Supporting Information

for

Nickel-Catalyzed Cross-Coupling of 2-Fluorobenzofurans with Arylboronic Acids via Aromatic C–F Bond Activation

Takeshi Fujita*[1], Haruna Yabuki[2], Ryutaro Morioka[2], Kohei Fuchibe[2], and Junji Ichikawa[3]

[1]The Institute for Solid State Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan

[2]Division of Chemistry, Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8571

[3]Sagami Chemical Research Institute, 2743-1 Hayakawa, Ayase, Kanagawa 252-1193, Japan

Email: tfujita@issp.u-tokyo.ac.jp

* Corresponding author

Detailed experimental procedures and spectral data

1. General Statement

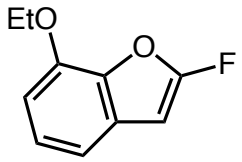
^{1}H NMR, ^{13}C NMR, and ^{19}F NMR were recorded on a Bruker Avance 500 or a JEOL ECS-400 spectrometer. Chemical shift values are given in ppm relative to internal Me_4Si (for ^{1}H NMR: δ = 0.00 ppm), $CDCl_3$ (for ^{13}C NMR: δ = 77.0 ppm), and C_6F_6 (for ^{19}F NMR: δ = 0.0 ppm). IR spectra were recorded on a Horiba FT-730 spectrometer. Mass spectra were measured on a JEOL JMS-T100GCV or a JEOL JMS-T200GC spectrometer.

Column chromatography was conducted on silica gel (Silica Gel 60 N, Kanto Chemical Co., Inc.). Toluene and *N*,*N*-dimethylformamide (DMF) were purified by a solvent-purification system (GlassContour) equipped with columns of activated alumina and supported-copper catalyst (Q-5) before use. 1,4-Dioxane and methanol were distilled from sodium, and stored over molecular sieves 4A. Unless otherwise noted, materials were obtained from commercial sources and used directly without further purifications.

2. Preparation of 2-Fluorobenzofurans

2-Fluorobenzofuran (**1a**) [1], 2-fluoronaphtho[2,1-*b*]furan (**1b**) [1], 2-fluoro-7-methoxybenzofuran (**1c**) [1], 2-fluorobenzo[*b*]thiophene (**4**) [2], 5-bromo-2-fluorobenzofuran (**1e**) [1], 2-chlorobenzofuran (**1a-Cl**) [3], 2-bromobenzofuran (**1a-Br**) [4], and 2-iodobenzofuran (**1a-I**) [5] were prepared according to the literature procedures, and their spectral data showed good agreement with the literature data.

7-Ethoxy-2-benzofuran (1d)

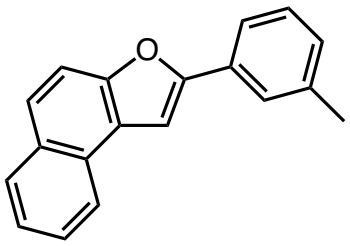


To a DMF (415 mL) solution of 2-(2,2-difluorovinyl)-6-ethoxyphenol (2.75 g, 13.7 mmol) was added DBU (2.46 mL, 16.5 mmol). After stirring at 100 °C for 2 h, water (250 mL) was added to the mixture. Organic materials were extracted with diethyl ether three times. The combined extracts were washed with brine and dried over Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by silica gel column chromatography (pentane/diethyl ether = 10/1) to give **1d** (1.65 g, 67%) as a colorless liquid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.13 (dd, J = 8.1, 7.8 Hz, 1H), 7.04 (dd, J = 7.8, 1.0 Hz, 1H), 6.77 (d, J = 8.1 Hz, 1H), 5.83 (d, J_{HF} = 6.7 Hz, 1H), 4.23 (q, J = 7.0 Hz, 2H), 1.50 (t, J = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 160.2 (d, J_{CF} = 280 Hz), 144.1, 136.8, 129.6, 124.2, 112.9 (d, J_{CF} = 5 Hz), 107.3, 78.7 (d, J_{CF} = 13 Hz), 64.6, 14.9. ^{19}F NMR (470 MHz, $CDCl_3$): δ 49.5 (d, J_{FH} = 7 Hz, 1F). IR (neat): 3136, 3060, 2983, 2933, 1643, 1496, 1439, 1396, 1340, 1296, 1196, 1082, 1018, 978, 893, 783, 727, 658, 607, 555 cm^{-1}. HRMS (EI): m/z Calcd for $C_{10}H_9FO_2$ $[M]^+$: 180.0587; Found: 180.0592.

3. Synthesis of 2-Arylbenzofurans

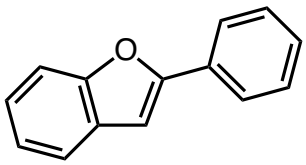
2-(3-Methylphenyl)naphtho[2,1-*b*]furan (3bb)



To the mixture of 2-fluoronaphtho[2,1-*b*]furan (**1b**, 56 mg, 0.30 mmol), (3-methylphenyl)boronic acid (**2b**, 41 mg, 0.30 mmol), $Ni(cod)_2$ (4.2 mg, 0.015 mmol), PCy_3 (8.2 mg, 0.029 mmol), 1,5-cyclooctadiene (1.8 μL, 0.015 mmol), and K_2CO_3 (50 mg, 0.36 mmol) were added toluene (3.0 mL) and H_2O (0.6 mL). After stirring at room temperature for 13 h, the reaction mixture was diluted with H_2O. Organic materials were extracted with diethyl ether three times. The combined extracts were washed with brine and dried over Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by silica gel column chromatography (hexane/EtOAc = 10/1) to give **3bb** (76 mg, 98%) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.75–7.67 (m, 4H), 7.58 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.49–7.46 (m, 2H), 7.35 (dd, *J* = 7.7, 7.6 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.6, 152.3, 138.5, 130.5, 130.4, 129.1, 128.8, 128.7, 127.6, 126.2, 125.3, 125.1, 124.6, 124.5, 123.4, 121.9, 112.3, 100.3, 21.5. IR (KBr): 3051, 1606, 1487, 1387, 1280, 1255, 1163, 1053, 991, 935, 789, 690 cm^{-1}. HRMS (EI): *m*/*z* Calcd for $C_{19}H_{14}O$ $[M]^+$: 258.1045; Found: 258.1035.

2-Phenylbenzofuran (3aa)



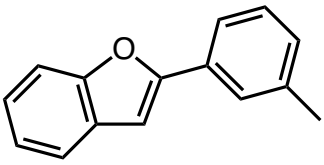
Compound **3aa** was synthesized by the method described for compound **3bb** using 2-fluorobenzofuran (**1a**, 28 mg, 0.20 mmol), phenylboronic acid (**2a**, 29 mg, 0.24 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), PCy_3 (5.6 mg, 0.020 mmol), 1,5-cyclooctadiene (1.2 μL, 0.010 mmol), K_2CO_3 (55 mg, 0.40 mmol), toluene (2.0 mL), and H_2O (0.4 mL).

A white solid, 31 mg, 77% yield.

^1H NMR (500 MHz, $CDCl_3$): δ 7.85 (d, *J* = 7.8 Hz, 2H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.43 (dd, *J* = 7.8, 7.5 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.29–7.20 (m, 2H), 7.00 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.9, 154.8, 130.4, 129.2, 128.8, 128.5, 124.9, 124.2, 122.9, 120.9, 111.1, 101.3.

Spectral data for this compound showed good agreement with literature data [6].

2-(3-Methylphenyl)benzofuran (3ab)



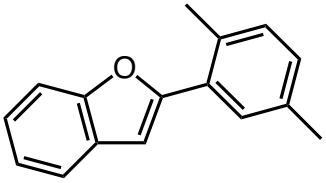
Compound **3ab** was synthesized by the method described for compound **3bb** using 2-fluorobenzofuran (**1a**, 28 mg, 0.20 mmol), (3-methylphenyl)boronic acid (**2b**, 33 mg, 0.24 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), PCy_3 (5.6 mg, 0.020 mmol), 1,5-cyclooctadiene (1.2 μL, 0.010 mmol), K_2CO_3 (55 mg, 0.40 mmol), toluene (2.0 mL), and H_2O (0.4 mL).

A white solid, 41 mg, 96% yield.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.69 (s, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.33 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.29–7.21 (m, 2H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.00 (s, 1H), 2.42 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 156.1, 154.8, 138.4, 130.3, 129.3, 129.2, 128.7, 125.5, 124.1, 122.9, 122.1, 120.8, 111.1, 101.2, 21.5.

Spectral data for this compound showed good agreement with literature data [7].

2-(2,5-Dimethylphenyl)benzofuran (3ac)



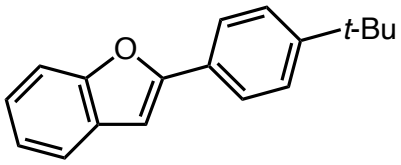
Compound **3ac** was synthesized by the method described for compound **3bb** using 2-fluorobenzofuran (**1a**, 27 mg, 0.20 mmol), (2,5-dimethylphenyl)boronic acid (**2c**, 36 mg, 0.24 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), PCy_3 (5.6 mg, 0.020 mmol), 1,5-cyclooctadiene (1.2 μL, 0.010 mmol), K_2CO_3 (55 mg, 0.40 mmol), toluene (2.0 mL), and H_2O (0.4 mL).

A white solid, 37 mg, 83% yield.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.68 (s, 1H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.30–7.22 (m, 2H), 7.17 (d, *J* = 7.8 Hz, 1H), 7.09 (d, *J* = 7.8 Hz, 1H), 6.87 (s, 1H), 2.53 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.8, 154.3, 135.5, 132.7, 131.2, 129.6, 129.3, 129.2, 128.6, 124.1, 122.7, 120.8, 111.0, 104.9, 21.4, 21.0.

Spectral data for this compound showed good agreement with literature data [6].

2-[4-(*tert*-Butyl)phenyl]benzofuran (3ad)



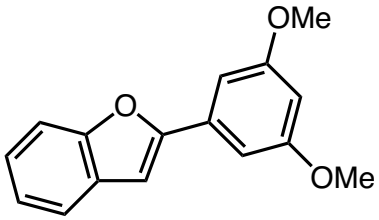
Compound **3ad** was synthesized by the method described for compound **3bb** using 2-fluorobenzofuran (**1a**, 29 mg, 0.21 mmol), [4-(*tert*-butyl)phenyl]boronic acid (**2d**, 43 mg, 0.24 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), PCy_3 (5.6 mg, 0.020 mmol), 1,5-cyclooctadiene (1.2 μL, 0.010 mmol), K_2CO_3 (57 mg, 0.41 mmol), toluene (2.0 mL), and H_2O (0.4 mL).

A white solid, 53 mg, 99% yield.

^1H NMR (500 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.27–7.19 (m, 2H), 6.96 (s, 1H), 1.35 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 156.1, 154.8, 151.8, 129.3, 127.7, 125.7, 124.7, 124.0, 122.8, 120.7, 111.1, 100.7, 34.7, 31.2.

Spectral data for this compound showed good agreement with literature data [8].

2-(3,5-Dimethoxyphenyl)benzofuran (3ae)



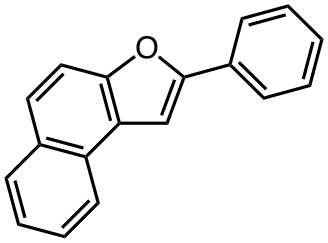
Compound **3ae** was synthesized by the method described for compound **3bb** using 2-fluorobenzofuran (**1a**, 28 mg, 0.20 mmol), (3,5-dimethoxyphenyl)boronic acid (**2e**, 44 mg, 0.24 mmol), $Ni(cod)_2$ (5.5 mg, 0.020 mmol), PCy_3 (11 mg, 0.040 mmol), 1,5-cyclooctadiene (2.5 μL, 0.020 mmol), K_2CO_3 (55 mg, 0.40 mmol), toluene (2.0 mL), and H_2O (0.4 mL).

A colorless oil, 38 mg, 73% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 7.6 Hz, 1H) 7.52 (d, *J* = 8.1 Hz, 1H), 7.30–7.23 (m, 2H), 7.04–7.02 (m, 3H), 6.48 (t, *J* = 2.2 Hz, 1H), 3.88 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 161.0, 155.6, 154.7, 132.1, 129.0, 124.3, 122.9, 120.9, 111.1, 102.9, 101.8, 101.0, 55.4.

Spectral data for this compound showed good agreement with literature data [8].

2-Phenylnaphtho[2,1-*b*]furan (3ba)



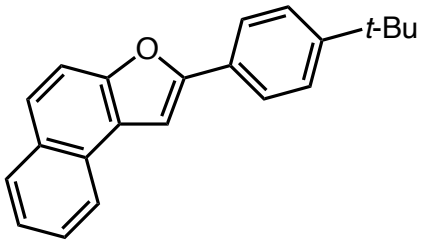
Compound **3ba** was synthesized by the method described for compound **3bb** using 2-fluoronaphtho[2,1-*b*]furan (**1b**, 56 mg, 0.30 mmol), phenylboronic acid (**2a**, 38 mg, 0.31 mmol), $Ni(cod)_2$ (4.2 mg, 0.015 mmol), PCy_3 (8.4 mg, 0.030 mmol), 1,5-cyclooctadiene (1.8 μL, 0.015 mmol), K_2CO_3 (50 mg, 0.36 mmol), toluene (3.0 mL), and H_2O (0.6 mL).

A white solid, 71 mg, 96% yield.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 (d, *J* = 8.2 Hz, 1H) 7.95–7.91 (m, 3H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.68 (d, *J* = 9.0 Hz, 1H), 7.59 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H), 7.51–7.45 (m, 4H), 7.35 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.3, 152.3, 130.6, 130.4, 128.80, 128.76, 128.2, 127.6, 126.2, 125.1, 124.6, 124.52, 124.48, 123.4, 112.2, 100.4.

Spectral data for this compound showed good agreement with literature data [8].

2-[4-(*tert*-Butyl)phenyl]naphtho[2,1-*b*]furan (3bd)



Compound **3bd** was synthesized by the method described for compound **3bb** using 2-fluoronaphtho[2,1-*b*]furan (**1b**, 55 mg, 0.30 mmol), [4-(*tert*-butyl)phenyl]boronic acid (**2d**, 54 mg, 0.30 mmol), $Ni(cod)_2$ (4.3 mg, 0.016 mmol), PCy_3 (8.2 mg, 0.029 mmol), 1,5-cyclooctadiene (1.8 μL, 0.015 mmol), K_2CO_3 (51 mg, 0.37 mmol), toluene (3.0 mL), and H_2O (0.6 mL).

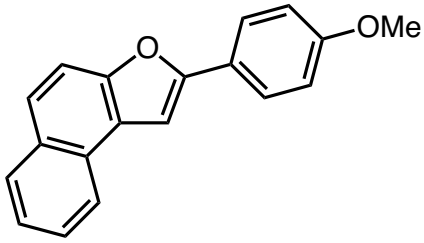
A white solid, 84 mg, 94% yield.

^1H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.86–7.84 (m, 2H), 7.68–7.66 (m, 2H), 7.57–7.55 (m, 1H), 7.49–7.46 (m, 4H), 1.36 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 155.6, 152.2, 151.5, 130.4, 128.8, 127.9, 127.6, 127.4, 126.1, 125.8, 124.8, 124.6, 124.5, 123.5, 112.3, 99.8, 34.7, 31.3.

Spectral data for this compound showed good agreement with literature data [9].

2-(4-Methoxyphenyl)naphtho[2,1-*b*]furan (3bf)



Compound **3bf** was synthesized by the method described for compound **3bb** using 2-fluoronaphtho[2,1-*b*]furan (**1b**, 39 mg, 0.21 mmol), (4-methoxyphenyl)boronic acid (**2f**, 38 mg, 0.25 mmol), $Ni(cod)_2$ (2.8 mg, 0.010 mmol), PCy_3 (5.6 mg, 0.020 mmol), 1,5-

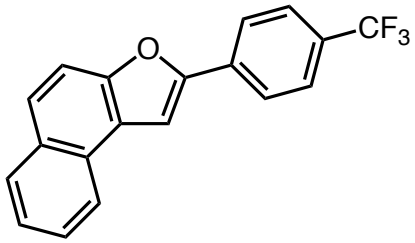
cyclooctadiene (1.2 μL, 0.010 mmol), K_2CO_3 (55 mg, 0.40 mmol), toluene (2.0 mL), and H_2O (0.4 mL).

A white solid, 54 mg, 94% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.8 Hz, 2H), 7.70–7.65 (m, 2H), 7.59–7.47 (m, 2H), 7.36 (s, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 159.8, 155.5, 152.0, 130.4, 128.7, 127.5, 126.12, 126.06, 124.7, 124.5, 124.4, 123.52, 123.45, 114.3, 112.2, 98.8, 55.3.

Spectral data for this compound showed good agreement with literature data [10].

2-[4-(Trifluoromethyl)phenyl]naphtho[2,1-*b*]furan (3bg)



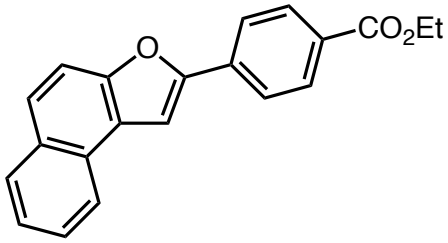
Compound **3bg** was synthesized by the method described for compound **3bb** using 2-fluoronaphtho[2,1-*b*]furan (**1b**, 56 mg, 0.30 mmol), [4-(trifluoromethyl)phenyl]boronic acid (**2g**, 57 mg, 0.30 mmol), $Ni(cod)_2$ (17 mg, 0.060 mmol), PCy_3 (34 mg, 0.12 mmol), 1,5-cyclooctadiene (7.4 μL, 0.060 mmol), K_3PO_4 (76 mg, 0.36 mmol), toluene (3.0 mL), and H_2O (0.6 mL).

A white solid, 74 mg, 78% yield.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.3 Hz, 2H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.78–7.69 (m, 4H), 7.63–7.61 (m, 2H), 7.52 (dd, *J* = 8.0, 7.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.6, 152.8, 133.8, 130.5, 129.8 (q, J_{CF} = 32 Hz), 128.9, 127.6, 126.6, 126.2, 125.9 (q, J_{CF} = 4 Hz), 124.9, 124.6, 124.3, 124.1 (q, J_{CF} = 271 Hz), 123.4, 112.3, 102.4. ^{19}F NMR (470 MHz, $CDCl_3$): δ 100.3 (s). IR (KBr): 3066,

2929, 1616, 1412, 1325, 1169, 1128, 1072, 1012, 922, 841, 802, 750, 675, 594 cm^{-1}. HRMS (EI): *m*/*z* Calcd for $C_{19}H_{11}F_3O$ $[M]^+$: 312.0762; Found: 312.0770.

Ethyl 4-(naphtho[2,1-*b*]furan-2-yl)benzoate (3bh)

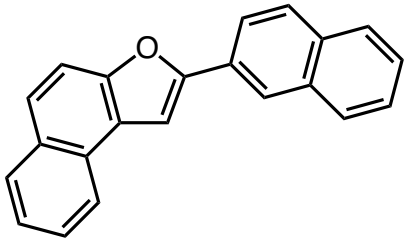


Compound **3bh** was synthesized by the method described for compound **3bb** using 2-fluoronaphtho[2,1-*b*]furan (**1b**, 38 mg, 0.20 mmol), [4-(ethoxycarbonyl)phenyl]boronic acid (**2h**, 47 mg, 0.24 mmol), $Ni(cod)_2$ (2.9 mg, 0.011 mmol), PCy_3 (5.7 mg, 0.020 mmol), 1,5-cyclooctadiene (1.2 μL, 0.010 mmol), K_2CO_3 (57 mg, 0.41 mmol), toluene (2.0 mL), and H_2O (0.4 mL).

