# *Supporting Information*

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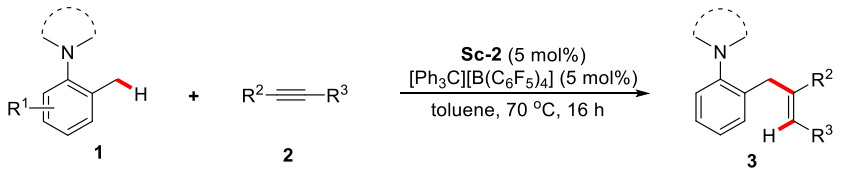
## 1. General Information

All manipulations of air- and moisture-sensitive compounds were performed under dry nitrogen atmosphere in an mBRAUN Labmaster glovebox. Nitrogen was purified by being passed through a dry column (4 Å molecular sieves, Nikka Seiko Co.) and a Gasclean GC-XR column (Nikka Seiko Co.). The nitrogen in the glovebox was constantly circulated through a copper/molecular sieves catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored by an $O_2/H_2O$ Combi-Analyzer (Mbraun) to ensure both were always below 0.1 ppm. Solvents (THF, Hexane and Toluene) (dehydrated, stabilizer-free) were obtained from Kanto Kagaku Co., purified by an mBRAUN SPS-800 solvent purification system, and dried over fresh Na chips in a glovebox. The commercially available internal alkynes and anilines were obtained from Tokyo Chemical Industry Co., Ltd., dried with $CaH_2$ before use. Other internal alkynes and 2-methyl anilines were prepared from corresponding literatures (*Org. Lett.* **2013**, *15*, 1654; *ACS Catal.* **2020**, *10*, 10495). Half-sandwich complexes **Sc-1**~ **Sc-4**, **Y-2**, **Sm-2**, and **Lu-2** were also prepared according to the literature procedure (*J. Am. Chem. Soc*., **1978**, *100*, 8068; *Chem. Eur. J.* **2011**, *17*, 5033; *Organometallics* **2011**, *30*, 2513; *Chem. Commun*. **2007**, 4137). Silica gel column chromatography was performed with Silica Gel 60 N (spherical, neutral, 40-50 μm) obtained from Kanato Chemical Co. All $^1$H NMR and $^{13}$C NMR spectra of organic products were recorded on Bruker AVANCE III HD 500 NMR (500 MHz) instrument. The $^1$H NMR Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as standard. The $^{13}$C NMR chemical shifts were given using $CDCl_3$ (77.16 ppm) or $C_6D_6$ (128.0 ppm) as the internal standard. The data are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, coupling constant(s) in Hz, integration). High Resolution Mass Spectra were obtained on a Bruker microTOF-Q III (ESI$^+$).

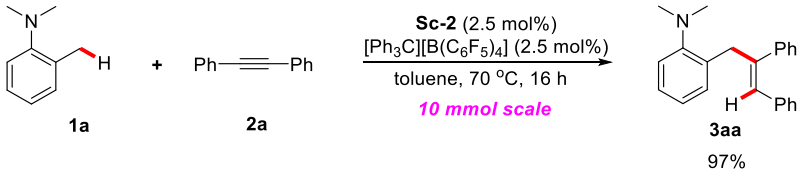
## 2. Representative procedure for scandium-catalyzed benzylic C−H Addition of 2-methyl anilines to internal alkynes



In a glovebox, $[Ph_3C][B(C_6F_5)_4]$ (9.2 mg, 0.01 mmol in 0.5 mL toluene) was added to a stirred toluene solution (1.5 mL) of **Sc-2** (4.5 mg, 0.01 mmol) in a Schlenk tube. After 10 min, to this tube was added 2-methyl anilines **1** (0.2 mmol, 1.0 equiv.) and alkynes **2** (0.4 mmol, 2 equiv.). After that, the tube was sealed, taken outside, and stirred at 70 °C for 16 h. Then, the mixture was concentrated and purified by silica gel column chromatography (hexane/acetone = 50:1) to obtain the desired product **3**.

**3. Representative procedure for gram scale synthesis of 3aa and its transformation**

**(1) Gram scale synthesis of 3aa**

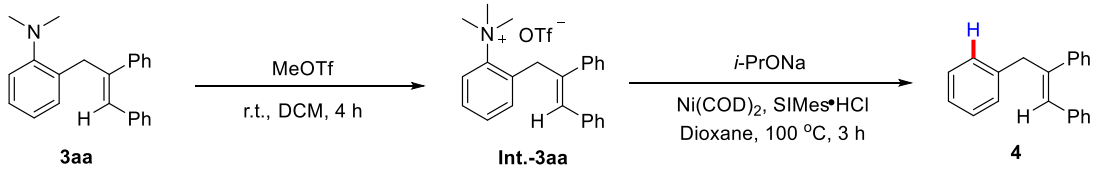



**1a** **2a** **3aa**

97%

In a glovebox, $[Ph_3C][B(C_6F_5)_4]$ (230 mg, 0.25 mmol in 25 mL toluene) was added to a stirred toluene solution (25 mL) of **Sc-2** (112.5 mg, 0.25 mmol) in a Schlenk tube. After 10 min, to this tube was added 2-methyl aniline **1a** (10 mmol, 1.0 equiv.) and diphenylacetylene **2a** (12 mmol, 1.2 equiv.). After that, the tube was sealed, taken outside, and stirred at 70 °C for 16 h. Then, the mixture was concentrated and purified by silica gel column chromatography (hexane/acetone = 50:1) to obtain the desired product **3a** (97% yield).

**(2) Removal of dialkyl amino group in product 3aa**

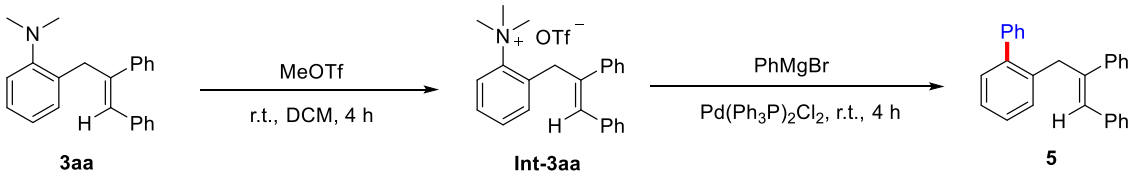



**3aa** **Int.-3aa** **4**

To a dry 20 mL Schlenk tube equipped with a magnetic stir bar was charged product **3aa** (0.20 mmol) and $CH_2Cl_2$ (2 mL). To the resultant stirring solution was added dropwise methyl trifluoromethanesulfonate (50 mg, 1.2 equiv) at r.t. The solution was stirred at r.t. for 4 h, at which time TLC analysis indicated complete consumption of **3aa**. The reaction mixture was concentrated to remove $CH_2Cl_2$ and the residue was washed with MTBE and hexanes, and dried under vacuum to give product **Int.-3aa** as thick oil, which was used directly for the next step. In a glovebox, a dry 20 mL Schlenk tube equipped with a magnetic stir bar was charged with obtained product **Int.-3aa**, $Ni(COD)_2$ (6.9 mg, 0.025 mmol, 10 mol%), SIMes·HCl (9.2 mg, 0.025 mmol, 10 mol%), *i*-PrONa

(68 mg, 0.75 mmol, 3 equiv) and dioxane (2 mL). The Schlenk tube was taken out of the glovebox and was heated to 100 °C and stirred for 3 h. The solvent was removed in vacuo and the residue was purified by silica gel chromatography (hexanes) to afford the desired products **4** (58% yield, *E*/*Z* = 3:1).

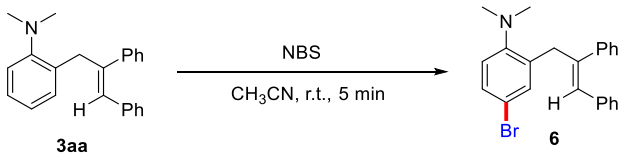
**(3) Kumada-type cross-coupling starting from product 3aa with phenyl Grignard reagent**




**3aa** **Int-3aa** **5**

To a dry 20 mL Schlenk tube equipped with a magnetic stir bar was charged product **3aa** (0.20 mmol) and $CH_2Cl_2$ (2 mL). To the resultant stirring solution was added dropwise methyl trifluoromethanesulfonate (50 mg, 1.2 equiv) at r.t. The solution was stirred at r.t. for 4 h, at which time TLC analysis indicated complete consumption of **3aa**. The reaction mixture was concentrated to remove $CH_2Cl_2$ and the residue was washed with MTBE and hexanes, and dried under vacuum to give product **Int-3aa** as thick oil, which was used directly for the next step. In a glovebox, to a dry 20 mL Schlenk tube equipped with a magnetic stir bar was charged obtained product **Int-3aa**, $PdCl_2(PPh_3)_2$ (3.5 mg, 0.005 mmol) and THF (1.5 mL), and the resultant slurry was stirred for 5 minutes. Then phenylmagnesium bromide (0.5 M solution in THF, 0.5 mL, 0.25 mmol) was added dropwise at r.t. The solution was stirred at r.t for 4 h. The reaction mixture was quenched by the addition of water (5 mL) and 2N HCl (1 mL), and extracted with MTBE. The organic extract was dried (MgSO4), filtered, and concentrated, and the crude product was purified by silica gel chromatography to afford the desired products **5** (65% yield).

**(4) Regioselective bromination of 3aa**



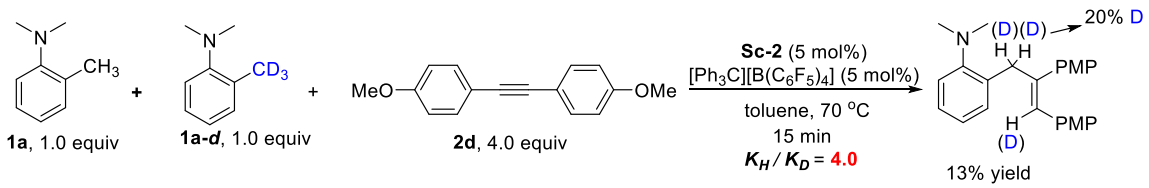

**3aa** **6**

NBS (0.21 mmol in $CH_3CN$ 1 mL) was added dropwise to a solution of **3aa** (0.2 mmol) in $CH_3CN$ (2 mL) in a 20 mL Schlenk tube with a magnetic stir bar. The reaction mixture was stirred at 25 °C until completion of the material as indicated by TLC. Then the solvents were removed in vacuo and the residue was directly purified by silica gel

chromatography using Hexane/acetone as the eluent to afford the desired bromination product **6** (96% yield).

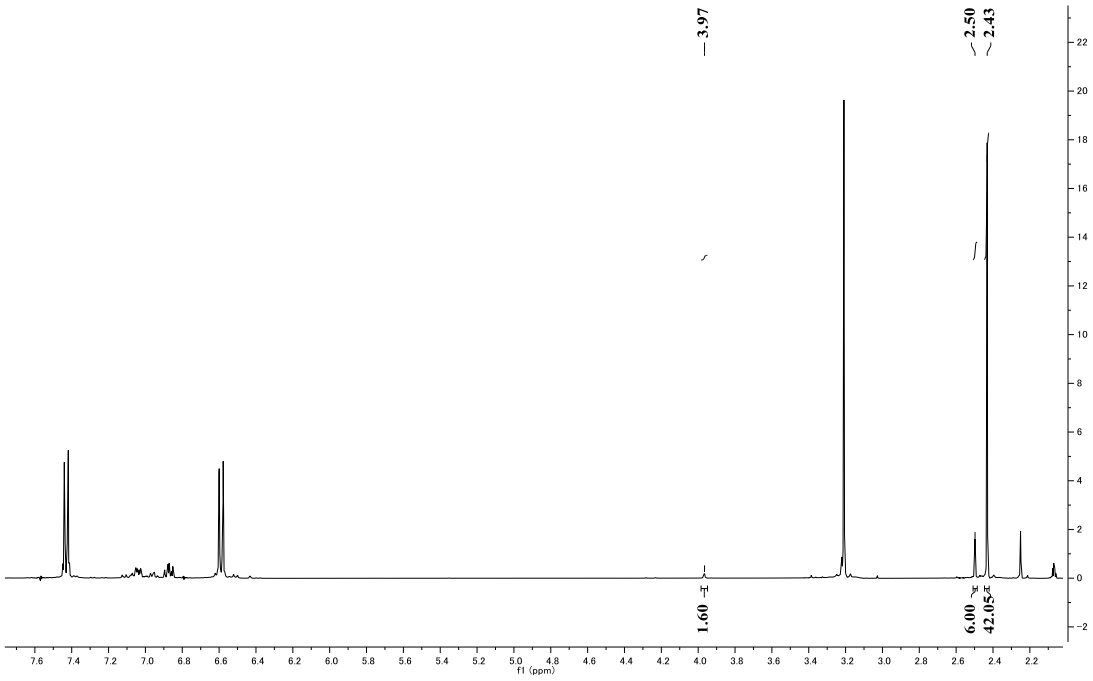
**4. Kinetic isotope effect experiments**

**(1) Intermolecular competition experiment**



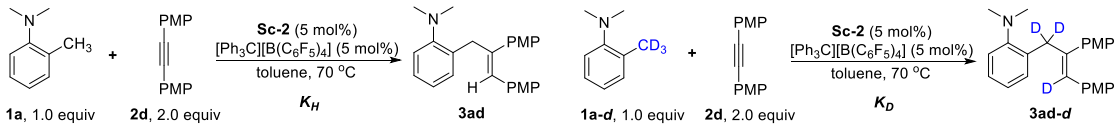

**1a**, 1.0 equiv + **1a-*d***, 1.0 equiv + **2d**, 4.0 equiv → 13% yield

In a glovebox, $[Ph_3C][B(C_6F_5)_4]$ (18.4 mg, 0.02 mmol in 1.0 mL toluene) was added to a stirred toluene solution (3.0 mL) of **Sc-2** (9.0 mg, 0.02 mmol) in a Schlenk tube. After 10 min, to this tube was added 2-methyl anilines **1a** (0.2 mmol, 1.0 equiv.), anilines **1a-*d*** (0.2 mmol, 1.0 equiv.) and alkynes **2d** (0.8 mmol, 2 equiv.). After that, the tube was sealed, taken outside, and stirred at 70 °C for 15 min. Then, the mixture was concentrated and purified by silica gel column chromatography (hexane/acetone = 40:1) to obtain the desired product **3ad-*d***, in which 99% deuterium was incorporated at the alkenyl and benzylic position. The D content (20%) of the methylene group in the product founded by $^1$H NMR reveals that the KIE value is 4.0.



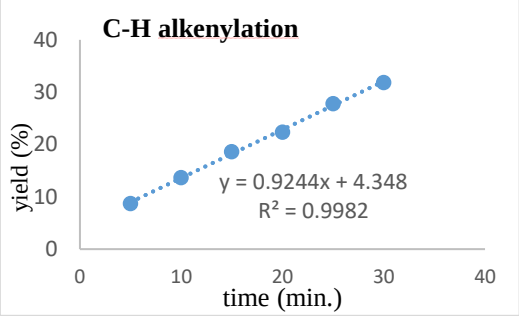
**(2) Initial rates of two side-by-side reactions**

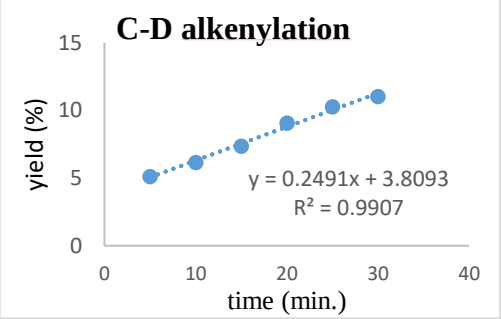
In a glovebox, a solution of $[Ph_3C][B(C_6F_5)_4]$ (9.2 mg, 0.01 mmol), and **Sc-2** (4.5 mg, 0.01 mmol) in toluene-$d_8$ (1 mL) was divided equally into two NMR tubes. To one tube was added the mixture of 2-methyl aniline **1a** (13.5 mg, 0.1 mmol) and internal alkyne **2d** (47.6 mg, 0.20 mmol) in toluene-$d_8$ (0.3 mL). To the other tube was added the mixture of deuterated aniline **1a-*d*$_3$** (16.5 mg, 0.1 mmol) and internal alkyne (47.6 mg, 0.20 mmol) in toluene-$d_8$ (0.3 mL). These tubes were sealed, taken out of the glovebox, and monitored by an NMR spectrometer at 70 ° C. Initial rates were calculated by comparing the $^1$H NMR integration of the methylene group and the *N*,*N*-dimethyl group. A KIE value of 3.70 was found in these side-by-side reactions.



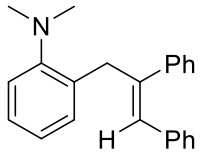

**1a**, 1.0 equiv **2d**, 2.0 equiv **3ad** **1a-*d***, 1.0 equiv **2d**, 2.0 equiv **3ad-*d***

$$k_H / k_D = 0.9244/0.2491 = 3.70$$



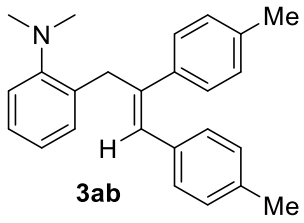




## 5. Analytic Data for Synthesized Compounds



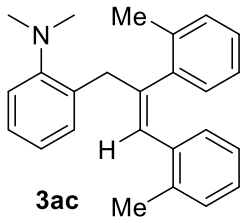

**3aa**

**3aa**; white solid; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.30 (d, *J* = 7.5 Hz, 1H), 7.24–7.15 (m, 6H), 7.11–7.00 (m, 5H), 6.91 (d, *J* = 7.5 Hz, 1H), 6.35 (s, 1H), 3.91 (s, 2H), 2.65 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.18, 142.66, 141.68, 137.52, 133.78, 131.15, 129.02, 128.58, 128.31, 127.77, 127.57, 127.06, 126.81, 126.11, 123.14, 119.68, 45.06, 41.10; HRMS (ESI) m/z calcd. for $C_{23}H_{24}N$ $[M+H]^+$ = 314.1903, found = 314.1920.



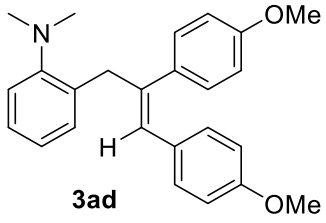

**3ab**

**3ab**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.30 (d, *J* = 7.0 Hz, 1H), 7.19–7.16 (m, 1H), 7.10–6.99 (m, 6H), 6.88 (d, *J* = 8.0 Hz, 2H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.28 (s, 1H), 3.87 (s, 2H), 2.65 (s, 6H), 2.30 (s, 3H), 2.22 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.13, 141.59, 138.82, 136.27, 135.67, 134.78, 133.97, 131.14, 129.03, 128.88, 128.49, 128.42, 127.27, 126.93, 123.04, 119.53, 45.03, 41.14, 21.20, 21.05; HRMS (ESI) m/z calcd. for $C_{25}H_{28}N$ $[M+H]^+$ = 342.2216, found = 342.2229.




**3ac**

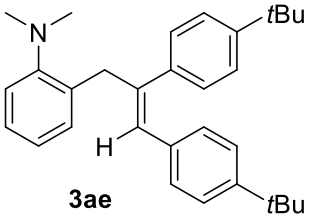
**3ac**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.27–7.19 (m, 3H), 7.13–7.08 (m, 4H), 7.04–7.01 (m, 3H), 6.93–6.90 (m, 1H), 6.74–6.71 (m, 1H), 6.61 (d, *J* = 7.5 Hz, 1H), 6.34 (s, 1H), 3.85 (br, 2H), 2.66 (s, 6H), 2.20 (s, 3H), 2.02 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.41, 142.32, 141.08, 136.69, 135.79, 135.22, 133.78, 131.62, 129.99, 129.50, 129.02, 128.35, 127.17, 126.63, 126.17, 126.11, 125.47, 125.05, 123.19, 119.82, 45.29, 40.96, 19.92, 19.16; HRMS (ESI) m/z calcd. for $C_{25}H_{28}N$ $[M+H]^+$ = 342.2216, found = 342.2229.




**3ad**

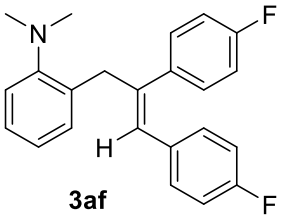
**3ad**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.30–7.29 (m, 1H), 7.19–7.15 (m, 1H), 7.10–7.07 (m, 3H), 7.01–6.99 (m, 1H), 6.88 (d, *J* = 7.0 Hz, 2H), 6.76 (d, *J* = 8.5 Hz, 2H), 6.63 (d, *J* = 8.5 Hz, 1H), 6.27 (s, 1H), 3.86 (s, 2H), 3.77 (s, 3H), 3.71 (s, 3H), 2.65 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 158.33, 157.81, 153.08, 140.10, 134.07, 134.01,

131.00, 130.39, 130.11, 129.76, 126.89, 126.81, 123.04, 119.50, 113.72, 113.24, 55.09, 45.03, 41.02; HRMS (ESI) m/z calcd. for $C_{25}H_{28}NO_2$ $[M+H]^+$ = 373.2036, found = 373.2035.



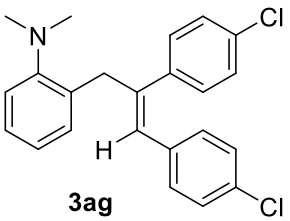
**3ae**

**3ae**; white solid; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.32 (d, *J* = 7.5 Hz, 1H), 7.28–7.25 (m, 2H), 7.21–7.18 (m, 1H), 7.11–7.08 (m, 5H), 7.03–7.00 (m, 1H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.25 (s, 1H), 3.86 (s, 2H), 2.63 (s, 6H), 1.31 (s, 9H), 1.23 (s, 9H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.17, 149.63, 148.98, 141.73, 139.03, 134.65, 134.06, 131.27, 128.58, 127.99, 127.10, 126.93, 125.24, 124.70, 123.04, 119.53, 45.02, 41.49, 34.38, 34.36, 31.38, 31.23; HRMS (ESI) m/z calcd. for $C_{31}H_{39}N$ $[M+H]^+$ = 426.3156, found = 426.3158.



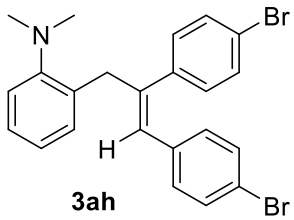
**3af**

**3af**; white solid; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.26 (d, *J* = 7.5 Hz, 1H), 7.20–7.17 (m, 1H), 7.11–7.06 (m, 3H), 7.03–6.99 (m, 1H), 6.92–6.85 (m, 4H), 6.79–6.76 (m, 2H), 6.35 (s, 1H), 3.87 (s, 2H), 2.63 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 161.79 (d, *J* = 244.38 Hz), 161.24 (d, *J* = 244.75 Hz), 153.14, 141.40, 137.016 (d, *J* = 3.38 Hz), 133.56, 133.39 (d, *J* = 3.12 Hz), 130.87, 130.50 (d, *J* = 7.75 Hz), 130.26 (d, *J* = 7.63 Hz), 127.19, 126.79, 123.24, 119.80, 115.31 (d, *J* = 21.13 Hz), 114.76 (d, *J* = 21.25 Hz), 45.06, 40.87; HRMS (ESI) m/z calcd. for $C_{23}H_{22}F_2N$ $[M+H]^+$ = 350.1715, found = 350.1719.



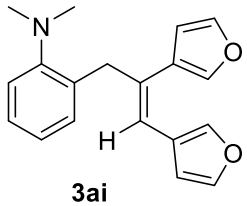
**3ag**

**3ag**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.25 (d, *J* = 8.0 Hz, 1H), 7.20–7.18 (m, 3H), 7.11–7.00 (m, 6H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.34 (s, 1H), 3.87 (s, 2H), 2.63 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.14, 142.18, 139.46, 135.68, 133.35, 132.83, 132.02, 130.83, 130.26, 130.00, 128.62, 128.10, 127.30, 126.95, 123.31, 119.89, 45.06, 40.74; HRMS (ESI) m/z calcd. for $C_{23}H_{22}Cl_2N$ $[M+H]^+$ = 382.1124, found = 382.1125.



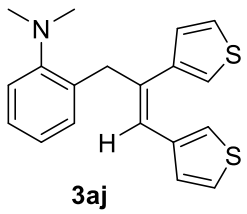
**3ah**

**3ah**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.34 (d, *J* = 8.5 Hz, 2H), 7.24–7.17 (m, 4H), 7.10 (d, *J* = 7.5 Hz, 1H), 7.02–6.98 (m, 3H), 6.78 (d, *J* = 8.5 Hz, 2H), 6.32 (s, 1H), 3.86 (s, 2H), 2.63 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.13, 142.31, 139.91, 136.09, 133.29, 131.57, 131.06, 130.81, 130.59, 130.31, 127.31, 126.97, 123.31, 121.03, 120.22, 119.89, 45.05, 40.70; HRMS (ESI) m/z calcd. for $C_{23}H_{22}Br_2N$ $[M+H]^+$ = 469.0035, found = 469.0039.



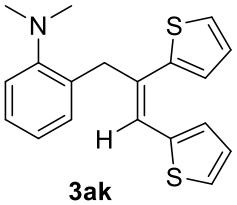
**3ai**

**3ai**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.30–7.25 (m, 4H), 7.20–7.17 (m, 2H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.01–6.99 (m, 1H), 6.26 (s, 1H), 6.20 (s, 1H), 6.19 (s, 1H), 3.77 (s, 2H), 2.65 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 152.94, 142.34, 142.19, 141.17, 140.26, 133.77, 132.27, 130.41, 127.03, 124.65, 123.05, 122.74, 119.33, 118.56, 111.00, 110.47, 44.95, 40.03; HRMS (ESI) m/z calcd. for $C_{19}H_{20}NO_2$ $[M+H]^+$ = 294.1489, found = 294.1489.



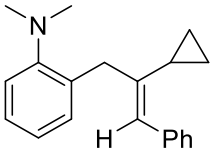
**3aj**

**3aj**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.30–7.27 (m, 2H), 7.22–7.19 (m, 1H), 7.11 (d, *J* = 8.0 Hz, 1H), 7.05–7.01 (m, 2H), 6.98–6.96 (m, 1H), 6.87–6.84 (m, 3H), 6.85 (s, 1H), 3.87 (s, 2H), 2.62 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.24, 141.42, 140.39, 133.76, 133.33, 130.81, 127.88, 127.29, 126.99, 126.90, 126.15, 126.05, 125.71, 124.07, 123.19, 119.73, 45.02, 41.71; HRMS (ESI) m/z calcd. for $C_{19}H_{20}NS_2$ $[M+H]^+$ = 326.1032, found = 326.1033.



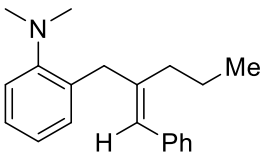

**3ak**

**3ak**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.31–7.27 (m, 2H), 7.23–7.20 (m, 1H), 7.11 (d, *J* = 8.0 Hz, 1H), 7.05–7.01 (m, 2H), 6.98–6.97 (m, 1H), 6.87–6.85 (m, 3H), 6.65 (s, 1H), 3.87 (s, 2H), 2.62 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.26, 141.43, 140.40, 133.78, 133.34, 130.82, 127.89, 127.30, 127.00, 126.91, 126.15, 126.07, 125.72, 124.08, 123.19, 119.73, 45.03, 41.72; HRMS (ESI) m/z calcd. for $C_{19}H_{20}NS_2$ $[M+H]^+$ = 326.1032, found = 326.1033.



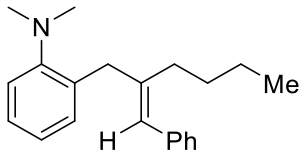

**3al**

**3al**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.41 (d, *J* = 7.5 Hz, 2H), 7.32–7.27 (m, 3H), 7.21–7.16 (m, 2H), 7.10 (d, *J* = 7.5 Hz, 1H), 7.03–6.99 (m, 1H), 6.27 (s, 1H), 3.33 (s, 2H), 2.68 (s, 6H), 1.91–1.85 (m, 2H), 0.64–0.55 (m, 4H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 152.57, 142.01, 138.47, 134.32, 130.54, 129.08, 127.99, 127.89, 126.78, 125.85, 122.91, 119.13, 44.89, 34.67, 13.94, 6.31; HRMS (ESI) m/z calcd. for $C_{21}H_{24}N$ $[M+H]^+$ = 288.1906, found = 288.1908.



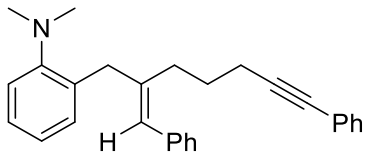

**3am**

**3am**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.31–7.28 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.21–7.16 (m, 4H), 7.12 (d, *J* = 8.0 Hz, 1H), 7.03–7.00 (m, 1H), 6.24 (s, 1H), 3.60 (s, 2H), 2.69 (s, 6H), 2.19–2.16 (m, 2H), 1.57–1.49 (m, 3H), 0.89 (t, *J* = 7.0 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.14, 143.34, 138.64, 134.38, 130.73, 128.62, 128.02, 126.83, 126.71, 125.88, 123.03, 119.34, 45.03, 38.08, 33.28, 21.55, 14.23; HRMS (ESI) m/z calcd. for $C_{20}H_{26}N$ $[M+H]^+$ = 280.2060, found = 280.2060.



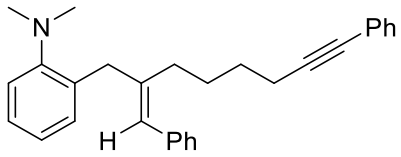

**3an**

**3an**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.31–7.28 (m, 2H), 7.25–7.16 (m, 5H), 7.12 (d, *J* = 8.0 Hz, 1H), 7.03–7.00 (m, 1H), 6.23 (s, 1H), 3.60 (s, 2H), 2.70 (s, 6H), 2.21–2.17 (m, 2H), 1.53–1.46 (m, 2H), 1.33–1.25 (m, 2H), 0.85 (t, *J* = 7.5 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.14, 143.54, 138.64, 134.38, 130.76, 128.61, 128.01, 126.82, 126.51, 125.86, 123.03, 119.33, 45.03, 38.08, 30.91, 30.48, 22.85, 13.94; HRMS (ESI) m/z calcd. for $C_{21}H_{28}N$ $[M+H]^+$ = 294.2216, found = 294.2227.



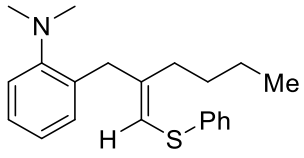

**3ao**

**3ao**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.31–7.25 (m, 10H), 7.22–7.19 (m, 1H), 7.17–7.12 (m, 2H), 6.30 (s, 1H), 3.63 (s, 2H), 2.70 (s, 6H), 2.39–2.36 (m, 4H), 1.85–1.79 (m, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.15, 142.29, 138.35, 134.22, 131.55, 130.64, 128.63, 128.13, 128.10, 127.46, 127.41, 126.94, 126.02, 123.92, 123.15, 119.46, 89.93, 80.93, 45.06, 38.13, 30.43, 27.35; HRMS (ESI) m/z calcd. for $C_{28}H_{30}N$ $[M+H]^+$ = 380.2373, found = 380.2386.



