Supporting Information

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General Methods.

^{1}H-NMR spectra were recorded on Varian 400 (400 MHz) spectrometer. Chemical shifts are reported in ppm from TMS with the solvent resonance as the internal standard (deuterochloroform: 7.26 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sext = sextet, sept = septet, p = pseudo, b = broad, m = multiplet, dm = double multiplet), coupling constants (Hz). ^{13}C-NMR spectra were recorded on a Varian 400 (100 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from TMS with the solvent as the internal standard (deuterochloroform: 77.0 ppm).

GC-MS spectra were taken by EI ionization at 70 eV on a Hewlett-Packard 5971 with GC injection. They are reported as: *m/z* (rel. intensity). LC-electrospray ionization mass spectra were obtained with an Agilent Technologies MSD1100 (nebulizer: 15.0 PSI, dry Gas: 5.0 L/min, dry temperature: 325 °C, capillary voltage positive scan: 4000 mA, capillary voltage negative scan: 3500 mA) single-quadrupole mass spectrometer. Chromatographic purification was done with 240-400 mesh silica gel. Anhydrous solvents were supplied by Sigma Aldrich in Sureseal® bottles and used without any further purification. Commercially available chemicals were purchased from Sigma Aldrich, Stream, TCI, Alfa Aeser and Fluorochem and used without any further purification. Melting points were determined with Bibby Stuart Scientific Melting Point Apparatus SMP 3 and are not corrected.

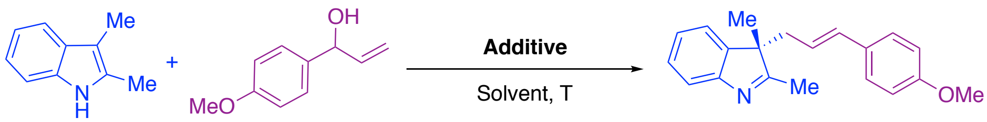
Indole **1a** was purchased from Merck-Aldrich and Fluorochem and used as received. Indoles **1h** and **1i** were purchased from Alfa Aeser and used as received.

Graphene oxide was purchased from Graphenea as powder and as water dispersion (4 mg/mL). The latter was dried before use.

FT-IR spectra were recorded on Brucker Alpha System spectrometer.

XPS spectra were acquired by using a Phoibos 100 hemispherical energy analyzer (Specs) using Mg K_α radiation ($\hbar\omega$ =1253.6 eV). The X-ray power was 125 W. The spectra were recorded in the constant analyser energy (CAE) mode with analyser pass energies of 10 eV for the high-resolution spectra. Charging effects were corrected by energy calibration on C 1s at 285.0 eV. Overall resolution of 0.9 eV was determined on Ag $3d_{5/2}$. The base pressure in the analysis chamber during analysis was 1×10^{-9} mbar. High resolution XPS spectra of C 1s were analysed by CasaXPS (Casa software, Ltd), the curve fitting was carried out using Gaussian/Lorentzian curves shape (GL(30)) for C-O groups with a full width half-maximum of 1.4 eV and an asymmetric Voigt for the C-C sp^2. The C 1s peak revealed the relative amounts of functional groups:[1] aromatic carbon (C−C sp^2, 284.4 eV), aliphatic carbon (C−C sp^3, 285.0 eV), hydroxyl (C−OH, 285.7 eV), epoxy (C−O−C, 286.7 eV), carbonyl (C=O, 288.0 eV), carboxyl (O−C=O, 289.1 eV) and aromatic carbons near vacancies (C-C* sp^2, 283.5).[2] More detail on consistency of the fitting procedure are reported in our previous work on C 1s fit.[1] GO was measured as a dry powder in solid tablet form

Table S1. Optimization reaction conditions



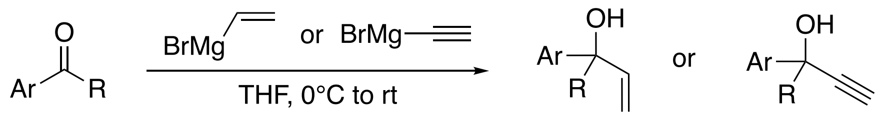
1a (+/-)-**2a** (+/-)-**3aa**

Run[a]	Additive	Solvent	T (°C)	Time (h)	Yield (%) **3aa**[b]
1[c]	GO (25 % wt, flakes)	CH_3Cl	105	5	37
2[c]	GO (50 % wt, flakes)	Toluene	105	8	traces
3[c][d]	GO (50 % wt, flakes)	DMF	105	2	--
4[c][e]	GO (25 % wt, flakes)	EtOH	105	2	--
5[f]	GO (50 % wt, flakes)	Toluene : H_2O (7:3)	105	Overnight	traces
6[f]	GO (25 % wt, flakes)	CH_3Cl : H_2O (1:4)	55	5	67
7[f]	GO (25 % wt, flakes)	Dioxane : H_2O (4:1)	55	5	66
8[f]	GO (25 % wt, flakes)	THF : H_2O (4:1)	55	5	30
9	GO (10 % wt, powder)	CH_3CN : H_2O (4:1)	55	6	68
10[f]	Grafite (25 % wt)	CH_3CN : H_2O (4:1)	55	6	traces
11[f]	*p*-TsOH (pH = 4)	CH_3CN : H_2O (4:1)	55	6	traces
12[f]	Styrene oxide (1 eq)	CH_3CN : H_2O (4:1)	55	6	--
13	Styrene oxide (1 eq), AcOH (pH = 4)	CH_3CN : H_2O (4:1)	55	6	27
14	Used GO (10 % wt, powder)	CH_3CN : H_2O (4:1)	55	36	12
15	Regenerated GO (10 % wt, powder)	CH_3CN : H_2O (4:1)	55	36	63

[a] All the reactions were carried out with reagent grade solvents, unless otherwise specified (**1a**/**2a** = 1/2 on 0.15 mmol of **1a**, 0.1 M). [b] Determined after flash chromatography. [c] **1a**/**2a** = 1/1.5. [d] Decomposition of indole **1a** was observed. [e] Alcohol **2a** decomposed. [f] **1a**/**2a** = 1/3.

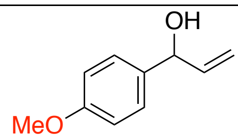
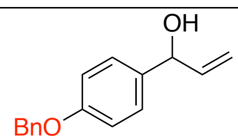
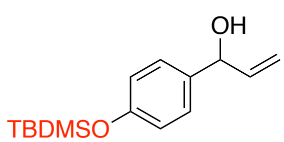
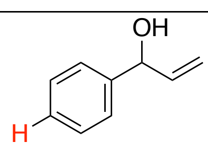
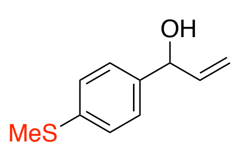
General procedure for the synthesis of allylic alcohols 2a-p and propargylic alcohols 4a-c.

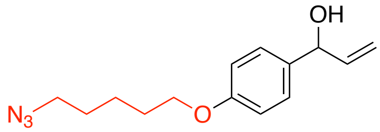
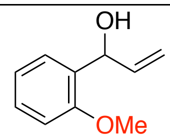
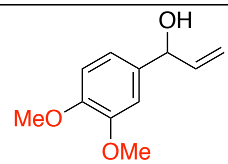
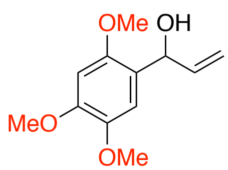
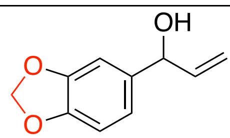
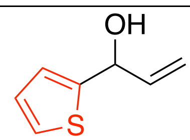
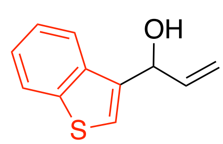
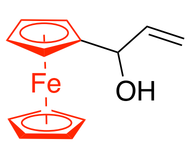
All alcohols were synthetized via addition of vinyl- or ethynylmagnesium bromide to the corresponding carbonyl compound according to literature procedures.[3a,3e]

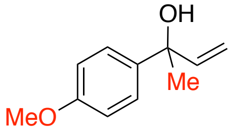
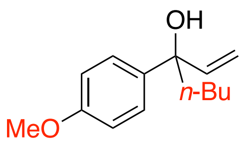
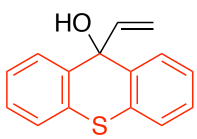
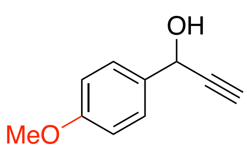
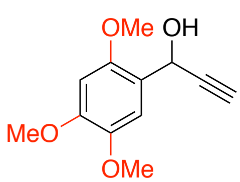
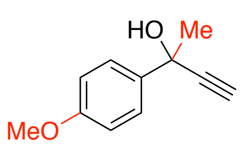


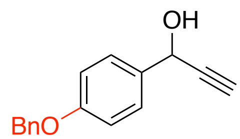
2 **4**

In a flame-dried three-necked round bottom flask, equipped with a dropping funnel, were added anhydrous THF (2.5 mL, 0.8 M) and carbonyl compound (2 mmol, 1 eq) under N_2 atmosphere and the mixture was cooled to 0 °C. Then vinylmagnesium bromide (1 M in THF, 2.4 mL, 2.4 mmol, 1.2 eq) or ethynylmagnesium bromide (0.5 M in THF, 4.8 mL, 2.4 mmol, 1.2 eq) was added dropwise. After the addition the ice bath was removed, and the mixture was allowed to warm at room temperature and stirred for 1-5 h. The reaction was quenched with a saturated aqueous NH_4Cl solution, extracted with EtOAc and the combined organic phases were washed with brine and then dried over Na_2SO_4. Solvent was removed by rotary evaporation and the crude was purified by column chromatography to give the desired product.

	**2a.** Pale yellow oil; yield = 88% (289 mg, *c*Hex:EtOAc 3:1).[3a]
	**2b.** White solid; yield = 67% (322 mg, *c*Hex:EtOAc 4:1).[3b]
	**2c.** Yellow oil; yield = 50% (264 mg, *c*Hex:EtOAc 8:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.23 – 7.18 (m, 2H), 6.82 – 6.77 (m, 2H), 6.03 (ddd, *J* = 17.1, 10.3, 5.7 Hz, 1H), 5.31 (d, *J* = 17.1 Hz, 1H), 5.17 (d, *J* = 10.3 Hz, 1H), 5.13 (d, *J* = 5.7 Hz, 1H), 1.92 (brs, 1H), 0.97 (s, 9H), 0.18 (s, 6H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 155.27, 140.34, 135.35, 127.57, 120.06, 114.71, 74.89, 25.65 (9C), 18.17 -4.45 (6C). ***LC-MS*** (m/z): $[M-OH]^+$ = 247.0. ***Anal. Calc.*** for ($C_{15}H_{24}O_2Si$: 264.44): C, 68.13; H, 9.15; found: C, 68.31; H, 9.26.
	**2d.** Colourless oil; yield = 80% (215 mg, *c*Hex:AcOEt = 4:1).[3c]
	**2e.** Pale yellow solid; yield = 83% (314 mg, *c*Hex:EtOAc = 4:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 6.00 (ddd, *J* = 17.1, 10.3, 5.9 Hz, 1H), 5.31 (d, *J* = 17.1 Hz, 1H), 5.17 (d, *J* = 10.3 Hz, 1H), 5.13 (d, *J* = 5.9 Hz, 1H), 2.46 (s, 3H), 2.14 (brs, 1H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 140.07, 139.48, 137.83, 126.86, 126.73, 115.17, 74.88, 15.89 (3C). ***LC-***

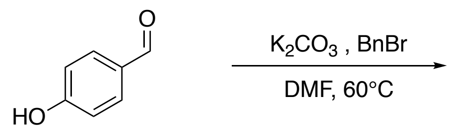
	MS (m/z): [M-OH]$^+$ = 163.0; [M+OH]$^+$ = 197.0; [M+K]$^+$ = 219.0. ***Anal. Calc.*** for ($C_{10}H_{12}OS$: 180.27): C, 66.63; H, 6.71; found: C, 66.55; H, 6.81.
	**2f.** Pale yellow oil; yield = 65% (349 mg, *c*Hex:EtOAc = 4:1).[3a]
	**2g.** Colourless oil; yield = 68% (223 mg, *c*Hex:EtOAc = 4:1).[3b]
	**2h.** White solid; yield = 69% (268 mg, *c*Hex:EtOAc = 2.5:1).[3b]
	**2i.** Pale yellow solid; yield = 80% (359 mg, *c*Hex:EtOAc = 1.5:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 6.85 (s, 1H), 6.51 (s, 1H), 6.07 (ddd, *J* = 17.1, 10.4, 5.4 Hz, 1H), 5.38 (dddd, *J* = 17.2, 5.5 Hz, 1.5 Hz, 1,5 Hz, 1H), 5.29 (ddd, *J* = 17.2, 1.5 Hz, 1,5 Hz, 1H), 5.14 (ddd, *J* = 10.4, 1.5 Hz, 1.5 Hz, 1H), 3.86 (s, 3H), 3.82 (s, 6H), 2.58 (d, *J* = 5.5 Hz, 1H).***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 150.80, 148.92, 143.13, 139.72, 122.47, 114.10, 111.28, 97.68, 70.27, 56.48 (3C), 56.31 (3C), 56.12 (3C). ***LC-MS*** (m/z): 207.0 [M-OH]$^+$, 247.0 [M+Na]$^+$, 471.0 [2M+Na]$^+$. ***Anal. Calc.*** for ($C_{12}H_{16}O_4$: 224.26): C, 64.27; H, 7.19; found: C, 64.16; H, 7.25.
	**2j.** Yellow oil; yield = 70% (250 mg, *n*Hex:EtOAc 4:1). Spectral data match those reported in the literature.[3b]
	**2k.** Yellow oil; yield = 51 % (143 mg, *c*Hex:EtOAc = 6:1). Spectral data match those reported in the literature.[3c]
	**2l.** Yellow oil; yield = 65% (247 mg, *c*Hex:EtOAc = 4:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$)) δ 7.92 – 7.87 (m, 1H), 7.87 – 7.82 (m, 1H), 7.47 – 7.30 (m, 3H), 6.18 (ddd, *J* = 17.2, 10.3, 5.7 Hz, 1H), 5.53 (d, *J* = 5.7 Hz, 1H), 5.45 (d, *J* = 17.2 Hz, 1H), 5.28 (d, *J* = 10.3 Hz, 1H), 2.30 (s, 1H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 138.38, 136.07, 134.88, 134.63, 121.91, 121.49, 120.68, 120.29, 120.00, 113.53, 68.10. ***LC-MS*** (m/z): [M-OH]$^+$ = 173.0. ***Anal. Calc.*** for ($C_{11}H_{10}OS$: 190.26): C, 69.44; H, 5.30; found: C, 69.21; H, 5.18.
	**2m.** Red oil; yield = 60% (291 mg, *n*Hex:EtOAc = 6:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 6.07 (ddd, *J* = 17.1, 10.4, 5.9 Hz, 1H), 5.31 (d, *J* = 17.1 Hz, 1H), 5.16 (d, *J* = 10.4 Hz, 1H), 4.84 (dd, *J* = 5.9 Hz, 5.1 Hz, 1H), 4.21 – 4.14 (m, 9H), 1.91 (d, *J* = 5.1 Hz, 1H).***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 139.59, 114.99, 91.80, 70.65, 68.41 (5C), 68.19, 68.15, 66.69, 66.47. ***LC-MS*** (m/z): [M]$^+$ = 242.0.

	Anal. Calc. for ($C_{13}H_{14}FeO$: 242.10): C, 64.50; H, 5.83; found: C, 64.31; H, 5.58.
	**2n.** Pale yellow oil; yield = 88% (314 mg, *c*Hex:EtOAc = 25:1). Spectral data match those reported in the literature.[3d]
	**2o.** Colourless oil; yield = 60% (264 mg, *c*Hex:EtOAc = 20:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.9 Hz, 1H), 6.86 (d, *J* = 8.9 Hz, 1H), 6.16 (dd, *J* = 17.2, 10.7 Hz, 1H), 5.26 (dd, *J* = 17.2, 1.0 Hz, 1H), 5.12 (dd, *J* = 10.7, 1.0 Hz, 1H), 3.78 (s, 3H), 1.94 – 1.80 (m, 2H), 1.78 (s, 1H), 1.33 – 1.03 (m, 4H), 0.85 (t, *J* = 7.1 Hz, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 158.33, 144.47, 137.87, 126.57, 113.44, 112.17, 55.20, 41.81, 25.78, 22.99, 14.00. ***LC-MS*** (m/z): $[M-OH]^+$ = 203.0. ***Anal. Calc.*** for ($C_{14}H_{20}O_2$: 220.31): C, 76.33; H, 9.15; found: C, 76.18; H, 9.01.
	**2p.** Pale yellow solid; yield = 70% (336 mg, *c*Hex:EtOAc = 6:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 7.8, 1.2 Hz, 2H), 7.39 (dd, *J* = 7.6, 1.1 Hz, 2H), 7.31 (ddd, *J* = 7.6, 7.6, 1.4 Hz, 2H), 7.24 (ddd, *J* = 7.5, 7.5,1.5 Hz, 2H), 5.91 (dd, *J* = 17.1, 10.2 Hz, 1H), 5.03 (dd, *J* = 10.2, 0.8 Hz, 1H), 4.79 (dd, *J* = 17.1, 0.8 Hz, 1H), 2.73 (brs, 1H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 138.53, 138.24, 130.64, 127.49, 126.65, 126.18, 125.74, 114.45, 75.42. ***LC-MS*** (m/z): 223.0 $[M-OH]^+$. ***Anal. Calc.*** for ($C_{15}H_{12}OS$: 240.32): C, 74.97; H, 5.03; found: C, 74.79; H, 5.21.
	**4a.** Pale yellow oil which solidifies on standing; yield = 90% (291 mg, *c*Hex:EtOAc = 3.4:1). Spectral data match those reported in the literature.[3e]
	**4b.** White solid; yield = 75% (333 mg, *c*Hex:EtOAc = 1.5:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.13 (s, 1H), 6.52 (s, 1H), 5.67 (dd, *J* = 5.9, 2.2 Hz, 1H), 3.88 (s, 3H), 3.86 (s, 3H), 3.85 (s, 3H), 2.81 (d, *J* = 5.9 Hz, 1H), 2.60 (d, *J* = 2.3 Hz, 1H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 151.05, 149.92, 143.09, 119.87, 111.77, 97.59, 83.37, 73.92, 60.32, 56.54, 56.44, 56.19. ***GC-MS*** (m/z): 222 (100) $[M]^+$, 205 (58) $[M-OH]^+$, 191 (31) $[M-OMe]^+$. ***Anal. Calc.*** for ($C_{12}H_{14}O_4$: 222.24): C, 64.85; H, 6.35; found: C, 64.71; H, 6.20.
	**4c.** Pale yellow solid; yield = 36% (127 mg, *c*Hex:EtOAc = 4:1). Spectral data match those reported in the literature.[3f]

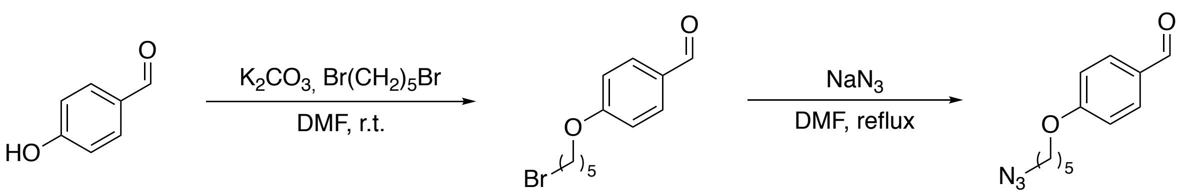
	**4e.** White solid; yield = 68% (324 mg, *c*Hex:EtOAc = 5:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.49 – 7.44 (m, 2H), 7.44 – 7.35 (m, 4H), 7.35 – 7.29 (m, 1H), 7.01 – 6.93 (m, 2H), 5.40 (dd, *J* = 5.7, 1.9 Hz, 1H), 5.07 (s, 2H), 2.65 (d, *J* = 2.2 Hz, 1H), 2.21 (d, *J* = 5.9 Hz, 1H).***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 158.97, 136.79, 132.60, 128.58 (2C), 128.07 (2C), 127.99, 127.40 (2C), 114.96 (2C), 83.64, 74.64, 70.05, 64.01.***GC-MS*** (m/z): 238 (6) $[M]^+$, 91 (100), 65 (13). ***Anal. Calc.*** for ($C_{16}H_{14}O_2$: 238.29): C, 80.65; H, 5.92; found: C, 80.33; H, 5.68.

Procedure for the synthesis of aldehyde precursors and propagylic alcohol 4d.

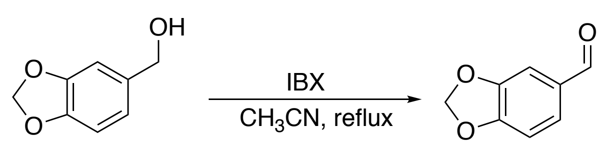
Alcohol **2b**: This compound was synthetized from 4-hydroxybenzaldehyde according to literature procedure.[4a]



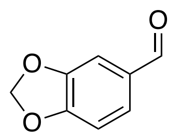
Alcohol **2f**: This compound was synthetized from 4-hydroxybenzaldehyde according to know literature procedures.[3a]



Alcohol **2f**: This compound was synthetized by oxidation of piperonol using IBX.

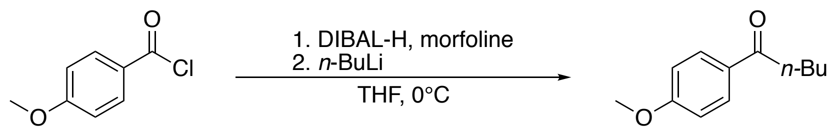


In a flame-dried two-necked round bottom flask were added anhydrous CH_3CN (7.5 mL, 0.4 M), piperonol (475 mg, 3 mmol, 1 eq) and IBX (1.68 g, 6mmol, 2 eq) under N_2 atmosphere. The mixture was refluxed overnight. The reaction mixture was filtered on a pad of Celite and the solvent was removed under vacuum. The crude was then dissolved in CH_2Cl_2 and washed with a saturated $NaHCO_3$ aqueous solution, then with a $Na_2S_2O_3$ aqueous solution (1 M) and dried over Na_2SO_4. Solvent was removed by rotary evaporation and the crude was purified by column chromatography.

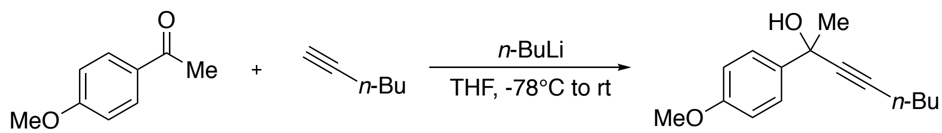


Yellow oil; yield = 86% (387 mg, *n*Hex:EtOAc = 6:1). Spectral data match those reported in the literature.[4b]

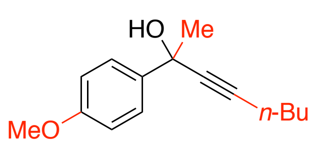
Alcohol **2o**: This compound was synthetized from 4-methoxybenzoyl chloride according to know literature procedures.[4c]



Alcohol **4d**: This compound was synthetized from 4-methoxyacetophenone and hex-1-yne according to a general known procedure.[4d]



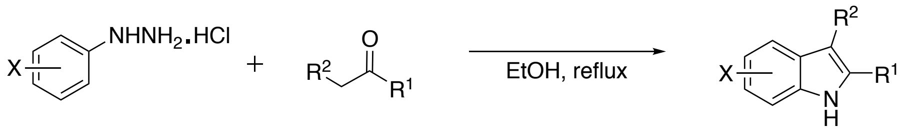
In a flame-dried three-necked round bottom flask were added anhydrous THF (4 mL) and hex-1-yne (0.49 mL, 4.4 mmol, 2.2 eq). *n*-BuLi (2.5 M in Hex, 1.6 mL, 4 mmol, 2 eq) was added dropwise at -78°C and the mixture was stirred at -78°C for 1 hour. Then a solution of 4-methoxyacetophenone (300 mg, 2 mmol, 1 eq) in THF (2.5 mL) was added dropwise at -78°C. After the addition the mixture was allowed to warm to room temperature and stirred overnight. The reaction was quenched with a saturated aqueous NH_4Cl solution, extracted with EtOAc and the combined organic phases were washed with brine and then dried over Na_2SO_4. Solvent was removed by rotary evaporation and the crude was purified by column chromatography to give the desired product.



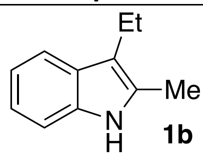
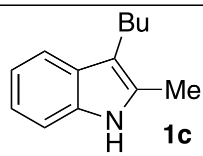
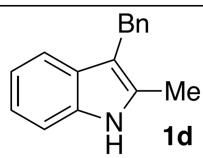
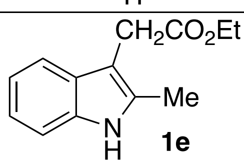
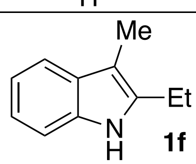
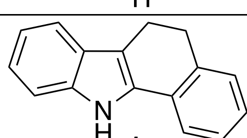
4d. Pale yellow oil; yield = 51% (238 mg, *n*Hex:EtOAc = 6:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.6 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 3.79 (s, 3H), 2.26 (t, *J* = 7.0 Hz, 2H), 2.22 (s, 1H), 1.72 (s, 3H), 1.57 – 1.38 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 158.94, 138.45, 126.22, 113.42, 85.48, 83.85, 69.66, 55.27, 33.41, 30.72, 21.96, 18.39, 13.56. ***GC-MS*** (m/z): 214 (100) $[M-H_2O]^+$, 172 (36), 128 (56). ***Anal. Calc.*** for ($C_{15}H_{20}O_2$: 232.32): C, 77.55; H, 8.68; found: C, 77.21; H, 8.57.

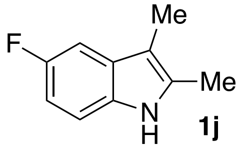
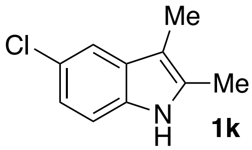
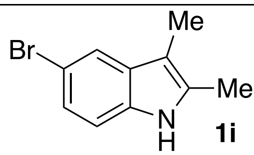
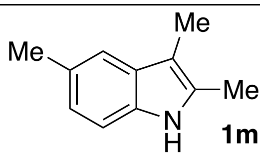
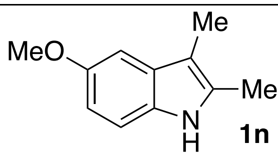
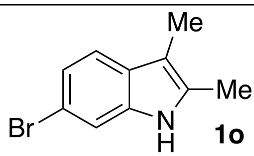
General procedure for the synthesis of 2,3-disubstituted indoles 1b-c, 1e-g e 1j-o.

Indoles were synthetized from aryl hydrazines and ketones using Fischer's indole synthesis. All commercially available carbonyl compounds were used without further purification.



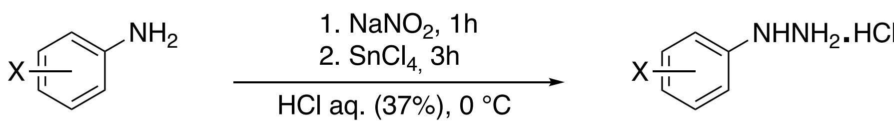
A Schenk tube was charged with aryl hydrazine hydrochloride (3 mmol, 1.5 eq), ketone (2mmol, 1 eq) and reagent grade ethanol (4 mL, 0.5 M). The reaction mixture was stirred at refluxed until complete consumption of the ketone.
After cooling, the solvent was removed under vacuum, the crude was dissolved in ethyl acetate and washed with 2M aqueous HCl, saturated aqueous $NaHCO_3$, deionized water, brine and dried over Na_2SO_4. Solvent was removed by rotary evaporation and (when necessary) the crude was purified by column chromatography to give the desired indole.

Compound	Conditions	Ref.
 **1b**	Pale brown solid, yield = 46% (147 mg, *n*Hex:Acetone = 16:1).	[5a]
 **1c**	Yellow oil, yield = 49% (184 mg, *n*Hex:Acetone = 10:1)	[5b]
 **1d**	Pale orange solid, yield = 50% (221 mg, *c*Hex:AcOEt = 4:1)	[5a]
 **1e**	Yellow oil, yield = 48% (209 mg, *n*Hex:Acetone = 3.5:1).	[5c]
 **1f**	Yellow oil, yield = 52% (166 mg, *n*Hex:Acetone = 16:1).	[5a]
 **1g**	Pale brown solid, yield = 64% (281 mg, *n*Hex:Acetone = 10:1).	[5d]

 **1j**	Pale brown solid, yield = 59 % (193 mg, *c*Hex:AcOEt = 12:1).	[5e]
 **1k**	White solid, yield = 54% (194 mg, *c*Hex:AcOEt = 8:1).	[5f]
 **1i**	Orange solid, yield = 67% (300 mg, No purification)	[5f]
 **1m**	Brown solid, yield = 93% (296 mg, No purification)	[5f]
 **1n**	Pale brown solid, yield = 44% (154 mg, *n*Hex:Acetone = 8:1)	[5f]
 **1o**	Pale brown solid, yield = 30% (135 mg, *n*Hex:AcOEt = 10:1).	[5f]

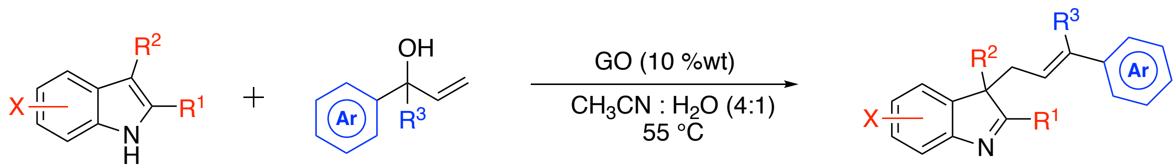
General procedure for the synthesis of aryl hydrazines

Aryl hydrazines were synthetized the from corresponding commercially available anilines that were used without further purification.[6]



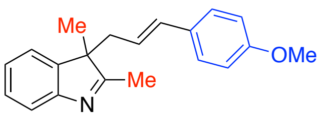
A one neck round-bottom flask is charged with aniline (1 eq) then HCl (37%) is added dropwise at 0 °C (for hydrazine **4f** at -15 °C). An aqueous solution of $NaNO_2$ (1.5 eq, 2 M) is added dropwise and the solution is stirred for 1h at 0°C (for hydrazine **4f** at -15 °C). Then a solution of $SnCl_4$ (3 eq, 1 M) in aqueous conc. HCl (37%) is added in one portion and the mixture is stirred for another 3 hours at 0 °C. The solution is then filtered and the solid is washed with a small amount of deionized water (0 °C) and then Et_2O to yield the hydrochloride salt of the desired aryl hydrazine. The obtained hydrochloride salts were employed in the synthesis of the indoles without further purifications.

General procedure for the allylic dearomatization of indoles

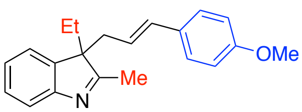


1 **2** **3**

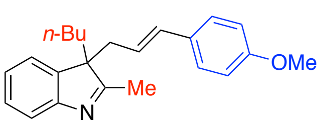
A screw-capped vial is charged with CH_3CN (1.2 mL), allylic alcohol **2** (0.3 mmol, 2 eq), indole **1** (0.15 mmol, 1 eq), GO dried flakes (10 wt% with respect to indole) and deionized water (0.3 mL). The reaction mixture was stirred at 55 °C (unless otherwise noted) until complete consumption of indole (*vide infra* for reaction times). The mixture was then filtered on a Gooch funnel and the GO washed with EtOAc. The collected organic layers were dried over Na_2SO_4 and evaporated to dryness under vacuum. The crude was purified by column chromatography to give the desired product **3**.



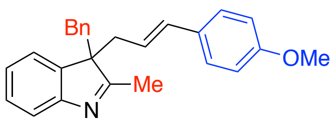
3aa. Yellow oil, yield = 70% (31 mg, 6 h, *n*Hex:Et_2O = 1:1.8). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.6 Hz, 1H), 7.33 – 7.25 (m, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.07 (d, *J* = 8.6 Hz, 2H), 6.75 (d, *J* = 8.6 Hz, 2H), 6.25 (d, *J* = 15.7 Hz, 1H), 5.47 (ddd, *J* = 15.7, 8.0, 6.7 Hz, 1H), 3.74 (s, 3H), 2.72 (dd, *J* = 13.9, 6.7 Hz, 1H), 2.48 (dd, *J* = 13.9, 8.0 Hz, 1H), 2.28 (s, 3H), 1.33 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.67, 158.95, 154.09, 143.47, 132.53, 129.78, 127.72, 127.23, 124.99, 121.91, 121.87, 119.85, 113.81, 57.74, 55.22, 40.34, 21.61, 16.00. ***LC-MS*** (m/z): 147.2 $[C_{10}H_{11}O]^+$, 314.2 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{20}H_{21}NO$: 291.39): C, 82.44; H, 7.26; found: C, 82.31; H, 7.31.



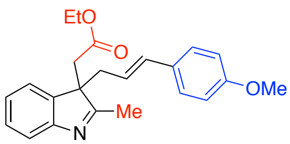
3ba. Pale yellow oil, yield = 68% (31 mg, 16 h, *n*Hex:Et_2O = 1:2). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.6 Hz, 1H), 7.29 (dt, *J* = 7.6, 1.4 Hz, 1H), 7.25-7.21 (m, 1H), 7.18 (dt, *J* = 7.5, 0.8 Hz, 1H), 7.09 – 7.00 (m, 2H), 6.77 – 6.68 (m, 2H), 6.23 (d, *J* = 15.6 Hz, 1H), 5.41 (ddd, *J* = 15.6, 8.0, 6.6 Hz, 1H), 3.73 (s, 3H), 2.75 (ddd, *J* = 13.9, 6.6, 1.4 Hz, 1H), 2.49 (ddd, *J* = 13.9, 8.0, 0.8 Hz, 1H), 2.24 (s, 3H), 2.01 (dq, *J* = 15.0, 7.4 Hz, 1H), 1.84 (dq, *J* = 15.0, 7.4 Hz, 1H), 0.37 (t, *J* = 7.4 Hz, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 185.54, 158.89, 155.24, 141.38, 132.29, 129.84, 127.68, 127.19, 124.88, 122.01, 121.87, 119.71, 113.77, 62.99, 55.21, 40.01, 28.85, 16.30, 8.12. ***LC-MS*** (m/z): 147.2 $[C_{10}H_{11}O]^+$, 328.2 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{21}H_{23}NO$: 305.42): C, 82.58; H, 7.59; found: C, 82.36; H, 7.69.



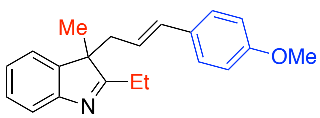
3ca. Yellow oil, yield = 61% (31 mg, overnight, Hex:Et_2O = 1:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.24 (d, *J* = 7.3Hz, 1H), 7.18 (t, *J* = 7.3 Hz, 1H), 7.05 (d, *J* = 8.5 Hz, 2H), 6.73 (d, *J* = 8.6 Hz, 2H), 6.22 (d, *J* = 15.7 Hz, 1H), 5.40 (ddd, *J* = 15.7, 8.1, 6.6 Hz, 1H), 3.73 (s, 3H), 2.74 (dd, *J* = 13.9, 6.6 Hz, 1H), 2.48 (dd, *J* = 13.9, 8.1 Hz, 1H), 1.95 (td, *J* = 12.9, 4.6 Hz, 1H), 1.78 (td, *J* = 12.8, 4.6 Hz, 1H), 1.21 – 1.06 (m, 2H), 0.80 – 0-63 (m, 4H), 0.63 – 0.49 (m, 1H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 185.80, 158.89, 155.04, 141.81, 132.31, 129.84, 127.64, 127.20, 124.87, 121.98, 121.81, 119.71, 113.77, 62.42, 55.21, 40.29, 35.70, 25.80, 22.81, 16.35, 13.73.
LC-MS (m/z): 147.0 $[C_{10}H_{11}O]^+$, 356.2 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{23}H_{27}NO$: 333.48): C, 82.84; H, 8.16; found: C, 82.65; H, 8.02.



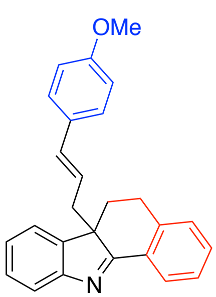
3da. Pale yellow oil, yield = 47% (26 mg, 7h, *n*Hex:Et_2O = 1:1.1, then *n*Hex:Acetone 4:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.6 Hz, 1H), 7.25 (ddd, 8.4, 7.7, 3.7 Hz, 1H), 7.19 – 7.12 (m, 2H), 7.10 – 6.99 (m, 5H), 6.79 – 6.68 (m, 4H), 6.27 (d, *J* = 15.7 Hz, 1H), 5.34 (ddd, *J* = 15.7, 8.1, 6.5 Hz, 1H), 3.73 (s, 3H), 3.28 (d, *J* = 13.6 Hz, 1H), 2.95 (d, *J* = 13.6 Hz, 1H), 2.89 (dd, *J* = 14.0, 6.5 Hz, 1H), 2.68 (dd, *J* = 14.0, 8.1 Hz, 1H), 2.34 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 184.60, 158.94, 154.97, 140.90, 135.79, 132.57, 129.73, 129.30, 127.85, 127.75, 127.23, 126.65, 124.61, 122.92, 121.51, 119.82, 113.77, 63.03, 55.22, 42.01, 39.70, 16.96. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 390.0 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{26}H_{25}NO$: 367.49): C, 84.98; H, 6.86; found: C, 84.71; H, 6.71.



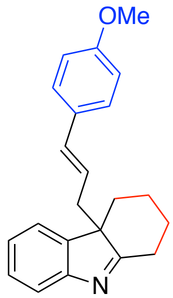
3ea. Yellow oil, yield = 57% (31 mg, *n*Hex:Et_2O = 1:3). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.6 Hz, 1H), 7.30 (m, 2H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.07 (d, *J* = 8.6 Hz, 2H), 6.75 (d, *J* = 8.6 Hz, 2H), 6.25 (d, *J* = 15.7 Hz, 1H), 5.45 (ddd, *J* = 15.7, 7.7, 6.7 Hz, 1H), 3.81 (q, *J* = 7.1 Hz, 2H), 3.74 (s, 3H), 2.95 (d, *J* = 14.5 Hz, 1H), 2.81-2.72 (m, 2H), 2.46 (dd, *J* = 13.8, 7.7 Hz, 1H), 2.34 (s, 3H), 0.88 (t, *J* = 7.1 Hz, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 184.30, 169.22, 159.06, 154.78, 140.15, 133.37, 129.55, 128.24, 127.30, 124.94, 122.50, 120.66, 119.98, 113.83, 60.46, 59.39, 55.23, 39.83, 39.82, 16.42, 13.66. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 386.0 $[M+Na]^+$, 749.2 $[2M+Na]^+$. ***Anal. Calc.*** for ($C_{23}H_{25}NO_3$: 363.46): C, 76.01; H, 6.93; found: C, 75.85; H, 6.81.



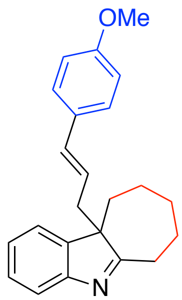
3fa. Pale yellow oil, yield = 68% (31 mg, 16 h, *n*Hex:Acetone = 3.5:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.7 Hz, 1H), 7.29 (dt, *J* = 7.5, 1.4 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.18 (ddd, *J* = 7.5, 7.5, 0.9 Hz, 1H), 7.05 (d, *J* = 8.7 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 6.23 (d, *J* = 15.7 Hz, 1H), 5.41 (ddd, *J* = 15.6, 8.0, 6.7 Hz, 1H), 2.75 (ddd, *J* = 13.9, 6.6, 1.3 Hz, 1H), 2.49 (ddd, *J* = 14.0, 8.1, 0.9 Hz, 1H), 2.24 (s, 3H), 2.00 (dq, *J* = 14.9, 7.5 Hz, 1H), 1.84 (dq, *J* = 14.5, 7.3 Hz, 1H), 0.37 (t, *J* = 7.4 Hz, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 185.54, 158.90, 155.21, 141.37, 132.30, 129.84, 127.67, 127.19, 124.88, 122.01, 121.87, 119.71, 113.78, 62.99, 55.21, 40.00, 28.84, 16.28, 8.11. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 328.2 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{21}H_{23}NO$: 305.42): C, 82.58; H, 7.59; found: C, 82.31; H, 7.71.



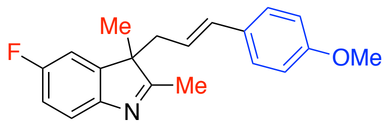
3ga. White solid, yield = 35% (19 mg, *n*Hex:Acetone = 6.5:1). ***M.p.*** = 51.2-53.5 °C. ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.46 – 7.28 (m, 5H), 7.14 (d, *J* = 8.6 Hz, 2H), 6.79 (d, *J* = 8.6 Hz, 2H), 6.18 (d, *J* = 15.7 Hz, 1H), 5.81 (ddd, *J* = 15.7, 7.6, 7.3 Hz, 1H), 3.35 (ddd, *J* = 18.0, 12.5, 5.7 Hz, 1H), 3.00 (dd, *J* = 17.9, 5.9 Hz, 1H), 2.73 (dd, *J* = 13.7, 7.6 Hz, 1H), 2.58 (dd, *J* = 13.5, 5.3 Hz, 1H), 2.24 (dd, *J* = 13.7, 7.3 Hz, 1H), 1.75 (ddd, *J* = 13.2, 12.5, 6.1 Hz, 1H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 180.31, 156.39, 153.20, 140.81, 137.16, 130.43, 128.51, 127.46, 127.39, 126.41, 125.55, 124.67, 124.28, 123.55, 122.33, 119.92, 119.24, 118.28, 111.30, 53.11, 52.69, 33.55, 27.05, 23.17. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 218 $[C_{16}H_{11}N]^+$,388.0 $[M+Na]^+$, 404.3 $[M+K]^+$. ***Anal. Calc.*** for ($C_{26}H_{23}NO$: 365.48): C, 85.45; H, 6.34; found: C, 85.21; H, 6.23.



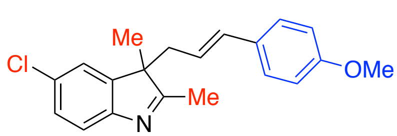
3ha. White solid, yield = 75% (36 mg, 6 h, *n*Hex:Et_2O = 1:1.5). ***M.p.*** = 124.5-125.3 °C. ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.1 Hz, 1H), 7.34 – 7.26 (m, 2H), 7.17 (dt, *J* = 7.1, 0.5 Hz 1H), 7.08 (d, *J* = 8.7 Hz, 2H), 6.75 (d, *J* = 8.7 Hz, 2H), 6.25 (d, *J* = 15.7 Hz, 1H), 5.49 (ddd, 15.6, 7.4, 6.5 Hz, 1H), 3.74 (s, 3H), 2.88 (brs d, *J* = 8.7 Hz, 1H), 2.77 (ddd, *J* = 13.6, 6.5, 0.8 Hz, 1H), 2.66 – 2.50 (m, 2H), 2.41 (dd, *J* = 13.3, 1.8 Hz, 1H), 2.20 (brs d, *J* = 13.1 Hz, 1H), 1.86 (tq, 13.6, 3.6 Hz 1H), 1.69 (brs, 1H), 1.43 (tq, 13.6, 3.6 Hz 1H), 1.16 (td, *J* = 13.5, 4.0 Hz, 1H). ***^{13}C NMR*** (100 MHz, $CDCl_3$)) δ 188.85, 158.91, 154.84, 144.70, 132.48, 129.87, 127.61, 127.21, 124.60, 122.00, 121.61, 120.18, 113.80, 57.88, 55.22, 36.62, 36.57, 30.17, 28.80, 21.08. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 340.2 $[M+Na]^+$. ***Anal. Calc***. for ($C_{22}H_{23}NO$: 317.43): C, 83.24; H, 7.30; found: C, 83.03; H, 7.41.



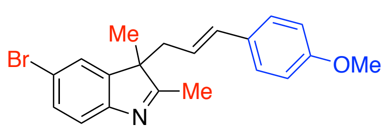
3ia. Pale yellow oil, yield = 58% (29 mg, overnight, *n*Hex:Acetone = 4.5:1). ***^{1}H* NMR** (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.6 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 7.1 Hz, 1H), 7.16 (t, *J* = 7.3 Hz, 1H), 7.08 (d, *J* = 8.5 Hz, 2H), 6.75 (d, *J* = 8.5 Hz, 2H), 6.21 (d, *J* = 15.7 Hz, 1H), 5.54 (ddd, 15.7, 7.9, 6.9 Hz, 1H), 3.75 (s, 3H), 2.93 (ddd, *J* = 13.2, 5.7, 4.1 Hz, 1H), 2.72 (dd, *J* = 13.6, 6.9 Hz, 1H), 2.63 (ddd, 14.0, 10.8, 3.6 Hz, 1H), 2.47 (dd, *J* = 13.6, 7.9 Hz, 1H), 2.18 – 1.97 (m, 2H), 1.91 – 1.78 (m, 2H), 1.79 – 1.69 (m, 1H), 1.68 – 1.53 (m, 1H), 1.52 – 1.40 (m, 1H), 0.73 (dt, *J* = 14.5, 10.7 Hz, 1H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 190.71, 158.89, 154.89, 143.80, 132.49, 129.93, 127.68, 127.21, 124.81, 121.92, 121.89, 119.74, 113.80, 62.40, 55.22, 40.74, 34.74, 31.59, 30.49, 28.64, 24.63. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 354.2 $[M+Na]^+$. ***Anal. Calc***. for ($C_{23}H_{25}NO$: 331.46): C, 83.34; H, 7.60; found: C, 83.55; H, 7.51.



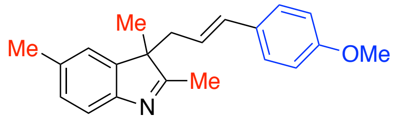
3ja. Pale yellow oil, yield = 92% (43 mg, 7 h, *n*Hex:Et_2O = 1:2.3). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.42 (dd, J_{H-F} = 9.1, J_{H-H} 4.6 Hz, 1H), 7.07 (d, *J* = 8.7 Hz, 2H), 7.02 – 6.91 (m, 2H), 6.75 (d, *J* = 8.7 Hz, 2H), 6.25 (d, *J* = 15.7 Hz, 1H), 5.42 (ddd, *J* = 15.5, 7.8, 6.9 Hz, 1H), 3.74 (s, 3H), 2.68 (ddd, *J* = 14.1, 6.9, 1.2 Hz, 1H), 2.49 (dd, *J* = 14.0, 7.9 Hz, 1H), 1.32 (s, 3H).***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.31 (d, J_{C-F} = 3.7 Hz, 1C), 161.02 (d, J_{C-F} = 243.5 Hz, 1C), 159.03, 150.18, 145.52 (d, J_{C-F} = 8.5 Hz, 1C), 132.85, 129.61, 127.25, 121.25, 120.43 (d, J_{C-F} = 8.9 Hz, 1C), 114.26 (d, J_{C-F} = 23.6 Hz, 1C), 113.83, 109.59(d, J_{C-F} = 24.4 Hz, 1C), 58.34, 55.21, 40.26, 21.58, 15.98. ***^{19}F* NMR** (377 MHz, $CDCl_3$) -117.62 (td, J_{F-H} = 9.2, 5.2 Hz). ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 332.2 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{20}H_{20}FNO$: 309.38): C, 77.64; H, 6.52; found: C, 77.42; H, 6.71.



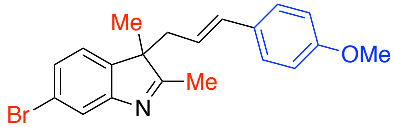
3ka. Pale yellow oil, yield = 77% (38 mg, 4 h, *n*Hex:Et_2O = 1:1.8). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.0 Hz, 1H), 7.29 – 7.20 (m, 2H), 7.07 (d, *J* = 8.7 Hz, 2H), 6.75 (d, *J* = 8.7 Hz, 2H), 6.25 (d, *J* = 15.7 Hz, 1H), 5.39 (ddd, *J* = 15.6, 7.9, 6.8 Hz, 1H), 3.74 (s, 3H), 2.70 (ddd, *J* = 14.0, 6.7, 1.3 Hz, 1H), 2.50 (ddd, *J* = 14.1, 8.0, 0.9 Hz, 1H), 2.26 (s, 3H), 1.32 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 187.06, 159.04, 152.79, 145.37, 132.91, 130.81, 129.57, 127.90, 127.27, 122.39, 121.18, 120.71, 113.84, 58.30, 55.22, 40.25, 21.59, 16.04 ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$. ***Anal. Calc***. for ($C_{20}H_{20}ClNO$: 325.84): C, 73.72; H, 6.19; found: C, 73.51; H, 6.01.



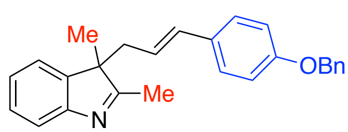
3la. Yellow oil, yield = 75% (42 mg, 4 h, *n*Hex:Et_2O = 1:1.8). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.41 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 8.7 Hz, 2H), 6.75 (d, *J* = 8.8 Hz, 2H), 6.25 (d, *J* = 15.7 Hz, 1H), 5.39 (ddd, *J* = 15.5, 8.0, 6.7 Hz, 1H), 3.74 (s, 3H), 2.70 (ddd, *J* = 14.0, 6.7, 1.4 Hz, 1H), 2.50 (ddd, *J* = 14.1, 8.0, 1.0 Hz, 1H), 2.25 (s, 3H), 1.32 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 187.07, 159.05, 153.27, 145.78, 132.92, 130.81, 129.57, 127.28, 125.26, 121.23, 121.17, 118.75, 113.84, 58.36, 55.23, 40.25, 21.59, 16.06. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 392.0/394.0 $[M+Na]^+$. ***Anal. Calc***. for ($C_{20}H_{20}BrNO$: 370.29): C, 64.87; H, 5.44; found: C, 64.71; H, 5.31.



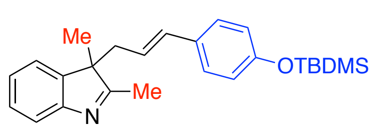
3ma. Yellow oil, yield = 60% (28 mg, 7 h, *n*Hex:Et_2O = 1:1.1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.6 Hz, 1H), 7.14 – 7.04 (m, 4H), 6.75 (d, *J* = 8.6 Hz, 2H), 6.26 (d, *J* = 15.7 Hz, 1H), 5.44 (ddd, *J* = 15.7, 8.1, 6.3 Hz, 1H), 3.74 (s, 3H), 2.70 (dd, *J* = 14.0, 6.3 Hz, 1H), 2.48 (dd, *J* = 14.0, 8.1 Hz, 1H), 2.38 (s, 3H), 2.24 (s, 3H), 1.31 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 185.54, 158.91, 152.08, 143.67, 134.62, 132.32, 129.86, 128.28, 127.22, 122.65, 122.15, 119.37, 113.79, 57.53, 55.22, 40.41, 21.81, 21.48, 15.98. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 328.0 $[M+Na]^+$. ***Anal. Calc***. for ($C_{21}H_{23}NO$: 305.42): C, 82.58; H, 7.59; found: C, 82.31; H, 7.41.



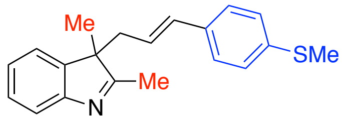
3na. Pale yellow oil, yield = 70% (39 mg, 4h, *n*Hex:Et_2O = 1:1.3, then Hex:Acetone 4:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 1.5 Hz, 1H), 7.31 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.13 (d, *J* = 7.9 Hz, 1H), 7.08 (d, *J* = 8.7 Hz, 2H), 6.76 (d, *J* = 8.7 Hz, 2H), 6.24 (d, *J* = 15.7 Hz, 1H), 5.43 (ddd, *J* = 15.7, 8.0, 6.6 Hz, 1H), 3.75 (s, 3H), 2.70 (ddd, *J* = 13.9, 6.6, 0.9 Hz, 1H), 2.46 (dd, *J* = 13.9, 8.0 Hz, 1H), 2.27 (s, 3H), 1.31 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 188.45, 159.06, 155.73, 142.46, 132.88, 129.55, 127.78, 127.27, 123.29, 123.08, 121.25, 121.06, 113.86, 57.79, 55.24, 40.17, 21.48, 16.11*.* ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 392.0/394.0 $[M+Na]^+$. ***Anal. Calc***. for ($C_{20}H_{20}BrNO$: 370.29): C, 64.87; H, 5.44; found: C, 64.88; H, 5.37.



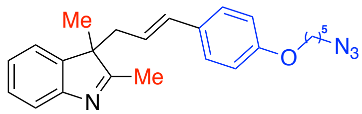
3ab. Pale yellow oil, yield = 65% (36 mg, 16 h, *n*Hex:Et_2O = 1:1.8). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.25 (m, 7H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 8.7 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 6.24 (d, *J* = 15.8 Hz, 1H), 5.48 (ddd, *J* = 15.8, 8.1, 6.7 Hz, 1H), 5.01 (s, 2H), 2.73 (ddd, *J* = 13.9, 6.7, 1.1 Hz, 1H), 2.48 (dd, *J* = 14.1, 8.1 Hz, 1H), 2.28 (s, 3H), 1.34 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.57, 158.15, 154.27, 143.52, 136.91, 132.48, 130.06, 128.54, 127.91, 127.72, 127.38, 127.25, 124.95, 122.08, 121.90, 119.89, 114.79, 69.97, 57.74, 40.35, 21.64, 16.04. ***LC-MS*** (m/z): 91.0 $[Bn]^+$, 145.0 $[C_{10}H_{11}N]^+$, 223.2 $[C_{16}H_{15}O]^+$, 390.2 $[M+Na]^+$, 406.0 $[2M+Na]^+$. ***Anal. Calc***. for ($C_{26}H_{25}NO$: 367.49): C, 84.98; H, 6.86; found: C, 84.71; H, 6.71.



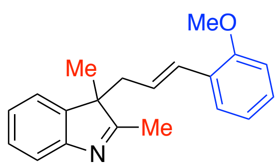
3ac. Yellow oil, yield = 66% (39 mg, 36h, *n*Hex:Et_2O = 1.2:1). ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.26 (m, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.01 (d, *J* = 8.5 Hz, 1H), 6.68 (d, *J* = 8.5 Hz, 1H), 6.25 (d, *J* = 15.7 Hz, 1H), 5.45 (ddd, *J* = 15.7, 8.1, 6.6 Hz, 1H), 2.72 (ddd, *J* = 14.0, 6.6, 1.3 Hz, 1H), 2.47 (ddd, *J* = 14.0, 8.1, 0.7 Hz, 1H), 2.27 (s, 1H), 1.33 (s, 1H), 0.95 (s, 9H), 0.15 (s, 6H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.62, 155.06, 154.24, 143.52, 132.60, 130.32, 127.70, 127.17, 124.96, 122.02, 121.88, 119.98, 119.87, 77.32, 77.00, 76.69, 57.73, 40.35, 25.64, 21.66, 18.17, 16.03, -4.46. ***LC-MS*** (m/z): 247.0 $[C_{15}H_{23}Si]^+$, 414.0 $[M+Na]^+$. ***Anal. Calc***. for ($C_{25}H_{33}NOSi$: 391.63): C, 76.67; H, 8.49; found: C, 76.65; H, 8.41.



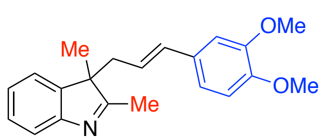
3ae. Yellow oil, yield = 51% (24 mg, 70°C, 36h, *n*Hex:Et_2O = 1:1.8). ***[1]H NMR*** (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.23 (m, 2H), 7.21 – 7.14 (m, 1H), 7.10 (d, *J* = 8.5 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 2H), 6.24 (d, *J* = 15.7 Hz, 1H), 5.55 (ddd, *J* = 15.7, 8.2, 6.8 Hz, 1H), 2.73 (dd, *J* = 14.0, 6.8 Hz, 1H), 2.49 (dd, *J* = 14.2, 8.2 Hz, 1H), 2.42 (s, 3H), 2.27 (s, 3H), 1.33 (s, 3H). ***[13]C NMR*** (100 MHz, $CDCl_3$) δ 186.43, 154.22, 143.38, 137.34, 133.96, 132.46, 127.76, 126.63, 126.50, 125.00, 123.65, 121.87, 119.91, 57.69, 40.33, 21.65, 16.00, 15.89. ***LC-MS*** (m/z): 163.0 $[C_{10}H_{11}S]^+$, 330.0 $[M+Na]^+$, 346.0 $[M+K]^+$. ***Anal. Calc***. for ($C_{20}H_{21}NS$: 307.46): C, 78.13; H, 6.88; found: C, 78.01; H, 6.93.



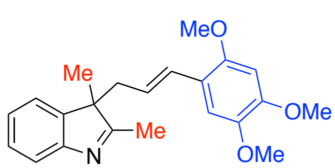
3af. Orange oil which solidifies on standing, yield = 76% (44 mg, 4 h, *n*Hex:Et_2O = 1:1.8). ***[1]H NMR*** (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.33 – 7.22 (m, 2H), 7.18 (dt, *J* = 7.4, 0.8 Hz, 1H), 7.06 (d, *J* = 8.7 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 6.24 (d, *J* = 15.7 Hz, 1H), 5.46 (ddd, *J* = 15.7, 8.0, 6.7 Hz, 1H), 3.90 (t, *J* = 6.3 Hz, 2H), 3.27 (t, *J* = 6.8 Hz, 2H), 2.72 (ddd, *J* = 13.9, 6.7, 1.3 Hz, 1H), 2.47 (ddd, *J* = 14.0, 8.0, 0.9 Hz, 1H), 2.27 (s, 3H), 1.81 – 1.71 (m, 2H), 1.68 – 1.59 (m, 2H), 1.57 – 1.46 (m, 2H), 1.33 (s, 3H). ***[13]C NMR*** (100 MHz, $CDCl_3$ δ 186.60, 158.33, 154.24, 143.51, 132.50, 129.75, 127.69, 127.23, 124.94, 121.90, 121.87, 119.86, 114.37, 67.53, 57.74, 51.30, 40.35, 28.74, 28.60, 23.33, 21.64, 16.03. ***LC-MS*** (m/z): 244.0 $[C_{14}H_{18}N_3O]^+$, 411.0 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{24}H_{28}N_4O$: 388.52): C, 74.20; H, 7.26; found: C, 74.11; H, 7.39.



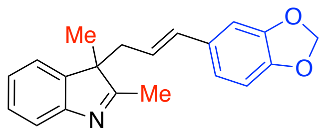
3ag. Yellow oil, yield = 40% 17.5 mg, *n*Hex:Et_2O = 1:1.4). ***M.p.*** = 132.5-135.5 °C. ***[1]H NMR*** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 6.9 Hz, 2H), 7.22 – 7.07 (m, 3H), 6.84 – 6.74 (m, 2H), 6.63 (d, *J* = 15.9 Hz, 1H), 5.58 (ddd, *J* = 15.9, 8.0, 6.7 Hz, 1H), 3.76 (s, 3H), 2.76 (dd, *J* = 13.9, 6.7 Hz, 1H), 2.52 (dd, *J* = 13.9, 8.0 Hz, 1H), 2.28 (s, 3H), 1.34 (s, 3H). ***[13]C NMR*** (100 MHz, $CDCl_3$) δ 184.13, 153.76, 151.68, 141.00, 125.69, 125.41, 125.08, 124.16, 123.63, 122.36, 122.35, 119.37, 117.98, 117.25, 108.17, 55.19, 52.84, 38.14, 19.05, 13.48. ***LC-MS*** (m/z): 147.0 $[C_{10}H_{11}O]^+$, 292.2 $[M+H]^+$. ***Anal. Calc.*** for ($C_{20}H_{21}NO$: 291.39): C, 82.44; H, 7.26; found: C, 82.24; H, 7.51.



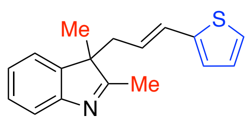
3ah. Pale yellow oil, yield = 76% (37 mg, overnight, *n*Hex:Et_2O = 1:6). ***[1]H NMR*** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.22 (m, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 6.74 – 6.65 (m, 2H), 6.64 (s, 1H), 6.23 (d, *J* = 15.7 Hz, 1H), 5.44 (ddd, *J* = 15.7, 7.9, 6.7 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 2.72 (ddd, *J* = 13.9, 6.7, 1.0 Hz, 1H), 2.48 (ddd, *J* = 13.9, 7.9, 0.6 Hz, 1H), 2.27 (s, 3H), 1.33 (s, 3H). ***[13]C NMR*** (100 MHz, $CDCl_3$) δ 186.52, 154.24, 148.85, 148.56, 143.47, 132.77, 130.15, 127.70, 124.96, 122.24, 121.90, 119.84, 118.98, 111.06, 108.95, 57.74, 55.87, 55.77, 40.30, 21.63, 16.02. ***LC-MS*** (m/z): 177.0 $[C_{11}H_{13}O_2]^+$, 344.0 $[M+Na]^+$, 665.2 $[2M+Na]^+$. ***Anal. Calc***. for ($C_{21}H_{15}NO_2$: 321.42): C, 78.47; H, 7.21; found: C, 78.62; H, 7.33.



