Supporting Information

Open-Air Oxidative Mizoroki-Heck Reaction of Arylsulfonyl hydrazides with Alkenes

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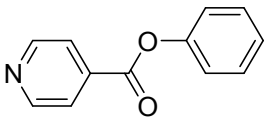
1. General considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All oxidative heck reactions were performed in an open vessel. A vial (approx. 40 mL volume) fitted with an air condenser as cooler was in the presence of Telfon coated magnetic stirrer bar (4 mm x 10 mm). All arylsulfonyl hydrazides except trimethylbenzenesulfonohydrazide were synthesized according to the literatutre report.[1] Phenyl isonicotinate was produced by the following procedures. Thin layer chromatography was performed on Merck precoated silica gel 60 F_{254} plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected Büchi Melting Point B-545 instrument. NMR spectra were recorded on a Brüker spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C and 376 MHz for ^{19}F). Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). ^{19}F NMR chemical shifts were determined relative to $CFCl_3$ as the external standard and low field is positive. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a HP 5989B Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on a Brüker APEX 47e FTICR mass spectrometer (ESI-MS). GC-MS analysis was conducted on a HP 5973 GCD system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from HP 6890 GC-FID system. All yields reported refer to isolated yield of compounds estimated to be greater than 95% purity as determined by capillary gas

chromatography (GC) or ^{1}H NMR. Compounds described in the literature were characterized by comparison of their ^{1}H, ^{13}C and/or ^{19}F NMR spectra to the previously reported data. The procedures in this section are representative, and thus the yields may differ from those reported in tables.

2. General procedure for the preparation of phenyl isonicotinate (L9)

Phenyl isonicotinate (L9)[2]



Thionyl chloride (5.95 g, 50 mmol) was added dropwise to isonicotinic acid (6.15 g, 50 mmol) and triethylamine (5.05 g, 50 mmol) in chloroform (200 mL). The mixture was refluxed for 2 h and cooled down to room temperature. Then a THF solution of sodium phenoxide (Sodium hydride (4.80 g, 60% in mineral oil, 120 mmol, 1.2 equiv.) was suspended in THF (100 mL) under nitrogen and cooled to 0^{o}C in an ice bath. Phenol (8.78 mL, 100 mmol) was added dropwise to the THF solution and stirred for 1 h.) was added dropwise to the resulting isonicotinyl chloride solution, cooled by salt and ice water. The solution was further refluxed for 2 h, and then water (100 mL) and ethyl acetate (200 mL) was added. The organic layer was successively washed with 1M sodium hydroxide solution and then washed with saturated brine solution. The organic layer was concentrated under vacuum and pass through a calica pad (5 x 3 cm) (Eluents = EtOAc: Hexane = 1: 9). The organic layer was concentrated. A white solid was obtained and then further washed with small amount of cool hexane and dry under vacuum. 4.2 g (42% yield) product yield of phenyl isonicotinate was obtained. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.23 (m, 2H), 7.26-7.32 (m, 1H), 7.42-7.47 (m, 2H), 7.99-8.00 (m, 2H), 8.84-8.86 (m, 2H); ^{13}C

NMR (100 MHz,$CDCl_3$) δ 121.3, 123.1, 126.3, 129.6, 136.8, 150.4, 150.8, 163.4; MS (EI): *m/z* (relative intensity) 199.0 (M^+, 37), 106.0 (100), 78.0 (50), 65.0 (7), 51.0 (24).

3. General procedure for the reaction condition screening without pyridine ligand

All reagents were weighted in air and the reactions were performed in an open vessel. Palladium source (0.03 mmol), 4-methylbenzenesulfonyl hydrazide (0.0838 g, 0.45 mmol) and styrene (34.4 μL, 0.3 mmol) were loaded into a 40 mL vial equipped with a Teflon-coated magnetic stir bar. The solvent (3 mL) was added at room temperature. The vial was fitted with an air condenser as cooler and then placed into a preheated oil bath (90 ^oC) and vigorously stirred for 16 h. After the completion of reaction, the reaction vial was allowed to cool at room temperature. Ethyl acetate (~10 mL) and dodecane (68.4 μL, internal standard) were added. The organic layer was subjected to GC analysis. The GC yield obtained was previously calibrated by anthentic sample/dodecane calibration curve.

4. General procedure for the reaction condition screening with pyridine ligand

All reagents were weighted in air and the reactions were performed in an open vessel. $Pd(OAc)_2$ (0.0068 g, 0.03 mmol) and pyridine ligand (Pd:L = 1:2) were loaded into a 40 mL vial equipped with a Teflon-coated magnetic stir bar. Precomplexation was applied by adding DMF (1 mL) in to the vial. The palladium complex stock solution was stirred for 10 minutes. 4-methylbenzenesulfonyl hydrazide (0.0838 g, 0.45 mmol) and styrene (34.4 μL, 0.3 mmol) were loaded into the vial. DMF (2 mL) was added with continuous stirring at room temperature. The vial was fitted with an air condenser as cooler and then placed into a preheated oil bath which the temperature was indicated in the table and vigorously stirred for 16 h.

After the completion of reaction, the reaction vial was allowed to cool at room temperature. Ethyl acetate (~10 mL) and dodecane (68.4 μL, internal standard) were added. The organic layer was subjected to GC analysis. The GC yield obtained was previously calibrated by anthentic sample/dodecane calibration curve.

5. General procedure for the oxidative Heck reaction of arylsulfonyl hydrazides with alkenes

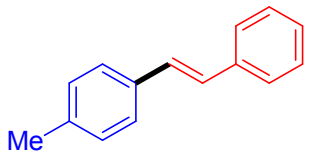
All reagents were weighted in air and the reactions were performed in an open vessel. $Pd(OAc)_2$ (0.0068 g, 0.03 mmol) and phenyl isonicotinate (Pd:L = 1:2) were loaded into a 40 mL vial equipped with a Teflon-coated magnetic stir bar. Precomplexation was applied by adding DMF (1 mL) in to the vial. The palladium complex stock solution was stirred for 10 minutes. Arylsulfonyl hydrazide (0.45 mmol) and alkenes (0.3 mmol) were loaded into the vial. DMF (2 mL) was added with continuous stirring at room temperature. The vial was fitted with an air condenser as cooler and then placed into a preheated oil bath which the temperature was indicated in the table and vigorously stirred for 16 h. After the completion of reaction, the reaction vial was allowed to cool at room temperature. Ethyl acetate (~10 mL) was added. The organic layer was subjected to GC analysis. After analyzing GC spectra, the crude product in the organic layer was extracted and the vial washed with ethyl acetate. The filtrate was concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel (230 - 400 mesh) to afford the desired product.

6. General procedure for the kinetic study of the oxidative Heck reaction of 4-methylbenzenesulfonyl hydrazide with styrene.

For the reaction with pyridine ligand ***L9***, $Pd(OAc)_2$ (0.0068 g, 0.03 mmol) and phenyl isonicotinate (Pd:L = 1:2) were loaded into a 25 mL reaction tube (tube A) with a narrow opening (4 mm) equipped with a Teflon-coated magnetic stir bar (3 x 8 mm). DMF (1 mL) was added to the reaction tube and the mixture was stirred for 10 minutes. During that time, *for the reaction without pyridine ligand* ***L9***, $Pd(OAc)_2$ (0.0068 g, 0.03 mmol), 4-methylbenzenesulfonyl hydrazide (0.0838 g, 0.45 mmol), styrene (34.4 μL, 0.3 mmol), and 1,4-dimethoxybenzene (internal standard, 0.0414 g, 0.3 mmol) were loaded into another 25 mL reaction tube (tube B) with a narrow opening (4 mm) equipped with a Teflon-coated magnetic stir bar (3 x 8 mm). After 10 minutes, 4-methylbenzenesulfonyl hydrazide (0.0838 g, 0.45 mmol), styrene (34.4 μL, 0.3 mmol), 1,4-dimethoxybenzene (internal standard, 0.0414 g, 0.3 mmol) and additional DMF (2 mL) were added into tube A meanwhile DMF (3 mL) was added to tube B. Tube A and B were allowed to stir at room temperature for 1 min. The tubes were then placed into a preheated oil bath (90 ^{o}C) with vigorous stirring. For the reaction time (data points) indicated in the Scheme 2, reaction mixtures (0.05 mL) in each reaction tube were taken up, diluted with ethyl acetate (0.5 mL) and then subjected to GC analysis. The GC yield obtained was previously calibrated by anthentic sample/1,4-dimethoxybenzene calibration curve.

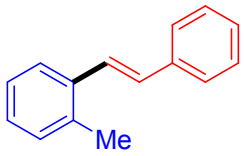
7. Characterization data of coupling products

Benzene, 1-methyl-4-[(1*E*)-2-phenylethenyl]- (Table 3, compound 3ak)[3]



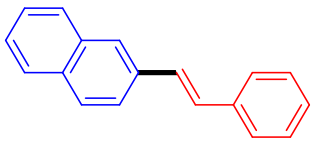
Eluents (Hexane, R_f= 0.56) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2,45 (s, 3H), 7.12-7.21 (m, 2H), 7.26 (d, *J*= 8.0 Hz, 2H), 7.31-7.36 (m, 1H), 7.44 (t, *J*= 6.8 Hz, 2H), 7.51 (d, *J*= 8.0 Hz, 2H), 7.59 (d, *J*= 7.6 Hz, 2H) ; ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.2, 126.4, 127.4, 127.7, 128.6, 129.4, 134.5, 137.5; MS (EI): *m/z* (relative intensity) 194.1 (M^+, 96), 179.0 (100), 165.0 (12), 152.0 (9), 115.0 (11).

Benzene, 1-methyl-2-[(1*E*)-2-phenylethenyl]- (Table 3, compound 3bk)[4]



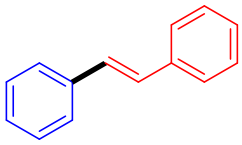
Eluents (Hexane, R_f= 0.56) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.52 (s, 3H), 7.07-7.11 (d, *J*= 16 Hz, 1H), 7.26-7.38 (m, 4H), 7.41-7.47 (m, 3H), 7.61 (d, *J*= 8.0 Hz, 2H), 7.69 (d, *J*= 6.8 Hz, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 19.9, 125.3, 126.2, 126.5, 127.5, 128.6, 130.0, 130.4, 135.8, 136.4, 137.6; MS (EI): *m/z* (relative intensity) 194.1 (M^+, 79), 179.0 (100), 165.0 (13), 152.0 (8), 115.0 (22).

Naphthalene, 2-[(1*E*)-2-phenylethenyl]- (Table 3, compound 3ck)[3]



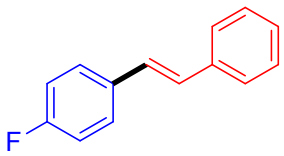
Eluents (Hexane, R_f= 0.38) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.35 (m, 3H), 7.41-7.45 (m, 2H), 7.47-7.56 (m, 2H), 7.60-7.62 (m, 2H), 7.77-7.80 (m, 1H), 7.85-7.89 (m, 4H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 14.2, 21.0, 29.7, 60.4, 123.5, 125.9, 126.3, 126.6, 127.7, 128.0, 128.3, 128.7, 129.0, 171.1; MS (EI): *m/z* (relative intensity) 230.1 (M^+, 100), 215.0 (23), 202.0 (11), 114.1 (3), 101.0 (9)

Benzene, 1,1'-(1*E*)-1,2-ethenediylbis- (Table 3, compound 3dk)[3]



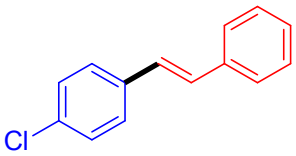
Eluents (Hexane, R_f= 0.50) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (s, 2H), 7.30-7.34 (m, 2H), 7.40-7.44 (m, 4H), 7.57-7.59 (m, 4H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 126.4, 127.5, 128.6, 137.3; MS (EI): *m/z* (relative intensity) 180.0 (M^+, 100), 165.0 (49), 152.0 (13), 89.0 (27), 76.0 (20), 51.0 (19).

Benzene, 1-fluoro-4-[(1*E*)-2-phenylethenyl]- (Table 3, compound 3ek)[3]



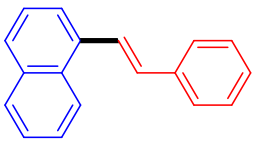
Eluents (Hexane, R_f= 0.44) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04-7.14 (m, 4H), 7.28-7.33 (m, 1H), 7.39-7.43 (m, 2H), 7.49-7.55 (m, 4H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 115.5, 115.7, 126.4, 127.4, 127.6, 127.9, 128.4, 133.5, 137.1, 161.1, 163.5; ^{19}F NMR (400 MHz,$CDCl_3$) δ -114.2; MS (EI): *m/z* (relative intensity) 198.0 (M^+, 100), 183.0 (38), 170.0 (8), 120.0 (5), 98.0 (10).

Benzene, 1-chloro-4-[(1*E*)-2-phenylethenyl]- (Table 3, compound 3fk)[3]



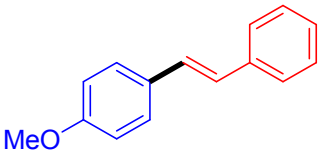
Eluents (Hexane, R_f=0.49) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) □δ 7.06-7.15 (m, 2H), 7.28-7.43 (m, 5H), 7.46-7.49 (m, 2H), 7.53-7.55 (m, 2H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 126.5, 127.3, 127.6, 127.8, 128.7, 128.8, 129.3, 133.1, 135.8, 136.9; MS (EI): *m/z* (relative intensity) 214.0 (M^+, 78), 178.0 (100), 152.0 (14), 115.0 (2), 76.0 (18).

Naphthalene, 1-[(1*E*)-2-phenylethenyl]- (Table 3, compound 3gk)[3]



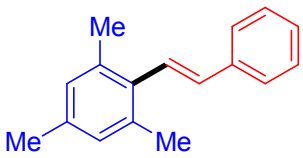
Eluents (Hexane, R_f= 0.54) was used for flash column chromatography. Yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, *J*= 16.0 Hz, 1H), 7.36-7.38 (m, 1H), 7.45-7.48 (m, 2H), 7.53-7.62 (m, 3H), 7.66-7.68 (m, 2H), 7.81 (d, *J*= 7.2 Hz, 1H), 7.86 (d, *J*= 8.4 Hz, 1H), 7.92-7.97 (m, 2H), 8.28 (d, *J*= 8.6 Hz, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 123.6, 123.7, 125.7, 125.8, 126.1, 126.7, 127.7, 128.0, 128.6, 128.7, 131.4, 131.7, 133.7, 135.0, 137.6; MS (EI): *m/z* (relative intensity) 229.1 (M^+, 100), 215.0 (18), 202.0 (13), 152.0 (21), 128.0 (5).

Benzene, 1-methoxy-4-[(1*E*)-2-phenylethenyl]- (Table 3, compound 3hk)[3]



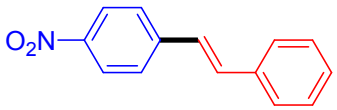
Eluents (EtOAc: Hexane = 1: 20, R_f= 0.40) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.87 (s, 3H), 6.93-6.97 (m, 2H), 7.01-7.14 (m, 2H), 7.26-7.31 (m, 1H), 7.38-7.41 (m, 2H), 7.49-7.55 (m, 4H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 55.29, 114.13, 126.2, 126.6, 127.2, 127.7, 128.2, 128.6, 130.1, 137.6, 159.3; MS (EI): *m/z* (relative intensity) 210.1 (M^+, 100), 195.0 (18), 179.0 (15), 165.0 (38), 152.0 (23).

Benzene, 1,3,5-trimethyl-2-[(1*E*)-2-phenylethenyl]- (Table 3, compound 3ik)[3]



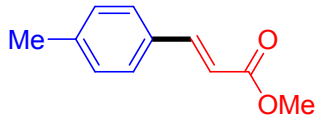
Eluents (Hexane, R_f= 0.50) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.36 (s, 3H), 2.41 (s, 6H), 7.66 (d, *J*= 16.8 Hz, 1H), 6.97 (s, 2H), 7.17 (d, *J*= 16.8 Hz, 1H), 7.33-7.36 (m, 1H), 7.42-7.45 (m, 2H), 7.57 (d, *J*= 7.2 Hz, 2H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 20.9, 126.2, 126.8, 127.4, 128.6, 133.6, 133.9, 136.1, 136.2, 137.7; MS (EI): *m/z* (relative intensity) 222.1 (M^+, 91), 207.1 (100), 192.0 (78), 178.0 (9), 144.0 (9).

Benzene, 1-nitro-4-[(1*E*)-2-phenylethenyl]- (Table 3, compound jk)[3]



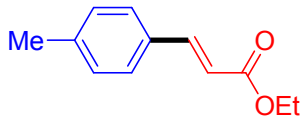
Eluents (EtOAc: Hexane = 1: 9, R_f= 0.70) was used for flash column chromatography. Yellow solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (d, *J*= 16.4 Hz, 1H), 7.27-7.45 (m, 4H), 7.56-7.59 (m, 2H), 7.64-7.67 (m, 2H), 8.22-8.26 (m, 2H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 124.1, 126.3, 126.8, 127.0, 128.9, 133.3, 136.2, 143.8, 146.8; MS (EI): *m/z* (relative intensity) 225.0 (M^+, 83), 207.0 (9), 178.0 (100), 165.0 (13), 152.0 (25).

2-Propenoic acid, 3-(4-methylphenyl)-, methyl ester, (2*E*)- (Table 3, compound 3al)[5]



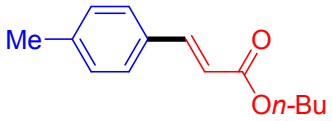
Eluents (EtOAc: Hexane = 1: 9, R_f= 0.53) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.40 (s, 3H), 3.82 (s, 3H), 6.42 (d, *J*= 16.0 Hz, 1H), 7.21 (d, *J*= 8.0 Hz, 2H), 7.44 (d, *J*= 8.0 Hz, 2H), 7.70 (d, *J*= 16.0 Hz, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.4, 51.6, 116.7 128.0, 129.6, 131.6, 140.7, 144.8, 167.6; MS (EI): *m/z* (relative intensity) 176.0 (M^+, 63), 161.0 (6), 145.0 (100), 115.0 (50), 91.0 (20).

2-Propenoic acid, 3-(4-methylphenyl)-, ethyl ester, (2*E*)- (Table 3, compound 3am)[6]



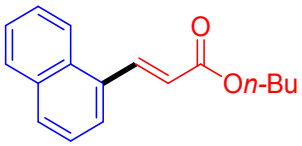
Eluents (EtOAc: Hexane = 1: 20, R_f= 0.52) was used for flash column chromatography. Yellow liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.36 (t, *J*= 7.2 Hz, 3H), 2.39 (s, 3H), 4.26 – 4.31 (m, 2H), 6.42 (d, *J*= 16.0 Hz, 1H), 7.21 (d, *J*= 8.0 Hz, 2H), 7.44 (d, *J*= 8.0 Hz, 2H), 7.69 (d, *J*= 15.6 Hz, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 14.3, 21.4, 60.4 117.1, 128.0, 129.6, 131.7, 140.6, 144.5, 167.1; MS (EI): *m/z* (relative intensity) 190.0 (M^+, 48), 175.0 (3), 162.0 (13), 145.0 (100), 115.0 (46).

2-Propenoic acid, 3-(4-methylphenyl)-, butyl ester, (2*E*)- (Table 3, compound 3an)[3]



Eluents (EtOAc: Hexane = 1: 20, R_f= 0.52) was used for flash column chromatography. Colorless liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.99 (t, *J*= 7.6 Hz, 3H), 1.44-1.49 (m, 2H), 1.69 – 1.73 (m, 2H), 2.39 (s, 3H), 4.23 (t, *J*= 6.4 Hz, 2H), 6.42 (d, *J*= 16.0 Hz, 1H), 7.21 (d, *J*= 8.0 Hz, 2H), 7.45 (d, *J*= 8.0 Hz, 2H), 7.68 (d, *J*=16.0 Hz, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 13.7, 19.1, 21.4 30.7, 64.2, 117.1, 128.0, 129.5, 131.7, 140.5, 144.5, 167.2; MS (EI): *m/z* (relative intensity) 218.1 (M^+, 26), 162.0 (95), 145.0 (100), 115.0 (51), 91.0 (25).

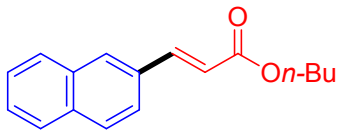
2-Propenoic acid, 3-(1-naphthalenyl)-, butyl ester, (2*E*)- (Table 3, compound 3gn)[7]



Eluents (EtOAc: Hexane = 1: 20, R_f= 0.64) was used for flash column chromatography. Yellow liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.04 (t, *J*= 7.2 Hz, 3H), 1.49-1.54 (m, 2H), 1.74-1.79 (m, 2H), 4.31 (t, *J*= 6.4 Hz, 2H), 6.58 (d, *J*= 15.6 Hz, 1H), 7.49-7.63 (m, 3H), 7.78 (d, *J*= 6.8 Hz, 1H), 7.91 (t, *J*= 7.2 Hz, 2H), 8.23 (d, *J*= 8.4 Hz, 1H), 8.57 (d, *J*= 15.6 Hz, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 13.7, 19.2, 30.8, 64.5, 120.9, 123.3, 124.9, 125.4, 126.1, 126.8, 128.7, 130.4, 131.4, 131.8, 133.6,

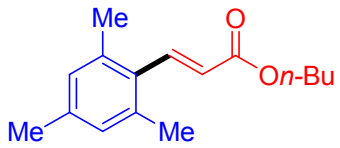
141.5, 166.9; MS (EI): *m/z* (relative intensity) 254.1 (M^+, 27), 198.0 (7), 181.0 (25), 153.0 (100), 76.1 (5).

2-Propenoic acid, 3-(2-naphthalenyl)-, butyl ester, (2*E*)- (Table 3, compound 3cn)[5]



Eluents (EtOAc: Hexane = 1: 20, R_f= 0.60) was used for flash column chromatography. Colorless liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02 (t, *J*= 7.2 Hz, 3H), 1.47-1.53 (m, 2H), 1.71-1.77 (m, 2H), 4.28 (t, *J*= 6.8 Hz, 2H), 6.59 (d, *J*= 16.0 Hz, 1H), 7.52-7.54 (m, 2H), 7.68 (d, *J*= 8.4 Hz, 1H), 7.83-7.94 (m, 5H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 1.0, 13.7, 19.2, 30.8, 64.4, 118.4, 123.4, 126.6, 127.1, 127.7, 128.5, 128.6, 129.8, 131.9, 133.2, 134.1, 144.5, 167.1; MS (EI): *m/z* (relative intensity) 254.1 (M^+, 52), 198.0 (100), 181.0 (70), 152.0 (65), 127.0 (11).

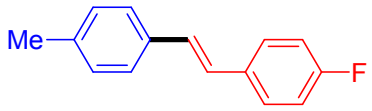
2-Propenoic acid, 3-(2,4,6-trimethylphenyl)-, butyl ester, (2*E*)- (Table 3, compound 3in)[5]



Eluents (EtOAc: Hexane = 1: 20, R_f= 0.49) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.01 (t, *J*= 7.6 Hz,

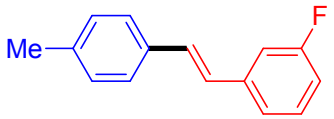
3H), 1.45-1.51 (m, 2H), 1.70-1.75 (m, 2H), 2.32 (s, 3H), 2.36 (s, 6H), 4.25 (t, *J*= 6.8 Hz, 2H), 6.09 (d, *J*= 16.4Hz, 1H), 6.92 (s, 2H), 7.87 (d, *J*= 16.4Hz, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 13.7, 19.2, 20.9, 21.0, 30.7, 64.3, 123.1, 129.1, 130.9, 136.7, 138.2, 143.1, 167.0; MS (EI): *m/z* (relative intensity) 246.1 (M^+, 27), 231.1 (5), 173.0 (100), 144.1 (52), 129.0 (39).

Benzene, 1-fluoro-4-[(1*E*)-2-(4-methylphenyl)ethenyl]- (Table 3, compound 3ao)[8]



Eluents (Hexane, R_f= 0.56) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 7.05-7.11 (m, 4H), 7.22 (d, *J*= 8.0 Hz, 2H), 7.45 (d, *J*= 8.0 Hz, 2H), 7.49-7.52 (m, 2H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.2, 115.4, 115.6, 126.3, 126.4, 127.7, 127.8, 128.4, 129.4, 133.6, 134.3, 137.5, 160.9, 163.4; ^{19}F NMR (400 MHz,$CDCl_3$) δ -114.6; MS (EI): *m/z* (relative intensity) 212.1 (M^+, 100), 197.0 (67), 177.0 (18), 115.0 (8), 91.1 (10).

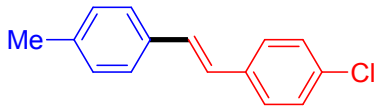
Benzene, 1-fluoro-3-[2-(4-methylphenyl)ethenyl]-, (*E*)- (Table 3, compound 3ap)[9]



Eluents (Hexane, R_f= 0.56) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.42 (s, 3H), 6.96-7.01 (m, 1H), 7.04-7.15 (m, 2H),

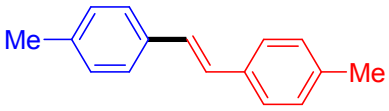
7.22-7.38 (m, 5H), 7.46 (d, *J*= 8.0 Hz, 2H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.3, 112.5, 112.7, 114.0, 114.2, 122.3, 126.5, 126.8, 129.4, 130.0, 134.0, 138.0, 139.9, 162.0, 164.4; ^{19}F NMR (400 MHz,$CDCl_3$) δ -113.5; MS (EI): *m/z* (relative intensity) 212.1 (M^+, 100), 197.0 (88), 177.0 (24), 115.0 (8), 91.1 (10).

Benzene, 1-chloro-4-[(1*E*)-2-(4-methylphenyl)ethenyl]- (Table 3, compound 3aq)[3]



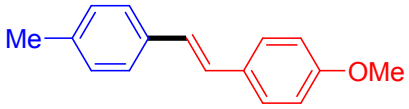
Eluents (Hexane, R_f= 0.56) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.39 (s, 3H), 7.00-7.11 (m, 2H), 7.20 (d, *J*= 7.6 Hz, 2H), 7.33-7.36 (m, 2H), 7.42-7.47 (m, 4H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.3, 126.4, 126.5, 127.5, 128.8, 129.3, 129.4, 132.9, 134.2, 136.1, 137.8; MS (EI): *m/z* (relative intensity) 228.0 (M^+, 100), 213.0 (16), 192.0 (26), 178.0 (95), 94.7 (12).

Benzene, 1,1'-(1*E*)-1,2-ethenediylbis[4-methyl- (Table 3, compound 3ar)[3]



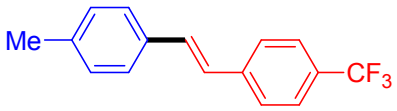
Eluents (Hexane, R_f= 0.56) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.42 (s, 6H), 7.10 (s, 2H), 7.22 (d, *J*= 8.0 Hz, 4H), 7.46 (d, *J*= 8.0 Hz, 4H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.2, 126.3, 127.6, 129.3, 134.7, 137.2; MS (EI): *m/z* (relative intensity) 208.1 (M^+, 100), 193.0 (57), 178.0 (59), 152.0 (5), 115.0 (13).

Benzene, 1-methoxy-4-[(1*E*)-2-(4-methylphenyl)ethenyl]- (Table 3, compound 3as)[3]



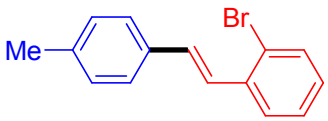
Eluents (EtOAc: Hexane = 1: 20, R_f= 0.48) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.40 (s, 3H), 3.86 (s, 3H), 6.92-6.96 (m, 2H), 6.97-7.09 (m, 2H), 7.20 (d, *J*= 7.6 Hz, 2H), 7.42-7.50 (m, 4H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.2, 55.3, 114.1, 126.1, 126.5, 127.2, 127.6, 129.3, 130.3, 134.8, 137.0, 159.1; MS (EI): *m/z* (relative intensity) 224.1 (M^+, 100), 209.0 (25), 194.0 (5), 178.0 (9), 165.0 (33).

Benzene, 1-[(1*E*)-2-(4-methylphenyl)ethenyl]-4-(trifluoromethyl)- (Table 3, compound 3at)[9]



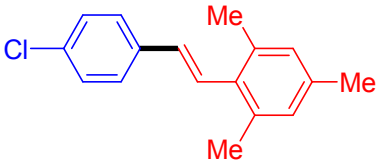
Eluents (Hexane, R_f= 0.56) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 7.10 (d, *J*= 16.4 Hz, 1H), 7.18-7.23 (m, 3H), 7.46 (d, *J*= 8.4 Hz, 2H), 7.59-7.64 (m, 4H); ^{13}C NMR (100 MHz,$CDCl_3$) δ , 21.3, 125.6, 126.1, 126.4, 126.7, 128.8, 129.5, 131.1, 133.8, 138.3, 141.0; ^{19}F NMR (400 MHz,$CDCl_3$) δ -62.4; MS (EI): *m/z* (relative intensity) 262.1 (M^+, 100), 247.0 (41), 227.0 (18), 115.0 (7), 91.0 (8).

