α-Fluoroamine Synthesis via P(III)-Mediated Deoxygenative Geminal Fluorosulfonimidation of 1,2-Diketones

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Electronic Supplementary Information

1. General Experimental

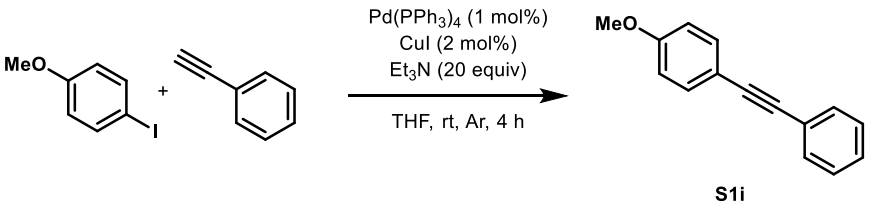
All glasswares were oven-dried (140 °C), and the round-bottom flasks used for the reactions were flame-dried. All reactions were performed under atmosphere of dry Ar or N_2 unless otherwise noted. Tetrahydrofuran (THF), diethyl ether (Et_2O), toluene, and dichloromethane (CH_2Cl_2) were dried by percolation through a column packed with neutral alumina and a column packed with Q5 reactant, a supported copper catalyst for scavenging oxygen, under a positive pressure of Ar. 1,2-Dichloroethane (1,2-DCE) and α,α,α-trifluorotoluene ($PhCF_3$) were distilled from CaH_2 under Ar. Dimethyl sulfoxide (DMSO) was dried over 3Å MS. Solvents for workup and chromatography were: ethyl acetate (EtOAc, Daejung, Extra Pure), hexanes (Duksan, Extra Pure), CH_2Cl_2 (Daejung, Extra Pure), Et_2O (Daejung, Extra pure), and *n*-pentane (Daejung, Extra Pure). Quenching solutions and drying reagents for workup were: NaCl (Daejung, Extra Pure), NH_4Cl (OCI, Extra Pure), $NaHCO_3$ (OCI, Extra Pure), $NaHSO_3$ (Daejung, Extra Pure), and $MgSO_4$ (Duksan, Extra Pure). Column chromatography was performed using Merck 230–400 mesh silica gel and Acros 50–200 μm aluminum oxide. Analytical thin-layer chromatography (TLC) was conducted on Merck silica gel or aluminum oxide 60 F_{254} TLC plates and visualized with UV (254 nm) as well as *p*-anisaldehyde or potassium permanganate ($KMnO_4$) staining solutions. Kugelrohr distillation was carried out using a Büchi B585 glass oven, and temperatures reported are air bath temperatures (ABT). Triethylamine was freshly distilled from CaH_2 under Ar. Phenylacetylene and 4-*tert*-butylphenylacetylene were distilled under Ar. 4-Iodobenzotrifluoride was distilled under reduced pressure. 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) was distilled from CaH_2 under reduced pressure. The following reagents were recrystallized from the indicated solvent: 4,4'-dimethylbenzil (**1a**, hexanes), 4,4'-dimethoxybenzil (**1b**, *i*-PrOH), benzil (**1c**, EtOH), 4,4'-difluorobenzil (**1d**, EtOH), 3,3'-dimethoxybenzil (**1e**, *i*-PrOH), 2,2'-furil (**1j**, EtOH), and 2,2'-thenil (**1k**, EtOH). The following reagents were used as received: 4-ethynylanisole (Acros, 99%), iodomethane (Aldrich, 99%), $Pd(PPh_3)_4$ (Acros, 99%), CuI (Aldrich, 98%), $Ru[(cymene)Cl_2]_2$ (Alfa, 98%), Oxone® (Alfa), 2,2,6,6-tetramethyl-1-piperidinyloxyl (TEMPO, Alfa, 98%), acetylene-dicarboxylic acid (Alfa, 97%, Aldrich, 95%), $Pd(PPh_3)_2Cl_2$ (TCI, >98%), 1,4-bis(diphenylphosphino)butane (dppb, TCI, >98%), *N*-fluorobenzenesulfonimide ($(PhSO_2)_2NF$, TCI, >98%, TCI, >97%), and 2-naphthaldehyde (Acros, 98%). *n*-Butyllithium (2.5 M in hexanes, Aldrich) was filtered and titrated against butylated hydroxytoluene (BHT) with fluorene as an indicator. ^1H, ^{13}C, ^{19}F, and ^{31}P NMR spectra were recorded on a JEOL ESC400 spectrometer (400 MHz, ^1H; 100 MHz, ^{13}C; 376 MHz, ^{19}F; 162 MHz, ^{31}P). Chemical shifts are referenced to residual chloroform (7.26 ppm, ^1H; 77.23 ppm, ^{13}C), acetonitrile (1.94 ppm, ^1H), acetone (206.26 ppm, ^{13}C), dichloromethane (53.50 ppm, ^{13}C), hexafluorobenzene (–164.90 ppm, ^{19}F), and triphenyl phosphate (–17.57 ppm, ^{31}P). Chemical shifts are reported in ppm. Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). Coupling constants, *J*, are reported in Hertz. HRMS (FAB and EI) was performed on a JEOL JMS-700 MStation mass spectrometer with magnetic sector-electric sector double focusing mass analyzer at Korea Basic Science Institute (KBSI), Daegu center. HRMS (ESI) was analyzed by a liquid chromatography electrospray ionization quadrupole time-of-flight mass spectroscopy (LC-ESI-QTOF-MS, Bruker impact II) in both positive and negative ESI modes at GIST Central Research Facilities (GCRF). Data are reported in the form of *m/z*. Elemental analysis was conducted on an Elementar UNICUBE at GCRF. X-ray crystallographic data for **4a** were collected using a Bruker APEX-II CCD-based diffractometer with graphite-monochromated MoKα radiation (λ = 0.7107 Å) at Chonnam National University.

2. Experimental Procedures

2.1. Preparation of 1,2-Diketones

Known compounds (**1f–h**, **1l**, and **2**) were prepared according to the previously reported procedure.[1]

1-(4-Methoxyphenyl)-2-phenylethyne (S1i):[1]



S1i

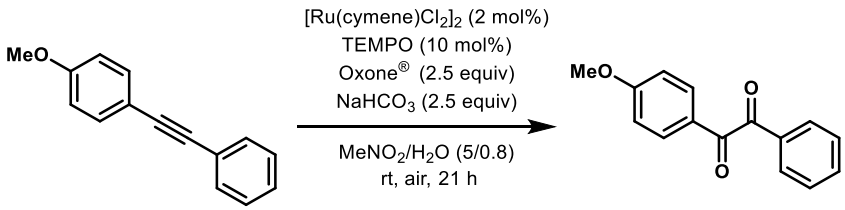
To a vigorously stirred mixture of 4-iodoanisole (1.17 g, 5.00 mmol), CuI (20 mg, 0.10 mmol), and $Pd(PPh_3)_4$ (58 mg, 0.050 mmol) in THF (2.5 mL) were added phenylacetylene (580 μL, 5.25 mmol) and Et_3N (14.0 mL, 100 mmol) at rt. After 4 h, the reaction mixture was filtered through celite, rinsed with EtOAc (40 mL), and concentrated under reduced pressure. The residue was dissolved in EtOAc (40 mL), washed with sat. aq. NH_4Cl (50 mL × 3), dried over $MgSO_4$ (7 g), filtered through a glass frit, and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2, ϕ = 4.0 cm, l = 10 cm, CH_2Cl_2:hexanes = 1:4, R_f = 0.6, UV 254 nm) to give **S1i** (1.03 g, 99%) as pale yellow solid.

Data for 1-(4-methoxyphenyl)-2-phenylethyne (**S1i**):[2] SJB-02-006

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 7.52–7.46 (m, 4H), 7.36–7.31 (m, 3H), 6.88 (d, J = 7.3, 2H), 3.83 (s, 3H).

1-(4-Methoxyphenyl)-2-phenylethane -1,2-dione (1i):[1]



S1i **1i**

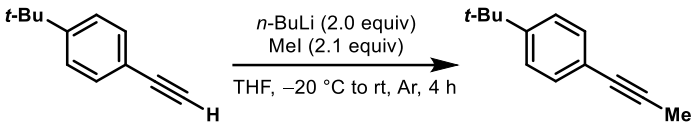
To a vigorously stirred mixture **S1i** (1.03 g, 2.90 mmol), Oxone® (7.47 g, 12.3 mmol), and $NaHCO_3$ (1.03 g, 12.3 mmol) in $MeNO_2$ (95 mL) and DI water (15 mL) were added $[Ru(cymene)Cl_2]_2$ (60 mg, 0.098 mmol) and TEMPO (78 mg, 0.49 mmol) at rt under air. After 21 h, the reaction mixture was quenched by sat. aq. $NaHSO_3$ (100 mL) and extracted with EtOAc (50 mL × 3). The combined organic layers were dried over $MgSO_4$ (13 g), filtered through a glass frit, and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2, ϕ = 4.5 cm, l = 10 cm, CH_2Cl_2:hexanes = 1:2, R_f = 0.3, UV 254 nm) to give **1i** (1.03 mg, 88%) as yellow solid.

Data for 1-(4-methoxyphenyl)-2-phenylethane-1,2-dione (**1i**):[2] SJB-02-008

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 7.99–7.94 (m, 4H), 7.67–7.63 (m, 1 H), 7.51 (t, J = 7.8, 2H), 6.99–6.97 (m, 2H), 3.89 (s, 3H).

1-(4-*tert*-Butylphenyl)-1-propyne (S1m):[1]



S1m

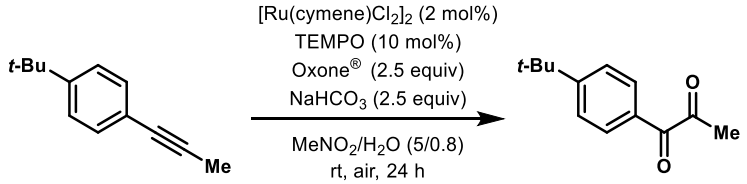
To a stirred solution of 4-*tert*-butylphenylacetylene (900 μL, 5.00 mmol) in THF (33 mL) was added *n*-BuLi (1.34 M in hexanes, 7.5 mL, 10.0 mmol) dropwise at –20 ℃. After 1 h, MeI (660 μL, 10.0 mmol) was added, and then the reaction mixture was warmed to rt. After 4 h, the reaction mixture was quenched by sat. aq. NH_4Cl (40 mL) and extracted with Et_2O (30 mL × 3). The combined organic layers were washed with brine (30 mL), dried over $MgSO_4$ (10 g), filtered through a glass frit, and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2, ϕ = 4.0 cm, l = 10 cm, pentane, R_f = 0.5, UV 254 nm) to give **S1m** (845 mg, 98%) as a colorless oil.

Data for 1-(4-*tert*-butylphenyl)-1-propyne (**S1m**): [3] SJB-01-068

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 7.35–7.28 (m, 4H), 2.04 (s, 3H), 1.30 (s, 9H).

1-(4-*tert*-Butylphenyl)propane-1,2-dione (1m):[1]



S1m **1m**

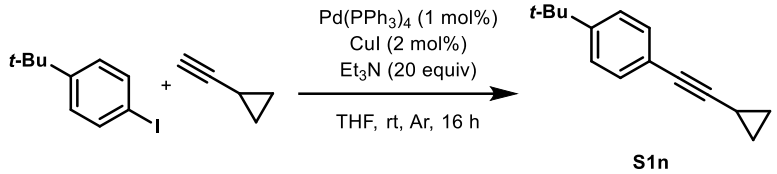
To a vigorously stirred mixture of **S1m** (845 mg, 4.90 mmol), Oxone® (7.48 g, 12.3 mmol), and $NaHCO_3$ (1.05 g, 12.3 mmol) in $MeNO_2$ (95 mL) and DI water (15 mL) were added $[Ru(cymene)Cl_2]_2$ (61 mg, 0.098 mmol) and TEMPO (78 mg, 0.49 mmol) at rt under air. After 24 h, the reaction mixture was quenched by sat. aq. $NaHSO_3$ (100 mL), diluted with CH_2Cl_2 (50 mL), washed with brine (50 mL × 2), dried over $MgSO_4$ (15 g), filtered through a glass frit, and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2, ϕ = 4.0 cm, l = 12 cm, CH_2Cl_2:hexanes = 1:3, R_f = 0.2, UV 254 nm) to give **1m** (692 mg, 69%) as a yellow oil.

Data for 1-(4-*tert*-butylphenyl)-1-propane-1,2-dione (**1m**):[4] SJB-01-070

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 7.96–7.94 (m, 2H), 7.53–7.50 (m, 2H), 2.51 (s, 3H), 1.35 (s, 9H).

1-Cycloproyl-2-(4-*tert*-butyl)phenylethyne (S1n):[1]



S1n

To a vigorously stirred mixture of CuI (20 mg, 0.10 mmol) and $Pd(PPh_3)_4$ (58 mg, 0.050 mmol) in THF (2.5 mL) were added cyclopropylacetylene (445 μL, 5.25 mmol), 1-*tert*-butyl-4-iodobezene (890 μL, 5.00 mmol), and Et_3N (14.0 mL, 100 mmol) at rt. After 16 h, the reaction mixture was filtered through celite, rinsed with EtOAc (40 mL), and concentrated under reduced pressure. The residue was dissolved in EtOAc (40 mL), washed with sat. aq. NH_4Cl (50 mL × 3), dried over $MgSO_4$ (7 g), filtered through a glass frit, and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2, ϕ = 4.0 cm, l = 10 cm, hexanes, R_f = 0.3, UV 254 nm) to give **S1n** (985 mg, 99%) as a pale yellow oil.

Data for 1-cyclopropyl-2-(4-*tert*-butyl)phenylethyne (**S1n**): SJB-02-011

^{1}H NMR: (400 MHz, $CDCl_3$)

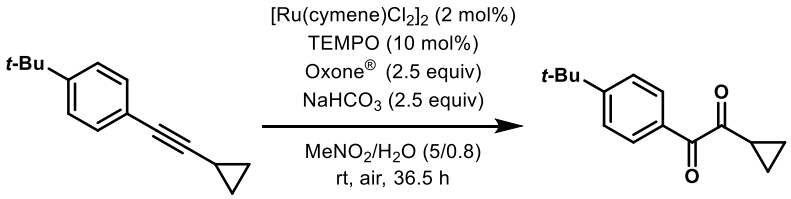
δ 7.40–7.33 (m, 4H), 1.53–1.49 (m, 1H), 1.36 (s, 9H), 0.93–0.81 (m, 4H).

^{13}C NMR: (100 MHz, $CDCl_3$)

δ 150.6, 131.5, 125.3, 121.1, 92.7, 76.0, 34.8, 31.3, 8.7, 0.4.

HRMS (ESI): Calcd for $C_{30}H_{37}$ $[2M+H]^+$: 397.2896; Found: 397.2891.

1-Cycloproyl-2-(4-*tert*-butyl)phenylethane-1,2-dione (1n):[1]



S1n **1n**

To a vigorously stirred mixture of **S1n** (835 mg, 4.20 mmol), Oxone® (6.40 g, 10.5 mmol), and $NaHCO_3$ (885 mg, 10.5 mmol) in $MeNO_2$ (90 mL) and DI water (15 mL) were added $[Ru(cymene)Cl_2]_2$ (51 mg, 0.084 mmol) and TEMPO (67 mg, 0.42 mmol) at rt under air. After 36.5 h, the reaction mixture was quenched by sat. aq. $NaHSO_3$ (100 mL) and extracted with EtOAc (50 mL × 3). The combined organic layers were dried over $MgSO_4$ (15 g), filtered through a glass frit, and concentrated under reduced pressure. The residue was purified by column chromatography (SiO_2, ϕ = 4.5 cm, l = 10 cm, CH_2Cl_2:hexanes = 1:3, R_f = 0.3, UV 254 nm) to give **1n** (775 mg, 80%) as pale yellow solid.

Data for 1-cyclopropyl-2-(4-*tert*-butyl)phenylethane-1,2-dione (**1n**): SJB-02-013

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 7.94–7.92 (m, 2H), 7.52–7.50 (m, 2H), 2.56–2.49 (m, 1H), 1.35–1.31 (m, 11H) 1.22–1.53 (m, 2H).

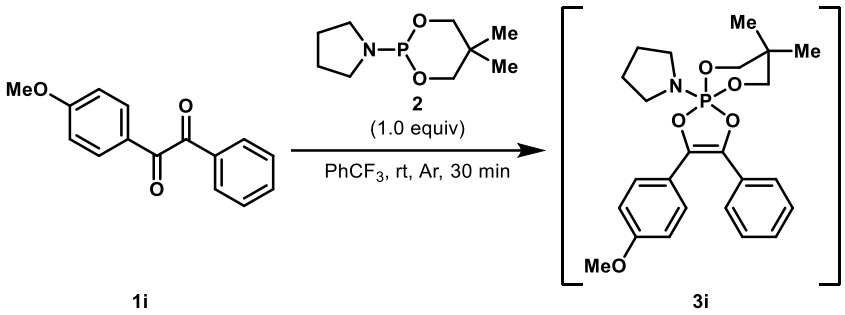
^{13}C NMR: (100 MHz, $CDCl_3$)

δ 203.0, 192.2, 158.6, 130.3, 129.6, 125.9, 35.4, 31.0, 18.7, 13.2.

HRMS (ESI): Calcd for $C_{15}H_{19}O_2$ $[M+H]^+$: 231.1385; Found: 231.1380.

2.2 Formation of Dioxaphospholenes

Dioxaphospholene 3i:[1]



To a stirred solution of **1i** (0.50 mmol) in $PhCF_3$ (0.4 mL) was added a solution of **2** (0.50 mmol) in $PhCF_3$ (0.6 mL then rinsed with 0.3 mL) at rt. After 30 min, $CDCl_3$ (1 mL) was added, and the reaction mixture was analyzed by ^1H and ^{31}P NMR spectroscopy.

Data for **3i**: SJB-02-010

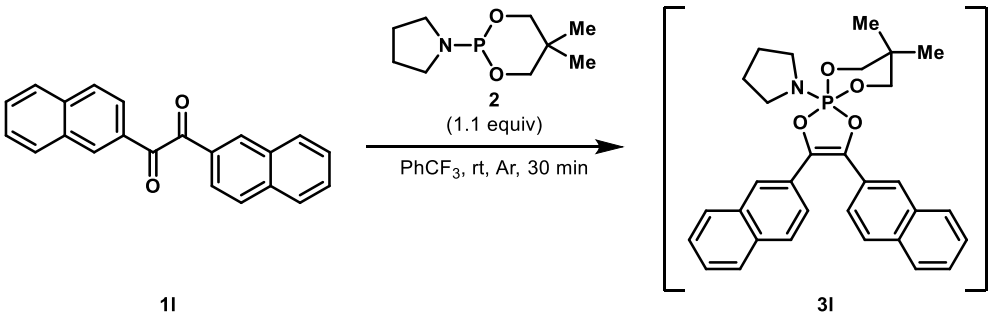
^1H NMR: (400 MHz, $CDCl_3$)

δ 7.64–7.17 (m, 7H), 6.85–6.82 (m, 2H), 3.90–3.85 (m, 4H), 3.81 (s, 3H), 3.51–3.48 (m, 4H), 1.77–1.76 (m, 4H), 3.81 (s, 3H), 3.51–3.48 (m, 4H), 1.77–1.76 (m, 4H), 1.09 (s, 3H), 1.01 (s, 3H).

^{31}P NMR: (162 MHz, $CDCl_3$)

δ –49.3.

Dioxaphospholene 3l:[1]



To a stirred solution of **1l** (0.30 mmol) in $PhCF_3$ (0.25 mL) was added a solution of **2** (0.33 mmol) in $PhCF_3$ (0.3 mL then rinsed with 0.2 mL) at rt. After 30 min, $CDCl_3$ (1 mL) was added, and the reaction mixture was analyzed by ^1H and ^{31}P NMR spectroscopy.

Data for **3k**: SJB-02-067

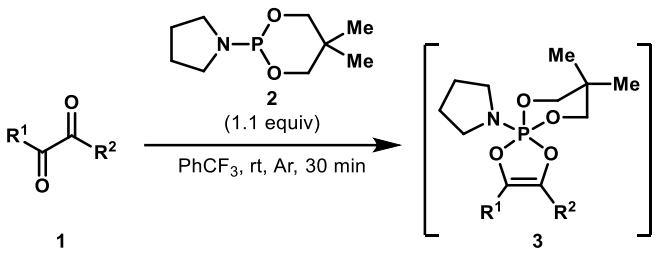
^1H NMR: (400 MHz, $CDCl_3$)

δ 8.27 (s, 2H), 7.89–7.49 (m, 12H), 4.16–4.03 (m, 4H), 3.71–3.60 (m, 4H), 1.88 (s, 4H), 1.23 (s, 3H), 1.14 (s, 3H).

^{31}P NMR: (162 MHz, $CDCl_3$)

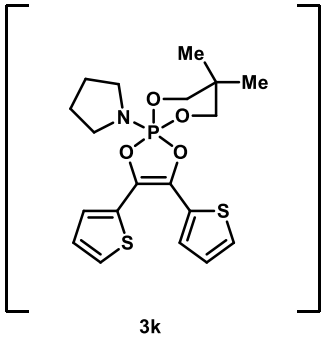
δ –48.9.

Dioxaphospholenes 3k, 3m, and 3n:[1]



To a stirred solution of **1** (0.50 mmol) in $PhCF_3$ (0.4 mL) was added a solution of **2** (0.55 mmol) in $PhCF_3$ (0.6 mL then rinsed with 0.3 mL) at rt. After 30 min, $CDCl_3$ (1 mL) was added, and the reaction mixture was analyzed by ^1H and ^{31}P NMR spectroscopy.

Data for **3k**: SJB-02-066



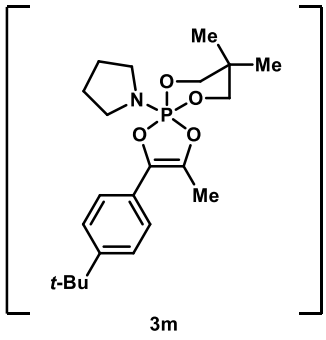
^1H NMR: (400 MHz, $CDCl_3$)

δ 7.69–7.29 (m, 4H), 7.07–7.05 (m, 2H), 3.99–3.79 (m, 4H), 3.55–3.52 (m, 4H), 1.80–1.79 (m, 4H), 1.11 (s, 3H), 1.04 (s, 3H).

^{31}P NMR: (162 MHz, $CDCl_3$)

δ –49.6.

Data for **3m**: SJB-02-063



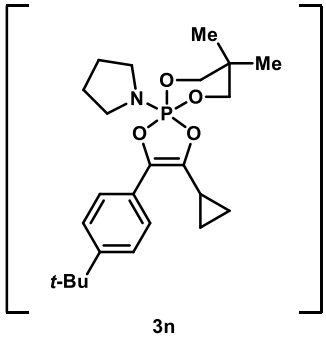
^1H NMR: (400 MHz, $CDCl_3$)

δ 7.67–7.42 (m, 4H), 4.03–3.73 (m, 4H), 3.48 (m, 4H), 2.25 (s, 3H), 1.78–1.77 (m, 4H), 1.38 (s, 9H), 1.09 (s, 3H), 1.03 (s, 3H).

^{31}P NMR: (162 MHz, $CDCl_3$)

δ –48.8.

Data for **3n**: SJB-02-016



^1H NMR: (400 MHz, $CDCl_3$)

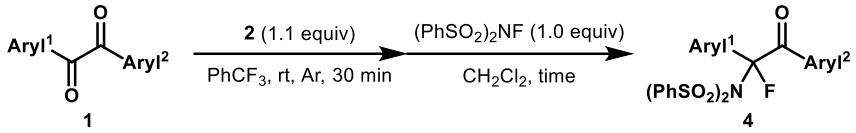
δ 7.65–7.47 (m, 2H), 7.39–7.37 (m, 2H), 3.90–3.75 (m, 4H), 3.37 (m, 4H), 1.97–1.90 (m, 1H), 1.77–1.66 (m, 4H), 1.34 (s, 9H), 1.02 (s, 3H), 0.99 (s, 3H), 0.89–0.82 (m, 4H).

^{31}P NMR: (162 MHz, $CDCl_3$)

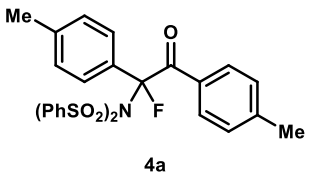
δ –49.6.

2.3. Geminal Fluorosulfonimidation of Aryl-Aryl 1,2-Diketones

General procedure for 4a–4f, 4h, 4i, 4k, and 4l:



To a mixture of **1** (1.00 mmol) and **2** (224 mg, 1.10 mmol) was added $PhCF_3$ (2.5 mL) at rt. After stirring for 30 min, a solution of $(PhSO_2)_2NF$ (315 mg, 1.00 mmol) in CH_2Cl_2 (2.5 mL) was added dropwise. After the given *time*, the reaction mixture was diluted with EtOAc (50 mL) and washed with brine (50 mL × 3). The combined aqueous layers were extracted with EtOAc (100 mL). The combined organic extracts were dried over $MgSO_4$ (10 g), filtered through a glass frit, and concentrated under reduced pressure. The residue was purified by column chromatography to give **4** along with a small amount of recovered **1**.



4a

time = 15 min; Column chromatography (SiO_2, ϕ = 3.5 cm, l = 12 cm, EtOAc:hexanes = 1:5 , R_f = 0.3, UV 254 nm) afforded **4a** along with recovered **1a** (14 mg, 6%). Further purification by recrystallization (EtOH) gave **4a** (414 mg, 77%) as white crystals, which were analyzed by elemental analysis and X-ray crystallography.

Data for *N*-[1-fluoro-1,2-bis(4-methylphenyl)-2-oxoethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4a**): YRS-03-007

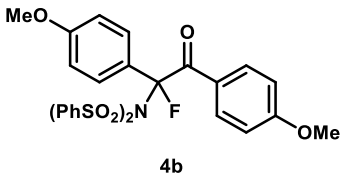
^{1}H NMR: (400 MHz, $CDCl_3$, 40 °C)
δ 8.04–7.72 (m, 4H), 7.65 (dd, *J* = 8.4, 2.0, 2H), 7.60 (t, *J* = 7.4, 2H), 7.46 (t, *J* = 7.8, 4H), 7.10 (d, *J* = 8.4, 4H), 6.85 (d, *J* = 8.0, 2H), 2.31 (s, 3H), 2.28 (s, 3H).

^{13}C NMR: (100 MHz, CD_2Cl_2, 40 °C)
δ 191.3 (d, *J* = 30.5), 144.1, 140.8, 140.5, 134.0, 131.4 (d, *J* = 2.9), 130.1 (d, *J* = 6.6), 129.2 (d, *J* = 9.5), 128.9, 128.8, 128.5, 128.3, 125.7 (d, *J* = 23.9), 106.0 (d, *J* = 231.7), 21.4, 20.9.

^{19}F NMR: (376 MHz, $CDCl_3$, 40 °C)
δ –115.0.

HRMS (ESI): Calcd for $C_{28}H_{24}FNO_5S_2Na$ $[M+Na]^+$, $C_{28}H_{24}FNO_5S_2K$ $[M+K]^+$: 560.0972, 576.0712;
Found: 560.0975, 576.0710.

EA: Calcd: C = 62.55, H = 4.50; Found: C = 63.05, H = 4.00.



4b

time = 1 h; Column chromatography (SiO_2, ϕ = 4 cm, *l* = 12 cm, EtOAc:hexanes = 1:2, R_f = 0.4, UV 254 nm) afforded **4b** along with recovered **1b** (83 mg, 31%). In this case, the complete removal of residual solvents from the product was difficult. Thus, the chromatographed material was repeatedly diluted with CH_2Cl_2 and concentrated under reduced pressure 5 times. Then, the residue was dried using a Büchi B585 glass oven (200 mTorr, 60 °C) for 13 h to give **4b** (380 mg, 67%) as beige solid.

Data for *N*-[1-fluoro-1,2-bis(4-methoxyphenyl)-2-oxoethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4b**): SJB-01-095

^{1}H NMR: (400 MHz, $CDCl_3$)

δ.8.00–7.81 (m, 4H), 7.79 (dd, *J* = 9.0, 1.8, 2H), 7.59 (t, *J* = 7.2, 2H), 7.49–7.47 (m, 4H), 7.21–7.07 (m, 2H), 6.79 (d, *J* = 8.8, 2H), 6.55 (m, 2H), 3.78 (s, 3H), 3.75 (s, 3H).

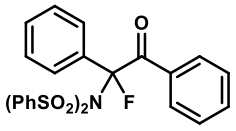
^{13}C NMR: (100 MHz, $CDCl_3$)

δ 190.2 (d, *J* = 29.5), 163.3, 161.0, 140.6, 133.9, 132.6 (d, *J* = 6.7), 131.0 (d, *J* = 9.5), 128.8, 128.4, 126.6 (d, *J* = 3.8), 120.5 (d, *J* = 24.8), 113.6, 113.2, 106.2 (d, *J* = 231.7), 55.5, 55.4.

^{19}F NMR: (376 MHz, $CDCl_3$)

δ –113.3.

HRMS (FAB): Calcd for $C_{28}H_{24}FNO_7S_2H$ $[M+H]^+$: 570.1056; Found: 570.1051



4c

time = 12 h; Column chromatography (SiO_2, ϕ = 3.5 cm, *l* = 12 cm, EtOAc:hexanes = 1:5 → 1:2, R_f = 0.2 in EtOAc:hexanes = 1:5, UV 254 nm) afforded **4c** along with recovered **1c** (58 mg, 28%). Further purification by recrystallization (EtOH) gave **4c** (330 mg, 61%) as white crystals.

Data for *N*-(1-fluoro-1,2-diphenyl-2-oxoethyl)-*N*-(phenylsulfonyl)benzenesulfonimide (**4c**): YRS-03-054

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 8.00–7.80 (m, 4H), 7.72–7.70 (m, 2H), 7.60 (t, *J* = 7.4, 2H) 7.49–7.41 (m, 5H), 7.32–7.24 (m, 5H), 7.09–7.06 (m, 2H).

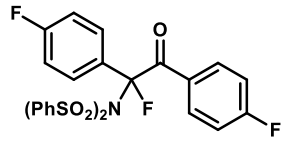
^{13}C NMR: (100 MHz, $CDCl_3$)

δ 192.5 (d, *J* = 30.5), 140.9, 134.7, 134.0, 132.8, 130.3, 130.2 (d, *J* = 5.7), 129.7 (d, *J* = 9.5), 129.3 (d, *J* = 23.8), 128.9, 128.7, 128.3, 128.0, 105.9 (d, *J* = 232.6).

^{19}F NMR: (376 MHz, $CDCl_3$)

δ –115.7.

HRMS (ESI): Calcd for $C_{26}H_{20}FNO_5S_2Na$ $[M+Na]^+$: 532.0665; Found: 532.0656.



4d

time = 1 h; Column chromatography (SiO_2, ϕ = 3.5 cm, l = 12 cm, EtOAc:hexanes = 1:5 → 1:2, R_f = 0.3 in EtOAc:hexanes = 1:5, UV 254 nm) afforded **4d** along with recovered **1d** (21 mg, 9%). Further purification by recrystallization (EtOH) gave **4d** (429 mg, 79%) as white crystals, which were analyzed by elemental analysis.

Data for *N*-[1-fluoro-1,2-bis(4-fluorophenyl)-2-oxoethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4d**): YRS-03-051

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 8.20–7.84 (m, 4H), 7.81–7.77 (m, 2H), 7.63–7.62 (m, 2H), 7.52–7.50 (m, 4H), 7.27–7.25 (m, 2H), 7.00 (td, *J* = 8.7, 2.3, 2H), 6.77 (t, *J* = 7.6, 2H).

^{13}C NMR: (100 MHz, $CDCl_3$)

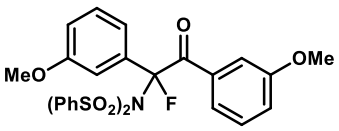
δ 190.9 (d, *J* = 30.5), 165.7 (d, *J* = 254.5), 164.0 (d, *J* = 251.7), 140.7, 134.2, 133.0 (dd, *J* = 9.3, 6.9), 131.9 (dd, *J* = 9.3, 6.7), 130.6 (dd, *J* = 3.6), 129.0, 128.7, 124.9 (dd, *J* = 24.8, 3.3), 115.6 (dd, *J* = 21.8, 1.1), 115.1 (dd, *J* = 21.9, 1.9), 105.6 (d, *J* = 232.2).

^{19}F NMR: (376 MHz, $CDCl_3$)

δ –107.8, –112.6, –114.4.

HRMS (ESI): Calcd for $C_{26}H_{18}F_3NO_5S_2Na$ $[M+Na]^+$, $C_{26}H_{18}F_3NO_5S_2K$ $[M+K]^+$: 568.0476, 584.0216; Found: 568.0469, 584.0206.

