Supporting Information

Perfluorohalogenated Naphthalenes: Synthesis, Crystal Structure, and Intermolecular Interaction

Naoya Ohtsuka,[1,2] Hino Ota,[1,2] Satoshi Sugiura,[1] Shuya Kakinuma,[1] Haruki Sugiyama,[1,2]

Toshiyasu Suzuki,[1] Norie Momiyama[1,2]*

momiyama@ims.ac.jp

[1]*Institute for Molecular Science Okazaki, Aichi 444-8787, Japan*

[2]*SOKENDAI (The Graduate University for Advanced Studies), Okazaki, Aichi 444-8787, Japan*

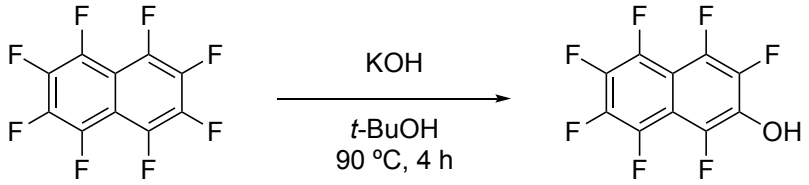
Table of contents

1. General Information

Unless otherwise noted, all reactions were carried out under an atmosphere of standard grade nitrogen gas (oxygen <10 ppm) in flame-dried glassware with magnetic stirring. Anhydrous THF, CH_2Cl_2, toluene and diethyl ether were supplied from Kanto Chemical Co., Inc. as "Dehydrated solvent system". Other reagents were purchased from commercial suppliers and used without further purification. Purification of reaction products was carried out by column chromatography on silica gel 60 (spherical, neutral, 100-210 μm; KANTO and Merck). Analytical thin layer chromatography (TLC) was performed on E. Merck precoated (0.25 mm) silica gel 60-F254 plates. Visualization was accomplished with UV light and a phosphomolybdic acid solution in ethanol by heating. ^{1}H NMR spectra were recorded on a JEOL ECA-400 (400 MHz) spectrometer at ambient temperature. NMR solvent was purchased from CIL ($CDCl_3$). Data are reported as follows: chemical shifts are reported in ppm from tetramethylsilane on the δ scale, with solvent resonance employed as internal standard ($CDCl_3$ 7.26 ppm, DMSO-d_6 2.49 ppm), multiplicity (b = broad, s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, and m = multiplet), integration, coupling constant (Hz) and assignment. ^{13}C NMR spectra were recorded on a JEOL ECA-400 (100 MHz) or JEOL ECA-600 (151 MHz), spectrometer at ambient temperature. Chemical shifts are reported in ppm from tetramethylsilane on the δ scale, with solvent resonance employed as internal standard ($CDCl_3$ 77.0 ppm, DMSO-d_6 39.5 ppm). ^{19}F NMR spectra were recorded on a JEOL ECS-400 (376 MHz) spectrometer. Chemical shifts are reported in ppm from the α,α,α-trifluorotoluene (–63.72 ppm) resonance as external standard. Infrared (IR) spectra were recorded on a Jasco FT/IR-460 plus using ATR. Melting points were recorded on a Büchi Melting point B-540. High-resolution mass spectra (HRMS) analysis was performed on a JEOL JMS-700 (double-focusing magnetic sector mass analyzer: EB) with the fast atom bombardment (FAB) using 3-nitrobenzyl alcohol as the matrix at the Instrument Center, Institute for Molecular Science. X-ray diffraction measurements were made on a Rigaku XtaLAB Synergy Custom diffractometer using multi-layer mirror monochromated Mo-Kα radiation. Data were collected and processed using CrysAlis^{Pro} (Rigaku Oxford Diffraction)[S1]. The structure was solved by a dual-space program[S2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. Calculations were performed using the CrystalStructure[S3] crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7[S4].

2. Synthesis and characterization of substrates

Synthesis of 1,3,4,5,6,7,8-heptafluoronaphthalen-2-ol (S2)



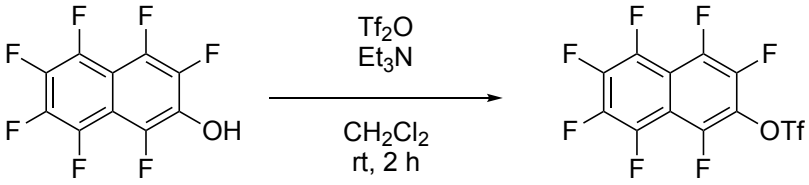
S1 **S2**

KOH (6.69 g, 119 mmol, 2.0 equiv.) was added to the solution of octafluoronaphthalene **S1** (16.9 g, 59.6 mmol, 1.0 equiv.) in *t*-BuOH (60 mL). The mixture was stirred at 90 °C for 4 h. After cooling to room temperature, H_2O (100 mL) was added to the mixture. The resulting mixture was acidified with 2M HCl aq. (pH <1, 60 mL) and extracted with Et_2O (30 mL×3). The combined organic layer was washed with brine (150 mL), dried over with Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane / ethyl acetate = 5:1 as eluent) to give a 1,3,4,5,6,7,8-heptafluoronaphthalen-2-ol **S2** (12.8 g, 47.5 mmol, 79%) as a brown solid.

R_f = 0.43 (hexane / ethyl acetate = 3:1). M.p. = 106-108 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 5.92 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –147.1 (ddd, *J* = 57.8, 17.3, 11.5 Hz, 1F), –147.9- –148.3 (m, 2F), –149.3- –149.6 (m, 1F), –153.9 (s, 1F), –156.1 (s, 1F), –158.1 (t, *J* = 18.8 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, DMSO-d_6): δ141.2, 140.7, 140.6, 140.4, 139.5, 138.0, 136.7, 135.3, 107.2, 103.0. IR (ATR): 3340, 1660, 1471, 1402, 1196, 1112, 935, 784 cm^{-1}. HRMS(FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HF_7O$ 269.9916, found 269.9922.

Synthesis of 2-[(trifluoromethanesulfonyl)oxy]-1,3,4,5,6,7,8-heptafluoronaphthalene (S3)



S2 **S3**

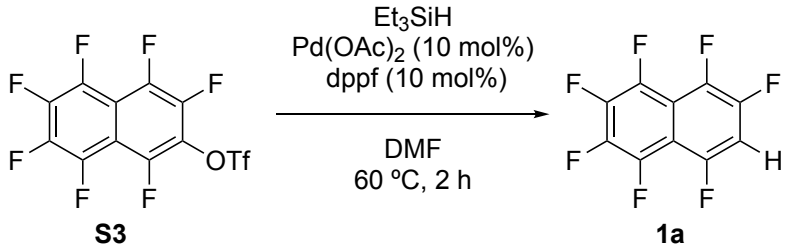
To a solution of 1,3,4,5,6,7,8-heptafluoronaphthalen-2-ol **S2** (6.37 g, 23.6 mmol, 1.0 equiv.) in CH_2Cl_2 (50 mL) was added triethylamine (6.54 mL, 47.2 mmol, 2.0 equiv.) and trifluoromethanesulfonic anhydride (5.80 mL 35.4 mmol, 1.5 equiv.) at 0 °C. The reaction mixture was stirred at room temperature for 2 h. The mixture was quenched with sat. NH_4Cl aq. (50 mL) at 0 ºC and extracted with CH_2Cl_2 (30 mL×3). The combined organic layer was washed with brine (150 mL), dried over with Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane / ethyl acetate = 40:1 as eluent)

to give a 2-[(trifluoromethanesulfonyl)oxy]-1,3,4,5,6,7,8-heptafluoronaphthalene **S3** (8.66 g, 21.5 mmol, 91%) as a pale yellow oil.

R_f = 0.63 (hexane / ethyl acetate = 5:1).

^{19}F NMR (376 MHz, $CDCl_3$): δ –73.5 (s, 3F), –132.2 (d, *J* = 63.6 Hz, 1F), –143.5 (dt, *J* = 63.6 , 20.2 Hz, 1F), –144.4 (ddd, *J* = 56.4, 20.2, 17.3 Hz, 1F), –144.8 (dt, *J* = 60.7, 17.3 Hz, 1F), –146.9 (s, 1F), –150.6- –150.8 (m, 1F), –151.8 (s, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 146.0, 141.7, 141.5, 141.3, 141.0, 140.7, 139.7, 125.4, 118.6, 110.5, 107.3. IR (ATR): 1654, 1458, 1412, 1216, 1122, 948, 823, 778, 726, 697 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{11}F_{10}SO_3$ 401.9408, found: 401.9408.

Synthesis of 1,2,3,4,5,6,8-heptafluoronaphthalene (1a)

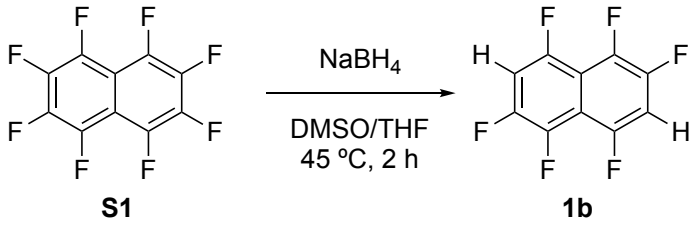


To a solution of 2-[(trifluoromethanesulfonyl)oxy]-1,3,4,5,6,7,8-heptafluoronaphthalene **S3** (10.0 g, 24.9 mmol, 1.0 equiv.) in DMF (50 mL) was added Et_3SiH (20.0 mL, 124 mmol, 5.0 equiv.), dppf (1.38 g, 2.49 mmol, 10 mol%) and $Pd(OAc)_2$ (555 mg, 2.49 mmol, 10 mol %) at 0 °C. After stirring at 0 ºC for 10 min, the reaction mixture was allowed warm to 60 °C and stirred for 2 h. After cooling to room temperature, H_2O (60 mL) was added to the mixture, then the resulting suspension was filtered through a pad of Celite while washing with Et_2O (30 mL). The filtrate was extracted with Et_2O (30 mL×3). The combined organic layer was washed with H_2O (100 mL) and brine (150 mL), dried over Na_2SO_4, and concentrated under reduced pressure after the filtration. The crude product was purified by column chromatography on silica gel (hexane 100% as eluent) to give 1,2,3,4,5,6,8-heptafluoronaphthalene **1a** (5.37 g, 21.2 mmol, 85%) as a white solid.

R_f = 0.45 (hexane). M. p. = 56-58 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (dt, *J* = 10.4, 5.8 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –117.1- –117.4 (m, 1F), –134.5- –134.7 (m, 1F), –145.0 (dt, *J* = 63.6, 17.3 Hz, 1F), –146.7 (dt, *J* = 58.8, 16.6 Hz, 1F), –150.2- –150.5 (m, 1F), –153.8 (dd, *J* = 21.7, 15.9 Hz, 1F), –155.6 (dd, *J* = 21.7, 15.9 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.6 (d, *J* = 6.7 Hz), 146.8 (d, *J* = 6.7 Hz), 141.4, 141.3, 140.4 (d, *J* = 6.7 Hz), 139.9, 138.5, 112.2, 108.2 (d, *J* = 5.8 Hz), 104.9 (d, *J* = 168.7 Hz). IR (ATR): 1650, 1401, 1138, 923, 845, 781, 701 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HF_7$ 263.9966, found 263.9967.

Synthesis of 1,2,4,5,6,8-hexafluoronaphtahlene (1b) [S5]



1b was synthesized according to literature.[S5]

A solution of $NaBH_4$ (1.25 g, 33.0 mmol, 2.2 equiv.) in DMSO (90 mL) was added to a solution of octafluoronaphthalene **S1** (4.08 g, 15.0 mmol, 1.0 equiv.) in THF (60 mL) at room temperature. The mixture was warmed up to 45 ºC and stirred for 2 h. After cooling to room temperature, the mixture was diluted with ethyl acetate (100 mL). The mixture was washed with brine (50 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane 100% as eluent) to furnish the 1,2,4,5,6,8-hexafluoronaphthalene **1b** as mixture with 1,2,4,5,7,8-hexafluoronaphthalene **1c** (**1b**:**1c** = 90:10). The mixture was further purified by recrystallization (EtOH / H_2O) to give a 1,2,4,5,6,8-hexafluoronaphthalene **1b** (1.16 g, 4.95 mmol, 33%) as a colorless solid.

R_f = 0.33 (hexane). M.p. = 66–69 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23-7.15 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –117.8- –118.2 (m, 2F), –136.7- –136.9 (m, 2F), –149.3- –149.7 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.6 (d, *J* = 6.7 Hz), 146.1 (d, *J* = 6.7 Hz), 140.6 (d, *J* = 7.7 Hz), 113.0 (d, *J* = 5.8 Hz), 105.6 (d, *J* = 167.7 Hz).

Synthesis of 3,6-dibromonaphthalene-2,7-diol (S5) [S6]

The **S5** was synthesized according to literature. [S6]

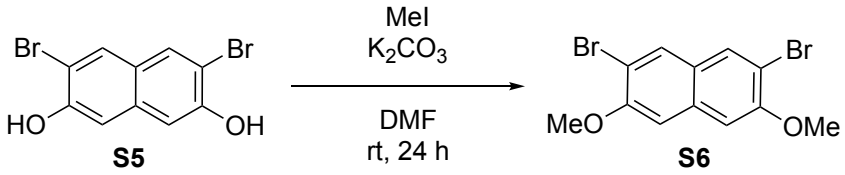
bromine (10.2 mL, 200 mmol, 4.0 equiv.) was added slowly to a solution of naphthalene-2,7-diol **S4** (8.01 g, 50.0 mmol, 1.0 equiv.) in acetic acid (250 mL) and H_2O (28 mL) at room temperature. The reaction mixture was stirred at 80 °C for 4 h followed by stirred at room temperature for 13 h. tin powder (20.8 g, 175 mmol, 3.5 equiv.) was added to the resulting suspension. The reaction mixture was warmed to 130 °C and stirred for 6 h. The hot mixture was transferred to 1000 mL Erlenmeyer flask. After cooling to room temperature, H_2O (700 mL) was added to the mixture. The resulting suspension was filtered by Kiriyama. The residue was washed with H_2O and dissolved in ethyl acetate (600 mL). The organic layer was washed with H_2O (300 mL) and brine (150 mL), dried over Na_2SO_4 and concentrated under reduced pressure after filtration to give a 3,6-dibromonaphthalene-2,7-diol **S5**

(13.3 g, 42.0 mmol, 84%) as a light brown solid. The **S5** was used to next reaction without further purification.

R_f = 0.20 (hexane / ethyl acetate = 1:1). M.p. = 155–159 ºC.

^{1}H NMR (400 MHz, DMSO-d_6): δ 10.53 (brs, 2H), 8.02 (s, 2H), 7.06 (s, 2H).

Synthesis of 2,7-dibromo-3,6-dimethoxynaphthalene (S6) [S7]

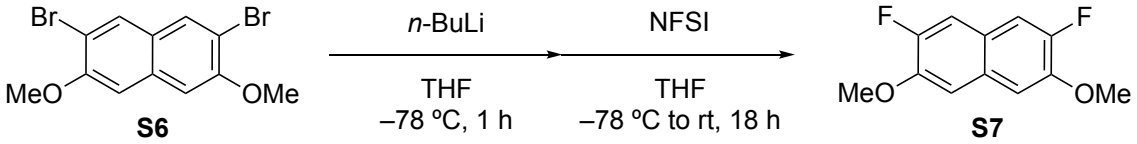


To a solution of 3,6-dibromonaphthalene-2,7-diol **S5** (12.8 g, 40.3 mmol, 1.0 equiv.) in DMF (80 mL) was added K_2CO_3 (16.7 g, 121 mmol, 3.0 equiv.) and iodomethane (7.52 mL, 121 mmol, 3.0 equiv.). The mixture was stirred at room temperature for 24 h. H_2O (150 mL) was added to the mixture and extracted with ethyl acetate (100 mL× 3). The combined organic layer was washed with H_2O (50 mL x 3) and brine (50 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by short pass silica pad (CH_2Cl_2 100% as eluent) to give a 2,7-dibromo-3,6-dimethoxynaphthalene **S6** (13.9 g, 40.0 mmol, 99%) as a white solid.

R_f = 0.33 (hexane / ethyl acetate = 3:1). M. p. =130-133 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (s, 2H), 7.06 (s, 2H), 3.99 (s, 6H).

Synthesis of 2,7-difluoro-3,6-dimethoxynaphthalene (S7)



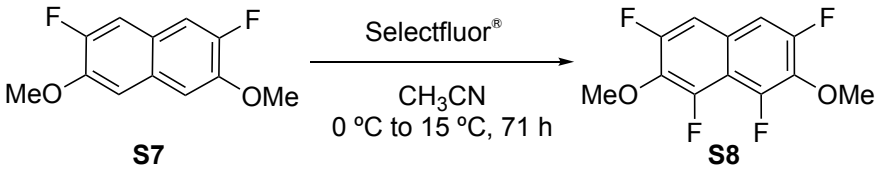
A solution of 2,7-dibromo-3,6-dimethoxynaphthalene **S6** (6.92 g, 20.0 mmol, 1.0 equiv.) in THF (50 mL) was cooled to –78 ºC. 1.6 M *n*-BuLi in hexane (32.0 mL, 50.0 mmol, 2.5 equiv.) was added dropwise to the solution over 20 min at –78 °C. The mixture was stirred at –78 °C for 1 h. A solution of NFSI (18.6 g, 60.0 mmol, 3.0 equiv.) in THF (50 mL) was added dropwise to the resulting suspension over 30 min at –78 ºC. The reaction mixture was allowed warm to room temperature and stirred for 18 h. The mixture was quenched with sat. NH_4Cl aq. (100 mL) and extracted with ethyl acetate (100 mL×3). The combined organic layer was washed with brine (75 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The residual crude product was suspended in CH_2Cl_2 then through the silica pad (CH_2Cl_2 as eluent) to remove an insoluble white solid. The filtrate was concentrated under reduced pressure, then the residual crude product was purified by column

chromatography on silica gel (hexane / ethyl acetate = 6:1 as eluent) to give a 2,7-difluoro-3,6-dimethoxynaphthalene **S7** (2.34 g, 10.4 mmol, 52%) as a light brown solid.

R_f = 0.33 (hexane / ethyl acetate = 3:1). M.p. = 132–133 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (d, *J* = 11.9 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 3.98 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –137.4 (t, *J* = 10.1 Hz, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 151.4 (d, *J* = 247.8 Hz), 147.4 (d, *J* = 13.4 Hz), 128.2, 122.5 (t, *J* = 8.6 Hz), 111.5 (dd, *J* = 19.2, 4.8 Hz), 107.4, 55.9. IR (ATR): 1518, 1435, 1406, 1263, 1149, 1025, 895, 765, 667, 607 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{12}H_{10}F_2O_2$ 224.0649, found 224.0659.

Synthesis of 1,3,6,8-tetrafluoro-2,7-dimethoxynaphthalene (S8)



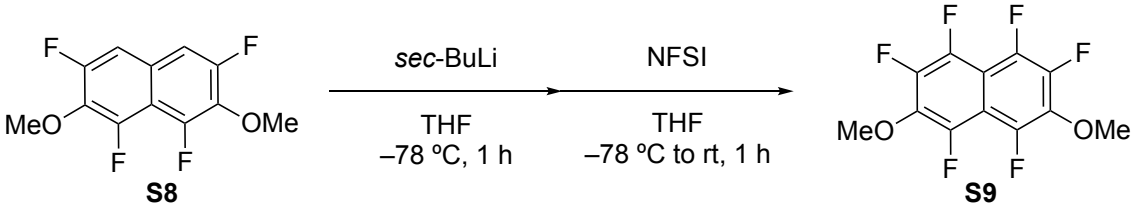
S7 **S8**

Selectfluor® (17.7 g, 50.0 mmol, 2.5 equiv.) was added to a solution of 2,7-difluoro-3,6-dimethoxynaphthalene **S7** (4.48 g, 20.0 mmol, 1.0 equiv.) in CH_3CN (200 mL) at 0 °C. The mixture was warmed to 15 °C and stirred for 71 h. The reaction mixture was poured into ice-water (250 mL) then extracted with ethyl acetate (100 mL×3). The combined organic layer was washed with brine (100 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane / CH_2Cl_2 = 8:1 as eluent) to give a 1,3,6,8-tetrafluoro-2,7-dimethoxynaphthalene **S8** (1.39 g, 5.34 mmol, 27%) as a white solid.

R_f = 0.31 (hexane / CH_2Cl_2 = 5:1). M. p. = 113–115 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (d, *J* = 10.5 Hz, 2H), 4.09 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –128.4 (d, *J* = 11.6 Hz, 2F), –135.5 (s, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 154.9 (d, *J* = 5.8 Hz), 149.3, 134.9, 124.6, 110.2, 107.3 (d, *J* = 170.6 Hz), 62.3 (q, *J* = 145.7 Hz). IR(ATR): 1685, 1633, 1582, 1507, 1465, 1409, 1348, 1264, 1234, 1207, 1160, 1069, 985, 956, 870, 807, 789, 705, 572 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{12}H_8F_4O_2$ 260.0460, found 260.0469.

Synthesis of 1,2,4,5,7,8-hexafluoro-3,6-dimethoxynaphthalene (S9)

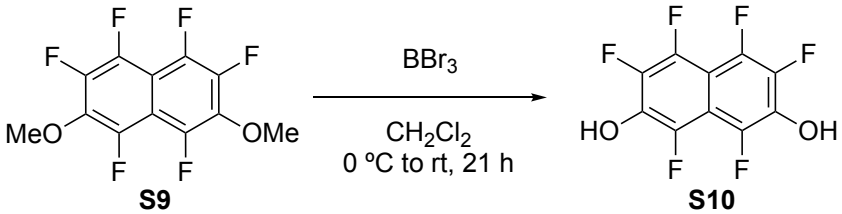


A solution of 1,3,6,8-tetrafluoro-2,7-dimethoxynaphthalene **S8** (260 mg, 1.00 mmol, 1.0 equiv.) in THF (10 mL) was cooled to –78 ºC. 1.2 M *sec*-BuLi in cyclohexane / hexane (2.10 mL, 2.52 mmol, 2.5 equiv.) was added dropwise to the solution at –78 °C. The reaction mixture was stirred at –78 °C for 1 h. NFSI (946 mg, 3.00 mmol, 3.0 equiv.) was added to the mixture one portion. The mixture was allowed warmed to room temperature and stirred for 18 h. The mixture was quenched with sat. NH_4Cl aq. (15 mL) and extracted with ethyl acetate (20 mL×3). The combined organic layer was washed with brine (15 mL), dried over Na_2SO_4 and concentrated under reduced pressure after filtration. The residual crude product was purified by column chromatography on silica gel (hexane / ethyl acetate = 10:1 as eluent) to give a 1,2,4,5,7,8-hexafluoro-3,6-dimethoxynaphthalene **S9** as a light brown solid (257 mg, 0.869 mmol, 87%)

R_f = 0.34 (hexane / ethyl acetate = 10:1). M.p. = 92–94 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.14 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –141.3- –141.4 (m, 2F), –149.2- –149.3 (m, 2F), –151.9- –152.0 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 144.6, 142.5, 141.1, 136.0, 108.2, 106.4, 62.5 (q, J = 146.7 Hz). IR (ATR): 1648, 1515, 1462, 1393, 1167, 1111, 950, 772 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{12}H_6F_6O_2$ 296.0272, found 296.0272.

Synthesis of 1,3,4,5,6,8-hexafluoronaphthalene-2,7-diol (19)

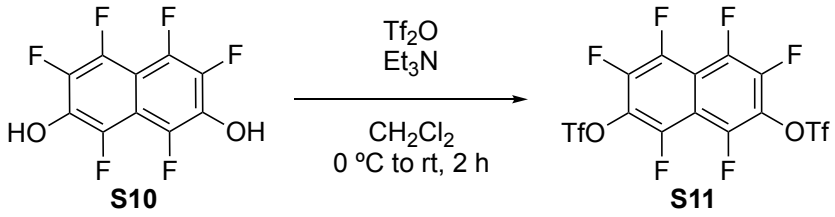


1.0 M BBr_3 in CH_2Cl_2 (2.35 mL, 2.35 mmol, 3.0 equiv.) was added to a solution of 1,2,4,5,7,8-hexafluoro-3,6-dimethoxynaphthalene **S9** (233 mg, 0.786 mmol, 1.0 equiv.) in CH_2Cl_2 (4.0 mL) at 0 °C. The reaction mixture was warmed to room temperature and stirred for 21 h. After cooling to 0 °C, H_2O (10 mL) was added carefully to the mixture. The mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane / ethyl acetate = 1:1 as eluent) to give a 1,3,4,5,6,8-hexafluoronaphthalene-2,7-diol **S10** (170 mg, 0.634 mmol, 81%) as a brownish solid.

R_f = 0.31 (hexane / ethyl acetate = 1:1). M. p. = 176–177 ºC

^{1}H NMR (400 MHz, DMSO-d_6): δ 11.44 (brs, 2H). ^{19}F NMR (376 MHz, DMSO-d_6): δ –148.5- –148.6 (m, 2F), –152.1 (s, 2F), –156.8 (s, 2F). ^{13}C {^{19}F} NMR (100 MHz, DMSO-d_6): δ 140.5, 139.4, 139.4, 134.0, 107.7, 99.9. IR (ATR): 2995, 1659, 1467, 1387, 1246, 1197, 1112, 931, 789, 743 cm^{-1}. HRMS (FAB/EB) *m/z* [M]$^+$ calcd for $C_{10}H_2F_6O_2$ 267.9959, found 267.9957.

Synthesis of 1,2,4,5,7,8-hexafluoro-3,6-bis[trifluoromehanesulfonyloxy]naphthalene (S11)

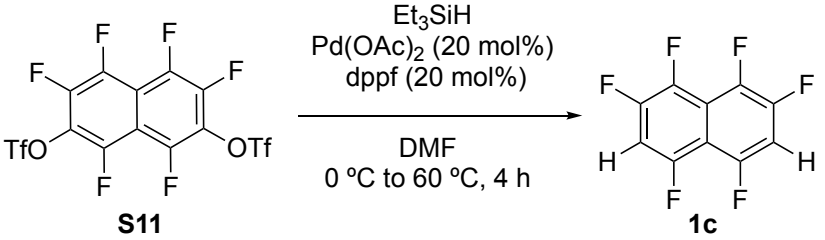


To a solution of 1,3,4,5,6,8-hexafluoronaphthalene-2,7-diol **S10** (186 mg, 0.694 mmol, 1.0 equiv.) in CH_2Cl_2 (7.0 mL) was added triethylamine (290 μL, 2.09 mmol, 3.0 equiv.) and trifluoromethansulufonic anhydride (290 μL, 1.77 mmol, 2.5 equiv.) at 0 °C. The reaction mixture was warmed to room temperature and stirred for 18 h. After cooling to 0 °C, the reaction mixture was quenched with H_2O, and extracted with CH_2Cl_2 (10 mL×3). The combined organic layer was washed with brine (15 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane / ethyl acetate = 30:1 as eluent) to give a 1,2,4,5,7,8-hexafluoro-3,6-bis[trifluoromehanesulfonyloxy]-naphthalene **S11** as a brown solid. (280 mg, 0.526 mmol, 76%)

R_f = 0.43 (hexane / ethyl acetate = 5:1). M. p. = 51–53 ºC.

^{19}F NMR (376 MHz, $CDCl_3$): δ –73.3 (s, 6F), –130.0 (s, 2F), –143.2 (s, 2F), –143.4- –143.5 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 146.4, 142.4, 141.4, 125.8, 118.6, 113.5, 107.0. IR (ATR): 1648, 1437, 1408, 1208, 1126, 1035, 947, 839, 818, 792, 754, 690 cm^{-1}. HRMS (FAB/EB) *m/z* [M]$^+$ calcd for $C_{12}F_{12}O_6S_2$ 531.8945, found 531.8925.

Synthesis of 1,2,4,5,7,8-hexafluoronaphthalene (1c)



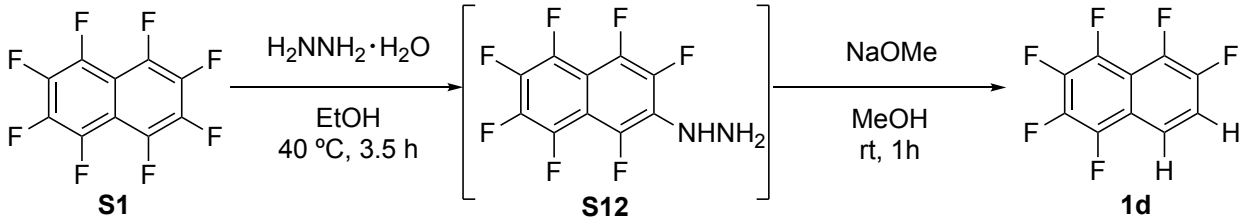
To a solution of 1,2,4,5,7,8-hexafluoro-3,6-bis[trifluoromehanesulfonyloxy]naphthalene **S11** (830 mg, 1.56 mmol, 1.0 equiv.) in DMF (3.0 mL) was added dppf (173 mg, 0.312 mmol, 20 mol%),

triethylsilane (2.50 mL, 15.7 mmol, 10 equiv.) and $Pd(OAc)_2$ (70.0 mg, 0.312 mmol, 20 mol%) at 0 °C. After stirring at 0 ºC for 10 min, the reaction mixture was allowed warm to 60 °C and stirred for 4 h. After cooling to room temperature, H_2O (10 mL) was added to the mixture, and the resulting suspension was filtered through the Celite pad. The residue was washed with Et_2O (10 mL) then the filtrate was extracted with Et_2O (30 mL×3). The combined organic layer was washed with H_2O (30 mL) and brine (30 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane as eluent) to give a 1,2,4,5,7,8-hexafluoronaphthalene **1c** as a white solid (196 mg, 0.830 mmol, 53%).

R_f = 0.34 (hexane). M. p. = 40–42 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.12–7.09 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –116.1- –116.3 (m, 2F), –133.8- –133.9 (m 2F), –151.0- –151.2 (br, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.8, 147.5 (d, *J* = 6.7 Hz), 140.6 (d, *J* = 6.7 Hz), 117.0, 109.3, 103.7 (d, *J* = 169.7 Hz). IR (ATR): 1649, 1488, 1401, 1380, 1161, 1078, 891, 846, 701, 687 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}H_2F_6$ 236.0061, found 236.0059.

Synthesis of 1,2,3,4,5,6-hexafluotonaphthalene (1d) [S8]

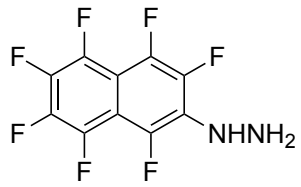


Hydrazine monohydrate (2.00 mL, 40.0 mmol, 4.0 equiv.) was added to a solution of octafluoronaphthalene **S1** (2.83 g, 10.0 mmol, 1.0 equiv.) in EtOH (12 mL). The mixture was stirred at 40 °C for 3.5 h. After cooling to room temperature, the mixture was quenched with H_2O (50 mL) and extracted with CH_2Cl_2 (30 mL×3). The combined organic layer was washed with H_2O (50 mL) and brine (50 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration to afford (1,3,4,5,6,7,8-heptafluoro-2-naphthalenyl) hydrazine **S12** as crude product. The **S12** was used to next step without further purification.

NaOMe (5.0 M in MeOH, 7.20 mL, 36.0 mmol, 3.6 equiv.) was added dropwise to a solution of (1,3,4,5,6,7,8-heptafluoro-2-naphthalenyl)hydrazine **S12** (2.75 g, 10.0 mmol, 1.0 equiv.) in MeOH (70 mL) at 0 °C. The reaction mixture was stirred at room temperature for 1 h while the generated-nitrogen gas was removed. The reaction mixture was quenched with H_2O (100 mL) at 0 °C and extracted with CH_2Cl_2 (30 mL×3). The combined organic layer was washed with H_2O (100 mL) and brine (50 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The residual crude product

was purified by column chromatography on silica gel (hexane as eluent) to give a 1,2,3,4,5,6-hexafluotonaphthalene **1d** (1.66 g, 70.3 mmol, 70%) as a colorless oil.

Characterization of **S12**

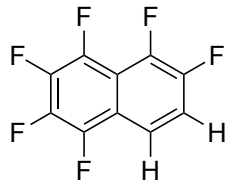


S12

R_f = 0.50 (hexane / ethyl acetate = 3:1).

^{1}H NMR (400 MHz, $CDCl_3$): δ 5.51 (s, 1H), 4.10 (brs, 2H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –143.4- –143.6 (m, 1F), –147.5 (dt, *J* = 36.1, 19.3 Hz, 1F), –148.2 (dt, *J* = 62.6, 15.2 Hz, 1F), –149.4 (dt, *J* = 36.8, 18.3 Hz, 1F), –150.2 (s, 1F), –156.6 (t, *J* = 18.8 Hz, 1F), –159.0 (t, *J* = 18.8 Hz, 1F).

Characterization of **1d**



1d

R_f = 0.43 (hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (m, 1H), 7.46 (dd, *J* = 9.4, 7.1 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –138.0 (s, 1F), –145.6 (dd, *J* = 57.8, 17.3 Hz, 1F), –147.3- –147.7 (m, 1F), –148.7 (t, *J* = 17.3 Hz, 1F), –156.2 (t, *J* = 17.3 Hz, 1F), –158.3- –158.5 (m, 1F).

3. Preparation for Magnesium amide reagents

TMP_2Mg[S9]

A 100 mL two-neck round-bottomed flask was flame-dried under vacuo. The flask was backfilled with nitrogen gas three times. THF (25 mL) and 2,2,6,6-tetramethylpiperidine (1.62 mL, 10.0 mmol, 1.9 equiv.) were charged into the flask, dibutylmagnesium (1.0 M in heptane, 5.00 mL, 5.00 mmol, 1.0 equiv.) was added dropwise. The mixture was refluxed for 24 h to afford a pale yellow solution of TMP_2Mg (0.1 M in THF). The TMP_2Mg was titrated against benzoic acid using 4-phenylazodiphenylamine as indicator.

$TMP_2Mg{\cdot}2LiBr$[S10]

A 30 mL two-neck round-bottomed flask was charged with Mg powder (122 mg, 5.00 mmol, 1.0 equiv.). The flask was flame-dried under vacuo. Then, the flask was backfilled with nitrogen gas three times. THF (5.0 mL) and 1,2-dibromoehtane (430 μL, 5.00 mmol, 1.0 equiv.) were added to the flask at room temperature. The mixture was refluxed for 1 h to give a $MgBr_2$ in THF. In another 30 mL two neck flask, 2,2,6,6-tetramethylpiperidine (1.70 mL, 10.0 mmol, 2.0 equiv.) and THF (5.0 mL) were charged. After cooling to –78 ºC, *n*-BuLi (1.58 M in hexane, 6.33 mL, 10.0 mol, 2.0 equiv.) was added dropwise to the solution at −78 °C. The resulting mixture was warmed to 0 °C and stirred for 30 min. The resulting solution was transferred to the $MgBr_2$ in THF via cannula at 0 ºC. The mixture was stirred at 0 °C for 30 min, then warmed to room temperature and stirred for 30 min to afford a $TMP_2Mg{\cdot}2LiBr$ (0.20 M in THF) as a light brown solution. The $TMP_2Mg{\cdot}2LiBr$ was titrated at 0 °C against benzoic acid using 4-phenylazodiphenylamine as indicator.

$TMP_2Mg{\cdot}2LiCl$[S11]

A 100 mL two-neck round-bottomed flask was charged with Mg powder (122 mg, 5.00 mmol, 1.0 equiv.). The flask was flame-dried under vacuo. Then, the flask was backfilled with nitrogen gas three times. THF (20 mL) and 1,2-dichloroehtane (400 μL, 5.00 mol, 1.0 equiv.) were added to the flask at room temperature. The reaction mixture was refluxed for 1 h to give a $MgCl_2$ in THF. In another 30 mL two neck flask, 2,2,6,6-tetramethylpiperidine (1.70 mL, 10.0 mmol, 2.0 equiv.) and THF (5.0 mL) were charged. After cooling to –78 ºC, *n*-BuLi (1.58 M in hexane, 6.33 mL, 10.0 mol, 2.0 equiv.) was added dropwise to the solution at −78 °C. The reaction mixture was warmed to 0 °C and stirred for 30 min. The resulting solution was transferred to the $MgCl_2$ in THF via cannula at 0ºC. The mixture was stirred at 0 °C for 30 min, then warmed to room temperature and stirred for 1 h to afford a

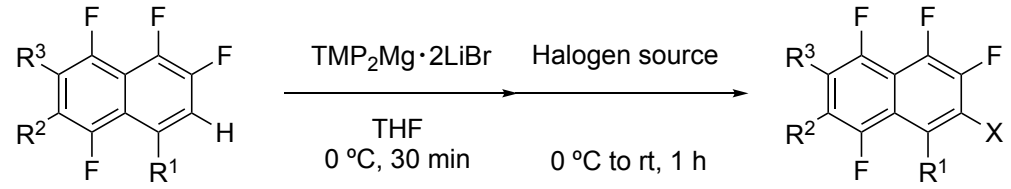
$TMP_2Mg·2LiCl$ (0.10 M in THF) as a pale yellow solution. The $TMP_2Mg·2LiCl$ was titrated at 0 °C against benzoic acid using 4-phenylazodiphenylamine as indicator.

TMPMgCl·LiCl[S12]

A flame-dried 50 mL two-neck round-bottom flask was charged with *i*-PrMgCl·LiCl (1.3 M in THF, 7.60 mL, 10.0 mmol, 1.0 equiv.). Then, 2,2,6,6-tetramethylpiperidine (1.70 mL, 10.0 mmol, 1.0 equiv.) was added dropwise to the solution at room temperature. The reaction mixture was stirred at room temperature for 48 h to afford a TMPMgCl·LiCl (0.60 M in THF) as a yellow solution. The TMPMgCl·LiCl was titrated at 0 °C against benzoic acid using 4-phenylazodiphenylamine as indicator.

4. Halogenation reaction for polyfluoronaphthalenes.

General procedure:

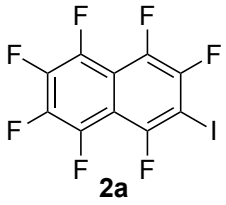


1a: $R^1 = R^2 = R^3 = F$
1b: $R^1 = R^2 = F$, $R^3 = H$
1c: $R^1 = R^3 = F$, $R^2 = H$
1d: $R^1 = H$, $R^2 = R^3 = F$

2: $R^1 = R^2 = R^3 = F$
3: $R^1 = R^2 = F$, $R^3 = X$
4: $R^1 = R^3 = F$, $R^2 = X$
5: $R^1 = H$, $R^2 = R^3 = F$
6: $R^1 = R^2 = F$, $R^3 = H$
7: $R^1 = R^3 = F$, $R^2 = H$

$TMP_2Mg·2LiBr$ was added to a solution of polyfluoronaphthalene **1** in THF at 0 °C. The mixture was stirred at 0 °C for 30 min, then halogen source was added to the reaction mixture at once. The mixture was stirred at room temperature for 1 h, quenched with 2 M HCl aq. (30 mL) at 0 ºC and extracted with Et_2O (10 mL×3). The combined organic layer was washed with sat. Na_2SO_3 aq. (30 mL) and brine (30 mL), dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The residual crude product was purified by column chromatography on silica gel (hexane as eluent) to give corresponding perflurorohalogenated-naphthalene (**2-7**).

1,2,3,4,5,6,8-Heptafluoro-7-iodonaphthalene (2a)



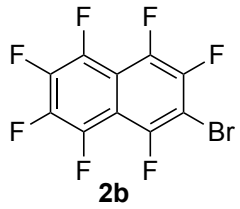
2a

2a was synthesized according to general procedure using 1,2,3,4,5,6,8-heptafuluoronaphthalene **1a** (127 mg, 0.500 mmol, 1.0 equiv.), THF (4 mL), $TMP_2Mg·2LiBr$ (0.20 M in THF, 3.00 mL, 0.600 mmol, 1.2 equiv.), and I_2 (305 mg, 1.20 mmol, 2.4 equiv.) to give **2a** (173 mg, 0.455 mmol, 91%) as a white solid.

R_f = 0.43 (hexane). M.p. = 61–63 ºC

^{19}F NMR (376 MHz, $CDCl_3$): δ –96.9 (dd, *J* = 66.5, 17.3 Hz, 1F), –116.4- –116.5 (m, 1F), –144.1 (dt, *J* = 66.5, 17.3 Hz, 1F), –146.3 (dt, *J* = 59.7, 16.6 Hz, 1F), –147.0- –147.3 (m, 1F), –152.9- –153.1 (m, 1F), –155.1 (s, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.9, 147.0, 141.4, 140.6, 140.1, 139.8, 138.8, 111.7, 107.7, 72.7. IR (ATR): 1650, 1487, 1399, 1254, 1161, 1107, 946, 889, 739, 686, 665 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}F_7I$ 379.8933, found 379.8932.

2-Bromo-1,3,4,5,6,7,8-heptafluoronaphthalene (2b)



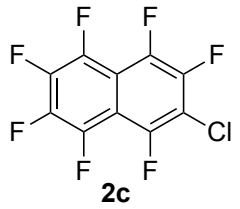
2b

2b was synthesized according to general procedure using 1,2,3,4,5,6,8-heptafuluoronaphthalene **1a** (254 mg, 1.00 mmol, 1.0 equiv.), THF (8.0 mL) $TMP_2Mg{\cdot}2LiBr$ (0.20 M in THF, 6.00 mL, 1.20 mmol, 1.2 equiv.), and Br_2 (260 μL, 5.00 mmol, 5.0 equiv.) to give **2b** (310 mg, 0.930 mmol, 93%) as a white solid.

R_f = 0.44 (hexane). M. p. = 64–65 ºC.

^{19}F NMR (376 MHz, $CDCl_3$): δ –111.4 (dd, *J* = 66.5, 14.4 Hz, 1F), –128.6- –128.8 (m, 1F), –144.4 (dt, *J* = 66.5, 17.3 Hz, 1F), –146.1 (dt, *J* = 59.7, 15.9 Hz, 1F), –146.7- –147.1 (m, 1F), –153.1 (dd, *J* = 20.2, 17.3 Hz, 1F), –154.7 (dd, *J* = 23.1, 14.5 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 150.2, 145.1, 141.4, 140.7, 140.7, 139.9, 139.0, 110.7, 107.9, 99.6. IR (ATR): 1638, 1522, 1483, 1398, 1252, 1156, 1106, 948, 897, 744 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}BrF_7$ 331.9072, found 331.9062.

2-Chloro-1,3,4,5,6,7,8-heptafluoronaphthalene (2c)



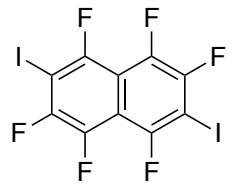
2c

2c was synthesized according to general procedure using 1,2,3,4,5,6,8-heptafuluoronaphthalene **1a** (127 mg, 0.50 mmol, 1.0 equiv.), THF (4.0 mL) $TMP_2Mg{\cdot}2LiBr$ (0.20 M in THF, 3.00 mL, 0.60 mmol, 1.2 equiv.), and $PhSO_2Cl$ (150 μL, 1.20 mmol, 2.4 equiv.) to give **2c** (126 mg, 0.435 mmol, 87%) as a white solid.

R_f = 0.50 (hexane). M. p. = 66–67 ºC

^{19}F NMR (376 MHz, $CDCl_3$): δ –120.1 (dd, *J* = 66.5, 17.3 Hz, 1F), –136.1- –136.2 (m, 1F), –144.6 (dt, *J* = 64.5, 16.6 Hz, 1F), –146.0 (dt, *J* = 59.7, 16.6 Hz, 1F), –146.9- –147.1 (m, 1F), –153.1- –153.3 (m, 1F), –154.6- –154.7 (m, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 149.3, 144.4, 141.3, 141.0, 140.9, 139.8, 139.1, 111.4, 109.9, 107.7. IR (ATR): 1639, 1477, 1393, 1162, 1105, 916, 750 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}ClF_7$ 287.9577, found 287.9585.

1,2,4,5,6,8-Hexafluoro-3,7-diiodonaphthalene (3a)



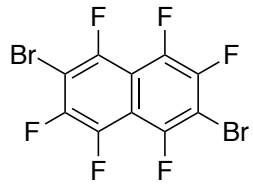
3a

3a was synthesized according to general procedure using 1,2,4,5,6,8-hexafluoronaphthalene **1b** (47.0 mg, 0.200 mmol, 1.0 equiv.), THF (1.5 mL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 2.10 mL, 0.480 mmol, 2.4 equiv.), and I_2 (244 mg, 0.960 mmol, 4.8 equiv.) to give **3a** (90.1 mg, 0.184 mmol, 92%) as a white solid.

R_f = 0.35 (hexane). M. p. = 180–183 ºC

^{19}F NMR (376 MHz, $CDCl_3$): δ –97.3 (dd, *J* = 66.1, 20.2 Hz, 2F), –116.9- –117.0 (m, 2F), –145.3- –145.7 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 153.0, 146.6, 138.9, 111.9, 74.2. IR (ATR): 1608, 1473, 1375, 1118, 942, 899 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}F_6I_2$ 487.7994, found 487.7990.

2,6-Dibromo-1,3,4,5,7,8-hexafluoronaphthalene (3b)



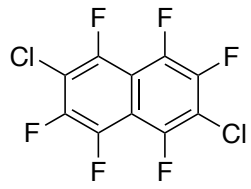
3b

3b was synthesized according to general procedure using 1,2,4,5,6,8-hexafluoronaphthalene **1b** (47.0 mg, 0.200 mmol, 1.0 equiv.), THF (1.5 mL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 2.10 mL, 0.480 mmol, 2.4 equiv.), and Br_2 (100 μL, 2.00 mmol, 10.0 equiv.) to give **3b** (65.1 mg, 0.166 mmol, 83%) as a white solid.

R_f =0.40 (hexane). M. p. = 133–135 ºC.