Benzene, 1-bromo-2-[(1*E*)-2-(4-methylphenyl)ethenyl]- (Table 3, compound 3au)[10]



Eluents (Hexane, R_f= 0.56) was used for flash column chromatography. Colorless liquid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 7.06 (d, *J*= 16.0 Hz, 1H), 7.12-7.16 (m, 1H), 7.20-7.23 (m, 2H), 7.32-7.36 (m, 1H), 7.44-7.50 (m, 3H), 7.60- 7.63 (m, 1H), 7.69-7.71 (m, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.3, 124.0, 126.5, 127.5, 128.5, 128.9, 129.4, 131.4, 132.9, 133.0, 134.2, 137.3, 138.0; MS (EI): *m/z* (relative intensity) 272.0 (M^+, 38), 193.0 (23), 178.0 (100), 165.0 (12), 115.0 (7).

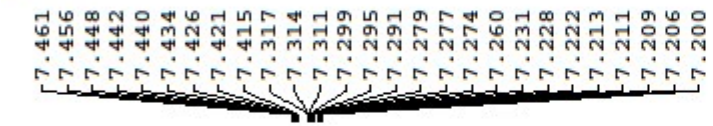
Benzene, 1-chloro-4-[(1*E*)-2-(1,3,5-trimethylphenyl)ethenyl]- (Table 3, compound 3fv)

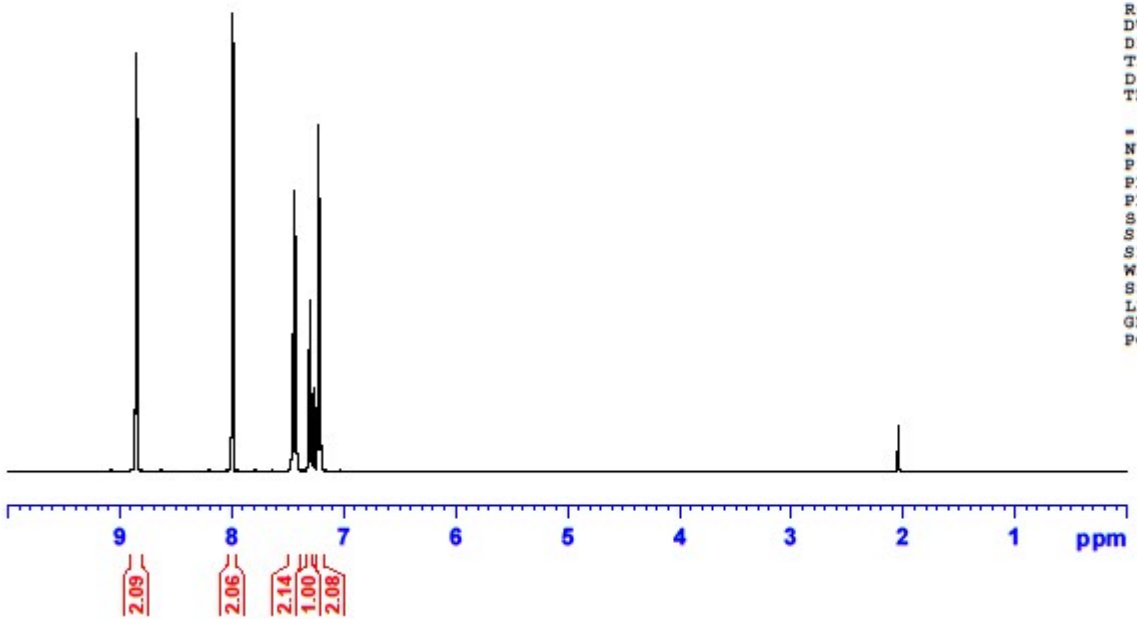


Eluents (Hexane, R_f= 0.55) was used for flash column chromatography. White solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.35 (s, 3H), 2.40 (s, 6H), 6.60 (d, *J*= 16.8 Hz, 1H), 6.97 (s, 2H), 7.13 (d, *J*= 16.4 Hz, 1H), 7.37-7.40 (m, 2H), 7.45-7.48 (m, 2H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 21.0, 127.4, 127.6, 132.3, 133.0, 133.6, 136.1, 136.2, 136.5; MS (EI): *m/z* (relative intensity) 256.0 (M^+, 63), 241.0 (23), 221.1 (27), 206.0 (100), 191.0 (15); IR (KBr, cm^{-1}) 3027, 1631, 1489, 981, 812; HRMS (ESI) calcd. for $C_{17}H_{17}Cl$ [M + H^+]: 256.1019, found 256.1018.

8. ^{1}H, ^{13}C, ^{19}F, HRMS and IR spectra

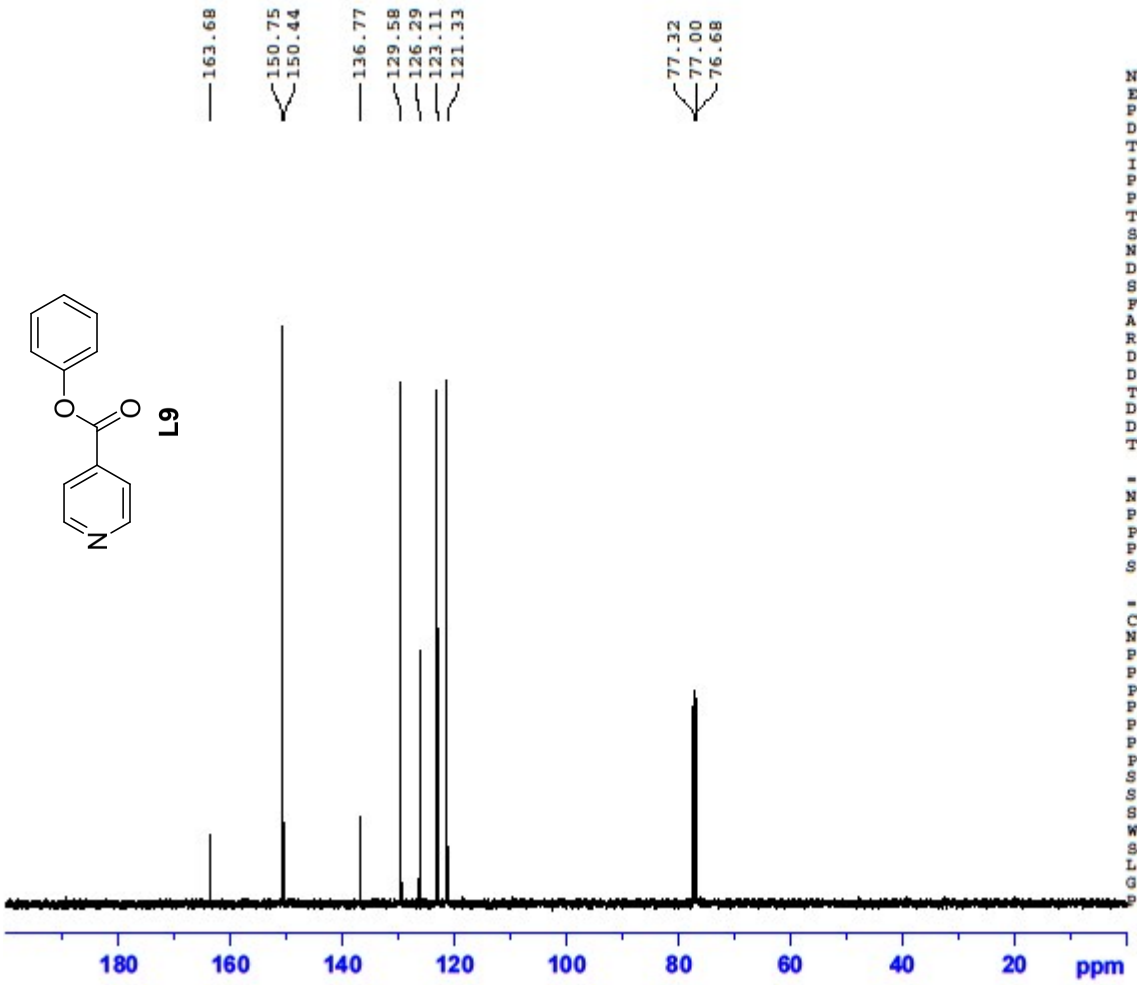
phenyl ester





NAME	Standard 1H	
EXPNO	189	
PROCNO	1	
Date_	20120508	
Time	13.45	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	9	
DS	2	
SWH	8012.820	Hz
FIDRES	0.244532	Hz
AQ	2.0447731	sec
RG	57	
DW	62.400	usec
DE	6.50	usec
TE	298.7	K
D1	1.00000000	sec
TD0	1	
--------	CHANNEL f1	--------
NUC1	1H	
P1	14.70	usec
PL1	0.00	dB
PL1W	11.88122272	W
SFO1	400.1320007	MHz
SI	32768	
SF	400.1300094	MHz
WDW	EM	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	

phenyl ester



NAME	Standard 13C
EXPNO	54
PROCNO	1
Date_	20120508
Time	13.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	92
DS	2
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	256
DW	19.800 usec
DE	6.50 usec
TE	298.9 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
--------	CHANNEL f1 --------
NUC1	13C
P1	9.50 usec
PL1	-2.00 dB
PL1W	58.52175522 W
SFO1	100.6228298 MHz
--------	CHANNEL f2 --------
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	15.00 dB
PL2W	11.88122272 W
PL12W	0.37571725 W
PL13W	0.37571725 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127772 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

