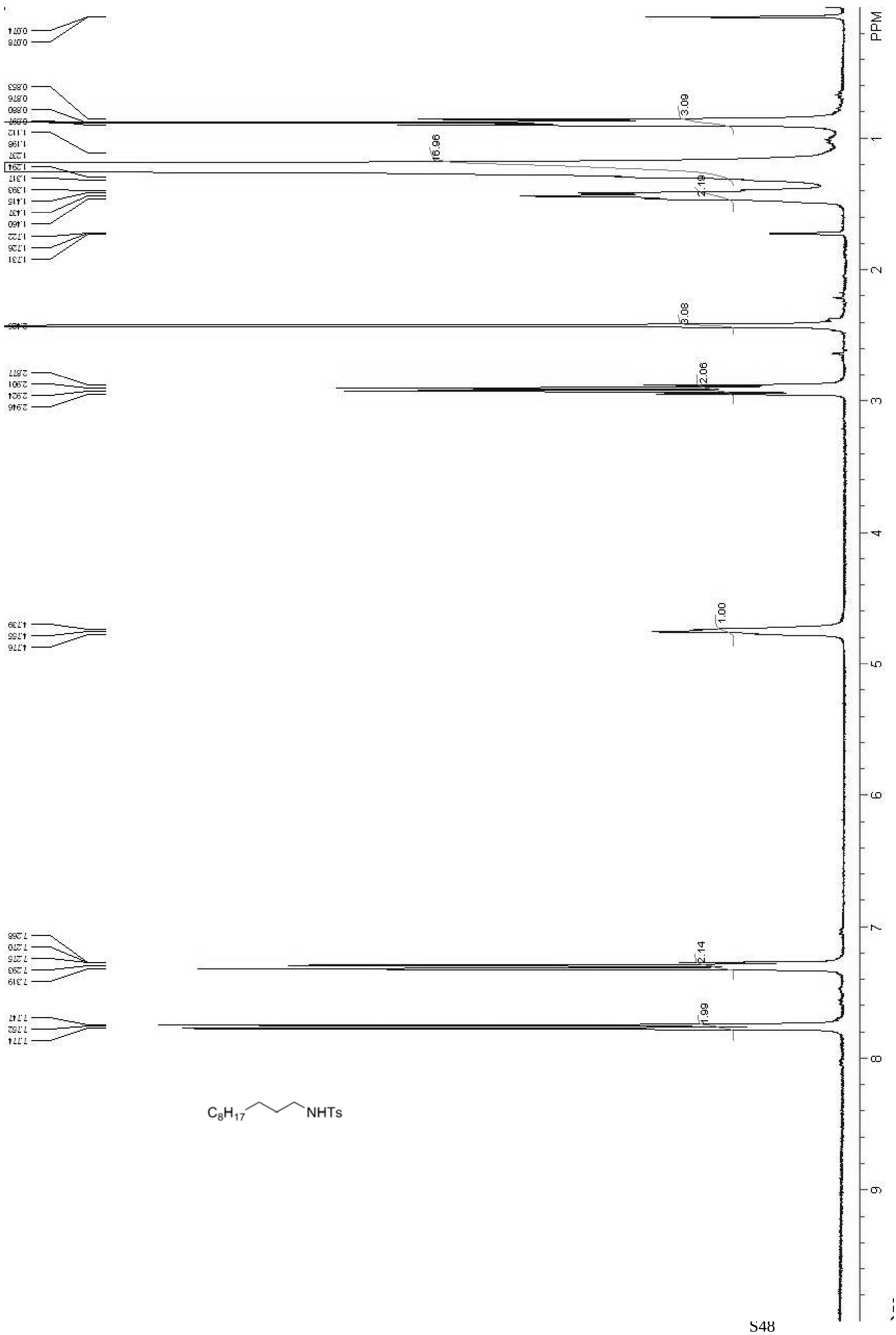

PPM
50
100
150
C8H17
N
COOMe
Ts

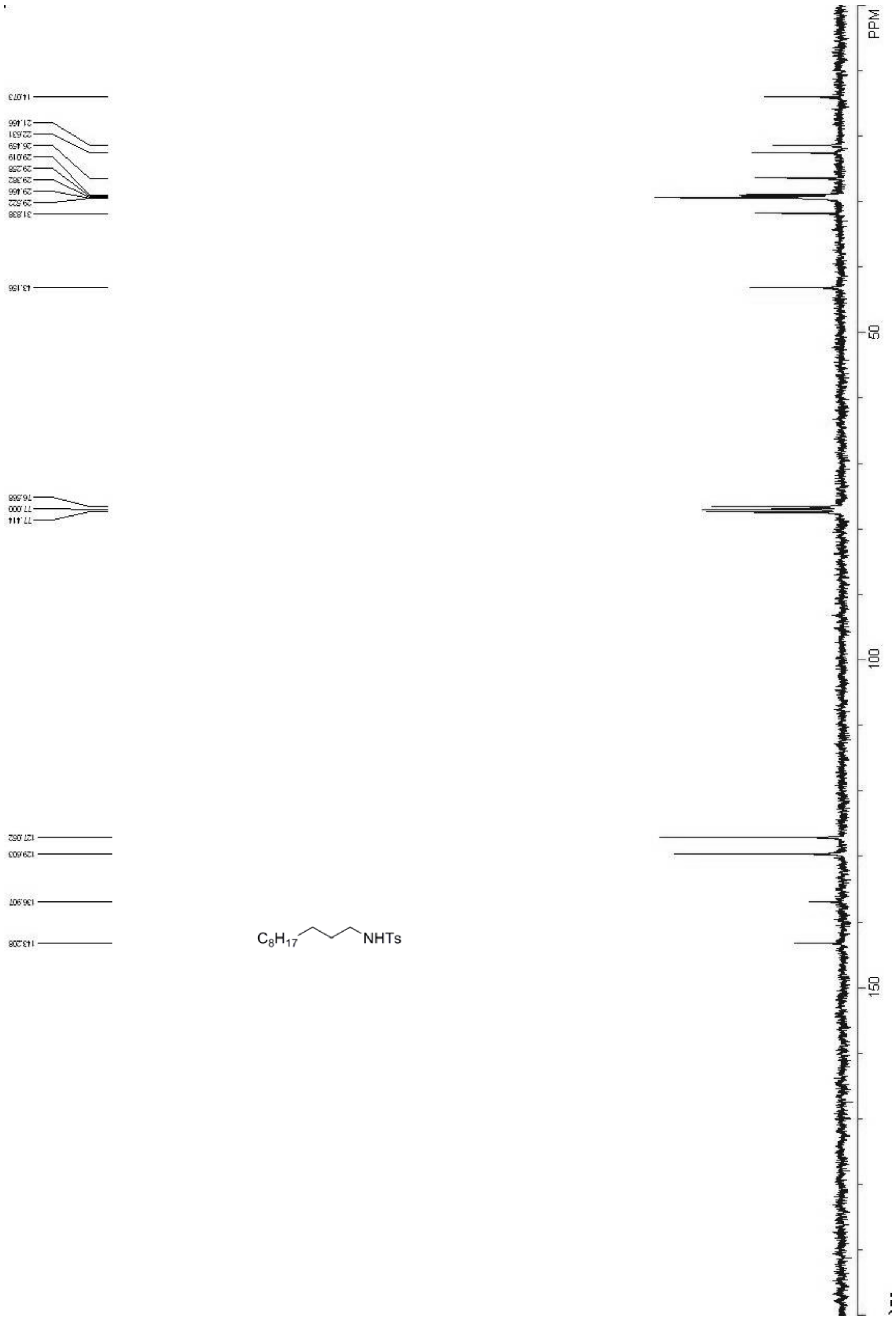

+ nonallylic isomers
PPM

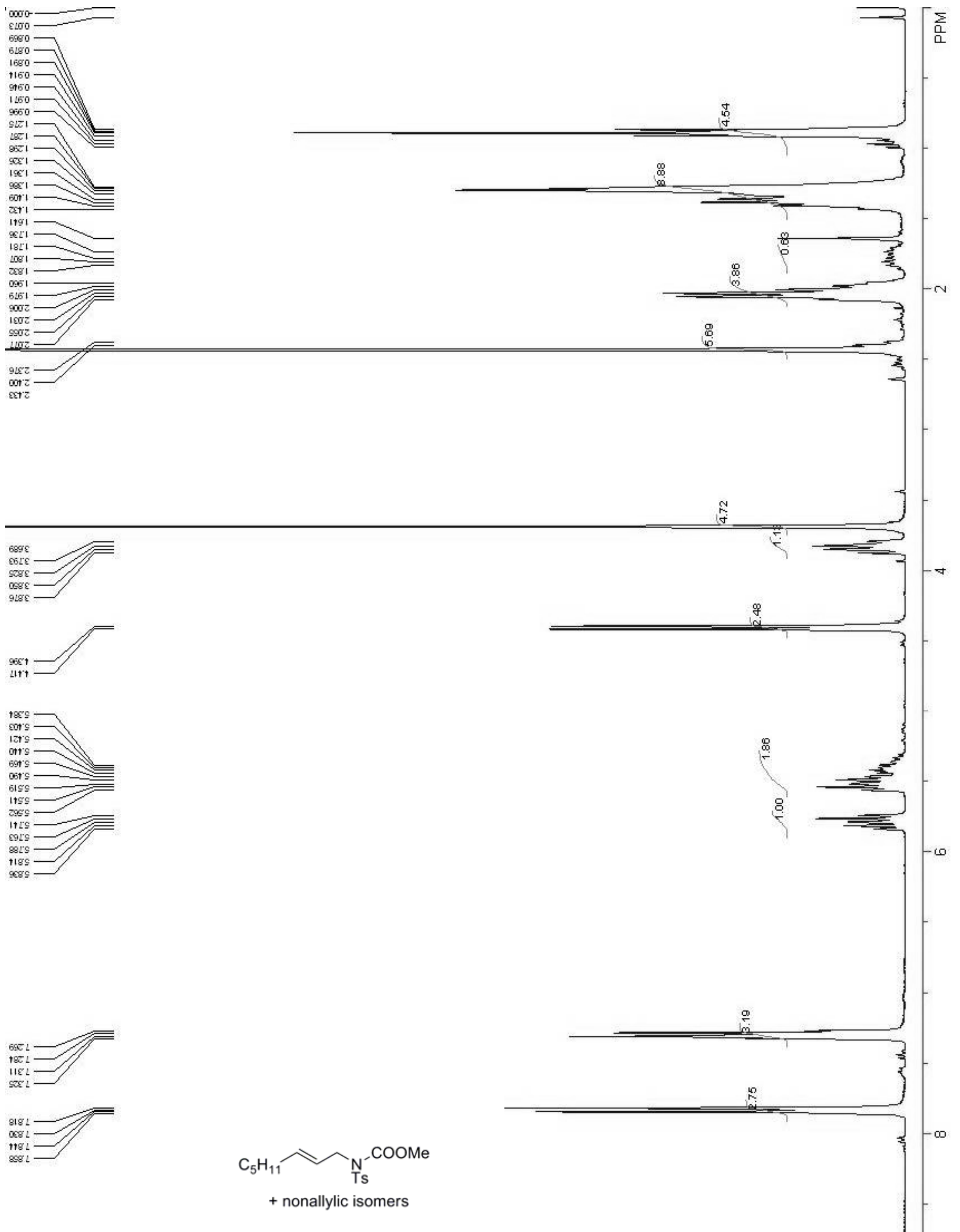

PPM
C8H17 N COOtBu Ts
3.56
27.83
2.05
3.15
2.00
2.11
1.99
2
4
6
8

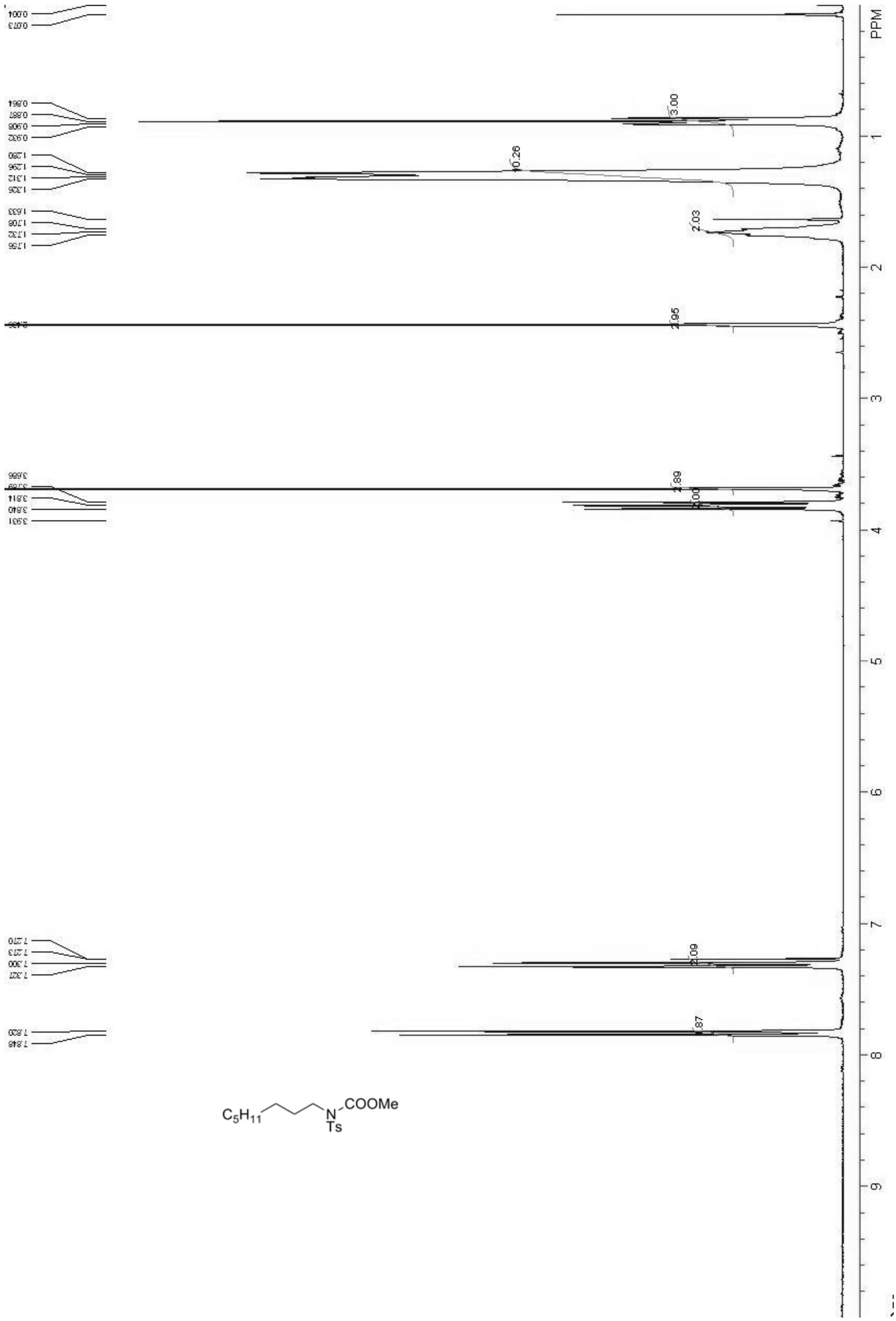

14.072
21.532
22.620
26.620
27.783
29.161
29.274
29.494
30.141
31.837
47.188
76.578
77.000
77.417
83.874
127.701
129.121
137.478
143.890
150.912
C_8H_{17}
N
COO^{t}Bu
Ts
PPM
50
100
150