A white solid, 35 mg, 54% yield.

^1H NMR (400 MHz, $CDCl_3$): δ 8.19–8.13 (m, 3H), 7.99–7.95 (m, 3H), 7.77 (d, *J* = 9.4 Hz, 1H), 7.70 (d, *J* = 9.4 Hz, 1H), 7.65 (s, 1H), 7.62 (ddd, *J* = 8.4, 6.8, 0.8 Hz, 1H), 7.51 (ddd, *J* = 8.2, 6.8, 1.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 154.2, 152.9, 134.5, 130.5, 130.2, 129.8, 128.9, 127.6, 126.6, 126.1, 124.8, 124.4, 124.3, 123.4, 112.3, 102.5, 61.1, 14.4. IR (KBr): 3057, 2981, 1712, 1608, 1410, 1367, 1279, 1178, 1105, 1022, 989, 856, 810, 768, 690 cm^{-1}. HRMS (FD): *m*/*z* Calcd for $C_{21}H_{16}O_3$ $[M]^+$: 316.1099; Found: 316.1105.

2-(Naphthalen-2-yl)naphtho[2,1-*b*]furan (3bi)



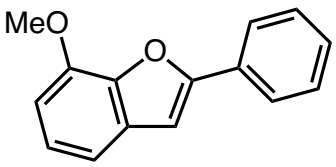
Compound **3bi** was synthesized by the method described for compound **3bb** using 2-fluoronaphtho[2,1-*b*]furan (**1b**, 56 mg, 0.30 mmol), 2-naphthylboronic acid (**2i**, 51 mg, 0.30 mmol), $Ni(cod)_2$ (4.1 mg, 0.015 mmol), PCy_3 (8.5 mg, 0.030 mmol), 1,5-cyclooctadiene (1.8 μL, 0.015 mmol), K_2CO_3 (50 mg, 0.36 mmol), toluene (3.0 mL), methanol (0.6 mL), and H_2O (0.6 mL).

A white solid, 62 mg, 70% yield.

^1H NMR (500 MHz, $CDCl_3$): δ 8.42 (s, 1H), 8.21 (d, *J* = 8.2 Hz, 1H), 8.01–7.92 (m, 4H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.65 (s, 1H), 7.62 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.55–7.51 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.4, 152.5, 133.5, 133.1, 130.5, 128.8, 128.6, 128.4, 127.9, 127.8, 127.6, 126.7, 126.4, 126.3, 125.4, 124.63, 124.61, 123.5, 123.4, 122.7, 112.3, 101.1.

Spectral data for this compound showed good agreement with literature data [11].

7-Methoxy-2-phenylbenzofuran (3ca)



Compound **3ca** was synthesized by the method described for compound **3bb** using 2-fluoro-7-methoxybenzofuran (**1c**, 56 mg, 0.33 mmol), phenylboronic acid (**2a**, 37 mg, 0.31 mmol), $Ni(cod)_2$ (4.1 mg, 0.015 mmol), PCy_3 (8.1 mg, 0.029 mmol), 1,5-

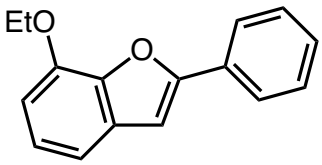
cyclooctadiene (1.8 μL, 0.015 mmol), K_2CO_3 (50 mg, 0.36 mmol), toluene (3.0 mL), and H_2O (0.6 mL).

A white solid, 46 mg, 67% yield.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89 (d, *J* = 7.4 Hz, 2H), 7.44 (dd, *J* = 7.9, 7.4 Hz, 2H), 7.36–7.33 (m, 1H), 7.19–7.13 (m, 2H), 7.01 (s, 1H), 6.80 (d, *J* = 6.7 Hz, 1H), 4.05 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 156.0, 145.3, 144.1, 130.9, 130.3, 128.7, 128.5, 125.0, 123.6, 113.3, 106.6, 101.6, 56.1.

Spectral data for this compound showed good agreement with literature data [12].

7-Ethoxy-2-phenylbenzofuran (3da)



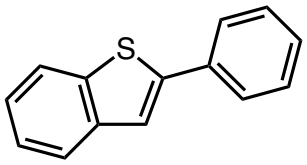
Compound **3da** was synthesized by the method described for compound **3bb** using 7-ethoxy-2-fluorobenzofuran (**1d**, 54 mg, 0.30 mmol), phenylboronic acid (**2a**, 37 mg, 0.31 mmol), $Ni(cod)_2$ (4.1 mg, 0.015 mmol), PCy_3 (8.1 mg, 0.029 mmol), 1,5-cyclooctadiene (1.8 μL, 0.015 mmol), K_2CO_3 (50 mg, 0.36 mmol), toluene (3.0 mL), and H_2O (0.6 mL).

A colorless oil, 46 mg, 65% yield.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.0 Hz, 2H), 7.44 (dd, *J* = 8.0, 7.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 7.12 (dd, *J* = 7.8, 7.6 Hz, 1H), 7.00 (s, 1H), 6.80 (d, *J* = 7.8 Hz, 1H), 4.32 (q, *J* = 7.0 Hz, 2H), 1.54 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.9, 144.5, 144.3, 131.0, 130.4, 128.7, 128.5, 125.0, 123.5, 113.2, 108.1, 101.6, 64.7, 15.0.

Spectral data for this compound showed good agreement with literature data [12].

2-Phenylbenzo[*b*]thiophene (5)



Compound **5** was synthesized by the method described for compound **3bb** using 2-fluorobenzo[*b*]thiophene (**4**, 45 mg, 0.29 mmol), phenylboronic acid (**2a**, 37 mg, 0.30 mmol), $Ni(cod)_2$ (17 mg, 0.060 mmol), PCy_3 (34 mg, 0.12 mmol), K_2CO_3 (50 mg, 0.36 mmol), toluene (3.0 mL), and H_2O (0.6 mL).

A white solid, 29 mg, 48% yield.

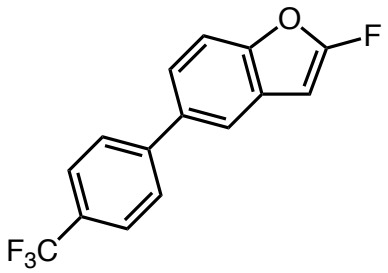
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.54 (s, 1H), 7.42 (dd, *J* = 7.9, 7.5 Hz, 2H), 7.36–7.29 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 144.2, 140.7, 139.5, 134.3, 128.9, 128.2, 126.5, 124.5, 124.3, 123.5, 122.2, 119.4.

Spectral data for this compound showed good agreement with literature data [13].

4. Orthogonal Coupling Reactions of Aromatic C–F and C–Br Bonds

2-Fluoro-5-[4-(trifluoromethyl)phenyl]benzofuran (1f)

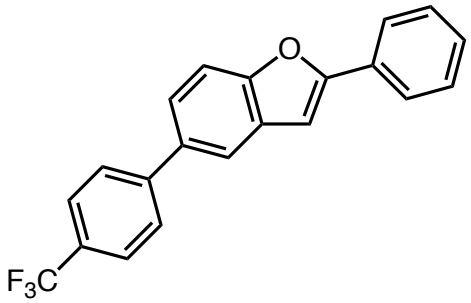


To the mixture of 5-bromo-2-fluorobenzofuran (**1e**, 357 mg, 1.66 mmol), [4-(trifluoromethyl)phenyl)]boronic acid (**2g**, 453 mg, 2.39 mmol), $Pd(PPh_3)_4$ (92 mg, 0.080 mmol), K_3PO_4 (1.27 g, 5.98 mmol), and H_2O (0.18 mL, 10 mmol) was added 1,4-dioxane (5.3 mL). After stirring at 80 °C for 12 h, the reaction mixture was diluted

with H_2O. Organic materials were extracted with dichloromethane three times. The combined extracts were washed with brine and dried over Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by silica gel column chromatography (hexane) to give **1f** (444 mg, 95%) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.73–7.65 (m, 5H), 7.47–7.43 (m, 2H), 5.91 (d, J_{HF} = 6.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 160.9 (d, J_{CF} = 281 Hz), 147.7, 144.9, 135.9, 129.2 (q, J_{CF} = 32 Hz), 128.6 (d, J_{CF} = 3 Hz), 127.6, 125.7 (q, J_{CF} = 4 Hz), 124.3 (q, J_{CF} = 272 Hz), 123.0 (d, J_{CF} = 4 Hz), 119.5 (d, J_{CF} = 6 Hz), 111.3, 78.6 (d, J_{CF} = 14 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): δ 100.5 (s, 3F), 52.3 (d, J_{FH} = 7 Hz, 1F). IR (KBr): 3149, 1637, 1468, 1323, 1165, 1124, 1068, 976, 843, 810, 777, 671 cm^{-1}. HRMS (EI): *m*/*z* Calcd for $C_{15}H_8F_4O$ $[M]^+$: 280.0511; Found: 280.0522.

2-Phenyl-5-[4-(trifluoromethyl)phenyl]benzofuran (3fa)



Compound **3fa** was synthesized by the method described for compound **3bb** using 2-fluoro-5-[4-(trifluoromethyl)phenyl]benzofuran (**1f**, 85 mg, 0.30 mmol), phenylboronic acid (**2a**, 38 mg, 0.31 mmol), $Ni(cod)_2$ (4.2 mg, 0.015 mmol), PCy_3 (8.2 mg, 0.029 mmol), 1,5-cyclooctadiene (1.8 μL, 0.015 mmol), K_2CO_3 (50 mg, 0.36 mmol), toluene (3.0 mL), and H_2O (0.6 mL).

A white solid, 83 mg, 81% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, *J* = 6.8 Hz, 2H), 7.78 (d, *J* = 1.6 Hz, 1H), 7.75–7.69 (m, 4H), 7.60 (d, *J* = 8.8 Hz, 1H), 7.52–7.45 (m, 3H), 7.38 (t, *J* = 7.4 Hz, 1H),

7.08 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 154.9, 145.2, 135.1, 130.2, 129.9, 129.0 (q, J_{CF} = 32 Hz), 128.85, 128.85, 127.6, 125.7 (q, J_{CF} = 4 Hz), 125.0, 124.5 (q, J_{CF} = 270 Hz), 123.9, 119.6, 111.5, 101.3. ^{19}F NMR (376 MHz, $CDCl_3$): δ 99.4 (s). Spectral data for this compound showed good agreement with literature data [14].

5. References

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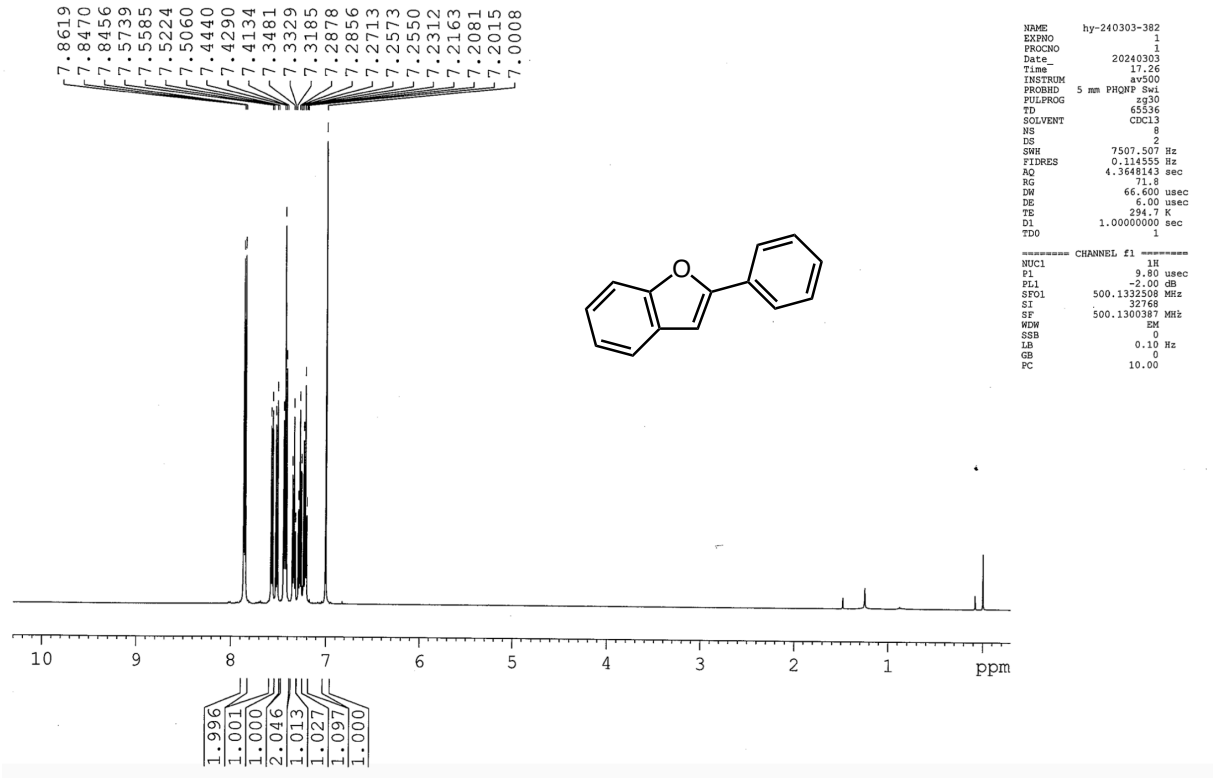
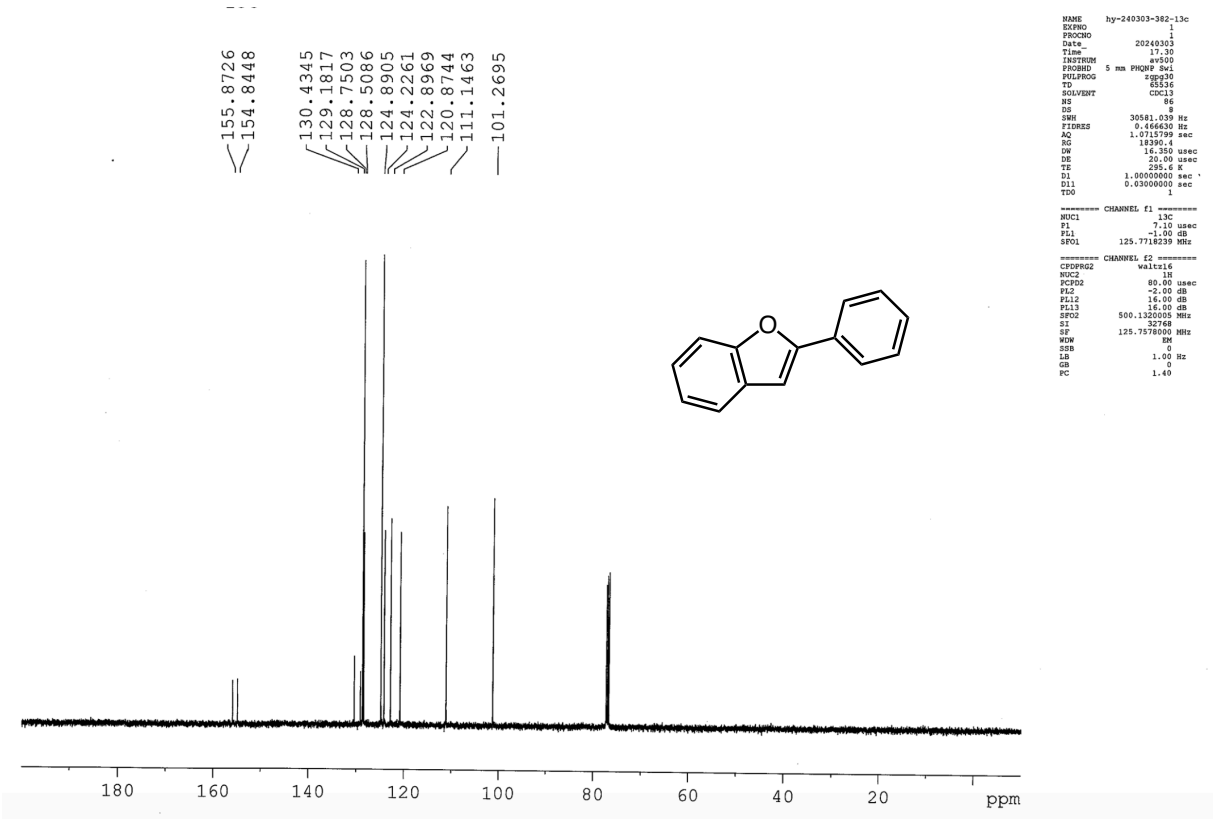
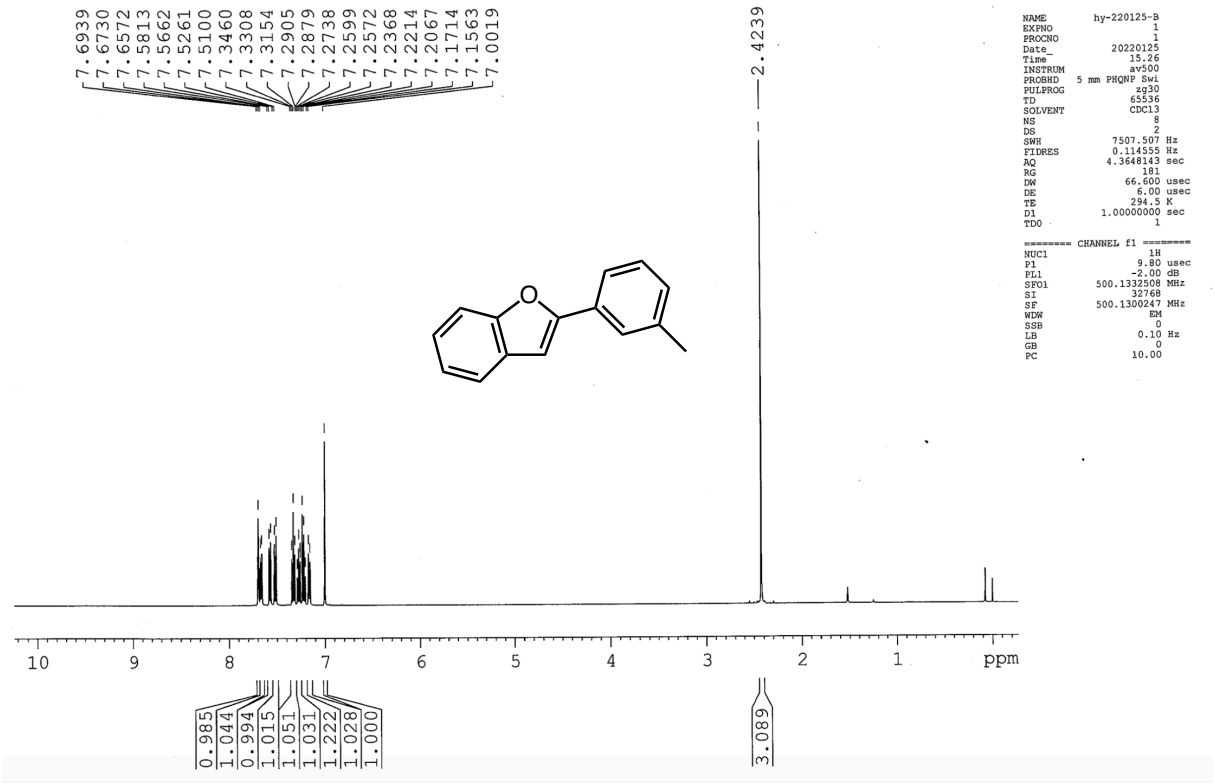
6. ^{1}H, ^{13}C, and ^{19}F NMR Charts

