

Contents

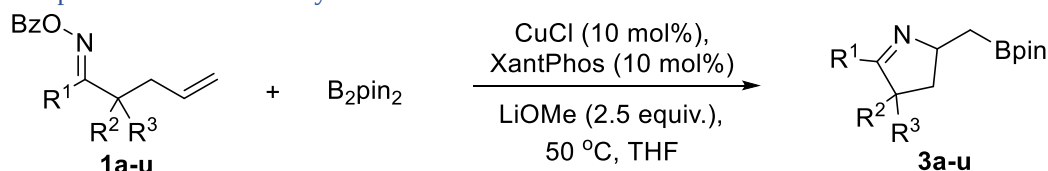
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1. General conditions

All solvents and commercially available reagents were purchased from Sigma-Aldrich, Abcr, Acros, TCI or Alfa Aesar and used without further purification. Anhydrous solvents were purchased from Sigma-Aldrich and used as received. NMR spectra were recorded on Bruker Avance 300 and Bruker ARX 400 spectrometers. Chemical shifts (ppm) are given relative to solvent: references for CDCl₃ were 7.26 ppm (¹H NMR) and 77.00 ppm (¹³C NMR). Multiplets were assigned as s (singlet), br.s (broad singlet), d (doublet), t (triplet), q (quartet), sept (septuplet), dd (doublet of doublet), dt (doublet of triplets), td (triplet of doublets) and m (multiplet). GC-yields were calculated using hexadecane as internal standard. All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210. The data are given as mass units per charge (m/z). Gas chromatography analysis was performed on an Agilent HP-7890A instrument with an FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d. 0.25 μm film thickness) using argon as carrier gas. The products were isolated from the reaction mixture by column chromatography on silica gel 60, 0.063-0.2 mm, 70-230 mesh (Merck). γ,δ-Unsaturated aromatic oxime esters were readily accessible from the corresponding ketones, aldehydes, and nitriles.^[1-5] In the ¹³C NMR, the signal of the borylated carbon was not clearly observed due to the quadrupolar relaxation.

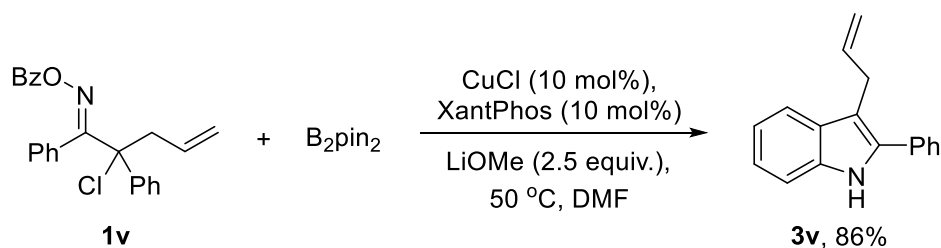
2. General procedures

2.1 General procedure for aminoborylation reactions



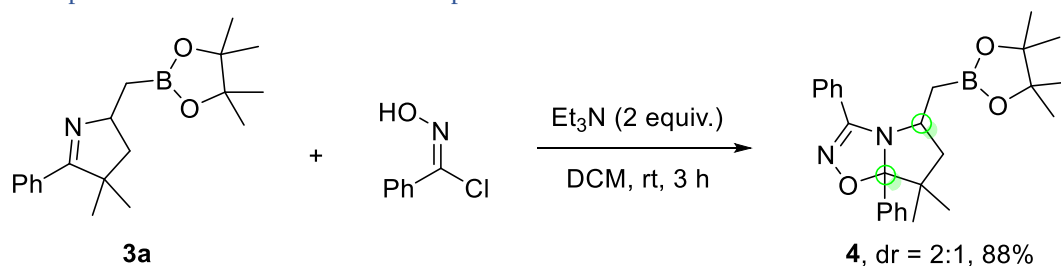
To each screw-cap vial (8 ml) equipped with a septum, a small cannula, and a stirring bar was added oxime ester **1a-u** (0.2 mmol), CuCl (2.0 mg, 10 mol%), XantPhos (11.6 mg, 10 mol%), B₂pin₂ (76 mg, 0.3 mmol) and LiOMe (19 mg, 0.5 mmol). The vials then were purged with argon three times before added dry THF (2 mL). These vials were placed on an alloy plate and the reaction was performed for 20 hours at 50 °C (a aluminum block). Afterward, the vials were cooled to room temperature, then the organic phase was removed under reduced pressure and the crude products were purified by column chromatography on silica gel (eluent: pentane/ethyl acetate = 5:1 to 2:1).

1 mmol scale: To each screw-cap vial (8 ml) equipped with a septum, a small cannula, and a stirring bar was added oxime ester **1a** (1.0 mmol), CuCl (5.0 mg, 5 mol%), XantPhos (29 mg, 5 mol%), B₂pin₂ (318 mg, 1.25 mmol) and LiOMe (95 mg, 2.25 mmol). The vials then were purged with argon three times before added dry THF (5 mL). These vials were placed on an alloy plate and the reaction was performed for 20 hours at 50 °C (a aluminum block). Afterward, the vials were cooled to room temperature, then the organic phase was removed under reduced pressure and the crude products were purified by column chromatography on silica gel (eluent: pentane/ethyl acetate = 5:1 to 2:1) to give the product **3a** in 85% yield (266.2 mg).



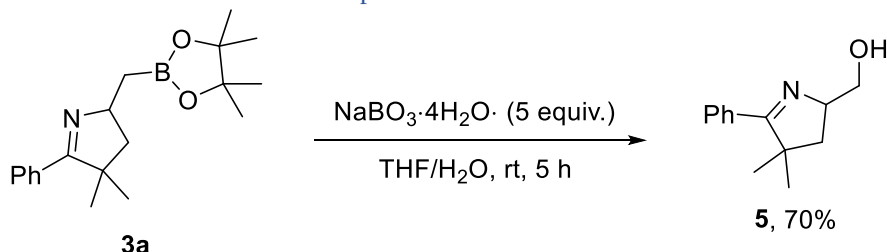
To each screw-cap vial (8 ml) equipped with a septum, a small cannula, and a stirring bar was added oxime ester **1v** (0.2 mmol), CuCl (2.0 mg, 10 mol%), XantPhos (11.6 mg, 10 mol%), B_2pin_2 (76 mg, 0.3 mmol) and LiOMe (19 mg, 0.5 mmol). The vials then were purged with argon three times before added dry DMF (2 mL). These vials were placed on an alloy plate and the reaction was performed for 20 hours at 50 °C (a aluminum block). Afterward, the vials were cooled to room temperature, then the organic phase was removed under reduced pressure and the crude products were purified by column chromatography on silica gel (eluent: pentane/ethyl acetate = 10:1) to give the product **3v** in 86% yield (40.1 mg).

2.2 General procedure of 3a transform into compound 4



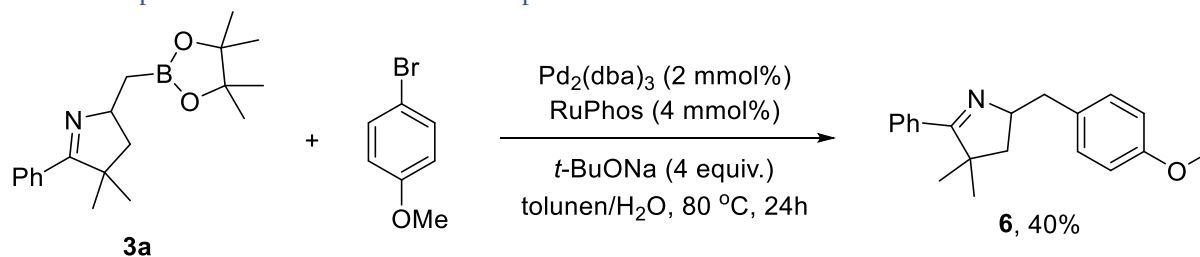
The reaction was performed according to an adapted version of a literature procedure.^[5] To a screw-cap vial equipped with a magnetic stirring bar were added **3a** (31.3 mg, 0.1 mmol, 1.0 equiv.), N-hydroxybenzimidoyl chloride (0.15 mmol, 23.4 mg, 1.5 equiv.), Et_3N (0.2 mmol, 20.2 mg, 2.0 equiv.) and CH_2Cl_2 (2.0 mL). The mixture was stirred at rt for 3 h. The solvent was removed in vacuo, and the crude products were purified by column chromatography on silica gel (eluent: pentane/ethyl acetate = 5:1 to 1:1) to give the product **4** in 88% yield (38.1 mg).

2.3 General procedure of 3a transform into compound 5



The reaction was performed according to an adapted version of a literature procedure.^[6] To a screw-cap vial equipped with a magnetic stirring bar were added **3a** (47 mg, 0.15 mmol, 1.0 equiv.), $NaBO_3 \cdot 4H_2O$ (0.9 mmol, 138.5 mg, 6.0 equiv.) and THF/ H_2O = 1:1 (2.0 mL). The mixture was stirred at rt for 5 h. The solvent was removed in vacuo, and the crude products were purified by column chromatography on silica gel (eluent: pentane/ethyl acetate = 2:1 to 0:1) to give the product **5** in 70% yield (21.3 mg).

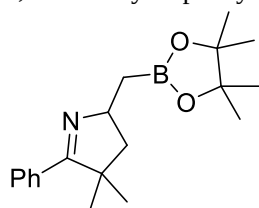
2.4 General procedure of 3a transform into compound 6



The reaction was performed according to an adapted version of a literature procedure.^[6] To a screw-cap vial equipped with a magnetic stirring bar were charged with $\text{Pd}_2(\text{dba})_3$ (2.70 mg, 2.0 mol %), RuPhos (2.8 mg, 4.0 mol%), NaOtBu (72.1 mg, 0.75 mmol, 5.0 equiv), and **3a** (47 mg, 0.15 mmol, 1.0 equiv.). The vial was purged with argon three times before added Toluene/ H_2O = 10:1 (0.55 mL), and 4-bromoanisole (28 mL, 0.23 mmol, 1.5 equiv). Then the reaction was stirred at 80 °C for 24 h. After reaction, the reaction allowed to cool to room temperature and was diluted with ethyl acetate (5 mL) and washed with water (10 mL). The aqueous layer was washed with ethyl acetate and the combined organic phase were dried over Na_2SO_4 and concentrated. The residue was purified by flash chromatography (eluent: pentane/ethyl acetate = 10:1 to 5:1) to give **6** in 40% yield (17.6 mg).

3. Analytical data

4,4-Dimethyl-5-phenyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2H-pyrrole (**3a**)



56.3 mg, colorless oil, yield: 90%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

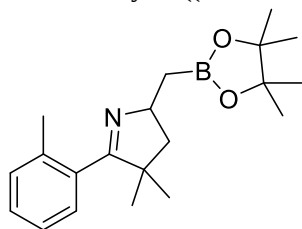
¹H NMR (300 MHz, CDCl_3) δ 7.74 – 7.62 (m, 2H), 7.38 – 7.29 (m, 3H), 4.25 – 4.13 (m, 1H), 2.15 (dd, J = 12.4, 6.7 Hz, 1H), 1.54 (dd, J = 15.4, 5.2 Hz, 1H), 1.52 (dd, J = 12.4, 8.8 Hz, 1H), 1.33 (s, 3H), 1.32 (s, 3H), 1.26 (s, 12H), 1.08 (dd, J = 15.4, 9.8 Hz, 1H).

¹³C NMR (75 MHz, CDCl_3) δ 178.1, 135.0, 129.1, 127.9, 127.9, 83.0, 64.7, 50.7, 49.9, 27.3, 26.0, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl_3) δ 33.7.

HR-MS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{28}\text{BNO}_2$ $[\text{M}+\text{H}]^+$: 313.2328; found: 313.2333.

4,4-Dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-5-(*o*-tolyl)-3,4-dihydro-2H-pyrrole (**3b**)



53.7 mg, colorless oil, yield: 82%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

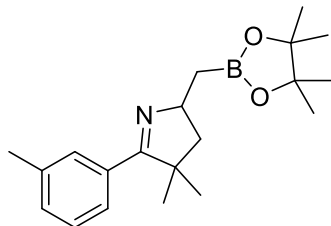
¹H NMR (300 MHz, CDCl_3) δ 7.24 – 7.17 (m, 2H), 7.17 – 7.10 (m, 2H), 4.25 (m, 1H), 2.29 (s, 3H), 2.17 (dd, J = 12.5, 6.9 Hz, 1H), 1.64 (dd, J = 15.5, 4.8 Hz, 1H), 1.50 (dd, J = 12.5, 8.5 Hz, 1H), 1.26 (s, 12H), 1.17 (s, 3H), 1.14 (s, 3H), 1.07 (dd, J = 15.5, 10.3 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 179.8, 136.3, 135.3, 130.3, 127.9, 127.5, 124.7, 83.1, 65.7, 52.9, 47.8, 26.8, 25.5, 24.9, 24.7, 19.9.

¹¹B NMR (96 MHz, CDCl₃) δ 33.5.

HR-MS (ESI-TOF) calcd. for C₂₀H₃₀BNO₂ [M+H]⁺: 327.2484; found: 327.2485.

4,4-Dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-5-(*m*-tolyl)-3,4-dihydro-2*H*-pyrrole (**3c**)



54.3 mg, colorless oil, yield: 83%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

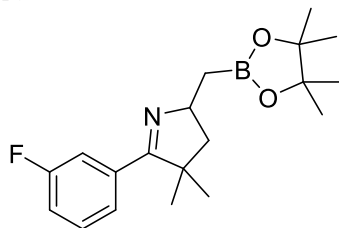
¹H NMR (300 MHz, CDCl₃) δ 7.54 – 7.49 (m, 1H), 7.48 – 7.42 (m, 1H), 7.25 – 7.19 (m, 1H), 7.19 – 7.13 (m, 1H), 4.23 – 4.11 (m, 1H), 2.34 (s, 3H), 2.14 (dd, *J* = 12.4, 6.7 Hz, 1H), 1.55 (dd, *J* = 15.4, 5.0 Hz, 1H), 1.51 (dd, *J* = 12.4, 8.8 Hz, 1H), 1.32 (s, 3H), 1.31 (s, 3H), 1.26 (s, 12H), 1.07 (dd, *J* = 15.4, 9.9 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 178.3, 137.6, 134.9, 129.8, 128.7, 127.7, 124.7, 83.0, 64.6, 50.7, 49.9, 27.3, 26.0, 24.9, 24.6, 21.4.

¹¹B NMR (96 MHz, CDCl₃) δ 33.5.

HR-MS (ESI-TOF) calcd. for C₂₀H₃₀BNO₂ [M+H]⁺: 327.2484; found: 327.2478.

5-(3-Fluorophenyl)-4,4-dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2*H*-pyrrole (**3d**)



54.3 mg, colorless oil, yield: 82%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

¹H NMR (300 MHz, CDCl₃) ¹H NMR (300 MHz, Chloroform-*d*) δ 7.48 – 7.36 (m, 2H), 7.34 – 7.25 (m, 1H), 7.09 – 6.98 (m, 1H), 4.24 – 4.11 (m, 1H), 2.15 (dd, *J* = 12.5, 6.7 Hz, 1H), 1.52 (dd, *J* = 12.5, 8.7 Hz, 1H), 1.48 (dd, *J* = 15.4, 5.5 Hz, 1H), 1.31 (s, 3H), 1.30 (s, 3H), 1.25 (s, 12H), 1.08 (dd, *J* = 15.4, 9.5 Hz, 1H).

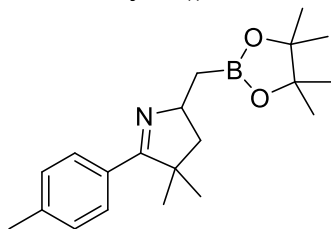
¹³C NMR (75 MHz, CDCl₃) δ 176.9 (d, *J* = 2.2 Hz), 162.4 (d, *J* = 245.4 Hz), 137.2 (d, *J* = 7.5 Hz), 129.5 (d, *J* = 8.1 Hz), 123.5 (d, *J* = 3.0 Hz), 116.0 (d, *J* = 21.2 Hz), 115.0 (d, *J* = 22.5 Hz), 83.0, 64.8, 50.7, 49.9, 27.2, 25.9, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl₃) δ 33.7.

¹⁹F NMR (282 MHz, CDCl₃) δ -113.2.

HR-MS (ESI-TOF) calcd. for C₁₉H₂₇BFNO₂ [M+H]⁺: 331.2233; found: 331.2233.

4,4-Dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-5-(*p*-tolyl)-3,4-dihydro-2*H*-pyrrole (**3e**)



49.7 mg, colorless oil, yield: 76%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

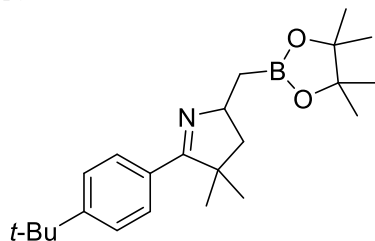
¹H NMR (300 MHz, CDCl₃) δ 7.64 – 7.58 (m, 2H), 7.18 – 7.12 (m, 2H), 4.23 – 4.11 (m, 1H), 2.35 (s, 3H), 2.13 (dd, *J* = 12.4, 6.7 Hz, 1H), 1.53 (dd, *J* = 15.4, 5.2 Hz, 1H), 1.51 (dd, *J* = 12.4, 8.8 Hz, 1H), 1.33 (s, 3H), 1.33 (s, 3H), 1.26 (s, 12H), 1.07 (dd, *J* = 15.4, 9.8 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 177.9, 139.1, 132.1, 128.7, 127.9, 83.0, 64.5, 50.6, 50.1, 27.4, 26.0, 24.9, 24.7, 21.3.

¹¹B NMR (96 MHz, CDCl₃) δ 33.0.

HR-MS (ESI-TOF) calcd. for C₂₀H₃₀BNO₂ [M+H]⁺: 327.2484; found: 327.2487.

5-(4-(*tert*-Butyl)phenyl)-4,4-dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2H-pyrrole (**3f**)



57.6 mg, colorless oil, yield: 78%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

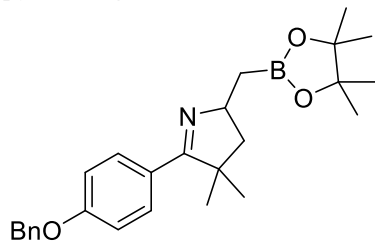
¹H NMR (300 MHz, CDCl₃) δ 7.69 – 7.63 (m, 2H), 7.38 – 7.32 (m, 2H), 4.23 – 4.10 (m, 1H), 2.14 (dd, *J* = 12.4, 6.7 Hz, 1H), 1.53 (dd, *J* = 15.3, 5.5 Hz, 1H), 1.51 (dd, *J* = 12.4, 8.8 Hz, 1H), 1.35 (s, 3H), 1.33 (s, 3H), 1.31 (s, 9H), 1.27 (s, 6H), 1.26 (s, 6H), 1.06 (dd, *J* = 15.3, 9.8 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 177.7, 152.2, 132.0, 127.7, 124.9, 83.0, 64.5, 50.6, 50.1, 34.6, 31.2, 27.4, 26.1, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl₃) δ 34.0.

HR-MS (ESI-TOF) calcd. for C₂₃H₃₆BNO₂ [M+H]⁺: 369.2953; found: 369.2956.

5-(4-(Benzyloxy)phenyl)-4,4-dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2H-pyrrole (**3g**)



36.1 mg, colorless oil, yield: 43%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

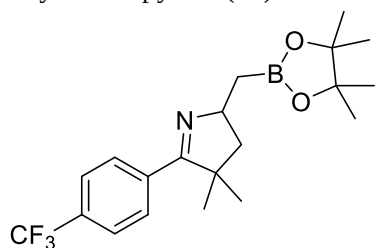
¹H NMR (400 MHz, CDCl₃) δ 7.73 – 7.68 (m, 2H), 7.44 – 7.32 (m, 5H), 6.97 – 6.92 (m, 2H), 5.08 (s, 2H), 4.20 – 4.11 (m, 1H), 2.14 (dd, *J* = 12.4, 6.7 Hz, 1H), 1.53 (dd, *J* = 15.4, 5.2 Hz, 1H), 1.51 (dd, *J* = 12.4, 8.7 Hz, 1H), 1.35 (s, 3H), 1.34 (s, 3H), 1.27 (s, 6H), 1.26 (s, 6H), 1.06 (dd, *J* = 15.4, 9.8 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 177.2, 159.7, 136.7, 129.5, 128.6, 128.0, 127.5, 114.3, 83.0, 69.9, 64.3, 50.5, 50.3, 27.5, 26.1, 24.9, 24.7.

¹¹B NMR (128 MHz, CDCl₃) δ 33.4.

HR-MS (ESITOF) calcd. for C₂₆H₃₄BNO₃ [M+H]⁺: 419.2746; found: 419.2746.

4,4-Dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-5-(4-(trifluoromethyl)phenyl)-3,4-dihydro-2H-pyrrole (**3h**)



53.4 mg, colorless oil, yield: 70%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

¹H NMR (300 MHz, CDCl₃) δ 7.83 – 7.72 (m, 2H), 7.63 – 7.56 (m, 2H), 4.28 – 4.16 (m, 1H), 2.17 (dd, *J* = 12.5, 6.7 Hz, 1H), 1.55 (dd, *J* = 12.5, 8.7 Hz, 1H), 1.50 (dd, *J* = 15.4, 5.6 Hz, 1H), 1.32 (s, 3H), 1.31 (s, 3H), 1.26 (s, 12H), 1.11 (dd, *J* = 15.4, 9.4 Hz, 1H).

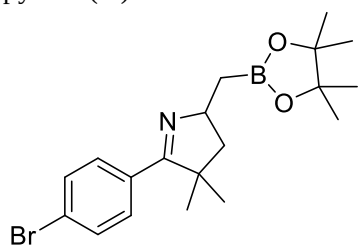
¹³C NMR (75 MHz, CDCl₃) δ 177.2, 138.6, 131.0 (q, *J* = 32.6 Hz), 128.3, 124.9 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 272.0 Hz), 83.1, 65.1, 50.8, 49.8, 27.1, 25.9, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl₃) δ 32.7.

¹⁹F NMR (282 MHz, CDCl₃) δ -62.8.

HR-MS (ESI-TOF) calcd. for C₂₀H₂₇BF₃NO₂ [M+H]⁺: 381.2201; found: 381.2202.

5-(4-Bromophenyl)-4,4-dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2H-pyrrole (**3i**)



69.8 mg, colorless oil, yield: 89%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

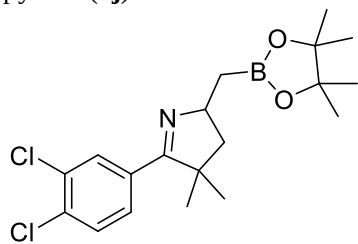
¹H NMR (300 MHz, CDCl₃) δ 7.58 – 7.52 (m, 2H), 7.47 – 7.41 (m, 2H), 4.21 – 4.09 (m, 1H), 2.12 (dd, *J* = 12.5, 6.8 Hz, 1H), 1.50 (dd, *J* = 12.5, 8.8 Hz, 1H), 1.46 (dd, *J* = 15.4, 5.3 Hz, 1H), 1.29 (s, 3H), 1.28 (s, 3H), 1.23 (s, 12H), 1.06 (dd, *J* = 15.4, 9.5 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) ¹³C NMR (75 MHz, CDCl₃) δ 177.0, 133.8, 131.1, 129.5, 123.5, 83.0, 64.7, 50.6, 49.9, 27.2, 25.9, 24.8, 24.6.

¹¹B NMR (96 MHz, CDCl₃) δ 33.2.

HR-MS (ESI-TOF) calcd. for C₁₉H₂₇BBrNO₂ [M+H]⁺: 391.1433; found: 391.1437.

5-(3,4-Dichlorophenyl)-4,4-dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2H-pyrrole (**3j**)



47.4 mg, colorless oil, yield: 62%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

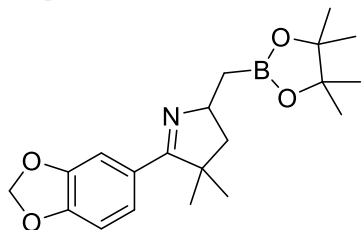
¹H NMR (300 MHz, CDCl₃) δ 7.86 – 7.70 (m, 1H), 7.53 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 4.23 – 4.12 (m, 1H), 2.15 (dd, *J* = 12.5, 6.8 Hz, 1H), 1.52 (dd, *J* = 12.5, 8.3 Hz, 1H), 1.46 (dd, *J* = 15.4, 5.1 Hz, 1H), 1.31 (s, 3H), 1.30 (s, 3H), 1.25 (s, 12H), 1.09 (dd, *J* = 15.4, 9.3 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 175.9, 134.9, 133.4, 132.3, 130.0, 130.0, 127.1, 83.1, 64.9, 50.6, 50.0, 27.2, 25.9, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl₃) δ 33.5.

HR-MS (ESI-TOF) calcd. for C₁₉H₂₆BCl₂NO₂ [M+H]⁺: 381.1548; found: 381.1548.

5-(Benzo[d][1,3]dioxol-5-yl)-4,4-dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2H-pyrrole (**3k**)



37.9 mg, colorless oil, yield: 53%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

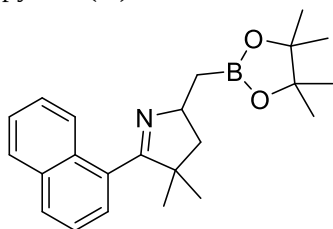
¹H NMR (300 MHz, CDCl₃) δ 7.26 (d, *J* = 1.8 Hz, 1H), 7.23 (dd, *J* = 8.0, 1.8 Hz, 1H), 6.77 (d, *J* = 8.1 Hz, 1H), 5.95 (s, 2H), 4.20 – 4.07 (m, 1H), 2.12 (dd, *J* = 12.4, 6.7 Hz, 1H), 1.50 (dd, *J* = 12.4, 8.8 Hz, 1H), 1.48 (dd, *J* = 15.4, 5.4 Hz, 1H), 1.32 (s, 3H), 1.31 (s, 3H), 1.25 (s, 12H), 1.05 (dd, *J* = 15.4, 9.6 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 177.1, 148.4, 147.4, 129.0, 122.1, 108.6, 107.7, 101.1, 83.0, 64.2, 50.5, 50.3, 27.4, 26.1, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl₃) δ 33.7.

HR-MS (ESI-TOF) calcd. for C₂₀H₂₈BNO₄ [M+H]⁺: 357.2226; found: 357.2225.

4,4-Dimethyl-5-(naphthalen-1-yl)-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2H-pyrrole (**3l**)



62.5 mg, colorless oil, yield: 86%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

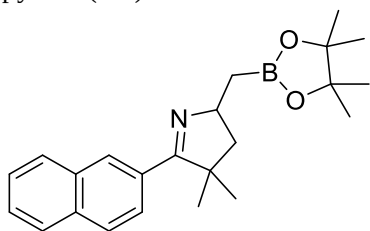
¹H NMR (300 MHz, CDCl₃) δ 8.02 – 7.93 (m, 1H), 7.85 – 7.79 (m, 2H), 7.49 – 7.41 (m, 3H), 7.35 (dd, *J* = 7.1, 1.3 Hz, 1H), 4.47 – 4.34 (m, 1H), 2.28 (dd, *J* = 12.5, 6.9 Hz, 1H), 1.73 (dd, *J* = 15.6, 4.7 Hz, 1H), 1.67 (dd, *J* = 12.5, 8.6 Hz, 1H), 1.29 (s, 12H), 1.23 (s, 3H), 1.15 (s, 3H), 1.17 (dd, *J* = 15.6, 10.0 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 179.1, 133.5, 133.4, 132.0, 128.3, 128.0, 126.0, 126.0, 125.7, 125.0, 124.4, 83.1, 66.0, 53.1, 47.9, 26.9, 25.5, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl₃) δ 33.7.

HR-MS (ESI-TOF) calcd. for C₂₃H₃₀BNO₂ [M+H]⁺: 363.2484; found: 363.2484.

4,4-Dimethyl-5-(naphthalen-2-yl)-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2H-pyrrole (**3m**)



67.6 mg, colorless oil, yield: 93%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

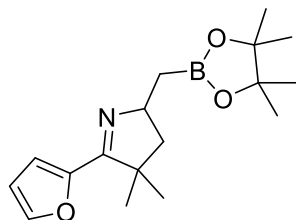
¹H NMR (300 MHz, CDCl₃) δ 8.17 (s, 1H), 7.92 – 7.79 (m, 4H), 7.53 – 7.43 (m, 2H), 4.33 – 4.19 (m, 1H), 2.21 (dd, *J* = 12.4, 6.7 Hz, 1H), 1.59 (dd, *J* = 12.4, 8.9 Hz, 1H), 1.58 (dd, *J* = 15.4, 5.2 Hz, 1H), 1.44 (s, 3H), 1.42 (s, 3H), 1.28 (s, 12H), 1.15 (dd, *J* = 15.4, 9.7 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 177.9, 133.6, 132.8, 132.4, 128.5, 127.6, 127.5, 127.4, 126.5, 126.1, 125.8, 83.0, 64.8, 50.8, 50.2, 27.5, 26.2, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl₃) δ 33.7.

HR-MS (ESI-TOF) calcd. for C₂₃H₃₀BNO₂ [M+H]⁺: 363.2484; found: 363.2477.

5-(Furan-2-yl)-4,4-dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2*H*-pyrrole (**3n**)



30.9 mg, colorless oil, yield: 51%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

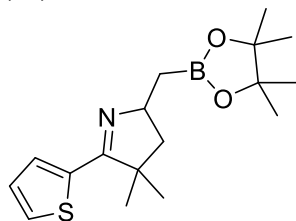
¹H NMR (300 MHz, CDCl₃) δ 7.48 (d, *J* = 1.4 Hz, 1H), 6.87 (d, *J* = 3.5 Hz, 1H), 6.44 (dd, *J* = 3.5, 1.8 Hz, 1H), 4.27 – 4.15 (m, 1H), 2.14 (dd, *J* = 12.6, 7.0 Hz, 1H), 1.64 (dd, *J* = 15.4, 4.7 Hz, 1H), 1.46 (dd, *J* = 12.6, 8.4 Hz, 1H), 1.41 (s, 3H), 1.29 (s, 3H), 1.26 (s, 6H), 1.25 (s, 6H), 1.01 (dd, *J* = 15.4, 10.7 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) ¹³C NMR (75 MHz, CDCl₃) δ 168.7, 149.3, 143.7, 112.2, 111.2, 83.1, 65.8, 50.3, 48.8, 27.5, 25.9, 24.9, 24.6.

¹¹B NMR (96 MHz, CDCl₃) δ 33.2.

HR-MS (ESI-TOF) calcd. for C₁₇H₂₆BNO₃ [M+H]⁺: 303.2120; found: 303.2122.

4,4-Dimethyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-5-(thiophen-2-yl)-3,4-dihydro-2*H*-pyrrole (**3o**)



56.8 mg, colorless oil, yield: 89%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

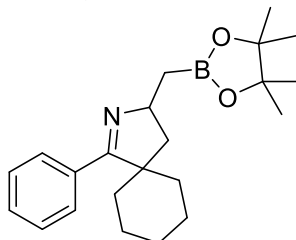
¹H NMR (300 MHz, CDCl₃) δ 7.41 (dd, *J* = 3.8, 1.0 Hz, 1H), 7.30 (dd, *J* = 5.1, 1.0 Hz, 1H), 7.00 (dd, *J* = 5.1, 3.7 Hz, 1H), 4.23 – 4.11 (m, 1H), 2.15 (dd, *J* = 12.6, 7.1 Hz, 1H), 1.53 (dd, *J* = 12.6, 8.3 Hz, 1H), 1.45 (dd, *J* = 15.3, 5.7 Hz, 1H), 1.43 (s, 3H), 1.32 (s, 3H), 1.24 (s, 6H), 1.23 (s, 6H), 1.06 (dd, *J* = 15.3, 9.5 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 171.8, 138.6, 128.0, 127.2, 127.1, 82.9, 65.1, 50.5, 49.8, 27.7, 26.1, 24.8, 24.6.

¹¹B NMR (96 MHz, CDCl₃) δ 33.6.

HR-MS (ESI-TOF) calcd. for C₁₇H₂₆BNO₂S [M+H]⁺: 319.1892; found: 319.1898.

1-Phenyl-3-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-2-azaspiro[4.5]dec-1-ene (**3p**)



65.0 mg, colorless oil, yield: 92%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

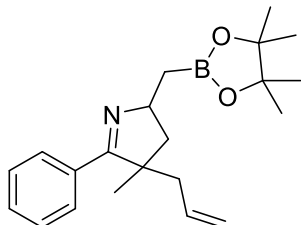
¹H NMR (300 MHz, CDCl₃) δ 7.55 – 7.48 (m, 2H), 7.36 – 7.27 (m, 3H), 4.24 – 4.12 (m, 1H), 2.41 (dd, *J* = 12.7, 7.1 Hz, 1H), 1.81 – 1.43 (m, 9H), 1.34 (dd, *J* = 12.7, 8.4 Hz, 1H), 1.25 (s, 12H), 1.19 – 1.13 (m, 2H), 1.07 (dd, *J* = 15.4, 9.9 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 179.0, 136.0, 128.5, 128.0, 127.7, 83.0, 65.3, 56.7, 42.8, 35.7, 31.8, 25.6, 24.9, 24.6, 24.5, 23.3, 23.1.

¹¹B NMR (96 MHz, CDCl₃) δ 33.9.

HR-MS (ESI-TOF) calcd. for C₂₂H₃₂BNO₂ [M+H]⁺: 353.2641; found: 353.2631.

4-Allyl-4-methyl-5-phenyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2*H*-pyrrole (**3q**)



48.8 mg, colorless oil, dr = 1:1, yield: 72%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

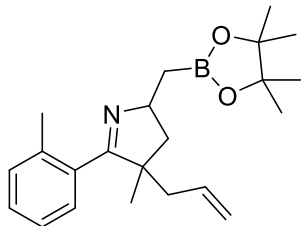
¹H NMR (300 MHz, CDCl₃) δ 7.73 – 7.63 (m, 4H), 7.39 – 7.30 (m, 6H), 5.82 – 5.53 (m, 2H), 5.11 – 4.90 (m, 4H), 4.27 – 4.08 (m, 2H), 2.47 – 2.24 (m, 5H), 1.96 (dd, *J* = 12.5, 6.7 Hz, 1H), 1.67 (dd, *J* = 12.6, 8.9 Hz, 1H), 1.56 – 1.39 (m, 3H), 1.36 (s, 3H), 1.33 (s, 3H), 1.27 – 1.23 (m, 24H), 1.09 (m, 2H).

¹³C NMR (75 MHz, CDCl₃) δ 177.2, 176.8, 135.2, 134.5, 134.3, 129.2, 129.1, 128.0, 128.0, 127.8, 118.0, 117.9, 83.0, 65.4, 64.8, 54.8, 54.3, 46.0, 45.8, 43.5, 43.3, 26.2, 24.9, 24.7, 24.7, 24.2.

¹¹B NMR (96 MHz, CDCl₃) δ 33.1.

HR-MS (ESI-TOF) calcd. for C₂₁H₃₀BNO₂ [M+H]⁺: 339.2484; found: 339.2489.

4-Allyl-4-methyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-5-(*o*-tolyl)-3,4-dihydro-2*H*-pyrrole (**3r**)



49.5 mg, colorless oil, dr = 1:1, yield: 70%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

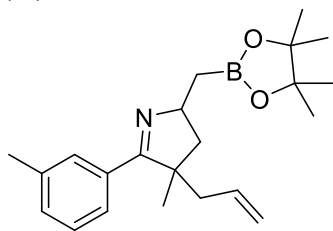
¹H NMR (300 MHz, CDCl₃) δ 7.22 – 7.17 (m, 4H), 7.17 – 7.10 (m, 4H), 5.86 – 5.58 (m, 2H), 5.12 – 4.92 (m, 4H), 4.31 – 4.15 (m, 2H), 2.38 – 2.29 (m, 7H), 2.24 – 1.98 (m, 4H), 1.65 – 1.53 (m, 3H), 1.35 (dd, *J* = 12.8, 8.1 Hz, 2H), 1.26 (s, 12H), 1.25 (s, 12H), 1.17 (s, 3H), 1.11 – 1.02 (m, 5H).

¹³C NMR (75 MHz, CDCl₃) δ 178.7, 178.4, 136.5, 136.5, 135.4, 135.4, 134.4, 134.3, 130.5, 130.4, 127.9, 127.9, 127.4, 127.4, 124.8, 124.8, 118.1, 117.7, 83.0, 66.3, 65.9, 56.4, 56.0, 44.9, 43.9, 43.4, 42.0, 24.8, 24.7, 24.7, 24.6, 22.6, 20.1, 20.0.

¹¹B NMR (96 MHz, CDCl₃) δ 33.9.

HR-MS (ESI-TOF) calcd. for C₂₂H₃₂BNO₂ [M+H]⁺: 353.2641; found: 353.2635.

4-Allyl-4-methyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-5-(*m*-tolyl)-3,4-dihydro-2*H*-pyrrole (**3s**)



55.1 mg, colorless oil, dr = 1:1, yield: 78%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

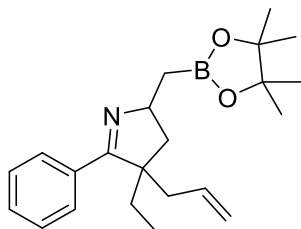
¹H NMR (300 MHz, CDCl₃) δ 7.53 – 7.40 (m, 4H), 7.25 – 7.14 (m, 4H), 5.82 – 5.53 (m, 2H), 5.12 – 4.91 (m, 4H), 4.26 – 4.06 (m, 2H), 2.44 – 2.25 (m, 11H), 1.95 (dd, *J* = 12.5, 6.7 Hz, 1H), 1.65 (dd, *J* = 13.0, 9.1 Hz, 1H), 1.56 – 1.37 (m, 3H), 1.35 (s, 3H), 1.32 (s, 3H), 1.26 (s, 12H), 1.25 (s, 12H), 1.13 – 1.03 (m, 2H).