PPM
2
4
6
8
C_8H_{17}
N
COOBn
Ts
+ nonallylic isomers

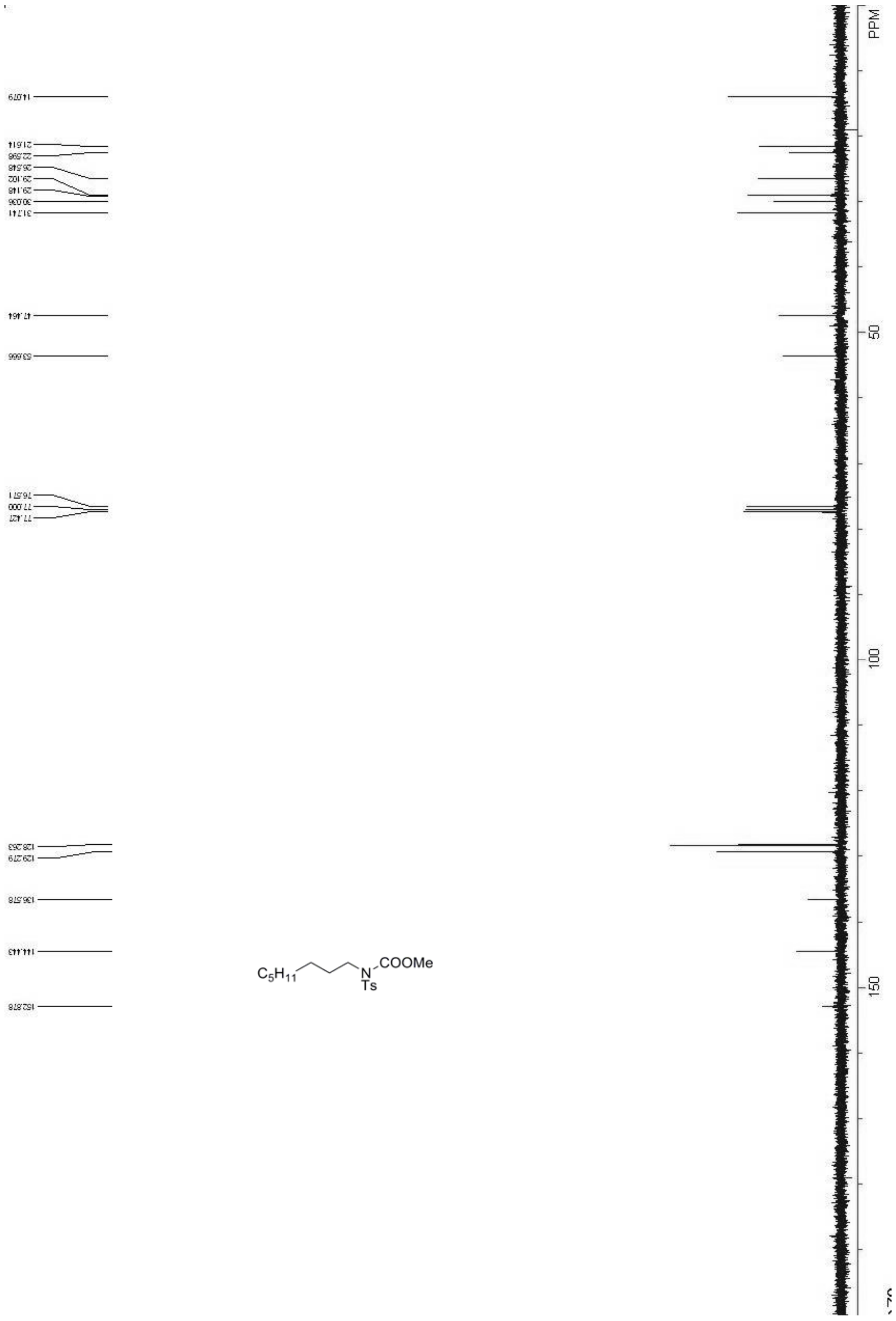

PPM
C8H17 NHTs


14.073
21.466
22.631
26.459
29.019
29.258
29.382
29.466
29.522
31.838
43.166
76.588
77.000
77.414
127.062
129.603
136.907
143.208
C8H17
NHTs
PPM
50
100
150

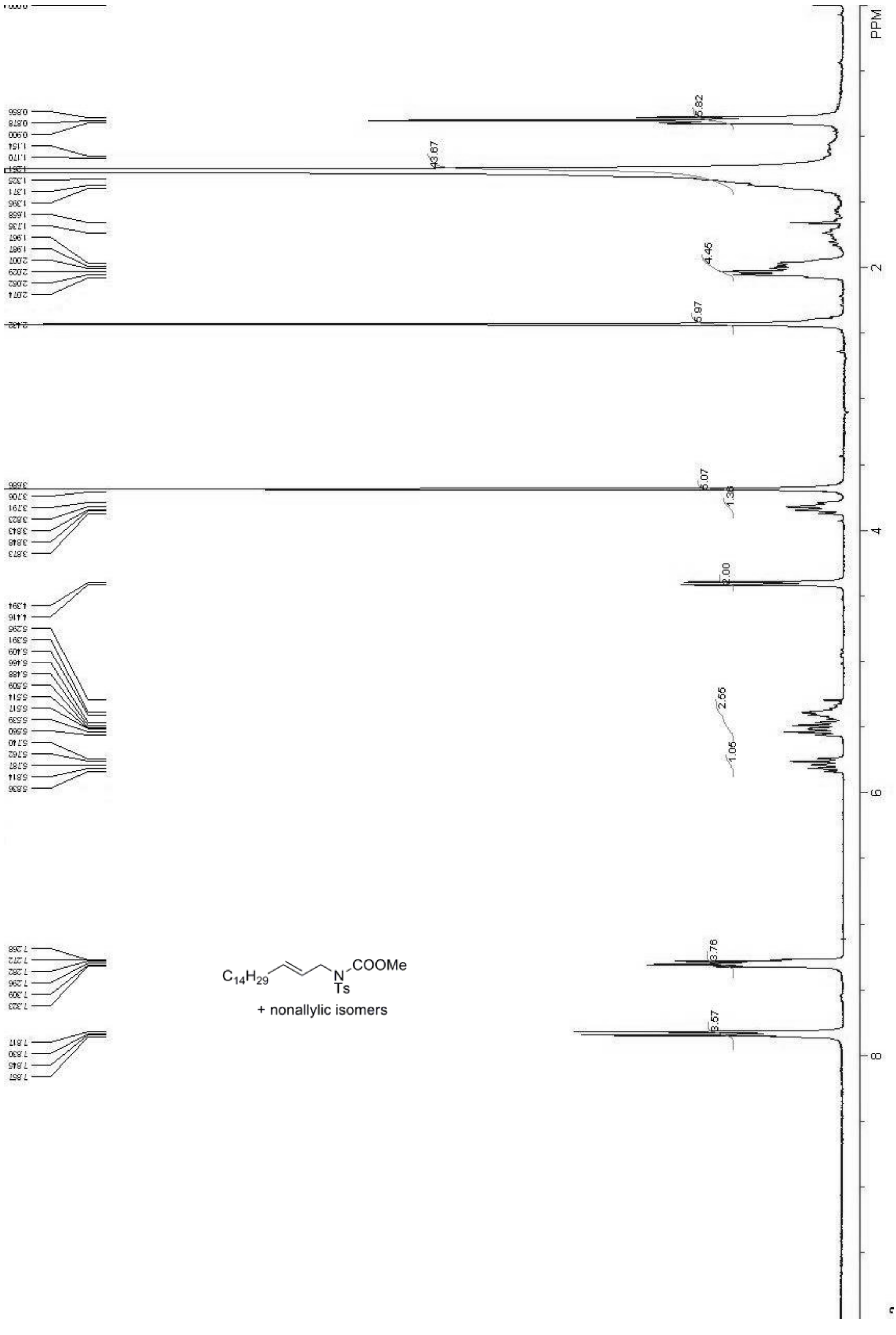

C5H11
N
COOMe
Ts
+ nonallylic isomers
PPM

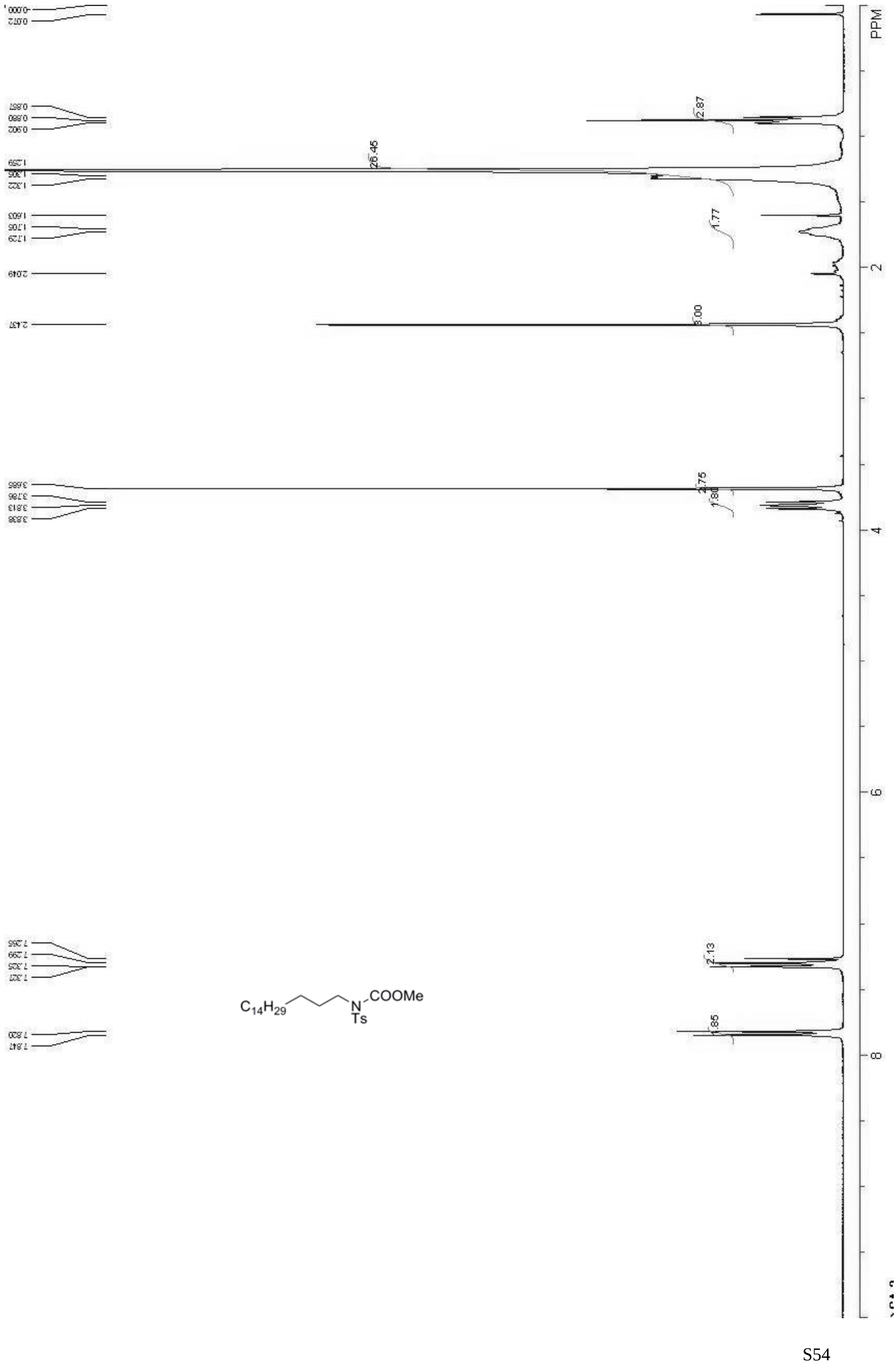


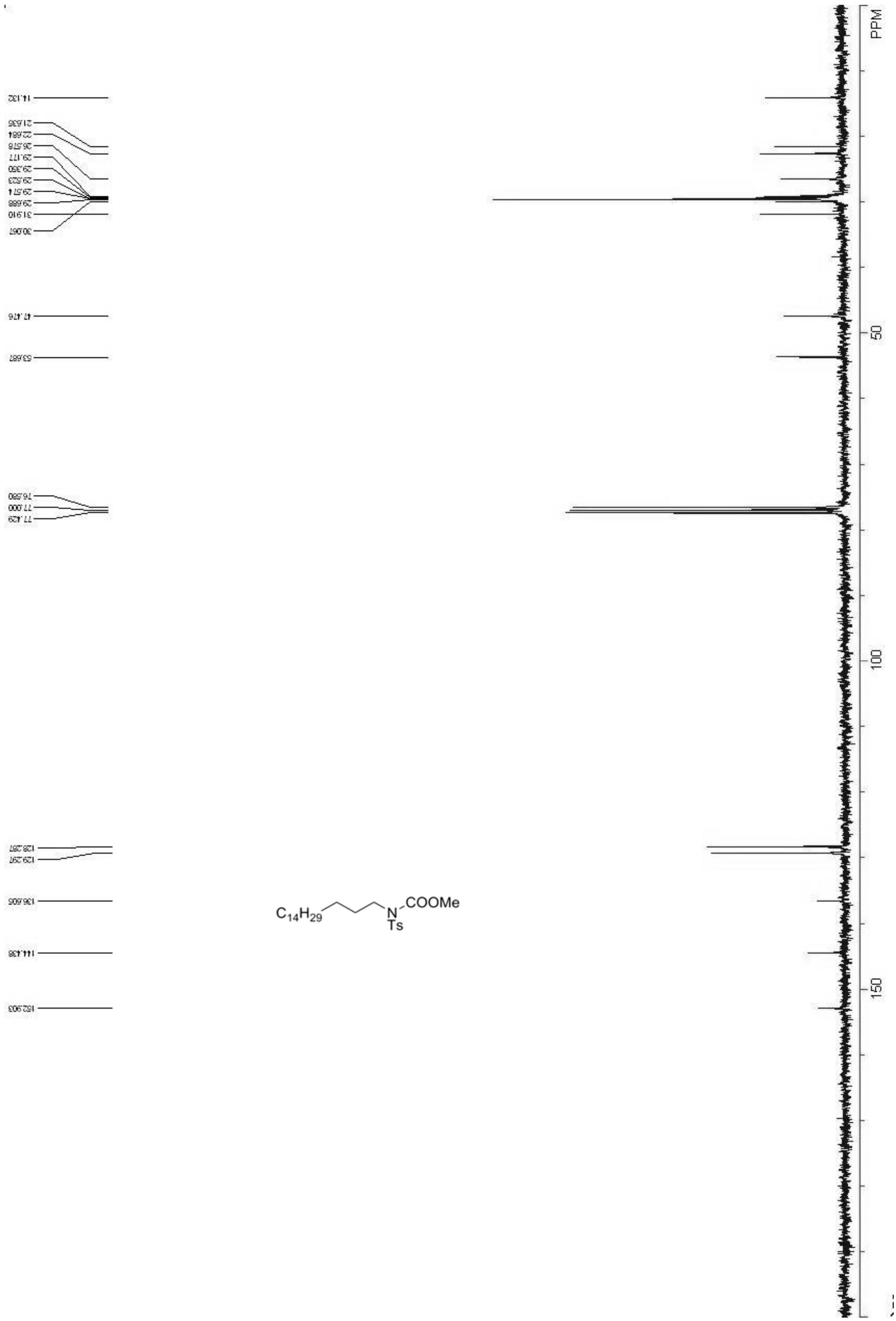
C5H11
N
COOMe
Ts
PPM



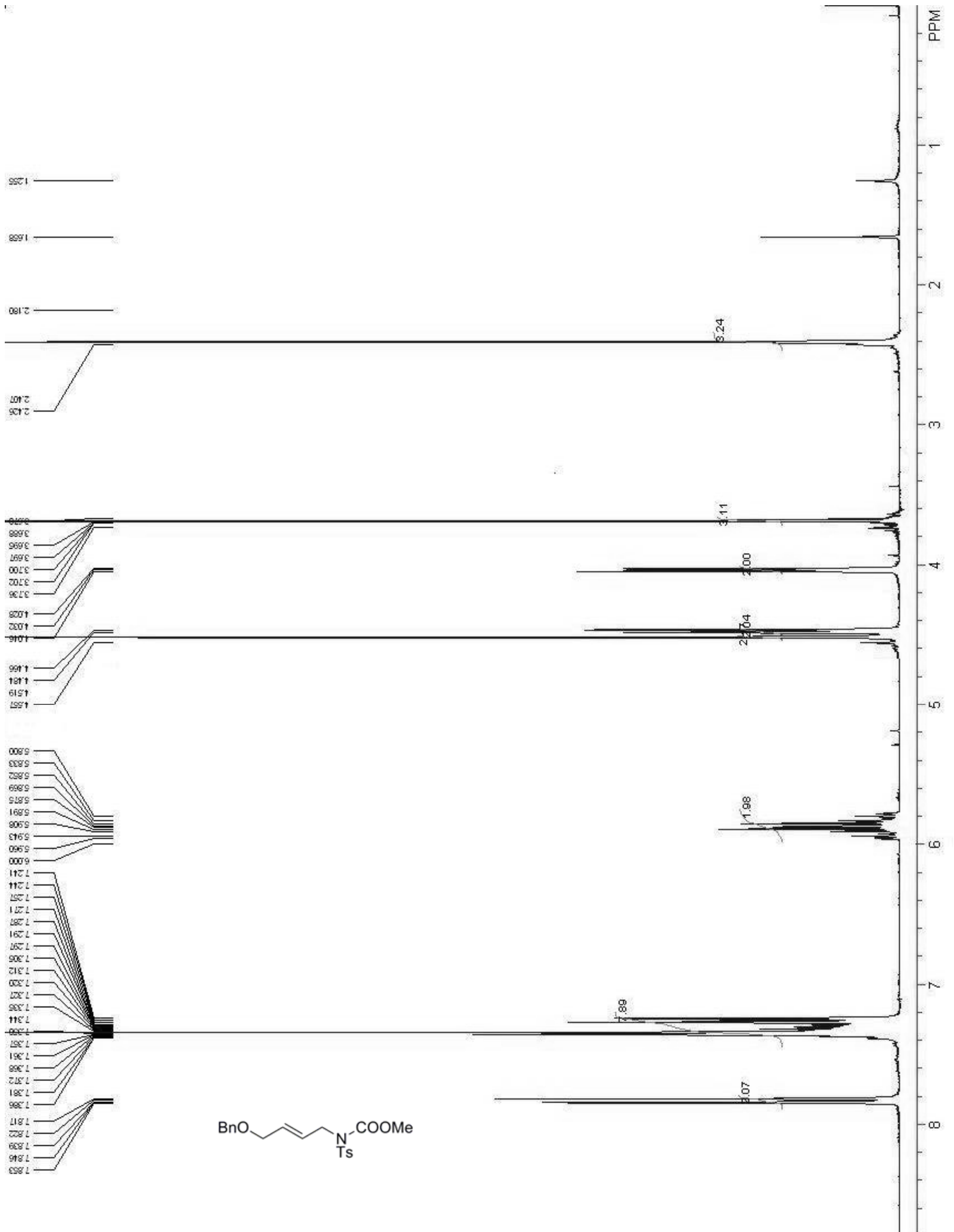
14.079
21.514
22.598
26.518
29.102
29.148
30.036
31.741
47.464
53.666
76.571
77.000
77.427
128.263
129.279
136.578
144.413
152.818
C_5H_{11}
N
COOMe
Ts
PPM
50
100
150

