Supporting Information

Rhodium(III)-Catalyzed Unreactive C(sp^3)-H Alkenylation of *N*-alkyl-1*H*-pyrazoles with Alkynes

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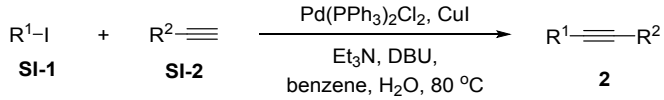
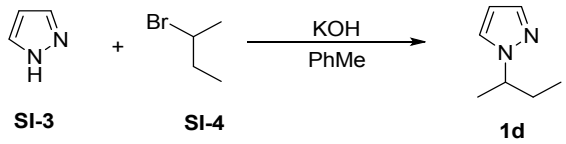
General Information

The ^{1}H NMR, ^{13}C NMR and ^{19}F NMR were recorded with Bruker 400 MHz spectrometer instruments in $CDCl_3$. The chemical shifts (δ) of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR were measured in ppm, referenced to residual ^{1}H and ^{13}C signals of nondeuterated $CDCl_3$ (δ = 7.26 and 77.00), as internal standards. All solvents were obtained from commercial sources and were purified according to standard procedures. Purification of products was accomplished by silica gel (200~300 mesh). Thin layer chromatography (TLC) was performed on Merck silica gel GF254 plates and visualized by UV-light (254 nm). HRMS were recorded on VG ZAB-HS mass spectrometer with ESI resource. Alkynes **2b**, **2c**, **2d**, **2e**, **2f**, **2h**, **2i**, **2j**, **2k**, **2l**, **2m**, **2n**, **2o**, **2t, 2u, 2v** and 1-(*sec*-butyl)-1*H*-pyrazole **1d** were synthesized according to the literature procedures. Other alkynes and 1-(*tert*-butyl)-1*H*-pyrazole **1a**, 1-isopropyl-1*H*-pyrazole **1b**, 1-ethyl-1*H*-pyrazole **1c** were commercially available. All solvents were obtained from commercial sources and were purified according to standard procedures.

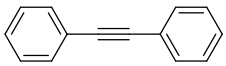
Preparation of Starting Materials



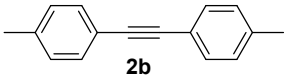
The preparation of the symmetrical and unsymmetrical alkyne by the coupling of iodide derivatives with alkyne derivatives. In a 50 mL vessel with $Pd(PPh_3)_2Cl_2$ (0.6 mmol, 0.06 equiv.), DBU (60 mmol, 6.0 equiv.), CuI (0.6 mmol, 0.06 equiv.) and H_2O (4.0 mmol, 0.4 equiv.) in benzene (25 mL), **SI-1** (10 mmol, 1.0 equiv.), **SI-2** (10 mmol, 1.0 equiv.) were added, respectively. The resulting product was extracted with diethyl ether (30 mL). The solution was concentrated in vacuo and the residue was purified by column chromatography on basic silica gel (petroleum ether) to afford the desired pure products **2**.



In a 50 mL vessel with **SI-3** (15 mmol, 1.0 equiv.) and KOH (15 mmol, 1.0 equiv.), Toluene (10 mL) and **SI-4** (18 mmol, 1.2 equiv.) were added, respectively. The reaction was performed at 90 °C. The resulting product was extracted with DCM (30 mL). The organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated to dryness to obtain the desired product **1d** in a pure form. (*Ultrason. Sonochem*. **2016**, *32*, 432.)



2a



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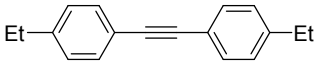

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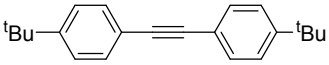
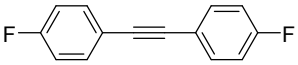


2d



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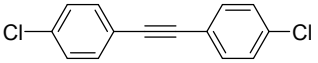

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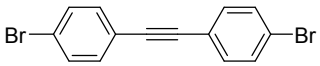

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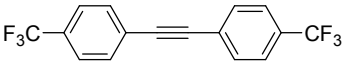

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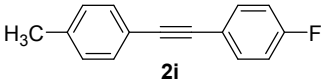

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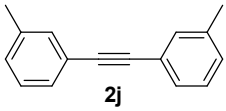

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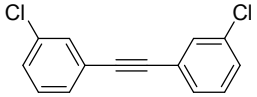

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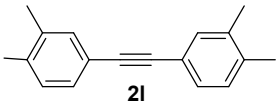

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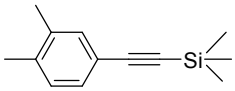

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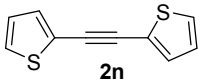

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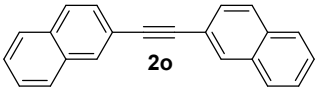

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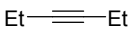

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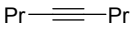
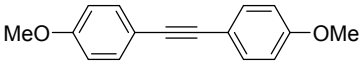


2q

2r

2s



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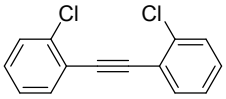
2u



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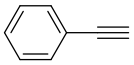

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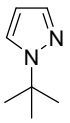

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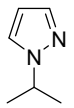

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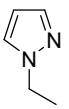

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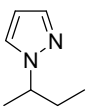

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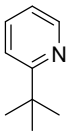

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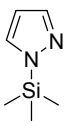

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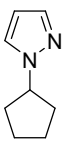
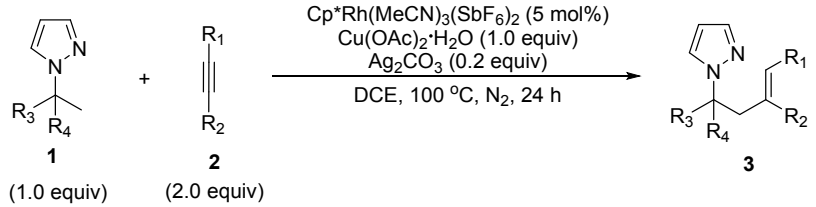


1g

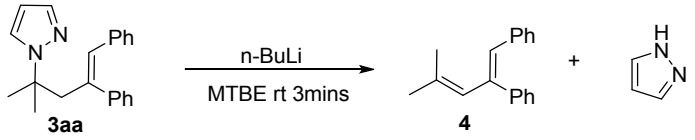
Synthesis of 3

General Procedure:

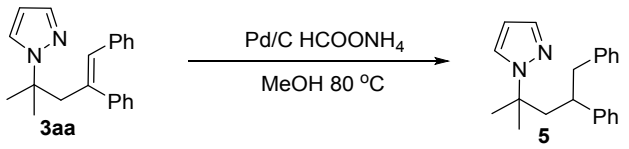


A sealed tube contained $[Cp^*Rh(CH_3CN)_3](SbF_6)_2$ (5 mol%, 0.01 mmol), Ag_2CO_3 (0.04 mmol, 0.2 equiv.), $Cu(OAc)_2{\cdot}H_2O$ (0.2 mmol, 1.0 equiv.) and **2** (0.4 mmol, 2.0 equiv.) was evacuated and purged with nitrogen gas three times. Then, **1** (0.2 mmol, 1.0 equiv.) in DCE (2.0 mL) were added to the system via syringe under a nitrogen atmosphere and the reaction was allowed to stir at 100 °C for 24 h. The reaction solution was concentrated in vacuo and the residue was purified by column chromatography on basic silica gel (petroleum ether/ethyl acetate, 70:1) to afford the desired pure products **3**.

Further Transformations of 3aa



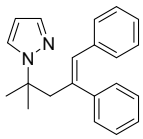
To a stirred solution of **3aa** (0.2 mmol, 1.0 equiv.) in MTBE (1.0 ml) under argon was added dropwise n-butylithium (1.6 M in hexane, 1.0 mL) at room temperature for 3 mins. Then the reaction mixture was concentrated in vacuo. The resulting residue was purified by column chromatography (PE) on silica gel to give the product **4** (PE, 40.7 mg, Isolated yield: 87%) as a colorless liquid.



To an oven-dried 50 mL screw-capped vial was added substrate **3aa** (0.2 mmol, 1.0 equiv.), HCO_2NH_4 (2.0 mmol, 10.0 equiv.), Pd/C (0.02 mmol, 0.1 equiv.), in MeOH (2.0 mL). The mixture was stirred for 8 h at 80 °C under air followed by cooling. The resulting residue was purified by column chromatography (PE:EA / 70:1) on silica gel to give the product **5** (PE:EA = 70:1, 49 mg, Isolated yield: 80%) as a colorless oil.

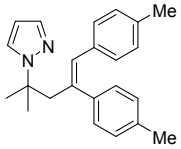
Characterization of Products

(Z)-1-(2-methyl-4,5-diphenylpent-4-en-2-yl)-1H-pyrazole (**3aa**)



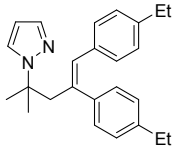
Yellow oil. (49 mg, 81%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 1.6 Hz, 1H), 7.39 (d, *J* = 2.4 Hz, 1H), 7.19 (d, *J* = 7.2 Hz, 3H), 7.09 (m, 2H), 7.04 (m, 3H), 6.76 (m, 2H), 6.16 (t, *J* = 2.0 Hz, 1H), 5.94 (s, 1H), 3.11 (s, 2H), 1.51 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 138.7, 137.8, 137.2, 130.7, 129.0, 128.9, 128.3, 127.7, 126.8, 126.7, 126.3, 104.2, 61.6, 52.3, 27.9; HRMS: Calcd for $C_{21}H_{22}N_2$: [M+H$^+$] 303.1861, found 303.1861.

(Z)-1-(2-methyl-4,5-di-p-tolylpent-4-en-2-yl)-1H-pyrazole (**3ab**)



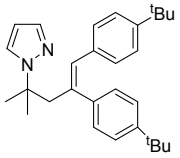
Yellow oil. (60 mg, 91%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 1.2 Hz, 1H), 7.39 (d, *J* = 2.4 Hz, 1H), 7.00 (d, *J* = 2.4 Hz, 4H), 6.86 (d, *J* = 8.0 Hz, 2H), 6.67 (d, *J* = 8.0 Hz, 2H), 6.16 (t, *J* = 2.0 Hz, 1H), 5.84 (s, 1H), 3.05 (s, 2H), 2.31 (s, 3H), 2.22 (s, 3H), 1.49 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 138.4, 136.9, 136.3, 135.8, 134.5, 130.5, 129.0, 128.8, 128.8, 128.4, 126.8, 104.1, 61.7, 52.4, 27.9, 21.2, 21.1; HRMS: Calcd for $C_{23}H_{26}N_2$: [M+H$^+$] 331.2174, found 331.2174.

(Z)-1-(4,5-bis(4-ethylphenyl)-2-methylpent-4-en-2-yl)-1H-pyrazole (**3ac**)



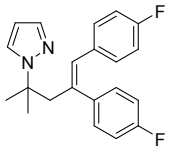
Yellow oil. (63 mg, 88%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 1.6 Hz, 1H), 7.37 (d, *J* = 2.4 Hz, 1H), 7.02 (d, *J* = 0.8 Hz, 4H), 6.89 (d, *J* = 8.0 Hz, 2H), 6.71 (d, *J* = 8.0 Hz, 2H), 6.14 (t, *J* = 2.0 Hz, 1H), 5.87 (s, 1H), 3.07 (s, 2H), 2.61 (t, *J* = 7.4 Hz, 2H), 2.52 (d, *J* = 7.4 Hz, 2H), 1.50 (s, 6H), 1.23 (t, *J* = 7.4 Hz, 3H), 1.15 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 142.2, 138.6, 138.6, 136.9, 134.7, 130.2, 130.2, 128.8, 127.7, 127.7, 127.2, 126.7, 104.1, 61.7, 52.5, 28.5, 28.4, 27.9, 15.4, 15.3; HRMS: Calcd for $C_{25}H_{30}N_2$: [M+H$^+$] 359.2487, found 359.2487.

(Z)-1-(4,5-bis(4-(tert-butyl)phenyl)-2-methylpent-4-en-2-yl)-1H-pyrazole (**3ad**)



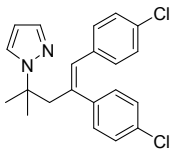
Yellow oil. (42 mg, 51%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.35 (d, *J* = 2.0 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.74 (d, *J* = 8.0 Hz, 2H), 6.11 (s, 1H), 5.87 (s, 1H), 3.07 (s, 2H), 1.51 (s, 6H), 1.31 (s, 9H), 1.23 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 149.2, 138.6, 138.3, 137.0, 134.3, 130.1, 128.6, 128.4, 126.7, 125.1, 124.6, 104.1, 61.6, 52.6, 34.5, 34.4, 31.4, 31.2, 27.9; HRMS: Calcd for $C_{29}H_{38}N_2$: [M+H$^+$] 415.3113, found 415.3113.

(Z)-1-(4,5-bis(4-fluorophenyl)-2-methylpent-4-en-2-yl)-1H-pyrazole (**3ae**)



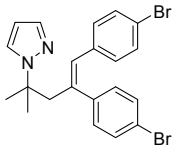
Yellow oil (41 mg, 60%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 1.2 Hz, 1H), 7.32 (d, *J* = 2.0 Hz, 1H), 7.02 – 6.94 (m, 2H), 6.86 (t, *J* = 8.8 Hz, 2H), 6.79 – 6.65 (m, 4H), 6.11 (t, *J* = 2.0 Hz, 1H), 5.93 (s, 1H), 3.07 (s, 2H), 1.52 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, *J* = 41.0 Hz), 160.3 (d, *J* = 41.0 Hz), 138.7, 136.8 (d, *J* = 1.0 Hz), 136.6 (d, *J* = 3.5 Hz), 133.1 (d, *J* = 3.2 Hz), 130.5 (d, *J* = 8.0 Hz), 130.4 (d, *J* = 8.0 Hz), 129.9, 126.6, 115.3 (d, *J* = 21.2 Hz), 114.7 (d, *J* = 21.2 Hz), 104.3, 61.4, 52.1, 27.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.15, -115.39; HRMS: Calcd for $C_{21}H_{20}F_2N_2$: [M+H$^+$] 339.1673, found 339.1666.

(Z)-1-(4,5-bis(4-chlorophenyl)-2-methylpent-4-en-2-yl)-1H-pyrazole (**3af**)



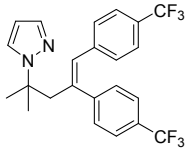
Yellow oil (31 mg, 42%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 1.6 Hz, 1H), 7.31 (d, *J* = 2.4 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.66 (d, *J* = 8.4 Hz, 2H), 6.12 (t, *J* = 2.0 Hz, 1H), 5.90 (s, 1H), 3.07 (s, 2H), 1.51 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.0, 138.8, 137.4, 135.3, 132.8, 132.2, 130.2, 130.1, 130.0, 128.6, 128.0, 126.7, 104.3, 61.3, 51.9, 27.9; HRMS: Calcd for $C_{21}H_{20}Cl_2N_2$: [M+H$^+$] 371.1082, found 371.1083.

(Z)-1-(4,5-bis(4-bromophenyl)-2-methylpent-4-en-2-yl)-1H-pyrazole (**3ag**)



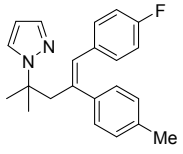
Yellow oil. (39 mg, 42%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 1.6 Hz, 1H), 7.32 – 7.28 (m, 3H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.89 (d, *J* = 8.4 Hz, 2H), 6.60 (d, *J* = 8.4 Hz, 2H), 6.12 (t, *J* = 2.0 Hz, 1H), 5.88 (s, 1H), 3.07 (s, 2H), 1.51 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 138.8, 137.5, 135.7, 131.6, 131.0, 130.5, 130.5, 130.1, 126.7, 121.0, 120.4, 104.3, 61.3, 51.9, 27.9; HRMS: Calcd for $C_{21}H_{20}Br_2N_2$: [M+H$^+$] 461.0051, found 461.0051.

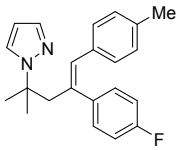
(Z)-1-(2-methyl-4,5-bis(4-(trifluoromethyl)phenyl)pent-4-en-2-yl)-1H-pyrazole (**3ah**)



Yellow oil. (18 mg, 20%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 2.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 2.0 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 6.09 – 6.04 (m, 2H), 3.16 (s, 2H), 1.54 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 140.2, 139.0, 138.9, 130.6, 129.3 (q, *J* = 32.3 Hz), 129.2, 129.1, 128.6 (q, *J* = 32.3 Hz), 126.6, 125.4, 125.3 (q, *J* = 3.7 Hz), 124.9 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 270.5 Hz), 104.4, 61.2, 52.0, 28.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.59, -62.60; HRMS: Calcd for $C_{23}H_{20}F_6N_2$: [M+H$^+$] 439.1609, found 439.1614.

(Z)-1-(5-(4-fluorophenyl)-2-methyl-4-(p-tolyl)pent-4-en-2-yl)-1H-pyrazole and *(Z)-1-(4-(4-fluorophenyl)-2-methyl-5-(p-tolyl)pent-4-en-2-yl)-1H-pyrazole* (**3ai** and **3ai'**)

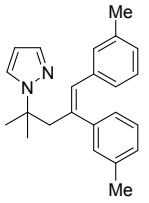




Yellow oil. (35 mg, 52%, 5:4); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 1.2 Hz, 1H), 7.49 (d, *J* = 1.6 Hz, 0.8H), 7.38 (d, *J* = 2.0 Hz, 1H), 7.31 (d, *J* = 2.0 Hz, 0.8H), 7.01 (m, 4H), 6.96 (s, 1.6H), 6.94 (s, 0.8H), 6.85 – 6.84 (m, 4H), 6.73 (d, *J* = 2.0 Hz, 1.8H), 6.71 (s, 2H), 6.66 (s, 1H), 6.64 (s, 0.8H), 6.17 (t, *J* = 2.0 Hz, 1H), 6.09 (t, *J* = 2.0 Hz, 0.8H), 5.97 (s, 0.8H), 5.79 (s, 1H), 3.07 (s, 1.6H), 3.05 (s, 2H), 2.30 (s, 3H), 2.23 (s, 2.4H), 1.52 (s, 4.9H), 1.48 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 138.0, 137.6 (d, *J* = 0.8 Hz), 137.0 (d, *J* = 3.4 Hz), 136.6, 136.1, 136.0, 134.1, 133.4 (d, *J* = 3.3 Hz), 131.0, 130.5 (d, *J* = 7.7 Hz), 130.4 (d, *J* = 7.7 Hz), 129.8, 129.1, 129.1,

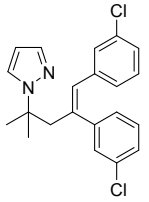
128.8, 128.5, 126.8, 126.6, 115.2 (d, J = 21.0 Hz), 114.6 (d, J = 21.2 Hz), 104.2, 104.1, 61.7, 61.4, 52.2, 52.2, 27.9, 27.9, 21.2, 21.1, 21.1, 21.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.52, -115.82; HRMS: Calcd for $C_{22}H_{23}FN_2$: [M+H$^+$] 335.1924, found 335.1925.

(Z)-1-(2-methyl-4,5-di-m-tolylpent-4-en-2-yl)-1H-pyrazole (**3aj**)



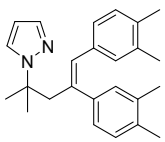
Yellow oil. (50 mg, 75%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.37 (d, J = 2.0 Hz, 1H), 7.06 (t, J = 7.6 Hz, 1H), 6.98 – 6.84 (m, 5H), 6.61 (s, 1H), 6.55 (d, J = 7.6 Hz, 1H), 6.14 (s, 1H), 5.90 (s, 1H), 3.09 (s, 2H), 2.25 (s, 3H), 2.15 (s, 3H), 1.52 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 138.6, 137.8, 137.7, 137.1, 137.1, 130.6, 129.8, 129.3, 128.0, 127.5, 127.0, 126.7, 126.1, 125.9, 104.1, 61.6, 52.4, 27.9, 21.3; HRMS: Calcd for $C_{23}H_{26}N_2$: [M+H$^+$] 331.2174, found 331.2169.

(Z)-1-(4,5-bis(3-chlorophenyl)-2-methylpent-4-en-2-yl)-1H-pyrazole (**3ak**)



Yellow oil. (24 mg, 33%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 1.2 Hz, 1H), 7.32 (d, J =1.6 Hz, 1H), 7.14 – 7.13 (m, 1H), 7.09 (t, J = 7.6 Hz, 1H), 7.05 – 7.01 (m, 1H), 7.00 (t, J = 1.6 Hz, 1H), 6.96 (t, J = 7.6 Hz, 1H), 6.88 – 6.87 (m, 1H), 6.75 (t, J = 2.0 Hz, 1H), 6.57 (d, J = 8.0 Hz, 1H), 6.16 – 6.05 (m, 1H), 5.90 (s, 1H), 3.09 (s, 2H), 1.54 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.2, 138.8, 138.5, 138.1, 134.2, 133.8, 130.2, 130.2, 129.5, 129.0, 128.9, 128.6, 127.2, 127.0, 126.7, 104.3, 61.2, 51.8, 27.9; HRMS: Calcd for $C_{21}H_{20}Cl_2N_2$: [M+H$^+$] 371.1082, found 371.1085.

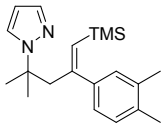
(Z)-1-(4,5-bis(3,4-dimethylphenyl)-2-methylpent-4-en-2-yl)-1H-pyrazole (**3al**)



Yellow oil. (33 mg, 46%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 1.6 Hz, 1H), 7.38 (d, J = 2.4 Hz, 1H), 6.94 (d, J = 8.0 Hz, 1H), 6.88 (s, 1H), 6.82 (d, J = 8.0 Hz, 1H), 6.78 (d, J = 8.0 Hz, 1H),

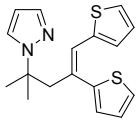
6.61 (s, 1H), 6.51 (d, *J* = 7.6 Hz, 1H), 6.15 (t, *J* = 2.0 Hz, 1H), 5.83 (s, 1H), 3.05 (s, 2H), 2.23 (s, 3H), 2.18 (s, 3H), 2.14 (s, 3H), 2.07 (s, 3H), 1.51 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.9, 138.6, 136.9, 136.3, 135.6, 134.9, 134.9, 134.5, 130.4, 130.1, 129.8, 129.4, 128.9, 126.7, 126.5, 126.1, 104.0, 61.7, 52.5, 27.9, 19.7, 19.6, 19.5, 19.3; HRMS: Calcd for $C_{25}H_{30}N_2$: [M+H$^+$] 359.2487, found 359.2488.