EA: Calcd: C = 57.24, H = 3.33; Found: C = 57.31, H = 3.39.



4e

time = 12 h; Column chromatography (SiO_2, ϕ = 4.0 cm, l = 12 cm, EtOAc:hexanes = 1:2, R_f = 0.4, UV 254 nm) afforded **4e** along with recovered **1e** (114 mg, 42%). In this case, the complete removal of residual solvents from the product was difficult. Thus, the chromatographed material was repeatedly diluted with CH_2Cl_2 and concentrated under reduced pressure 5 times. Then, the residue was dried using a Büchi B585 glass oven (200 mTorr, 60 °C) for 12 h to give **4b** (285 mg, 50%) as off-white solid.

Data for *N*-[1-fluoro-1,2-bis(3-methoxyphenyl)-2-oxoethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4e**): SJB-01-086

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 8.20–7.70 (m, 4H), 7.60 (t, *J* = 7.2, 2H), 7.49–7.47 (m, 4H), 7.32–7.29 (m, 2H), 7.22–7.18 (m, 1H), 7.04–6.98 (m, 3H), 6.81 (dd, *J* = 8.2, 2.6, 1H), 6.75–6.60 (m, 1H), 3.74 (s, 3H), 3.57 (s, 3H).

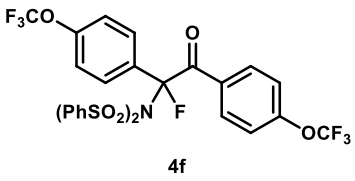
^{13}C NMR: (100 MHz, $CDCl_3$)

δ 192.0 (d, *J* = 31.4), 159.3, 158.9, 140.6, 135.5 (d, *J* = 3.8), 134.0, 130.3 (d, *J* = 24.3), 129.2, 129.0, 128.9, 128.5, 122.6 (d, *J* = 6.7), 122.0 (d, *J* = 9.5), 119.4, 116.6, 114.9 (d, *J* = 4.8), 114.7 (d, *J* = 9.5), 105.6 (d, *J* = 233.6), 55.4, 55.2.

^{19}F NMR: (376 MHz, $CDCl_3$)

δ –114.6.

HRMS (ESI): Calcd for $C_{28}H_{24}FNO_7S_2Na$ $[M+Na]^+$: 592.0876; Found: 592.0874.



4f

time = 12 h; Column chromatography (SiO_2, ϕ = 3.5 cm, *l* = 12 cm, EtOAc:hexanes = 1:5, R_f = 0.4, UV 254 nm) afforded **4f** along with recovered **1f** (50 mg, 14%). The residual solvent was removed by freeze-drying (MeCN) to give **4f** (504 mg, 74%) as white solid.

Data for *N*-[1-fluoro-2-oxo-1,2-bis(4-(trifluoromethoxy)phenyl)ethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4f**): YRS-03-055

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 8.14–7.72 (m, 6 H), 7.65 (t, *J* = 7.2, 2H), 7.52–7.50 (m, 4H), 7.37–7.22 (m, 2H), 7.16 (d, *J* = 8.0, 2H), 6.99–6.83 (m, 2H).

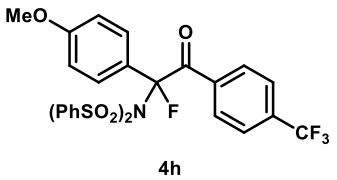
^{13}C NMR: (100 MHz, CD_3COCD_3)

δ 191.6 (d, *J* = 31.5), 153.0, 151.4, 141.1, 135.6, 133.7, 133.3 (d, *J* = 5.7), 132.5 (d, *J* = 9.5), 130.2, 129.1, 128.2 (d, *J* = 25.7), 121.3, 121.28 (q, *J* = 255.5), 121.23 (q, *J* = 256.2), 121.0, 106.0 (d, *J* = 232.6).

^{19}F NMR: (376 MHz, $CDCl_3$)

δ –60.78, –60.80, –115.4.

HRMS (ESI): Calcd for $C_{28}H_{21}F_4NO_6S_2Na$ $[M+Na]^+$: 700.0311; Found: 700.0302.



4h

time = 1 h; Column chromatography (SiO_2, ϕ = 3.5 cm, *l* = 12 cm, EtOAc:hexanes = 1:2, R_f = 0.5, UV 254 nm) afforded **4h** along with recovered **1h** (205 mg, 67%). The residual solvent was removed by freeze-drying (MeCN) to give **4h** (152 mg, 25%) as beige solid.

Data for *N*-[1-fluoro-1-(methoxyphenyl)-2-oxo-2-(4-(trifluoromethyl)pheny)lethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4h**): YRS-03-053

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 8.03–7.81 (m, 4H), 7.77 (d, *J* = 8.0, 2H), 7.63 (t, *J* = 7.4, 2H), 7.57 (d, *J* = 8.8, 2H), 7.51–7.49 (m, 4H), 7.21–7.02 (m, 2H), 6.67–6.51 (m, 2H), 3.78 (s, 3H).

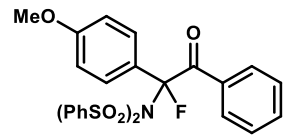
^{13}C NMR: (100 MHz, CD_2Cl_2)

δ 191.5 (d, *J* = 32.4), 161.4, 140.2, 137.7, 134.2, 133.6 (q, *J* = 32.4), 131.1 (d, *J* = 9.5), 130.2 (d, *J* = 5.7), 128.9, 128.3, 125.1 (d, *J* = 3.8), 123.7 (q, *J* = 271.3), 119.1 (d, *J* = 24.8), 113.5, 105.5 (d, *J* = 229.8), 55.5.

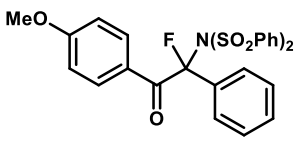
^{19}F NMR: (376 MHz, $CDCl_3$)

δ –66.5, –115.3.

HRMS (ESI): Calcd for $C_{28}H_{21}F_4NO_6S_2Na$ $[M+Na]^+$: 630.0644; Found: 630.0635.



4ia



4ib

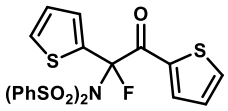
time = 1 h; Column chromatography (SiO_2, ϕ = 4.0 cm, *l* = 12 cm, EtOAc:hexanes = 1:5 → 1:2, R_f = 0.2 in EtOAc:hexanes = 1:5, UV 254 nm) afforded a mixture of **4ia** and **4ib** along with recovered **1i** (83 mg, 35%). In this case, the complete removal of residual solvents from the product was difficult. Thus, the chromatographed material was repeatedly diluted with CH_2Cl_2 and concentrated under reduced pressure 5 times. Then, the residue was dried using a Büchi B585 glass oven (200 mTorr, 65 °C) for 12 h to give a mixture of **4ia** and **4ib** (257 mg, 48%, 63:37 rr) as beige solid. The isomeric ratio was determined by integration of the MeO peaks in the ^{1}H NMR spectrum (δ 3.79 for **4ib**, δ 3.76 for **4ia**). Accurate full assignment was difficult. Copies of ^{1}H and ^{13}C NMR spectra are given at the end of the ESI.

Data for *N*-[1-fluoro-1-(4-methoxyphenyl)-2-oxo-2-phenylethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4ia**) and *N*-[1-fluoro-2-(4-methoxyphenyl)-2-oxo-1-phenylethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4ib**): SJB-02-024

^{19}F NMR: (376 MHz, CD_3CN)

δ –112.0 (**4ib**), –112.2 (**4ia**).

HRMS (ESI): Calcd for $C_{27}H_{22}FNO_6S_2NH_4$ $[M+NH_4]^+$, $C_{27}H_{22}FNO_6S_2Na$ $[M+Na]^+$: 557.1217, 562.0771; Found: 557.1206, 562.0757.



4k

time = 3 h; Column chromatography (SiO_2, ϕ = 4.0 cm, *l* = 7.0 cm, EtOAc:hexanes = 1:1, R_f = 0.7, UV 254 nm) afforded **4k**. In this case, the complete removal of residual solvents from the product was difficult. Thus, the chromatographed material was repeatedly diluted with CH_2Cl_2 and concentrated under reduced pressure 5 times. Then, the residue was dried using a Büchi B585 glass oven (200 mTorr, 40 °C) for 30 min to give **4k** (153 mg, 29%) as red solid.

Data for *N*-[1-fluoro-2-oxo-1,2-bis(2-thienyl)ethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4k**): SJB-02-054

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 7.93–7.91 (m, 5H), 7.66–7.60 (m, 3H), 7.50 (t, *J* = 7.8, 4H), 7.30–7.29 (m, 1H), 7.07 (t, *J* = 4.4, 1H), 6.68–6.67 (m, 2H).

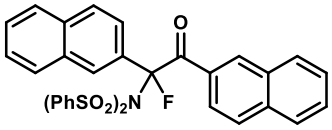
^{13}C NMR: (100 MHz, $CDCl_3$)

δ 183.1 (d, *J* = 28.6), 140.2, 137.81, 137.76, 135.66 (d, *J* = 5.7), 135.59 (d, *J* = 1.9), 134.1, 132.9 (d, *J* = 5.8), 131.6 (d, *J* = 28.1), 131.0, 129.0, 128.5, 126.7, 104.2 (d, *J* = 228.8).

^{19}F NMR: (376 MHz, $CDCl_3$)

δ –103.1.

HRMS (FAB): Calcd for $C_{22}H_{16}NO_5S_4$ $[M–F]^+$: 501.9911; Found: 501.9914.



4l

time = 1 h; Column chromatography (SiO_2, ϕ = 4.0 cm, *l* = 12 cm, EtOAc:hexanes = 1:5, R_f = 0.3, UV 254 nm) afforded **4l** along with recovered **1l** (30 mg, 10%). In this case, the complete removal of residual solvents from the product was difficult. Thus, the chromatographed material was repeatedly diluted with CH_2Cl_2 and concentrated under reduced pressure 5 times. The residue was dried using a Büchi B585 glass oven (200 mTorr, 60 °C) for 13 h to give **4l** (474 mg, 78%) as pale yellow solid.

Data for *N*-[1-fluoro-1,2-bis(2-naphthyl)-2-oxoethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4l**): SJB-02-048

^{1}H NMR: (400 MHz, $CDCl_3$)

δ 8.39 (s, 2H), 8.30–6.80 (m, 22H).

^{13}C NMR: (100 MHz, $CDCl_3$)

δ 192.0 (d, *J* = 30.5), 140.6, 135.3, 134.1, 133.7, 132.14, 132.09, 131.9, 131.5 (d, *J* = 1.9), 130.4, 130.3, 129.8, 129.1, 128.8, 128.7, 128.6, 128.1 (d, *J* = 9.6), 127.8, 127.6, 127.5, 126.6 (d, *J* = 9.5), 126.4 (d, *J* = 24.8), 125.7 (d, *J* = 3.8) 125.6, 125.5, 106.2 (d, *J* = 232.6).

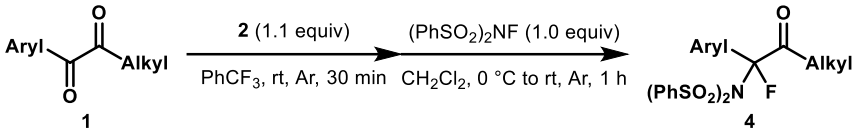
^{19}F NMR: (376 MHz, $CDCl_3$)

δ –114.5.

HRMS (ESI): Calcd for $C_{68}H_{48}F_2N_2O_{10}S_4NH_4$ $[2M+NH_4]^+$, $C_{34}H_{24}FNO_5S_2Na$ $[M+Na]^+$, $C_{34}H_{24}FNO_5S_2NH_4$ $[M+NH_4]^+$: 1236.2504, 632.0978, 627.1424; Found: 1236.2498, 632.0969, 627.1418.

2.4. Geminal Fluorosulfonimidation of Aryl-Alkyl 1,2-Diketones

General procedure for 4m and 4n:



To a solution of **1** (1.00 mmol) in $PhCF_3$ (0.5 mL) was added a solution of **2** (224 mg, 1.10 mmol) in $PhCF_3$ (1.5 mL then rinsed with 0.5 mL) at rt. After stirring for 30 min, a solution of $(PhSO_2)_2NF$ (315 mg, 1.00 mmol) in CH_2Cl_2 (2.5 mL) was added dropwise at 0 °C, and then the reaction mixture was warmed to rt. After 1 h, the reaction mixture was diluted with EtOAc (50 mL) and washed with brine (50 mL × 3). The combined aqueous layers were extracted with EtOAc (100 mL). The combined organic extracts were dried over $MgSO_4$ (10 g), filtered through a glass frit, and concentrated under reduced pressure. The residue was purified by column chromatography to give **4** along with recovered **1**.

4m

Column chromatography (SiO_2, ϕ = 4.0 cm, l = 12 cm, EtOAc:hexanes = 1:5, R_f = 0.4, UV 254 nm) afforded **4m** along with recovered **1m** (95 mg, 47%). To remove the residual grease, an additional flash column chromatography (SiO_2, ϕ = 4.0 cm, l = 12 cm, EtOAc:distilled hexanes = 1:10, R_f = 0.3, UV 254 nm) was performed. In this case, the complete removal of residual solvents from the product was difficult. Thus, the chromatographed material was repeatedly diluted with CH_2Cl_2 and concentrated under reduced pressure 5 times. Then, the residue was dried using a Büchi B585 glass oven (200 mTorr, 65 °C) for 12 h to give **4m** (120 mg, 24%) as white solid.

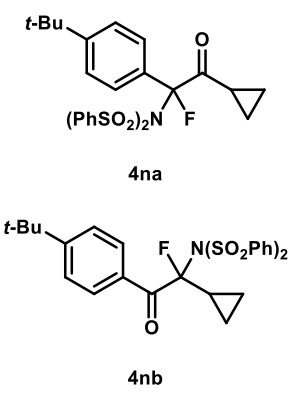
Data for *N*-[2-(4-*tert*-butylphenyl)-1-fluoro-1-methyl-2-oxoethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4m**): SJB-01-098

^{1}H NMR: (400 MHz, $CDCl_3$)
δ 7.75 (d, J = 7.2, 4H), 7.58 (t, J = 7.6, 2H), 7.42 (t, J = 7.8, 4H), 7.09–7.02 (m, 4H), 2.23 (d, J = 4.4, 3H). 1.27 (s, 9H).

^{13}C NMR: (100 MHz, $CDCl_3$)
δ 199.4 (d, J = 33.4), 153.4, 140.4, 134.0, 129.2 (d, J = 9.5), 128.9, 128.4, 124.8 (d, J = 24.8), 124.6 (d, J = 2.1), 104.4 (d, J = 229.8), 34.7, 31.2, 24.9.

^{19}F NMR: (376 MHz, $CDCl_3$)
δ –121.3.

HRMS (ESI): Calcd for $C_{25}H_{26}FNO_5S_2NH_4$ $[M+NH_4]^+$, $C_{25}H_{26}FNO_5S_2Na$ $[M+Na]^+$: 521.1580, 526.1134;
Found: 521.1576, 526.1124.



Column chromatography (SiO_2, ϕ = 4.0 cm, l = 12 cm, EtOAc:hexanes = 1:5, R_f = 0.24 and R_f = 0.16, UV 254 nm) afforded a mixture of **4na** and **4nb** along with recovered **1n** (16 mg, 7%). In this case, the complete removal of residual solvents from the product was difficult. Thus, the chromatographed material was repeatedly diluted with CH_2Cl_2 and concentrated under reduced pressure 5 times. Then, the residue was dried using a Büchi B585 glass oven (200 mTorr, 65 °C) for 13 h to give a mixture of **4na** and **4nb** (401 mg, 76%, 78:22 rr) as white solid. The isomeric ratio was determined by integration of the phenyl peaks in ^{1}H NMR spectra (δ 8.16–8.14 for **4nb**, δ 7.77–7.75 for **4na**). Accurate full assignment was difficult. A copy of ^{13}C NMR spectrum is given at the end of SI.

Data for *N*-[1-(4-*tert*-butylphenyl)-2-cyclopropyl-1-fluoro-2-oxoethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4na**):
SJB-02-050

^{1}H NMR: (400 MHz, $CDCl_3$)
δ 7.76 (d, J = 8.0, 4H), 7.59–7.55 (m, 2H), 7.42 (t, J = 7.6, 4H), 7.06–7.01 (m, 4H), 2.35–2.28 (m, 1H), 1.34–1.23 (m, 10H), 1.12–1.05 (m, 1H), 0.88–0.81 (m, 1H), 0.81–0.72 (m, 1H).

^{19}F NMR: (376 MHz, $CDCl_3$)
δ –121.7.

HRMS (ESI): Calcd for $C_{54}H_{56}F_2N_2O_{10}S_4Na$ $[2M+Na]^+$, $C_{27}H_{28}FNO_5S_2Na$ $[M+Na]^+$, $C_{27}H_{28}FNO_5S_2NH_4$ $[M+NH_4]^+$: 1081.2684, 552.1291, 547.1737; Found: 1081.2674, 552.1284, 547.1734.

Data for *N*-[2-(4-*tert*-butylphenyl)-1-cyclopropyl-1-fluoro-2-oxoethyl]-*N*-(phenylsulfonyl)benzenesulfonimide (**4nb**):
SJB-02-050

^{1}H NMR: (400 MHz, $CDCl_3$)
δ 8.15 (d, J = 8.0, 4H), 8.01–7.99 (m, 2H), 7.68–7.64 (m, 2H), 7.60–7.55 (m, 4H), 7.06–7.01 (m, 2H), 1.35–1.32 (m, 10H), 0.49–0.47 (m, 2H), 0.37–0.30 (m, 1H), 0.29–0.26 (m, 1H).

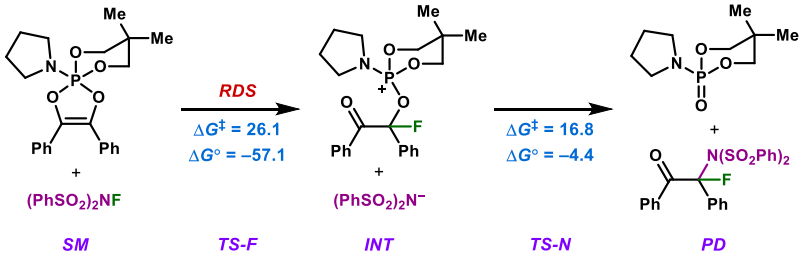
^{19}F NMR: (376 MHz, $CDCl_3$)
δ –121.7.

HRMS (ESI): Calcd for $C_{54}H_{56}F_2N_2O_{10}S_4Na$ $[2M+Na]^+$, $C_{27}H_{28}FNO_5S_2Na$ $[M+Na]^+$, $C_{27}H_{28}FNO_5S_2NH_4$ $[M+NH_4]^+$: 1081.2684, 552.1291, 547.1737; Found: 1081.2674, 552.1284, 547.1734.

3. DFT Calculation

Approximate transition structures for the electrophilic fluorination of benzil-derived dioxaphospholene was obtained by the PM7 semi-empirical method using MOPAC 2016.[5] These saddle points were refined by DFT calculation at the M062X-D3[6,7]/6-31+G(d,p) level of theory using the Gaussian 16 suite of programs.[8] Four different approaches of NFSI onto the C=C double bond of dioxaphospholene were examined, and the most stable TS was selected. Each phenyl ring in this structure was replaced by a methyl group, and then saddle point optimizations was performed for the fluorination of 1-phenyl-1,2-propanedione at each nucleophilic carbon. These TSs were verified by the presence of a single negative frequency as well as the Intrinsic Reaction Coordinate (IRC) calculation at the same level of theory. The reactants and the products from the IRC profiles were further optimized to give the ground state structures that lack imaginary frequency. Subsequently, the TS for the nucleophilic amination was located by a relaxed coordinate scan from the α-oxyphosphonium intermediate. In all of these calculations, the solvent effect was considered with the polarizable continuum model (PCM) for CH_2Cl_2.[9] More precise single point energies for the optimized structures were obtained with def2TZVP basis set[10] after thermal free energy correction. The 3-D illustrations were produced using CYLview 1.0b.[11]

3.1. Geminal Fluorosulfonimidation of Diphenyl 1,2-Diketone (Benzil)



- computed data for ***SM***

: total free energy = –3304.800348 Hartree

: relative free energy = 0.0 kcal/mol

: no imaginary frequency

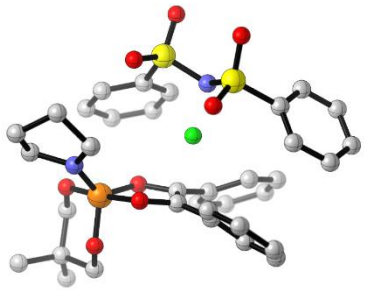
: Cartesian coordinates

Atom	X	Y	Z
C	3.84210200	2.36464300	-1.20654700
C	1.63585700	2.04098200	-2.18552800
N	2.72222000	1.41336700	-1.38826500
P	2.68405300	-0.11715200	-0.75703400
O	3.50601300	-1.31233500	-1.51546400
O	3.90850500	0.29064800	0.29946000
C	4.18605000	-2.31073600	-0.73775700
C	5.25894200	-1.72678300	0.17957300
H	4.62753800	-2.99593500	-1.46721600
H	3.44214000	-2.86333600	-0.14620500
C	4.57046900	-0.69542500	1.07478500
H	5.30833100	-0.16355100	1.68715100
H	3.85243700	-1.18725500	1.74587800
O	1.30345200	-0.44519300	-1.75599300

O	1.82962000	-0.76320800	0.51681900
C	0.40533800	-1.26679500	-1.15467400
C	0.66326600	-1.42209000	0.15783200
C	-0.67181200	-1.77550300	-2.01182100
C	-0.07993300	-2.01110100	1.27295800
C	-1.48134400	-1.97507300	1.31655400
C	0.61984600	-2.54807200	2.36232900
C	-0.06689500	-3.05553900	3.46269800
C	-1.46167900	-3.02739600	3.49421700
C	-2.16526100	-2.48585000	2.41608600
C	-1.26931500	-3.02382800	-1.78980900
C	-2.25655900	-3.49138900	-2.65217600
C	-2.65813200	-2.72425200	-3.74837200
C	-2.05963200	-1.48475700	-3.97939400
C	-1.07013200	-1.01325200	-3.11910600
H	-0.94575000	-3.63395600	-0.95156000
H	-2.70565500	-4.46416800	-2.47520000
H	-3.42571000	-3.09395600	-4.42102000
H	-2.36413200	-0.88245100	-4.82957200
H	-0.59894000	-0.05101600	-3.29385100
H	1.70614800	-2.55372700	2.34338400
H	0.48805000	-3.46932600	4.29916100
H	-1.99659300	-3.41796800	4.35408900
H	-3.25054900	-2.44464600	2.43553900
H	-2.03288900	-1.53132400	0.49326800
H	0.66742000	1.90545300	-1.70048200
H	1.58812300	1.59183000	-3.18299600
C	2.04346200	3.51134600	-2.26259200
C	3.56928100	3.44438000	-2.25051600
H	4.80184500	1.86637400	-1.34583000
H	3.82814000	2.78587400	-0.19322200
C	5.83424500	-2.84862500	1.04377300
C	6.36022600	-1.06243000	-0.64933800
N	-2.17290400	1.48155300	0.50676100
F	-1.28532100	0.73396700	-0.26776500
S	-1.26251200	2.91274100	0.99932600
S	-3.59794800	1.69776300	-0.52300300
O	-3.16364900	1.73481300	-1.90357900
O	-4.30796400	2.79973700	0.09372800
O	-0.73928100	3.60373400	-0.16582500
O	-2.15921800	3.57741300	1.92456700
C	0.04439400	2.09012600	1.85766900
C	-4.39871500	0.16388400	-0.17329200
C	-4.19616000	-0.91591700	-1.02880300
C	-4.81596700	-2.12384400	-0.71088800
C	-5.17729000	0.08369900	0.98159300
C	-5.78594700	-1.13042200	1.27971000
C	-5.60385700	-2.22846600	0.43499000
H	-6.08065200	-3.17365600	0.67357500
H	-4.67814900	-2.98007900	-1.36161700

H	-5.30445400	0.95209100	1.61962600
H	-6.40095100	-1.21960500	2.16848500
H	-3.57302100	-0.81478000	-1.91345200
C	1.35629000	2.42842800	1.53909000
C	2.38016200	1.87575200	2.30561000
C	2.07882400	0.98631500	3.33442600
C	0.75507500	0.64246400	3.61840500
C	-0.28311400	1.20390100	2.88442500
H	1.56322000	3.10968200	0.71947900
H	3.41146900	2.11875800	2.07785900
H	2.88320100	0.54949800	3.91823900
H	0.52905500	-0.06339800	4.41037900
H	-1.31887400	0.95743800	3.09648000
H	5.05374500	-3.33492300	1.63941400
H	6.58981900	-2.45263200	1.73035900
H	6.31345400	-3.61117700	0.42097200
H	7.12048000	-0.62473000	0.00645200
H	6.84927100	-1.79787600	-1.29701200
H	5.95102900	-0.26852400	-1.27983200
H	1.67915100	4.04949100	-1.37991200
H	1.62991700	3.99989200	-3.14753400
H	3.93946600	3.11997600	-3.22935200
H	4.04978600	4.39158900	-1.99555400

- computed data for ***TS-F***



: total free energy = –3304.758701 Hartree

: relative free energy = 26.13 kcal/mol

: a single imaginary frequency at –743.46 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
C	-3.76236400	2.20700800	1.36759200
C	-1.50436300	2.06986900	2.29353900
N	-2.55082400	1.35842600	1.50645500
P	-2.42921800	-0.14592900	0.86322500
O	-3.04868800	-1.43272900	1.64314400
O	-3.70692400	0.12430000	-0.13963800
C	-3.67196900	-2.49841100	0.90010600
C	-4.83710900	-2.02262500	0.03547700
H	-4.00894500	-3.21334500	1.65515500

H	-2.90661800	-2.98412700	0.27844500
C	-4.29978600	-0.92973300	-0.88815600
H	-5.11204200	-0.47458900	-1.46546700
H	-3.56394600	-1.33976300	-1.59330300
O	-0.94448900	-0.36887900	1.83301300
O	-1.51816000	-0.69306900	-0.43633300
C	-0.02994400	-1.09028100	1.22424200
C	-0.30709900	-1.23467700	-0.13617100
C	1.06148100	-1.61119900	2.04770900
C	0.31957900	-2.01369100	-1.20792900
C	1.71310000	-2.09046500	-1.35157000
C	-0.50516000	-2.65725900	-2.14022900
C	0.05300400	-3.39117200	-3.18379900
C	1.43844800	-3.47972300	-3.31322600
C	2.26419700	-2.82580100	-2.39558700
C	1.67203200	-2.84397800	1.78088000
C	2.65666000	-3.32821000	2.63621300
C	3.03794100	-2.59041200	3.75832400
C	2.42113000	-1.36825700	4.03383900
C	1.43041600	-0.88157700	3.18716700
H	1.36296600	-3.43230700	0.92341100
H	3.12270700	-4.28632100	2.42971300
H	3.80821800	-2.97129000	4.42160900
H	2.71268900	-0.79470800	4.90757700
H	0.94597700	0.06821600	3.38742500
H	-1.58364300	-2.57417600	-2.04643000
H	-0.59546900	-3.88808500	-3.89822200
H	1.87435500	-4.04648000	-4.12963800
H	3.34353600	-2.87423700	-2.50106700
H	2.35767900	-1.55674300	-0.65914500
H	-0.53476100	2.00127400	1.79992600
H	-1.42989000	1.63430000	3.29547900
C	-2.02270200	3.50386800	2.34981100
C	-3.53800900	3.31946200	2.38828800
H	-4.66463300	1.62551700	1.55904600
H	-3.82920500	2.60717800	0.34977200
C	-5.33348500	-3.19645700	-0.80920900
C	-5.96065600	-1.47292600	0.91723000
N	1.91895800	1.70368800	-0.82496800
F	0.94897000	0.40545900	-0.17295900
S	0.84145800	2.95335500	-1.17996000
S	3.08904600	1.93446200	0.36839400
O	2.54842600	1.83889200	1.71720200
O	3.82569300	3.14036100	-0.00533300
O	0.26695300	3.56050100	0.01735200
O	1.52407000	3.82728000	-2.13197500
C	-0.41058200	2.01949500	-2.02281100
C	4.05859400	0.48695200	0.02704800
C	4.25803400	-0.44697100	1.03648400
C	5.02075600	-1.58056900	0.74823400

C	4.58840600	0.32998900	-1.25447100
C	5.33844900	-0.80801000	-1.52735400
C	5.55168000	-1.76167200	-0.52697700
H	6.13577000	-2.64972600	-0.74654500
H	5.18821100	-2.32204200	1.52193500
H	4.40298000	1.07699200	-2.01988300
H	5.75300000	-0.95447300	-2.51916600
H	3.81763900	-0.29414000	2.01643800
C	-1.73677500	2.31984600	-1.73777100
C	-2.73543100	1.66774600	-2.46061100
C	-2.39450400	0.72190600	-3.42370600
C	-1.05374700	0.42016400	-3.67887300
C	-0.04487500	1.07674600	-2.98335200
H	-1.97461400	3.04417500	-0.96454000
H	-3.77710100	1.88588600	-2.25060400
H	-3.17602900	0.20935800	-3.97651000
H	-0.79269400	-0.32904800	-4.41917500
H	1.00147700	0.85224700	-3.16574600
H	-4.53678700	-3.59498000	-1.44717200
H	-6.15963900	-2.87901100	-1.45354600
H	-5.69810700	-4.00702700	-0.17016500
H	-6.78725400	-1.10814600	0.29874800
H	-6.34644400	-2.25657700	1.57749400
H	-5.60568500	-0.64622500	1.53850700
H	-1.72423600	4.03483300	1.43979100
H	-1.62274800	4.04411100	3.21051300
H	-3.85322500	2.98440400	3.38254700
H	-4.09807900	4.22189900	2.13396600

- computed data for ***INT***

: total free energy = –3304.891289 Hartree

: relative free energy = –57.07 kcal/mol

: no imaginary frequency

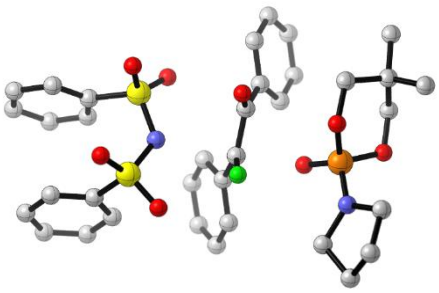
: Cartesian coordinates

Atom	X	Y	Z
C	2.78310900	3.52214200	0.48337600
C	4.39865200	3.18519900	-1.35417800
N	3.57583300	2.53056800	-0.29941400
P	3.65816800	0.97114300	0.00804100
O	3.74908400	0.19629500	-1.34925400
O	4.91802600	0.56131300	0.85837100
C	4.31776400	-1.15346200	-1.43415900
C	5.59295100	-1.30148000	-0.60390000
H	4.51093600	-1.29700800	-2.49744300
H	3.54276600	-1.85407900	-1.11097800
C	5.31936600	-0.84569400	0.82942300
H	6.21890700	-0.89135700	1.44318200

H	4.52676800	-1.43826300	1.30149400
O	1.00951000	-1.03154800	-1.53592800
O	2.44113800	0.50662500	0.91277100
C	1.12703000	-1.07245100	-0.33537200
C	1.07968100	0.27377300	0.44636400
C	1.46208000	-2.33111700	0.39363600
C	0.17941800	0.36127800	1.65486300
C	-0.80244900	-0.59964700	1.90213700
C	0.34316400	1.43865700	2.52842600
C	-0.46175100	1.54978000	3.65980700
C	-1.42170700	0.57331200	3.92692500
C	-1.59128500	-0.49475600	3.04702400
C	1.93705700	-2.36210000	1.71217600
C	2.29614500	-3.57725100	2.29193700
C	2.17134700	-4.76245700	1.56764900
C	1.68575400	-4.73647400	0.25814000
C	1.33526700	-3.52591400	-0.32759600
H	2.03629600	-1.45022500	2.29186100
H	2.66965600	-3.59606600	3.31036100
H	2.44744000	-5.70733900	2.02495700
H	1.57735000	-5.65945000	-0.30158000
H	0.94622100	-3.48208300	-1.33905800
H	1.10381200	2.18635500	2.33111600
H	-0.33181900	2.39034100	4.33334300
H	-2.04015900	0.64866500	4.81602900
H	-2.34656800	-1.24804300	3.24864100
H	-0.96451200	-1.41490100	1.20233700
H	4.36499900	2.59822500	-2.27324500
H	5.43491600	3.27736300	-1.01216600
C	3.72947700	4.55235800	-1.47497200
C	3.31734700	4.86040700	-0.03360000
H	2.94946600	3.39235400	1.55489800
H	1.72299300	3.39159300	0.25235500
C	5.94360400	-2.79291600	-0.56368300
C	6.73661100	-0.48848900	-1.21807600
N	-1.82898200	0.08462500	-0.99009400
F	0.81668200	1.26737500	-0.43662600
S	-2.60719600	1.44587600	-1.36741200
S	-2.35031900	-1.35275900	-1.50001500
O	-1.61207300	-2.34705700	-0.69861100
O	-2.29116100	-1.52973500	-2.95740200
O	-1.65345500	2.54727400	-1.18655400
O	-3.33326600	1.38773400	-2.64697700
C	-3.84956300	1.66248500	-0.09400800
C	-4.07163900	-1.49808100	-1.03214200
C	-4.38094200	-1.61016200	0.32313200
C	-5.71551100	-1.68071900	0.70864000
C	-5.06297800	-1.44488500	-2.00480300
C	-6.39968300	-1.52074900	-1.60867500
C	-6.72359000	-1.63797500	-0.25817800

