Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information to

An unprecedented Pd-catalyzed *trans*-addition of boronic acids to ynamides

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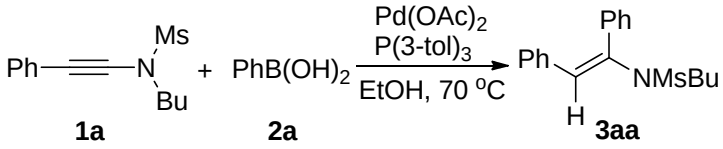
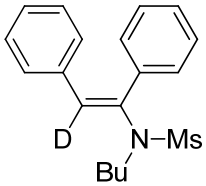
General: Solvents were purified or dried in a standard manner. Column chromatography was performed using silica gel (300–400 mesh). ^{1}H NMR and ^{13}C NMR spectra are recorded on a 400 or 600 MHz NMR spectrometers. Chemical shifts were reported in ppm downfield from tetramethylsilane with the solvent resonance as the internal standard. All melting points were determined by a micro melting point apparatus and are uncorrected. High-resolution mass spectral (HRMS) analyses were carried out using a TOF MS instrument with an ESI or APCI source.

General procedure for the Pd-catalyzed synthesis of enamides:



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

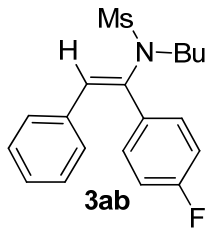
Compound ***3aa***. To a mixture of P(3-tol)$_3$ (9.1 mg, 0.03 mmol), Pd(OAc)$_2$ (3.4 mg, 0.015 mmol), and **2a** (54.9 mg, 0.45 mmol) in 1.5 mL of EtOH was added **1a** (75.3 mg, 0.3 mmol) under N_2 atmosphere. After stirring at 70 °C for 5 h, the reaction mixture was quenched with 5 mL of water, extracted with ethyl acetate, washed with brine, dried over anhydrous Na_2SO_4 and concentrated. Column chromatography on silica gel gave **3aa** as a white solid (92 mg, 93% yield); mp: 106–108 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.91 (t, J = 7.4 Hz, 3 H), 1.30–1.38 (m, 2 H), 1.58–1.64 (m, 2 H), 3.04 (s, 3 H), 3.36 (t, J = 7.5 Hz, 2 H), 6.79 (s, 1 H), 7.00–7.07 (m, 2 H), 7.10–7.17 (m, 3 H), 7.29–7.39 (m, 5 H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 13.9, 19.8, 30.9, 40.7, 47.8, 127.3, 128.1, 128.6, 128.7, 129.3, 129.5, 129.9, 135.2, 135.3, 137.6; MS (EI, *m*/*z*): 330 (6), 329 (M^+, 33), 251 (19), 250 (100), 206 (26); HRMS (APCI) calcd for $C_{19}H_{24}NO_2S$ $(M+H)^+$ 330.1528, found 330.1523.



3aa-*d* (95% D)

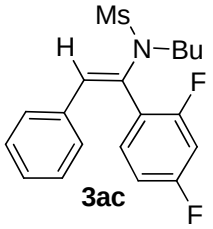
Compound ***3aa***-*d*. It was prepared from **1a** and $(PhBO)_3$ by using CD_3OD as the solvent, 86 mg, 87% yield, white solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.92 (t, J = 7.4 Hz, 3 H), 1.30–1.38 (m, 2 H), 1.58–1.64 (m, 2 H), 3.05 (s, 3 H), 3.37 (t, J = 7.5 Hz, 2 H), 6.80 (s,

0.05 H), 7.00–7.07 (m, 2 H), 7.10–7.17 (m, 3 H), 7.29–7.39 (m, 5 H); MS (EI, *m*/*z*): 331 (5), 330 (M^+, 27), 329 (62), 251 (83), 207 (24).



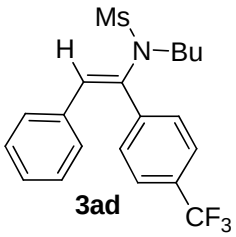
3ab

Compound ***3ab***. 94 mg, 90% yield, white solid, mp: 113–115 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.92 (t, J = 7.4 Hz, 3 H), 1.32–1.39 (m, 2 H), 1.57–1.63 (m, 2 H), 3.06 (s, 3 H), 3.37 (t, J = 7.5 Hz, 2 H), 6.77 (s, 1 H), 6.97–7.04 (m, 2 H), 7.02–7.06 (m, 2 H), 7.15–7.18 (m, 3 H), 7.36–7.41 (m, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.7, 40.6, 47.8, 115.6 (d, J = 21.5 Hz), 127.4, 128.1, 129.2, 129.4, 131.3, 131.7 (d, J = 8.3 Hz), 135.1, 136.8, 162.6 (d, J = 249.2 Hz); ^{19}F NMR ($CDCl_3$, 565 MHz) δ -111.9; MS (EI, *m*/*z*): 348 (6), 347 (M^+, 31), 268 (100), 224 (26), 212 (77); HRMS (APCI) calcd for $C_{19}H_{23}FNO_2S$ $(M+H)^+$ 348.1434, found 348.1428.



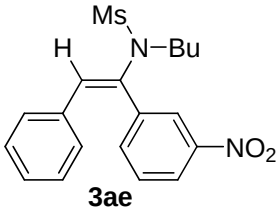
3ac

Compound ***3ac***. 97 mg, 89% yield, yellow oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.91 (t, J = 7.4 Hz, 3 H), 1.29–1.41 (m, 2 H), 1.59–1.71 (m, 2 H), 3.03 (s, 3 H), 3.36 (t, J = 7.4 Hz, 2 H), 6.79 (dd, J = 10.3, 2.4 Hz, 1 H), 6.89 (td, J = 8.6, 2.5 Hz, 1 H), 6.93 (s, 1 H), 6.99–7.02 (m, 2 H), 7.11–7.17 (m, 3 H), 7.43 (dd, J = 15.0, 8.4 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.9, 40.0 (d, J = 2.3 Hz), 48.1, 104.4 (t, J = 25.7 Hz), 112.1 (dd, J = 21.3, 3.6 Hz), 119.7 (dd, J = 15.2, 3.8 Hz), 127.7, 128.2, 128.6, 130.5, 132.0, 133.2 (dd, J = 9.6, 4.6 Hz), 134.9, 160.4 (dd, J = 251.9, 11.7 Hz), 163.2 (dd, J = 251.4, 11.4 Hz); ^{19}F NMR ($CDCl_3$, 565 MHz) δ -107.8 (d, J = 8.7 Hz), -108.2 (d, J = 8.6 Hz); MS (EI, *m*/*z*): 366 (5), 365 (M^+, 29), 286 (100), 242 (25), 230 (89); HRMS (APCI) calcd for $C_{19}H_{22}F_2NO_2S$ $(M+H)^+$ 366.1339, found 366.1341.



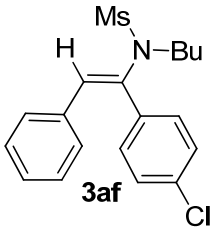
3ad

Compound ***3ad***. 100 mg, 84% yield, yellow oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.92 (t, J = 7.4 Hz, 3 H), 1.32–1.38 (m, 2 H), 1.59–1.64 (m, 2 H), 3.09 (s, 3 H), 3.38 (t, J = 7.6 Hz, 2 H), 6.86 (s, 1 H), 7.01–7.05 (m, 2 H), 7.16–7.23 (m, 3 H), 7.50 (d, J = 8.2 Hz, 2 H), 7.54 (d, J = 8.4 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.7, 40.5, 48.2, 122.9, 124.7, 125.4 (q, J = 3.7 Hz), 127.8, 128.3, 129.3, 130.3, 130.9, 134.7, 136.6, 139.3; ^{19}F NMR ($CDCl_3$, 565 MHz) δ -62.64; MS (EI, *m*/*z*): 398 (4), 397 (M^+, 25), 319 (20), 318 (100), 274 (27), 262 (79); HRMS (APCI) calcd for $C_{20}H_{23}F_3NO_2S$ $(M+H)^+$ 398.1402, found 398.1408.



3ae

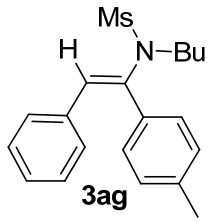
Compound ***3ae***. 92 mg, 82% yield, white solid, mp: 119–121 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.95 (t, J = 7.4 Hz, 3 H), 1.36–1.43 (m, 2 H), 1.65–1.70 (m, 2 H), 3.12 (s, 3 H), 3.46 (t, J = 7.5 Hz, 2 H), 6.92 (s, 1 H), 7.04–7.07 (m, 2 H), 7.17–7.21 (m, 3 H), 7.48 (t, J = 8.0 Hz, 1 H), 7.75 (d, J = 7.7 Hz, 1 H), 8.16 (dd, J = 8.2, 1.4 Hz, 1 H), 8.21 (s, 1 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.8, 30.7, 40.0, 48.7, 123.3, 124.5, 128.1, 128.5, 129.1, 129.5, 131.3, 134.3, 135.9, 136.0, 137.9, 148.2; MS (EI, *m*/*z*): 375 (6), 374 (M^+, 24), 329 (21), 294 (43), 250 (29); HRMS (APCI) calcd for $C_{19}H_{23}N_2O_4S$ $(M+H)^+$ 375.1379, found 375.1376.



3af

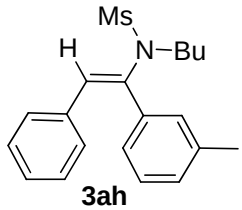
Compound ***3af***. 93 mg, 85% yield, white solid, mp: 113–115 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.91 (t, J = 7.4 Hz, 3 H), 1.31–1.37 (m, 2 H), 1.57–1.62 (m, 2 H), 3.06 (s, 3 H),

3.36 (t, J = 7.5 Hz, 2 H), 6.78 (s, 1 H), 7.04–7.07 (m, 2 H), 7.15–7.18 (m, 3 H), 7.29 (d, J = 8.5 Hz, 2 H), 7.31 (d, J = 8.4 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.8, 40.7, 48.0, 127.6, 128.2, 128.8, 129.2, 129.9, 131.2, 133.9, 134.5, 135.0, 136.7; MS (EI, m/z): 365 (10), 363 (M^+, 30), 286 (30), 284 (100), 240 (23); HRMS (APCI) calcd for $C_{19}H_{23}ClNO_2S$ $(M+H)^+$ 364.1138, found 364.1134.



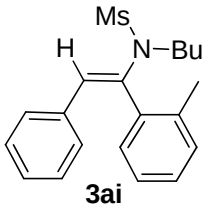
3ag

Compound ***3ag***. 94 mg, 91% yield, yellow oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.92 (t, J = 7.4 Hz, 3 H), 1.32–1.38 (m, 2 H), 1.59–1.64 (m, 2 H), 2.35 (s, 3 H), 3.05 (s, 3 H), 3.36 (t, J = 7.3 Hz, 2 H), 6.77 (s, 1 H), 7.06 (d, J = 7.6 Hz, 2 H), 7.09–7.17 (m, 5 H), 7.25 (d, J = 7.7 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 19.7, 21.3, 30.9, 40.7, 47.7, 127.2, 128.0, 128.9, 129.2, 129.3, 129.7, 132.2, 135.5, 137.6, 138.7; MS (EI, m/z): 344 (6), 343 (M^+, 31), 264 (80), 220 (16), 208 (42); HRMS (APCI) calcd for $C_{20}H_{26}NO_2S$ $(M+H)^+$ 344.1684, found 344.1683.



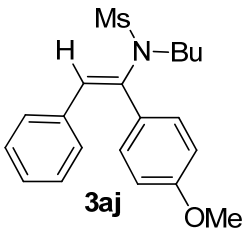
3ah

Compound ***3ah***. 94 mg, 91% yield, yellow oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.93 (t, J = 7.4 Hz, 3 H), 1.34–1.38 (m, 2 H), 1.61–1.66 (m, 2 H), 2.30 (s, 3 H), 3.06 (s, 3 H), 3.31–3.39 (m, 2 H), 6.80 (s, 1 H), 7.00–7.08 (m, 2 H), 7.09–7.24 (m, 7 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 21.3, 30.8, 40.6, 47.6, 127.0, 127.2, 127.9, 128.4, 129.2, 129.3, 129.5, 130.1, 135.0, 135.3, 137.5, 138.2; MS (EI, m/z): 344 (6), 343 (M^+, 34), 281 (2), 264 (92), 220 (17), 208 (52); HRMS (APCI) calcd for $C_{20}H_{26}NO_2S$ $(M+H)^+$ 344.1684, found 344.1684.



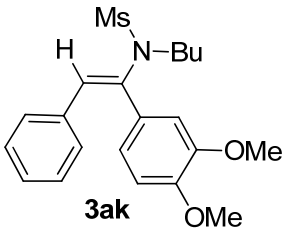
3ai

Compound ***3ai***. 91 mg, 89% yield, yellow oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.91 (t, J = 7.4 Hz, 3 H), 1.29–1.35 (m, 2 H), 1.66–1.71 (m, 2 H), 2.05 (s, 3 H), 2.99 (s, 3 H), 3.21–3.50 (m, 2 H), 6.81 (s, 1 H), 6.88–6.92 (m, 2 H), 7.09–7.15 (m, 4 H), 7.24–7.31 (m, 2 H), 7.37–7.41 (m, 1 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 19.6, 19.9, 31.4, 40.9, 48.3, 125.3, 126.3, 127.2, 128.1, 128.1, 128.5, 128.8, 129.8, 130.8, 134.7, 135.5, 137.4; MS (EI, *m*/*z*): 344 (3), 343 (M^+, 13), 264 (59), 220 (13), 208 (28); HRMS (APCI) calcd for $C_{20}H_{26}NO_2S$ $(M+H)^+$ 344.1684, found 344.1682.



3aj

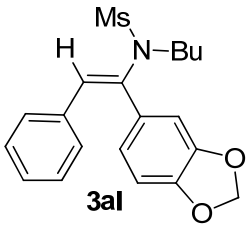
Compound ***3aj***. 90 mg, 84% yield, yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.93 (t, J = 7.4 Hz, 3 H), 1.32–1.41 (m, 2 H), 1.58–1.66 (m, 2 H), 3.07 (s, 3 H), 3.39 (t, J = 7.5 Hz, 2 H), 3.83 (s, 3 H), 6.73 (s, 1 H), 6.85 (d, J = 8.8 Hz, 2 H), 7.02–7.22 (m, 5 H), 7.31 (d, J = 8.8 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 19.7, 30.8, 40.7, 47.7, 55.1, 113.9, 127.1, 127.3, 128.1, 128.3, 129.2, 131.2, 135.6, 137.5, 159.8; MS (EI, *m*/*z*): 360 (3), 359 (M^+, 15), 280 (22), 209 (15), 197 (100); HRMS (APCI) calcd for $C_{20}H_{26}NO_3S$ $(M+H)^+$ 360.1633, found 360.1626.



3ak

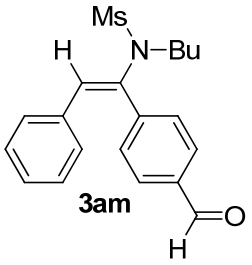
Compound ***3ak***. 103 mg, 88% yield, white solid, mp: 143–145 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.90 (t, J = 7.4 Hz, 3 H), 1.30–1.36 (m, 2 H), 1.56–1.61 (m, 2 H), 3.05 (s, 3 H), 3.37 (t, J = 7.4 Hz, 2 H), 3.63 (s, 3 H), 3.86 (s, 3 H), 6.69 (s, 1 H), 6.78 (d, J = 8.3 Hz, 1 H), 6.83 (d, J = 1.9 Hz, 1 H), 6.93 (dd, J = 8.3, 1.9 Hz, 1 H), 7.05–7.16 (m, 5 H); ^{13}C

NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.8, 40.7, 47.8, 55.6, 55.7, 110.8, 113.0, 122.4, 127.2, 127.5, 128.0, 128.4, 129.2, 135.6, 137.6, 148.6, 149.3; MS (EI, *m*/*z*): 390 (4), 389 (M^+, 20), 310 (19), 239 (15), 227 (100); HRMS (APCI) calcd for $C_{21}H_{28}NO_4S$ $(M+H)^+$ 390.1739, found 390.1740.



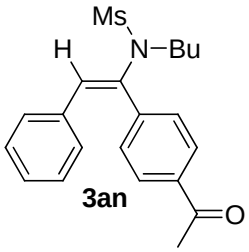
3al

Compound ***3al***. 103 mg, 92% yield, white solid, mp: 149–151 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.92 (t, J = 7.4 Hz, 3 H), 1.31–1.37 (m, 2 H), 1.57–1.62 (m, 2 H), 3.05 (s, 3 H), 3.37 (t, J = 7.4 Hz, 2 H), 5.96 (s, 2 H), 6.70 (s, 1 H), 6.72 (d, J = 8.0 Hz, 1 H), 6.83–6.86 (m, 2 H), 7.08 (d, J = 6.8 Hz, 2 H), 7.14–7.18 (m, 3 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.8, 40.7, 47.7, 101.2, 108.4, 109.9, 124.0, 127.2, 128.1, 128.6, 129.2, 135.4, 137.2, 147.8, 147.9; MS (EI, *m*/*z*): 374 (4), 373 (M^+, 21), 294 (28), 223 (12), 211 (100); HRMS (APCI) calcd for $C_{20}H_{24}NO_4S$ $(M+H)^+$ 374.1426, found 374.1422.



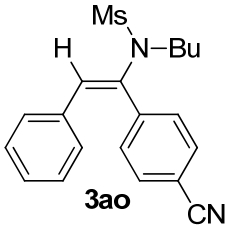
3am

Compound ***3am***. 93 mg, 87% yield, colorless oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.90 (t, J = 7.4 Hz, 3 H), 1.31–1.36 (m, 2 H), 1.58–1.63 (m, 2 H), 3.08 (s, 3 H), 3.38 (t, J = 7.4 Hz, 2 H), 6.87 (s, 1 H), 6.99–7.04 (m, 2 H), 7.11–7.16 (m, 3 H), 7.53 (t, J = 8.1 Hz, 2 H), 7.78 (d, J = 8.1 Hz, 2 H), 9.97 (s, 1 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.7, 40.4, 48.3, 127.9, 128.3, 129.3, 129.7, 130.5, 131.1, 134.6, 135.9, 136.7, 142.0, 191.6; MS (EI, *m*/*z*): 358 (5), 357 (M^+, 24), 278 (92), 234 (18), 222 (42), 207 (38); HRMS (APCI) calcd for $C_{20}H_{24}NO_3S$ $(M+H)^+$ 358.1477, found 358.1475.



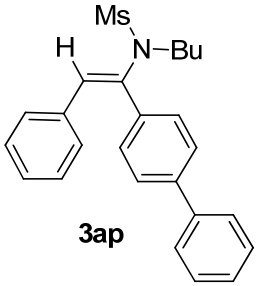
3an

Compound ***3an***. 92 mg, 83% yield, colorless oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.90 (t, J = 7.4 Hz, 3 H), 1.29–1.38 (m, 2 H), 1.56–1.65 (m, 2 H), 2.58 (s, 3 H), 3.07 (s, 3 H), 3.36 (t, J = 7.5 Hz, 2 H), 6.84 (s, 1 H), 7.01–7.04 (m, 2 H), 7.13–7.16 (m, 3 H), 7.46 (d, J = 8.3 Hz, 2 H), 7.86 (d, J = 8.3 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 26.6, 30.8, 40.5, 48.2, 127.8, 128.3, 128.5, 129.3, 130.1, 130.8, 134.8, 136.8, 136.8, 140.5, 197.5; MS (EI, *m*/*z*): 372 (5), 371 (M^+, 26), 293 (19), 292 (86), 281 (11); HRMS (APCI) calcd for $C_{21}H_{26}NO_3S$ $(M+H)^+$ 372.1633, found 372.1632.



3ao

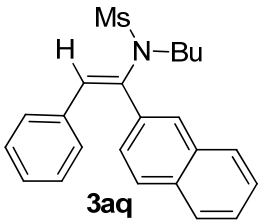
Compound ***3ao***. 93 mg, 88% yield, colorless oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.91 (t, J = 7.4 Hz, 3 H), 1.31–1.38 (m, 2 H), 1.56–1.64 (m, 2 H), 3.08 (s, 3 H), 3.37 (t, J = 7.5 Hz, 2 H), 6.85 (s, 1 H), 6.98–7.06 (m, 2 H), 7.16–7.21 (m, 3 H), 7.48 (d, J = 8.3 Hz, 2 H), 7.55 (d, J = 8.4 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.7, 40.3, 48.5, 112.0, 118.4, 128.1, 128.4, 129.2, 130.5, 131.4, 132.2, 134.4, 136.4, 140.7; MS (EI, *m*/*z*): 355 (4), 354 (M^+, 17), 281 (8), 275 (75), 231 (28), 219 (79); HRMS (APCI) calcd for $C_{20}H_{23}N_2O_2S$ $(M+H)^+$ 355.1480, found 355.1477.



3ap

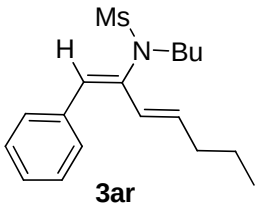
Compound ***3ap***. 103 mg, 85% yield, white solid, mp: 145–147 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.95 (t, J = 6.6 Hz, 3 H), 1.29–1.46 (m, 2 H), 1.58–1.74 (m, 2 H), 3.10 (s, 3 H),

3.43 (t, J = 6.2 Hz, 2 H), 6.84 (s, 1 H), 7.13–7.19 (m, 5 H), 7.35–7.39 (m, 1 H), 7.46 (d, J = 6.0 Hz, 4 H), 7.57 (d, J = 7.3 Hz, 2 H), 7.63 (d, J = 6.8 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 19.8, 30.9, 40.7, 47.9, 126.9, 127.1, 127.4, 127.6, 128.1, 128.8, 129.3, 129.5, 130.3, 134.1, 135.4, 137.4, 140.1, 141.2; MS (EI, *m*/*z*): 406 (3), 405 (M^+, 13), 329 (21), 271 (64), 253 (33); HRMS (APCI) calcd for $C_{25}H_{28}NO_2S$ $(M+H)^+$ 406.1841, found 406.1839.



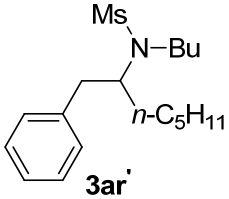
3aq

Compound ***3aq***. 98 mg, 86% yield, white solid, mp: 139–141 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.94 (t, J = 7.4 Hz, 3 H), 1.35–1.39 (m, 2 H), 1.65–1.70 (m, 2 H), 3.13 (s, 3 H), 3.43 (t, J = 7.1 Hz, 2 H), 6.91 (s, 1 H), 7.11–7.14 (m, 5 H), 7.44 (d, J = 8.5 Hz, 1 H), 7.48–7.53 (m, 2 H), 7.76 (d, J = 8.5 Hz, 1 H), 7.80 (d, J = 7.9 Hz, 1 H), 7.83 (d, J = 7.9 Hz, 1 H), 7.93 (s, 1 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 19.7, 30.8, 40.8, 47.8, 126.2, 126.7, 127.4, 127.4, 127.6, 128.1, 128.1, 128.3, 129.2, 129.3, 129.7, 132.7, 133.2, 133.2, 135.2, 137.5; MS (EI, *m*/*z*): 380 (6), 379 (M^+, 26), 300 (54), 256 (11), 244 (29); HRMS (APCI) calcd for $C_{23}H_{26}NO_2S$ $(M+H)^+$ 380.1684, found 380.1684.



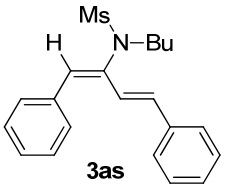
3ar

Compound ***3ar***. 76 mg, 79% yield, colorless oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.87–0.98 (m, 6 H), 1.32–1.40 (m, 2 H), 1.42–1.49 (m, 2 H), 1.55–1.66 (m, 2 H), 2.10–2.21 (m, 2 H), 3.01 (s, 3 H), 3.49 (t, J = 7.6 Hz, 2 H), 6.10–6.18 (m, 1 H), 6.41 (d, J = 15.4 Hz, 1 H), 6.57 (s, 1 H), 7.26–7.43 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 13.6, 19.8, 22.1, 31.0, 34.6, 39.1, 49.5, 124.0, 127.6, 128.2, 129.2, 130.3, 135.3, 136.5, 137.0; MS (EI, *m*/*z*): 322 (3), 321 (M^+, 22), 243 (18), 242 (100), 198 (24); HRMS (APCI) calcd for $C_{18}H_{28}NO_2S$ $(M+H)^+$ 322.1841, found 322.1844.



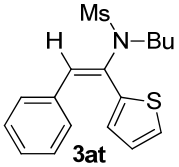
3ar'

Compound ***3ar'***. Treatment of **3ar** with 10% of Pd/C in EtOH under H_2 (balloon) at room temperature for 10 h gave 74 mg (76% yield) of **3ar'** as colorless oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.87 (t, J = 6.8 Hz, 3 H), 0.95 (t, J = 7.4 Hz, 3 H), 1.22–1.36 (m, 7 H), 1.39–1.43 (m, 1 H), 1.52–1.61 (m, 3 H), 1.67–1.73 (m, 1 H), 2.29 (s, 3 H), 2.76–2.85 (m, 2 H), 3.00–3.06 (m, 1 H), 3.09–3.17 (m, 1 H), 3.98–4.02 (m, 1 H), 7.19–7.24 (m, 3 H), 7.27–7.32 (m, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.8, 14.1, 20.5, 22.5, 26.4, 31.6, 33.1, 33.7, 39.9, 40.5, 43.5, 61.4 (NCH), 126.7, 128.6, 129.3, 139.1; HRMS (APCI) calcd for $C_{18}H_{32}NO_2S$ $(M+H)^+$ 326.2154, found 326.2154. The NMR measurements of **3ar'** further confirmed the regioselectivity reported in this paper.



3as

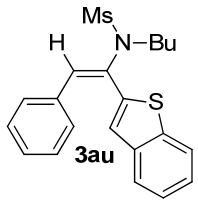
Compound ***3as***. 75 mg, 70% yield, colorless oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.97 (t, J = 7.3 Hz, 3 H), 1.39–1.44 (m, 2 H), 1.65–1.71 (m, 2 H), 3.12 (s, 3 H), 3.62 (t, J = 7.6 Hz, 2 H), 6.81 (s, 1 H), 7.01 (d, J = 15.8 Hz, 1 H), 7.20 (d, J = 15.8 Hz, 1 H), 7.27–7.32 (m, 1 H), 7.34–7.40 (m, 3 H), 7.42–7.48 (m, 6 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.9, 19.9, 31.0, 39.2, 49.8, 122.6, 127.0, 128.0, 128.2, 128.5, 128.6, 129.5, 132.6, 133.2, 135.2, 136.4, 137.2 ; HRMS (APCI) calcd for $C_{21}H_{26}NO_2S$ $(M+H)^+$ 356.1684, found 356.1683.



3at

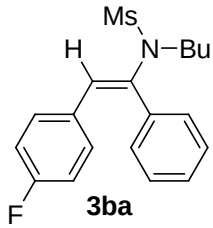
Compound ***3at***. 82 mg, 82% yield, yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.93 (t, J = 7.4 Hz, 3 H), 1.33–1.41 (m, 2 H), 1.60–1.68 (m, 2 H), 3.02 (s, 3 H), 3.43 (t, J = 7.4 Hz, 2 H), 6.85 (s, 1 H), 6.91–6.97 (m, 1 H), 7.03 (dd, J = 3.6, 1.1 Hz, 1 H), 7.16–7.24 (m, 5 H), 7.32 (dd, J = 5.1, 1.1 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 13.7, 19.8, 31.0, 39.9, 48.2, 127.2, 127.3, 127.9, 128.3, 129.2, 129.5, 130.5, 132.4, 135.0, 137.9; MS (EI, m/z): 336 (3),

335 (M^+, 16), 256 (54), 212 (11), 200 (42); HRMS (APCI) calcd for $C_{17}H_{22}NO_2S_2$ $(M+H)^+$ 336.1092, found 336.1088.



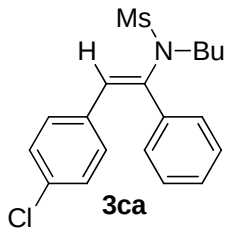
3au

Compound ***3au***. 89 mg, 77% yield, yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 0.94 (t, J = 7.4 Hz, 3 H), 1.35–1.41 (m, 2 H), 1.64–1.71 (m, 2 H), 3.08 (s, 3 H), 3.47 (t, J = 7.4 Hz, 2 H), 6.96 (s, 1 H), 7.21–7.29 (m, 5 H), 7.31–7.35 (m, 3 H), 7.68 (dd, J = 5.9, 3.1 Hz, 1 H), 7.76 (dd, J = 5.9, 3.2 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 13.7, 19.8, 31.1, 40.2, 48.3, 122.3, 124.1, 124.5, 125.1, 126.5, 128.2, 128.4, 129.2, 129.4, 133.6, 134.7, 138.1, 139.2, 140.4; MS (EI, *m*/*z*): 386 (3), 385 (M^+, 19), 306 (50), 250 (27), 234 (40), 223 (100); HRMS (APCI) calcd for $C_{21}H_{24}NO_2S_2$ $(M+H)^+$ 386.1248, found 386.1245.



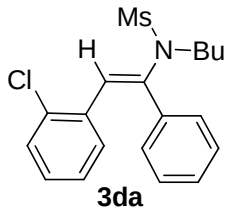
3ba

Compound ***3ba***. 89 mg, 86% yield, white solid, mp: 116–118 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.90 (t, J = 7.4 Hz, 3 H), 1.28–1.36 (m, 2 H), 1.57–1.63 (m, 2 H), 3.04 (s, 3 H), 3.34 (t, J = 7.4 Hz, 2 H), 6.75 (s, 1 H), 6.82 (t, J = 8.7 Hz, 2 H), 6.99 (dd, J = 8.6, 5.5 Hz, 2 H), 7.30–7.34 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.8, 40.7, 47.6, 115.1 (d, J = 21.5 Hz), 127.4, 128.4, 128.6, 128.7, 128.8, 129.8, 131.0 (d, J = 8.0 Hz), 134.9, 161.8 (d, J = 247.9 Hz); ^{19}F NMR ($CDCl_3$, 565 MHz) δ -113.81; MS (EI, *m*/*z*): 348 (5), 347(M^+, 25), 268 (100), 224 (19), 212 (80); HRMS (APCI) calcd for $C_{19}H_{23}FNO_2S$ $(M+H)^+$ 348.1434, found 348.1436.



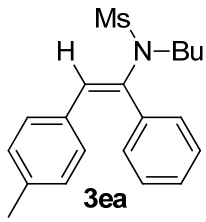
3ca

Compound ***3ca***. 99 mg, 91% yield, white solid, mp: 121–123 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.89 (t, J = 7.4 Hz, 3 H), 1.29–1.35 (m, 2 H), 1.56–1.61 (m, 2 H), 3.04 (s, 3 H), 3.34 (t, J = 7.4 Hz, 2 H), 6.73 (s, 1 H), 6.94 (d, J = 8.5 Hz, 2 H), 7.09 (d, J = 8.5 Hz, 2 H), 7.29–7.36 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.8, 40.7, 47.6, 127.9, 128.2, 128.7, 128.9, 129.7, 130.5, 132.9, 133.8, 134.8, 138.2; MS (EI, *m*/*z*): 365 (6), 363 (M^+, 19), 284 (58), 249 (20), 228 (29); HRMS (APCI) calcd for $C_{19}H_{23}ClNO_2S$ $(M+H)^+$ 364.1138, found 364.1137.



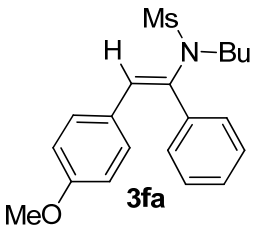
3da

Compound ***3da***. 100 mg, 92% yield, white solid, mp: 131–133 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.92 (t, J = 7.4 Hz, 3 H), 1.34–1.40 (m, 2 H), 1.58–1.62 (m, 2 H), 3.15 (s, 3 H), 3.38 (t, J = 7.3 Hz, 2 H), 6.86 (s, 1 H), 6.88 (dd, J = 7.8, 1.7 Hz, 1 H), 6.88–6.94 (m, 1 H), 7.07–7.12 (m, 1 H), 7.20–7.31 (m, 5 H), 7.35 (dd, J = 8.0, 0.8 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 19.7, 30.6, 40.8, 47.8, 126.3, 126.3, 128.3, 128.6, 128.7, 129.1, 129.8, 131.2, 133.7, 134.4, 134.6, 139.7; MS (EI, *m*/*z*): 365 (9), 363 (M^+, 29), 284 (66), 249 (14), 228 (20); HRMS (APCI) calcd for $C_{19}H_{23}ClNO_2S$ $(M+H)^+$ 364.1138, found 364.1133



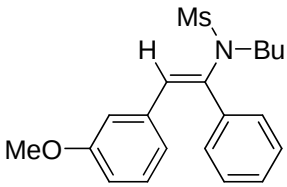
3ea

Compound ***3ea***. 91 mg, 89% yield, white solid, mp: 103–105 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.91 (t, J = 7.3 Hz, 3 H), 1.32–1.36 (m, 2 H), 1.57–1.62 (m, 2 H), 2.26 (s, 3 H), 3.02 (s, 3 H), 3.35 (t, J = 7.5 Hz, 2 H), 6.75 (s, 1 H), 6.92 (d, J = 8.2 Hz, 2 H), 6.95 (d, J = 8.2 Hz, 2 H), 7.28–7.38 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 19.8, 21.1, 30.9, 40.6, 47.8, 128.6, 128.8, 129.2, 129.2, 129.7, 129.9, 132.4, 135.5, 136.7, 137.3; MS (EI, *m*/*z*): 344 (5), 343 (M^+, 24), 265 (23), 264 (100), 220 (19), 207 (11); HRMS (APCI) calcd for $C_{20}H_{26}NO_2S$ $(M+H)^+$ 344.1684, found 344.1688.



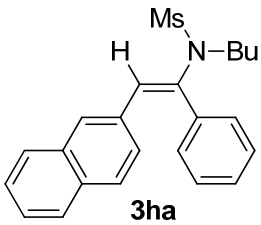
3fa

Compound ***3fa***. 92 mg, 85% yield, white solid, mp: 117–119 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.94 (t, J = 7.4 Hz, 3 H), 1.34–1.39 (m, 2 H), 1.61–1.68 (m, 2 H), 3.04 (s, 3 H), 3.37 (t, J = 7.4 Hz, 2 H), 3.76 (s, 3 H), 6.70 (d, J = 8.7 Hz, 2 H), 6.76 (s, 1 H), 7.00 (d, J = 8.7 Hz, 2 H), 7.28–7.39 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.8, 40.5, 47.7, 55.1, 113.5, 127.6, 128.5, 128.6, 129.5, 129.8, 130.6, 135.5, 135.6, 158.8; MS (EI, *m*/*z*): 360 (2), 359 (M^+, 11), 280 (68), 236 (8), 224 (12), 207 (29); HRMS (APCI) calcd for $C_{20}H_{26}NO_3S$ $(M+H)^+$ 360.1633, found 360.1620.



3ga

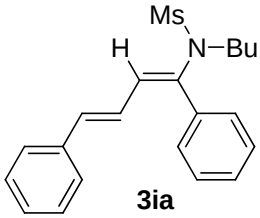
Compound ***3ga***. 94 mg, 87% yield, white solid, mp: 126–128 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.92 (t, J = 7.4 Hz, 3 H), 1.31–1.38 (m, 2 H), 1.58–1.64 (m, 2 H), 3.04 (s, 3 H), 3.37 (t, J = 7.4 Hz, 2 H), 3.53 (s, 3 H), 6.53 (s, 1 H), 6.63–6.67 (m, 1 H), 6.67–6.71 (m, 1 H), 6.78 (s, 1 H), 7.06 (t, J = 7.9 Hz, 1 H), 7.29–7.40 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.8, 40.6, 47.7, 54.8, 113.8, 113.8, 122.0, 128.6, 128.7, 129.0, 129.3, 129.8, 135.3, 136.5, 137.7, 159.0; MS (EI, *m*/*z*): 360 (3), 359 (M^+, 22), 283 (58), 204 (65), 162 (100); HRMS (APCI) calcd for $C_{20}H_{26}NO_3S$ $(M+H)^+$ 360.1633, found 360.1626.



3ha

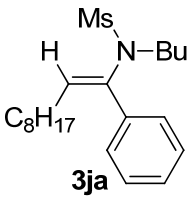
Compound ***3ha***.102 mg, 90% yield, white solid, mp: 117–119 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.93 (t, J = 7.4 Hz, 3 H), 1.35–1.38 (m, 2 H), 1.62–1.67 (m, 2 H), 3.09 (s, 3 H), 3.40 (t, J = 7.5 Hz, 2 H), 6.96 (s, 1 H), 7.08 (dd, J = 8.6, 1.6 Hz, 1 H), 7.29–7.33 (m, 3 H), 7.39–7.42 (m, 4 H), 7.54 (d, J = 8.6 Hz, 1 H), 7.59 (s, 1 H), 7.64–7.65 (m, 1 H), 7.71–7.72

(m, 1 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 19.8, 30.9, 40.8, 47.9, 126.1, 126.1, 126.8, 127.4, 127.4, 127.8, 128.6, 128.8, 128.9, 129.3, 129.9, 132.4, 132.9, 133.1, 135.2, 137.9; MS (EI, *m*/*z*): 380 (9), 379 (M^+, 35), 301 (27), 300 (100), 281 (11); HRMS (APCI) calcd for $C_{23}H_{26}NO_2S$ $(M+H)^+$ 380.1684, found 380.1678.



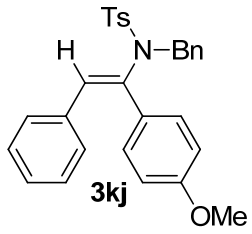
3ia

Compound ***3ia***. 81 mg, 76% yield, white solid, mp: 123–125 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.91 (t, J = 7.4 Hz, 3 H), 1.31–1.35 (m, 2 H), 1.56–1.59 (m, 2 H), 3.07 (s, 3 H), 3.38–3.41 (m, 2 H), 6.65 (d, J = 11.1 Hz, 1 H), 6.75 (d, J = 15.6 Hz, 1 H), 6.92 (dd, J = 15.6, 11.1 Hz, 1 H), 7.18–7.23 (m, 1 H), 7.26–7.33 (m, 4 H), 7.39–7.48 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.7, 30.9, 40.3, 48.3, 124.8, 126.5, 127.8, 128.5, 128.5, 128.7, 128.8, 129.6, 135.0, 135.5, 136.9, 138.1; MS (EI, *m*/*z*): 356 (3), 355 (M^+, 16), 232 (33), 217 (30), 207 (29); HRMS (APCI) calcd for $C_{21}H_{26}NO_2S$ $(M+H)^+$ 356.1684, found 356.1682.



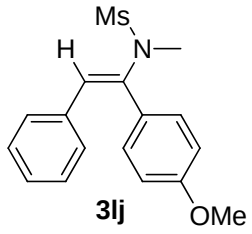
3ja

Compound ***3ja***. 96 mg, 88% yield, colorless oil; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.85–0.91 (m, 8 H), 1.21–1.32 (m, 10 H), 1.39–1.42 (m, 2 H), 1.52–1.56 (m, 2 H), 2.13–2.16 (m, 2 H), 2.92 (s, 3 H), 3.29 (t, J = 7.4 Hz, 2 H), 5.83 (t, J = 7.7 Hz, 1 H), 7.31–7.38 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.7, 14.0, 19.7, 22.6, 28.6, 29.1, 29.1, 29.3, 29.6, 30.6, 31.8, 40.1, 48.0, 126.5, 128.1, 128.2, 129.2, 132.5, 135.7; MS (EI, *m*/*z*): 366 (2), 365 (M^+, 4), 350 (47), 286 (39), 210 (33), 186 (44); HRMS (APCI) calcd for $C_{21}H_{36}NO_2S$ $(M+H)^+$ 366.2467, found 366.2468.



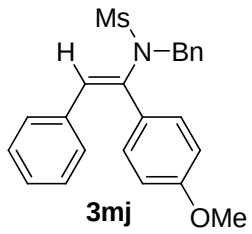
3kj

Compound ***3kj***. 112 mg, 80% yield, white solid, mp: 149–151 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 2.50 (s, 3 H), 3.79 (s, 3 H), 4.57 (s, 2 H), 6.52 (s, 1 H), 6.69 (d, J = 8.7 Hz, 2 H), 6.80 (s, 2 H), 6.84 (d, J = 8.7 Hz, 2 H), 6.86–6.92 (m, 2 H), 7.09–7.12 (m, 2 H), 7.20–7.24 (m, 2 H), 7.29–7.33 (m, 2 H), 7.36 (d, J = 8.1 Hz, 2 H), 7.84 (d, J = 8.2 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 21.5, 52.1, 55.1, 113.6, 114.7, 116.0, 126.9, 127.5, 127.7, 127.9, 128.3, 128.9, 129.1, 129.5, 131.2, 135.8, 136.5, 136.9, 143.5, 149.7, 159.5; MS (EI, *m*/*z*): 470 (2), 469 (M^+, 10), 350 (46), 281 (10), 209 (100); HRMS (APCI) calcd for $C_{29}H_{28}NO_3S$ $(M+H)^+$ 470.1790, found 470.1787.



3lj

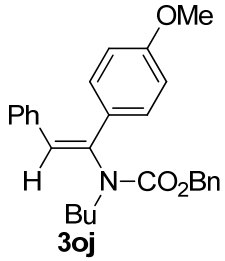
Compound ***3lj***. 77 mg, 81% yield, white solid, mp: 111–113 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 3.01 (s, 3 H), 3.13 (s, 3 H), 3.83 (s, 3 H), 6.69 (s, 1 H), 6.86 (d, J = 8.6 Hz, 2 H), 7.07 (d, J = 7.0 Hz, 2 H), 7.14–7.18 (m, 3 H), 7.31 (d, J = 8.6 Hz, 2 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 37.0, 39.0, 55.1, 113.9, 126.3, 127.1, 127.4, 128.0, 129.0, 131.1, 135.5, 139.8, 159.8; MS (EI, *m*/*z*): 318 (4), 317 (M^+, 27), 238 (38), 223 (13), 197 (100); HRMS (APCI) calcd for $C_{17}H_{20}NO_3S$ $(M+H)^+$ 318.1164, found 318.1162.



3mj

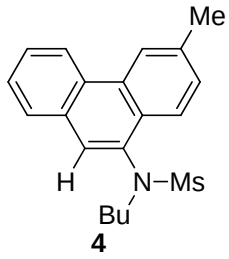
Compound ***3mj***. 90 mg, 76% yield, white solid, mp: 131–133 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 3.00 (s, 3 H), 3.81 (s, 3 H), 4.54 (s, 2 H), 6.53 (s, 1 H), 6.82 (d, J = 8.5 Hz, 2 H), 6.99 (d, J = 6.0 Hz, 2 H), 7.10–7.14 (m, 3 H), 7.23 (d, J = 8.4 Hz, 2 H), 7.33–7.38 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 41.6, 51.9, 55.1, 113.9, 127.1, 127.8, 128.0, 128.5,

128.7, 128.9, 129.0, 129.1, 131.4, 135.5, 136.4, 137.6, 159.8; MS (EI, *m*/*z*): 394 (3), 393 (M^+, 15), 314 (39), 223 (32), 209 (36), 197 (100); HRMS (APCI) calcd for $C_{23}H_{24}NO_3S$ $(M+H)^+$ 394.1477, found 394.1473.



3oj

Compound ***3oj***. 85 mg, 68% yield, yellow oil, *E*/*Z* = 83:17 (determined by GC or crude NMR); Data of (*E*)-isomer: ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.94 (t, J = 7.4 Hz, 3 H), 1.32–1.39 (m, 2 H), 1.62–1.68 (m, 2 H), 3.44 (t, J = 7.4 Hz, 2 H), 3.83 (s, 3 H), 5.16 (s, 2 H), 6.54 (s, 1 H), 6.77 (d, J = 8.5 Hz, 2 H), 7.12 (d, J = 7.5 Hz, 2 H), 7.16–7.21 (m, 5 H), 7.23–7.32 (m, 5 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.9, 20.0, 30.5, 48.2, 55.2, 67.1, 113.7, 126.8, 126.9, 127.5, 127.7, 128.1, 128.2, 128.4, 129.1, 130.6, 136.2, 136.7, 138.8, 155.9, 159.5; MS (EI, *m*/*z*): 416 (1), 415 (M^+, 5), 324 (43), 280 (18), 125 (16); HRMS (APCI) calcd for $C_{27}H_{30}NO_3$ $(M+H)^+$ 416.2226, found 416.2224.

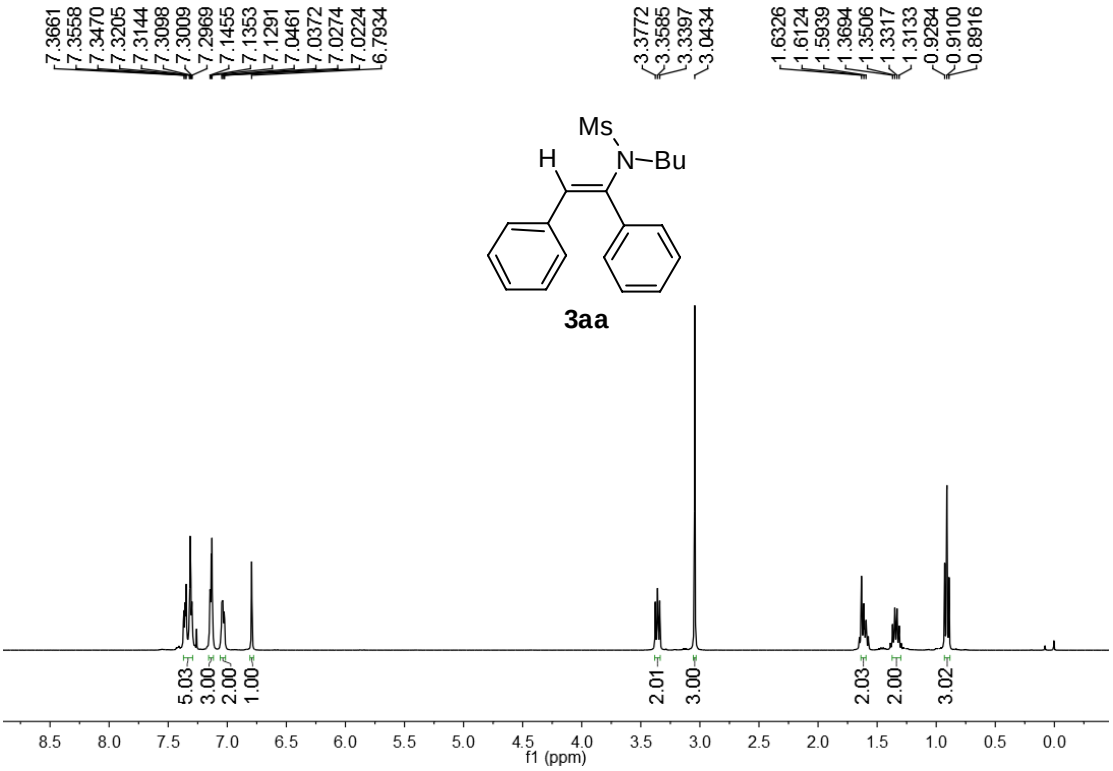


4

Compound ***4***. The title compound was prepared from **3ag** according to the method described in the literature[1] in 70% yield (72 mg) as a white solid, mp 109−111 °C; ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.85 (t, J = 7.4 Hz, 3 H), 1.30–1.37 (m, 2 H), 1.52–1.64 (m, 2 H), 2.64 (s, 3 H), 3.06 (s, 3 H), 3.73–3.84 (m, 2 H), 7.54 (d, J = 8.3 Hz, 1 H), 7.59–7.62 (m, 1 H), 7.66–7.72 (m, 1 H), 7.75 (s, 1 H), 7.89 (d, J = 7.8 Hz, 1 H), 8.20 (d, J = 8.3 Hz, 1 H), 8.52 (s, 1 H), 8.70 (d, J = 8.3 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 13.6, 19.9, 21.9, 31.0, 38.2, 51.8, 122.6, 122.7, 124.4, 126.5, 126.9, 127.4, 128.7, 128.9, 128.9, 130.4,

[1] (a) G. H. Hakimelahi, C. B. Boyce and H. S. Kasmai, *Helv. Chim. Acta*, 1977, **60**, 342. (b) Z. Lu, W. Cui, S. Xia, Y. Bai, F. Luo and G. Zhu, *J. Org. Chem.*, 2012, **77**, 9871.

