Amine-catalyzed and functional group-controlled chemo- and regioselective synthesis of multi-functionalized CF_3-benzene *via* a metal-free process

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Supporting Information

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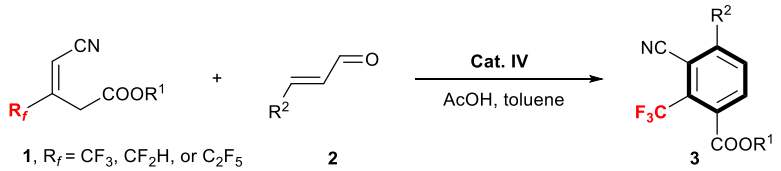
1. General methods

- Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded with Bruker Avance III 400 MHz spectrometers. Proton chemical shifts are reported in parts per million (δ scale), and are referenced using residual protium in the NMR solvent ($CDCl_3$: δ 7.26). Data are reported as follows: chemical shift [multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br s = broad singlet), coupling constant(s) (Hz), integration].
- Carbon-13 nuclear magnetic resonance (^{13}C NMR) spectra were recorded with Bruker Avance 400 MHz spectrometers. Carbon chemical shifts are reported in parts per million (δ scale), and are referenced using the carbon resonances of the solvent ($CDCl_3$: δ 77.0). Data are reported as follows: chemical shift [multiplicity (if not singlet), assignment (C_q = fully substituted carbon)].
- High resolution mass spectra (HRMS) were recorded on a Waters SYNAPT G2 or Agilent G1969-85000 using an electrospray (ESI) ionization source.
- Column chromatography was performed on silica gel (400-500 mesh) eluting with ethyl acetate and petroleum ether. TLC was performed on glass-backed silica plates. UV light and I_2 were used to visualize products.
- Melting points were determined on a Mel-Temp apparatus and are uncorrected.

2. The synthesis of CF3-functionalized multi-substituted benzenes

2.1 Procedure for 3

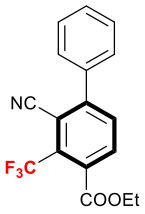


1, R_f = CF_3, CF_2H, or C_2F_5 **2** **3**

The reaction was carried out with **1** (0.20 mmol) and **2** (0.30 mmol), amine catalyst **IV** (0.05 mmol) and AcOH (0.08 mmol) in toluene (2 mL) under an open atmosphere at 70 °C for 8 h. Then the reaction mixture was concentrated and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 80:1) to

give the final CF_3-functionlized tetra-substuted benzenes **3**, which was further analyzed by ^1H NMR, ^{13}C HMR, HRMS analysis.

ethyl 2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3a

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.20 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3a** as a white solid with 76% yield (48.6 mg). m.p. 68-70 ºC.

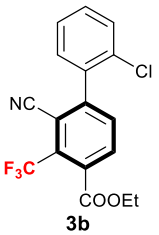
NMR and HRMS data for the product **3a**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.80 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.53-7.50 (m, 5H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.4 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 149.8, 136.6, 133.4, 132.9 (q, *J* = 2.0 Hz), 132.2, 131.2 (d, *J* = 36.0 Hz), 129.8, 129.0, 128.9, 122.1 (d, *J* = 274.0 Hz), 114.5, 110.3 (d, *J* = 2.0 Hz), 62.9, 13.9 ppm.

HRMS (ESI): *m/z* calculated for $C_{17}H_{12}F_3NO_2$+Na 342.0718, found 342.0714.

ethyl 2'-chloro-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3b

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.20 mmol) and 2-chlorocinnamaldehyde (50.0 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3b** as a white solid with 73% yield (51.6 mg). m.p. 68-70 ºC.

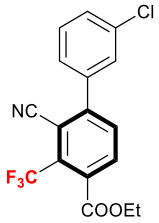
NMR and HRMS data for the product **3b**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.56 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.48-7.40 (m, 2H), 7.34 (dd, *J* = 7.6, 2.0 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 147.2, 135.5, 134.0, 133.6 (q, *J* = 2.0 Hz), 132.8, 132.0, 131.1, 130.8, 130.7 (d, *J* = 32.0 Hz), 130.2, 127.2, 122.0 (d, *J* = 274.0 Hz), 113.7, 112.0 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}ClF_3NO_2$+Na 376.0328, found 376.0325.

ethyl 3'-chloro-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3c

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.20 mmol) and 3-chlorocinnamaldehyde (50.0 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3c** as a white solid with 78% yield (54.9 mg). m.p. 89-91 °C.

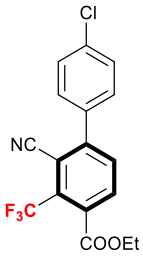
NMR and HRMS data for the product **3c**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.52-7.45 (m, 3H), 7.42 (dt, *J* = 7.2, 1.6 Hz, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 148.1, 138.2, 135.0, 133.5 (d, *J* = 3.0 Hz), 133.2, 132.4, 131.3 (d, *J* = 33.0 Hz), 130.2, 130.0, 129.0, 127.2, 122.0 (d, *J* = 274.0 Hz), 114.1, 110.4 (d, *J* = 3.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}ClF_3NO_2$+Na 376.0328, found 376.0326.

ethyl 4'-chloro-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3d

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.20 mmol) and 4-chlorocinnamaldehyde (50.0 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3d** as a white solid with 77% yield (54.2 mg). m.p. 94-96 ºC.

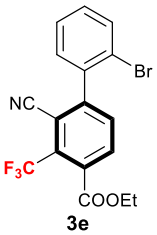
NMR and HRMS data for the product **3d**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.53-7.50 (m, 2H), 7.48-7.45 (m, 2H), 4.43 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm;

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 148.5, 136.3, 134.9,133.3 (d, *J* = 2.0 Hz), 133.2， 132.4, 131.3 (d, *J* = 33.0 Hz), 130.3, 129.3, 122.0 (d, *J* = 275.0 Hz), 114.3, 110.3 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm;

HRMS (ESI): m/z calculated for $C_{17}H_{11}ClF_3NO_2$+Na 376.0328, found 376.0331.

ethyl 2'-bromo-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3e

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 2-bromocinnamaldehyde (63.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3e** as a white solid with 71% yield (56.5 mg). m.p. 96-98 ºC.

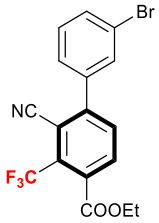
NMR and HRMS data for the product **3e**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.0, 1.2 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.47 (td, *J* = 7.2, 1.2 Hz, 1H), 7.40-7.31 (m, 2H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 148.8, 137.5, 133.9, 133.6 (q, *J* = 2.0 Hz), 133.4, 132.0, 131.2, 130.7, 130.6 (d, *J* = 33.0 Hz), 127.8, 122.5, 122.0 (, *J* = 274.0 Hz), 113.6, 110.9 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}BrF_3NO_2$+Na 419.9823, found 419.9819.

ethyl 3'-bromo-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3f

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-bromocinnamaldehyde (63.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3f** as a white solid with 76% yield (60.3 mg). m.p. 102-104 °C.

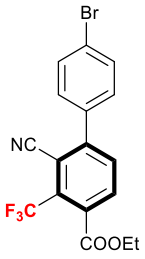
NMR and HRMS data for the product **3f**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.0, 1.2 Hz, 1H), 7.67-7.63 (m, 2H), 7.49-7.47 (m, 1H), 7.40 (td, *J* = 8.0, 0.4 Hz, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 148.0, 138.4, 133.5 (q, *J* = 2.0 Hz), 133.3, 132.8, 132.4, 131.8, 131.3 (d, *J* = 32.0 Hz), 130.4, 127.7, 123.0, 122.0 (d, *J* = 274.0 Hz), 114.1, 110.4 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}BrF_3NO_2$+Na 419.9823, found 419.9821.

ethyl 4'-bromo-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3g

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 4-bromocinnamaldehyde (63.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3g** as a white solid with 78% yield (61.8 mg). m.p. 101-103 ºC.

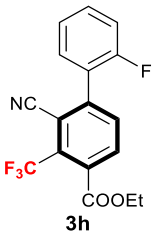
NMR and HRMS data for the product **3g**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.81 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.68-7.65 (m, 2H), 7.41-7.38 (m, 2H), 4.43 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 148.5, 135.4, 133.3 (q, *J* = 2.0 Hz), 133.2, 132.4, 132.2, 131.3 (d, *J* = 33.0 Hz), 130.5, 124.5, 122.0 (, *J* = 274.0 Hz), 114.3, 110.2 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}BrF_3NO_2$+Na 419.9823, found 419.9826.

ethyl 2-cyano-2'-fluoro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3h

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 2-fluorocinnamaldehyde (45.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3h** as a white solid with 72% yield (48.7 mg). m.p. 82-84 ºC.

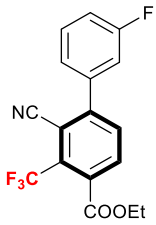
NMR and HRMS data for the product **3h**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.54-7.48 (m, 1H), 7.40 (td, *J* = 7.6, 1.6 Hz, 1H), 7.33-7.28 (m, 1H), 7.24 (d, *J* = 8.8 Hz, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 159.3 (d, *J* = 248.0 Hz), 143.9, 134.2, 133.6 (q, *J* = 2.0 Hz), 132.1, 132.0 (d, *J* = 8.0 Hz), 131.1 (d, *J* = 2.0 Hz), 131.0 (d, *J* = 33.0 Hz), 124.7 (d, *J* = 4.0 Hz), 124.3 (d, *J* = 15.0 Hz), 122.0 (d, *J* = 274.0 Hz), 116.4 (d, *J* = 21.0 Hz), 113.9, 111.8 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}F_4NO_2$+Na 360.0624, found 360.0621.

ethyl 2-cyano-3'-fluoro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3i

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-fluorocinnamaldehyde (45.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3i** as a white solid with 73% yield (49.1 mg). m.p. 95-97 ºC.

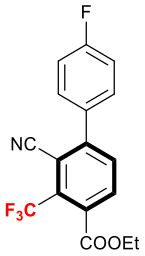
NMR and HRMS data for the product **3i**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.54-7.48 (m, 1H), 7.33-7.30 (m, 1H), 7.25-7.20 (m, 2H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 162.7 (d, *J* = 247.0 Hz), 148.3, 138.4 (d, *J* = 7.0 Hz), 133.5 (q, *J* = 2.0 Hz), 133.3, 132.4, 131.3 (d, *J* = 32.0 Hz), 130.7 (d, *J* = 8.0 Hz), 124.8 (d, *J* = 3.0 Hz), 122.0 (d, *J* = 274.0 Hz), 116.8 (d, *J* = 21.0 Hz), 116.2 (d, *J* = 22.0 Hz), 114.1, 110.4 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}F_4NO_2$+Na 360.0624, found 360.0625.

ethyl 2-cyano-4'-fluoro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3j

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 4-fluorocinnamaldehyde (45.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3j** as a white solid with 75% yield (50.7 mg). m.p. 44-46 ºC.

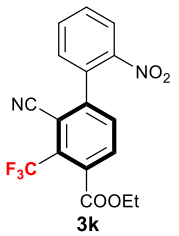
NMR and HRMS data for the product **3j**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.80 (d, *J* = 8.4 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.51 (dd, *J* = 8.4, 5.2 Hz, 2H), 7.24-7.20 (m, 2H), 4.43 (q, *J* = 7.2 Hz, 2H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 163.6 (d, *J* = 279.0 Hz), 148.7, 133.3, 133.1 (q, *J* = 2.0 Hz), 132.6 (d, *J* = 3.0 Hz), 132.3, 131.2 (d, *J* = 32.0 Hz), 131.0 (d, *J* = 9.0 Hz), 122.0 (q, *J* = 274.0 Hz), 116.2 (d, *J* = 22.0 Hz), 114.4, 110.3 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}F_4NO_2$+Na 360.0624, found 360.0627.

ethyl 2-cyano-2'-nitro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3k

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 2-nitrocinnamaldehyde (53.2 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered

3k as a white solid with 64% yield (46.3 mg). m.p. 74-76 °C.

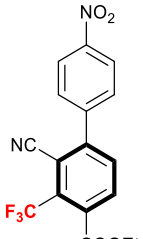
NMR and HRMS data for the product **3k**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.29 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.80 (td, *J* = 7.6, 1.2 Hz, 1H), 7.73 (td, *J* = 8.0, 1.6 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.41 (dd, *J* = 7.2, 1.2 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.0, 147.4, 146.9, 134.0, 133.6 (q, *J* = 2.0 Hz), 132.5, 132.1, 132.0, 131.9, 130.9, 130.8 (q, *J* = 33.0 Hz), 125.5, 121.9 (q, *J* = 274.0 Hz), 113.6, 111.1 (d, *J* = 2.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}F_3N_2O_4$+Na 387.0569, found 387.0570.

ethyl 2-cyano-4'-nitro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3l

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 4-nitrocinnamaldehyde (53.2 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3l** as a white solid with 68% yield (49.5 mg). m.p. 140-142 °C.

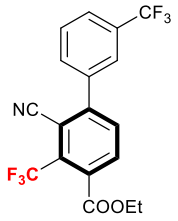
NMR and HRMS data for the product **3l**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.41-8.39 (m, 2H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.73-7.70 (m, 2H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.9, 148.6, 147.1, 142.6, 134.2 (d, *J* = 2.0 Hz), 133.1, 132.7, 131.5 (d, *J* = 33.0 Hz), 130.2, 124.2, 121.8 (d, *J* = 274.0 Hz), 113.9, 110.4 (d, *J* = 2.0 Hz), 63.2, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{11}F_3N_2O_4$+Na 387.0569, found 387.0569.

ethyl 2-cyano-3,3'-bis(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3m

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(trifluoromethyl) cinnamaldehyde (60.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3m** as a white solid with 70% yield (53.9 mg). m.p. 58-60 ^oC.

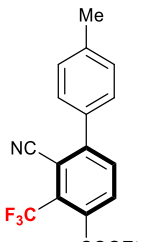
NMR and HRMS data for the product **3m**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.76-7.74 (m, 3H), 7.68 (t, *J* = 8.0 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 148.0, 137.3, 133.7 (d, *J* = 2.0 Hz), 133.3, 132.5, 132.4 (d, *J* = 1.0 Hz), 131.6 (q, *J* = 33.0 Hz), 131.4 (q, *J* = 32.0 Hz), 129.6, 126.5 (q, *J* = 1.6 Hz), 125.9 (q, *J* = 1.6 Hz), 123.7 (d, *J* = 271.0 Hz), 121.9 (d, *J* = 274.0 Hz), 114.1, 110.5 (d, *J* = 2.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{18}H_{11}F_6NO_2$+Na 410.0592, found 410.0591.

ethyl 2-cyano-4'-methyl-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3n

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and trans-4-methylcinnamaldehyde (43.9 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3n** as a white solid with 81% yield (53.7 mg). m.p. 62-64 °C.

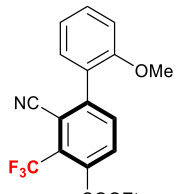
NMR and HRMS data for the product **3n**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.43-7.41 (m, 2H), 7.34-7.32 (m, 2H), 4.43 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.5, 149.8, 140.0, 133.7, 133.3, 132. 7 (d, *J* = 2.0 Hz), 132.1, 131.1 (d, *J* = 32.0 Hz), 129.6, 129.0, 122.1 (d, *J* = 274.0 Hz), 114.7, 110.1 (d, *J* = 3.0 Hz), 62.9, 21.3, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{18}H_{14}F_3NO_2$+Na 356.0874, found 356.0877.

ethyl 2-cyano-2'-methoxy-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3o

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 2-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3o** as a white solid with 79% yield (55.4 mg). m.p. 86-87 °C.

NMR and HRMS data for the product **3o**:

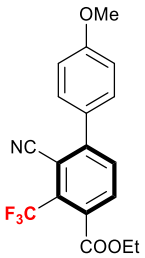
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.77 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.47 (td, *J* = 8.4, 1.6 Hz, 1H), 7.23 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.10-7.03 (m, 2H), 4.43 (q, *J* = 7.2 Hz, 2H), 3.83 (s, 3H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.6, 156.4, 147.1, 134.2, 132.6 (d, *J* = 2.0 Hz), 131.9, 131.4, 130.6, 130.5 (d, *J* = 33.0 Hz), 125.7, 122.2 (d, *J* = 274.0 Hz), 120.9, 114.4,

112.3 (d, J = 2.0 Hz), 111.5, 62.8, 55.5, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{18}H_{14}F_3NO_3$+Na 372.0823, found 372.0825.

ethyl 2-cyano-4'-methoxy-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3p

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3p** as a white solid with 83% yield 57.8 mg). m.p. 101-103 ºC.

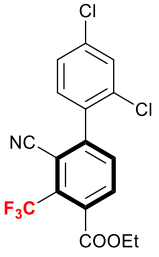
NMR and HRMS data for the product **3p**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.76 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.50-7.46 (m, 2H), 7.06-7.02 (m, 2H), 4.42 (q, J = 7.2 Hz, 2H), 3.88 (s, 3H), 1.40 (t, J = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.5, 160.9, 149.5, 133.3, 132.4 (d, J = 3.0 Hz), 132.1, 131.2 (d, J = 32.0 Hz), 130.4, 128.8, 122.1 (d, J = 274.0 Hz), 114.8, 114.4, 109.9 (d, J = 2.0 Hz), 62.9, 55.4, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{18}H_{14}F_3NO_3$+Na 372.0823, found 372.0821.

ethyl 2',4'-dichloro-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3q

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-

(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(2,4-dichlorophenyl) acrylaldehyde (60.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3q** as a white solid with 76% yield (59.1 mg). m.p. 110-112 ^{o}C.

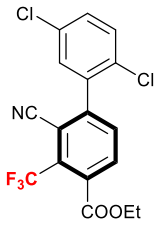
NMR and HRMS data for the product **3q**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.84 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 2.0 Hz, 1H), 7.42 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 146.1, 136.7, 133.9, 133.9, 133.7, 133.3 (d, *J* = 3.0 Hz), 132.2, 131.6, 130.9 (d, *J* = 33.0 Hz), 130.2, 127.7, 121.9 (d, *J* = 274.0 Hz), 113.6, 112.0 (d, *J* = 2.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{10}Cl_2F_3NO_2$+Na 409.9938, found 409.9937.

ethyl 2',5'-dichloro-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3r

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(2,5-dichlorophenyl)acrylaldehyde (60.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3r** as a white solid with 74% yield (57.2 mg). m.p. 134-136 ^{o}C.

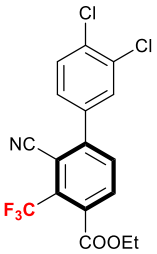
NMR and HRMS data for the product **3r**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85 (dd, *J* = 8.0, 0.4 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.44 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.32 (d, *J* = 2.8 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.0, 145.8, 136.8, 134.0 (q, *J* = 3.0 Hz), 133.7, 133.2, 132.3, 131.3, 131.2, 130.9 (d, *J* = 33.0 Hz), 130.6, 121.9 (d, *J* = 274.0 Hz), 113.4, 112.0 (d, *J* = 2.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{10}Cl_2F_3NO_2$+Na 409.9938, found 409.9940.

ethyl 3',4'-dichloro-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3s

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(3,4-dichlorophenyl)acrylaldehyde (60.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3s** as a white solid with 77% yield (59.6 mg). m.p. 118-120 ºC.

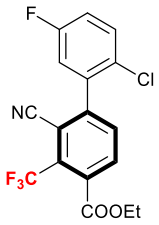
NMR and HRMS data for the product **3s**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.63-7.59 (m, 2H), 7.39 (dd, *J* = 8.4, 2.4 Hz, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.40 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 147.0, 136.2, 134.6, 133.7 (d, *J* = 2.0 Hz), 133.4, 133.1, 132.5, 131.4 (d, *J* = 33.0 Hz), 131.02, 130.8, 128.2, 121.9 (d, *J* = 274.0 Hz), 114.0, 110.4 (d, *J* = 2.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{10}Cl_2F_3NO_2$+Na 409.9938, found 409.9941.

ethyl 2'-chloro-2-cyano-5'-fluoro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3t

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(2-chloro-4-fluorophenyl)acrylaldehyde (55.4 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3t** as a white solid with 75% yield (55.4 mg). m.p. 65-67 °C.

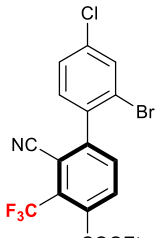
NMR and HRMS data for the product **3t**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85 (dd, *J* = 8.0, 0.4 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.53 (dd, *J* = 8.8, 4.8 Hz, 1H), 7.18 (ddd, *J* = 8.8, 7.6, 3.2 Hz, 1H), 7.08 (dd, *J* = 8.0, 2.8 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 161.0 (d, *J* = 248.0 Hz), 146.0, 136.9 (d, *J* = 8.0 Hz), 134.0 (q, *J* = 2.0 Hz), 133.7, 132.3, 131.7 (d, *J* = 8.0 Hz), 130.9 (d, *J* = 33.0 Hz), 128.1 (d, *J* = 4.0 Hz), 121.9 (q, *J* = 274.0 Hz), 118.3 (d, *J* = 23.0 Hz), 118.0 (d, *J* = 24.0 Hz), 113.4, 111.9 (d, *J* = 2.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{10}ClF_4NO_2$+Na 394.0234, found 394.0235.

ethyl 2'-bromo-4'-chloro-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3u

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(2-bromo-4-

chlorophenyl)acrylaldehyde (73.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3u** as a white solid with 73% yield (62.8 mg). m.p. 102-104 °C.

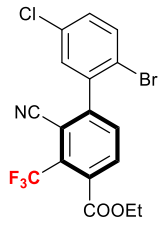
NMR and HRMS data for the product **3u**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.84 (dd, *J* = 8.0, 0.4 Hz, 1H), 7.77 (d, *J* = 2.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.46 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 147.7, 136.6, 136.0, 133.9, 133.2, 132.2, 131.4, 130.8 (d, *J* = 33.0 Hz), 128.3, 126.0 (d, *J* = 4.0 Hz), 123.1, 121.9 (d, *J* = 275.0 Hz), 113.5, 111.9 (d, *J* = 2.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{10}BrClF_3NO_2$+Na 453.9433, found 453.9435.

ethyl 2'-bromo-5'-chloro-2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3v

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(2-bromo-5-chlorophenyl)acrylaldehyde (73.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3v** as a white solid with 72% yield (62.3 mg). m.p. 156-158 °C.

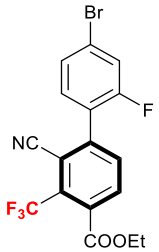
NMR and HRMS data for the product **3v**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85 (dd, *J* = 8.0, 0.4 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.36 (dd, *J* = 8.4, 2.8 Hz, 1H), 7.32 (d, *J* = 2.8 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 147.4, 138.9, 134.5, 134.0 (d, *J* = 3.0 Hz), 134.0, 133.6, 132.3, 131.3, 130.8 (d, *J* = 33.0 Hz), 130.6, 121.9 (d, *J* = 274.0 Hz), 120.6, 113.4, 111.9 (d, *J* = 2.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{10}BrClF_3NO_2$+Na 453.9433, found 453.9431.

ethyl 4'-bromo-2-cyano-2'-fluoro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3w

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(4-bromo-2-fluorophenyl)acrylaldehyde (68.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3w** as a white solid with 70% yield (58.1 mg). m.p. 98-100 ºC.

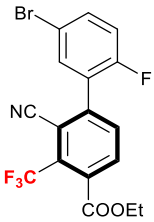
NMR and HRMS data for the product **3w**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.84 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.49-7.45 (m, 2H), 7.31-7.27 (m, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 159.1 (d, *J* = 253.0 Hz), 142.7, 134.0, 133.9 (q, *J* = 2.0 Hz), 132.3, 132.0 (d, *J* = 3.0 Hz), 131.1 (d, *J* = 33.0 Hz), 128.2 (d, *J* = 3.0 Hz), 124.9 (d, *J* = 9.0 Hz), 123.4, 121.9 (q, *J* = 274.0 Hz), 120.2 (d, *J* = 25.0 Hz), 113.8, 111.7 (d, *J* = 1.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{10}BrF_4NO_2$+Na 437.9729, found 437.9727.

ethyl 5'-bromo-2-cyano-2'-fluoro-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3x

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(5-bromo-2-fluorophenyl)acrylaldehyde (68.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3x** as a white solid with 71% yield (58.7 mg). m.p. 74-76 °C.

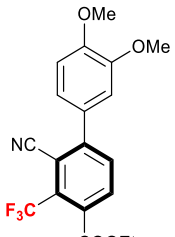
NMR and HRMS data for the product **3x**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85 (dd, *J* = 8.0, 0.4 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.62 (ddd, *J* = 7.6 4.8, 2.8 Hz, 1H), 7.52 (dd, *J* = 6.4, 2.4 Hz, 1H), 7.16 (t, *J* = 8.8 Hz, 1H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.0, 158.5 (d, *J* = 249 Hz), 142.3, 134.9 (d, *J* = 8.0 Hz), 134.1 (q, *J* = 3.0 Hz), 133.9, 13.6 (d, *J* = 2.0 Hz), 132.4, 131.1 (d, *J* = 33.0 Hz), 126.3 (d, *J* = 16.0 Hz), 121.9 (d, *J* = 275.0 Hz), 118.2 (d, *J* = 23.0 Hz), 117.1 (d, *J* = 3.0 Hz), 113.6, 111.9 (d, *J* = 1.0 Hz), 63.1, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{10}BrF_4NO_2$+Na 437.9729, found 437.9730.

ethyl 2-cyano-3',4'-dimethoxy-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3y

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(3,4-dimethoxyphenyl)acrylaldehyde (57.7 mg, 0.3 mmol). Purification of the crude product

via column chromatography delivered **3y** as a white solid with 79% yield (60.2 mg). m.p. 128-130 ºC.

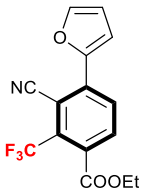
NMR and HRMS data for the product **3y**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.75 (q, *J* = 8.4 Hz, 2H), 7.11-7.05 (m, 2H), 7.00 (d, *J* = 8.0 Hz, 1H), 4.43 (q, *J* = 7.2 Hz, 2H), 3.95 (d, *J* = 2.0 Hz, 6H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.5, 150.4, 149.5, 149.1, 133.3, 132.5, 132.1, 131.2 (d, *J* = 32.0 Hz), 129.0, 122.1 (d, *J* = 274.0 Hz), 122.0, 114.8, 112.2, 111.4, 110.0 (d, *J* = 2.0 Hz), 62.9, 56.2, 56.0, 13.9 ppm.

HRMS (ESI): calcd. For $C_{19}H_{16}F_3NO_4$+Na 402.0929, found 402.0926.

ethyl 3-cyano-4-(furan-2-yl)-2-(trifluoromethyl)benzoate



3z

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(furan-2-yl)acrylaldehyde (36.6 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3z** as a white solid with 67% yield (41.4 mg). m.p. 86-87 ºC.

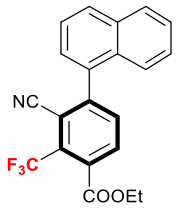
NMR and HRMS data for the product **3z**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.15 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 0.4 Hz, 1H), 7.58 (d, *J* = 3.6 Hz, 1H), 6.63 (dd, *J* = 3.6, 1.2 Hz, 1H), 4.41 (q, *J* = 7.2 Hz, 2H), 1.39 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 147.8, 144.7, 136.8, 132.4, 129.1, 122.1 (d, *J* = 274.0 Hz), 115.0, 113.8, 112.9, 111.7, 110.5, 105.0 (d, *J* = 2.0 Hz), 62.9, 13.9 ppm.

HRMS (ESI): calcd. For $C_{15}H_{10}F_3NO_3$+Na 332.0510, found 332.0515.

ethyl 3-cyano-4-(naphthalen-1-yl)-2-(trifluoromethyl)benzoate



3aa

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(naphthalen-1-yl)acrylaldehyde (54.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3aa** as a white solid with 71% yield (52.6 mg). m.p. 99-101 ^{o}C.

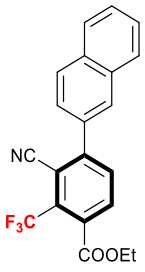
NMR and HRMS data for the product **3aa**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.00 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.61-7.53 (m, 2H), 7.50-7.45 (m, 2H), 7.39 (d, *J* = 8.4 Hz, 1H), 4.47 (q, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ =166.4, 148.8, 134.7, 134.1, 133.7, 133.3 (d, *J* = 2.0 Hz), 131.8, 131.0, 130.9 (d, *J* = 32.0 Hz), 130.2, 128.8, 127.7, 127.2, 126.5, 125.2, 124.6, 122.1 (d, *J* = 274.0 Hz), 113.9, 112.3 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{21}H_{14}F_3NO_2$+Na 392.0874, found 392.0876.

ethyl 3-cyano-4-(naphthalen-2-yl)-2-(trifluoromethyl)benzoate



3ab

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(naphthalen-2-yl)acrylaldehyde (54.7 mg, 0.3 mmol). Purification of the crude product *via* column

chromatography delivered **3ab** as a white solid with 73% yield (53.8 mg). m.p. 110-111 ^{o}C.

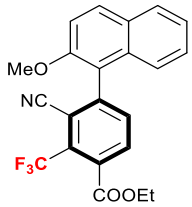
NMR and HRMS data for the product **3ab**:

^{1}H NMR (400 MHz, $CDCl_3$): δ =7.99 (d, *J* = 8.8 Hz, 2H), 7.92 (dd, *J* = 8.8, 5.2 Hz, 2H), 7.85-7.80 (m, 2H), 7.62-7.55 (m, 2H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.41 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ =166.4, 149. 8, 133.9, 133.6, 133.5, 133.0, 133.0 (d, *J* = 3.0 Hz), 132.2, 131.3 (d, *J* = 32.0 Hz), 128.9, 128.9, 128.5, 127.8, 127.4, 127.0, 125.9, 122.1 (d, *J* = 274.0 Hz), 114.6, 110.5 (d, *J* = 2.0 Hz), 63.0, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{21}H_{14}F_3NO_2$+Na 392.0874, found 392.0871.

ethyl 3-cyano-4-(2-methoxynaphthalen-1-yl)-2-(trifluoromethyl)benzoate



3ac

Prepared according to the general procedure using ethyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (41.4 mg, 0.2 mmol) and 3-(2-methoxynaphthalen-1-yl)acrylaldehyde (63.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3ac** as a white solid with 64% yield (50.9 mg). m.p. 148-149^{o}C.

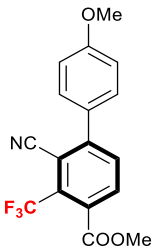
NMR and HRMS data for the product **3ac**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.01 (d, *J* = 9.0 Hz, 1H), 7.88-7.56 (m, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.42-7.37 (m, 3H), 7.17 (d, *J* = 7.8 Hz, 1H), 4.47 (q, *J* = 7.2 Hz, 2H), 3.92 (s, 3H), 1.44 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ =166.7, 154.2, 145.6, 135.5, 132.9, 132.4, 132.0, 131.8, 130.8 (d, *J* = 22.0 Hz), 128.9, 128.5, 127.6, 124.0, 123.3, 122.2 (d, *J* = 282.0 Hz), 118.8, 114.2, 113.7, 112.9, 62.9, 56.4, 13.9 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}F_3NO_3$+Na 422.0980, found 422.0982.

methyl 2-cyano-4'-methoxy-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3ad

Prepared according to the general procedure using methyl (*E*)-4-cyano-3-(trifluoromethyl)but-3-enoate (38.6 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3ad** as a white solid with 74% yield (49.7 mg). m.p. 127-128 °C.

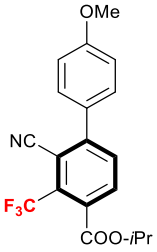
NMR and HRMS data for the product **3ad**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.76 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.49-7.47 (m, 2H), 7.05-7.03 (m, 2H), 3.97 (s, 3H), 3.88 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 160.8, 149.4, 133.2, 132.9 (d, *J* = 3.0 Hz), 132.1, 131.0 (d, *J* = 33.0 Hz) 130.4, 128.8, 122.2 (d, *J* = 274.0 Hz), 114.8, 114.4, 109.9 (d, *J* = 2.0 Hz), 71.0, 55.4, 21.5 ppm.

HRMS (ESI): m/z calculated for $C_{17}H_{12}F_3NO_3$+Na 358.0667, found 358.0665.

isopropyl 2-cyano-4'-methoxy-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3ae

Prepared according to the general procedure using isopropyl *(E)*-4-cyano-3-(trifluoromethyl)but-3-enoate (44.2 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography

delivered **3ae** as a white solid with 72% yield (52.1 mg). m.p. 82-83 °C.

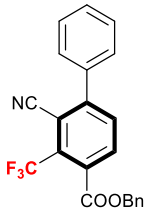
NMR and HRMS data for the product **3ae**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.75 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.49-7.46 (m, 2H), 7.06-7.02 (m, 2H), 5.31-5.25 (m, 1H), 3.88 (s, 3H), 1.38 (d, *J* = 6.4 Hz, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 160.8, 149.4, 133.2, 132.9 (d, *J* = 2.0 Hz), 132.1, 131.0 (d, *J* = 32.0 Hz), 130.4, 128.8, 122.2 (d, *J* = 274.0 Hz), 114.8, 114.4, 109.9 (d, *J* = 2.0 Hz), 71.0, 55.4, 21.5 ppm.

HRMS (ESI): m/z calculated for $C_{19}H_{16}F_3NO_3$+Na 386.0980, found 386.0975.

benzyl 2-cyano-3-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



3af

Prepared according to the general procedure using benzyl *(E)*-4-cyano-3-(trifluoromethyl)but-3-enoate (53.8 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3af** as a white solid with 73% yield (55.7 mg). m.p. 91-93 °C.

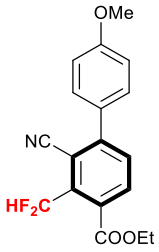
NMR and HRMS data for the product **3af**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.79 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.53-7.49 (m, 5H), 7.44-7.36 (m, 5H), 5.38 (s, 2H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.2, 149.9, 136.5, 134.5, 133.4, 132.5, 132.2, 131.2 (q, *J* = 31.5 Hz), 129.8, 128.9, 128.8, 128.74, 128.71, 122.0 (d, *J* = 274.5 Hz), 114.4, 110.3, 68.7 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{14}F_3O_2$+Na 404.0874, found 404.0870.

ethyl 2-cyano-3-(difluoro-λ^3-methyl)-4'-methoxy-[1,1'-biphenyl]-4-carboxylate



3ag

Prepared according to the general procedure using ethyl *(E)*-4-cyano-3-(difluoro-λ^3-methyl)but-3-enoate (37.8 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product via column chromatography delivered **3ag** as a white solid with 78% yield (51.7 mg). m.p. 103-105 °C.

NMR and HRMS data for the product **3ag**:

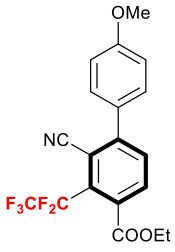
^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.11 (d, *J* = 8.4 Hz, 1H), 7.64 (t, *J* = 53.4 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.52-7.49 (m, 2H), 7.05-7.03 (m, 2H), 4.45 (q, *J* = 7.2 Hz, 2H), 3.88 (s, 3H), 1.43 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 165.1, 160.8, 150.6, 137.9 (t, *J* = 22.5 Hz), 133.7, 132.0, 130.4, 129.7 (d, *J* = 3.0 Hz), 129.0, 115.5, 114.4, 110.83 (t, *J* = 238.5 Hz), 110.3, 62.6, 55.4, 14.1 ppm.

^{19}F NMR (564 MHz, $CDCl_3$): δ = -110.24 (d, *J* = 50.76 Hz, 2F).

HRMS (ESI): m/z calculated for $C_{18}H_{15}F_2NO_3$+Na 354.0918, found 354.0915.

ethyl 2-cyano-4'-methoxy-3-(perfluoroethyl)-[1,1'-biphenyl]-4-carboxylate



3ah

Prepared according to the general procedure using ethyl *(E)*-3-(cyanomethylene)-4,4,5,5,5-pentafluoropentanoate (51.4 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **3ah** as a white solid with 66% yield (53.1 mg). m.p. 118-120 °C.

NMR and HRMS data for the product **3ah**:

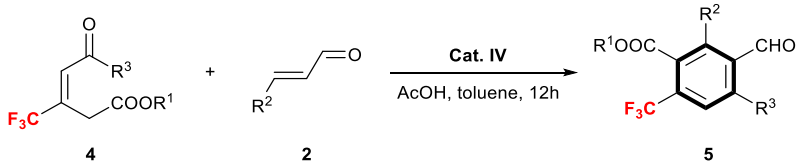
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.72-7.69 (m, 2H), 7.46-7.44 (m, 2H), 7.03-7.02 (m, 2H), 4.41 (q, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 1.37 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.7, 160.8, 149.9, 134.3 (t, *J* = 4.5 Hz), 133.7, 132.2, 130.5, 128.8, 128.7 (t, *J* = 22.5 Hz), 118.9 (d, *J* = 286.5 Hz), 114.9, 114.4, 113.1 (d, *J* = 40.5 Hz), 111.1, 62.8, 55.4, 13.8 ppm.

^{19}F NMR (564 MHz, $CDCl_3$): δ = -81.0 (s, 3F), -105.2 (s, 2F).

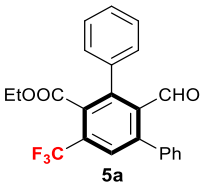
HRMS (ESI): m/z calculated for $C_{19}H_{14}F_5NO_3$+Na 422.0792, found 422.0788.

2.2 Procedure for 5



The reaction was carried out with **4** (0.20 mmol) and **2** (0.30 mmol), amine catalyst **IV** (0.05 mmol) and AcOH (0.08 mmol) in toluene (2 mL) under an open atmosphere at 70 °C for 12 h. Then the reaction mixture was concentrated and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) to give the final CF_3-functionlized penta-substuted benzenes **5**, which was further analyzed by ^{1}H NMR, ^{13}C HMR, HRMS analysis.

ethyl 2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5a** as a white solid with 75% yield (59.4 mg). m.p. 84-86 °C.

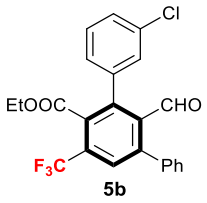
NMR and HRMS data for the product **5a**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.75 (s, 1H), 7.48-7.45 (m, 3H), 7.42-7.40 (m, 3H), 7.35-7.33 (m, 2H), 7.31-7.28 (m, 2H), 4.00 (q, *J* = 7.2 Hz, 2H), 0.99 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 192.0, 165.9, 144.7, 142.1, 137.5, 136.9, 135.1, 133.0 (d, *J* = 2.0 Hz), 129.8. 129.5, 129.4 (d, *J* = 32.0 Hz), 128.7, 128.64, 128.62, 128.1, 128.0 (d, *J* = 4.0 Hz), 122.9 (d, *J* = 273.0 Hz), 62.0, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{17}F_3O_3$+Na 421.1027, found 421.1025.

ethyl 3''-chloro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5b

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-chlorocinnamaldehyde (50.0 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5b** as a white solid with 74% yield (63.7 mg). m.p. 130-132 ºC.

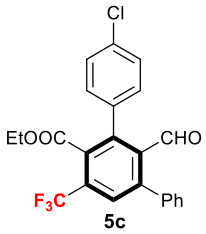
NMR and HRMS data for the product **5b**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.83 (s, 1H), 7.79 (s, 1H), 7.50-7.47 (m, 3H), 7.41-7.38 (m, 1H), 7.36-7.32 (m, 3H), 7.31 (t, *J* = 1.6 Hz, 1H), 7.19-7.17 (m, 1H), 4.06 (q, *J* = 7.2 Hz, 2H), 1.06 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.6, 165.6, 145.3, 140.1, 137.1, 136.9, 136.5, 134.0, 133.1 (d, *J* = 2.0 Hz), 129.7, 129.8 (d, *J* = 32.0 Hz), 129.6, 129.3, 129.0, 128.8, 128.7, 128.4 (q, *J* = 5.0 Hz), 128.1, 122.8 (q, *J* = 273.0 Hz), 62.2, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}ClF_3O_3$+Na 455.0638, found 455.0641.

ethyl 4''-chloro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5c

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 4-chlorocinnamaldehyde (50.0 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5c** as a white solid with 79% yield (68.6 mg). m.p. 96-98 ºC.

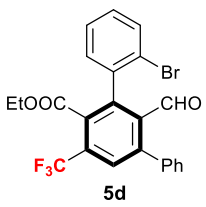
NMR and HRMS data for the product **5c**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.81 (s, 1H), 7.78 (s, 1H), 7.48-7.47 (m, 3H), 7.40-7.38 (m, 2H), 7.36-7.34 (m, 2H), 7.24-7.22 (s, 2H), 4.04 (q, *J* = 7.2 Hz, 2H), 1.05 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.7, 165.7, 145.2, 140,4, 136.9, 136.7, 134.8, 133.8, 133.1 (d, *J* = 2.0 Hz), 131,1, 129.6 (d, *J* = 32.0 Hz), 129.5, 129.0, 128.8, 128.3, 128.2 (q, *J* = 5.0 Hz), 122.8 (q, *J* = 273.0 Hz), 62.2, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}ClF_3O_3$+Na 455.0638, found 455.0635.

ethyl 2''-bromo-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5d

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 2-bromocinnamaldehyde (63.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5d** as a white solid with 70% yield (67.1 mg). m.p. 86-88 ºC.

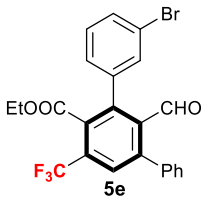
NMR and HRMS data for the product **5d**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.83 (s, 1H), 7.83 (s, 1H), 7.55 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.53-7.49 (m, 3H), 7.40-7.36 (m, 3H), 7.34- 7.28 (m, 2H), 4.00 (q, *J* = 7.2 Hz, 2H), 1.01 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.8, 165.4, 145.4, 140.1, 136.8, 136.7, 136.2, 132.7 (d, *J* = 2.0 Hz), 132.3, 131.2, 130.1 (d, *J* = 32.0 Hz), 130.0, 129.7, 129.1, 128.9, 128.6 (q, *J* = 4.0 Hz), 127.0, 123.6, 122.8 (d, *J* = 273.0 Hz), 62.0, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}BrF_3O_3$+Na 499.0133, found 499.0116.

ethyl 3''-bromo-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5e

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-bromocinnamaldehyde (63.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5e** as a white solid with 75% yield (71.3 mg). m.p. 134-136 °C.

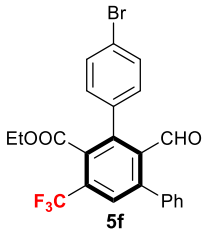
NMR and HRMS data for the product **5e**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.79 (s, 1H), 7.55 (ddd, *J* = 8.0, 2.0, 1.2 Hz, 1H), 7.50-7.46 (m, 4H), 7.36-7.34 (m, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 7.6, 1.2 Hz, 1H), 4.06 (q, *J* = 7.2 Hz, 2H), 1.07 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.5, 165.6, 145.3, 140.0, 137.3, 136.9, 136.4, 133.1 (d, *J* = 2.0 Hz), 132.5, 131.6, 129.7 (d, *J* = 32.0 Hz), 129.6, 129.5, 129.0, 128.8, 128.5, 128.4 (q, *J* = 4.0 Hz), 122.8 (d, *J* = 273.0 Hz), 122.1, 62.2, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}BrF_3O_3$+Na 499.0133, found 499.0140.

ethyl 4''-bromo-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5f

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 4-bromocinnamaldehyde (63.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5f** as a white solid with 80% yield (76.2 mg). m.p. 102-104 °C.

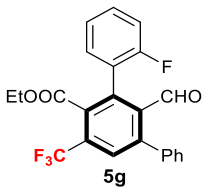
NMR and HRMS data for the product **5f**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.81 (s, 1H), 7.78 (s, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.50-7.47 (m, 3H), 7.36-7.34 (m, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 4.04 (q, *J* = 7.2 Hz, 2H), 1.05 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.7, 165.7, 145.3, 140.4, 136.9, 136.6, 134.3, 133.0 (d, *J* = 1.0 Hz), 131.3, 131.2, 129.6 (q, *J* = 33.0 Hz), 129.6, 129.0, 128.8, 128.3 (q, *J* = 4.0 Hz), 123.0, 122.8 (q, *J* = 273.0 Hz), 62.2, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}BrF_3O_3$+Na 499.0133, found 499.0130.

ethyl 2''-fluoro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5g

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 2-fluorocinnamaldehyde (45.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5g** as a white solid with 71% yield (58.9 mg). m.p. 100-102 °C.

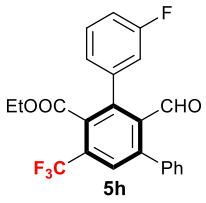
NMR and HRMS data for the product **5g**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.84 (s, 1H), 7.83 (s, 1H), 7.52-7.48 (m, 3H), 7.42-7.37 (m, 3H), 7.27 (td, *J* = 7.6, 2.0 Hz, 1H), 7.19 (td, *J* = 7.6, 1.2 Hz, 1H), 7.14-7.09 (m, 1H), 4.06-3.98 (m, 2H), 1.01 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.2, 165.6, 159.6 (d, *J* = 246.0 Hz), 145.6, 136.6, 136.5, 134.9, 133.6 (d, *J* = 2.0 Hz), 131.1 (d, *J* = 3.0 Hz), 130.7 (d, *J* = 8.0 Hz), 130.1 (d, *J* = 32.0 Hz), 129.8, 129.1, 128.6 (q, *J* = 5.0 Hz), 123.8 (d, *J* = 4.0 Hz), 123.6 (d, *J* = 17.0 Hz), 122.8 (q, *J* = 273.0 Hz), 115.2 (d, *J* = 21.0 Hz), 62.1, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}F_4O_3$+Na 439.0933, found 439.0930.

ethyl 3''-fluoro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5h

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-fluorocinnamaldehyde (45.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5h** as a white solid with 76% yield (63.4 mg). m.p. 102-104 ºC.

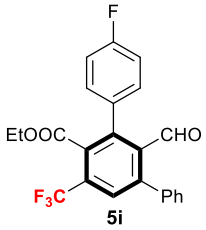
NMR and HRMS data for the product **5h**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.79 (s, 1H), 7.51-7.46 (m, 3H), 7.40-7.34 (m, 3H), 7.14-7.02 (m, 3H), 4.05 (q, *J* = 7.2 Hz, 2H), 1.05 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.6, 165.6, 162.2 (d, *J* = 246.0 Hz), 145.2, 140.3, 137.4 (d, *J* = 8.0 Hz), 137.0, 136.6, 133.0 (d, *J* = 1.0 Hz), 129.7 (d, *J* = 8.0 Hz), 129.6, 128.9, 128.8, 128.4 (q, *J* = 5.0 Hz), 125.7 (d, *J* = 3.0 Hz), 122.8 (q, *J* = 273.0 Hz), 117.1 (d, *J* = 22.0 Hz), 115.6 (d, *J* = 21.0 Hz), 62.1, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}F_4O_3$+Na 439.0933, found 439.0932.

ethyl 4''-fluoro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5i

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 4-fluorocinnamaldehyde (45.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5i** as a white solid with 82% yield (68.5 mg). m.p. 98-100 °C.

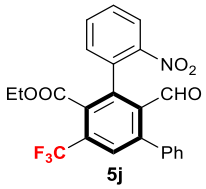
NMR and HRMS data for the product **5i**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.81 (s, 1H), 7.78 (s, 1H), 7.49-7.47 (m, 3H), 7.36-7.34 (m, 2H), 7.29-7.25 (m, 2H), 7.13-7.07 (m, 2H), 4.04 (q, *J* = 7.2 Hz, 2H), 1.05 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.9, 165.8, 162.8 (d, *J* = 247.0 Hz), 145.1, 140.7, 137.1, 136.9, 133.3, 131.6 (d, *J* = 9.0 Hz), 131.1 (d, *J* = 4.0 Hz), 129.6, 129.5 (d, *J* = 32.0 Hz), 128.9, 128.8, 128.2 (q, *J* = 5.0 Hz), 122.8 (q, *J* = 273.0 Hz), 115.1 (d, *J* = 21.0 Hz), 62.1, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}F_4O_3$+Na 439.0933, found 439.0934.

ethyl 2'-formyl-2''-nitro-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5j

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 2-nitrocinnamaldehyde (53.2

mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5j** as a white solid with 72% yield (63.7 mg). m.p. 80-81 °C.

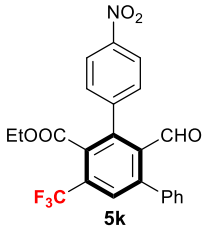
NMR and HRMS data for the product **5j**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.80 (s, 1H), 8.24 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.87 (s, 1H), 7.66 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.60 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.54-7.50 (m, 3H), 7.45-7.42 (m, 2H), 7.32 (dd, *J* = 7.6, 1.6 Hz, 1H), 4.01-3.85 (m, 2H), 0.99 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.9, 165.4, 148.0, 146.8, 137.9, 136.1, 134.9 (d, *J* = 1.0 Hz), 133.0, 132.2, 131.8, 133.4 (d, *J* = 2.0 Hz), 130.4 (d, *J* = 33.0 Hz), 130.0, 129.5, 129.4, 129.0, 128.5 (q, *J* = 5.0 Hz), 124.5, 122.7 (q, *J* = 273.0 Hz), 62.2, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}F_3NO_5$+Na 466.0878, found 466.0879.

ethyl 2'-formyl-4''-nitro-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5k

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 4-nitrocinnamaldehyde (53.2 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5k** as a white solid with 75% yield (66.2 mg). m.p. 150-152 °C.

NMR and HRMS data for the product **5k**:

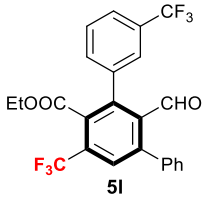
^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 8.28-8.26 (m, 2H), 7.88 (s, 1H), 7.53-7.51 (m, 3H), 7.47-7.44 (m, 2H), 7.40-7.38 (m, 2H), 4.02 (q, *J* = 7.2 Hz, 2H), 1.05 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.9, 165.4, 148.0, 146.8, 137.9, 136.1, 134.9 (d,

J = 1.0 Hz), 133.0, 132.2, 131.8, 133.4 (d, J = 2.0 Hz), 130.4 (d, J = 33.0 Hz), 130.0, 129.5, 129.4, 129.0, 128.5 (q, J = 5.0 Hz), 124.5, 122.7 (q, J = 273.0 Hz), 62.2, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}F_3NO_5$+Na 466.0878, found 466.0881.

ethyl 2'-formyl-3'',5'-bis(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5l

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-trifluoromethylcinnamaldehyde (60.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5l** as a white solid with 69% yield (64.8 mg). m.p. 142-144 ºC.

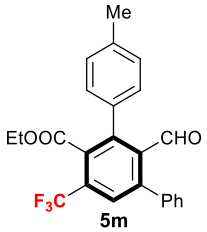
NMR and HRMS data for the product **5l**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.83 (s, 1H), 7.83 (d, J = 7.6 Hz, 1H), 7.58-7.47 (m, 6H), 7.39-7.36 (m, 2H), 4.05-3.95 (m, 2H), 1.01 (t, J = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.4, 165.5, 145.8, 139.9, 136.6, 136.4, 136.3 (d, J = 1.0 Hz), 133.3 (d, J = 2.0 Hz), 133.2 (d, J = 1.0 Hz), 130.4 (d, J = 33.0 Hz), 130.0, 129.7, 129.2, 128.9, 128.5 (d, J = 4.0 Hz), 128.4, 126.4 (q, J = 3.0 Hz), 125.2 (q, J = 4.0 Hz), 122.7 (d, J = 273.0 Hz), 122.5, 62.2, 13.4 ppm.

HRMS (ESI): m/z calculated for $C_{24}H_{16}F_6O_3$+Na 489.0901, found 489.0906.

ethyl 2'-formyl-4''-methyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5m

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 4-methylcinnamaldehyde (43.9 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5m** as a white solid with 83% yield (68.6 mg). m.p. 101-103 °C.

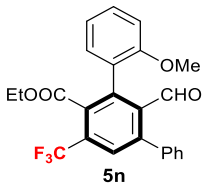
NMR and HRMS data for the product **5m**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.81 (s, 1H), 7.73 (s, 1H), 7.46-7.42 (m, 3H), 7.34-7.32 (m, 2H), 7.23-7.17 (m, 4H), 4.03 (q, *J* = 7.2 Hz, 2H), 2.39 (s, 3H), 1.02 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 192.2, 166.0, 144.5, 142.3, 138.6, 137.7, 137.1, 133.1 (d, *J* = 2.0 Hz), 132.0, 129.7, 129.4, 129.3 (d, *J* = 32.0 Hz), 128.8, 128.6, 127.9 (q, *J* = 5.0 Hz), 122.7 (q, *J* = 273.0 Hz), 62.0, 21.3, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{24}H_{19}F_3O_3$+Na 435.1184, found 435.1188.

ethyl 2'-formyl-2''-methoxy-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5n

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 2-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5n** as a white solid with 80% yield (68.2 mg). m.p. 108-110 °C.

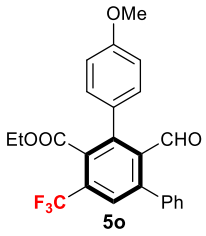
NMR and HRMS data for the product **5n**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.78 (s, 1H), 7.74 (s, 1H), 7.48-7.44 (m, 3H), 7.41-7.7.35 (m, 3H), 7.23 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.02 (td, *J* = 7.6, 0.8 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 4.00 (q, *J* = 7.2 Hz, 2H), 3.72 (s, 3H), 0.99 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.6, 166.0, 156.2, 144.2, 138.4, 137.5, 137.2, 133.0 (d, *J* = 2.0 Hz), 130.7, 130.4, 129.9 (d, *J* = 33.0 Hz), 129.6, 128.7, 127.9 (q, *J* = 5.0 Hz), 124.5, 123.0 (d, *J* = 273.0 Hz), 120.5, 110.7, 61.8, 55.6, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{24}H_{19}F_3O_4$+Na 451.1133, found 451.1135.

ethyl 2'-formyl-4''-methoxy-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5o

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5o** as a white solid with 84% yield (72.3 mg). m.p. 88-90 ºC.

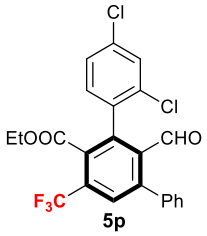
NMR and HRMS data for the product **5o**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.81 (s, 1H), 7.72 (s, 1H), 7.48-7.44 (m, 3H), 7.34-7.32 (m, 2H), 7.24-7.20 (m, 2H), 6.95-6.93 (m, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 3.84 (s, 3H), 1.05 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 192.3, 166.0, 159.9, 144.5, 142.0, 137.7, 137.3, 133.2 (d, *J* = 2.0 Hz), 131.1, 129.4, 129.3 (d, *J* = 32.0 Hz), 128.6, 127.8 (d, *J* = 4.0 Hz), 127.0, 122.9 (q, *J* = 273.0 Hz), 113.6, 62.0, 55.3, 13.7 ppm.

HRMS (ESI): m/z calculated for $C_{24}H_{19}F_3O_4$+Na 451.1133, found 451.1131.

ethyl 2'',4''-dichloro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5p

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(2,4-dichlorophenyl)acrylaldehyde (60.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5p** as a white solid with 75% yield (69.7 mg). m.p. 90-92 °C.

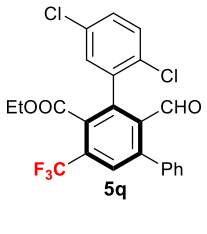
NMR and HRMS data for the product **5p**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.81 (s, 1H), 7.86 (s, 1H), 7.52-7.49 (m, 3H), 7.46 (d, *J* = 2.0 Hz, 1H), 7.39 (dd, *J* = 7.6, 4.0 Hz, 2H), 7.32 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 1.07 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.6, 165.3, 146.0, 137.1, 136.3, 136.1, 135.2, 134.2, 133.6, 131.7, 130.3 (d, *J* = 33.0 Hz), 129.8, 129.3, 129.1, 129.0, 128.9, 128.8 (d, *J* = 4.0 Hz), 126.8, 122.7 (d, *J* = 273.0 Hz), 62.2, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{15}Cl_2F_3O_3$+Na 489.0248, found 489.0246.

ethyl 2'',5''-dichloro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5q

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(2,5-dichlorophenyl)acrylaldehyde (60.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5q** as a white solid with 71% yield (66.4 mg). m.p. 172-174 °C.

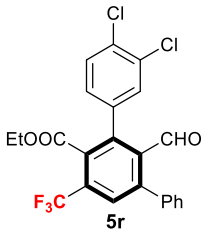
NMR and HRMS data for the product **5q**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.86 (s, 1H), 7.53-7.50 (m, 3H), 7.41-7.37 (m, 2H), 7.36-7.34 (m, 2H), 7.32-7.31 (m, 1H), 4.08 (qd, *J* = 7.2, 2.8 Hz, 2H), 1.08 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.5, 165.2, 146.0, 136.9, 136.6, 136.2, 135.9, 132.8 (d, *J* = 2.0 Hz), 132.4, 131.8, 130.8, 130.5, 130.2, 129.9, 129.8, 129.3, 129.0, 128.9 (d, *J* = 5.0 Hz), 122.7 (d, *J* = 273.0 Hz), 62.2, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{15}Cl_2F_3O_3$+Na 489.0248, found 489.0247.

ethyl 3'',4''-dichloro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5r

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(3,4-dichlorophenyl)acrylaldehyde (60.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5r** as a white solid with 74% yield (69.1 mg). m.p. 146-148 ºC.

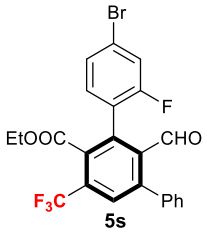
NMR and HRMS data for the product **5r**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.82 (s, 1H), 7.51-7.47 (m, 4H), 7.40 (d, *J* = 2.0 Hz, 1H), 7.37-7.35 (m, 2H),7.13 (dd, *J* = 8.0, 2.0 Hz, 1H), 4.08 (qd, *J* = 7.2, 2.4 Hz, 2H), 1.10 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.4, 165.5, 145.8, 138.8, 136.5, 136.3, 135.4, 133.1 (d, *J* = 2.0 Hz), 132.9, 132.3, 131.4, 129.9, 129.7, 129.2, 128.9, 128.6 (q, *J* = 5.0 Hz), 122.7 (d, *J* = 273.0 Hz), 62.3, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{15}Cl_2F_3O_3$+Na 489.0248, found 489.0250.

ethyl 4''-bromo-2''-fluoro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5s

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(4-bromo-2-fluorophenyl)acrylaldehyde (68.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5s** as a white solid with 76% yield (75.2 mg). m.p. 136-137 ºC.

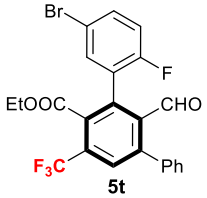
NMR and HRMS data for the product **5s**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.86 (s, 1H), 7.53-7.49 (m, 3H), 7.40-7.33 (m, 3H), 7.13 (dd, *J* = 8.8, 1.6 Hz, 1H) , 7.13 (t, *J* = 7.6 Hz, 3H), 4.07 (q, *J* = 7.2 Hz, 2H), 1.08 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.9, 165.4, 159.5 (d, *J* = 249.0 Hz), 146.1, 136.2, 133.7, 133.5 (d, *J* = 1.0 Hz), 131.9 (d, *J* = 4.0 Hz), 130.3 (d, *J* = 32.0 Hz), 129.8, 129.3, 129.0, 128.9 (d, *J* = 5.0 Hz), 127.2 (d, *J* = 3.0 Hz), 126.0, 123.3 (d, *J* = 9.0 Hz), 123.0 (d, *J* = 17.0 Hz), 122.7 (d, *J* = 273.0 Hz), 118.9 (d, *J* = 25.0 Hz), 62.3, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{15}BrF_4O_3$+Na 517.0038, found 517.0041.

ethyl 5''-bromo-2''-fluoro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5t

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-

(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(5-bromo-2-fluorophenyl)acrylaldehyde (68.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5t** as a white solid with 73% yield (71.9 mg). m.p. 140-142 °C.

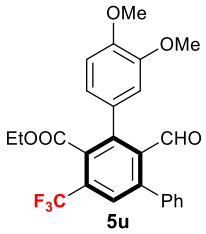
NMR and HRMS data for the product **5t**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.83 (s, 1H), 7.86 (s, 1H), 7.53-7.49 (m, 4H), 7.41-7.38 (m, 3H), 7.01 (t, *J* = 8.8 Hz, 1H), 4.15-4.07 (m, 2H), 1.11 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.8, 165.3, 158.8 (d, *J* = 246.0 Hz), 146.2, 136.12, 136.09, 133.54 (d, *J* = 2.0 Hz), 133.47, 133.41 (d, *J* = 6.0 Hz), 133.2, 130.4 (d, *J* = 33.0 Hz), 129.8, 129.3, 129.1 (d, *J* = 4.0 Hz), 129.0, 125.9 (d, *J* = 18.0 Hz), 122.7 (d, *J* = 273.0 Hz), 116.9 (d, *J* = 24.0 Hz), 116.2 (d, *J* = 4.0 Hz), 62.3, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{15}BrF_4O_3$+Na 517.0038, found 517.0043.

ethyl 2'-formyl-3'',4''-dimethoxy-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5u

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(3,4-dimethoxyphenyl)acrylaldehyde (57.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5u** as a white solid with 78% yield (71.3 mg). m.p. 110-111 °C.

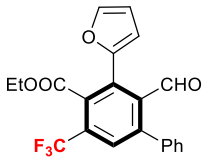
NMR and HRMS data for the product **5u**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.72 (s, 1H), 7.47-7.44 (m, 3H), 7.34-7.32 (m, 2H), 6.92-6.90 (m, 1H), 6.86-6.84 (m, 2H), 4.10-4.04 (m, 2H), 3.92 (s, 3H), 3.86 (s, 3H), 1.07 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 192.3, 166.1, 149.4, 148.6, 144.3, 142.0, 137.7, 137.4, 133.0 (d, *J* = 2.0 Hz), 129.4, 129.3 (d, *J* = 33.0 Hz), 128.6, 127.9 (q, *J* = 4.0 Hz), 127.1, 122.9 (d, *J* = 273.0 Hz), 122.8, 113.2, 110.7, 62.1, 56.0, 55.9, 13.7 ppm.

HRMS (ESI): m/z calculated for $C_{25}H_{21}F_3O_5$+Na: 481.1239, found 481.1236

ethyl 2-formyl-3-(furan-2-yl)-5-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



5v

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(furan-2-yl)acrylaldehyde (36.6 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5v** as a white solid with 64% yield (49.8 mg). m.p. 76-77 ºC.

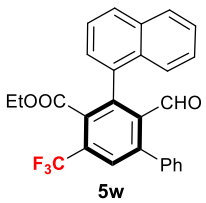
NMR and HRMS data for the product **5v**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.91 (s, 1H), 7.76 (s, 1H), 7.55 (dd, *J* = 2.0, 0.8 Hz, 1H), 7.49-7.45 (m, 3H), 7.35-7.32 (m, 2H), 6.58 (dd, *J* = 3.2, 0.8 Hz, 1H), 6.53 (dd, *J* =3.2, 1.6 Hz, 1H), 4.26 (q, *J* = 7.2, 2.4 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.5, 165.9, 146.9, 144.8, 144.0, 137.5, 137.0, 132.8 (d, *J* = 2.0 Hz), 130.5, 129.8 (d, *J* = 32.0 Hz), 129.5, 128.9 (d, *J* = 4.0 Hz), 128.8, 128.7, 122.7 (d, *J* = 273.0 Hz), 113.0, 111.6, 62.4, 13.8 ppm.

HRMS (ESI): m/z calculated for $C_{21}H_{15}F_3O_4$+Na 411.0820, found 411.0822.

ethyl 2-formyl-3-(naphthalen-1-yl)-5-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



5w

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(naphthalen-1-yl)acrylaldehyde (54.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5w** as a white solid with 69% yield (61.7 mg). m.p. 110-112 ^{o}C.

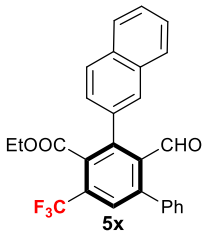
NMR and HRMS data for the product **5w**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.67 (s, 1H), 7.90 (dd, *J* = 12.8, 8.4 Hz, 1H), 7.85 (s, 1H), 7.53-7.45 (m, 5H), 7.43-7.38 (m, 5H), 3.77-3.68 (m, 2H), 0.55 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.4, 165.6, 144.8, 140.8, 137.5, 137.3, 133.7 (d, *J* = 2.0 Hz), 133.1, 132.5, 132.4, 129.9 (d, *J* = 33.0 Hz), 129.5, 129.2, 128.7, 128.6, 128.5 (d, *J* = 5.0 Hz), 128.3, 128.2, 126.8, 126.2, 125.7, 124.8, 122.9 (d, *J* = 273.0 Hz), 62.6, 13.0 ppm.

HRMS (ESI): m/z calculated for $C_{27}H_{19}F_3O_3$+Na 471.1184, found 471.1182.

ethyl 2-formyl-3-(naphthalen-2-yl)-5-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



5x

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(naphthalen-2-yl)acrylaldehyde (54.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5x** as a white solid with 72% yield (64.5 mg). m.p. 116-118 ^{o}C.

NMR and HRMS data for the product **5x**:

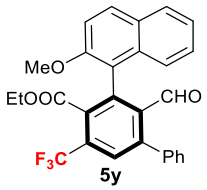
^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.83 (s, 1H), 7.89-7.87 (m, 2H), 7.83-7.81 (m, 1H),

7.79 (s, 1H), 7.77-7.76 (m, 1H), 7.54-7.52 (m, 2H), 7.49-7.45 (m, 3H), 7.42 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.38-7.35 (m, 2H), 3.96-3.87 (m, 2H), 0.86 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.9, 165.9, 144.8, 142.1, 137.5, 137.0, 133.2 (d, *J* = 2.0 Hz), 132.9, 132.7, 132.6, 129.5 (d, *J* = 32.0 Hz), 129.4, 129.3, 129.1, 128.7, 128.6, 128.1, 128.0 (d, *J* = 4.0 Hz), 127.8, 127.7, 127.5, 126.8, 126.7, 122.9 (d, *J* = 273.0 Hz), 62.0, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{27}H_{19}F_3O_3$+Na 471.1184, found 471.1181.

ethyl 2-formyl-3-(2-methoxynaphthalen-1-yl)-5-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate



5y

Prepared according to the general procedure using ethyl ethyl (*E*)-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (57.3 mg, 0.2 mmol) and 3-(2-methoxynaphthalen-1-yl)acrylaldehyde (63.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5y** as a white solid with 61% yield (58.6 mg). m.p. 119-121 ^{o}C.

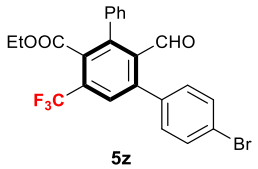
NMR and HRMS data for the product **5y**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.69 (s, 1H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.83 (s, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.47-7.46 (m, 3H), 7.42-7.31 (m, 5H), 7.21 (d, *J* = 8.4 Hz, 1H), 3.86 (s, 3H), 3.73-3.64 (m, 2H), 0.55 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.6, 165.6, 154.6, 144.8, 137.8, 137.7, 137.6, 133.9 (d, *J* = 2.0 Hz), 133.4, 131.0, 130.1 (d, *J* = 32.0 Hz), 129.5, 128.6, 128.5, 128.4 (d, *J* = 4.0 Hz), 127.9, 127.0, 124.7, 123.8, 123.0 (d, *J* = 273.0 Hz), 117.5, 112.7, 100.0, 61.4, 56.5, 13.0 ppm.

HRMS (ESI): m/z calculated for $C_{28}H_{21}F_3O_4$+Na 501.1290, found 501.1287.

ethyl 4-bromo-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5z

Prepared according to the general procedure using ethyl ethyl (E)-5-(4-bromophenyl)-5-oxo-3-(trifluoromethyl)pent-3-enoate (73.0 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5z** as a white solid with 76% yield (72.2 mg). m.p. 135-136 ºC.

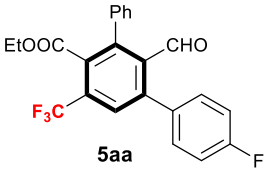
NMR and HRMS data for the product **5z**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.78 (s, 1H), 7.70 (s, 1H), 7.60-7.58 (m, 2H), 7.44-7.42 (m, 3H), 7.31-7.29 (m, 2H), 7.22-7.20 (m, 2H), 4.01 (q, *J* = 7.2 Hz, 2H), 0.99 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 191.8, 165.7, 143.1, 142.8, 136.7, 136.6, 134.6, 133.2, 131.7, 130.9, 129.8, 129.6 (d, *J* = 33.0 Hz), 128.9, 128.2, 127.9 (d, *J* = 4.5 Hz), 123.1, 122.7 (d, *J* = 273.0 Hz), 62.1, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}BrF_3O_3$+Na 499.0133, found 499.0129.

ethyl 4-fluoro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5aa

Prepared according to the general procedure using ethyl ethyl (E)-5-(4- fluorophenyl)-5-oxo-3-(trifluoromethyl)pent-3-enoate (60.9 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5aa** as a white solid with 74% yield (61.4 mg). m.p. 107-109 ºC.

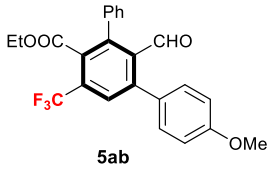
NMR and HRMS data for the product **5aa**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.79 (s, 1H), 7.71 (s, 1H), 7.43-7.41 (m, 3H), 7.33-7.30 (m, 4H), 7.17-7.14 (m, 2H), 4.01 (q, *J* = 7.2 Hz, 2H), 0.99 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 191.9, 165.8, 162.9 (d, *J* = 247.5 Hz), 143.3, 142.6, 136.8, 134.7, 133.6 (d, *J* = 1.5 Hz), 133.1, 131 (d, *J* = 7.5 Hz), 129.8, 129.5 (d, *J* = 31.5 Hz), 128.8, 128.2, 128.1 (d, *J* = 4.5 Hz), 122.8 (d, *J* = 273.0 Hz), 115.7 (d, *J* = 22.5 Hz), 62.1, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{16}F_4O_3$+Na 439.0933, found 439.0930.

ethyl 2'-formyl-4-methoxy-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5ab

Prepared according to the general procedure using ethyl ethyl (*E*)-5-(4-methoxyphenyl)-5-oxo-3-(trifluoromethyl)pent-3-enoate (63.3 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5ab** as a white solid with 77% yield (66.3 mg). m.p. 77-79 °C.

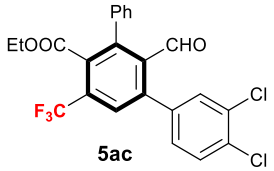
NMR and HRMS data for the product **5ab**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.81 (s, 1H), 7.75 (s, 1H), 7.41-7.40 (m, 3H), 7.29-7.28 (m, 4H), 7.01-6.98 (m, 2H), 3.99 (q, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 0.98 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 192.3, 166.0, 160.1, 144.4, 141.9, 136.8, 135.2, 132.5, 130.9, 129.3, 129.4, 129.2 (d, *J* = 10.5 Hz), 128.5, 128.0, 127.9, 122.9 (d, *J* = 273.0 Hz), 114.2, 61.9, 55.4, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{24}H_{19}F_3O_4$+Na 451.4133, found 451.1134.

ethyl 3,4-dichloro-2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5ac

Prepared according to the general procedure using ethyl (E)-5-(3,4-dichlorophenyl)-5-oxo-3-(trifluoromethyl)pent-3-enoate (71.0 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5ac** as a white solid with 72% yield (67.1 mg). m.p. 123-124 ºC.

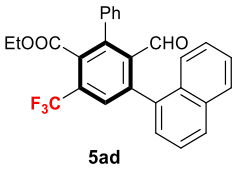
NMR and HRMS data for the product **5ac**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.78 (s, 1H), 7.67 (s, 1H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.46-7.43 (m, 4H), 7.32-7.30 (m, 2H), 7.15 (dd, *J* = 8.4, 2.4 Hz, 1H), 4.02 (q, *J* = 7.2 Hz, 2H), 0.99 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 191.4, 165.5, 143.3, 141.6, 138.0, 136.4, 134.2, 133.6, 133.0, 132.8, 130.9, 130.4, 129.9, 129.7, 129.1, 128.6, 128.3, 128.0 (d, *J* = 4.5 Hz), 122.6 (d, *J* = 273.0 Hz), 62.2, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{15}Cl_2F_3O_3$+Na 521.0510, found 521.0509.

ethyl 6-formyl-5-(naphthalen-1-yl)-3-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylate



5ad

Prepared according to the general procedure using ethyl (*E*)-5-(naphthalen-1-yl)-5-oxo-3-(trifluoromethyl)pent-3-enoate (67.3 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5ad** as a white solid with 70% yield (54.7 mg). m.p. 96-97 ºC.

NMR and HRMS data for the product **5ad**:

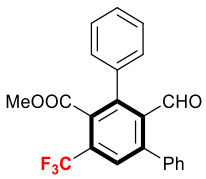
^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.85 (s, 1H), 7.93-7.51 (m, 5H), 7.57-7.53 (m, 2H), 7.43-7.41 (m, 4H), 7.35-7.31 (m, 2H), 4.02 (q, *J* = 7.2 Hz, 2H), 1.00 (t, *J* = 7.2 Hz, 3H)

ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 192.0, 165.9, 144.7, 142.3, 136.9, 135.1, 135.0, 133.0, 132.9, 129.8, 129.5 (d, *J* = 33.0 Hz), 128.9, 128.6, 128.4, 128.3, 128.5, 128.1, 127.8, 127.0, 126.9, 122.9 (d, *J* = 273.0 Hz), 62.0, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{27}H_{19}F_3O_3$+Na 471.1184, found 471.1186.

methyl 2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5ae

Prepared according to the general procedure using methyl *(E)*-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (54.4 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5ae** as a white solid with 71% yield (54.7 mg). m.p. 119-121 °C.

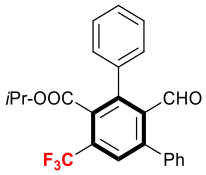
NMR and HRMS data for the product **5ae**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.76 (s, 1H), 7.48-7.46 (m, 3H), 7.43-7.42 (m, 3H), 7.36-7.34 (m, 2H), 7.29-7.28 (m, 2H), 3.54 (s, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 192.0, 166.4, 144.8, 142.2, 137.4, 136.8, 135.0, 132.7, 129.6, 129.4, 128.7, 128.6, 128.1, 128.0 (d, *J* = 4.5 Hz), 122.8 (d, *J* = 273.0 Hz), 52.6 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{15}F_3O_3$+Na 407.0871, found 407.0872.

isopropyl 2'-formyl-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-4'-carboxylate



5af

Prepared according to the general procedure using isopropyl *(E)*-5-oxo-5-phenyl-3-(trifluoromethyl)pent-3-enoate (60.1 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **5af** as a white solid with 67% yield (55.2 mg). m.p. 102-103 ºC.

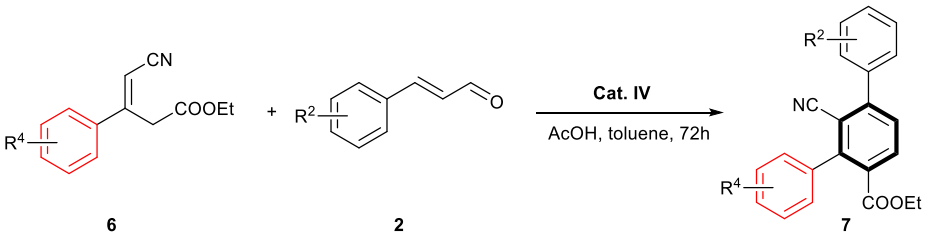
NMR and HRMS data for the product **5af**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.81 (s, 1H), 7.75 (s, 1H), 7.47 (m, 3H), 7.42-7.70 (m, 3H), 7.35-7.33 (m, 2H), 7.32-7.30 (m, 2H), 4.92-4.88 (m, 1H), 0.98 (d, *J* = 6.0 Hz, 6H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 192.11, 165.33, 144.5, 141.9, 137.5, 136.8, 135.0, 133.2, 129.9, 129.4, 129.2 (d, *J* = 10.5 Hz), 128.6, 128.6, 128.1, 128.0 (d, *J* = 4.5 Hz), 122.9 (d, *J* = 273.0 Hz), 70.0, 29.7, 21.1 ppm.