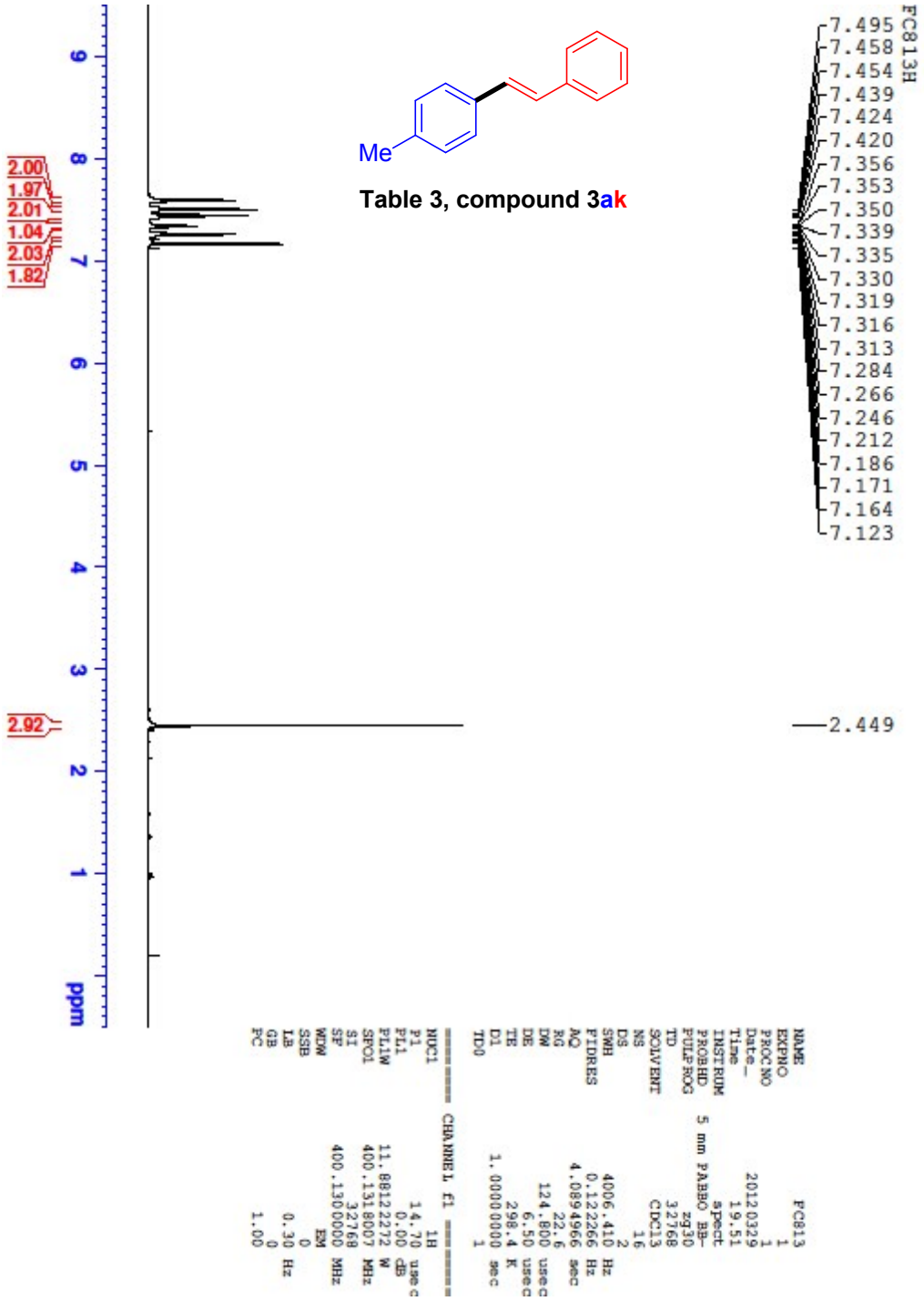


Table 3, compound 3ak

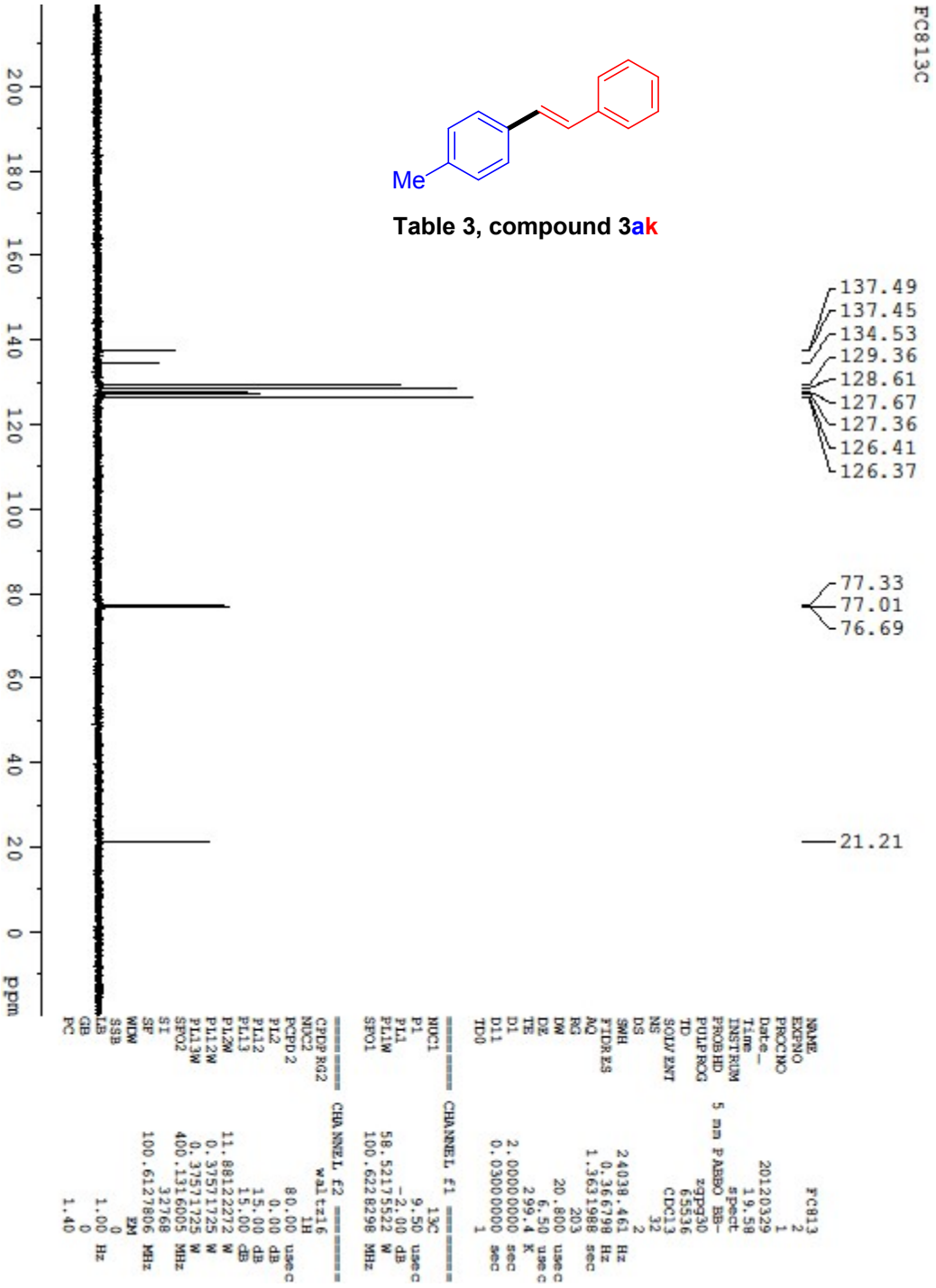


Table 3, compound 3ak

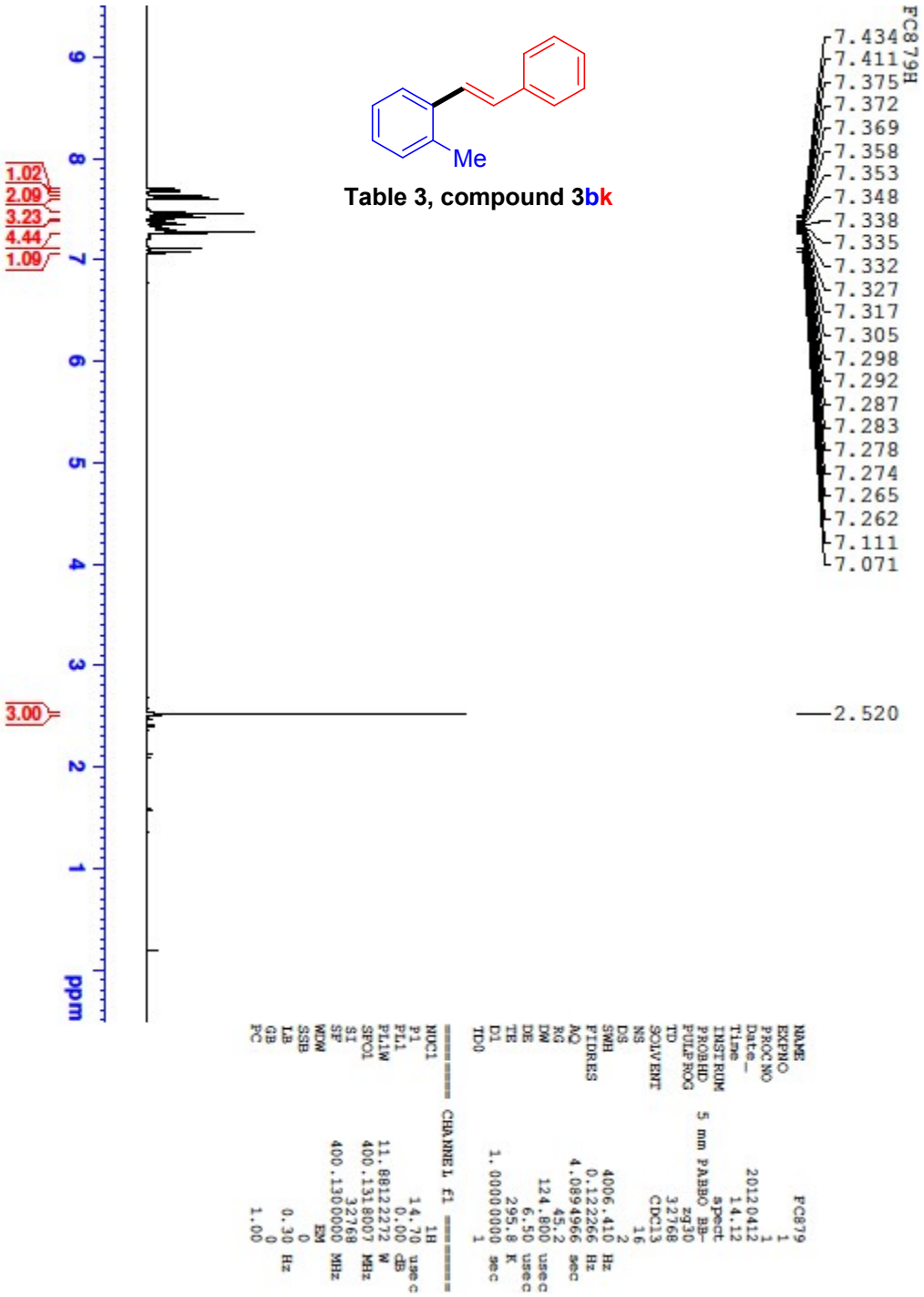


Table 3, compound 3bk

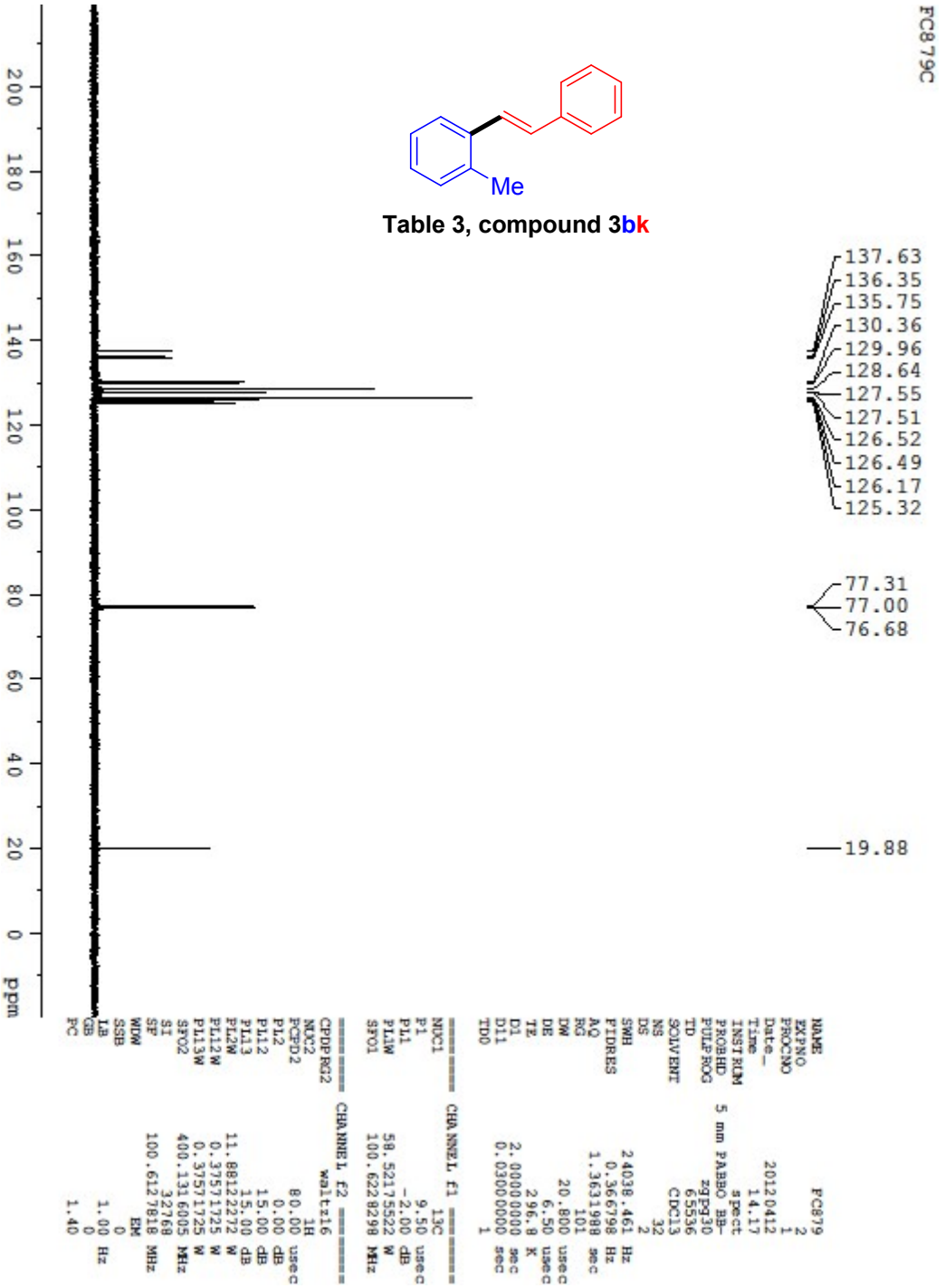


Table 3, compound 3bk

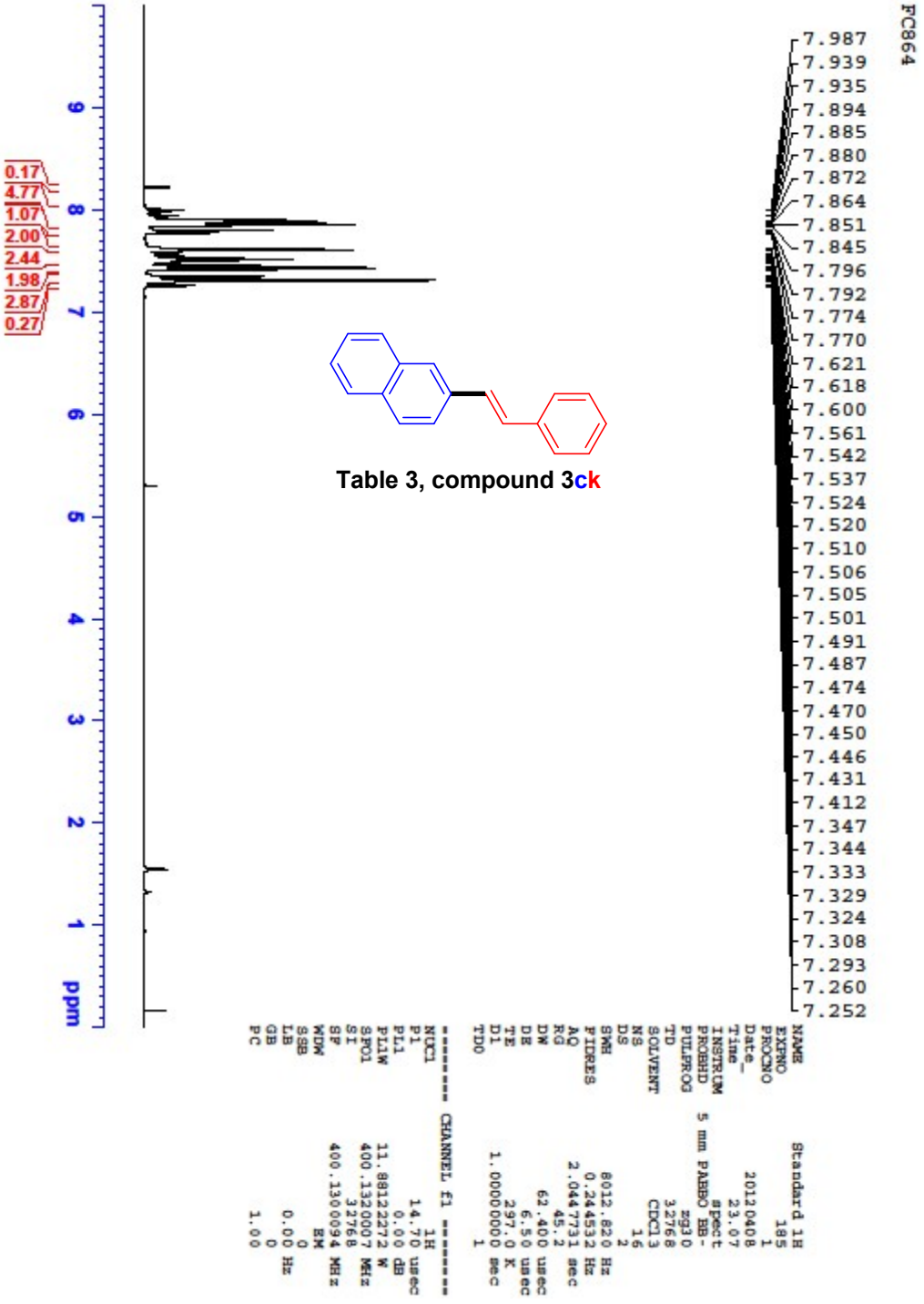


Table 3, compound 3ck

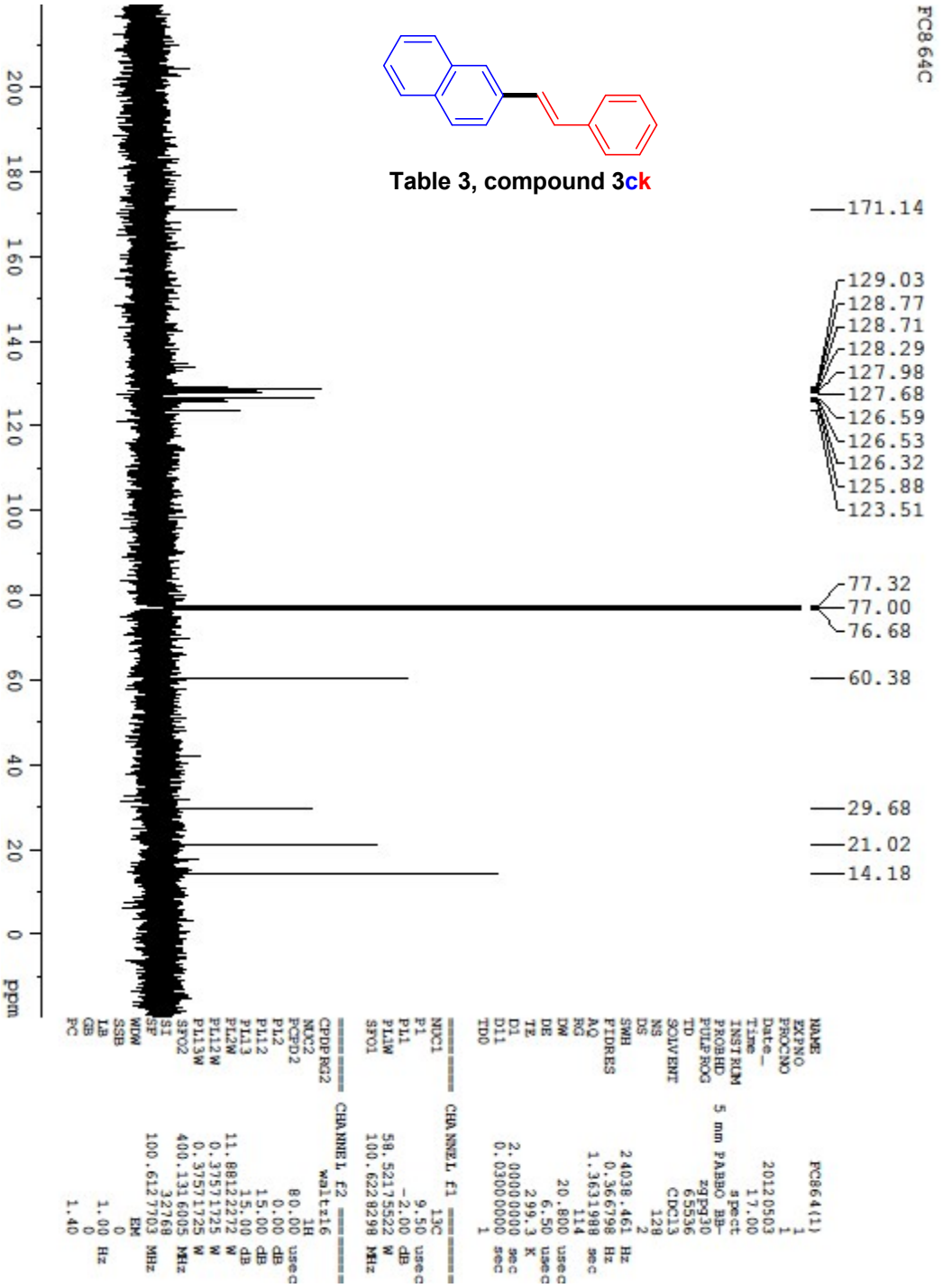


Table 3, compound 3ck

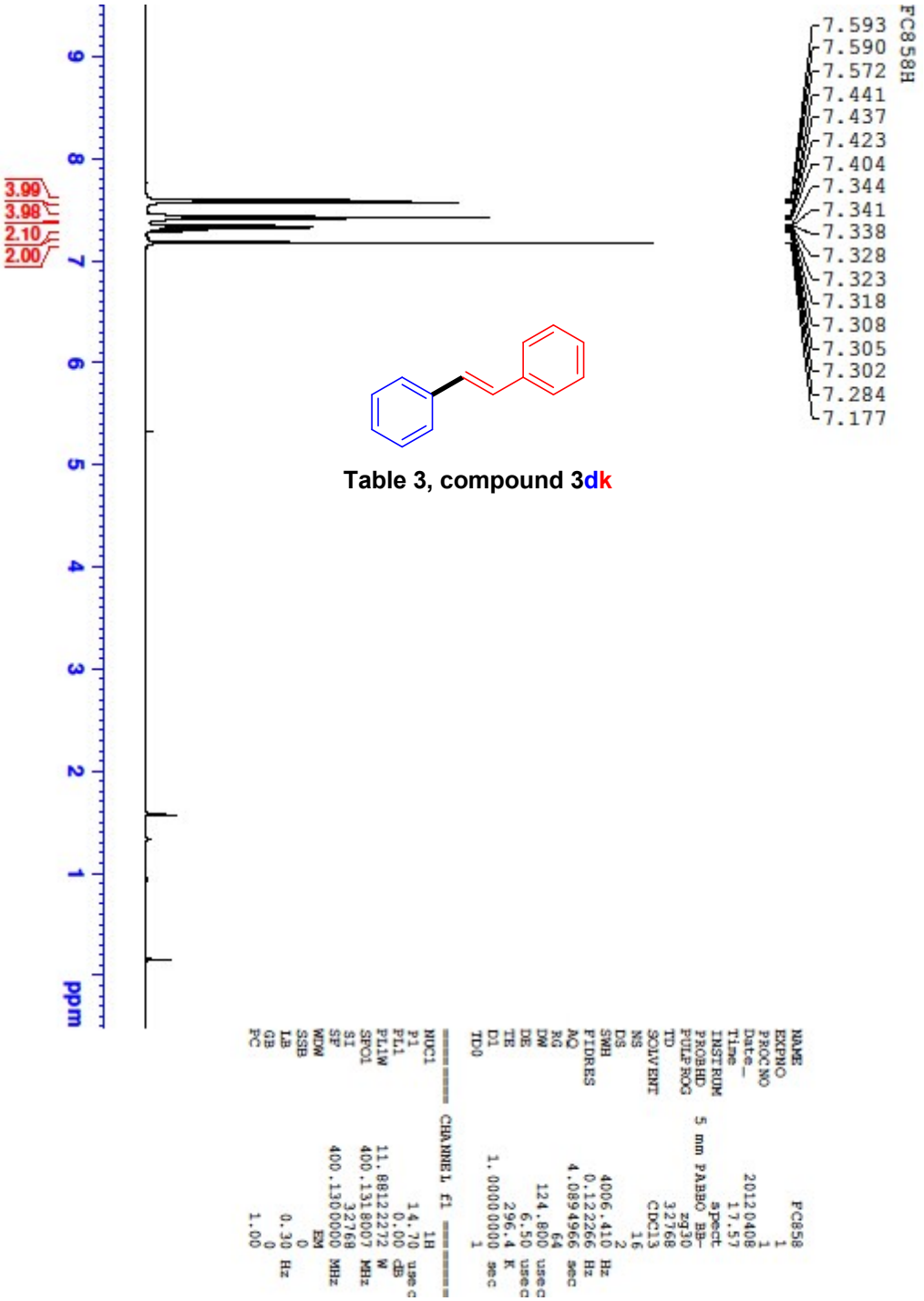


Table 3, compound 3dk

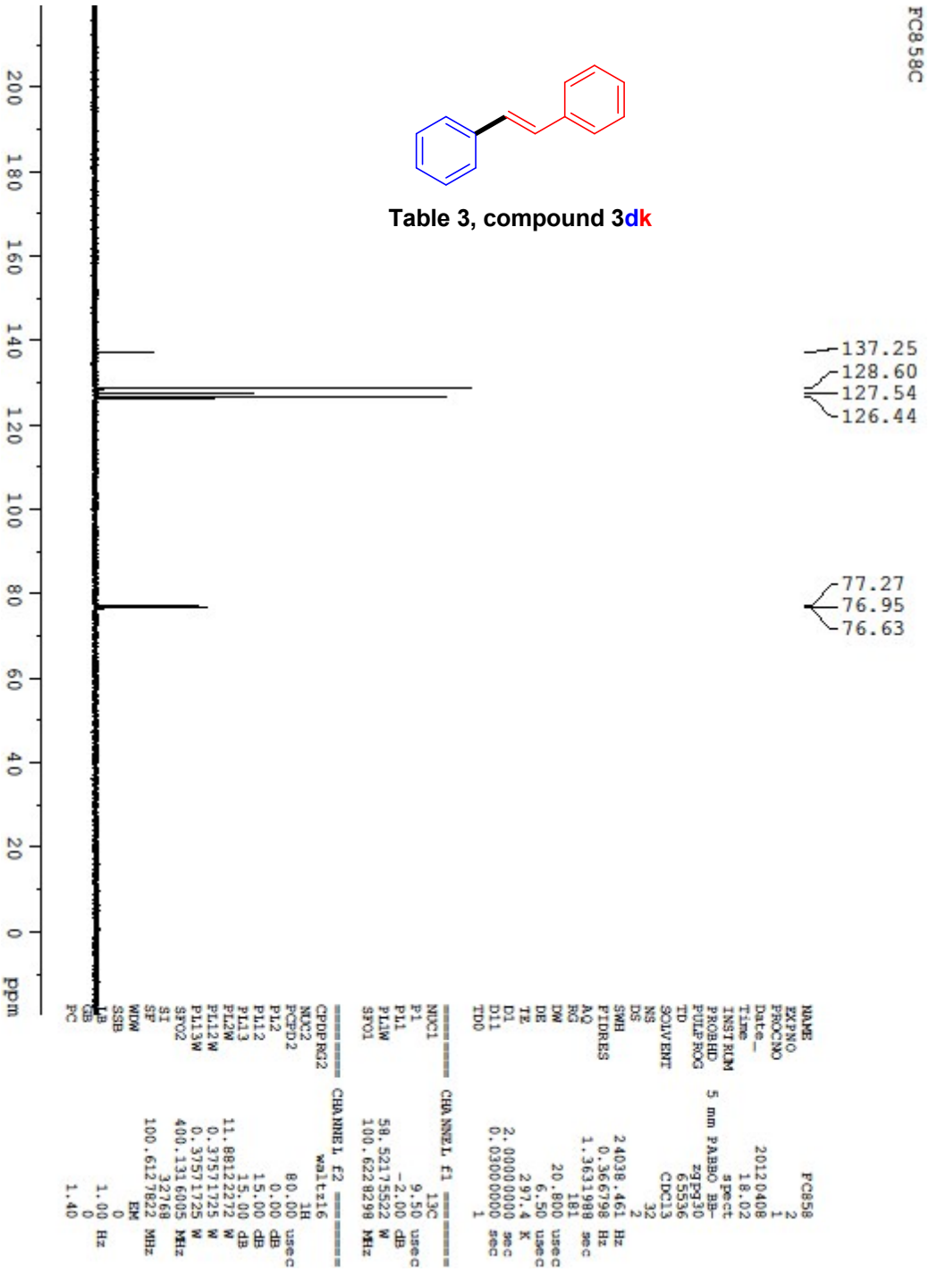


Table 3, compound 3dk

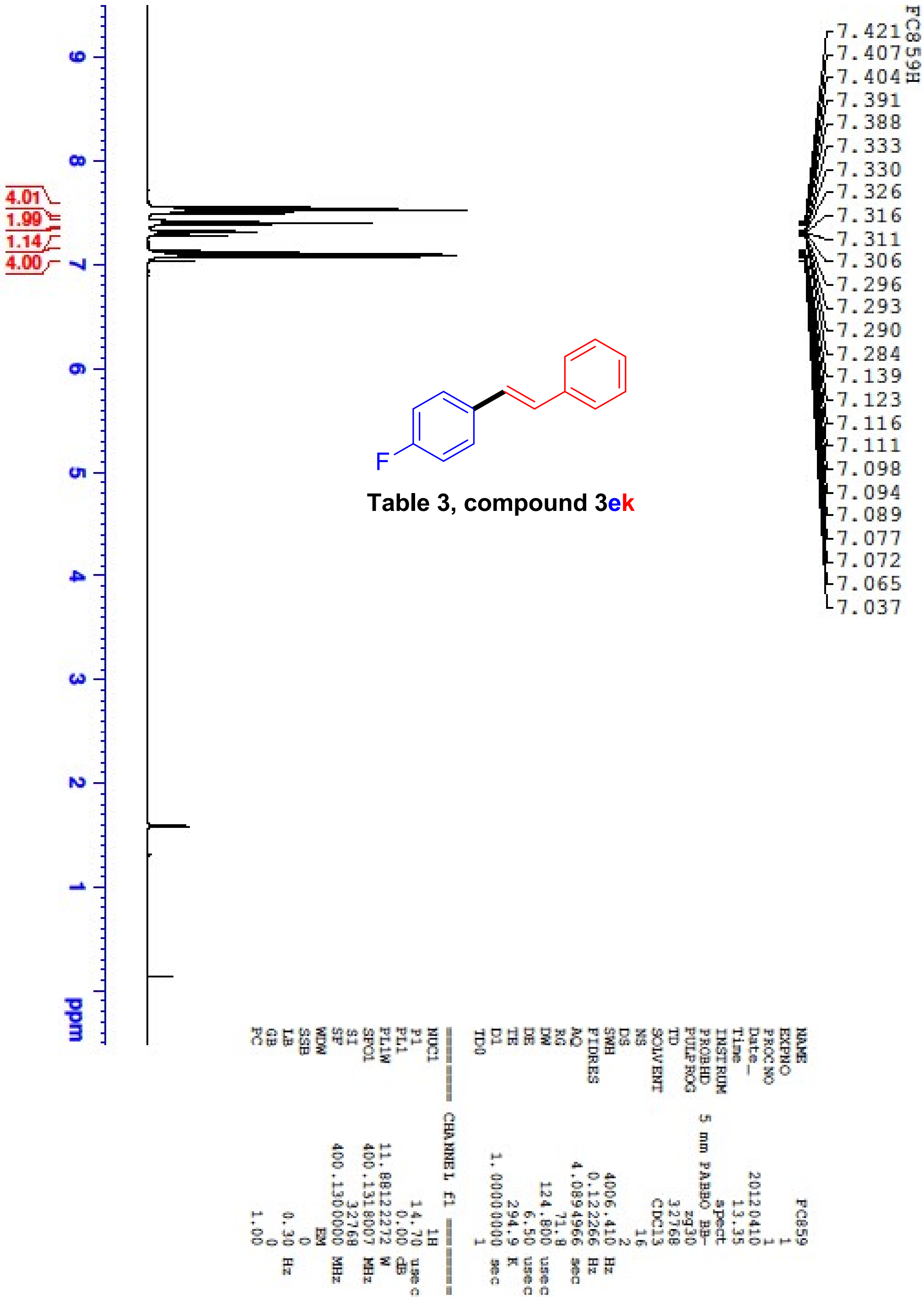


Table 3, compound 3ek

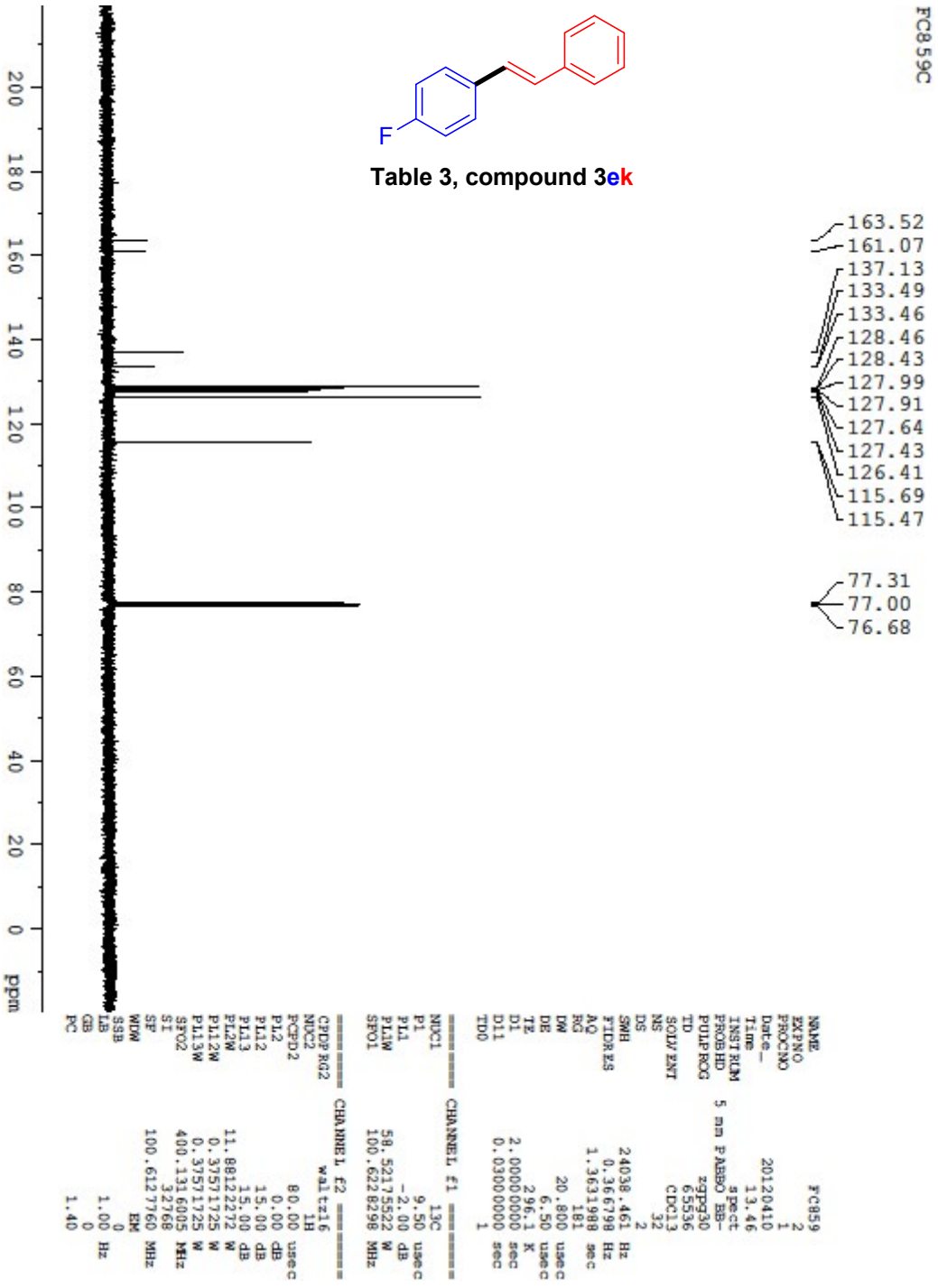


Table 3, compound 3ek

FC859F
F
Table 3, compound 3ek
1.00
-114.19
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200 ppm
NAME FC959
EXPNO 3
PROCNO 1
Date_ 20120410
Time 14.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 1290
DW 5.600 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.46071164 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.13160055 MHz
SI 65536
SF 376.49836600 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Table 3, compound 3fk

NAME	FC860
EXPNO	1
PROCNO	1
Date_	20120410
Time	13.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	2
SWH	4006.410 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	71.8
DW	124.800 usec
DE	6.50 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
======	CHANNEL f1 ======
NUC1	1H
P1	14.70 usec
PL1	0.00 dB
PL1W	11.88122272 W
SFO1	400.1318007 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
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GB	0
PC	1.00

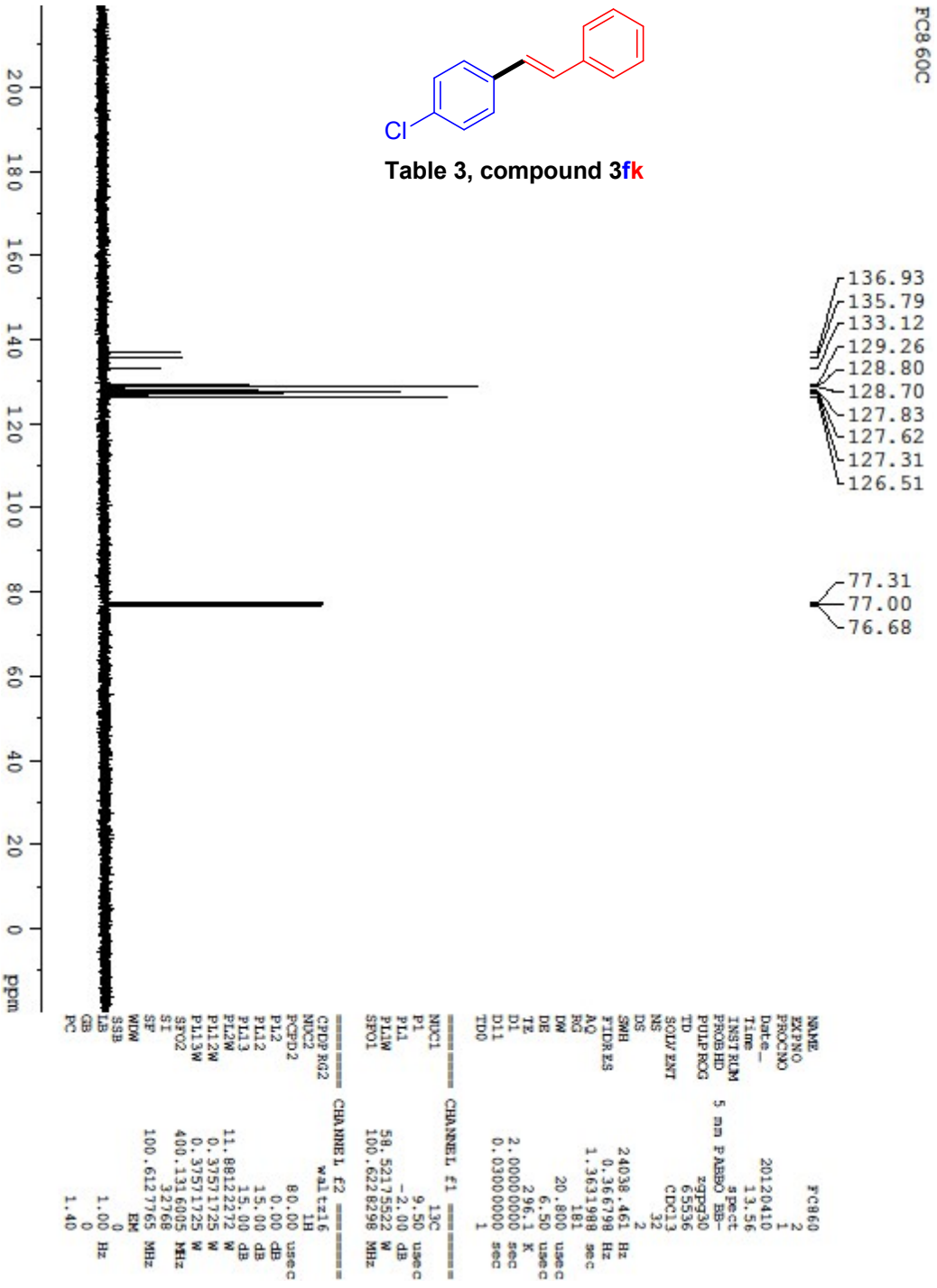


Table 3, compound 3fk

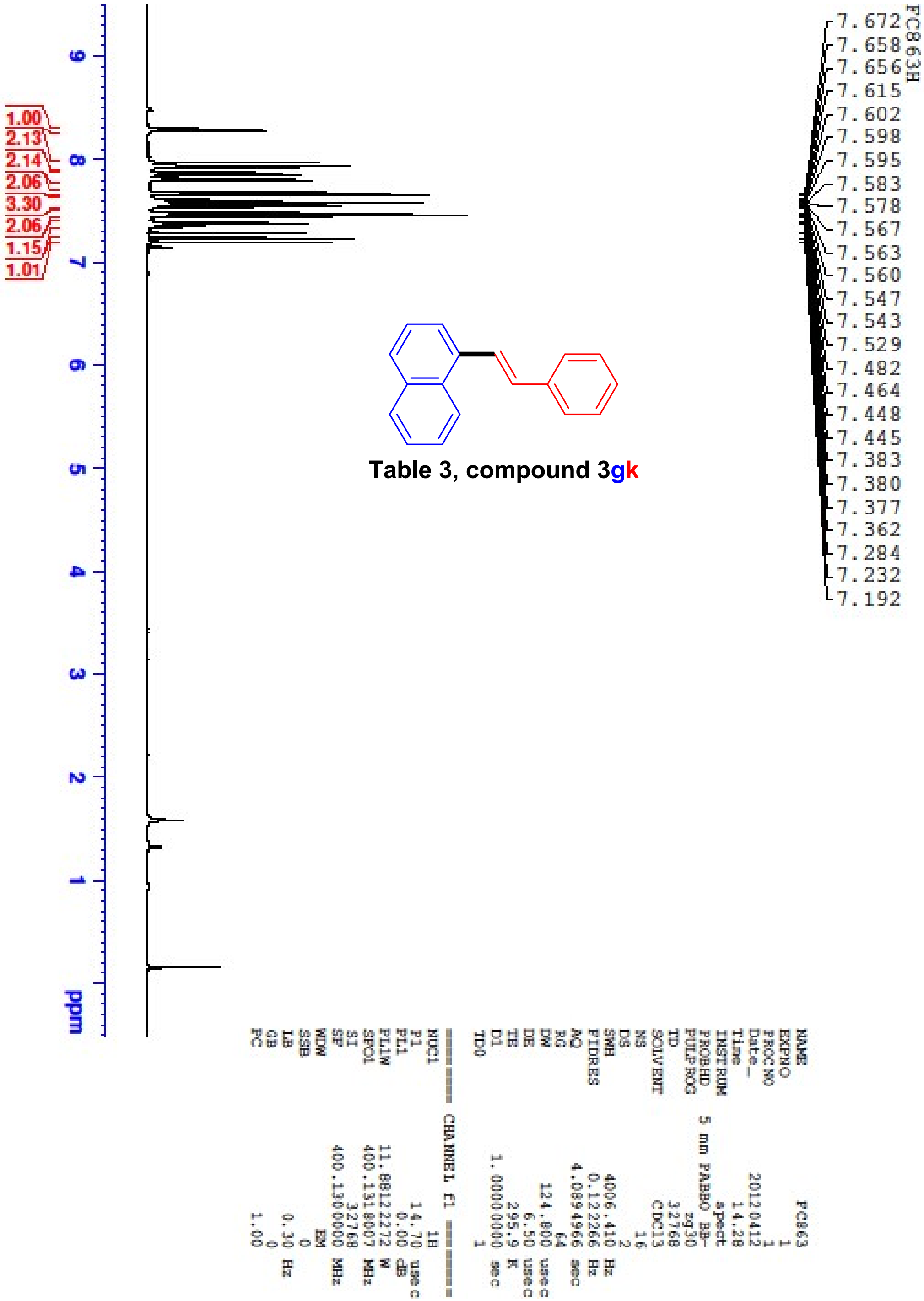


Table 3, compound 3gk

FC8 63C

137.57
134.97
133.68
131.72
131.36
128.71
128.58
128.00
127.74
126.65
126.05
125.79
125.76
125.65
123.73
123.58
77.30
76.98
76.66

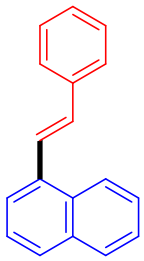


Table 3, compound 3gk

NAME	FC863	
EXPNO	2	
PROCNO	1	
Date_	20120412	
Time	14.30	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	32	
DS	2	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	101	
DW	20.800	usec
DE	6.50	usec
TE	296.8	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
========	CHANNEL f1	========
NUC1	13C	
P1	9.50	usec
PL1	-2.00	dB
PL1W	58.52175522	W
SFO1	100.6228298	MHz
========	CHANNEL f2	========
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.00	dB
PL12	15.00	dB
PL13	15.00	dB
PL2W	11.88122272	W
PL12W	0.37571725	W
PL13W	0.37571725	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127787	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