131.3, 131.7, 134.7, 137.2; MS (EI, *m*/*z*): 342 (6), 341 (M^+, 30), 263 (19), 262 (100), 220 (60); HRMS (APCI) calcd for $C_{20}H_{24}NO_2S$ $(M+H)^+$ 342.1528, found 342.1532.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7.0461
7.0372
7.0274
7.0224
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3.3772
3.3585
3.3397
3.0434
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1.6124
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1.3694
1.3506
1.3317
1.3133
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0.9100
0.8916
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H
N–Bu
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1.00
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3.00
2.03
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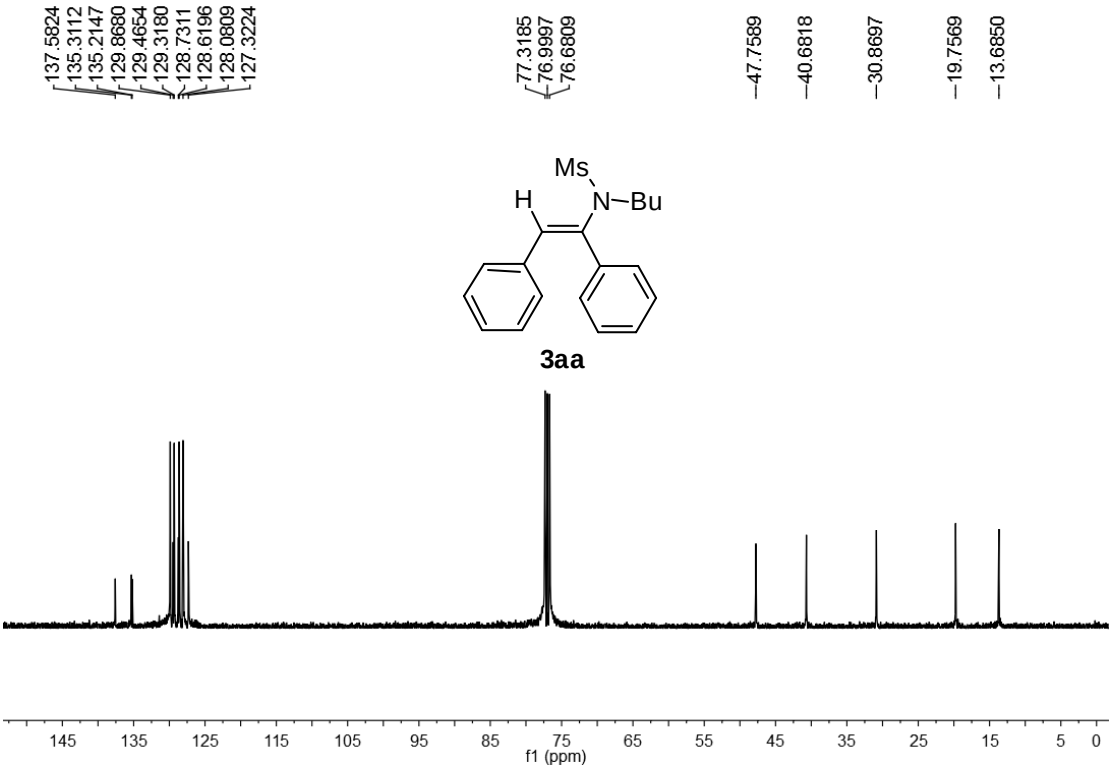
f1 (ppm)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76.9997
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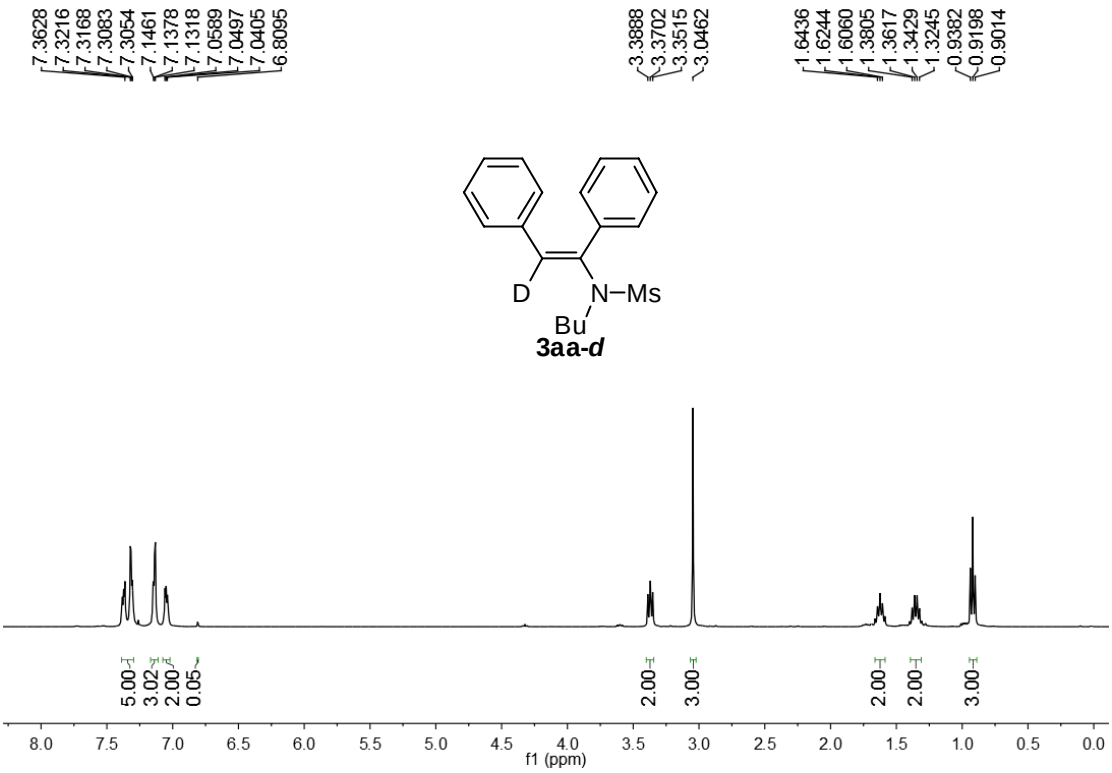
Ms
H
N–Bu
3aa
f1 (ppm)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3.3515
3.0462
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1.3429
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N−Ms
Bu
3aa-d
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3.02
2.00
0.05
2.00
3.00
2.00
2.00
3.00
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7.0
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6.0
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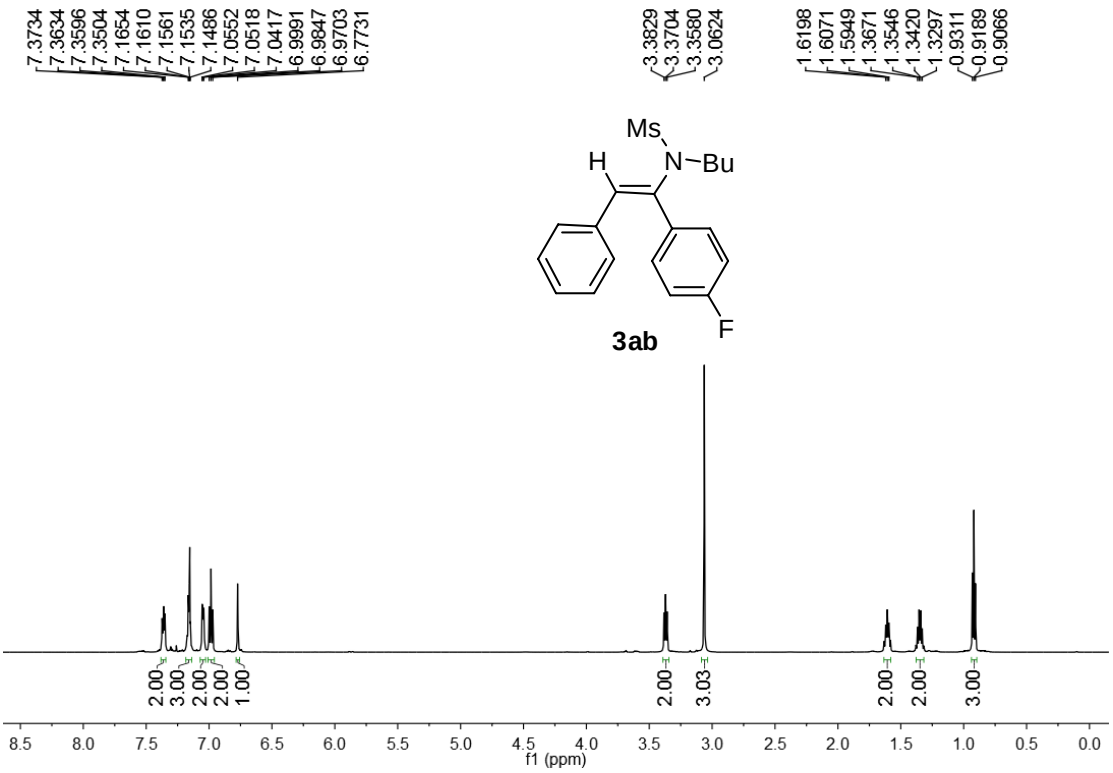
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N−Bu
F
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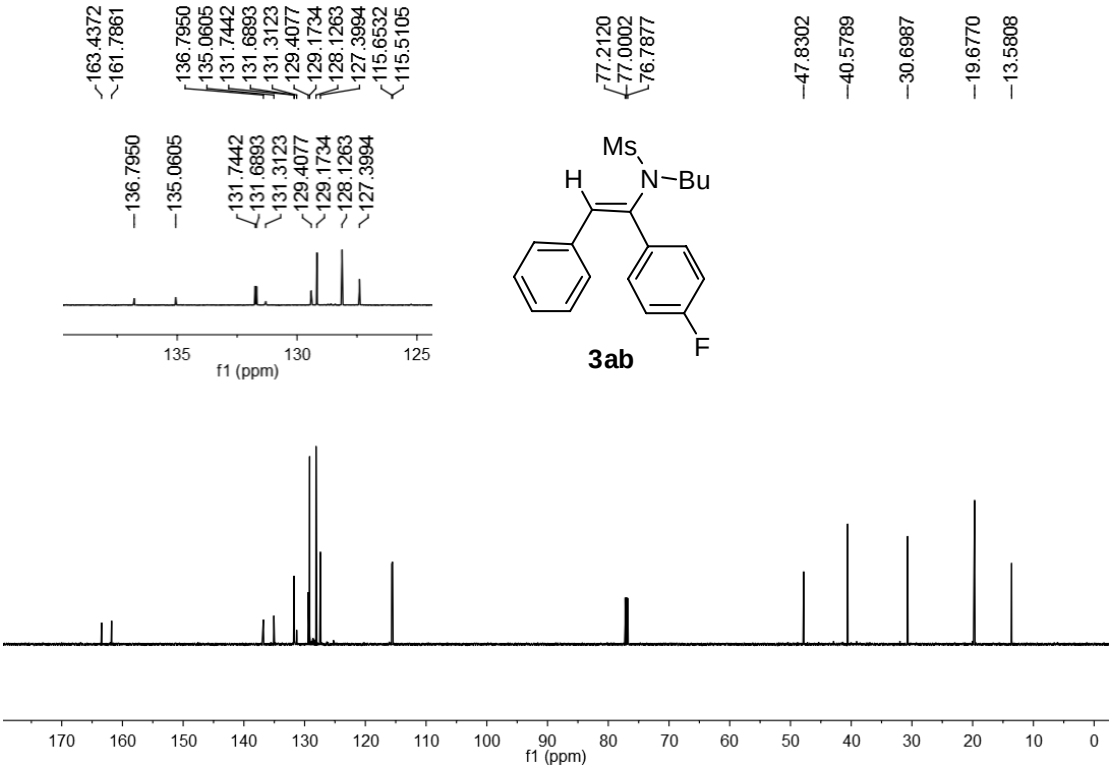
f1 (ppm)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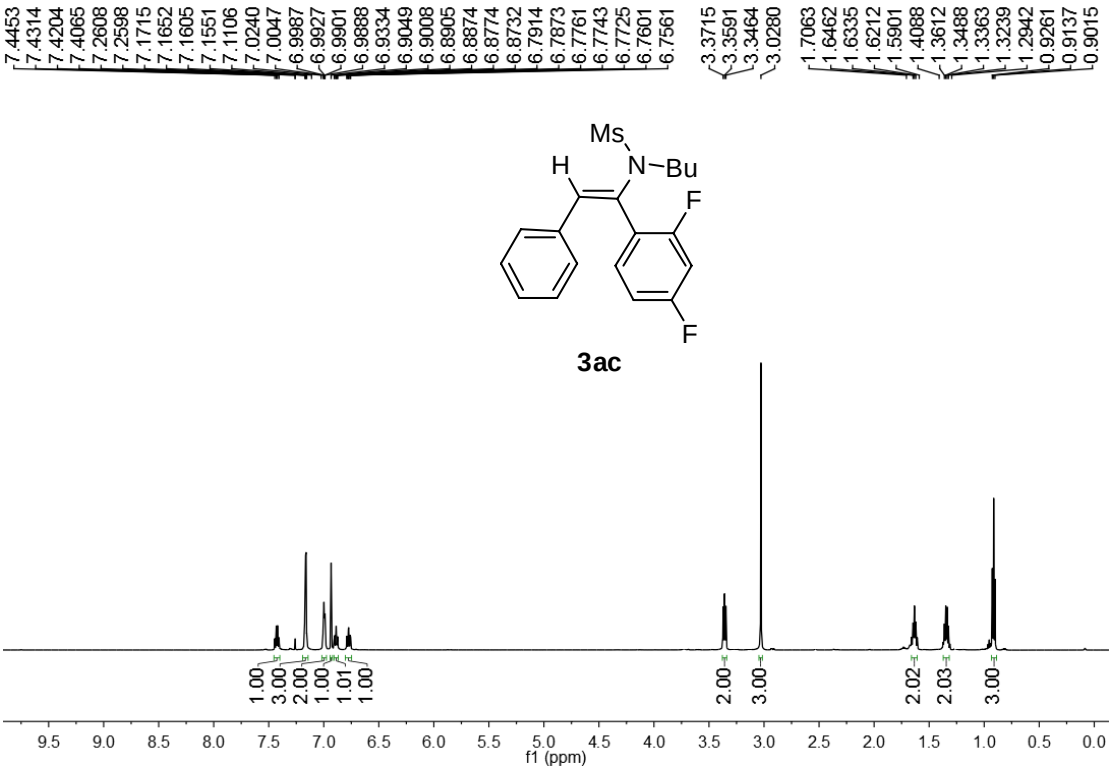
H
N−Bu
F
3ab
f1 (ppm)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N–Bu
F
F
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2.00
1.00
1.01
1.00
2.00
3.00
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2.03
3.00
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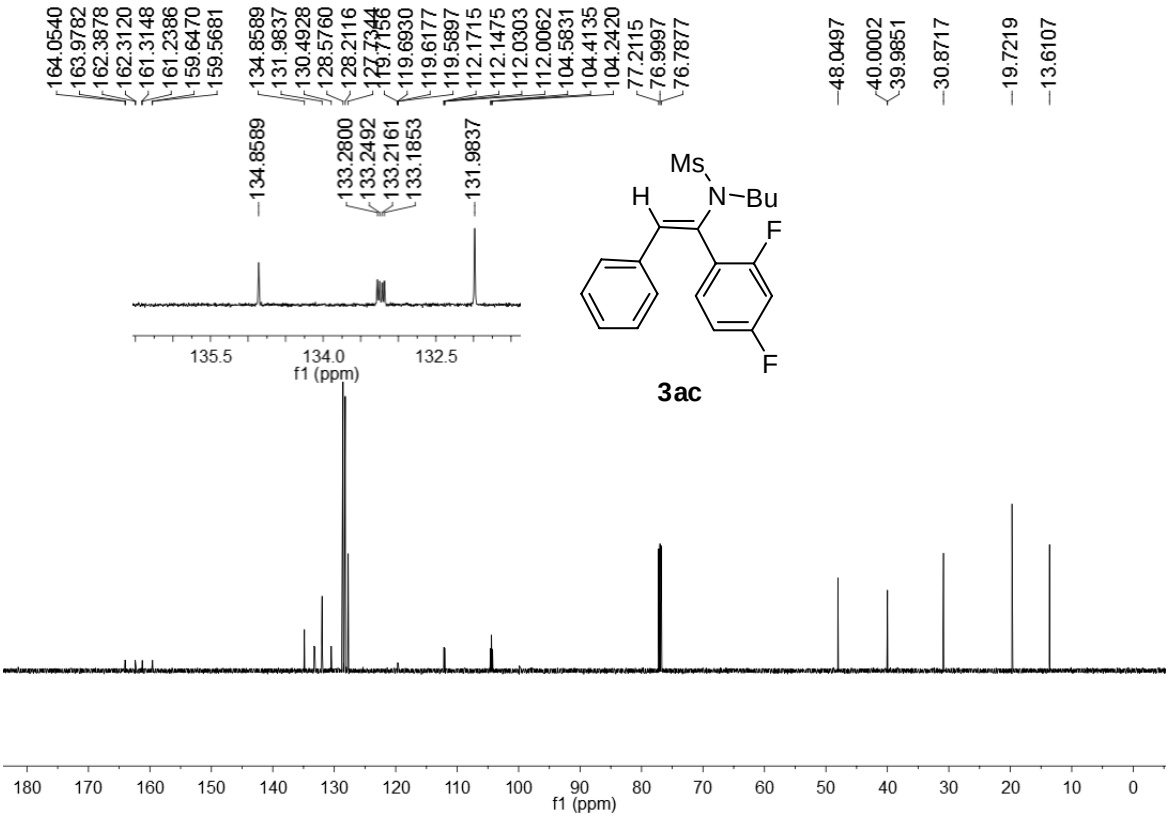
f1 (ppm)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119.6177
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112.0062
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104.2420
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N–Bu
F
F
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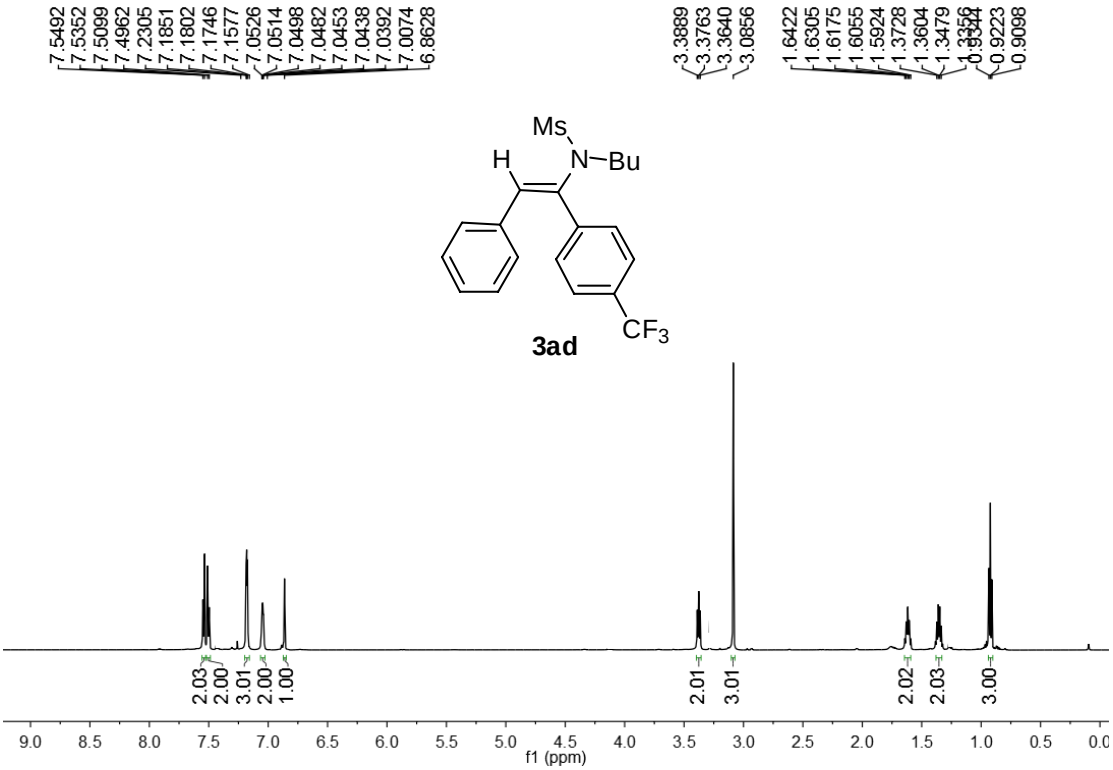
f1 (ppm)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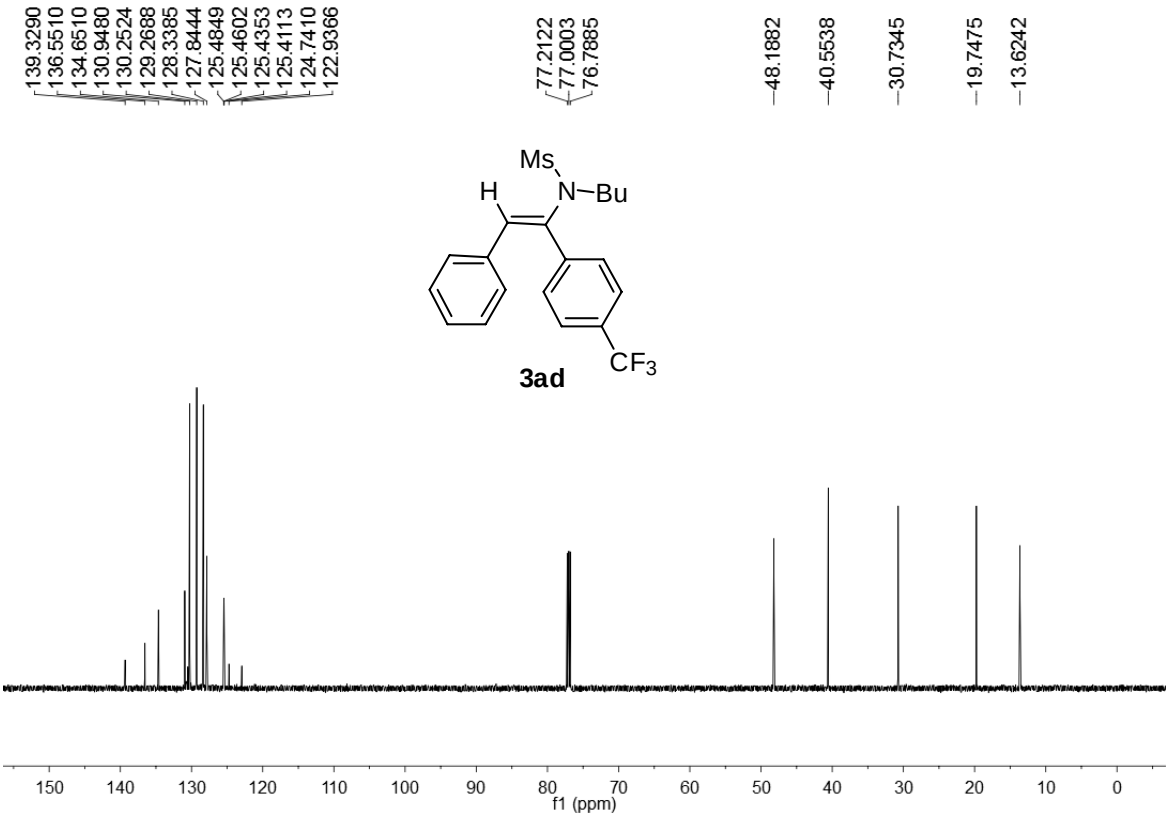
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N–Bu
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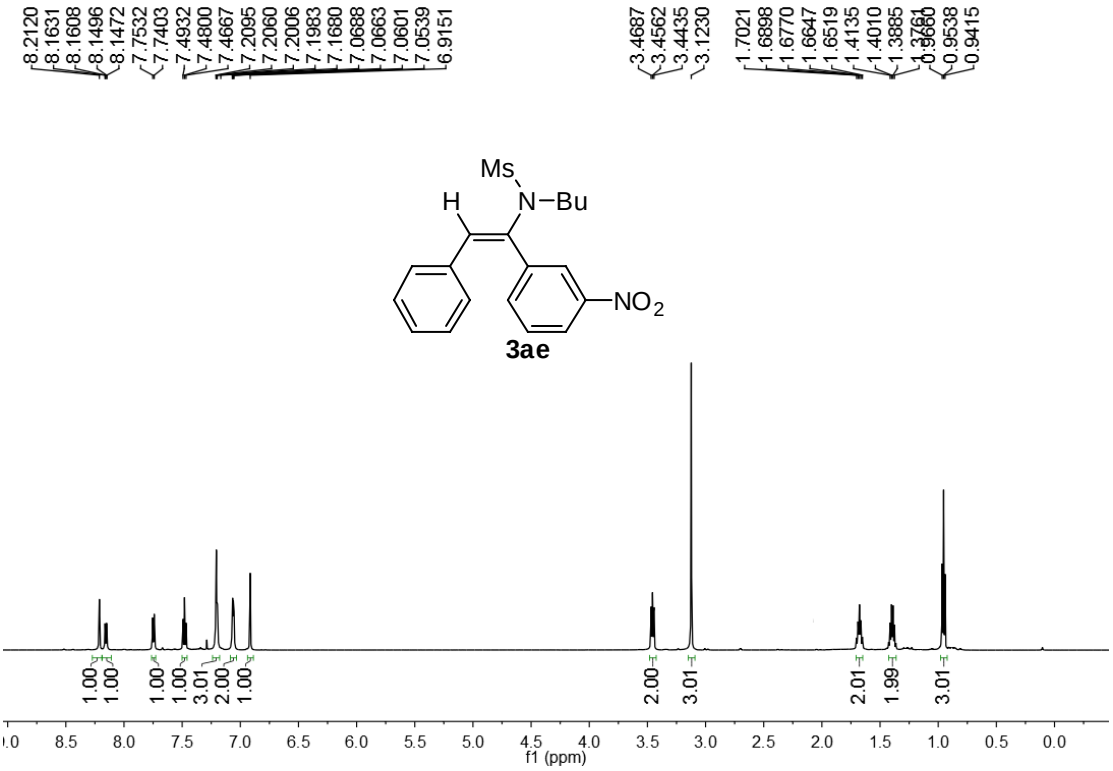
3ad
f1 (ppm)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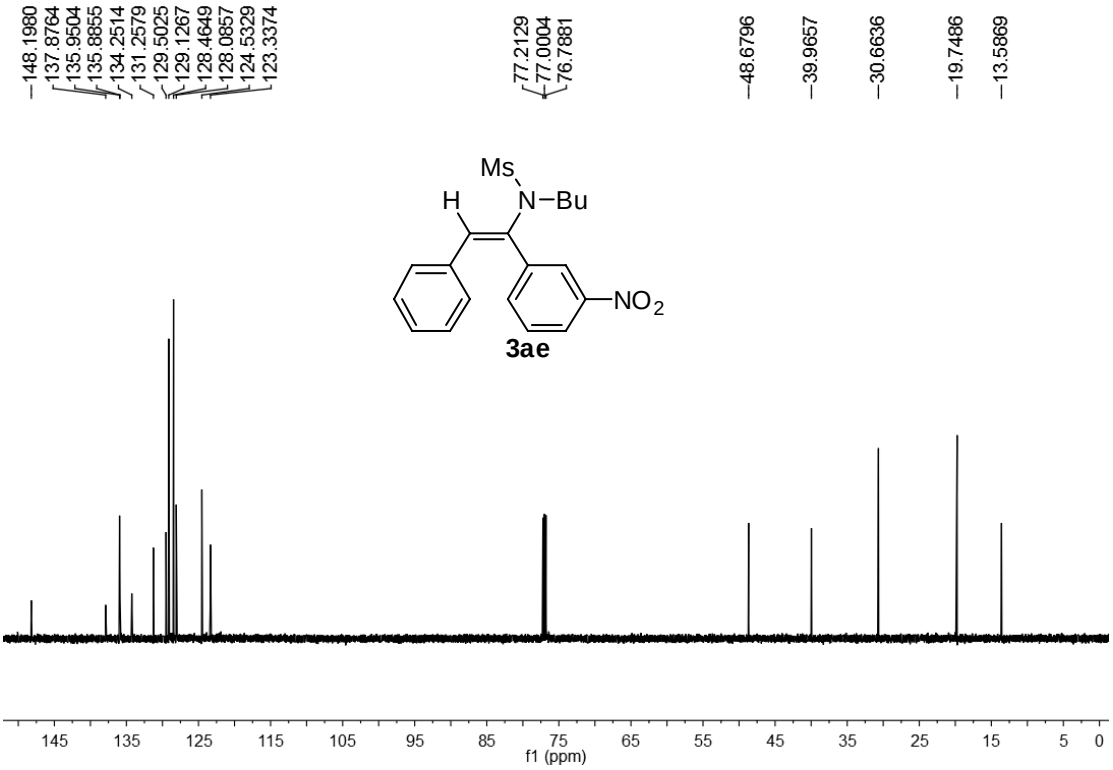
f1 (ppm)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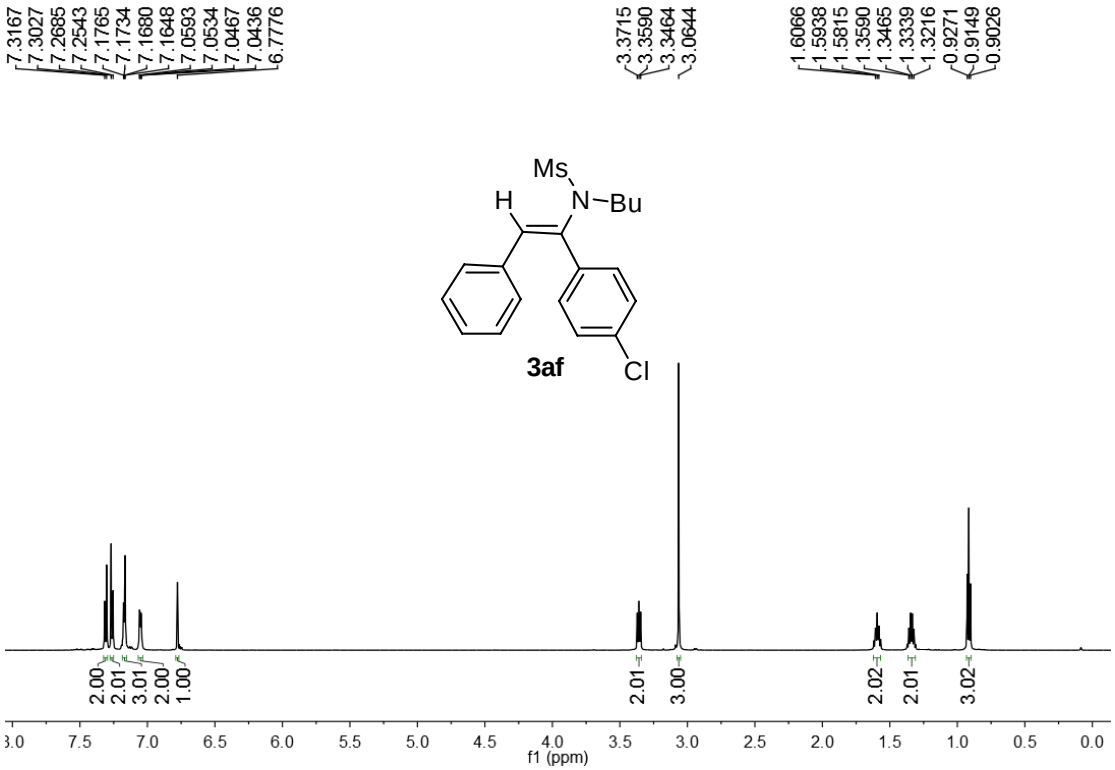
f1 (ppm)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0.9026
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N–Bu
3af
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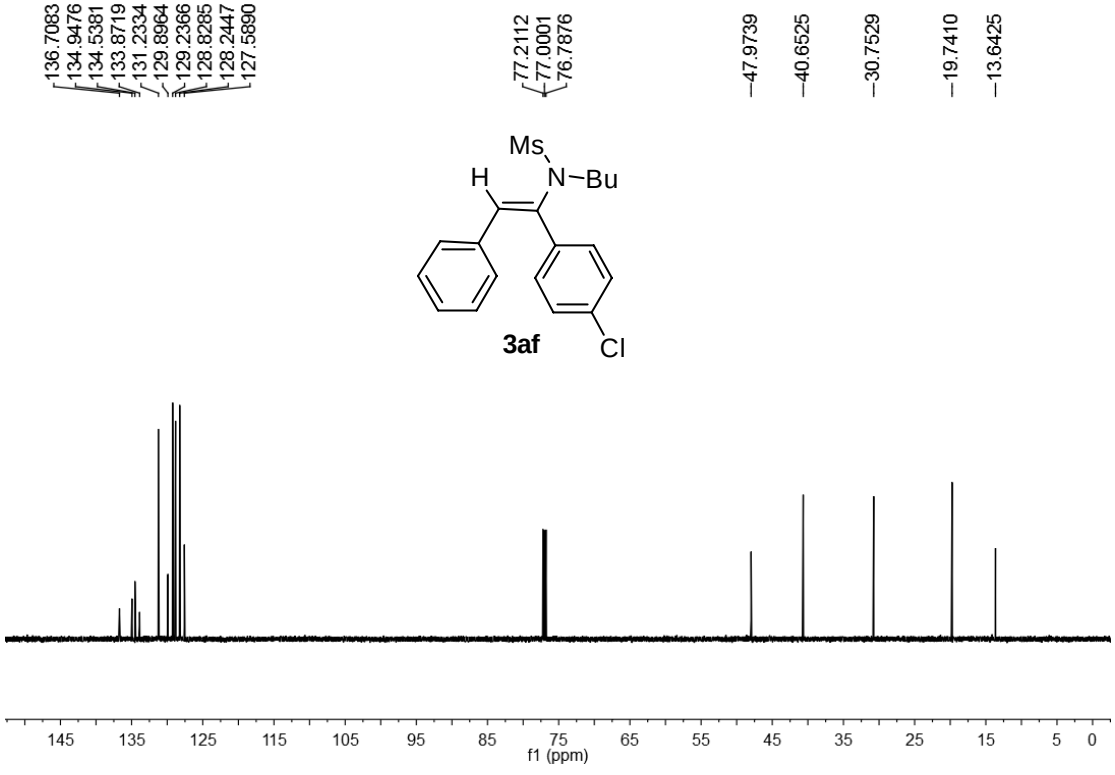
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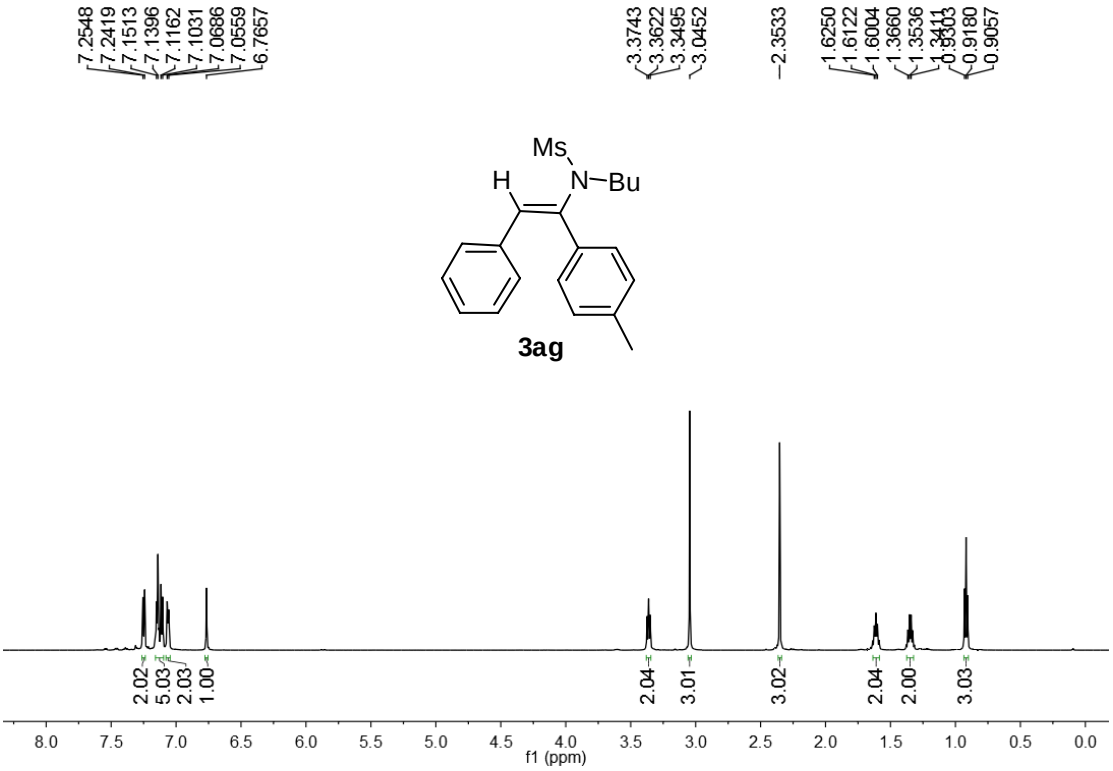
N–Bu
3af
Cl
f1 (ppm)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N–Bu
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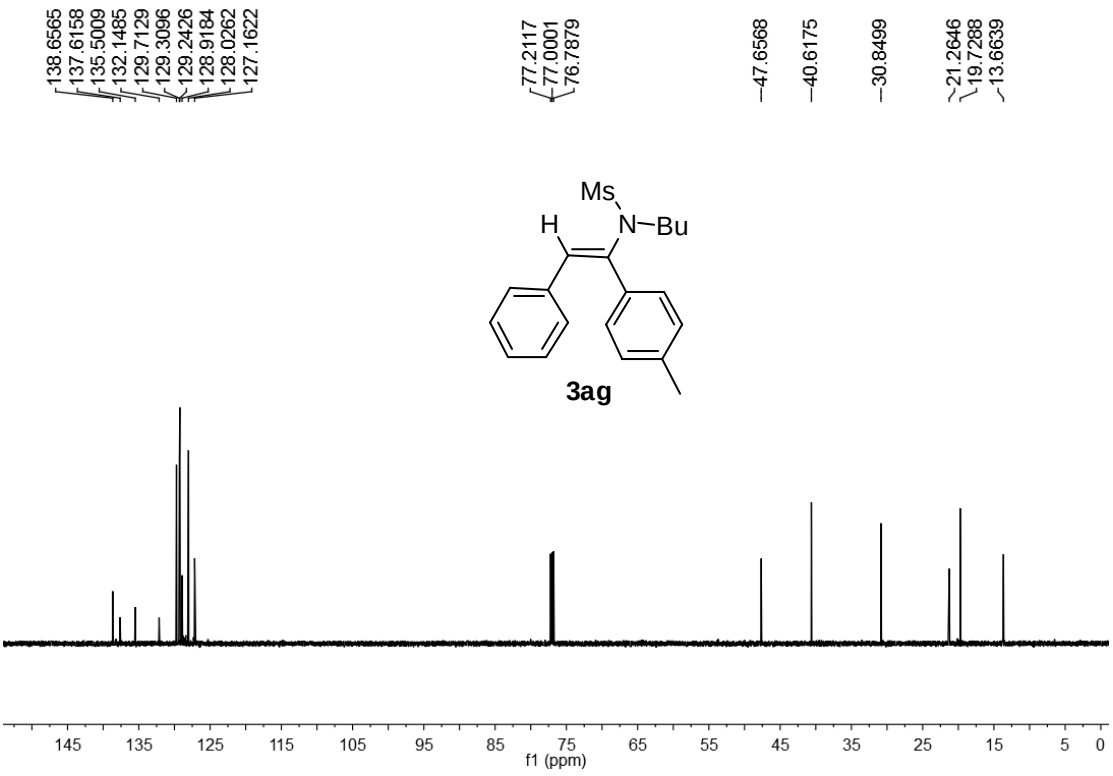
3.03
f1 (ppm)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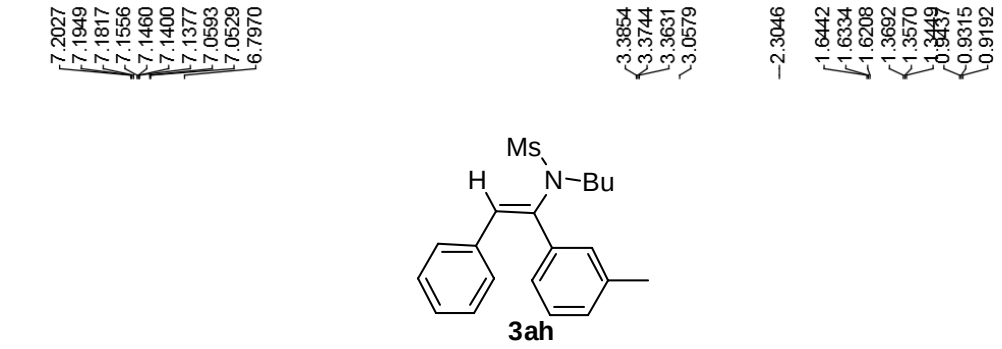
H
N–Bu
3ag
f1 (ppm)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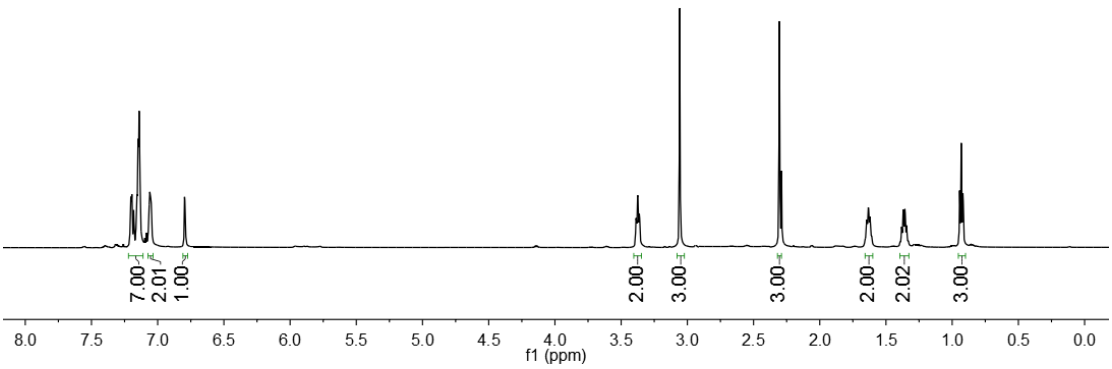
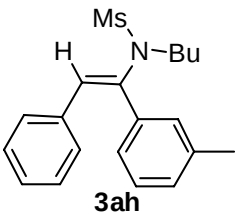
Ms
H
N–Bu

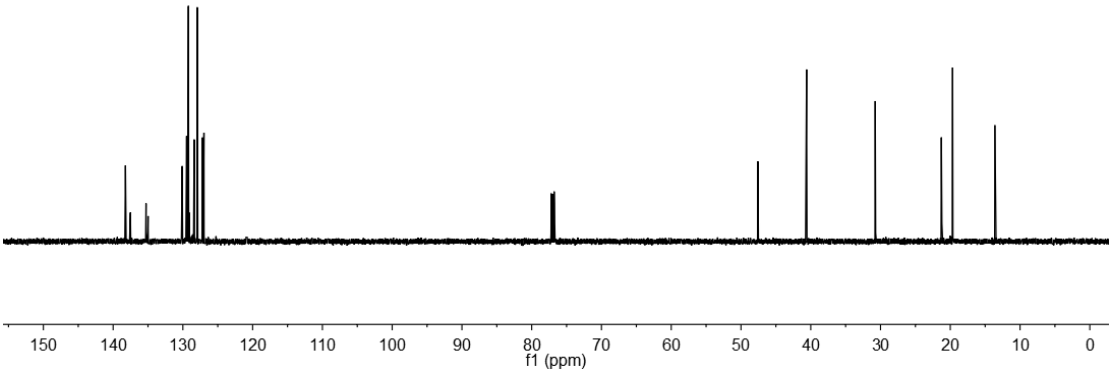
3ah


7.00
2.01
1.00
2.00
3.00
3.00
2.00
2.02
3.00
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)


138.2315
137.5253
135.2825
134.9887
130.0982
129.4622
129.2688
129.2081
128.3818
127.9447
127.1978
126.9784
77.2092
76.9997
76.7860
47.5846
40.5958
30.7578
21.2765
19.6657
13.6016


Ms
H
N–Bu

3ah


150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.3987
7.3956
7.3094
7.2750
7.2722
7.2638
7.2600
7.2519
7.1380
7.1354
7.1240
7.1111
7.1060
7.1004
6.9086
6.9048
6.9012
6.8989
6.8927
6.8054
3.4911
3.3561
3.2451
2.9852
2.0490
1.7032
1.6903
1.6775
1.3414
1.3290
1.3166
1.3045
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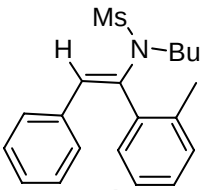
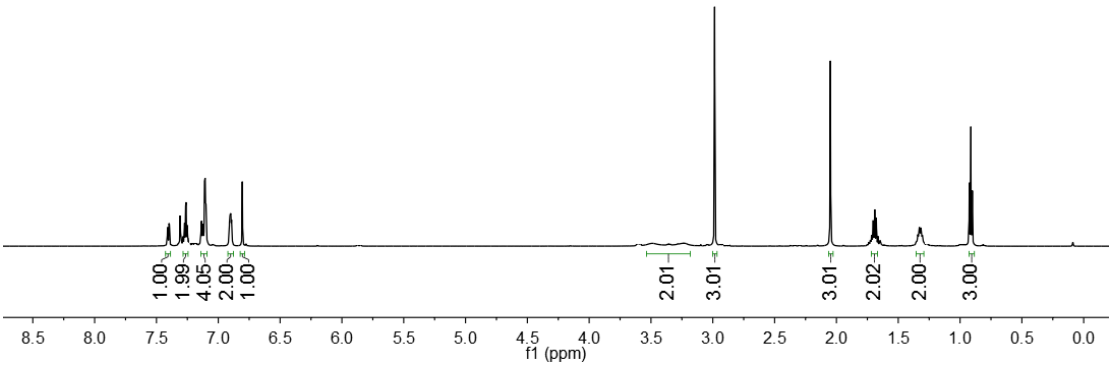
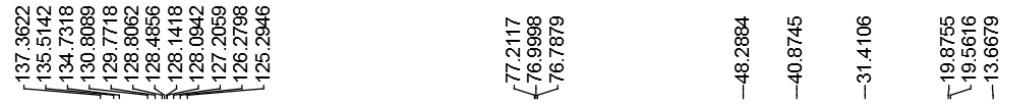
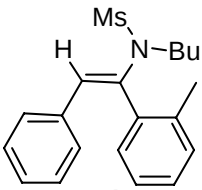
0.9130
0.9007