HRMS (ESI): m/z calculated for $C_{24}H_{19}F_3O_3$+Na 435.1184, found 435.1186.

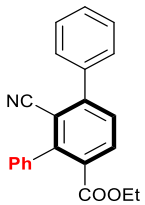
2.3 Procedure for 7



6 2 7

The reaction was carried out with **6** (0.20 mmol) and **2** (0.30 mmol), amine catalyst **IV** (0.05 mmol) and AcOH (0.08 mmol) in toluene (2 mL) under an open atmosphere at 70 ºC for 72 h. Then the reaction mixture was concentrated and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 80:1) to give the final diaryl substituted benzenes **7**, which was further analyzed by ^{1}H NMR, ^{13}C HMR, HRMS analysis.

ethyl 2'-cyano-[1,1':3',1''-terphenyl]-4'-carboxylate



7a

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and cinnamaldehyde (39.7 mg, 0.3 mmol). Purification of the crude product via column chromatography delivered **7a** as a white solid with 68% yield (44.3 mg). m.p. 78-79 ºC.

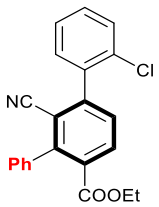
NMR and HRMS data for the product **7a**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.08 (d, *J* = 8.0 Hz, 1H), 7.59 (dd, *J* = 12.0, 3.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.53-7.41 (m, 6H), 7.38-7.36 (m, 2H), 4.04 (q, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 148.9, 147.0, 137.8, 137.7, 133.3, 131.6, 129.2. 129.0, 128.9, 128.8, 128.7, 128.6, 128.2, 116.8, 113.3, 61.4, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{17}NO_2$+Na 350.1157, found 350.1160.

ethyl 2-chloro-2'-cyano-[1,1':3',1''-terphenyl]-4'-carboxylate



7b

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 2-chlorocinnamaldehyde (50.0 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7b** as a white solid with 61% yield (43.8 mg). m.p. 108-109 ºC.

NMR and HRMS data for the product **7b**:

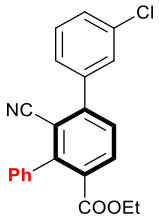
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.08 (d, *J* = 8.0 Hz, 1H), 7.55-7.52 (m, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.46-7.43 (m, 3H), 7.42-7.38 (m, 5H), 4.06 (q, *J* = 7.2 Hz, 2H), 0.95

(t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 146.4, 146.3, 137.4, 136.7, 132.9, 132.8, 132.4, 130.9, 130.5, 130.1, 129.6, 129.0, 128.7, 128.3, 127.1, 126.1, 116.1, 61.6, 13.6 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}ClNO_2$+Na 384.0767, found 384.0770.

ethyl 3-chloro-2'-cyano-[1,1':3',1''-terphenyl]-4'-carboxylate



7c

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 3-chlorocinnamaldehyde (50.0 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7c** as a white solid with 63% yield (45.6 mg). m.p. 126-128 ºC.

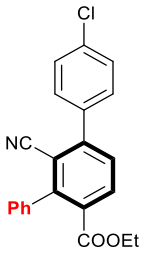
NMR and HRMS data for the product **7c**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.08 (d, *J* = 8.0 Hz, 1H), 7.56-7.55 (m, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.51-7.44 (m, 6H), 7.37-7.35 (m, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.6, 147.3, 147.1, 139.4, 137.5, 134.7, 133.4, 132.2, 130.1, 129.4, 129.0, 128.9, 128.7, 128.6, 128.3, 127.2, 116.5, 113.4, 61.5, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}ClNO_2$+Na 384.0767, found 384.0768.

ethyl 4-chloro-2'-cyano-[1,1':3',1''-terphenyl]-4'-carboxylate



7d

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 4-chlorocinnamaldehyde (50.0 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7d** as a white solid with 66% yield (47.5 mg). m.p. 104-106 ºC.

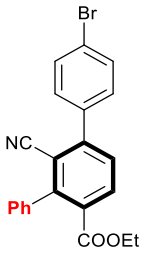
NMR and HRMS data for the product **7d**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.09 (d, *J* = 8.4 Hz, 1H), 7.55-7.52 (m, 3H), 7.49-7.46 (m, 5H), 7.37-7.35 (m, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.7, 147.6, 147.1, 137.5, 136.0, 135.6, 133.4, 131.9, 130.2, 129.1, 128.8, 128.7, 128.6, 128.3, 116.7, 113.2, 61.5, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}ClNO_2$+Na 384.0767, found 384.0771.

ethyl 4-bromo-2'-cyano-[1,1':3',1''-terphenyl]-4'-carboxylate



7e

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 4-bromocinnamaldehyde (63.3 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7e** as a white solid with 67% yield (54.3 mg). m.p. 118-120 ºC.

NMR and HRMS data for the product **7e**:

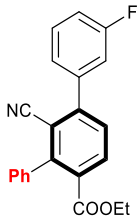
^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.09 (d, *J* = 7.8 Hz, 1H), 7.66-7.64 (m, *2*H), 7.53 (d,

J = 8.4 Hz, 1H), 7.48-7.46 (m, 5H), 7.37-7.35 (m, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.7, 147.6, 147.1, 137.5, 136.5, 133.4, 132.0, 132.0, 130.5, 128.8, 128.7, 128.6, 128.3, 123. 9, 116.7, 113.2, 61.5, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}BrNO_2$+Na 428.0262, found 428.0262.

ethyl 2'-cyano-3-fluoro-[1,1':3',1''-terphenyl]-4'-carboxylate



7f

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 3-fluorocinnamaldehyde (45.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7f** as a white solid with 65% yield (44.7 mg). m.p. 72-74 ºC.

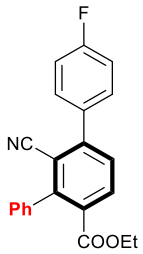
NMR and HRMS data for the product **7f**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.09 (d, *J* = 7.8 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.49-7.47 (m, 4H), 7.38-7.36 (m, 3H), 7.30-7.28 (m, 1H), 7.20-7.17 (m, 1H), 4.05 (q, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.7, 162.6 (d, *J* = 246.0 Hz), 147.4 (d, *J* = 1.5 Hz), 147.1, 139.7 (d, *J* = 7.5 Hz), 137.5, 133.4, 132.1, 130.5 (d, *J* = 9.0 Hz), 128.8 (d, *J* = 33.0 Hz), 128.7, 128.3, 124.8 (d, *J* = 3.0 Hz), 116.5, 116.3, 116.2 (d, *J* = 3.0 Hz), 116.0, 113.3, 61.6, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}FNO_2$+Na 368.1063, found 368.1064.

ethyl 2'-cyano-4-fluoro-[1,1':3',1''-terphenyl]-4'-carboxylate



7g

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 4-fluorocinnamaldehyde (45.1 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7g** as a white solid with 64% yield (44.1 mg). m.p. 70-72 ºC.

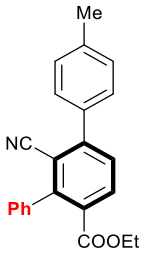
NMR and HRMS data for the product **7g**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.08 (d, *J* = 7.8 Hz, 1H), 7.58 (dd, *J* = 9.0, 4.8 Hz, 2H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.47-7.46 (m, 3H), 7.37-7.36 (m, 2H), 7.22-7.19 (m, 2H), 4.05 (q, *J* = 7.2 Hz, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.7, 163.4 (d, *J* = 247.5 Hz), 147.8, 147.1, 137.6, 133.7 (d, *J* = 3.0 Hz), 133.4, 131.7, 130.9, 130.8, 128.9, 128.7, 128.6, 128.3, 116.8, 116.0, 115.9, 113.3, 61.5, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}FNO_2$+Na 368.1063, found 368.1060.

ethyl 2'-cyano-4-methyl-[1,1':3',1''-terphenyl]-4'-carboxylate



7h

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 4-methylcinnamaldehyde (43.9 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7h** as a white solid with 72% yield (49.2 mg). m.p. 81-82 ºC.

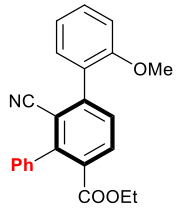
NMR and HRMS data for the product **7h**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.06 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.50-7.48 (m, 2H), 7.46-7.43 (m, 3H), 7.37-7.35 (m, 2H), 7.31-7.29 (m, 2H), 4.04 (q, *J* = 7.2 Hz, 2H), 2.42 (s, 3H), 0.93 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 149.0, 147.0, 139.3, 137.9, 134.8, 133.2, 131.3, 129.5, 128.9, 128.8, 128.7, 128.6, 128.2, 117.0, 113.2, 61.4, 21.3, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{19}NO_2$+Na 364.1313, found 364.1313

ethyl 2'-cyano-2-methoxy-[1,1':3',1''-terphenyl]-4'-carboxylate



7i

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 2-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7i** as a white solid with 70% yield (50.3 mg). m.p. 158-160 ^oC.

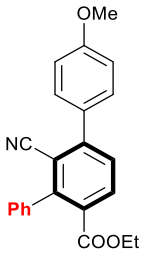
NMR and HRMS data for the product **7i**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.06 (d, *J* = 8.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.47-7.42 (m, 4H), 7.38 (d, *J* = 7.2 Hz, 1H), 7.30 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.07 (t, *J* = 7.2 Hz, 1H), 7.03 (d, *J* = 7.2 Hz, 1H), 4.04 (q, *J* = 7.2 Hz, 2H), 3.85 (s, 3H), 0.94 (t, *J* = 7.8 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 167.0, 156.4, 146.2, 146.0, 137.8, 132.9, 131.4, 130.8, 130.7, 129.8, 128.8, 128.5, 128.2, 126.8, 120.8, 116.8, 115.2, 111.3, 61.4, 55.5, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{19}NO_3$+Na 380.1263, found 380.1261.

ethyl 2'-cyano-4-methoxy-[1,1':3',1''-terphenyl]-4'-carboxylate



7j

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7j** as a white solid with 74% yield (52.6 mg). m.p. 98-100 ºC.

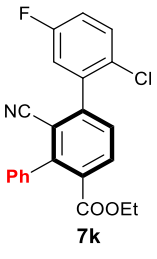
NMR and HRMS data for the product **7j**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.06 (d, *J* = 8.4 Hz, 1H), 7.57-7.52 (m, 3H), 7.49-7.43 (m, 3H), 7.38-7.35 (m, 2H), 7.05-7.00 (m, 2H), 4.04 (q, *J* = 7.2 Hz, 2H), 3.86 (s, 3H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 160.5, 148.6, 147.1, 137.9, 133.3, 131.1, 130.3, 130.0, 128.8, 128.7, 128.6, 128.2, 117.1, 114.3, 113.1, 61.4, 55.4, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{19}NO_3$+Na 380.1263, found 380.1264.

ethyl 2-chloro-2'-cyano-5-fluoro-[1,1':3',1''-terphenyl]-4'-carboxylate



7k

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-phenylbut-3-enoate (43.1 mg, 0.2 mmol) and 3-(2-chloro-5-fluorophenyl)acrylaldehyde (55.4 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7k** as a white solid with 62% yield (47.4 mg). m.p. 132-134 ºC.

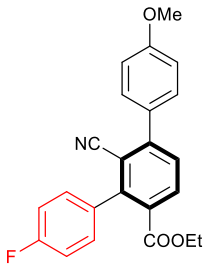
NMR and HRMS data for the product **7k**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.10 (d, *J* = 7.8 Hz, 1H), 7.50-7.45 (m, , 5H), 7.38-7.33 (m, 2H), 7.14-7.11 (m, 2H), 4.07 (q, *J* = 7.2 Hz, 2H), 0.95 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.7, 161.0 (d, *J* = 165.0 Hz), 146.4, 145.1, 138.1 (d, *J* = 5.0 Hz), 137.2, 133.1, 132.8, 131.5 (d, *J* = 5.0 Hz), 129.3, 128.8, 128.7 (d, *J* = 5.0 Hz), 128.3, 128.0 (d, *J* = 2.0 Hz), 118.0 (d, *J* = 16.0 Hz), 117.7 (d, *J* = 14.0 Hz), 115.8, 114.8, 61.6, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{15}ClFNO_2$+Na 402.0673, found 402.0674.

ethyl 2'-cyano-4''-fluoro-4-methoxy-[1,1':3',1''-terphenyl]-4'-carboxylate



7l

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-(4-fluorophenyl)but-3-enoate (46.7 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7l** as a white solid with 71% yield (53.5 mg). m.p. 127-128 °C.

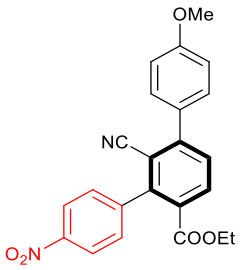
NMR and HRMS data for the product **7l**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.08 (d, *J* = 7.8 Hz, 1H), 7.55-7.53 (m, 3H), 7.36-7.33 (m, 2H), 7.18-7.15 (m, 2H), 7.04-7.02 (m, 2H), 4.08 (q, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 1.02 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 166.5, 162.9 (d, *J* = 247.5 Hz), 160.5, 148.7, 146.1, 133.9, 133.5, 130.9, 130.5 (d, *J* = 7.5 Hz), 130.3, 129.8, 129.1, 117.1, 115.4 (d, *J* = 7.5 Hz), 114.3, 113.2, 61.5, 55.4, 13.7 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}FNO_2$+Na 398.1168, found 398.1165.

ethyl 2'-cyano-4''-nitro-[1,1':3',1''-terphenyl]-4'-carboxylate



7m

Prepared according to the general procedure using ethyl ethyl (*E*)-4-cyano-3-(4-nitrophenyl)but-3-enoate (52.1 mg, 0.2 mmol) and 4-methoxycinnamaldehyde (48.7 mg, 0.3 mmol). Purification of the crude product *via* column chromatography delivered **7m** as a white solid with 69% yield (52.1 mg). m.p. 162-163 °C.

NMR and HRMS data for the product **7m**:

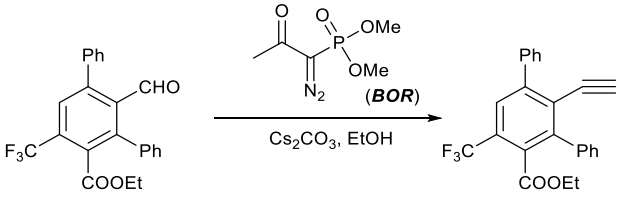
^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.36-8.34 (m, 2H), 8.23 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.57-7.53 (m, 5H), 7.05-7.03 (m, 2H), 4.11 (q, *J* = 7.2 Hz, 2H), 3.88 (s, 3H), 1.06 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (150 MHz, $CDCl_3$): δ = 165.4, 160.8, 149.2, 147.8, 145.3, 144.9, 134.1, 130.3, 129.9, 129.6, 129.3, 123.5, 116.6, 114.4, 112.8, 61.7, 55.4, 13.7 ppm.

HRMS (ESI): m/z calculated for $C_{22}H_{16}FNO_2$+Na 425.1113, found 425.1118.

3. Synthetic transformations of 5a

3.1 Procedure of terminal alkyne **8**



5a **8**

To a solution of **5a** (39.8 mg, 0.10 mmol) in ethyl alcohol (2 mL) was added BOR (48.0 mg, 0.2 mmol) and Cs_2CO_3 (97.7 mg, 0.30 mmol). The mixture was stirred at room temperature. When the reaction was complete (based on TLC monitoring), the reaction mixture was concentrated and the residue was purified by flash

chromatography on silica gel (petroleum ether/ethyl acetate = 6:1) to give **8** as a white solid in 83% yield (32.7 mg). m.p. 78-79 °C.

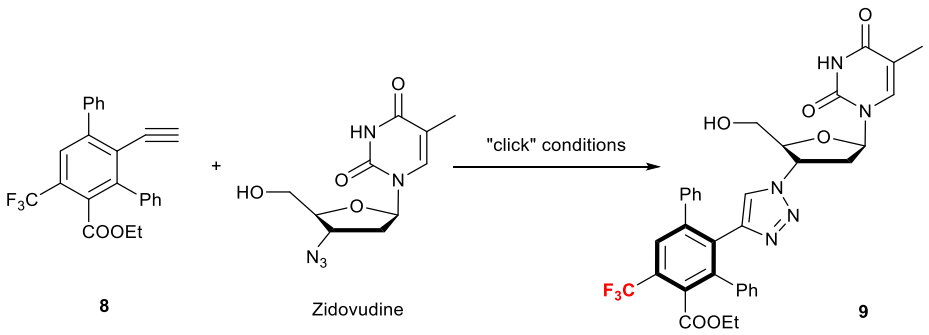
NMR and HRMS data for the product **8**:

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.69 (s, 1H), 7.59-7.58 (m, 2H), 7.48-7.43 (m, 3H), 7.41-7.37 (m, 5H), 4.00 (q, *J* = 7.2 Hz, 2H), 2.99 (s, 1H), 0.97 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 146.4, 144.8, 138.8, 137.3, 131.5, 129.5, 129.2, 128.5, 128.3, 128.2, 127.8, 126.7 (d, *J* = 33.0 Hz), 129.3 (d, *J* = 4.5 Hz), 124.6, 123.2 (d, *J* = 271.5 Hz), 87.5, 80.0, 61.8, 13.5 ppm.

HRMS (ESI): m/z calculated for $C_{23}H_{17}F_3O_3$+Na 417.1078, found 417.1079.

3.2 Procedure of CF_3-functionalized multi-substituted benzene-bridged Zidovudine **9**



To a solution of **8** (39.4 mg, 0.10 mmol) in THF (1.0 mL) was added Zidovudine (26.7 mg, 0.10 mmol), a freshly prepared solution of $CuSO_4$•$5H_2O$ (25.0 mg, 0.10 mmol) and sodium ascorbate (19.8 mg, 0.10 mmol) in H_2O (1.0 mL). When the reaction was complete (based on TLC monitoring), the reaction mixture was concentrated and the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate = 6:1) to give **9** as a white solid in 81% yield (53.6 mg). m.p. 153-154 °C.

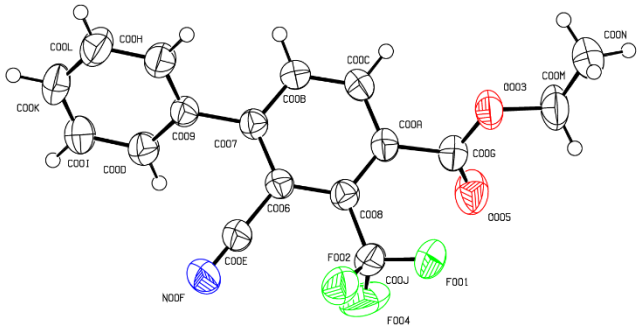
NMR and HRMS data for the product **9**:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.81 (s, 1H), 7.79 (s, 1H), 7.25-7.16 (m, 10H), 7.11-7.09 (m, 1H), 6.83 (s, 1H), 5.97 (t, *J* = 6.8 Hz, 1H), 5.11-5.06 (m, 1H), 4.00 (q, *J* = 7.2 Hz, 2H), 3.87-3.85 (m, 1H), 3.78 (dd, *J* = 12.4, 2.0 Hz, 1H), 3.33 (dd, *J* = 12.4, 2.0 Hz, 1H), 2.96 (br, 1H), 2.81-2.64 (m, 2H), 1.89 (s, 3H), 0.96 (t, *J* = 7.2 Hz, 3H) ppm.

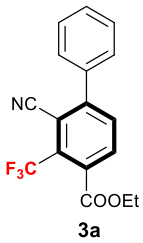
^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.5, 163.4, 150.2, 144.4, 144.0, 142.1, 139.5, 137.9, 137.2, 132.8, 132.0, 130.0 (d, *J* = 6.0 Hz), 129.4, 128.1, 127.7 (d, *J* = 2.0 Hz), 127.6 (d, *J* = 3.0 Hz), 127.0 (d, *J* = 4.0 Hz), 123.7, 123.4 (d, *J* = 273.0 Hz), 111.3, 89.1, 85.3, 61.8, 61.2, 58.6, 36.7, 31.6, 22.7, 14.1, 13.5, 12.4 ppm.

HRMS (ESI): m/z calculated for $C_{34}H_{30}F_3N_5O_6$+Na 684.2046, found 684.2047.

4. Crystal data of 3a



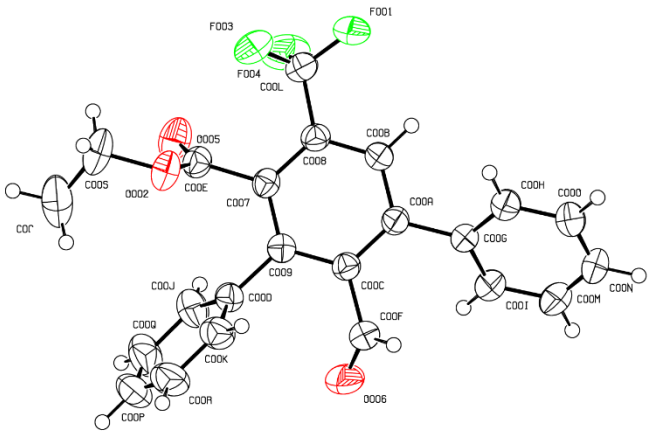
≡

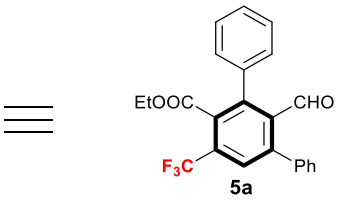


3a

Empirical formula	$C_{17}H_{12}F_3NO_2$
Formula weight	319.28
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	7.9917(5)
b/Å	8.3050(6)
c/Å	11.8750(7)
α/°	107.623(6)
β/°	97.098(5)
γ/°	91.682(5)
Volume/Å^3	743.55(9)
Z	2
ρ_{calc}g/cm^3	1.426
μ/mm^{-1}	1.025
F(000)	328.0
Crystal size/mm^3	0.8 × 0.6 × 0.5
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	11.186 to 145.5
Index ranges	-9 ≤ h ≤ 9, -10 ≤ k ≤ 10, -9 ≤ l ≤ 14
Reflections collected	6956
Independent reflections	2880 [R_{int} = 0.0222, R_{sigma} = 0.0211]
Data/restraints/parameters	2880/0/209
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0570, wR_2 = 0.1626
Final R indexes [all data]	R_1 = 0.0624, wR_2 = 0.1702
Largest diff. peak/hole / e Å^{-3}	0.27/-0.32

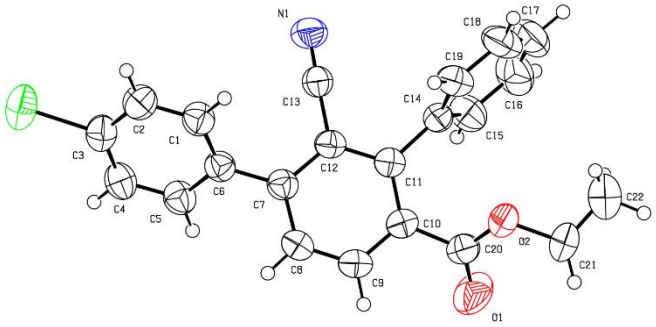
5. Crystal data of 5a

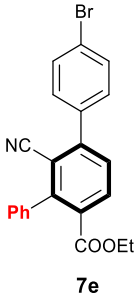




Empirical formula	$C_{23}H_{17}F_3O_3$
Formula weight	398.36
Temperature/K	293.8(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	17.2218(6)
b/Å	13.2420(4)
c/Å	17.2998(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3945.3(2)
Z	8
ρ_{calc}g/cm^3	1.341
μ/mm^{-1}	0.909
F(000)	1648.0
Crystal size/mm^3	0.75 × 0.6 × 0.5
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.856 to 144.854
Index ranges	-21 ≤ h ≤ 13, -10 ≤ k ≤ 16, -13 ≤ l ≤ 21
Reflections collected	11346
Independent reflections	3809 [R_{int} = 0.0276, R_{sigma} = 0.0225]
Data/restraints/parameters	3809/0/263
Goodness-of-fit on F^2	1.085
Final R indexes [I>=2σ (I)]	R_1 = 0.0650, wR_2 = 0.1607
Final R indexes [all data]	R_1 = 0.0739, wR_2 = 0.1709
Largest diff. peak/hole / e Å^{-3}	0.30/-0.53

6. Crystal data of 7e

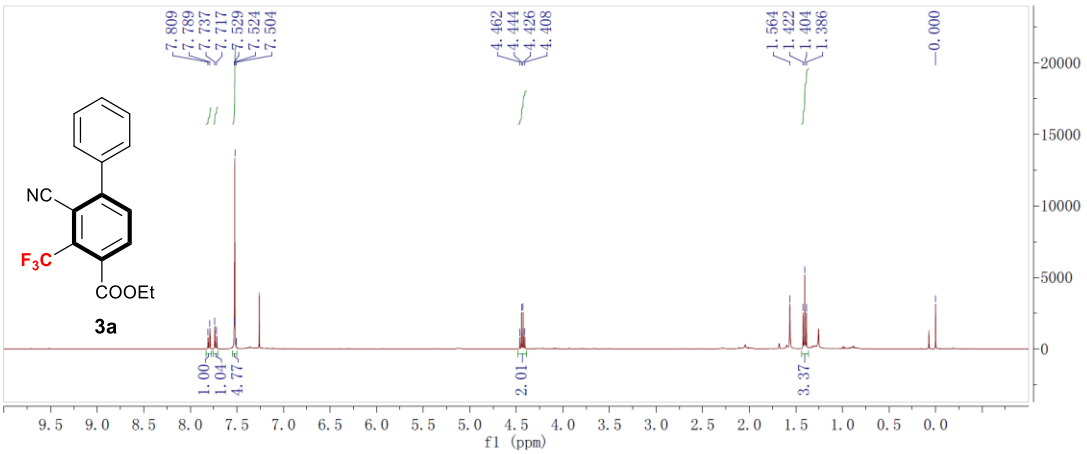


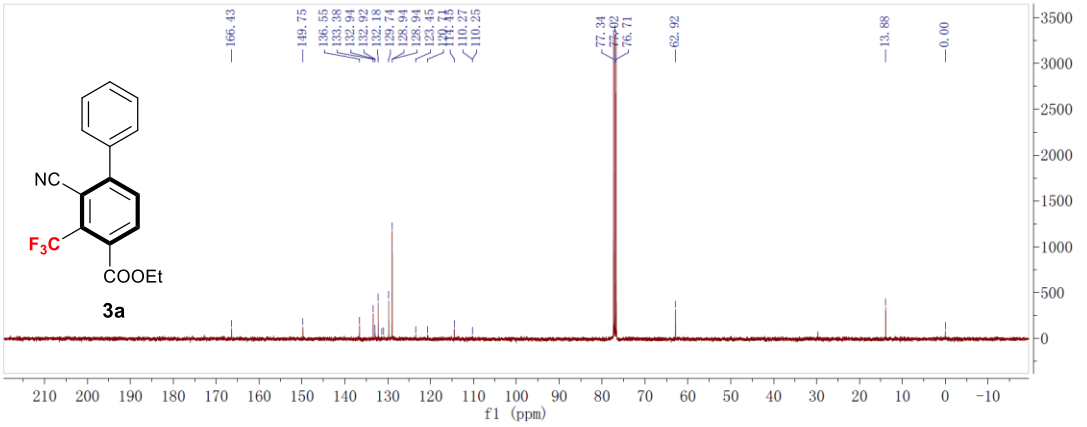


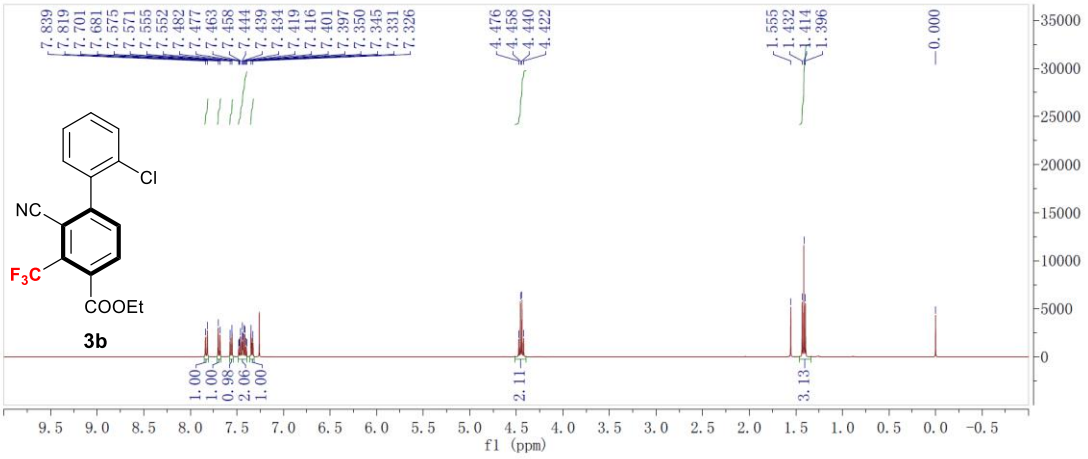
7e

Empirical formula	$C_{22}H_{15}BrNO_2$
Formula weight	405.26
Temperature/K	292.4(5)
Crystal system	monoclinic
Space group	I2/a
a/Å	15.8840(6)
b/Å	7.2300(2)
c/Å	32.8613(11)
α/°	90
β/°	90.675(3)
γ/°	90
Volume/Å^3	3773.5(2)
Z	8
ρ_{calc}g/cm^3	1.427
μ/mm^{-1}	3.089
F(000)	1640.0
Crystal size/mm^3	0.6 × 0.4 × 0.3
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.77 to 145.068
Index ranges	-19 ≤ h ≤ 16, -5 ≤ k ≤ 8, -36 ≤ l ≤ 40
Reflections collected	10640
Independent reflections	3658 [R_{int} = 0.0337, R_{sigma} = 0.0270]
Data/restraints/parameters	3658/0/236
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0582, wR_2 = 0.1593
Final R indexes [all data]	R_1 = 0.0641, wR_2 = 0.1688
Largest diff. peak/hole / e Å^{-3}	0.47/-0.75

7. NMR spectra



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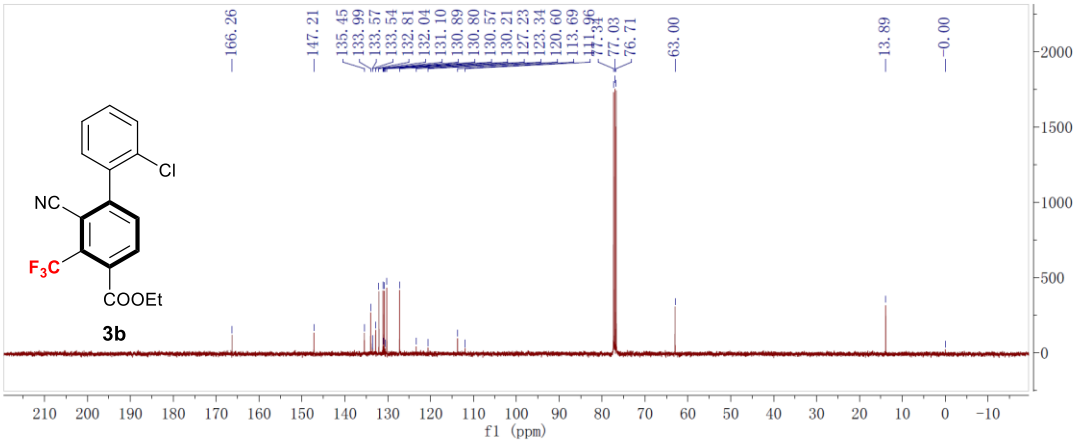
7.819
7.701
7.681
7.575
7.571
7.555
7.552
7.482
7.477
7.463
7.458
7.444
7.439
7.434
7.419
7.416
7.401
7.397
7.350
7.345
7.331
7.326
4.476
4.458
4.440
4.422
1.555
1.432
1.414
1.396
0.000
Cl
NC
F3C
COOEt
3b
1.00
1.00
0.98
2.06
1.00
2.11
3.13
f1 (ppm)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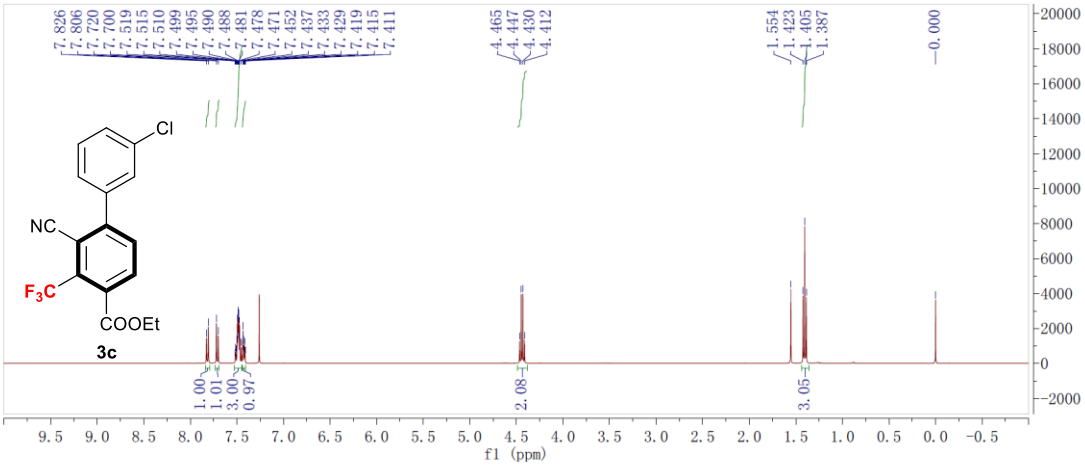
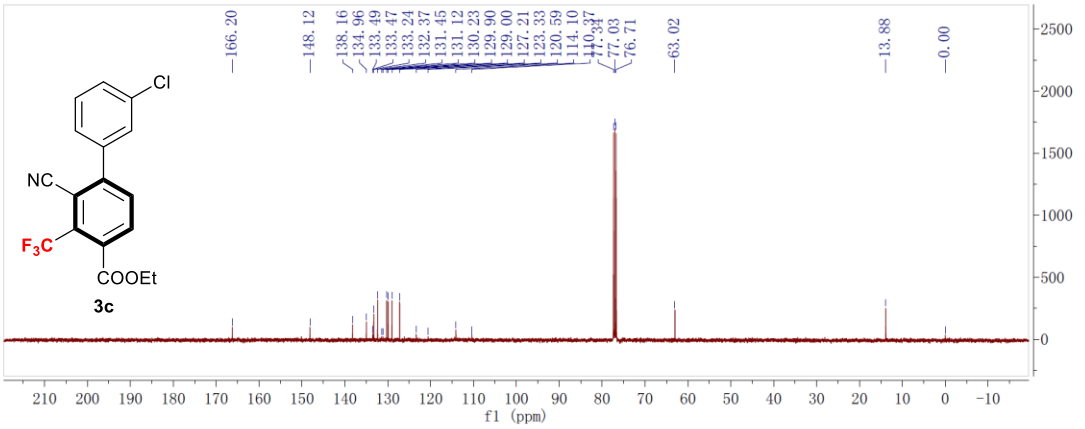
147.21
135.45
133.99
133.57
133.54
132.81
132.04
131.10
130.89
130.80
130.57
130.21
127.23
123.34
120.60
113.69
77.03
76.71
63.00
13.89
0.00
Cl
NC
F3C
COOEt
3b
f1 (ppm)


7.826
7.806
7.720
7.700
7.519
7.515
7.510
7.499
7.495
7.490
7.488
7.481
7.478
7.471
7.452
7.437
7.433
7.429
7.419
7.415
7.411
4.465
4.447
4.430
4.412
1.554
1.423
1.405
1.387
0.000
Cl
NC
F3C
COOEt
3c
1.00
1.01
3.00
0.97
2.08
3.05
f1 (ppm)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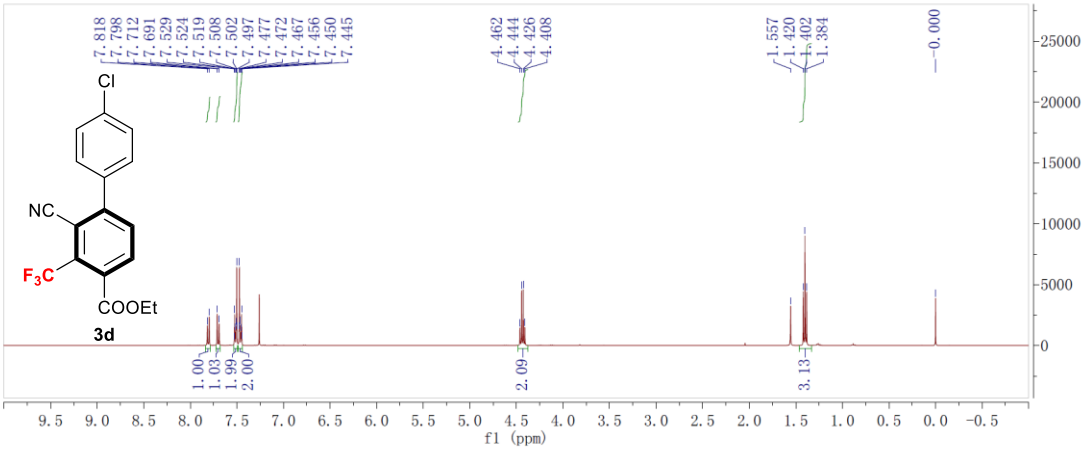
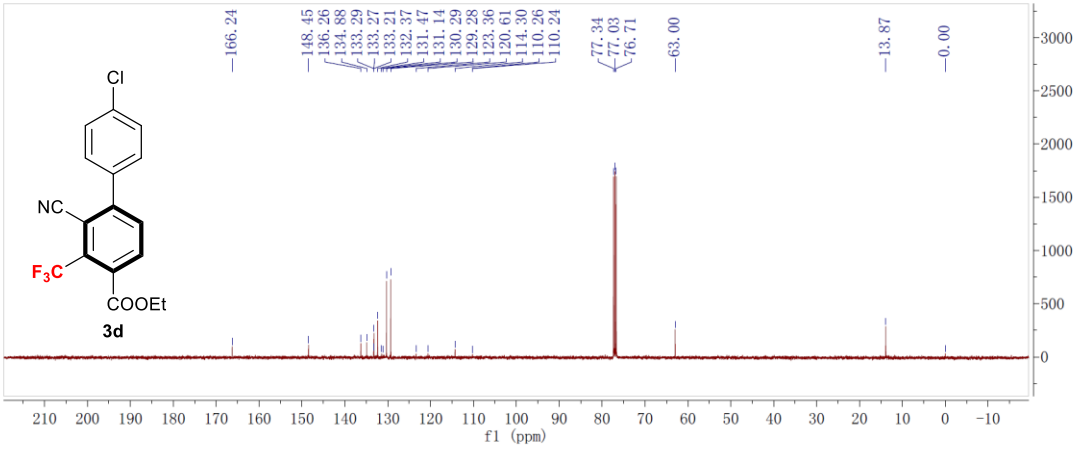
138.16
134.96
133.49
133.47
133.24
132.37
131.45
131.12
130.23
129.90
129.00
127.21
123.33
120.59
114.10
77.03
76.71
63.02
13.88
0.00
Cl
NC
F3C
COOEt
3c
f1 (ppm)


7.818
7.798
7.712
7.691
7.529
7.524
7.519
7.508
7.502
7.497
7.477
7.472
7.467
7.456
7.450
7.445
4.462
4.444
4.426
4.408
1.557
1.420
1.402
1.384
-0.000
Cl
NC
F3C
COOEt
3d
1.00
1.03
1.99
2.00
2.09
3.13
f1 (ppm)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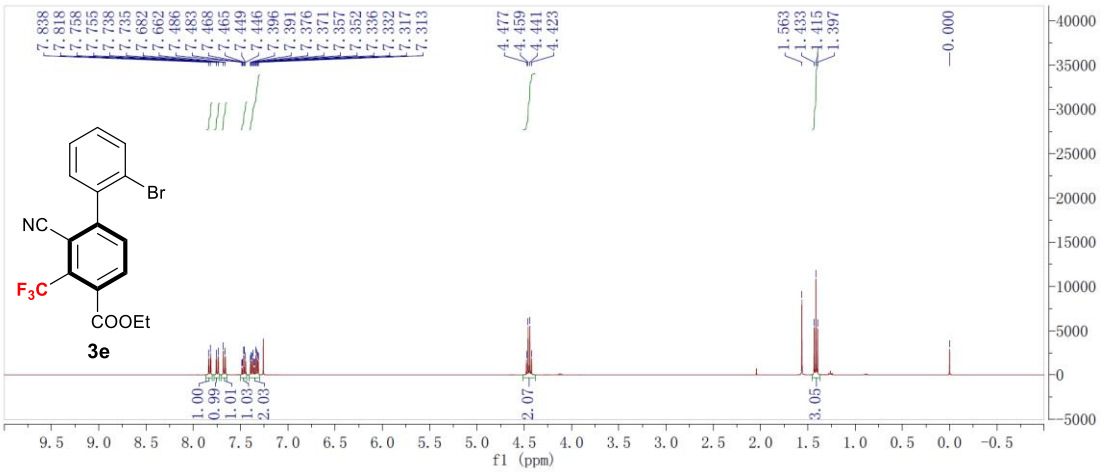
148.45
136.26
134.88
133.29
133.27
133.21
132.37
131.47
131.14
130.29
129.28
123.36
120.61
114.30
110.26
110.24
77.34
77.03
76.71
63.00
13.87
0.00
Cl
NC
F3C
COOEt
3d
f1 (ppm)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7.818
7.758
7.755
7.738
7.735
7.682
7.662
7.486
7.483
7.468
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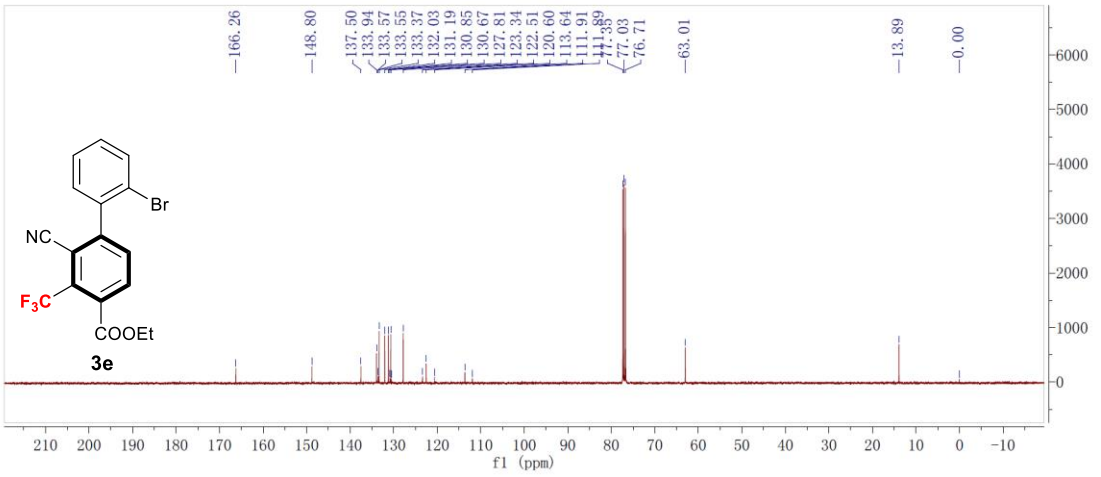
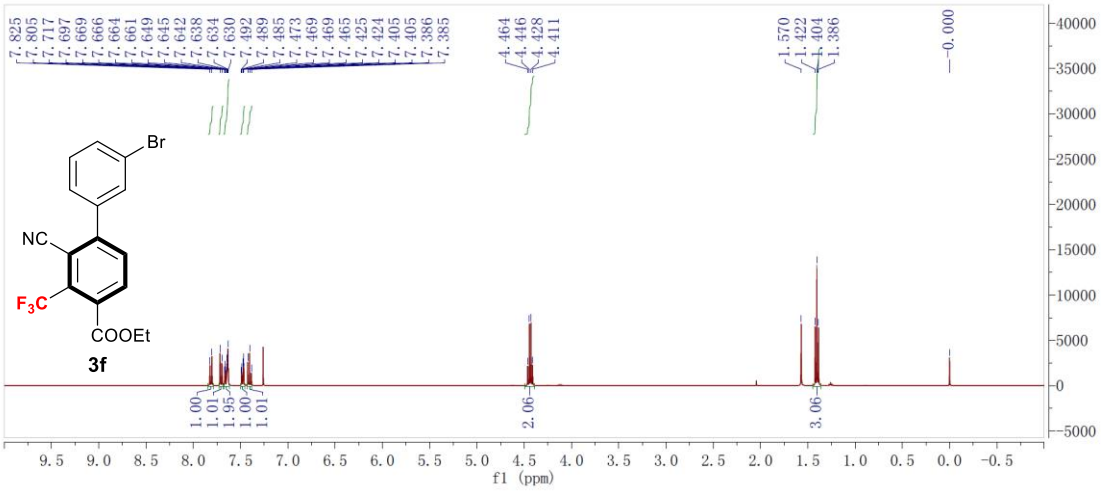
7.449
7.446
7.396
7.391
7.376
7.371
7.357
7.352
7.336
7.332
7.317
7.313
4.477
4.459
4.441
4.423
1.563
1.433
1.415
1.397
0.000
Br
NC
F3C
COOEt
3e
1.00
0.99
1.01
1.03
2.03
2.07
3.05
f1 (ppm)


166.26
148.80
137.50
133.94
133.57
133.55
133.37
132.03
131.19
130.85
130.67
127.81
123.34
122.51
120.60
113.64
111.91
77.35
77.03
76.71
63.01
13.89
0.00
Br
NC
F3C
COOEt
3e
f1 (ppm)


7.825
7.805
7.717
7.697
7.669
7.666
7.664
7.661
7.649
7.645
7.642
7.638
7.634
7.630
7.492
7.489
7.485
7.473
7.469
7.469
7.465
7.425
7.424
7.405
7.405
7.386
7.385
4.464
4.446
4.428
4.411
1.570
1.422
1.404
1.386
0.000
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NC
F3C
COOEt
3f
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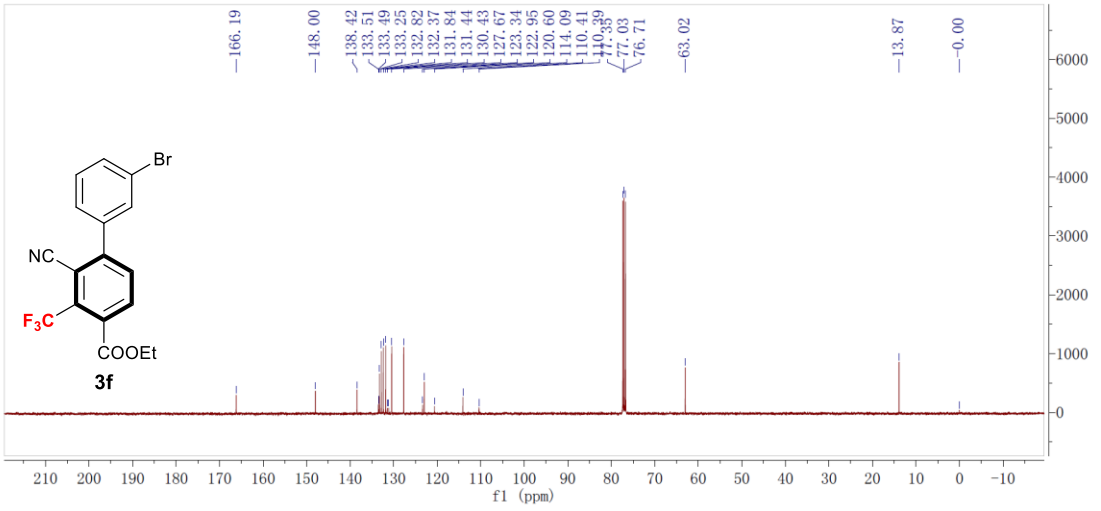
1.01
1.95
1.00
1.01
2.06
3.06
f1 (ppm)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132.37
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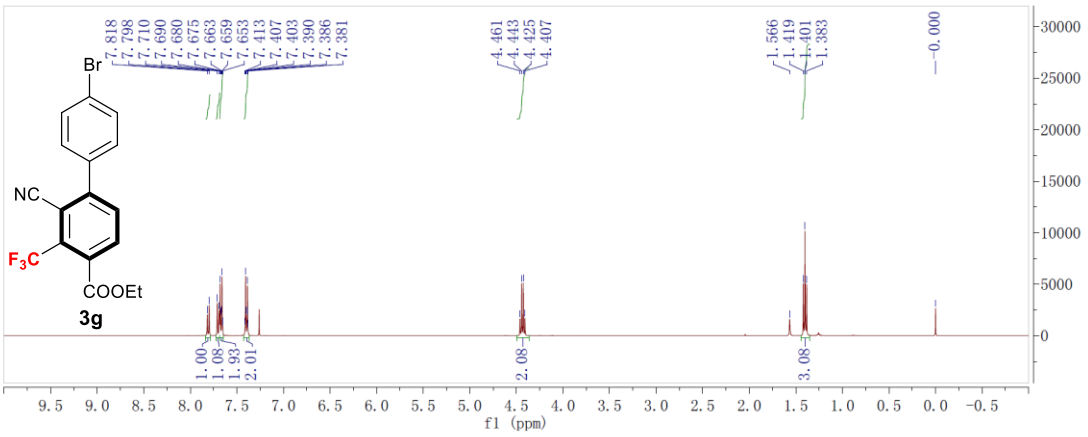
123.34
122.95
120.60
114.09
110.41
77.35
77.03
76.71
63.02
13.87
0.00
Br
NC
F3C
COOEt
3f
f1 (ppm)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NC
F3C
COOEt
3g
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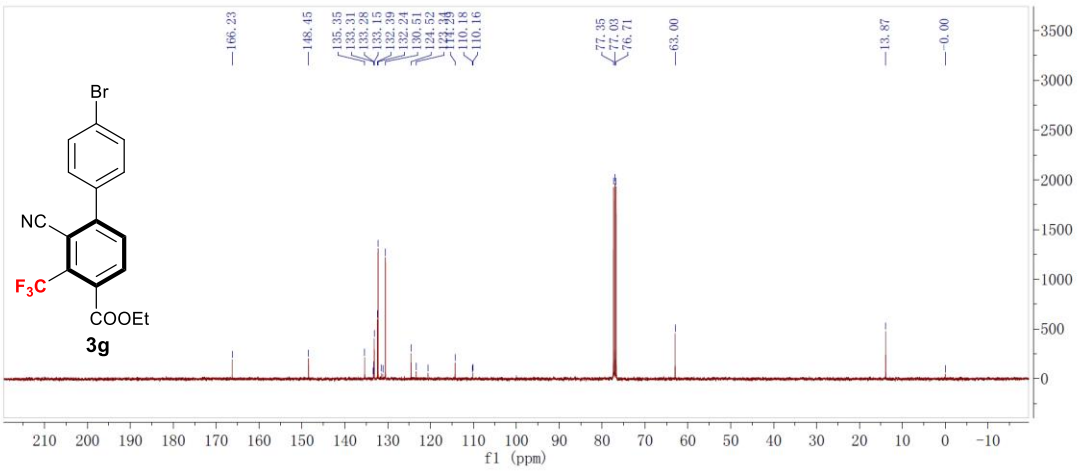
7.675
7.663
7.659
7.653
7.413
7.407
7.403
7.390
7.386
7.381
4.461
4.443
4.425
4.407
1.566
1.419
1.401
1.383
0.000
1.00
1.08
1.93
2.01
2.08
3.08
f1 (ppm)