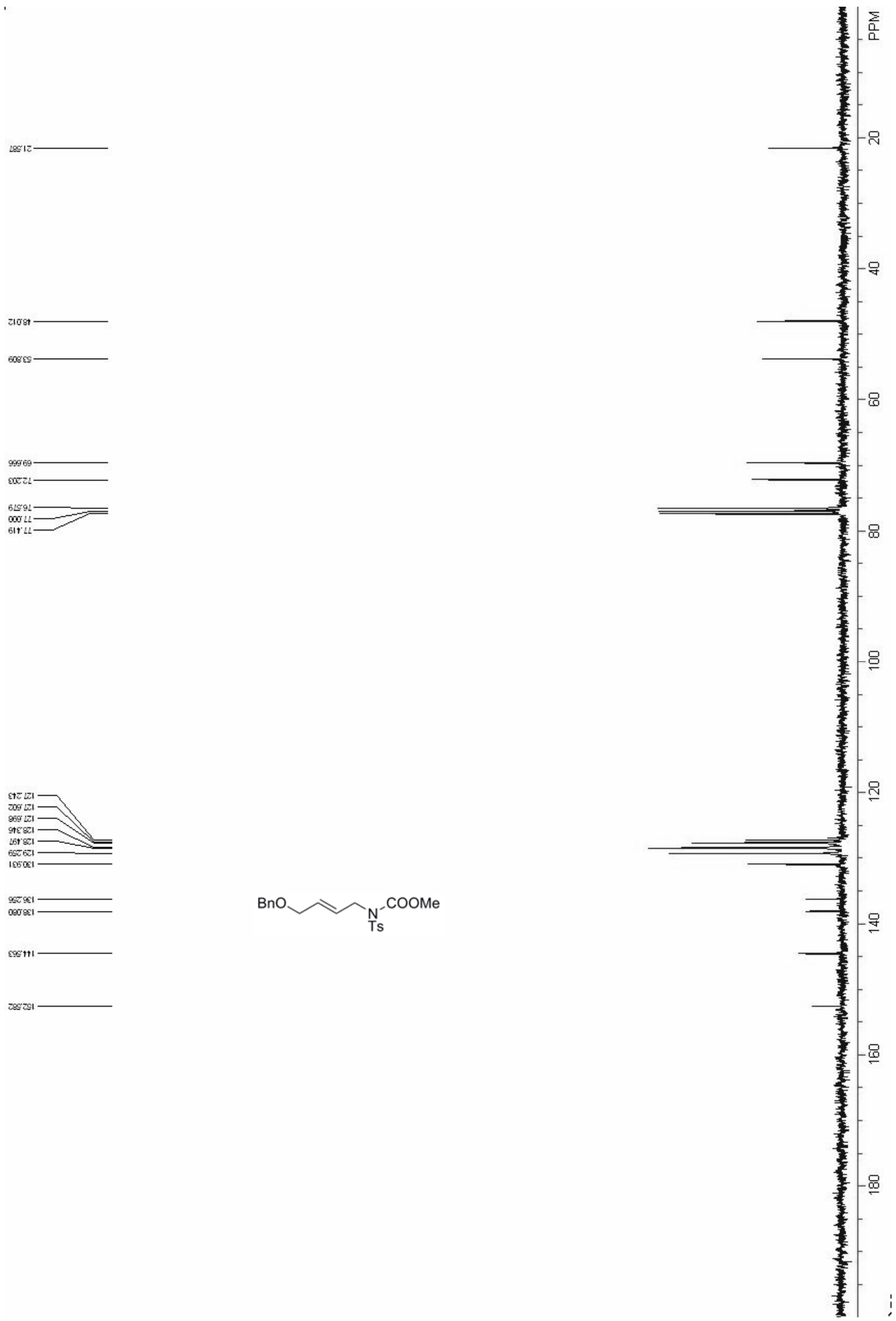

PPM
$C_{14}H_{29}$
N
COOMe
Ts
+ nonallylic isomers

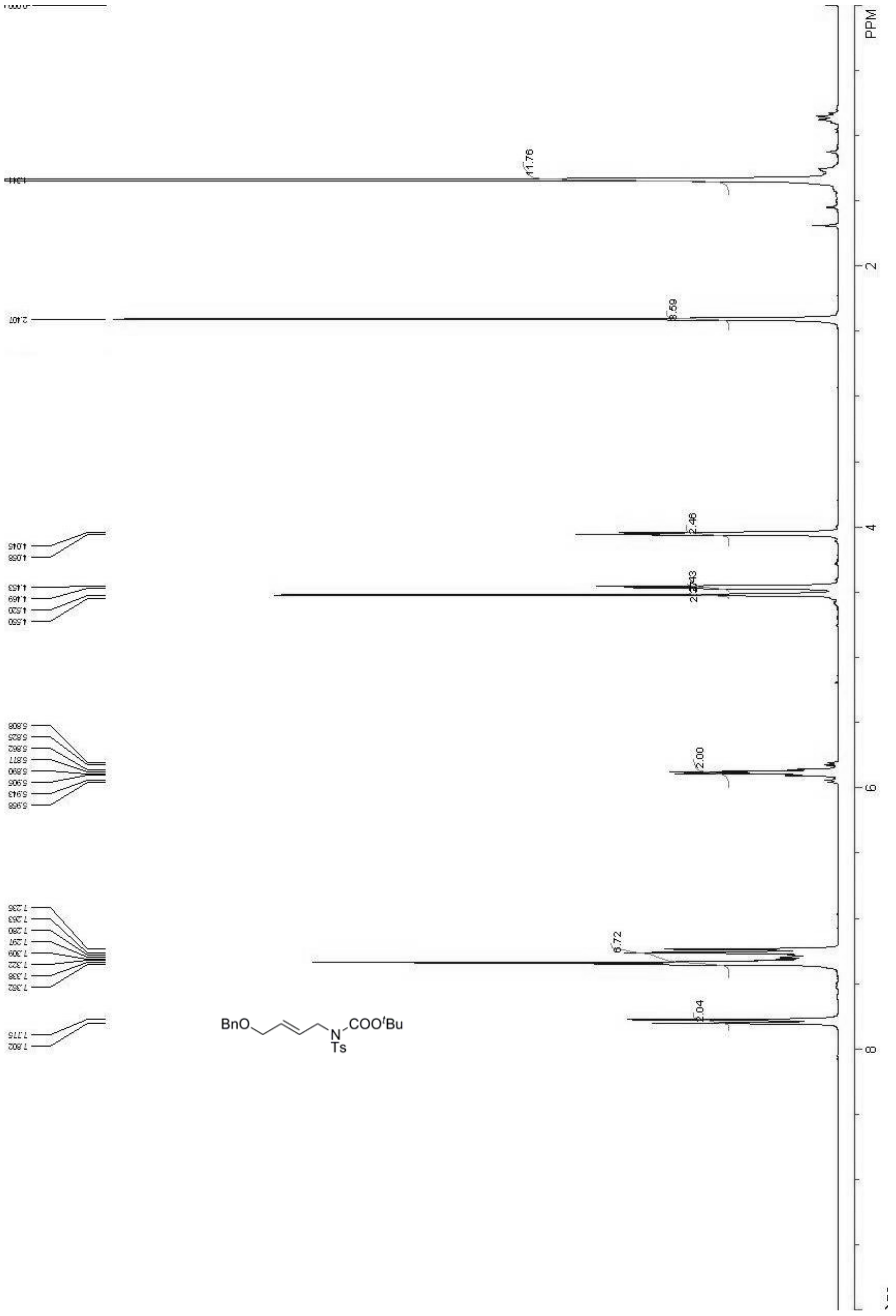


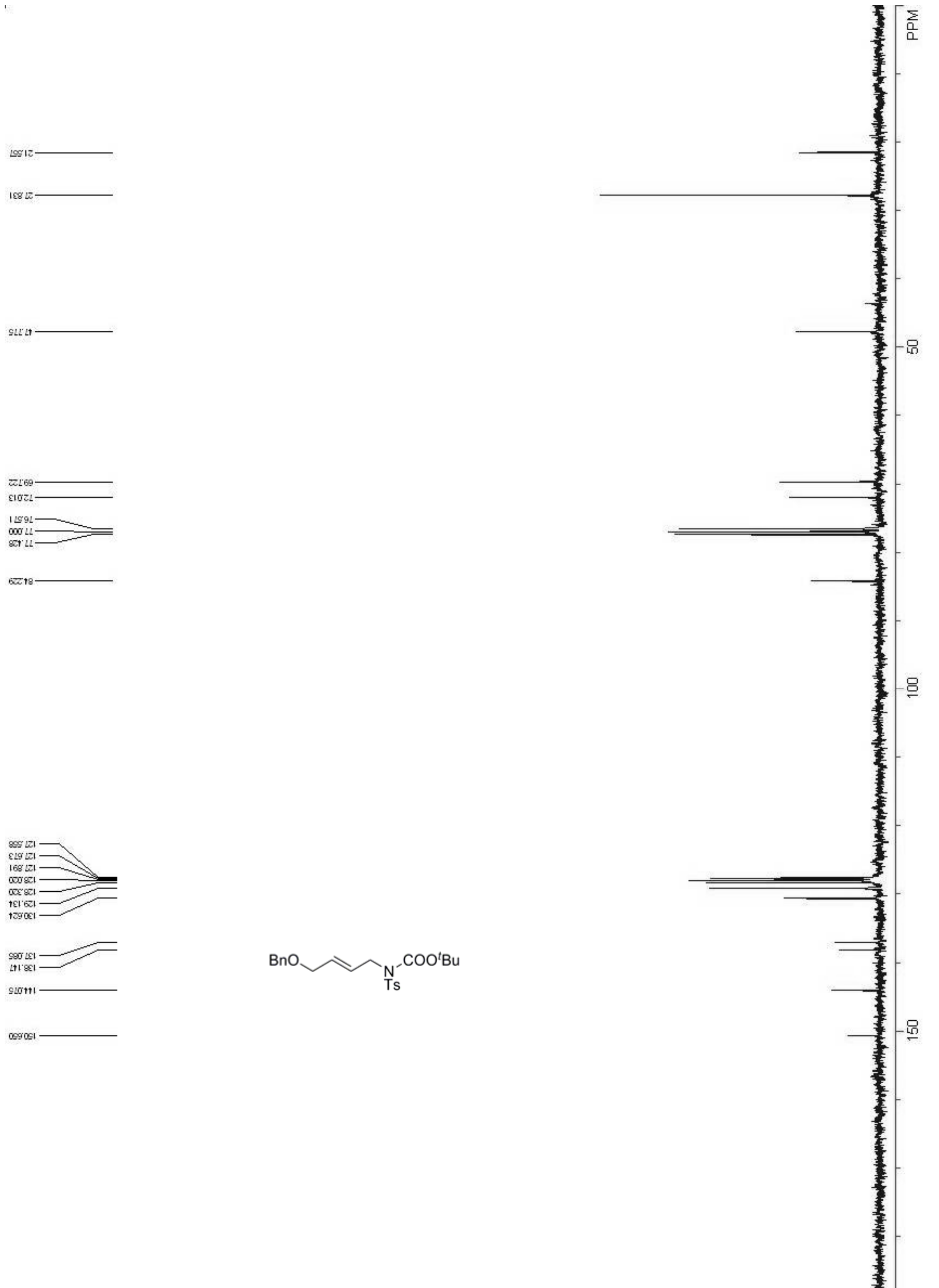


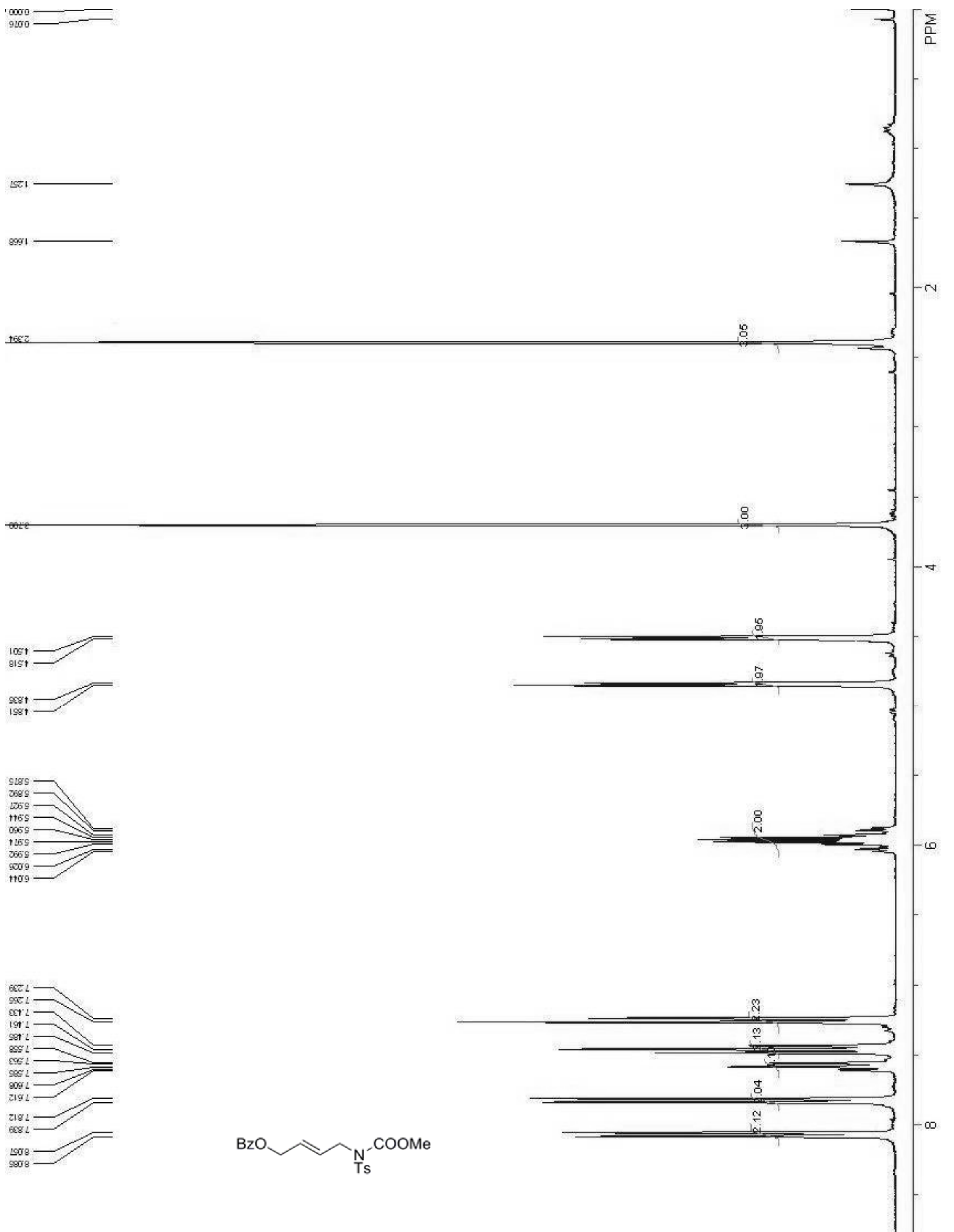
14.132
21.535
22.684
26.578
29.117
29.350
29.523
29.571
29.688
31.910
30.067
47.476
53.687
76.580
77.000
77.429
128.287
129.297
136.605
144.438
152.903
C14H29
N
COOMe
Ts
PPM
50
100
150