^{19}F NMR (376 MHz, $CDCl_3$): δ –111.6 (dd, *J* = 66.5, 17.3 Hz, 2F), –128.9- –129.0 (m, 2F), –145.4- –145.7 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 150.4, 144.9, 140.0, 111.0, 100.7. IR (ATR): 1618, 1386, 1132, 913, 668 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}{}^{79}Br^{81}BrF_6$ 393.8250, found 393.8250.

2,6-Dichloro-1,3,4,5,7,8-hexafluoronaphtalene (3c)



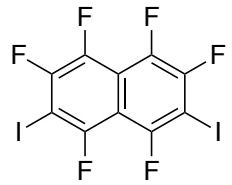
3c

3c was synthesized according to general procedure using 1,2,4,5,6,8-hexafluoronaphthalene **1b** (47.0 mg, 0.200 mmol, 1.0 equiv.), THF (1.5 mL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 2.10 mL, 0.480 mmol, 2.4 equiv.), and $PhSO_2Cl$ (155 µL, 1.20 mmol, 6.0 equiv.) to give **3c** (56.0 mg, 0.184 mmol, 92%) as a white solid.

R_f = 0.38 (hexane). M. p. = 101–102 ºC.

^{19}F NMR (376 MHz, $CDCl_3$): δ –120.2 (dd, *J* = 63.6, 17.3 Hz, 2F), –136.2- –136.4 (m, 2F), –145.6- –146.0 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 149.3, 144.3, 140.4, 112.3, 110.1. IR (ATR): 1624, 1390, 1139, 915, 791, 702 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}Cl_2F_6$ 303.9281, found 303.9275.

1,2,4,5,7,8-Hexafluoro-3,6-diiodonaphthalene (4a)



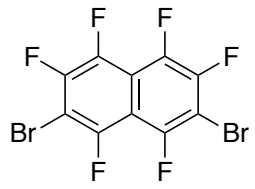
4a

4a was synthesized according to general procedure using 1,2,4,5,7,8-hexafluoronaphthalene **1c** (4.6 mg, 0.02 mmol, 1.0 equiv.), THF (150 µL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 210 µL, 0.048 mmol, 2.4 equiv.), and I_2 (25.0 mg, 0.096 mmol, 4.8 equiv.) to give **4a** (8.40 mg, 0.017 mmol, 86%) as a white solid.

R_f = 0.33 (hexane). M. p. = 149–150 ºC

^{19}F NMR (376 MHz, $CDCl_3$): δ –94.7 (dd, *J* = 11.6, 8.7 Hz, 2F), –114.9 (d, *J* = 8.7 Hz 2F), –147.2- –147.4 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.2, 147.7, 140.1, 116.0, 108.2, 71.9. IR (ATR): 1626, 1382, 1124, 900 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}F_6I_2$ 487.7994, found 487.7977.

2,7-Dibromo-1,3,4,5,6,8-hexafluoronaphthalene (4b)



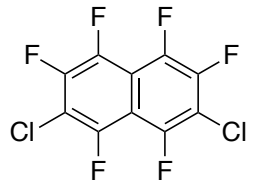
4b

4b was synthesized according to general procedure using 1,2,4,5,7,8-hexafluoronaphthalene **1c** (23.6 mg, 0.100 mmol, 1.0 equiv.), THF (770 µL), $TMP_2Mg{\cdot}2LiBr$ (0.24 M in THF, 1.0 mL, 0.240 mmol, 2.4 equiv.), and Br_2 (50 µL, 1.00 mmol, 10.0 equiv.) to give **4b** (36.0 mg, 0.091 mmol, 91%) as a white solid.

R_f = 0.44 (hexane). M. p. = 102–105 ºC

^{19}F NMR (376 MHz, $CDCl_3$): δ –109.6 (dd, *J* = 11.6, 8.7 Hz, 2F), –1267.2 (d, *J* = 8.7 Hz, 2F), –146.8- –147.0 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 149.7, 145.7, 140.8, 113.9, 108.5, 99.2. IR (ATR): 1628, 1461, 1386, 1130, 933, 858 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}Br_2F_6$ 391.8271, found 391.8269.

2,7-Dichloro-1,3,4,5,6,8-hexafluoronaphthalene (4c)



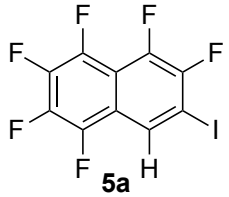
4c

4c was synthesized according to general procedure using 1,2,4,5,7,8-hexafluoronaphthalene **1c** (23.6 mg, 0.100 mmol, 1.0 equiv.), THF (770 µL), $TMP_2Mg{\cdot}2LiBr$ (0.24 M in THF, 1.0 mL, 0.240 mmol, 2.4 equiv.), and $PhSO_2Cl$ (80 µL, 0.60 mmol, 6.0 equiv.) to give **4b** (28.1 mg, 0.092 mmol, 92%) as a white solid.

R_f = 0.42 (hexane). M. p. = 80–81 ºC

^{19}F NMR (376 MHz, $CDCl_3$): δ –118.7 (dd, *J* = 11.6, 8.7 Hz, 2F), –134.9 (dd, *J* = 11.6, 5.8 Hz, 2F), –146.9- –147.0 (m, 2F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 148.8, 145.0, 141.0, 122.5, 111.2, 108.0. IR (ATR): 1636, 1470, 1392, 1134, 1094, 943, 898, 742 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}Cl_2F_6$ 303.9281, found 303.9287.

1,2,3,4,5,6-Hexafluoro-7-iodonaphthalene (5a)



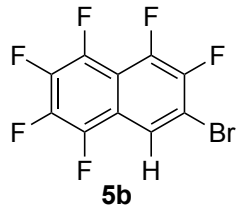
5a

5a was synthesized according to general procedure using 1,2,3,4,5,6-hexafluoronaphthalene **1d** (118 mg, 0.500 mmol, 1.0 equiv.), THF (4 mL), $TMP_2Mg{\cdot}2LiBr$ (0.20 M in THF, 3.00 mL, 0.600 mmol, 1.2 equiv.), and I_2 (305 mg, 1.20 mmol, 2.4 equiv.) to give **5a** (153 mg, 0.423 mmol, 84%) as a white solid.

R_f = 0.44 (hexane). M. p. = 40–43 ºC.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (d, *J* = 5.0 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –118.1- –118.2 (m, 1F), –141.2 (dd, *J* = 52.0, 17.3 Hz, 1F), –146.6- –146.9 (m, 1F), –148.5 (t, *J* = 17.3 Hz, 1F), –155.1 (t, *J* = 15.9 Hz, 1F), –156.4 (dt, *J* = 14.5, 8.7 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ147.6 (d, *J* = 10.5 Hz), 143.1, 141.1, 140.7 (d, *J* = 4.8 Hz), 139.6, 138.1, 126.0 (d, *J* = 174.4 Hz), 118.5, 111.5 (d, *J* = 7.7 Hz), 84.0 (d, *J* = 5.8 Hz). IR (ATR): 1655, 1459, 1416, 1223, 1124, 951, 827 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HF_6I$ 361.9027, found 361.9028.

7-Bromo-1,2,3,4,5,6-hexafluoronaphthalene (5b)



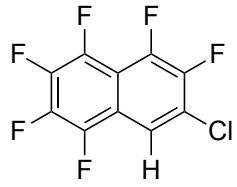
5b

5b was synthesized according to general procedure using 1,2,3,4,5,6-hexafluoronaphthalene **1d** (118 mg, 0.500 mmol, 1.0 equiv.), THF (4 mL), $TMP_2Mg{\cdot}2LiBr$ (0.20 M in THF, 3.00 mL, 0.600 mmol, 1.2 equiv.), and Br_2 (130 μL, 2.52 mmol, 5.0 equiv.) to give **5b** (144 mg, 0.457 mmol, 92%) as a white solid.

R_f = 0.50 (hexane). M. p. = 34–35 ºC

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 5.7 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –130.7 (s, 1F), –140.9 (dd, *J* = 52.0, 17.3 Hz, 1F), –146.7 (ddd, *J* = 52.0, 17.3, 5.8 Hz, 1F), –148.3 (t, *J* = 15.9 Hz, 1F), –155.2 (t, *J* = 17.3 Hz, 1F), –156.1 (dt, *J* = 14.5, 8.7 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$,): δ 145.7 (d, *J* = 10.5 Hz), 144.3, 141.2, 141.0 (d, *J* = 3.8 Hz), 139.4, 138.3, 119.7 (d, *J* = 173.5 Hz), 117.3, 112.2, 110.8 (d, *J* = 6.7 Hz). IR (ATR): 1625, 1518, 1475, 1416, 1373, 1140, 1058, 990, 906, 867, 797, 739 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HBrF_6$ 315.9145, found 315.9151.

7-Chloro-1,2,3,4,5,6-hexafluoronaphthalene (5c)



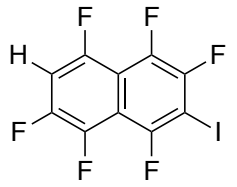
5c

5c was synthesized according to general procedure using 1,2,3,4,5,6-hexafluoronaphthalene **1d** (118 mg, 0.500 mmol, 1.0 equiv.), THF (4 mL), $TMP_2Mg{\cdot}2LiBr$ (0.20 M in THF, 3.00 mL, 0.600 mmol, 1.2 equiv.), and $PhSO_2Cl$ (190 μL, 1.50 mmol, 3.0 equiv.) to give **5c** (124 mg, 0.458 mmol, 92%) as a white solid.

R_f = 0.50 (hexane). M. p. = 35–37 ºC.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 6.2 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –138.5 (s, 1F), –141.0 (dd, *J* = 52.0, 14.5 Hz, 1F), –146.8 (ddd, *J* = 52.0, 17.3, 5.8 Hz 1F), –148.2 (t, *J* = 17.3 Hz, 1F), –155.4 (dd, *J* = 20.2, 17.3 Hz, 1F), –156.1 (dd, *J* = 28.8, 8.7 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 145.0 (d, *J* = 9.6 Hz), 144,8, 141.2, 141.1 (d, *J* = 3.8 Hz), 139.4, 138.4, 124.4 (d, *J* = 5.8 Hz), 116.6 (d, *J* = 173.5 Hz), 116.6, 110.3 (d, *J* = 8.6 Hz). IR (ATR): 1631, 1520, 1480, 1377, 1266, 1147, 1058, 991, 934, 910. 867, 797, 756 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HClF_6$ 269.9671, found 269.9676.

1,3,4,5,7,8-Hexafluoro-2-iodonaphthalene (6a)



6a

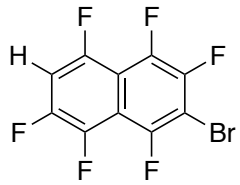
6a was synthesized according to general procedure using 1,2,4,5,6,8-hexafluoronaphthalene **1b** (118 mg, 0.500 mmol, 1.0 equiv.), THF (4 mL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 1.10 mL, 0.250 mmol, 0.5 equiv.), and I_2 (152 mg, 0.60 mmol, 1.2 equiv.) to give **6a** (175 mg, 0.485 mmol, 97%) as a white solid.

R_f = 0.31 (hexane). M. p. = 56–58 ºC.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.21 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –97.7 (dd, *J* = 66.5, 20.2 Hz, 1F), –117.5- –117.8 (m, 1F), –118.6- –118.8 (m, 1F), –135.1- –135.2 (m, 1F), –146.2- –146.5 (m, 1F), –148.4- –148.8 (m, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.9, 152.6, 146.4 (d, *J* = 5.8 Hz), 146.3, 139.9, 139.6, 112.5 (d, *J* = 6.7 Hz), 112.4, 105.8 (d, *J* = 168.7 Hz), 74.0. IR (ATR): 1653,

1619, 1382, 1160, 1121, 890, 843, 732 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HF_6I$ 361.9027, found 361.9022.

2-Bromo-1,3,4,5,7,8-hexafluoronaphthalene (6b)



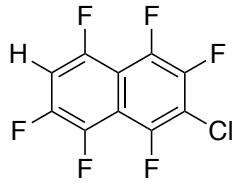
6b

6b was synthesized according to general procedure using 1,2,4,5,6,8-hexafluoronaphthalene **1b** (118 mg, 0.500 mmol, 1.0 equiv.), THF (4 mL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 1.10 mL, 0.250 mmol, 0.5 equiv.), and Br_2 (70 µL, 1.25 mmol, 2.5 equiv.) to give **6b** (151 mg, 0.480 mmol, 96%) as a white solid.

R_f = 0.38 (hexane). M. p. = 53–55 ºC.

^1H NMR (400 MHz, $CDCl_3$): δ 7.26-7.19 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –112.2 (dd, *J* = 65.4, 17.4 Hz, 1F), –117.2- –117.6 (m, 1F), –130.8- –131.0 (m, 1F), –134.7- –134.9 (m, 1F), –146.1 (ddd, *J* = 60.7, 17.3, 14.5 Hz, 1F), –148.9 (ddd, *J* = 63.6, 20.2, 5.8 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.6 (d, *J* = 6.7 Hz), 150.3, 146.7 (d, *J* = 6.7 Hz), 144.3, 140.8, 139.8, 112.6, 111.4 (d, *J* = 4.8 Hz), 105.7 (d, *J* = 169.7 Hz), 100.5. IR (ATR): 1625, 1386, 1125, 893, 846, 740, 666 cm^{-1}. HRMS (FAB/EB) $[M]^+$ calcd for $C_{10}HBrF_6$ 313.9166, found 313.9171.

2-Chloro-1,3,4,5,7,8-hexafluoronaphthalene (6c)



6c

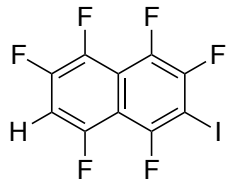
6c was synthesized according to general procedure using 1,2,4,5,6,8-hexafluoronaphthalene **1b** (118 mg, 0.500 mmol, 1.0 equiv.), THF (4 mL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 1.10 mL, 0.250 mmol, 0.5 equiv.), and $PhSO_2Cl$ (95 µL, 0.75 mmol, 1.5 equiv.) to give **6c** (122 mg, 0.465 mmol, 93%) as a white solid.

R_f = 0.38 (hexane). M. p. = 54–56 ºC

^1H NMR (400 MHz, $CDCl_3$): δ 7.26-7.18 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –117.2- –117.5 (m, 1F), –120.9 (dd, *J* = 63.6, 17.3 Hz, 1F), –134.6- –134.8 (m, 1F), –138.3- –138.5 (m, 1F), –146.2 (ddd, *J* = 63.6, 17.4, 5.8 Hz, 1F), –148.9- –149.3 (m, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.6 (d, *J*

= 5.8 Hz), 149.3, 146.8 (d, *J* = 6.7 Hz), 143.7, 141.0, 139.9 (d, *J* = 6.7 Hz), 112.4, 112.2, 110.7(d, *J* = 5.8 Hz), 105.7 (d, *J* = 168.7 Hz). IR (ATR): 1633, 1390, 1125, 900, 849, 808, 751, 683 cm^{-1}. HRMS (FAB/EB) $[M]^+$ calcd for $C_{10}HClF_6$ 269.9671, found 269.9681.

1,3,4,5,6,8-Hexafluoro-2-iodonaphthalene (7a)



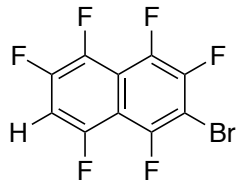
7a

7a was synthesized according to general procedure using 1,2,4,5,7,8-hexafluoronaphthalene **1c** (23.6 mg, 0.100 mmol, 1.0 equiv.), THF (770 µL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 215 µL, 0.050 mmol, 0.5 equiv.), and I_2 (30.5 mg, 0.12 mmol, 1.2 equiv.) to give **7a** (23.1 mg, 0.064 mmol, 64%, 77% purity) as a white solid. ***7a*** *was obtained as mixture with* ***1c*** *and these compounds were not able to be isolated. Therefore,* ***7a*** *was characterized as mixture with* ***1c****.*

R_f = 0.33 (hexane)

^1H NMR (400 MHz, $CDCl_3$): δ 7.18-7.11 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –95.7 (dd, *J* = 78.0, 17.3 Hz, 1F), –115.1- –115.4 (m, 1F), –115.8 (d, *J* = 23.1 Hz, 1F), –132.8- –133.0 (m, 1F), –147.7 (ddd, *J* = 57.8, 17.3, 5.8 Hz, 1F), –150.5 (ddd, *J* = 63.6, 20.2, 5.8 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 153.2, 151.9 (d, *J* = 7.7 Hz), 147.6 (d, *J* = 6.7 Hz), 147.5, 140.7, 140.1, 116.5, 108.8 (d, *J* = 6.7 Hz), 104.3 (d, *J* = 168.7), 71.1. IR (ATR): 1650, 1474, 1381, 1118, 1081, 910, 884, 840, 779, 745, 701cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HF_6I$ 361.9027, found 361.9036.

2-Bromo-1,3,4,5,6,8-hexafluoronaphthalene (7b)



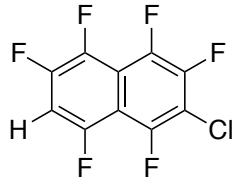
7b

7b was synthesized according to general procedure using 1,2,4,5,7,8-hexafluoronaphthalene **1c** (23.6 mg, 0.100 mmol, 1.0 equiv.), THF (770 µL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 215 µL, 0.050 mmol, 0.5 equiv.), and Br_2 (13 µL, 0.12 mmol, 1.2 equiv.) to give **7b** (18.5 mg, 0.059 mmol, 59%, 74% purity) as a white solid. ***7b*** *was obtained as mixture with* ***1c*** *and these compounds were not able to be isolated. Therefore,* ***7b*** *was characterized as mixture with* ***1c****.*

R_f = 0.38 (hexane)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18-7.10 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –110.3 (dd, *J* = 72.3, 20.2 Hz, 1F), –115.4- –115.8 (m, 1F), –128.0 (d, *J* = 17.3 Hz, 1F), –133.0- –133.1 (m, 1F), –147.6 (ddd, *J* = 57.8, 17.3 Hz, 1F), –150.4 (ddd, *J* = 57.8, 14.5, 5.8 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.0 (d, *J* = 7.7 Hz), 150.6, 147.5 (d, *J* = 6.7 Hz), 145.7, 140.9, 115.5, 108.9, 104.7 (d, *J* = 166.8 Hz), 99.9 (d, *J* = 5.8 Hz), 98.1. IR (ATR): 1632, 1464, 1388, 1081, 936, 915, 741, 661 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HBrF_6$ 313.9166, found 313.9173.

2-Chloro-1,3,4,5,6,8-hexafluoronaphthalene (7c)



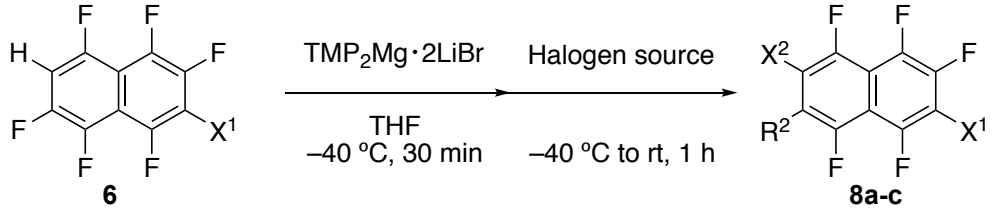
7c

7a was synthesized according to general procedure using 1,2,4,5,7,8-hexafluoronaphthalene **1c** (23.6 mg, 0.100 mmol, 1.0 equiv.), THF (770 µL), $TMP_2Mg{\cdot}2LiBr$ (0.23 M in THF, 215 µL, 0.050 mmol, 0.5 equiv.), and $PhSO_2Cl$ (20 µL, 0.15 mmol, 1.5 equiv.) to give **7c** (13.4 mg, 0.049 mmol, 49%, 74% purity) as a white solid. ***7c** was obtained as mixture with **1c** and these compounds were not able to be isolated. Therefore, **7c** was characterized as mixture with **1c**.*

R_f = 0.37 (hexane)

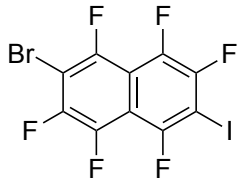
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20-7.14 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$): δ –115.7- –116.0 (m, 1F), –119.0 (dd, *J* = 66.5, 20.2 Hz, 1F), –133.1- –133.3 (m, 1F), –135.5 (dd, *J* = 11.6, 5.8 Hz, 1F), –147.7 (ddd, *J* = 57.8, 17.3, 5.8 Hz, 1F), –150.3 (ddd, *J* = 57.8, 20.2, 5.8 Hz, 1F). ^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 152.2 (d, *J* = 5.8 Hz), 149.7, 147.5 (d, *J* = 6.7 Hz), 145.1, 141.2, 140.6, 114.9, 110.1, 108.7 (d, *J* = 5.8 Hz), 104.8 (d, *J* = 169.7 Hz). IR (ATR): 1642, 1480, 1440, 1390, 1262, 1085, 907, 815, 764, 701 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}HClF_6$ 269.9671, found 269.9677.

General procedure for synthesis of hetero-dihalogenated F_6 Naphthalenes



$TMP_2Mg·2LiBr$ (0.5 equiv.) was added to a solution of 3-halogenated-1,2,4,5,6,8-hexafluoronaphthalene **6** (1.0 equiv.) in THF at –40 ºC. The mixture was stirred at –40 ºC for 30 min, then corresponding halogen source was added to the mixture. The reaction mixture was warmed to room temperature and stirred for 1 h, quenched with 2M-HCl aq. (5 mL) at 0 ºC and extracted with Et_2O (5 mL x 3). The combined organic layer was washed with sat. Na_2SO_3 aq. (5 mL) and brine, dried over Na_2SO_4, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane as eluent) to give **8**.

3-Bromo-1,2,4,5,6,8-hexafluoro-7-iodonaphthalene (8a)



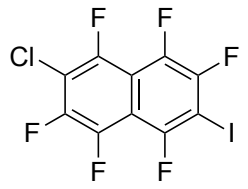
8a

8a was synthesized according to general procedure for heterohalogenation using 1,3,4,5,7,8-hexafluoro-2-iodonaphthalene **6a** (108 mg, 0.30 mmol, 1.0 equiv.), $TMP_2Mg·2LiBr$ (0.24 M in THF, 625 μL, 0.15 mmol, 0.5 equiv.), THF (2.5 mL) and Br_2 (40 μL, 0.75 mmol, 2.5 equiv.). The product was further purified by reprecipitation with hexane after column chromatography on silica gel to give **8a** (81.9 mg, 0.186 mmol, 62%) as a white solid.

R_f = 0.37 (hexane). M.p. = 156–157 ºC.

^{19}F NMR (376 MHz, $CDCl_3$): δ –97.2 (dd, J = 72.3, 14.5 Hz, 1F), –111.8 (dd, J = 66.5, 14.5 Hz, 1F), –116.6- –116.8 (m, 1F), –129.2- –129.3 (m, 1F), –145.3 (ddd, J = 72.3, 23.1, 5.8 Hz, 1F), –145.8 (ddd, J = 66.5, 17.3, 5.8 Hz, 1F).^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 153.0, 150.4, 146.9, 144.7, 139.8, 139.1, 112.1, 110.8, 100.8, 74.0. IR (ATR): 1636, 1471, 1385, 1095, 943, 900, 743 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}BrF_6I$ 439.8132, found 439.8140.

3-Chloro-1,2,4,5,6,8-hexafluoro-7-iodonaphthalene (8b)



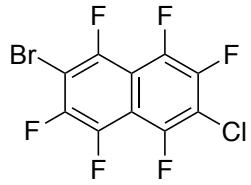
8b

8b was synthesized according to general procedure for heterohalogenation using 2-chloro-1,3,4,5,7,8-hexafluoronaphthalene **6c** (27.1 mg, 0.10 mmol, 1.0 equiv.), $TMP_2Mg{\cdot}2LiBr$ (0.24 M in THF, 220 µL, 0.05 mmol, 0.5 equiv.), THF (770 µL) and I_2 (30.5 mg, 0.12 mmol, 1.2 equiv.) to give **8b** (35.4 mg, 0.089 mmol, 89%) as a white solid.

R_f = 0.37 (hexane). M. p. = 125–126 ºC.

^{19}F NMR (376 MHz, $CDCl_3$): δ –97.1 (dd, *J* = 66.4, 20.2 Hz, 1F), –116.5- –116.7 (m, 1F), –120.5 (dd, *J* = 63.5, 14.5 Hz, 1F), –136.7- –136.9 (m, 1F), –145.3 (ddd, *J* = 72.3, 17.3, 5.8 Hz, 1F), –146.0 (ddd, *J* = 66.5, 17.3, 5.8 Hz 1F).^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 153.0, 149.4, 146.9, 144.0, 140.1, 139.2, 112.5, 111.9, 110.1, 73.9. IR (ATR): 1614, 1422, 1382, 1129, 908, 700 cm^{-1}. HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}ClF_6I$ 395.8637, found 395.8631.

3-Bromo-7-chloro-1,2,4,5,6,8-hexafluoronaphthalene (8c)



8c

8c was synthesized according to general procedure for heterohalogenation using 2-chloro-1,3,4,5,7,8-hexafluoronaphthalene **6c** (81.0 mg, 0.30 mmol, 1.0 equiv.), $TMP_2Mg{\cdot}2LiBr$ (0.24 M in THF, 625 µL, 0.15 mmol, 0.5 equiv.), THF (2.5 mL) and Br_2 (40 µL, 0.75 mmol, 2.5 equiv.) to give **8c** (89.0 mg, 0.267 mmol, 89%) as a white solid.

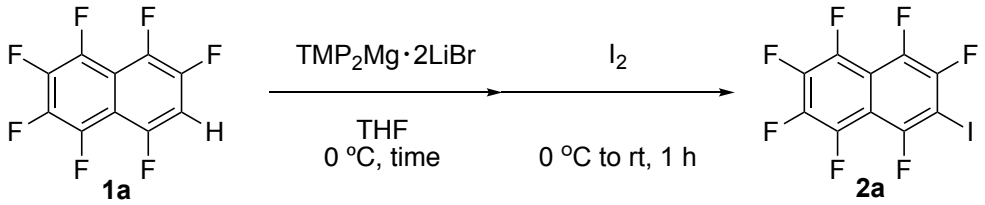
R_f = 0.36 (hexane). M. p. = 112–114 ºC.

^{19}F NMR (376 MHz, $CDCl_3$): δ –111.6 (dd, *J* = 66.4, 17.3 Hz, 1F), –120.3 (dd, *J* = 63.6, 17.3 Hz, 1F), –128.7- –128.9 (m, 1F), –136.4- –136.5 (m, 1F), –145.7 (dt, *J* = 72.3, 17.3 Hz, 2F).^{13}C {^{19}F} NMR (101 MHz, $CDCl_3$): δ 150.3, 149.4, 145.0, 144.2, 140.3, 140.1, 112.4, 110.8, 110.3, 100.6. IR (ATR): 1615, 1472, 1386, 1130, 901, 790, 745, 701 cm^{-1}.

HRMS (FAB/EB) *m/z* $[M]^+$ calcd for $C_{10}BrClF_6$ 347.8776, found 347.8785.

5. Optimization of halogenation reaction

Table S1. Initial study of iodination for 1a using $TMP_2Mg\cdot 2LiBr$

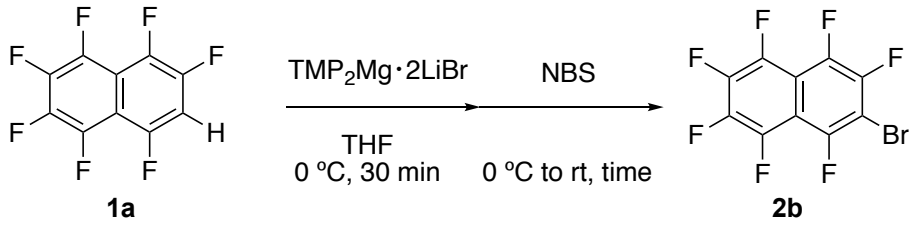


Entry	$TMP_2Mg\cdot 2LiBr$ (equiv.)	Time (h)	I_2 (equiv.)	Yield [b] (%)
1	1.2	4.0	6.0	13
2	1.2	2.0	6.0	63
3	1.2	1.0	6.0	86
4	1.2	0.5	6.0	90
5	1.2	0.5	4.8	89
6	1.2	0.5	2.4	91
7	1.2	0.5	1.2	44
8	0.6	0.5	1.2	85
9	0.5	0.5	1.0	66

[a]Reaction was conducted in THF (0.13 M) under the indicated conditions with 0.50 mmol of **1a**.

[b] Isolated yield.

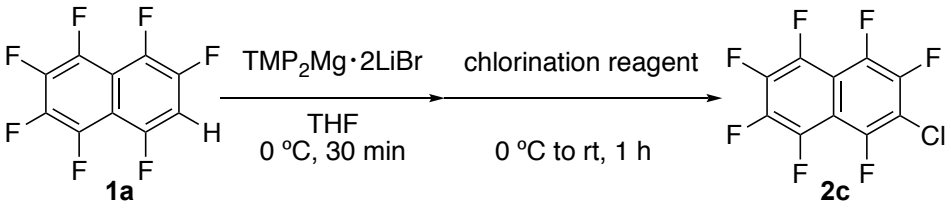
Table S2. Bromination of 1a using *N*-bromosuccinimide (NBS)[a]

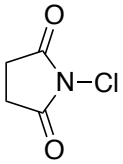
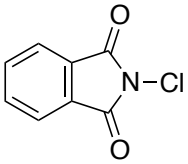
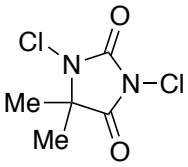
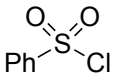


Entry	NBS (equiv.)	Method	Time (h)	Yield[b] (%)
1	3.0	A[c]	1.0	4
2	3.0	B[d]	1.0	12
3	5.0	B[d]	1.0	12
4	5.0	B[d]	18	16

[a]Reaction was conducted in THF (0.13 M) under the indicated conditions with 0.50 mmol of **1a** and 1.2 equiv. of $TMP_2Mg\cdot 2LiBr$. [b]Yield was determined by ^{19}F NMR using C_6F_6 as internal standard. [c]Method A: a solution of NBS in THF was added. [d]Method B: NBS was added in one portion.

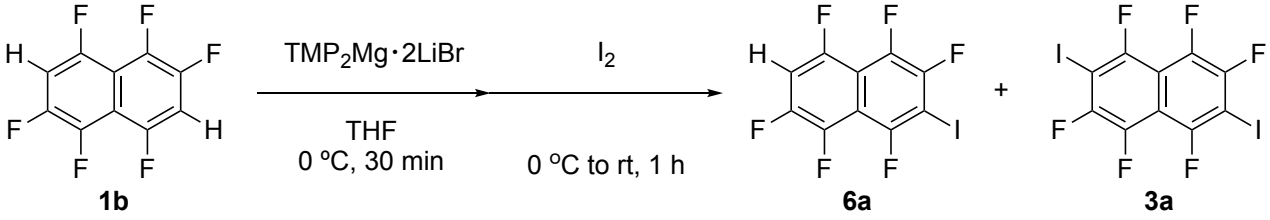
Scheme S1. Optimization of chlorination reagent[a]



chlorination reagent	 NCS	 NCPI	 DCDMH	 $PhSO_2Cl$
Yield of **2c**	18% yield[b]	13% yield[b]	24% yield[b]	89% yield[c]

[a]Reaction was conducted in THF (0.13 M) under the indicated conditions with 0.50 mmol of **1a**, 1.2 equiv. of $TMP_2Mg·2LiBr$ and 3.0 equiv. of chlorination reagent. [b] Yield was determined by ^{19}F NMR using C_6F_6 as internal standard. [c]Isolated yield.

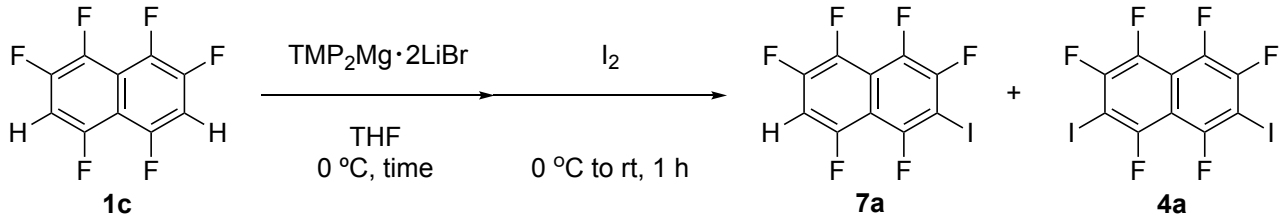
Table S3. Optimization for synthesis of monohalogenated 3,7- F_6 naphthalene



Entry	$TMP_2Mg·2LiBr$ (equiv.)	I_2 (equiv.)	Yield[b] (%)	
			6a	**3a**
1	1.2	2.4	0	92
2	0.5	1.2	97	<1

[a]Reaction was conducted in THF (0.13 M) under the indicated conditions with 0.50 mmol of **1b**. [b]Isolated yield.

Table S4. Optimization for synthesis of monohalogenated 3,6- F_6 naphthalene[a]



Entry	$TMP_2Mg·2LiBr$ (equiv.)	Time (h)	I_2 (equiv.)	Yield[b] (%)		Recovery of **1c**[c] (%)
				7a	**4a**	
1	1.2	0.5	2.4	0	84	0
2	0.5	0.5	1.2	64	0	30
3	0.5	2	1.2	50	0	41
4	0.75	0.5	1.5	73	5	12

[a]Reaction was conducted in THF (0.13 M) under the indicated conditions with 0.10 mmol of **1c**. [b]Yield was determined by ^{19}F NMR using C_6F_6 as internal standard. [c]Recovery of **1c** was determined by ^{19}F NMR using C_6F_6 as internal standard.

6. X-ray diffraction analysis

A solution of **3a** in hexane/CH_2Cl_2 was left standing for several weeks during slow evaporation to give colorless crystal.

Figure S1. ORTEP diagram of 1,2,4,5,6,8-hexafluoro-3,7-diiodonaphthalene **3a** (CCDC 2278634) [Thermal ellipsoids are drawn at the 50% probability level.]

Table S5. Crystallographic data of **3a**

Chemical formula	$C_{10}F_6I_2$
Formula weight	487.91
Temperature/K	113
Crystal system	Monoclinic
Space group	$C2_1/c$ (#14)
a/Å	10.2667(9)
b/Å	6.0444(4)
c/Å	8.9912(6)
α/°	90
β/°	94.075(7)
γ/°	90
Volume/Å^3	556.55(7)
Z	2
ρ_{calc} g/cm^3	2.911
μ/mm^{-1}	0.073
F(000)	440.00
Crystal size/mm^3	0.010 × 0.010× 0.010
Radiation	MoKα (λ = 0.71073Å)
θ range for data collection/°	3.89 to 30.34
Index ranges	$-11 \le h \le 13,\ -5 \le k \le 8,\ -11 \le l \le 8$
Reflections collected	3857

Independent reflections	1444 [R_{int} = 0.0392, R_{sigma} = 0.0474]
Data/restraints/parameters	1444/0/82
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0332, wR_2 = 0.0711
Final R indexes [all data]	R_1 = 0.0433, wR_2 = 0.0755
Largest diff. peak/hole / e Å^{-3}	0.93/−0.98

4a was crystallized by sublimation under the vacuo (<1 Torr) using heating-gun to afford thin plate-shaped colorless crystals. The crystal structure of **4a** is highly disordered by layer slippings. FigureS3s are XRD maps of the (h1l) and (h2l) planes drawn using CrysAlis$^{Pro\ S13}$ software. The broad peaks of diffuse scattering are observed at the positions of l=odd in the maps. The diffuse scattering suggested that the periodicity along the *a*-axis is imperfect. The crystal structure of **4a** is considered to consist of the multiple crystal domains shifted by 1/2 in the *c*-axis. (FigureS4). Thus, the crystal structure was analyzed as twin and refined with some strong restraints and constraints.

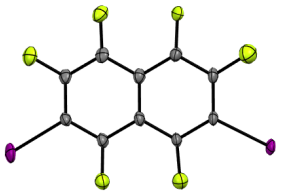


Figure S2. ORTEP diagram of 1,2,4,5,7,8-hexafluoro-3,6-diiodonaphthalene **4a** (CCDC 2278633) [Thermal ellipsoids are drawn at the 50% probability level.]

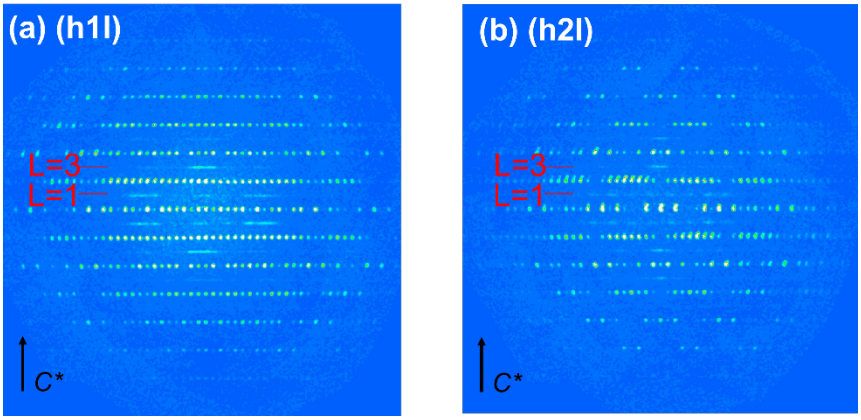


Figure S3(a)(b). A precession-like image of reciprocal space (h1l) plane (a) and (h2l) plane (b) reconstructed with the UNWARP procedure of the CrysAlis^{Pro} software,

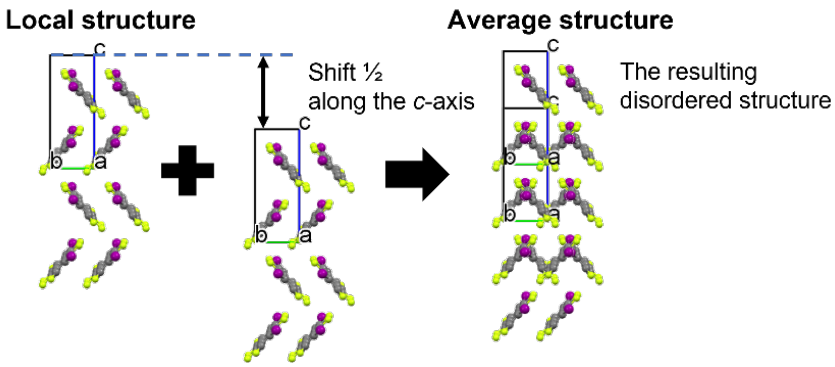


Figure S4 The disordered structure (average structure) model of **4a**, consisted of crystal domains of the local structures shifted by 1/2 along the *c*-axis direction.

Table S6. Crystallographic data of **4a**

Chemical formula	$C_{10}F_6I_2$
Formula weight	487.90
Temperature/K	123
Crystal system	Monoclinic
Space group	*Cc* (#9)
a/Å	43.5510(12)
b/Å	4.4515(19)
c/Å	11.3608(4)
α/°	90
β/°	90.067(3)
γ/°	90
Volume/Å^3	2202.51(14)
Z	8
ρ_{calc} g/cm^3	2.943
μ/mm^{-1}	5.769
F(000)	1760.0
Crystal size/mm^3	0.050 × 0.040× 0.010
Radiation	MoKα (λ = 0.71073 Å)
θ range for data collection/°	2.81 to 28.28
Index ranges	$-58 \le h \le 58,\ -5 \le k \le 5,\ -15 \le l \le 15$
Reflections collected	25044
Independent reflections	5413 [R_{int} = 0.0853, R_{sigma} = 0.0602]

Data/restraints/parameters	5413/1022/554
Goodness-of-fit on F^2	1.167
Final R indexes [$I>=2\sigma\ (I)$]	$R_1 = 0.0956$, $wR_2 = 0.2158$
Final R indexes [all data]	$R_1 = 0.1114$, $wR_2 = 0.2243$
Largest diff. peak/hole / e Å^{-3}	3.12/−2.67

A solution of **1,4-diiodotetrafluorobenzene** in CH_2Cl_2 was left standing for several days during slow evaporation to give colorless crystal.

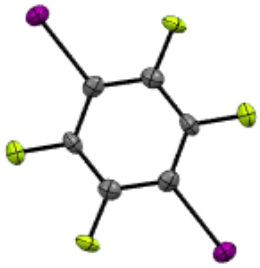


Figure S5. ORTEP diagram of 1,4-diiodotetrafluorobenzene (CCDC 2278632) [Thermal ellipsoids are drawn at the 50% probability level.]

Table S7. Crystallographic data of **1,4-diiodotetrafluorobenzene**

Chemical formula	$C_6F_4I_2$
Formula weight	200.93
Temperature/K	123
Crystal system	Monoclinic
Space group	$P2_1/c$ (#14)
a/Å	7.9881(8)
b/Å	6.0289(4)
c/Å	9.0193(10)
α/°	90
β/°	100.291(9)
γ/°	90
Volume/Å^3	427.38(7)
Z	4
ρ_{calc} g/cm^3	3.123

μ/mm^{-1}	7.363
F(000)	356.0
Crystal size/mm^3	0.200 × 0.086× 0.074
Radiation	MoKα (λ = 0.71073Å)
θ range for data collection/°	2.59 to 25.34
Index ranges	$-8 \le h \le 9,\ -7 \le k \le 5,\ -10 \le l \le 10$
Reflections collected	2554
Independent reflections	769 [R_{int} = 0.0553, R_{sigma} = 0.0461]
Data/restraints/parameters	769/0/55
Goodness-of-fit on F^2	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0327, wR_2 = 0.0818
Final R indexes [all data]	R_1 = 0.0361, wR_2 = 0.0848
Largest diff. peak/hole / e Å^{-3}	0.92/−0.79

7. Calculation of crystal data.

The calculation of crystal data was performed at CE-B3LYP/6-311G(d,p) level using CrystalExplorer 21.5.[S14]

Operation details are as follows:

1) Open the CIF file using CrystalExplorer 21.5.

2) Calculate the wave function of the central molecule at CE-B3LYP/6-311G(d,p) level.

3) Generate a cluster model consisting of molecules within 3.8 Å of the central molecule.

4) Calculate interaction energies with the central molecule at CE-B3LYP/6-311G(d,p) level.