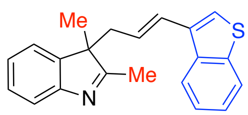
3ai. White oil, yield = 81% (43 mg, 2 h, 25 °C, *n*Hex:AcOEt = 1:2). ***[1]H NMR*** (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.6 Hz, 1H), 7.31 – 7.25 (m, 2H), 7.17 (t, *J* = 7.4 Hz, 1H), 6.57 (s, 1H), 6.53 (d, *J* = 15.8 Hz, 1H), 6.40 (s, 1H), 5.41 (ddd, *J* = 15.8, 8.0, 6.7 Hz, 1H), 3.82 (s, 3H), 3.73 (s, 3H), 3.70 (s, 3H), 2.73 (dd, *J* = 13.8, 6.7 Hz, 1H), 2.51 (dd, *J* = 13.8, 8.0 Hz, 1H), 2.27 (s, 3H), 1.33 (s, 3H).***[13]C NMR*** (100 MHz, $CDCl_3$) δ 186.75, 154.22, 151.02, 149.21, 143.60, 143.28, 127.61, 127.47, 124.95, 122.82, 121.96, 119.70, 118.26, 110.32, 98.02, 57.89, 56.75, 56.51, 56.05, 40.71, 21.58, 16.02. ***LC-MS*** (m/z): 207.2 $[C_{12}H_{15}O_3]^+$, 374.4 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{22}H_{25}NO_3$: 351.45): C, 75.19; H, 7.17; found: C, 75.08; H, 7.31.



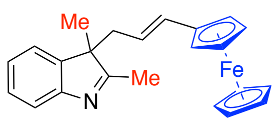
3aj. Yellow oil, yield = 66% (30 mg, 16 h, *n*Hex:Et_2O = 1:2.4). ***^1H NMR*** (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.34 – 7.23 (m, 2H), 7.18 (td, *J* = 7.4, 0.7 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 1.5 Hz, 1H), 6.58 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.21 (d, *J* = 15.7 Hz, 1H), 5.88 (s, 2H), 5.42 (ddd, *J* = 15.7, 8.1, 6.7 Hz, 1H), 2.71 (ddd, *J* = 13.9, 6.7, 1.3 Hz, 1H), 2.46 (ddd, *J* = 13.9, 8.1, 0.9 Hz, 1H), 2.27 (s, 3H), 1.33 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.47, 154.23, 147.80, 146.90, 143.41, 132.63, 131.45, 127.75, 124.97, 122.37, 121.85, 120.57, 119.90, 108.09, 105.49, 100.92, 57.71, 40.24, 21.62, 16.01. ***LC-MS*** (m/z): 144.2 $[C_{10}H_{10}N]^+$, 161.0 $[C_{10}H_{19}O_2]^+$, 328.0 $[M+Na]^+$. ***Anal. Calc***. for ($C_{20}H_9NO_2$: 305.38): C, 78.66; H, 6.27; found: C, 78.41; H, 6.42.



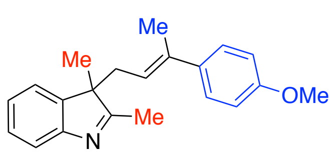
3ak. Pale yellow oil, yield = 63% (25 mg, 36h, *n*Hex:Et_2O = 1:1.7). ***^1H NMR*** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.6 Hz, 1H), 7.28 (m, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.04 (d, *J* = 4.7 Hz, 1H), 6.85 (dd, *J* = 4.7, 3.3 Hz, 1H), 6.77 (d, *J* = 3.3 Hz, 1H), 6.42 (d, *J* = 15.5 Hz, 1H), 5.52 (ddd, *J* = 15.5, 8.1, 6.9 Hz, 1H), 2.69 (dd, *J* = 13.9, 6.9 Hz, 1H), 2.43 (dd, *J* = 13.9, 8.1 Hz, 1H), 2.27 (s, 3H), 1.33 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.31, 154.19, 143.28, 141.93, 127.79, 127.16, 126.23, 125.01, 124.92, 123.95, 123.76, 121.94, 119.95, 57.57, 40.13, 21.47, 16.00. ***LC-MS*** (m/z): 123.0 $[C_7H_7S]^+$, 268.0 $[M+H]^+$. ***Anal. Calc.*** for ($C_{17}H_{17}NS$: 267.39): C, 76.36; H, 6.41; found: C, 76.24; H, 6.19.



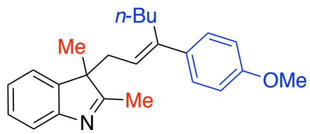
3al. Yellow oil, yield = 53% (25 mg, 70 °C, 36 h, *n*Hex:Et_2O = 1:1.6). ***^1H NMR*** (400 MHz, $CDCl_3$) δ 7.78 (m, 1H), 7.59 – 7.51 (m, 2H), 7.36 – 7.26 (m, 4H), 7.20 (t, *J* = 7.1 Hz, 1H), 7.12 (s, 1H), 6.51 (d, *J* = 15.8 Hz, 1H), 5.61 (ddd, *J* = 15.8, 8.0, 6.7 Hz, 1H), 2.82 (ddd, *J* = 13.9, 6.7, 1.2 Hz, 1H), 2.59 (ddd, *J* = 13.9, 8.0, 0.8 Hz, 1H), 2.32 (s, 3H), 1.38 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.36, 154.29, 143.34, 140.23, 137.52, 133.70, 127.84, 126.32, 125.42, 125.09, 124.29, 124.10, 122.74, 121.90, 121.82, 121.59, 119.96, 57.80, 40.63, 21.68, 16.03. ***LC-MS*** (m/z): 173.0 $[C_{11}H_9S]^+$, 318.0 $[M+H]^+$, 340.2 $[M+Na]^+$. ***Anal. Calc.*** for ($C_{21}H_{19}NS$: 317.45): C, 73.46 H, 6.03; found: C, 73.61; H, 5.89.



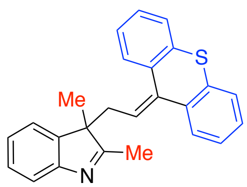
3am. Red oil which solidifies on standing, yield = 61% (34 mg, 1 h, 25 °C, *n*Hex:Et_2O = 1.2:1, then *n*Hex:Acetone 5:1). ***^1H NMR*** (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 1H), 7.33 – 7.27 (m, 2H), 7.21 (t, *J* = 7.3 Hz, 1H), 5.96 (d, *J* = 15.5 Hz, 1H), 5.15 (ddd, *J* = 15.5, 7.6, 7.2 Hz, 1H), 4.12 – 4.01 (m, 4H), 3.88 (s, 5H), 2.61 (dd, *J* = 13.9, 7.6 Hz, 1H), 2.44 (dd, *J* = 13.8, 7.2 Hz, 1H), 2.31 (s, 3H), 1.32 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.36, 154.39, 143.66, 130.30, 127.77, 124.94, 121.80, 121.01, 119.88, 82.78, 69.02 (5C), 68.35, 68.25, 66.73, 65.96, 57.89, 40.50, 21.95, 16.02. ***LC-MS*** (m/z): 225.0 $[C_{13}H_{13}Fe]^+$, 369.0 $[M]^+$. ***Anal. Calc***. for ($C_{23}H_{23}FeN$: 369.29): 74.81; H, 6.28; found: C, 74.66; H, 6.15.



3an. Pale yellow oil, yield = 72% (33 mg, 6 h, *n*Hex:Et_2O = 1:1.5). ***^1H NMR*** (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.28 (m, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.04 (d, *J* = 8.8 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 5.01 (ddd, *J* = 7.6, 7.0, 1.1 Hz, 1H), 3.74 (s, 3H), 2.74 (dd, *J* = 14.7, 7.0 Hz, 1H), 2.54 (dd, *J* = 14.7, 7.6 Hz, 1H), 2.29 (s, 3H), 1.88 (s, 3H), 1.36 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.90, 158.61, 154.06, 143.64, 136.92, 135.96, 127.72, 126.72, 125.04, 121.80, 120.19, 119.74, 113.45, 57.77, 55.21, 35.80, 21.68, 16.31, 15.82. ***LC-MS*** (m/z): 161.2 $[C_1H_{13}O]^+$, 344.2 $[M+K]^+$. ***Anal. Calc.*** for ($C_{21}H_{23}NO$: 305.42): C, 82.58; H, 7.59; found: C, 82.37; H, 7.71.

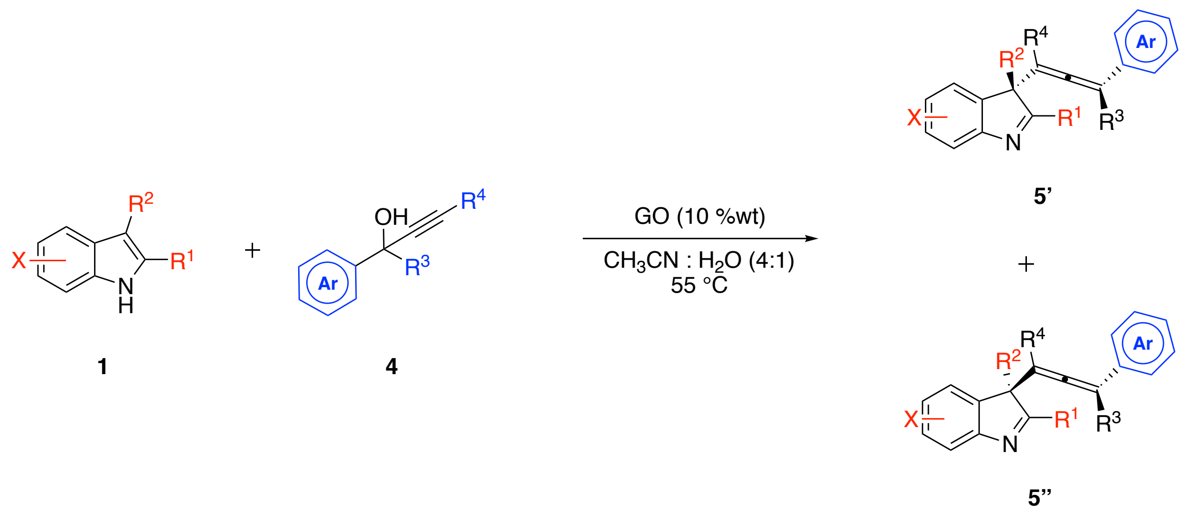


3ao. Yellow solid, yield = 80% (42 mg, 5 h, *c*Hex:AcOEt = 3:1). ***M.p.*** = 162.7-163.6 °C. ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.6 Hz, 1H), 7.27 (m, 2H), 7.15 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.73 (d, *J* = 8.8 Hz, 2H), 4.85 (t, *J* = 7.1 Hz, 1H), 3.74 (s, 2H), 2.73 (dd, *J* = 14.9, 7.0 Hz, 1H), 2.53 (dd, *J* = 14.9, 7.3 Hz, 1H), 2.36 – 2.28 (m, 2H), 2.27 (s, 3H), 1.35 (s, 3H), 1.29 – 1.18 (m, 2H), 1.18 – 1.07 (m, 2H), 0.82 (t, *J* = 7.2 Hz, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.72, 158.49, 154.36, 143.70, 142.41, 135.25, 127.67, 127.31, 124.96, 121.81, 120.57, 119.79, 113.43, 57.66, 55.17, 35.48, 30.64, 29.85, 22.76, 21.79, 15.92, 13.93. ***LC-MS*** (m/z): 203.2 $[C_{14}H_{19}O]^+$, 370.2 $[M+Na]^+$. ***Anal. Calc***. for ($C_{24}H_{29}NO$: 347.50): C, 82.95; H, 8.41; found: C, 82.76; H, 8.21.

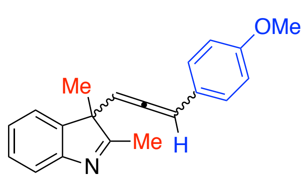


3ap. White solid, yield = 84% (46 mg, 5 h, 25 °C, *n*Hex:AcOEt = 2:1). ***M.p.*** = 61.8-62.6 °C. ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.6 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.29 (m, 3H), 7.26 – 7.20 (m, 3H), 7.18 (dd, *J* = 7.3, 0.8 Hz, 1H), 7.16 – 7.08 (m, 3H), 5.07 (dd, *J* = 8.6, 5.9 Hz, 1H), 3.02 (dd, *J* = 15.2, 5.9 Hz, 1H), 2.86 (dd, *J* = 15.2, 8.6 Hz, 1H), 2.05 (s, 3H), 1.28 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 186.46, 154.44, 143.18, 138.19, 138.17, 134.17, 133.40, 131.74, 128.52, 127.87, 127.14, 126.89, 126.82, 126.74, 125.77, 125.73, 125.37, 125.25, 125.14, 121.63, 119.93, 77.33, 77.02, 76.70, 57.86, 36.15, 22.22, 15.70. ***LC-MS*** (m/z): 223.0 $[C_{15}H_{11}S]^+$, 390.0 $[M+Na]^+$, 757.2 $[2M+Na]^+$. ***Anal. Calc.*** for ($C_{25}H_{21}NS$: 367.51): C, 81.71; H, 5.76; found: C, 81.91; H, 5.65.

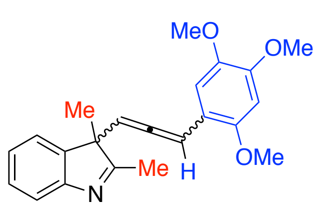
General procedure for the allenylic dearomatization of indoles



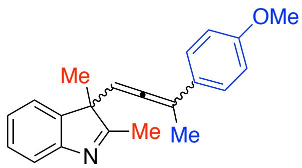
A screw-capped vial is charged with CH_3CN (0.8 mL), propargylic alcohol **4** (0.3 mmol, 3 eq), indole **1** (0.10 mmol, 1 eq), GO dried flakes (10 wt% with respect to indole) and deionized water (0.2 mL). The reaction mixture was stirred at 55 °C (unless otherwise noted) until complete consumption of indole (*vide infra* for reaction times). The mixture was then filtered on a Gooch funnel and the GO washed with EtOAc. The collected organic layers were dried over Na_2SO_4 and evaporated to dryness under vacuum. The crude was purified by column chromatography to give the desired product as a mixture of two diastereomers **5'** and **5''**.



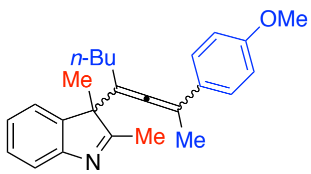
5aa' + 5aa''. Yellow oil, yield = 54% (15.6 mg, 48 h, *n*Hex:Acetone = 6:1), *d.r.* = 58:42. ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.57 – 7.50 (m, 1H), 7.39 – 7.27 (m, 2H), 7.27 – 7.14 (m, 3H), 6.93 – 6.82 (m, 2H), 6.41 – 6.33 (m, 1H), 5.35 – 5.29 (m, 1H), 3.84 – 3.76 (m, 3H), 2.38 – 2.28 (m, 3H), 1.42 – 1.38 (m, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 204.99, 204.87, 185.73, 185.50, 159.11, 159.08, 154.12, 154.08, 144.07, 143.91, 128.09, 128.05, 127.85, 127.82, 125.98, 125.94, 125.45, 125.38, 122.42, 122.24, 120.01, 119.96, 114.29, 97.97, 97.01, 96.79, 58.02, 55.30, 20.51, 20.22, 15.97, 15.89. ***GC-MS*** (m/z): 289 (28) $[M]^+$, 274. (4) $[M-Me]^+$, 145 (100) $[M-C_{10}H_{10}N]^+$. ***Anal. Calc***. for ($C_{20}H_{19}NO$: 289.38): C, 83.01; H, 6.62; found: C, 82.82; H, 6.46.



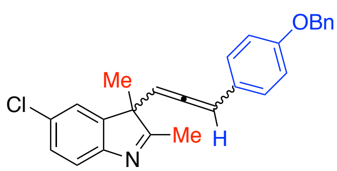
5ab' + 5ab''. Orange oil, yield = 78% (27.8 mg, 3 h, *n*Hex:AcOEt = 1:1). *d.r.* = 77:23. ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.55 – 7.49 (m, 1H), 7.34 – 7.27 (m, 2H), 7.21 – 7.15 (m, 1H), 6.81 – 6.73 (m, 2H), 6.50 – 6.48 (m, 1H), 5.40 – 5.32 (m, 1H), 3.89 – 3.86 (m, 3H), 3.84 – 3.79 (m, 3H), 3.72 (s, 3H), 2.38 – 2.30 (m, 3H), 1.41 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 205.09, 185.51, 154.03, 150.68, 149.32, 144.33, 143.53, 128.06, 127.97, 125.40, 125.31, 122.26, 122.18, 120.02, 119.97, 113.54, 110.15, 97.97, 96.52, 92.36, 58.03, 57.93, 56.78, 56.14, 56.12, 20.54, 20.37, 15.96. ***GC-MS*** (m/z): 349 (22) $[M]^+$, 205 (100) $[M-C_{10}H_{10}N]^+$, 144 (94) $[C_{10}H_{10}N]^+$. ***Anal. Calc***. for ($C_{22}H_{23}NO_3$: 349.43): C, 75.62; H, 6.63; found: C, 75.46; H, 6.29.



5ac' + 5ac''. Orange oil, yield = 94% (28.4 mg, 12 h, *n*Hex:AcOEt = 2.8:1), *d.r.* = 80:20 ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 1H), 7.36 – 7.25 (m, 4H), 7.23 – 7.16 (m, 1H), 6.92 – 6.84 (m, 2H), 5.22 – 5.16 (m, 1H), 3.82 – 3.79 (m, 3H), 2.35 – 2.30 (m, 3H), 2.18 – 2.11 (m, 3H), 1.39 – 1.36 (m, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 204.11, 204.10, 185.95, 158.81, 158.79, 154.11, 154.05, 144.29, 144.22, 128.67, 128.62, 127.99, 127.93, 126.79, 126.73, 125.36, 125.33, 122.28, 119.93, 119.90, 113.90, 104.37, 104.30, 94.85, 94.67, 58.49, 58.41, 55.29, 20.43, 20.22, 17.67, 17.52, 16.02, 15.78. ***GC-MS*** (m/z): 303 (15) $[M]^+$, 288 (8) $[M-Me]^+$, 159 (100) $[M-C_{10}H_{10}N]^+$. ***Anal. Calc***. for ($C_{21}H_{21}NO$: 303.41): C, 83.13; H, 6.98; found: C, 83.01; H, 6.75.



5ad' + 5ad''. Orange oil, yield = 74% (26.6 mg, 6 h, *n*Hex:AcOEt = 4:1), *d.r.* = 56:44. ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.60 – 7.51 (m, 1H), 7.47 – 7.36 (m, 2H), 7.36 – 7.16 (m, 3H), 6.97 – 6.85 (m, 2H), 3.86 – 3.77 (m, 3H), 2.34 – 2.24 (m, 3H), 2.25 – 2.19 (m, 3H), 1.46 – 1.38 (m, 1H), 1.32 – 1.23 (m, 4H), 1.23 – 1.13 (m, 2H), 1.13 – 0.99 (m, 2H), 0.71 – 0.63 (m, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 202.20, 202.12, 186.62, 158.64, 158.60, 154.80, 154.74, 144.01, 143.90, 129.78, 129.70, 127.90, 127.88, 126.57, 126.51, 125.38, 125.35, 122.10, 122.03, 119.94, 119.88, 113.94, 113.90, 107.85, 107.65, 104.95, 104.85, 61.91, 61.82, 55.33, 55.31, 29.78, 27.77, 27.70, 22.28, 22.19, 20.73, 20.68, 18.20, 17.75, 16.16, 15.71, 13.82, 13.79. ***GC-MS*** (m/z): 359 (10) $[M]^+$, 344 (2) $[M-Me]^+$, 215 (100) $[M-C_{10}H_{10}N]^+$. ***Anal. Calc.*** for ($C_{25}H_{29}NO$: 359.22): C, 83.52; H, 8.13; found: C, 83.31; H, 8.01.



5be' + 5be''. Pale yellow oil, yield = 40% (16.1 mg, 4 days, *n*Hex:Et_2O = 1:1.8), *d.r.* = 72:28. ***^{1}H NMR*** (400 MHz, $CDCl_3$) δ 7.47 – 7.35 (m, 5H), 7.35 – 7.25 (m, 3H), 7.25 – 7.19 (m, 2H), 6.99 – 6.92 (m, 2H), 6.39 (d, *J* = 6.3 Hz, 1H), 5.33 – 5.27 (m, 1H), 5.09 – 5.05 (m, 2H), 2.37 – 2.27 (m, 3H), 1.39 (s, 3H). ***^{13}C NMR*** (100 MHz, $CDCl_3$) δ 205.14, 204.94, 186.24, 186.08, 158.42, 158.37, 152.65, 152.60, 145.83, 145.74, 136.80, 131.23, 128.58, 128.26, 128.22, 127.98, 127.91, 127.89, 127.41, 127.39, 125.94, 125.87, 123.00, 122.85, 120.86, 120.80, 115.32, 115.30, 98.35, 98.26, 96.37, 96.21, 70.07, 58.37, 20.26, 20.22, 15.99, 15.89. ***LC-MS*** (m/z): 221.2 $[C_{16}H_{13}O]^+$, 400.2/402.2 $[M+H]^+$. ***Anal. Calc.*** for ($C_{26}H_{22}ClNO$: 399.92): C, 78.09; H, 5.55; found: C, 77.35; H, 5.42.

Gram scale reaction and recycling of GO (entry 17, Table 1)

In a Schlenk tube are added in a sequence reagent grade CH_3CN (28 mL), allylic alcohol **2a** (1.64 g, 10 mmol), indole **1a** (725 mg, 5 mmol), GO (72.5 mg, 10 % wt, powder) and deionized water (7 mL). The reaction mixture was stirred at 55 °C overnight. The mixture was then filtered on a Gooch funnel and the GO washed with EtOAc. The filtrate was concentrated by rotary evaporation to remove CH_3CN and then extracted with EtOAC. The collected organic layers were dried over Na_2SO_4 and evaporated to dryness under vacuum. The crude was purified by column chromatography to give the desired product **3aa** in 78% yield (1.135 g). The graphene recovered from the mixture by filtration was then washed with water, acetone, methanol and DCM. Then, GO was suspended in DCM and stirred for 2 hours at room temperature. The mixture was filtered on a Gooch funnel, and the GO washed with some fresh DCM. This process was repeated 3 times; after that the GO was dried under vacuum for 4 hours.

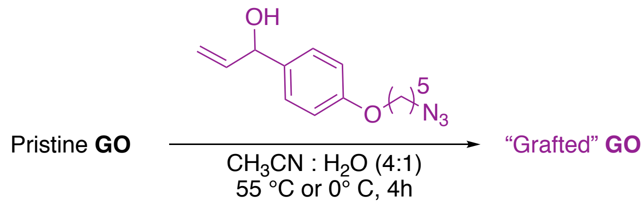
The so obtained GO was used in place of pristine GO in the model reaction which was set up according to the general procedure. The product **3aa** was isolated in 12% yield (36 h).

GO regeneration

The used GO was sonicated in 1 M HCl, following the procedure described by C.-H. Chen *et al.* for the regeneration of epoxides.[7]

The so obtained GO was used in place of pristine GO in the model reaction. The product **3aa** was isolated in 63 % yield (36 h).

Grafting experiments



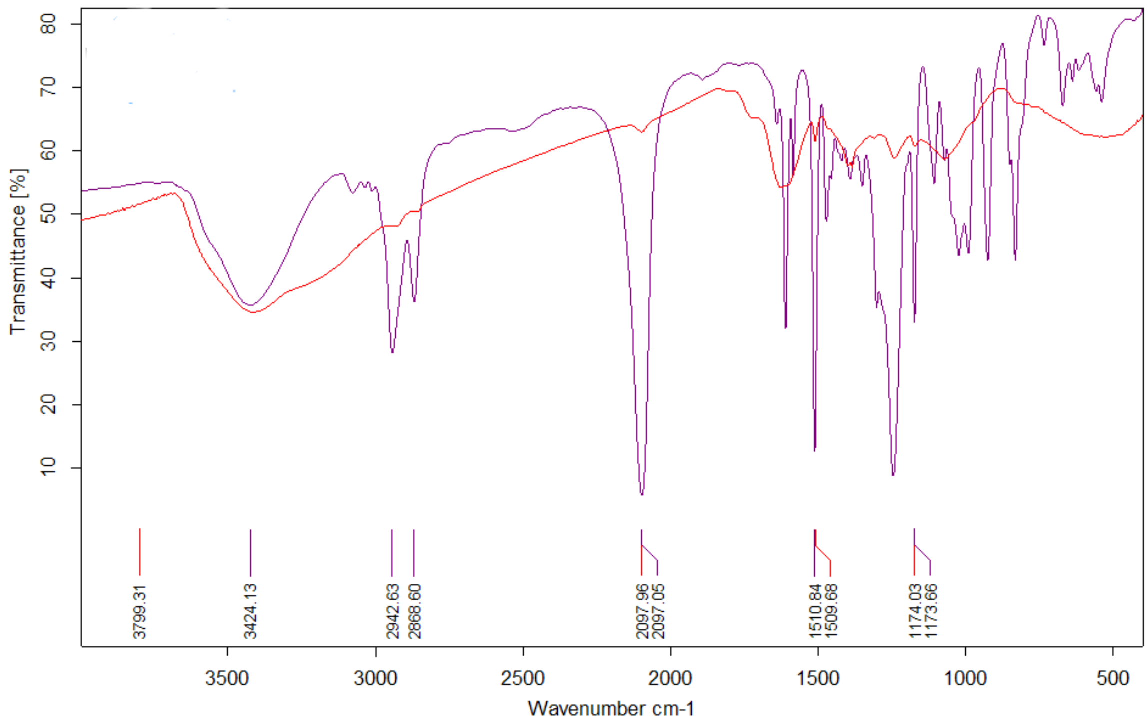
In a screw-capped vial are added in a sequence: CH_3CN (3 mL), allylic alcohol **2f** (76 mg, 0.75 mmol), GO (5.4 mg) and deionized water (0.75 mL). The reaction mixture was stirred at 55 °C for 4 hours. The mixture was then filtered, and the recovered GO was washed with water, acetone, methanol and DCM. The GO was then suspended in DCM and the suspension was stirred for 2 hours at room temperature. The solvent was removed by pipette, and the graphene was washed again with some fresh DCM. This process was repeated 3 times; after that the GO was dried under vacuum for 4 hours.

The reaction was also performed at 0° C following the same procedure.

FT-IR analysis and spectra

FT-IR spectra of various samples were acquired using transmission mode. The samples were prepared grinding GO (*ca.* 0.5 mg) with KBr and then pressing them into disks.

a)



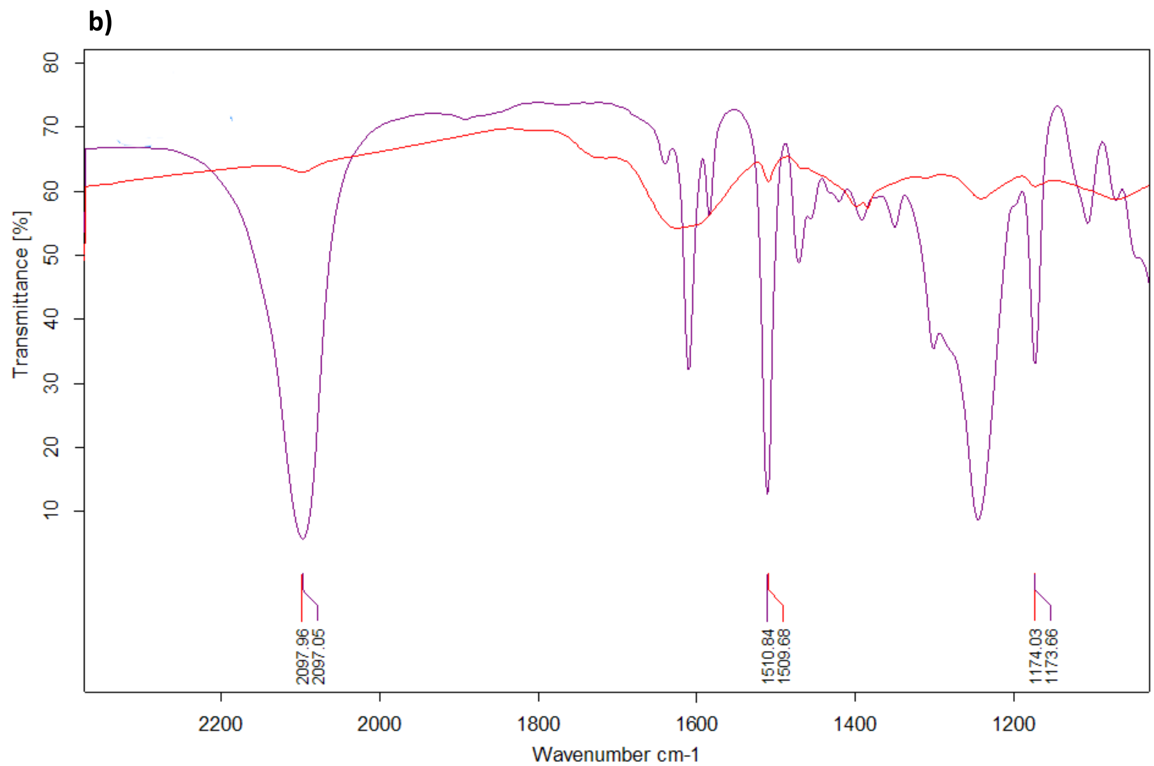


Figure S1. a) Violet: alcohol **2f**. Red: GO + **2f** after 6 h in $CH_3CN:H_2O$ 4:1 at 55 °C. b) Zoomed region showing characteristic peaks of alcohol **2f** matching with the "grafted" GO peaks.

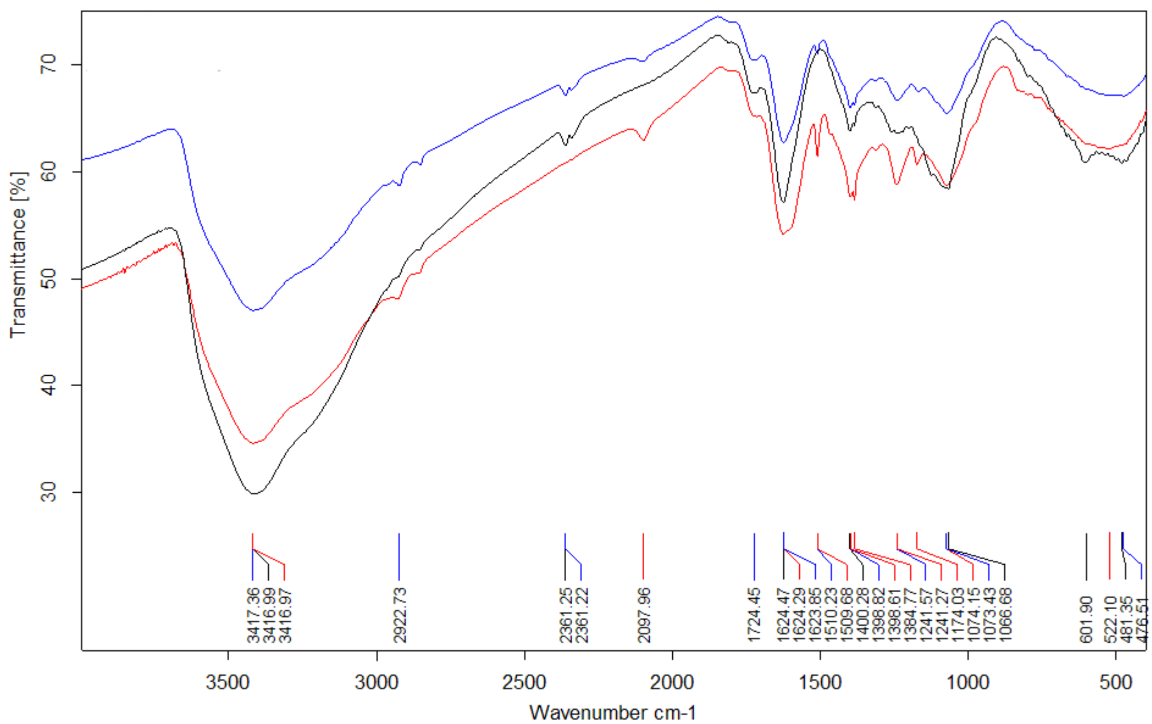


Figure S2. Black: pristine GO. Blue: GO + **2f** after 6 h in CH_3CN:H_2O 4:1 at 0 °C. Red: GO + **2f** after 6 h in CH_3CN:H_2O 4:1 at 55 °C. The peaks associated with alcohol **2f** (2098, 1510, 1174 cm^{-1}) are completely absent in pristine GO.

XPS-analysis

The O:C ratio was obtained from the fit of C 1s peak, the general trends of all functional groups are reported in Table S2 and Figures S3/S4.
XPS N 1s of azide is reported to be a double peak with 4 eV relative shift, the high energy peak corresponding to the central nitrogen (N=<u>N</u>=N) is between 405-403 eV, while the two-external nitrogen (<u>N</u>=N=<u>N</u>) are in the 401-399 eV region. The pristine GO present a residual amounts (<0.7% at.) of indole and amino groups in the region 402-399 eV (Figure S5).[8]
The C1s peak in Figure S6 support the grafting of **2f**, the decrease of epoxy group confirms the epoxy ring open, as already observed in Figure 2 for GO after **2a**. Moreover, no increase of hydroxyl group was observed.
The epoxidation of GO was confirmed by the increase of epoxy group after the HCl treatment (Figure S7) from 24% of reacted GO (GO after **1a**+**2a**) up to 30%.

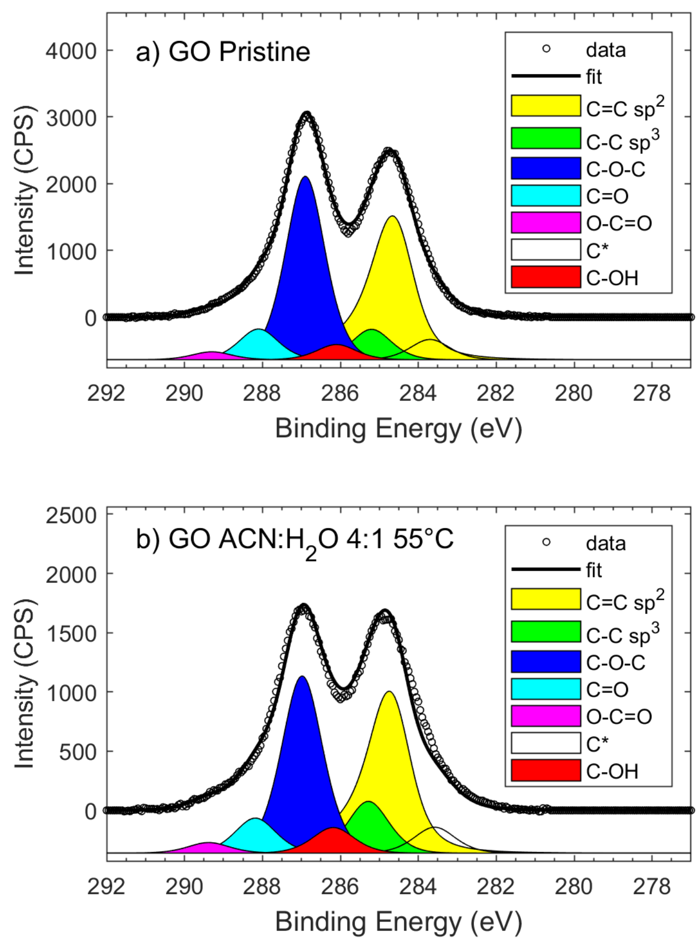


Figure S3. C 1s spectrum of GO: a) as given and b) after 5 h in ACN:H_2O 4:1 at 55 °C.

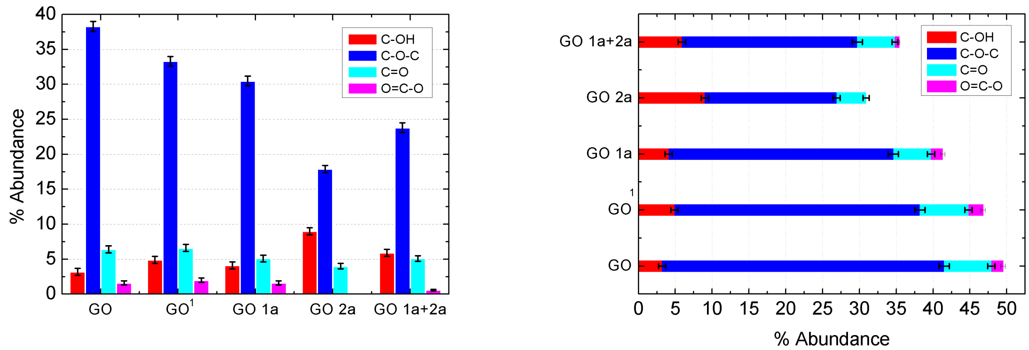


Figure S4. XPS fit of C 1s of GO after different experimental conditions. Only C-O groups are reported.

Table S2. XPS fit of C 1s of GO after different experimental conditions. The components used in fit are: aromatic carbon (C–C sp^2, 284.4 eV), aliphatic carbon (C–C sp^3, 285.0 eV), hydroxyl (C–OH, 285.7 eV), epoxy (C–O–C, 286.7 eV), carbonyl (C=O, 288.0 eV), carboxyl (O–C=O, 289.1 eV) and aromatic carbons near vacancies (C-C* sp^2, 283.5).

Sample	C-C sp^2	C-C sp^3	C=C*	C-OH	C-O-C	C=O	O=C-O	O/C_{fit}
GO	39.9±0.8	10.5±0.5	4.2±0.3	3.2±0.3	38.3±0.8	6.4±0.4	1.6±0.2	0.32±0.02
GO (solvent)	38.7±0.8	14.6±0.5	4.9±0.3	4.9±0.3	33.3±0.8	6.6±0.4	2.0±0.2	0.32±0.02
GO after **1a**	42.5±0.8	16.3±0.5	5.4±0.4	4.1±0.3	30.5±0.8	5.1±0.4	1.6±0.2	0.28±0.02
GO after **2a**	45.5±0.8	23.6±0.6	3.9±0.3	9.0±0.5	17.9±0.6	4.0±0.3	0.0±0.2	0.22±0.01
GO after **1a**+**2a**	39.1±0.8	25.5±0.6	8.8±0.5	5.9±0.4	23.8±0.7	5.1±0.4	0.6±0.2	0.24±0.02
Regenerated GO	37.4±0.8	12.2±0.5	9.5±0.5	3.4±0.3	30.2±0.8	5.5±0.3	1.8±0.2	0.28±0.02
GO + **2f** 0°C	28.7±0.7	14.4±0.5	5.2±0.4	10.1±0.5	33.2±0.8	5.6±0.4	2.7±0.3	0.38±0.02
GO + **2f** 55 °C	39.1±0.8	16.8±0.5	0.4±0.2	5.7±0.4	30.8±0.8	3.1±0.3	2.4±0.2	0.29±0.02

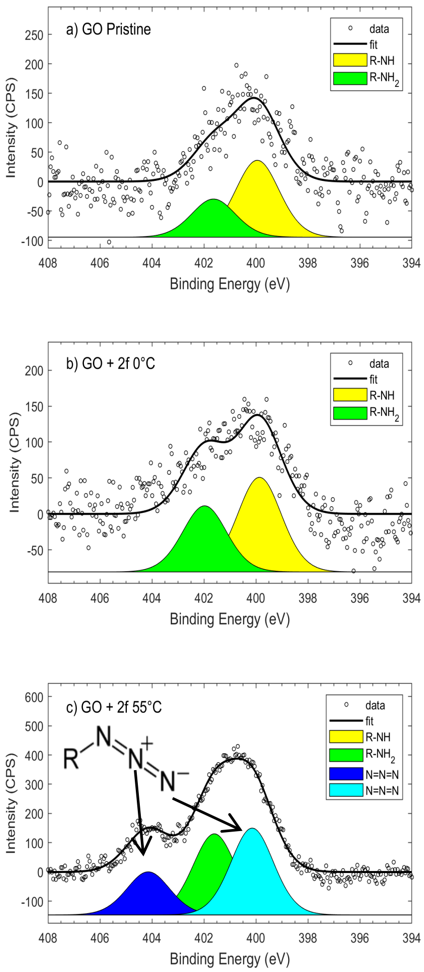


Figure S5. XPS N 1s signal of a) pristine GO, b) GO + **2f** after 6 h in $CH_3CN:H_2O$ 4:1 at 0 °C and c) GO + **2f** after 6 h in $CH_3CN:H_2O$ 4:1 at 55 °C.

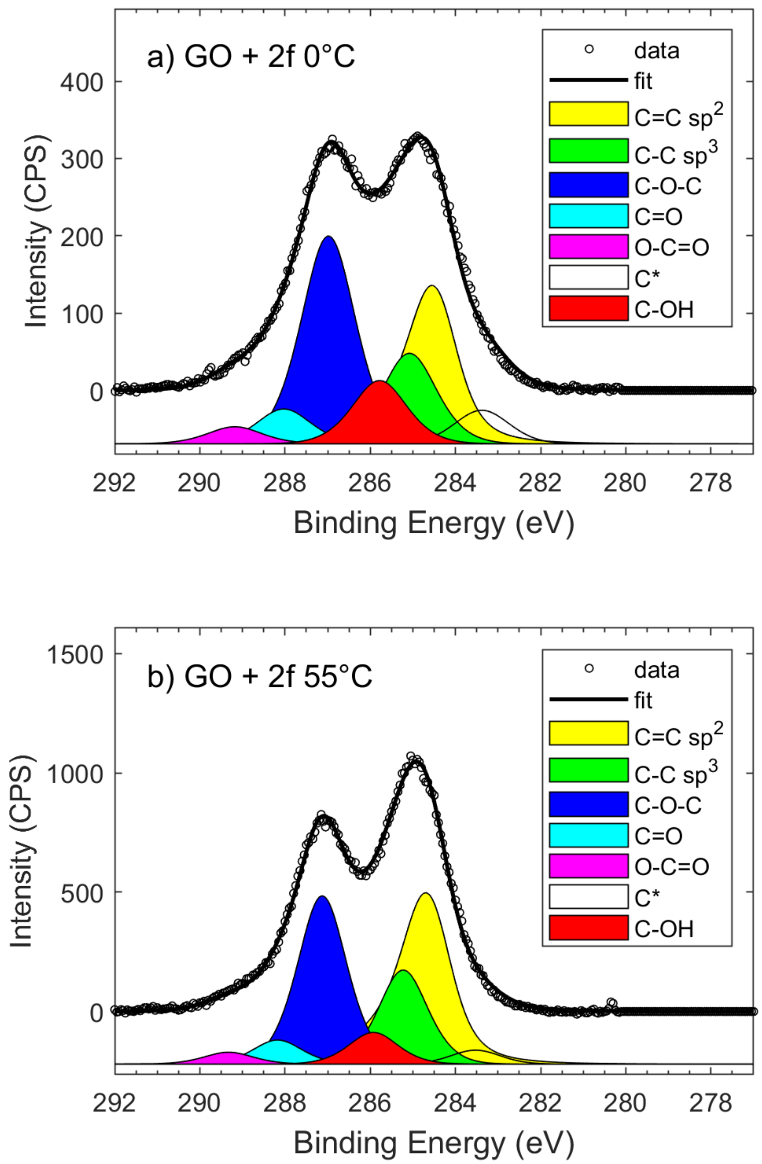


Figure S6. XPS C 1s signal of a) GO + **2f** after 6 h in $CH_3CN:H_2O$ 4:1 at 0 °C and b) GO + **2f** after 6 h in $CH_3CN:H_2O$ 4:1 at 55 °C.

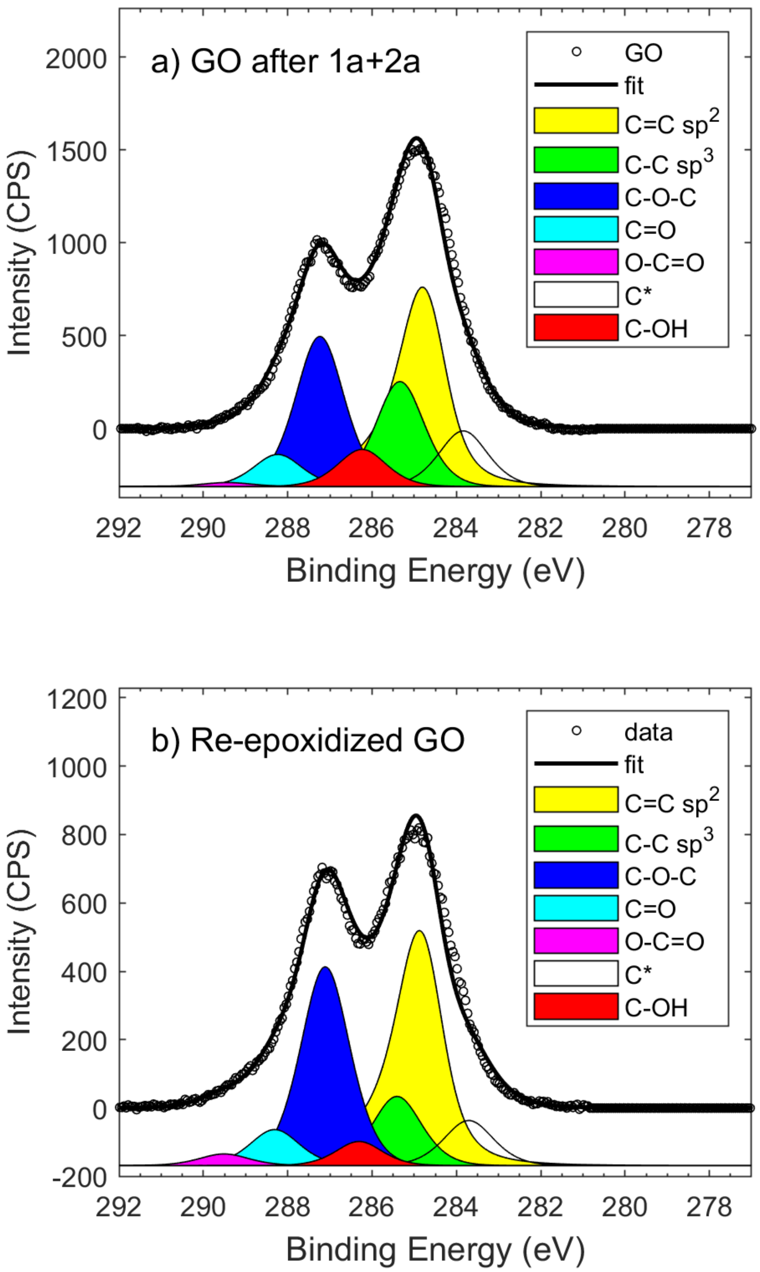


Figure S7. XPS C 1s signal of a) GO after **1a**+**2a** and b) Re-epoxidized GO.

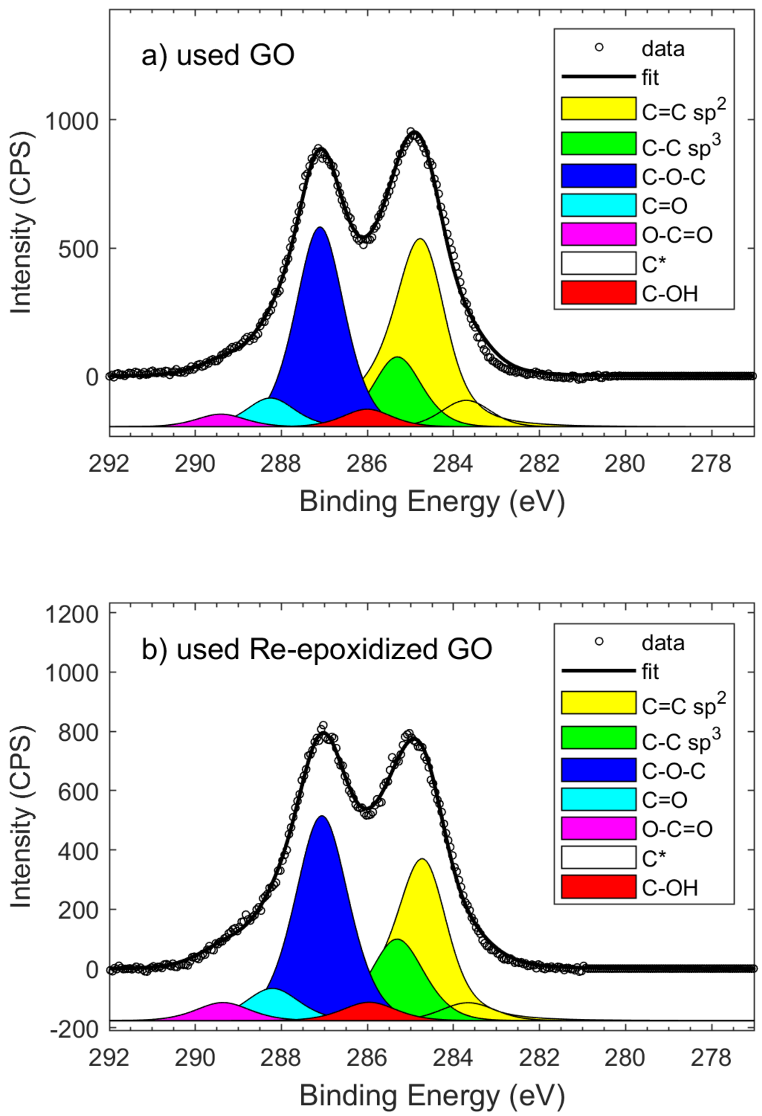


Figure S8. XPS C 1s signal of a) used GO and b) used Re-epoxidized GO.

Computational details

All calculations were carried out using the combined quantum mechanical and molecular mechanical (QM/MM) method in the ONIOM formalism, as implemented within the Gaussian 16 program suite.[9] The coupled QM/MM method adopted here is a two-layer ONIOM scheme, where the reactive region is treated at DFT level using the density functional M06-2X (a functional able to account for π-π interactions) and 6-1G*basis set.[10] The remaining region is treated using the UFF force field.[11] The global potential can be referred as M06-2X/6-31G*:UFF potential. ONIOM calculations were performed considering mechanical and electrostatic embedding. In the MM calculations partial atomic (point) charges were used to compute the electrostatic interactions. These charges were calculated using the QEq formalism.[12] Frequency calculations were carried out at the same level of theory to check the nature of critical points. The presence of the solvent (water) is taken in account employing the polarizable continuum model (PCM) using the integral equation formalism variant (IEFPCM).[13]

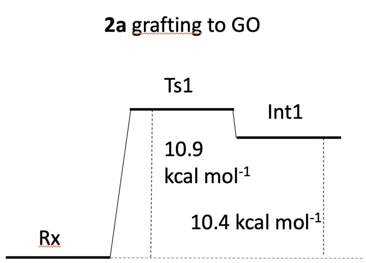


Figure S9. Energy profile for the covalent grafting of **2a** to the GO surface.

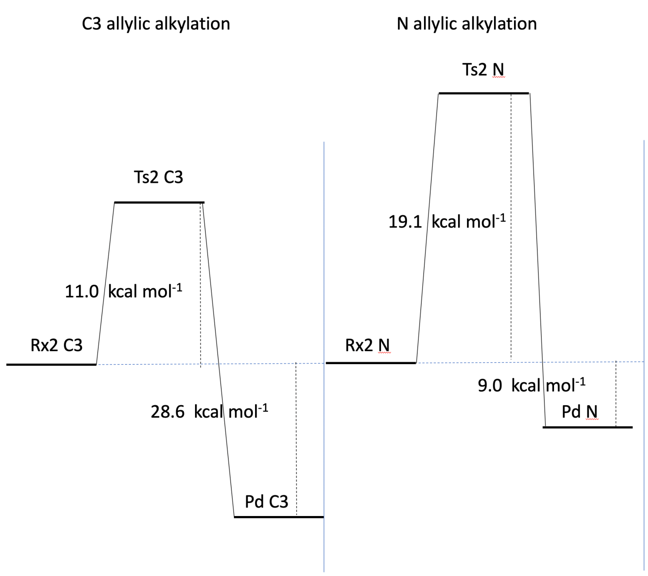


Figure S10. Energy profiles for the C3/N allylic alkylation of **1a**

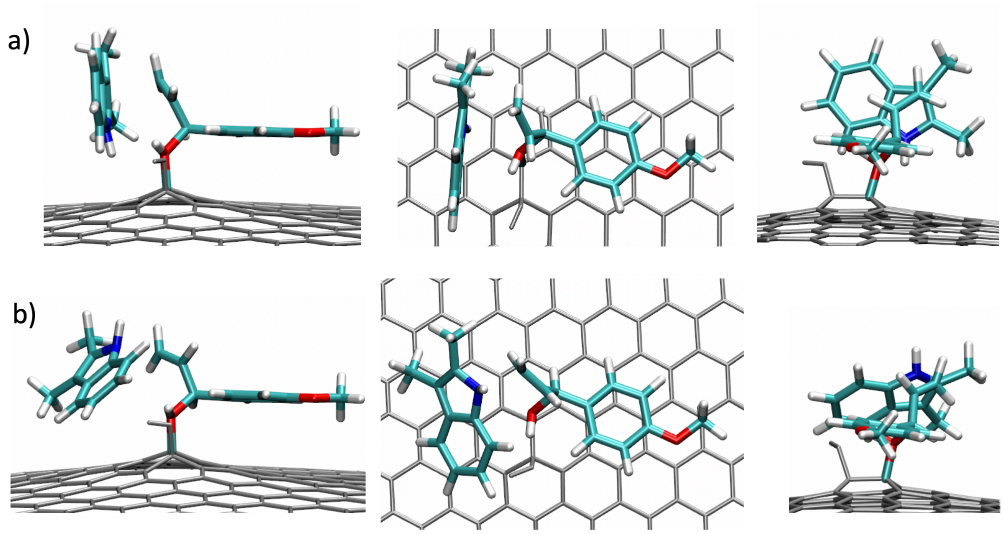


Figure S11. Side view (left), top view (center) and front view (right) of the identified transition states for the C(3) (a, Ts2 C3) and (N) (b, Ts2 N) allylic alkylation of **1a**.

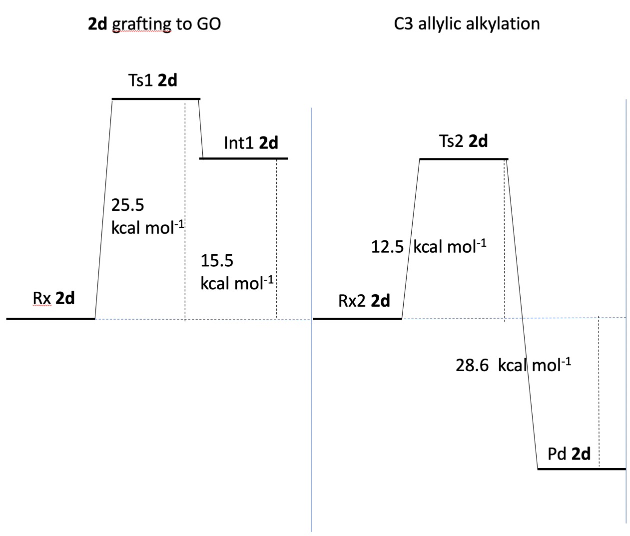


Figure S12. Energy profiles for the a) covalent grafting of **2d** to the GO surface and b) C3 allylic alkylation of **1a**

Crystallographic data collection and structure determination for 3ha.

The X-ray intensity data were measured on a Bruker Apex II CCD diffractometer using MoKα radiation. Cell dimensions and the orientation matrix were initially determined from a least-squares refinement on reflections measured in three sets of 20 exposures, collected in three different regions, and eventually refined against all data. A full sphere of reciprocal space was scanned by 0.3steps. The software SMART[14] was used for collecting frames of data, indexing reflections and determination of lattice parameters. The collected frames were then processed for integration by the SAINT program[14] and an empirical absorption correction was applied using SADABS[15]. The structures were solved by direct methods (SIR 2014)[16] and subsequent Fourier syntheses and refined by full-matrix least-squares on F^2 (SHELXTL)[17] using anisotropic thermal parameters for all non-hydrogen atoms. The hydrogen atoms were placed in calculated positions, refined with isotropic thermal parameters U(H)= 1.2 Ueq(C) or U(H)= 1.5 Ueq(methyl) and allowed to ride on their carrier carbons. Crystal data and details of data collections for compound **3ha** are reported in Table S1. Molecular drawings were generated using Mercury[18]. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC) as supplementary publication number CCDC 1964157. Copies of the data can be obtained free of charge upon request (www.ccdc.cam.ac.uk/).

Table S3. Crystal data and structure refinement for compound **3ha**.

Compound	**3ha**
Formula	$C_{22}H_{23}NO$
Fw	317.41
T, K	296
λ, Å	0.71073
Crystal symmetry	Monoclinic
Space group	$P2_1/c$
a, Å	9.577(2)
b, Å	10.592(2)
c, Å	16.415(3)
α	90
β	91.56(3)
γ	90
Cell volume, $Å^3$	1664.5(6)
Z	4
D_C, Mg m^{-3}	1.267
μ(Mo-K_α), mm^{-1}	0.077
F(000)	680
Crystal size/ mm	0.30 x 0.10 x 0.05
θ limits, °	2.127 - 24.495

Reflections collected	14923
Unique obs. Reflections [$F_o > 4\sigma(F_o)$]	2453 [R(int) = 0.0705]
Goodness-of-fit-on F^2	1.375
R_1 (F)^a, wR_2 (F^2)^b [$I > 2\sigma(I)$]	0.1073, 0.2281
Largest diff. peak and hole, e. Å^{-3}	0.224 and -0.247

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$.[b] $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$ where $w = 1/[\sigma^2(F_o^2) + (aP)^2+ bP]$ where $P = (F_o^2 + F_c^2)/3$.