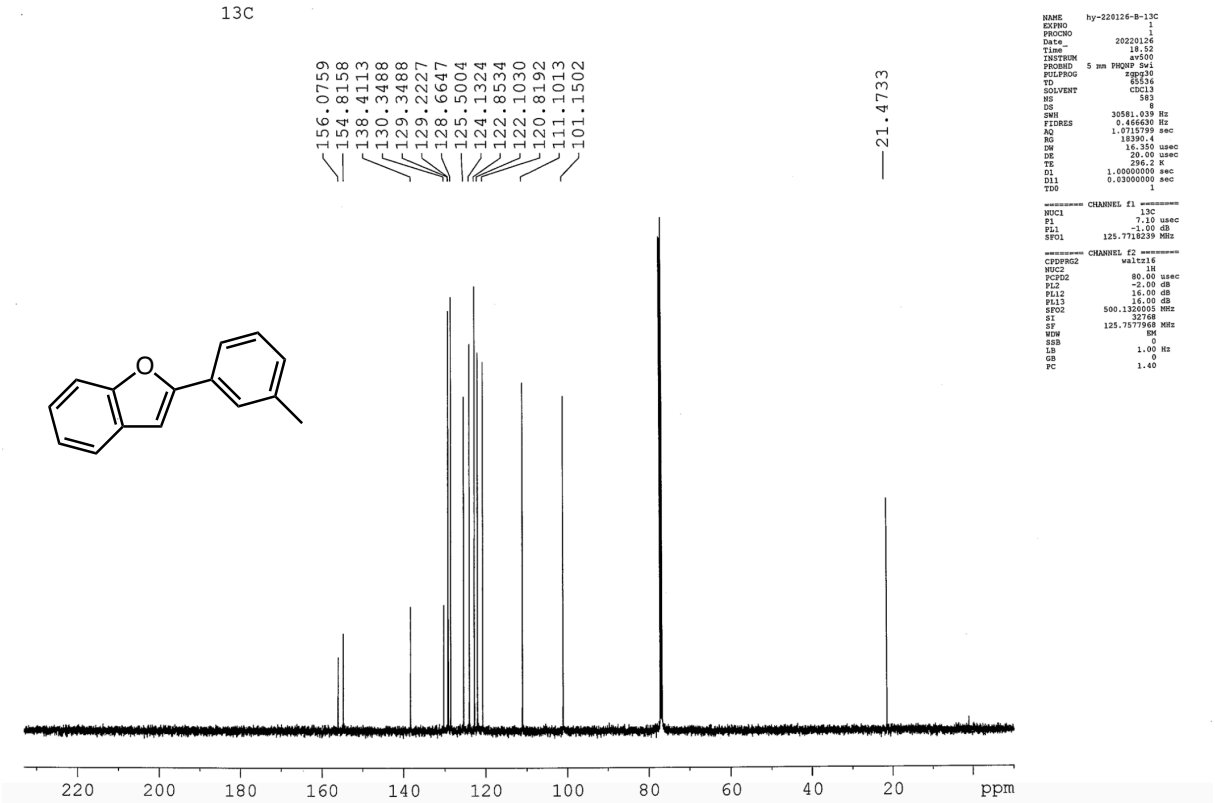
2-Phenylbenzofuran (3aa)



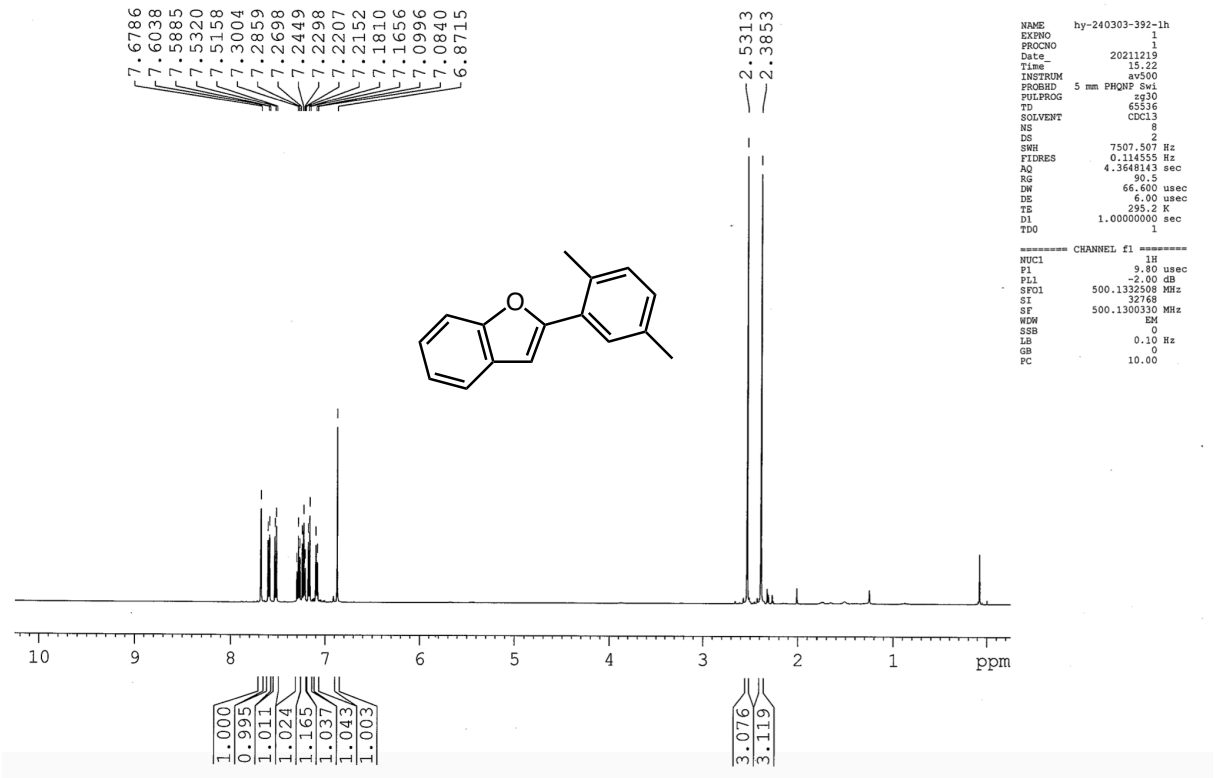


2-(3-Methylphenyl)benzofuran (3ab)





2-(2,5-Dimethylphenyl)benzofuran (3ac)

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D1             1.00000000 sec
TD0                      1

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PL1                -2.00 dB
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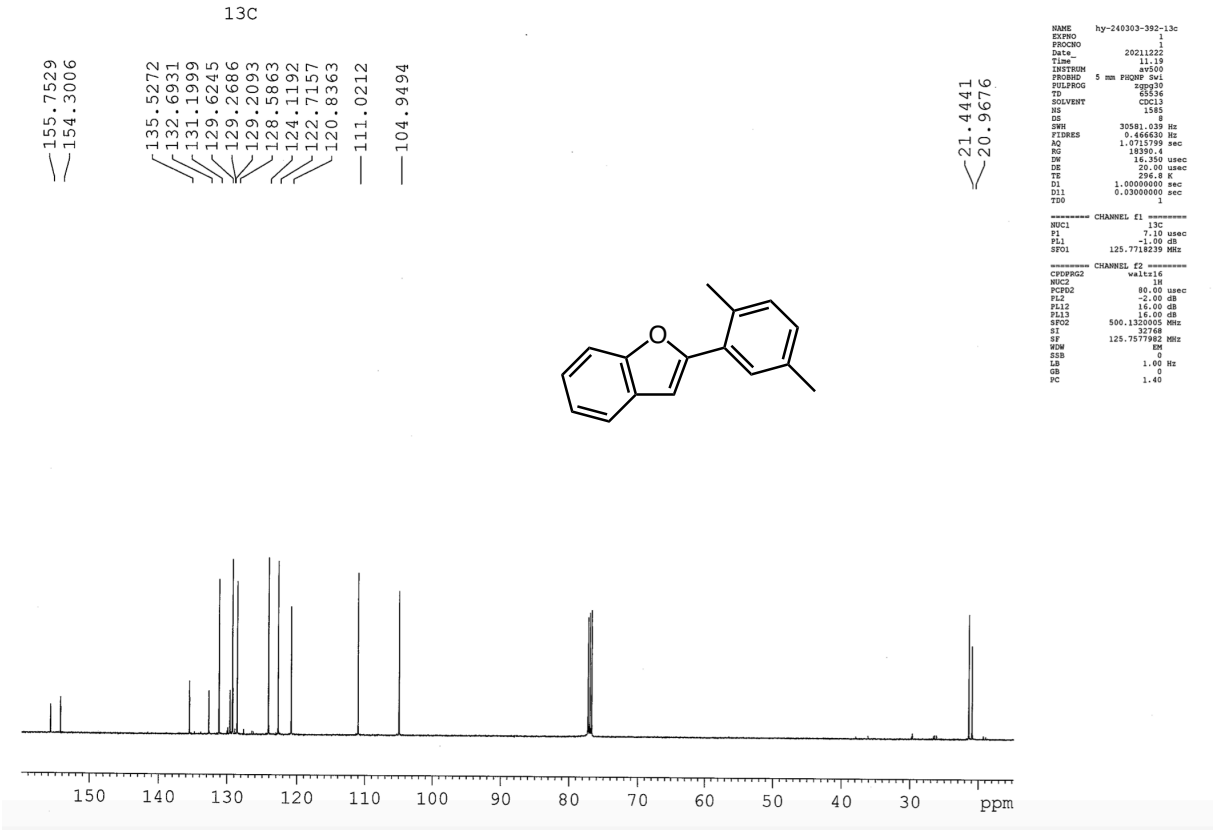


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TE                296.8 K
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D11            0.03000000 sec
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PL1                -1.00 dB
SFO1          125.7718239 MHz

======== CHANNEL f2 ========
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NUC2                   1H
PCPD2              80.00 usec
PL2                -2.00 dB
PL12               16.00 dB
PL13               16.00 dB
SFO2          500.1320005 MHz
SI                   32768
SF            125.7577982 MHz
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SSB                     0
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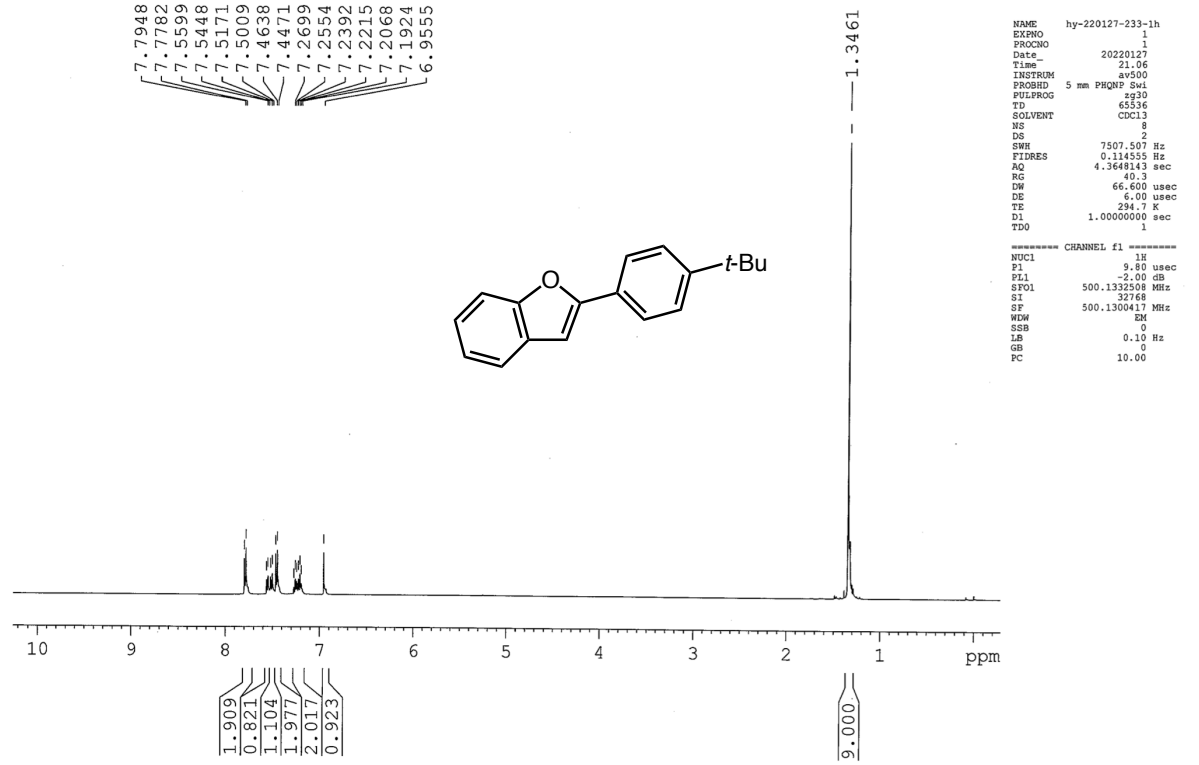
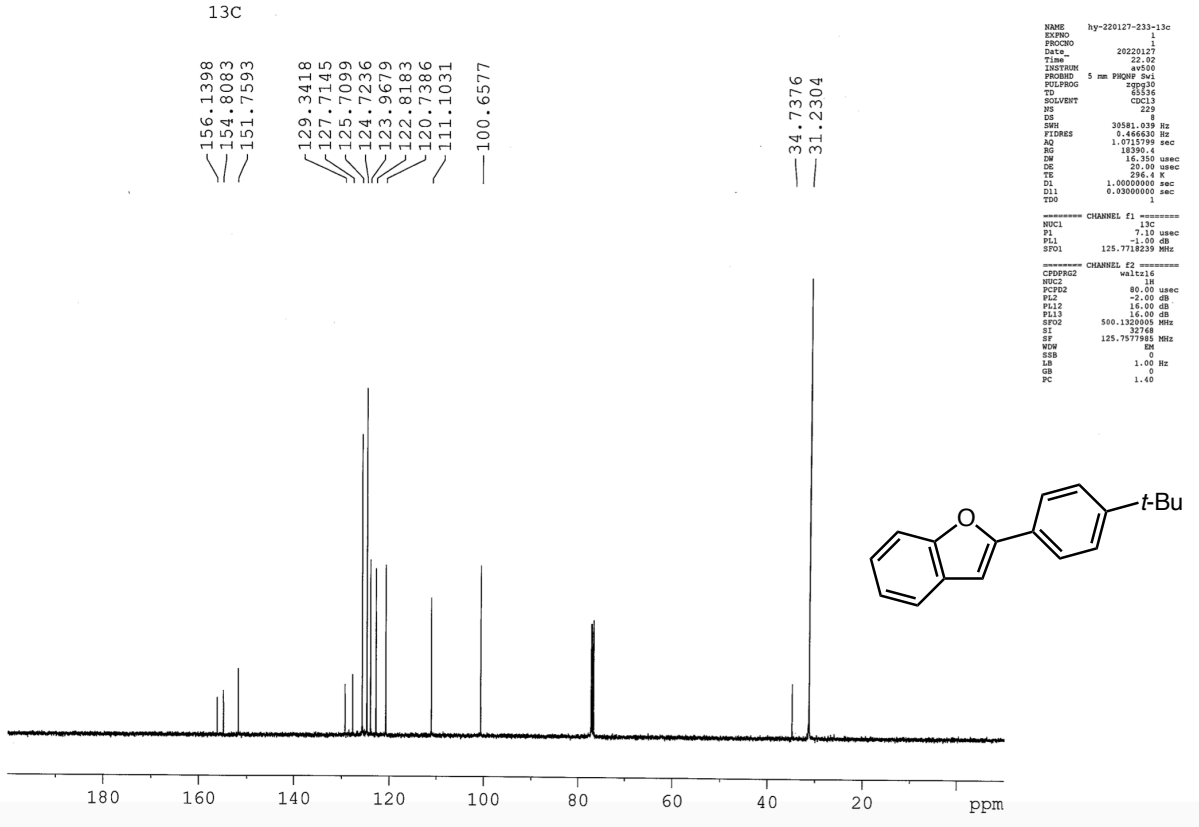
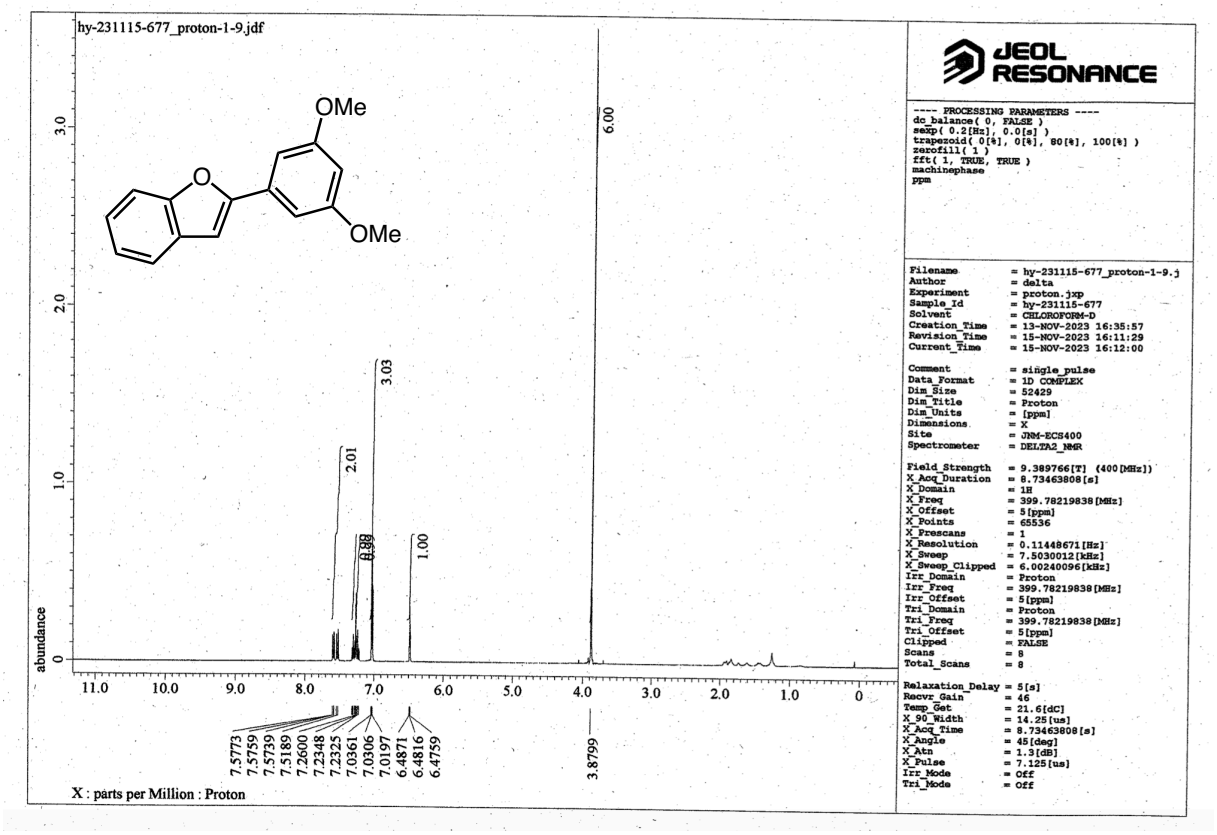
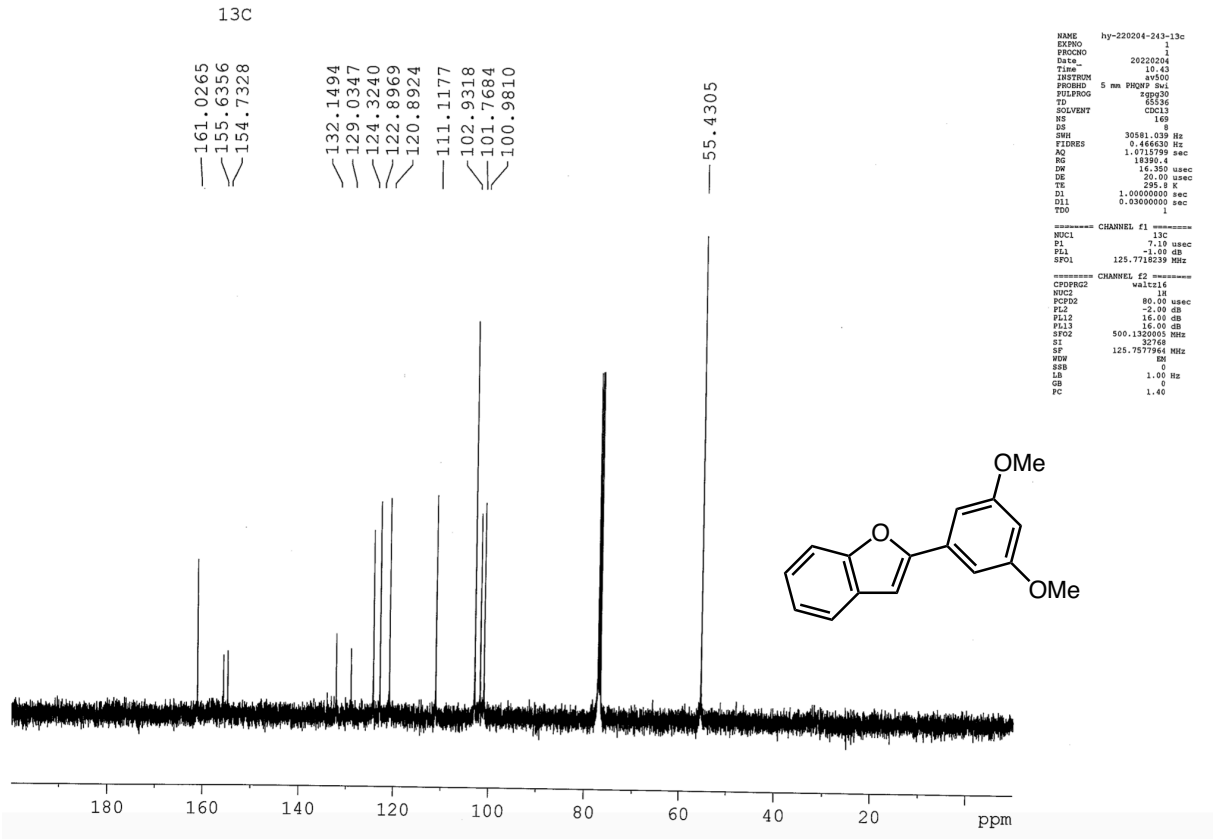
2-[4-(*tert*-Butyl)phenyl]benzofuran (3ad)