CE-B3LYP was employed for all crystal data calculations using Crystal Explorer21.5, which included energy decomposition analysis. HF was not utilized in the current calculation. Spackman P. R. and co-workers reported that CE-B3LYP is suitable in terms of accuracy, comparable to B3LYP-D2.[S14]

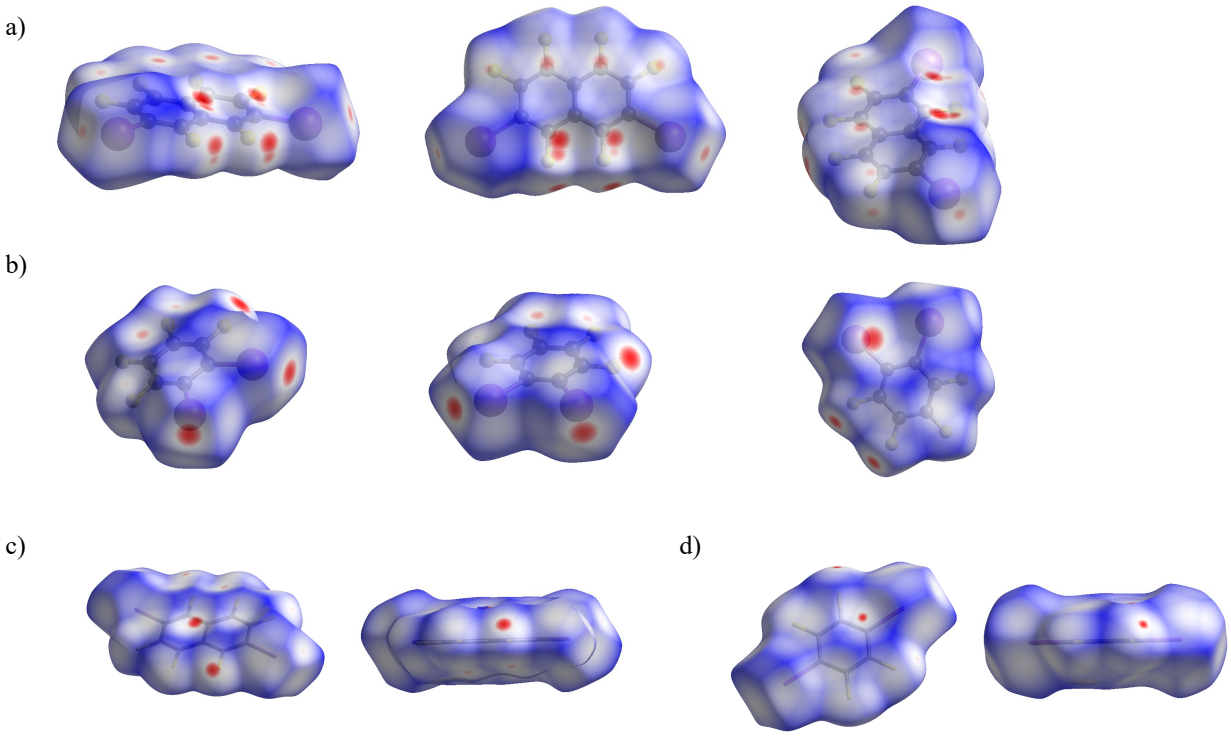
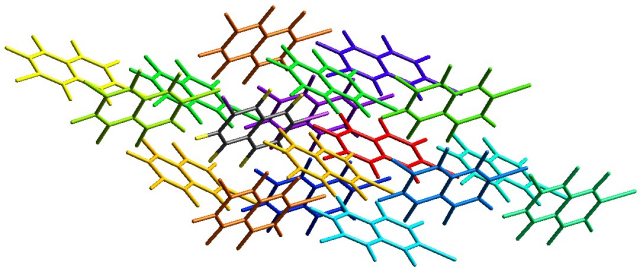
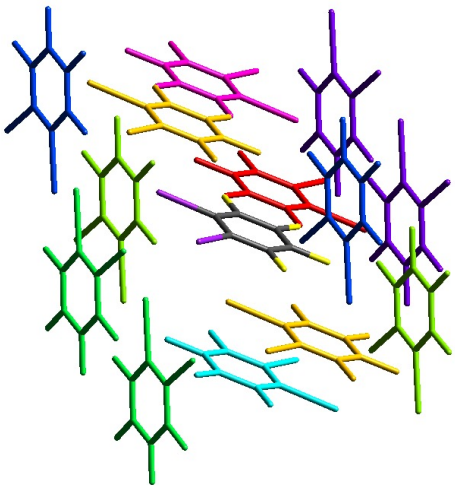


Figure S6. Hirshfeld surfaces mapped on d_{norm}. a) 3,6-I_2F_6Naphthalene (**4a**): color scale: –0.167 a.u.(red) to 1.0178 a.u. (blue). b)1,2-TFIB: color scale: –0.1253 a.u. (red) to 0.8530 a.u. (blue). c) 3,7-I_2F_6Naphthalene (**3a**): color scale: –0.0845 a.u.(red) to 0.8962 a.u. (blue). d) 1,4-TFIB: color scale: –0.0262 a.u. (red) to 0.9311 a.u. (blue)



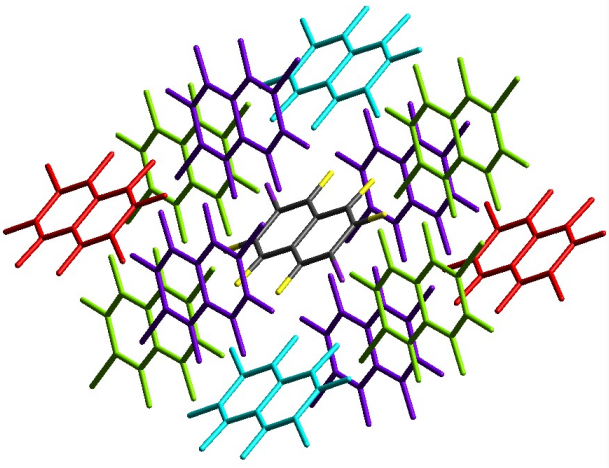
N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
1	-	11.34	B3LYP/6-311G(d,p)	-7.4	-0.3	-11.0	17.3	-1.4
2	x, y, z	4.45	B3LYP/6-311G(d,p)	-20.1	-2.1	-68.8	61.6	-29.4
2	x, -y, z+1/2	6.57	B3LYP/6-311G(d,p)	-6.2	-0.7	-26.5	18.9	-14.5
1	-	11.27	B3LYP/6-311G(d,p)	-11.4	-0.5	-11.6	24.4	0.9
1	-	11.21	B3LYP/6-311G(d,p)	-12.0	-0.5	-11.5	29.2	5.2
1	-	11.49	B3LYP/6-311G(d,p)	-7.5	-0.5	-10.7	14.4	-4.3
2	x, -y, z+1/2	5.79	B3LYP/6-311G(d,p)	-6.8	-0.7	-30.7	17.7	-20.5
1	x+1/2, y+1/2, z	21.89	B3LYP/6-311G(d,p)	0.1	-0.0	-0.0	0.0	0.1
1	x+1/2, -y+1/2, z+1/2	22.54	B3LYP/6-311G(d,p)	0.0	-0.0	-0.0	0.0	0
1	-	12.55	B3LYP/6-311G(d,p)	0.4	-0.0	-1.1	0.0	-0.7
1	-	11.52	B3LYP/6-311G(d,p)	-2.4	-0.0	-6.2	6.7	-1.9
1	-	14.06	B3LYP/6-311G(d,p)	-0.0	-0.0	-0.3	0.0	-0.3
1	-	11.81	B3LYP/6-311G(d,p)	-3.3	-0.1	-6.2	6.2	-3.4
1	-	14.03	B3LYP/6-311G(d,p)	0.2	-0.0	-0.3	0.0	-0.1
0	x, y, z	4.45	B3LYP/6-311G(d,p)	-18.4	-2.0	-67.1	57.2	-30.3
0	x, -y, z+1/2	5.82	B3LYP/6-311G(d,p)	-6.7	-0.7	-29.6	16.6	-20.4
0	x, -y, z+1/2	6.50	B3LYP/6-311G(d,p)	-6.6	-0.8	-27.8	21.3	-13.9

Figure S7. Intermolecular interaction and lattice energy for 3,6-I_2F_6Naphthalene.



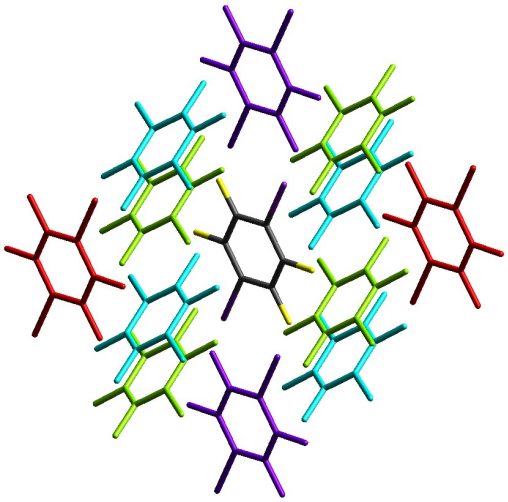
N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
1	-x, -y, -z	9.52	B3LYP/6-311G(d,p)	0.6	-0.1	-7.5	3.4	-3.6
2	x, y, z	5.77	B3LYP/6-311G(d,p)	-11.6	-0.5	-28.4	26.5	-14.0
2	x+1/2, -y+1/2, z+1/2	8.23	B3LYP/6-311G(d,p)	-1.1	-0.2	-9.7	5.7	-5.3
2	-x+1/2, y+1/2, -z+1/2	5.10	B3LYP/6-311G(d,p)	-22.6	-0.8	-27.4	51.8	1.0
1	-x, -y, -z	7.98	B3LYP/6-311G(d,p)	-2.2	-0.2	-8.9	6.8	-5.3
2	x+1/2, -y+1/2, z+1/2	7.66	B3LYP/6-311G(d,p)	-8.7	-0.5	-12.2	18.0	-3.4
2	-x+1/2, y+1/2, -z+1/2	7.21	B3LYP/6-311G(d,p)	-3.7	-0.4	-17.6	9.8	-11.9
1	-x, -y, -z	6.96	B3LYP/6-311G(d,p)	-6.9	-0.3	-20.2	13.8	-13.6

Figure S8. Intermolecular interaction and lattice energy for 1,2-TFIB



N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
2	x, y, z	10.27	B3LYP/6-311G(d,p)	-3.0	-0.2	-10.4	8.6	-5.0
4	-x, y+1/2, -z+1/2	11.32	B3LYP/6-311G(d,p)	-9.5	-0.6	-11.7	20.1	-1.7
2	x, y, z	6.04	B3LYP/6-311G(d,p)	-14.8	-1.0	-38.6	27.9	-26.5
4	-x, y+1/2, -z+1/2	5.42	B3LYP/6-311G(d,p)	-13.2	-1.0	-37.7	30.4	-21.5

Figure S9. Intermolecular interaction and lattice energy for 3,7-I_2F_6Naphthalene (**3a**)



	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	7.99	B3LYP/6-311G(d,p)	-2.5	-0.2	-10.0	8.3	-4.4
	4	-x, y+1/2, -z+1/2	8.96	B3LYP/6-311G(d,p)	-9.1	-0.6	-11.7	19.2	-2.2
	4	-x, y+1/2, -z+1/2	5.42	B3LYP/6-311G(d,p)	-10.1	-0.5	-26.1	23.1	-13.6
	2	x, y, z	6.03	B3LYP/6-311G(d,p)	-9.8	-0.4	-25.6	20.8	-15.0

Figure S10. Intermolecular interaction and lattice energy for 1,4-TFIB

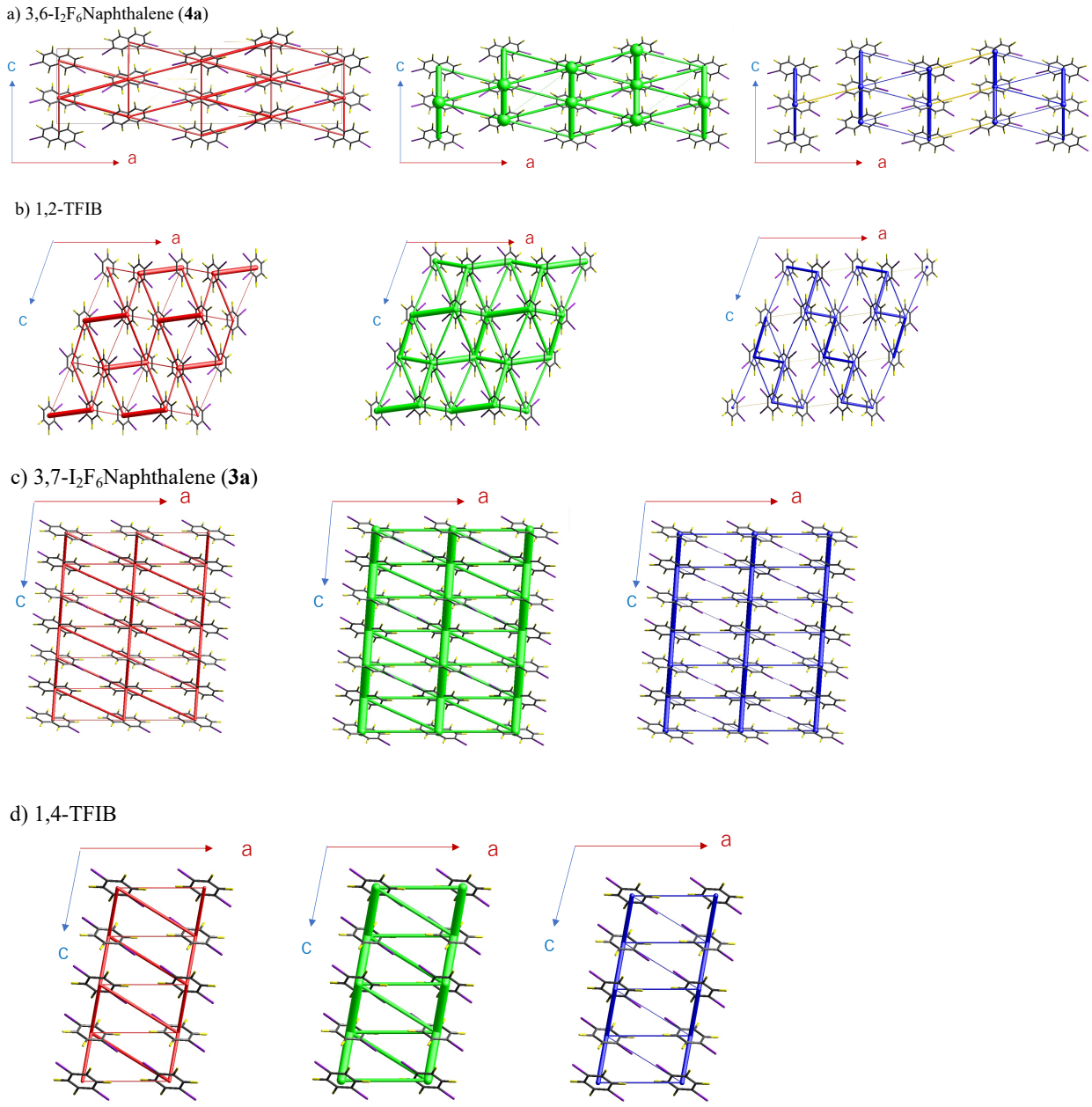


Figure S11. Energy framework diagrams views along with *c* axis. Same scale was used for all graphs. For energy framework tube size is 160. Red: electrostatic energy (E_{ele}). Green: Dispersion energy (E_{dis}). Blue: total energy (E_{tot}). a) 3,6-I_2F_6Naphthalene (**4a**). b)1,2-TFIB. c) 3,7-I_2F_6Naphthalene. d) 1,4-TFIB.

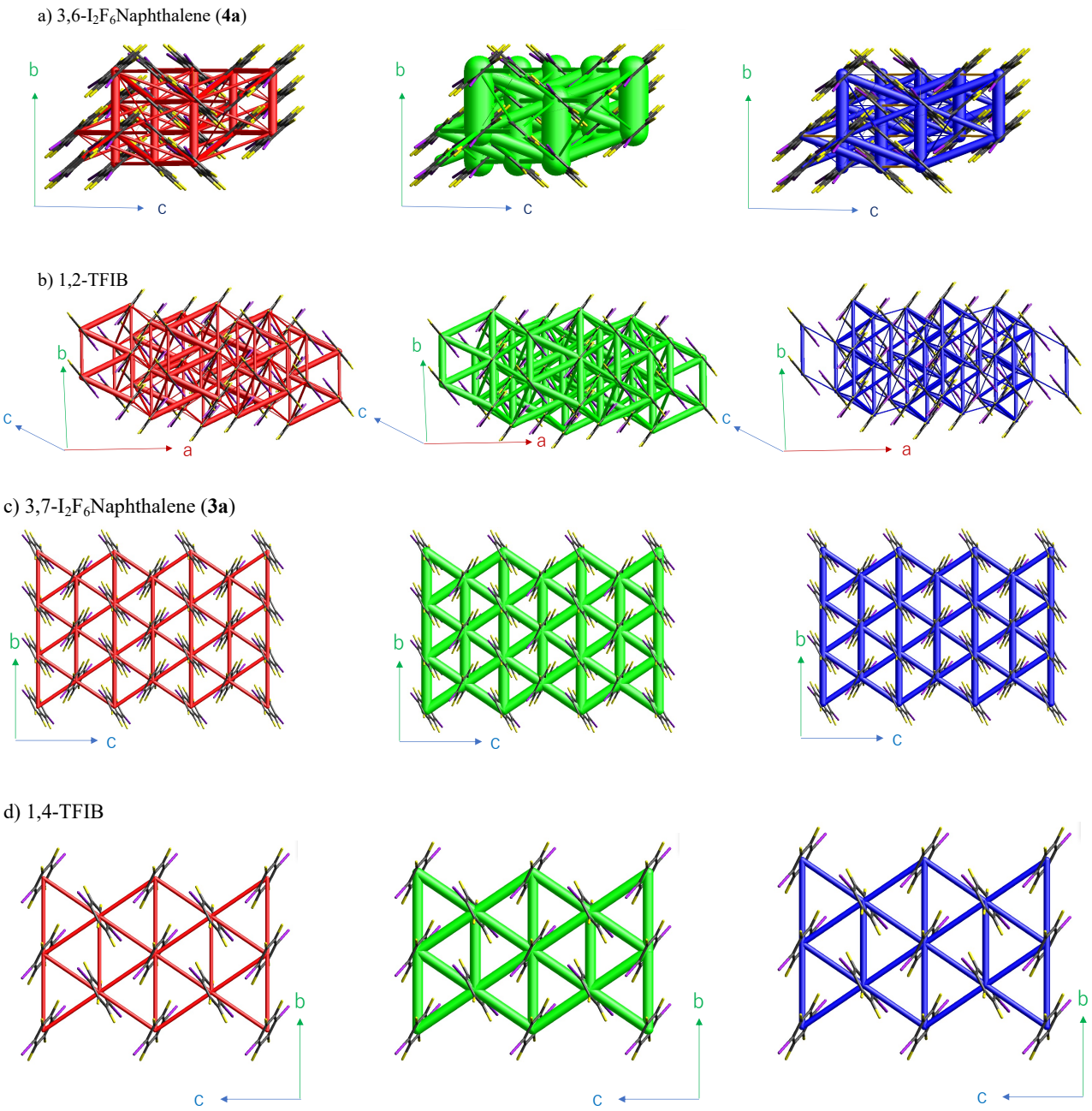


Figure S12. Energy framework diagrams viewed along with *b* axis. Same scale was used for all graphs. For energy framework tube size is 160. Red: electrostatic energy (*E*_ele). Green: Dispersion energy (*E*_dis). Blue: total energy (*E*_tot). a) 3,6-I_2F_6Naphthalene (**4a**). b)1,2-TFIB

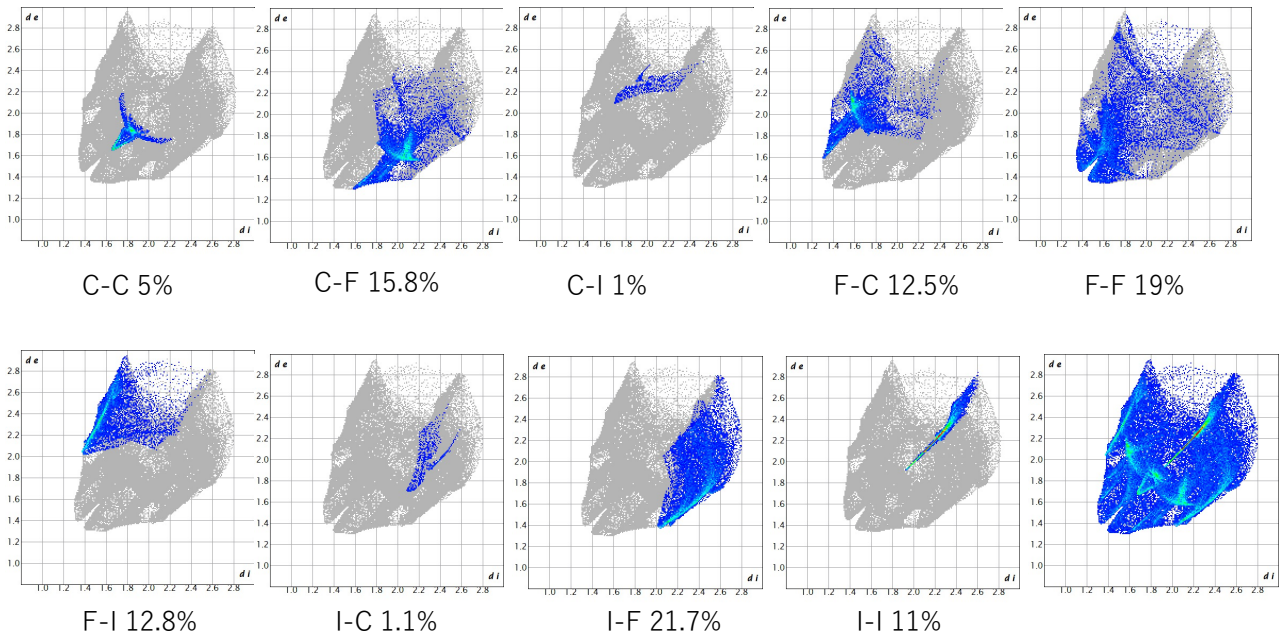


Figure S13. 2-D fingerprint plot for 3,6-I_2F_6Naphthalene(**4a**) and individual contributions (inside atom–outside atom xx%).

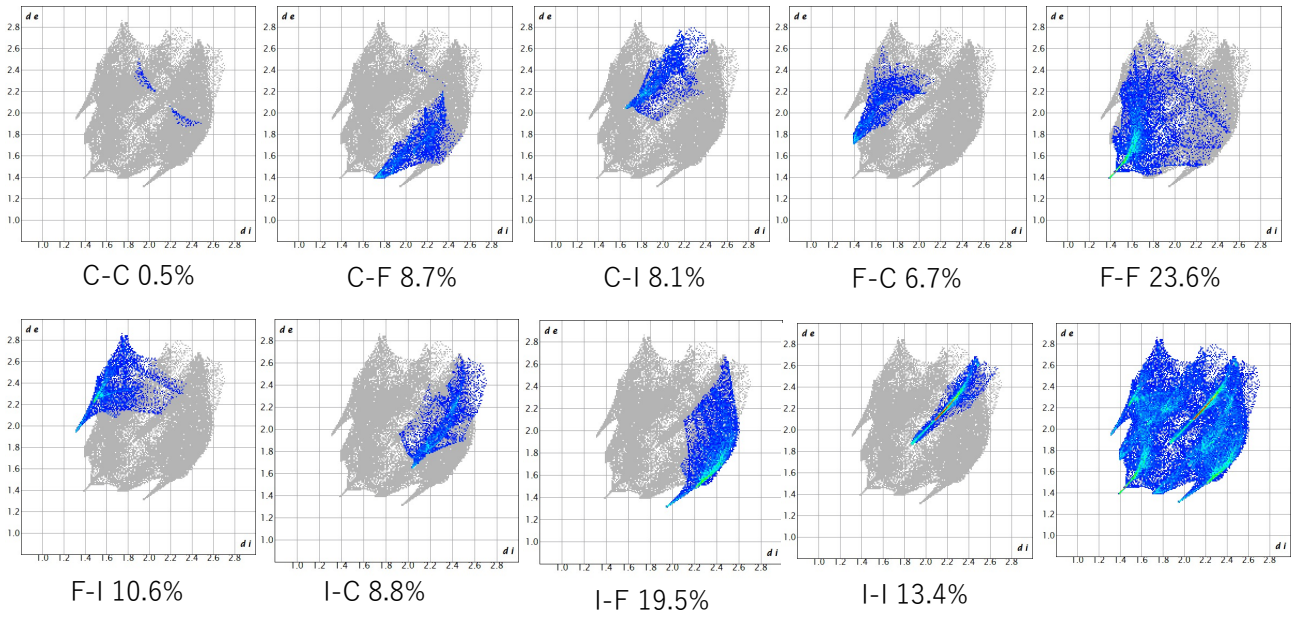


Figure S14. 2-D fingerprint plot for 1,2-TFIB and individual contributions (inside atom–outside atom xx%)

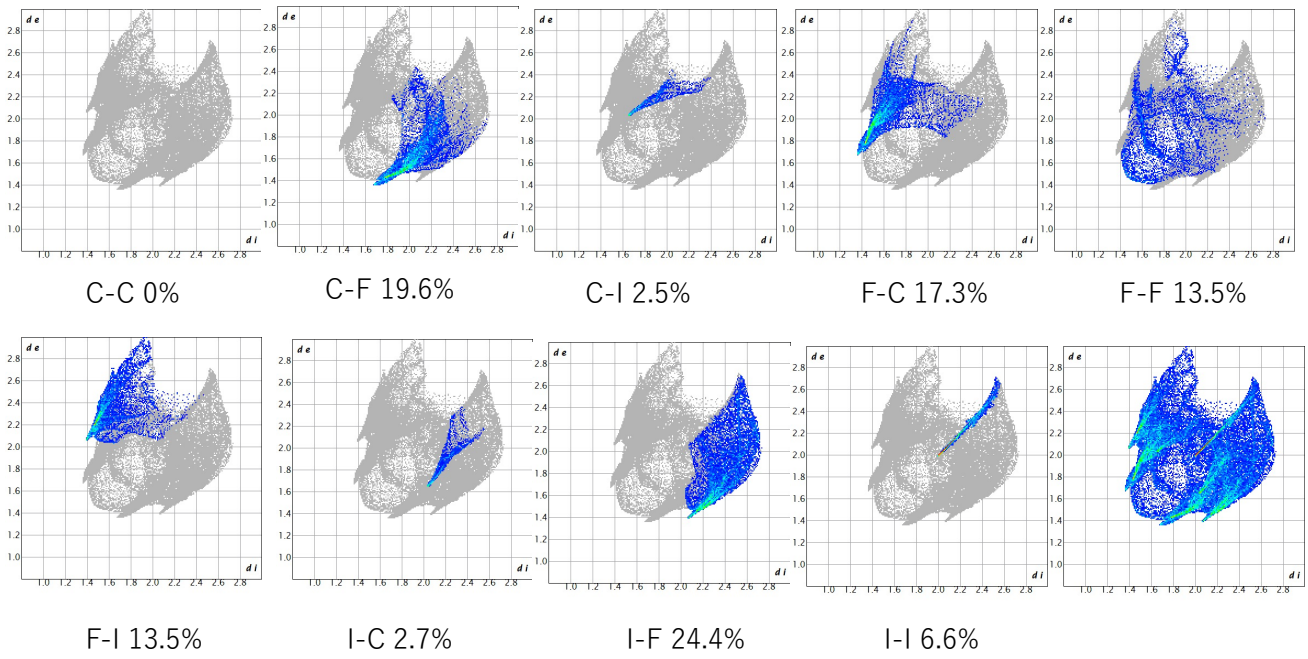


Figure S15. 2-D fingerprint plot for 3,7-I_2F_6Naphthalene and individual contributions (inside atom–outside atom xx%)

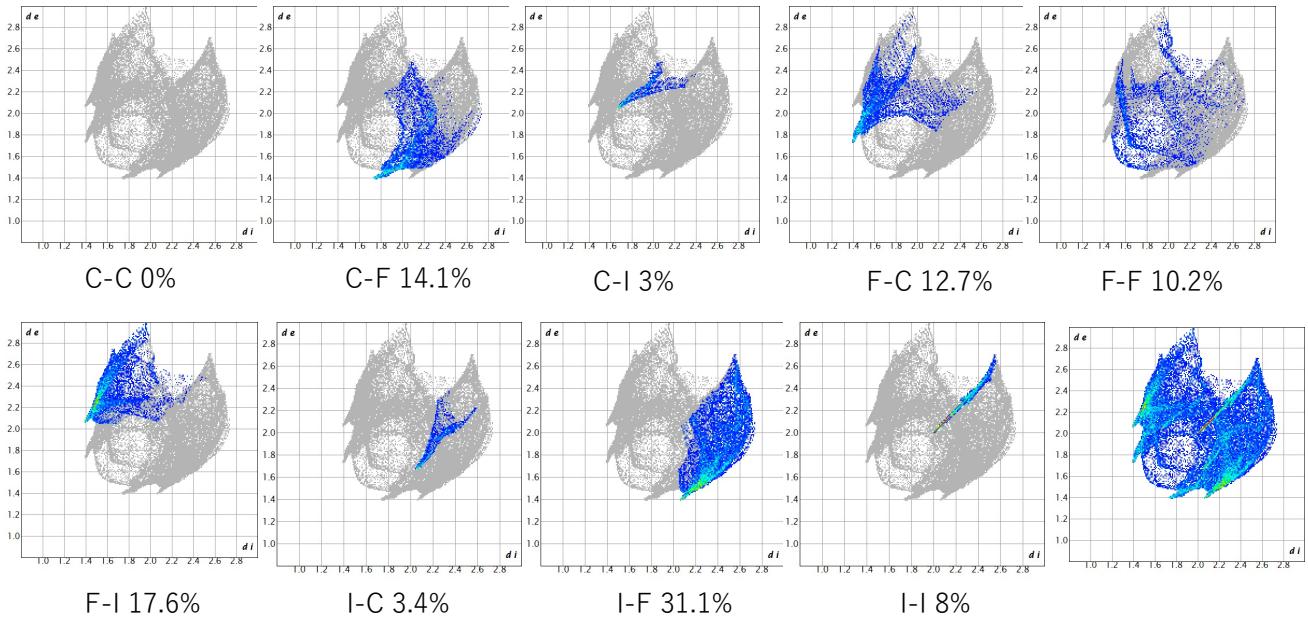


Figure S16. 2-D fingerprint plot for 1,4-TFIB and individual contributions (inside atom–outside atom xx%)

8. DFT calculation

Computational Analysis.

All molecular geometries were optimized by the M06-2X functional with Grimme's D3 dispersion correction[S15] using the SDD basis set (iodine) and 6-311+G(d,p) for all other atoms. The SMD18 solvation model[S16,S17] was used with THF as the solvent. The stationary geometries were checked by the vibration analyses after the geometry optimization procedures. The stationary geometries and their energies were refined using Gaussian 16 software package.[S18]

Computational Details.

The table shows total energy *E*, enthalpy *H*, and Gibbs free energy *G* (hartree) at the SMD18(THF)/M06-2X-D3/6-311+G(d,p)-SDD level.

Table S00.

compound	*E*	*H*	*G*
3a	-1002.7545816	-1002.659778	-1002.722157
4a	-1002.7546768	-1002.659938	-1002.722854
1,4-TFIB	-650.6662727	-650.606631	-650.658938
1,2-TFIB	-650.6599711	-650.600539	-650.652780

10. References

[S1] CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation. (2015). Tokyo 196-8666, Japan.

[S2] SHELXT Version 2014/5: Sheldrick, M. G.; *Acta Cryst*. **2014**, *A70,* C1437.

[S3] CrystalStructure 4.3: Crystal Structure Analysis Package, Rigaku Corporation (2000-2018). Tokyo 196-8666, Japan.

[S4] SHELXL Version 2014/7: Sheldrick, M. G.; *Acta Cryst*. **2008**, *A64,* 112−122**.**

[S5] Schoch, T. D.; Mondal, M.; Weaver, J. D. *Org. Lett.* **2021**, *23*, 1588–1593.

[S6] Kiel, G. R.; Bergman, H. M.; Tilley, T. D. *Chem. Sci.* **2020**, *11*, 3028–3035.

[S7] Storch, J.; Bernard, M.; Sýkora, J.; Karban, J.; Čermák, J *Eur. J. Org. Chem.* **2013**, *2013*, 260–263.

[S8] Morrison, D. J.; Riegel, S. D.; Piers, W. E.; Parveza, M.; McDonald R. *Chem. Commun*. **2006**, 2875–2877.

[S9] Eaton, P. E.; Lee, C. H.; Xiong, Y. *J. Am. Chem. Soc.* **1989**, *111*, 8016–8018.

[S10] Momiyama, N.; Okamoto, H.; Shimizu, M.; Terada. M. *Chirality* **2015**, *27*, 464–475.

[S11] Clososki, G. C.; Rohbogner, C. J.; Knochel, P. *Angew. Chem. Int. Ed.* **2007**, *46*, 7681–7684.

[S12] Mosrin, M.; Knochel, P. *Org. Lett.* **2008**, *10*, 2497–2500

[S13] Agilent (2014).*CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, Oxfordshire, England.

[S14] Spackman, P. R.; Turner, M. J.; McKinnon, J. J.; Wolff, S. K.; Grimwood, D. J.; Jayatilaka, D.; Spackman, M. *J. Appl. Cryst.* **2021**, *54*, 1006–1011.

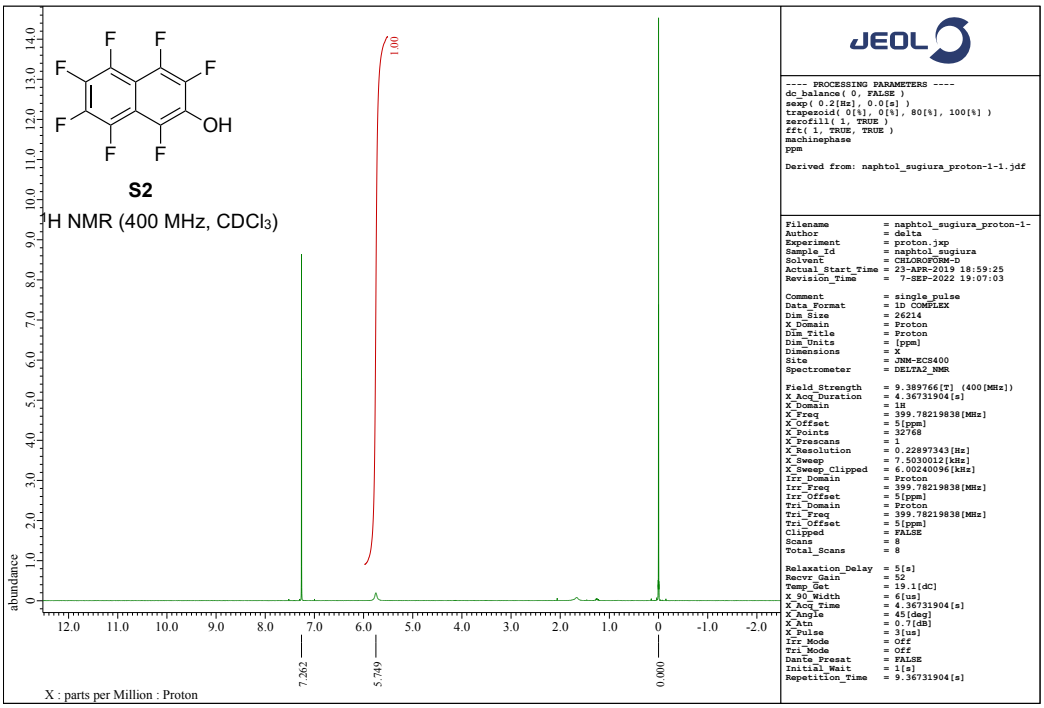
[S15] Grimme, S.; Antony, J.; Ehrlich S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.

[S16] Engelage, E.; Schulz, N.; Heinen, F.; Huber, S. M.; Truhlar, D. G.; Cramer, C. J. *Chem. Eur. J.* **2018**, 24, 15983–15987.

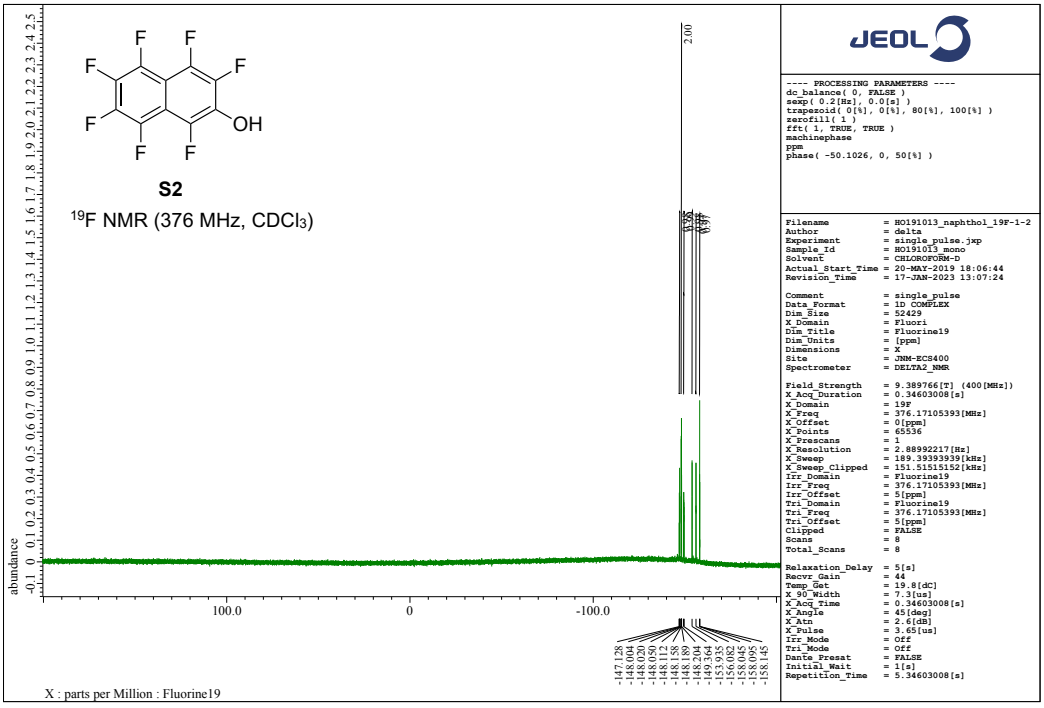
[S17] Heinen, F.; Engelage, E.; Cramer, C. J.; Huber, S. M. *J. Am. Chem. Soc*. **2020**, *142*, 8633–8640.

[S18] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J.V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo,

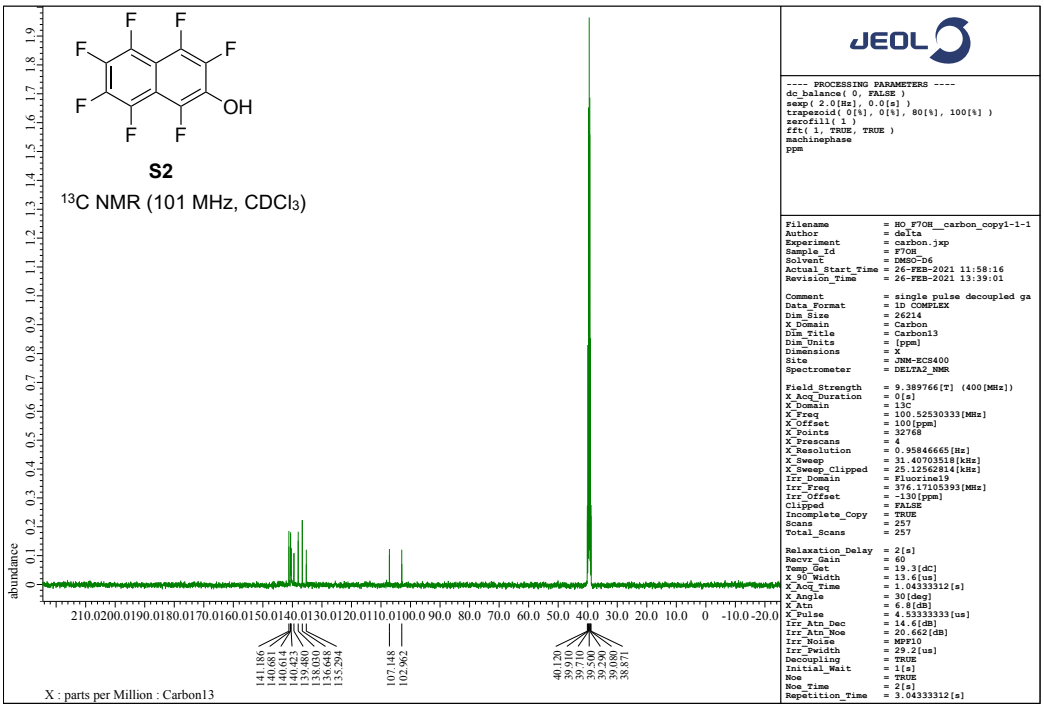
R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

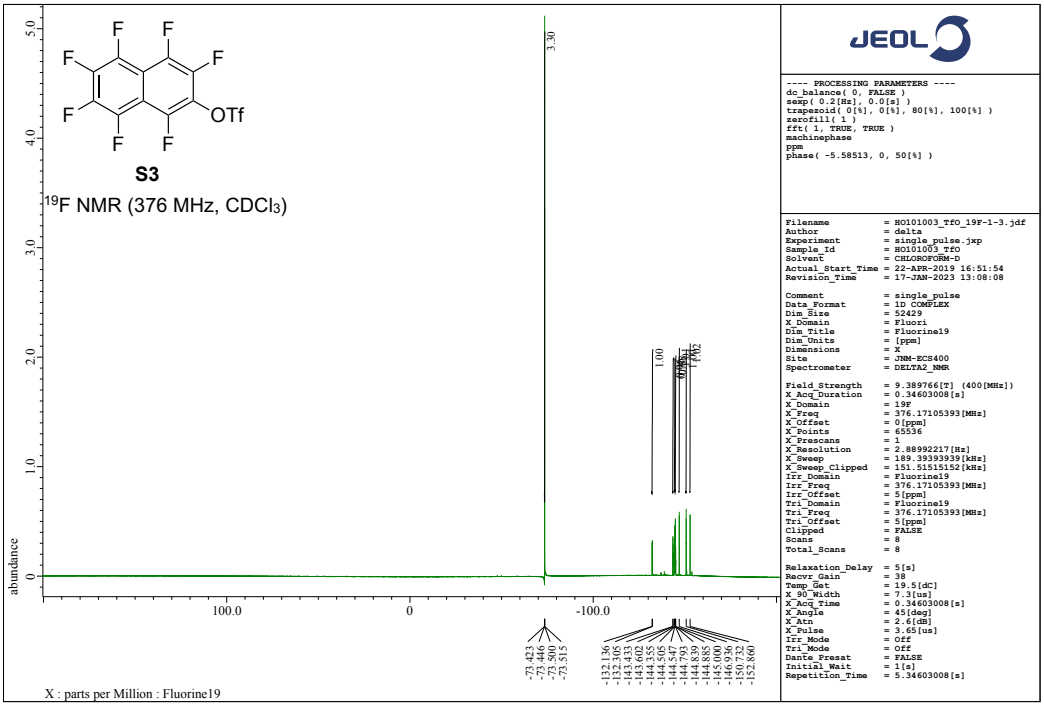


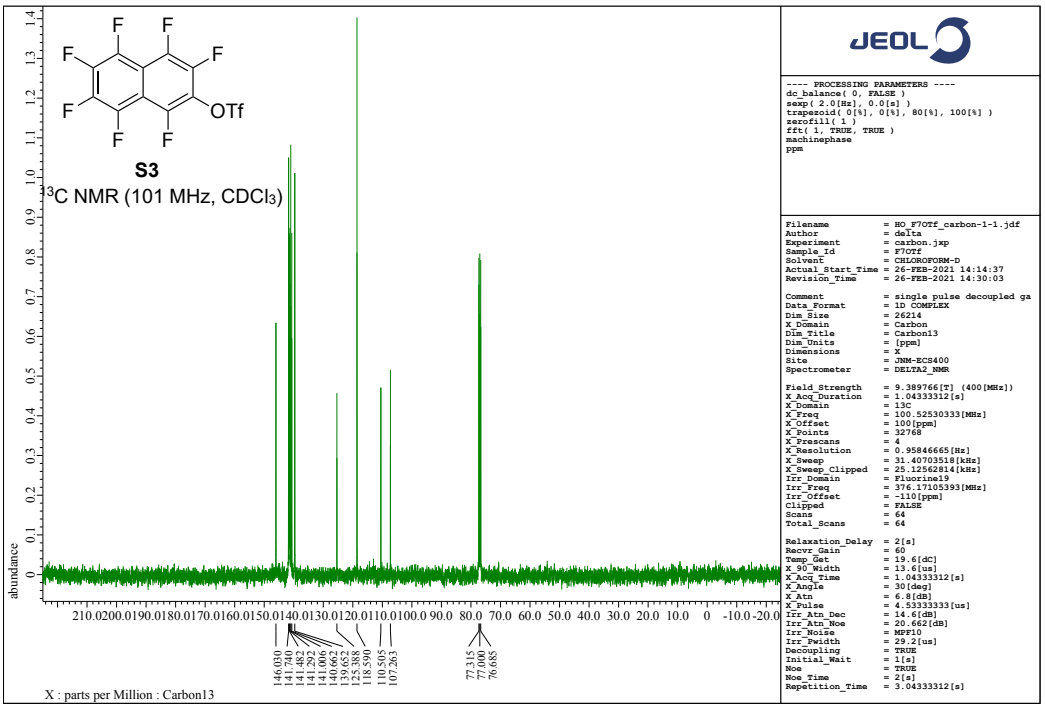

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: naphtol_sugiura_proton-1-1.jdf

Filename            = naphtol_sugiura_proton-1-
Author              = delta
Experiment          = proton.jxp
Sample_Id           = naphtol_sugiura
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 23-APR-2019 18:59:25
Revision_Time       =  7-SEP-2022 19:07:03

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 4.36731904[s]
X_Domain            = 1H
X_Freq              = 399.78219838[MHz]
X_Offset            = 5[ppm]
X_Points            = 32768
X_Prescans          = 1
X_Resolution        = 0.22897343[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          = 52
Temp_Get            = 19.1[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 4.36731904[s]
X_Angle             = 45[deg]
X_Atn               = 0.7[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 9.36731904[s]
```

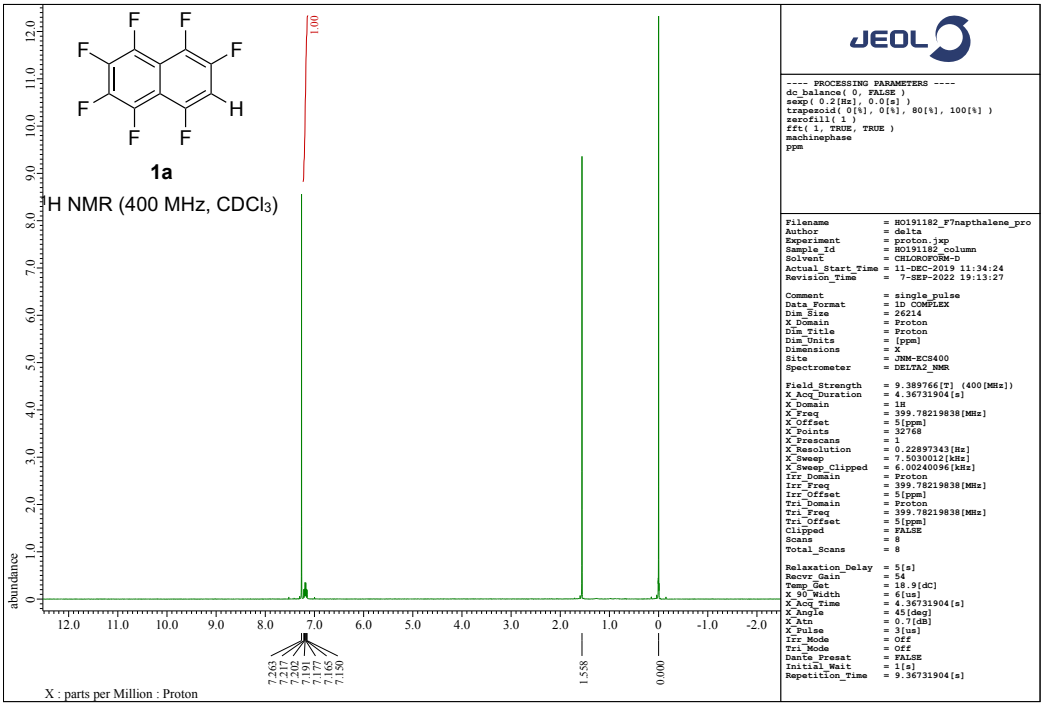


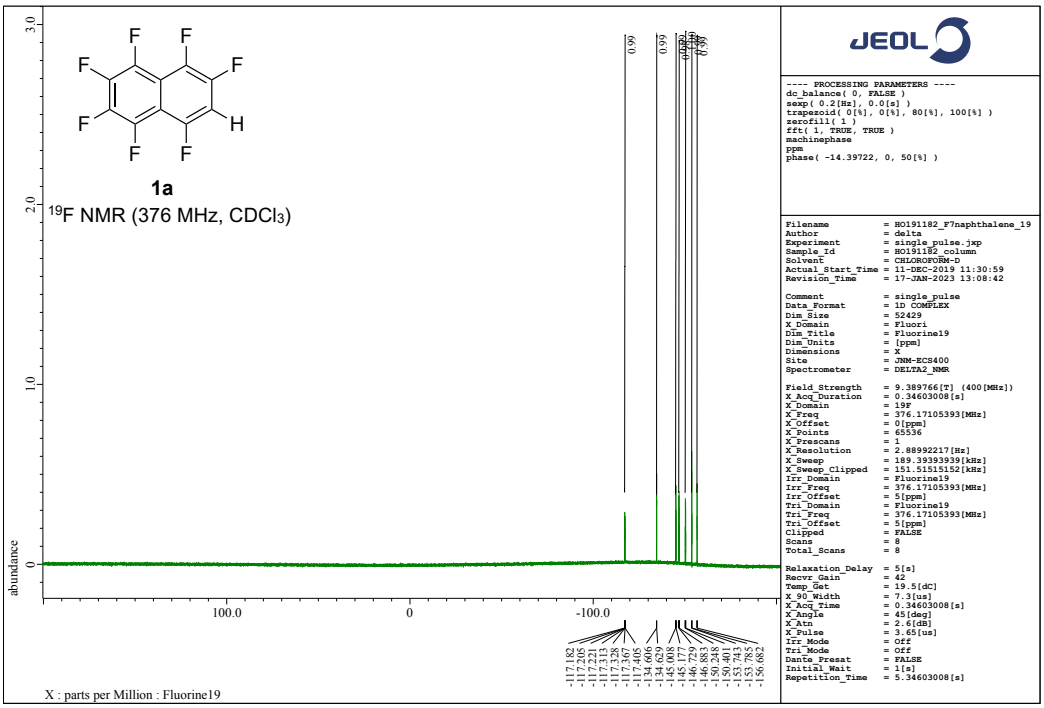

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -50.1026, 0, 50[%] )

Filename            = H0191013_naphthol_19F-1-2
Author              = delta
Experiment          = single_pulse.jxp
Sample_Id           = H0191013_mono
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 20-MAY-2019 18:06:44
Revision_Time       = 17-JAN-2023 13:07:24

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 52429
X_Domain            = Fluori
Dim_Title           = Fluorine19
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 0.34603008[s]
X_Domain            = 19F
X_Freq              = 376.17105393[MHz]
X_Offset            = 0[ppm]
X_Points            = 65536
X_Prescans          = 1
X_Resolution        = 2.88992217[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          = 44
Temp_Get            = 19.8[dC]
X_90_Width          = 7.3[us]
X_Acq_Time          = 0.34603008[s]
X_Angle             = 45[deg]
X_Atn               = 2.6[dB]
X_Pulse             = 3.65[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 5.34603008[s]
```