H	-7.76454200	-1.69115100	0.04545200
H	-5.97040700	-1.76283300	1.76049700
H	-4.78323100	-1.34154400	-3.04765600
H	-7.18520200	-1.48370000	-2.35662200
H	-3.58194700	-1.63410000	1.05880000
C	-3.42517000	1.78748800	1.22816300
C	-4.37798100	1.93371300	2.23188800
C	-5.73761100	1.95774600	1.90832900
C	-6.14492700	1.83714000	0.58101400
C	-5.19723600	1.68714600	-0.43258800
H	-2.36385400	1.76103100	1.46258600
H	-4.05968200	2.02699900	3.26588300
H	-6.47821700	2.06937700	2.69421100
H	-7.20122400	1.84920200	0.33084900
H	-5.49169100	1.57678700	-1.47098100
H	5.14675100	-3.37833000	-0.09176600
H	6.86892100	-2.94901800	-0.00164500
H	6.09616200	-3.17493000	-1.57730000
H	7.63765900	-0.57615600	-0.60383300
H	6.96590800	-0.86221900	-2.22000000
H	6.48607100	0.57311800	-1.30245100
H	2.84630800	4.47576000	-2.11597800
H	4.40688400	5.29663500	-1.89628700
H	4.19143700	5.16401800	0.55048400
H	2.56082000	5.64294600	0.04002900

- computed data for ***TS-N***



: total free energy = –3304.864452 Hartree

: relative free energy = –40.23 kcal/mol

: a single imaginary frequency at –153.53 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
C	-3.24640100	-3.48038800	0.15446700
C	-5.26518500	-2.85354500	-1.09552300
N	-4.10094200	-2.37101000	-0.32343200
P	-3.86022600	-0.81657000	0.04011600
O	-3.95103100	-0.02450900	-1.34642700
O	-5.15597400	-0.30428800	0.83487600
C	-4.25023400	1.39385600	-1.33161200

C	-5.51153800	1.71055400	-0.52536900
H	-4.37119100	1.67250500	-2.38035000
H	-3.38707700	1.92964200	-0.92313500
C	-5.35211400	1.12966000	0.88150100
H	-6.25439400	1.28409200	1.47656100
H	-4.49885800	1.58623300	1.40129400
O	-0.99533800	1.09051800	-1.60304800
O	-2.59444100	-0.57052800	0.81899700
C	-0.91055300	1.02702100	-0.39961000
C	-0.50097900	-0.35806100	0.14999300
C	-1.24658700	2.16639600	0.49709900
C	0.13306300	-0.70257100	1.38549800
C	0.86673800	0.26196500	2.10213700
C	0.03258900	-2.02830800	1.84676900
C	0.62808700	-2.37525200	3.05016300
C	1.34725100	-1.41477700	3.76947300
C	1.48027700	-0.10775600	3.29046900
C	-1.70266400	2.02849200	1.81405000
C	-2.06993800	3.16094800	2.53911600
C	-1.98113800	4.42611100	1.96033700
C	-1.52356700	4.56525500	0.64757100
C	-1.16073300	3.44037800	-0.08198500
H	-1.81086600	1.04693300	2.25956100
H	-2.43341800	3.04965100	3.55537300
H	-2.26838800	5.30405100	2.53038300
H	-1.44598000	5.54913400	0.19727600
H	-0.79079400	3.52848800	-1.09760800
H	-0.52725700	-2.75633100	1.27012700
H	0.54178000	-3.38824200	3.42626900
H	1.81910700	-1.69172900	4.70703500
H	2.06638600	0.61816600	3.84325400
H	0.99588900	1.25862800	1.69027600
H	-5.38108000	-2.27403100	-2.01489700
H	-6.17933300	-2.76063600	-0.49727400
C	-4.91323600	-4.32044800	-1.35226800
C	-4.12197600	-4.70923200	-0.09975200
H	-2.99231900	-3.34911300	1.20876800
H	-2.32358000	-3.52530600	-0.43470500
C	-5.62347000	3.23255200	-0.40593300
C	-6.74829000	1.12058700	-1.20796800
N	1.90005700	-0.04217800	-0.93734100
F	-0.68503900	-1.29400400	-0.70799000
S	2.67748000	-1.34287400	-1.51041500
S	2.40565900	1.46659900	-1.24125900
O	1.64603200	2.30200900	-0.29267500
O	2.32743800	1.84996000	-2.65463700
O	1.73855900	-2.46216100	-1.36566500
O	3.29884800	-1.13439800	-2.82457000
C	4.01287600	-1.65712400	-0.35945600
C	4.12512000	1.56336200	-0.76839800

C	4.44931600	1.45358300	0.58380700
C	5.78723300	1.49651200	0.96018100
C	5.10122400	1.70549400	-1.74775600
C	6.44091600	1.75285500	-1.35815400
C	6.78086000	1.64874900	-0.01090900
H	7.82428200	1.68001500	0.28693600
H	6.05652300	1.40622500	2.00761900
H	4.80971600	1.77521500	-2.79025800
H	7.21554200	1.86713300	-2.10939700
H	3.66226600	1.32929900	1.32298200
C	3.68592200	-1.90042500	0.97294200
C	4.70526900	-2.13433100	1.88951900
C	6.03750700	-2.12392200	1.46676700
C	6.34825400	-1.88138300	0.13018900
C	5.33136200	-1.64468600	-0.79665000
H	2.64474900	-1.90104800	1.28045300
H	4.46209800	-2.32326200	2.93089800
H	6.83315700	-2.30288200	2.18313500
H	7.38379200	-1.86636800	-0.19466800
H	5.55057900	-1.44181600	-1.83968800
H	-4.74857400	3.65672300	0.10057100
H	-6.51794100	3.50734200	0.16158000
H	-5.69920000	3.68984400	-1.39736000
H	-7.64704900	1.33461100	-0.62094200
H	-6.87619800	1.55751000	-2.20315600
H	-6.66412400	0.03569100	-1.31956500
H	-4.27551500	-4.39830700	-2.23851800
H	-5.80264600	-4.93316200	-1.50949400
H	-4.80414900	-4.85904600	0.74345300
H	-3.52556600	-5.61409500	-0.22945400

- computed data for ***PD***

: total free energy = –3304.898369 Hartree

: relative free energy = –61.51 kcal/mol

: no imaginary frequency

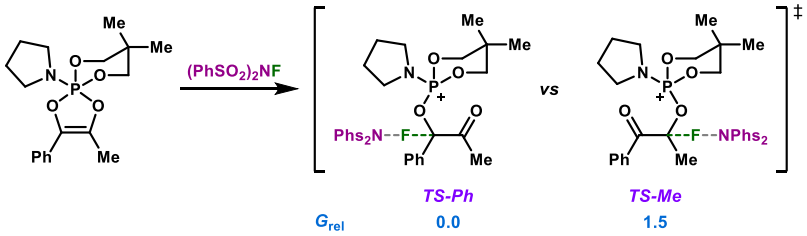
: Cartesian coordinates

Atom	X	Y	Z
C	3.22795400	3.40403100	-0.43839500
C	5.38002300	2.65187400	-1.34164200
N	4.21150700	2.30273800	-0.51242500
P	3.87101700	0.79355300	-0.01871700
O	3.99035300	-0.13459300	-1.33202400
O	5.17136700	0.32393100	0.82011800
C	4.11540800	-1.55433400	-1.10169300
C	5.34701300	-1.88352100	-0.25270700
H	4.18737600	-2.01151900	-2.09167600
H	3.20259700	-1.91484200	-0.61415200

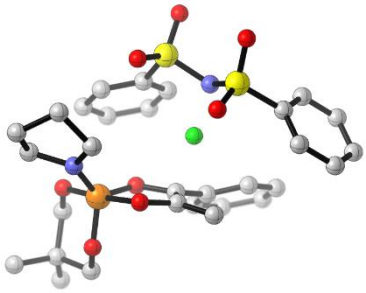
C	5.25715800	-1.09757100	1.05957800
H	6.15406200	-1.24575200	1.66577800
H	4.37823600	-1.41371100	1.63874000
O	0.96203700	-1.04339700	-1.54488200
O	2.59562400	0.65339500	0.72966200
C	0.55008600	-0.97849900	-0.41175500
C	-0.36618400	0.28560200	-0.09900700
C	0.92215900	-2.02147600	0.60007300
C	-0.54879100	0.60389700	1.36673700
C	-1.35353400	-0.23922400	2.13549700
C	0.08543300	1.69760200	1.94915200
C	-0.09115100	1.94790200	3.31033400
C	-0.88516800	1.10054900	4.08459700
C	-1.51547100	0.00278100	3.49580700
C	1.36402700	-1.74818900	1.90019000
C	1.80424700	-2.79072800	2.71552800
C	1.79933400	-4.10507000	2.25029600
C	1.36614600	-4.37999300	0.95226400
C	0.94087300	-3.34211200	0.12932200
H	1.41603300	-0.72786200	2.25690900
H	2.15934000	-2.56839100	3.71694200
H	2.13971000	-4.91110900	2.89310900
H	1.36539200	-5.39913400	0.57927700
H	0.60921000	-3.53973400	-0.88428800
H	0.71839000	2.32985000	1.33859200
H	0.39630500	2.80359200	3.76637900
H	-1.01583400	1.29725000	5.14410900
H	-2.13940400	-0.65533300	4.09178900
H	-1.84640400	-1.08826400	1.66748300
H	5.60884100	1.84721100	-2.04593000
H	6.25685900	2.82238800	-0.70561400
C	4.93492500	3.94137400	-2.03666700
C	4.01589000	4.59097000	-0.99722900
H	2.89976500	3.55895700	0.59199000
H	2.34954600	3.18182800	-1.05469500
C	5.31270700	-3.37684800	0.07824400
C	6.62945600	-1.51669300	-1.00317800
N	-1.71618700	0.18409000	-0.73091900
F	0.30795700	1.29441500	-0.73753100
S	-2.65634200	1.64225700	-0.83933900
S	-2.15007400	-1.15949300	-1.72805400
O	-1.55605200	-2.29719100	-1.03404900
O	-1.82457800	-0.89814300	-3.11718200
O	-1.77552800	2.74870700	-0.52508700
O	-3.32538300	1.55181300	-2.12688500
C	-3.89109100	1.57948300	0.44108700
C	-3.90821400	-1.32869600	-1.56026700
C	-4.40246400	-1.90900200	-0.39401100
C	-5.77205800	-2.13871600	-0.29770000
C	-4.72441700	-0.99733000	-2.63838500

C	-6.09127800	-1.24022200	-2.52883300
C	-6.61106900	-1.80385400	-1.36135100
H	-7.67757600	-1.98850100	-1.28302100
H	-6.18057600	-2.58124800	0.60420300
H	-4.29243700	-0.55437700	-3.52863900
H	-6.74852000	-0.98966000	-3.35422200
H	-3.73109500	-2.17954900	0.41424700
C	-3.55503700	2.02979400	1.71780800
C	-4.54271500	2.04320400	2.69777000
C	-5.84010300	1.62775600	2.39267300
C	-6.16280300	1.20898200	1.10237700
C	-5.18539000	1.18635600	0.11032900
H	-2.54793000	2.37065300	1.93685900
H	-4.29712100	2.38480900	3.69776300
H	-6.60571600	1.64378700	3.16158200
H	-7.17544100	0.90319900	0.86097200
H	-5.42571600	0.88616600	-0.90410800
H	4.39545300	-3.64119600	0.61768700
H	6.17073900	-3.65322800	0.69964500
H	5.35405900	-3.97397400	-0.83846800
H	7.50927600	-1.74966900	-0.39430600
H	6.69926100	-2.08362000	-1.93722500
H	6.65426400	-0.45076700	-1.24679200
H	4.36439100	3.69685900	-2.93868500
H	5.78067600	4.57066500	-2.32100800
H	4.61478900	5.04709100	-0.20171300
H	3.35963800	5.35544600	-1.41768700

3.2. Geminal Fluorosulfonimidation of Methyl Phenyl 1,2-Diketone (1-Phenyl-1,2-propanedione)



- computed data for ***TS-Ph***



: total free energy = –3113.074461 Hartree

: relative free energy = 0.00 kcal/mol

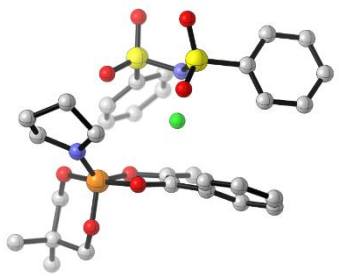
: a single imaginary frequency at –731.91 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
C	-3.49938600	-2.64723000	-0.40222400
C	-1.35690700	-2.70778400	-1.57604400
N	-2.39674600	-1.82895300	-0.96949800
P	-2.36251700	-0.18967600	-0.89187700
O	-3.17391100	0.70808600	-1.98002600
O	-3.51307500	-0.17282400	0.28809600
C	-3.81420900	1.93089200	-1.56530000
C	-4.84703200	1.71819700	-0.46079300
H	-4.28202300	2.32903800	-2.46940300
H	-3.03874500	2.63602500	-1.23382200
C	-4.12913600	1.03902300	0.70534500
H	-4.83945400	0.76497400	1.49302800
H	-3.37263500	1.70651900	1.13987800
O	-0.99954900	-0.22998600	-2.05888100
O	-1.39393500	0.81777800	0.02929300
C	-0.07853300	0.66855200	-1.80978300
C	-0.26138100	1.27890100	-0.57445800
C	0.96913500	0.87513100	-2.83599600
C	0.37989100	2.43525400	0.04648600
C	1.74977100	2.70008600	-0.10925900
C	-0.39646700	3.29042700	0.84302500
C	0.17755000	4.40581900	1.44539300
C	1.53396400	4.67885100	1.26694800
C	2.31548400	3.82066900	0.49161900
H	-1.44996300	3.07231200	0.98768600
H	-0.43506100	5.06050500	2.05706100
H	1.98264800	5.54696000	1.73889600
H	3.37698800	4.01157900	0.36810300
H	2.37940800	2.00858800	-0.66116400
H	-0.35927200	-2.41077400	-1.25301200
H	-1.41069900	-2.65233200	-2.66783200
C	-1.73414500	-4.09770900	-1.07221200
C	-3.25770700	-4.03262300	-0.99501500
H	-4.46898900	-2.22787000	-0.67210200
H	-3.43296100	-2.66572500	0.69141800
C	-5.36898400	3.08162100	-0.00689300
C	-5.99239600	0.83935100	-0.96809800
N	2.34966400	-1.09687100	0.73913100
F	1.18171200	-0.17003000	-0.13952000
S	1.45605500	-2.23231900	1.62162800
S	3.38742300	-1.63282300	-0.47751400
O	2.67967000	-2.01213700	-1.69417700
O	4.28543700	-2.60572200	0.13912700
O	0.84618800	-3.24778500	0.76873500
O	2.32565500	-2.67392600	2.70872100

C	0.18926000	-1.16669400	2.26219200
C	4.22210000	-0.09247200	-0.77374800
C	4.34291800	0.35528700	-2.08533900
C	4.98278800	1.57298500	-2.31732300
C	4.73725800	0.62170400	0.30810200
C	5.37673100	1.83166500	0.06042400
C	5.49068000	2.30935900	-1.24797300
H	5.98086900	3.25978400	-1.43301300
H	5.08020000	1.94344500	-3.33208900
H	4.61950500	0.24638100	1.31939700
H	5.77622900	2.40709700	0.88882100
H	3.94142400	-0.23447500	-2.90221500
C	-1.11994900	-1.63128000	2.23046700
C	-2.11584600	-0.84898100	2.81511800
C	-1.79249800	0.37821300	3.38733300
C	-0.47168700	0.83561400	3.38797500
C	0.53738300	0.05773600	2.83183200
H	-1.34777300	-2.58091300	1.75558800
H	-3.14473100	-1.19188100	2.79918800
H	-2.57336000	0.98827500	3.83120800
H	-0.22703700	1.79979700	3.82142500
H	1.56822400	0.39810400	2.82166000
H	-4.55675200	3.71925300	0.35929800
H	-6.09799700	2.95996800	0.80073600
H	-5.86600700	3.60057900	-0.83275000
H	-6.72305300	0.66823800	-0.17075300
H	-6.50540300	1.32540000	-1.80447100
H	-5.62308800	-0.13121100	-1.31015000
H	-1.30575700	-4.25495000	-0.07644300
H	-1.35940300	-4.88193700	-1.73342100
H	-3.68999900	-4.09094600	-1.99995900
H	-3.70184200	-4.81933900	-0.38135400
H	1.54967300	1.77881800	-2.65307400
H	0.49526400	0.93424600	-3.81877000
H	1.63409200	0.00368000	-2.82491600

- computed data for ***TS-Me***



: total free energy = –3113.072060 Hartree

: relative free energy = 1.51 kcal/mol

: a single imaginary frequency at –769.45 cm^{-1}

: Cartesian coordinates

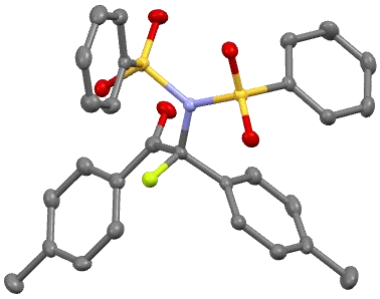
Atom	X	Y	Z
C	3.01829500	-0.59079400	2.68853300
C	0.95517000	0.70273300	2.79679800
N	2.12380000	0.33331600	1.94887300
P	2.35274600	0.77359200	0.38585000
O	3.26332500	2.08504600	0.07691500
O	3.53475900	-0.36860300	0.17833100
C	4.17430900	2.10962800	-1.03626300
C	5.19812800	0.97906300	-0.98390900
H	4.66151700	3.08703200	-0.98591300
H	3.59333500	2.05452200	-1.96723100
C	4.41055500	-0.32984500	-0.94366100
H	5.08508500	-1.18577900	-0.83277300
H	3.83236500	-0.45436200	-1.86949400
O	0.94492600	1.85607700	0.53469900
O	1.64418700	0.24428400	-1.04082100
C	0.14799200	1.84841000	-0.51682700
C	0.49685600	0.86218500	-1.42830600
C	-0.97496700	2.78003700	-0.52164700
C	0.01703400	0.50203800	-2.78696900
C	-1.60429300	3.18877500	-1.70693700
C	-2.68672900	4.06224700	-1.65397100
C	-3.14516700	4.54040700	-0.42500500
C	-2.50682200	4.15340700	0.75525500
C	-1.42421600	3.28137900	0.71005400
H	-1.23703700	2.85041100	-2.66914500
H	-3.16820800	4.37578800	-2.57474200
H	-3.99213800	5.21822400	-0.38802200
H	-2.85905700	4.52510800	1.71185800
H	-0.93329800	2.95729500	1.62133600
H	0.02089500	0.50291500	2.27405600
H	1.00627500	1.76815900	3.04580600
C	1.11161200	-0.16342900	4.04680900
C	2.62099900	-0.37405500	4.14462000
H	4.06432700	-0.35987000	2.49147600
H	2.82162900	-1.62290900	2.37653300
C	6.04478500	1.01932500	-2.25630100
C	6.08014500	1.11536700	0.25903900
N	-1.88169500	-1.54712200	0.16349800
F	-0.90206000	-0.24253200	-0.42201300
S	-0.70076400	-2.64626600	0.69036400
S	-2.89671400	-0.80557500	1.30805800
O	-2.26859800	0.36923400	1.89479000
O	-3.39125600	-1.86012500	2.18771800
O	0.22273400	-2.04772300	1.64656500
O	-1.40153900	-3.87214700	1.06235000
C	0.13445200	-2.90108700	-0.85397500
C	-4.19376400	-0.28225400	0.21720600

C	-4.15608400	1.00770400	-0.30248500
C	-5.17207700	1.39902900	-1.17326400
C	-5.20130900	-1.19049000	-0.10075700
C	-6.20995000	-0.78252400	-0.96890500
C	-6.19243300	0.50753500	-1.50402300
H	-6.98168200	0.81956900	-2.18036400
H	-5.16370700	2.40189800	-1.58753700
H	-5.19480300	-2.18651000	0.33013000
H	-7.00887400	-1.46961500	-1.22601300
H	-3.35544800	1.68496500	-0.02246800
C	1.50962600	-2.71052700	-0.90430300
C	2.17131100	-2.99096500	-2.10106400
C	1.45577000	-3.43183900	-3.21180800
C	0.06990000	-3.60625600	-3.14074500
C	-0.60263300	-3.34745500	-1.95182100
H	2.04738200	-2.34012200	-0.03698500
H	3.24662700	-2.86084600	-2.16158800
H	1.97690300	-3.64317400	-4.14003200
H	-0.48312500	-3.94845300	-4.00884900
H	-1.67660700	-3.48327200	-1.87353500
H	5.42478100	0.92320800	-3.15407500
H	6.77255100	0.20143400	-2.25519200
H	6.59859700	1.96134700	-2.32237700
H	6.79474400	0.28735200	0.31189200
H	6.64424600	2.05335800	0.22577300
H	5.47949700	1.10955700	1.17258000
H	0.60933200	-1.12214000	3.89195300
H	0.68054700	0.32061800	4.92615600
H	3.10871500	0.52737900	4.53287900
H	2.90563500	-1.22011500	4.77434600
H	0.18770600	-0.56994100	-2.92834300
H	0.56637300	1.04854200	-3.56102400
H	-1.05010000	0.69859300	-2.88863500

4. X-ray Crystallographic Data

Reflection data for **4a** were collected using a Bruker APEX-II CCD-based diffractometer with graphite-monochromated MoKα radiation (λ = 0.7107 Å). The hemisphere of the reflection data was collected as ω scan frames at 0.5°/frame and an exposure time of 5 s/frame. The cell parameters were determined and refined using the APEX2 program.[12] The data were corrected for Lorentz and polarization effects, and an empirical absorption correction was applied using the SADABS program.[13] The compound structure was solved by direct methods and refined by full matrix least-squares using the SHELXTL program package[14] and Olex2[15] with anisotropic thermal parameters for all non-hydrogen atoms. The relevant data are summarized in Table S1. CCDC 2110574 contains the supplementary crystallographic data for this study. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic data and parameters for **4a**.



Identification code	JWJ05_0m
CCDC #	2110574
Empirical formula	$C_{28}H_{24}FNO_5S_2$
Formula weight	537.60
Temperature/K	100
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.7215(2)
b/Å	18.6021(5)
c/Å	20.0805(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2510.75(12)
Z	4
ρ_{calc}g/cm^3	1.422
μ/mm^{-1}	0.260
F(000)	1120.0
2Θ range for data collection/°	7.618 to 51.904
Index ranges	$-8 \le h \le 8$, $-22 \le k \le 22$, $-24 \le l \le 24$
Reflections collected	31857
Independent reflections	4877 [R_{int} = 0.0439, R_{sigma} = 0.0283]
Data/restraints/parameters	4877/0/336
Goodness-of-fit on F^2	1.130
Final R indexes [I>=2σ (I)]	^{a}R_1 = 0.0342, ^{b}wR_2 = 0.0794
Final R indexes [all data]	^{a}R_1 = 0.0399, ^{b}wR_2 = 0.0820
Largest diff. peak/hole / e Å^{-3}	0.34/-0.31
Flack parameter	0.49(2)

^{a} $R_1 = \sum||Fo| - |Fc||/\sum|Fo|$. ^{b} $wR_2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