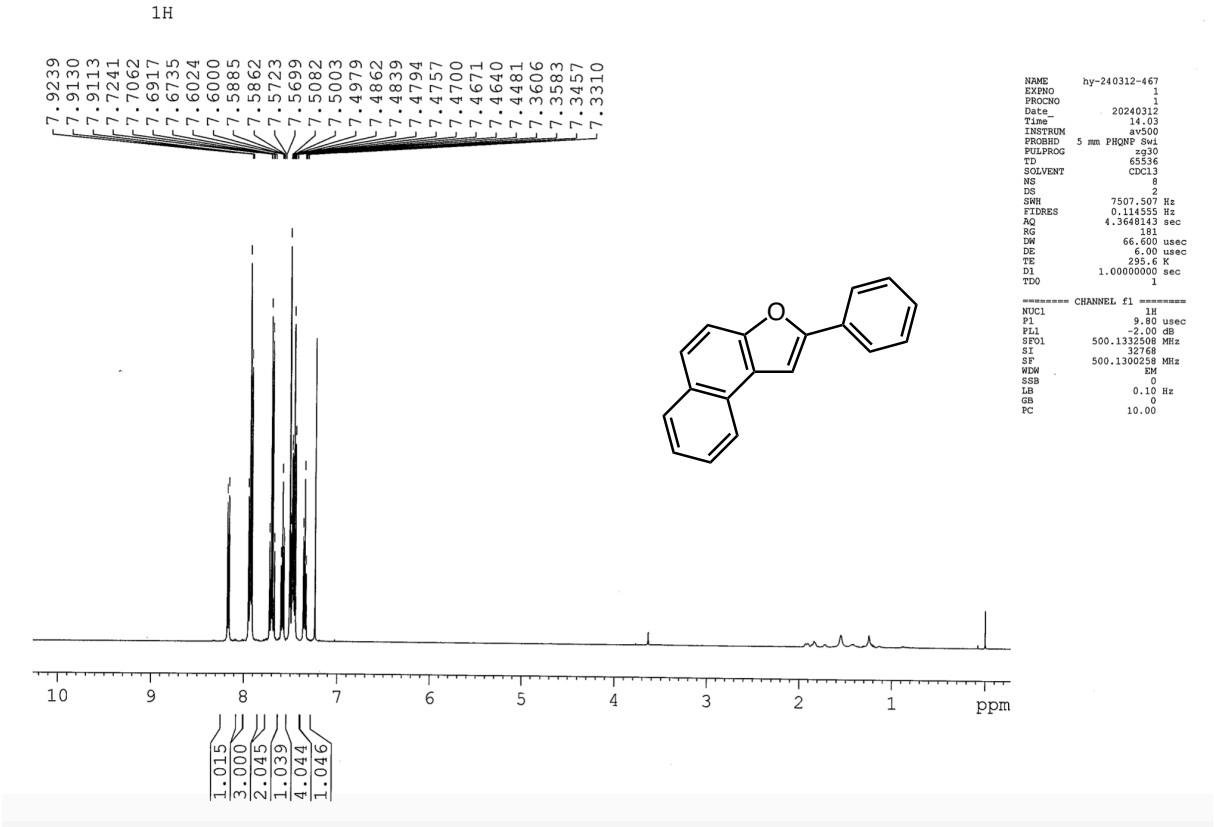


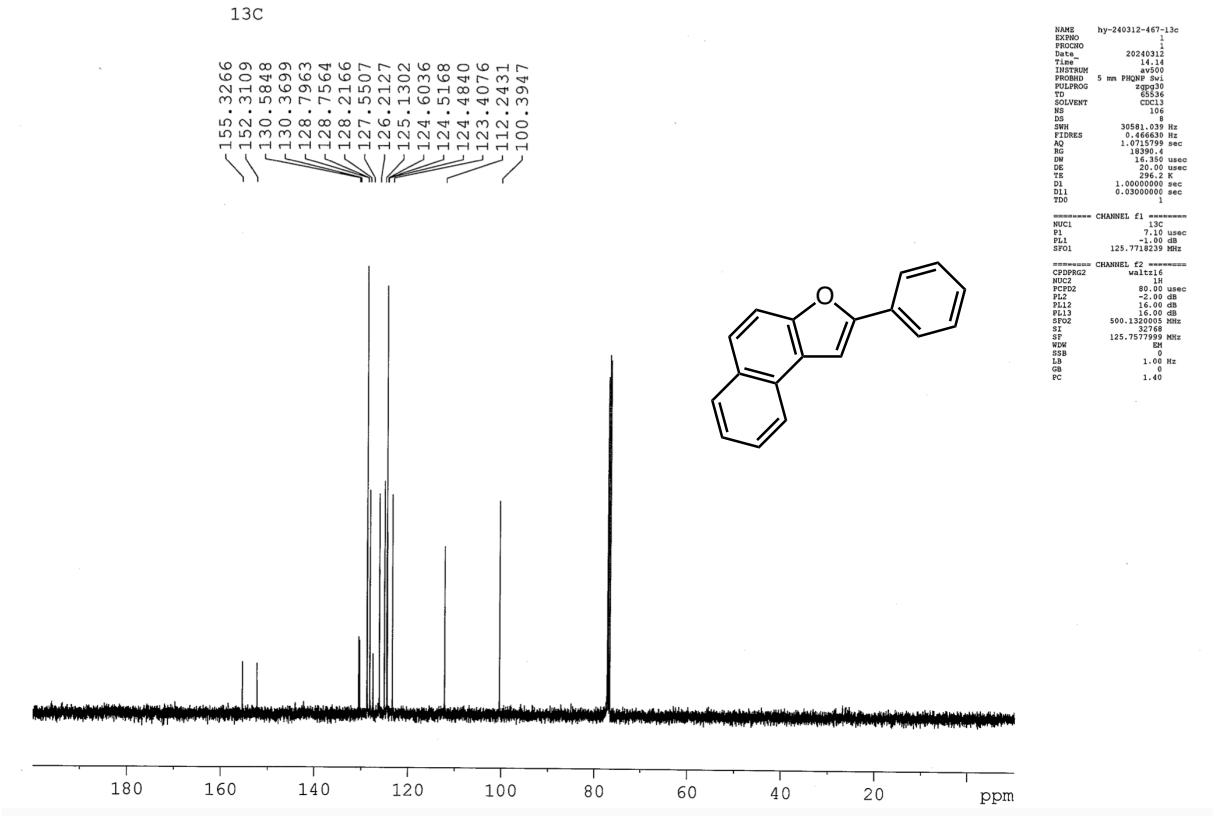
2-(3,5-Dimethoxyphenyl)benzofuran (3ae)



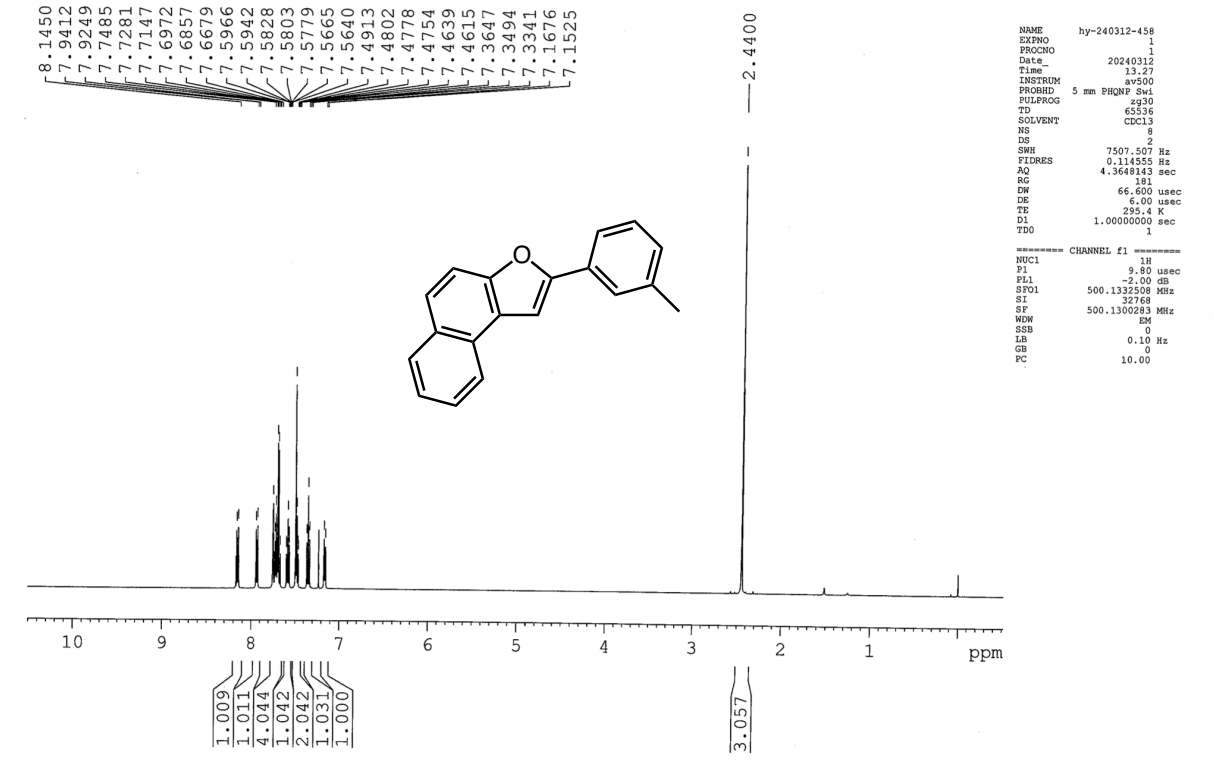


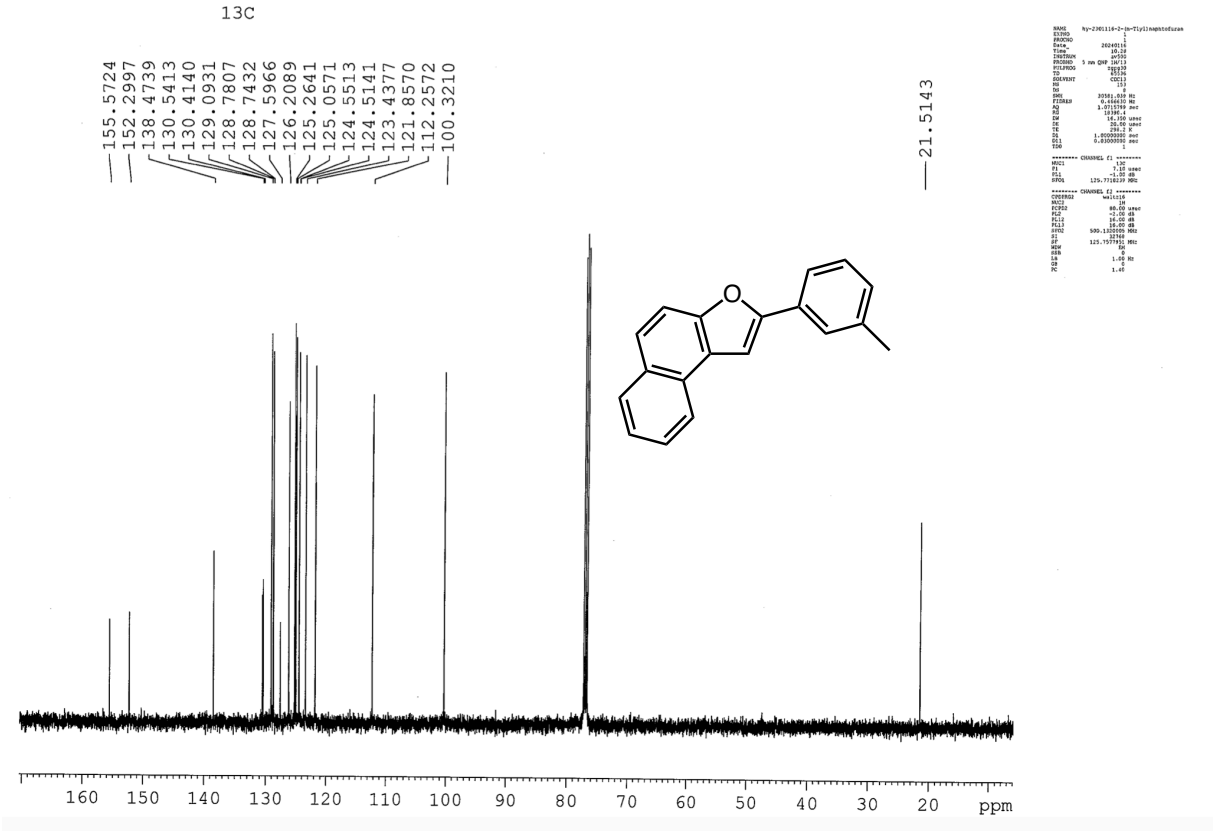
2-Phenylnaphtho[2,1-*b*]furan (3ba)