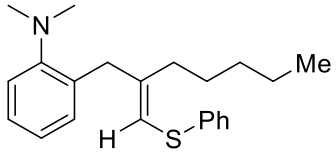

**3ap**

**3ap**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.38–7.36 (m, 2H), 7.30–7.17 (m, 10H), 7.12 (d, *J* = 7.5 Hz, 1H), 7.03–7.00 (m, 1H), 6.27 (s, 1H), 3.62 (s, 2H), 2.68 (s, 6H), 2.35 (t, *J* = 7.0 Hz, 2H), 2.23 (d, *J* = 7.5 Hz, 2H), 1.72–1.66 (m, 2H), 1.61–1.56 (m, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.15, 142.94, 138.51, 134.29, 131.52, 130.70, 128.60, 128.15, 128.07, 127.46, 126.93, 126.89, 125.98, 124.03, 123.09, 119.40, 90.17, 80.70, 45.04, 38.04, 30.50, 28.75, 27.40, 19.15; HRMS (ESI) m/z calcd. for $C_{29}H_{32}N$ $[M+H]^+$ = 394.2529, found = 394.2536.



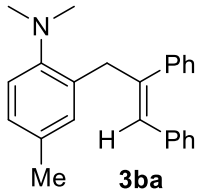

**3aq**

**3aq**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.26–7.25 (m, 4H), 7.20–7.17 (m, 2H), 7.15–7.10 (m, 2H), 7.03–7.00 (m, 1H), 5.86 (s, 1H), 3.60 (s, 2H), 2.68 (s, 6H), 2.26 (t, *J* = 7.5 Hz, 2H), 1.48–1.42 (m, 2H), 1.38–1.30 (m, 2H), 0.91 (t, *J* = 7.5 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.10, 146.82, 137.59, 133.49, 130.77, 128.80, 127.78, 127.12, 125.46, 123.16, 119.47, 117.06, 45.07, 37.77, 32.24, 30.13, 22.67, 13.99; HRMS (ESI) m/z calcd. for $C_{21}H_{28}NS$ $[M+H]^+$ = 326.1937, found = 326.1951.



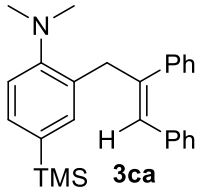

**3ar**

**3ar**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.26–7.25 (m, 4H), 7.20–7.17 (m, 2H), 7.15–7.10 (m, 2H), 7.03–7.00 (m, 1H), 5.87 (s, 1H), 3.60 (s, 2H), 2.68 (s, 6H), 2.25 (t, *J* = 7.5 Hz, 2H), 1.50–1.44 (m, 2H), 1.34–1.30 (m, 4H), 0.88 (t, *J* = 6.5 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.10, 146.90, 137.61, 133.50, 130.77, 128.80, 127.79, 127.12, 125.47, 123.16, 119.47, 117.05, 45.08, 37.77, 32.42, 31.71, 27.57, 22.50, 14.01; HRMS (ESI) m/z calcd. for $C_{22}H_{30}NS$ $[M+H]^+$ = 340.2094, found = 340.2098.



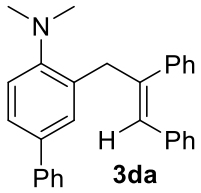

**3ba**

**3ba**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.24–7.20 (m, 3H), 7.17–7.15 (m, 2H), 7.11 (s, 2H), 7.08–6.99 (m, 5H), 6.91 (d, *J* = 7.0 Hz, 2H), 6.32 (s, 1H), 3.87 (s, 2H), 2.61 (s, 6H), 2.28 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 150.76, 142.86, 141.83, 137.59, 133.78, 132.59, 131.77, 129.02, 128.57, 128.31, 127.76, 127.66, 127.39, 126.79, 126.08, 119.68, 45.30, 41.03, 20.83; HRMS (ESI) m/z calcd. for $C_{24}H_{26}N$ $[M+H]^+$ = 328.2060, found = 328.2060.



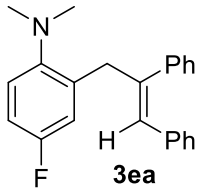
**3ca**

**3ca**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.37 (s, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.24–7.15 (m, 5H), 7.09–7.04 (m, 4H), 6.91 (d, *J* = 7.0 Hz, 2H), 6.39 (s, 1H), 3.91 (s, 2H), 2.69 (s, 6H), 0.21 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.78, 142.65, 141.64, 137.60, 136.57, 133.74, 132.49, 132.14, 129.02, 128.68, 128.32, 127.78, 127.58, 126.81, 126.09, 118.80, 44.86, 41.26, -1.01; HRMS (ESI) m/z calcd. for $C_{26}H_{32}NSi$ $[M+H]^+$ = 386.2299, found = 386.2320.



**3da**

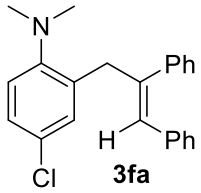
**3da**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.53–7.51 (m, 3H), 7.43–7.37 (m, 3H), 7.30–7.15 (m, 7H), 7.08–7.02 (m, 3H), 6.92 (d, *J* = 6.5 Hz, 1H), 6.42 (s, 1H), 3.96 (s, 2H), 2.70 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 152.56, 142.53, 141.60, 141.07, 137.46, 135.73, 133.80, 129.94, 129.06, 128.64, 128.38, 127.79, 127.71, 126.88, 126.83, 126.69, 126.17, 125.69, 119.88, 45.04, 41.35; HRMS (ESI) m/z calcd. for $C_{29}H_{28}N$ $[M+H]^+$ = 390.2216, found = 390.2218.



**3ea**

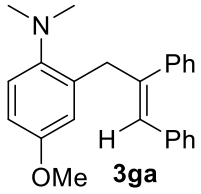
**3ea**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.25–7.19 (m, 3H), 7.14–7.13 (m, 2H), 7.10–7.00 (m, 5H), 6.93 (d, *J* = 7.0 Hz, 1H), 6.87–6.84 (m, 1H), 6.39 (s, 1H), 3.90 (s,

2H), 2.58 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 159.10 (d, *J* = 239.88 Hz), 149.18 (d, *J* = 2.38 Hz), 141.91, 141.15, 137.29, 136.67 (d, *J* = 7.25 Hz), 129.04, 128.61, 128.35, 128.07, 127.83, 126.95, 126.30, 121.29 (d, *J* = 8.25 Hz), 117.06 (d, *J* = 22.00 Hz), 113.44 (d, *J* = 21.75 Hz), 45.43, 40.90; HRMS (ESI) m/z calcd. for $C_{23}H_{23}NF$ $[M+H]^+$ = 332.1809, found = 332.1821.



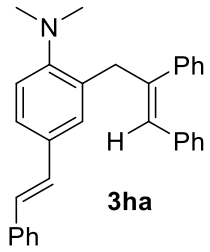
**3fa**

**3fa**; white solid; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.28–7.20 (m, 4H), 7.14–7.06 (m, 6H), 7.01 (d, *J* = 7.5 Hz, 1H), 6.93 (d, *J* = 7.5 Hz, 2H), 6.37 (s, 1H), 3.87 (s, 2H), 2.61 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 151.76, 141.84, 141.16, 137.24, 135.84, 130.72, 129.05, 128.56, 128.38, 128.31, 128.04, 127.83, 127.00, 126.98, 126.33, 121.10, 45.00, 40.90; HRMS (ESI) m/z calcd. for $C_{23}H_{23}NCl$ $[M+H]^+$ = 348.1514, found = 348.1517.



**3ga**

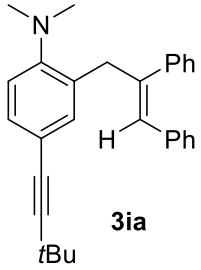
**3ga**; white solid; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.24–7.15 (m, 5H), 7.08–7.04 (m, 4H), 6.92 (d, *J* = 7.0 Hz, 2H), 6.84 (d, *J* = 3.0 Hz, 1H), 6.75–6.72 (m, 1H), 6.37 (s, 1H), 3.90 (s, 2H), 3.73 (s, 3H), 2.58 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 155.71, 146.59, 142.48, 141.55, 137.53, 135.95, 129.03, 128.68, 128.31, 127.77, 127.73, 126.82, 126.13, 121.09, 116.12, 112.18, 55.38, 45.67, 41.09; HRMS (ESI) m/z calcd. for $C_{24}H_{26}NO$ $[M+H]^+$ = 344.2009, found = 344.2007.



**3ha**

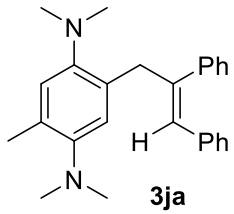
**3ha**; white solid; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.49–7.48 (m, 2H), 7.44 (s, 1H), 7.36–7.32 (m, 3H), 7.26–7.18 (m, 6H), 7.09–7.04 (m, 5H), 6.98–6.93 (m, 3H), 6.40 (s, 1H),

3.91 (s, 2H), 2.68 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 152.94, 142.55, 141.68, 137.70, 137.48, 133.57, 132.02, 129.63, 129.09, 128.62, 128.43, 127.83, 127.68, 127.22, 127.08, 126.93, 126.32, 126.22, 125.23, 119.73, 44.94, 41.34; HRMS (ESI) m/z calcd. for $C_{31}H_{30}N$ $[M+H]^+$ = 416.2373, found = 416.2375.



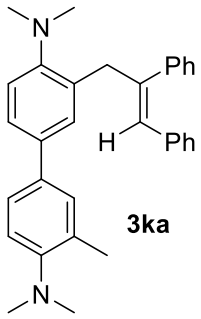

**3ia**

**3ia**; white solid; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.34 (d, *J* = 1.5 Hz, 1H), 7.26–7.21 (m, 4H), 7.17–7.15 (m, 2H), 7.09–7.04 (m, 3H), 6.97 (d, *J* = 7.5 Hz, 1H), 6.91 (d, *J* = 7.0 Hz, 2H), 6.29 (s, 1H), 3.83 (s, 2H), 2.62 (s, 6H), 1.30 (s, 9H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 152.67, 142.54, 141.73, 137.44, 134.52, 133.14, 130.55, 129.05, 128.49, 128.39, 127.79, 127.40, 126.88, 126.16, 119.33, 118.32, 97.34, 79.04, 44.79, 41.11, 31.14, 27.91; HRMS (ESI) m/z calcd. for $C_{29}H_{32}N$ $[M+H]^+$ = 394.2529, found = 394.2526.



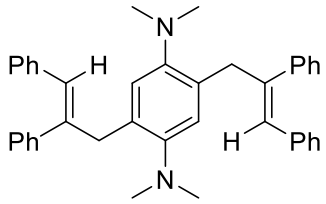

**3ja**

**3ja**; white solid; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.23–7.15 (m, 5H), 7.11–7.02 (m, 3H), 6.93–6.91 (m, 4H), 6.39 (s, 1H), 3.87 (s, 2H), 2.62 (s, 6H), 2.60 (s, 6H), 2.28 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 148.14, 148.01, 142.89, 141.74, 137.67, 131.73, 130.74, 129.00, 128.72, 128.30, 127.77, 127.44, 126.75, 126.05, 122.48, 121.12, 45.45, 44.58, 40.97, 17.96; HRMS (ESI) m/z calcd. for $C_{26}H_{31}N_2$ $[M+H]^+$ = 371.2482, found = 371.2484.



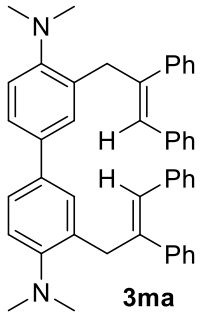

**3ka**

**3ka**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.46 (d, *J* = 2.0 Hz, 1H), 7.39–7.37 (m, 1H), 7.32–7.31 (m, 2H), 7.27–7.18 (m, 5H), 7.14 (d, *J* = 7.0 Hz, 1H), 7.08–7.03 (m, 4H), 6.91 (d, *J* = 7.0 Hz, 1H), 6.41 (s, 1H), 3.95 (s, 2H), 2.72 (s, 6H), 2.69 (s, 6H), 2.37 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 152.01, 151.66, 142.64, 141.71, 137.53, 135.75, 135.24, 133.76, 132.13, 129.69, 129.07, 128.69, 128.37, 127.76, 127.63, 126.85, 126.12, 125.37, 124.72, 119.84, 118.53, 45.13, 44.26, 41.36, 18.60; HRMS (ESI) m/z calcd. for $C_{32}H_{35}N_2$ $[M+H]^+$ = 447.2795, found = 447.2796.



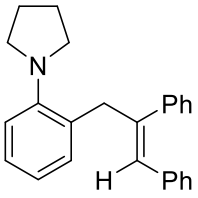

**3la**

**3la**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.22–7.16 (m, 6H), 7.11–7.04 (m, 10H), 6.95 (s, 2H), 6.91 (d, *J* = 6.5 Hz, 1H), 6.36 (s, 2H), 3.86 (s, 4H), 2.54 (s, 12H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 148.57, 142.90, 141.60, 137.63, 132.50, 128.99, 128.68, 128.25, 127.78, 127.39, 126.71, 126.07, 122.50, 45.40, 41.06; HRMS (ESI) m/z calcd. for $C_{40}H_{41}N_2$ $[M+H]^+$ = 549.3264, found = 549.3262.



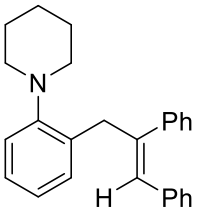

**3ma**

**3ma**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.43 (d, *J* = 7.0 Hz, 2H), 7.35–7.33 (m, 2H), 7.23–7.17 (m, 10H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.06–7.01 (m, 6H), 6.90–6.89 (m, 4H), 6.40 (s, 2H), 3.94 (s, 4H), 2.68 (s, 12H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 152.09, 142.60, 141.64, 137.51, 135.70, 133.75, 129.66, 129.06, 128.67, 128.35, 127.77, 127.63, 126.83, 126.10, 125.39, 119.85, 45.11, 41.32; HRMS (ESI) m/z calcd. for $C_{40}H_{41}N_2$ $[M+H]^+$ = 549.3264, found = 549.3262.



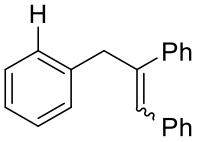

**3na**

**3na**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.27–7.21 (m, 4H), 7.18–7.15 (m, 3H), 7.08–7.03 (m, 3H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.93–6.89 (m, 3H), 6.29 (s, 1H), 3.84 (s, 2H), 3.16–3.14 (m, 4H), 1.92–1.87 (m, 4H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 149.63, 142.68, 141.91, 137.59, 132.01, 130.47, 129.05, 128.50, 128.40, 127.77, 127.58, 127.02, 126.87, 126.09, 120.96, 117.41, 51.74, 42.81, 24.92; HRMS (ESI) m/z calcd. for $C_{25}H_{26}N$ $[M+H]^+$ = 340.2060, found = 340.2062.



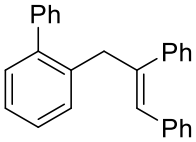

**3oa**

**3oa**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.28–7.13 (m, 7H), 7.08–6.99 (m, 5H), 6.90 (d, *J* = 7.0 Hz, 2H), 6.35 (s, 1H), 3.89 (s, 2H), 2.78–2.76 (m, 4H), 1.72–1.65 (m, 4H), 1.54 (s, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.38, 143.03, 141.66, 137.57, 134.31, 131.02, 129.00, 128.58, 128.28, 127.77, 127.11, 127.05, 126.75, 126.07, 123.30, 120.43, 54.15, 41.06, 26.78, 24.38; HRMS (ESI) m/z calcd. for $C_{26}H_{28}N$ $[M+H]^+$ = 354.2216, found = 354.2208.



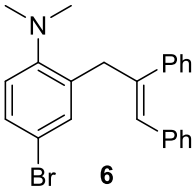

**4** (*E*/*Z* = 3:1)

**3oa**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.49 (d, *J* = 7.5 Hz, 2H), 7.35–7.15 (m, 12H), 7.11 (s, 1H), 7.07–7.05 (m, 1H), 4.13 (s, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 142.43, 139.67, 139.05, 137.73, 130.31, 129.24, 128.58, 128.49, 128.36, 128.34, 127.26, 126.96, 126.49, 125.92, 30.10; HRMS (ESI) m/z calcd. for $C_{23}H_{26}N$ $[M+H]^+$ = 316.2060, found = 316.2070.



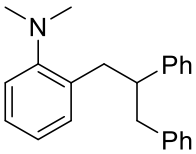

**5**

**5**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.39–7.25 (m, 10H), 7.18–7.17 (m, 3H), 7.05–7.02 (m, 3H), 6.90–6.88 (m, 2H), 6.81 (d, *J* = 6.5 Hz, 2H), 6.06 (s, 1H), 3.71 (s, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 142.70, 142.66, 141.69, 141.36, 137.31, 136.17, 130.73, 130.09, 129.18, 128.96, 128.40, 128.37, 127.96, 127.74, 127.26, 126.88, 126.83, 126.37, 126.16, 43.90; HRMS (ESI) m/z calcd. for $C_{27}H_{23}$ $[M+H]^+$ = 345.1795, found = 345.1796.



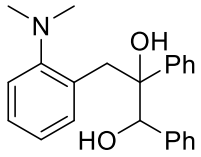

**6**

**6**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.41 (d, *J* = 1.5 Hz, 1H), 7.28–7.19 (m, 4H), 7.13 (d, *J* = 7.0 Hz, 2H), 7.09–7.04 (m, 3H), 6.95–6.92 (m, 3H), 6.36 (s, 1H), 3.86 (s, 2H), 2.60 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 152.23, 141.82, 141.14, 137.20, 136.17, 133.67, 129.97, 129.04, 128.53, 128.38, 128.03, 127.82, 126.97, 126.32, 121.50, 116.08, 44.88, 40.88; HRMS (ESI) m/z calcd. for $C_{23}H_{23}NBr$ $[M+H]^+$ = 392.1008, found = 392.1010.




**7**

**7**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.18–7.15 (m, 4H), 7.11–7.01 (m, 8H), 6.96 (d, *J* = 7.5 Hz, 1H), 6.88–6.85 (m, 1H), 3.35–3.29 (m, 1H), 3.13–3.09 (m, 1H), 2.96–2.91 (m, 3H), 2.55 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 153.18, 145.02, 140.92, 135.74, 130.36, 129.12, 127.90, 126.62, 125.84, 125.60, 123.22, 119.76, 48.45, 45.01, 42.67, 37.42; HRMS (ESI) m/z calcd. for $C_{23}H_{26}N$ $[M+H]^+$ = 316.2060, found = 316.2064.




**8**

**8**; white solid; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 8.22 (br, 1H), 7.13–7.03 (m, 11H), 7.00–6.97 (m, 1H), 6.84–6.81 (m, 1H), 6.73 (d, *J* = 7.5 Hz, 1H), 4.88 (s, 1H), 3.94 (br, 1H), 3.83 (d, *J* = 14.5 Hz, 1H), 3.26 (d, *J* = 14.5 Hz, 1H), 2.71 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 151.29, 142.68, 140.53, 133.92, 133.26, 127.97, 127.69, 127.23, 127.04, 126.93, 126.49, 126.02, 125.21, 120.01, 80.43, 44.98, 43.37; HRMS (ESI) m/z calcd. for $C_{23}H_{26}NO_2$ $[M+H]^+$ = 348.1958, found = 348.1957.

## 6. X-ray Crystallographic Studies

Suitable crystals for an X-ray diffraction study were obtained as described below. These were manipulated under a microscope in a glovebox filled with nitrogen. Data collections were performed at –100 ˚C on a Bruker D8 QUEST diffractometer equipped with a CMOS area detector, using a IμS (Incoatec Microfocus Source) microfocus sealed tube with Mo Kα radiation (λ = 0.71073 Å) at 173 K. The Bravais lattice and the unit cell parameters were S64 determined by the Bruker APEX3 software package.[1] The raw frame data were processed, and absorption corrections were done using SAINT and SADABS embedded in Bruker APEX3 to yield the reflection data (hkl) file. All of the structures were solved using SIR-2014[2] and SHELXL-2017.[3] Structural refinement was performed using the WINGX-Version 2014.1 system,[4] on $F^2$ anisotropically for all of the non-hydrogen atoms by the fullmatrix least-squares method. The analytical scattering factors for neutral atoms S70 were used throughout the analysis. The hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. The residual electron densities were of no chemical significance. CCDC number 2168988 (**3la**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.uk/data_request/cif.

**X-ray structure of 3la**

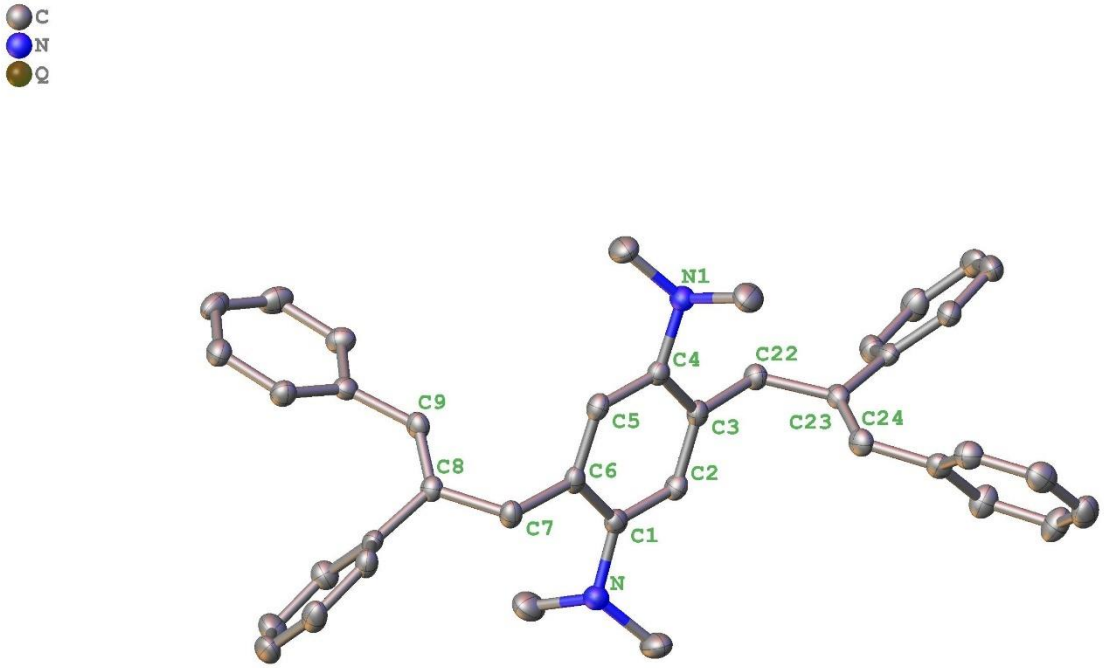



**Fig. S1.** X-ray structure of **3la**

**Crystal data and structure refinement for 3la**

Bond precision: C-C = 0.0019 Å
Wavelength = 0.71073
Cell: a=10.4940(3) b=11.0423(3) c=15.0933(5)
alpha=70.036(1) beta=85.293(1) gamma=71.406(1)
Temperature: 296 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1557.37(8) | 1557.37(8) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C40 H40 N2 | C40 H40 N2 |
| Sum formula | C40 H40 N2 | C40 H40 N2 |
| Mr | 548.74 | 548.74 |
| Dx,g cm-3 | 1.170 | 1.170 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.067 | 0.067 |
| F000 | 588.0 | 588.0 |
| F000' | 588.20 | |
| h,k,lmax | 12,13,17 | 12,13,17 |
| Nref | 5522 | 5512 |
| Tmin,Tmax | 0.961,0.967 | 0.722,0.745 |
| Tmin' | 0.961 | |

Correction method= # Reported T Limits: Tmin=0.722 Tmax=0.745
AbsCorr = MULTI-SCAN
Data completeness= 0.998 Theta(max)= 25.060
R(reflections)= 0.0368( 4944) wR2(reflections)= 0.0997( 5512)
S = 1.032 Npar= 383

**References**

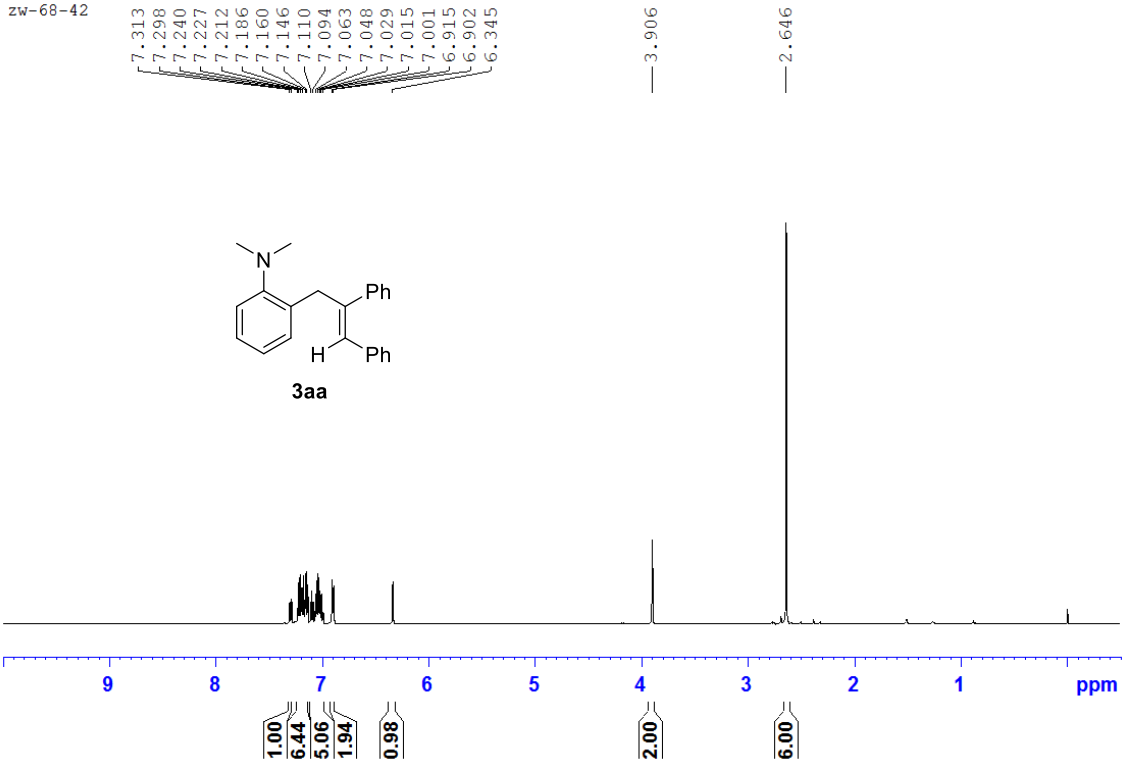
1. APEX3 v2016.1-0, Bruker AXS Inc., Madison, **2016**.

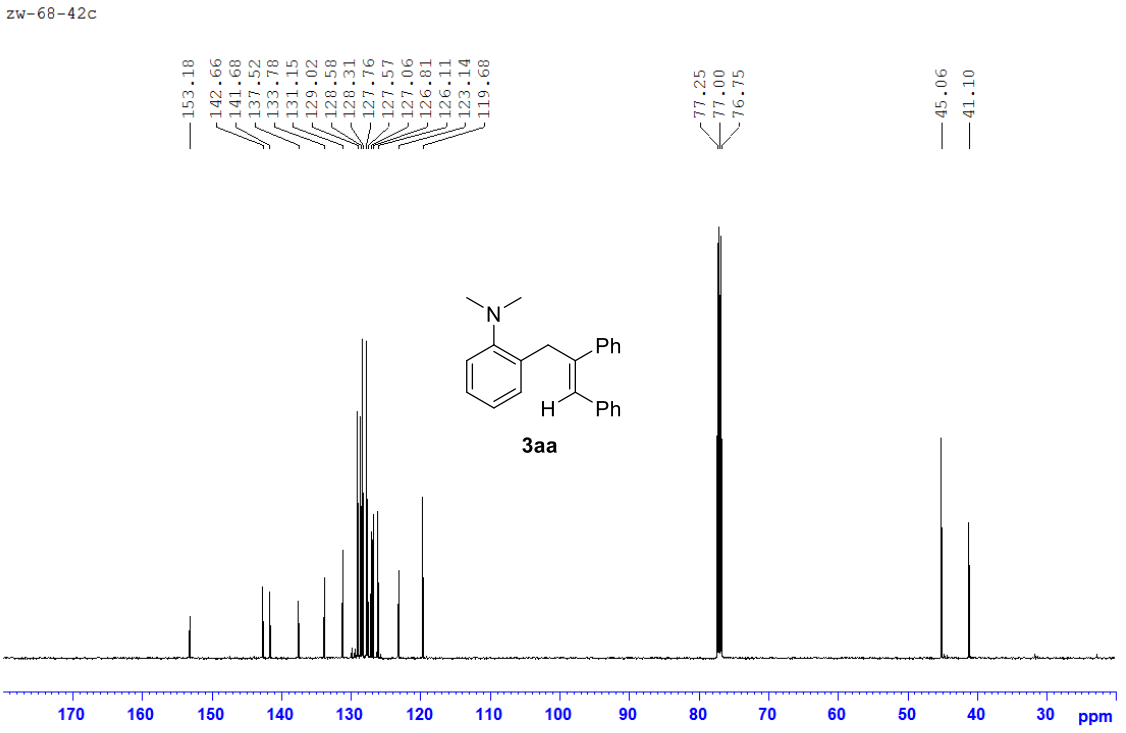
2. Burla, M. C.; Caliandro, R.; Carrozzini, B.; Cascarano, G. L.; Cuocci, C.; Giacovazzo, C.; Mallamo, M.; Mazzone, A.; Polidori, G. SIR-2014, version 14.07.