¹³C NMR (75 MHz, CDCl₃) δ 177.2, 176.8, 137.7, 137.6, 135.2, 134.6, 134.4, 129.9, 129.8, 128.9, 128.7, 127.8, 127.8, 124.8, 124.6, 117.9, 117.8, 83.0, 83.0, 65.4, 64.8, 54.8, 54.3, 46.0, 45.7, 43.6, 43.3, 26.2, 24.9, 24.7, 24.6, 24.2, 21.4.

¹¹B NMR (96 MHz, CDCl₃) δ 32.9.

HR-MS (ESI-TOF) calcd. for C₂₂H₃₂BNO₂ [M+H]⁺: 353.2641; found: 353.2639.

4-Allyl-4-ethyl-5-phenyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2*H*-pyrrole (**3t**)



45.2 mg, colorless oil, dr = 5:3, yield: 64%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

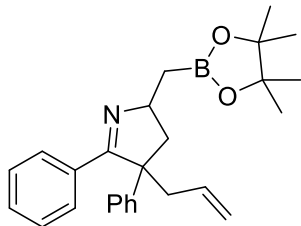
¹H NMR (300 MHz, CDCl₃) δ 7.76 – 7.66 (m, 3.2H), 7.39 – 7.29 (m, 4.8H), 5.82 – 5.67 (m, 1H), 5.67 – 5.53 (m, 0.6H), 5.12 – 4.91 (m, 3.2H), 4.24 – 4.06 (m, 1.6H), 2.54 – 2.42 (m, 1.6H), 2.42 – 2.26 (m, 1.6H), 2.21 – 2.07 (m, 1.6H), 1.85 – 1.43 (m, 6.4H), 1.27 (s, 12H), 1.26 (s, 7.2H), 1.10 – 1.00 (m, 1.6H), 0.91 (t, *J* = 7.5 Hz, 1.8H), 0.81 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (75 MHz, CDCl₃) δ 174.9, 174.8, 135.6, 134.8, 134.4, 129.2, 128.1, 128.1, 127.9, 117.9, 117.8, 83.0, 66.3, 65.7, 59.8, 59.7, 43.4, 43.3, 42.4, 42.0, 31.8, 30.7, 24.9, 24.7, 9.3.

¹¹B NMR (96 MHz, CDCl₃) δ 33.6.

HR-MS (ESI-TOF) calcd. for C₂₂H₃₂BNO₂ [M+H]⁺: 353.2641; found: 353.2639.

4-Allyl-4,5-diphenyl-2-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-3,4-dihydro-2*H*-pyrrole (**3u**)



36.9 mg, colorless oil, dr = 5:1, yield: 46%. Eluent: pentane/ethyl acetate = 5/1 to 2/1.

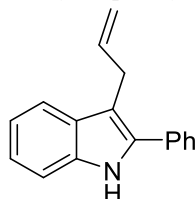
¹H NMR (300 MHz, CDCl₃) δ 7.51 – 7.43 (m, 2H), 7.37 – 7.28 (m, 4H), 7.26 – 7.20 (m, 2H), 7.19 – 7.11 (m, 2H), 5.79 – 5.62 (m, 1H), 5.12 – 5.01 (m, 2H), 4.33 – 4.20 (m, 1H), 2.91 (dt, *J* = 7.4, 1.2 Hz, 2H), 2.67 (dd, *J* = 13.4, 7.9 Hz, 1H), 1.85 (dd, *J* = 13.4, 7.6 Hz, 1H), 1.59 (dd, *J* = 15.4, 5.5 Hz, 1H), 1.26 (s, 6H), 1.25 (s, 6H), 1.17 (dd, *J* = 15.4, 9.8 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 172.3, 147.4, 133.7, 133.5, 129.4, 128.9, 128.6, 127.8, 126.5, 126.2, 118.6, 83.1, 67.4, 62.2, 50.7, 40.6, 24.9, 24.7.

¹¹B NMR (96 MHz, CDCl₃) δ 34.3.

HR-MS (ESI-TOF) calcd. for C₂₆H₃₂BN₂O₂ [M+H]⁺: 401.2641; found: 401.2632.

3-Allyl-2-phenyl-1*H*-indole (**3v**)⁷



40.1 mg, colorless solid, yield: 86%. Eluent: pentane/ethyl acetate = 10/1.

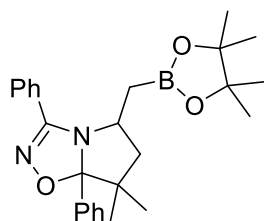
¹H NMR (300 MHz, CDCl₃) δ 7.99 (br.s, 1H), 7.55 – 7.51 (m, 1H), 7.50 – 7.47 (m, 2H), 7.41 – 7.36 (m, 2H), 7.32 – 7.27 (m, 2H), 7.16 – 7.10 (m, 1H), 7.08 – 7.02 (m, 1H), 6.15 – 5.94 (m, 1H), 5.04 (dq, *J* = 6.5, 1.8 Hz, 1H), 4.99 (t, *J* = 1.8 Hz, 1H), 3.56 (dt, *J* = 5.6, 1.8 Hz, 2H).

¹³C NMR (75 MHz, CDCl₃) δ 137.4, 135.9, 134.8, 133.0, 129.4, 128.8, 127.8, 127.6, 122.3, 119.6, 119.4, 115.2, 110.8, 110.5, 28.9.

GC-MS (EI, 70eV): *m/z*(%) = 233 (M⁺, 100), 218 (27), 206 (100), 191 (9), 178 (15), 156 (11), 128 (17), 108 (18), 77 (15).

HR-MS (ESI-TOF) calcd. for C₁₇H₁₅N [M+H]⁺: 234.1283; found: 234.1287.

7,7-Dimethyl-3,7a-diphenyl-5-((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl)-5,6,7,7a-tetrahydropyrrolo [1,2-*d*][1,2,4]oxadiazole (**4**)



38.1 mg, colorless solid, dr = 2:1, yield: 88%. Eluent: pentane/ethyl acetate = 5/1 to 1/1.

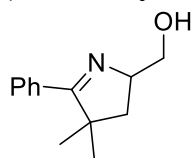
¹H NMR (300 MHz, CDCl₃) *Data for the major diastereomer*: δ 7.83 – 7.75 (m, 2H), 7.72 – 7.66 (m, 2H), 7.43 – 7.23 (m, 6H), 3.77 – 3.66 (m, 1H), 2.24 (dd, *J* = 12.8, 7.7 Hz, 1H), 1.69 (dd, *J* = 12.8, 5.7 Hz, 1H), 1.59 (dd, *J* = 15.6, 5.1 Hz, 1.5H), 1.50 (dd, *J* = 15.6, 11.2 Hz, 1H), 1.29 (s, 3H), 1.20 (s, 12H), 0.78 (s, 3H). *Characteristic signals for the minor isomer*: 4.18 – 4.03 (m, 1H), 1.99 (dd, *J* = 11.9, 5.1 Hz, 1H), 1.28 (s, 3H), 1.18 (s, 12H), 1.06 (dd, *J* = 14.7, 4.0 Hz, 1H), 0.81 (s, 3H), 0.72 (dd, *J* = 14.7, 12.3 Hz, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 160.5, 141.6, 130.5, 128.6, 128.4, 127.7, 127.4, 127.3, 126.2, 112.6, 83.3, 59.3, 47.3, 45.8, 27.4, 24.9, 24.5, 24.0.

¹¹B NMR (96 MHz, CDCl₃) δ 33.5.

HR-MS (ESI-TOF) calcd. for C₂₆H₃₃BN₂O₃ [M+H]⁺: 432.2699; found: 432.2693.

(4,4-Dimethyl-5-phenyl-3,4-dihydro-2*H*-pyrrol-2-yl)methanol (**5**)



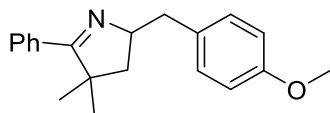
21.3 mg, yellow oil, yield: 70%. Eluent: pentane/ethyl acetate = 2/1 to 0/1.

¹H NMR (300 MHz, CDCl₃) δ 7.73 – 7.59 (m, 2H), 7.43 – 7.32 (m, 3H), 4.21 – 4.09 (m, 1H), 3.93 (dd, *J* = 11.2, 4.1 Hz, 1H), 3.57 (dd, *J* = 11.2, 6.5 Hz, 1H), 2.89 (br.s, 1H), 1.96 (dd, *J* = 12.5, 7.0 Hz, 1H), 1.68 (dd, *J* = 12.5, 8.9 Hz, 1H), 1.33 (s, 3H), 1.33 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ 181.4, 134.5, 129.6, 128.1, 127.8, 69.8, 65.9, 50.7, 43.3, 27.0, 26.0.

HR-MS (ESI-TOF) calcd. for C₁₃H₁₇NO [M+H]⁺: 204.1388; found: 204.1390.

2-(4-Methoxybenzyl)-4,4-dimethyl-5-phenyl-3,4-dihydro-2*H*-pyrrole (**6**)



17.6 mg, yellow solid, yield: 40%. Eluent: pentane/ethyl acetate = 10/1 to 5/1.

¹H NMR (400 MHz, CDCl₃) δ 7.74 – 7.67 (m, 2H), 7.41 – 7.36 (m, 3H), 7.23 – 7.19 (m, 2H), 6.89 – 6.83 (m, 2H), 4.29 – 4.21 (m, 1H), 3.80 (s, 3H), 3.30 (dd, *J* = 13.5, 5.2 Hz, 1H), 2.70 (dd, *J* = 13.5, 8.8 Hz, 1H), 1.94 (dd, *J* = 12.5, 6.7 Hz, 1H), 1.60 (dd, *J* = 12.5, 8.7 Hz, 1H), 1.31 (s, 3H), 1.27 (s, 3H).

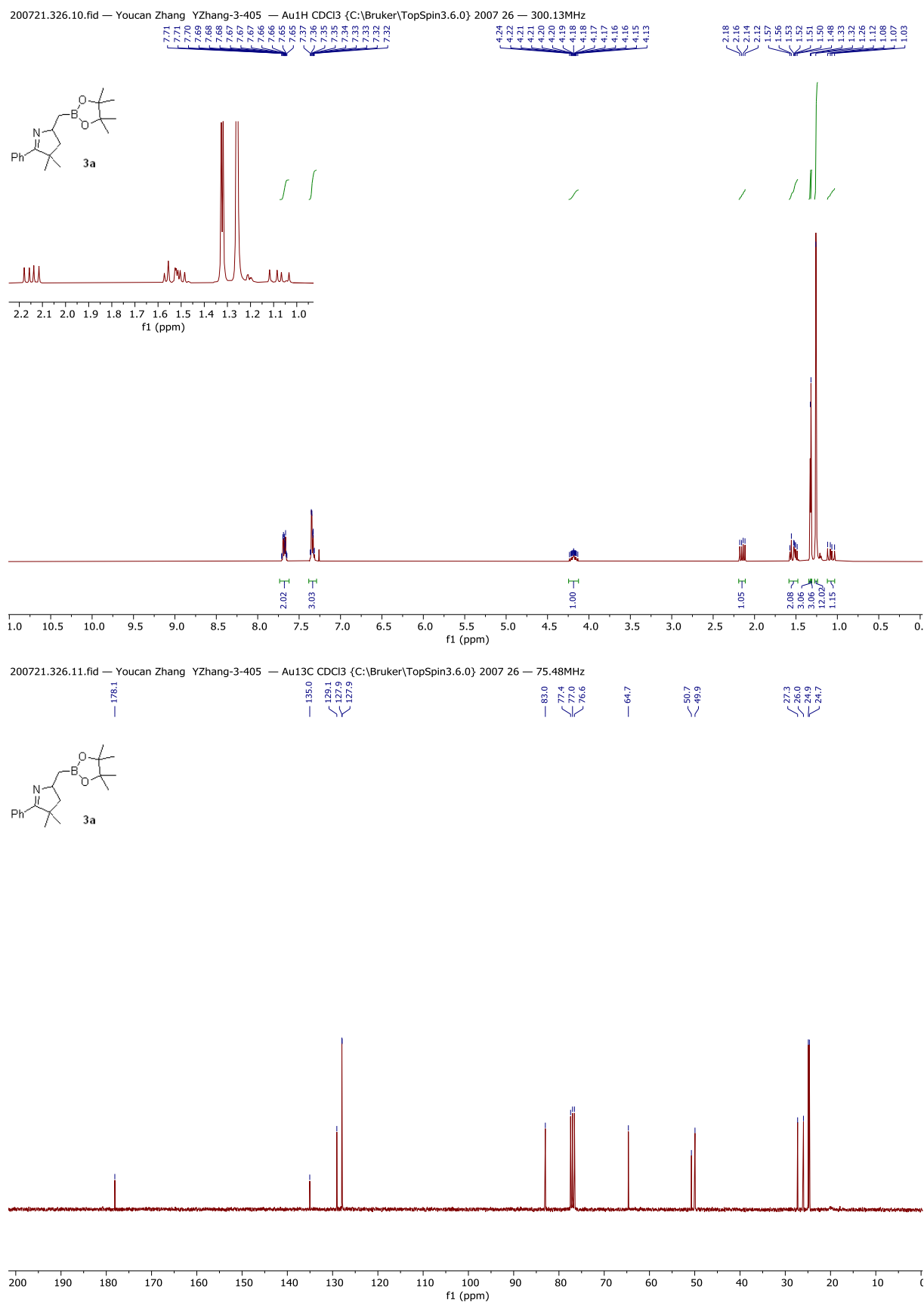
¹³C NMR (101 MHz, CDCl₃) δ 179.4, 158.0, 134.9, 131.6, 130.3, 129.3, 128.1, 127.8, 113.6, 69.5, 55.2, 50.3, 47.3, 41.9, 27.2, 26.0.

HR-MS (ESI-TOF) calcd. for C₂₀H₂₃NO [M+H]⁺: 294.1858; found: 294.1861.

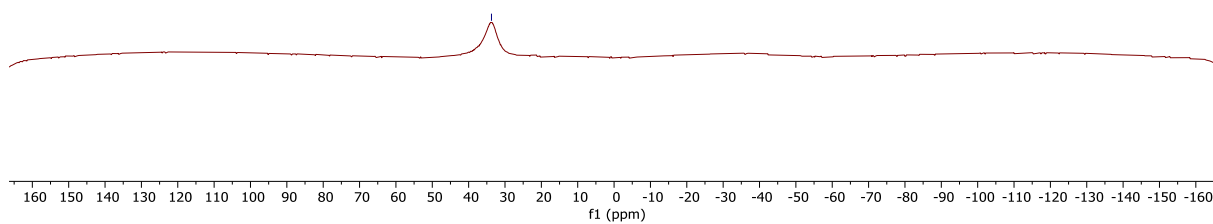
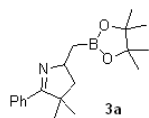
4. Reference

- [1] Liu, R.-H.; Wei, D.; Han, B.; Yu, W. *ACS Catalysis* **2016**, 6, 6525–6530.
- [2] Wang, L.; Wang C. *J. Org. Chem.* **2019**, 84, 6547–6556.
- [3] Zhang, M.; Liu, S.; Li, H.; Guo, Y.; Li, N.; Guan, M.; Mehfooz, H.; Zhao, J.; Zhang, Q. *Chem. Eur. J.* **2019**, 25, 12620–12627.
- [4] Cai, S.-H.; Xie, J.-H.; Song, S.; Ye, L.; Feng, C.; Loh, T.-P. *ACS Catalysis* **2016**, 6, 5571–5574.
- [5] Zhang, Y.; Yin, Y.; Wang H.; Wu, X.-F. *Chem. Commun.* **2020**, 56, 7045–7048.
- [6] Yuan, Y.; Wu, F.-P.; Xu, J.-X.; Wu, X.-F. *Angew. Chem. Int. Ed.* **2020**, 59, 2 – 9
- [7] Du, W.; Zhao, M.-N.; Ren, Z.-H.; Wang, Y.-Y.; Guan, Z.-H. *Chem. Commun.* **2014**, 50, 7437–7439.

5. ^1H -, ^{13}C -, ^{11}B - and ^{19}F -NMR spectra and HR-MS data copy of products



— 33.7



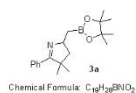
ESI-TOF Accurate Mass Report

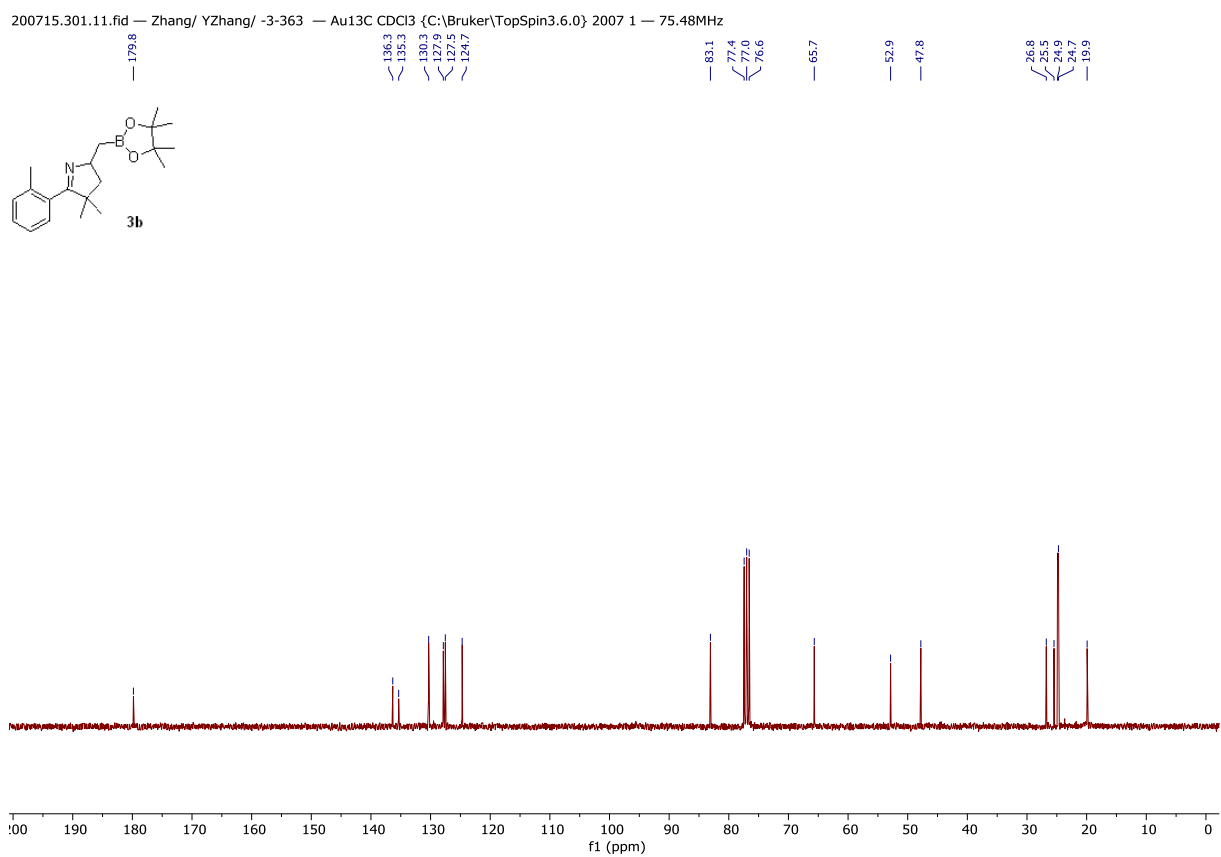
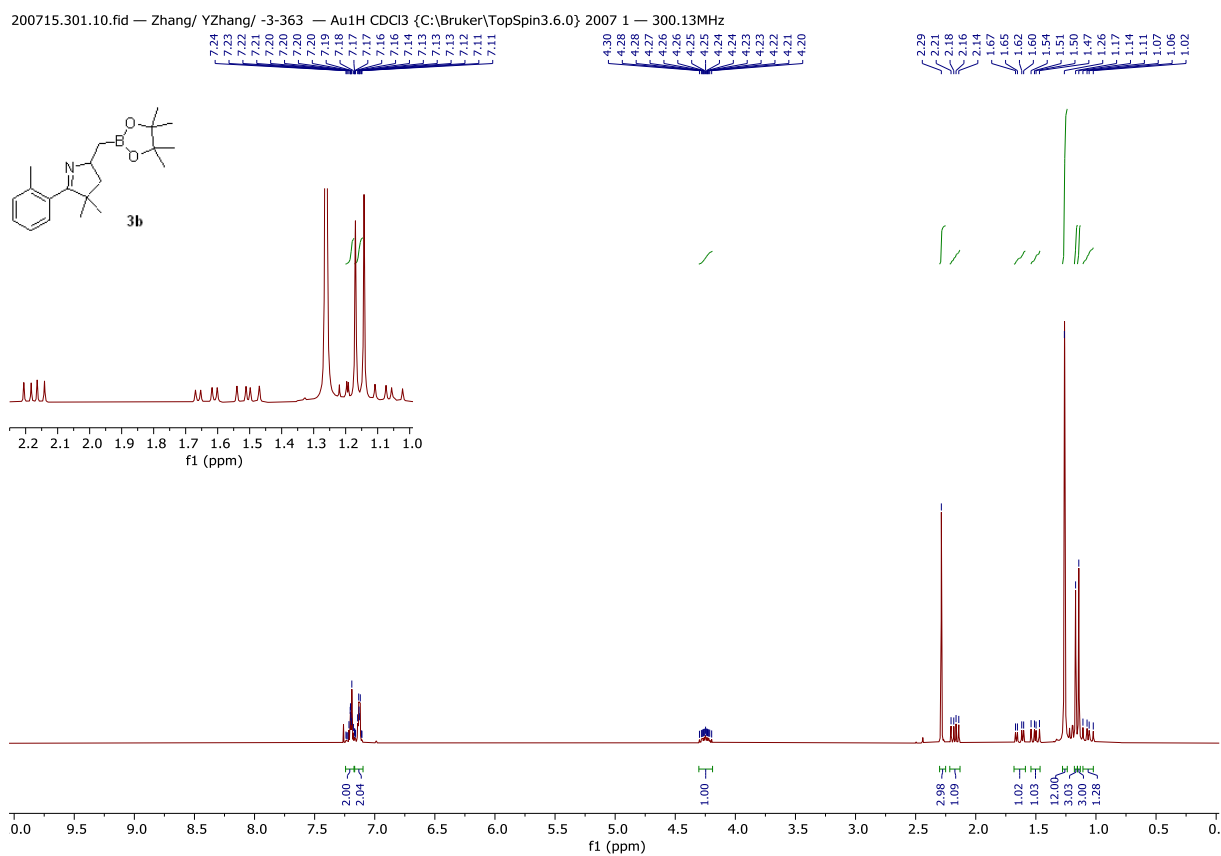
Page 1

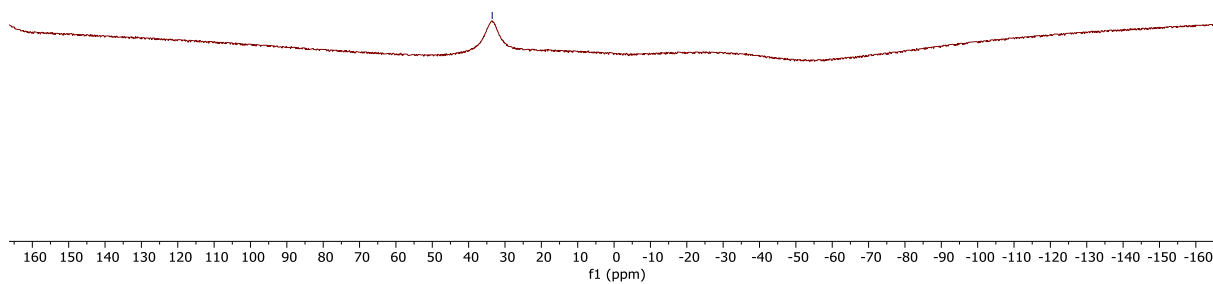
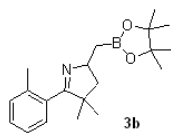
Results file: E:\Projects\2007.PRO\SampleDB\2007.rpt
Last modified: Thursday, July 09, 2020 14:31:26

Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
141	20070910	YZ-137+141	Youcan Zhang	312.2249	C19H28BNO2	313.2328	313.2333	1.6	0.5
				332.1889	C22H24N2O	333.1967	333.1964	-0.9	-0.3

Chemical Formula: C₁₉H₂₈BNO₂





ESI-TOF Accurate Mass Report

File:20080516

Vial:1.F.5

Description:MeOH/0.1% HCOOH in H2O 90:10

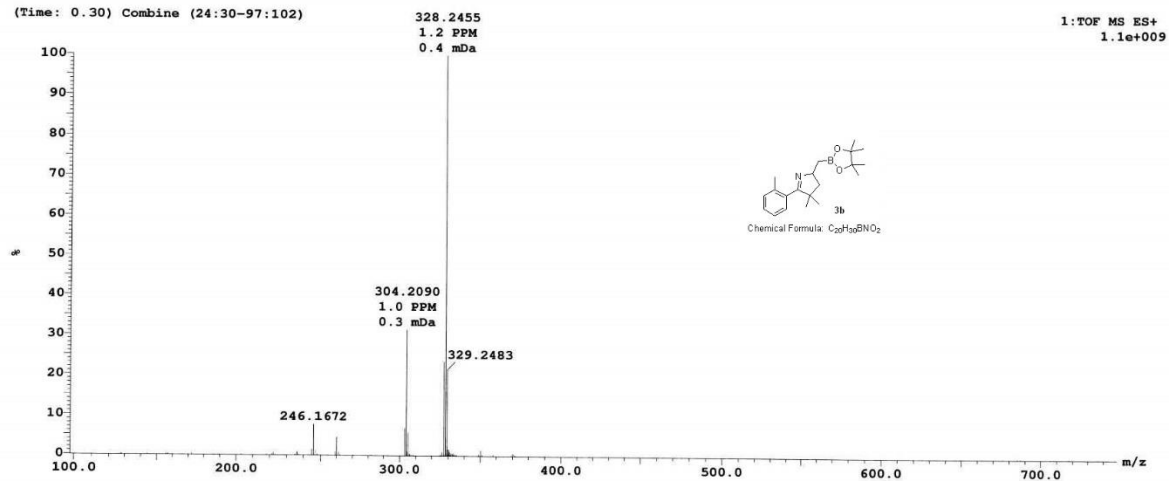
Sample Name:YZ-363+367
Date:05-Aug-2020

UserName:Youcan Zhang
Time:16:33:09

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Sample Report (continued):

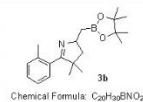
(Time: 0.30) Combine (24:30-97:102)



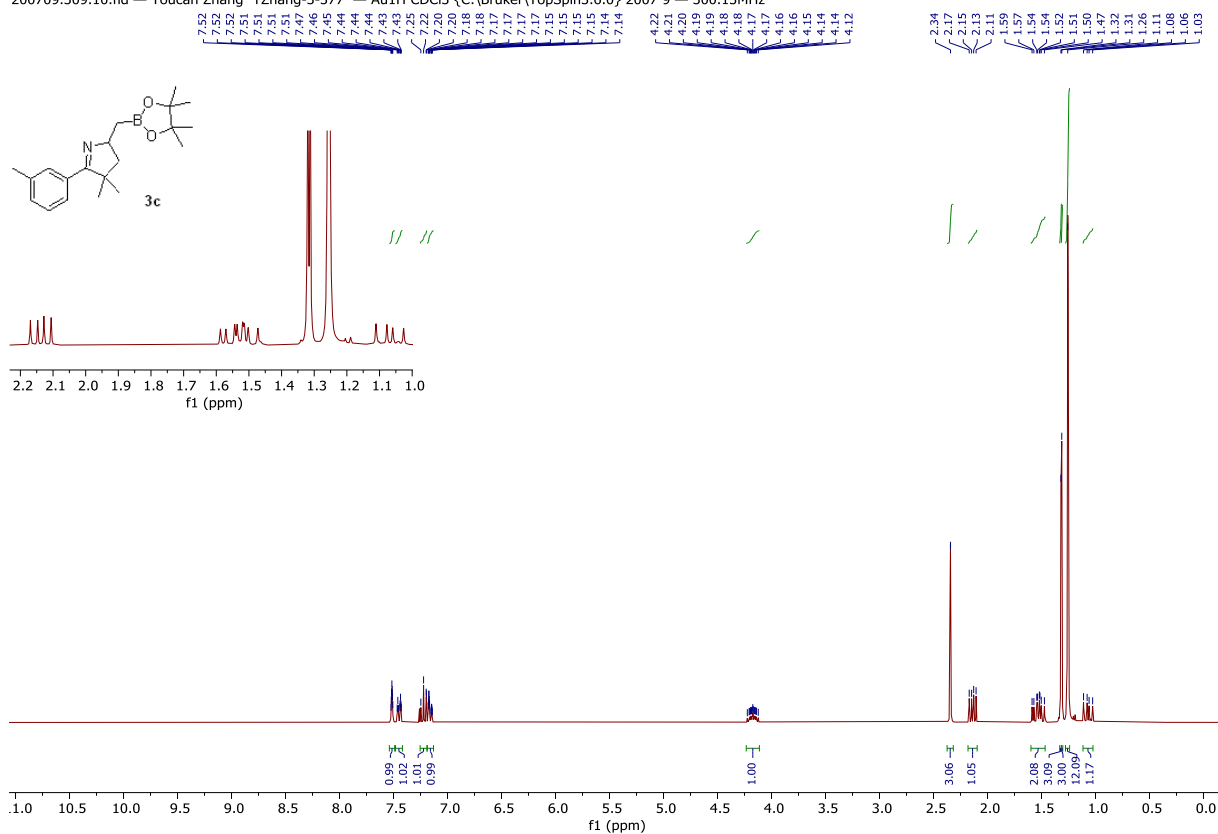
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:35:42

Sample Summary:

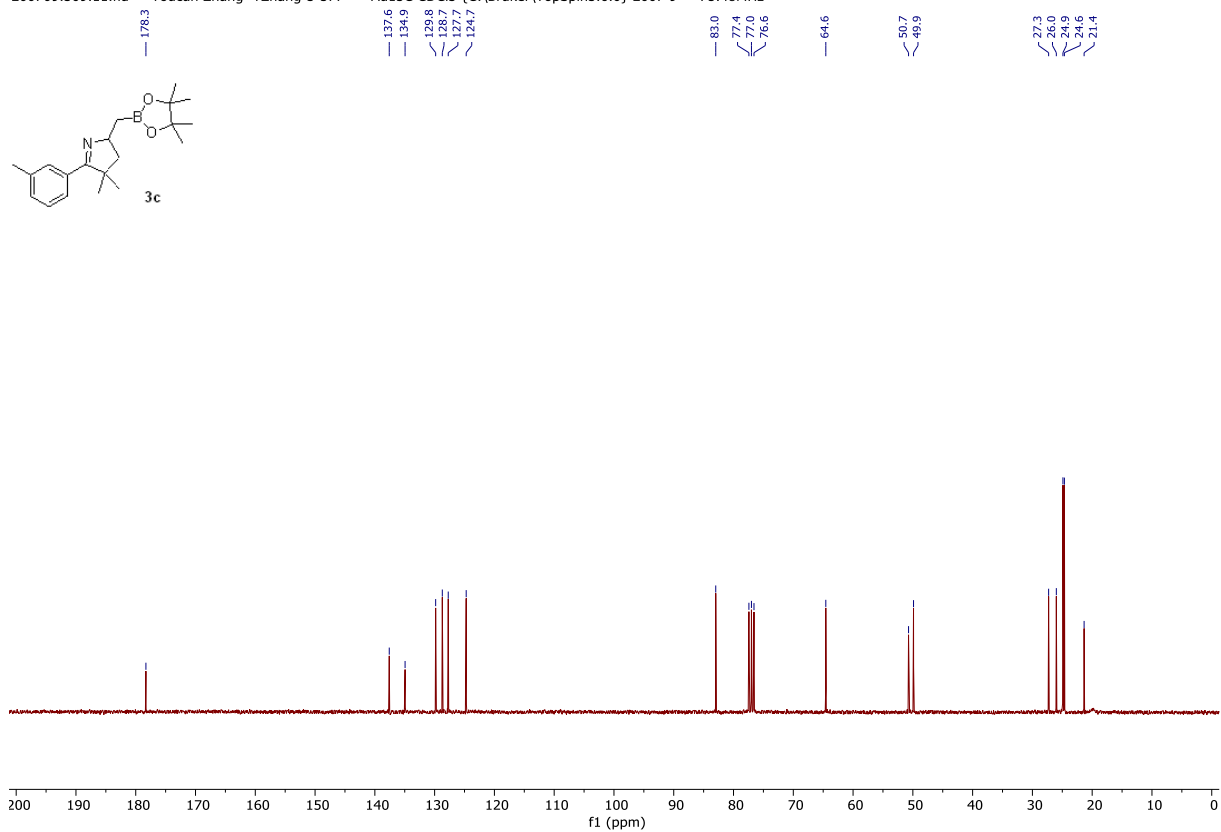
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
80	20080516	YZ-363+367	Youcan Zhang	302.2042	C17H26BNO3	303.2120	303.2122	0.7	0.2
				326.2406	C20H30BNO2	304.2087	304.2091	1.3	0.4
						327.2484	327.2485	0.3	0.1
						328.2451	328.2455	1.2	0.4



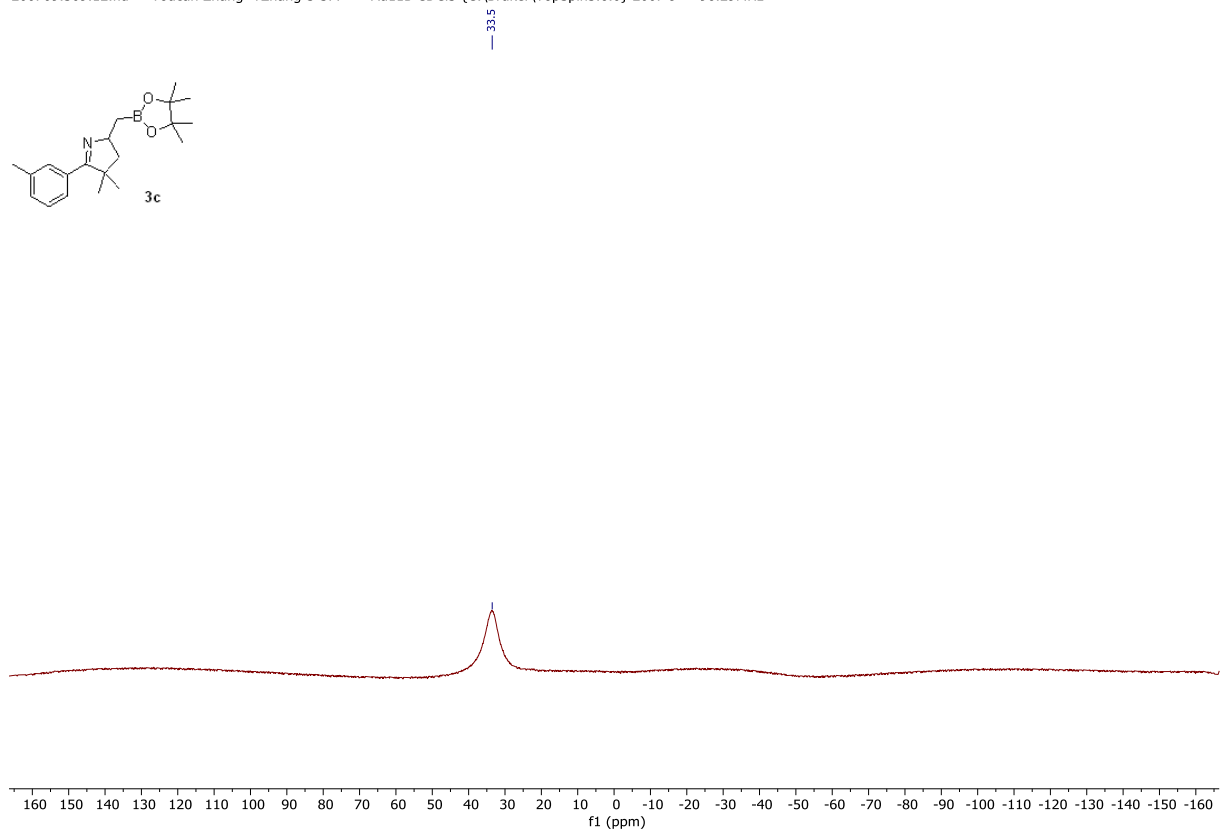
200709.309.10.fid — Youcan Zhang YZhang-3-377 — Au1H CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 9 — 300.13MHz



200709.309.11.fid — Youcan Zhang YZhang-3-377 — Au13C CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 9 — 75.48MHz



200709.309.12.fid — Youcan Zhang YZhang-3-377 — Au11B CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 9 — 96.29MHz