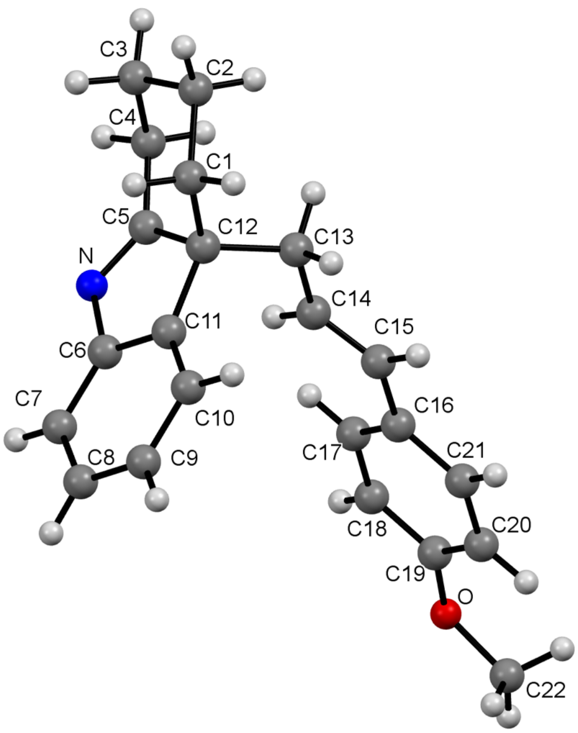


Figure S13. Crystal structure of **3ha**

Cartesian coordinates of critical points

RX

GOp

C	10.298423	9.439151	-0.238560
C	9.063521	10.075325	-0.276167
C	10.373434	8.048615	-0.185164
C	9.201622	7.257021	-0.165348
C	10.451247	5.039400	-0.077872
C	9.238858	5.759314	-0.112185
C	10.477952	3.701940	-0.043629
C	9.295566	2.937371	-0.044506
C	10.496113	0.690081	-0.173844
C	9.308163	1.432095	-0.041896
C	10.493016	-0.647329	-0.176186
C	9.300897	-1.391384	-0.043126
C	10.475735	-3.647477	-0.090985
C	9.289690	-2.890200	-0.050387
C	10.460081	-4.981859	-0.150717
C	9.253833	-5.715497	-0.171571
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C	10.339234	-9.312169	-0.507535
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C	6.648167	9.977207	-0.297636
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C	6.802799	2.839415	0.038727
C	8.087163	0.727652	0.055188
C	6.817829	1.486027	0.108105
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C	6.799868	-5.679823	-0.051956
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C	4.314914	2.852680	0.148882
C	5.551146	0.732656	0.227786
C	4.338250	1.445702	0.276378
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C	4.363221	-1.406921	0.387614
C	5.613804	-3.553350	0.159903
C	4.331775	-2.816930	0.321161
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C	4.354979	-5.652111	0.098149
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C	1.812751	7.042046	-0.159162
C	3.056659	4.948263	-0.009042
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C	3.090623	3.546813	0.120646
C	1.818736	2.810584	0.242226
C	3.073631	0.698057	0.457019
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C	-0.584009	-7.046864	0.082449
C	0.646342	-9.146702	-0.137732
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C	-4.311422	-0.718602	0.359521
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C	-4.337864	-3.578925	0.232679
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C	-6.849503	3.537491	0.052296
C	-8.063248	2.815241	0.034619
C	-6.849004	0.669367	0.152657
C	-8.062530	1.388612	0.069725
C	-6.824090	-0.755031	0.149076
C	-8.031590	-1.486950	0.065361
C	-6.778968	-3.599869	0.052771
C	-8.010264	-2.909116	0.020219
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C	-7.963597	-5.739925	-0.158920
C	-6.685498	-7.831615	-0.256710
C	-7.927807	-7.159072	-0.273130
C	-6.640816	-9.236206	-0.379744
C	-7.824103	-9.964292	-0.507145
C	-9.189265	9.281823	-0.167034
C	-10.330841	10.097945	-0.177073
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2a

O	-1.038166	-0.720021	3.743396
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Int1

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Rx2 C3

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Rx2 N

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Ts2 C3

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Ts2 N

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Pd N

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C	10.784617	1.800946	-0.437454
C	9.838659	4.094052	-0.302991
C	11.105472	4.717059	-0.319736
C	10.114802	6.939393	-0.417188
C	11.238930	6.097977	-0.380379
C	10.229073	8.359221	-0.507424
C	11.453114	9.039084	-0.600029
H	-12.117790	-8.386977	-1.450645
H	-10.097601	-9.776799	-1.382473
H	-11.993875	-5.992202	-1.178529
H	-11.813913	-3.956160	-0.728145
H	-11.591100	-1.678343	-0.517444
H	-11.325118	0.378511	-0.789133
H	-11.060546	2.640965	-0.735665
H	-10.851783	4.635146	-0.281894
H	-10.571728	6.882571	-0.354645
H	-10.314255	8.911710	-0.618051
H	-9.906837	11.270375	-0.757344
H	-7.630243	12.176849	-0.713849
H	-7.697692	-9.982325	-1.167277
H	-5.235683	11.839083	-0.598718
H	-5.316530	-10.226137	-0.993961
H	-2.843684	11.528852	-0.512695
H	-2.911626	-10.505345	-0.870743
H	-0.445573	11.234201	-0.463494
H	-0.489385	-10.783454	-0.790970
H	1.955783	10.955726	-0.452952
H	1.927688	-11.053798	-0.754603
H	4.359198	10.693851	-0.476528
H	4.322362	-11.339634	-0.773584
H	6.762744	10.445770	-0.524267
H	6.688563	-11.651809	-0.826218
H	9.142832	10.221161	-0.585998
H	10.251627	-10.769889	-0.797133
H	8.987927	-12.080055	-0.900435
H	10.553950	-8.698440	-0.717676
H	10.858832	-6.388406	-0.545340
H	11.105465	-4.352148	-0.214606
H	11.364988	-2.091989	-0.137286
H	11.548698	-0.089974	-0.562056

H	11.786031	2.156774	-0.610203
H	12.029247	4.167690	-0.262309
H	12.246800	6.479013	-0.388604
H	12.414590	8.554733	-0.624423
H	11.480813	10.120480	-0.665135
O	-0.364817	1.372752	2.632042
H	0.137802	2.203138	2.682196
O	-0.757334	-0.889364	2.721480
C	-0.862094	-2.121277	3.627292
H	-0.353505	-0.091246	3.166782
C	-2.229788	-2.726589	3.453826
C	-2.405202	-4.102343	3.317366
C	-3.688321	-4.635060	3.198903
C	-4.797437	-3.796549	3.215516
C	-4.626519	-2.420072	3.370780
C	-3.349856	-1.889504	3.496977
H	-1.549515	-4.769255	3.302612
H	-3.815605	-5.705635	3.078657
H	-5.794131	-4.210853	3.106215
H	-5.488932	-1.761674	3.386300
H	-3.214437	-0.814726	3.593607
C	0.325801	-3.017694	3.506487
H	0.303974	-3.782203	2.739460
C	1.365620	-2.909638	4.329359
H	1.402641	-2.160003	5.116288
H	2.218358	-3.575388	4.248181
H	-0.814367	-1.595525	4.587134

Rx2 2d

C	-9.994307	-9.510178	-1.332269
C	-8.742201	-10.113715	-1.328877
C	-10.111287	-8.128661	-1.190728
C	-8.965950	-7.314431	-1.033713
C	-10.280458	-5.142372	-0.836406
C	-9.047873	-5.825271	-0.882084
C	-10.345202	-3.809419	-0.740798
C	-9.184615	-3.013591	-0.685566
C	-10.444667	-0.803054	-0.810044
C	-9.240727	-1.511646	-0.641303
C	-10.485902	0.532175	-0.767051
C	-9.327773	1.306136	-0.547133
C	-10.589926	3.512876	-0.469431
C	-9.374813	2.801778	-0.484909
C	-10.626694	4.848889	-0.481936
C	-9.449505	5.628830	-0.505290
C	-10.684062	7.797382	-0.672320
C	-9.478526	7.055749	-0.572129
C	-10.672674	9.189713	-0.738593

C	-9.471787	9.886497	-0.715038
C	-7.586736	-9.336900	-1.186063
C	-6.332132	-9.955640	-1.198411
C	-7.690528	-7.929498	-1.037073
C	-6.516954	-7.152364	-0.897128
C	-7.851562	-5.077625	-0.766933
C	-6.597931	-5.743588	-0.758841
C	-7.930017	-3.660104	-0.659333
C	-6.698771	-2.850788	-0.504275
C	-8.045305	-0.774746	-0.479649
C	-6.753238	-1.497098	-0.402362
C	-8.080925	0.649267	-0.433192
C	-6.890491	1.412099	-0.304690
C	-8.166033	3.526414	-0.422278
C	-6.931278	2.841004	-0.323452
C	-8.201503	4.949827	-0.444705
C	-6.995937	5.684684	-0.408779
C	-8.254318	7.777578	-0.555259
C	-7.021628	7.094212	-0.469131
C	-8.260154	9.194744	-0.627354
C	-7.056183	9.908031	-0.617897
C	-5.164325	-9.199982	-1.063834
C	-3.913411	-9.837864	-1.096514
C	-5.253140	-7.798719	-0.906115
C	-4.003781	-7.008083	-0.754305
C	-5.342393	-4.959984	-0.595952
C	-4.087965	-5.613044	-0.586185
C	-5.400162	-3.560826	-0.456631
C	-4.223793	-2.829667	-0.272512
C	-5.515353	-0.702231	-0.223302
C	-4.284131	-1.367961	-0.124674
C	-5.579590	0.705341	-0.169337
C	-4.401509	1.451782	-0.013227
C	-5.737225	3.600398	-0.241102
C	-4.440457	2.917814	-0.080674
C	-5.761253	5.009985	-0.307212
C	-4.550640	5.747911	-0.275816
C	-5.809778	7.826499	-0.454713
C	-4.573397	7.152229	-0.365150
C	-5.833351	9.236238	-0.536253
C	-4.633606	9.960114	-0.543682
C	-2.726344	-9.106238	-0.975636
C	-1.478145	-9.746810	-1.040983
C	-2.795745	-7.632640	-0.786901
C	-1.597509	-6.897915	-0.656909
C	-2.906072	-4.863137	-0.415858
C	-1.652671	-5.508551	-0.454255
C	-2.985195	-3.474753	-0.233296

C	-1.753393	-2.692400	0.015718
C	-3.036519	-0.618112	0.145002
C	-1.845358	-1.316316	0.285876
C	-3.097738	0.778625	0.194679
C	-1.957515	1.542507	0.347383
C	-3.243187	3.645009	-0.027636
C	-1.961321	2.930813	0.162677
C	-3.243206	5.043804	-0.153121
C	-2.077289	5.748456	-0.173889
C	-3.365368	7.888573	-0.376863
C	-2.120681	7.225675	-0.306083
C	-3.401991	9.297463	-0.473776
C	-2.206469	10.028130	-0.508301
C	-0.286097	-9.013752	-0.942116
C	0.961560	-9.646467	-1.038402
C	-0.345965	-7.543533	-0.742689
C	0.848234	-6.793306	-0.668321
C	-0.459257	-4.772264	-0.329875
C	0.790749	-5.400963	-0.473960
C	-0.522369	-3.322259	-0.061485
C	0.668200	-2.578153	-0.017309
C	-0.614001	-0.639646	0.800652
C	0.651112	-1.216602	0.229863
C	-0.666933	0.937787	0.854387
C	0.552108	1.625741	0.280648
C	-0.774658	3.641460	0.102511
C	0.473713	2.993033	0.109036
C	-0.819774	5.101844	-0.090521
C	0.392252	5.821854	-0.200161
C	-0.919548	7.963759	-0.360224
C	0.329993	7.303809	-0.325784
C	-0.968703	9.372185	-0.461630
C	0.220406	10.109232	-0.522935
C	2.152438	-8.905040	-0.974975
C	3.395551	-9.539083	-1.084110
C	2.100583	-7.427909	-0.799181
C	3.252136	-6.706124	-0.773965
C	1.987663	-4.649821	-0.454987
C	3.224418	-5.305848	-0.619868
C	1.958905	-3.254444	-0.280719
C	3.148525	-2.506286	-0.310105
C	1.809938	-0.431519	0.082602
C	3.105167	-1.105905	-0.171398
C	1.763268	0.948231	0.109753
C	2.998896	1.744077	-0.104710
C	1.713571	3.782635	-0.101773
C	2.920215	3.152504	-0.170561
C	1.605477	5.190725	-0.208041

C	2.852014	5.993518	-0.340042
C	1.522766	8.050501	-0.412053
C	2.776171	7.398038	-0.419487
C	1.461897	9.460093	-0.504450
C	2.643412	10.206020	-0.586370
C	4.588919	-8.800393	-1.051932
C	5.818620	-9.455918	-1.163141
C	4.559486	-7.395937	-0.913011
C	5.763949	-6.651230	-0.905144
C	4.424301	-4.558504	-0.626289
C	5.737222	-5.244205	-0.778797
C	4.377284	-3.161329	-0.487981
C	5.625728	-2.372389	-0.527533
C	4.279768	-0.335970	-0.272665
C	5.578163	-1.024820	-0.440458
C	4.233507	1.074876	-0.243543
C	5.492095	1.862962	-0.382941
C	4.174580	3.938769	-0.327753
C	5.425563	3.279404	-0.403946
C	4.106567	5.345024	-0.384358
C	5.292149	6.104315	-0.488098
C	3.960719	8.157517	-0.518375
C	5.218064	7.512113	-0.546964
C	3.888440	9.565732	-0.594229
C	5.062608	10.318624	-0.684418
C	7.017650	-8.731426	-1.143933
C	8.234158	-9.406950	-1.248677
C	6.998006	-7.325308	-1.023120
C	8.210265	-6.600709	-1.015579
C	6.946084	-4.497400	-0.793176
C	8.183063	-5.181115	-0.915963
C	6.919649	-3.079582	-0.678379
C	8.104856	-2.314399	-0.724723
C	6.818313	-0.218963	-0.513832
C	8.054186	-0.892379	-0.645713
C	6.744977	1.202010	-0.488044
C	7.928630	1.974778	-0.559379
C	6.613287	4.043579	-0.500237
C	7.864765	3.394405	-0.551838
C	6.548579	5.457416	-0.532770
C	7.735628	6.225355	-0.623743
C	6.397623	8.280019	-0.643734
C	7.658826	7.646027	-0.680944
C	6.311913	9.686723	-0.708199
C	7.473368	10.454220	-0.797895
C	9.454146	-8.717691	-1.232356
C	10.621742	-9.486351	-1.354790
C	9.449977	-7.296528	-1.106177

C	10.638110	-6.545670	-1.051312
C	9.395578	-4.454160	-0.927680
C	10.610496	-5.160636	-0.958199
C	9.350510	-2.958989	-0.882923
C	10.505483	-2.168640	-1.041575
C	9.250310	-0.150789	-0.730686
C	10.457557	-0.835413	-0.971235
C	9.188028	1.338548	-0.624486
C	10.349432	2.126788	-0.556441
C	9.063360	4.155789	-0.593845
C	10.292405	3.459818	-0.542410
C	8.997367	5.578905	-0.662137
C	10.150841	6.381472	-0.797951
C	8.839851	8.432939	-0.783509
C	10.074291	7.766715	-0.850502
C	8.739931	9.855844	-0.831534
C	9.847573	10.714191	-0.906510
H	-10.883334	-10.117465	-1.450032
H	-8.676873	-11.189510	-1.443634
H	-11.109859	-7.726750	-1.215345
H	-11.221114	-5.666054	-0.873021
H	-11.331472	-3.377250	-0.697842
H	-11.377131	-1.306841	-1.005248
H	-11.448998	0.985318	-0.934612
H	-11.541552	3.008482	-0.433568
H	-11.609083	5.288955	-0.465282
H	-11.656058	7.337747	-0.714364
H	-11.606392	9.733491	-0.814534
H	-9.490351	10.968865	-0.771261
H	-6.264984	-11.032056	-1.318734
H	-7.071428	10.991400	-0.679086
H	-3.863746	-10.913639	-1.228441
H	-4.658360	11.042595	-0.614038
H	-1.434248	-10.821015	-1.184522
H	-2.239334	11.109872	-0.585537
H	1.006480	-10.721262	-1.177066
H	0.179460	11.190874	-0.598560
H	3.435361	-10.616617	-1.203263
H	2.593702	11.287922	-0.652915
H	5.843212	-10.535957	-1.264914
H	5.003799	11.400772	-0.739943
H	8.228622	-10.488454	-1.345079
H	7.387400	11.535809	-0.840415
H	11.616828	-9.075575	-1.381607
H	10.566151	-10.564729	-1.446425
H	11.613812	-7.002446	-1.070004
H	11.565571	-4.665902	-0.895510
H	11.468845	-2.604847	-1.249339

H	11.385630	-0.311060	-1.132000
H	11.331153	1.685069	-0.496297
H	11.240946	3.963982	-0.471631
H	11.141542	5.972595	-0.894768
H	11.009046	8.291280	-0.960910
H	10.871765	10.381788	-0.917081
H	9.712133	11.788781	-0.943865
O	-0.647646	1.288999	2.272000
O	-0.454241	-1.050964	2.305213
C	-1.267111	-2.035166	3.127357
H	-0.087282	2.076363	2.379519
C	-0.637747	-2.013965	4.482704
C	-2.734204	-1.698576	3.154434
H	-1.082624	-2.984807	2.622815
C	-3.651014	-2.739886	3.001648
C	-5.017999	-2.484710	3.047737
C	-5.475133	-1.182690	3.241769
C	-4.561277	-0.145415	3.416554
C	-3.193527	-0.401818	3.388086
H	-3.292615	-3.752269	2.828940
H	-5.723338	-3.297870	2.913046
H	-4.914014	0.868983	3.572316
H	-2.495054	0.422285	3.506298
C	-0.139541	-3.113494	5.041678
H	-0.685627	-1.072926	5.030047
H	0.247888	-3.104506	6.054003
H	-0.115492	-4.062982	4.512055
N	2.334508	-2.190045	3.069569
H	1.805652	-2.190218	2.209630
H	-0.335297	-0.163789	2.773827
C	2.429482	-1.103140	3.904677
C	2.674141	-3.339174	3.765177
C	3.044597	-3.005706	5.042295
C	2.888331	-1.576524	5.154752
C	3.077455	-0.662449	6.200609
C	2.170880	0.250688	3.672188
C	2.357678	1.131741	4.728235
C	2.802099	0.679272	5.983267
H	3.438343	-1.000427	7.167787
H	2.946141	1.395772	6.784661
H	2.181339	2.193082	4.577650
H	1.881465	0.601447	2.686121
C	2.617377	-4.659527	3.070451
H	2.726730	-5.481215	3.779484
H	1.658254	-4.788228	2.551270
H	3.412291	-4.752150	2.322628
C	3.529593	-3.911826	6.129941
H	3.486820	-4.962043	5.830868

H	4.566557	-3.687303	6.400676
H	2.925932	-3.798354	7.037446
H	-6.540315	-0.977962	3.257071

Ts2 2d

C	-10.266370	-9.176630	-1.412087
C	-9.036009	-9.822829	-1.391872
C	-10.337743	-7.791819	-1.270959
C	-9.167414	-7.017302	-1.097620
C	-10.408501	-4.800482	-0.919543
C	-9.199861	-5.525869	-0.947407
C	-10.428192	-3.465667	-0.826954
C	-9.241559	-2.710400	-0.757343
C	-10.420735	-0.457103	-0.909812
C	-9.245777	-1.206997	-0.717923
C	-10.415862	0.879088	-0.869520
C	-9.235530	1.612511	-0.629361
C	-10.420829	3.861433	-0.567294
C	-9.231134	3.108913	-0.568109
C	-10.411054	5.197942	-0.582245
C	-9.207213	5.936612	-0.593682
C	-10.363267	8.145968	-0.783383
C	-9.185680	7.363380	-0.665176
C	-10.302617	9.536795	-0.854377
C	-9.078704	10.191592	-0.817810
C	-7.856848	-9.086141	-1.232469
C	-6.624477	-9.747656	-1.229032
C	-7.914123	-7.675943	-1.083823
C	-6.716566	-6.939633	-0.928217
C	-7.980142	-4.819871	-0.816297
C	-6.750729	-5.528772	-0.791012
C	-8.010976	-3.400139	-0.711705
C	-6.754790	-2.633483	-0.541705
C	-8.028143	-0.511665	-0.539201
C	-6.763529	-1.278260	-0.443507
C	-8.014481	0.912979	-0.495685
C	-6.800078	1.634629	-0.352274
C	-7.998932	3.791463	-0.490512
C	-6.790325	3.064028	-0.374232
C	-7.984416	5.215077	-0.516017
C	-6.754570	5.907876	-0.466777
C	-7.937471	8.042394	-0.635329
C	-6.730455	7.317118	-0.531705
C	-7.893151	9.458584	-0.712374
C	-6.665512	10.129798	-0.690667
C	-5.433532	-9.032529	-1.079868
C	-4.205453	-9.712977	-1.100020
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C	8.341217	7.020515	-0.580299
C	7.174994	9.169400	-0.581892
C	8.398240	9.835226	-0.664490
C	8.720513	-9.418451	-1.402673
C	9.817468	-10.282224	-1.543843
C	8.838348	-8.004514	-1.253328

C	10.086545	-7.358577	-1.198081
C	9.027154	-5.171985	-1.027749
C	10.177468	-5.978169	-1.081992
C	9.109695	-3.680138	-0.958688
C	10.325212	-2.988736	-1.124772
C	9.251849	-0.878708	-0.755888
C	10.392312	-1.658205	-1.030494
C	9.319275	0.607006	-0.621434
C	10.545211	1.289812	-0.550609
C	9.439447	3.422116	-0.545226
C	10.604081	2.622003	-0.514809
C	9.496474	4.846115	-0.593240
C	10.714553	5.547851	-0.724142
C	9.585499	7.703975	-0.677989
C	10.757694	6.934914	-0.758503
C	9.608567	9.130576	-0.708528
C	10.786085	9.891056	-0.776524
H	-11.654664	-9.099096	-1.576310
H	-9.546185	-10.352968	-1.572262
H	-11.679513	-6.698313	-1.335414
H	-11.614736	-4.627505	-1.046311
H	-11.528425	-2.336133	-0.878450
H	-11.385725	-0.269858	-1.200292
H	-11.257740	2.021797	-1.131182
H	-11.185080	4.040584	-0.601100
H	-11.055704	6.319122	-0.612941
H	-10.922155	8.366081	-0.844389
H	-10.665897	10.749832	-0.910949
H	-8.452778	11.798346	-0.816942
H	-7.129716	-10.399437	-1.444664
H	-6.043138	11.612091	-0.686578
H	-4.726762	-10.482527	-1.356857
H	-3.636734	11.455679	-0.583428
H	-2.298837	-10.591640	-1.323687
H	-1.222501	11.315893	-0.516961
H	0.138622	-10.694946	-1.330287
H	1.193586	11.190677	-0.495136
H	2.563965	-10.795157	-1.370051
H	3.607378	11.082131	-0.522906
H	4.967574	-10.919568	-1.444639
H	6.018784	10.989431	-0.596302
H	7.347354	-11.075423	-1.538284
H	8.405665	10.920576	-0.694514
H	10.844248	-9.958330	-1.567247
H	9.669378	-11.350192	-1.653132
H	11.019698	-7.895960	-1.235566
H	11.171626	-5.567113	-1.020655
H	11.243903	-3.501546	-1.358754

H	11.358579	-1.211171	-1.200312
H	11.485181	0.763281	-0.506182
H	11.593397	3.040576	-0.445339
H	11.666122	5.056783	-0.830554
H	11.733849	7.378216	-0.866809
H	11.777843	9.471805	-0.793798
H	10.743853	10.973664	-0.801135
O	-0.608903	1.363465	2.261126
O	-0.609994	-1.037891	2.150672
C	-1.855968	-3.371485	4.532288
H	-0.712390	2.329456	2.289860
C	-0.954982	-2.971580	5.436395
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C	-4.027462	-3.232458	3.354699
C	-5.134133	-2.526727	2.892468
C	-5.187576	-1.143168	3.033291
C	-4.126877	-0.469136	3.639880
C	-3.036110	-1.179320	4.127562
H	-3.988573	-4.312404	3.236386
H	-5.953729	-3.057898	2.419109
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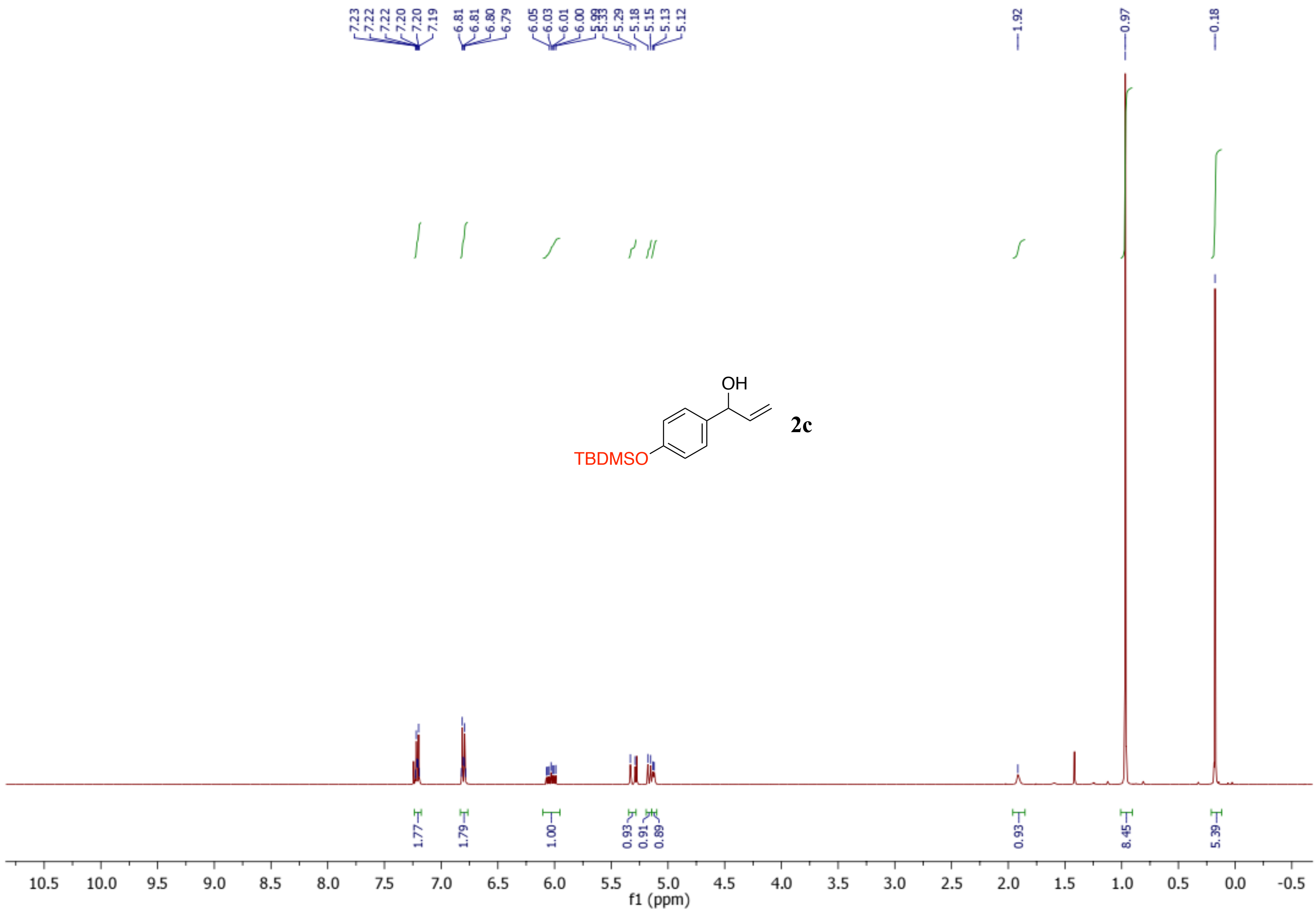
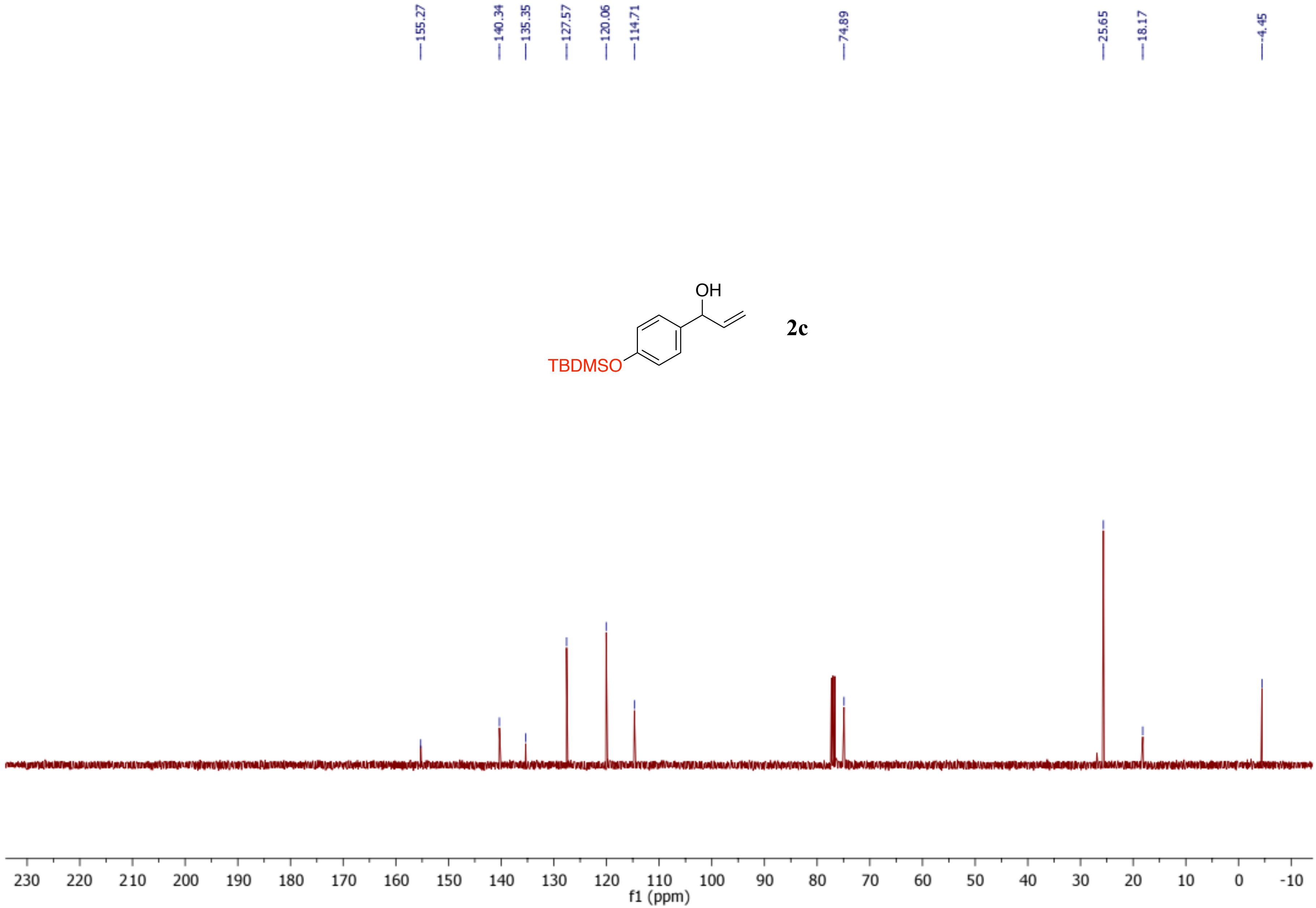
H	-2.224033	-0.644002	4.616347
C	0.172522	-3.839834	5.922617
H	-1.001043	-1.964671	5.846868
H	0.310381	-3.732709	7.004517
H	-0.041163	-4.896802	5.725570
N	1.371003	-2.409029	3.248259
H	1.068257	-2.196997	2.289592
H	-1.277034	-0.533596	2.647903
C	1.647659	-1.386061	4.193605
C	1.340386	-3.584600	3.783158
C	1.556578	-3.481525	5.271372
C	1.826650	-2.002219	5.428831
C	2.113378	-1.222008	6.538258
C	1.720757	-0.020978	3.981529
C	2.012854	0.749090	5.106825
C	2.211387	0.160803	6.359309
H	2.253753	-1.663961	7.520115
H	2.437452	0.792386	7.211673
H	2.081336	1.826827	5.005437
H	1.525101	0.419371	3.009514
C	1.039943	-4.814288	3.009366
H	0.701879	-5.618201	3.664295
H	0.271187	-4.601667	2.260904
H	1.944326	-5.154693	2.491492
C	2.661931	-4.406389	5.787526
H	2.419690	-5.454663	5.588732

H	3.623363	-4.168972	5.325339
H	2.761046	-4.281769	6.868894
H	-6.046118	-0.589208	2.666709

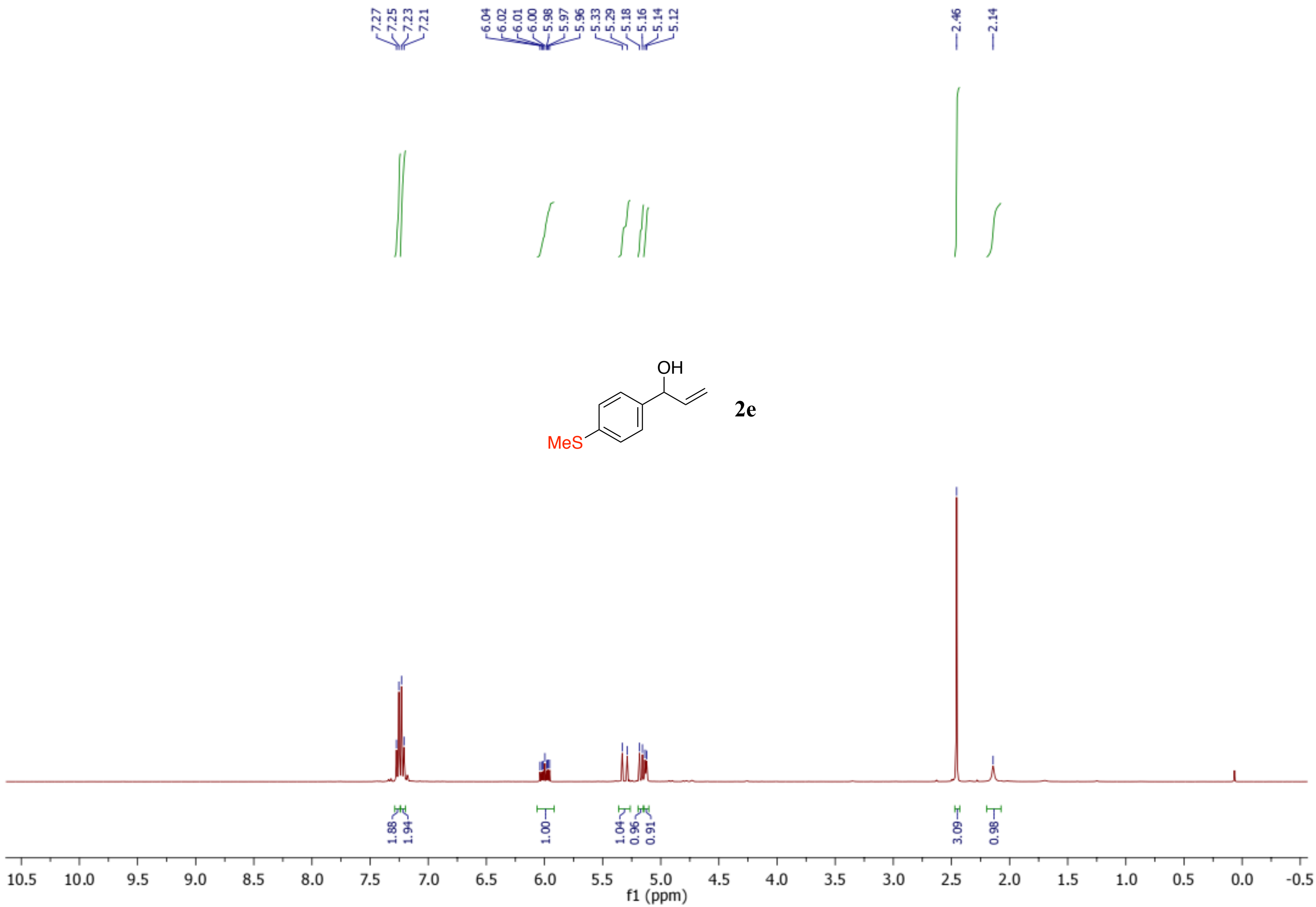
NMR Spectra of new compounds



7.23
7.22
7.22
7.20
7.20
7.19
6.81
6.81
6.80
6.79
6.05
6.03
6.01
6.00
5.99
5.33
5.29
5.18
5.15
5.13
5.12
1.92
0.97
0.18
OH
TBDMSO
2c
1.77
1.79
1.00
0.93
0.91
0.89
0.93
8.45
5.39
10.5 10.0 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 0.0 -0.5
f1 (ppm)



155.27
140.34
135.35
127.57
120.06
114.71
74.89
25.65
18.17
-4.45
OH
TBDMSO
2c
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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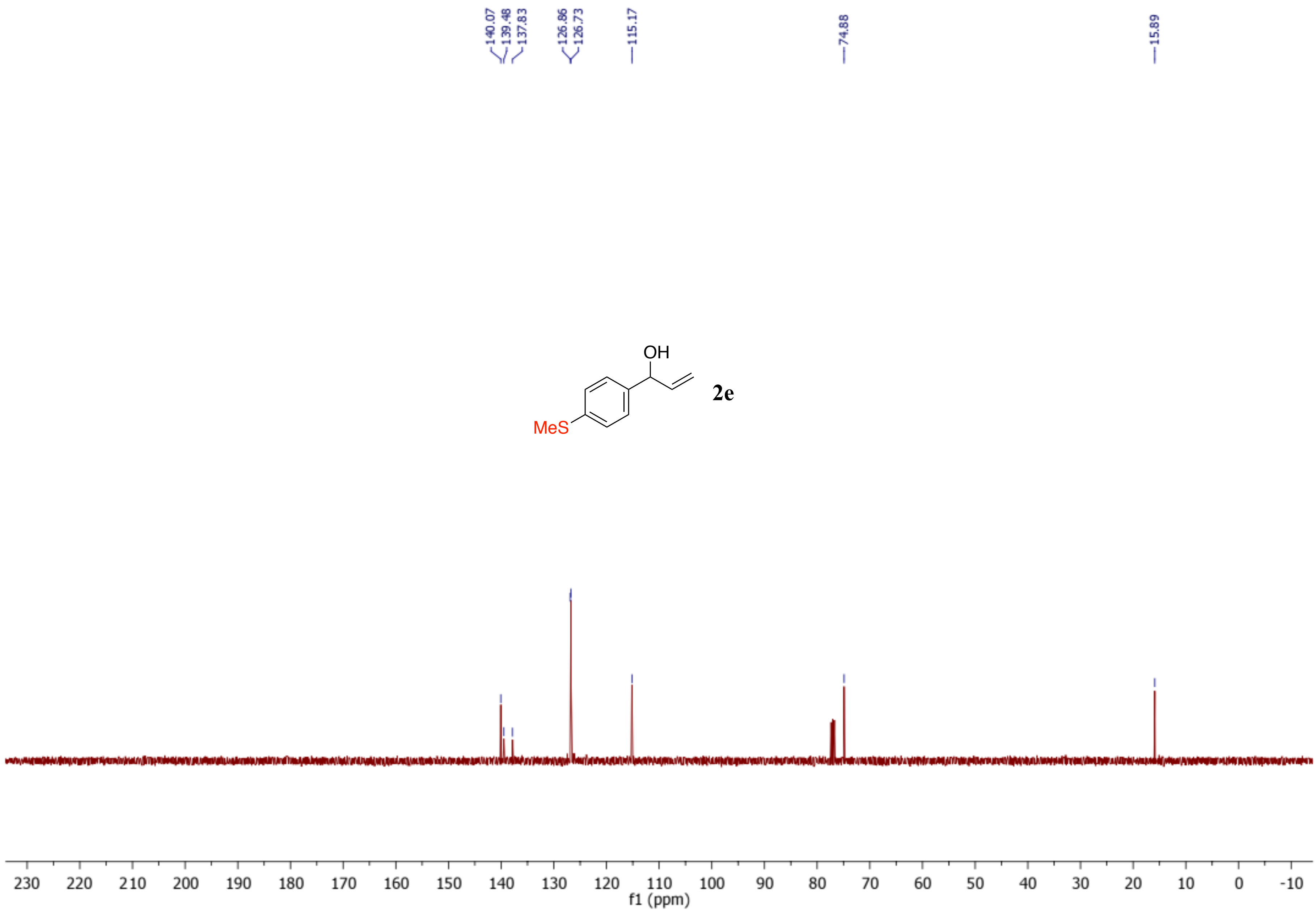
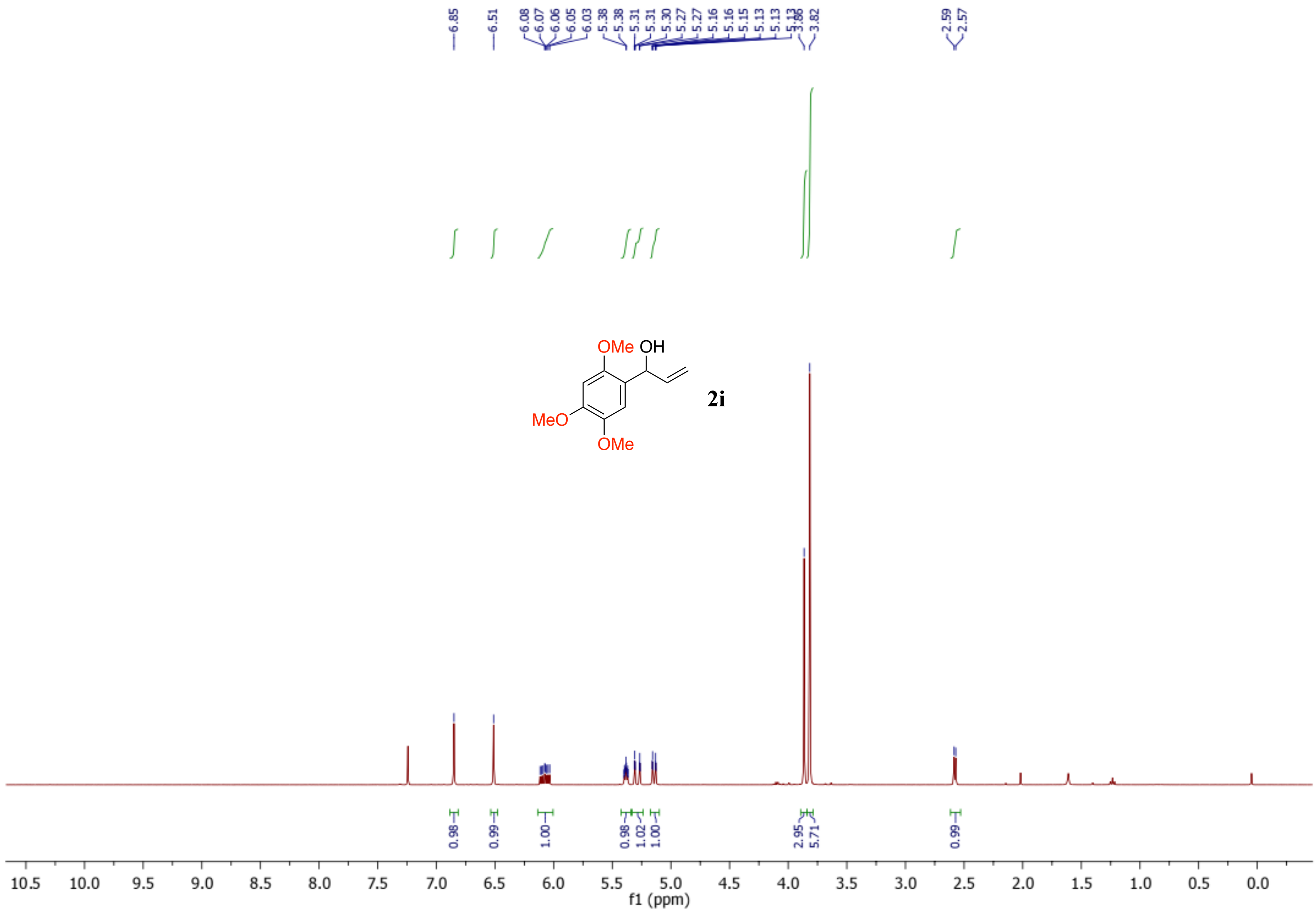
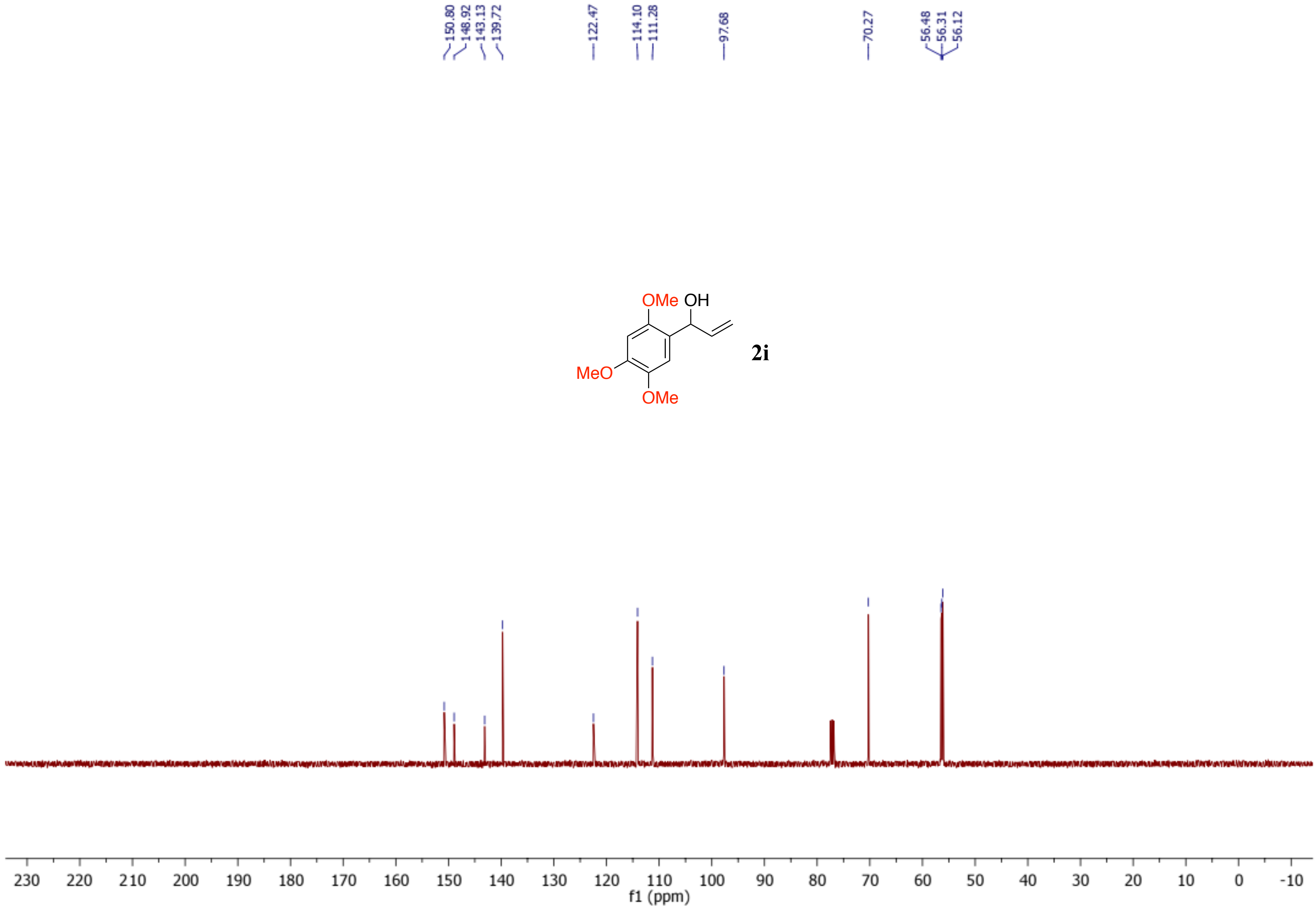
7.25
7.23
7.21
6.04
6.02
6.01
6.00
5.98
5.97
5.96
5.33
5.29
5.18
5.16
5.14
5.12
2.46
2.14
OH
MeS
2e
1.88
1.94
1.00
1.04
0.96
0.91
3.09
0.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

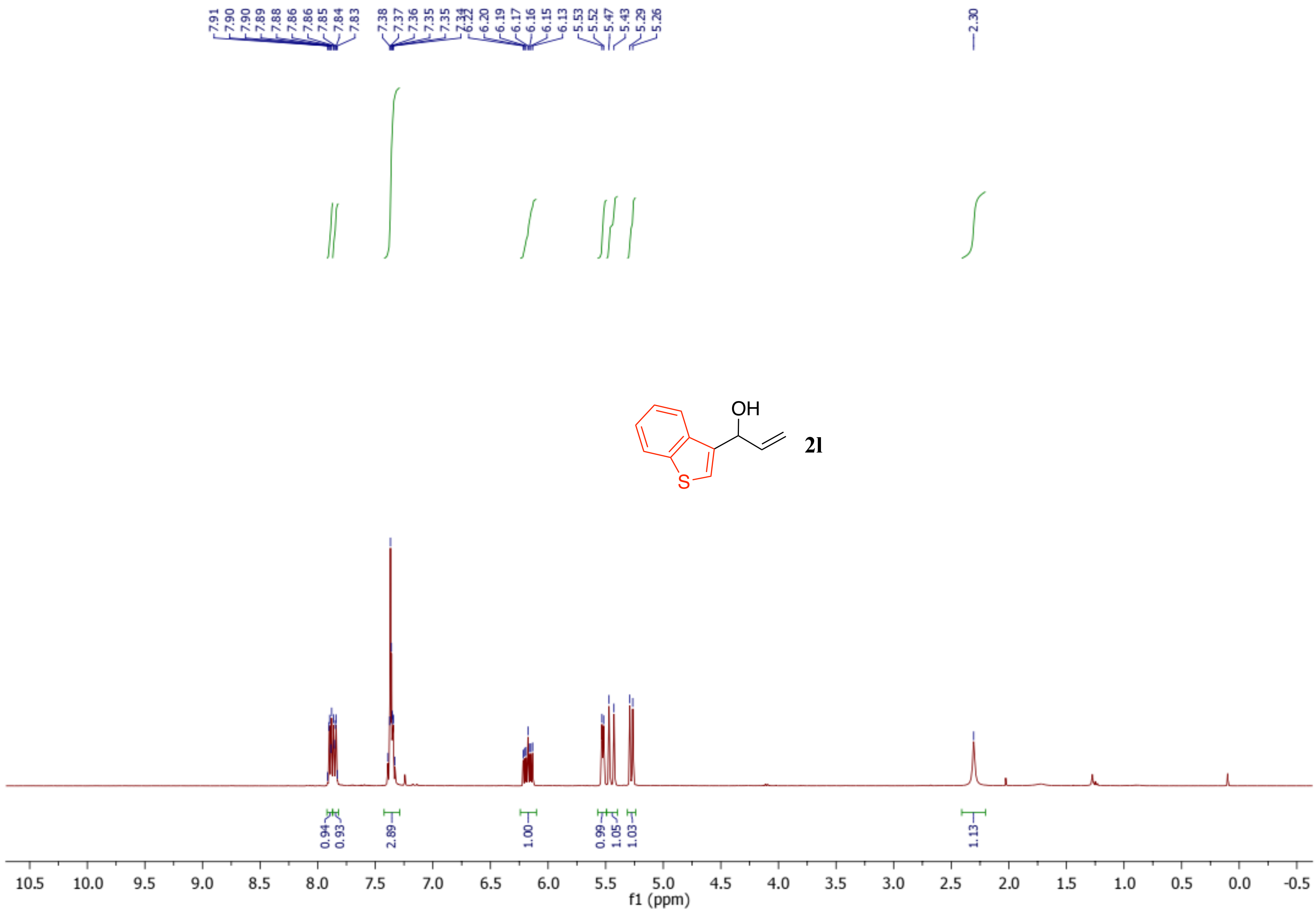

140.07
139.48
137.83
126.86
126.73
115.17
74.88
15.89
OH
MeS
2e
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



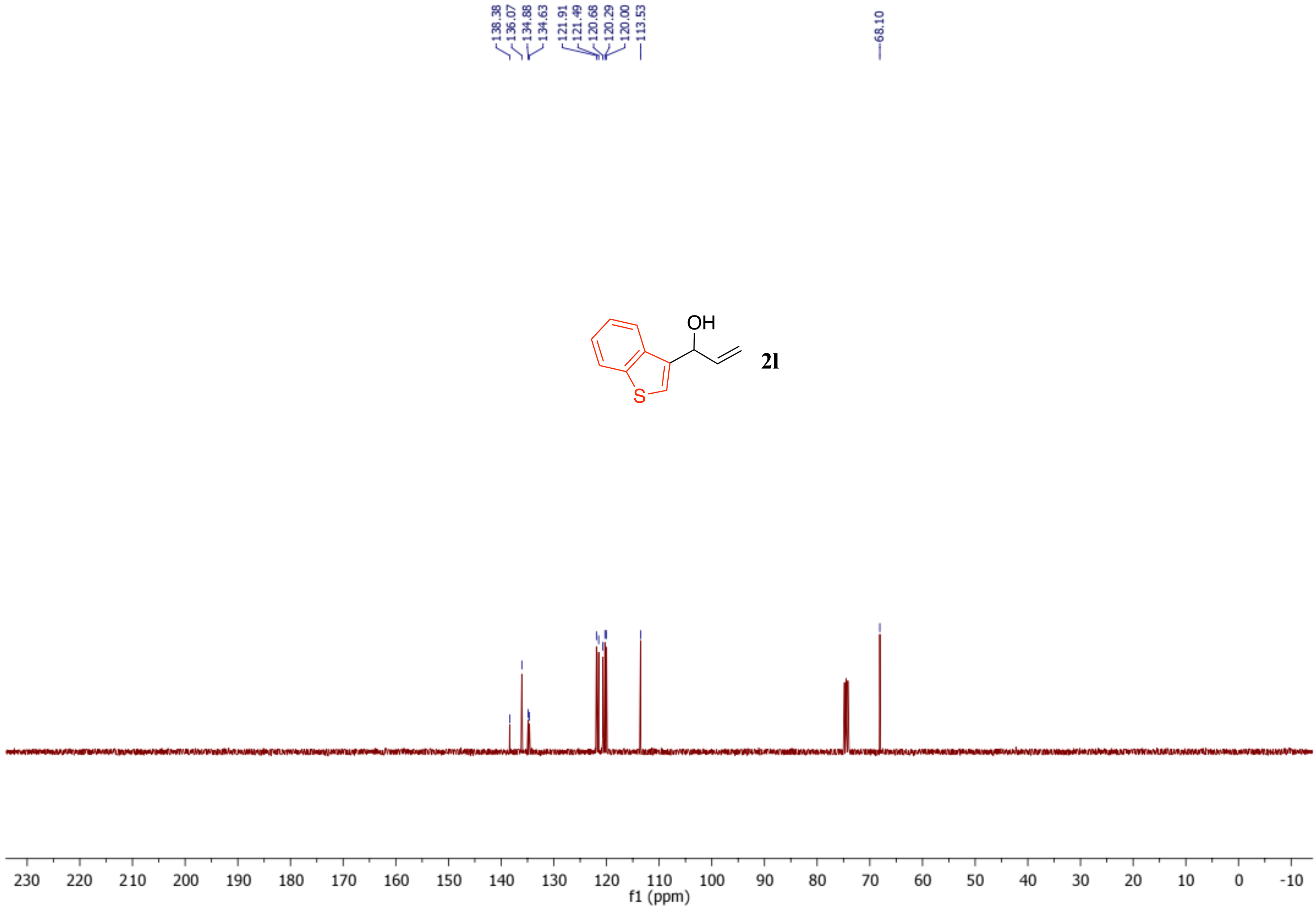
6.85
6.51
6.08
6.07
6.06
6.05
6.03
5.38
5.38
5.31
5.31
5.30
5.27
5.27
5.16
5.16
5.15
5.13
5.13
3.86
3.82
2.59
2.57
OMe
OH
MeO
OMe
0.98
0.99
1.00
0.98
1.02
1.00
2.95
5.71
0.99
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

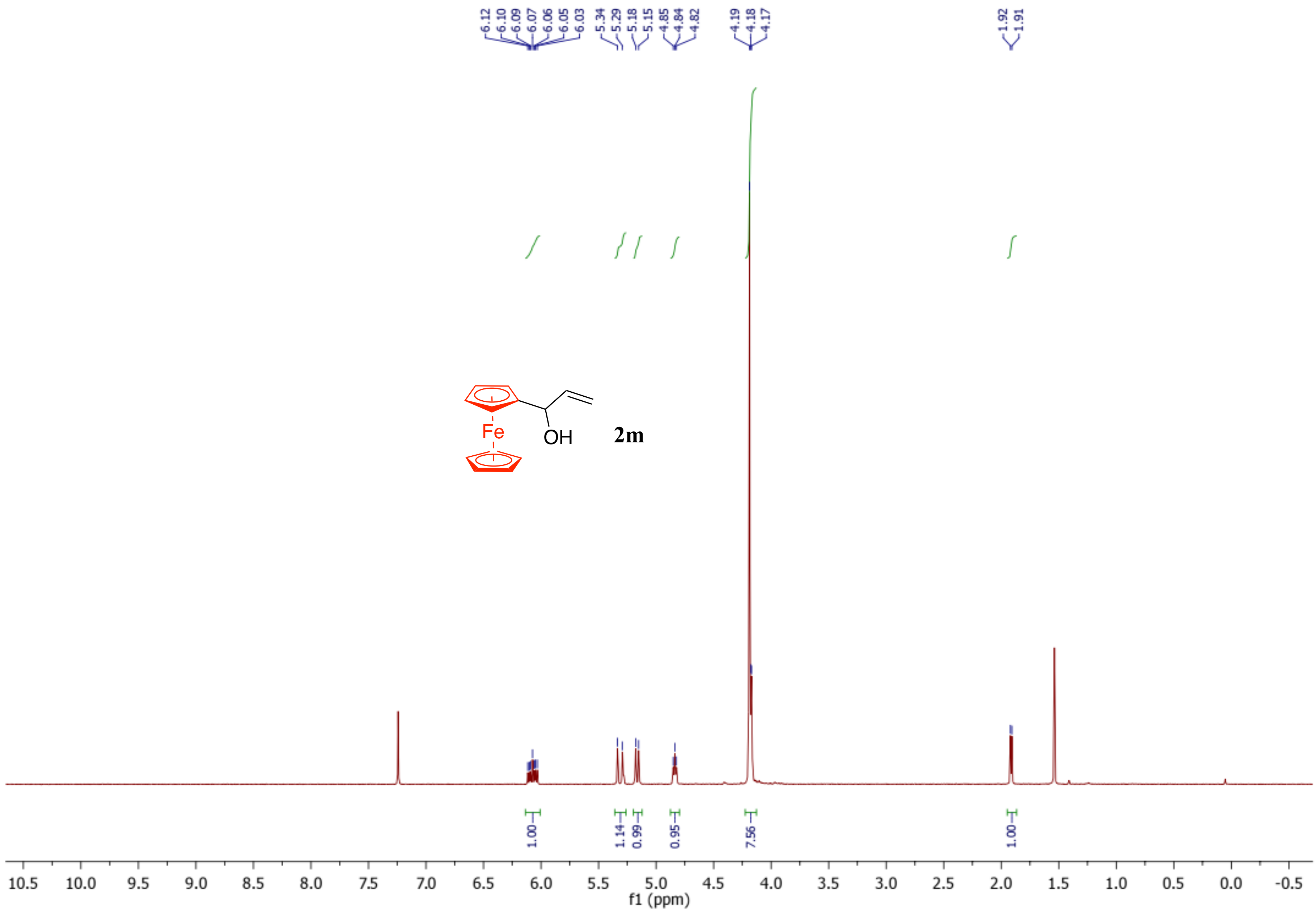
2i

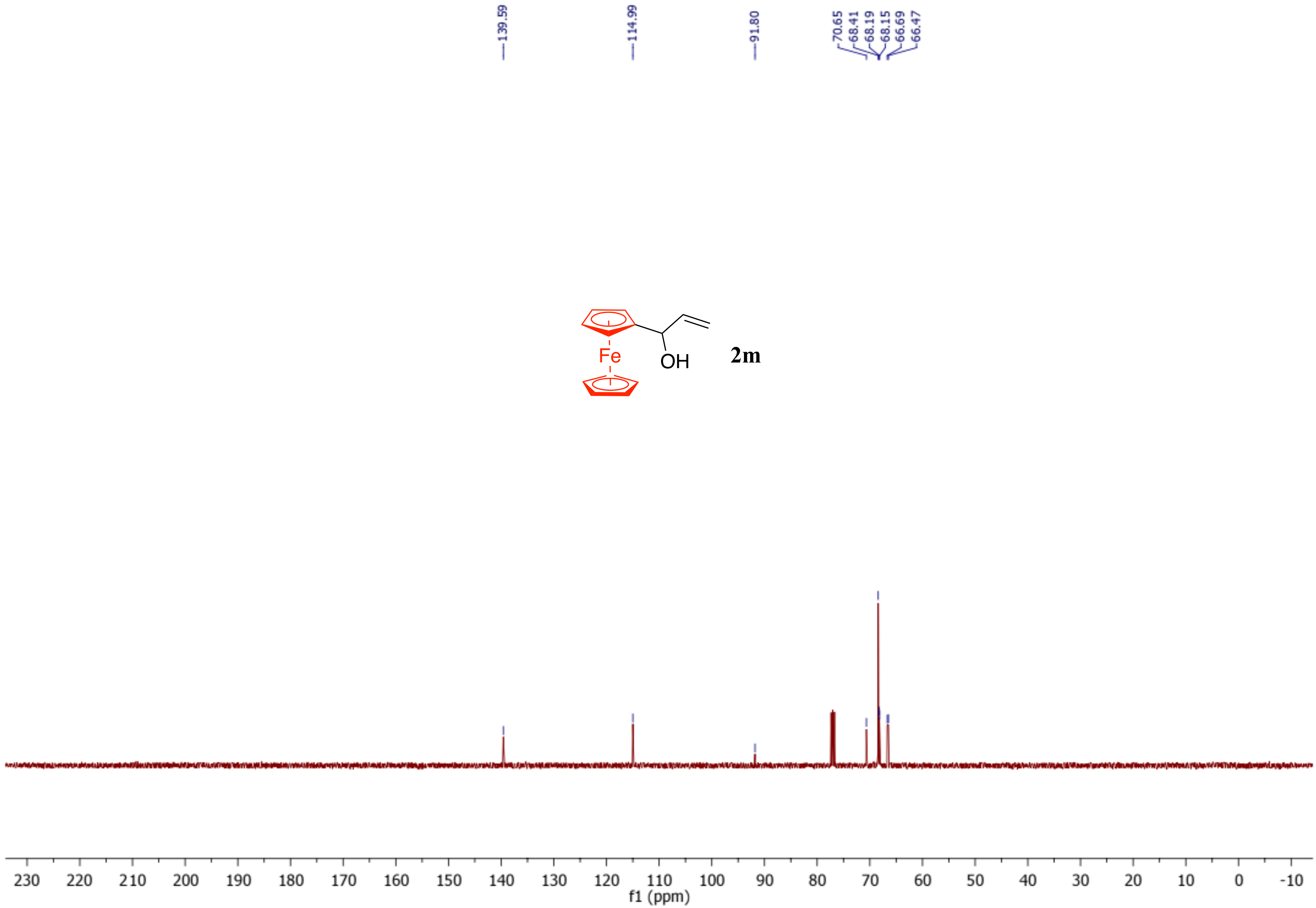

150.80
148.92
143.13
139.72
122.47
114.10
111.28
97.68
70.27
56.48
56.31
56.12
OMe
OH
MeO
OMe
2i
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