(Z)-1-(5-(3,4-dimethylphenyl)-2-methyl-4-(trimethylsilyl)pent-4-en-2-yl)-1H-pyrazole (**3am**)



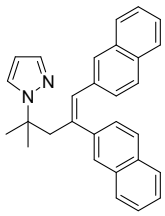
Yellow oil. (31 mg, 48%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 1.6 Hz, 1H), 7.45 (d, *J* =2.0 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.63 – 6.55 (m, 2H), 6.26 – 6.20 (m, 1H), 5.48 – 5.41 (m, 1H), 2.49 (s, 1H), 2.47 (s, 1H), 2.24 (s, 3H), 2.23 (s, 3H), 1.51 (s, 6H), -0.04 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 139.4, 138.6, 135.9, 134.8, 133.3, 129.2, 128.8, 126.2, 125.0, 104.4, 60.5, 42.5, 27.6, 19.8, 19.3, -1.7; HRMS: Calcd for $C_{20}H_{30}N_2Si$: [M+H$^+$] 327.2257, found 327.2255.

1-(2-methyl-4,5-di(thiophen-2-yl)pent-4-en-2-yl)-1H-pyrazole (**3an**)



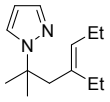
Yellow oil. (43 mg, 68%, Z:E = 3:2); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 1.2 Hz, 1H), 7.49 (d, *J* = 1.6 Hz, 0.6H), 7.44 (d, *J* = 2.0 Hz, 1H), 7.34 (d, *J* = 5.2 Hz, 1H), 7.28 (d, *J* = 4.8 Hz, 0.63H), 7.25 (d, *J* = 2.4 Hz, 0.63H), 7.09 (d, *J* = 3.2 Hz, 1.2H), 7.03-7.02 (m, 2.4H), 6.97 (dd, *J* = 5.0, 3.6 Hz, 1H), 6.89 (d, *J* = 3.2 Hz, 1H), 6.82 (dd, *J* = 4.8, 3.6 Hz, 1H), 6.77 – 6.75 (m, 0.6H), 6.74 – 6.73 (m, 1H), 6.53 (d, *J* = 3.6 Hz, 0.6H), 6.17 (t, *J* = 2.0 Hz, 1H), 6.07 (s, 1H), 5.99 (t, *J* = 2.0 Hz, 0.6H), 3.53 (s, 1.2H), 3.04 (s, 2H), 1.66 (s, 4H), 1.59 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.4, 142.3, 139.8, 139.8, 138.9, 138.8, 130.4, 129.2, 128.8, 128.5, 127.6, 127.3, 127.1, 126.9, 126.8, 126.8, 126.5, 126.3, 126.0, 125.7, 125.2, 124.1, 123.9, 123.6, 104.4, 104.4, 61.6, 61.2, 53.0, 43.2, 27.8, 27.7; HRMS: Calcd for $C_{17}H_{18}N_2S_2$: [M+H$^+$] 315.0990, found 315.0994.

1-(2-methyl-4,5-di(naphthalen-2-yl)pent-4-en-2-yl)-1H-pyrazole (**3ao**)



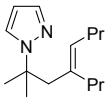
Yellow oil. (31 mg, 38%, Z:E = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.68 (m, 7.51H), 7.67 – 7.40 (m, 12.08H), 7.40 – 7.31 (m, 5.04H), 7.29 (d, *J* = 1.6 Hz, 0.51H), 7.18 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.07 (d, *J* = 2.0 Hz, 0.5H), 7.02 (s, 0.5H), 6.81 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.19 (s, 1H), 6.12 – 6.07 (m, 0.5H), 5.76 – 5.72 (m, 1H), 3.57 (s, 1.02H), 3.28 (s, 2H), 1.54 (s, 6H), 1.44 (s, 3.08H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 140.0, 138.8, 138.7, 138.6, 138.0, 135.4, 134.8, 133.6, 133.5, 133.4, 133.4, 133.2, 132.5, 132.5, 132.3, 132.1, 131.1, 128.2, 128.1, 128.0, 127.9, 127.9, 127.8, 127.7, 127.6, 127.4, 127.2, 127.0, 126.8, 126.2, 126.0, 125.9, 125.8, 125.8, 125.6, 125.3, 125.2, 104.2, 61.7, 61.2, 52.5, 41.7, 29.7, 28.4, 28.0; HRMS: Calcd for $C_{29}H_{26}N_2$: [M+H$^+$] 403.2174, found 403.2179.

(E)-1-(4-ethyl-2-methylhept-4-en-2-yl)-1H-pyrazole (**3ap**)



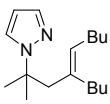
Yellow oil. (31 mg, 76%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 1.2 Hz, 1H), 7.39 (d, *J* = 2.4 Hz, 1H), 6.17 (t, *J* = 2.0 Hz, 1H), 4.79 (t, *J* = 7.2 Hz, 1H), 2.48 (s, 2H), 1.93 (m, 2H), 1.57 (s, 6H), 1.44 (m, 2H), 0.88 (t, *J* = 7.6 Hz, 3H), 0.78 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 136.5, 136.4, 131.6, 126.6, 104.3, 60.9, 48.3, 27.8, 23.3, 20.9, 14.6, 13.5; HRMS: Calcd for $C_{13}H_{22}N_2$: [M+H$^+$] 207.1861, found 207.1854.

(E)-1-(2-methyl-4-propyloct-4-en-2-yl)-1H-pyrazole (**3aq**)



Yellow oil. (34 mg, 72%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 1.2 Hz, 1H), 7.40 (dd, *J* = 2.4, 0.4 Hz, 1H), 6.20 – 6.15 (m, 1H), 4.84 (t, *J* = 7.2 Hz 1H), 2.49 (s, 2H), 1.90 (m, 2H), 1.57 (s, 6H), 1.39 (m, 2H), 1.31 – 1.17 (m, 4H), 0.86 (t, *J* = 7.6 Hz, 3H), 0.74 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 135.3, 130.5, 126.5, 104.3, 61.0, 48.7, 32.3, 30.0, 29.9, 27.8, 23.1, 21.9, 14.0, 13.9; HRMS: Calcd for $C_{15}H_{26}N_2$: [M+H$^+$] 235.2174, found 235.2174.

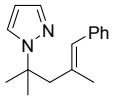
(E)-1-(4-butyl-2-methylnon-4-en-2-yl)-1H-pyrazole (**3ar**)



Yellow oil. (35 mg, 66%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 1.2 Hz, 1H), 7.39 (d, *J* = 2.0 Hz, 1H), 6.17 (t, *J* = 2.0 Hz, 1H), 4.83 (t, *J* = 7.2 Hz, 1H), 2.49 (s, 2H), 1.92 (q, *J* = 7.2 Hz, 2H),

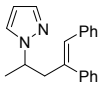
1.57 (s, 6H), 1.39 (d, J = 7.2 Hz, 2H), 1.27 (dd, J = 7.2, 3.2 Hz, 2H), 1.24 (d, J = 3.2 Hz, 2H), 1.19 – 1.10 (m, 4H), 0.85 (t, J = 7.2 Hz, 3H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 135.4, 135.3, 130.5, 126.5, 104.3, 61.0, 48.7, 32.3, 30.0, 29.9, 27.9, 23.1, 21.9, 14.0, 13.9; HRMS: Calcd for $C_{17}H_{30}N_2$: [M+H$^+$] 263.2487, found 263.2481.

(E)-1-(2,4-dimethyl-5-phenylpent-4-en-2-yl)-1H-pyrazole (**3as**)



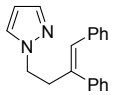
Yellow oil. (42 mg, 88%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 1.6 Hz, 1H), 7.48 (d, J = 2.4 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.20 – 7.14 (m, 3H), 6.23 (t, J = 2.0 Hz, 1H), 5.98 (s, 1H), 2.74 (s, 2H), 1.67 (s, 6H), 1.43 (d, J = 1.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 138.1, 134.7, 129.6, 128.8, 128.0, 126.6, 126.1, 104.5, 60.9, 53.1, 27.9, 18.6; HRMS: Calcd for $C_{16}H_{20}N_2$: [M+H$^+$] 241.1705, found 241.1702.

(Z)-1-(4,5-diphenylpent-4-en-2-yl)-1H-pyrazole (**3ba**)



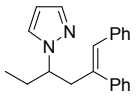
Yellow oil. (47 mg, 82%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (s, 1H), 7.32 – 7.27 (m, 4H), 7.16 – 7.11 (m, 2H), 7.05 (dd, J = 5.2, 1.6 Hz, 3H), 6.85 – 6.76 (m, 2H), 6.24 (s, 1H), 6.19 (t, J = 2.0 Hz, 1H), 4.27 – 4.21 (m, 1H), 3.19 – 3.14 (m, 1H), 2.92 – 2.87 (m, 1H), 1.52 (d, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 139.0, 138.4, 137.0, 129.4, 128.9, 128.8, 128.7, 128.1, 127.8, 127.3, 126.4, 104.4, 56.1, 48.1, 20.9; HRMS: Calcd for $C_{20}H_{20}N_2$: [M+H$^+$] 289.1705, found 289.1699.

(Z)-1-(3,4-diphenylbut-3-en-1-yl)-1H-pyrazole (**3ca**)



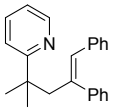
Yellow oil. (29 mg, 53%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 1.6 Hz, 1H), 7.34 – 7.27 (m, 4H), 7.19 – 7.16 (m, 2H), 7.11 – 7.03 (m, 3H), 6.86 – 6.84 (m, 2H), 6.32 (s, 1H), 6.21 (t, J = 2.0 Hz, 1H), 4.15 (t, J = 7.2 Hz, 2H), 3.07 (t, J = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 138.5, 136.9, 129.3, 129.1, 129.0, 128.8, 128.8, 127.9, 127.4, 126.5, 105.0, 50.5, 41.3; HRMS: Calcd for $C_{19}H_{18}N_2$: [M+H$^+$] 275.1548, found 275.1549.

(Z)-1-(5,6-diphenylhex-5-en-3-yl)-1H-pyrazole (**3da**)



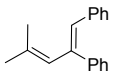
Yellow oil. (13 mg, 22%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 1.6 Hz, 1H), 7.31 – 7.27 (m, 3H), 7.21 (d, *J* = 2.0 Hz, 1H), 7.12 – 7.10 (m, 2H), 7.04 – 7.03 (m, 3H), 6.78 – 6.76 (m, 2H), 6.19 – 6.18 (m, 2H), 3.90 (m, 1H), 3.16 – 3.10 (m, 1H), 2.96 (m, 1H), 2.07 – 1.97 (m, 1H), 1.86 – 1.76 (m, 1H), 0.69 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 139.2, 138.4, 137.0, 129.3, 128.9, 128.9, 128.6, 127.7, 127.2, 126.3, 104.1, 62.5, 46.5, 28.3, 10.6; HRMS: Calcd for $C_{21}H_{22}N_2$: [M+H$^+$] 303.1861, found 303.1859.

(Z)-2-(2-methyl-4,5-diphenylpent-4-en-2-yl)pyridine (**3ea**)



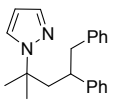
Yellow oil. (45 mg, 71%);^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.39 (m, 1H), 7.43 – 7.37 (m, 1H), 7.08 – 6.93 (m, 10H), 6.76 – 6.74 (m, 2H), 6.19 (s, 1H), 3.03 (d, *J* = 1.6 Hz, 2H), 1.33 (s, 3H), 1.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 148.4, 141.4, 140.6, 137.5, 135.5, 129.9, 129.0, 129.0, 128.0, 127.6, 126.3, 126.0, 120.4, 120.1, 53.1, 41.7, 28.1; HRMS: Calcd for $C_{23}H_{23}N$: [M+H$^+$] 314.1909, found 314.1915.

(Z)-(4-methylpenta-1,3-diene-1,2-diyl)dibenzene(**4**)



Colorless oil. (41 mg, 87%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.24 (m, 3H), 7.20 – 7.16 (m, 2H), 7.14 – 7.04 (m, 3H), 6.98 – 6.93 (m, 2H), 6.47 (s, 1H), 5.96 – 5.95 (m, 1H), 1.85 (d, *J* = 1.2 Hz, 3H), 1.63 (d, *J* = 1.2 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 140.8, 140.3, 137.5, 136.1, 129.3, 129.2, 128.5, 128.4, 127.8, 127.0, 126.3, 27.2, 19.6; HRMS: Calcd for $C_{18}H_{18}$: [M+H$^+$] 235.1487, found 235.1478.

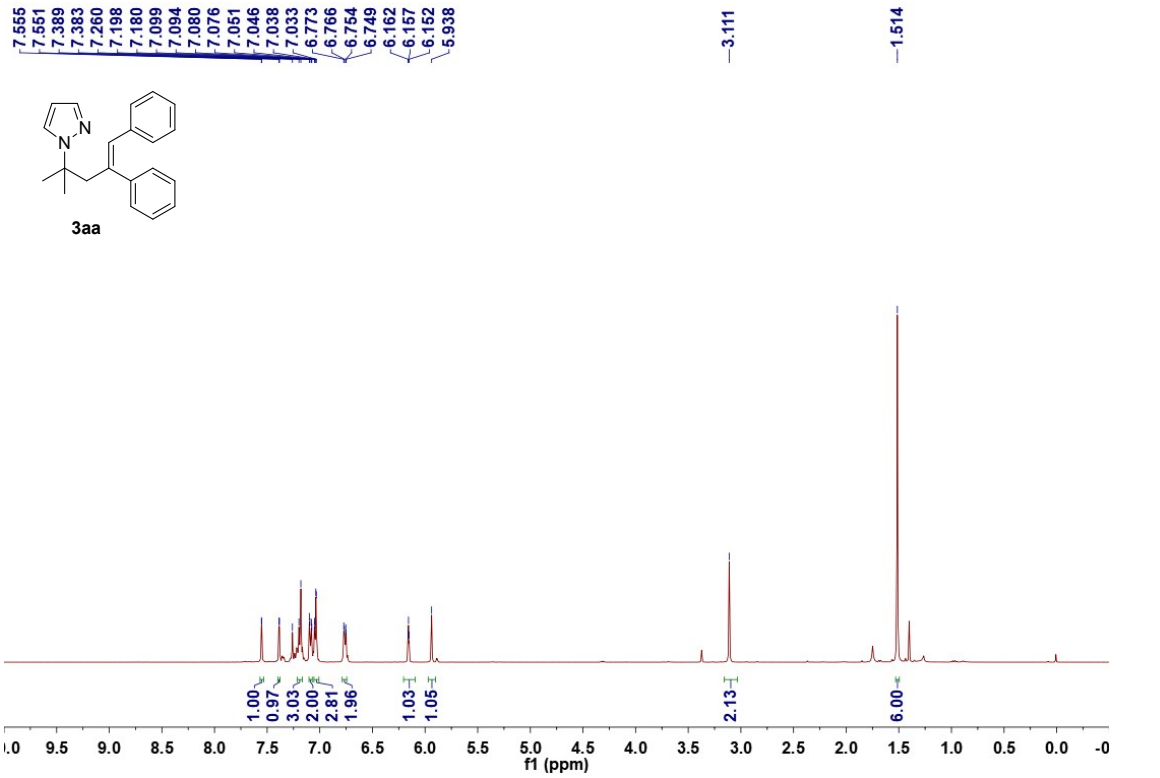
1-(2-methyl-4,5-diphenylpentan-2-yl)-1H-pyrazole(**5**)



Colorless oil. (49 mg, 80%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 1.6 Hz, 1H), 7.31 – 7.30 (m, 1H), 7.19 – 7.09 (m, 6H), 6.99 – 6.94 (m, 2H), 6.82 – 6.80 (m, 2H), 6.26 – 6.02 (m, 1H), 2.72 – 2.55 (m, 3H), 2.45 – 2.41 (m, 1H), 2.35 – 2.29 (m, 1H), 1.47 (s, 3H), 1.38 (s, 3H).^{13}C NMR (100

MHz, $CDCl_3$) δ 145.3, 140.1, 138.6, 129.1, 128.1, 127.9, 127.8, 126.2, 125.9, 125.7, 104.5, 60.8, 48.0, 45.3, 44.2, 29.5, 27.1; HRMS: Calcd for $C_{21}H_{24}N_2$: [M+H$^+$] 305.2018, found 305.2016.

NMR Spectra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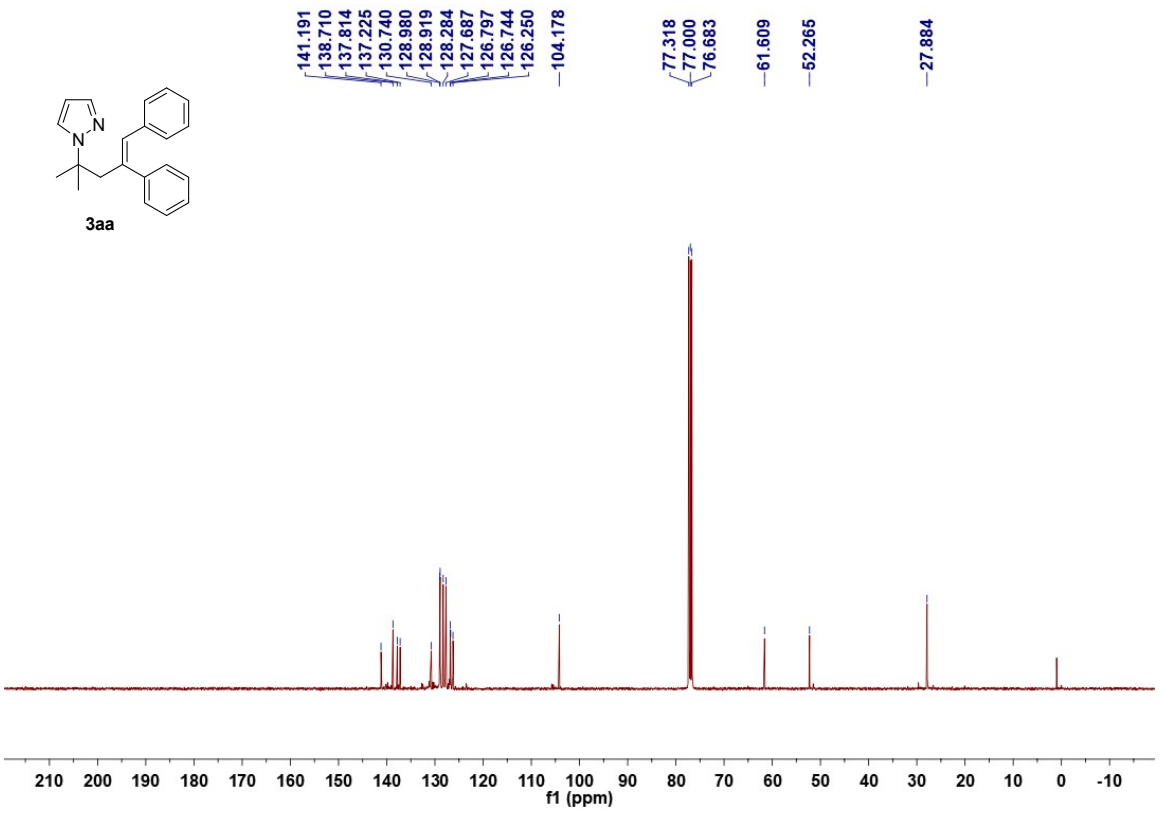
7.551
7.389
7.383
7.260
7.198
7.180
7.099
7.094
7.080
7.076
7.051
7.046
7.038
7.033
6.773
6.766
6.754
6.749
6.162
6.157
6.152
5.938
3.111
1.514
3aa
1.00
0.97
3.03
2.00
2.81
1.96
1.03
1.05
2.13
6.00
f1 (ppm)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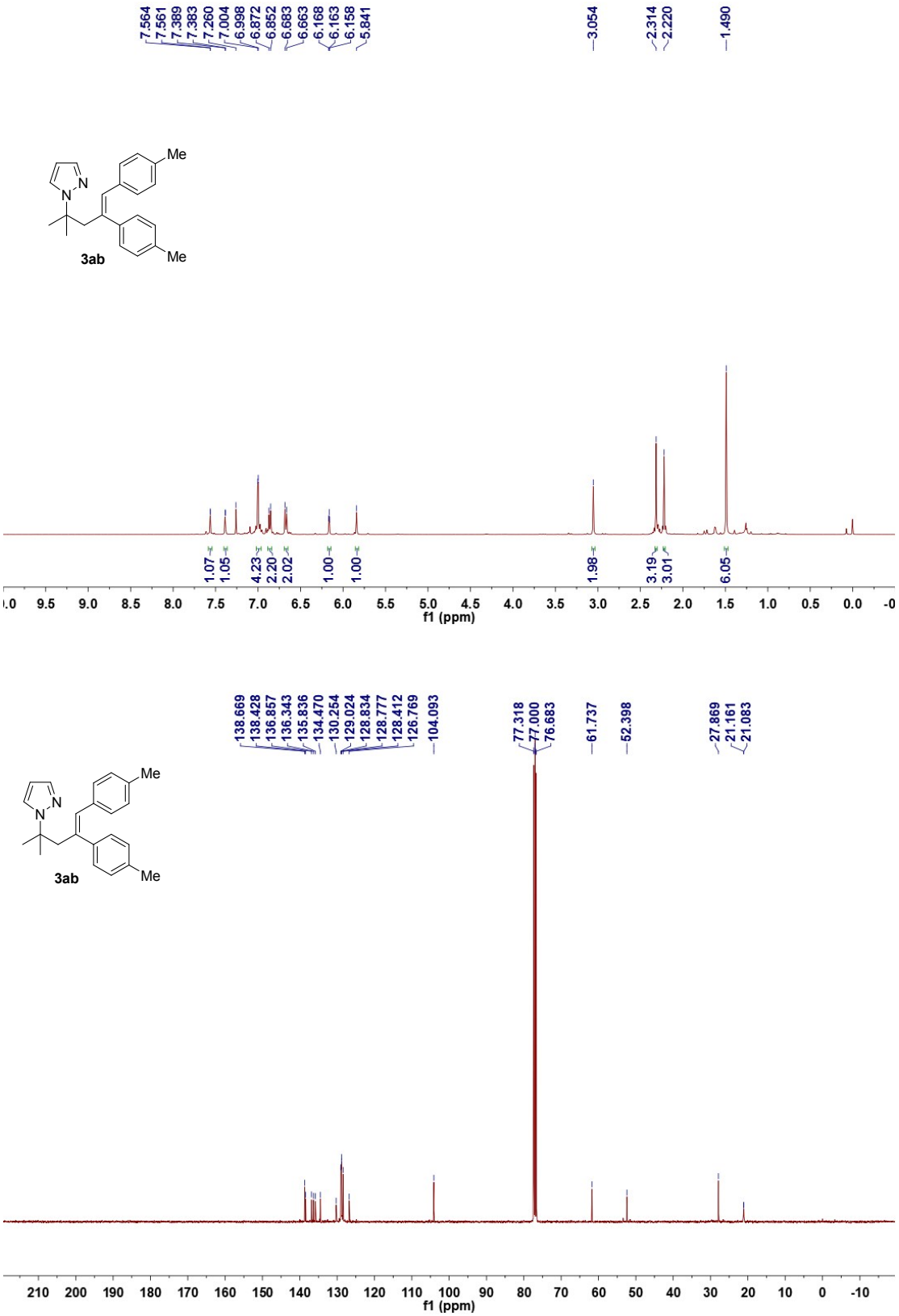
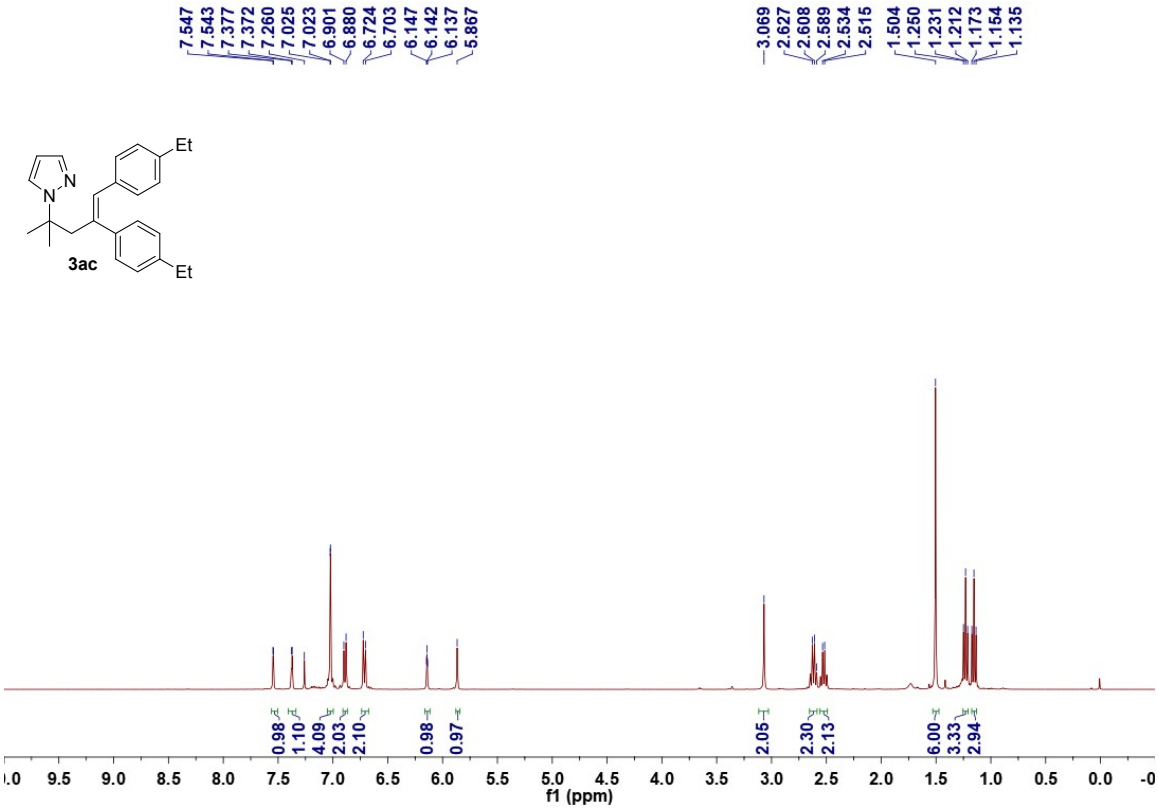
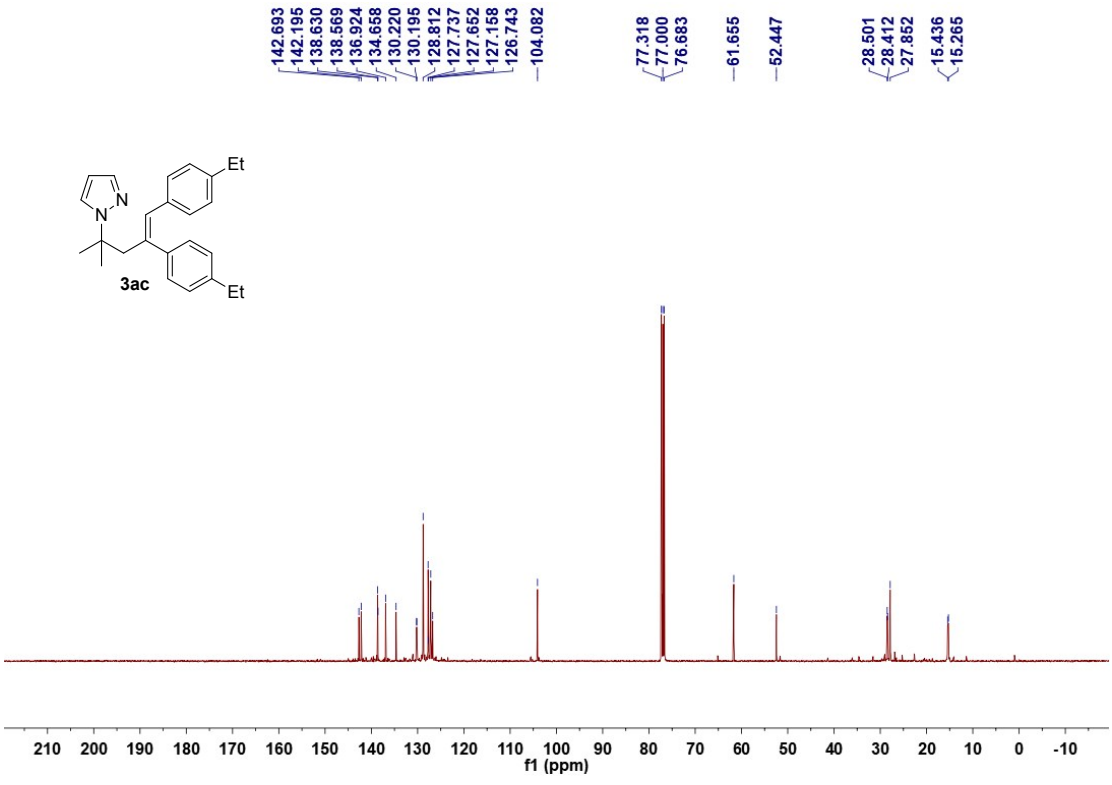
138.710
137.814
137.225
130.740
128.980
128.919
128.284
127.687
126.797
126.744
126.250
104.178
77.318
77.000
76.683
61.609
52.265
27.884
3aa
f1 (ppm)