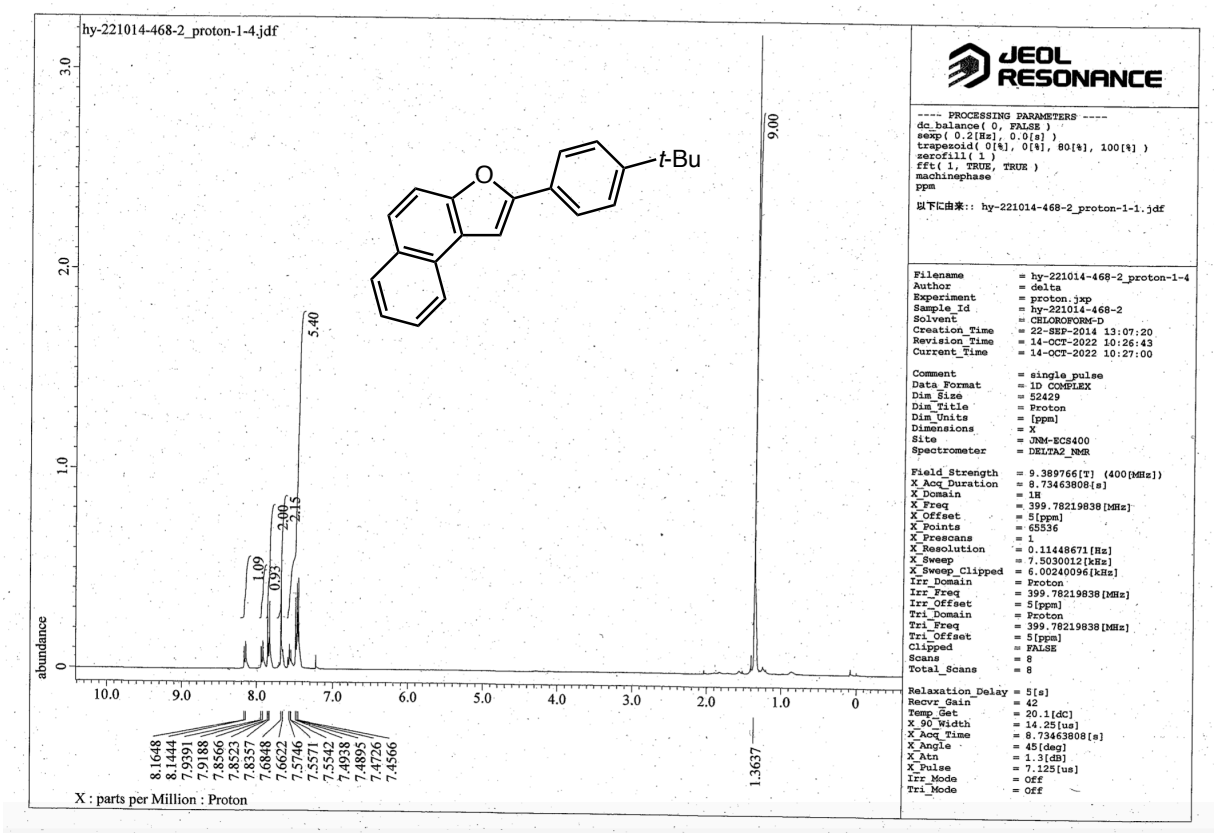


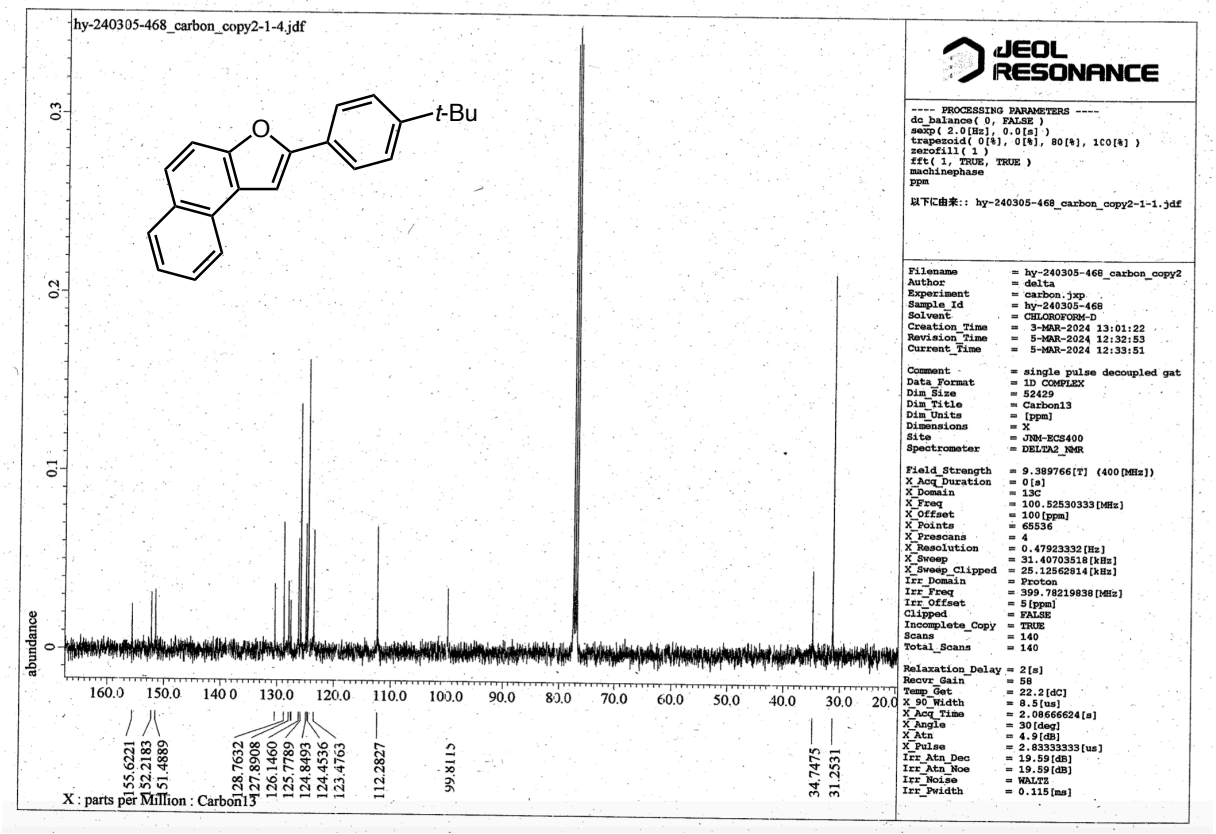
2-(3-Methylphenyl)naphtho[2,1-*b*]furan (3bb)



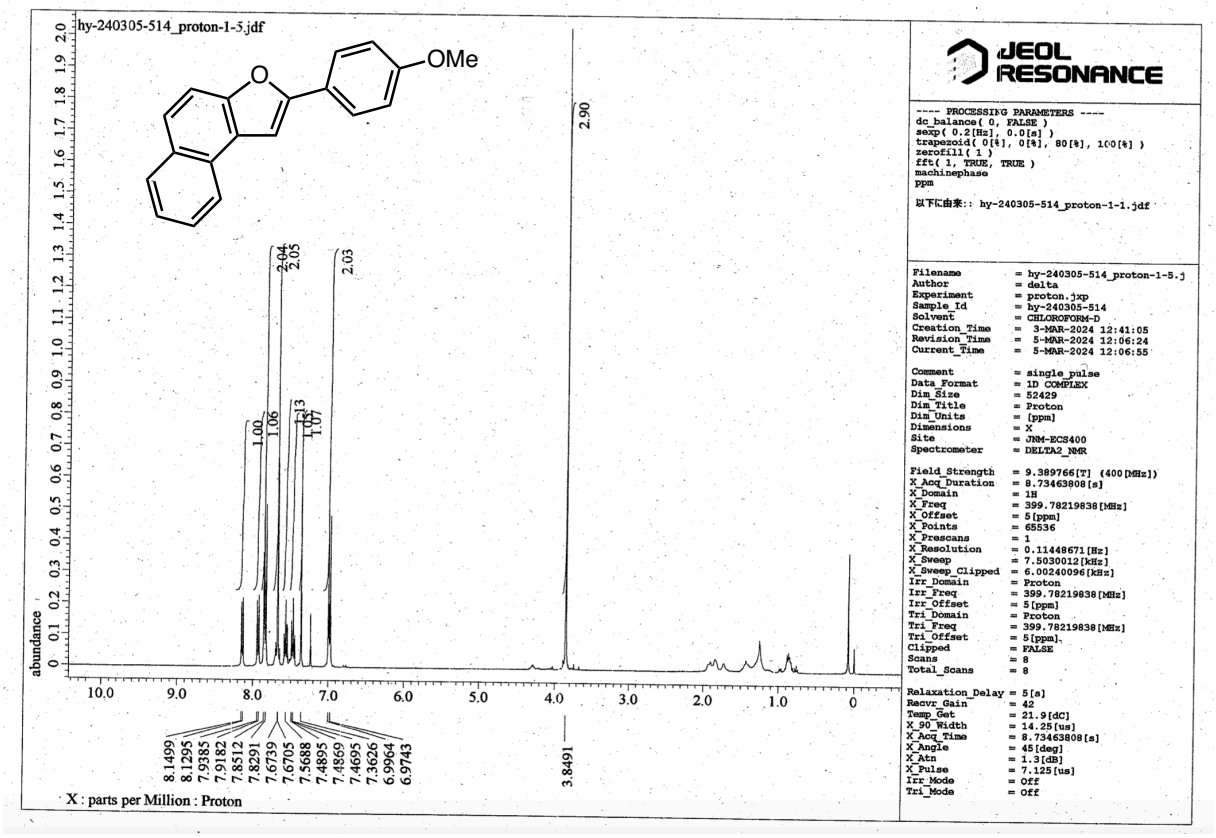


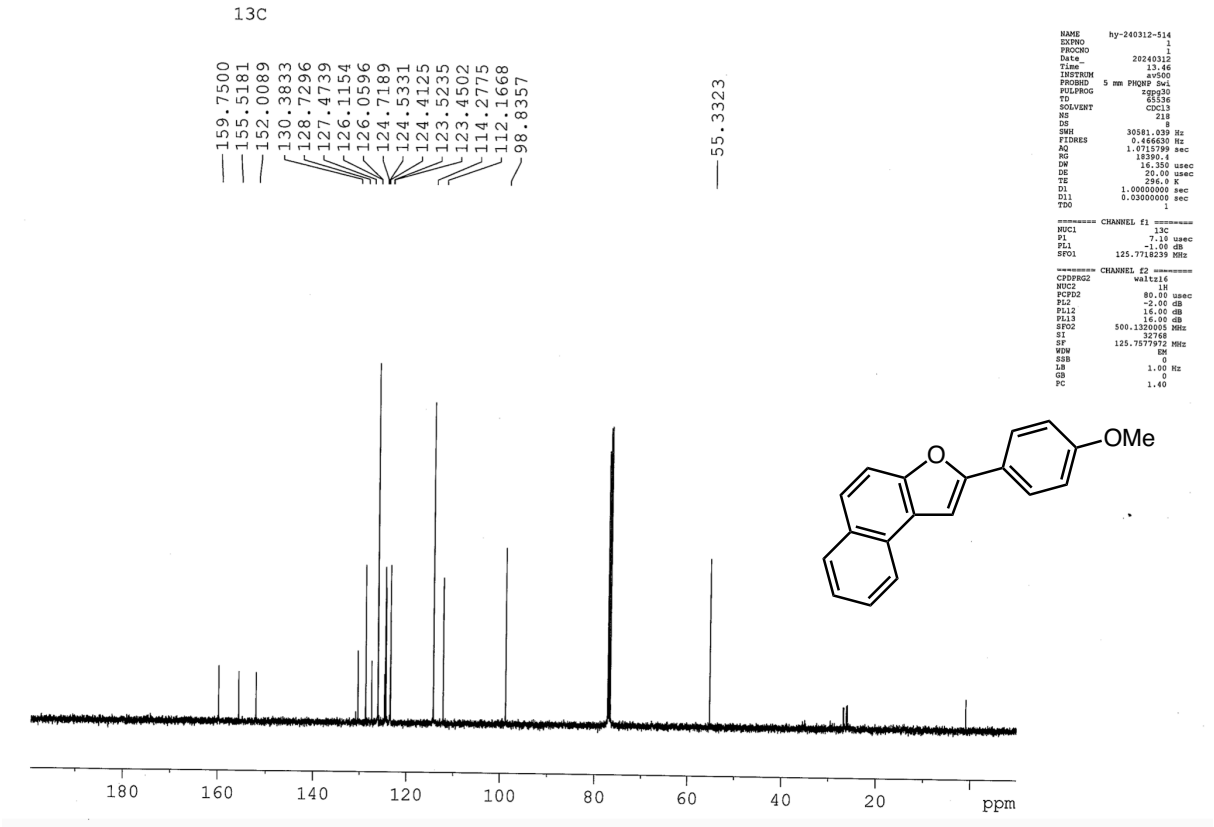
2-[4-(*tert*-Butyl)phenyl]naphtho[2,1-*b*]furan (3bd)



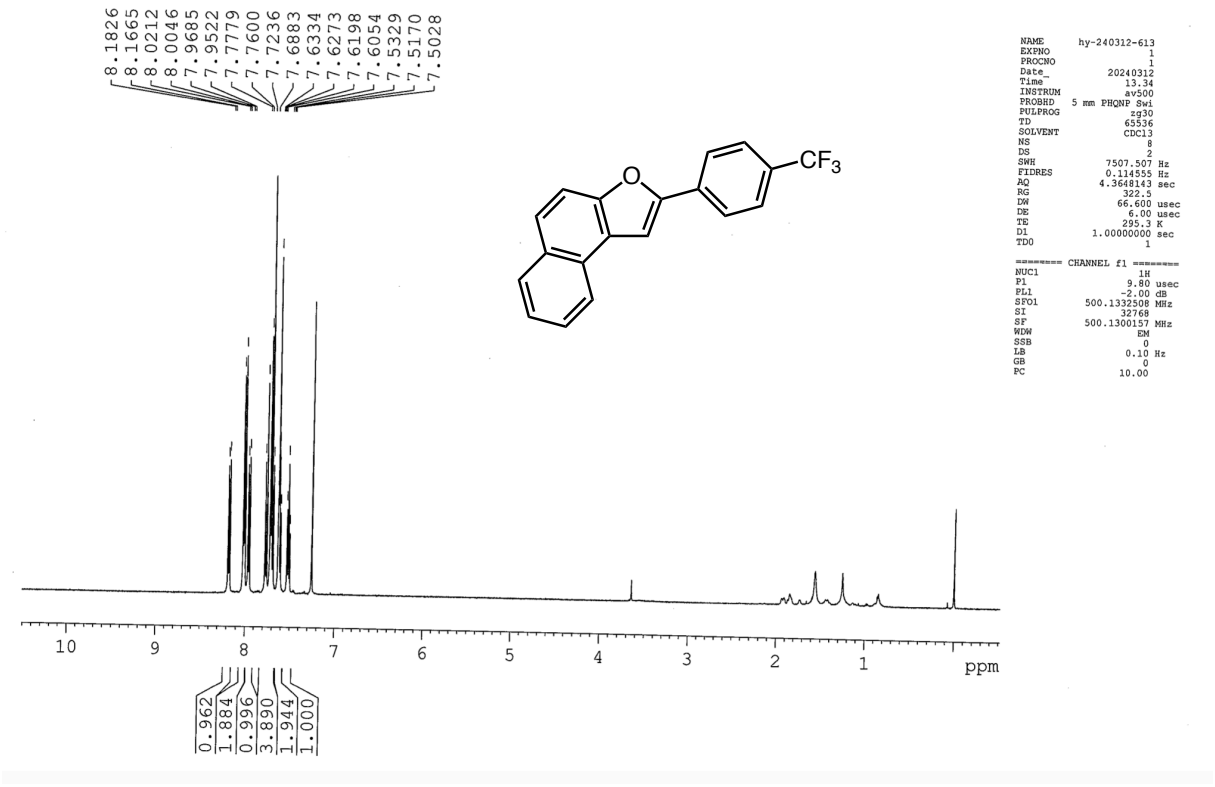


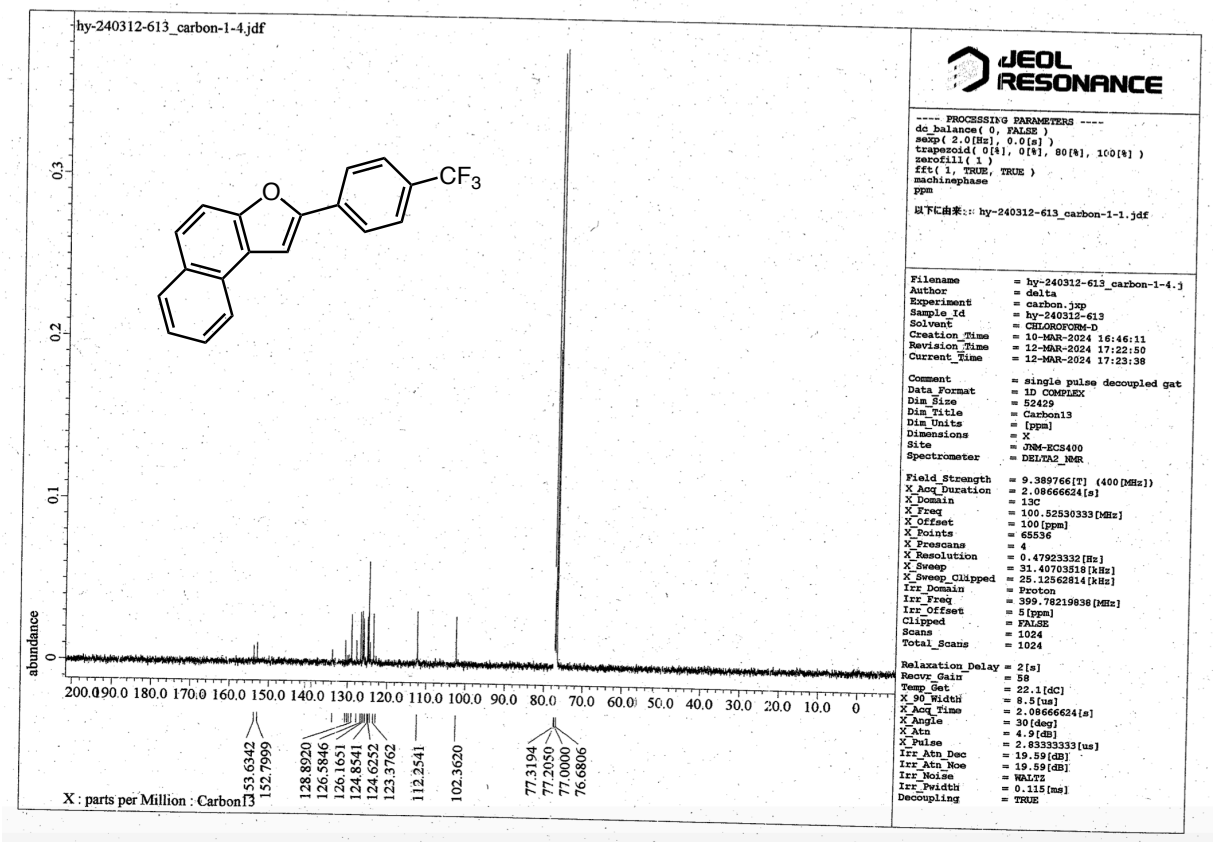
2-(4-Methoxyphenyl)naphtho[2,1-*b*]furan (3bf)

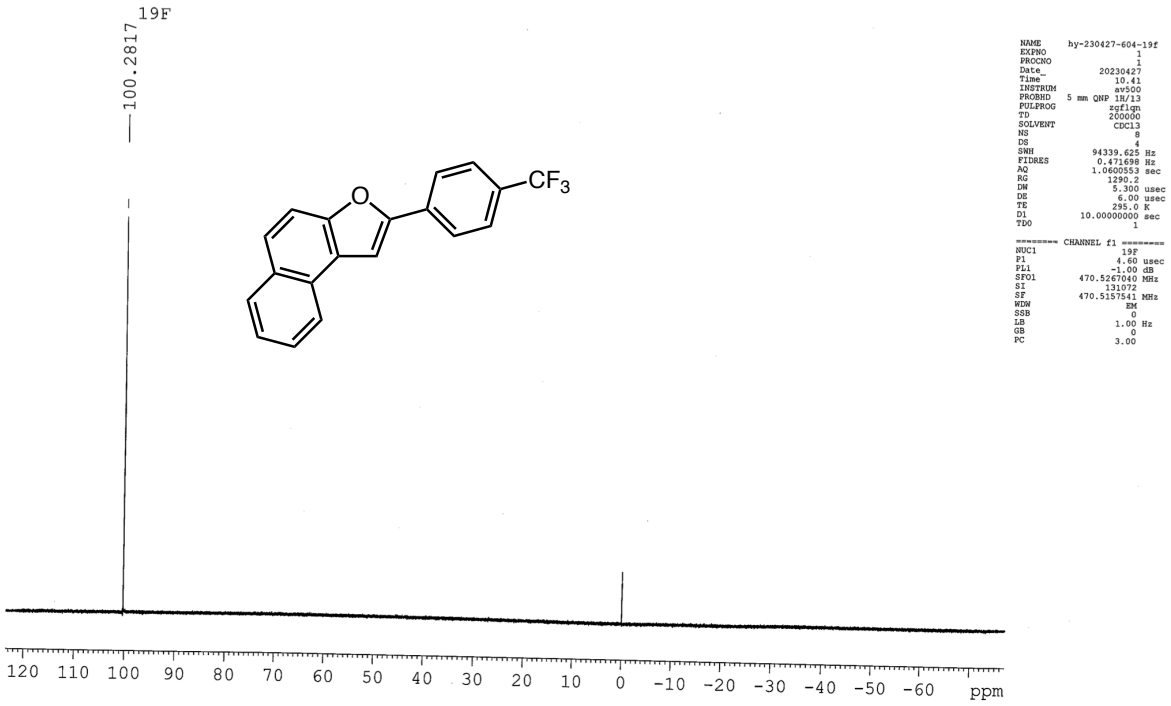




2-[4-(Trifluoromethyl)phenyl]naphtho[2,1-*b*]furan (3bg)