7.91
7.90
7.90
7.89
7.88
7.86
7.86
7.85
7.84
7.83
7.38
7.37
7.36
7.35
7.35
7.34
6.22
6.20
6.19
6.17
6.16
6.15
6.13
5.53
5.52
5.47
5.43
5.29
5.26
2.30
OH
S
2l
0.94
0.93
2.89
1.00
0.99
1.05
1.03
1.13
10.5
10.0
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
0.0
-0.5
f1 (ppm)


138.38
136.07
134.88
134.63
121.91
121.49
120.68
120.29
120.00
113.53
68.10
OH
S
2l
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


6.12
6.10
6.09
6.07
6.06
6.05
6.03
5.34
5.29
5.18
5.15
4.85
4.84
4.82
4.19
4.18
4.17
1.92
1.91
Fe
OH
2m
1.00
1.14
0.99
0.95
7.56
1.00
10.5 10.0 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 0.0 -0.5
f1 (ppm)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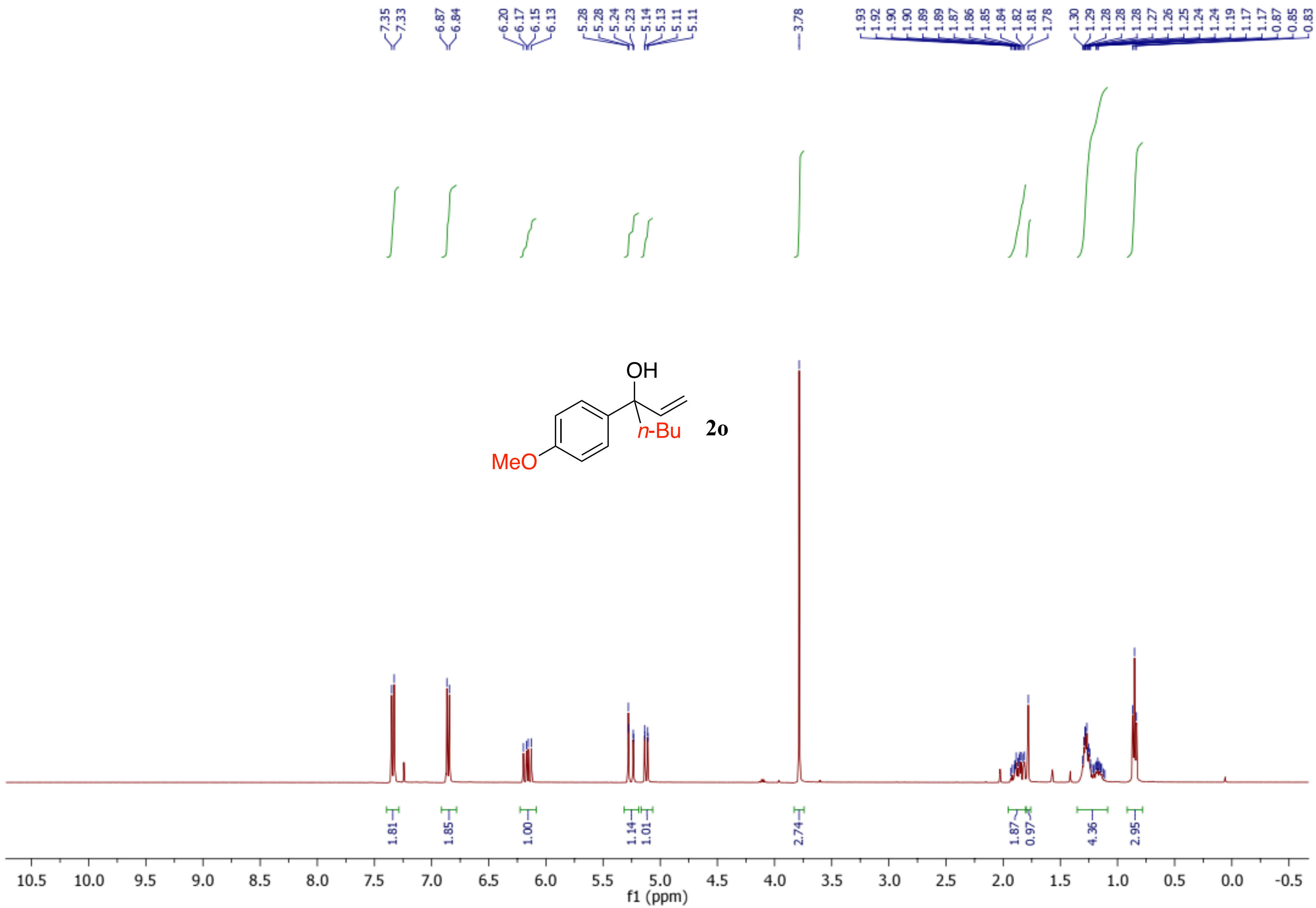
114.99
91.80
70.65
68.41
68.19
68.15
66.69
66.47
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
Fe
OH

2m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7.33
6.87
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6.20
6.17
6.15
6.13
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5.28
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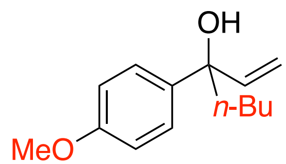
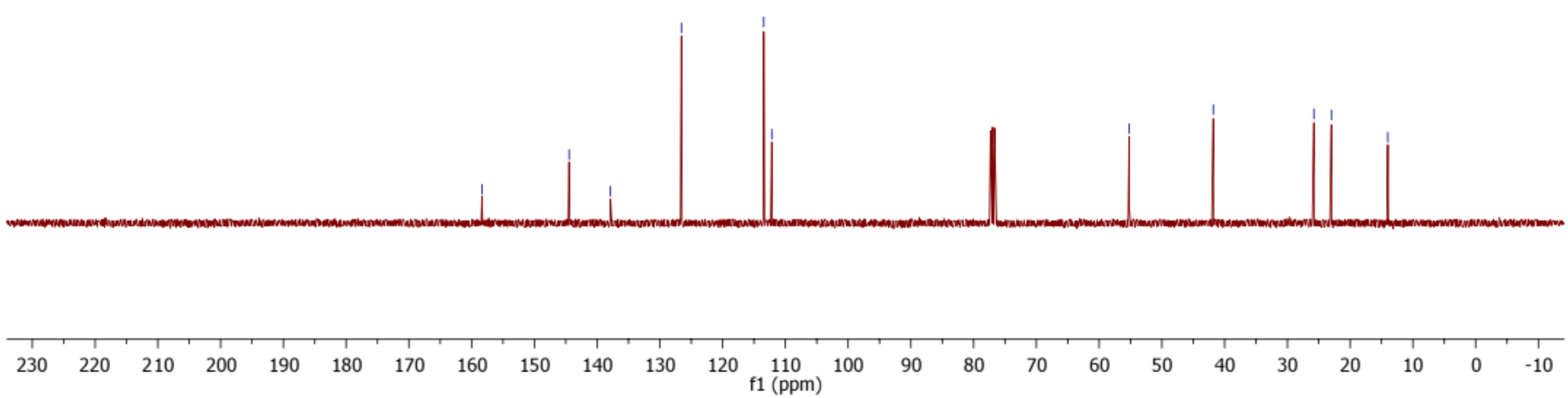
5.23
5.14
5.13
5.11
5.11
3.78
1.93
1.92
1.90
1.89
1.89
1.87
1.86
1.85
1.84
1.82
1.81
1.78
1.30
1.29
1.28
1.28
1.28
1.27
1.26
1.25
1.24
1.24
1.19
1.17
0.87
0.85
0.83
OH
MeO
n-Bu
2o
1.81
1.85
1.00
1.14
1.01
2.74
1.87
0.97
4.36
2.95
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

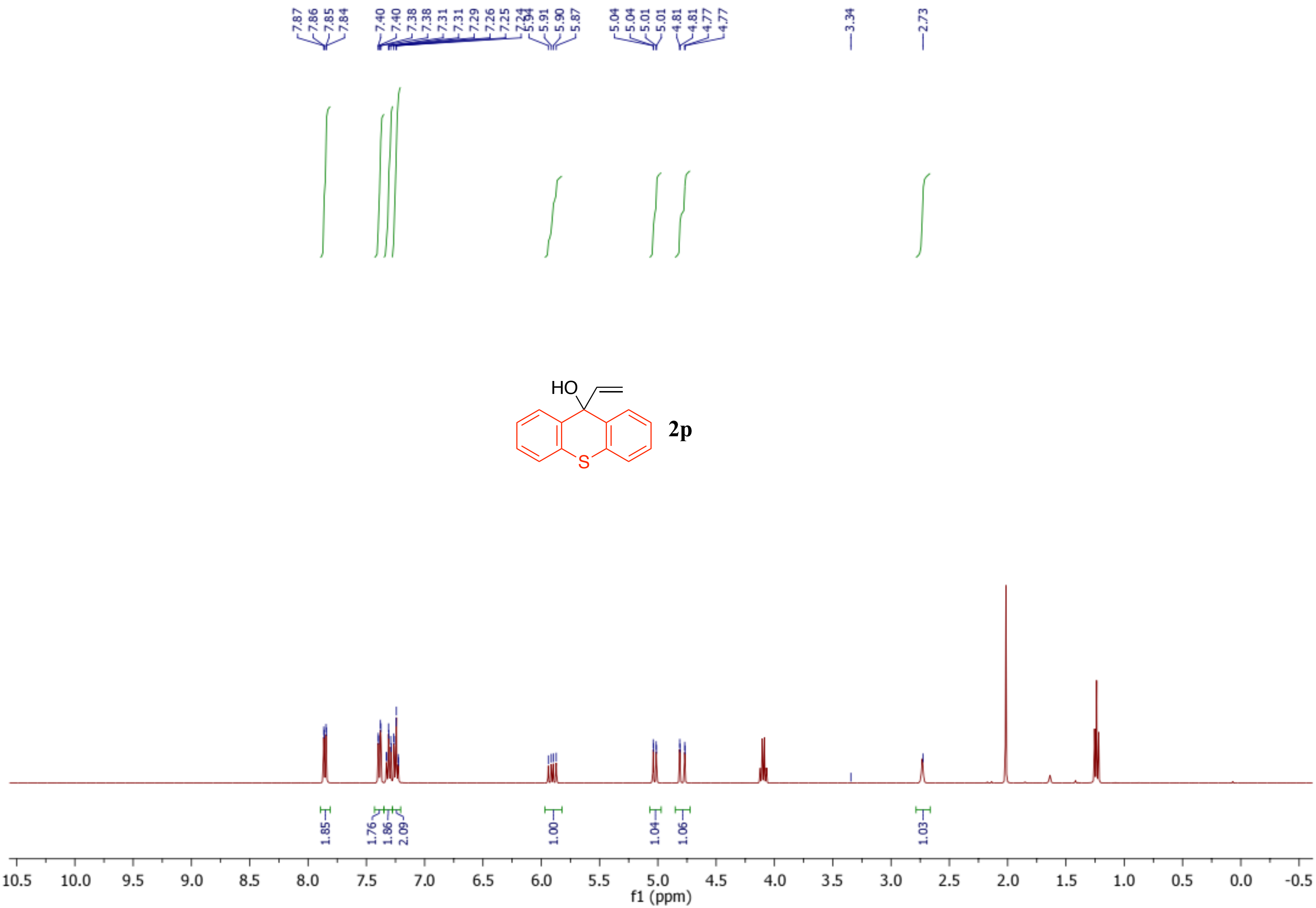


OH
MeO
n-Bu

2o



158.33
144.47
137.87
126.57
113.44
112.17
55.20
41.81
25.78
22.99
14.00
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.85
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7.40
7.38
7.38
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7.29
7.26
7.25
7.24
5.94
5.91
5.90
5.87
5.04
5.04
5.01
5.01
4.81
4.81
4.77
4.77
3.34
2.73
HO
S
2p
1.85
1.76
1.86
2.09
1.00
1.04
1.06
1.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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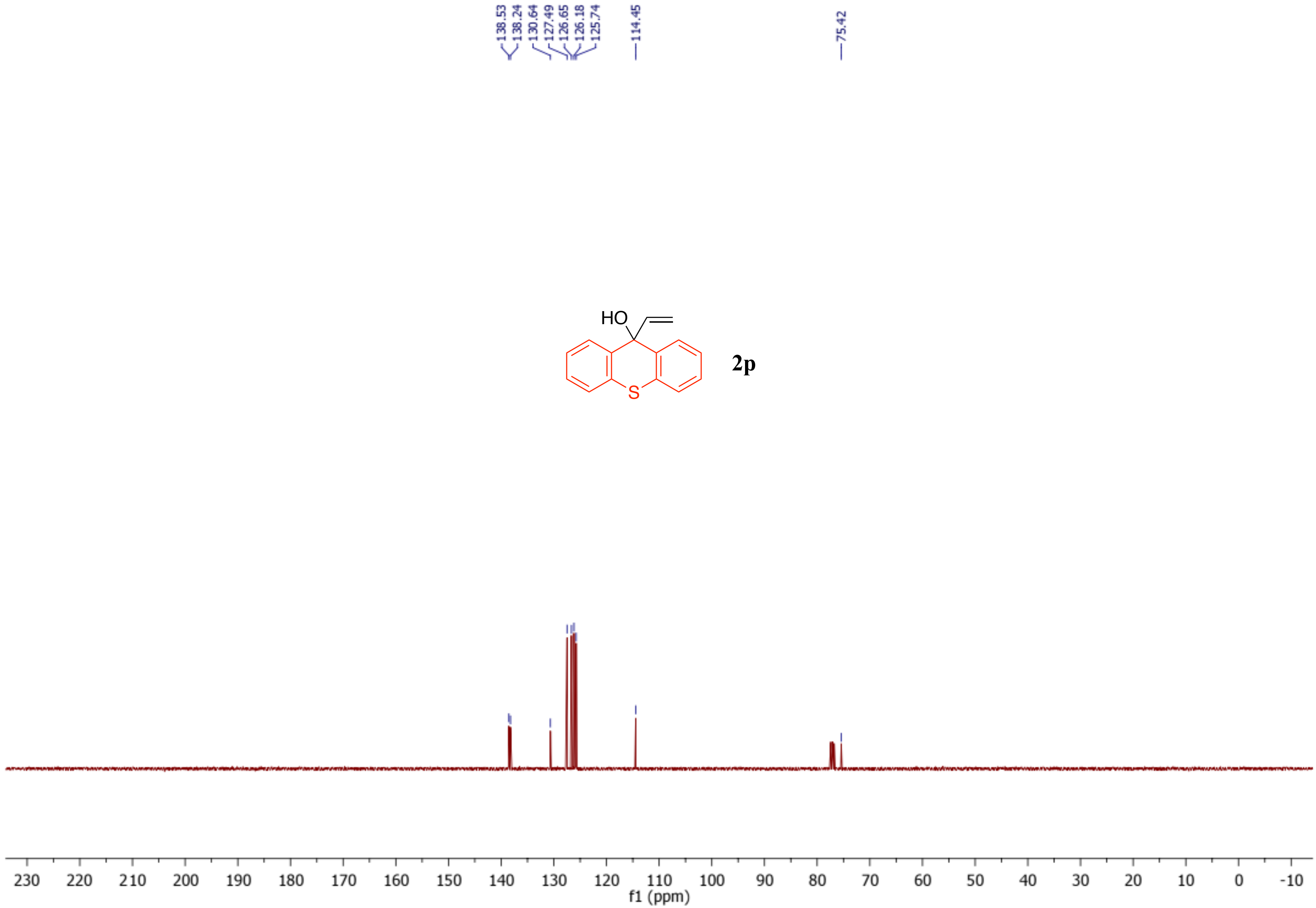
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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126.18
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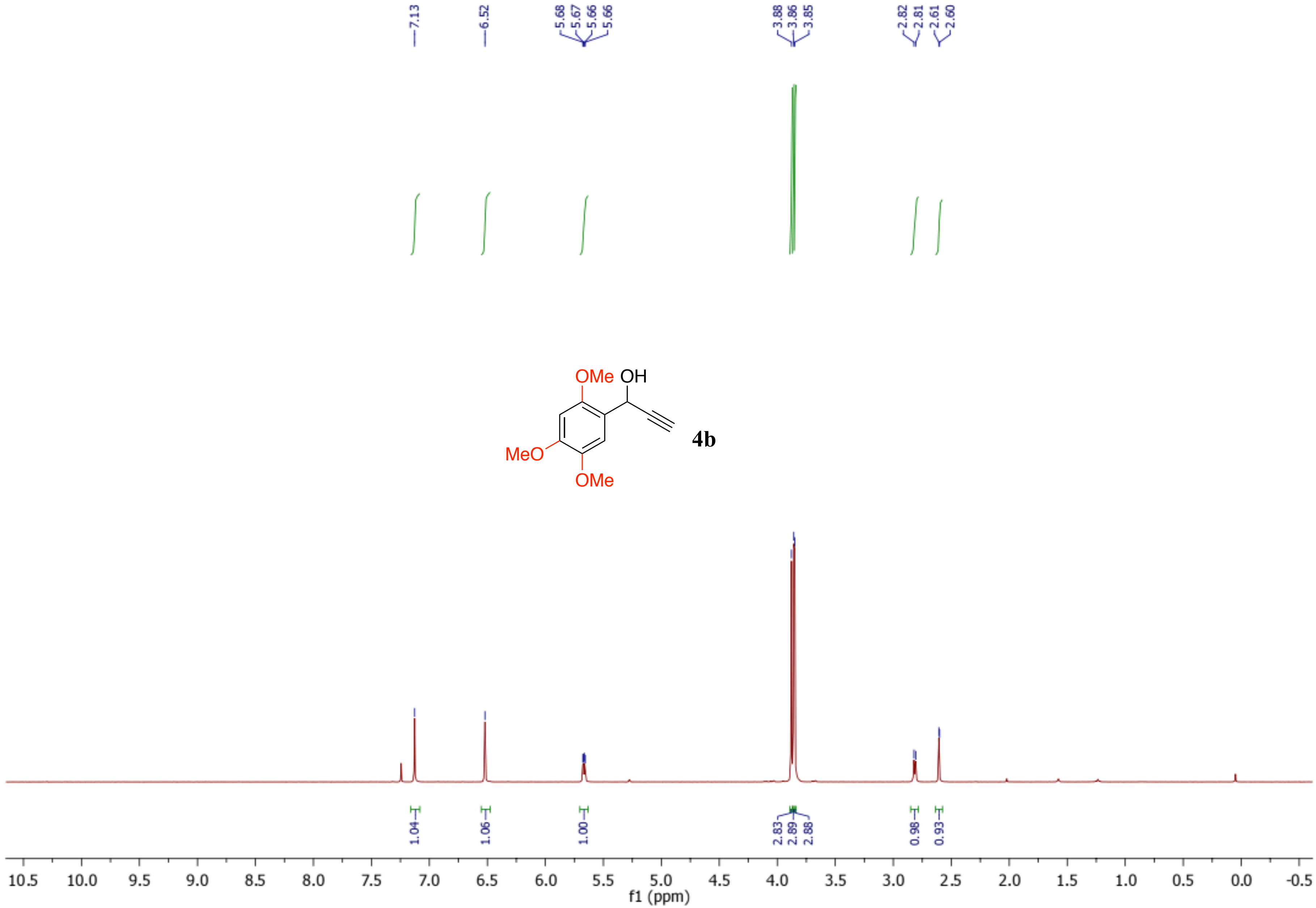
114.45
75.42
HO
S
2p
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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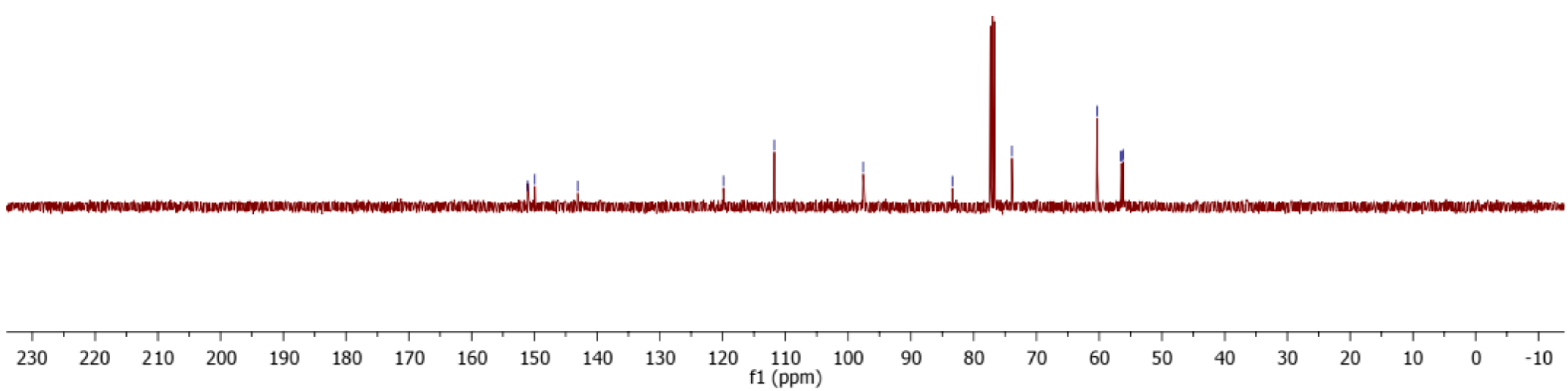
6.52
5.68
5.67
5.66
5.66
3.88
3.86
3.85
2.82
2.81
2.61
2.60
OMe
OH
MeO
OMe
4b
1.04
1.06
1.00
2.83
2.89
2.88
0.98
0.93
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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97.59
83.37
73.92
60.32
56.54
56.44
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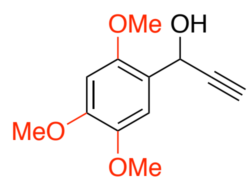
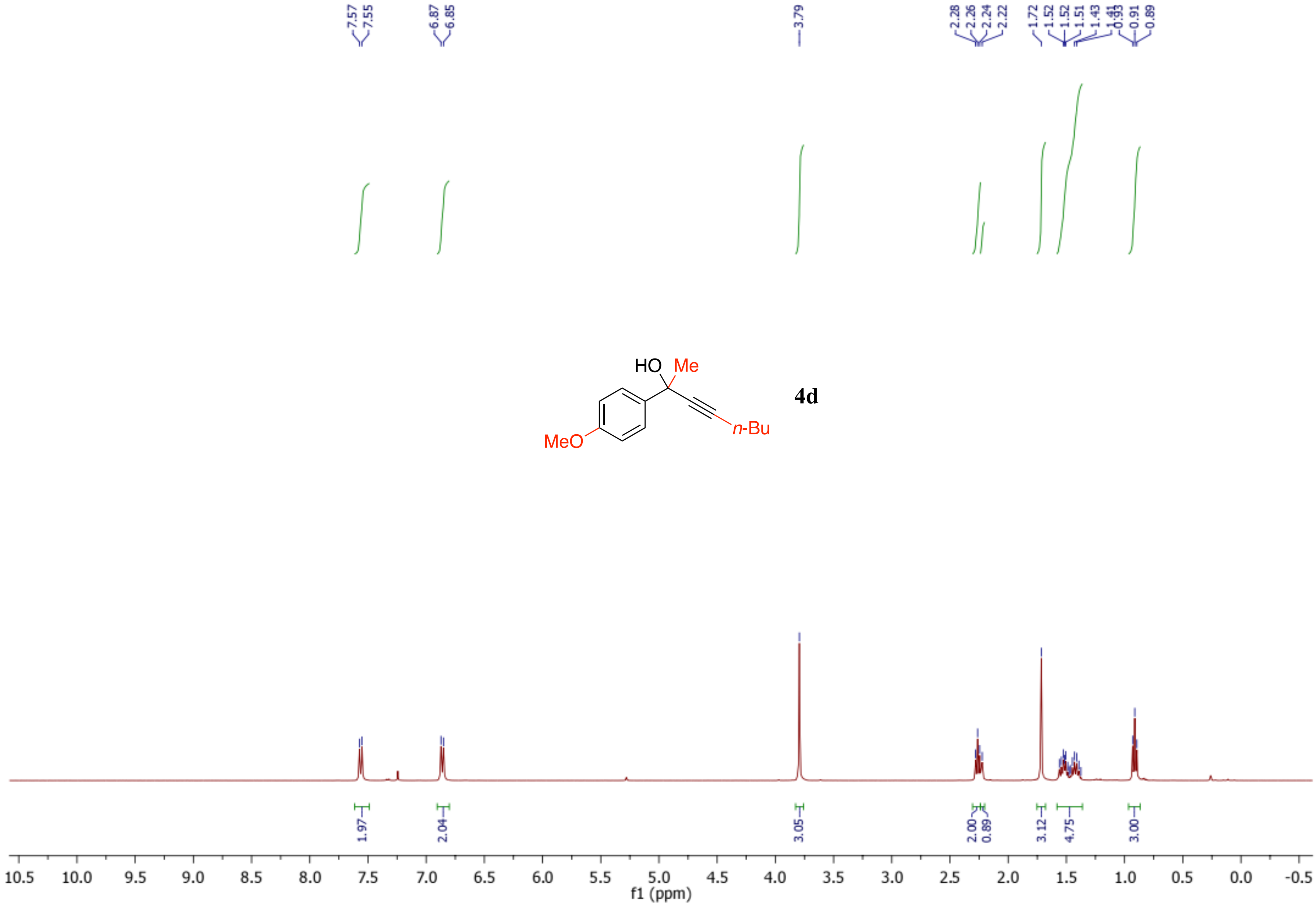
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OMe
OH
MeO
OMe

4b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2.24
2.22
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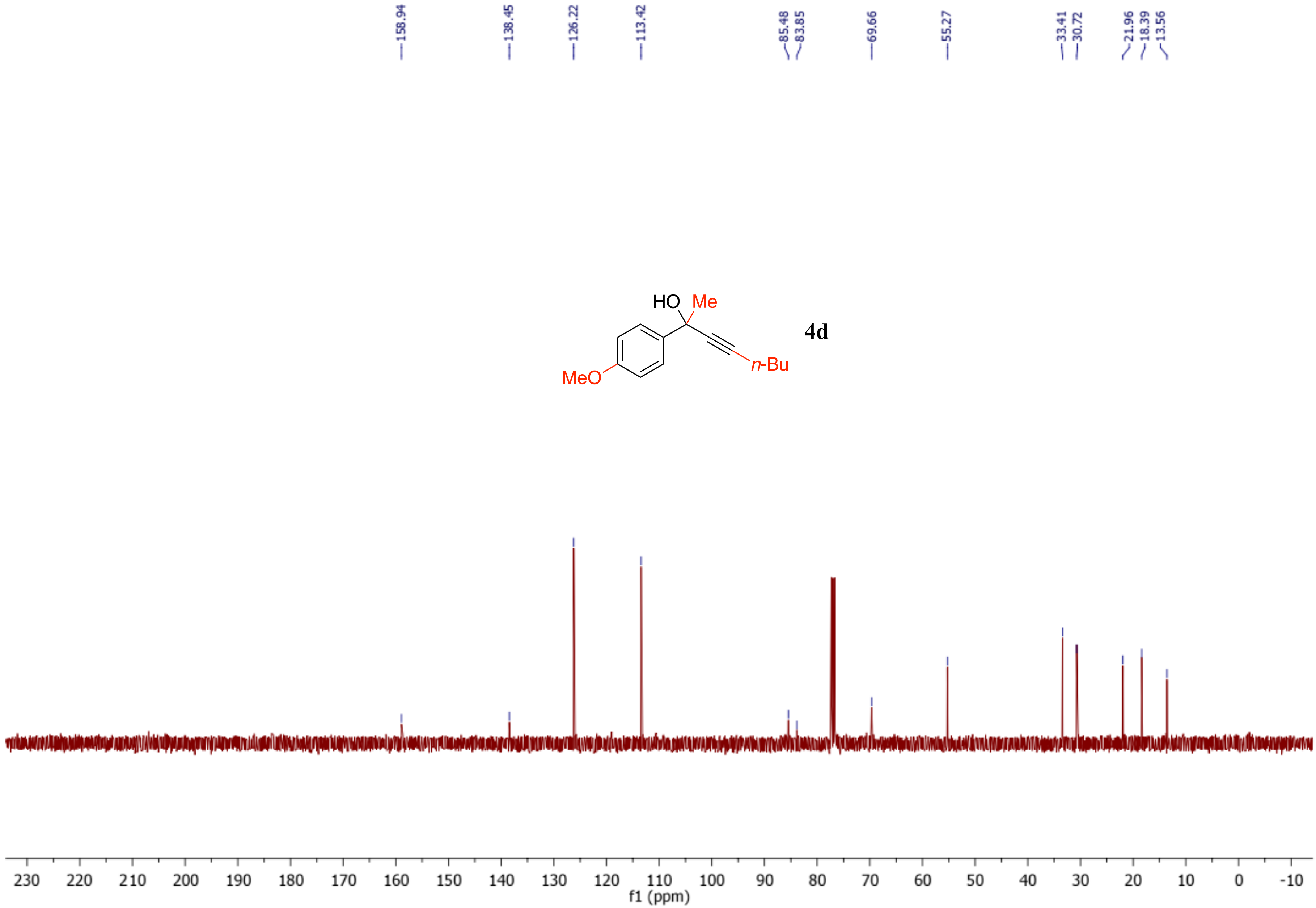
1.52
1.52
1.51
1.43
1.41
0.93
0.91
0.89
HO
Me
MeO
n-Bu
4d
1.97
2.04
3.05
2.00
0.89
3.12
4.75
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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Me
MeO
n-Bu
4d
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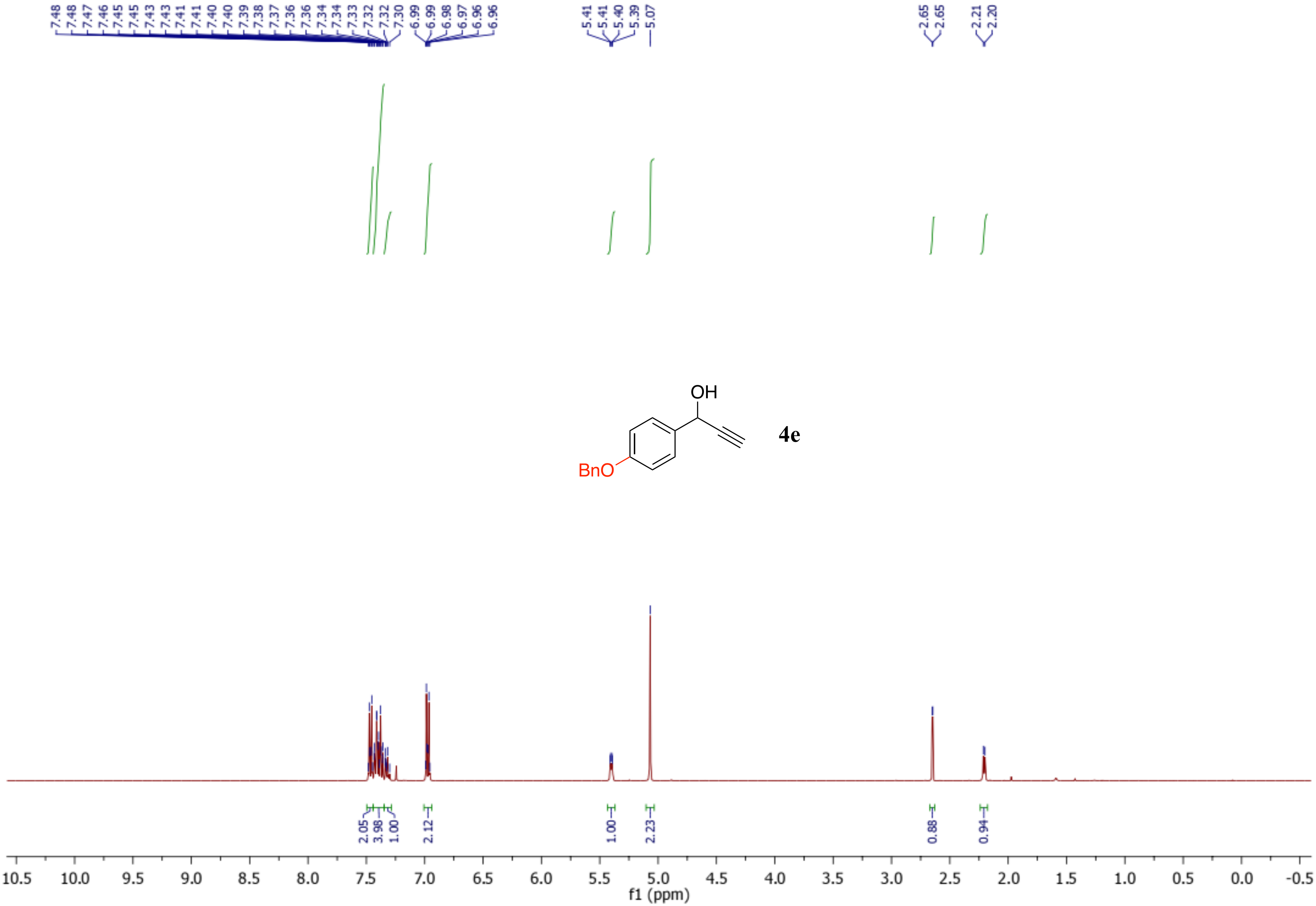
f1 (ppm)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7.36
7.36
7.34
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7.33
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2.65
2.21
2.20
OH
BnO
2.05
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1.00
2.12
1.00
2.23
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0.94
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10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.5
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1.5
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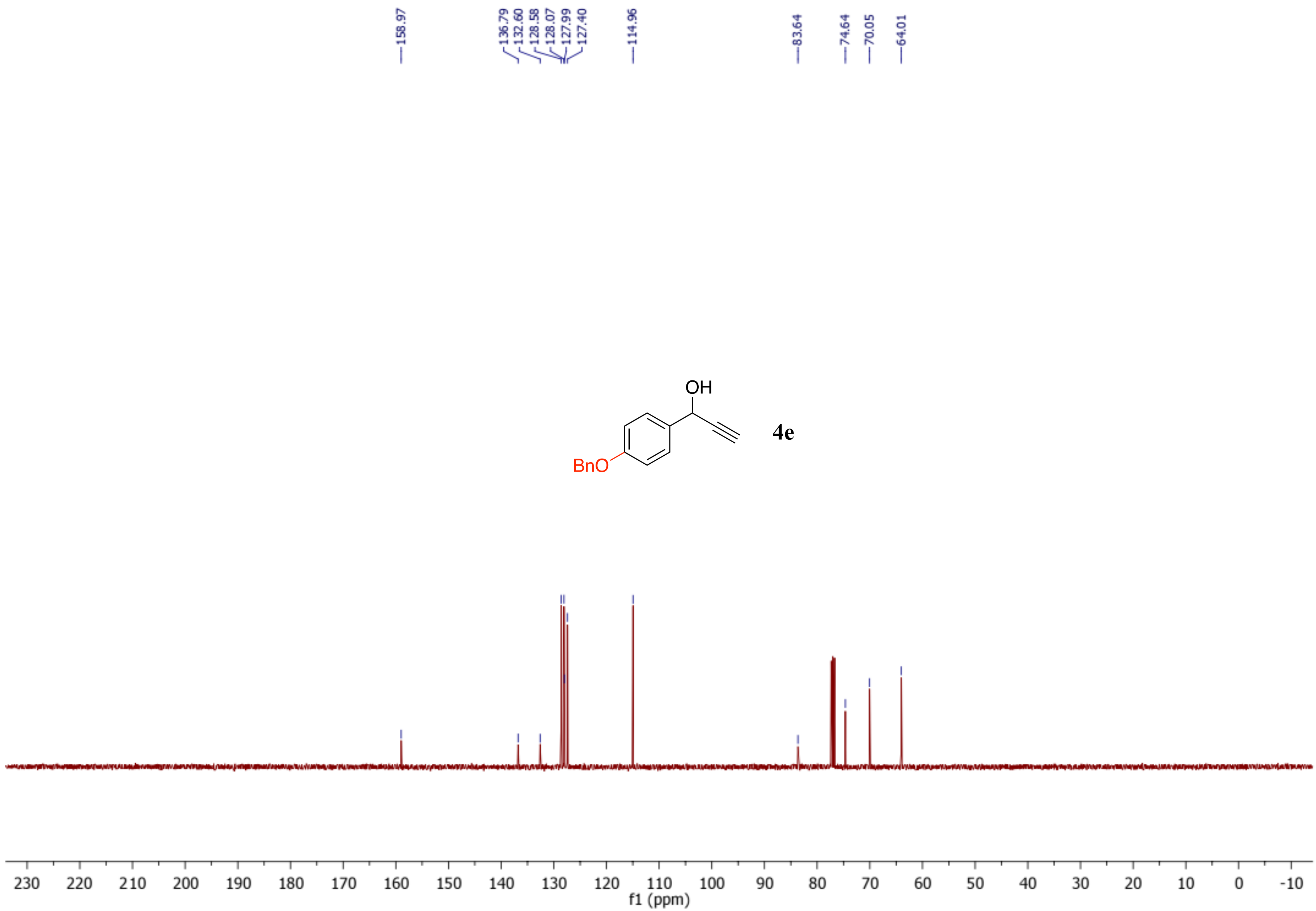
-0.5
f1 (ppm)

4e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83.64
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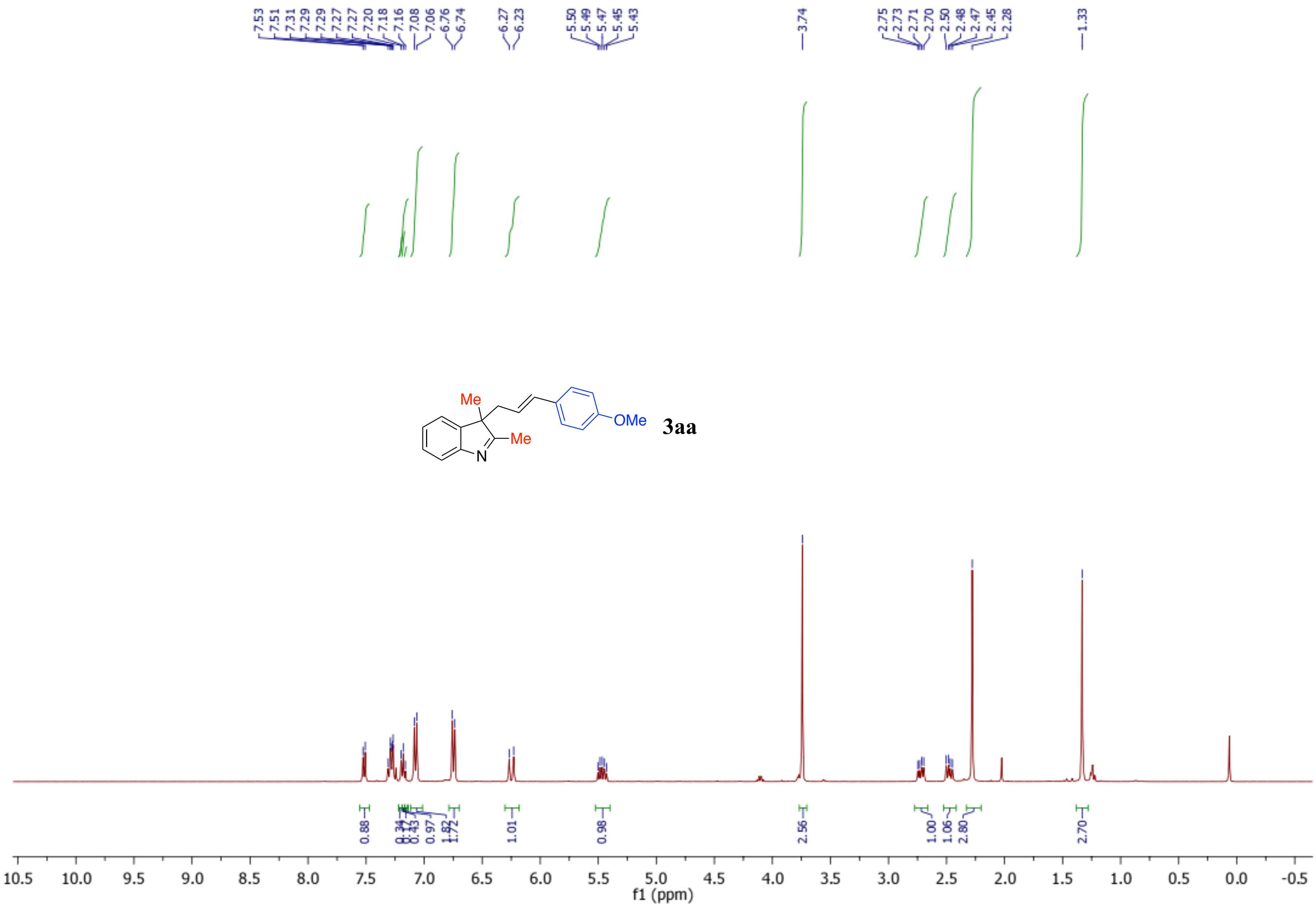
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
OH
BnO

4e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7.16
7.08
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6.76
6.74
6.27
6.23
5.50
5.49
5.47
5.45
5.43
3.74
2.75
2.73
2.71
2.70
2.50
2.48
2.47
2.45
2.28
1.33
Me
Me
N
OMe
0.88
0.97
1.82
1.72
1.01
0.98
2.56
1.00
1.06
2.80
2.70
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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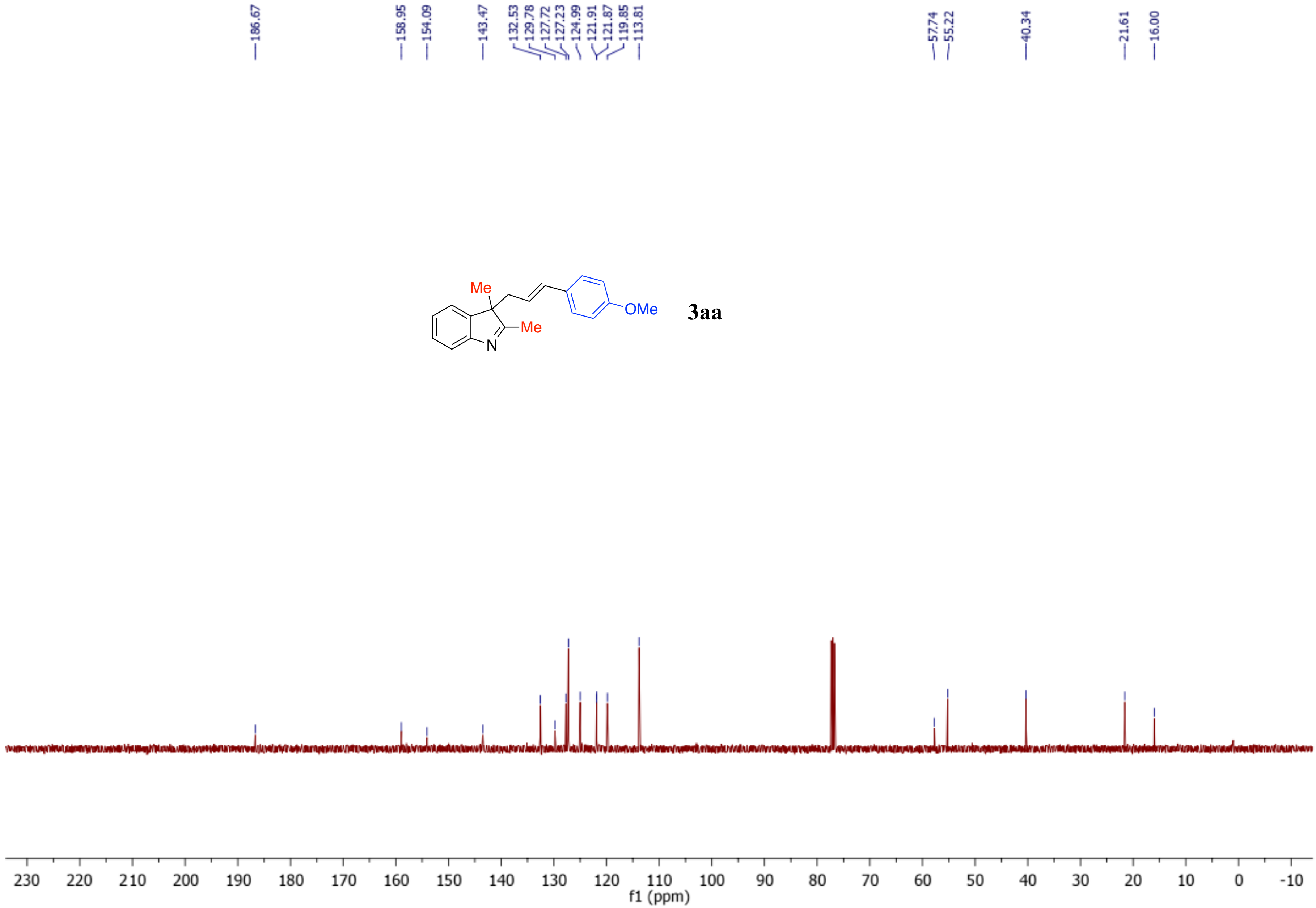
f1 (ppm)

3aa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113.81
57.74
55.22
40.34
21.61
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Me
N
OMe
3aa
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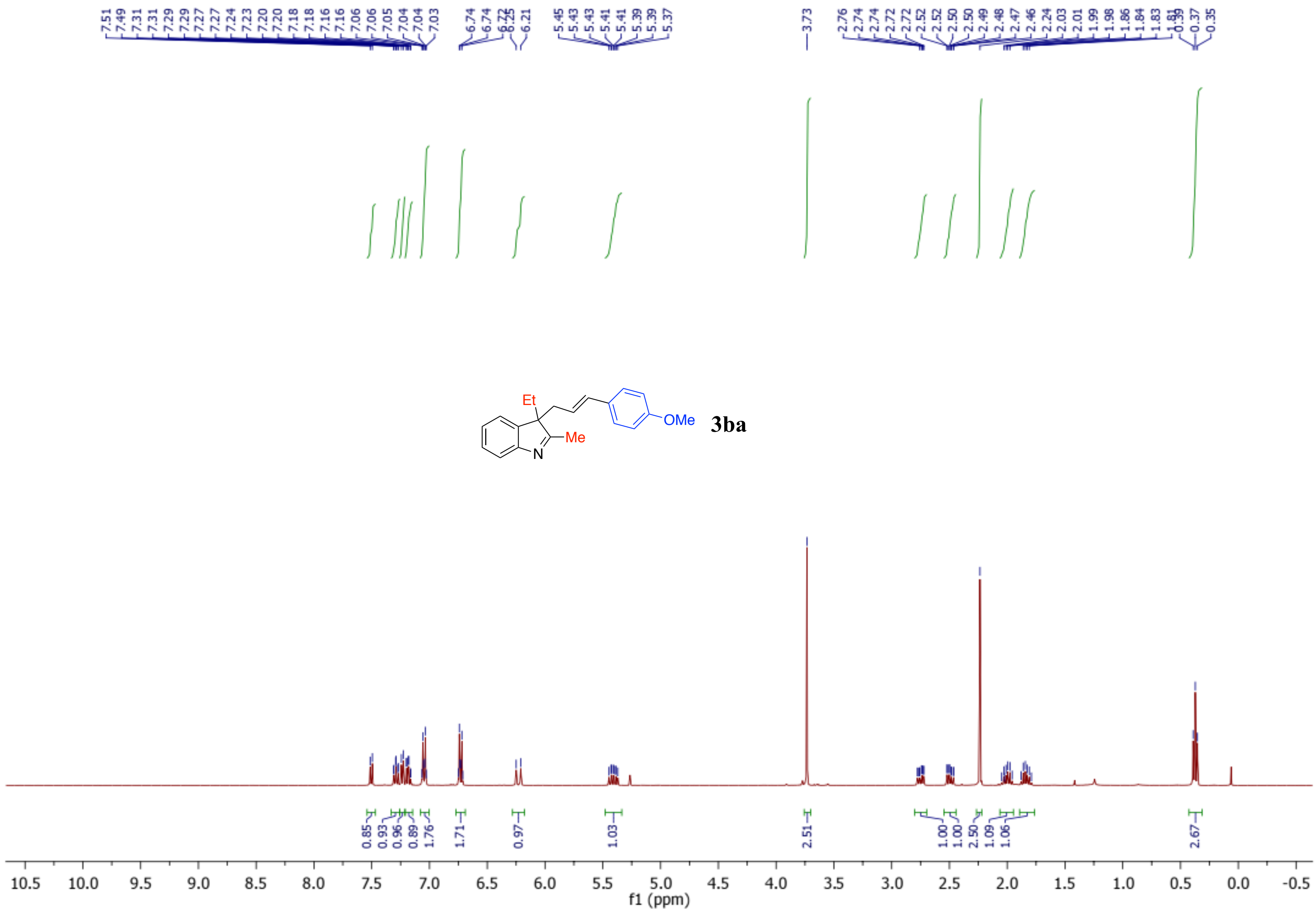
f1 (ppm)



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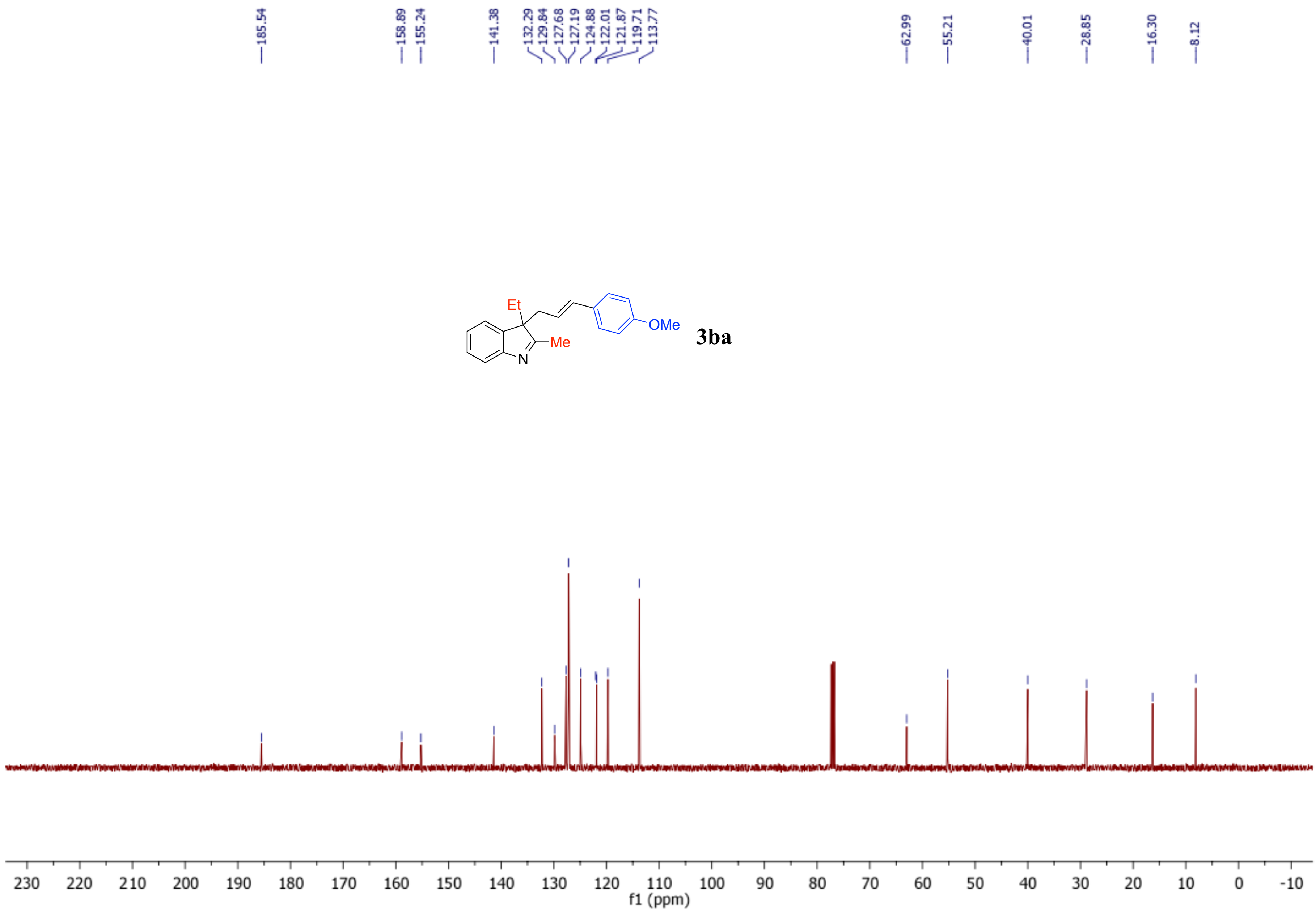
3.73
2.76 2.74 2.74 2.72 2.72 2.52 2.52 2.50 2.50 2.49 2.48 2.47 2.46 2.24 2.03 2.01 1.99 1.98 1.86 1.84 1.83 1.81 0.39 0.37 0.35
Et
Me
N
OMe
3ba
0.85 0.93 0.96 0.89 1.76 1.71 0.97 1.03 2.51 1.00 1.00 2.50 1.09 1.06 2.67
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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113.77
62.99
55.21
40.01
28.85
16.30
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Me
N
OMe
3ba
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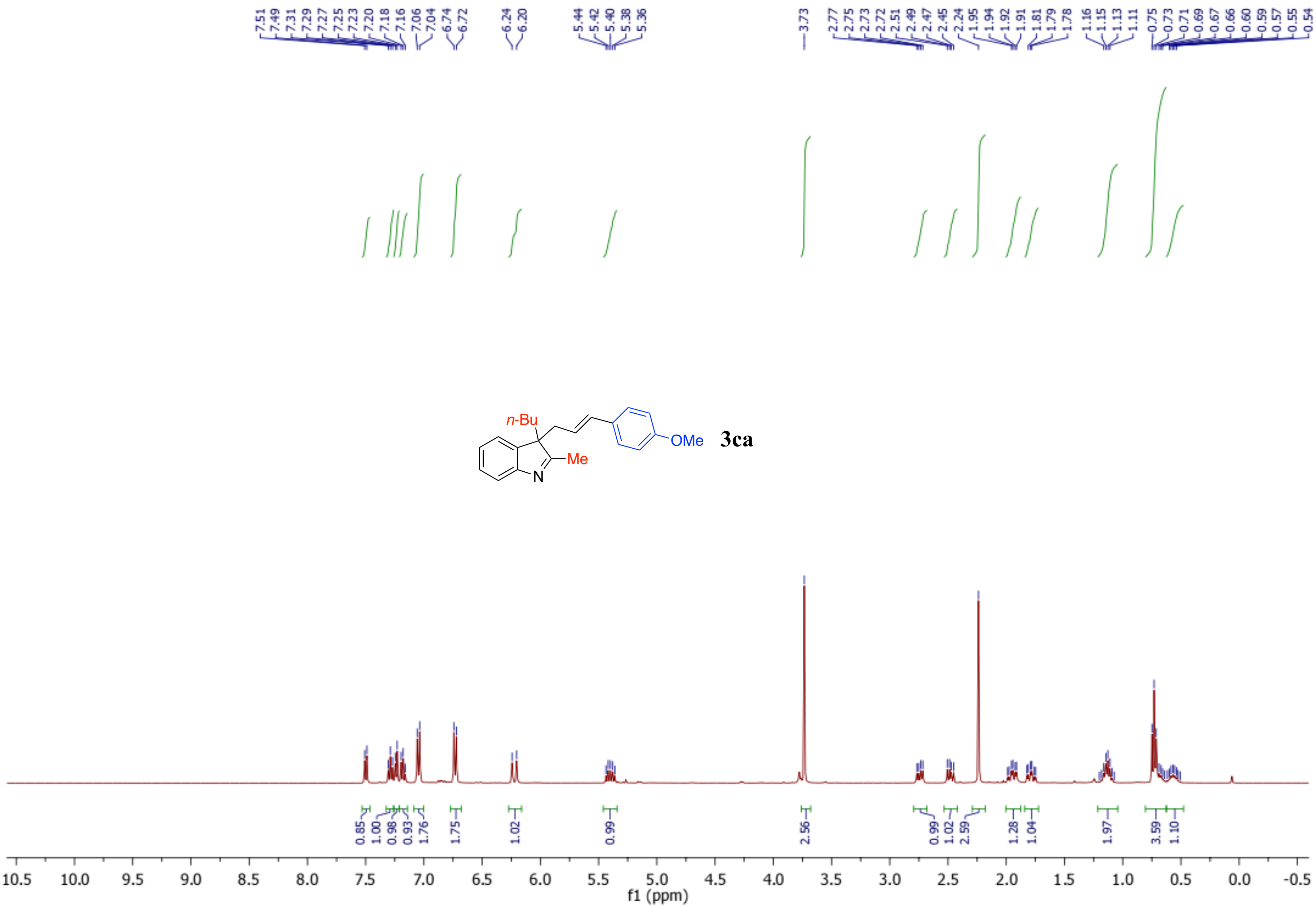
f1 (ppm)