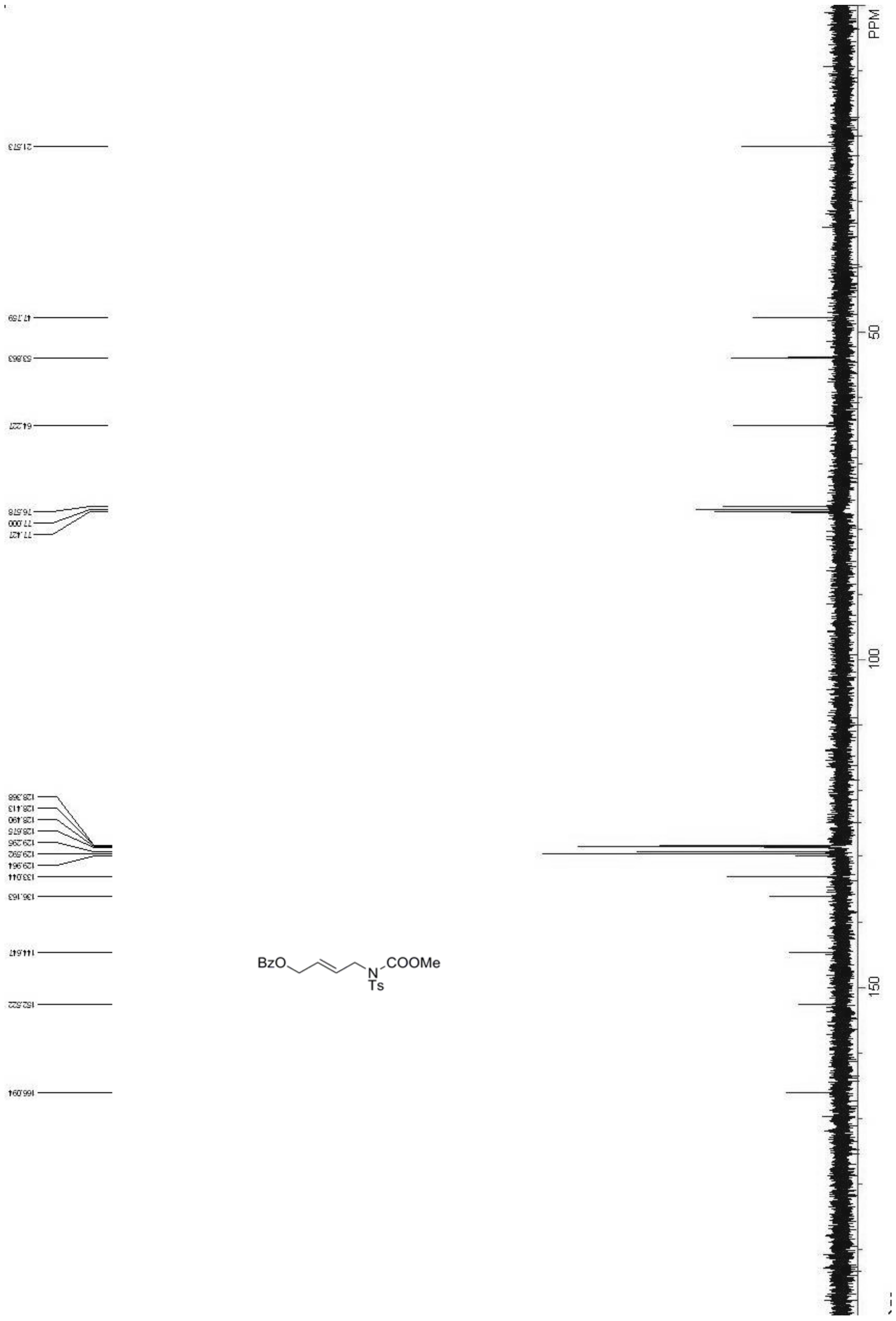

BnO
N
COOMe
Ts
PPM


BnO
N
COOMe
Ts
PPM

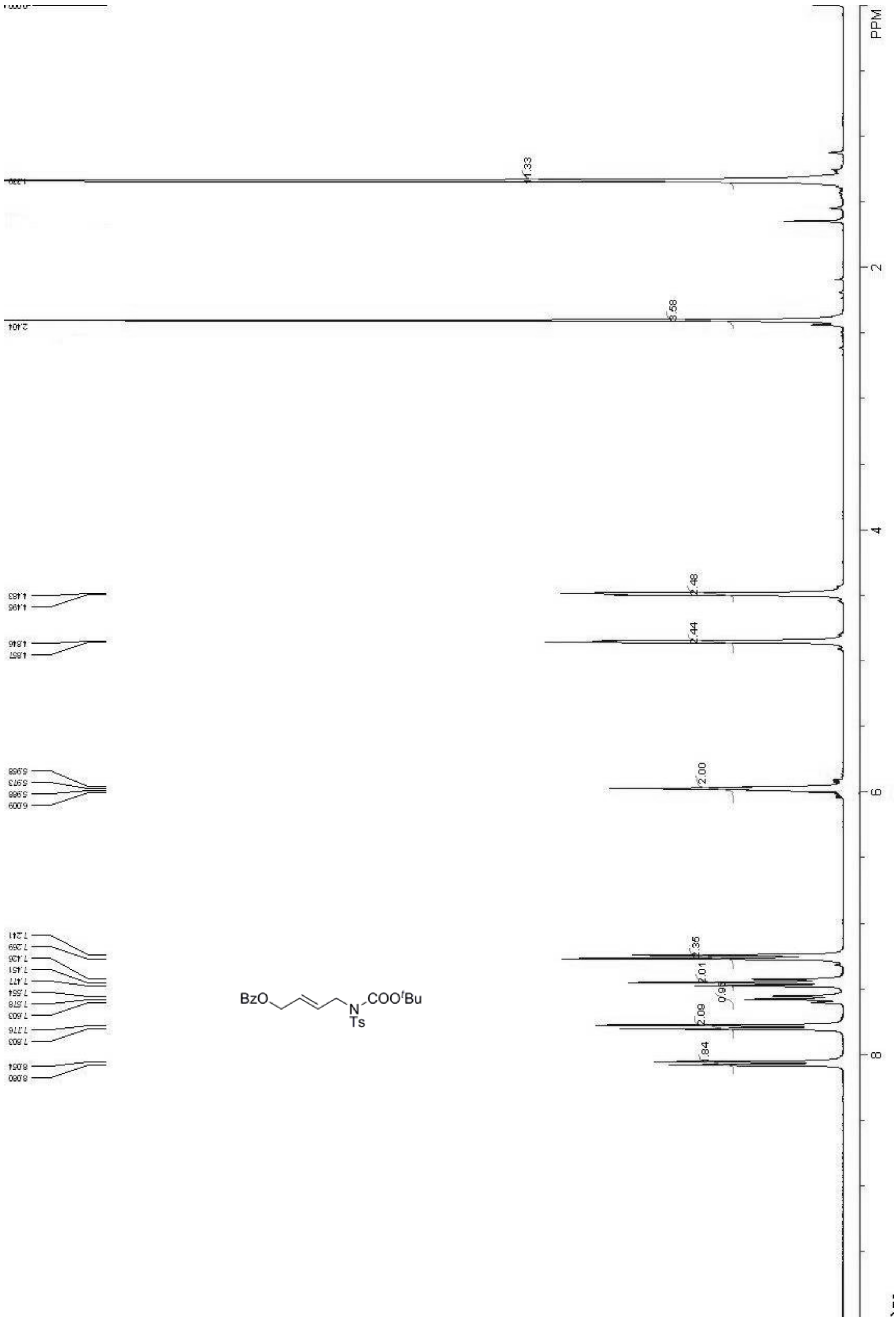

PPM
2
4
6
8
11.76
8.59
2.46
2.00
6.72
2.04
BnO
N
COO^{t}Bu
Ts

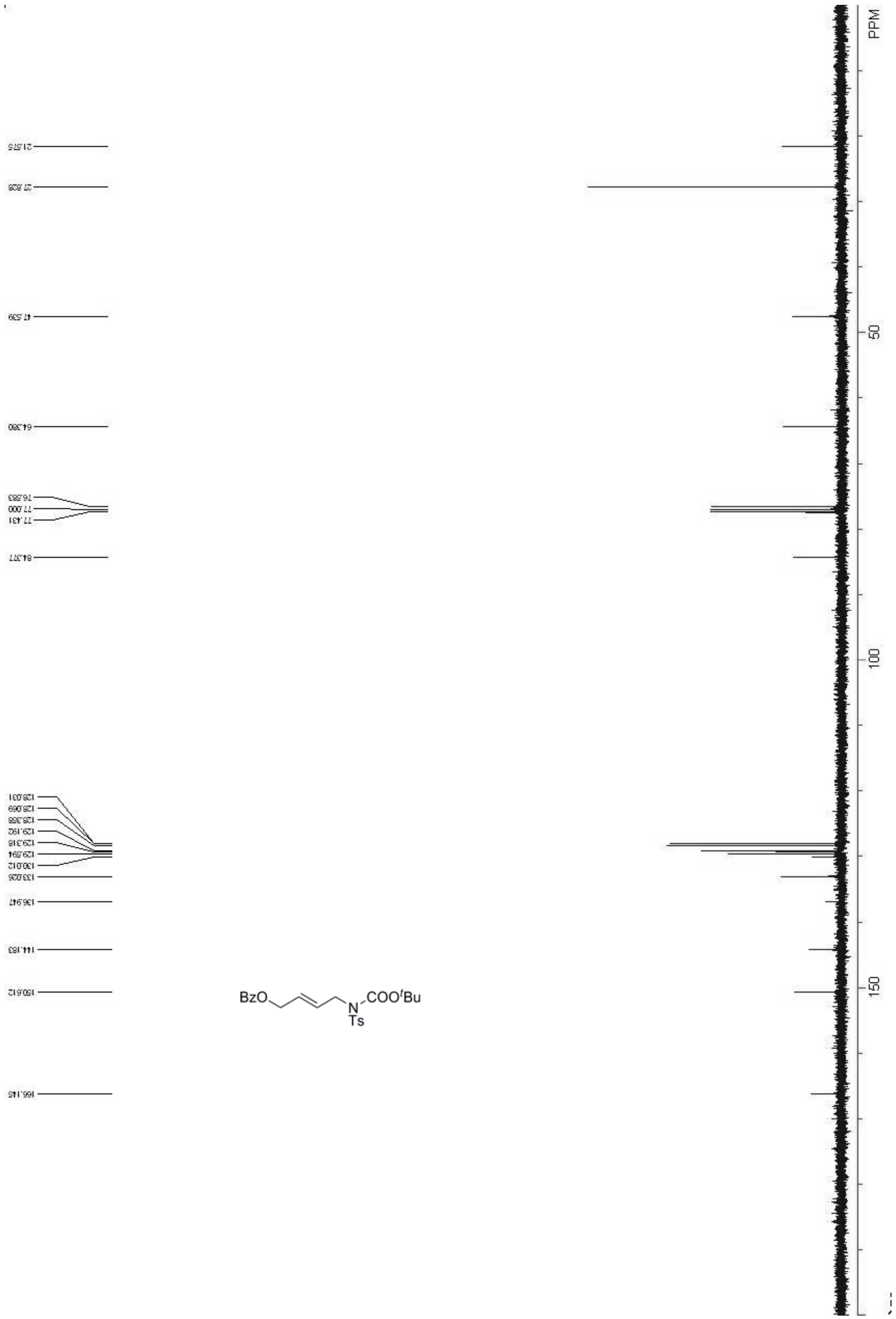

21.557
27.831
47.775
69.722
72.013
76.571
77.000
77.428
81.229
127.588
127.673
127.891
128.020
128.320
129.134
130.624
137.085
138.147
144.075
150.660
BnO
N
COO^{t}Bu
Ts
PPM
50
100
150