7.564
7.561
7.389
7.383
7.260
7.004
6.998
6.872
6.852
6.683
6.663
6.168
6.163
6.158
5.841
3.054
2.314
2.220
1.490
Me
Me
3ab
1.07
1.05
4.23
2.20
2.02
1.00
1.00
1.98
3.19
3.01
6.05
f1 (ppm)
138.669
138.428
136.857
136.343
135.836
134.470
130.254
129.024
128.834
128.777
128.412
126.769
104.093
77.318
77.000
76.683
61.737
52.398
27.869
21.161
21.083
Me
Me
3ab
f1 (ppm)


7.547
7.543
7.377
7.372
7.260
7.025
7.023
6.901
6.880
6.724
6.703
6.147
6.142
6.137
5.867
3.069
2.627
2.608
2.589
2.534
2.515
1.504
1.250
1.231
1.212
1.173
1.154
1.135
Et
N
N
3ac
Et
0.98
1.10
4.09
2.03
2.10
0.98
0.97
2.05
2.30
2.13
6.00
3.33
2.94
f1 (ppm)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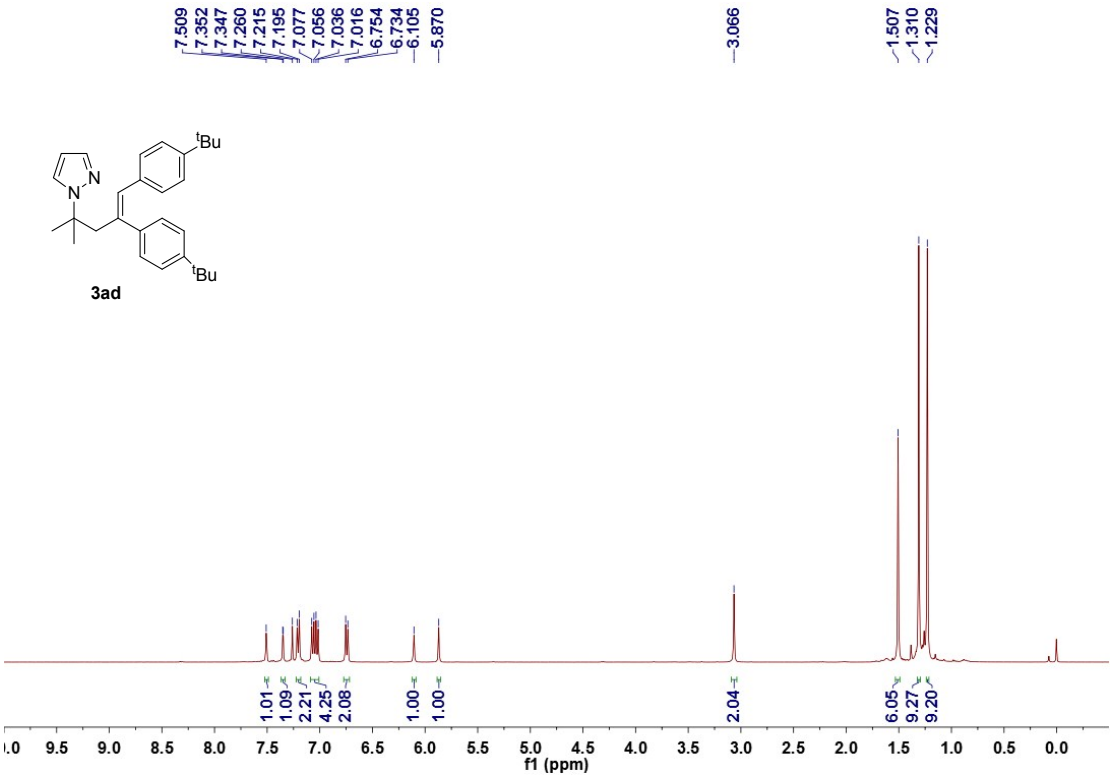
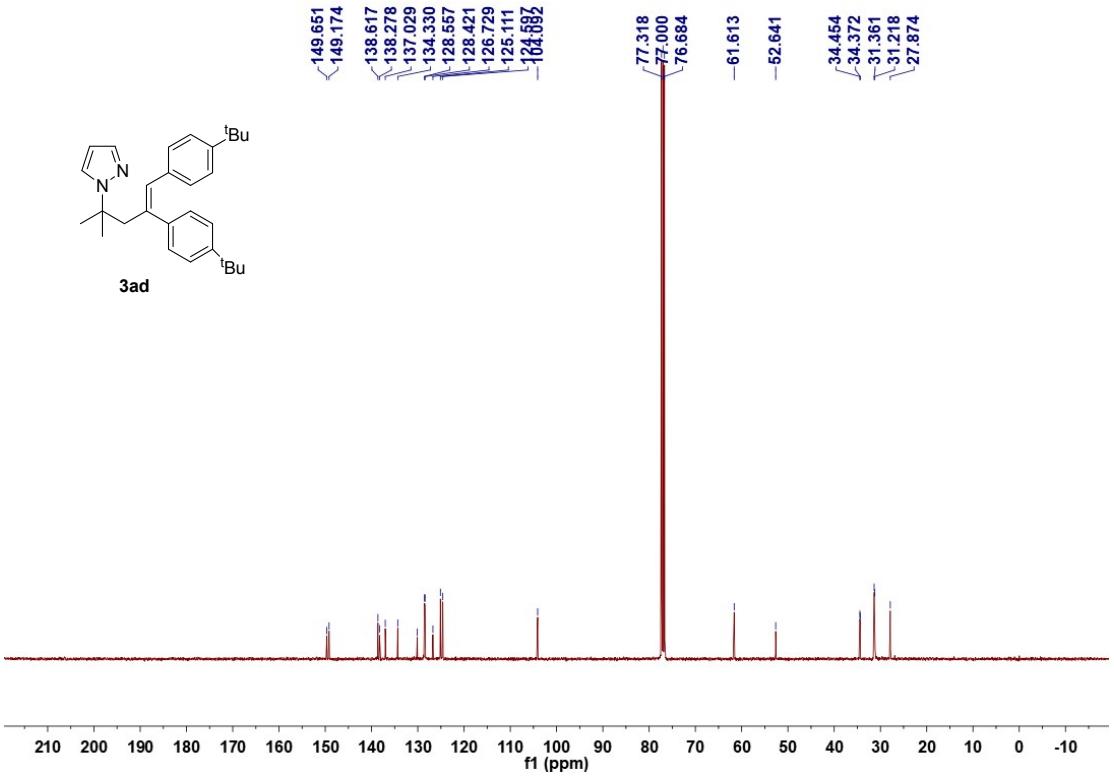
142.195
138.630
138.569
136.924
134.658
130.220
130.195
128.812
127.737
127.652
127.158
126.743
104.082
77.318
77.000
76.683
61.655
52.447
28.501
28.412
27.852
15.436
15.265
Et
N
N
3ac
Et
f1 (ppm)


7.509
7.352
7.347
7.260
7.215
7.195
7.077
7.056
7.036
7.016
6.754
6.734
6.105
5.870
3.066
1.507
1.310
1.229
tBu
tBu
3ad
1.01
1.09
2.21
4.25
2.08
1.00
1.00
2.04
6.05
9.27
9.20
f1 (ppm)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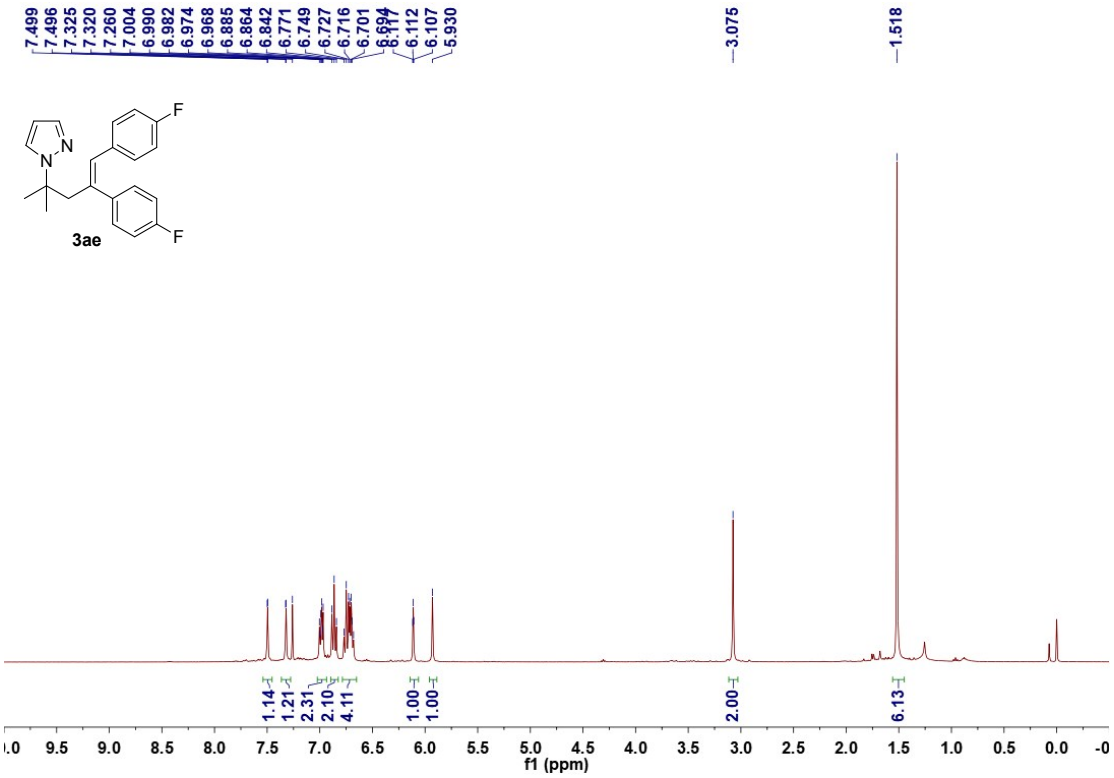
149.174
138.617
138.278
137.029
134.330
128.557
128.421
126.729
125.111
77.318
77.000
76.684
61.613
52.641
34.454
34.372
31.361
31.218
27.874
tBu
tBu
3ad
f1 (ppm)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7.496
7.325
7.320
7.260
7.004
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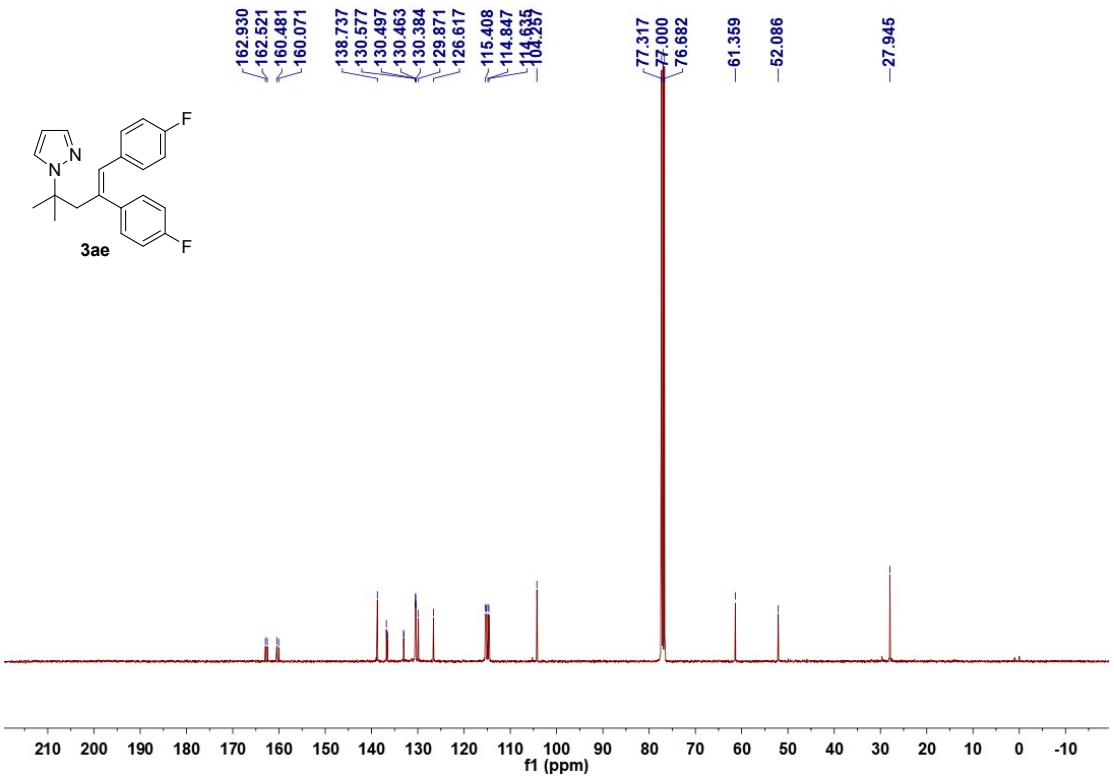
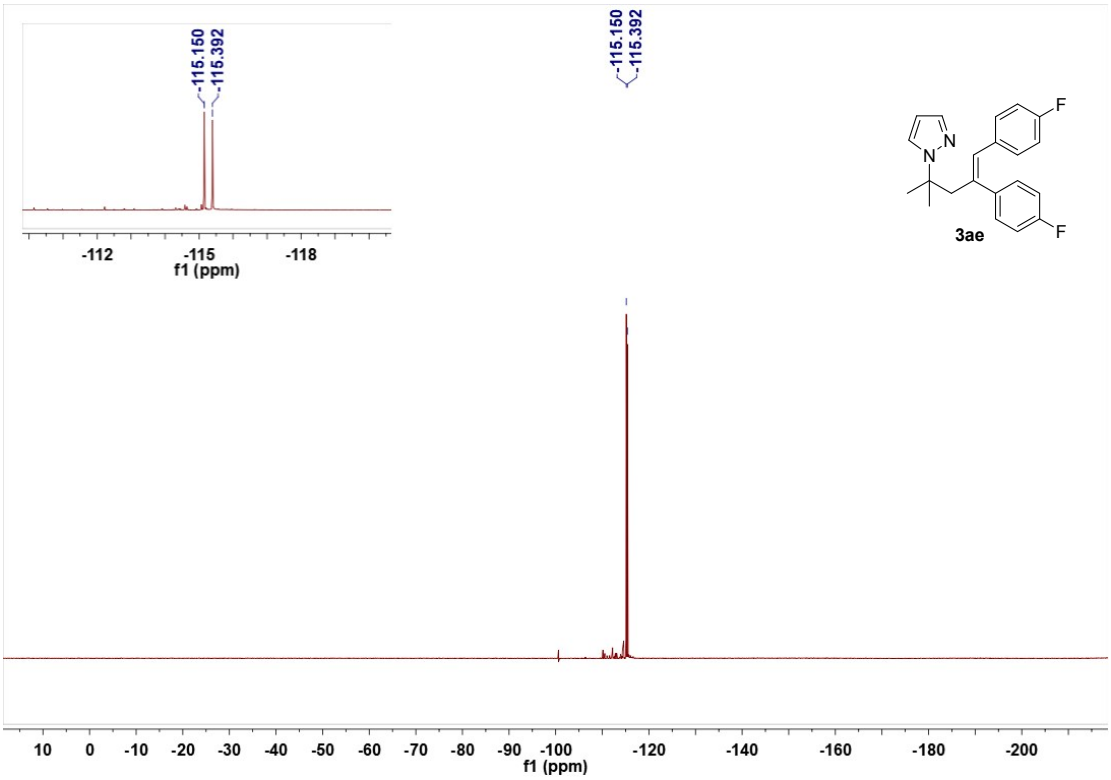
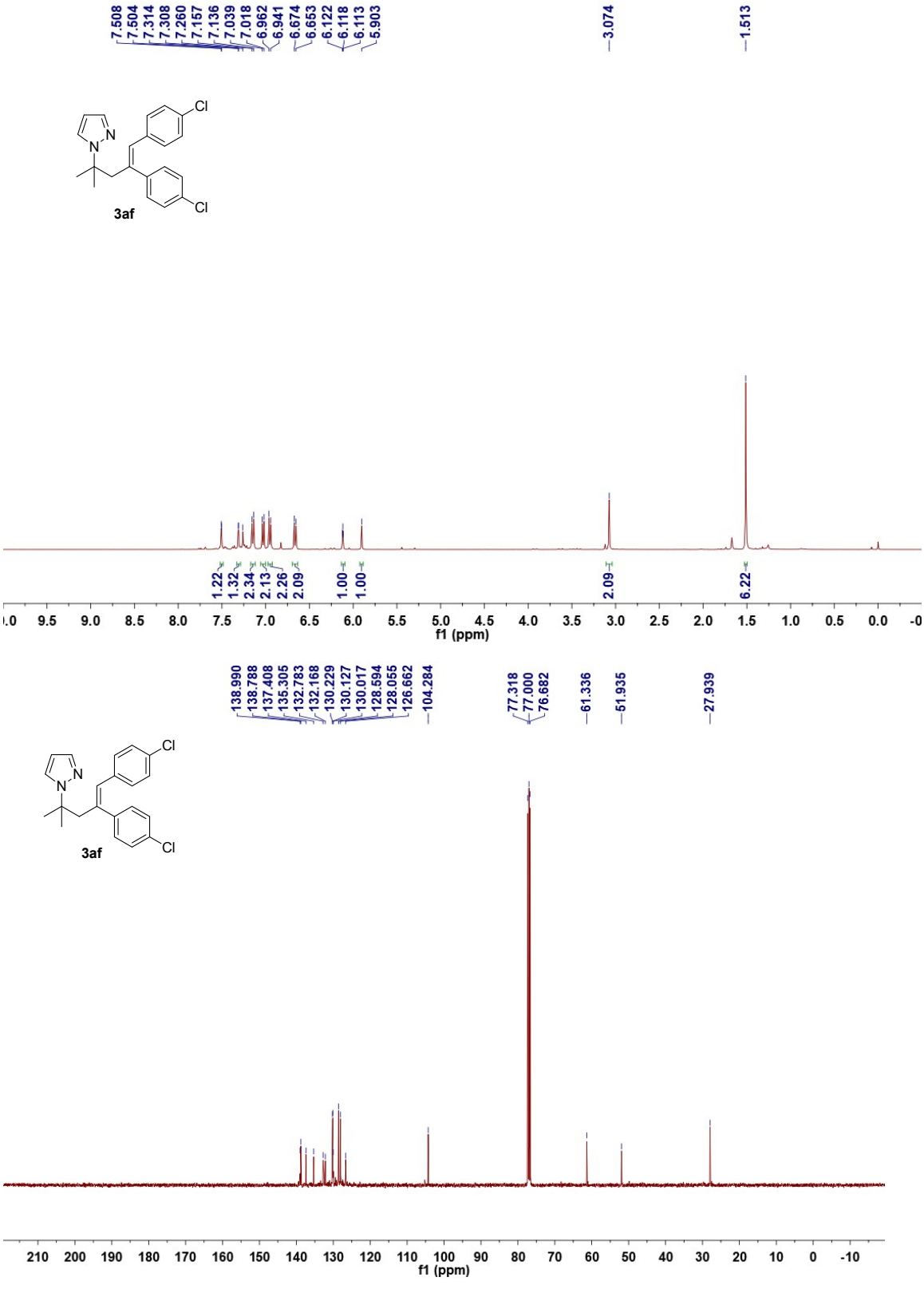
6.982
6.974
6.968
6.885
6.864
6.842
6.771
6.749
6.727
6.716
6.701
6.112
6.107
5.930
3.075
1.518
F
N
N
F
3ae
1.14
1.21
2.31
2.10
4.11
1.00
1.00
2.00
6.13
f1 (ppm)