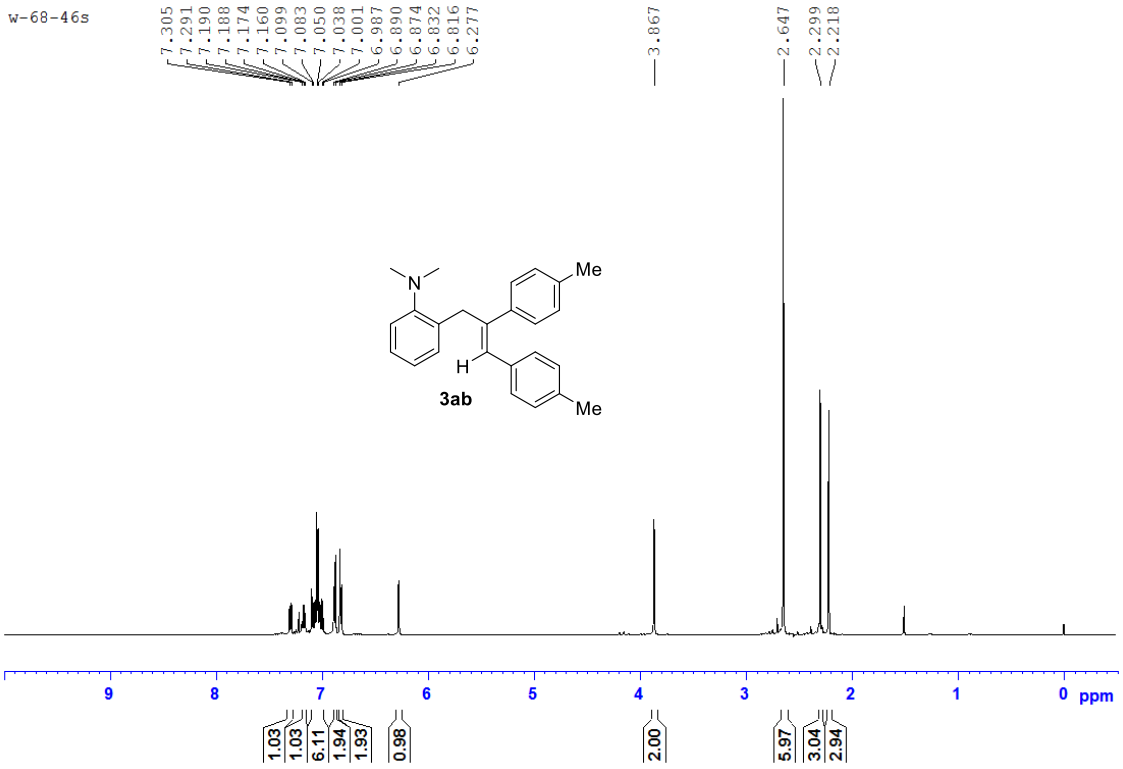
3. Sheldrick, G. M. SHELXL 2018/1, University of Göttingen, Germany, **2018**.

4. Farrugia, L. J. *J. Appl. Cryst*. **2012**, *45*, 849.

## 7. NMR spectra for the synthesized compounds

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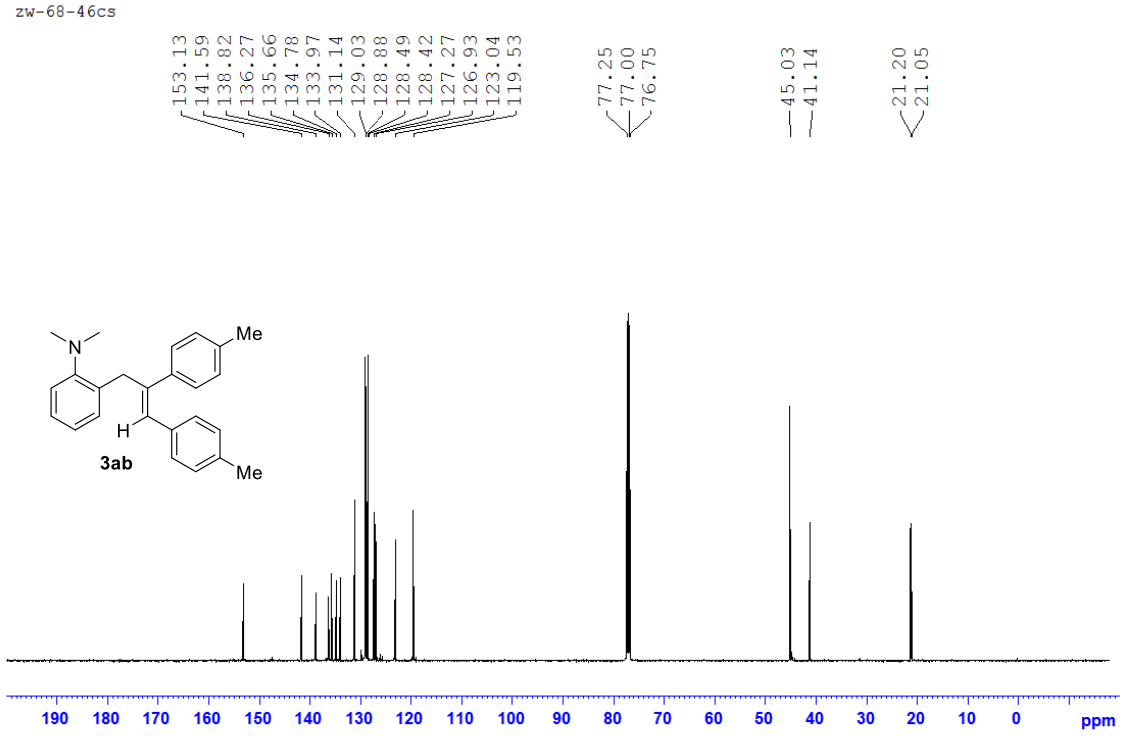
7.291
7.190
7.188
7.174
7.160
7.099
7.083
7.050
7.038
7.001
6.987
6.890
6.874
6.832
6.816
6.277
3.867
2.647
2.299
2.218
N
Me
H
Me
3ab
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.03
6.11
1.94
1.93
0.98
2.00
5.97
3.04
2.94


zw-68-46cs
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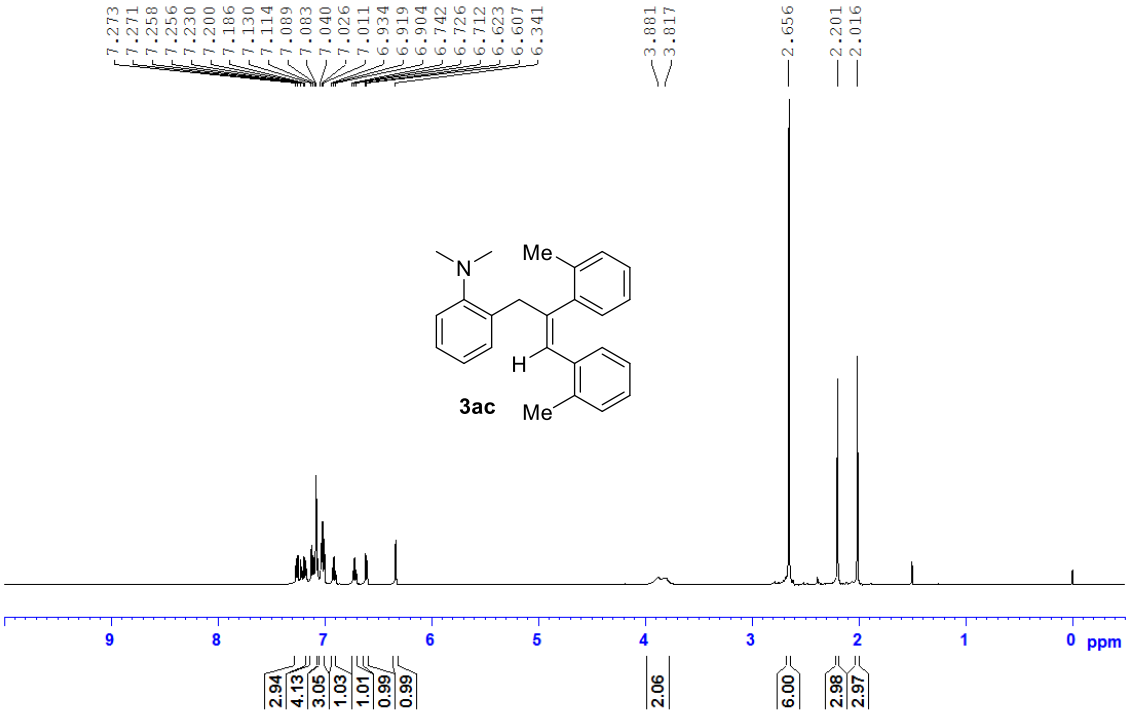
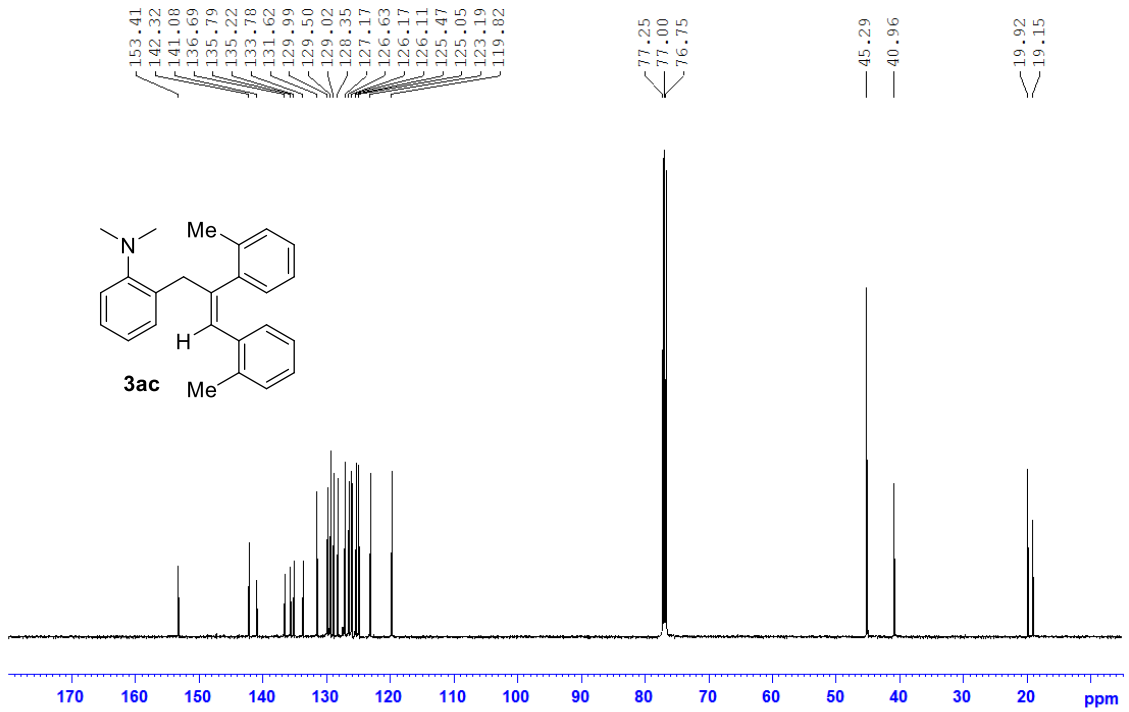
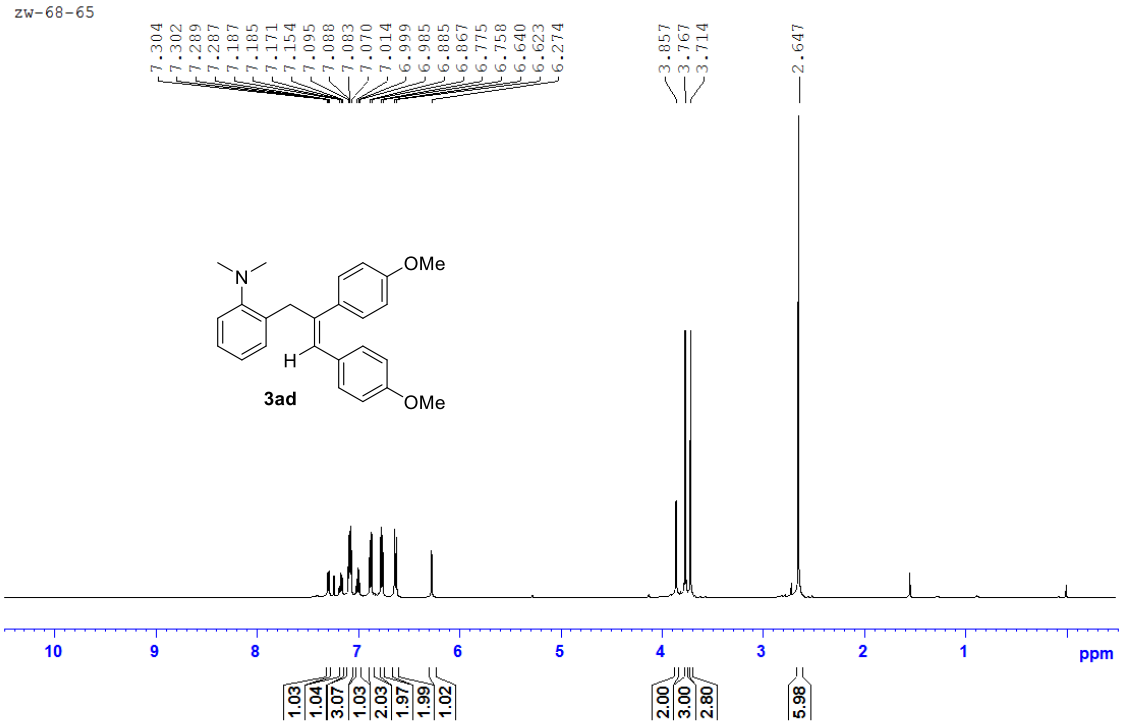
141.59
138.82
136.27
135.66
134.78
133.97
131.14
129.03
128.88
128.49
128.42
127.27
126.93
123.04
119.53
77.25
77.00
76.75
45.03
41.14
21.20
21.05
N
Me
H
Me
3ab
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

zw-68-68b




zw-68-68bc

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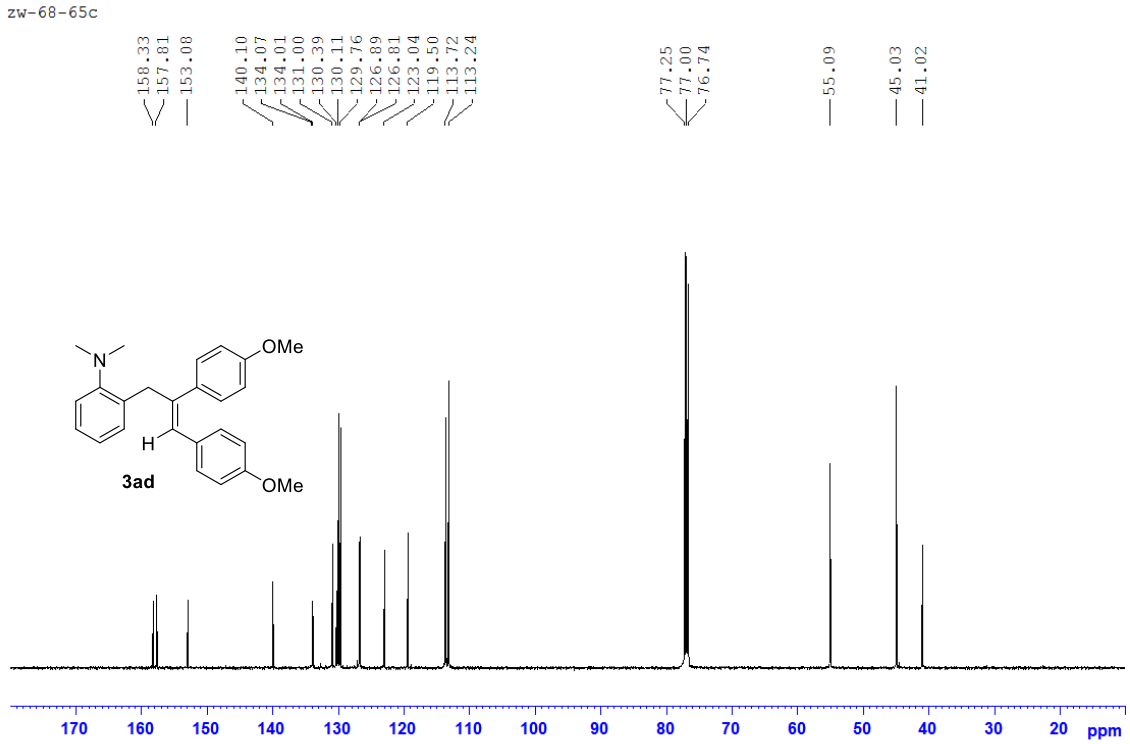
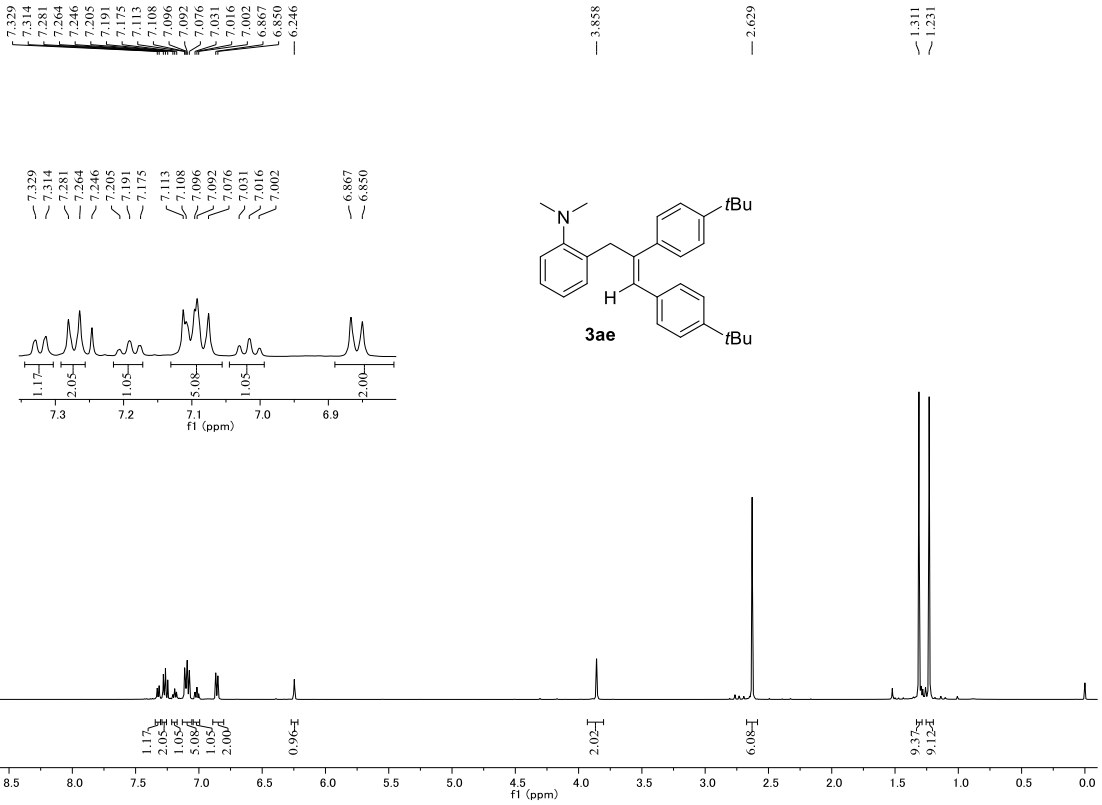
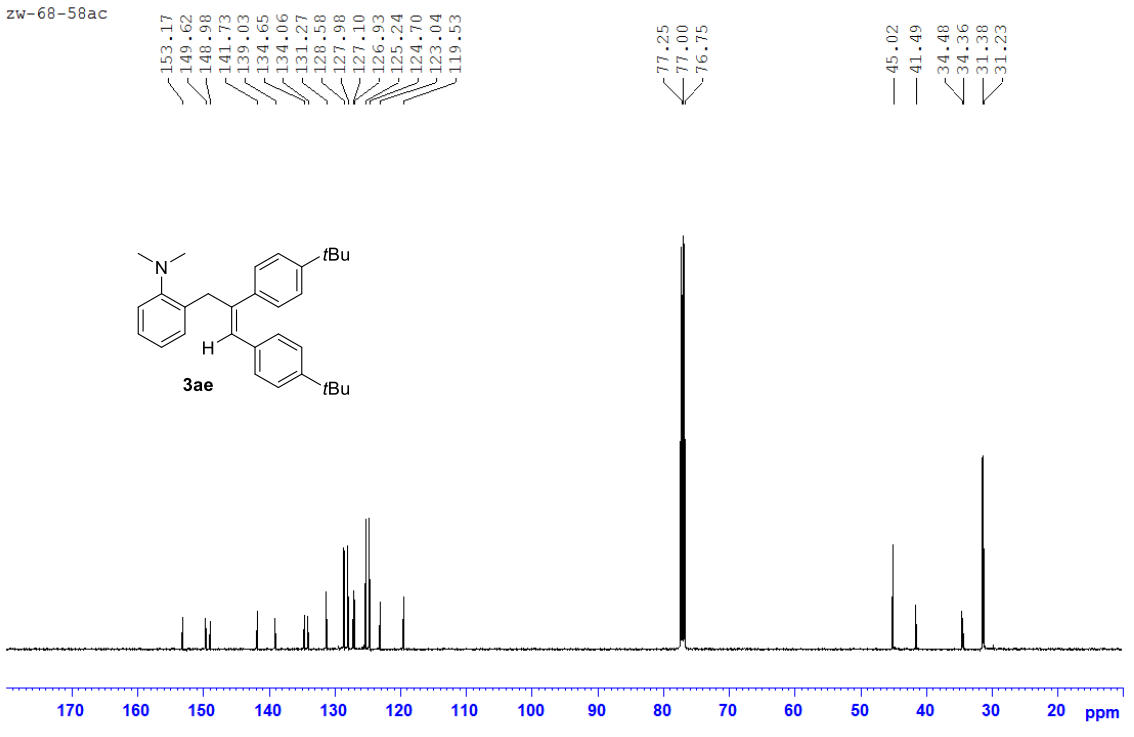
7.302
7.289
7.287
7.187
7.185
7.171
7.154
7.095
7.088
7.083
7.070
7.014
6.999
6.985
6.885
6.867
6.775
6.758
6.640
6.623
6.274
3.857
3.767
3.714
2.647
N
OMe
H
OMe
3ad
10
9
8
7
6
5
4
3
2
1
ppm
1.03
1.04
3.07
1.03
2.03
1.97
1.99
1.02
2.00
3.00
2.80
5.98


zw-68-65c
158.33
157.81
153.08
140.10
134.07
134.01
131.00
130.39
130.11
129.76
126.89
126.81
123.04
119.50
113.72
113.24
77.25
77.00
76.74
55.09
45.03
41.02
N
OMe
H
OMe
3ad
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.329
7.314
7.281
7.264
7.246
7.205
7.191
7.175
7.113
7.108
7.096
7.092
7.076
7.031
7.016
7.002
6.867
6.850
6.246
3.858
2.629
1.311
1.231
tBu
N
H
tBu
3ae
f1 (ppm)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139.03
134.65
134.06
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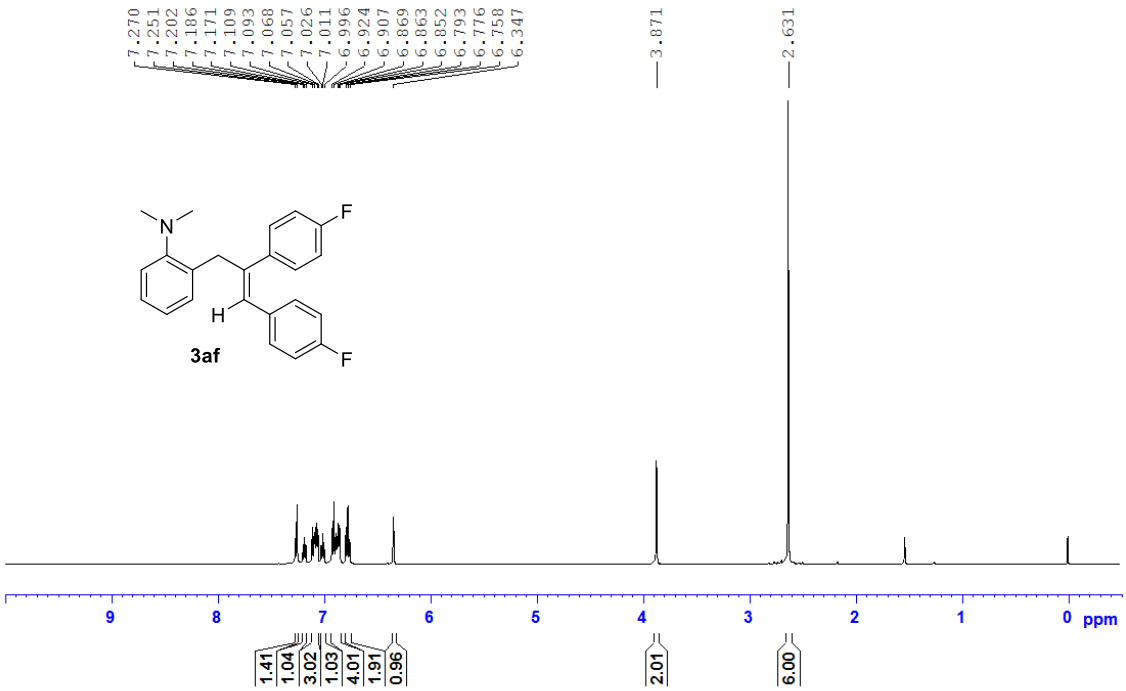
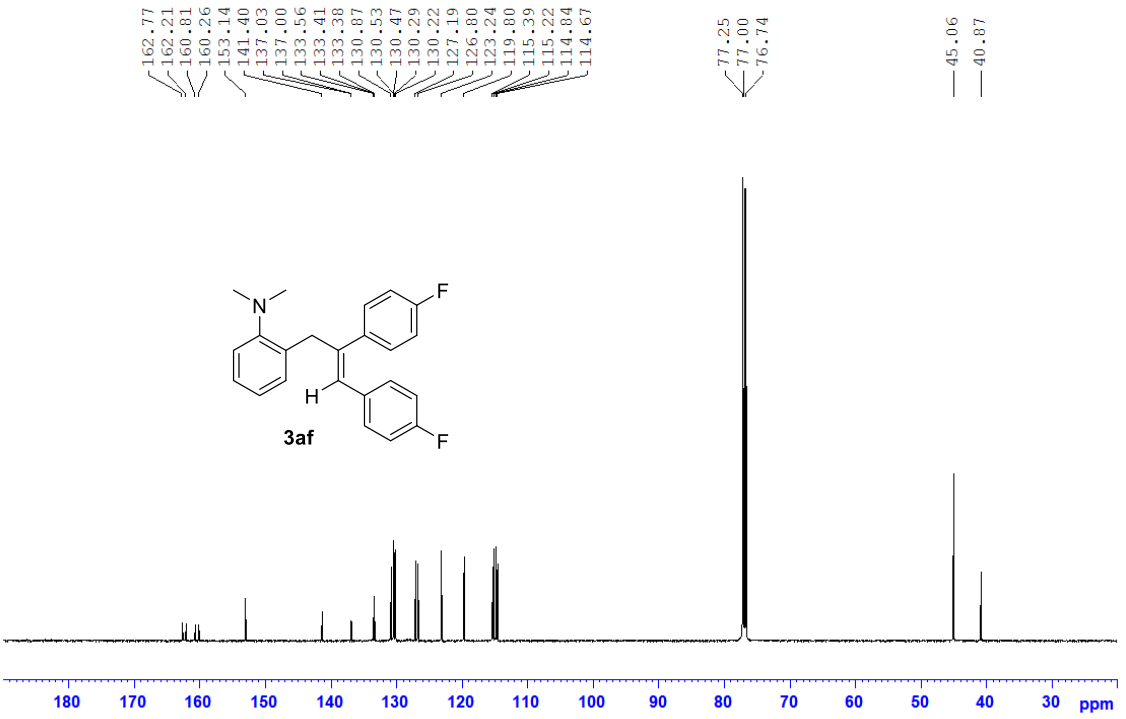
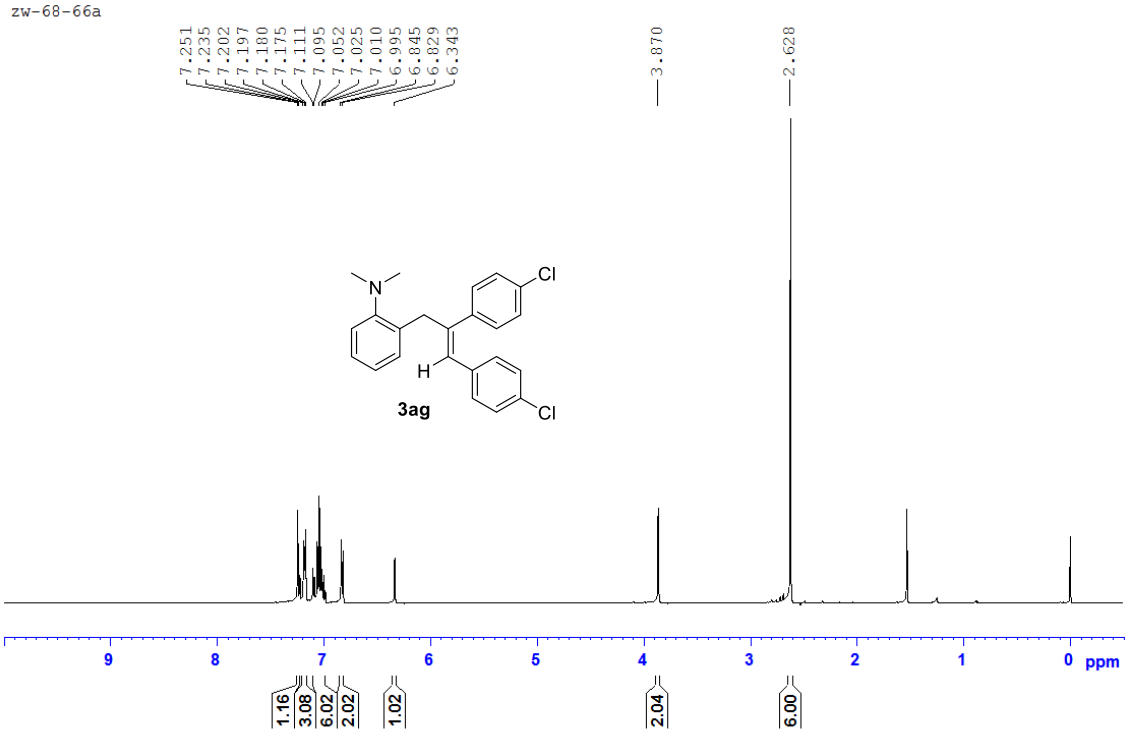
127.98
127.10
126.93
125.24
124.70
123.04
119.53
77.25
77.00
76.75
45.02
41.49
34.48
34.36
31.38
31.23
tBu
N
H
tBu
3ae
ppm