Br
NC
F3C
COOEt
3g
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135.35
133.31
133.28
133.15
132.39
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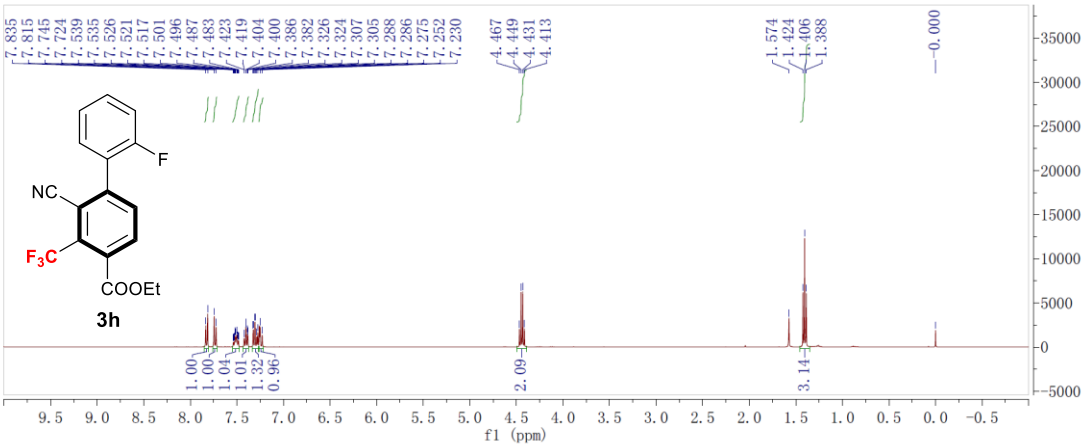
130.51
124.52
110.18
110.16
77.35
77.03
76.71
63.00
13.87
0.00
f1 (ppm)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7.526
7.521
7.517
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7.487
7.483
7.423
7.419
7.404
7.400
7.386
7.382
7.326
7.324
7.307
7.305
7.288
7.286
7.275
7.252
7.230
4.467
4.449
4.431
4.413
1.574
1.424
1.406
1.388
0.000
F
NC
F3C
COOEt
3h
1.00
1.00
1.04
1.01
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0.96
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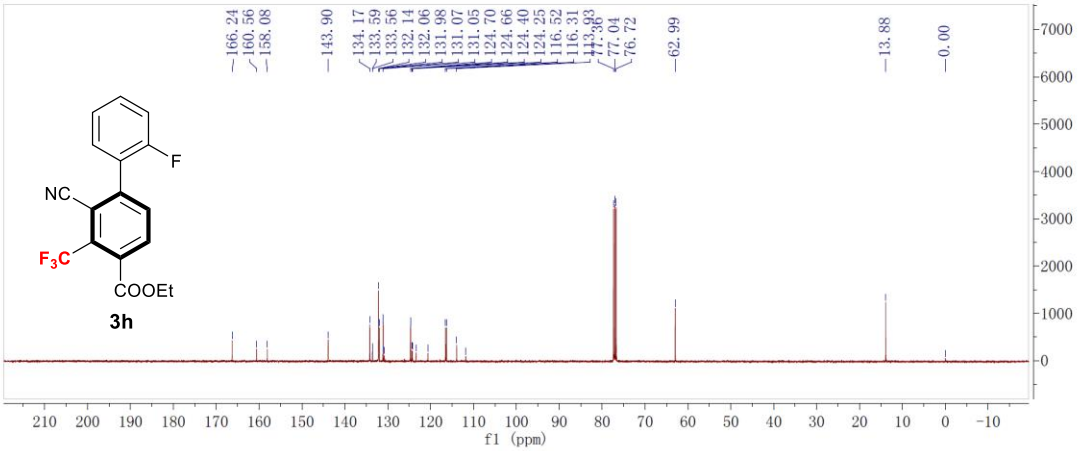
3.14
f1 (ppm)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132.14
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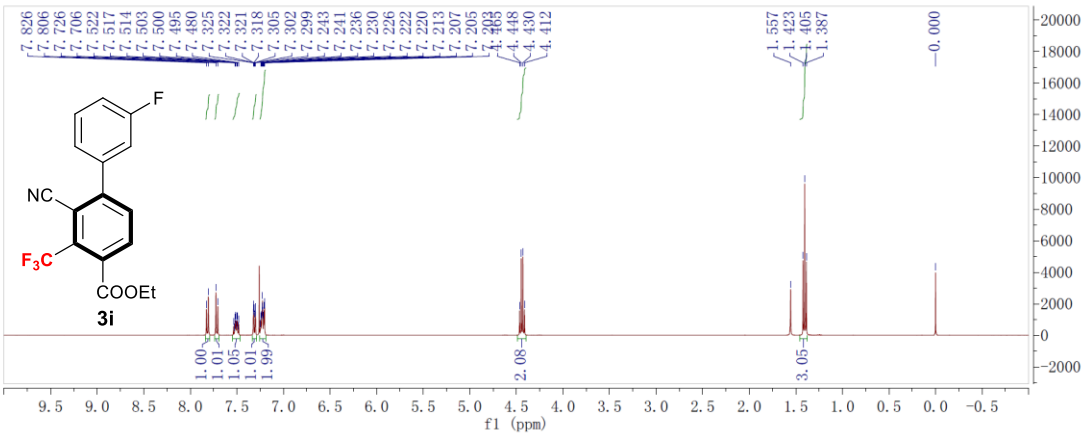
131.98
131.07
131.05
124.70
124.66
124.40
124.25
116.52
116.31
77.04
76.72
62.99
13.88
0.00
F
NC
F3C
COOEt
3h
f1 (ppm)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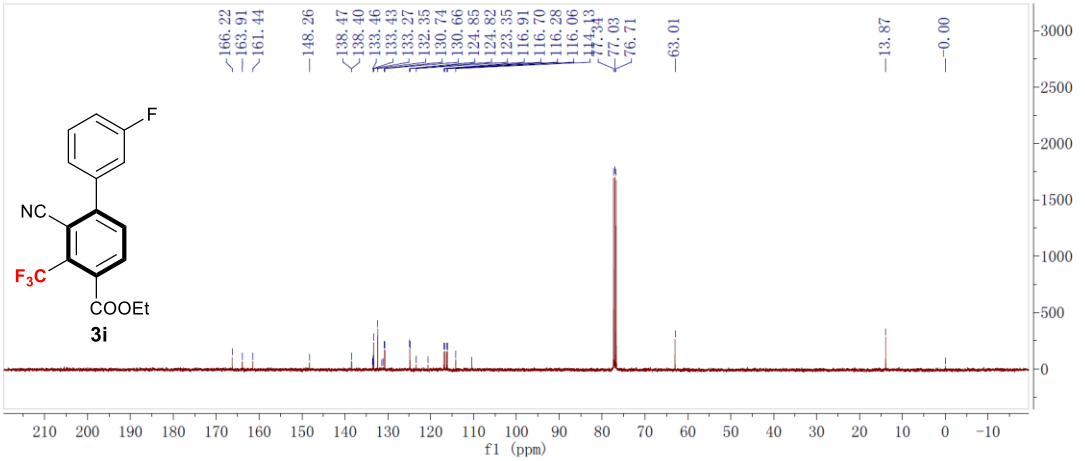
7.726
7.706
7.522
7.517
7.514
7.503
7.500
7.495
7.480
7.325
7.322
7.321
7.318
7.305
7.302
7.299
7.243
7.241
7.236
7.230
7.226
7.222
7.220
7.213
7.207
7.205
4.448
4.430
4.412
1.557
1.423
1.405
1.387
0.000
F
NC
F3C
COOEt
3i
1.00
1.01
1.05
1.01
1.99
2.08
3.05
f1 (ppm)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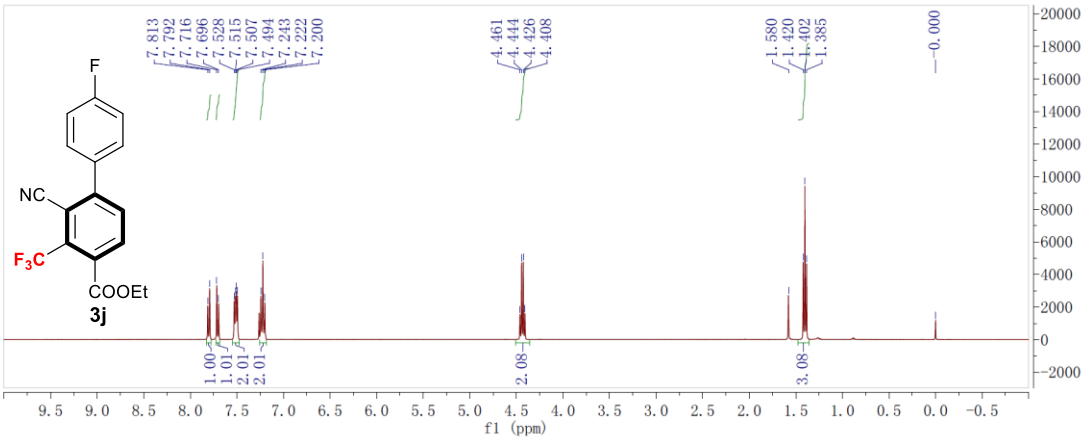
138.40
133.46
133.43
133.27
132.35
130.74
130.66
124.85
124.82
123.35
116.91
116.70
116.28
116.06
77.03
76.71
63.01
13.87
0.00
F
NC
F3C
COOEt
3i
f1 (ppm)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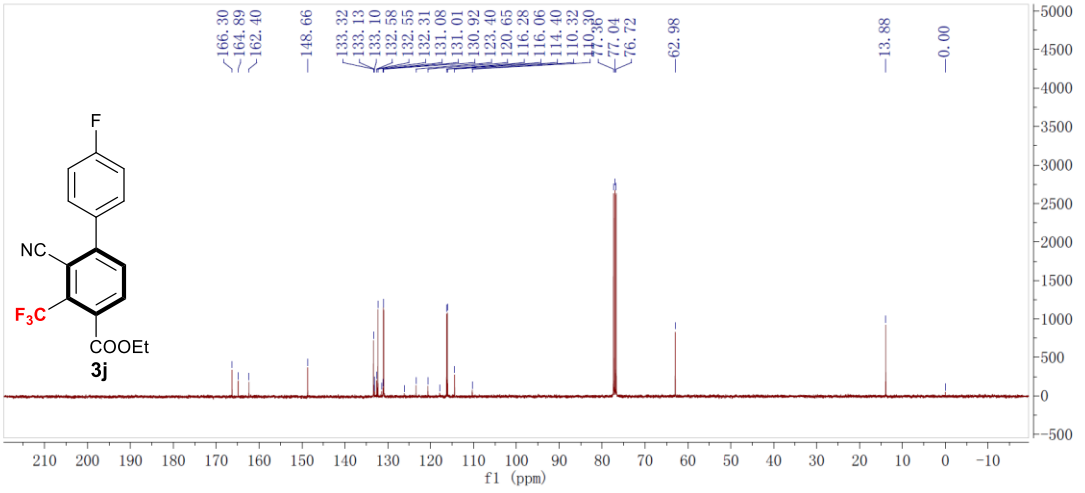
7.716
7.696
7.528
7.515
7.507
7.494
7.243
7.222
7.200
4.461
4.444
4.426
4.408
1.580
1.420
1.402
1.385
0.000
F
NC
F3C
COOEt
3j
1.00
1.01
2.01
2.01
2.08
3.08
f1 (ppm)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164.89
162.40
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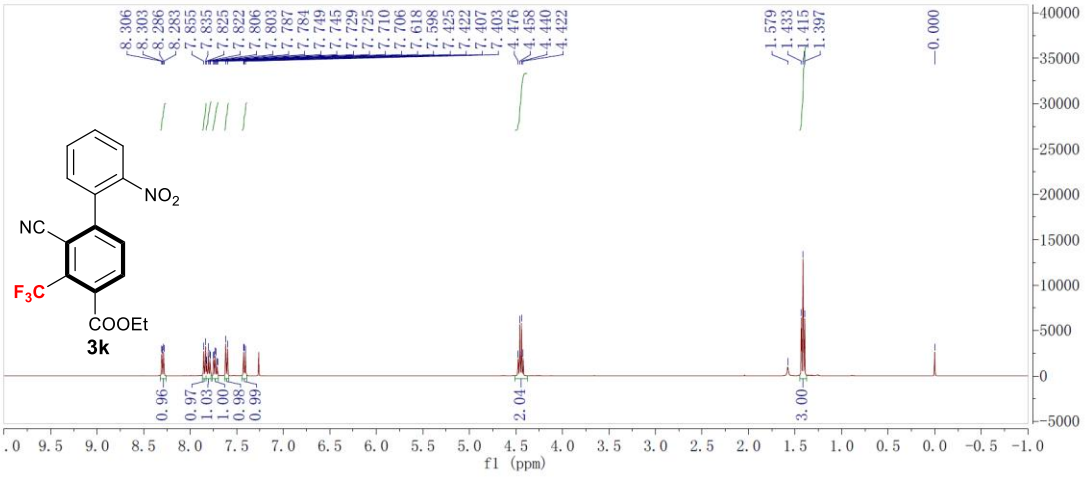
133.13
133.10
132.58
132.55
132.31
131.08
131.01
130.92
123.40
120.65
116.28
116.06
114.40
110.32
77.36
77.04
76.72
62.98
13.88
0.00
F
NC
F3C
COOEt
3j
f1 (ppm)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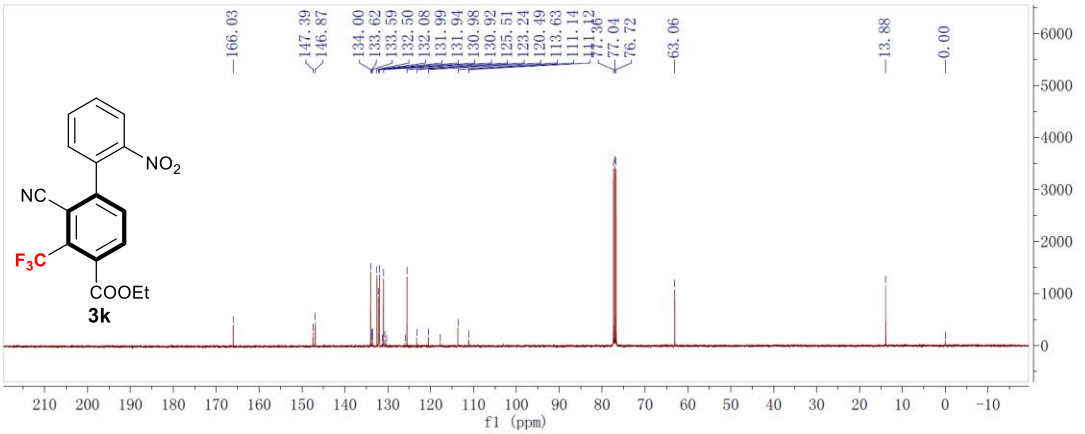
8.286
8.283
7.855
7.835
7.825
7.822
7.806
7.803
7.787
7.784
7.749
7.745
7.729
7.725
7.710
7.706
7.618
7.598
7.425
7.422
7.407
7.403
4.476
4.458
4.440
4.422
1.579
1.433
1.415
1.397
0.000
NO2
NC
F3C
COOEt
3k
0.96
0.97
1.03
1.00
0.98
0.99
2.04
3.00
f1 (ppm)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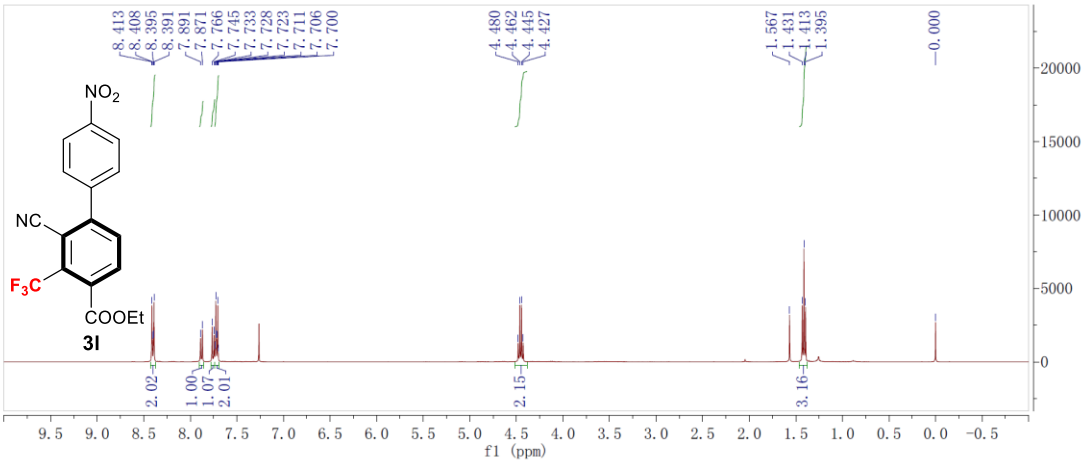
133.59
132.50
132.08
131.99
131.94
130.98
130.92
125.51
123.24
120.49
113.63
111.14
77.04
76.72
63.06
13.88
0.00
NO2
NC
F3C
COOEt
3k
f1 (ppm)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8.408
8.395
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7.745
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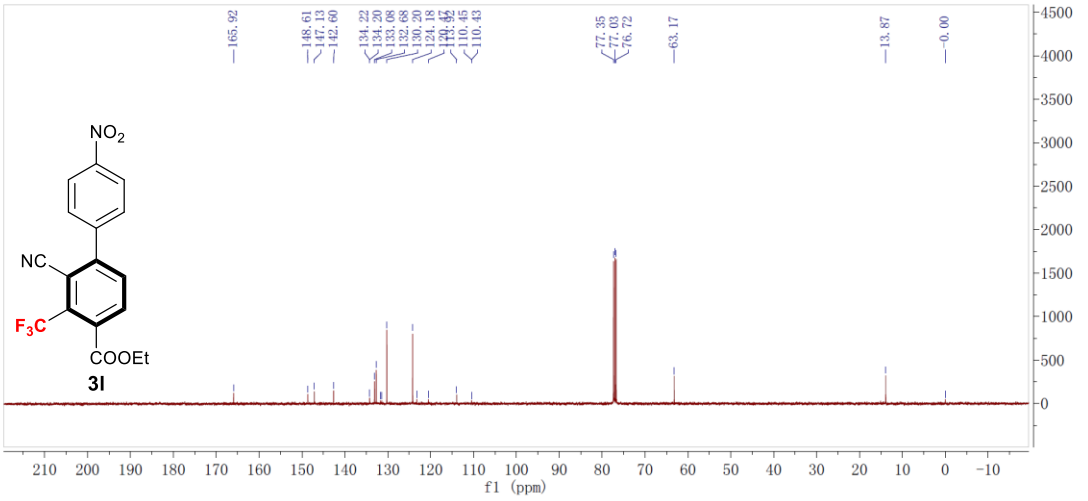
7.728
7.723
7.711
7.706
7.700
4.480
4.462
4.445
4.427
1.567
1.431
1.413
1.395
0.000
NO2
NC
F3C
COOEt
3l
2.02
1.00
1.07
2.01
2.15
3.16
f1 (ppm)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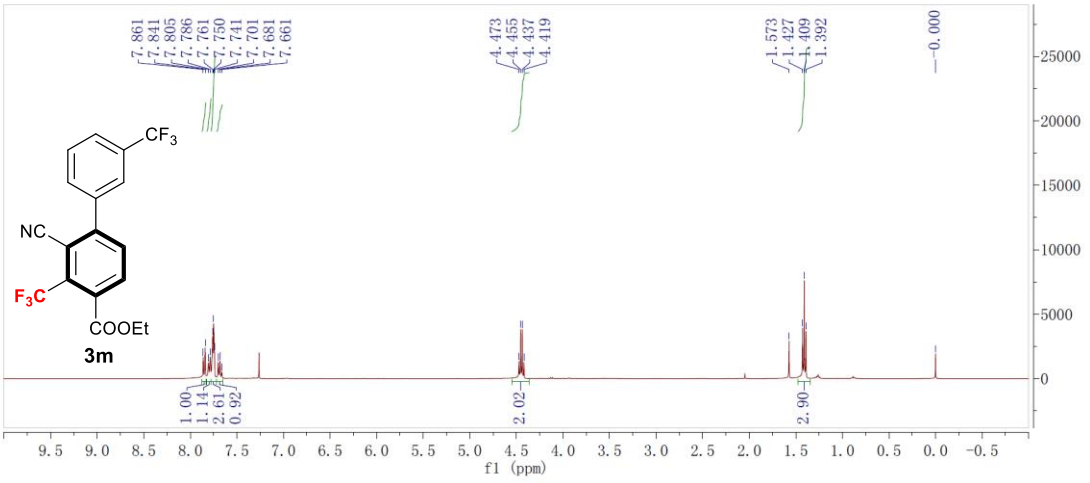
148.61
147.13
142.60
134.22
134.20
133.08
132.68
130.20
130.18
124.42
123.92
110.45
110.43
77.35
77.03
76.72
63.17
13.87
0.00
NO2
NC
F3C
COOEt
3l
f1 (ppm)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7.750
7.741
7.701
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7.661
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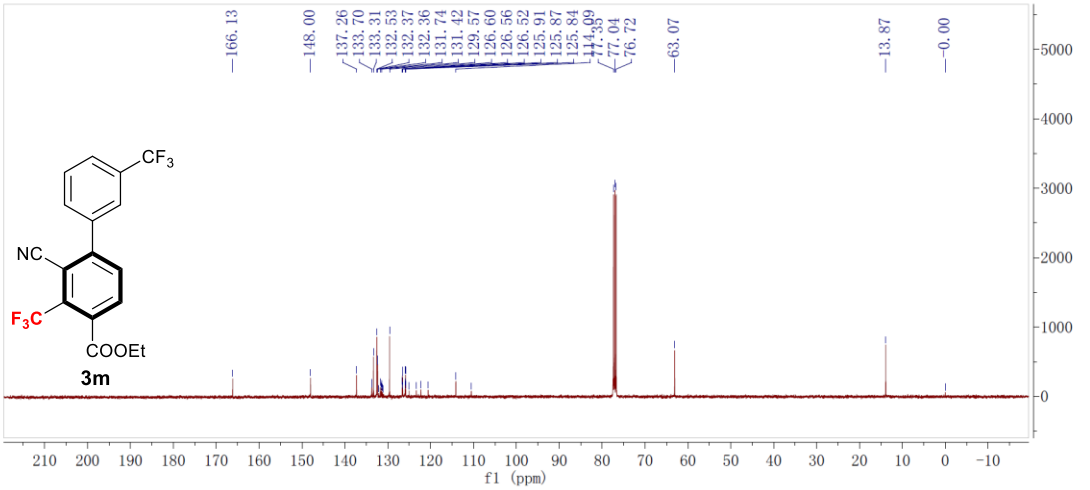
4.455
4.437
4.419
1.573
1.427
1.409
1.392
0.000
CF3
NC
F3C
COOEt
3m
1.00
1.14
2.61
0.92
2.02
2.90
f1 (ppm)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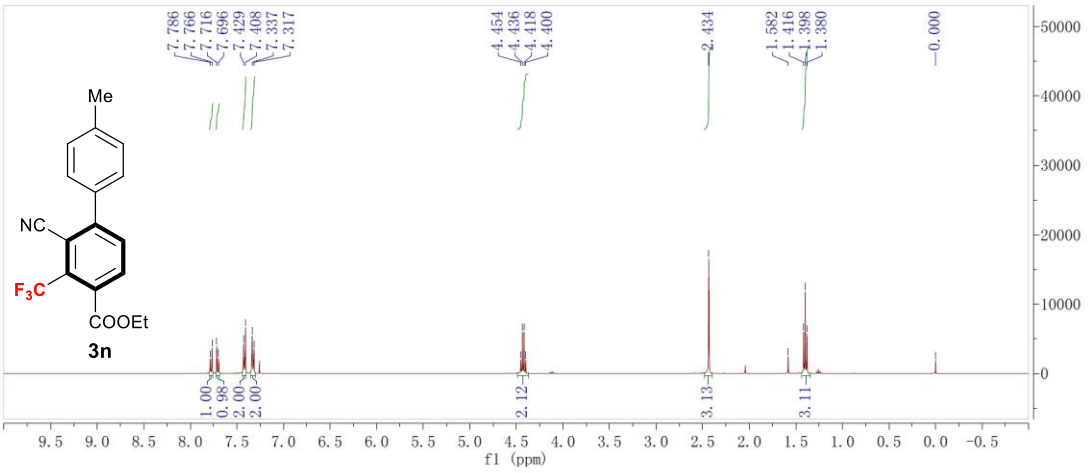
132.37
132.36
131.74
131.42
129.57
126.60
126.56
126.52
125.91
125.87
125.84
77.04
76.72
63.07
13.87
0.00
CF3
NC
F3C
COOEt
3m
f1 (ppm)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7.317
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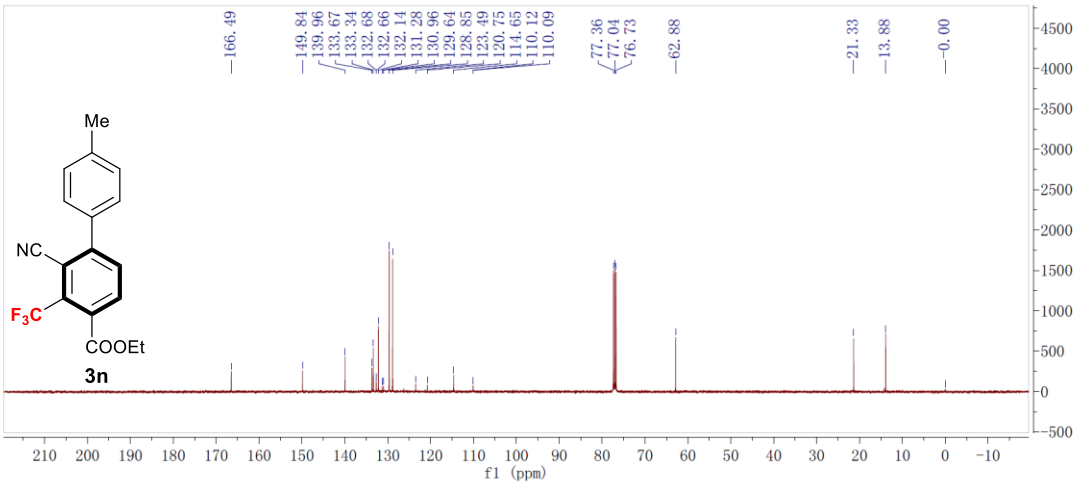
4.436
4.418
4.400
2.434
1.582
1.416
1.398
1.380
0.000
Me
NC
F3C
COOEt
3n
1.00
0.98
2.00
2.00
2.12
3.13
3.11
f1 (ppm)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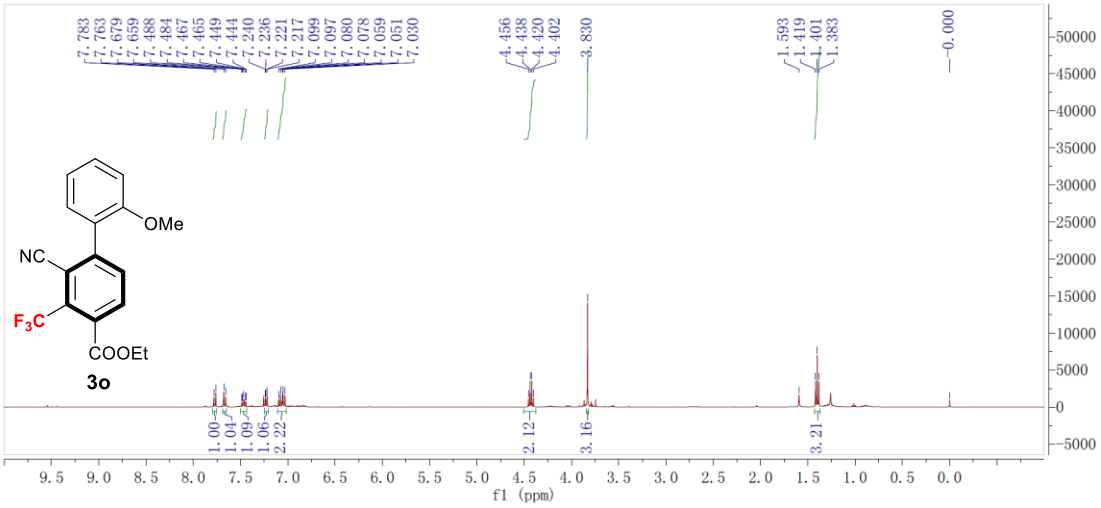
132.68
132.66
132.14
131.28
130.96
129.64
128.85
123.49
120.75
114.65
110.12
110.09
77.36
77.04
76.73
62.88
21.33
13.88
0.00
Me
NC
F3C
COOEt
3n
f1 (ppm)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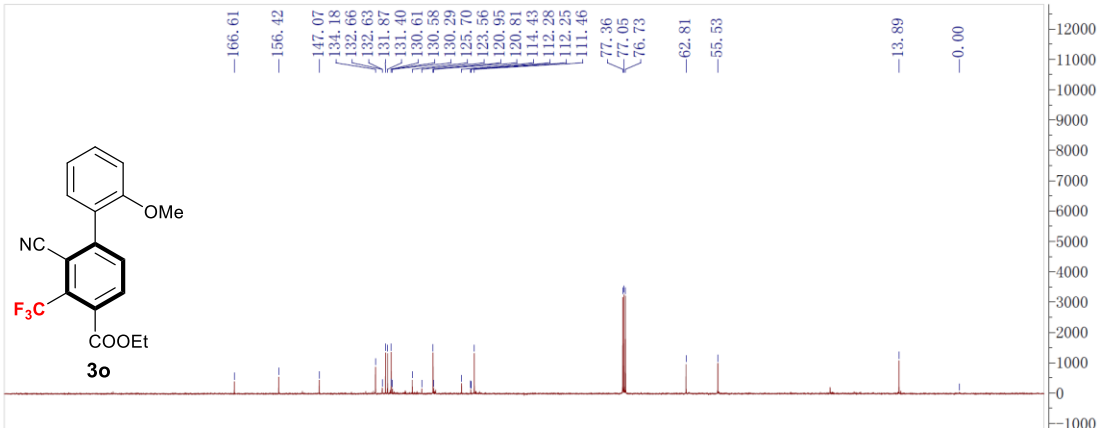
7.465
7.449
7.444
7.240
7.236
7.221
7.217
7.099
7.097
7.080
7.078
7.059
7.051
7.030
4.456
4.438
4.420
4.402
3.830
1.593
1.419
1.401
1.383
0.000
OMe
NC
F3C
COOEt
3o
1.00
1.04
1.09
1.06
2.22
2.12
3.16
3.21
f1 (ppm)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131.40
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130.58
130.29
125.70
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120.95
120.81
114.43
112.28
112.25
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76.73
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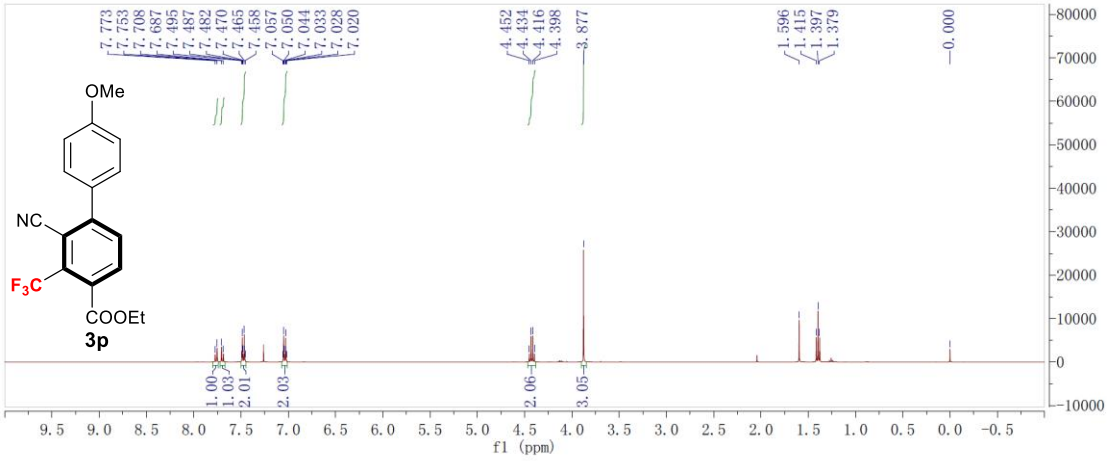
NC
F3C
COOEt
3o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7.487
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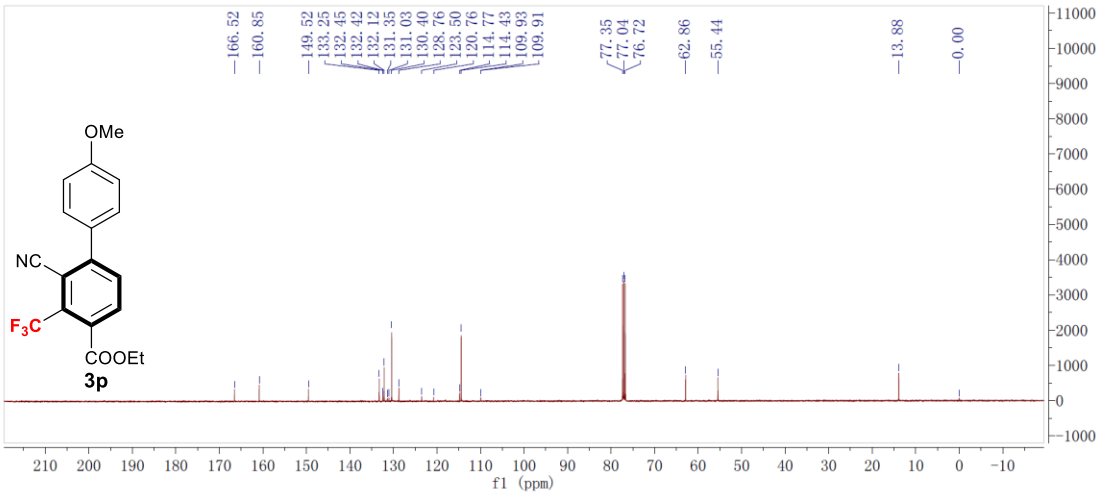
7.470
7.465
7.458
7.057
7.050
7.044
7.033
7.028
7.020
4.452
4.434
4.416
4.398
3.877
1.596
1.415
1.397
1.379
0.000
OMe
NC
F3C
COOEt
3p
1.00
1.03
2.01
2.03
2.06
3.05
f1 (ppm)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132.45
132.42
132.12
131.35
131.03
130.40
128.76
123.50
120.76
114.77
114.43
109.93
109.91
77.35
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76.72
62.86
55.44
13.88
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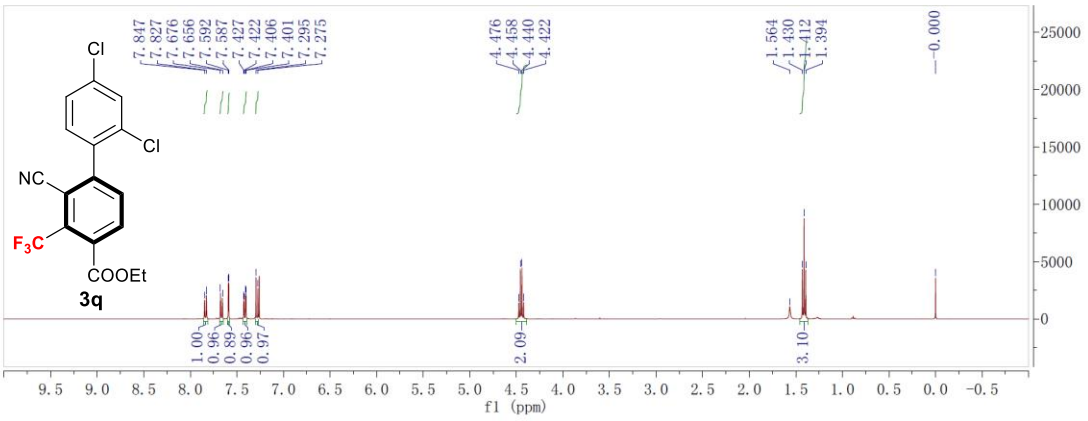
OMe
NC
F3C
COOEt
3p
f1 (ppm)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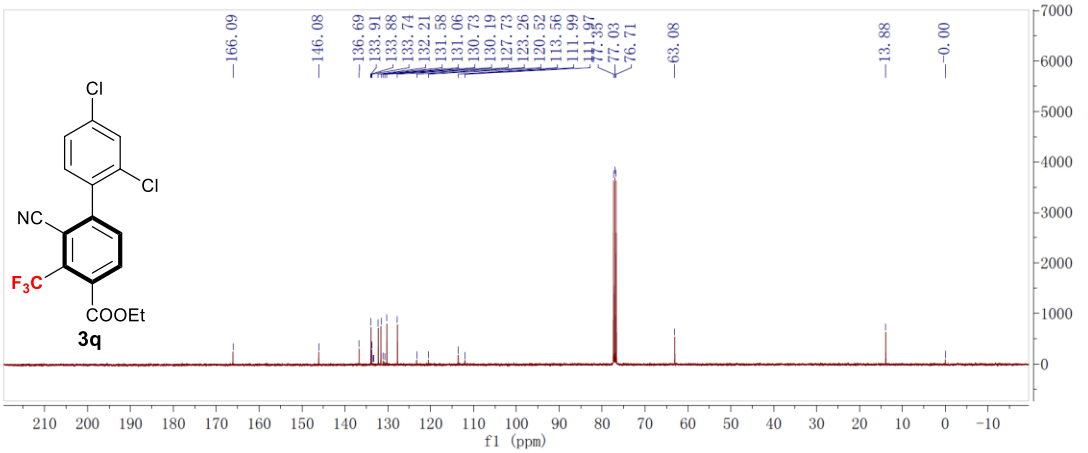
7.656
7.592
7.587
7.427
7.422
7.406
7.401
7.295
7.275
4.476
4.458
4.440
4.422
1.564
1.430
1.412
1.394
0.000
Cl
Cl
NC
F3C
COOEt
3q
1.00
0.96
0.89
0.96
0.97
2.09
3.10
f1 (ppm)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136.69
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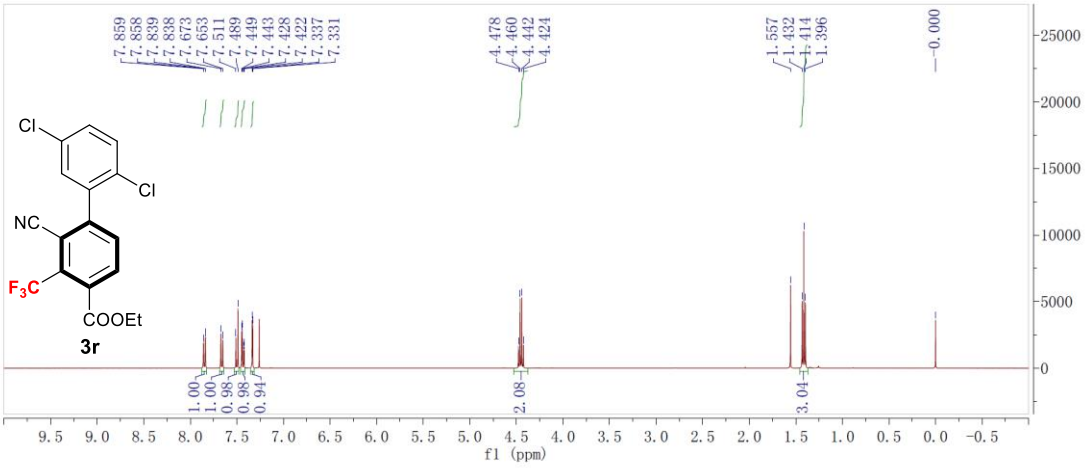
133.88
133.74
132.21
131.58
131.06
130.73
130.19
127.73
123.26
120.52
113.56
111.99
77.03
76.71
63.08
13.88
0.00
Cl
Cl
NC
F3C
COOEt
3q
f1 (ppm)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7.511
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7.449
7.443
7.428
7.422
7.337
7.331
4.478
4.460
4.442
4.424
1.557
1.432
1.414
1.396
0.000
Cl
Cl
NC
F3C
COOEt
3r
1.00
1.00
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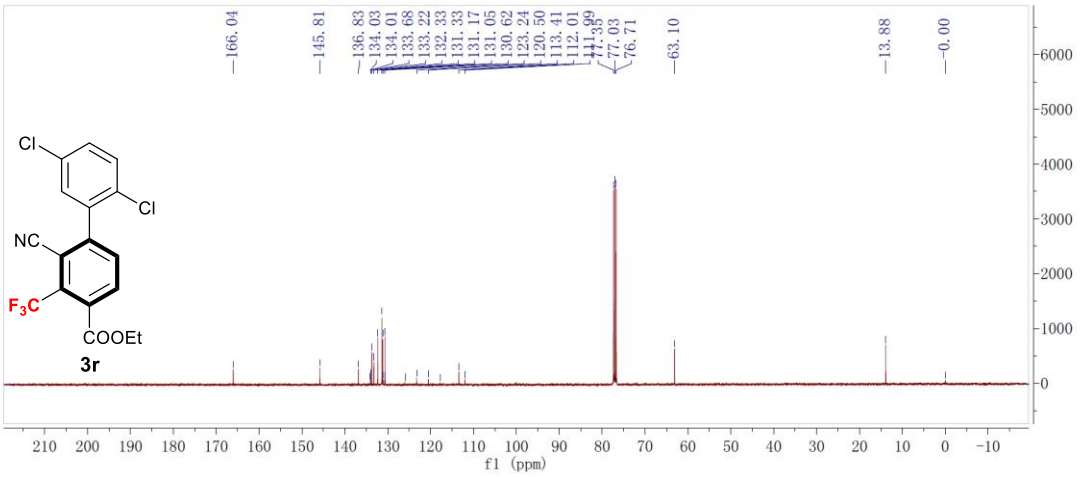
0.98
0.94
2.08
3.04
f1 (ppm)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134.01
133.68
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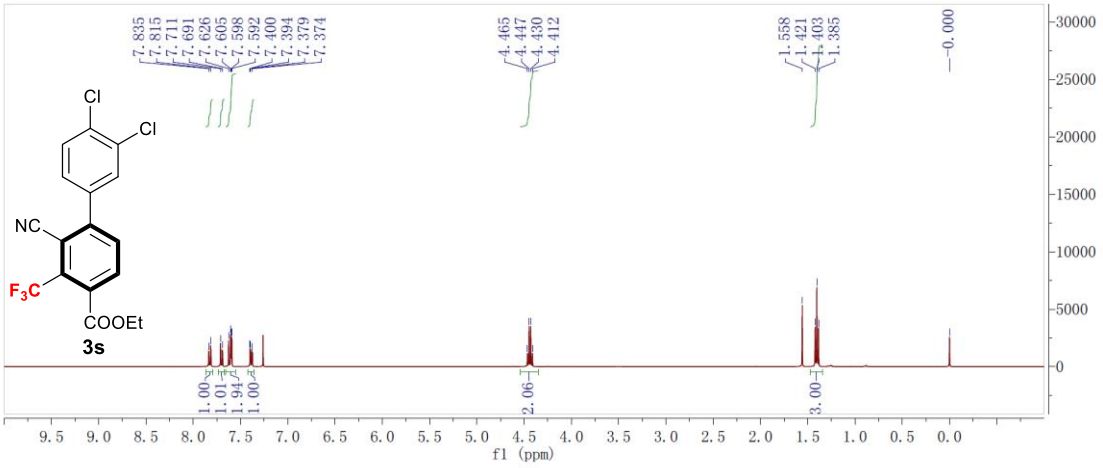
132.33
131.33
131.17
131.05
130.62
123.24
120.50
113.41
112.01
77.35
77.03
76.71
63.10
13.88
0.00
Cl
Cl
NC
F3C
COOEt
3r
f1 (ppm)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7.711
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7.605
7.598
7.592
7.400
7.394
7.379
7.374
4.465
4.447
4.430
4.412
1.558
1.421
1.403
1.385
0.000
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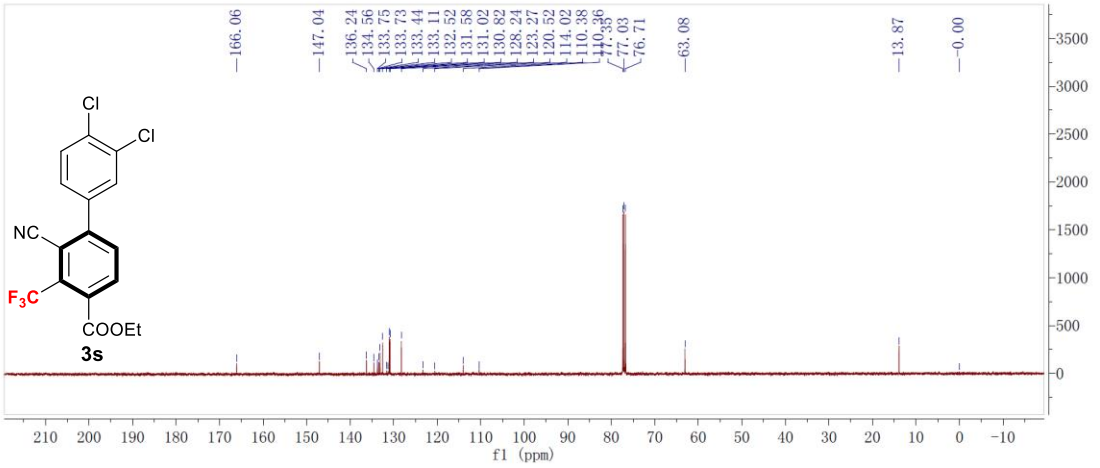
Cl
NC
F3C
COOEt
3s
1.00
1.01
1.94
1.00
2.06
3.00
f1 (ppm)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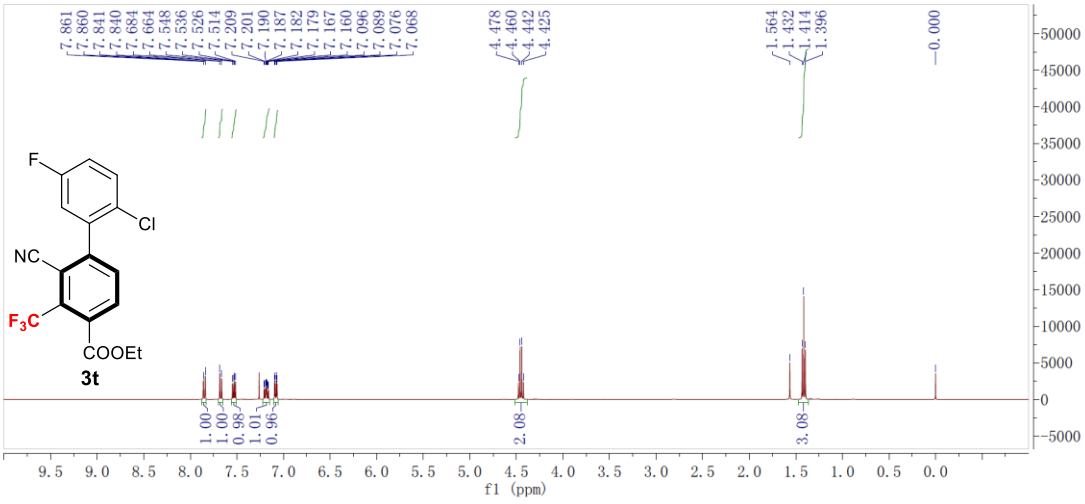
133.11
132.52
131.58
131.02
130.82
128.24
123.27
120.52
114.02
110.38
77.35
77.03
76.71
63.08
13.87
0.00
Cl
Cl
NC
F3C
COOEt
3s
f1 (ppm)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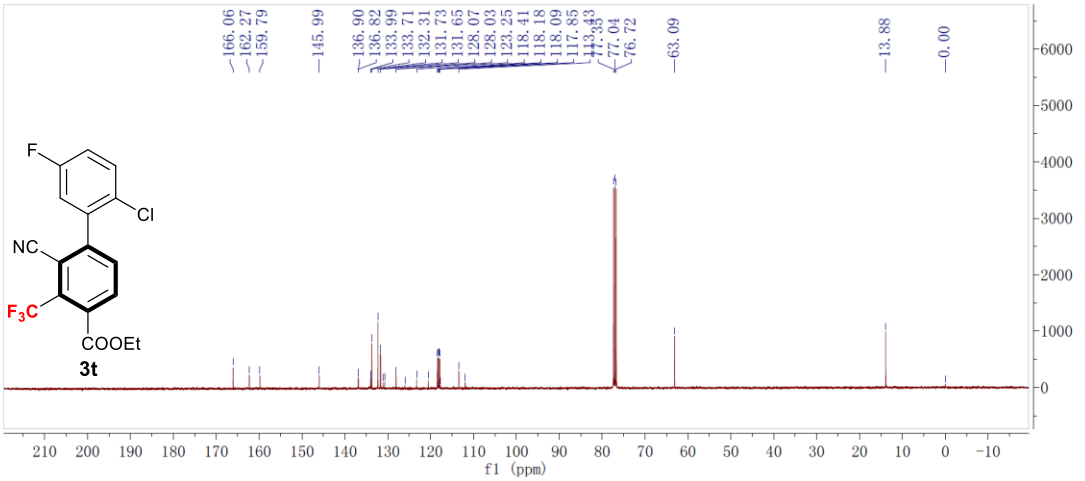
7.840
7.684
7.664
7.548
7.536
7.526
7.514
7.209
7.201
7.190
7.187
7.182
7.179
7.167
7.160
7.096
7.089
7.076
7.068
4.478
4.460
4.442
4.425
1.564
1.432
1.414
1.396
0.000
F
Cl
NC
F3C
COOEt
3t
1.00
1.00
0.98
1.01
0.96
2.08
3.08
f1 (ppm)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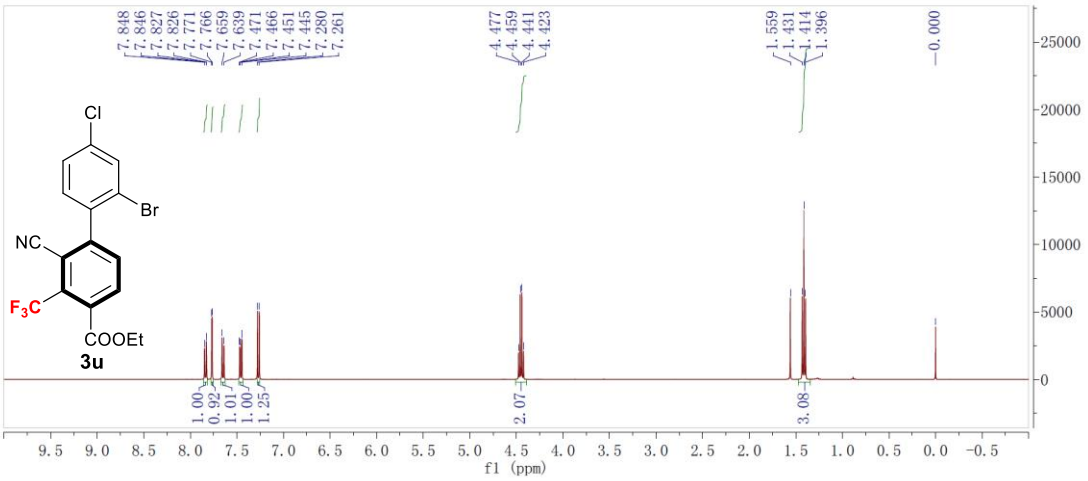
159.79
145.99
136.90
136.82
133.99
133.71
132.31
131.73
131.65
128.07
128.03
123.25
118.41
118.18
118.09
117.85
77.33
77.04
76.72
63.09
13.88
0.00
F
Cl
NC
F3C
COOEt
3t
f1 (ppm)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7.846
7.827
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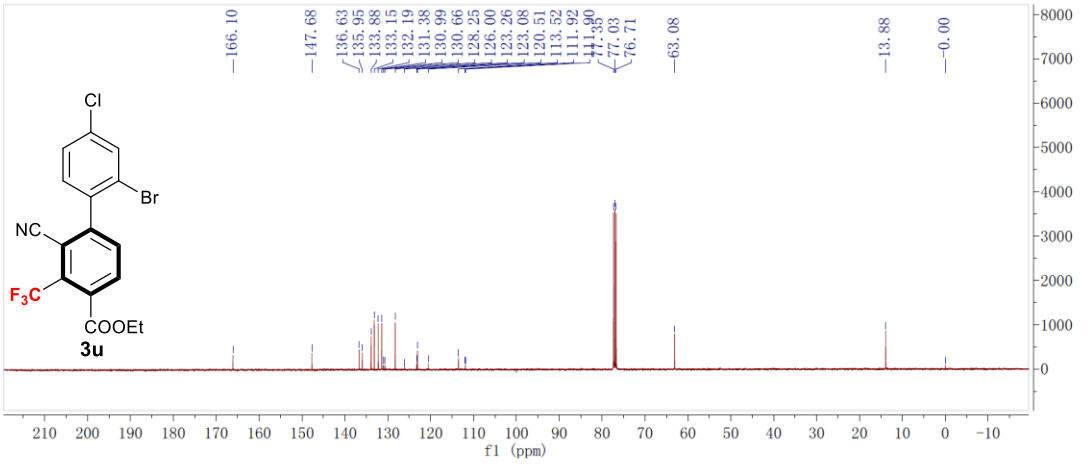
7.771
7.766
7.659
7.639
7.471
7.466
7.451
7.445
7.280
7.261
4.477
4.459
4.441
4.423
1.559
1.431
1.414
1.396
0.000
Cl
Br
NC
F3C
COOEt
3u
1.00
0.92
1.01
1.00
1.25
2.07
3.08
f1 (ppm)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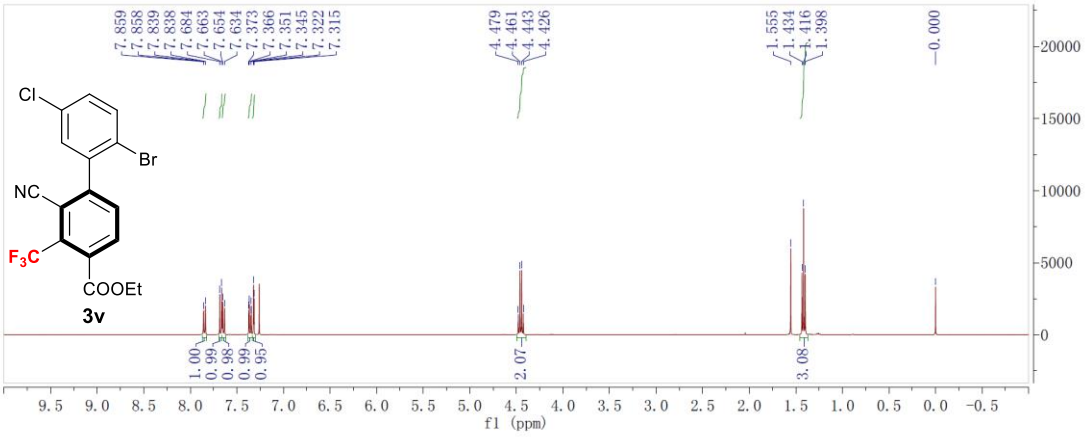
133.88
133.15
132.19
131.38
130.99
130.66
128.25
126.00
123.26
123.08
120.51
113.52
111.92
77.35
77.03
76.71
63.08
13.88
0.00
Cl
Br
NC
F3C
COOEt
3u
f1 (ppm)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7.858
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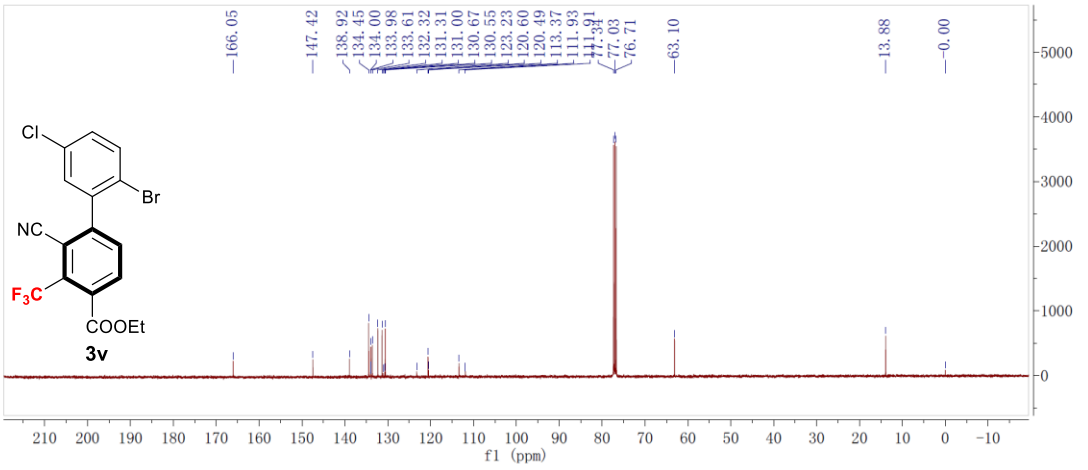
7.838
7.684
7.663
7.654
7.634
7.373
7.366
7.351
7.345
7.322
7.315
4.479
4.461
4.443
4.426
1.555
1.434
1.416
1.398
0.000
Cl
Br
NC
F3C
COOEt
3v
1.00
0.99
0.98
0.99
0.95
2.07
3.08
f1 (ppm)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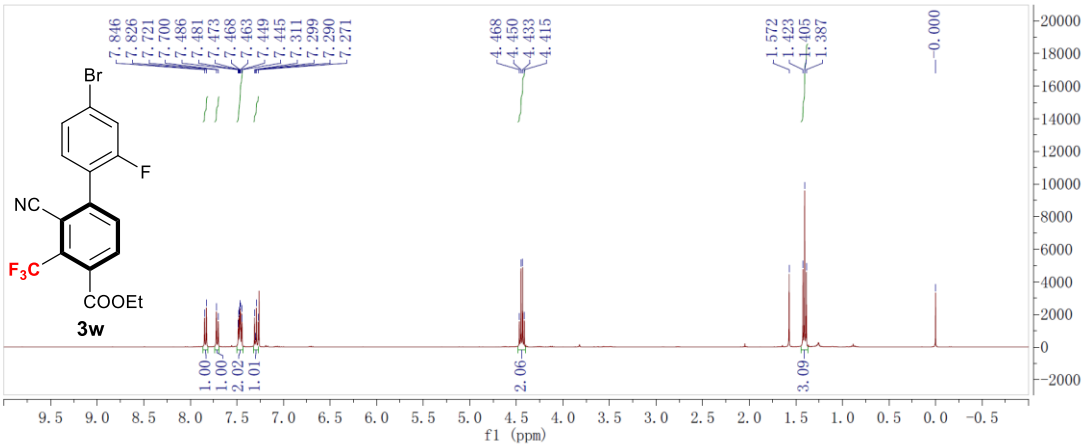
134.00
133.98
133.61
132.32
131.31
131.00
130.67
130.55
123.23
120.60
120.49
113.37
111.93
77.03
76.71
63.10
13.88
0.00
Cl
Br
NC
F3C
COOEt
3v
f1 (ppm)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7.826
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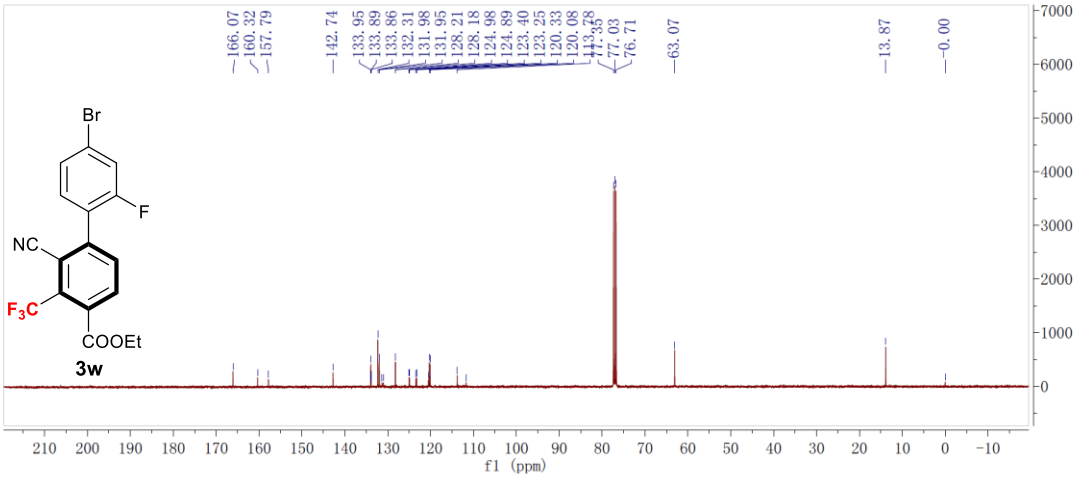
7.486
7.481
7.473
7.468
7.463
7.449
7.445
7.311
7.299
7.290
7.271
4.468
4.450
4.433
4.415
1.572
1.423
1.405
1.387
0.000
Br
F
NC
F3C
COOEt
3w
1.00
1.00
2.02
1.01
2.06
3.09
f1 (ppm)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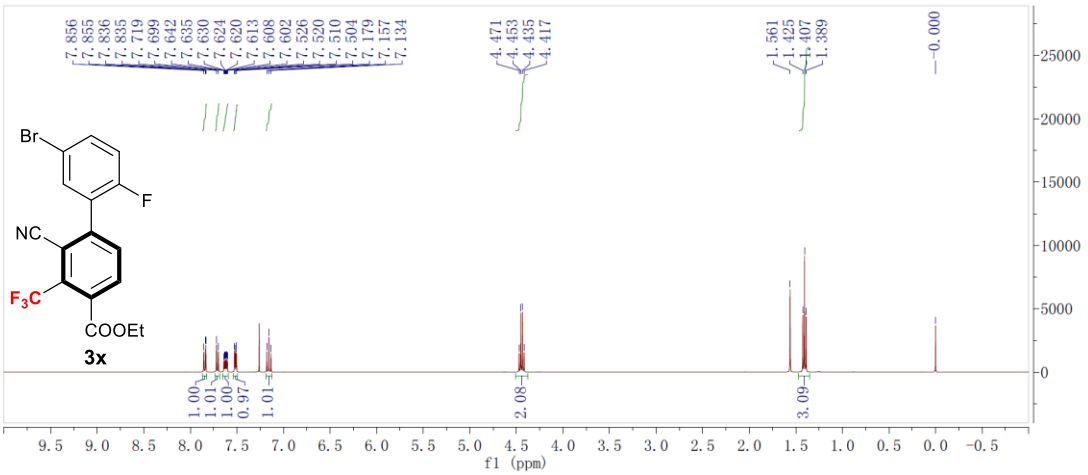
160.32
157.79
142.74
133.95
133.89
133.86
132.31
131.98
131.95
128.21
128.18
124.98
124.89
123.40
123.25
120.33
120.08
77.03
76.71
63.07
13.87
0.00
Br
F
NC
F3C
COOEt
3w
f1 (ppm)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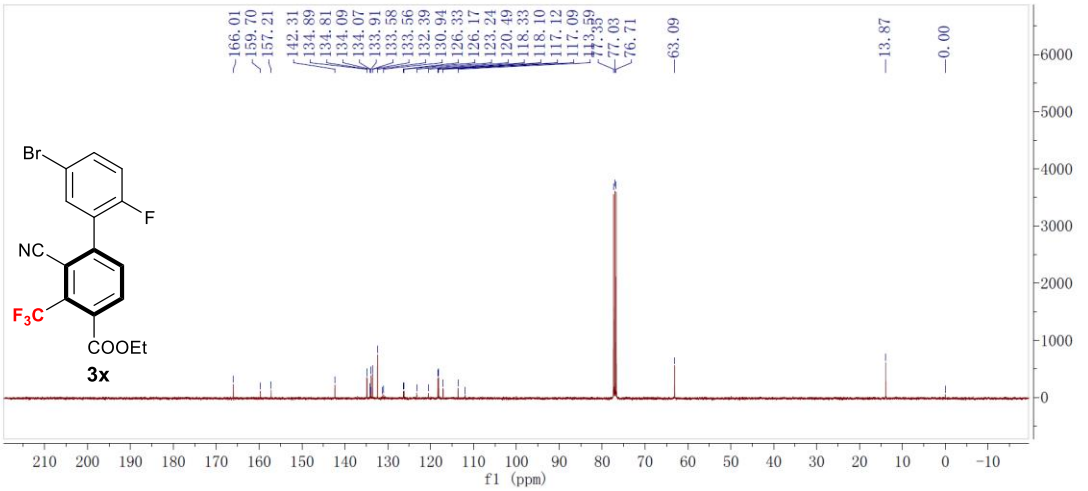
7.855
7.836
7.835
7.719
7.699
7.642
7.635
7.630
7.624
7.620
7.613
7.608
7.602
7.526
7.520
7.510
7.504
7.179
7.157
7.134
4.471
4.453
4.435
4.417
1.561
1.425
1.407
1.389
0.000
Br
F
NC
F3C
COOEt
3x
1.00
1.01
1.00
0.97
1.01
2.08
3.09
f1 (ppm)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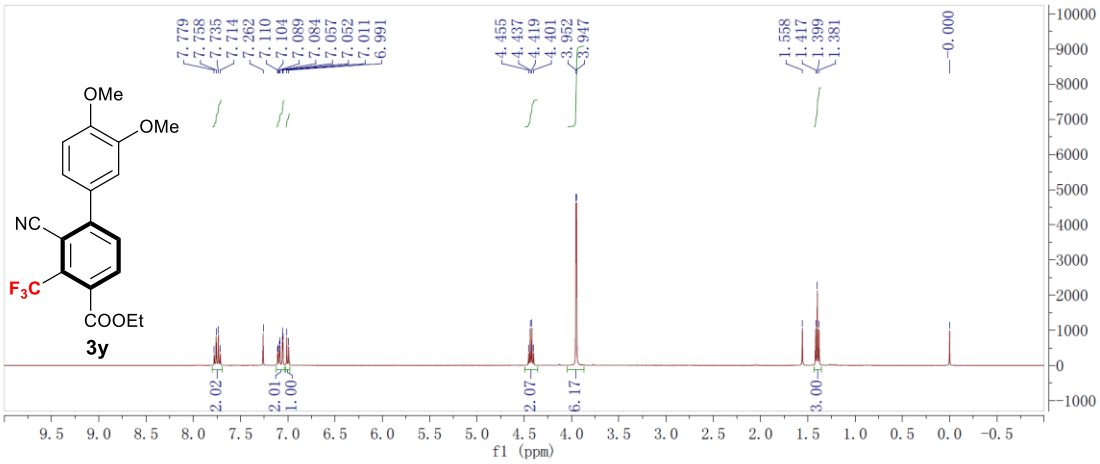
159.70
157.21
142.31
134.89
134.81
134.09
134.07
133.91
133.58
133.56
132.39
130.94
126.33
126.17
123.24
120.49
118.33
118.10
117.12
117.09
77.03
76.71
63.09
13.87
0.00
Br
F
NC
F3C
COOEt
3x
f1 (ppm)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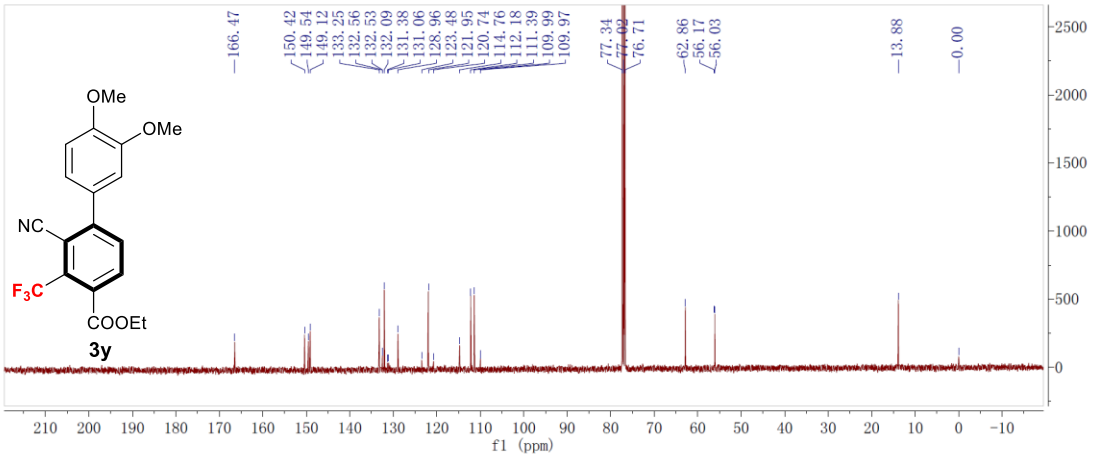
7.758
7.735
7.714
7.262
7.110
7.104
7.089
7.084
7.057
7.052
7.011
6.991
4.455
4.437
4.419
4.401
3.952
3.947
1.558
1.417
1.399
1.381
-0.000
OMe
OMe
NC
F3C
COOEt
3y
2.02
2.01
1.00
2.07
6.17
3.00
f1 (ppm)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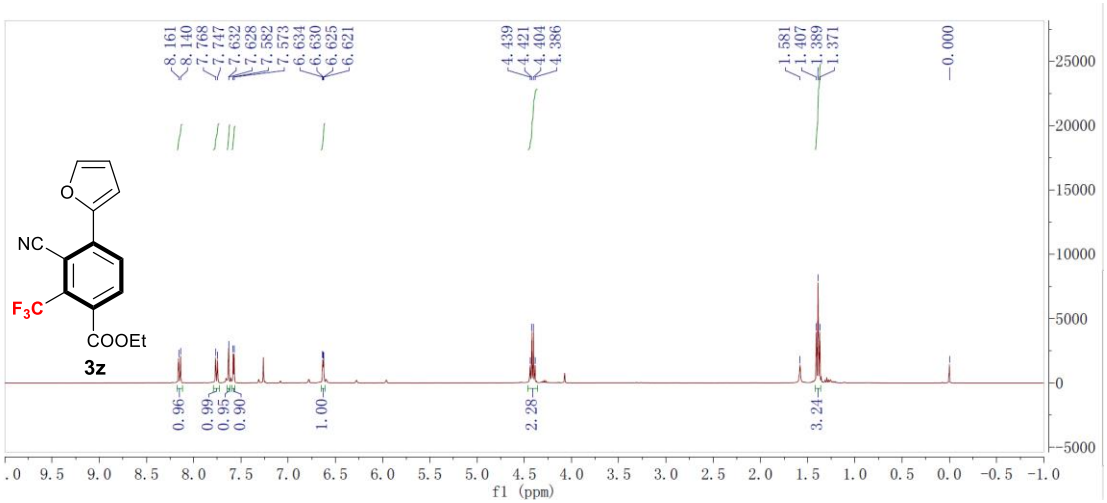
149.54
149.12
133.25
132.56
132.53
132.09
131.38
131.06
128.96
123.48
121.95
120.74
114.76
112.18
111.39
109.99
109.97
77.34
77.00
76.71
62.86
56.17
56.03
13.88
0.00
OMe
OMe
NC
F3C
COOEt
3y
f1 (ppm)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8.140
7.768
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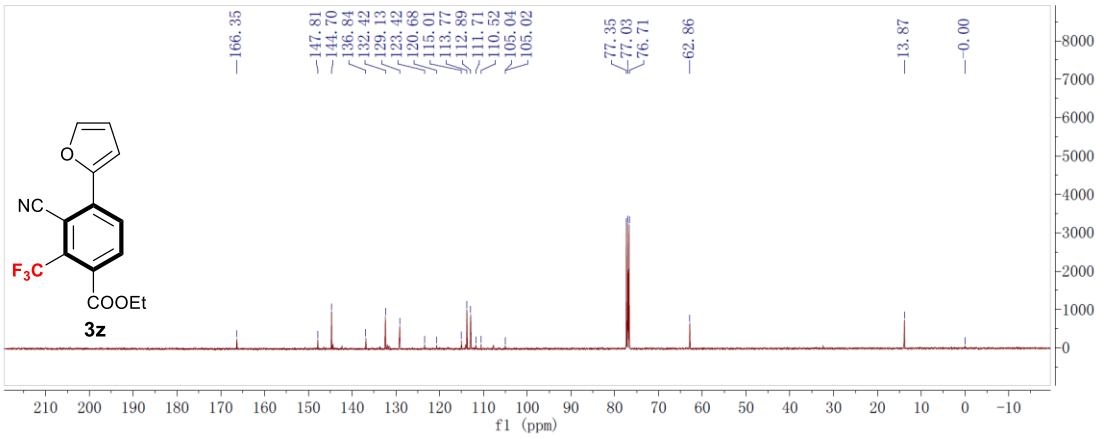
7.632
7.628
7.582
7.573
6.634
6.630
6.625
6.621
4.439
4.421
4.404
4.386
1.581
1.407
1.389
1.371
0.000
NC
F3C
COOEt
3z
0.96
0.99
0.95
0.90
1.00
2.28
3.24
f1 (ppm)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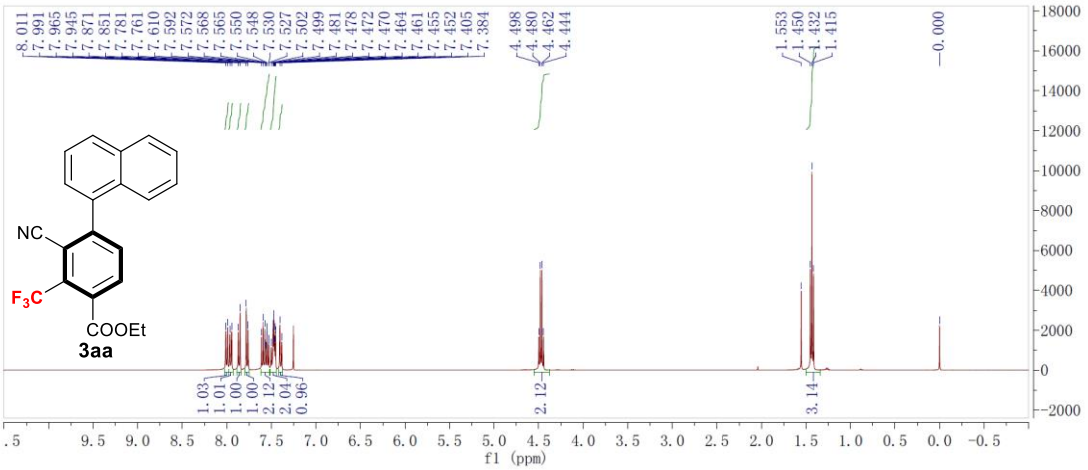
144.70
136.84
132.42
129.13
123.42
120.68
115.01
113.77
112.89
111.71
110.52
105.04
105.02
77.35
77.03
76.71
62.86
13.87
0.00
NC
F3C
COOEt
3z
f1 (ppm)


NC
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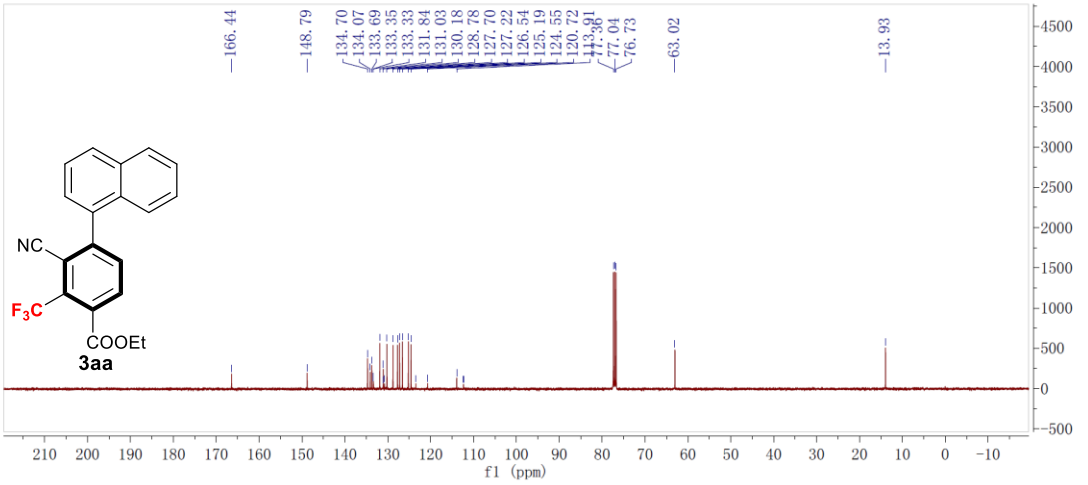
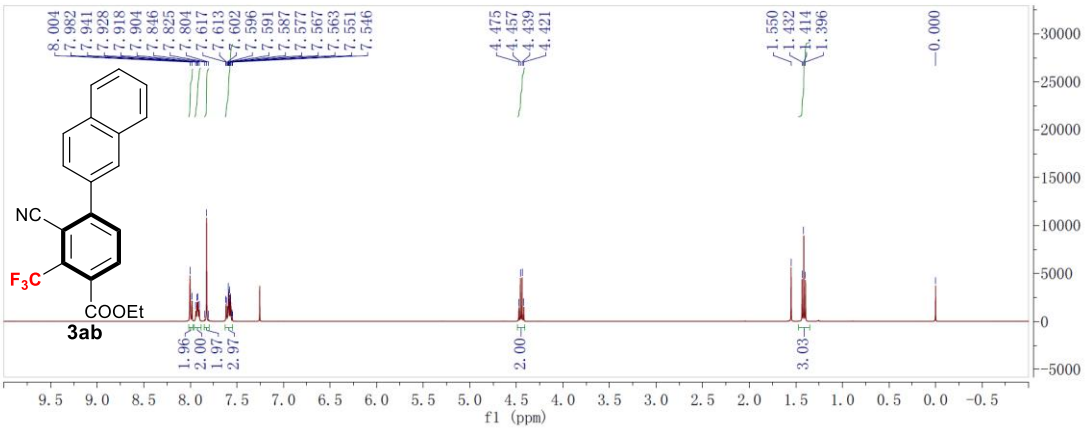
COOEt
3aa
f1 (ppm)


NC
F3C
COOEt
3aa
f1 (ppm)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7.928
7.918
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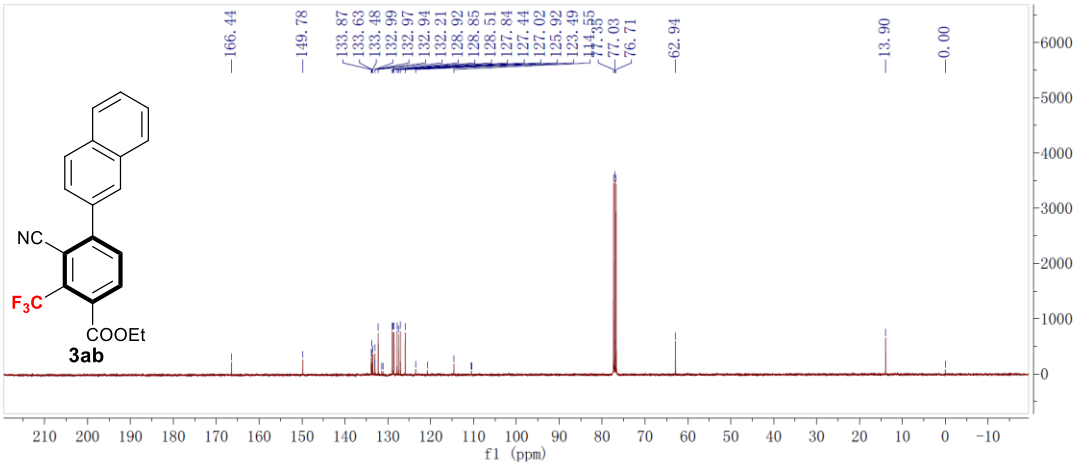
7.846
7.825
7.804
7.617
7.613
7.602
7.596
7.591
7.587
7.577
7.567
7.563
7.551
7.546
4.475
4.457
4.439
4.421
1.550
1.432
1.414
1.396
0.000
NC
F3C
COOEt
3ab
1.96
2.00
1.97
2.97
2.00
3.03
f1 (ppm)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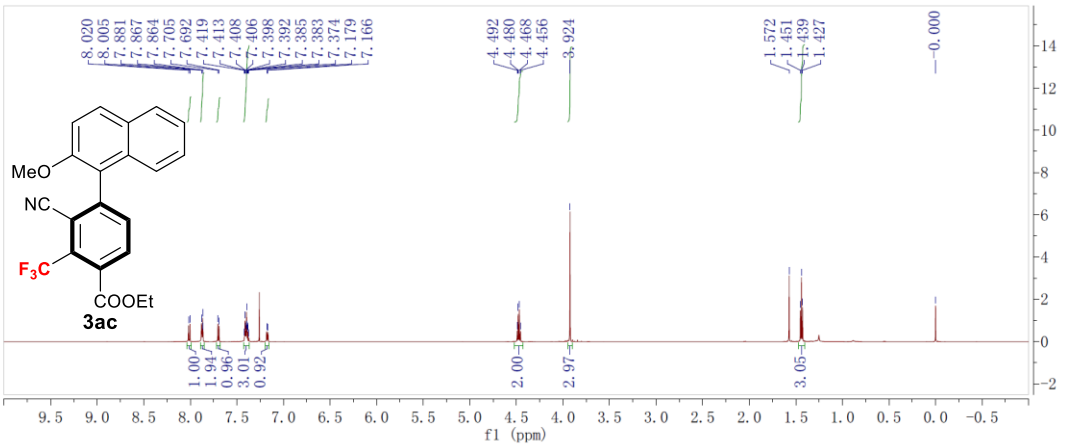
132.21
128.92
128.85
128.51
127.84
127.44
127.02
125.92
123.49
77.03
76.71
62.94
13.90
0.00
NC
F3C
COOEt
3ab
f1 (ppm)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7.419
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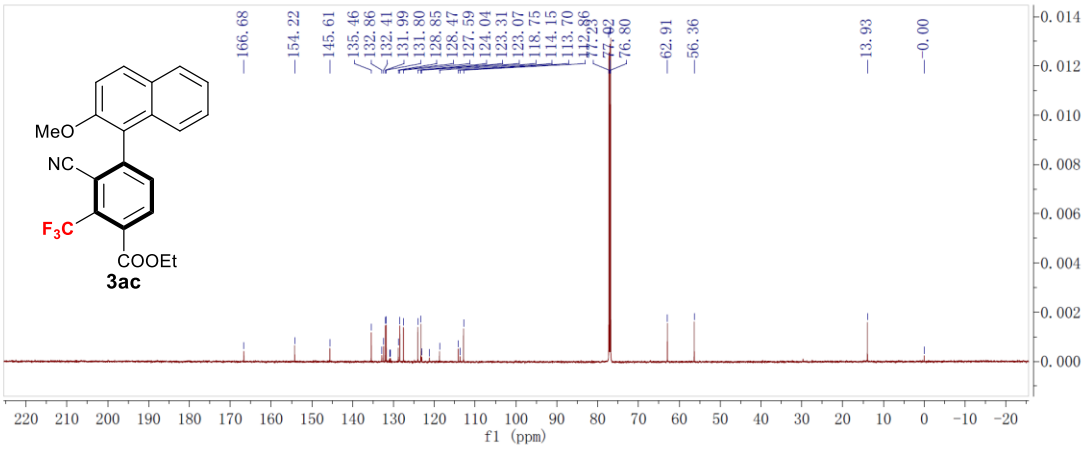
7.408
7.406
7.398
7.392
7.385
7.383
7.374
7.179
7.166
4.492
4.480
4.468
4.456
3.924
1.572
1.451
1.439
1.427
0.000
MeO
NC
F3C
COOEt
3ac
1.00
1.94
0.96
3.01
0.92
2.00
2.97
3.05
f1 (ppm)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132.41
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131.80
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128.47
127.59
124.04
123.31
123.07
118.75
114.15
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62.91
56.36
13.93
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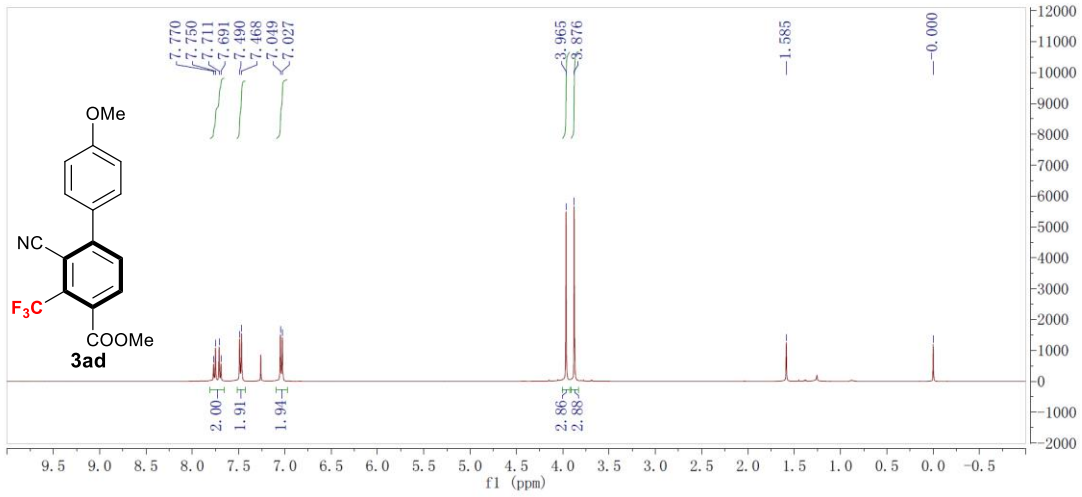
MeO
NC
F3C
COOEt
3ac
f1 (ppm)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7.490
7.468
7.049
7.027
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3.876
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0.000
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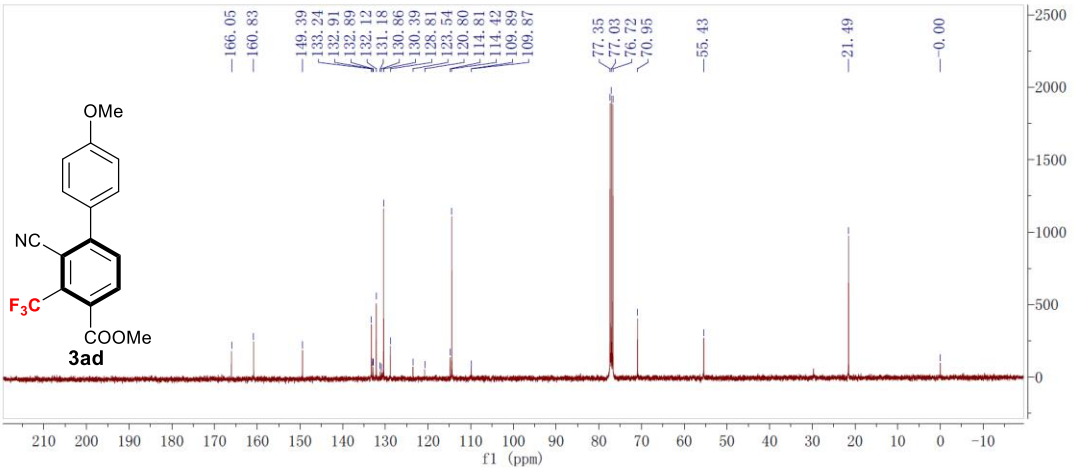
NC
F3C
COOMe
3ad
2.00
1.91
1.94
2.86
2.88
f1 (ppm)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132.89
132.12
131.18
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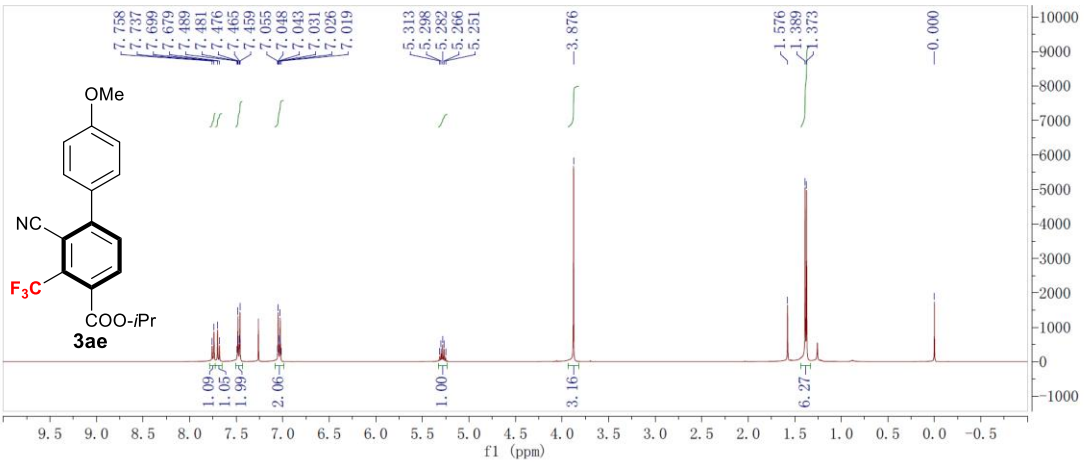
130.39
128.81
123.54
120.80
114.81
114.42
109.89
109.87
77.35
77.03
76.72
70.95
55.43
21.49
0.00
OMe
NC
F3C
COOMe
3ad
f1 (ppm)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7.465
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7.055
7.048
7.043
7.031
7.026
7.019
5.313
5.298
5.282
5.266
5.251
3.876
1.576
1.389
1.373
0.000
OMe
NC
F3C
COO-iPr
3ae
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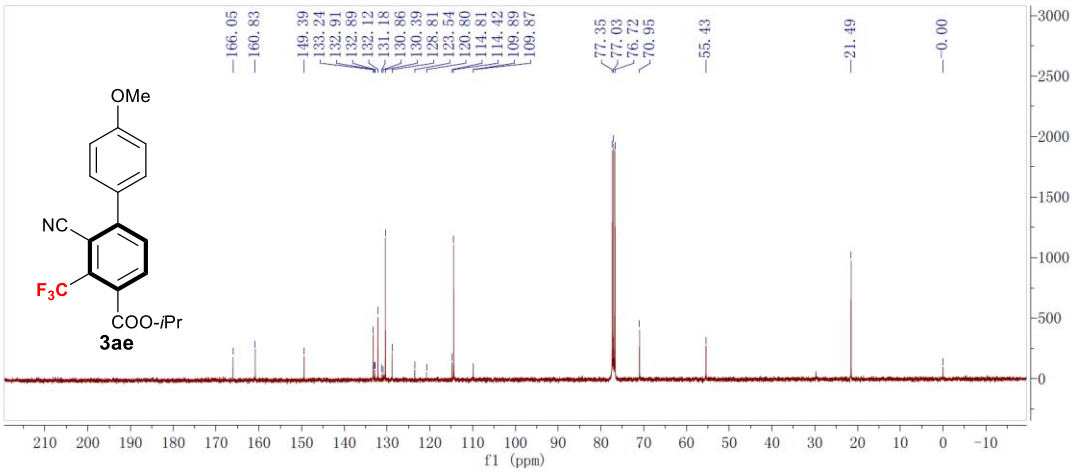
1.05
1.99
2.06
1.00
3.16
6.27
f1 (ppm)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133.24
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132.89
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131.18
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130.39
128.81
123.54
120.80
114.81
114.42
109.89
109.87
77.35
77.03
76.72
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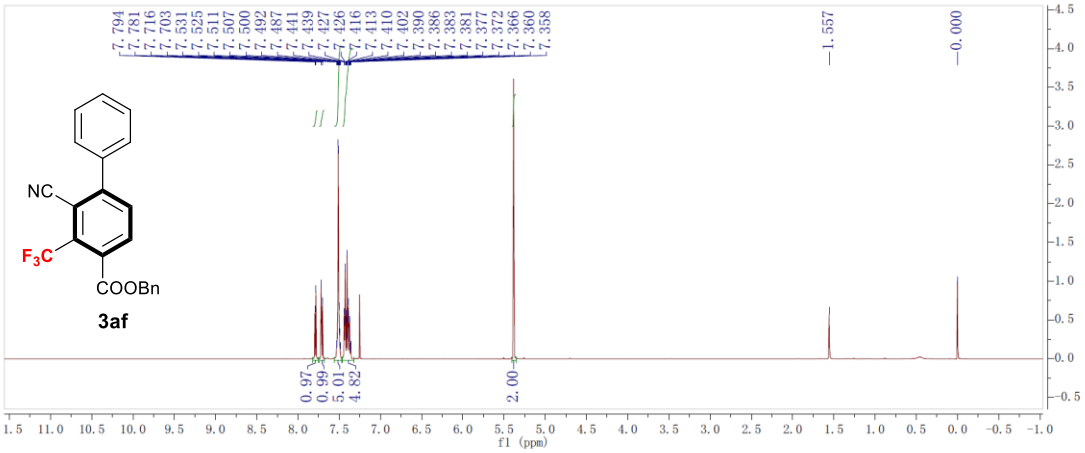
55.43
21.49
0.00
OMe
NC
F3C
COO-iPr
3ae
f1 (ppm)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7.507
7.500
7.492
7.487
7.441
7.439
7.427
7.426
7.416
7.413
7.410
7.402
7.390
7.386
7.383
7.381
7.377
7.372
7.366
7.360
7.358
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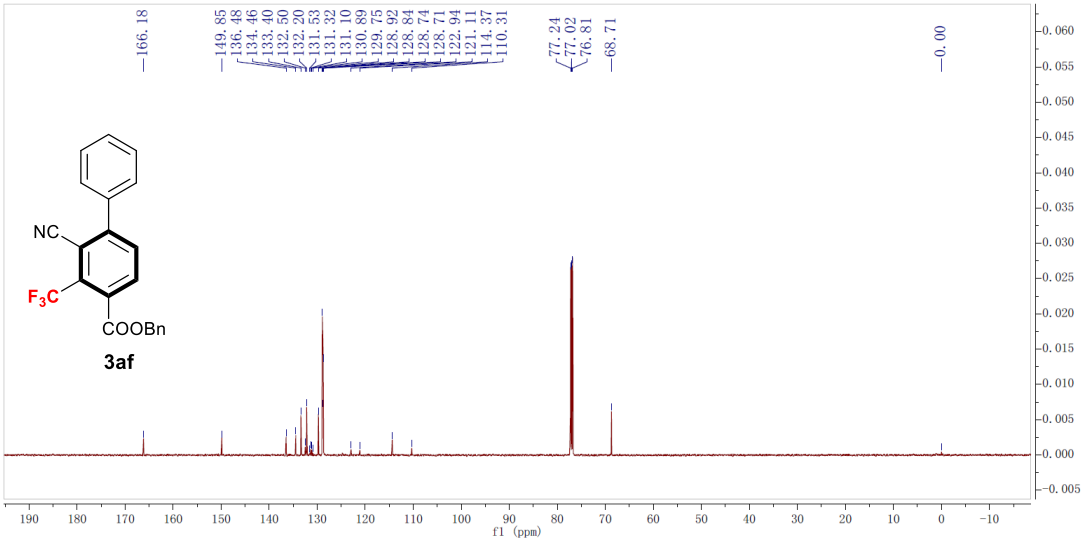
0.000
NC
F3C
COOBn
3af
0.97
0.99
5.01
4.82
2.00
f1 (ppm)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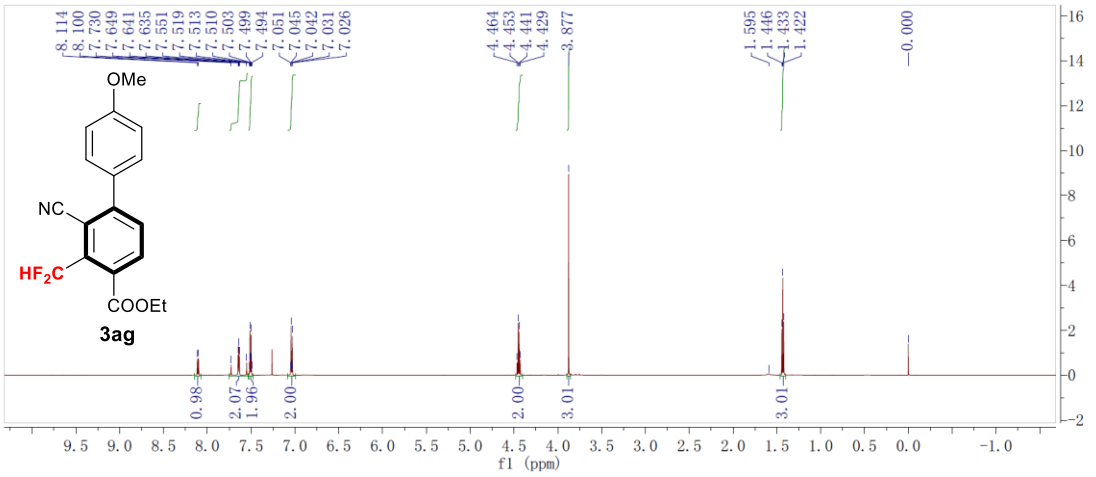
132.20
131.53
131.32
131.10
130.89
129.75
128.92
128.84
128.74
128.71
122.94
121.11
114.37
110.31
77.24
77.02
76.81
68.71
0.00
NC
F3C
COOBn
3af
f1 (ppm)


8.114
8.100
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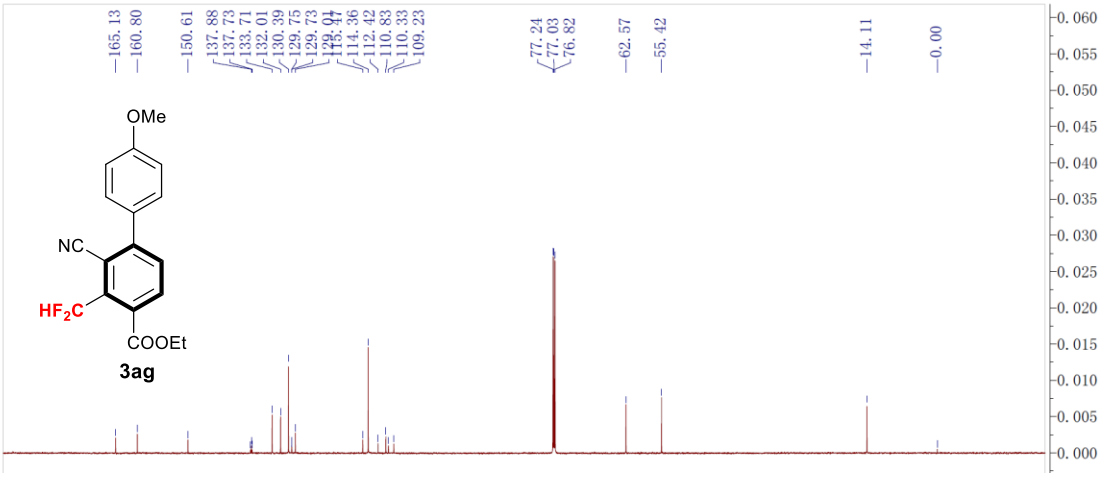
7.635
7.551
7.519
7.513
7.510
7.503
7.499
7.494
7.051
7.045
7.042
7.031
7.026
4.464
4.453
4.441
4.429
3.877
1.595
1.446
1.433
1.422
0.000
OMe
NC
HF2C
COOEt
3ag
0.98
2.07
1.96
2.00
2.00
3.01
3.01
f1 (ppm)