162.930
162.521
160.481
160.071
138.737
130.577
130.497
130.463
130.384
129.871
126.617
115.408
114.847
77.317
77.000
76.682
61.359
52.086
27.945
F
N
N
F
3ae
f1 (ppm)


-115.150
-115.392
-112
-115
-118
f1 (ppm)
-115.150
-115.392
F
N
N
F
3ae
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)


7.508
7.504
7.314
7.308
7.260
7.157
7.136
7.039
7.018
6.962
6.941
6.674
6.653
6.122
6.118
6.113
5.903
3.074
1.513
Cl
N
N
Cl
3af
1.22
1.32
2.34
2.13
2.26
2.09
1.00
1.00
2.09
6.22
f1 (ppm)
138.990
138.788
137.408
135.305
132.783
132.168
130.229
130.127
130.017
128.594
128.055
126.662
104.284
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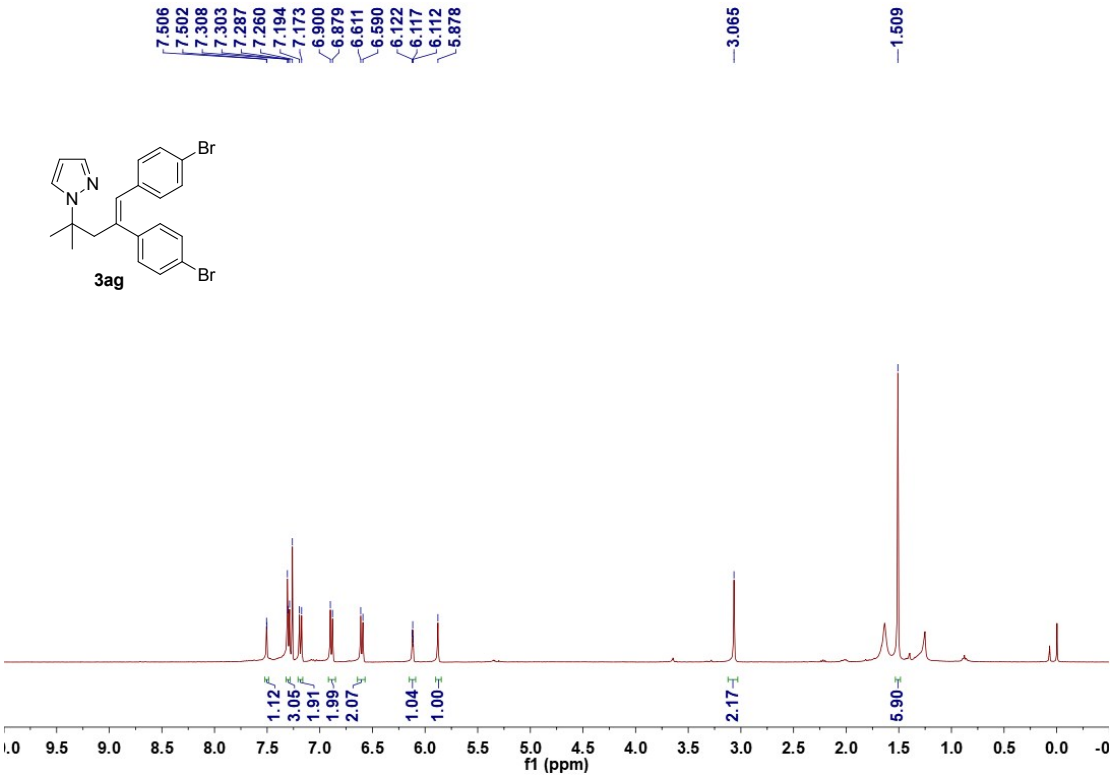
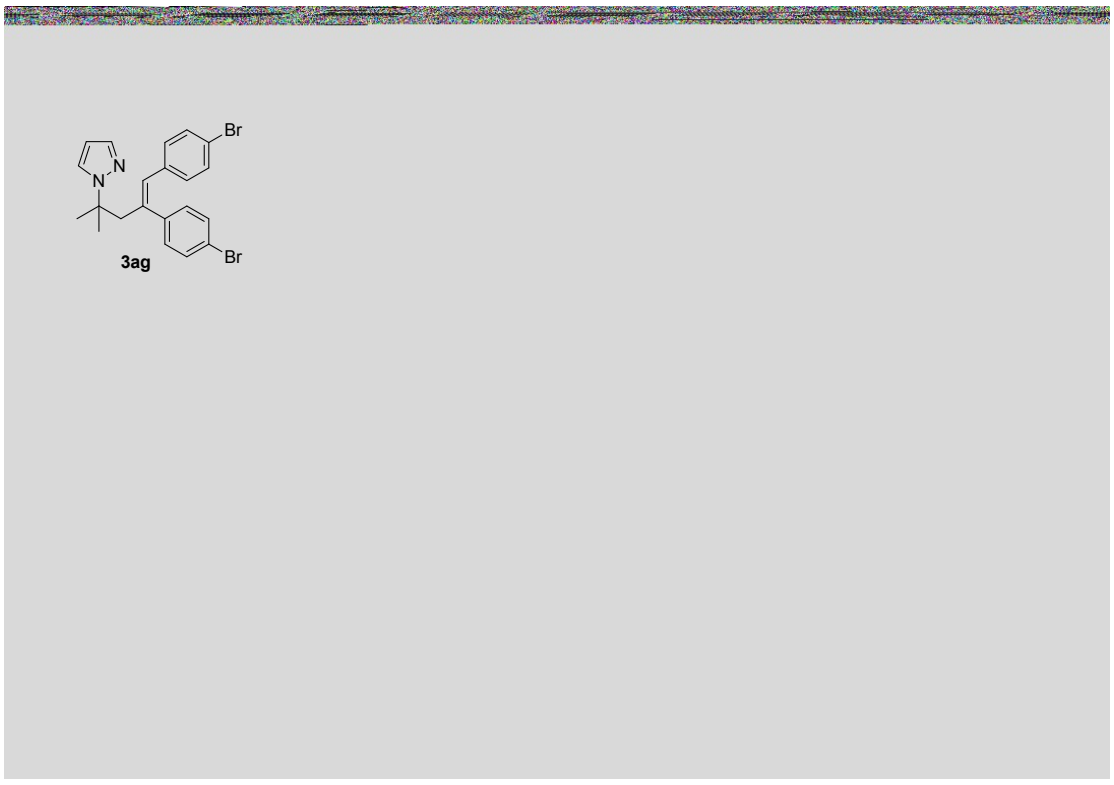
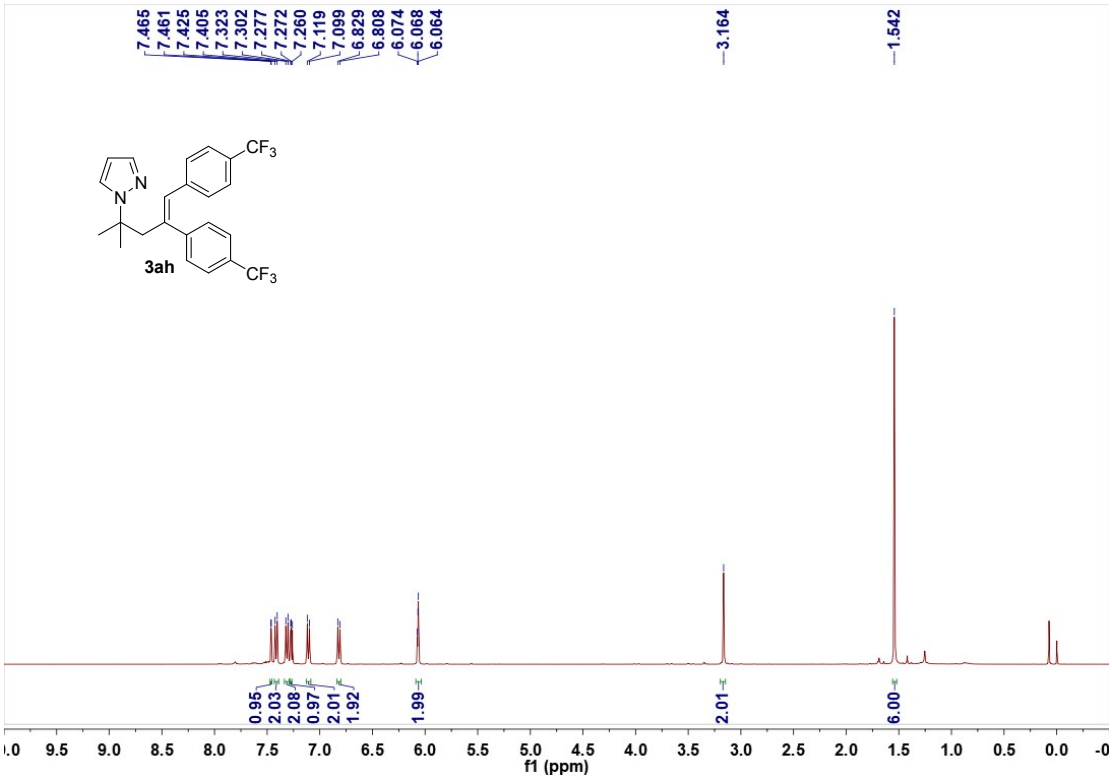
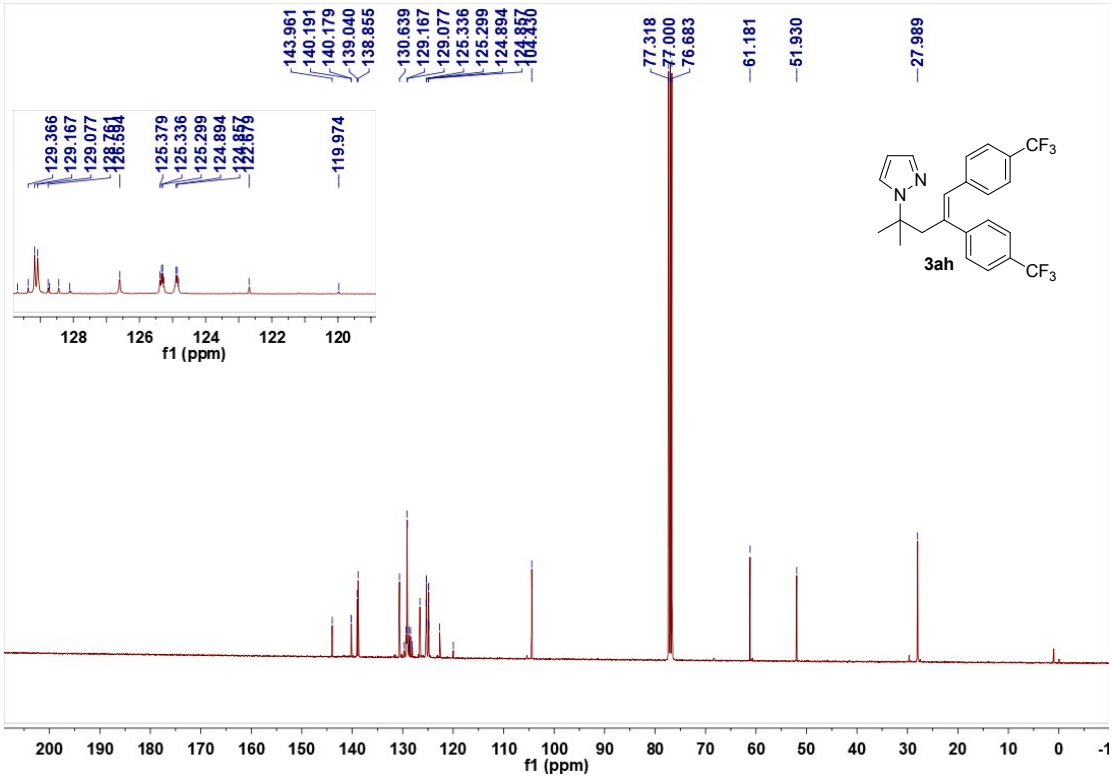
77.000
76.682
61.336
51.935
27.939
Cl
N
N
Cl
3af
f1 (ppm)


7.506
7.502
7.308
7.303
7.287
7.260
7.194
7.173
6.900
6.879
6.611
6.590
6.122
6.117
6.112
5.878
3.065
1.509
Br
N
N
Br
3ag
1.12
3.05
1.91
1.99
2.07
1.04
1.00
2.17
5.90
f1 (ppm)


Br
N
N
Br
3ag


7.465
7.461
7.425
7.405
7.323
7.302
7.277
7.272
7.260
7.119
7.099
6.829
6.808
6.074
6.068
6.064
3.164
1.542
CF3
N
N
3ah
CF3
0.95
2.03
2.08
0.97
2.01
1.92
1.99
2.01
6.00
f1 (ppm)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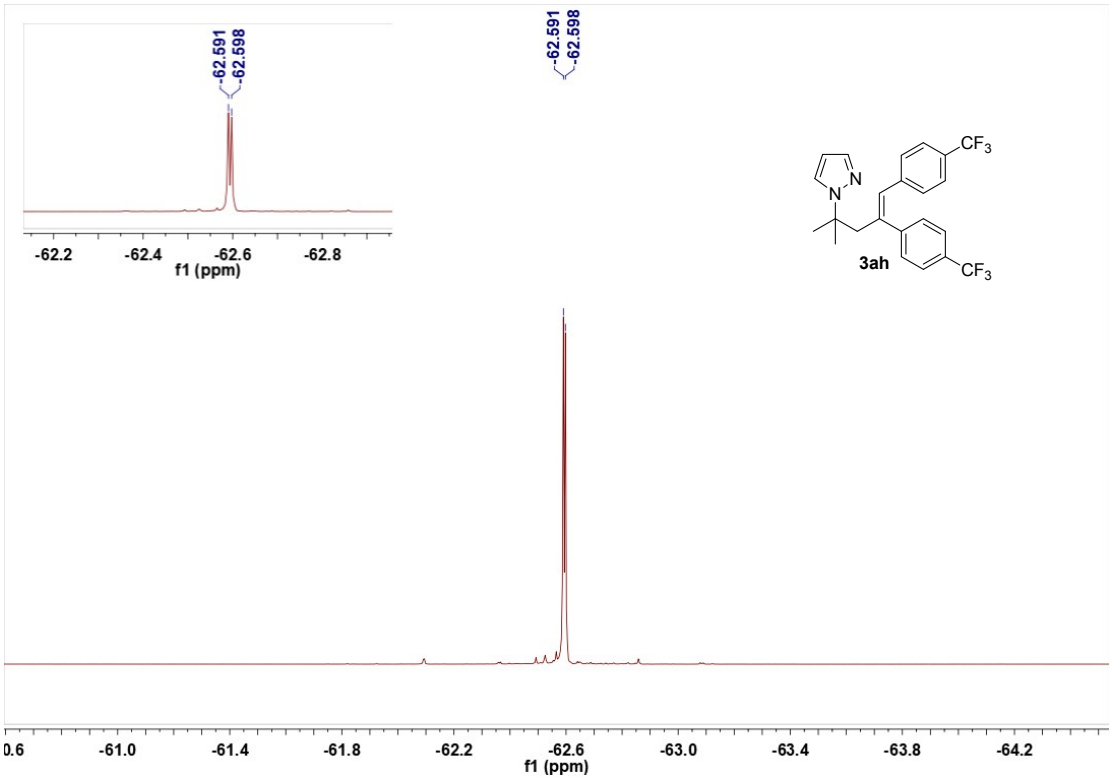
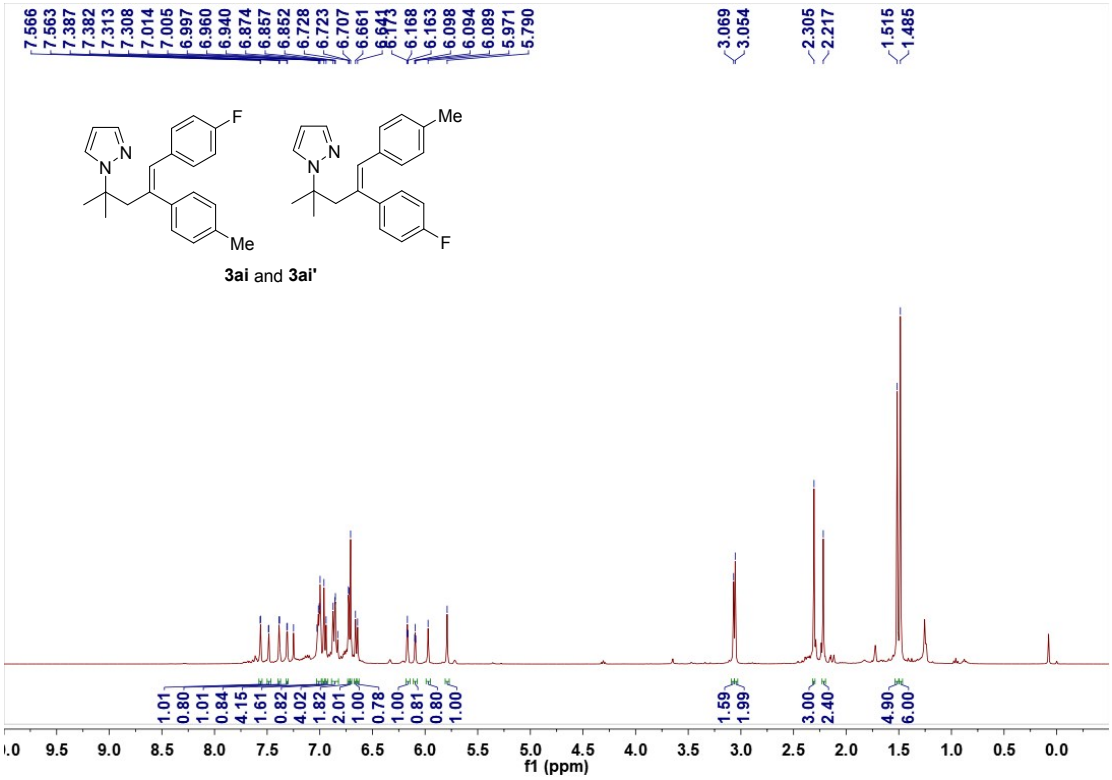
140.191
140.179
139.040
138.855
130.639
129.167
129.077
125.336
125.299
124.894
77.318
77.000
76.683
61.181
51.930
27.989
129.366
129.167
129.077
125.379
125.336
125.299
124.894
119.974
f1 (ppm)
CF3
N
N
3ah
CF3
f1 (ppm)