5. References

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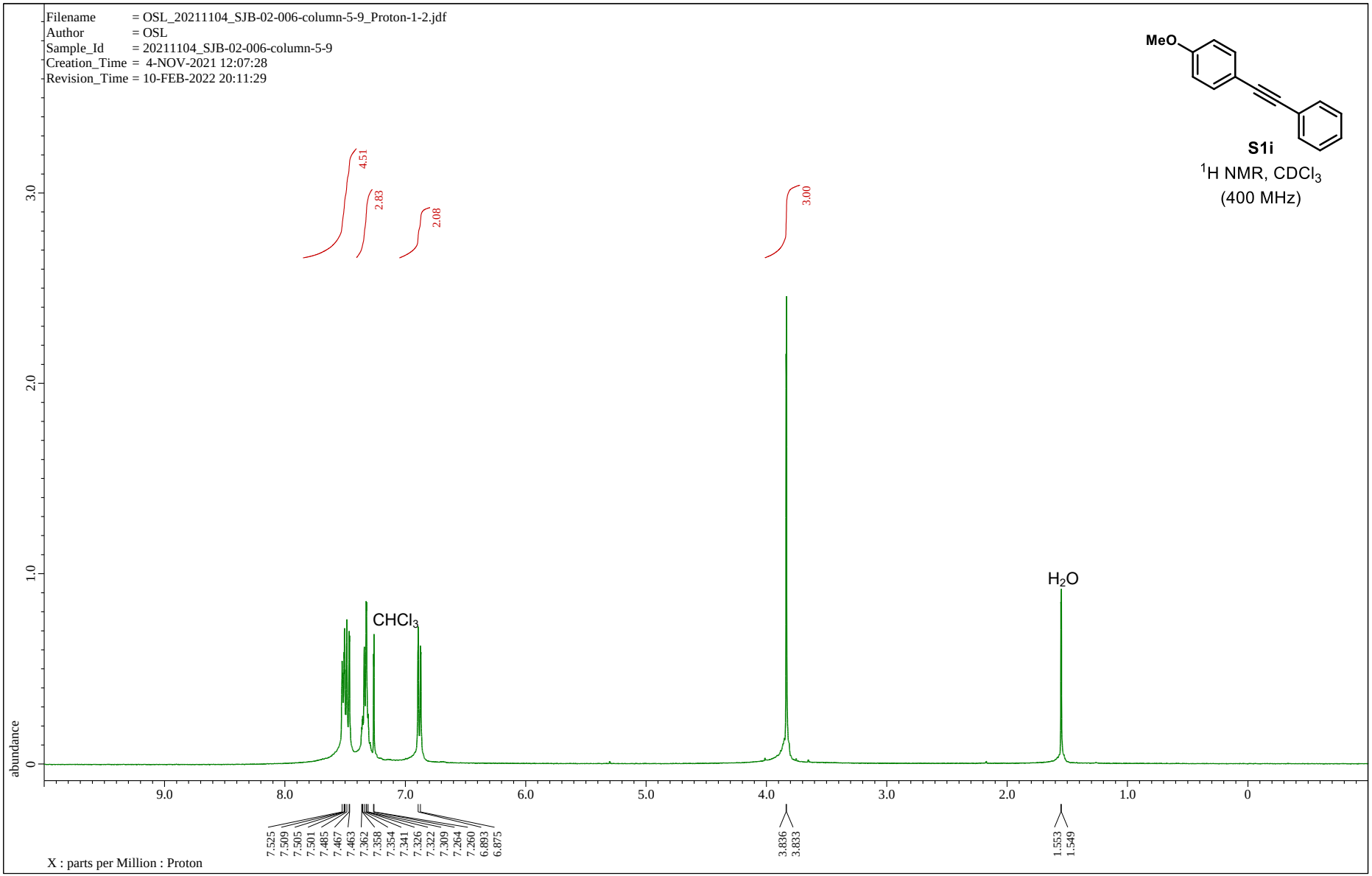
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2.83
2.08
3.00
CHCl3
H2O
abundance
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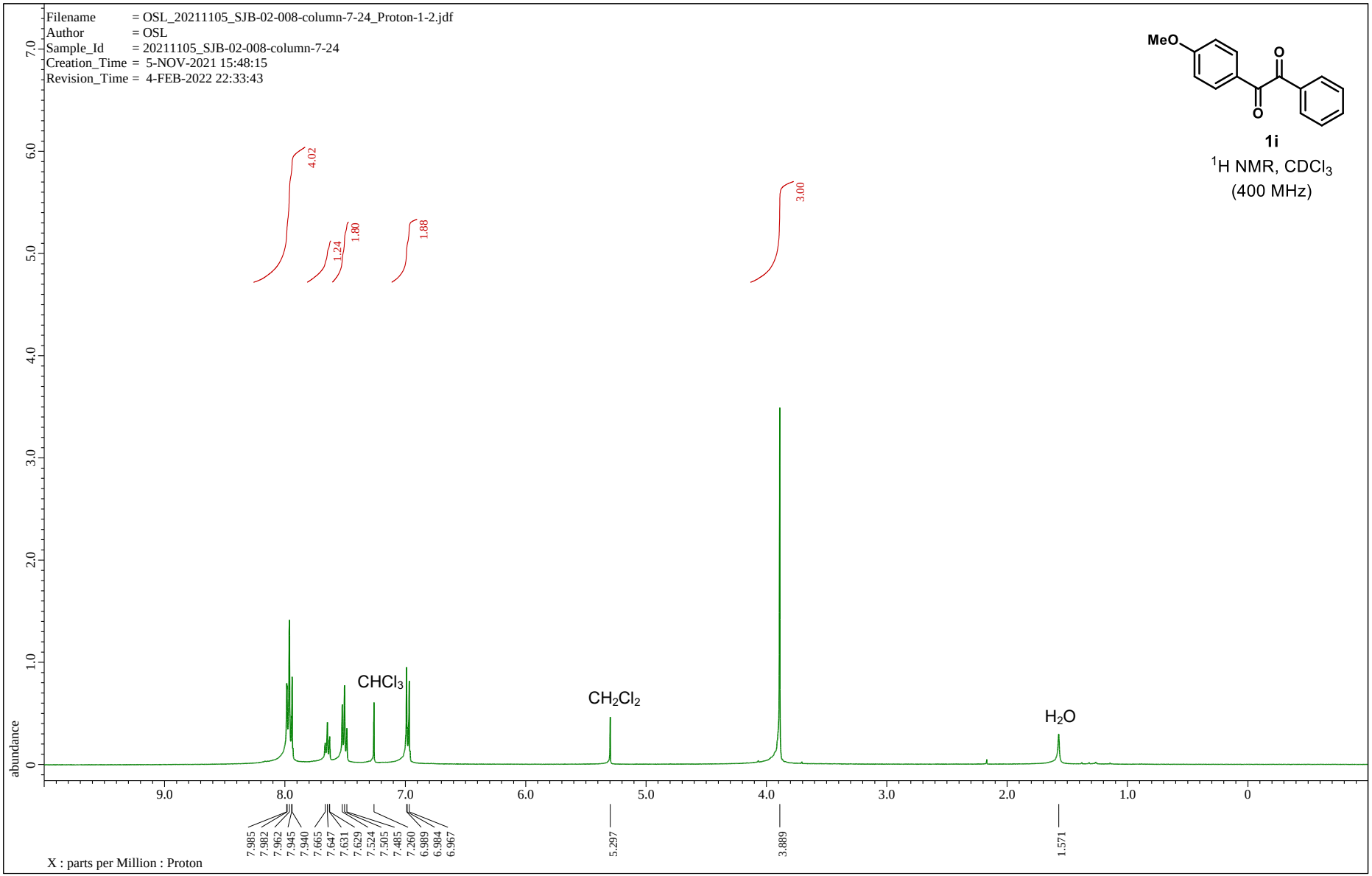
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.525
7.509
7.505
7.501
7.485
7.467
7.463
7.362
7.358
7.354
7.341
7.326
7.322
7.309
7.264
7.260
6.893
6.875
3.836
3.833
1.553
1.549
X : parts per Million : Proton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O
1i
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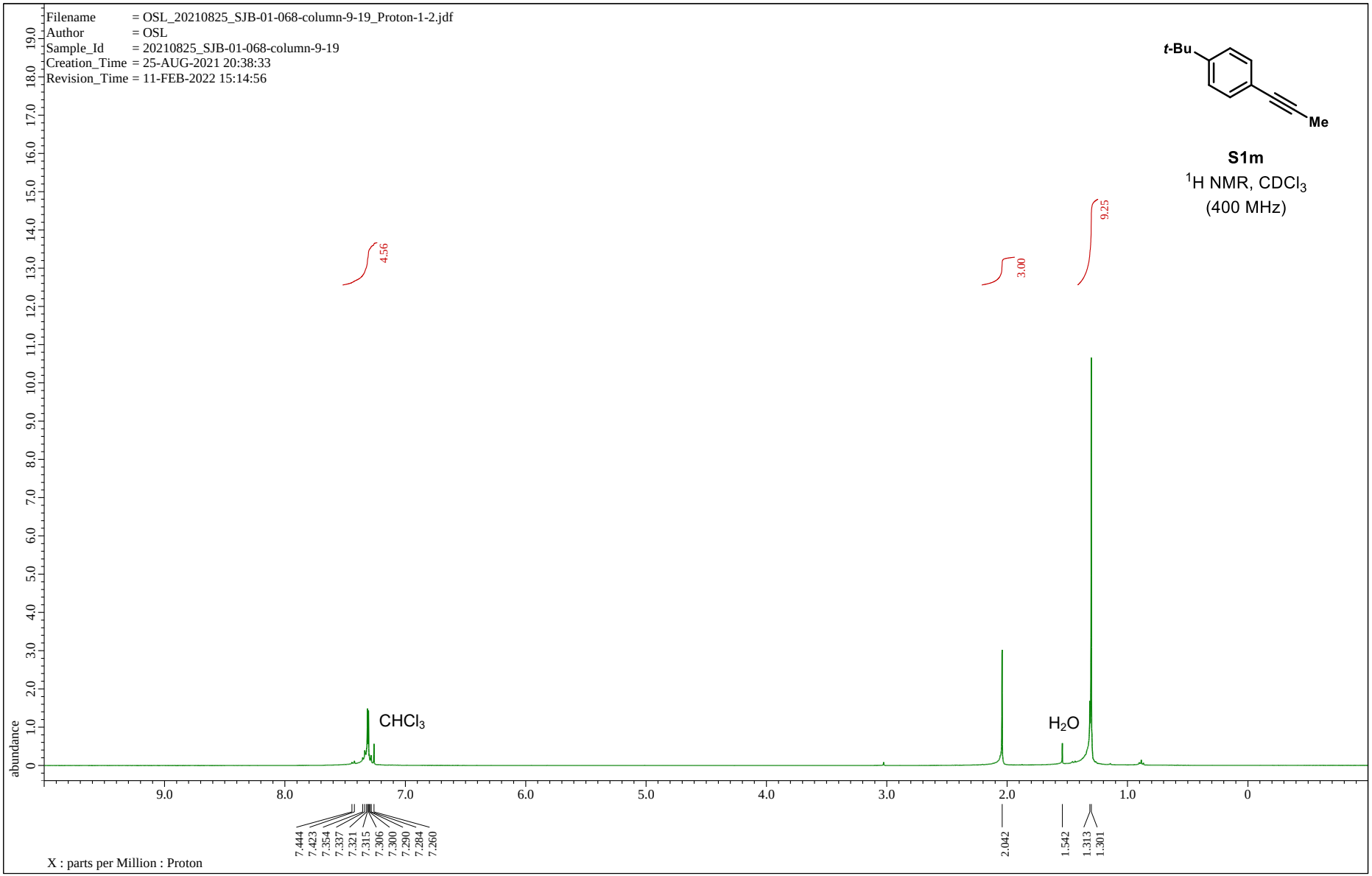
(400 MHz)
4.02
1.24
1.80
1.88
3.00
CHCl3
CH2Cl2
H2O
abundance
X : parts per Million : Proton
7.985
7.982
7.962
7.945
7.940
7.665
7.647
7.631
7.629
7.524
7.505
7.485
7.260
6.989
6.984
6.967
5.297
3.889
1.571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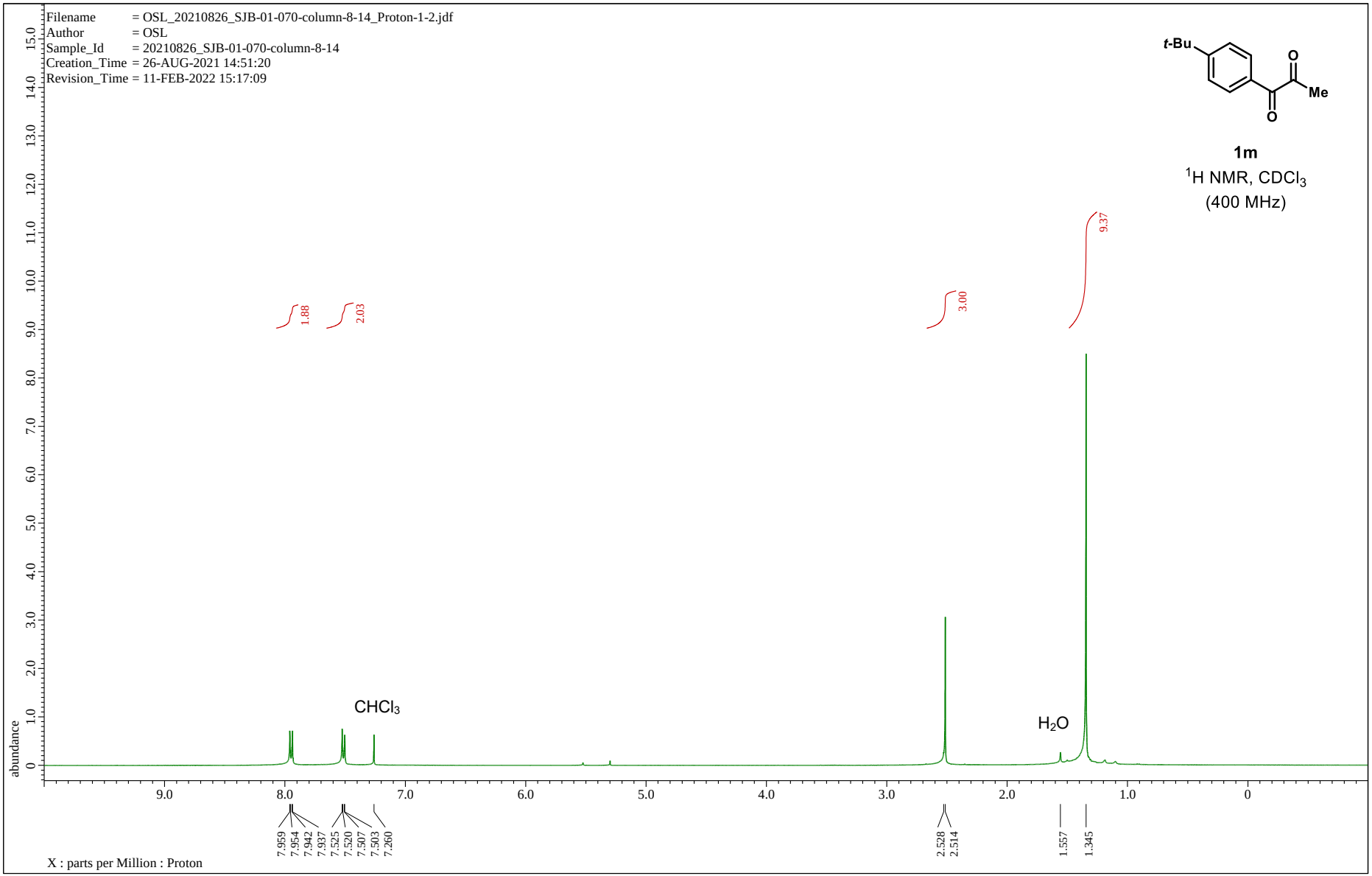
Me
S1m
1H NMR, CDCl3
(400 MHz)
4.56
3.00
9.25
CHCl3
H2O
abundance
X : parts per Million : Proton
7.444
7.423
7.354
7.337
7.321
7.315
7.306
7.300
7.290
7.284
7.260
2.042
1.542
1.313
1.301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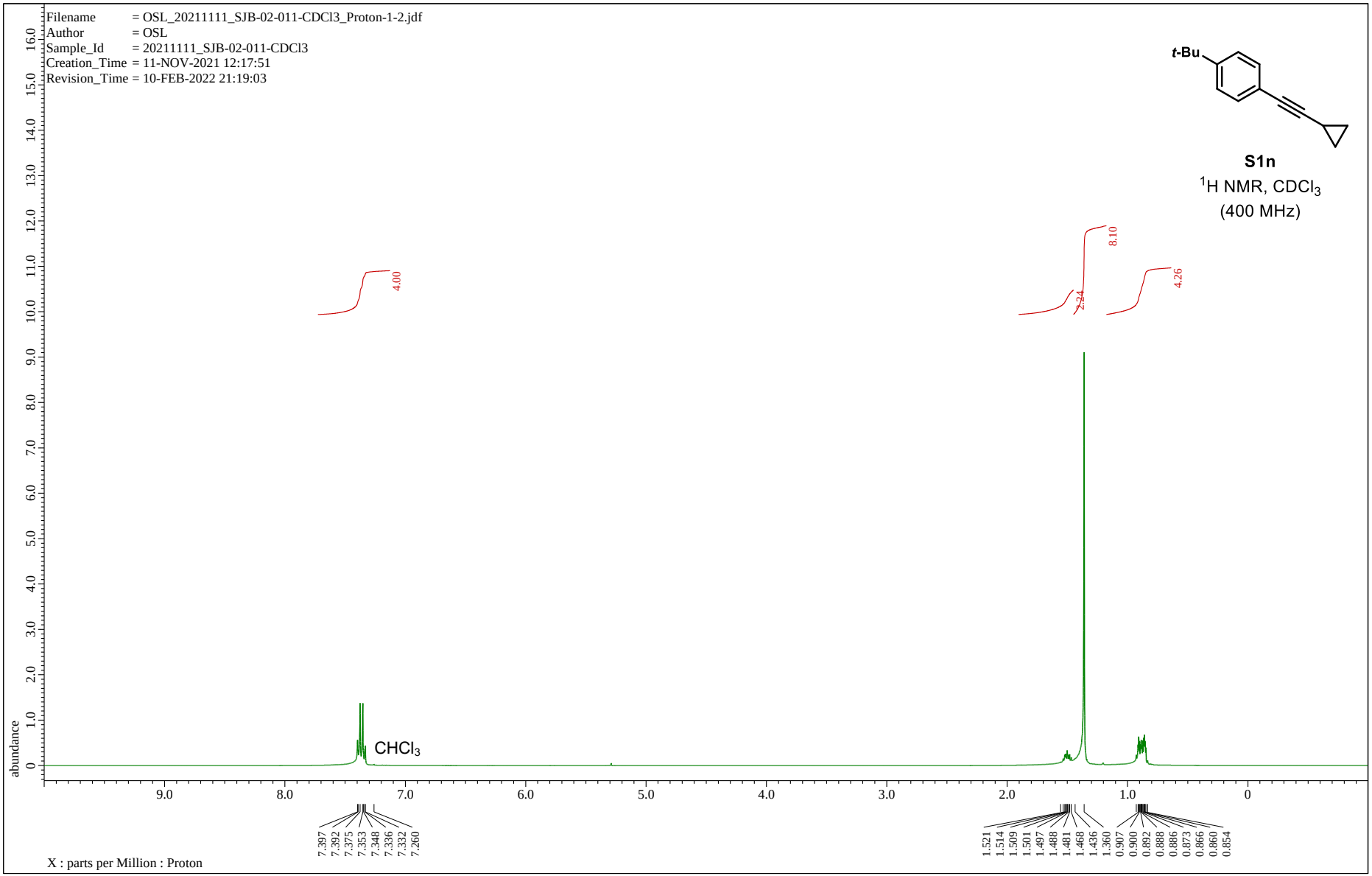
t-Bu
O
Me
O
1m
1H NMR, CDCl3
(400 MHz)
9.37
3.00
2.03
1.88
CHCl3
H2O
abundance
X : parts per Million : Proton
7.959
7.954
7.942
7.937
7.525
7.520
7.507
7.503
7.260
2.528
2.514
1.557
1.345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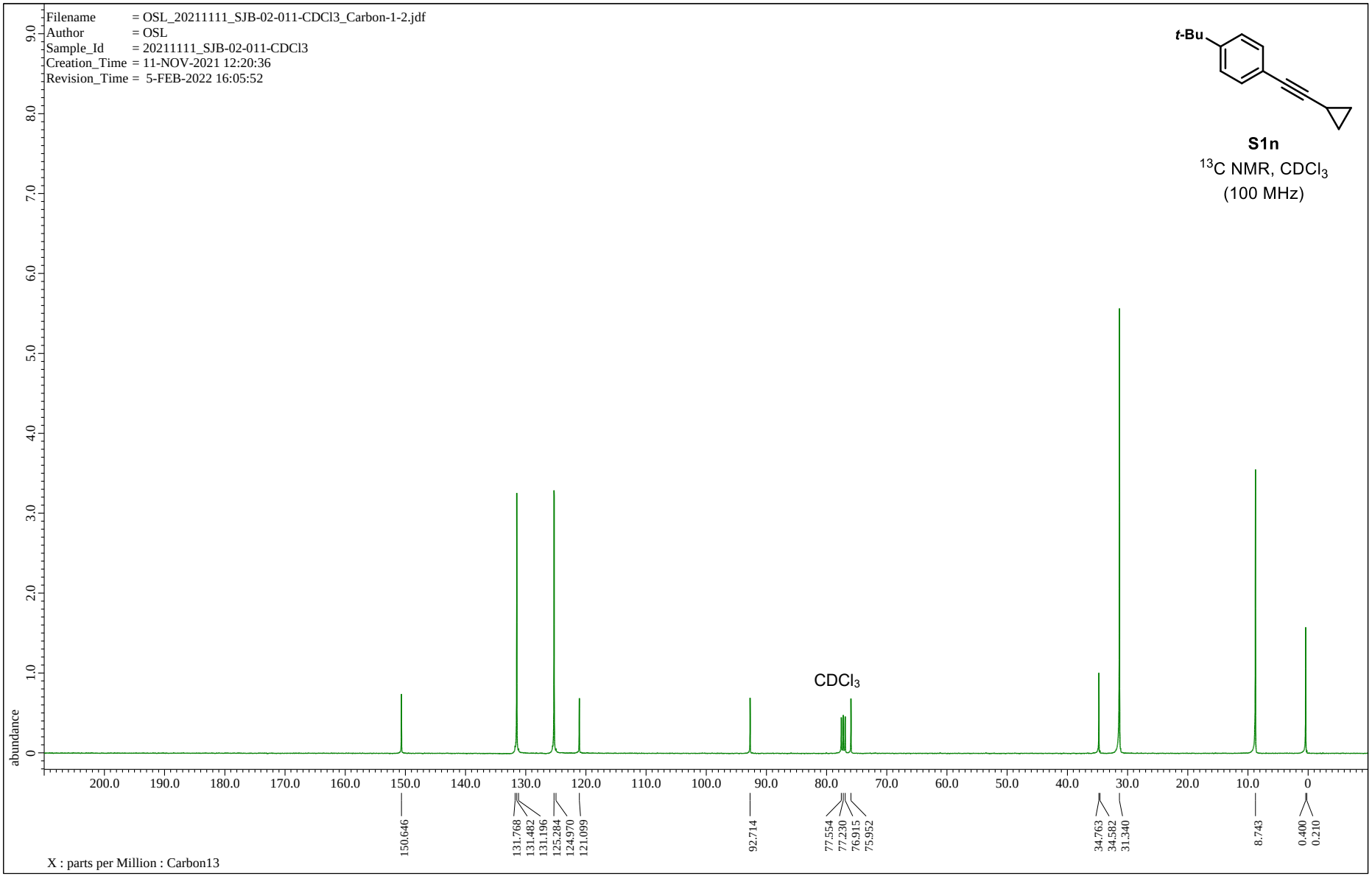
t-Bu
S1n
1H NMR, CDCl3
(400 MHz)
4.00
2.94
8.10
4.26
CHCl3
abundance
X : parts per Million : Proton
7.397
7.392
7.375
7.353
7.348
7.336
7.332
7.260
1.521
1.514
1.509
1.501
1.497
1.488
1.481
1.468
1.436
1.360
0.907
0.900
0.892
0.888
0.886
0.873
0.866
0.860
0.854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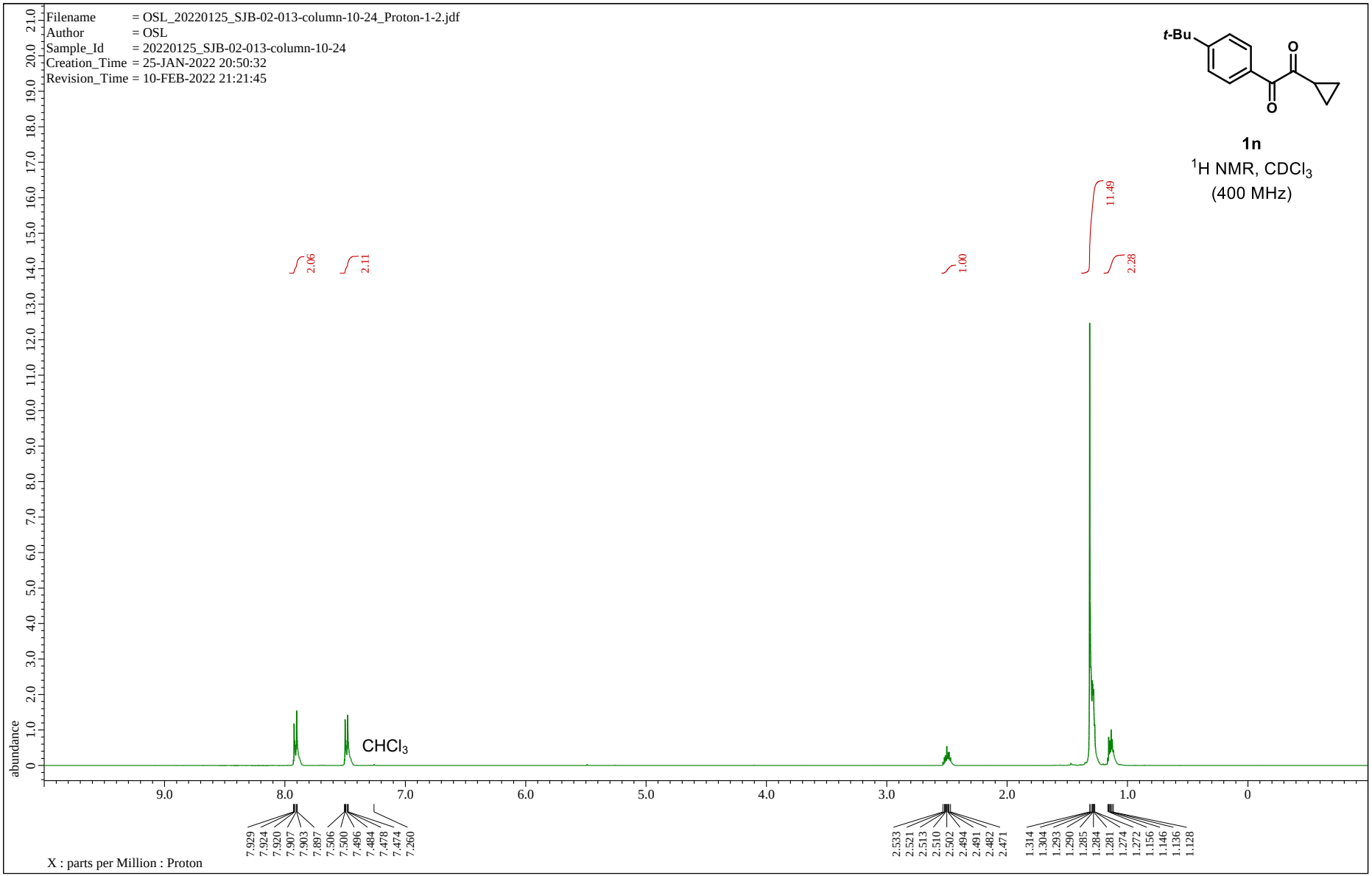
t-Bu
S1n
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
150.646
131.768
131.482
131.196
125.284
124.970
121.099
92.714
77.554
77.230
76.915
75.952
34.763
34.582
31.340
8.743
0.400
0.210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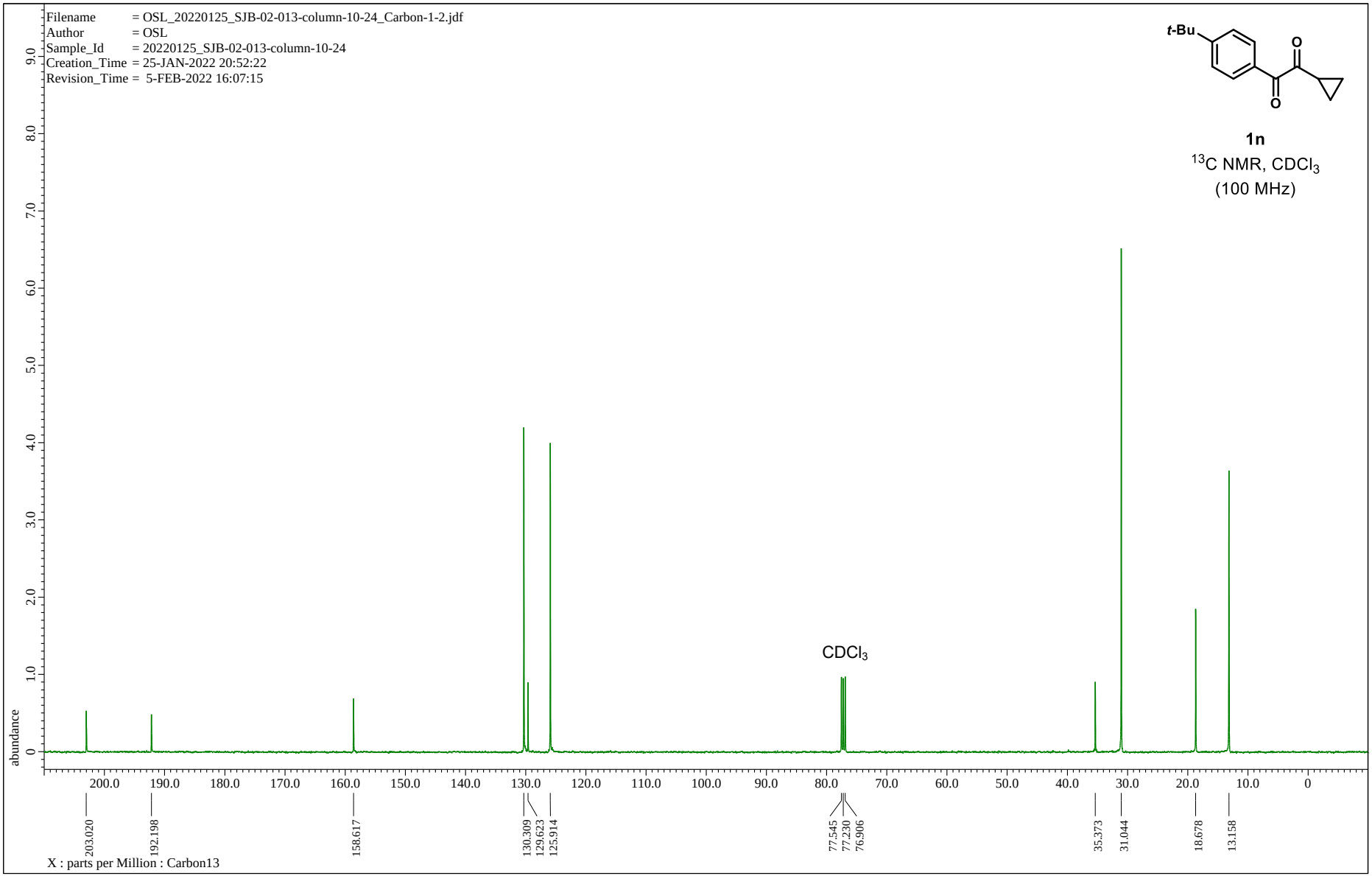
t-Bu
O
O
1n
1H NMR, CDCl3
(400 MHz)
2.06
2.11
1.00
11.49
2.28
CHCl3
abundance
X : parts per Million : Proton
7.929
7.924
7.920
7.907
7.903
7.897
7.506
7.500
7.496
7.484
7.478
7.474
7.260
2.533
2.521
2.513
2.510
2.502
2.494
2.491
2.482
2.471
1.314
1.304
1.293
1.290
1.285
1.284
1.281
1.274
1.272
1.156
1.146
1.136
1.128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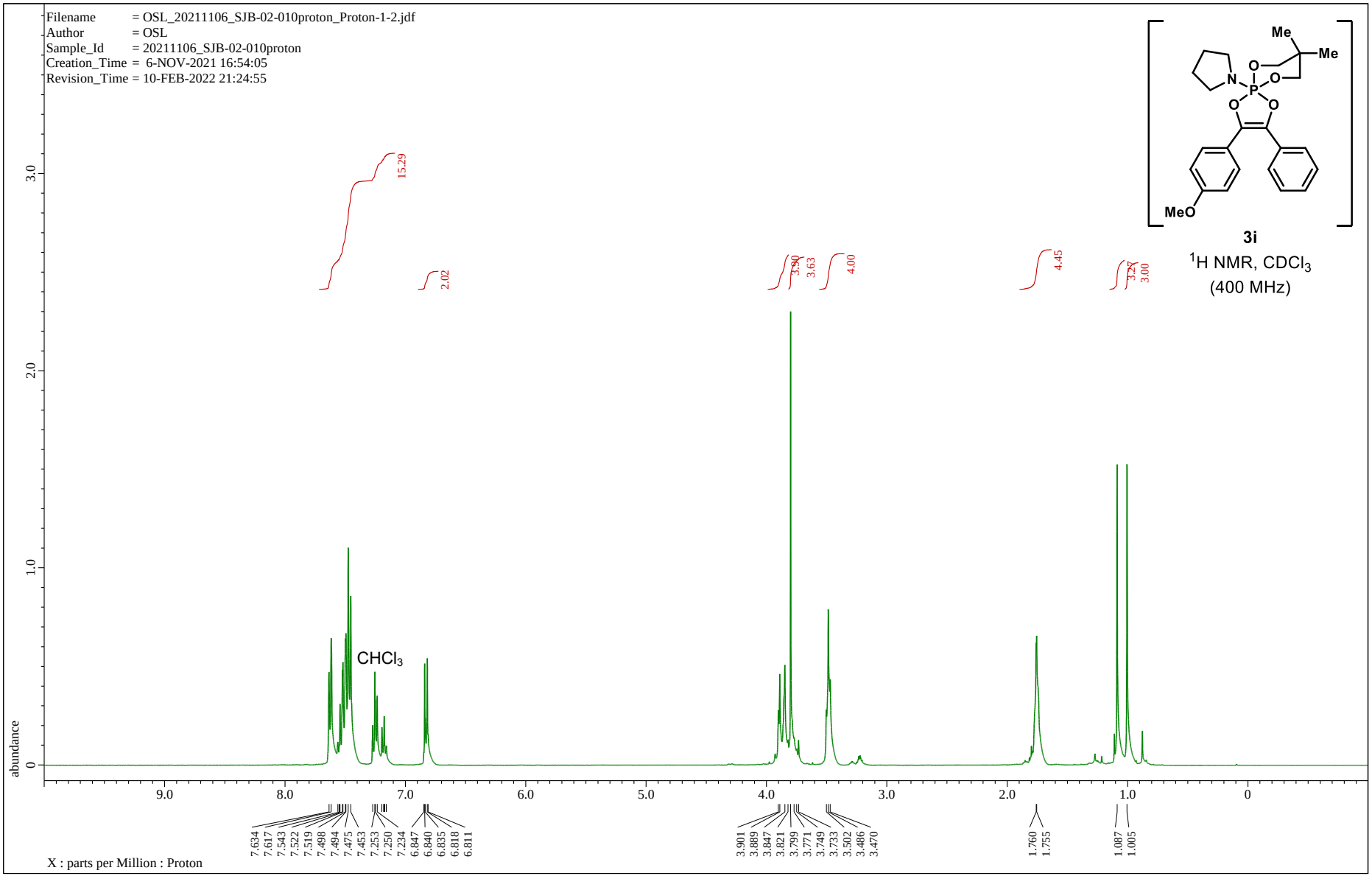