Ms
H
N–Bu

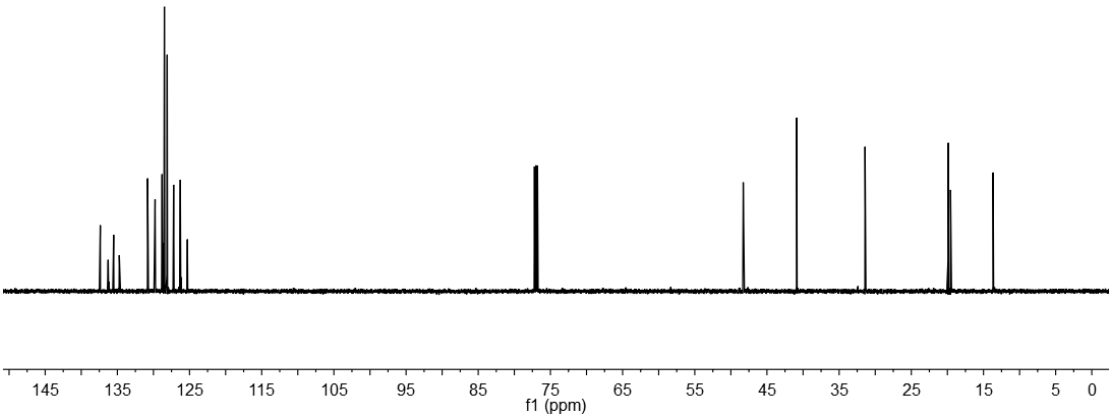
3ai

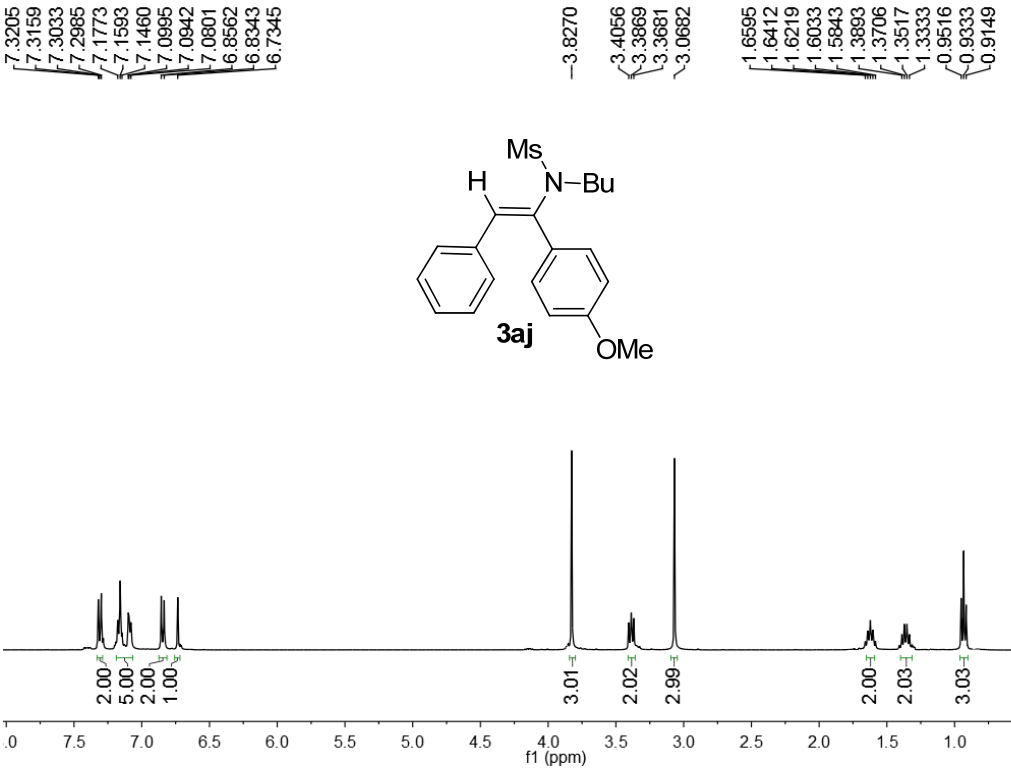

1.00
1.99
4.05
2.00
1.00
2.01
3.01
3.01
2.02
2.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

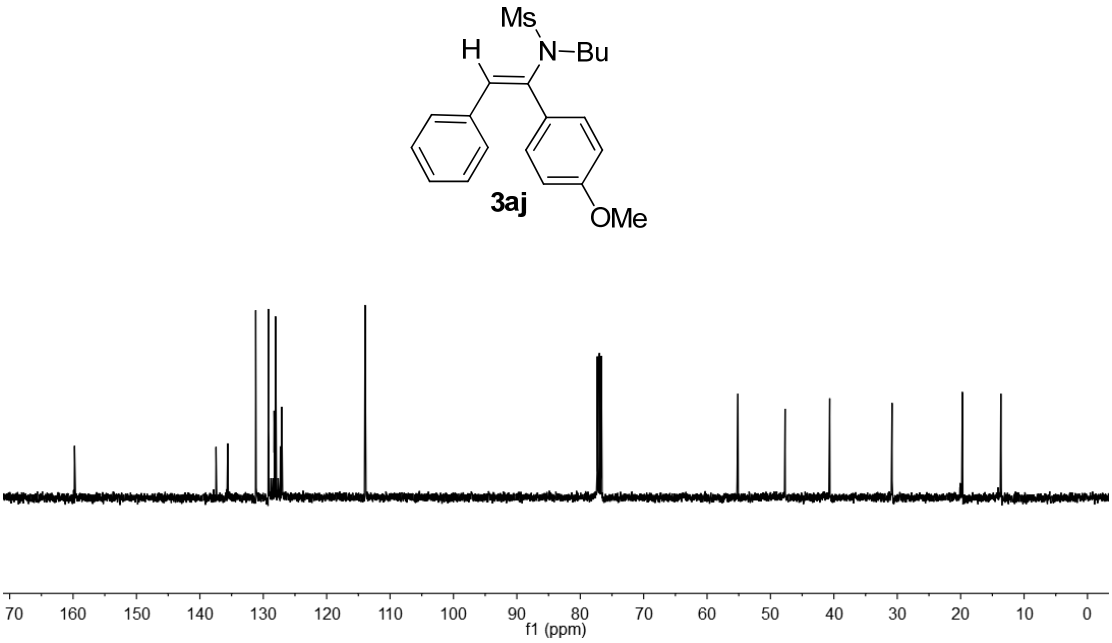

137.3622
135.5142
134.7318
130.8089
129.7718
128.8062
128.4856
128.1418
128.0942
127.2059
126.2798
125.2946
77.2117
76.9998
76.7879
48.2884
40.8745
31.4106
19.8755
19.5616
13.6679

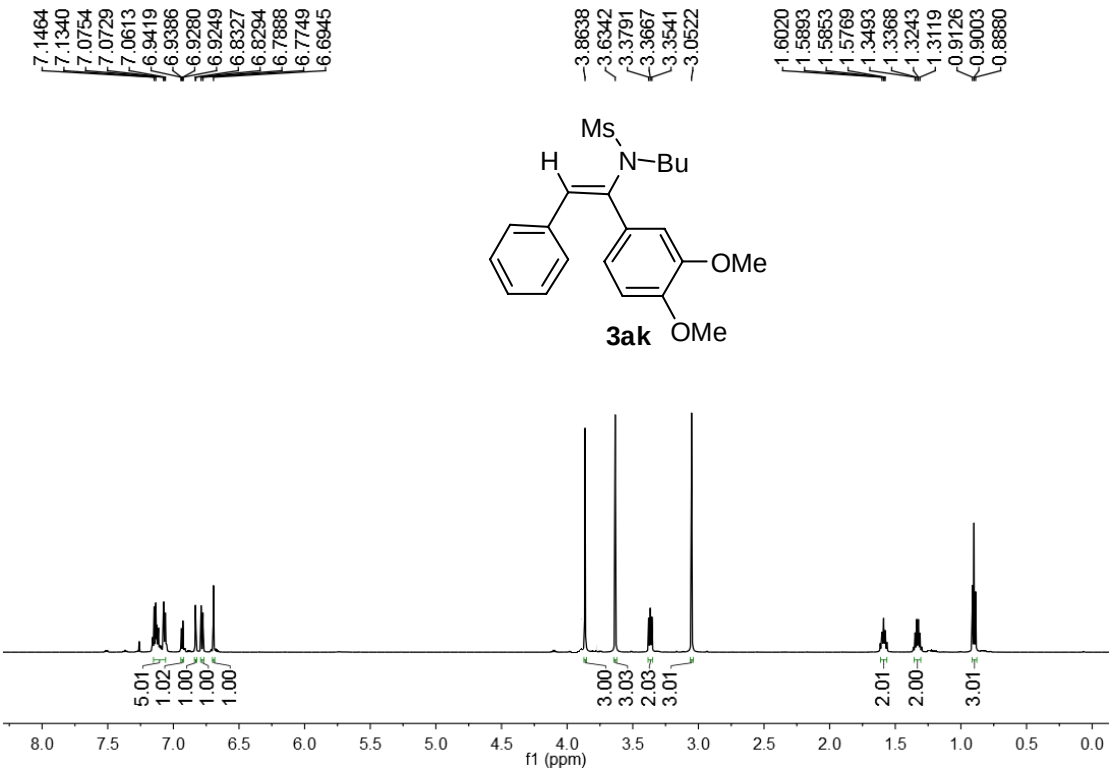

Ms
H
N–Bu

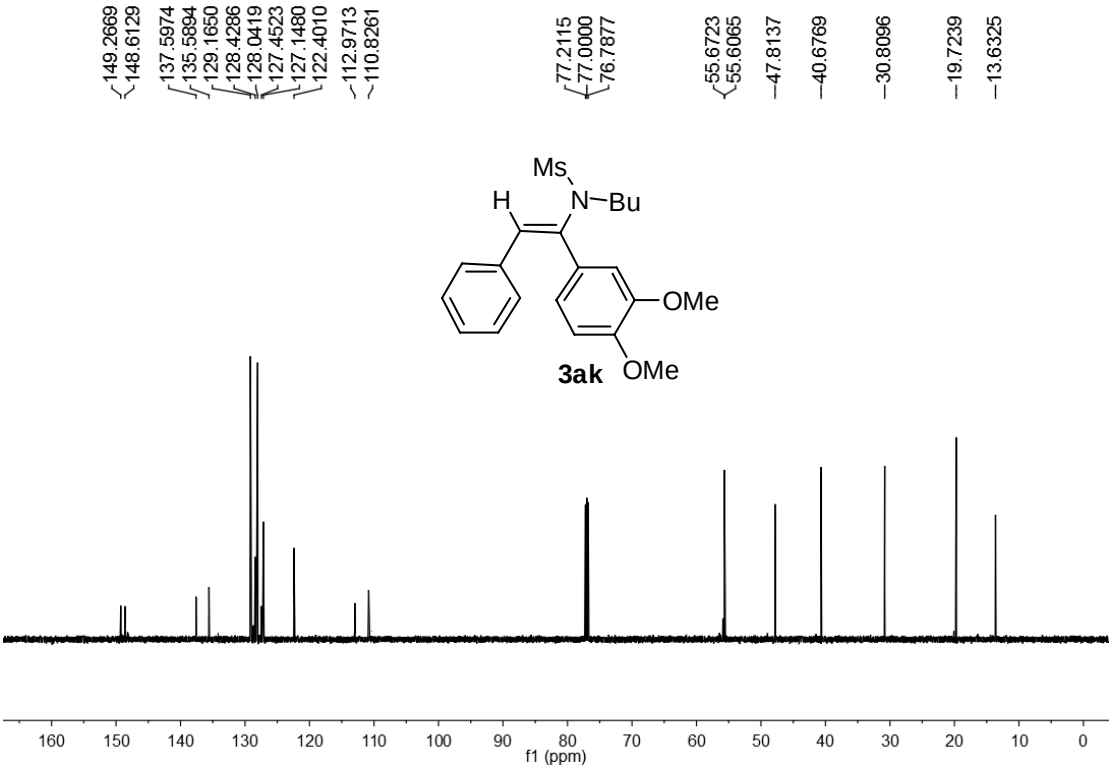
3ai

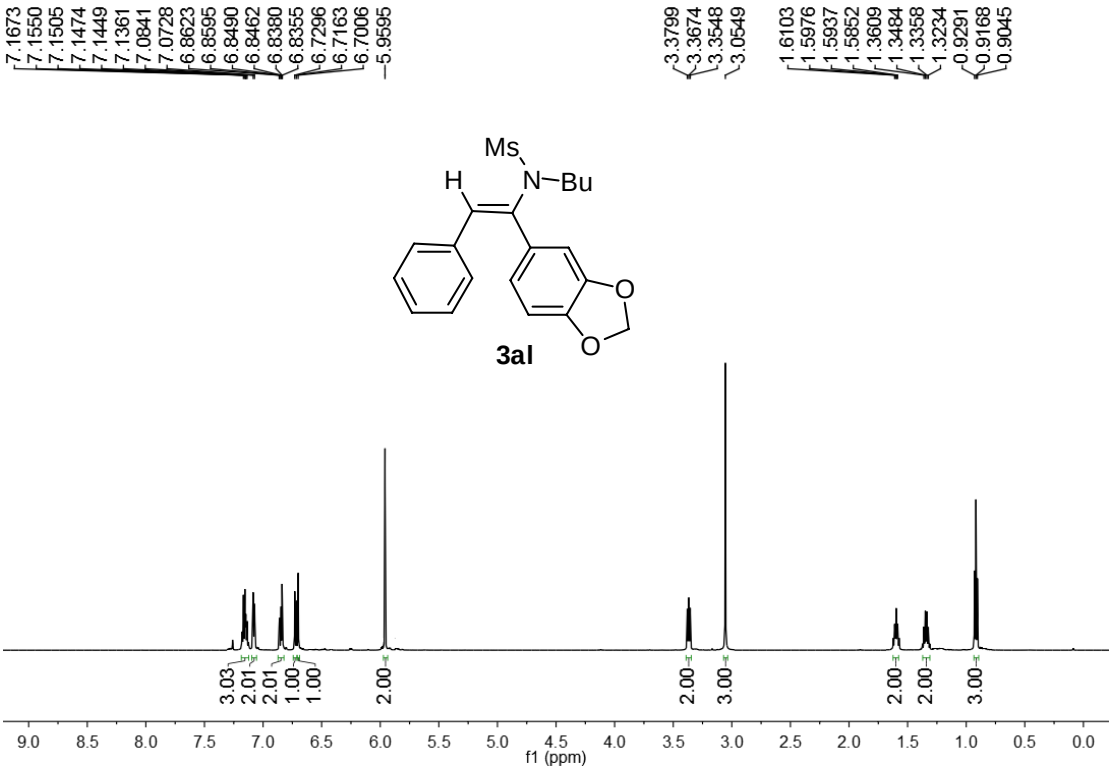

145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)


7.3205
7.3159
7.3033
7.2985
7.1773
7.1593
7.1460
7.0995
7.0942
7.0801
6.8562
6.8343
6.7345
3.8270
3.4056
3.3869
3.3681
3.0682
1.6595
1.6412
1.6219
1.6033
1.5843
1.3893
1.3706
1.3517
1.3333
0.9516
0.9333
0.9149
Ms
H
N–Bu
3aj
OMe
2.00
5.00
2.00
1.00
3.01
2.02
2.99
2.00
2.03
3.03
f1 (ppm)

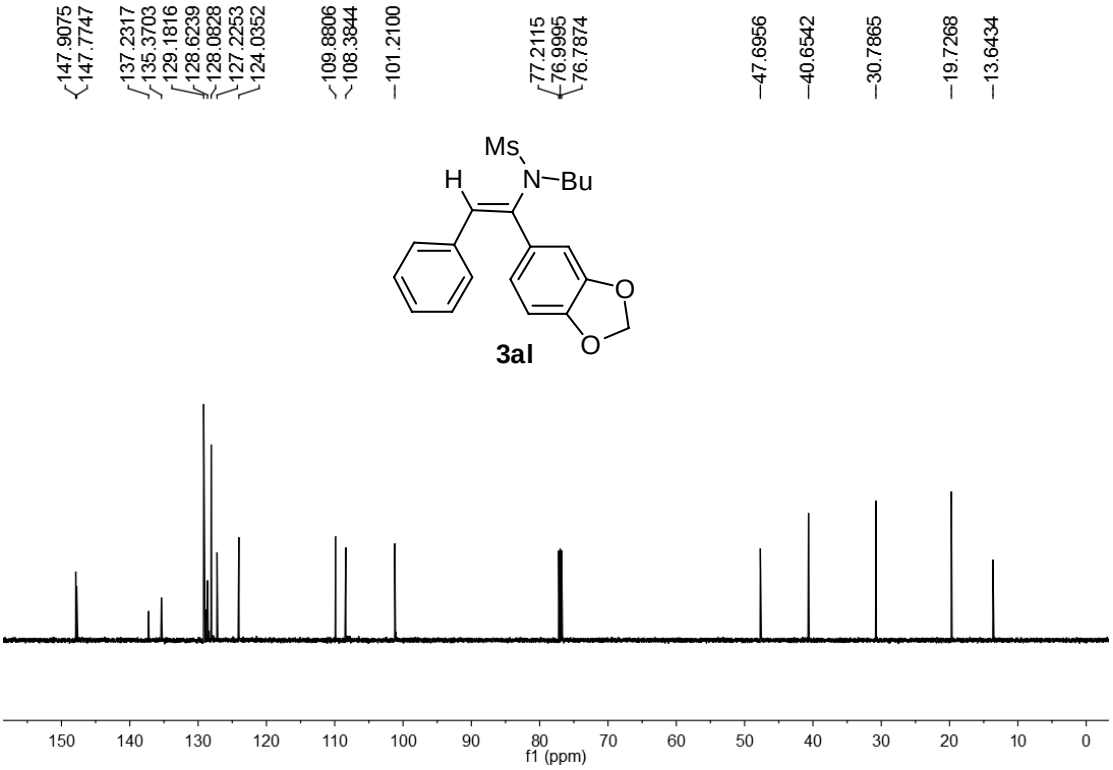

159.7699
137.4529
135.6017
131.1884
129.1957
128.2883
128.0554
127.2961
127.0944
113.9388
77.3182
77.0000
76.6822
55.1318
47.6965
40.6545
30.8302
19.7340
13.6631
Ms
H
N–Bu
3aj
OMe
f1 (ppm)


7.1464
7.1340
7.0754
7.0729
7.0613
6.9419
6.9386
6.9280
6.9249
6.8327
6.8294
6.7888
6.7749
6.6945
3.8638
3.6342
3.3791
3.3667
3.3541
3.0522
1.6020
1.5893
1.5853
1.5769
1.3493
1.3368
1.3243
1.3119
0.9126
0.9003
0.8880
Ms
H
N–Bu
OMe
OMe
3ak
5.01
1.02
1.00
1.00
1.00
3.00
3.03
2.03
3.01
2.01
2.00
3.01
f1 (ppm)

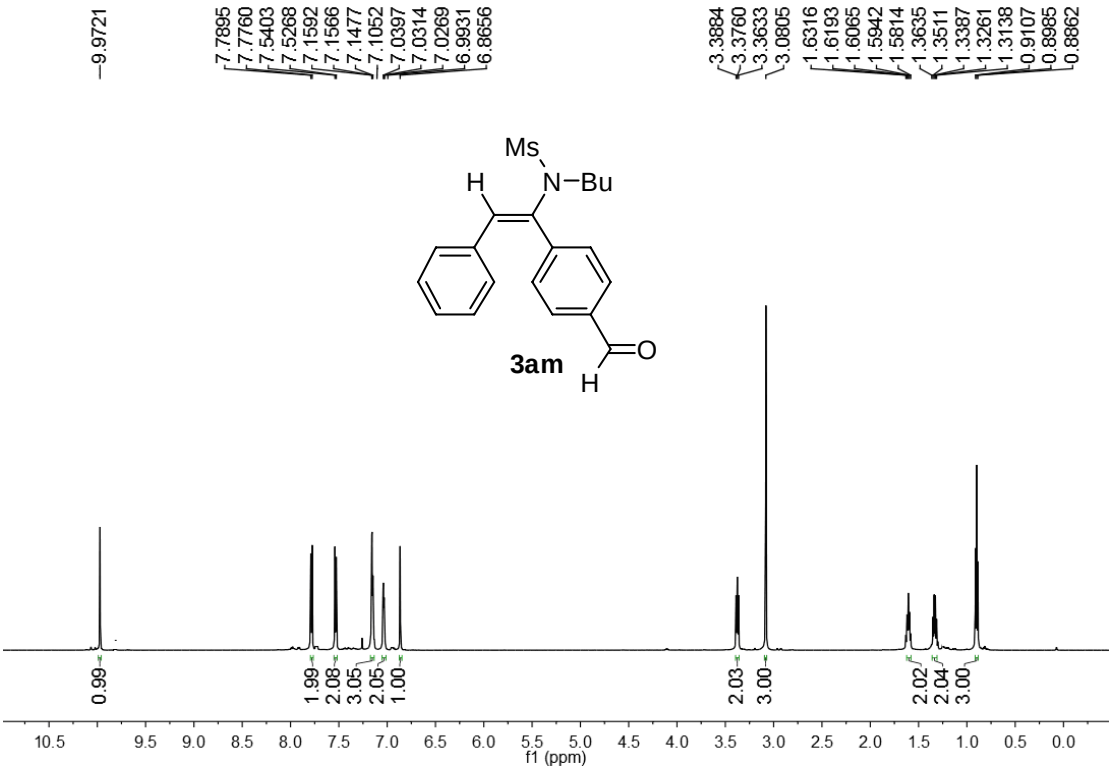

149.2669
148.6129
137.5974
135.5894
129.1650
128.4286
128.0419
127.4523
127.1480
122.4010
112.9713
110.8261
77.2115
77.0000
76.7877
55.6723
55.6065
47.8137
40.6769
30.8096
19.7239
13.6325
Ms
H
N–Bu
OMe
OMe
3ak
f1 (ppm)

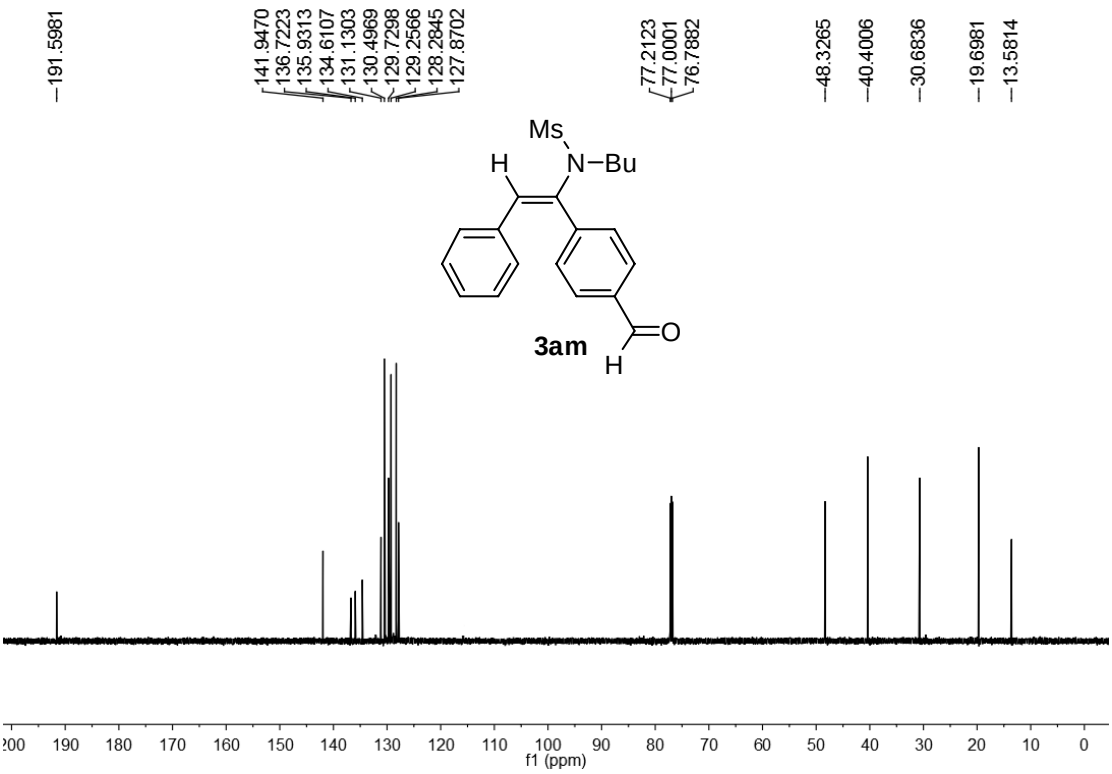

7.1673
7.1550
7.1505
7.1474
7.1449
7.1361
7.0841
7.0728
6.8623
6.8595
6.8490
6.8462
6.8380
6.8355
6.7296
6.7163
6.7006
5.9595
3.3799
3.3674
3.3548
3.0549
1.6103
1.5976
1.5937
1.5852
1.3609
1.3484
1.3358
1.3234
0.9291
0.9168
0.9045
Ms
H
N–Bu
O
O
3.03
2.01
2.01
1.00
1.00
2.00
2.00
3.00
2.00
2.00
3.00
9.0
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)

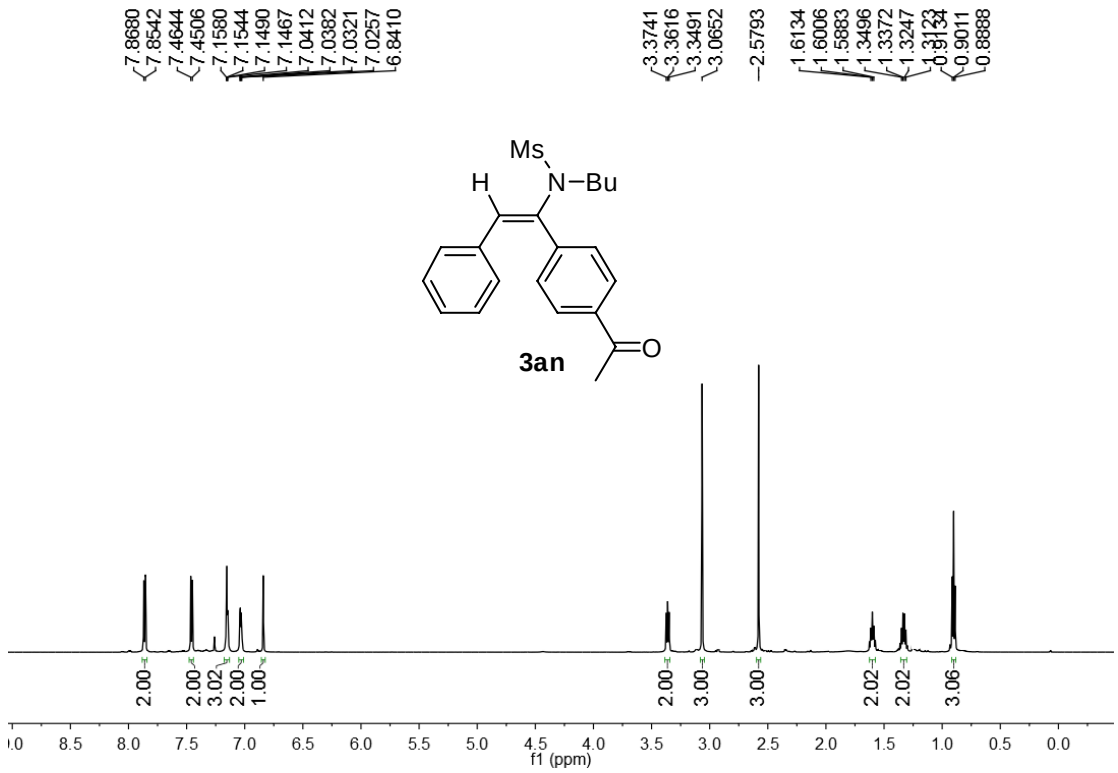
3al

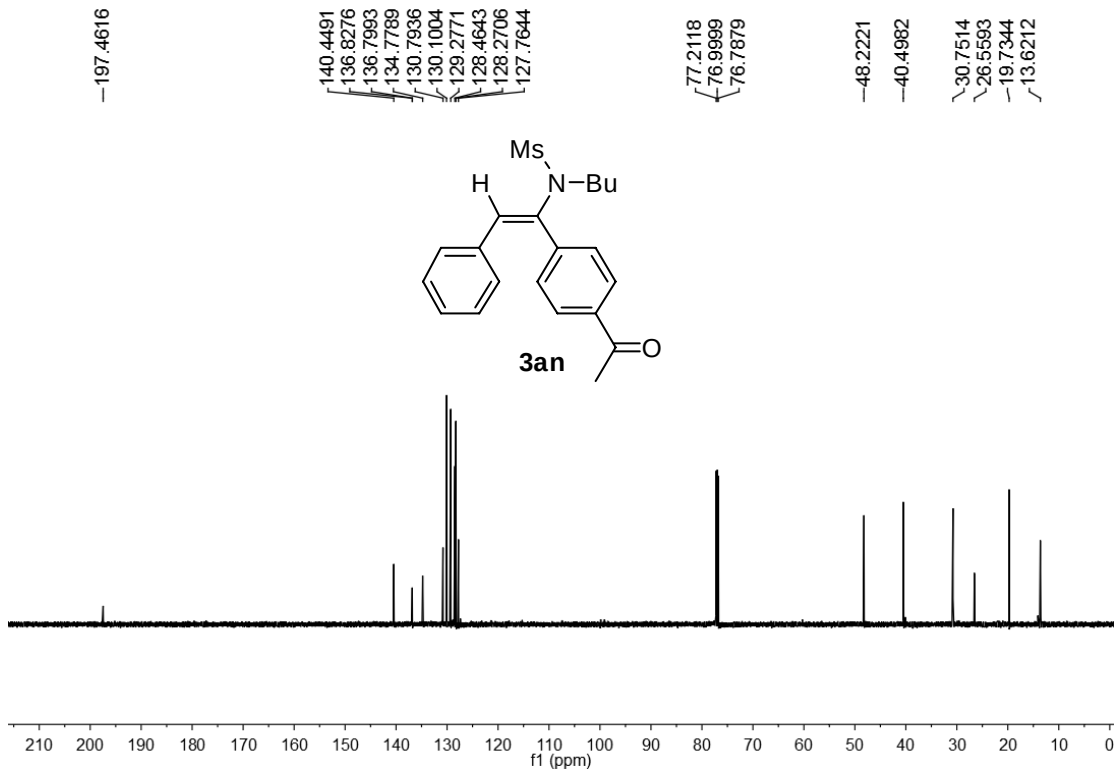

147.9075
147.7747
137.2317
135.3703
129.1816
128.6239
128.0828
127.2253
124.0352
109.8806
108.3844
101.2100
77.2115
76.9995
76.7874
47.6956
40.6542
30.7865
19.7268
13.6434
Ms
H
N–Bu
O
O
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3al


9.9721
7.7895
7.7760
7.5403
7.5268
7.1592
7.1566
7.1477
7.1052
7.0397
7.0314
7.0269
6.9931
6.8656
3.3884
3.3760
3.3633
3.0805
1.6316
1.6193
1.6065
1.5942
1.5814
1.3635
1.3511
1.3387
1.3261
1.3138
0.9107
0.8985
0.8862
Ms
H
N−Bu
O
H
3am
0.99
1.99
2.08
3.05
2.05
1.00
2.03
3.00
2.02
2.04
3.00
f1 (ppm)


191.5981
141.9470
136.7223
135.9313
134.6107
131.1303
130.4969
129.7298
129.2566
128.2845
127.8702
77.2123
77.0001
76.7882
48.3265
40.4006
30.6836
19.6981
13.5814
Ms
H
N−Bu
O
H
3am
f1 (ppm)


7.8680
7.8542
7.4644
7.4506
7.1580
7.1544
7.1490
7.1467
7.0412
7.0382
7.0321
7.0257
6.8410
3.3741
3.3616
3.3491
3.0652
2.5793
1.6134
1.6006
1.5883
1.3496
1.3372
1.3247
0.9011
0.8888
Ms
H
N−Bu
O
3an
2.00
2.00
3.02
2.00
1.00
2.00
3.00
3.00
2.02
2.02
3.06
f1 (ppm)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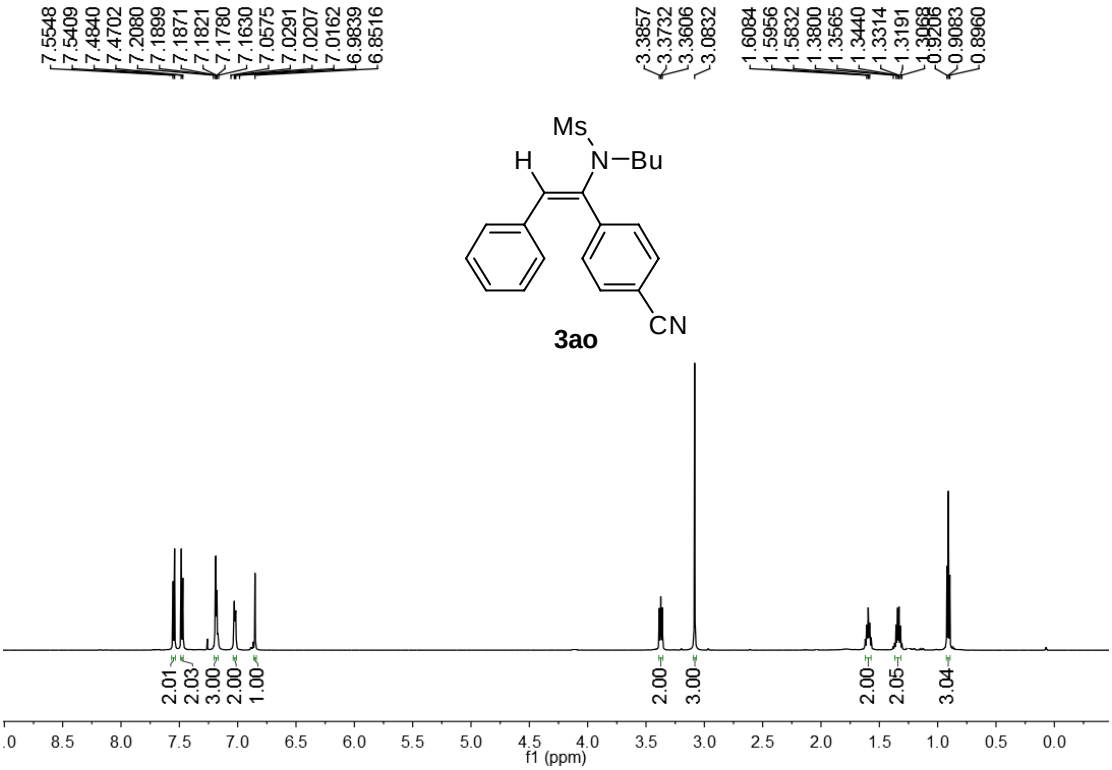
140.4491
136.8276
136.7993
134.7789
130.7936
130.1004
129.2771
128.4643
128.2706
127.7644
77.2118
76.9999
76.7879
48.2221
40.4982
30.7514
26.5593
19.7344
13.6212
Ms
H
N−Bu
O
3an
f1 (ppm)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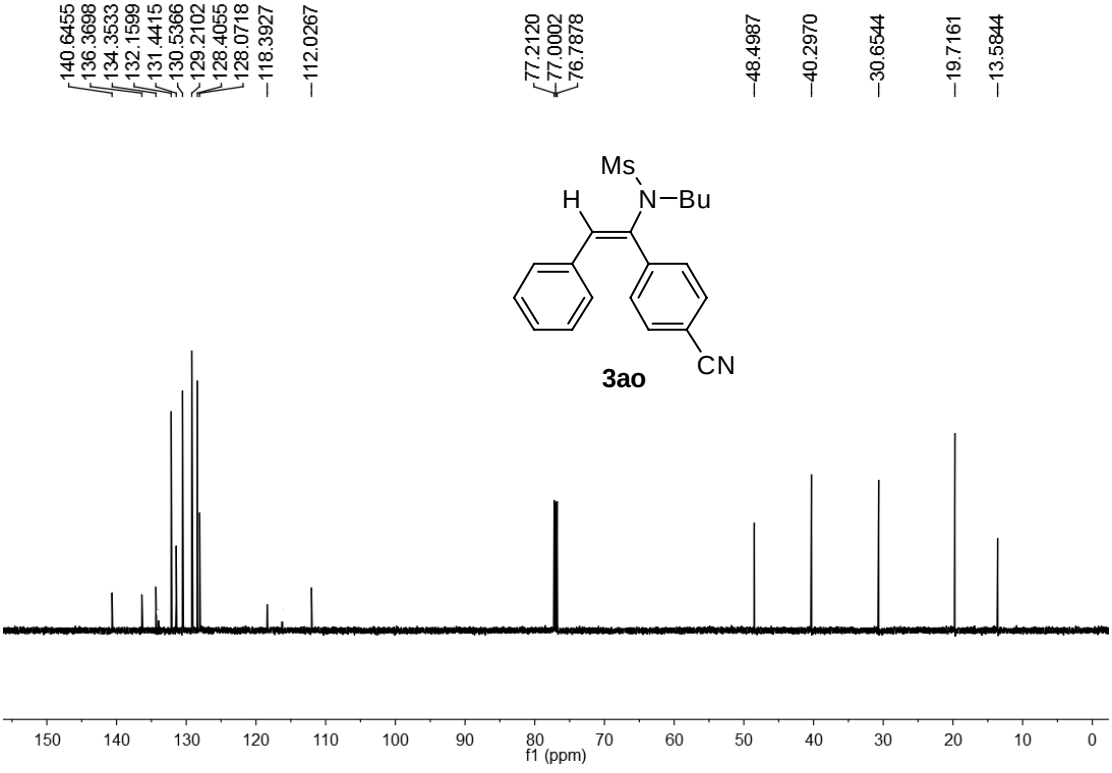
7.5409
7.4840
7.4702
7.2080
7.1899
7.1871
7.1821
7.1780
7.1630
7.0575
7.0291
7.0207
7.0162
6.9839
6.8516
3.3857
3.3732
3.3606
3.0832
1.6084
1.5956
1.5832
1.3800
1.3565
1.3440
1.3314
1.3191
0.9083
0.8960
Ms
H
N−Bu
CN
3ao
2.01
2.03
3.00
2.00
1.00
2.00
3.00
2.00
2.05
3.04
f1 (ppm)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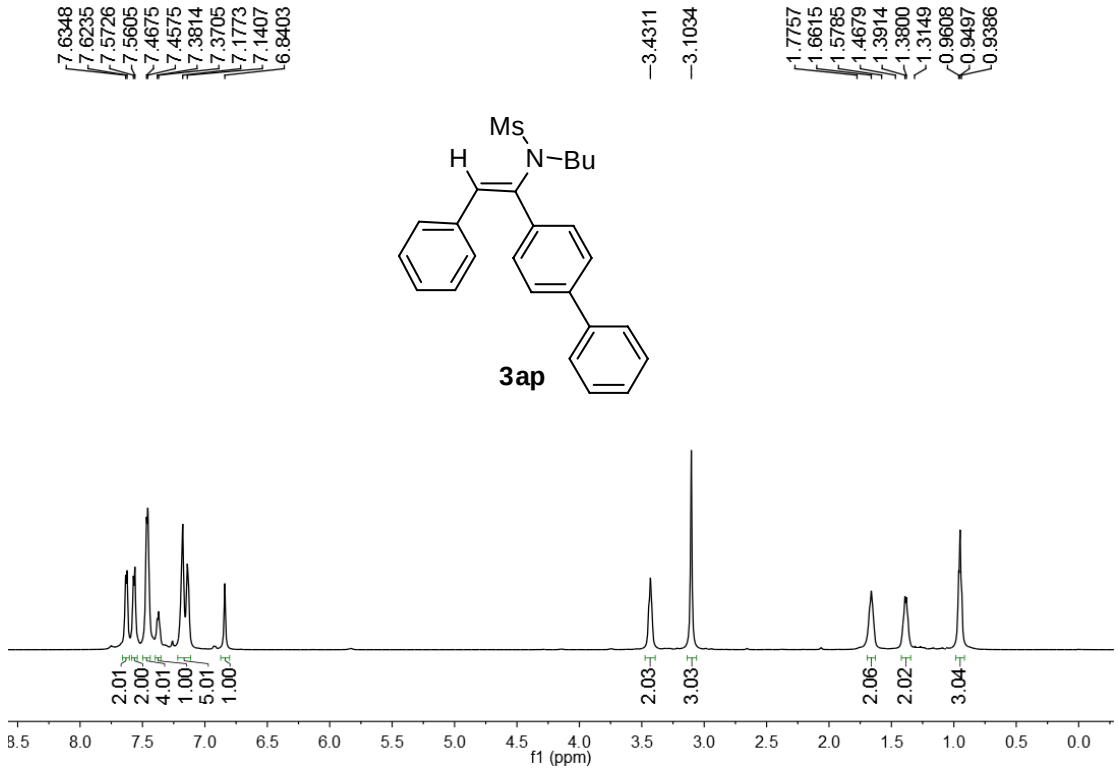
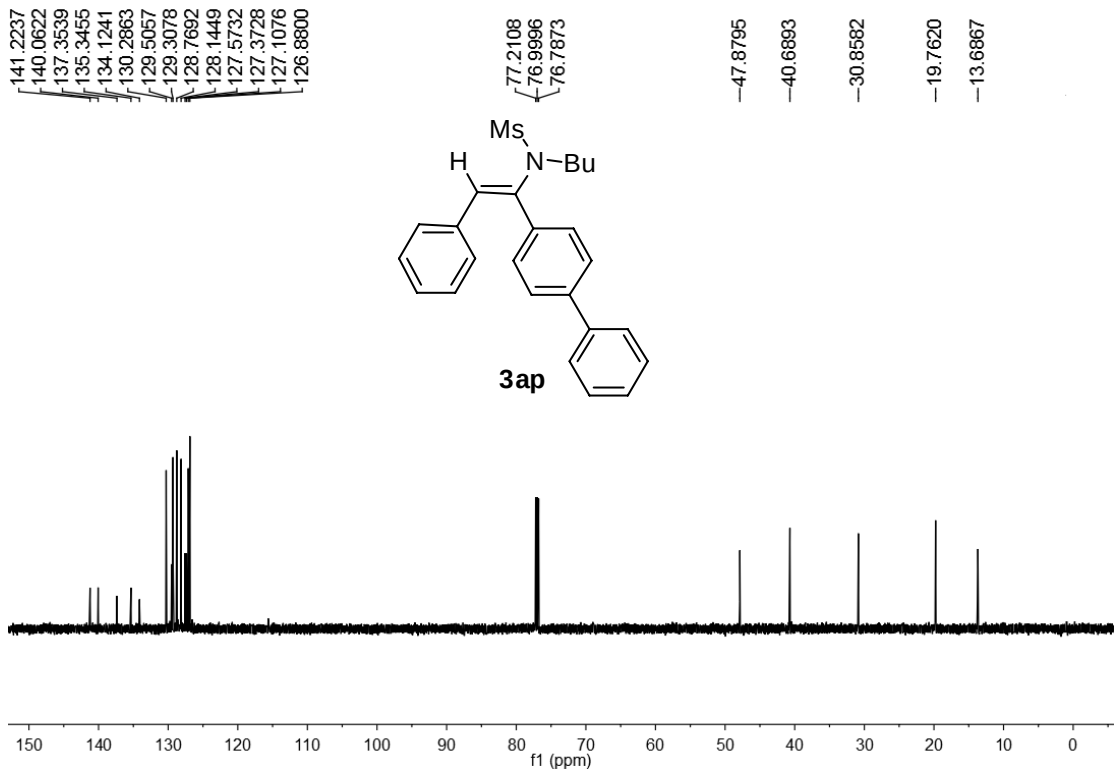
134.3533
132.1599
131.4415
130.5366
129.2102
128.4055
128.0718
118.3927
112.0267
77.2120
77.0002
76.7878
48.4987
40.2970
30.6544
19.7161
13.5844
Ms
H
N−Bu
CN
3ao
f1 (ppm)