zw-68-fp




zw-68-fcp

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7.202
7.197
7.180
7.175
7.111
7.095
7.052
7.025
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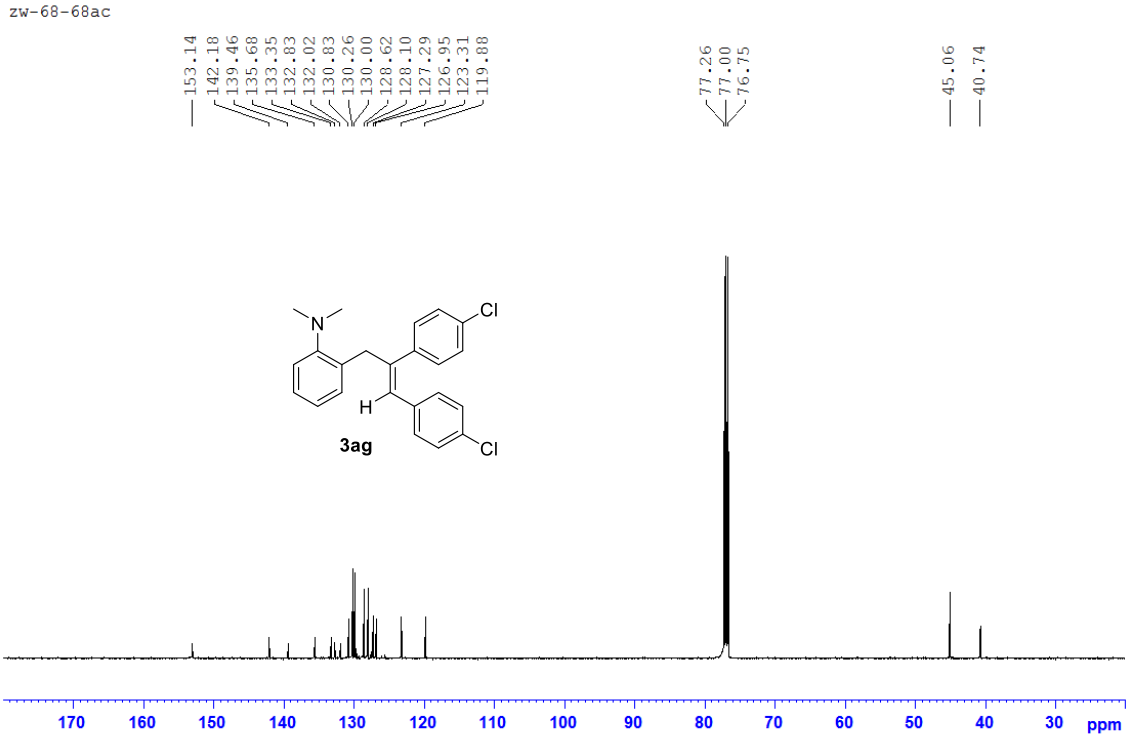
6.845
6.829
6.343
3.870
2.628
N
Cl
H
Cl
3ag
9
8
7
6
5
4
3
2
1
0
ppm
1.16
3.08
6.02
2.02
1.02
2.04
6.00


zw-68-68ac
153.14
142.18
139.46
135.68
133.35
132.83
132.02
130.83
130.26
130.00
128.62
128.10
127.29
126.95
123.31
119.88
77.26
77.00
76.75
45.06
40.74
N
Cl
H
Cl
3ag
170
160
150
140
130
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90
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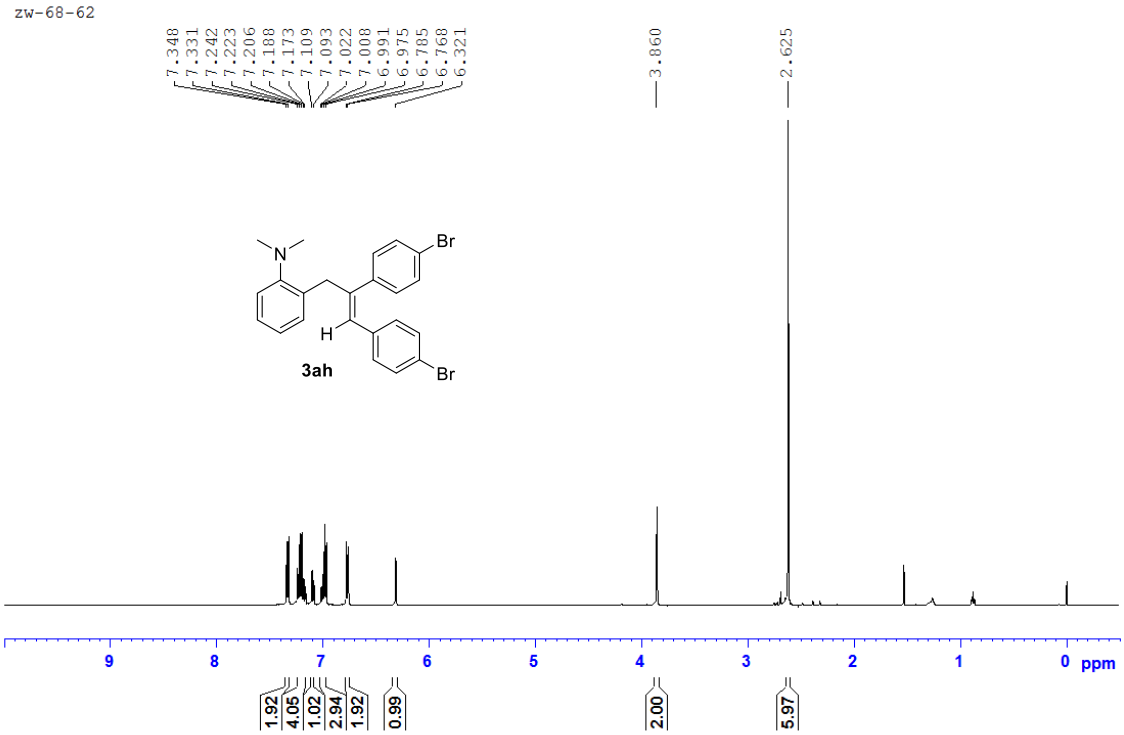
50
40
30
ppm


zw-68-62
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7.331
7.242
7.223
7.206
7.188
7.173
7.109
7.093
7.022
7.008
6.991
6.975
6.785
6.768
6.321
3.860
2.625
N
Br
H
Br
3ah
9
8
7
6
5
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3
2
1
0
ppm
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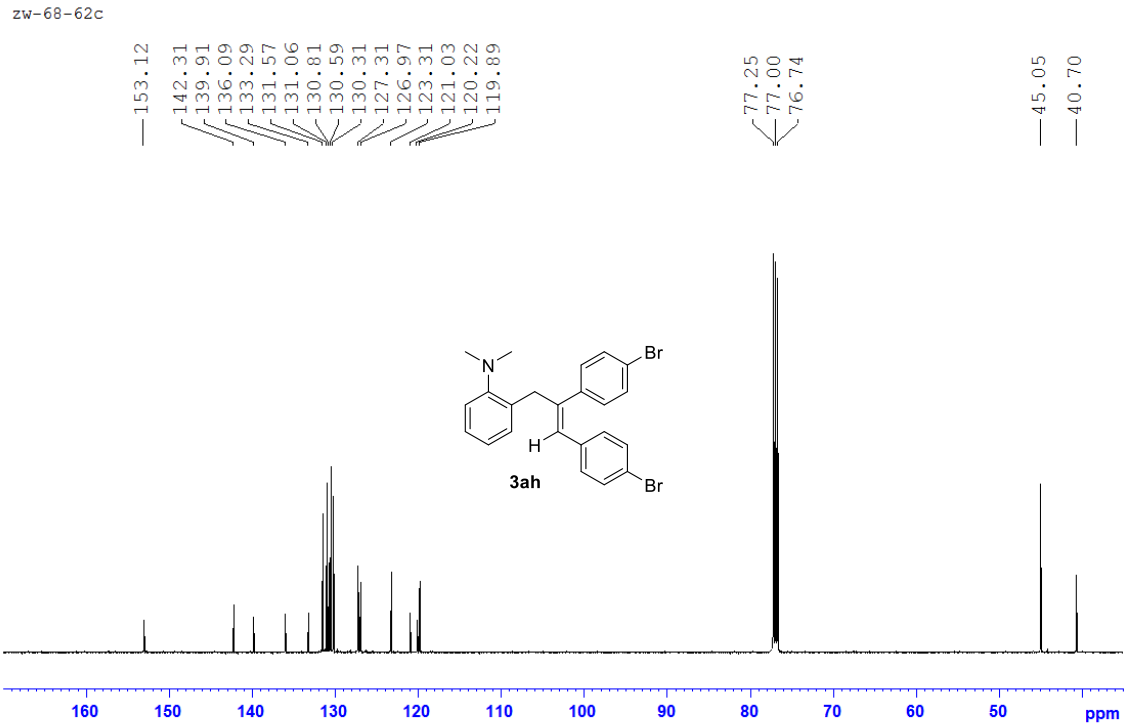
4.05
1.02
2.94
1.92
0.99
2.00
5.97


zw-68-62c
153.12
142.31
139.91
136.09
133.29
131.57
131.06
130.81
130.59
130.31
127.31
126.97
123.31
121.03
120.22
119.89
77.25
77.00
76.74
45.05
40.70
N
Br
H
Br
3ah
160
150
140
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120
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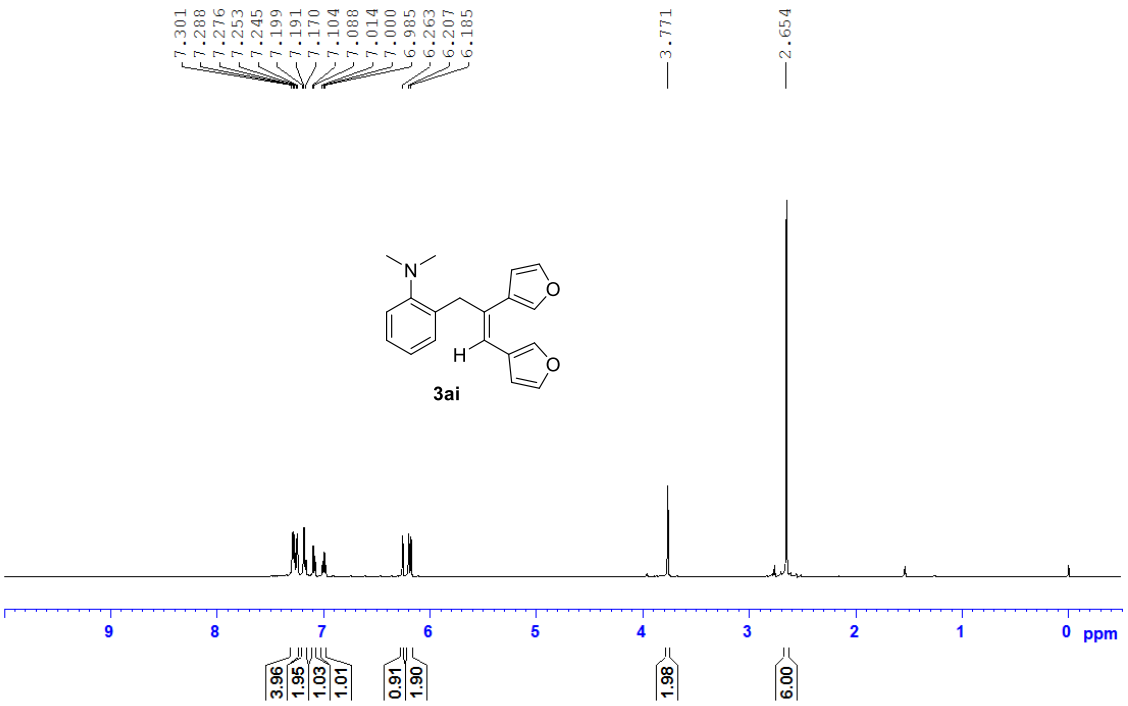
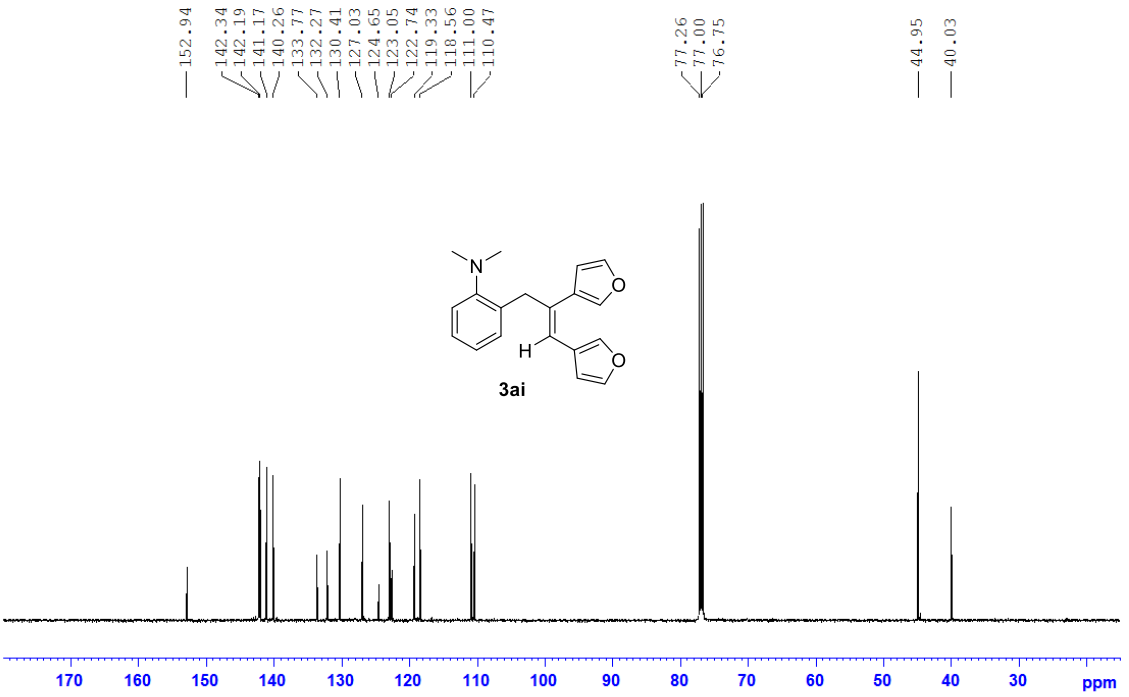
100
90
80
70
60
50
ppm

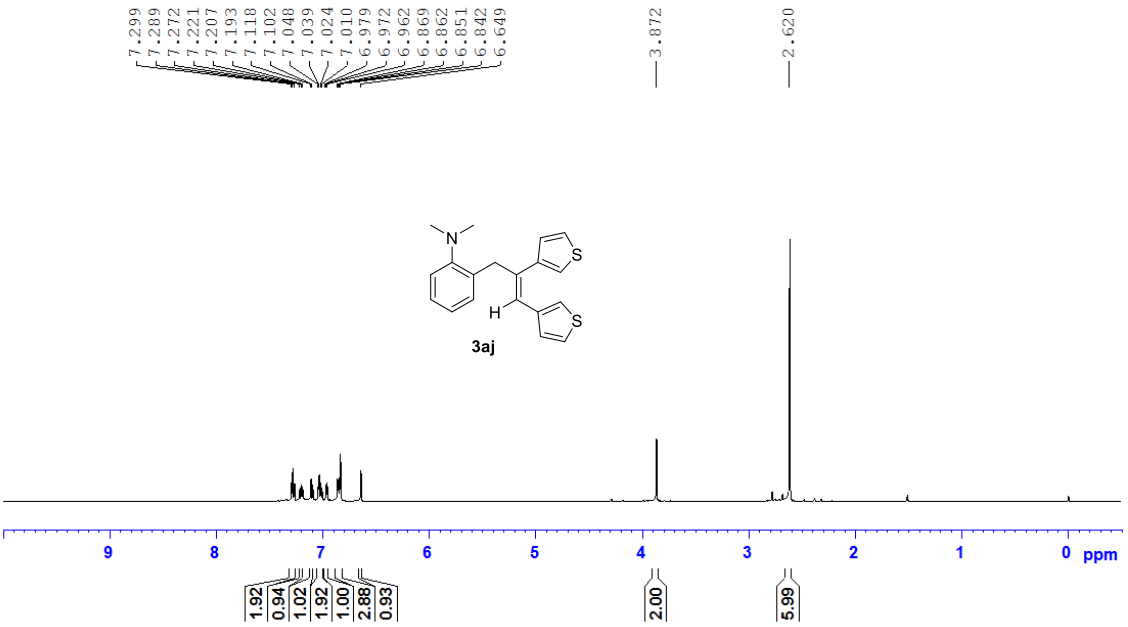
zw-68-86-2



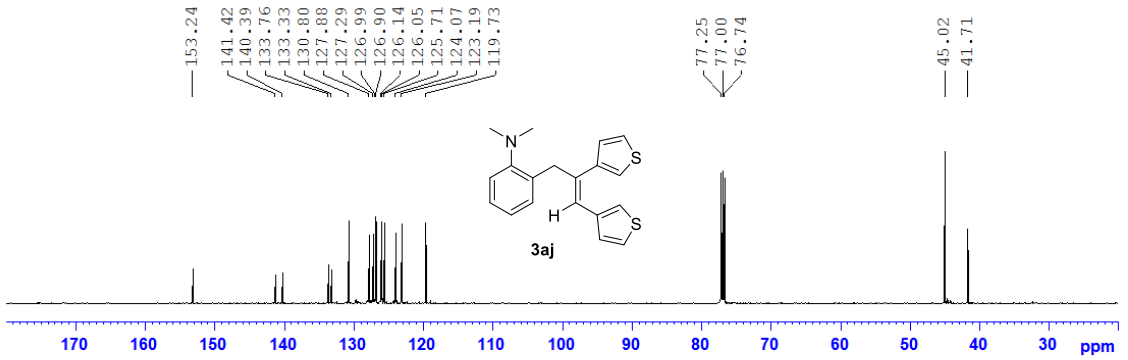

zw-68-86-2c

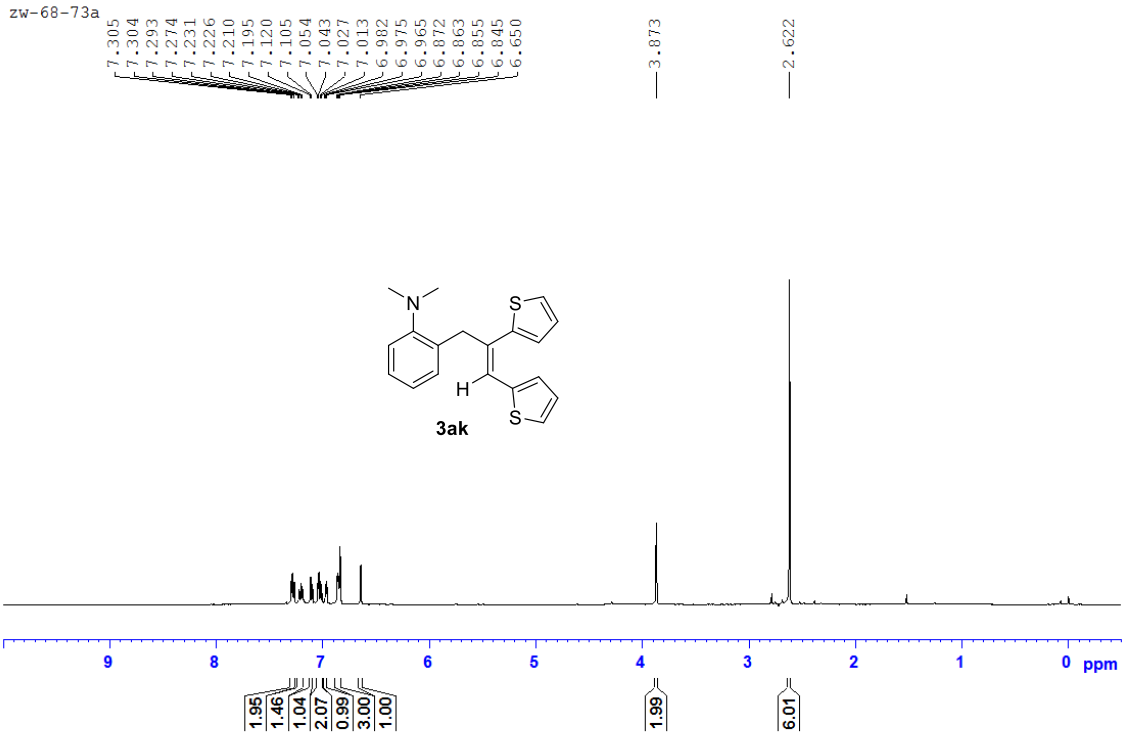


zw-68-77a




zw-68-77ac




zw-68-73a
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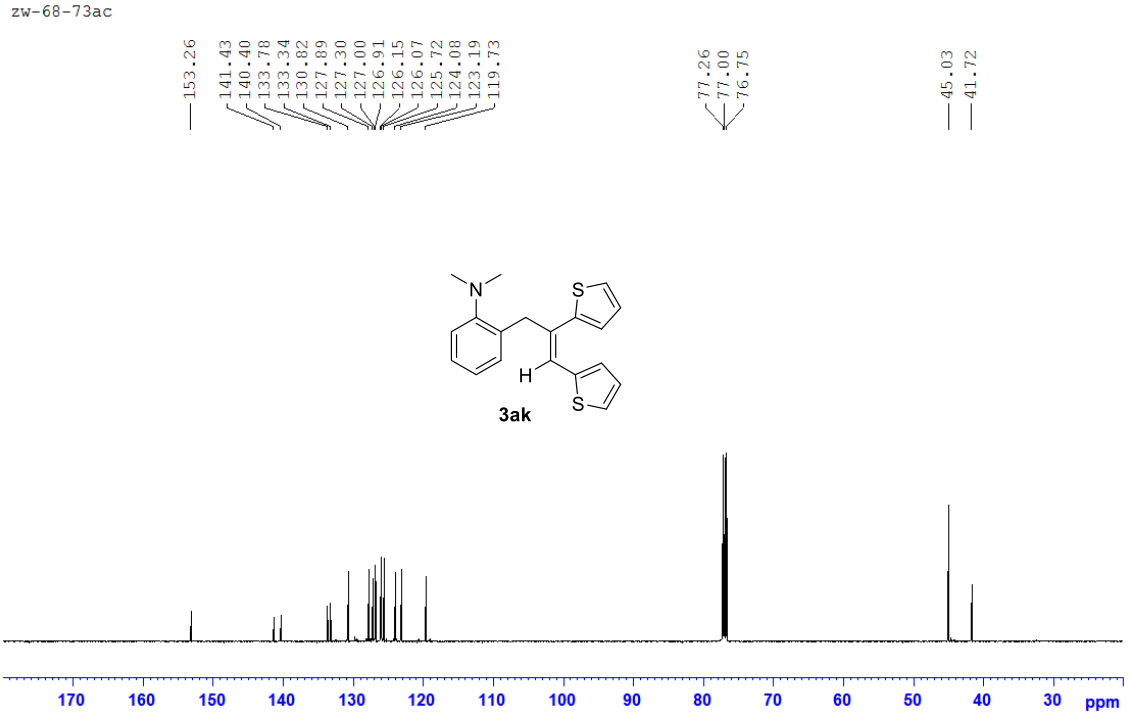
7.304
7.293
7.274
7.231
7.226
7.210
7.195
7.120
7.105
7.054
7.043
7.027
7.013
6.982
6.975
6.965
6.872
6.863
6.855
6.845
6.650
3.873
2.622
N
S
H
S
3ak
9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.46
1.04
2.07
0.99
3.00
1.00
1.99
6.01


zw-68-73ac
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141.43
140.40
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133.34
130.82
127.89
127.30
127.00
126.91
126.15
126.07
125.72
124.08
123.19
119.73
77.26
77.00
76.75
45.03
41.72
N
S
H
S
3ak
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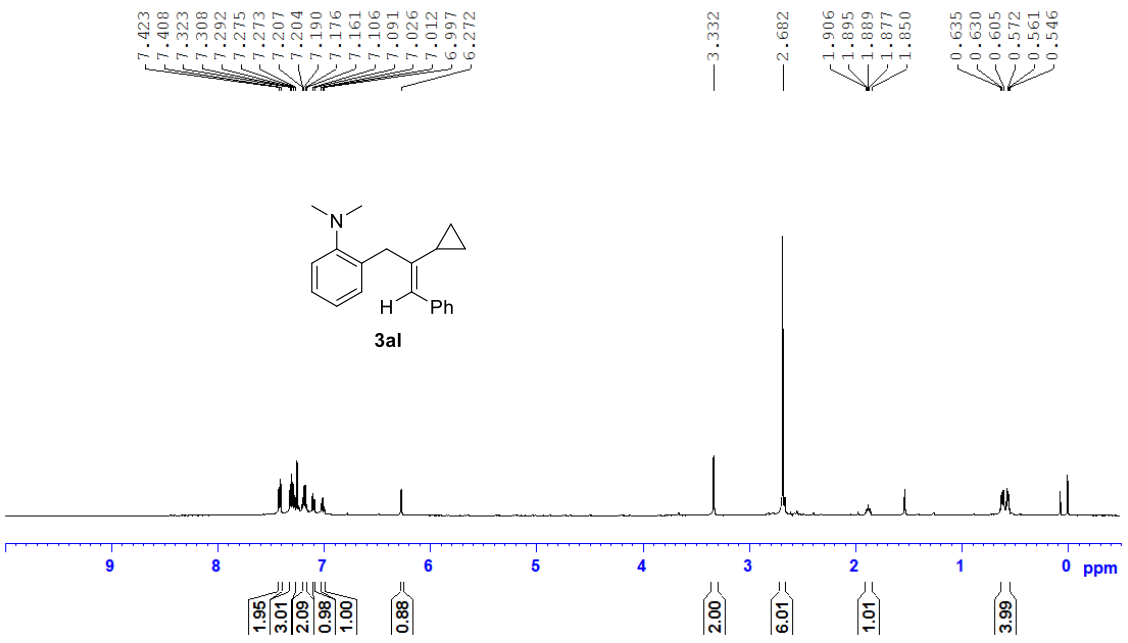
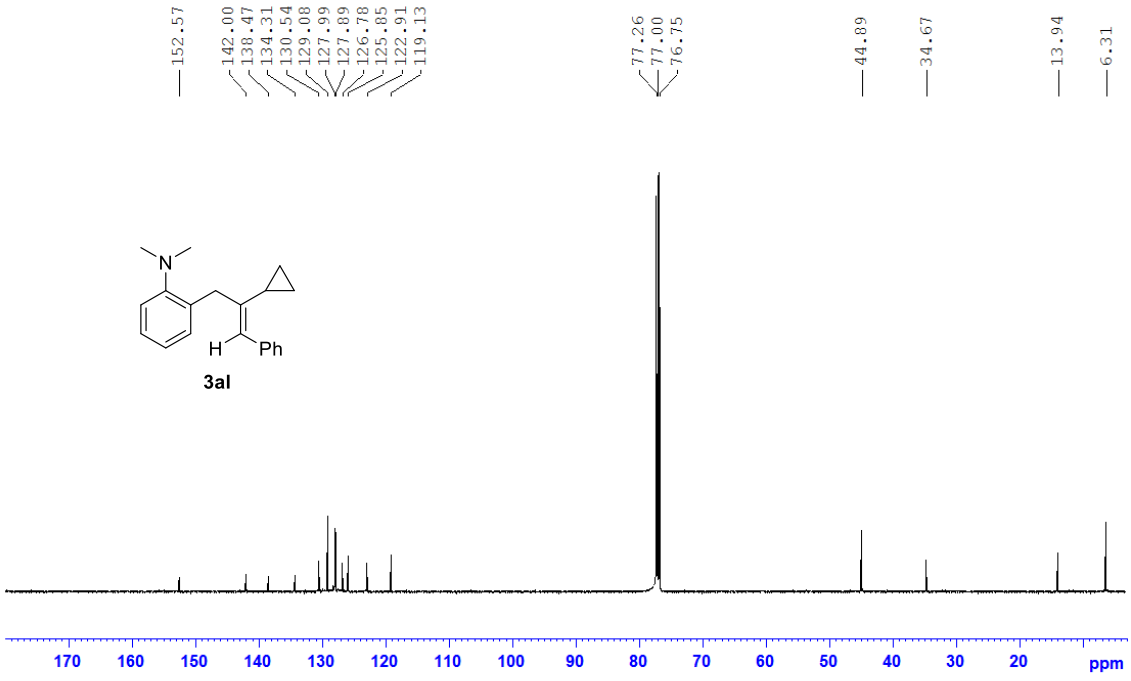
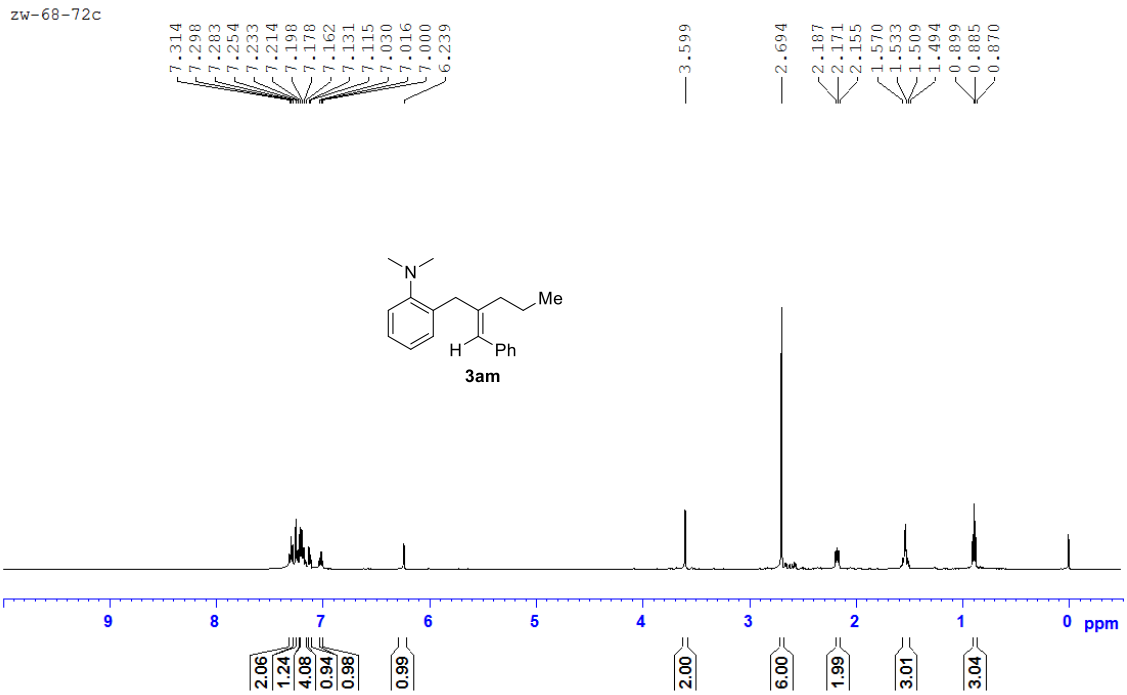
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