t-Bu
O
O
1n
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
203.020
192.198
158.617
130.309
129.623
125.914
77.545
77.230
76.906
35.373
31.044
18.678
13.158
X : parts per Million : Carbon13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Me
MeO
3i
1H NMR, CDCl3
(400 MHz)
15.29
2.02
3.90
3.63
4.00
4.45
3.28
3.00
CHCl3
abundance
X : parts per Million : Proton
7.634
7.617
7.543
7.522
7.519
7.498
7.494
7.475
7.453
7.253
7.250
7.234
6.847
6.840
6.835
6.818
6.811
3.901
3.889
3.847
3.821
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3.749
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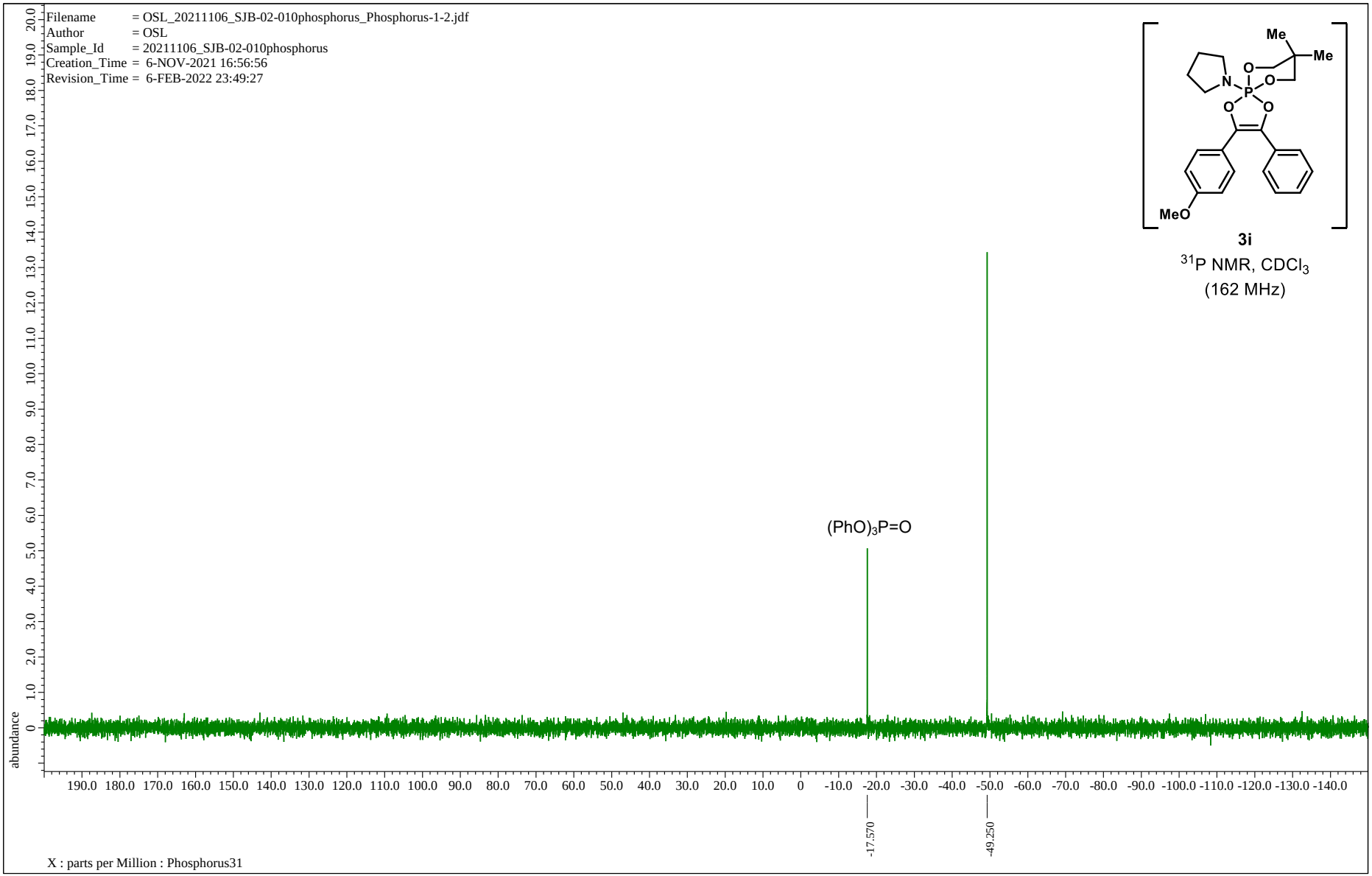
3.470
1.760
1.755
1.087
1.005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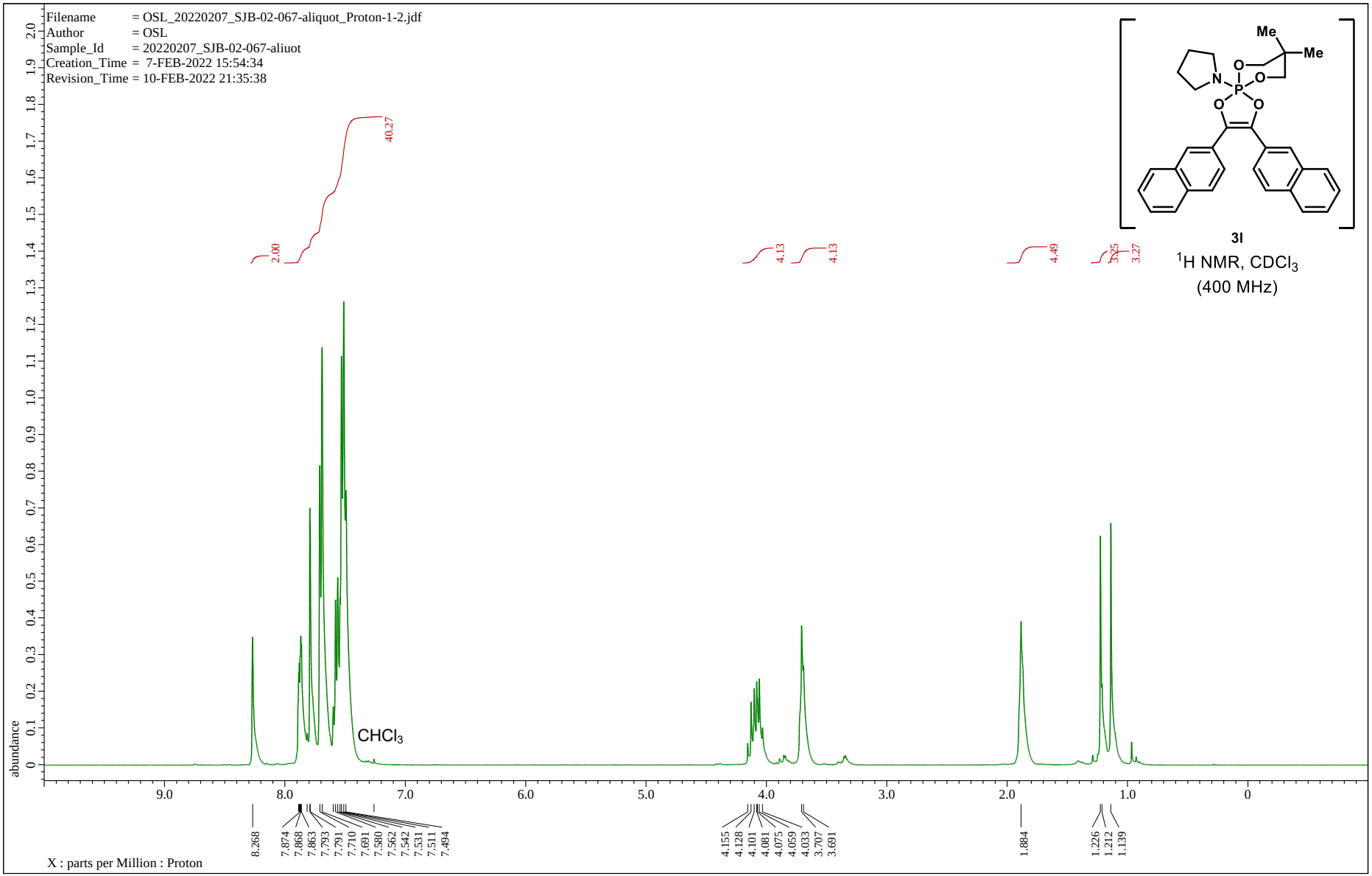
Me
O
N
P
O
O
O
O
MeO
3i
31P NMR, CDCl3
(162 MHz)
(PhO)3P=O
abundance
-17.570
-49.250
X : parts per Million : Phosphorus31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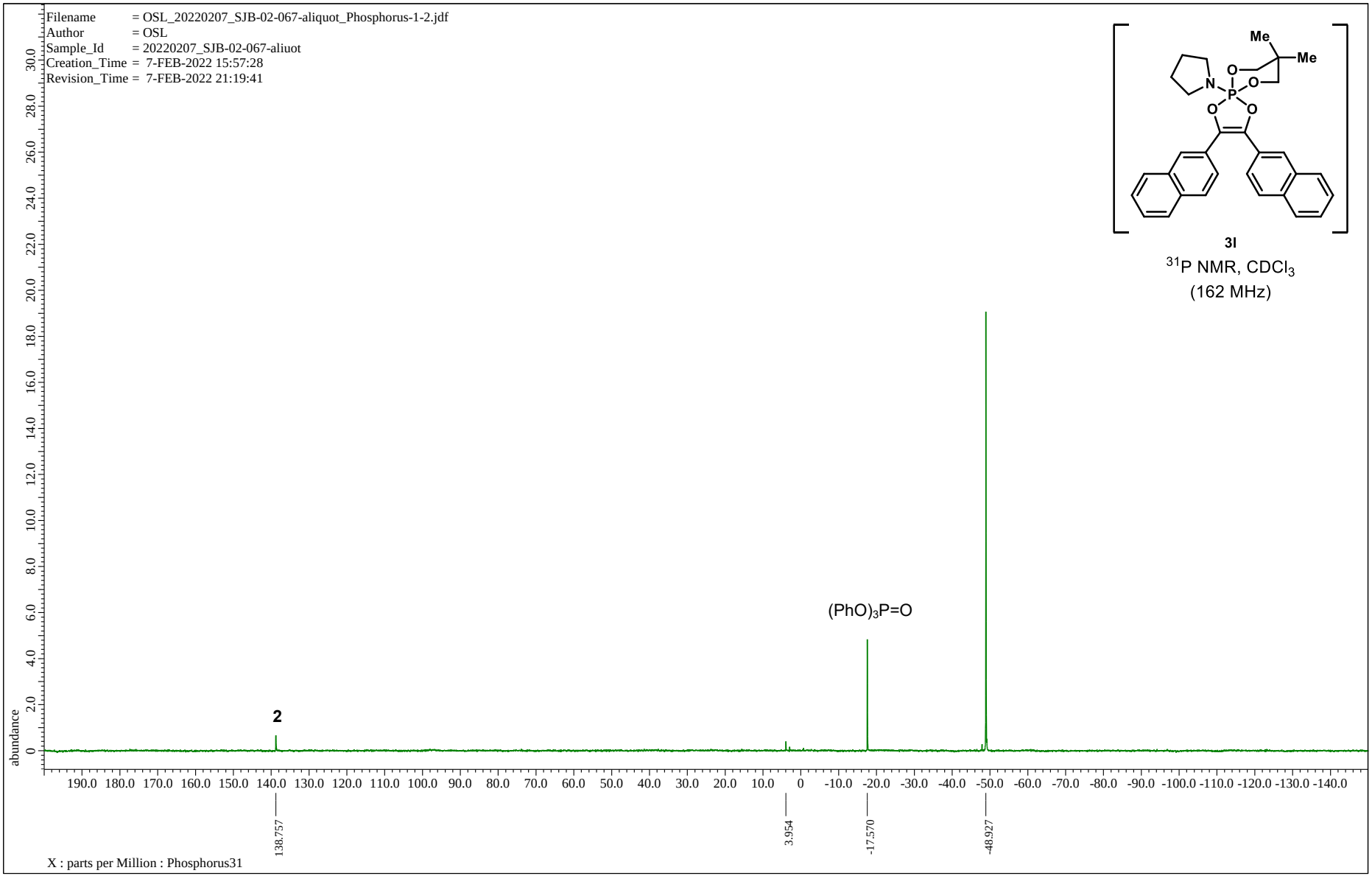
Me
O
O
N
P
O
O
3l
^{1}H NMR, $CDCl_3$
(400 MHz)
2.00
40.27
4.13
4.13
4.49
3.25
3.27
$CHCl_3$
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.268
7.874
7.868
7.863
7.793
7.791
7.710
7.691
7.580
7.562
7.542
7.531
7.511
7.494
4.155
4.128
4.101
4.081
4.075
4.059
4.033
3.707
3.691
1.884
1.226
1.212
1.139
X : parts per Million : Proton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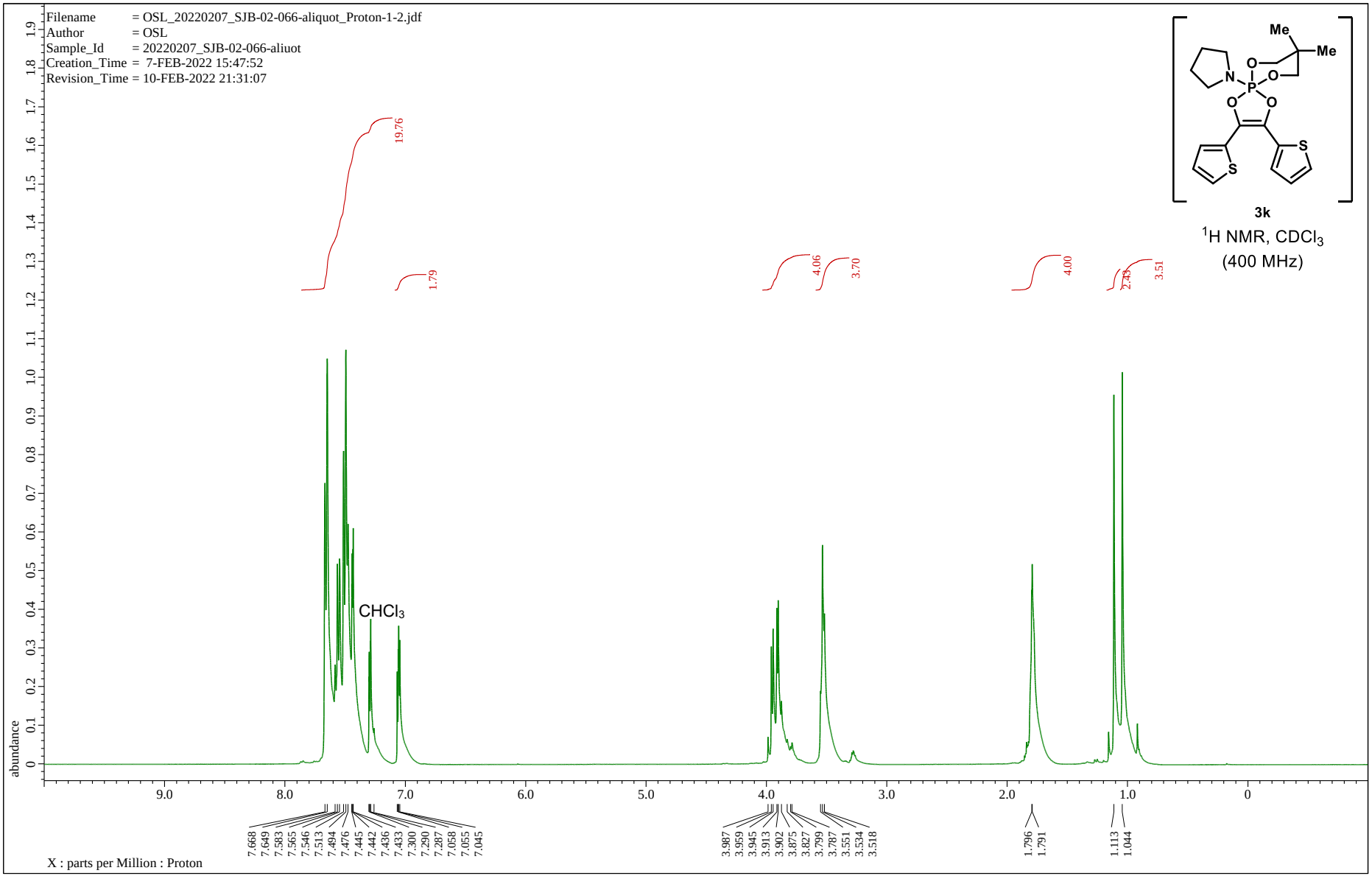
Me
Me
O
N
P
O
O
O
O
3l
31P NMR, CDCl3
(162 MHz)
(PhO)3P=O
2
abundance
138.757
3.954
-17.570
-48.927
X : parts per Million : Phosphorus31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P
O
O
O
O
S
S
3k
1H NMR, CDCl3
(400 MHz)
19.76
1.79
4.06
3.70
4.00
2.43
3.51
CHCl3
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.668
7.649
7.583
7.565
7.546
7.513
7.494
7.476
7.445
7.442
7.436
7.433
7.300
7.290
7.287
7.058
7.055
7.045
3.987
3.959
3.945
3.913
3.902
3.875
3.827
3.799
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3.518
1.796
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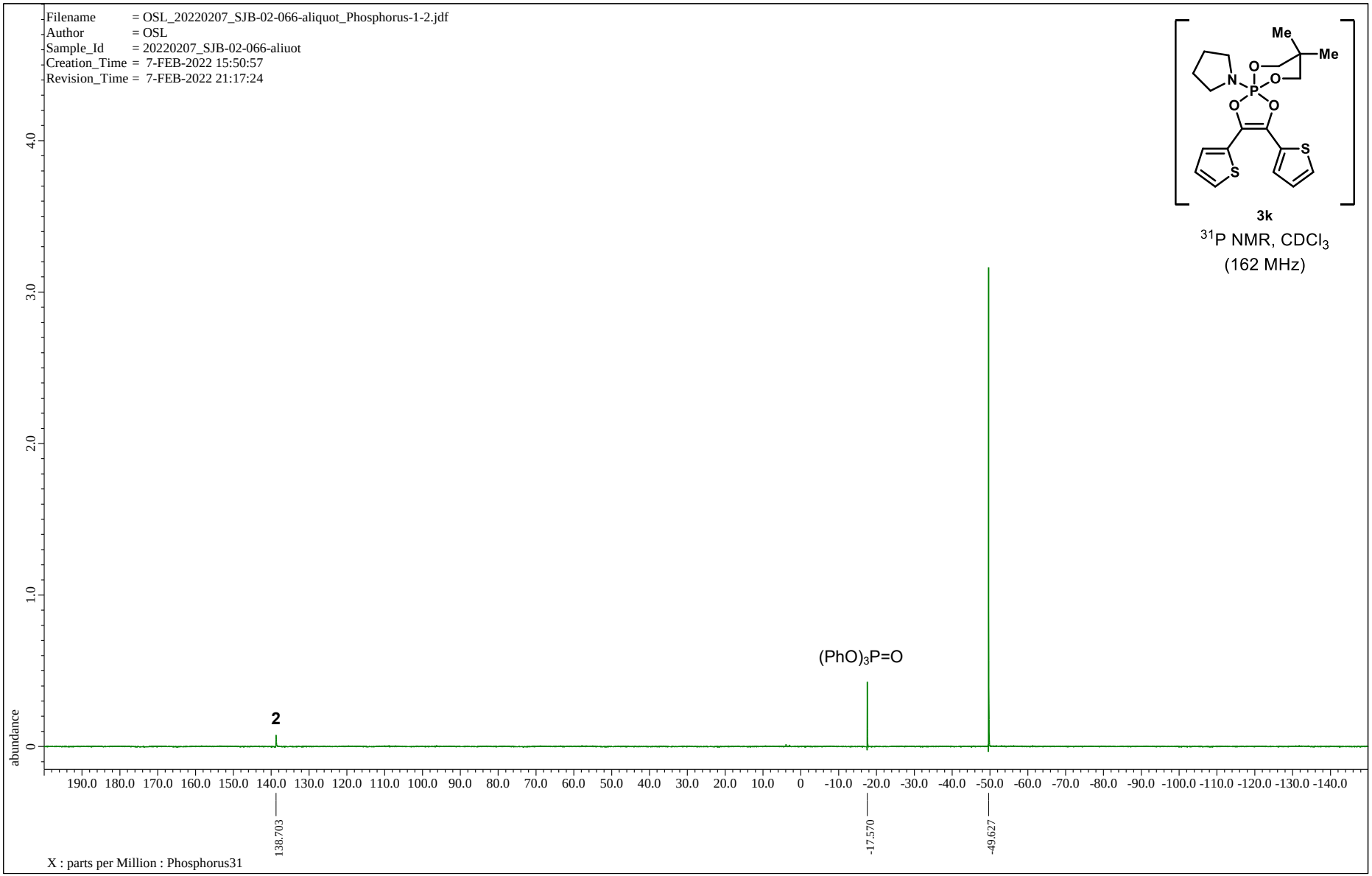
1.113
1.044
X : parts per Million : Proton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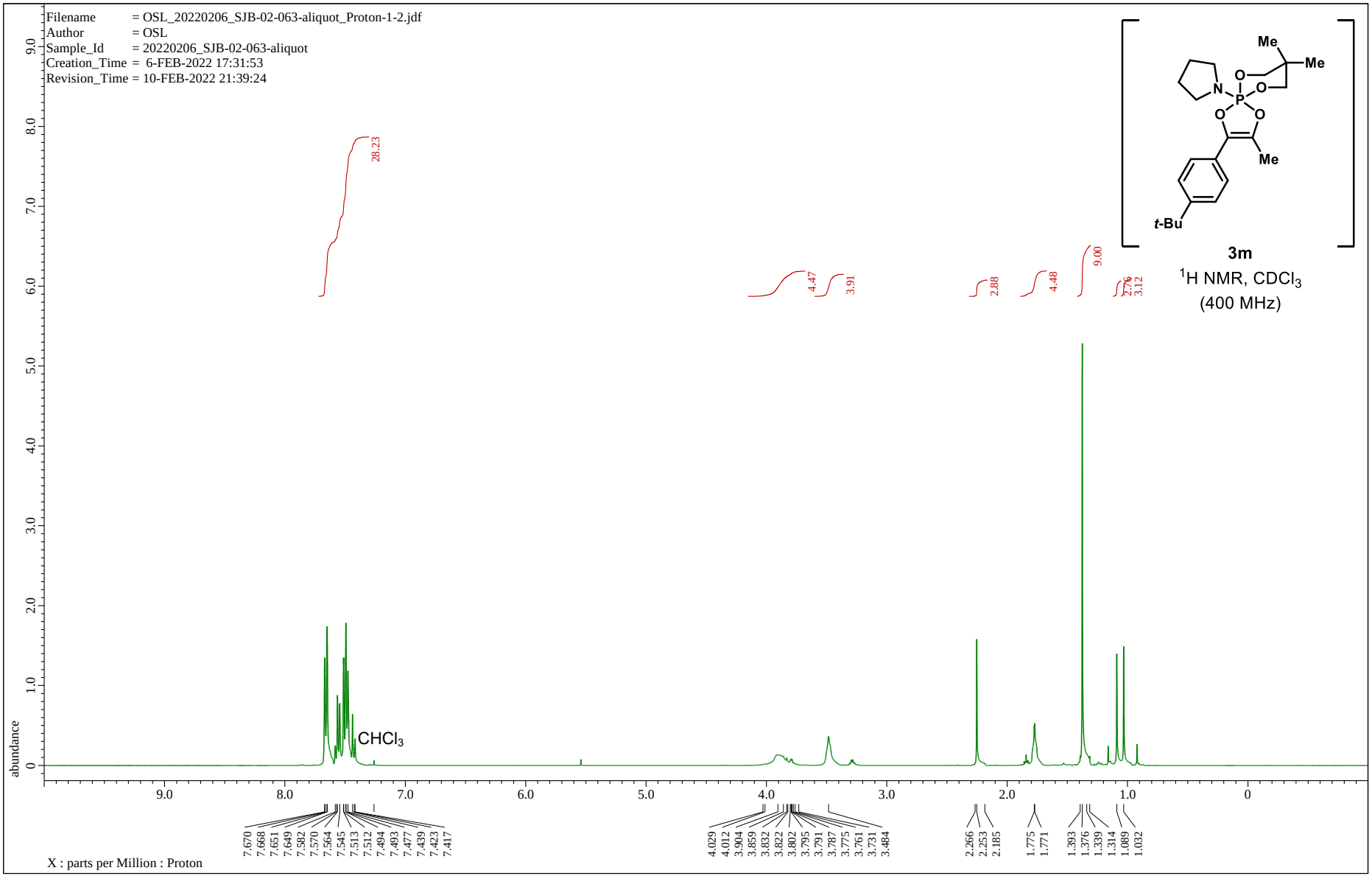
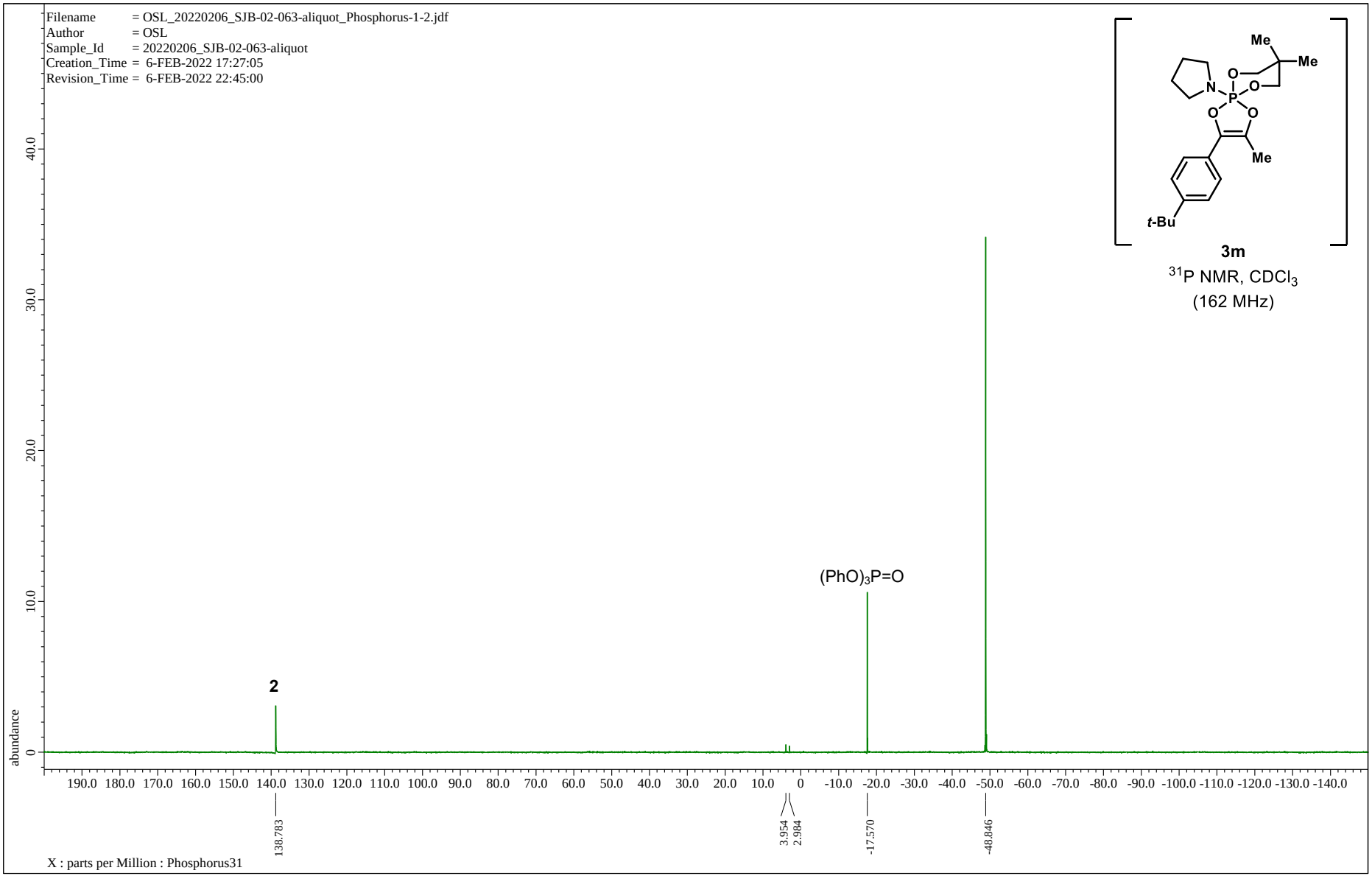
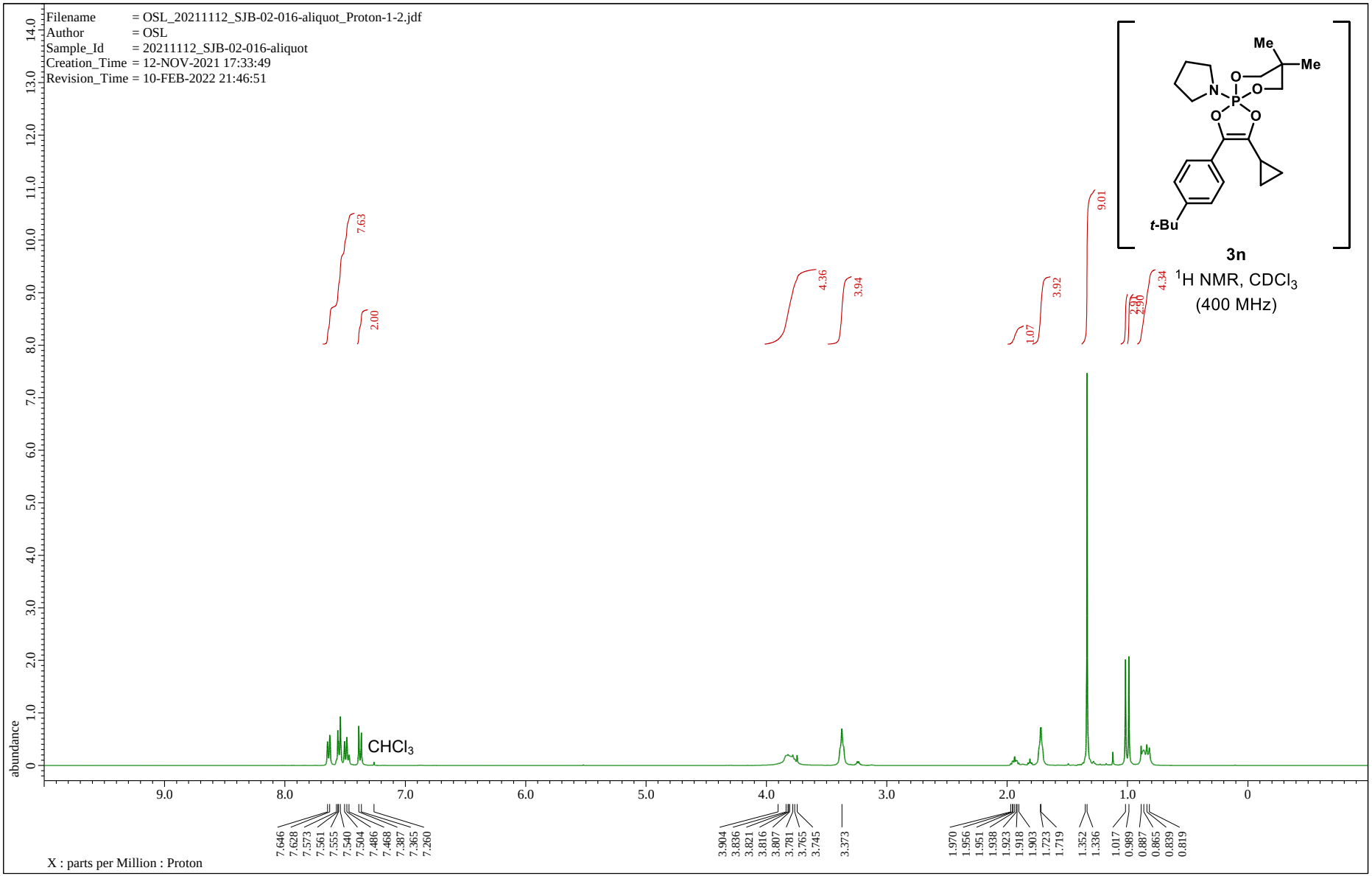
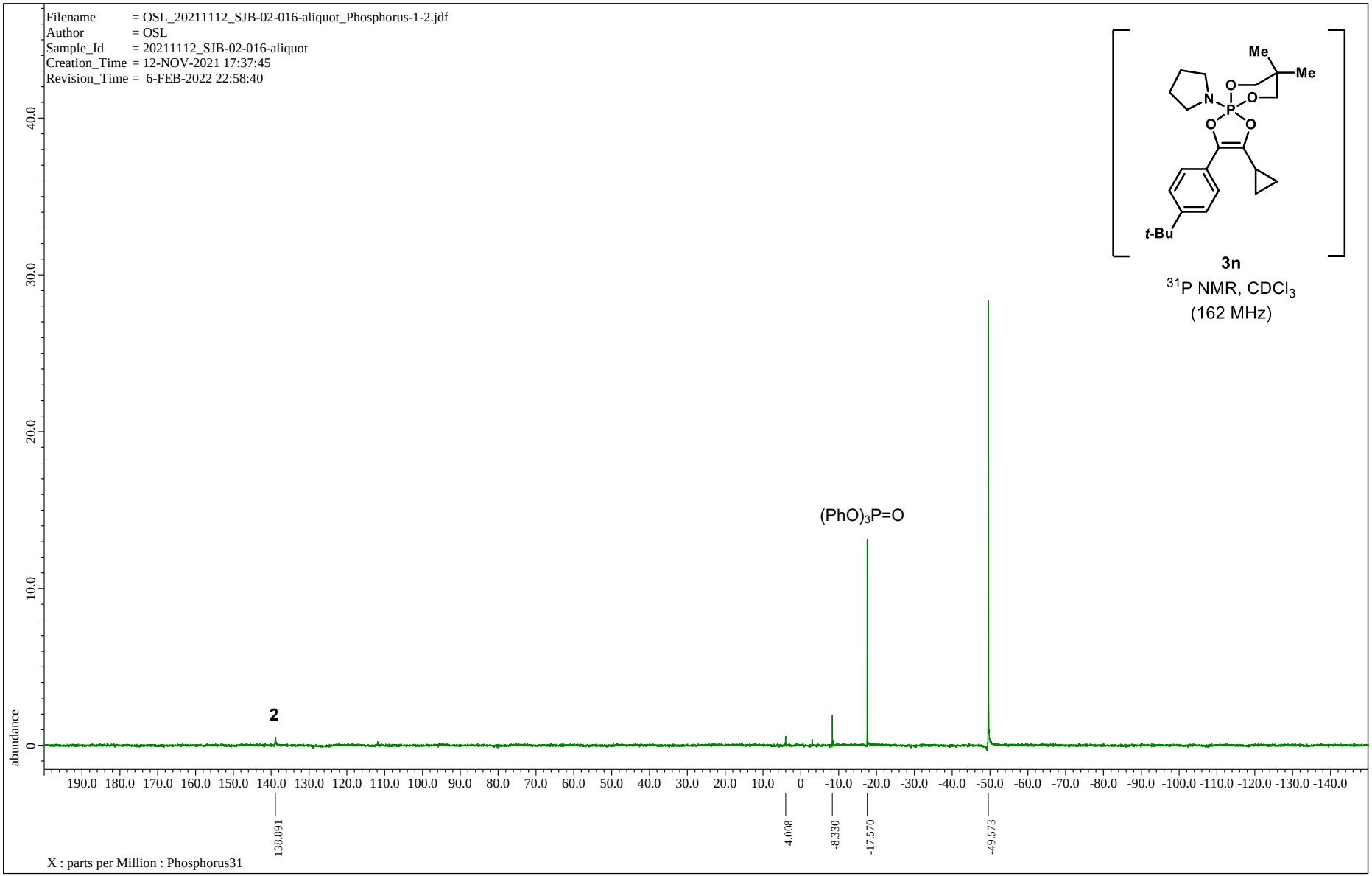
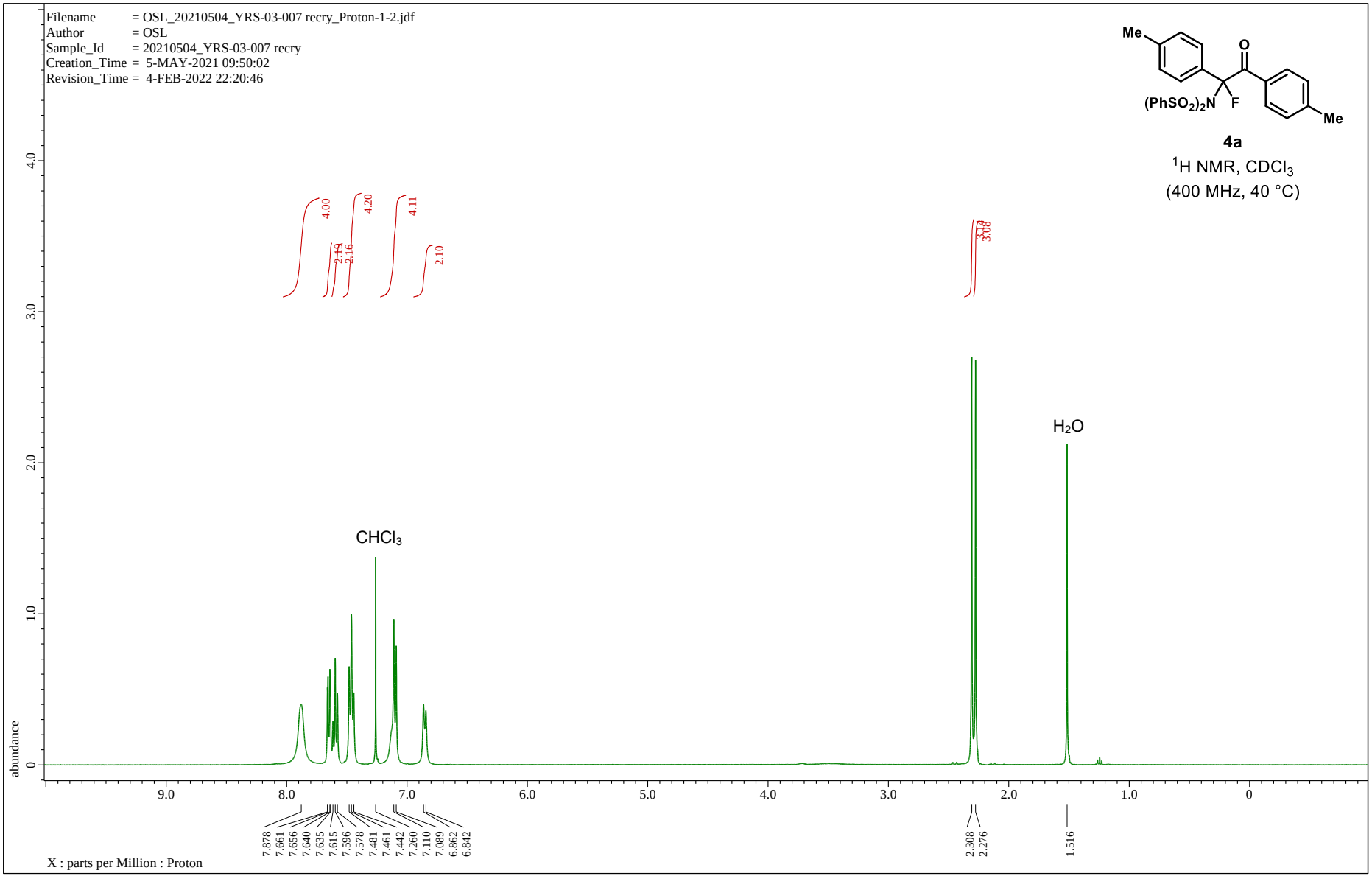
Me
N
O
O
P
O
O
S
S
3k
31P NMR, CDCl3
(162 MHz)
(PhO)3P=O
2
abundance
4.0
3.0
2.0
1.0
0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0
138.703
-17.570
-49.627
X : parts per Million : Phosphorus31