7.6348
7.6235
7.5726
7.5605
7.4675
7.4575
7.3814
7.3705
7.1773
7.1407
6.8403
3.4311
3.1034
1.7757
1.6615
1.5785
1.4679
1.3914
1.3800
1.3149
0.9608
0.9497
0.9386
Ms
H
N−Bu
3ap
2.01
2.00
4.01
1.00
5.01
1.00
2.03
3.03
2.06
2.02
3.04
f1 (ppm)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130.2863
129.5057
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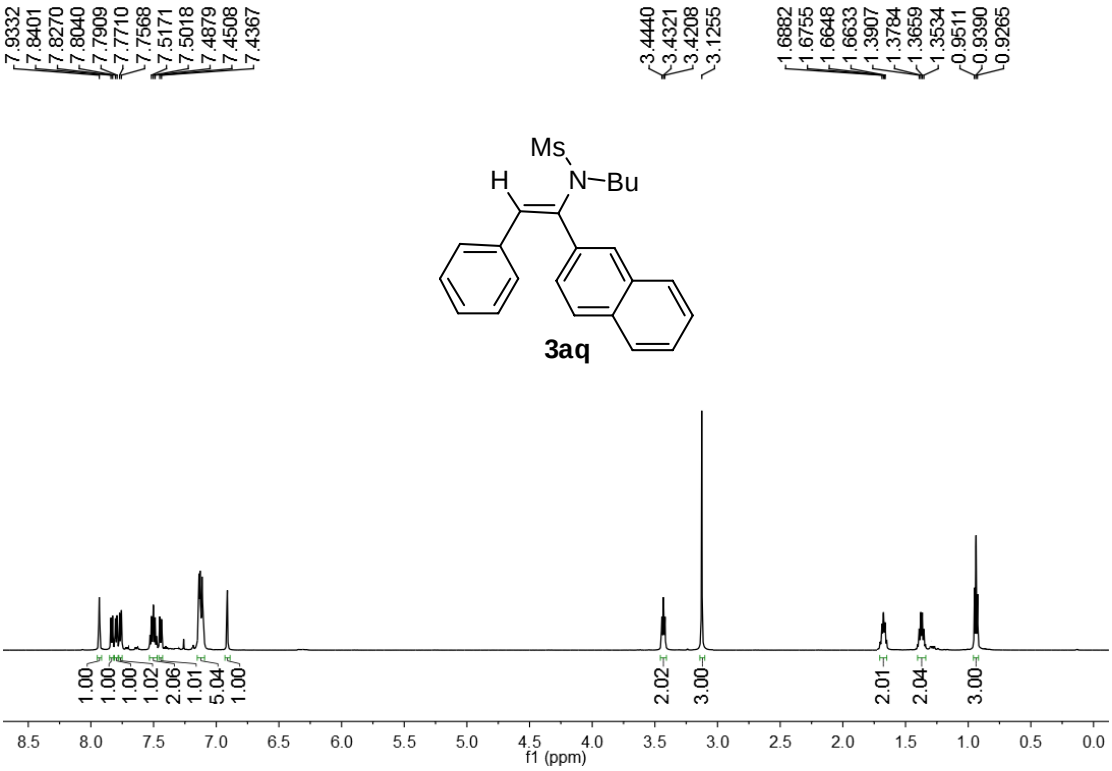
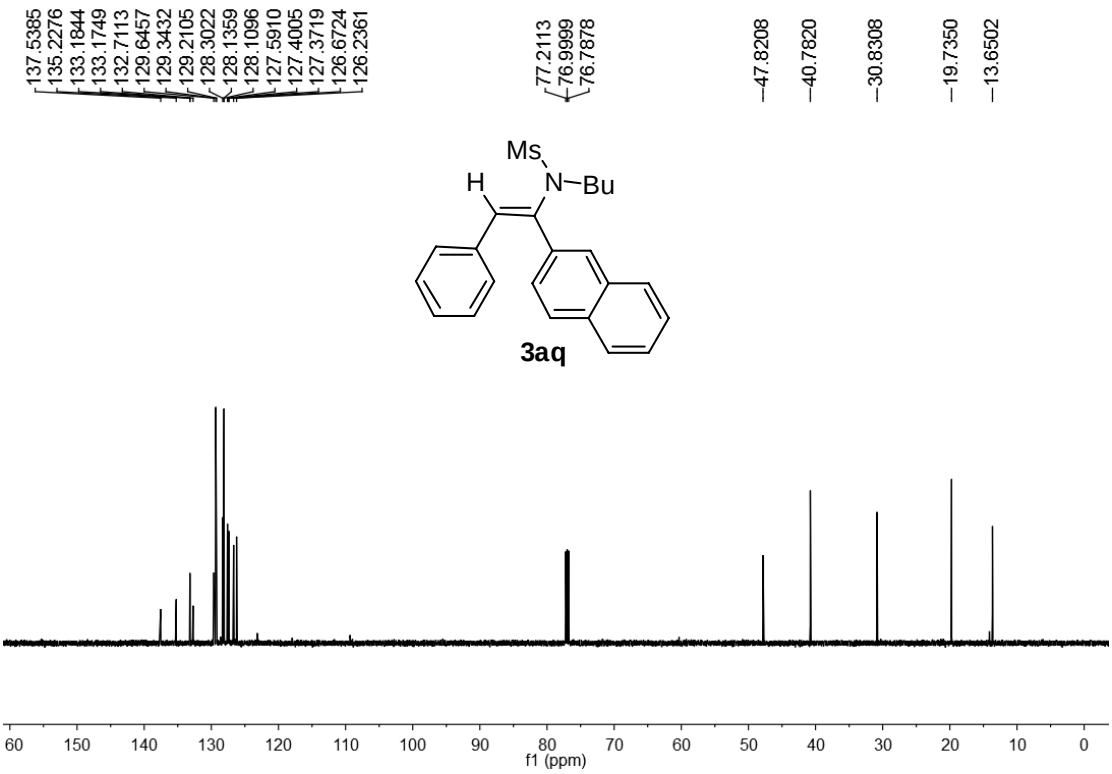
128.7692
128.1449
127.5732
127.3728
127.1076
126.8800
77.2108
76.9996
76.7873
47.8795
40.6893
30.8582
19.7620
13.6867
Ms
H
N−Bu
3ap
f1 (ppm)


7.9332
7.8401
7.8270
7.8040
7.7909
7.7710
7.7568
7.5171
7.5018
7.4879
7.4508
7.4367
3.4440
3.4321
3.4208
3.1255
1.6882
1.6755
1.6648
1.6633
1.3907
1.3784
1.3659
1.3534
0.9511
0.9390
0.9265
Ms
H
N–Bu
3aq
1.00
1.00
1.00
1.02
2.06
1.01
5.04
1.00
2.02
3.00
2.01
2.04
3.00
f1 (ppm)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133.1844
133.1749
132.7113
129.6457
129.3432
129.2105
128.3022
128.1359
128.1096
127.5910
127.4005
127.3719
126.6724
126.2361
77.2113
76.9999
76.7878
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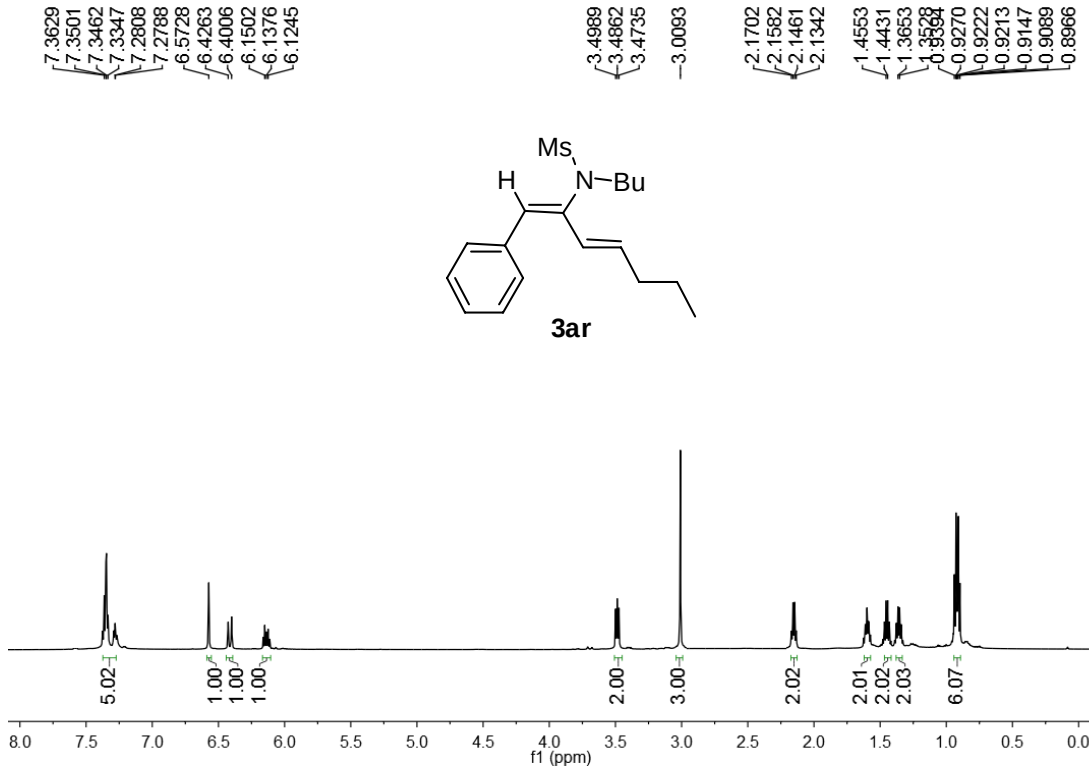
40.7820
30.8308
19.7350
13.6502
Ms
H
N–Bu
3aq
f1 (ppm)


7.3629
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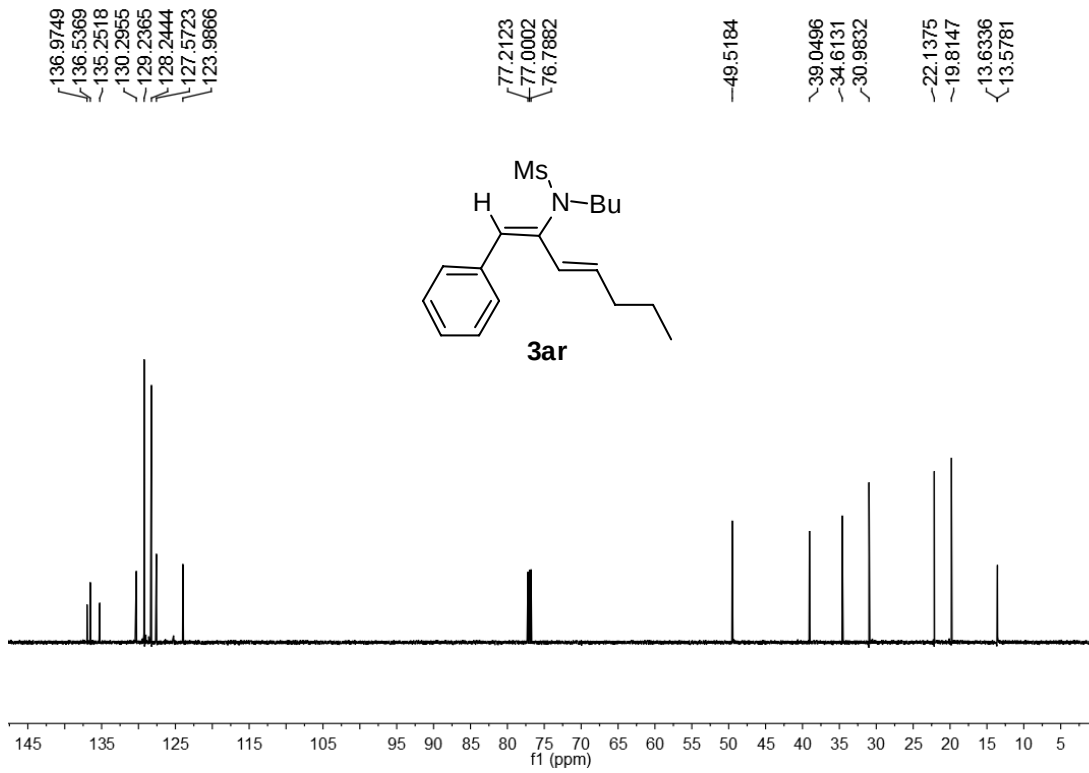
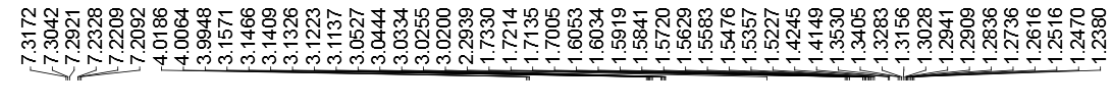
7.3462
7.3347
7.2808
7.2788
6.5728
6.4263
6.4006
6.1502
6.1376
6.1245
3.4989
3.4862
3.4735
3.0093
2.1702
2.1582
2.1461
2.1342
1.4553
1.4431
1.3653
1.3528
0.9394
0.9270
0.9222
0.9213
0.9147
0.9089
0.8966
Ms
H
N–Bu
3ar
5.02
1.00
1.00
1.00
2.00
3.00
2.02
2.01
2.02
2.03
6.07
f1 (ppm)


136.9749
136.5369
135.2518
130.2955
129.2365
128.2444
127.5723
123.9866
77.2123
77.0002
76.7882
49.5184
39.0496
34.6131
30.9832
22.1375
19.8147
13.6336
13.5781
Ms
H
N–Bu
3ar
f1 (ppm)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7.3042
7.2921
7.2328
7.2209
7.2092
4.0186
4.0064
3.9948
3.1571
3.1466
3.1409
3.1326
3.1223
3.1137
3.0527
3.0444
3.0334
3.0255
3.0200
2.2939
1.7330
1.7214
1.7135
1.7005
1.6053
1.6034
1.5919
1.5841
1.5720
1.5629
1.5583
1.5476
1.5357
1.5227
1.4245
1.4149
1.3530
1.3405
1.3283
1.3156
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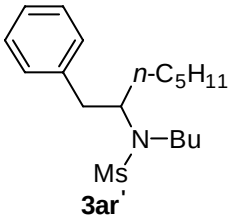
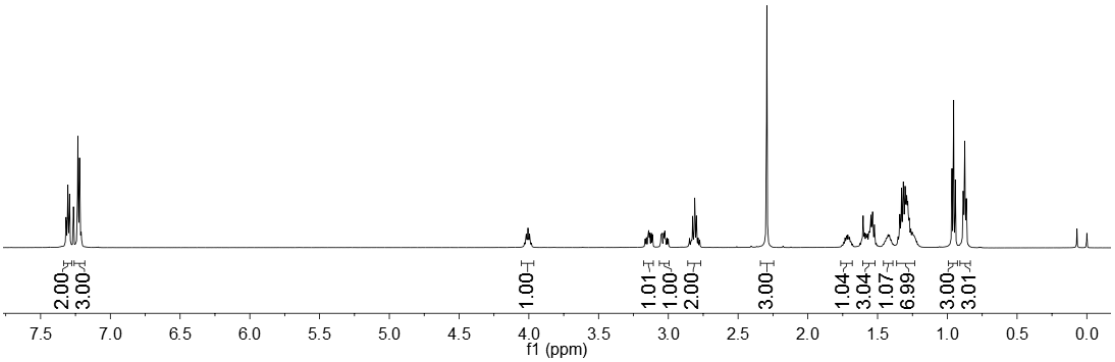
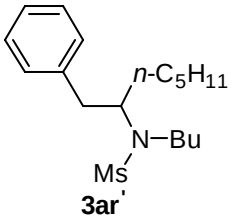
1.2941
1.2909
1.2836
1.2736
1.2616
1.2516
1.2470
1.2380


n-C5H11
N–Bu
Ms

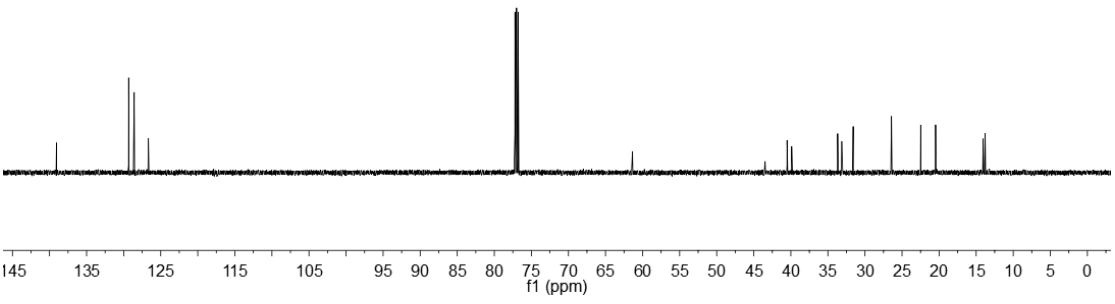
3ar'

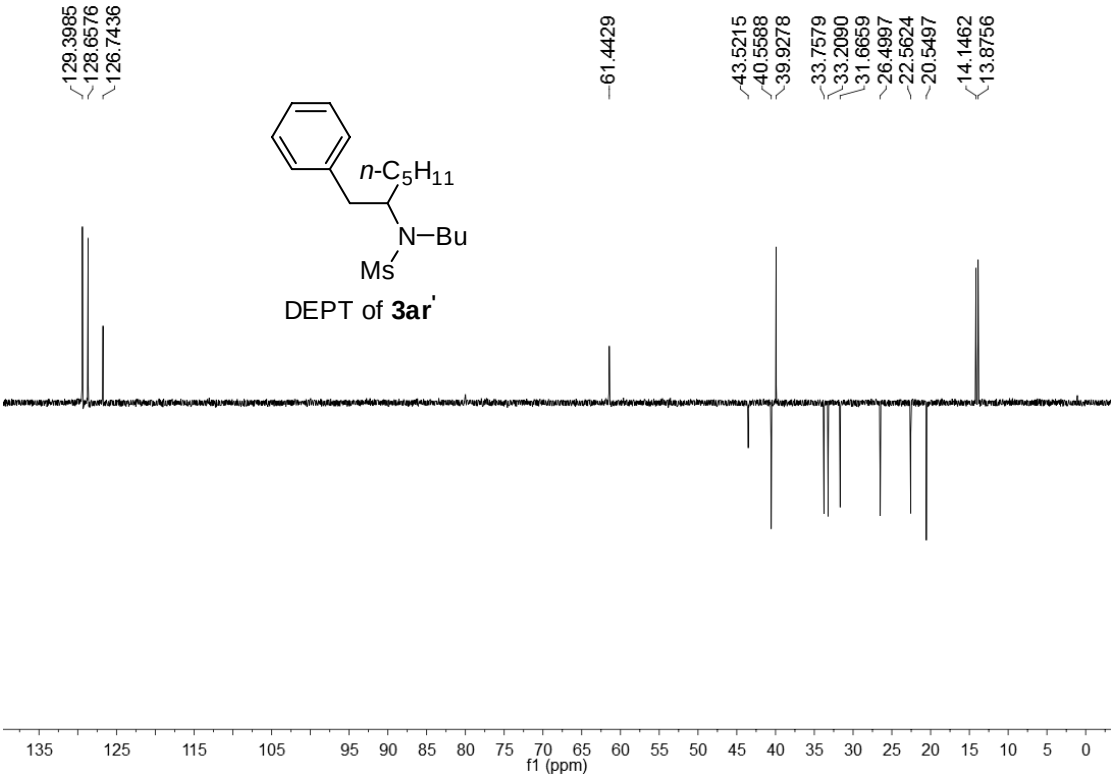

2.00
3.00
1.00
1.01
1.00
2.00
3.00
1.04
3.04
1.07
6.99
3.00
3.01
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


139.0664
129.3234
128.5794
126.6644
77.2114
76.9998
76.7881
61.3659
43.4740
40.5053
39.8860
33.6808
33.1272
31.5891
26.4288
22.4805
20.4718
14.0551
13.7874

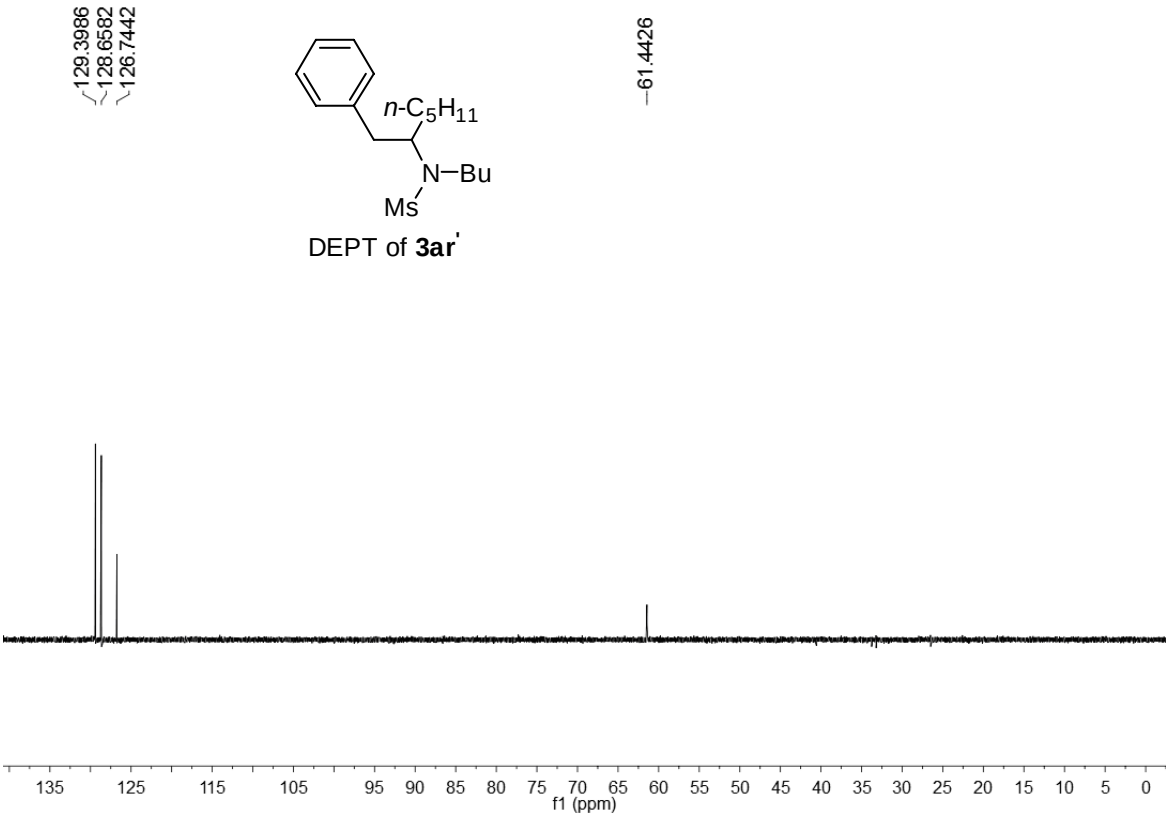

n-C5H11
N–Bu
Ms

3ar'

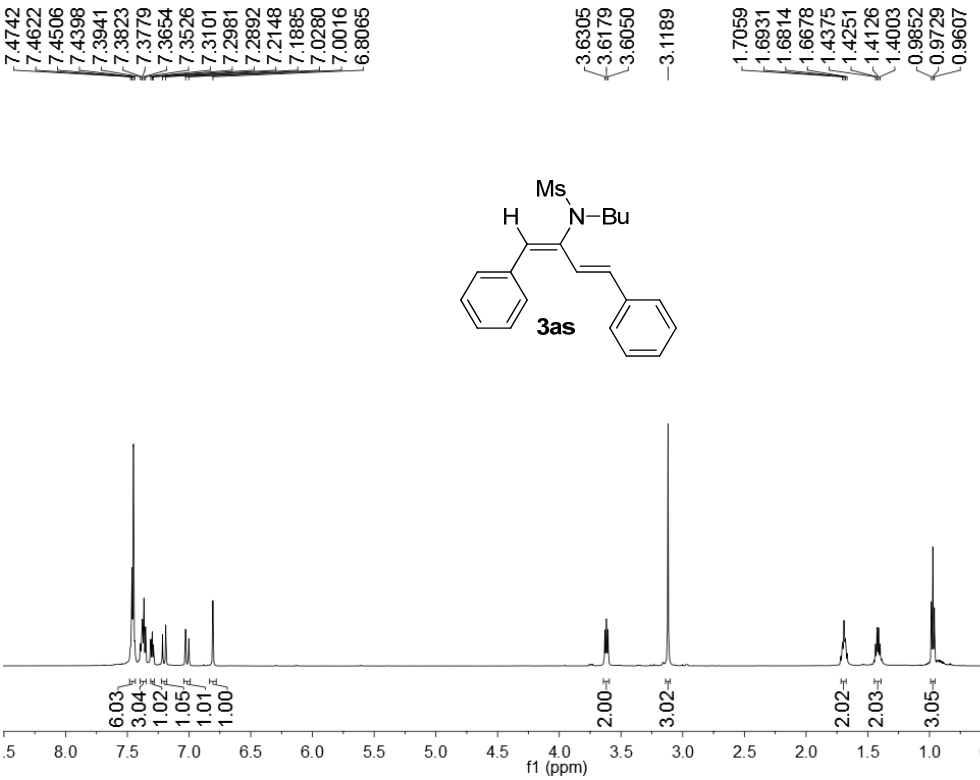

145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)



DEPT of **3ar'**



DEPT of **3ar'**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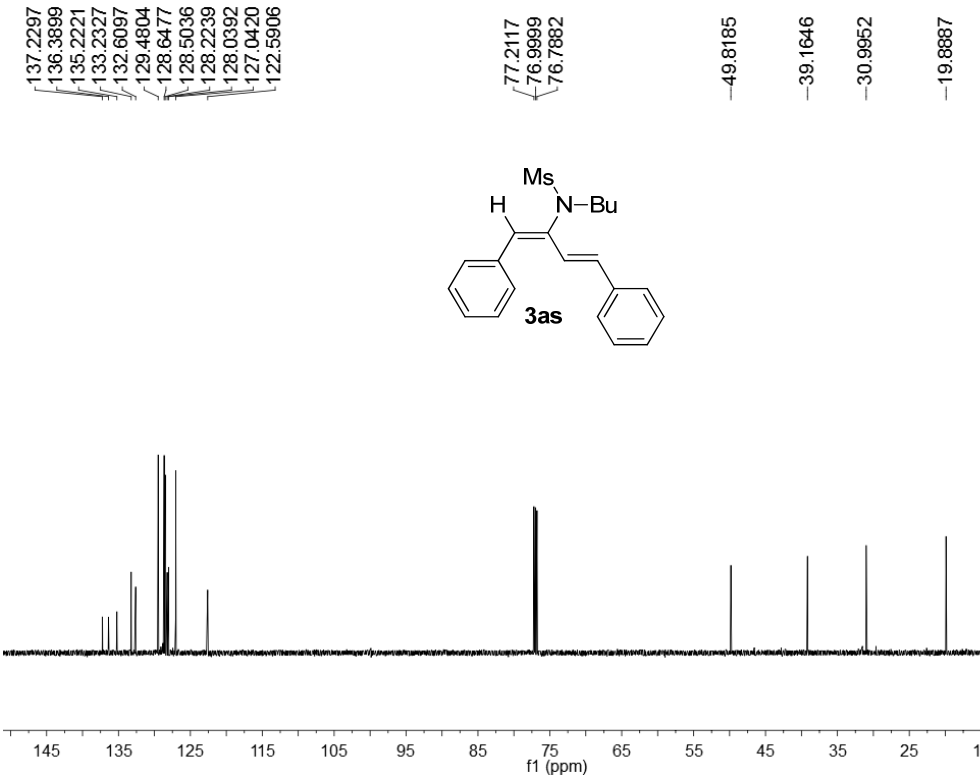
7.4398
7.3941
7.3823
7.3779
7.3654
7.3526
7.3101
7.2981
7.2892
7.2148
7.1885
7.0280
7.0016
6.8065
3.6305
3.6179
3.6050
3.1189
1.7059
1.6931
1.6814
1.6678
1.4375
1.4251
1.4126
1.4003
0.9852
0.9729
0.9607
Ms
H
N–Bu
3as
6.03
3.04
1.02
1.05
1.01
1.00
2.00
3.02
2.02
2.03
3.05
f1 (ppm)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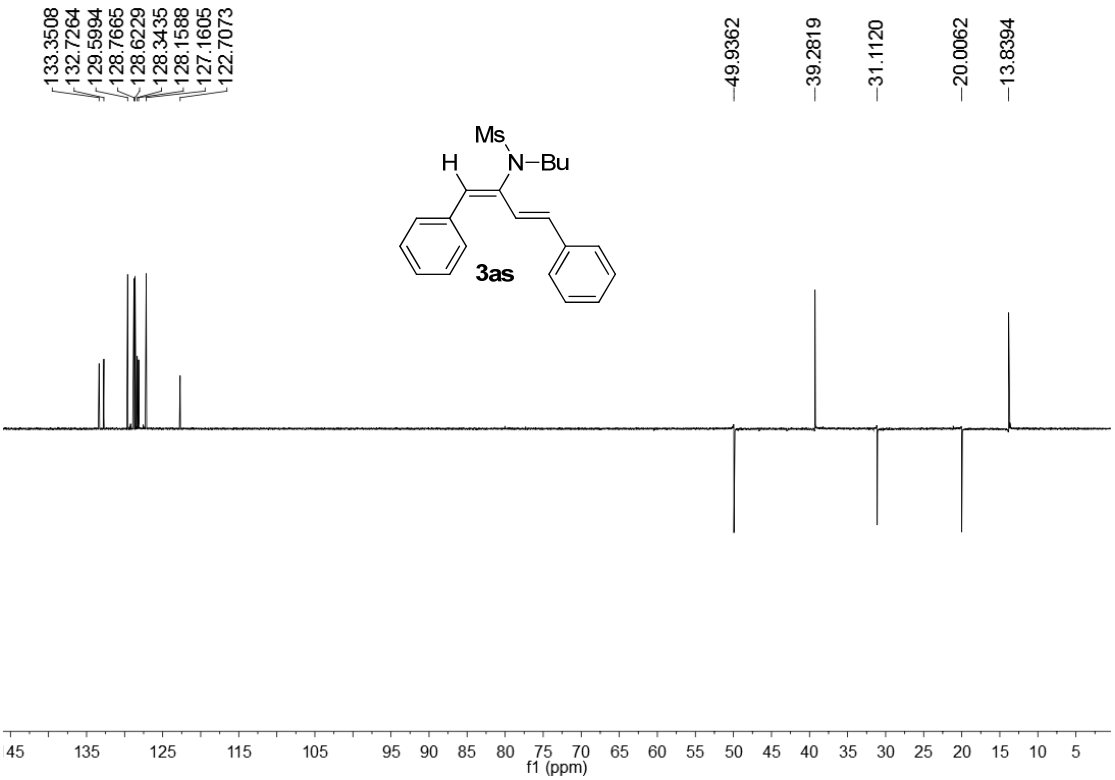
135.2221
133.2327
132.6097
129.4804
128.6477
128.5036
128.2239
128.0392
127.0420
122.5906
77.2117
76.9999
76.7882
49.8185
39.1646
30.9952
19.8887
13.7178
Ms
H
N–Bu
3as
f1 (ppm)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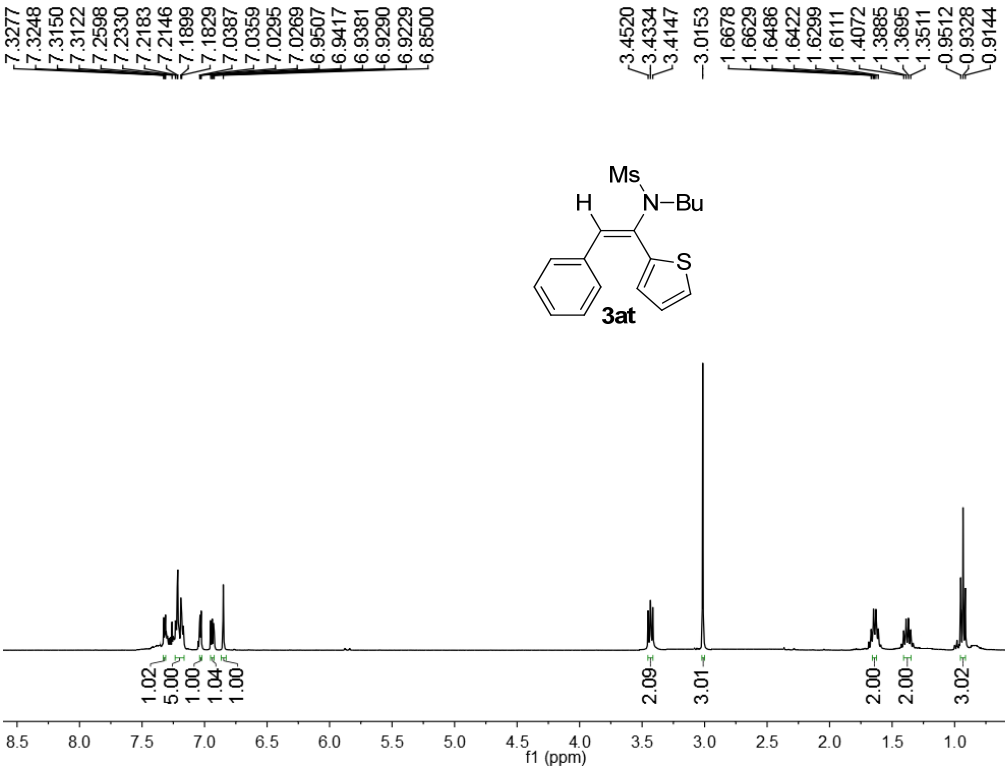
132.7264
129.5994
128.7665
128.6229
128.3435
128.1588
127.1605
122.7073
49.9362
39.2819
31.1120
20.0062
13.8394
Ms
H
N–Bu
3as
45
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
f1 (ppm)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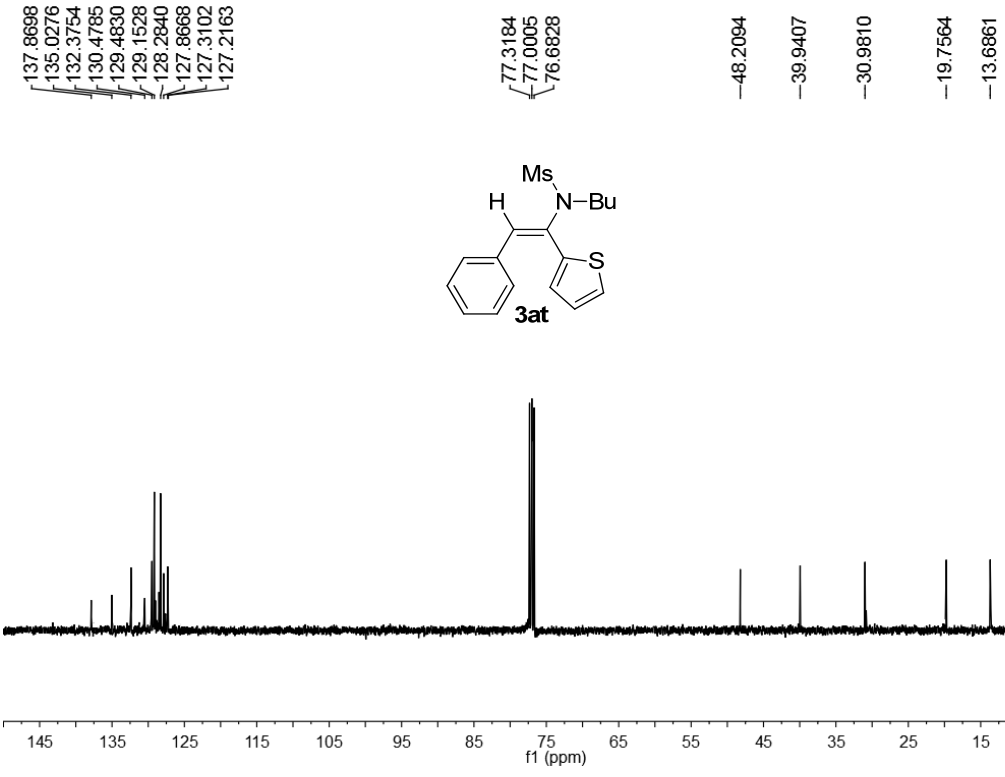
7.3248
7.3150
7.3122
7.2598
7.2330
7.2183
7.2146
7.1899
7.1829
7.0387
7.0359
7.0295
7.0269
6.9507
6.9417
6.9381
6.9290
6.9229
6.8500
3.4520
3.4334
3.4147
3.0153
1.6678
1.6629
1.6486
1.6422
1.6299
1.6111
1.4072
1.3885
1.3695
1.3511
0.9512
0.9328
0.9144
Ms
H
N–Bu
S
3at
1.02
5.00
1.00
1.04
1.00
2.09
3.01
2.00
2.00
3.02
f1 (ppm)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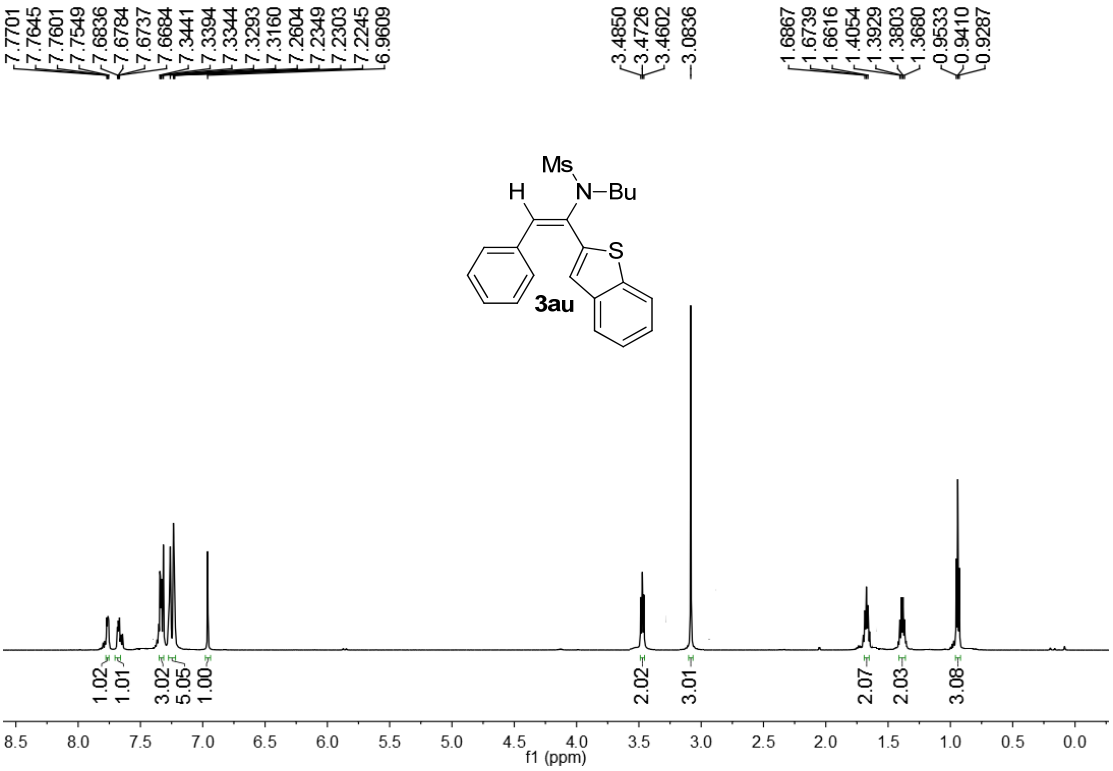
135.0276
132.3754
130.4785
129.4830
129.1528
128.2840
127.8668
127.3102
127.2163
77.3184
77.0005
76.6828
48.2094
39.9407
30.9810
19.7564
13.6861
Ms
H
N–Bu
S
3at
f1 (ppm)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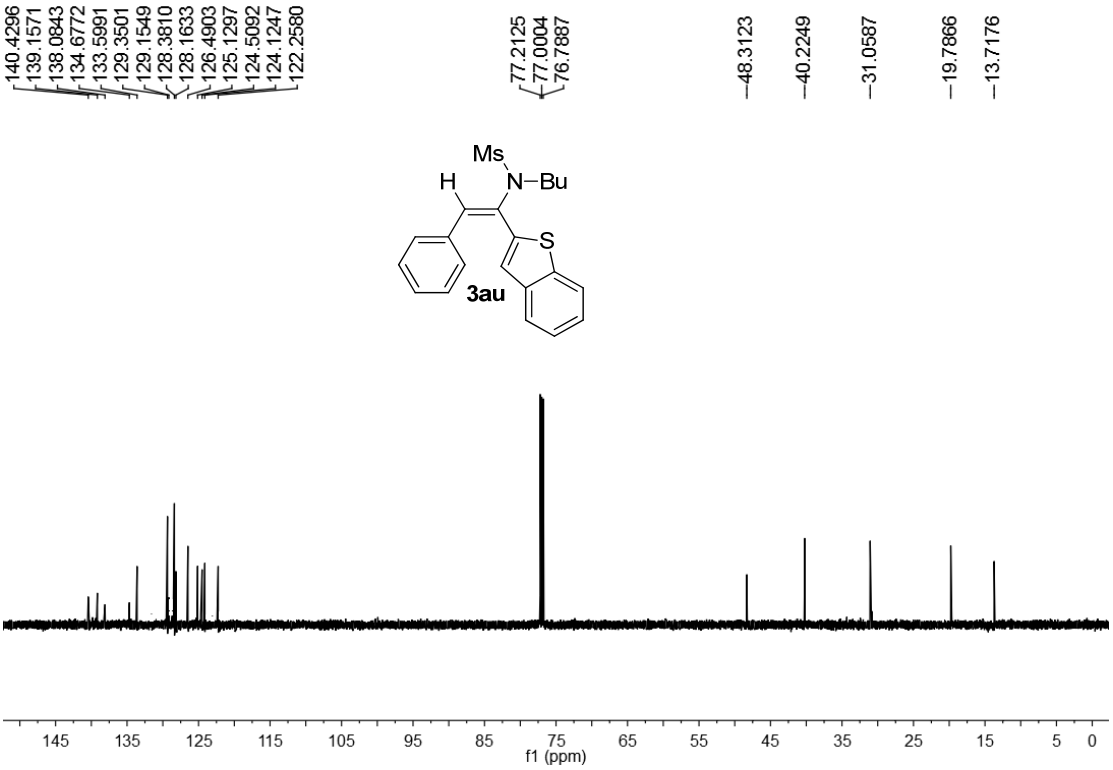
7.7645
7.7601
7.7549
7.6836
7.6784
7.6737
7.6684
7.3441
7.3394
7.3344
7.3293
7.3160
7.2604
7.2349
7.2303
7.2245
6.9609
3.4850
3.4726
3.4602
3.0836
1.6867
1.6739
1.6616
1.4054
1.3929
1.3803
1.3680
0.9533
0.9410
0.9287
Ms
H
N–Bu
S
3au
1.02
1.01
3.02
5.05
1.00
2.02
3.01
2.07
2.03
3.08
f1 (ppm)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138.0843
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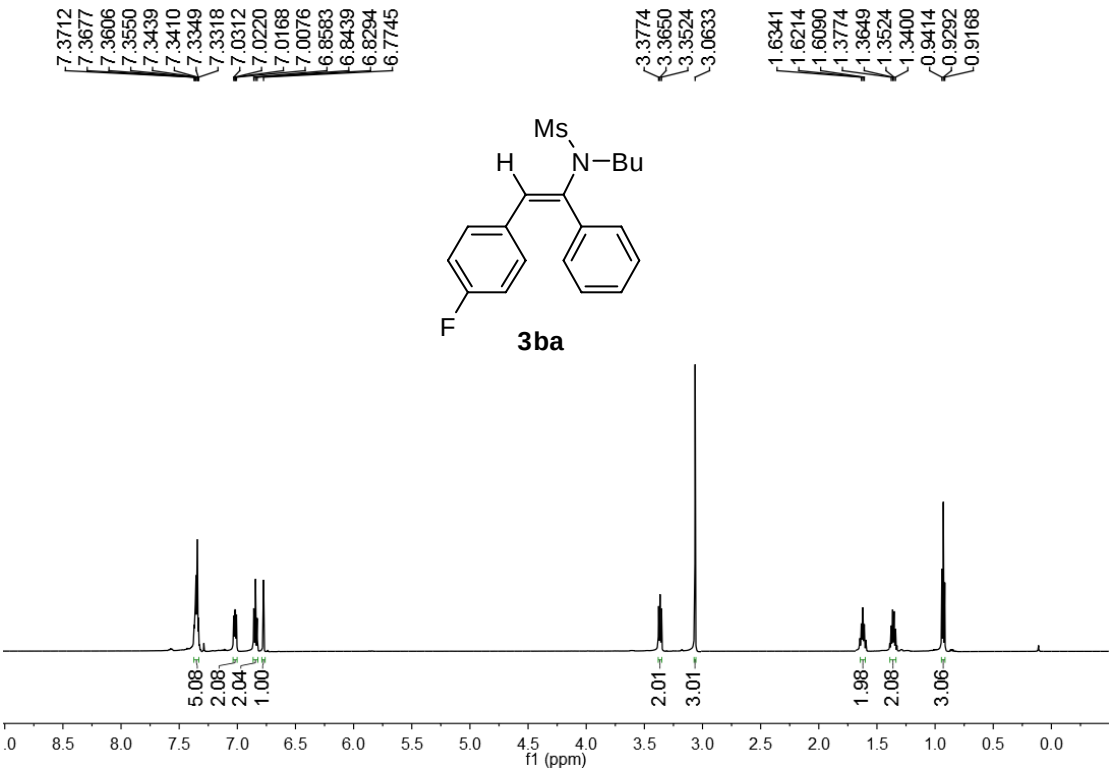
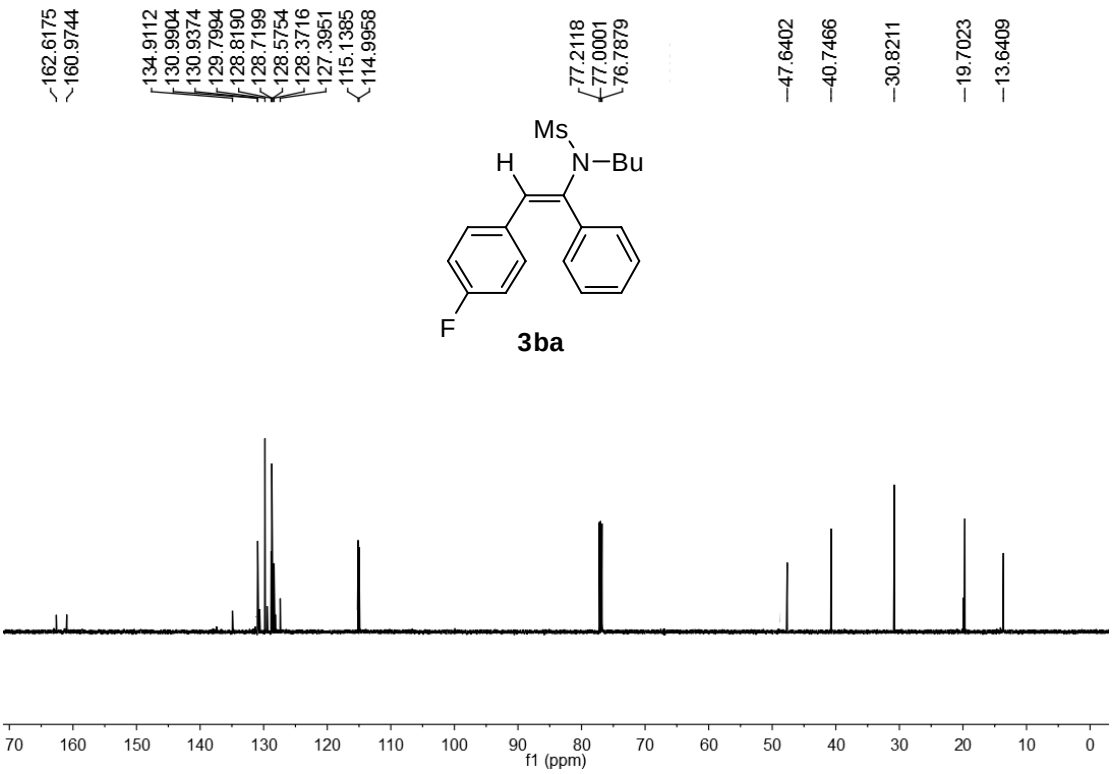
133.5991
129.3501
129.1549
128.3810
128.1633
126.4903
125.1297
124.5092
124.1247
122.2580
77.2125
77.0004
76.7887
48.3123
40.2249
31.0587
19.7866
13.7176
Ms
H
N–Bu
S
3au
f1 (ppm)