165.13
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150.61
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137.73
133.71
132.01
130.39
129.75
129.73
114.36
112.42
110.83
110.33
109.23
77.24
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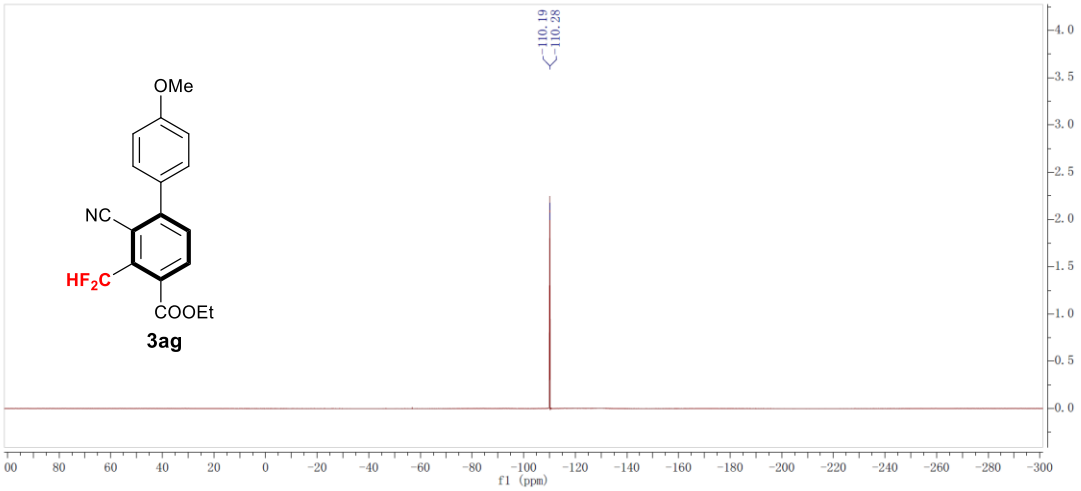
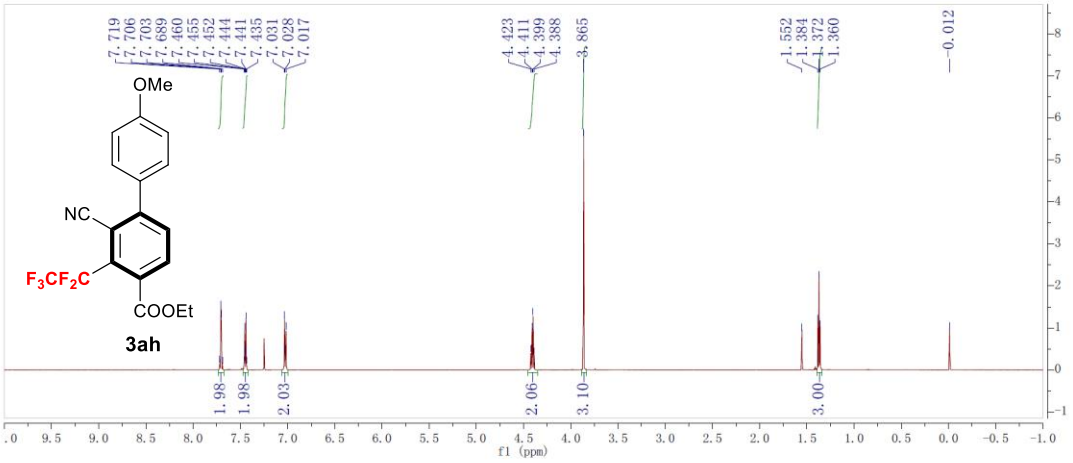
76.82
62.57
55.42
14.11
0.00
OMe
NC
HF2C
COOEt
3ag