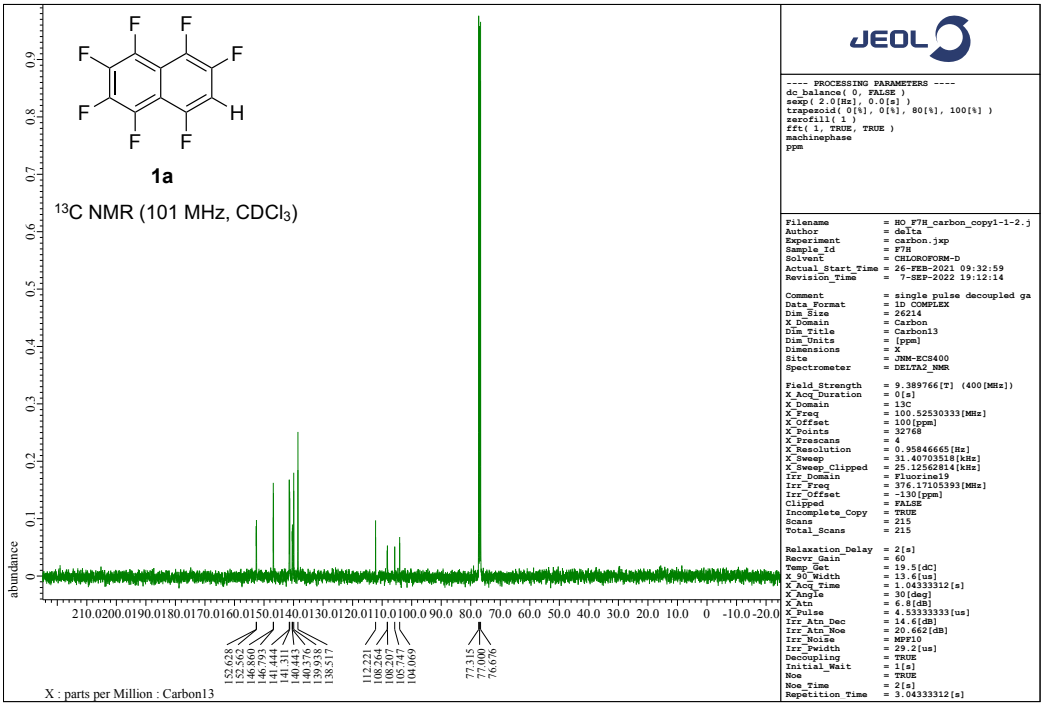

S2
13C NMR (101 MHz, CDCl3)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO_F7OH__carbon_copy1-1-1
Author = delta
Experiment = carbon.jxp
Sample_Id = F7OH
Solvent = DMSO-D6
Actual_Start_Time = 26-FEB-2021 11:58:16
Revision_Time = 26-FEB-2021 13:39:01
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 257
Total_Scans = 257
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.3[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
DecCoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

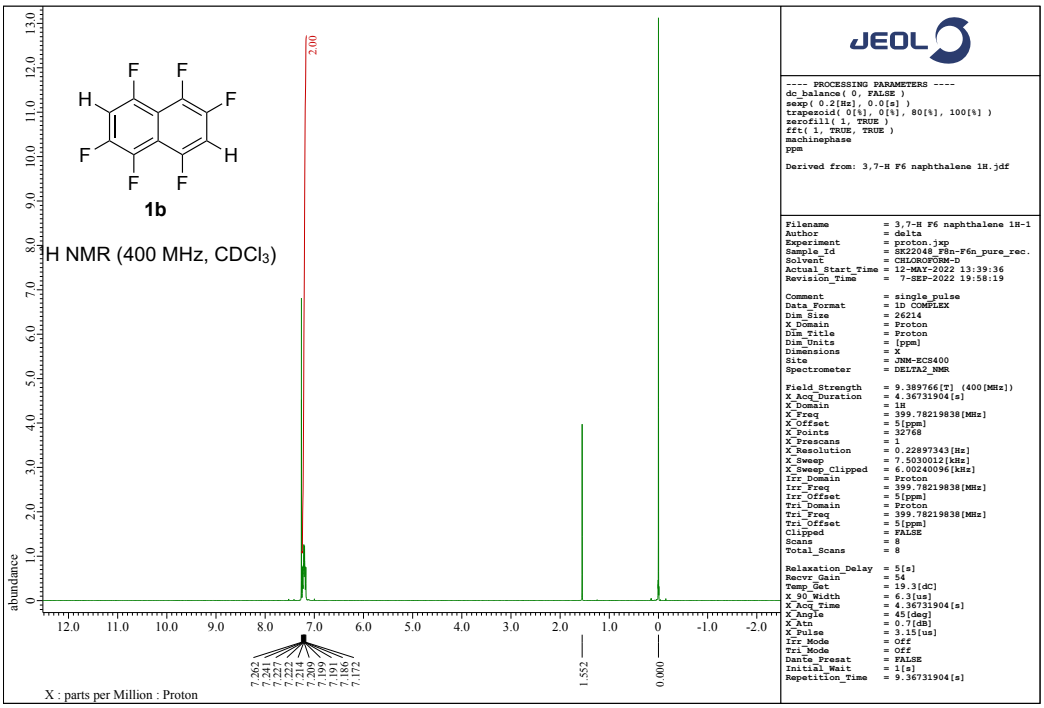

S3
19F NMR (376 MHz, CDCl3)
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-5.58513, 0, 50[%])
Filename = HO101003_TfO_19F-1-3.jdf
Author = delta
Experiment = single_pulse.jxp
Sample_Id = HO101003_TfO
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-APR-2019 16:51:54
Revision_Time = 17-JAN-2023 13:08:08
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 38
Temp_Get = 19.5[dC]
X_90_Width = 7.3[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 3.65[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

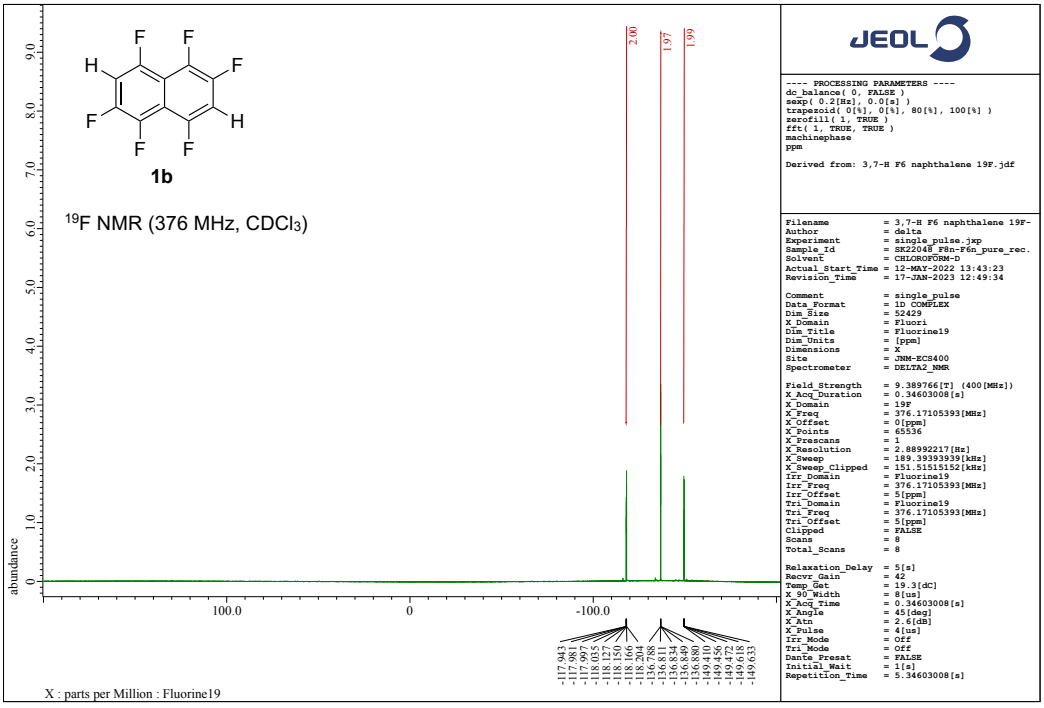

S3
^{13}C NMR (101 MHz, CDCl$_3$)
OTf
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO_F7OTf_carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = F7OTf
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-FEB-2021 14:14:37
Revision_Time = 26-FEB-2021 14:30:03
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -110[ppm]
Clipped = FALSE
Scans = 64
Total_Scans = 64
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.6[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

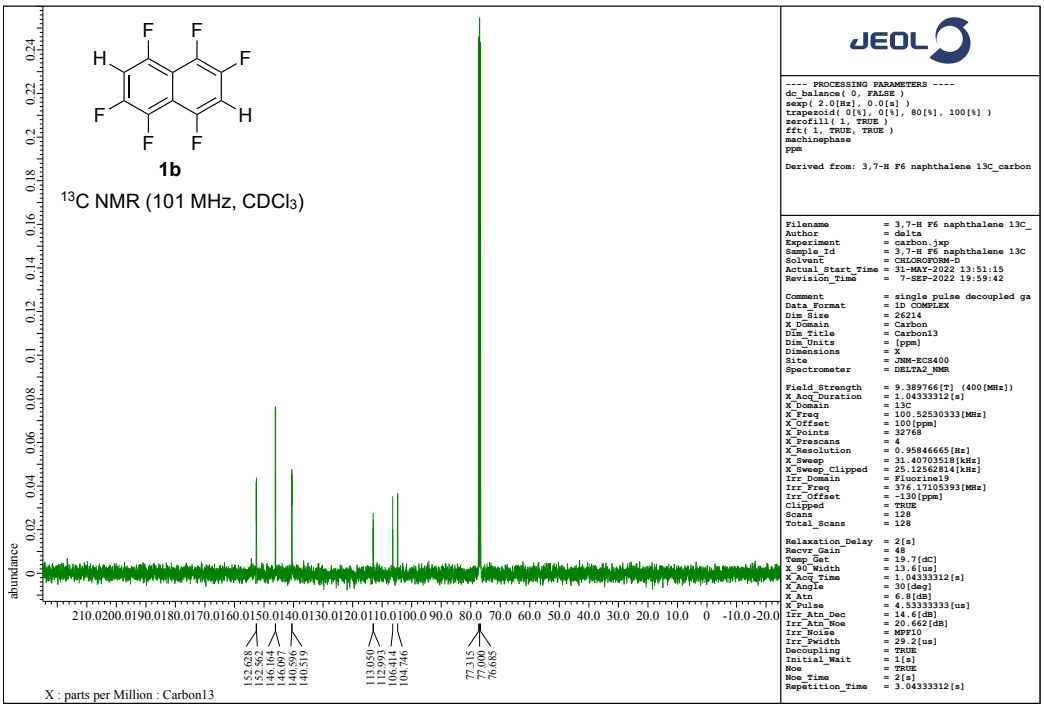

1a
^{1}H NMR (400 MHz, CDCl$_3$)
1.00
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO191182_F7napthalene_pro
Author = delta
Experiment = proton.jxp
Sample_Id = HO191182_column
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-DEC-2019 11:34:24
Revision_Time = 7-SEP-2022 19:13:27
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 54
Temp_Get = 18.9[dC]
X_90_Width = 6[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

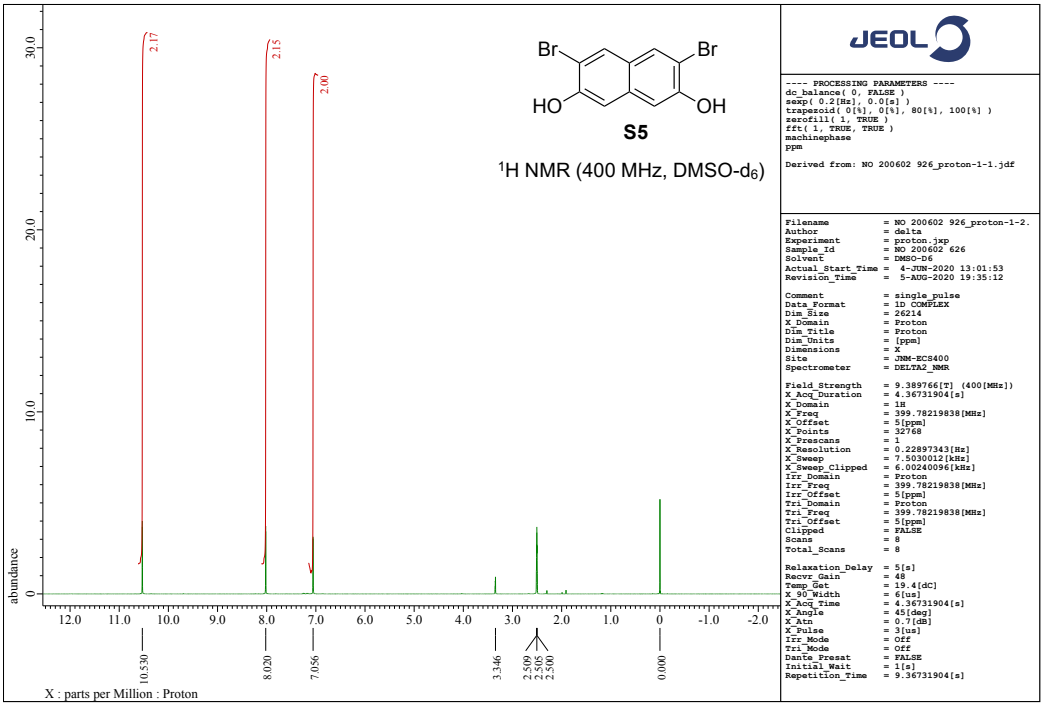

1a
19F NMR (376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-14.39722, 0, 50[%])
Filename = HO191182_F7naphthalene_19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = HO191182_column
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-DEC-2019 11:30:59
Revision_Time = 17-JAN-2023 13:08:42
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.5[dC]
X_90_Width = 7.3[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 3.65[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

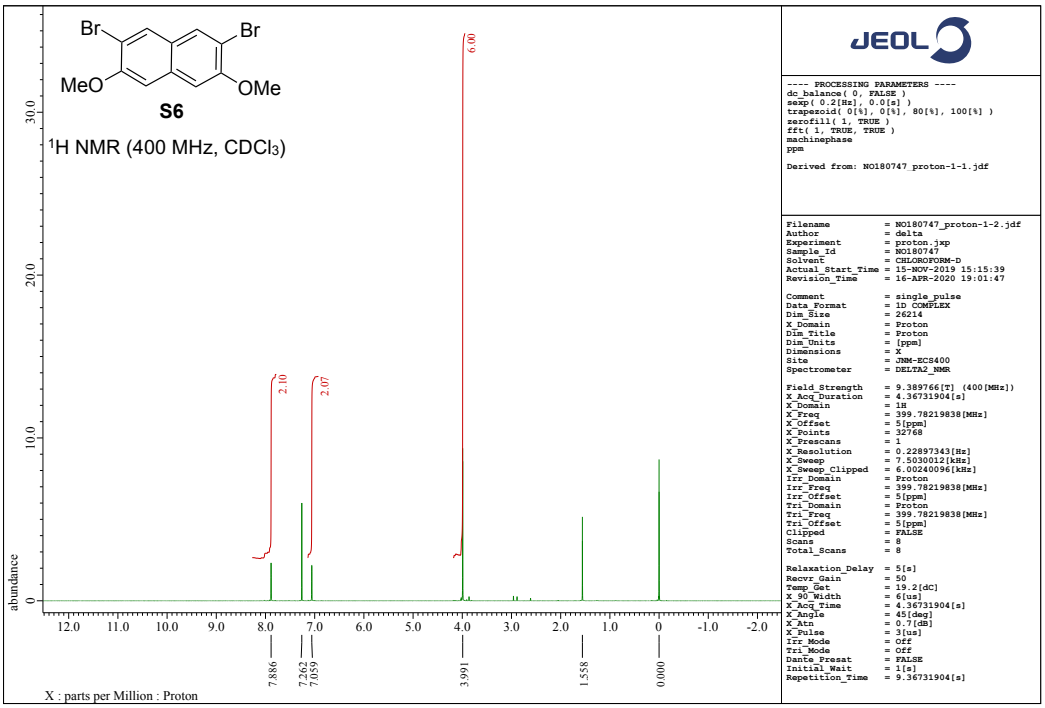

1a
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO_F7H_carbon_copy1-1-2.j
Author = delta
Experiment = carbon.jxp
Sample_Id = F7H
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-FEB-2021 09:32:59
Revision_Time = 7-SEP-2022 19:12:14
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 215
Total_Scans = 215
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.5[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_NoiSe = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

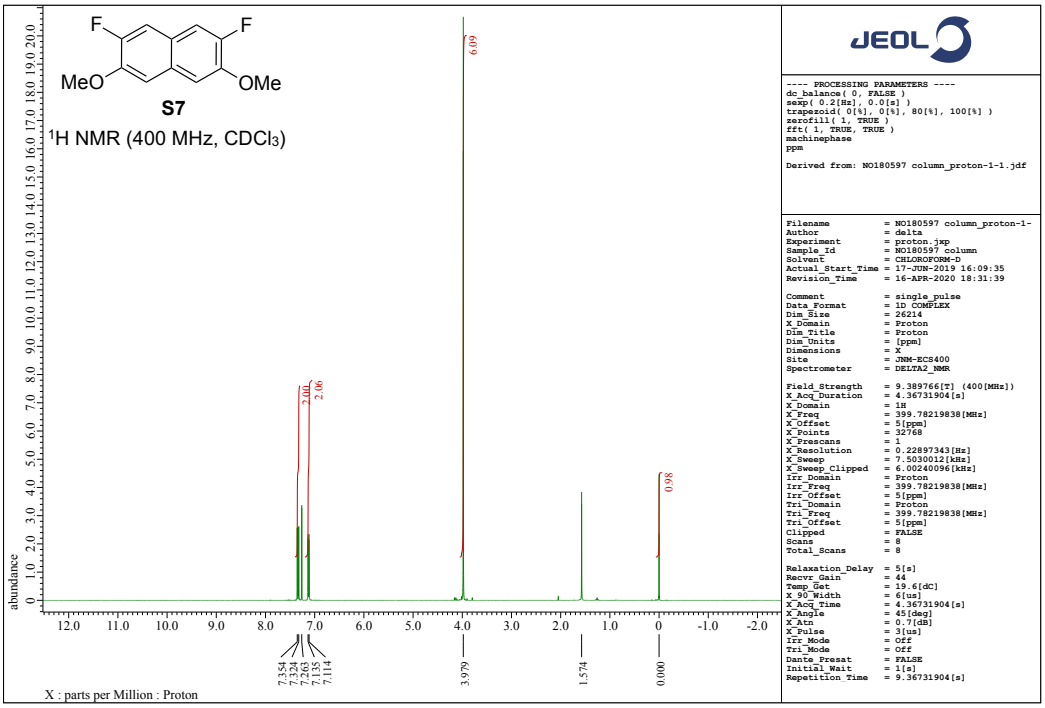

1b
^{1}H NMR (400 MHz, CDCl$_3$)
2.00
abundance
X : parts per Million : Proton
7.262
7.241
7.227
7.222
7.214
7.209
7.199
7.191
7.186
7.172
1.552
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-H F6 naphthalene 1H.jdf
Filename = 3,7-H F6 naphthalene 1H-1
Author = delta
Experiment = proton.jxp
Sample_Id = SK22048 F8n-F6n_pure_rec.
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-MAY-2022 13:39:36
Revision_Time = 7-SEP-2022 19:58:19
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 54
Temp_Get = 19.3[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

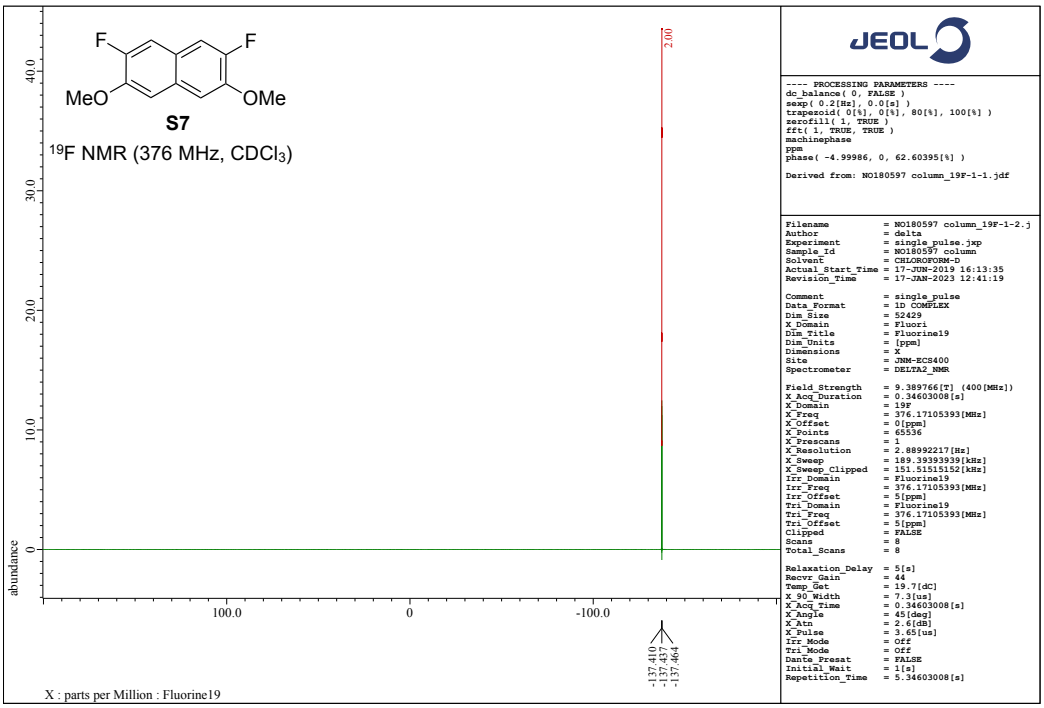

1b
^{19}F NMR (376 MHz, CDCl$_3$)
2.00
1.97
1.99
abundance
X : parts per Million : Fluorine19
-117.943
-117.981
-117.997
-118.055
-118.127
-118.150
-118.166
-118.204
-136.788
-136.811
-136.834
-136.849
-136.880
-149.410
-149.456
-149.472
-149.618
-149.633
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-H F6 naphthalene 19F.jdf
Filename = 3,7-H F6 naphthalene 19F-
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SK22048 F8n-F6n_pure_rec.
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-MAY-2022 13:43:23
Revision_Time = 17-JAN-2023 12:49:34
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.3[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

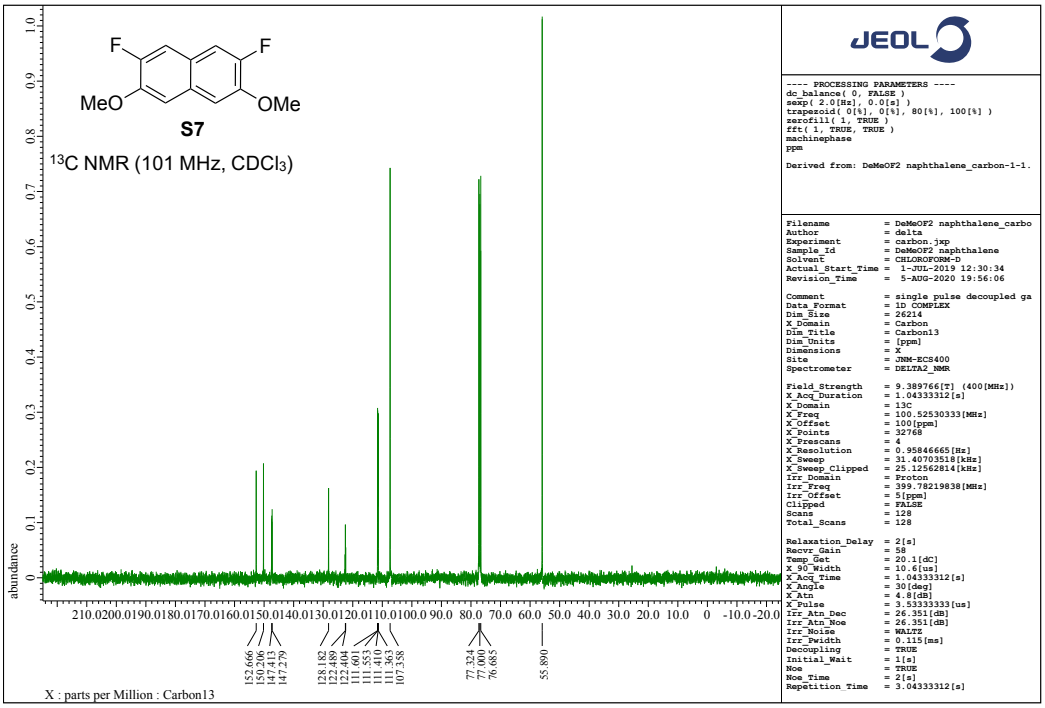

1b
13C NMR (101 MHz, CDCl3)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-H F6 naphthalene 13C_carbon
Filename = 3,7-H F6 naphthalene 13C_
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-H F6 naphthalene 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-MAY-2022 13:51:15
Revision_Time = 7-SEP-2022 19:59:42
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = TRUE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 19.7[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

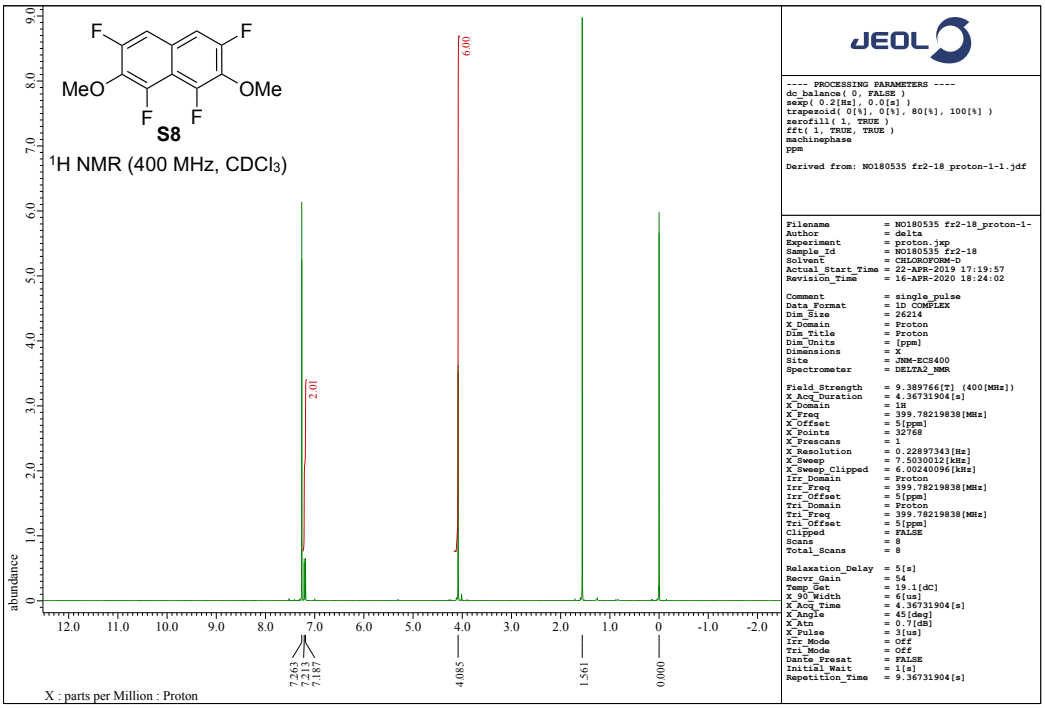

S5
1H NMR (400 MHz, DMSO-d6)
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO 200602 926_proton-1-1.jdf
Filename = NO 200602 926_proton-1-2.
Author = delta
Experiment = proton.jxp
Sample_Id = NO 200602 626
Solvent = DMSO-D6
Actual_Start_Time = 4-JUN-2020 13:01:53
Revision_Time = 5-AUG-2020 19:35:12
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 48
Temp_Get = 19.4[dC]
X_90_Width = 6[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
RepetitIon_Time = 9.36731904[s]

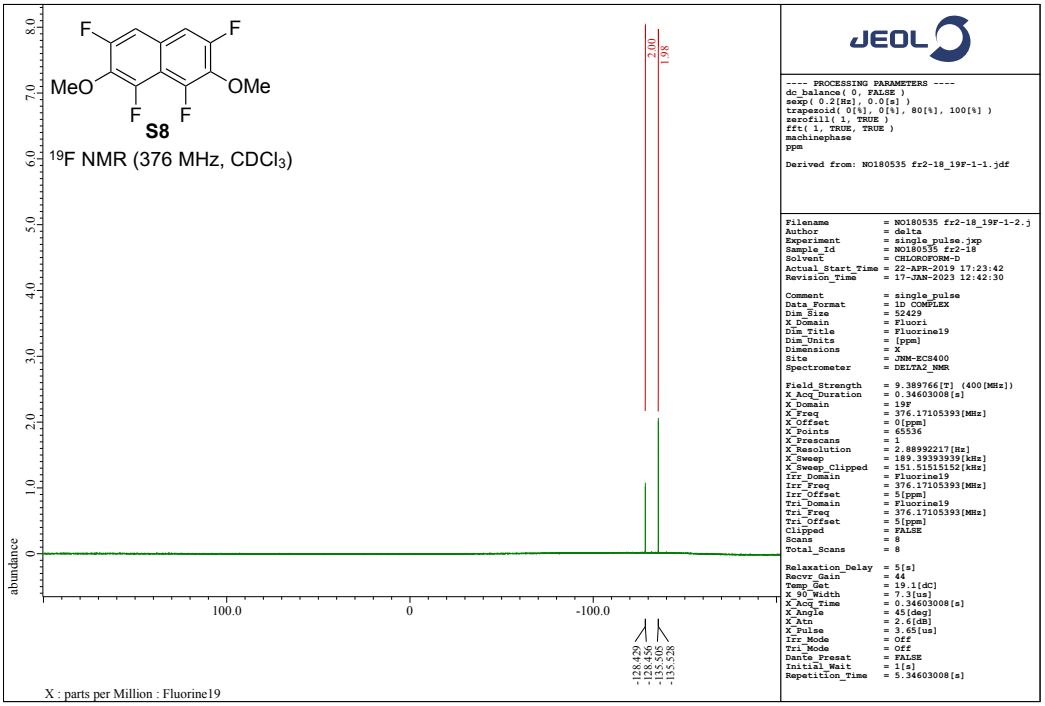

Br
Br
MeO
OMe
S6
1H NMR (400 MHz, CDCl3)
6.00
2.10
2.07
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
7.886
7.262
7.059
3.991
1.558
0.000
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO180747_proton-1-1.jdf
Filename = NO180747_proton-1-2.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = NO180747
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-NOV-2019 15:15:39
Revision_Time = 16-APR-2020 19:01:47
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 19.2[dC]
X_90_Width = 6[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

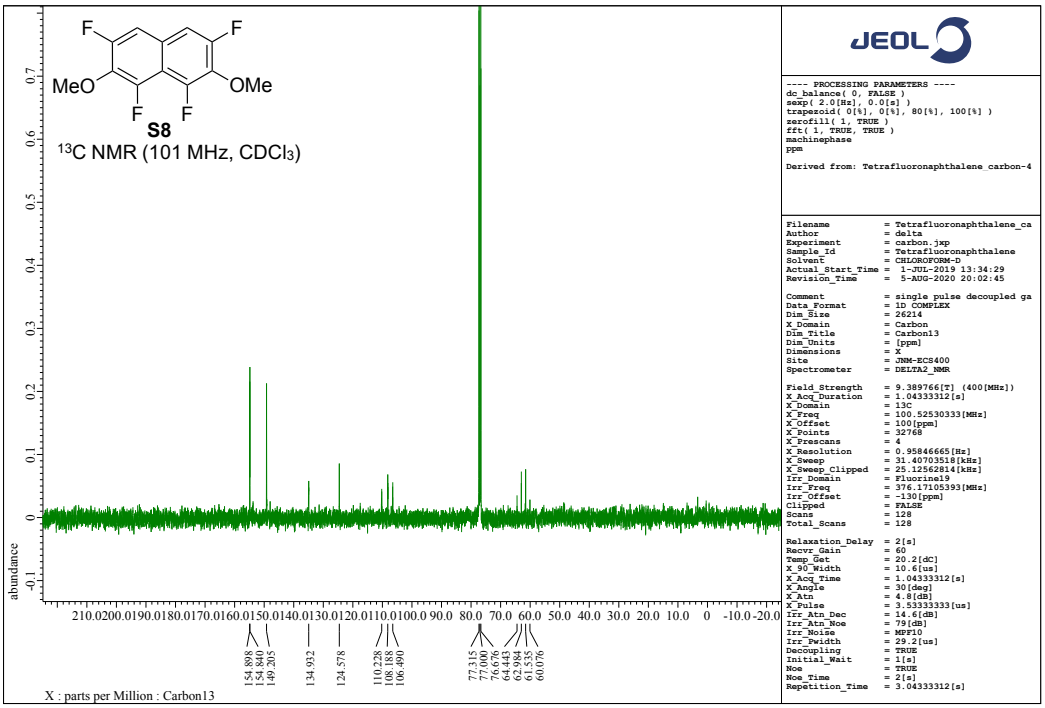

F
F
MeO
OMe
S7
1H NMR (400 MHz, CDCl3)
6.09
2.00
2.06
0.98
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
7.354
7.324
7.263
7.135
7.114
3.979
1.574
0.000
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO180597 column_proton-1-1.jdf
Filename = NO180597 column_proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = NO180597 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-JUN-2019 16:09:35
Revision_Time = 16-APR-2020 18:31:39
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 44
Temp_Get = 19.6[dC]
X_90_Width = 6[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

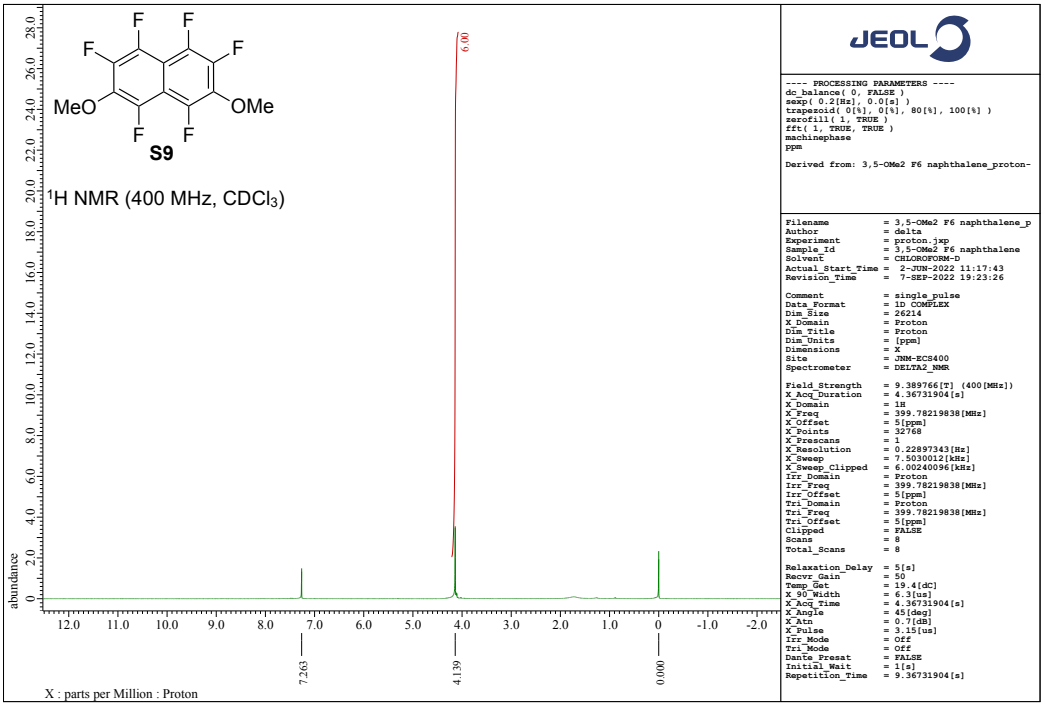

F
F
MeO
OMe
S7
19F NMR (376 MHz, CDCl3)
2.00
abundance
40.0
30.0
20.0
10.0
0
100.0
0
-100.0
-137.410
-137.451
-137.464
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-4.99986, 0, 62.60395[%])
Derived from: NO180597 column_19F-1-1.jdf
Filename = NO180597 column_19F-1-2.j
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO180597 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-JUN-2019 16:13:35
Revision_Time = 17-JAN-2023 12:41:19
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 44
Temp_Get = 19.7[dC]
X_90_Width = 7.3[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 3.65[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

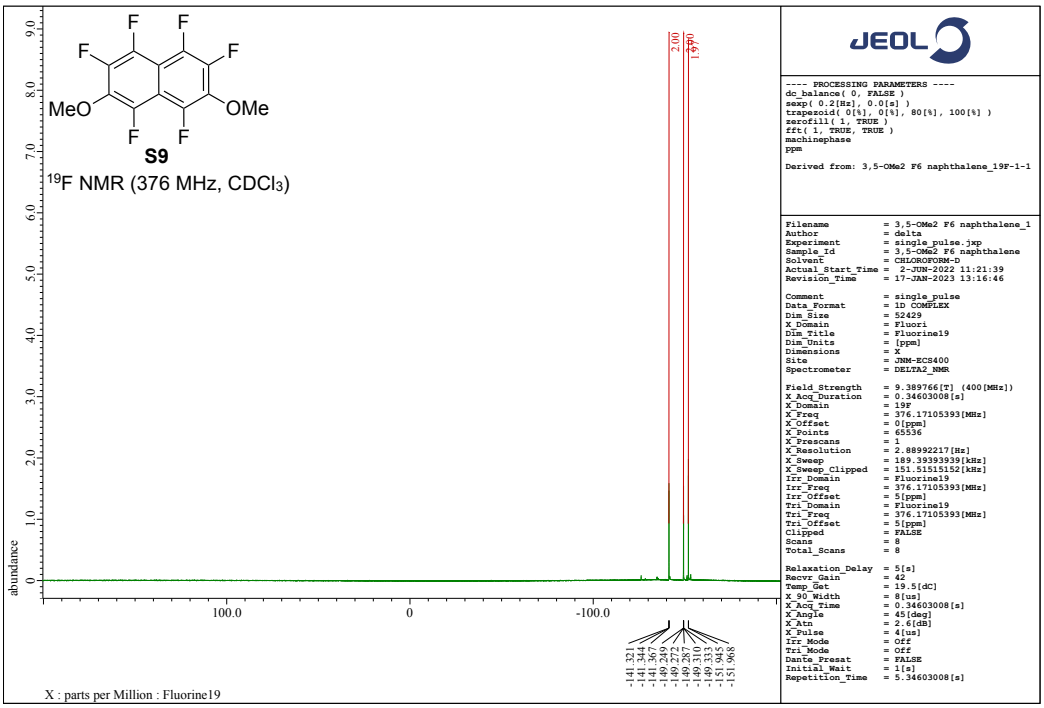

F
F
MeO
OMe
S7
13C NMR (101 MHz, CDCl3)
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
152.666
150.206
147.743
147.279
128.182
122.489
122.404
111.551
111.551
111.410
111.363
107.358
77.324
77.000
76.685
55.890
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: DeMeOF2 naphthalene_carbon-1-1.
Filename = DeMeOF2 naphthalene_carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = DeMeOF2 naphthalene
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-JUL-2019 12:30:34
Revision_Time = 5-AUG-2020 19:56:06
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 20.1[dC]
X_90_Width = 10.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 4.8[dB]
X_Pulse = 3.53333333[us]
Irr_Atn_Dec = 26.351[dB]
Irr_Atn_Noe = 26.351[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
DeCoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

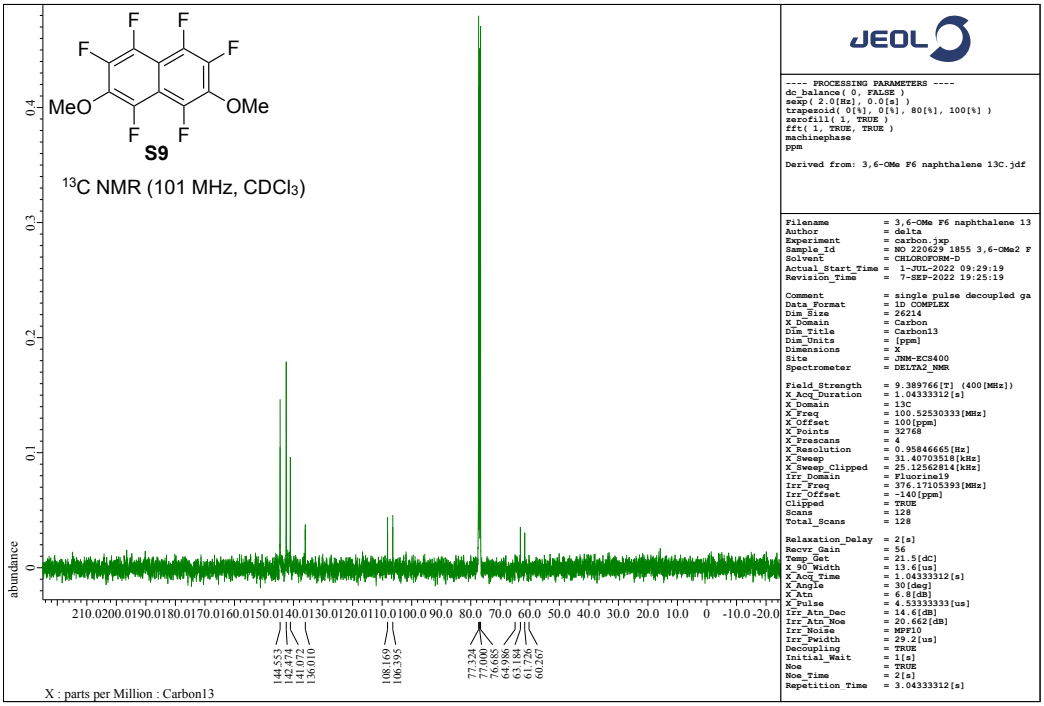

F
F
MeO
OMe
F
F
S8
1H NMR (400 MHz, CDCl3)
6.00
2.01
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
7.263
7.213
7.187
4.085
1.561
0.000
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO180535 fr2-18_proton-1-1.jdf
Filename = NO180535 fr2-18_proton-1-
Author = delta
Experiment = proton.jxp
Sample_Id = NO180535 fr2-18
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-APR-2019 17:19:57
Revision_Time = 16-APR-2020 18:24:02
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 54
Temp_Get = 19.1[dC]
X_90_Width = 6[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