7.3712
7.3677
7.3606
7.3550
7.3439
7.3410
7.3349
7.3318
7.0312
7.0220
7.0168
7.0076
6.8583
6.8439
6.8294
6.7745
3.3774
3.3650
3.3524
3.0633
1.6341
1.6214
1.6090
1.3774
1.3649
1.3524
1.3400
0.9414
0.9292
0.9168
Ms
H
N—Bu
F
3ba
5.08
2.08
2.04
1.00
2.01
3.01
1.98
2.08
3.06
f1 (ppm)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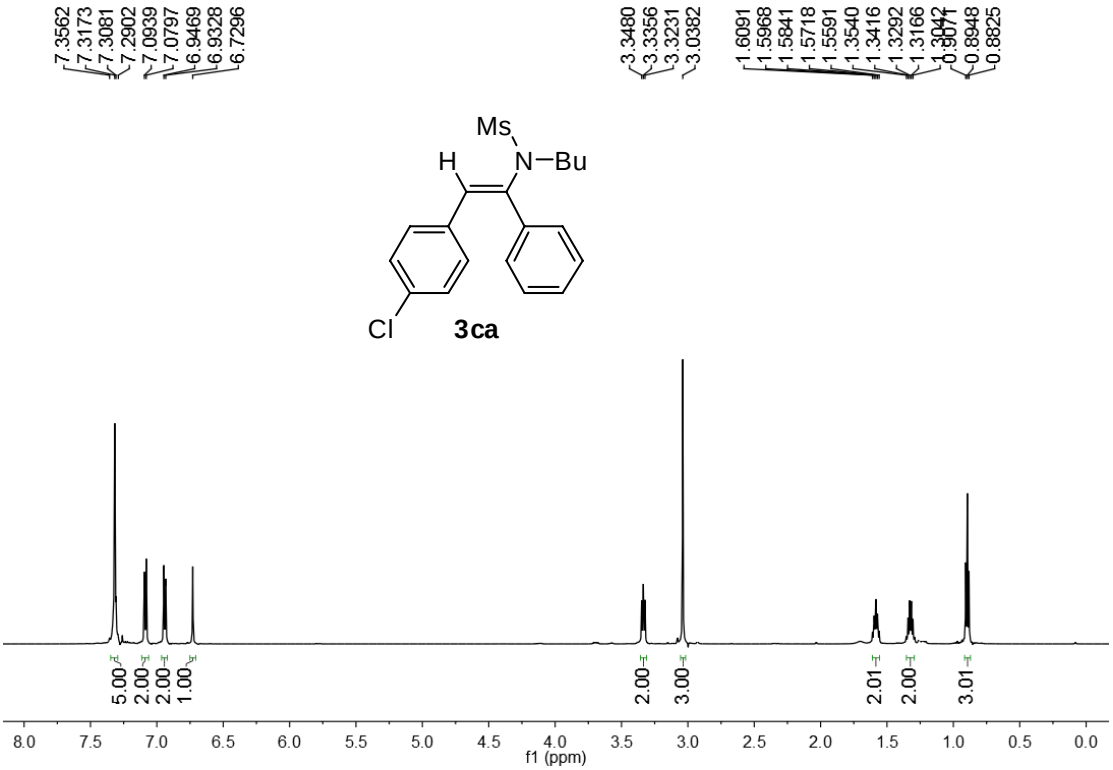
160.9744
134.9112
130.9904
130.9374
129.7994
128.8190
128.7199
128.5754
128.3716
127.3951
115.1385
114.9958
77.2118
77.0001
76.7879
47.6402
40.7466
30.8211
19.7023
13.6409
Ms
H
N—Bu
F
3ba
f1 (ppm)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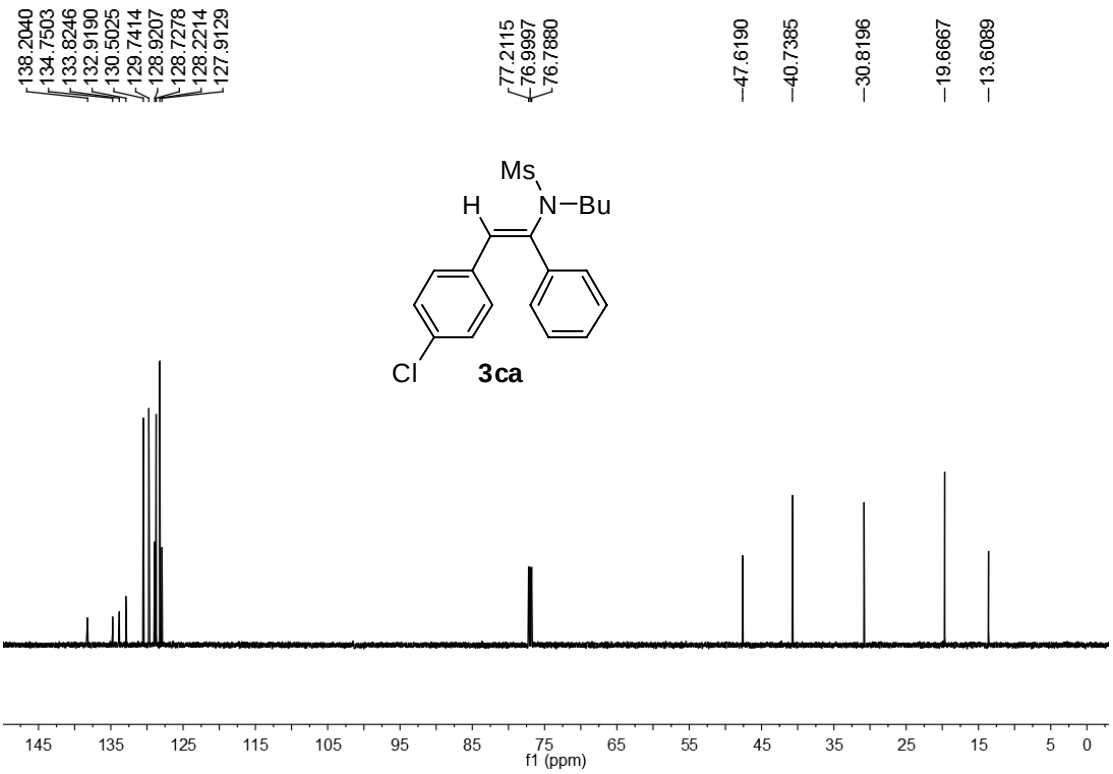
7.3081
7.2902
7.0939
7.0797
6.9469
6.9328
6.7296
3.3480
3.3356
3.3231
3.0382
1.6091
1.5968
1.5841
1.5718
1.5591
1.3540
1.3416
1.3292
1.3166
0.8948
0.8825
Ms
H
N−Bu
Cl
3ca
5.00
2.00
2.00
1.00
2.00
3.00
2.01
2.00
3.01
f1 (ppm)


138.2040
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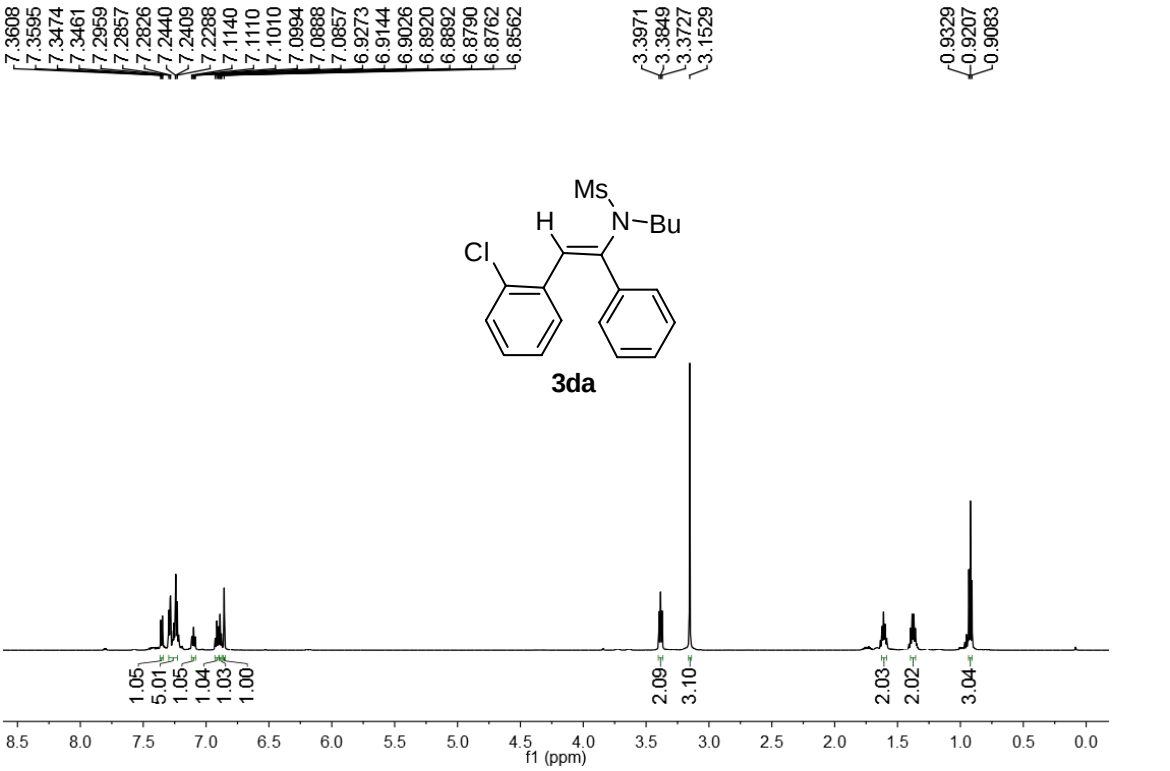
133.8246
132.9190
130.5025
129.7414
128.9207
128.7278
128.2214
127.9129
77.2115
76.9997
76.7880
47.6190
40.7385
30.8196
19.6667
13.6089
Ms
H
N−Bu
Cl
3ca
f1 (ppm)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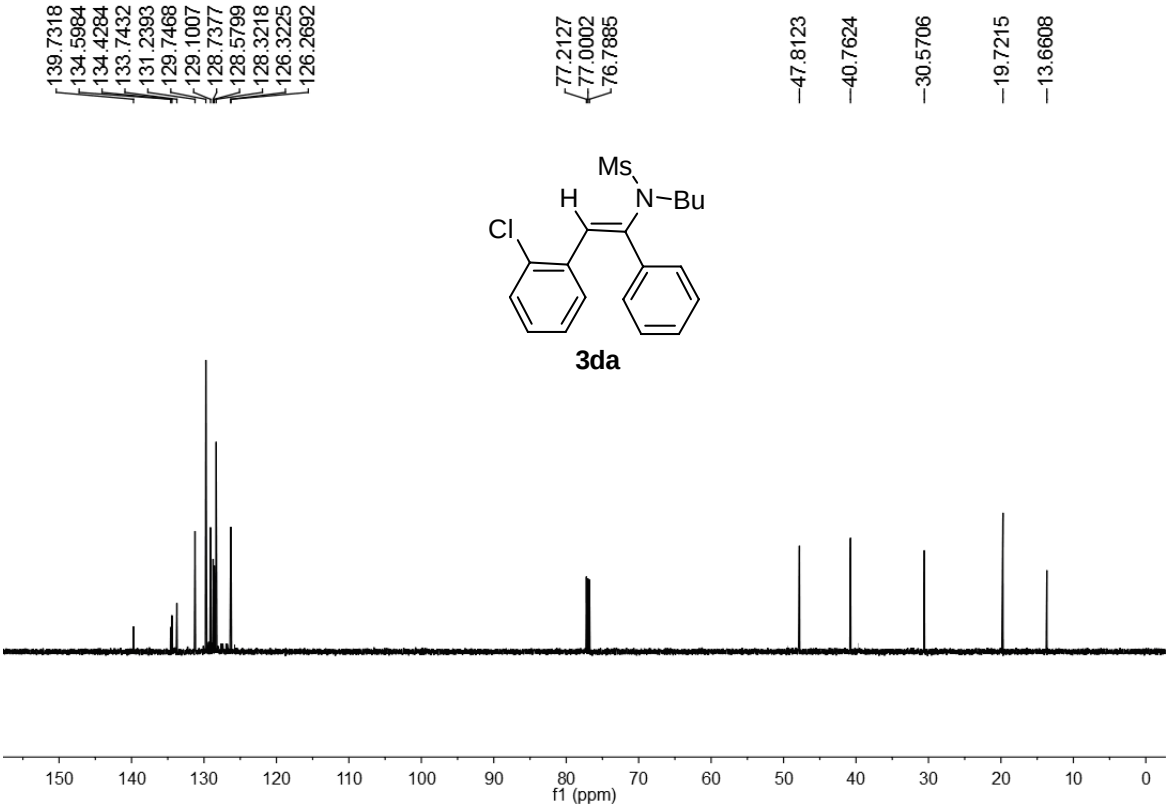
7.3461
7.2959
7.2857
7.2826
7.2440
7.2409
7.2288
7.1140
7.1110
7.1010
7.0994
7.0888
7.0857
6.9273
6.9144
6.9026
6.8920
6.8892
6.8790
6.8762
6.8562
3.3971
3.3849
3.3727
3.1529
0.9329
0.9207
0.9083
Ms
H
N–Bu
Cl
3da
1.05
5.01
1.05
1.04
1.03
1.00
2.09
3.10
2.03
2.02
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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134.4284
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129.1007
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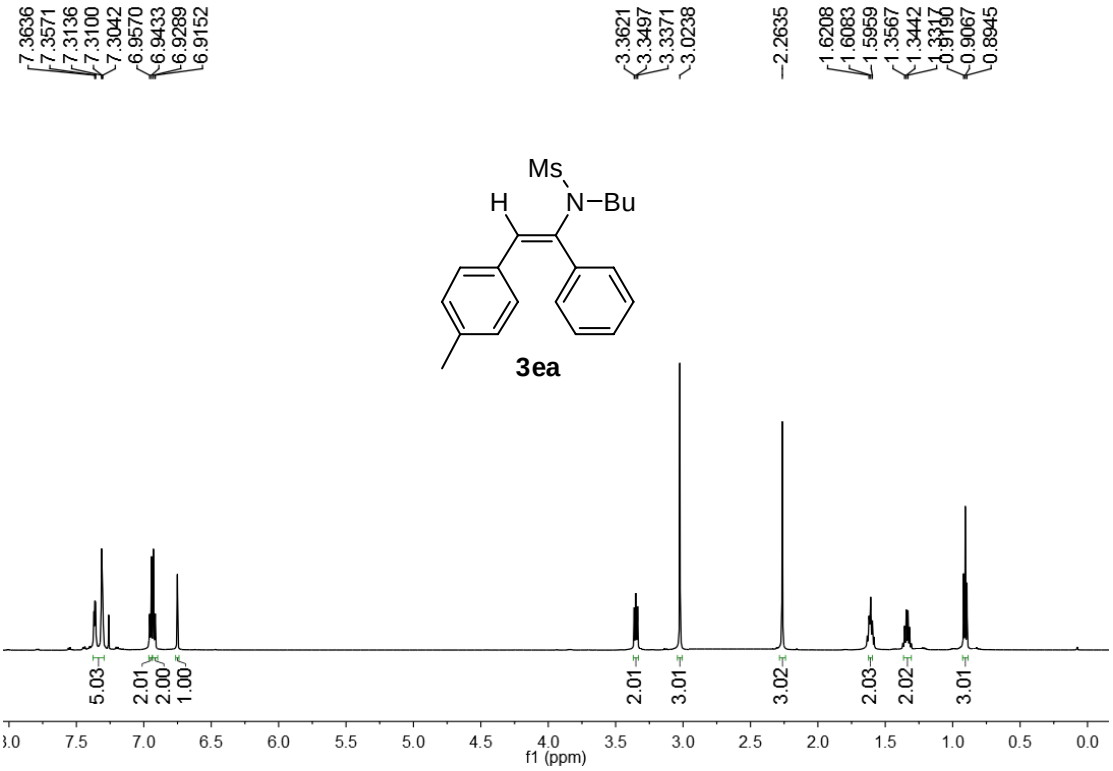
128.5799
128.3218
126.3225
126.2692
77.2127
77.0002
76.7885
47.8123
40.7624
30.5706
19.7215
13.6608
Ms
H
N–Bu
Cl
3da
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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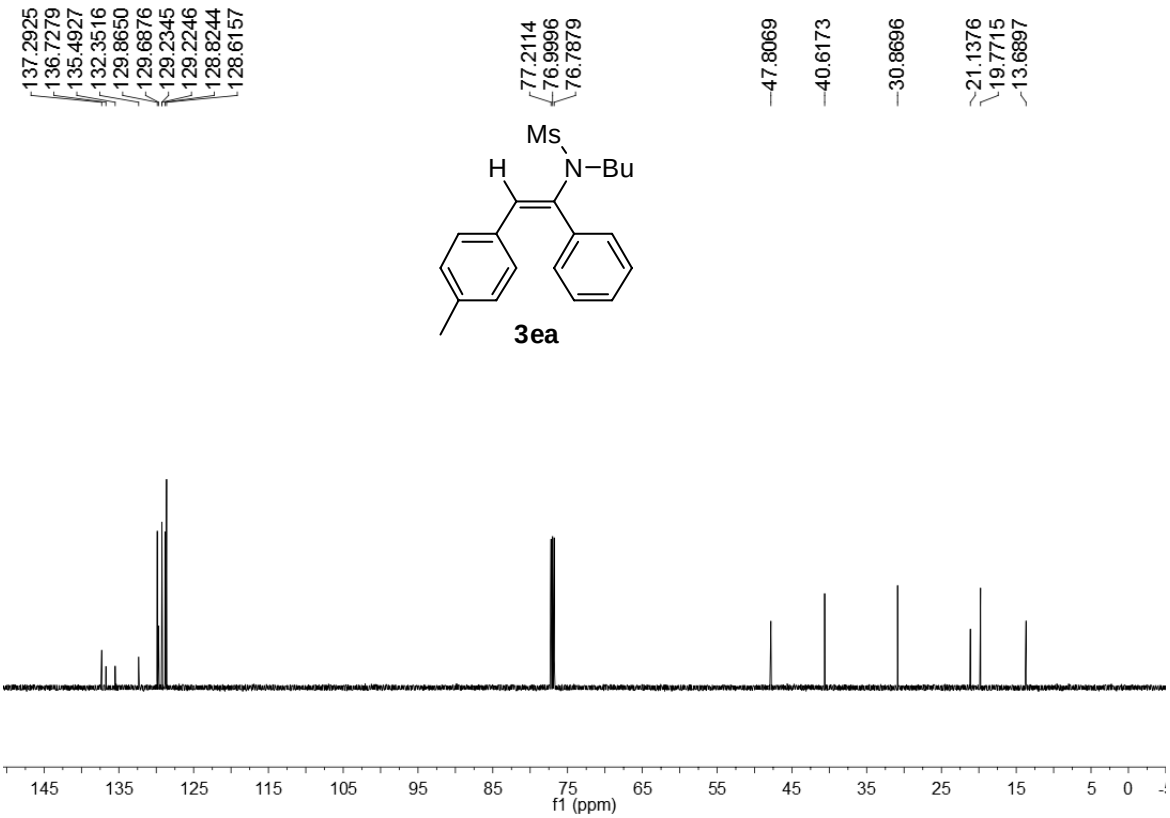
7.3100
7.3042
6.9570
6.9433
6.9289
6.9152
3.3621
3.3497
3.3371
3.0238
2.2635
1.6208
1.6083
1.5959
1.3567
1.3442
1.3317
0.9190
0.9067
0.8945
Ms
H
N−Bu
3ea
5.03
2.01
2.00
1.00
2.01
3.01
3.02
2.03
2.02
3.01
f1 (ppm)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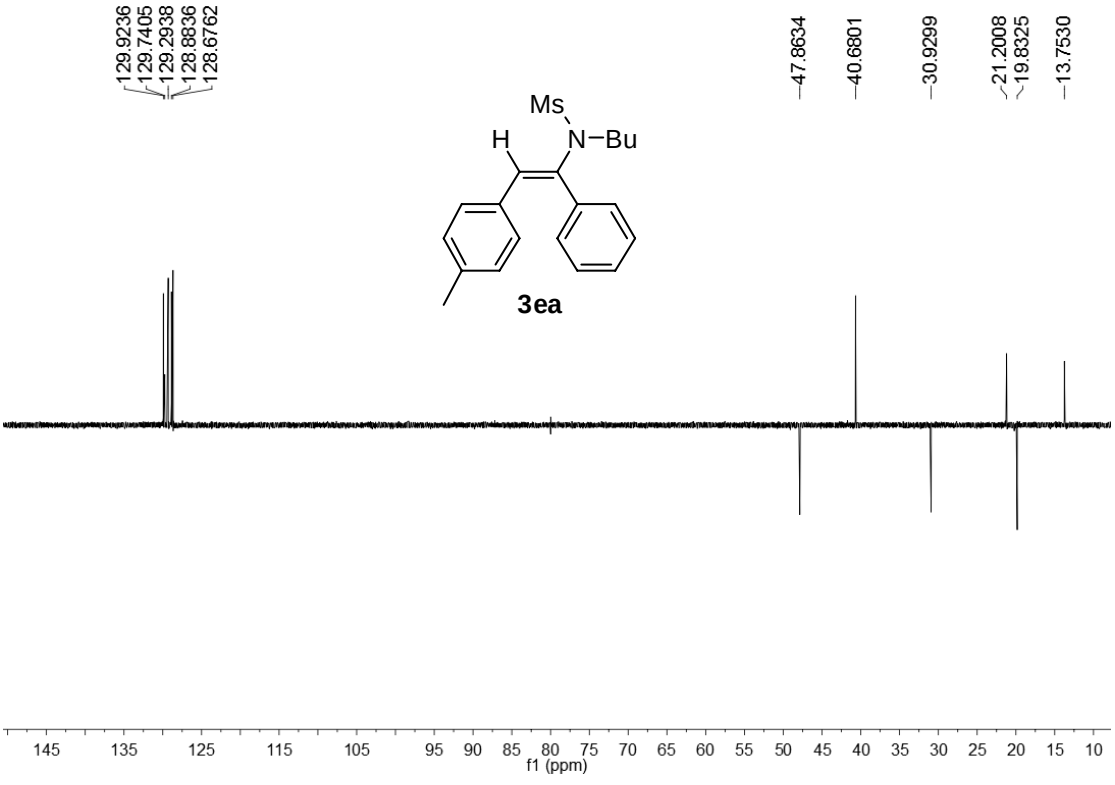
135.4927
132.3516
129.8650
129.6876
129.2345
129.2246
128.8244
128.6157
77.2114
76.9996
76.7879
47.8069
40.6173
30.8696
21.1376
19.7715
13.6897
Ms
H
N−Bu
3ea
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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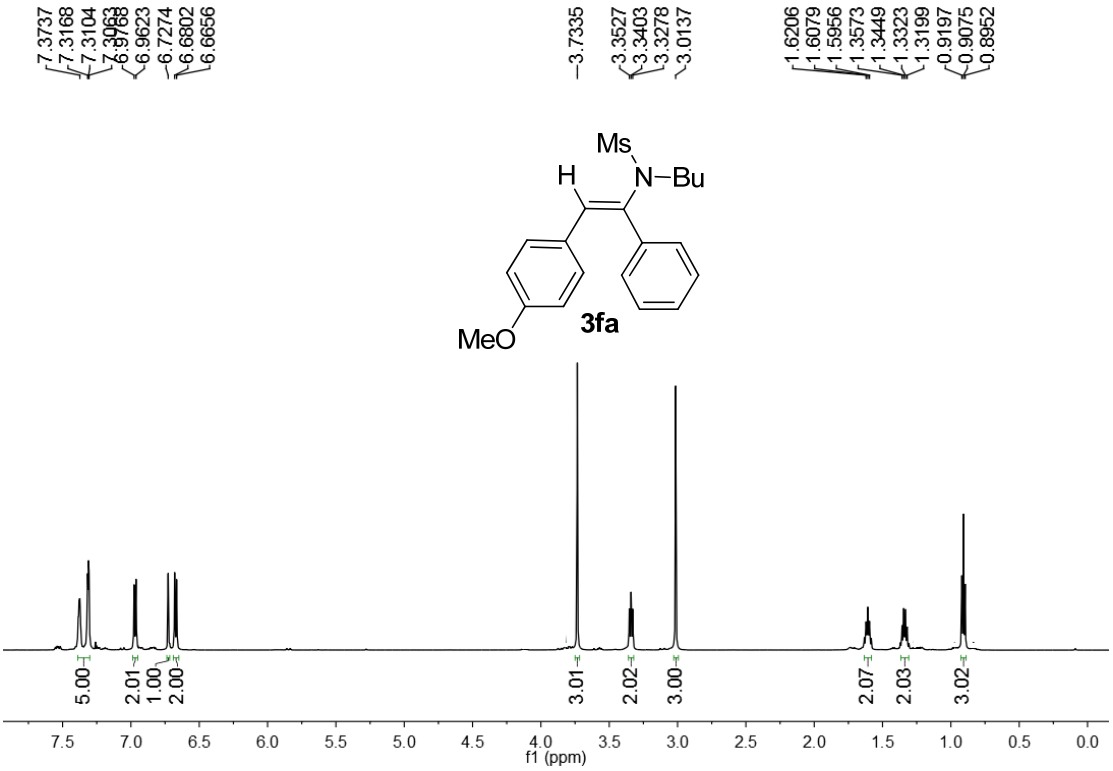
129.2938
128.8836
128.6762
47.8634
40.6801
30.9299
21.2008
19.8325
13.7530
Ms
H
N−Bu
3ea
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)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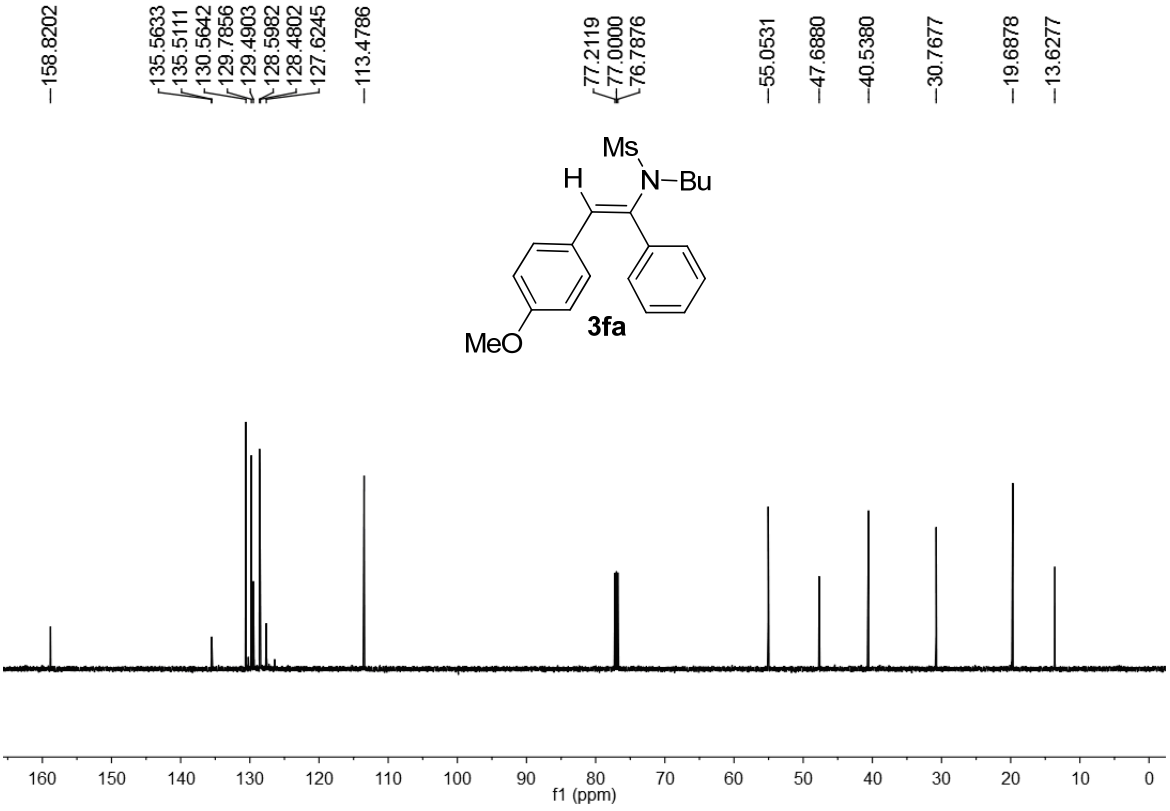
6.9768
6.9623
6.7274
6.6802
6.6656
3.7335
3.3527
3.3403
3.3278
3.0137
1.6206
1.6079
1.5956
1.3573
1.3449
1.3323
1.3199
0.9197
0.9075
0.8952
Ms
H
N–Bu
MeO
3fa
5.00
2.01
1.00
2.00
3.01
2.02
3.00
2.07
2.03
3.02
f1 (ppm)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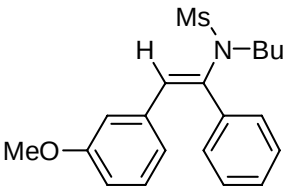
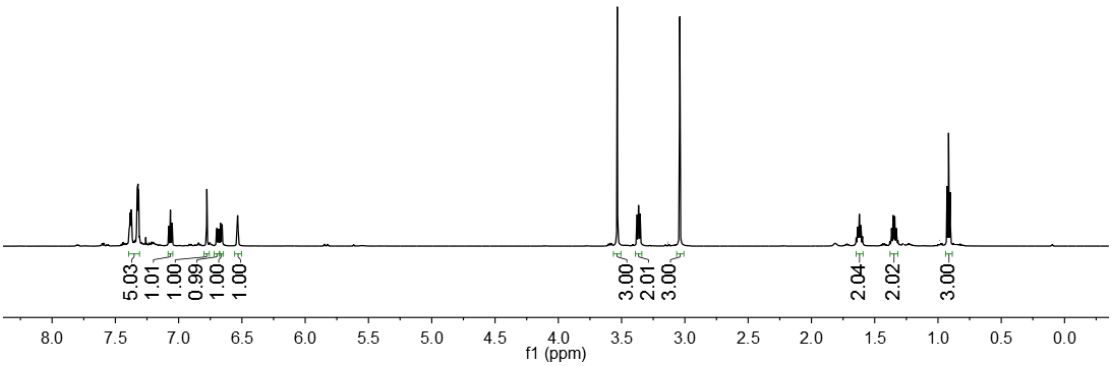
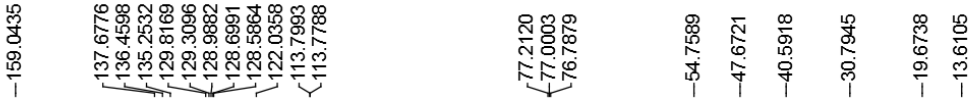
135.5111
130.5642
129.7856
129.4903
128.5982
128.4802
127.6245
113.4786
77.2119
77.0000
76.7876
55.0531
47.6880
40.5380
30.7677
19.6878
13.6277
Ms
H
N–Bu
MeO
3fa
f1 (ppm)


7.3833
7.3773
7.3734
7.3269
7.3207
7.3160
7.0781
7.0649
7.0516
6.7768
6.6998
6.6961
6.6862
6.6825
6.6693
6.6566
6.5341
3.5342
3.3784
3.3660
3.3535
3.0400
1.6342
1.6215
1.6091
1.3667
1.3542
1.3416
1.3292
0.9283
0.9161
0.9037


Ms
H
N—Bu
MeO

3ga


5.03
1.01
1.00
0.99
1.00
1.00
3.00
2.01
3.00
2.04
2.02
3.00
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)


159.0435
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136.4598
135.2532
129.8169
129.3096
128.9882
128.6991
128.5864
122.0358
113.7993
113.7788
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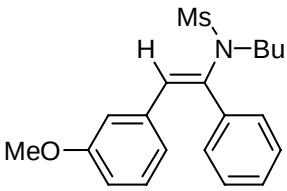
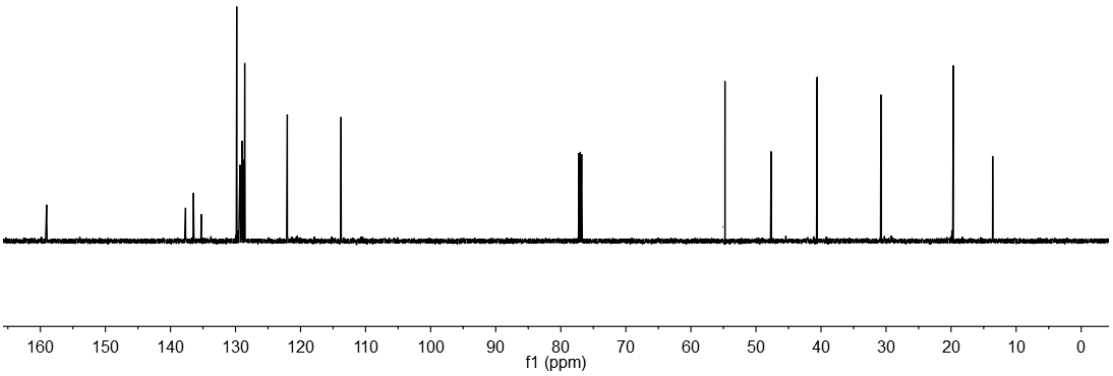
77.0003
76.7879
54.7589
47.6721
40.5918
30.7945
19.6738
13.6105