110.19
110.28
OMe
NC
HF2C
COOEt
3ag
f1 (ppm)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7.017
4.423
4.411
4.399
4.388
3.865
1.552
1.384
1.372
1.360
0.012
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NC
F3CF2C
COOEt
3ah
1.98
1.98
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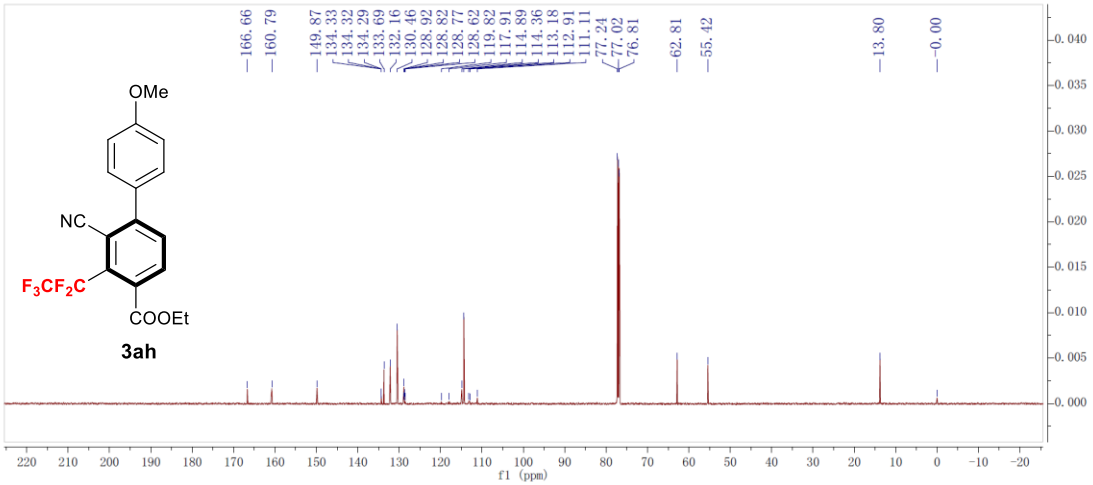
2.06
3.10
3.00
f1 (ppm)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128.77
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119.82
117.91
114.89
114.36
113.18
112.91
111.11
77.24
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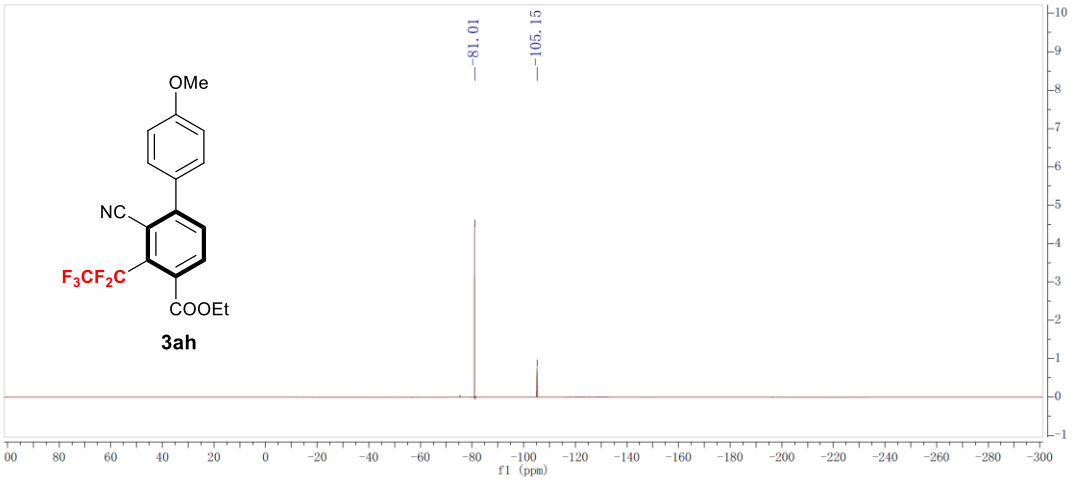
NC
F3CF2C
COOEt
3ah
f1 (ppm)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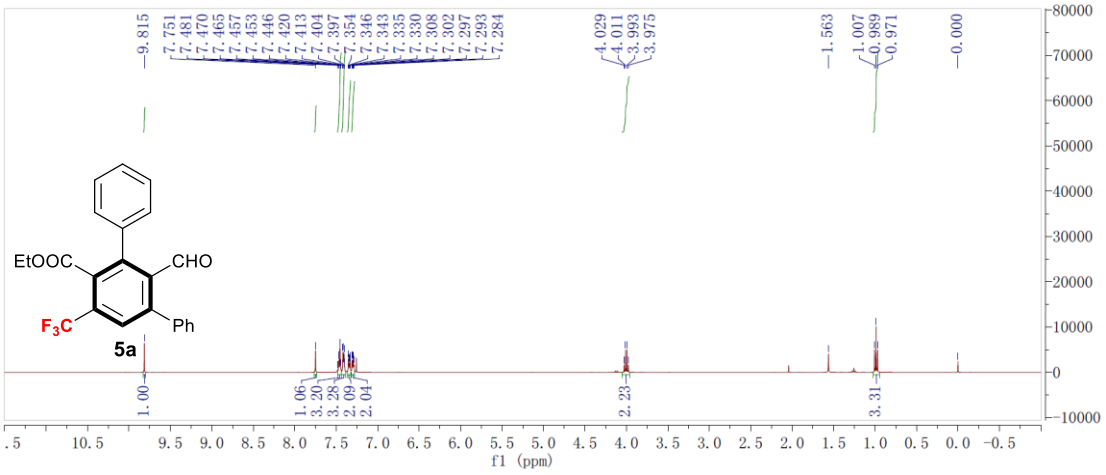
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7.404
7.397
7.354
7.346
7.343
7.335
7.330
7.308
7.302
7.297
7.293
7.284
4.029
4.011
3.993
3.975
1.563
1.007
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0.971
0.000
EtOOC
CHO
F3C
Ph
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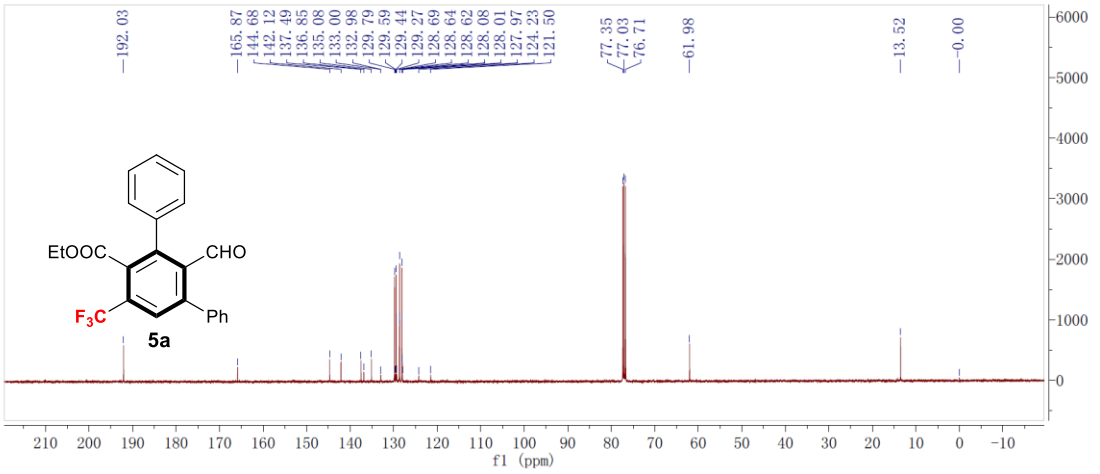
1.06
3.20
3.28
2.09
2.04
2.23
3.31
f1 (ppm)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128.64
128.62
128.08
128.01
127.97
124.23
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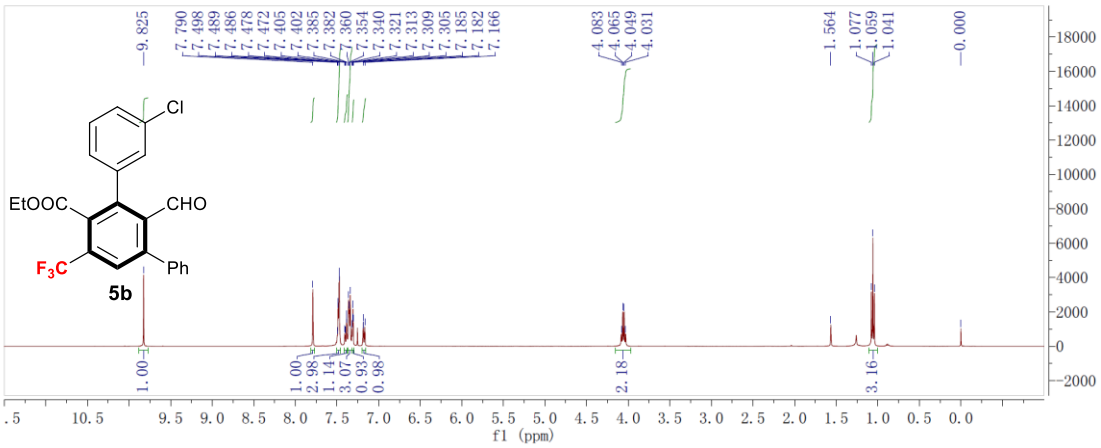
76.71
61.98
13.52
0.00
EtOOC
CHO
F3C
Ph
5a
f1 (ppm)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7.354
7.340
7.321
7.313
7.309
7.305
7.185
7.182
7.166
4.083
4.065
4.049
4.031
1.564
1.077
1.059
1.041
0.000
Cl
EtOOC
CHO
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Ph
5b
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2.98
1.14
3.07
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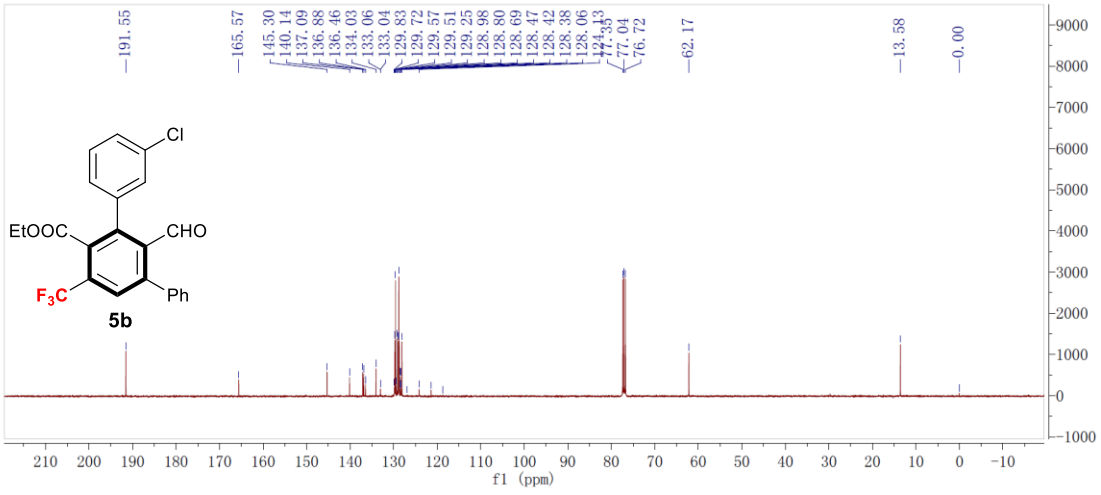
0.98
2.18
3.16
f1 (ppm)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129.57
129.51
129.25
128.98
128.80
128.69
128.47
128.42
128.38
128.06
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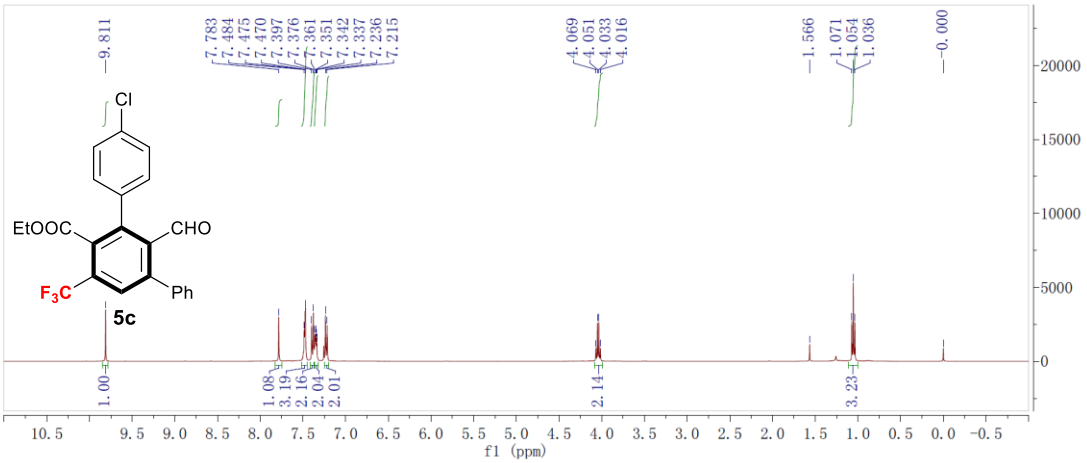
76.72
62.17
13.58
0.00
Cl
EtOOC
CHO
F3C
Ph
5b
f1 (ppm)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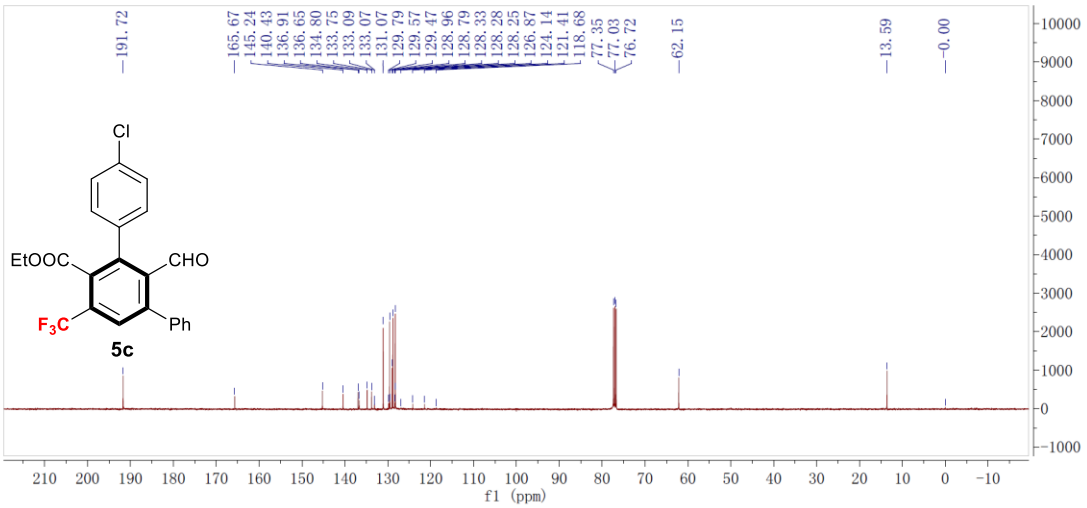
7.342
7.337
7.236
7.215
4.069
4.051
4.033
4.016
1.566
1.071
1.054
1.036
0.000
Cl
EtOOC
CHO
F3C
Ph
5c
1.00
1.08
3.19
2.16
2.04
2.01
2.14
3.23
f1 (ppm)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133.75
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133.07
131.07
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129.57
129.47
128.96
128.79
128.33
128.28
128.25
126.87
124.14
121.41
118.68
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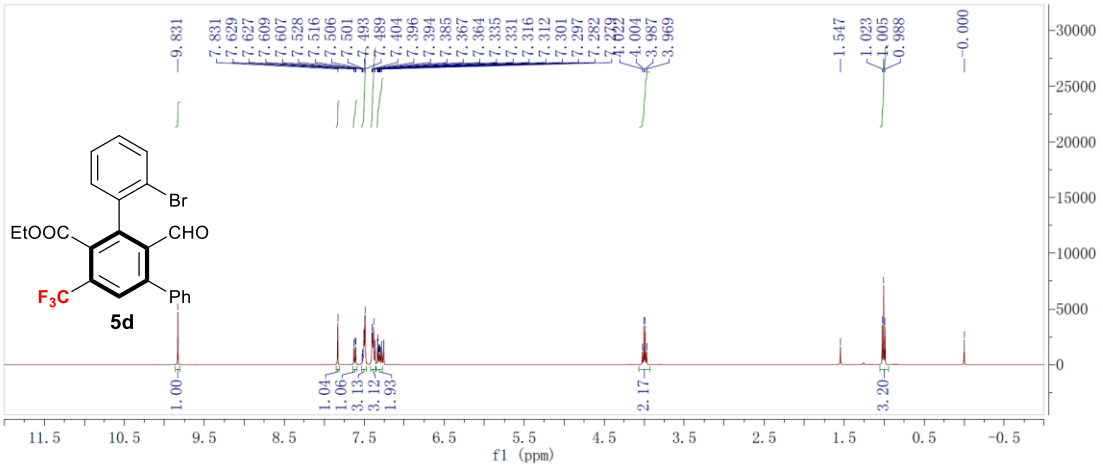
76.72
62.15
13.59
0.00
Cl
EtOOC
CHO
F3C
Ph
5c
f1 (ppm)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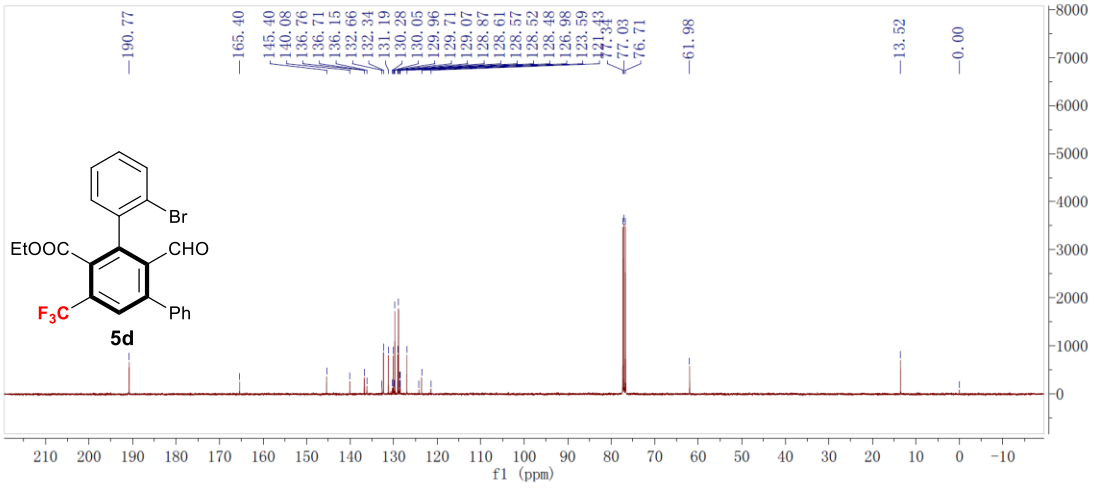
7.516
7.506
7.501
7.493
7.489
7.404
7.396
7.394
7.385
7.367
7.364
7.335
7.331
7.316
7.312
7.301
7.297
7.282
4.004
3.987
3.969
1.547
1.023
1.005
0.988
0.000
Br
EtOOC
CHO
F3C
Ph
5d
1.00
1.04
1.06
3.13
3.12
1.93
2.17
3.20
f1 (ppm)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130.28
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128.87
128.61
128.57
128.52
128.48
126.98
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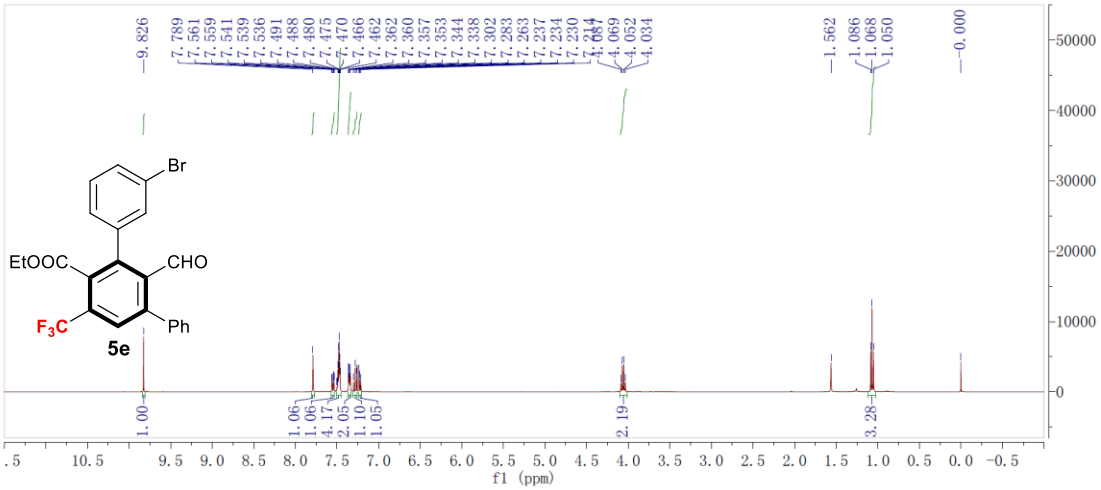
76.71
61.98
13.52
0.00
Br
EtOOC
CHO
F3C
Ph
5d
f1 (ppm)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7.462
7.362
7.360
7.357
7.353
7.344
7.338
7.302
7.283
7.263
7.237
7.234
7.230
4.069
4.052
4.034
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1.086
1.068
1.050
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Br
EtOOC
CHO
F3C
Ph
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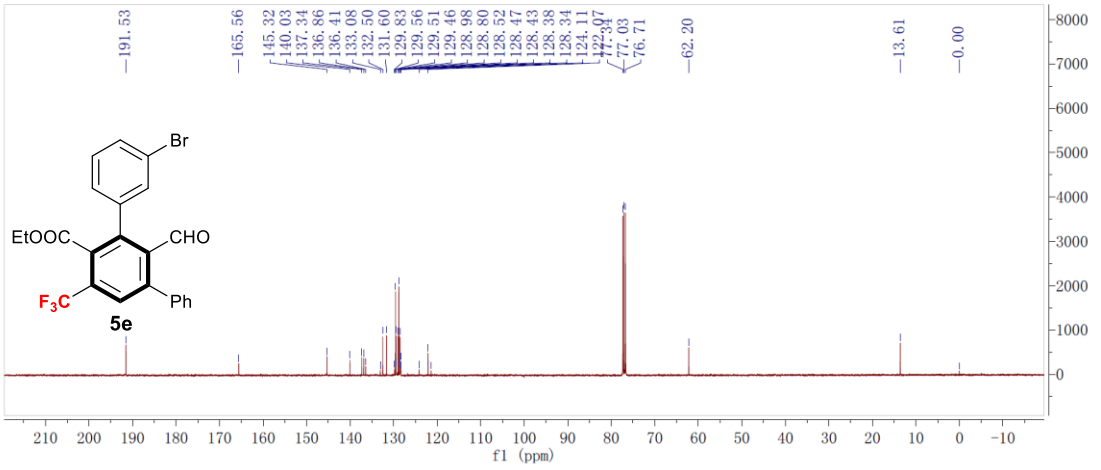
1.06
1.06
4.17
2.05
1.10
1.05
2.19
3.28
f1 (ppm)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128.98
128.80
128.52
128.47
128.43
128.38
128.34
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62.20
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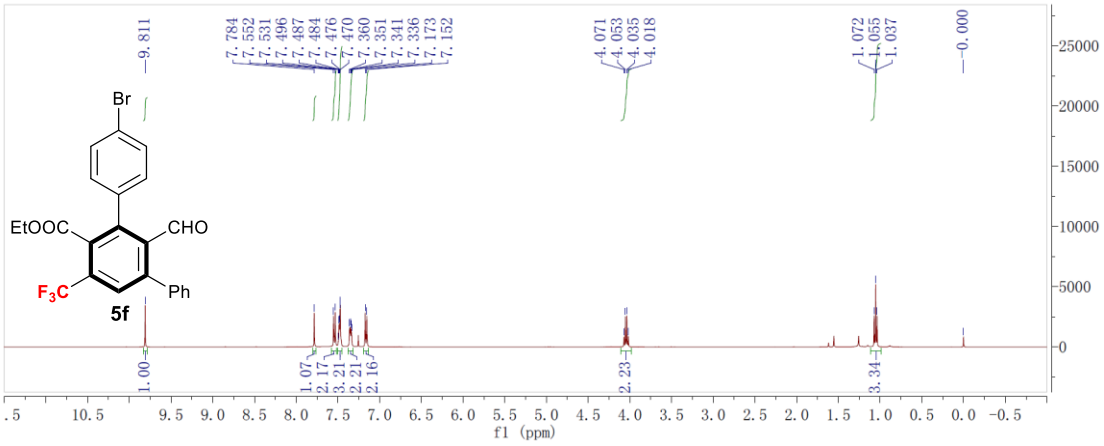
Br
EtOOC
CHO
F3C
Ph
5e
f1 (ppm)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4.071
4.053
4.035
4.018
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1.055
1.037
0.000
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EtOOC
CHO
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Ph
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1.07
2.17
3.21
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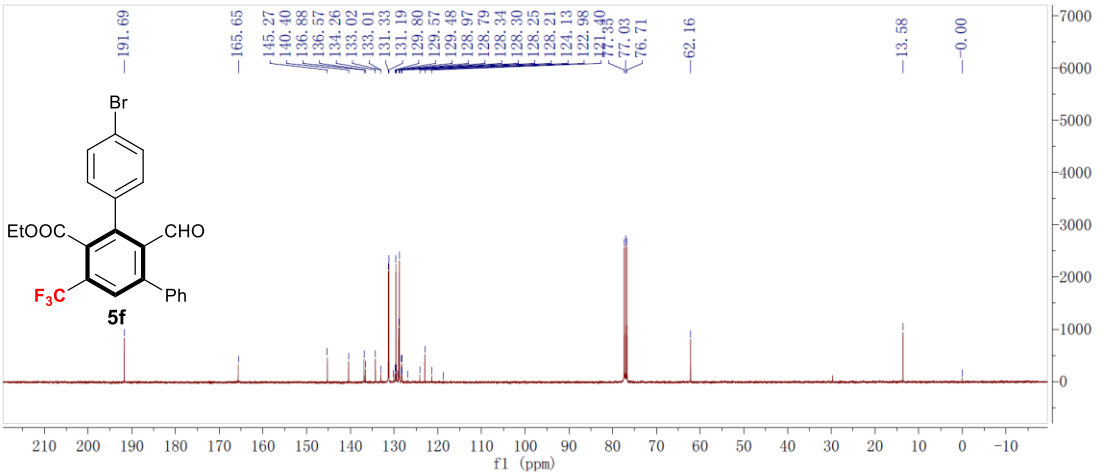
2.16
2.23
3.34
f1 (ppm)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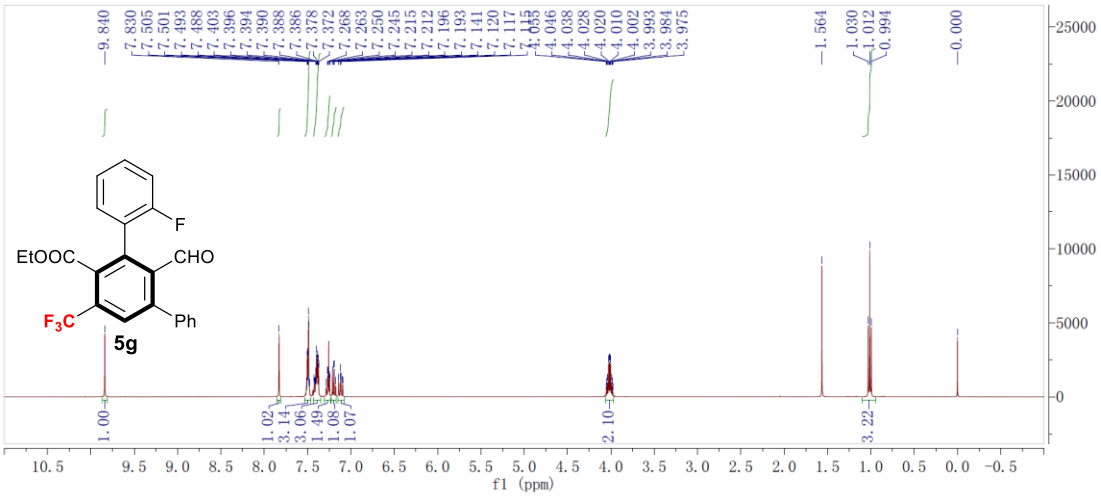
129.80
129.57
129.48
128.97
128.79
128.34
128.30
128.25
128.21
124.13
122.98
77.03
76.71
62.16
13.58
0.00
Br
EtOOC
CHO
F3C
Ph
5f
f1 (ppm)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7.372
7.268
7.263
7.250
7.245
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7.212
7.196
7.193
7.141
7.120
7.117
4.046
4.038
4.028
4.020
4.010
4.002
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3.984
3.975
1.564
1.030
1.012
0.994
0.000
F
EtOOC
CHO
F3C
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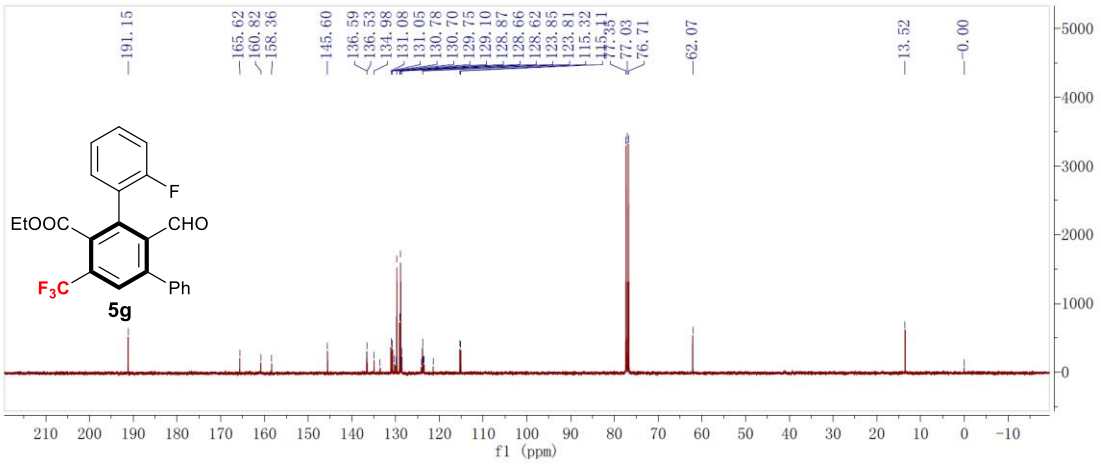
3.22
f1 (ppm)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128.87
128.66
128.62
123.85
123.81
115.32
115.11
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62.07
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-0.00
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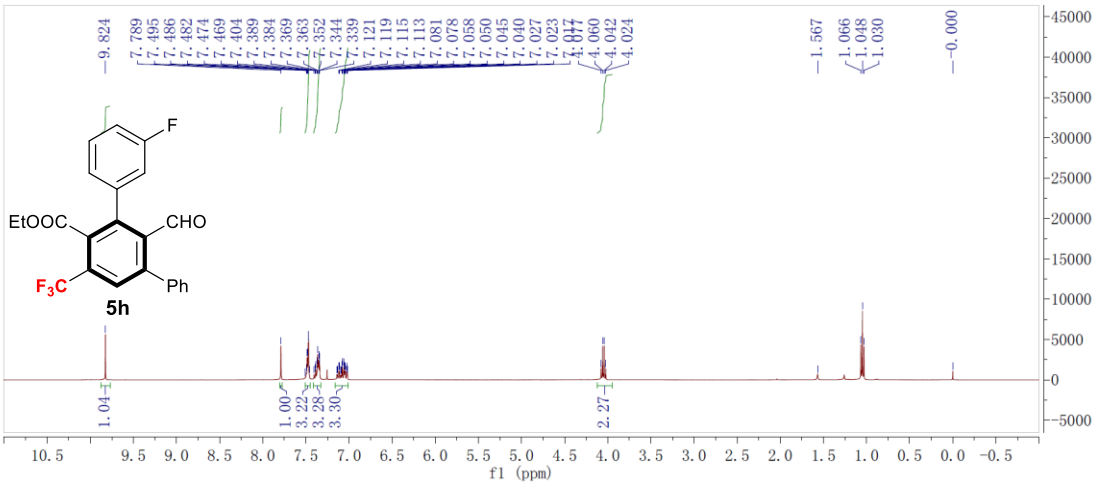
EtOOC
CHO
F3C
Ph
5g
f1 (ppm)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7.115
7.113
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7.078
7.058
7.050
7.045
7.040
7.027
7.023
4.060
4.042
4.024
1.567
1.066
1.048
1.030
0.000
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CHO
F3C
Ph
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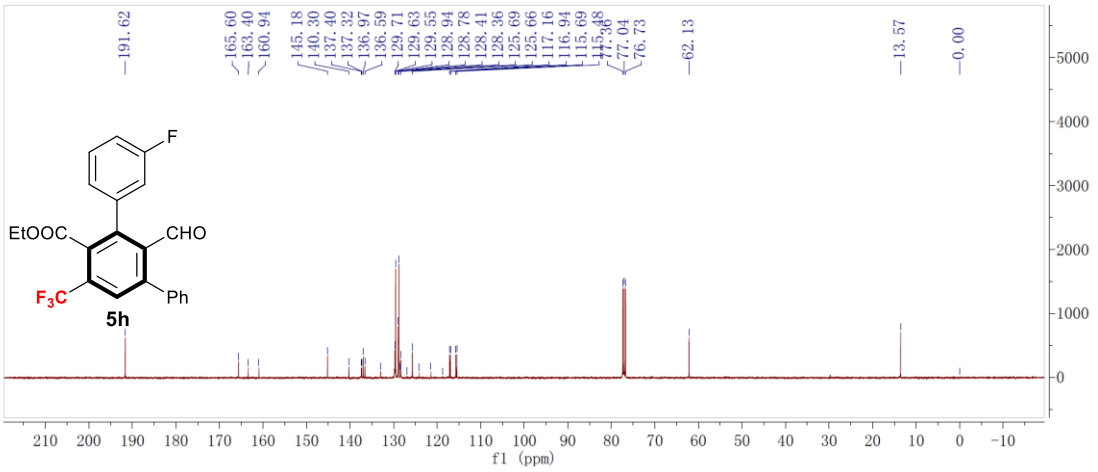
f1 (ppm)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129.71
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129.55
128.94
128.78
128.41
128.36
125.69
125.66
117.16
116.94
115.69
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76.73
62.13
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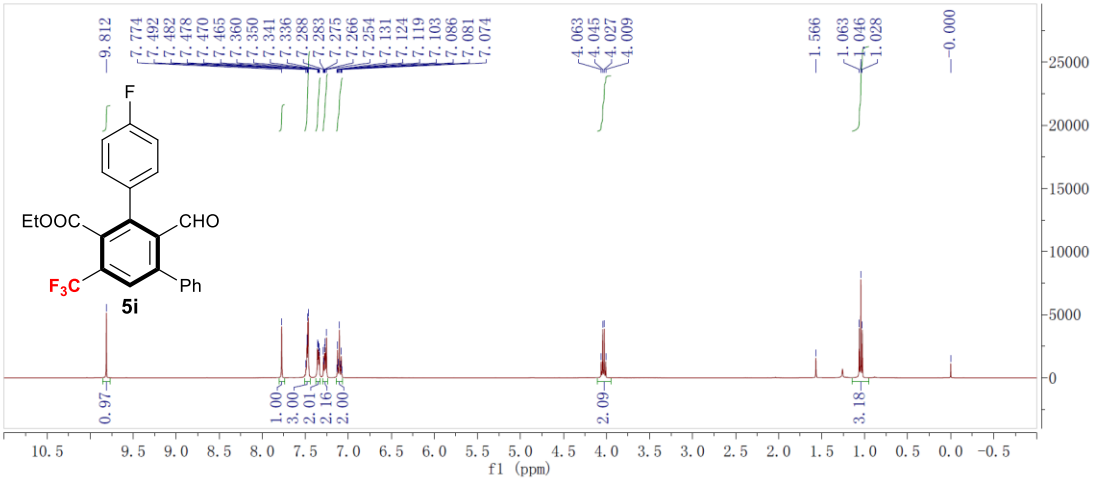
CHO
F3C
Ph
5h
f1 (ppm)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7.086
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7.074
4.063
4.045
4.027
4.009
1.566
1.063
1.046
1.028
0.000
F
EtOOC
CHO
F3C
Ph
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3.00
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2.00
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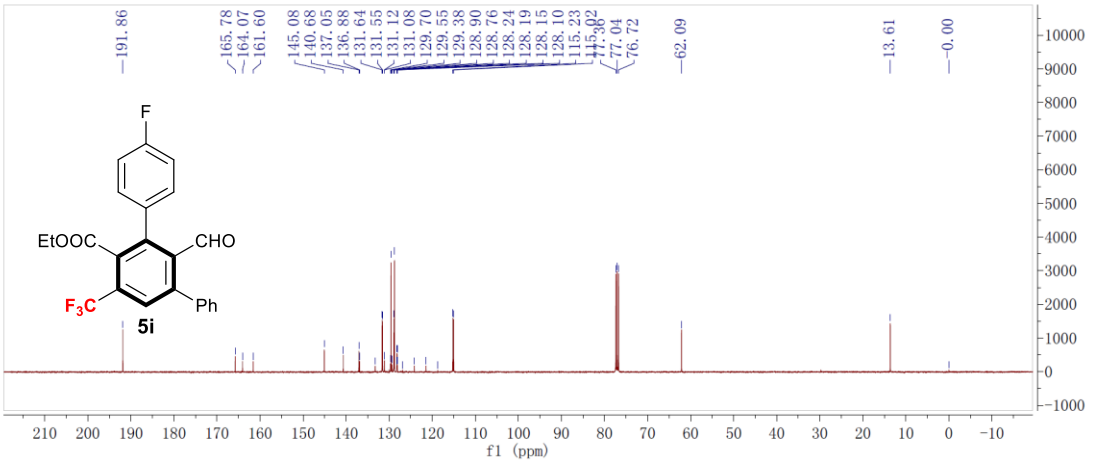
f1 (ppm)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129.38
128.90
128.76
128.24
128.19
128.15
128.10
115.23
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76.72
62.09
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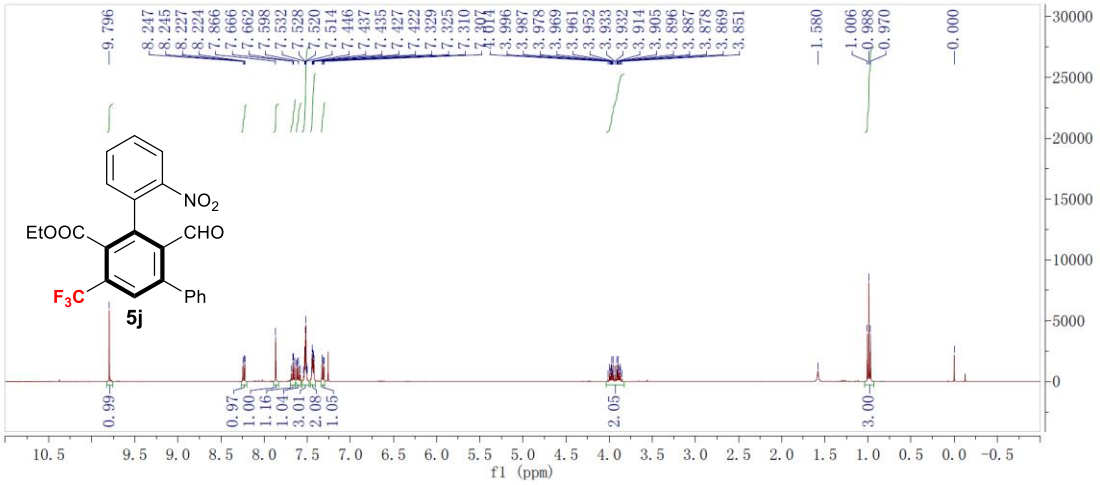
F
EtOOC
CHO
F3C
Ph
5i
f1 (ppm)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3.987
3.978
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3.933
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3.914
3.905
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0.970
0.000
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EtOOC
CHO
F3C
Ph
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1.05
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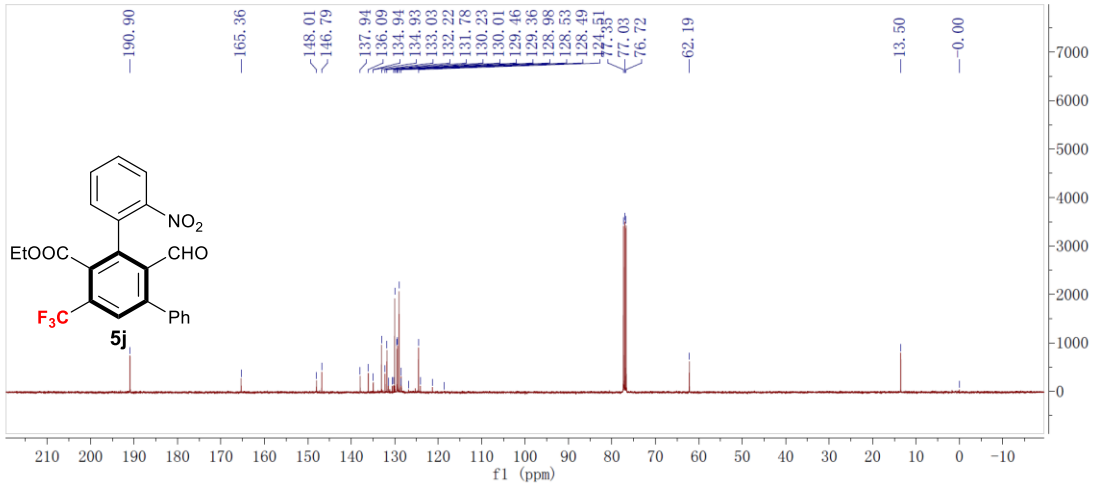
3.00
f1 (ppm)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130.01
129.46
129.36
128.98
128.53
128.49
124.51
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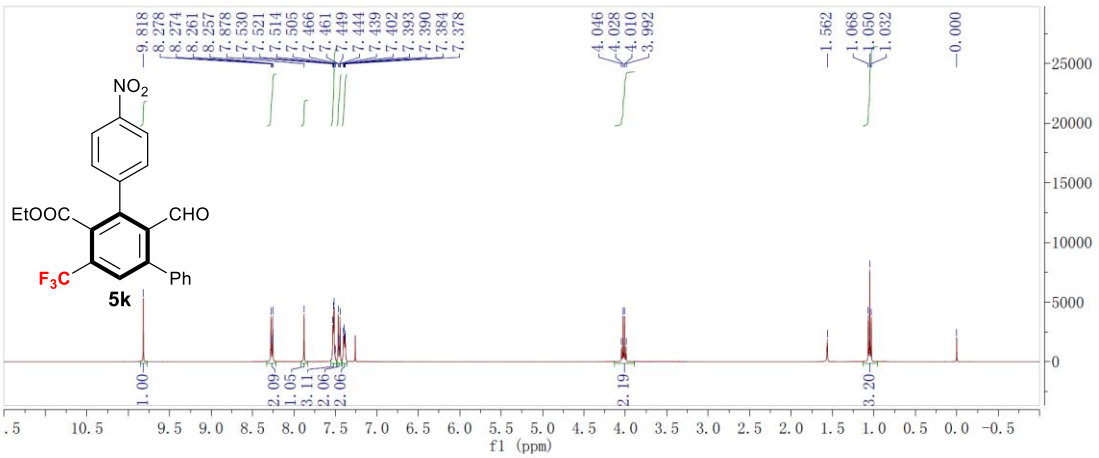
77.03
76.72
62.19
13.50
0.00
NO2
EtOOC
CHO
F3C
Ph
5j
f1 (ppm)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7.439
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7.393
7.390
7.384
7.378
4.046
4.028
4.010
3.992
1.562
1.068
1.050
1.032
0.000
NO2
EtOOC
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F3C
Ph
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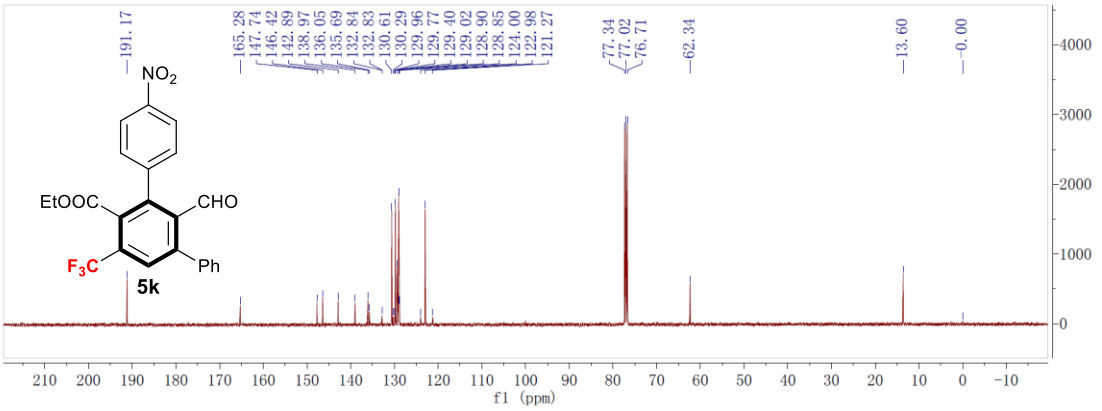
1.05
3.11
2.06
2.06
2.19
3.20
f1 (ppm)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129.40
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128.90
128.85
124.00
122.98
121.27
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0.00
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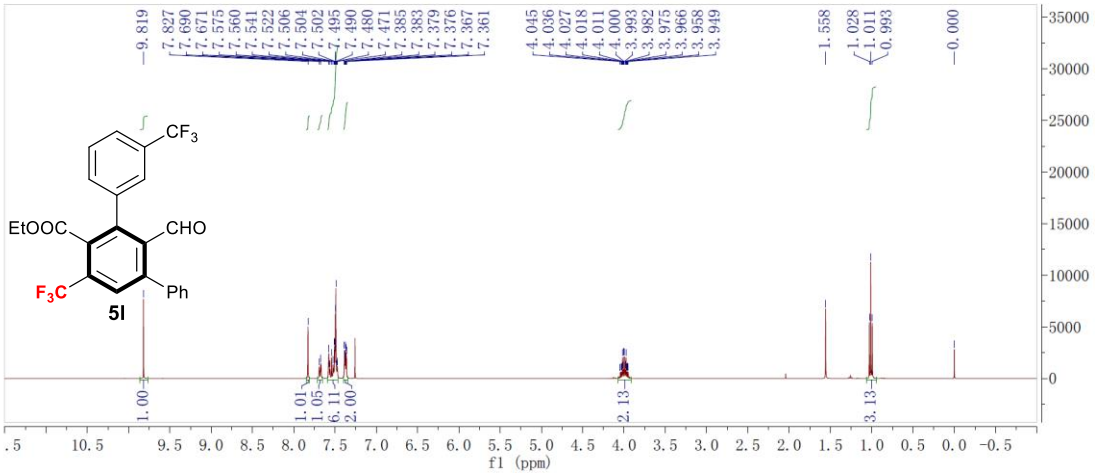
CHO
F3C
Ph
5k
f1 (ppm)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7.504
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4.027
4.018
4.011
4.000
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3.975
3.966
3.958
3.949
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CF3
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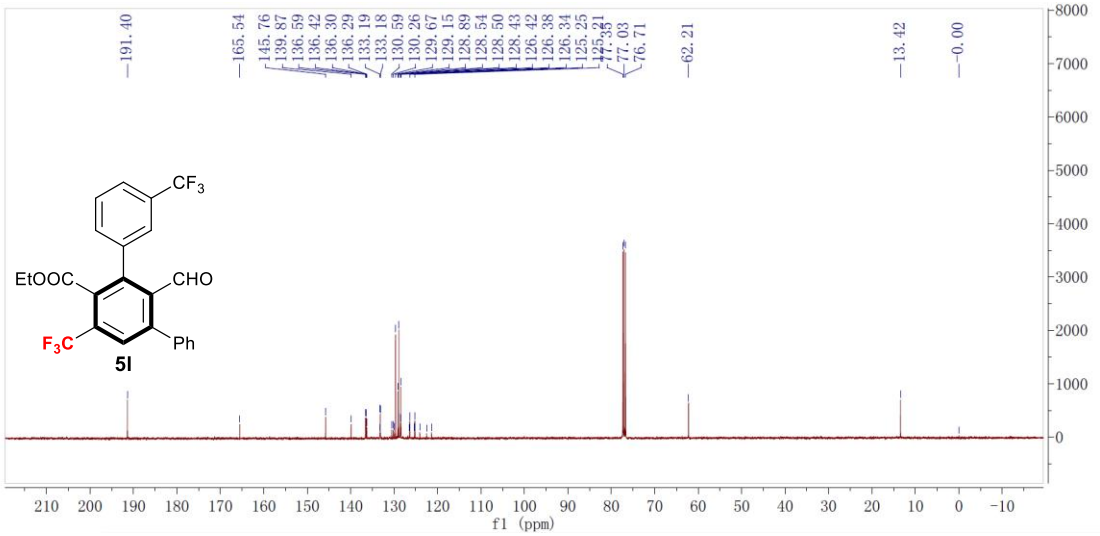
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128.54
128.50
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126.34
125.25
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CHO
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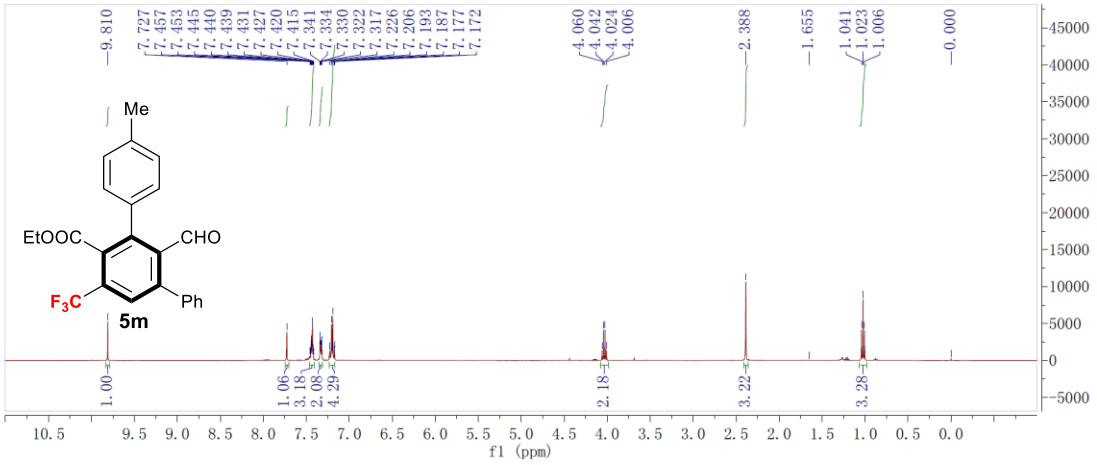
Ph
5l
f1 (ppm)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7.172
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4.024
4.006
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1.655
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0.000
Me
EtOOC
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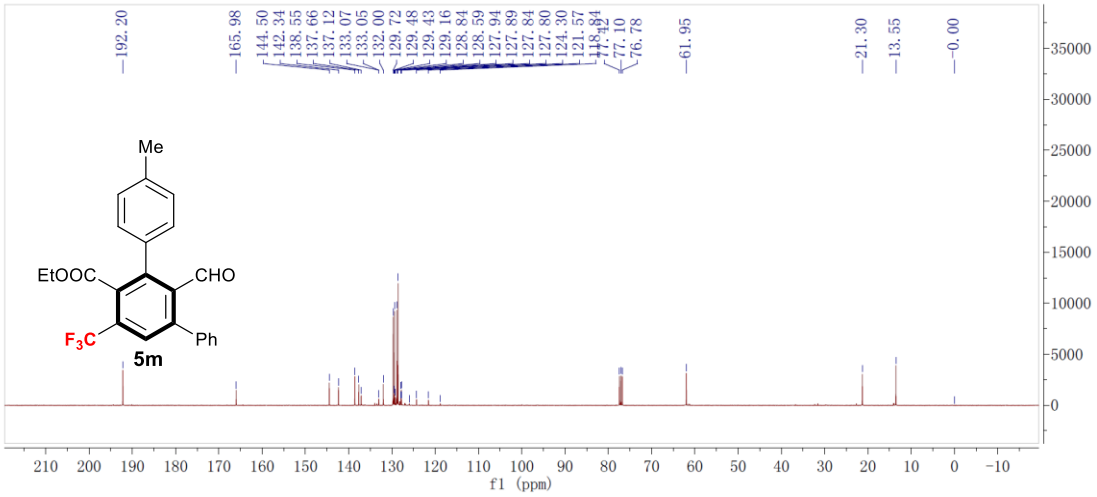
f1 (ppm)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128.84
128.59
127.94
127.89
127.84
127.80
124.30
121.57
77.42
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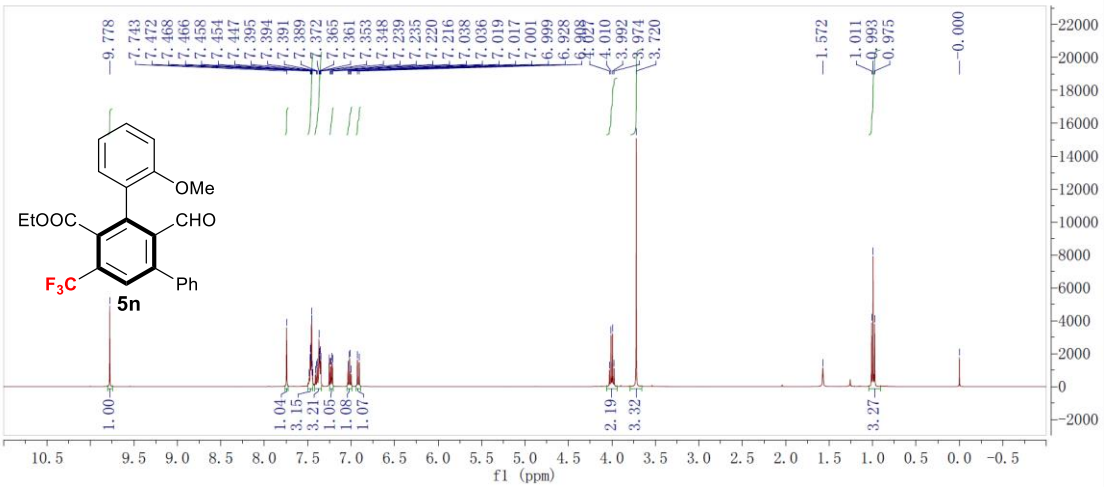
Me
EtOOC
CHO
F3C
Ph
5m
f1 (ppm)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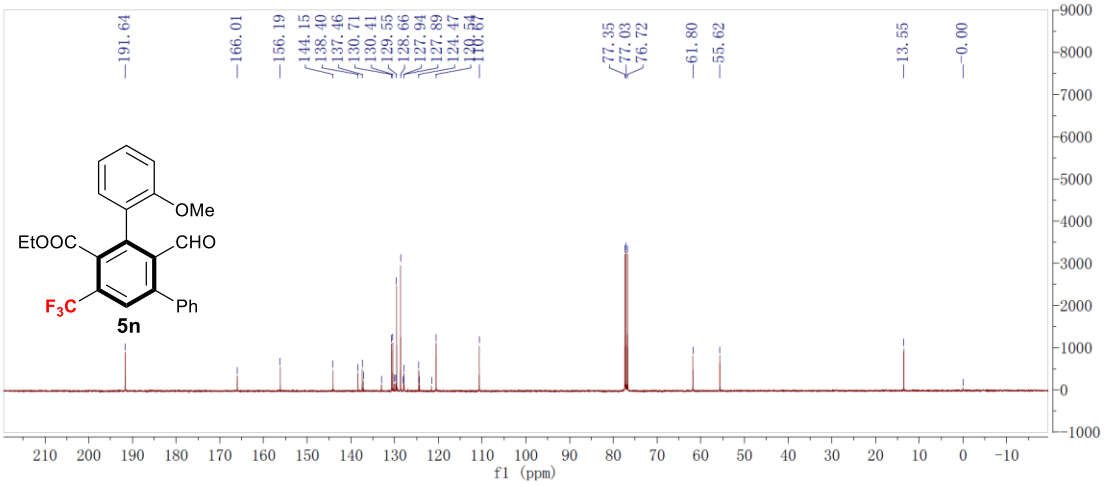
5n
f1 (ppm)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Ph
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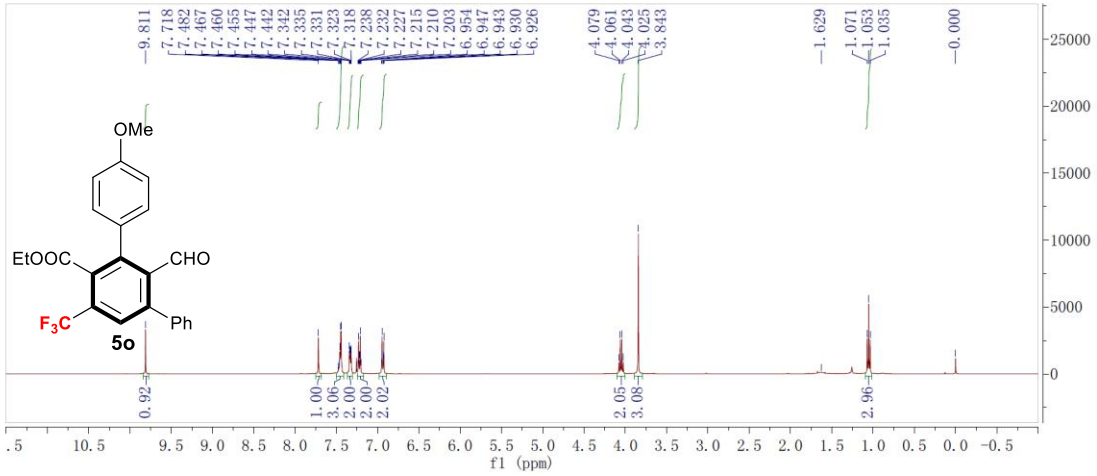
f1 (ppm)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4.025
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1.071
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1.035
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EtOOC
CHO
F3C
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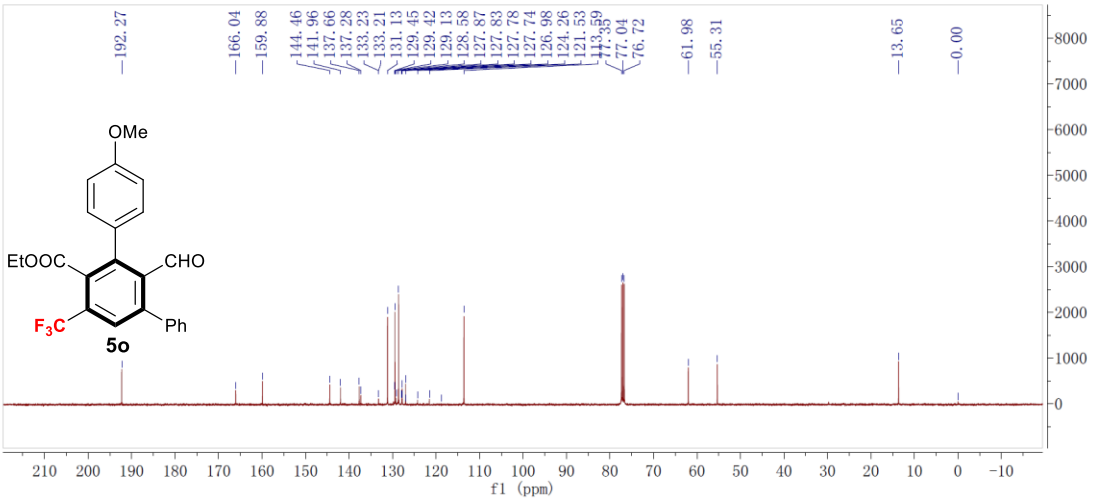
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127.87
127.83
127.78
127.74
126.98
124.26
121.53
77.35
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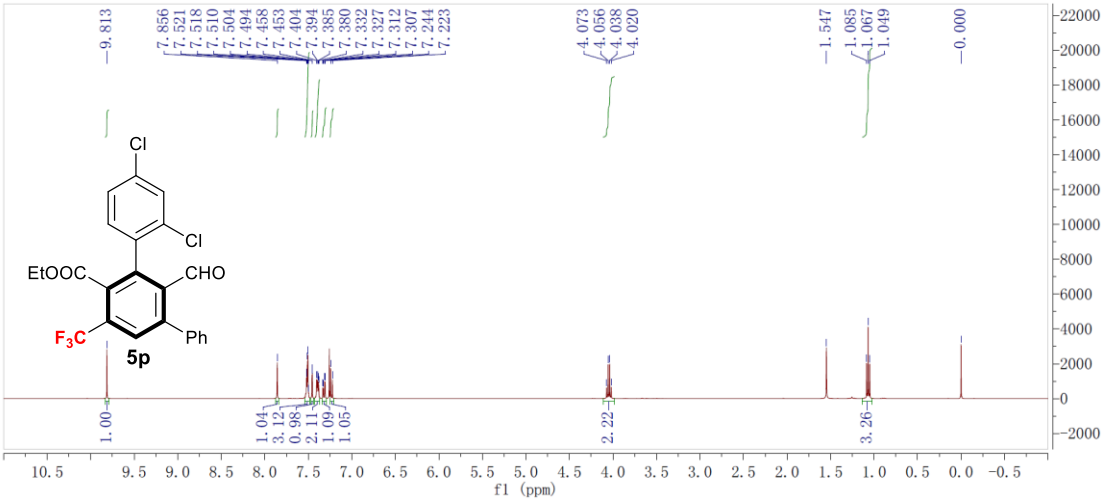
0.00
OMe
EtOOC
CHO
F3C
Ph
5o
f1 (ppm)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7.385
7.380
7.332
7.327
7.312
7.307
7.244
7.223
4.073
4.056
4.038
4.020
1.547
1.085
1.067
1.049
0.000
Cl
Cl
EtOOC
CHO
F3C
Ph
5p
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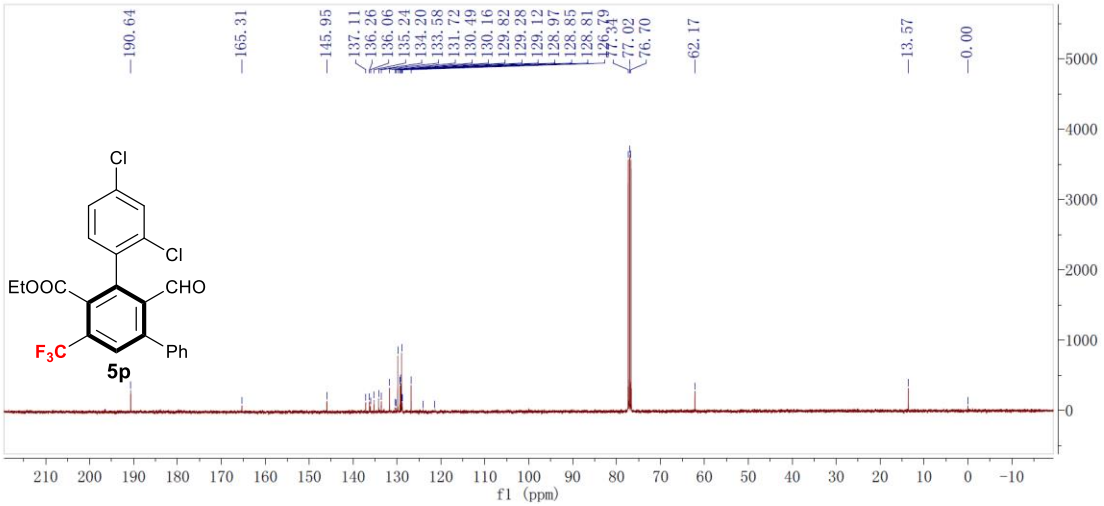
1.04
3.12
0.98
2.11
1.09
1.05
2.22
3.26
f1 (ppm)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129.12
128.97
128.85
128.81
126.79
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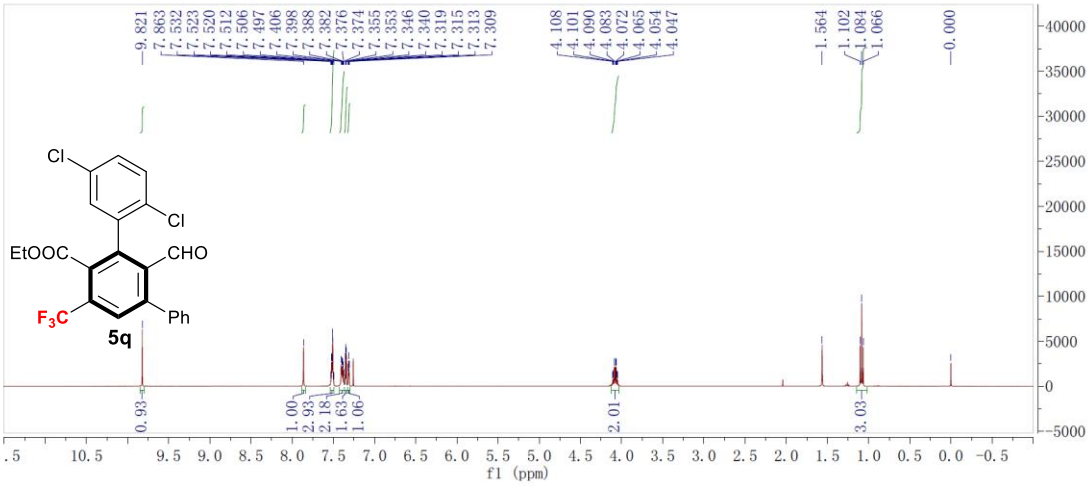
Cl
Cl
EtOOC
CHO
F3C
Ph
5p
f1 (ppm)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7.376
7.374
7.355
7.353
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7.340
7.319
7.315
7.313
7.309
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4.101
4.090
4.083
4.072
4.065
4.054
4.047
1.564
1.102
1.084
1.066
0.000
Cl
Cl
EtOOC
CHO
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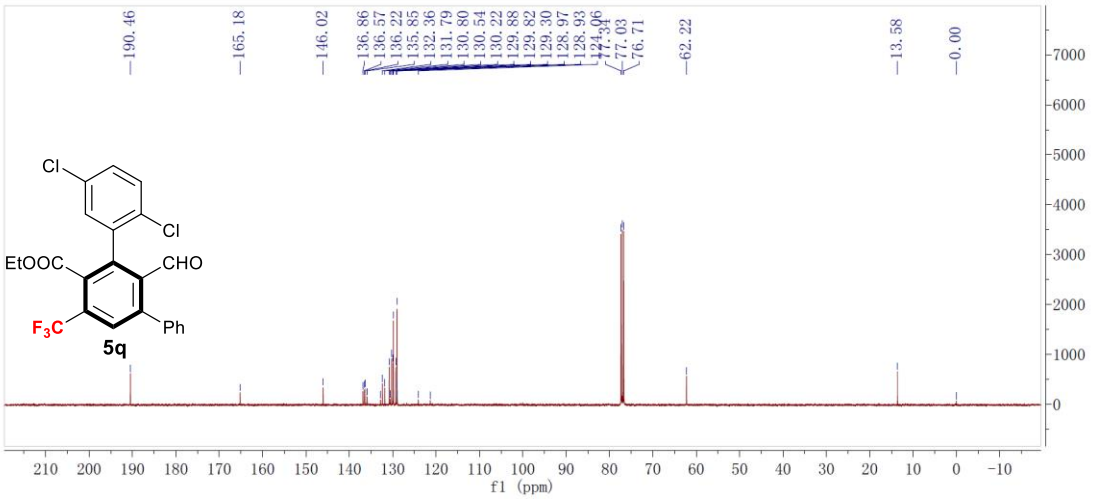
3.03
f1 (ppm)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129.30
128.97
128.93
124.06
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77.03
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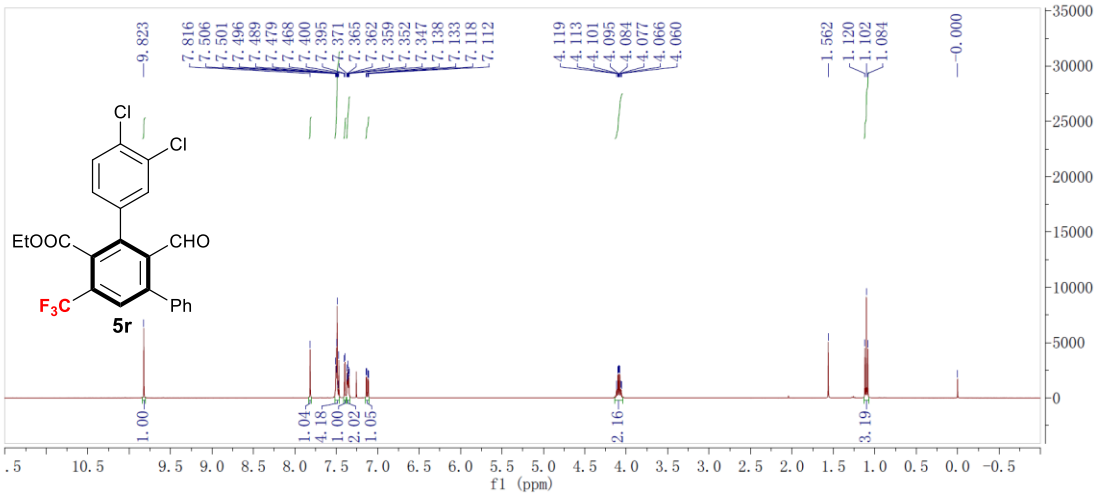
62.22
13.58
0.00
Cl
Cl
EtOOC
CHO
F3C
Ph
5q
f1 (ppm)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7.352
7.347
7.138
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4.113
4.101
4.095
4.084
4.077
4.066
4.060
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1.120
1.102
1.084
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Cl
Cl
EtOOC
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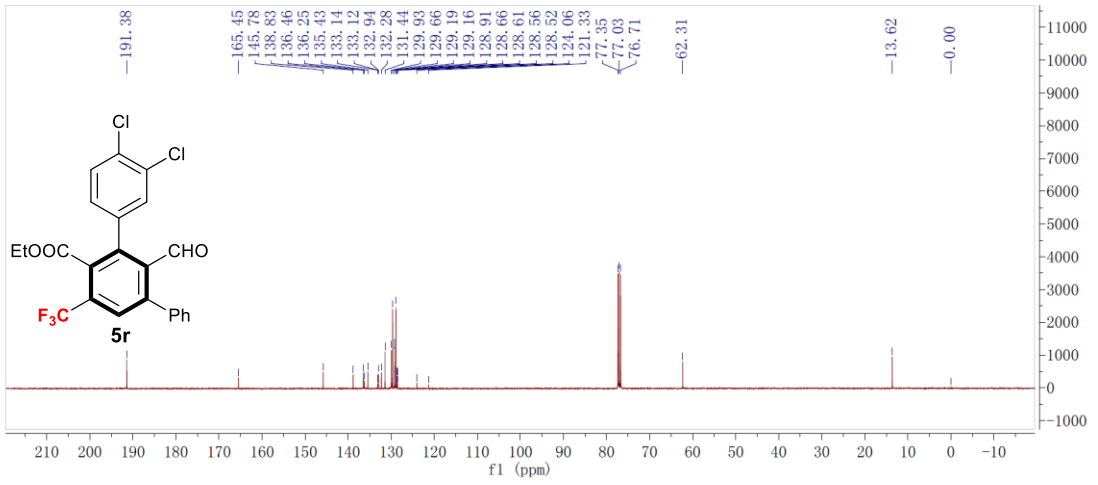
f1 (ppm)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129.66
129.19
129.16
128.91
128.66
128.61
128.56
128.52
124.06
121.33
77.35
77.03
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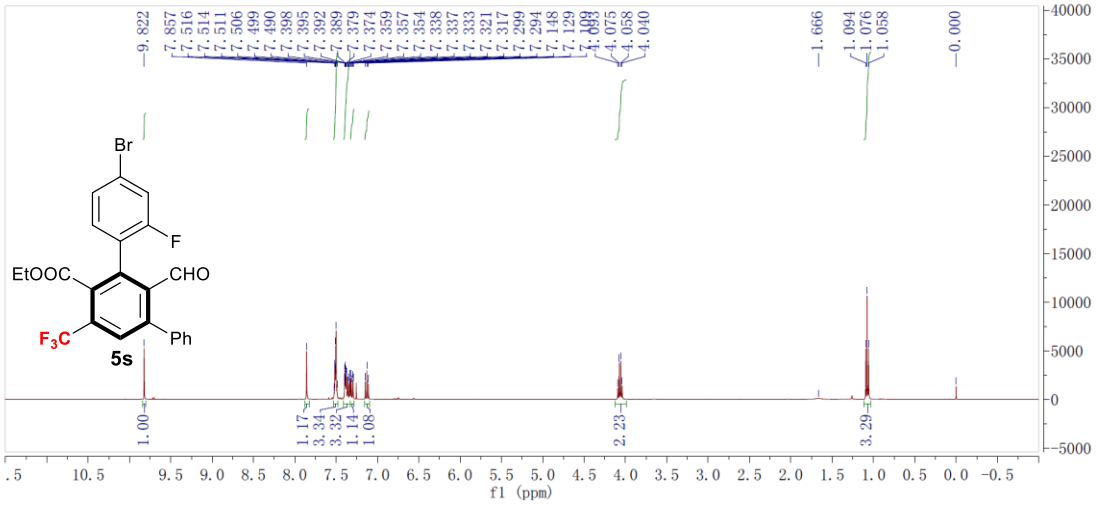
62.31
13.62
0.00
Cl
Cl
EtOOC
CHO
F3C
Ph
5r
f1 (ppm)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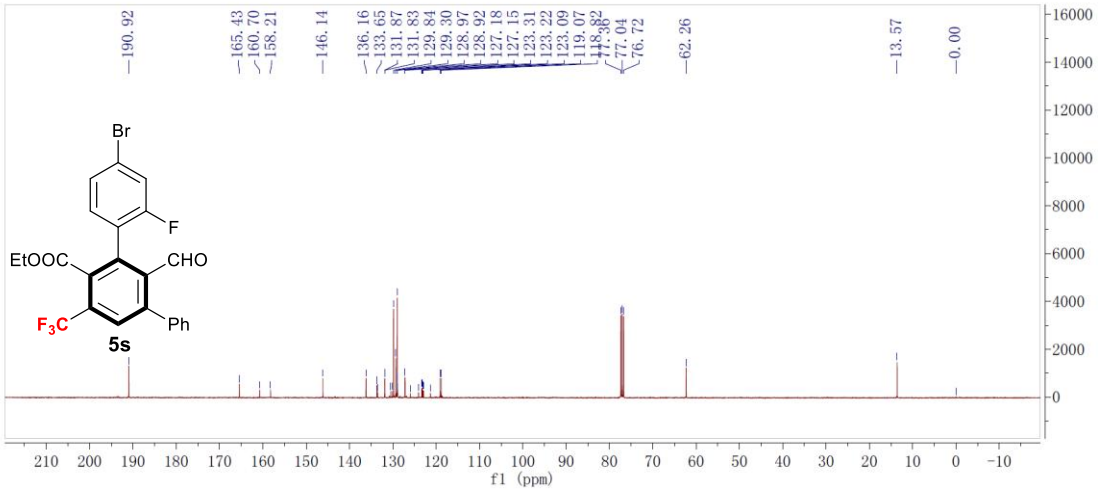
F
EtOOC
CHO
F3C
Ph
5s
f1 (ppm)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F
EtOOC
CHO
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Ph
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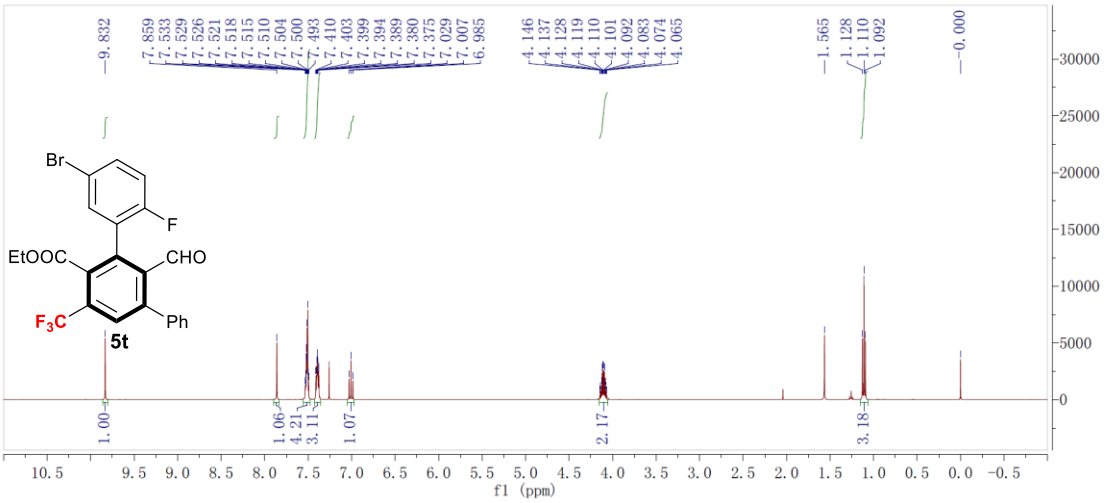
f1 (ppm)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7.380
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7.029
7.007
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4.137
4.128
4.119
4.110
4.101
4.092
4.083
4.074
4.065
1.565
1.128
1.110
1.092
0.000
Br
F
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CHO
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Ph
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1.07
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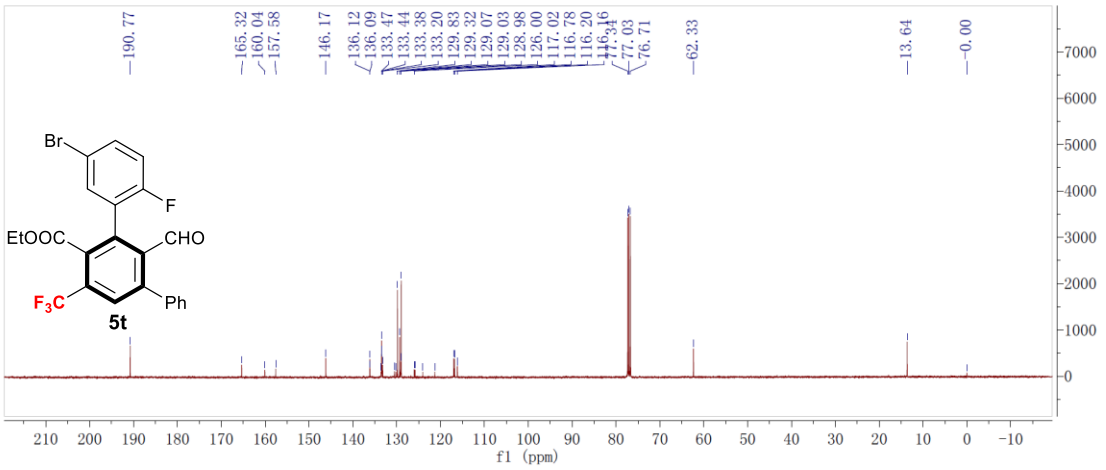
3.18
f1 (ppm)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129.03
128.98
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116.20
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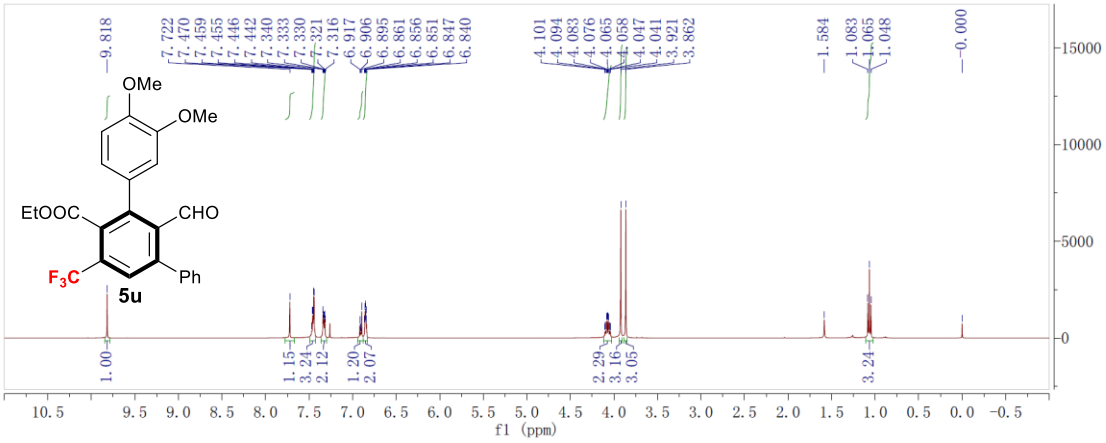
5t
f1 (ppm)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4.076
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1.065
1.048
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OMe
OMe
EtOOC
CHO
F3C
Ph
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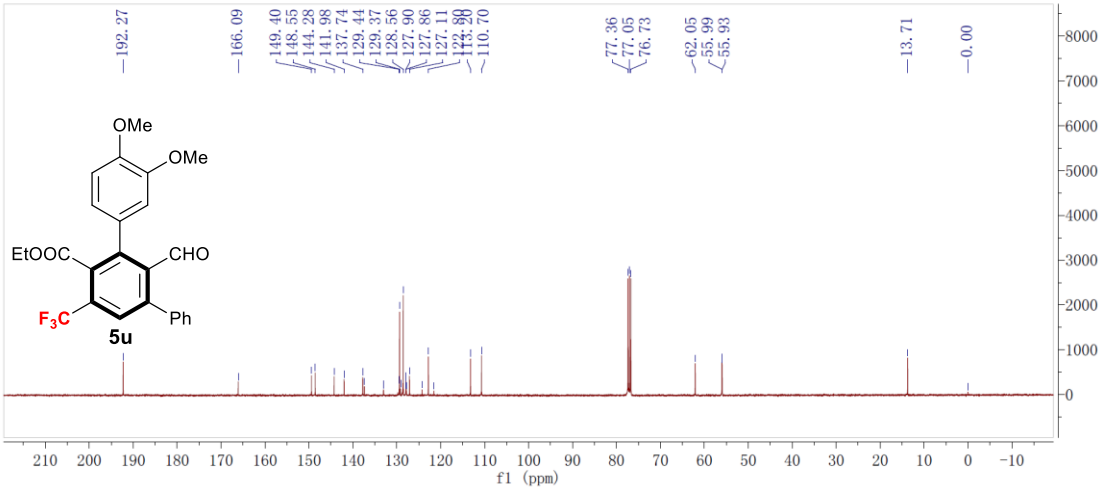
f1 (ppm)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127.11
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77.36
77.05
76.73
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13.71
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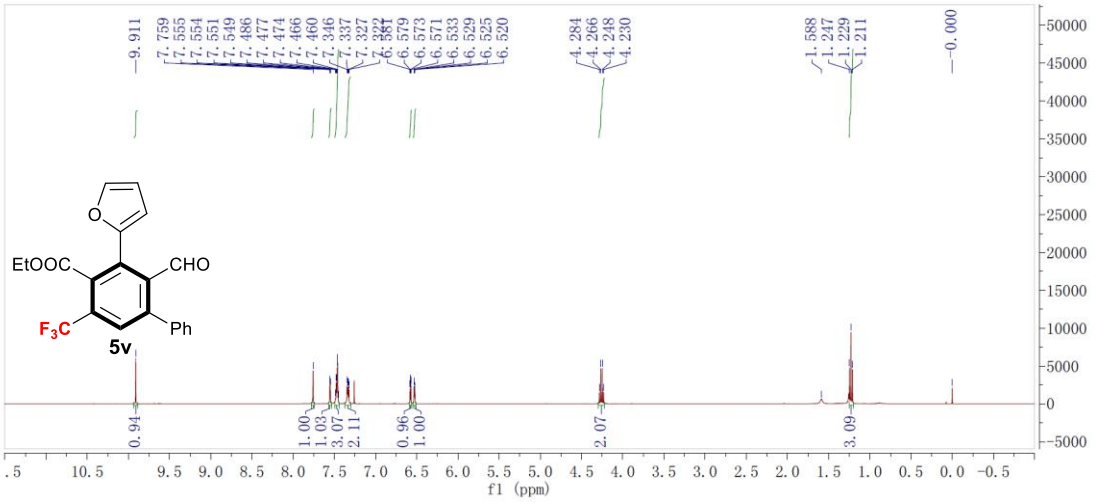
OMe
EtOOC
CHO
F3C
Ph
5u
f1 (ppm)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6.571
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6.529
6.525
6.520
4.284
4.266
4.248
4.230
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1.247
1.229
1.211
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EtOOC
CHO
F3C
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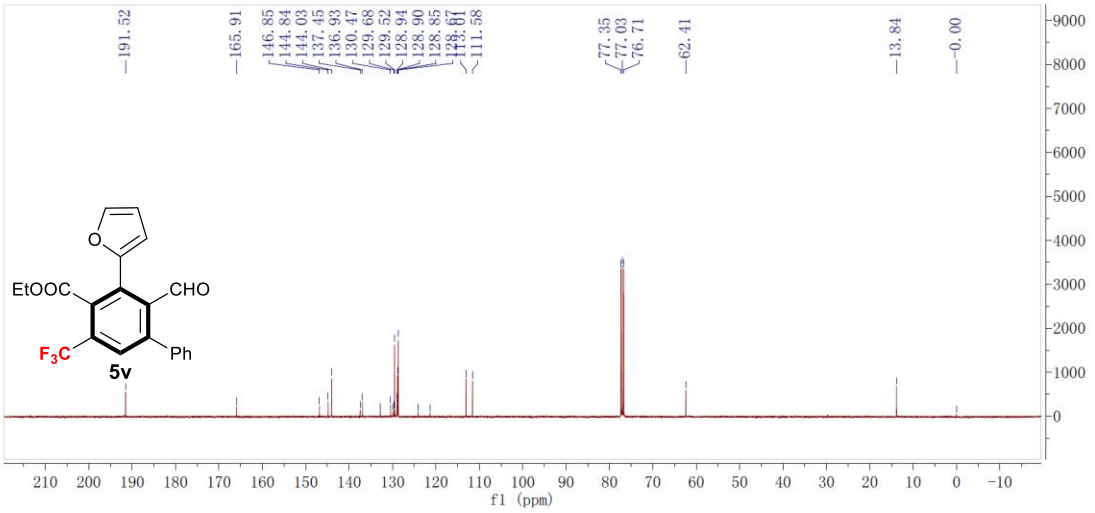
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128.90
128.85
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76.71
62.41
13.84
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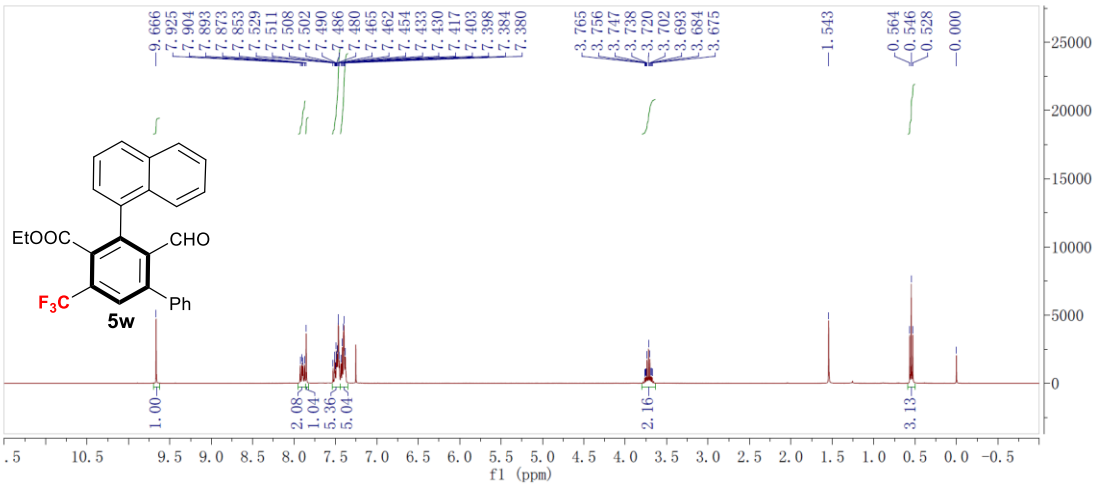
CHO
F3C
Ph
5v
f1 (ppm)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7.465
7.462
7.454
7.433
7.430
7.417
7.403
7.398
7.384
7.380
3.765
3.756
3.747
3.738
3.720
3.702
3.693
3.684
3.675
1.543
0.564
0.546
0.528
0.000
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CHO
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Ph
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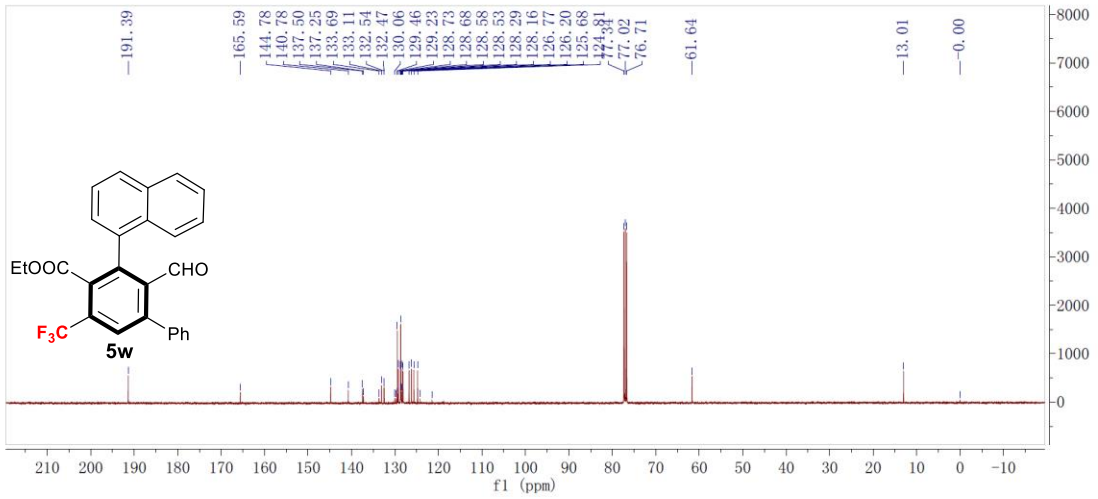
f1 (ppm)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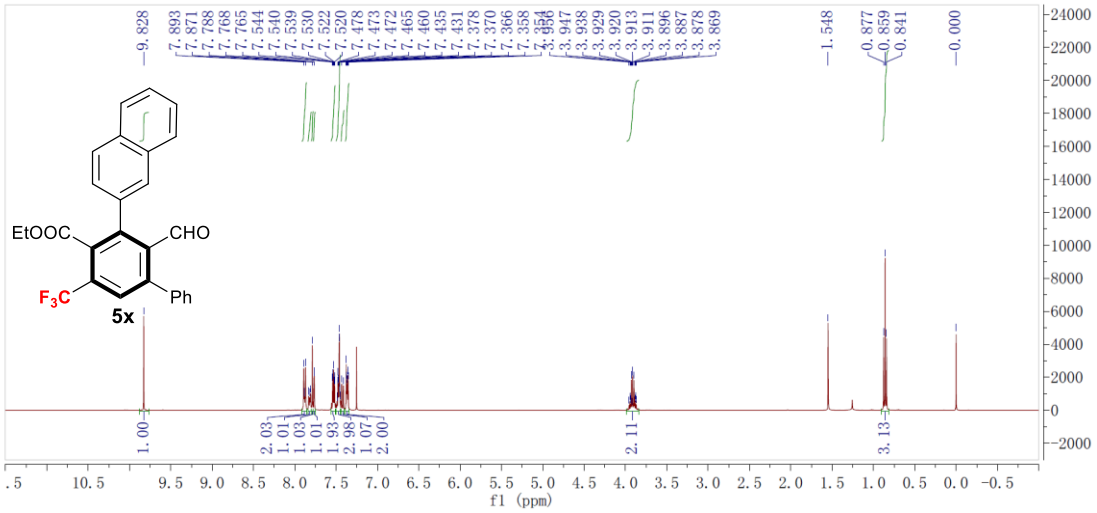
CHO
F3C
Ph
5w
f1 (ppm)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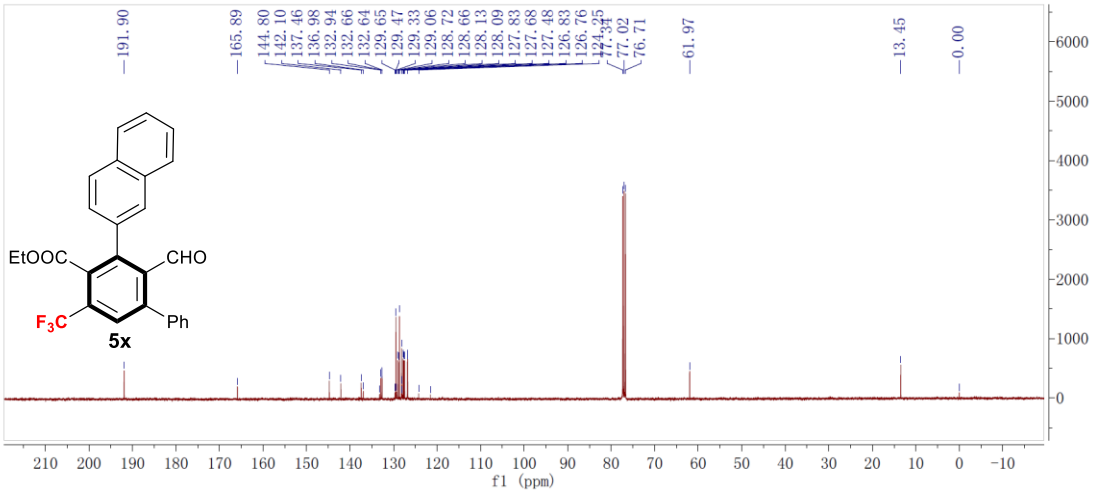
CHO
F3C
Ph
5x
f1 (ppm)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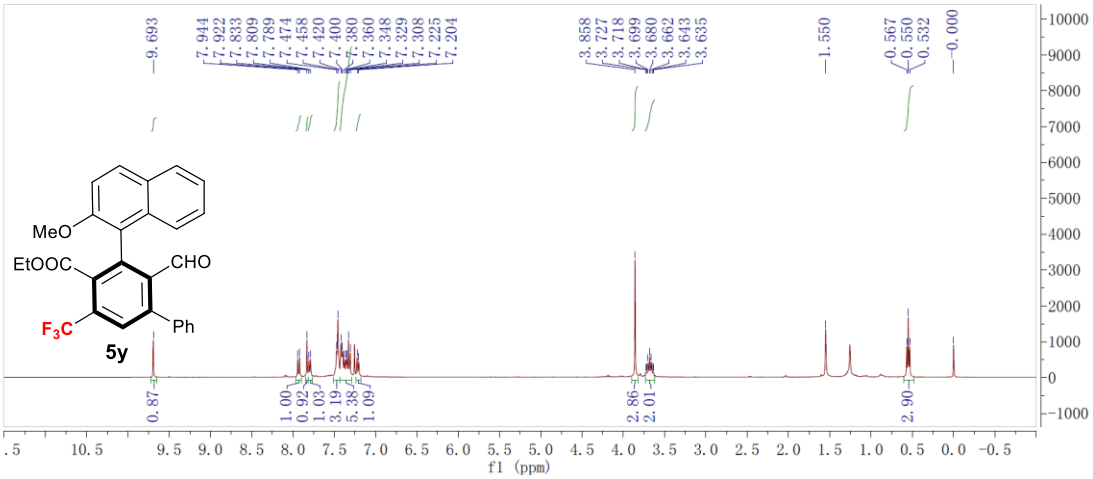
CHO
F3C
Ph
5x
f1 (ppm)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7.204
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3.727
3.718
3.699
3.680
3.662
3.643
3.635
1.550
0.567
0.550
0.532
0.000
MeO
EtOOC
CHO
F3C
Ph
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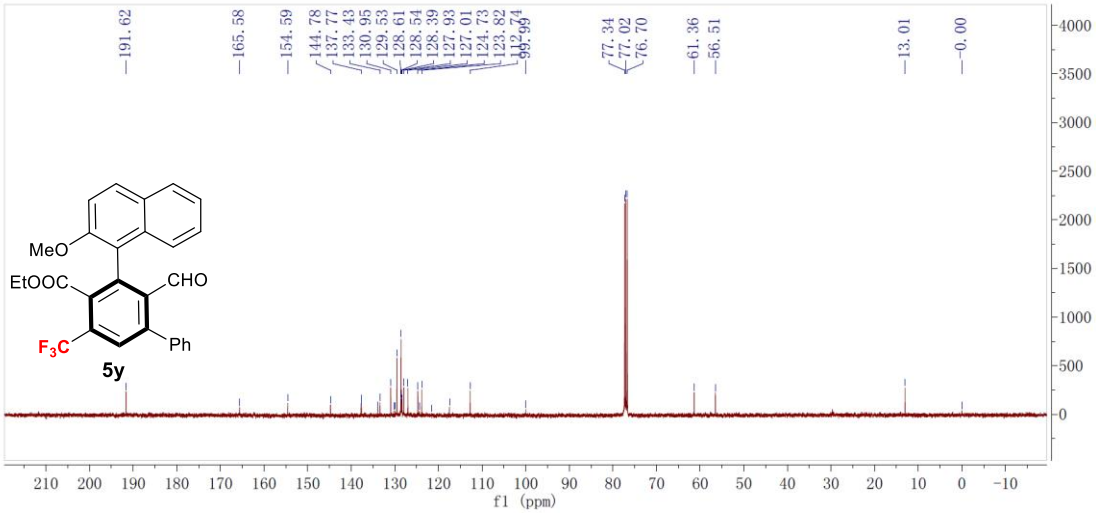
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123.82
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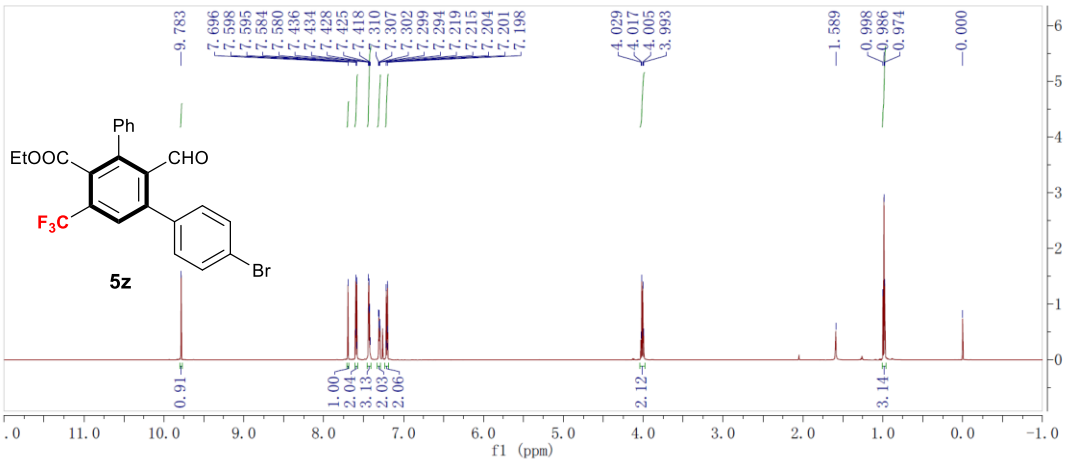
77.34
77.02
76.70
61.36
56.51
13.01
0.00
MeO
EtOOC
CHO
F3C
Ph
5y
f1 (ppm)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7.434
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7.425
7.418
7.310
7.307
7.302
7.299
7.294
7.219
7.215
7.204
7.201
7.198
4.029
4.017
4.005
3.993
1.589
0.998
0.986
0.974
0.000
Ph
EtOOC
CHO
F3C
Br
5z
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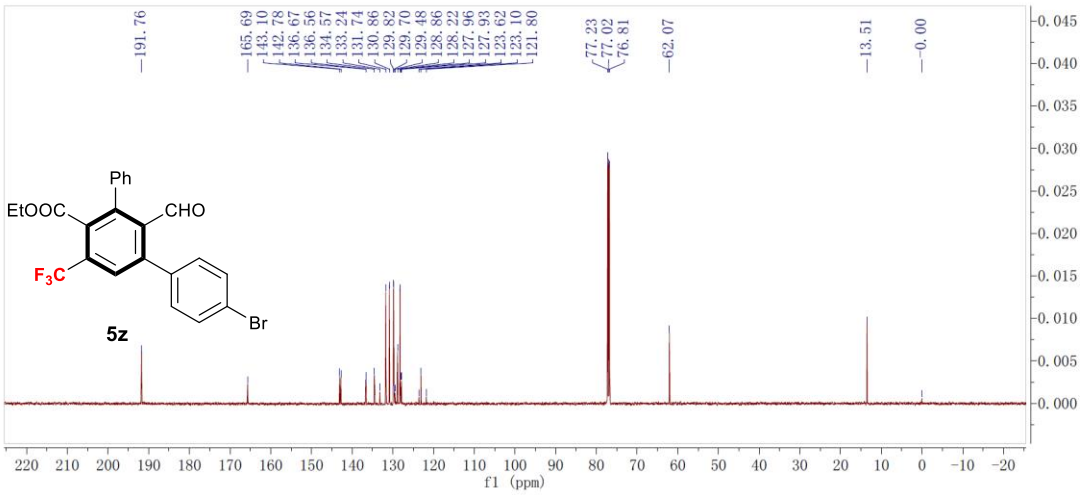
1.00
2.04
3.13
2.03
2.06
2.12
3.14
f1 (ppm)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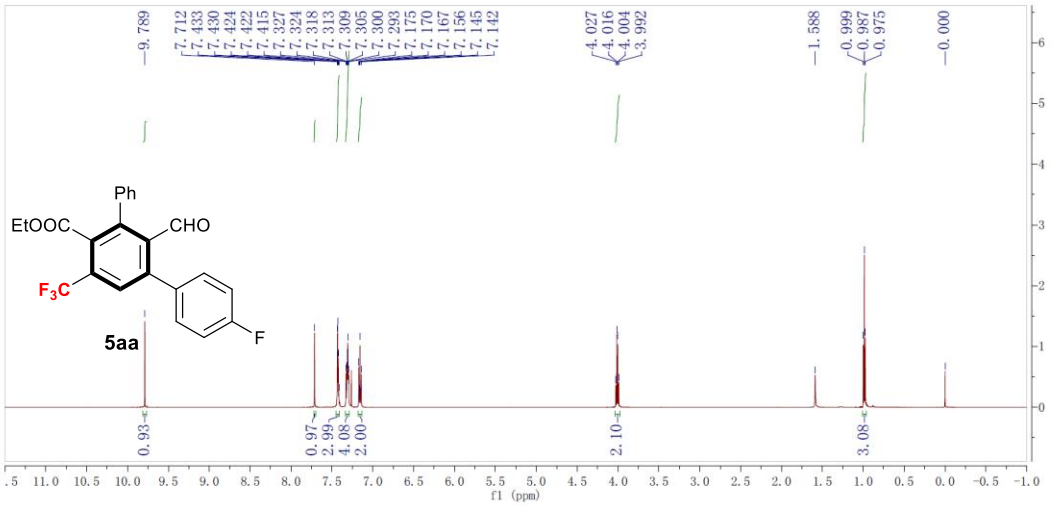
143.10
142.78
136.67
136.56
134.57
133.24
131.74
130.86
129.82
129.70
129.48
128.86
128.22
127.96
127.93
123.62
123.10
121.80
77.23
77.02
76.81
62.07
13.51
0.00
Ph
EtOOC
CHO
F3C
Br
5z
f1 (ppm)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7.433
7.430
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7.422
7.415
7.327
7.324
7.318
7.313
7.309
7.305
7.300
7.293
7.175
7.170
7.167
7.156
7.145
7.142
4.027
4.016
4.004
3.992
1.588
0.999
0.987
0.975
0.000
Ph
EtOOC
CHO
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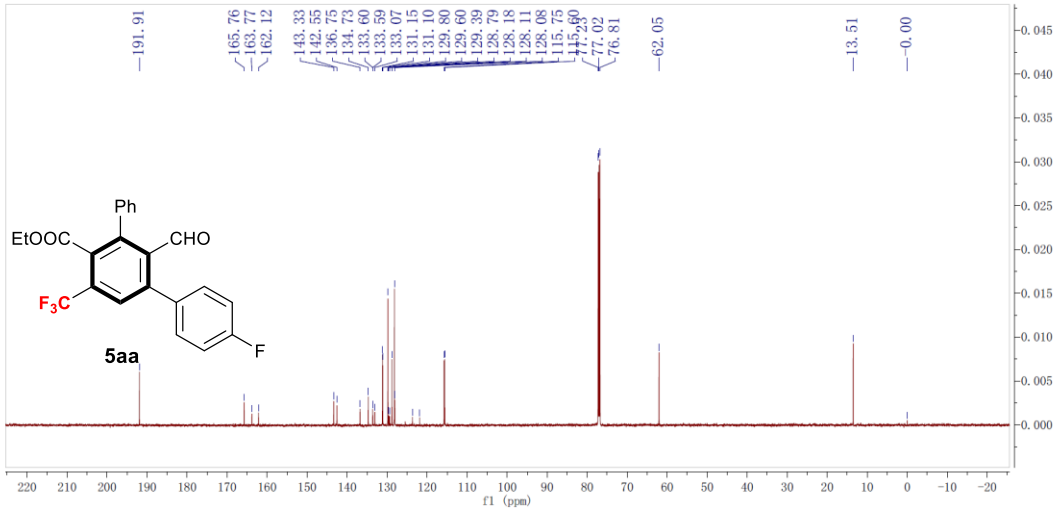
F
5aa
0.93
0.97
2.99
4.08
2.00
2.10
3.08
f1 (ppm)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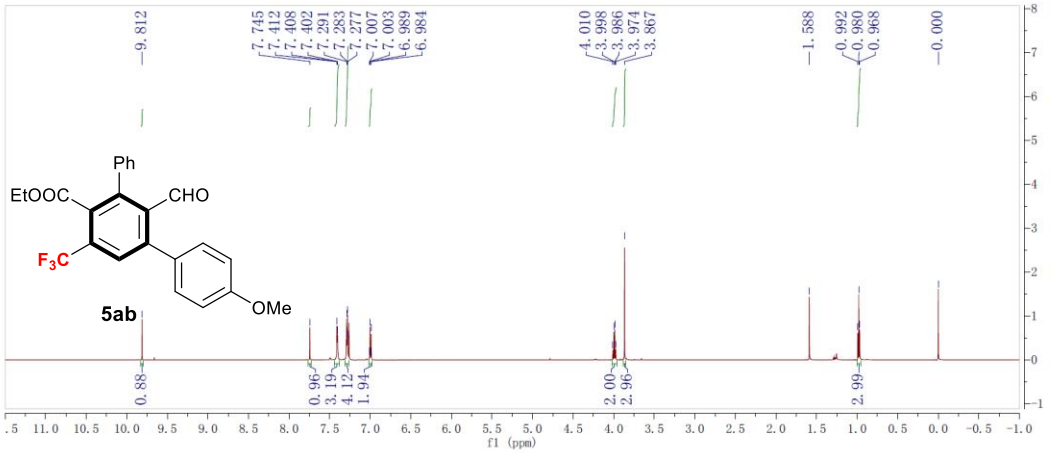
134.73
133.60
133.59
133.07
131.15
131.10
129.80
129.60
129.39
128.79
128.18
128.11
128.08
115.75
115.60
77.02
76.81
62.05
13.51
-0.00
Ph
EtOOC
CHO
F3C
F
5aa
f1 (ppm)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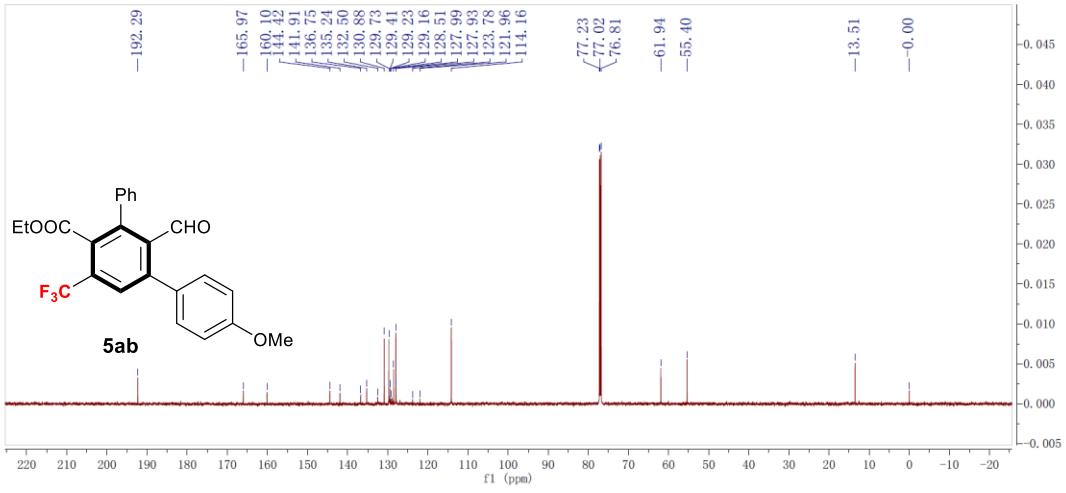
7.291
7.283
7.277
7.007
7.003
6.989
6.984
4.010
3.998
3.986
3.974
3.867
1.588
0.992
0.980
0.968
0.000
Ph
EtOOC
CHO
F3C
OMe
5ab
0.88
0.96
3.19
4.12
1.94
2.00
2.96
2.99
f1 (ppm)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136.75
135.24
132.50
130.88
129.73
129.41
129.23
129.16
128.51
127.99
127.93
123.78
121.96
114.16
77.23
77.02
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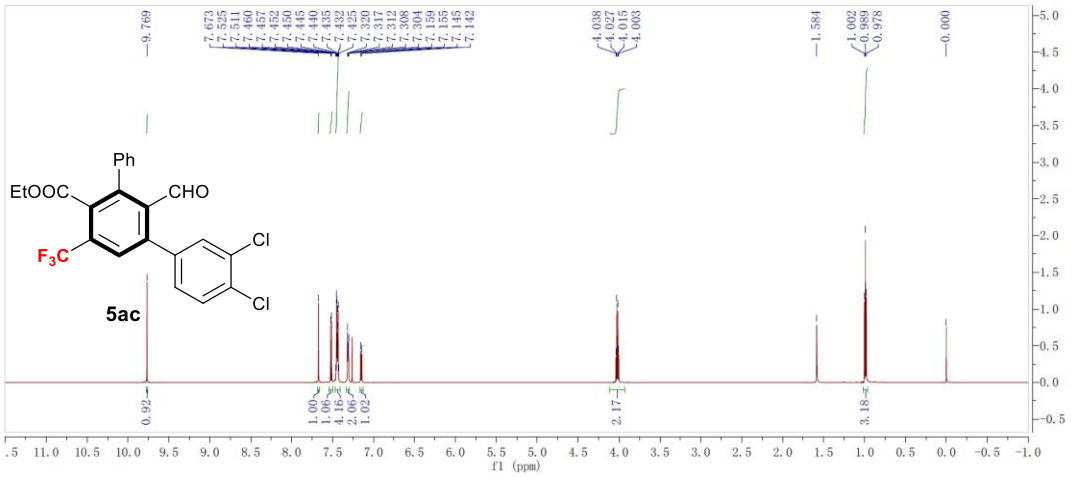
61.94
55.40
13.51
0.00
Ph
EtOOC
CHO
F3C
OMe
5ab
f1 (ppm)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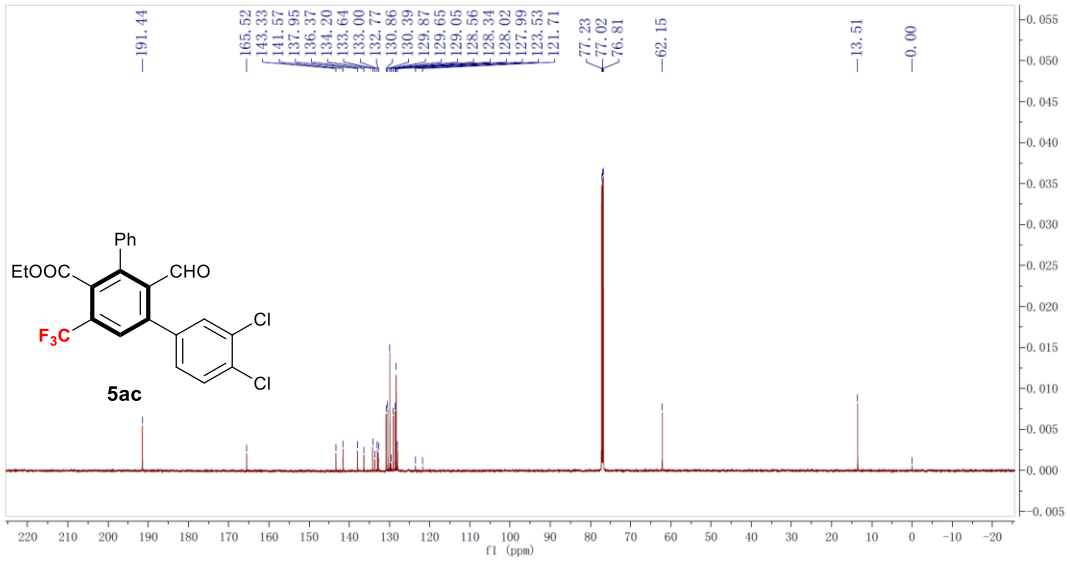
EtOOC
CHO
Cl
F_3C
Cl
5ac
f1 (ppm)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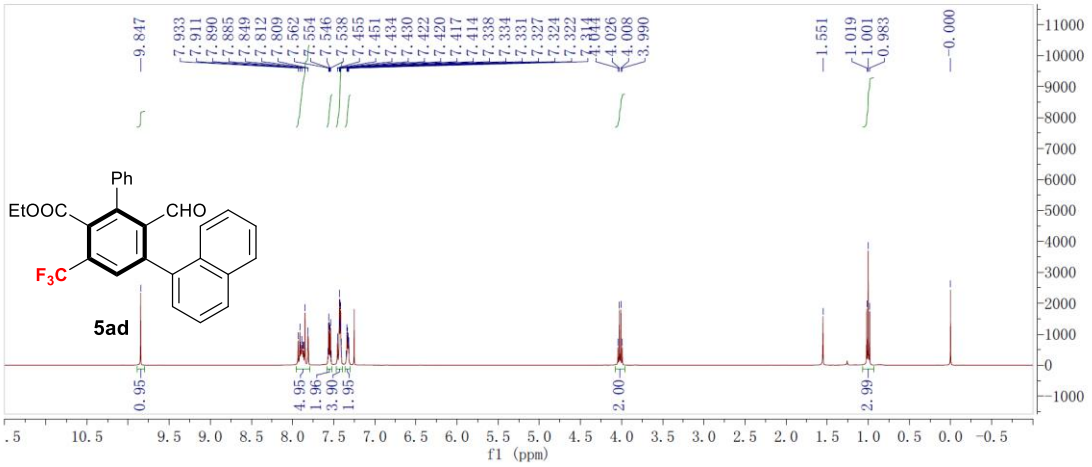
EtOOC
CHO
Cl
F_3C
Cl
5ac
f1 (ppm)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7.890
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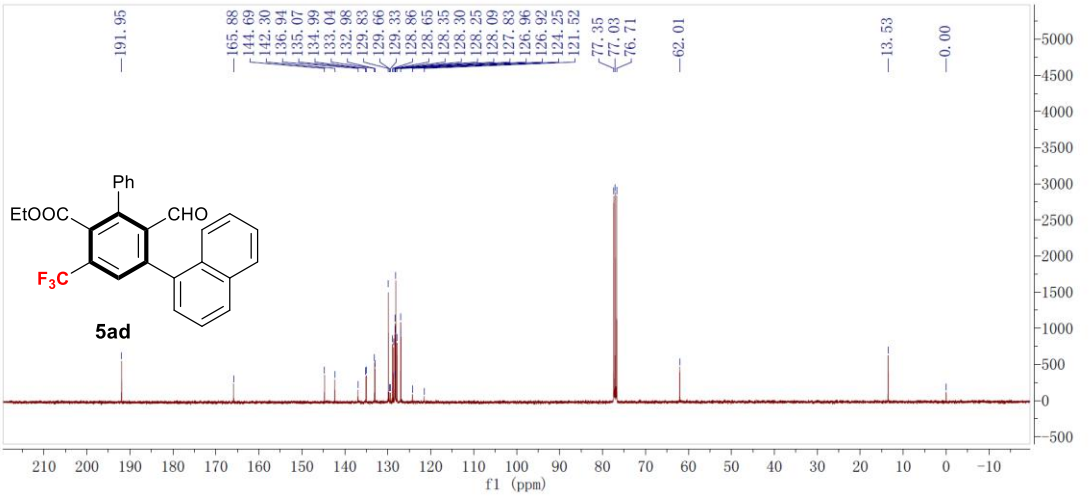
7.849
7.812
7.809
7.562
7.554
7.546
7.538
7.455
7.451
7.434
7.430
7.422
7.420
7.417
7.414
7.338
7.334
7.331
7.327
7.324
7.322
4.014
4.011
4.026
4.008
3.990
1.551
1.019
1.001
0.983
0.000
Ph
EtOOC
CHO
F3C
5ad
0.95
4.95
1.96
3.90
1.95
2.00
2.99
f1 (ppm)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135.07
134.99
133.04
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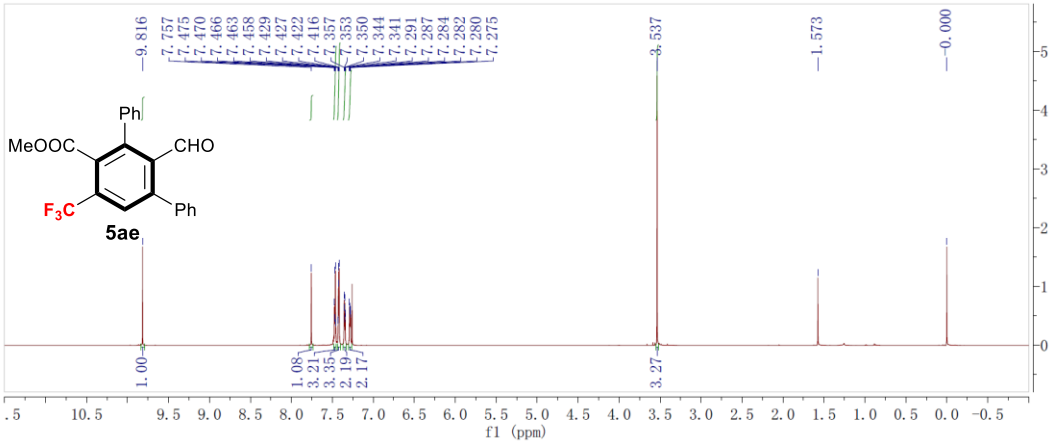
129.83
129.66
129.33
128.86
128.65
128.35
128.30
128.25
128.09
127.83
126.96
126.92
124.25
121.52
77.35
77.03
76.71
62.01
13.53
0.00
Ph
EtOOC
CHO
F3C
5ad
f1 (ppm)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7.466
7.463
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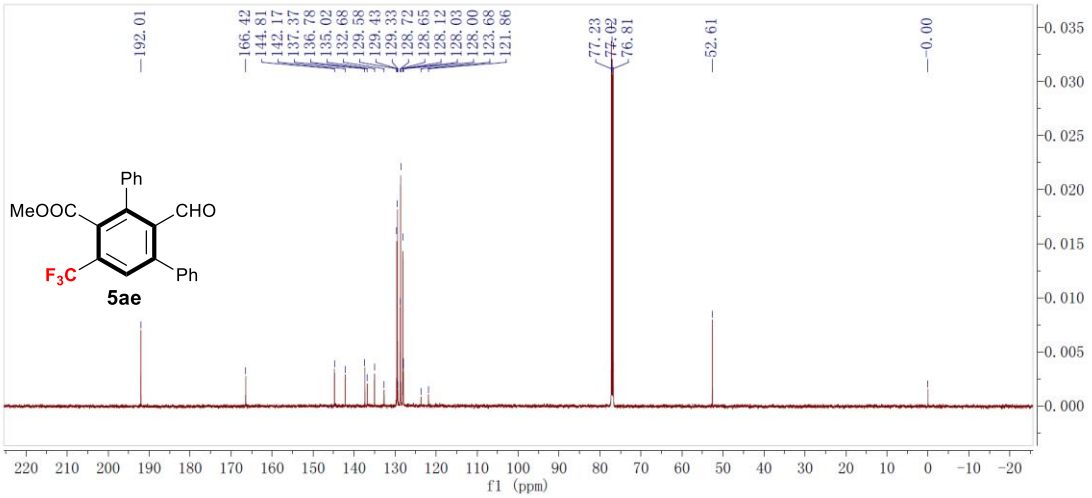
7.429
7.427
7.422
7.416
7.357
7.353
7.350
7.344
7.341
7.291
7.287
7.284
7.282
7.280
7.275
3.537
1.573
0.000
Ph
MeOOC
CHO
F3C
Ph
5ae
1.00
1.08
3.21
3.35
2.19
2.17
3.27
f1 (ppm)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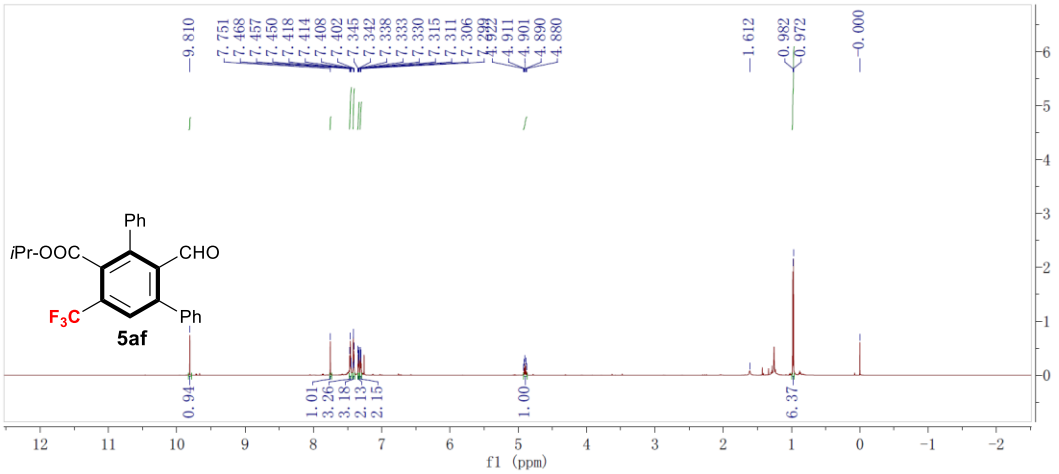
136.78
135.02
132.68
132.58
129.43
129.33
128.72
128.65
128.12
128.03
128.00
123.68
121.86
77.23
77.02
76.81
52.61
0.00
Ph
MeOOC
CHO
F3C
Ph
5ae
f1 (ppm)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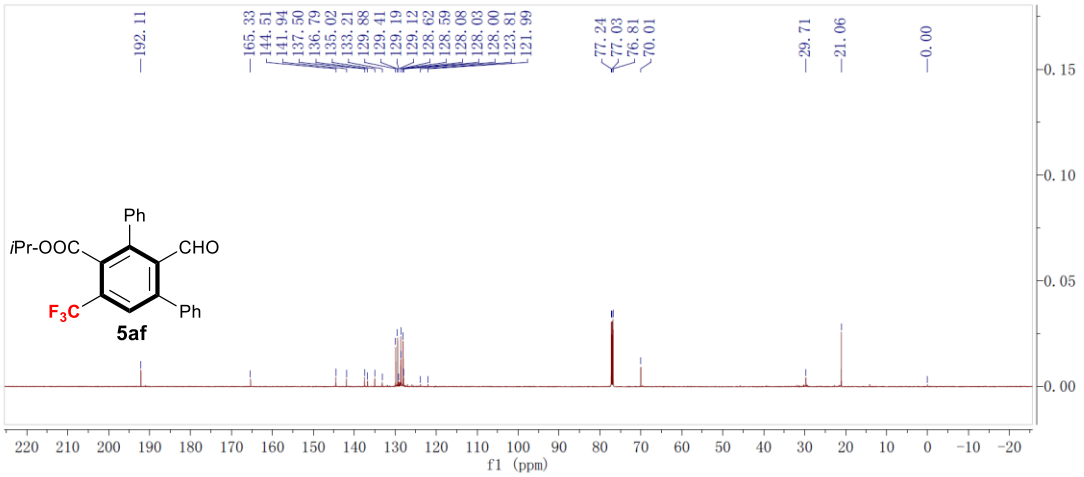
7.457
7.450
7.418
7.414
7.408
7.402
7.345
7.342
7.338
7.333
7.330
7.315
7.311
7.306
4.911
4.901
4.890
4.880
1.612
0.982
0.972
0.000
Ph
iPr-OOC
CHO
F3C
Ph
5af
0.94
1.01
3.26
3.18
2.13
2.15
1.00
6.37
f1 (ppm)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141.94
137.50
136.79
135.02
133.21
129.88
129.41
129.19
129.12
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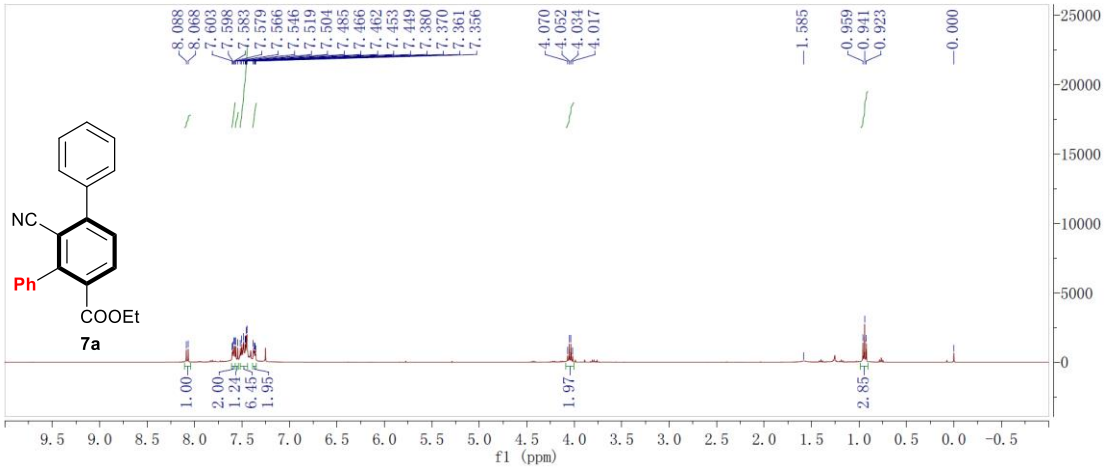
128.59
128.08
128.03
128.00
123.81
121.99
77.24
77.03
76.81
70.01
29.71
21.06
0.00
Ph
iPr-OOC
CHO
F3C
Ph
5af
f1 (ppm)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7.583
7.579
7.566
7.546
7.519
7.504
7.485
7.466
7.462
7.453
7.449
7.380
7.370
7.361
7.356
4.070
4.052
4.034
4.017
1.585
0.959
0.941
0.923
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7a
1.00
2.00
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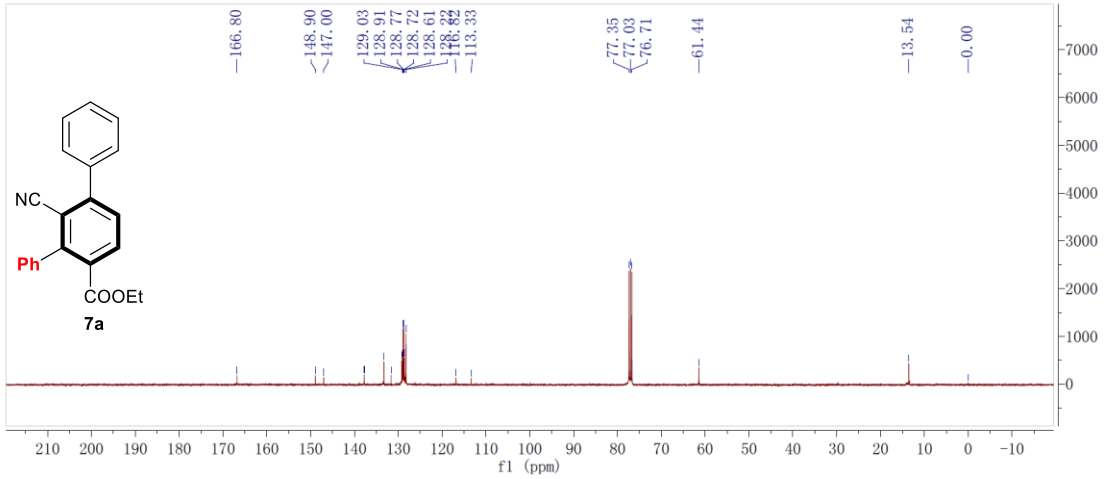
1.95
1.97
2.85
f1 (ppm)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128.72
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77.03
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61.44
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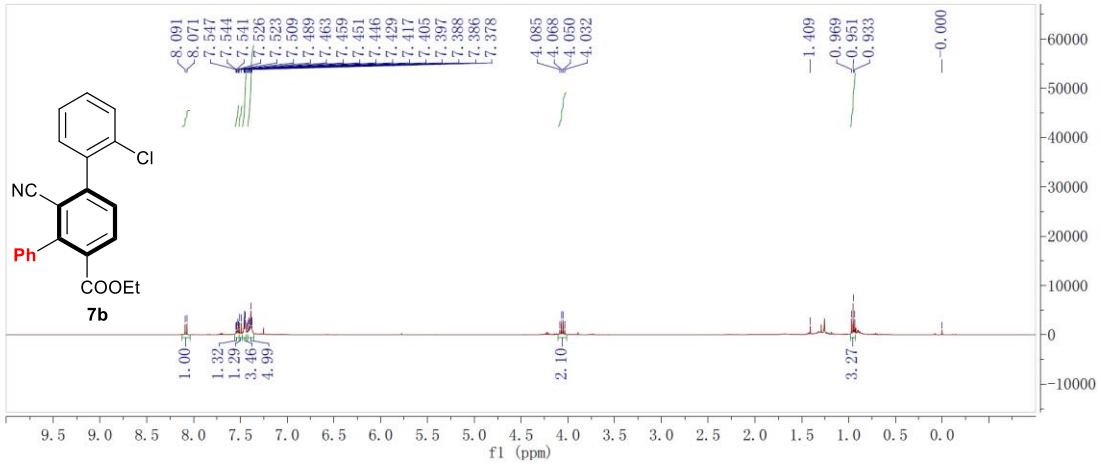
Ph
COOEt
7a
f1 (ppm)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7.509
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7.463
7.459
7.451
7.446
7.429
7.417
7.405
7.397
7.388
7.386
7.378
4.085
4.068
4.050
4.032
1.409
0.969
0.951
0.933
0.000
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7b
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1.32
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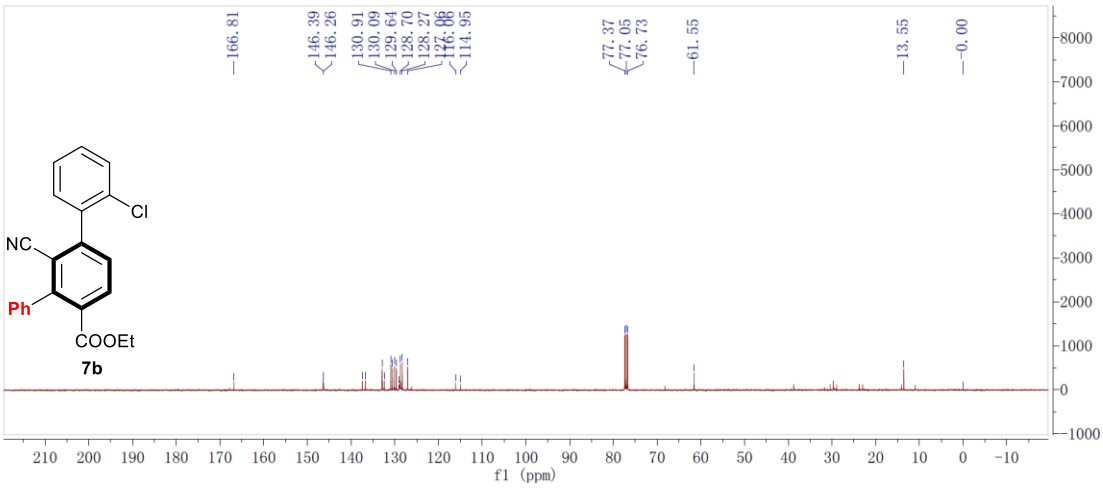
4.99
2.10
3.27
f1 (ppm)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129.64
128.70
128.27
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77.05
76.73
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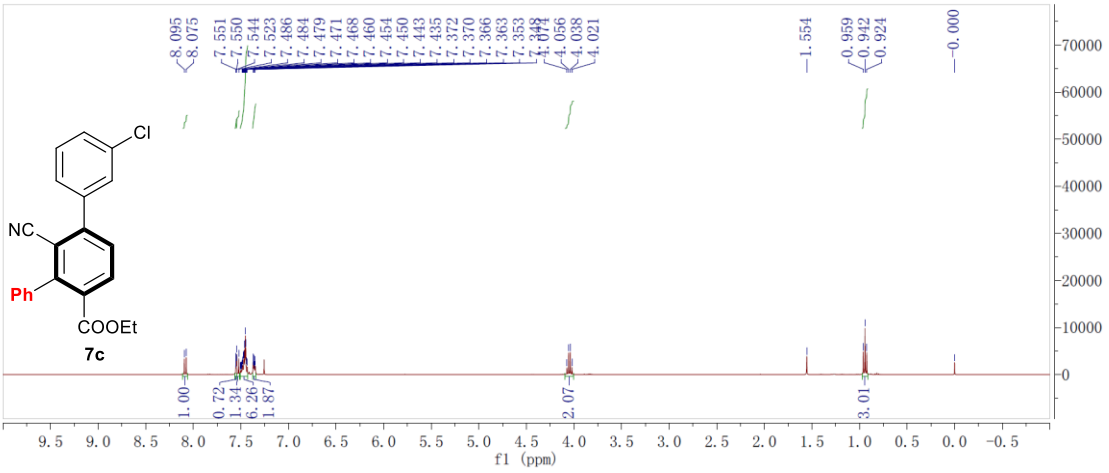
Cl
NC
Ph
COOEt
7b
f1 (ppm)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7.471
7.468
7.460
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7.450
7.443
7.435
7.372
7.370
7.366
7.363
7.353
4.056
4.038
4.021
1.554
0.959
0.942
0.924
0.000
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7c
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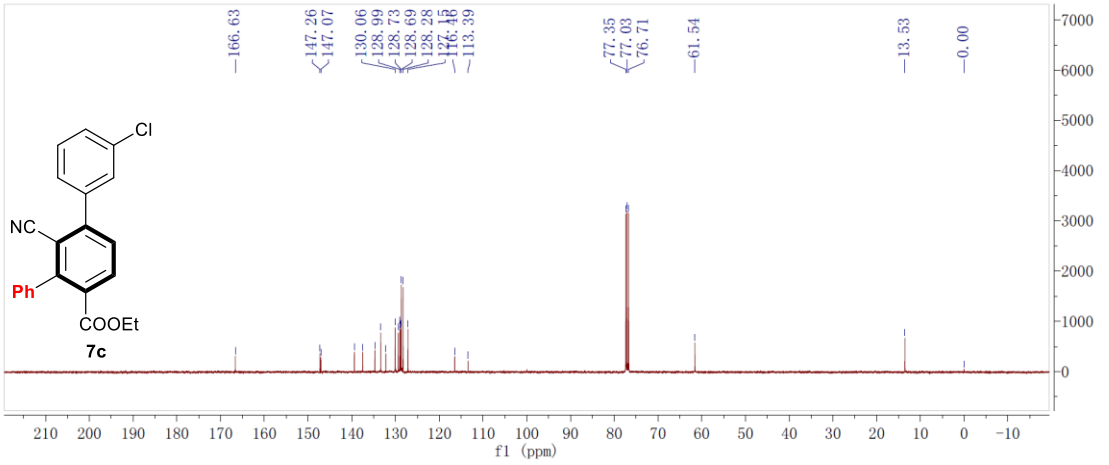
f1 (ppm)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76.71
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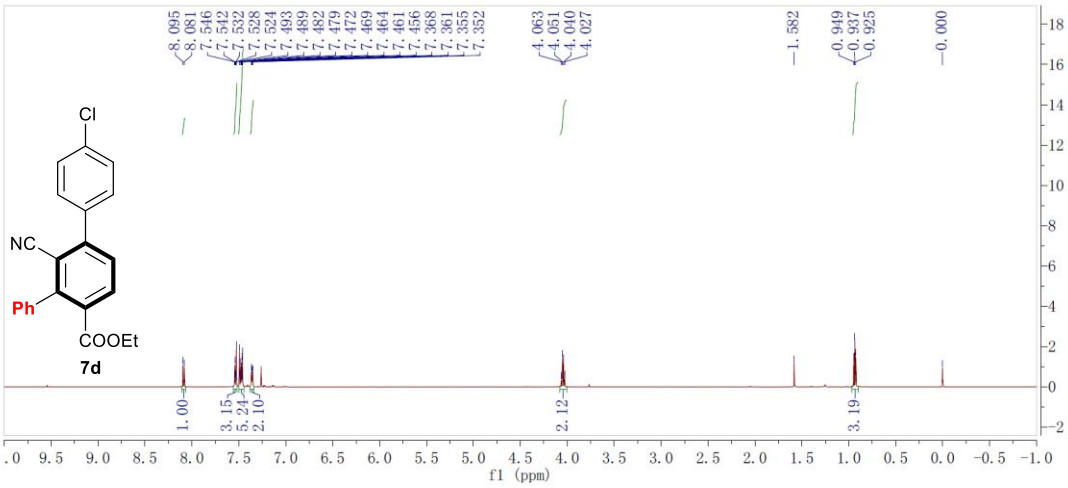
Cl
NC
Ph
COOEt
7c
f1 (ppm)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7.479
7.472
7.469
7.464
7.461
7.456
7.368
7.361
7.355
7.352
4.063
4.051
4.040
4.027
1.582
0.949
0.937
0.925
0.000
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Ph
COOEt
7d
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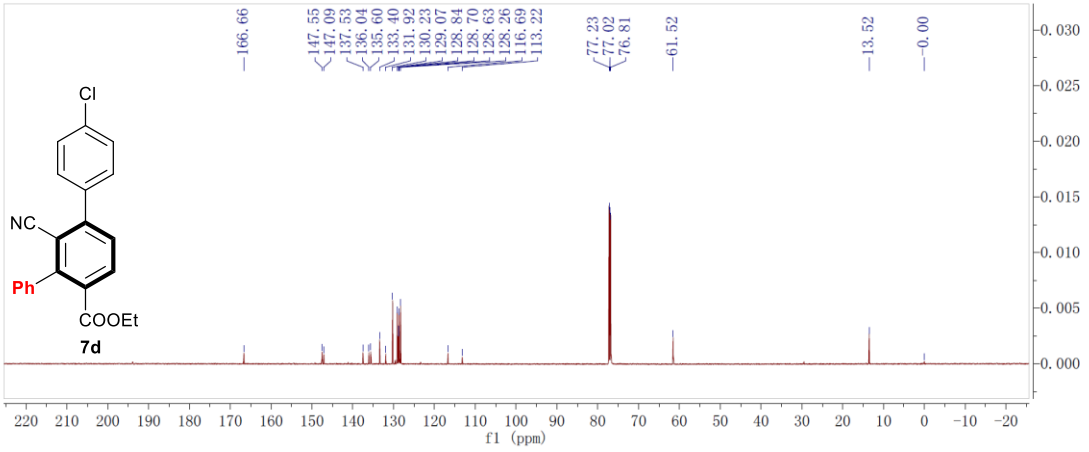
3.15
5.24
2.10
2.12
3.19
f1 (ppm)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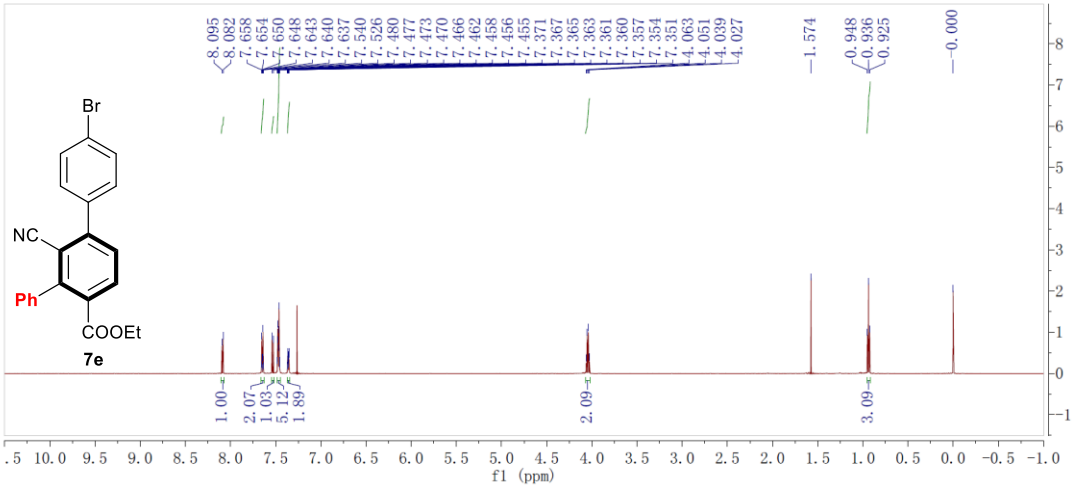
131.92
130.23
129.07
128.84
128.70
128.63
128.26
116.69
113.22
77.23
77.02
76.81
61.52
13.52
-0.00
Cl
NC
Ph
COOEt
7d
f1 (ppm)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7.526
7.480
7.477
7.473
7.470
7.466
7.462
7.458
7.456
7.455
7.371
7.367
7.365
7.363
7.361
7.360
7.357
7.354
7.351
4.063
4.051
4.039
4.027
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0.948
0.936
0.925
0.000
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Ph
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7e
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1.89
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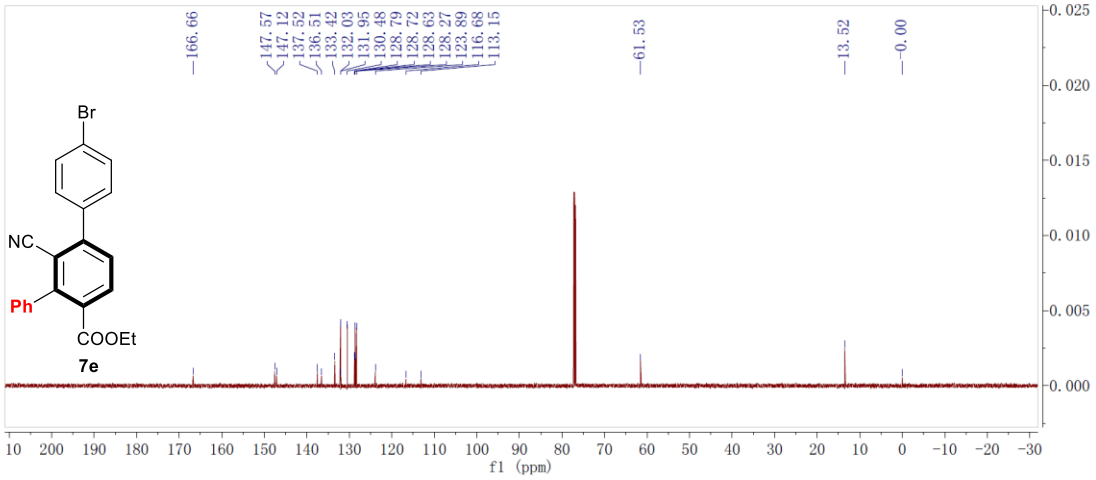
3.09
f1 (ppm)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128.72
128.63
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113.15
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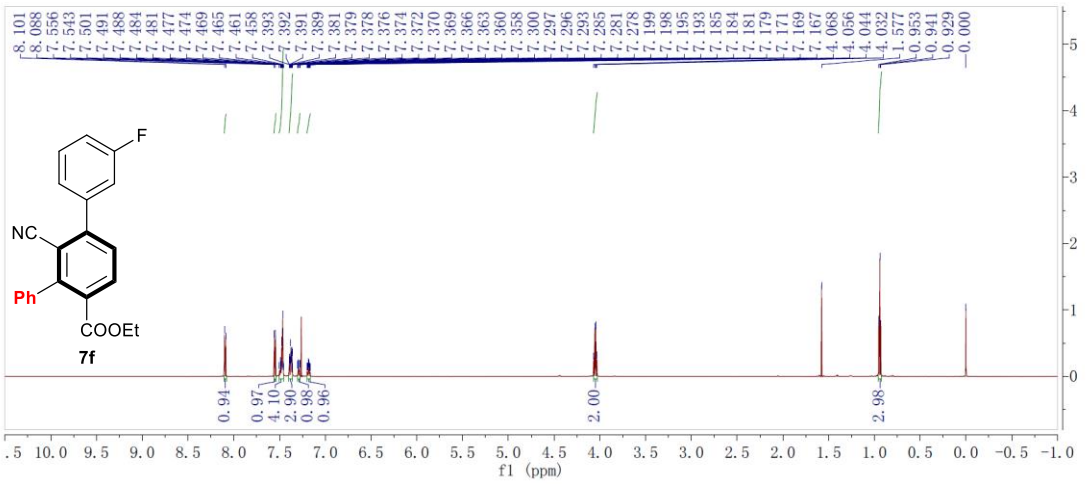
13.52
0.00
Br
NC
Ph
COOEt
7e
f1 (ppm)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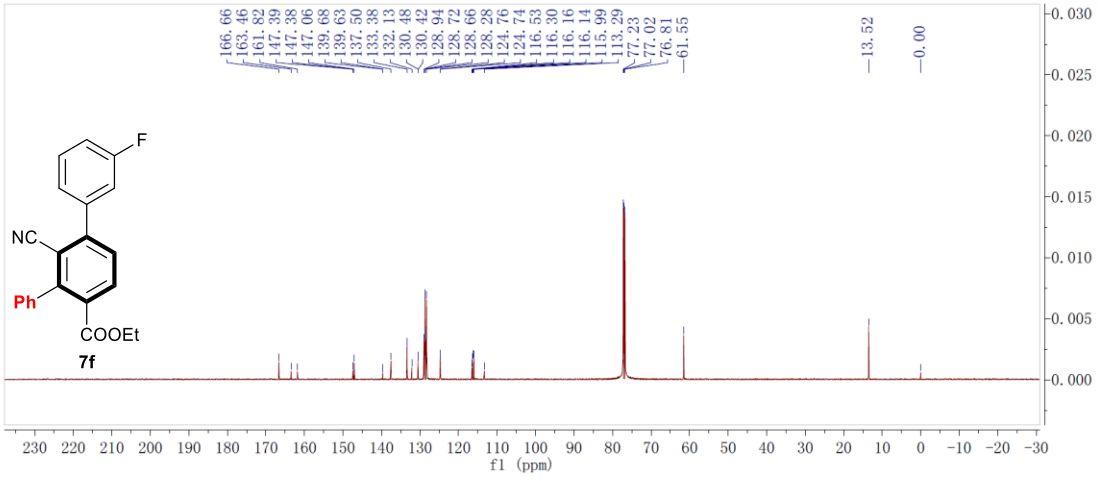
NC
Ph
COOEt
7f
f1 (ppm)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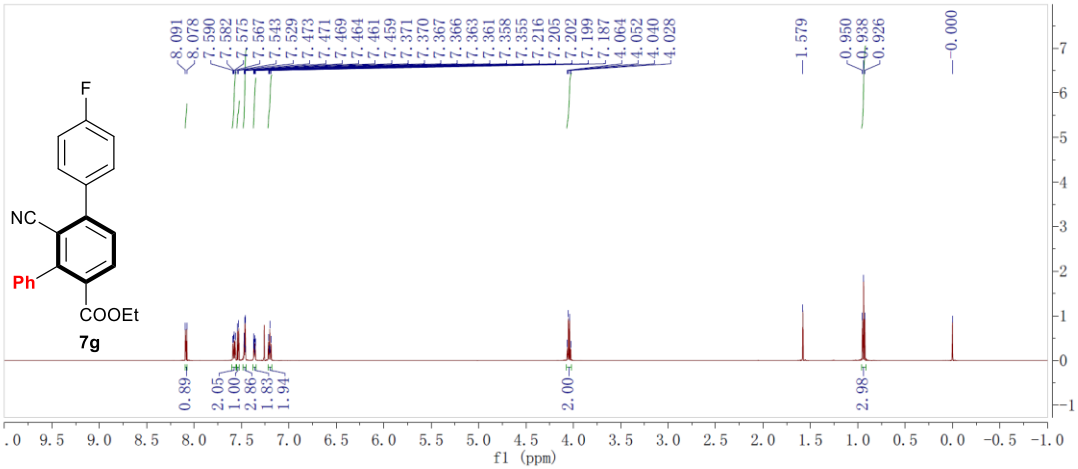
Ph
COOEt
7f
f1 (ppm)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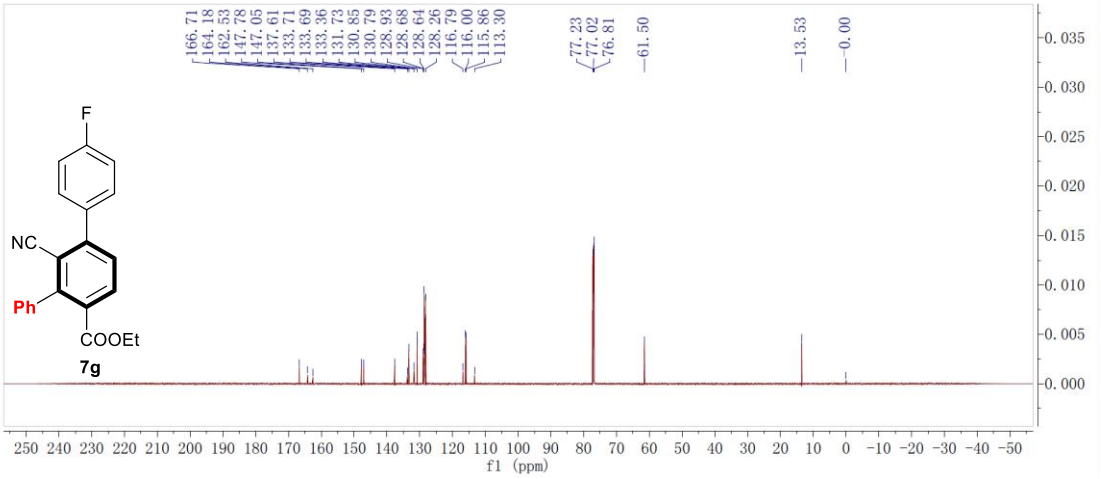
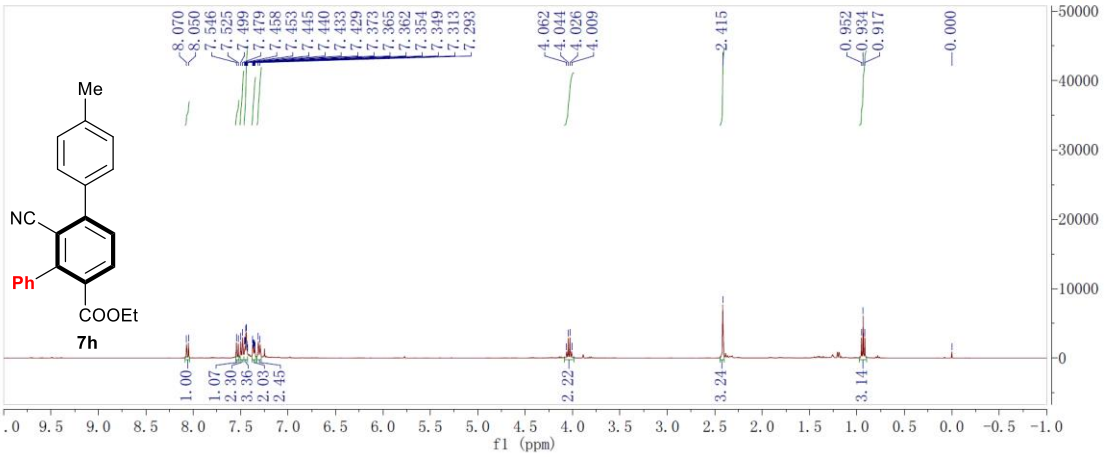
Ph
COOEt
7g
f1 (ppm)