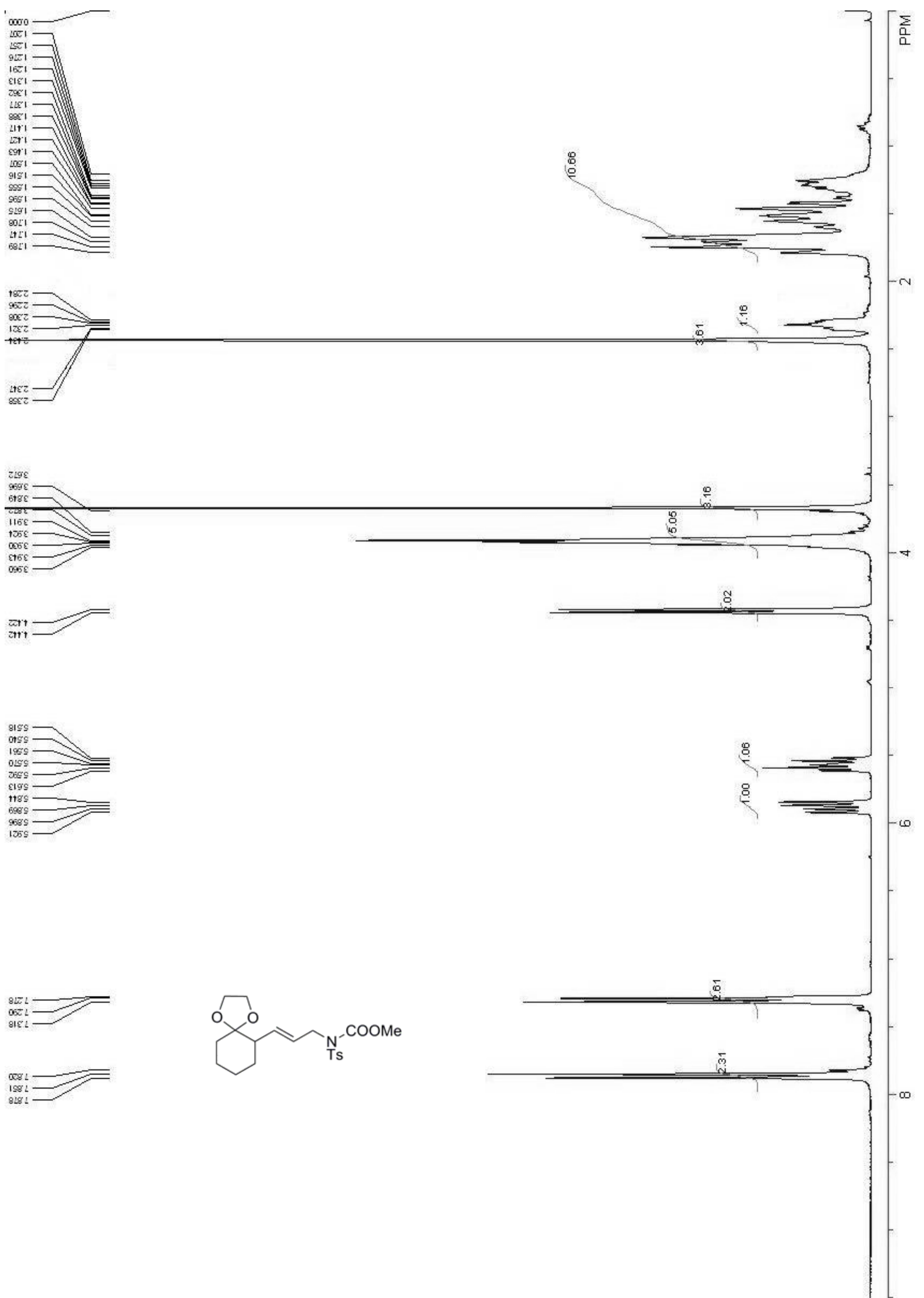

PPM
2
4
6
8
3.05
3.00
1.95
1.97
2.00
2.12
BzO
N
COOMe
Ts

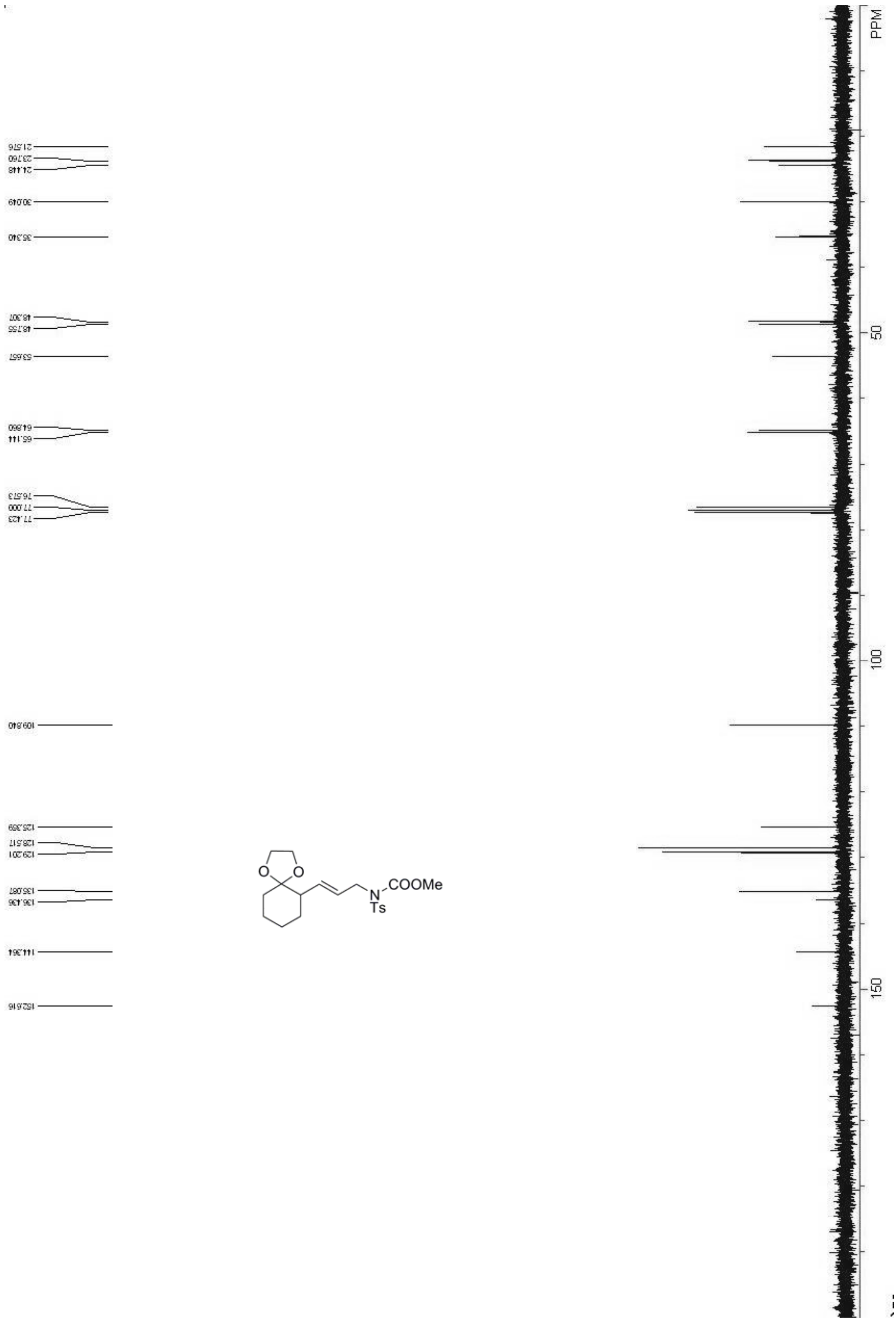


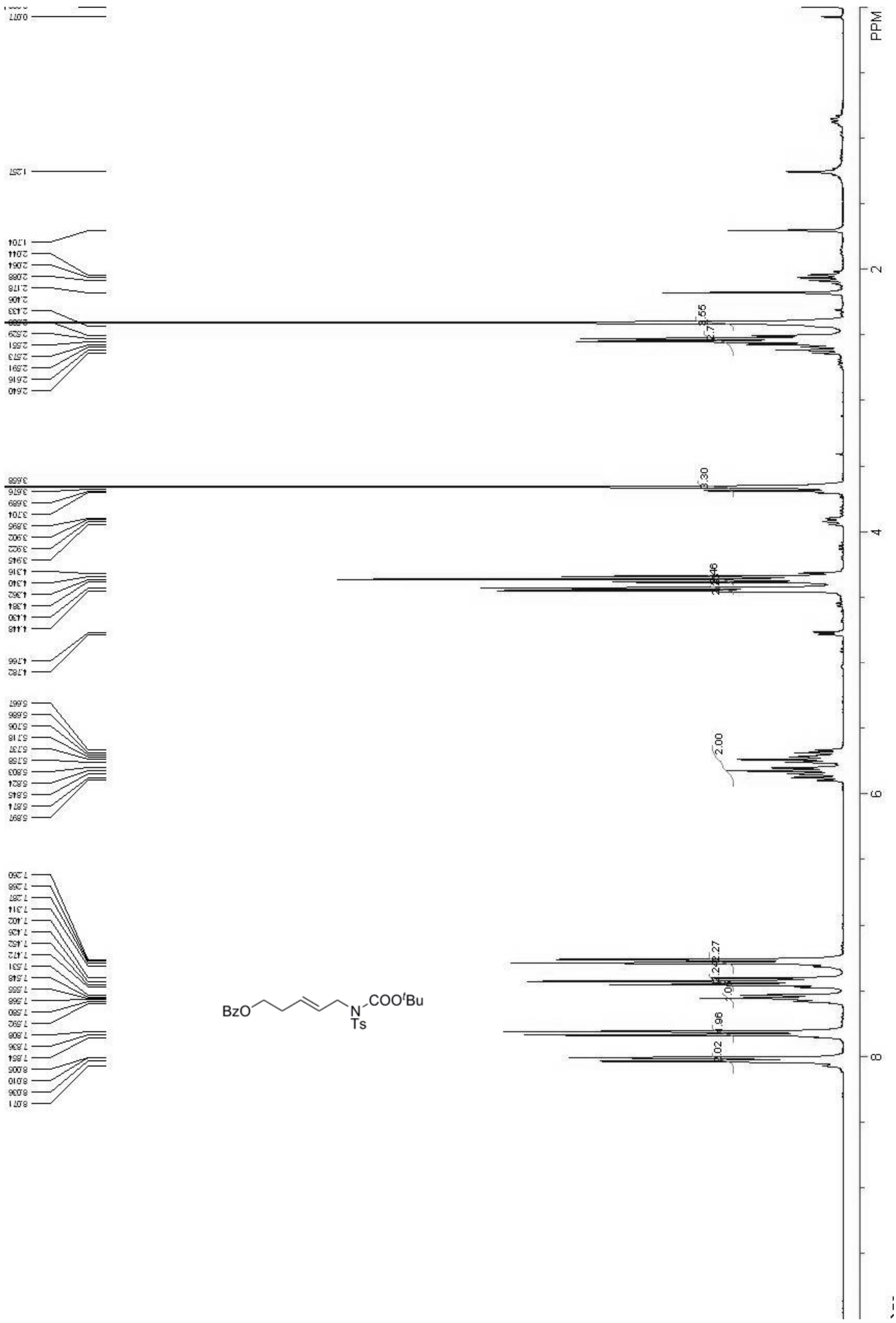
21.573
47.759
53.863
64.227
76.578
77.000
77.421
128.366
128.413
128.480
128.675
129.296
129.592
129.964
133.044
136.163
144.647
152.622
166.094
BzO
N
COOMe
Ts
PPM
50
100
150

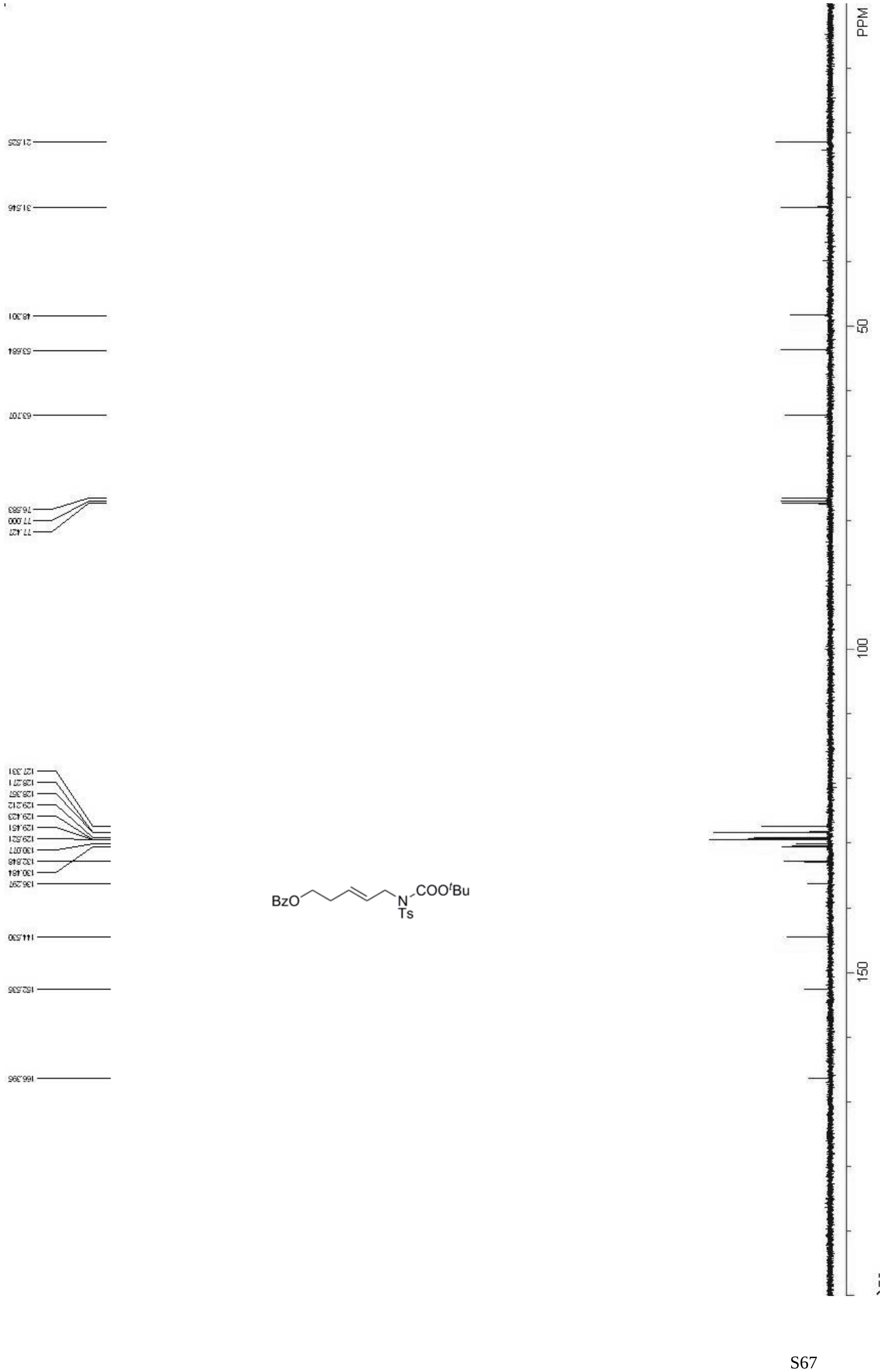

BzO
N
COO^{t}Bu
Ts

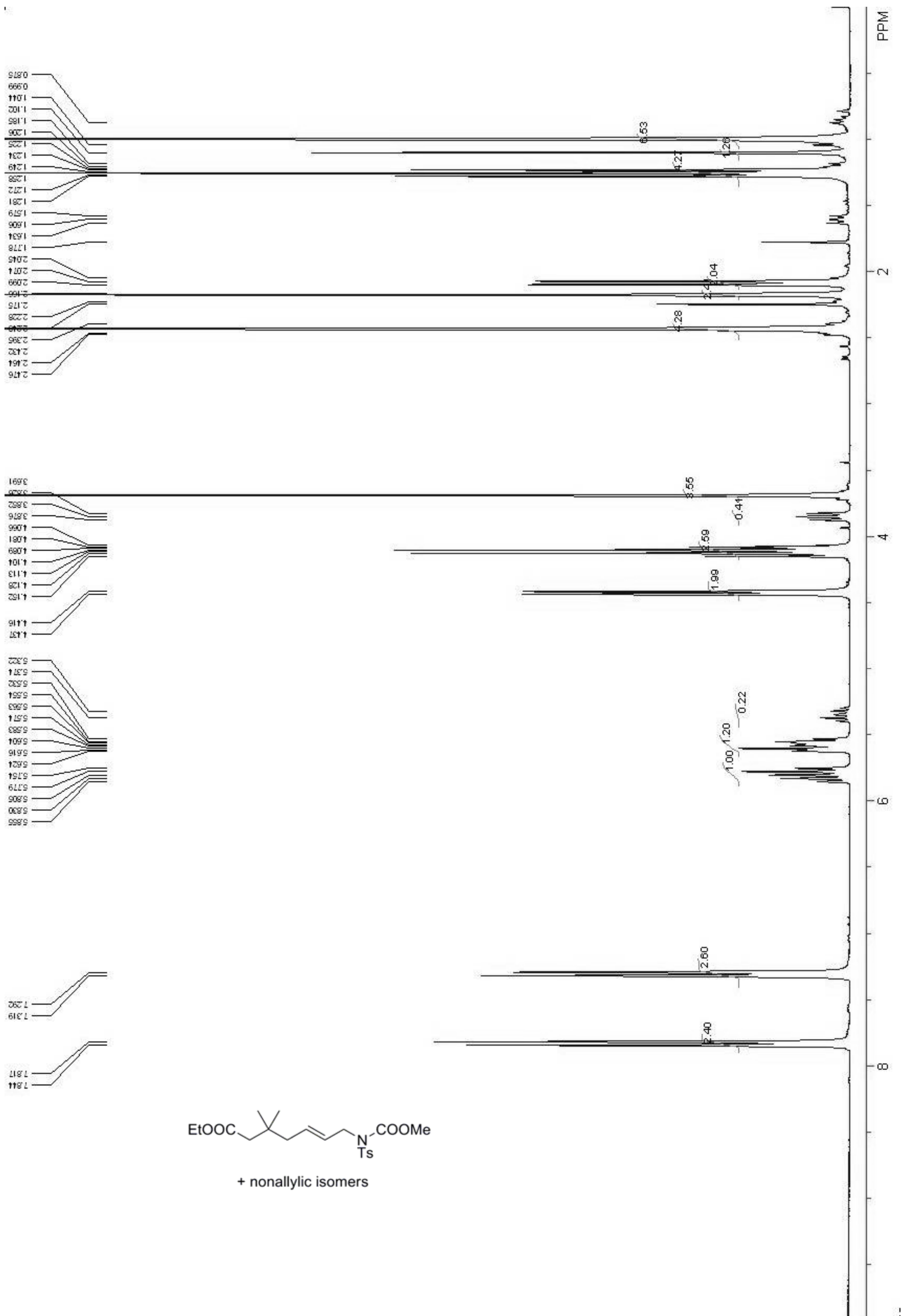

PPM
50
100
150
BzO
N
COO^{t}Bu
Ts

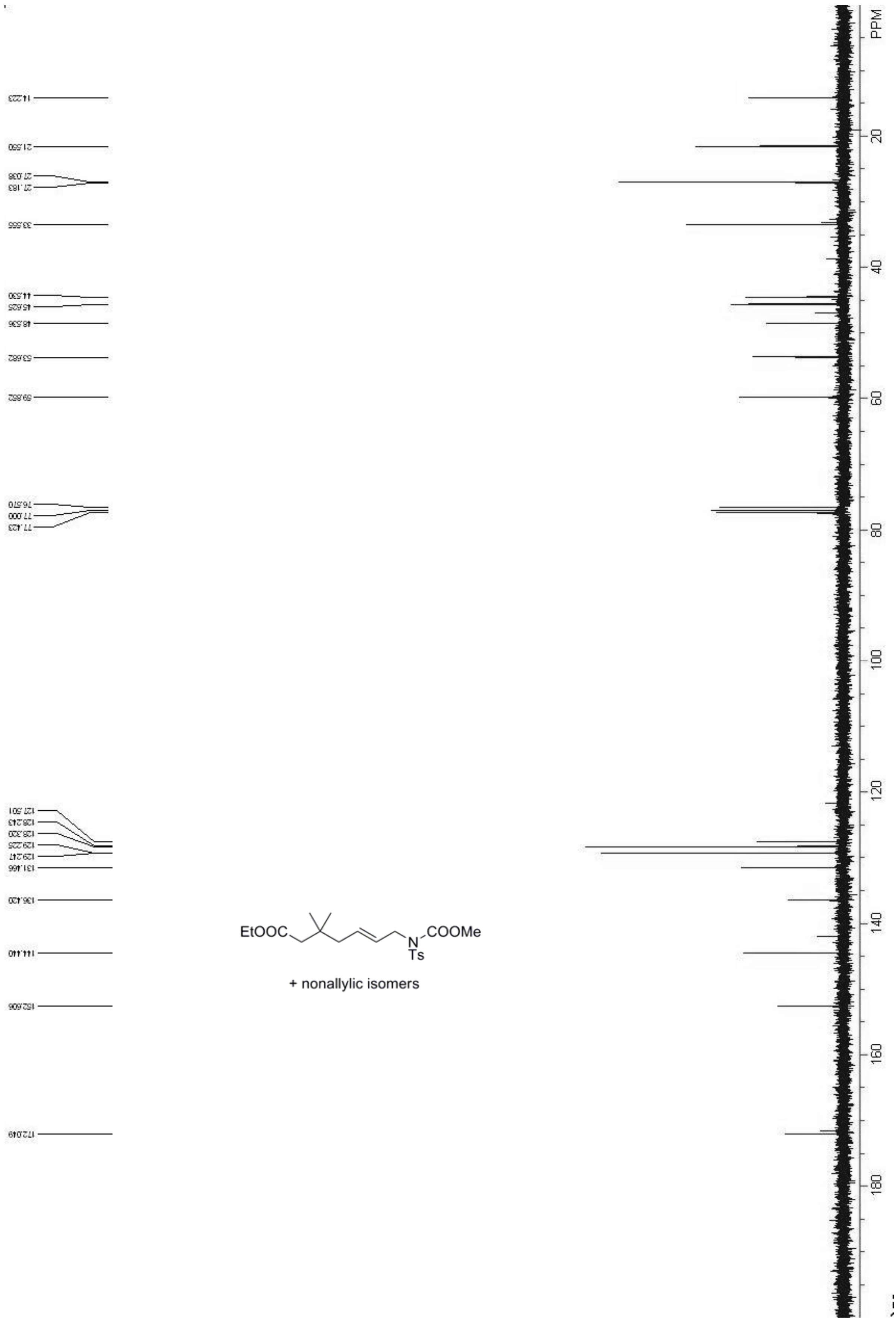

PPM
2
4
6
8
O
O
N
COOMe
Ts


PPM
50
100
150
21.576
23.760
24.448
30.049
35.340
48.307
48.755
53.657
64.860
65.144
76.573
77.000
77.423
109.840
125.399
128.517
129.201
135.087
136.436
144.364
152.616
O
O
N
COOMe
Ts