Ms
H
N—Bu
MeO

3ga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90
80
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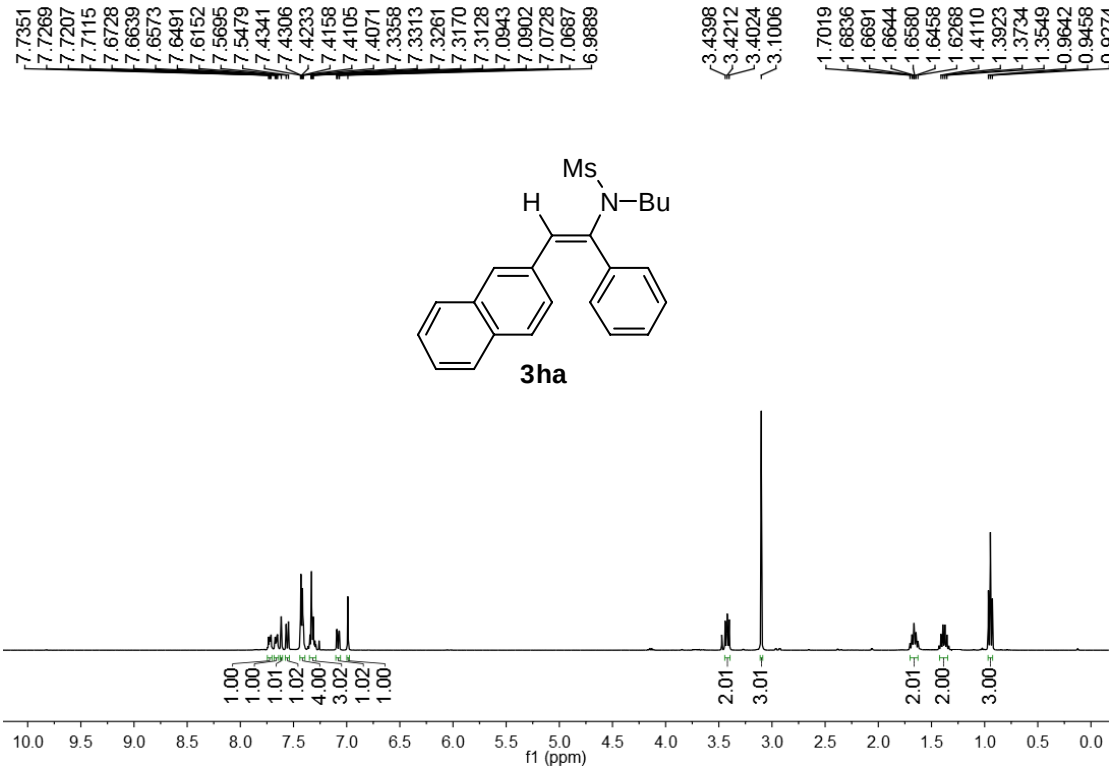
60
50
40
30
20
10
0
f1 (ppm)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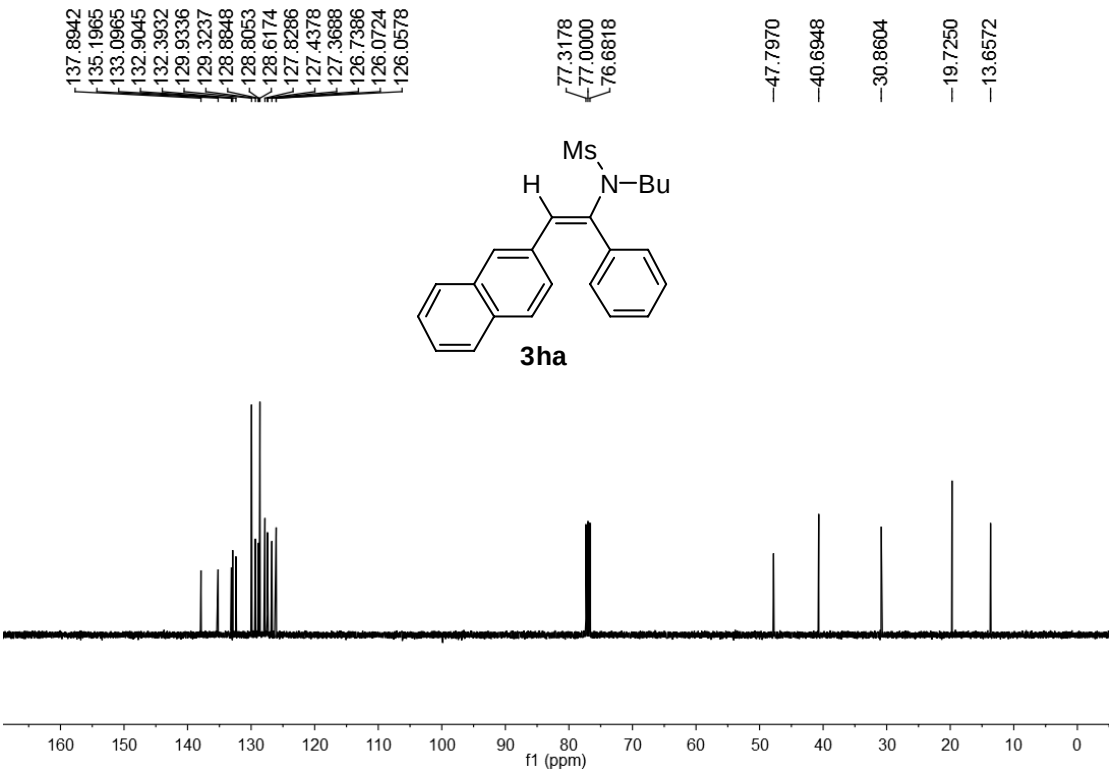
7.6573
7.6491
7.6152
7.5695
7.5479
7.4341
7.4306
7.4233
7.4158
7.4105
7.4071
7.3358
7.3313
7.3261
7.3170
7.3128
7.0943
7.0902
7.0728
7.0687
6.9889
3.4398
3.4212
3.4024
3.1006
1.7019
1.6836
1.6691
1.6644
1.6580
1.6458
1.6268
1.4110
1.3923
1.3734
1.3549
0.9642
0.9458
Ms
H
N—Bu
3ha
1.00
1.00
1.01
1.02
4.00
3.02
1.02
1.00
2.01
3.01
2.01
2.00
3.00
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)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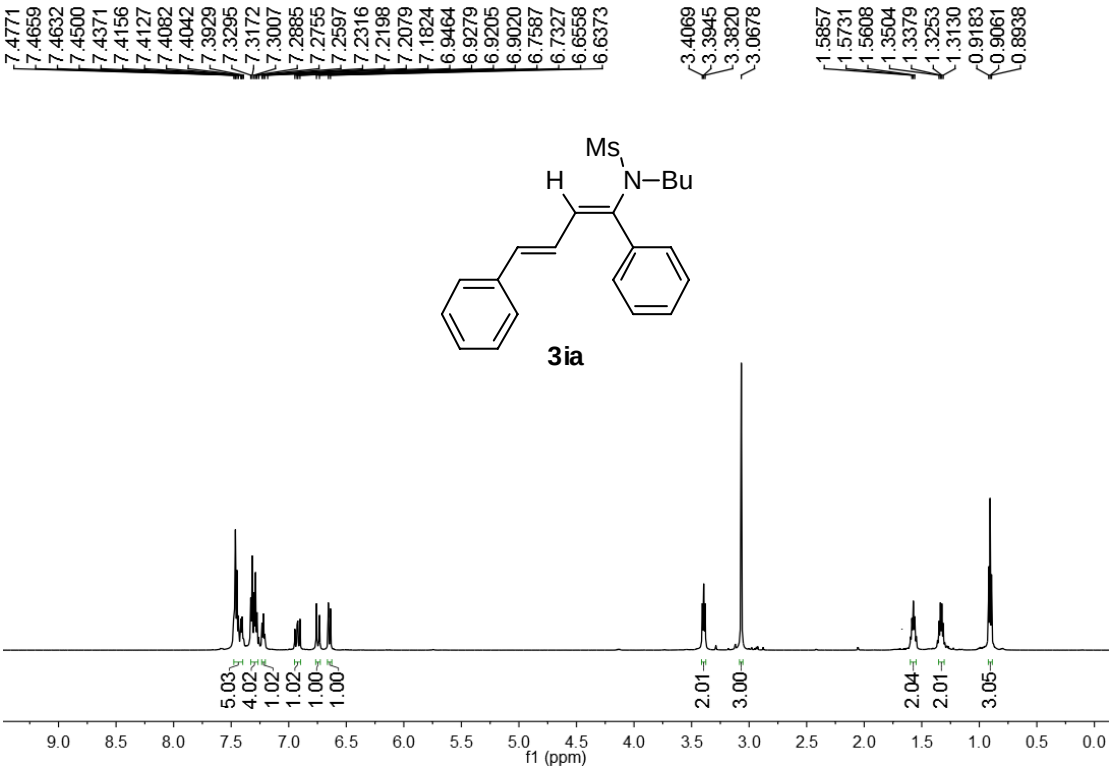
127.8286
127.4378
127.3688
126.7386
126.0724
126.0578
77.3178
77.0000
76.6818
47.7970
40.6948
30.8604
19.7250
13.6572
Ms
H
N—Bu
3ha
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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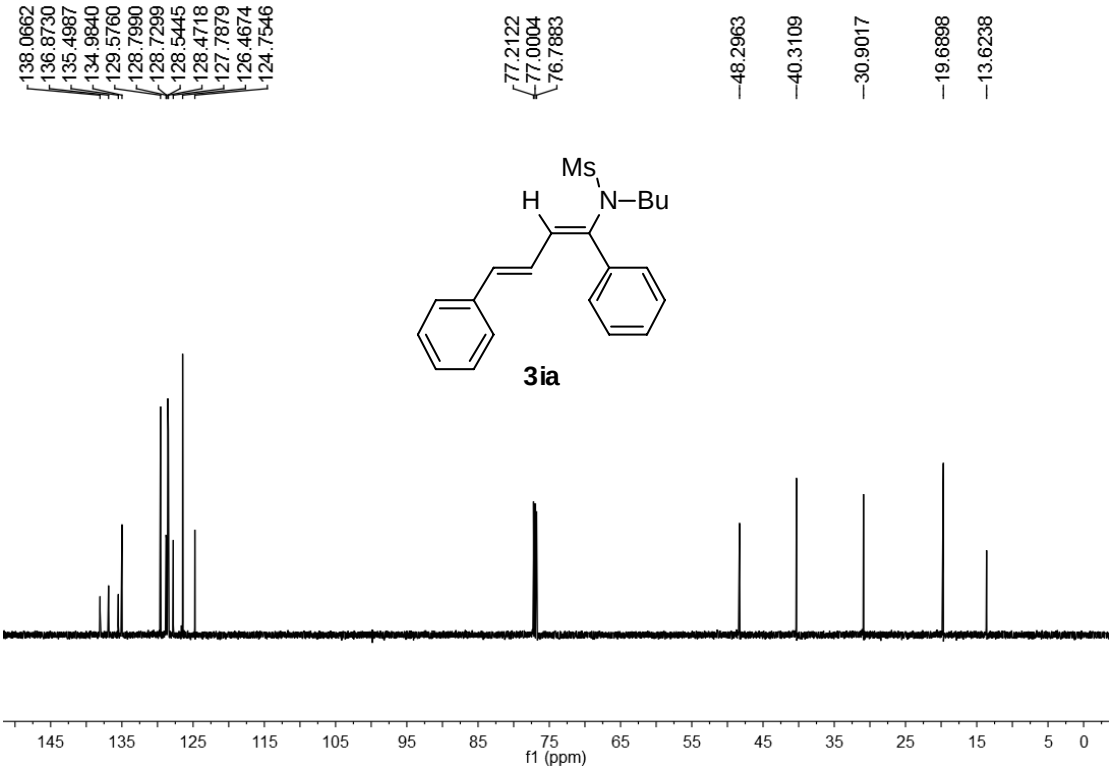
7.4500
7.4371
7.4156
7.4127
7.4082
7.4042
7.3929
7.3295
7.3172
7.3007
7.2885
7.2755
7.2597
7.2316
7.2198
7.2079
7.1824
6.9464
6.9279
6.9205
6.9020
6.7587
6.7327
6.6558
6.6373
3.4069
3.3945
3.3820
3.0678
1.5857
1.5731
1.5608
1.3504
1.3379
1.3253
1.3130
0.9183
0.9061
0.8938
Ms
H
N–Bu
3ia
5.03
4.02
1.02
1.02
1.00
1.00
2.01
3.00
2.04
2.01
3.05
f1 (ppm)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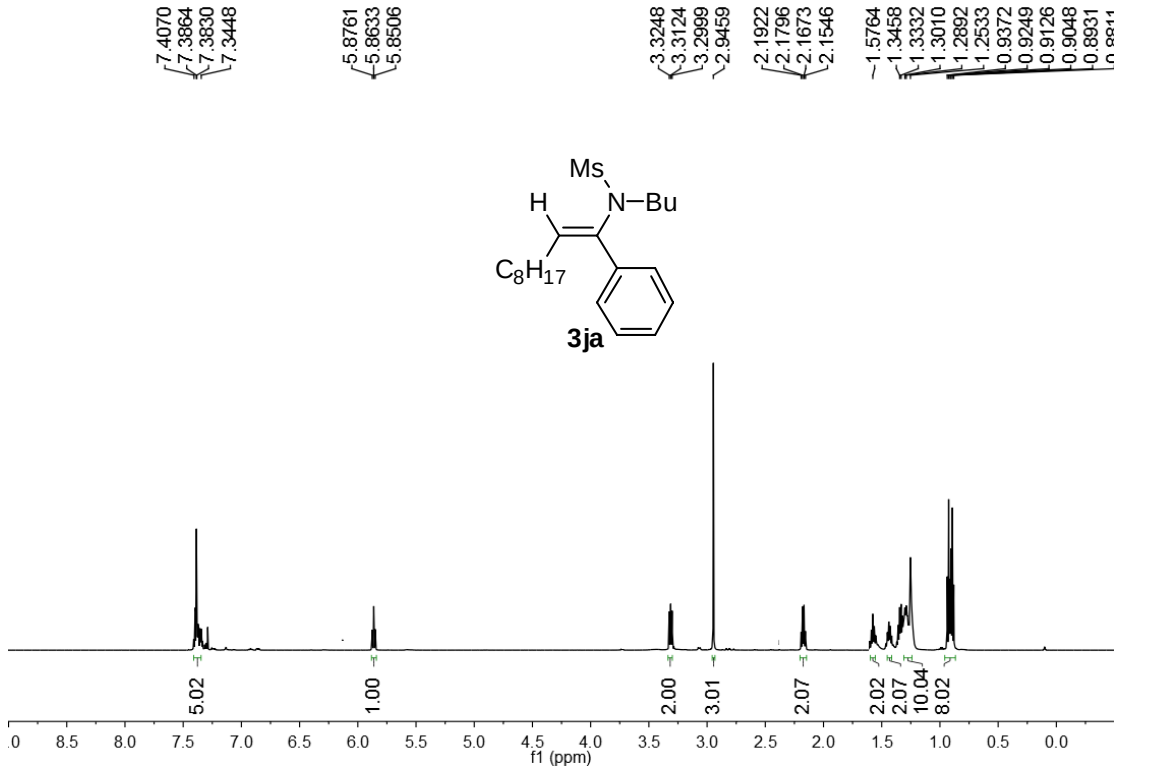
136.8730
135.4987
134.9840
129.5760
128.7990
128.7299
128.5445
128.4718
127.7879
126.4674
124.7546
77.2122
77.0004
76.7883
48.2963
40.3109
30.9017
19.6898
13.6238
Ms
H
N–Bu
3ia
f1 (ppm)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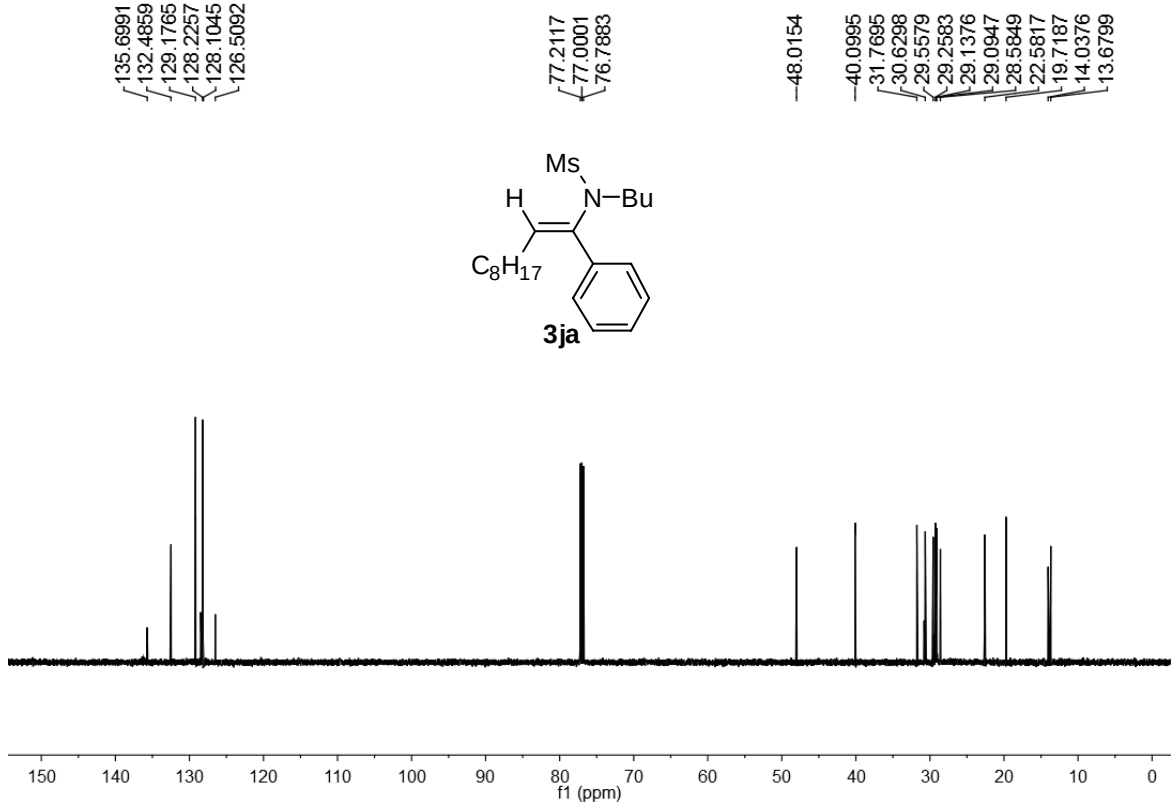
7.3864
7.3830
7.3448
5.8761
5.8633
5.8506
3.3248
3.3124
3.2999
2.9459
2.1922
2.1796
2.1673
2.1546
1.5764
1.3458
1.3332
1.3010
1.2892
1.2533
0.9372
0.9249
0.9126
0.9048
0.8931
Ms
H
N–Bu
C8H17
3ja
5.02
1.00
2.00
3.01
2.07
2.02
2.07
10.04
8.02
f1 (ppm)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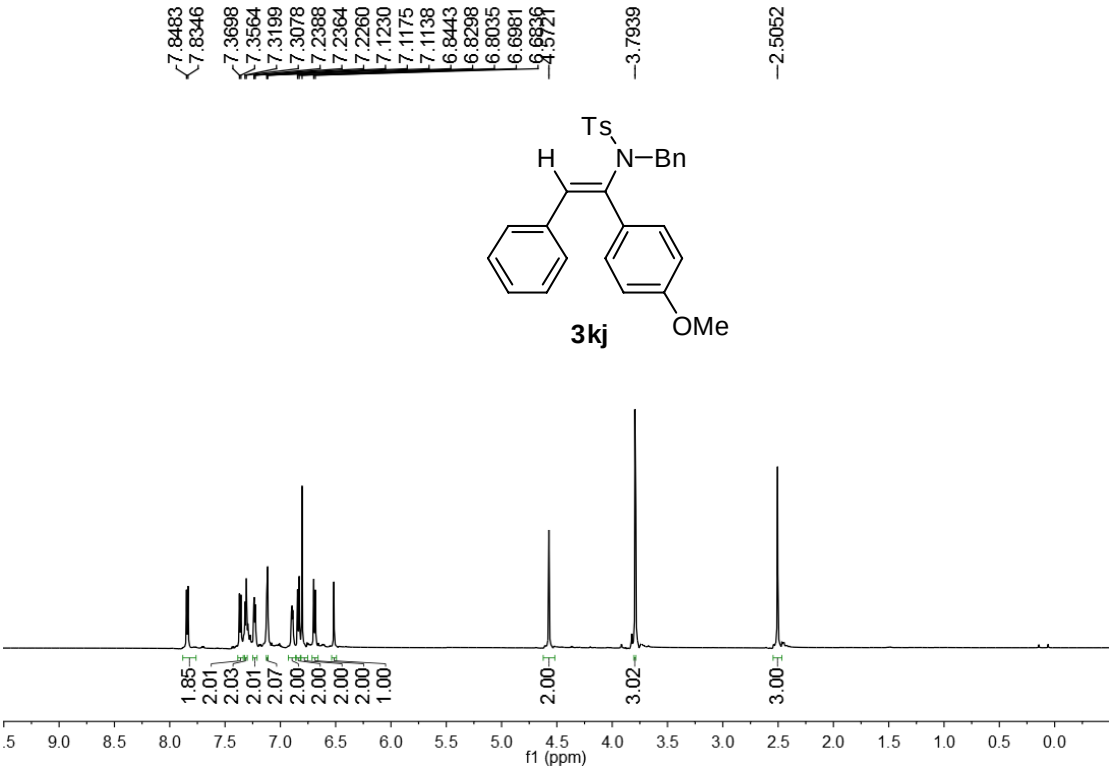
128.2257
128.1045
126.5092
77.2117
77.0001
76.7883
48.0154
40.0995
31.7695
30.6298
29.5579
29.2583
29.1376
29.0947
28.5849
22.5817
19.7187
14.0376
13.6799
Ms
H
N–Bu
C8H17
3ja
f1 (ppm)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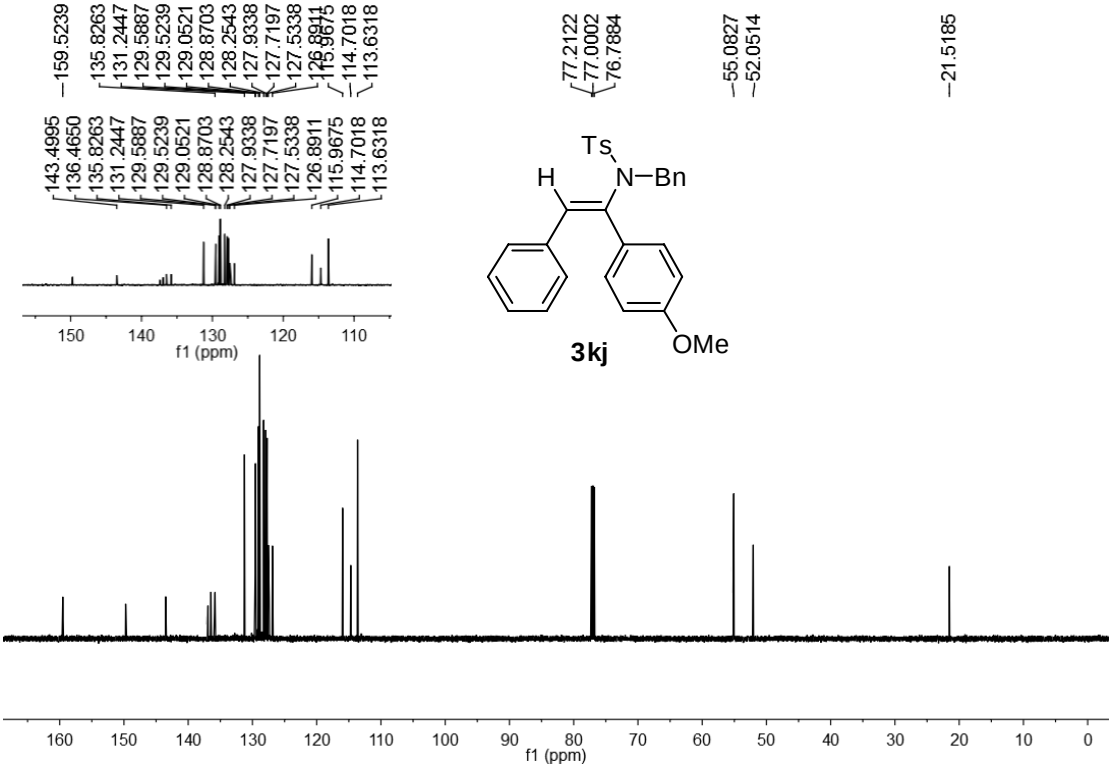
7.3698
7.3564
7.3199
7.3078
7.2388
7.2364
7.2260
7.1230
7.1175
7.1138
6.8443
6.8298
6.8035
6.6981
4.5721
3.7939
2.5052
Ts
H
N—Bn
OMe
3kj
1.85
2.01
2.03
2.01
2.07
2.00
2.00
2.00
2.00
1.00
2.00
3.02
3.00
f1 (ppm)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131.2447
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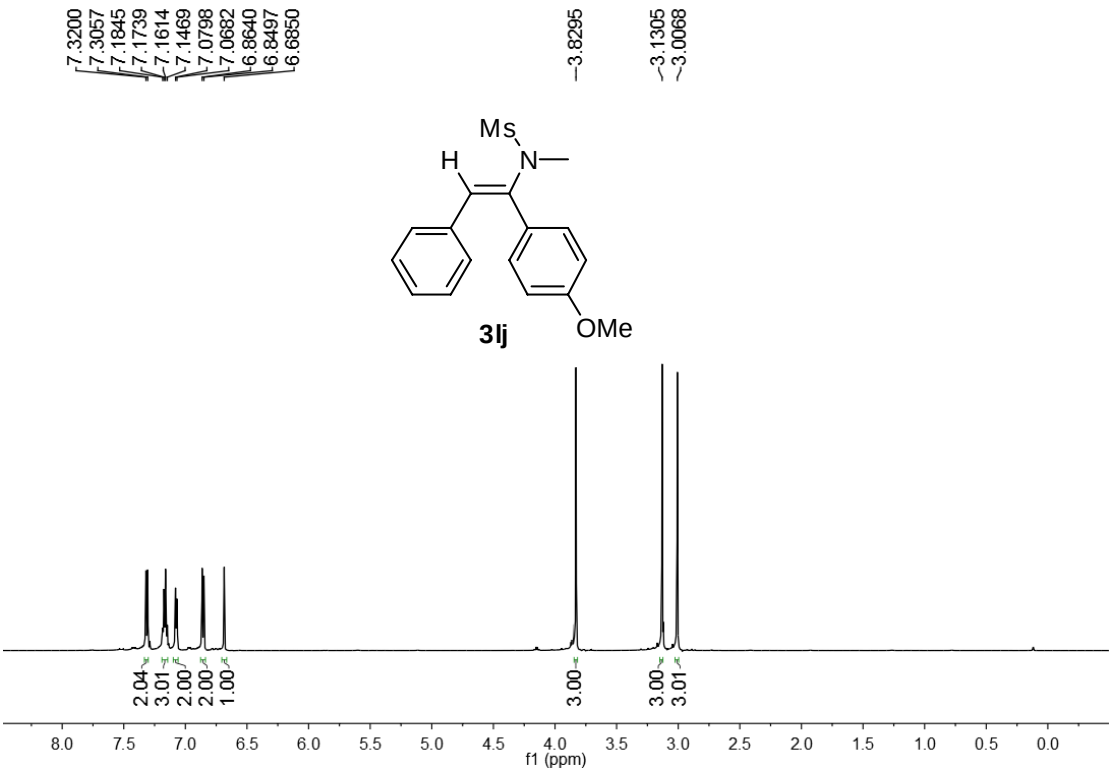
129.5239
129.0521
128.8703
128.2543
127.9338
127.7197
127.5338
126.8911
115.9675
114.7018
113.6318
77.2122
77.0002
76.7884
55.0827
52.0514
21.5185
143.4995
136.4650
Ts
H
N—Bn
OMe
3kj
f1 (ppm)
f1 (ppm)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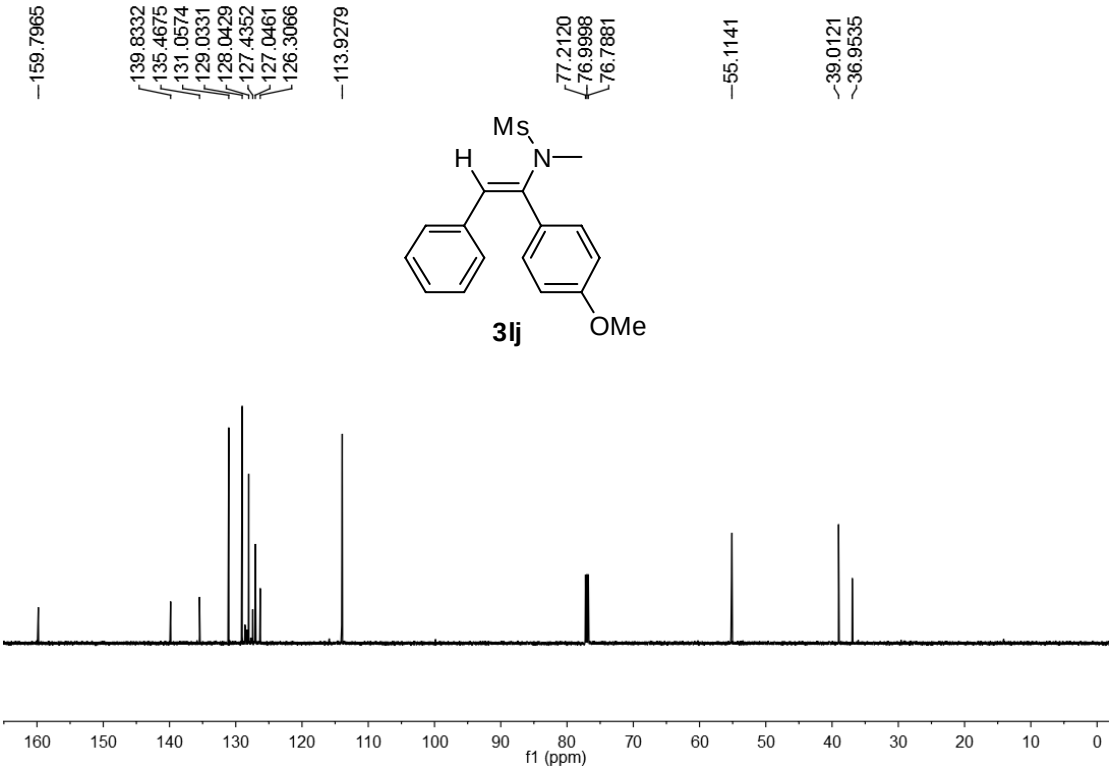
7.1739
7.1614
7.1469
7.0798
7.0682
6.8640
6.8497
6.6850
3.8295
3.1305
3.0068
Ms
H
N
OMe
3lj
2.04
3.01
2.00
2.00
1.00
3.00
3.00
3.01
f1 (ppm)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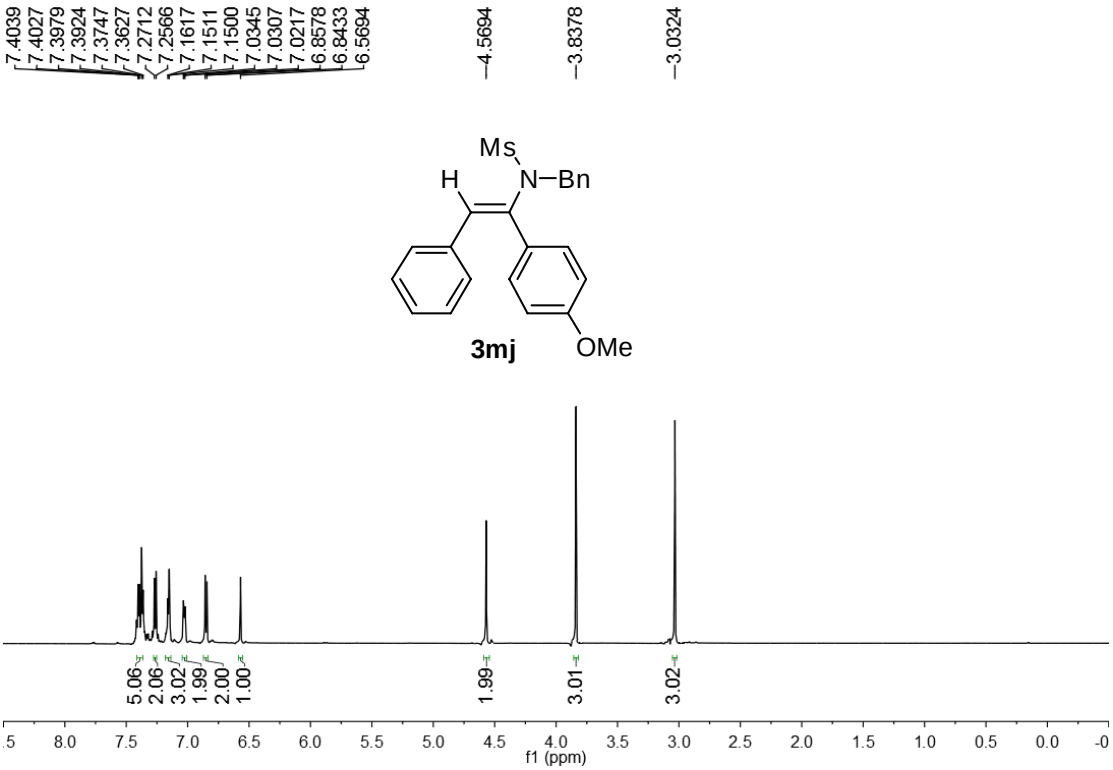
139.8332
135.4675
131.0574
129.0331
128.0429
127.4352
127.0461
126.3066
113.9279
77.2120
76.9998
76.7881
55.1141
39.0121
36.9535
Ms
H
N
OMe
3lj
f1 (ppm)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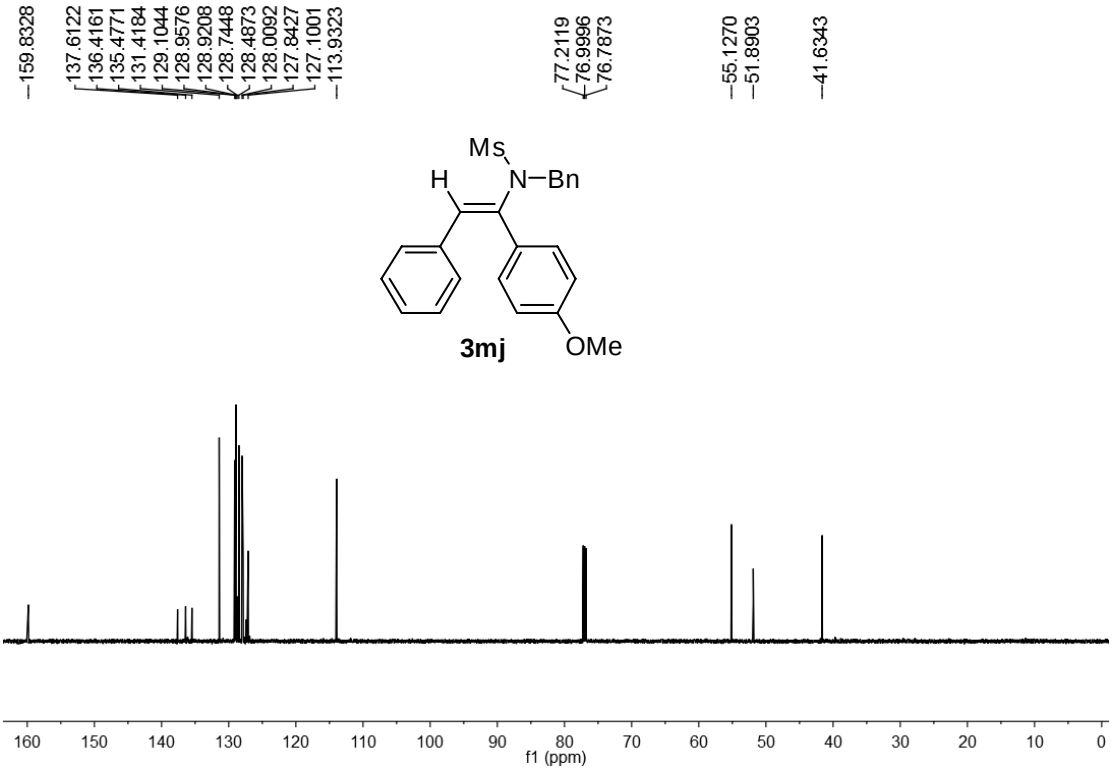
7.4027
7.3979
7.3924
7.3747
7.3627
7.2712
7.2566
7.1617
7.1511
7.1500
7.0345
7.0307
7.0217
6.8578
6.8433
6.5694
4.5694
3.8378
3.0324
Ms
H
N–Bn
OMe
3mj
5.06
2.06
3.02
1.99
2.00
1.00
1.99
3.01
3.02
f1 (ppm)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131.4184
129.1044
128.9576
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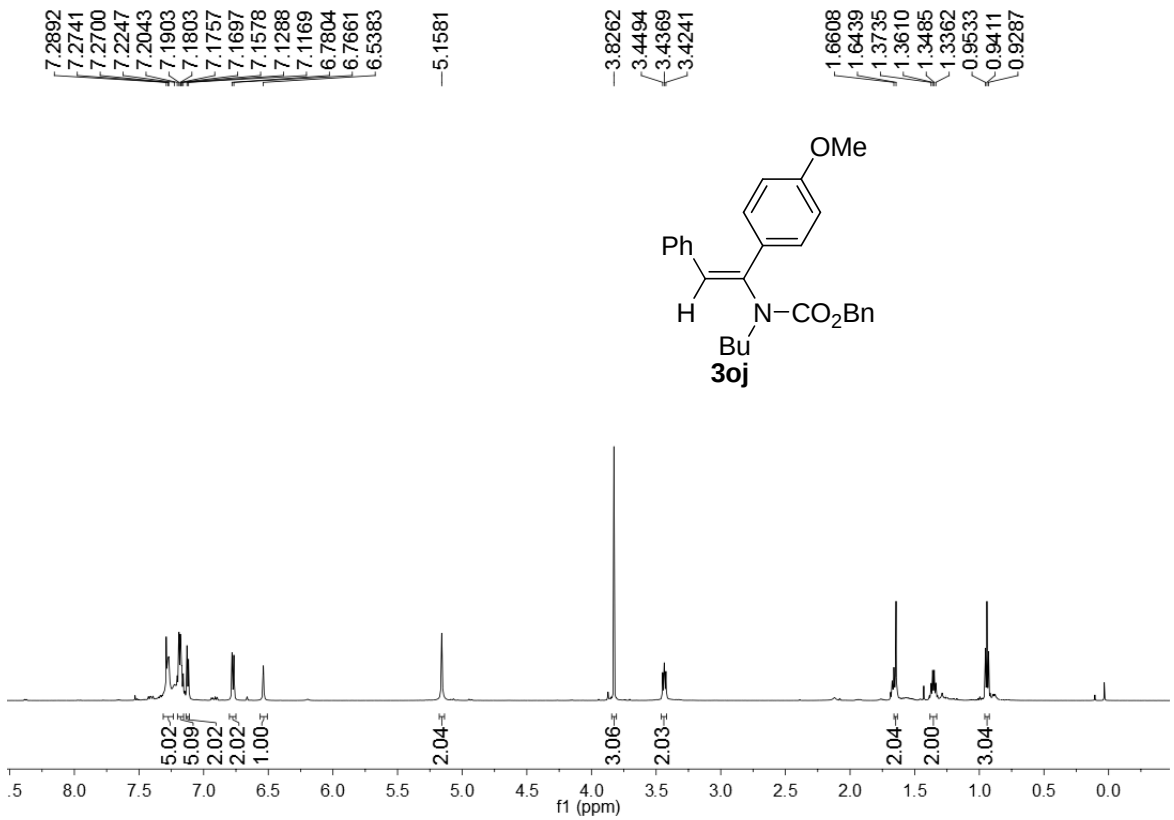
128.7448
128.4873
128.0092
127.8427
127.1001
113.9323
77.2119
76.9996
76.7873
55.1270
51.8903
41.6343
Ms
H
N–Bn
OMe
3mj
f1 (ppm)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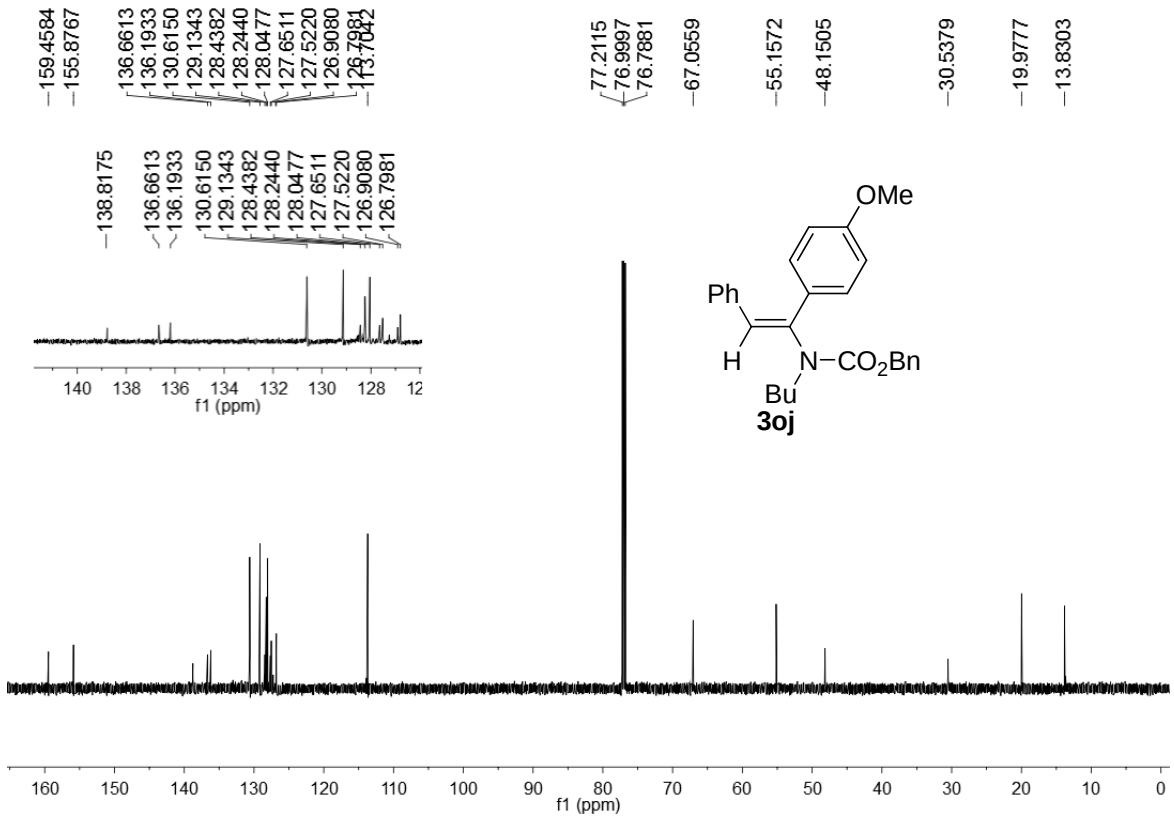
7.2043
7.1903
7.1803
7.1757
7.1697
7.1578
7.1288
7.1169
6.7804
6.7661
6.5383
5.1581
3.8262
3.4494
3.4369
3.4241
1.6608
1.6439
1.3735
1.3610
1.3485
1.3362
0.9533
0.9411
0.9287
OMe
Ph
H
N−CO2Bn
Bu
3oj
5.02
5.09
2.02
2.02
1.00
2.04
3.06
2.03
2.04
2.00
3.04
f1 (ppm)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136.1933
130.6150
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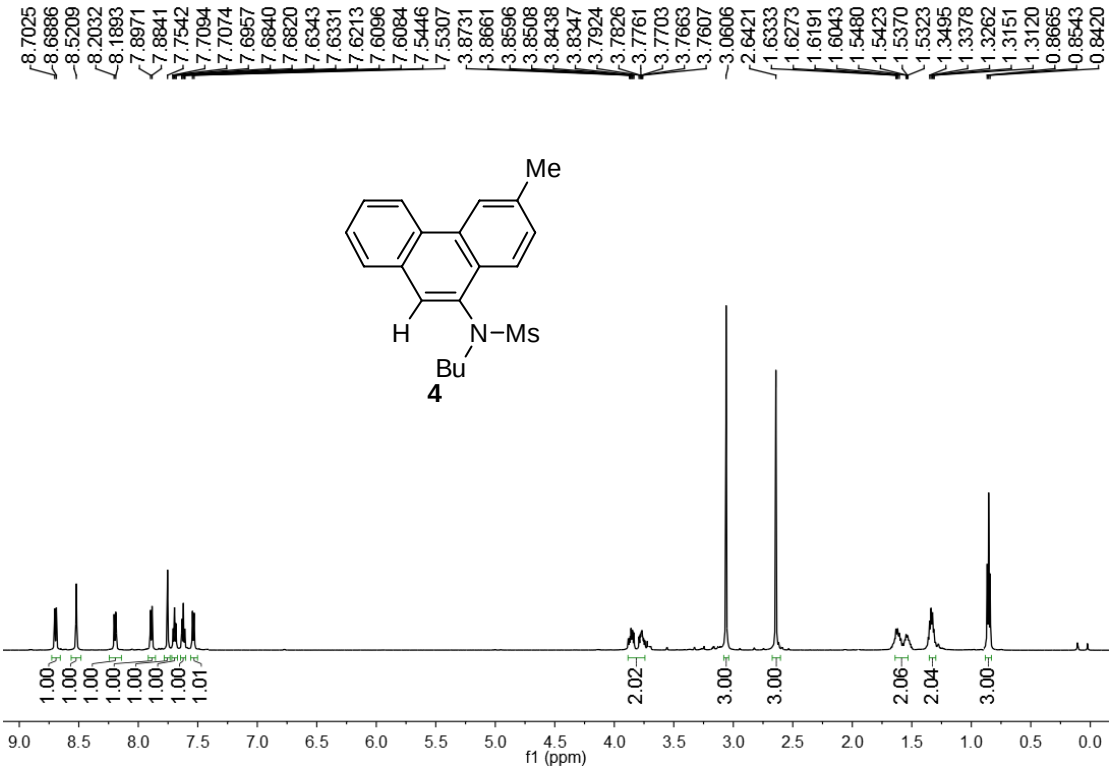
128.4382
128.2440
128.0477
127.6511
127.5220
126.9080
126.7981
113.7042
77.2115
76.9997
76.7881
67.0559
55.1572
48.1505
30.5379
19.9777
13.8303
138.8175
OMe
Ph
H
N−CO2Bn
Bu
3oj
f1 (ppm)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8.2032
8.1893
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7.8841
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7.7094
7.7074
7.6957
7.6840
7.6820
7.6343
7.6331
7.6213
7.6096
7.6084
7.5446
7.5307
3.8731
3.8661
3.8596
3.8508
3.8438
3.8347
3.7924
3.7826
3.7761
3.7703
3.7663
3.7607
3.0606
2.6421
1.6333
1.6273
1.6191
1.6043
1.5480
1.5423
1.5370
1.5323
1.3495
1.3378
1.3262
1.3151
1.3120
0.8665
0.8543
0.8420
Me
H
N−Ms
Bu
4
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.01
2.02
3.00
3.00
2.06
2.04
3.00
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)


137.2156
134.7195
131.7009
131.2843
130.0389
128.9412
128.8999
128.7031
127.4220
126.8581
126.4770
124.4372
122.6835
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38.1583
31.0051
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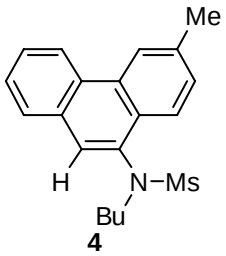
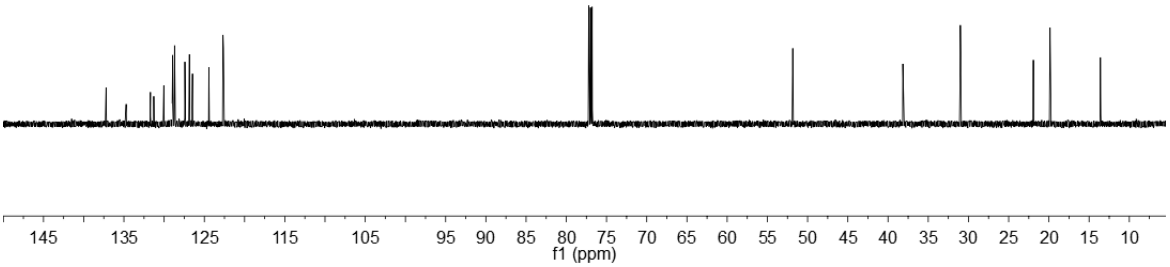
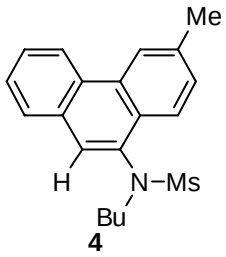
19.8600
13.5963

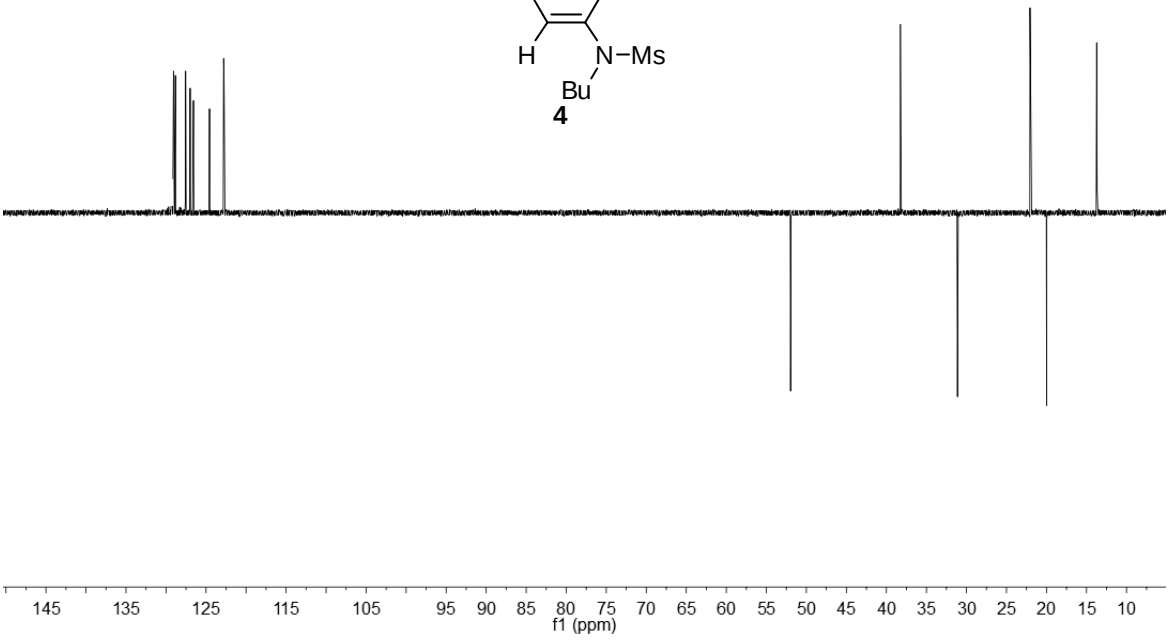

Me
H
N−Ms
Bu

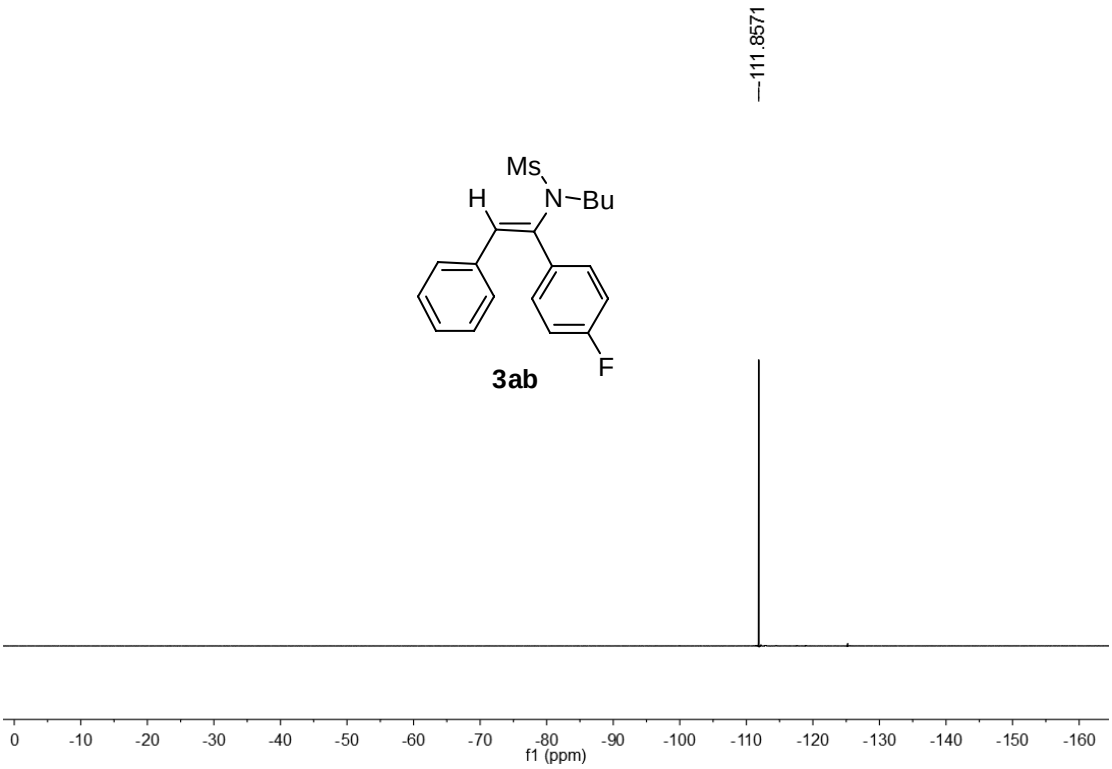
4


145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10
f1 (ppm)

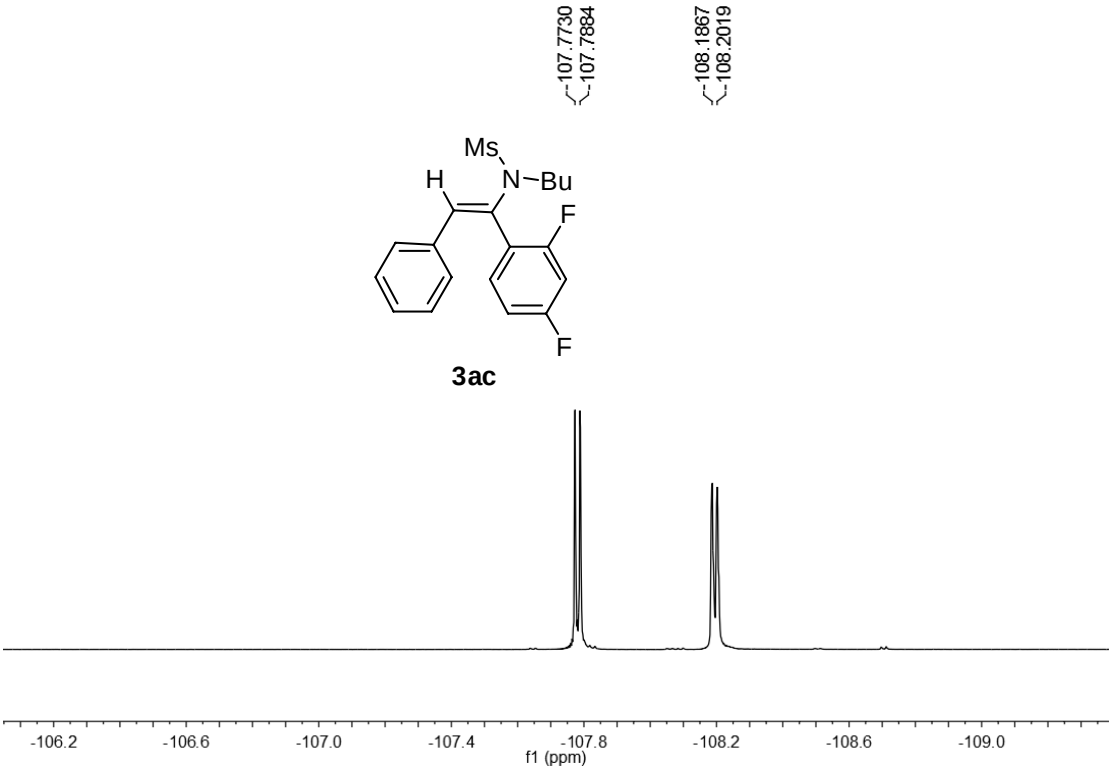

Me
H
N−Ms
Bu

4

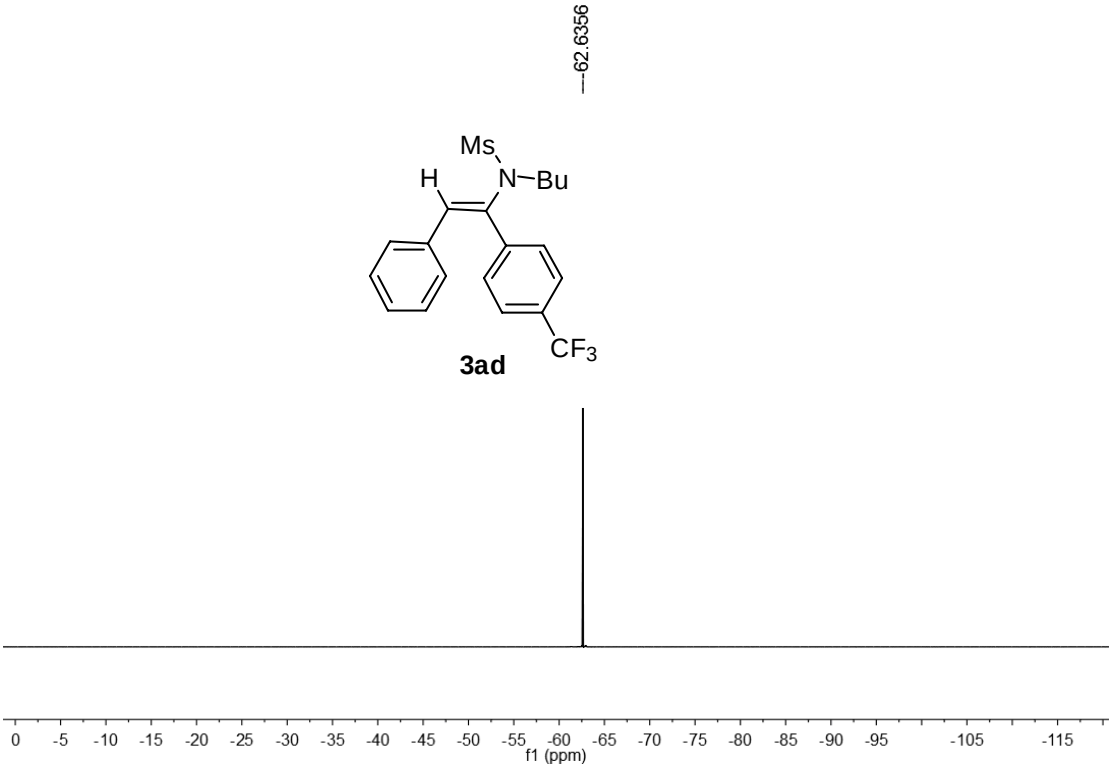

145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10
f1 (ppm)

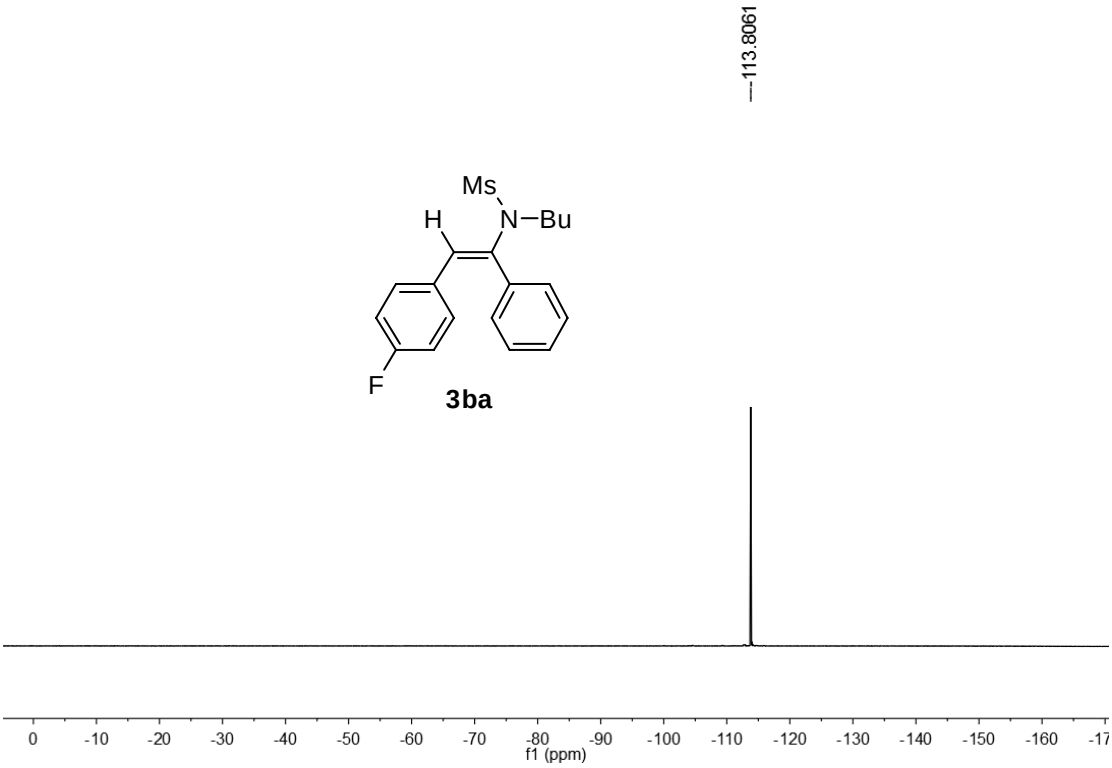

111.8571
Ms
H
N–Bu
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

3ab


107.7730
107.7884
108.1867
108.2019
Ms
H
N–Bu
F
F
-106.2
-106.6
-107.0
-107.4
-107.8
-108.2
-108.6
-109.0
f1 (ppm)

3ac


-62.6356
Ms
H
N–Bu
CF3
3ad
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115
f1 (ppm)


-113.8061
Ms
H
N–Bu
F
3ba
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -17
f1 (ppm)