F
NC
Ph
COOEt
7g
f1 (ppm)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7.365
7.362
7.354
7.349
7.313
7.293
4.062
4.044
4.026
4.009
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0.934
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Me
NC
Ph
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2.03
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2.22
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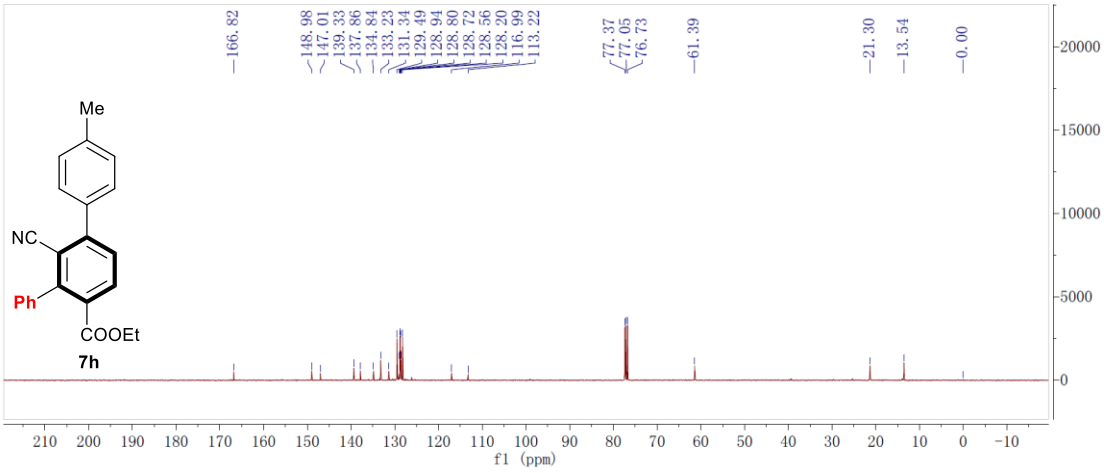
3.14
f1 (ppm)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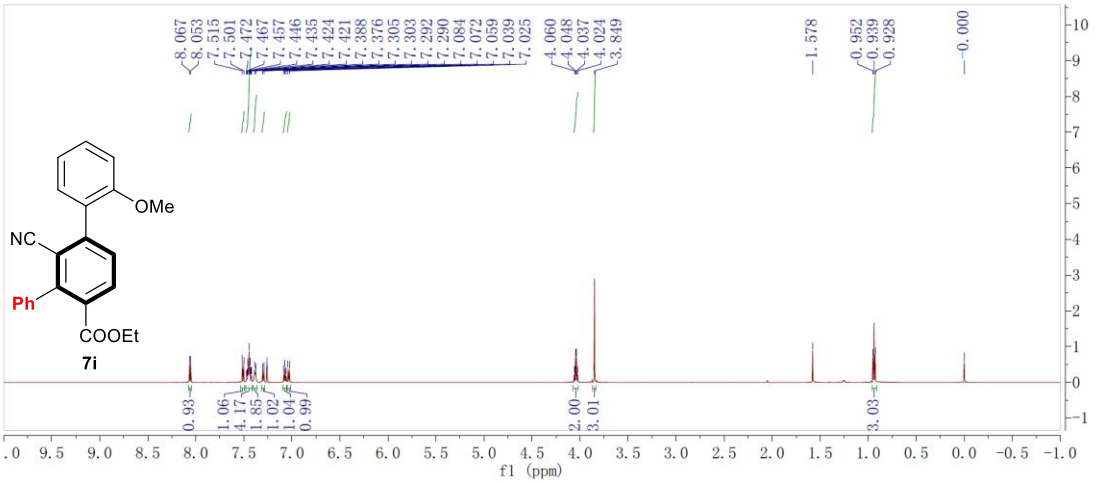
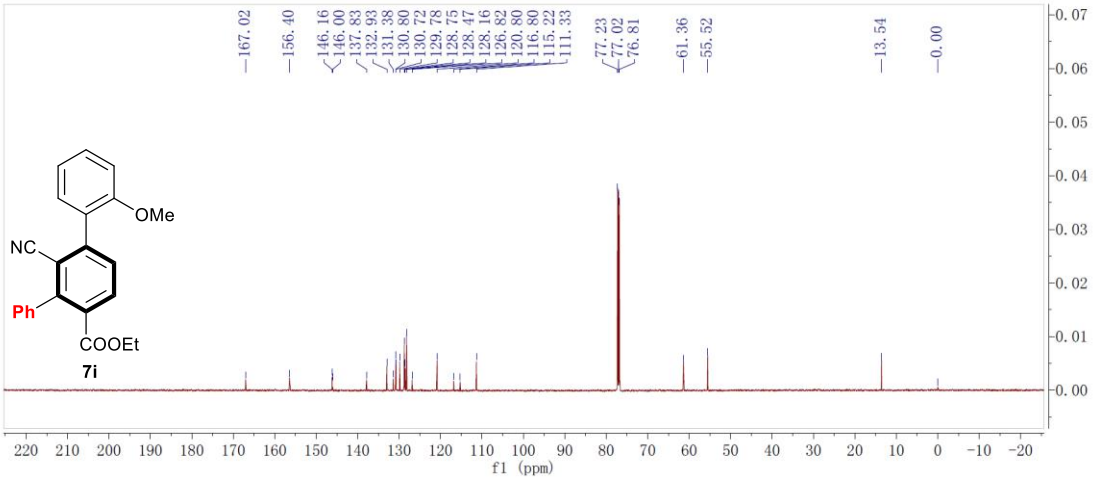
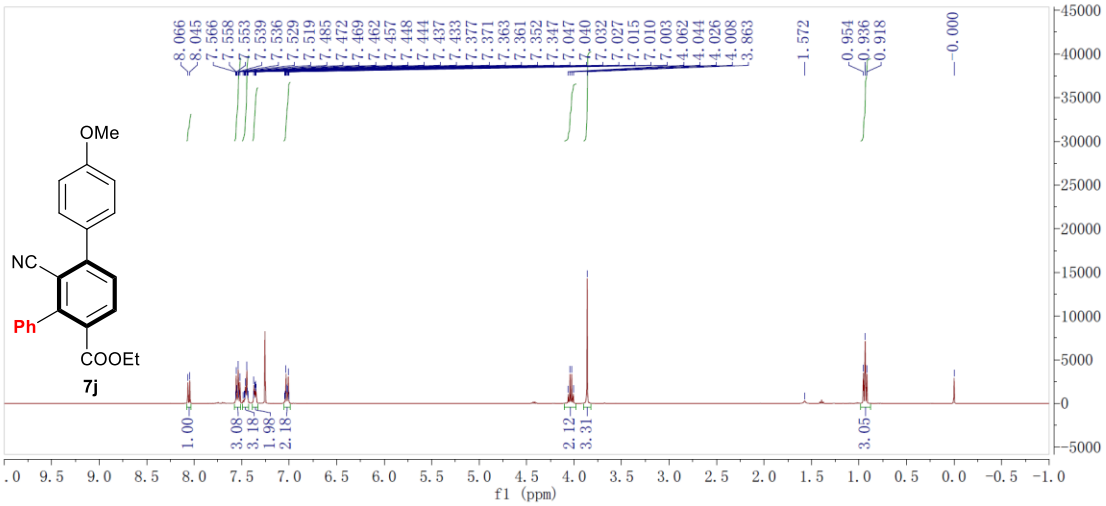
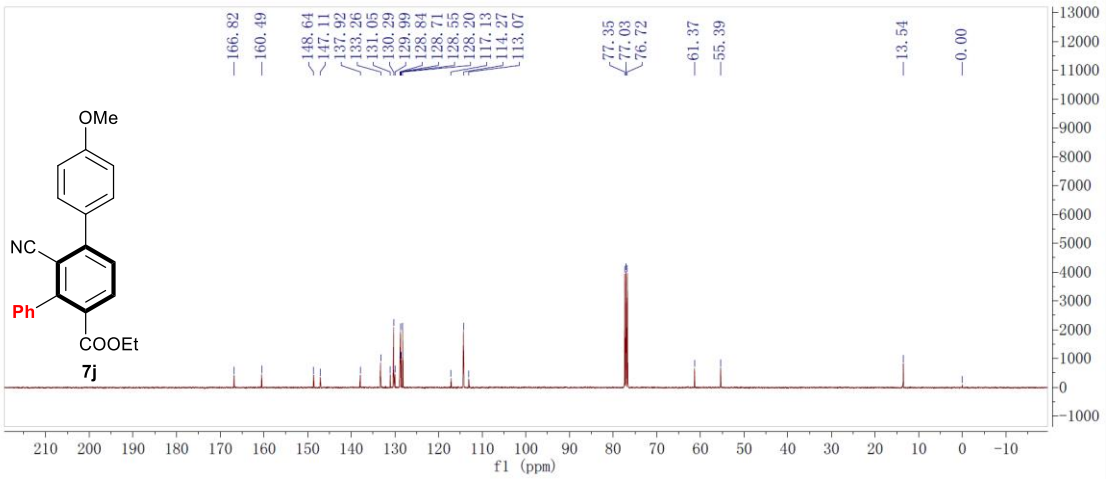
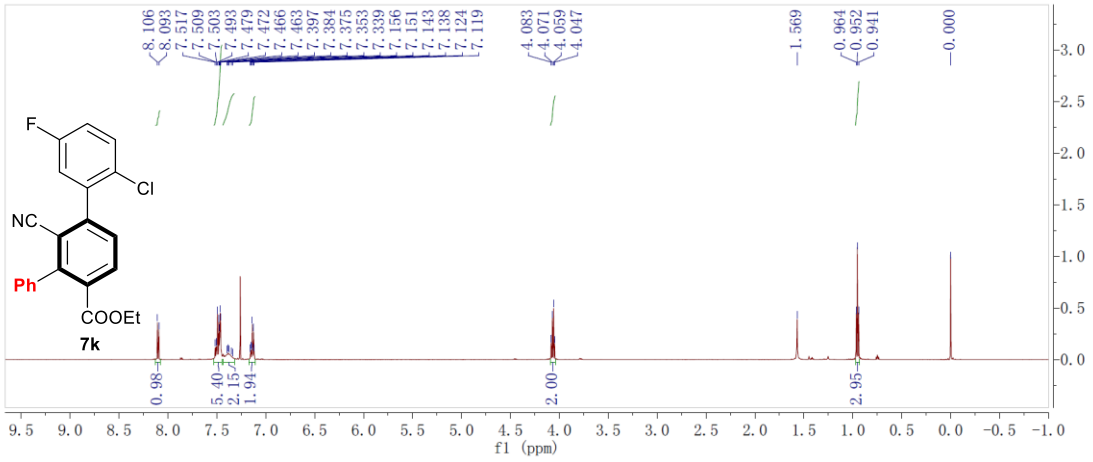
116.99
113.22
77.37
77.05
76.73
61.39
21.30
13.54
0.00
Me
NC
Ph
COOEt
7h
f1 (ppm)

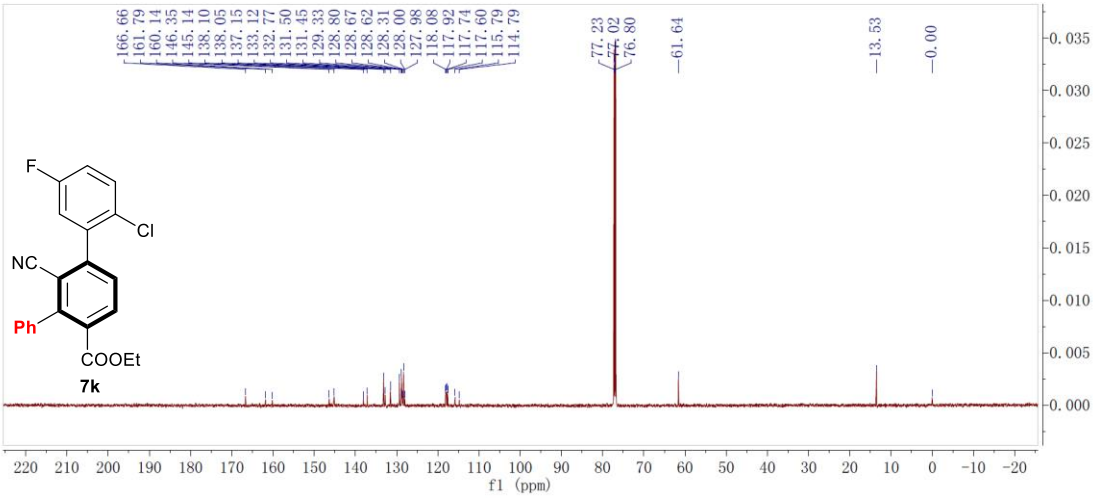

8.067
8.053
7.515
7.501
7.472
7.467
7.457
7.446
7.435
7.424
7.421
7.388
7.376
7.305
7.303
7.292
7.290
7.084
7.072
7.059
7.039
7.025
4.060
4.048
4.037
4.024
3.849
1.578
0.952
0.939
0.928
0.000
OMe
NC
Ph
COOEt
7i
0.93
1.06
4.17
1.85
1.02
1.04
0.99
2.00
3.01
3.03
f1 (ppm)

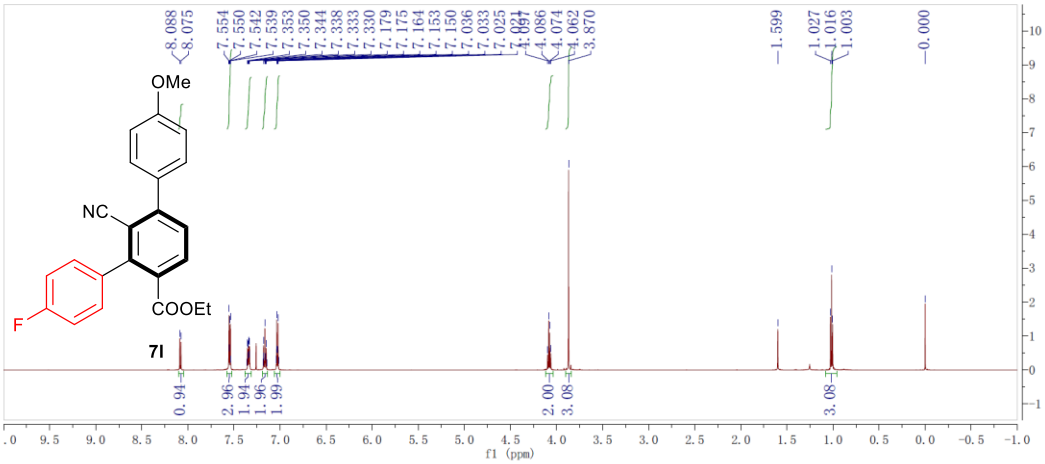

167.02
156.40
146.16
146.00
137.83
132.93
131.38
130.80
130.72
129.78
128.75
128.47
128.16
126.82
120.80
116.80
115.22
111.33
77.23
77.02
76.81
61.36
55.52
13.54
0.00
OMe
NC
Ph
COOEt
7i
f1 (ppm)

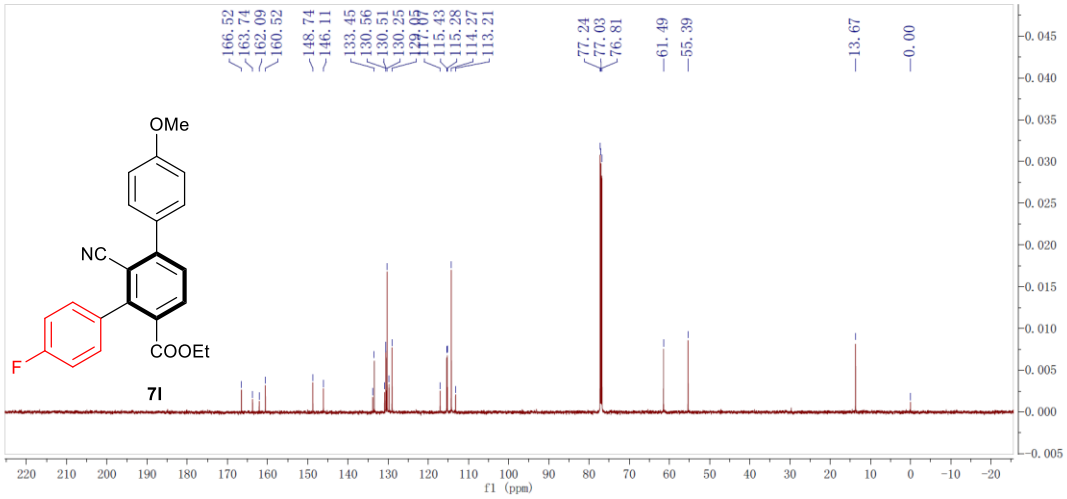

OMe
NC
Ph
COOEt
7j
f1 (ppm)

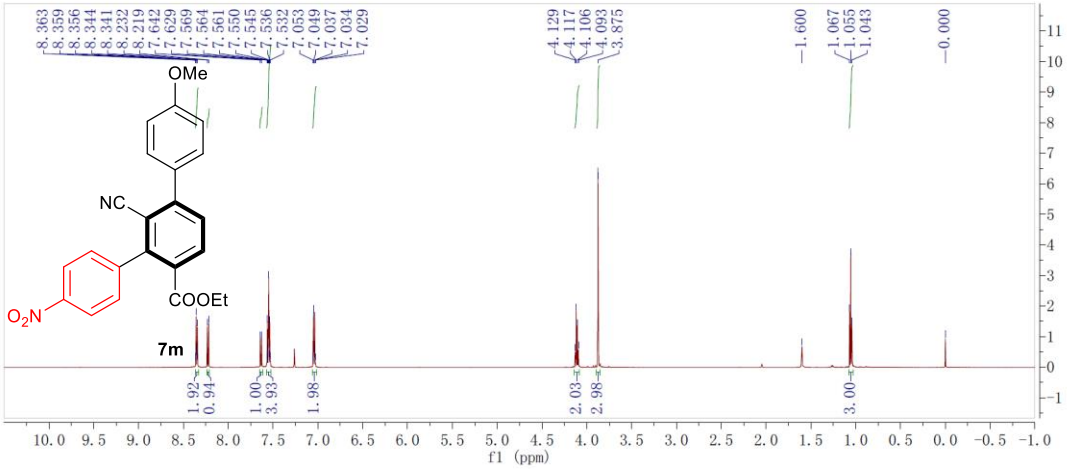

OMe
NC
Ph
COOEt
7j
f1 (ppm)

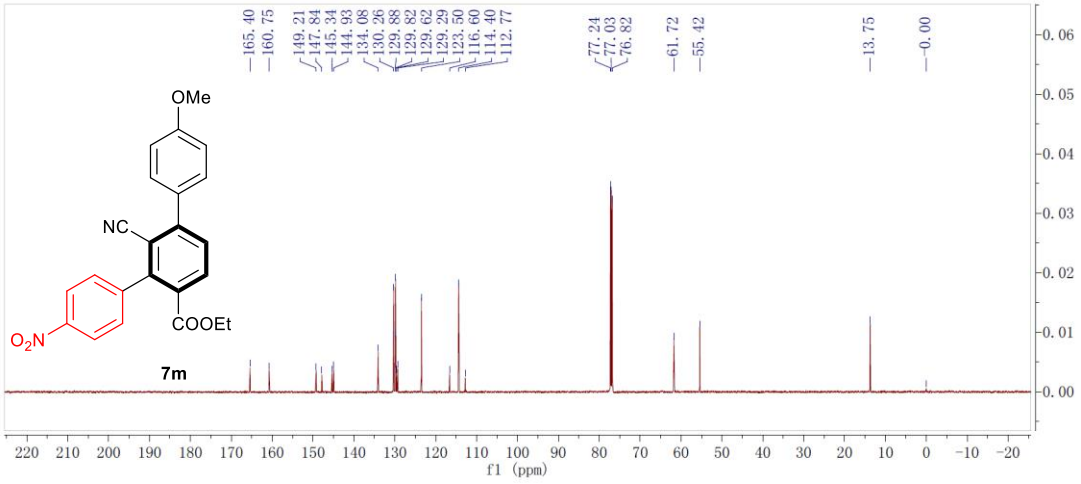

8.106
8.093
7.517
7.509
7.503
7.493
7.479
7.472
7.466
7.463
7.397
7.384
7.375
7.353
7.339
7.156
7.151
7.143
7.138
7.124
7.119
4.083
4.071
4.059
4.047
1.569
0.964
0.952
0.941
0.000
F
Cl
NC
Ph
COOEt
7k
0.98
5.40
2.15
1.94
2.00
2.95
f1 (ppm)


166.66
161.79
160.14
146.35
145.14
138.10
138.05
137.15
133.12
132.77
131.90
131.45
129.33
128.80
128.67
128.62
128.31
128.00
127.98
118.08
117.92
117.74
117.60
115.79
114.79
77.23
77.02
76.80
61.64
13.53
0.00
F
Cl
NC
Ph
COOEt
7k
f1 (ppm)

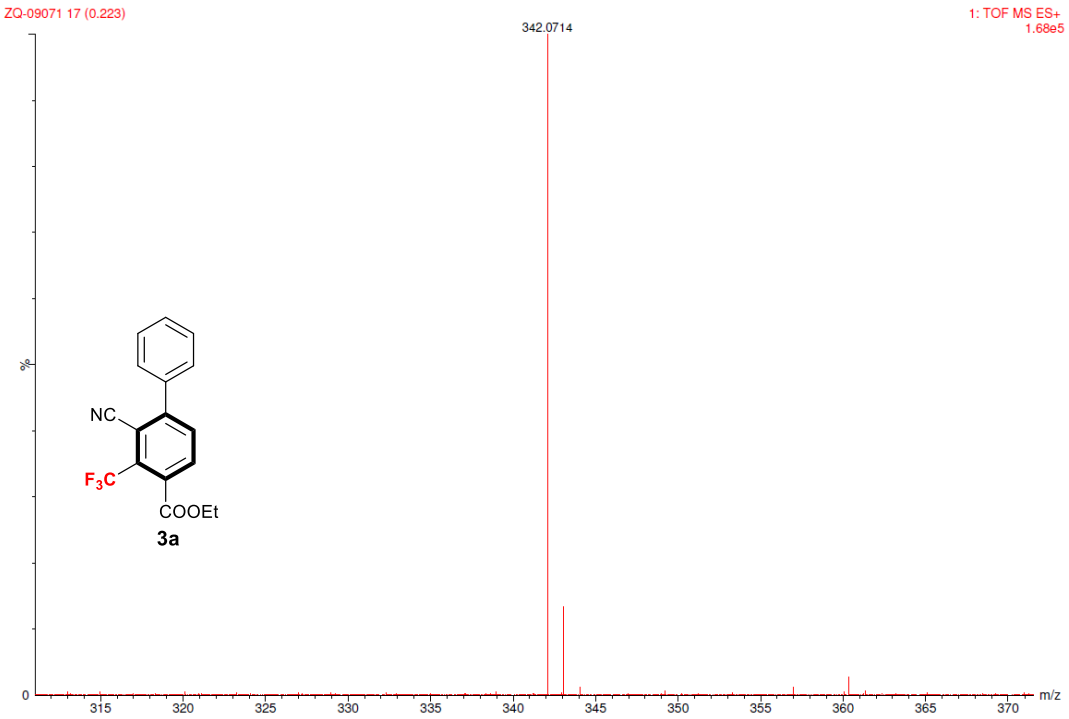

OMe
NC
COOEt
F
7l
f1 (ppm)

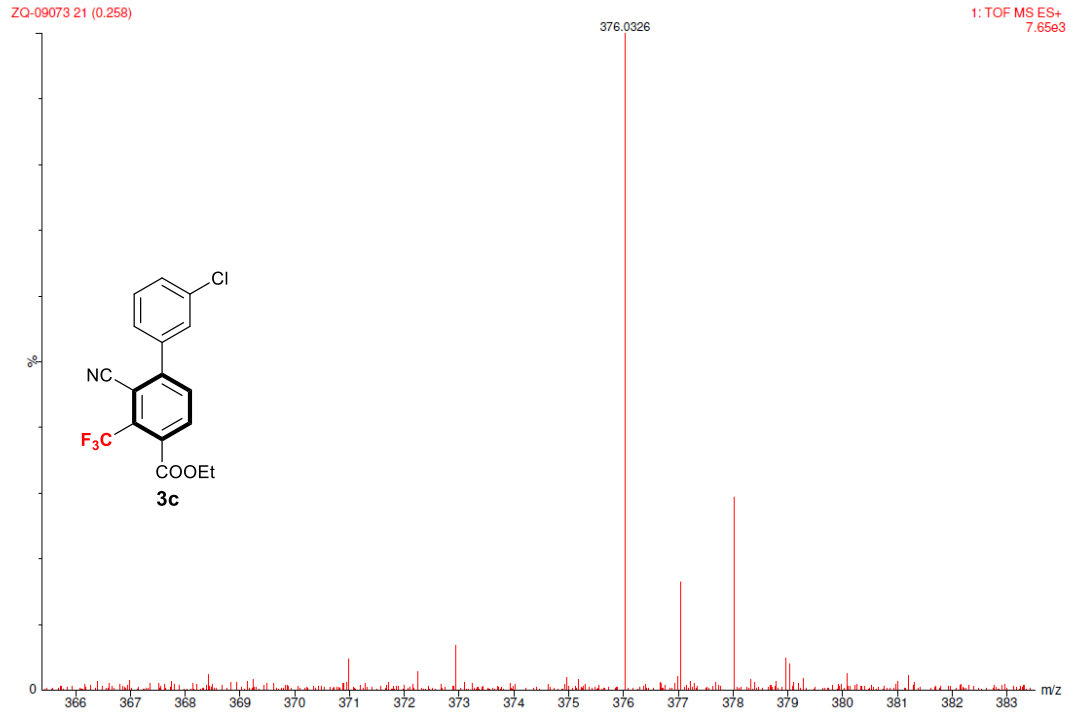

OMe
NC
COOEt
F
7l
f1 (ppm)

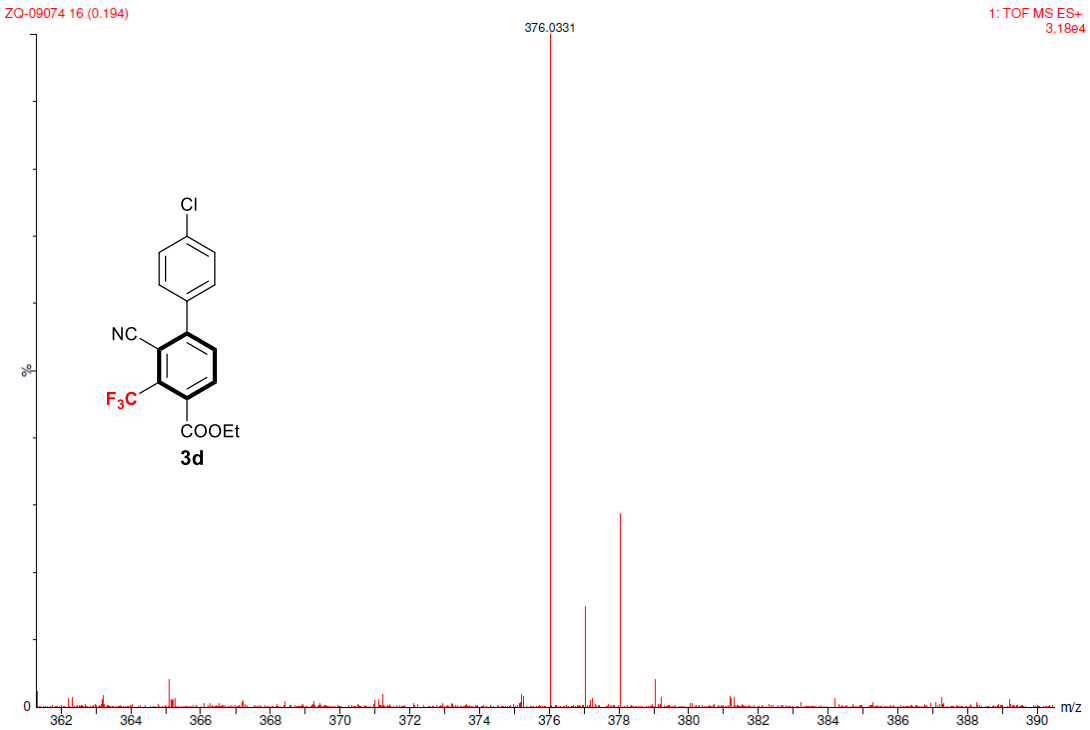

OMe
NC
COOEt
O_2N
7m
f1 (ppm)

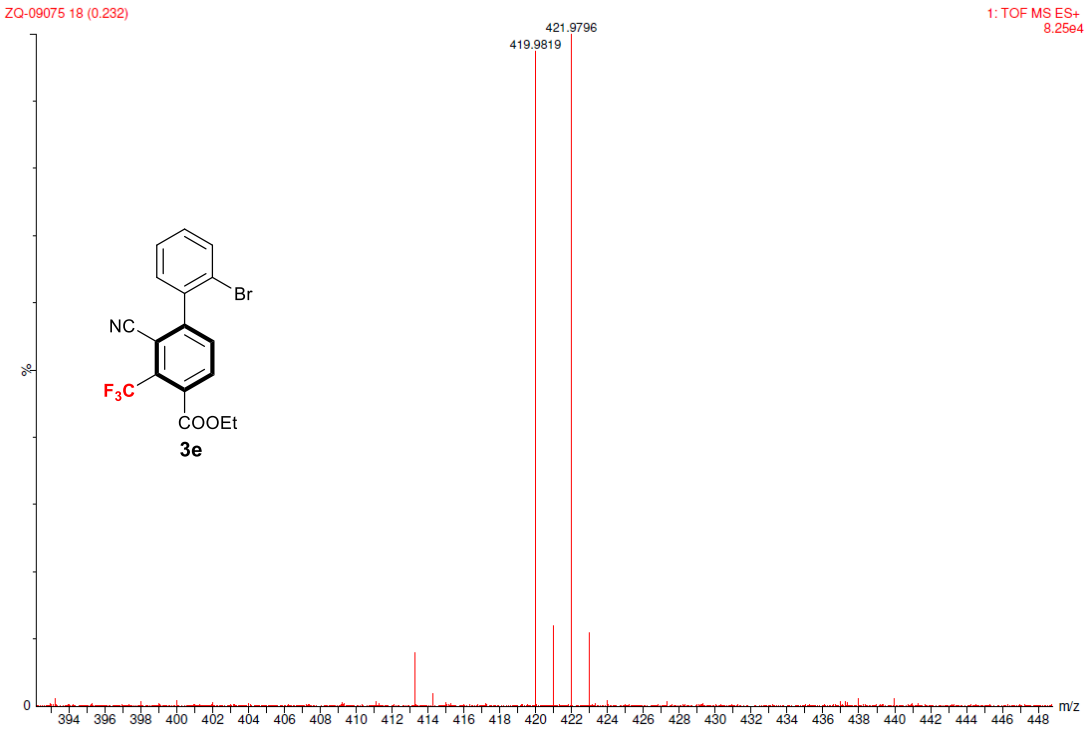

OMe
NC
COOEt
O_2N
7m
f1 (ppm)

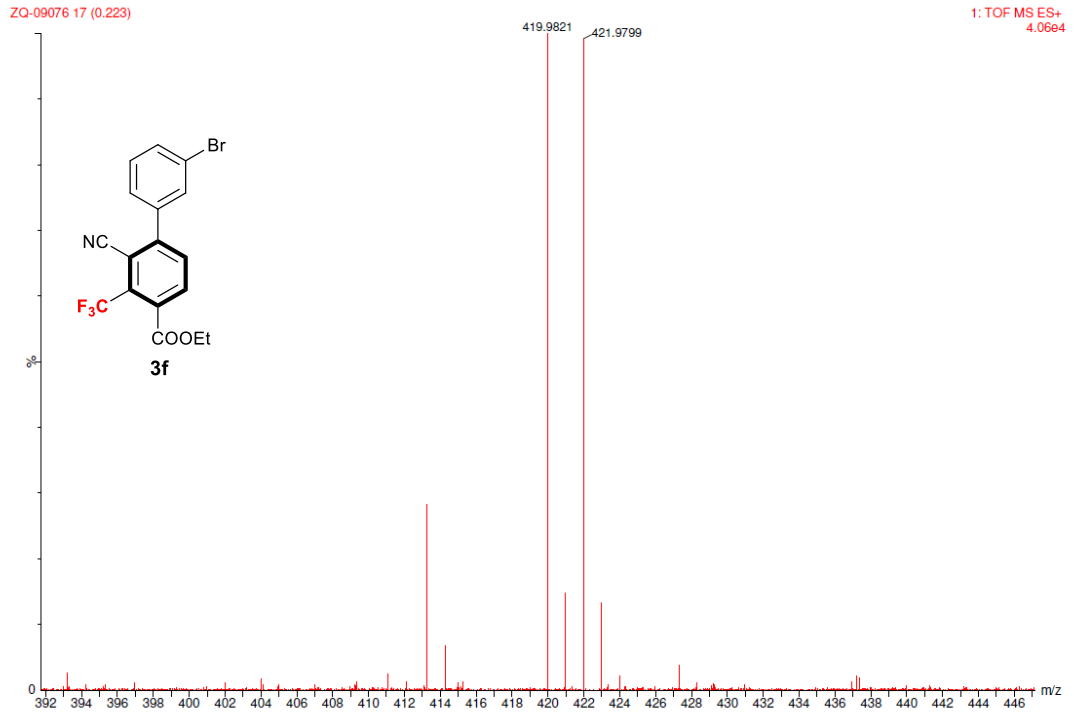
8. HRMS spectra

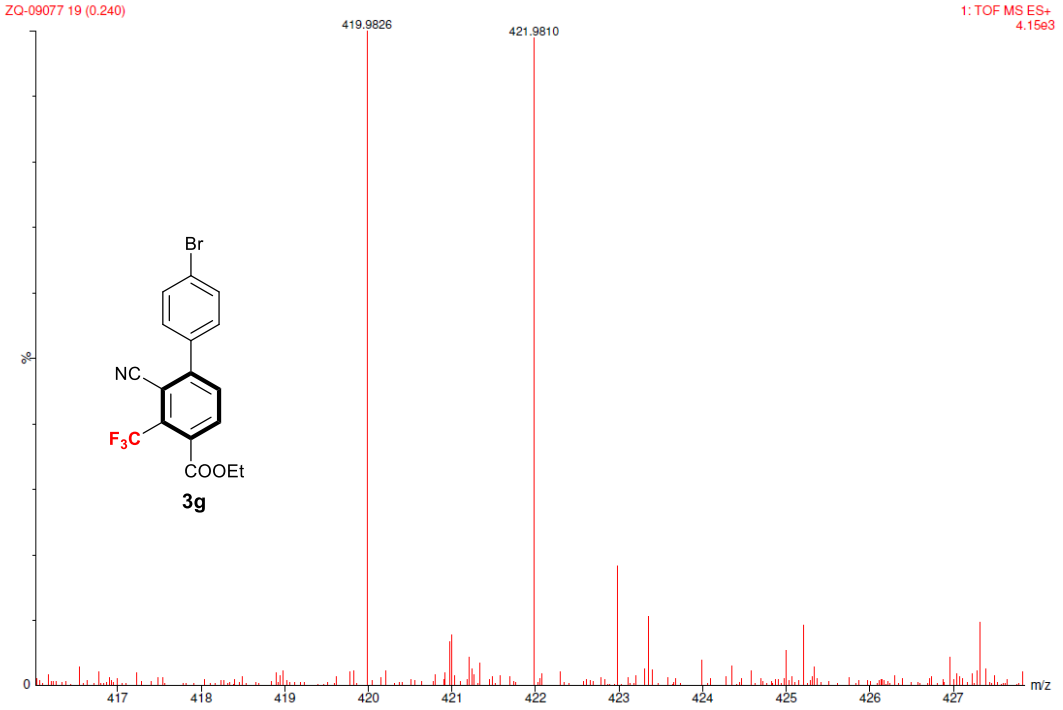


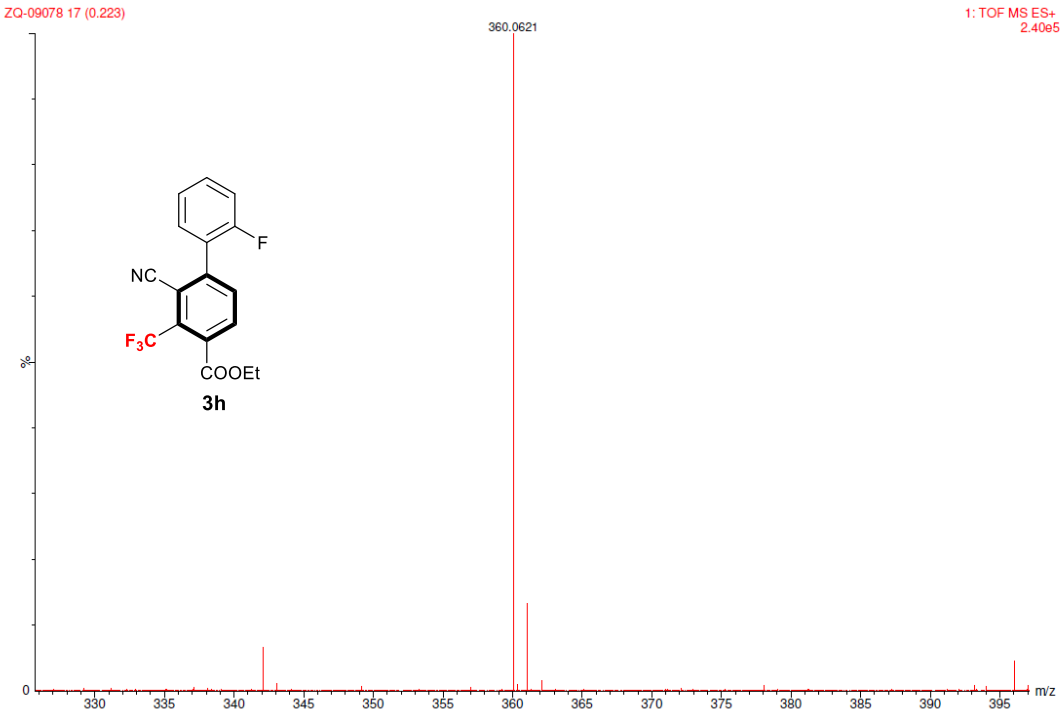

ZQ-09073 21 (0.258)
1: TOF MS ES+
7.65e3
376.0326
Cl
NC
F3C
COOEt
3c
%
0
366
367
368
369
370
371
372
373
374
375
376
377
378
379
380
381
382
383
m/z

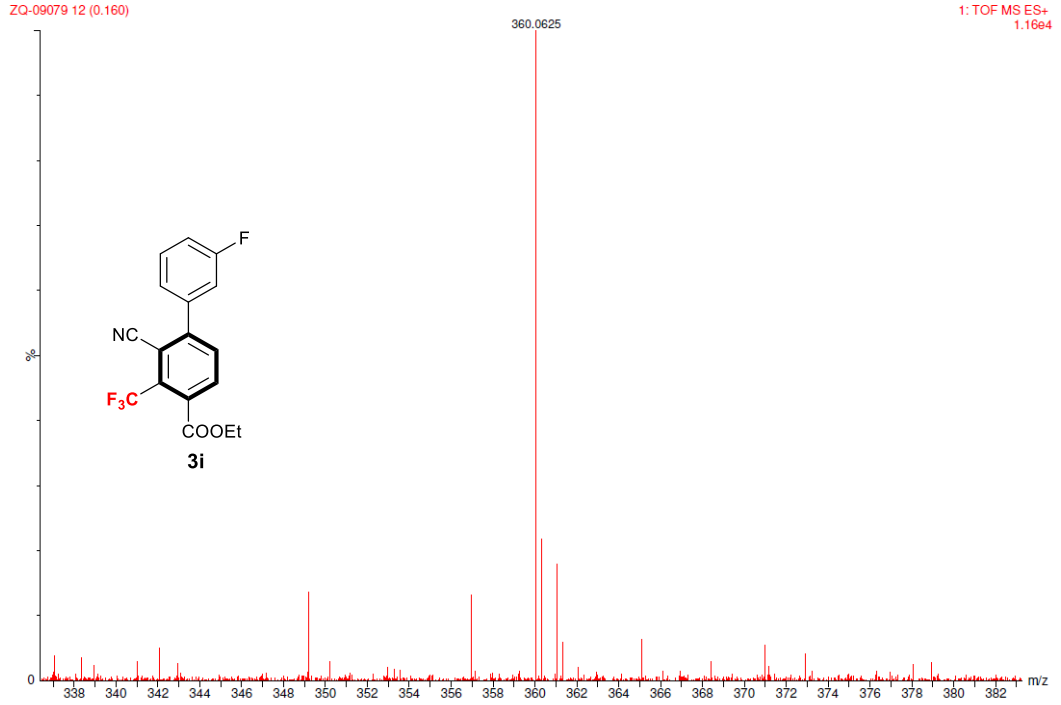

ZQ-09074 16 (0.194)
1: TOF MS ES+
3.18e4
376.0331
Cl
NC
F3C
COOEt
3d
%
0
362
364
366
368
370
372
374
376
378
380
382
384
386
388
390
m/z

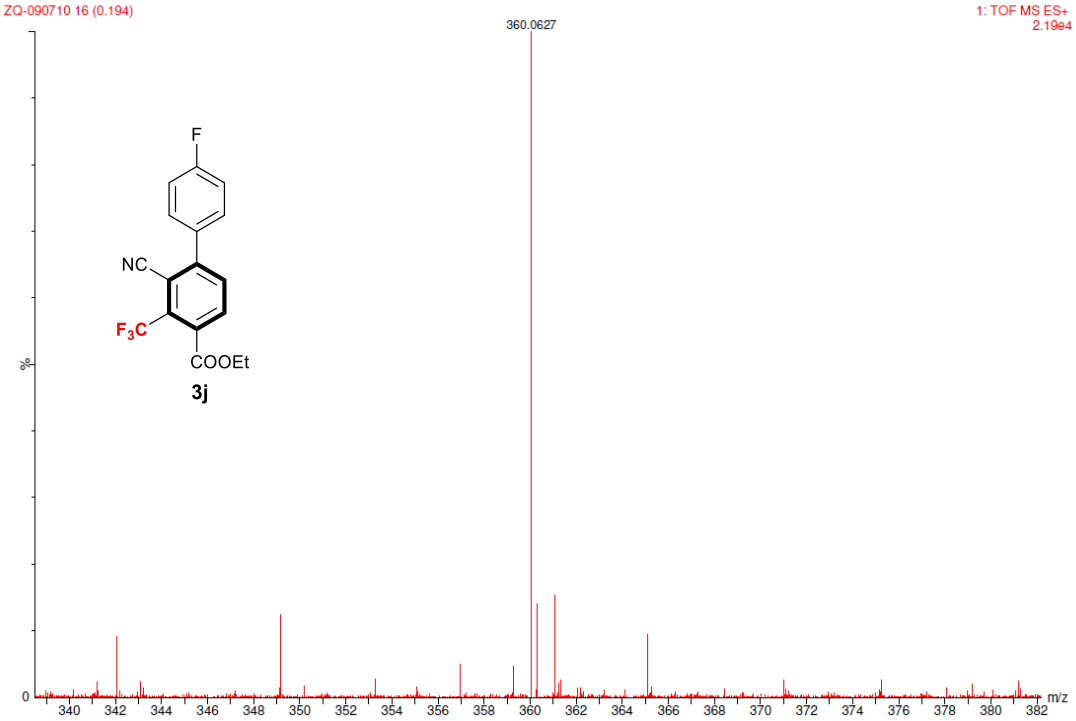

ZQ-09075 18 (0.232)
1: TOF MS ES+
8.25e4
421.9796
419.9819
Br
NC
F3C
COOEt
3e
%
0
394 396 398 400 402 404 406 408 410 412 414 416 418 420 422 424 426 428 430 432 434 436 438 440 442 444 446 448
m/z

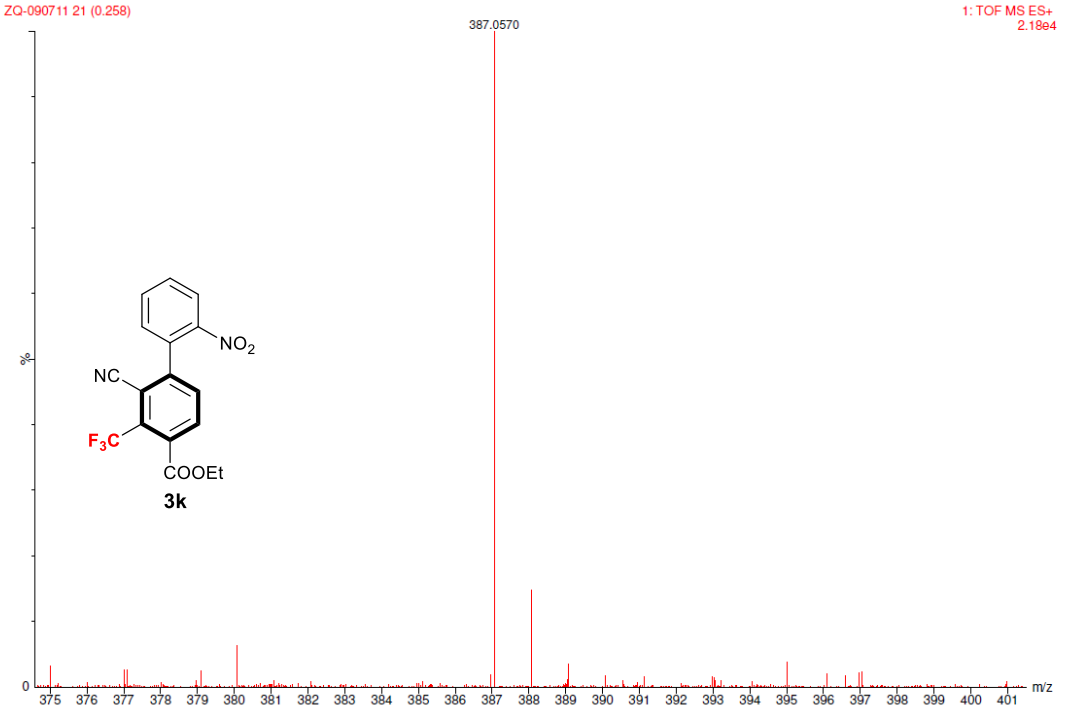

ZQ-09076 17 (0.223)
1: TOF MS ES+
4.06e4
419.9821
421.9799
Br
NC
F3C
COOEt
3f
%
0
392 394 396 398 400 402 404 406 408 410 412 414 416 418 420 422 424 426 428 430 432 434 436 438 440 442 444 446
m/z


ZQ-09077 19 (0.240)
1: TOF MS ES+
4.15e3
419.9826
421.9810
Br
NC
F3C
COOEt
3g
%
0
417
418
419
420
421
422
423
424
425
426
427
m/z

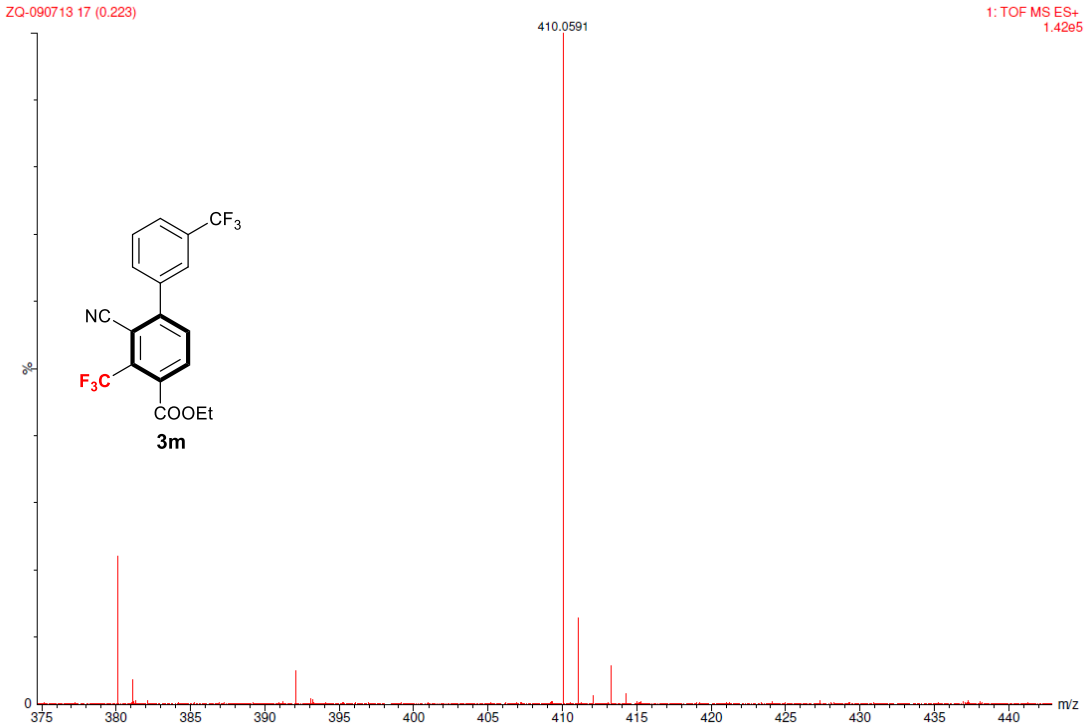

ZQ-09078 17 (0.223)
1: TOF MS ES+
2.40e5
360.0621
F
NC
F3C
COOEt
3h
%
0
330
335
340
345
350
355
360
365
370
375
380
385
390
395
m/z

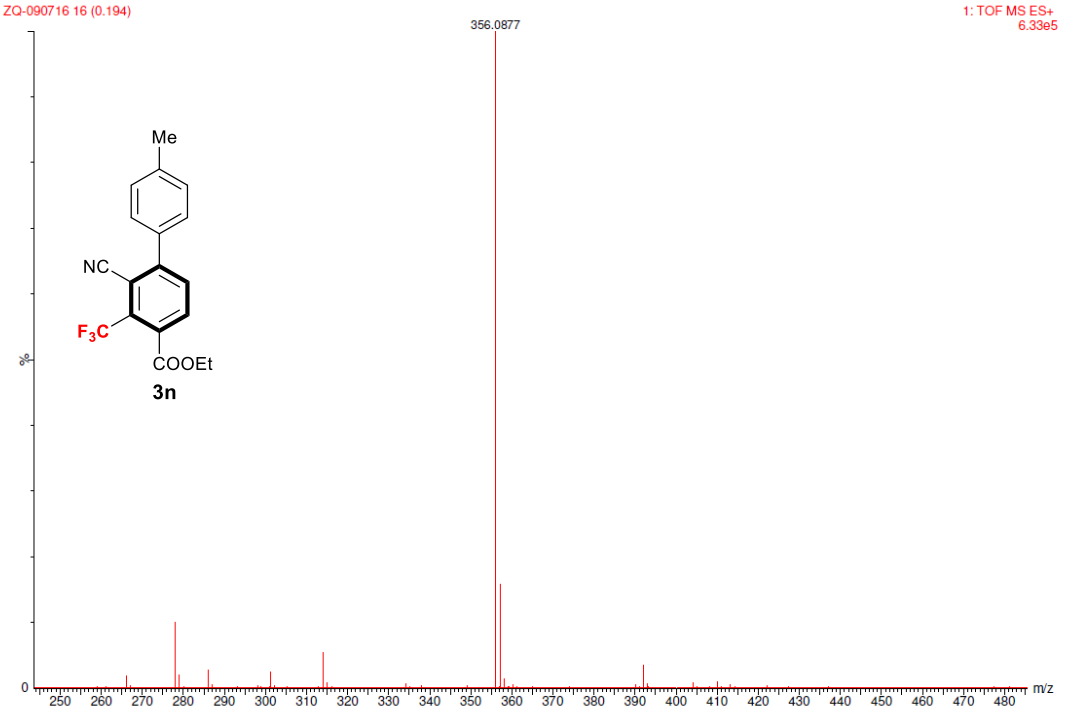

ZQ-09079 12 (0.160)
1: TOF MS ES+
1.16e4
360.0625
F
NC
F3C
COOEt
3i
%
0
338 340 342 344 346 348 350 352 354 356 358 360 362 364 366 368 370 372 374 376 378 380 382
m/z

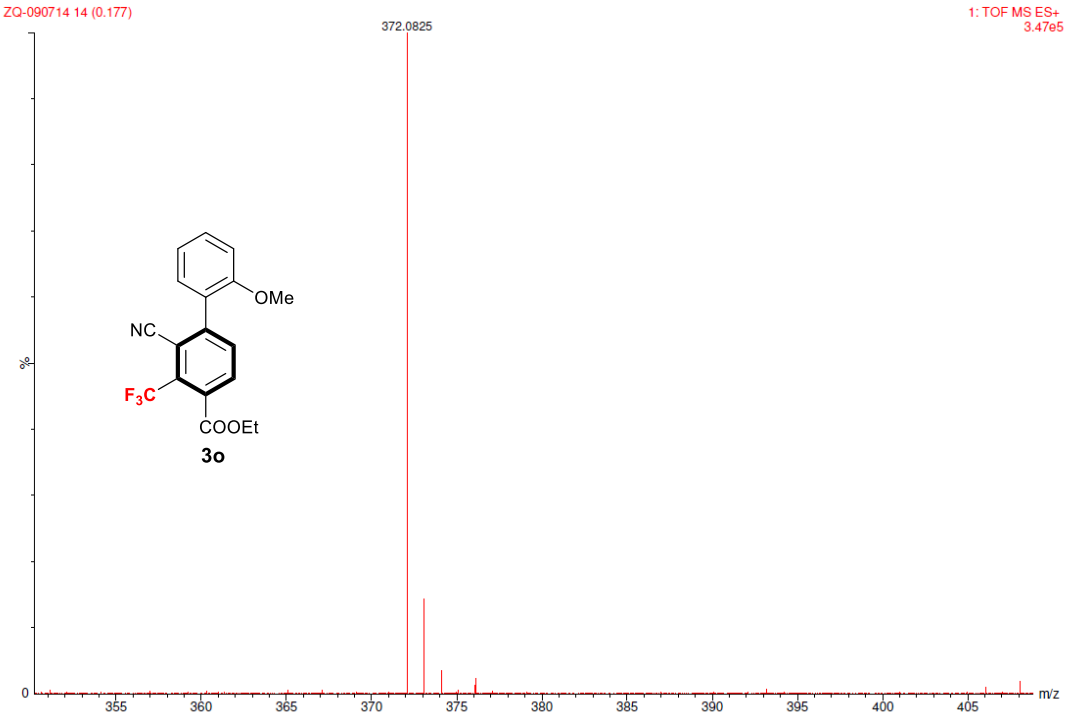

ZQ-090710 16 (0.194)
1: TOF MS ES+
2.19e4
360.0627
F
NC
F3C
COOEt
3j
%
0
340 342 344 346 348 350 352 354 356 358 360 362 364 366 368 370 372 374 376 378 380 382
m/z

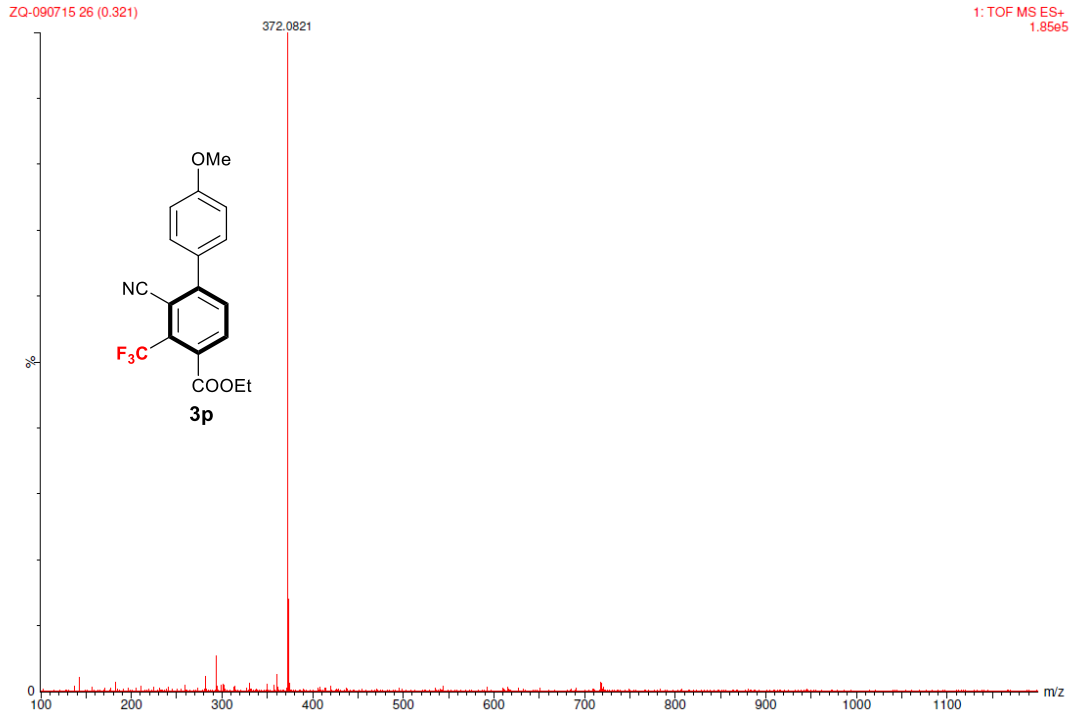

ZQ-090711 21 (0.258)
1: TOF MS ES+
2.18e4
387.0570
%
NC
NO_2
F_3C
COOEt
3k
0
375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401
m/z

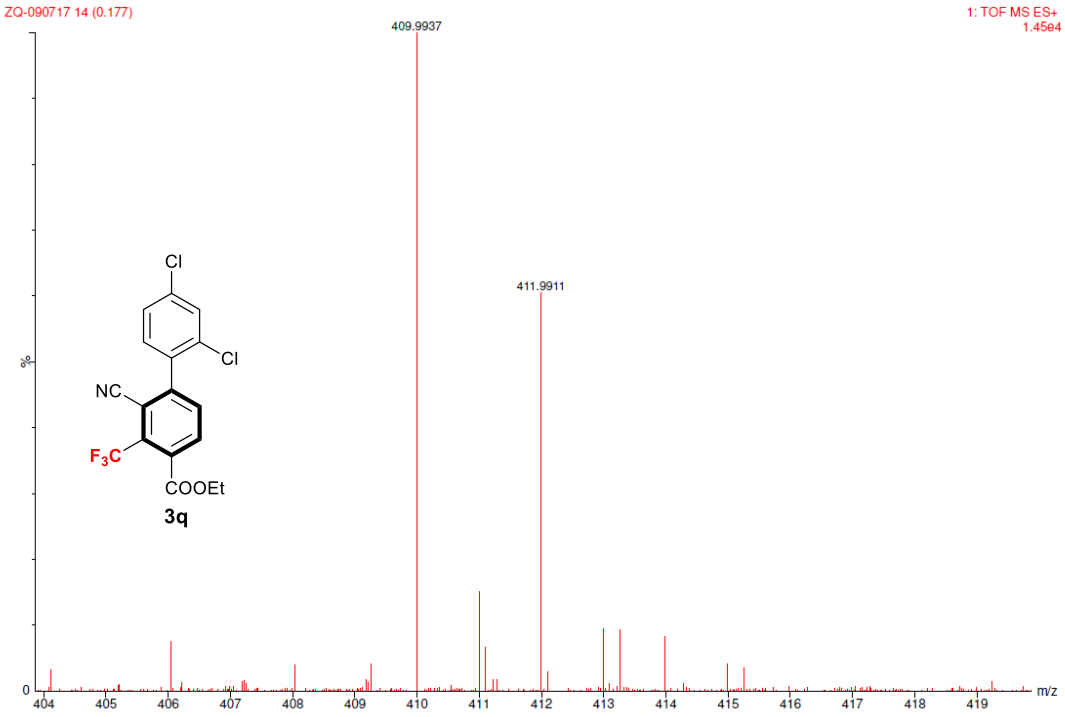

ZQ-090712 12 (0.159)
1: TOF MS ES+
2.43e3
387.0569
%
NO_2
NC
F_3C
COOEt
3l
0
385 386 387 388 389
m/z


ZQ-090713 17 (0.223)
1: TOF MS ES+
1.42e5
410.0591
CF3
NC
F3C
COOEt
3m
%
0
375 380 385 390 395 400 405 410 415 420 425 430 435 440
m/z

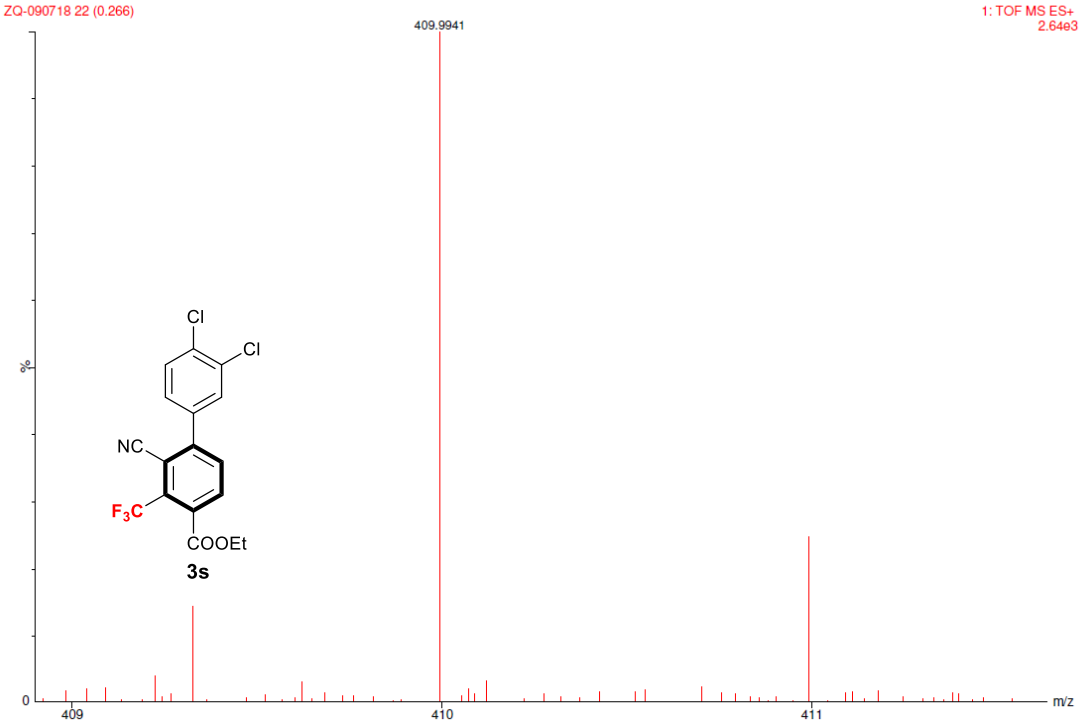

ZQ-090716 16 (0.194)
1: TOF MS ES+
6.33e5
356.0877
Me
NC
F3C
COOEt
3n
%
0
250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460 470 480
m/z

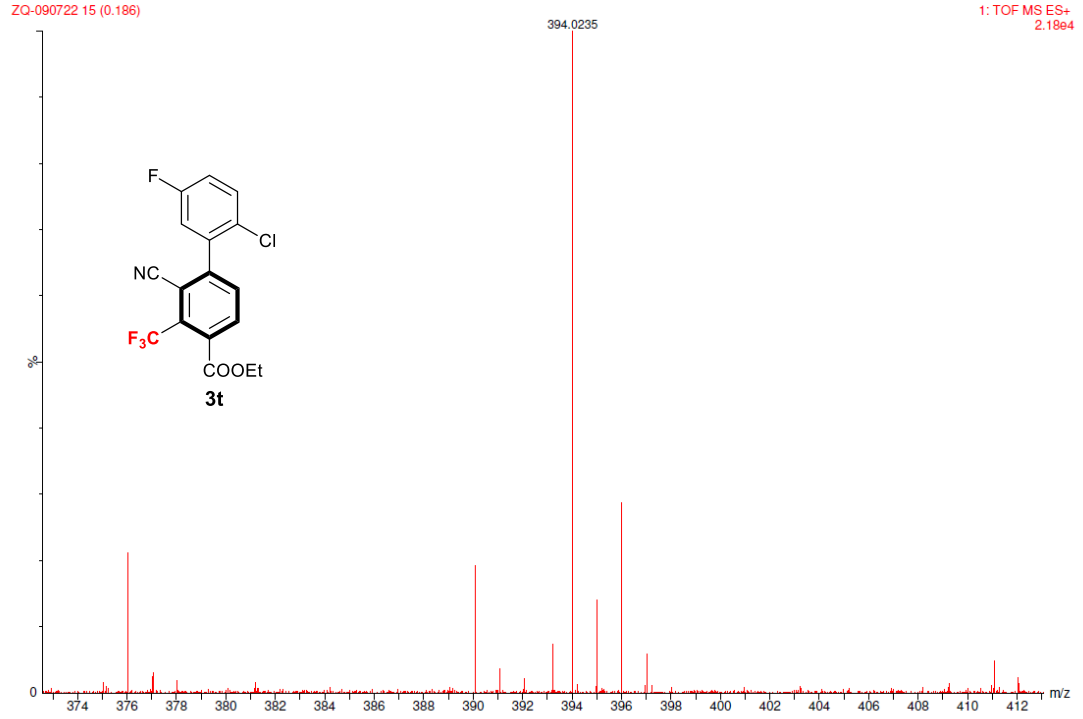

ZQ-090714 14 (0.177)
1: TOF MS ES+
3.47e5
372.0825
OMe
NC
F3C
COOEt
3o
%
0
355
360
365
370
375
380
385
390
395
400
405
m/z

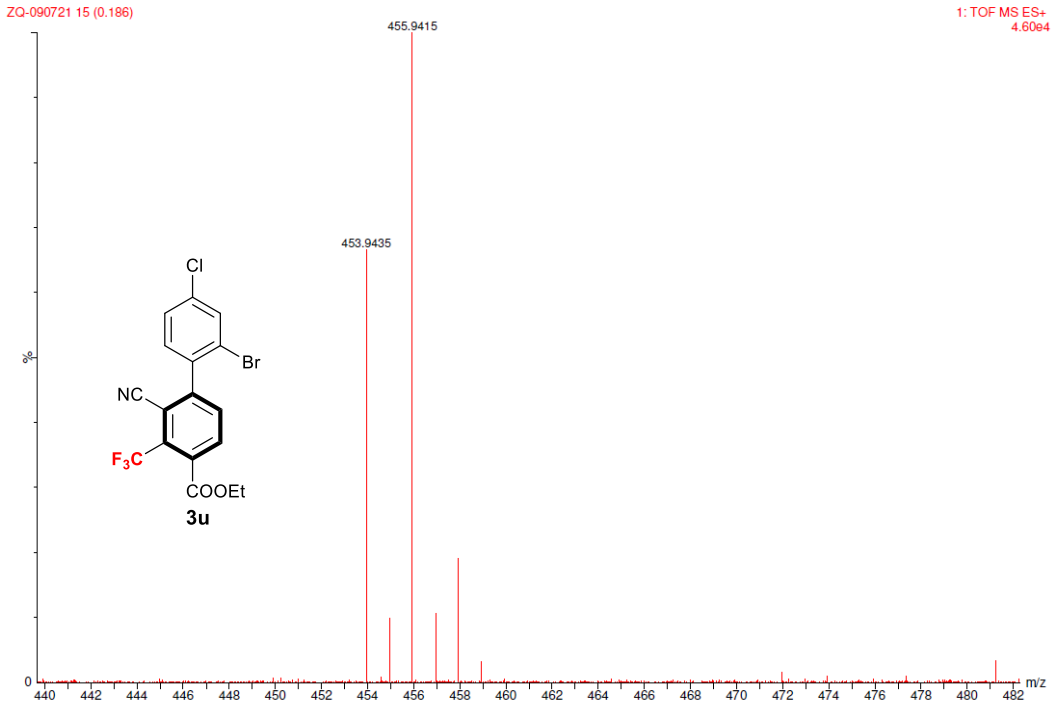

ZQ-090715 26 (0.321)
1: TOF MS ES+
1.85e5
372.0821
OMe
NC
F3C
COOEt
3p
%
0
100
200
300
400
500
600
700
800
900
1000
1100
m/z

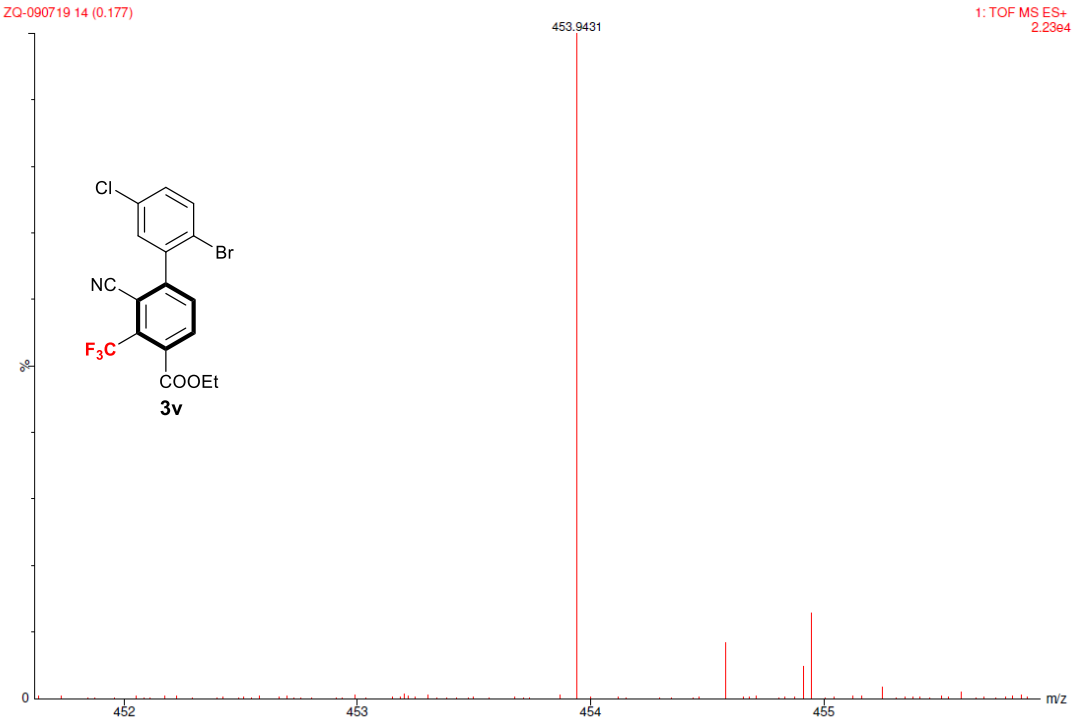

ZQ-090717 14 (0.177)
1: TOF MS ES+
1.45e4
409.9937
411.9911
Cl
Cl
NC
F3C
COOEt
3q
%
0
404
405
406
407
408
409
410
411
412
413
414
415
416
417
418
419
m/z