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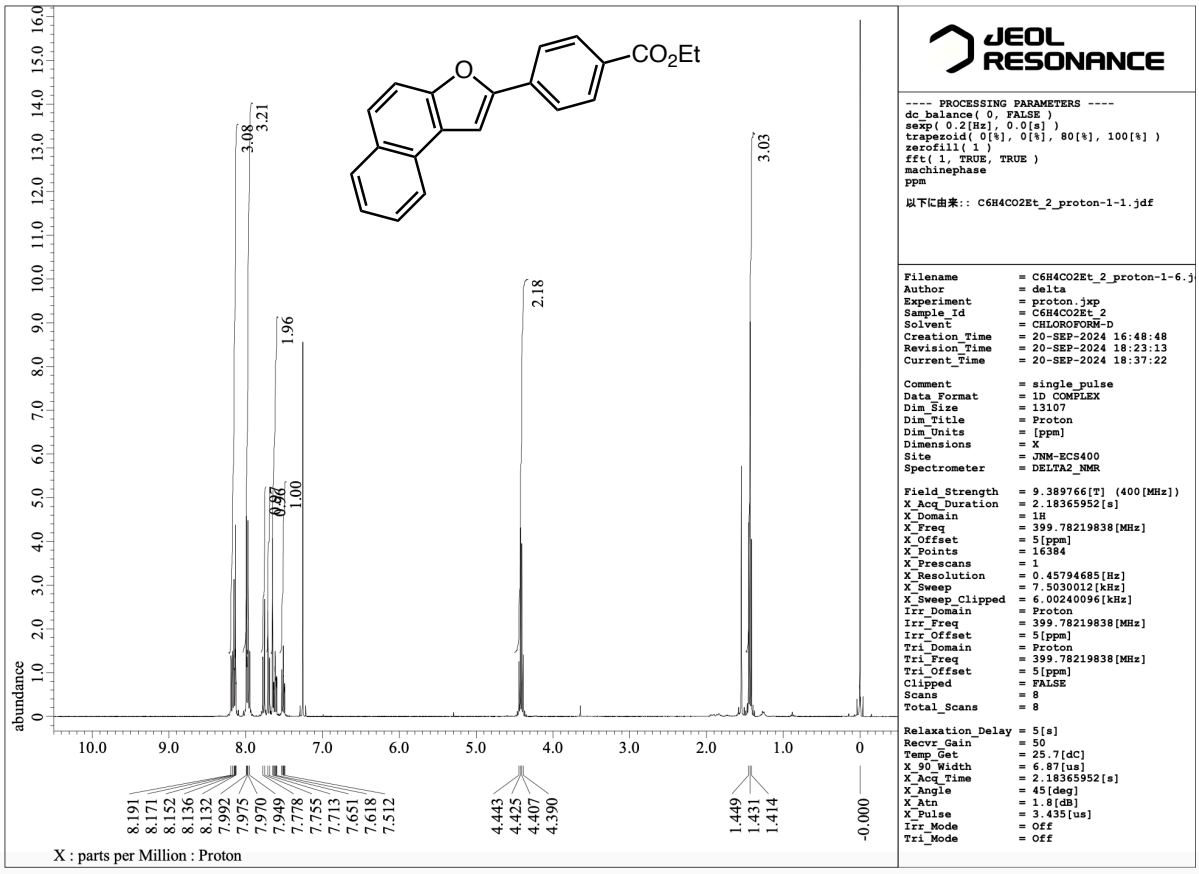
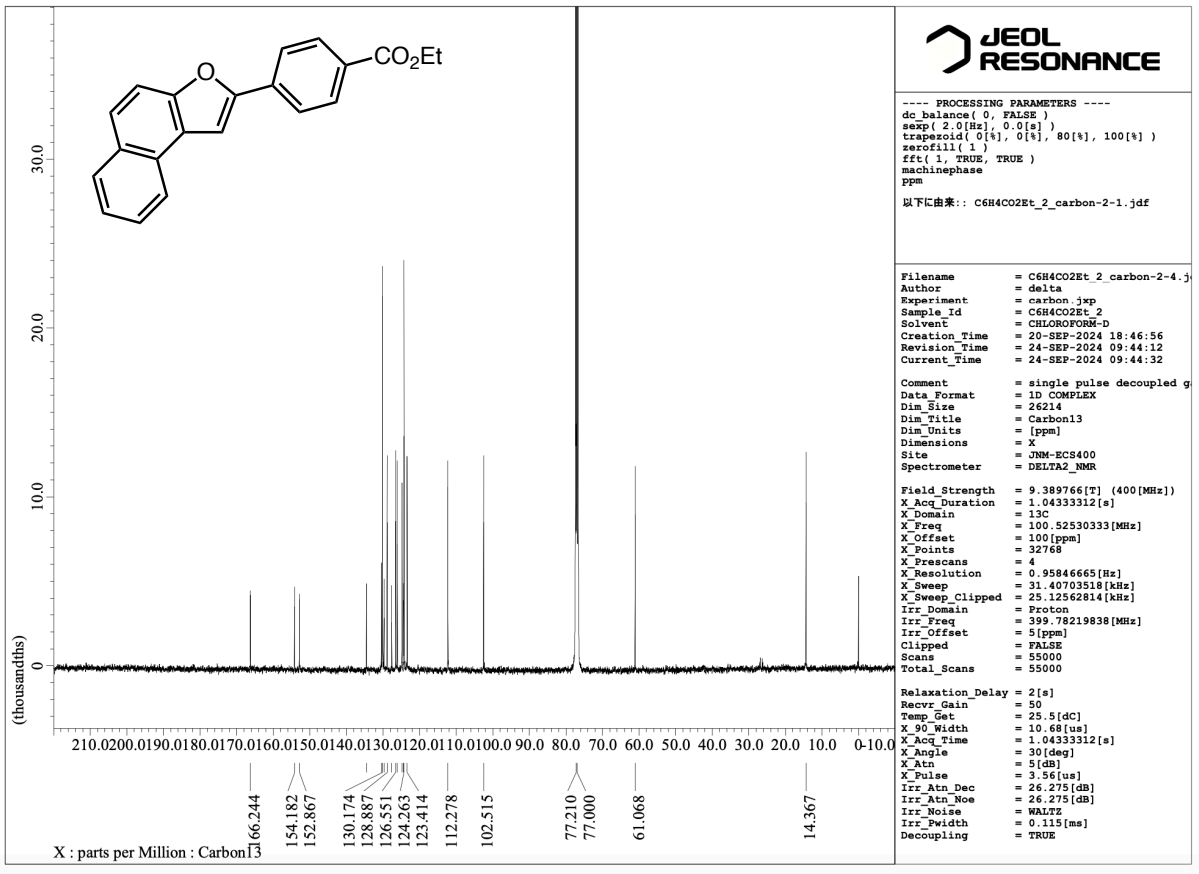
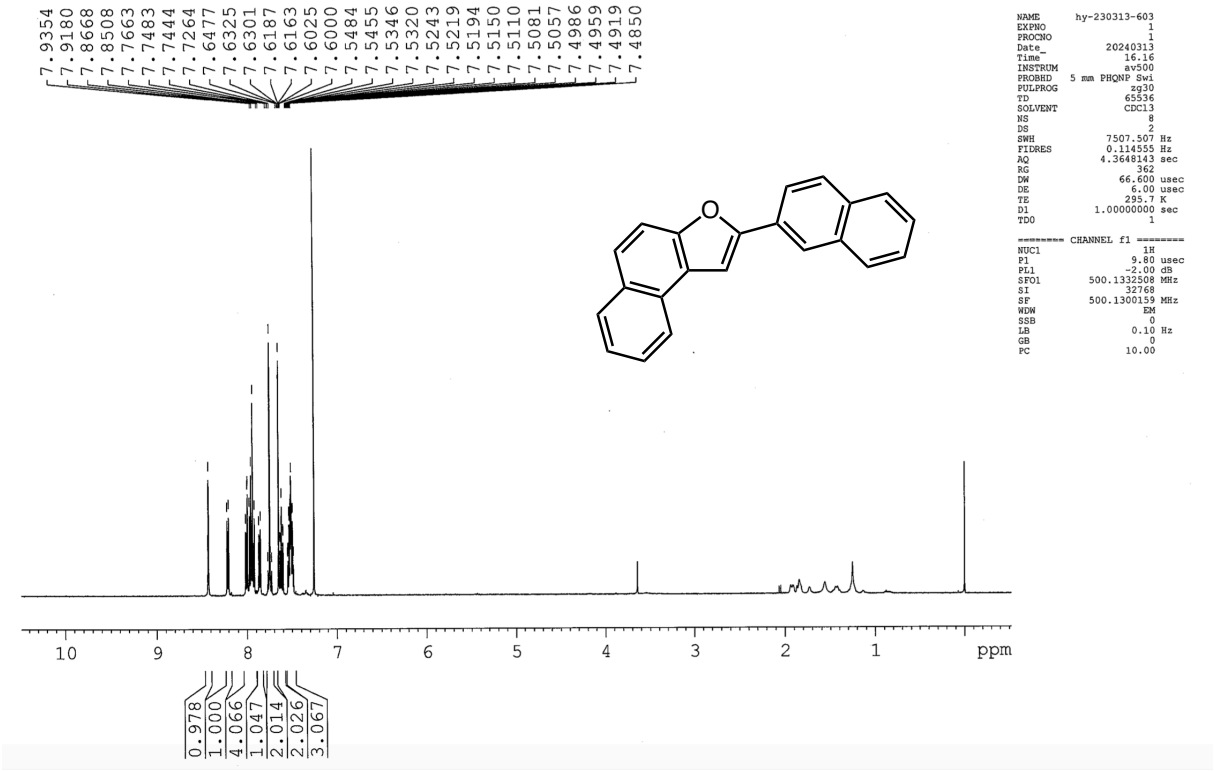
Ethyl 4-(naphtho[2,1-*b*]furan-2-yl)benzoate (3bh)

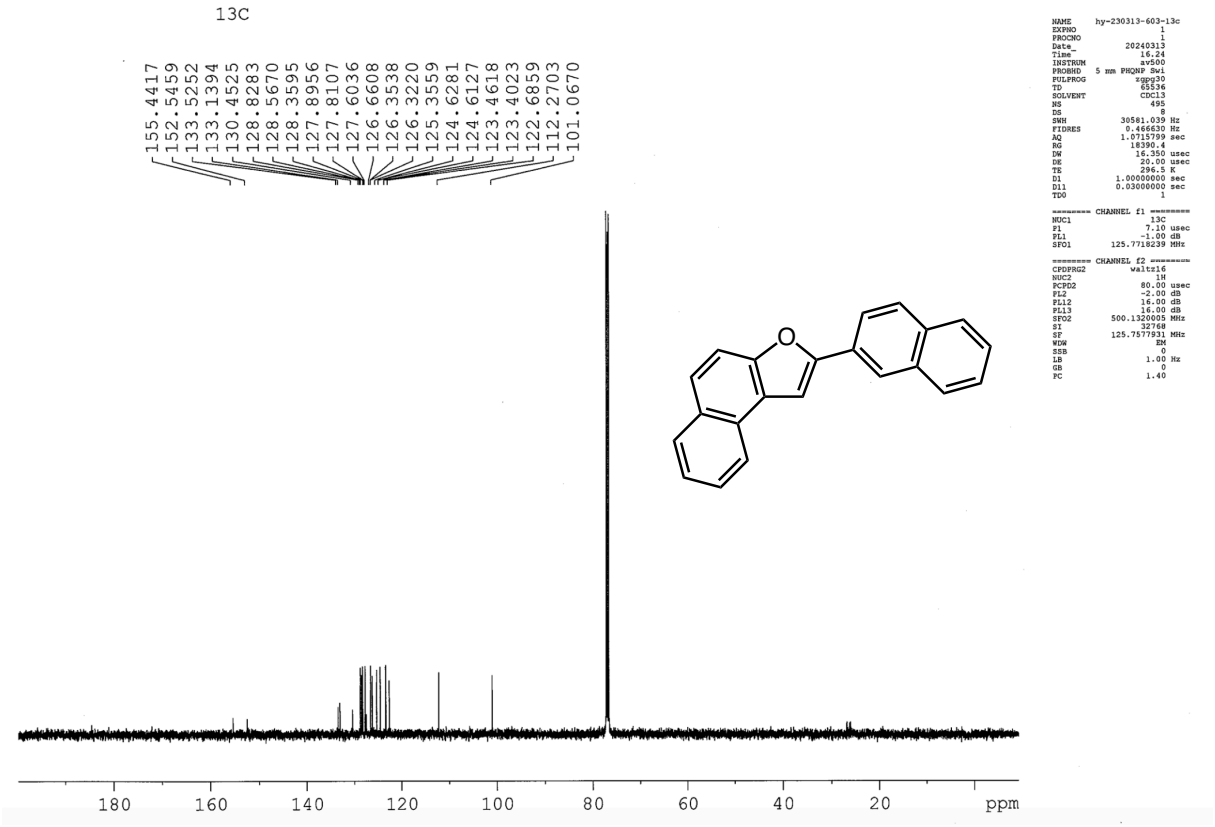




2-(Naphthalen-2-yl)naphtho[2,1-*b*]furan (3bi)

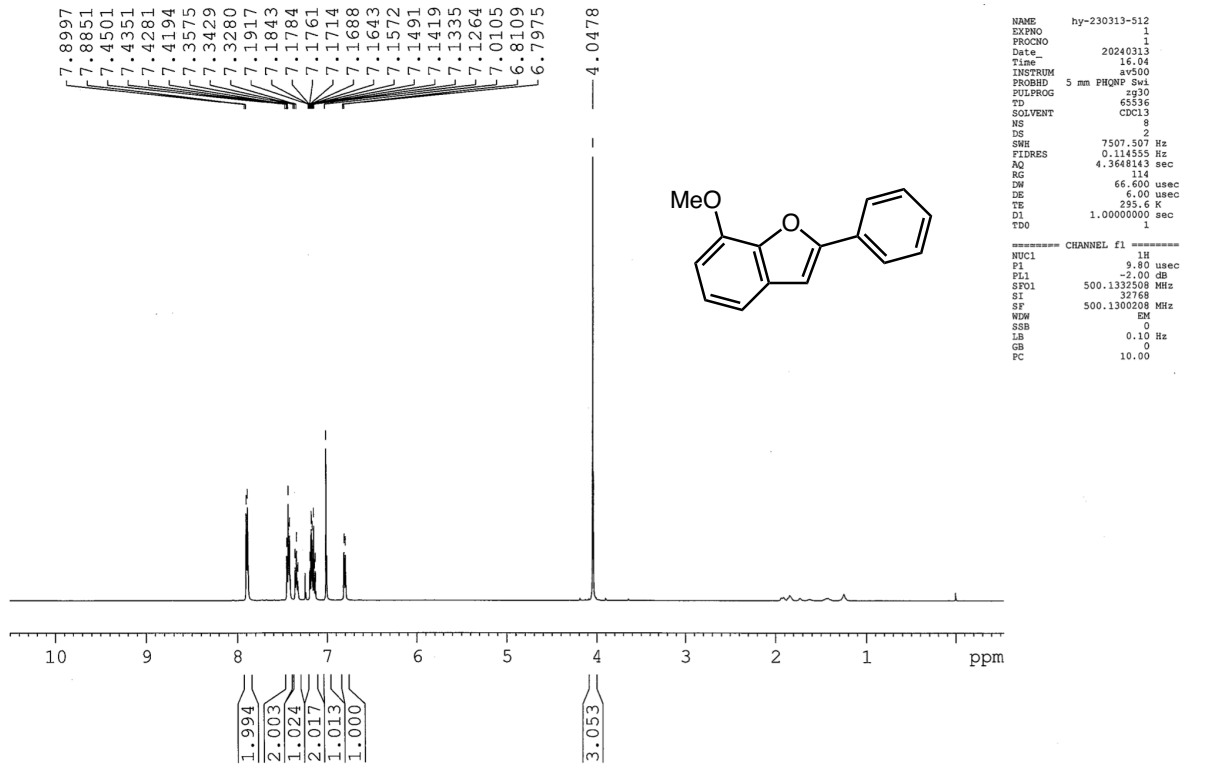



```
NAME          hy-230313-603
EXPNO                 1
PROCNO                1
Date_          20240313
Time              16.16
INSTRUM           av500
PROBHD   5 mm PHQNP Swi
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                    8
DS                    2
SWH           7507.507 Hz
FIDRES        0.114555 Hz
AQ            4.3648143 sec
RG                  362
DW               66.600 usec
DE                6.00 usec
TE               295.7 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                9.80 usec
PL1              -2.00 dB
SFO1        500.1332508 MHz
SI                32768
SF          500.1300159 MHz
WDW                  EM
SSB                   0
LB                 0.10 Hz
GB                    0
PC                10.00
```

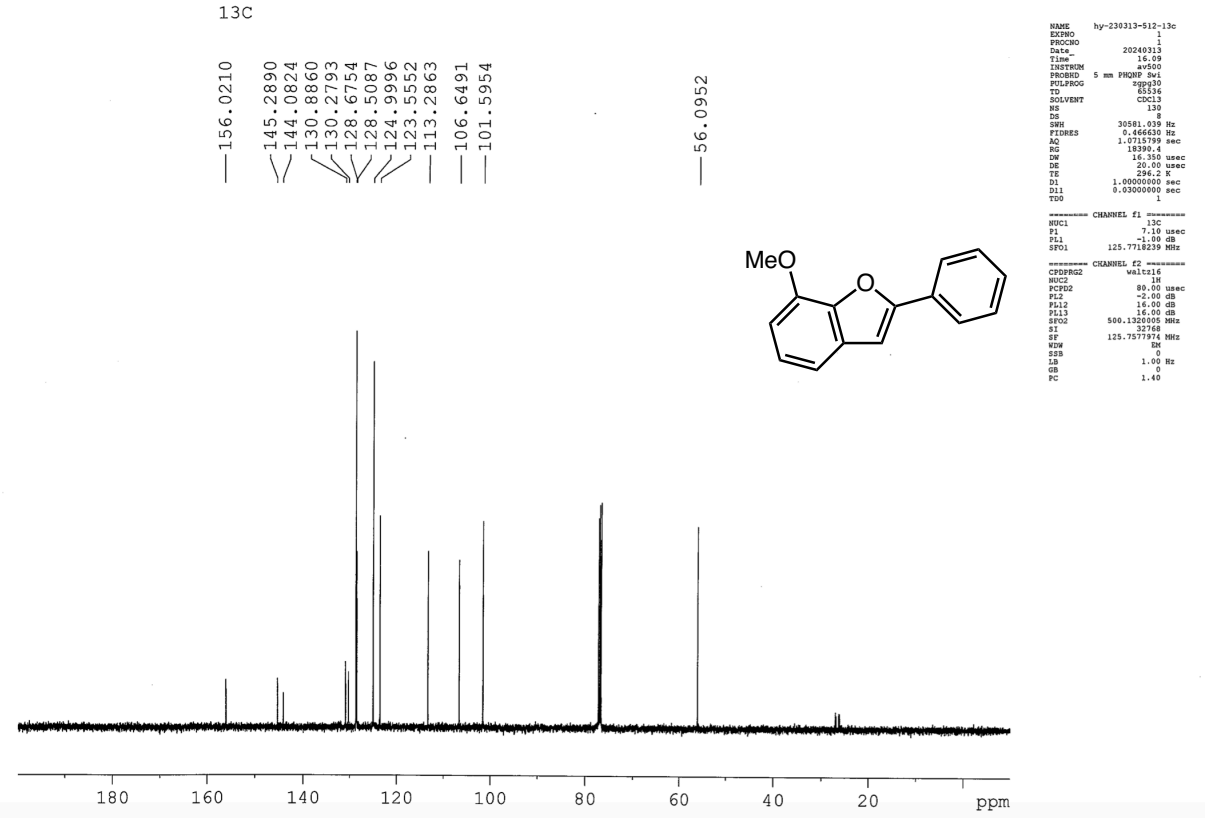



```
NAME          hy-230313-603-13c
EXPNO                 1
PROCNO                1
Date_          20240313
Time              16.24
INSTRUM           av500
PROBHD   5 mm PHQNP Swi
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  495
DS                    8
SWH           30581.039 Hz
FIDRES        0.466630 Hz
AQ            1.0715799 sec
RG               18390.4
DW               16.350 usec
DE                20.00 usec
TE               296.5 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                7.10 usec
PL1              -1.00 dB
SFO1        125.7718239 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2              -2.00 dB
PL12             16.00 dB
PL13             16.00 dB
SFO2        500.1320005 MHz
SI                32768
SF          125.7577931 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                1.40
```