-62.591
-62.598
-62.2
-62.4
-62.6
-62.8
f1 (ppm)
-62.591
-62.598
CF3
N
N
3ah
CF3
0.6
-61.0
-61.4
-61.8
-62.2
-62.6
-63.0
-63.4
-63.8
-64.2
f1 (ppm)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7.387
7.382
7.313
7.308
7.014
7.005
6.997
6.960
6.940
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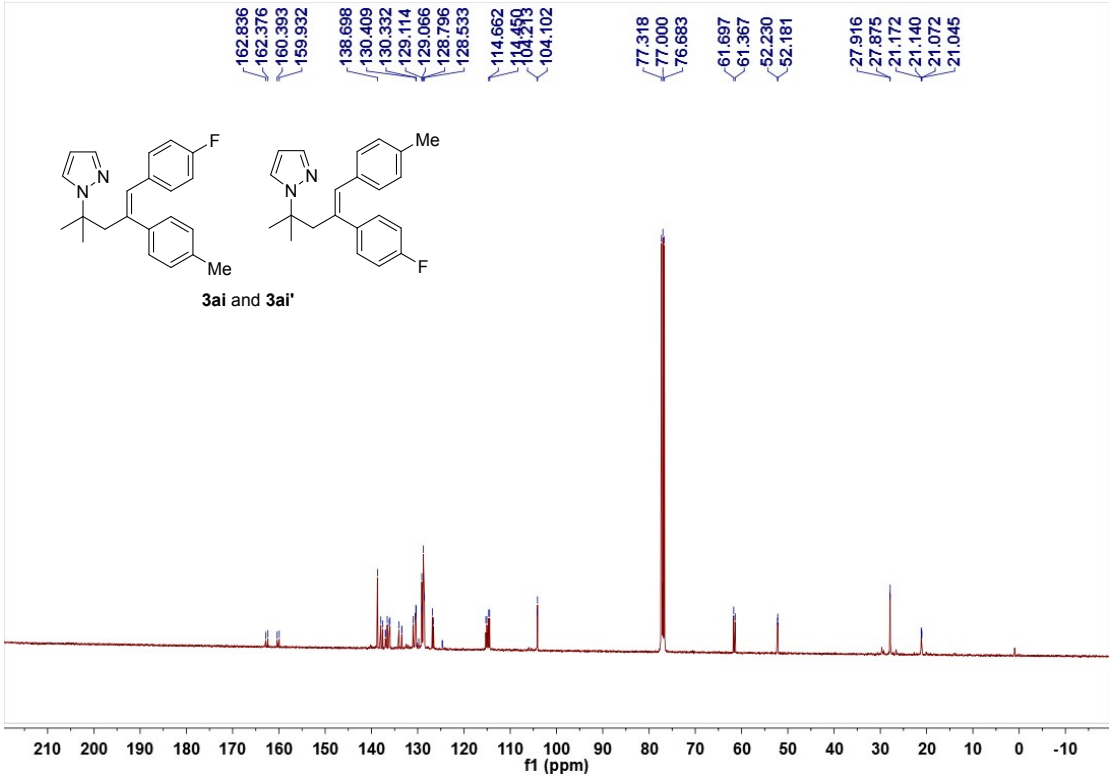
6.857
6.852
6.728
6.723
6.707
6.661
6.168
6.163
6.098
6.094
6.089
5.971
5.790
3.069
3.054
2.305
2.217
1.515
1.485
F
Me
N
N
Me
F
3ai and 3ai'
1.01
0.80
1.01
0.84
4.15
1.61
0.82
4.02
1.82
2.01
1.00
0.78
1.00
0.81
0.80
1.00
1.59
1.99
3.00
2.40
4.90
6.00
f1 (ppm)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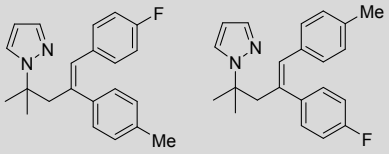
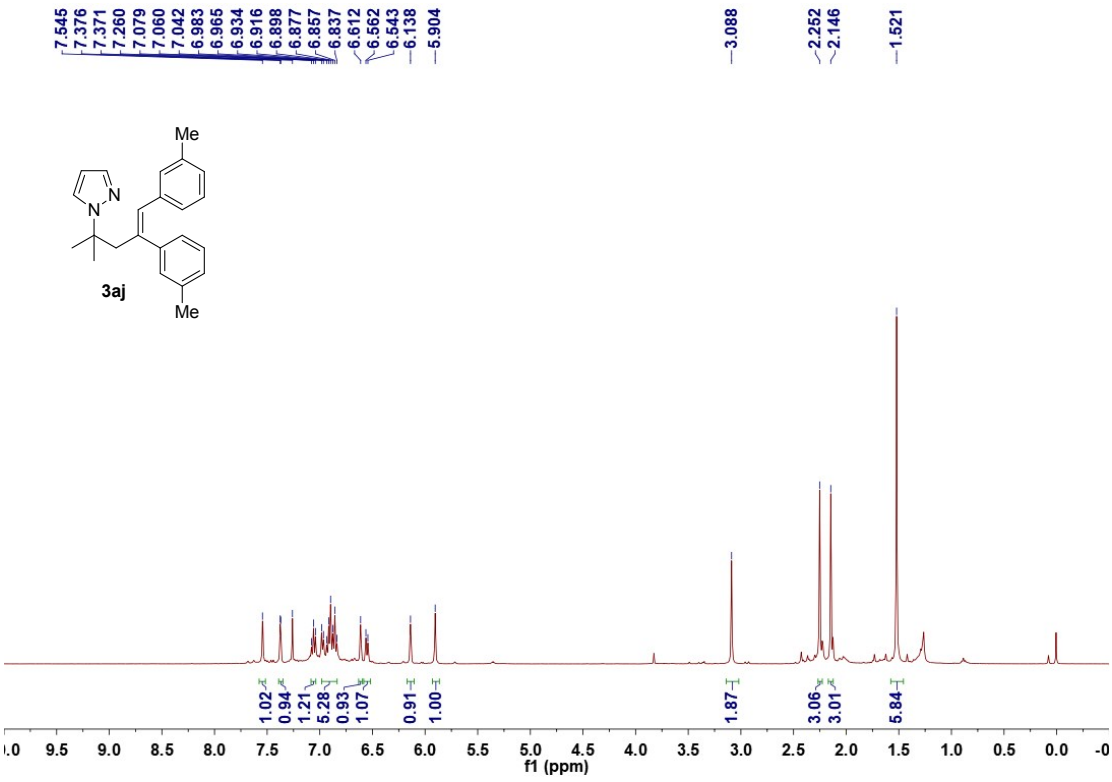
162.376
160.393
159.932
138.698
130.409
130.332
129.114
129.066
128.796
128.533
114.662
114.450
104.213
104.102
77.318
77.000
76.683
61.697
61.367
52.230
52.181
27.916
27.875
21.172
21.140
21.072
21.045
F
Me
N
N
Me
F
3ai and 3ai'
f1 (ppm)



3ai and **3ai'**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7.376
7.371
7.260
7.079
7.060
7.042
6.983
6.965
6.934
6.916
6.898
6.877
6.857
6.837
6.612
6.562
6.543
6.138
5.904
3.088
2.252
2.146
1.521
Me
N
N
3aj
Me
1.02
0.94
1.21
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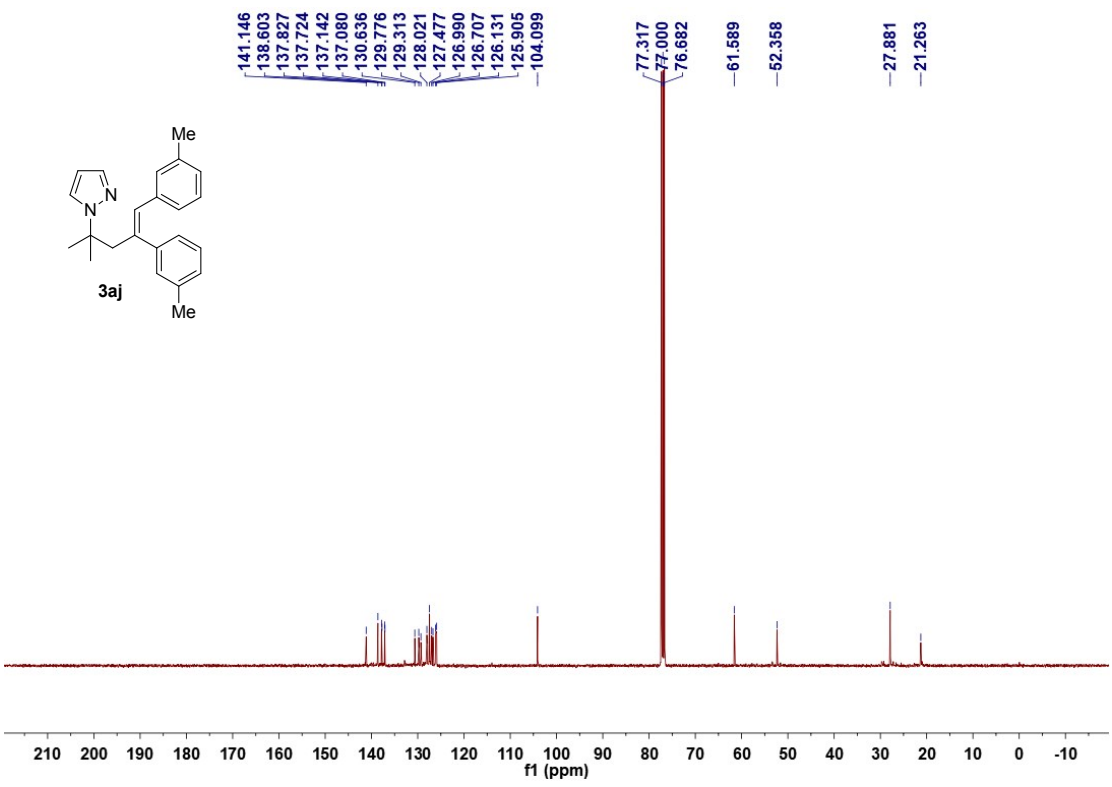
0.93
1.07
0.91
1.00
1.87
3.06
3.01
5.84
f1 (ppm)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138.603
137.827
137.724
137.142
137.080
130.636
129.776
129.313
128.021
127.477
126.990
126.707
126.131
125.905
104.099
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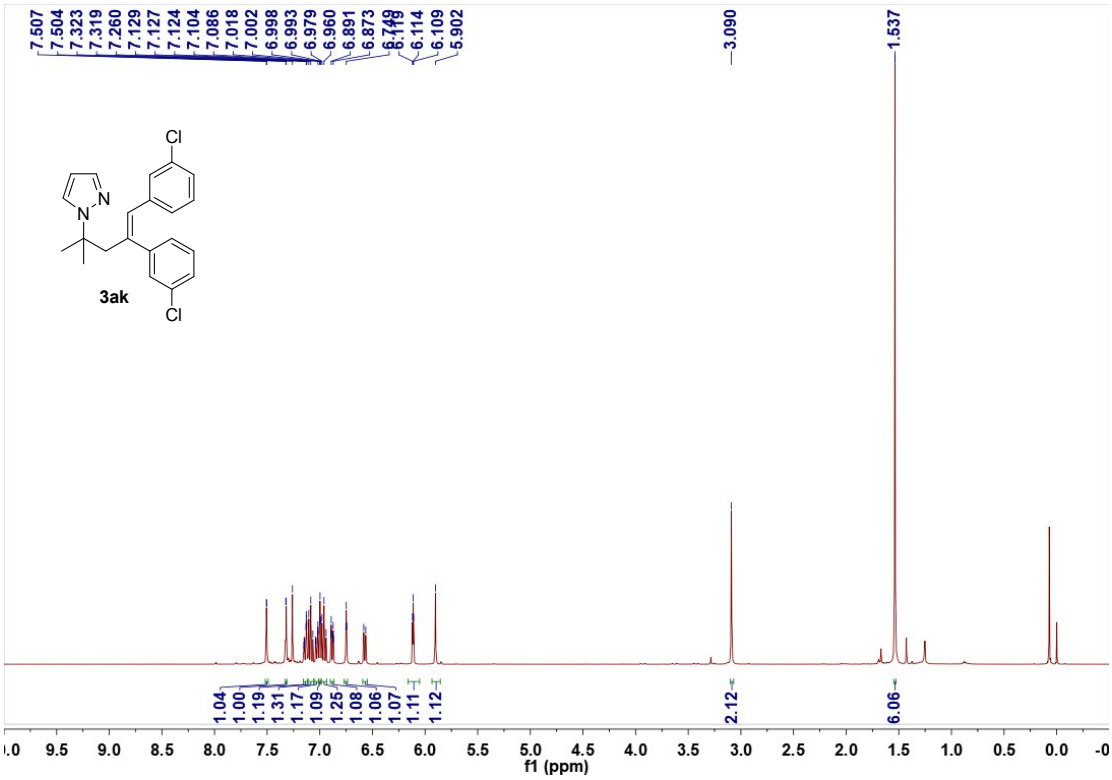
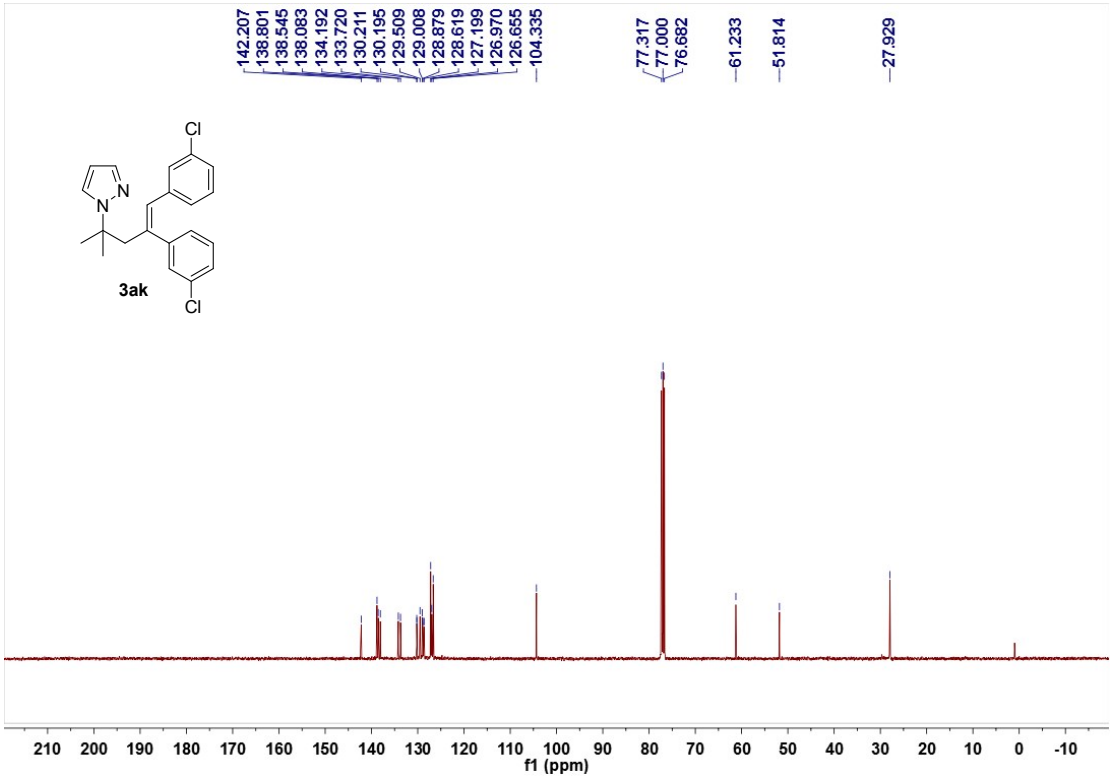
77.000
76.682
61.589
52.358
27.881
21.263
Me
N
N
3aj
Me
f1 (ppm)


7.507
7.504
7.323
7.319
7.260
7.129
7.127
7.124
7.104
7.086
7.018
7.002
6.998
6.993
6.979
6.960
6.891
6.873
6.114
6.109
5.902
3.090
1.537
Cl
N
N
3ak
Cl
1.04
1.00
1.19
1.31
1.17
1.09
1.25
1.08
1.06
1.07
1.11
1.12
2.12
6.06
f1 (ppm)


142.207
138.801
138.545
138.083
134.192
133.720
130.211
130.195
129.509
129.008
128.879
128.619
127.199
126.970
126.655
104.335
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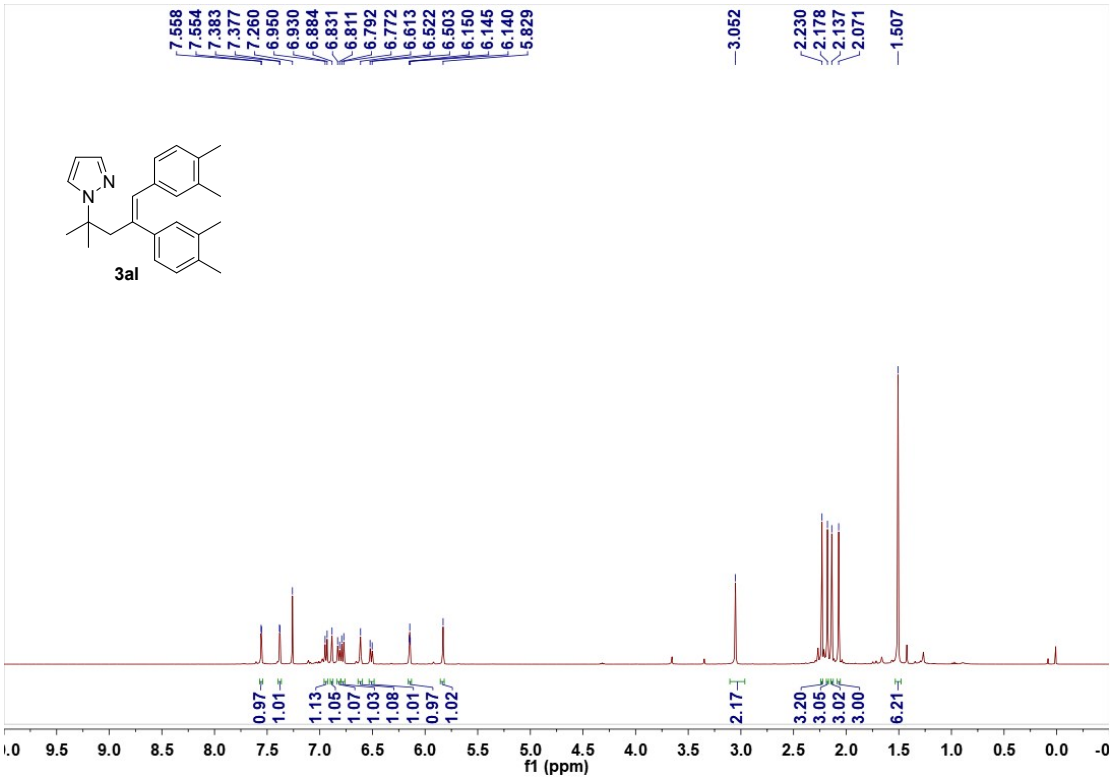
77.000
76.682
61.233
51.814
27.929
Cl
N
N
3ak
Cl
f1 (ppm)