ESI-TOF Accurate Mass Report

File:20080518

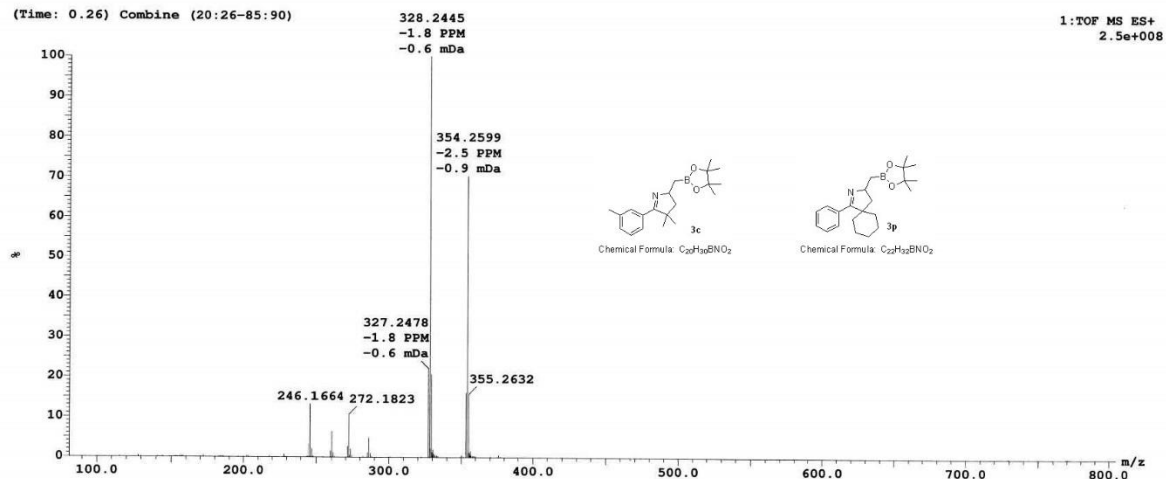
Vial:1:F.7

Description:MeOH/0.1% HCOOH in H₂O 90:10Sample Name:YZ-374+377
Date:05-Aug-2020UserName:Youcan Zhang
Time:16:58:58

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Sample Report:

(Time: 0.26) Combine (20:26-85:90)



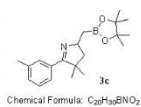
ESI-TOF Accurate Mass Report

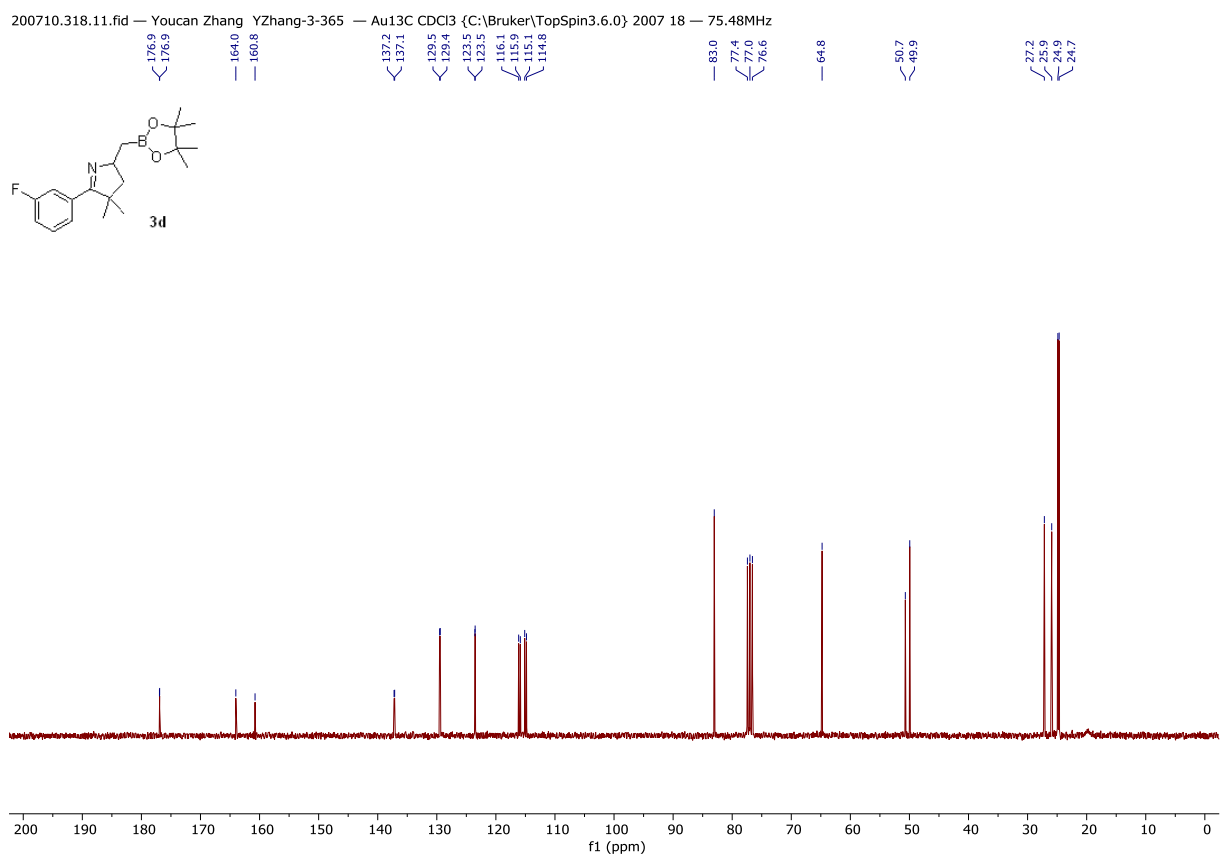
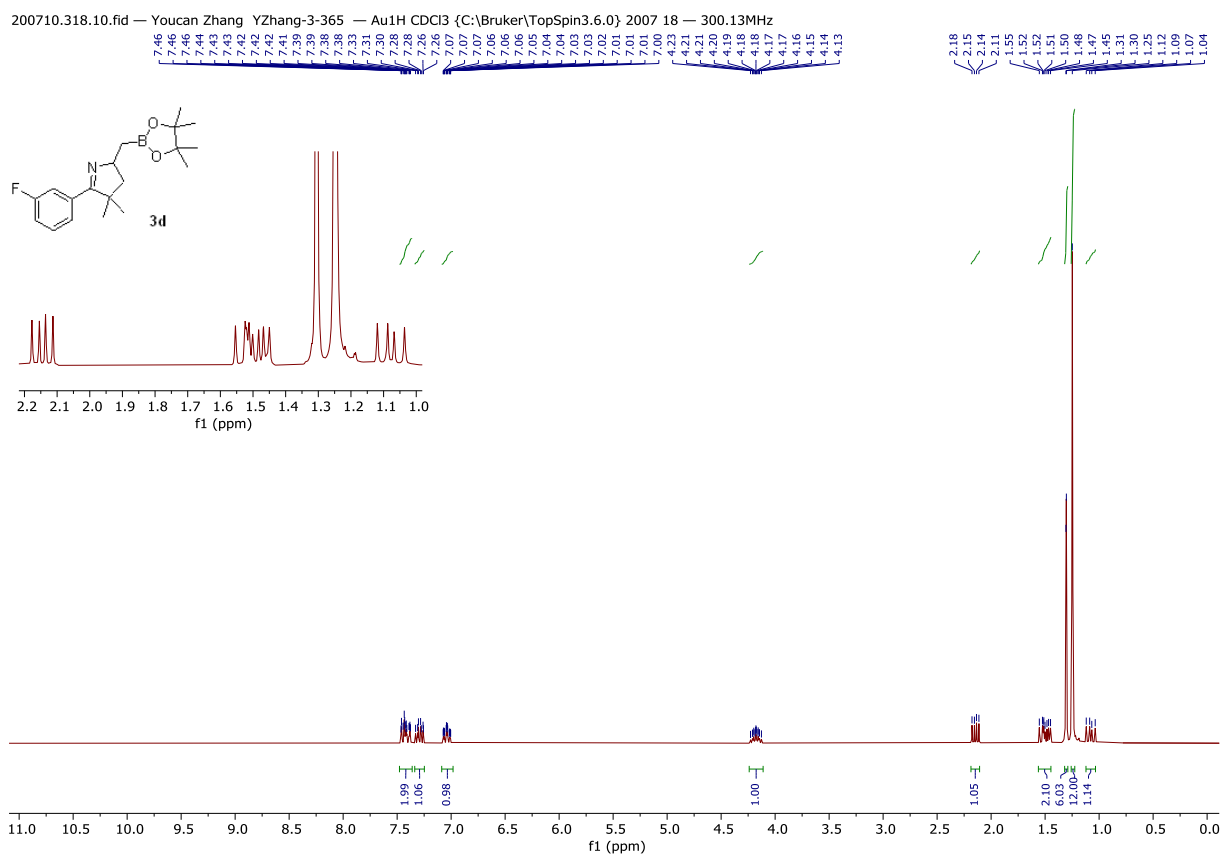
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 17:01:26

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Sample Summary:

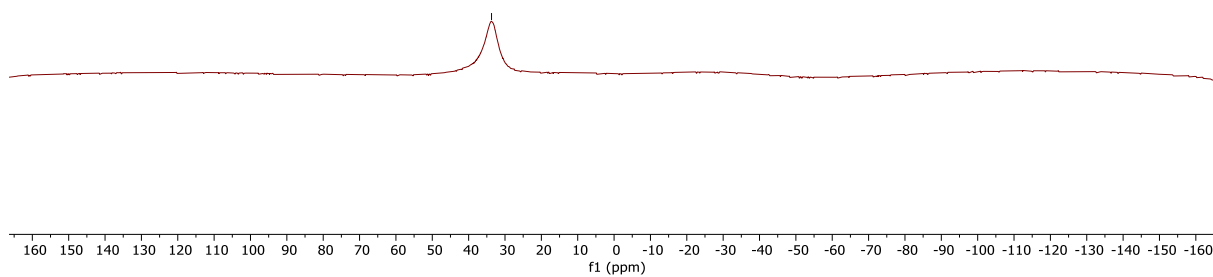
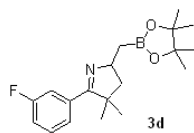
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
82	20080518	YZ-374+377	Youcan Zhang	326.2406	C20H30BNO2	327.2484	327.2478	-1.8	-0.6
				352.2563	C22H32BNO2	328.2451	328.2445	-1.8	-0.6
						353.2641	353.2631	-2.8	-1.0
						354.2608	354.2599	-2.5	-0.9





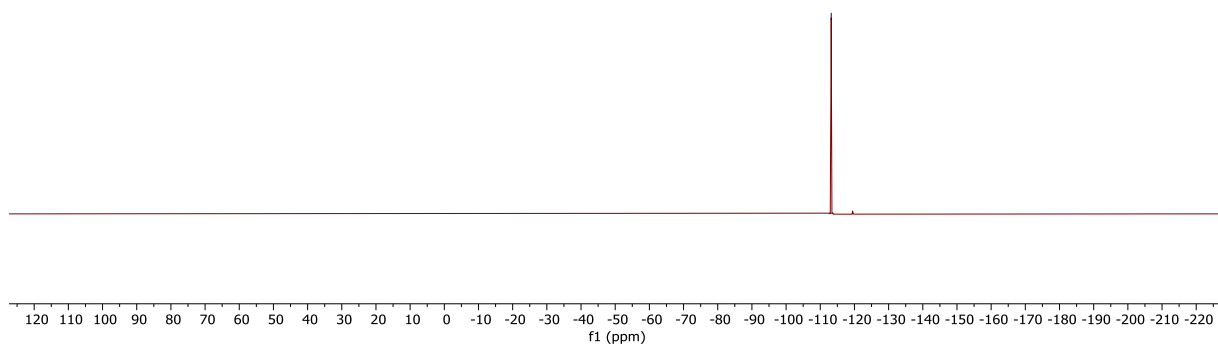
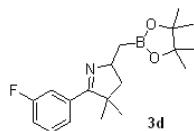
200710.318.12.fid — Youcan Zhang YZhang-3-365 — Au11B CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 18 — 96.29MHz

— 33.7



200713.322.10.fid — Youcan Zhang YZhang-3-365 — Au19F CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 22 — 282.39MHz

— -113.2



ESI-TOF Accurate Mass Report

File:20080515

Vial:1:F,4

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-365+372

Date:05-Aug-2020

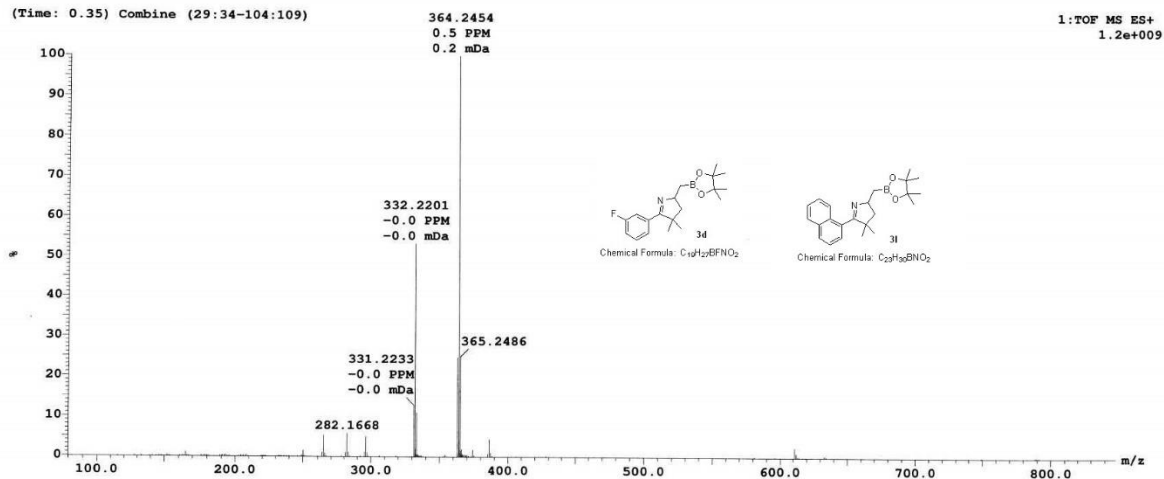
UserName:Youcan Zhang

Time:16:30:35

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Sample Report (continued):

(Time: 0.35) Combine (29:34-104:109)



ESI-TOF Accurate Mass Report

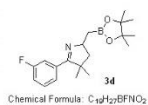
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt

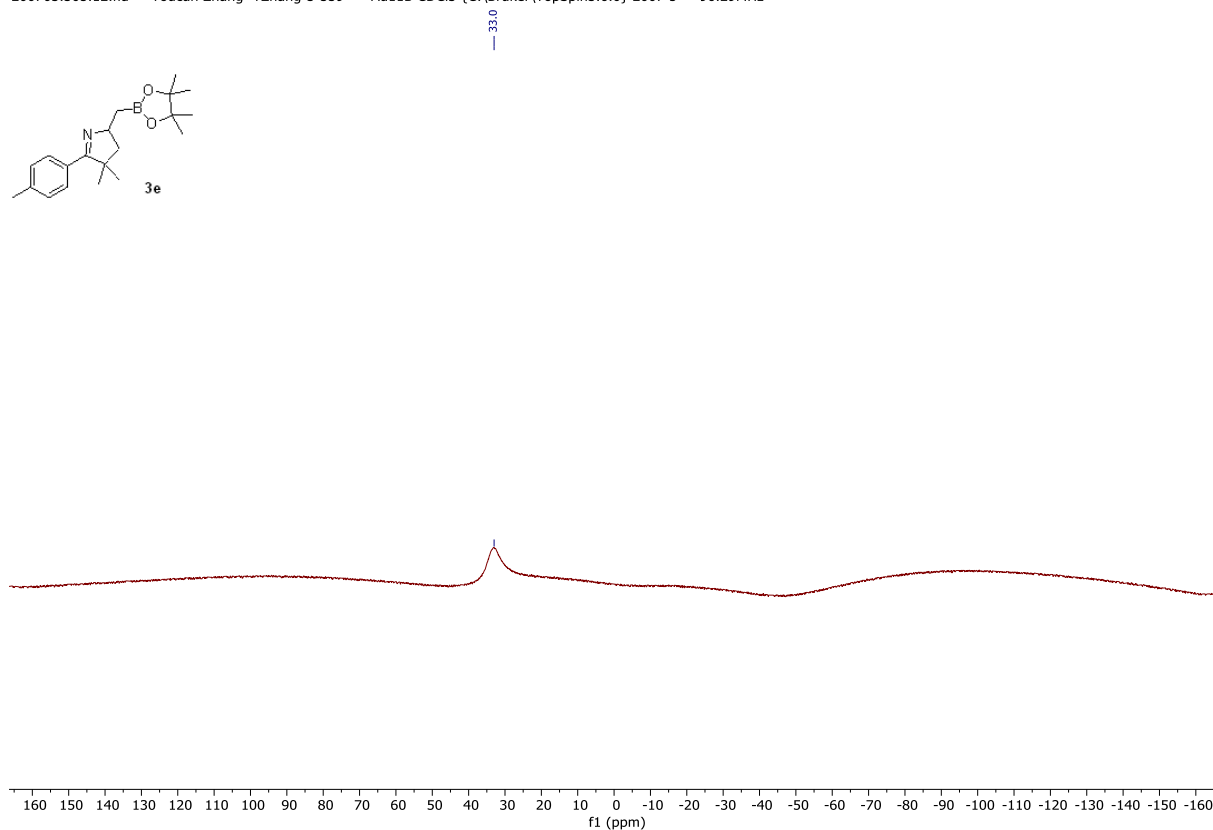
Last modified: Wednesday, August 05, 2020 16:33:07

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Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
79	20080515	YZ-365+372	Youcan Zhang	330.2155	<u>C19H27BNO2F</u>	331.2233	331.2233	0.0	0.0
				362.2406	C23H30BNO2	332.2201	332.2201	0.0	0.0
						363.2484	363.2484	0.0	0.0
						364.2452	364.2454	0.5	0.2





ESI-TOF Accurate Mass Report

File:20080510
Vial:1.E.7
Description:MeOH/0.1% HCOOH in H2O 90:10

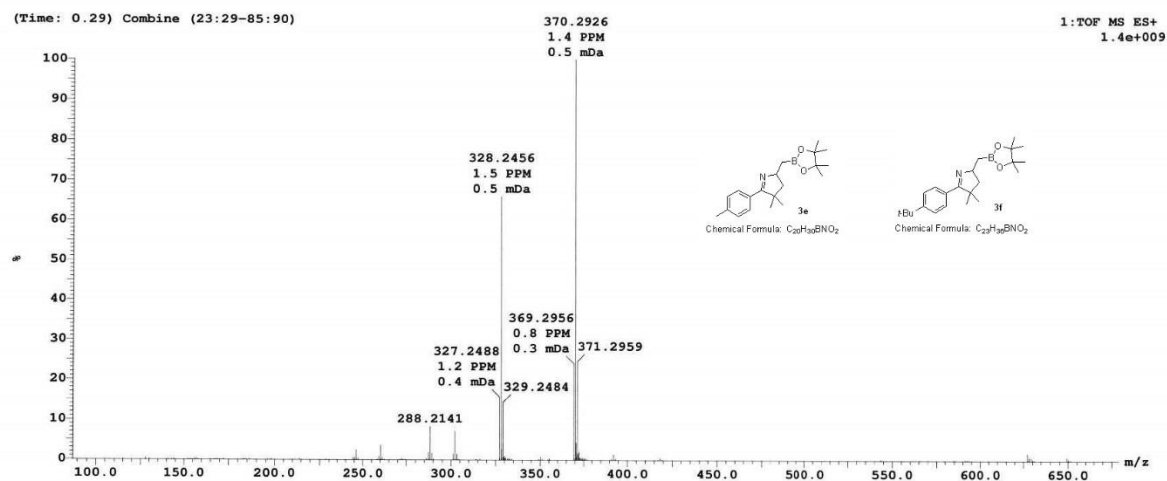
Sample Name:YZ-339+340
Date:05-Aug-2020

UserName:Youcan Zhang
Time:15:29:10

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Sample Report (continued):

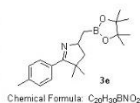
(Time: 0.29) Combine (23:29-85:90)



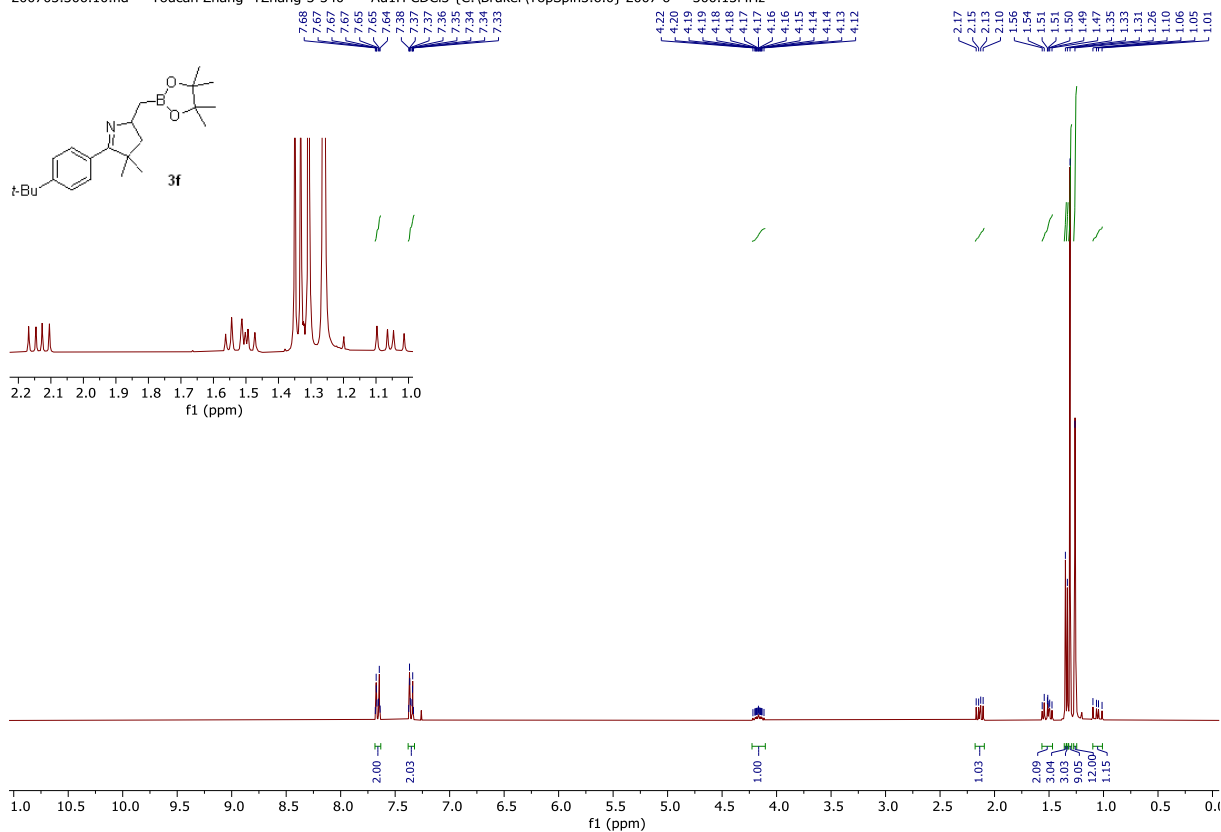
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:10:24

Sample Summary:

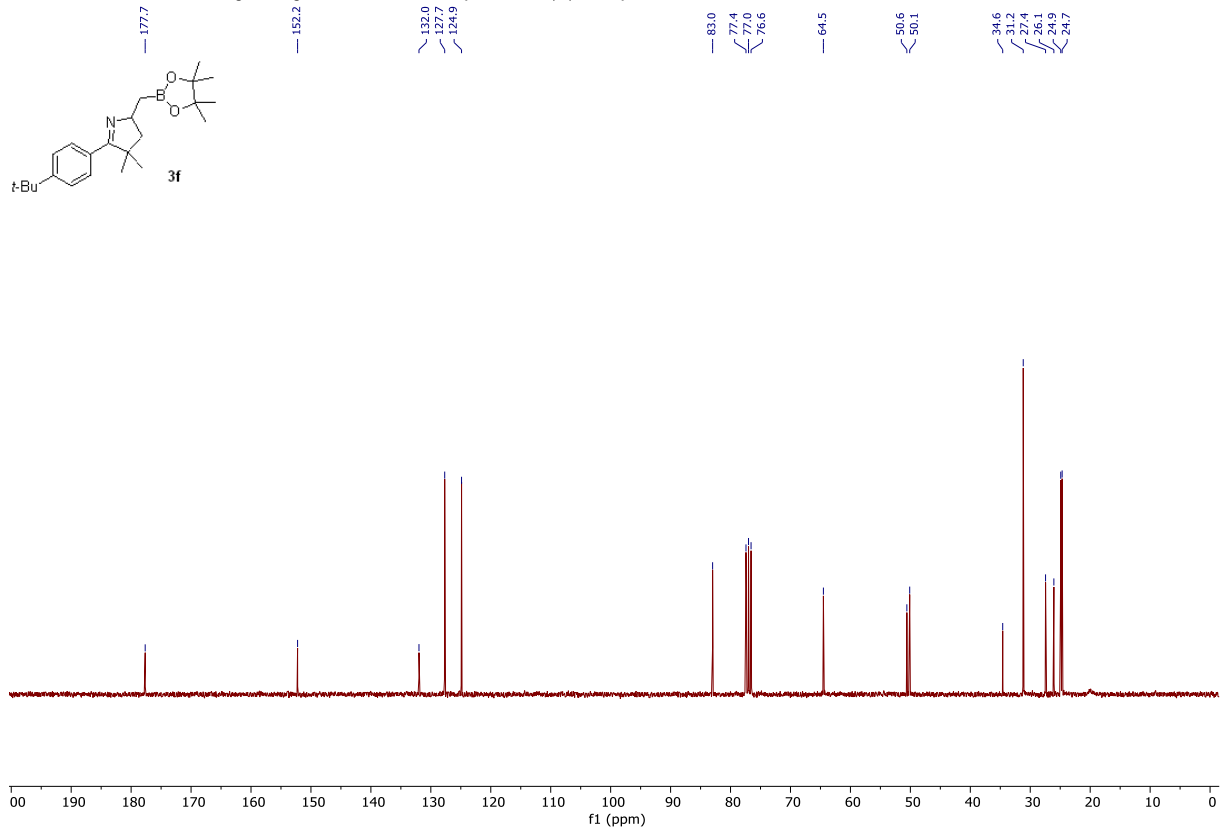
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
74	20080510	YZ-339+340	Youcan Zhang	326.2406	C20H30BNO2	327.2484	327.2487	0.9	0.3
						328.2451	328.2456	1.5	0.5
				368.2875	C23H36BNO2	369.2953	369.2956	0.8	0.3
						370.2921	370.2926	1.4	0.5



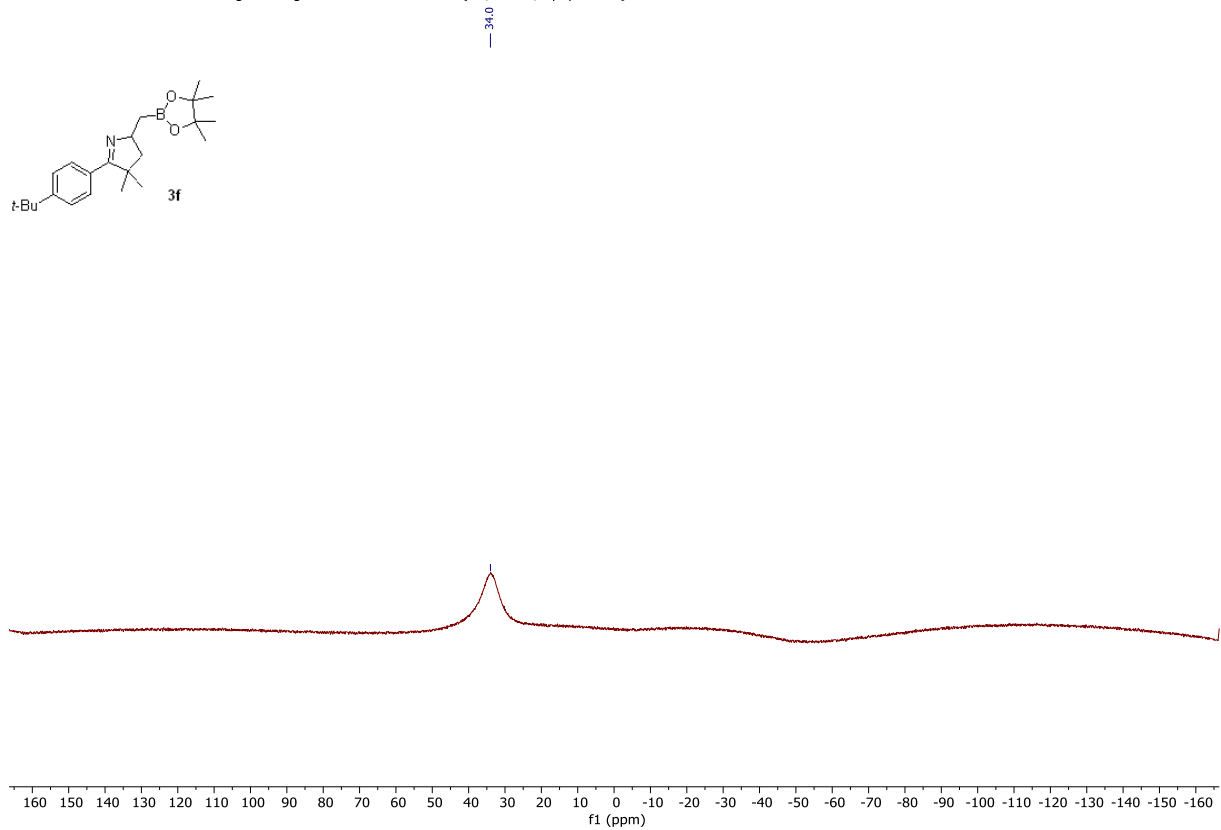
200703.306.10.fid — Youcan Zhang YZhang-3-340 — Au1H CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 6 — 300.13MHz



200703.306.11.fid — Youcan Zhang YZhang-3-340 — Au13C CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 6 — 75.48MHz



200703.306.12.fid — Youcan Zhang YZhang-3-340 — Au11B CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 6 — 96.29MHz



ESI-TOF Accurate Mass Report

File: 20080510

Vial: 1.E.7

Description: MeOH/0.1% HCOOH in H₂O 90:10

Sample Name: YZ-339+340

Date: 05-Aug-2020

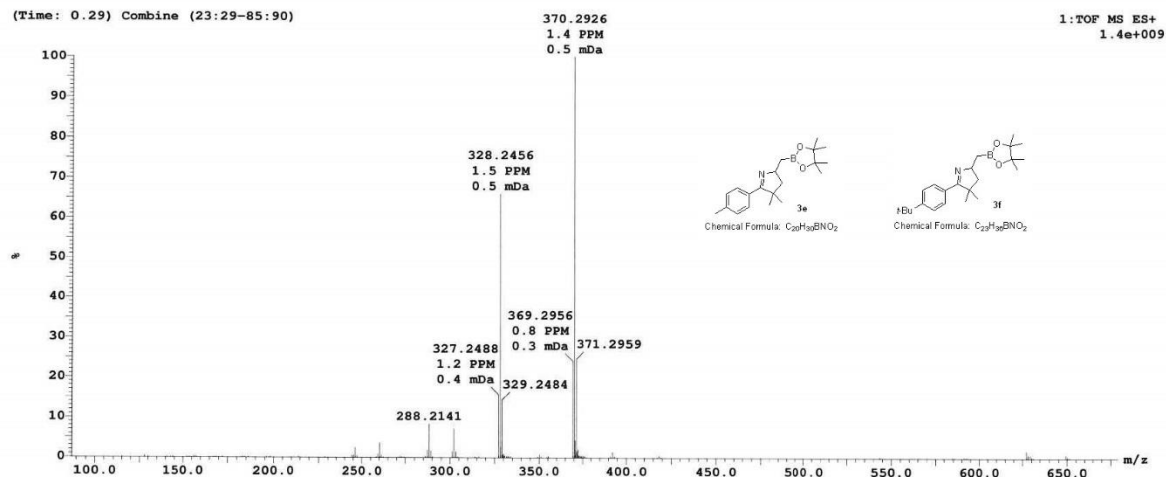
UserName: Youcan Zhang

Time: 15:29:10

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Sample Report (continued):

(Time: 0.29) Combine (23:29-85:90)



ESI-TOF Accurate Mass Report

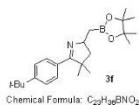
Page 1

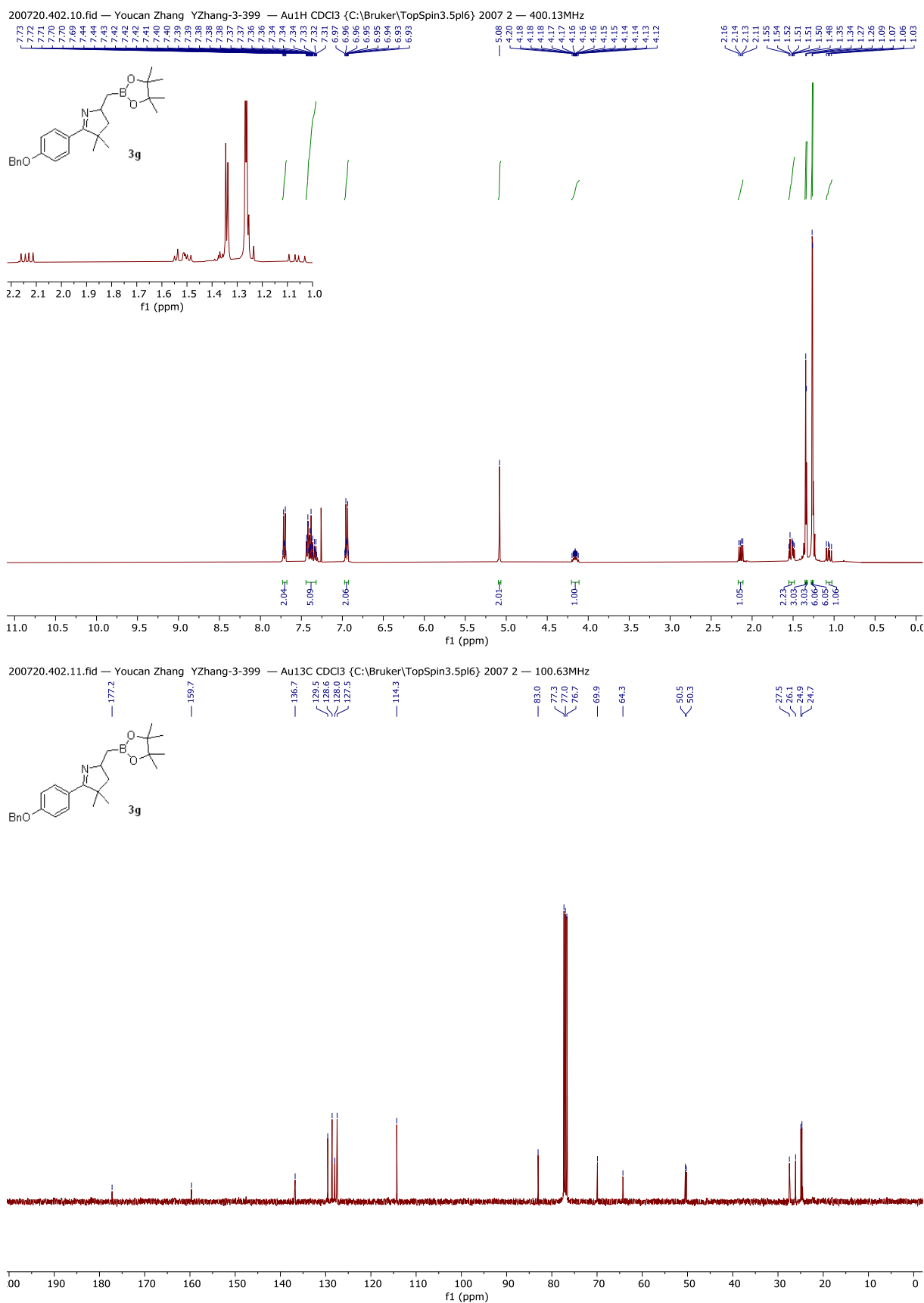
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt

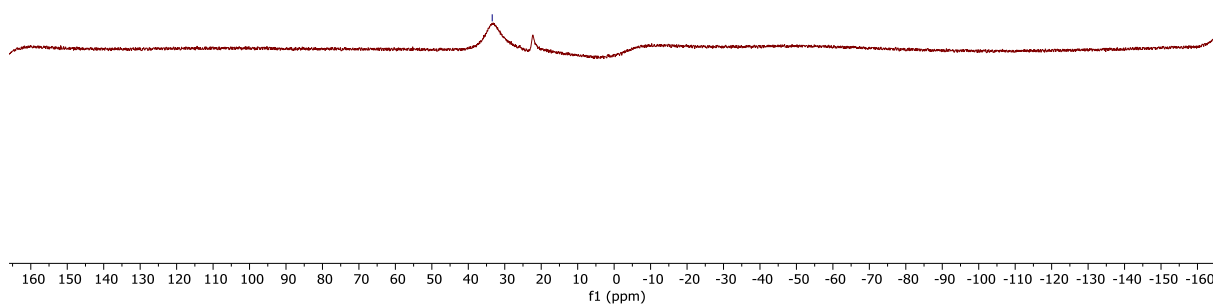
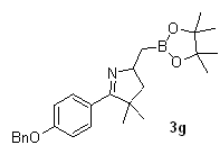
Last modified: Wednesday, August 05, 2020 16:10:24

Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
74	20080510	YZ-339+340	Youcan Zhang	326.2406	C ₂₀ H ₃₀ BNO ₂	327.2484	327.2487	0.9	0.3
				368.2875	C ₂₃ H ₃₆ BNO ₂	369.2953	369.2956	0.8	0.3
						370.2921	370.2926	1.4	0.5







ESI-TOF Accurate Mass Report

File:20080509
Vial:1.E.6
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-399
Date:05-Aug-2020

UserName:Youcan Zhang
Time:15:26:36

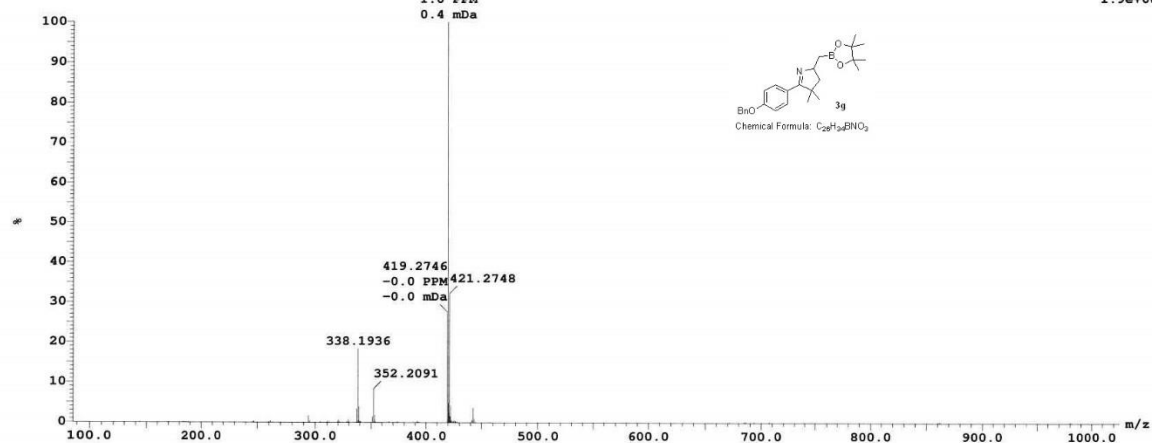
Page 2

Sample Report:

(Time: 0.27) Combine (21:27-89:94)

420.2719
1.0 PPM
0.4 mDa

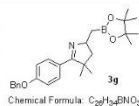
1:TOF MS ES+
1.9e+009



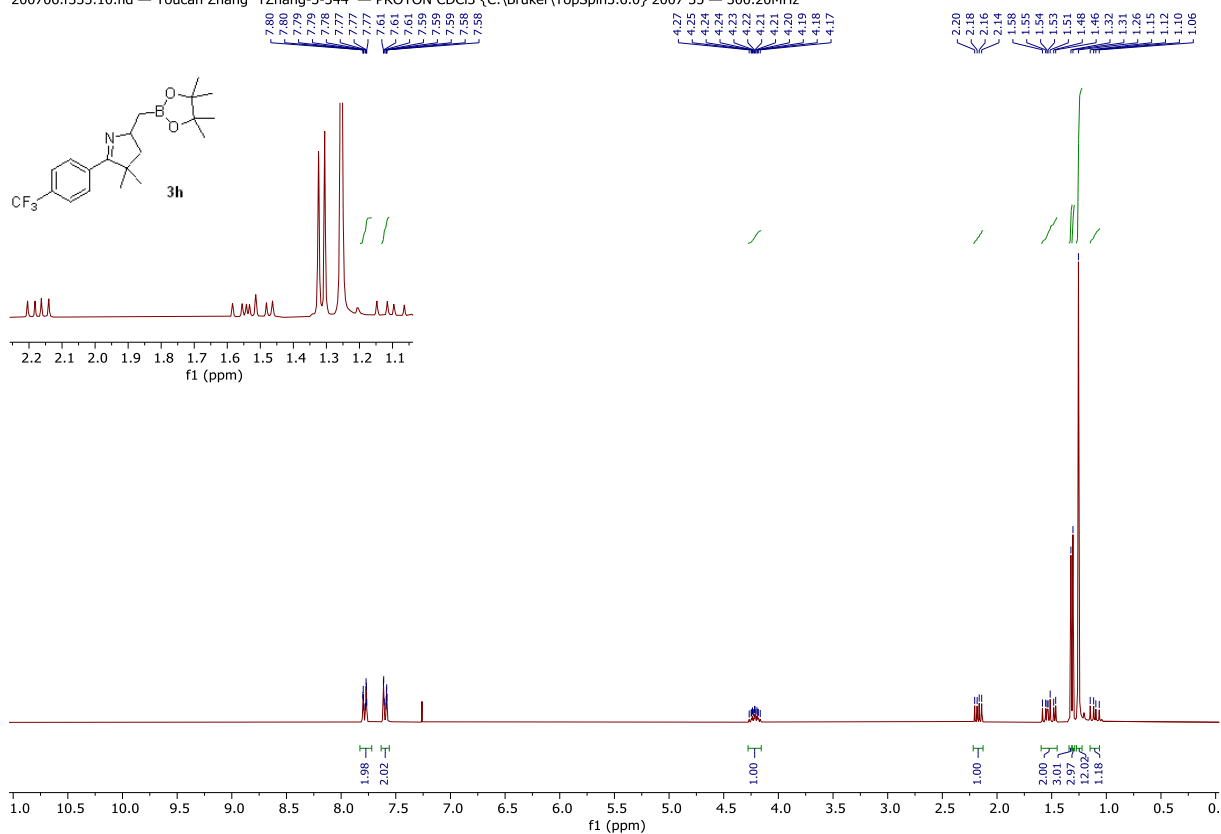
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:09:45

Sample Summary:

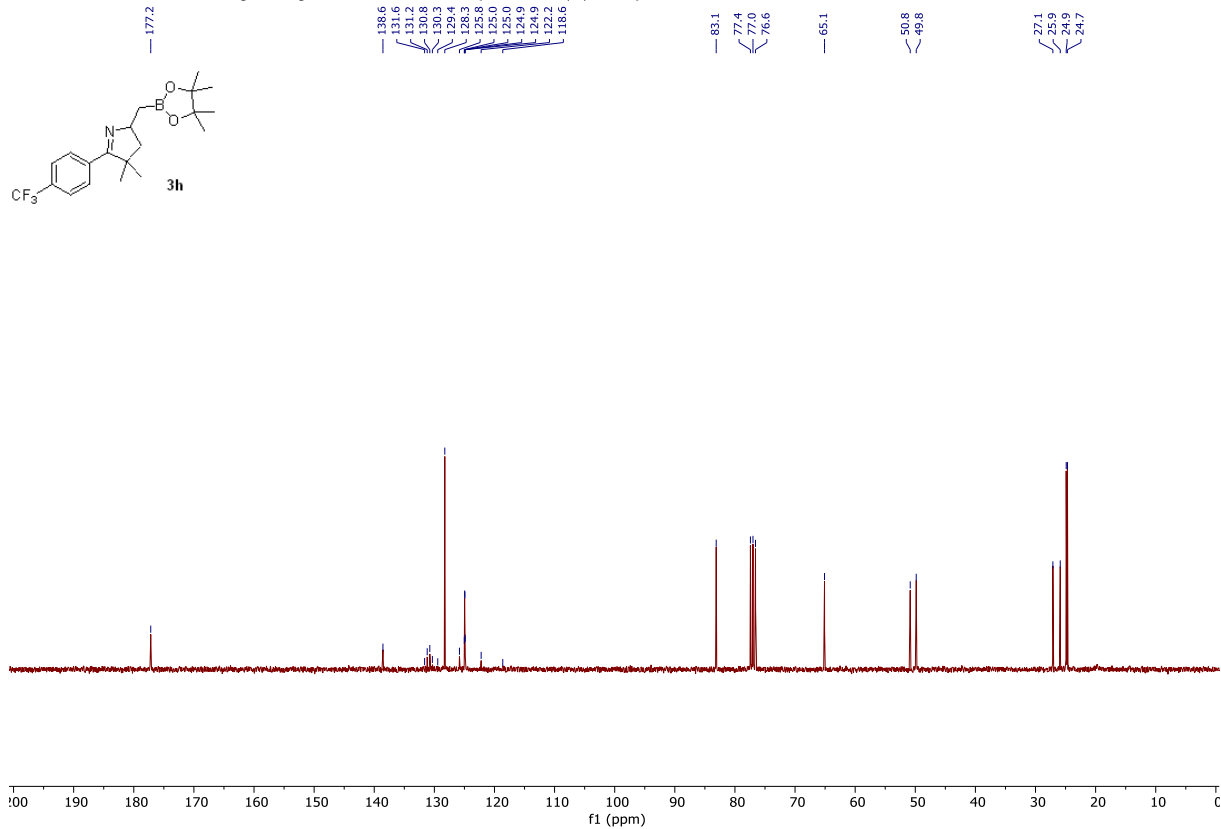
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
73	20080509	YZ-399	Youcan Zhang	418.2668	C ₂₆ H ₃₄ BN ₃ O ₃	419.2746 420.2715	419.2746 420.2719	0.0 1.0	0.0 0.4



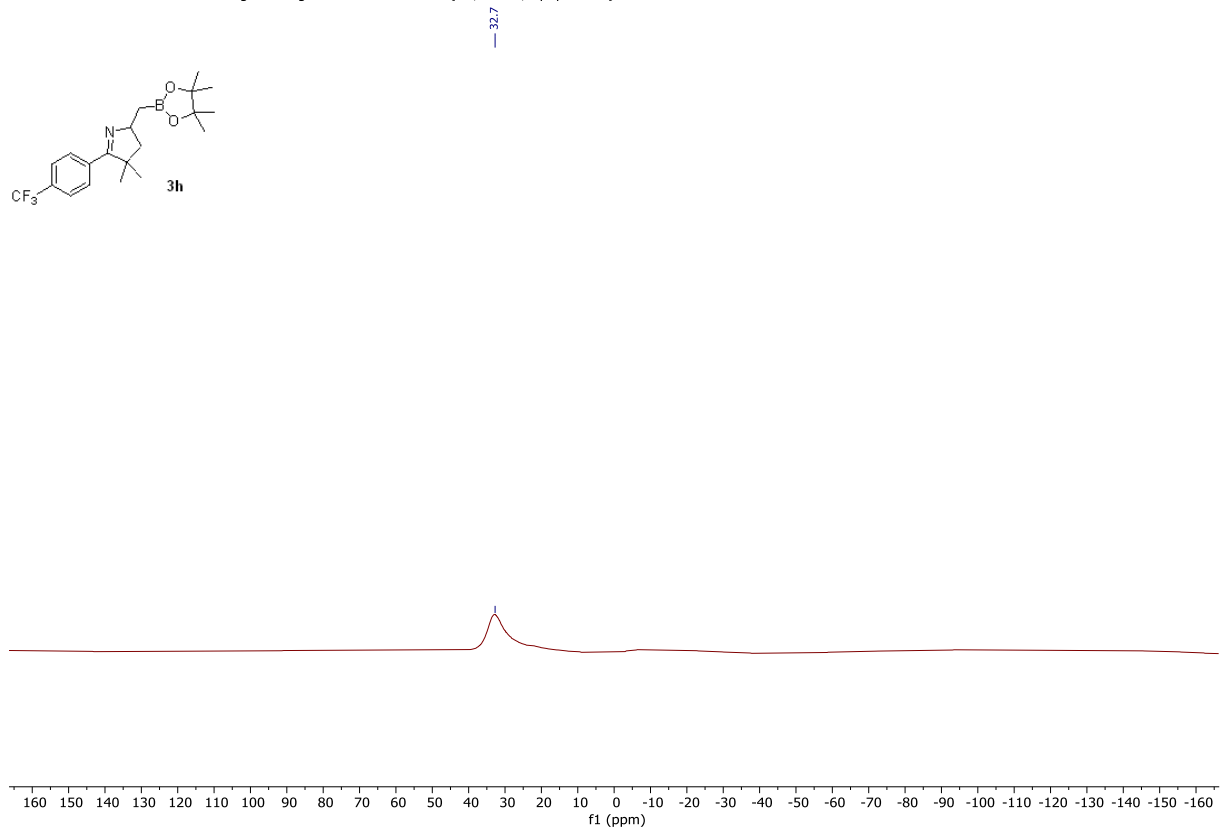
200706.f335.10.fid — Youcan Zhang YZhang-3-344 — PROTON CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 35 — 300.20MHz

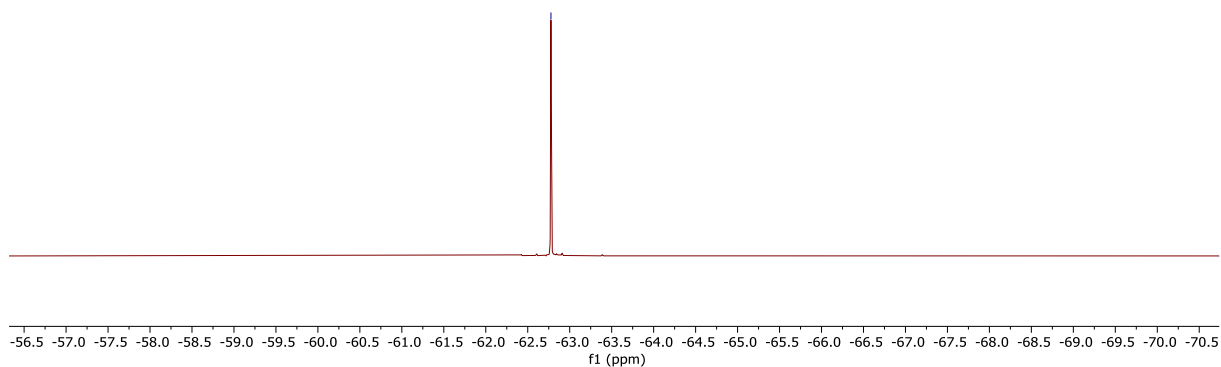
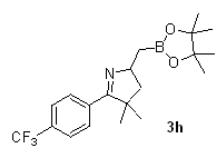


200706.f335.11.fid — Youcan Zhang YZhang-3-344 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2007 35 — 75.49MHz



200706.f335.12.fid — Youcan Zhang YZhang-3-344 — 11B CDCl3 {C:\Bruker\TopSpin3.6.0} 2007 35 — 96.32MHz





ESI-TOF Accurate Mass Report

File:20080511
Vial:1.E.8
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-343+344
Date:05-Aug-2020

UserName:Youcan Zhang
Time:16:13:49

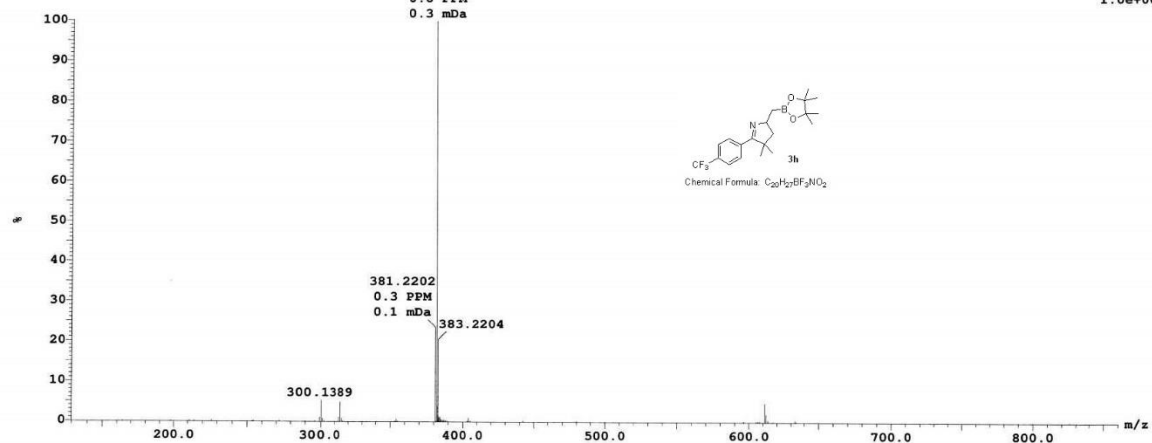
Page 3

Sample Report (continued):

(Time: 0.41) Combine (34:40-104:109)

382.2172
0.8 PPM
0.3 mDa

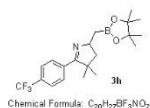
1:TOF MS ES+
1.0e+009



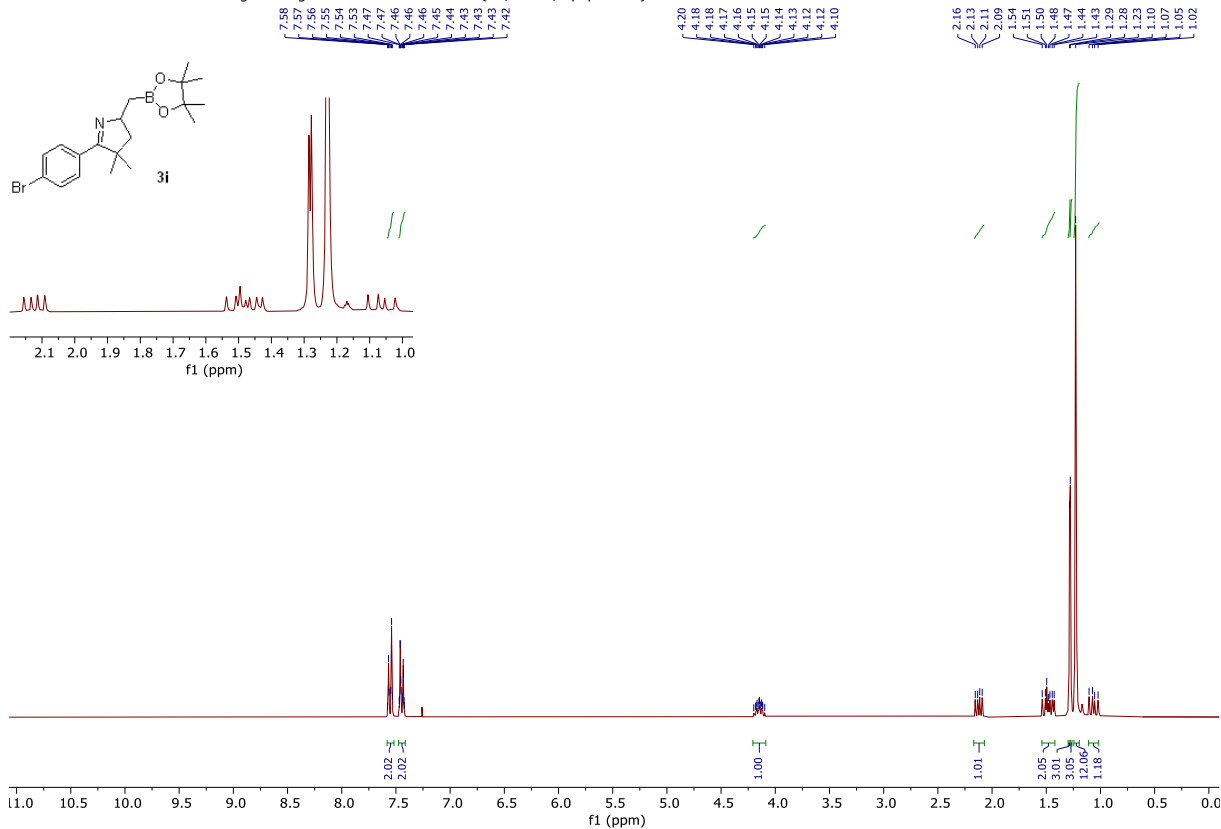
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:16:22

Sample Summary:

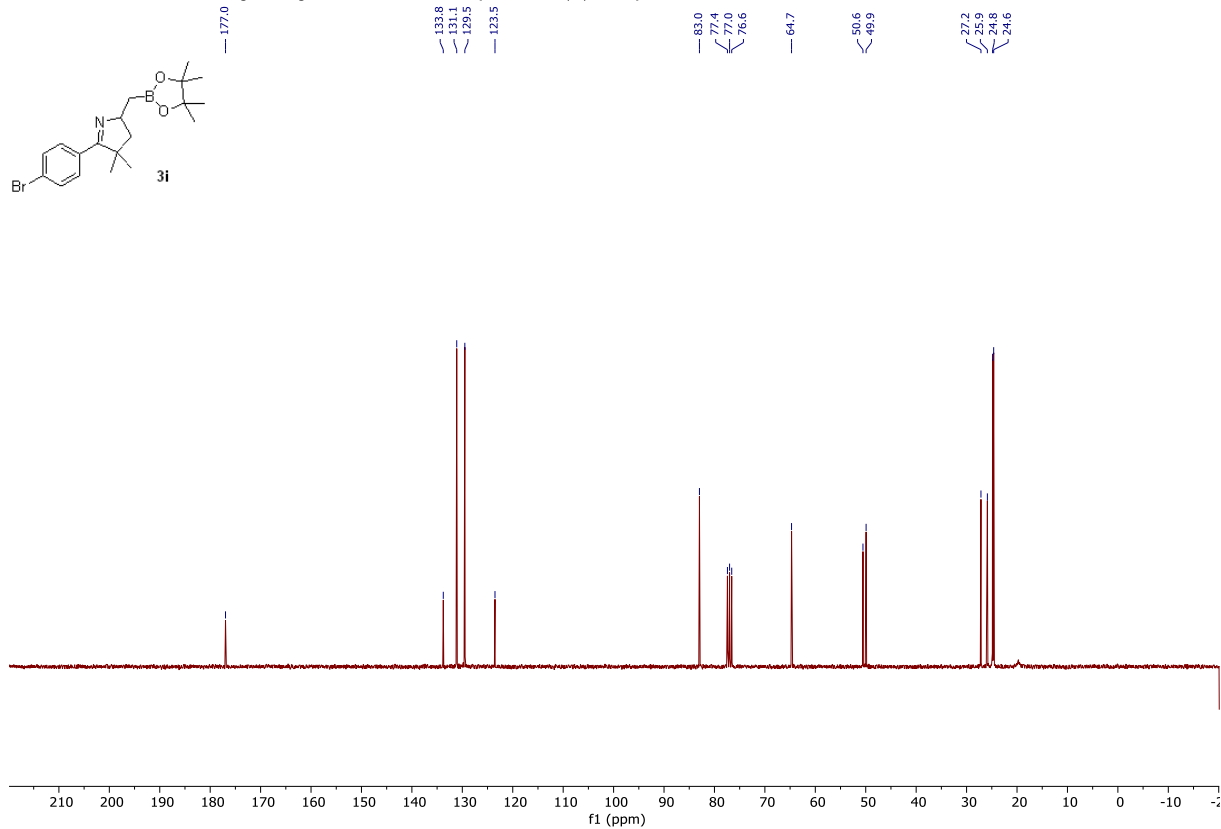
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
75	20080511	YZ-343+344	Youcan Zhang	352.2563	C22H32BNO2	353.2641	353.2639	-0.6	-0.2
				380.2123	C20H27BNO2F3	381.2201	381.2202	0.3	0.1
						382.2169	382.2172	0.8	0.3



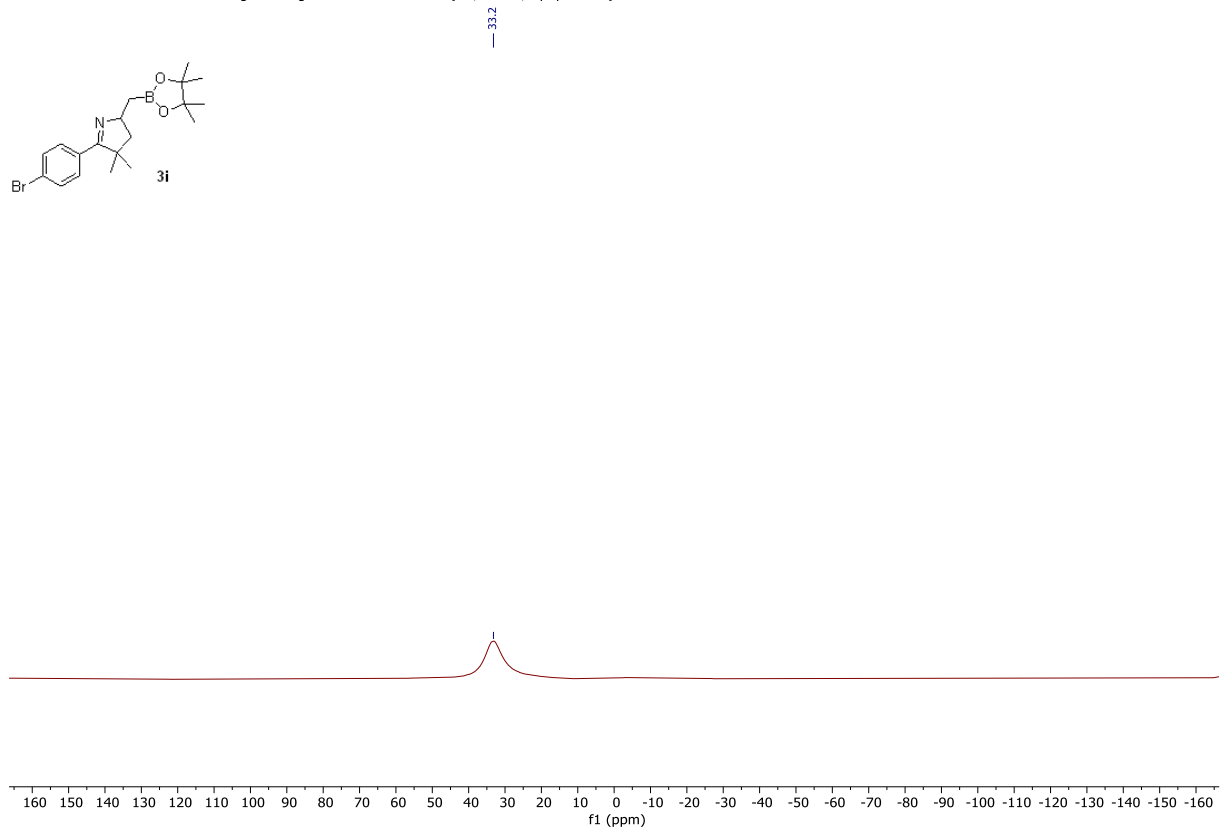
200706.f334.10.fid — Youcan Zhang YZhang-3-345 — PROTON CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 34 — 300.20MHz



200706.f334.11.fid — Youcan Zhang YZhang-3-345 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2007 34 — 75.49MHz



200706.f334.12.fid — Youcan Zhang YZhang-3-345 — 11B CDCl3 {C:\Bruker\TopSpin3.6.0} 2007 34 — 96.32MHz



ESI-TOF Accurate Mass Report

File:20080512

Vial:1.F.1

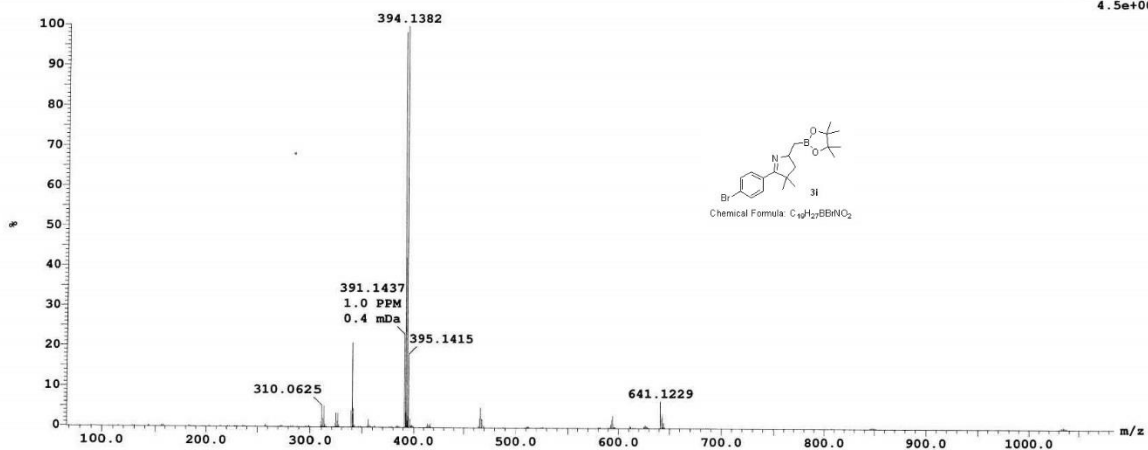
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-342+345
Date:05-Aug-2020UserName:Youcan Zhang
Time:16:19:39

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Sample Report (continued):

(Time: 0.33) Combine (27:33-95:99)

1:TOF MS ES+
4.5e+008

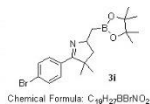
ESI-TOF Accurate Mass Report

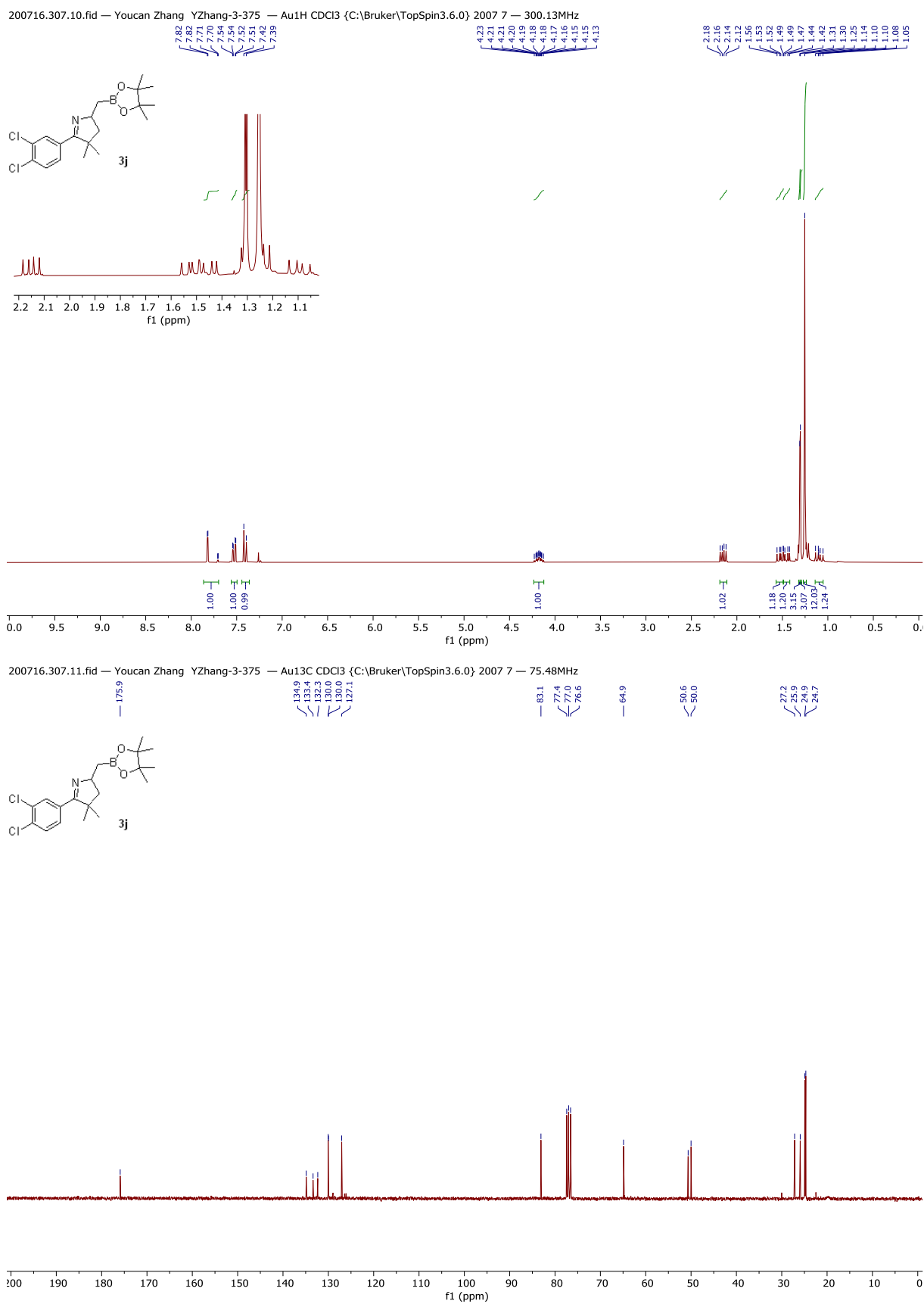
Page 1

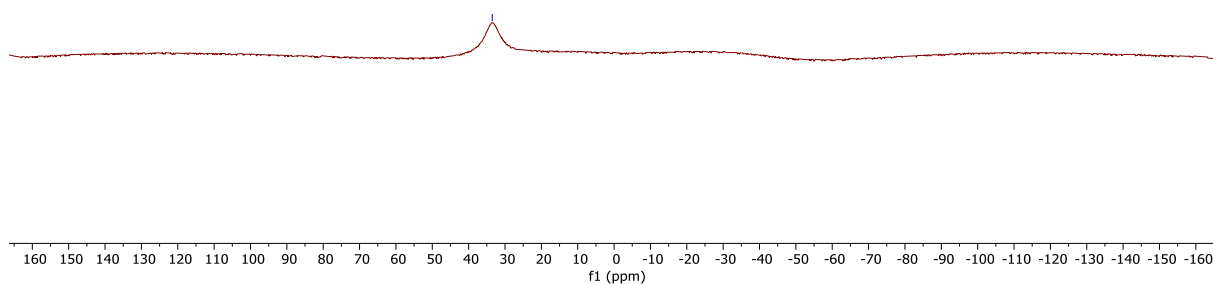
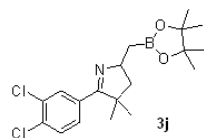
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:22:11

Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
76	20080512	YZ-342+345	Youcan Zhang	338.2406	C ₂₁ H ₃₀ BN ₂ O ₂	339.2484 340.2451	339.2489 340.2457	1.5 1.8	0.5 0.6
				390.1355	C ₁₉ H ₂₇ BN ₂ O ₂ Br	391.1433 392.1400	391.1437 392.1406	1.0 1.5	0.4 0.6







ESI-TOF Accurate Mass Report

File:20080507
Vial:1:E.4
Description:MeOH/0.1% HCOOH in H2O 90:10

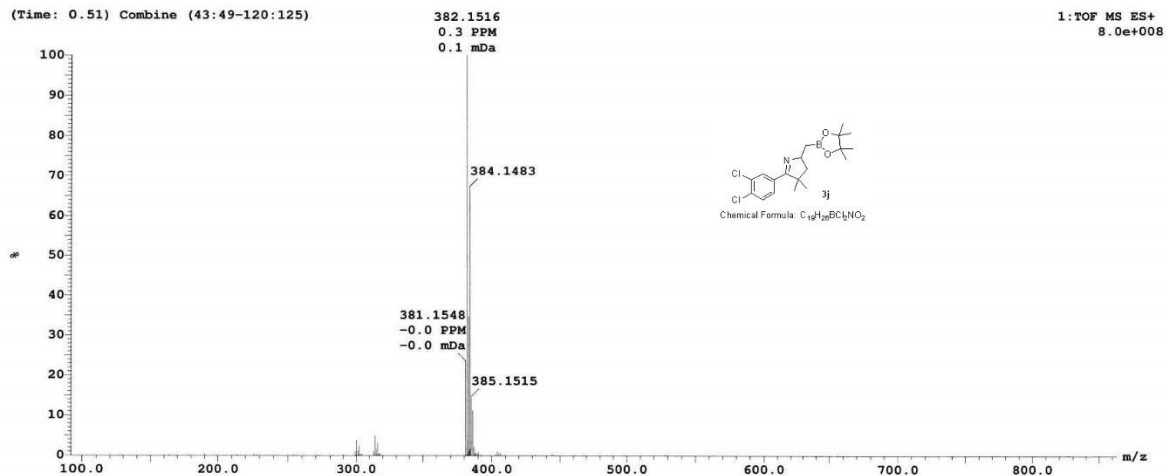
Sample Name:YZ-375
Date:05-Aug-2020

UserName:Youcan Zhang
Time:15:21:28

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Sample Report:

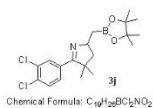
(Time: 0.51) Combine (43:49-120:125)