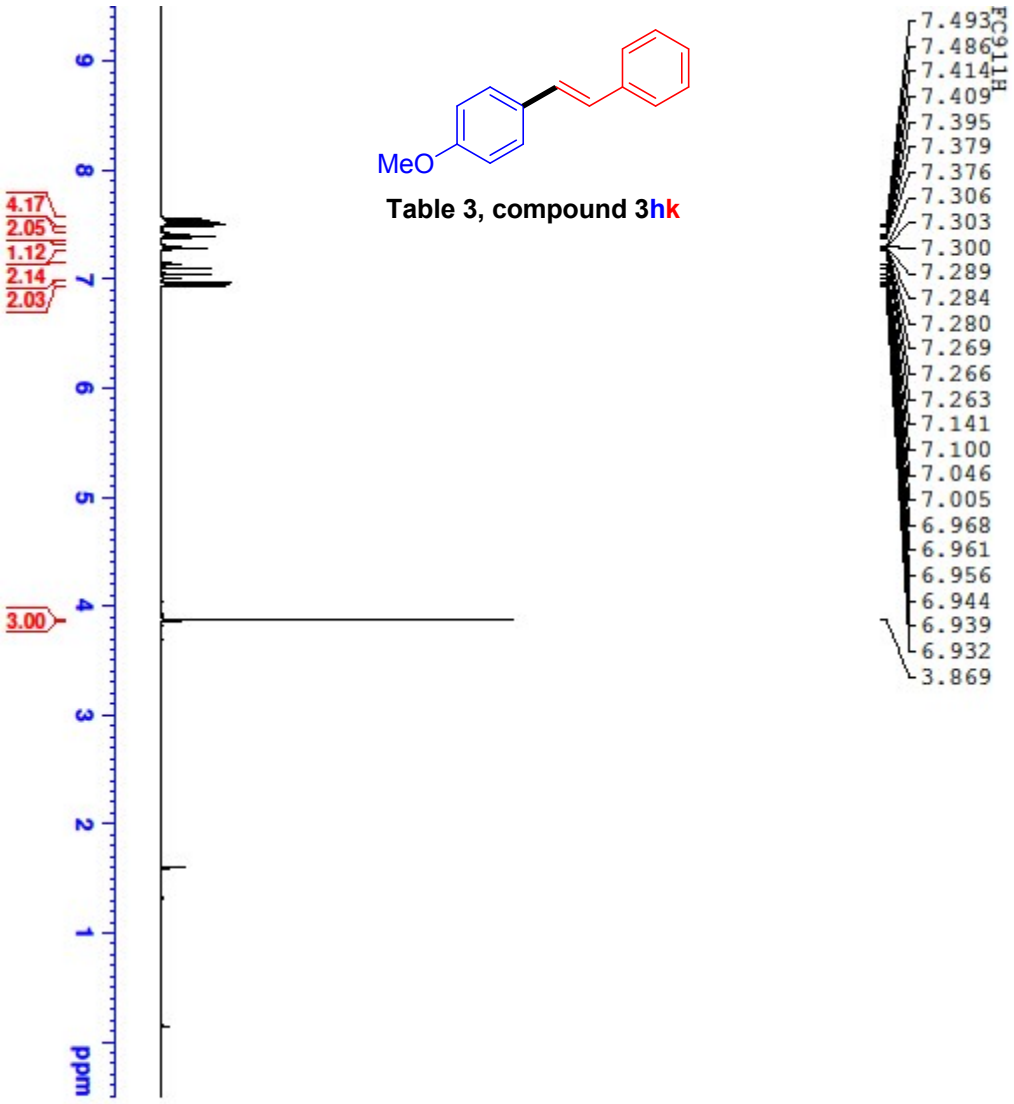


Table 3, compound 3hk

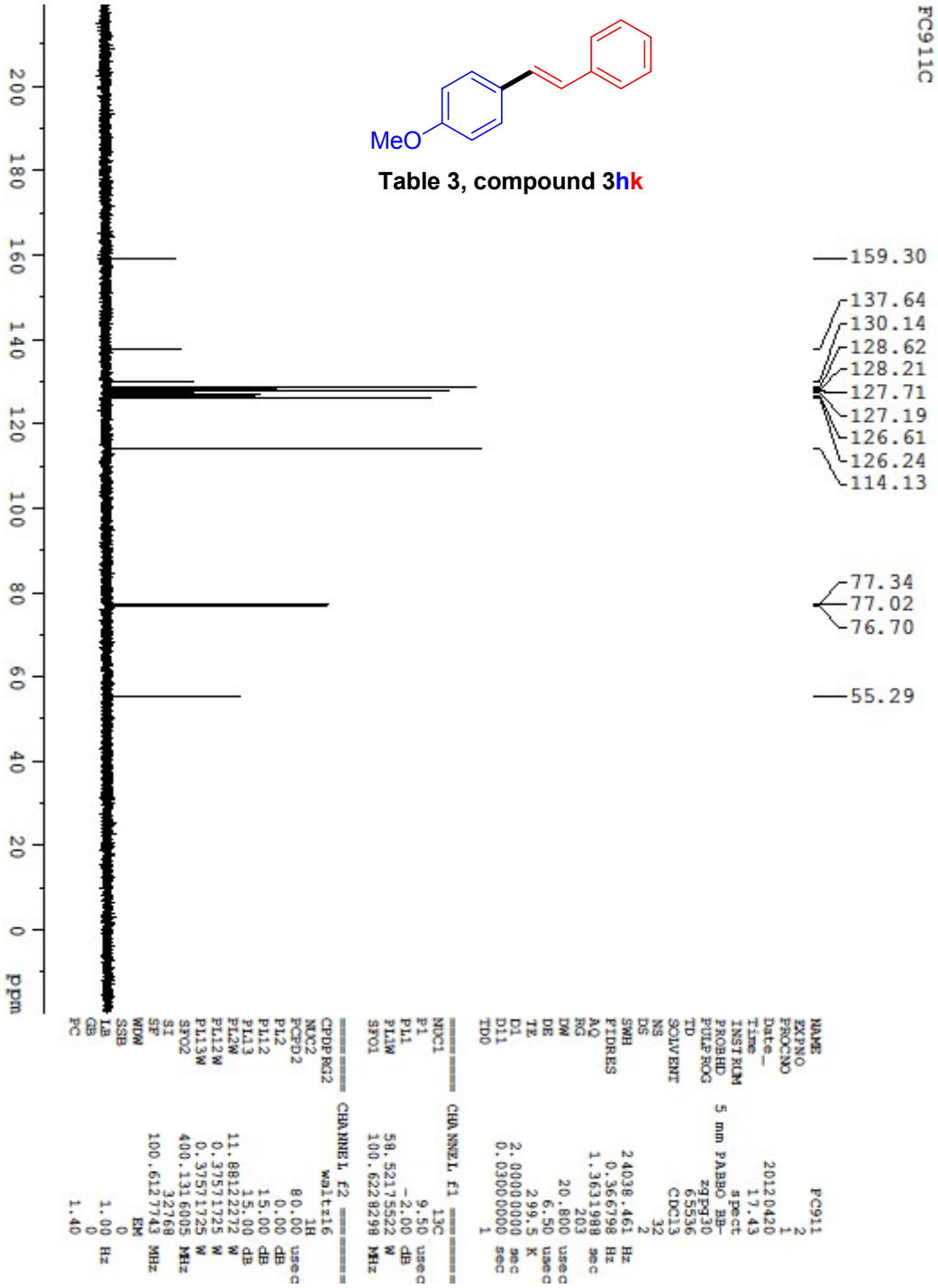
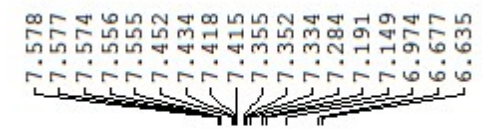


Table 3, compound 3hk

FC878H



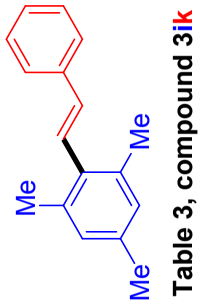
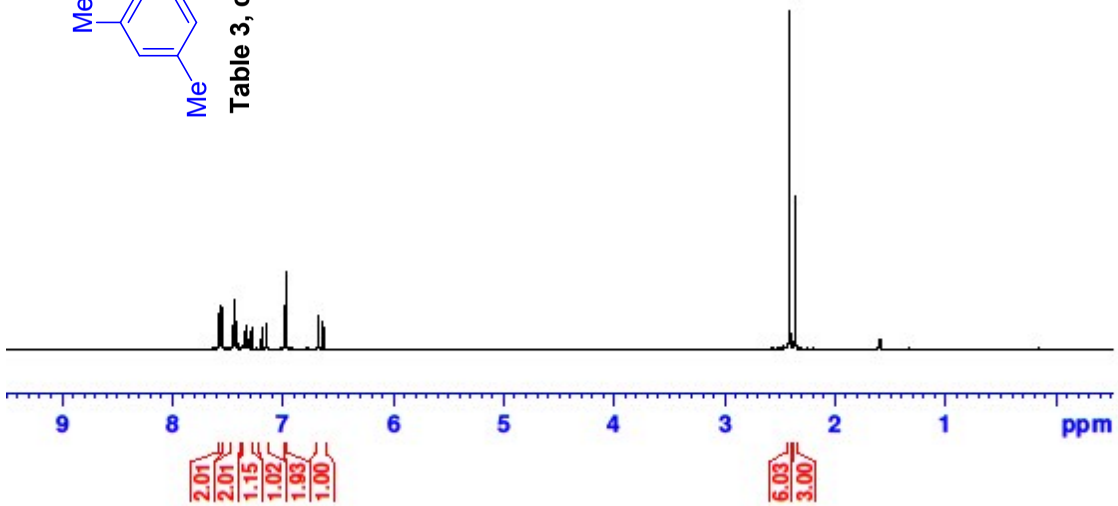


Table 3, compound 3ik

NAME	FC878	
EXPNO	1	
PROCNO	1	
Date_	20120412	
Time	14.21	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	4006.410	Hz
FIDRES	0.122266	Hz
AQ	4.0894966	sec
RG	64	
DW	124.800	usec
DE	6.50	usec
TE	295.9	K
D1	1.00000000	sec
TD0	1	
========	CHANNEL f1	========
NUC1	1H	
P1	14.70	usec
PL1	0.00	dB
PL1W	11.88122272	W
SFO1	400.1318007	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



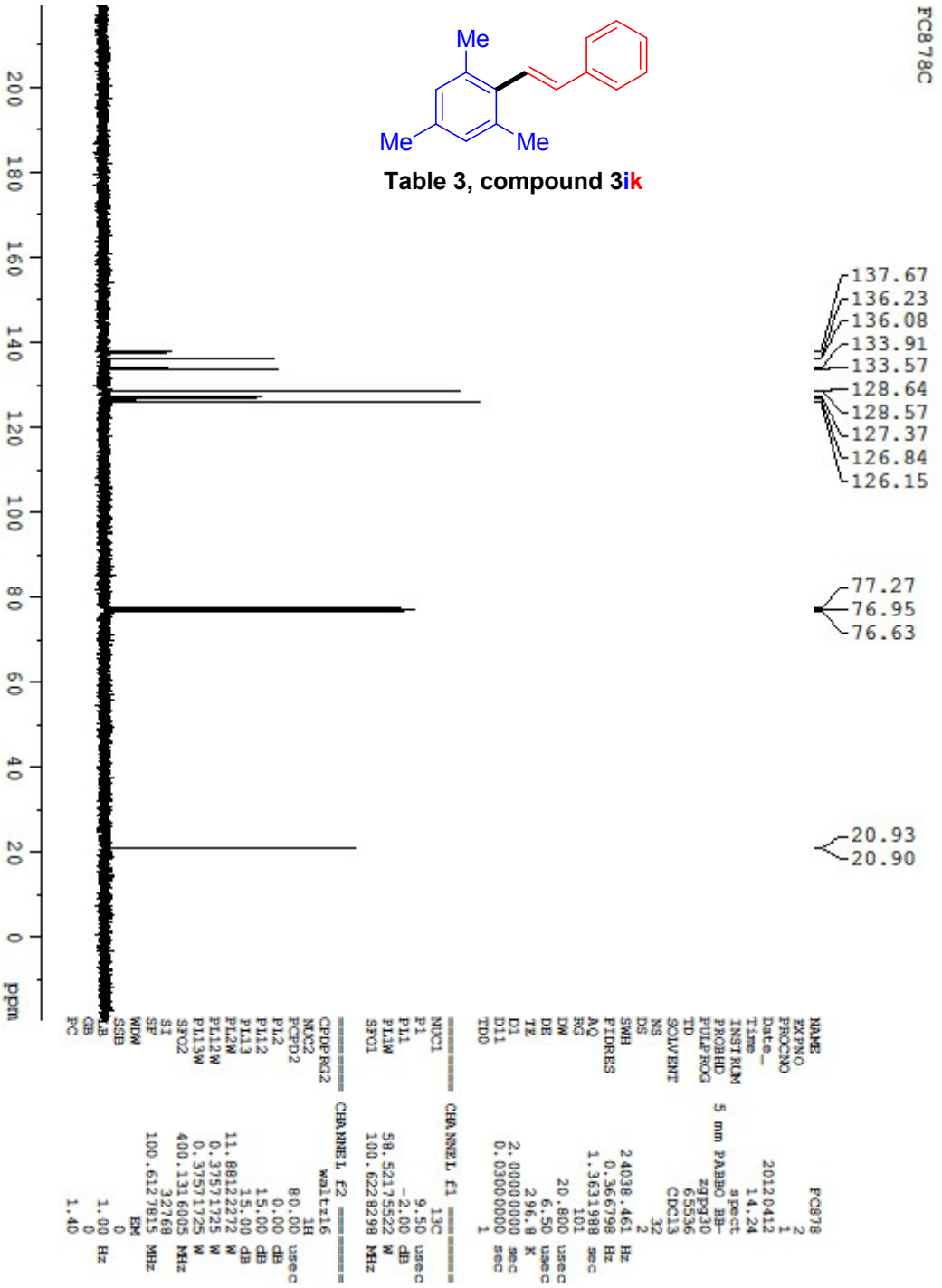


Table 3, compound 3ik

FC936H

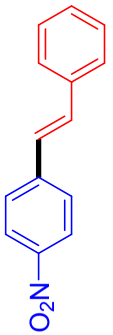
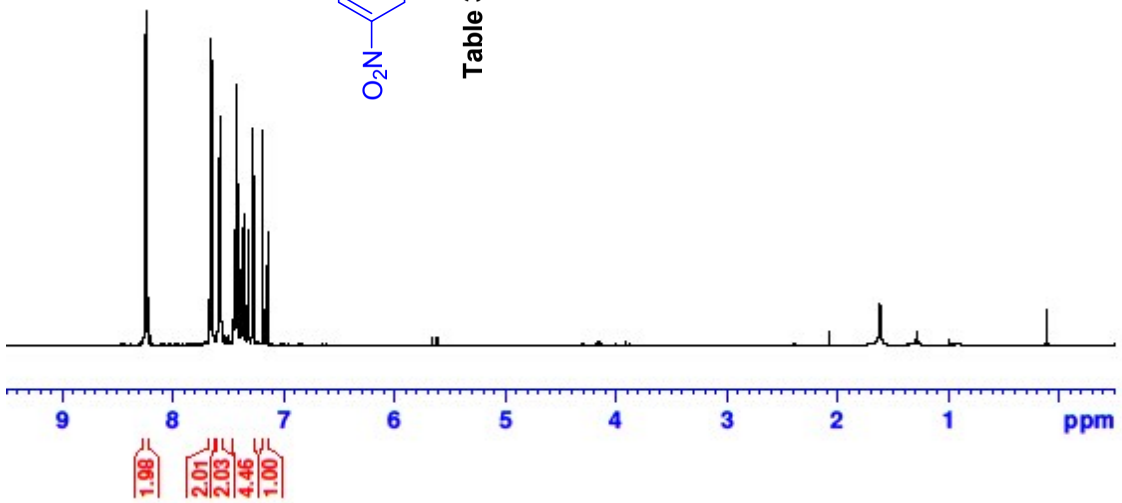


Table 3, compound 3jk

NAME	FC936	
EXPNO	1	
PROCNO	1	
Date_	20120425	
Time	13.32	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	4006.410	Hz
FIDRES	0.122266	Hz
AQ	4.0894966	sec
RG	114	
DW	124.800	usec
DE	6.50	usec
TE	298.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.70	usec
PL1	0.00	dB
PL1W	11.88122272	W
SFO1	400.1318007	MHz
SI	32768	
SF	400.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



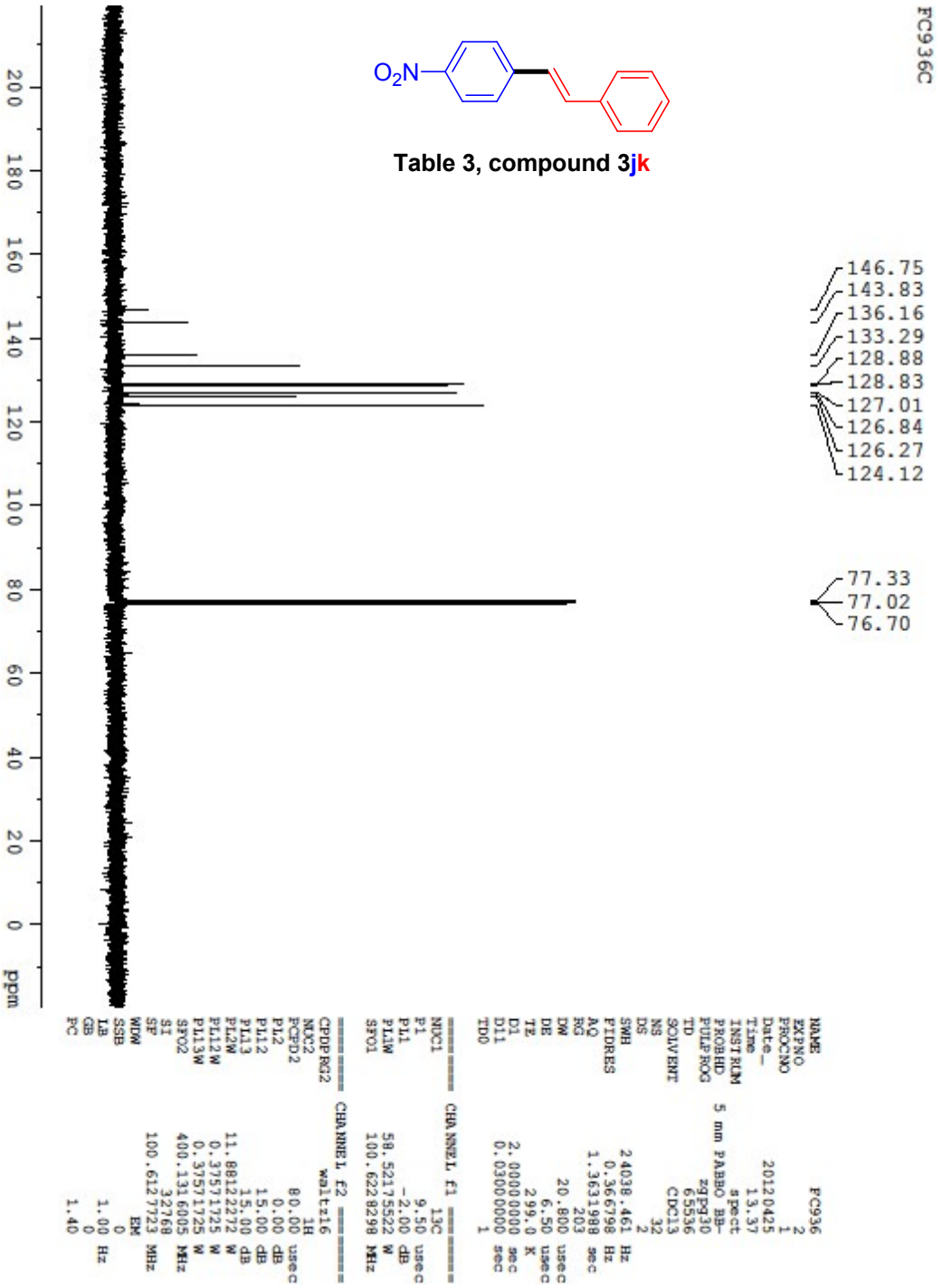


Table 3, compound 3jk

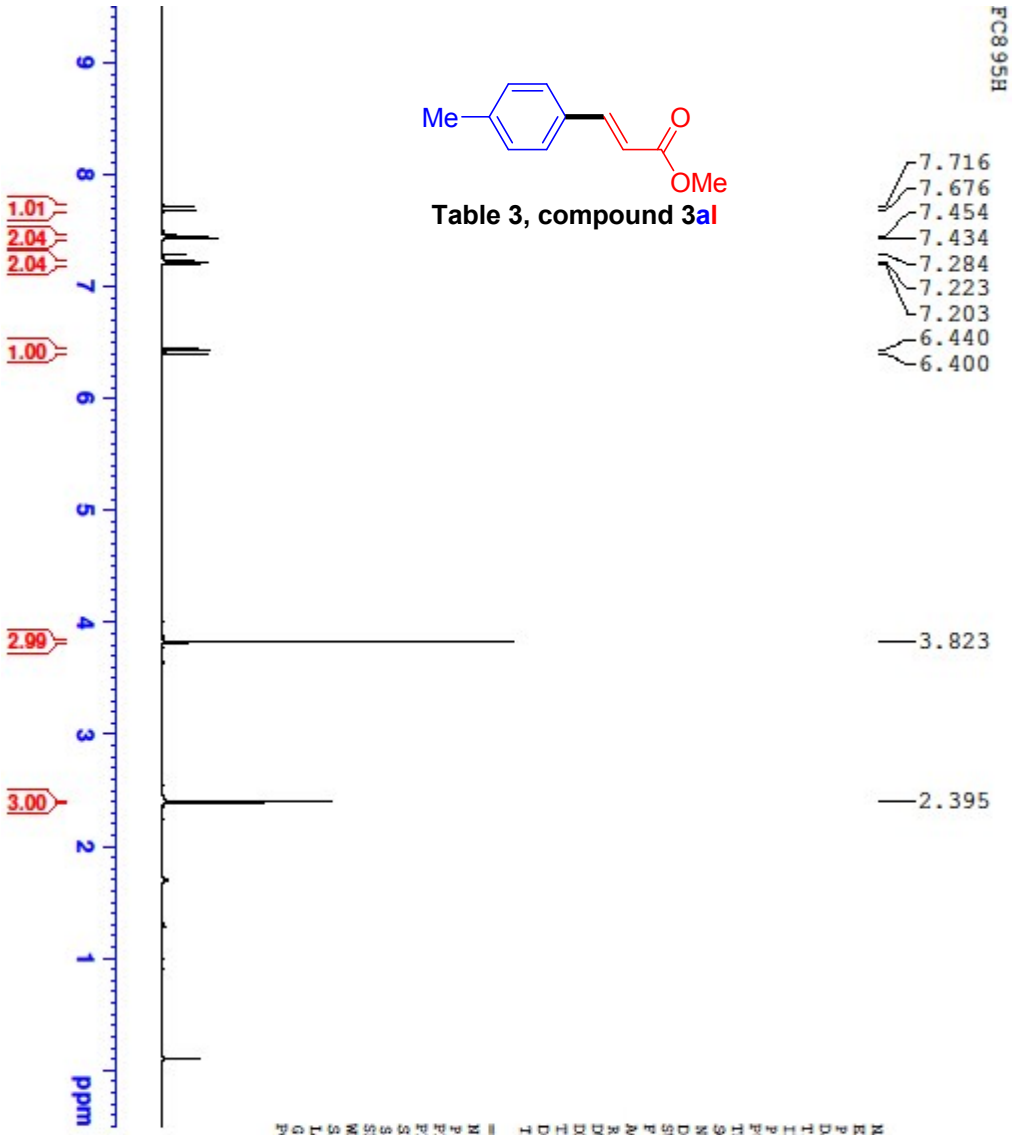


Table 3, compound 3al

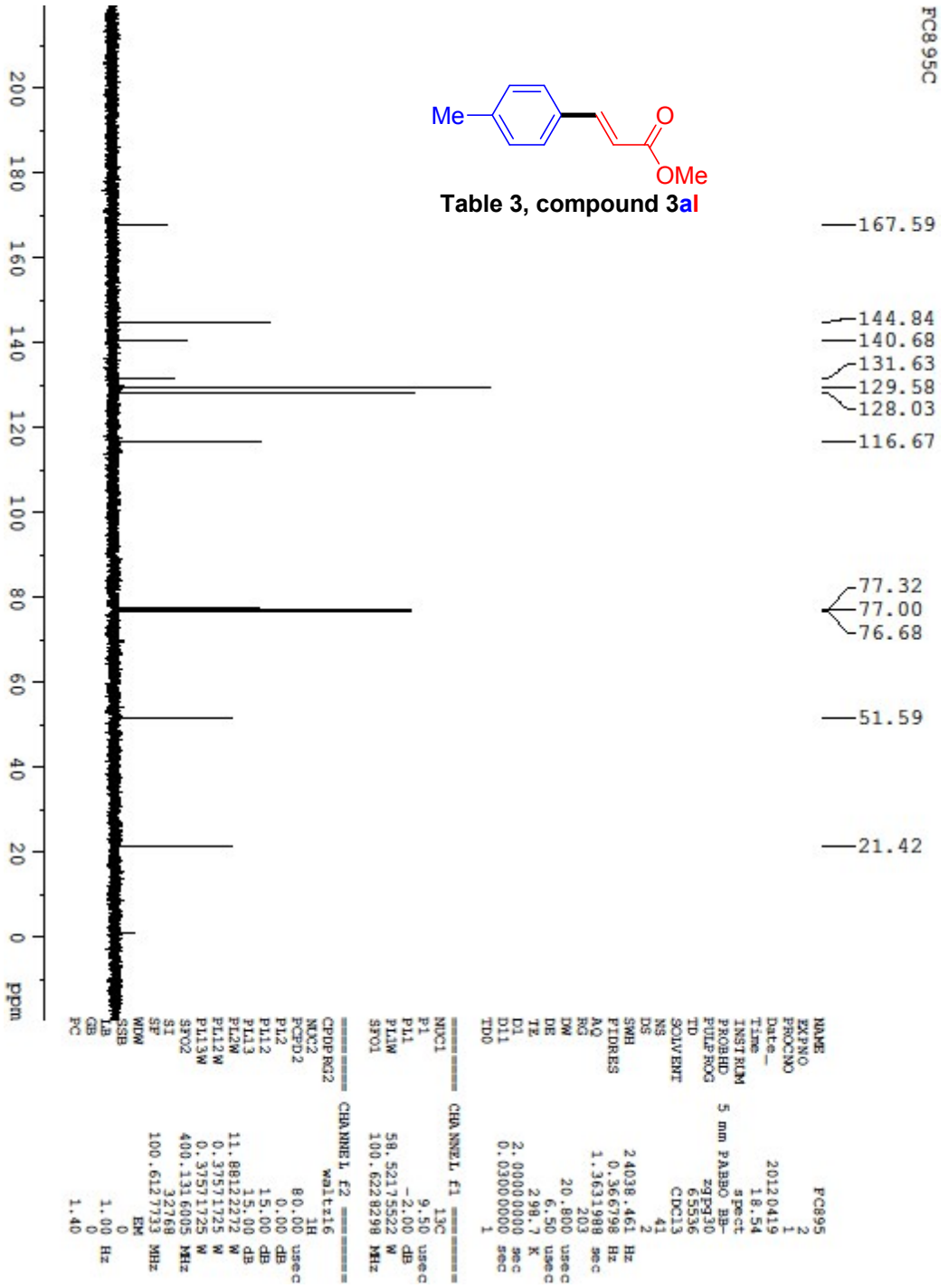
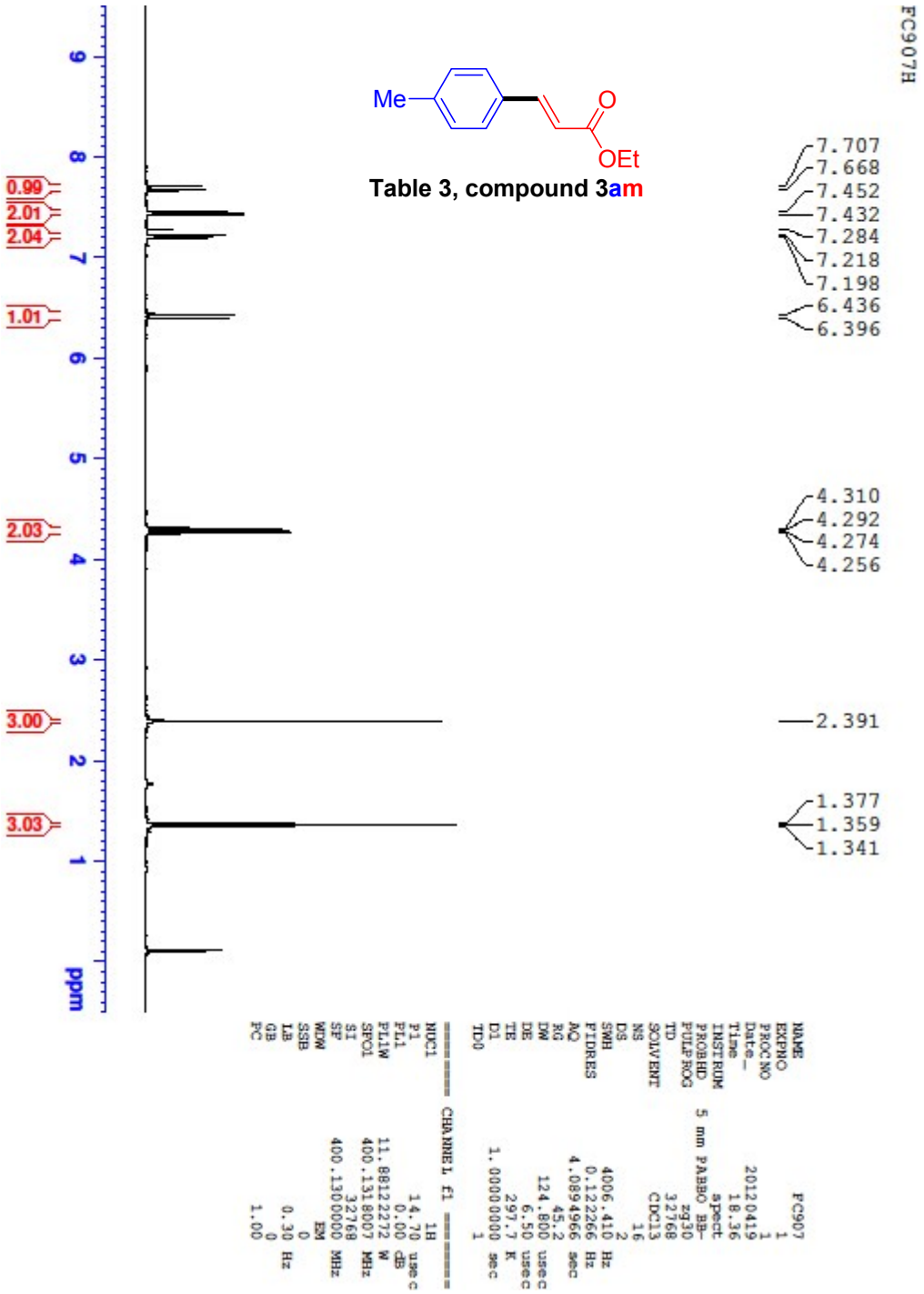