7.558
7.554
7.383
7.377
7.260
6.950
6.930
6.884
6.831
6.811
6.792
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6.613
6.522
6.503
6.150
6.145
6.140
5.829
3.052
2.230
2.178
2.137
2.071
1.507
3al
0.97
1.01
1.13
1.05
1.07
1.03
1.08
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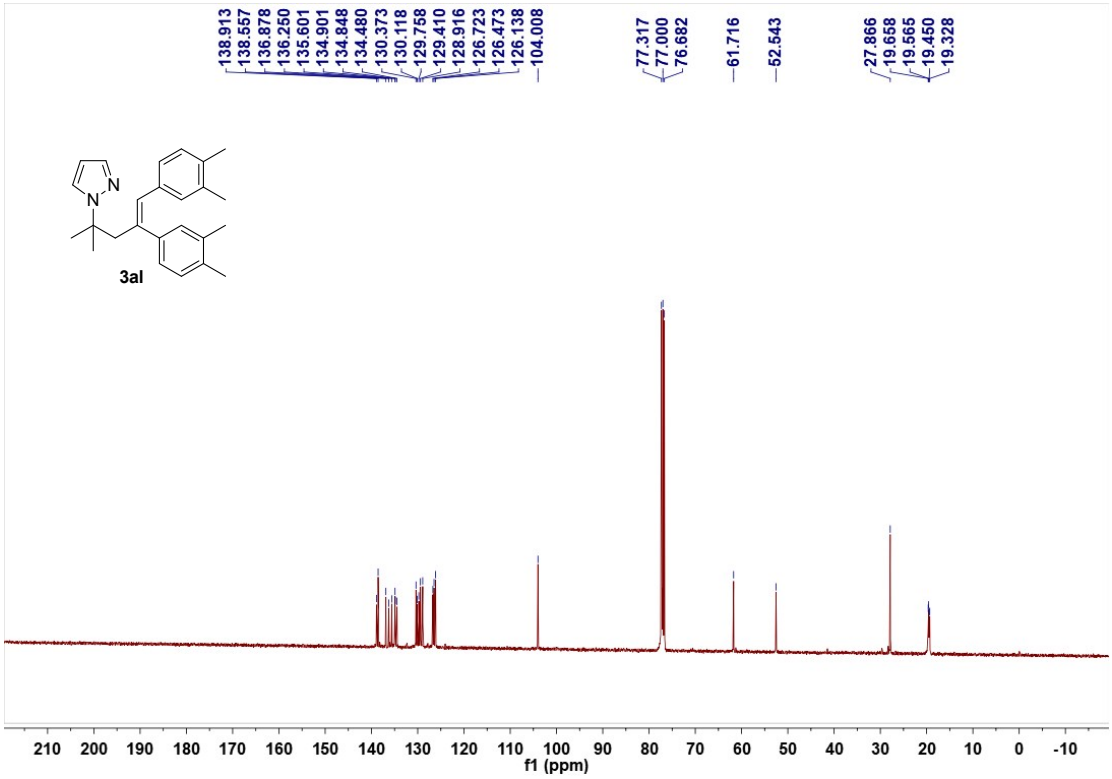
0.97
1.02
2.17
3.20
3.05
3.02
3.00
6.21
f1 (ppm)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136.878
136.250
135.601
134.901
134.848
134.480
130.373
130.118
129.758
129.410
128.916
126.723
126.473
126.138
104.008
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77.000
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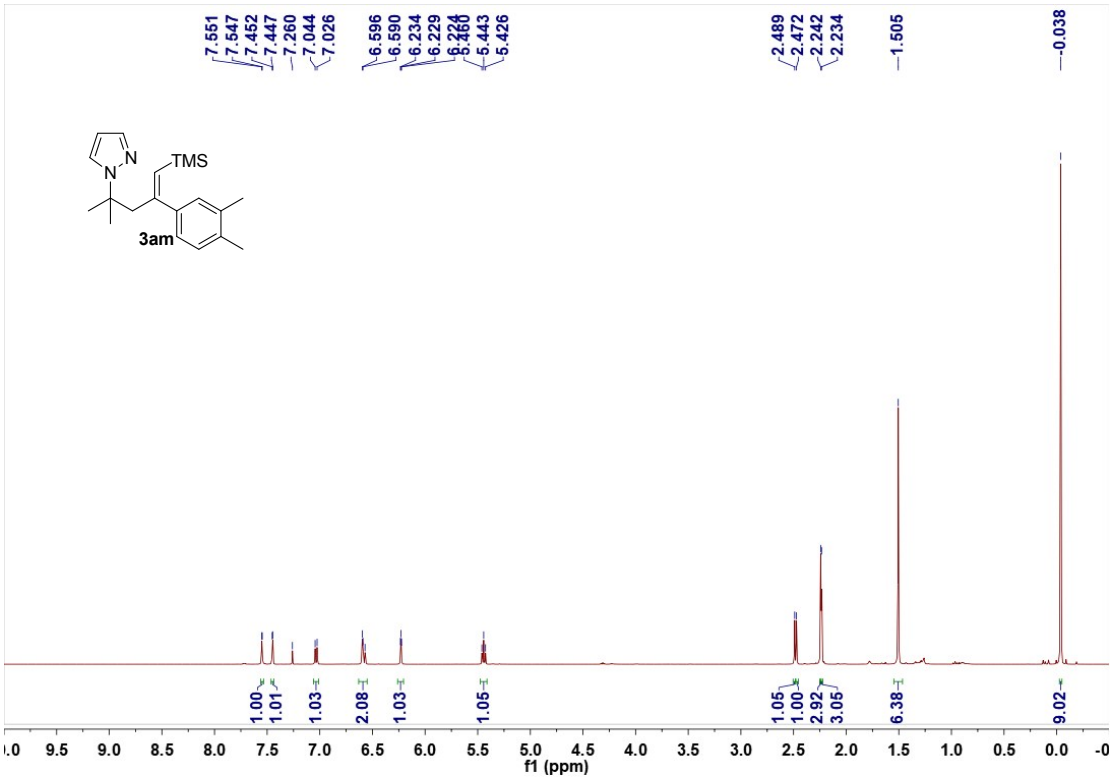
61.716
52.543
27.866
19.658
19.565
19.450
19.328
3al
f1 (ppm)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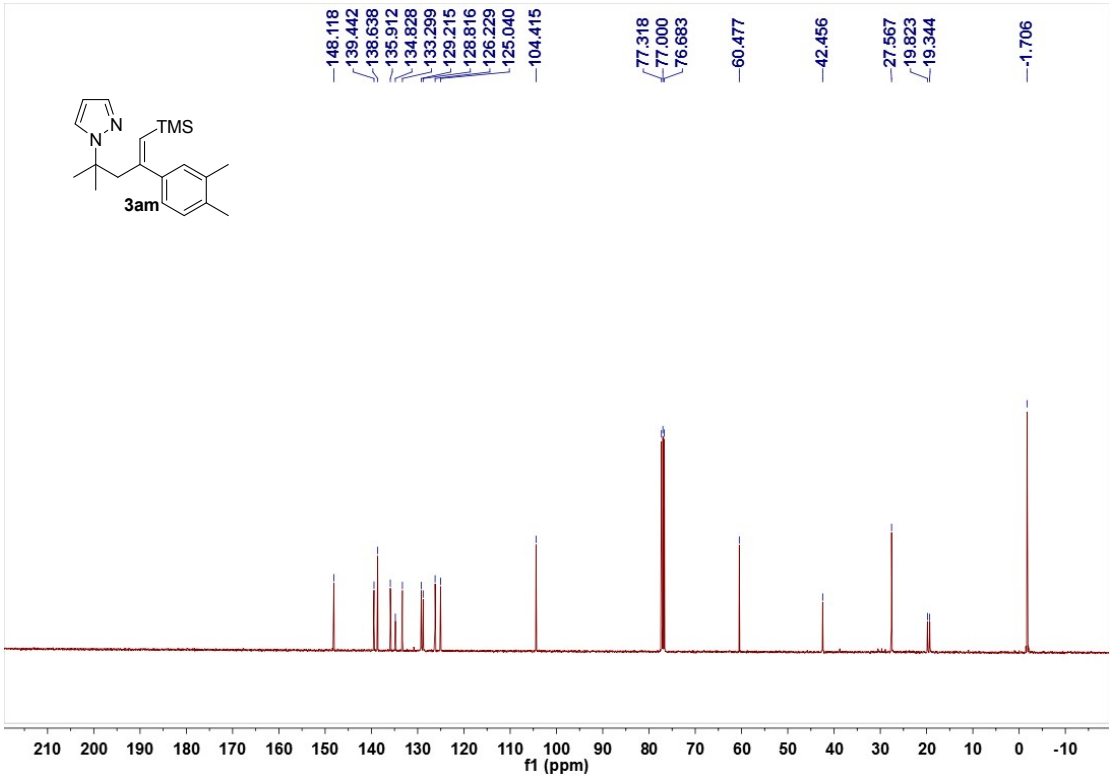
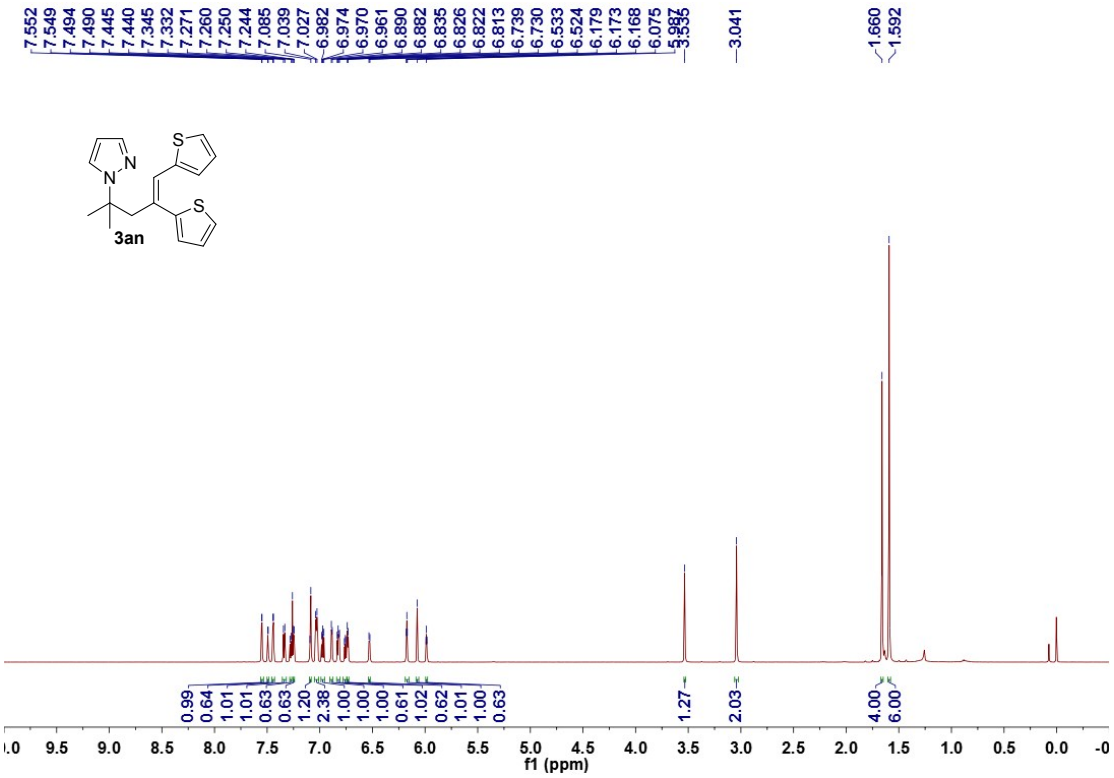
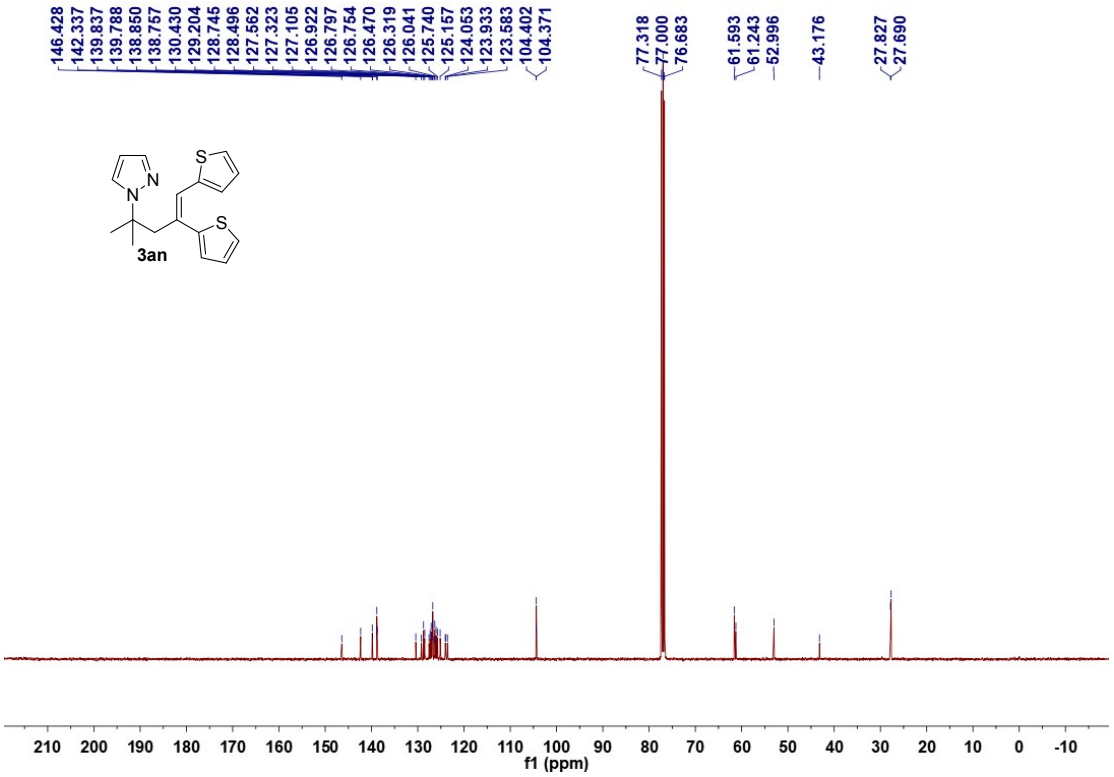
7.547
7.452
7.447
7.260
7.044
7.026
6.596
6.590
6.234
6.229
5.443
5.426
2.489
2.472
2.242
2.234
1.505
0.038
TMS
3am
1.00
1.01
1.03
2.08
1.03
1.05
1.05
1.00
2.92
3.05
6.38
9.02
f1 (ppm)


148.118
139.442
138.638
135.912
134.828
133.299
129.215
128.816
126.229
125.040
104.415
77.318
77.000
76.683
60.477
42.456
27.567
19.823
19.344
1.706
TMS
3am
f1 (ppm)