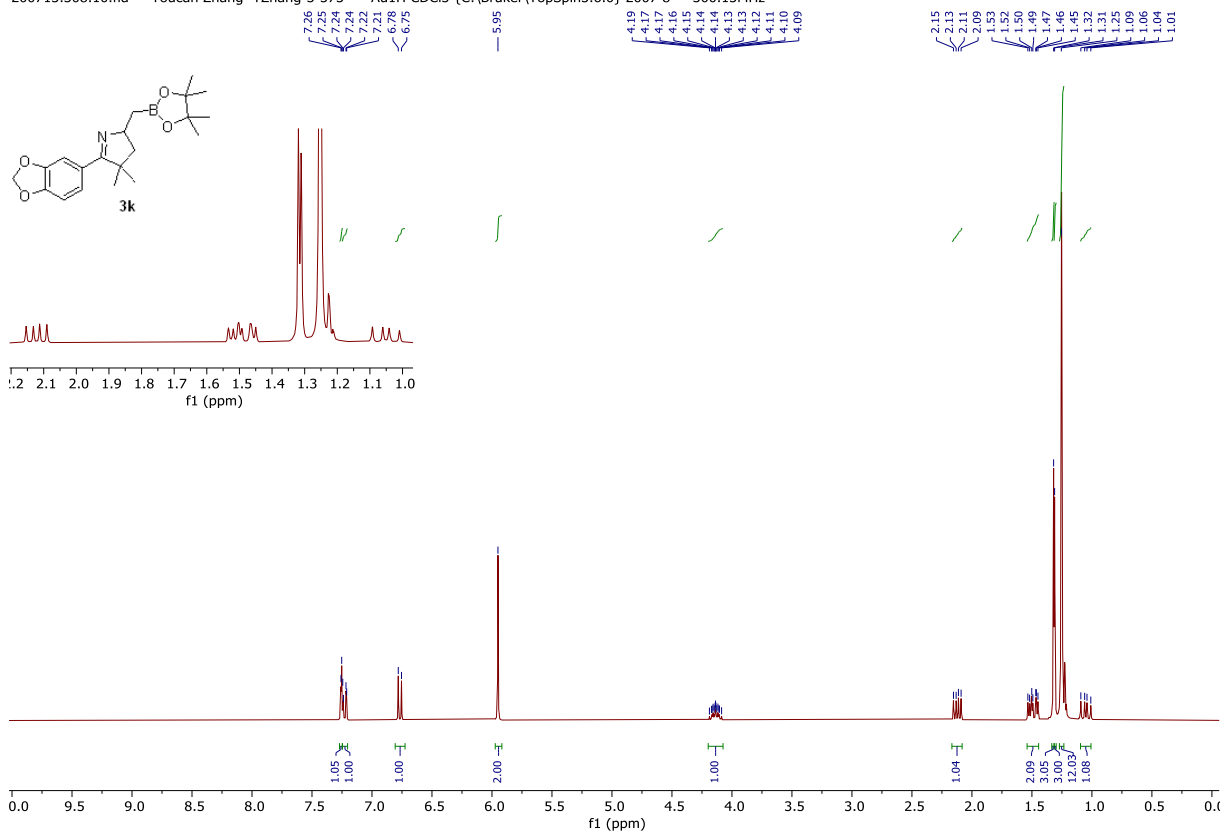
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:03:07

Sample Summary:

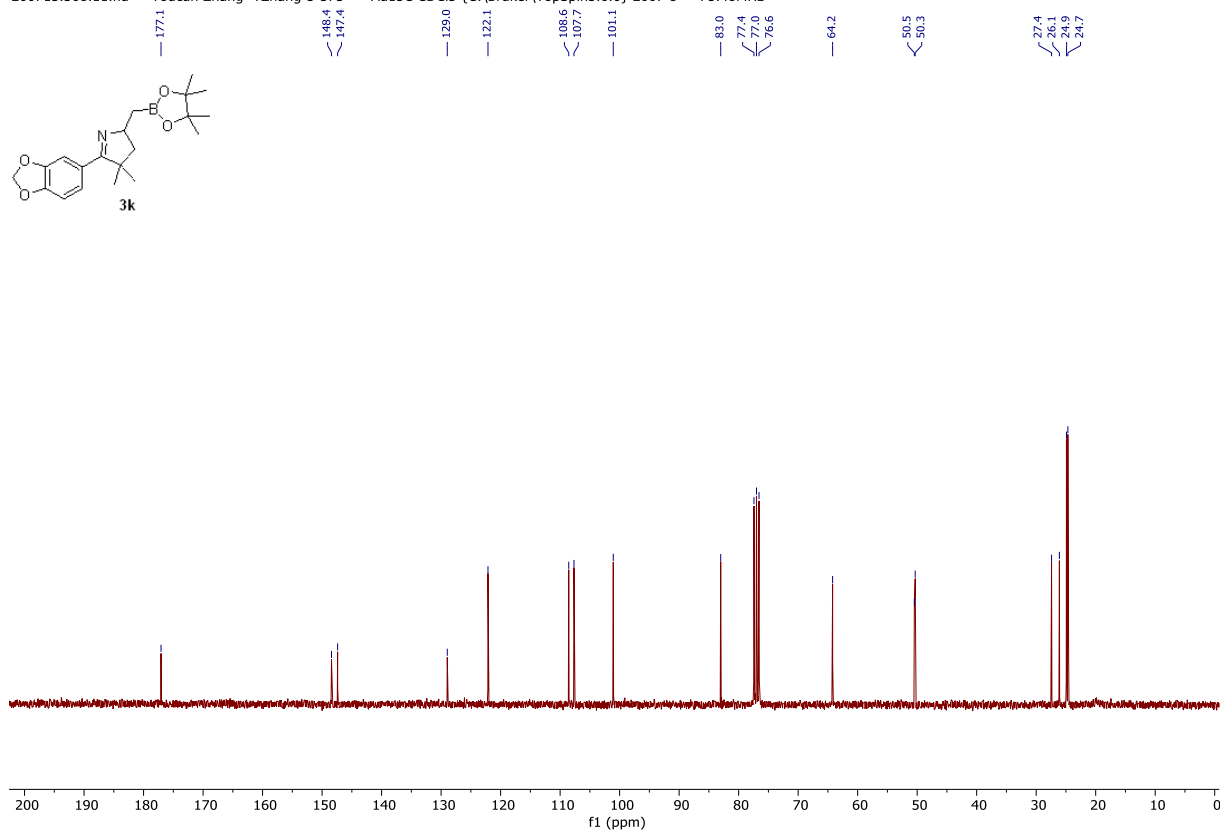
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
71	20080507	YZ-375	Youcan Zhang	380.1470	C ₁₉ H ₂₆ BN ₂ O ₂ C ₁₂	381.1548 382.1515	381.1548 382.1516	0.0 0.3	0.0 0.1



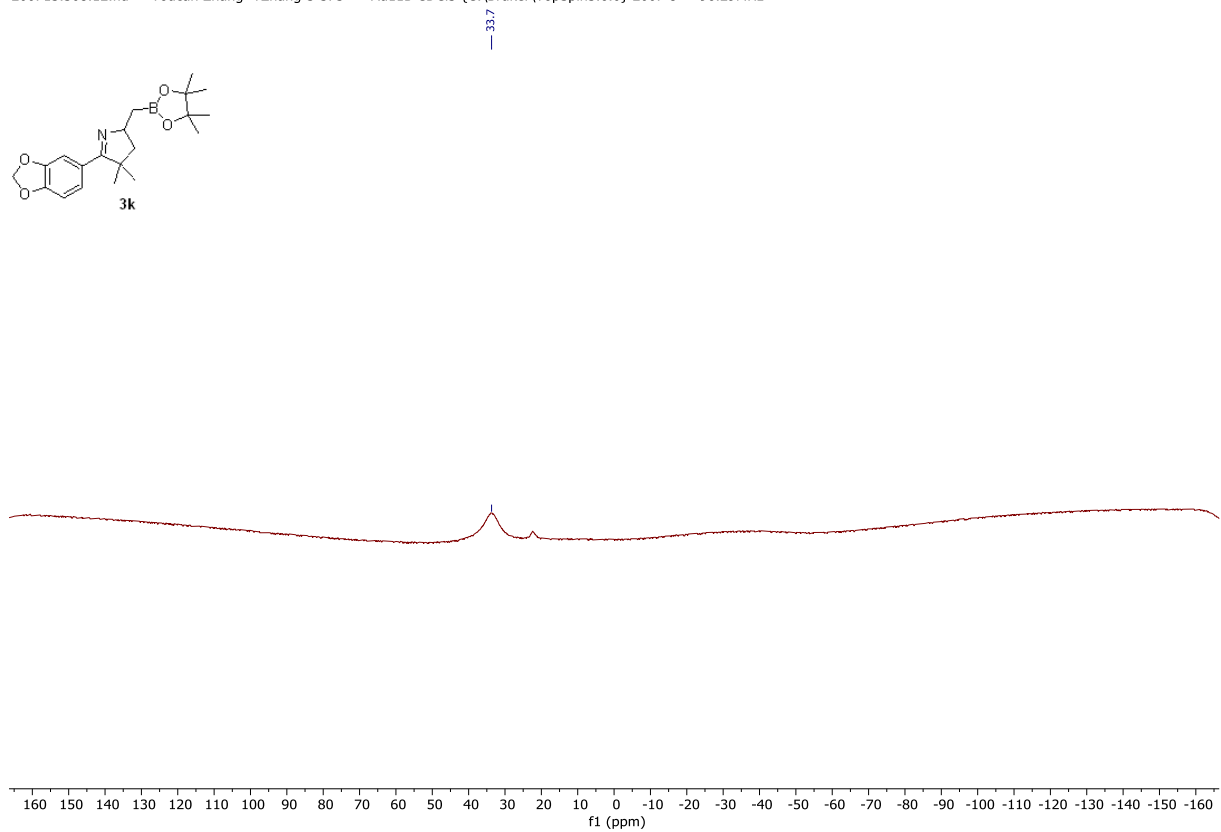
200713.308.10.fid — Youcan Zhang YZhang-3-373 — Au1H CDCI3 {C:\Bruker\TopSpin3.6.0} 2007 8 — 300.13MHz



200713.308.11.fid — Youcan Zhang YZhang-3-373 — Au13C CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 8 — 75.48MHz



200713.308.12.fid — Youcan Zhang YZhang-3-373 — Au11B CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 8 — 96.29MHz



ESI-TOF Accurate Mass Report

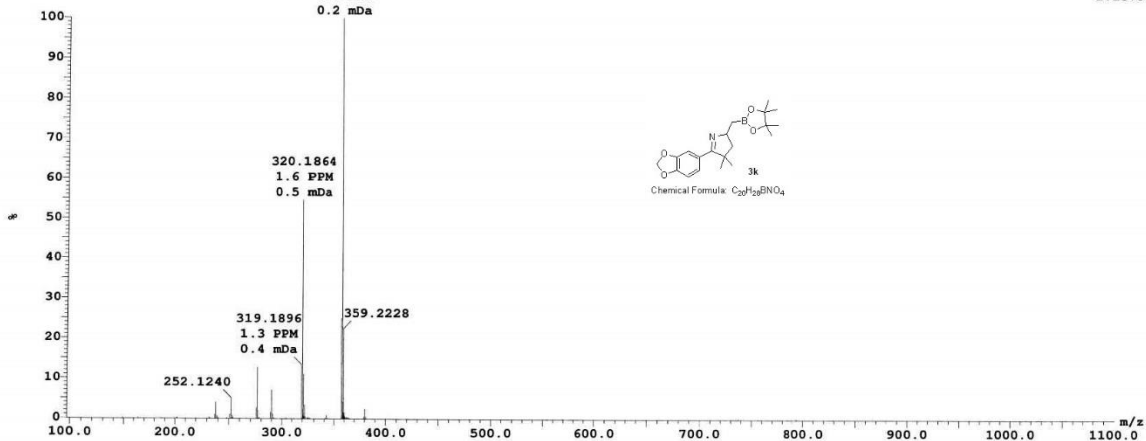
File:20080517

Vial:1.F.6

Description:MeOH/0.1% HCOOH in H₂O 90:10Sample Name:YZ-368+373
Date:05-Aug-2020UserName:Youcan Zhang
Time:16:35:44

Page 2

Sample Report:

(Time: 0.25) Combine (19:25-84:89) 358.2195
0.6 PPM
0.2 mDa1:TOF MS ES+
1.1e+009

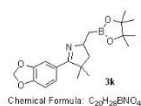
ESI-TOF Accurate Mass Report

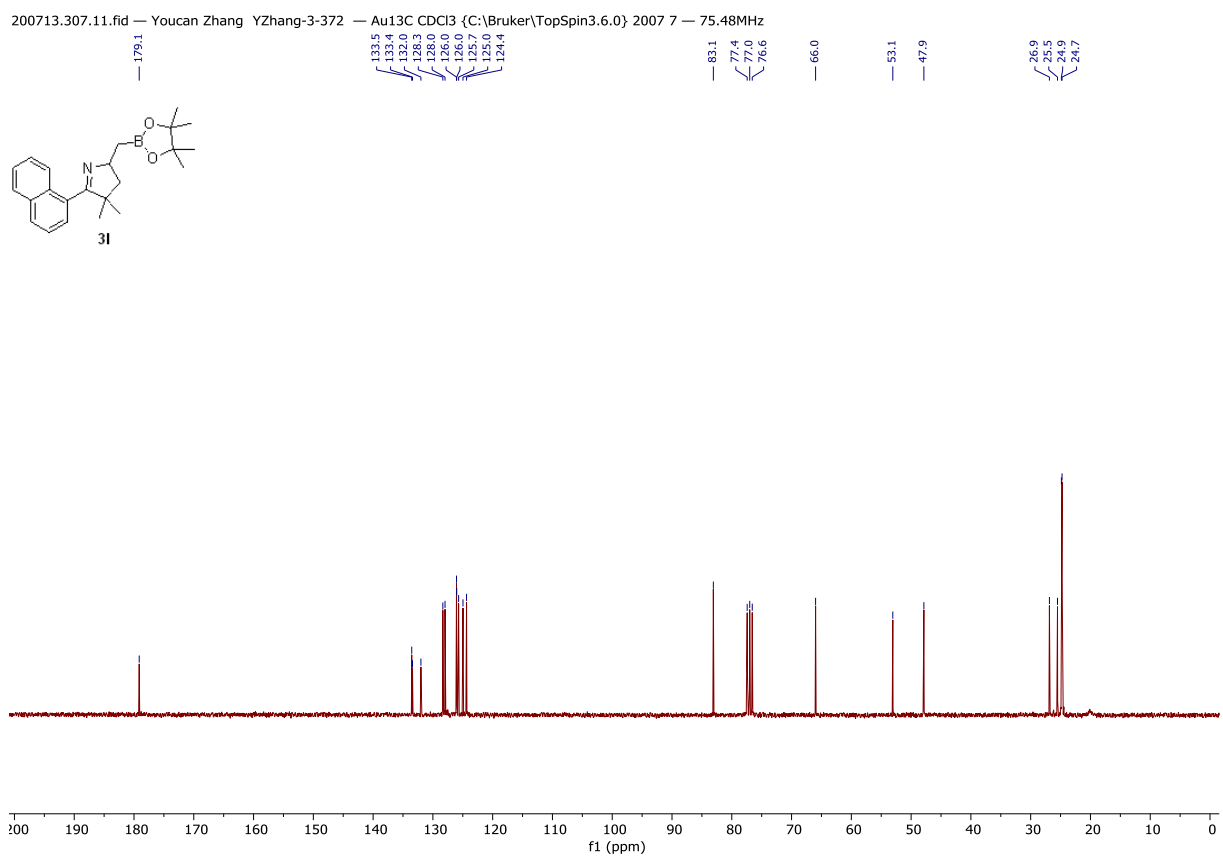
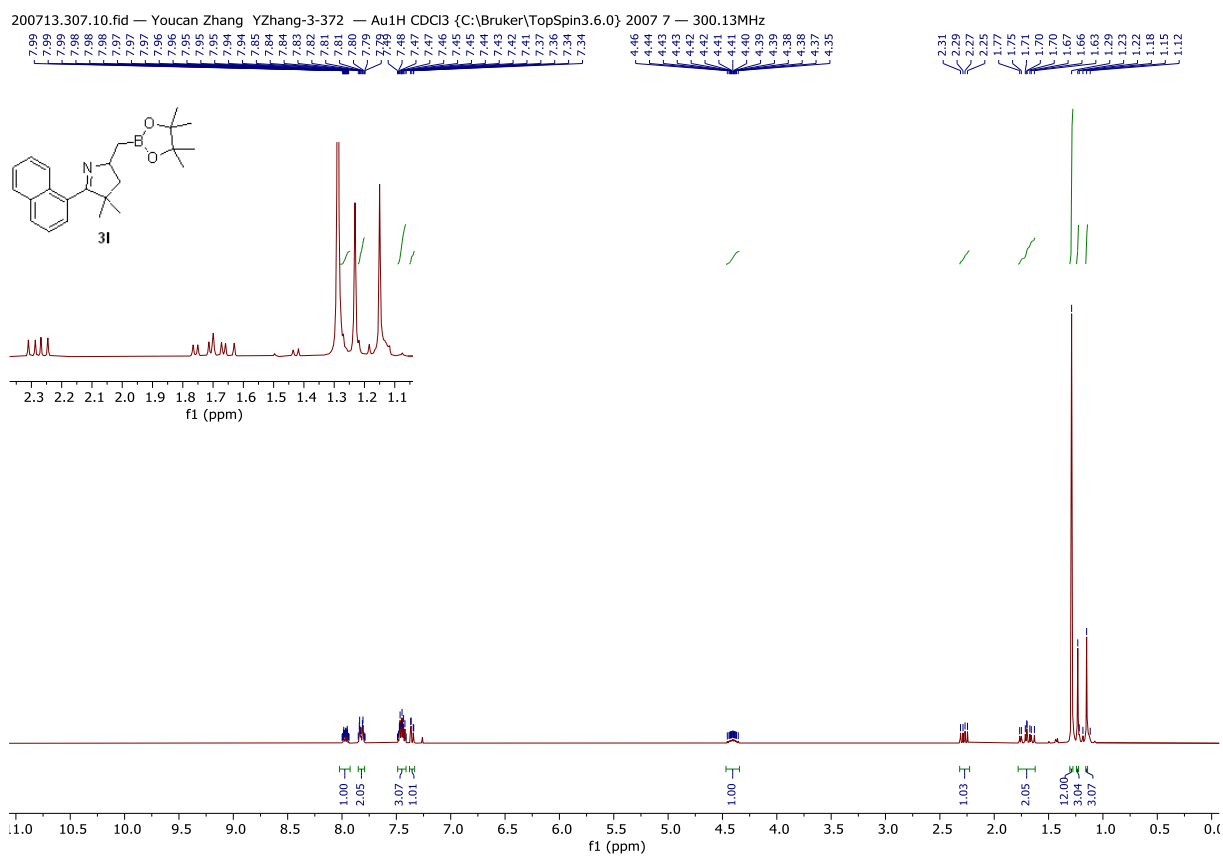
Page 1

Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:38:16

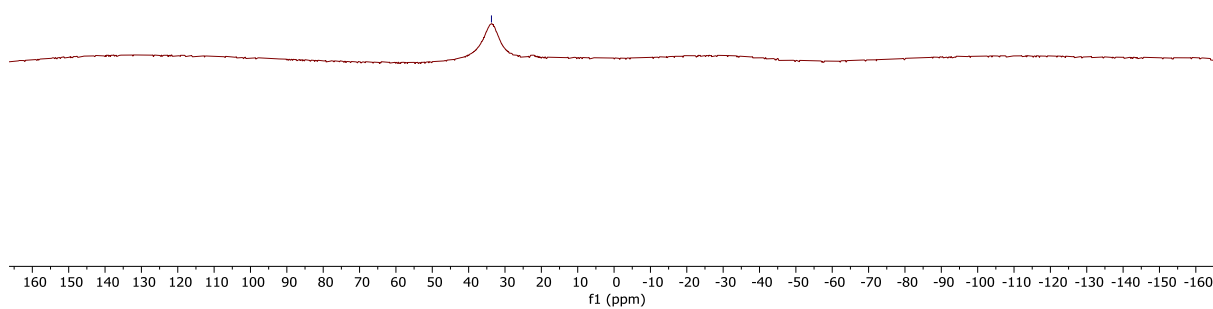
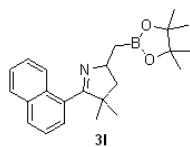
Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
81	20080517	YZ-368+373	Youcan Zhang	318.1814	C17H26BNO2S	319.1892	319.1898	1.9	0.6
				320.1859		320.1866	320.1866	2.2	0.7
				356.2148	C20H28BNO4	357.2226	357.2225	-0.3	-0.1
						358.2193	358.2195	0.6	0.2





— 33.7



ESI-TOF Accurate Mass Report

File:20080515

Vial:1.F.4

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-365+372
Date:05-Aug-2020

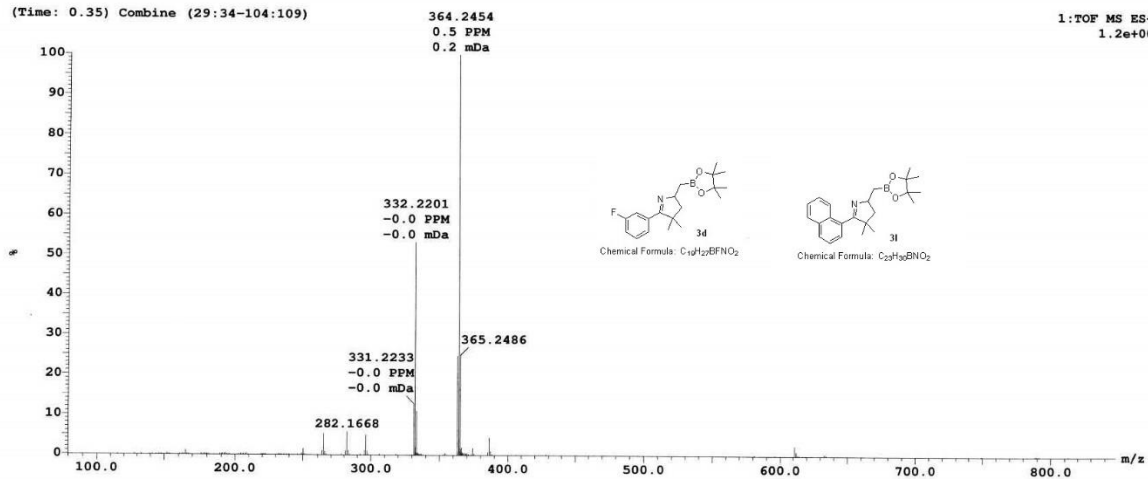
UserName:Youcan Zhang
Time:16:30:35

Page 3

Sample Report (continued):

(Time: 0.35) Combine (29:34-104:109)

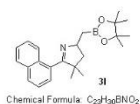
1:TOF MS ES+
1.2e+009



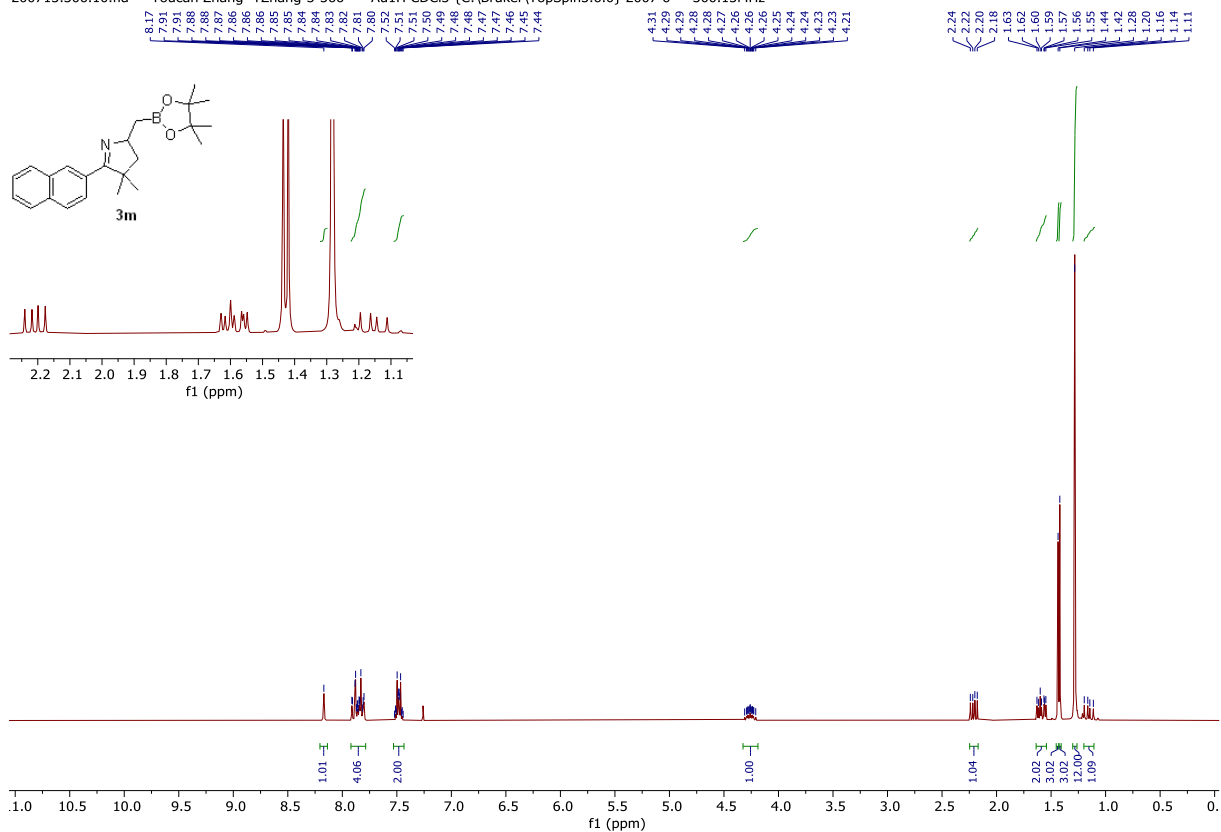
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:33:07

Sample Summary:

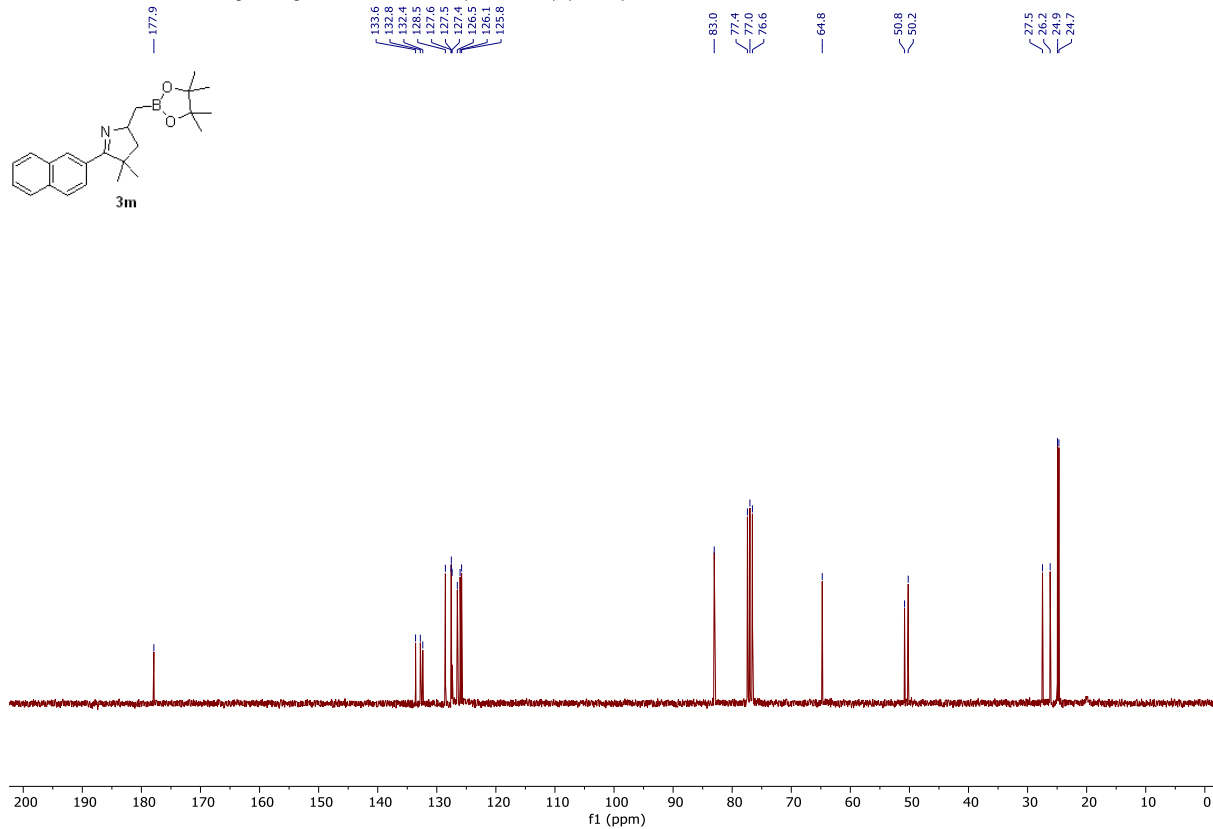
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
79	20080515	YZ-365+372	Youcan Zhang	330.2155	C ₁₉ H ₂₇ NO ₂ F	331.2233	331.2233	0.0	0.0
				362.2406	C ₂₃ H ₃₀ NO ₂	332.2201	332.2201	0.0	0.0
						363.2484	363.2484	0.0	0.0
						364.2452	364.2454	0.5	0.2



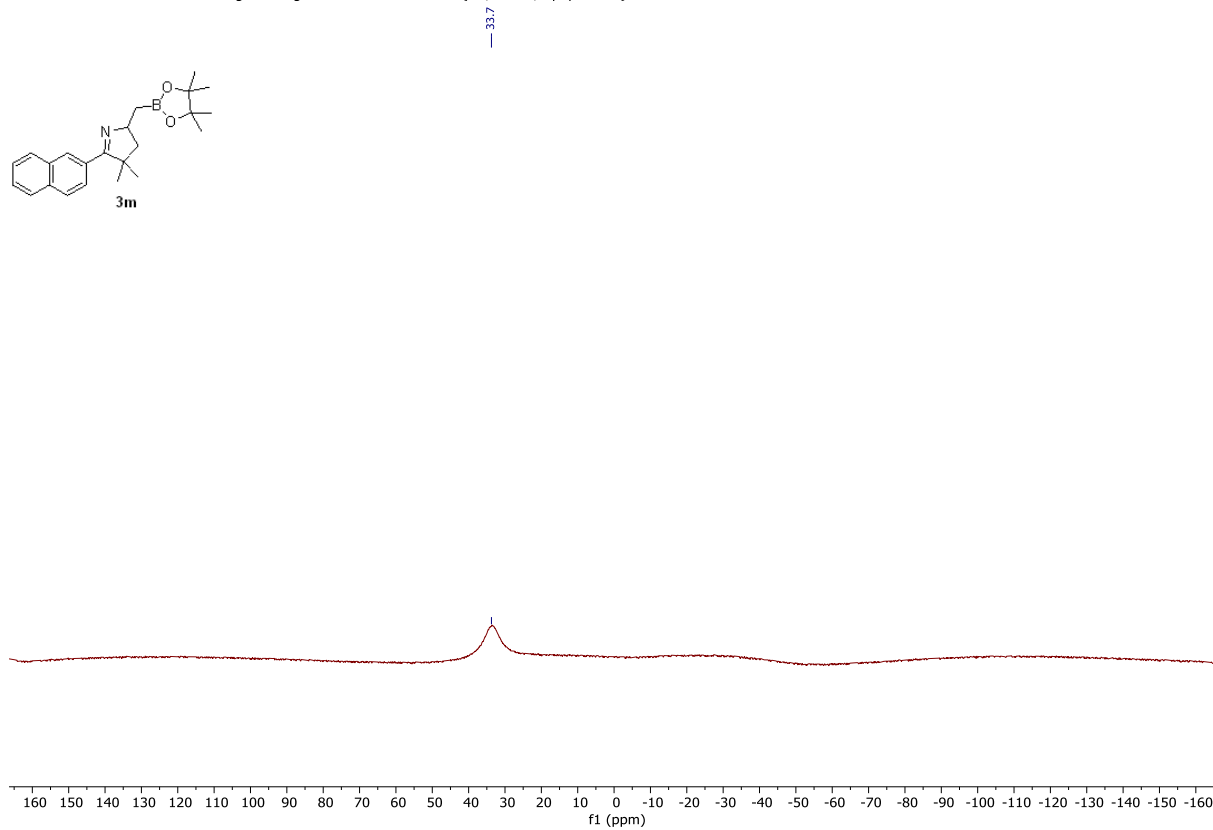
200713.306.10.fid — Youcan Zhang YZhang-3-366 — Au1H CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 6 — 300.13MHz



200713.306.11.fid — Youcan Zhang YZhang-3-366 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.0} 2007 6 — 75.48MHz



200713.306.12.fid — Youcan Zhang YZhang-3-366 — Au11B CDCl3 {C:\Bruker\TopSpin3.6.0} 2007 6 — 96.29MHz



ESI-TOF Accurate Mass Report

File:20080514

Vial:1-F.3

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-366+385

Date:05-Aug-2020

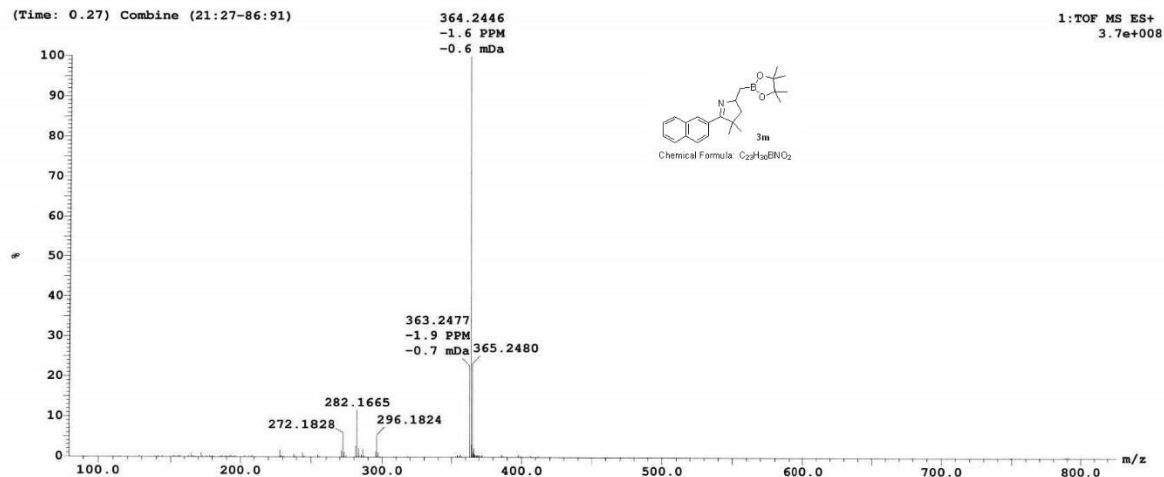
UserName:Youcan Zhang

Time:16:51:17

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Sample Report:

(Time: 0.27) Combine (21:27-86:91)



ESI-TOF Accurate Mass Report

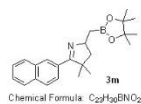
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt

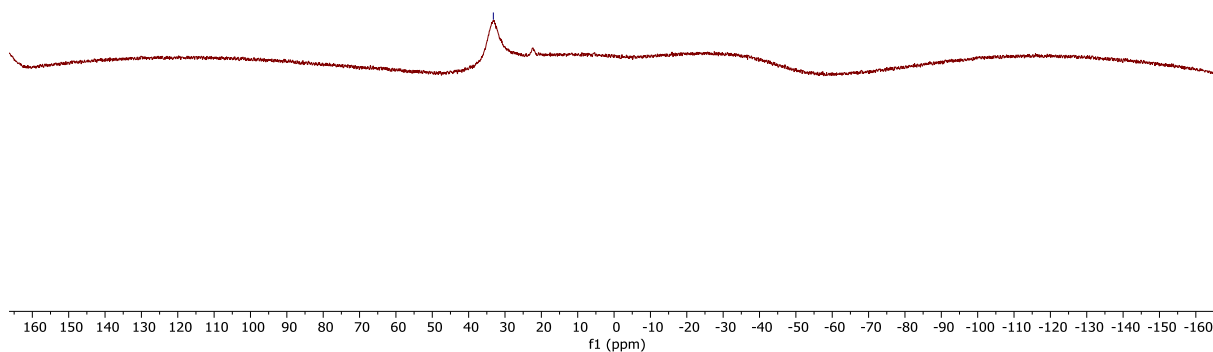
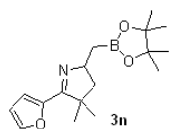
Last modified: Wednesday, August 05, 2020 16:53:46

Page 1

Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
78	20080514	YZ-366+385	Youcan Zhang	352.2563	C ₂₂ H ₃₂ BN ₂ O ₂	353.2641	353.2635	-1.7	-0.6
				362.2406	C ₂₃ H ₃₀ BN ₂ O ₂	354.2608	354.2603	-1.4	-0.5
						363.2484	363.2477	-1.9	-0.7
						364.2452	364.2446	-1.6	-0.6





ESI-TOF Accurate Mass Report

File:20080516

Vial:1.F.5

Description:MeOH/0.1% HCOOH in H2O 90:10

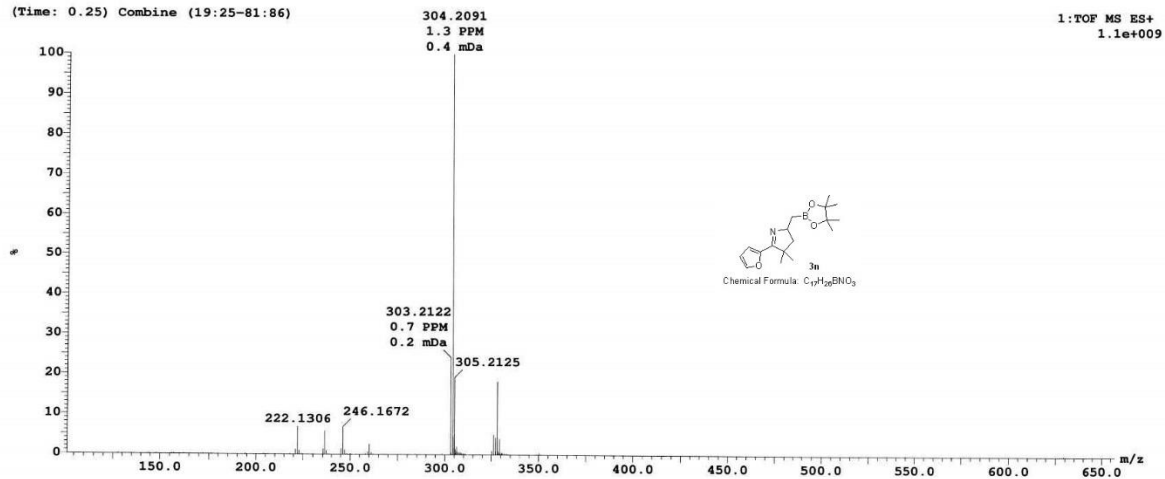
Sample Name:YZ-363+367
Date:05-Aug-2020

UserName:Youcan Zhang
Time:16:33:09

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Sample Report:

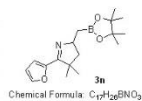
(Time: 0.25) Combine (19:25-81:86)



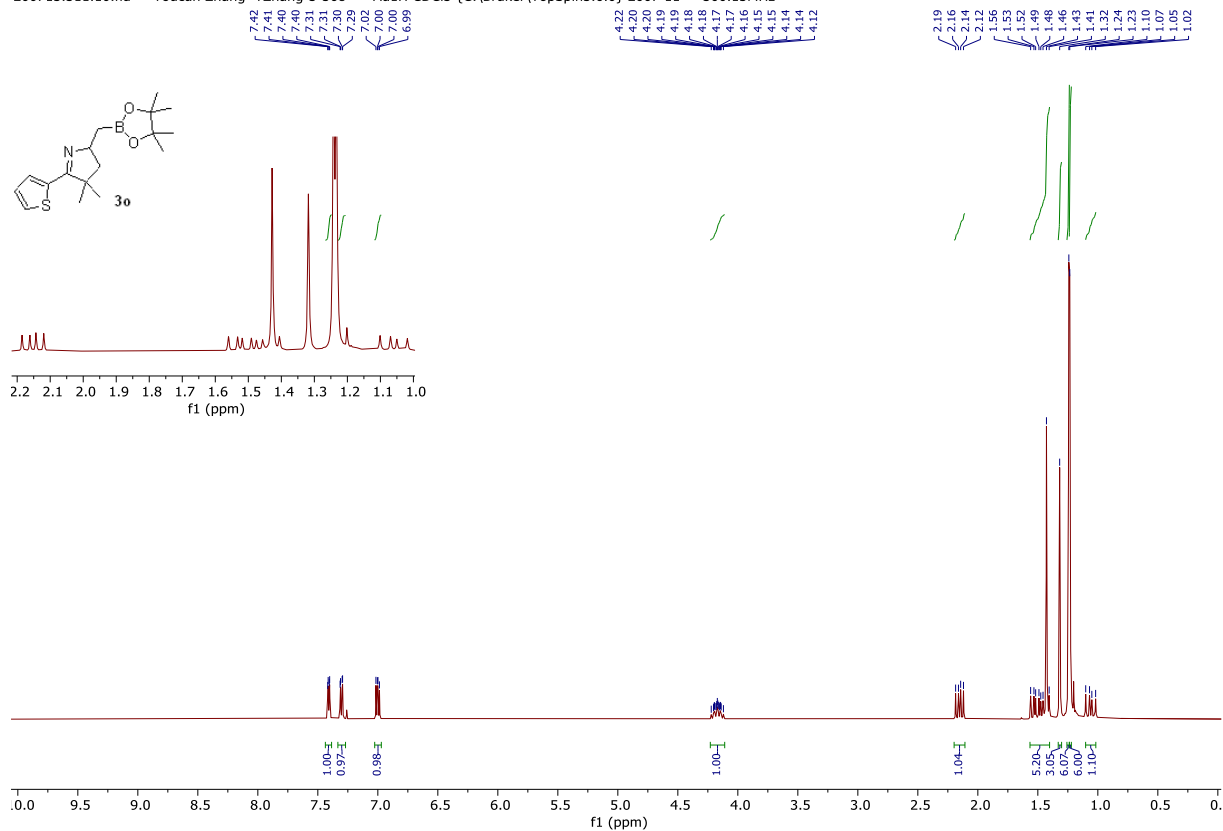
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:35:42

Sample Summary:

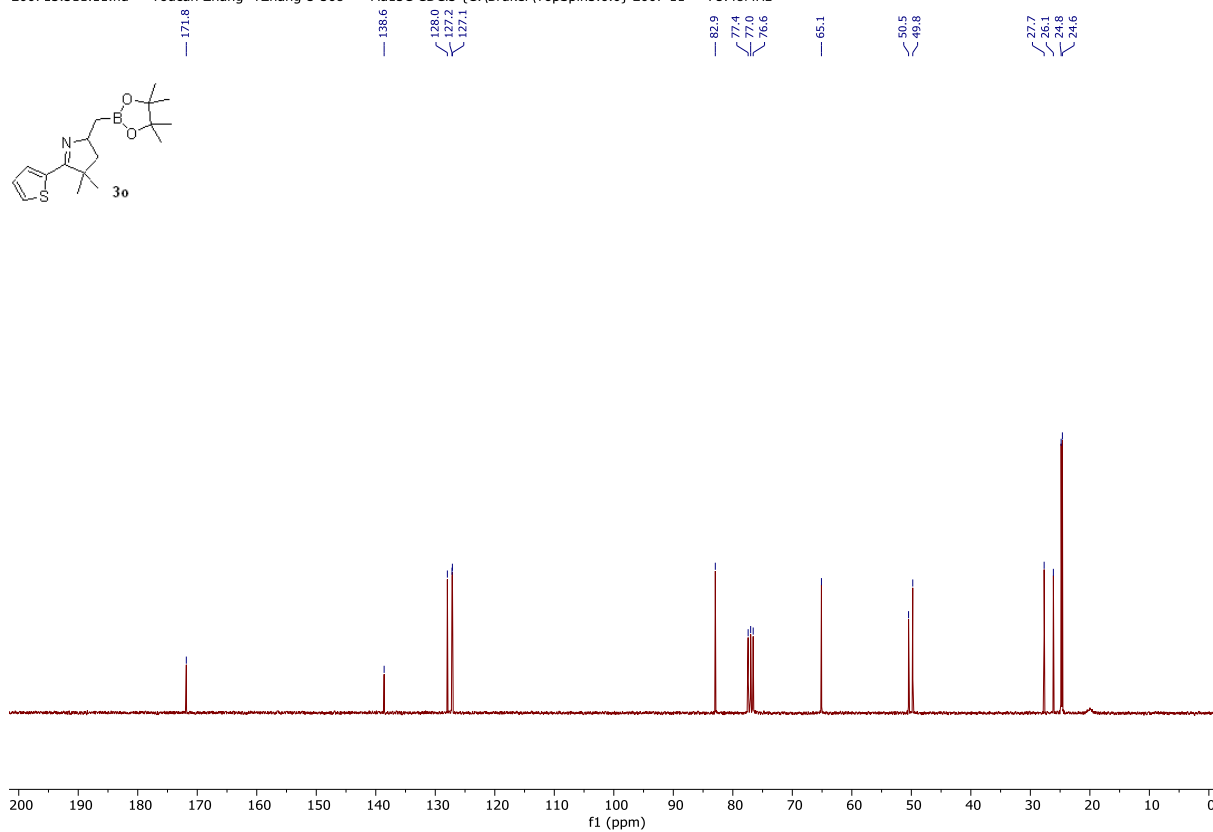
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
80	20080516	YZ-363+367	Youcan Zhang	302.2042	C17H26BNO3	303.2120	303.2122	0.7	0.2
				326.2406	C20H30BNO2	304.2087	304.2091	1.3	0.4
						327.2484	327.2485	0.3	0.1
						328.2451	328.2455	1.2	0.4



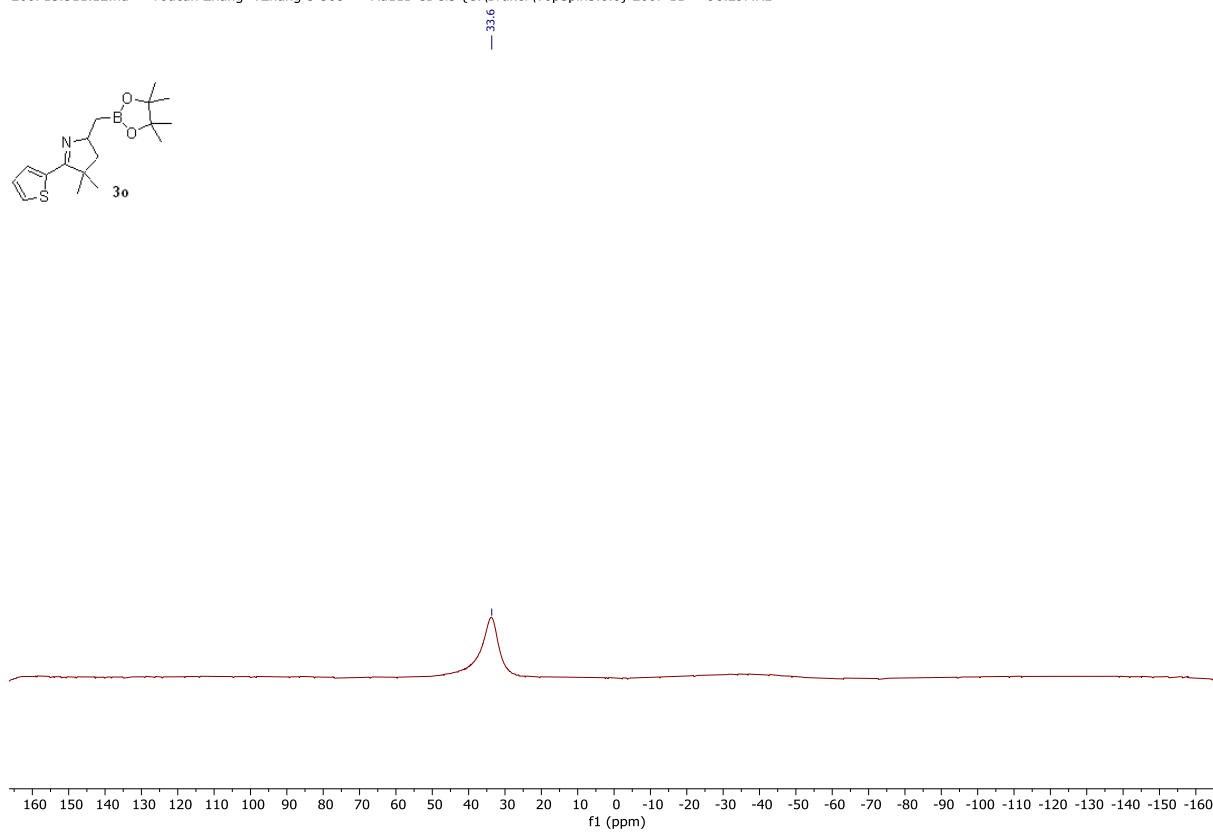
200713.311.10.fid — Youcan Zhang YZhang-3-368 — Au1H CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 11 — 300.13MHz



200713.311.11.fid — Youcan Zhang YZhang-3-368 — Au13C CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 11 — 75.48MHz



200713.311.12.fid — Youcan Zhang YZhang-3-368 — Au11B CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 11 — 96.29MHz



ESI-TOF Accurate Mass Report

File:20080517

Vial:1 F.6

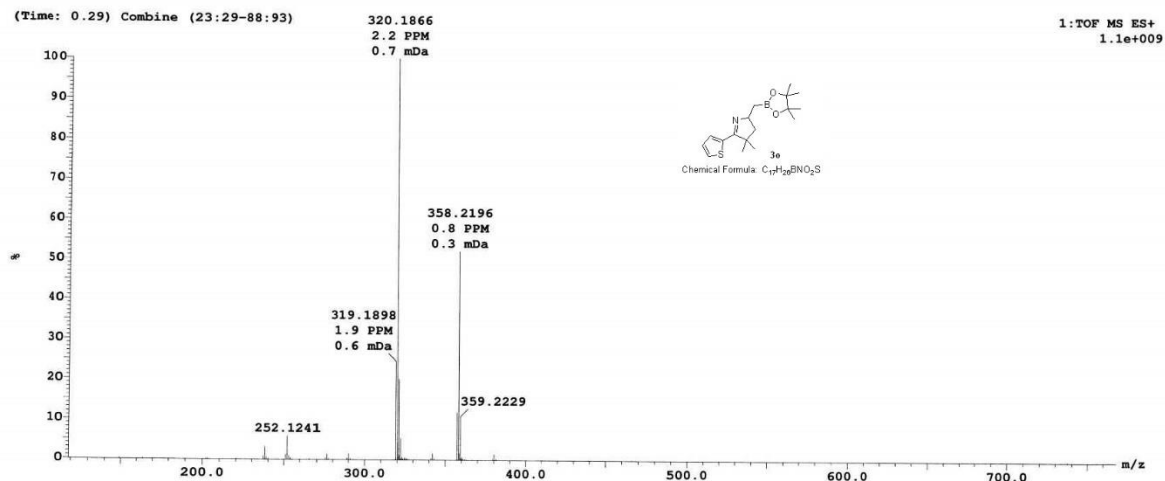
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-368+373
Date:05-Aug-2020UserName:Youcan Zhang
Time:16:35:44

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Sample Report (continued):

(Time: 0.29) Combine (23:29-88:93)



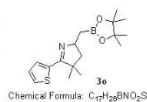
ESI-TOF Accurate Mass Report

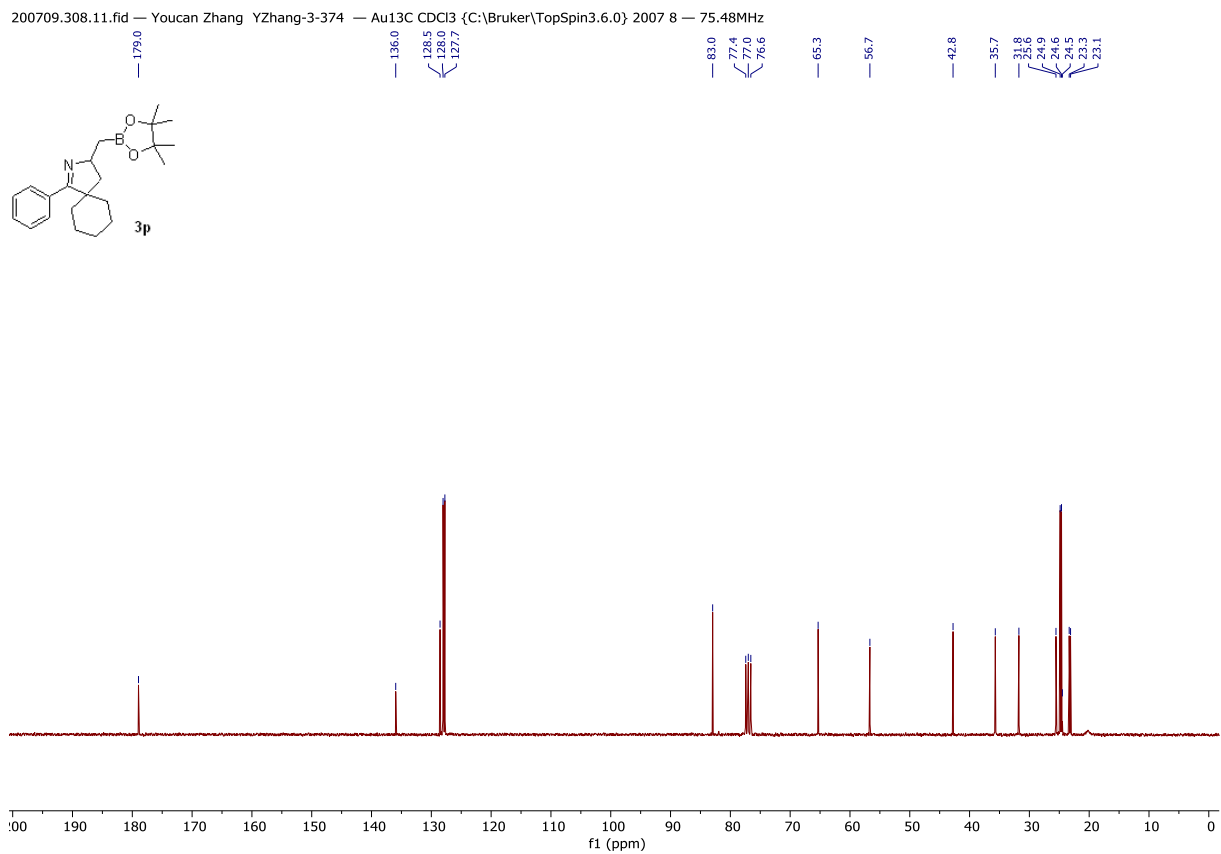
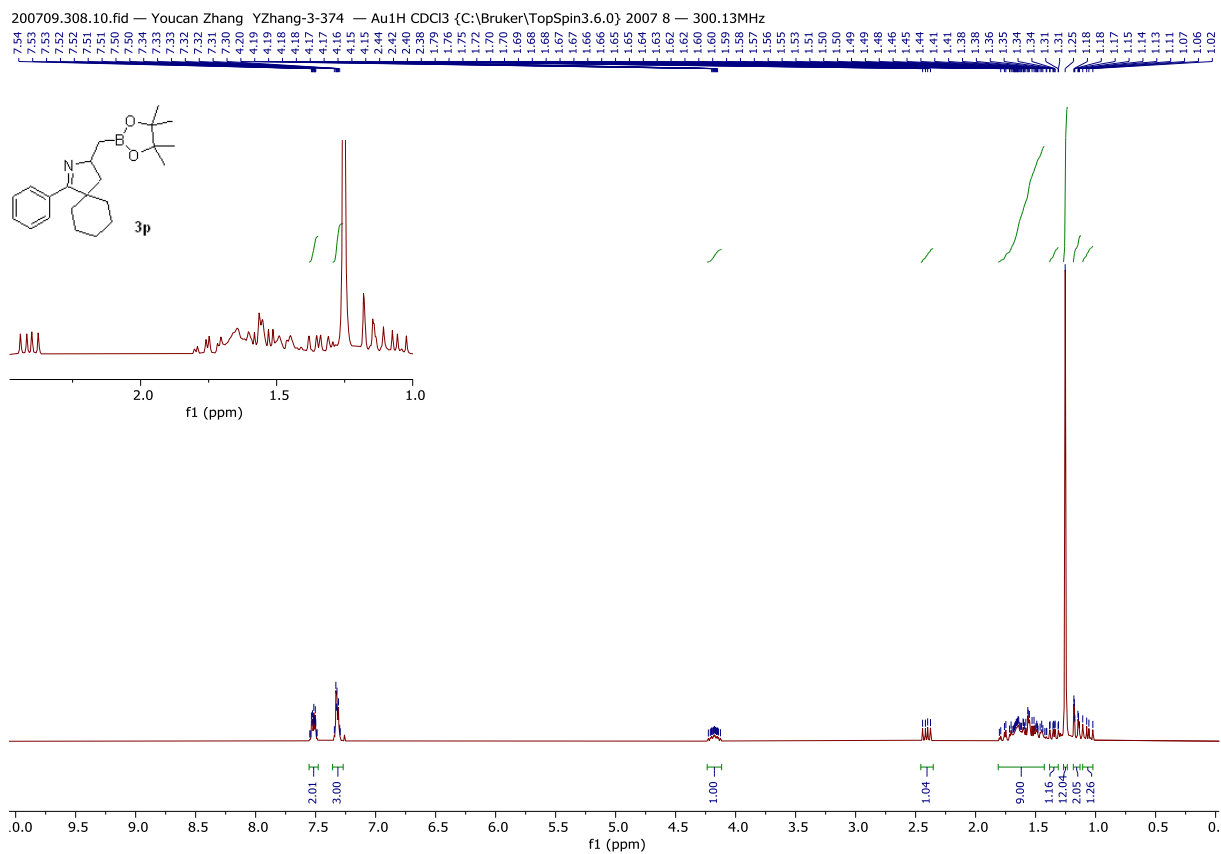
Page 1

Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:38:16

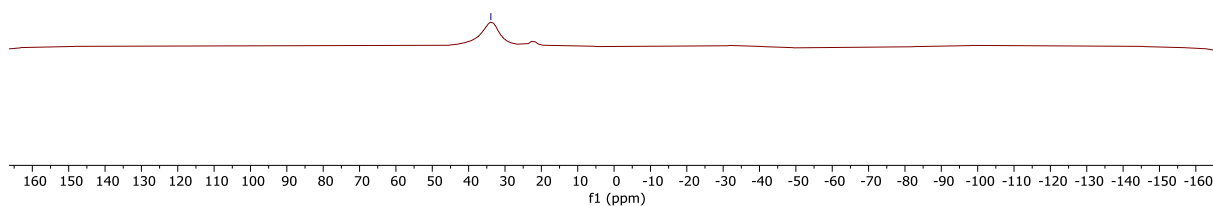
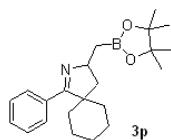
Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
81	20080517	YZ-368+373	Youcan Zhang	318.1814	C ₁₇ H ₂₆ NO ₂ S	319.1892	319.1898	1.9	0.6
						320.1859	320.1866	2.2	0.7
				356.2148	C ₂₀ H ₂₈ NO ₄	357.2226	357.2225	-0.3	-0.1
						358.2193	358.2195	0.6	0.2





— 33.9



ESI-TOF Accurate Mass Report

File:20080518

Vial:1:F.7

Description:MeOH/0.1% HCOOH in H2O 90:10

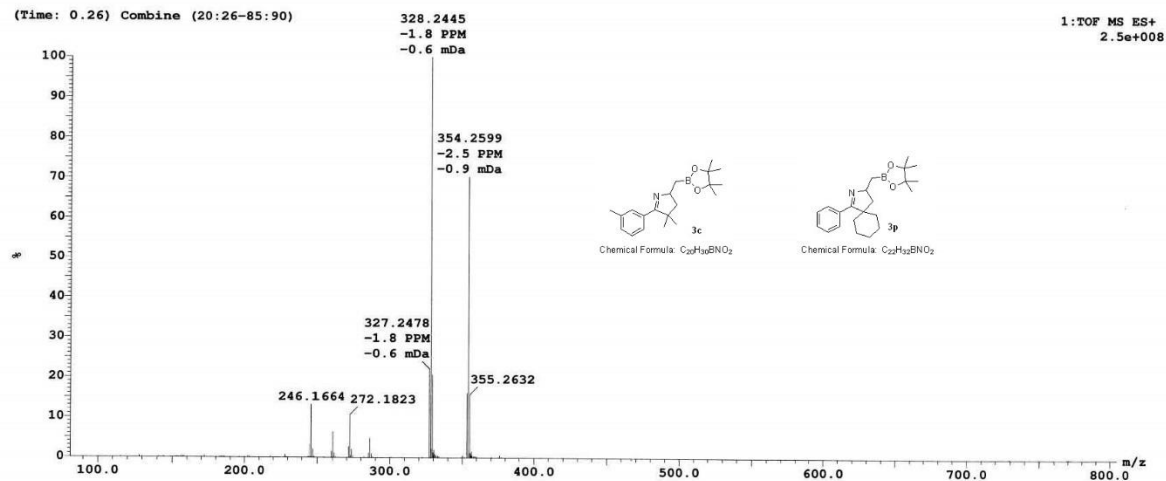
Sample Name:YZ-374+377
Date:05-Aug-2020

UserName:Youcan Zhang
Time:16:58:58

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Sample Report:

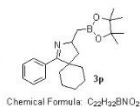
(Time: 0.26) Combine (20:26-85:90)



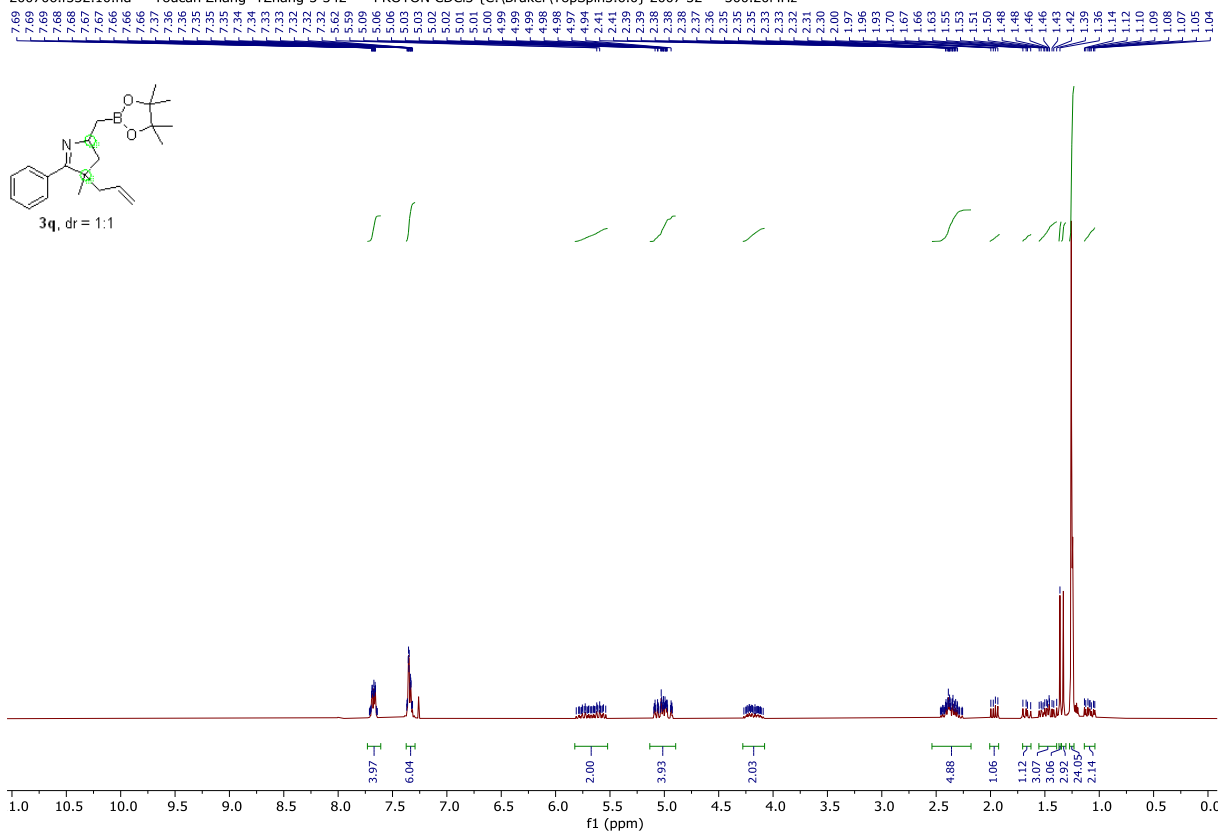
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 17:01:26

Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
82	20080518	YZ-374+377	Youcan Zhang	326.2406	C20H30BNO2	327.2484	327.2478	-1.8	-0.6
				352.2563	C22H32BNO2	353.2641	353.2631	-2.8	-1.0
						354.2608	354.2599	-2.5	-0.9



200706.f332.10.fid — Youcan Zhang YZhang-3-342 — PROTON CDCI3 {C:\Bruker\TopSpin3.6.0} 2007 32 — 300.20MHz



3q, dr = 1:1

¹H NMR (CDCl₃) peaks (ppm): 7.24, 7.17, 7.14, 7.07, 6.54, 6.48, 5.48, 5.43, 4.60, 4.58, 4.35, 4.33, 2.62, 2.49, 2.47, 2.42.

¹³C NMR (CDCl₃) peaks (ppm): 177.2, 176.8, 135.2, 134.2, 134.1, 134.3, 129.2, 129.1, 128.0, 128.0, 127.8, 118.5, 117.9, 83.0, 77.4, 77.0, 76.6, 65.4, 64.8, 54.8, 54.3, 46.0, 45.8, 43.5, 43.3, 26.2, 24.9, 24.7, 24.2.

3q, dr = 1:1

33.1

ESI-TOF Accurate Mass Report

File:20080512

Vial:1:F,1

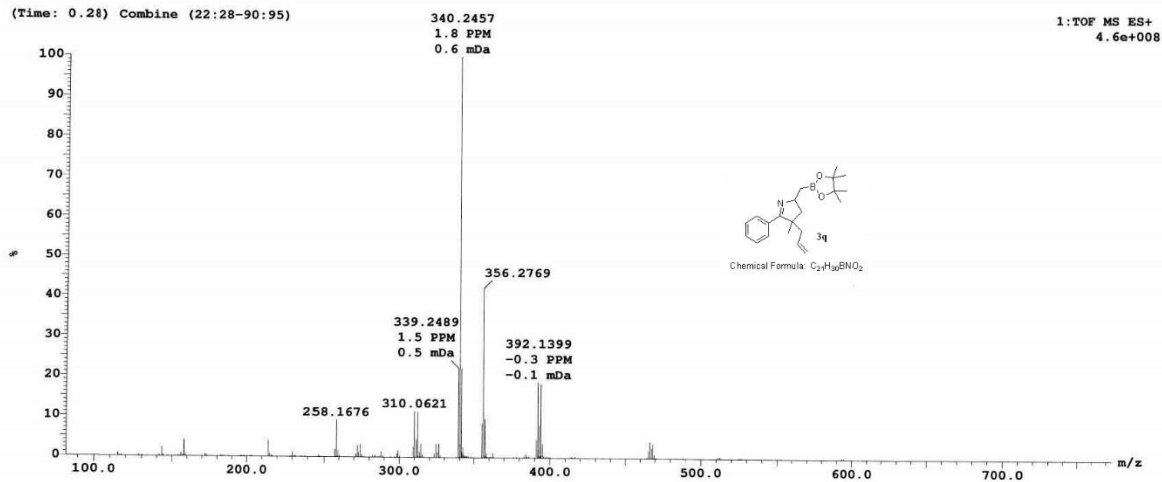
Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-342+345
Date:05-Aug-2020UserName:Youcan Zhang
Time:16:19:39

Page 2

Sample Report:

(Time: 0.28) Combine (22:28-90:95)



ESI-TOF Accurate Mass Report

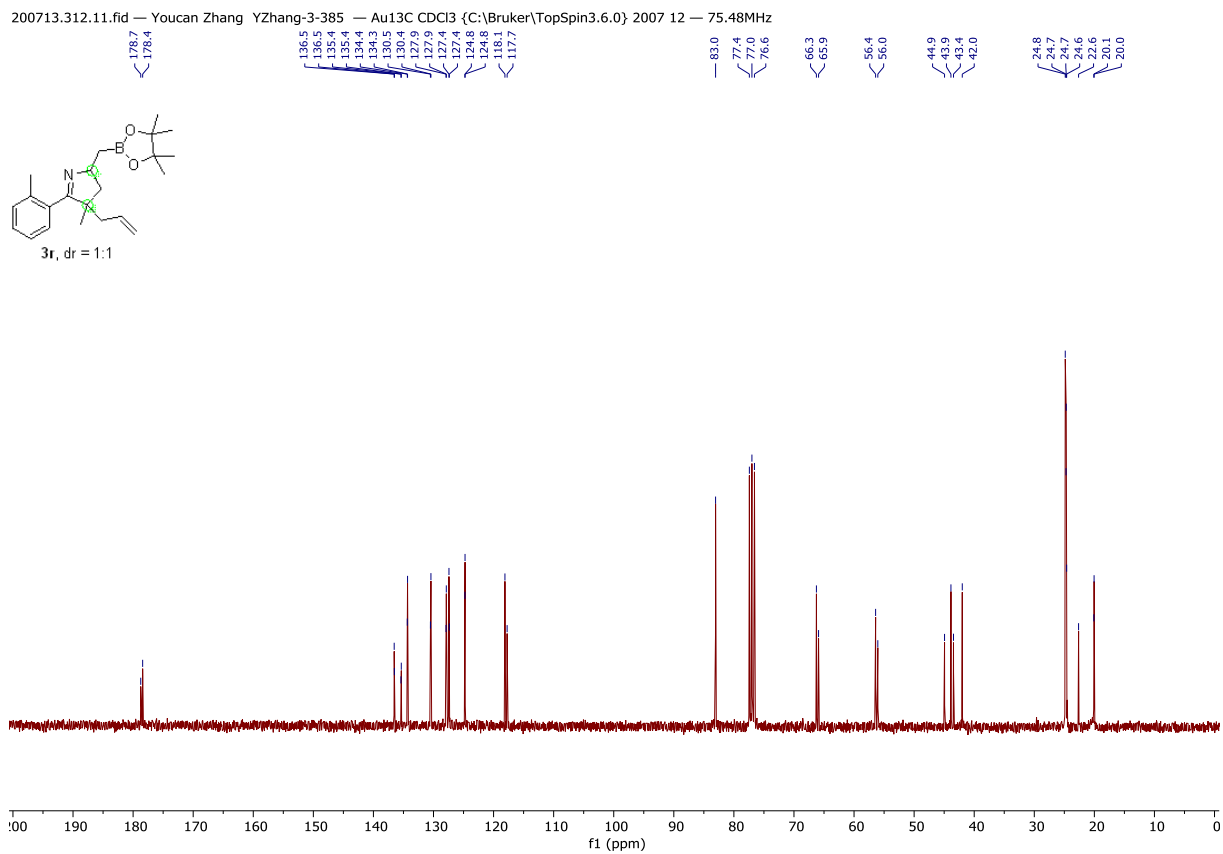
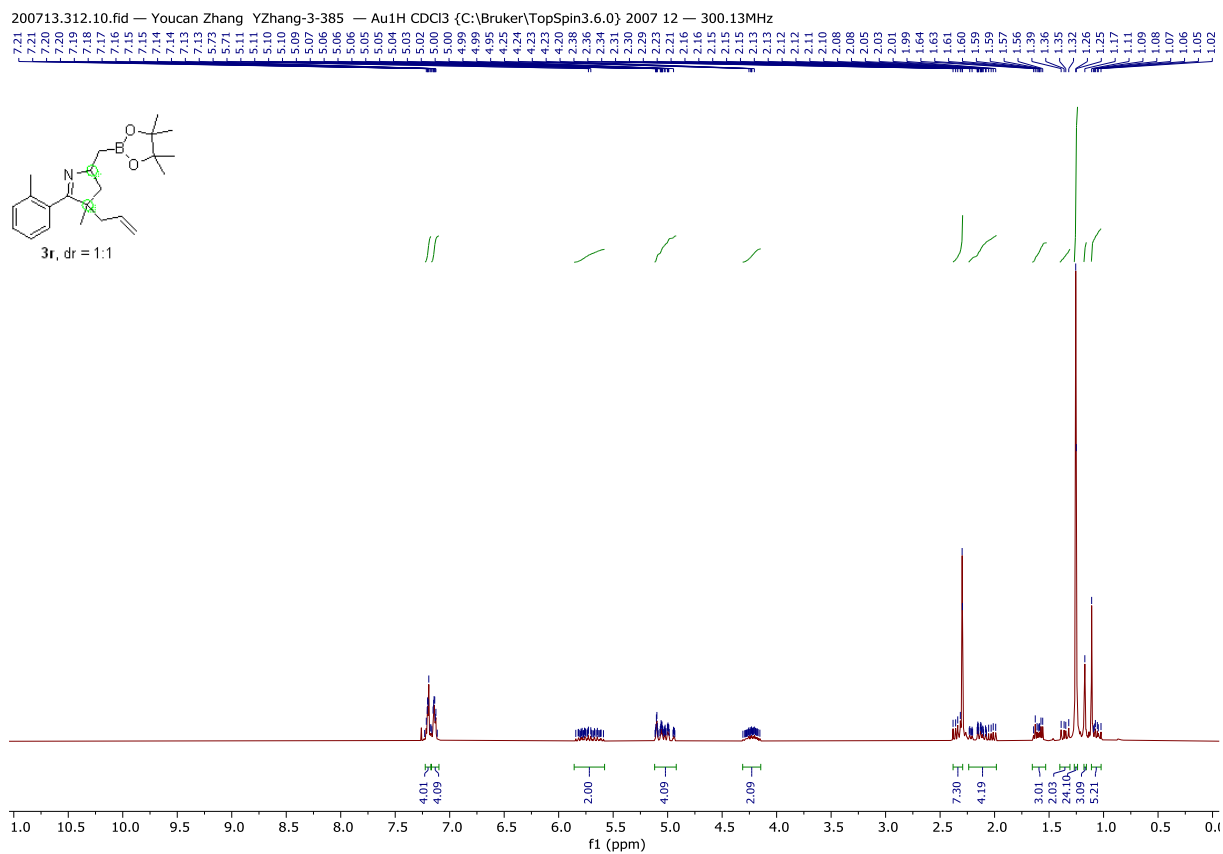
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:22:11

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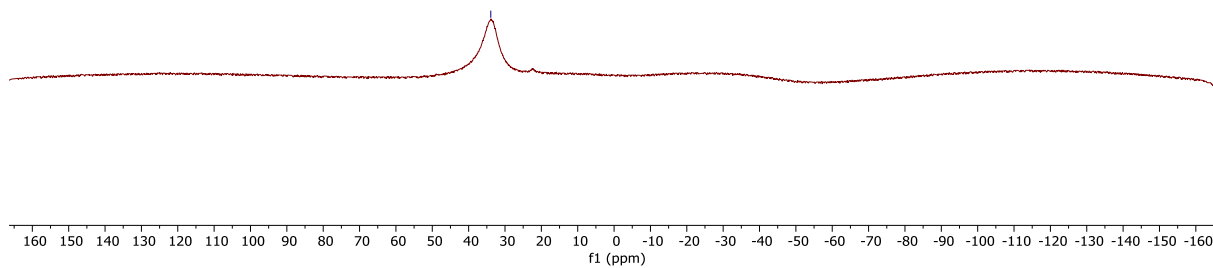
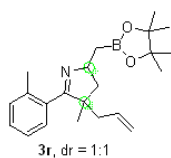
Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
76	20080512	YZ-342+345	Youcan Zhang	338.2406	C21H30BNO2	339.2484	339.2489	1.5	0.5
				390.1355	C19H27BNO2Br	340.2451	340.2457	1.8	0.6
						391.1433	391.1437	1.0	0.4
						392.1400	392.1406	1.5	0.6