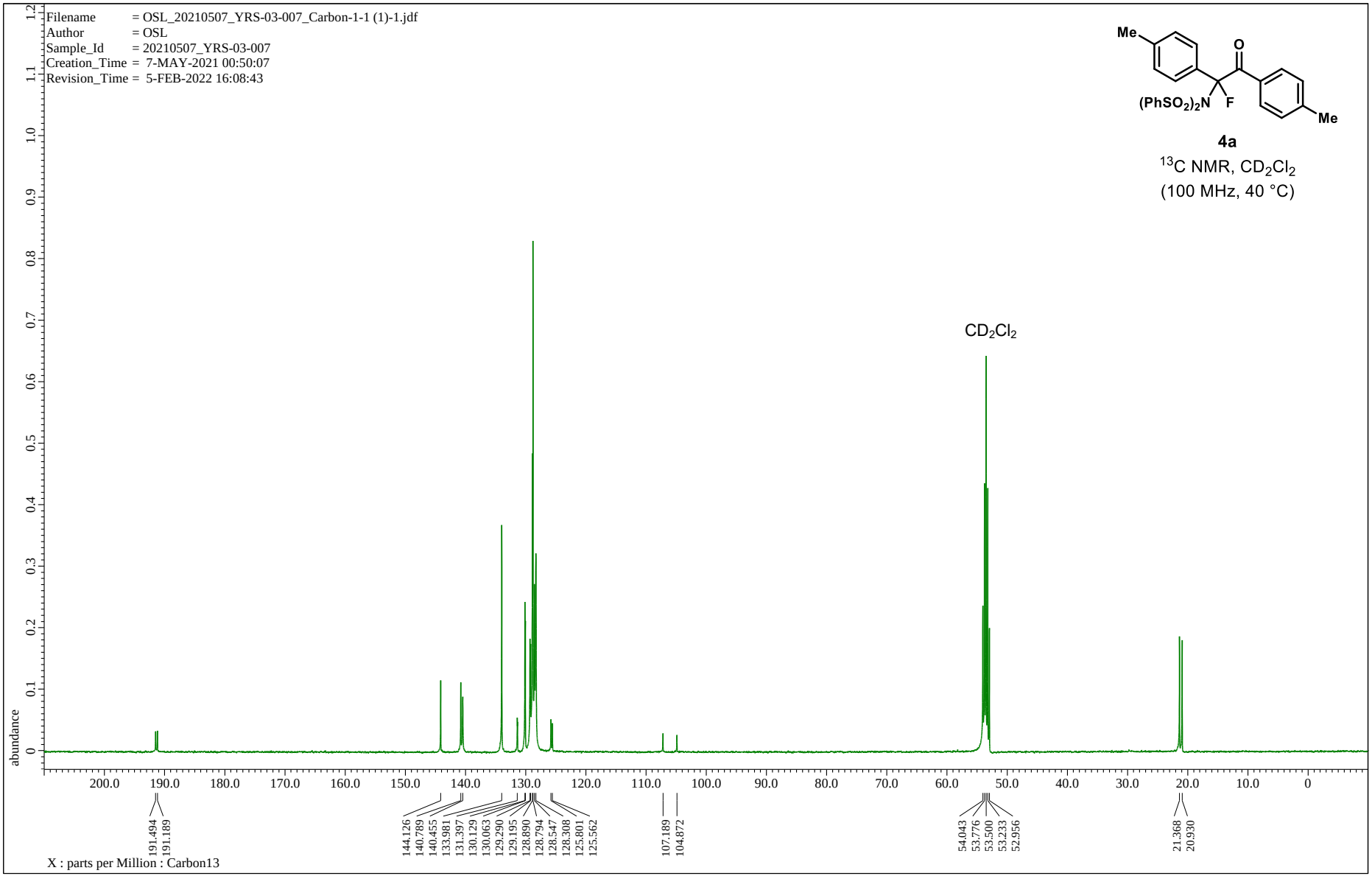

Filename = OSL_20220206_SJB-02-063-aliquot_Proton-1-2.jdf
Author = OSL
Sample_Id = 20220206_SJB-02-063-aliquot
Creation_Time = 6-FEB-2022 17:31:53
Revision_Time = 10-FEB-2022 21:39:24
Me
Me
Me
t-Bu
3m
1H NMR, CDCl3
(400 MHz)
28.23
4.47
3.91
2.88
4.48
9.00
2.76
3.12
CHCl3
abundance
X : parts per Million : Proton

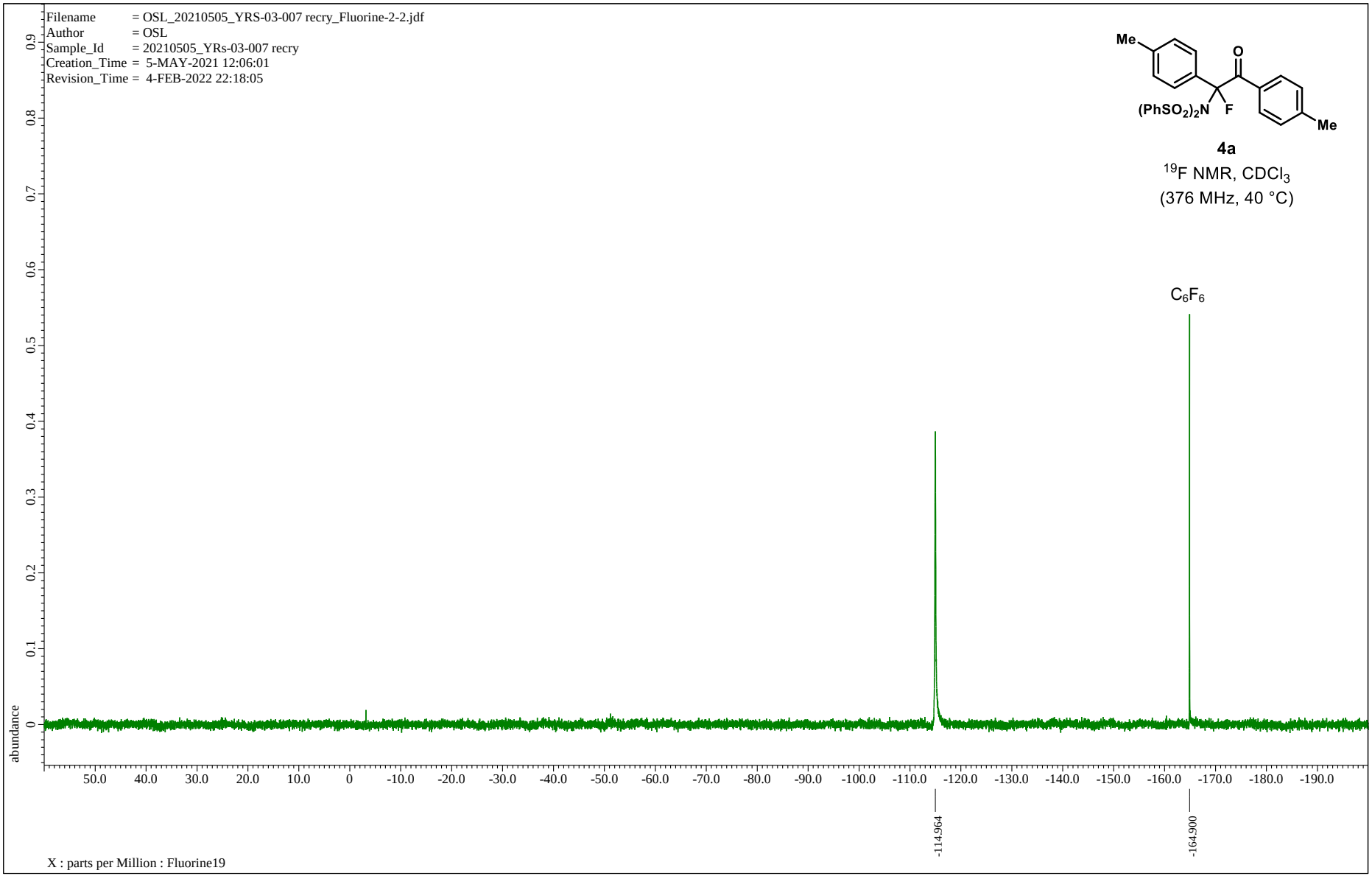

Filename = OSL_20220206_SJB-02-063-aliquot_Phosphorus-1-2.jdf
Author = OSL
Sample_Id = 20220206_SJB-02-063-aliquot
Creation_Time = 6-FEB-2022 17:27:05
Revision_Time = 6-FEB-2022 22:45:00
Me
Me
O
N
O
P
O
O
O
Me
t-Bu
3m
31P NMR, CDCl3
(162 MHz)
(PhO)3P=O
2
abundance
40.0
30.0
20.0
10.0
0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0
138.783
3.954
2.984
-17.570
-48.846
X : parts per Million : Phosphorus31

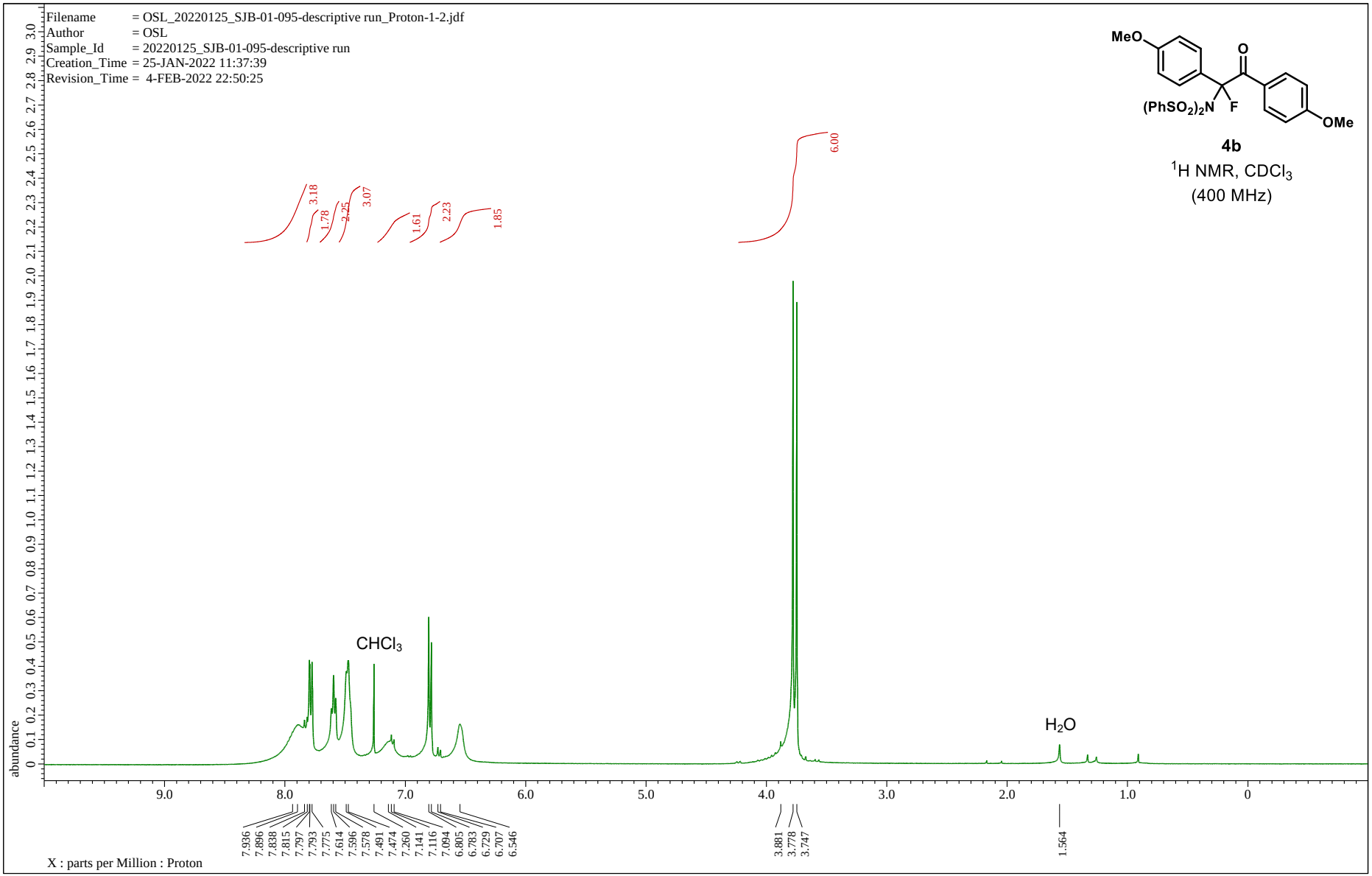

Filename = OSL_20211112_SJB-02-016-aliquot_Proton-1-2.jdf
Author = OSL
Sample_Id = 20211112_SJB-02-016-aliquot
Creation_Time = 12-NOV-2021 17:33:49
Revision_Time = 10-FEB-2022 21:46:51
Me
Me
t-Bu
3n
1H NMR, CDCl3
(400 MHz)
7.63
2.00
4.36
3.94
1.07
3.92
9.01
2.96
2.90
4.34
CHCl3
abundance
X : parts per Million : Proton
7.646
7.628
7.573
7.561
7.555
7.540
7.504
7.486
7.468
7.387
7.365
7.260
3.904
3.836
3.821
3.816
3.807
3.781
3.765
3.745
3.373
1.970
1.956
1.951
1.938
1.923
1.918
1.903
1.723
1.719
1.352
1.336
1.017
0.989
0.887
0.865
0.839
0.819

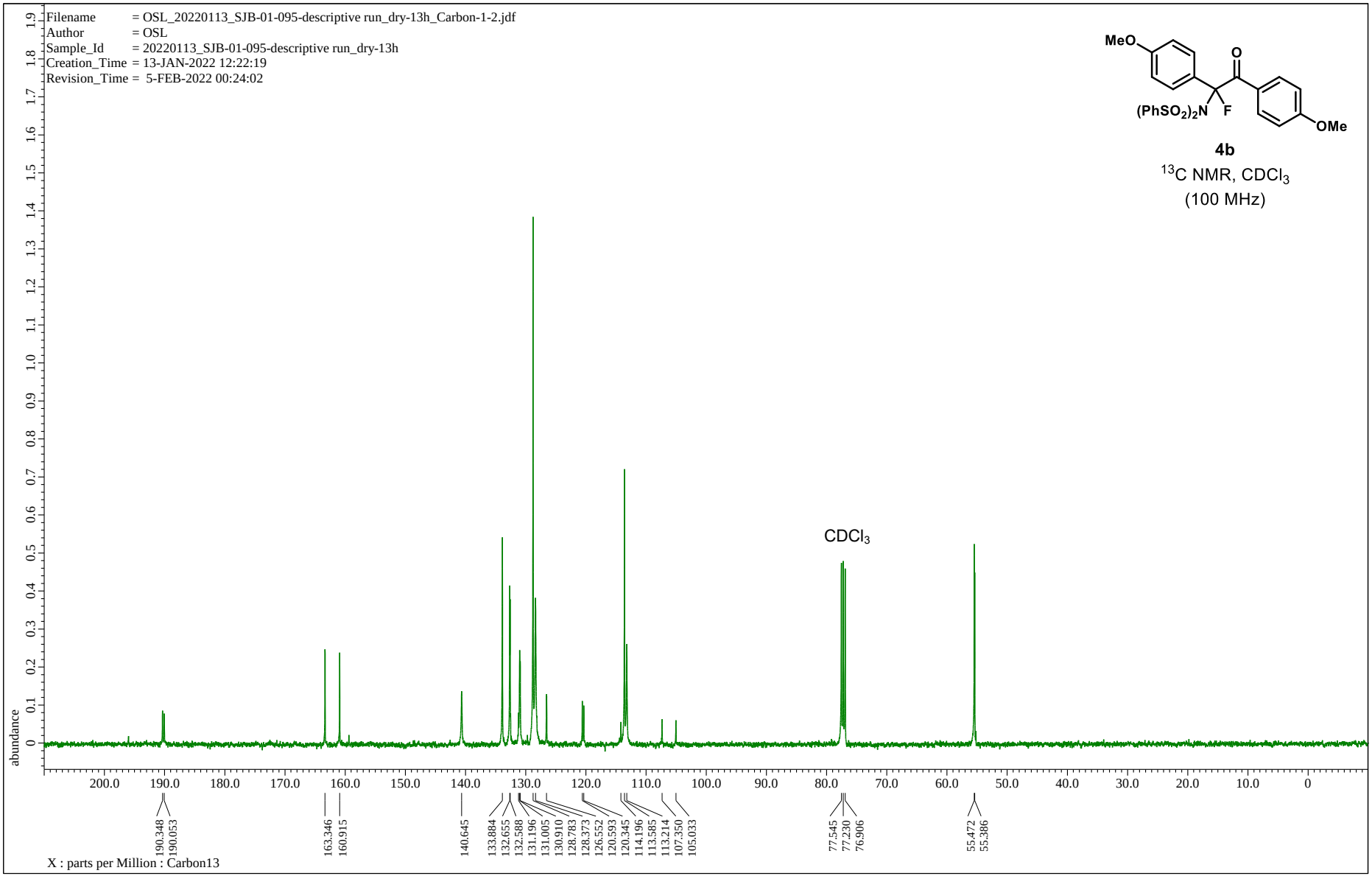

Filename = OSL_20211112_SJB-02-016-aliquot_Phosphorus-1-2.jdf
Author = OSL
Sample_Id = 20211112_SJB-02-016-aliquot
Creation_Time = 12-NOV-2021 17:37:45
Revision_Time = 6-FEB-2022 22:58:40
Me
Me
O
N
O
P
O
O
t-Bu
3n
31P NMR, CDCl3
(162 MHz)
(PhO)3P=O
2
abundance
40.0
30.0
20.0
10.0
0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0
138.891
4.008
-8.330
-17.570
-49.573
X : parts per Million : Phosphorus31

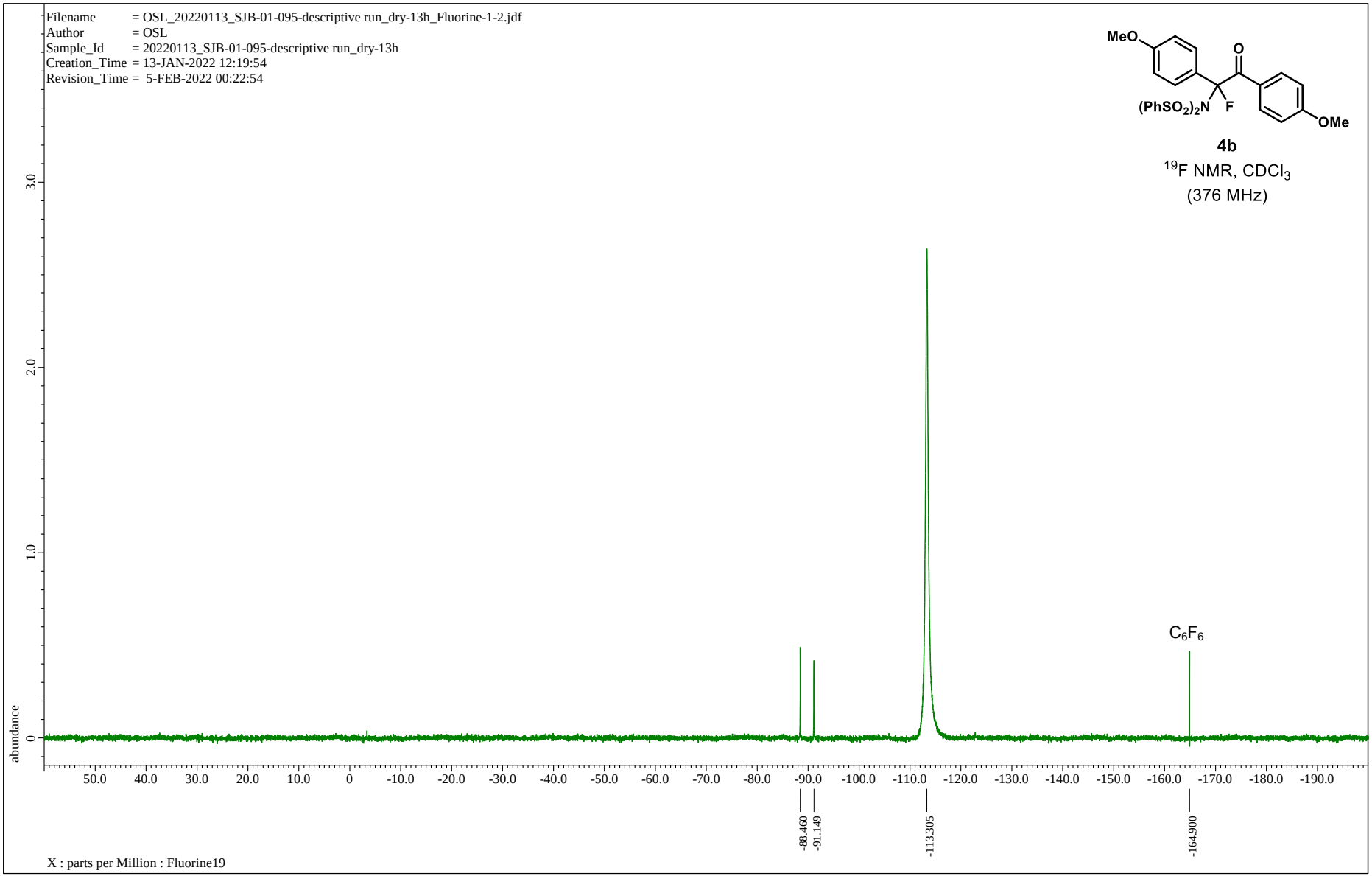

Filename = OSL_20210504_YRS-03-007 recry_Proton-1-2.jdf
Author = OSL
Sample_Id = 20210504_YRS-03-007 recry
Creation_Time = 5-MAY-2021 09:50:02
Revision_Time = 4-FEB-2022 22:20:46
Me
O
(PhSO2)2N
F
Me
4a
1H NMR, CDCl3
(400 MHz, 40 °C)
4.00
2.19
2.16
4.20
4.11
2.10
3.07
3.08
H2O
CHCl3
abundance
X : parts per Million : Proton
7.878
7.661
7.656
7.640
7.635
7.615
7.596
7.578
7.481
7.461
7.442
7.260
7.110
7.089
6.862
6.842
2.308
2.276
1.516

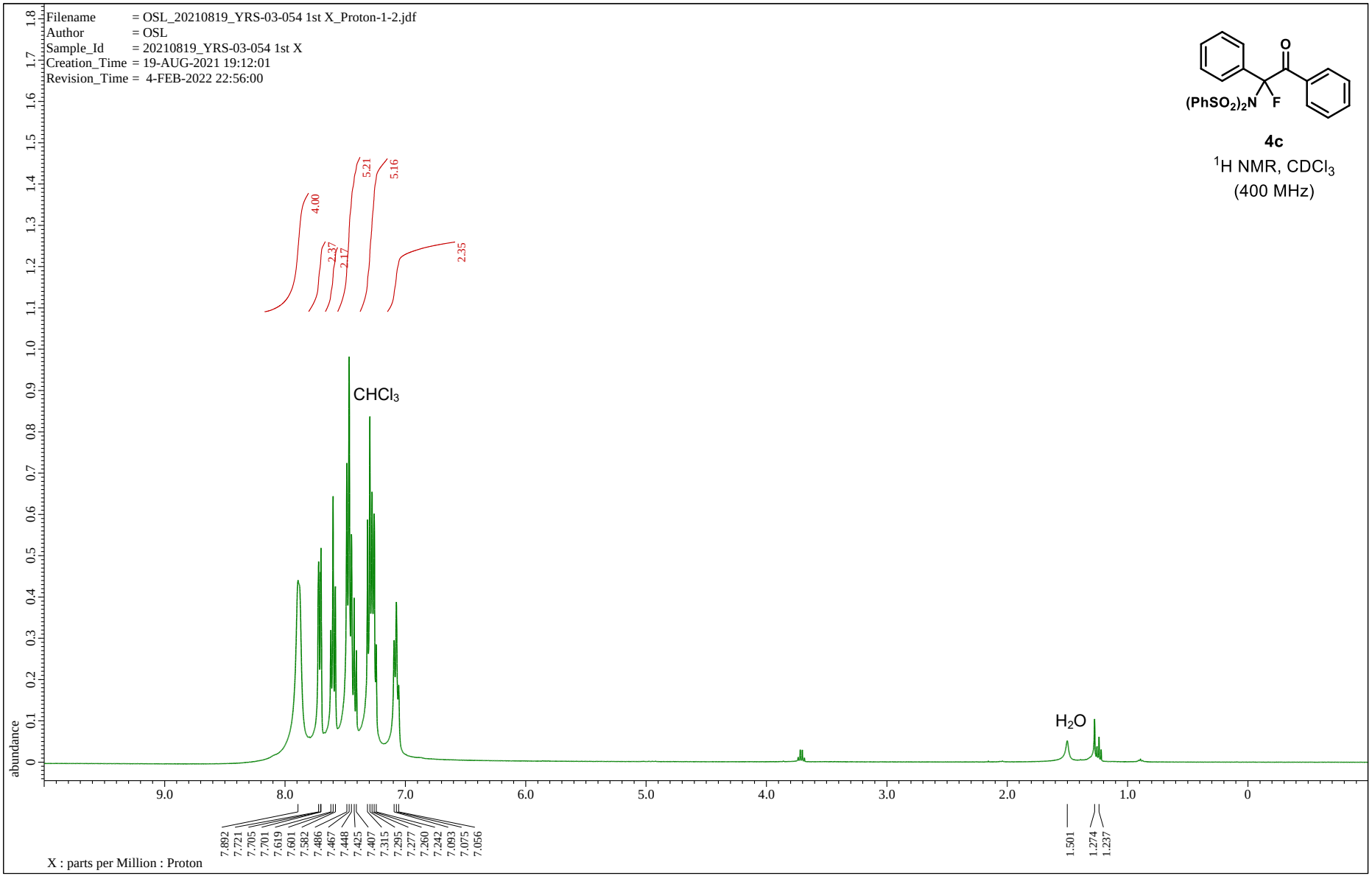

Filename = OSL_20210507_YRS-03-007_Carbon-1-1 (1)-1.jdf
Author = OSL
Sample_Id = 20210507_YRS-03-007
Creation_Time = 7-MAY-2021 00:50:07
Revision_Time = 5-FEB-2022 16:08:43
Me
O
(PhSO2)2N
F
Me
4a
13C NMR, CD2Cl2
(100 MHz, 40 °C)
CD2Cl2
abundance
X : parts per Million : Carbon13
191.494
191.189
144.126
140.789
140.455
133.981
131.397
130.129
130.063
129.290
129.195
128.890
128.794
128.547
128.308
125.801
125.562
107.189
104.872
54.043
53.776
53.500
53.233
52.956
21.368
20.930

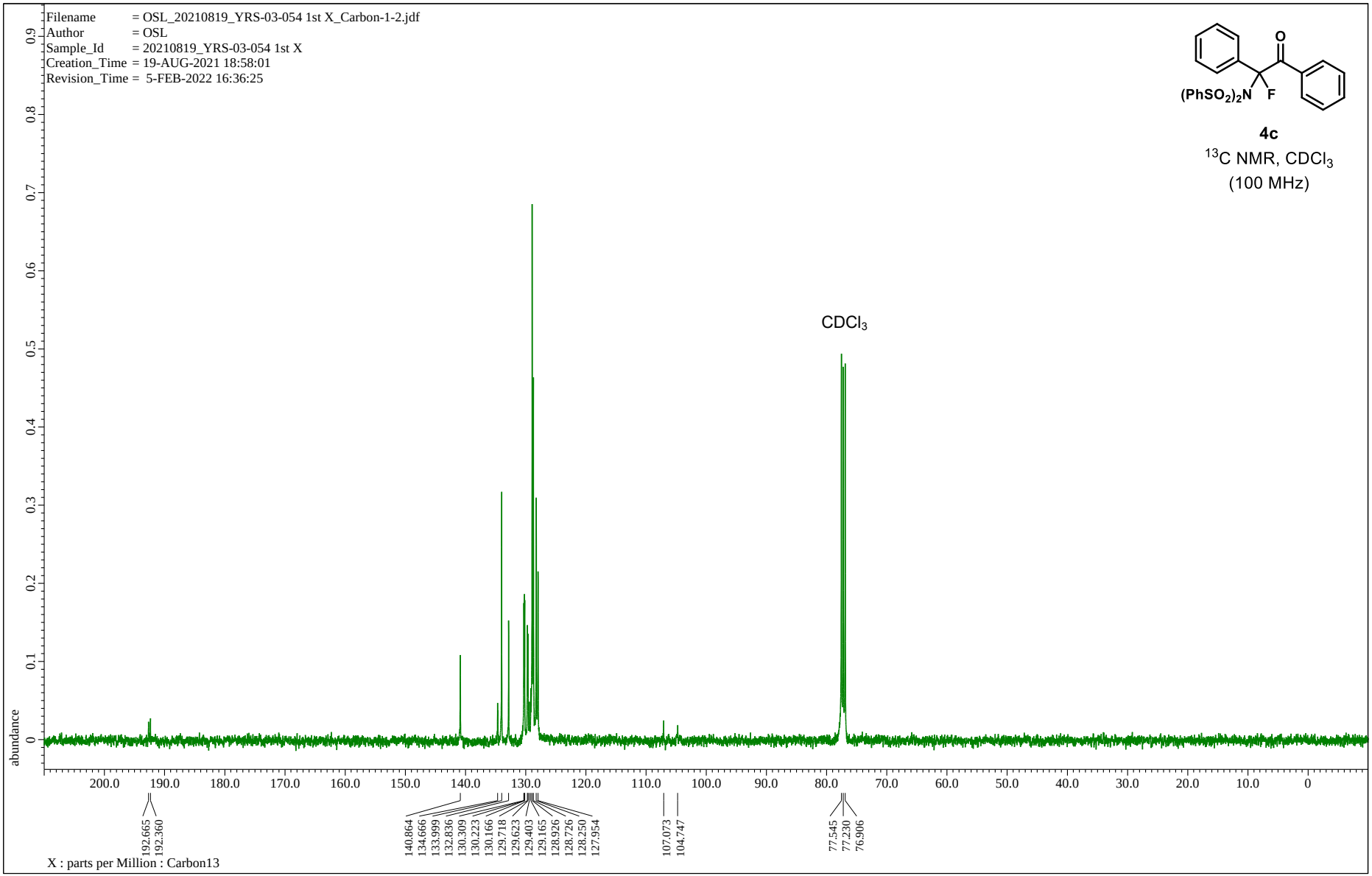

Filename = OSL_20210505_YRS-03-007 recry_Fluorine-2-2.jdf
Author = OSL
Sample_Id = 20210505_YRs-03-007 recry
Creation_Time = 5-MAY-2021 12:06:01
Revision_Time = 4-FEB-2022 22:18:05
Me
O
(PhSO2)2N
F
Me
4a
19F NMR, CDCl3
(376 MHz, 40 °C)
C6F6
abundance
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
-114.964
-164.900
X : parts per Million : Fluorine19