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6.74
6.72
6.24
6.20
5.44
5.42
5.40
5.38
5.36
3.73
2.77
2.75
2.73
2.72
2.51
2.49
2.47
2.45
2.24
1.95
1.94
1.92
1.91
1.81
1.79
1.78
1.16
1.15
1.13
1.11
0.75
0.73
0.71
0.69
0.67
0.66
0.60
0.59
0.57
0.55
0.54
n-Bu
Me
N
OMe
3ca
0.85
1.00
0.98
0.93
1.76
1.75
1.02
0.99
2.56
0.99
1.02
2.59
1.28
1.04
1.97
3.59
1.10
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
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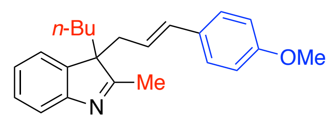
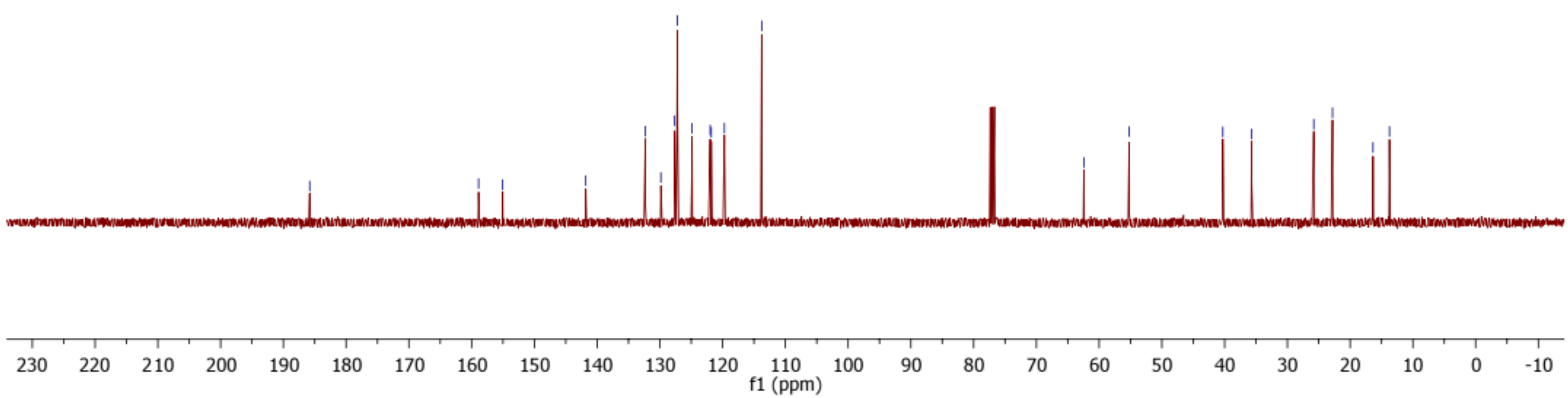
0.0
-0.5
f1 (ppm)


n-Bu
Me
N
OMe

3ca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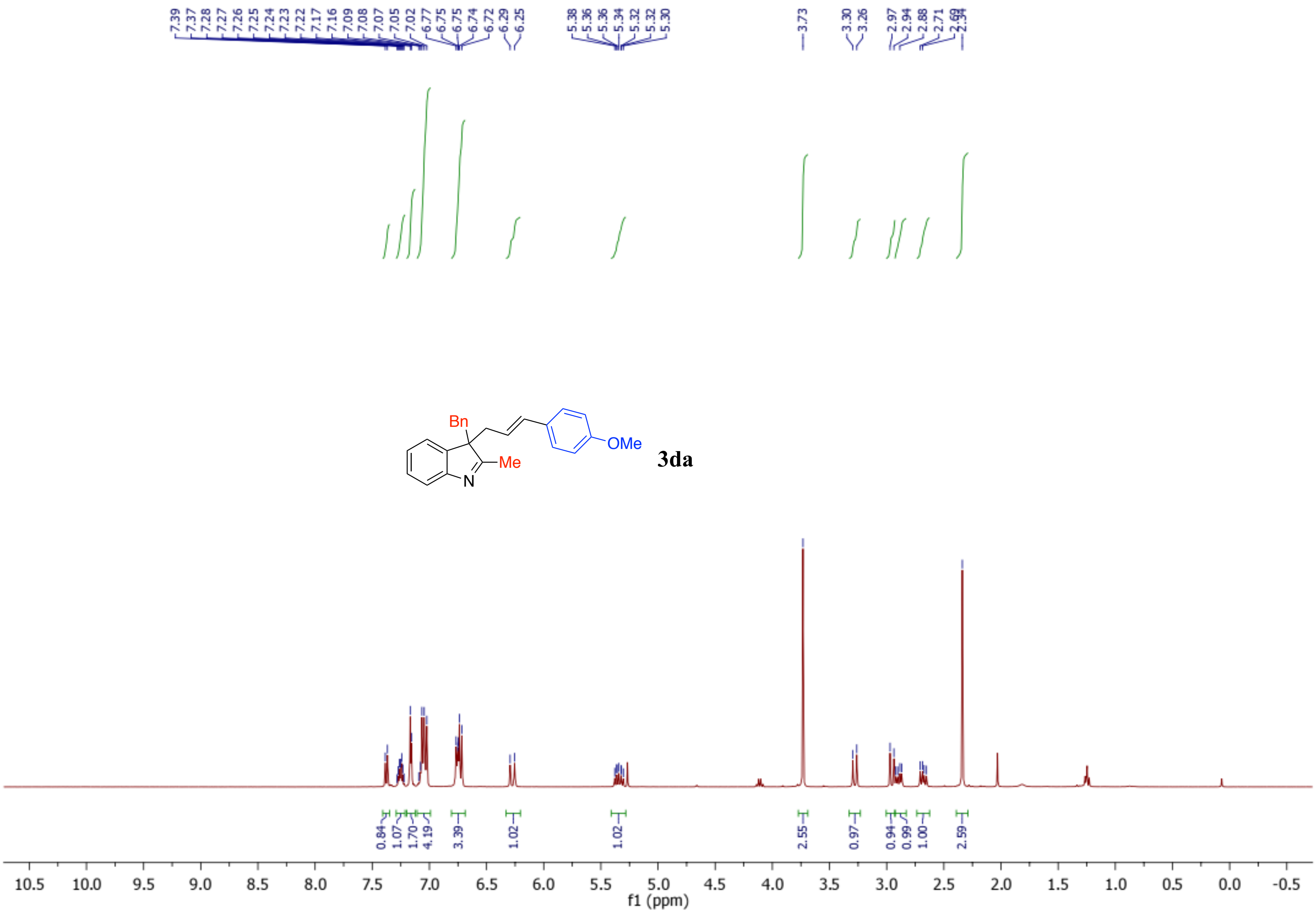
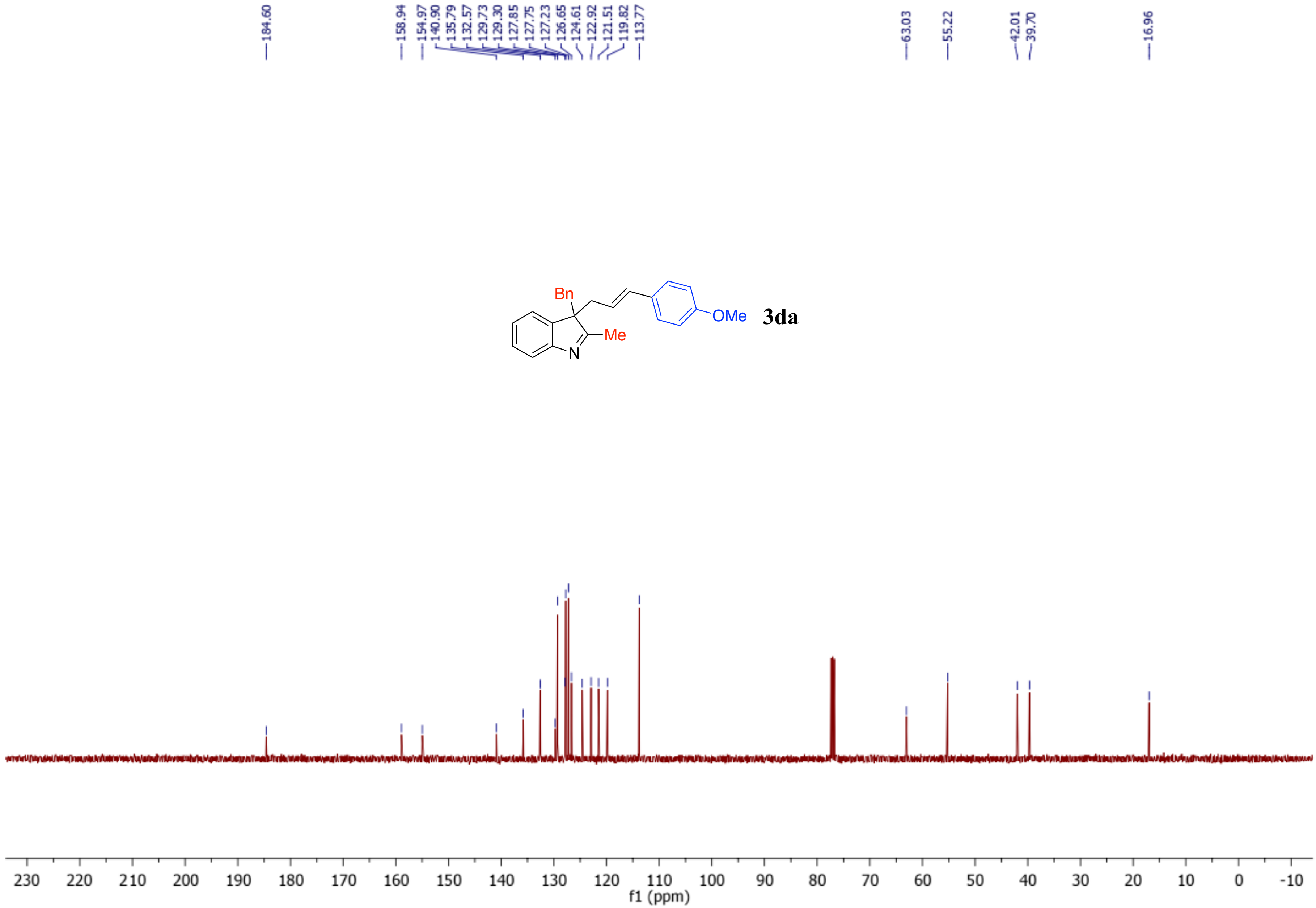
127.64
127.20
124.87
121.98
121.81
119.71
113.77
62.42
55.21
40.29
35.70
25.80
22.81
16.35
13.73
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



3da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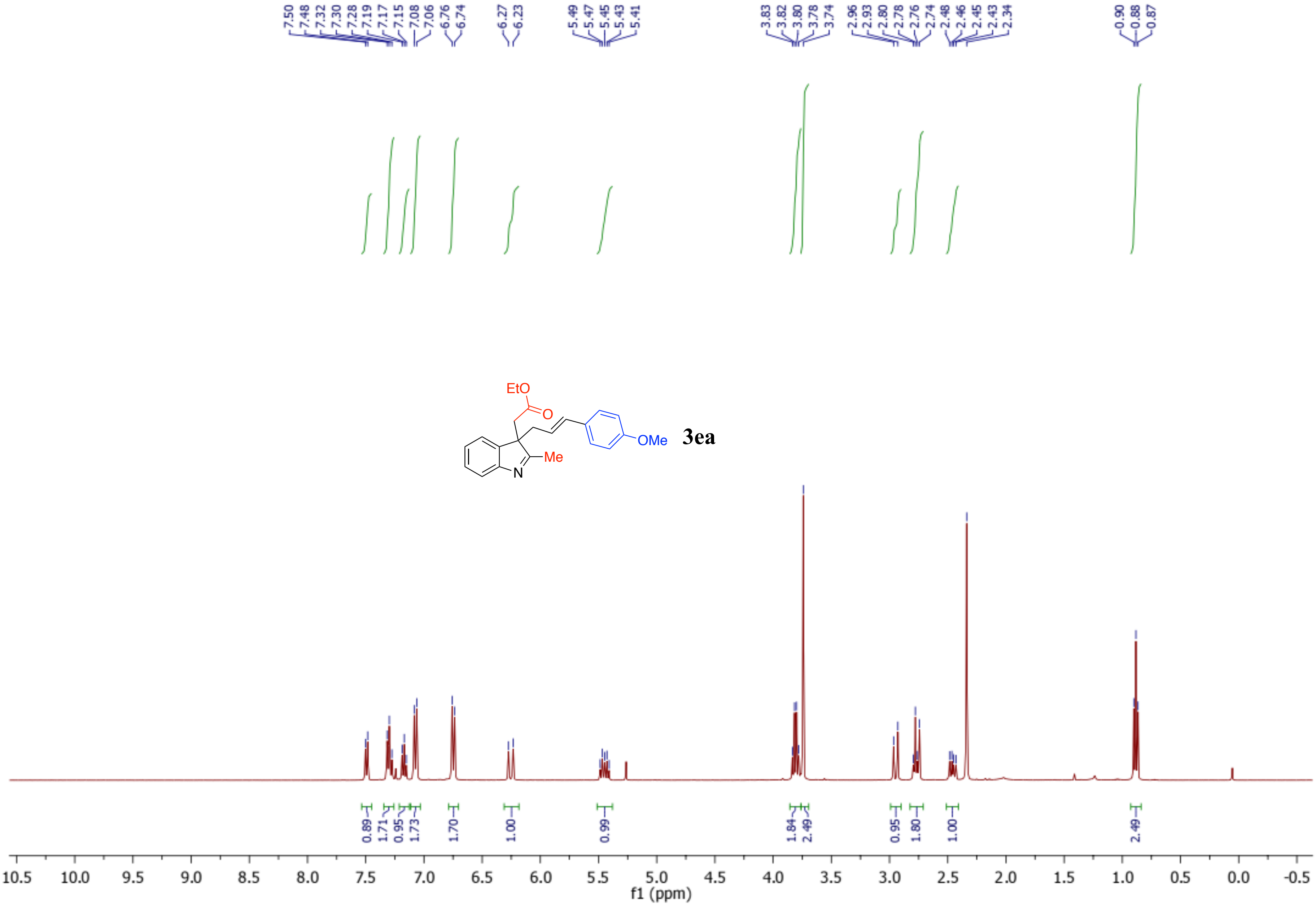
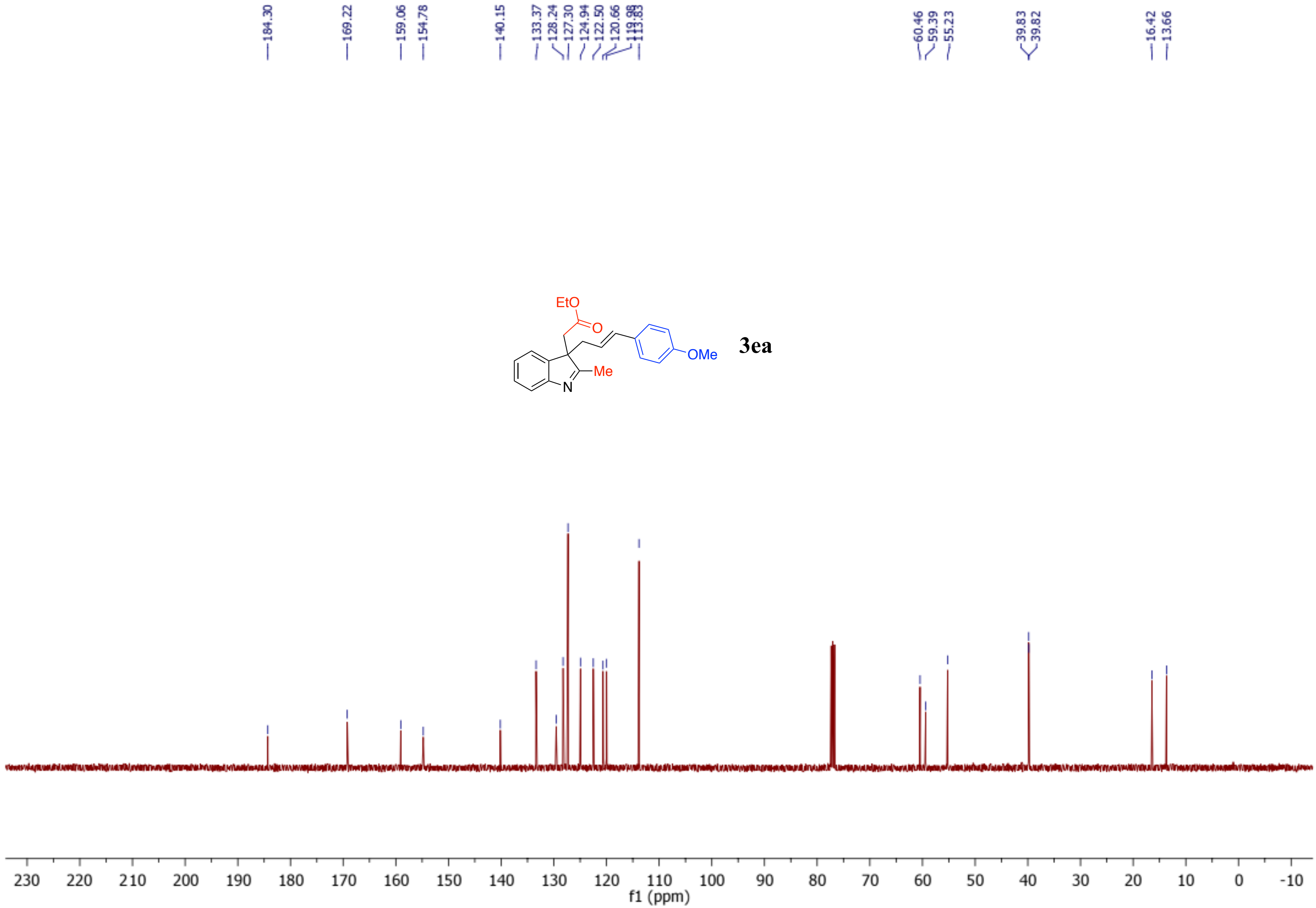
129.30
127.85
127.75
127.23
126.65
124.61
122.92
121.51
119.82
113.77
63.03
55.22
42.01
39.70
16.96
Bn
Me
N
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3da



7.50 7.48 7.32 7.30 7.28 7.19 7.17 7.15 7.08 7.06 6.76 6.74 6.27 6.23 5.49 5.47 5.45 5.43 5.41 3.83 3.82 3.80 3.78 3.74 2.96 2.93 2.80 2.78 2.76 2.74 2.48 2.46 2.45 2.43 2.34 0.90 0.88 0.87
EtO
O
OMe
Me
N
3ea
0.89 1.71 0.95 1.73 1.70 1.00 0.99 1.84 2.49 0.95 1.80 1.00 2.49
10.5 10.0 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 0.0 -0.5
f1 (ppm)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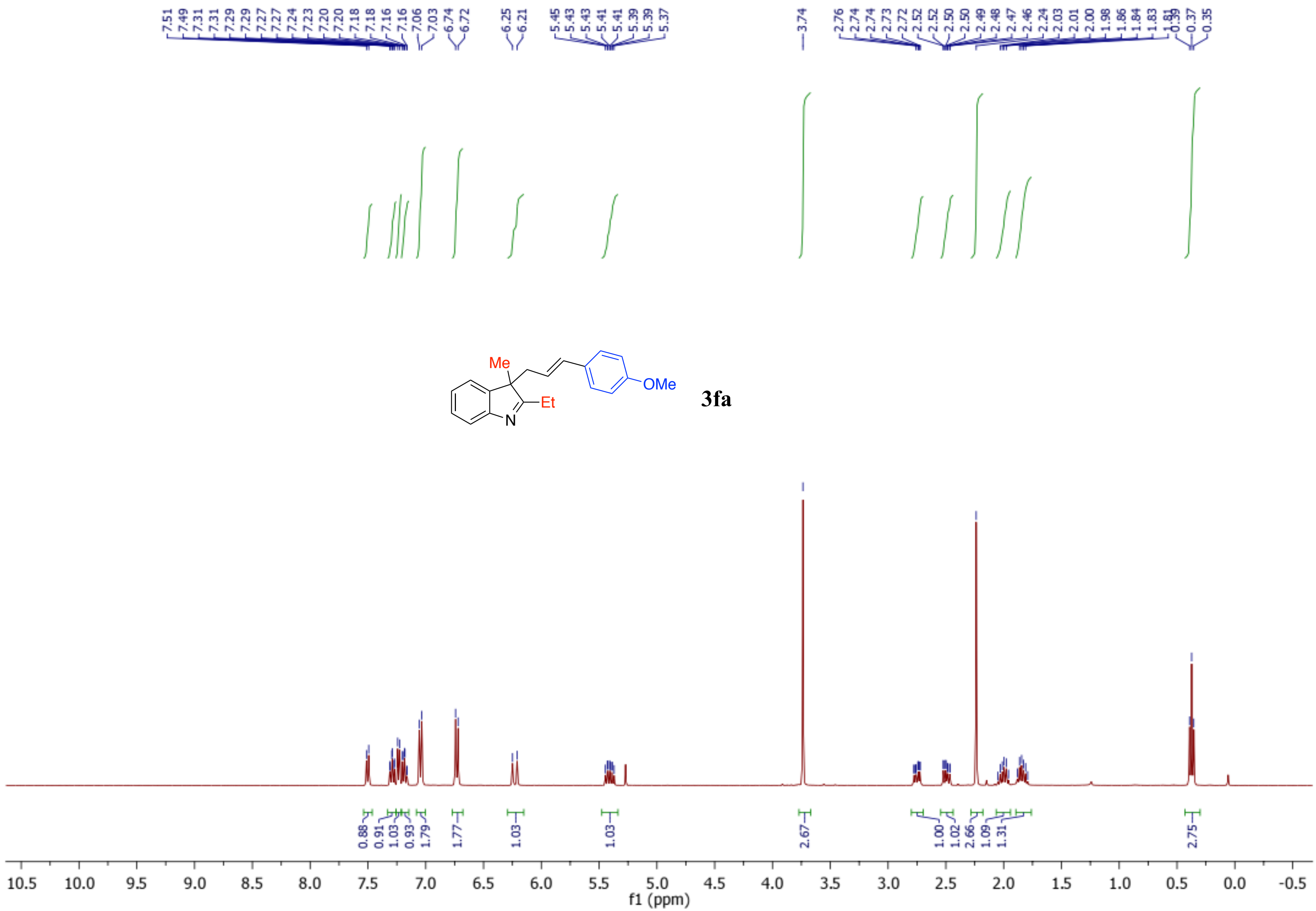
133.37
128.24
127.30
124.94
122.50
120.66
119.98
113.83
60.46
59.39
55.23
39.83
39.82
16.42
13.66
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
EtO
O
Me
N
OMe

3ea



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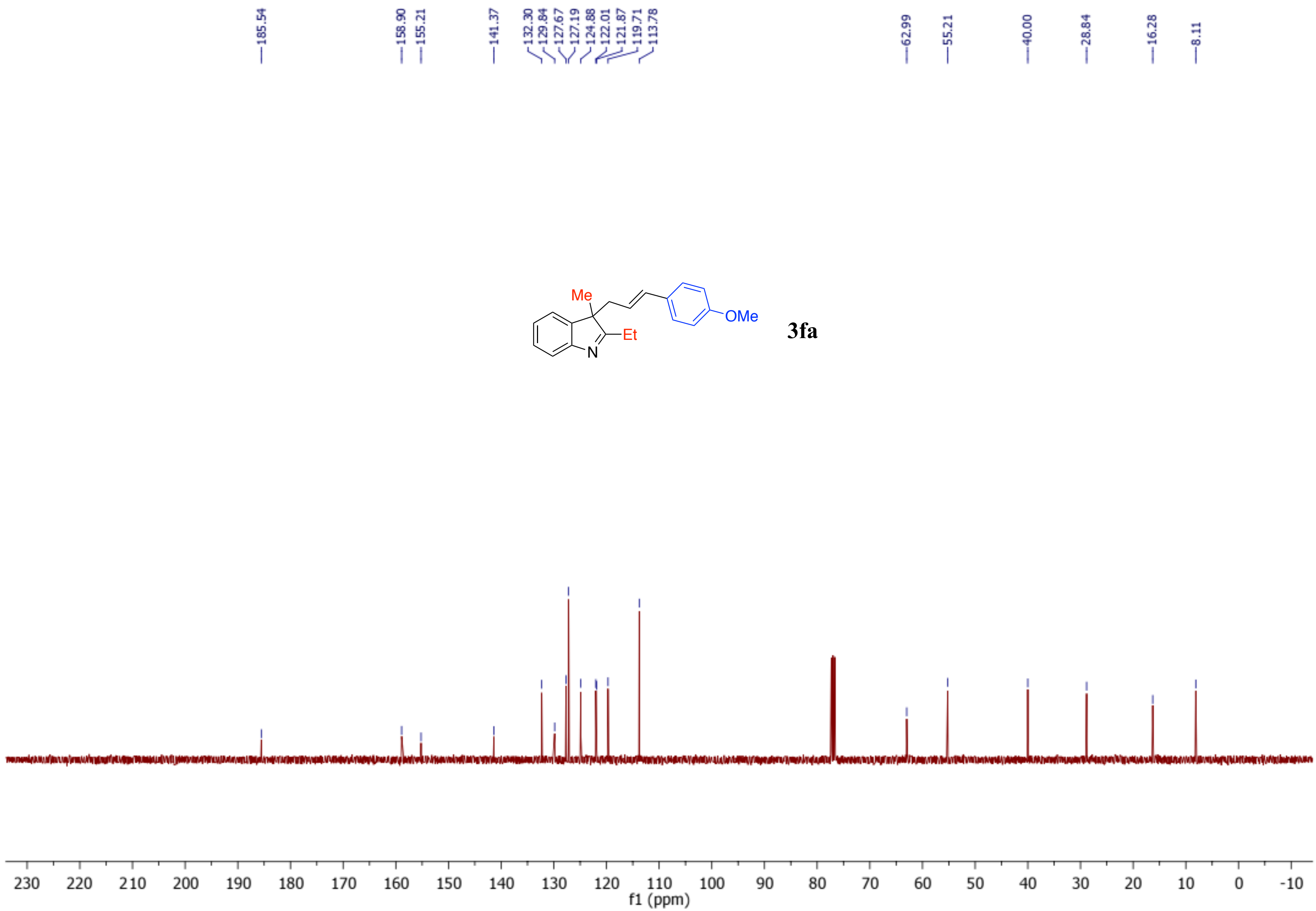
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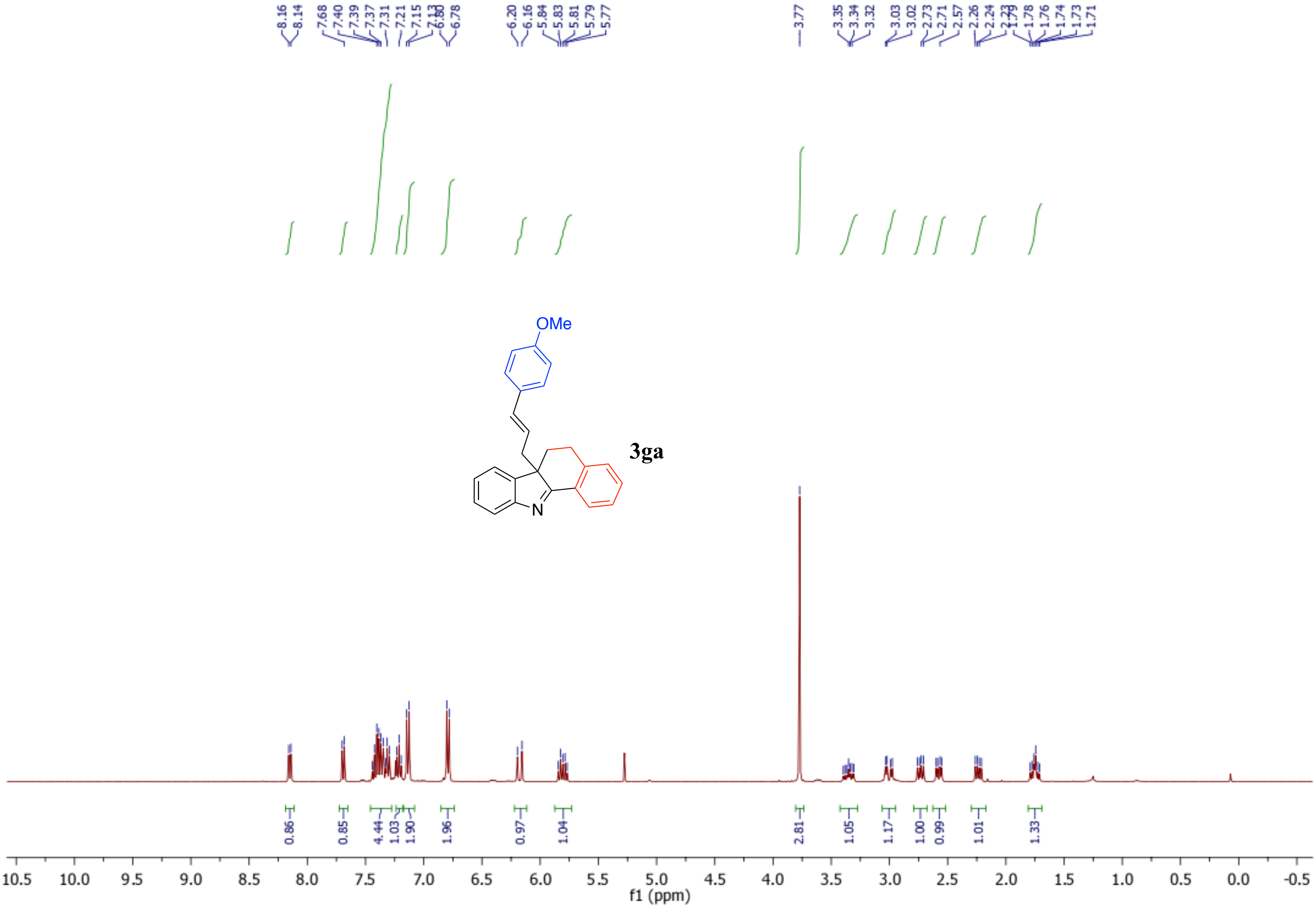
127.19
124.88
122.01
121.87
119.71
113.78
62.99
55.21
40.00
28.84
16.28
8.11
Me
Et
N
OMe
f1 (ppm)

3fa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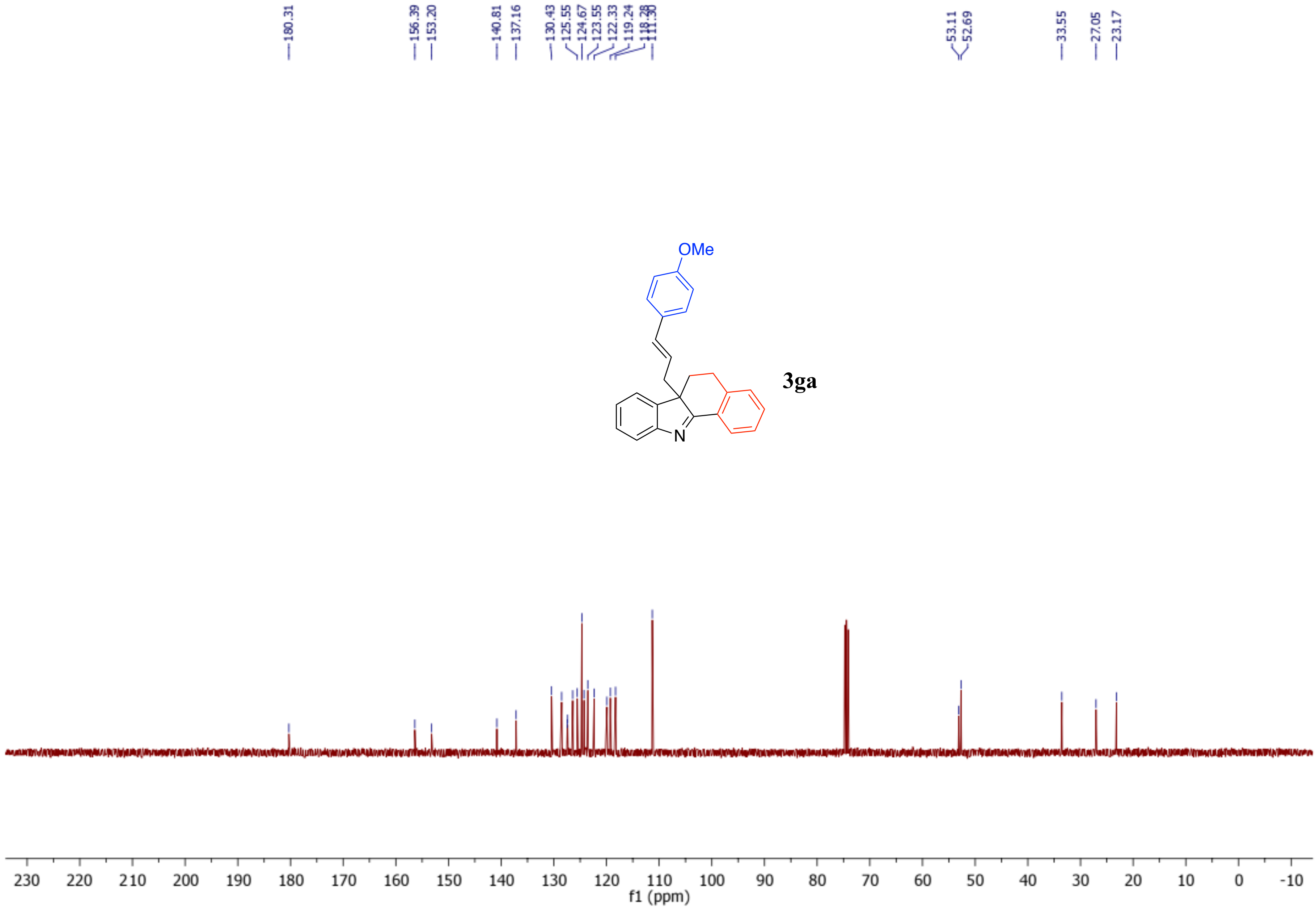
7.37
7.31
7.21
7.15
7.13
6.80
6.78
6.20
6.16
5.84
5.83
5.81
5.79
5.77
3.77
3.35
3.34
3.32
3.03
3.02
2.73
2.71
2.57
2.26
2.24
2.23
1.79
1.78
1.76
1.74
1.73
1.71
OMe
N
0.86
0.85
4.44
1.03
1.90
1.96
0.97
1.04
2.81
1.05
1.17
1.00
0.99
1.01
1.33
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

3ga



180.31
156.39
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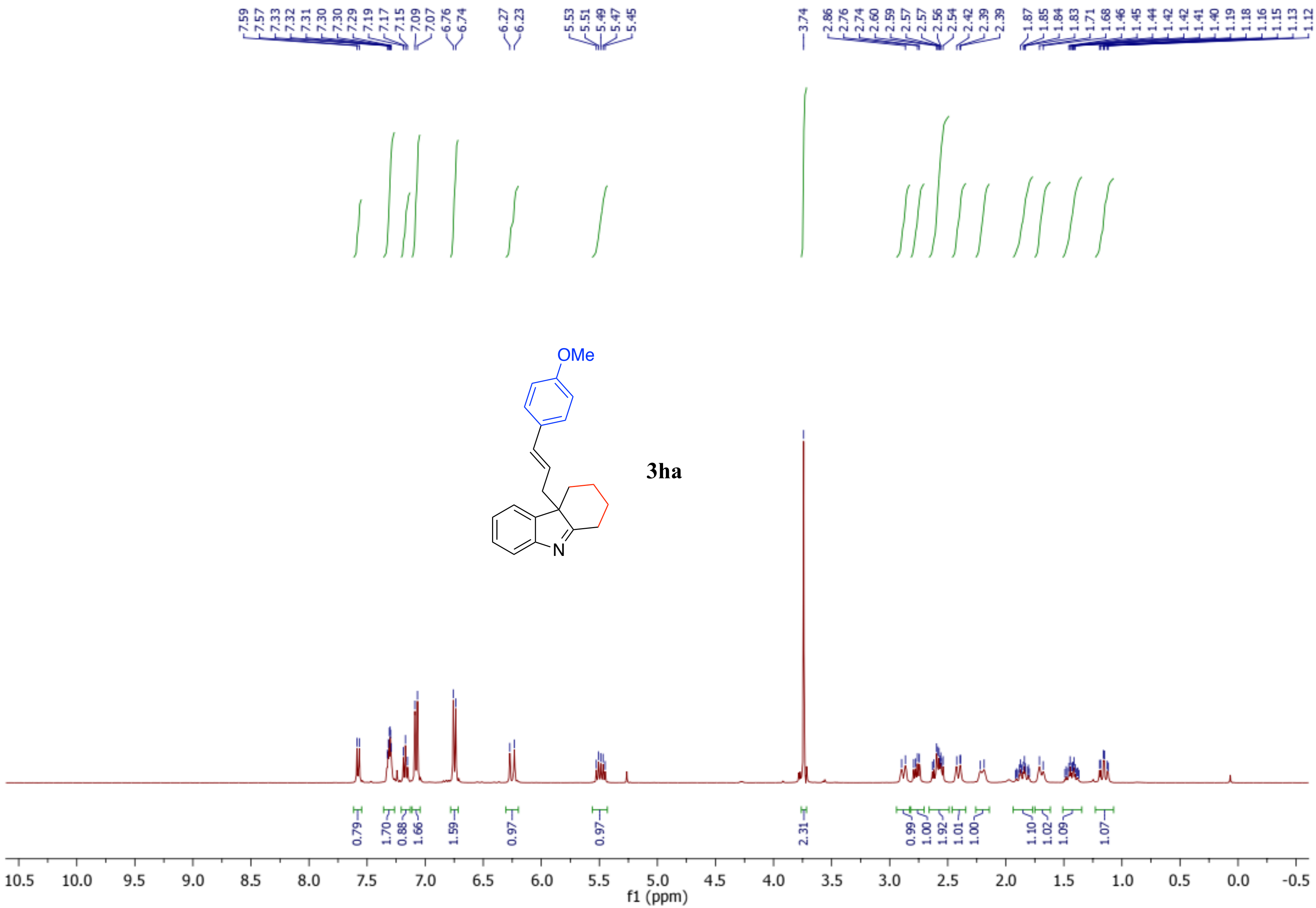
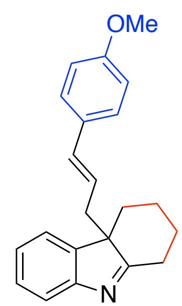
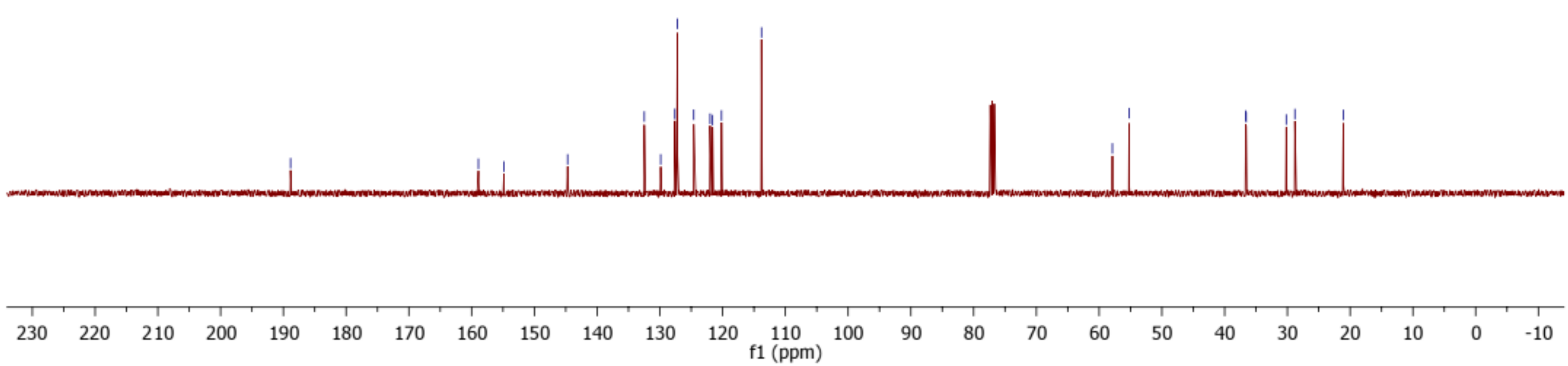
140.81
137.16
130.43
125.55
124.67
123.55
122.33
119.24
118.28
111.30
53.11
52.69
33.55
27.05
23.17
OMe
N
3ga
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



7.59 7.57 7.33 7.32 7.31 7.30 7.30 7.29 7.19 7.17 7.15 7.09 7.07 6.76 6.74 6.27 6.23 5.53 5.51 5.49 5.47 5.45
3.74
2.86 2.76 2.74 2.60 2.59 2.57 2.57 2.56 2.54 2.42 2.39 2.39 1.87 1.85 1.84 1.83 1.71 1.68 1.46 1.45 1.44 1.42 1.42 1.41 1.40 1.19 1.18 1.16 1.15 1.13 1.12
OMe
N
3ha
0.79 1.70 0.88 1.66 1.59 0.97 0.97 2.31 0.99 1.00 1.92 1.01 1.00 1.10 1.02 1.09 1.07
10.5 10.0 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 0.0 -0.5
f1 (ppm)



3ha



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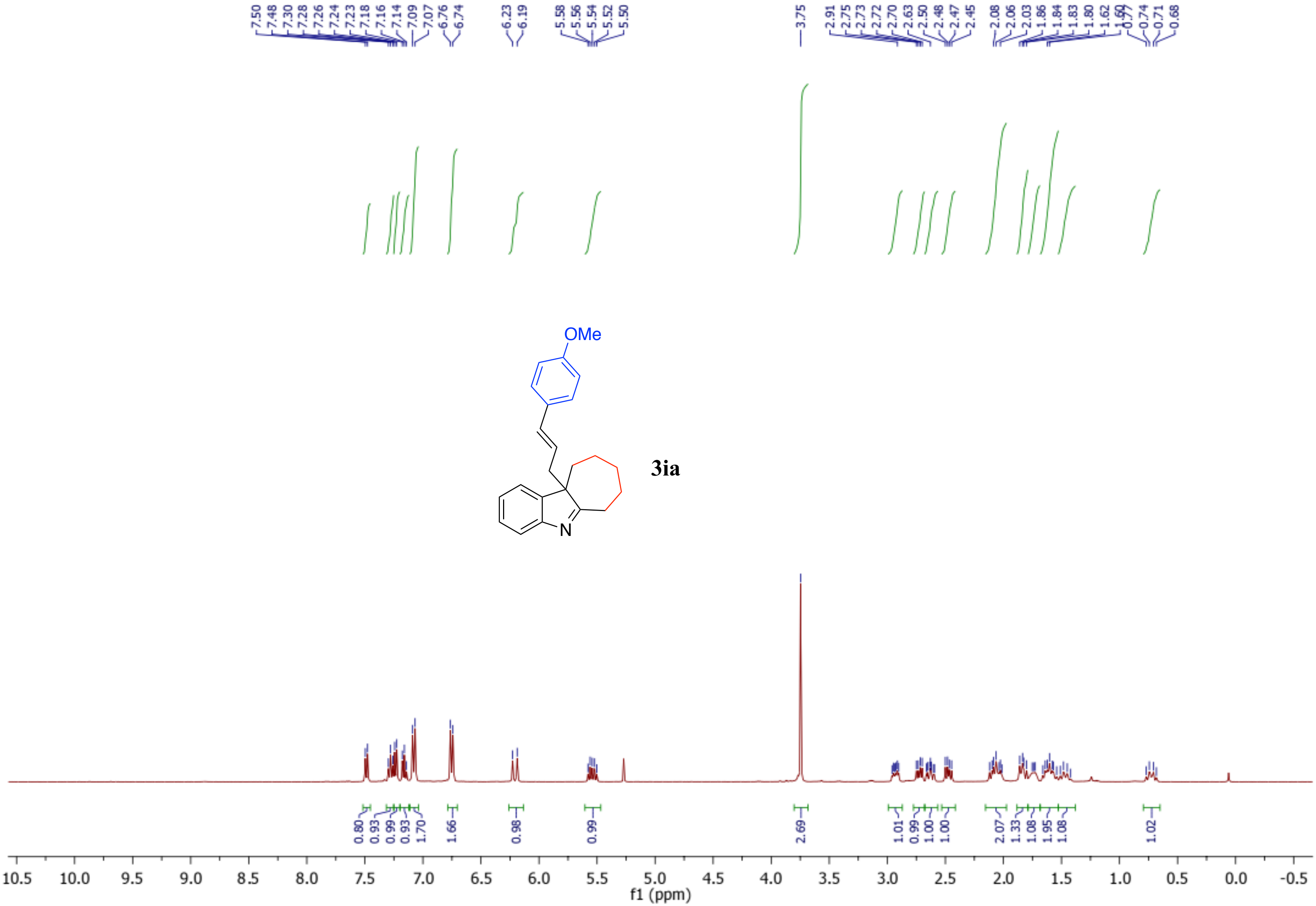
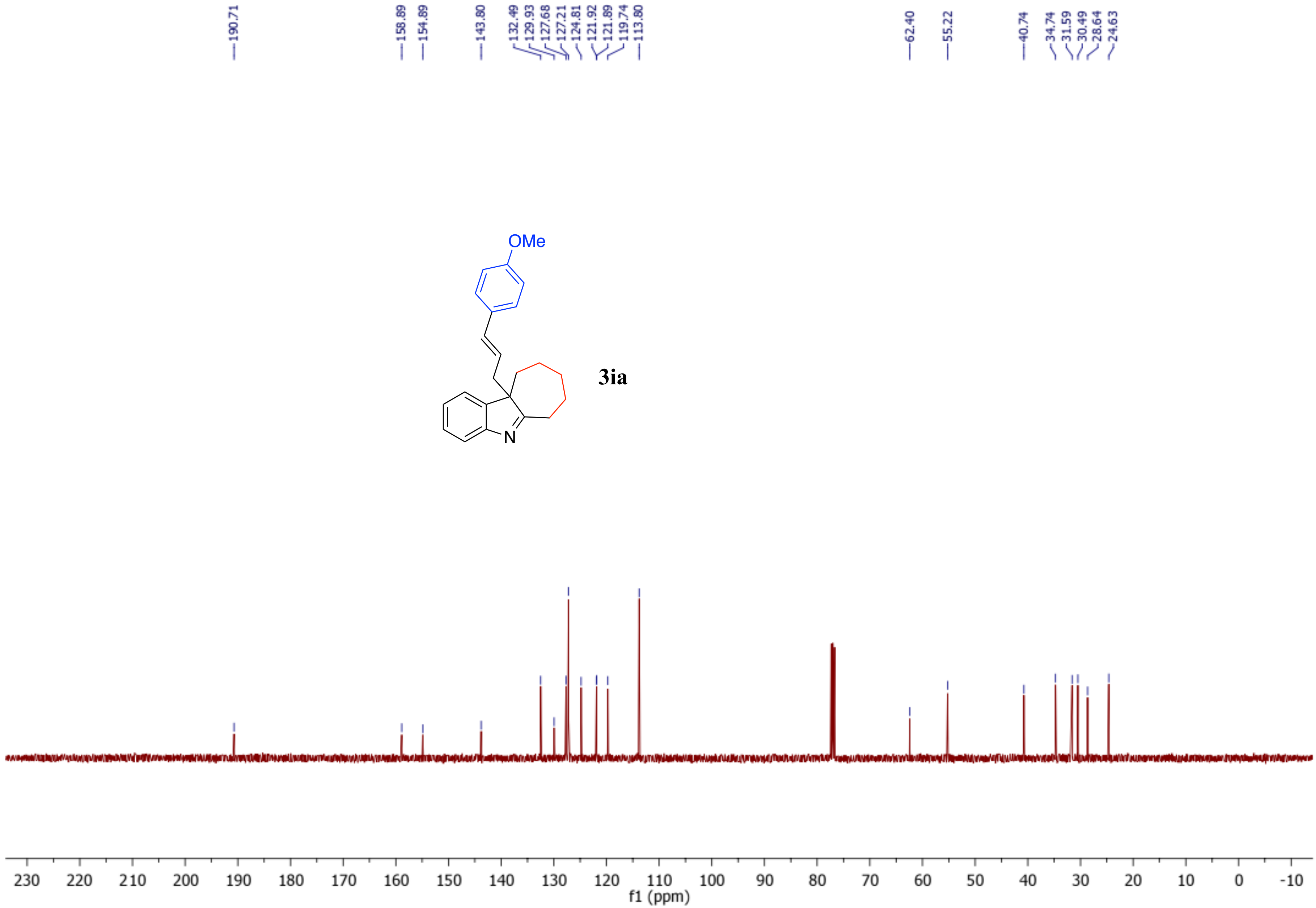
121.61
120.18
113.80
57.88
55.22
36.62
36.57
30.17
28.80
21.08
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



7.50 7.48 7.30 7.28 7.26 7.24 7.23 7.18 7.16 7.14 7.09 7.07 6.76 6.74 6.23 6.19 5.58 5.56 5.54 5.52 5.50 3.75 2.91 2.75 2.73 2.72 2.70 2.63 2.50 2.48 2.47 2.45 2.08 2.06 2.03 1.86 1.84 1.83 1.80 1.62 1.60 0.77 0.74 0.71 0.68
OMe
N
3ia
0.80 0.93 0.99 0.93 1.70 1.66 0.98 0.99 2.69 1.01 0.99 1.00 1.00 2.07 1.33 1.08 1.95 1.08 1.02
10.5 10.0 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 0.0 -0.5
f1 (ppm)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127.21
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121.89
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113.80
62.40
55.22
40.74
34.74
31.59
30.49
28.64
24.63
OMe
N
3ia
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

7.44
7.43
7.42
7.40
7.08
7.06
6.98
6.96
6.76
6.74
6.26
6.23
5.46
5.45
5.44
5.43
5.42
5.41
5.40
5.39
3.74
2.71
2.71
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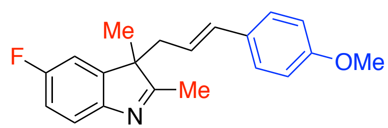
2.25
1.32

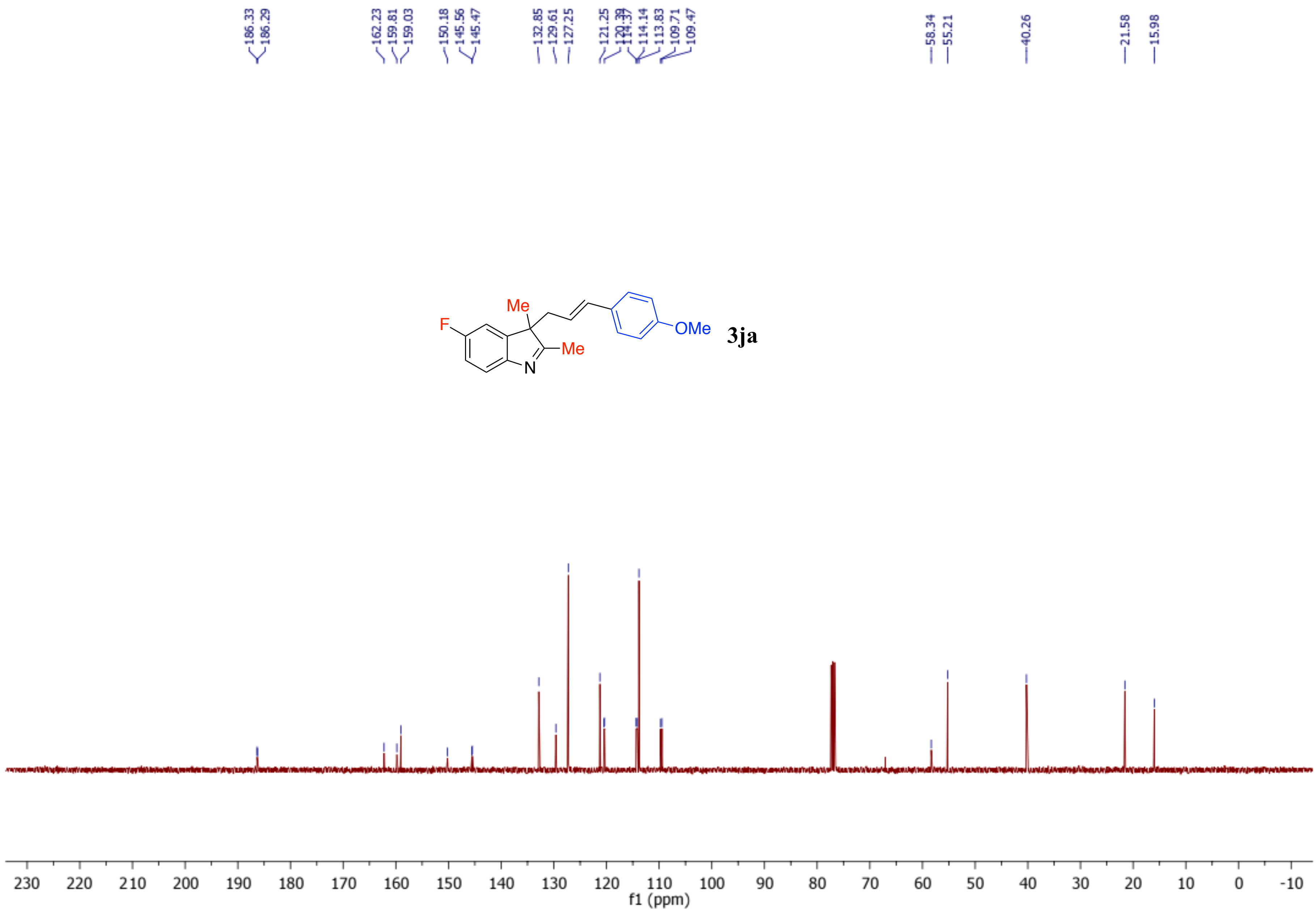


3ja

0.85 1.77 1.73 1.76 0.97 1.00 2.56 0.99 1.00 2.69 2.71

10.5 10.0 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 0.0 -0.5

f1 (ppm)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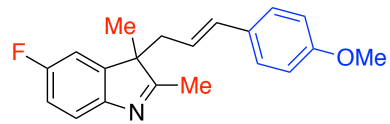
129.61
127.25
121.25
120.39
114.37
114.14
113.83
109.71
109.47
58.34
55.21
40.26
21.58
15.98
F
Me
Me
N
OMe
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3ja



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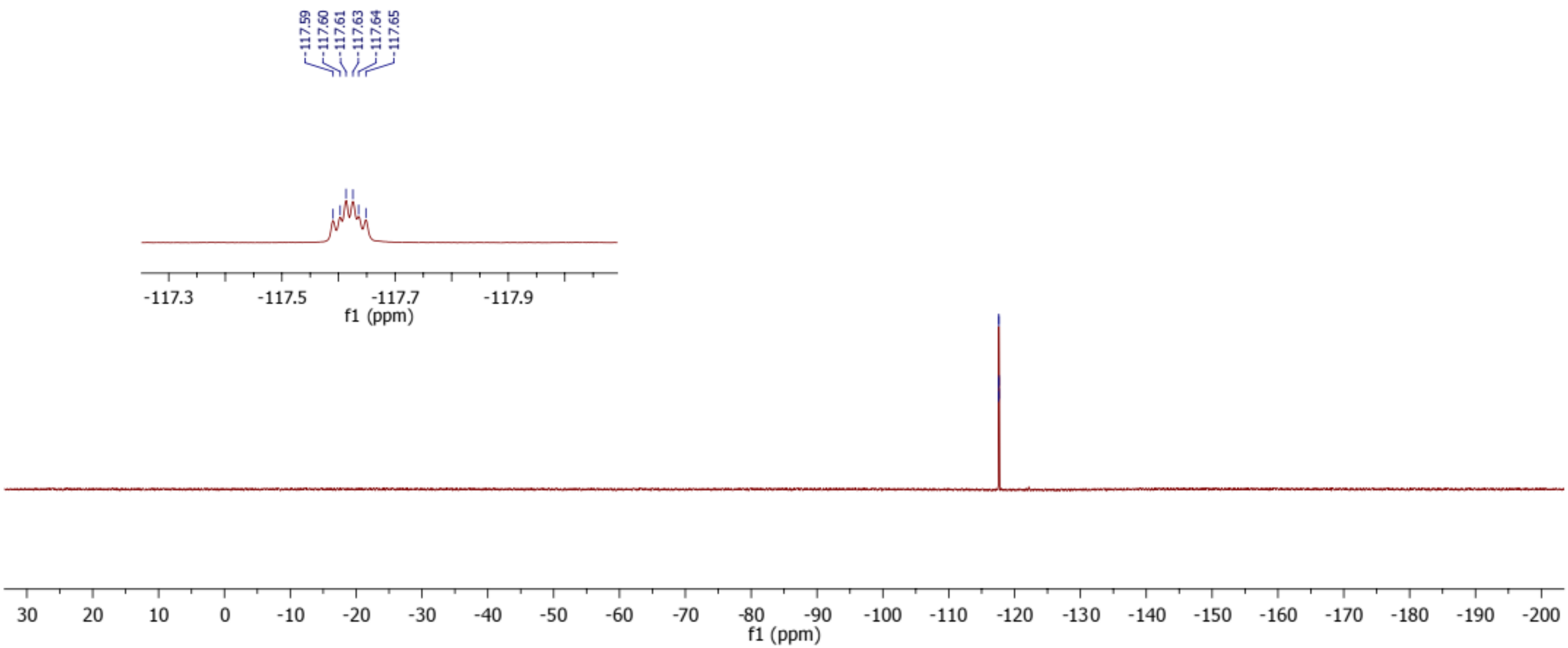
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-117.61
-117.63
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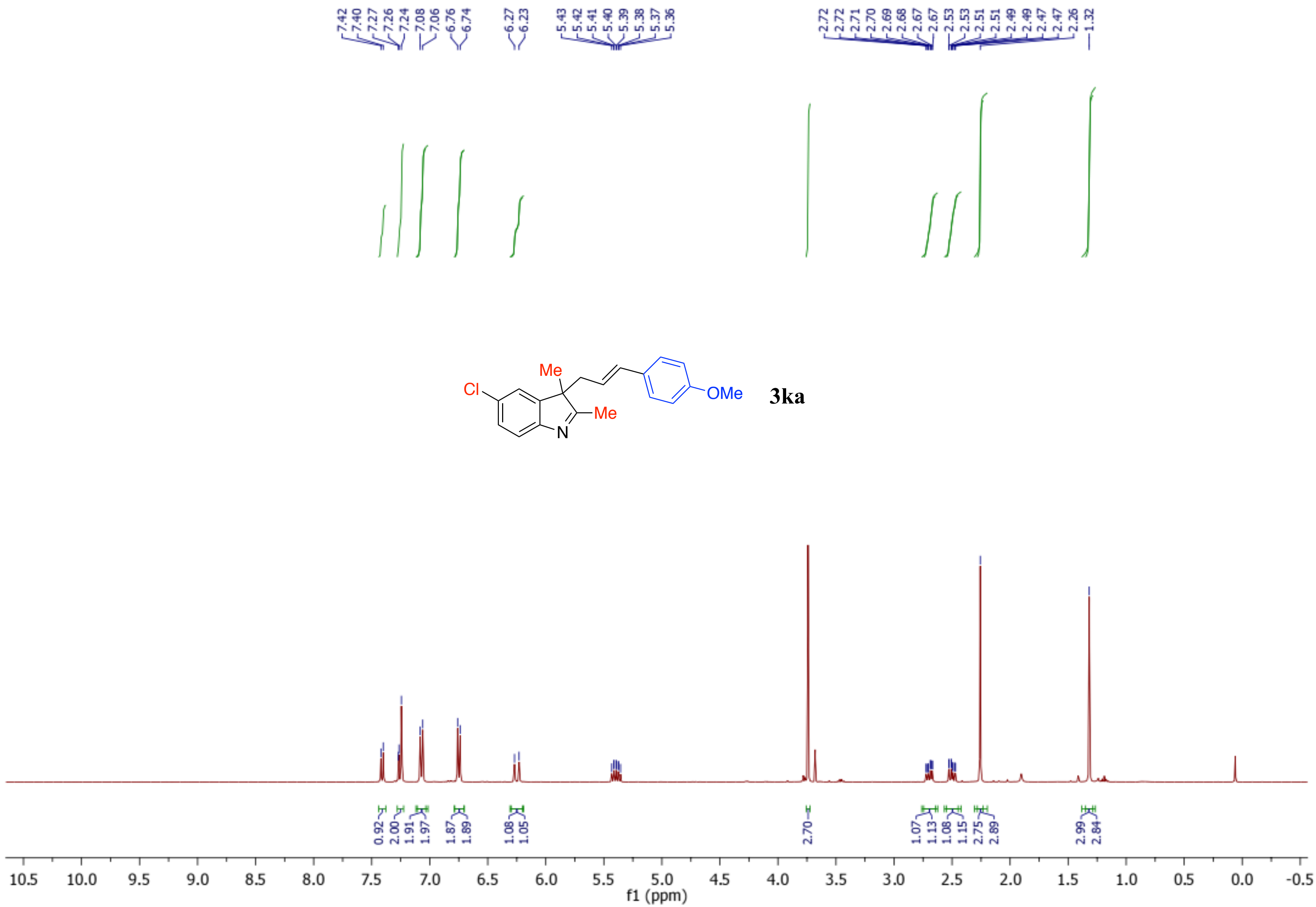
-117.65
-117.3
-117.5
-117.7
-117.9
f1 (ppm)
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)