7-Methoxy-2-phenylbenzofuran (3ca)

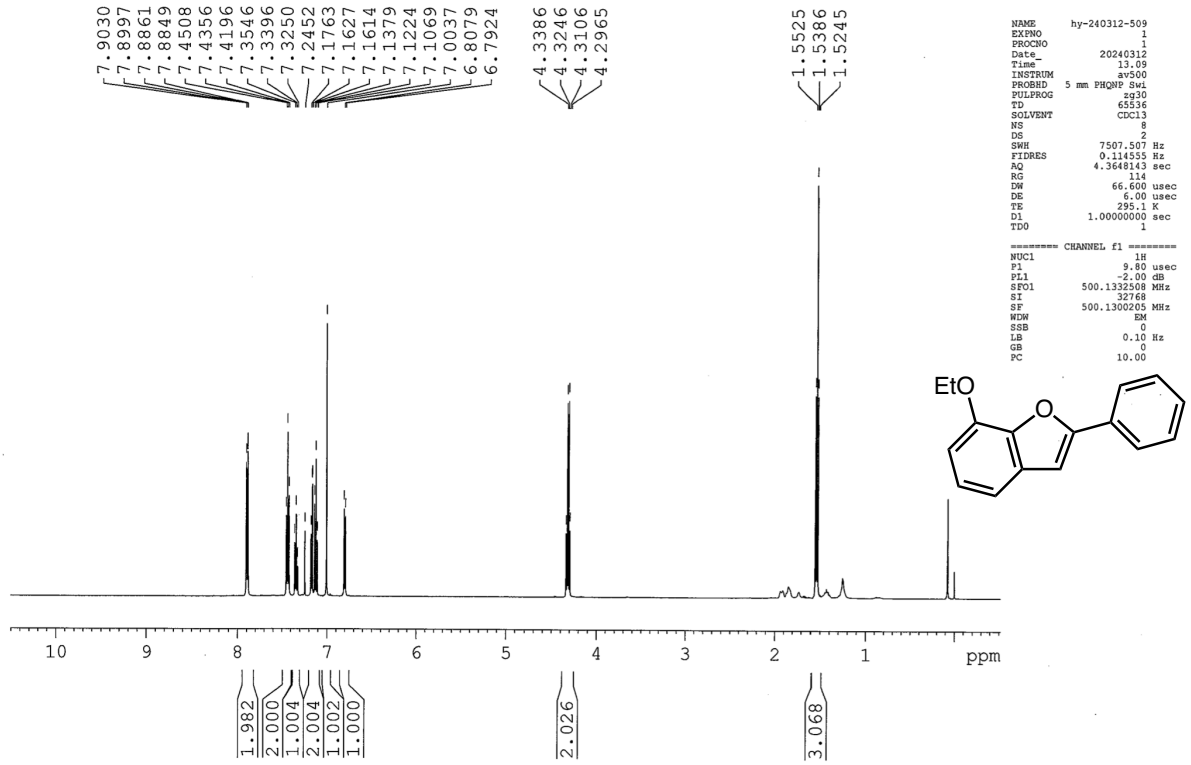


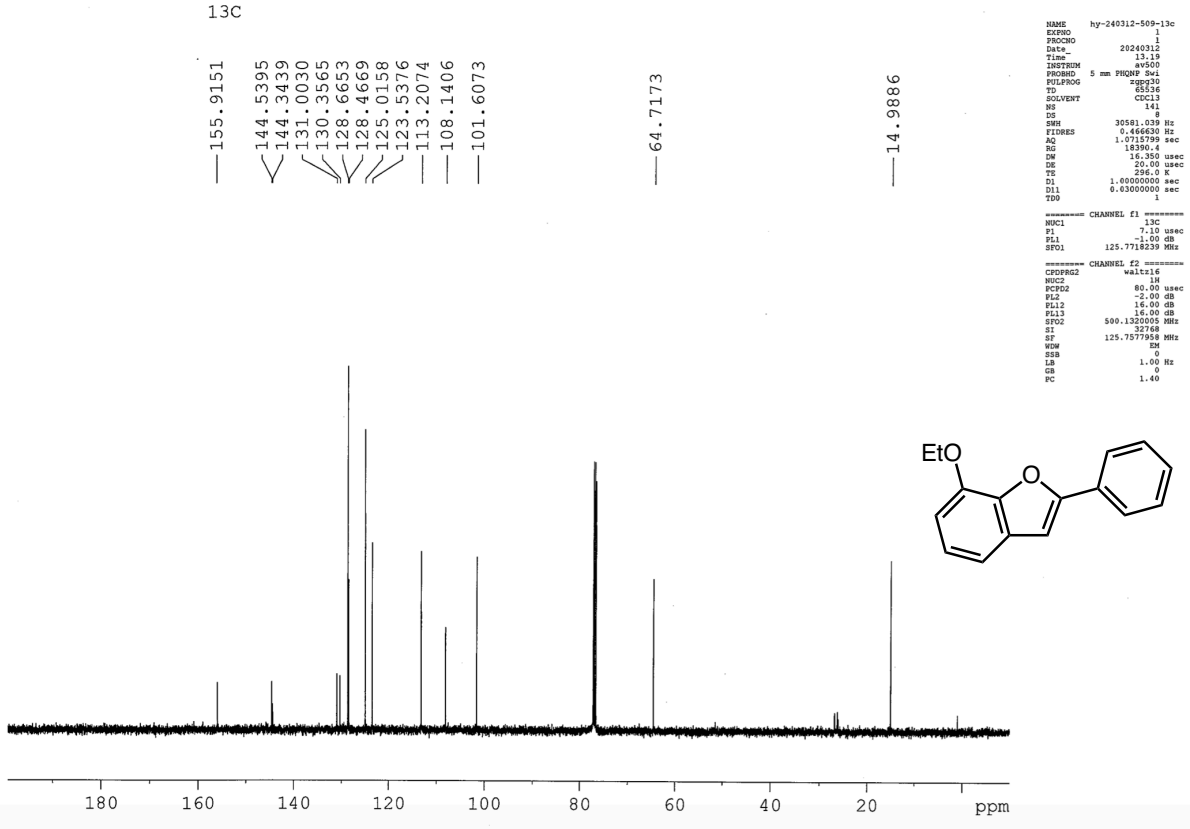

```
NAME          hy-230313-512
EXPNO                    1
PROCNO                   1
Date_             20240313
Time                 16.04
INSTRUM              av500
PROBHD   5 mm PHQNP Swi
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH              7507.507 Hz
FIDRES           0.114555 Hz
AQ               4.3648143 sec
RG                     114
DW                66.600 usec
DE                 6.00 usec
TE                 295.6 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                   9.80 usec
PL1                 -2.00 dB
SFO1          500.1332508 MHz
SI                   32768
SF            500.1300208 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                  10.00
```



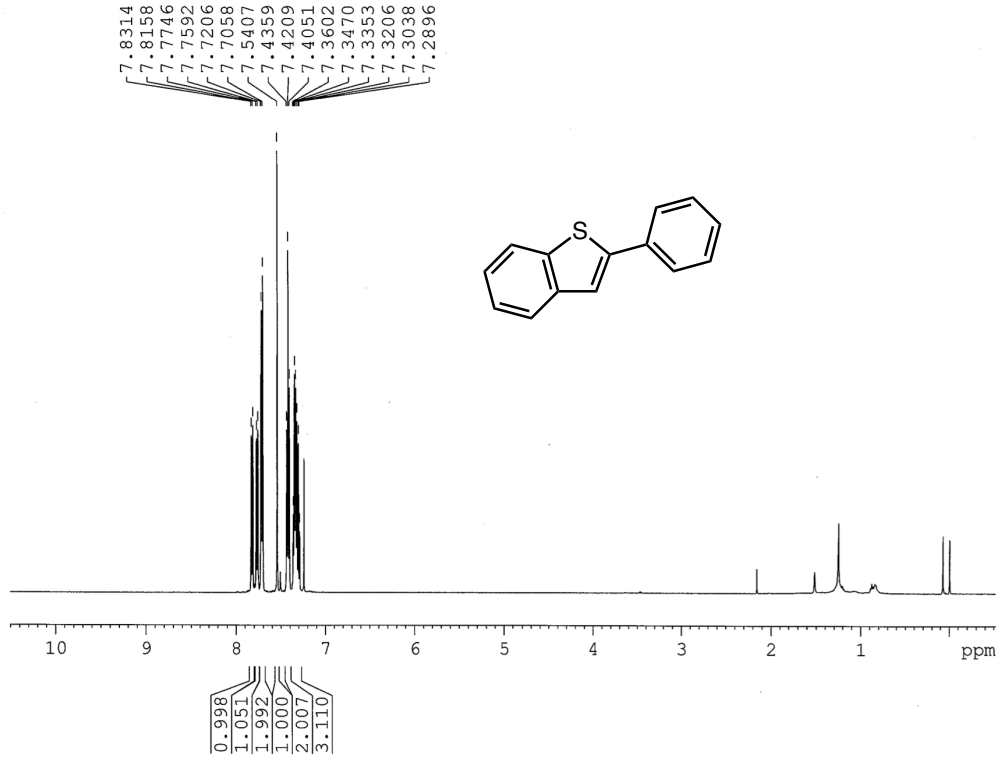

```
NAME          hy-230313-512-13c
EXPNO                    1
PROCNO                   1
Date_             20240313
Time                 16.09
INSTRUM              av500
PROBHD   5 mm PHQNP Swi
PULPROG          zgpg30
TD                  65536
SOLVENT              CDCl3
NS                     130
DS                       8
SWH              30581.039 Hz
FIDRES           0.466630 Hz
AQ               1.0715799 sec
RG                   18390.4
DW                16.350 usec
DE                20.00 usec
TE                 296.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.10 usec
PL1                 -1.00 dB
SFO1          125.7718239 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                 -2.00 dB
PL12                16.00 dB
PL13                16.00 dB
SFO2          500.1320005 MHz
SI                   32768
SF            125.7577974 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

7-Ethoxy-2-phenylbenzofuran (3da)

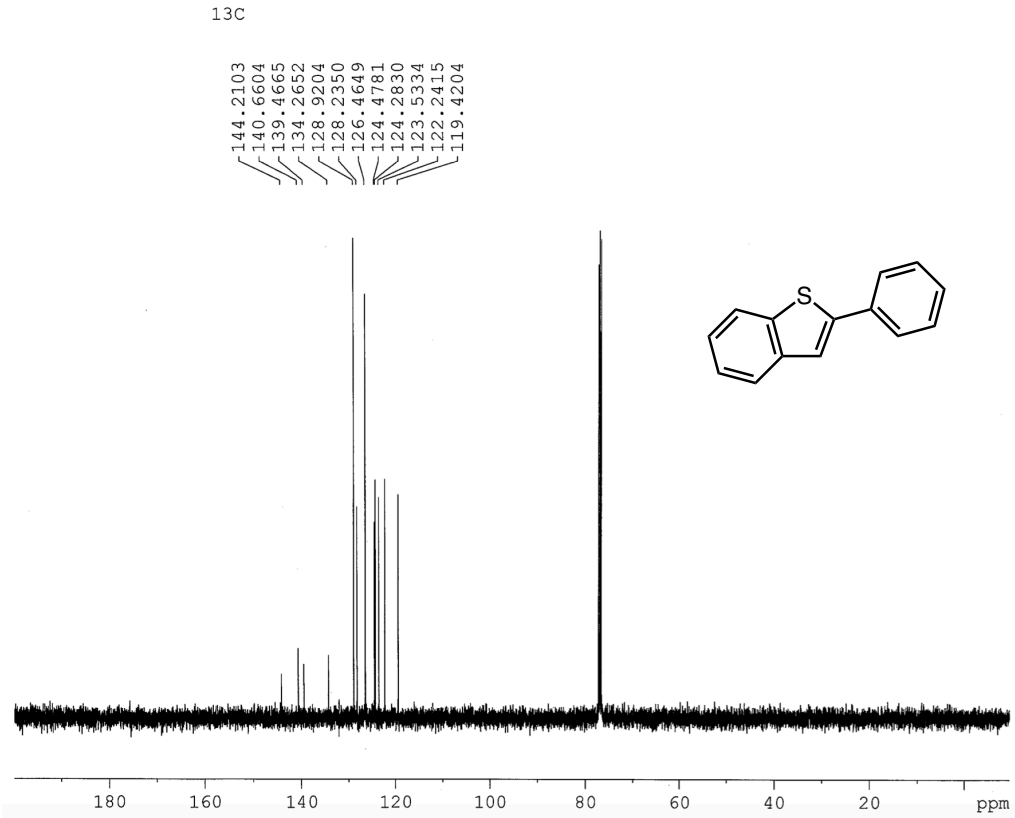




2-Phenylbenzo[*b*]thiophene (5)

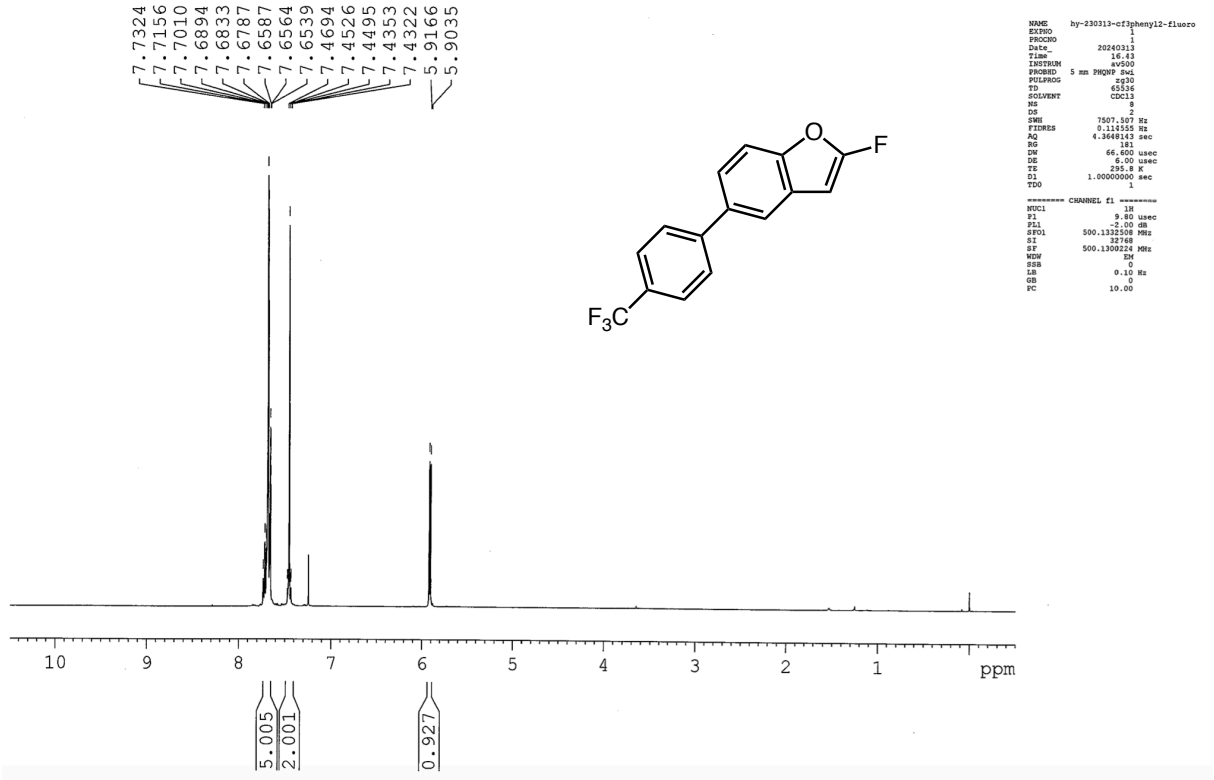


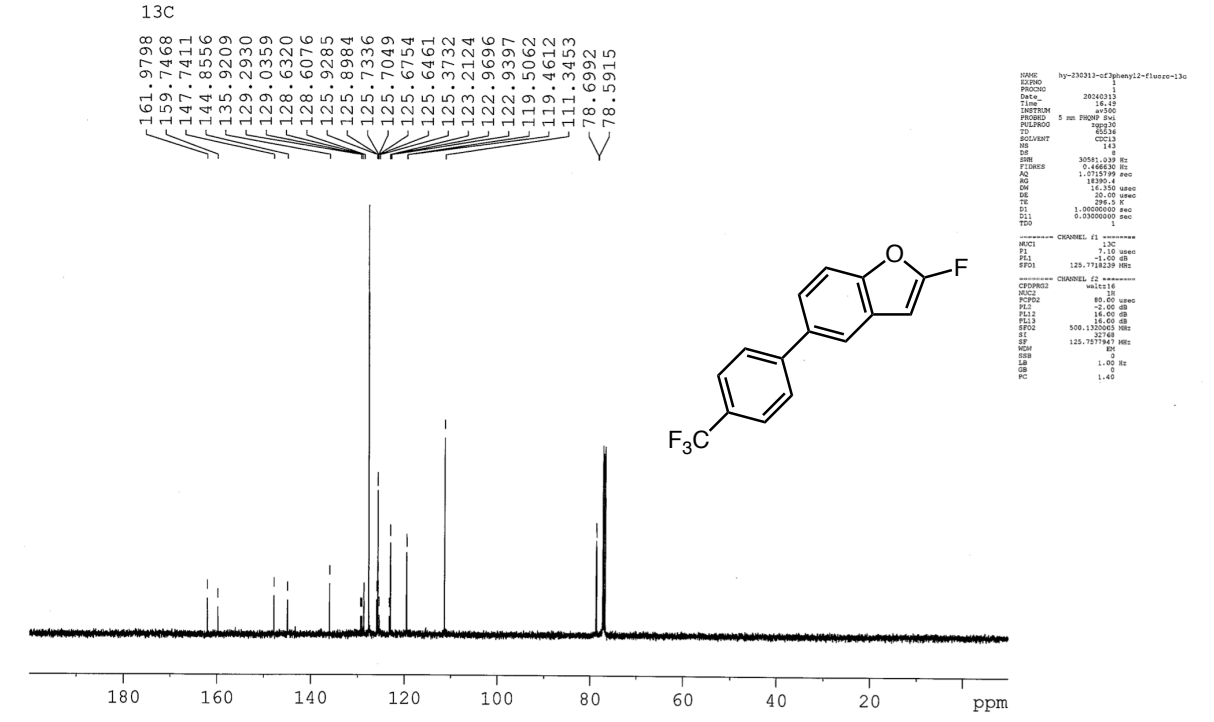