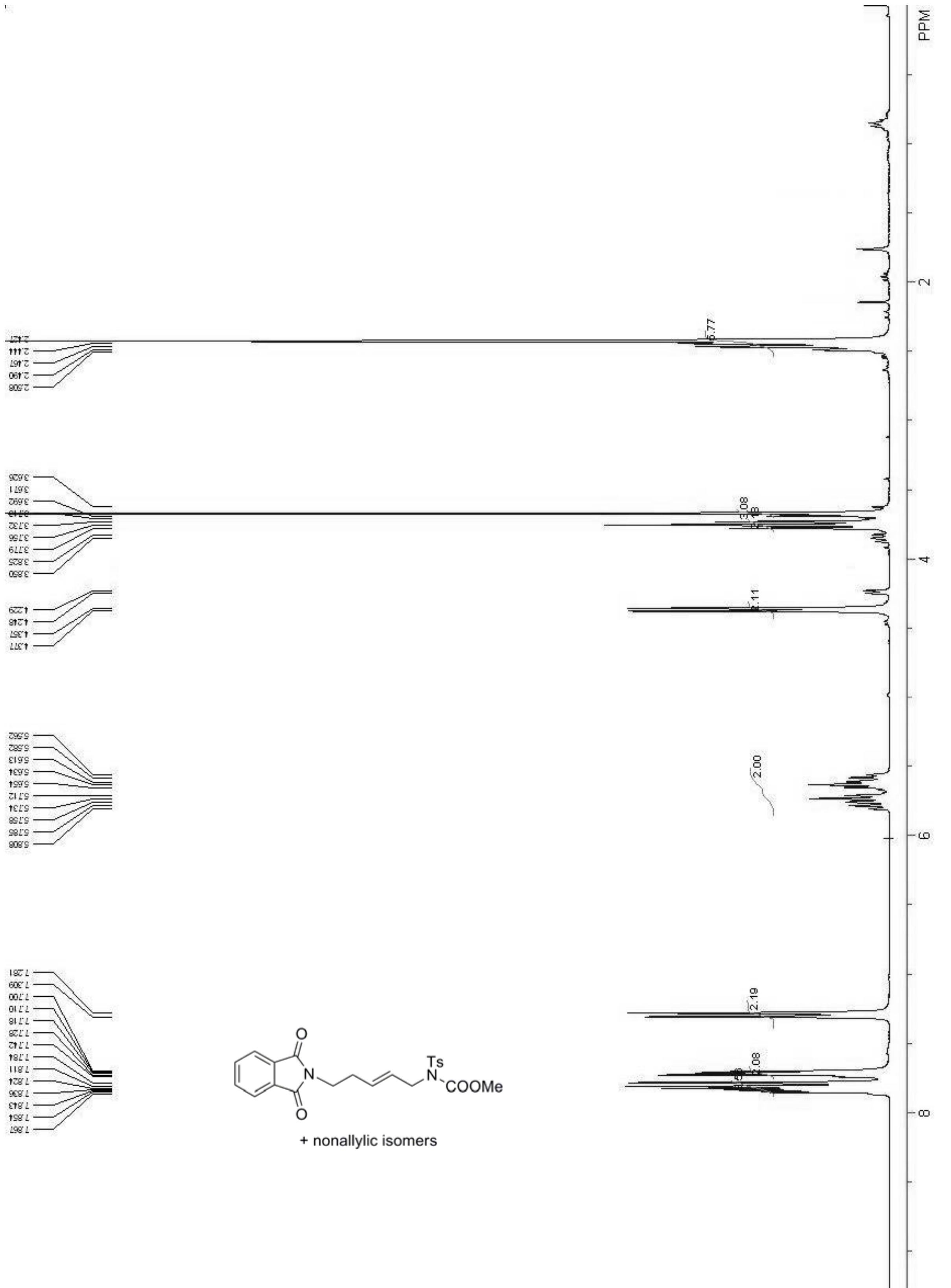

BzO
N
COOtBu
Ts
PPM

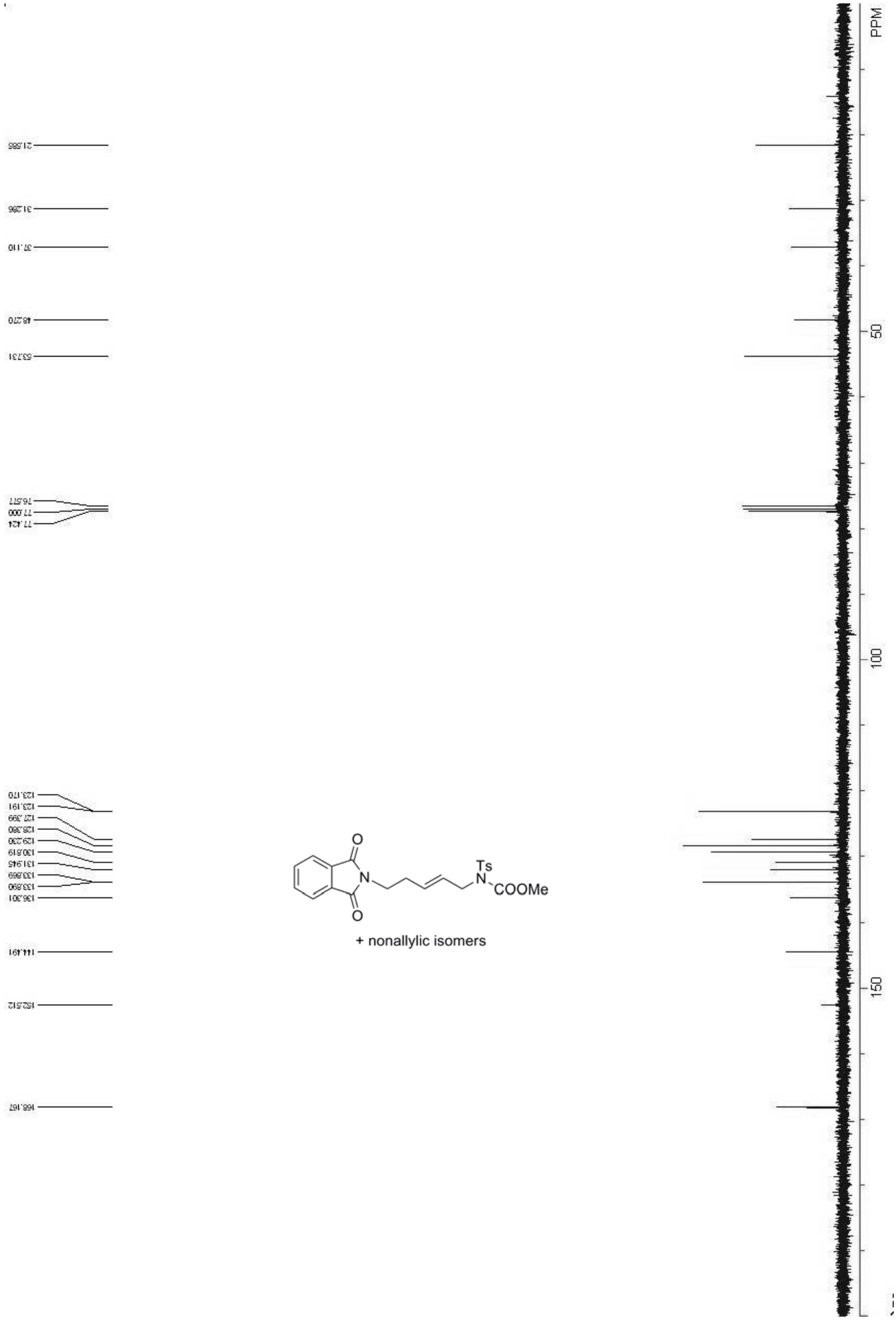

PPM
50
100
150
BzO
N
COO^{t}Bu
Ts


PPM
EtOOC
N
COOMe
Ts
+ nonallylic isomers

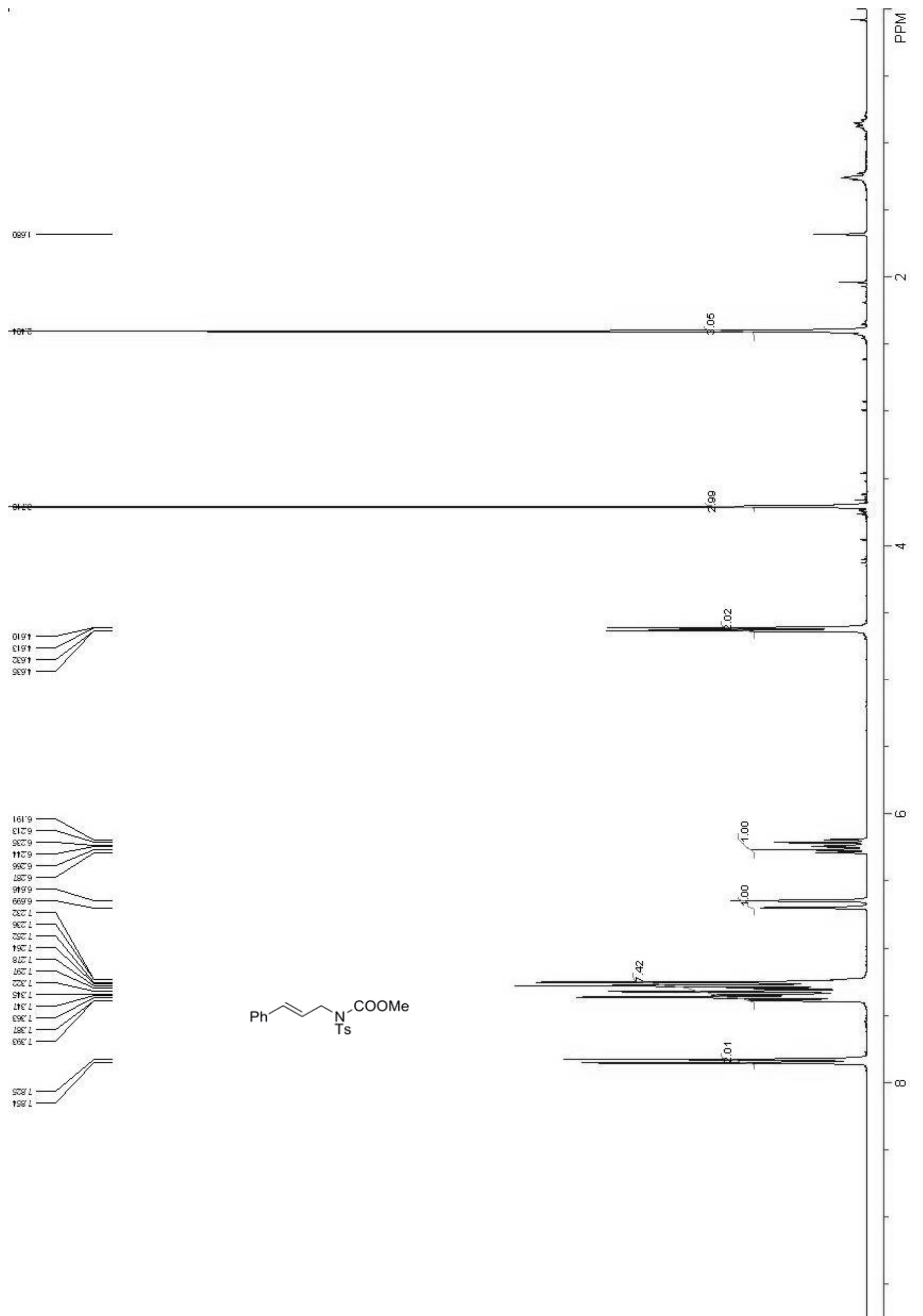


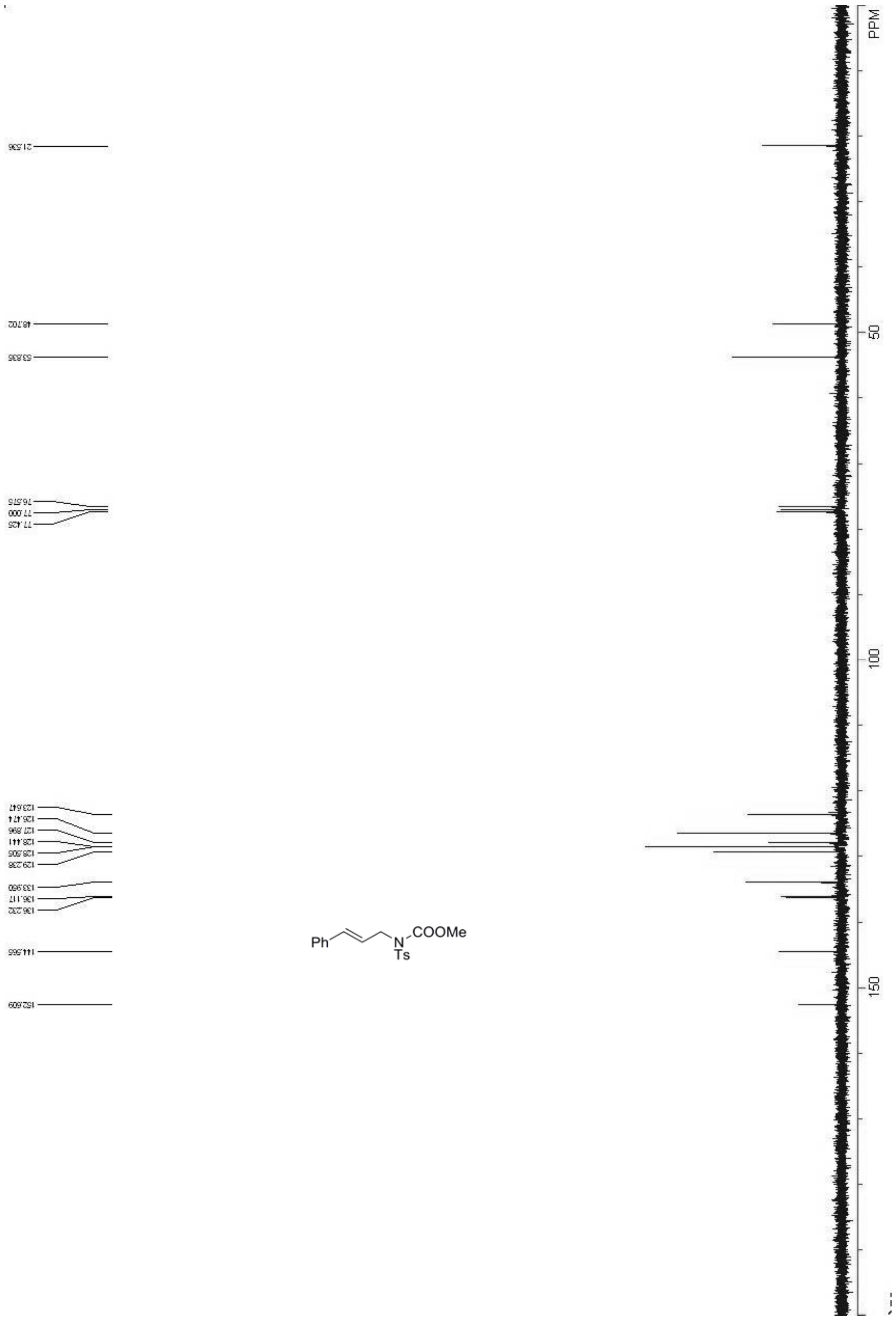
+ nonallylic isomers


Ts
N
COOMe
O
N
O
+ nonallylic isomers
PPM



21.885
31.296
37.110
48.270
53.731
76.577
77.000
77.421
123.170
123.191
127.399
128.380
129.230
130.819
131.945
133.869
133.890
136.301
144.491
152.512
168.167
O
N
O
Ts
N
COOMe
+ nonallylic isomers
PPM
50
100
150





PPM
50
100
150
21.536
48.702
53.835
76.575
77.000
77.425
123.647
125.474
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128.505
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144.565
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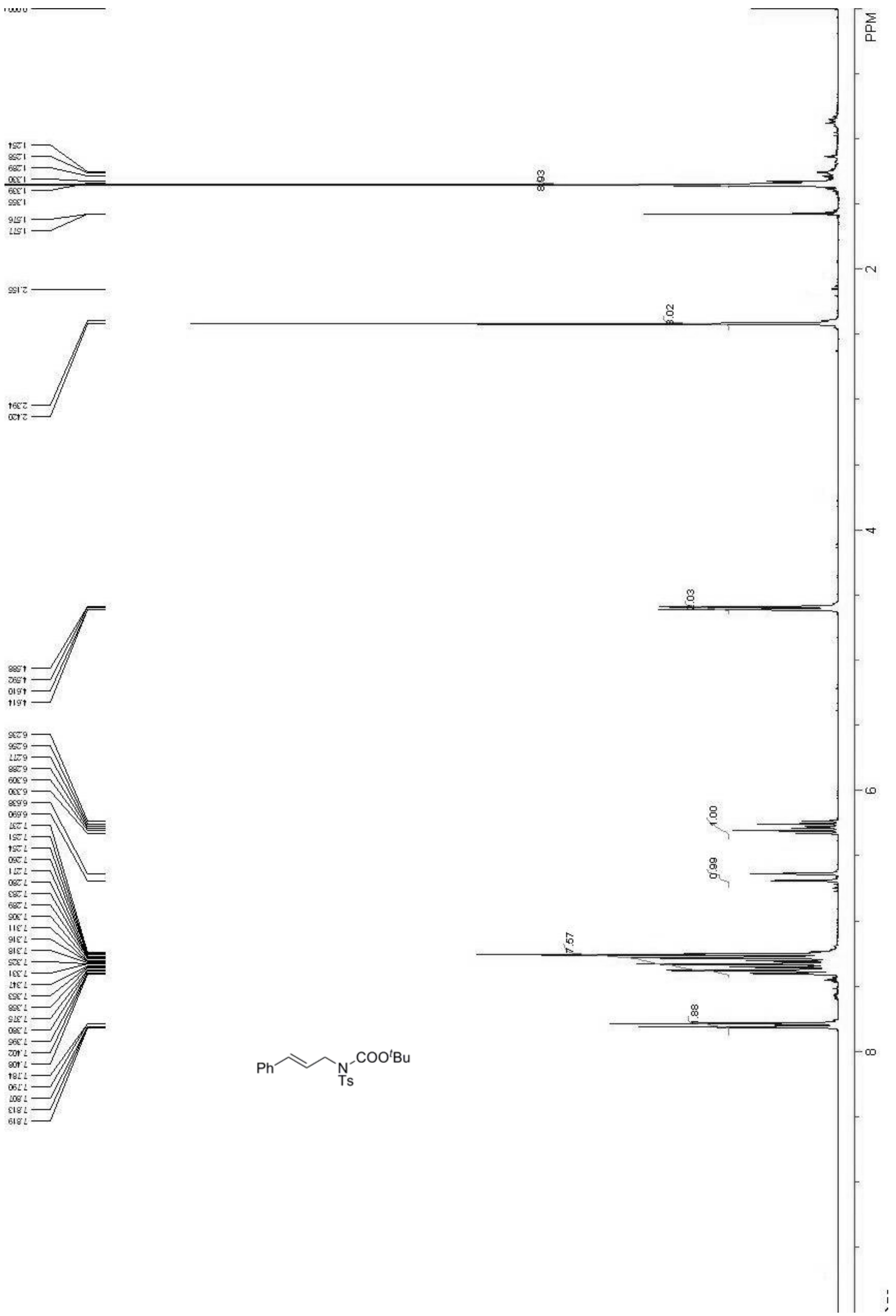
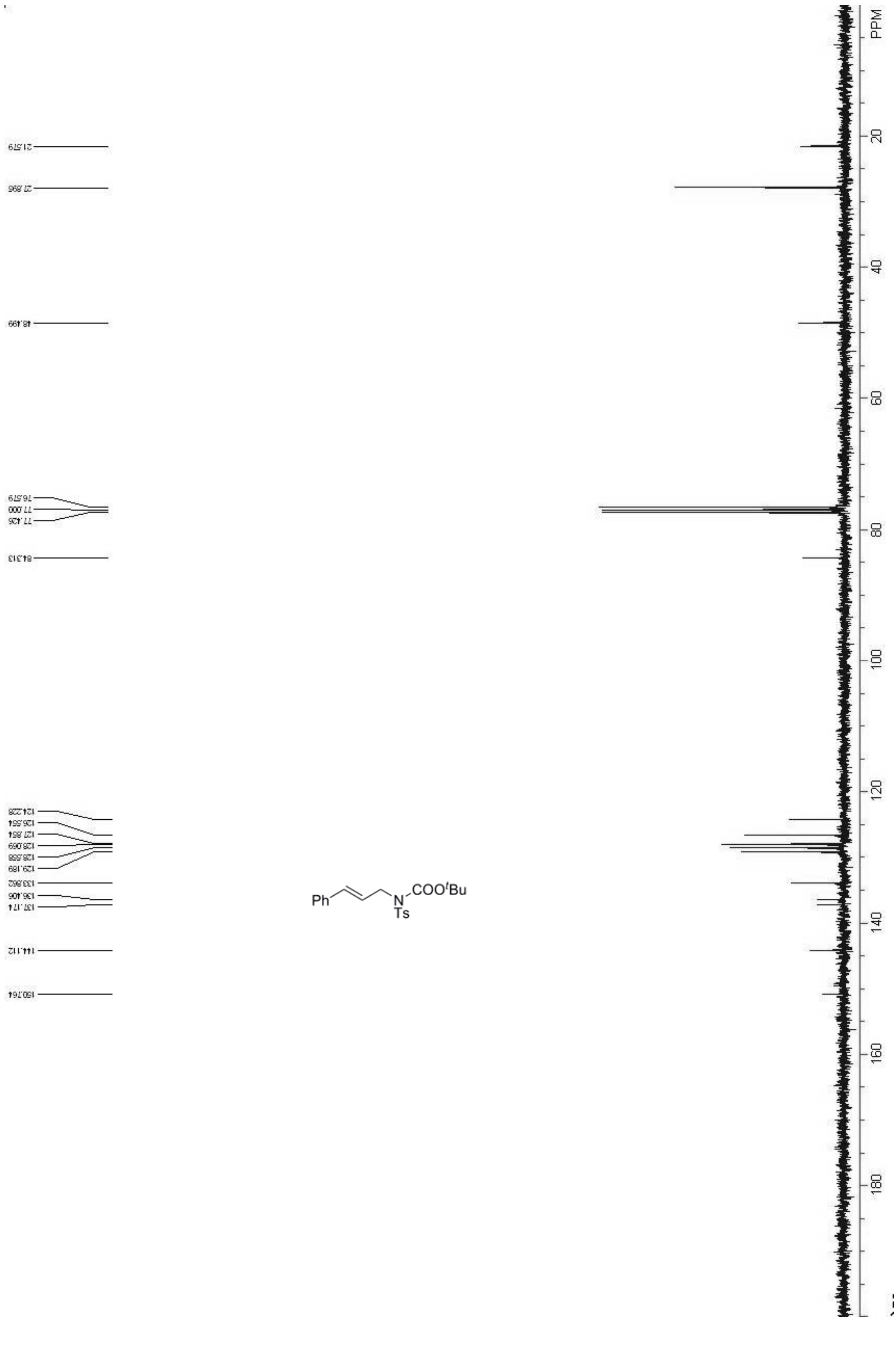
Ph
N
COOMe
Ts