8.2120
8.1631
8.1608
8.1496
8.1472
7.7532
7.7403
7.4932
7.4800
7.4667
7.2095
7.2060
7.2006
7.1983
7.1680
7.0688
7.0663
7.0601
7.0539
6.9151
3.4687
3.4562
3.4435
3.1230
1.7021
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1.6647
1.6519
1.4135
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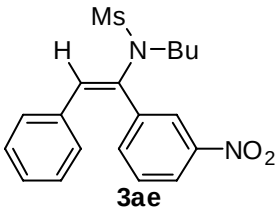
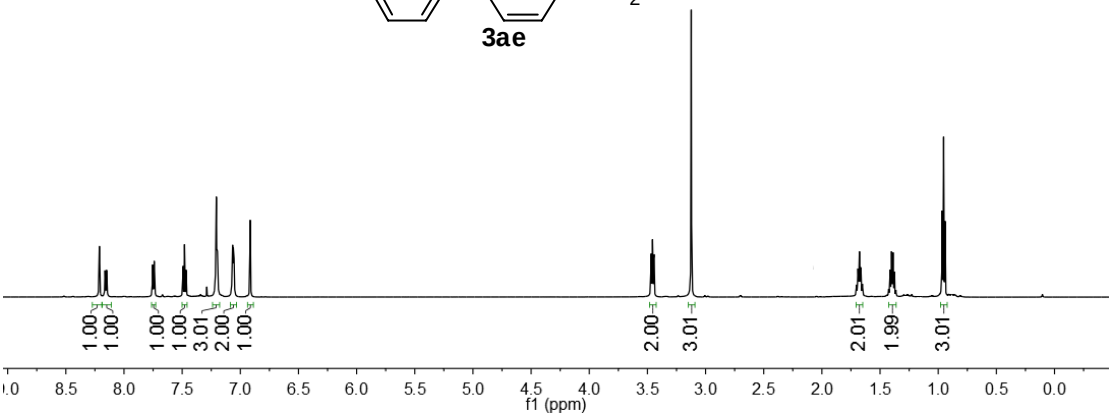
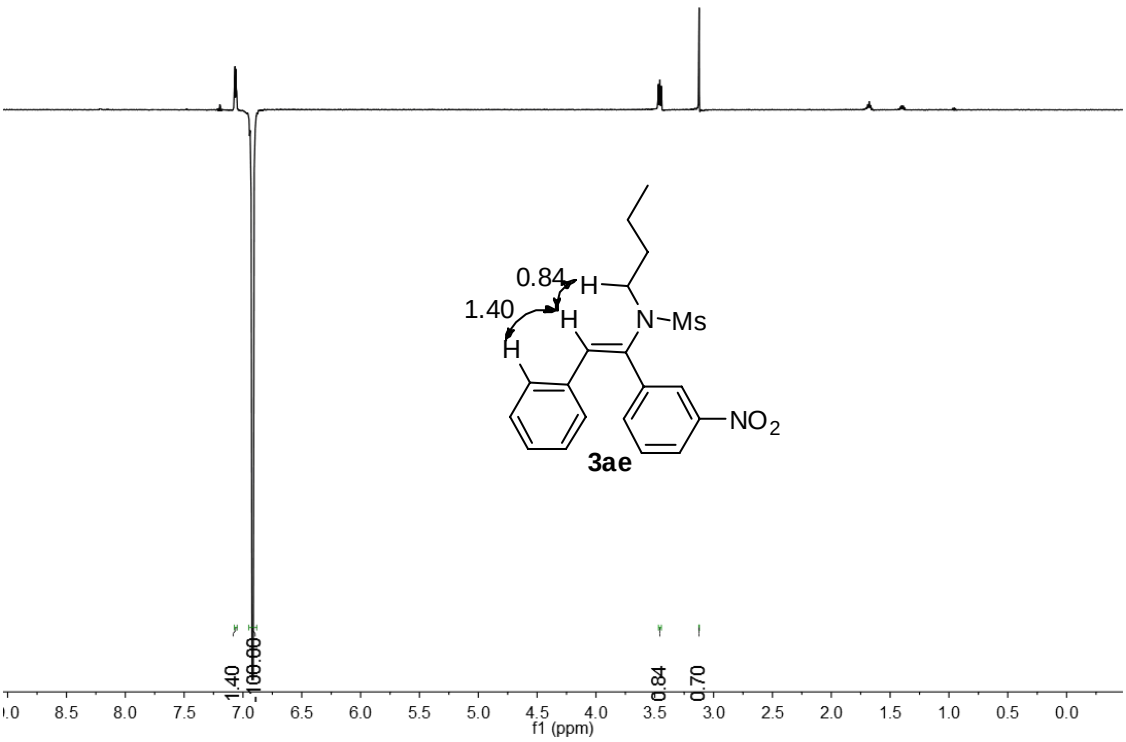
1.3885
0.9680
0.9538
0.9415

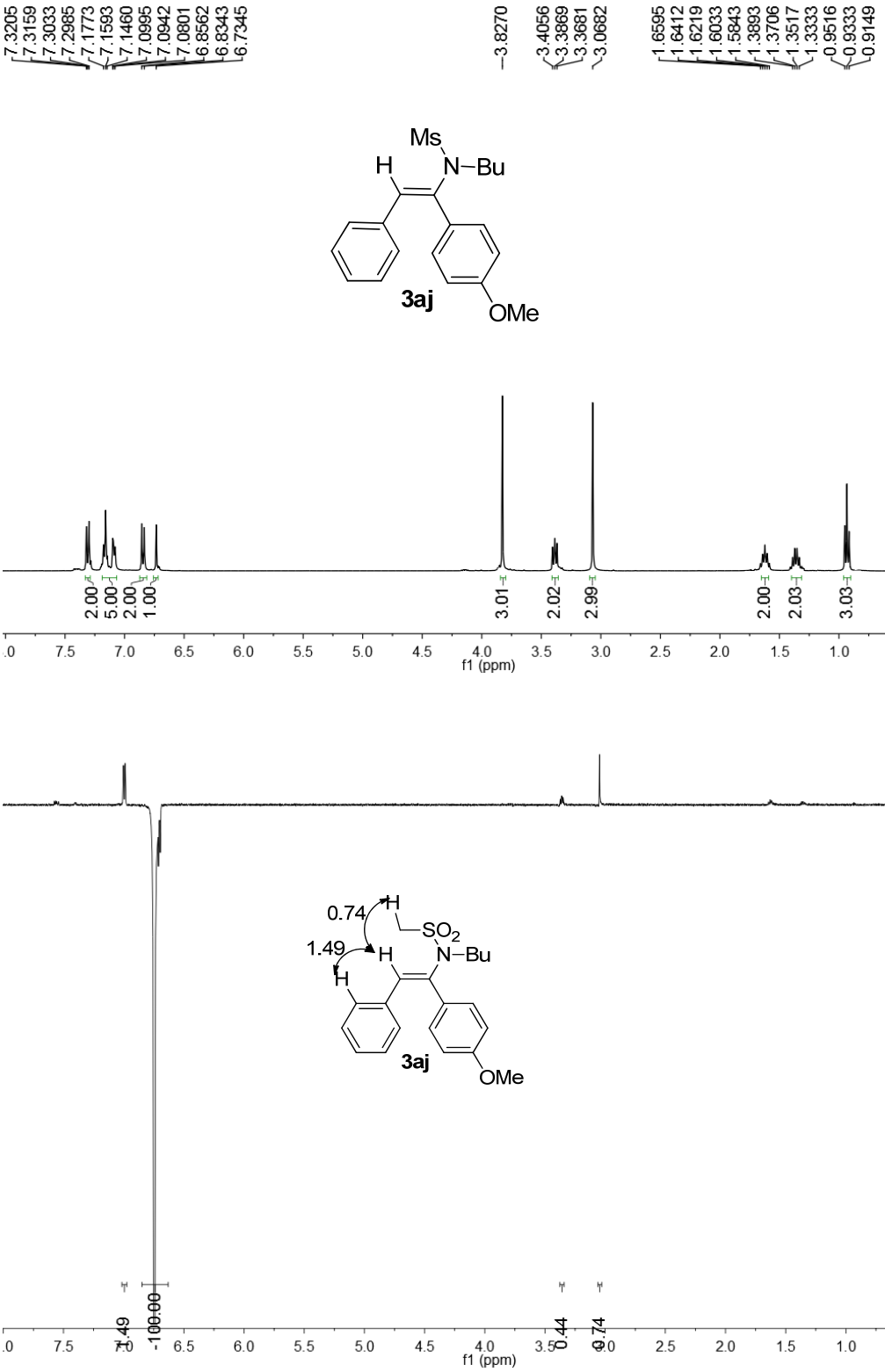

Ms
H
N−Bu
NO2

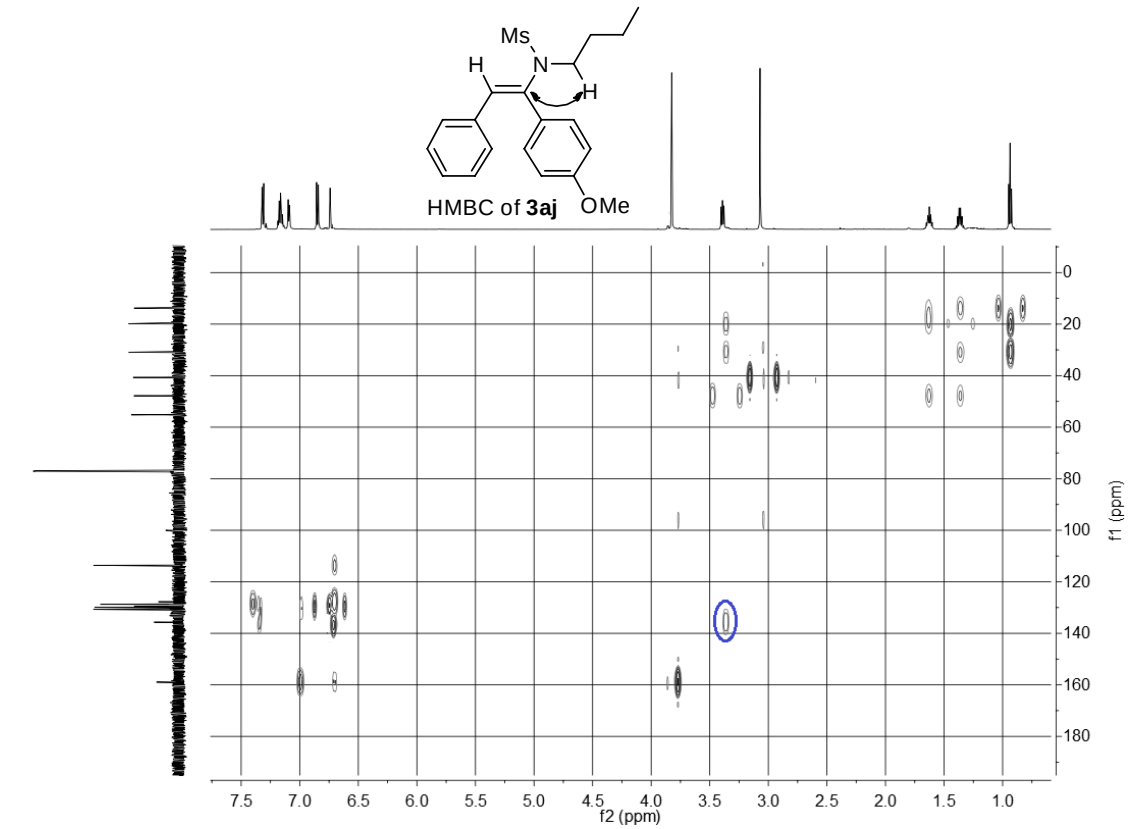
3ae

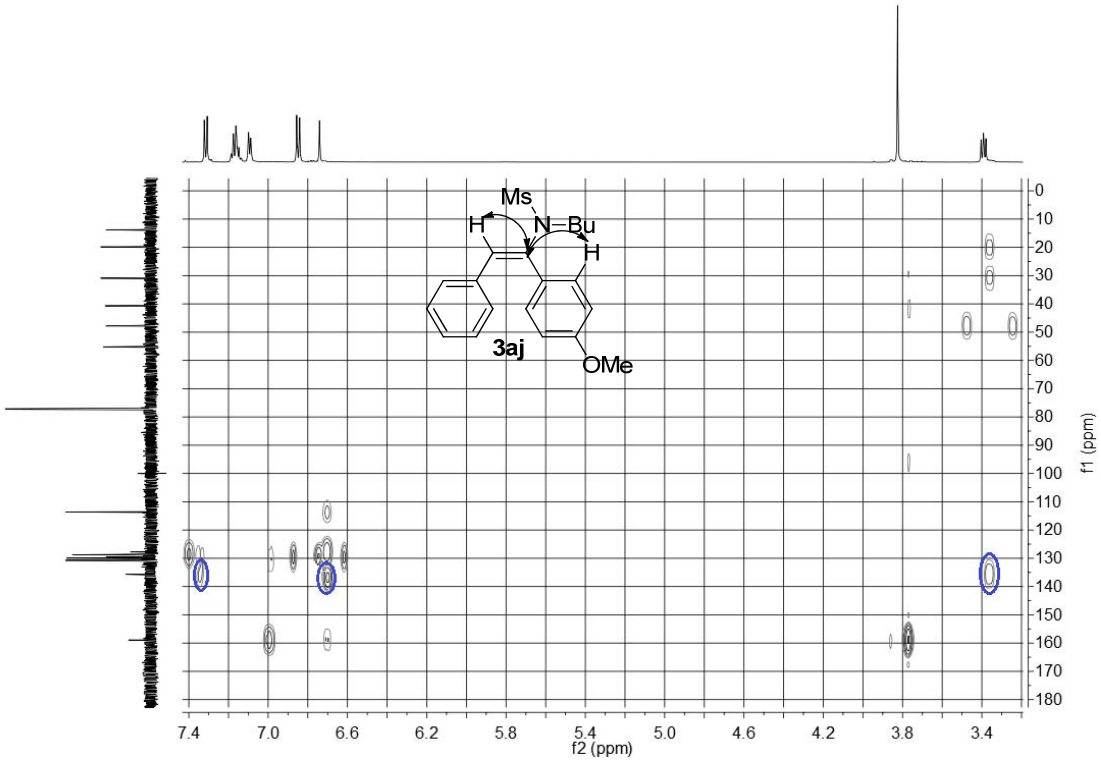

1.00
1.00
1.00
1.00
3.01
2.00
1.00
2.00
3.01
2.01
1.99
3.01
f1 (ppm)

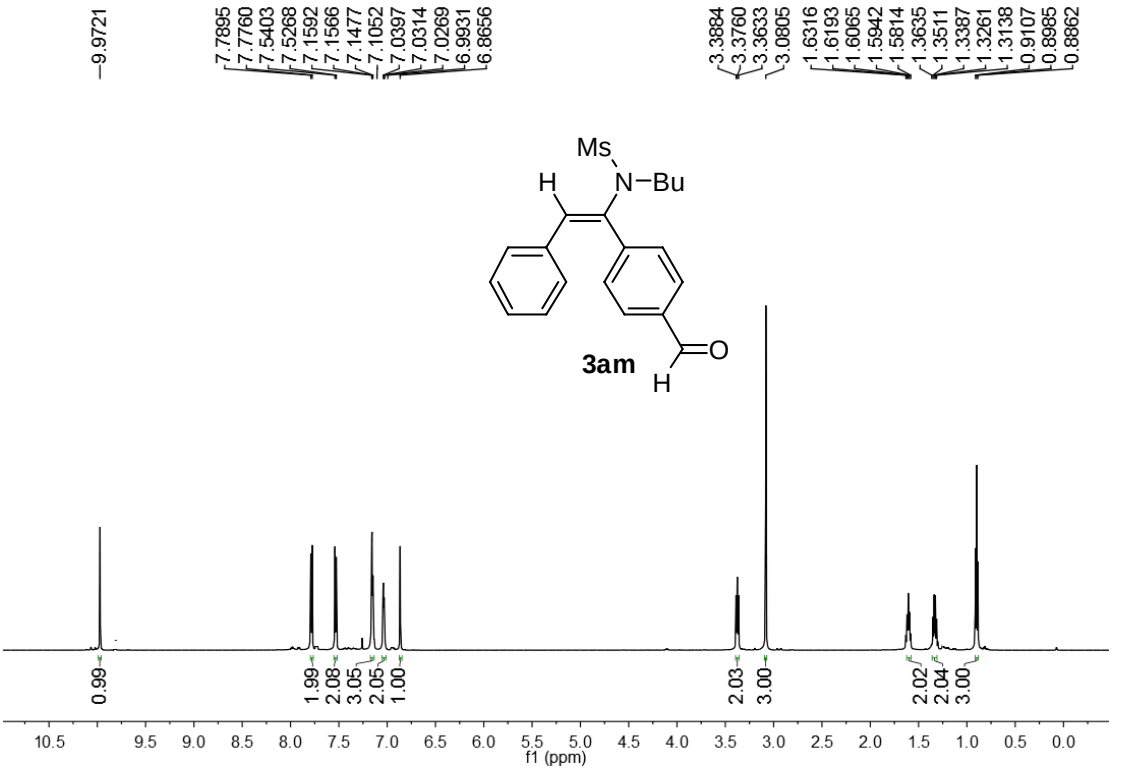

0.84
H
1.40
H
H
N−Ms
NO2
1.40
-100.00
0.84
0.70
f1 (ppm)

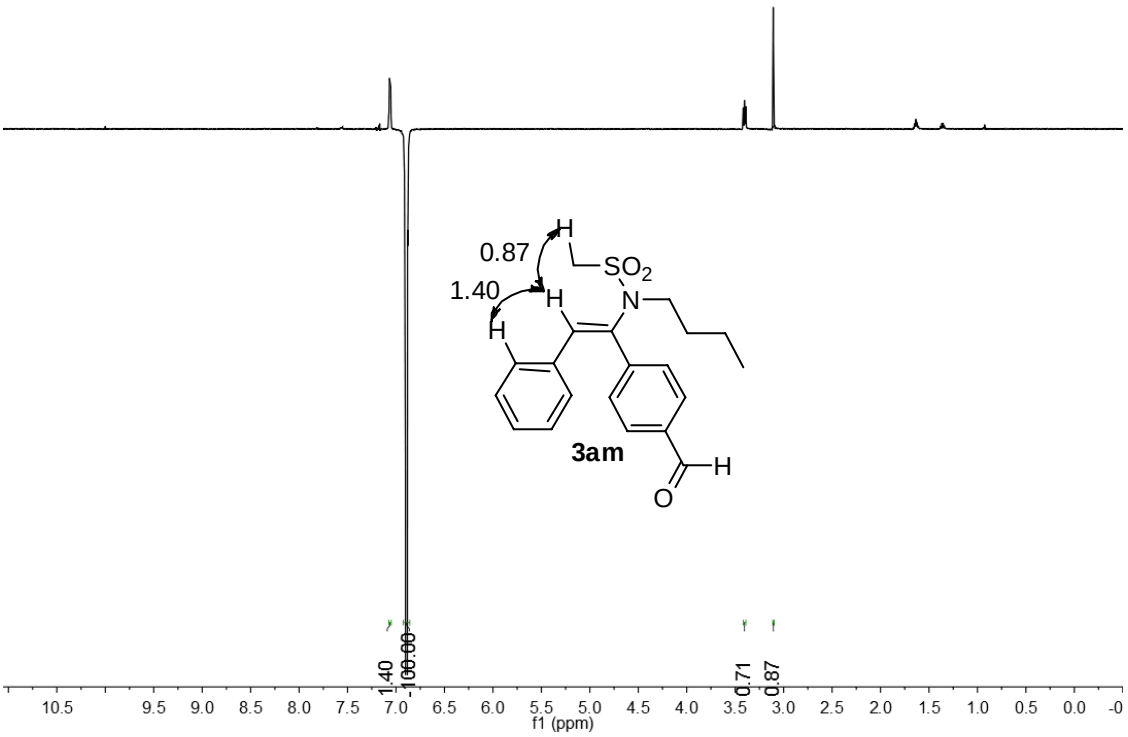
3ae

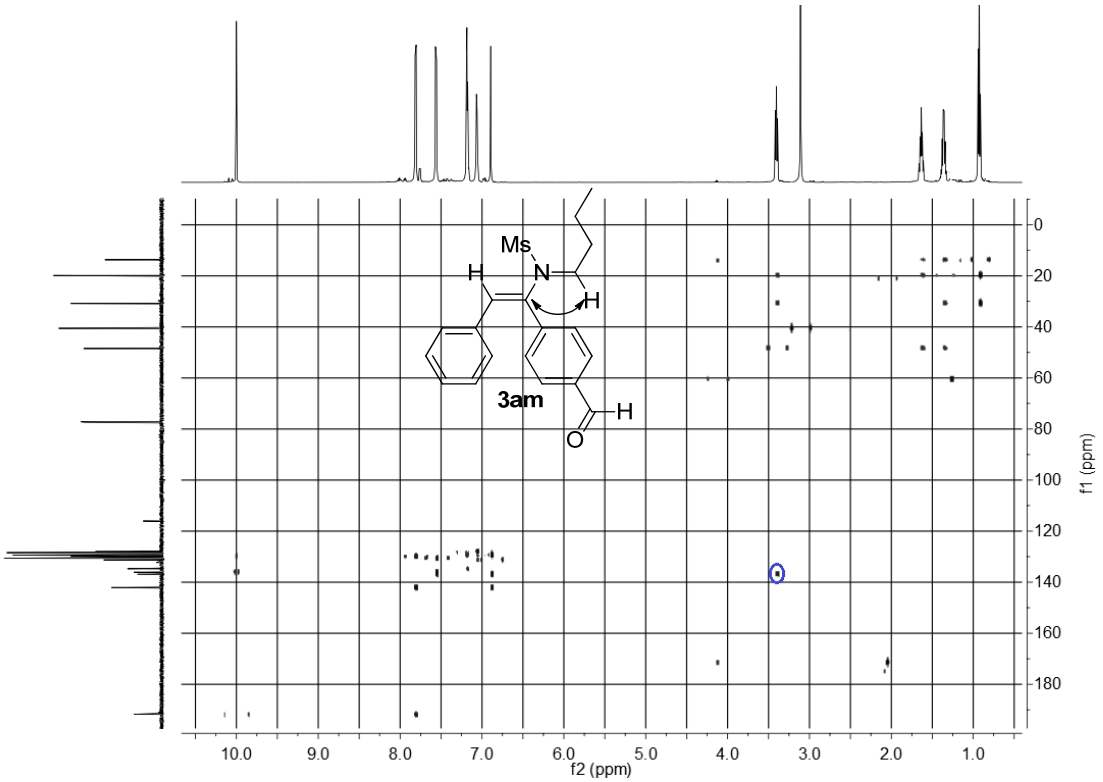

7.3205
7.3159
7.3033
7.2985
7.1773
7.1593
7.1460
7.0995
7.0942
7.0801
6.8562
6.8343
6.7345
3.8270
3.4056
3.3869
3.3681
3.0682
1.6595
1.6412
1.6219
1.6033
1.5843
1.3893
1.3706
1.3517
1.3333
0.9516
0.9333
0.9149
Ms
H
N−Bu
3aj
OMe
2.00
5.00
2.00
1.00
3.01
2.02
2.99
2.00
2.03
3.03
f1 (ppm)
0.74
1.49
H
SO2
N−Bu
3aj
OMe
-100.00
1.49
0.44
0.74
f1 (ppm)

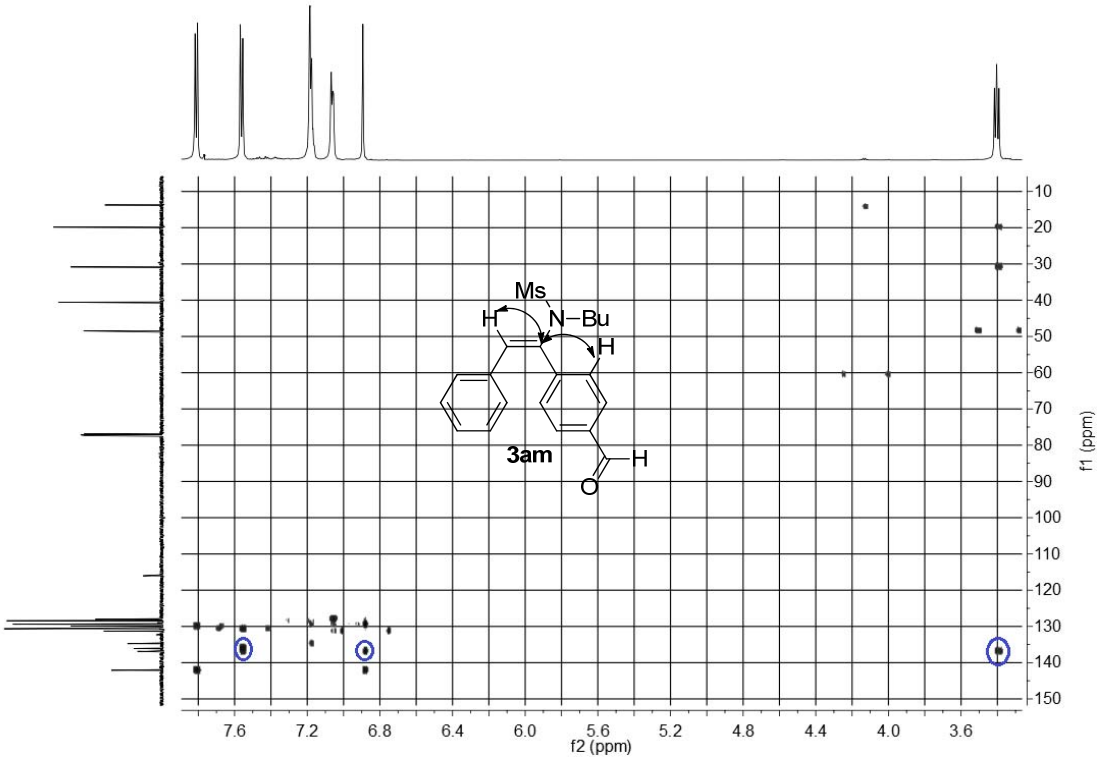

Ms
N
H
H
OMe
HMBC of 3aj
f2 (ppm)
f1 (ppm)

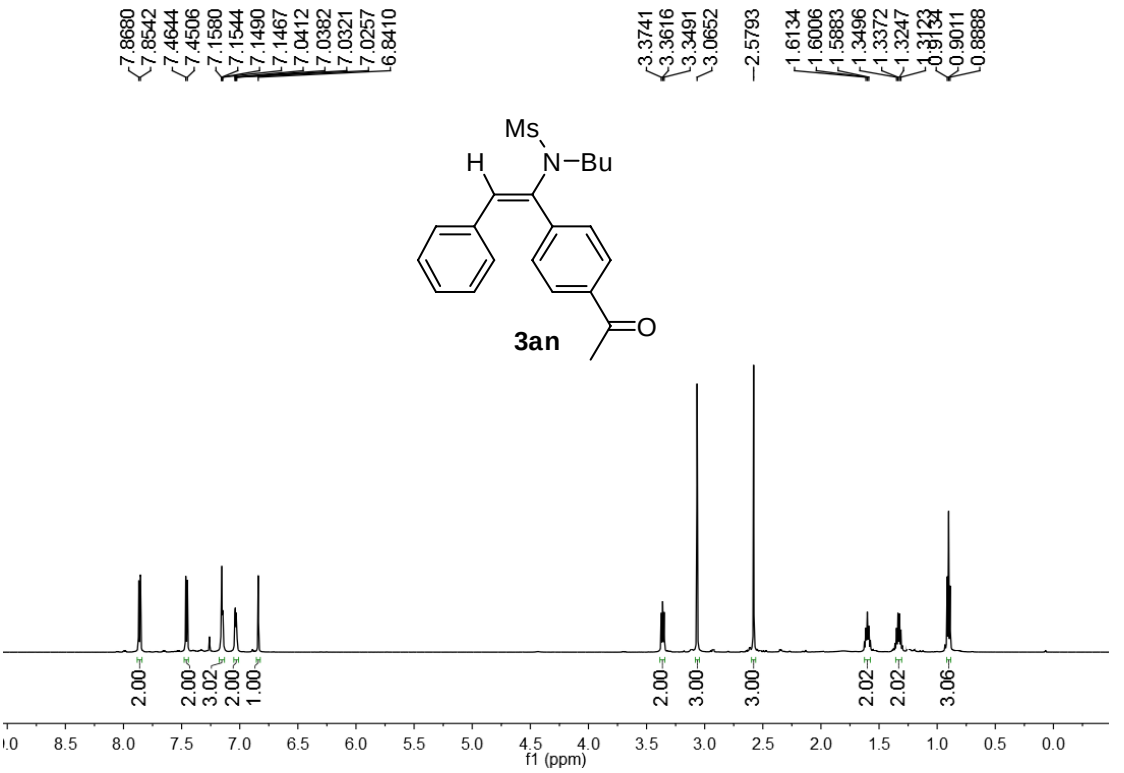

Ms
N
Bu
H
H
3aj
OMe
f2 (ppm)
f1 (ppm)

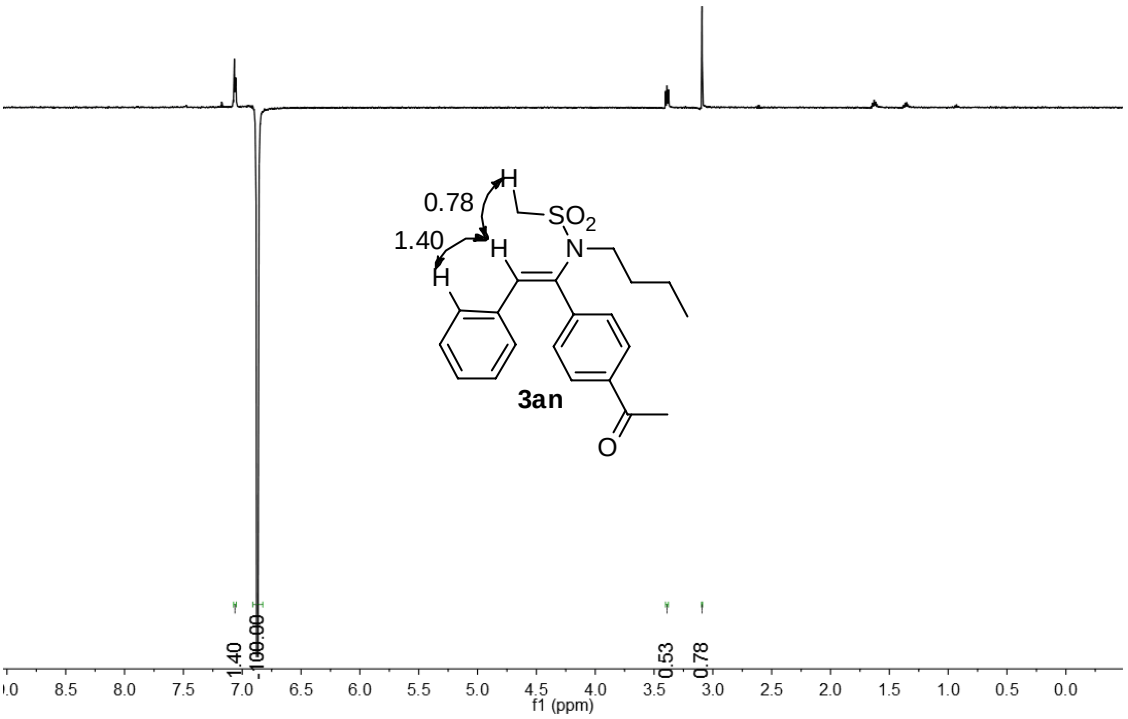

9.9721
7.7895
7.7760
7.5403
7.5268
7.1592
7.1566
7.1477
7.1052
7.0397
7.0314
7.0269
6.9931
6.8656
3.3884
3.3760
3.3633
3.0805
1.6316
1.6193
1.6065
1.5942
1.5814
1.3635
1.3511
1.3387
1.3261
1.3138
0.9107
0.8985
0.8862
Ms
H
N−Bu
O
H
3am
0.99
1.99
2.08
3.05
2.05
1.00
2.03
3.00
2.02
2.04
3.00
f1 (ppm)

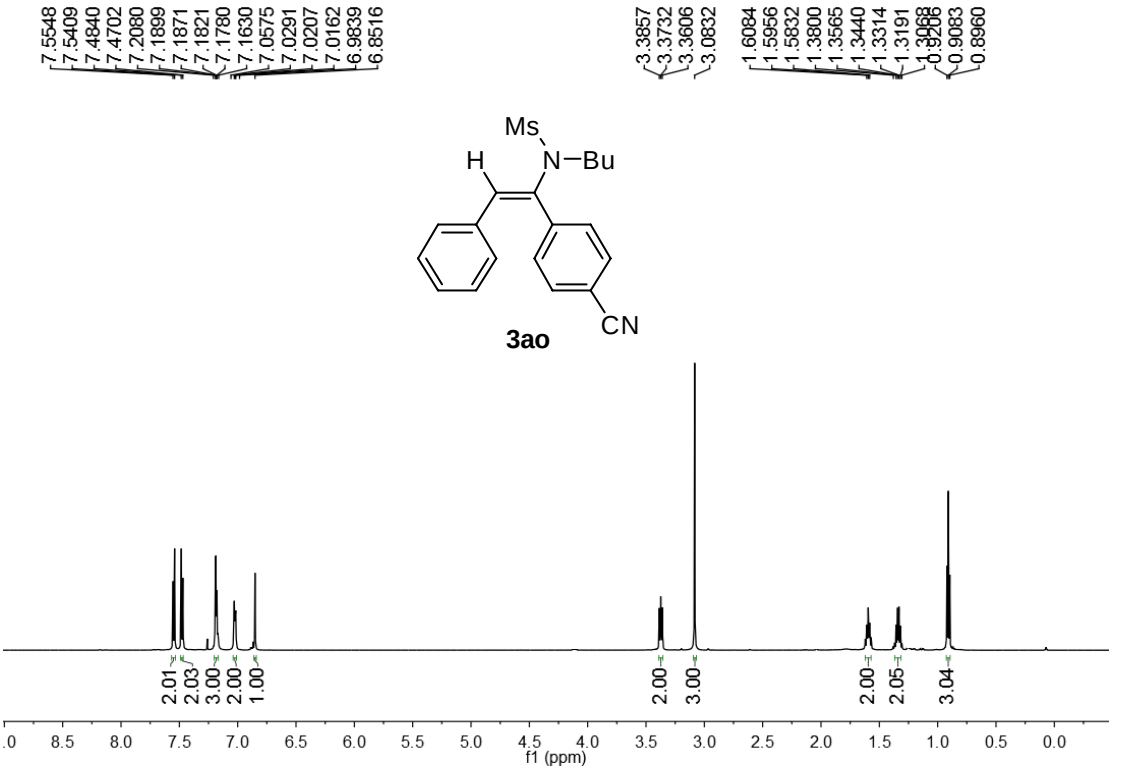

0.87
1.40
H
SO2
N
H
H
3am
O
H
1.40
100.00
0.71
0.87
f1 (ppm)

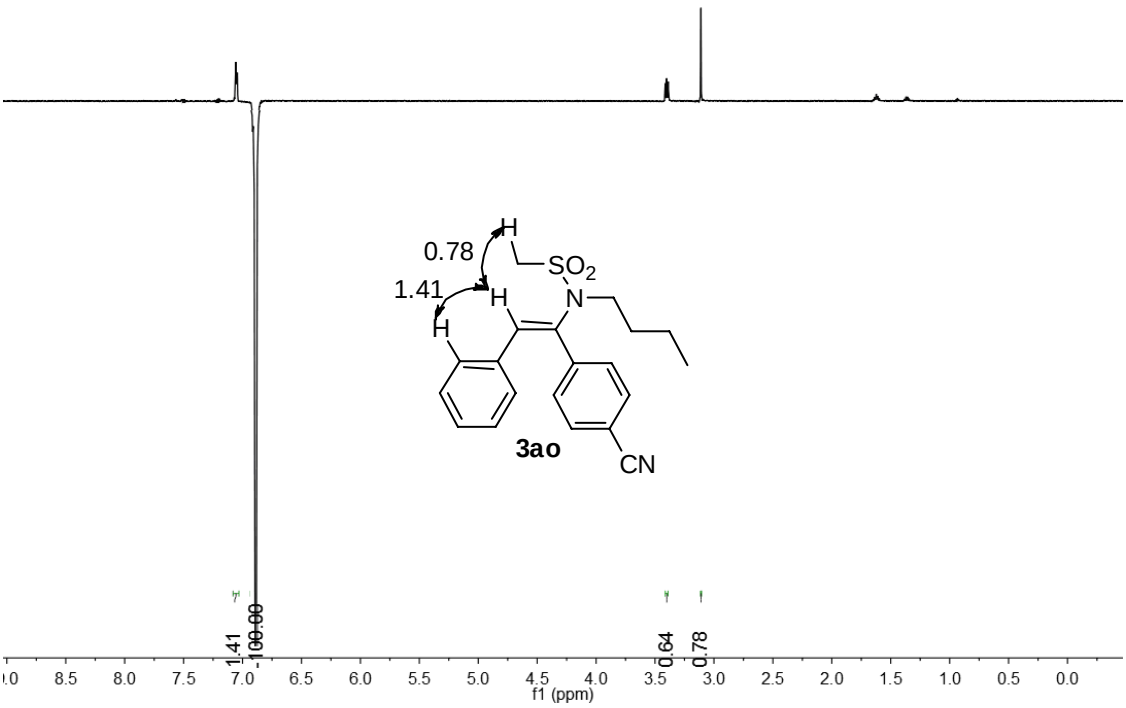

Ms
H
N
H
3am
H
O
f1 (ppm)
f2 (ppm)

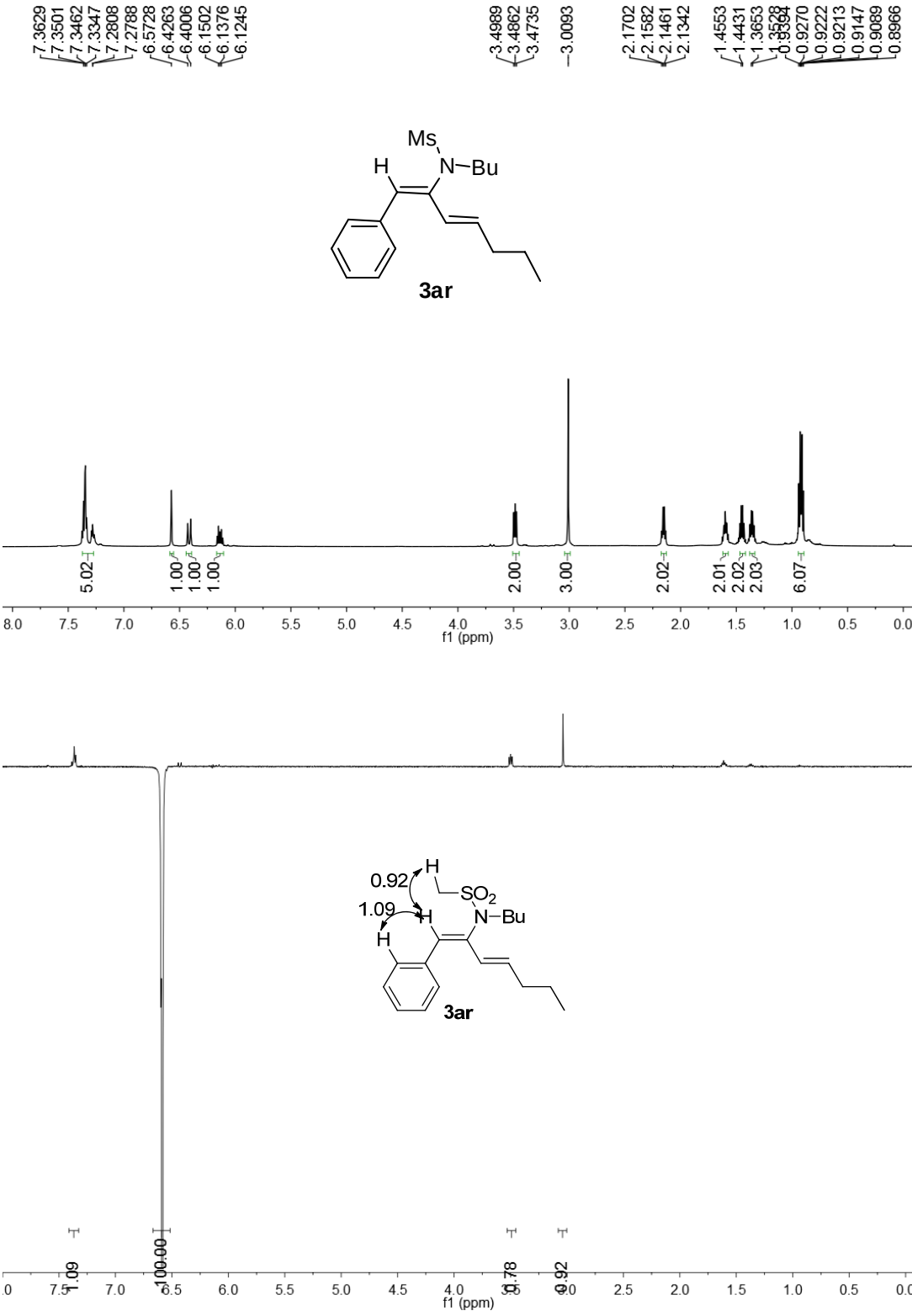

Ms
H
N–Bu
H
3am
H
O
f1 (ppm)
f2 (ppm)

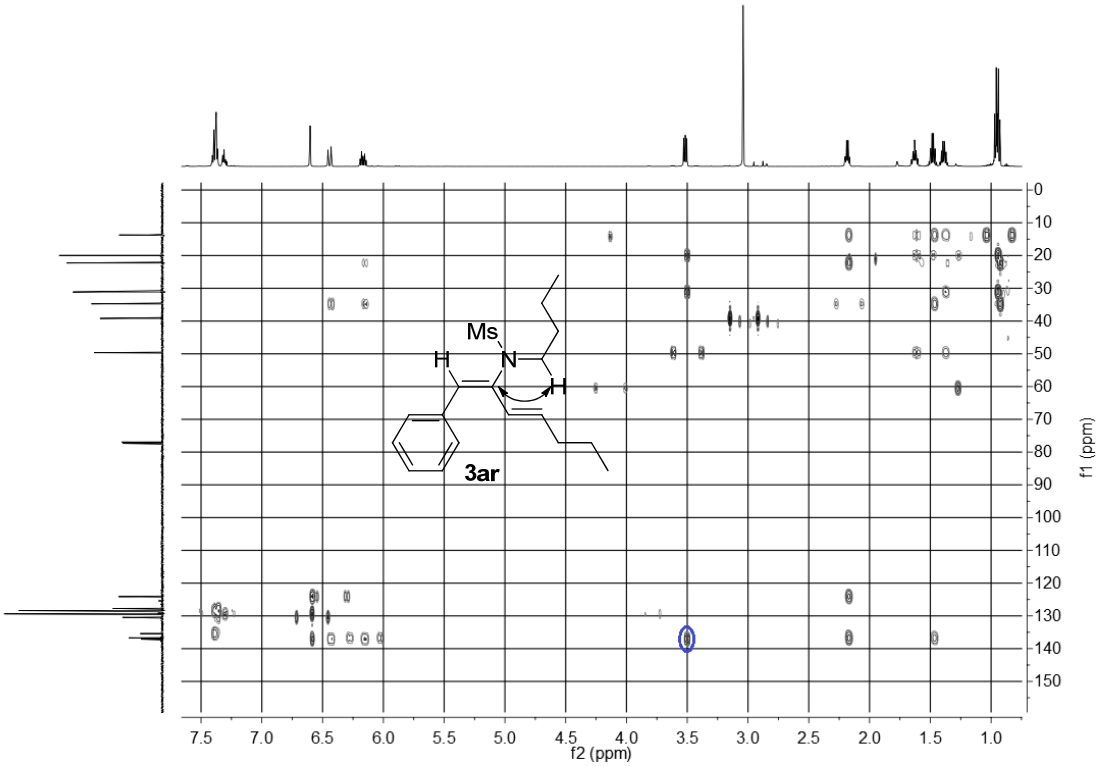

7.8680
7.8542
7.4644
7.4506
7.1580
7.1544
7.1490
7.1467
7.0412
7.0382
7.0321
7.0257
6.8410
3.3741
3.3616
3.3491
3.0652
2.5793
1.6134
1.6006
1.5883
1.3496
1.3372
1.3247
1.3123
0.9011
0.8888
Ms
H
N−Bu
O
3an
2.00
2.00
3.02
2.00
1.00
2.00
3.00
3.00
2.02
2.02
3.06
f1 (ppm)

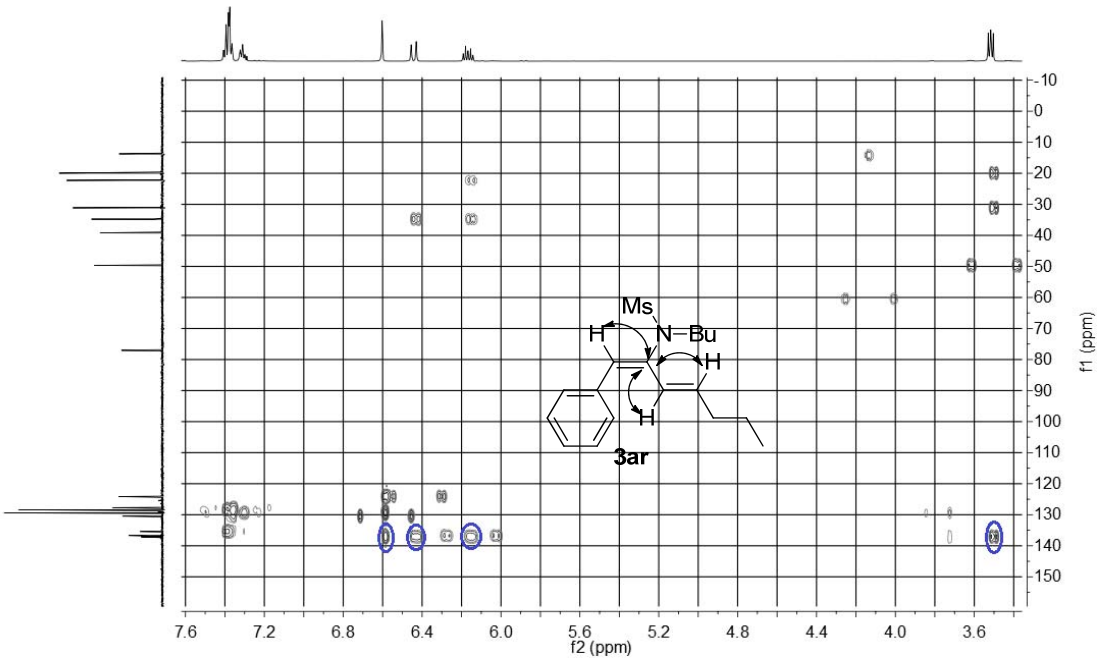

0.78
1.40
H
SO2
N
3an
O
1.40
1.00
0.53
0.78
f1 (ppm)


7.5548
7.5409
7.4840
7.4702
7.2080
7.1899
7.1871
7.1821
7.1780
7.1630
7.0575
7.0291
7.0207
7.0162
6.9839
6.8516
3.3857
3.3732
3.3606
3.0832
1.6084
1.5956
1.5832
1.3800
1.3565
1.3440
1.3314
1.3191
0.9083
0.8960
Ms
H
N—Bu
CN
3ao
2.01
2.03
3.00
2.00
1.00
2.00
3.00
2.00
2.05
3.04
f1 (ppm)

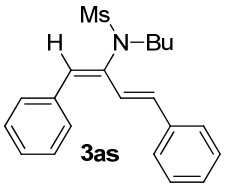

0.78
1.41
H
SO2
N
H
H
3ao
CN
1.41
100.00
0.64
0.78
f1 (ppm)