```
NAME          hy-240314-625
EXPNO                     1
PROCNO                    1
Date_              20240314
Time                  19.55
INSTRUM               av500
PROBHD   5 mm PHQNP Swi
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                        8
DS                        2
SWH               7507.507 Hz
FIDRES            0.114555 Hz
AQ                4.3648143 sec
RG                      181
DW                 66.600 usec
DE                  6.00 usec
TE                  295.9 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    1H
P1                   9.80 usec
PL1                 -2.00 dB
SFO1          500.1332508 MHz
SI                    32768
SF            500.1300234 MHz
WDW                     EM
SSB                      0
LB                    0.10 Hz
GB                       0
PC                   10.00
```

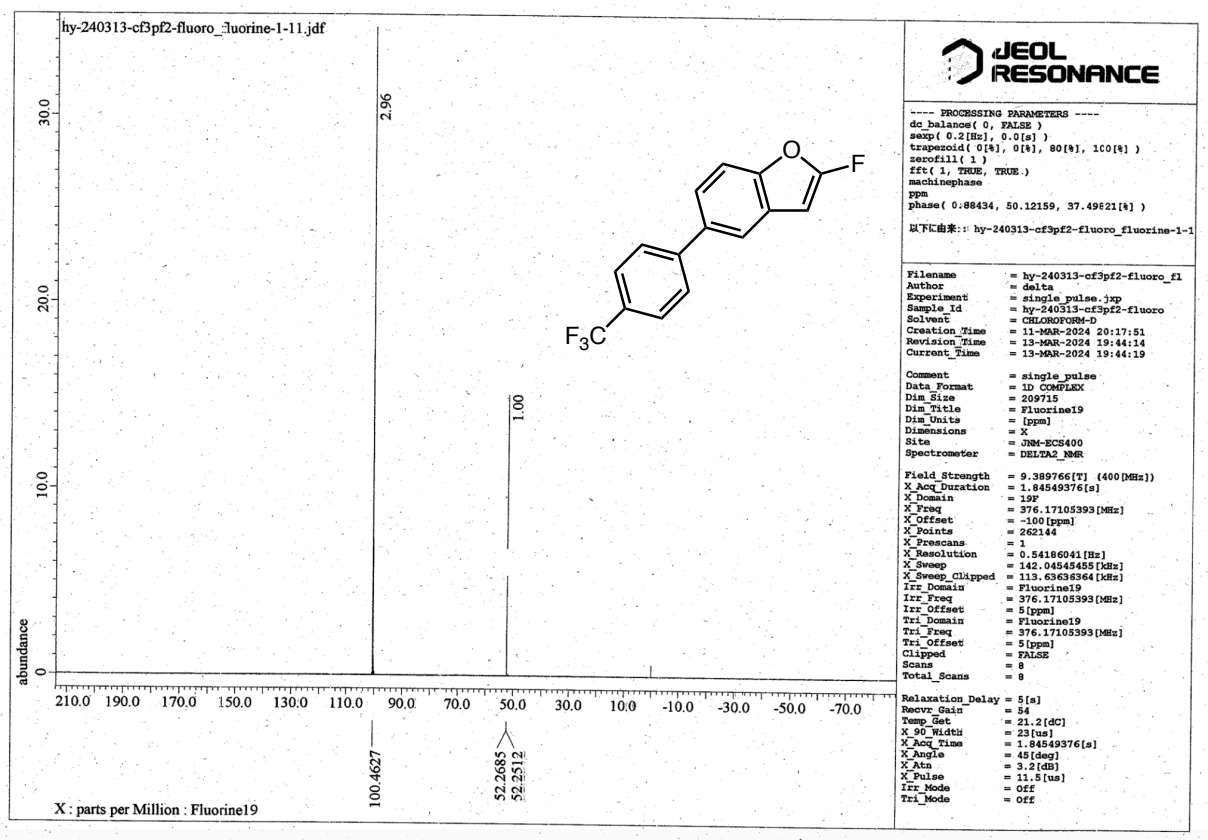



```
NAME          hy-240314-625-13c
EXPNO                     1
PROCNO                    1
Date_              20240314
Time                  19.59
INSTRUM               av500
PROBHD   5 mm PHQNP Swi
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                       73
DS                        8
SWH              30591.039 Hz
FIDRES            0.466630 Hz
AQ                1.0715799 sec
RG                   18390.4
DW                 16.350 usec
DE                  20.00 usec
TE                  296.3 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   7.10 usec
PL1                 -1.00 dB
SFO1          125.7718239 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                 -2.00 dB
PL12                16.00 dB
PL13                16.00 dB
SFO2          500.1320005 MHz
SI                    32768
SF            125.7577964 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

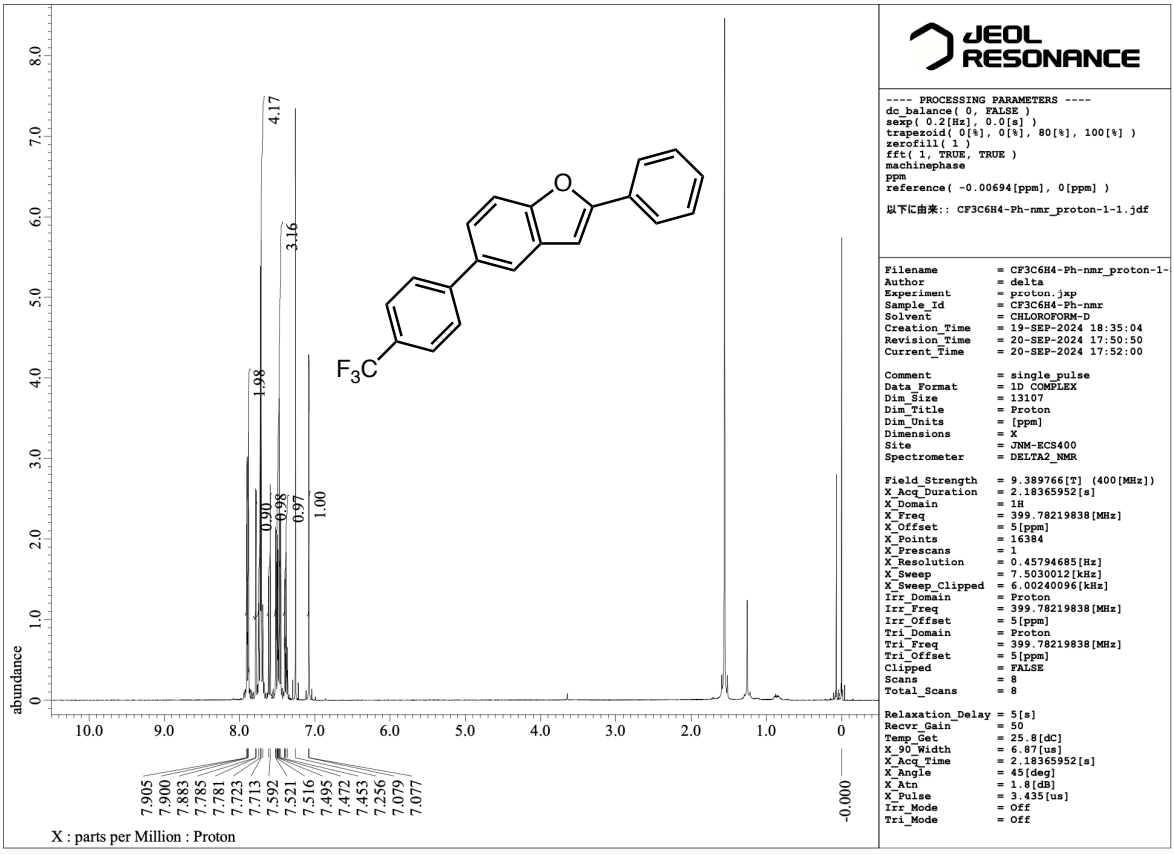
2-Fluoro-5-[4-(trifluoromethyl)phenyl]benzofuran (1f)



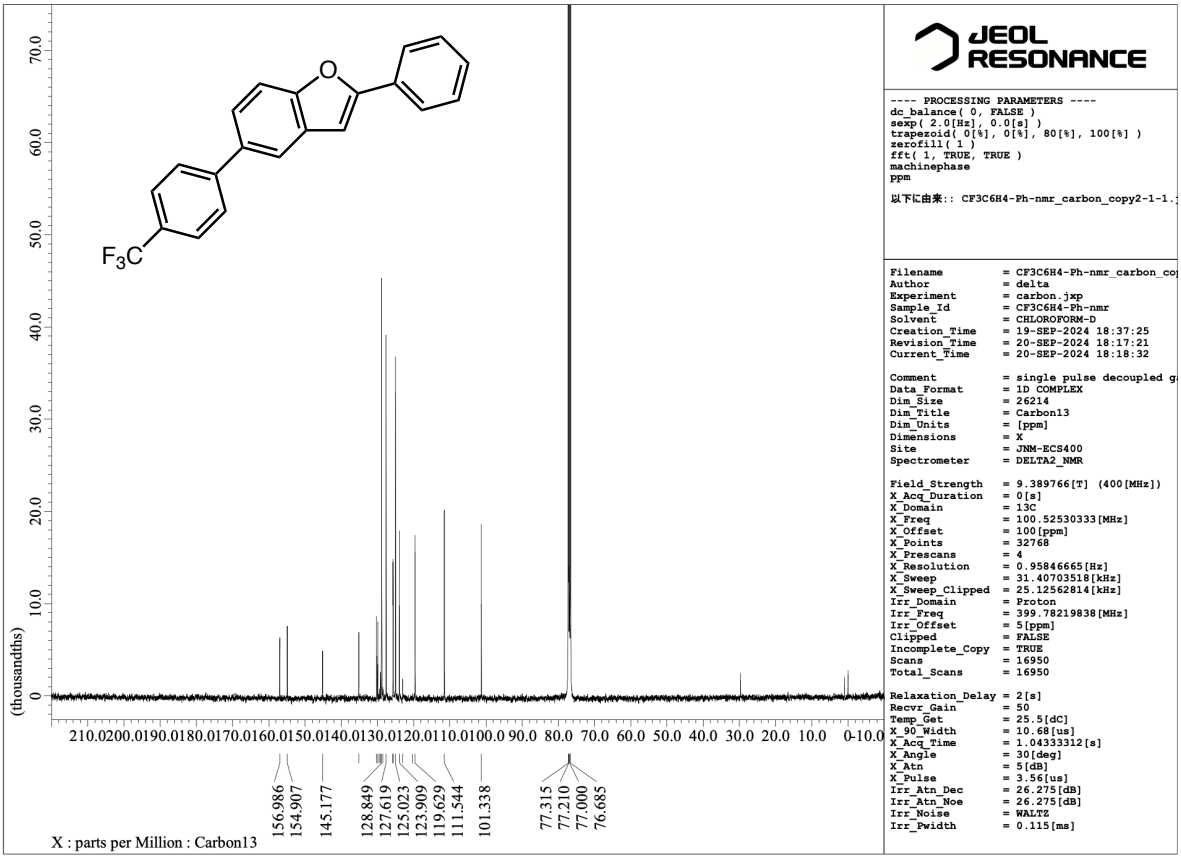



hy-240313-cf3pf2-fluoro_fluorine-1-11.jdf
2.96
1.00
O
F
F3C
abundance
30.0
20.0
10.0
0
210.0 190.0 170.0 150.0 130.0 110.0 90.0 70.0 50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0
100.4627
52.2685
52.2512
X : parts per Million : Fluorine19
JEOL RESONANCE
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(0.88434, 50.12159, 37.49821[%])
以下に由来:: hy-240313-cf3pf2-fluoro_fluorine-1-1
Filename = hy-240313-cf3pf2-fluoro_f1
Author = delta
Experiment = single_pulse.jxp
Sample_Id = hy-240313-cf3pf2-fluoro
Solvent = CHLOROFORM-D
Creation_Time = 11-MAR-2024 20:17:51
Revision_Time = 13-MAR-2024 19:44:14
Current_Time = 13-MAR-2024 19:44:19
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 209715
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.84549376[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = -100[ppm]
X_Points = 262144
X_Prescans = 1
X_Resolution = 0.54186041[Hz]
X_Sweep = 142.04545455[kHz]
X_Sweep_Clipped = 113.63636364[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 376.17105393[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 54
Temp_Get = 21.2[dC]
X_90_Width = 23[us]
X_Acq_Time = 1.84549376[s]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 11.5[us]
Irr_Mode = Off
Tri_Mode = Off

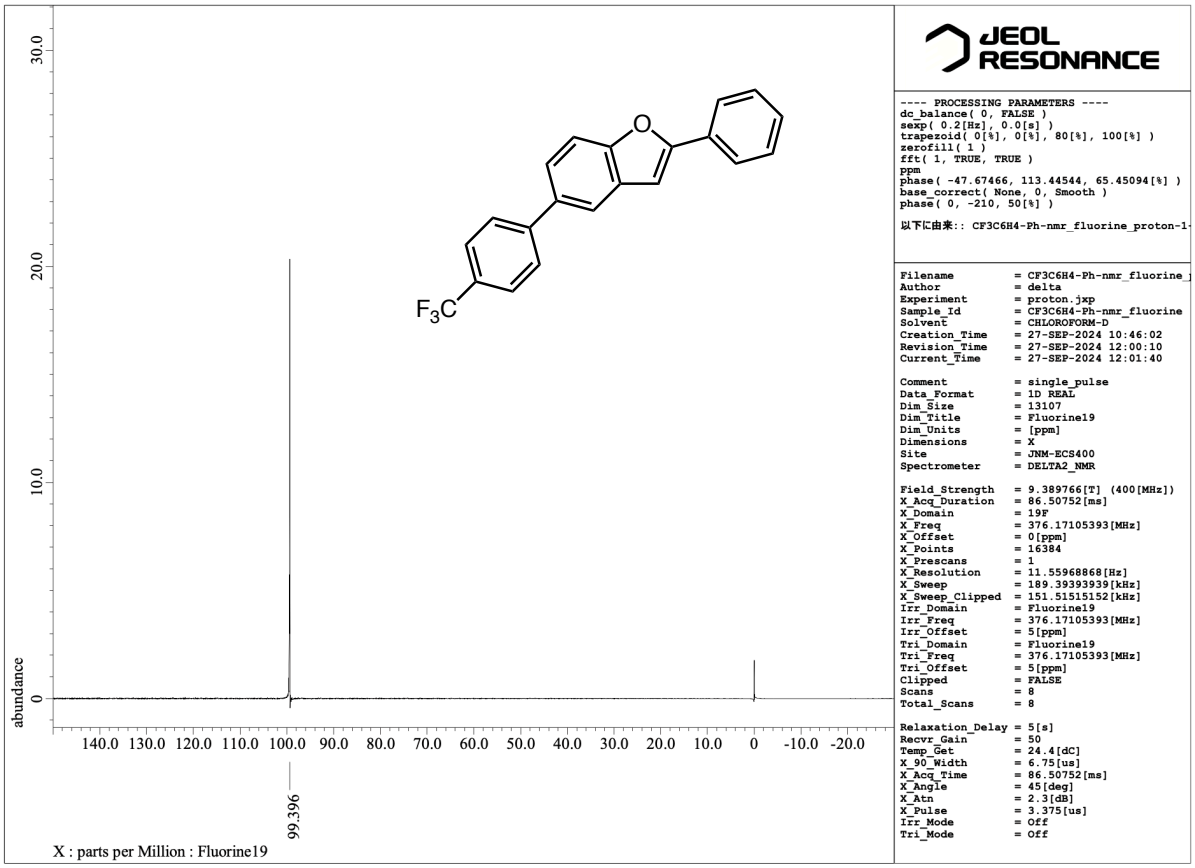
2-Phenyl-5-[4-(trifluoromethyl)phenyl]benzofuran (3fa)




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.00694[ppm], 0[ppm] )

以下に由来:: CF3C6H4-Ph-nmr_proton-1-1.jdf

Filename          = CF3C6H4-Ph-nmr_proton-1-
Author            = delta
Experiment        = proton.jxp
Sample_Id         = CF3C6H4-Ph-nmr
Solvent           = CHLOROFORM-D
Creation_Time     = 19-SEP-2024 18:35:04
Revision_Time     = 20-SEP-2024 17:50:50
Current_Time      = 20-SEP-2024 17:52:00

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 50
Temp_Get          = 25.8[dC]
X_90_Width        = 6.87[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1.8[dB]
X_Pulse           = 3.435[us]
Irr_Mode          = Off
Tri_Mode          = Off
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: CF3C6H4-Ph-nmr_carbon_copy2-1-1.j

Filename          = CF3C6H4-Ph-nmr_carbon_co
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = CF3C6H4-Ph-nmr
Solvent           = CHLOROFORM-D
Creation_Time     = 19-SEP-2024 18:37:25
Revision_Time     = 20-SEP-2024 18:17:21
Current_Time      = 20-SEP-2024 18:18:32

Comment           = single pulse decoupled g
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Incomplete_Copy   = TRUE
Scans             = 16950
Total_Scans       = 16950

Relaxation_Delay = 2[s]
Recvr_Gain        = 50
Temp_Get          = 25.5[dC]
X_90_Width        = 10.68[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 5[dB]
X_Pulse           = 3.56[us]
Irr_Atn_Dec       = 26.275[dB]
Irr_Atn_Noe       = 26.275[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
```



JEOL RESONANCE

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
ppm
phase( -47.67466, 113.44544, 65.45094[%] )
base_correct( None, 0, Smooth )
phase( 0, -210, 50[%] )

以下に由来:: CF3C6H4-Ph-nmr_fluorine_proton-1-
```

```
Filename          = CF3C6H4-Ph-nmr_fluorine_
Author            = delta
Experiment        = proton.jxp
Sample_Id         = CF3C6H4-Ph-nmr_fluorine
Solvent           = CHLOROFORM-D
Creation_Time     = 27-SEP-2024 10:46:02
Revision_Time     = 27-SEP-2024 12:00:10
Current_Time      = 27-SEP-2024 12:01:40

Comment           = single_pulse
Data_Format       = 1D REAL
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.17105393[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.17105393[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.17105393[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 50
Temp_Get          = 24.4[dC]
X_90_Width        = 6.75[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 2.3[dB]
X_Pulse           = 3.375[us]
Irr_Mode          = Off
Tri_Mode          = Off
```