zw-68-66




zw-68-66c




zw-68-72c
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7.283
7.254
7.233
7.214
7.198
7.178
7.162
7.131
7.115
7.030
7.016
7.000
6.239
3.599
2.694
2.187
2.171
2.155
1.570
1.533
1.509
1.494
0.899
0.885
0.870
N
Me
H
Ph
3am
9
8
7
6
5
4
3
2
1
0
ppm
2.06
1.24
4.08
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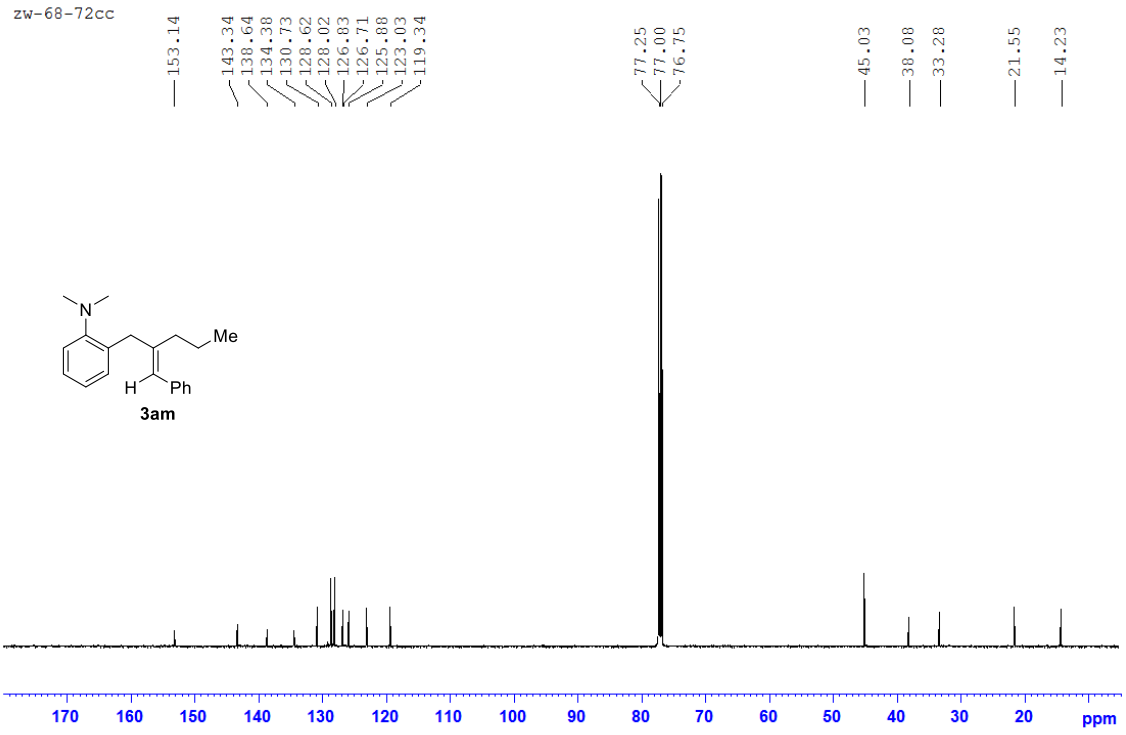
0.98
0.99
2.00
6.00
1.99
3.01
3.04


zw-68-72cc
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143.34
138.64
134.38
130.73
128.62
128.02
126.83
126.71
125.88
123.03
119.34
77.25
77.00
76.75
45.03
38.08
33.28
21.55
14.23
N
Me
H
Ph
3am
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160
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140
130
120
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100
90
80
70
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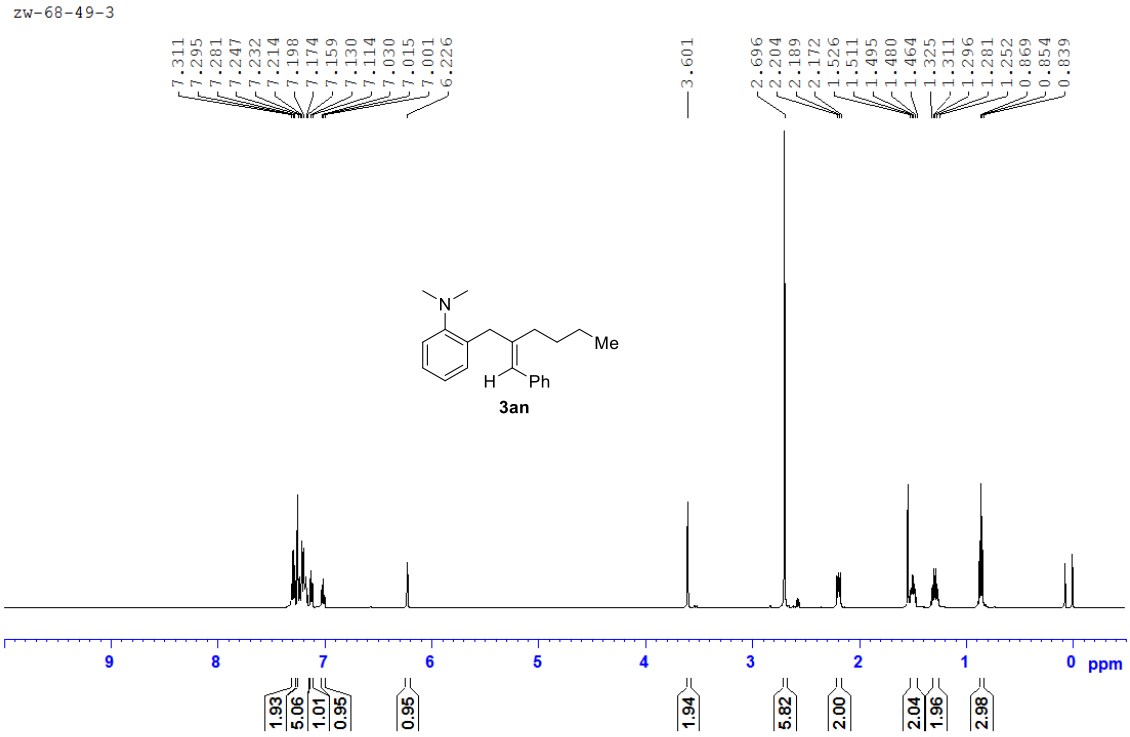
40
30
20
ppm


zw-68-49-3
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7.247
7.232
7.214
7.198
7.174
7.159
7.130
7.114
7.030
7.015
7.001
6.226
3.601
2.696
2.204
2.189
2.172
1.526
1.511
1.495
1.480
1.464
1.325
1.311
1.296
1.281
1.252
0.869
0.854
0.839
N
Me
H
Ph
3an
9
8
7
6
5
4
3
2
1
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ppm
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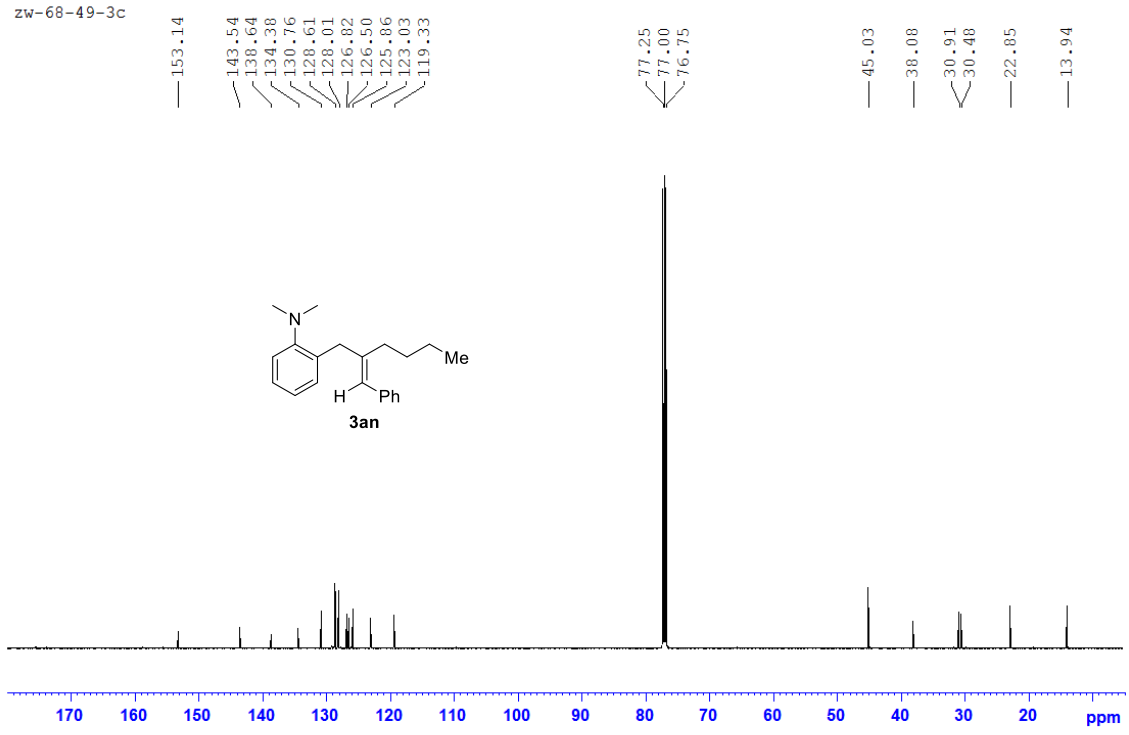
5.06
1.01
0.95
0.95
1.94
5.82
2.00
2.04
1.96
2.98


zw-68-49-3c
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77.25
77.00
76.75
45.03
38.08
30.91
30.48
22.85
13.94
N
Me
H
Ph
3an
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50
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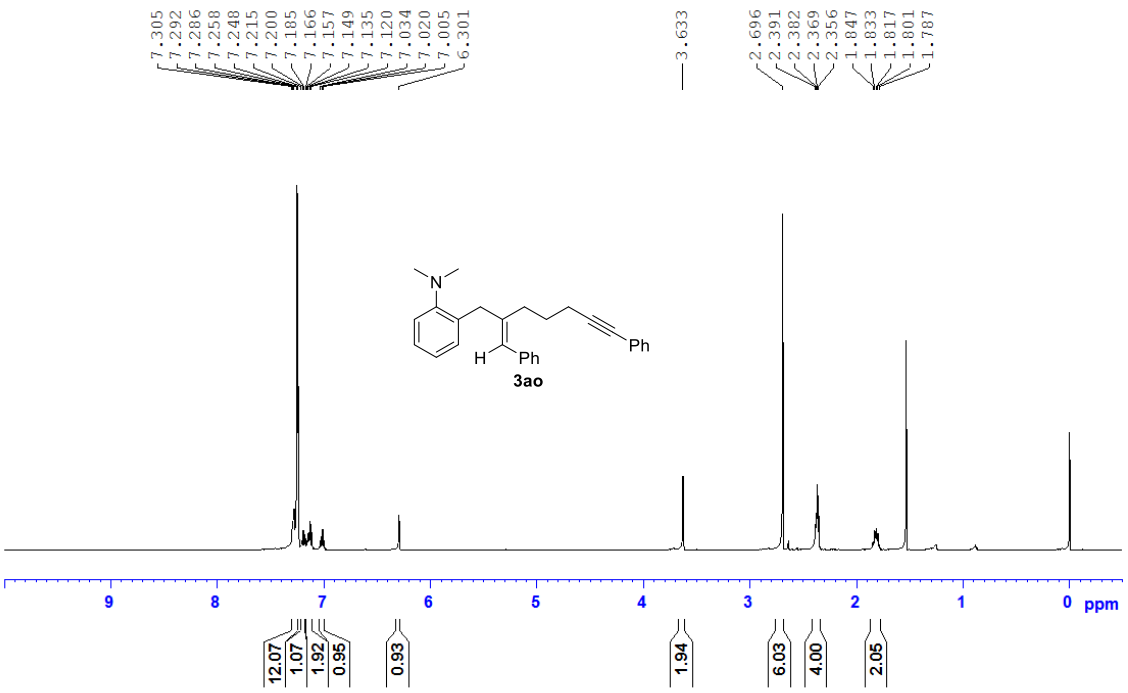
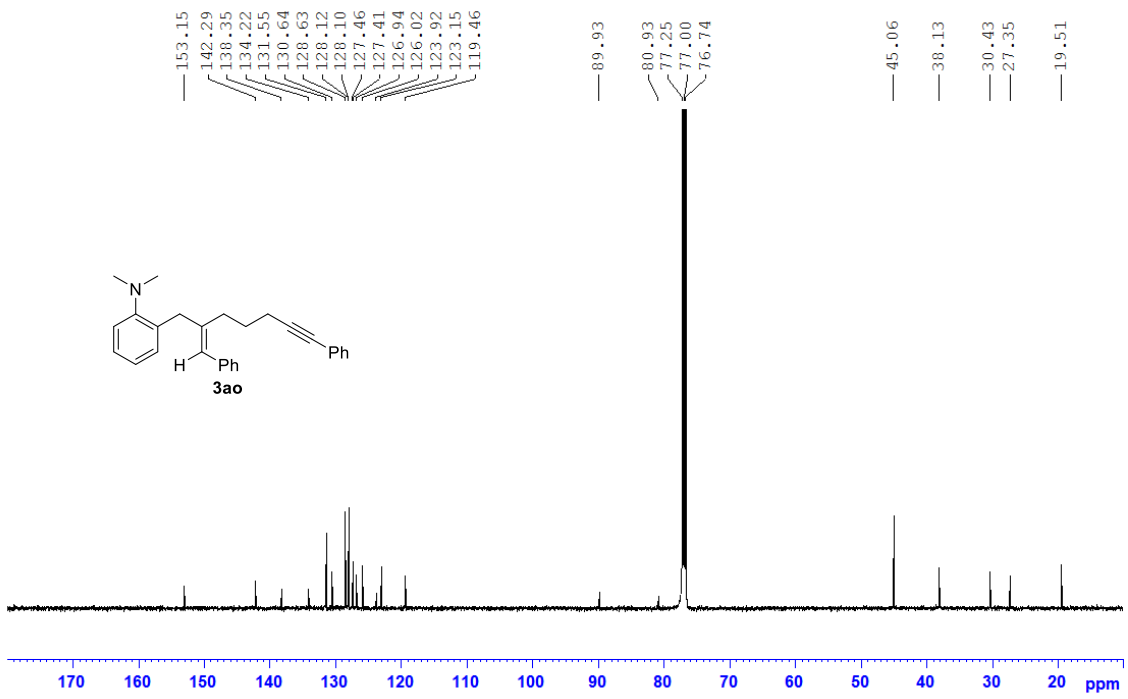
20
ppm