Table 3, compound 3al


FC907H
Me
O
OEt
Table 3, compound 3am
7.707
7.668
7.452
7.432
7.284
7.218
7.198
6.436
6.396
4.310
4.292
4.274
4.256
2.391
1.377
1.359
1.341
0.99
2.01
2.04
1.01
2.03
3.00
3.03
ppm
NAME FC907
EXPNO 1
PROCNO 1
Date_ 20120419
Time 18.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 45.2
DW 124.800 usec
DE 6.50 usec
TE 297.7 K
D1 1.0000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

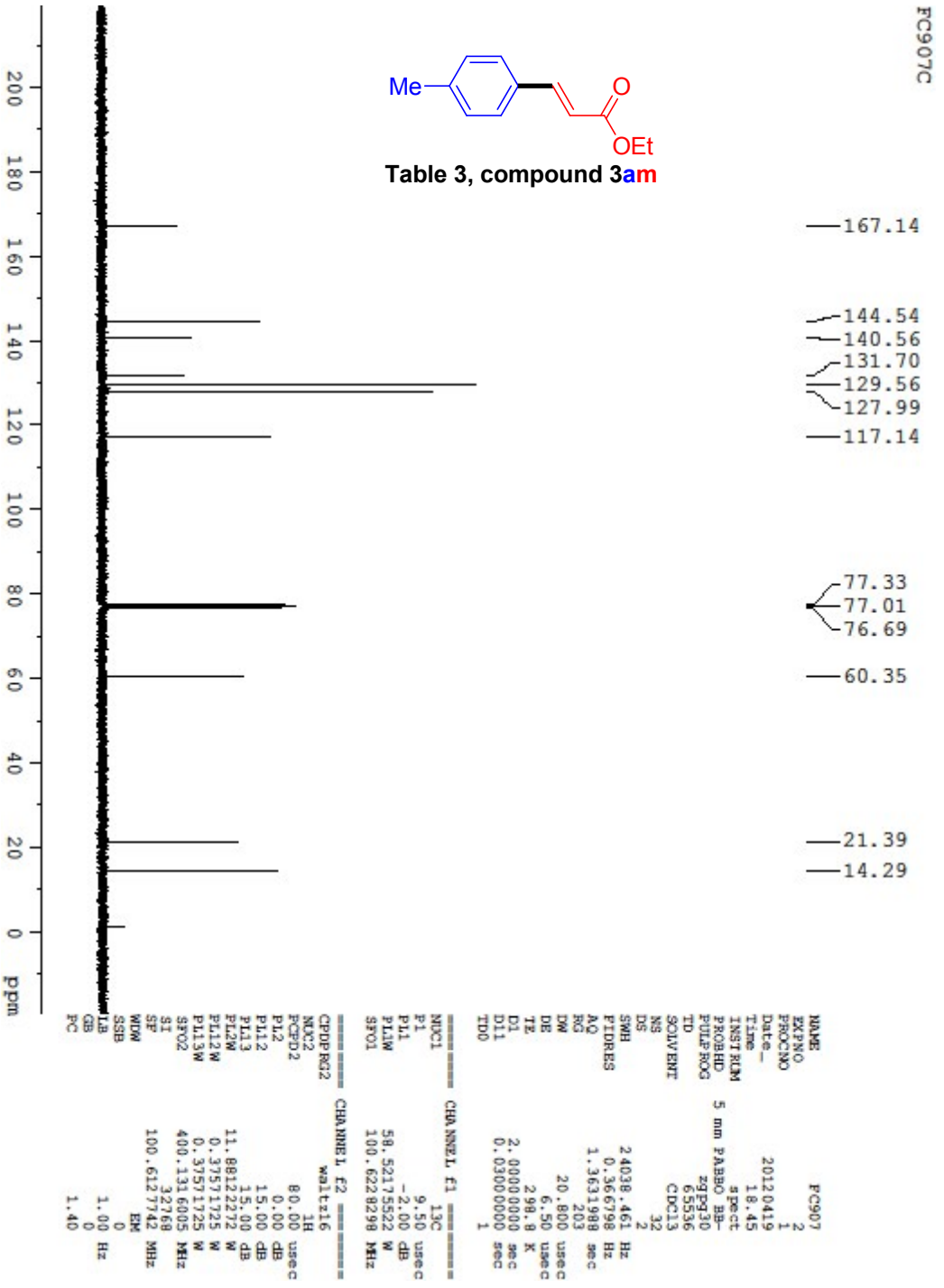


Table 3, compound 3am

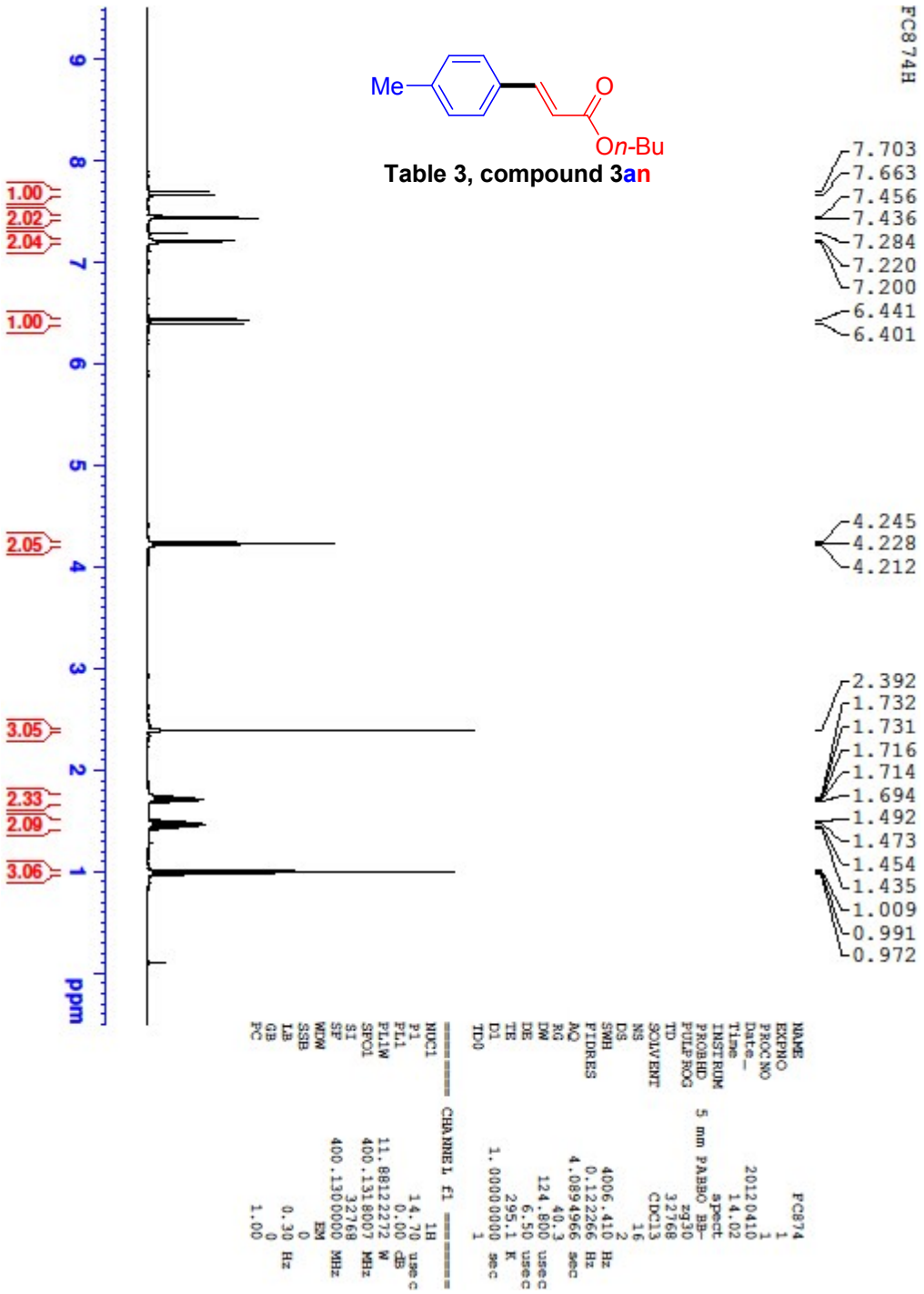


Table 3, compound 3an

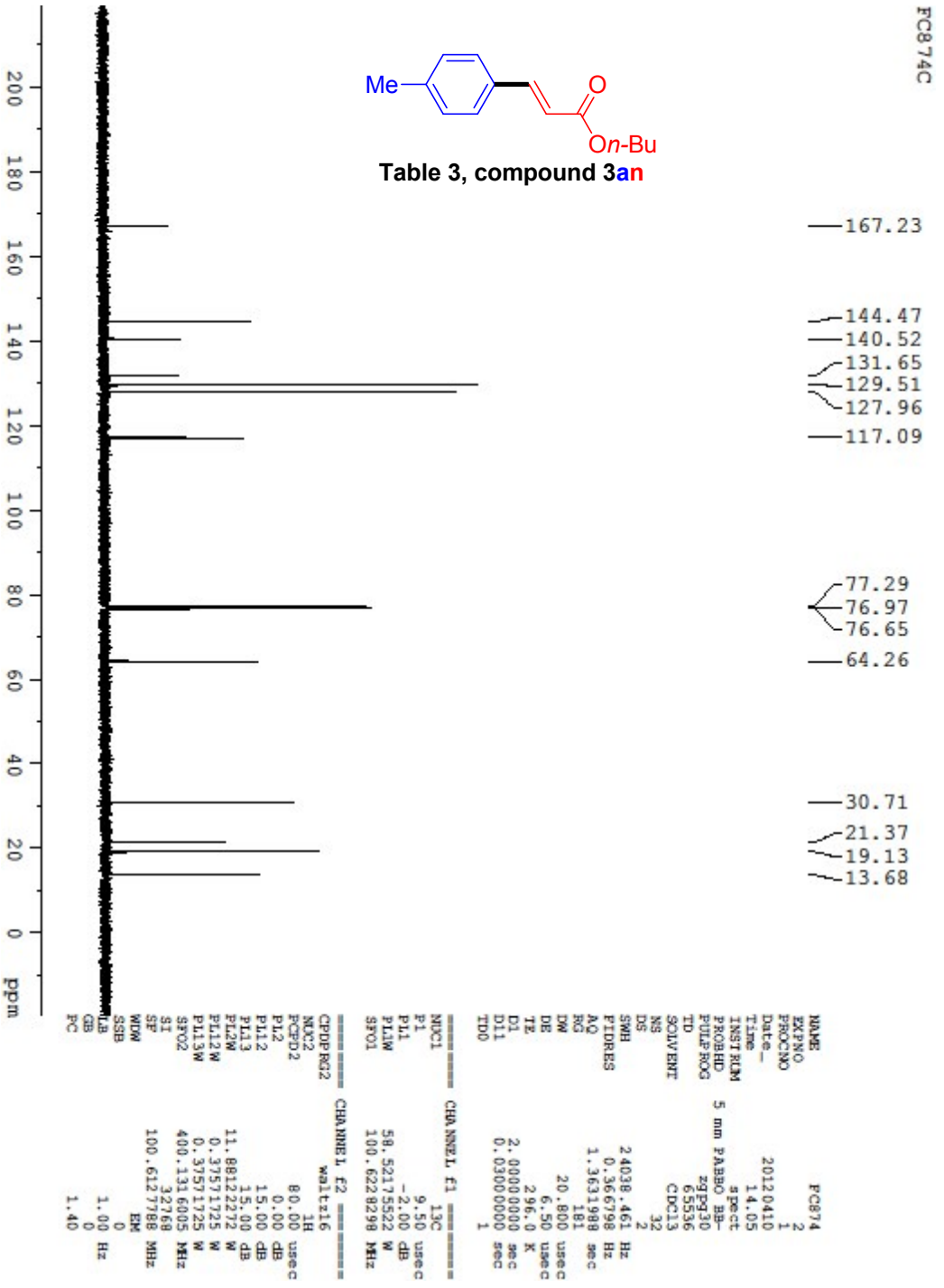
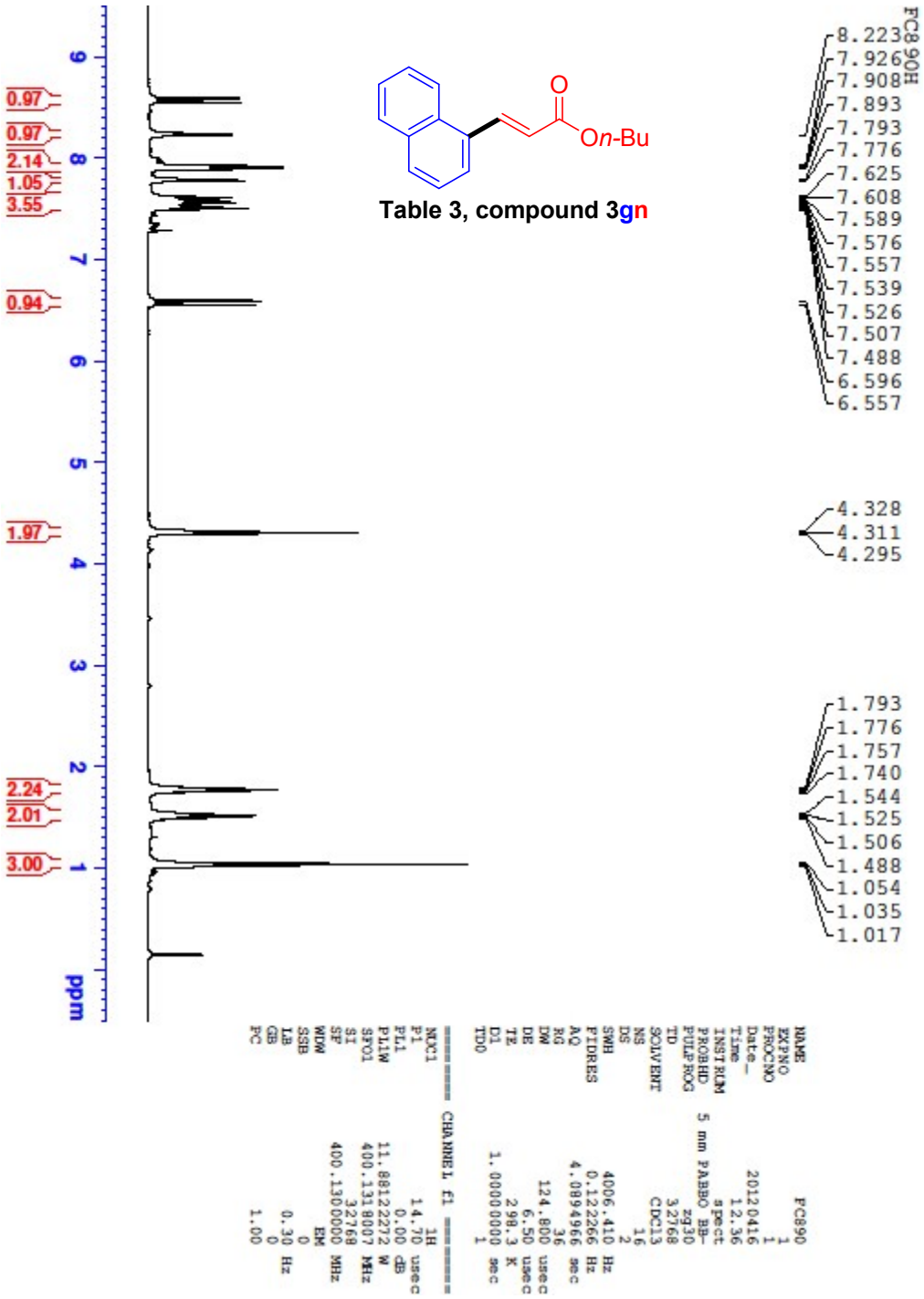


Table 3, compound 3an


FC890H
8.223
7.926
7.908
7.893
7.793
7.776
7.625
7.608
7.589
7.576
7.557
7.539
7.526
7.507
7.488
6.596
6.557
4.328
4.311
4.295
1.793
1.776
1.757
1.740
1.544
1.525
1.506
1.488
1.054
1.035
1.017
0.97
0.97
2.14
1.05
3.55
0.94
1.97
2.24
2.01
3.00
ppm
On-Bu
Table 3, compound 3gn
NAME FC890
EXPNO 1
PROCNO 1
Date_ 20120416
Time 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 36
DW 124.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.13190007 MHz
SI 32768
SF 400.13000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

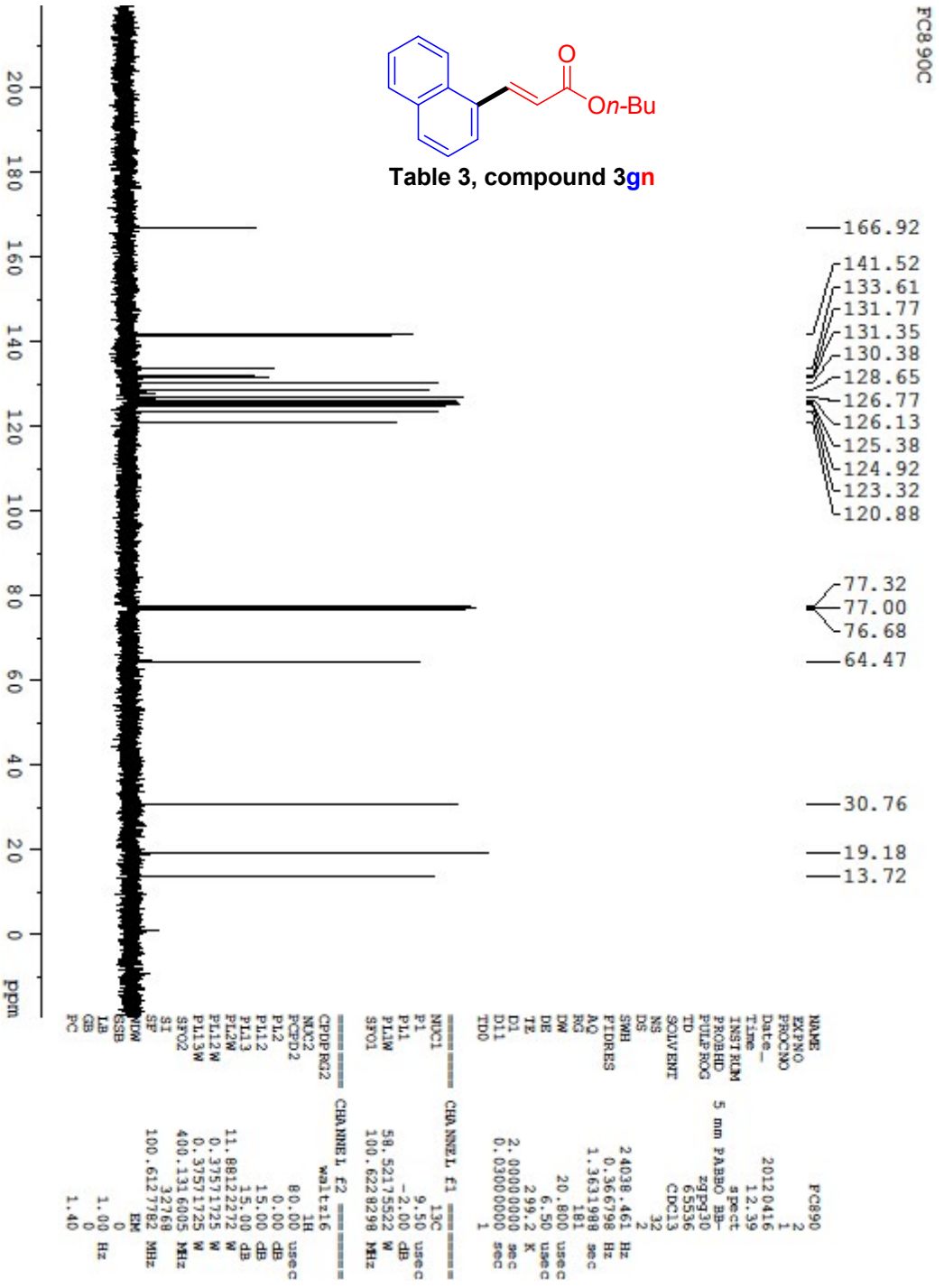
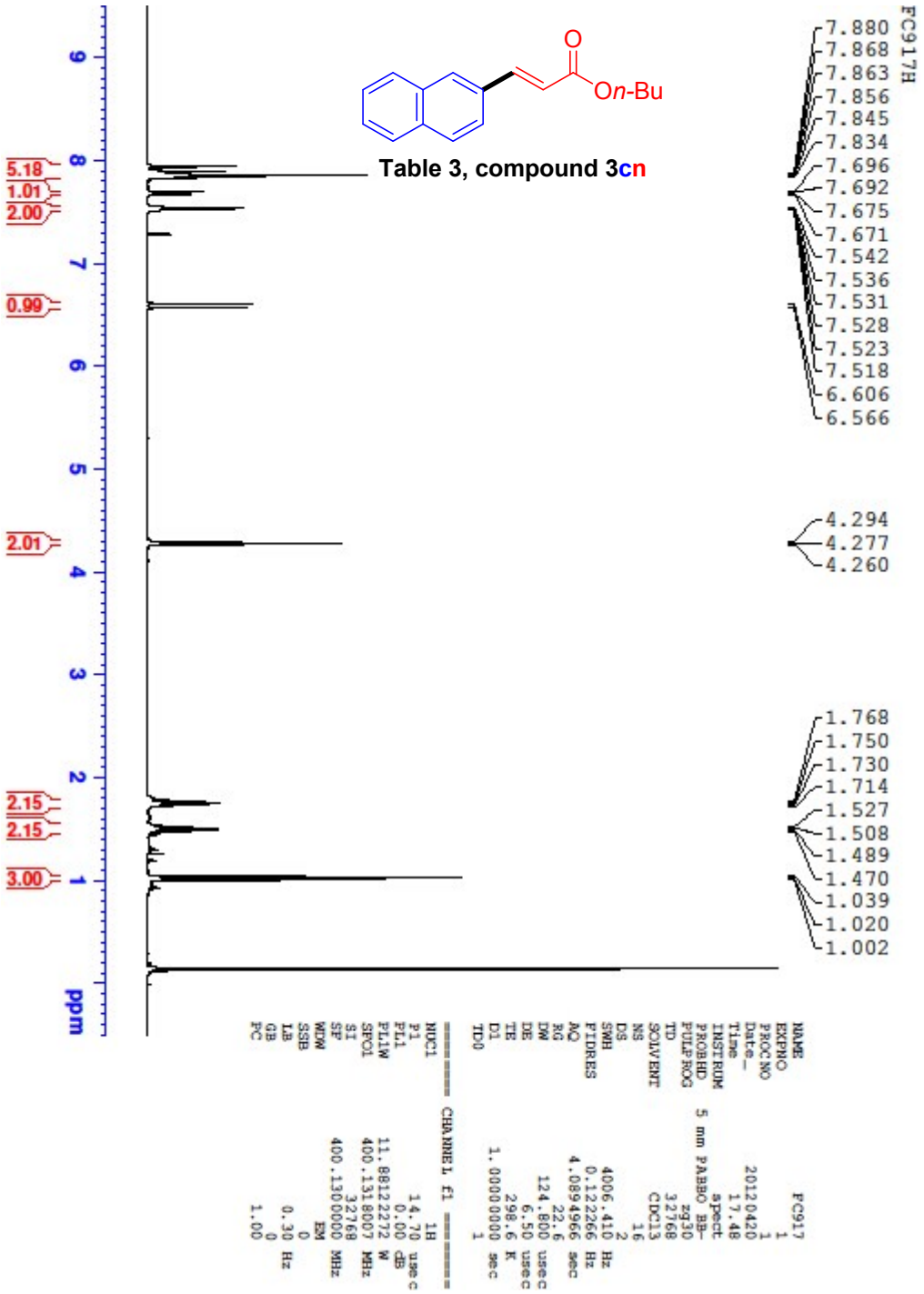


Table 3, compound 3gn


FC917H
O
On-Bu
Table 3, compound 3cn
7.880
7.868
7.863
7.856
7.845
7.834
7.696
7.692
7.675
7.671
7.542
7.536
7.531
7.528
7.523
7.518
6.606
6.566
4.294
4.277
4.260
1.768
1.750
1.730
1.714
1.527
1.508
1.489
1.470
1.039
1.020
1.002
5.18
1.01
2.00
0.99
2.01
2.15
2.15
3.00
ppm
NAME FC917
EXPNO 1
PROCNO 1
Date_ 20120420
Time 17.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 22.6
DW 124.800 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