— 33.9



ESI-TOF Accurate Mass Report

File:20080514

Vial:1.F.3

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-366+385

Date:05-Aug-2020

UserName:Youcan Zhang

Time:16:51:17

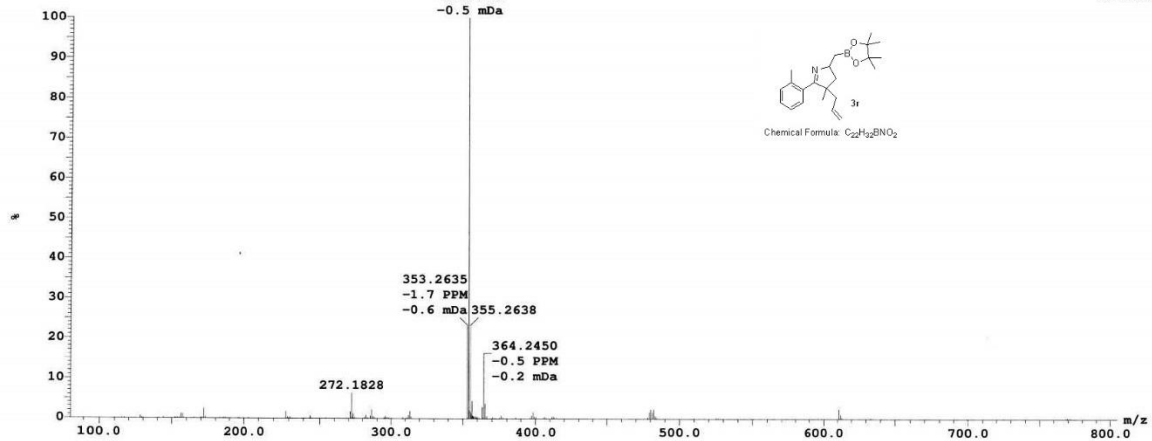
Page 3

Sample Report (continued):

(Time: 0.33) Combine (27:33-97:101)

354.2603
-1.4 PPM
-0.5 mDa

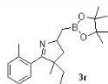
1:TOF MS ES+
2.7e+008



Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:53:46

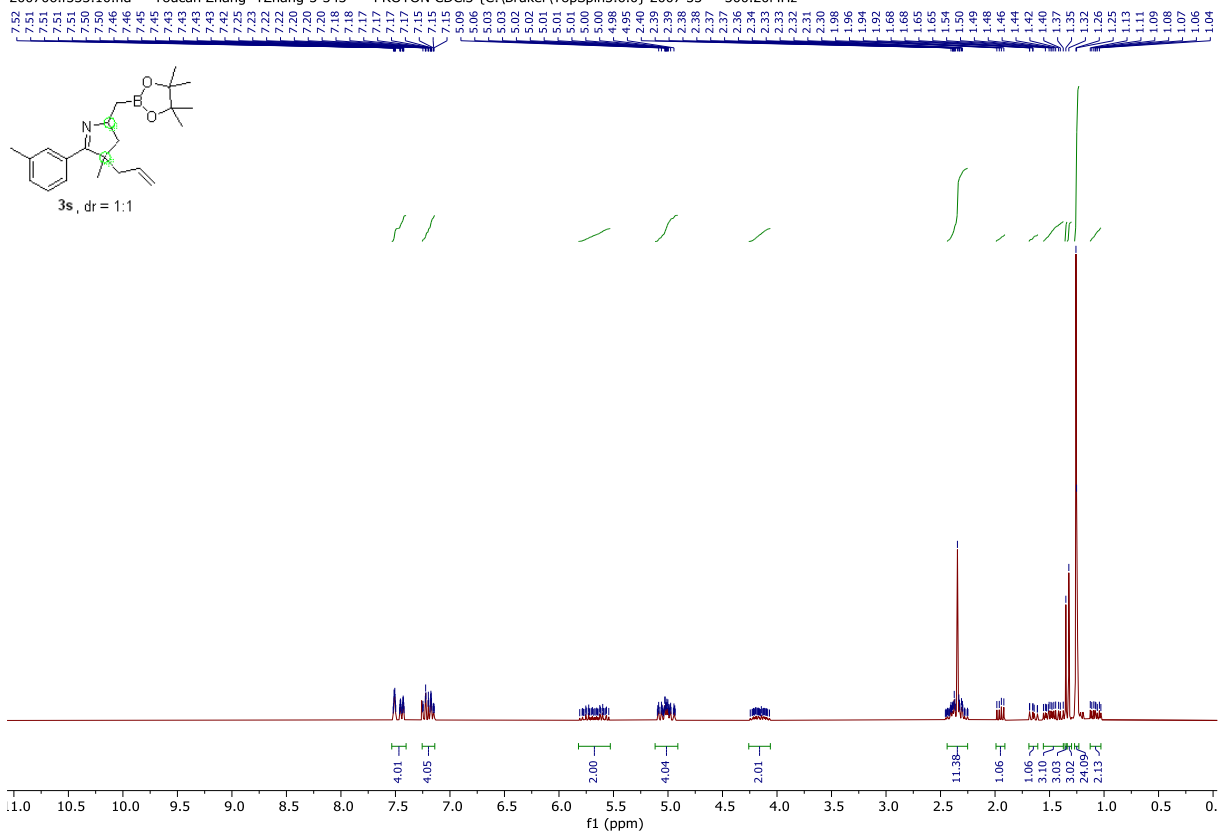
Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
78	20080514	Y2-366+385	Youcan Zhang	352.2563	C22H32BNO2	353.2641	353.2635	-1.7	-0.6
						354.2608	354.2603	-1.4	-0.5
				362.2406	C23H30BNO2	363.2484	363.2477	-1.9	-0.7
						364.2452	364.2446	-1.6	-0.6

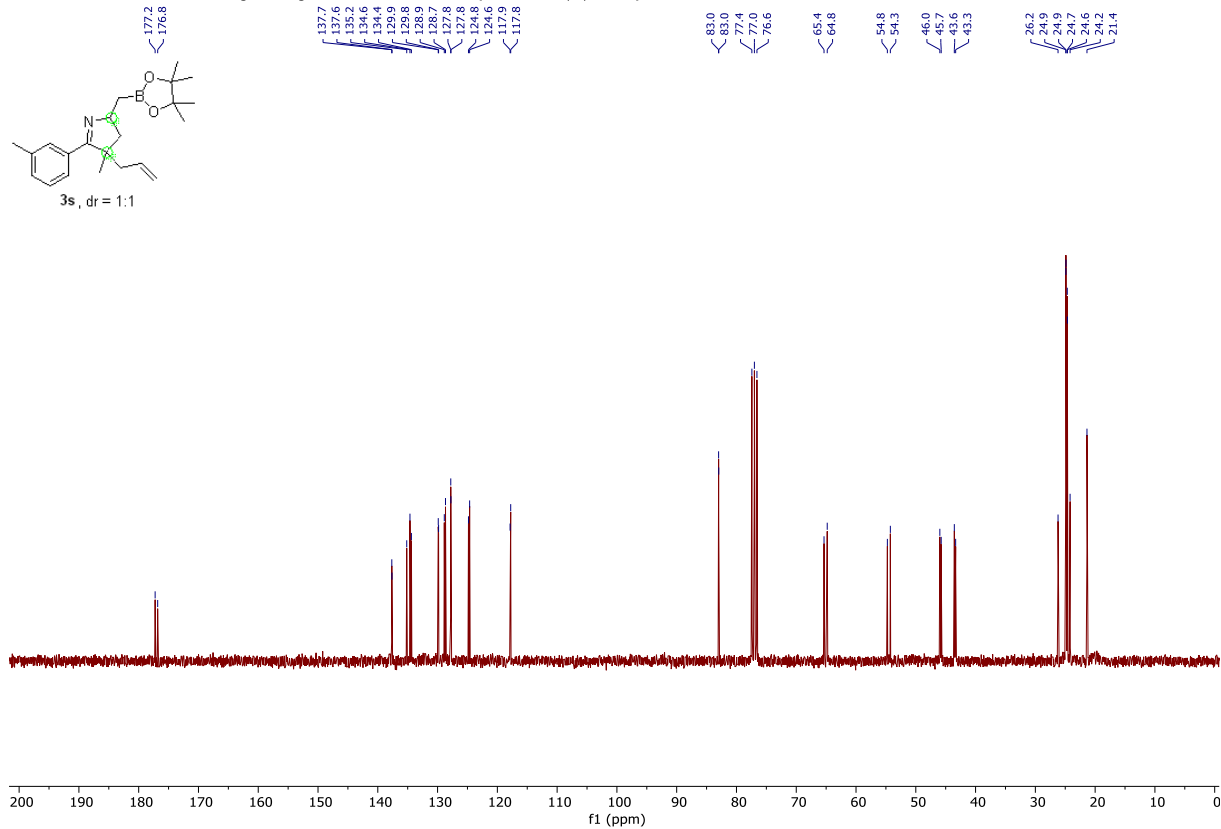


Chemical Formula: C₂₂H₃₂BNO₂

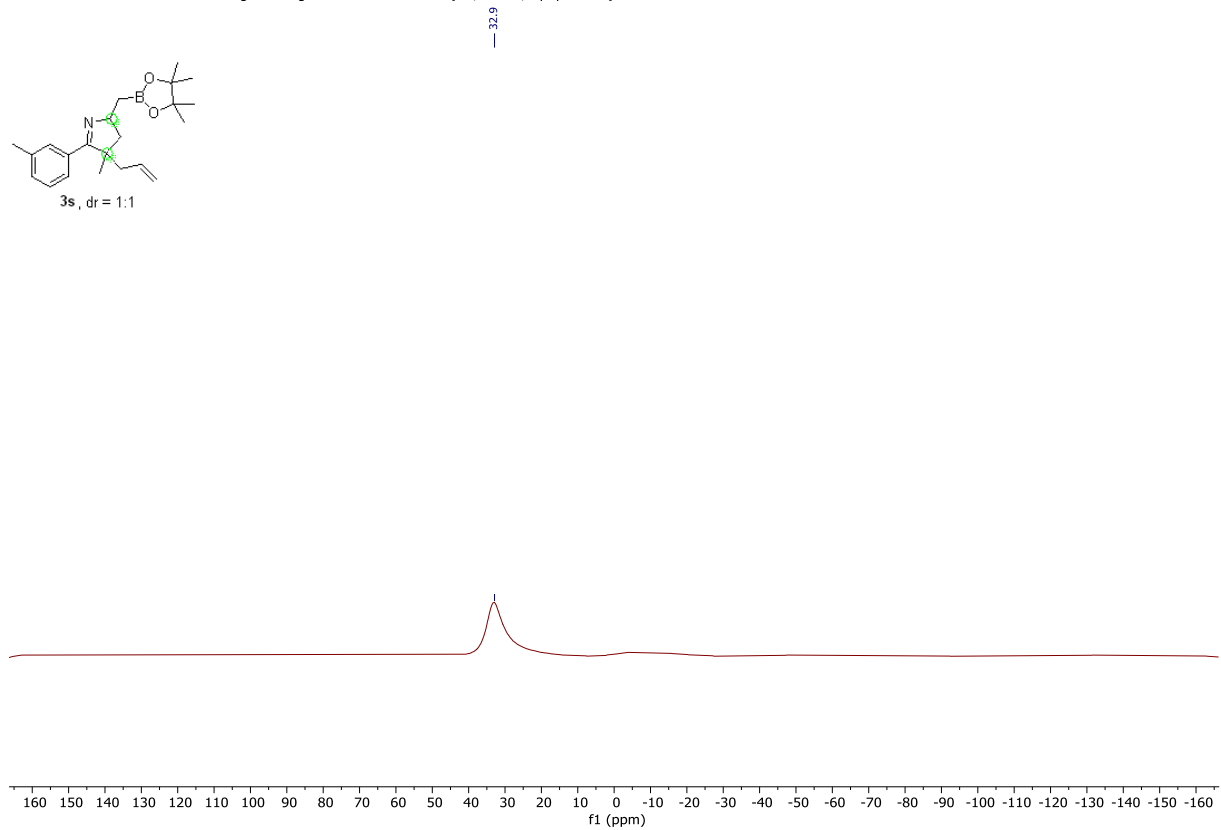
200706.f3333.10.fid — Youcan Zhang YZhang-3-343 — PROTON CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 33 — 300.20MHz



200706.f333.11.fid — Youcan Zhang YZhang-3-343 — C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2007 33 — 75.49MHz



200706.f333.12.fid — Youcan Zhang YZhang-3-343 — 11B CDCl3 {C:\Bruker\TopSpin3.6.0} 2007 33 — 96.32MHz



ESI-TOF Accurate Mass Report

File:20080511

Vial:1:E.8

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-343+344

Date:05-Aug-2020

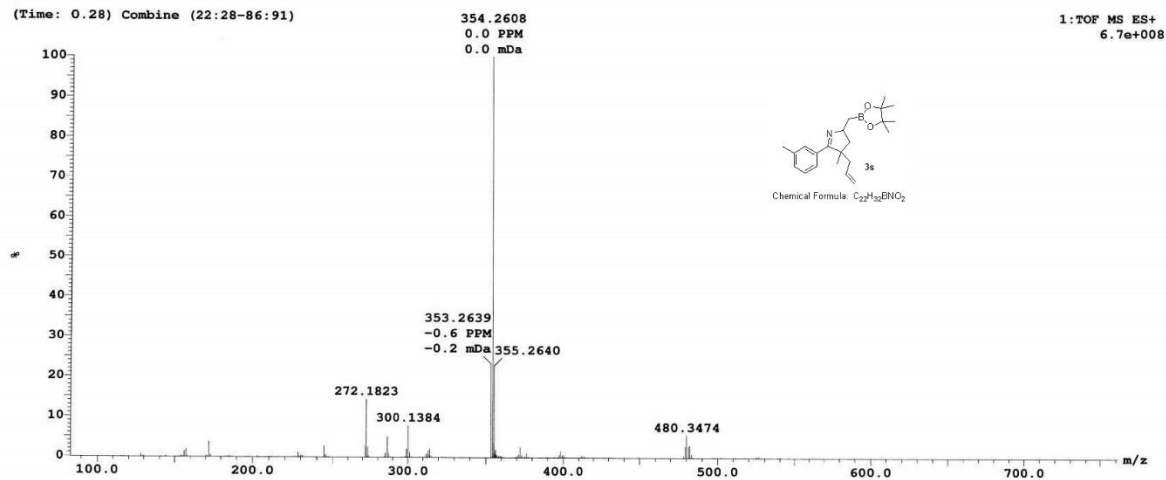
UserName:Youcan Zhang

Time:16:13:49

Page 2

Sample Report:

(Time: 0.28) Combine (22:28-86:91)



ESI-TOF Accurate Mass Report

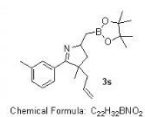
Page,1

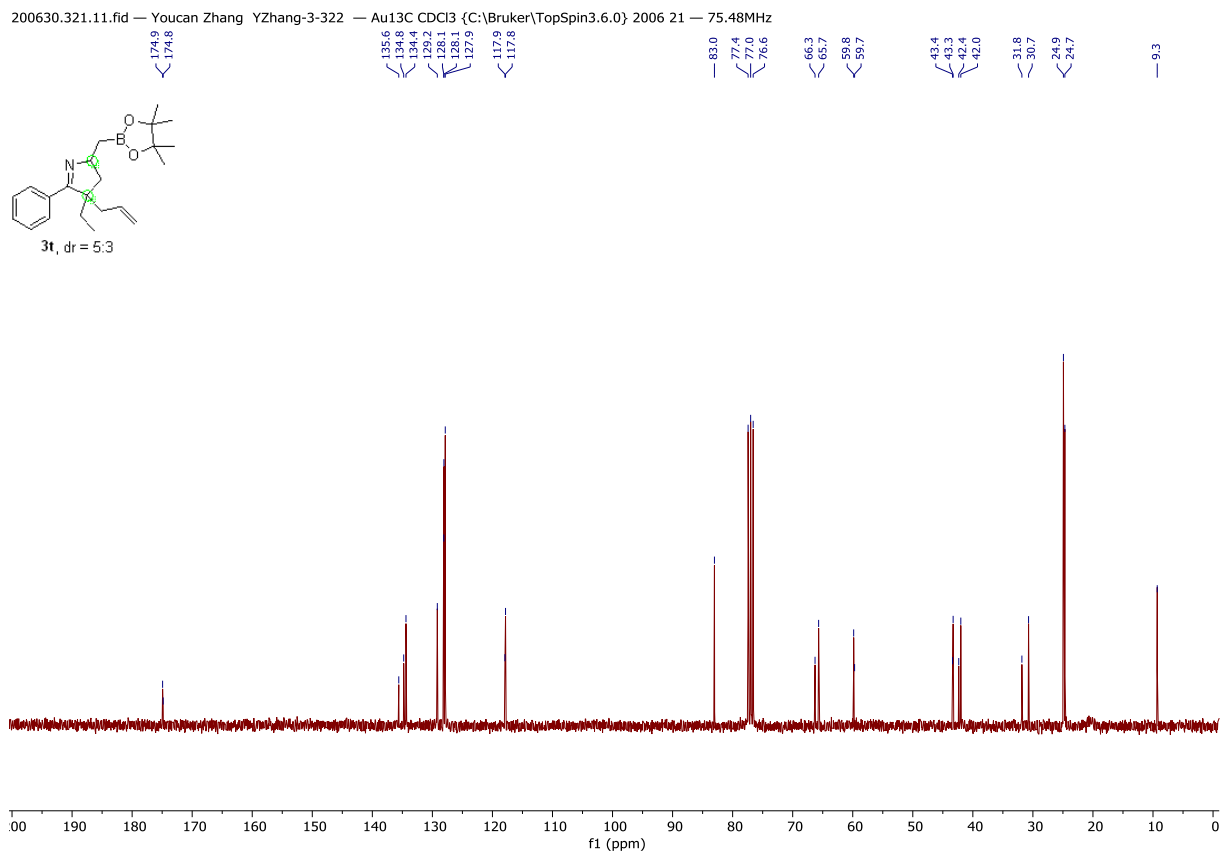
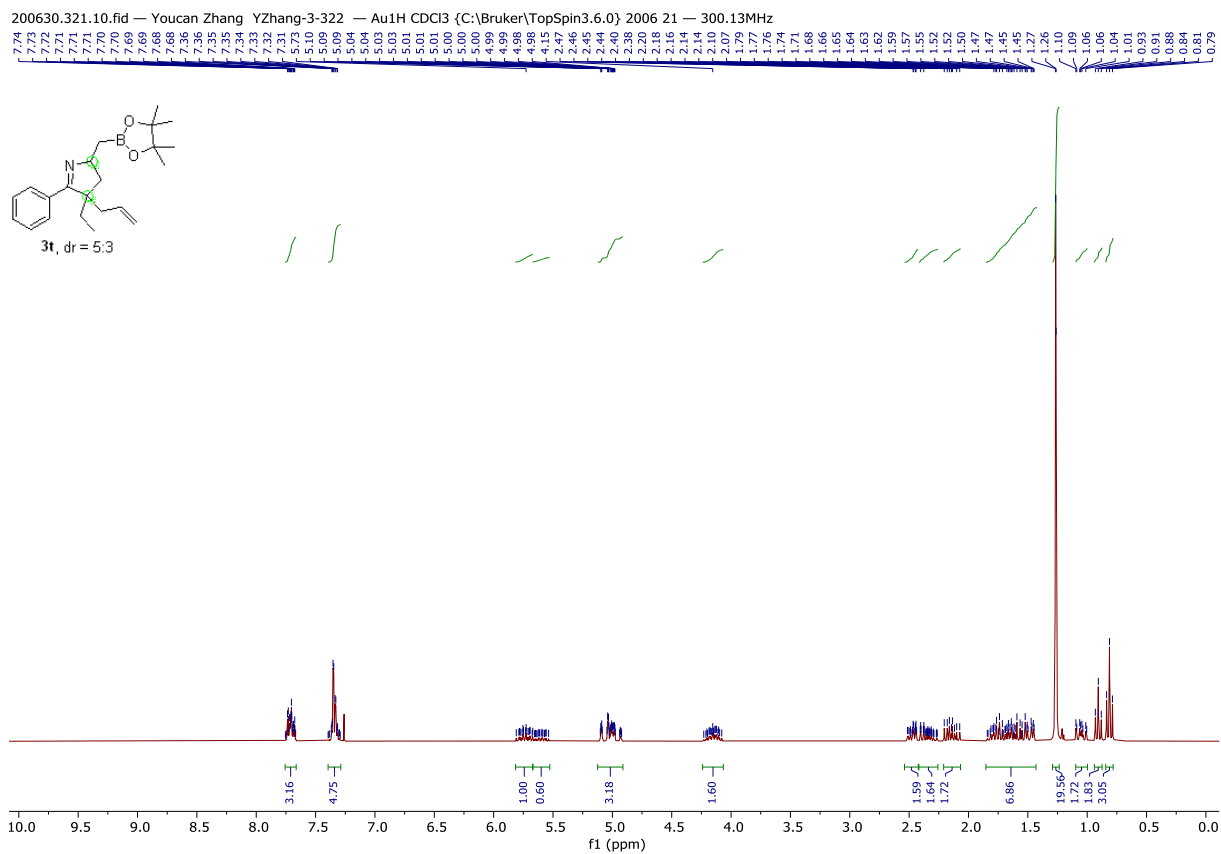
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt

Last modified: Wednesday, August 05, 2020 16:16:22

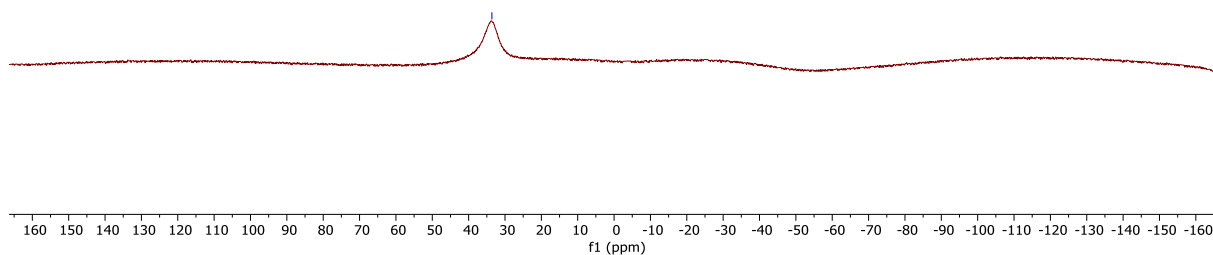
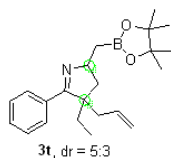
Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
75	20080511	YZ-343+344	Youcan Zhang	352.2563	<u>C22H32BNO2</u>	353.2641	353.2639	-0.6	-0.2
				380.2123	C20H27BNO2F3	354.2608	354.2608	0.0	0.0
						381.2201	381.2202	0.3	0.1
						382.2169	382.2172	0.8	0.3





— 33.6



ESI-TOF Accurate Mass Report

File:20080506

Vial:1:E,3

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-322
Date:05-Aug-2020

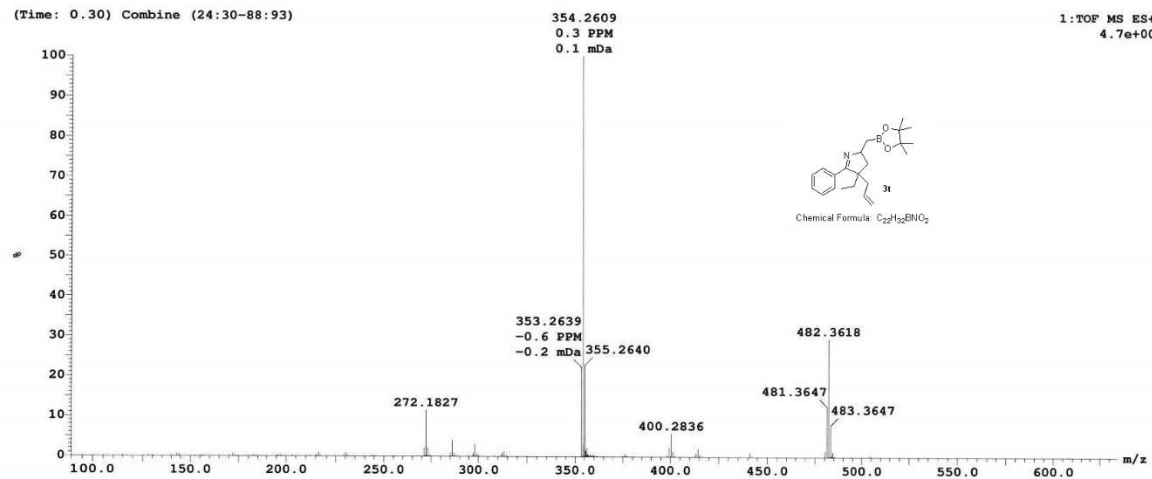
UserName:Youcan Zhang
Time:15:18:54

Page 2

Sample Report:

(Time: 0.30) Combine (24:30-88:93)

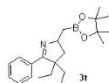
1:TOF MS ES+
4.7e+008



Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 15:54:36

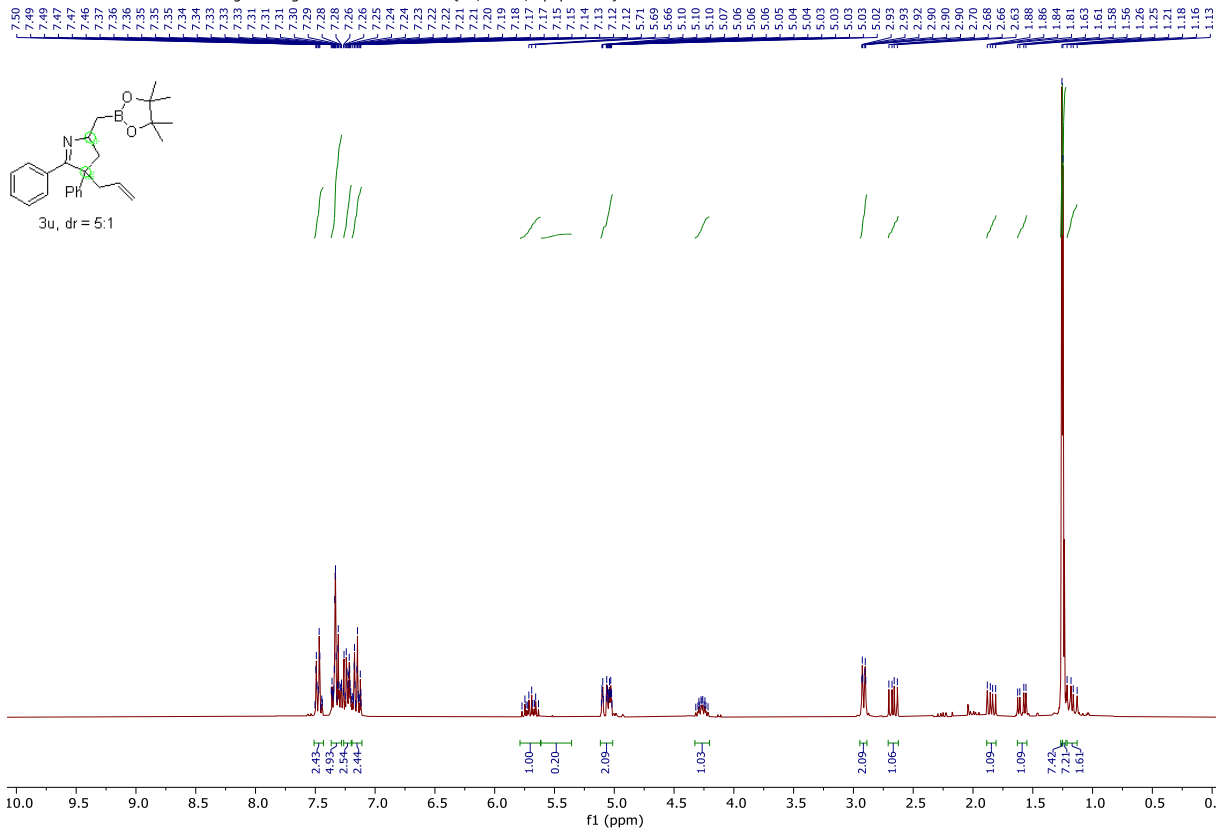
Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
70	20080506	YZ-322	Youcan Zhang	352.2563	C ₂₂ H ₃₂ BrNO ₂	353.2641 354.2608	353.2639 354.2609	-0.6 0.3	-0.2 0.1

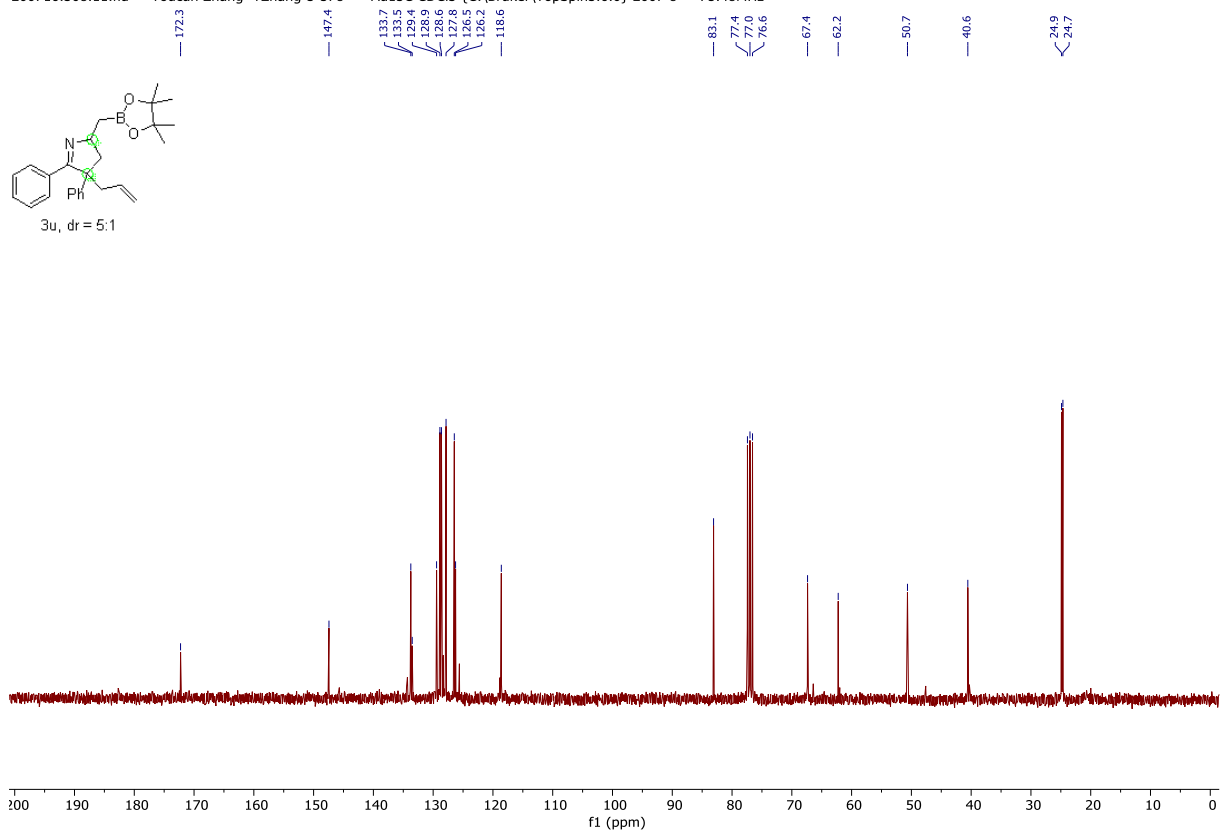


Chemical Formula: C₂₂H₃₂BrNO₂

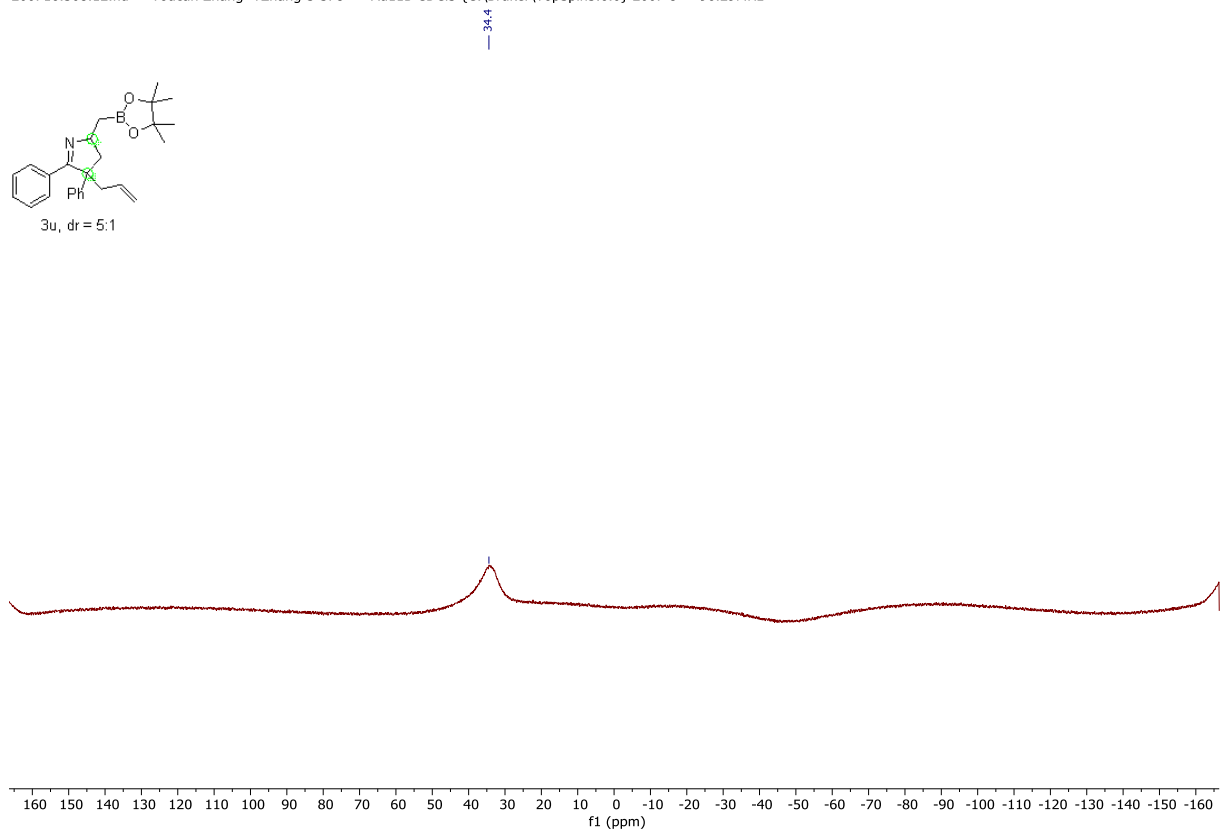
200716.308.10.fid — Youcan Zhang YZhang-3-378 — Au1H CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 8 — 300.13MHz



200716.308.11.fid — Youcan Zhang YZhang-3-378 — Au13C CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 8 — 75.48MHz



200716.308.12.fid — Youcan Zhang YZhang-3-378 — Au11B CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 8 — 96.29MHz



ESI-TOF Accurate Mass Report

File:20080508

Vial:1.E.5

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-378

Date:05-Aug-2020

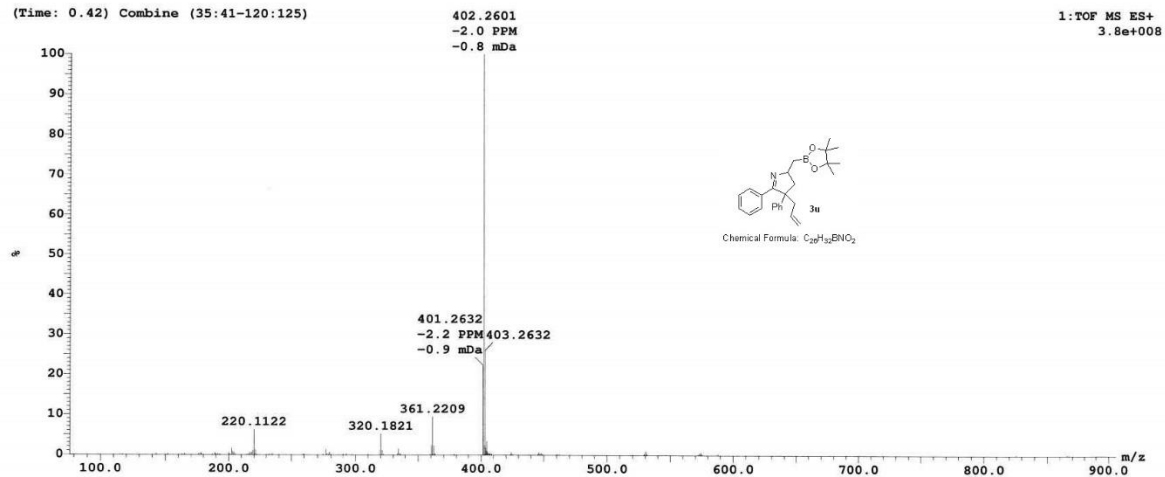
UserName:Youcan Zhang

Time:16:06:18

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Sample Report:

(Time: 0.42) Combine (35:41-120:125)