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6.76
6.74
6.27
6.23
5.43
5.42
5.41
5.40
5.39
5.38
5.37
5.36
2.72
2.72
2.71
2.70
2.69
2.68
2.67
2.67
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2.51
2.51
2.49
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2.47
2.47
2.26
1.32
Cl
Me
Me
N
OMe
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1.87
1.89
1.08
1.05
2.70
1.07
1.13
1.08
1.15
2.75
2.89
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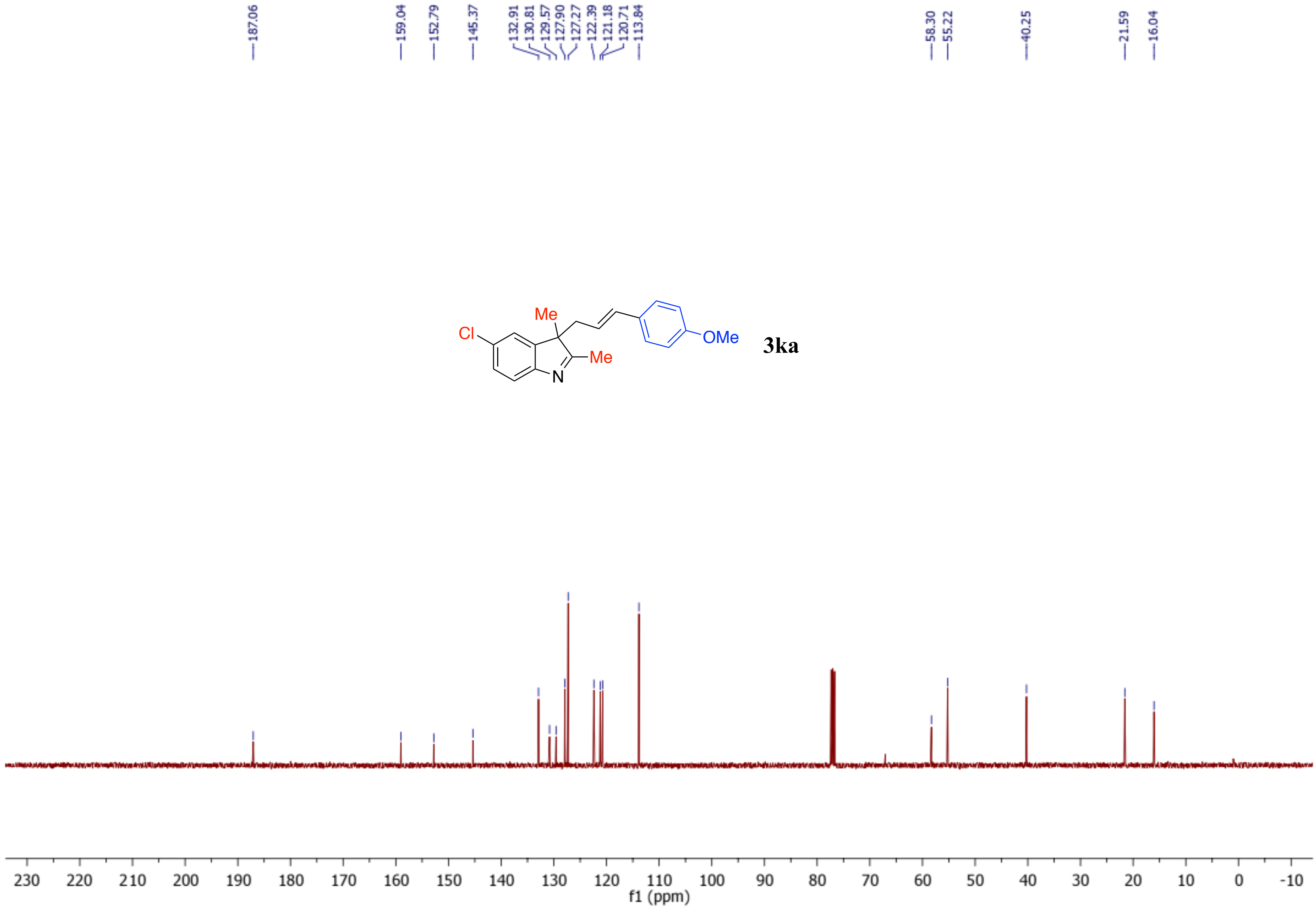
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

3ka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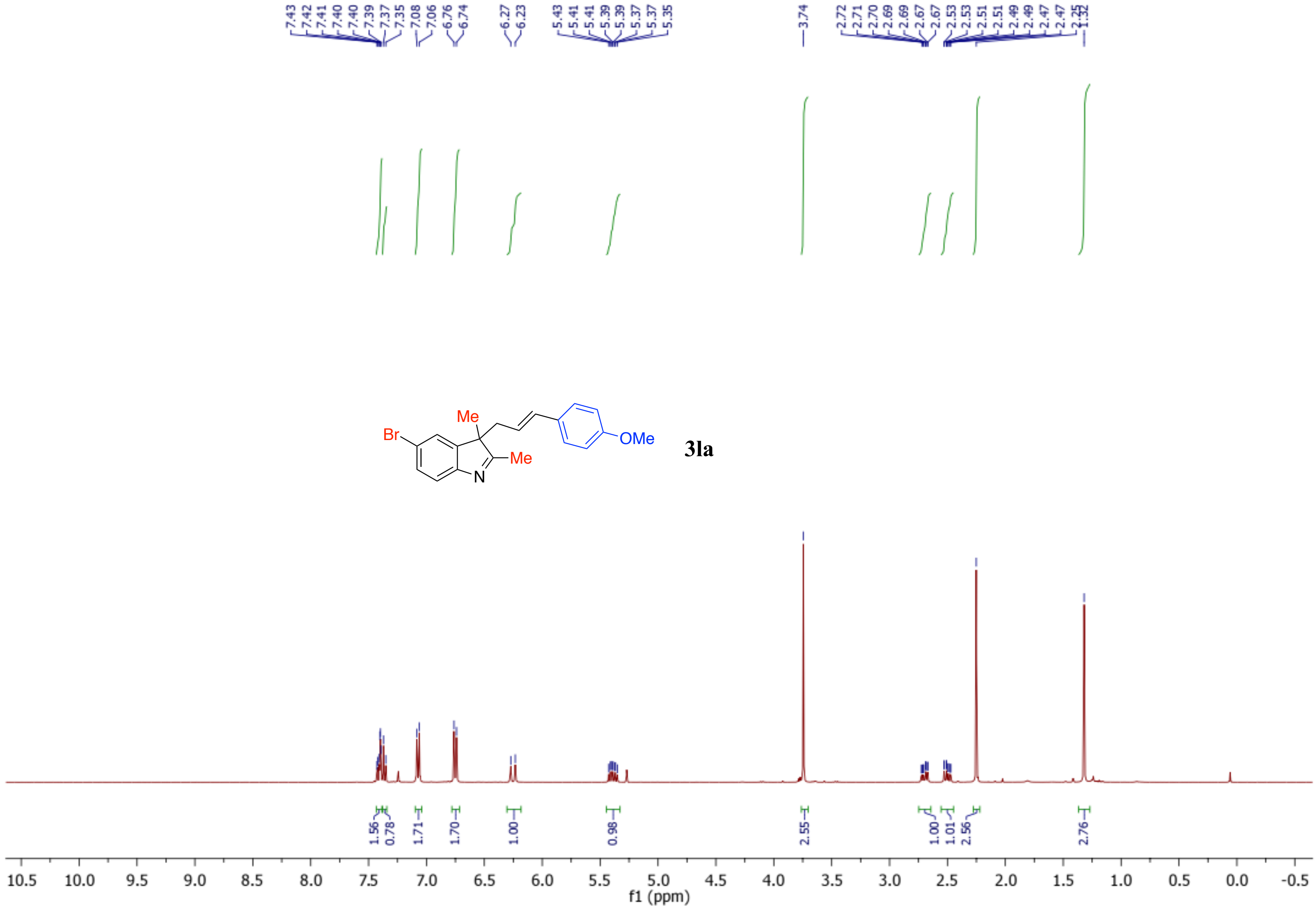
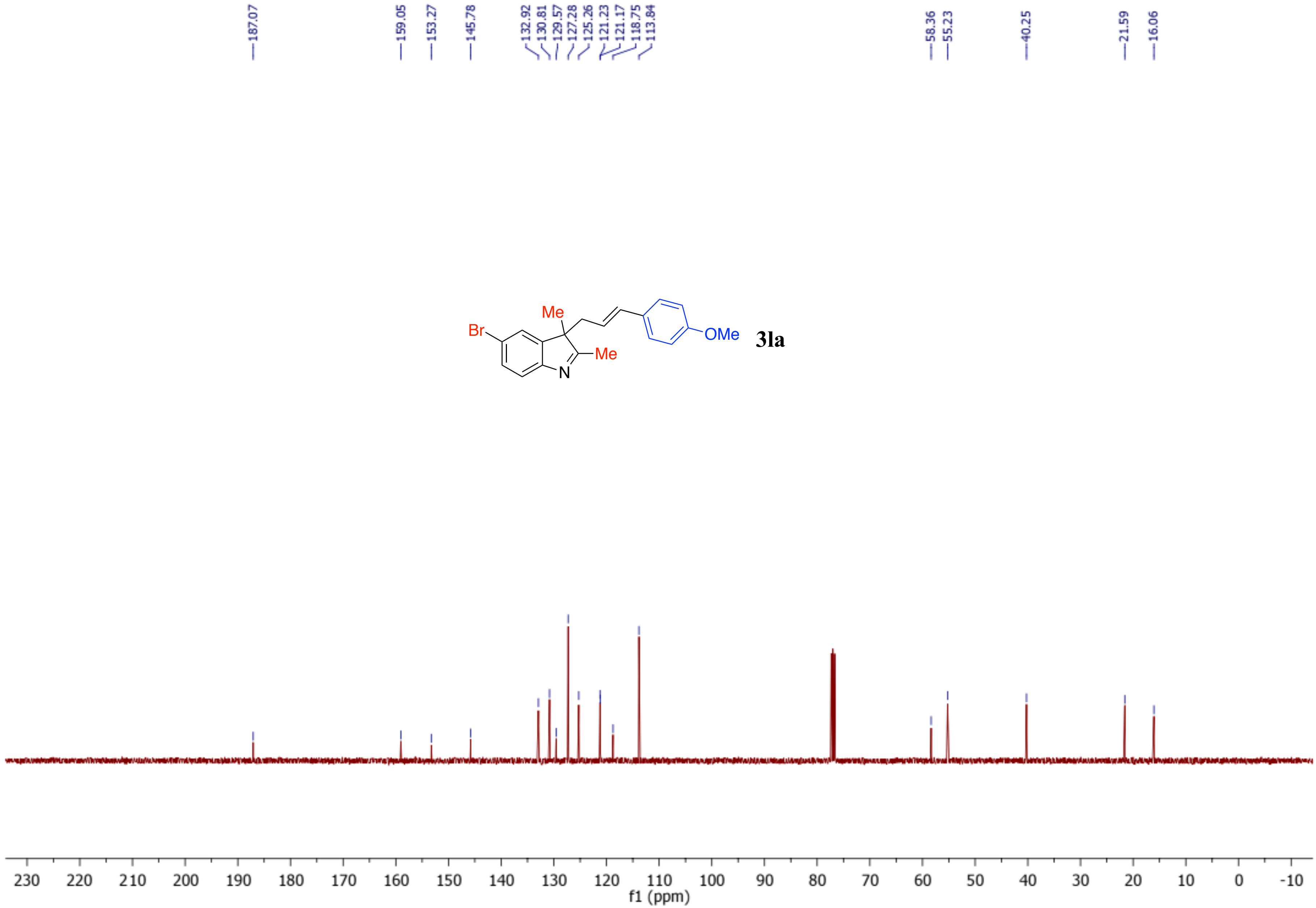
130.81
129.57
127.90
127.27
122.39
121.18
120.71
113.84
58.30
55.22
40.25
21.59
16.04
Cl
Me
Me
N
OMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ka



7.43 7.42 7.41 7.40 7.40 7.39 7.37 7.35 7.08 7.06 6.76 6.74
6.27 6.23
5.43 5.41 5.41 5.39 5.39 5.37 5.37 5.35
3.74
2.72 2.71 2.70 2.69 2.69 2.67 2.67 2.53 2.53 2.51 2.51 2.49 2.49 2.47 2.47 2.25 1.32
Br
Me
Me
N
OMe
1.56 0.78 1.71 1.70 1.00 0.98 2.55 1.00 1.01 2.56 2.76
10.5 10.0 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 0.0 -0.5
f1 (ppm)

3la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55.23
40.25
21.59
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Me
Me
N
OMe
3la
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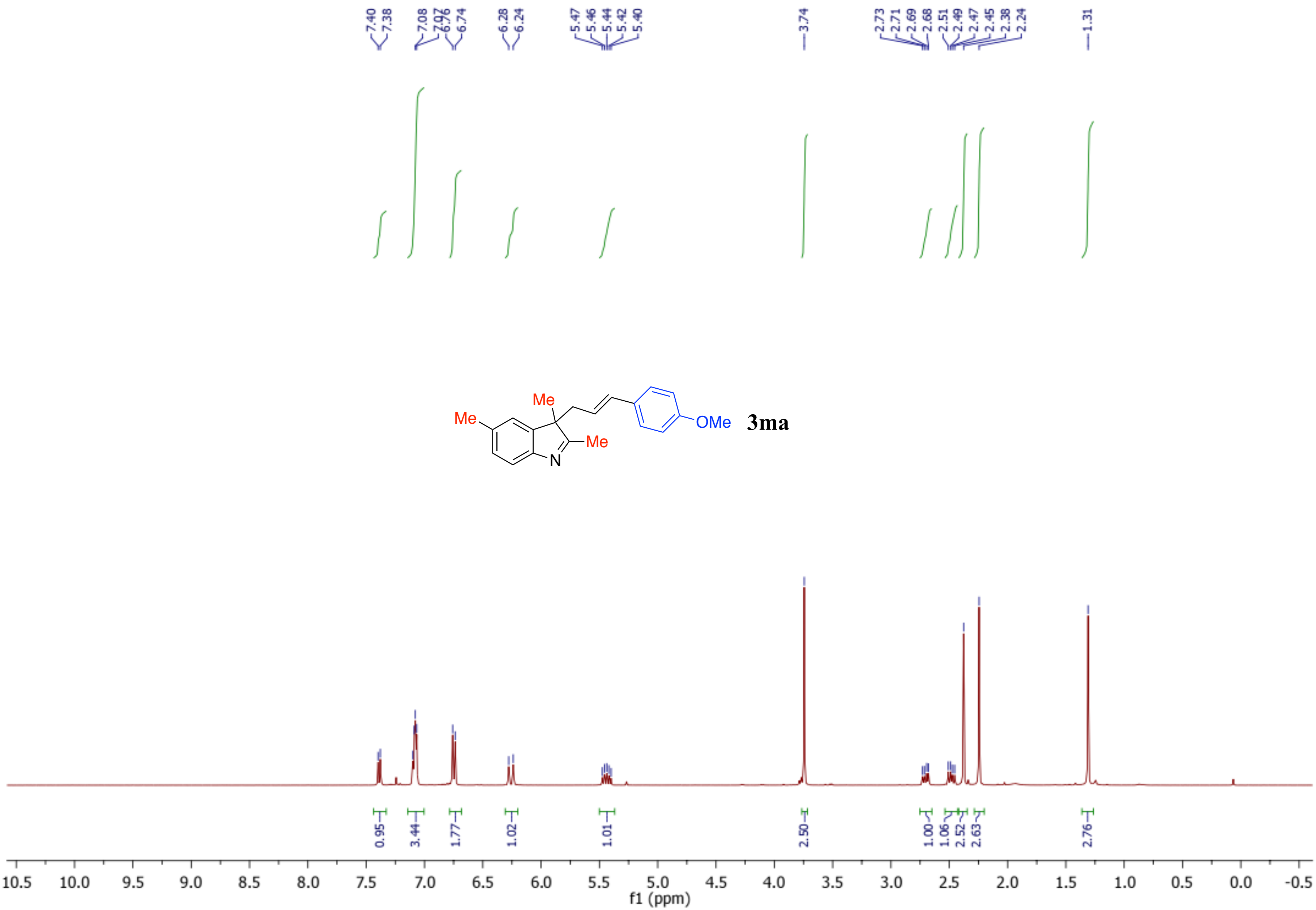
f1 (ppm)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3.74
2.73
2.71
2.69
2.68
2.51
2.49
2.47
2.45
2.38
2.24
1.31
Me
Me
Me
N
OMe
0.95
3.44
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1.00
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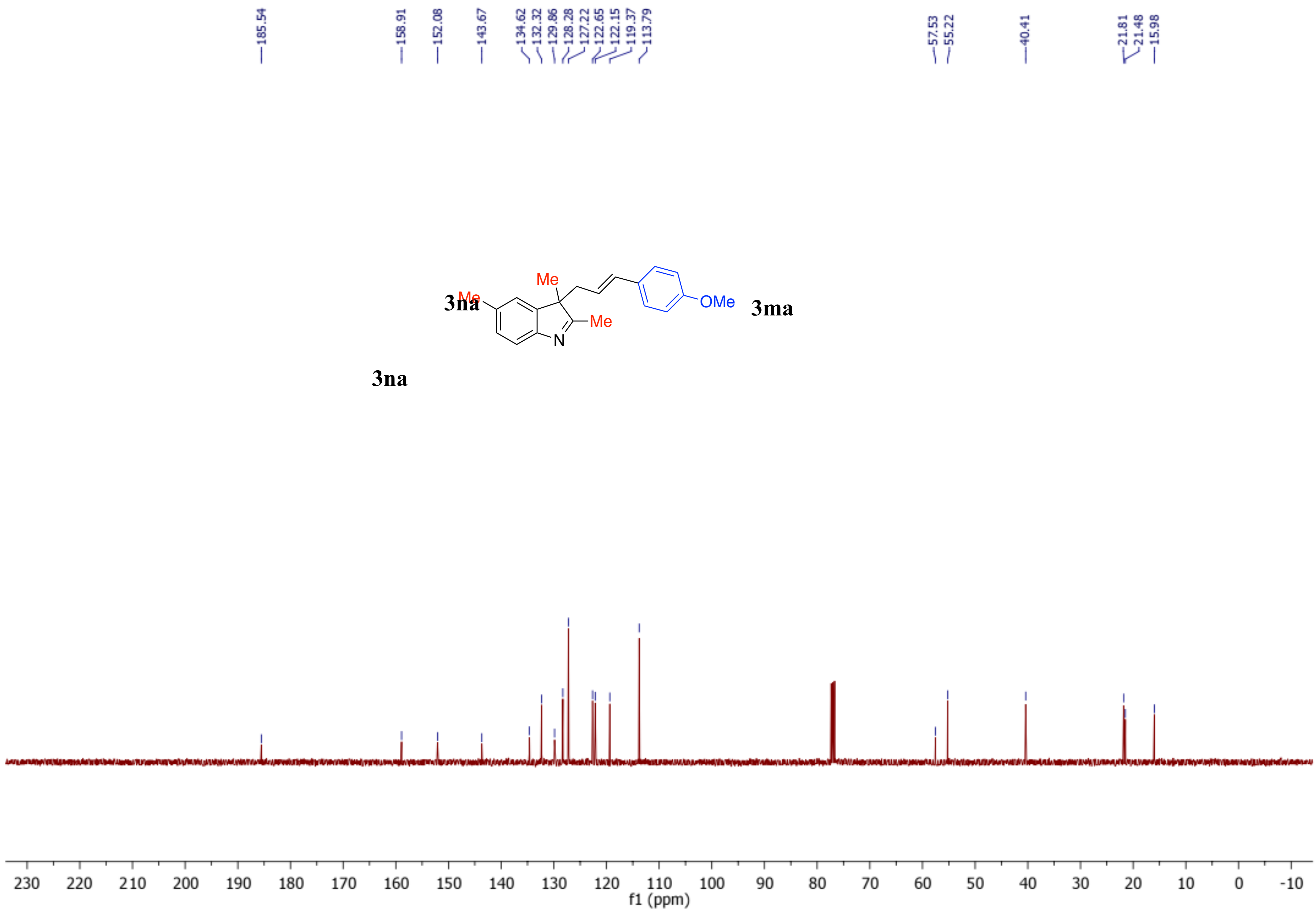
f1 (ppm)

3ma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113.79
57.53
55.22
40.41
21.81
21.48
15.98
3na
Me
Me
Me
N
OMe
3ma
3na
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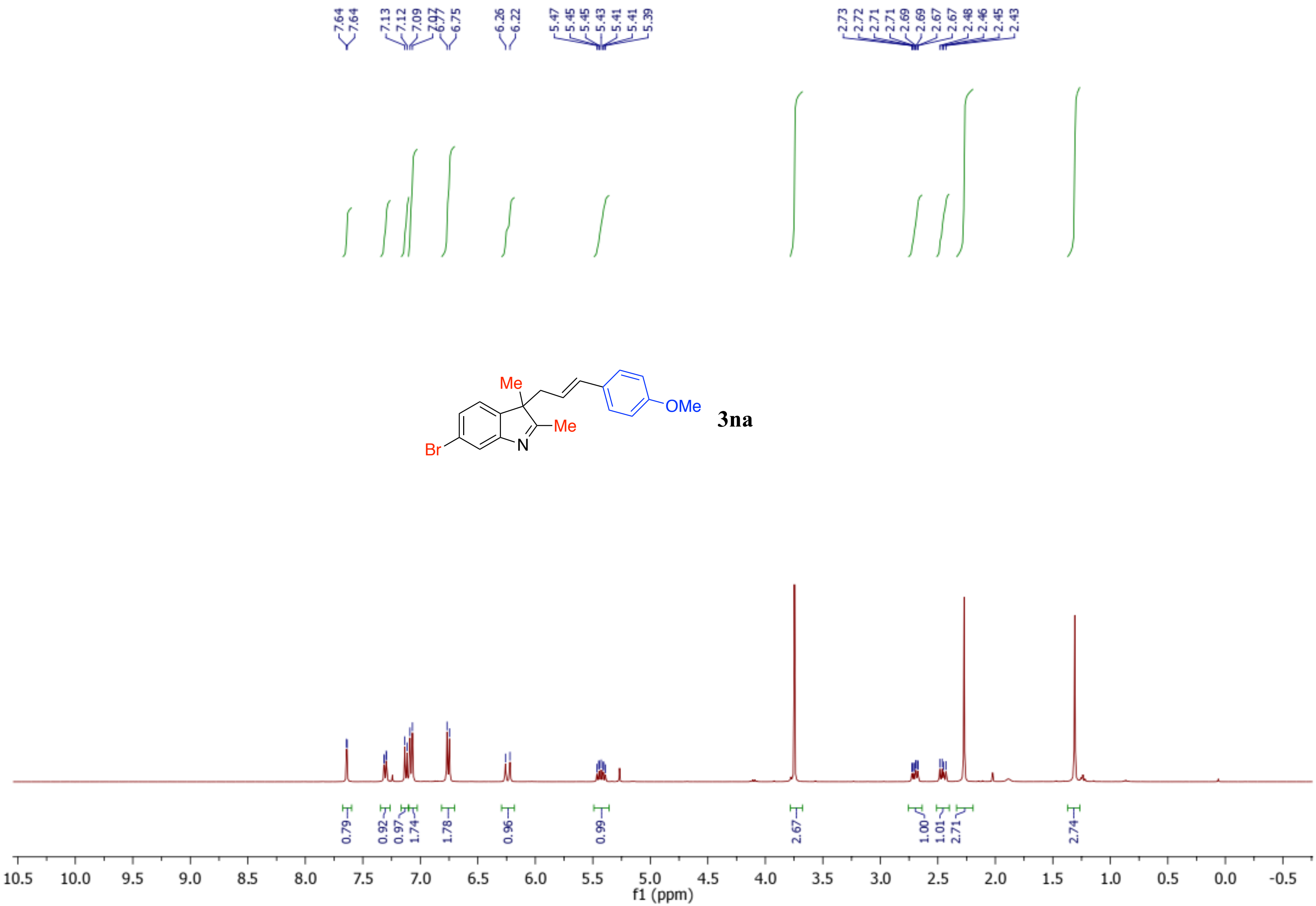
f1 (ppm)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5.41
5.39
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2.67
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2.46
2.45
2.43
Me
Me
Br
N
OMe
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0.97
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1.78
0.96
0.99
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1.00
1.01
2.71
2.74
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9.0
8.5
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7.0
6.5
6.0
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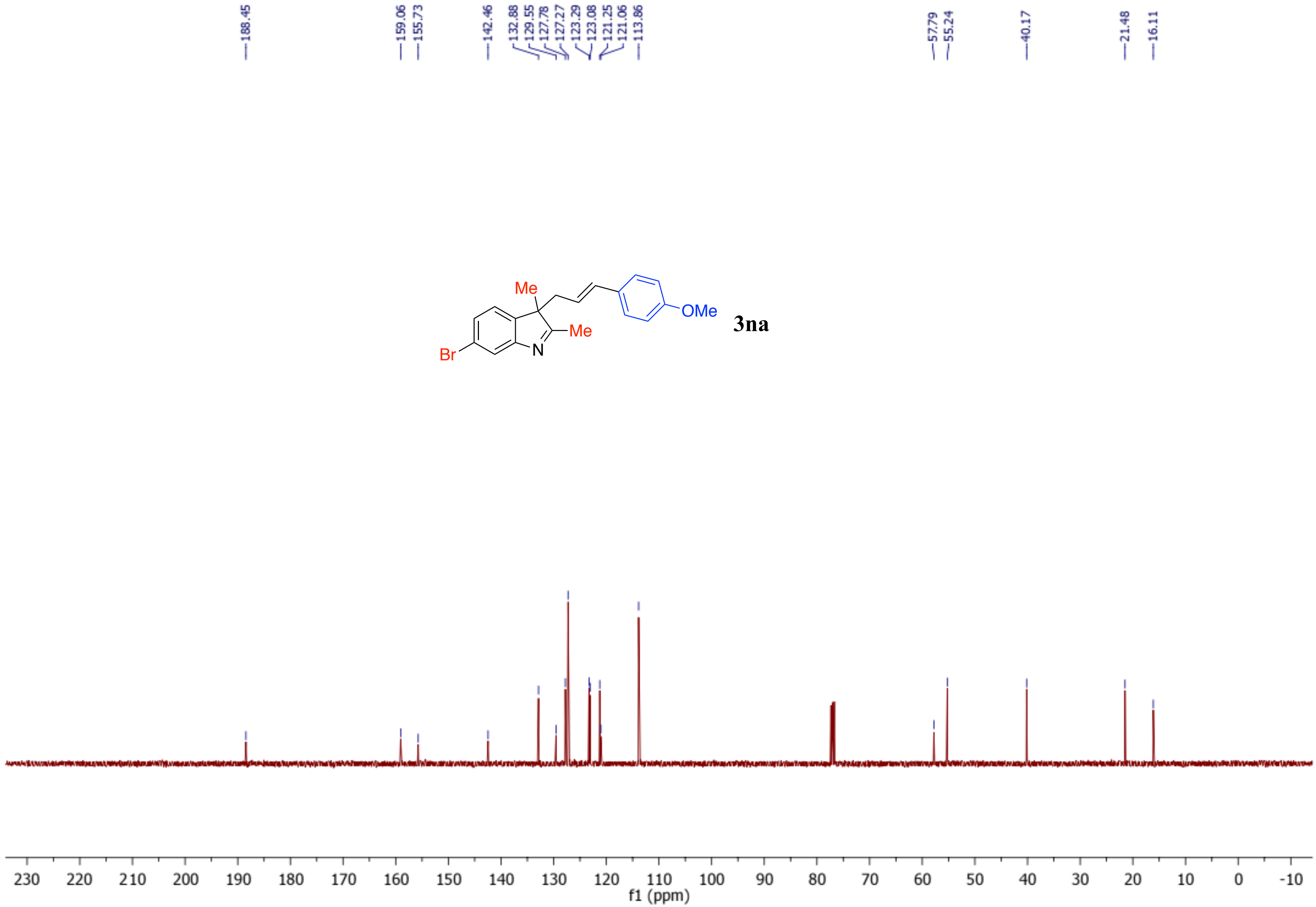
f1 (ppm)

3na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57.79
55.24
40.17
21.48
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Me
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Br
N
OMe
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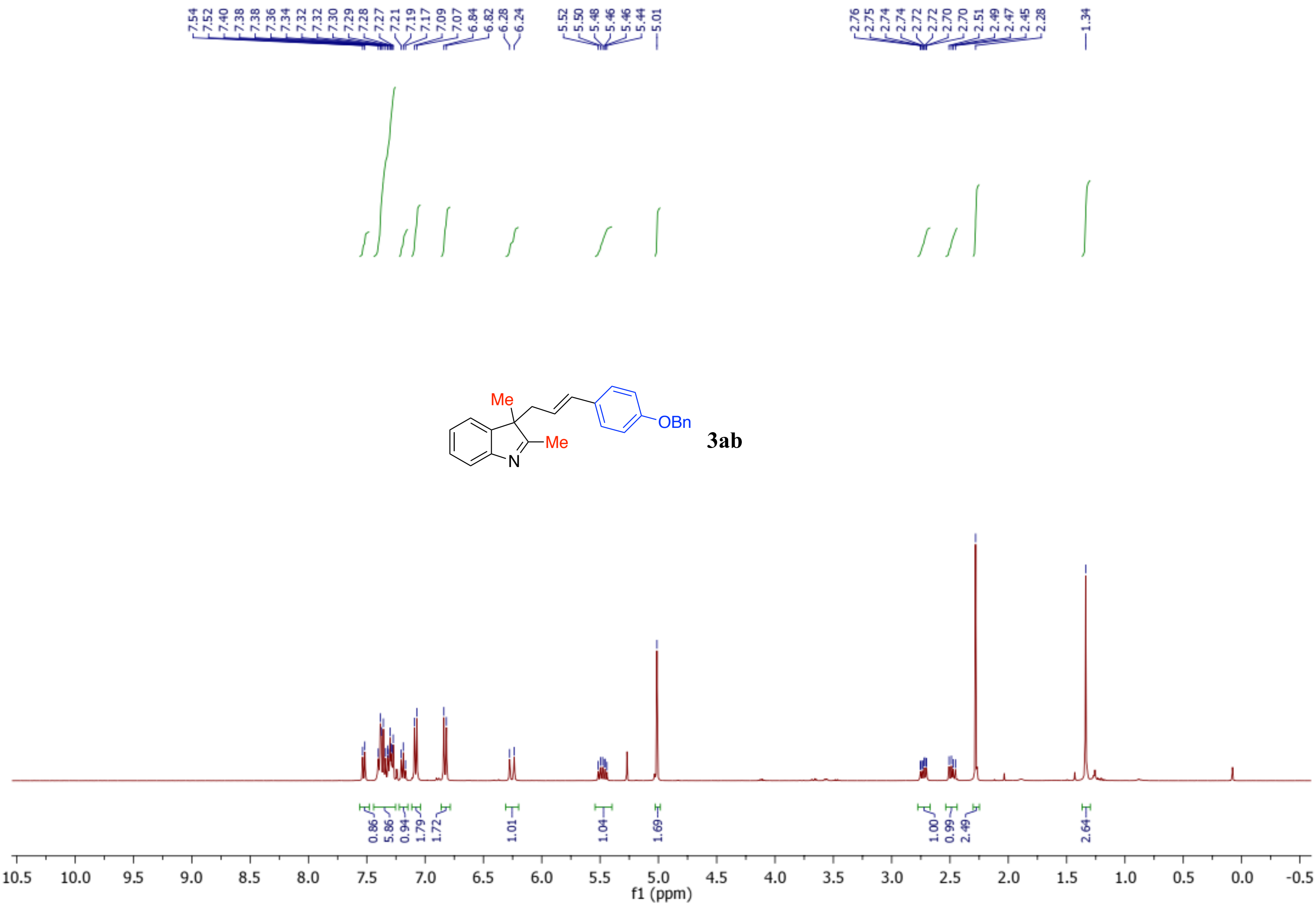
f1 (ppm)

3na



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7.19
7.17
7.09
7.07
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6.24
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5.50
5.48
5.46
5.46
5.44
5.01
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2.74
2.72
2.72
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2.70
2.51
2.49
2.47
2.45
2.28
1.34
Me
Me
N
OBn
3ab
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5.86
0.94
1.79
1.72
1.01
1.04
1.69
1.00
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9.0
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8.0
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6.0
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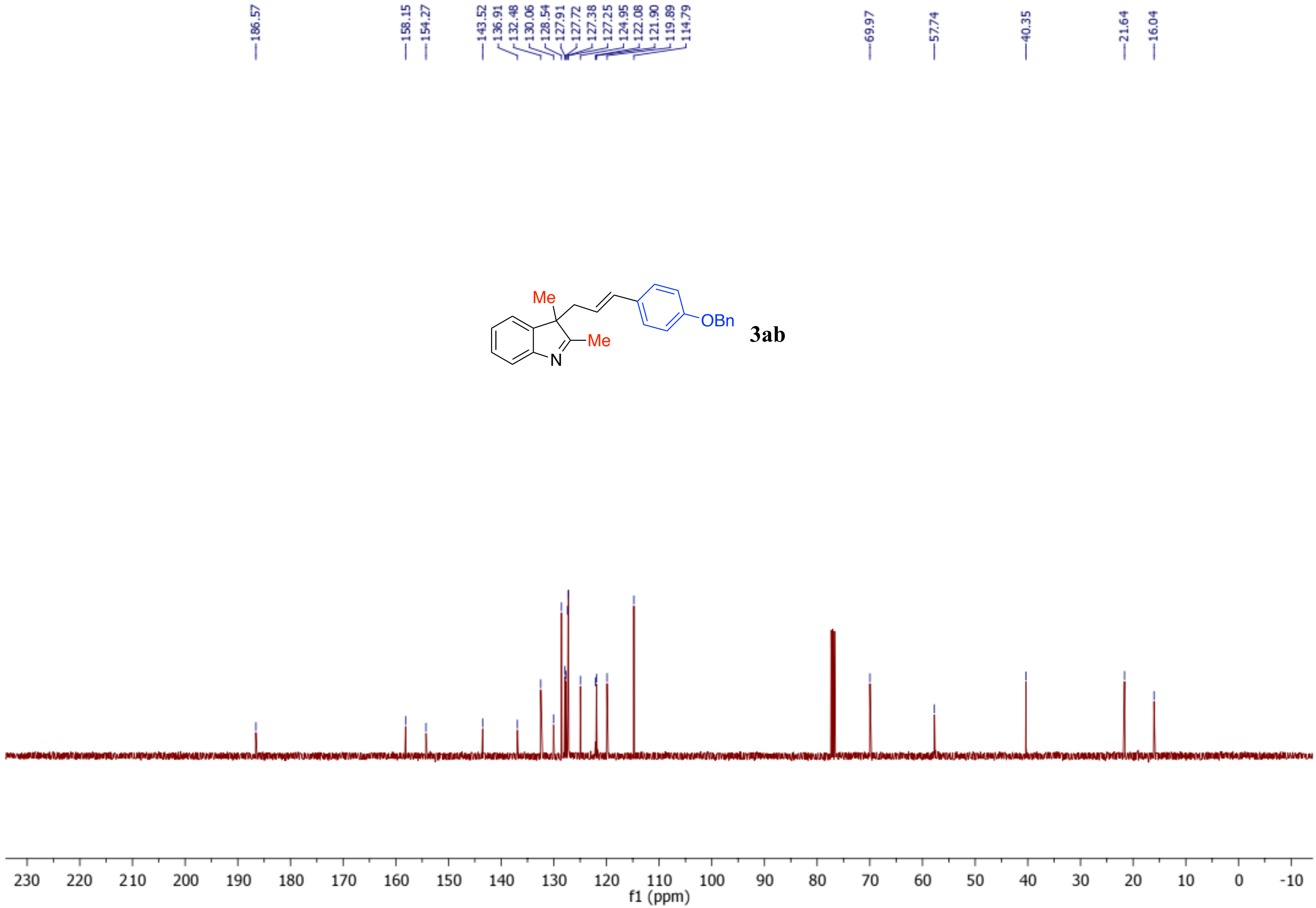
-0.5
f1 (ppm)



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122.08
121.90
119.89
114.79
69.97
57.74
40.35
21.64
16.04
Me
Me
N
OBn
230
220
210
200
190
180
170
160
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100
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80
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60
50
40
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20
10
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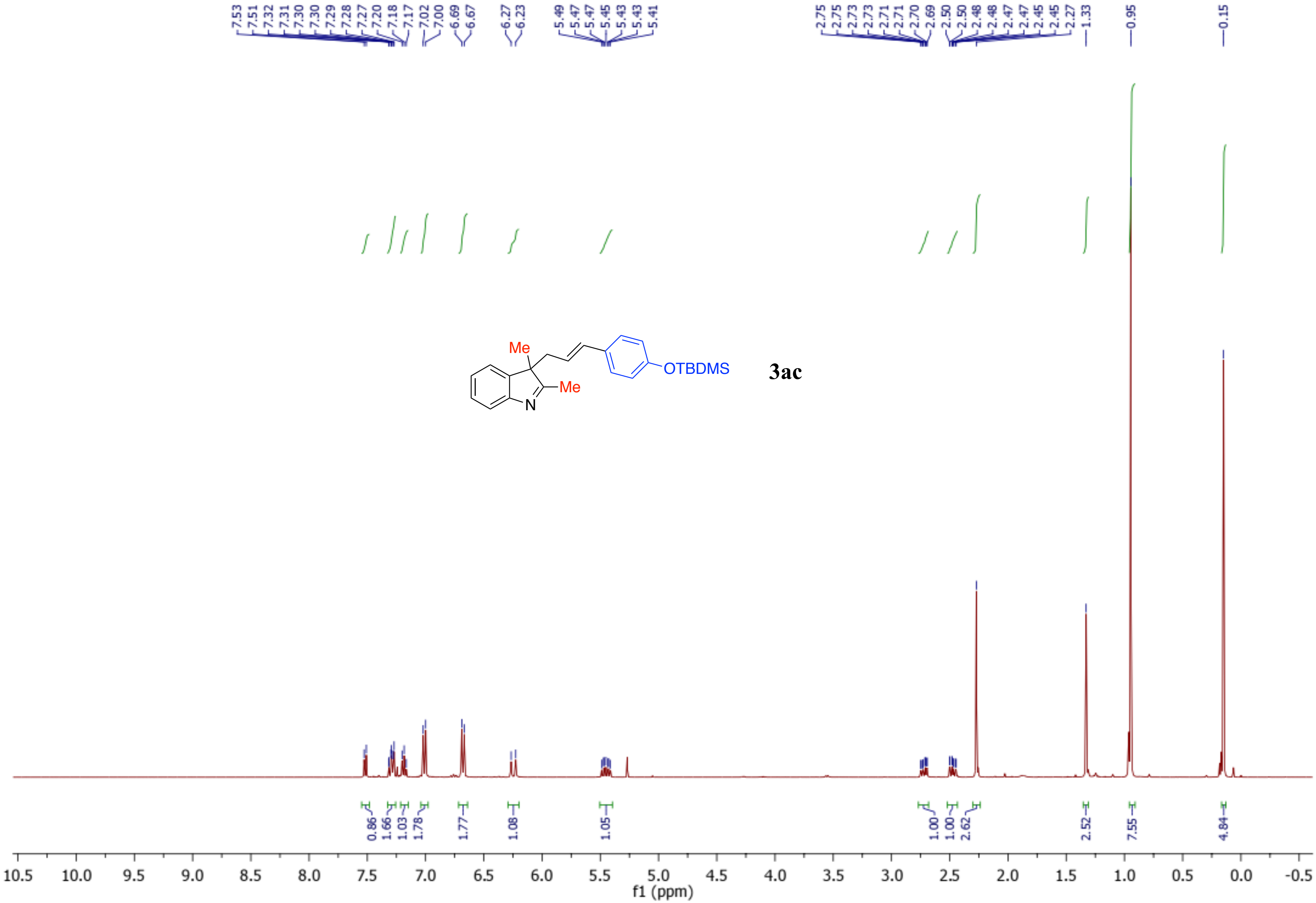
-10
f1 (ppm)

3ab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6.67
6.27
6.23
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5.47
5.47
5.45
5.43
5.43
5.41
2.75
2.75
2.73
2.73
2.71
2.71
2.70
2.69
2.50
2.50
2.48
2.47
2.47
2.45
2.45
2.27
1.33
0.95
0.15
Me
Me
N
OTBDMS
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1.66
1.03
1.78
1.77
1.08
1.05
1.00
1.00
2.62
2.52
7.55
4.84
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.5
2.0
1.5
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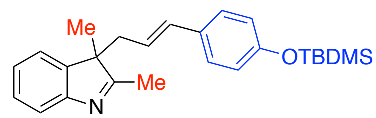
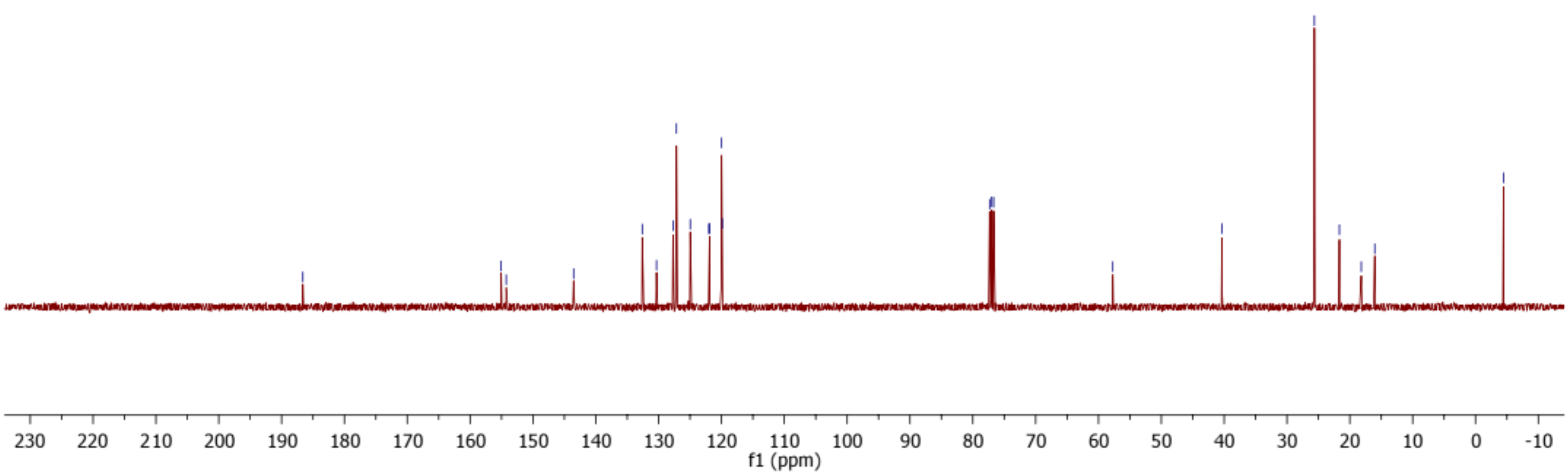
0.0
-0.5
f1 (ppm)

3ac


Me
Me
N
OTBDMS

3ac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143.52
132.60
130.32
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127.17
124.96
122.02
121.88
119.98
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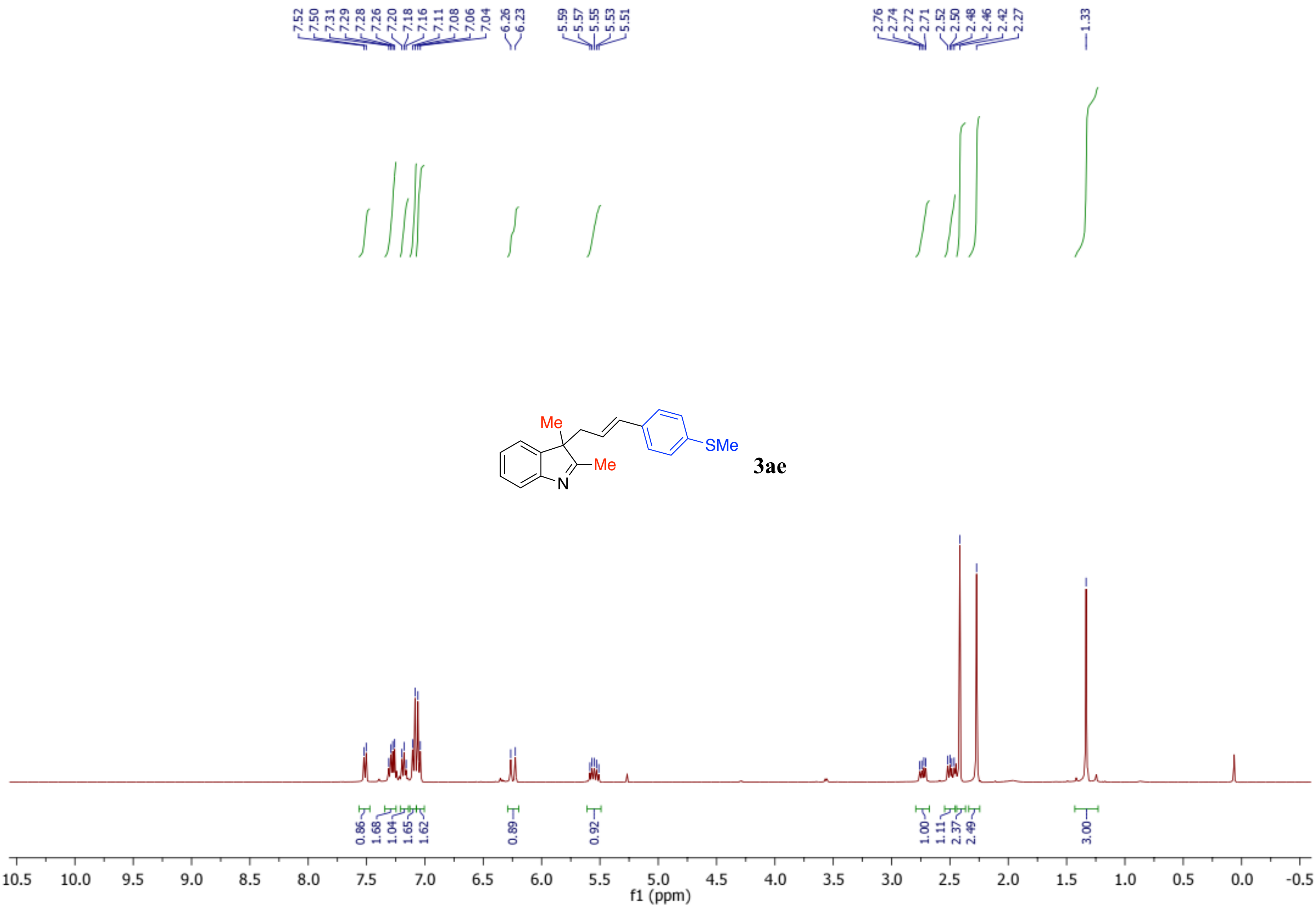
77.32
77.00
76.69
57.73
40.35
25.64
21.66
18.17
16.03
-4.46
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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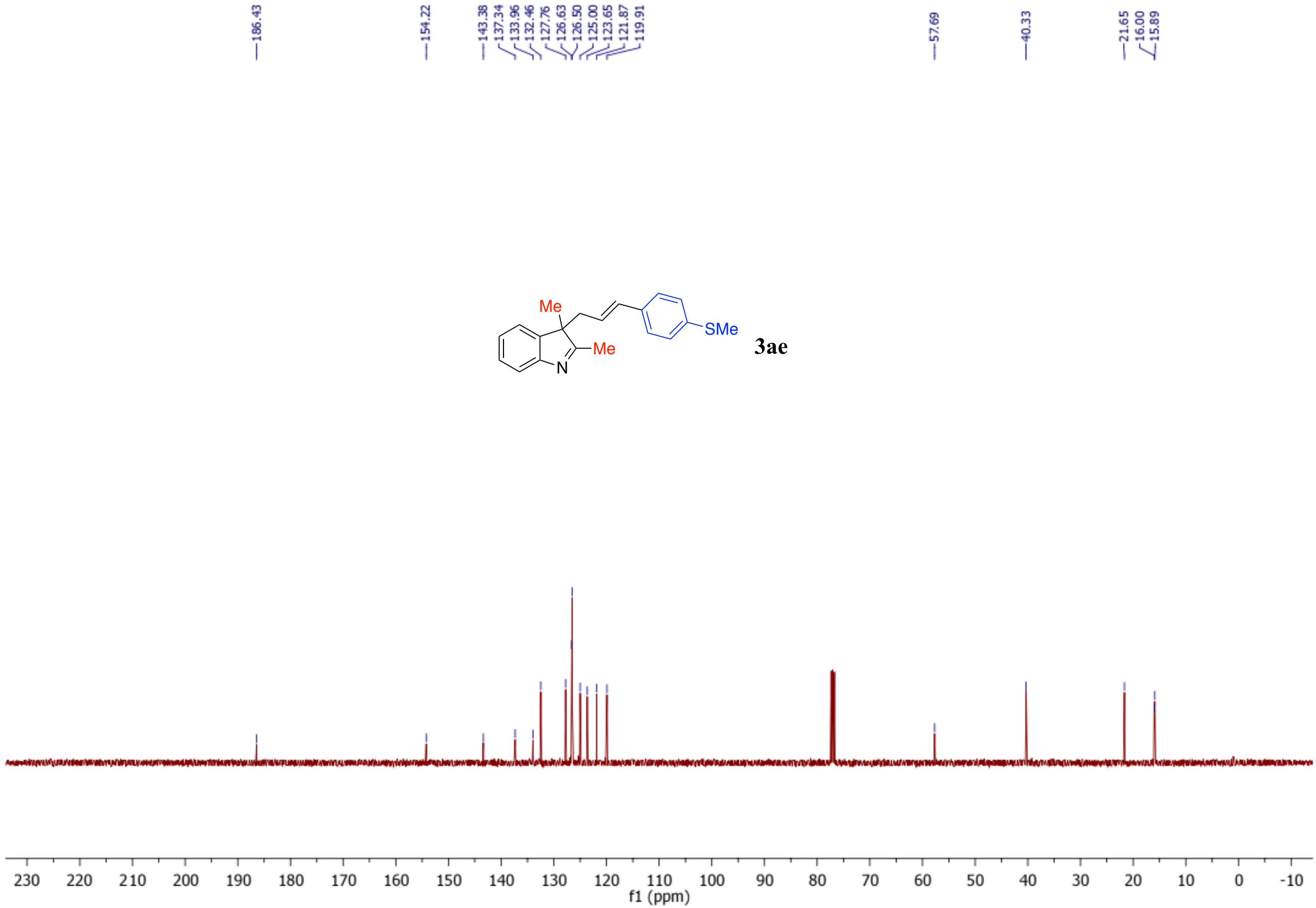
7.11
7.08
7.06
7.04
6.26
6.23
5.59
5.57
5.55
5.53
5.51
2.76
2.74
2.72
2.71
2.52
2.50
2.48
2.46
2.42
2.27
1.33
Me
Me
N
SMe
3ae
0.86
1.68
1.04
1.65
1.62
0.89
0.92
1.00
1.11
2.37
2.49
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



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143.38
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133.96
132.46
127.76
126.63
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125.00
123.65
121.87
119.91
57.69
40.33
21.65
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Me
N
SMe
3ae
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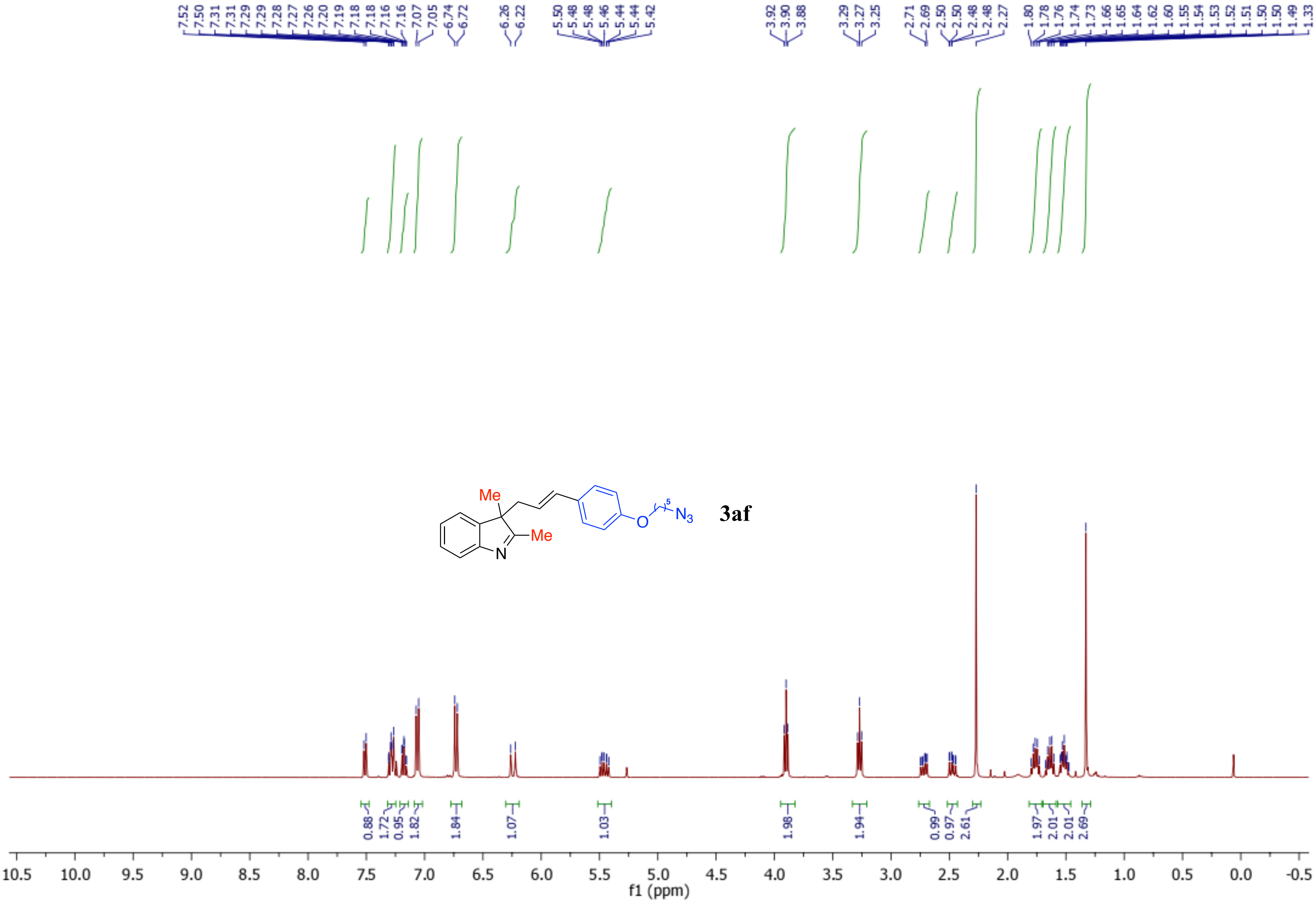
f1 (ppm)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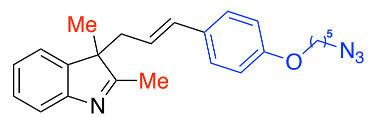
Me
Me
N
O
5
N3
3af
0.88 1.72 0.95 1.82 1.84 1.07 1.03 1.98 1.94 0.99 0.97 2.61 1.97 2.01 2.01 2.69
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



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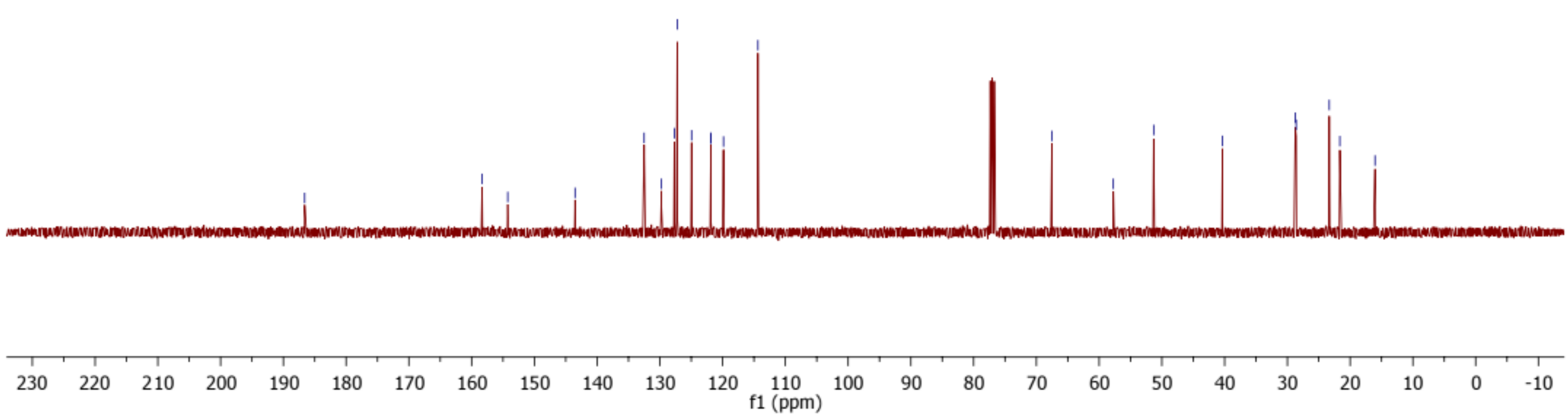
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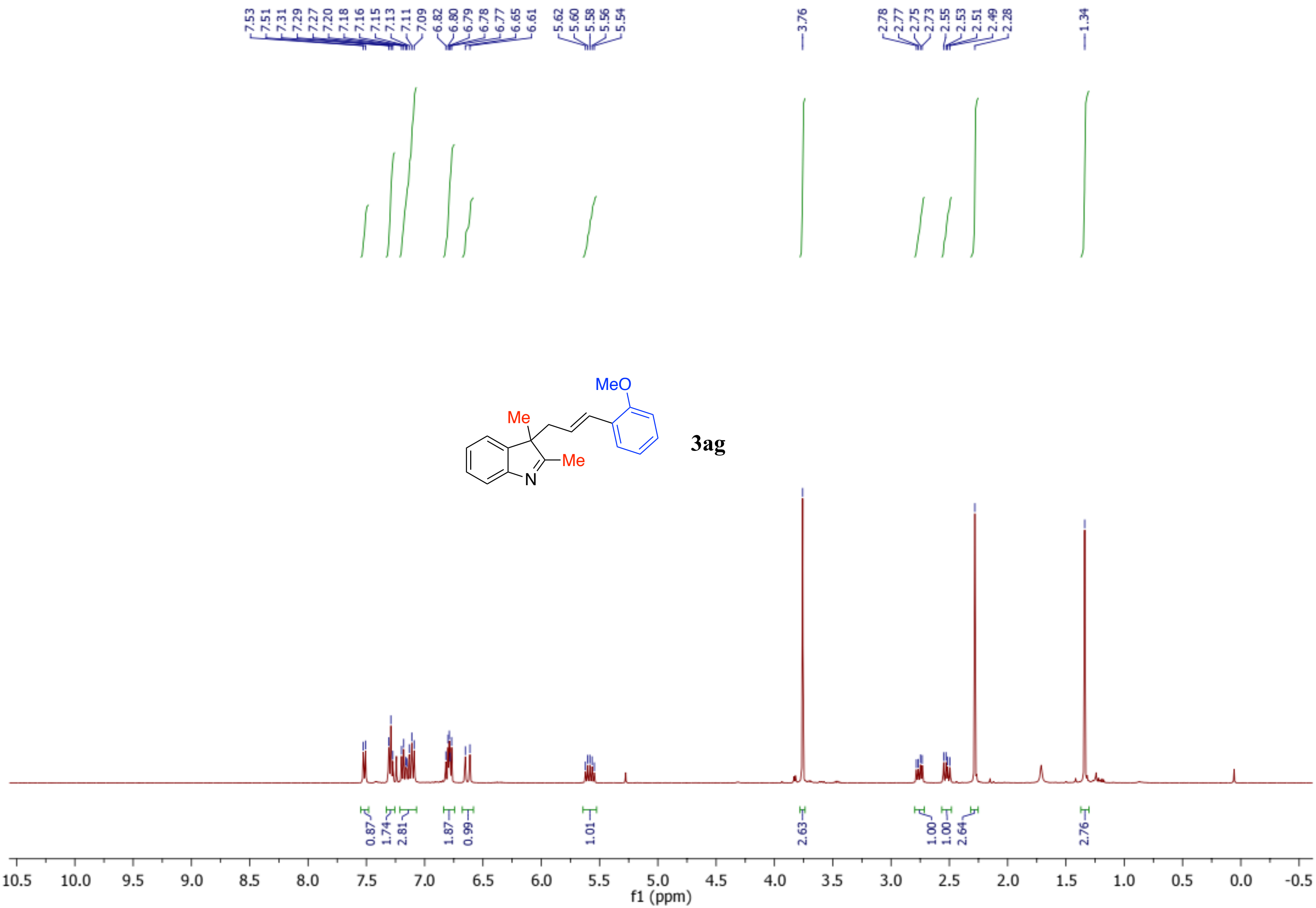
121.90
121.87
119.86
114.37
67.53
57.74
51.30
40.35
28.74
28.60
23.33
21.64
16.03
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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6.82
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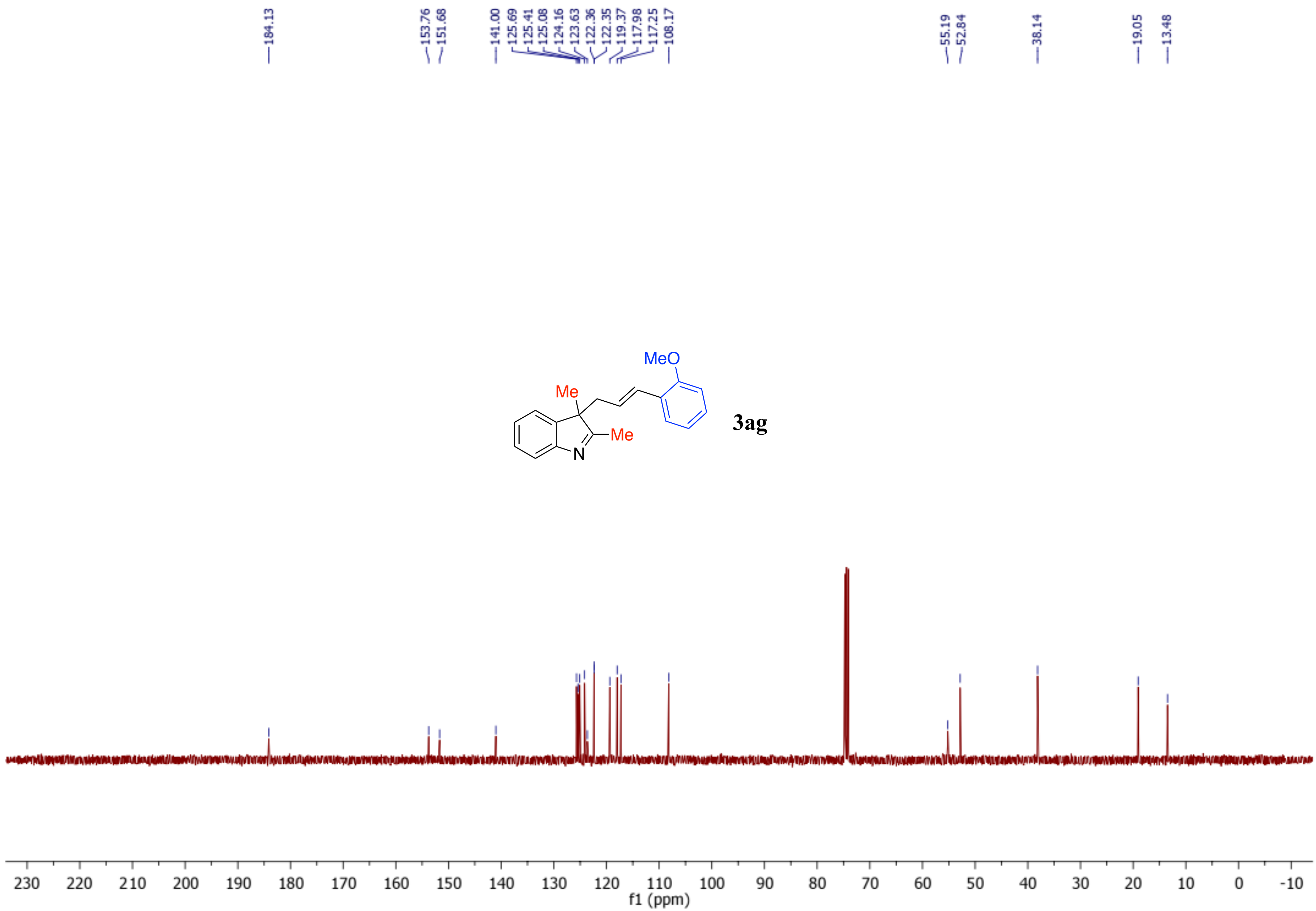
6.79
6.78
6.77
6.65
6.61
5.62
5.60
5.58
5.56
5.54
3.76
2.78
2.77
2.75
2.73
2.55
2.53
2.51
2.49
2.28
1.34
MeO
Me
Me
N
0.87
1.74
2.81
1.87
0.99
1.01
2.63
1.00
1.00
2.64
2.76
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3ag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122.36
122.35
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117.98
117.25
108.17
55.19
52.84
38.14
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13.48
MeO
Me
Me
N
3ag
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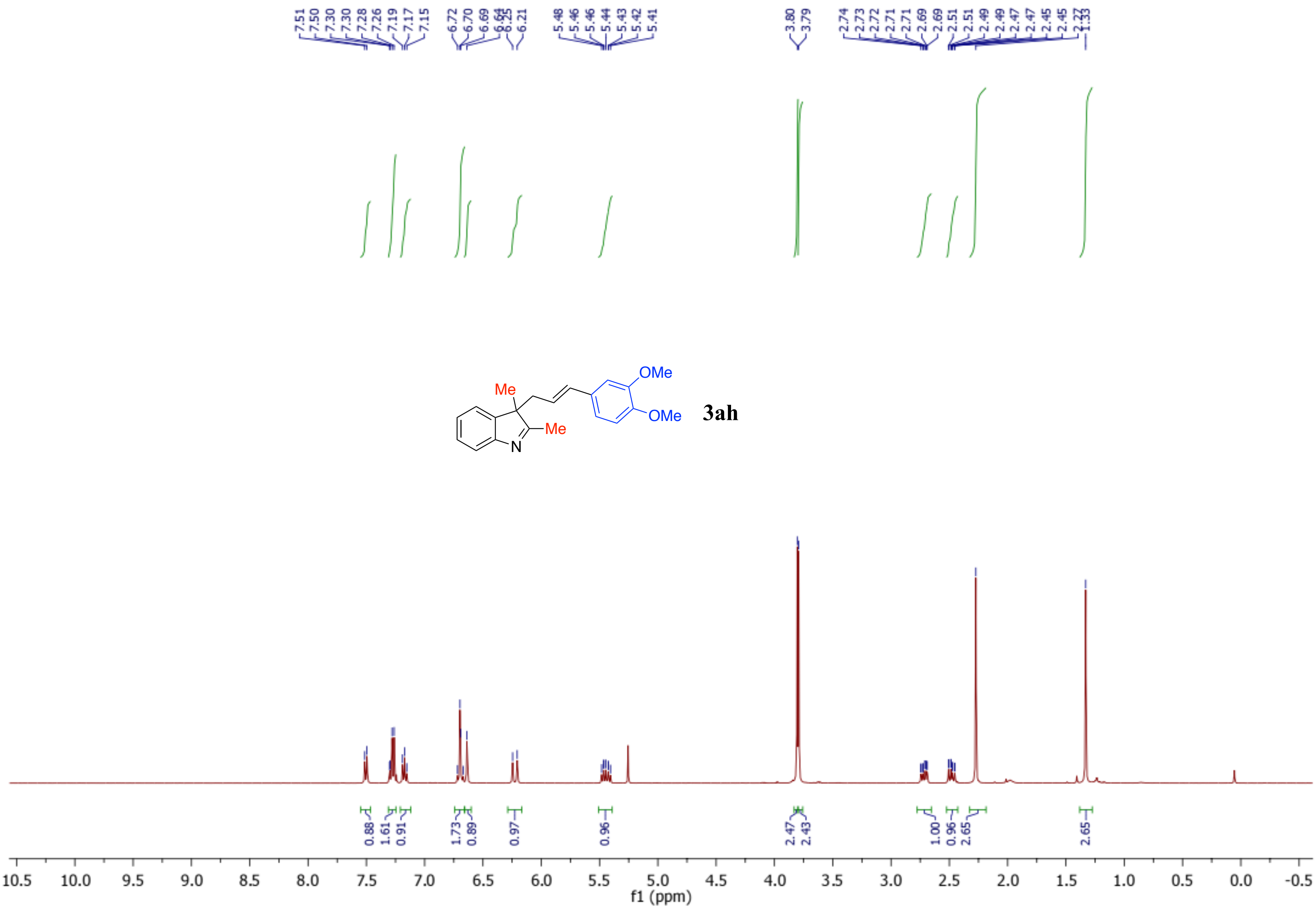
f1 (ppm)