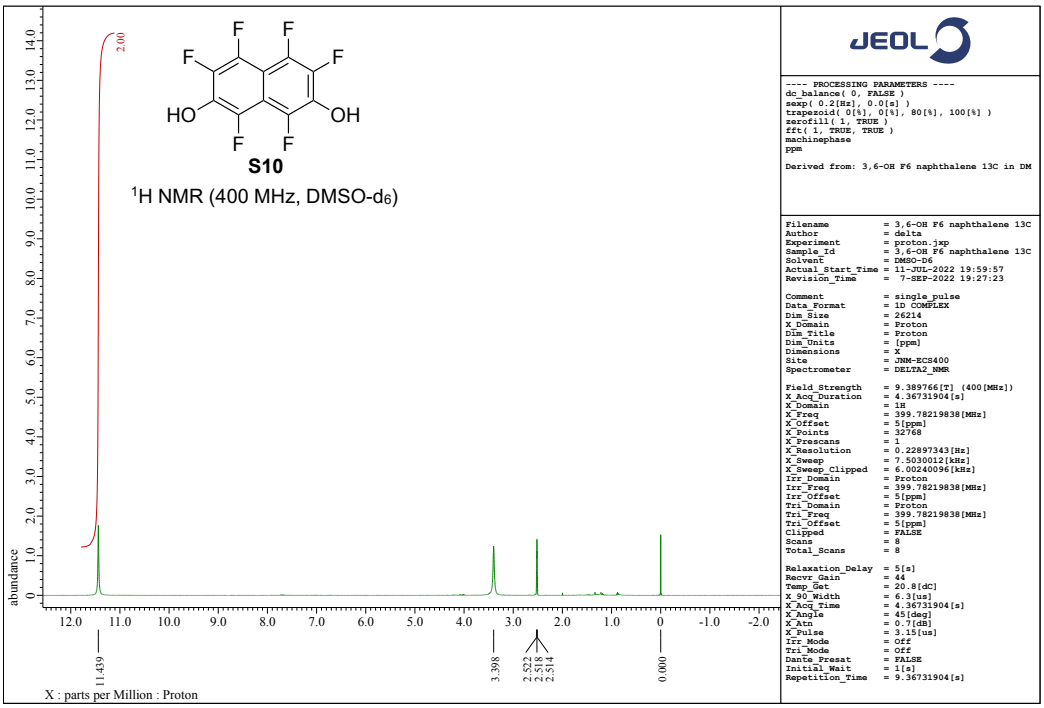

F
F
MeO
OMe
F
F
S8
19F NMR (376 MHz, CDCl3)
2.00
1.98
abundance
100.0 0 -100.0
-128.429
-128.456
-135.505
-135.528
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO180535 fr2-18_19F-1-1.jdf
Filename = NO180535 fr2-18_19F-1-2.j
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO180535 fr2-18
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-APR-2019 17:23:42
Revision_Time = 17-JAN-2023 12:42:30
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 44
Temp_Get = 19.1[dC]
X_90_Width = 7.3[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 3.65[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

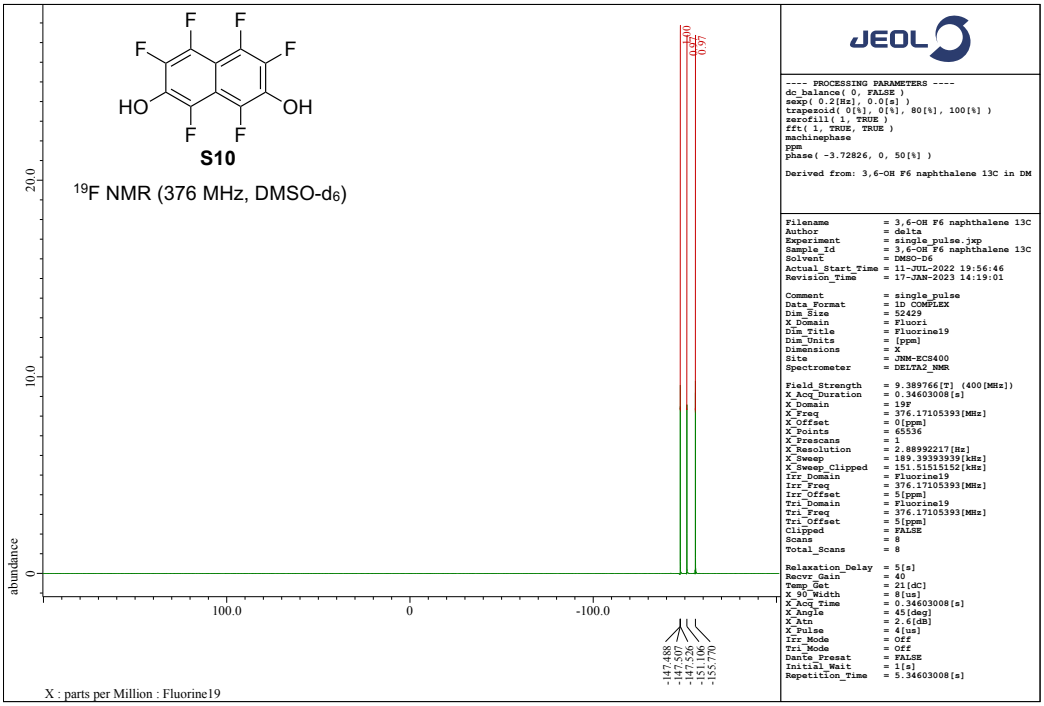

F
F
MeO
OMe
F
F
S8
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: Tetrafluoronaphthalene carbon-4
Filename = Tetrafluoronaphthalene_ca
Author = delta
Experiment = carbon.jxp
Sample_Id = Tetrafluoronaphthalene
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-JUL-2019 13:34:29
Revision_Time = 5-ADG-2020 20:02:45
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.2[dC]
X_90_Width = 10.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 4.8[dB]
X_Pulse = 3.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 79[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

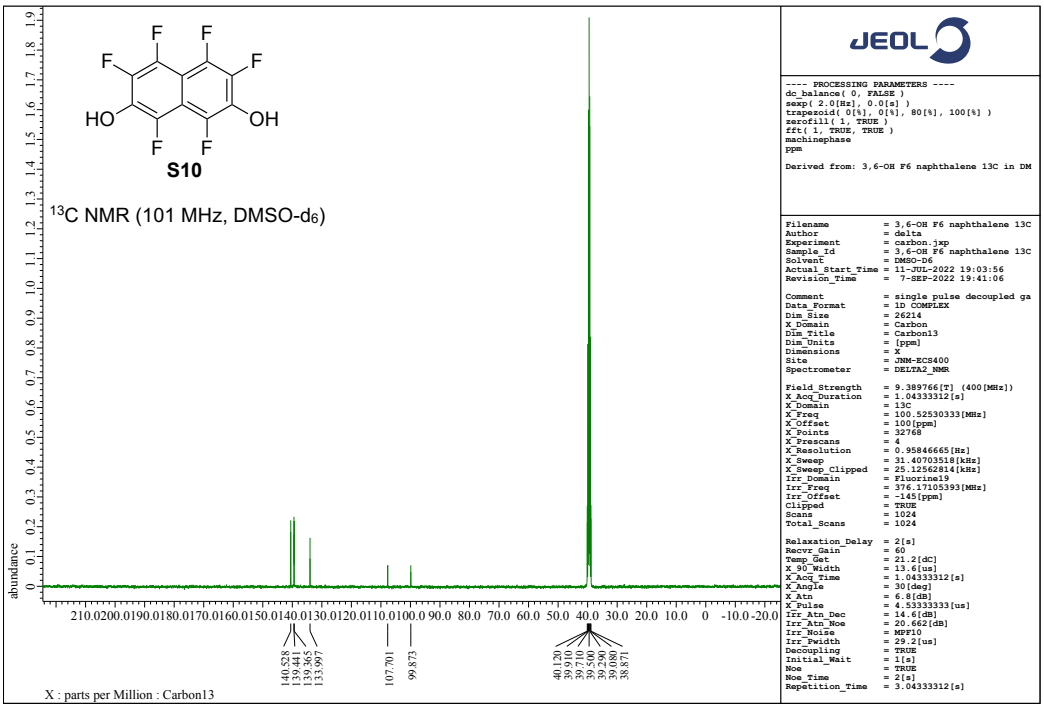

F
F
F
F
MeO
OMe
F
F
S9
1H NMR (400 MHz, CDCl3)
6.00
abundance
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,5-OMe2 F6 naphthalene_proton-
Filename = 3,5-OMe2 F6 naphthalene_p
Author = delta
Experiment = proton.jxp
Sample_Id = 3,5-OMe2 F6 naphthalene
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUN-2022 11:17:43
Revision_Time = 7-SEP-2022 19:23:26
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 19.4[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

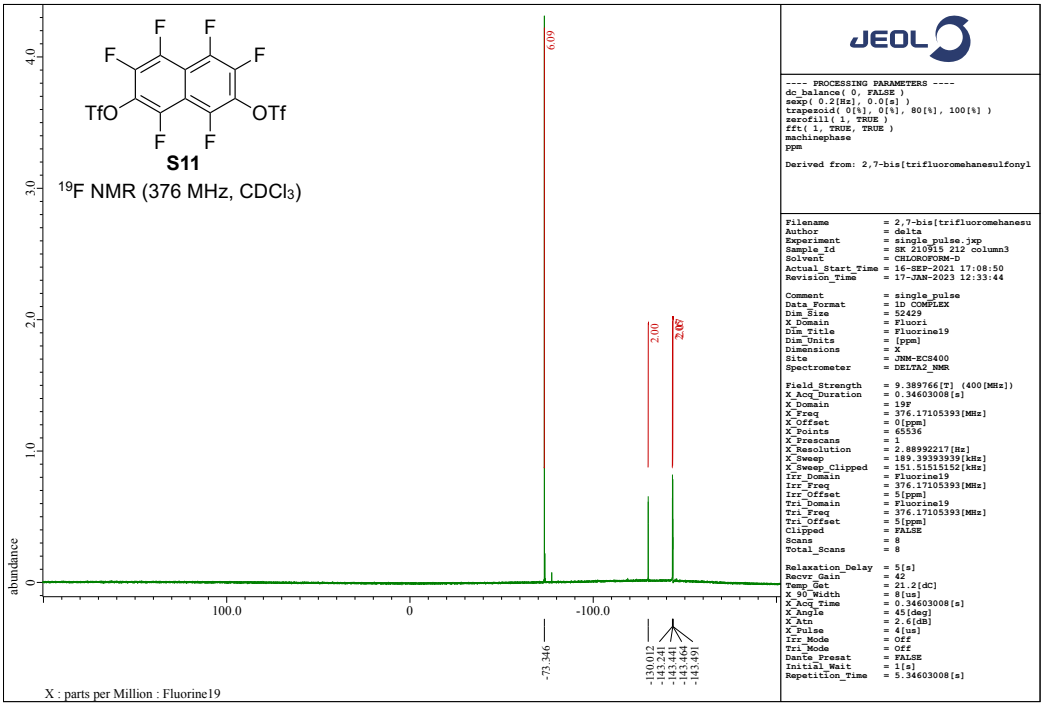

F
F
F
F
MeO
OMe
F
F
S9
19F NMR (376 MHz, CDCl3)
abundance
100.0
0
-100.0
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,5-OMe2 F6 naphthalene_19F-1-1
Filename = 3,5-OMe2 F6 naphthalene_1
Author = delta
Experiment = single_pulse.jxp
Sample_Id = 3,5-OMe2 F6 naphthalene
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUN-2022 11:21:39
Revision_Time = 17-JAN-2023 13:16:46
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.5[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

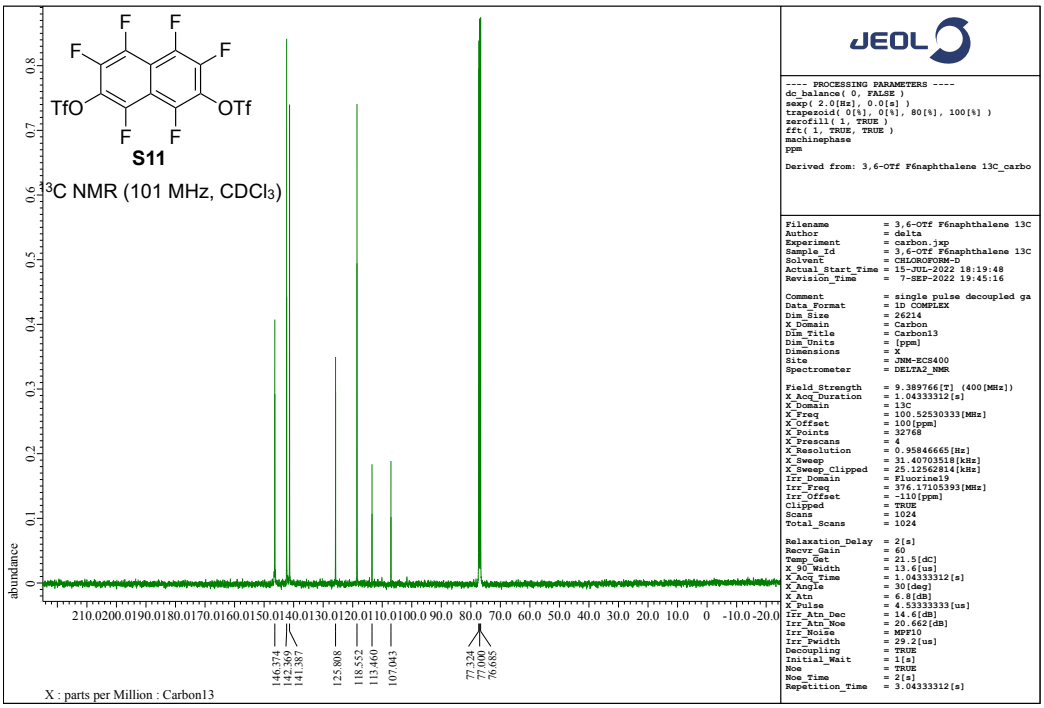

F
F
F
F
MeO
OMe
F
F
S9
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-OMe F6 naphthalene 13C.jdf
Filename = 3,6-OMe F6 naphthalene 13
Author = delta
Experiment = carbon.jxp
Sample_Id = NO 220629 1855 3,6-OMe2 F
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-JUL-2022 09:29:19
Revision_Time = 7-SEP-2022 19:25:19
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -140[ppm]
Clipped = TRUE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 21.5[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

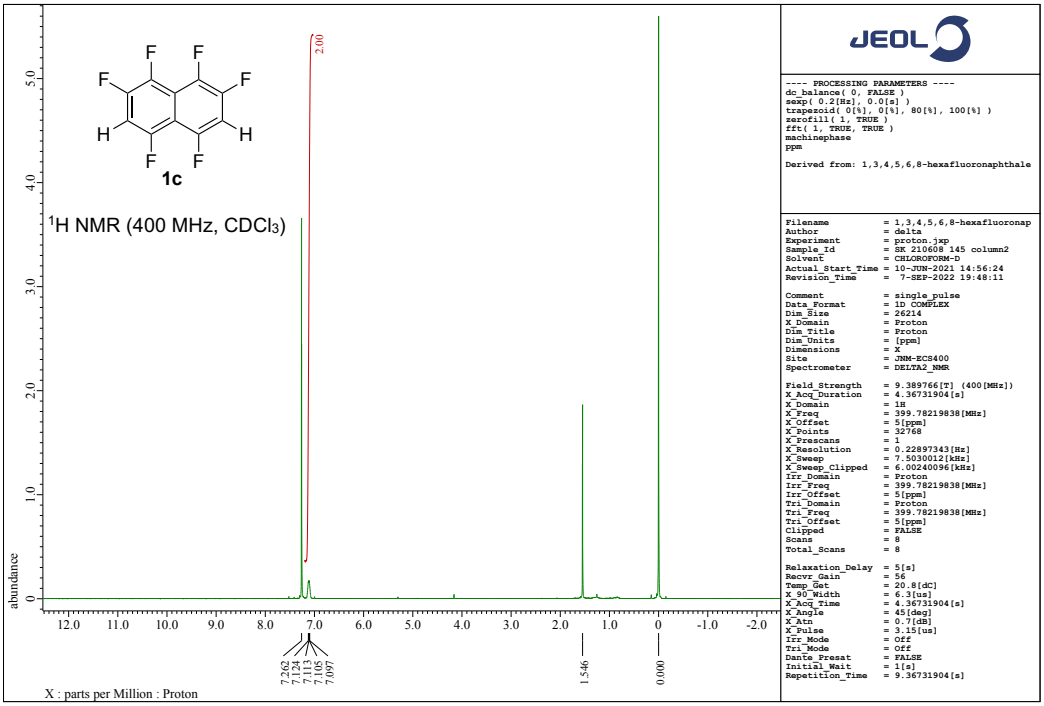

F
F
F
F
HO
OH
F
F
S10
1H NMR (400 MHz, DMSO-d6)
2.00
abundance
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
11.439
3.398
2.522
2.516
2.514
0.000
X : parts per Million : Proton
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-OH F6 naphthalene 13C in DM
Filename = 3,6-OH F6 naphthalene 13C
Author = delta
Experiment = proton.jxp
Sample_Id = 3,6-OH F6 naphthalene 13C
Solvent = DMSO-D6
Actual_Start_Time = 11-JUL-2022 19:59:57
Revision_Time = 7-SEP-2022 19:27:23
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 44
Temp_Get = 20.8[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

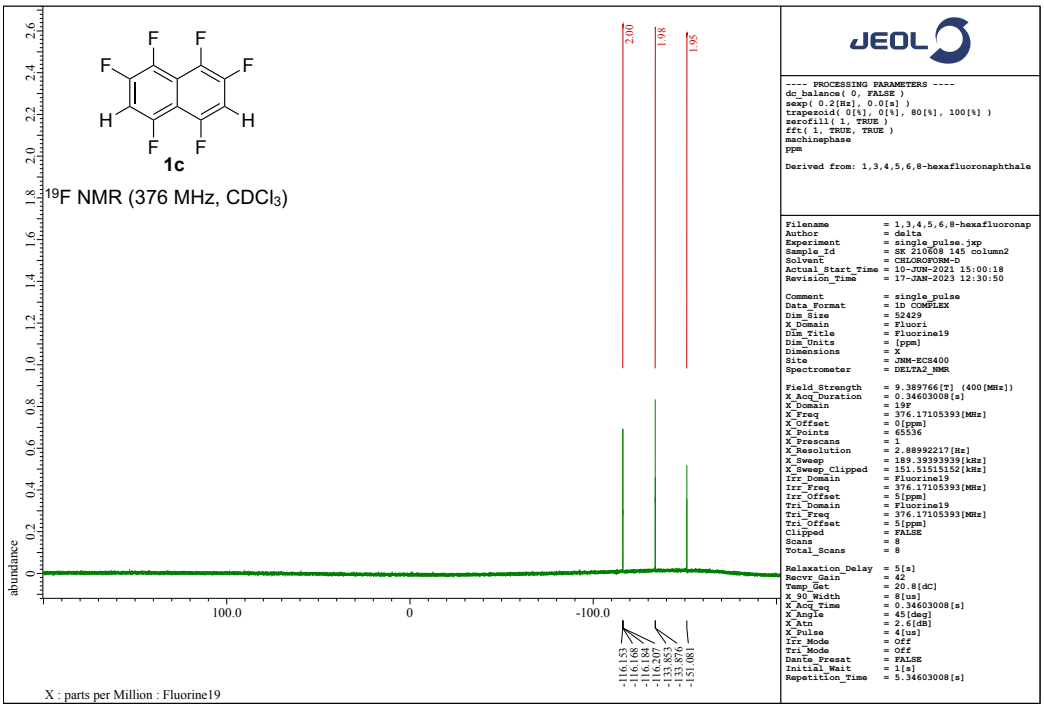

F
F
F
F
HO
OH
F
F
S10
19F NMR (376 MHz, DMSO-d6)
1.00
0.97
abundance
20.0
10.0
0
100.0
0
-100.0
-147.488
-147.507
-147.526
-151.106
-155.770
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-3.72826, 0, 50[%])
Derived from: 3,6-OH F6 naphthalene 13C in DM
Filename = 3,6-OH F6 naphthalene 13C
Author = delta
Experiment = single_pulse.jxp
Sample_Id = 3,6-OH F6 naphthalene 13C
Solvent = DMSO-D6
Actual_Start_Time = 11-JUL-2022 19:56:46
Revision_Time = 17-JAN-2023 14:19:01
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 40
Temp_Get = 21[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]


S10
13C NMR (101 MHz, DMSO-d6)
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-OH F6 naphthalene 13C in DM
Filename = 3,6-OH F6 naphthalene 13C
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,6-OH F6 naphthalene 13C
Solvent = DMSO-D6
Actual_Start_Time = 11-JUL-2022 19:03:56
Revision_Time = 7-SEP-2022 19:41:06
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -145[ppm]
Clipped = TRUE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.2[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

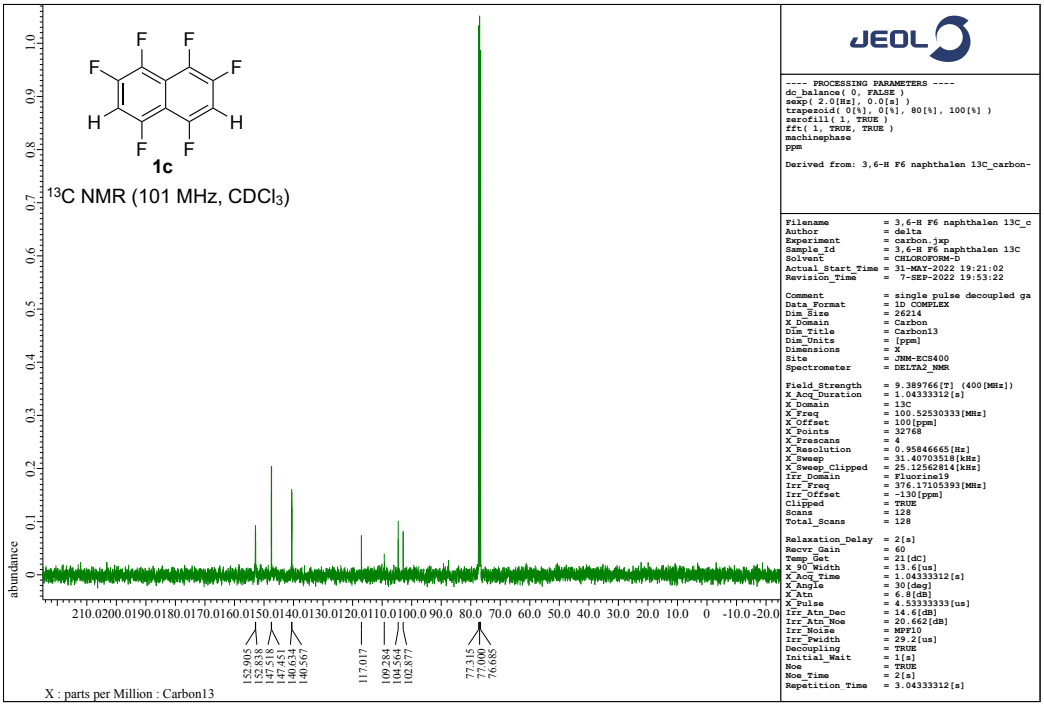

S11
19F NMR (376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 2,7-bis[trifluoromehanesulfonyl
Filename = 2,7-bis[trifluoromehanesu
Author = delta
Experiment = single_pulse.jxp
Sample_Id = SK 210915 212 column3
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-SEP-2021 17:08:50
Revision_Time = 17-JAN-2023 12:33:44
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 21.2[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]


S11
^{13}C NMR (101 MHz, CDCl$_3$)
abundance
X : parts per Million : Carbon13
146.374
142.869
141.387
125.808
118.552
113.460
107.043
77.324
77.000
76.685
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-OTf F6naphthalene 13C_carbo
Filename = 3,6-OTf F6naphthalene 13C
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,6-OTf F6naphthalene 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2022 18:19:48
Revision_Time = 7-SEP-2022 19:45:16
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -110[ppm]
Clipped = TRUE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.5[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

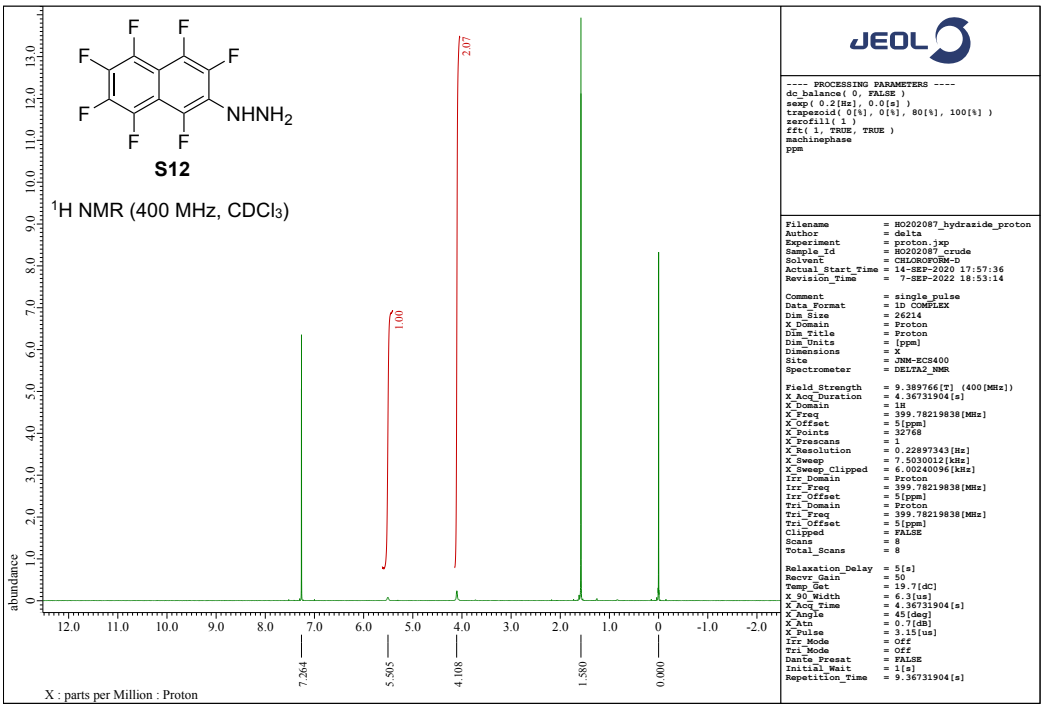

1c
^{1}H NMR (400 MHz, CDCl$_3$)
2.00
abundance
X : parts per Million : Proton
7.262
7.124
7.113
7.105
7.097
1.546
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 1,3,4,5,6,8-hexafluoronaphthale
Filename = 1,3,4,5,6,8-hexafluoronap
Author = delta
Experiment = proton.jxp
Sample_Id = RK 210608 145 column2
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-JUN-2021 14:56:24
Revision_Time = 7-SEP-2022 19:48:11
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 56
Temp_Get = 20.8[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

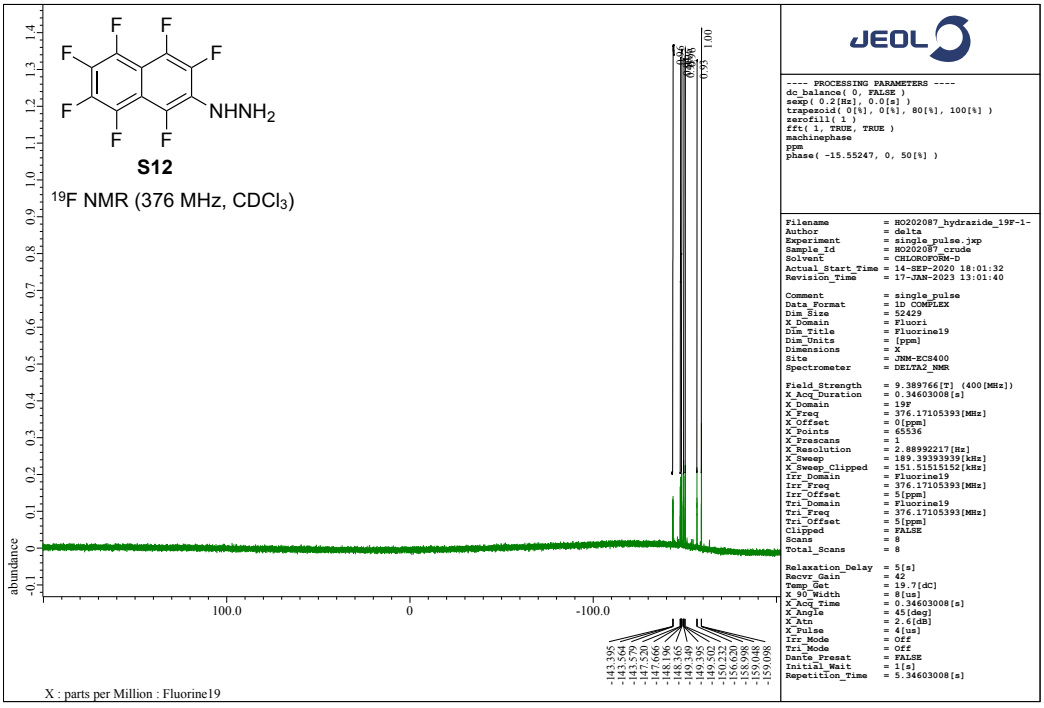


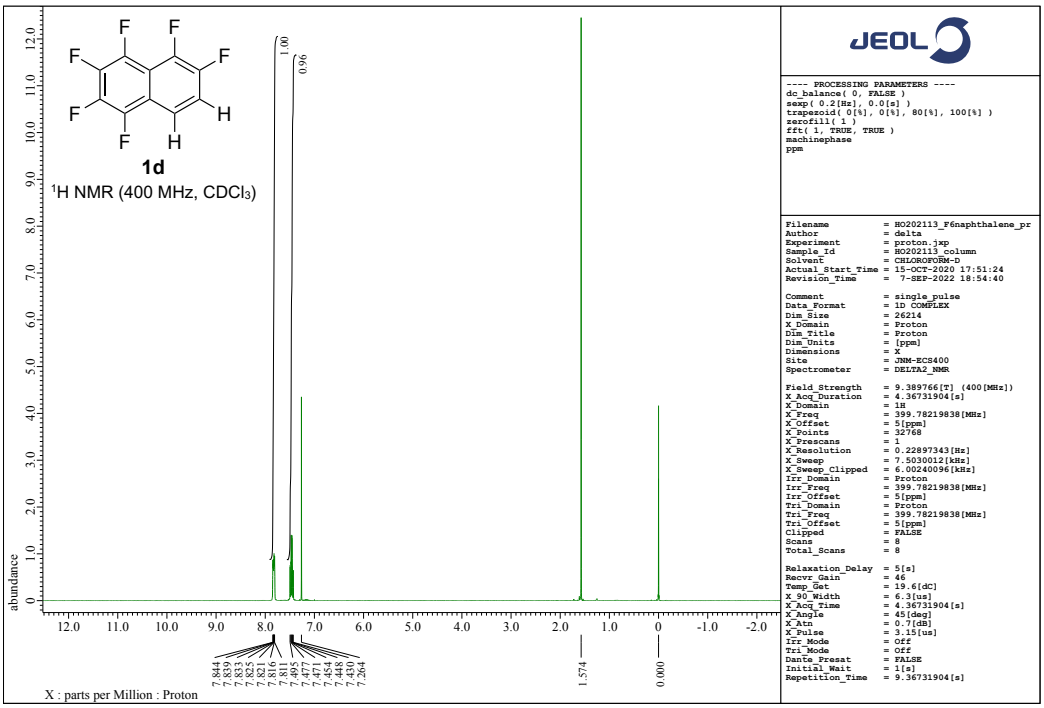

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: 1,3,4,5,6,8-hexafluoronaphthale

Filename            = 1,3,4,5,6,8-hexafluoronap
Author              = delta
Experiment          = single_pulse.jxp
Sample_Id           = SK 210608 145 column2
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 10-JUN-2021 15:00:18
Revision_Time       = 17-JAN-2023 12:30:50

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 52429
X_Domain            = Fluori
Dim_Title           = Fluorine19
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 0.34603008[s]
X_Domain            = 19F
X_Freq              = 376.17105393[MHz]
X_Offset            = 0[ppm]
X_Points            = 65536
X_Prescans          = 1
X_Resolution        = 2.88992217[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          = 42
Temp_Get            = 20.8[dC]
X_90_Width          = 8[us]
X_Acq_Time          = 0.34603008[s]
X_Angle             = 45[deg]
X_Atn               = 2.6[dB]
X_Pulse             = 4[us]
Irr_Mode            = Off
Tri_Mode            = Off
DanTe_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 5.34603008[s]
```

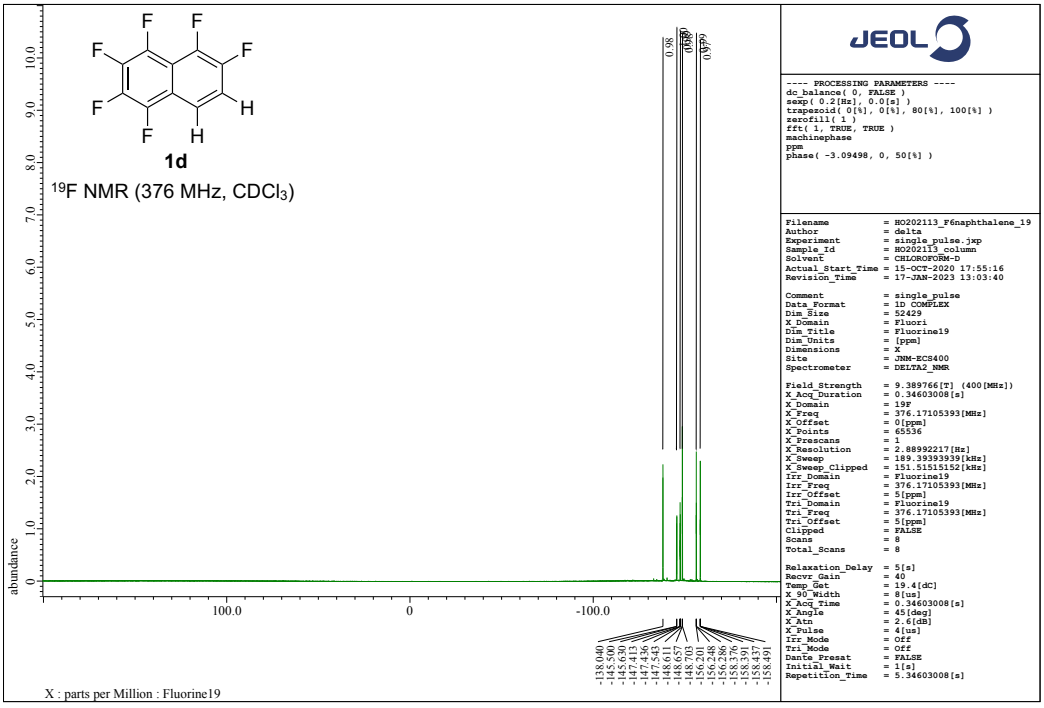


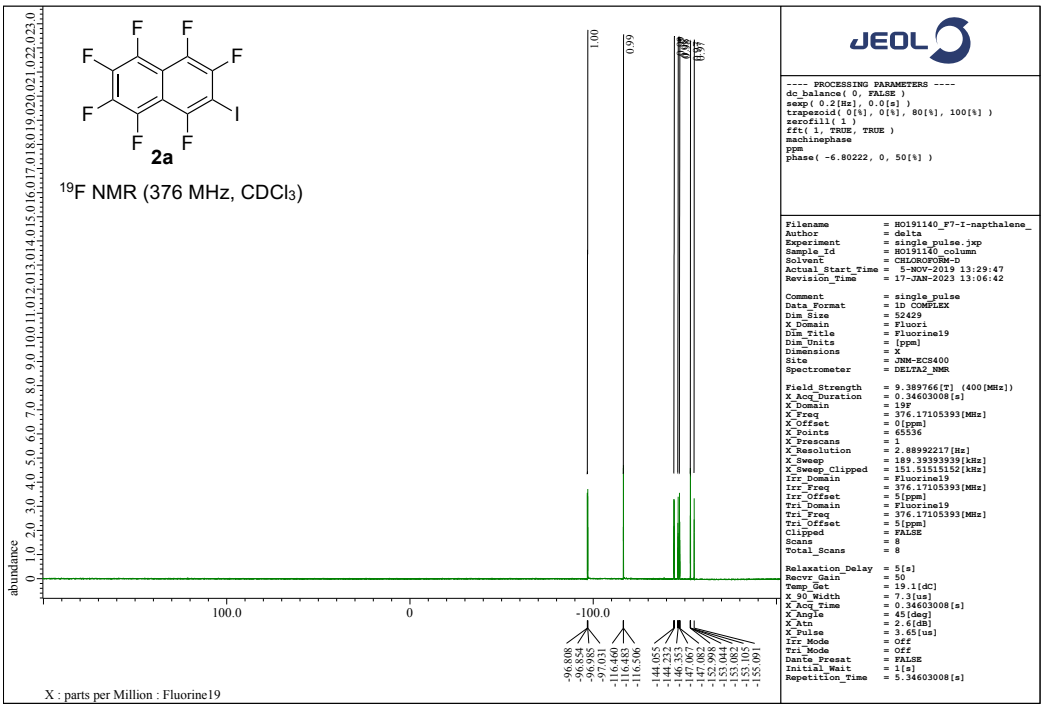

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: 3,6-H F6 naphthalen 13C_carbon-

Filename            = 3,6-H F6 naphthalen 13C_c
Author              = delta
Experiment          = carbon.jxp
Sample_Id           = 3,6-H F6 naphthalen 13C
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 31-MAY-2022 19:21:02
Revision_Time       =  7-SEP-2022 19:53:22

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

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 1.04333312[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          = Fluorine19
Irr_Freq            = 376.17105393[MHz]
Irr_Offset          = -130[ppm]
Clipped             = TRUE
Scans               = 128
Total_Scans         = 128

Relaxation_Delay    = 2[s]
Recvr_Gain          = 60
Temp_Get            = 21[dC]
X_90_Width          = 13.6[us]
X_Acq_Time          = 1.04333312[s]
X_Angle             = 30[deg]
X_Atn               = 6.8[dB]
X_Pulse             = 4.53333333[us]
Irr_Atn_Dec         = 14.6[dB]
Irr_Atn_Noe         = 20.662[dB]
Irr_Noise           = MPF10
Irr_Pwidth          = 29.2[us]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 3.04333312[s]
```


F
F
F
F
F
F
NHNH2
S12
1H NMR (400 MHz, CDCl3)
2.07
1.00
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.264
5.505
4.108
1.580
0.000
X : parts per Million : Proton
JEOL
---- 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
Filename = HO202087_hydrazide_proton
Author = delta
Experiment = proton.jxp
Sample_Id = HO202087_crude
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-SEP-2020 17:57:36
Revision_Time = 7-SEP-2022 18:53:14
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 19.7[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]


F
F
F
F
F
F
NHNH2
S12
19F NMR (376 MHz, CDCl3)
1.00
abundance
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
100.0
0
-100.0
-143.395
-143.564
-143.579
-147.520
-147.666
-148.196
-148.345
-149.349
-149.395
-149.502
-150.232
-158.670
-158.698
-159.048
-159.098
X : parts per Million : Fluorine19
JEOL
---- 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(-15.55247, 0, 50[%])
Filename = HO202087_hydrazide_19F-1-
Author = delta
Experiment = single_pulse.jxp
Sample_Id = HO202087_crude
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-SEP-2020 18:01:32
Revision_Time = 17-JAN-2023 13:01:40
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.7[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

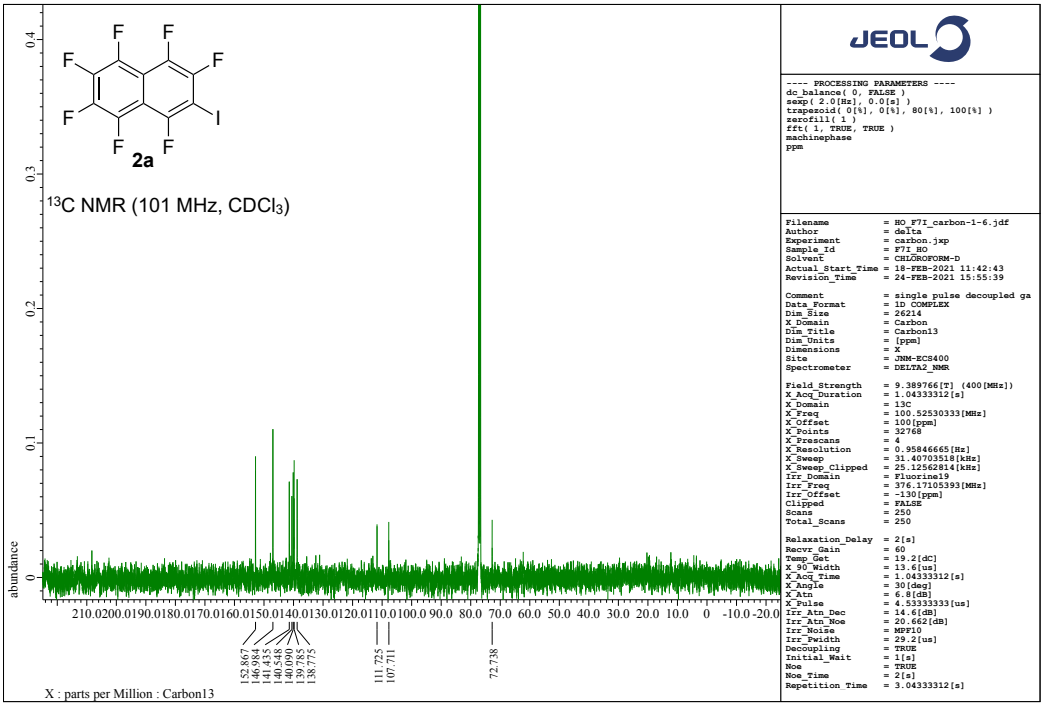

1d
1H NMR (400 MHz, CDCl3)
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = H0202113_F6naphthalene_pr
Author = delta
Experiment = proton.jxp
Sample_Id = H0202113_column
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-OCT-2020 17:51:24
Revision_Time = 7-SEP-2022 18:54:40
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 46
Temp_Get = 19.6[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]


1d
19F NMR (376 MHz, CDCl3)
X : parts per Million : Fluorine19
---- 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(-3.09498, 0, 50[%])
Filename = H0202113_F6naphthalene_19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = H0202113_column
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-OCT-2020 17:55:16
Revision_Time = 17-JAN-2023 13:03:40
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 40
Temp_Get = 19.4[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]



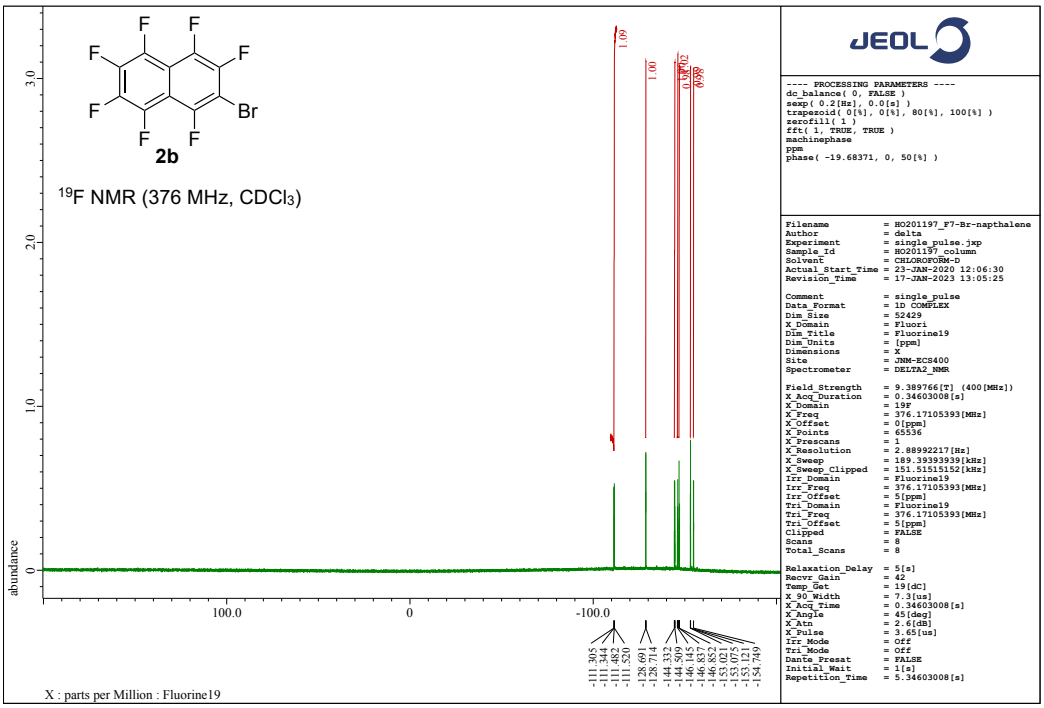

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -6.80222, 0, 50[%] )
```

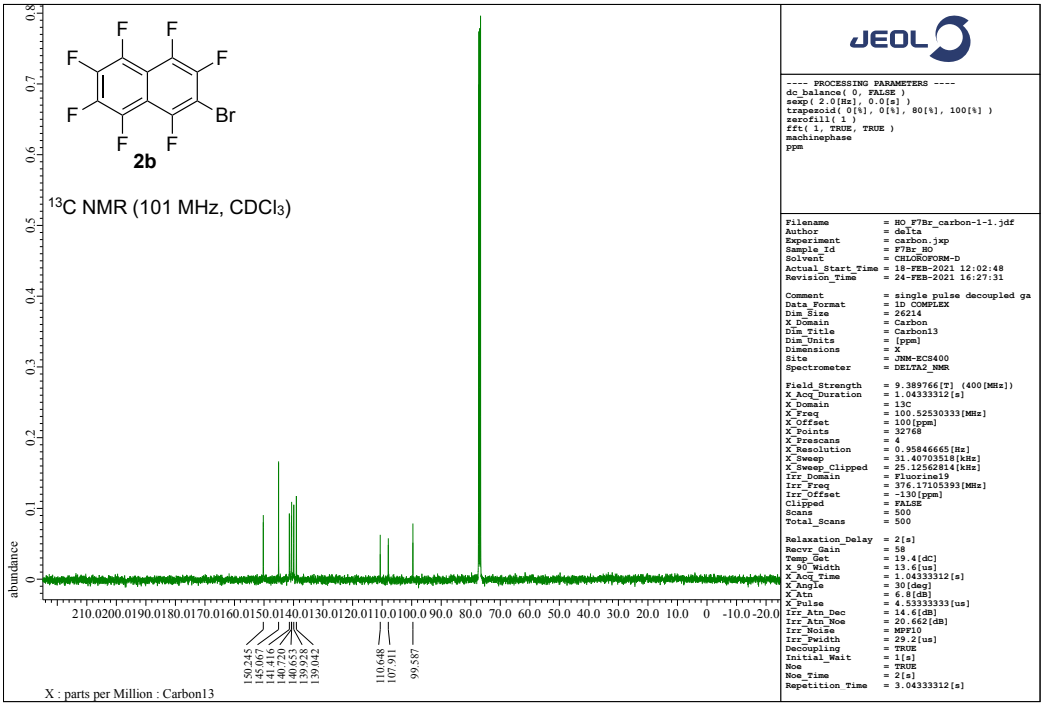
```
Filename            = H0191140_F7-I-napthalene_
Author              = delta
Experiment          = single_pulse.jxp
Sample_Id           = H0191140 column
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-NOV-2019 13:29:47
Revision_Time       = 17-JAN-2023 13:06:42