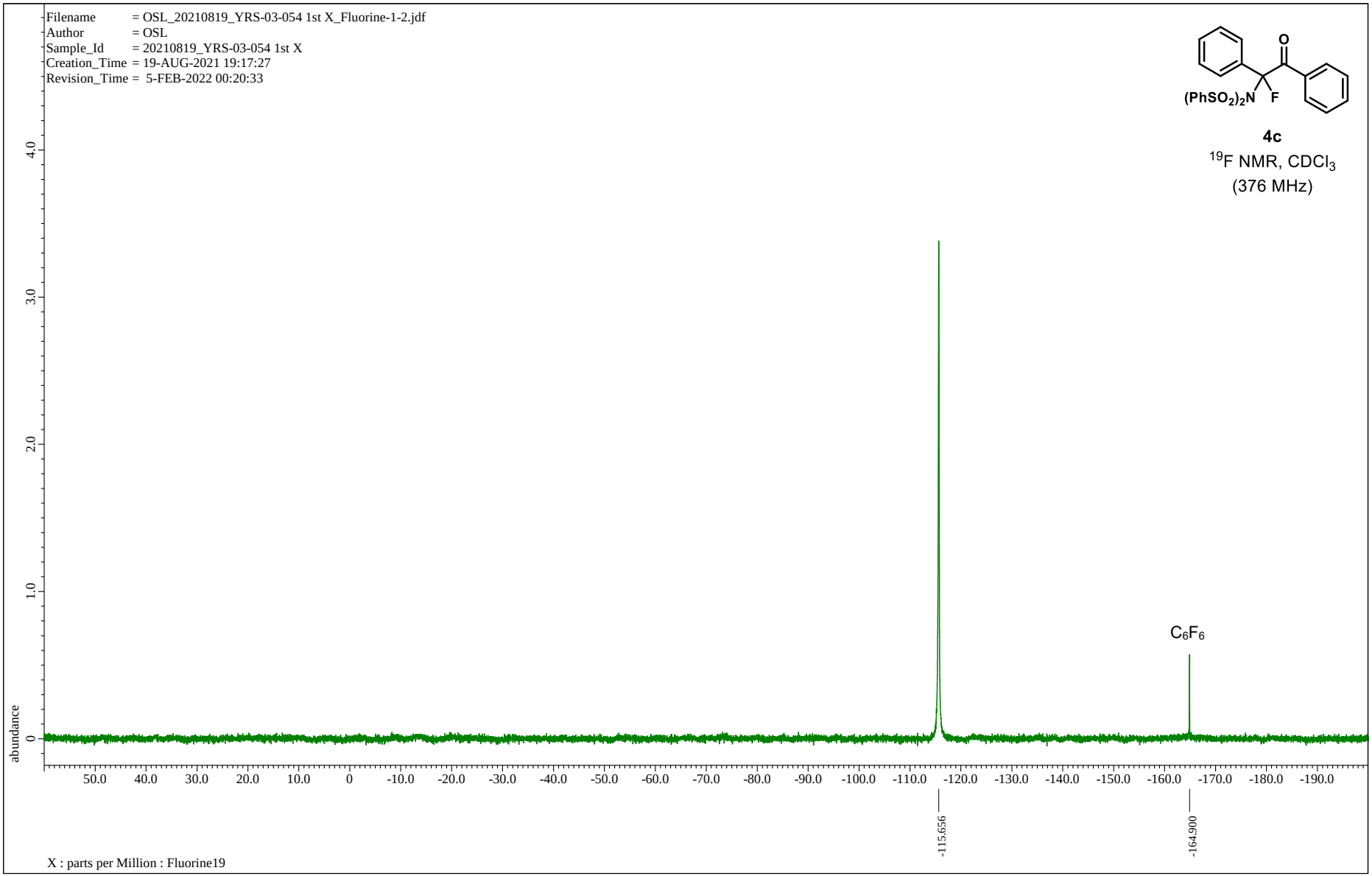

Filename = OSL_20220125_SJB-01-095-descriptive run_Proton-1-2.jdf
Author = OSL
Sample_Id = 20220125_SJB-01-095-descriptive run
Creation_Time = 25-JAN-2022 11:37:39
Revision_Time = 4-FEB-2022 22:50:25
MeO
O
(PhSO2)2N
F
OMe
4b
1H NMR, CDCl3
(400 MHz)
3.18
1.78
2.25
3.07
1.61
2.23
1.85
6.00
CHCl3
H2O
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.936
7.896
7.838
7.815
7.797
7.793
7.775
7.614
7.596
7.578
7.491
7.474
7.260
7.141
7.116
7.094
6.805
6.783
6.729
6.707
6.546
3.881
3.778
3.747
1.564
X : parts per Million : Proton

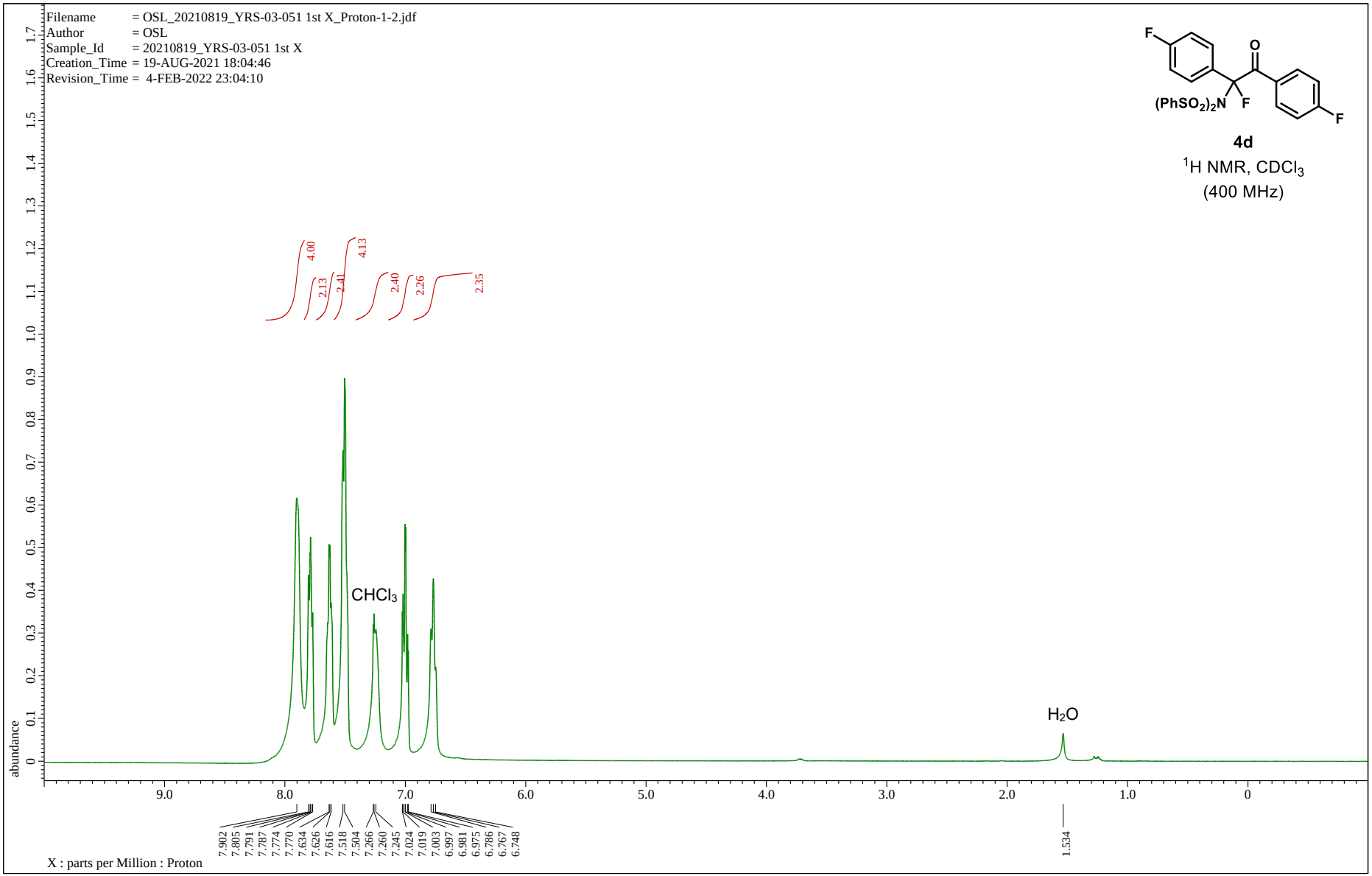

Filename = OSL_20220113_SJB-01-095-descriptive run_dry-13h_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20220113_SJB-01-095-descriptive run_dry-13h
Creation_Time = 13-JAN-2022 12:22:19
Revision_Time = 5-FEB-2022 00:24:02
MeO
O
(PhSO2)2N
F
OMe
4b
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
190.348
190.053
163.346
160.915
140.645
133.884
132.655
132.588
131.196
131.005
130.910
128.783
128.373
126.552
120.593
120.345
114.196
113.585
113.214
107.350
105.033
77.545
77.230
76.906
55.472
55.386

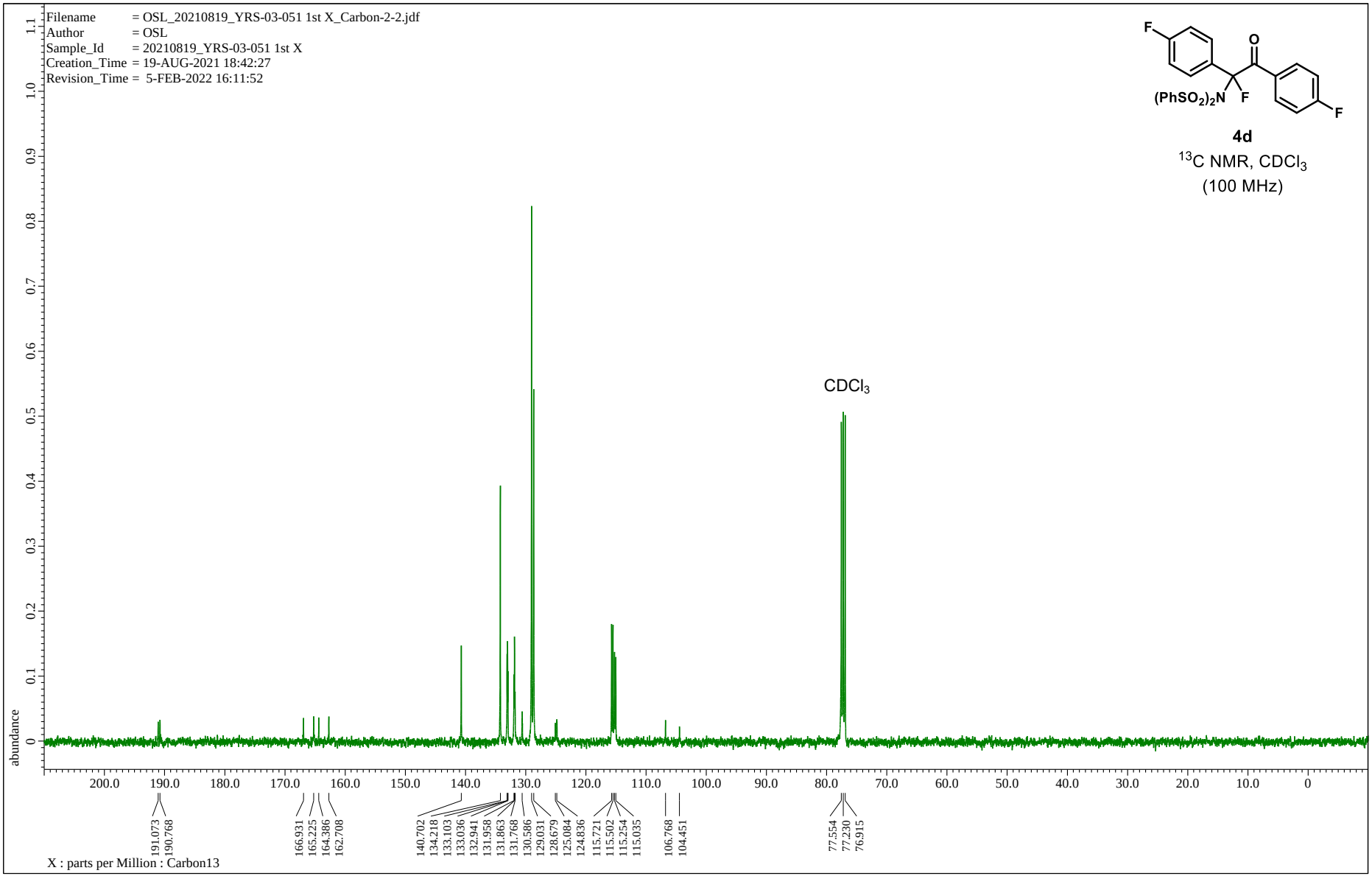

Filename = OSL_20220113_SJB-01-095-descriptive run_dry-13h_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20220113_SJB-01-095-descriptive run_dry-13h
Creation_Time = 13-JAN-2022 12:19:54
Revision_Time = 5-FEB-2022 00:22:54
MeO
O
(PhSO2)2N
F
OMe
4b
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
3.0
2.0
1.0
0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
-88.460
-91.149
-113.305
-164.900
X : parts per Million : Fluorine19

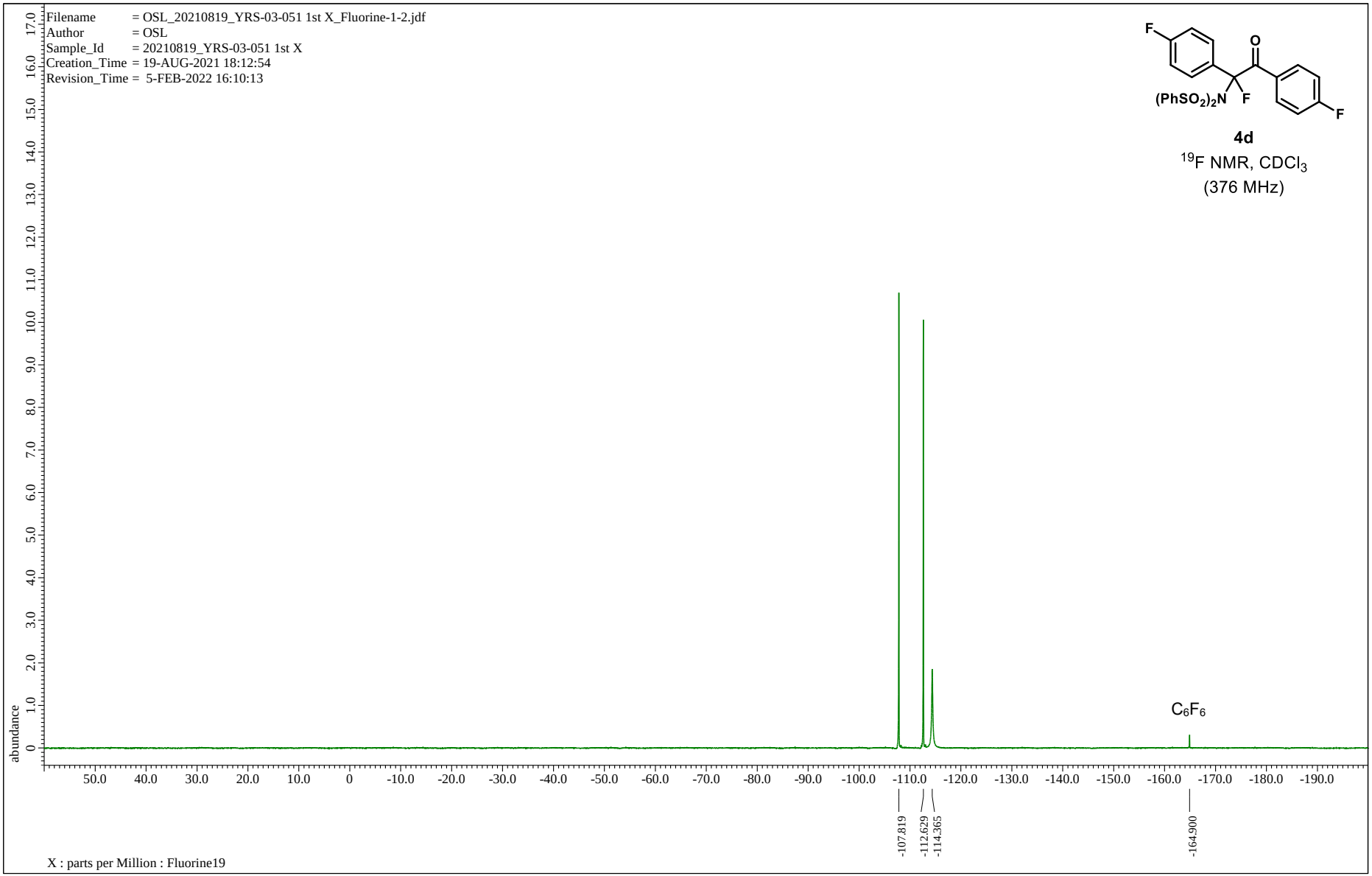

Filename = OSL_20210819_YRS-03-054 1st X_Proton-1-2.jdf
Author = OSL
Sample_Id = 20210819_YRS-03-054 1st X
Creation_Time = 19-AUG-2021 19:12:01
Revision_Time = 4-FEB-2022 22:56:00
(PhSO2)2N F
O
4c
1H NMR, CDCl3
(400 MHz)
4.00
2.37
2.17
5.21
5.16
2.35
CHCl3
H2O
abundance
X : parts per Million : Proton
7.892
7.721
7.705
7.701
7.619
7.601
7.582
7.486
7.467
7.448
7.425
7.407
7.315
7.295
7.277
7.260
7.242
7.093
7.075
7.056
1.501
1.274
1.237

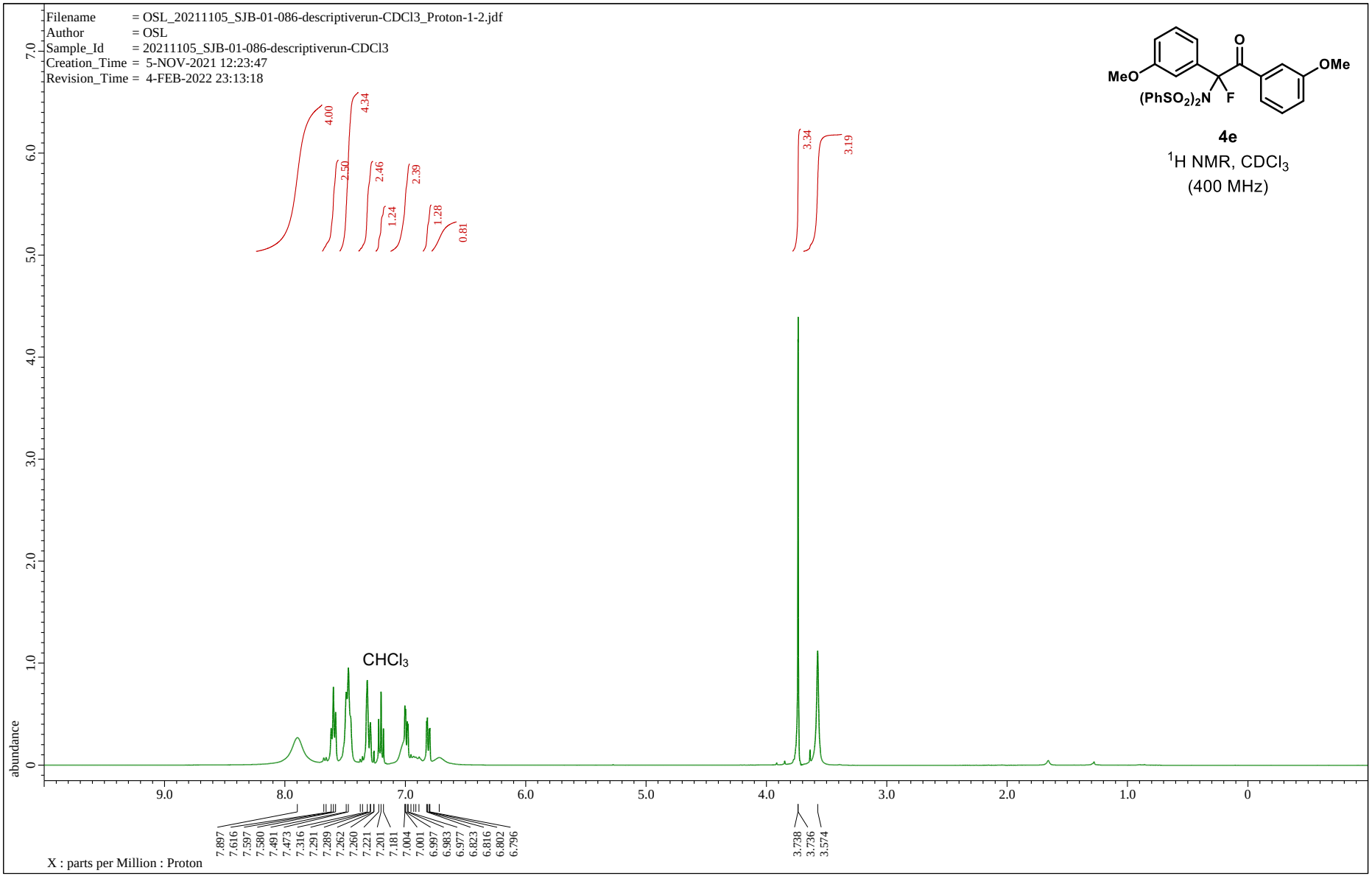

Filename = OSL_20210819_YRS-03-054 1st X_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20210819_YRS-03-054 1st X
Creation_Time = 19-AUG-2021 18:58:01
Revision_Time = 5-FEB-2022 16:36:25
(PhSO2)2N F
O
4c
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
192.665
192.360
140.864
134.666
133.999
132.836
130.309
130.223
130.166
129.718
129.623
129.403
129.165
128.926
128.726
128.250
127.954
107.073
104.747
77.545
77.230
76.906
X : parts per Million : Carbon13

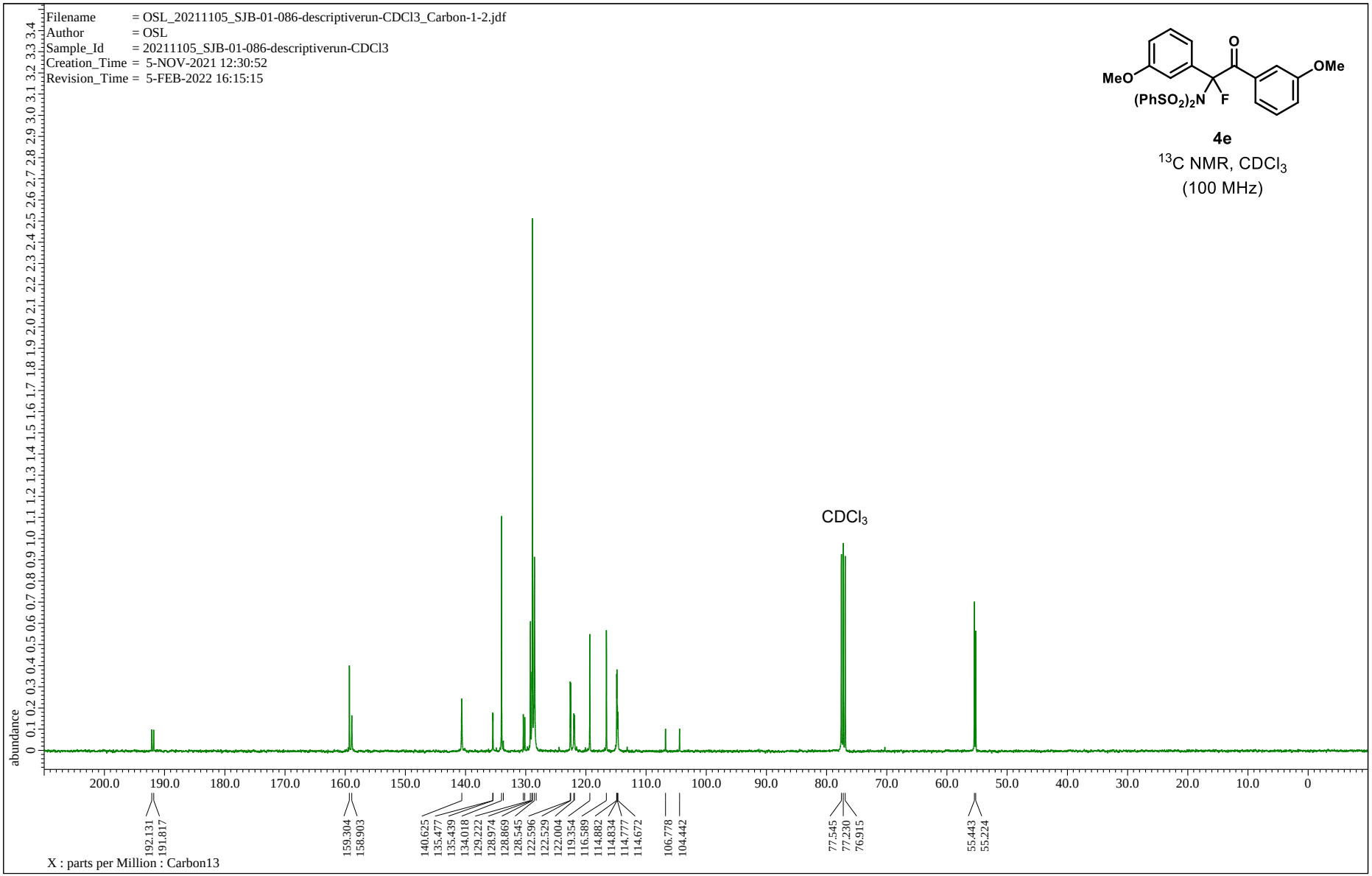

Filename = OSL_20210819_YRS-03-054 1st X_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20210819_YRS-03-054 1st X
Creation_Time = 19-AUG-2021 19:17:27
Revision_Time = 5-FEB-2022 00:20:33
(PhSO2)2N F
O
4c
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
4.0
3.0
2.0
1.0
0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
-115.656
-164.900
X : parts per Million : Fluorine19

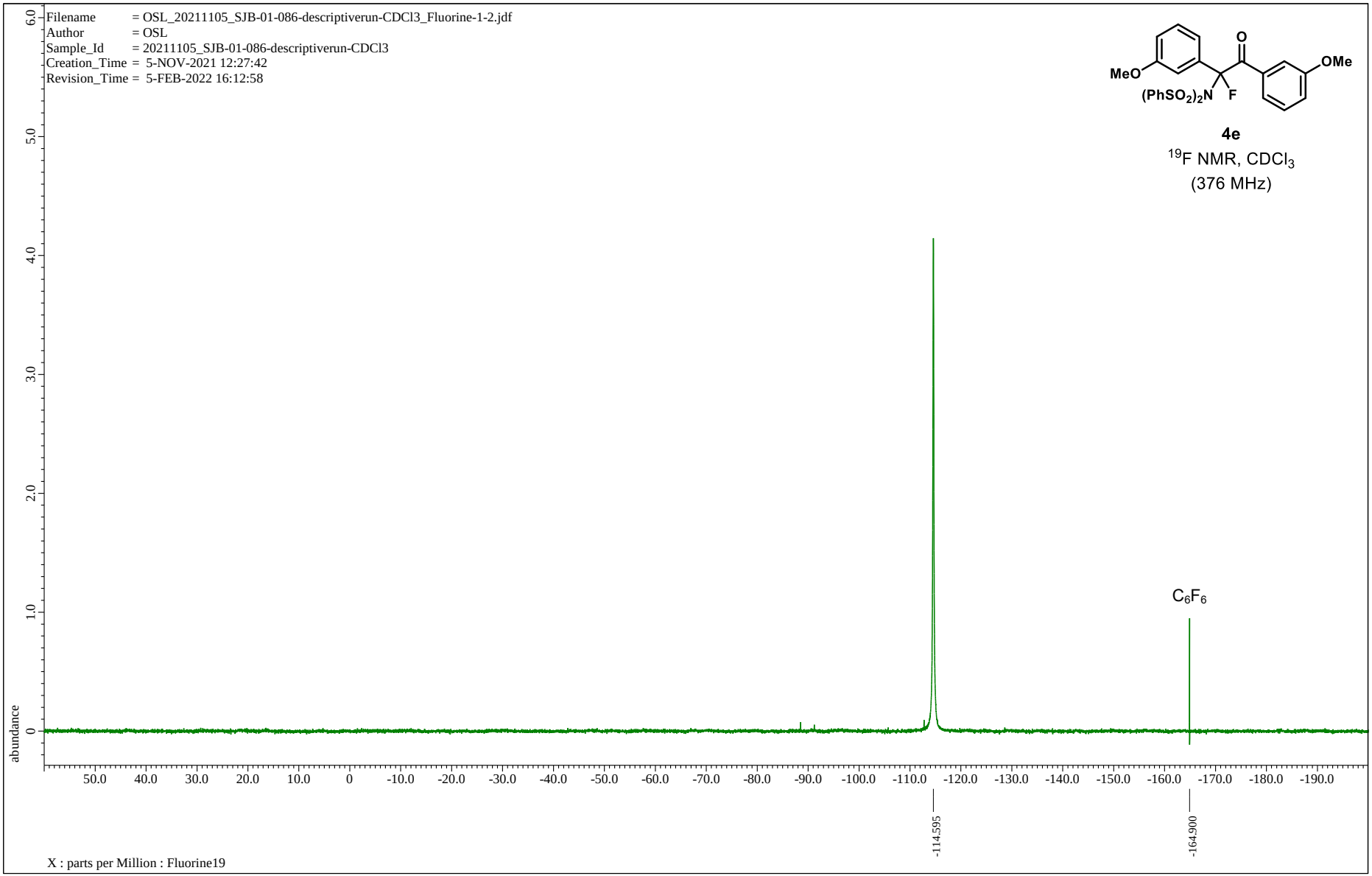

Filename = OSL_20210819_YRS-03-051 1st X_Proton-1-2.jdf
Author = OSL
Sample_Id = 20210819_YRS-03-051 1st X
Creation_Time = 19-AUG-2021 18:04:46
Revision_Time = 4-FEB-2022 23:04:10
F
O
(PhSO2)2N
F
F
4d
1H NMR, CDCl3
(400 MHz)
4.00
2.13
2.41
4.13
2.40
2.26
2.35
CHCl3
H2O
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.902
7.805
7.791
7.787
7.774
7.770
7.634
7.626
7.616
7.518
7.504
7.266
7.260
7.245
7.024
7.019
7.003
6.997
6.981
6.975
6.786
6.767
6.748
1.534
X : parts per Million : Proton