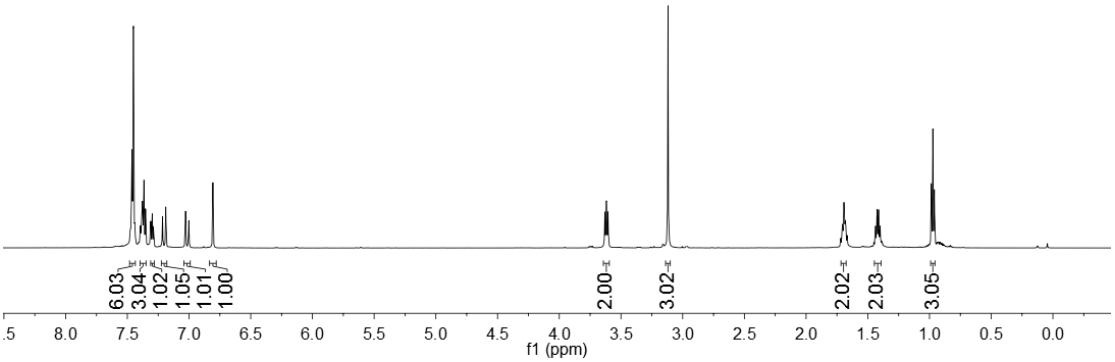

7.3629
7.3501
7.3462
7.3347
7.2808
7.2788
6.5728
6.4263
6.4006
6.1502
6.1376
6.1245
3.4989
3.4862
3.4735
3.0093
2.1702
2.1582
2.1461
2.1342
1.4553
1.4431
1.3653
1.3528
0.9394
0.9270
0.9222
0.9213
0.9147
0.9089
0.8966
Ms
H
N–Bu
3ar
5.02
1.00
1.00
1.00
2.00
3.00
2.02
2.01
2.02
2.03
6.07
f1 (ppm)
0.92
1.09
H
SO2
N–Bu
3ar
1.09
100.00
0.78
0.92
f1 (ppm)

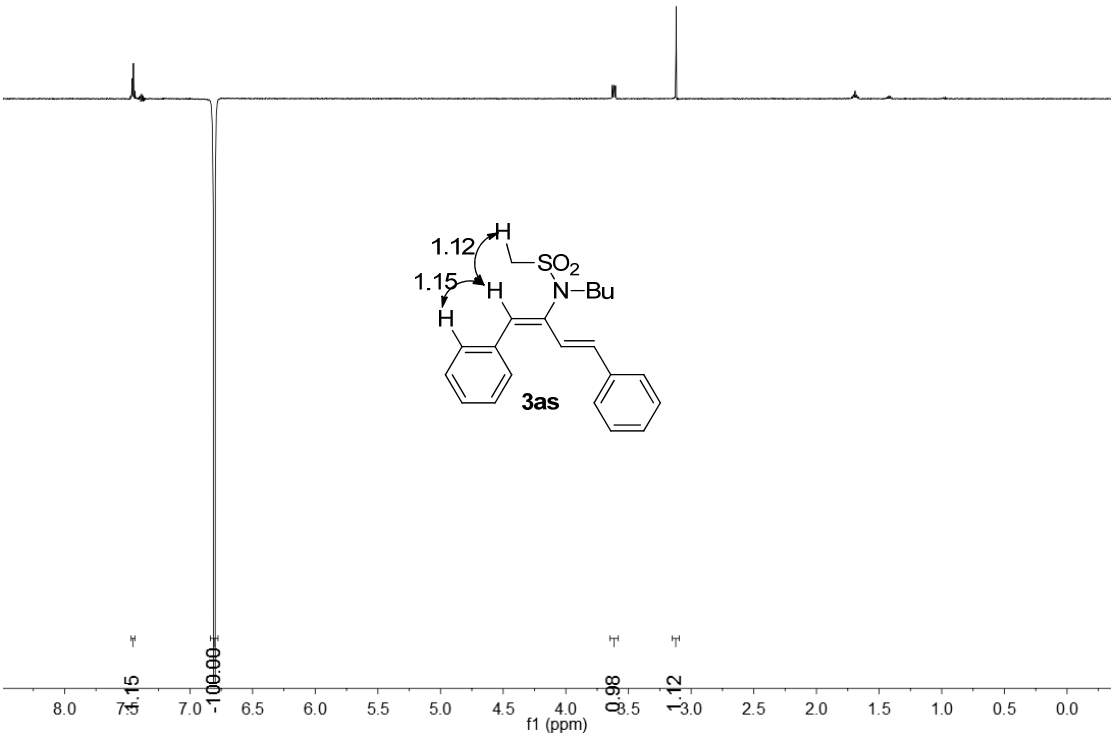

Ms
H
N
H
3ar
f1 (ppm)
f2 (ppm)

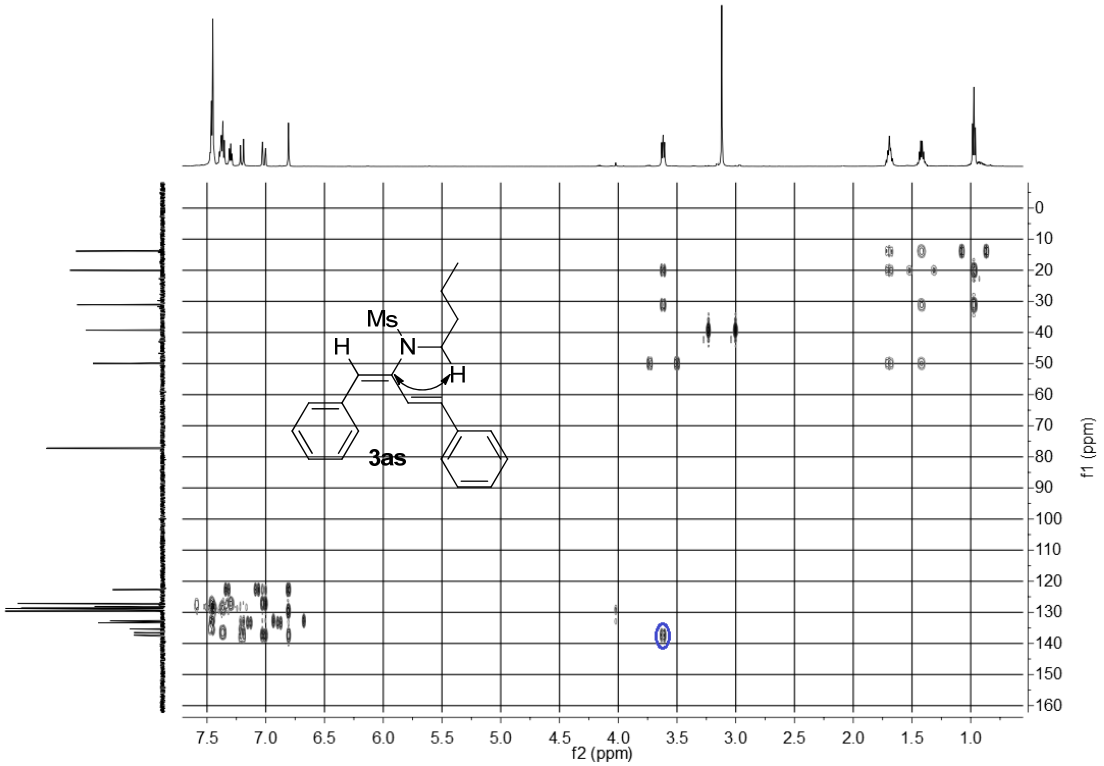

Ms
H
N–Bu
H
H
3ar
f1 (ppm)
f2 (ppm)

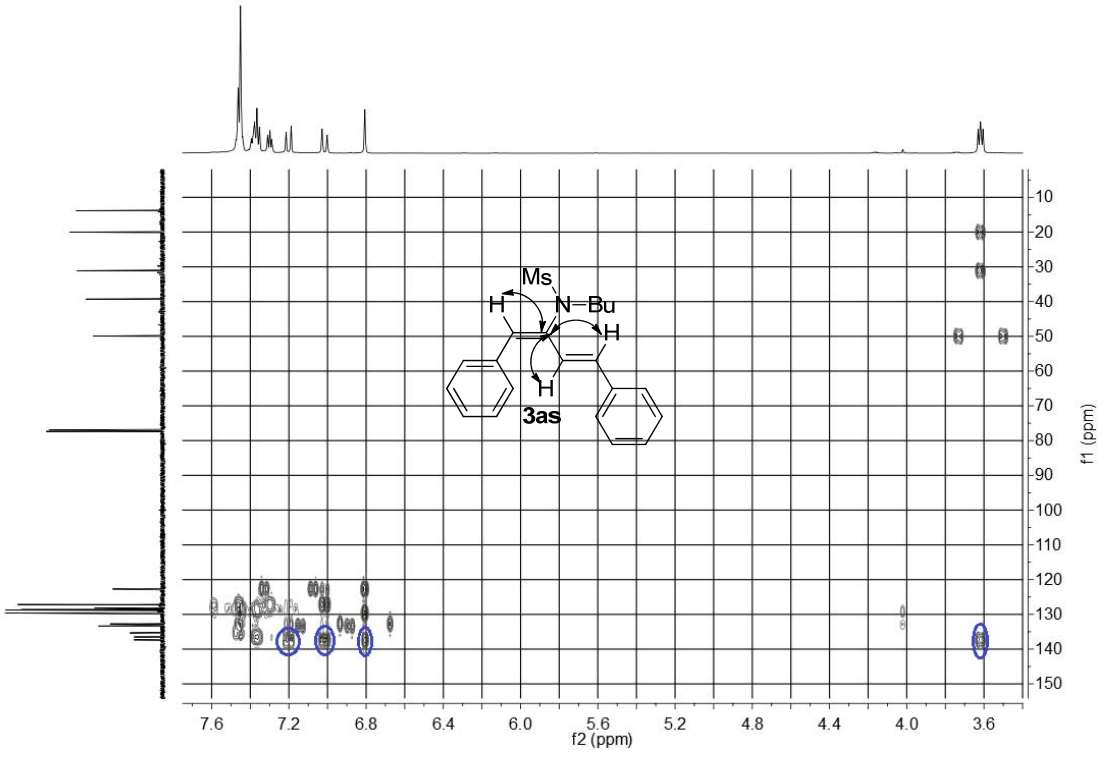

7.4742
7.4622
7.4506
7.4398
7.3941
7.3823
7.3779
7.3654
7.3526
7.3101
7.2981
7.2892
7.2148
7.1885
7.0280
7.0016
6.8065
3.6305
3.6179
3.6050
3.1189
1.7059
1.6931
1.6814
1.6678
1.4375
1.4251
1.4126
1.4003
0.9852
0.9729
0.9607

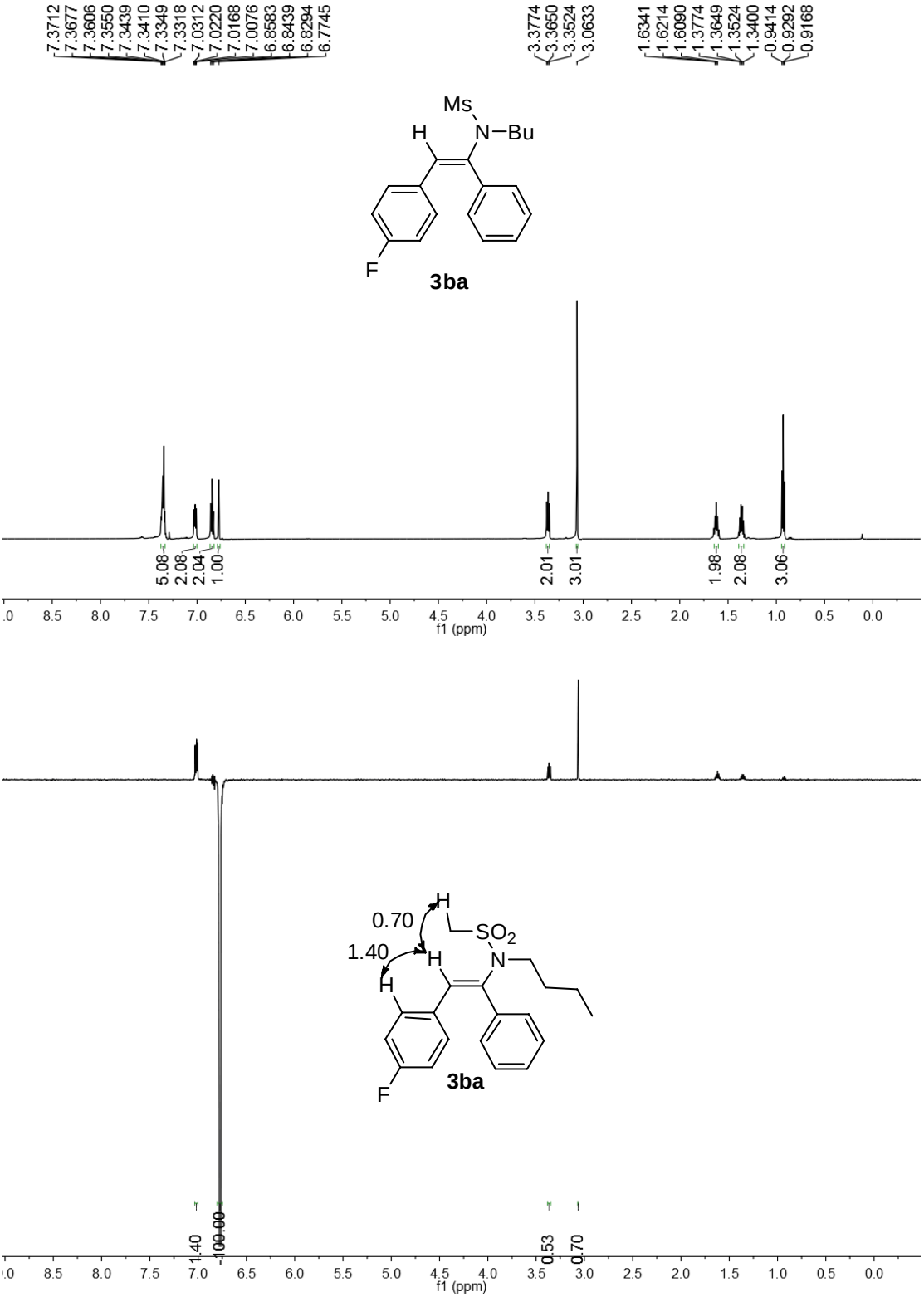

Ms
H
N–Bu
3as

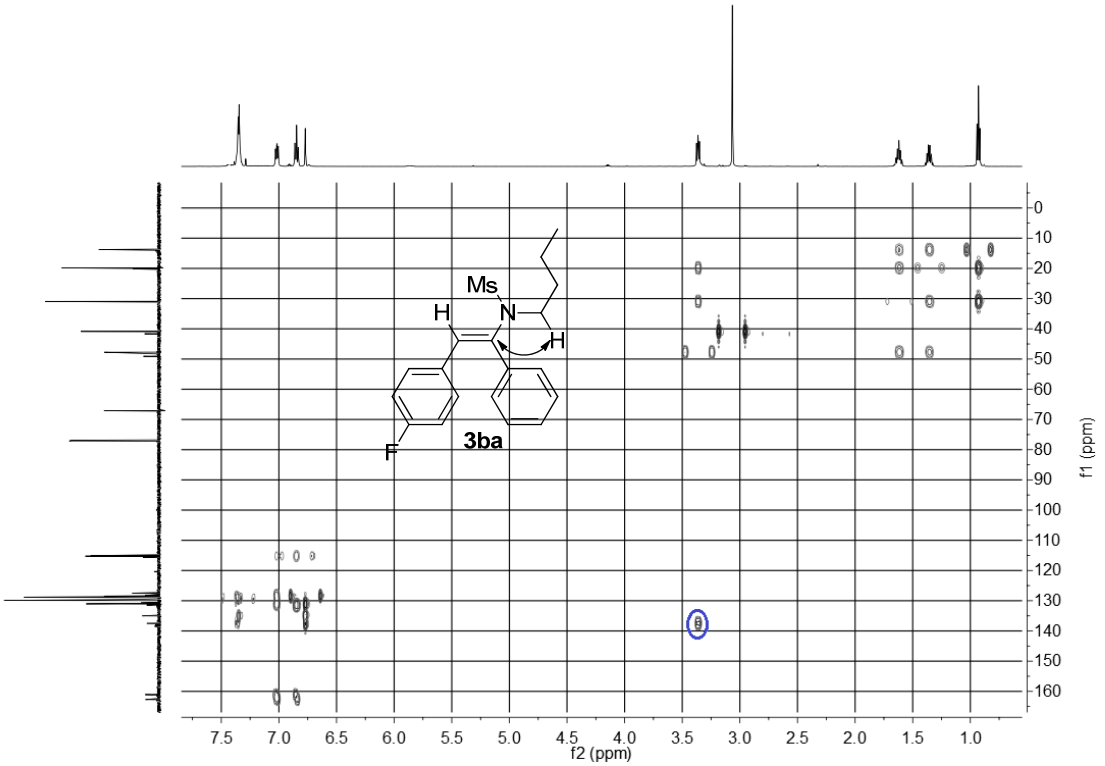

6.03
3.04
1.02
1.05
1.01
1.00
2.00
3.02
2.02
2.03
3.05
f1 (ppm)

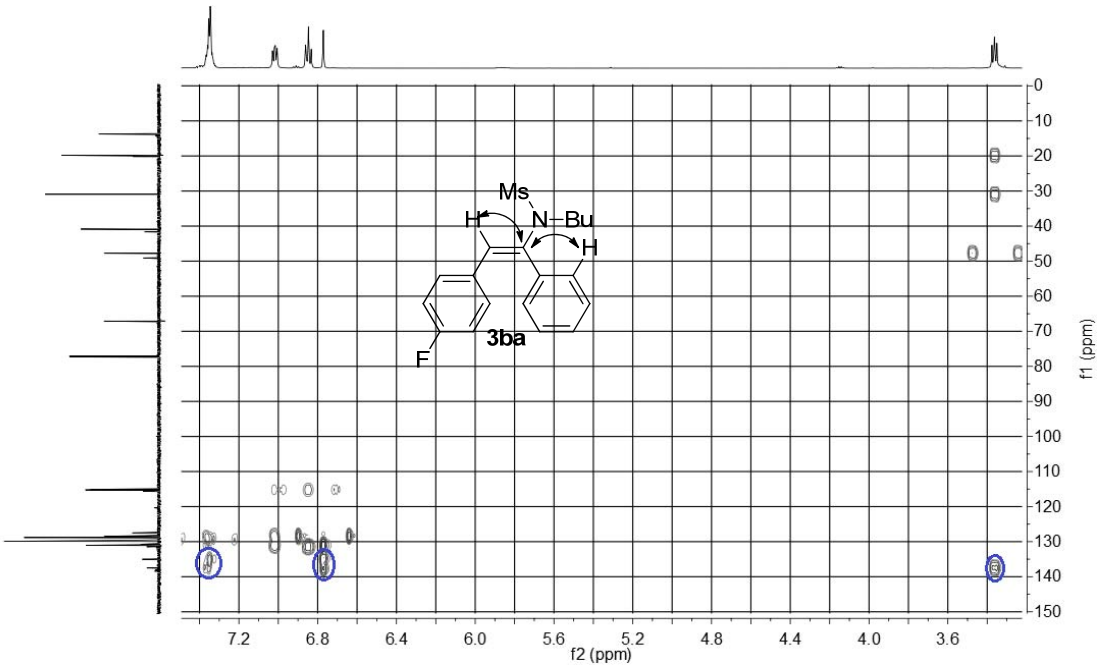

1.12
H
SO2
1.15
H
N–Bu
H
3as
1.15
-100.00
0.98
1.12
f1 (ppm)

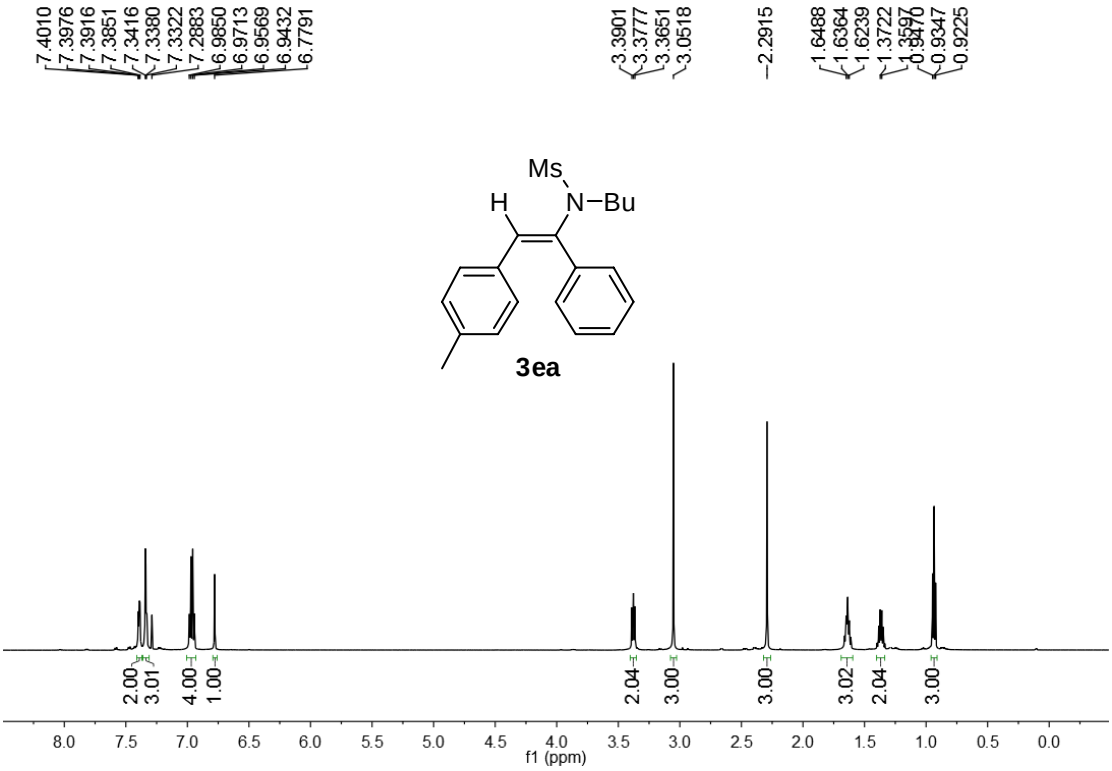

Ms
H
N
H
3as
f1 (ppm)
f2 (ppm)

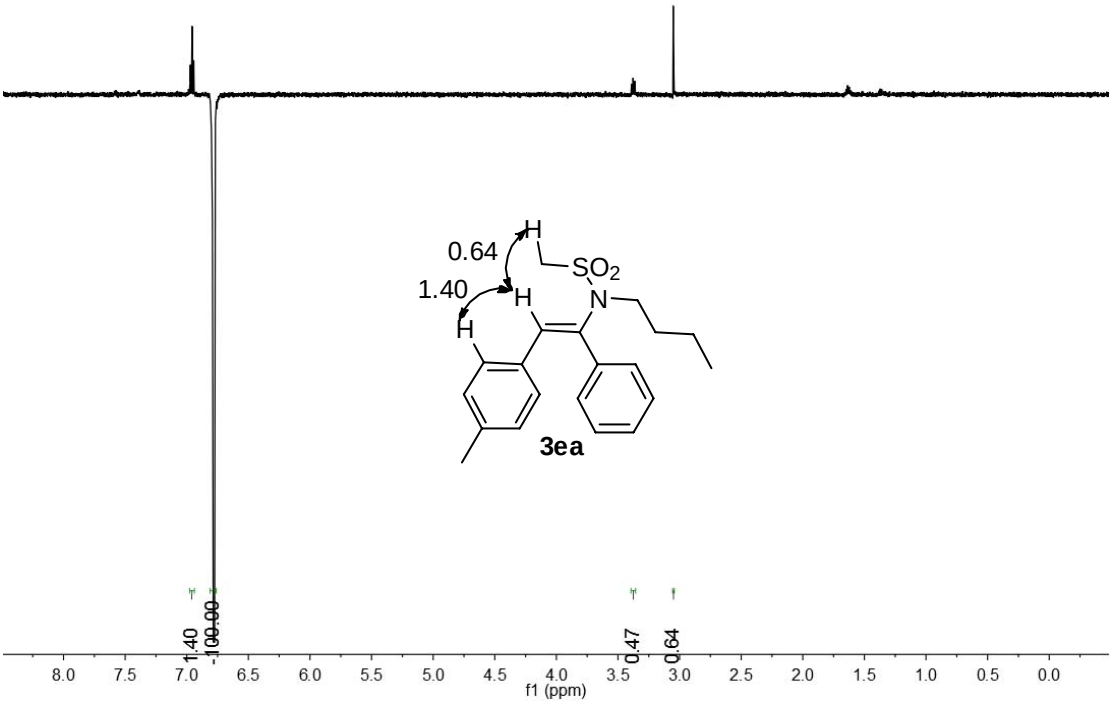

Ms
H
N-Bu
H
H
3as
f1 (ppm)
f2 (ppm)

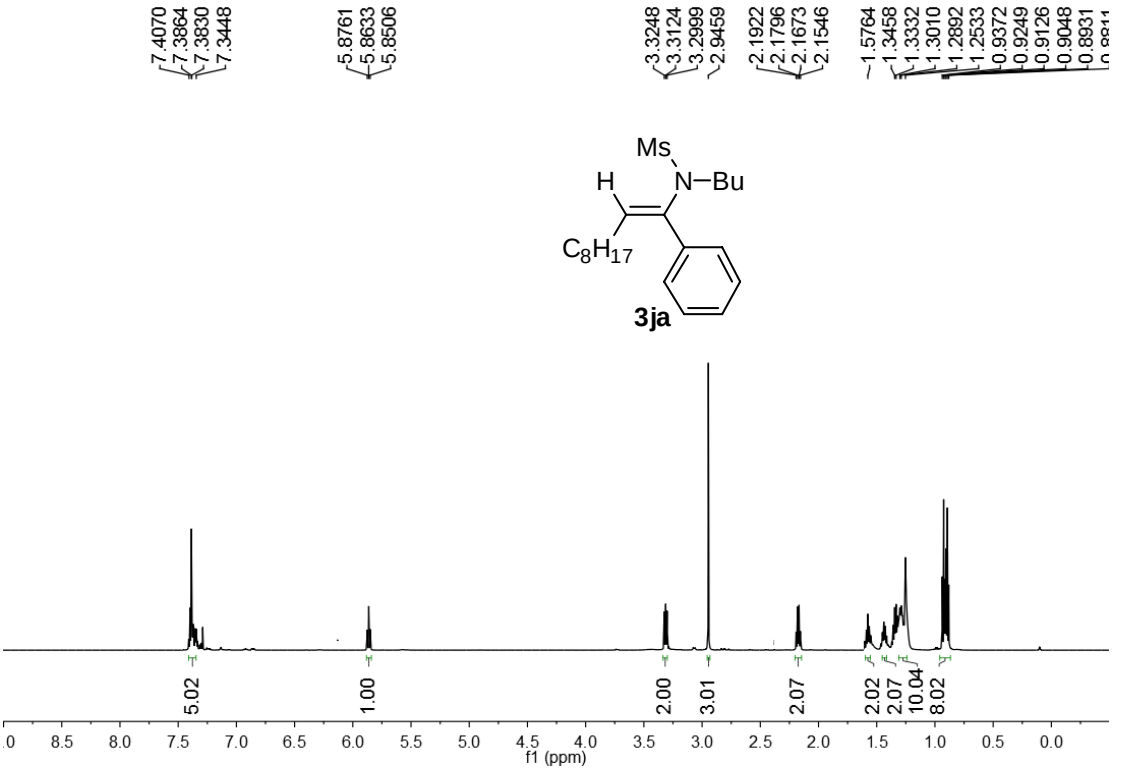

7.3712
7.3677
7.3606
7.3550
7.3439
7.3410
7.3349
7.3318
7.0312
7.0220
7.0168
7.0076
6.8583
6.8439
6.8294
6.7745
3.3774
3.3650
3.3524
3.0633
1.6341
1.6214
1.6090
1.3774
1.3649
1.3524
1.3400
0.9414
0.9292
0.9168
Ms
H
N−Bu
F
3ba
5.08
2.08
2.04
1.00
2.01
3.01
1.98
2.08
3.06
f1 (ppm)
0.70
1.40
H
SO2
N
3ba
1.40
100.00
0.53
0.70
f1 (ppm)

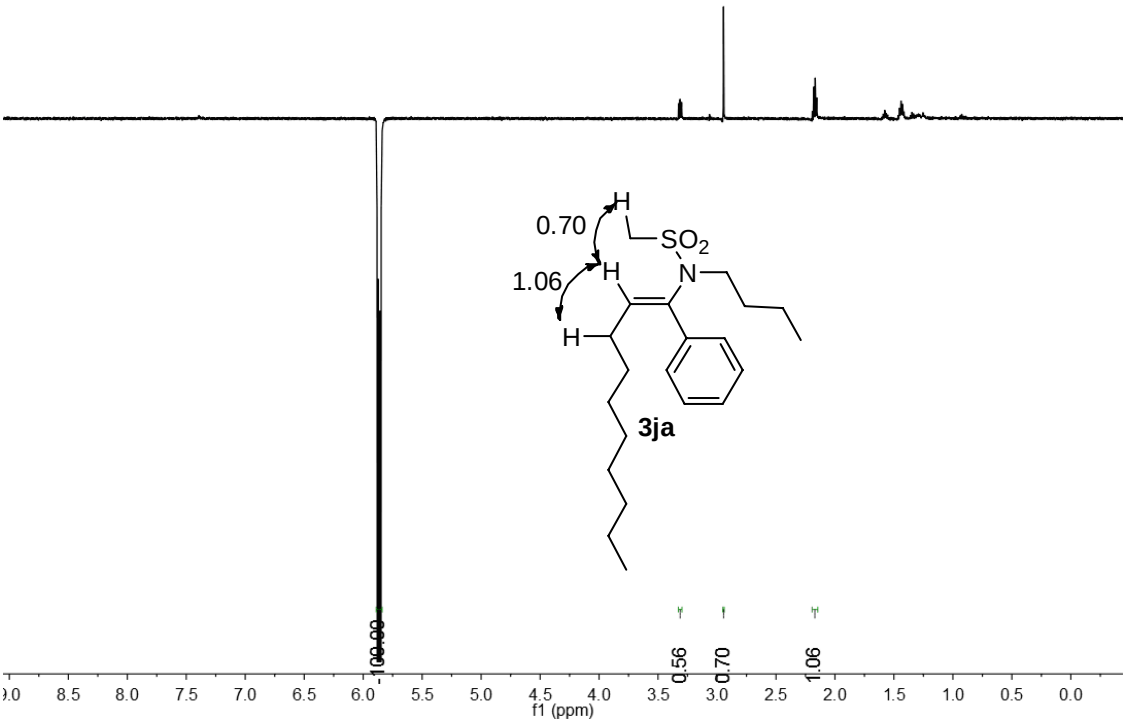


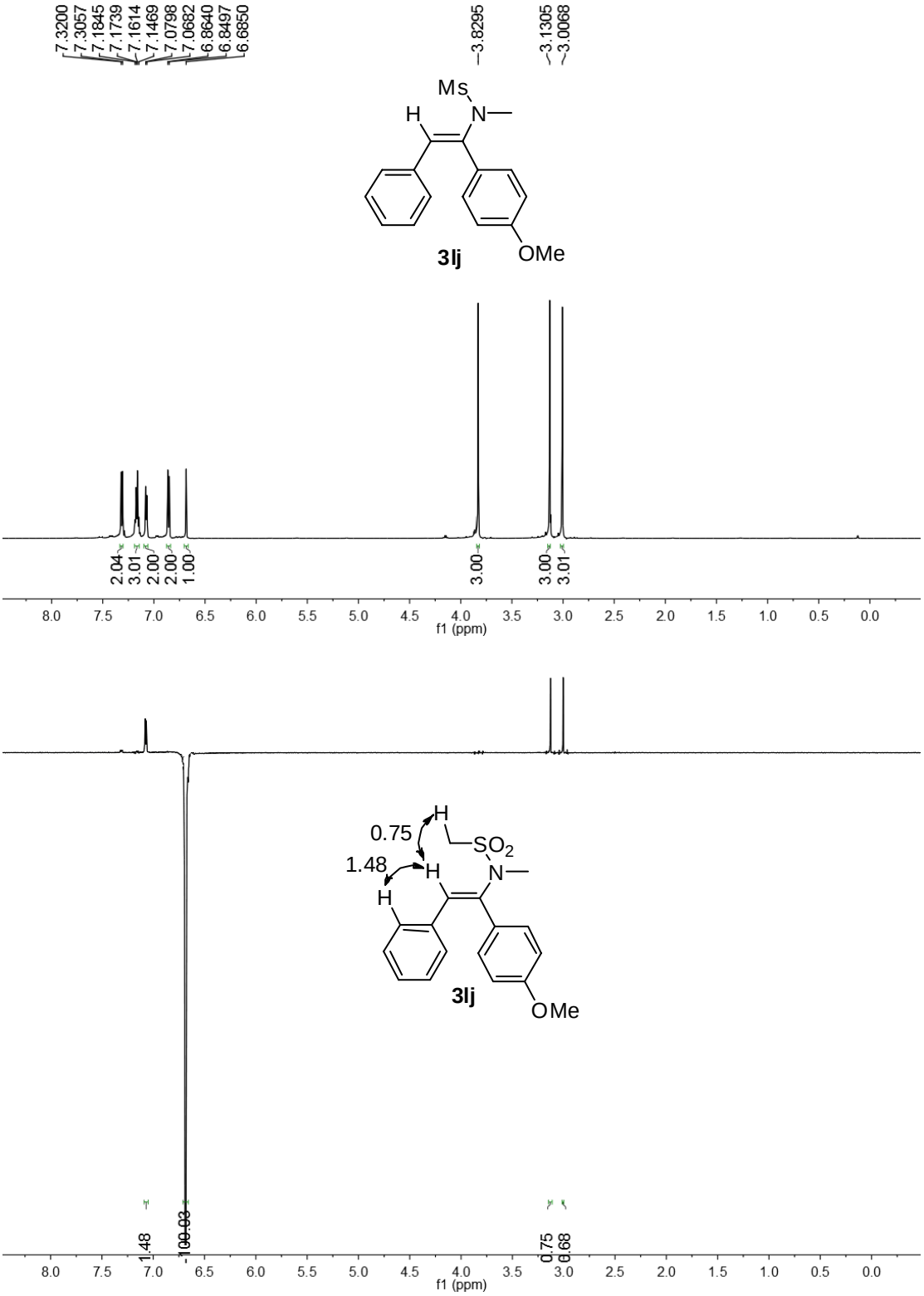


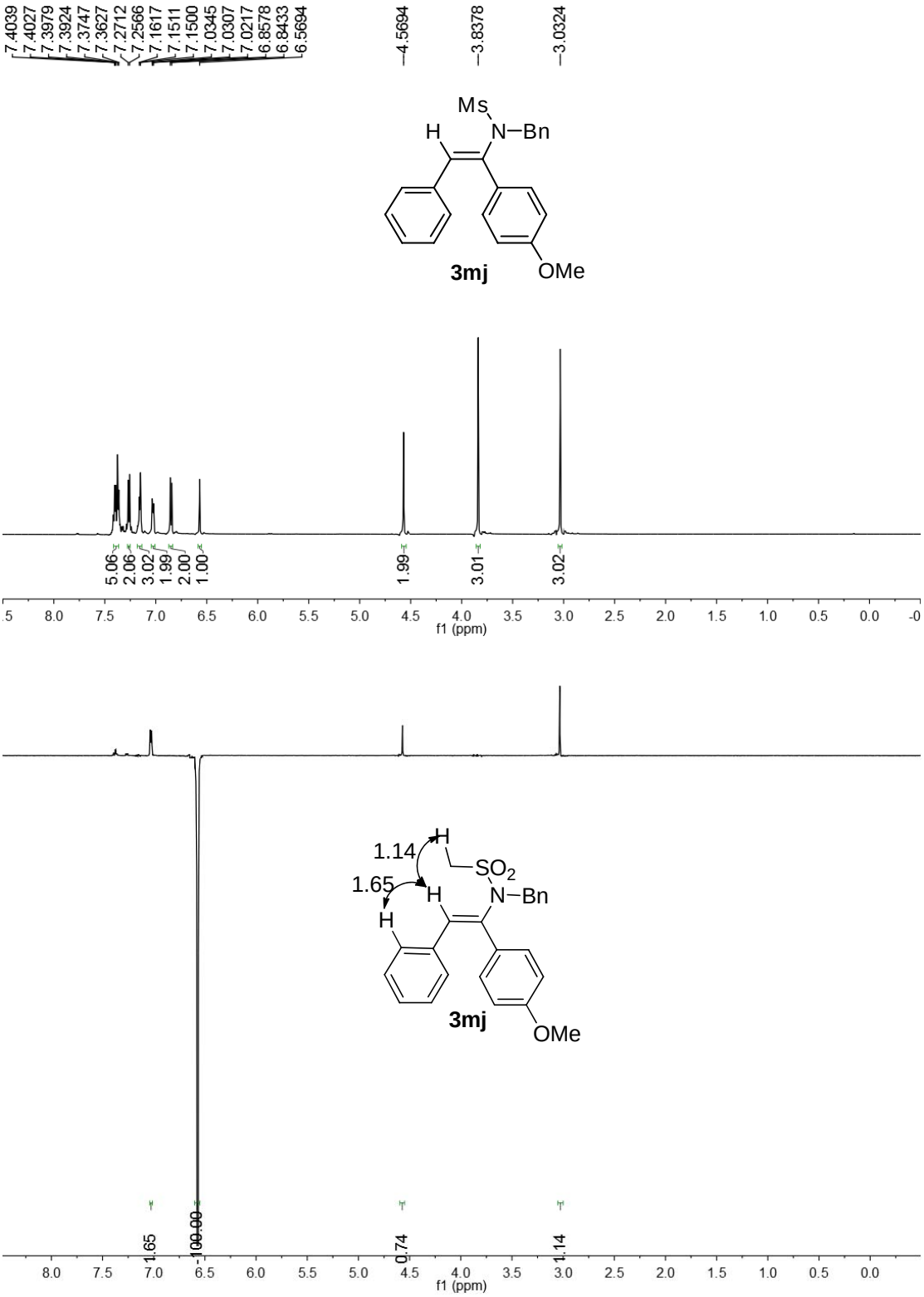

7.4010
7.3976
7.3916
7.3851
7.3416
7.3380
7.3322
7.2883
6.9850
6.9713
6.9569
6.9432
6.7791
3.3901
3.3777
3.3651
3.0518
2.2915
1.6488
1.6364
1.6239
1.3722
1.3597
0.9470
0.9347
0.9225
Ms
H
N−Bu
3ea
2.00
3.01
4.00
1.00
2.04
3.00
3.00
3.02
2.04
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

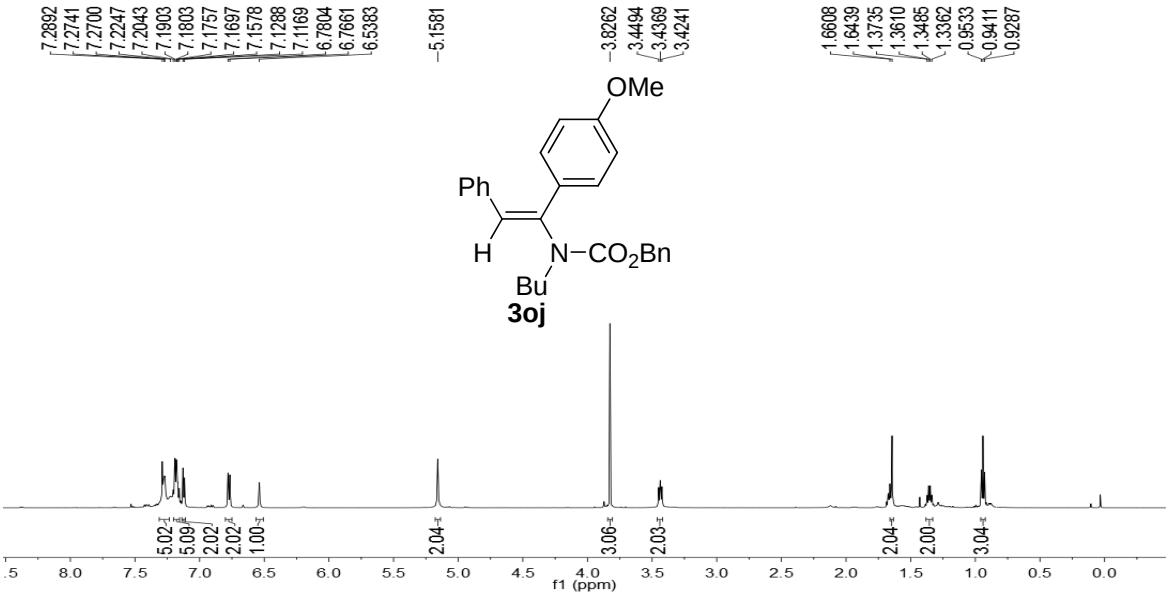

0.64
1.40
H
SO2
N
H
H
3ea
1.40
-100.00
0.47
0.64
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

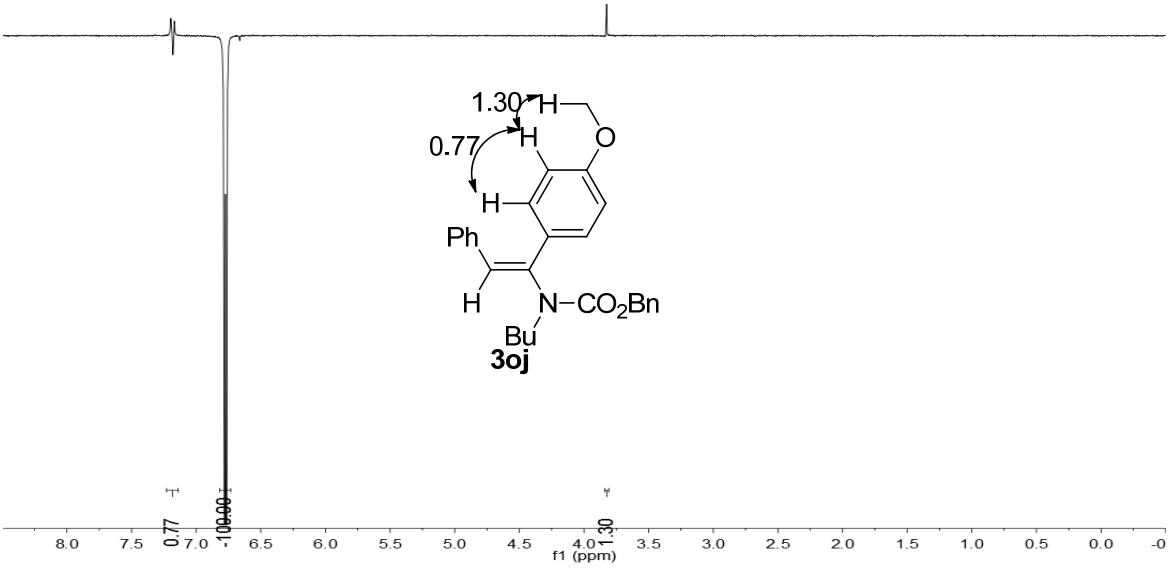

7.4070
7.3864
7.3830
7.3448
5.8761
5.8633
5.8506
3.3248
3.3124
3.2999
2.9459
2.1922
2.1796
2.1673
2.1546
1.5764
1.3458
1.3332
1.3010
1.2892
1.2533
0.9372
0.9249
0.9126
0.9048
0.8931
Ms
H
N–Bu
C8H17
3ja
5.02
1.00
2.00
3.01
2.07
2.02
2.07
10.04
8.02
f1 (ppm)

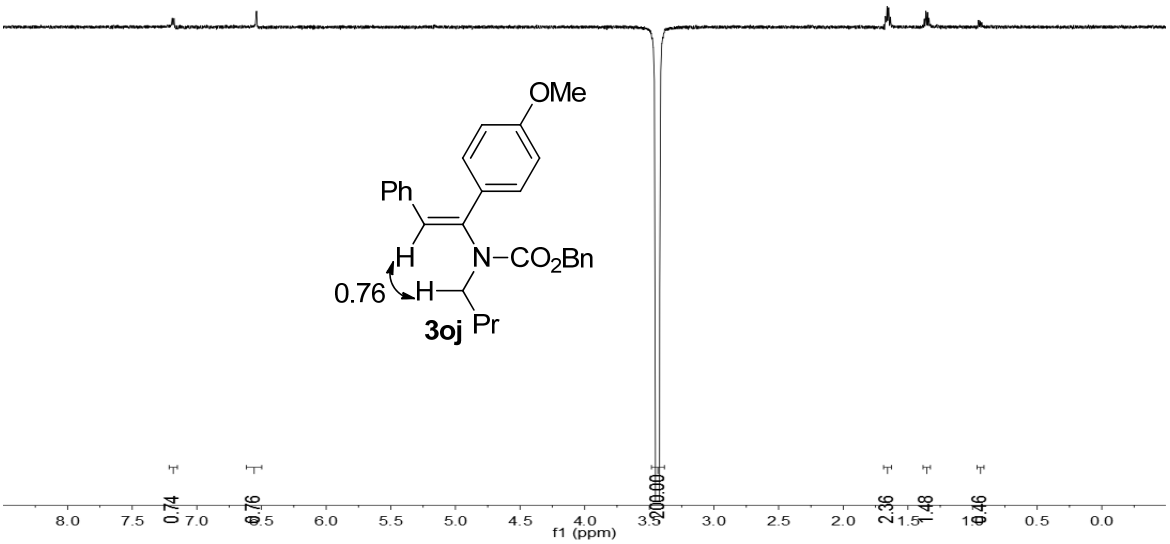

0.70
1.06
H
SO2
N
3ja
100.00
0.56
0.70
1.06
f1 (ppm)


7.3200
7.3057
7.1845
7.1739
7.1614
7.1469
7.0798
7.0682
6.8640
6.8497
6.6850
3.8295
3.1305
3.0068
Ms
H
N
OMe
3lj
2.04
3.01
2.00
2.00
1.00
3.00
3.00
3.01
f1 (ppm)
0.75
1.48
H
SO2
N
H
H
OMe
3lj
1.48
100.00
0.75
0.68
f1 (ppm)


7.4039
7.4027
7.3979
7.3924
7.3747
7.3627
7.2712
7.2566
7.1617
7.1511
7.1500
7.0345
7.0307
7.0217
6.8578
6.8433
6.5694
4.5694
3.8378
3.0324
Ms
H
N—Bn
OMe
3mj
5.06
2.06
3.02
1.99
2.00
1.00
1.99
3.01
3.02
f1 (ppm)
1.14
1.65
H
SO2
N—Bn
3mj
OMe
1.65
100.00
0.74
1.14
f1 (ppm)


7.2892
7.2741
7.2700
7.2247
7.2043
7.1903
7.1803
7.1757
7.1697
7.1578
7.1288
7.1169
6.7804
6.7661
6.5383
5.1581
3.8262
3.4494
3.4369
3.4241
1.6608
1.6439
1.3735
1.3610
1.3485
1.3362
0.9533
0.9411
0.9287
OMe
Ph
H
N−CO2Bn
Bu
3oj
5.02
5.09
2.02
2.02
1.00
2.04
3.06
2.03
2.04
2.00
3.04
f1 (ppm)


1.30
H
0.77
H
O
H
Ph
H
N−CO2Bn
Bu
3oj
0.77
-100.00
1.30
f1 (ppm)


OMe
Ph
H
N−CO2Bn
0.76
H
3oj
Pr
0.74
0.76
-200.00
2.36
1.48
0.46
f1 (ppm)