7.552
7.549
7.494
7.490
7.445
7.440
7.345
7.332
7.271
7.260
7.250
7.244
7.085
7.039
7.027
6.982
6.974
6.970
6.961
6.890
6.882
6.835
6.826
6.822
6.813
6.739
6.730
6.533
6.524
6.179
6.173
6.168
6.075
5.982
3.041
1.660
1.592
3an
0.99
0.64
1.01
1.01
0.63
0.63
1.20
2.38
1.00
1.00
1.00
0.61
1.02
0.62
1.01
1.00
0.63
1.27
2.03
4.00
6.00
f1 (ppm)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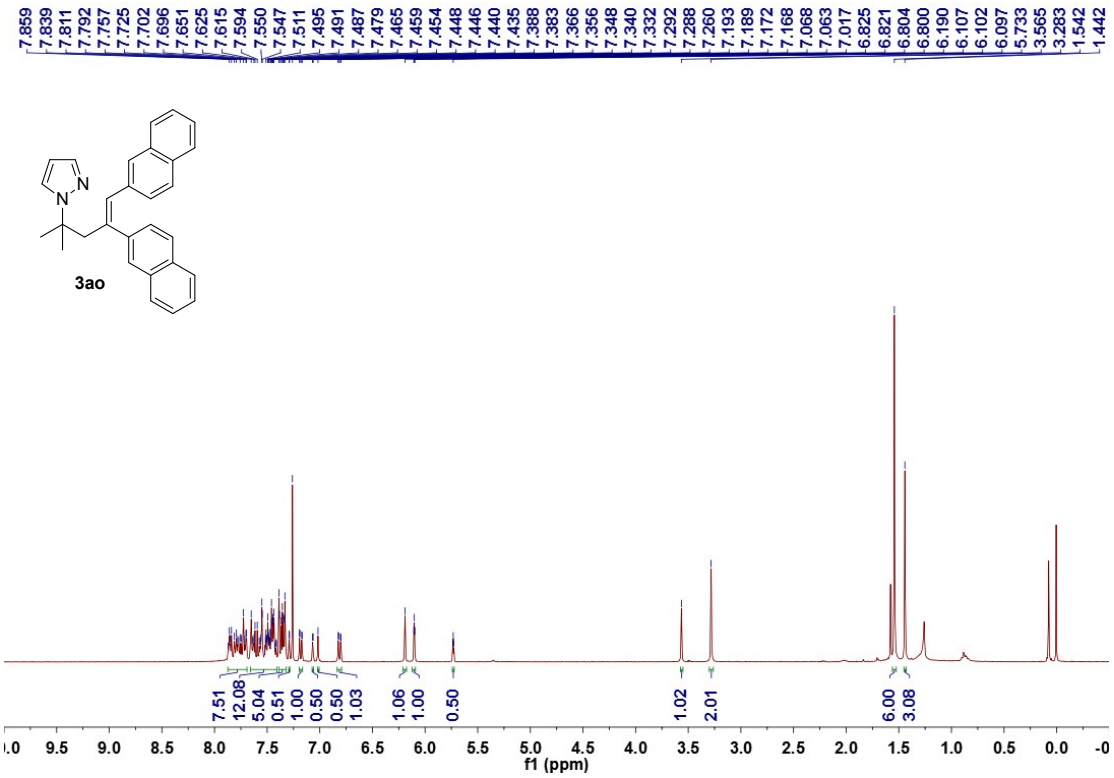
142.337
139.837
139.788
138.850
138.757
130.430
129.204
128.745
128.496
127.562
127.323
127.105
126.922
126.797
126.754
126.470
126.319
126.041
125.740
125.157
124.053
123.933
123.583
104.402
104.371
77.318
77.000
76.683
61.593
61.243
52.996
43.176
27.827
27.690
3an
f1 (ppm)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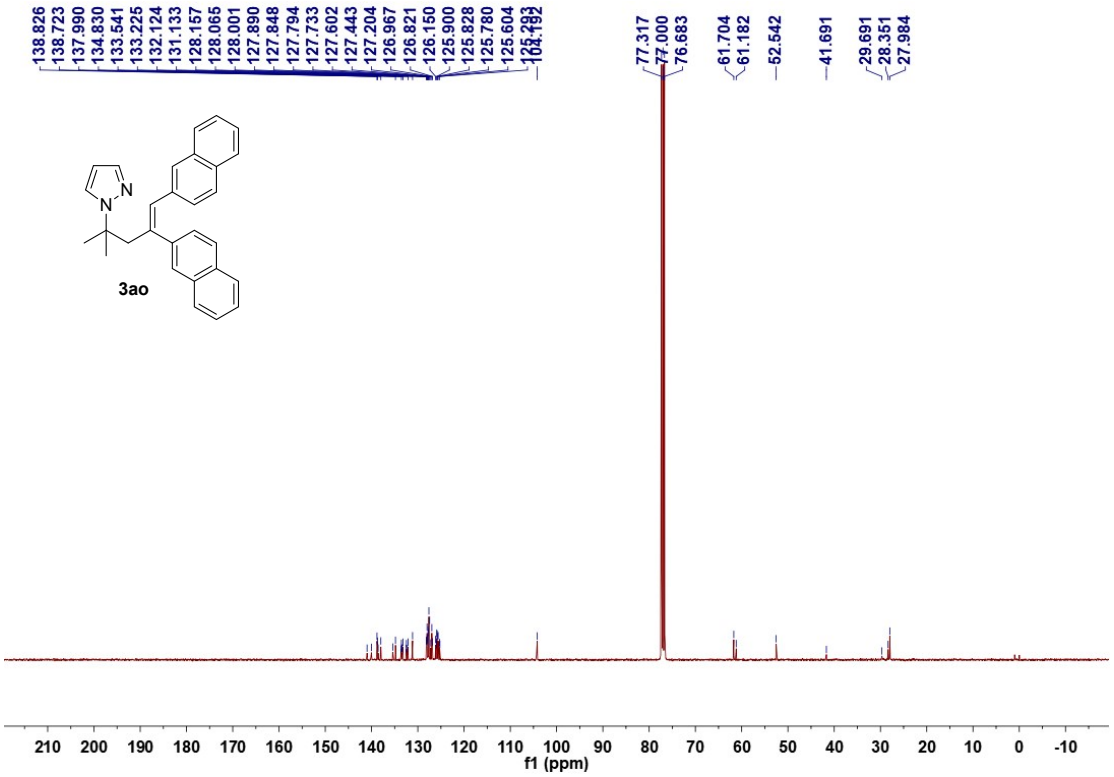
7.811
7.792
7.757
7.725
7.702
7.696
7.651
7.625
7.615
7.594
7.550
7.547
7.511
7.495
7.491
7.487
7.479
7.465
7.459
7.454
7.448
7.446
7.440
7.435
7.388
7.383
7.366
7.356
7.348
7.340
7.332
7.292
7.288
7.260
7.193
7.189
7.172
7.168
7.068
7.063
7.017
6.825
6.821
6.804
6.800
6.190
6.107
6.102
6.097
5.733
3.565
3.283
1.542
1.442
3ao
7.51
12.08
5.04
0.51
1.00
0.50
0.50
1.03
1.06
1.00
0.50
1.02
2.01
6.00
3.08
f1 (ppm)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138.723
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134.830
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133.225
132.124
131.133
128.157
128.065
128.001
127.890
127.848
127.794
127.733
127.602
127.443
127.204
126.967
126.821
126.150
125.900
125.828
125.780
125.604
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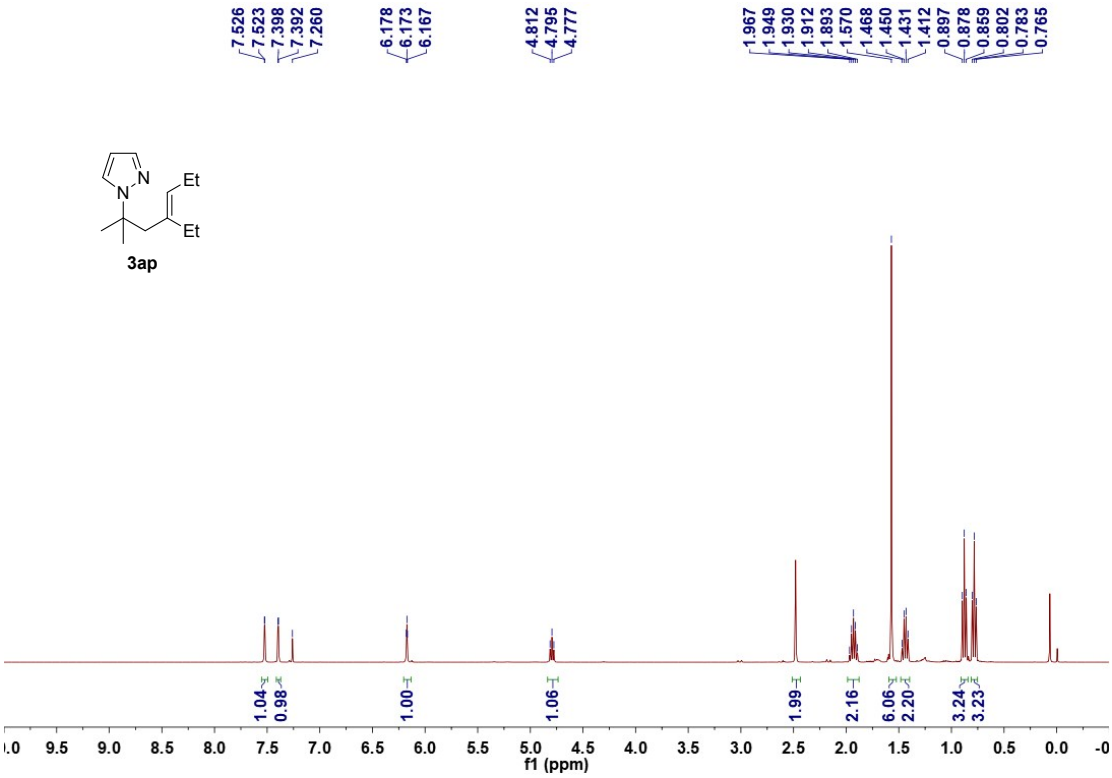
29.691
28.351
27.984
3ao
f1 (ppm)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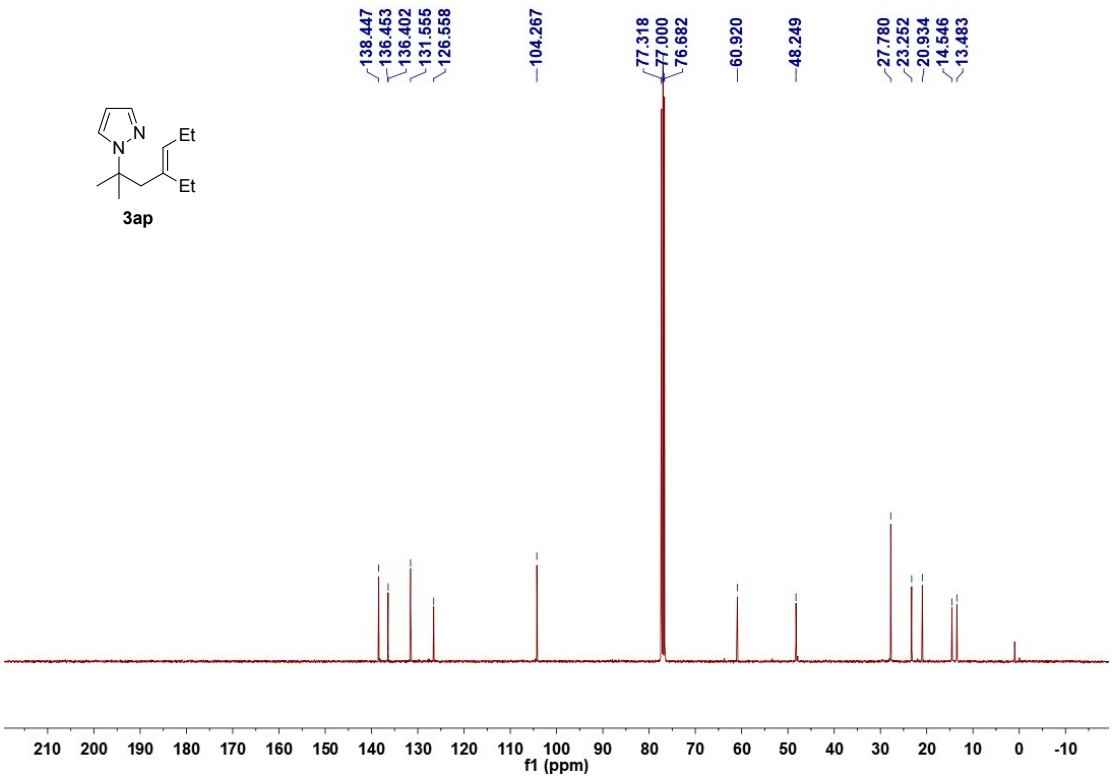
7.523
7.398
7.392
7.260
6.178
6.173
6.167
4.812
4.795
4.777
1.967
1.949
1.930
1.912
1.893
1.570
1.468
1.450
1.431
1.412
0.897
0.878
0.859
0.802
0.783
0.765
Et
Et
3ap
1.04
0.98
1.00
1.06
1.99
2.16
6.06
2.20
3.24
3.23
f1 (ppm)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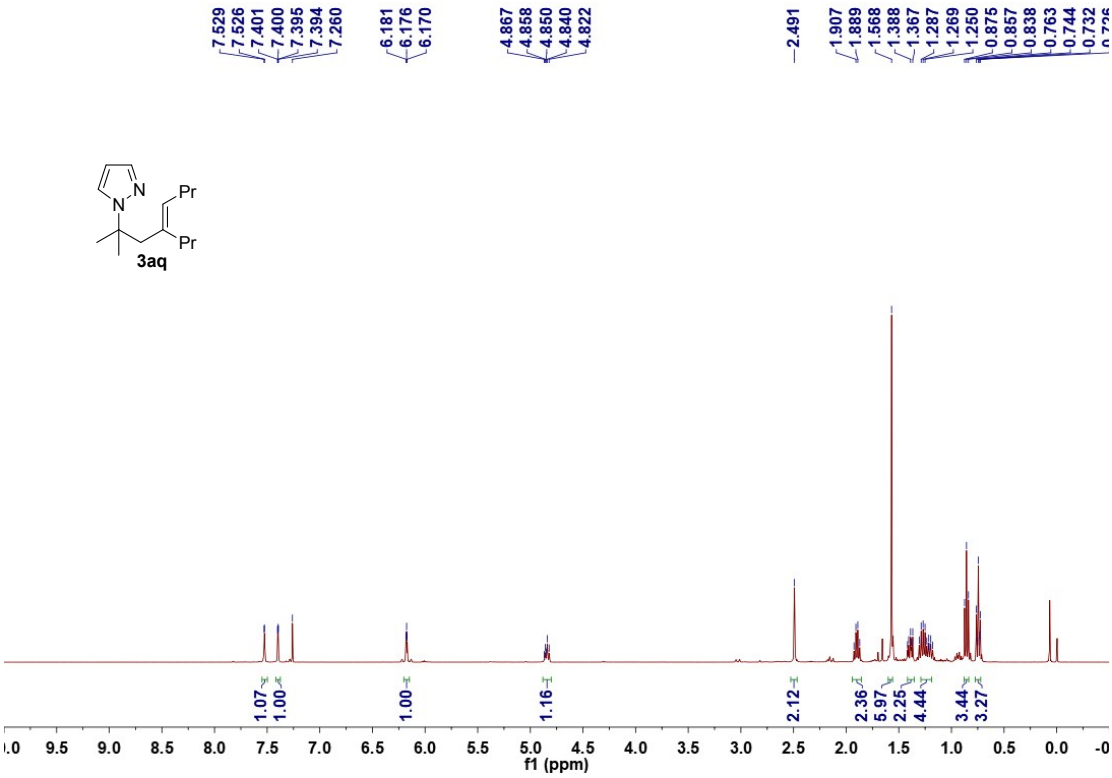
136.453
136.402
131.555
126.558
104.267
77.318
77.000
76.682
60.920
48.249
27.780
23.252
20.934
14.546
13.483
Et
Et
3ap
f1 (ppm)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7.394
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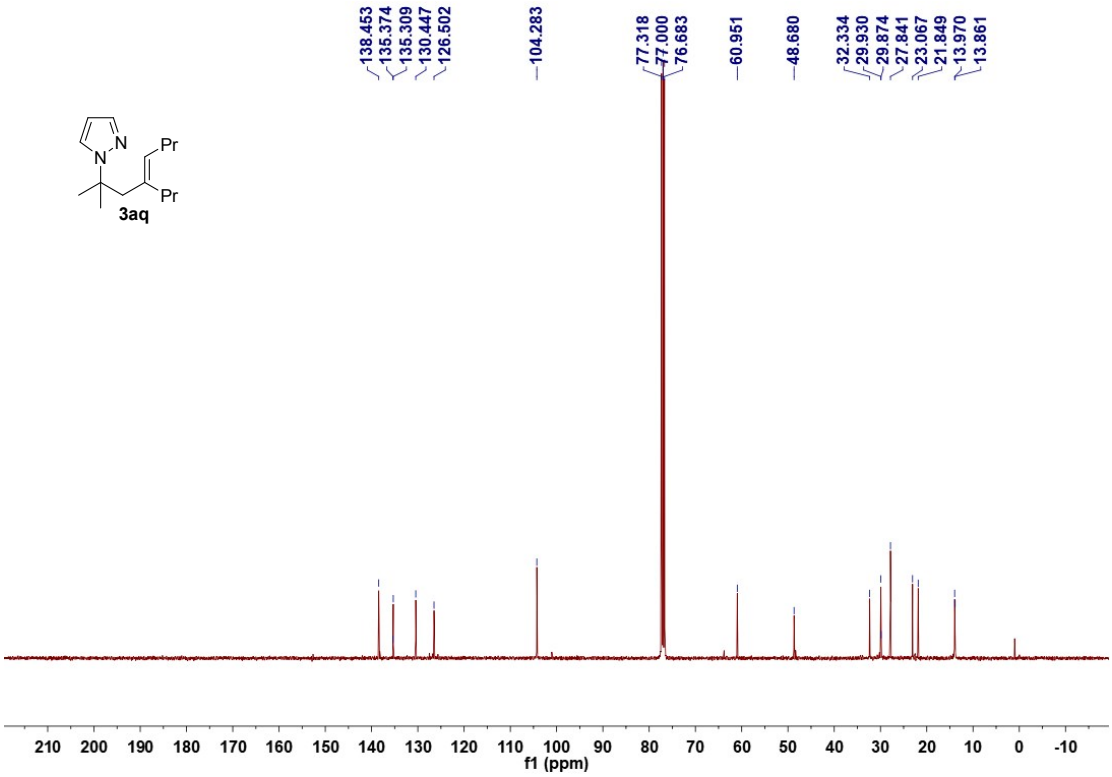
6.176
6.170
4.867
4.858
4.850
4.840
4.822
2.491
1.907
1.889
1.568
1.388
1.367
1.287
1.269
1.250
0.875
0.857
0.838
0.763
0.744
0.732
Pr
Pr
3aq
1.07
1.00
1.00
1.16
2.12
2.36
5.97
2.25
4.44
3.44
3.27
f1 (ppm)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77.000
76.683
60.951
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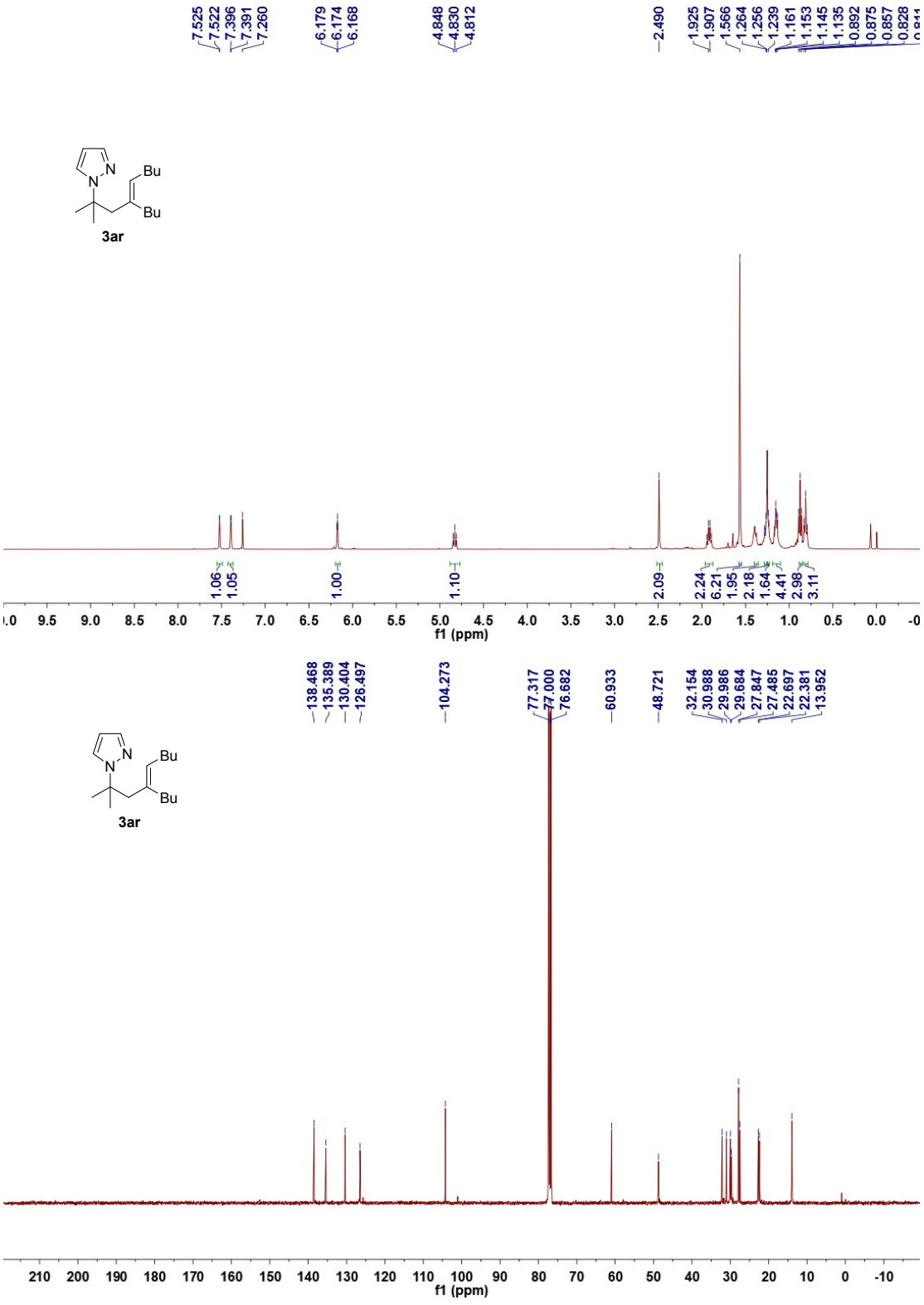
29.930
29.874
27.841
23.067
21.849
13.970
13.861
Pr
Pr
3aq
f1 (ppm)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7.391
7.260
6.179
6.174
6.168
4.848
4.830
4.812
2.490
1.925
1.907
1.566
1.264
1.256
1.239
1.161
1.153
1.145
1.135
0.892
0.875
0.857
0.828
Bu
Bu
3ar
1.06
1.05
1.00
1.10
2.09
2.24
6.21
1.95
2.18
1.64
4.41
2.98
3.11
f1 (ppm)
138.468
135.389
130.404
126.497
104.273
77.317
77.000
76.682
60.933
48.721
32.154
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29.684
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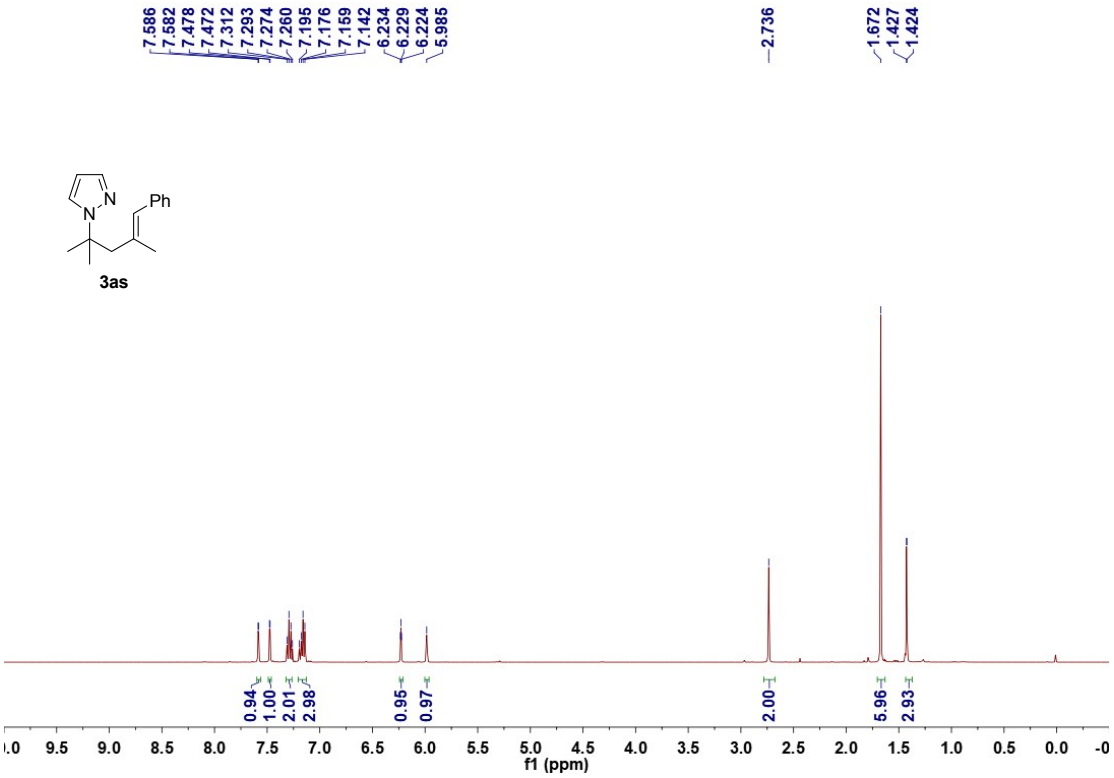
22.697
22.381
13.952
Bu
Bu
3ar
f1 (ppm)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7.472
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7.293
7.274
7.260
7.195
7.176
7.159
7.142
6.234
6.229
6.224
5.985
2.736
1.672
1.427
1.424
Ph
3as
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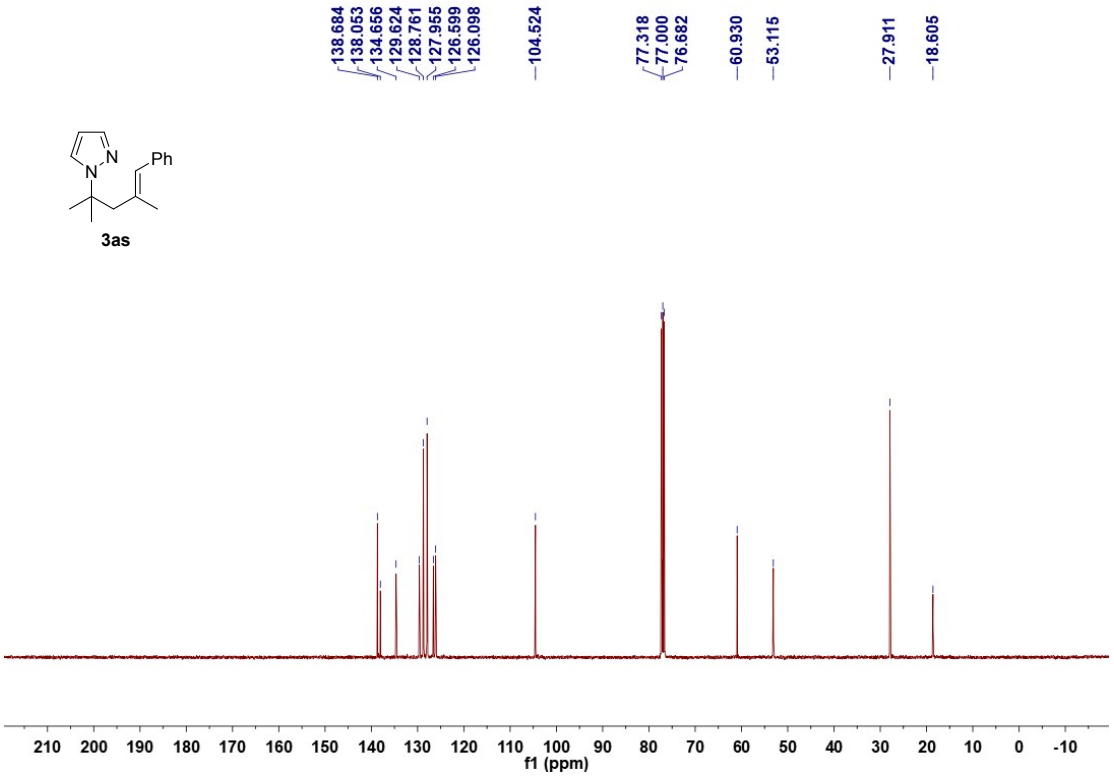
1.00
2.01
2.98
0.95
0.97
2.00
5.96
2.93
f1 (ppm)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128.761
127.955
126.599
126.098
104.524
77.318
77.000
76.682
60.930
53.115
27.911
18.605
Ph
3as
f1 (ppm)


7.562
7.324
7.318
7.302
7.284
7.271
7.265
7.260
7.149
7.145
7.129
7.057
7.053
7.045
7.040
6.819
6.811
6.801
6.245
6.197
6.192
6.187
4.269
4.252
4.232
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3.156
3.135
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2.906
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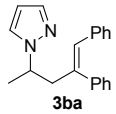
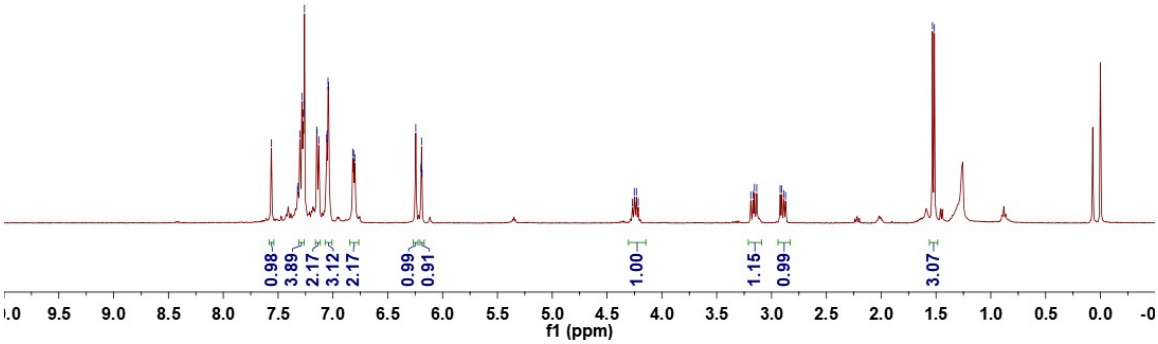
1.515


N
N
Ph
Ph

3ba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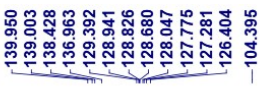
2.17
0.99
0.91
1.00
1.15
0.99
3.07
f1 (ppm)


139.950
139.003
138.428
136.963
129.392
128.941
128.826
128.680
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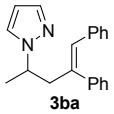
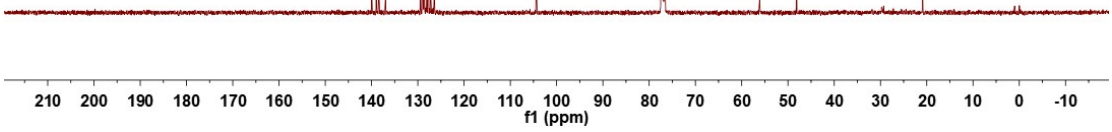
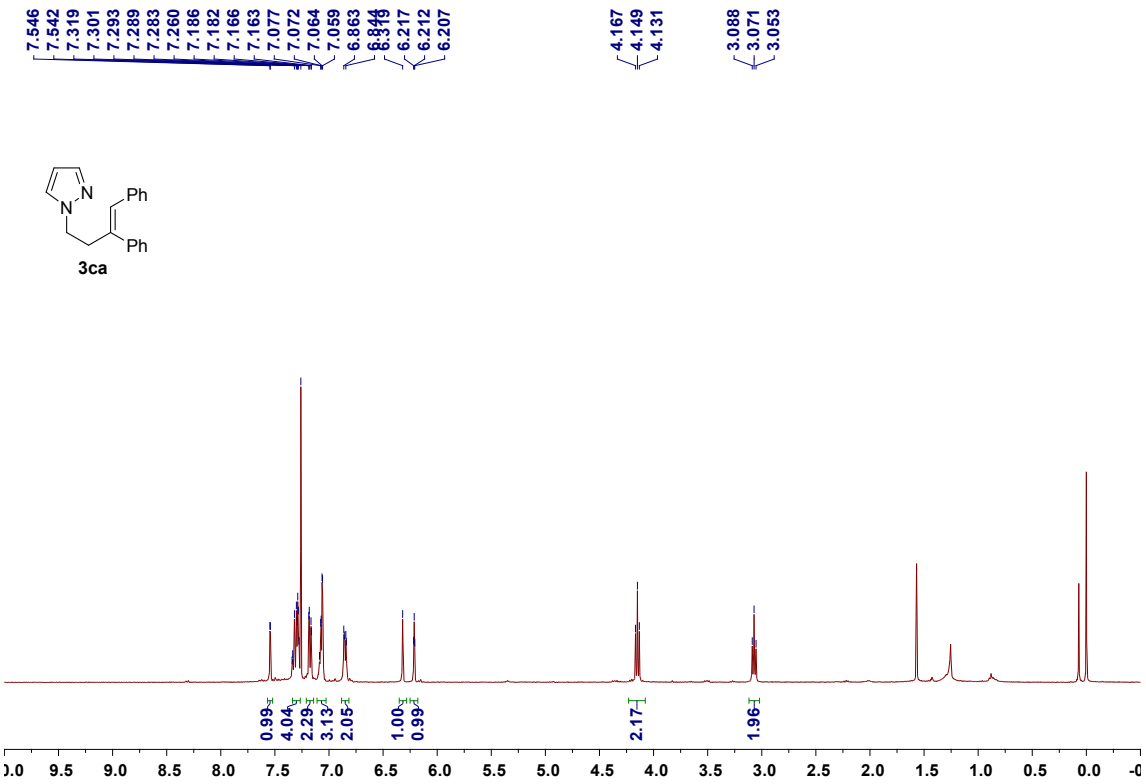
127.775
127.281
126.404
104.395
77.318
77.000
76.683
56.119
48.107
20.877