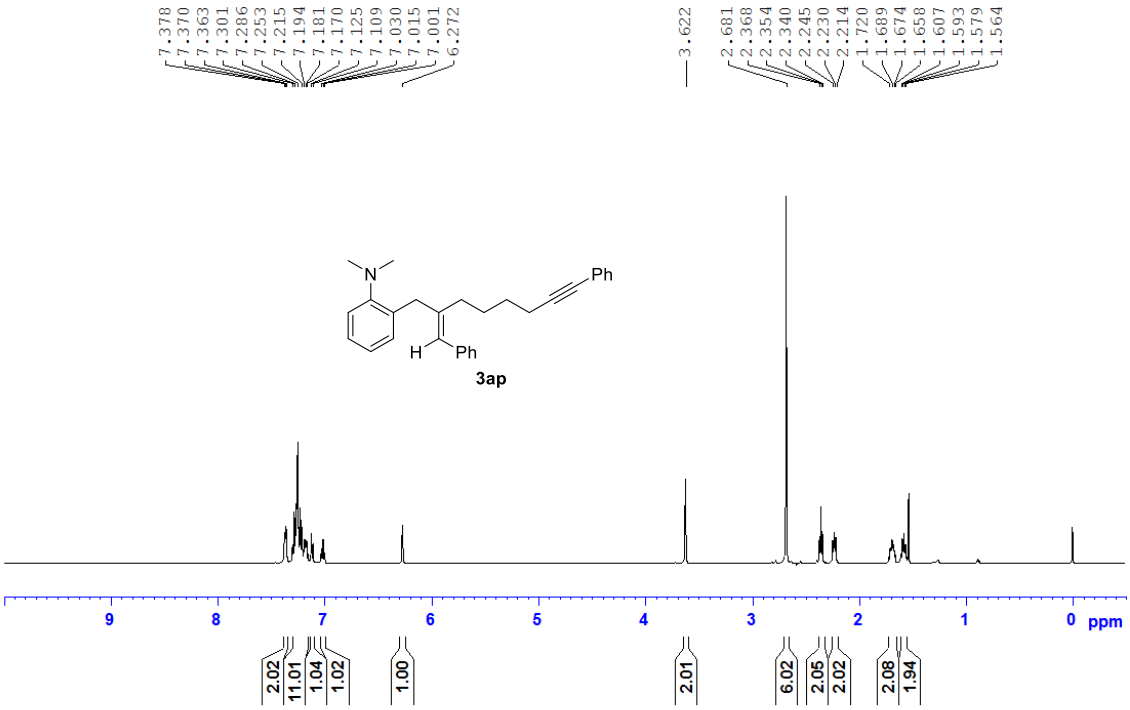
zw-68-140-1



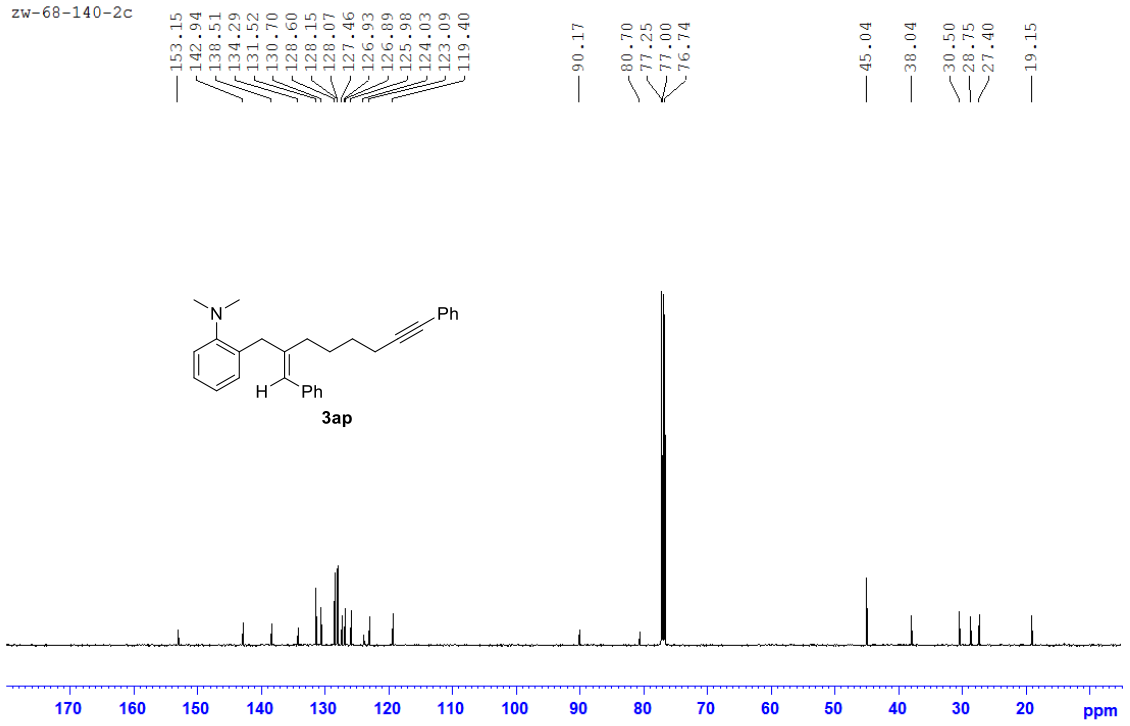

zw-68-140-1c



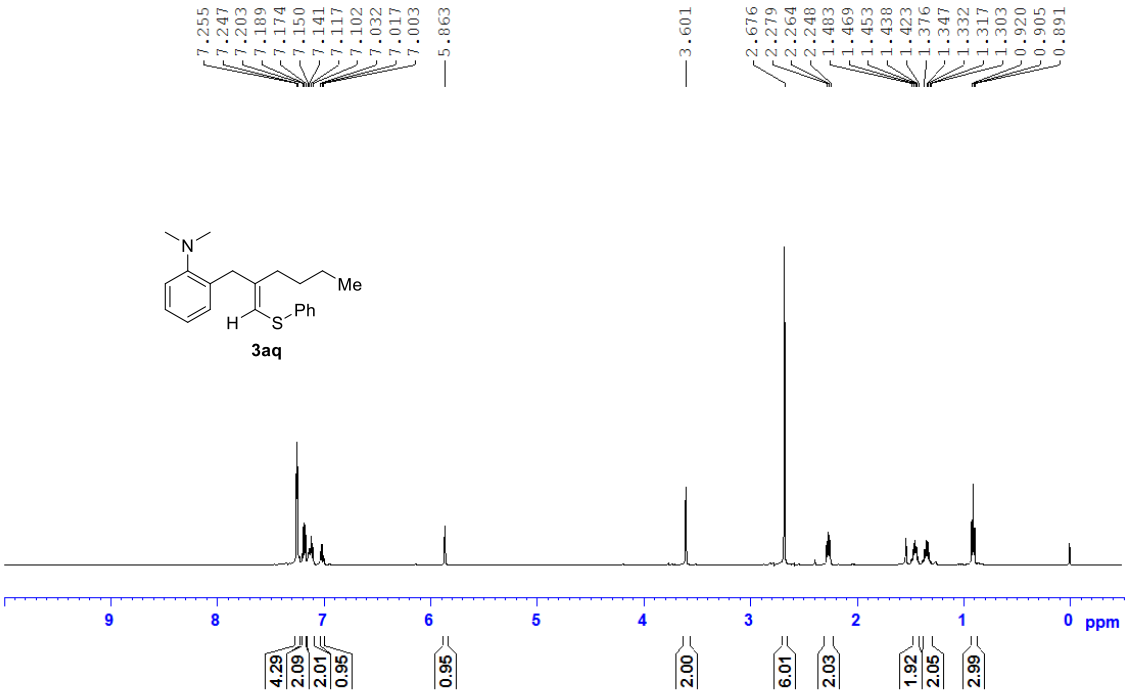
zw-68-140-2



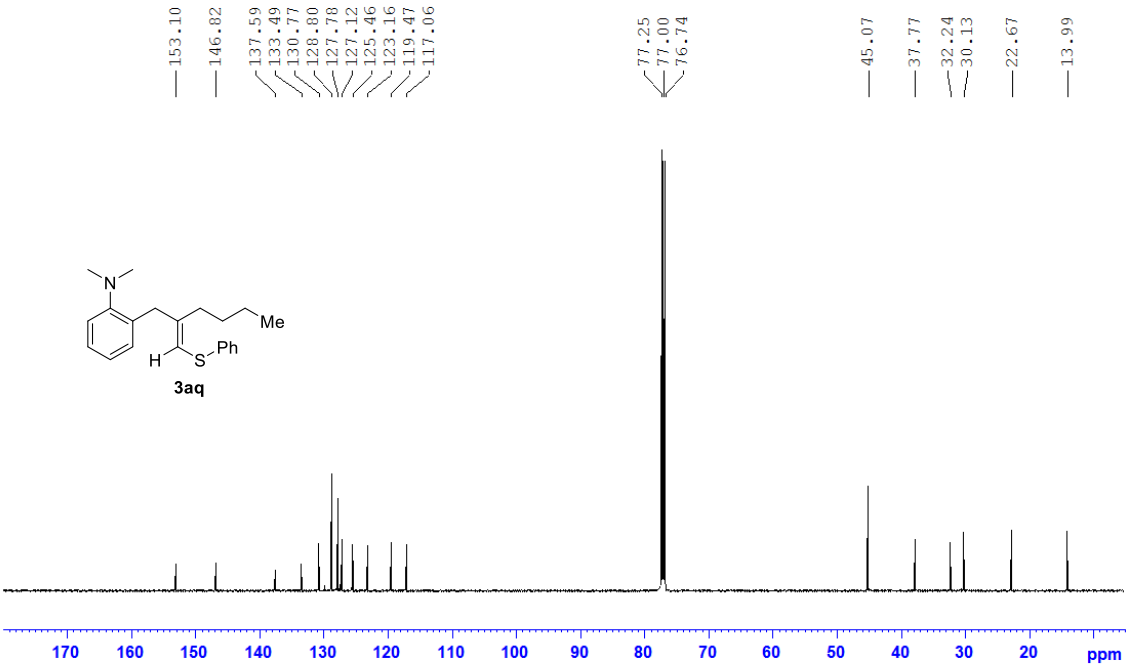

zw-68-140-2c



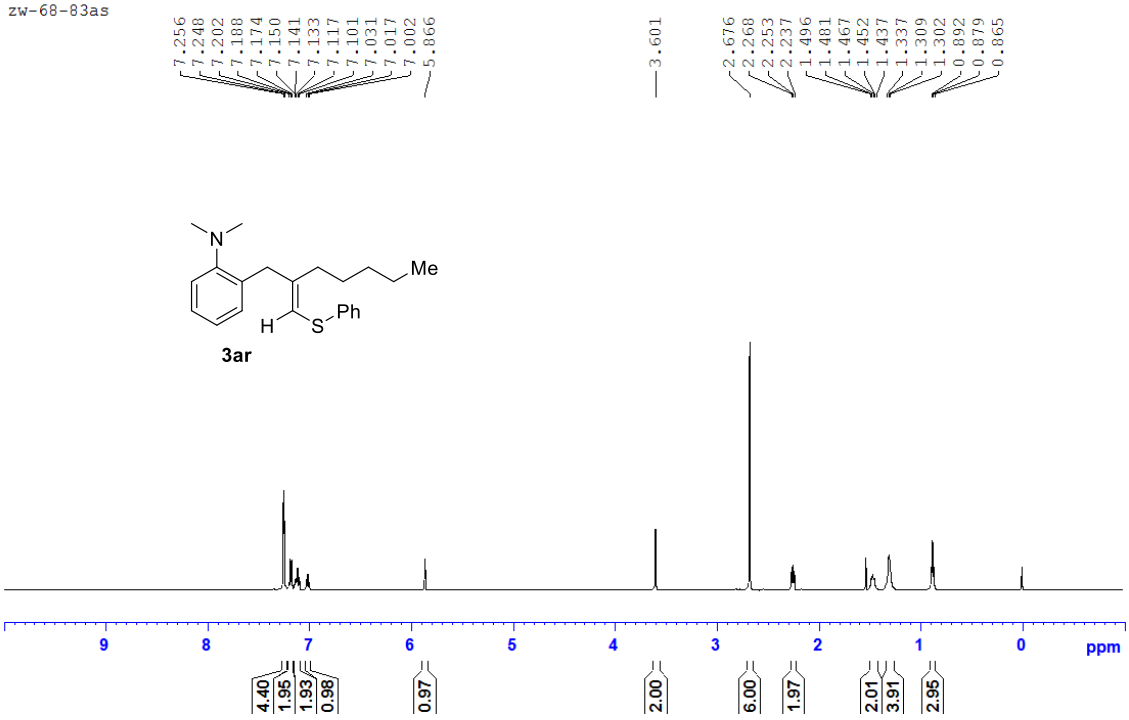
zw-68-80



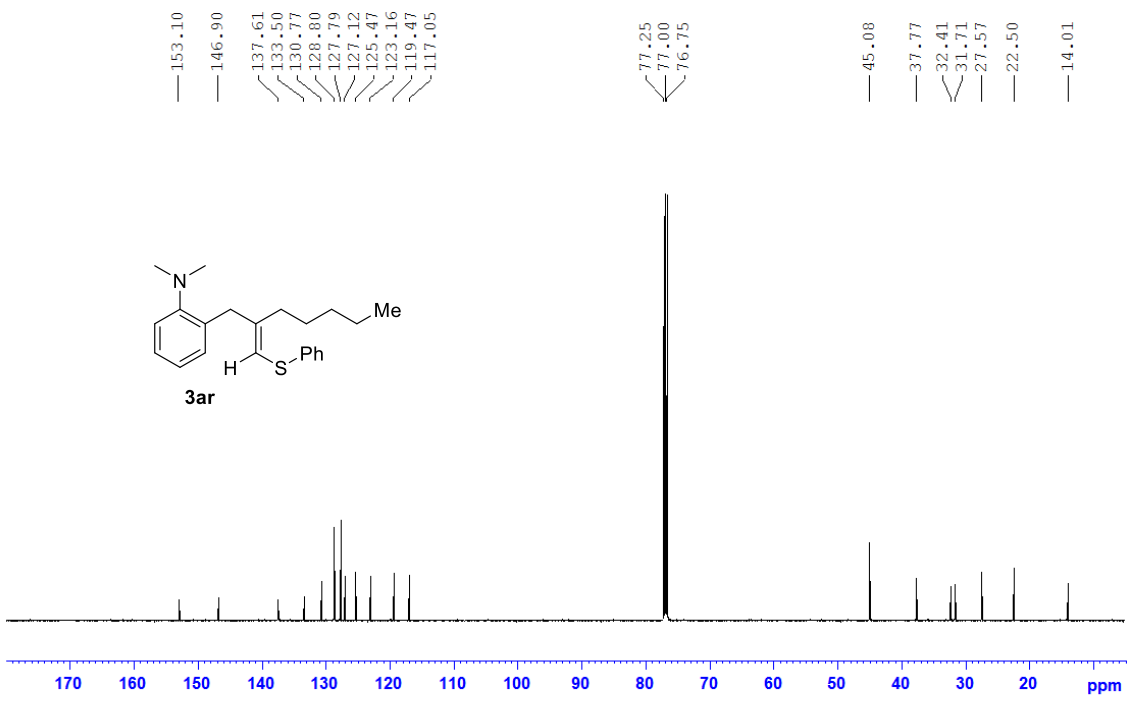

zw-68-81



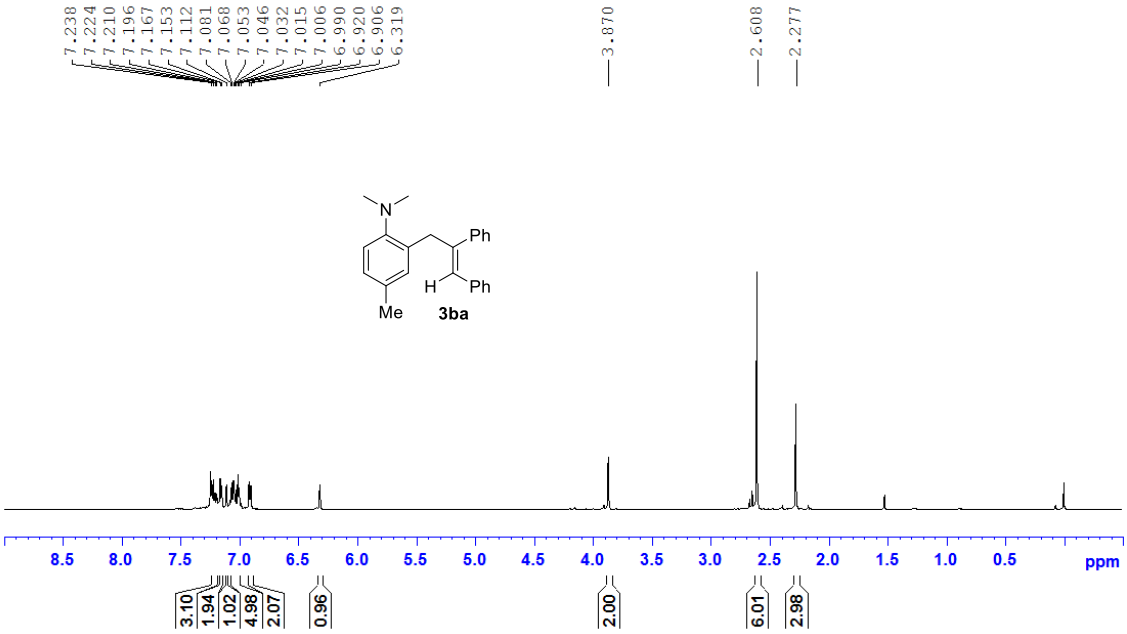
zw-68-83as



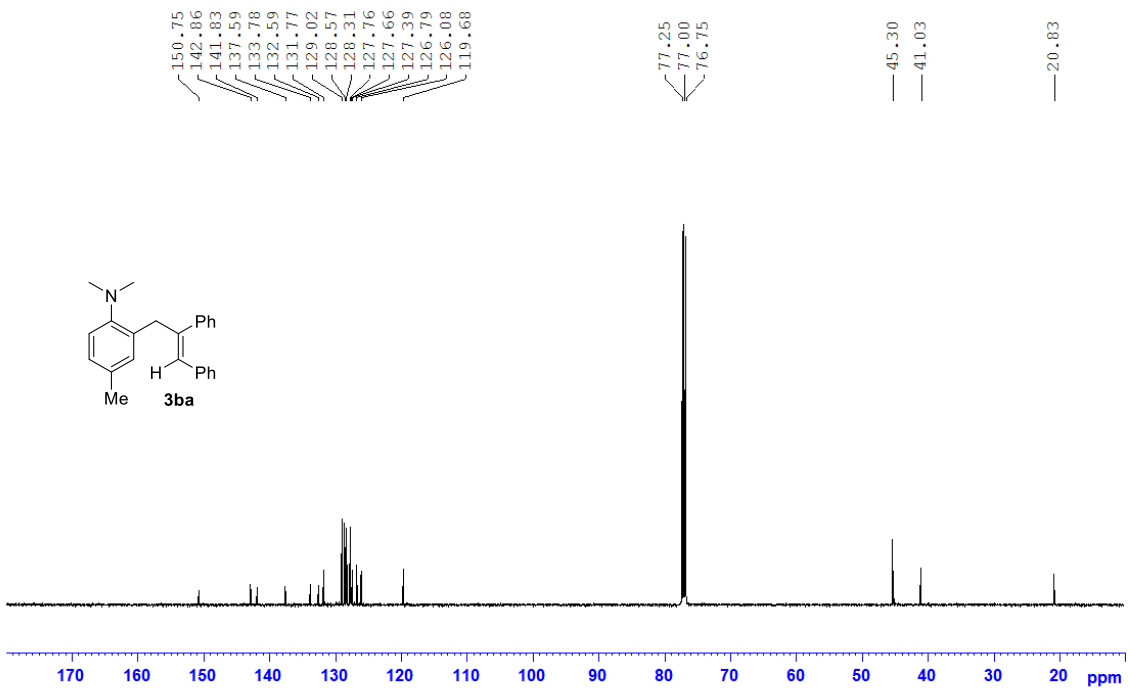

zw-68-83acs



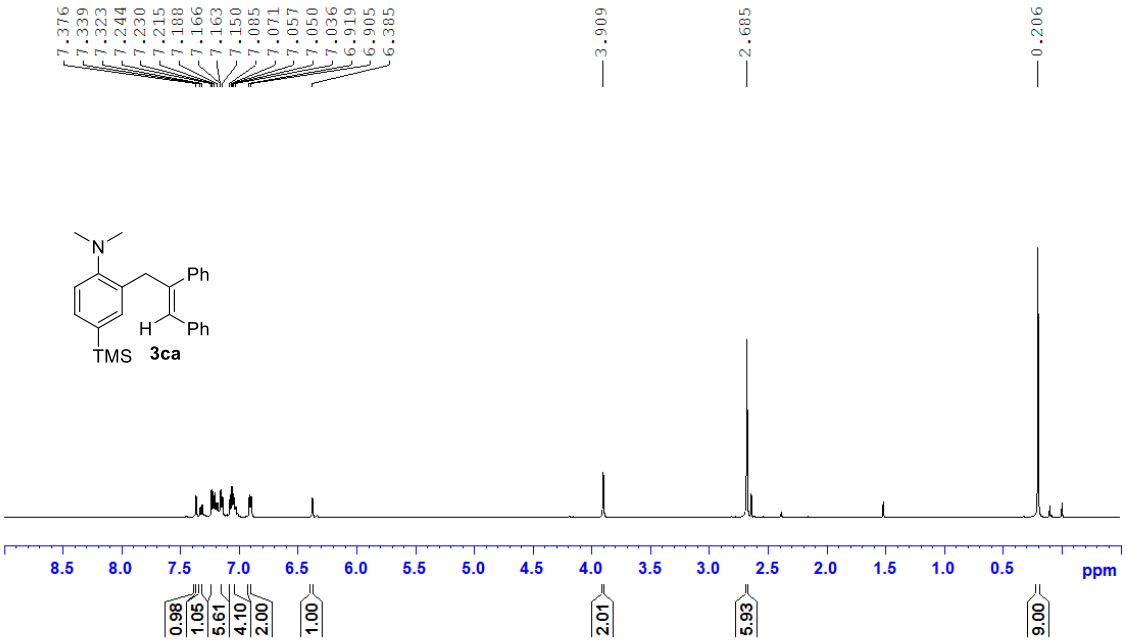
zw-68-106-3



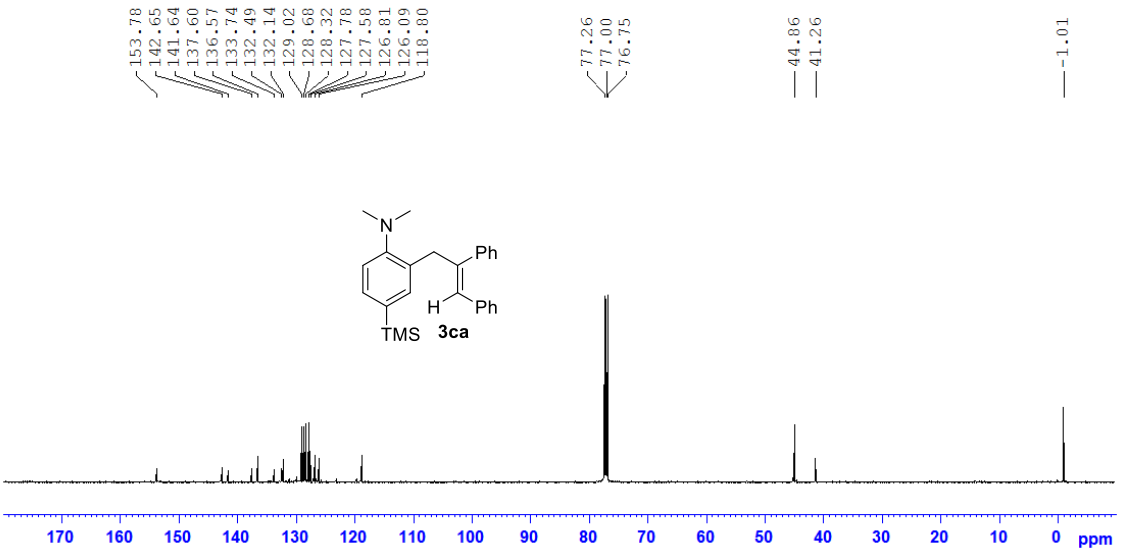

zw-68-106-3c



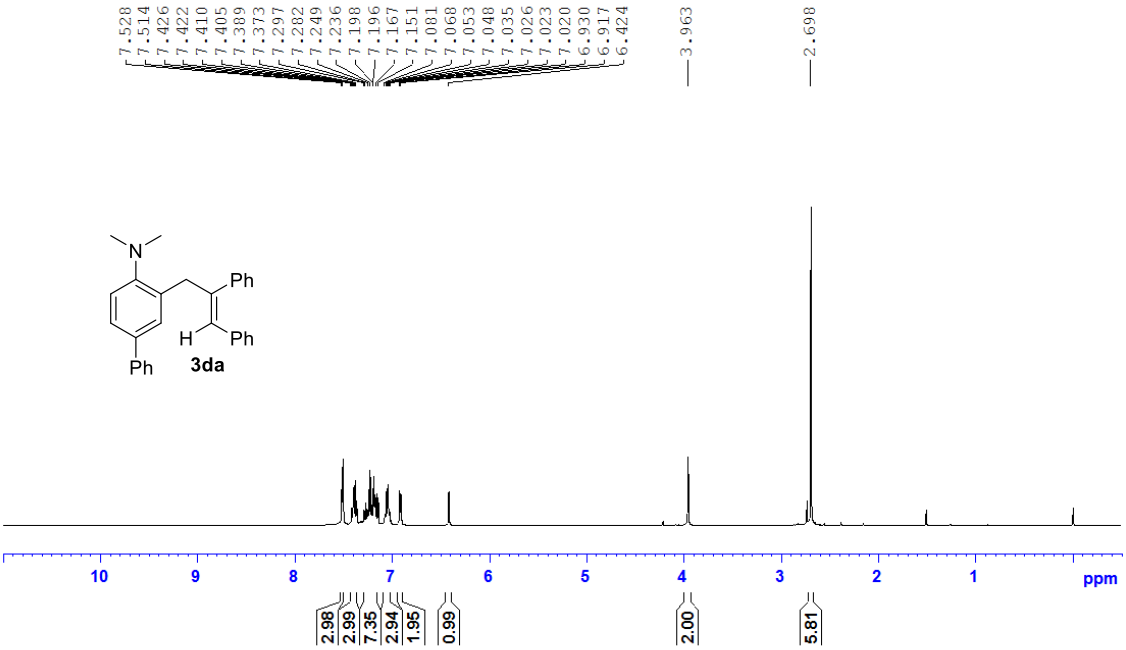
zw-68-117-1



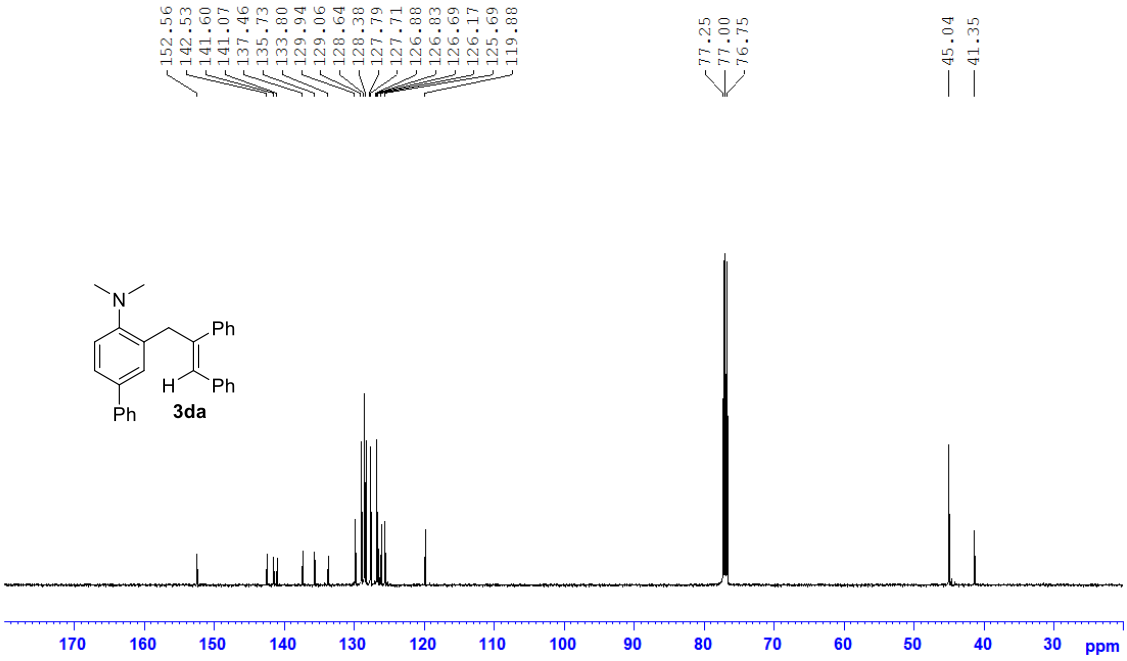

zw-68-117-1c



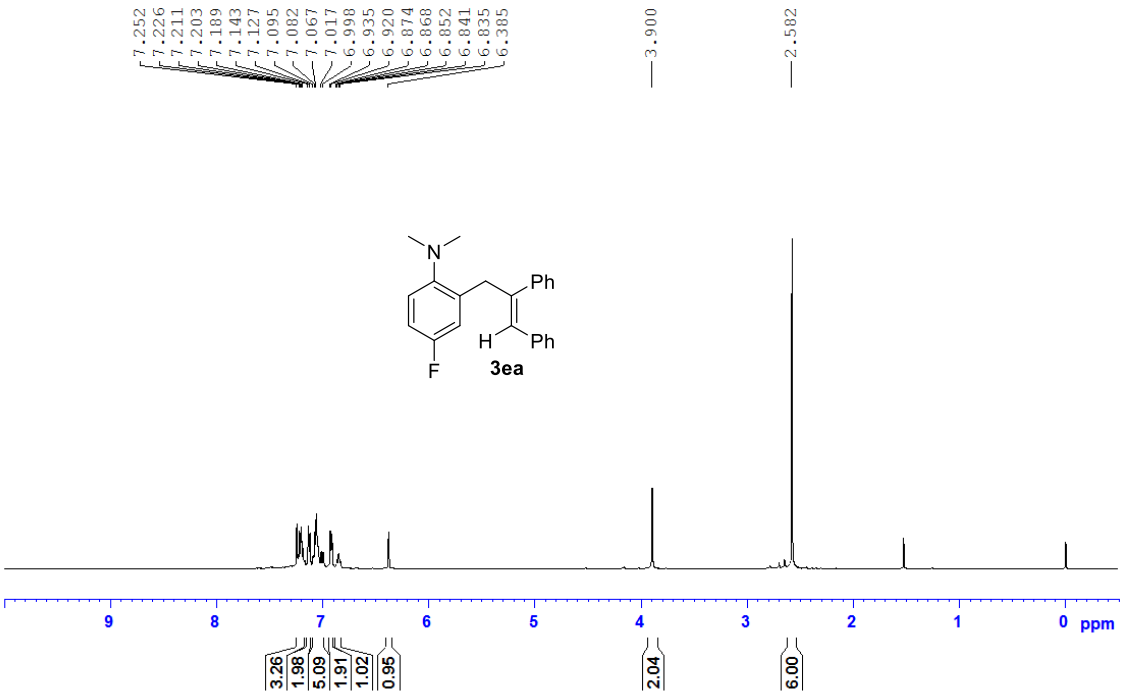
zw-68-109-1



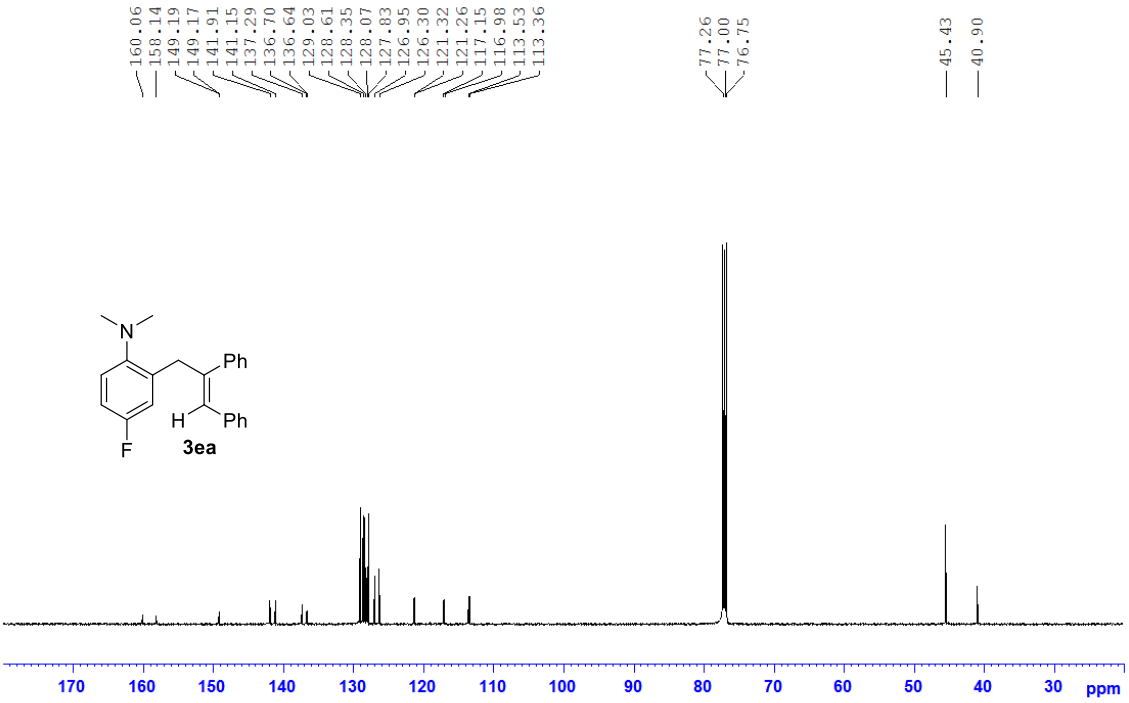

zw-68-109-1c



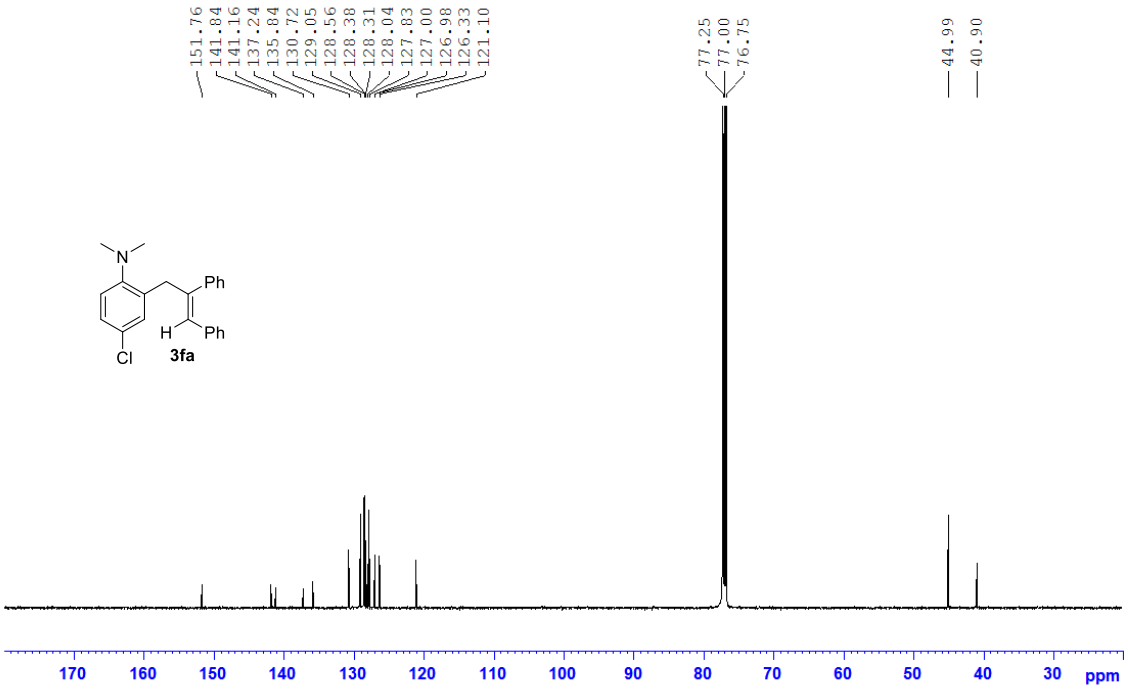
zw-68-110-2



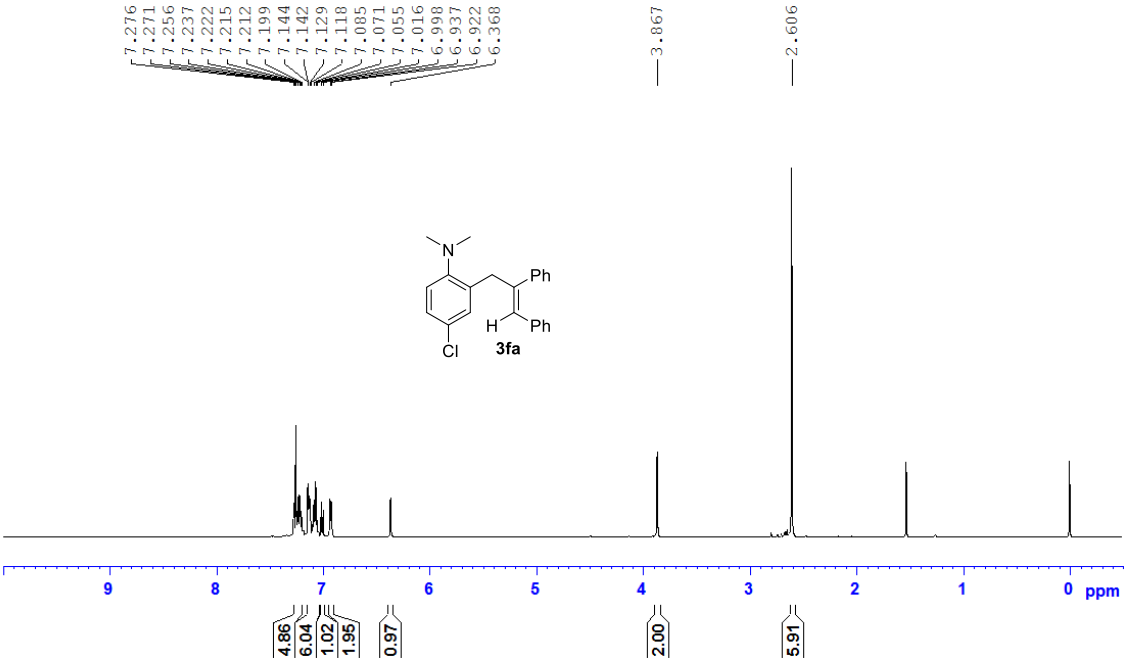

zw-68-110-2c



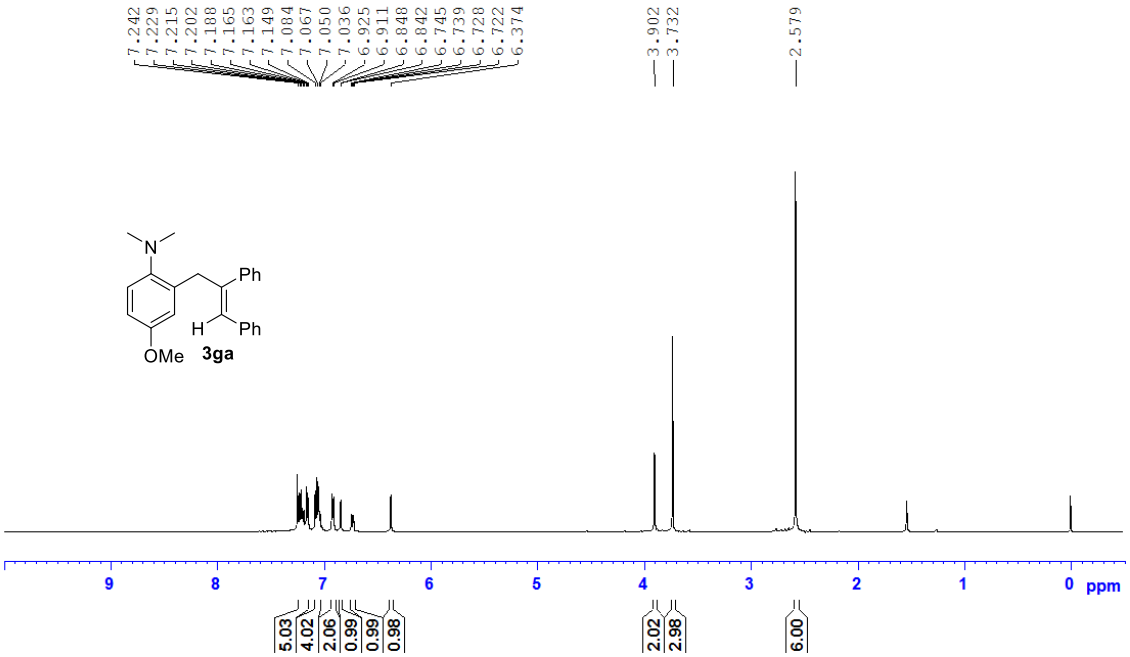
zw-68-112-1c