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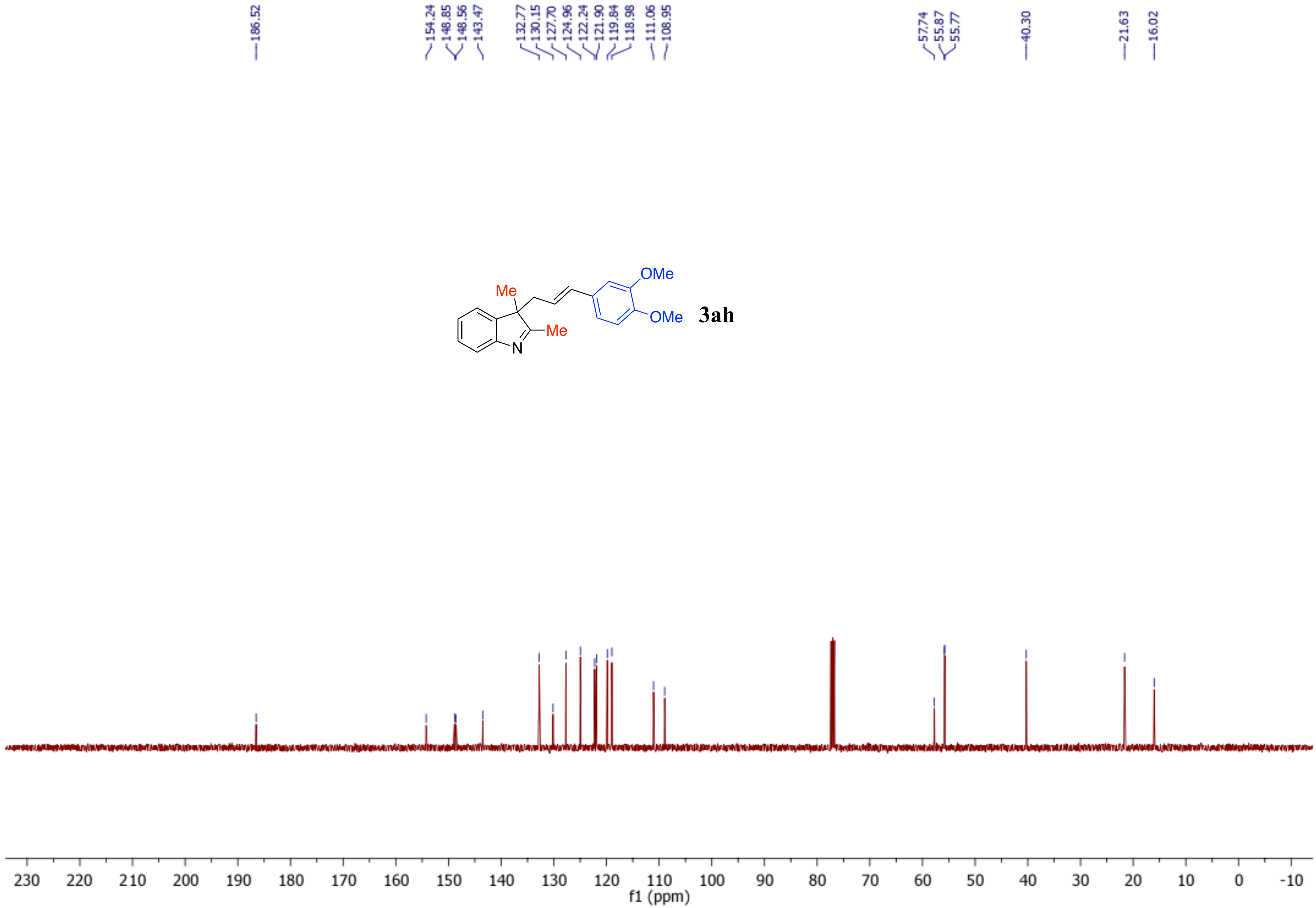
6.72 6.70 6.69 6.64 6.25 6.21
5.48 5.46 5.46 5.44 5.43 5.42 5.41
3.80 3.79
2.74 2.73 2.72 2.71 2.71 2.69 2.69 2.51 2.51 2.49 2.49 2.47 2.45 2.45 2.27 1.33
Me
Me
N
OMe
OMe
3ah
0.88 1.61 0.91 1.73 0.89 0.97 0.96 2.47 2.43 1.00 0.96 2.65 2.65
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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111.06
108.95
57.74
55.87
55.77
40.30
21.63
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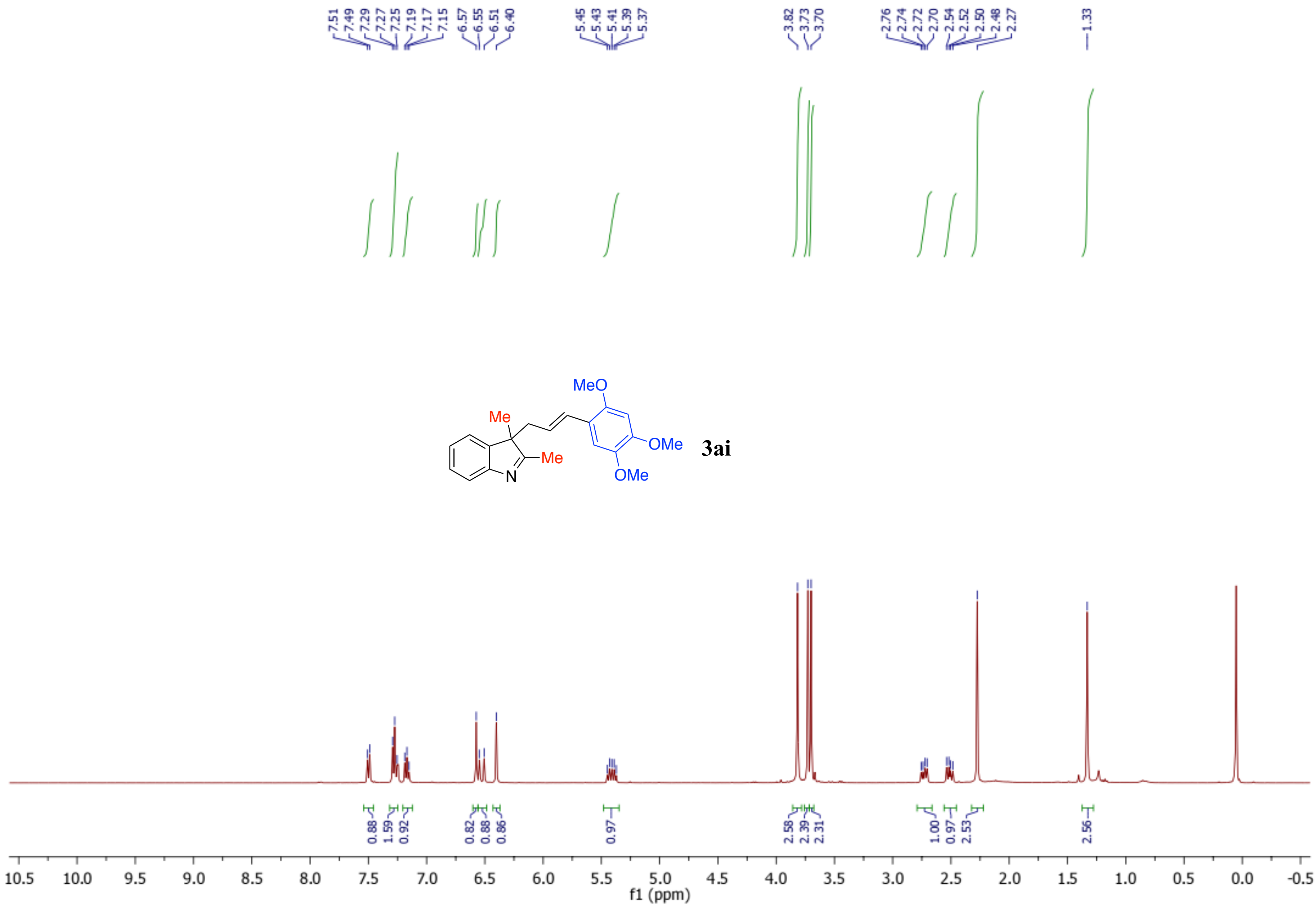
Me
Me
N
OMe
OMe
3ah
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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5.45 5.43 5.41 5.39 5.37
3.82 3.73 3.70
2.76 2.74 2.72 2.70 2.54 2.52 2.50 2.48 2.27
1.33
MeO
Me
Me
N
OMe
OMe
3ai
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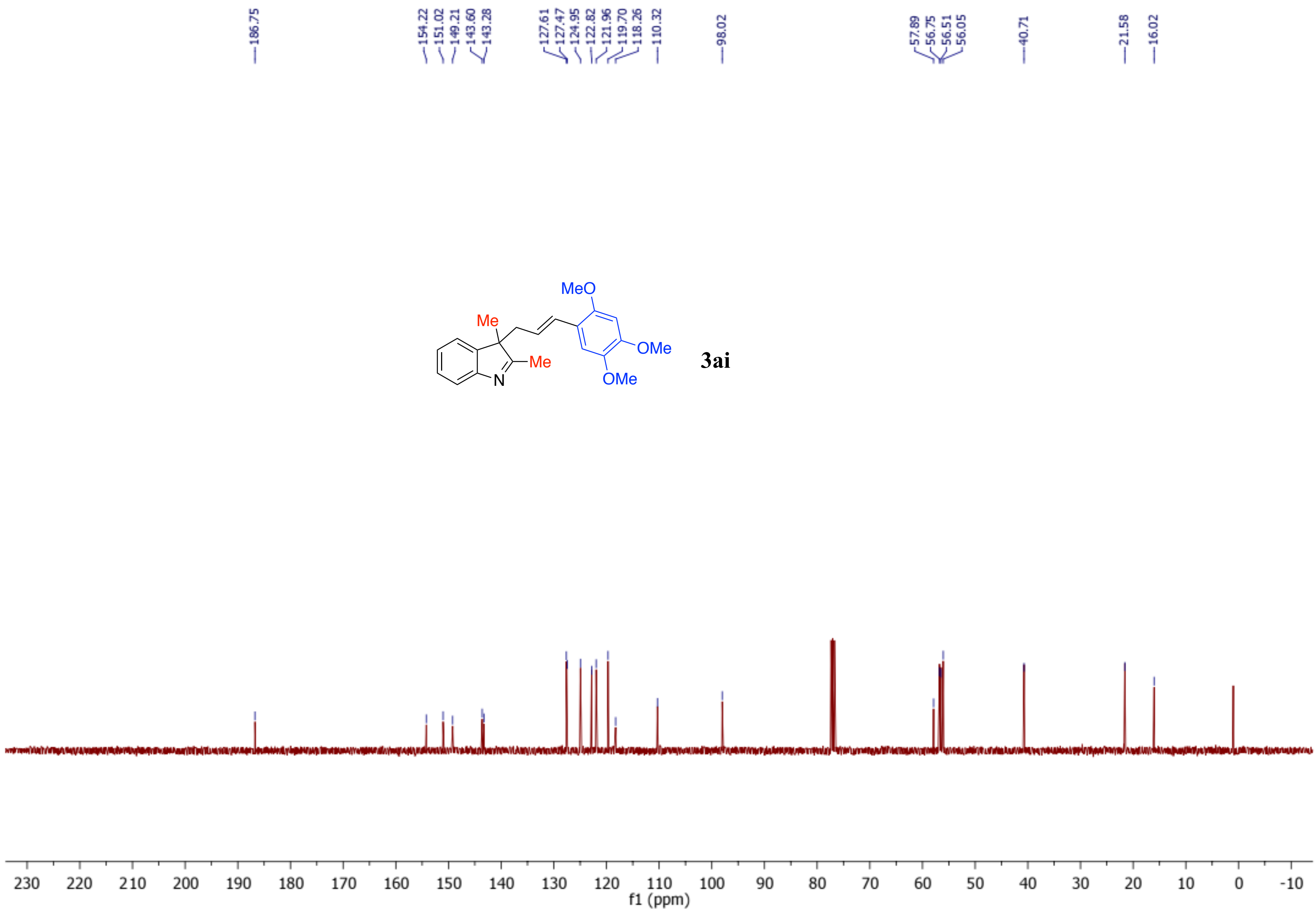
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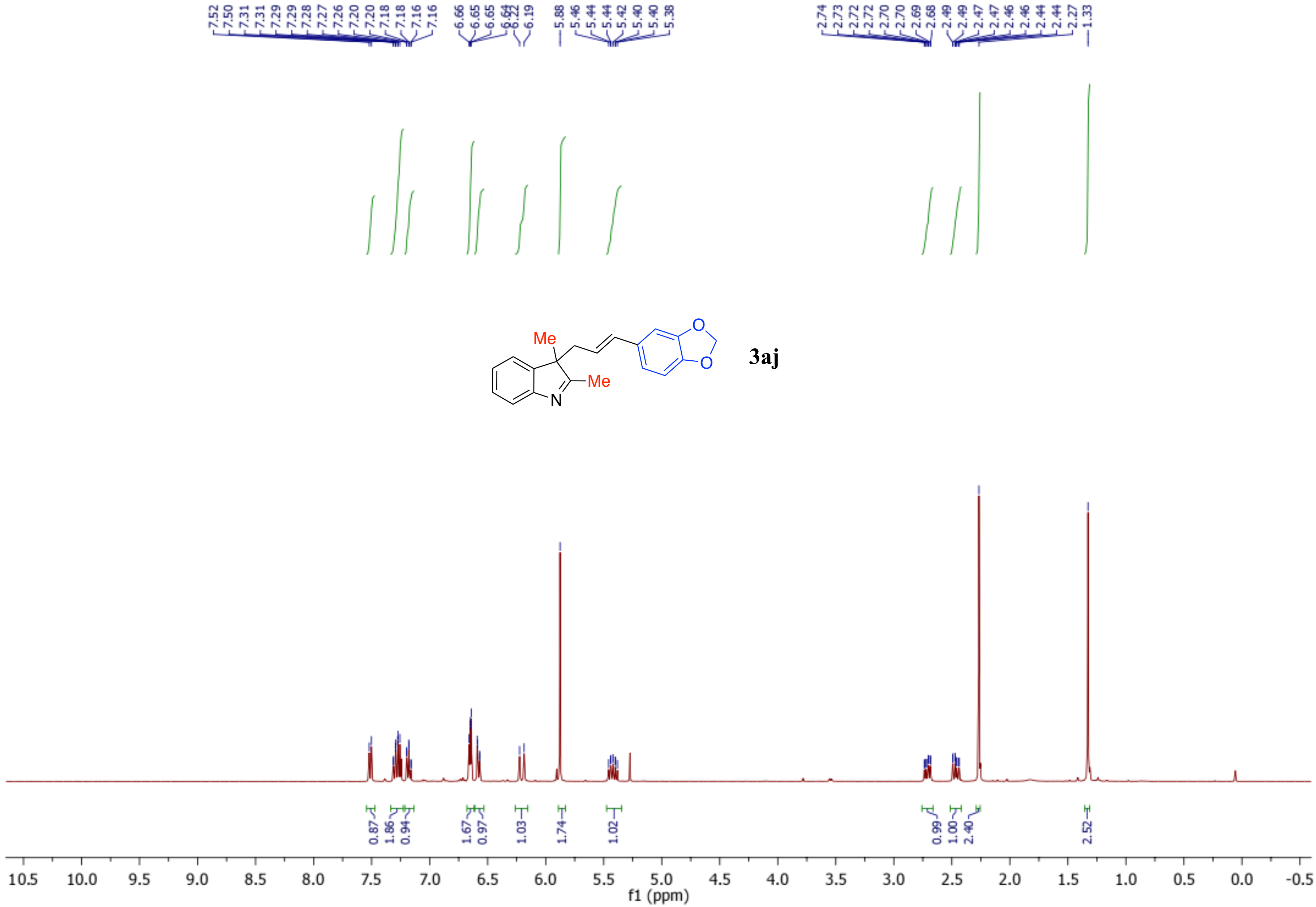
118.26
110.32
98.02
57.89
56.75
56.51
56.05
40.71
21.58
16.02
MeO
Me
OMe
Me
N
OMe
3ai
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



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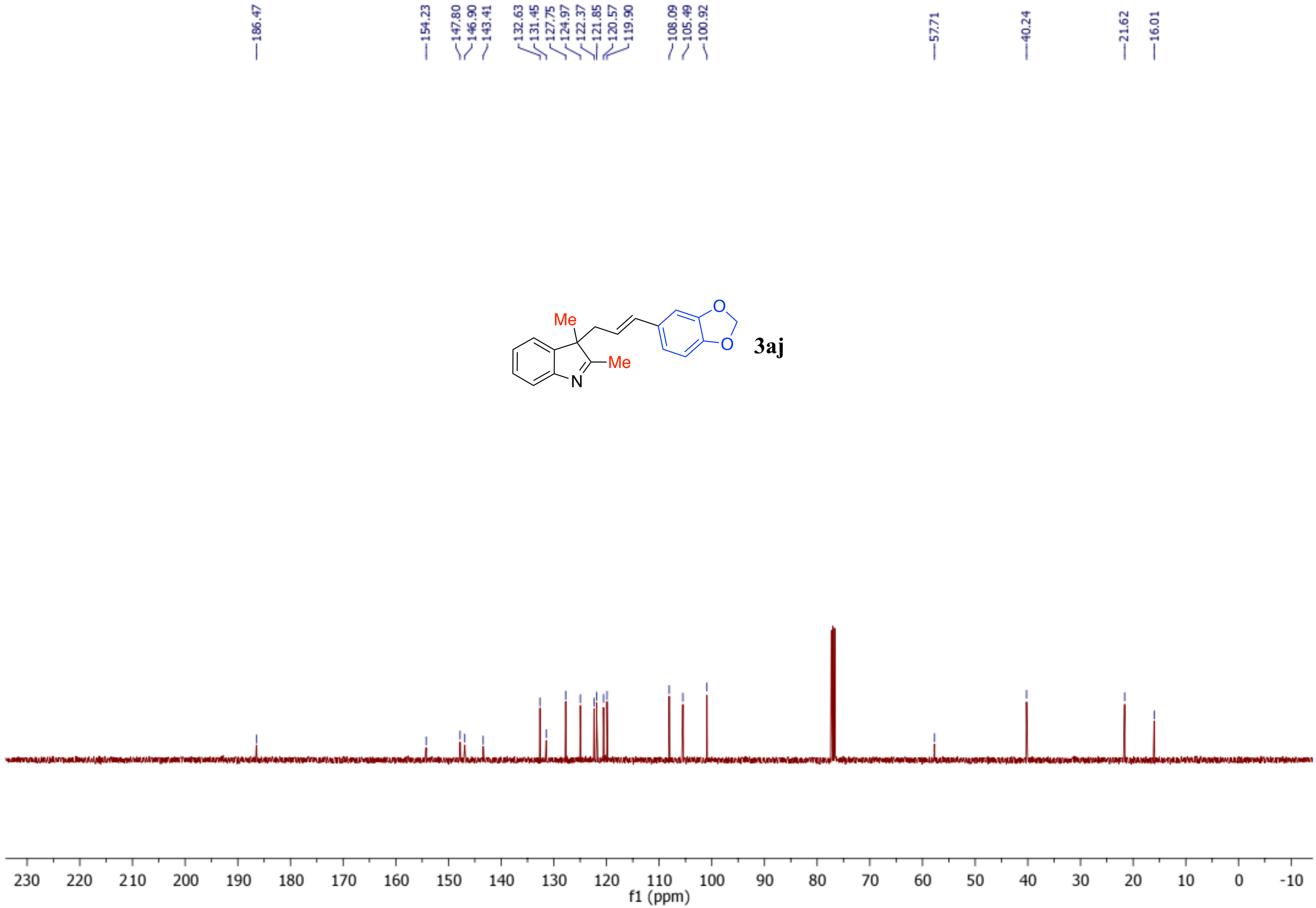

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119.90
108.09
105.49
100.92
57.71
40.24
21.62
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Me
Me
N
O
O
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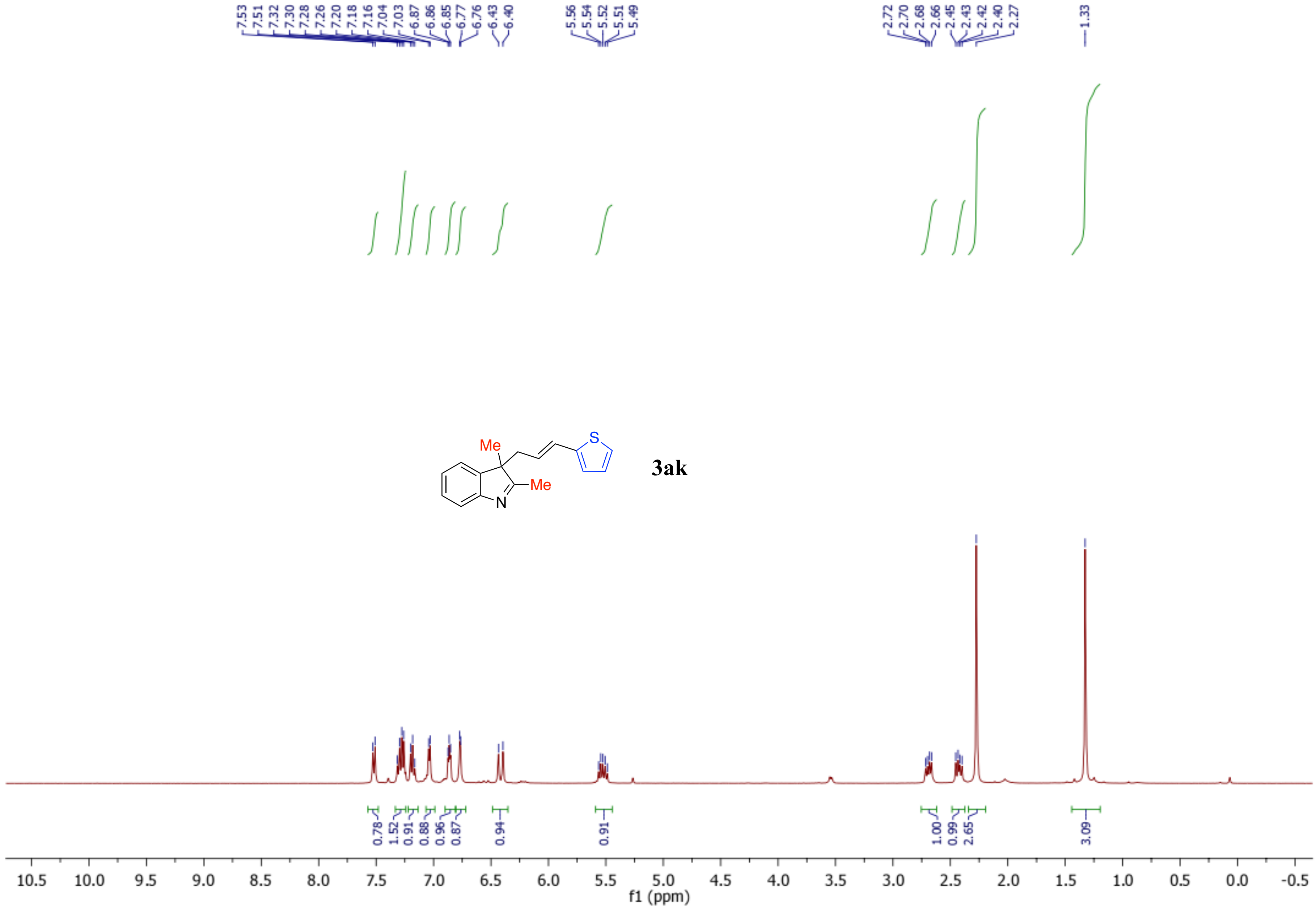
f1 (ppm)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6.86
6.85
6.77
6.76
6.43
6.40
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5.52
5.51
5.49
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2.68
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2.27
1.33
Me
Me
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S
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0.94
0.91
1.00
0.99
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3.09
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7.0
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5.5
5.0
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3.0
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2.0
1.5
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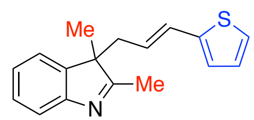
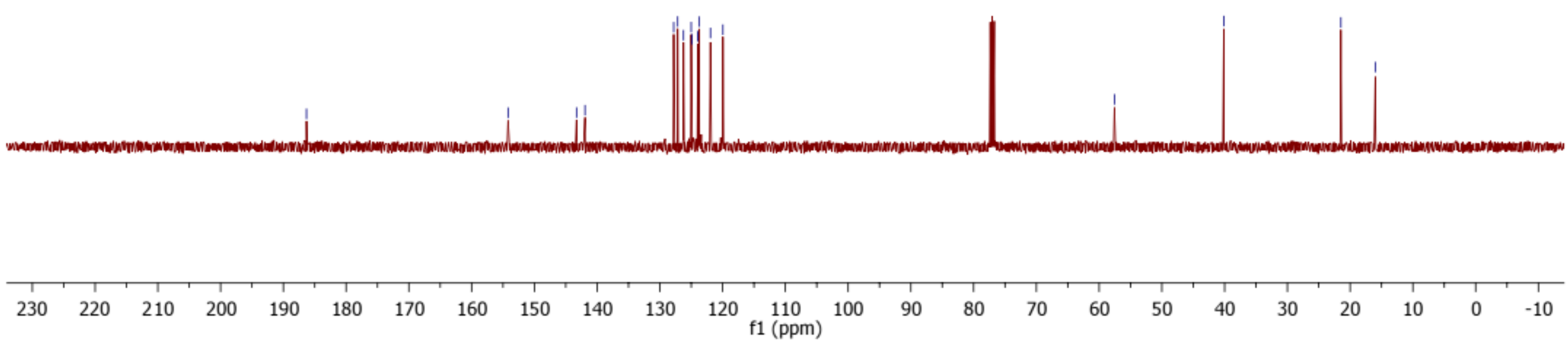
f1 (ppm)


Me
S
Me
N

3ak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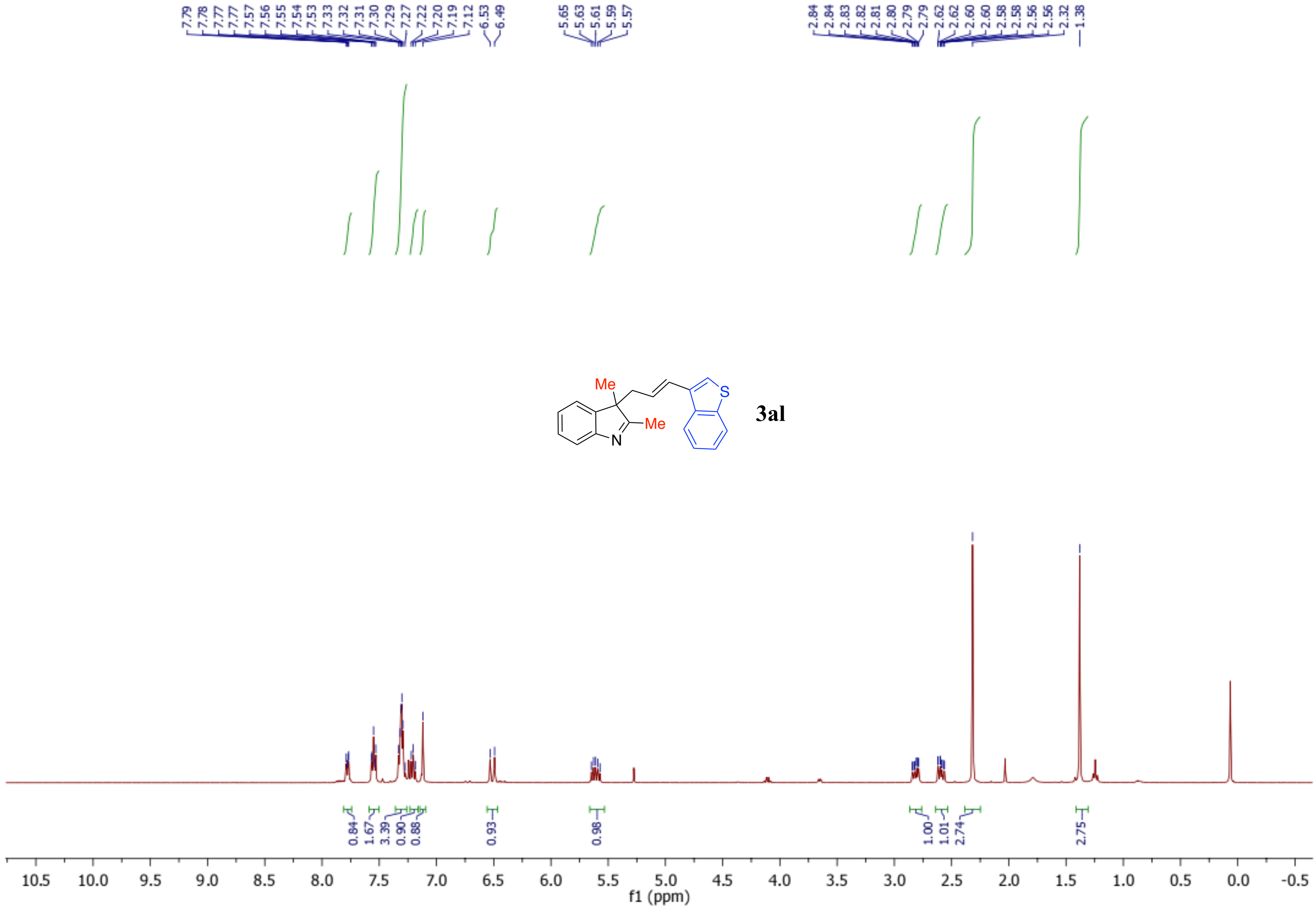
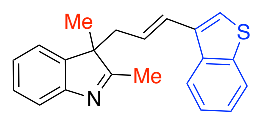
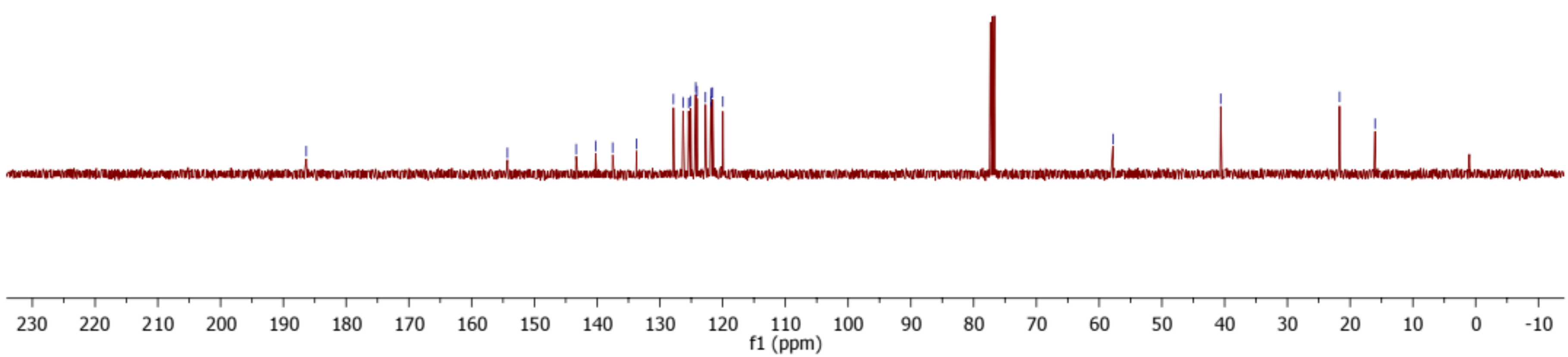
21.47
16.00
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.79 7.78 7.77 7.77 7.57 7.56 7.55 7.54 7.53 7.33 7.32 7.31 7.30 7.29 7.27 7.22 7.20 7.19 7.12 6.53 6.49
5.65 5.63 5.61 5.59 5.57
2.84 2.84 2.83 2.82 2.81 2.80 2.79 2.79 2.62 2.62 2.60 2.60 2.58 2.58 2.56 2.56 2.32 1.38
0.84 1.67 3.39 0.90 0.88 0.93 0.98 1.00 1.01 2.74 2.75
10.5 10.0 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 0.0 -0.5
f1 (ppm)
Me
Me
N
S

3al


Me
Me
N
S

3al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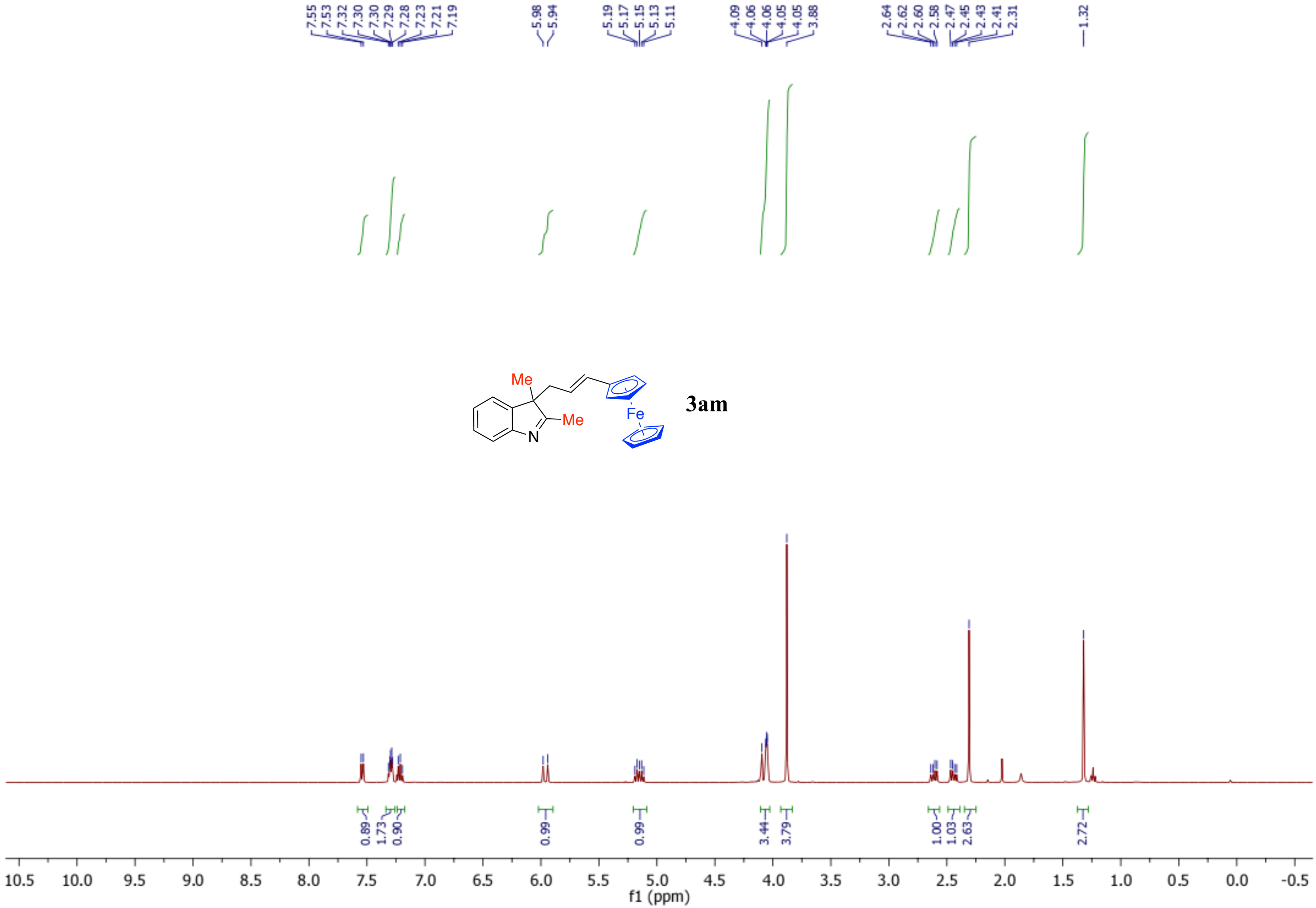
154.29
143.34
140.23
137.52
133.70
127.84
126.32
125.42
125.09
124.29
124.10
122.74
121.90
121.82
121.59
119.96
57.80
40.63
21.68
16.03
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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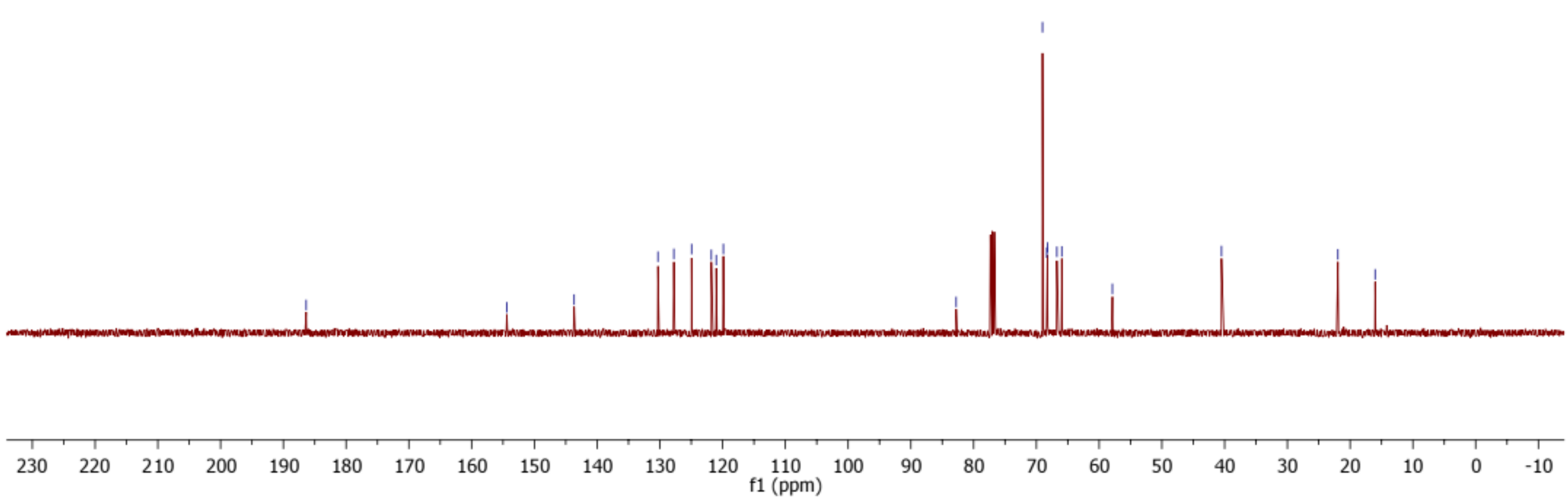
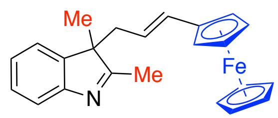
7.53
7.32
7.30
7.30
7.29
7.28
7.23
7.21
7.19
5.98
5.94
5.19
5.17
5.15
5.13
5.11
4.09
4.06
4.06
4.05
4.05
3.88
2.64
2.62
2.60
2.58
2.47
2.45
2.43
2.41
2.31
1.32
Me
Me
N
Fe
3am
0.89
1.73
0.90
0.99
0.99
3.44
3.79
1.00
1.03
2.63
2.72
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

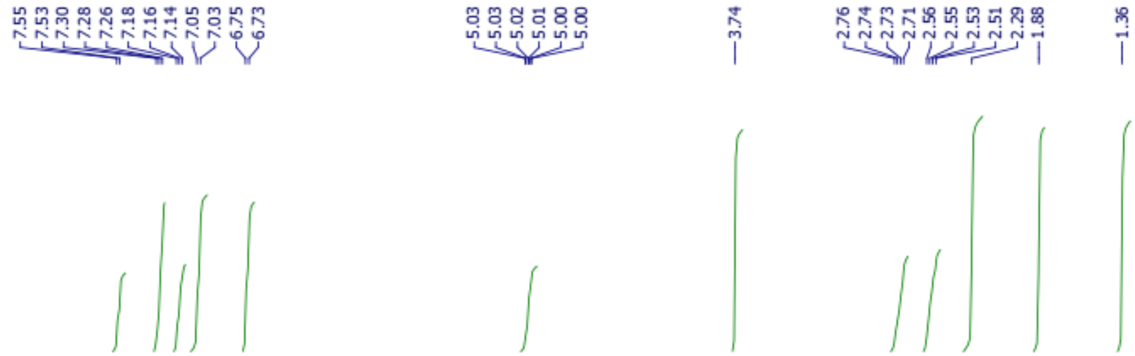


186.36
154.39
143.66
130.30
127.77
124.94
121.80
121.01
119.88
82.78
69.02
68.35
68.25
66.73
65.96
57.89
40.50
21.95
16.02
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

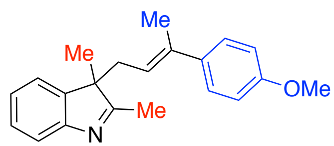


Me
Me
N
Fe

3am

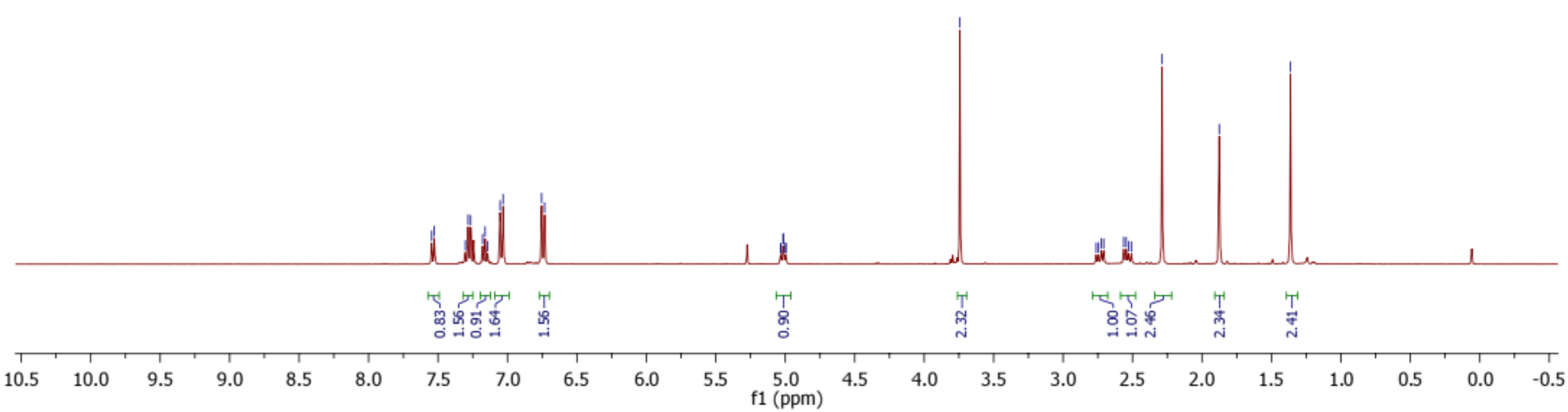


7.55
7.53
7.30
7.28
7.26
7.18
7.16
7.14
7.05
7.03
6.75
6.73
5.03
5.03
5.02
5.01
5.00
5.00
3.74
2.76
2.74
2.73
2.71
2.56
2.55
2.53
2.51
2.29
1.88
1.36

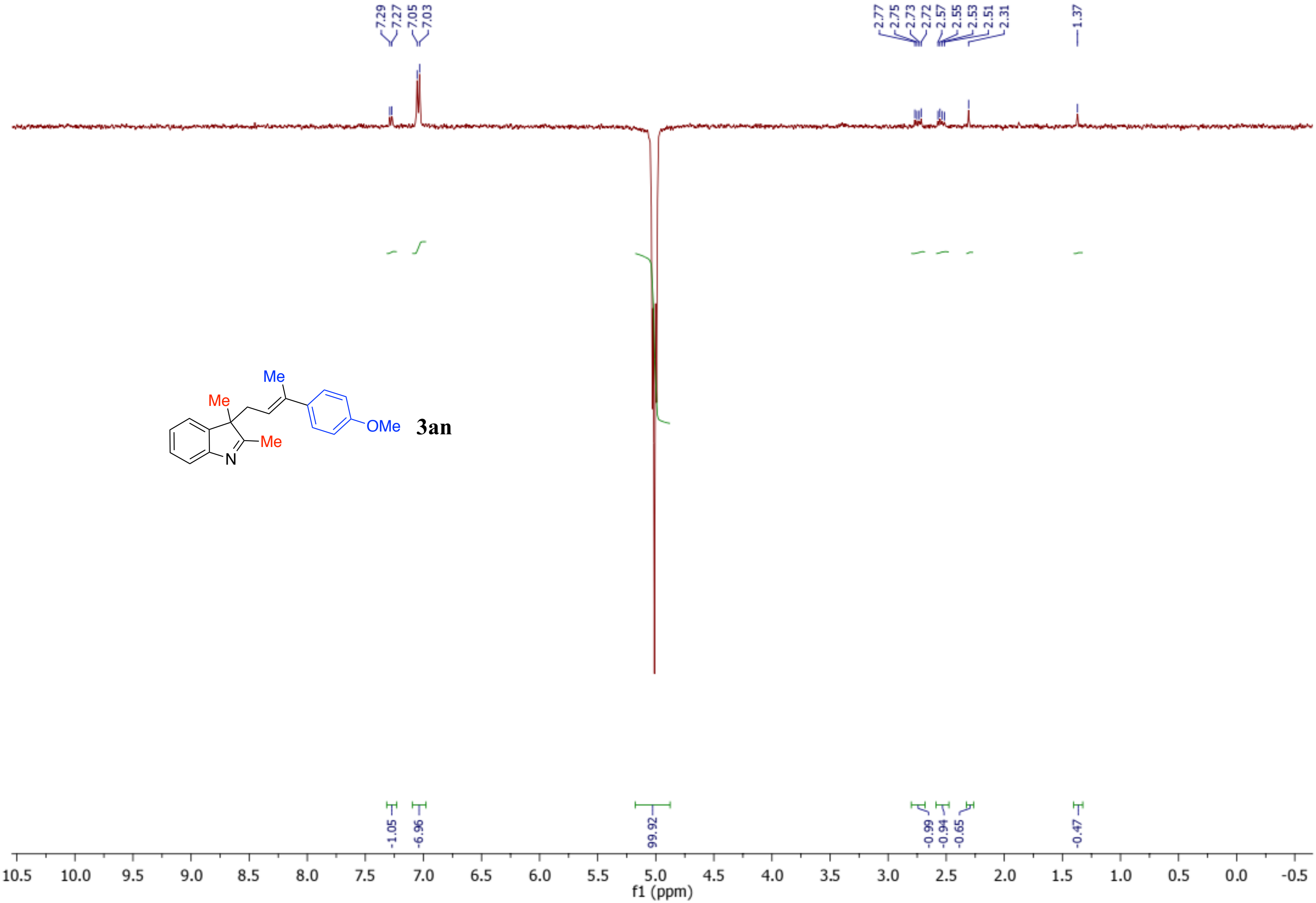


Me
Me
Me
N
OMe

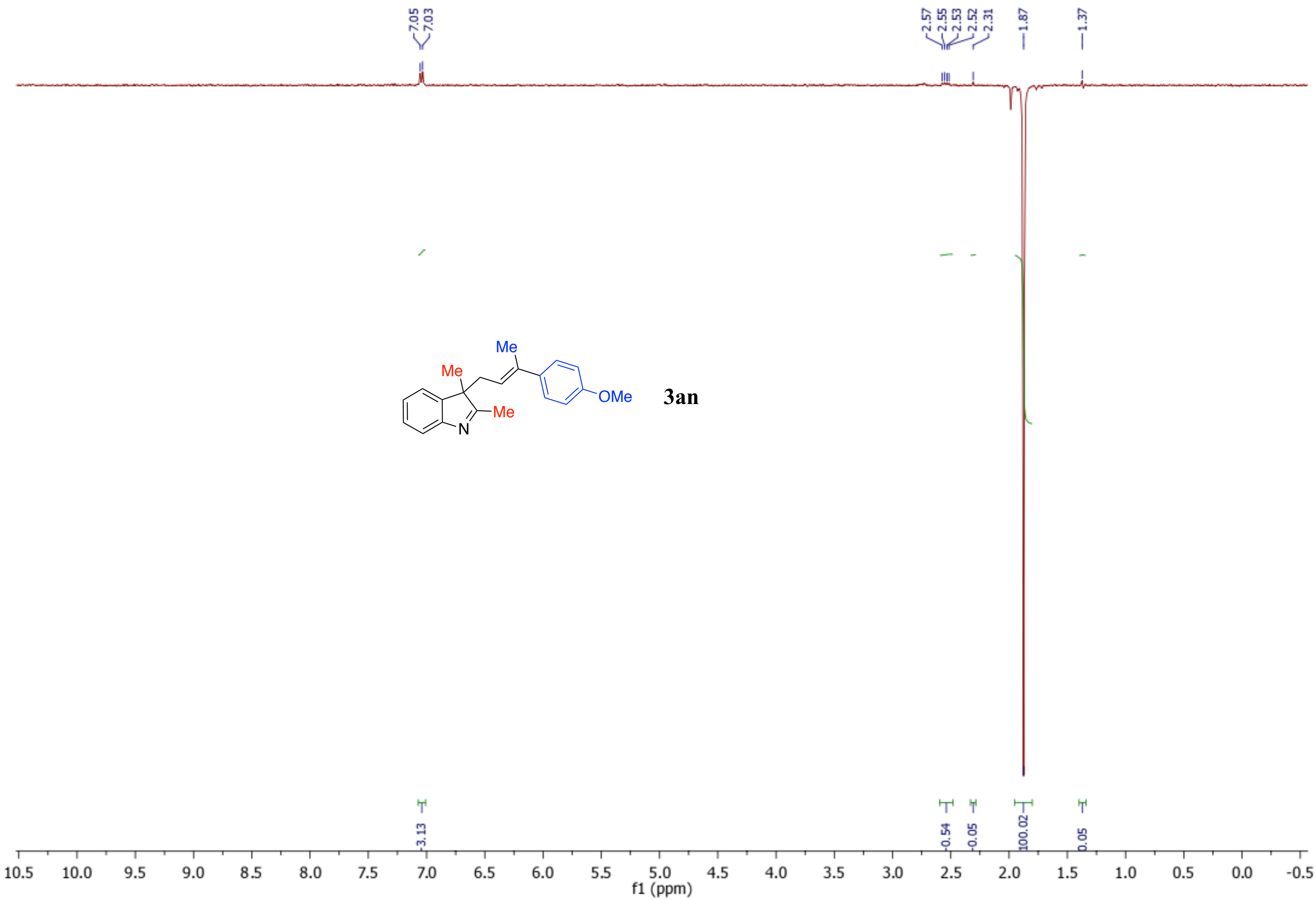
3an

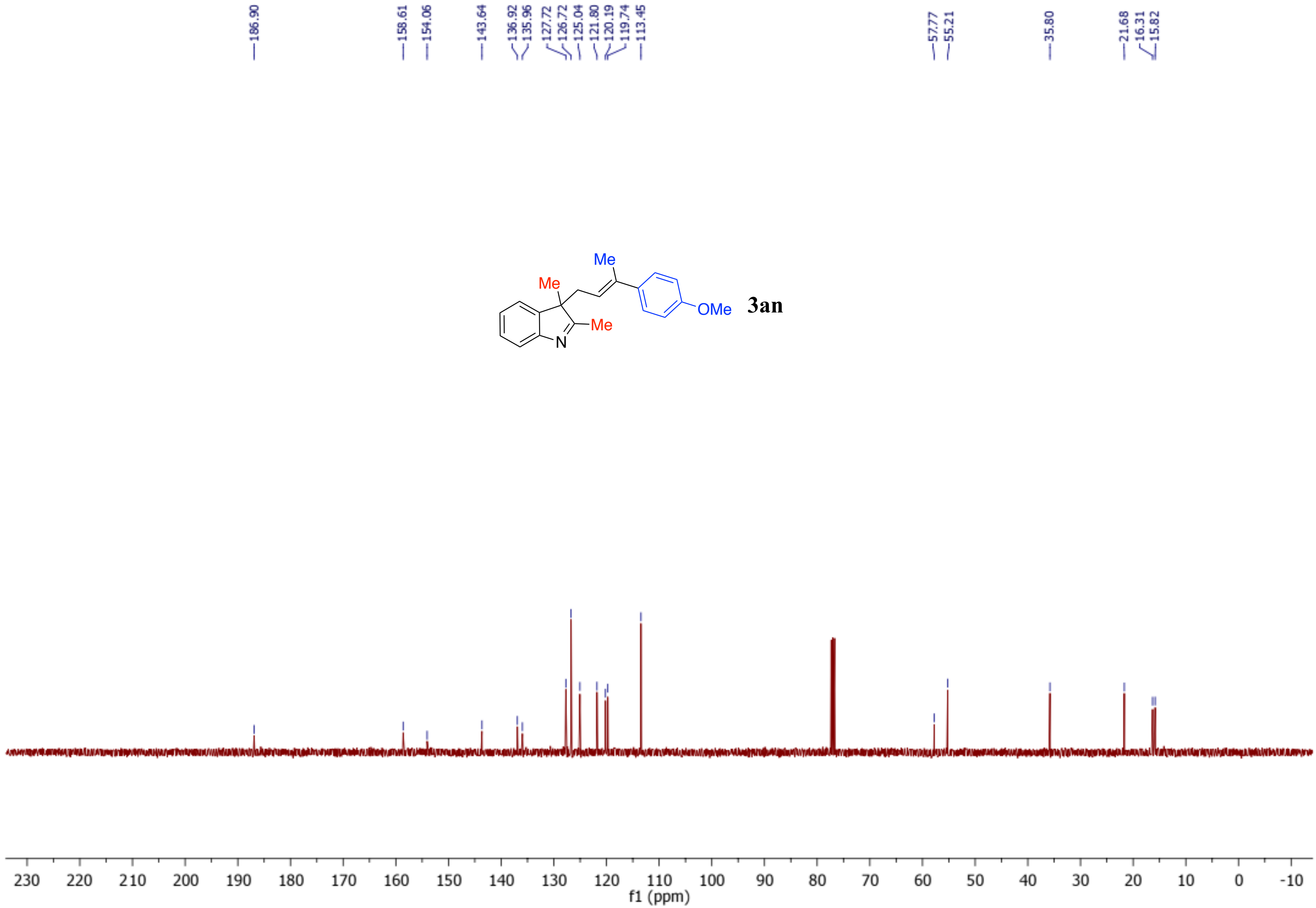


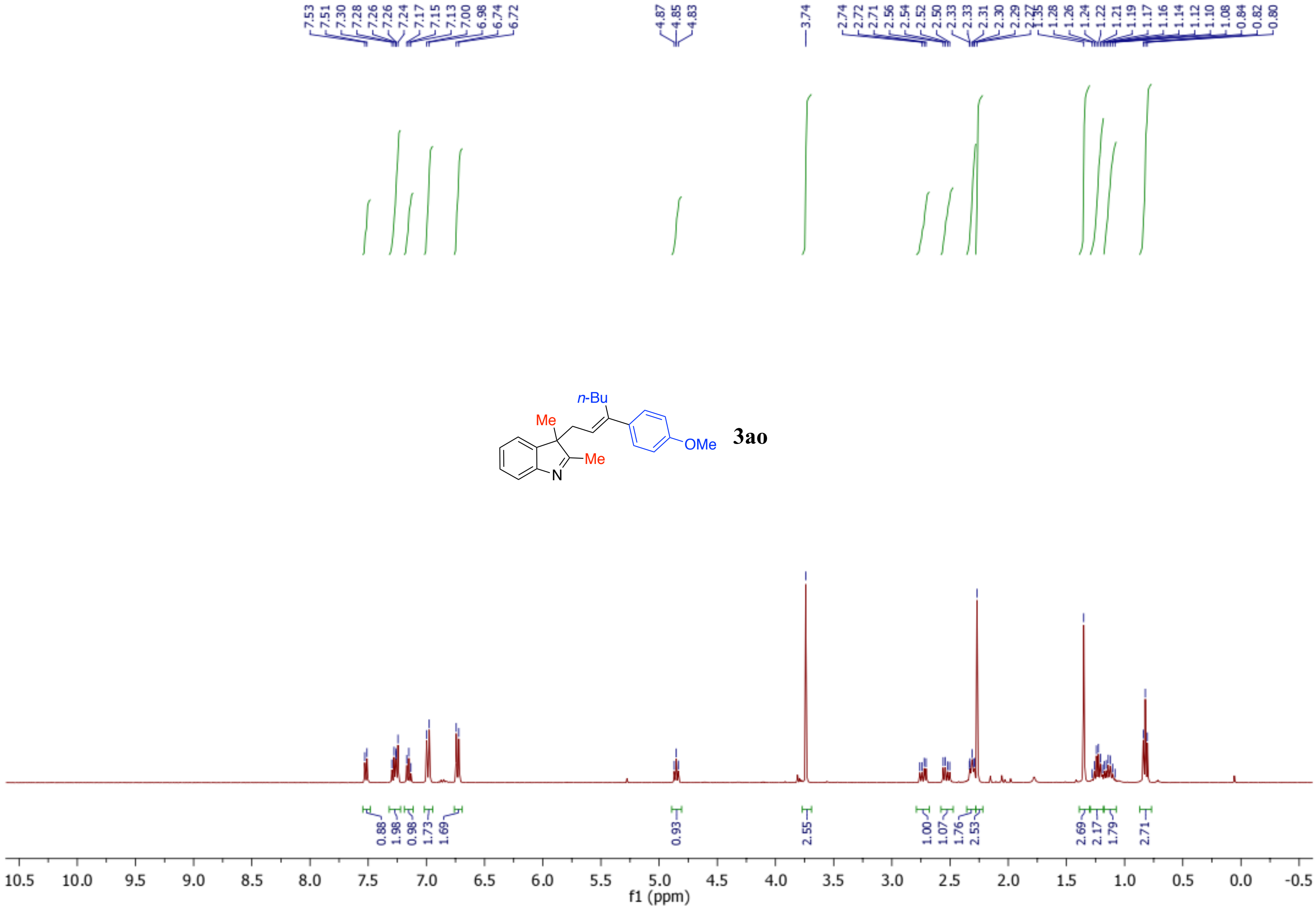
0.83
1.56
0.91
1.64
1.56
0.90
2.32
1.00
1.07
2.46
2.34
2.41
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