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 52429
X_Domain            = Fluori
Dim_Title           = Fluorine19
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 0.34603008[s]
X_Domain            = 19F
X_Freq              = 376.17105393[MHz]
X_Offset            = 0[ppm]
X_Points            = 65536
X_Prescans          = 1
X_Resolution        = 2.88992217[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            = 19.1[dC]
X_90_Width          = 7.3[us]
X_Acq_Time          = 0.34603008[s]
X_Angle             = 45[deg]
X_Atn               = 2.6[dB]
X_Pulse             = 3.65[us]
Irr_Mode            = Off
Tri_Mode            = Off
DanTe_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 5.34603008[s]
```

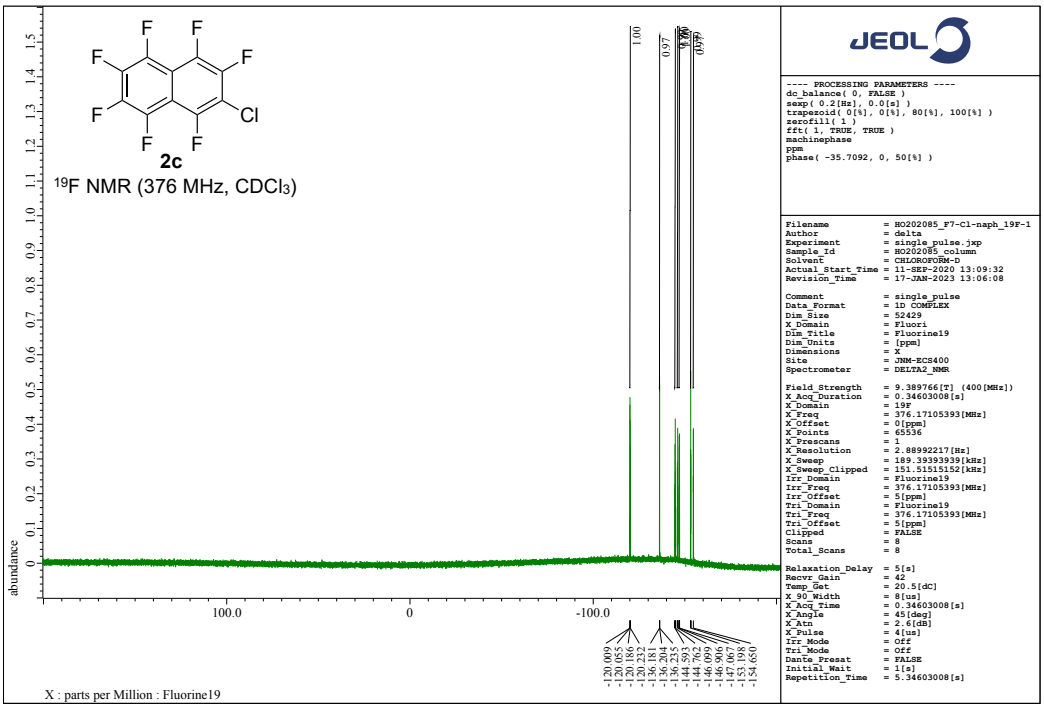


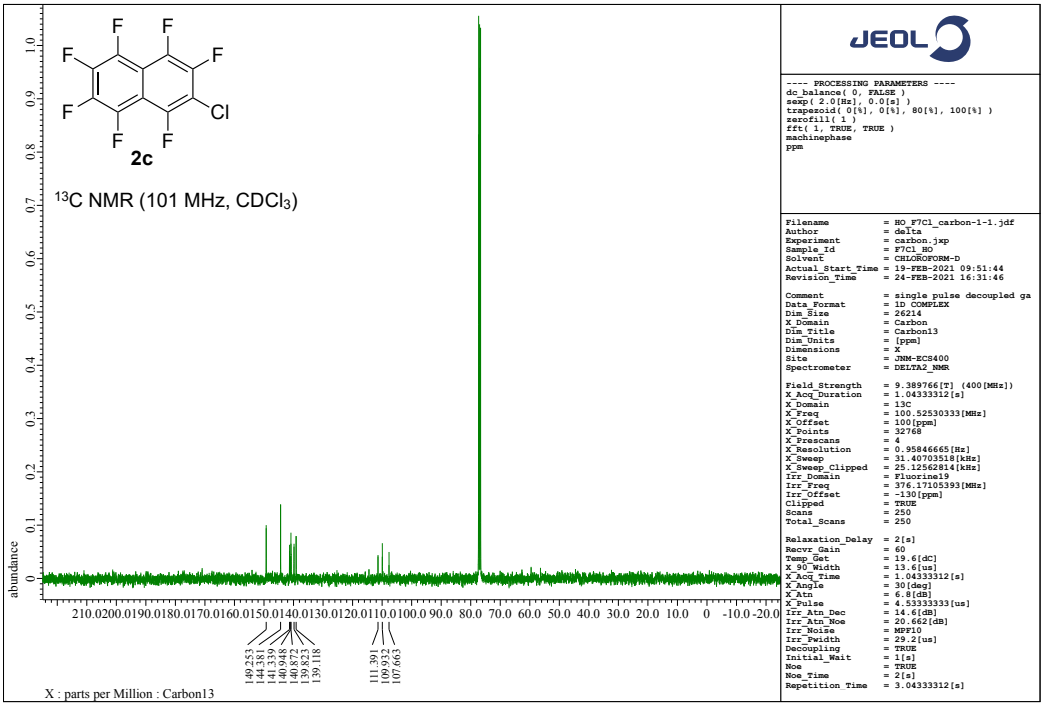

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

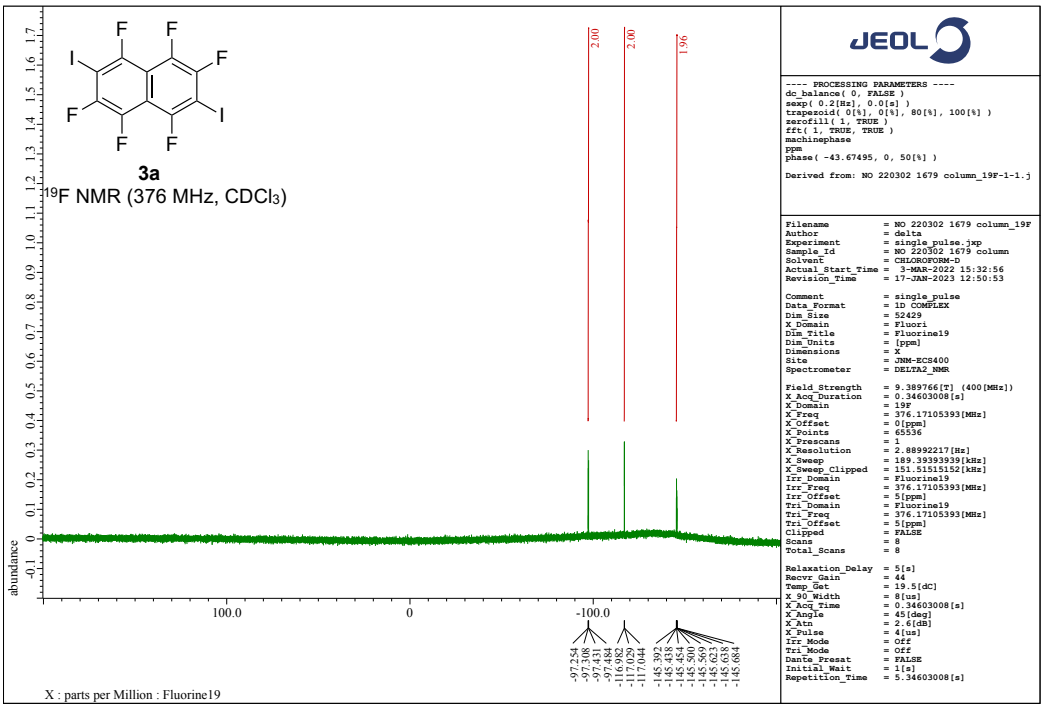
```
Filename            = HO_F7I_carbon-1-6.jdf
Author              = delta
Experiment          = carbon.jxp
Sample_Id           = F7I HO
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 18-FEB-2021 11:42:43
Revision_Time       = 24-FEB-2021 15:55:39

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

Field_Strength      = 9.389766[T] (400[MHz])
X_Acq_Duration      = 1.04333312[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          = Fluorine19
Irr_Freq            = 376.17105393[MHz]
Irr_Offset          = -130[ppm]
Clipped             = FALSE
Scans               = 250
Total_Scans         = 250