PPM
Ph
N
COO^{t}Bu
Ts



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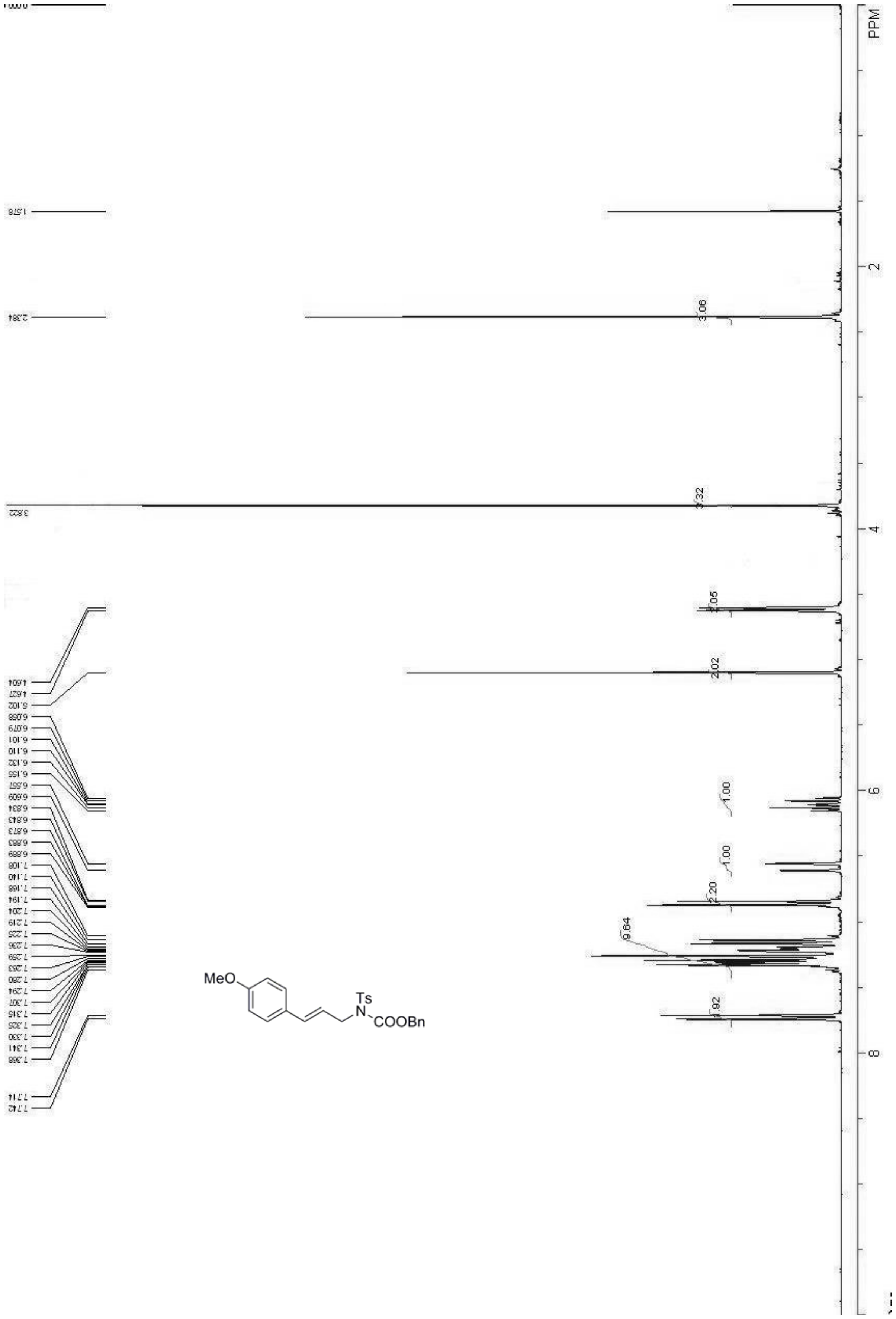
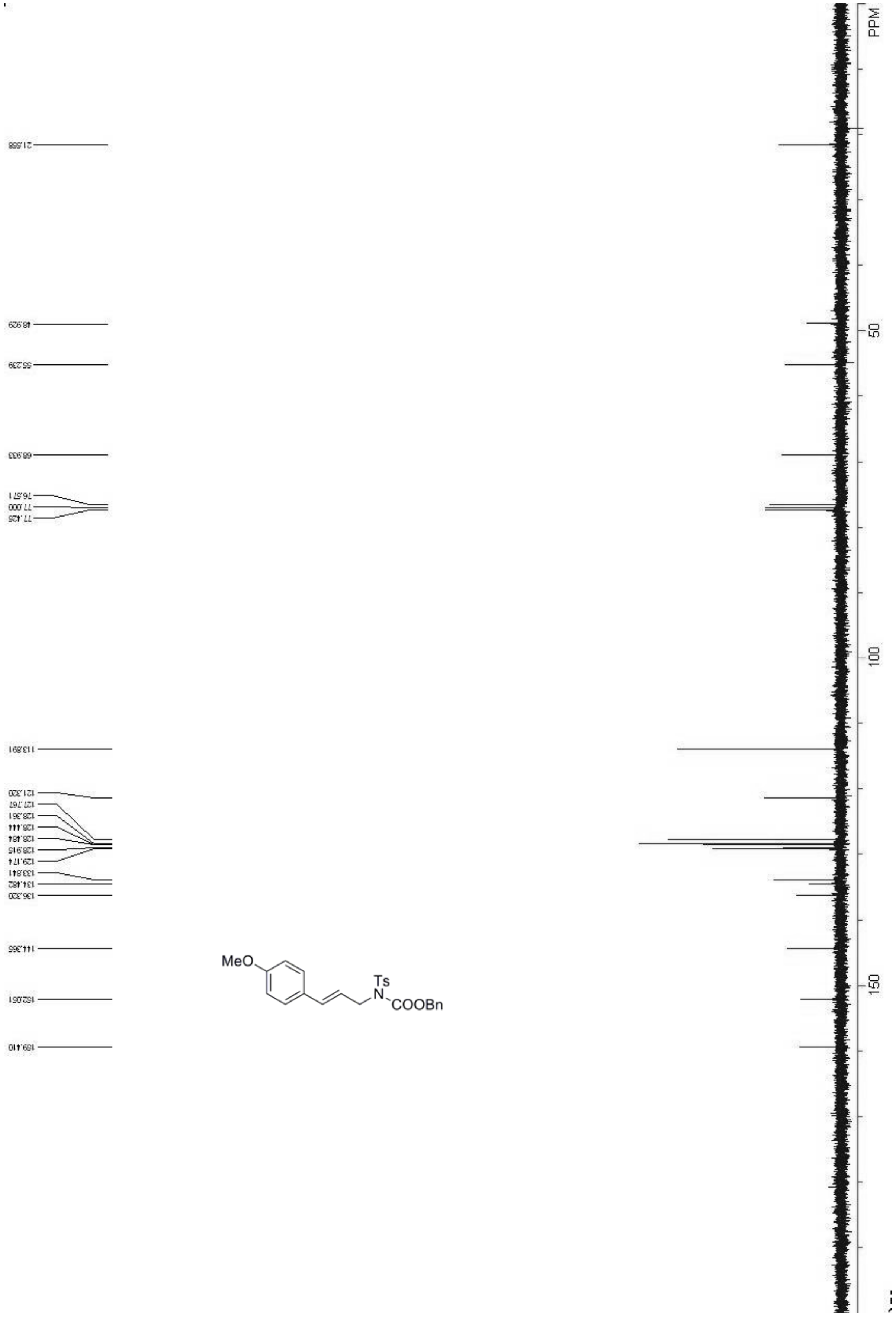
77.000
77.435
84.313
124.228
126.554
127.854
128.069
128.588
129.189
133.862
136.406
137.174
144.112
150.764
Ph
N
COO^{t}Bu
Ts
PPM
20
40
60
80
100
120
140
160
180


MeO
Ts
N
COOBn



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68.933
76.571
77.000
77.425
113.891
121.320
127.767
128.361
128.441
128.481
128.915
129.174
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134.482
136.320
144.365
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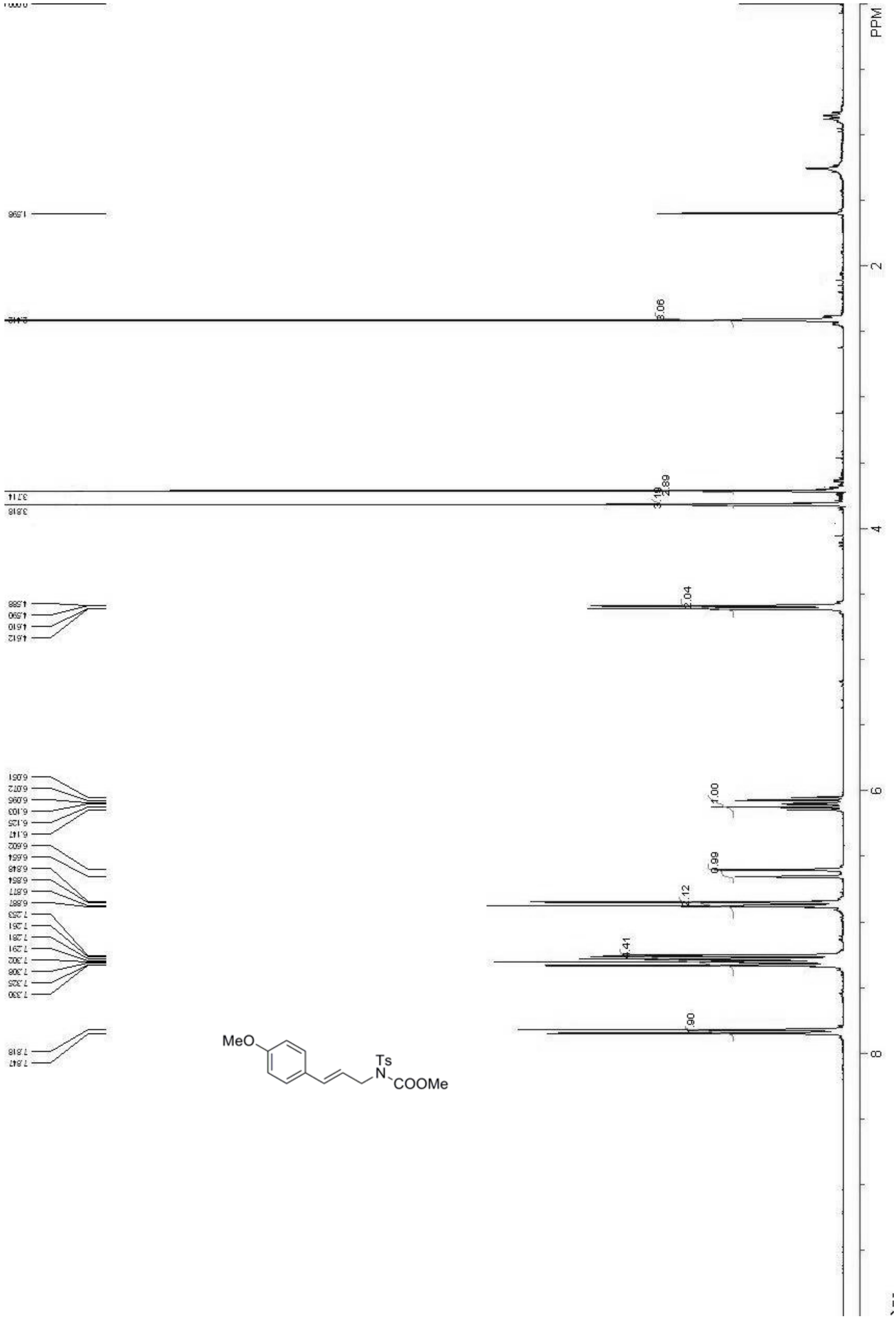
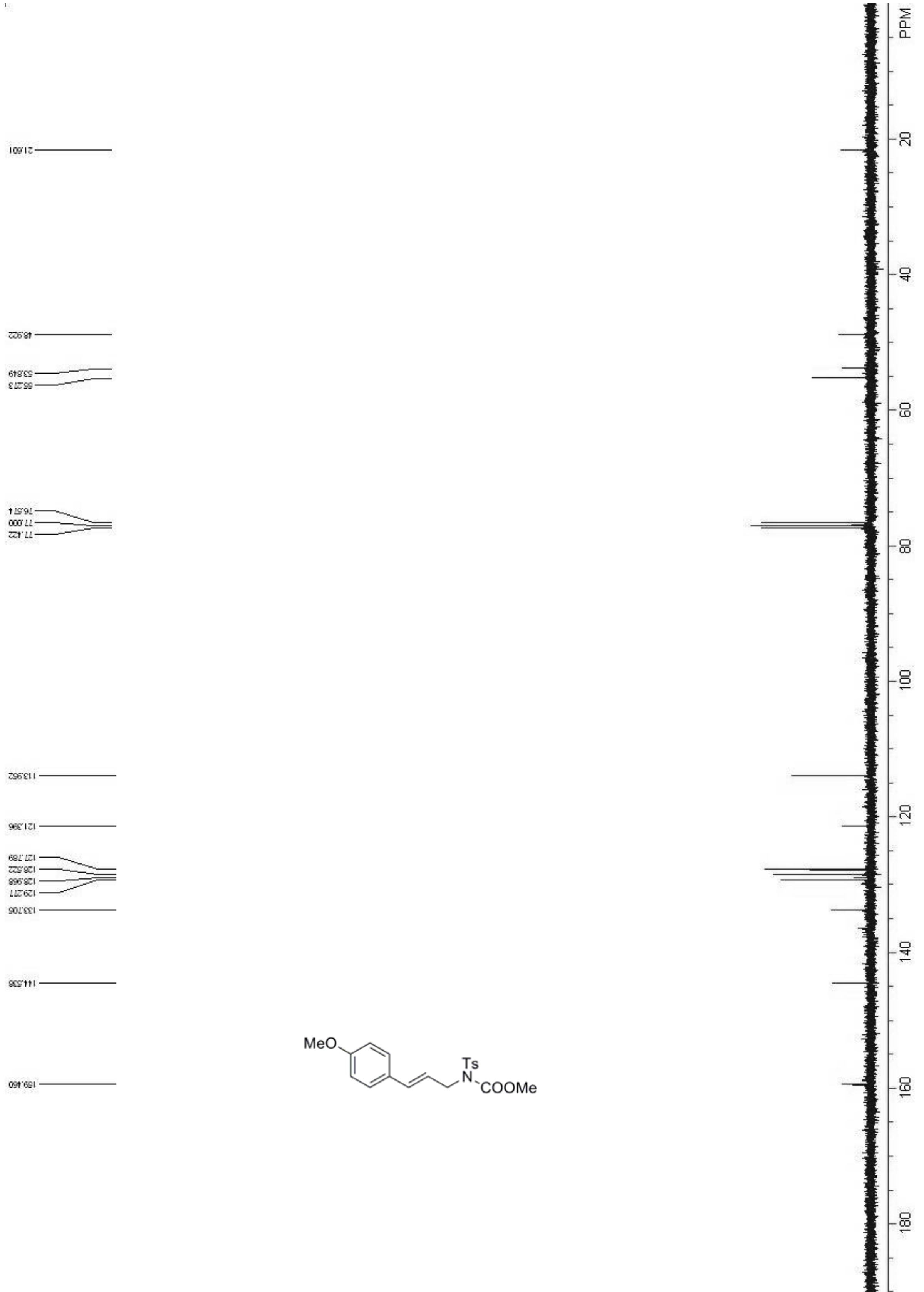
159.410
MeO
Ts
N
COOBn
PPM
50
100
150