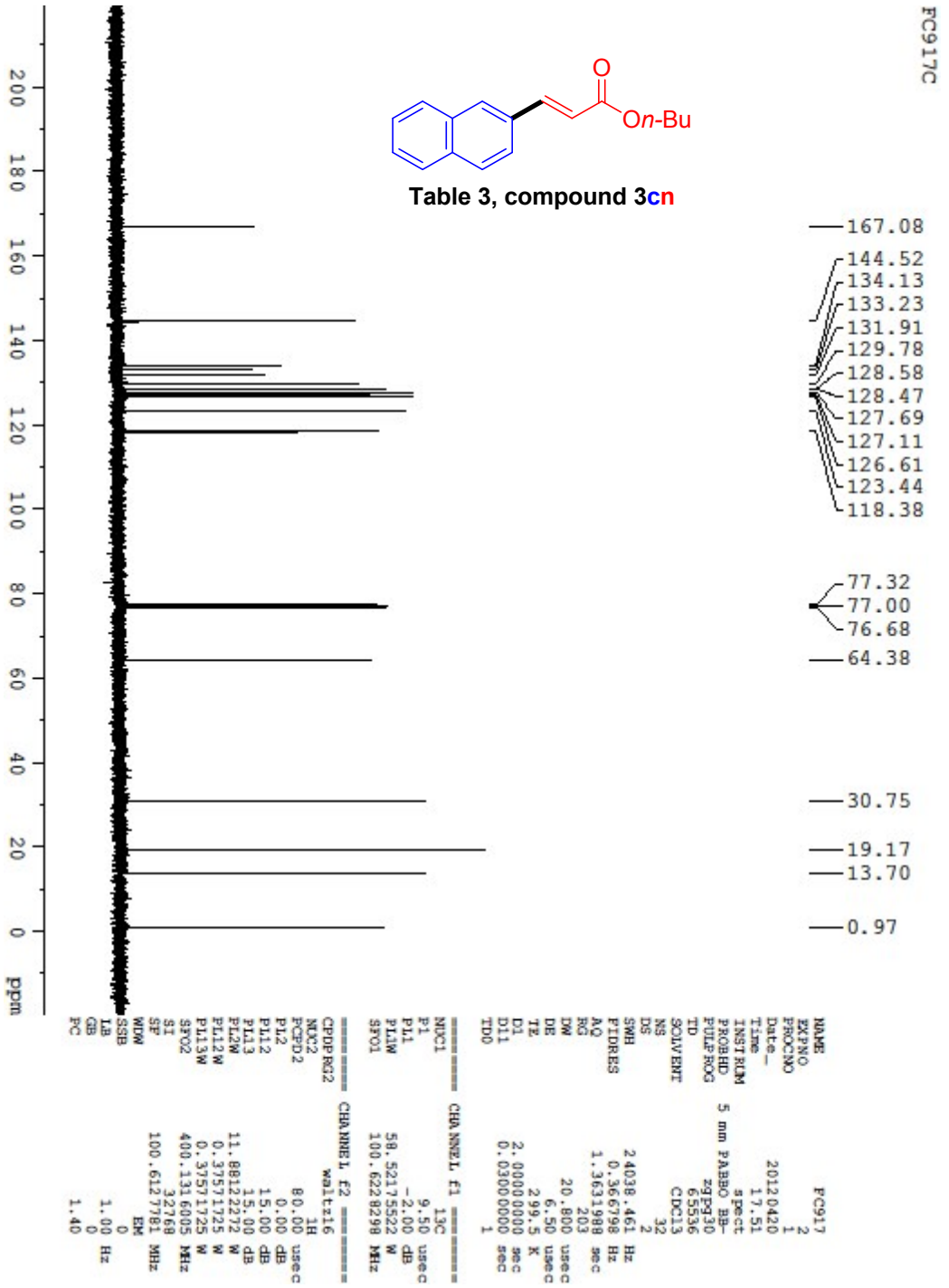


Table 3, compound 3cn

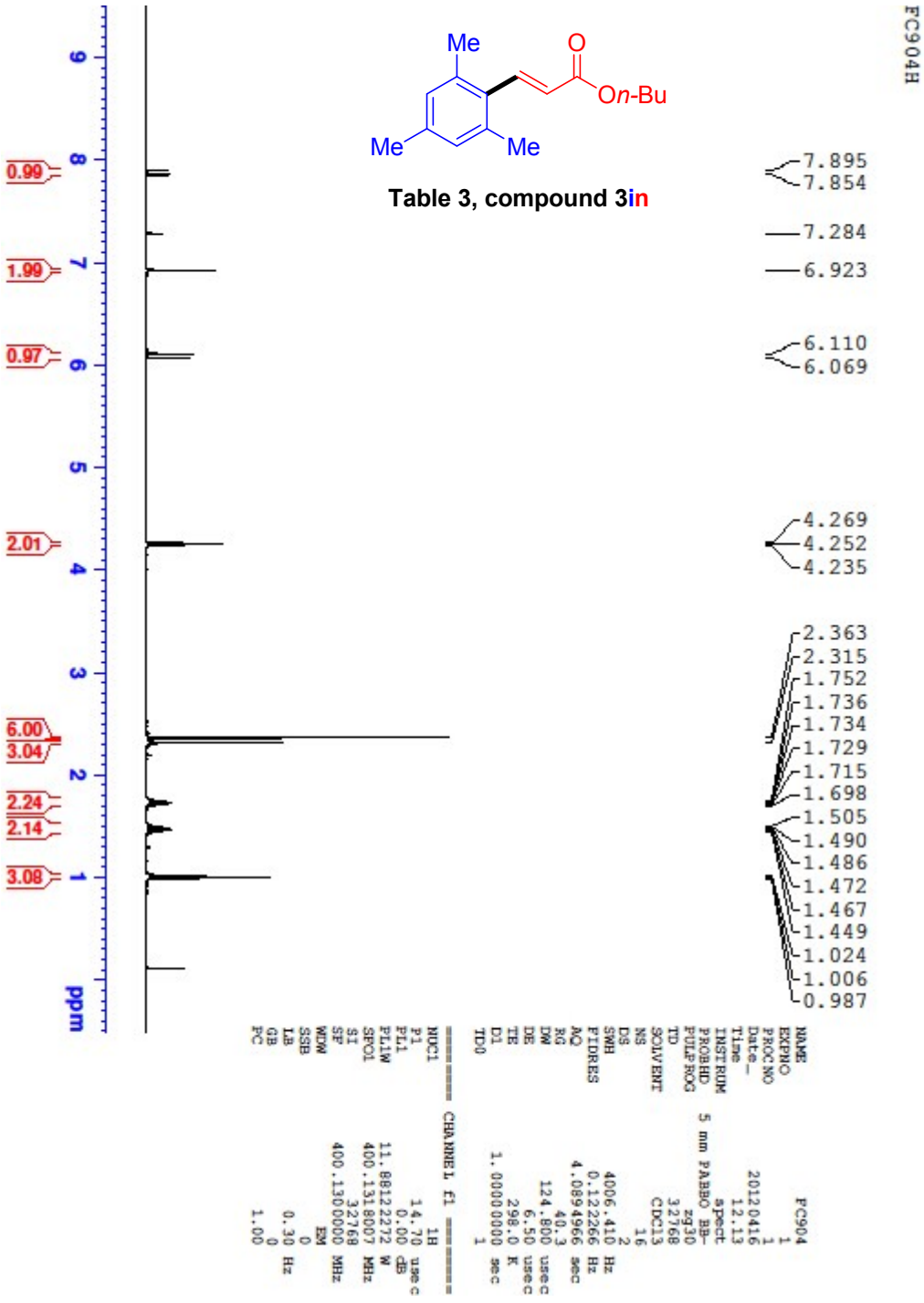


Table 3, compound 3in

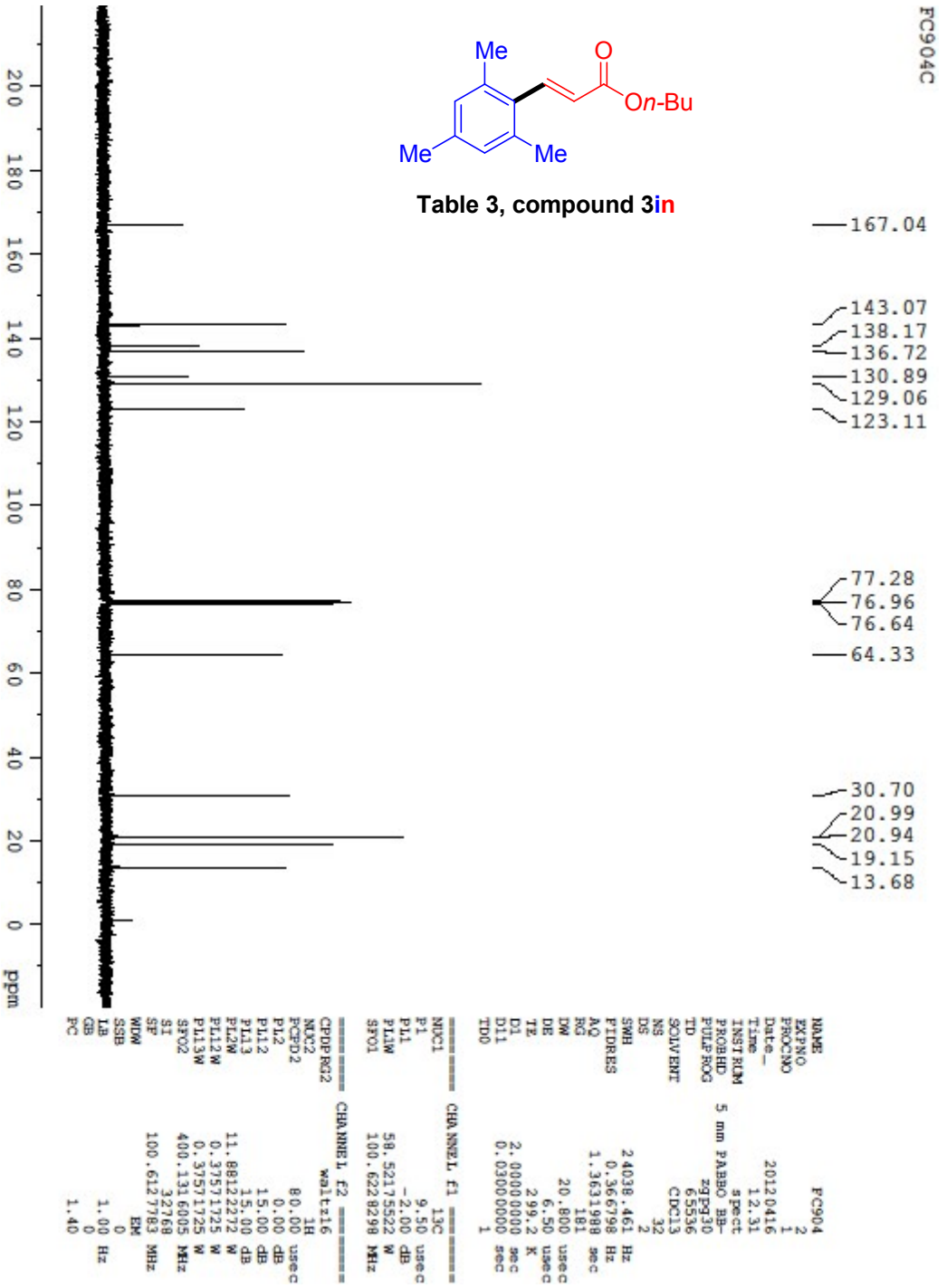
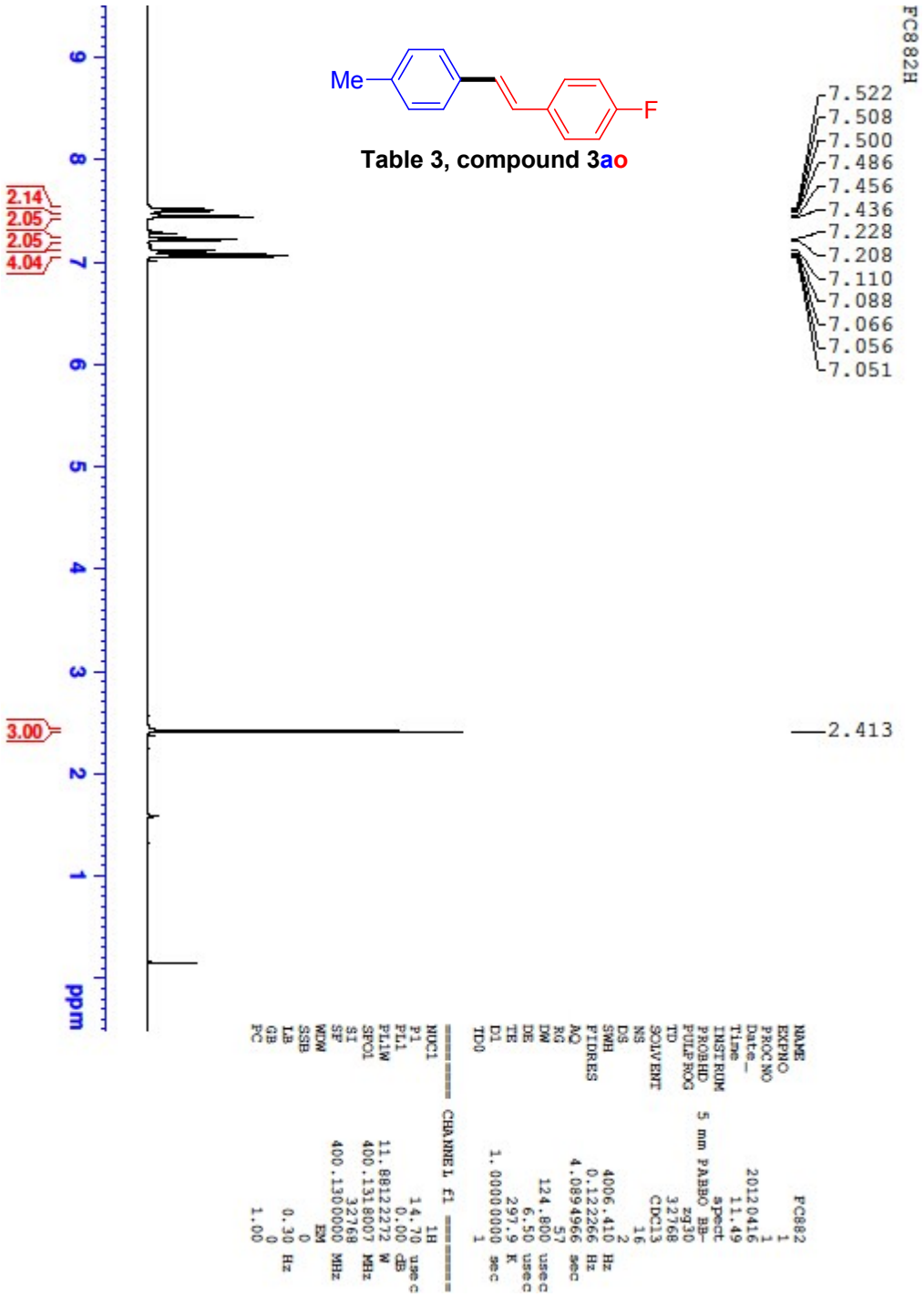


Table 3, compound 3in


Me
F
Table 3, compound 3ao
FC882H
7.522
7.508
7.500
7.486
7.456
7.436
7.228
7.208
7.110
7.088
7.066
7.056
7.051
2.413
2.14
2.05
2.05
4.04
3.00
ppm
NAME FC882
EXPNO 1
PROCNO 1
Date_ 20120416
Time 11.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 57
DW 124.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.0000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

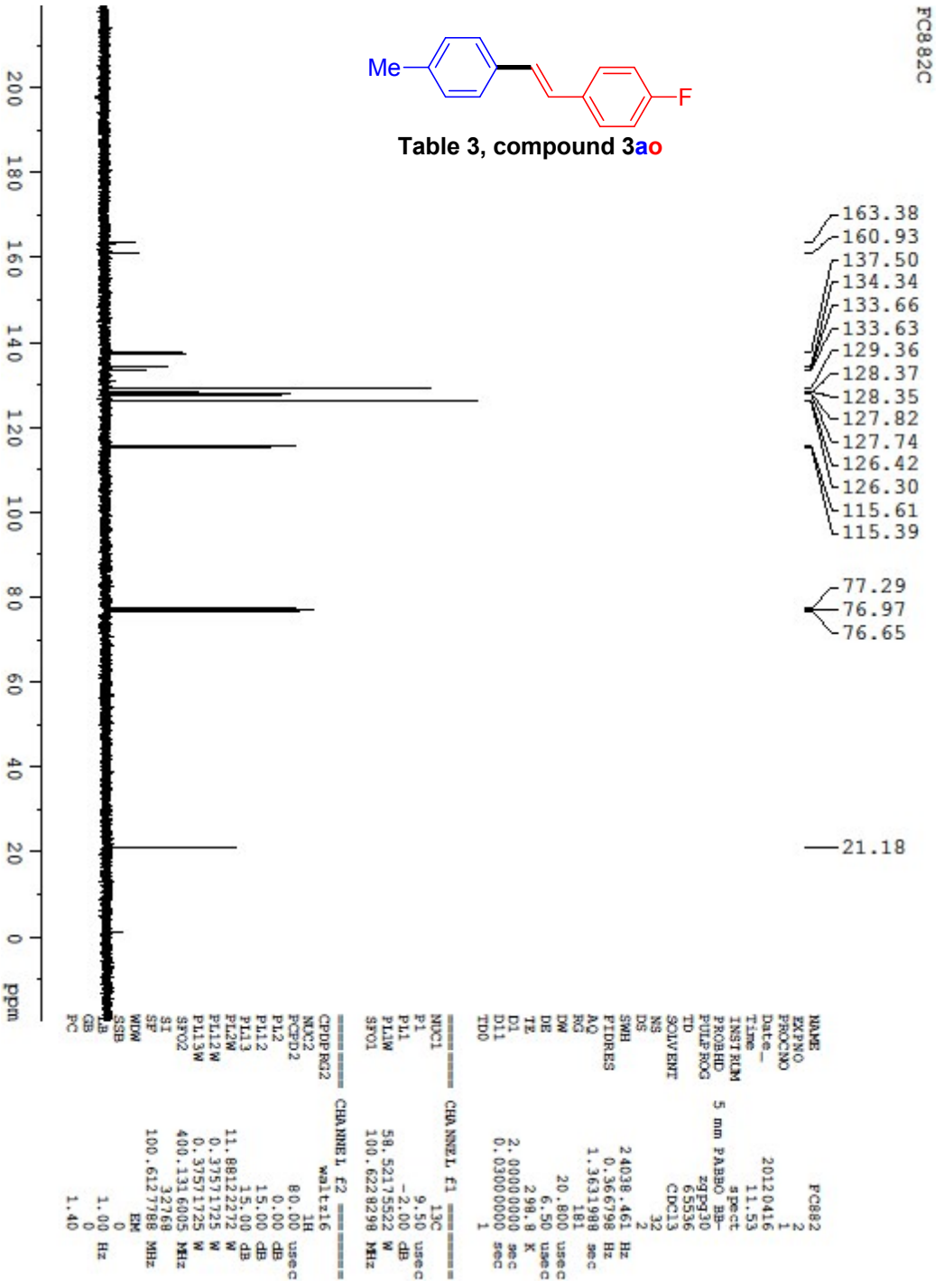


Table 3, compound 3ao

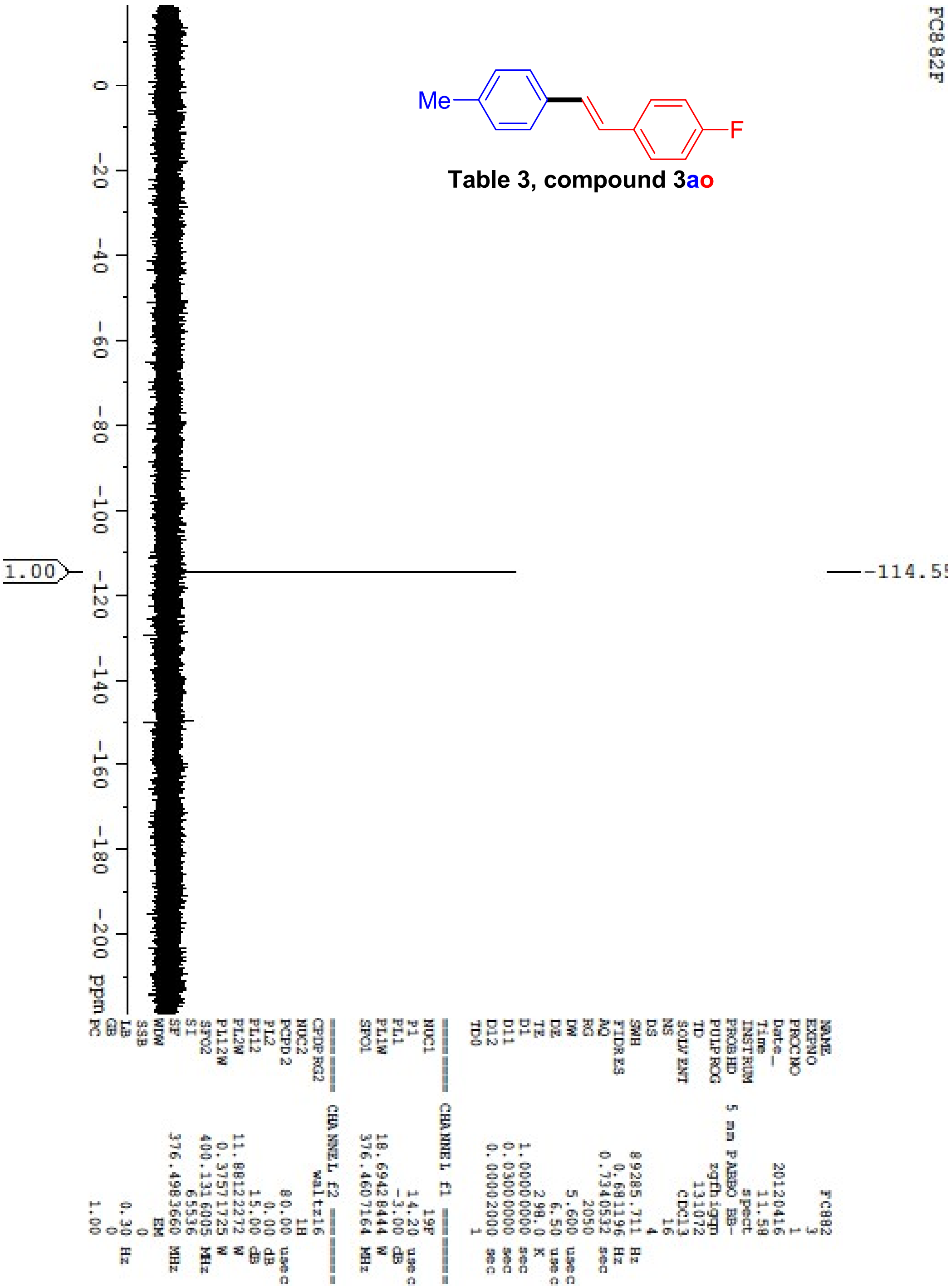


Table 3, compound 3ao

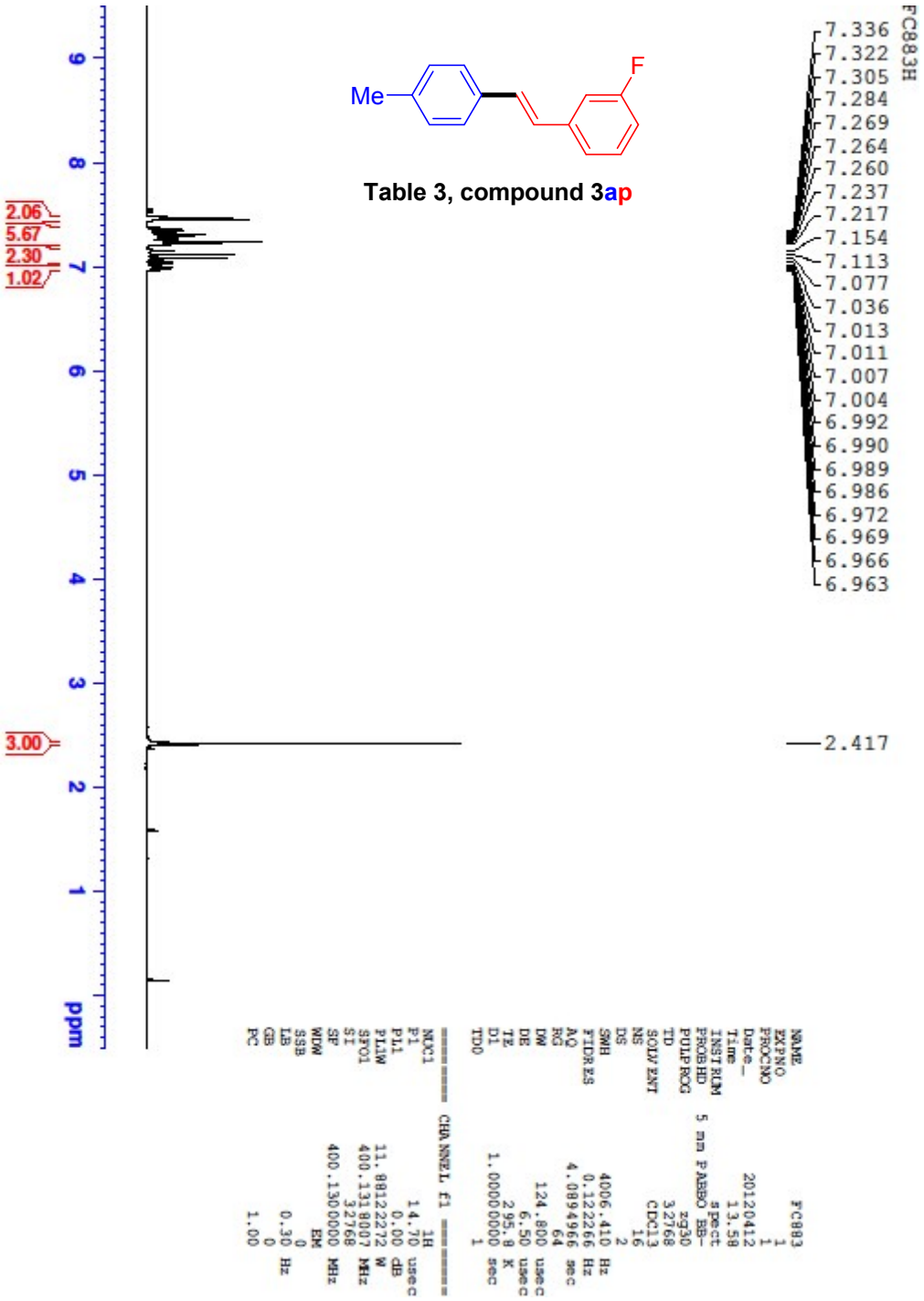


Table 3, compound 3ap

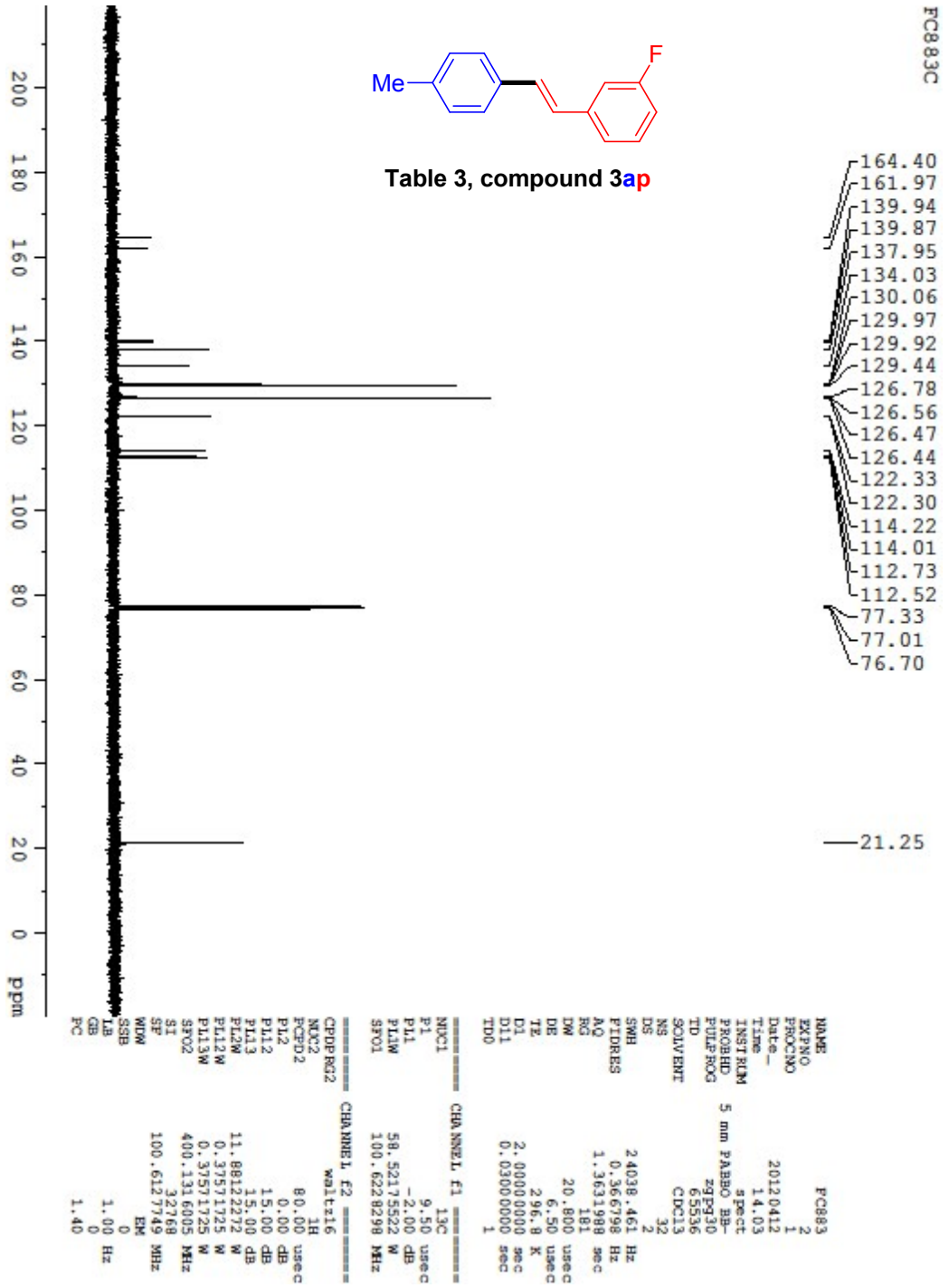


Table 3, compound 3ap

NAME	FC883
EXPNO	2
PROCNO	1
Date_	20120412
Time	14.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	181
DW	20.800 usec
DE	6.50 usec
TE	296.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

========	CHANNEL f1	========
NUC1	13C	
P1	9.50	usec
PL1	-2.00	dB
PL1W	58.52175522	W
SFO1	100.6228298	MHz

========	CHANNEL f2	========
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	0.00	dB
PL12	15.00	dB
PL13	15.00	dB
PL2W	11.88122272	W
PL12W	0.37571725	W
PL13W	0.37571725	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127749	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