ESI-TOF Accurate Mass Report

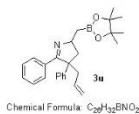
Page 1

Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt

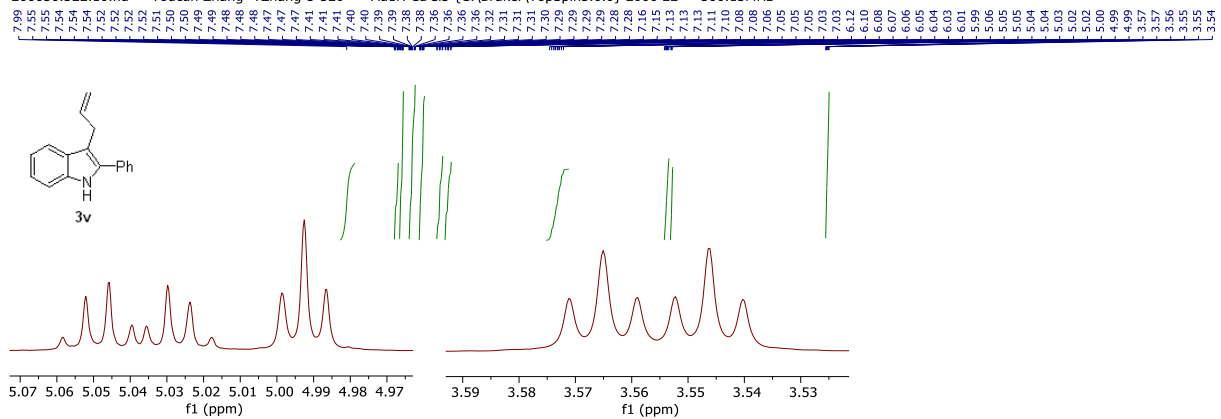
Last modified: Wednesday, August 05, 2020 16:08:47

Sample Summary:

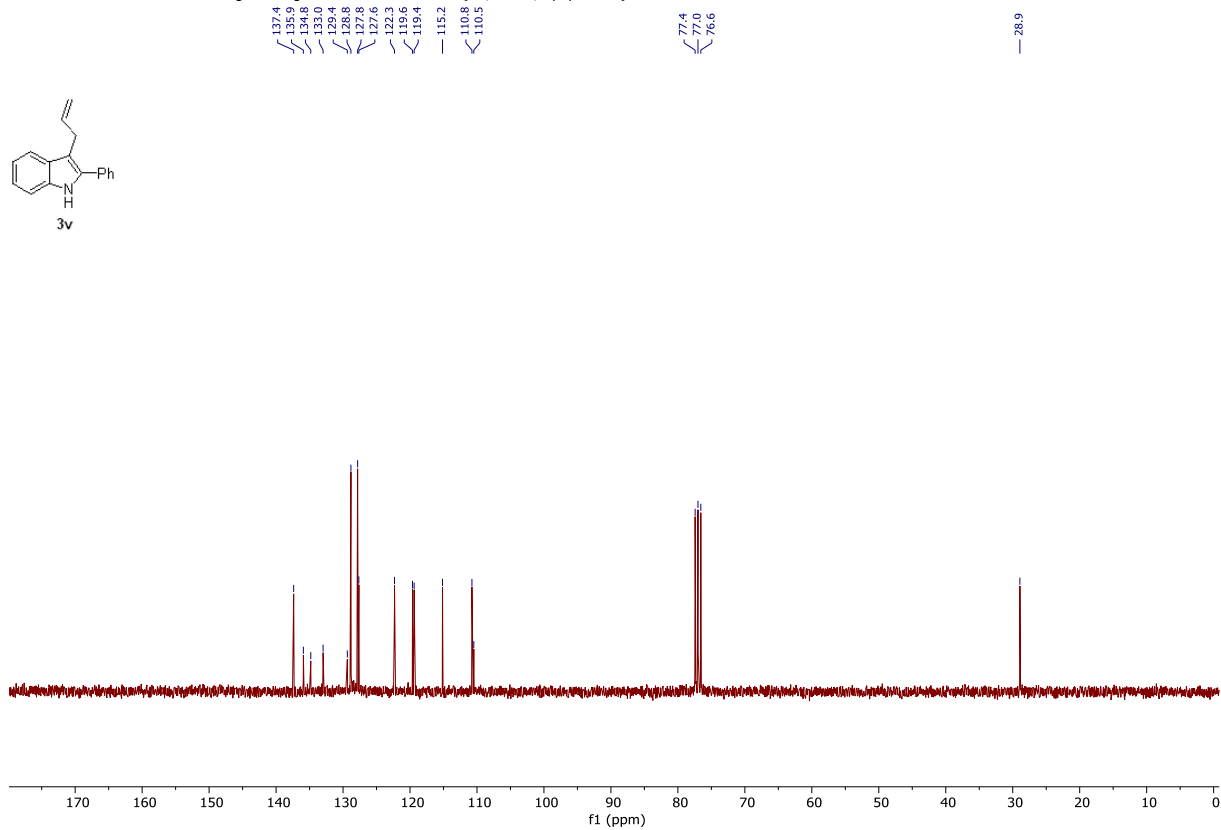
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
72	20080508	YZ-378	Youcan Zhang	400.2563	C ₂₆ H ₃₂ BNO ₂	401.2641 402.2609	401.2632 402.2601	-2.2 -2.0	-0.9 -0.8



200630.322.10.fid — Youcan Zhang YZhang-3-320 — Au1H CDCl₃ {C:\Bruker\TopSpin3.6.0} 2006 22 — 300.13MHz



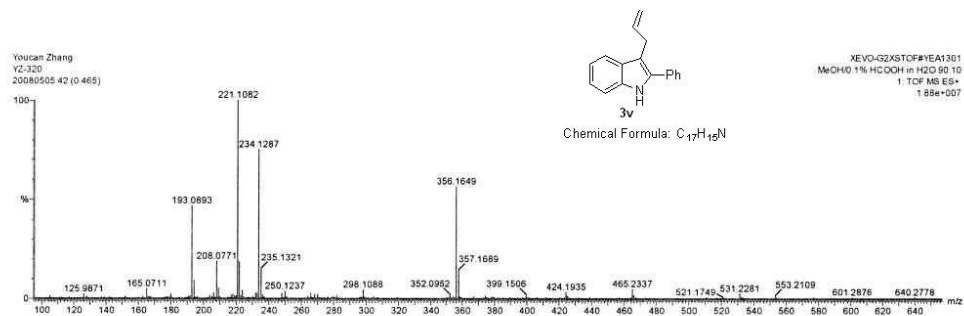
200630.322.11.fid — Youcan Zhang YZhang-3-320 — Au13C CDCl₃ {C:\Bruker\TopSpin3.6.0} 2006 22 — 75.48MHz

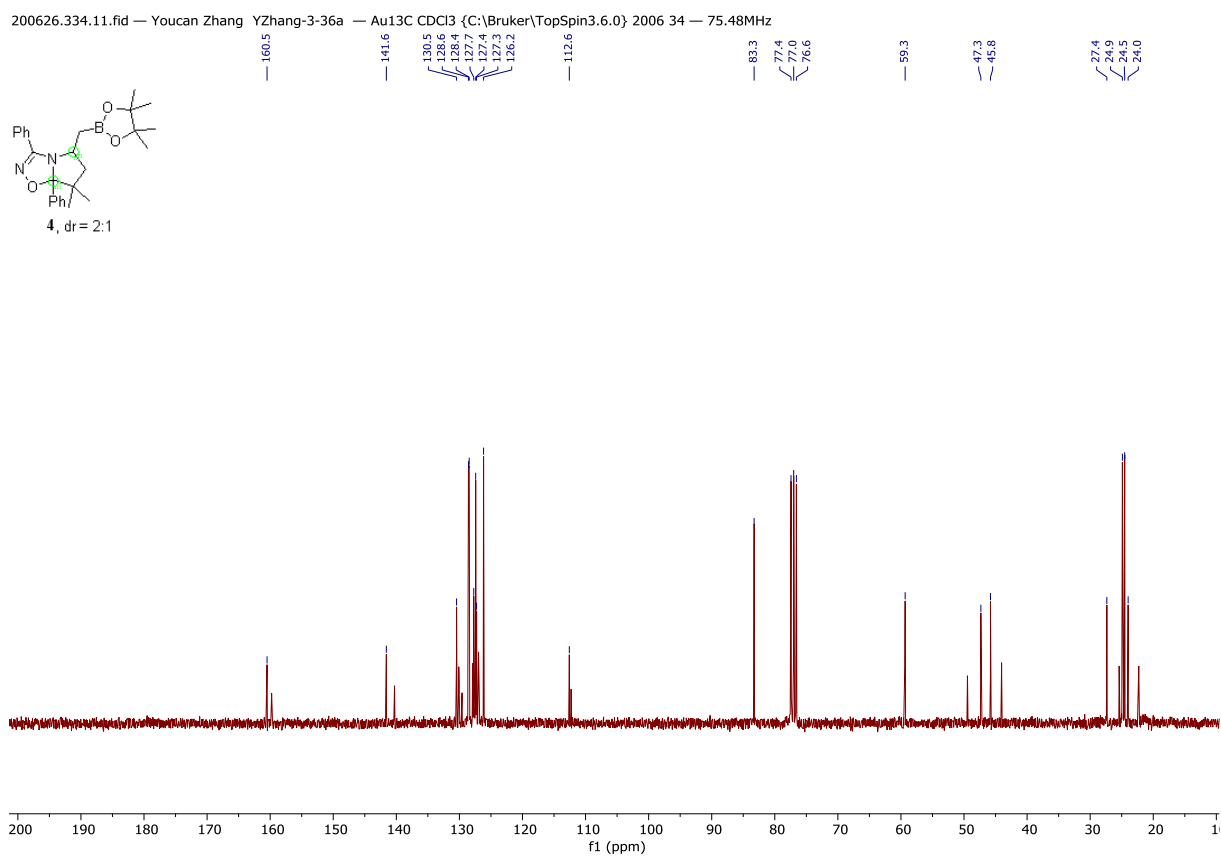
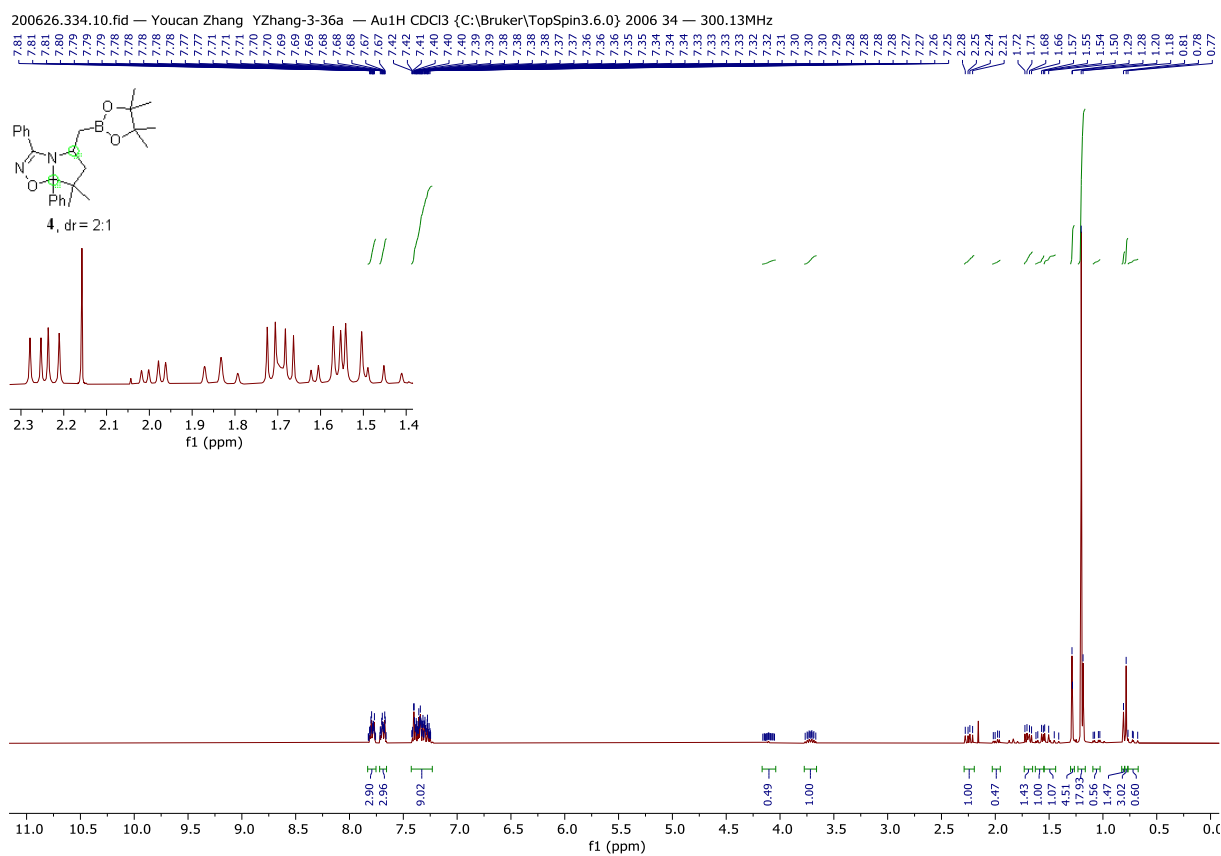


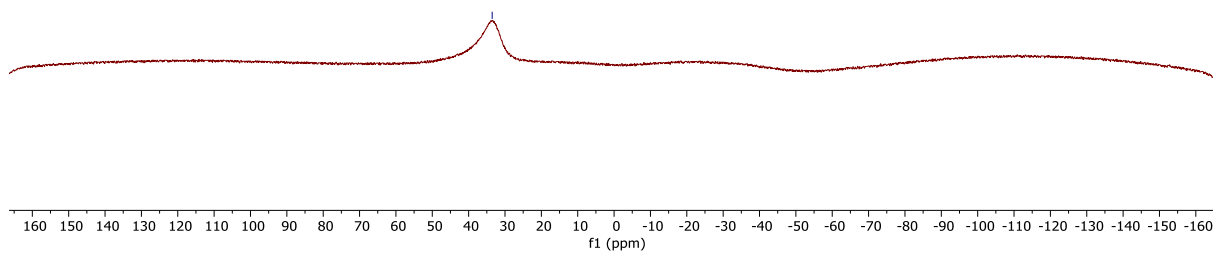
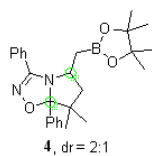
Elemental Composition Report

Youcan Zhang YZ-320

Mass	Calc. Mass	mDa	PPM	Formula
234.1287	234.1283	0.4	1.7	C ₁₇ H ₁₆ N (M+H) ⁺







ESI-TOF Accurate Mass Report

File:20080520

Vial:1:E,1

Description:MeOH/0.1% HCOOH in H₂O 90:10

Sample Name:YZ-36A

Date:05-Aug-2020

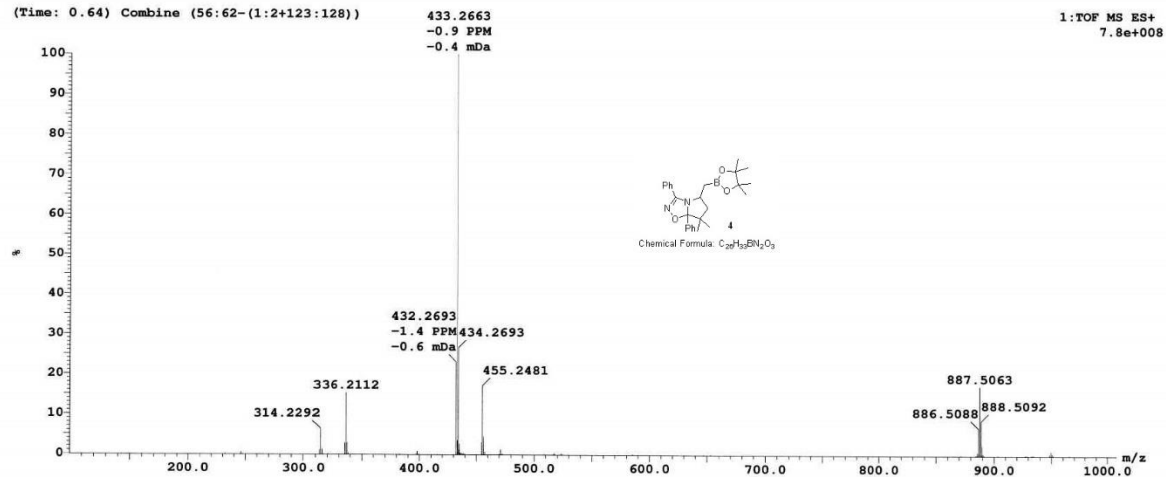
UserName:Youcan Zhang

Time:16:43:30

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Sample Report:

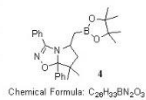
(Time: 0.64) Combine (56:62-(1:2+123:128))



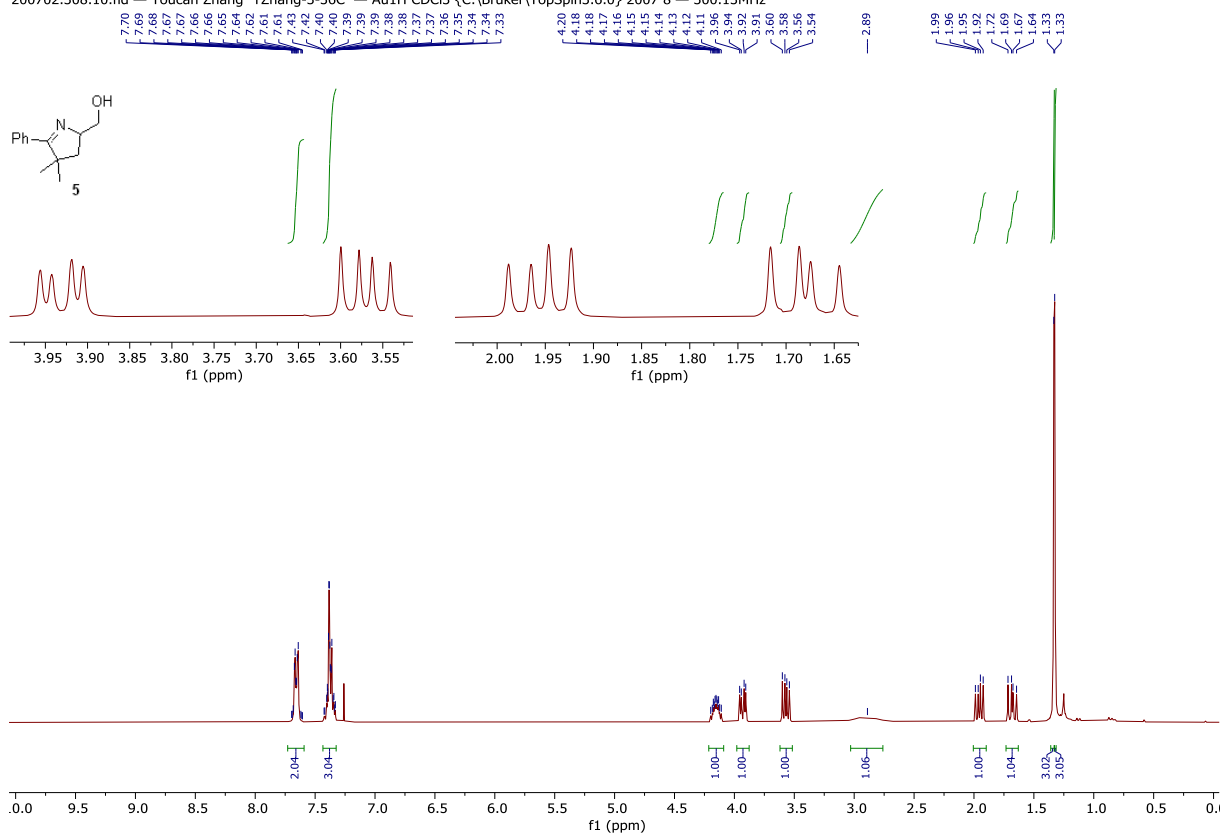
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:46:02

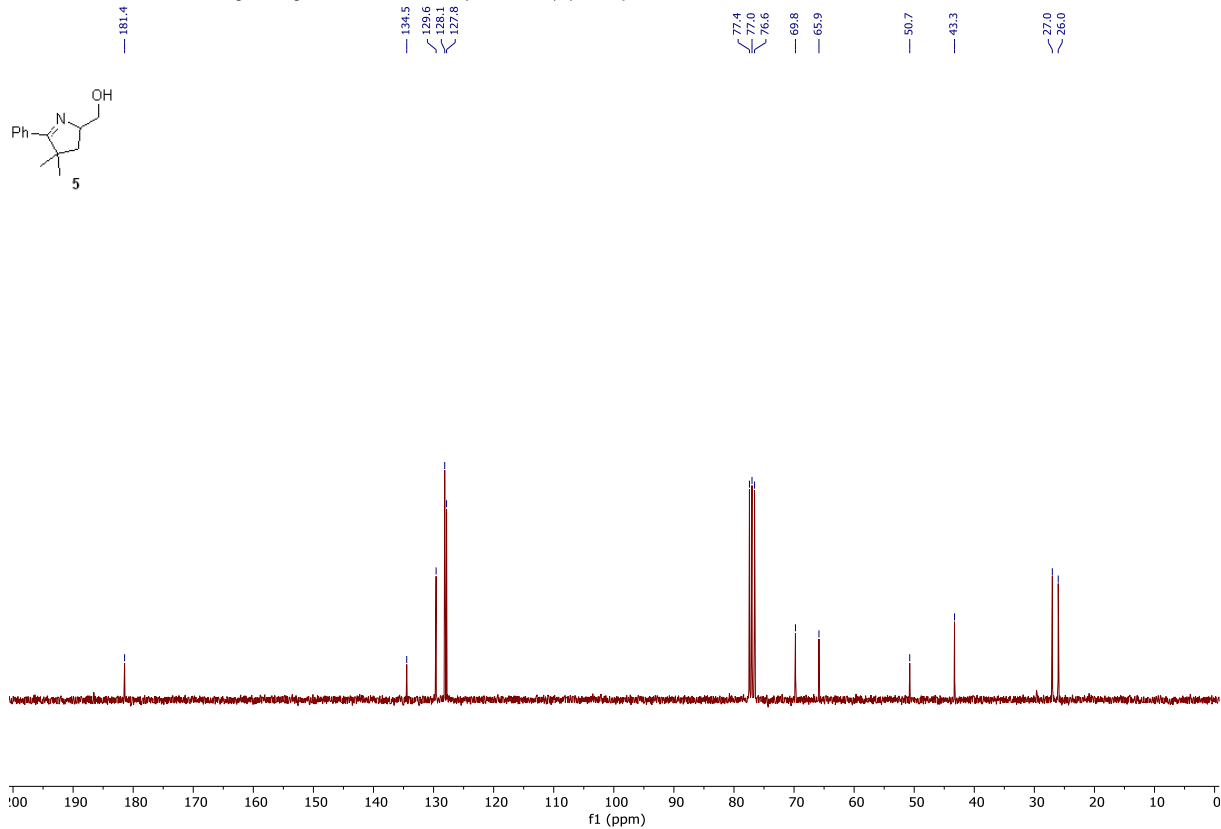
Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
84	20080520	YZ-36A	Youcan Zhang	431.2621	C ₂₆ H ₃₃ BN ₂ O ₃	432.2699 433.2667	432.2693 433.2663	-1.4 -0.9	-0.6 -0.4



200702.308.10.fid — Youcan Zhang YZhang-3-36C — Au1H CDCl₃ {C:\Bruker\TopSpin3.6.0} 2007 8 — 300.13MHz





ESI-TOF Accurate Mass Report

File:20080521

Vial:1.E.2

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-36C
Date:05-Aug-2020

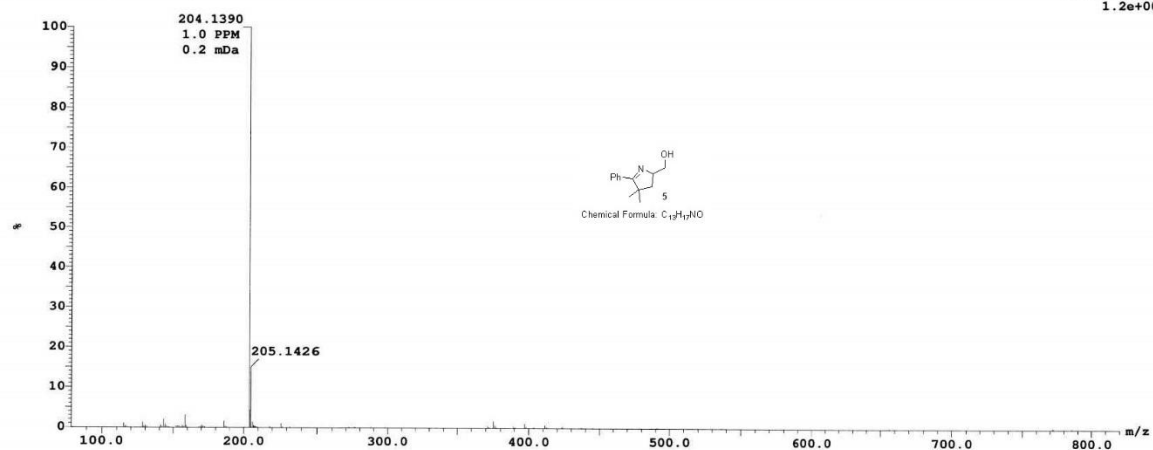
UserName:Youcan Zhang
Time:16:46:05

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Sample Report:

(Time: 0.27) Combine (21:27-86:91)

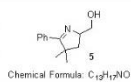
1:TOF MS ES+
1.2e+009



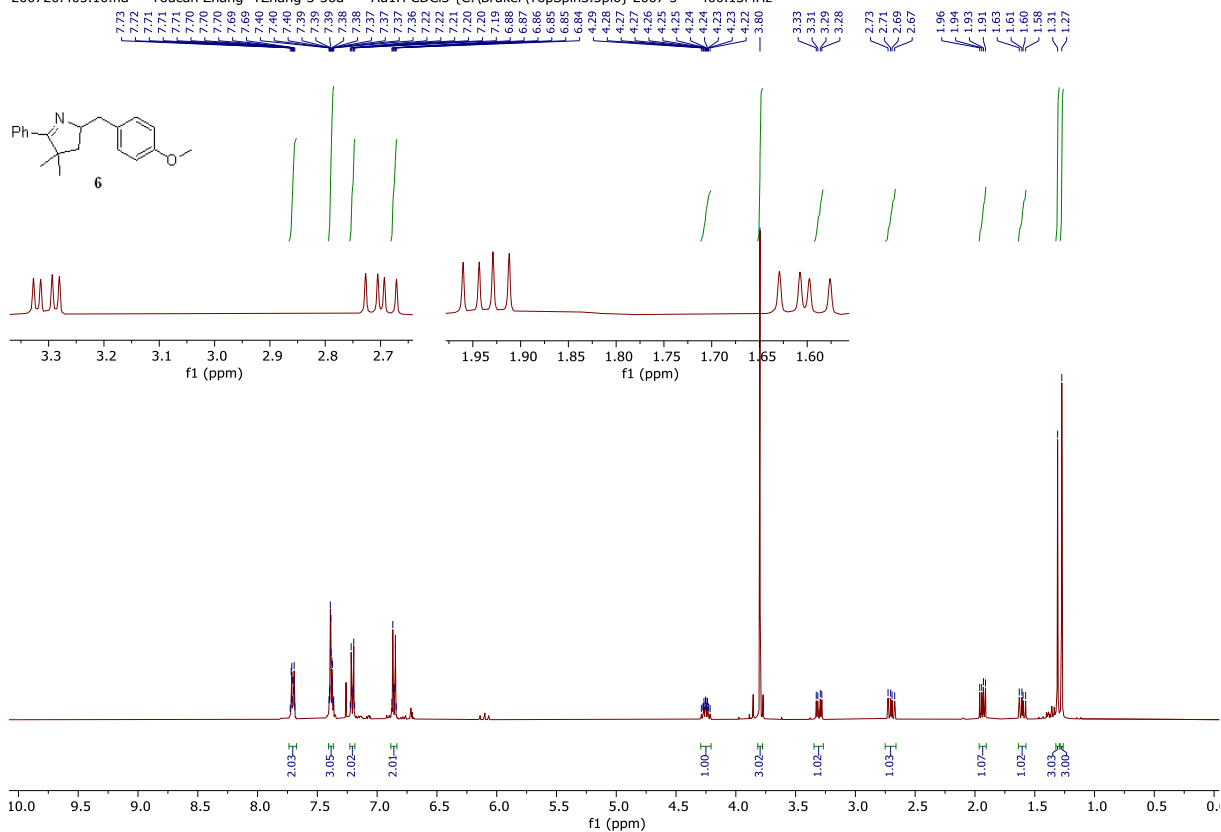
Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:48:37

Sample Summary:

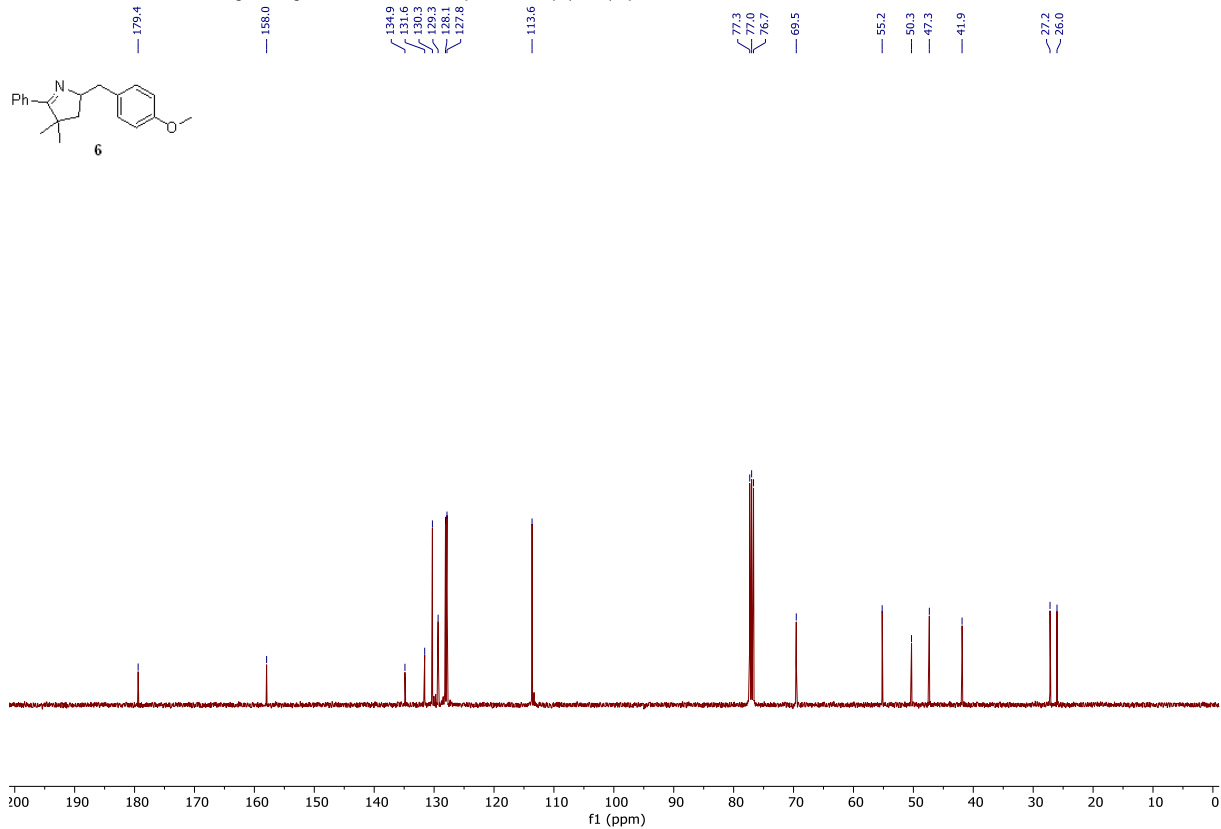
Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
85	20080521	YZ-36C	Youcan Zhang	203.1310	C ₁₃ H ₁₇ NO	204.1388	204.1390	1.0	0.2



200720.405.10.fid — Youcan Zhang YZhang-3-36d — Au1H CDCl₃ {C:\Bruker\TopSpin3.5\pl6} 2007 5 — 400.13MHz



200720.405.11.fid — Youcan Zhang YZhang-3-36d — Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2007 5 — 100.63MHz



ESI-TOF Accurate Mass Report

File:20080522

Vial:1:E.3

Description:MeOH/0.1% HCOOH in H2O 90:10

Sample Name:YZ-36D

Date:05-Aug-2020

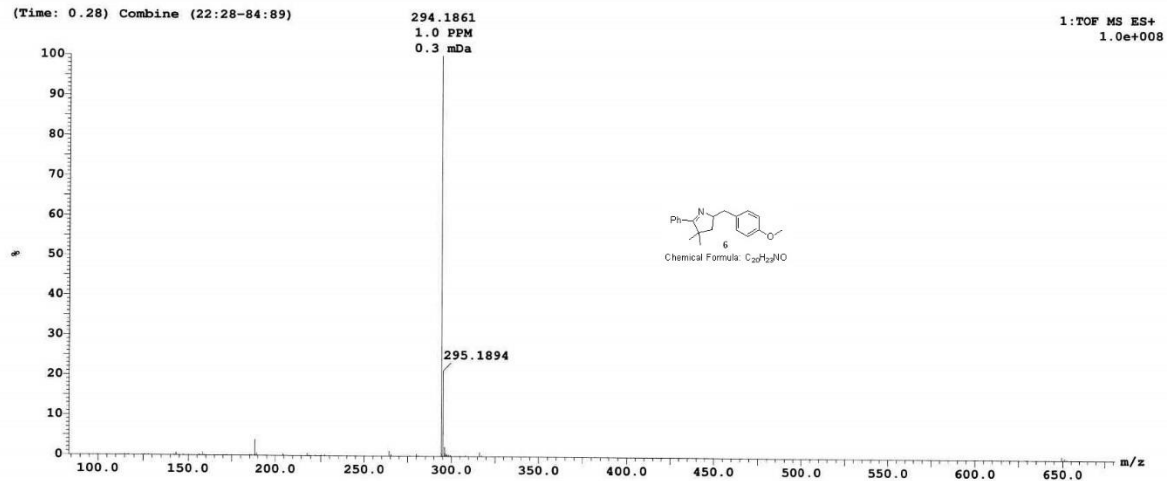
UserName:Youcan Zhang

Time:16:56:25

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Sample Report:

(Time: 0.28) Combine (22:28-84:89)



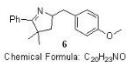
ESI-TOF Accurate Mass Report

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Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:58:53

Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
86	20080522	YZ-36D	Youcan Zhang	293.1780	C ₂₀ H ₂₃ NO	294.1858	294.1861	1.0	0.3



ESI-TOF Accurate Mass Report

Page 2

File:20080519
Vial:1.F.8
Description:MeOH/0.1% HCOOH in H₂O 90:10

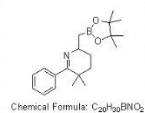
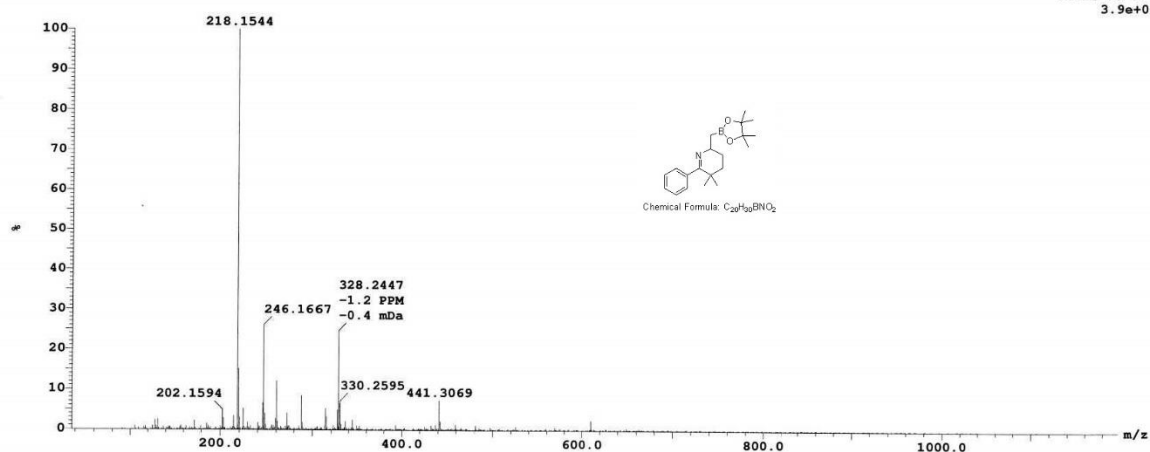
Sample Name:YZ-404
Date:05-Aug-2020

UserName:Youcan Zhang
Time:16:40:55

Sample Report:

(Time: 0.25) Combine (19:25-98:103)

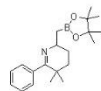
1:TOF MS ES+
3.9e+007



Results file: E:\Projects\2008.PRO\SampleDB\2008.rpt
Last modified: Wednesday, August 05, 2020 16:43:27

Sample Summary:

Sample	File	Sample Name	User	Target	Formula	Expected Mass	Observed Mass	Error PPM	Error mDa
83	20080519	YZ-404	Youcan Zhang	326.2406	C ₂₀ H ₃₀ BN ₂ O ₂	327.2484 328.2451	327.2479 328.2447	-1.5 -1.2	-0.5 -0.4



Chemical Formula: C₂₀H₃₀BN₂O₂