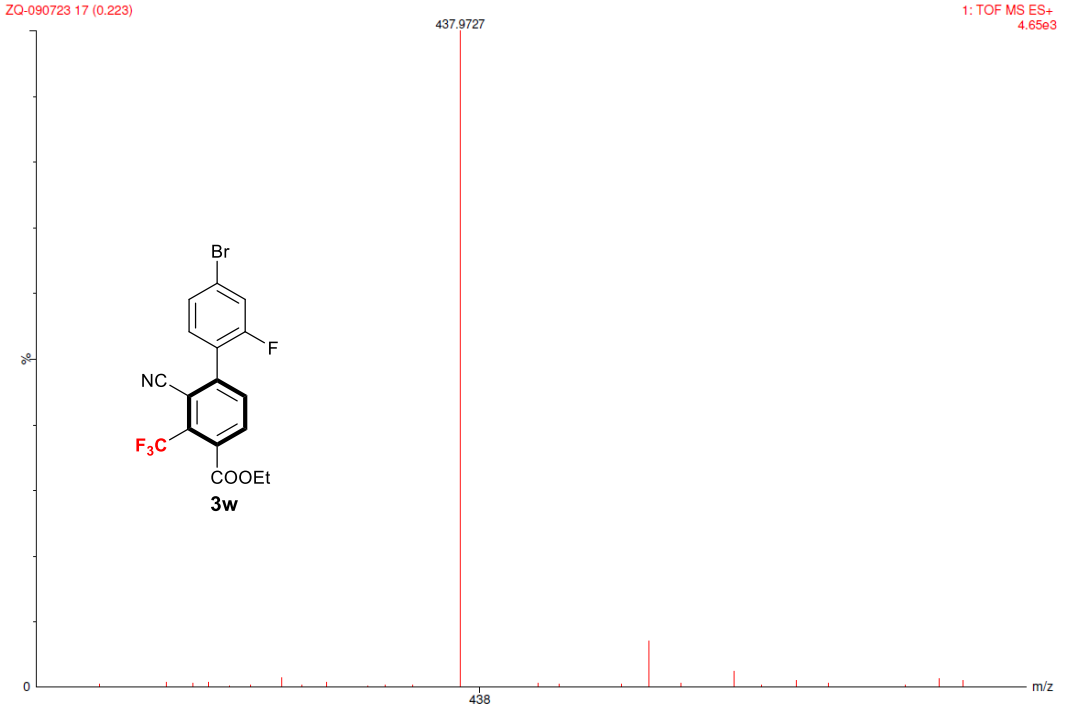

ZQ-090717 16 (0.194)
1: TOF MS ES+
1.78e4
409.9940
Cl
Cl
NC
F3C
COOEt
3r
%
0
409
410
411
m/z

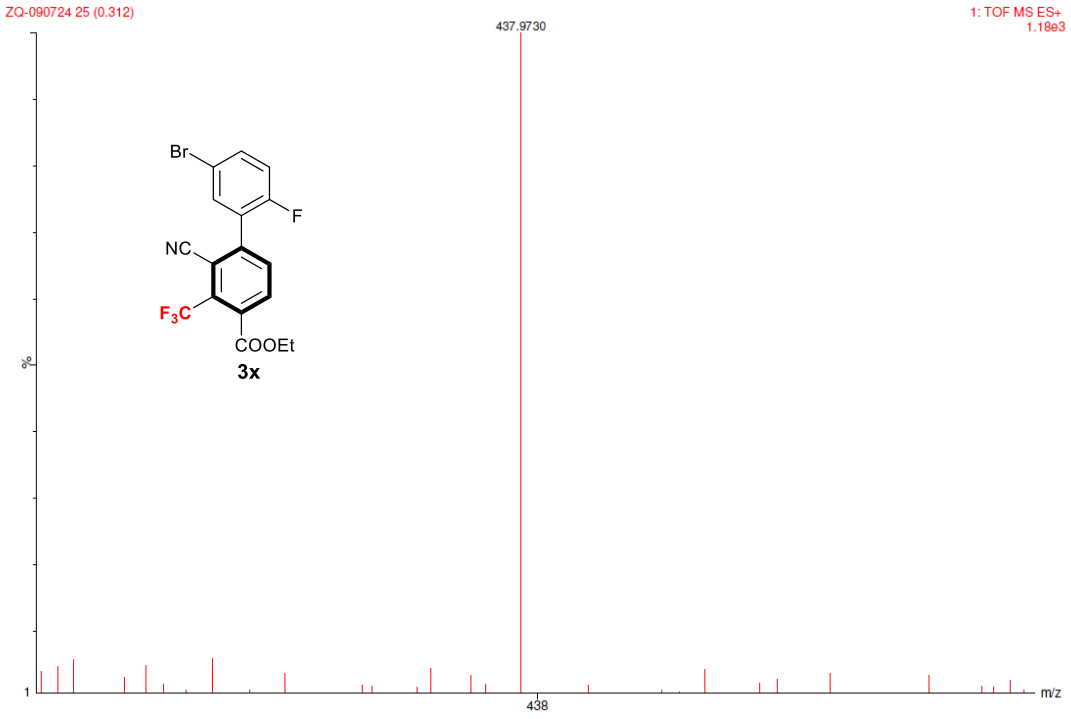

ZQ-090718 22 (0.266)
1: TOF MS ES+
2.64e3
409.9941
Cl
Cl
NC
F3C
COOEt
3s
%
0
409
410
411
m/z

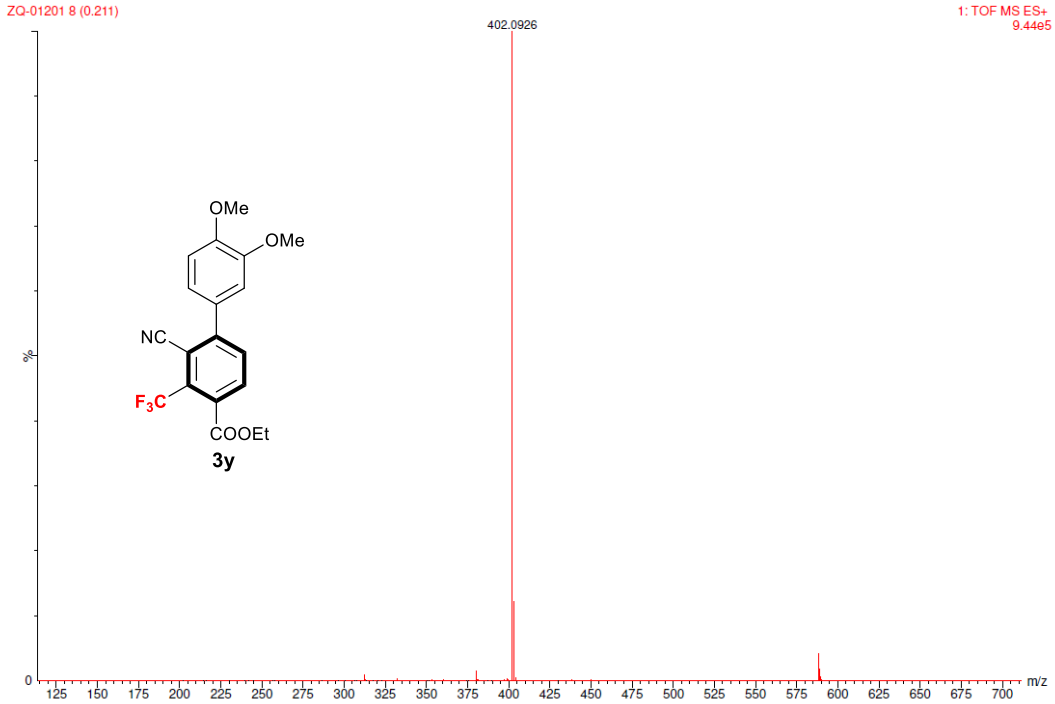

ZQ-090722 15 (0.186)
1: TOF MS ES+
2.18e4
394.0235
F
Cl
NC
F3C
COOEt
3t
%
0
374
376
378
380
382
384
386
388
390
392
394
396
398
400
402
404
406
408
410
412
m/z

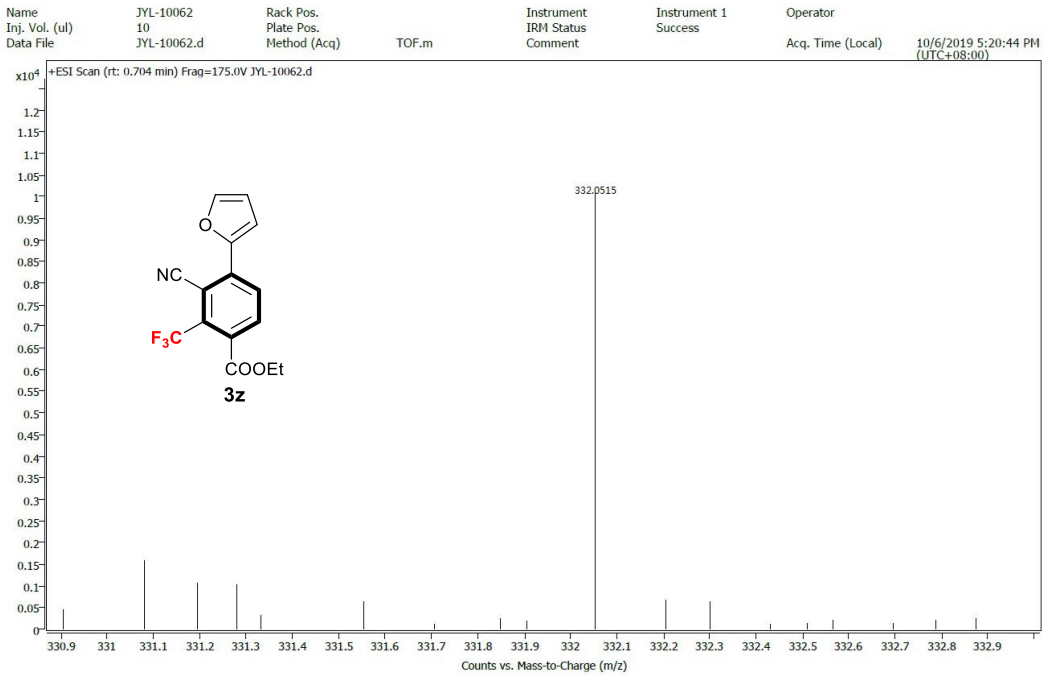

ZQ-090721 15 (0.186)
1: TOF MS ES+
4.60e4
455.9415
453.9435
Cl
Br
NC
F3C
COOEt
3u
%
0
440 442 444 446 448 450 452 454 456 458 460 462 464 466 468 470 472 474 476 478 480 482
m/z

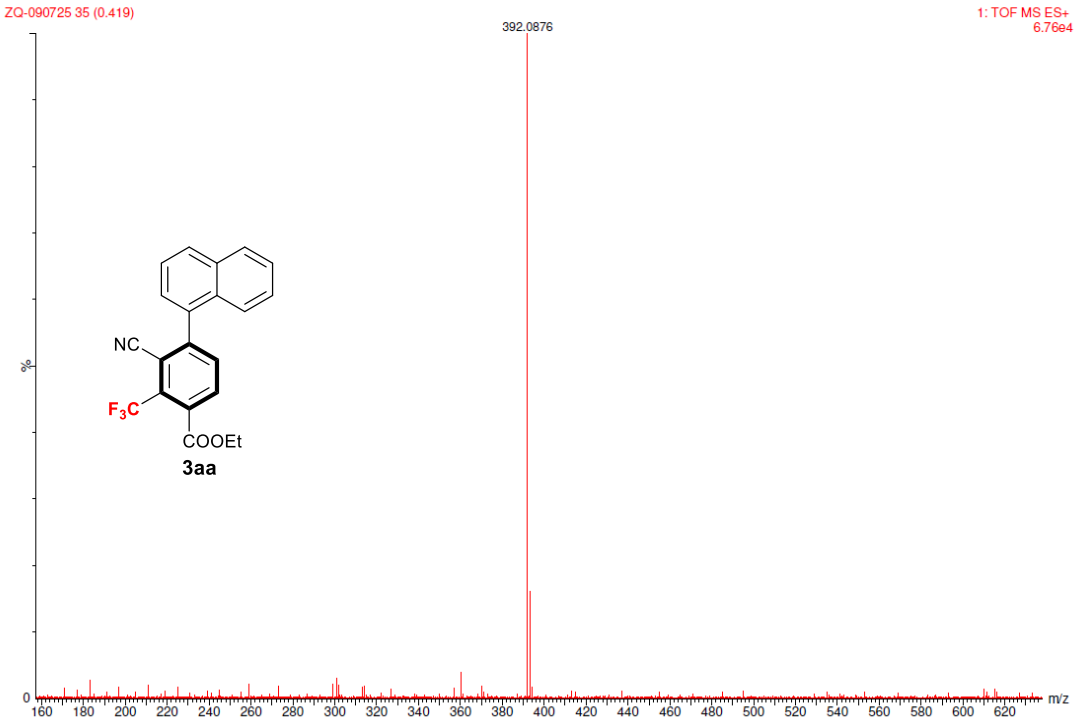

ZQ-090719 14 (0.177)
1: TOF MS ES+
2.23e4
453.9431
Cl
Br
NC
F3C
COOEt
3v
%
0
452
453
454
455
m/z

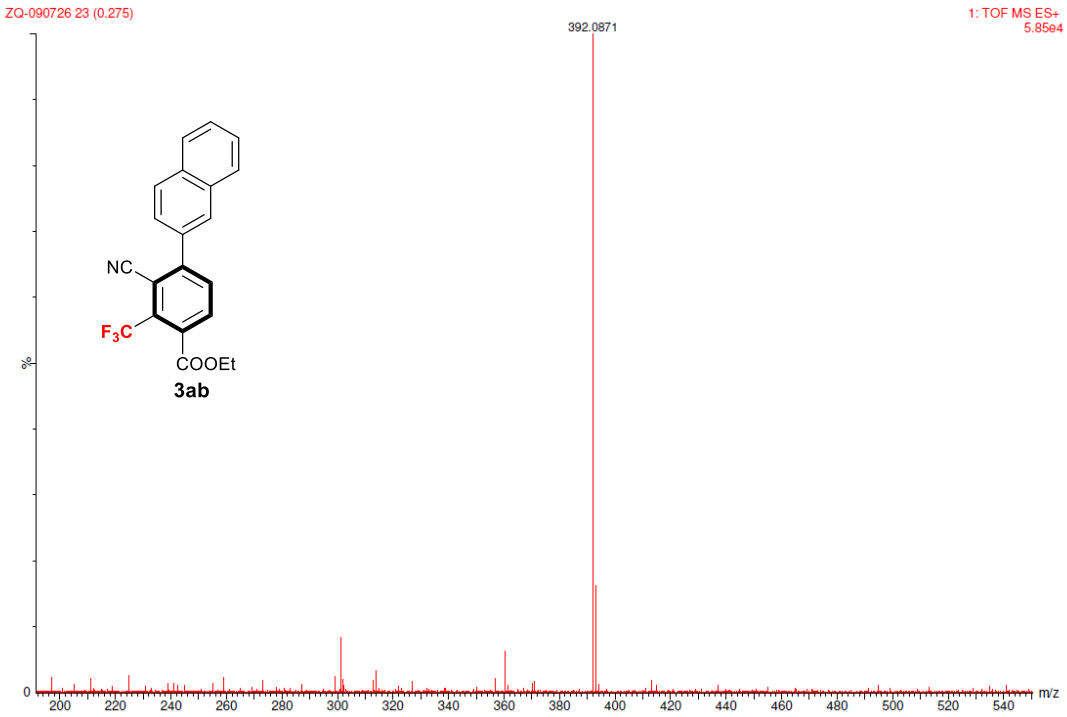

ZQ-090723 17 (0.223)
1: TOF MS ES+
4.65e3
437.9727
Br
F
NC
F3C
COOEt
3w
%
0
438
m/z

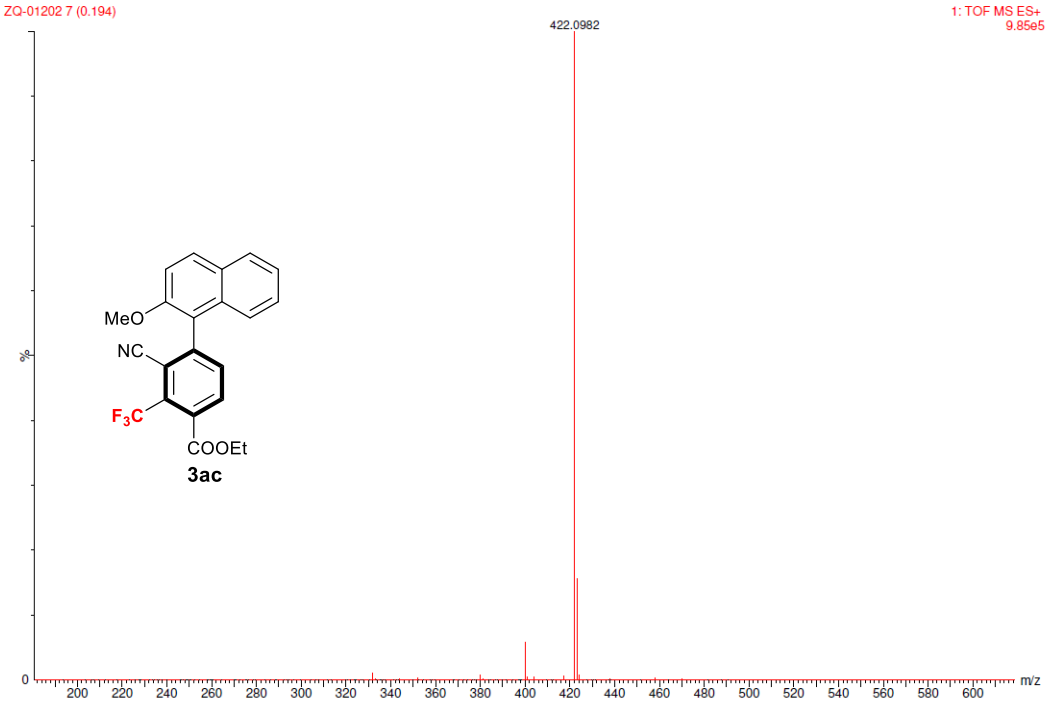

ZQ-090724 25 (0.312)
1: TOF MS ES+
1.18e3
437.9730
Br
F
NC
F3C
COOEt
3x
%
1
438
m/z

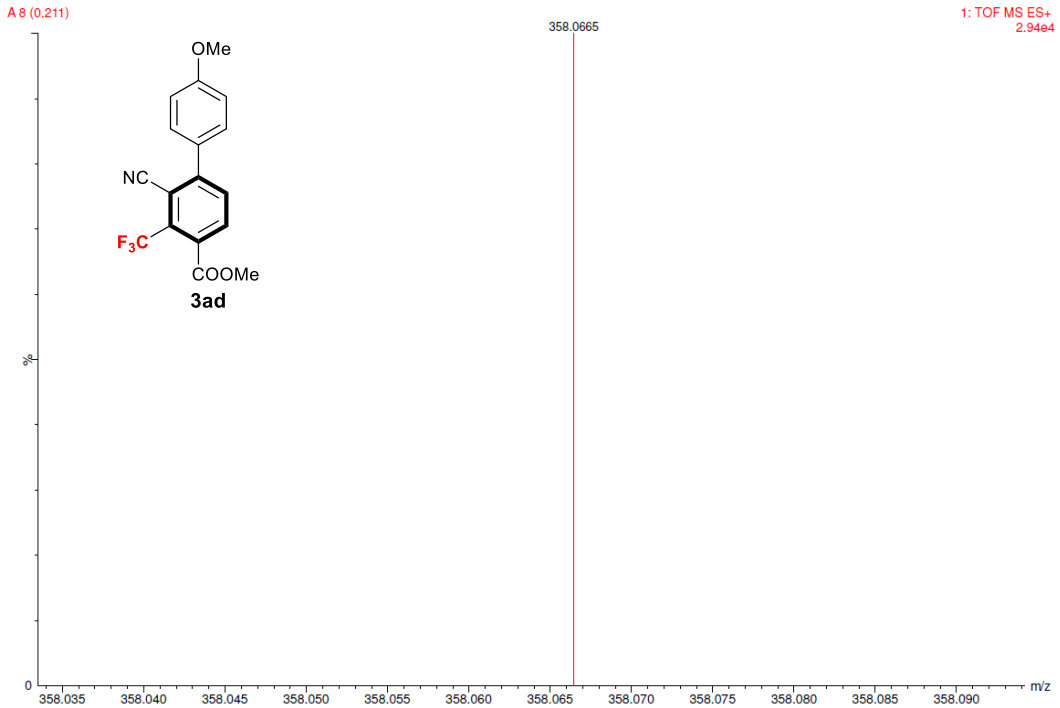

ZQ-01201 8 (0.211)
1: TOF MS ES+
9.44e5
402.0926
OMe
OMe
NC
F3C
COOEt
3y
%
0
125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700
m/z

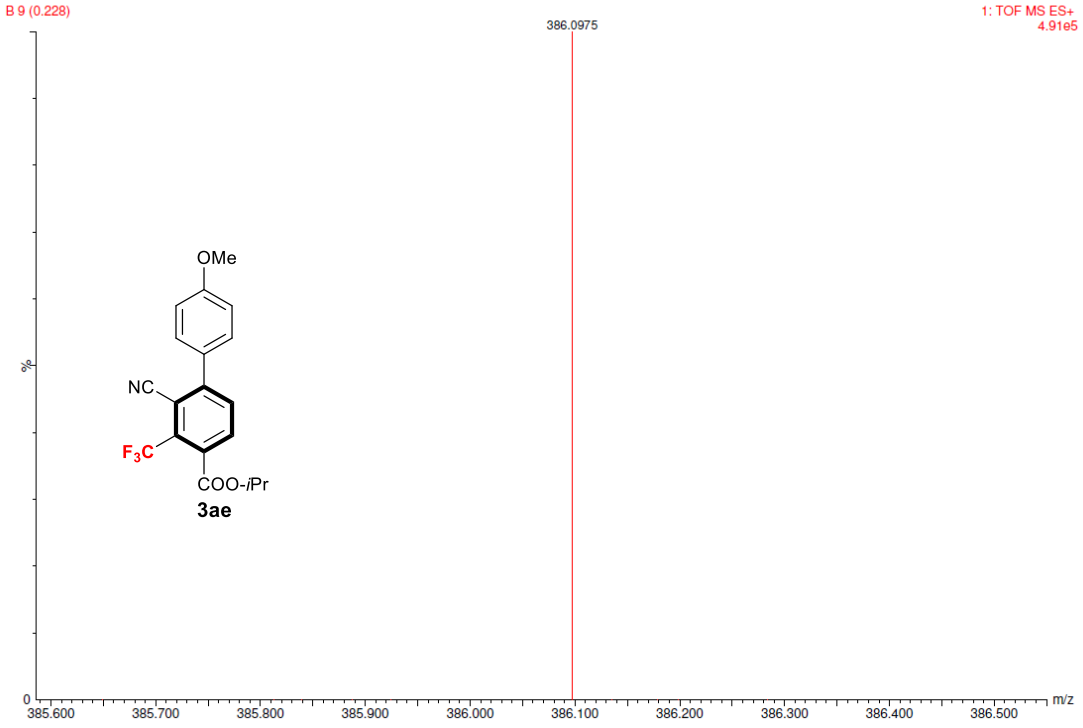

Name JYL-10062
Inj. Vol. (ul) 10
Data File JYL-10062.d
Rack Pos.
Plate Pos.
Method (Acq) TOF.m
Instrument
IRM Status
Comment
Instrument 1
Success
Operator
Acq. Time (Local) 10/6/2019 5:20:44 PM (UTC+08:00)
+ESI Scan (rt: 0.704 min) Frag=175.0V JYL-10062.d
x10^4
332.0515
O
NC
F3C
COOEt
3z
Counts vs. Mass-to-Charge (m/z)

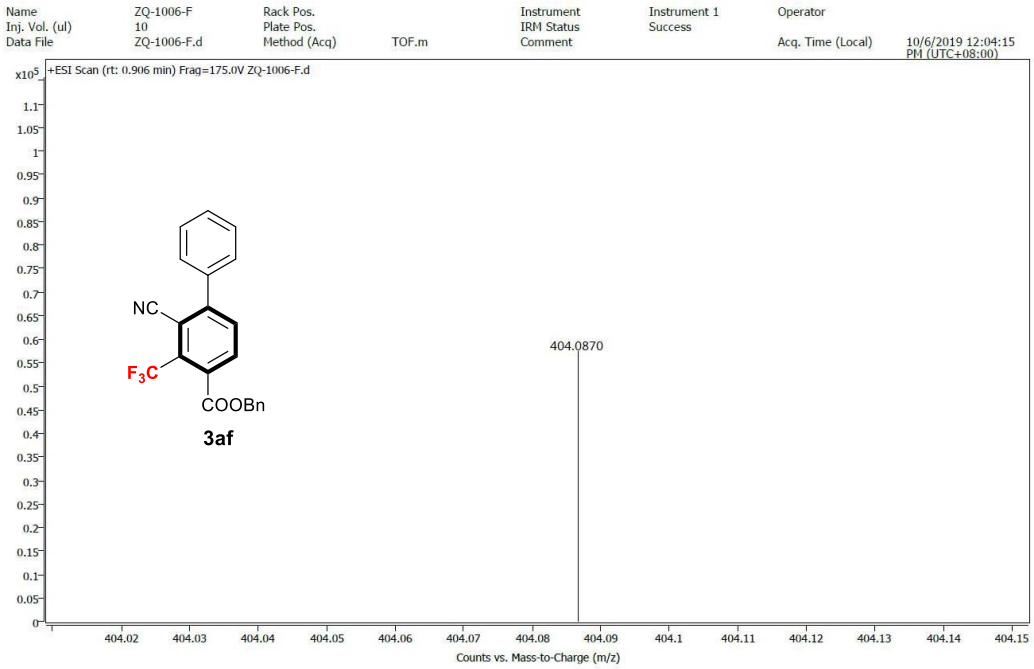

ZQ-090725 35 (0.419)
1: TOF MS ES+
6.76e4
392.0876
NC
F3C
COOEt
3aa
%
0
160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620
m/z


ZQ-090726 23 (0.275)
1: TOF MS ES+
5.85e4
392.0871
NC
F3C
COOEt
3ab
%
0
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540
m/z

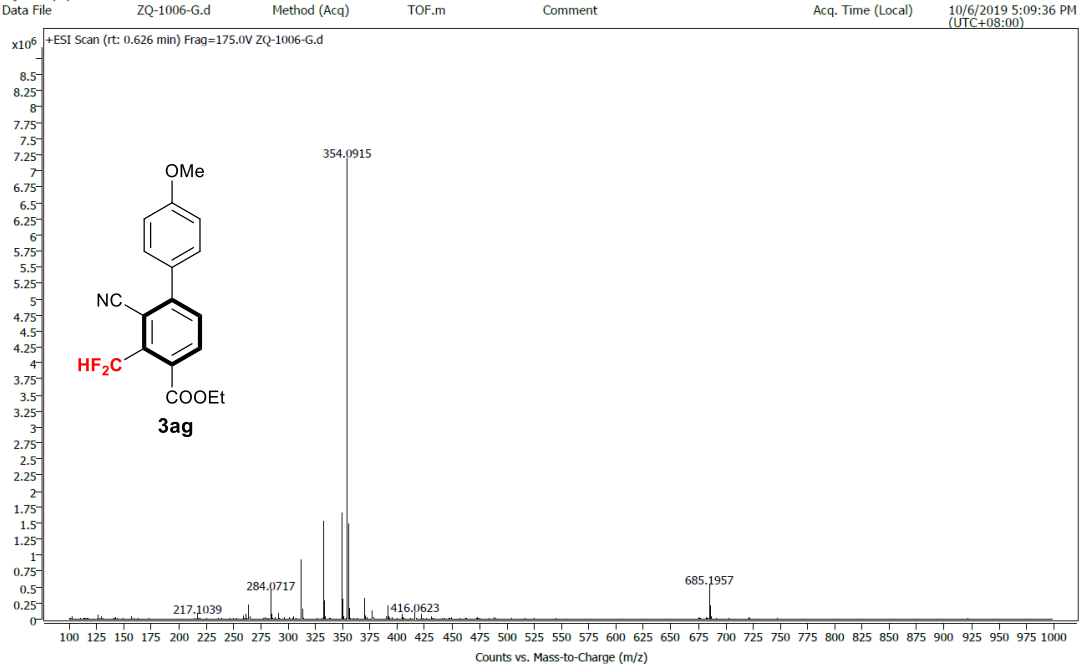

ZQ-01202 7 (0.194)
1: TOF MS ES+
9.85e5
422.0982
MeO
NC
F3C
COOEt
3ac
%
0
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600
m/z


A 8 (0.211)
1: TOF MS ES+
2.94e4
358.0665
OMe
NC
F3C
COOMe
3ad
%
0
358.035 358.040 358.045 358.050 358.055 358.060 358.065 358.070 358.075 358.080 358.085 358.090
m/z

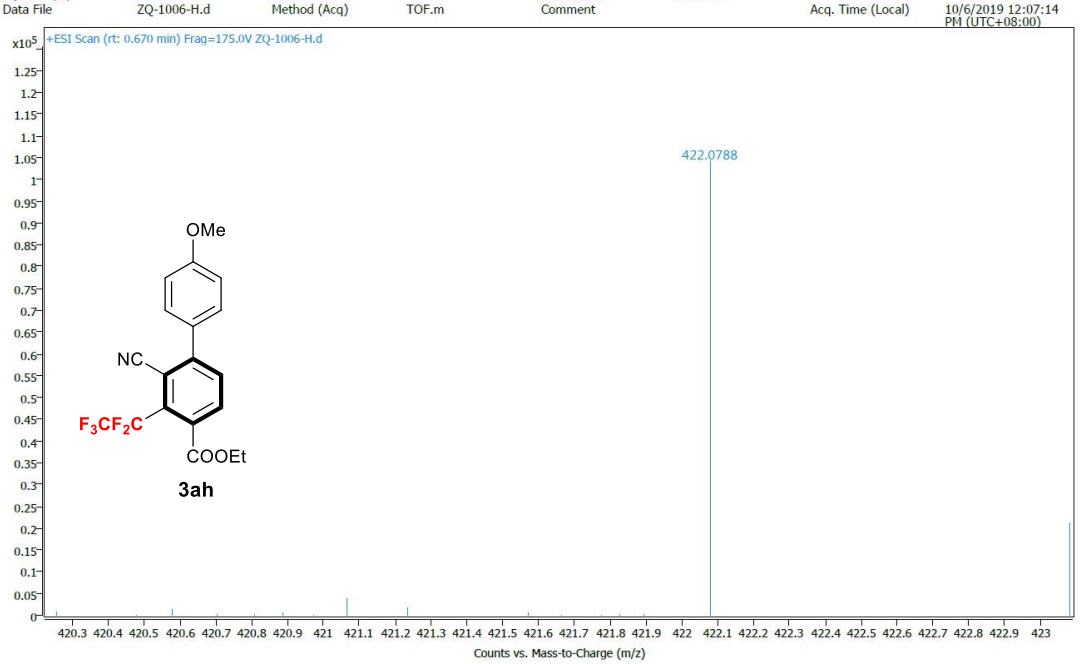

B 9 (0.228)
1: TOF MS ES+
4.91e5
386.0975
%
0
385.600
385.700
385.800
385.900
386.000
386.100
386.200
386.300
386.400
386.500
m/z
OMe
NC
F3C
COO-iPr
3ae

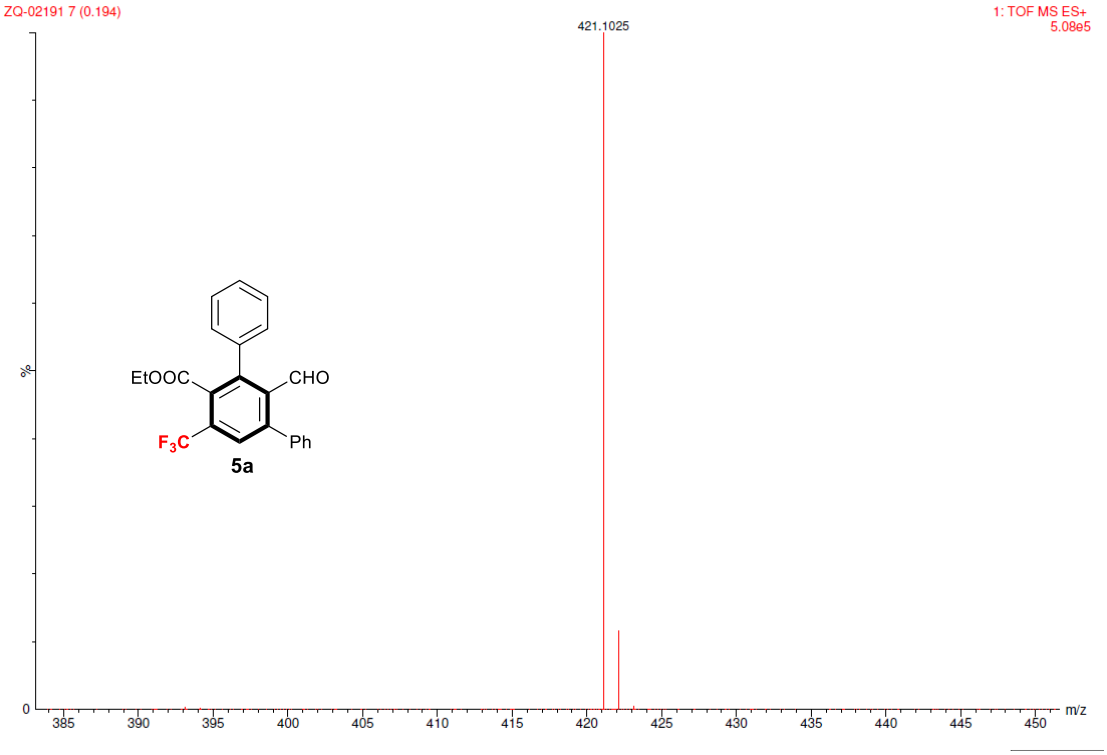

Name ZQ-1006-F
Rack Pos.
Instrument
Instrument 1
Operator
Inj. Vol. (ul) 10
Plate Pos.
IRM Status
Success
Data File ZQ-1006-F.d
Method (Acq) TOF.m
Comment
Acq. Time (Local) 10/6/2019 12:04:15 PM (UTC+08:00)
+ESI Scan (rt: 0.906 min) Frag=175.0V ZQ-1006-F.d
x10^5
404.0870
404.02
404.03
404.04
404.05
404.06
404.07
404.08
404.09
404.1
404.11
404.12
404.13
404.14
404.15
Counts vs. Mass-to-Charge (m/z)
NC
F3C
COOBn
3af

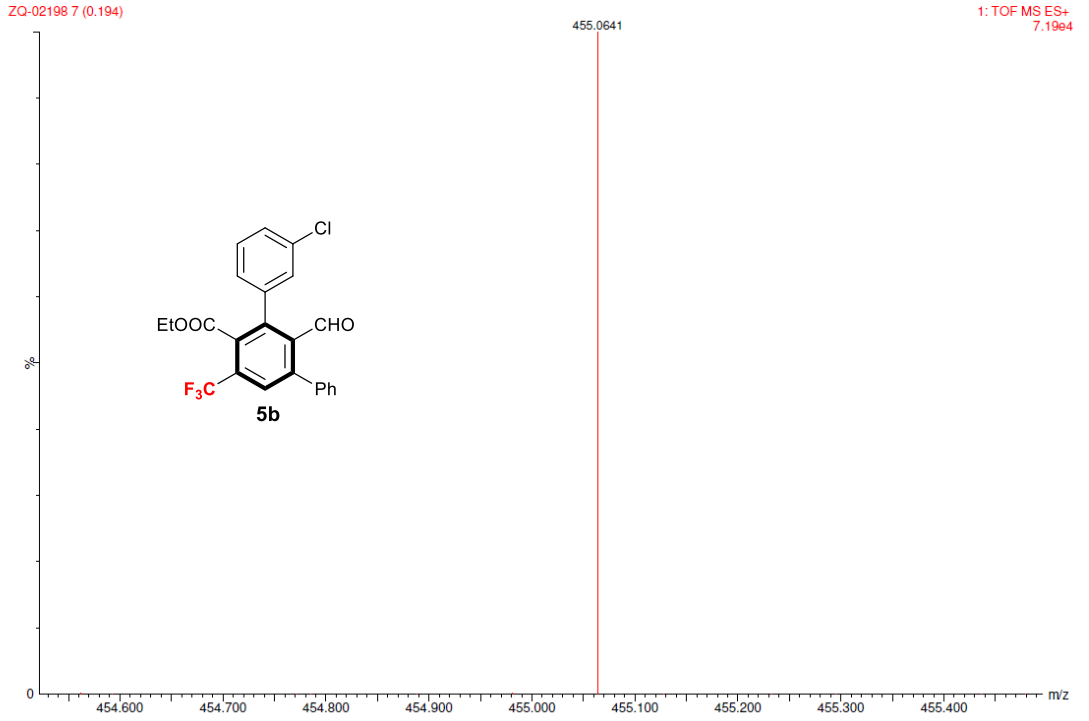
Name	ZQ-1006-G	Rack Pos.		Instrument	Instrument 1	Operator	
Inj. Vol. (ul)	10	Plate Pos.		IRM Status	Success		
Data File	ZQ-1006-G.d	Method (Acq)	TOF.m	Comment		Acq. Time (Local)	10/6/2019 5:09:36 PM (UTC+08:00)

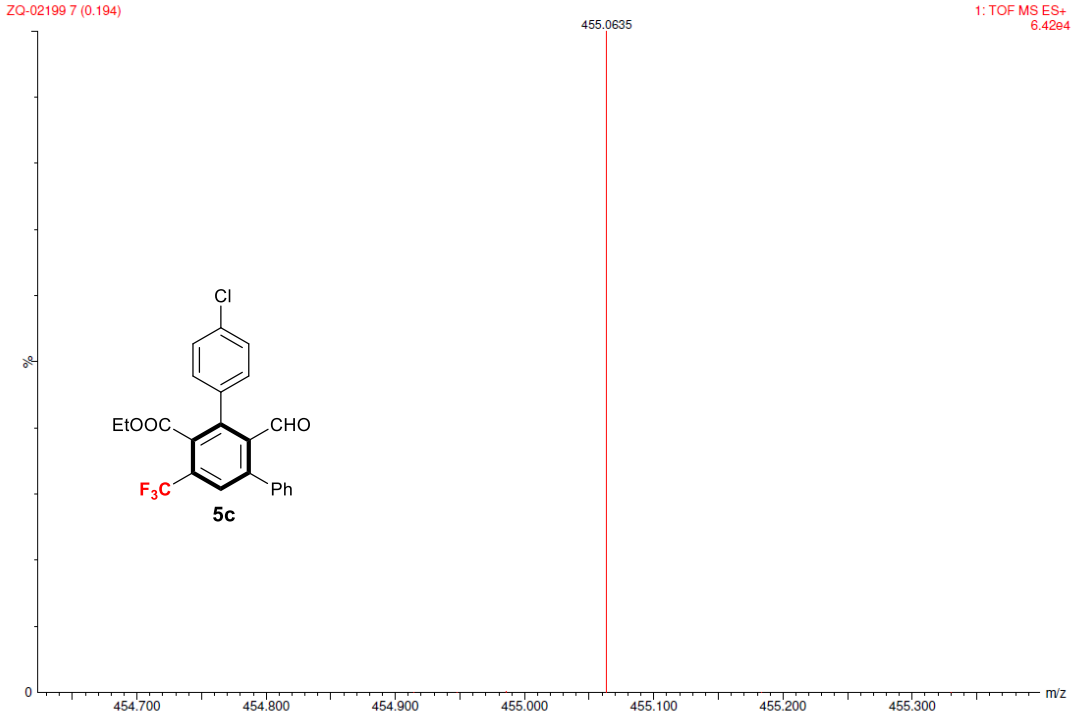


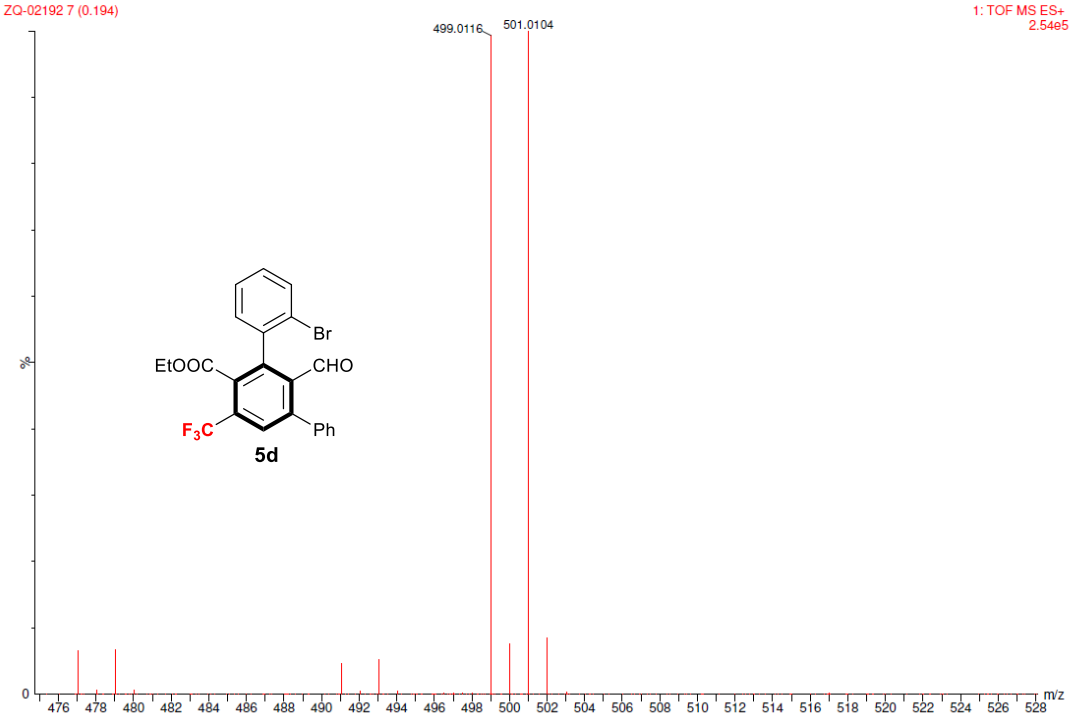
Name	ZQ-1006-H	Rack Pos.		Instrument	Instrument 1	Operator	
Inj. Vol. (ul)	10	Plate Pos.		IRM Status	Success		
Data File	ZQ-1006-H.d	Method (Acq)	TOF.m	Comment		Acq. Time (Local)	10/6/2019 12:07:14 PM (UTC+08:00)

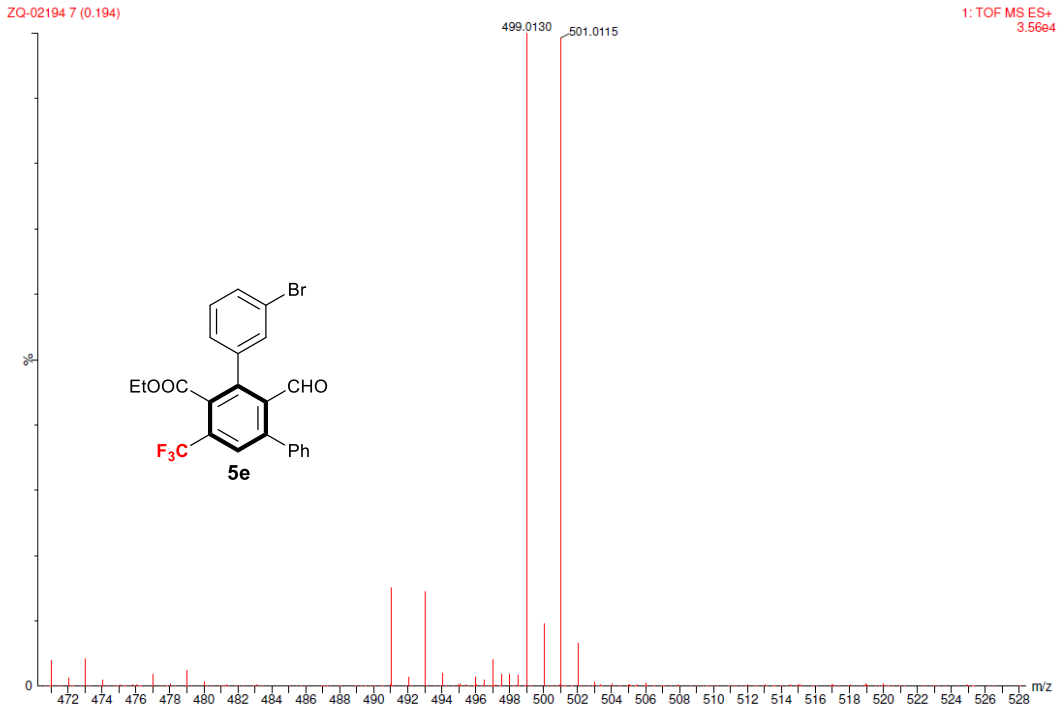


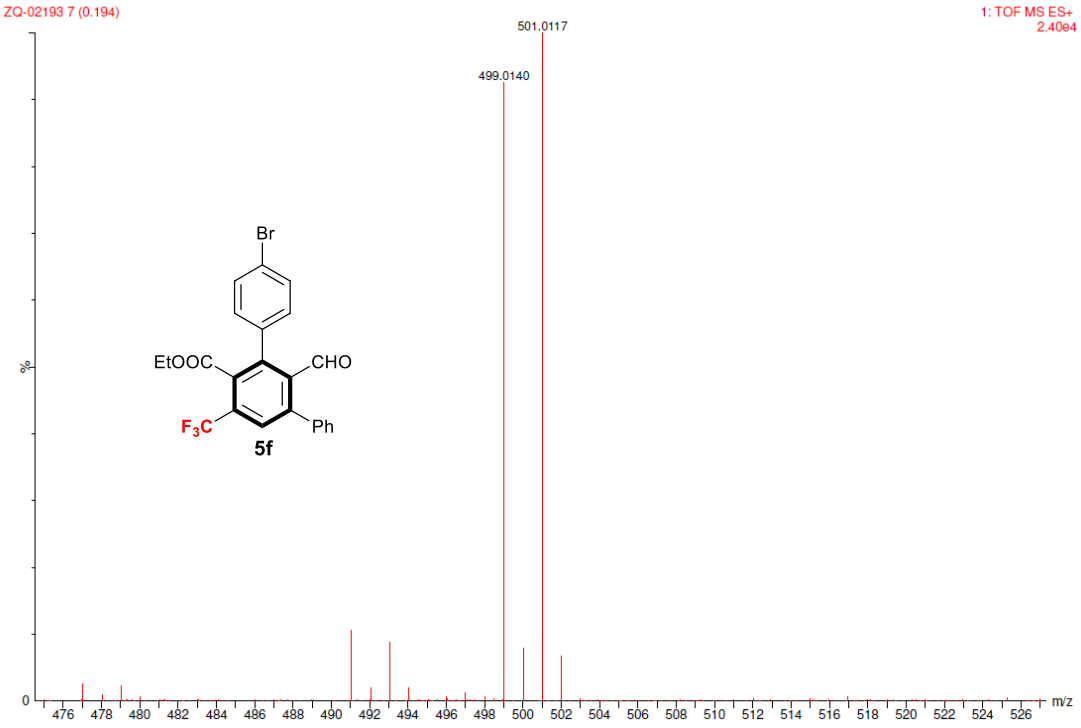

ZQ-02191 7 (0.194)
1: TOF MS ES+
5.08e5
421.1025
%
EtOOC
CHO
F3C
Ph
5a
0
385
390
395
400
405
410
415
420
425
430
435
440
445
450
m/z

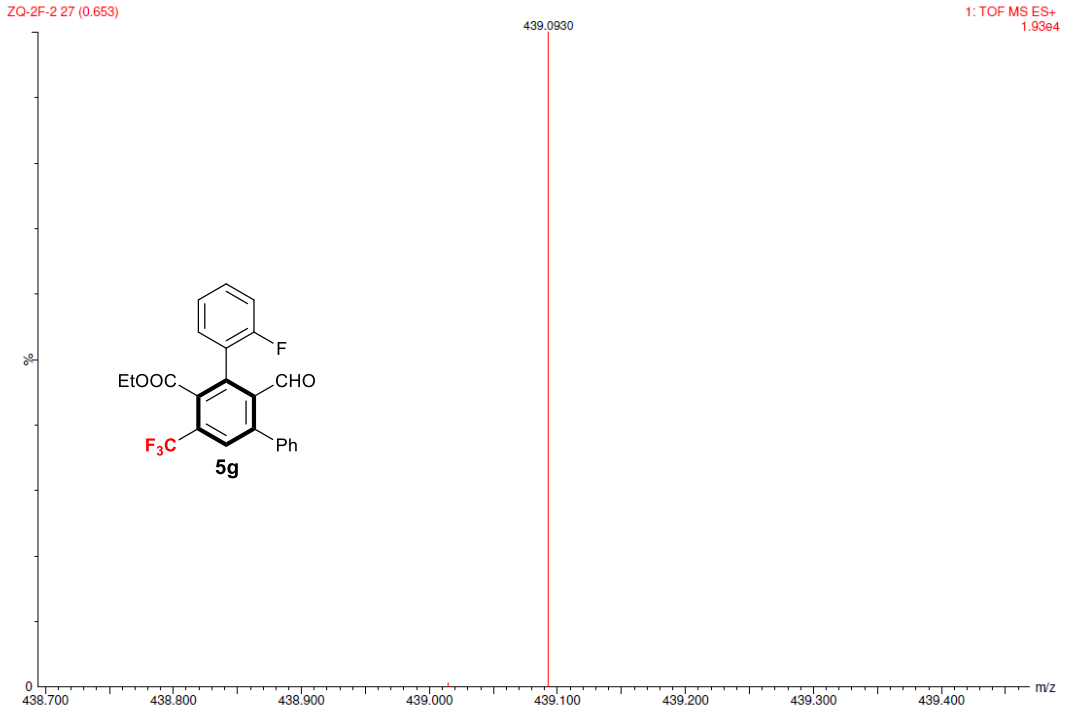

ZQ-02198 7 (0.194)
1: TOF MS ES+
7.19e4
455.0641
%
Cl
EtOOC
CHO
F3C
Ph
5b
0
454.600
454.700
454.800
454.900
455.000
455.100
455.200
455.300
455.400
m/z

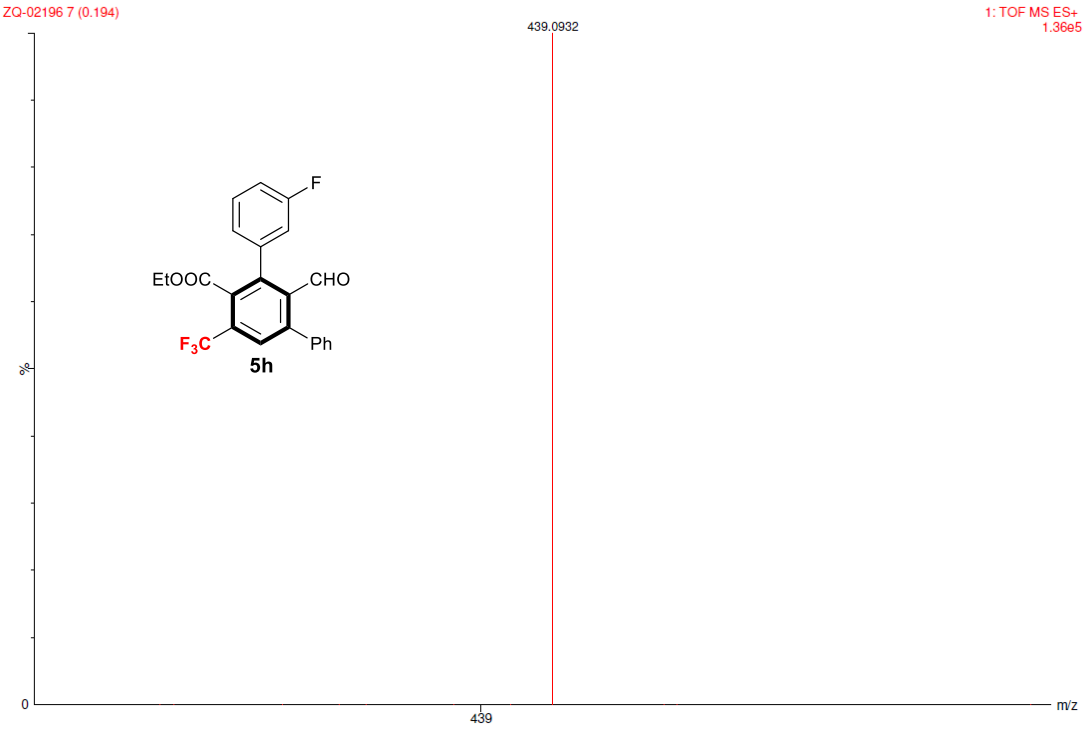

ZQ-02199 7 (0.194)
1: TOF MS ES+
6.42e4
455.0635
Cl
EtOOC
CHO
F3C
Ph
5c
%
0
454.700
454.800
454.900
455.000
455.100
455.200
455.300
m/z

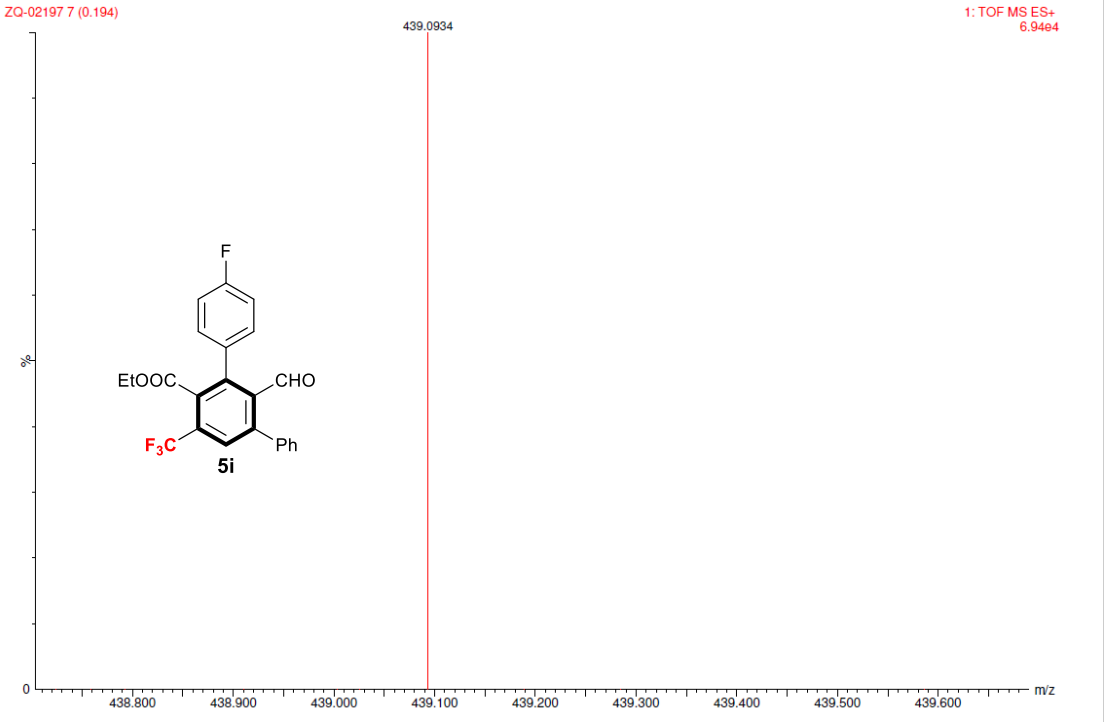

ZQ-02192 7 (0.194)
1: TOF MS ES+
2.54e5
499.0116
501.0104
Br
EtOOC
CHO
F3C
Ph
5d
%
0
476
478
480
482
484
486
488
490
492
494
496
498
500
502
504
506
508
510
512
514
516
518
520
522
524
526
528
m/z

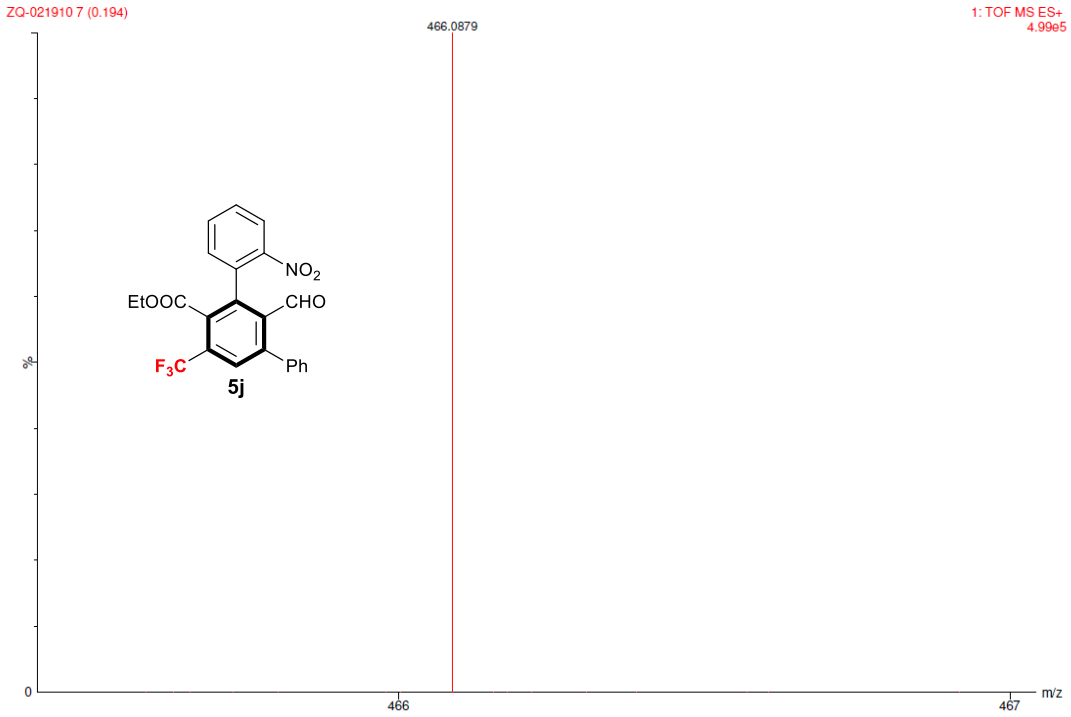

ZQ-02194 7 (0.194)
1: TOF MS ES+
3.56e4
499.0130
501.0115
Br
EtOOC
CHO
F3C
Ph
5e
%
0
m/z
472 474 476 478 480 482 484 486 488 490 492 494 496 498 500 502 504 506 508 510 512 514 516 518 520 522 524 526 528

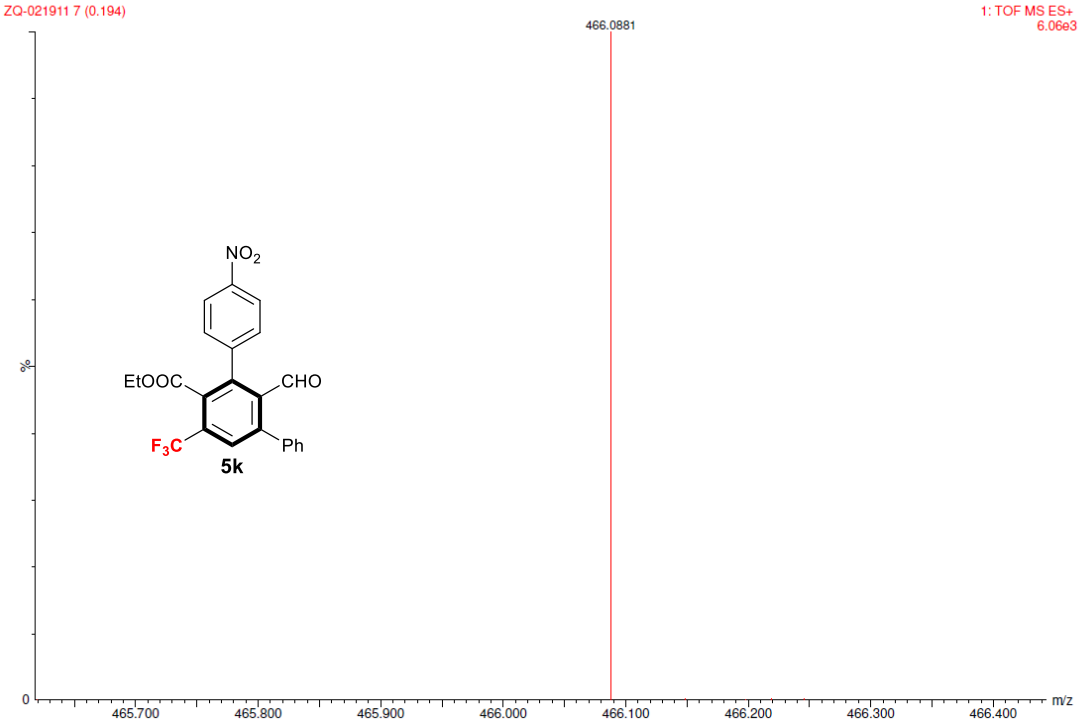

ZQ-02193 7 (0.194)
1: TOF MS ES+
2.40e4
501.0117
499.0140
Br
EtOOC
CHO
F3C
Ph
5f
%
0
m/z
476 478 480 482 484 486 488 490 492 494 496 498 500 502 504 506 508 510 512 514 516 518 520 522 524 526

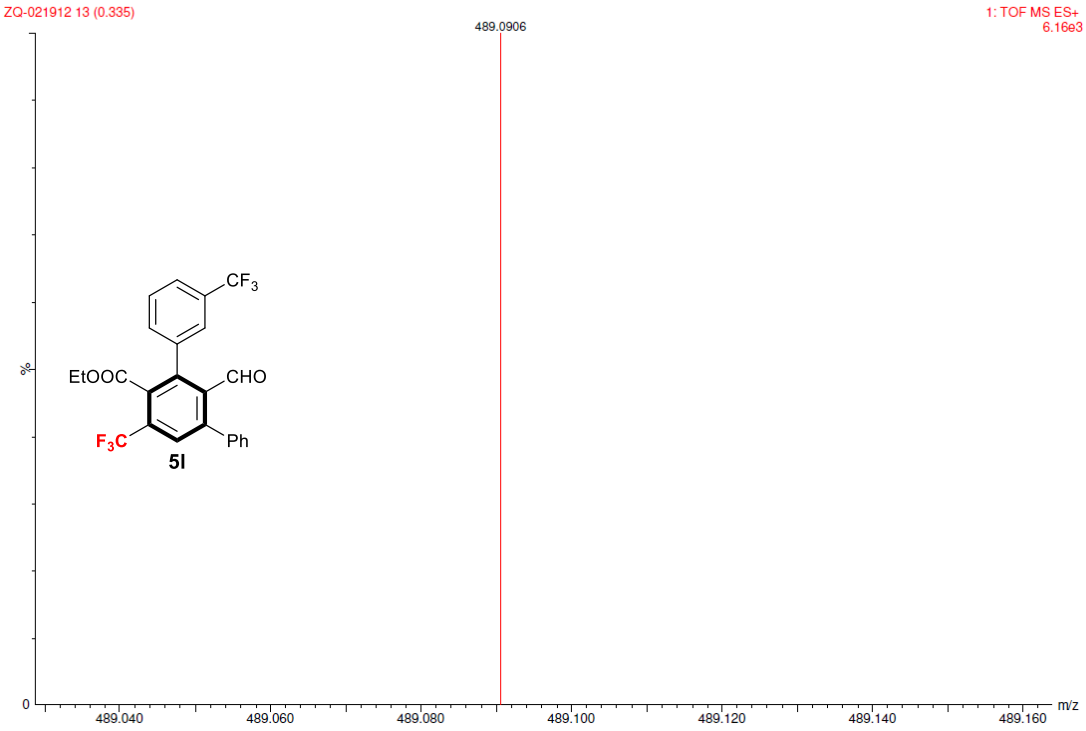

ZQ-2F-2 27 (0.653)
1: TOF MS ES+
1.93e4
439.0930
%
0
438.700
438.800
438.900
439.000
439.100
439.200
439.300
439.400
m/z
F
EtOOC
CHO
F3C
Ph
5g

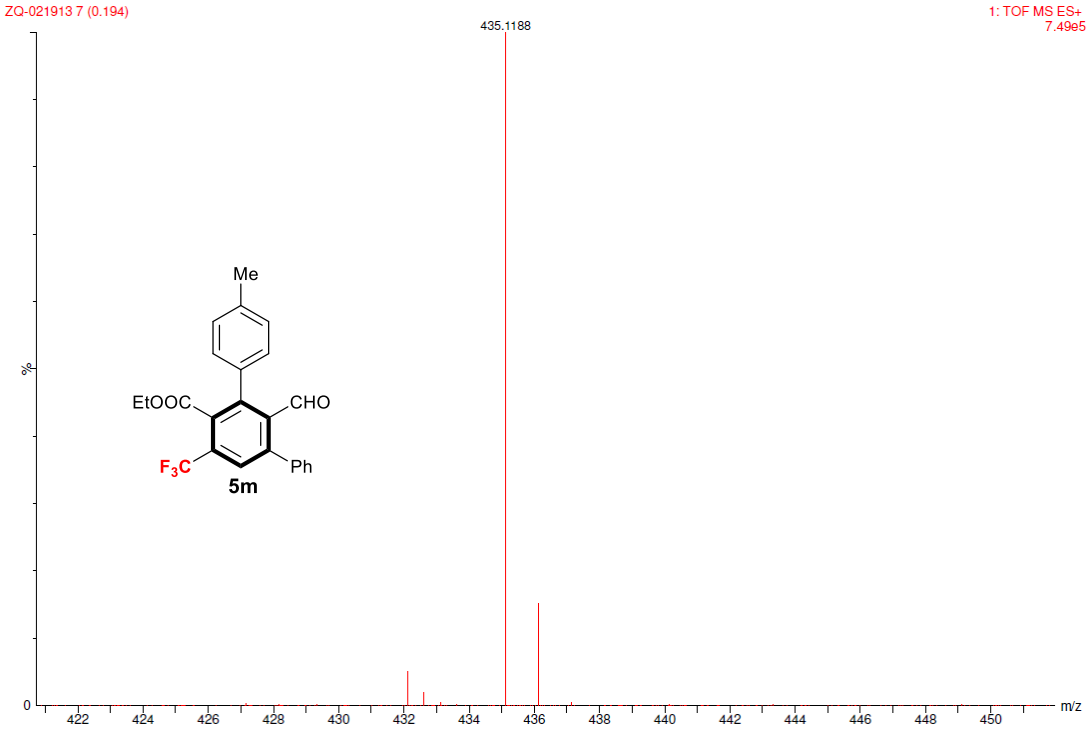

ZQ-02196 7 (0.194)
1: TOF MS ES+
1.36e5
439.0932
%
0
439
m/z
F
EtOOC
CHO
F3C
Ph
5h

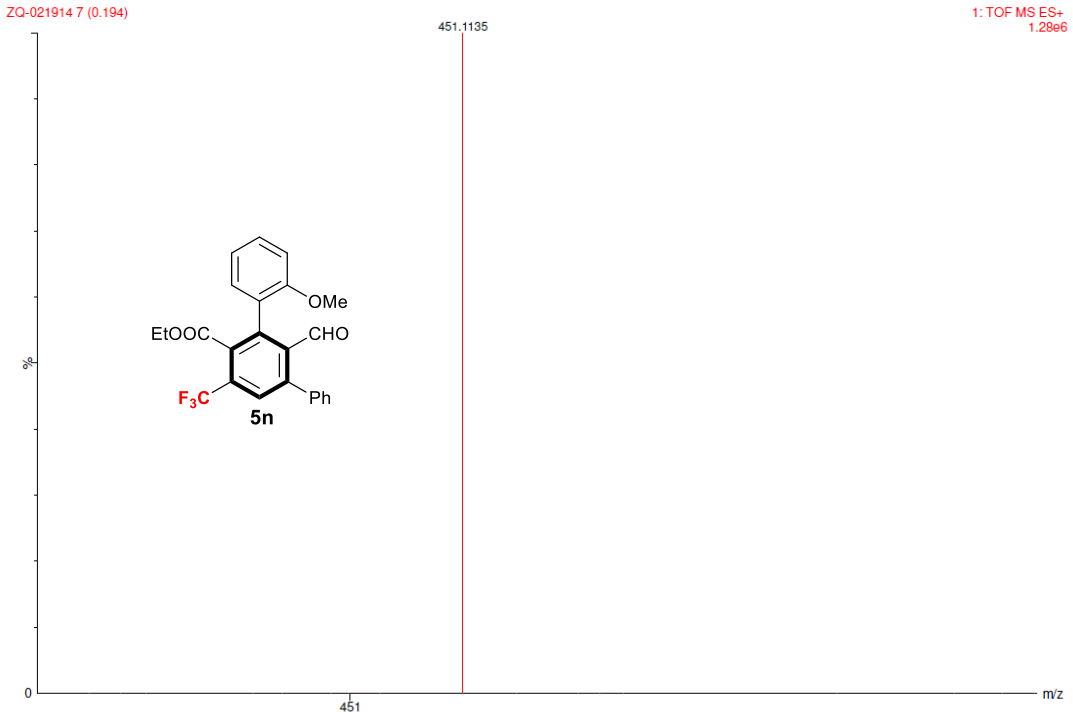

ZQ-02197 7 (0.194)
1: TOF MS ES+
6.94e4
439.0934
F
EtOOC
CHO
F3C
Ph
5i
%
0
438.800
438.900
439.000
439.100
439.200
439.300
439.400
439.500
439.600
m/z

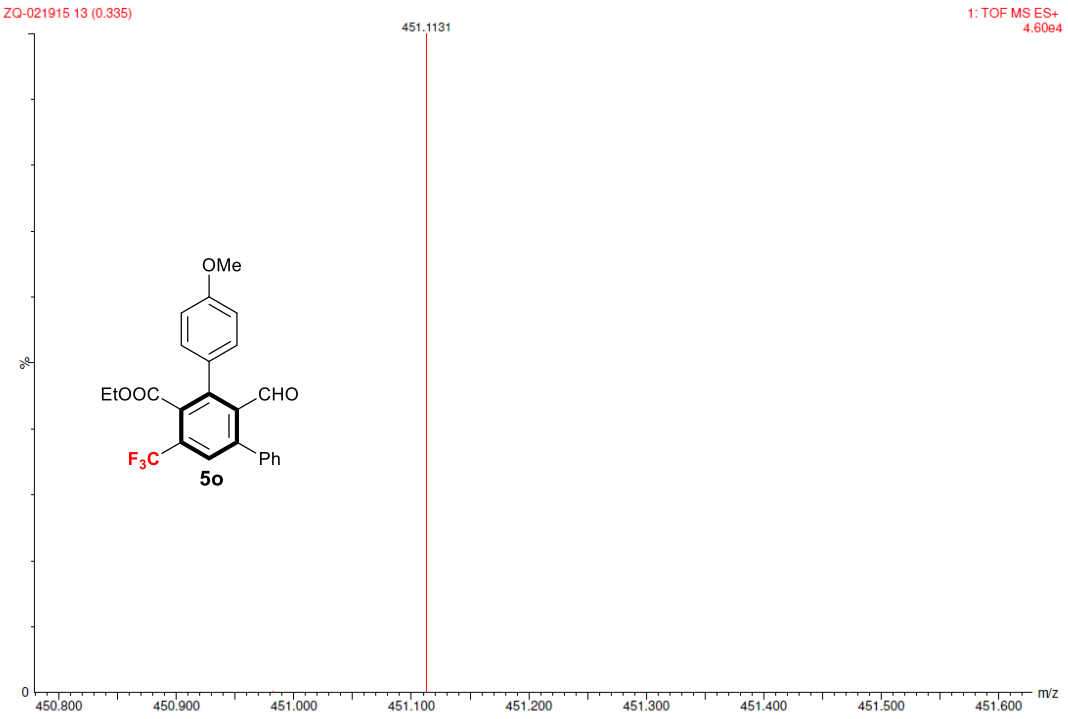

ZQ-021910 7 (0.194)
1: TOF MS ES+
4.99e5
466.0879
NO2
EtOOC
CHO
F3C
Ph
5j
%
0
466
467
m/z

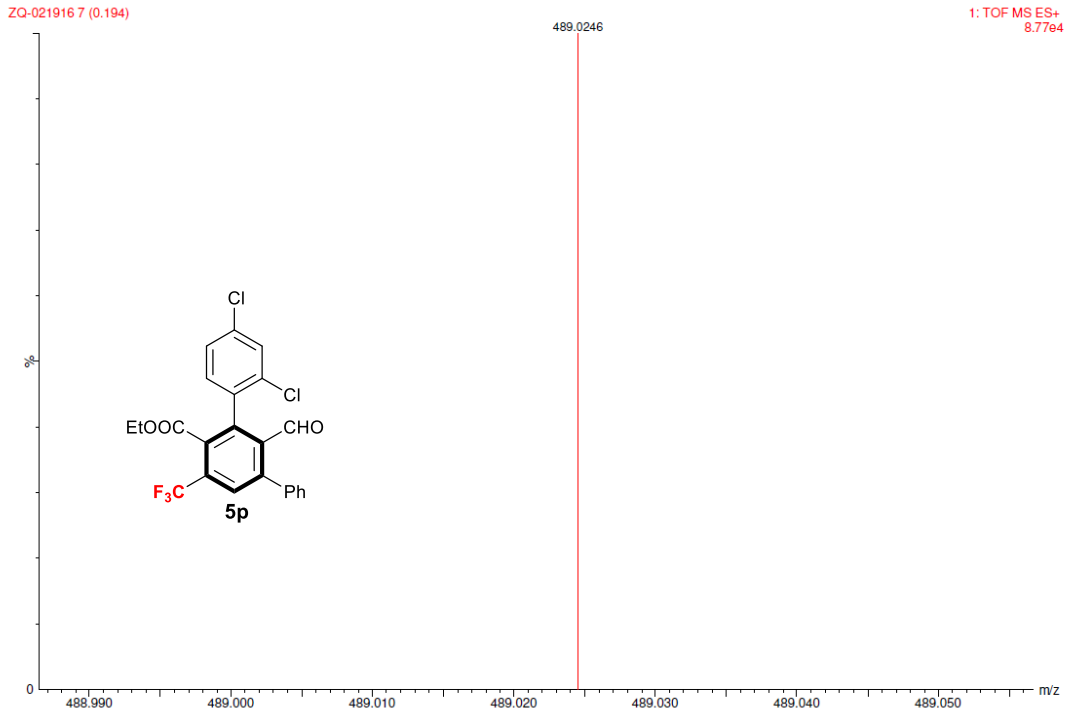

ZQ-021911 7 (0.194)
1: TOF MS ES+
6.06e3
466.0881
%
0
NO2
EtOOC
CHO
F3C
Ph
5k
465.700
465.800
465.900
466.000
466.100
466.200
466.300
466.400
m/z