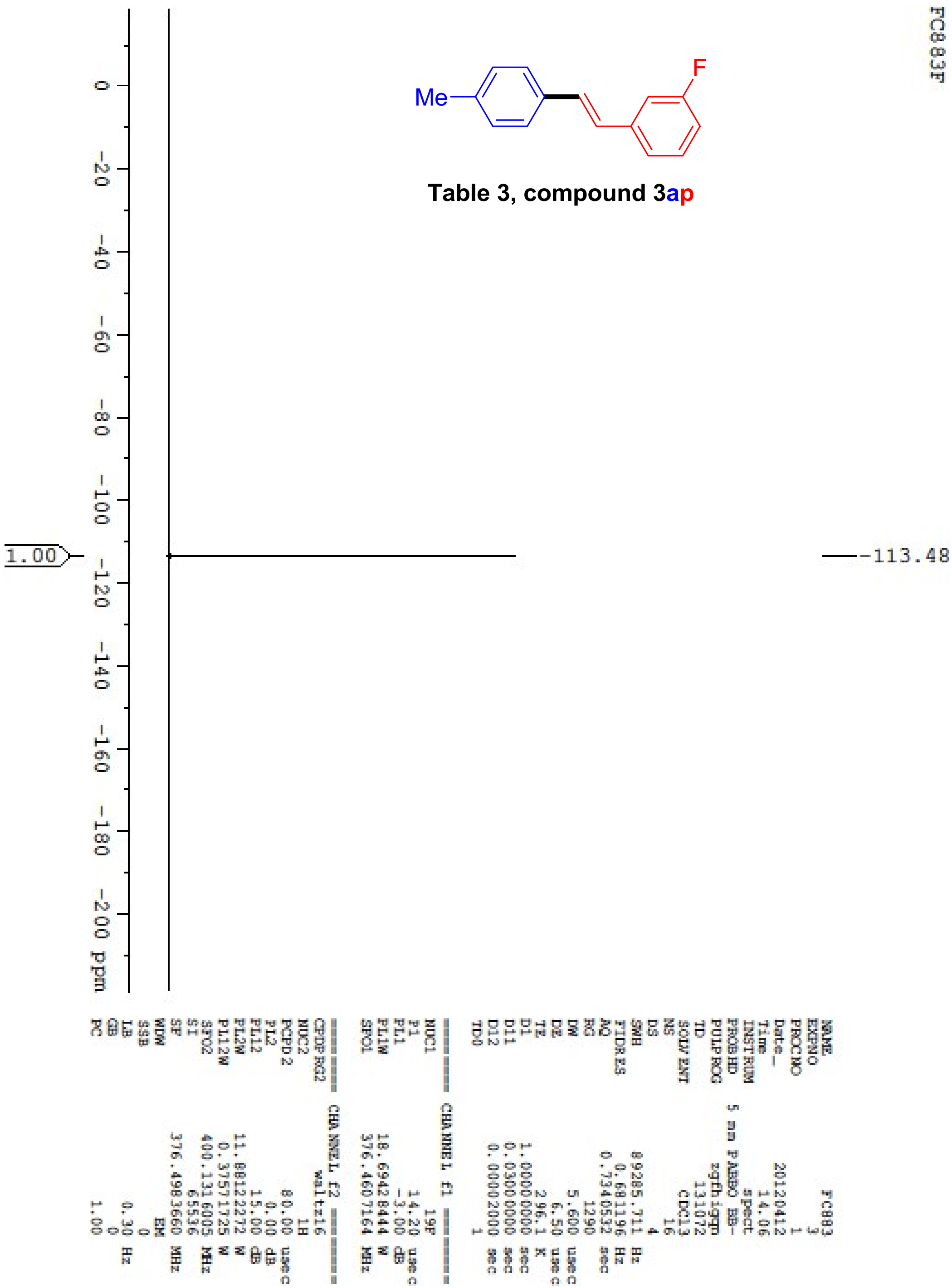


Table 3, compound 3ap

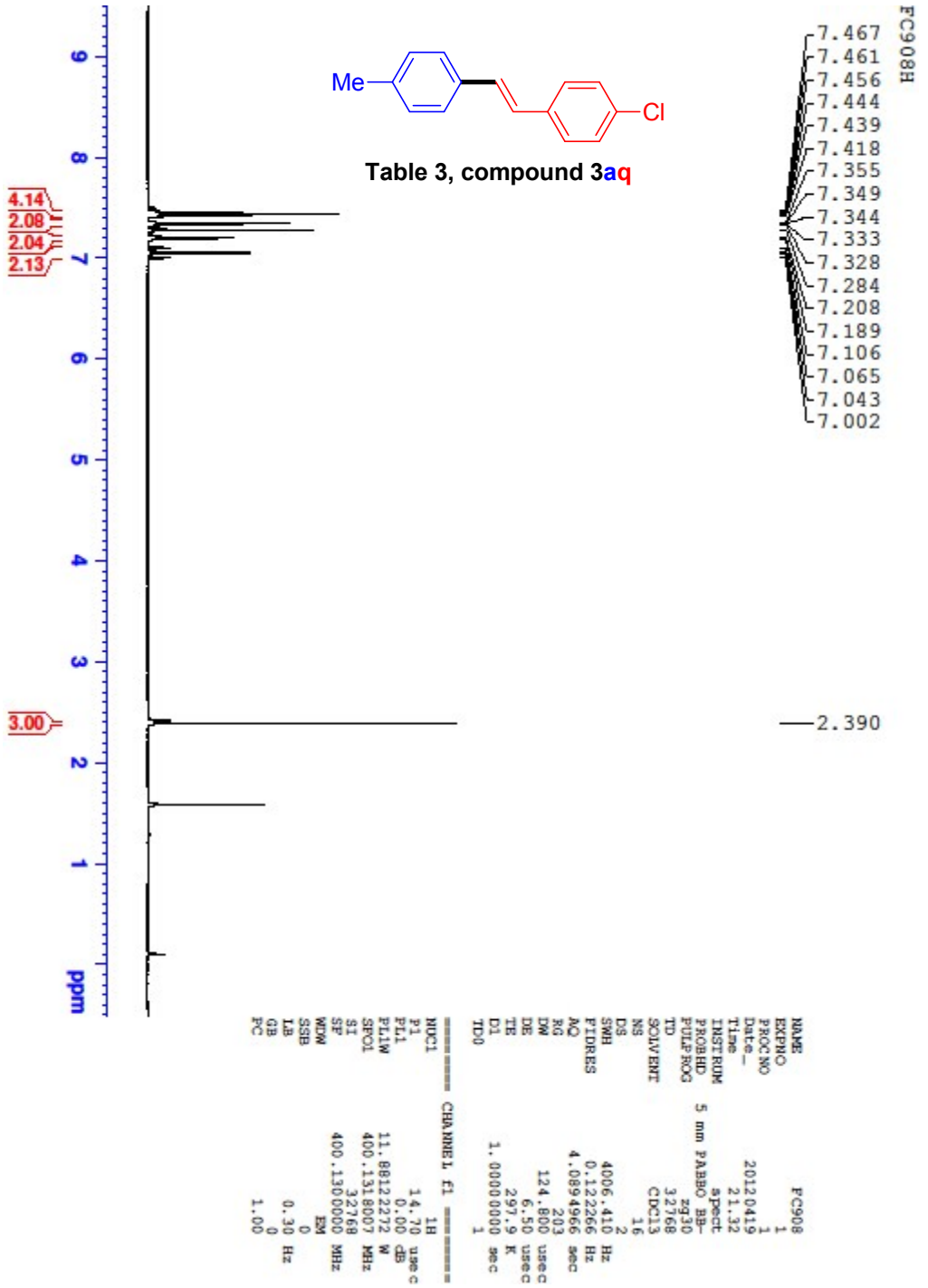


Table 3, compound 3aq

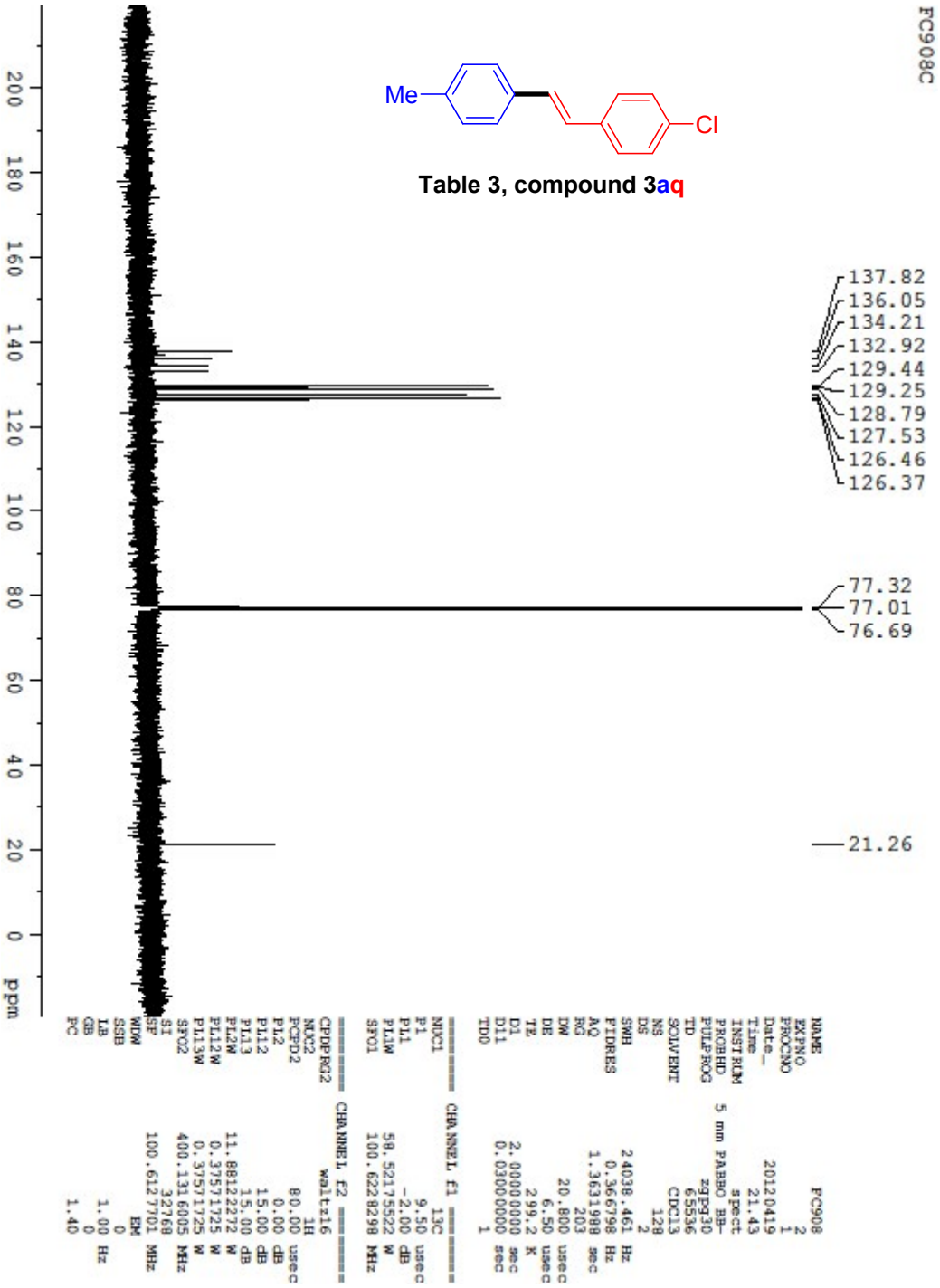
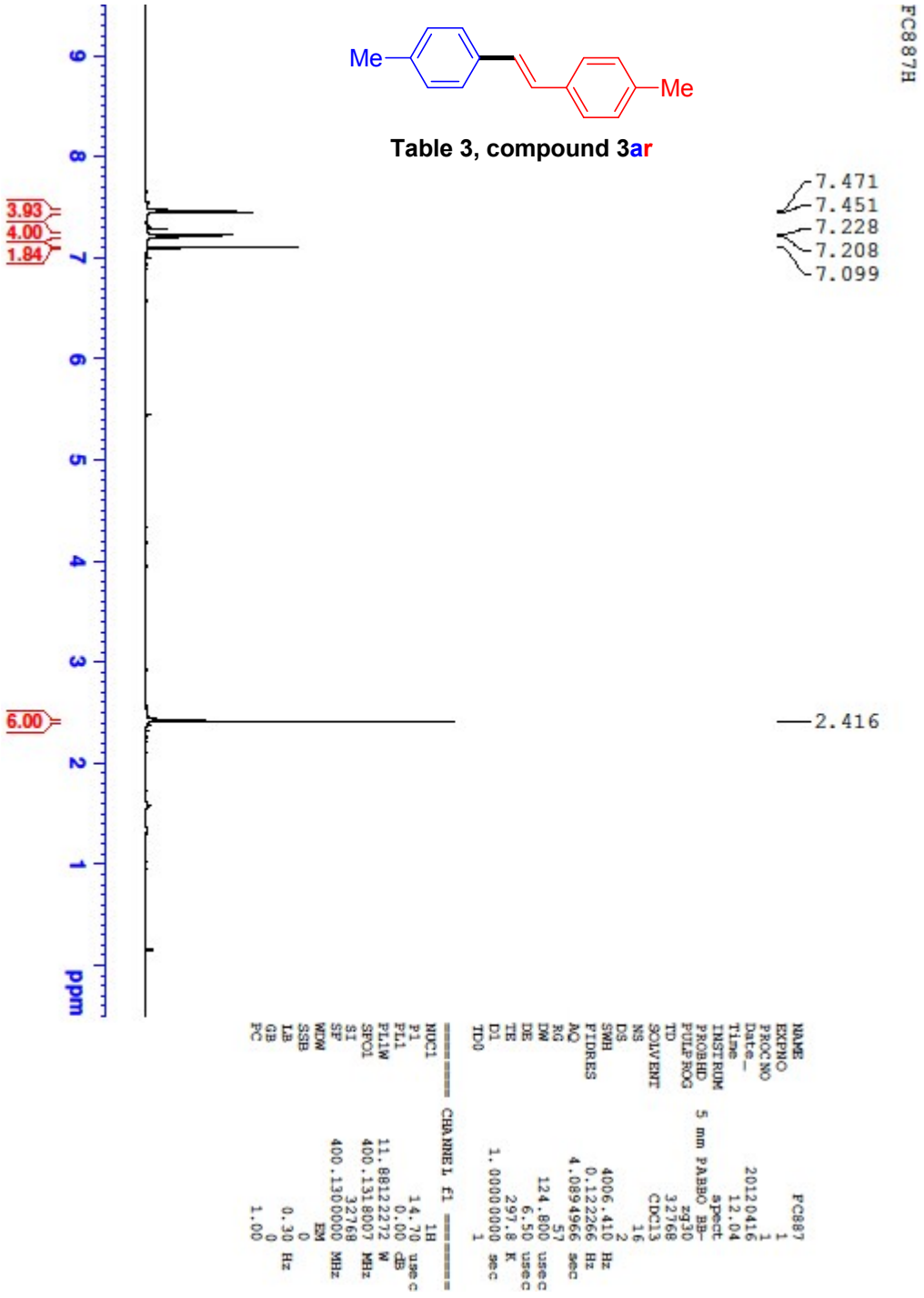


Table 3, compound 3aq


Me
Me
Table 3, compound 3ar
FC887H
7.471
7.451
7.228
7.208
7.099
2.416
3.93
4.00
1.84
6.00
ppm
NAME FC887
EXPNO 1
PROCNO 1
Date_ 20120416
Time 12.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 57
DW 124.800 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
CHANNEL f1 1H
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.98122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

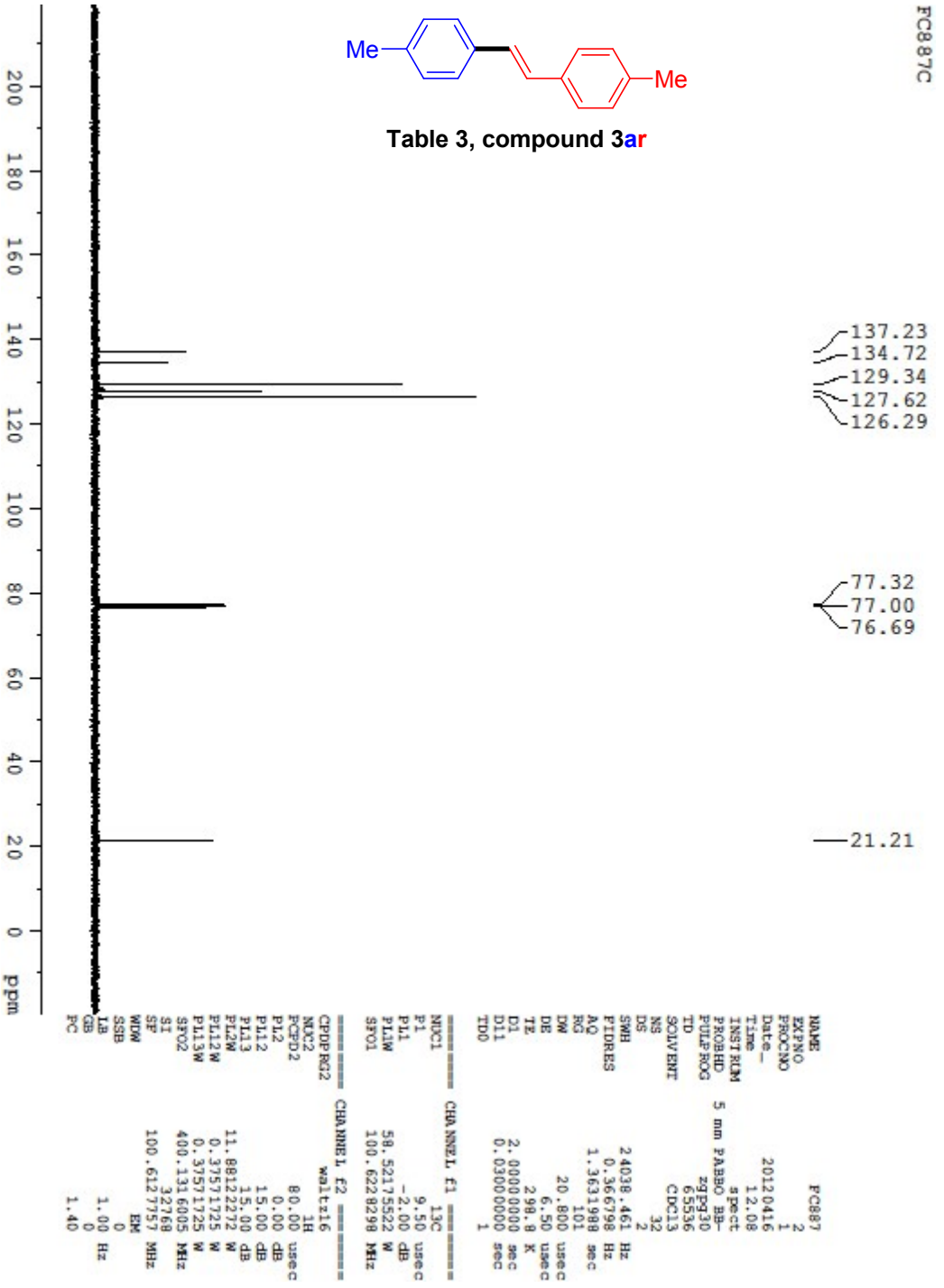


Table 3, compound 3ar

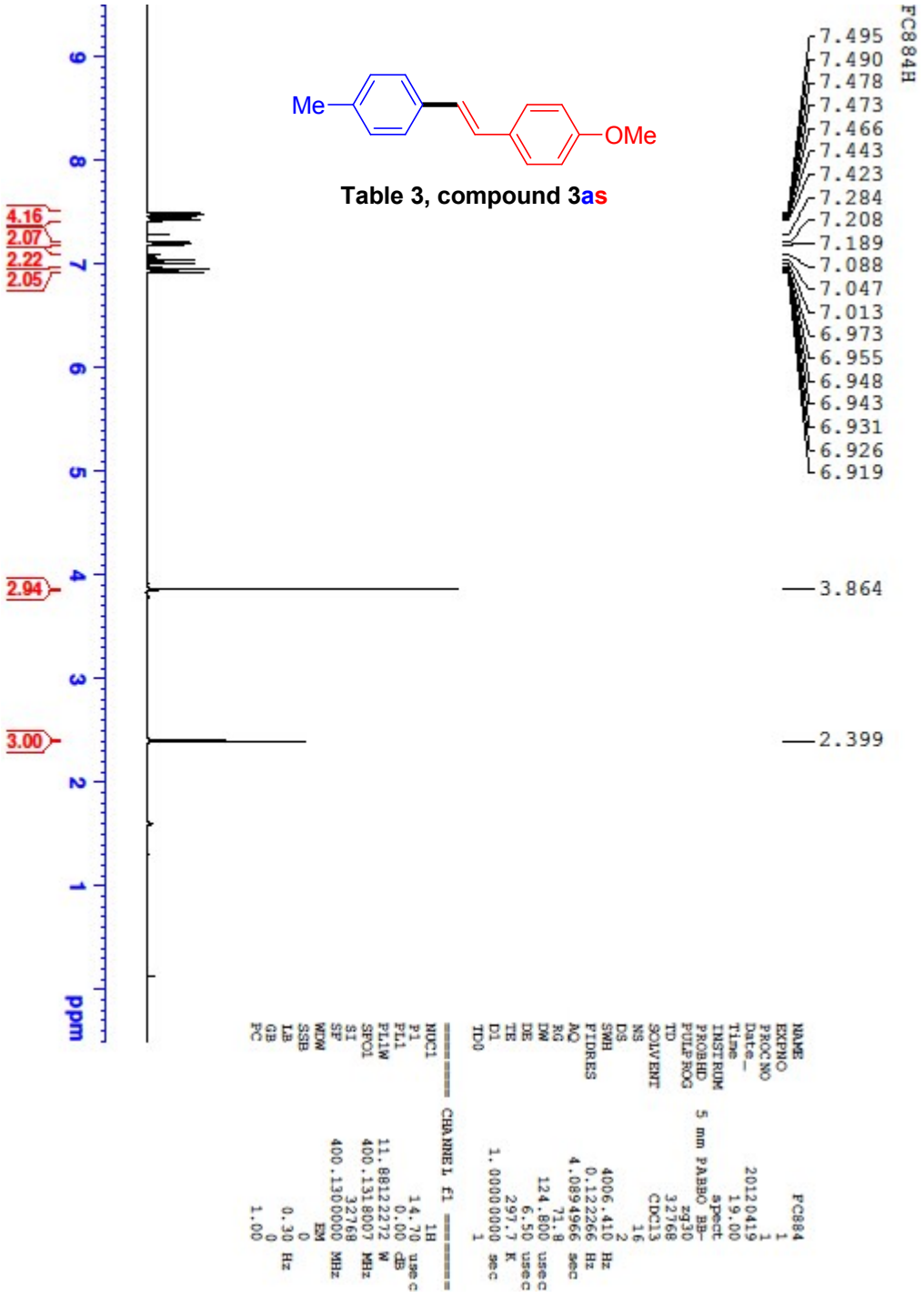


Table 3, compound 3as

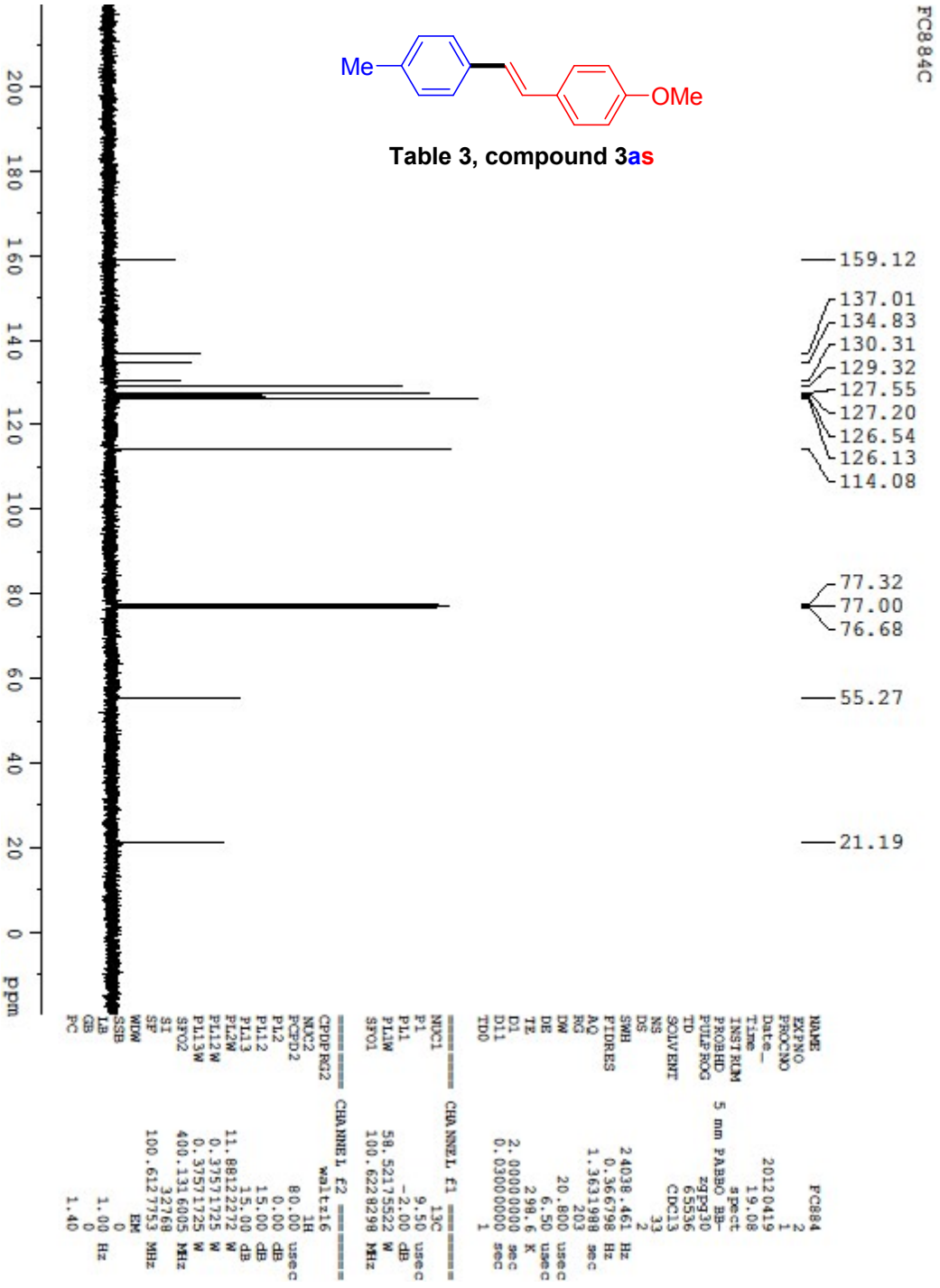
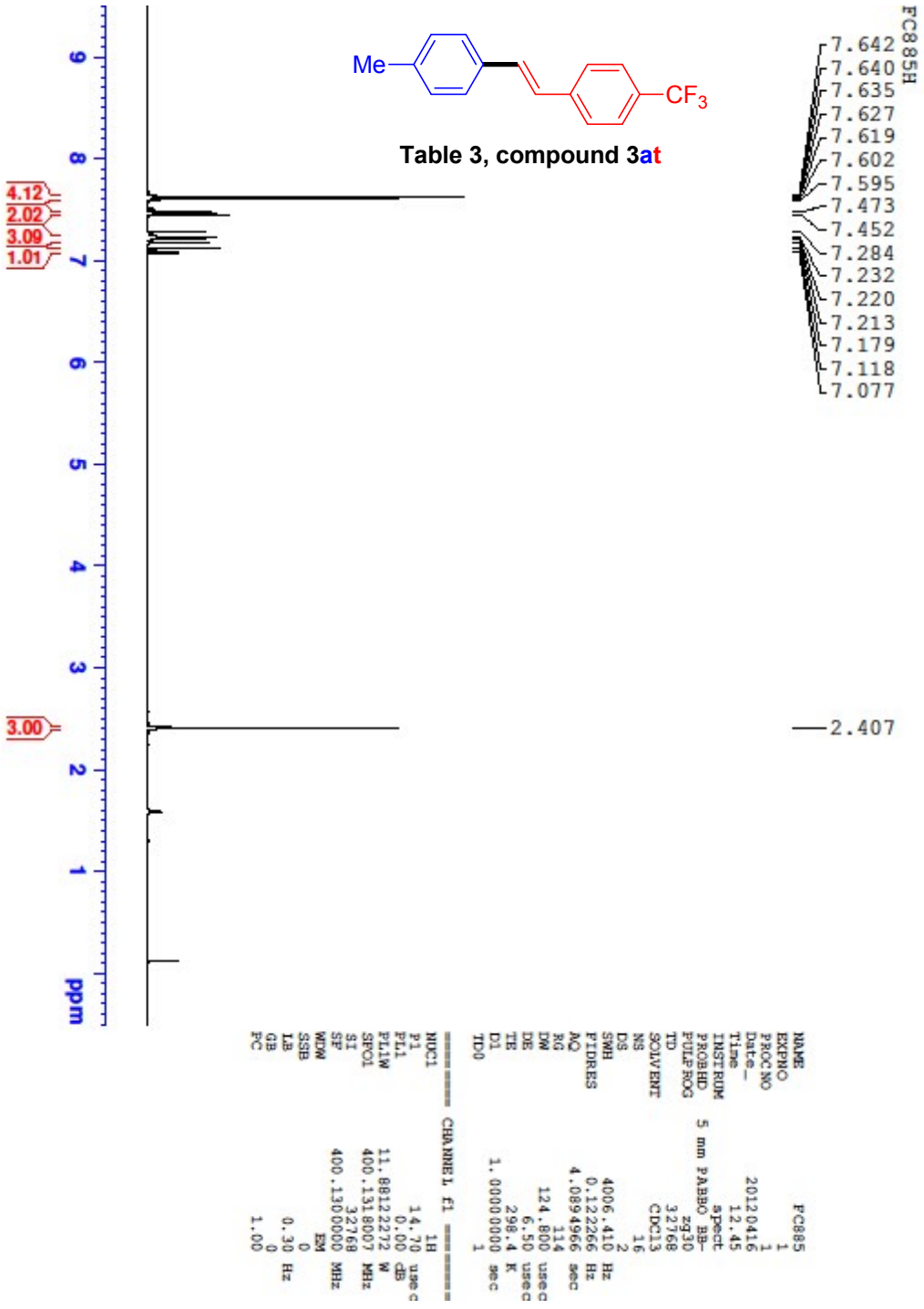