Relaxation_Delay    = 2[s]
Recvr_Gain          = 60
Temp_Get            = 19.2[dC]
X_90_Width          = 13.6[us]
X_Acq_Time          = 1.04333312[s]
X_Angle             = 30[deg]
X_Atn               = 6.8[dB]
X_Pulse             = 4.53333333[us]
Irr_Atn_Dec         = 14.6[dB]
Irr_Atn_Noe         = 20.662[dB]
Irr_Noise           = MPF10
Irr_Pwidth          = 29.2[us]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition_Time     = 3.04333312[s]
```

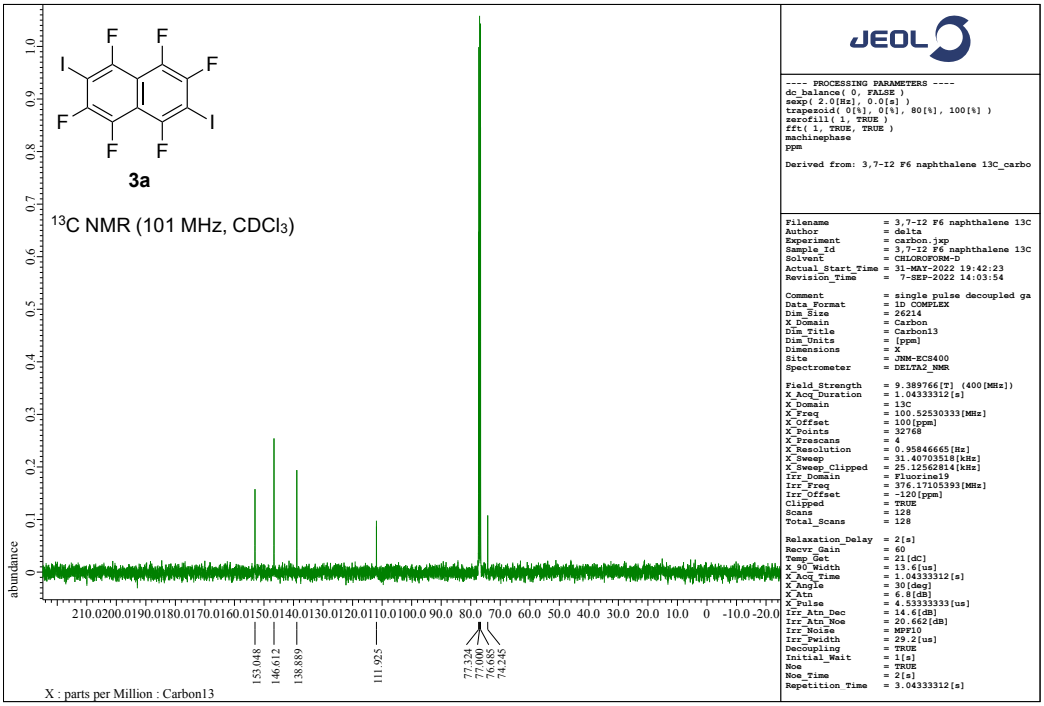

2b
^{19}F NMR (376 MHz, CDCl$_3$)
X : parts per Million : Fluorine19

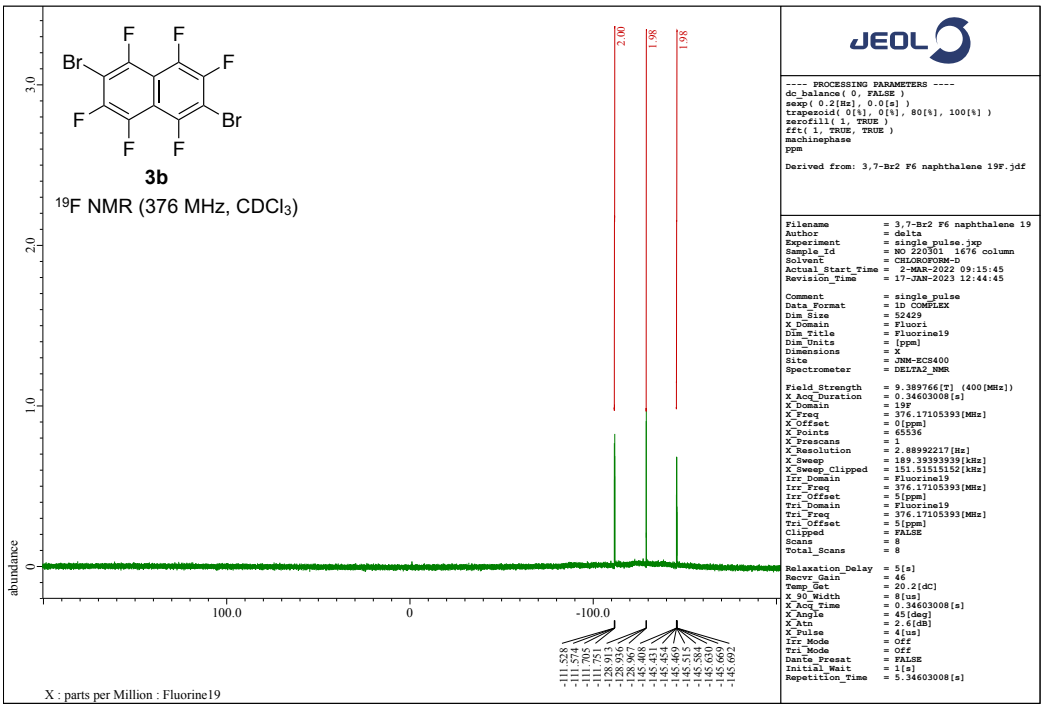

2b
^{13}C NMR (101 MHz, CDCl$_3$)
X : parts per Million : Carbon13

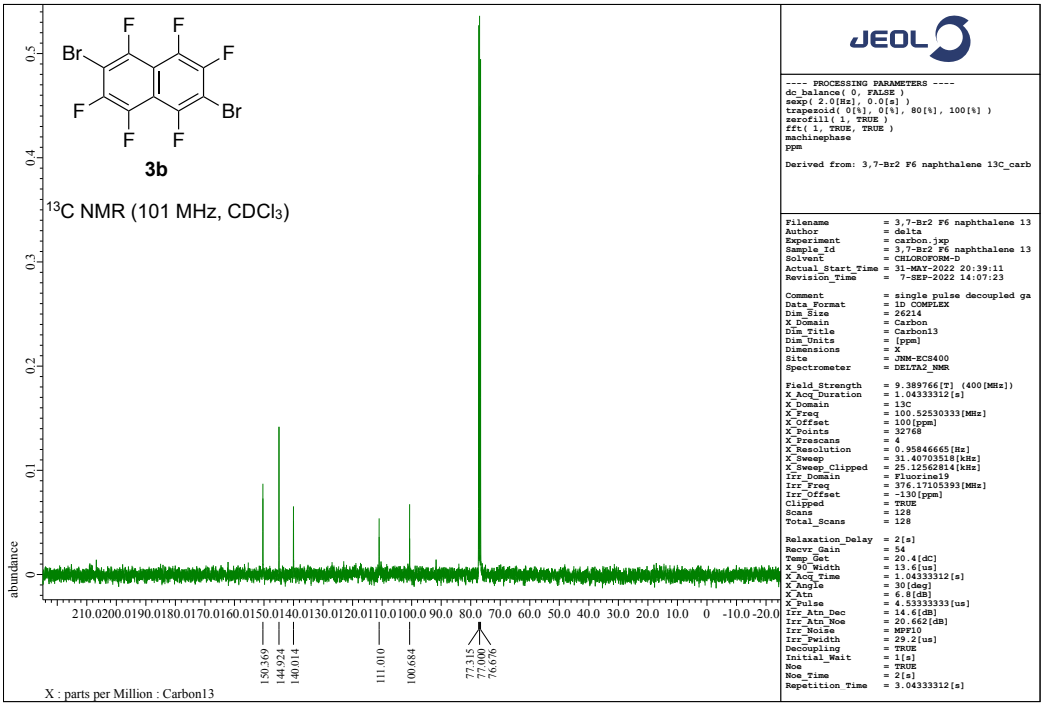

2c
19F NMR (376 MHz, CDCl3)
abundance
100.0
0
-100.0
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-35.7092, 0, 50[%])
Filename = HO202085_F7-Cl-naph_19F-1
Author = delta
Experiment = single_pulse.jxp
Sample_Id = HO202085_column
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2020 13:09:32
Revision_Time = 17-JAN-2023 13:06:08
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 20.5[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

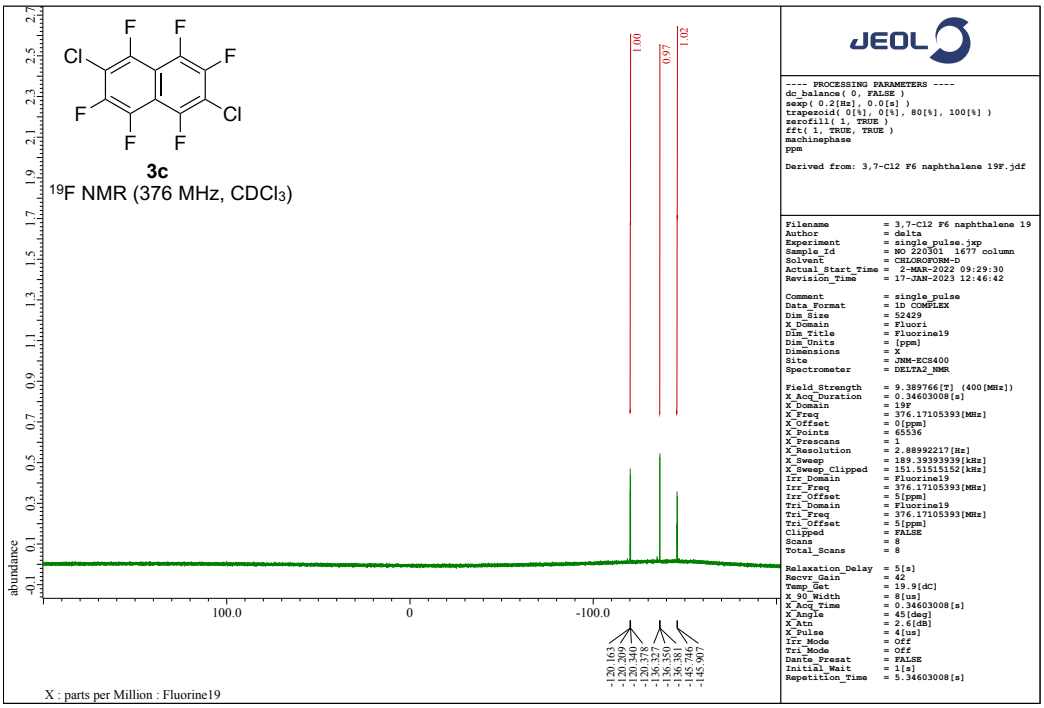

2c
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO_F7Cl_carbon-1-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = F7Cl_HO
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2021 09:51:44
Revision_Time = 24-FEB-2021 16:31:46
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = TRUE
Scans = 250
Total_Scans = 250
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.6[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

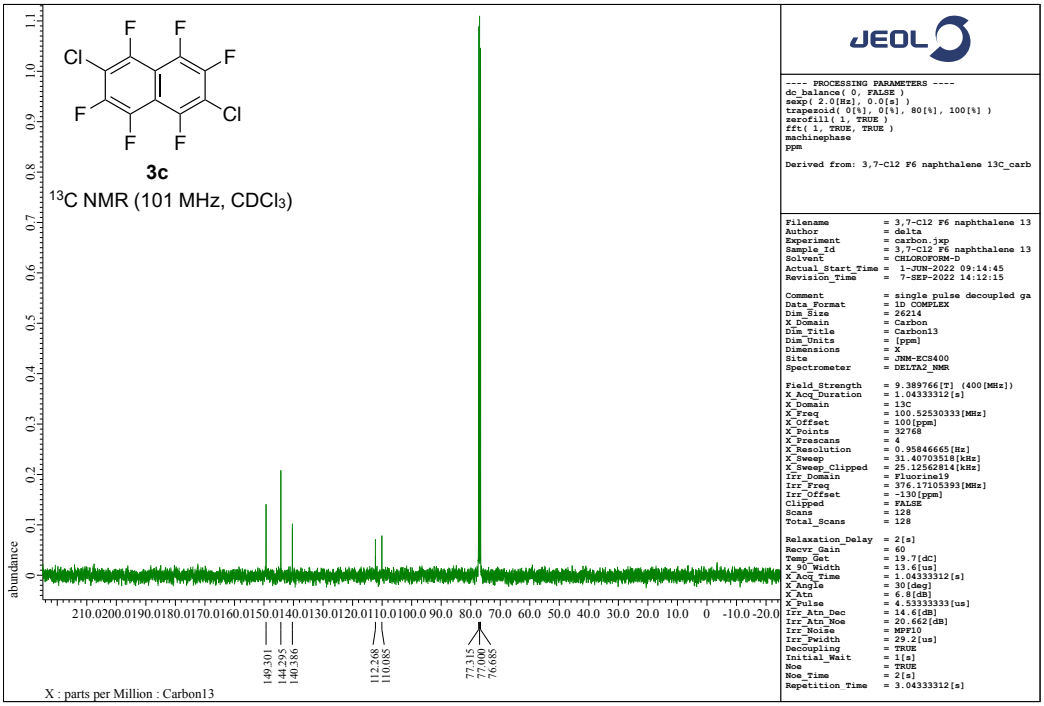

3a
19F NMR (376 MHz, CDCl3)
2.00
2.00
1.96
abundance
100.0
0
-100.0
-97.254
-97.308
-97.431
-97.484
-117.029
-117.044
-145.392
-145.438
-145.454
-145.507
-145.569
-145.623
-145.638
-145.684
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-43.67495, 0, 50[%])
Derived from: NO 220302 1679 column_19F-1-1.j
Filename = NO 220302 1679 column_19F
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220302 1679 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-MAR-2022 15:32:56
Revision_Time = 17-JAN-2023 12:50:53
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 44
Temp_Get = 19.5[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

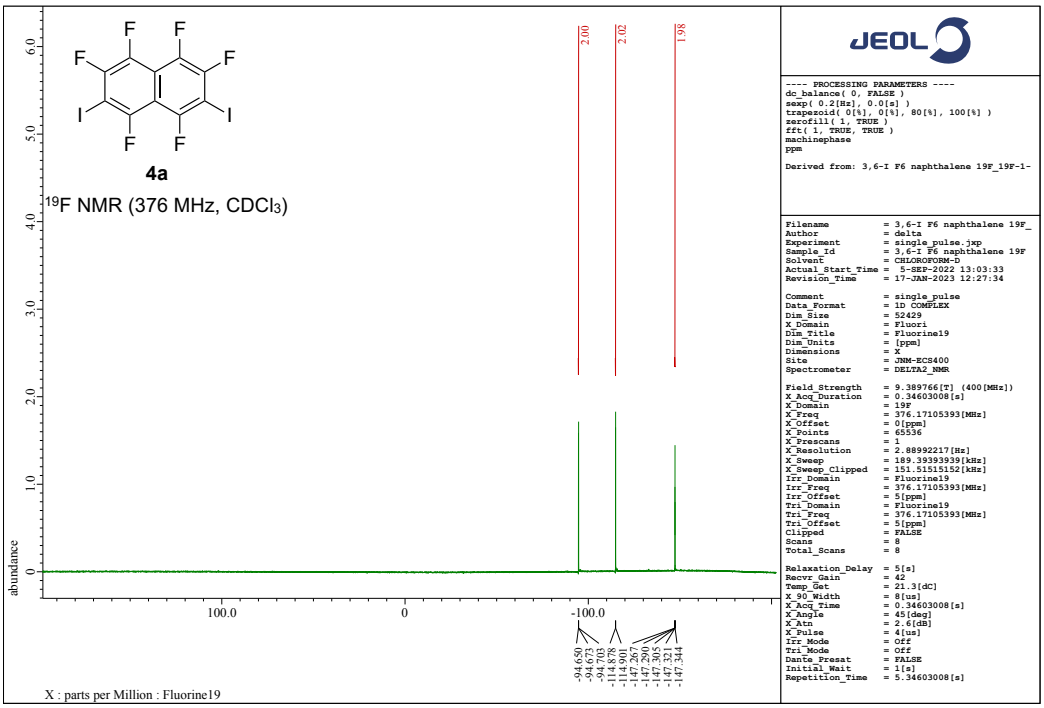

3a
13C NMR (101 MHz, CDCl3)
abundance
153.048
146.612
138.889
111.925
77.324
77.000
76.685
74.245
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-I2 F6 naphthalene 13C_carbo
Filename = 3,7-I2 F6 naphthalene 13C
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-I2 F6 naphthalene 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-MAY-2022 19:42:23
Revision_Time = 7-SEP-2022 14:03:54
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -120[ppm]
Clipped = TRUE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

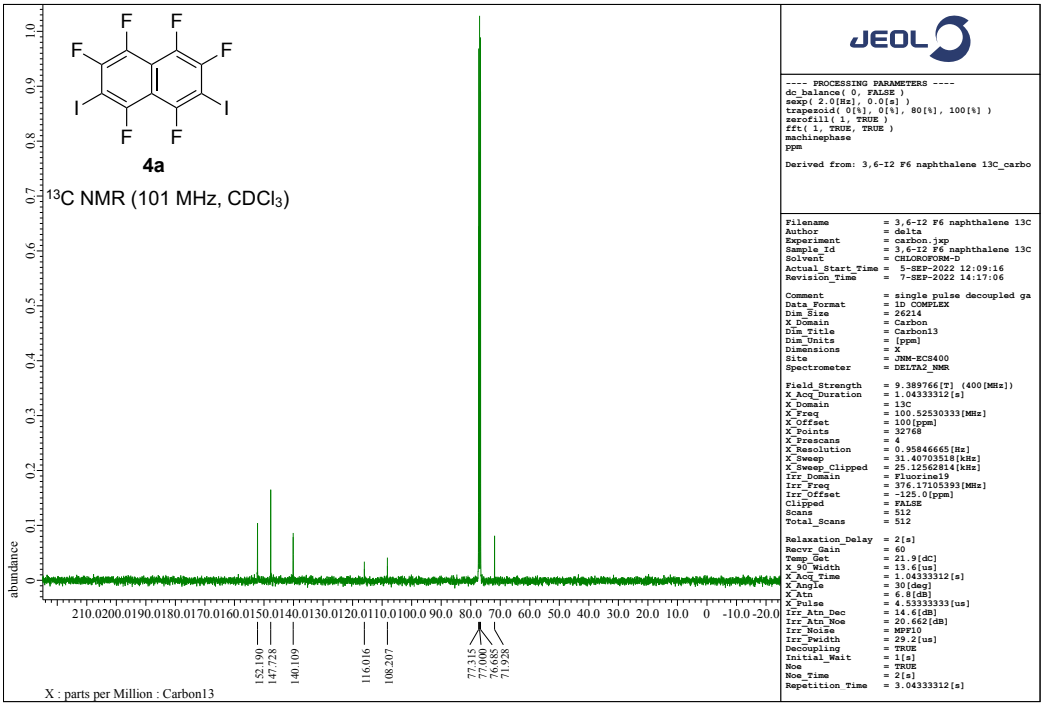

3b
19F NMR (376 MHz, CDCl3)
2.00
1.98
1.98
abundance
100.0
0
-100.0
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-Br2 F6 naphthalene 19F.jdf
Filename = 3,7-Br2 F6 naphthalene 19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220301 1676 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-MAR-2022 09:15:45
Revision_Time = 17-JAN-2023 12:44:45
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 46
Temp_Get = 20.2[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

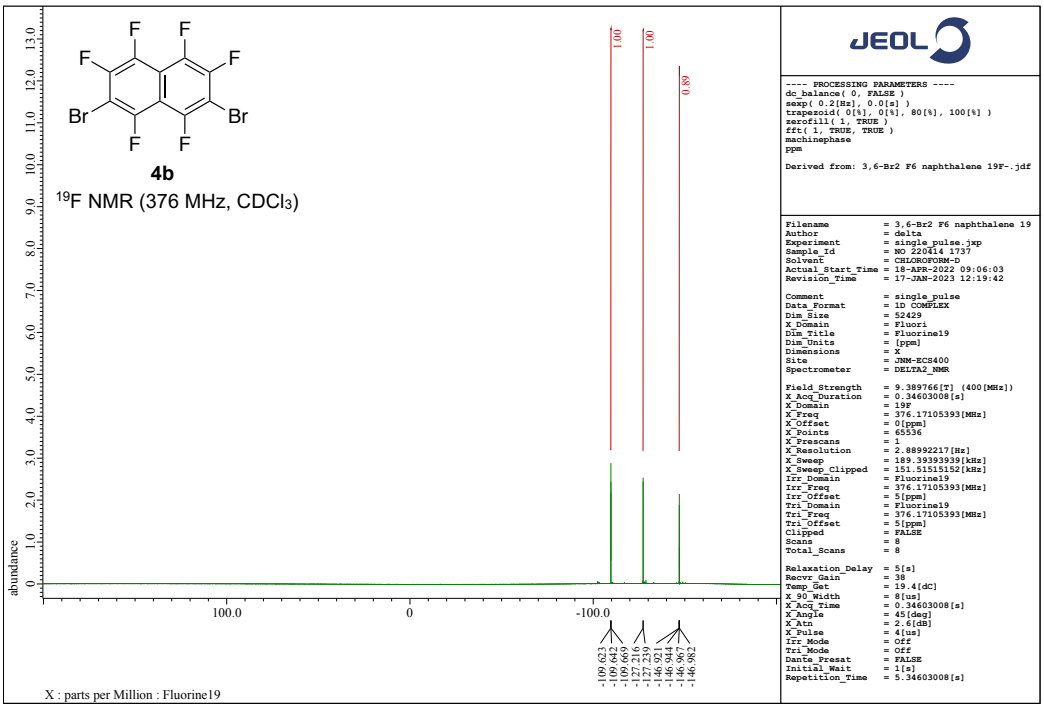

3b
13C NMR (101 MHz, CDCl3)
150.369
144.924
140.014
111.010
100.684
77.315
77.000
76.696
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-Br2 F6 naphthalene 13C_carb
Filename = 3,7-Br2 F6 naphthalene 13
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-Br2 F6 naphthalene 13
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-MAY-2022 20:39:11
Revision_Time = 7-SEP-2022 14:07:23
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = TRUE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 20.4[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

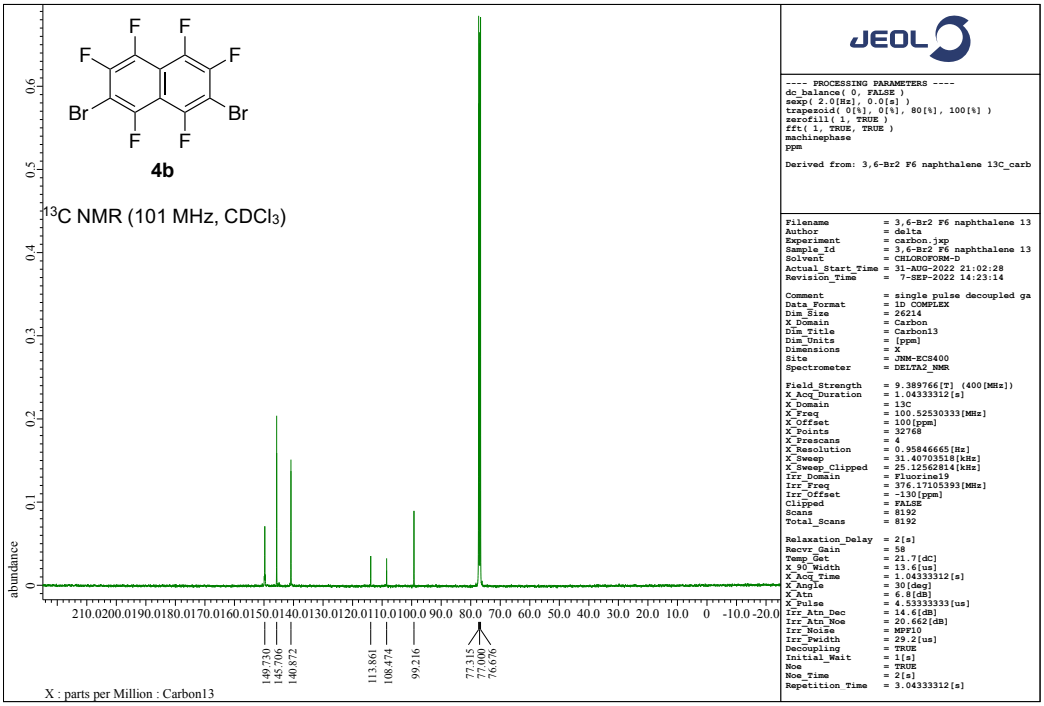

3c
19F NMR (376 MHz, CDCl3)
1.00
0.97
1.02
100.0
0
-100.0
-120.163
-120.309
-120.549
-120.758
-136.327
-136.350
-136.516
-136.761
-145.969
-145.907
abundance
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-Cl2 F6 naphthalene 19F.jdf
Filename = 3,7-Cl2 F6 naphthalene 19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220301 1677 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-MAR-2022 09:29:30
Revision_Time = 17-JAN-2023 12:46:42
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.9[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

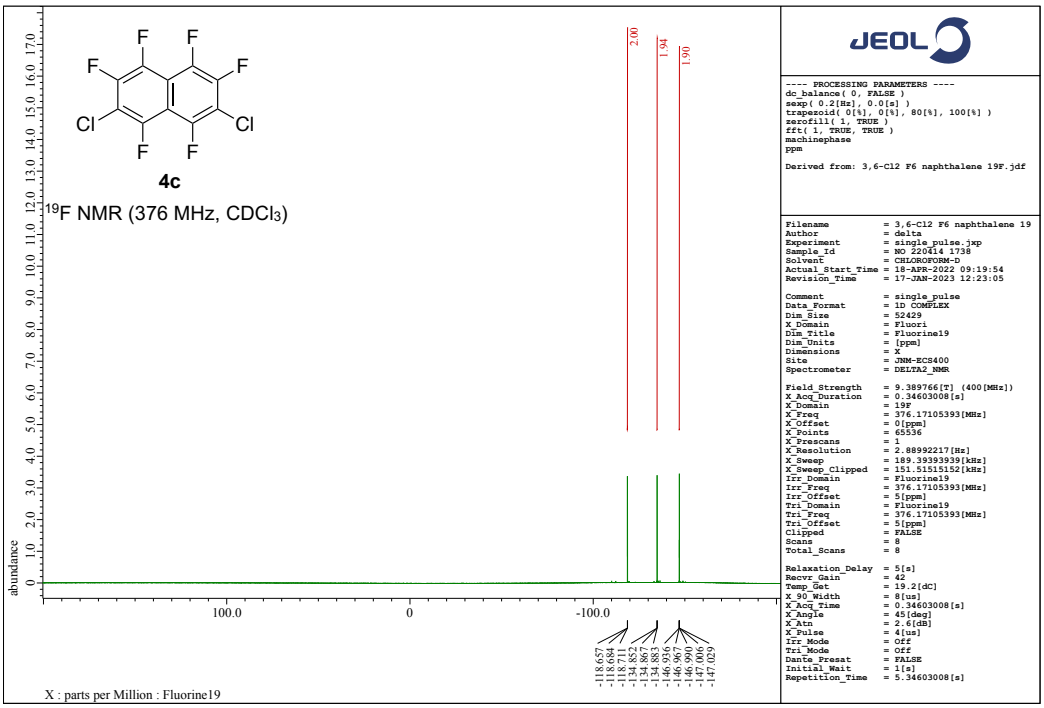

3c
13C NMR (101 MHz, CDCl3)
149.301
144.295
140.386
112.268
110.085
77.315
77.000
76.685
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-Cl2 F6 naphthalene 13C_carb
Filename = 3,7-Cl2 F6 naphthalene 13
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-Cl2 F6 naphthalene 13
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-JUN-2022 09:14:45
Revision_Time = 7-SEP-2022 14:12:15
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.7[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

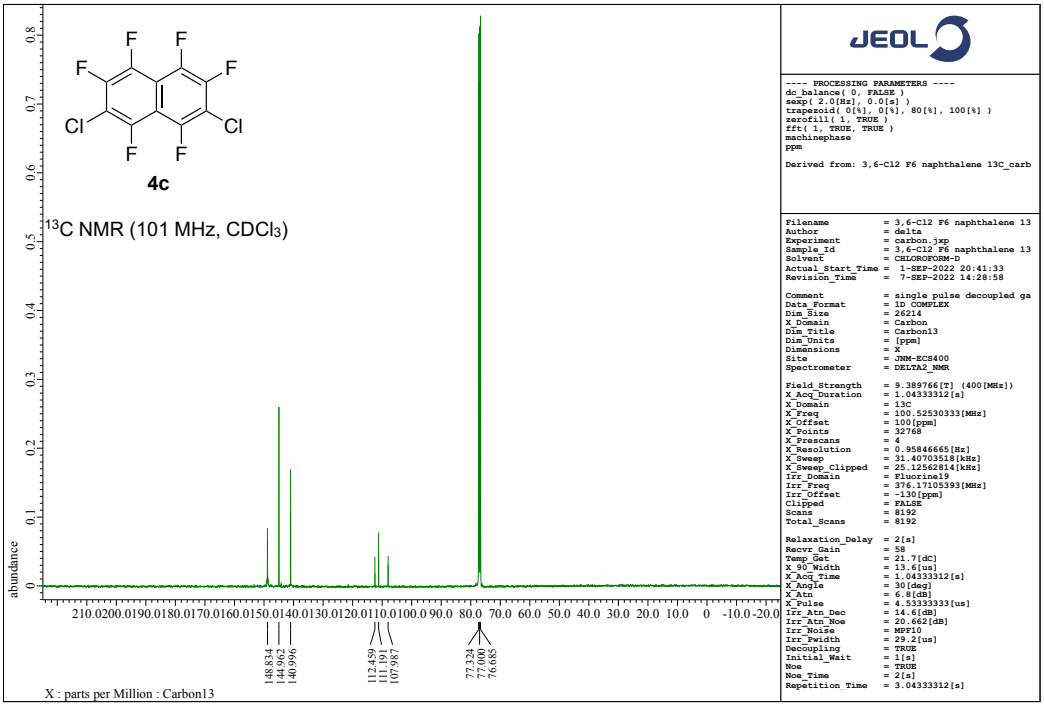

4a
19F NMR (376 MHz, CDCl3)
abundance
2.00
2.02
1.98
100.0
0
-100.0
-94.650
-94.673
-94.703
-114.878
-114.901
-114.925
-147.290
-147.305
-147.321
-147.344
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-I F6 naphthalene 19F_19F-1-
Filename = 3,6-I F6 naphthalene 19F_
Author = delta
Experiment = single_pulse.jxp
Sample_Id = 3,6-I F6 naphthalene 19F
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2022 13:03:33
Revision_Time = 17-JAN-2023 12:27:34
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 21.3[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

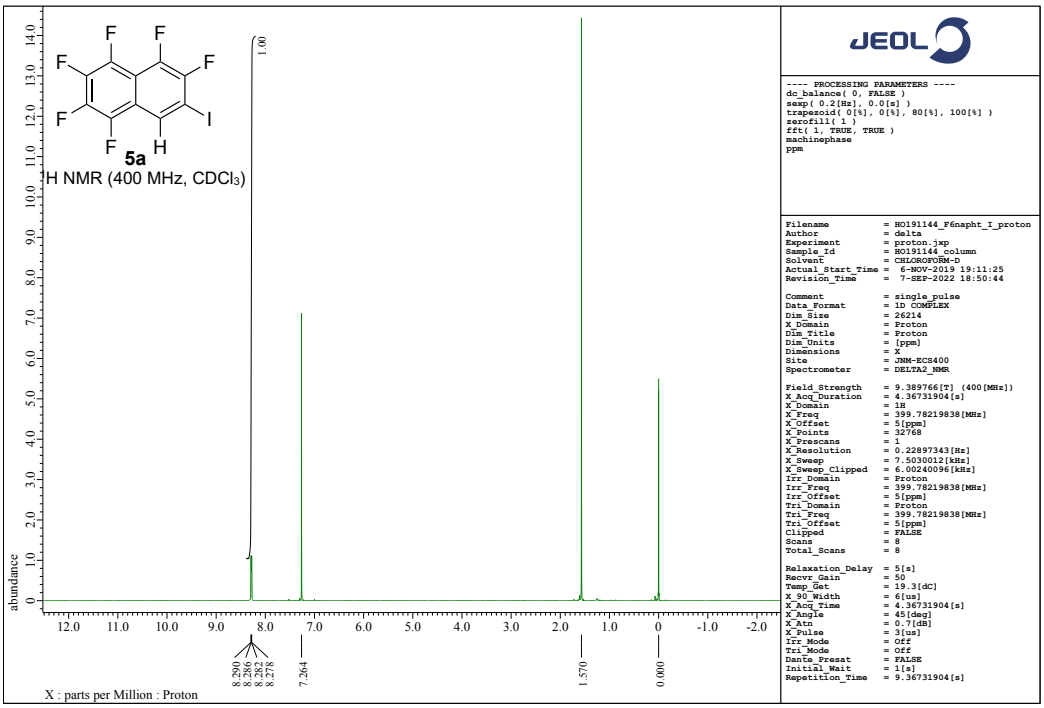

4a
13C NMR (101 MHz, CDCl3)
abundance
152.190
147.728
140.109
116.016
108.207
77.315
77.000
76.685
71.928
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-I2 F6 naphthalene 13C_carbo
Filename = 3,6-I2 F6 naphthalene 13C
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,6-I2 F6 naphthalene 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2022 12:09:16
Revision_Time = 7-SEP-2022 14:17:06
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -125.0[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.9[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

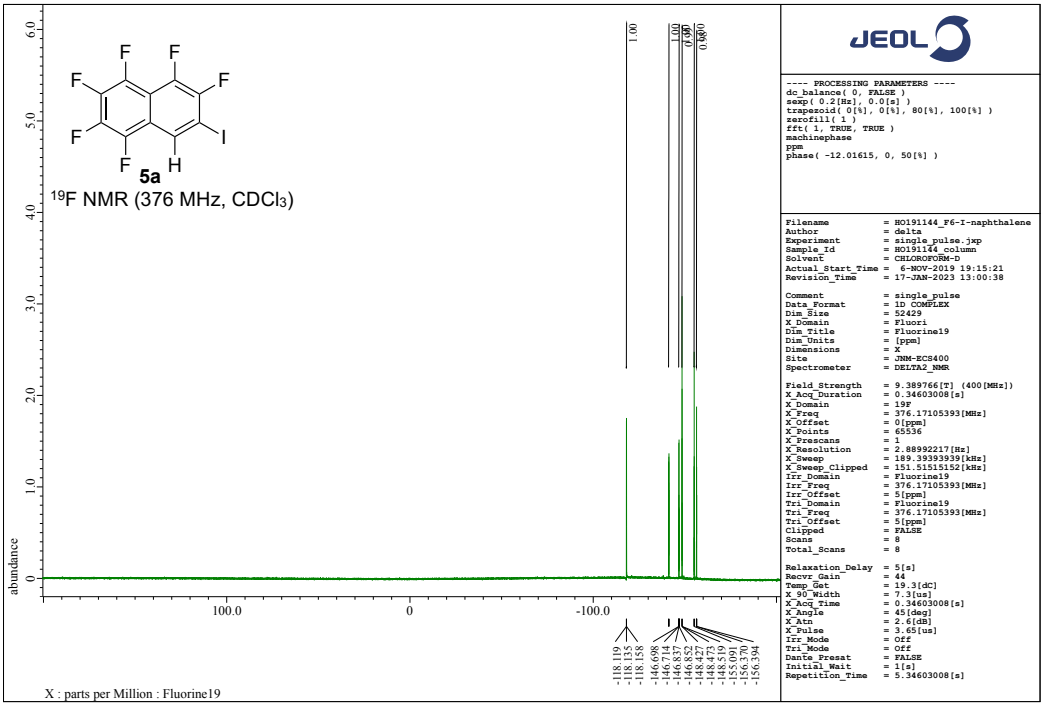

F
F
F
F
Br
Br
F
F
4b
19F NMR (376 MHz, CDCl3)
1.00
1.00
0.89
abundance
100.0
0
-100.0
-109.623
-109.642
-109.669
-127.219
-127.239
-146.921
-146.944
-146.967
-146.982
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-Br2 F6 naphthalene 19F-.jdf
Filename = 3,6-Br2 F6 naphthalene 19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220414 1737
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-APR-2022 09:06:03
Revision_Time = 17-JAN-2023 12:19:42
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 38
Temp_Get = 19.4[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

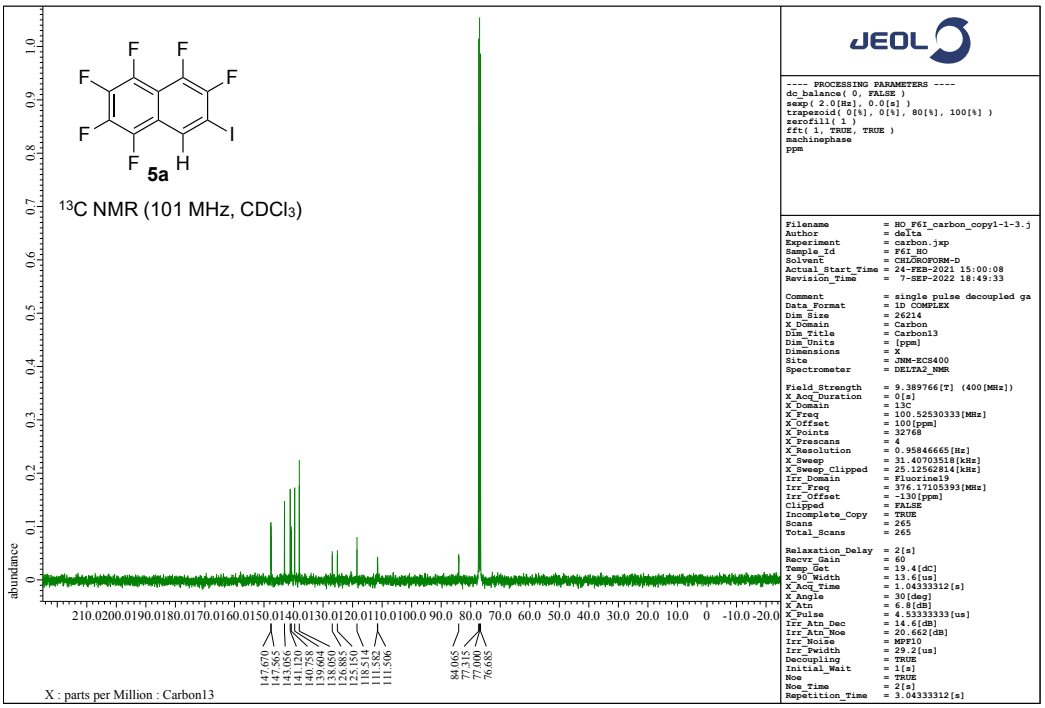

F
F
F
F
Br
Br
F
F
4b
13C NMR (101 MHz, CDCl3)
abundance
149.730
145.706
140.872
113.861
108.474
99.216
77.315
77.000
76.696
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-Br2 F6 naphthalene 13C_carb
Filename = 3,6-Br2 F6 naphthalene 13
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,6-Br2 F6 naphthalene 13
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-AUG-2022 21:02:28
Revision_Time = 7-SEP-2022 14:23:14
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 21.7[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

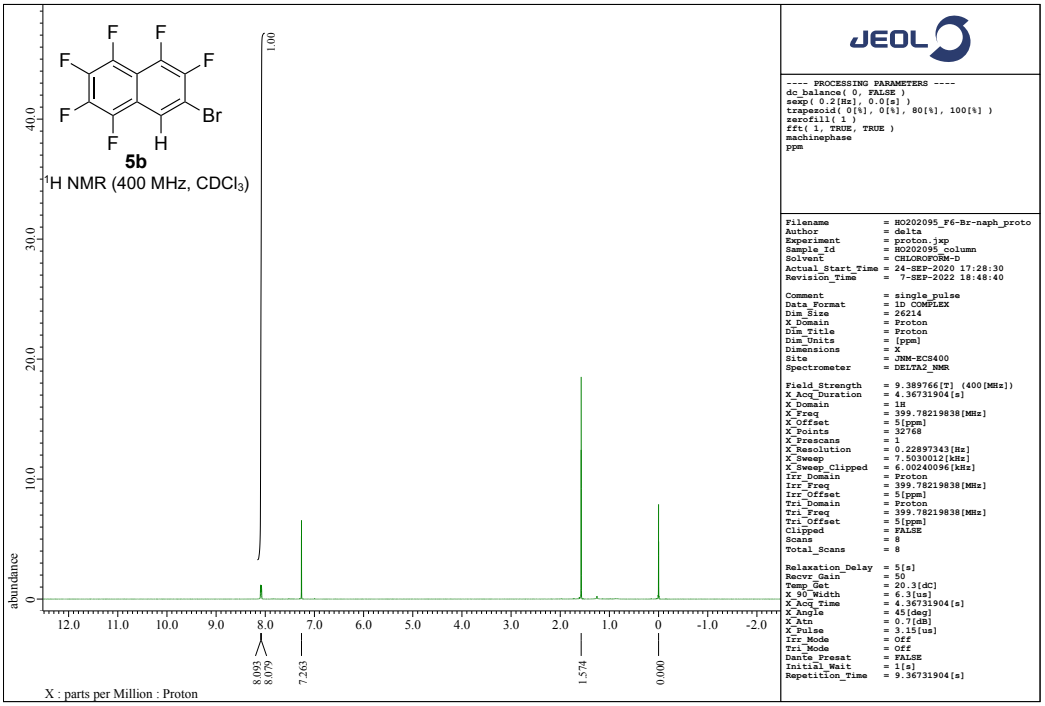

4c
19F NMR (376 MHz, CDCl3)
2.00
1.94
1.90
abundance
100.0
0
-100.0
-118.657
-118.694
-118.825
-134.867
-134.883
-146.956
-146.995
-146.990
-147.006
-147.029
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-Cl2 F6 naphthalene 19F.jdf
Filename = 3,6-Cl2 F6 naphthalene 19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220414 1738
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-APR-2022 09:19:54
Revision_Time = 17-JAN-2023 12:23:05
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.2[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

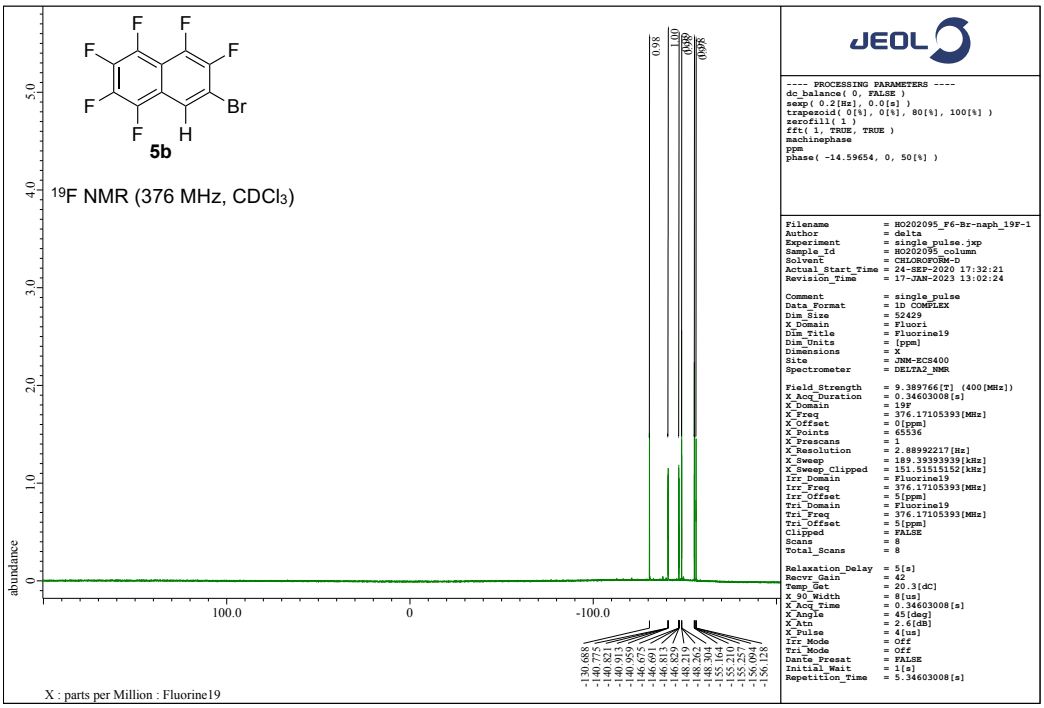

4c
13C NMR (101 MHz, CDCl3)
abundance
148.834
144.962
140.996
112.459
111.918
107.987
77.324
77.008
76.685
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-Cl2 F6 naphthalene 13C_carb
Filename = 3,6-Cl2 F6 naphthalene 13
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,6-Cl2 F6 naphthalene 13
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-SEP-2022 20:41:33
Revision_Time = 7-SEP-2022 14:28:58
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 21.7[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

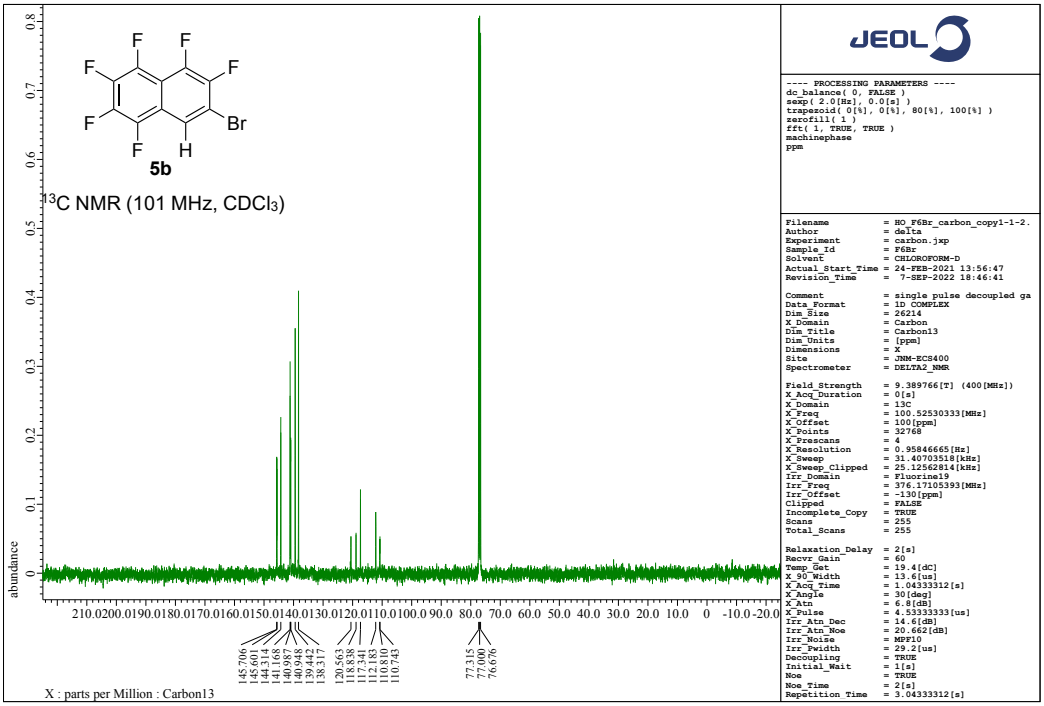

5a
1H NMR (400 MHz, CDCl3)
abundance
X : parts per Million : Proton
8.290
8.266
8.252
8.278
7.264
1.570
0.000
1.00
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = H0191144_F6napht_I_proton
Author = delta
Experiment = proton.jxp
Sample_Id = H0191144 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-NOV-2019 19:11:25
Revision_Time = 7-SEP-2022 18:50:44
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 19.3[dC]
X_90_Width = 6[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

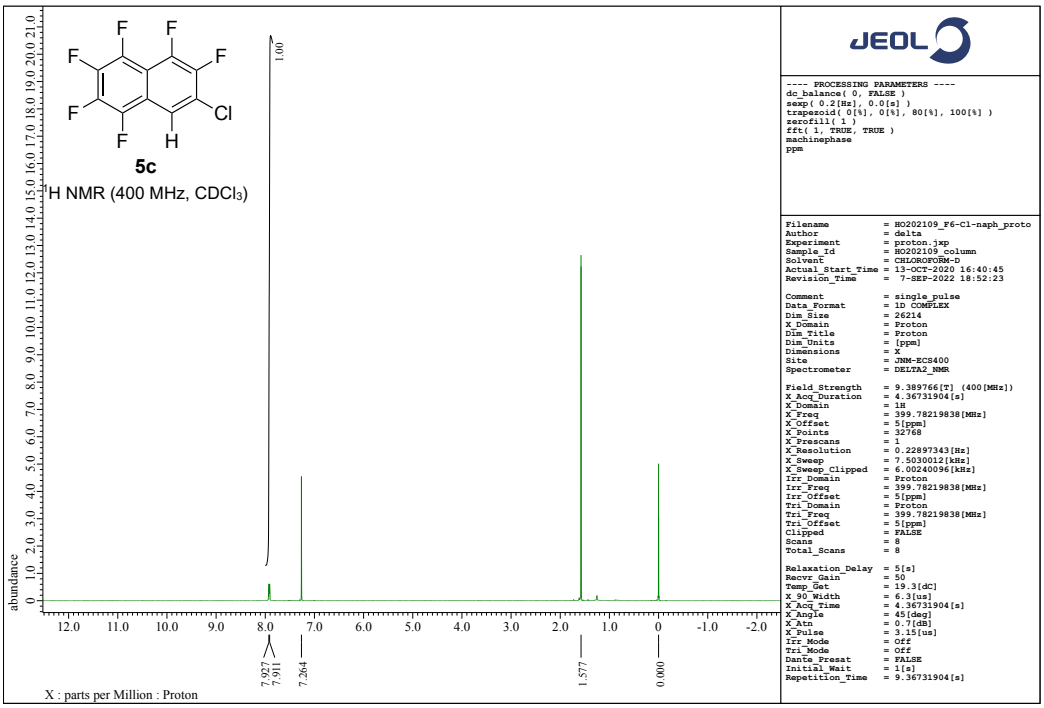

5a
19F NMR (376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19
-118.119
-118.135
-118.158
-146.698
-146.714
-146.737
-146.852
-148.427
-148.473
-148.519
-155.691
-156.370
-156.394
1.00
1.00
0.980
0.980
0.960
0.960
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-12.01615, 0, 50[%])
Filename = H0191144_F6-I-naphthalene
Author = delta
Experiment = single_pulse.jxp
Sample_Id = H0191144 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-NOV-2019 19:15:21
Revision_Time = 17-JAN-2023 13:00:38
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 44
Temp_Get = 19.3[dC]
X_90_Width = 7.3[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 3.65[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

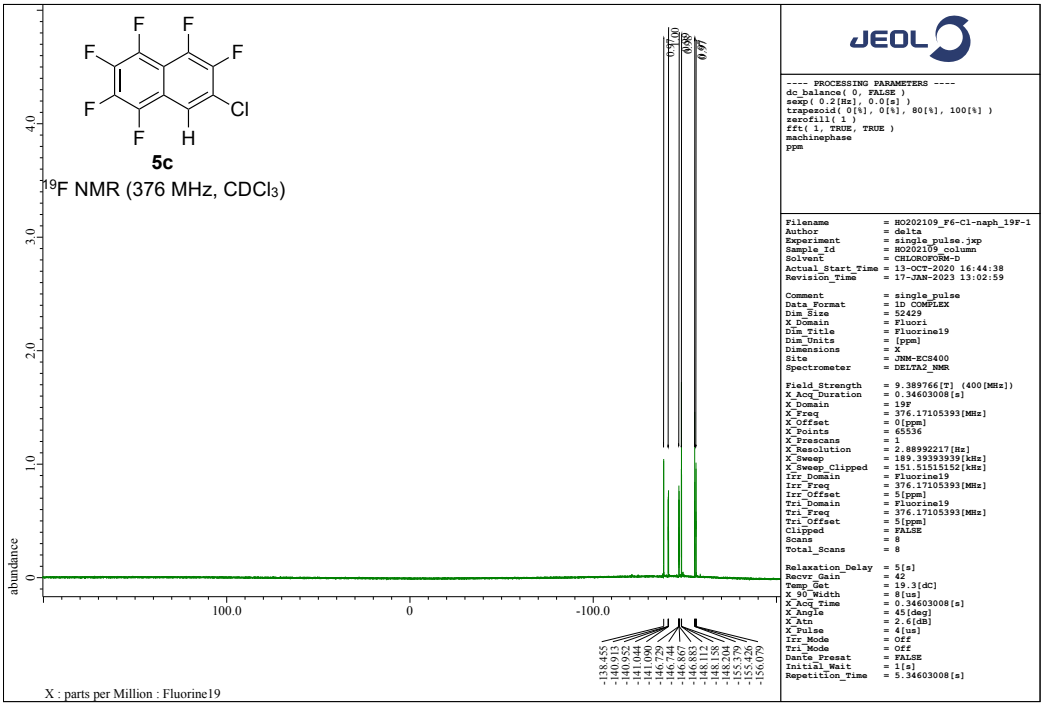

5a
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO_F6I_carbon_copy1-1-3.j
Author = delta
Experiment = carbon.jxp
Sample_Id = F6I_HO
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-FEB-2021 15:00:08
Revision_Time = 7-SEP-2022 18:49:33
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 265
Total_Scans = 265
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.4[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
DecCoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

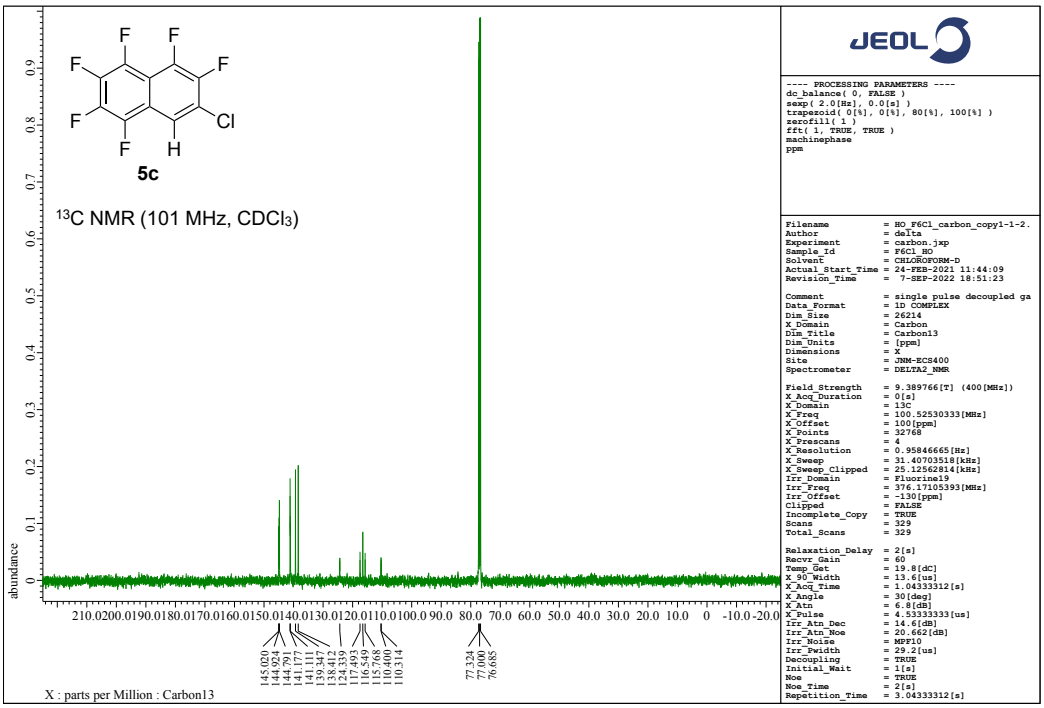

5b
1H NMR (400 MHz, CDCl3)
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO202095_F6-Br-naph_proto
Author = delta
Experiment = proton.jxp
Sample_Id = HO202095_column
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-SEP-2020 17:28:30
Revision_Time = 7-SEP-2022 18:48:40
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 20.3[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

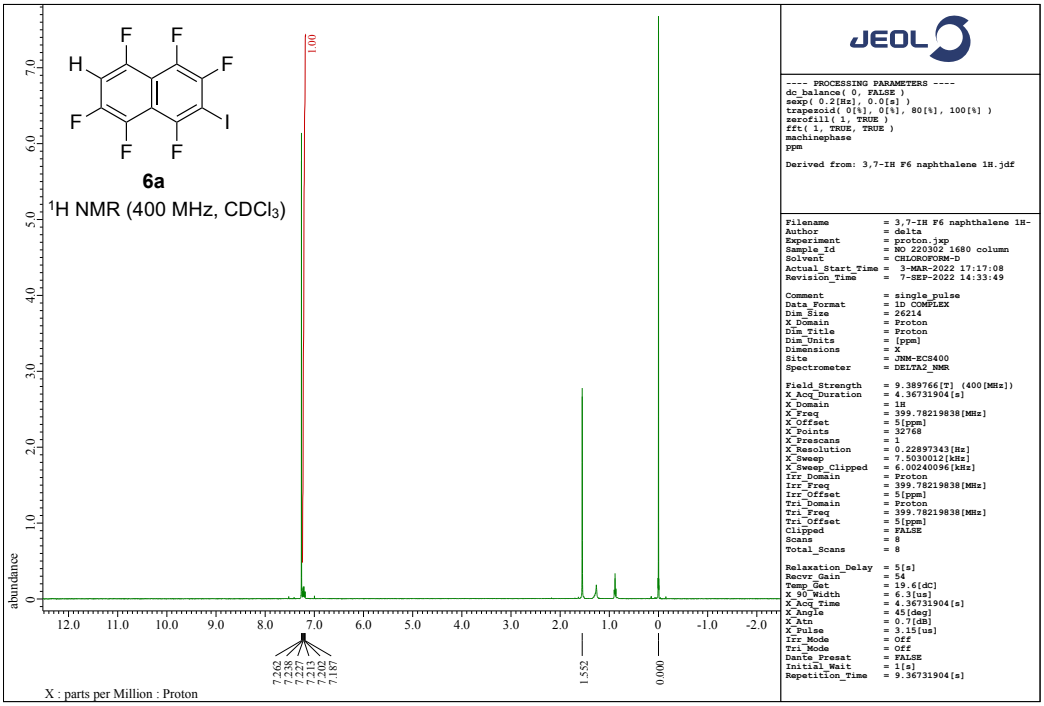

5b
19F NMR (376 MHz, CDCl3)
abundance
100.0
0
-100.0
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(-14.59654, 0, 50[%])
Filename = HO202095_F6-Br-naph_19F-1
Author = delta
Experiment = single_pulse.jxp
Sample_Id = HO202095 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-SEP-2020 17:32:21
Revision_Time = 17-JAN-2023 13:02:24
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 20.3[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

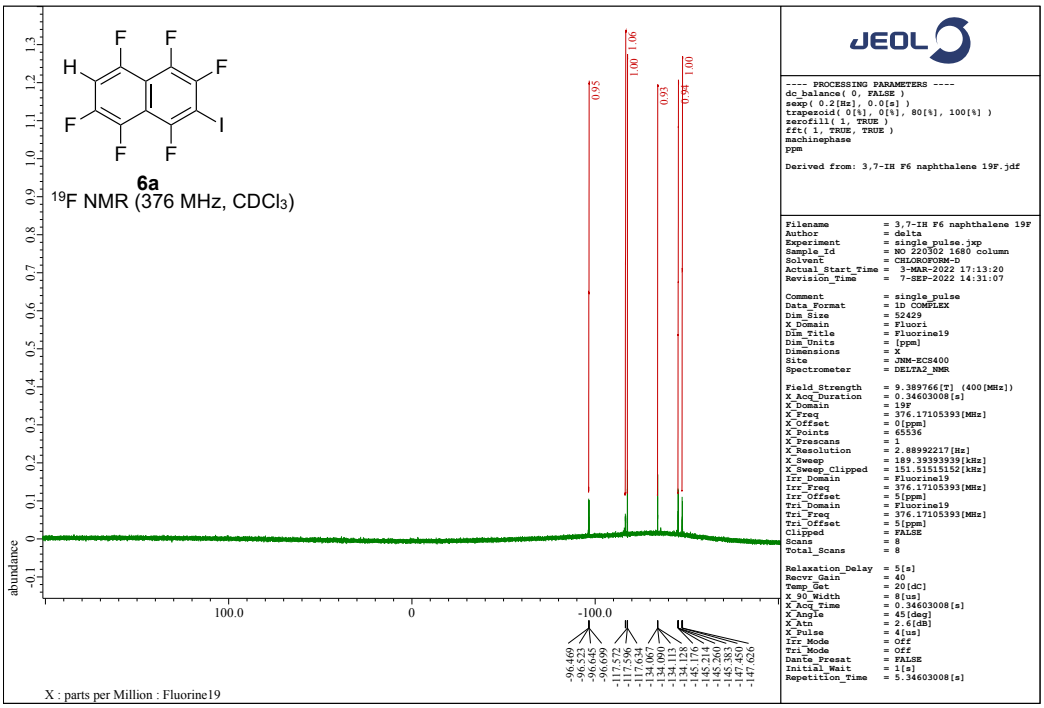

5b
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO_F6Br_carbon_copy1-1-2.
Author = delta
Experiment = carbon.jxp
Sample_Id = F6Br
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-FEB-2021 13:56:47
Revision_Time = 7-SEP-2022 18:46:41
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 255
Total_Scans = 255
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.4[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

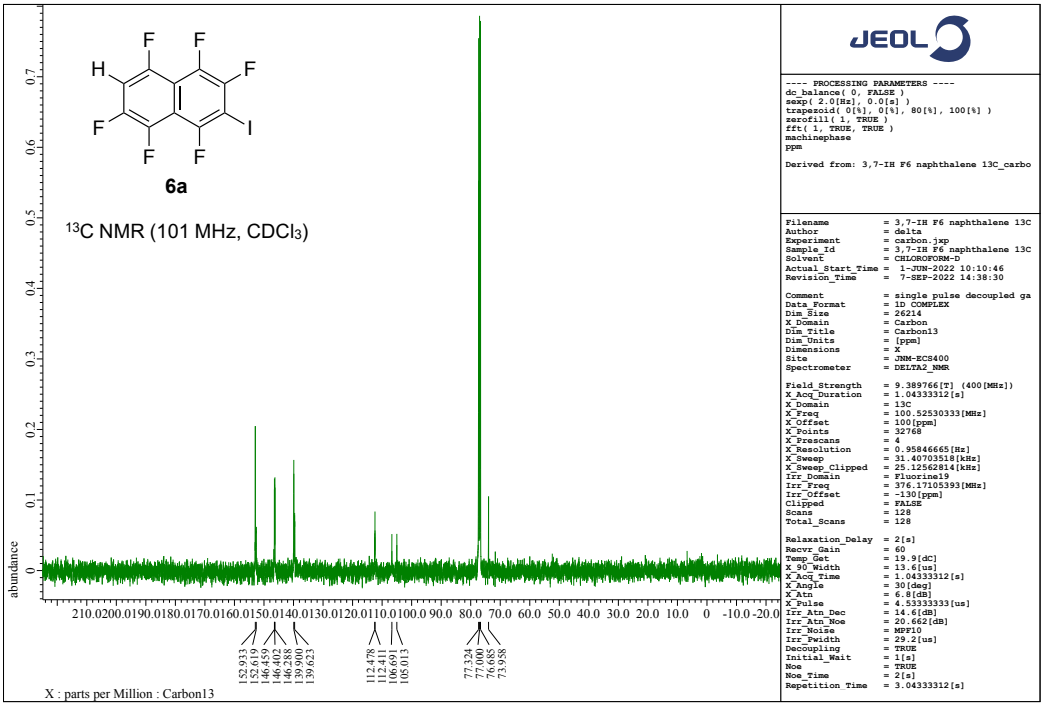

5c
^{1}H NMR (400 MHz, CDCl$_3$)
abundance
X : parts per Million : Proton
7.927
7.911
7.264
1.577
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO202109_F6-Cl-naph_proto
Author = delta
Experiment = proton.jxp
Sample_Id = HO202109_column
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-OCT-2020 16:40:45
Revision_Time = 7-SEP-2022 18:52:23
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 19.3[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

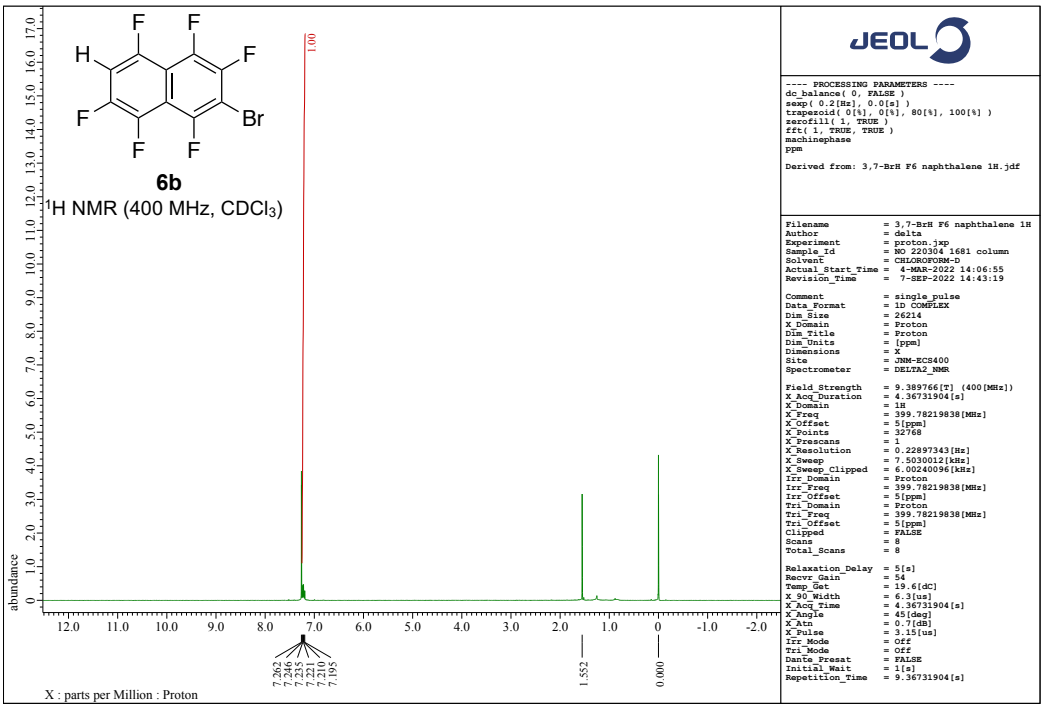

5c
^{19}F NMR (376 MHz, CDCl$_3$)
abundance
X : parts per Million : Fluorine19
-138.455
-140.913
-140.952
-141.044
-141.090
-146.729
-146.744
-146.867
-146.883
-148.112
-148.158
-148.204
-155.379
-155.426
-156.079
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO202109_F6-Cl-naph_19F-1
Author = delta
Experiment = single_pulse.jxp
Sample_Id = HO202109_column
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-OCT-2020 16:44:38
Revision_Time = 17-JAN-2023 13:02:59
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.3[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

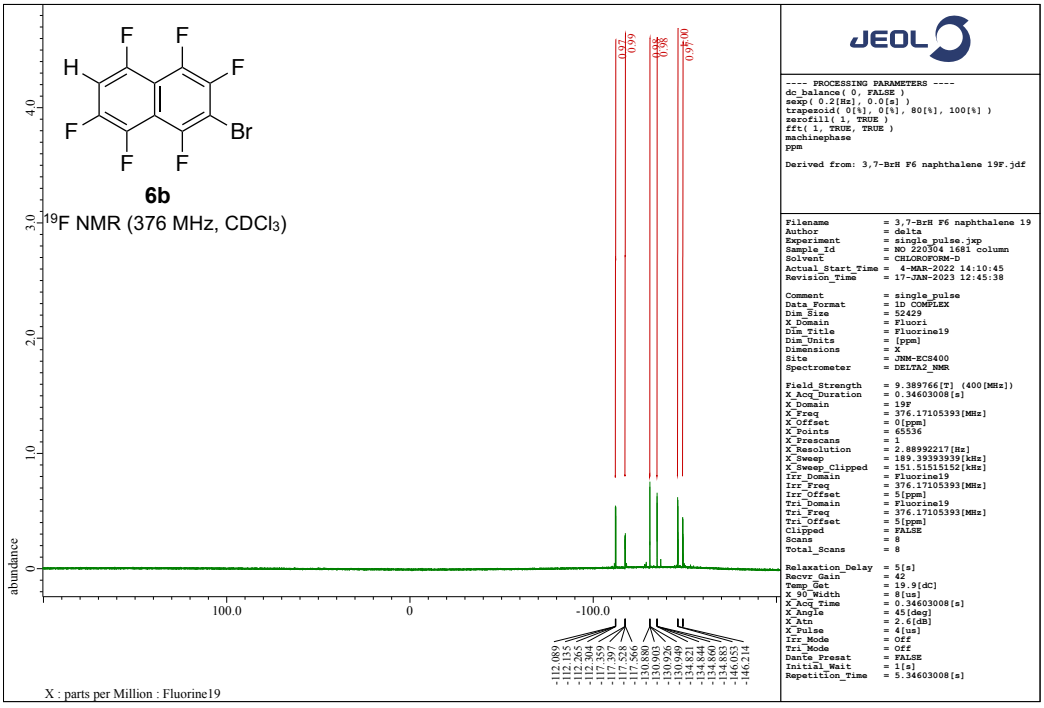

5c
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
145.020
144.924
144.791
141.177
141.111
139.347
138.412
124.359
124.253
116.549
115.768
110.400
110.314
77.324
77.000
76.685
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = HO_F6Cl_carbon_copy1-1-2.
Author = delta
Experiment = carbon.jxp
Sample_Id = F6Cl_HO
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-FEB-2021 11:44:09
Revision_Time = 7-SEP-2022 18:51:23
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Incomplete_Copy = TRUE
Scans = 329
Total_Scans = 329
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.8[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
DecCoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

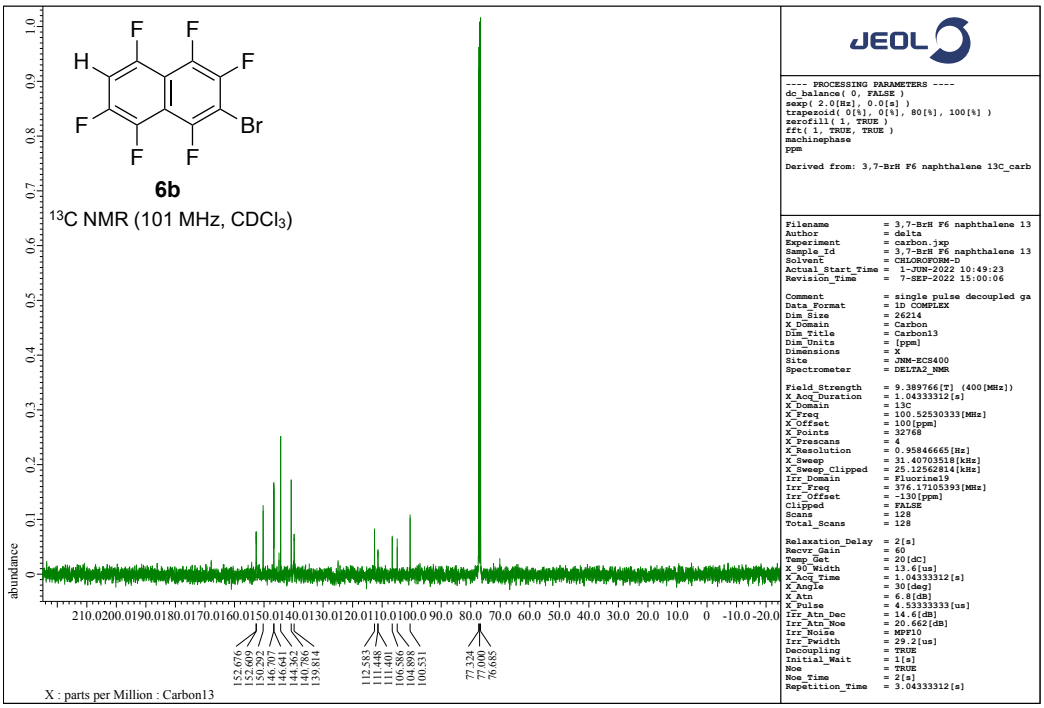

6a
1H NMR (400 MHz, CDCl3)
1.00
abundance
X : parts per Million : Proton
7.262
7.238
7.225
7.213
7.202
7.187
1.552
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-IH F6 naphthalene 1H.jdf
Filename = 3,7-IH F6 naphthalene 1H-
Author = delta
Experiment = proton.jxp
Sample_Id = NO 220302 1680 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-MAR-2022 17:17:08
Revision_Time = 7-SEP-2022 14:33:49
Comment = single pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 54