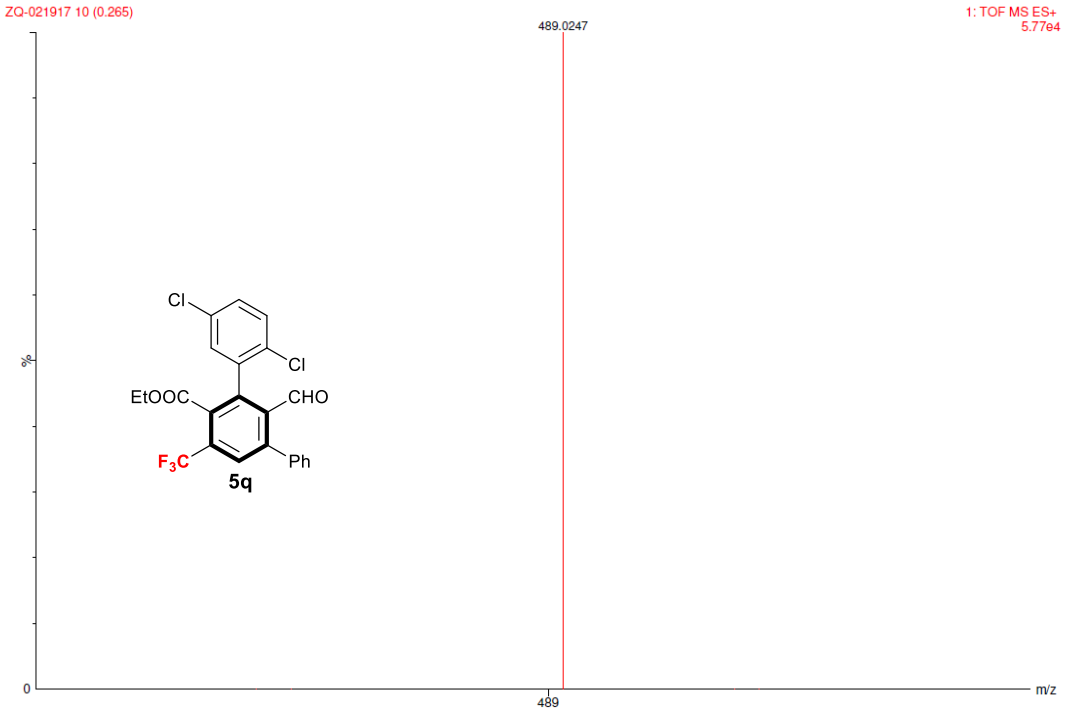

ZQ-021912 13 (0.335)
1: TOF MS ES+
6.16e3
489.0906
%
0
CF3
EtOOC
CHO
F3C
Ph
5l
489.040
489.060
489.080
489.100
489.120
489.140
489.160
m/z

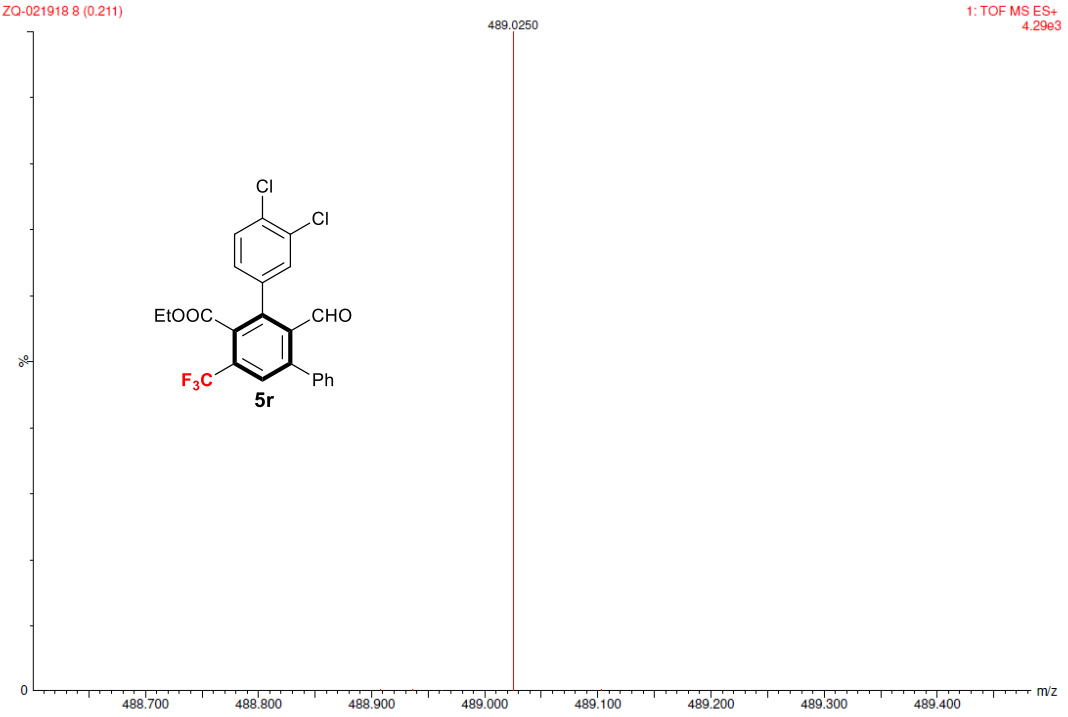

ZQ-021913 7 (0.194)
1: TOF MS ES+
7.49e5
435.1188
Me
EtOOC
CHO
F3C
Ph
5m
%
0
422
424
426
428
430
432
434
436
438
440
442
444
446
448
450
m/z

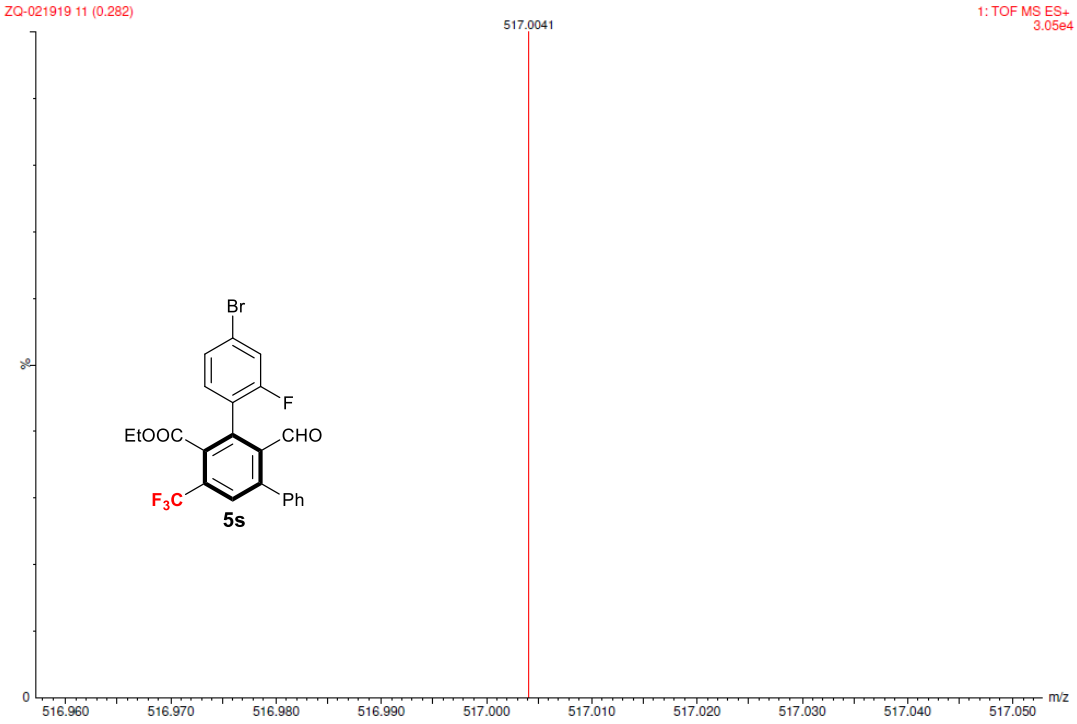

ZQ-021914 7 (0.194)
1: TOF MS ES+
1.28e6
451.1135
OMe
EtOOC
CHO
F3C
Ph
5n
%
0
451
m/z

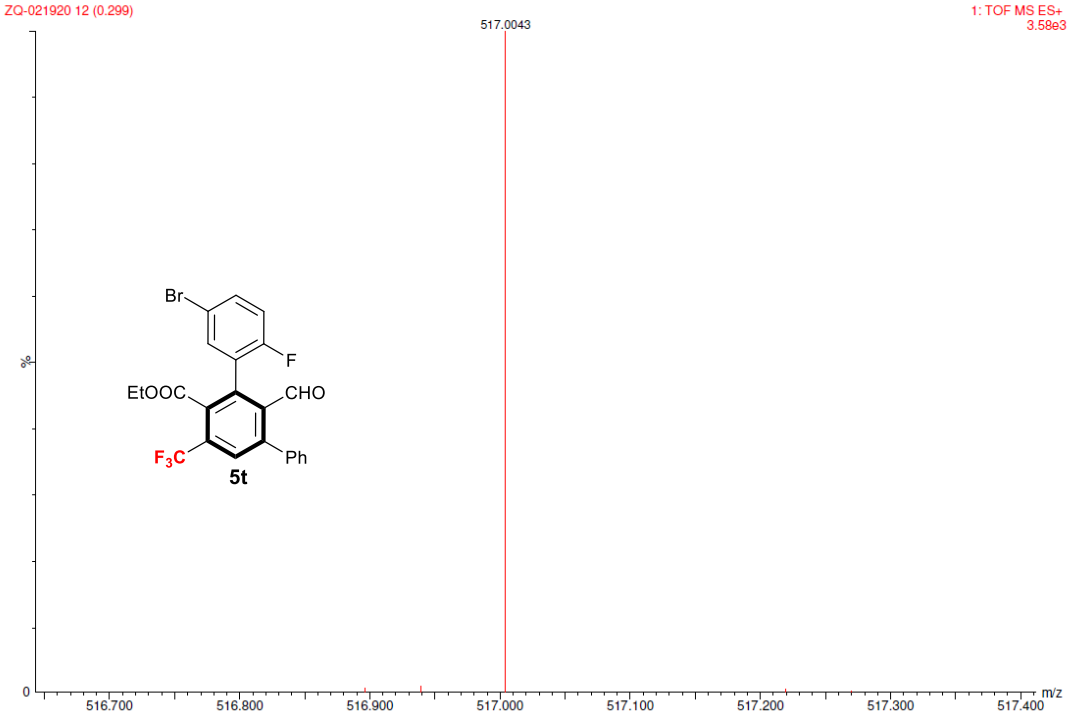

ZQ-021915 13 (0.335)
1: TOF MS ES+
4.60e4
451.1131
OMe
EtOOC
CHO
F3C
Ph
5o
%
0
450.800
450.900
451.000
451.100
451.200
451.300
451.400
451.500
451.600
m/z


ZQ-021916 7 (0.194)
1: TOF MS ES+
8.77e4
489.0246
Cl
Cl
EtOOC
CHO
F3C
Ph
5p
%
0
488.990
489.000
489.010
489.020
489.030
489.040
489.050
m/z


ZQ-021917 10 (0.265)
1: TOF MS ES+
5.77e4
489.0247
Cl
Cl
EtOOC
CHO
F3C
Ph
5q
%
0
489
m/z


ZQ-021918 8 (0.211)
1: TOF MS ES+
4.29e3
489.0250
Cl
Cl
EtOOC
CHO
F3C
Ph
5r
%
0
488.700
488.800
488.900
489.000
489.100
489.200
489.300
489.400
m/z

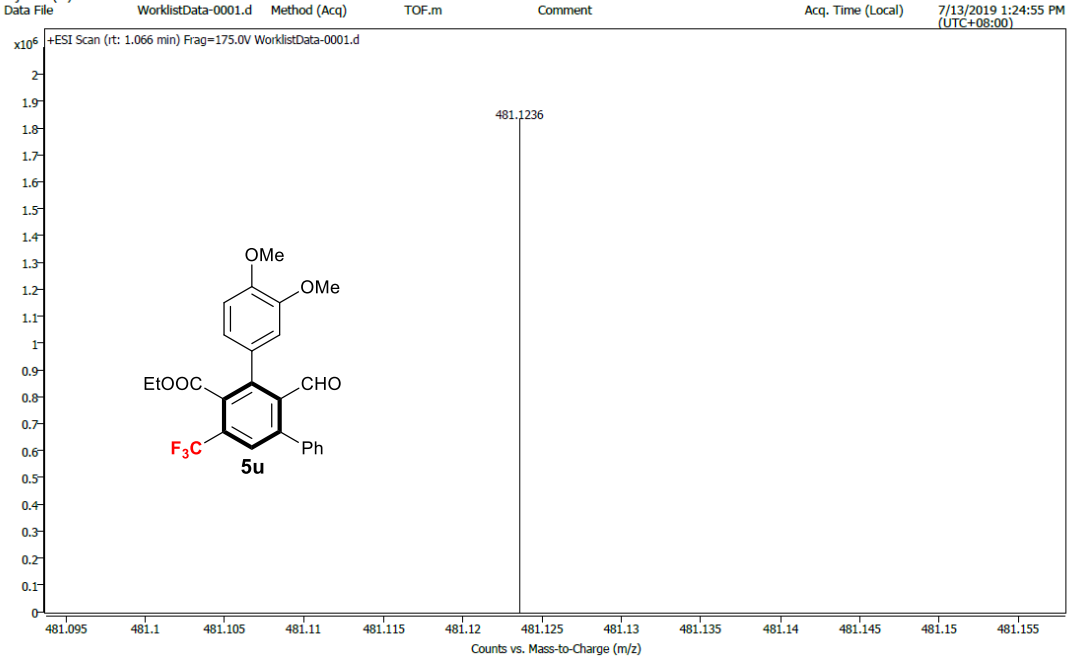

ZQ-021919 11 (0.282)
1: TOF MS ES+
3.05e4
517.0041
Br
F
EtOOC
CHO
F3C
Ph
5s
%
0
516.960
516.970
516.980
516.990
517.000
517.010
517.020
517.030
517.040
517.050
m/z


ZQ-021920 12 (0.299)
1: TOF MS ES+
3.58e3
517.0043
Br
F
EtOOC
CHO
F3C
Ph
5t
%
0
516.700
516.800
516.900
517.000
517.100
517.200
517.300
517.400
m/z

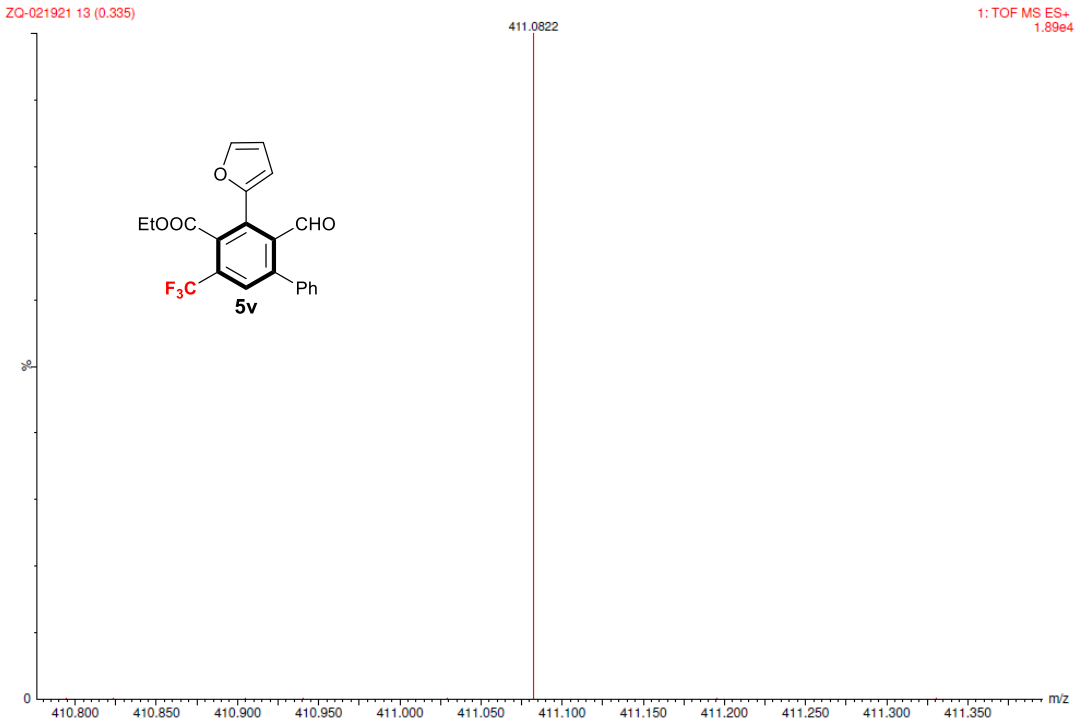
Spectrum Plot Report

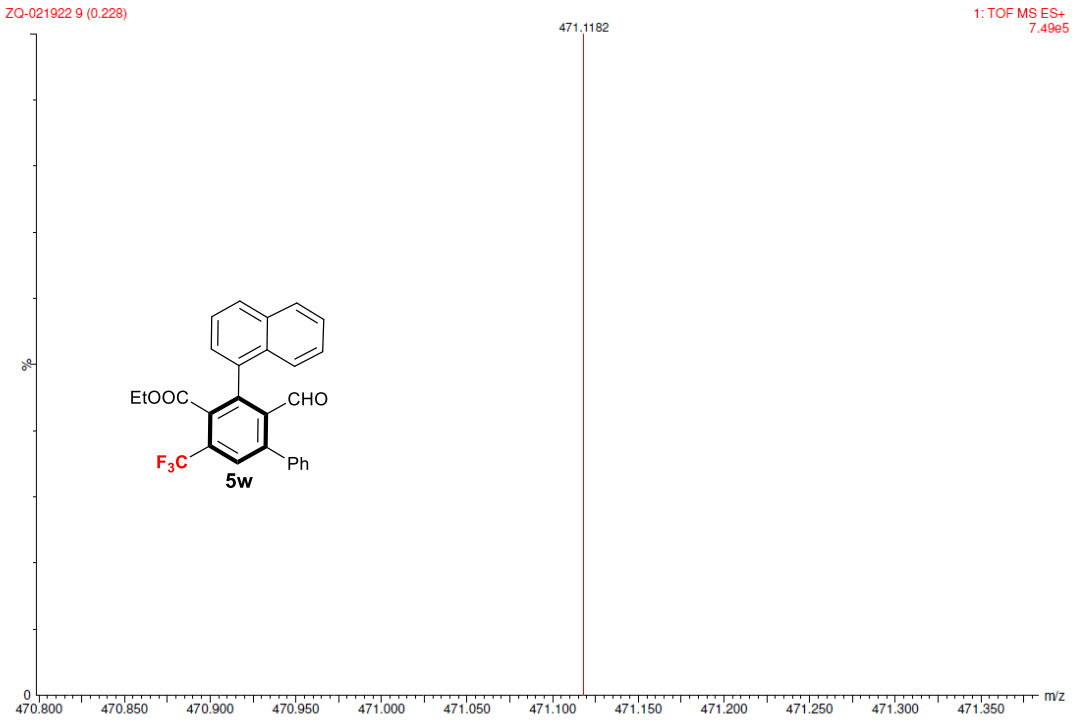
Agilent

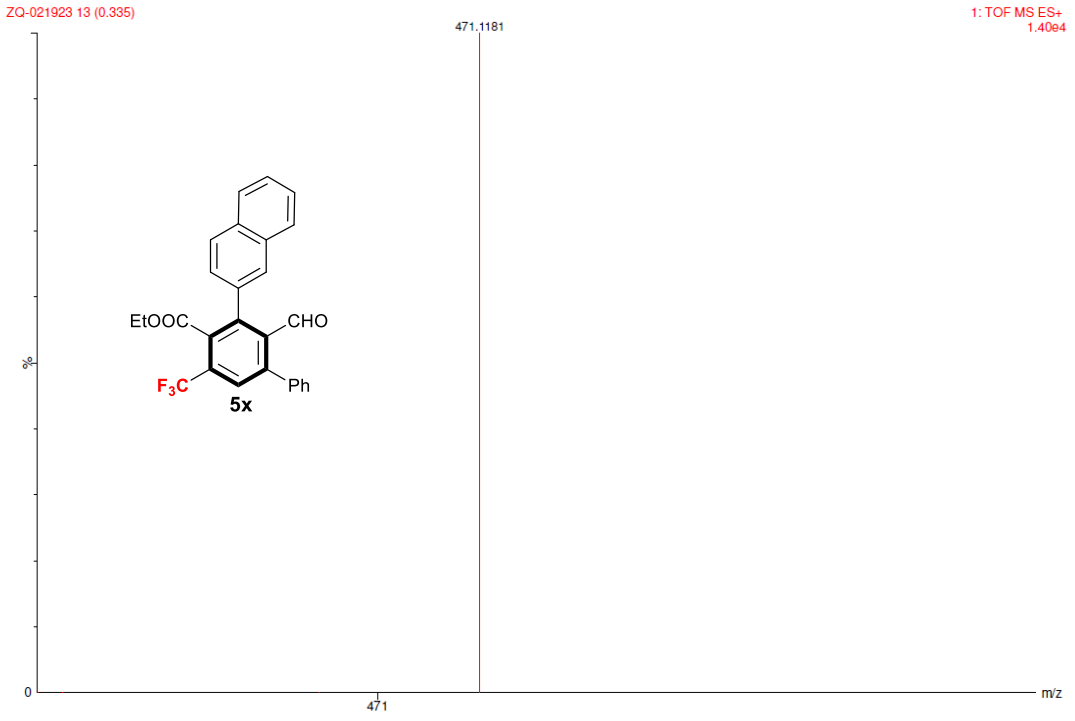
Name	zq-0711	Rack Pos.		Instrument	Instrument 1	Operator
Inj. Vol. (ul)	10	Plate Pos.		IRM Status	Success	
Data File	WorklistData-0001.d	Method (Acq)	TOF.m	Comment		Acq. Time (Local) 7/13/2019 1:24:55 PM (UTC+08:00)

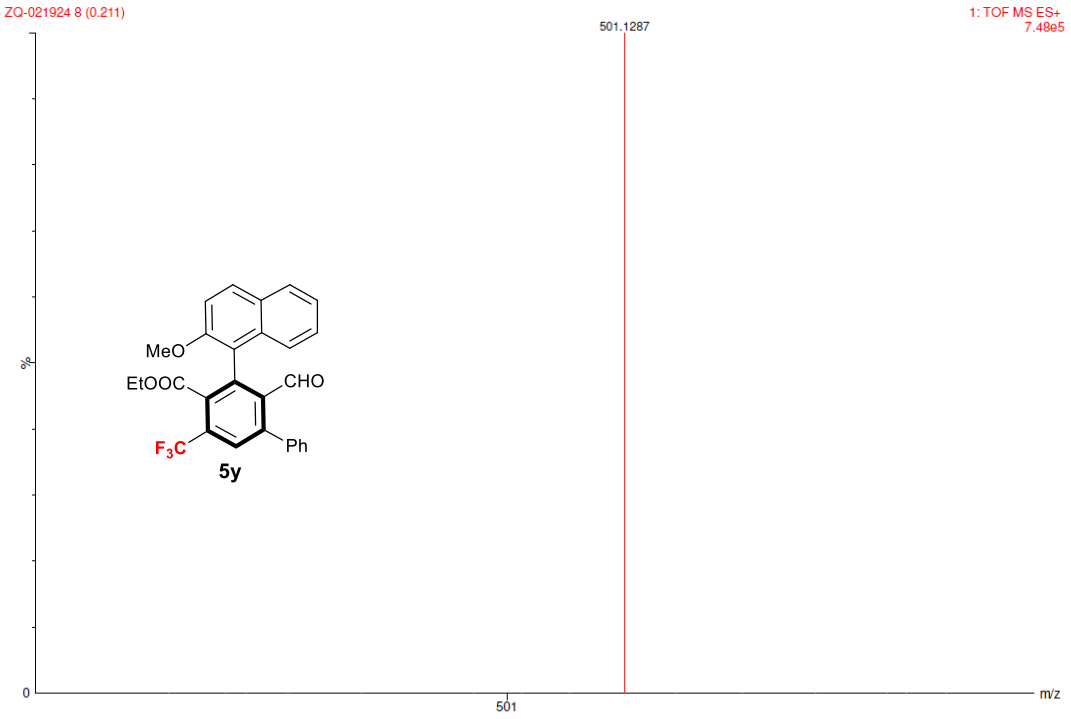


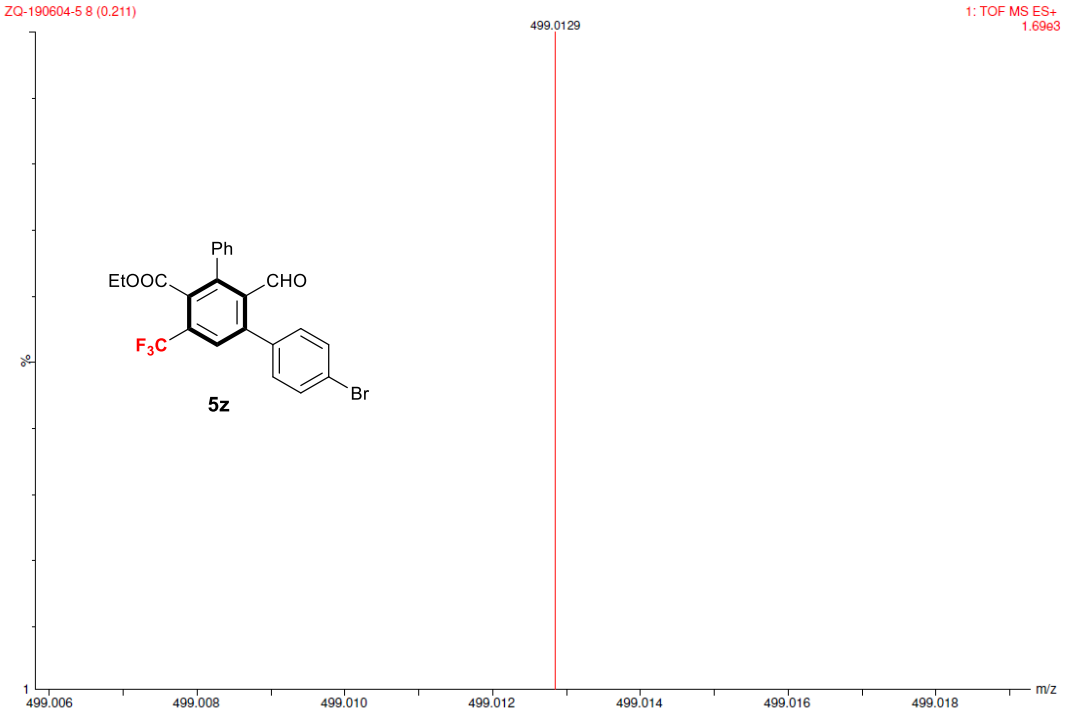
Generated at 4:11 PM on 7/13/2019

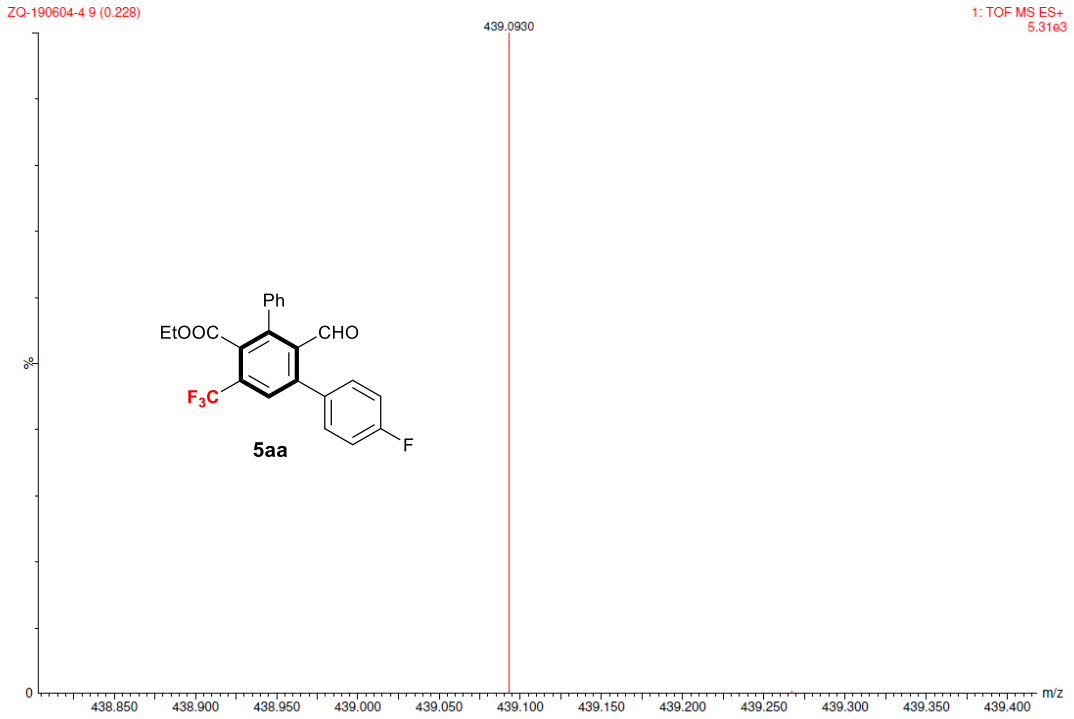


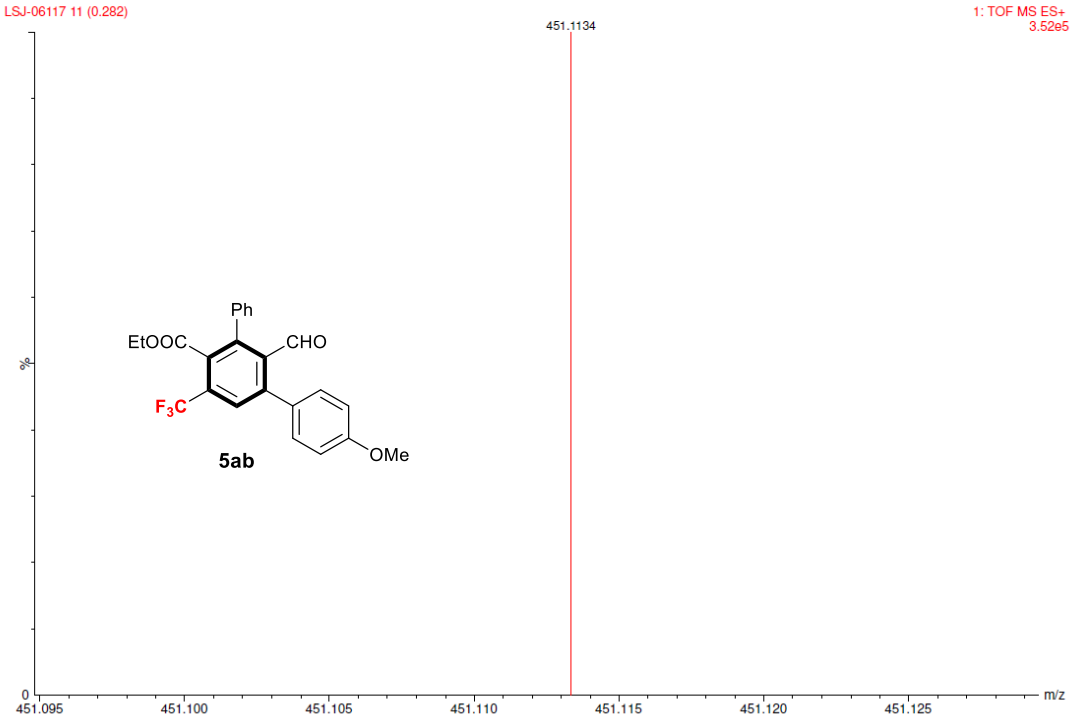

ZQ-021922 9 (0.228)
1: TOF MS ES+
7.49e5
471.1182
%
0
EtOOC
CHO
F3C
Ph
5w
470.800
470.850
470.900
470.950
471.000
471.050
471.100
471.150
471.200
471.250
471.300
471.350
m/z

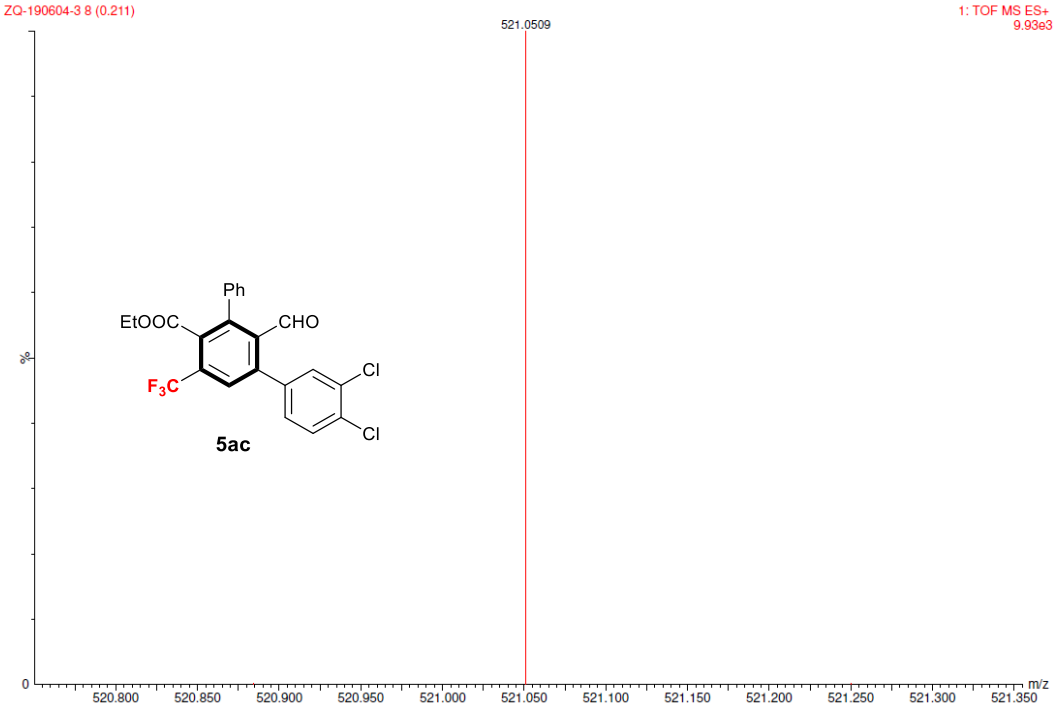

ZQ-021923 13 (0.335)
1: TOF MS ES+
1.40e4
471.1181
%
0
EtOOC
CHO
F3C
Ph
5x
471
m/z

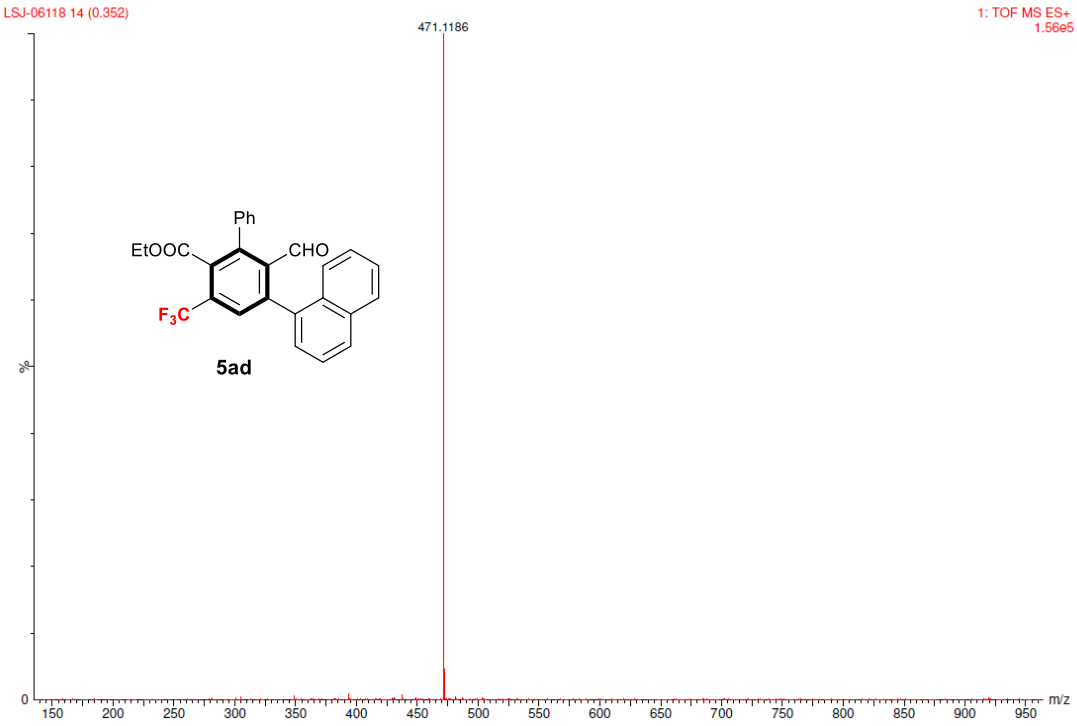

ZQ-021924 8 (0.211)
1: TOF MS ES+
7.48e5
501.1287
MeO
EtOOC
CHO
F3C
Ph
5y
%
0
501
m/z

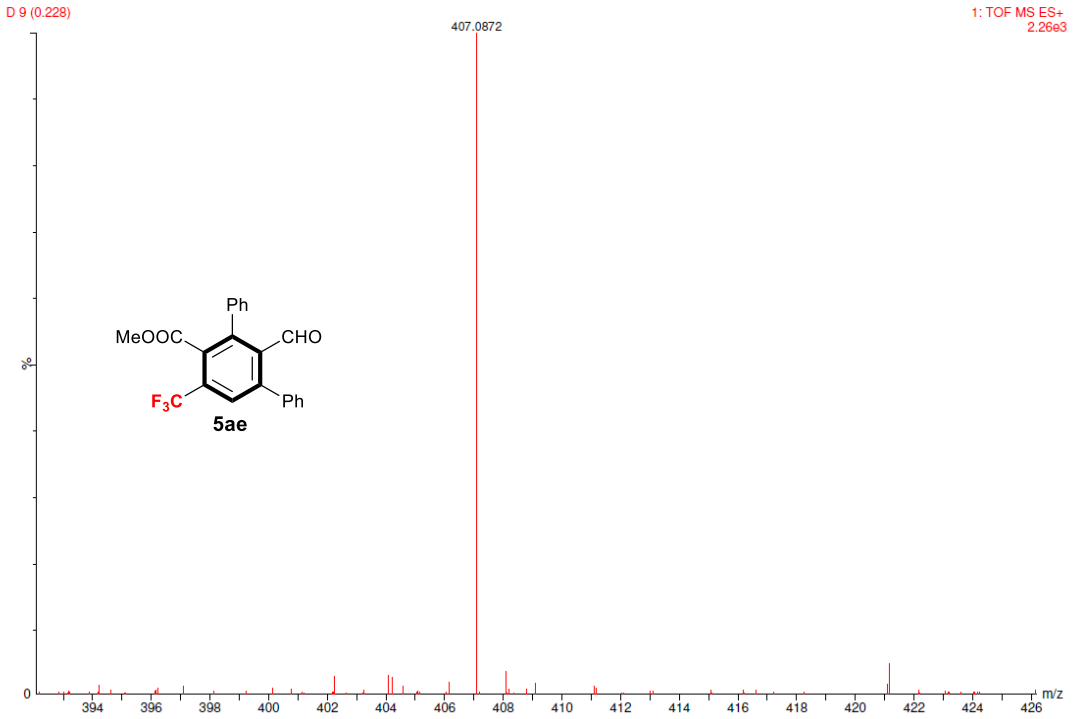

ZQ-190604-5 8 (0.211)
1: TOF MS ES+
1.69e3
499.0129
Ph
EtOOC
CHO
F3C
Br
5z
%
1
499.006
499.008
499.010
499.012
499.014
499.016
499.018
m/z

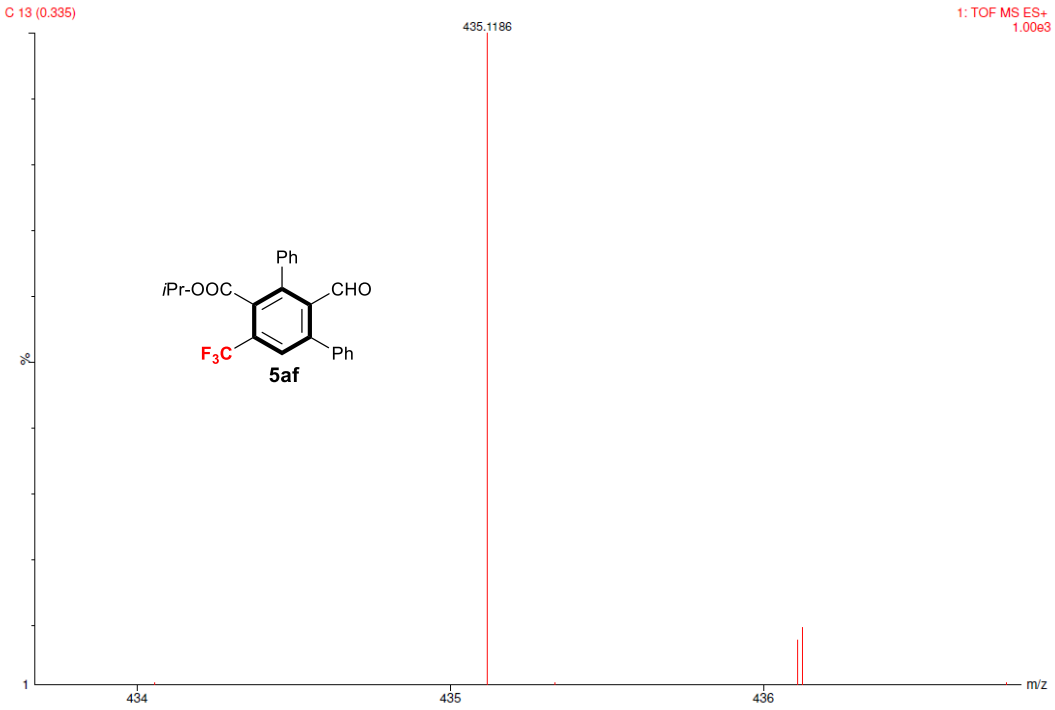

ZQ-190604-4 9 (0.228)
1: TOF MS ES+
5.31e3
439.0930
Ph
EtOOC
CHO
F3C
F
5aa
%
0
438.850
438.900
438.950
439.000
439.050
439.100
439.150
439.200
439.250
439.300
439.350
439.400
m/z

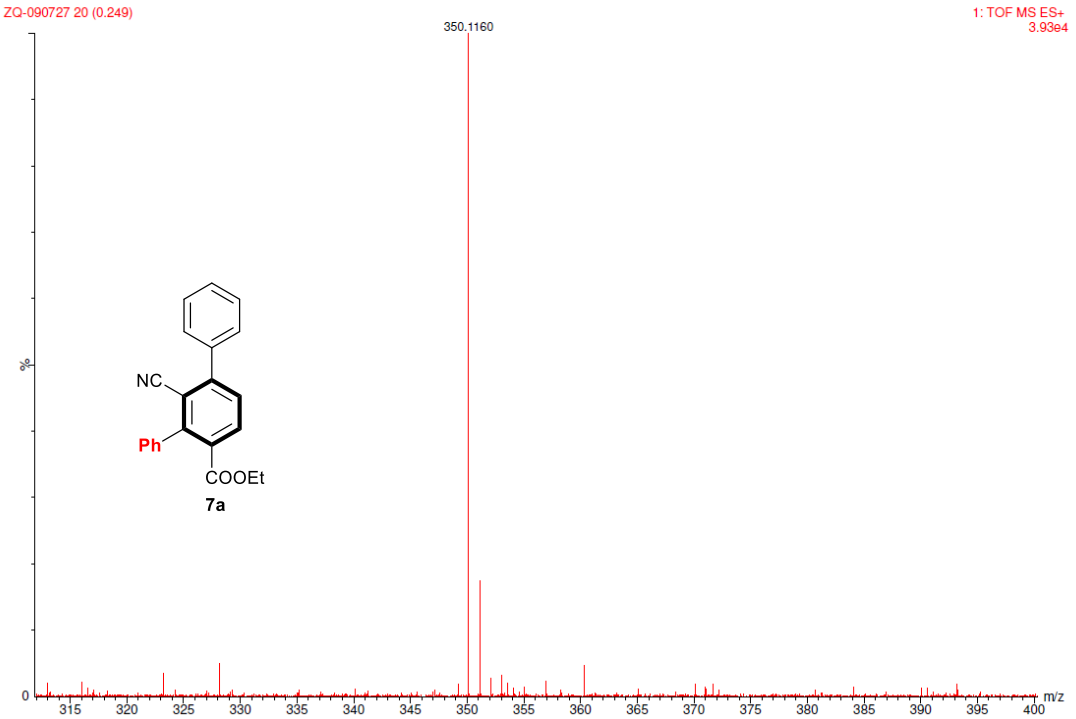

LSJ-06117 11 (0.282)
1: TOF MS ES+
3.52e5
451.1134
Ph
EtOOC
CHO
F3C
OMe
5ab
%
0
451.095
451.100
451.105
451.110
451.115
451.120
451.125
m/z

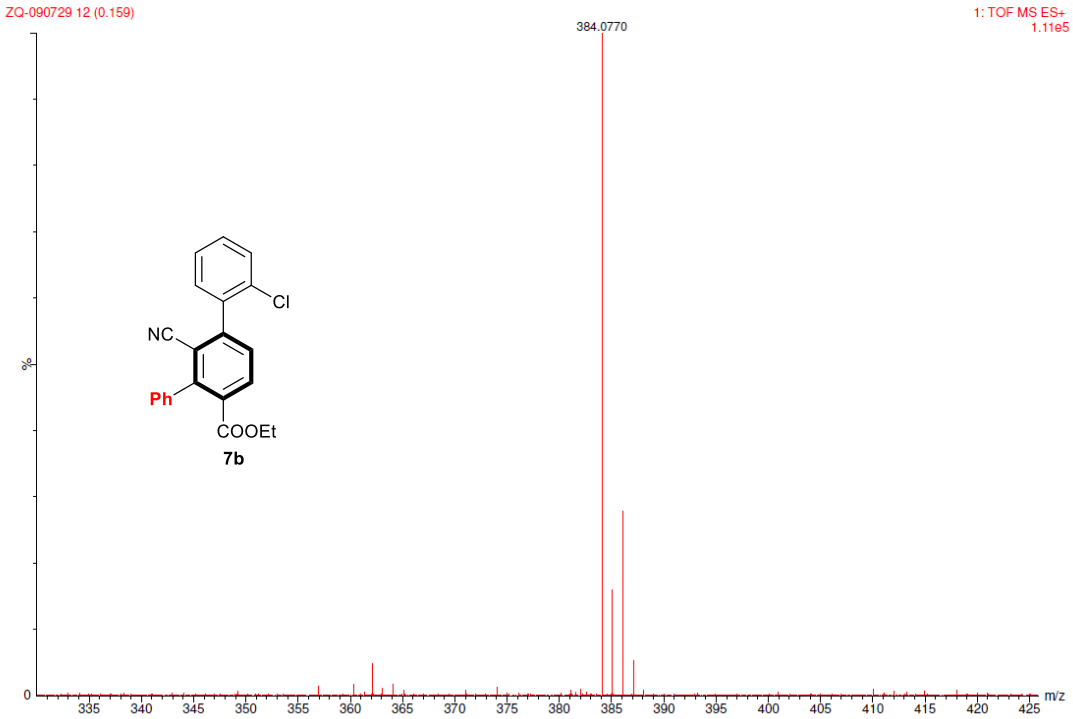

ZQ-190604-3 8 (0.211)
1: TOF MS ES+
9.93e3
521.0509
Ph
EtOOC
CHO
Cl
F3C
Cl
5ac
%
0
520.800
520.850
520.900
520.950
521.000
521.050
521.100
521.150
521.200
521.250
521.300
521.350
m/z

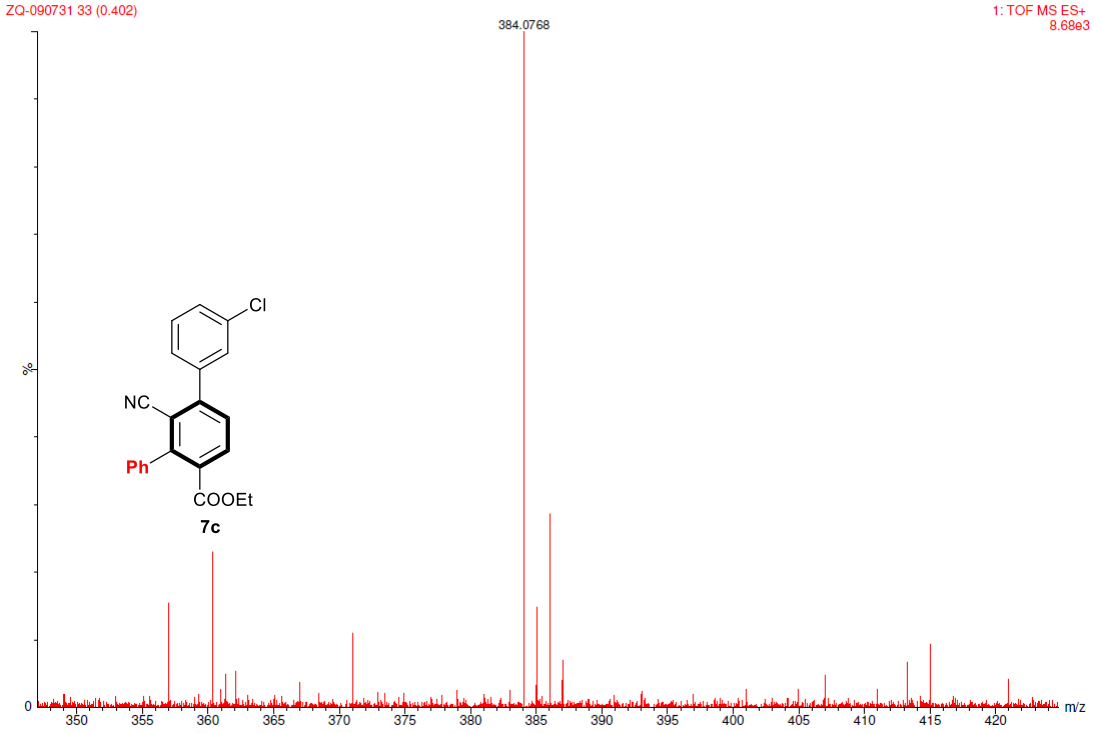

LSJ-06118 14 (0.352)
1: TOF MS ES+
1.56e5
471.1186
Ph
EtOOC
CHO
F3C
5ad
%
0
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
m/z

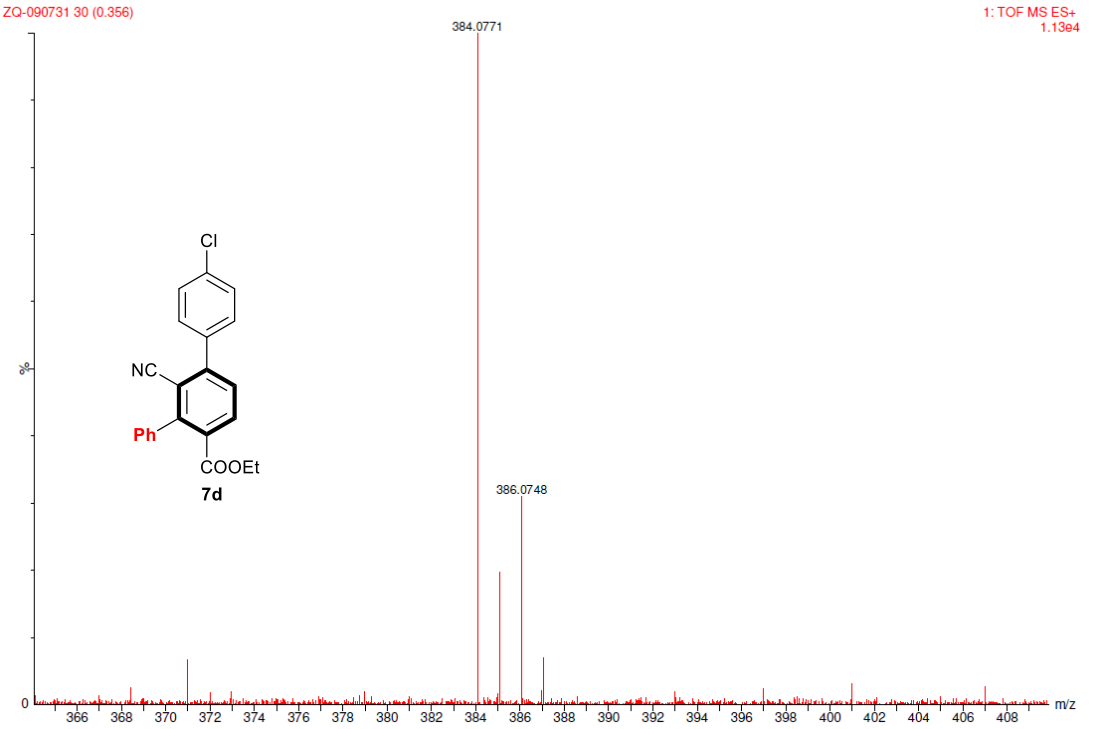

D 9 (0.228)
1: TOF MS ES+
2.26e3
407.0872
Ph
MeOOC
CHO
F3C
Ph
5ae
%
0
394
396
398
400
402
404
406
408
410
412
414
416
418
420
422
424
426
m/z


C 13 (0.335)
1: TOF MS ES+
1.00e3
435.1186
Ph
iPr-OOC
CHO
F3C
Ph
5af
%
1
434
435
436
m/z

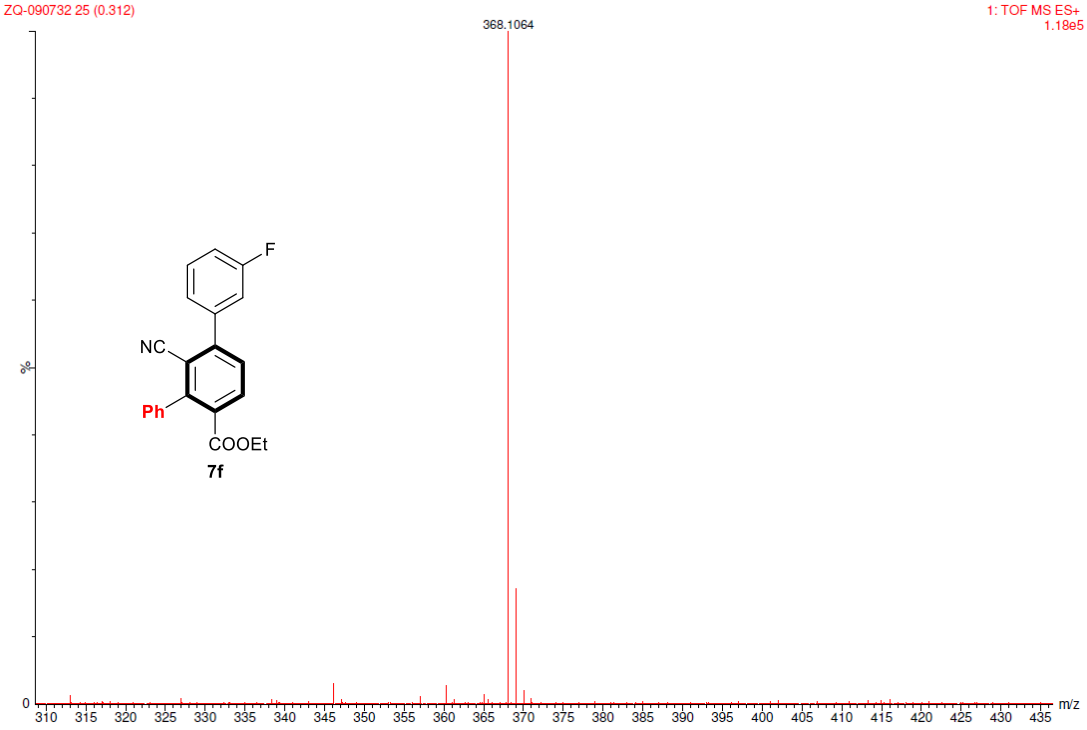

ZQ-090727 20 (0.249)
1: TOF MS ES+
3.93e4
350.1160
NC
Ph
COOEt
7a
%
0
315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400
m/z

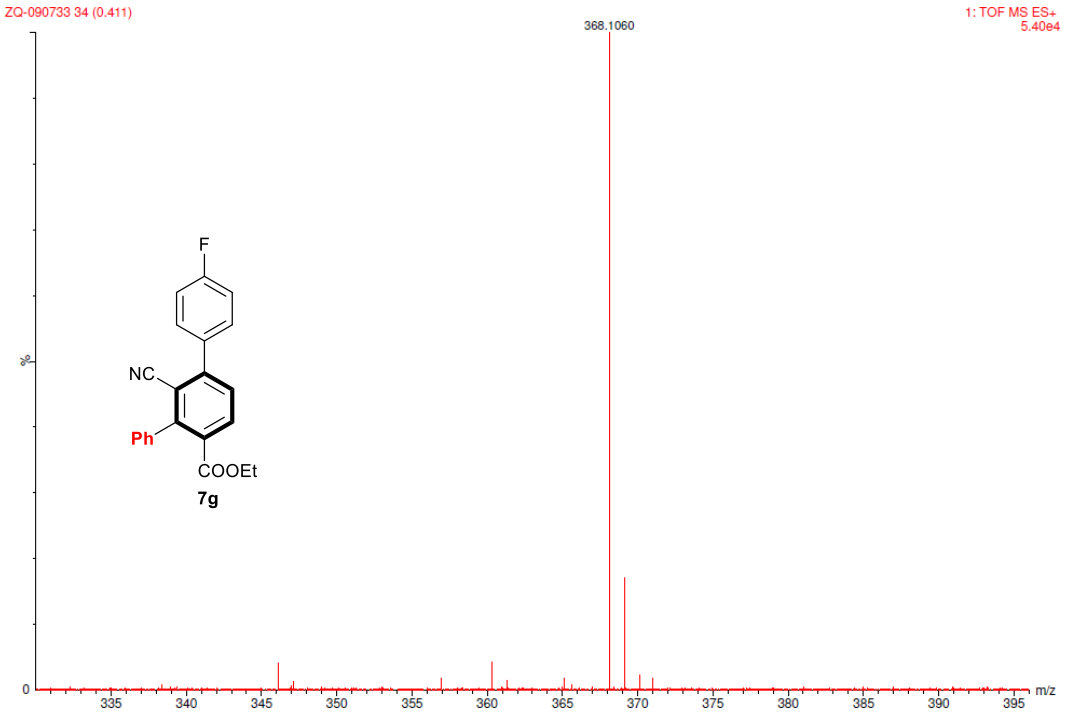

ZQ-090729 12 (0.159)
1: TOF MS ES+
1.11e5
384.0770
Cl
NC
Ph
COOEt
7b
%
0
335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425
m/z

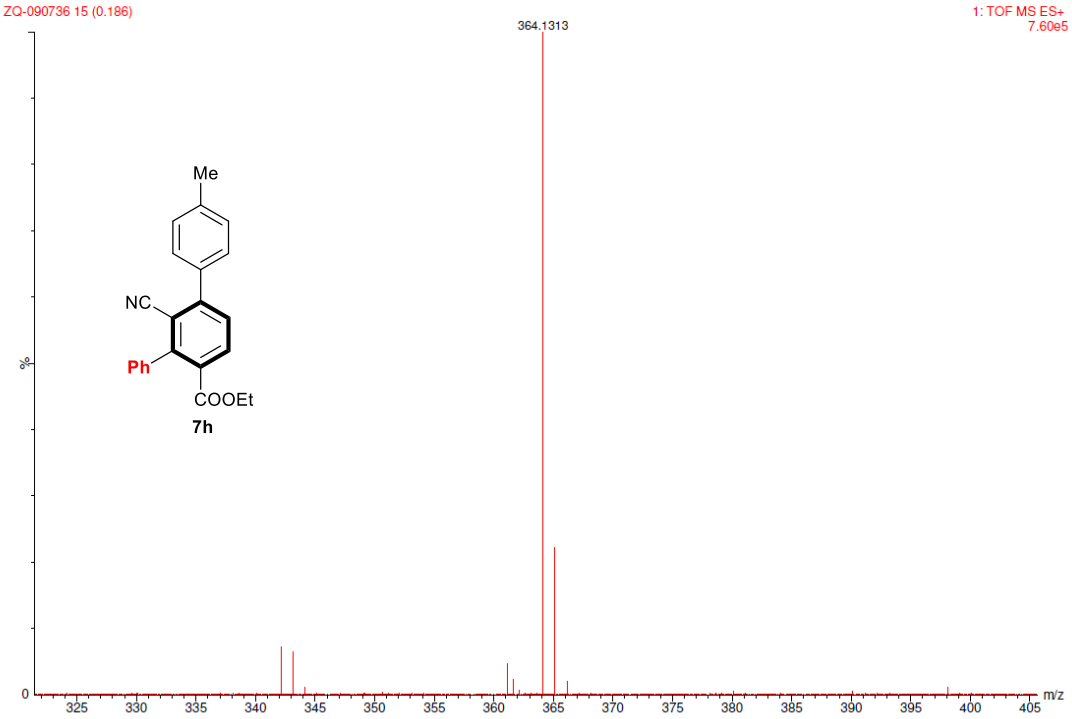

ZQ-090731 33 (0.402)
1: TOF MS ES+
8.68e3
384.0768
Cl
NC
Ph
COOEt
7c
%
0
350
355
360
365
370
375
380
385
390
395
400
405
410
415
420
m/z


ZQ-090731 30 (0.356)
1: TOF MS ES+
1.13e4
384.0771
386.0748
Cl
NC
Ph
COOEt
7d
%
0
366
368
370
372
374
376
378
380
382
384
386
388
390
392
394
396
398
400
402
404
406
408
m/z

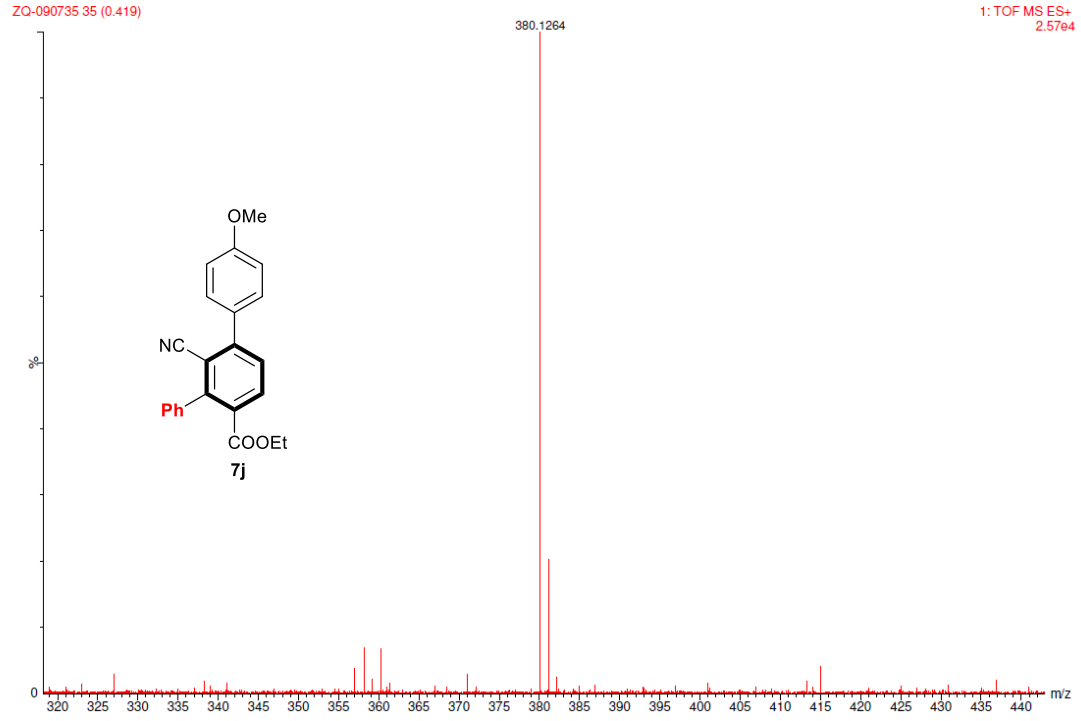

ZQ-090728 17 (0.223)
1: TOF MS ES+
4.68e5
428.0262
430.0251
Br
NC
Ph
COOEt
7e
%
0
m/z
410 412 414 416 418 420 422 424 426 428 430 432 434 436 438 440 442 444 446


ZQ-090732 25 (0.312)
1: TOF MS ES+
1.18e5
368.1064
F
NC
Ph
COOEt
7f
%
0
m/z
310 315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425 430 435

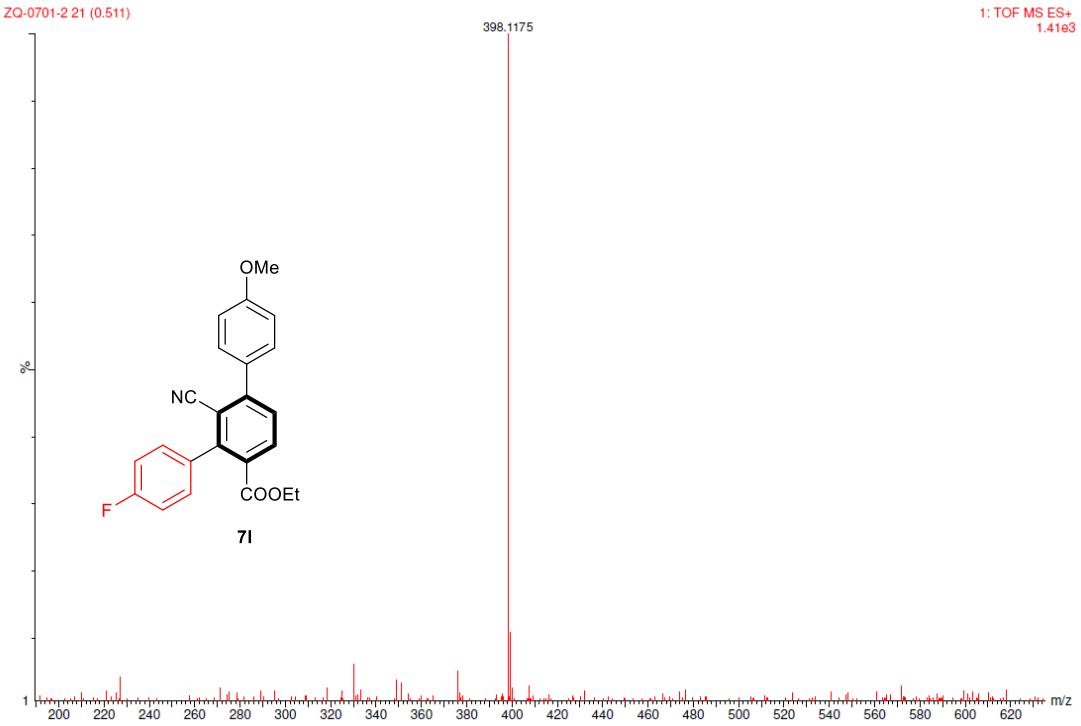

ZQ-090733 34 (0.411)
1: TOF MS ES+
5.40e4
368.1060
F
NC
Ph
COOEt
7g
%
0
335
340
345
350
355
360
365
370
375
380
385
390
395
m/z

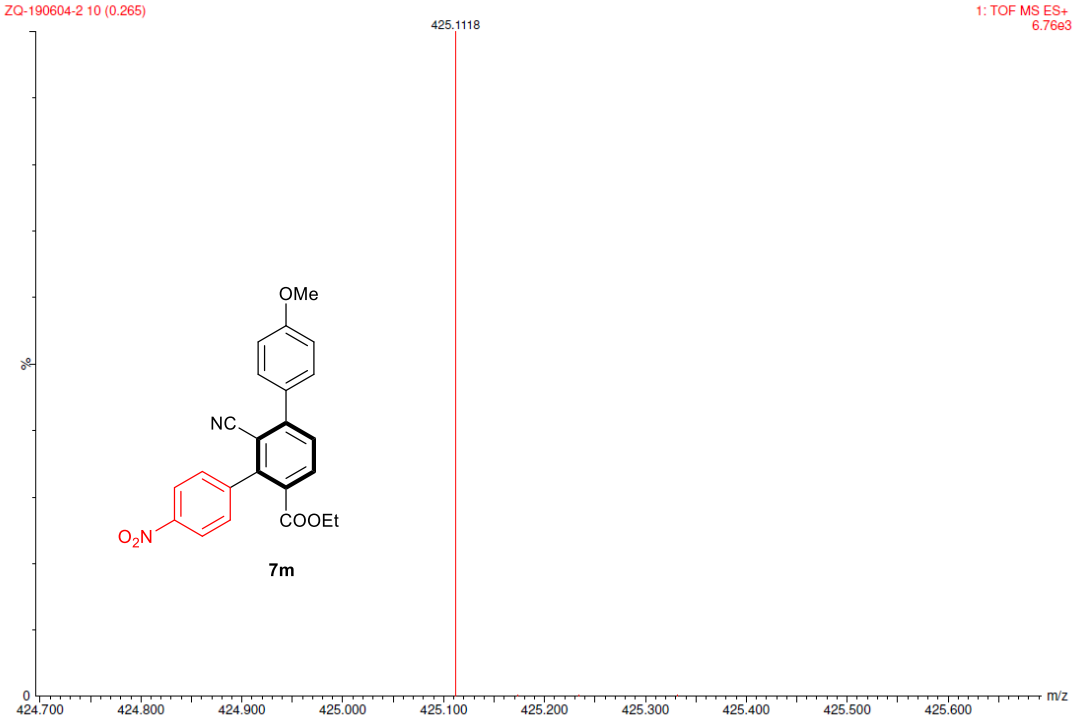

ZQ-090736 15 (0.186)
1: TOF MS ES+
7.60e5
364.1313
Me
NC
Ph
COOEt
7h
%
0
325
330
335
340
345
350
355
360
365
370
375
380
385
390
395
400
405
m/z


ZQ-090734 27 (0.330)
1: TOF MS ES+
3.45e5
380.1261
OMe
NC
Ph
COOEt
7i
%
0
300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460
m/z

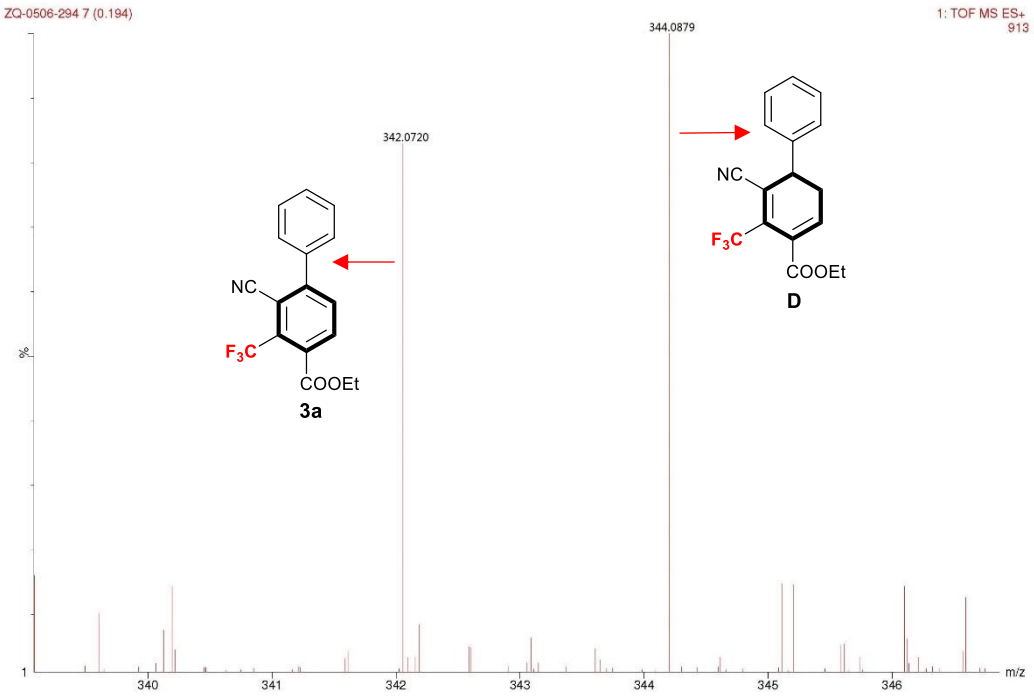

ZQ-090735 35 (0.419)
1: TOF MS ES+
2.57e4
380.1264
OMe
NC
Ph
COOEt
7j
%
0
320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425 430 435 440
m/z

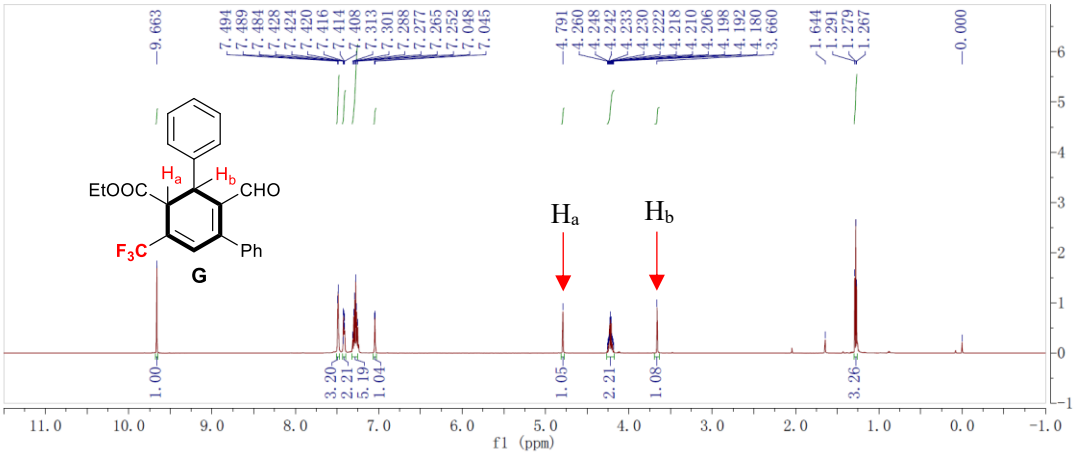

ZQ-01203 6 (0.157)
1: TOF MS ES+
1.23e5
402.0674
F
Cl
NC
Ph
COOEt
7k
%
0
160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700 720
m/z

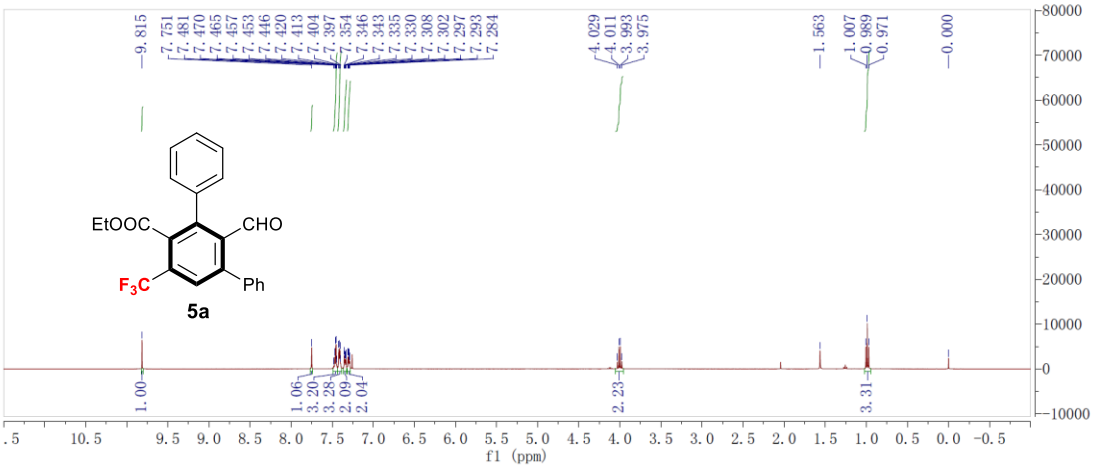

ZQ-0701-2 21 (0.511)
1: TOF MS ES+
1.41e3
398.1175
OMe
NC
F
COOEt
7l
%
1
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620
m/z


ZQ-190604-2 10 (0.265)
1: TOF MS ES+
6.76e3
425.1118
%
0
OMe
NC
COOEt
O2N
7m
424.700
424.800
424.900
425.000
425.100
425.200
425.300
425.400
425.500
425.600
m/z

9. Control experiments results




EtOOC
Ha
Hb
CHO
F3C
Ph
G
Ha
Hb
f1 (ppm)


EtOOC
CHO
F3C
Ph
5a
f1 (ppm)