Table 3, compound 3as


FC885H
7.642
7.640
7.635
7.627
7.619
7.602
7.595
7.473
7.452
7.284
7.232
7.220
7.213
7.179
7.118
7.077
2.407
4.12
2.02
3.09
1.01
3.00
ppm
Me
CF3
Table 3, compound 3at
NAME FC885
EXPNO 1
PROCNO 1
Date_ 20120416
Time 12.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4006.410 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 114
DW 124.800 usec
DE 6.50 usec
TE 298.4 K
D1 1.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
PL1W 11.88122272 W
SFO1 400.1318007 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

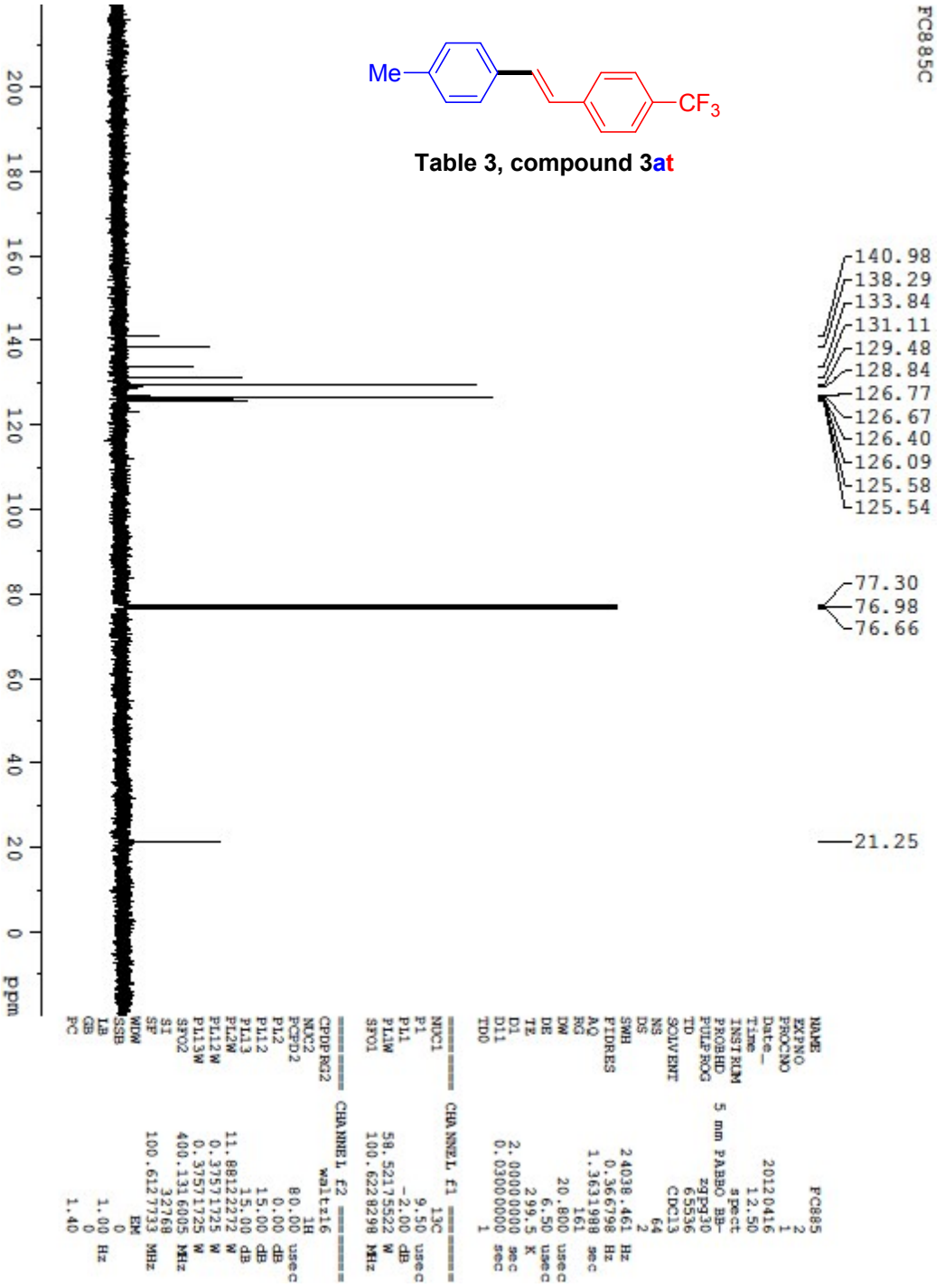
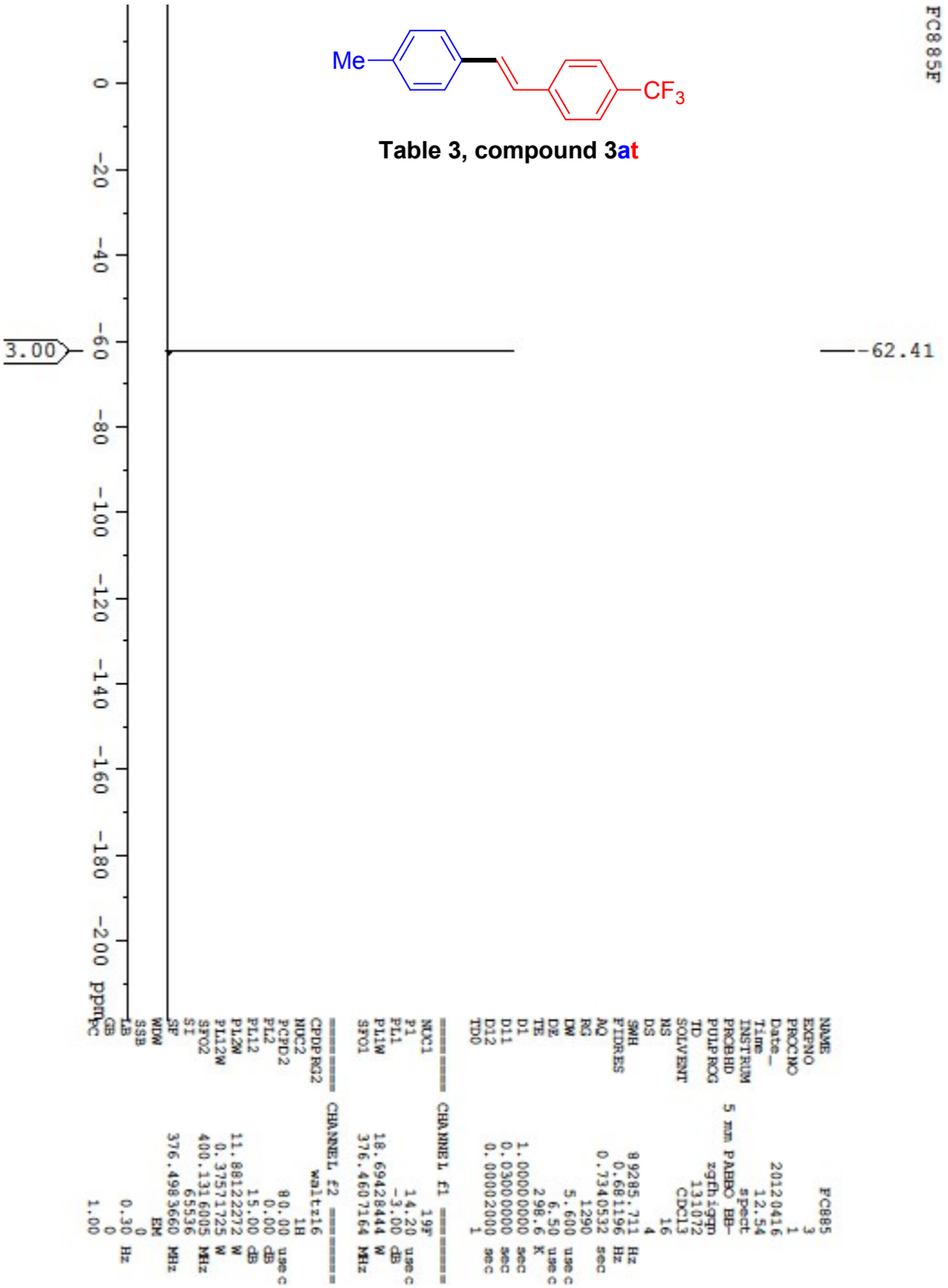


Table 3, compound 3at


Me
CF3
Table 3, compound 3at
FC085F
3.00
-62.41
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
NAME FC085
EXPNO 3
PROCNO 1
Date_ 20120416
Time 12.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 1290
DW 5.600 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
CHANNEL f1
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.46071764 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.13160055 MHz
SI 65536
SF 376.49836600 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

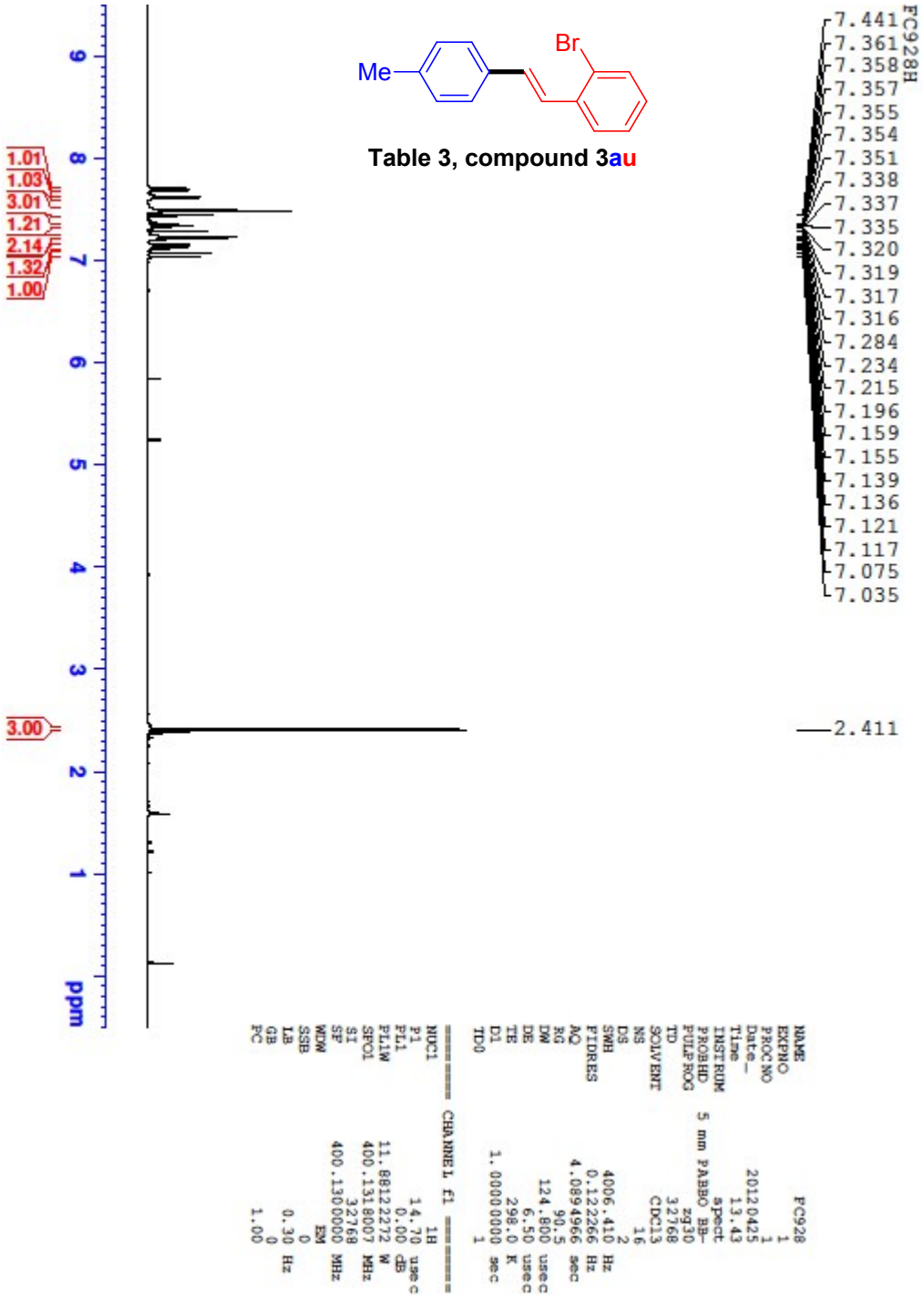


Table 3, compound 3au

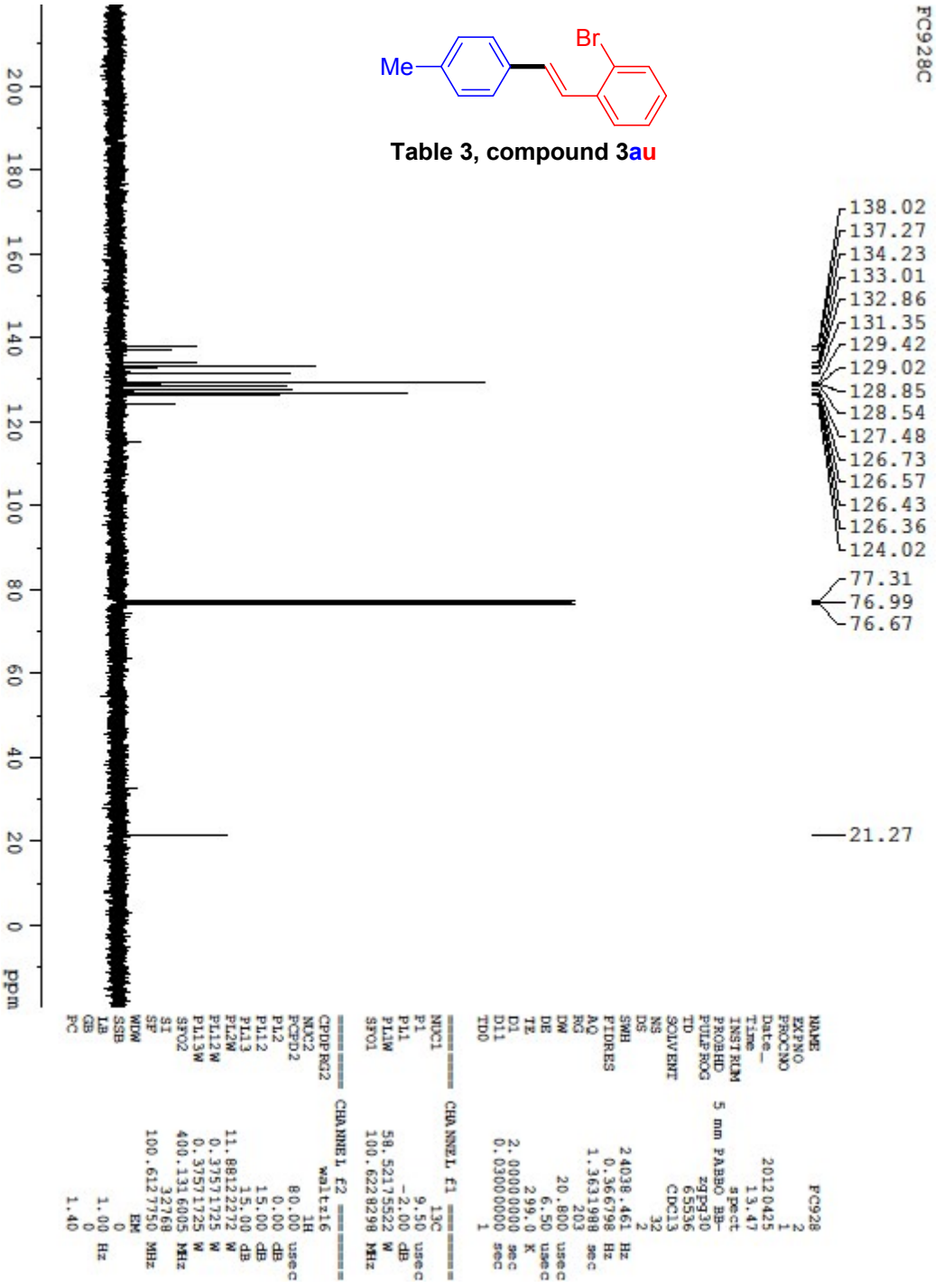


Table 3, compound 3au

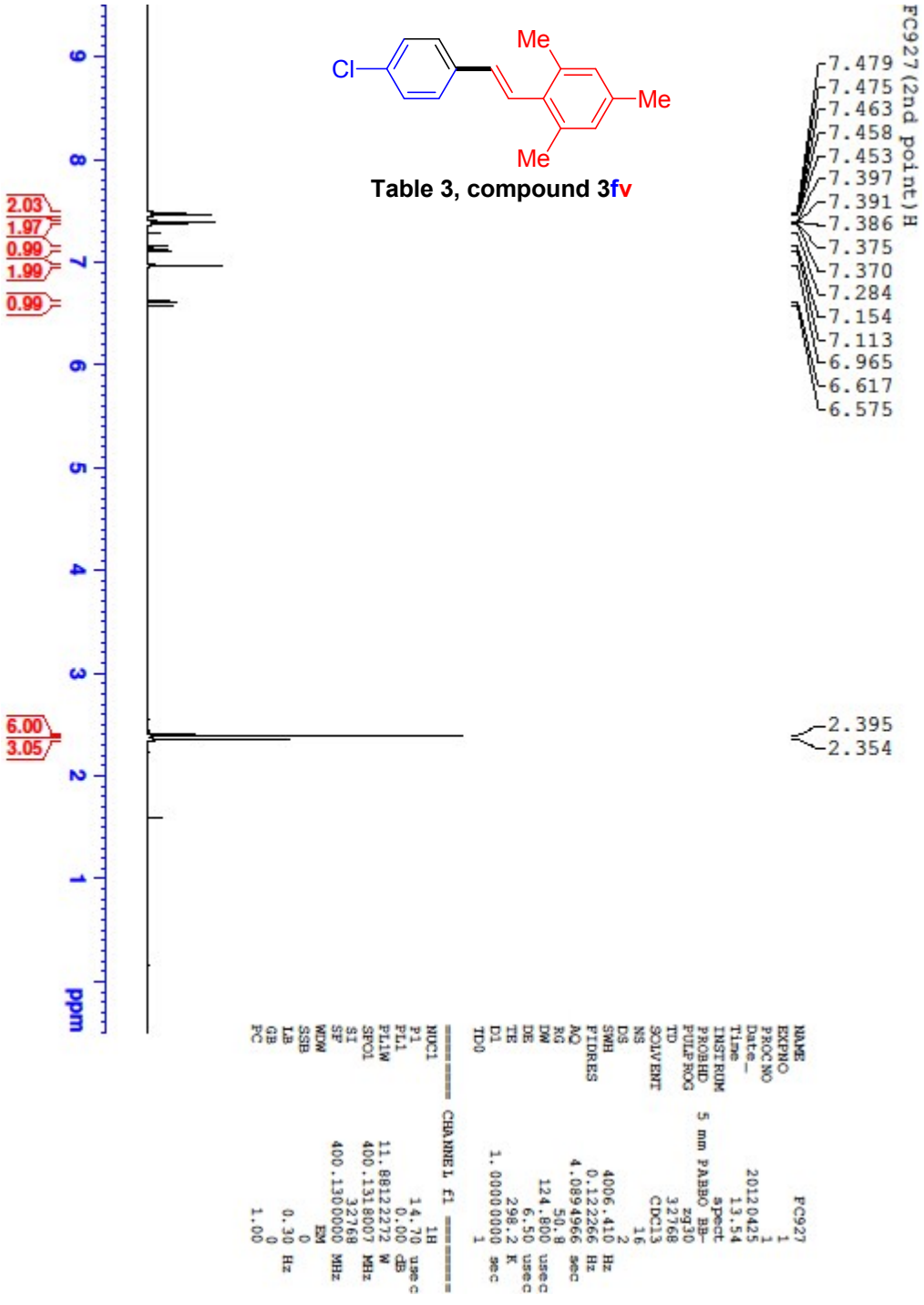


Table 3, compound 3fv

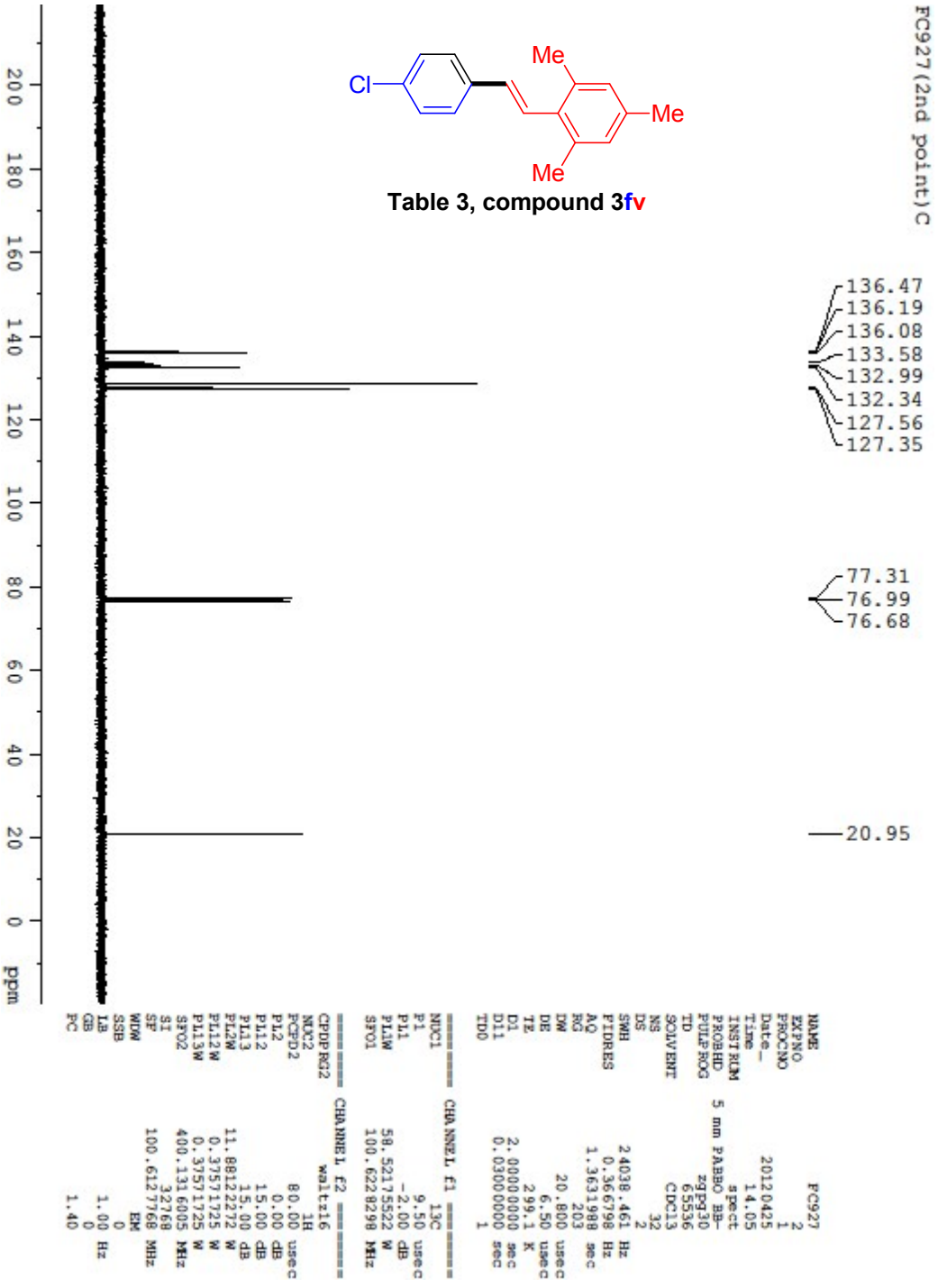
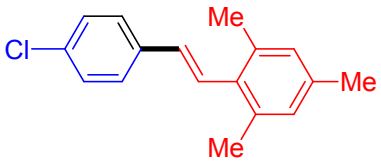


Table 3, compound 3fv



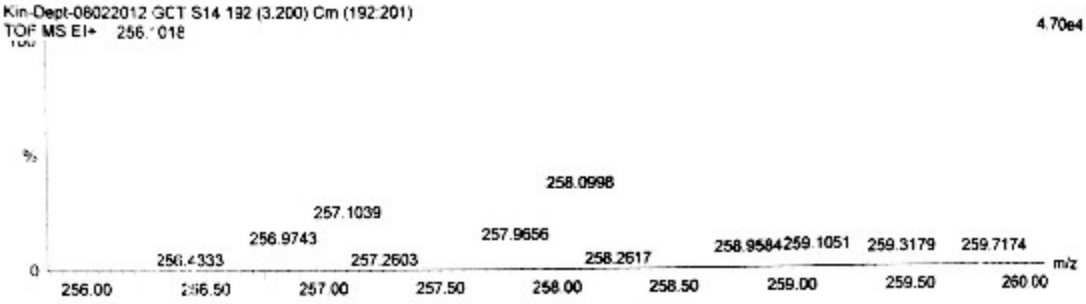
Elemental Composition Report

Table 3, compound 3fv

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 2-17 H: 0-17 Cl: 0-1

Kin-Dept-08022012 GCT S14 192 (3.200) Cm (192:201)
TOF MS EI+ 256.1018



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
256.1018	256.1019	-0.1	-0.4	9.0	41.7	C17 H17 Cl

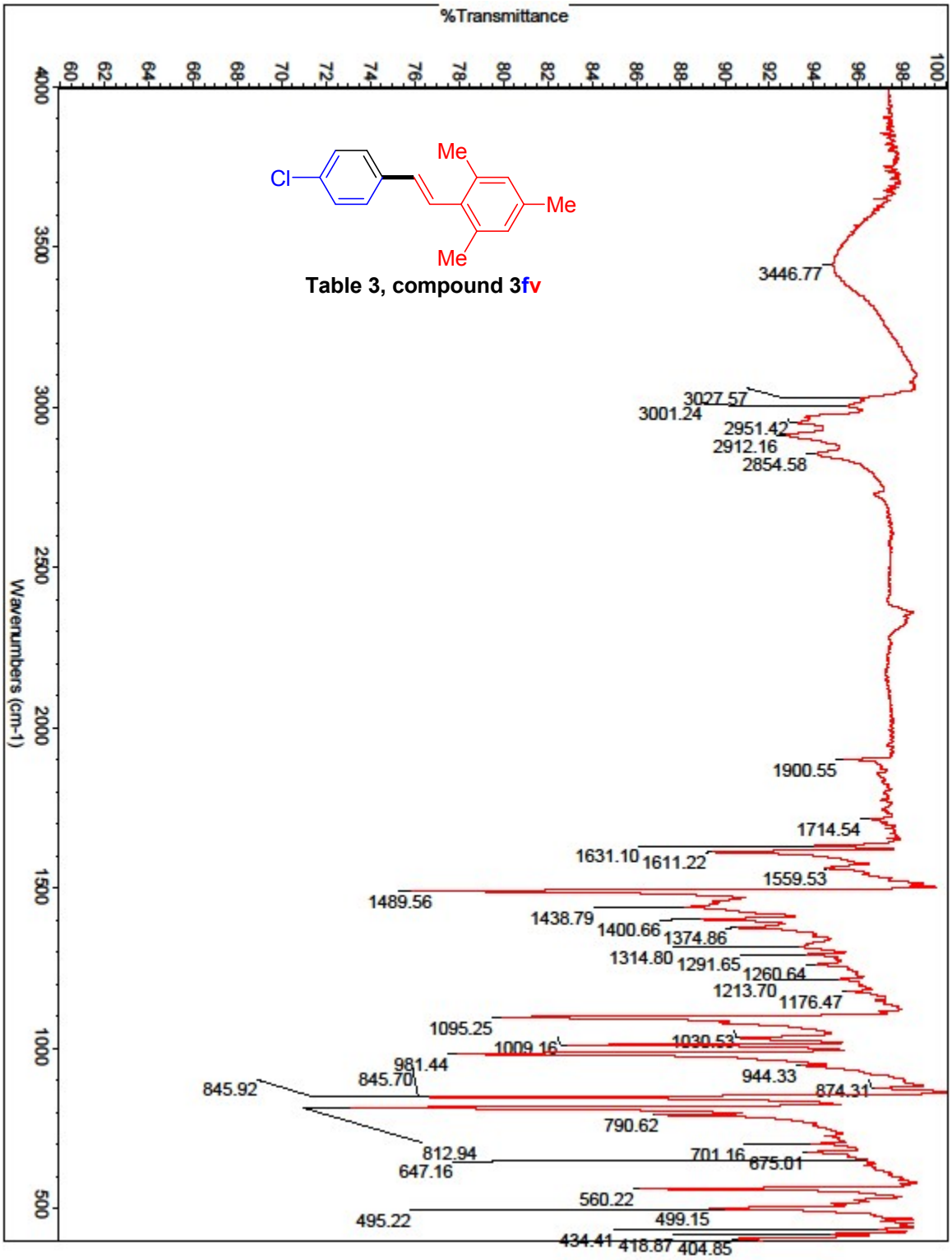


Table 3, compound 3fv

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