Temp_Get = 19.6[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

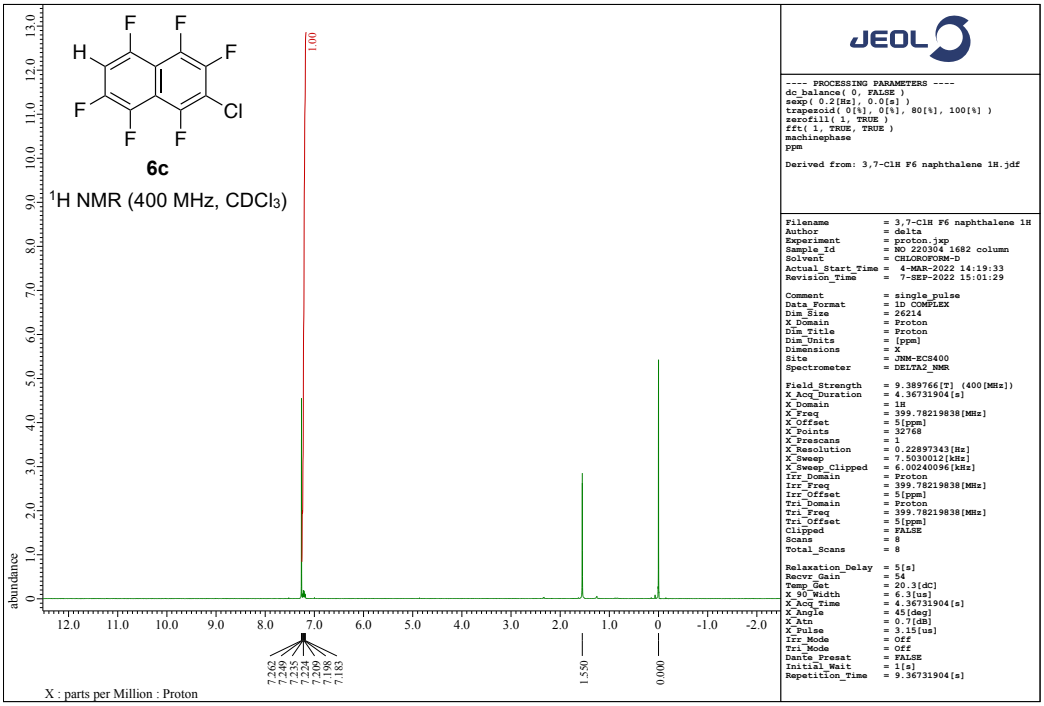

6a
19F NMR (376 MHz, CDCl3)
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-IH F6 naphthalene 19F.jdf
Filename = 3,7-IH F6 naphthalene 19F
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220302 1680 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-MAR-2022 17:13:20
Revision_Time = 7-SEP-2022 14:31:07
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 40
Temp_Get = 20[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

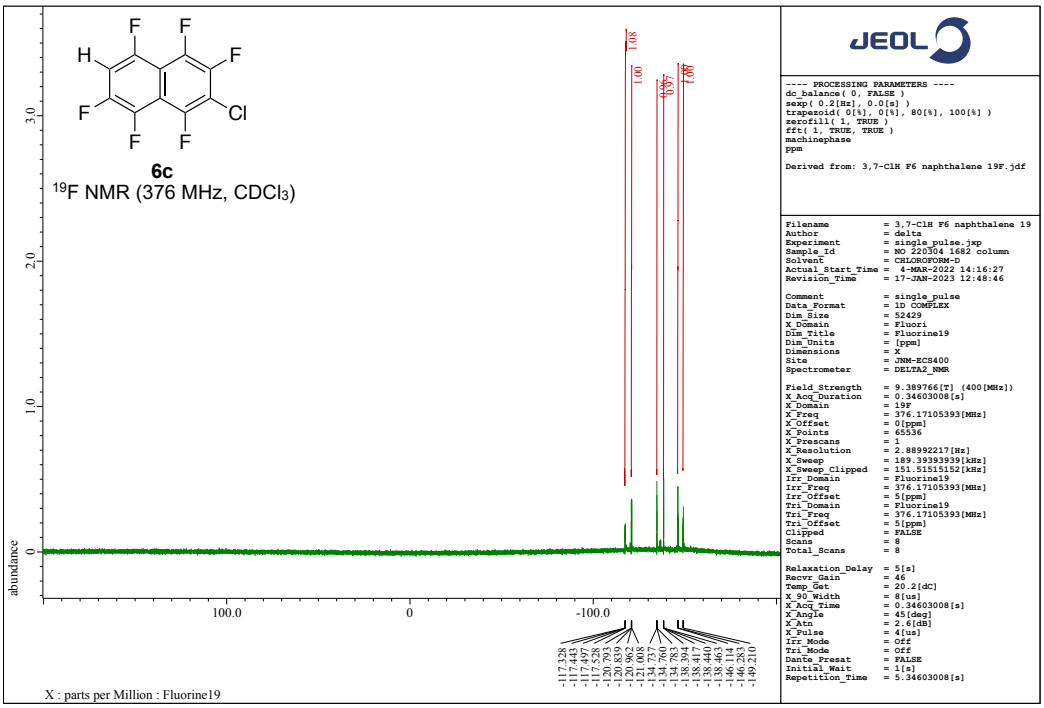

6a
13C NMR (101 MHz, CDCl3)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-IH F6 naphthalene 13C_carbo
Filename = 3,7-IH F6 naphthalene 13C
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-IH F6 naphthalene 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-JUN-2022 10:10:46
Revision_Time = 7-SEP-2022 14:38:30
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.9[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

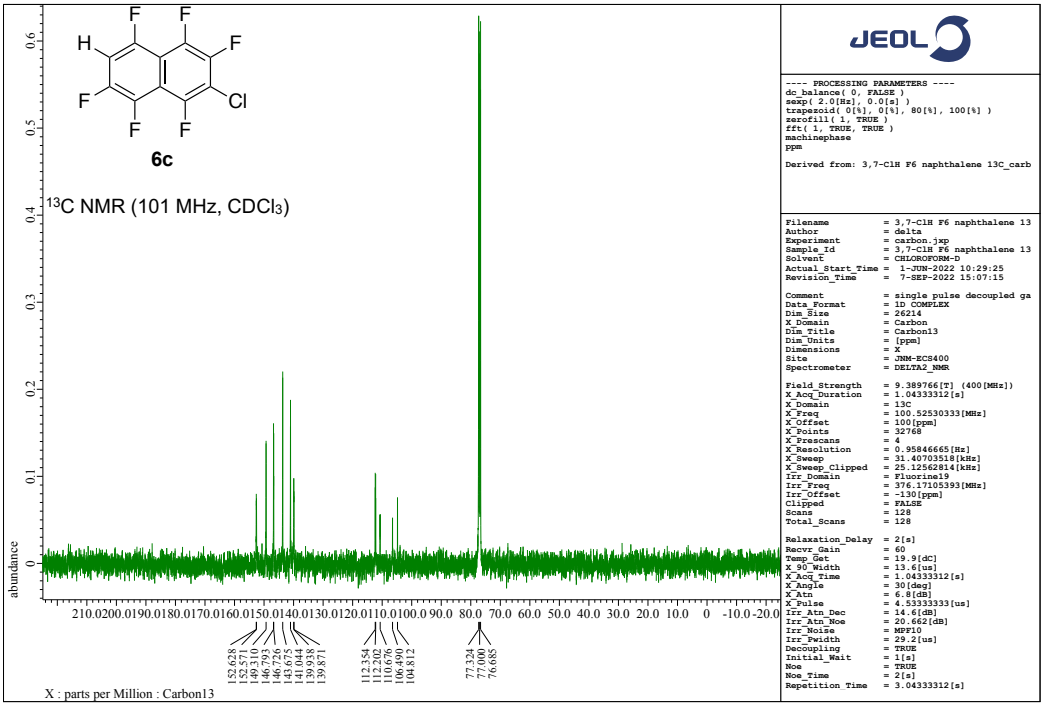

6b
^{1}H NMR (400 MHz, CDCl$_3$)
abundance
X : parts per Million : Proton
7.262
7.246
7.235
7.221
7.210
7.195
1.552
0.000
1.00
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-BrH F6 naphthalene 1H.jdf
Filename = 3,7-BrH F6 naphthalene 1H
Author = delta
Experiment = proton.jxp
Sample_Id = NO 220304 1681 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-MAR-2022 14:06:55
Revision_Time = 7-SEP-2022 14:43:19
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 54
Temp_Get = 19.6[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

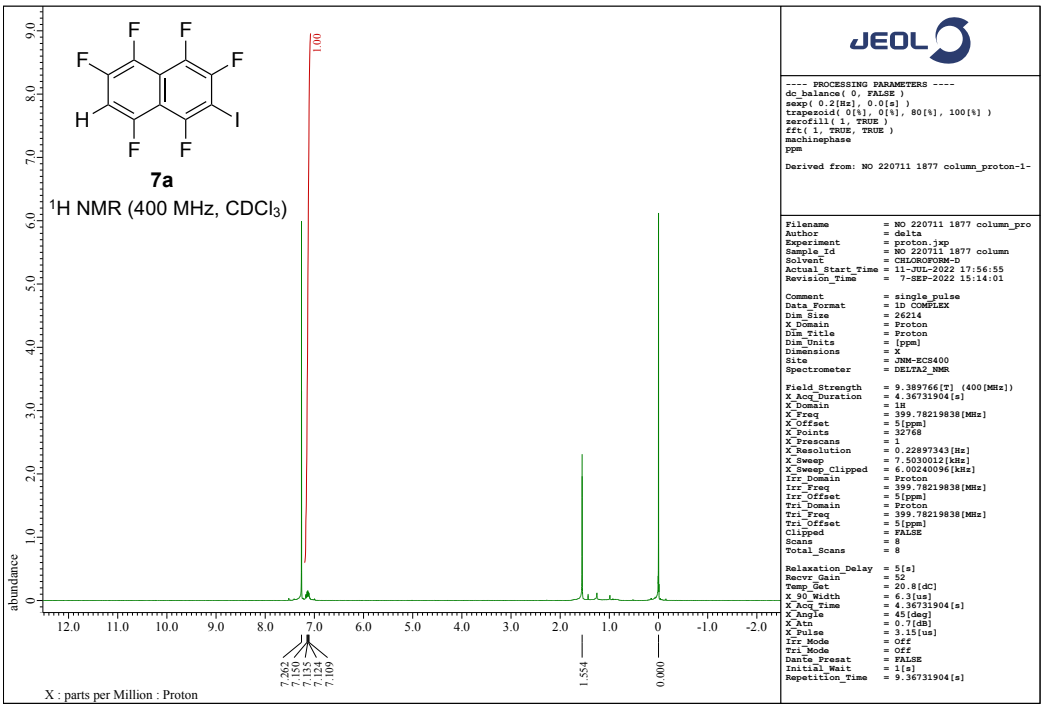

6b
^{19}F NMR (376 MHz, CDCl$_3$)
abundance
X : parts per Million : Fluorine19
-112.089
-112.135
-112.265
-112.304
-117.359
-117.397
-117.528
-117.566
-130.880
-130.903
-130.926
-134.949
-134.971
-134.844
-134.860
-134.883
-146.053
-146.214
0.97
0.99
0.98
0.98
0.97
1.00
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-BrH F6 naphthalene 19F.jdf
Filename = 3,7-BrH F6 naphthalene 19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220304 1681 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-MAR-2022 14:10:45
Revision_Time = 17-JAN-2023 12:45:38
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.9[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

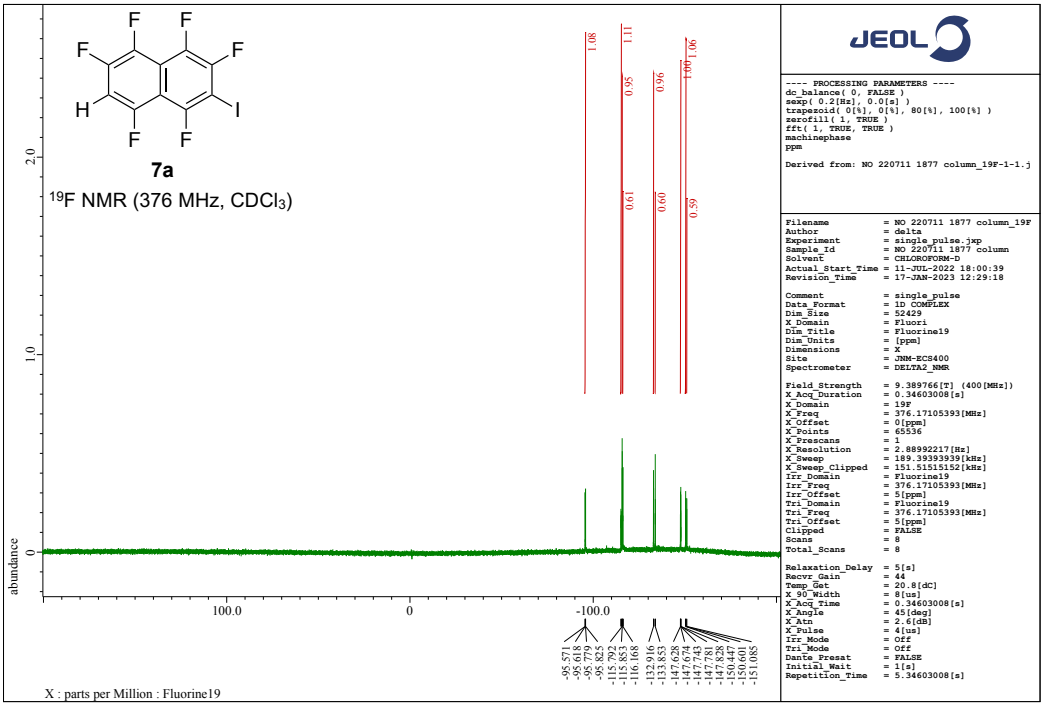

F
F
H
F
F
Br
F
F
6b
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
152.676
152.609
150.292
146.777
146.641
144.362
140.786
139.814
112.583
111.448
111.401
106.586
106.388
100.831
77.324
77.000
76.685
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-BrH F6 naphthalene 13C_carb
Filename = 3,7-BrH F6 naphthalene 13
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-BrH F6 naphthalene 13
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-JUN-2022 10:49:23
Revision_Time = 7-SEP-2022 15:00:06
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

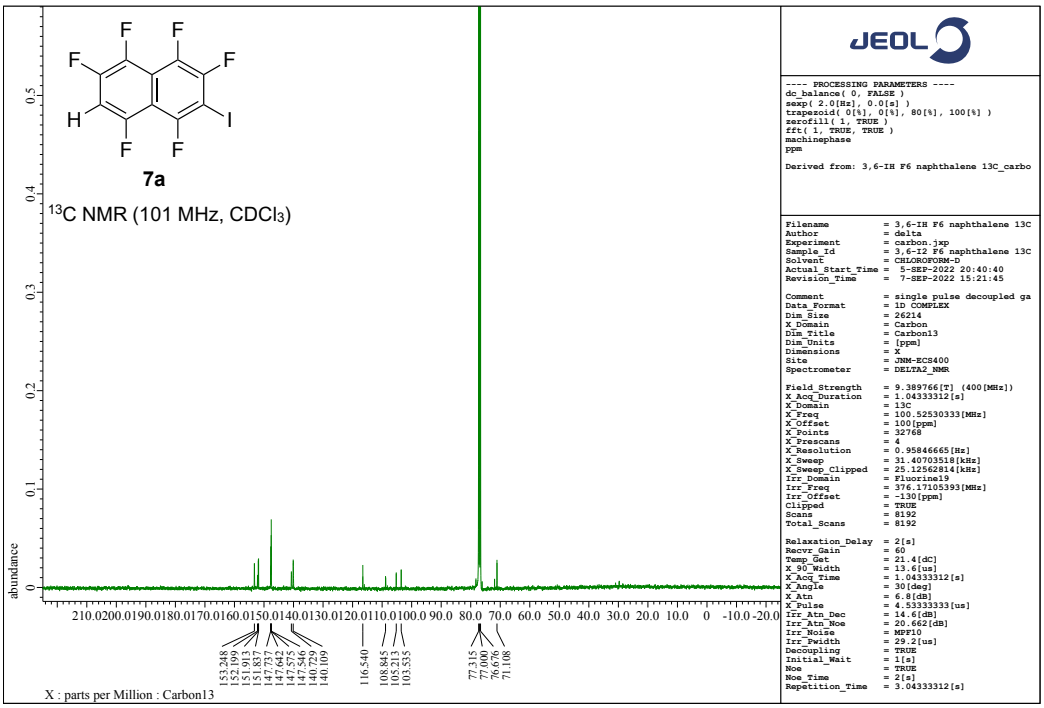

F
F
H
F
F
Cl
F
F
6c
1H NMR (400 MHz, CDCl3)
1.00
abundance
X : parts per Million : Proton
7.262
7.249
7.235
7.224
7.209
7.198
7.185
1.550
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-ClH F6 naphthalene 1H.jdf
Filename = 3,7-ClH F6 naphthalene 1H
Author = delta
Experiment = proton.jxp
Sample_Id = NO 220304 1682 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-MAR-2022 14:19:33
Revision_Time = 7-SEP-2022 15:01:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 54
Temp_Get = 20.3[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

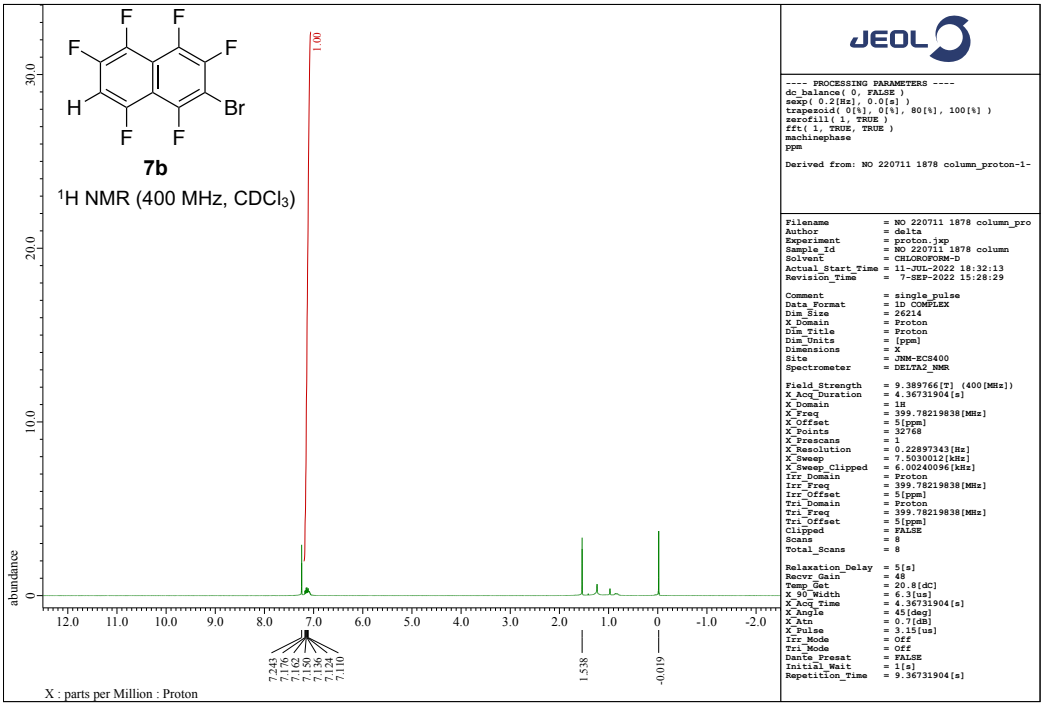

6c
19F NMR (376 MHz, CDCl3)
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-ClH F6 naphthalene 19F.jdf
Filename = 3,7-ClH F6 naphthalene 19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220304 1682 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-MAR-2022 14:16:27
Revision_Time = 17-JAN-2023 12:48:46
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 46
Temp_Get = 20.2[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

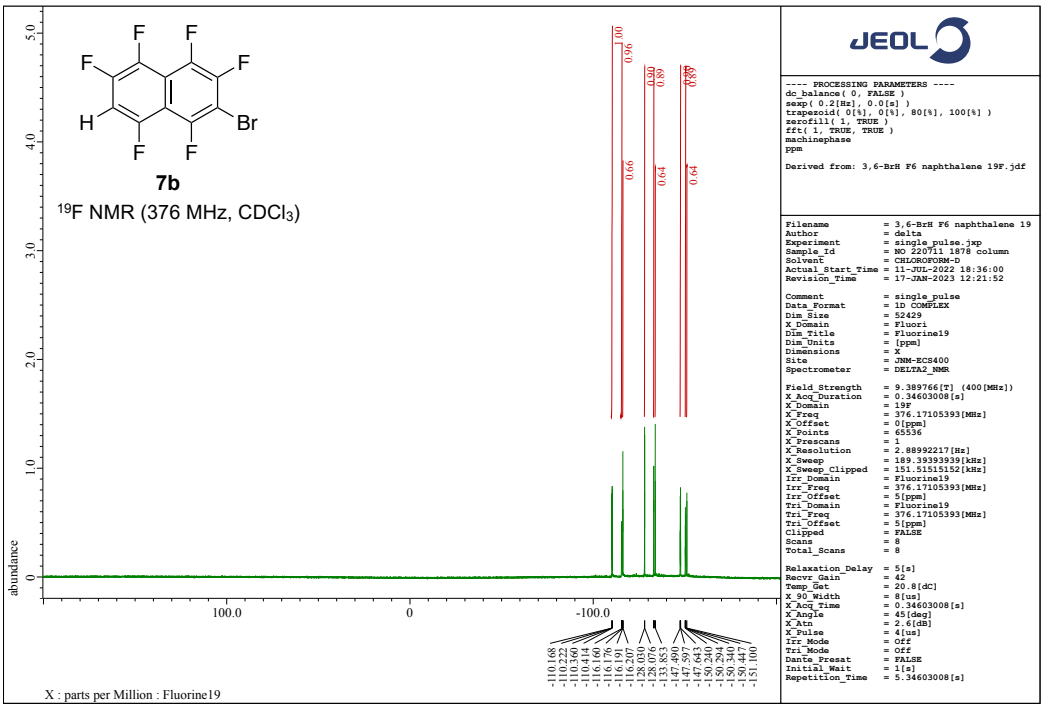

6c
13C NMR (101 MHz, CDCl3)
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-ClH F6 naphthalene 13C_carb
Filename = 3,7-ClH F6 naphthalene 13
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-ClH F6 naphthalene 13
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-JUN-2022 10:29:25
Revision_Time = 7-SEP-2022 15:07:15
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.9[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

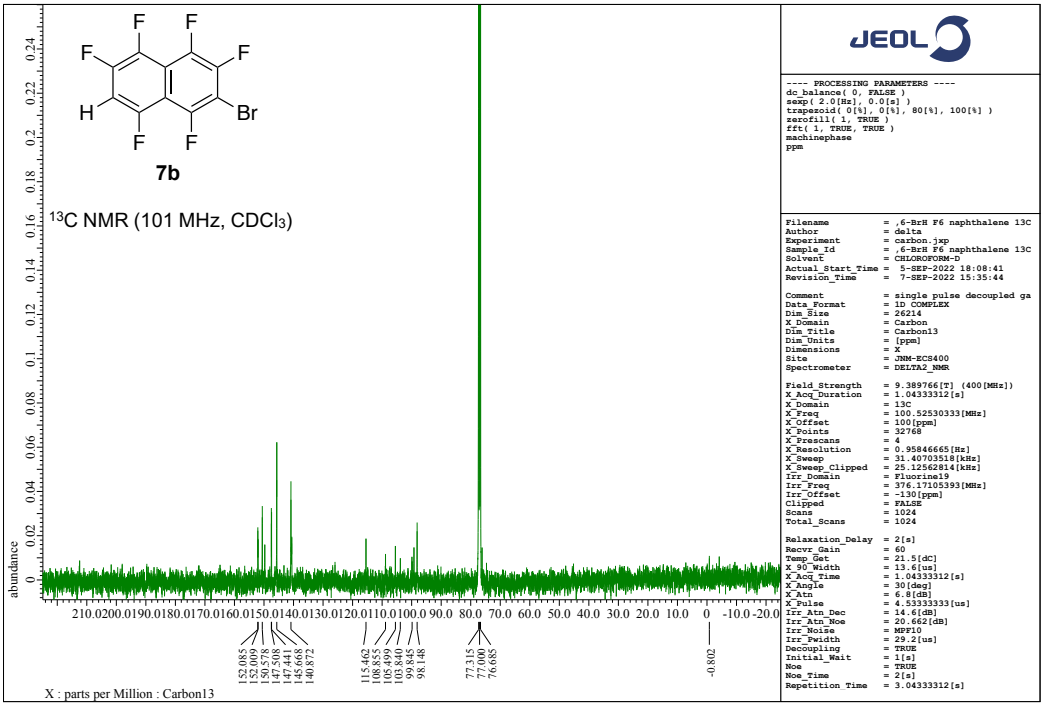

7a
1H NMR (400 MHz, CDCl3)
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO 220711 1877 column_proton-1-
Filename = NO 220711 1877 column_pro
Author = delta
Experiment = proton.jxp
Sample_Id = NO 220711 1877 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-JUL-2022 17:56:55
Revision_Time = 7-SEP-2022 15:14:01
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 52
Temp_Get = 20.8[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

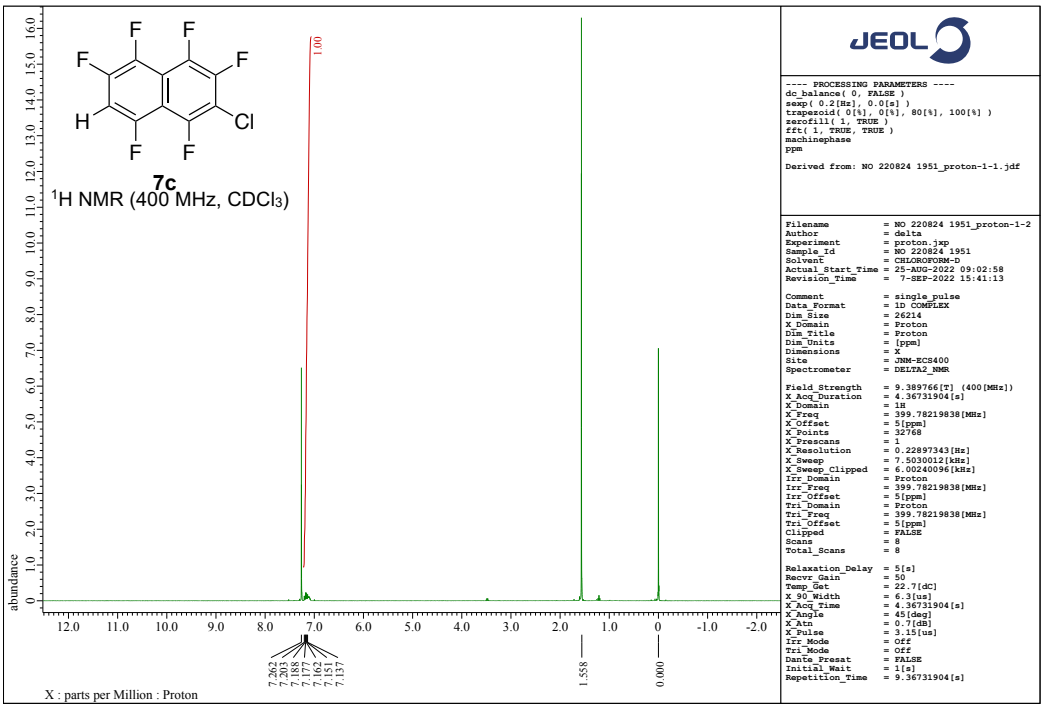

7a
19F NMR (376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO 220711 1877 column_19F-1-1.j
Filename = NO 220711 1877 column_19F
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220711 1877 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-JUL-2022 18:00:39
Revision_Time = 17-JAN-2023 12:29:18
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 44
Temp_Get = 20.8[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

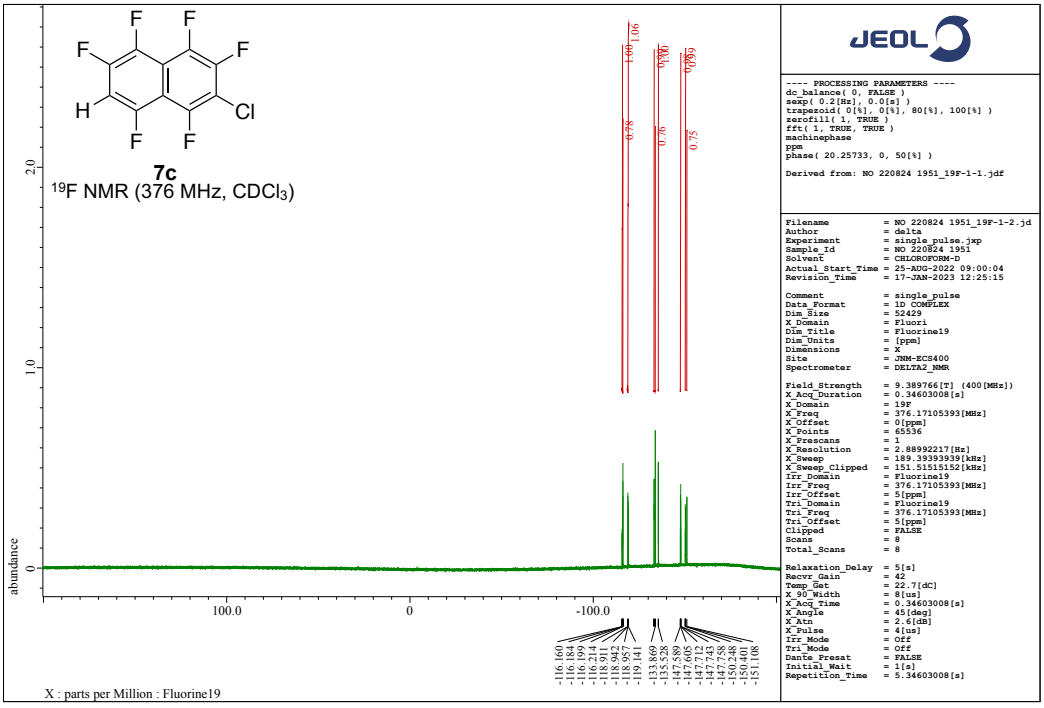

7a
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-IH F6 naphthalene 13C_carbo
Filename = 3,6-IH F6 naphthalene 13C
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,6-I2 F6 naphthalene 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2022 20:40:40
Revision_Time = 7-SEP-2022 15:21:45
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.4[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

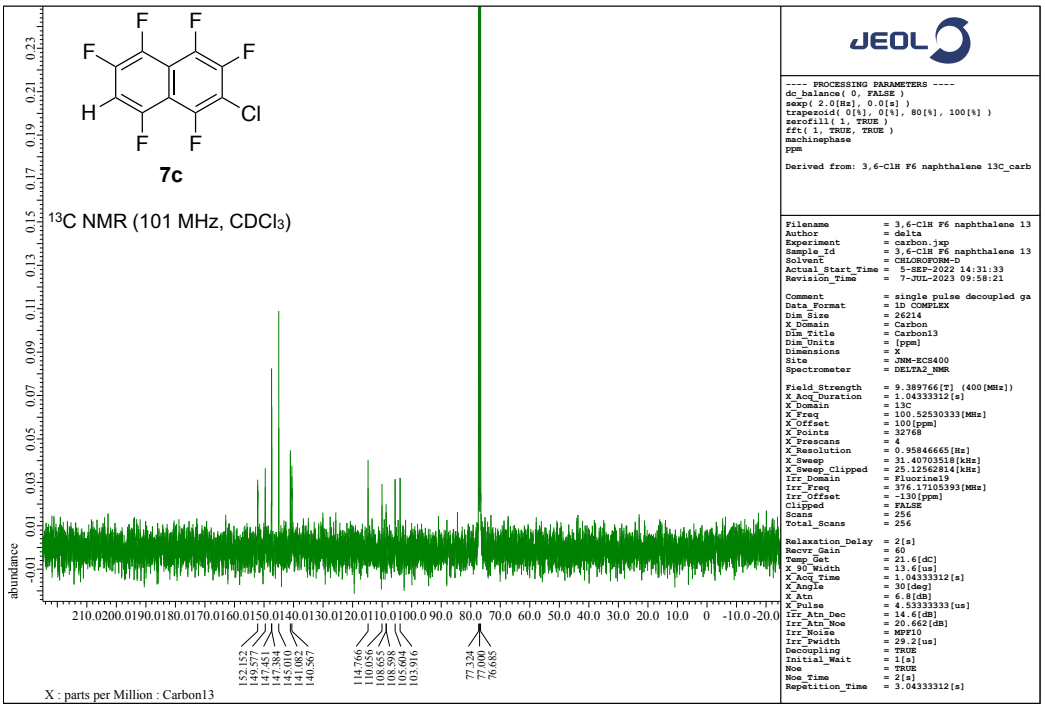

7b
1H NMR (400 MHz, CDCl3)
abundance
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO 220711 1878 column_proton-1-
Filename = NO 220711 1878 column_pro
Author = delta
Experiment = proton.jxp
Sample_Id = NO 220711 1878 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-JUL-2022 18:32:13
Revision_Time = 7-SEP-2022 15:28:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 48
Temp_Get = 20.8[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

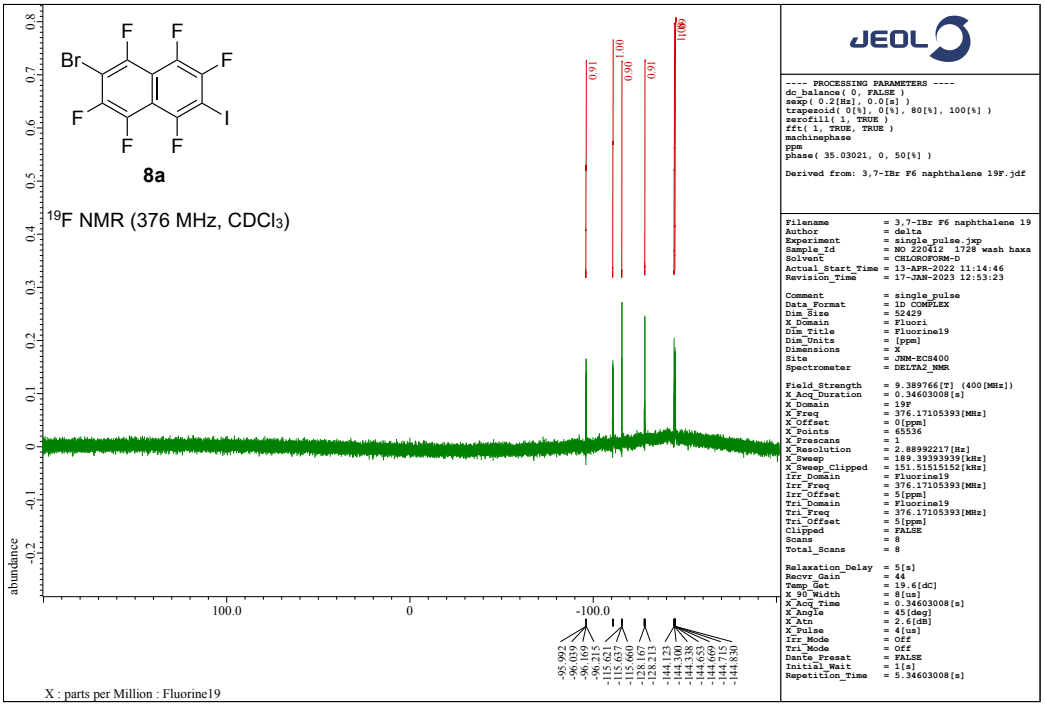

7b
19F NMR (376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,6-BrH F6 naphthalene 19F.jdf
Filename = 3,6-BrH F6 naphthalene 19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220711 1878 column
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-JUL-2022 18:36:00
Revision_Time = 17-JAN-2023 12:21:52
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 20.8[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
DanTe_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

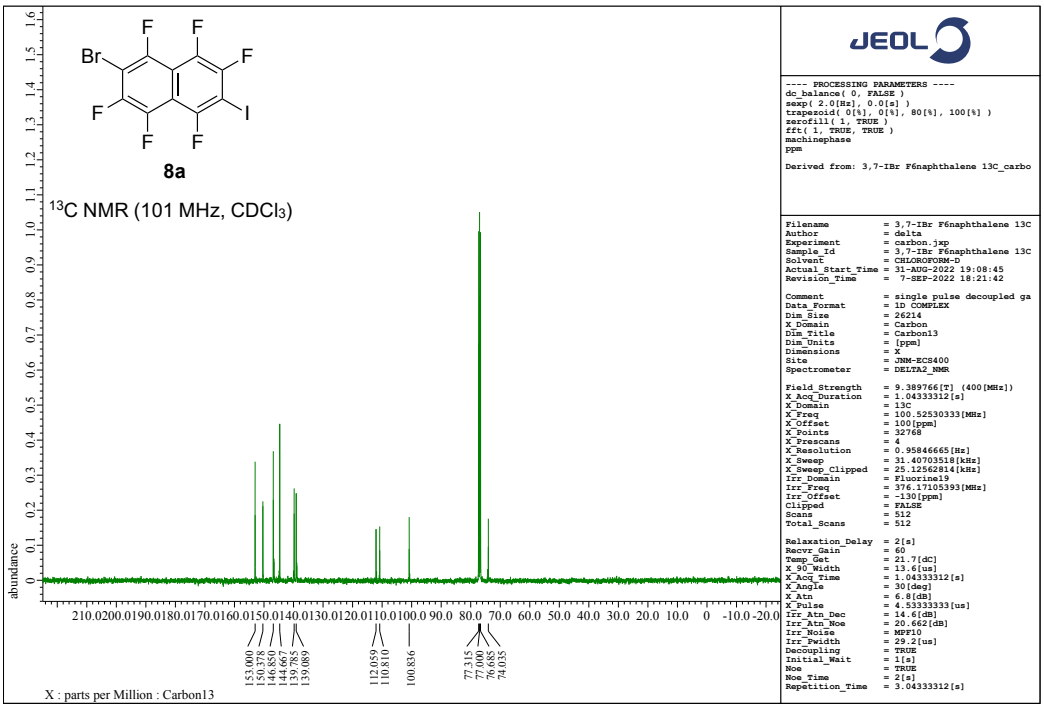

7b
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = ,6-BrH F6 naphthalene 13C
Author = delta
Experiment = carbon.jxp
Sample_Id = , 6-BrH F6 naphthalene 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2022 18:08:41
Revision_Time = 7-SEP-2022 15:35:44
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.5[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPF10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

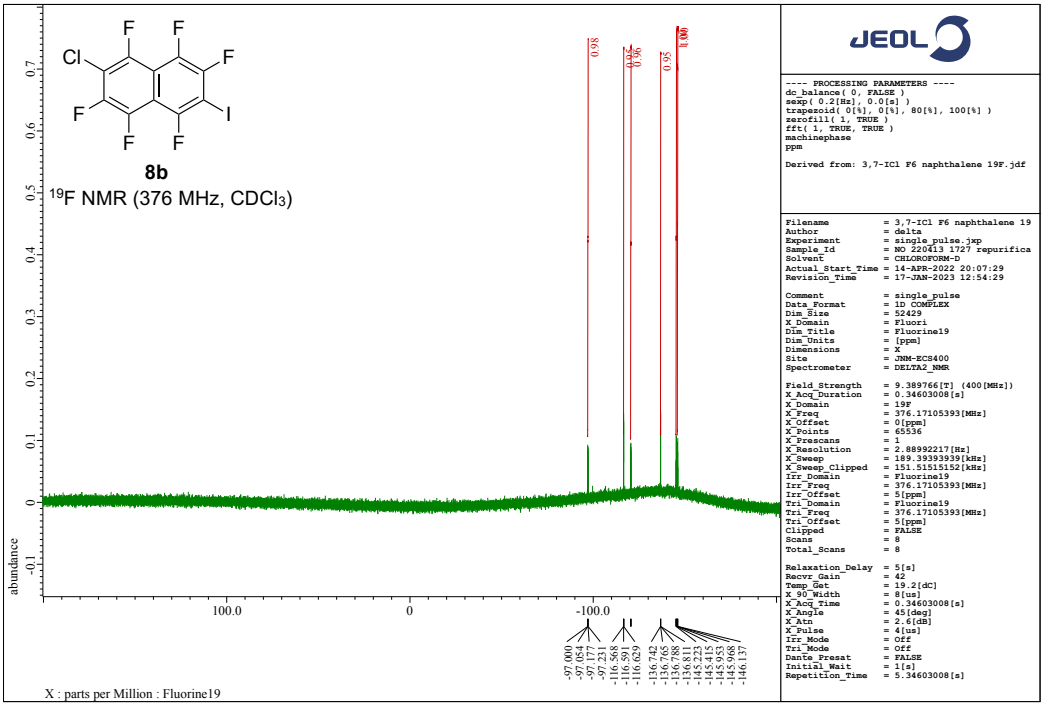

7c
1H NMR (400 MHz, CDCl3)
X : parts per Million : Proton
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: NO 220824 1951_proton-1-1.jdf
Filename = NO 220824 1951_proton-1-2
Author = delta
Experiment = proton.jxp
Sample_Id = NO 220824 1951
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-AUG-2022 09:02:58
Revision_Time = 7-SEP-2022 15:41:13
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.36731904[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22897343[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 = 22.7[dC]
X_90_Width = 6.3[us]
X_Acq_Time = 4.36731904[s]
X_Angle = 45[deg]
X_Atn = 0.7[dB]
X_Pulse = 3.15[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 9.36731904[s]

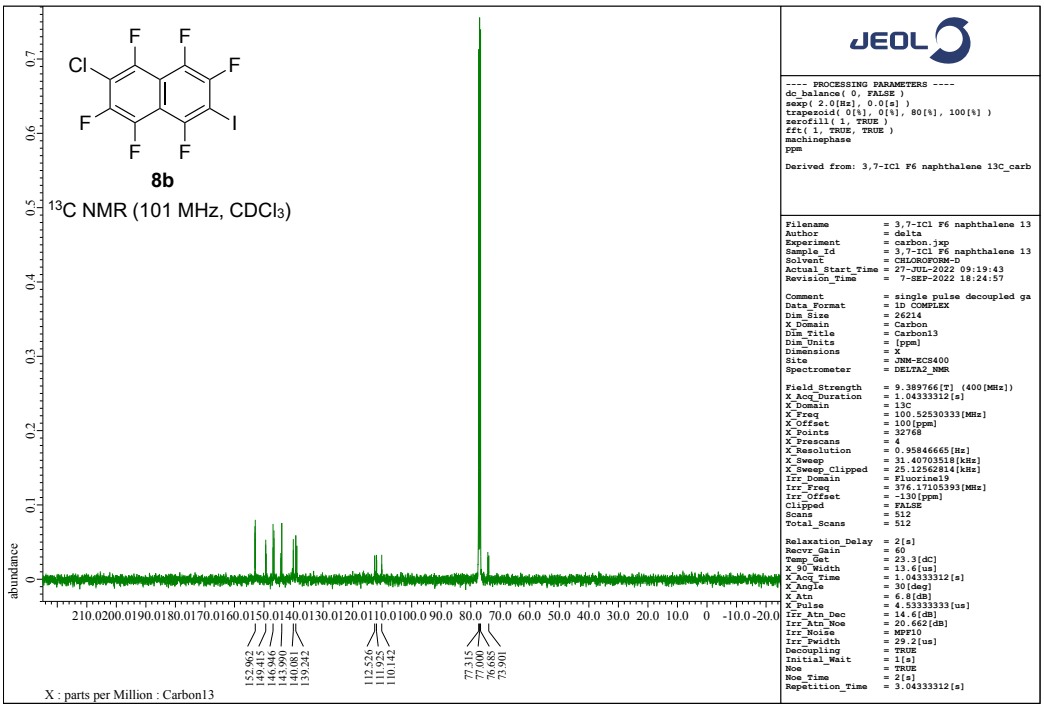

7c
19F NMR (376 MHz, CDCl3)
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(20.25733, 0, 50[%])
Derived from: NO 220824 1951_19F-1-1.jdf
Filename = NO 220824 1951_19F-1-2.jd
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220824 1951
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-AUG-2022 09:00:04
Revision_Time = 17-JAN-2023 12:25:15
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 22.7[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]

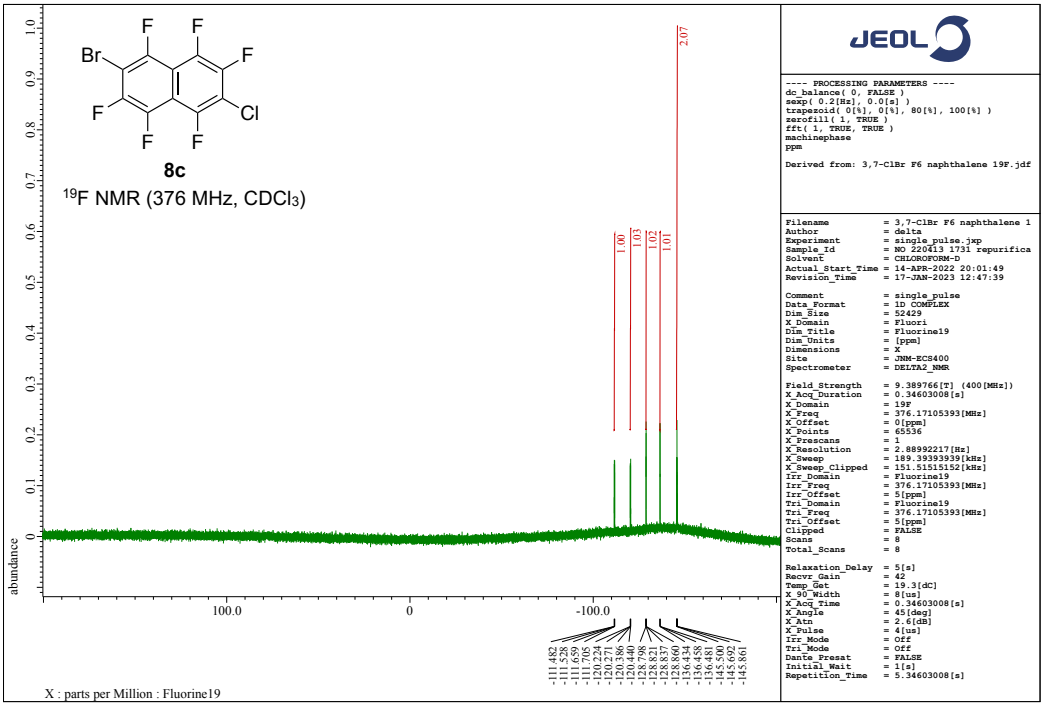

7c
13C NMR (101 MHz, CDCl3)
X : parts per Million : Carbon13

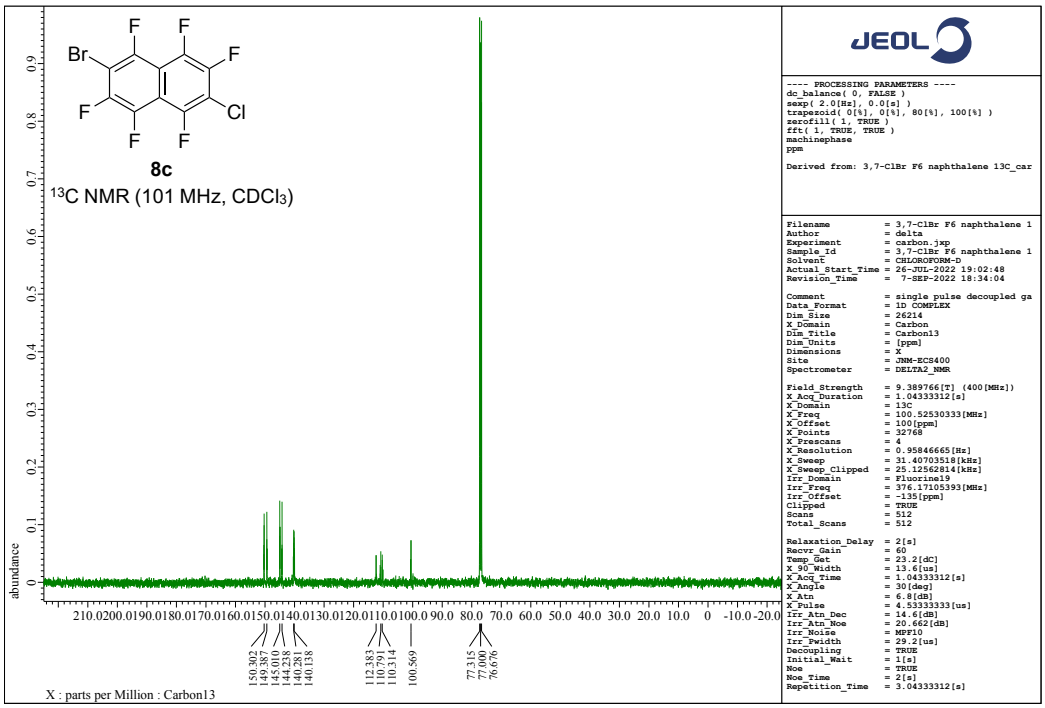

8a
19F NMR (376 MHz, CDCl3)
X : parts per Million : Fluorine19


F
F
Br
F
F
I
F
F
8a
13C NMR (101 MHz, CDCl3)
abundance
153.000
150.378
144.867
144.467
139.785
139.089
112.059
110.810
100.836
77.315
77.000
76.685
74.035
X : parts per Million : Carbon13
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-IBr F6naphthalene 13C_carbo
Filename = 3,7-IBr F6naphthalene 13C
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-IBr F6naphthalene 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-AUG-2022 19:08:45
Revision_Time = 7-SEP-2022 18:21:42
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.7[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]


F
F
Cl
F
F
I
F
F
8b
19F NMR (376 MHz, CDCl3)
abundance
0.98
0.97
0.96
0.95
1.00
-97.000
-97.074
-97.177
-97.231
-116.568
-116.591
-116.629
-136.742
-136.765
-136.788
-136.811
-145.223
-145.415
-145.968
-146.137
X : parts per Million : Fluorine19
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-ICl F6 naphthalene 19F.jdf
Filename = 3,7-ICl F6 naphthalene 19
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220513 1727 repurifica
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-APR-2022 20:07:29
Revision_Time = 17-JAN-2023 12:54:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.2[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]


F
F
Cl
F
F
I
F
F
8b
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-ICl F6 naphthalene 13C_carb
Filename = 3,7-ICl F6 naphthalene 13
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-ICl F6 naphthalene 13
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-JUL-2022 09:19:43
Revision_Time = 7-SEP-2022 18:24:57
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -130[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 23.3[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]


F
F
Br
F
F
F
Cl
F
F
8c
19F NMR (376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19
JEOL
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-ClBr F6 naphthalene 19F.jdf
Filename = 3,7-ClBr F6 naphthalene 1
Author = delta
Experiment = single_pulse.jxp
Sample_Id = NO 220513 1731 repurifica
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-APR-2022 20:01:49
Revision_Time = 17-JAN-2023 12:47:39
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.34603008[s]
X_Domain = 19F
X_Freq = 376.17105393[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 1
X_Resolution = 2.88992217[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 = 42
Temp_Get = 19.3[dC]
X_90_Width = 8[us]
X_Acq_Time = 0.34603008[s]
X_Angle = 45[deg]
X_Atn = 2.6[dB]
X_Pulse = 4[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 5.34603008[s]


F
F
Br
F
F
Cl
F
F
8c
13C NMR (101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
150.302
149.387
145.010
143.738
141.281
140.138
112.383
110.791
110.314
100.569
77.315
77.000
76.676
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: 3,7-ClBr F6 naphthalene 13C_car
Filename = 3,7-ClBr F6 naphthalene 1
Author = delta
Experiment = carbon.jxp
Sample_Id = 3,7-ClBr F6 naphthalene 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-JUL-2022 19:02:48
Revision_Time = 7-SEP-2022 18:34:04
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[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 = Fluorine19
Irr_Freq = 376.17105393[MHz]
Irr_Offset = -135[ppm]
Clipped = TRUE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 23.2[dC]
X_90_Width = 13.6[us]
X_Acq_Time = 1.04333312[s]
X_Angle = 30[deg]
X_Atn = 6.8[dB]
X_Pulse = 4.53333333[us]
Irr_Atn_Dec = 14.6[dB]
Irr_Atn_Noe = 20.662[dB]
Irr_Noise = MPP10
Irr_Pwidth = 29.2[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.04333312[s]

11. Cartesian coordinates

SMD18(THF)/M06-2X-D3/6-311+G(d,p)-SDD

3a	C	-2.534562	-0.146744	0.000042
	C	-1.639590	0.884974	0.000213
	C	-0.240580	0.669899	0.000133
	C	0.240565	-0.669876	-0.000133
	C	-0.703349	-1.722946	-0.000306
	C	-2.041967	-1.464776	-0.000221
	C	0.703367	1.722976	0.000306
	C	1.639587	-0.884971	-0.000213
	C	2.534551	0.146732	-0.000042
	C	2.041966	1.464796	0.000221
	F	-2.893453	-2.485852	-0.000394
	F	-0.306772	-2.994112	-0.000556
	F	2.091374	-2.137906	-0.000464
	F	-2.091448	2.137892	0.000464
	F	0.306804	2.994149	0.000556
	I	-4.603785	0.207112	0.000164
	I	4.603788	-0.207121	-0.000164
	F	2.893486	2.485836	0.000394
4a	C	-2.437575	0.013016	0.000078
	C	-1.248039	-0.658637	-0.000105
	C	0.000000	0.014176	-0.000038
	C	0.000000	1.438192	0.000240
	C	-1.240611	2.112838	0.000425
	C	-2.414904	1.419923	0.000349
	C	1.248039	-0.658637	-0.000200
	C	1.240611	2.112838	0.000322
	C	2.414904	1.419923	0.000159
	C	2.437574	0.013015	-0.000108
	F	-3.558580	2.096106	0.000527
	F	-1.288253	3.444438	0.000683
	F	1.288253	3.444438	0.000569
	F	3.558580	2.096106	0.000254
	F	-1.259208	-1.989713	-0.000347
	F	1.259208	-1.989713	-0.000441
	I	4.269744	-1.012027	-0.000322

	I	-4.269744	-1.012027	-0.000017
1,4-TFIB	C	-1.403460	0.000005	0.000006
	C	-0.692610	-1.189274	0.000009
	C	0.692611	-1.189274	0.000002
	C	1.403461	0.000006	0.000004
	C	0.692616	1.189275	0.000008
	C	-0.692616	1.189275	0.000003
	F	1.324748	2.359570	-0.000004
	F	-1.324748	2.359570	0.000001
	F	1.324758	-2.359562	0.000000
	F	-1.324757	-2.359562	-0.000002
	I	-3.501556	-0.000002	0.000001
	I	3.501556	-0.000002	-0.000003
1,2-TFIB	C	1.521395	1.373887	0.000005
	C	0.309917	0.698728	0.000004
	C	0.309763	-0.698770	0.000002
	C	1.521162	-1.374079	0.000002
	C	2.725613	-0.690269	0.000002
	C	2.725721	0.689851	0.000004
	F	3.873111	-1.354593	-0.000001
	F	3.873338	1.353984	0.000003
	I	-1.440737	-1.877702	-0.000003
	F	1.572051	-2.703831	-0.000003
	I	-1.440396	1.877918	0.000001
	F	1.572457	2.703605	0.000003