7.29
7.27
7.05
7.03
2.77
2.75
2.73
2.72
2.57
2.55
2.53
2.51
2.31
1.37
Me
Me
Me
N
OMe
1.05
6.96
99.92
0.99
0.94
0.65
0.47
10.5
10.0
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
0.0
-0.5
f1 (ppm)

3an

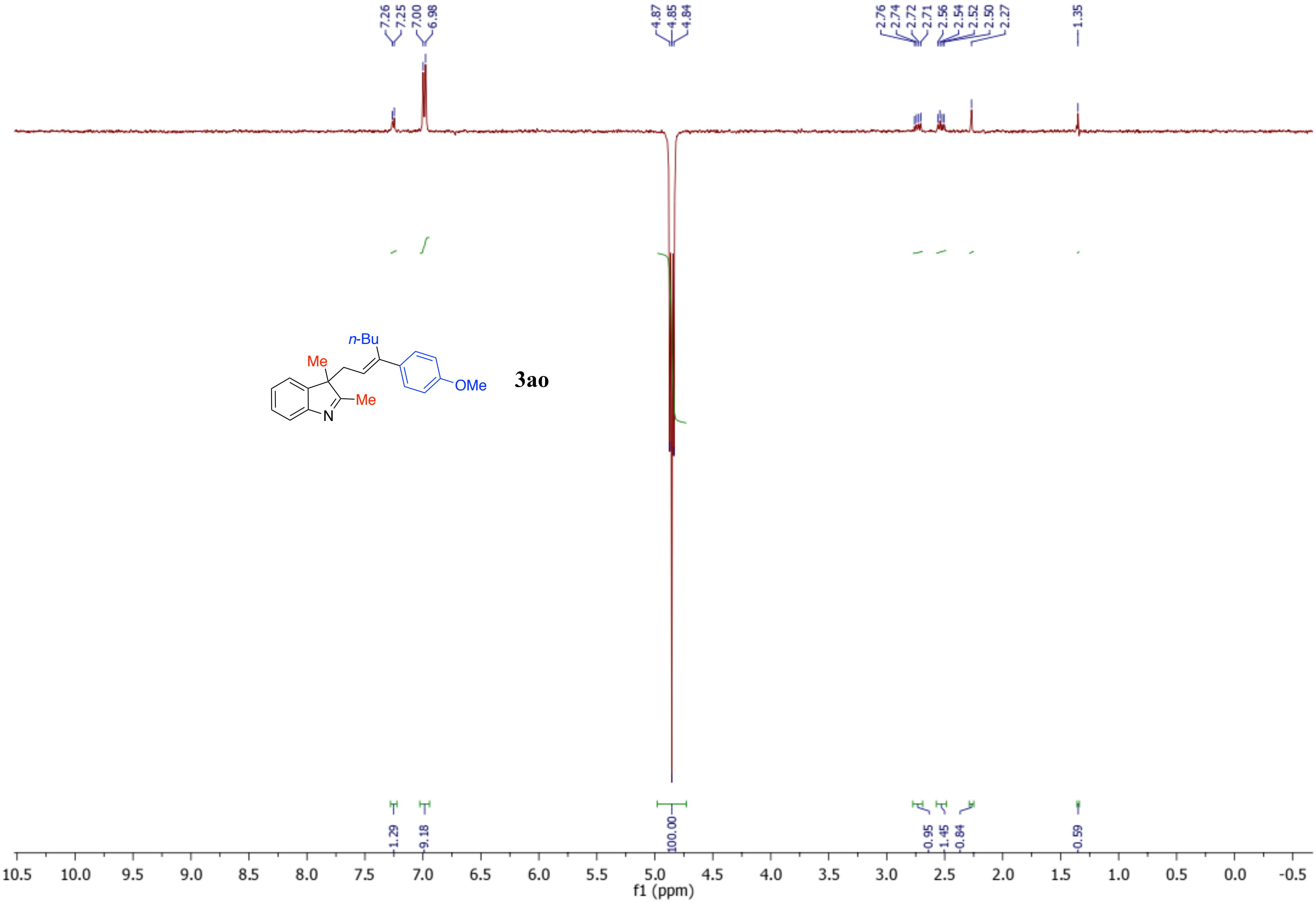

7.05
7.03
2.57
2.55
2.53
2.52
2.31
1.87
1.37
Me
Me
Me
OMe
N
3an
3.13
0.54
0.05
100.02
0.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

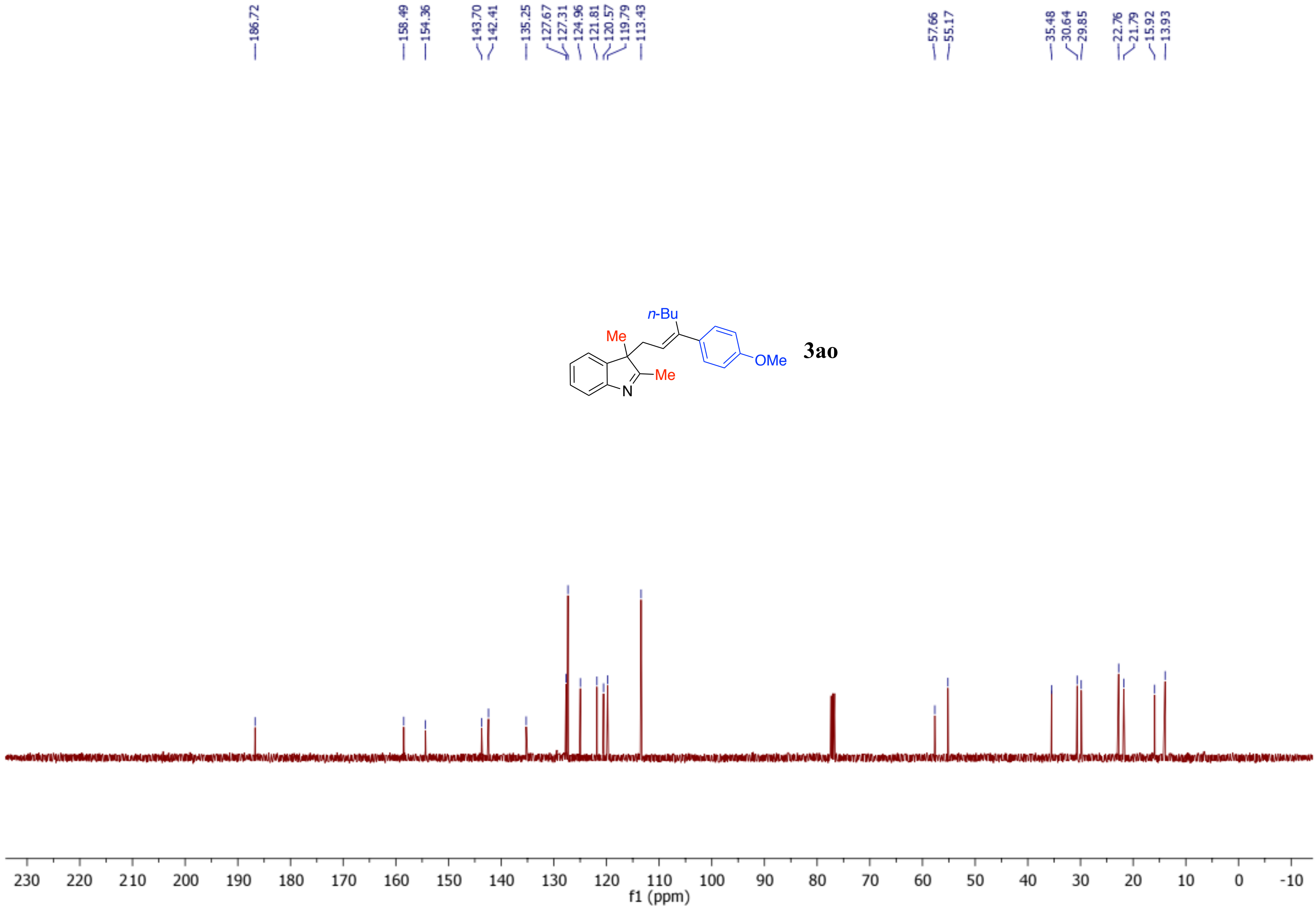

186.90
158.61
154.06
143.64
136.92
135.96
127.72
126.72
125.04
121.80
120.19
119.74
113.45
57.77
55.21
35.80
21.68
16.31
15.82
Me
Me
Me
OMe
N
3an
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



7.53
7.51
7.30
7.28
7.26
7.26
7.24
7.17
7.15
7.13
7.00
6.98
6.74
6.72
4.87
4.85
4.83
3.74
2.74
2.72
2.71
2.56
2.54
2.52
2.50
2.33
2.33
2.31
2.30
2.29
2.27
1.35
1.28
1.26
1.24
1.22
1.21
1.19
1.17
1.16
1.14
1.12
1.10
1.08
0.84
0.82
0.80
n-Bu
Me
Me
N
OMe
0.88
1.98
0.98
1.73
1.69
0.93
2.55
1.00
1.07
1.76
2.53
2.69
2.17
1.79
2.71
10.5
10.0
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
0.0
-0.5
f1 (ppm)

3ao


7.26
7.25
7.00
6.98
4.87
4.85
4.84
2.76
2.74
2.72
2.71
2.56
2.54
2.52
2.50
2.27
1.35
n-Bu
Me
Me
N
OMe
3ao
1.29
9.18
100.00
0.95
1.45
0.84
0.59
10.5
10.0
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
0.0
-0.5
f1 (ppm)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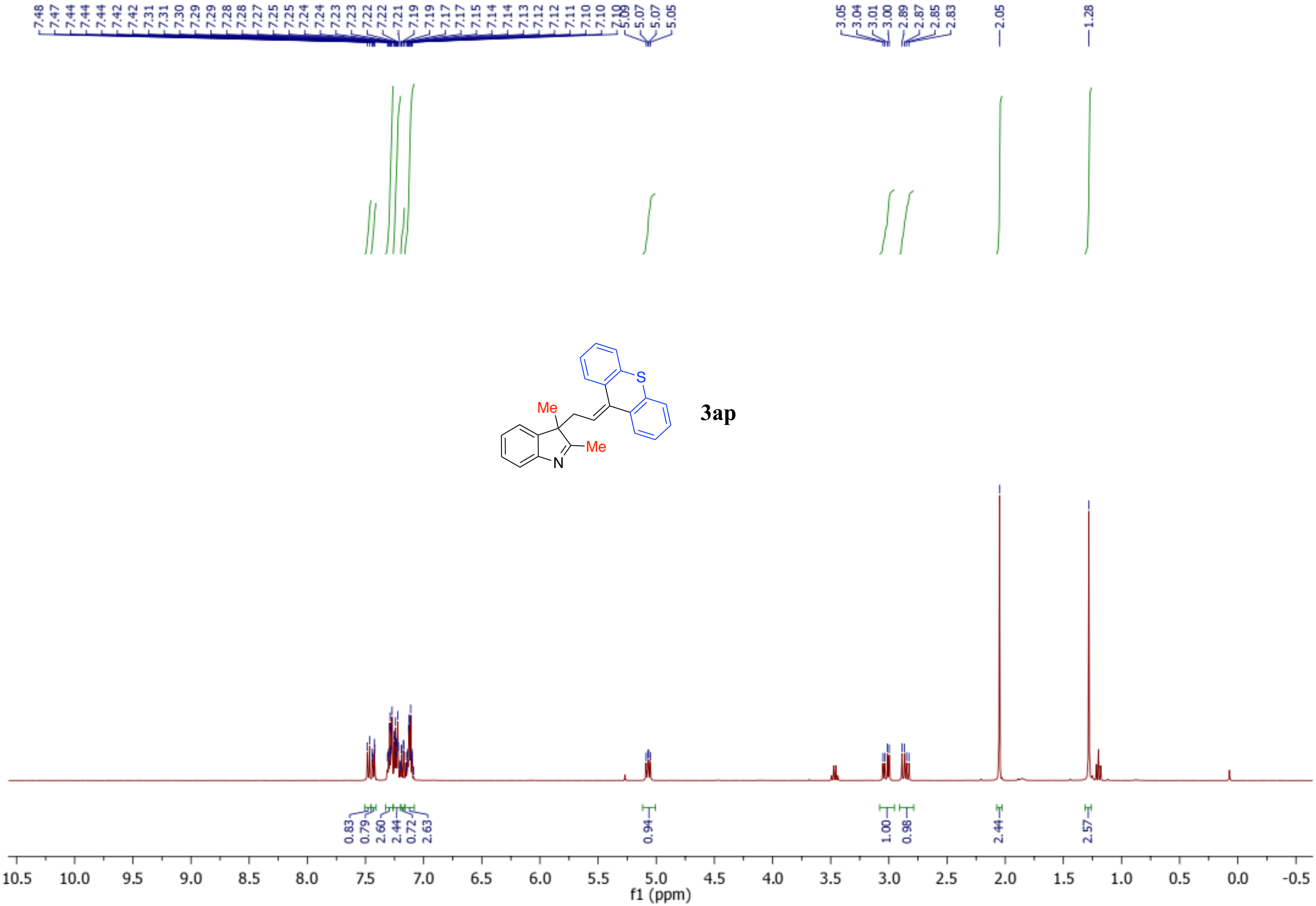
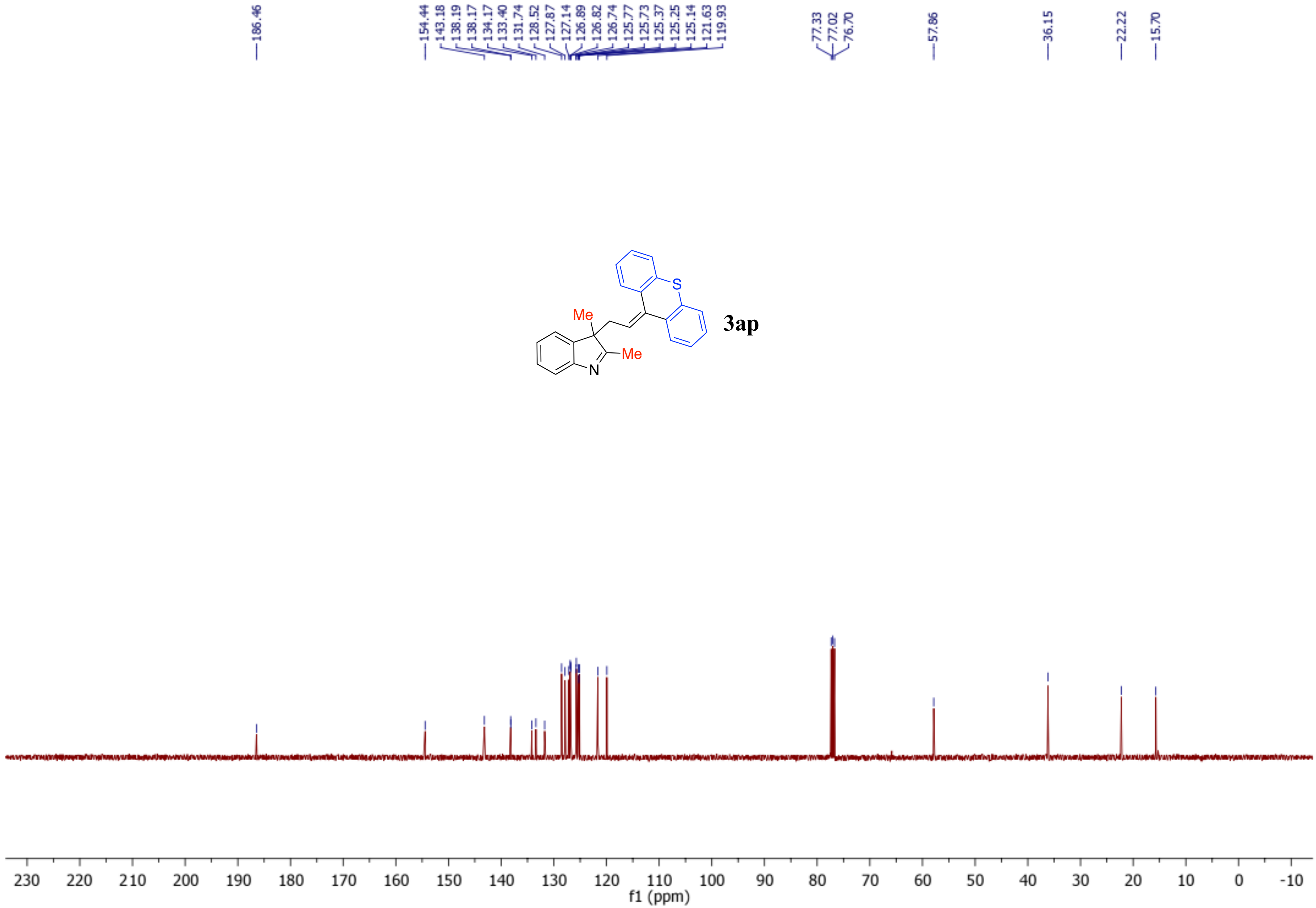
143.70
142.41
135.25
127.67
127.31
124.96
121.81
120.57
119.79
113.43
57.66
55.17
35.48
30.64
29.85
22.76
21.79
15.92
13.93
n-Bu
Me
Me
N
OMe
3ao
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



7.48 7.47 7.44 7.44 7.44 7.42 7.42 7.31 7.31 7.30 7.29 7.29 7.28 7.28 7.27 7.25 7.25 7.24 7.24 7.23 7.23 7.22 7.22 7.21 7.19 7.19 7.17 7.17 7.15 7.14 7.14 7.13 7.12 7.12 7.11 7.10 7.10 7.10 5.08 5.07 5.07 5.05
3.05 3.04 3.01 3.00 2.89 2.87 2.85 2.83
2.05
1.28
Me
Me
S
N
3ap
0.83 0.79 2.60 2.44 0.72 2.63
0.94
1.00 0.98
2.44
2.57
10.5 10.0 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 0.0 -0.5
f1 (ppm)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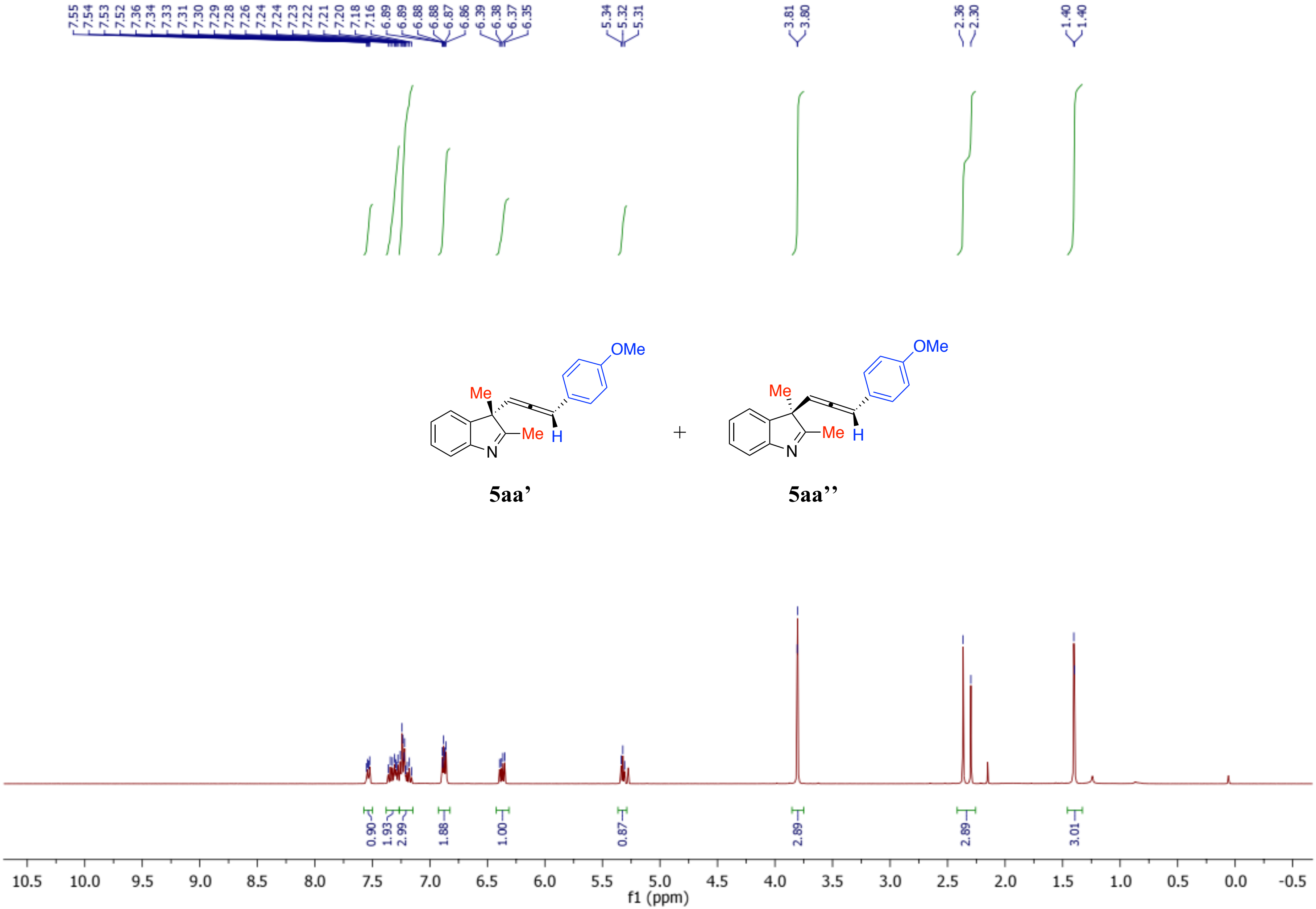
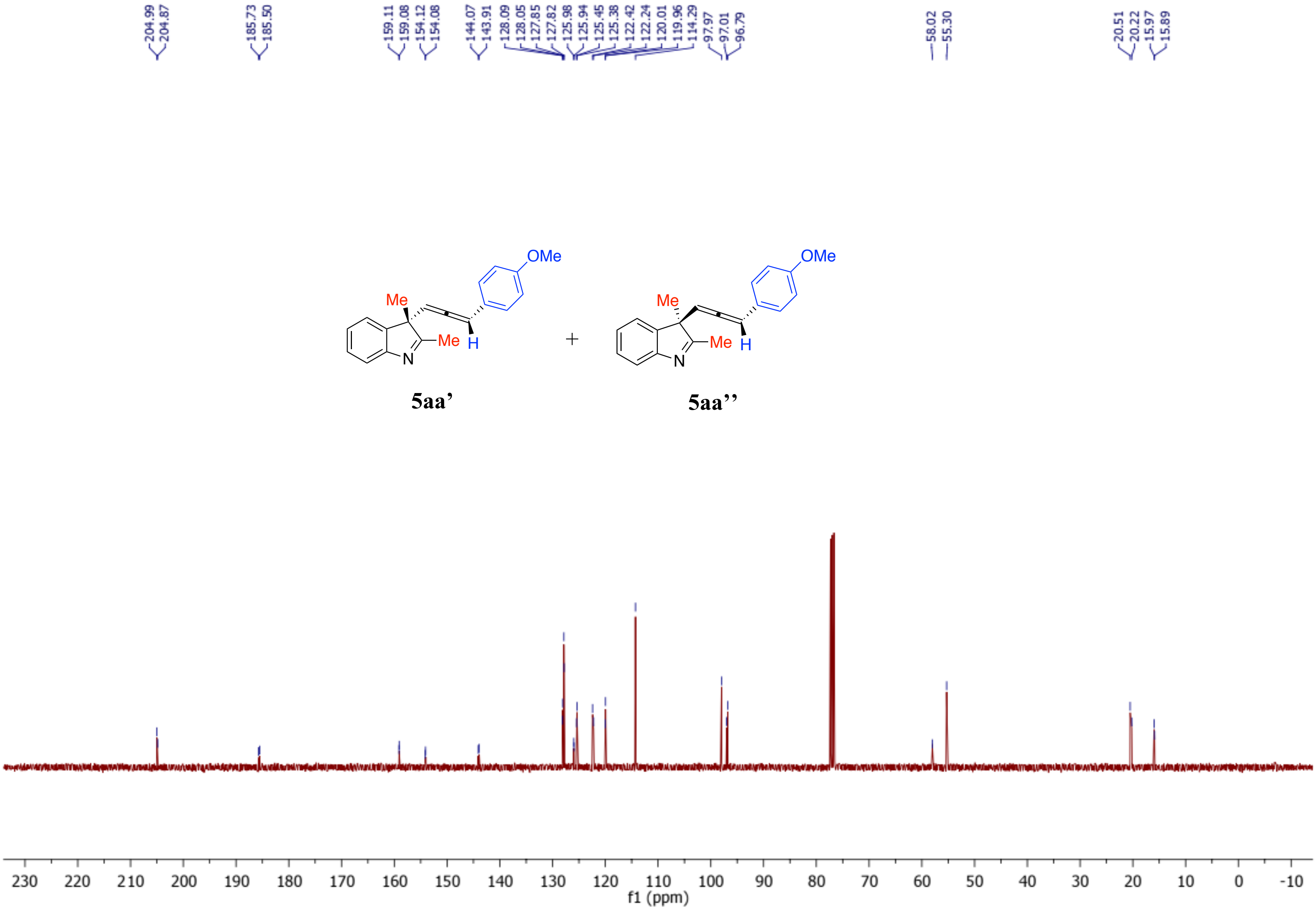
138.17
134.17
133.40
131.74
128.52
127.87
127.14
126.89
126.82
126.74
125.77
125.73
125.37
125.25
125.14
121.63
119.93
77.33
77.02
76.70
57.86
36.15
22.22
15.70
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
S
Me
Me
N

3ap


7.55 7.54 7.53 7.52 7.36 7.34 7.33 7.31 7.30 7.29 7.28 7.26 7.24 7.24 7.23 7.22 7.21 7.20 7.18 7.16 6.89 6.89 6.88 6.88 6.87 6.86 6.39 6.38 6.37 6.35
5.34 5.32 5.31
3.81 3.80
2.36 2.30
1.40 1.40
OMe
Me
Me
N
H
+
OMe
Me
Me
N
H
5aa’
5aa’’
0.90 1.93 2.99 1.88 1.00 0.87 2.89 2.89 3.01
10.5 10.0 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 0.0 -0.5
f1 (ppm)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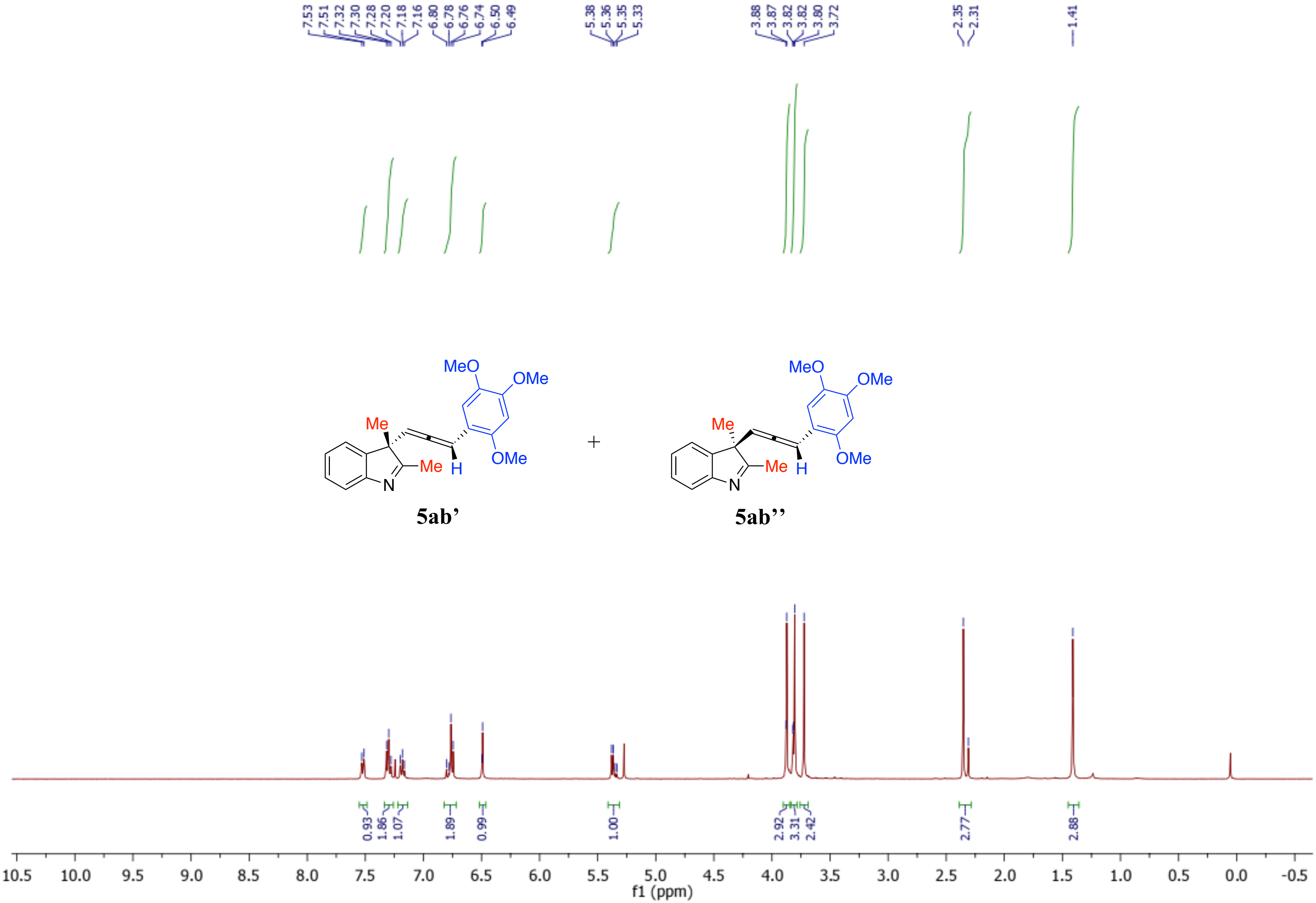
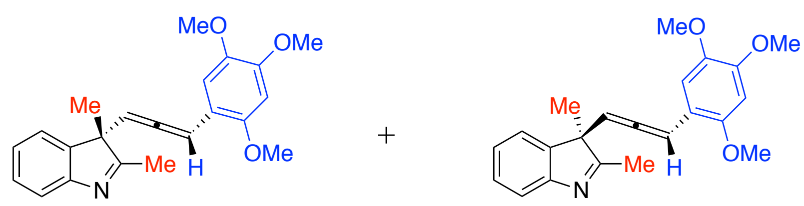
185.50
159.11
159.08
154.12
154.08
144.07
143.91
128.09
128.05
127.85
127.82
125.98
125.94
125.45
125.38
122.42
122.24
120.01
119.96
114.29
97.97
97.01
96.79
58.02
55.30
20.51
20.22
15.97
15.89
OMe
Me
Me
H
N
+
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

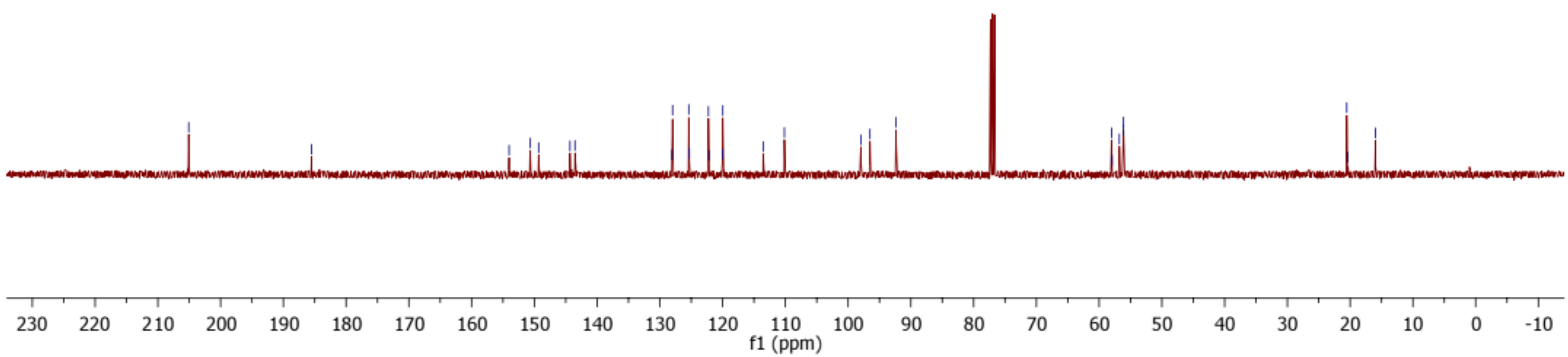
5aa' + **5aa''**

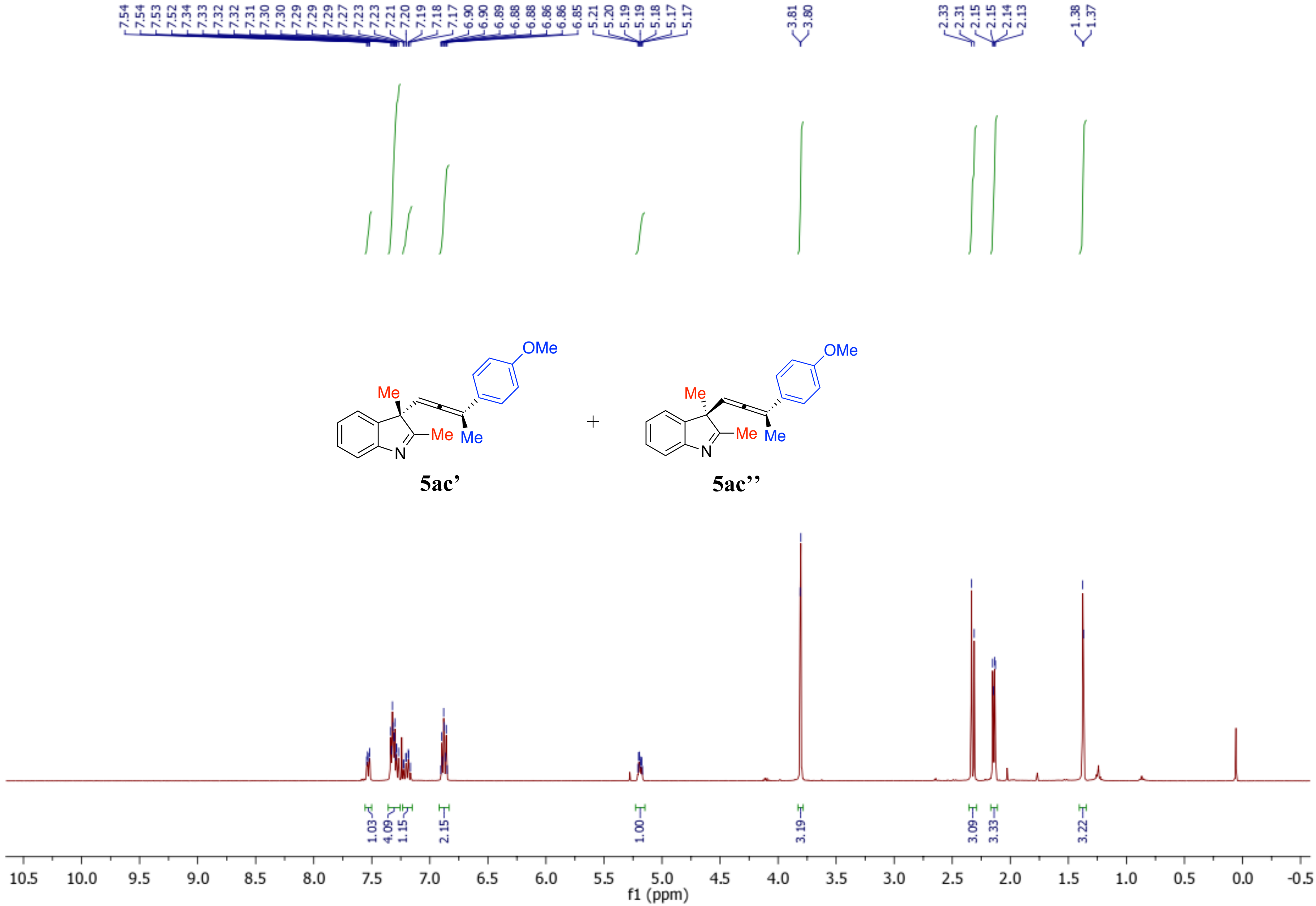

7.53
7.51
7.32
7.30
7.28
7.20
7.18
7.16
6.80
6.78
6.76
6.74
6.50
6.49
5.38
5.36
5.35
5.33
3.88
3.87
3.82
3.82
3.80
3.72
2.35
2.31
1.41
MeO
OMe
Me
Me
N
H
OMe
+
0.93
1.86
1.07
1.89
0.99
1.00
2.92
3.31
2.42
2.77
2.88
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

5ab' **5ab''**

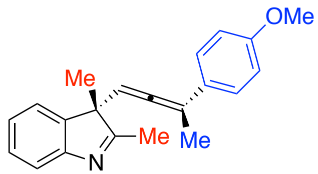

MeO
OMe
Me
Me
N
H
OMe
MeO
OMe
Me
Me
N
H
OMe

5ab’ + **5ab’’**


205.09
185.51
154.03
150.68
149.32
144.33
143.53
128.06
127.97
125.40
125.31
122.26
122.18
120.02
119.97
113.54
110.15
97.97
96.52
92.36
58.03
57.93
56.78
56.14
56.12
20.54
20.37
15.96
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OMe
Me
Me
Me
N
5ac'
OMe
Me
Me
Me
N
5ac''
f1 (ppm)

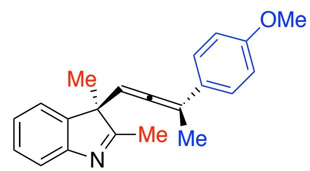
204.11
204.10
185.95
158.81
158.79
154.11
154.05
144.29
144.22
127.99
127.93
126.79
126.73
125.33
122.28
119.93
119.90
113.90
104.37
104.30
94.85
94.67
58.49
58.41
55.29
20.43
20.22
17.67
17.52
16.02
15.78



OMe
Me
Me
Me
N

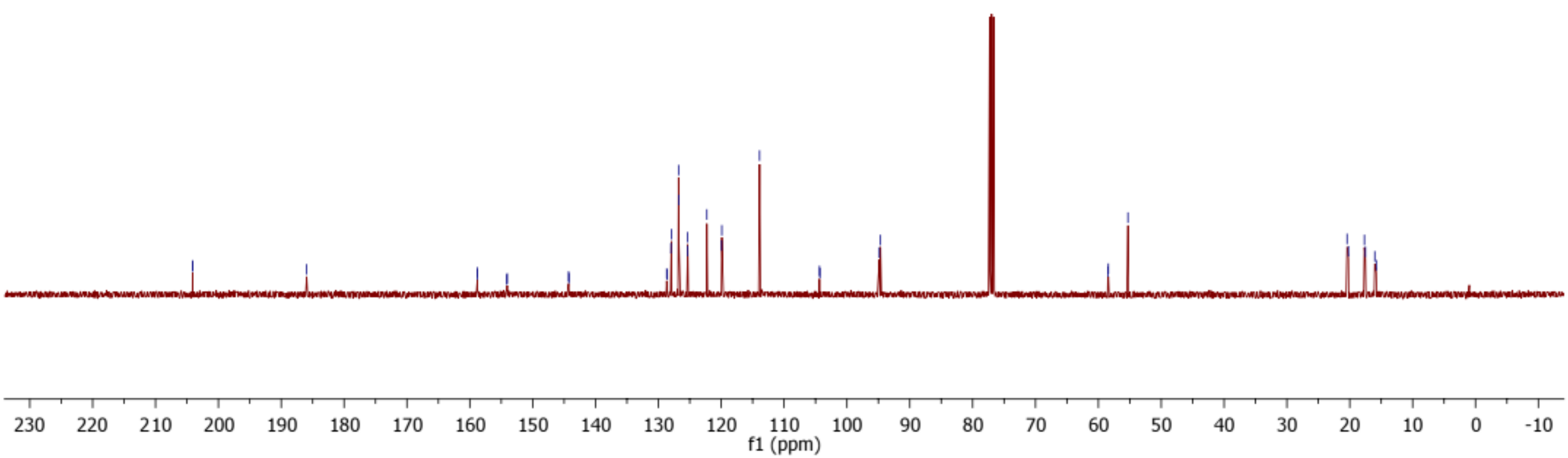
5ac’

+

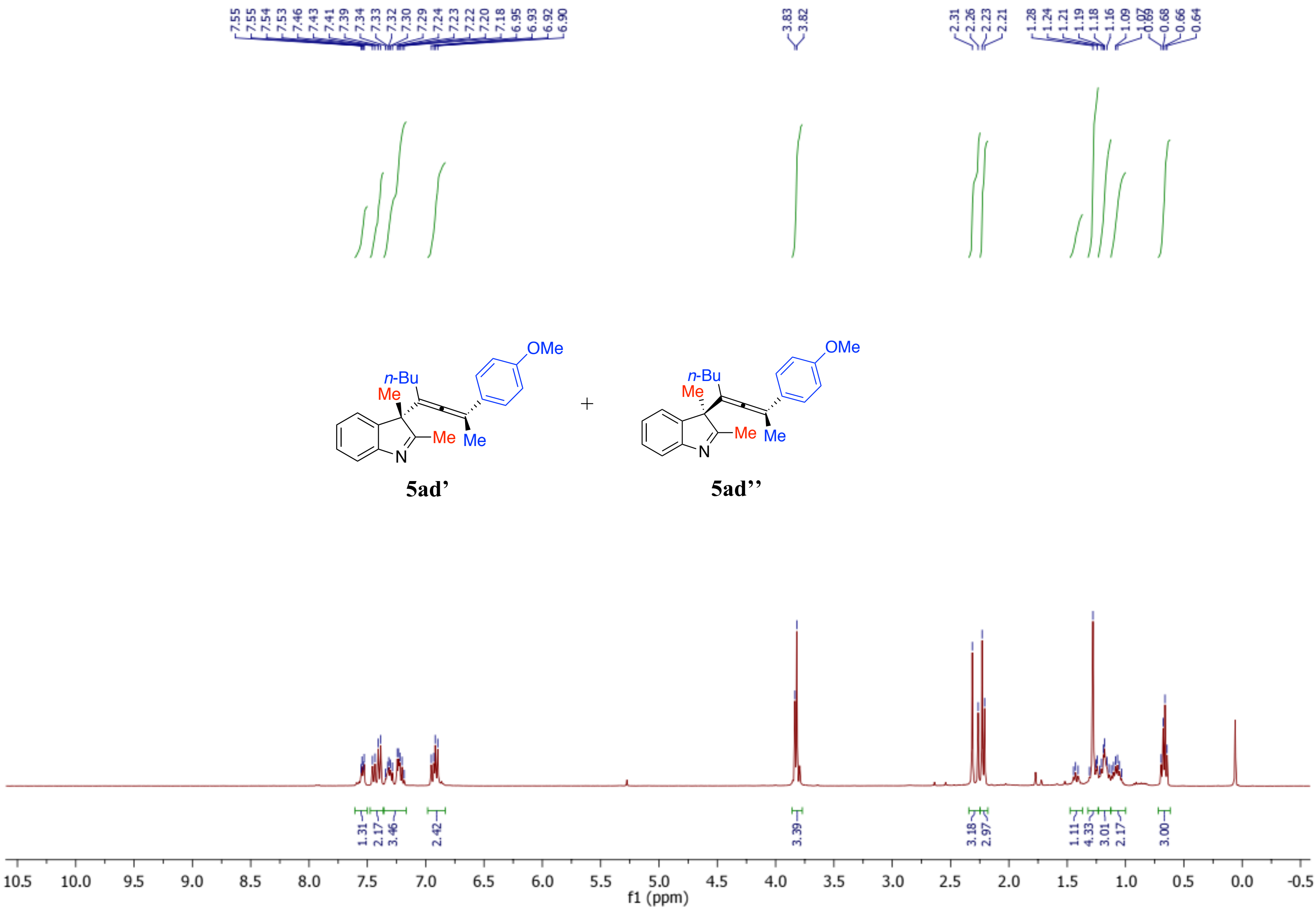


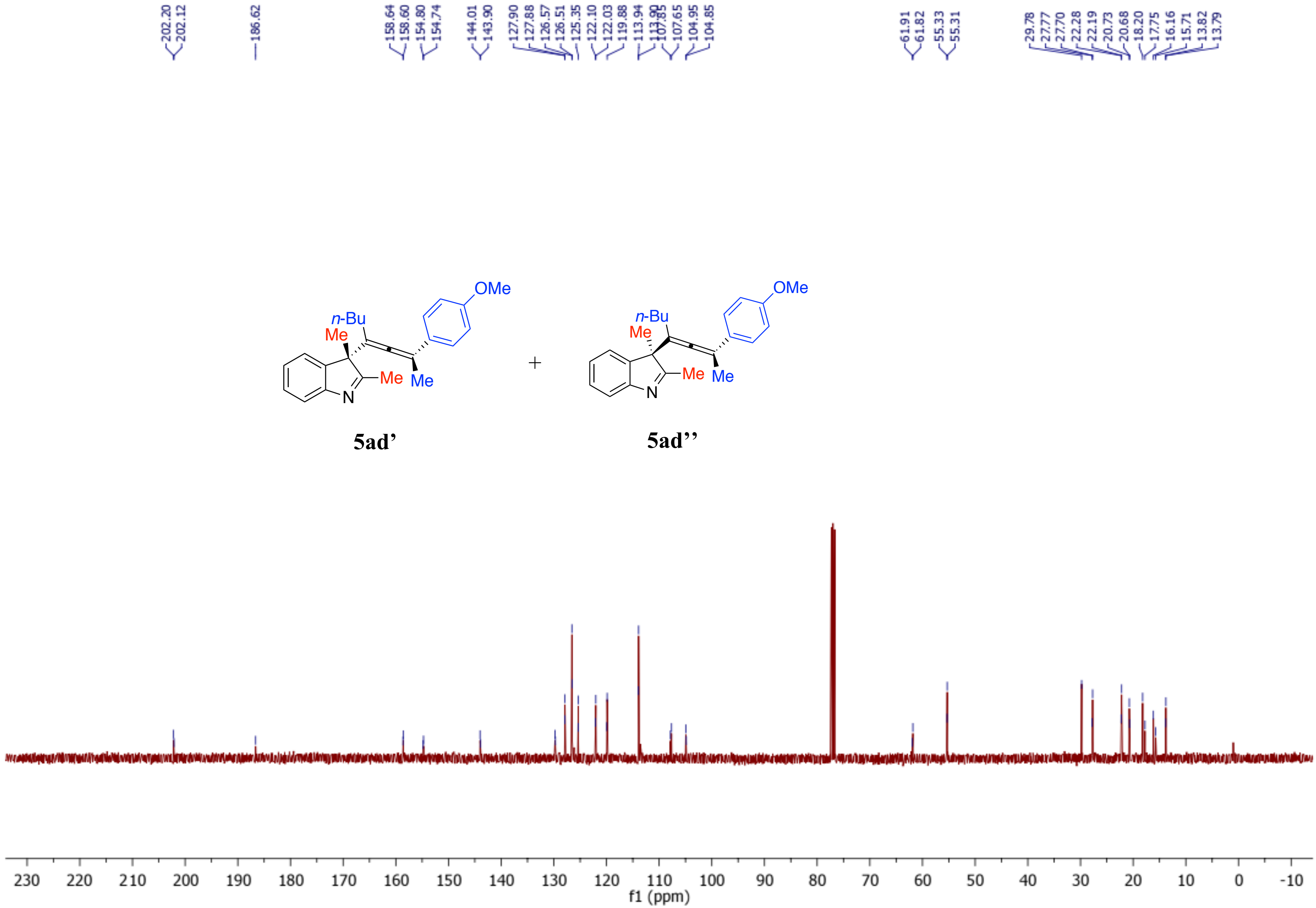
OMe
Me
Me
Me
N

5ac’’

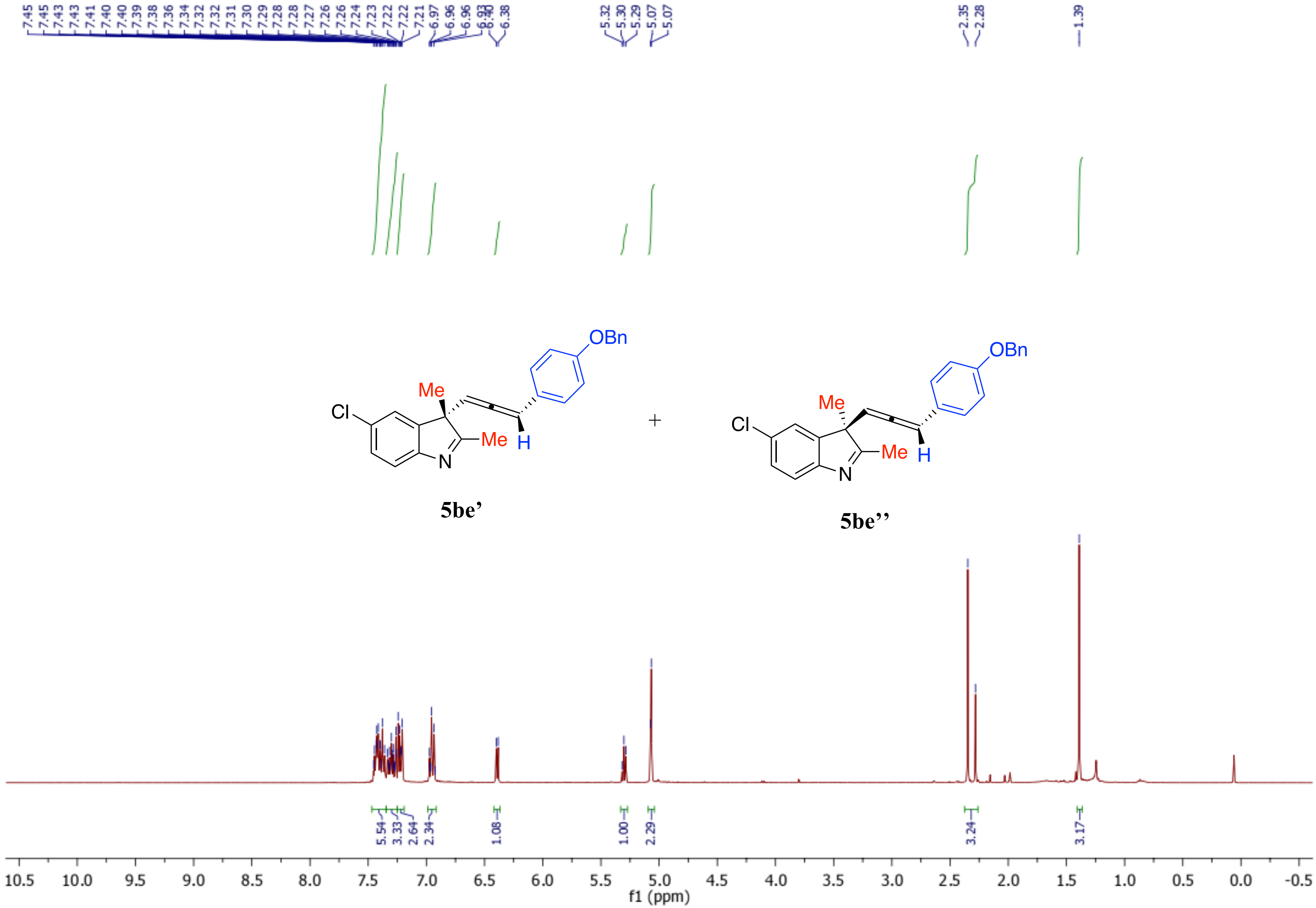


230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

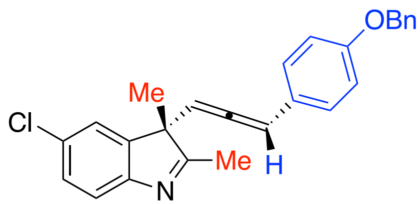

7.55 7.55 7.54 7.53 7.46 7.43 7.41 7.39 7.34 7.33 7.32 7.30 7.29 7.24 7.23 7.22 7.20 7.18 6.95 6.93 6.92 6.90
3.83 3.82
2.31 2.26 2.23 2.21
1.28 1.24 1.21 1.19 1.18 1.16 1.09 1.07 0.69 0.68 0.66 0.64
OMe
n-Bu
Me
Me
Me
N
5ad'
+
5ad''
1.31 2.17 3.46 2.42 3.39 3.18 2.97 1.11 4.33 3.01 2.17 3.00
10.5 10.0 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 0.0 -0.5
f1 (ppm)



202.20
202.12
186.62
158.64
158.60
154.80
154.74
144.01
143.90
127.90
127.88
126.57
126.51
125.35
122.10
122.03
119.88
113.94
113.90
107.85
107.65
104.95
104.85
61.91
61.82
55.33
55.31
29.78
27.77
27.70
22.28
22.19
20.73
20.68
18.20
17.75
16.16
15.71
13.82
13.79
OMe
n-Bu
Me
Me
Me
N
+
OMe
n-Bu
Me
Me
Me
N
5ad'
5ad''
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



7.45 7.45 7.43 7.43 7.41 7.40 7.40 7.39 7.38 7.36 7.34 7.32 7.32 7.31 7.30 7.29 7.28 7.28 7.27 7.26 7.26 7.24 7.23 7.22 7.22 7.21 6.97 6.96 6.96 6.93 6.40 6.38
5.32 5.30 5.29 5.07 5.07
2.35 2.28
1.39
OBn
Cl
Me
Me
N
H
5be'
+
5be''
5.54 3.33 2.64 2.34 1.08 1.00 2.29 3.24 3.17
10.5 10.0 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 0.0 -0.5
f1 (ppm)


OBn
Me
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5be'

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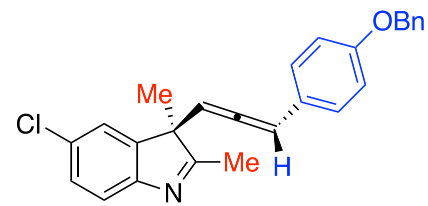
OBn
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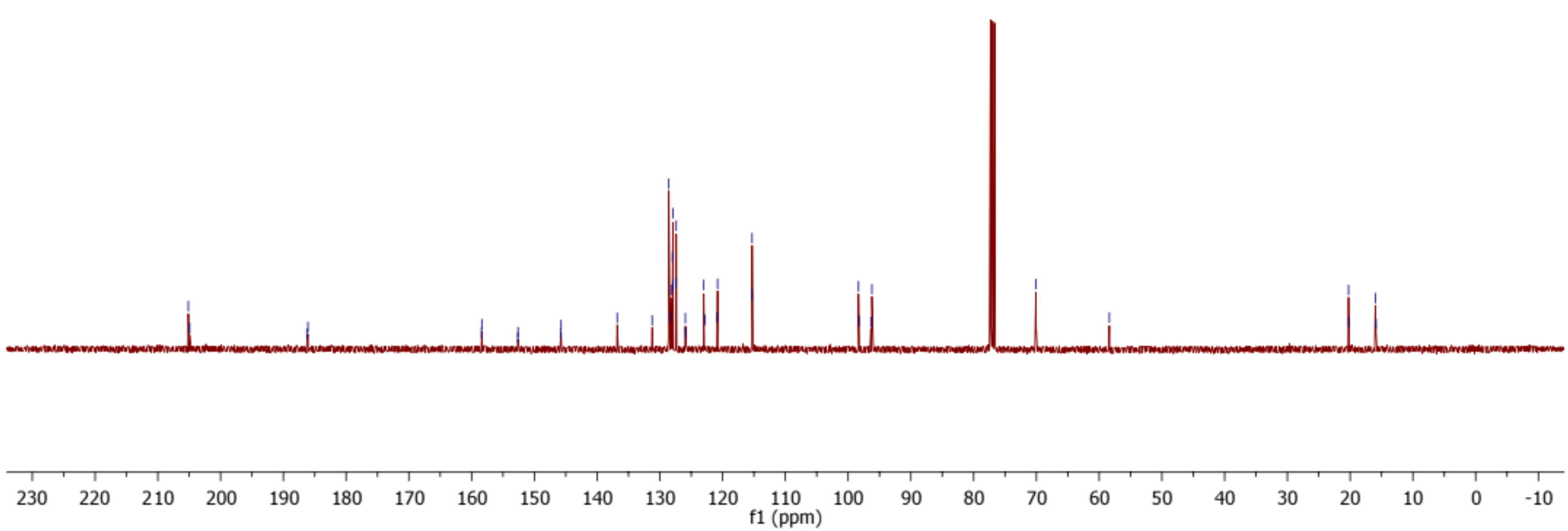
5be''


205.14
204.94
186.24
186.08
158.42
158.37
152.65
152.60
145.83
145.74
128.58
128.26
128.22
127.98
127.91
127.89
127.41
127.39
123.00
120.86
120.80
115.32
115.30
98.35
98.26
96.37
96.21
70.07
58.37
20.26
20.22
15.99
15.89
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

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