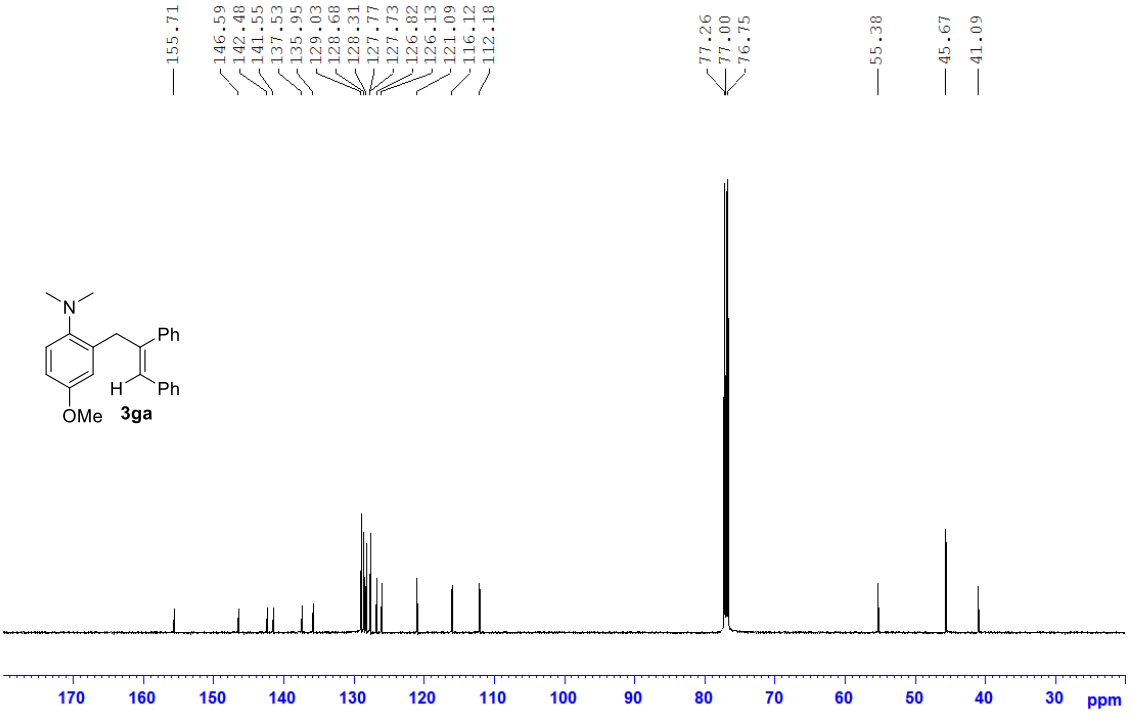

zw-68-112-1



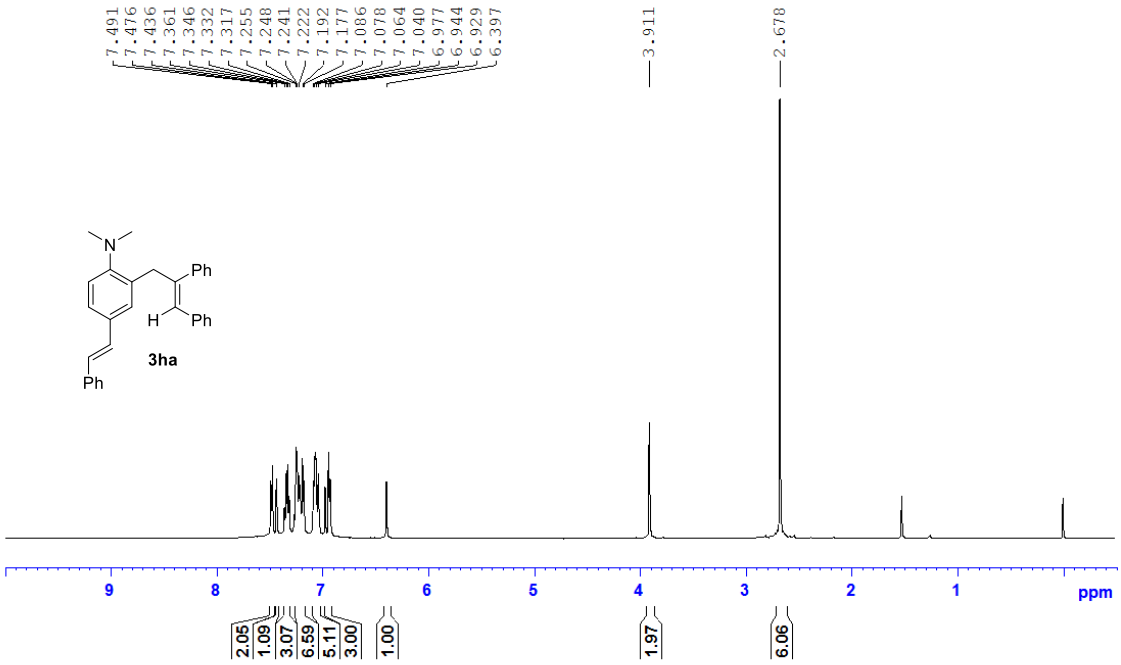
zw-68-115-1



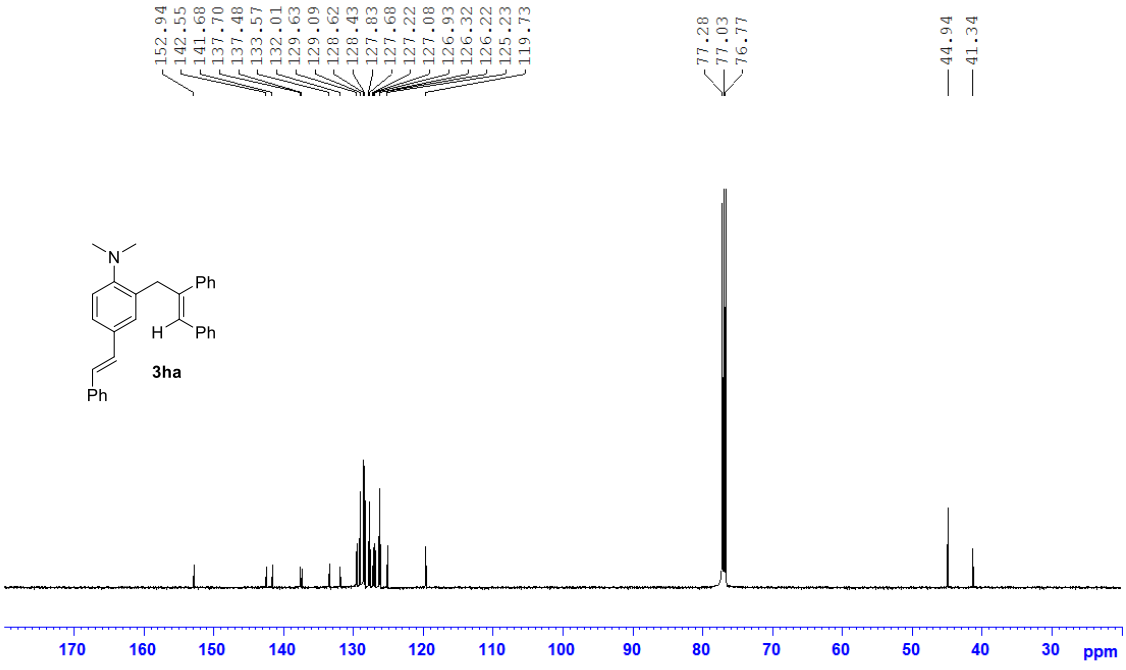

zw-68-115-1c



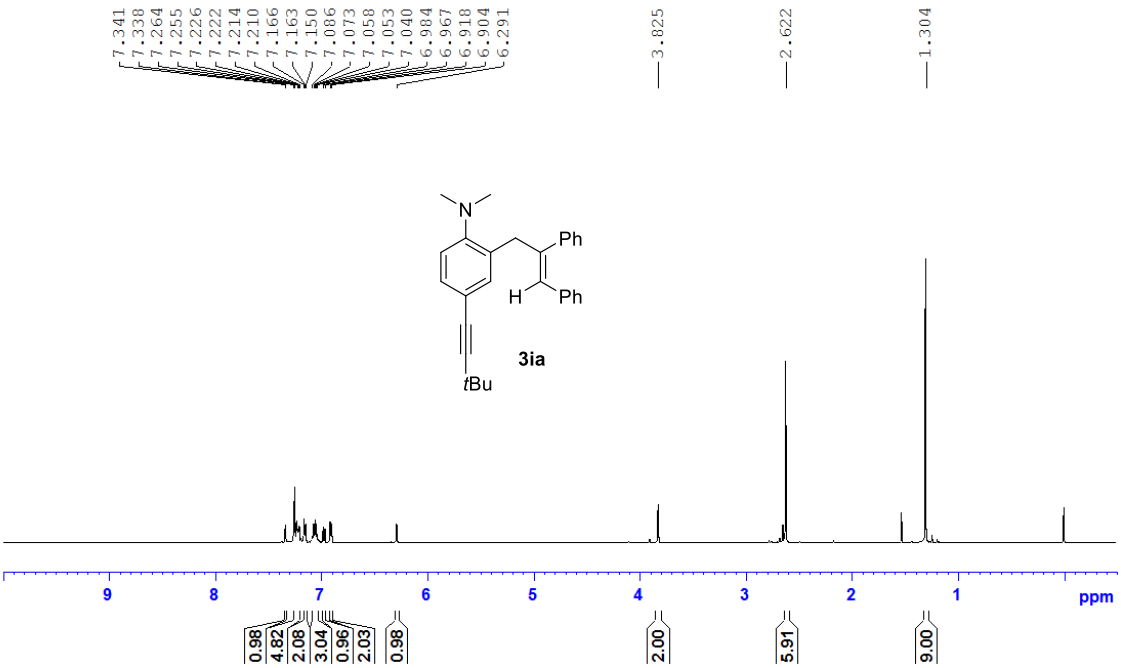
zw-68-110-1



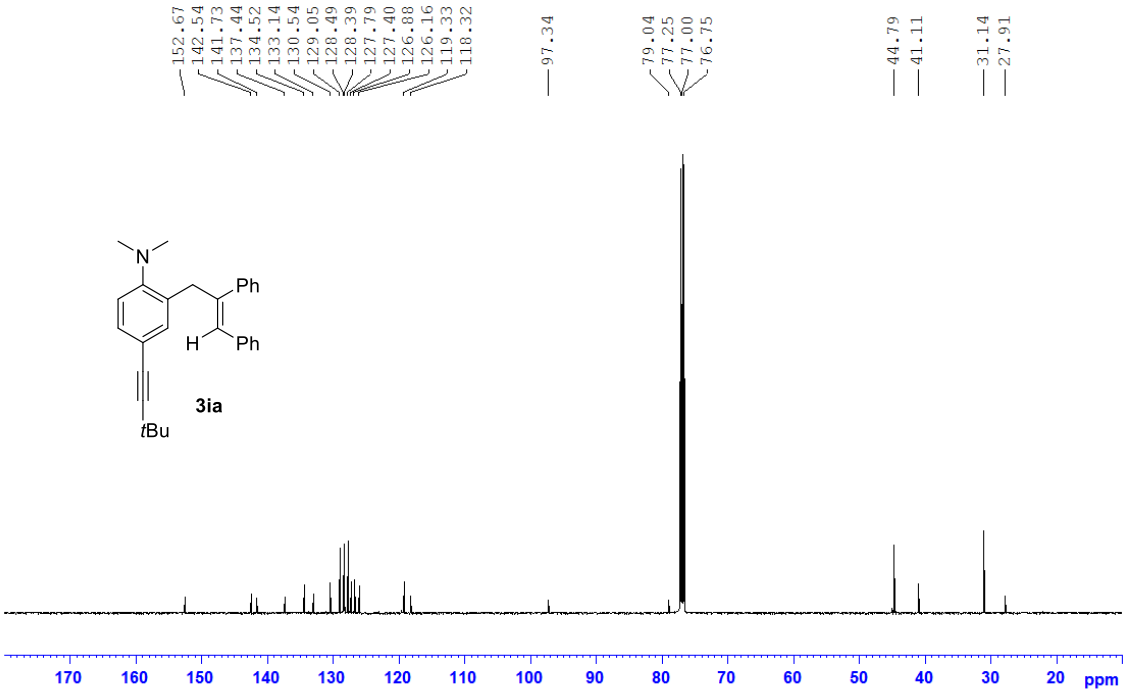

zw-68-110-1c



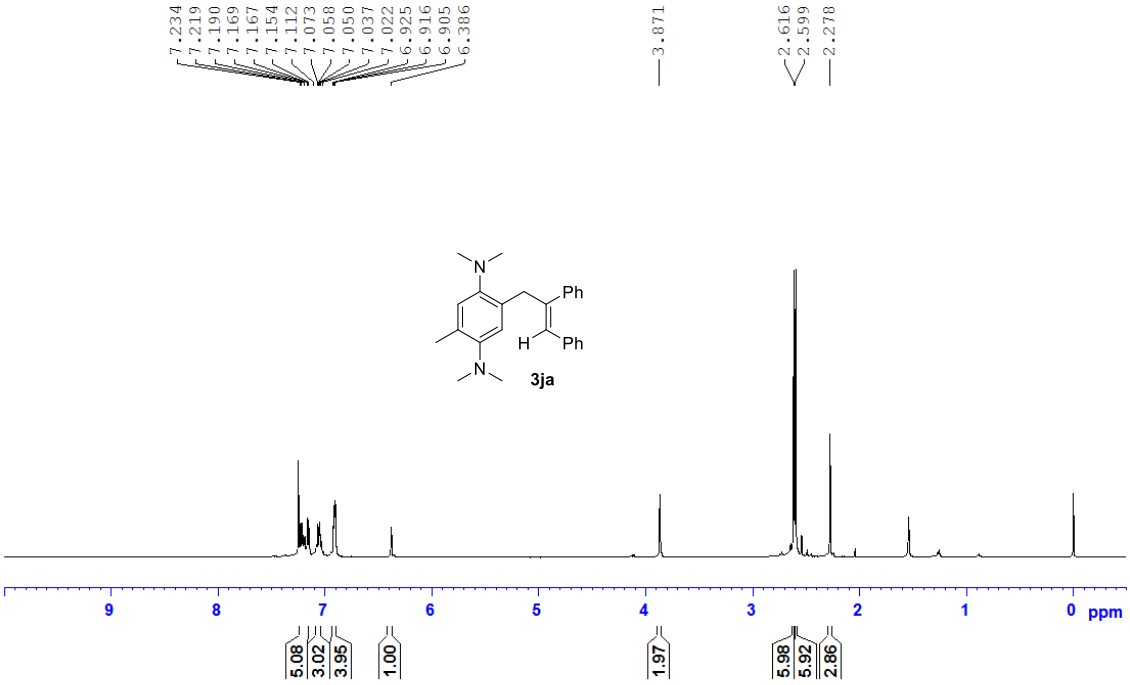
zw-68-113-1



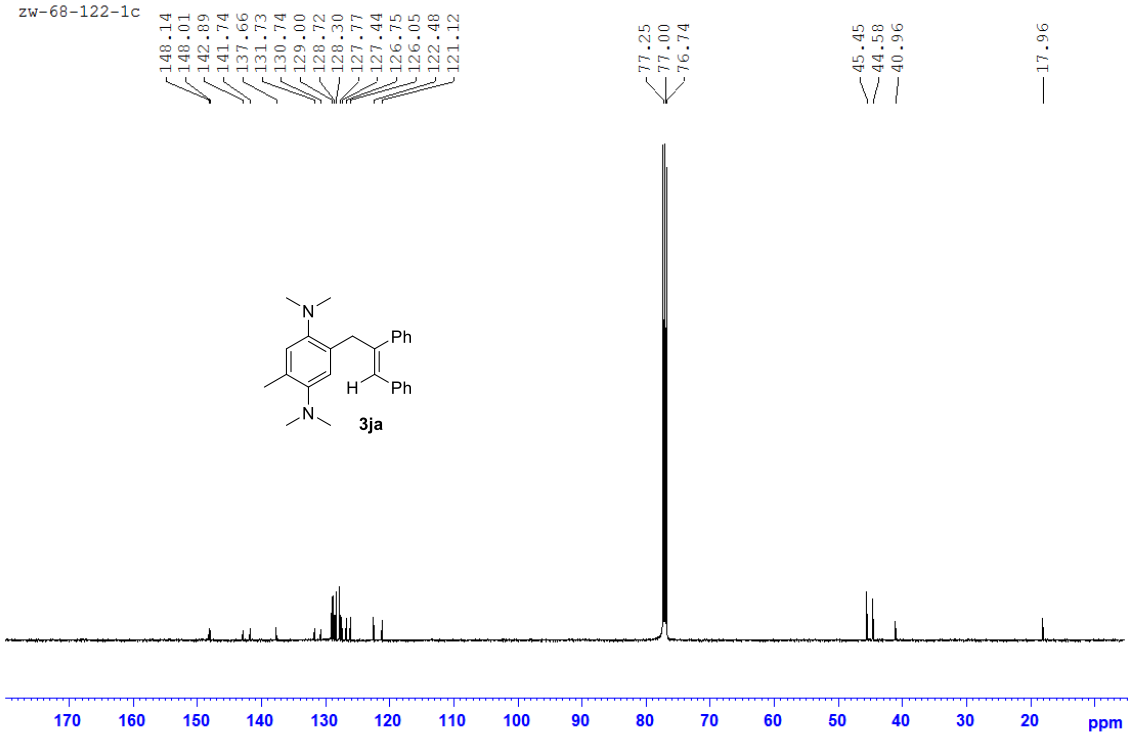

zw-68-113-1c



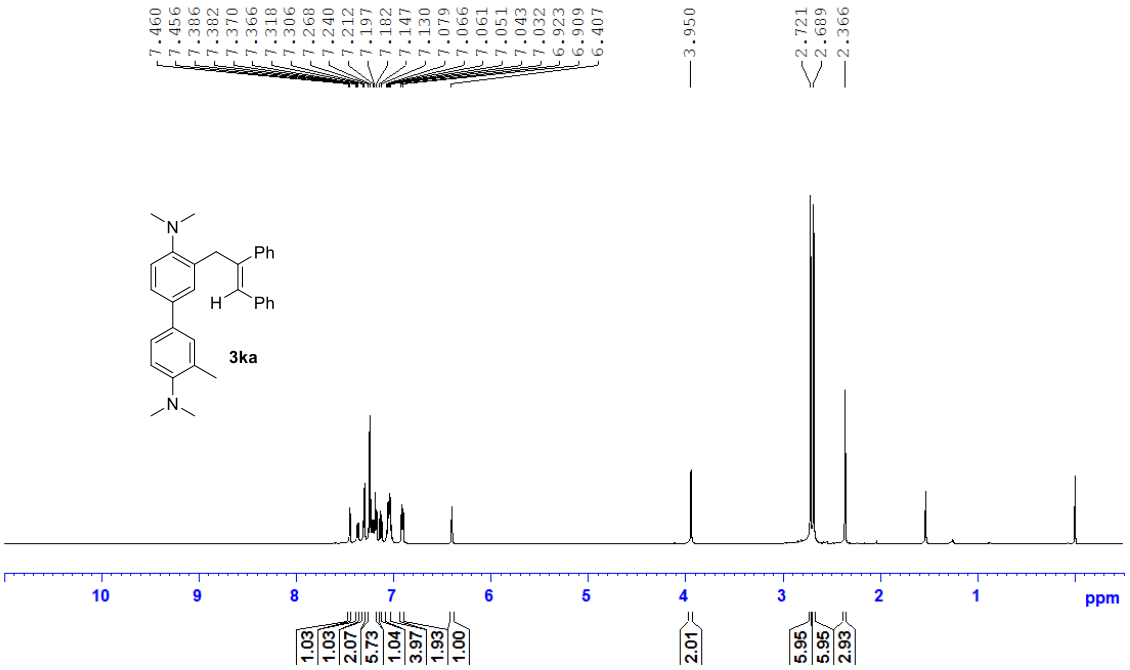
zw-68-122-1



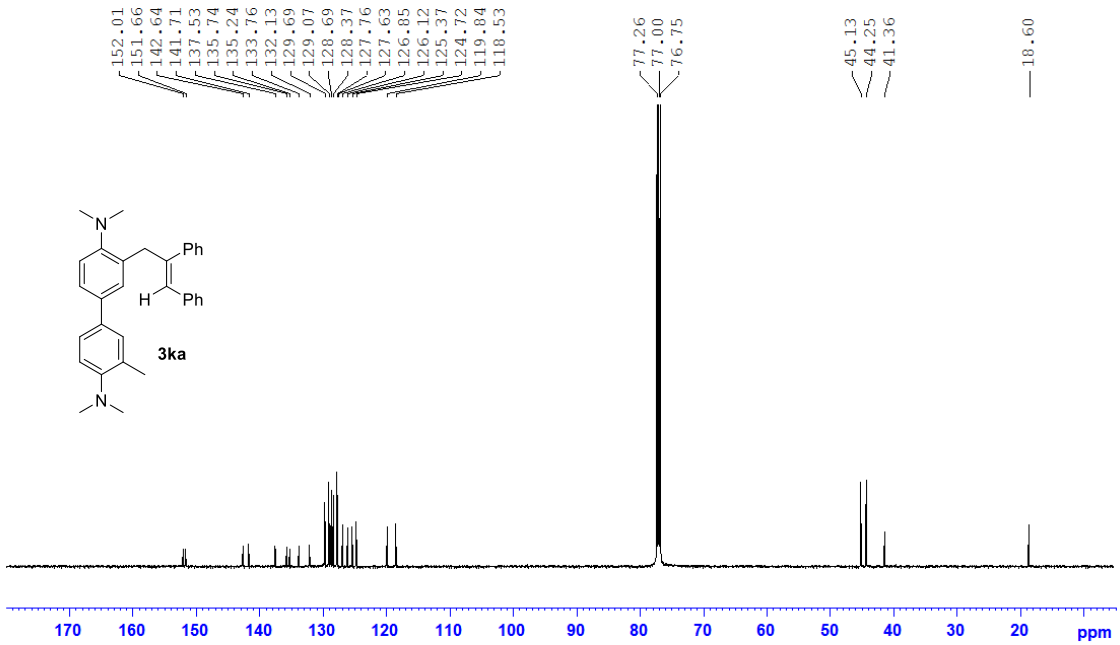

zw-68-122-1c



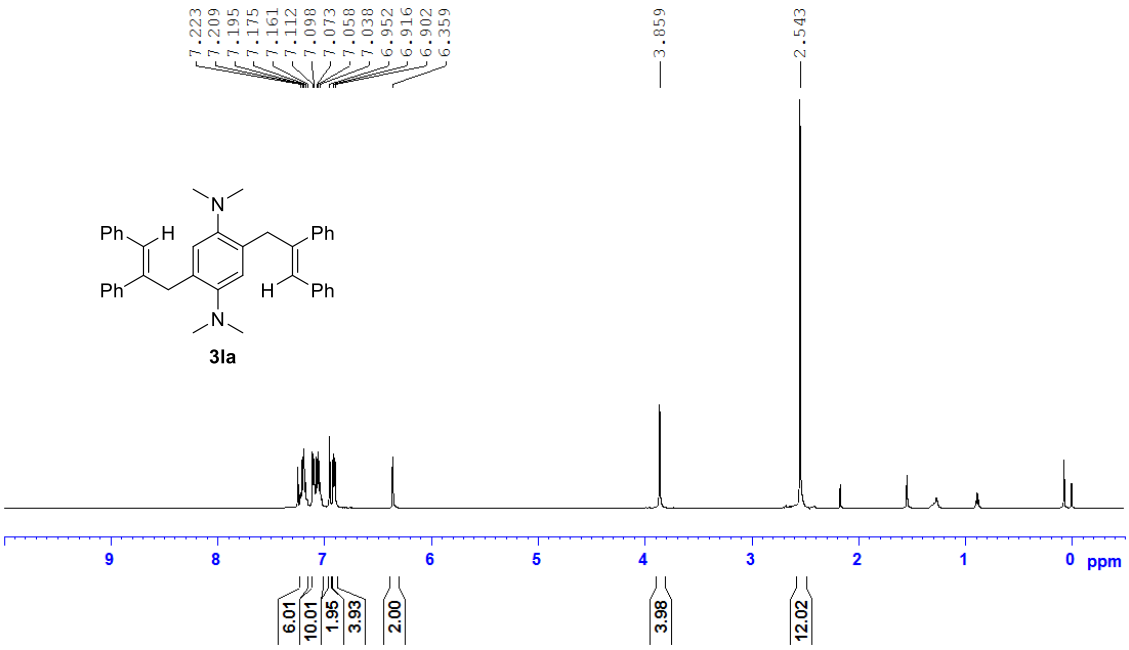
zw-68-122-2



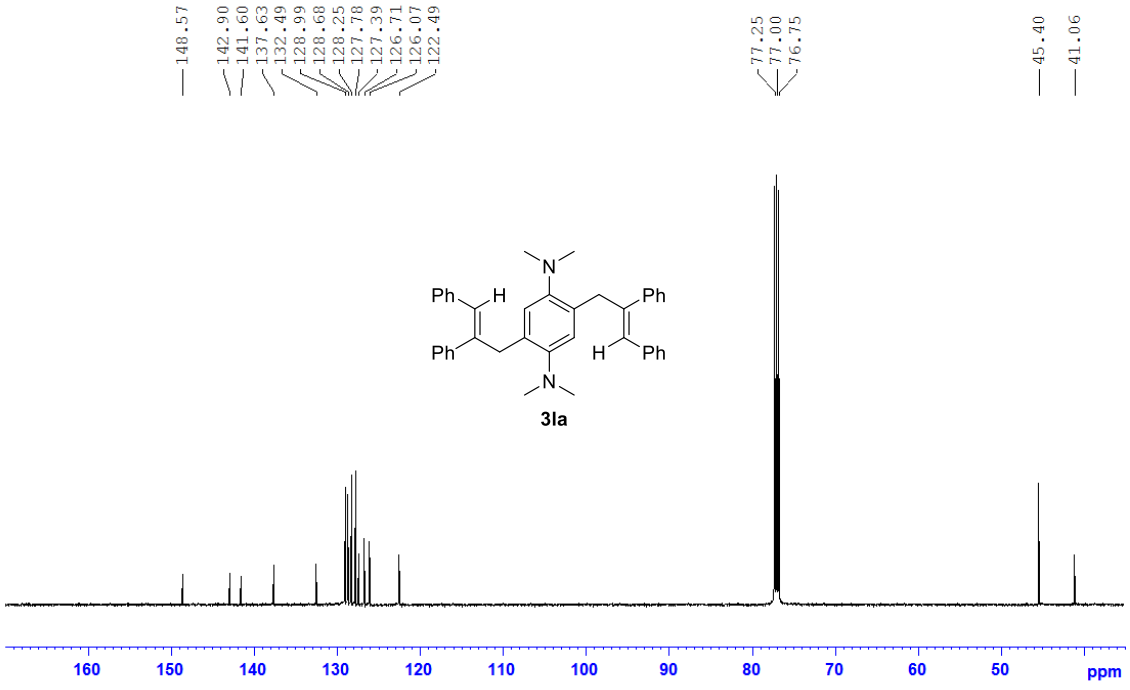

zw-68-122-2c



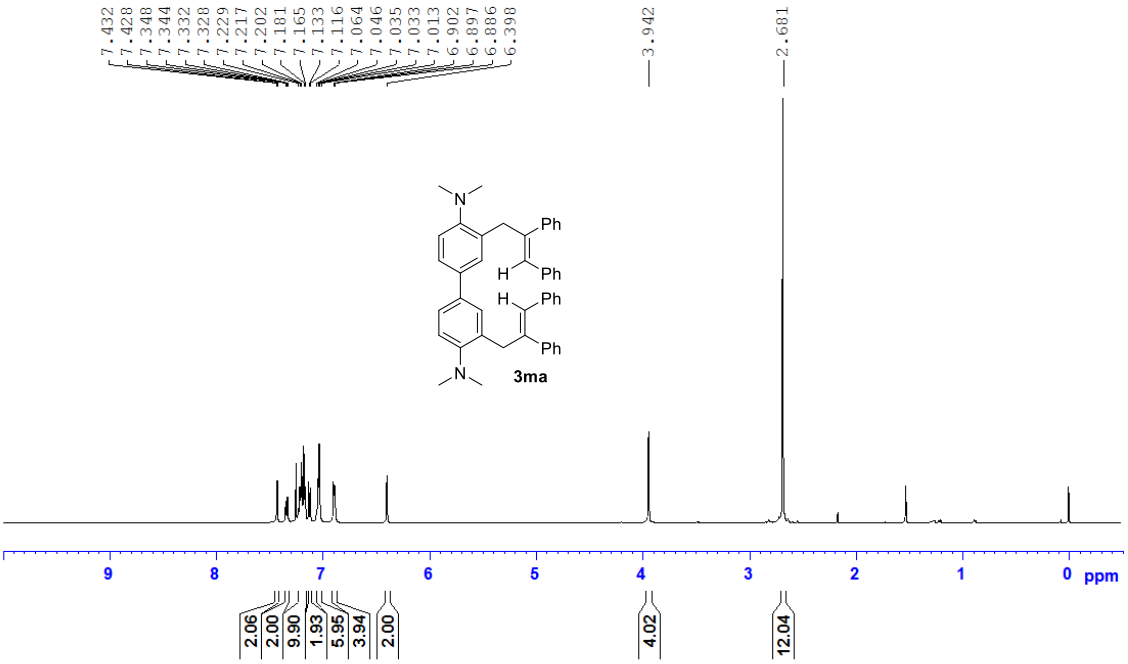
zw-68-119-1



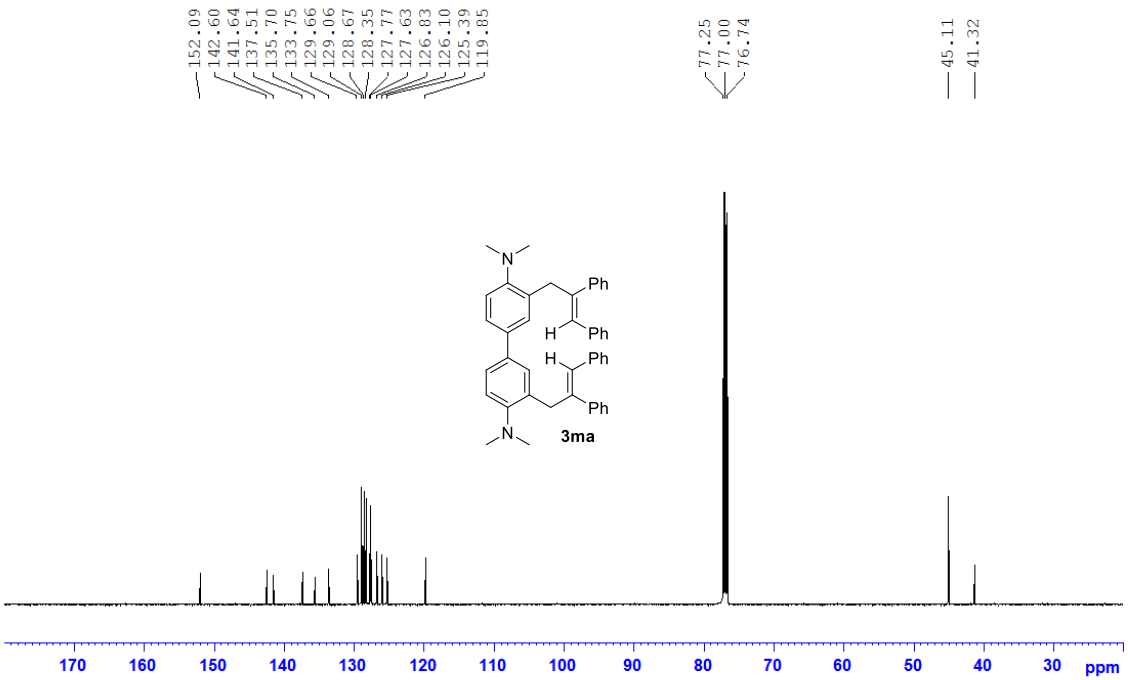

zw-68-119-1



zw-68-119-2




zw-68-119-2c



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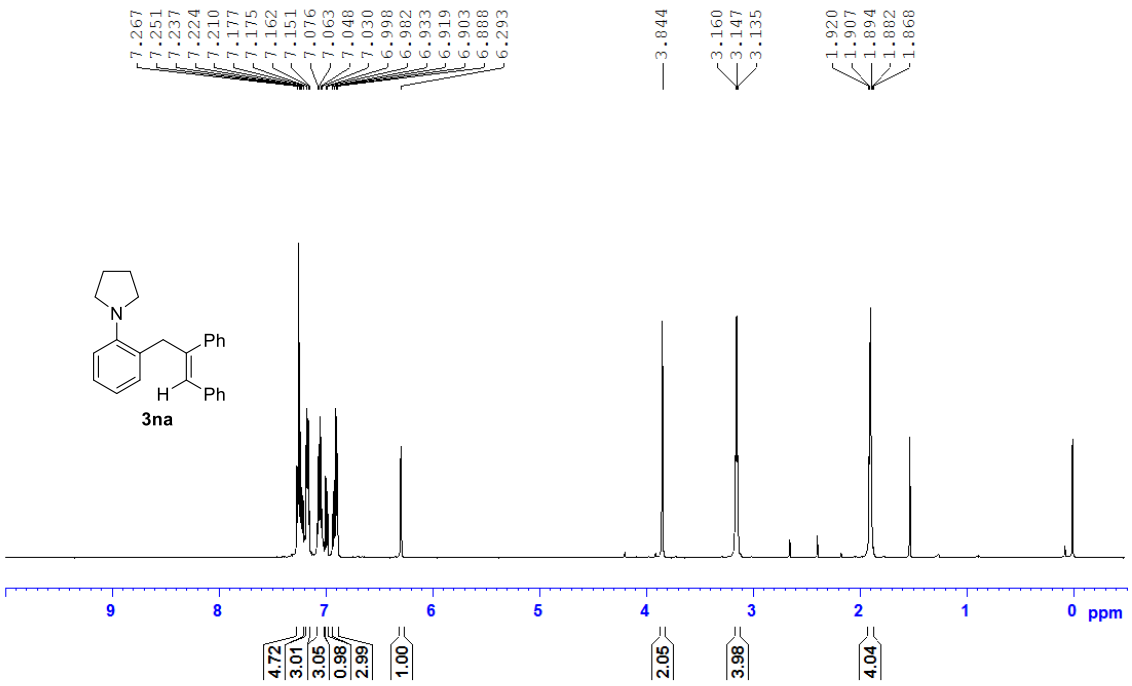


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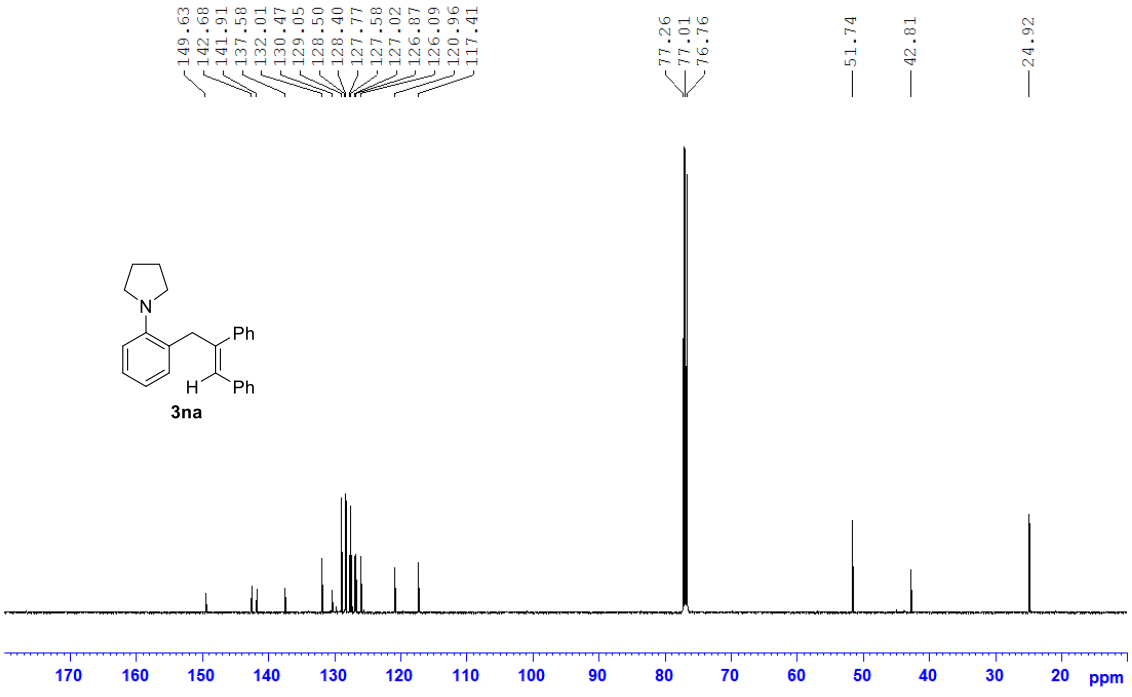