MeO
Ts
N
COOMe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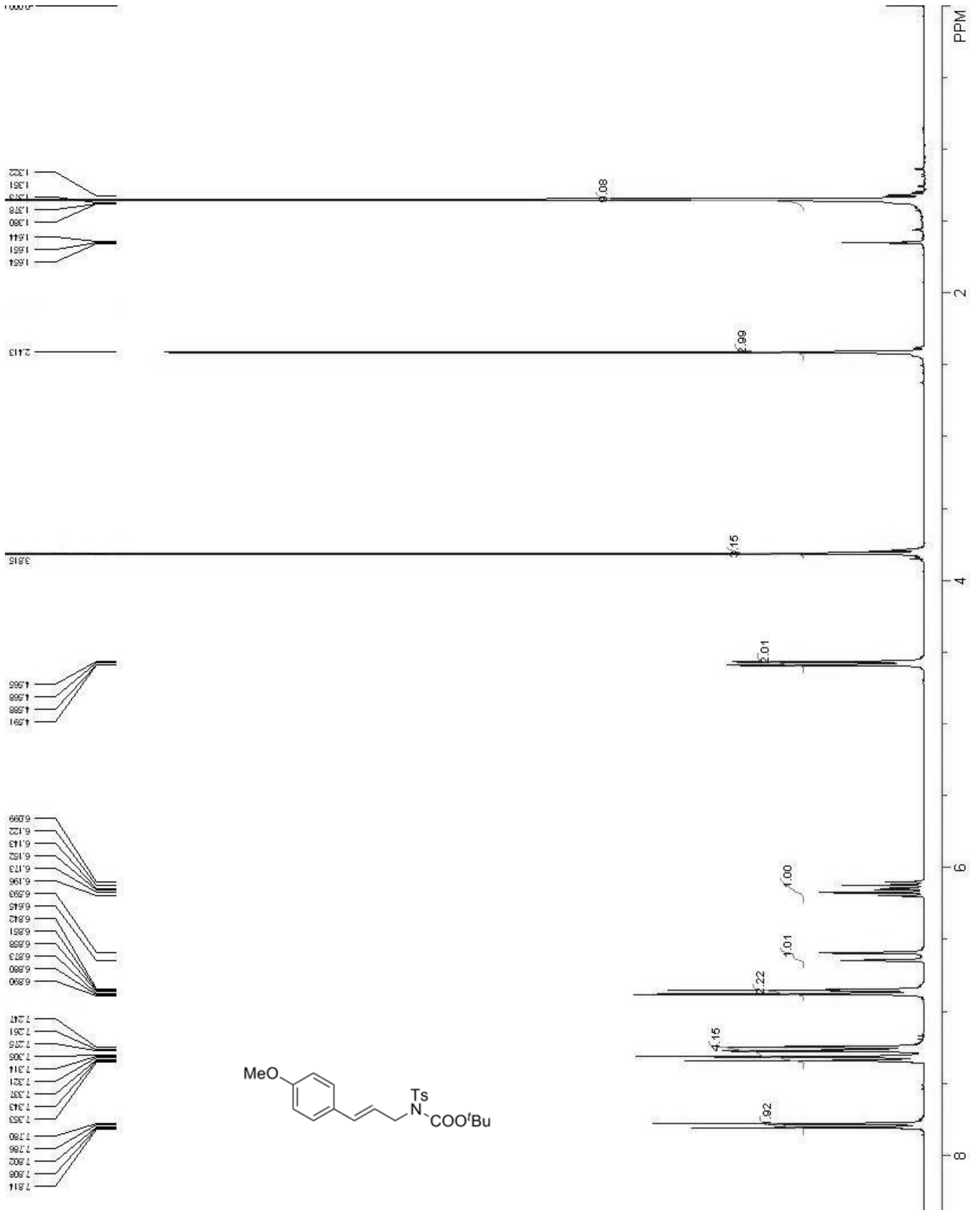
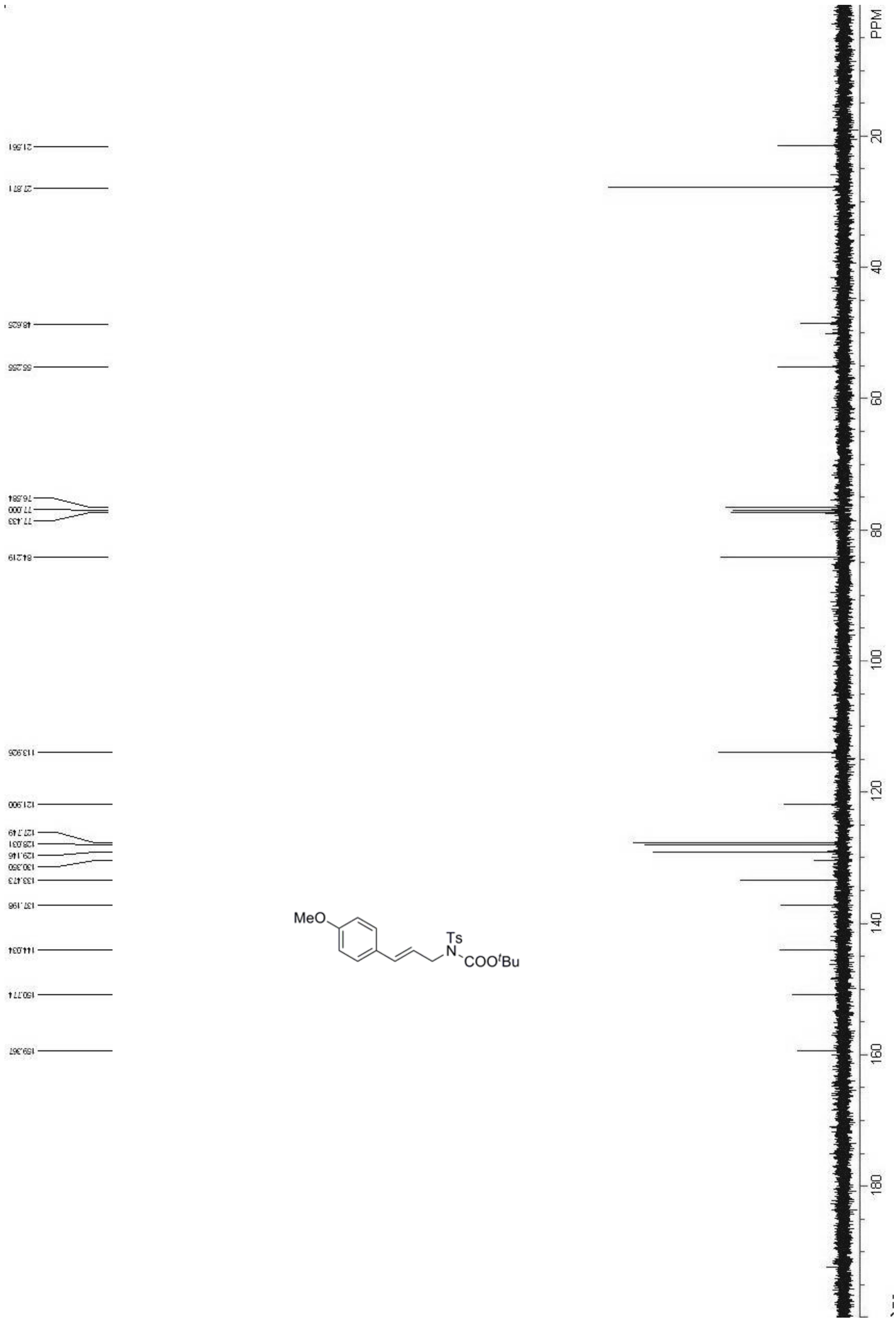
77.422
113.962
121.396
127.789
128.522
128.968
129.277
133.705
144.538
159.460
MeO
Ts
N
COOMe
PPM
20
40
60
80
100
120
140
160
180


PPM
2
4
6
8
9.08
2.99
3.15
2.01
1.00
1.01
2.22
4.15
1.92
MeO
Ts
N
COO^{t}Bu


MeO
Ts
N
COOtBu
PPM
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55.255
76.584
77.000
77.433
84.219
113.905
121.900
127.149
128.031
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137.196
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159.367
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100
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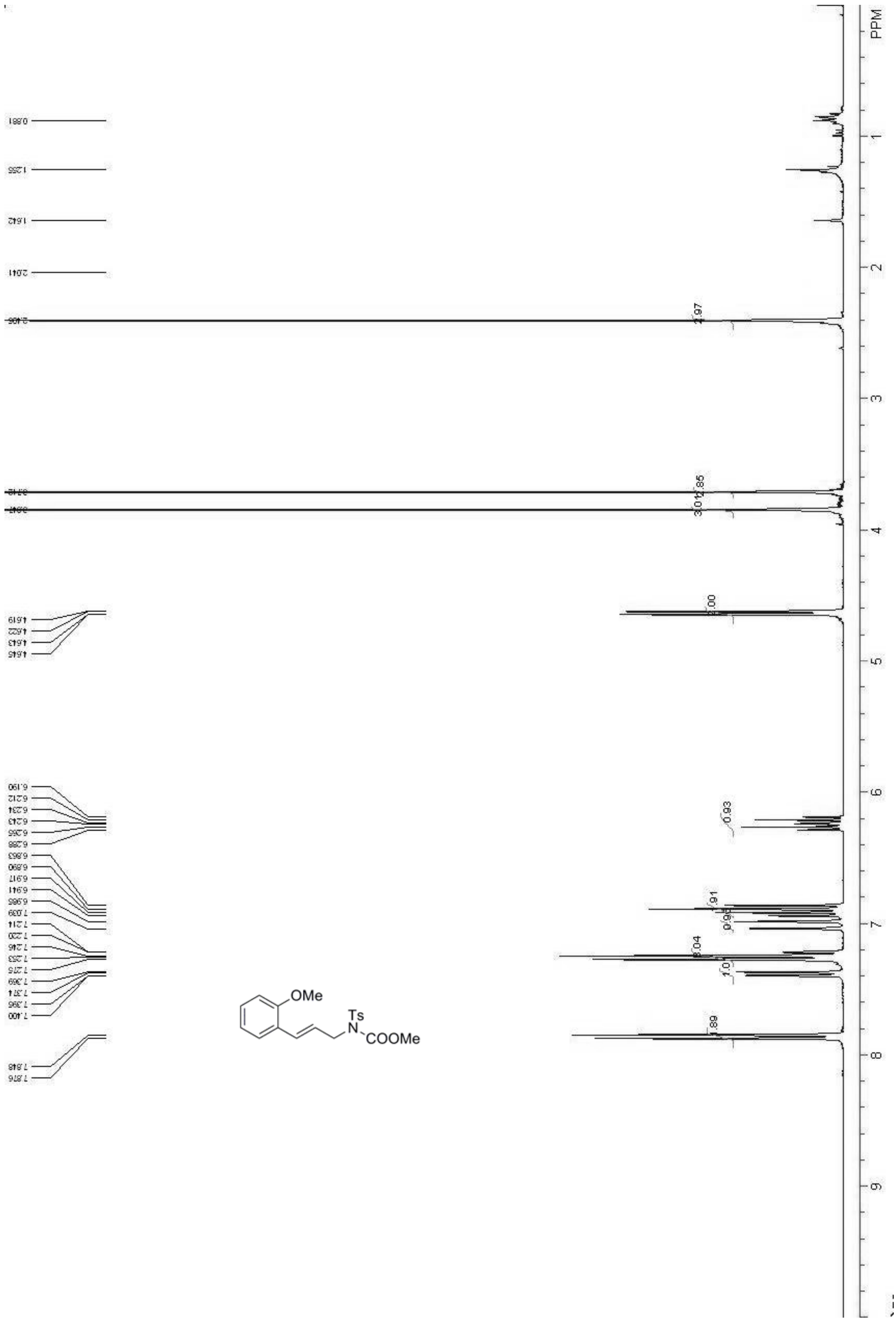

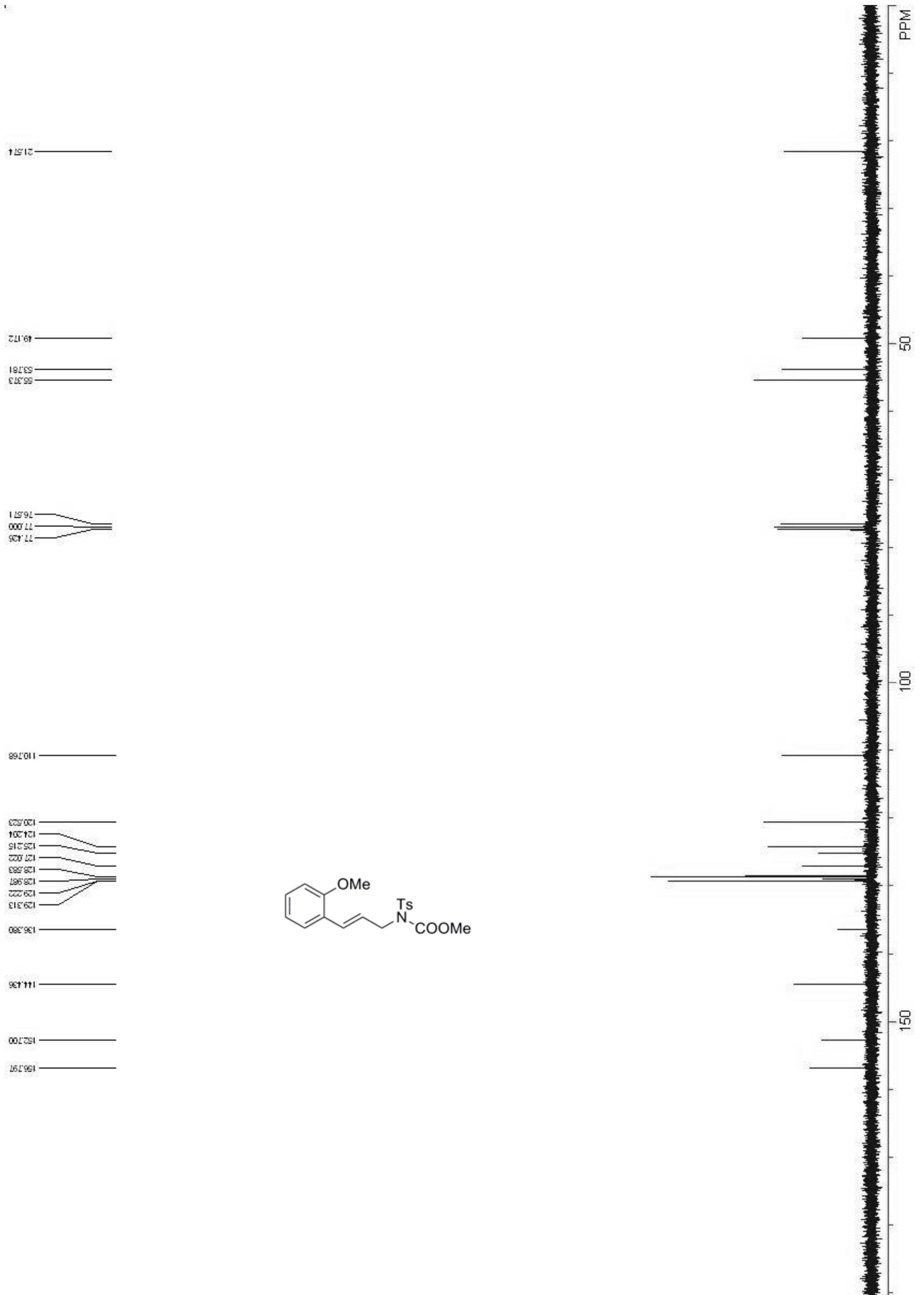
OMe
Ts
N
COOMe
PPM
50
100
150