N
N
Ph
Ph

3ba


f1 (ppm)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7.260
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7.077
7.072
7.064
7.059
6.863
6.217
6.212
6.207
4.167
4.149
4.131
3.088
3.071
3.053
Ph
Ph
3ca
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3.13
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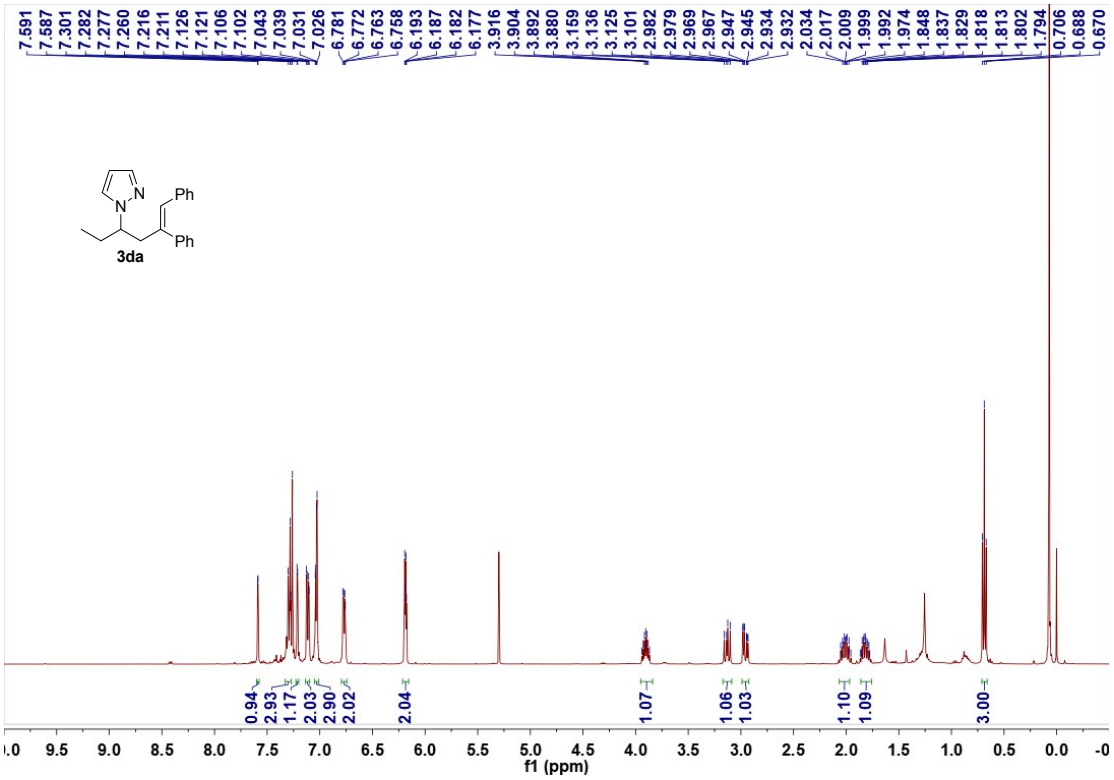
1.96
f1 (ppm)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7.277
7.260
7.216
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7.121
7.106
7.102
7.043
7.039
7.031
7.026
6.781
6.772
6.763
6.758
6.193
6.187
6.182
6.177
3.916
3.904
3.892
3.880
3.159
3.136
3.125
3.101
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2.947
2.945
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2.932
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2.017
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1.992
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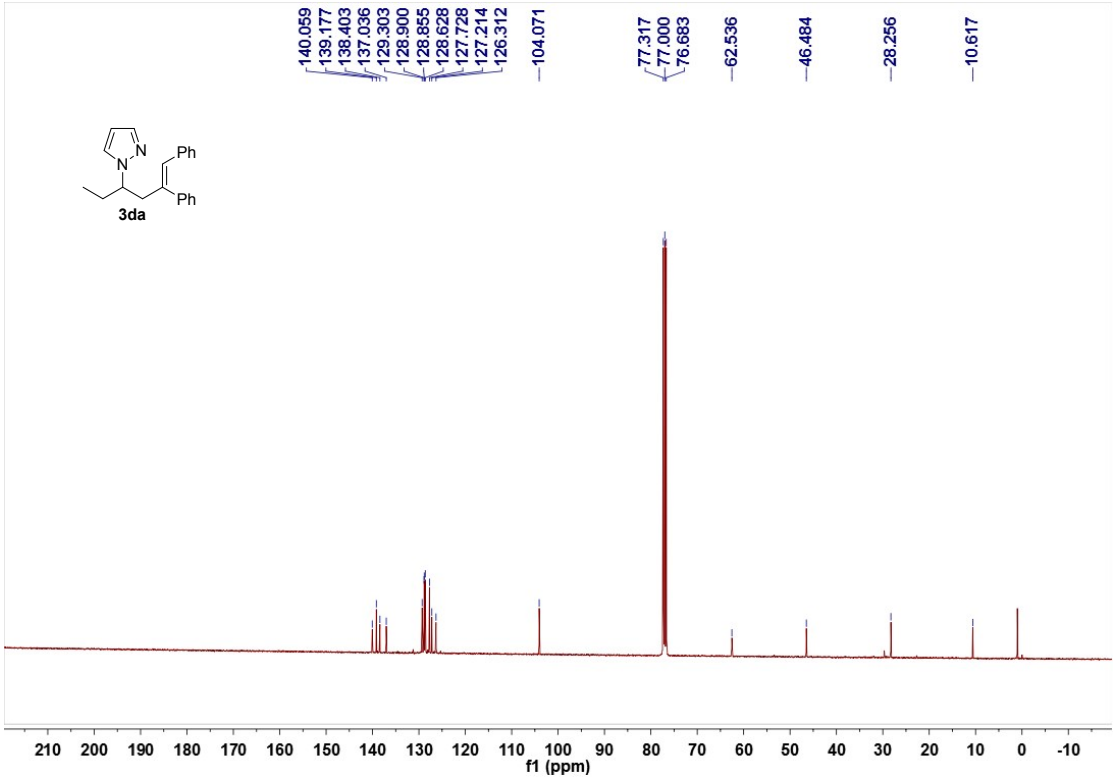
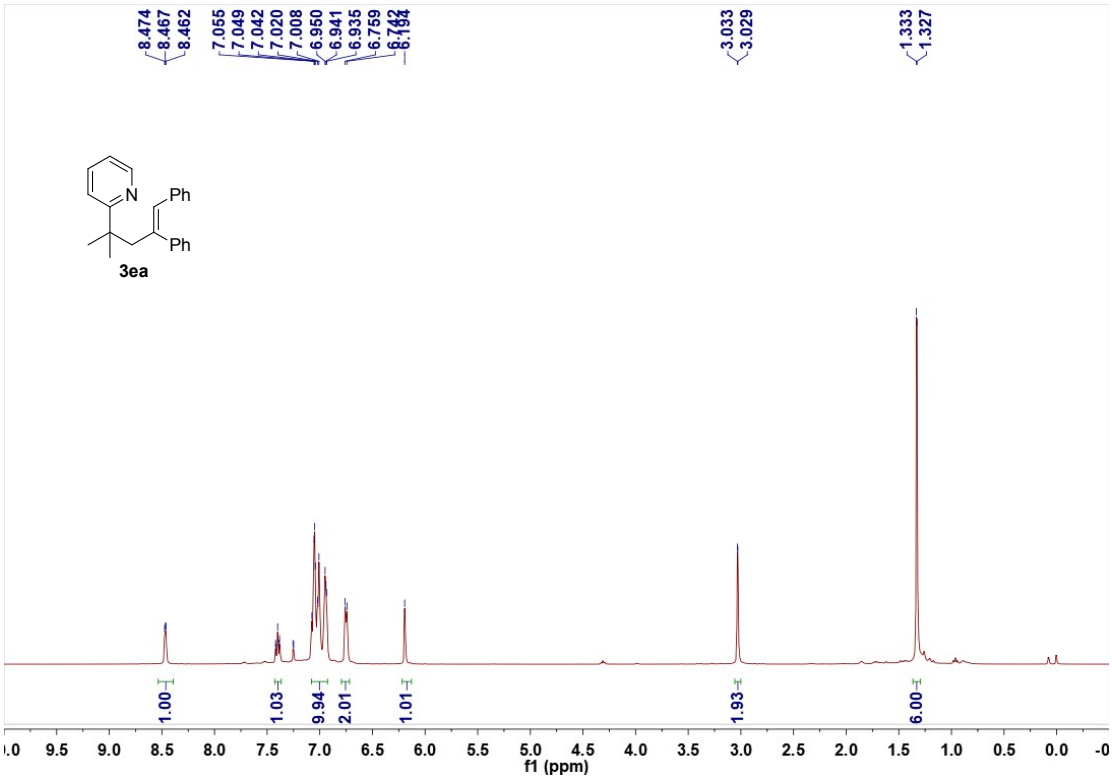
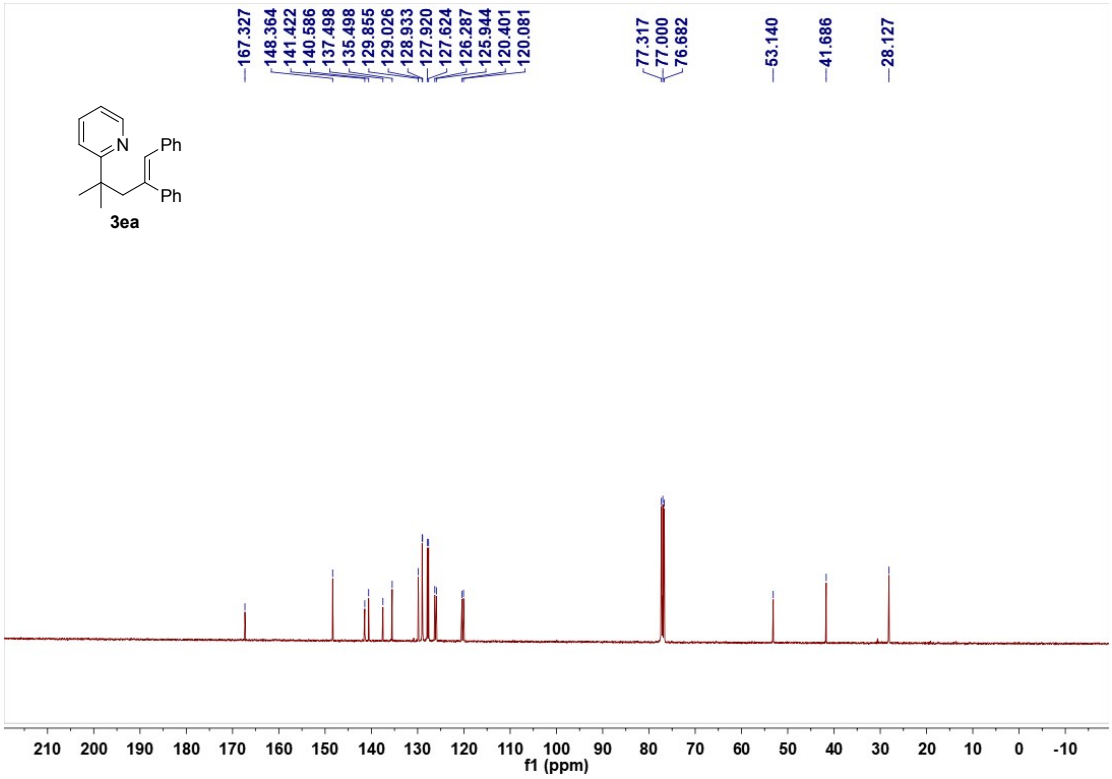
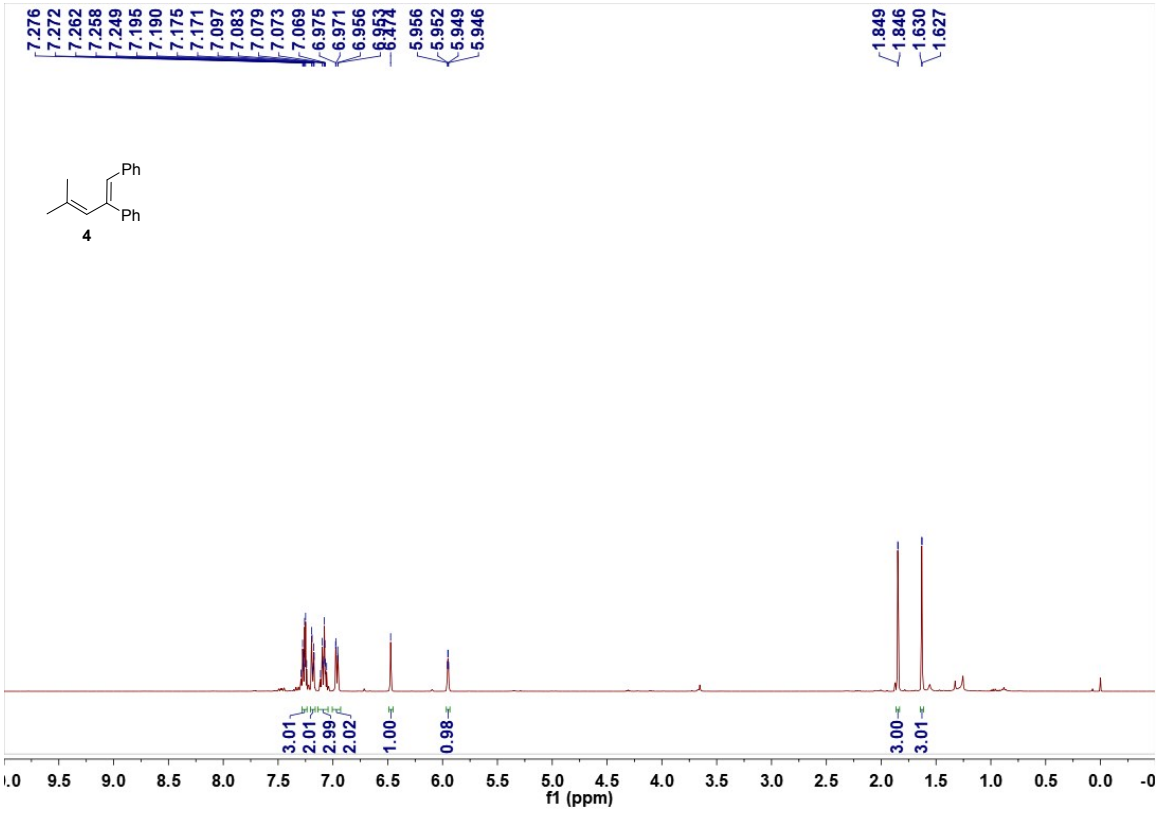
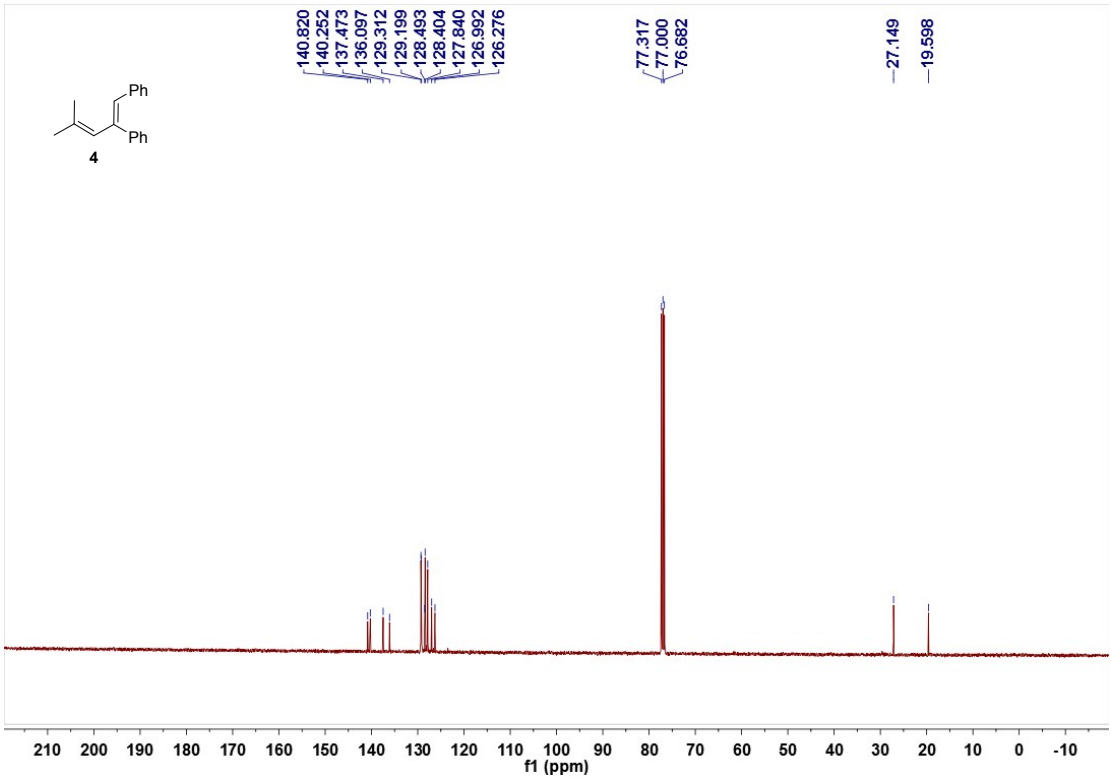
1.848
1.837
1.829
1.818
1.813
1.802
1.794
0.706
0.688
0.670
Ph
Ph
3da
0.94
2.93
1.17
2.03
2.90
2.02
2.04
1.07
1.06
1.03
1.10
1.09
3.00
f1 (ppm)

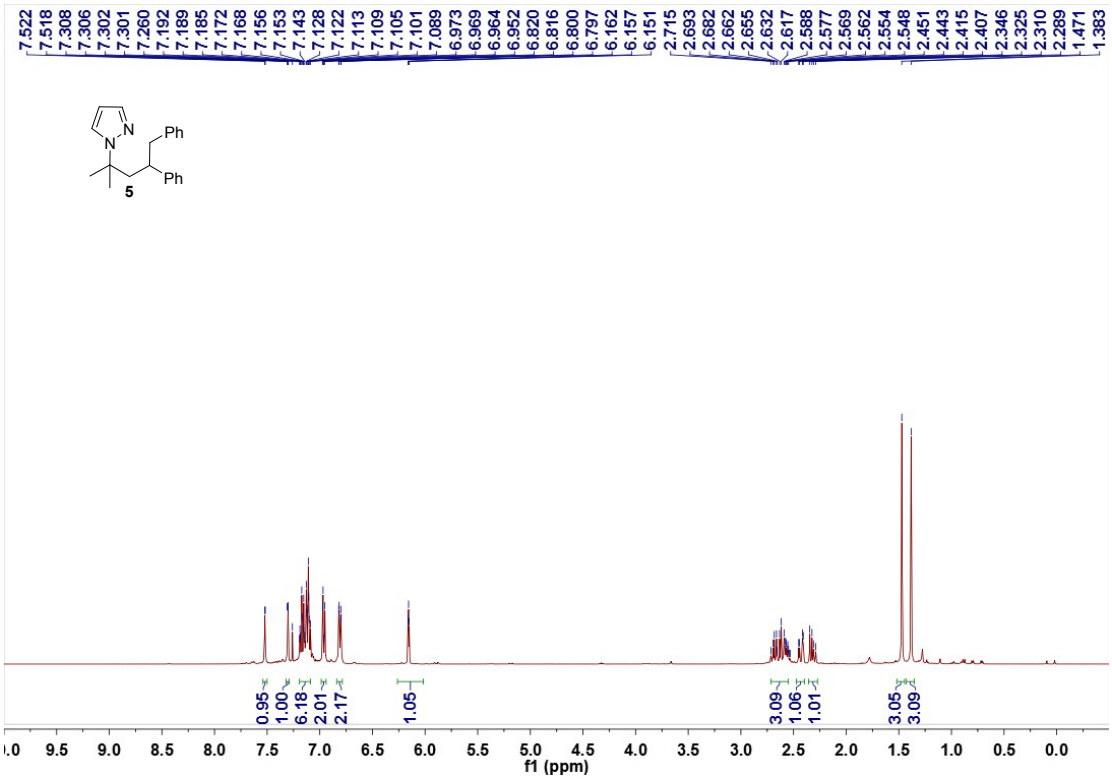

140.059
139.177
138.403
137.036
129.303
128.900
128.855
128.628
127.728
127.214
126.312
104.071
77.317
77.000
76.683
62.536
46.484
28.256
10.617
Ph
Ph
3da
f1 (ppm)

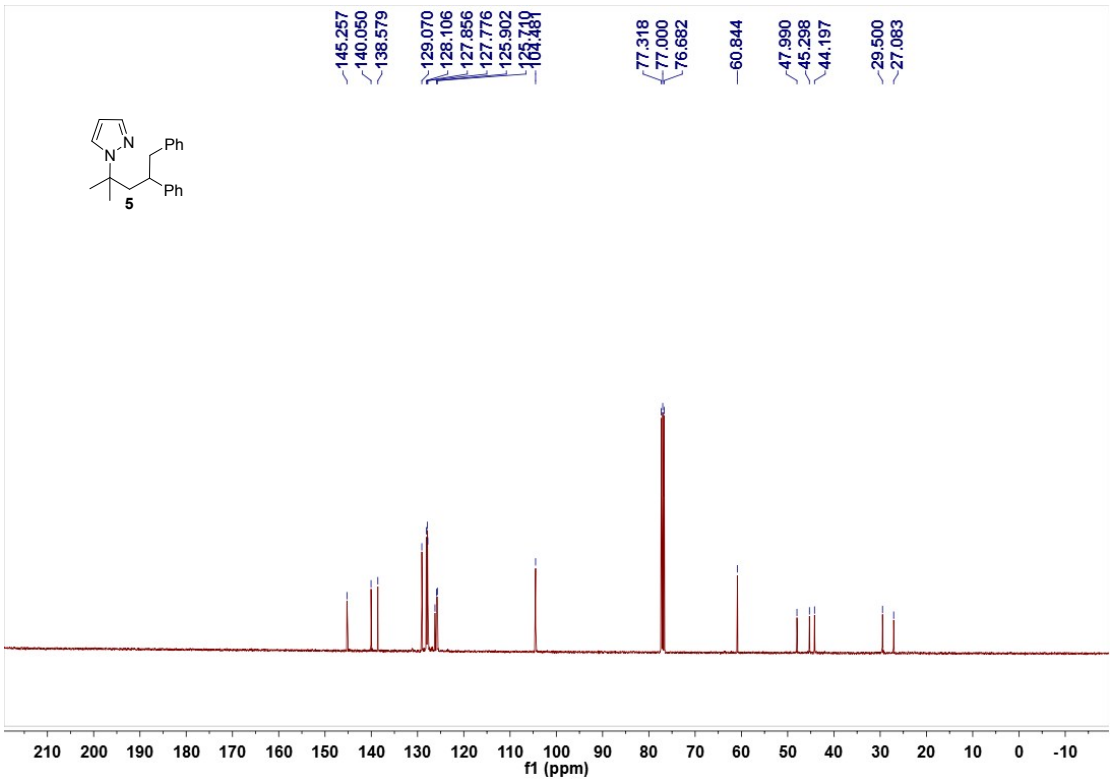

8.474
8.467
8.462
7.055
7.049
7.042
7.020
7.008
6.950
6.941
6.935
6.759
3.033
3.029
1.333
1.327
N
Ph
Ph
3ea
1.00
1.03
9.94
2.01
1.01
1.93
6.00
f1 (ppm)


167.327
148.364
141.422
140.586
137.498
135.498
129.855
129.026
128.933
127.920
127.624
126.287
125.944
120.401
120.081
77.317
77.000
76.682
53.140
41.686
28.127
N
Ph
Ph
3ea
f1 (ppm)


7.276
7.272
7.262
7.258
7.249
7.195
7.190
7.175
7.171
7.097
7.083
7.079
7.073
7.069
6.975
6.971
6.956
6.953
6.947
5.956
5.952
5.949
5.946
1.849
1.846
1.630
1.627
Ph
Ph
4
3.01
2.01
2.99
2.02
1.00
0.98
3.00
3.01
f1 (ppm)


140.820
140.252
137.473
136.097
129.312
129.199
128.493
128.404
127.840
126.992
126.276
77.317
77.000
76.682
27.149
19.598
Ph
Ph
4
f1 (ppm)


7.522
7.518
7.308
7.306
7.302
7.301
7.260
7.192
7.189
7.185
7.172
7.168
7.156
7.153
7.143
7.128
7.122
7.113
7.109
7.105
7.101
7.089
6.973
6.969
6.964
6.952
6.820
6.816
6.800
6.797
6.162
6.157
6.151
2.715
2.693
2.682
2.662
2.655
2.632
2.617
2.588
2.577
2.569
2.562
2.554
2.548
2.451
2.443
2.415
2.407
2.346
2.325
2.310
2.289
1.471
1.383
Ph
Ph
5
0.95
1.00
6.18
2.01
2.17
1.05
3.09
1.06
1.01
3.05
3.09
f1 (ppm)


145.257
140.050
138.579
129.070
128.106
127.856
127.776
125.902
77.318
77.000
76.682
60.844
47.990
45.298
44.197
29.500
27.083
Ph
Ph
5
f1 (ppm)

Noesy of 3am and 3as