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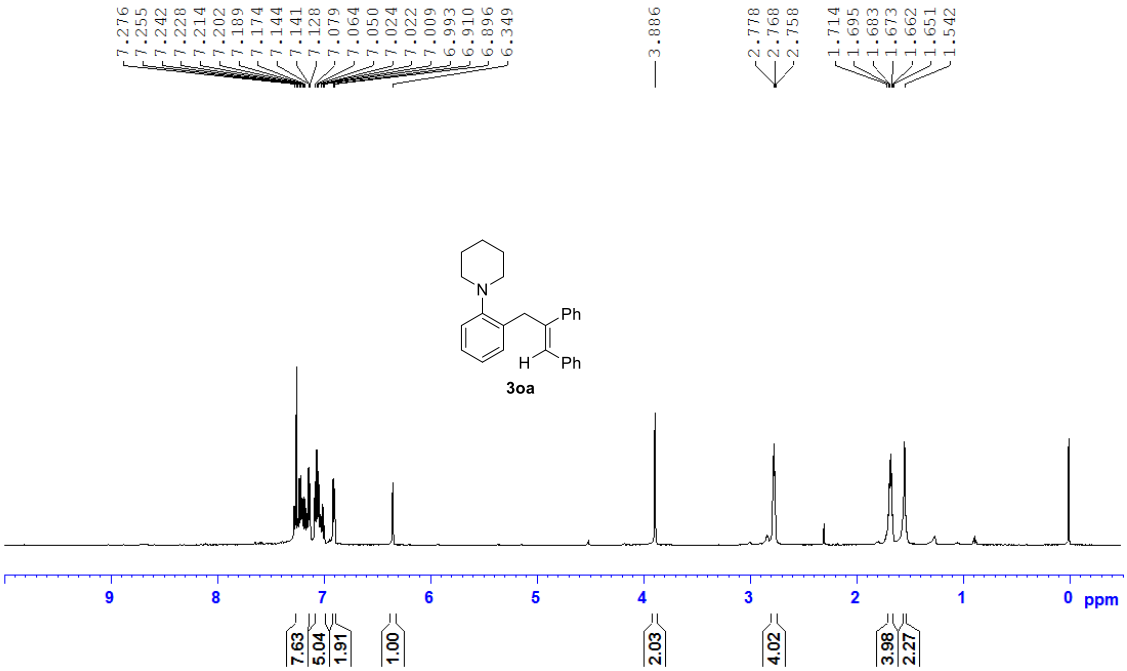


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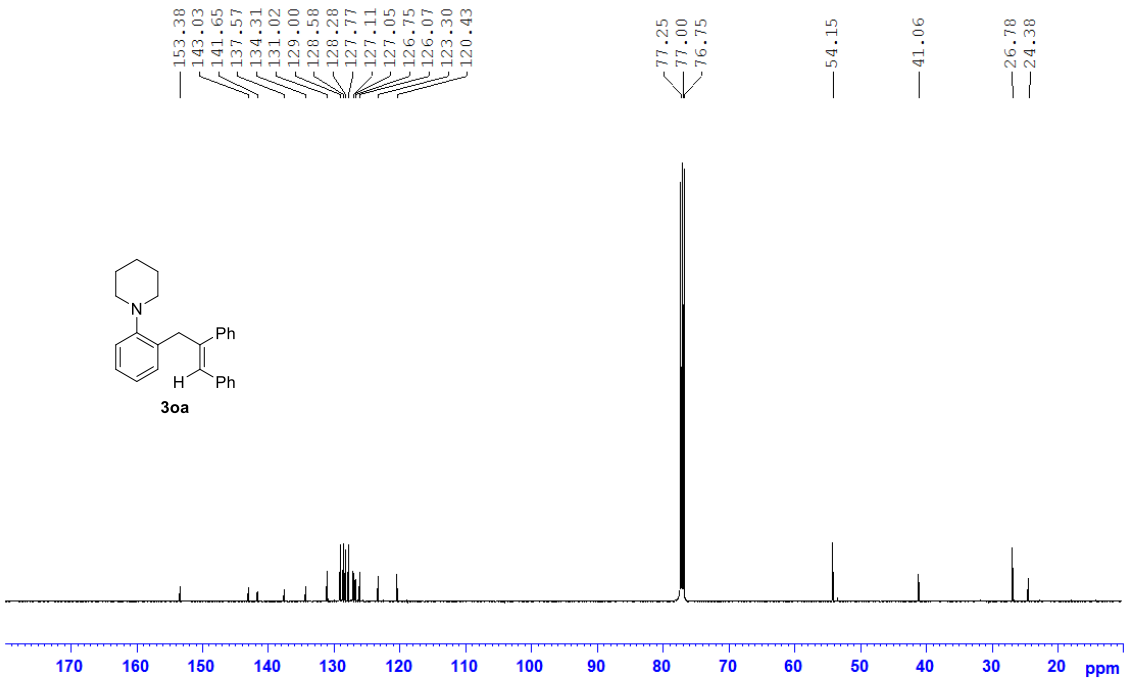

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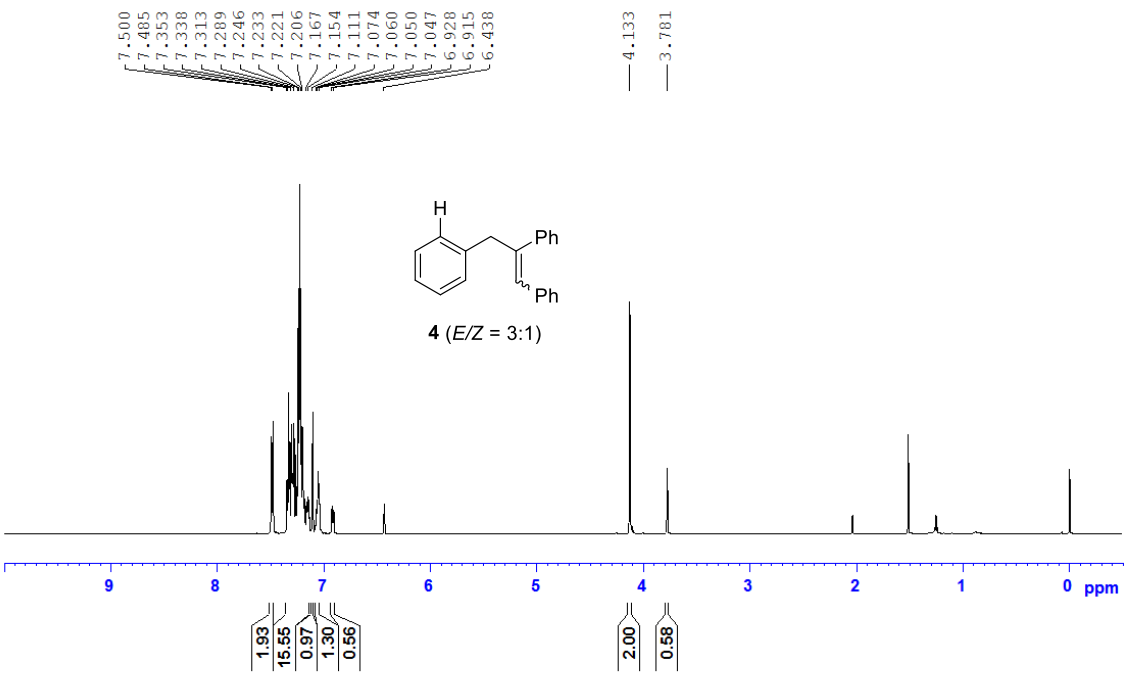


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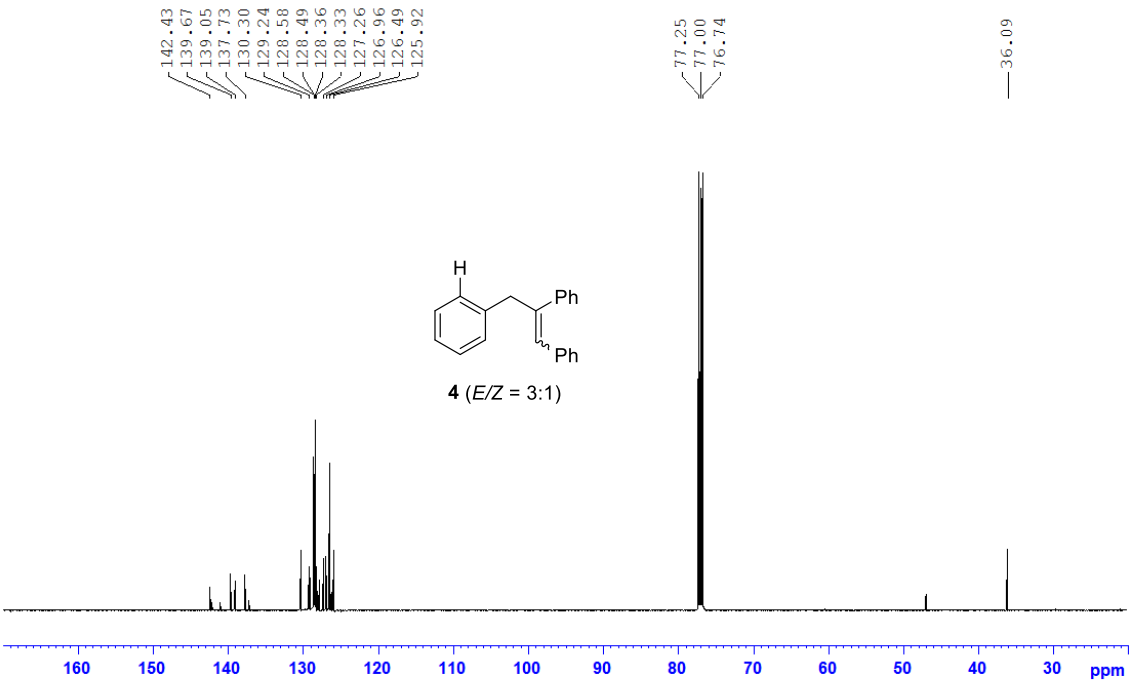

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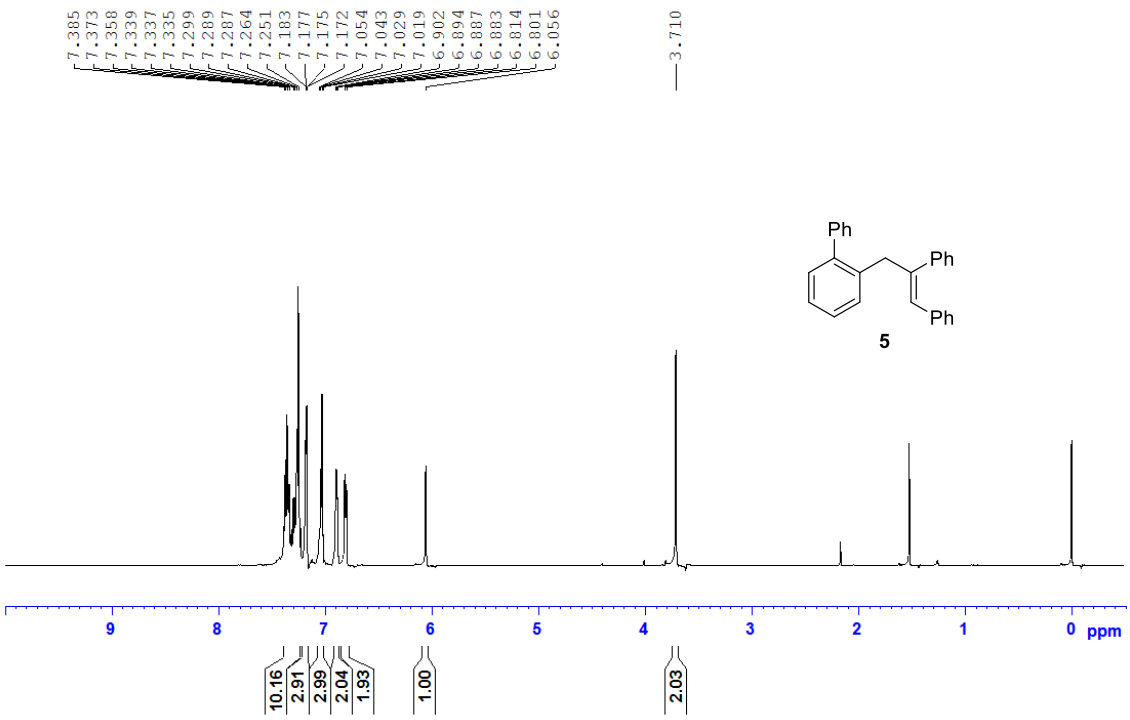


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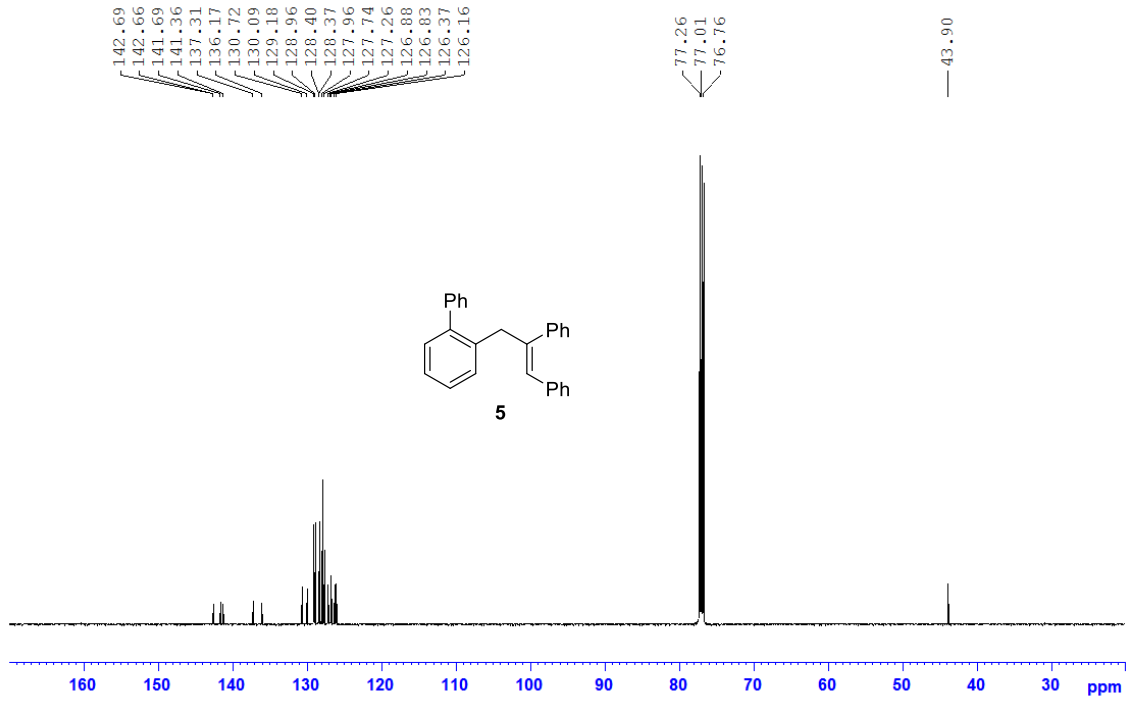

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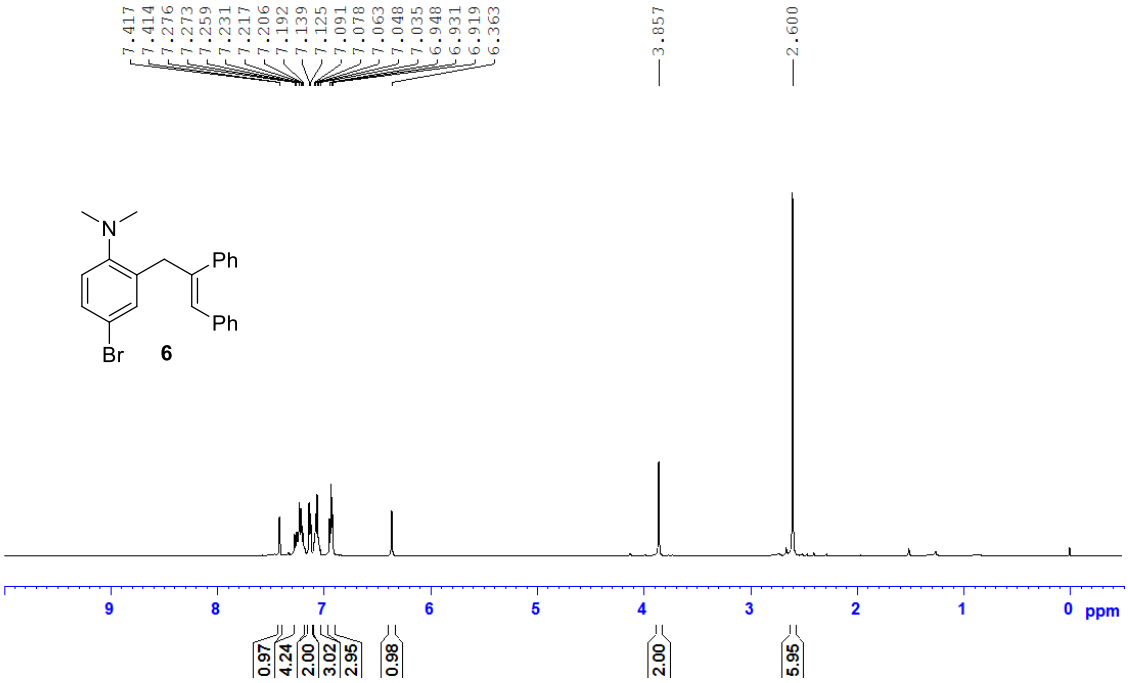


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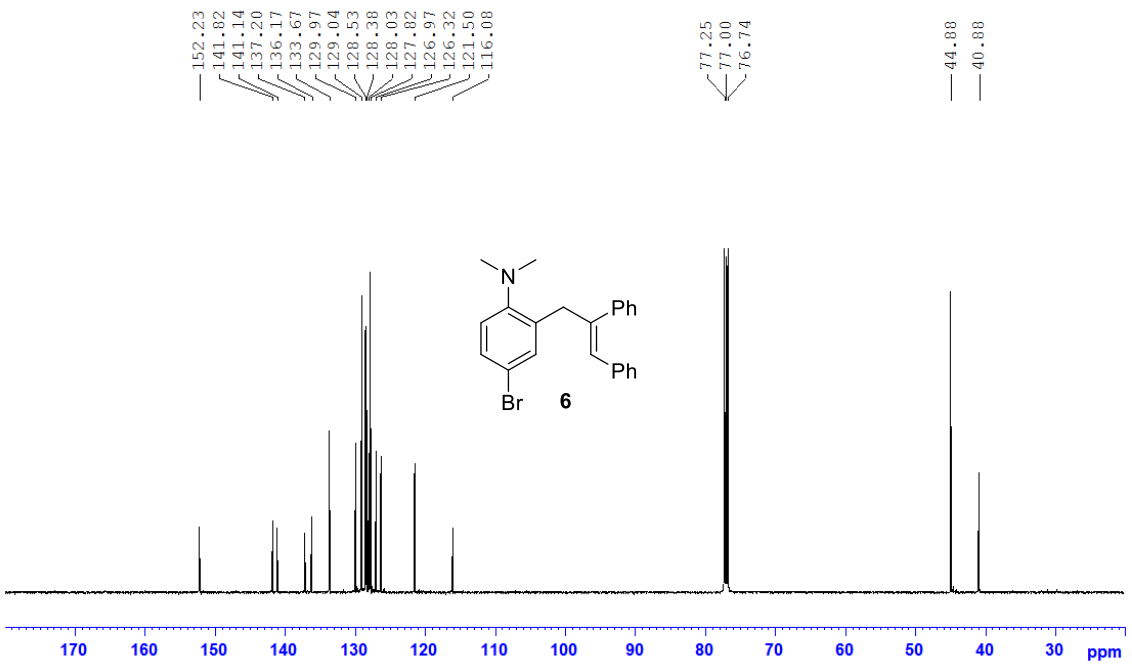

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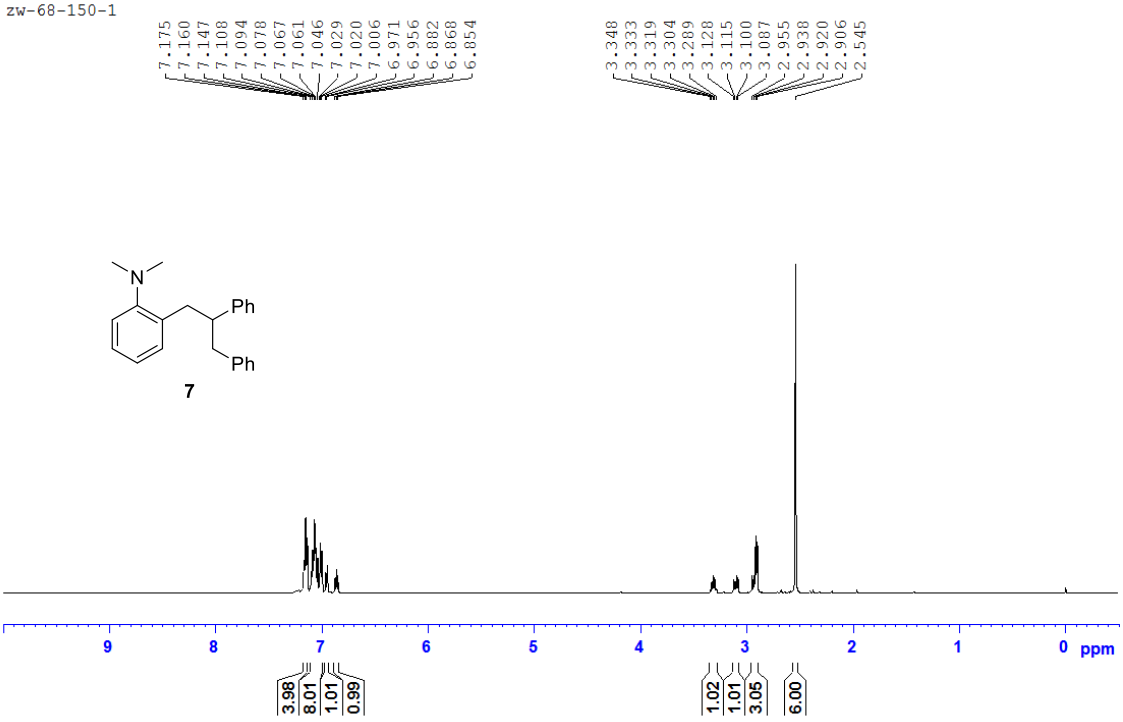


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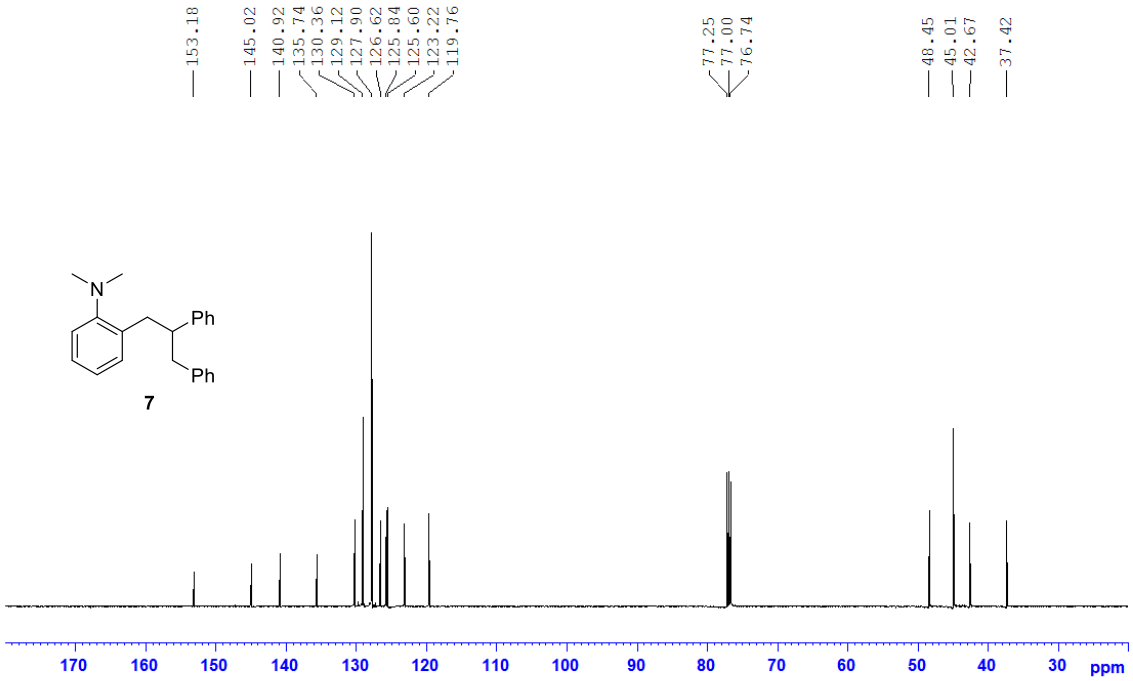

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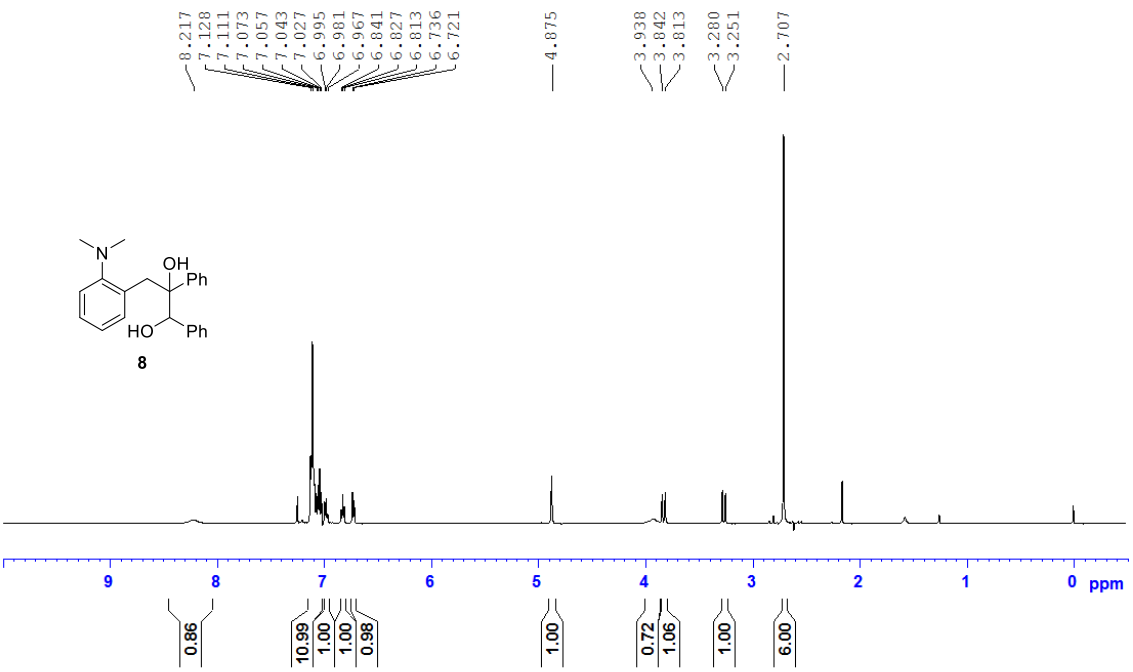


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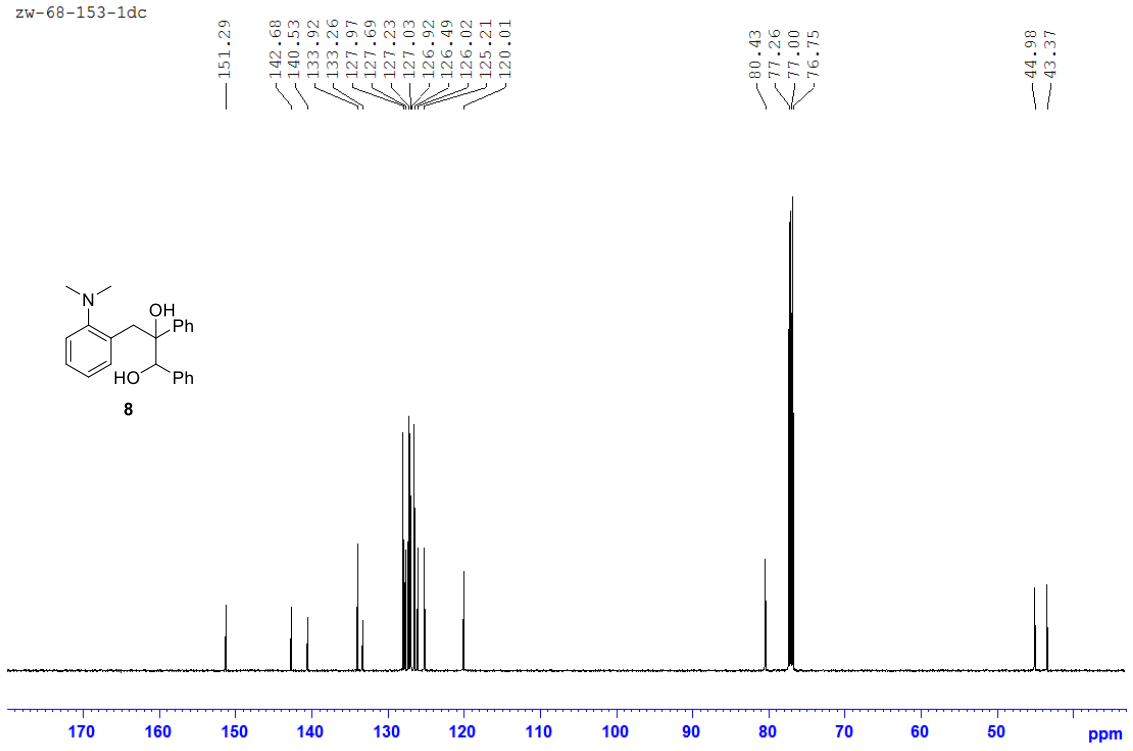


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