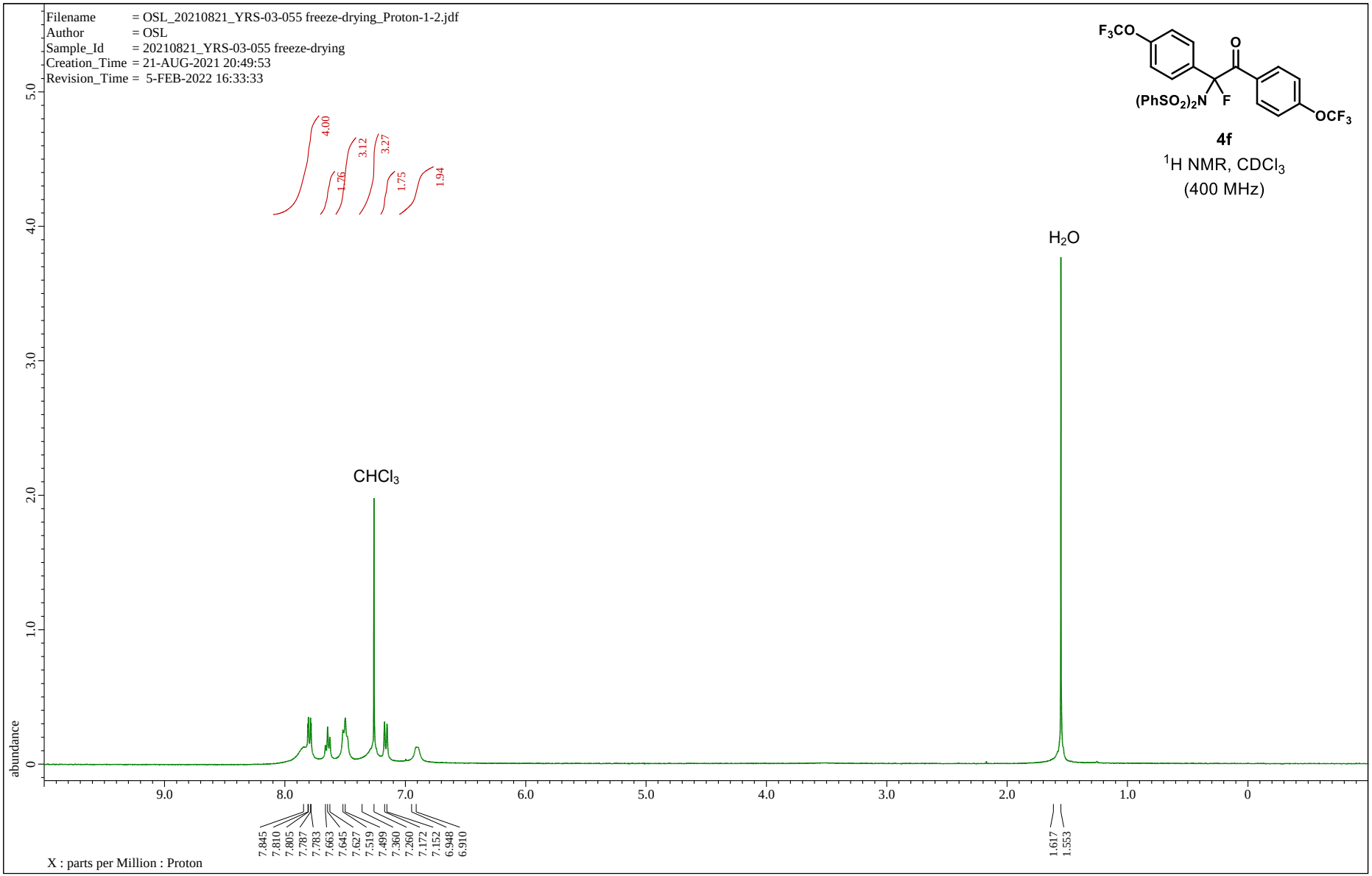

Filename = OSL_20210819_YRS-03-051 1st X_Carbon-2-2.jdf
Author = OSL
Sample_Id = 20210819_YRS-03-051 1st X
Creation_Time = 19-AUG-2021 18:42:27
Revision_Time = 5-FEB-2022 16:11:52
F
O
(PhSO2)2N
F
F
4d
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
191.073
190.768
166.931
165.225
164.386
162.708
140.702
134.218
133.103
133.036
132.941
131.958
131.863
131.768
130.586
129.031
128.679
125.084
124.836
115.721
115.502
115.254
115.035
106.768
104.451
77.554
77.230
76.915

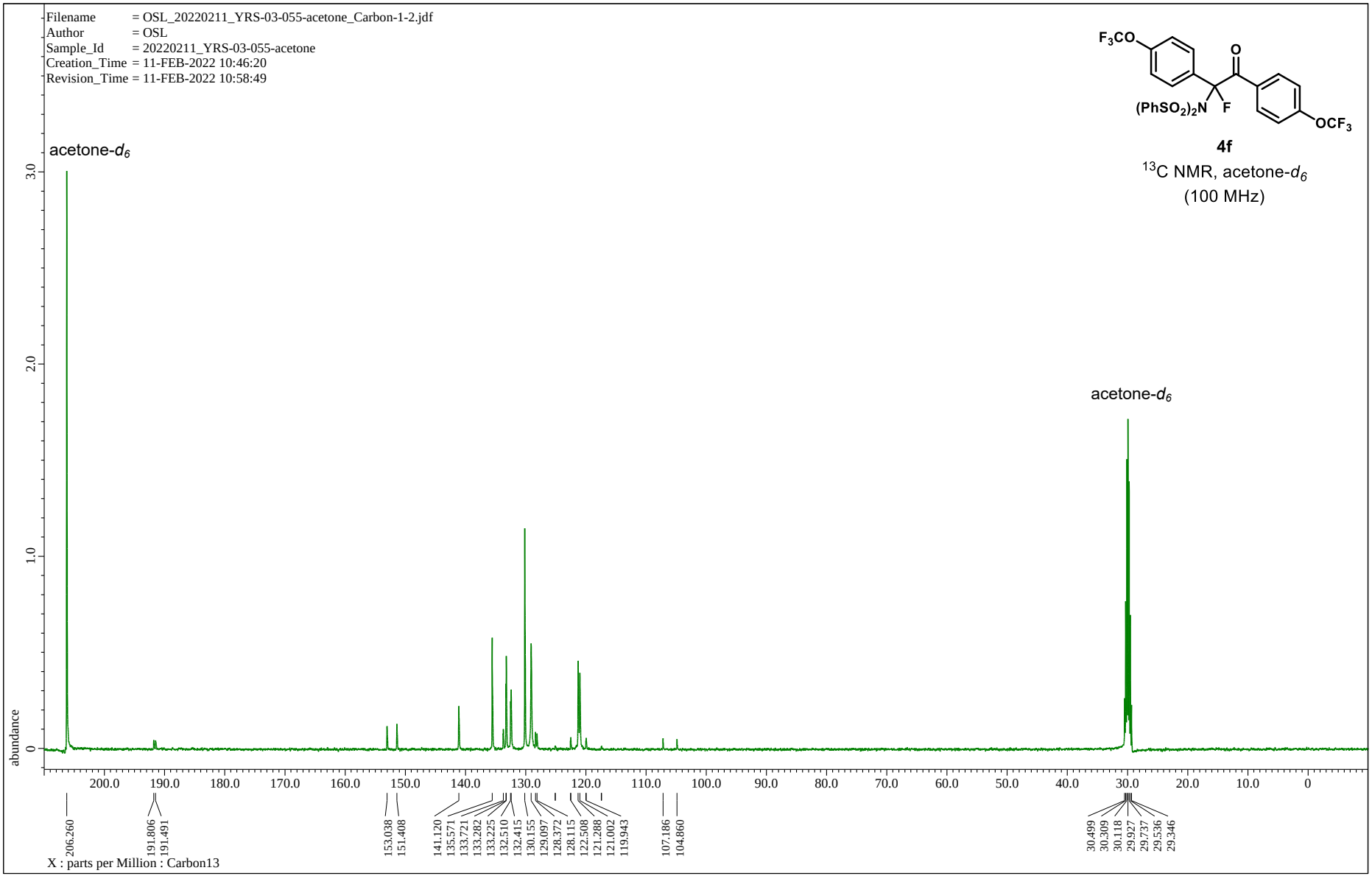

Filename = OSL_20210819_YRS-03-051 1st X_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20210819_YRS-03-051 1st X
Creation_Time = 19-AUG-2021 18:12:54
Revision_Time = 5-FEB-2022 16:10:13
F
O
(PhSO2)2N
F
F
4d
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
-107.819
-112.629
-114.365
-164.900
X : parts per Million : Fluorine19

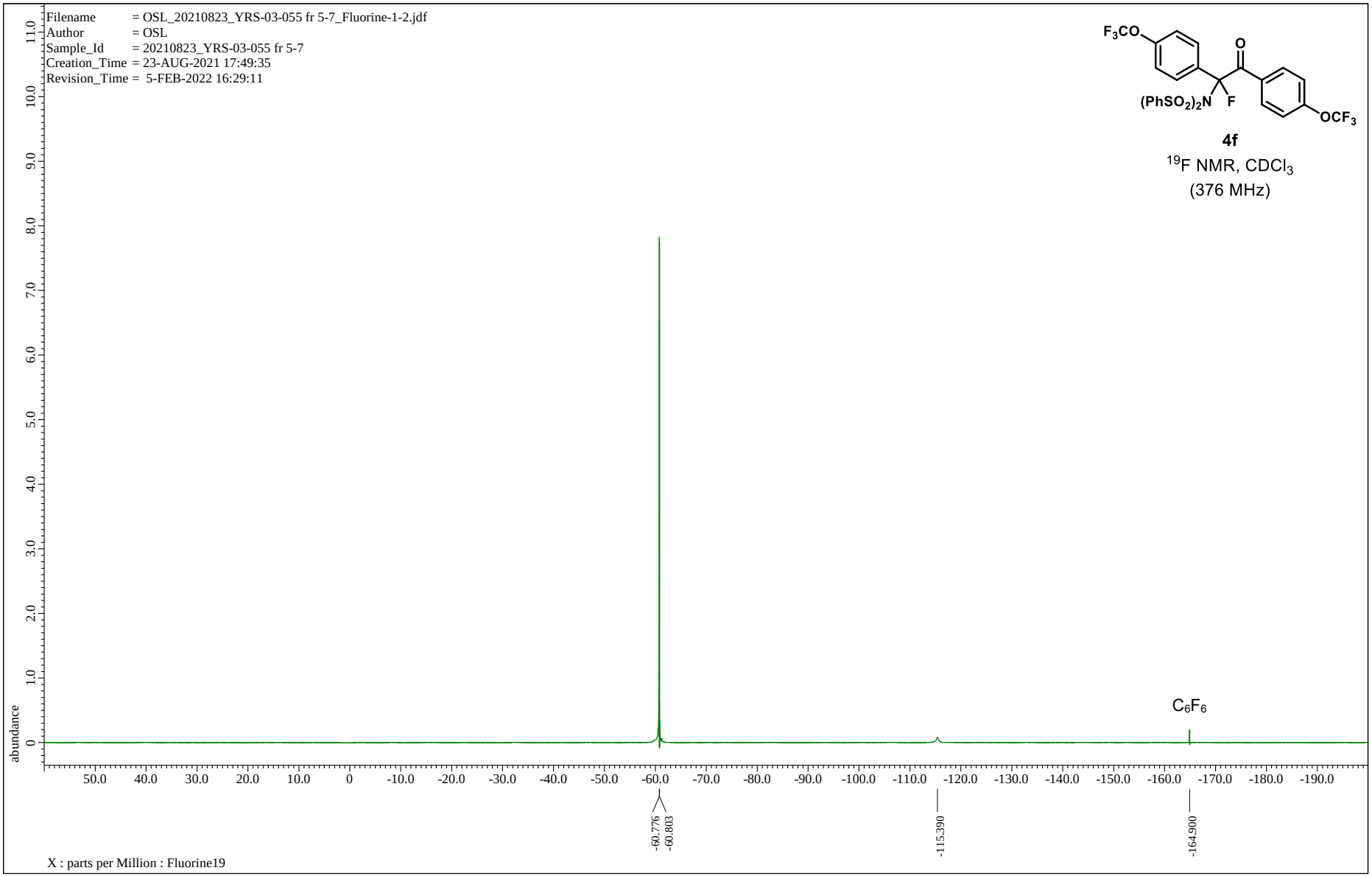

Filename = OSL_20211105_SJB-01-086-descriptiverun-CDCl3_Proton-1-2.jdf
Author = OSL
Sample_Id = 20211105_SJB-01-086-descriptiverun-CDCl3
Creation_Time = 5-NOV-2021 12:23:47
Revision_Time = 4-FEB-2022 23:13:18
MeO
OMe
O
F
(PhSO2)2N
4e
1H NMR, CDCl3
(400 MHz)
4.00
2.50
4.34
2.46
1.24
2.39
1.28
0.81
3.34
3.19
CHCl3
abundance
X : parts per Million : Proton
7.897
7.616
7.597
7.580
7.491
7.473
7.316
7.291
7.289
7.262
7.260
7.221
7.201
7.181
7.004
7.001
6.997
6.983
6.977
6.823
6.816
6.802
6.796
3.738
3.736
3.574

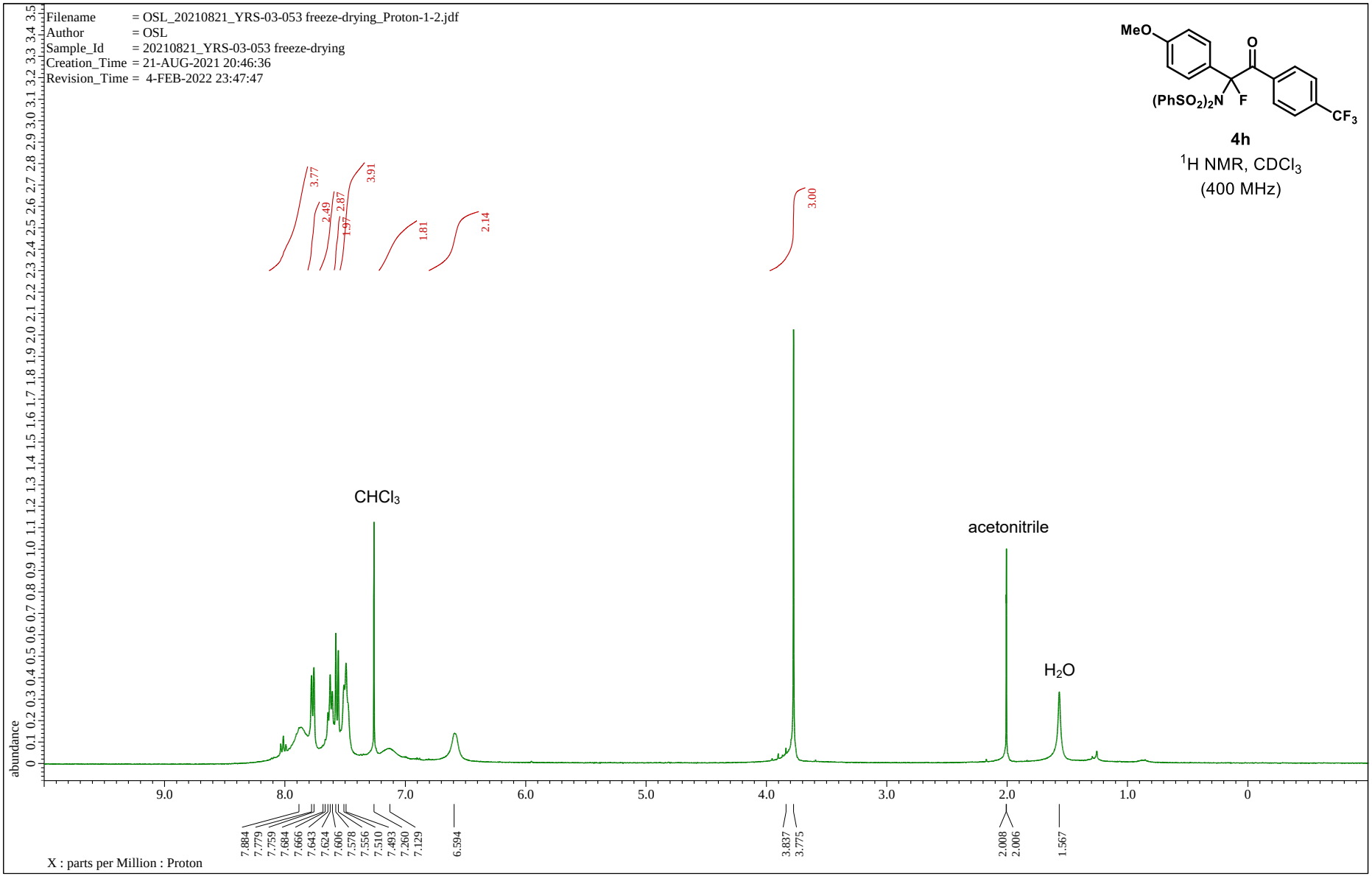

Filename = OSL_20211105_SJB-01-086-descriptiverun-CDCl3_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20211105_SJB-01-086-descriptiverun-CDCl3
Creation_Time = 5-NOV-2021 12:30:52
Revision_Time = 5-FEB-2022 16:15:15
MeO
OMe
O
(PhSO2)2N
F
4e
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
192.131
191.817
159.304
158.903
140.625
135.477
135.439
134.018
129.222
128.974
128.869
128.545
122.596
122.529
122.004
119.354
116.589
114.882
114.834
114.777
114.672
106.778
104.442
77.545
77.230
76.915
55.443
55.224

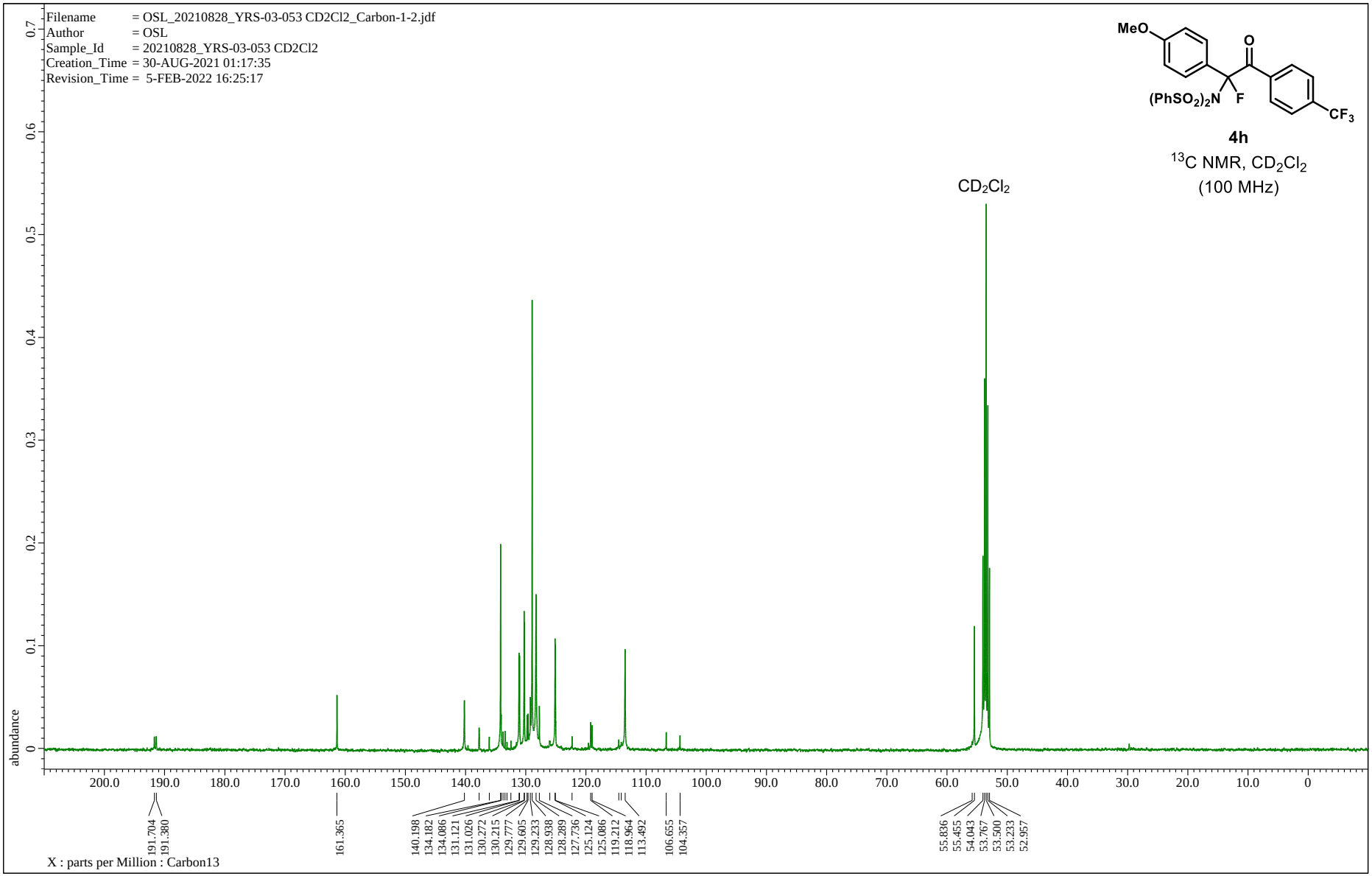

Filename = OSL_20211105_SJB-01-086-descriptiverun-CDCl3_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20211105_SJB-01-086-descriptiverun-CDCl3
Creation_Time = 5-NOV-2021 12:27:42
Revision_Time = 5-FEB-2022 16:12:58
MeO
OMe
O
(PhSO2)2N
F
4e
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
6.0
5.0
4.0
3.0
2.0
1.0
0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
-114.595
-164.900
X : parts per Million : Fluorine19

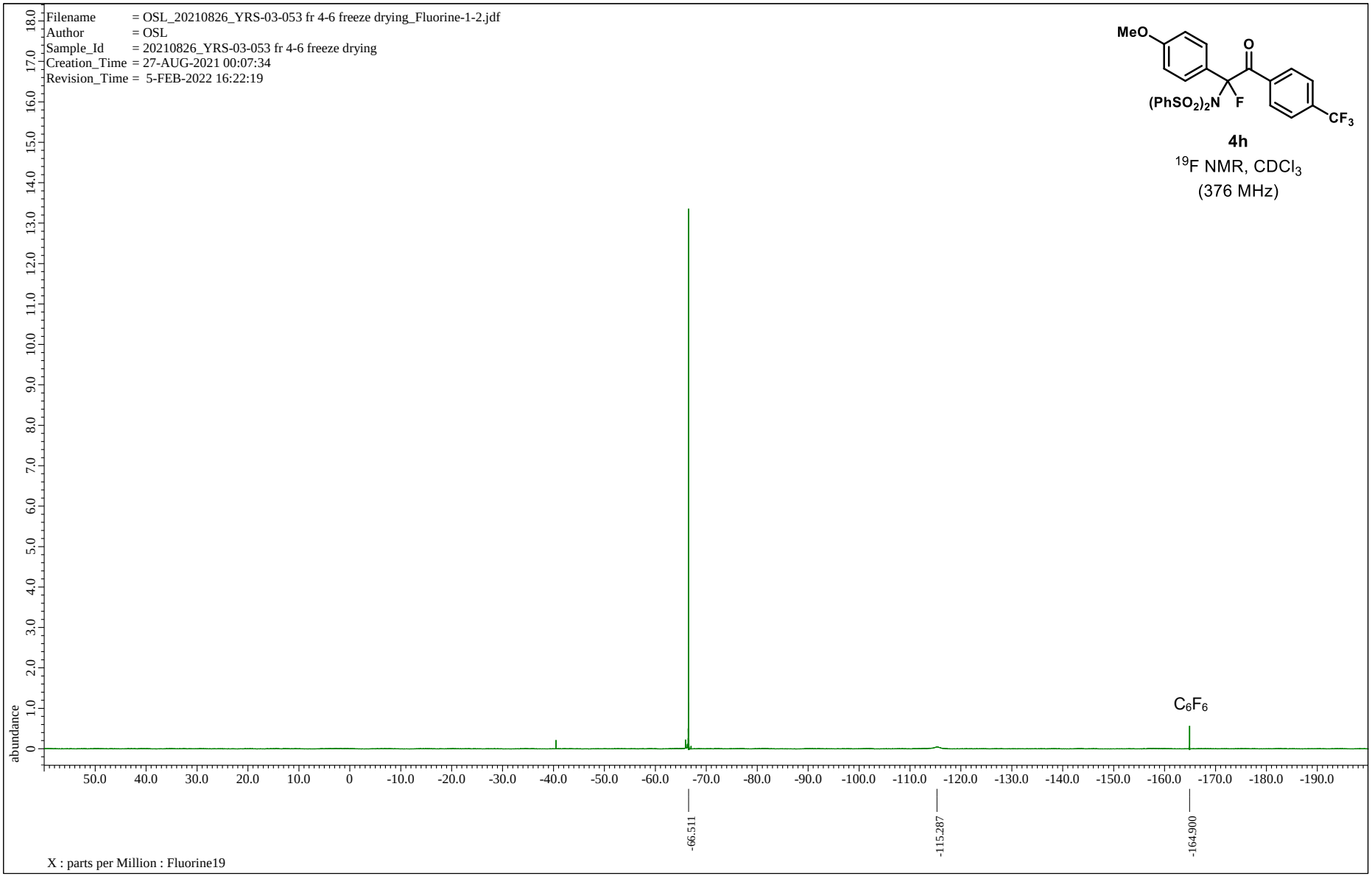

Filename = OSL_20210821_YRS-03-055 freeze-drying_Proton-1-2.jdf
Author = OSL
Sample_Id = 20210821_YRS-03-055 freeze-drying
Creation_Time = 21-AUG-2021 20:49:53
Revision_Time = 5-FEB-2022 16:33:33
F3CO
O
(PhSO2)2N
F
OCF3
4f
1H NMR, CDCl3
(400 MHz)
4.00
1.76
3.12
3.27
1.75
1.94
H2O
CHCl3
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.845
7.810
7.805
7.787
7.783
7.663
7.645
7.627
7.519
7.499
7.360
7.260
7.172
7.152
6.948
6.910
1.617
1.553
X : parts per Million : Proton

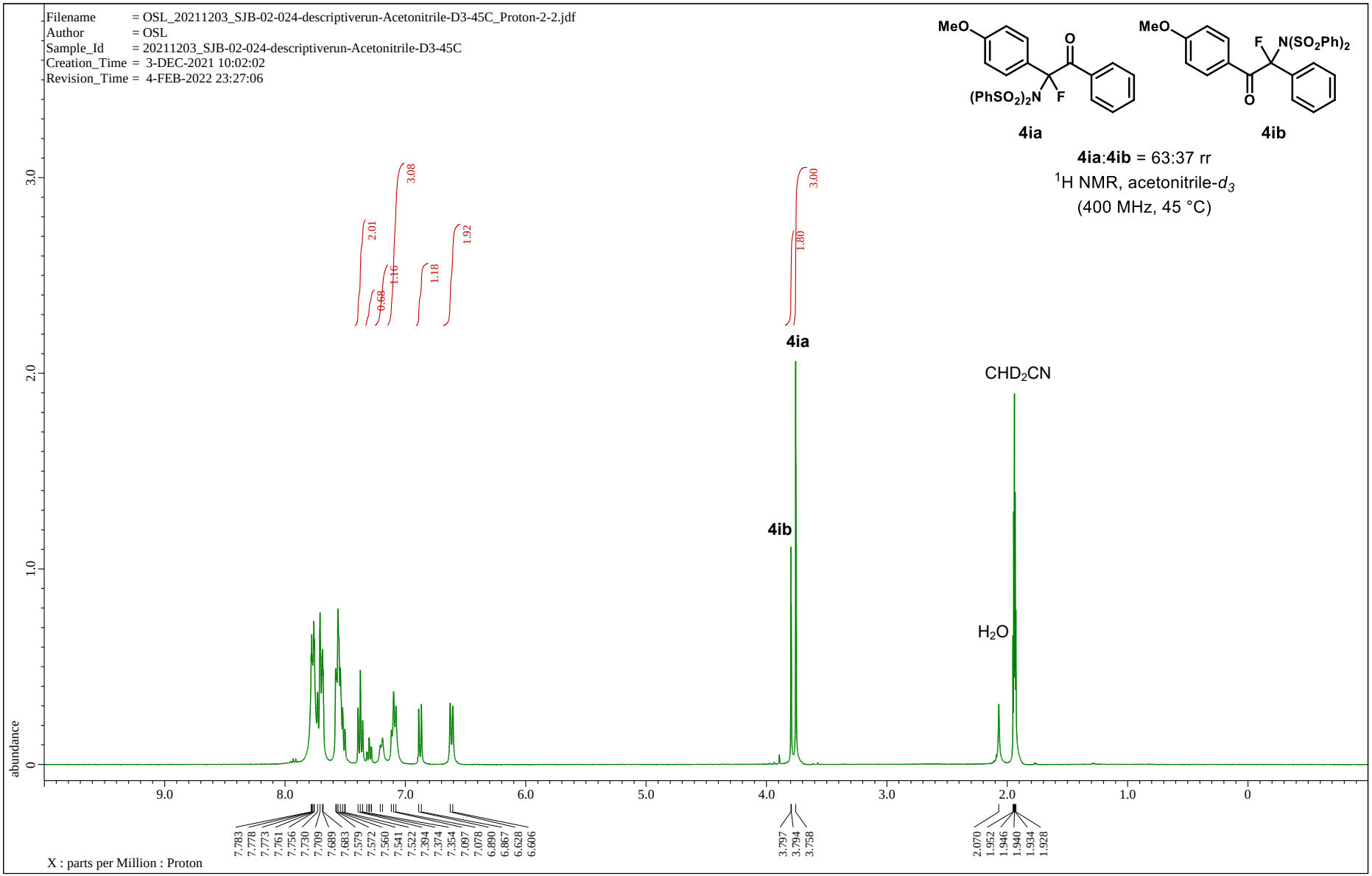

Filename = OSL_20220211_YRS-03-055-acetone_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20220211_YRS-03-055-acetone
Creation_Time = 11-FEB-2022 10:46:20
Revision_Time = 11-FEB-2022 10:58:49
F3CO
O
(PhSO2)2N
F
OCF3
4f
13C NMR, acetone-d6
(100 MHz)
acetone-d6
acetone-d6
abundance
3.0
2.0
1.0
0
200.0
190.0
180.0
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
206.260
191.806
191.491
153.038
151.408
141.120
135.571
133.721
133.282
133.225
132.510
132.415
130.155
129.097
128.372
128.115
122.508
121.288
121.002
119.943
107.186
104.860
30.499
30.309
30.118
29.927
29.737
29.536
29.346
X : parts per Million : Carbon13

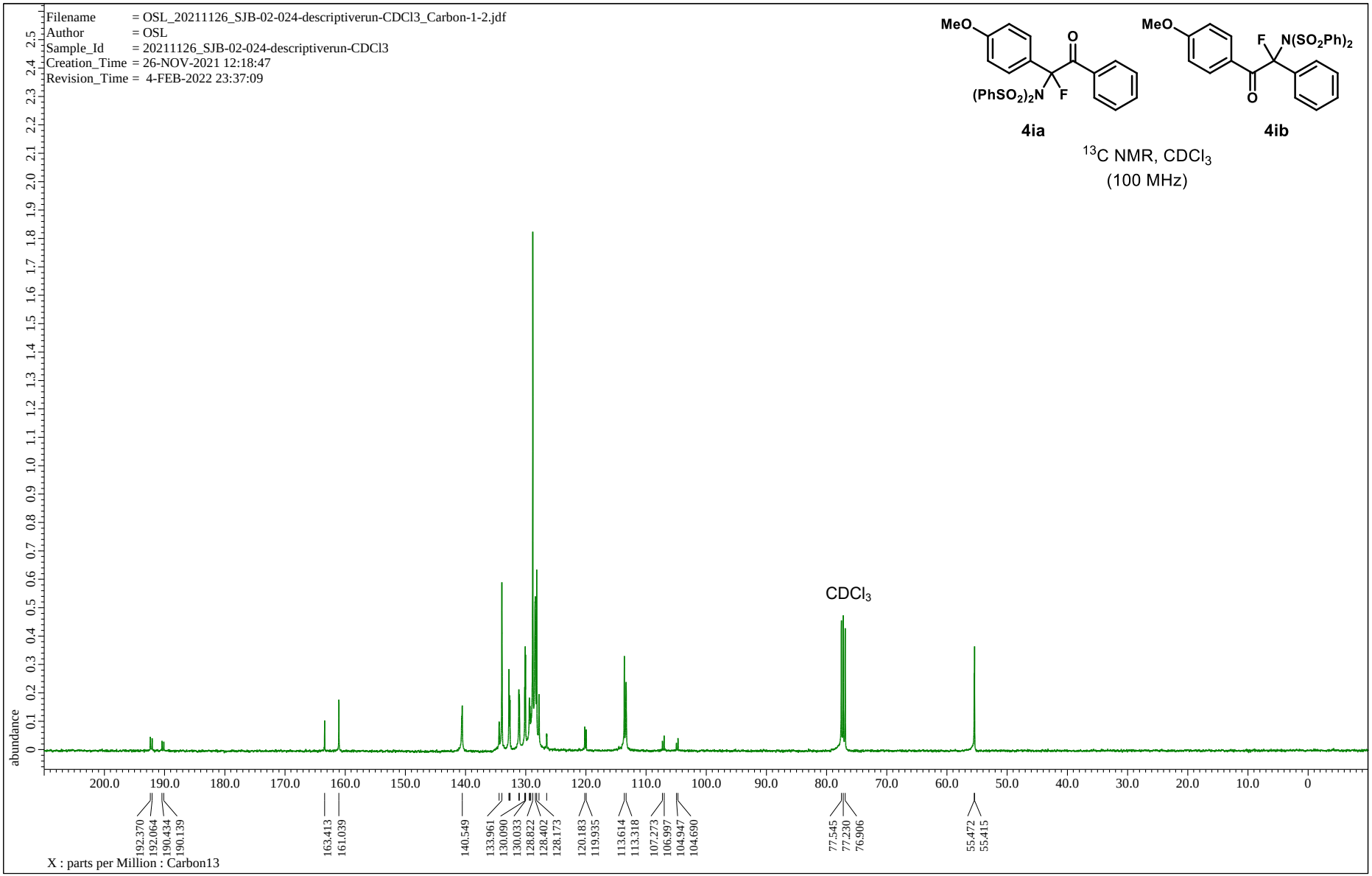

Filename = OSL_20210823_YRS-03-055 fr 5-7_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20210823_YRS-03-055 fr 5-7
Creation_Time = 23-AUG-2021 17:49:35
Revision_Time = 5-FEB-2022 16:29:11
F3CO
O
(PhSO2)2N
F
OCF3
4f
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
-60.776
-60.803
-115.390
-164.900
X : parts per Million : Fluorine19

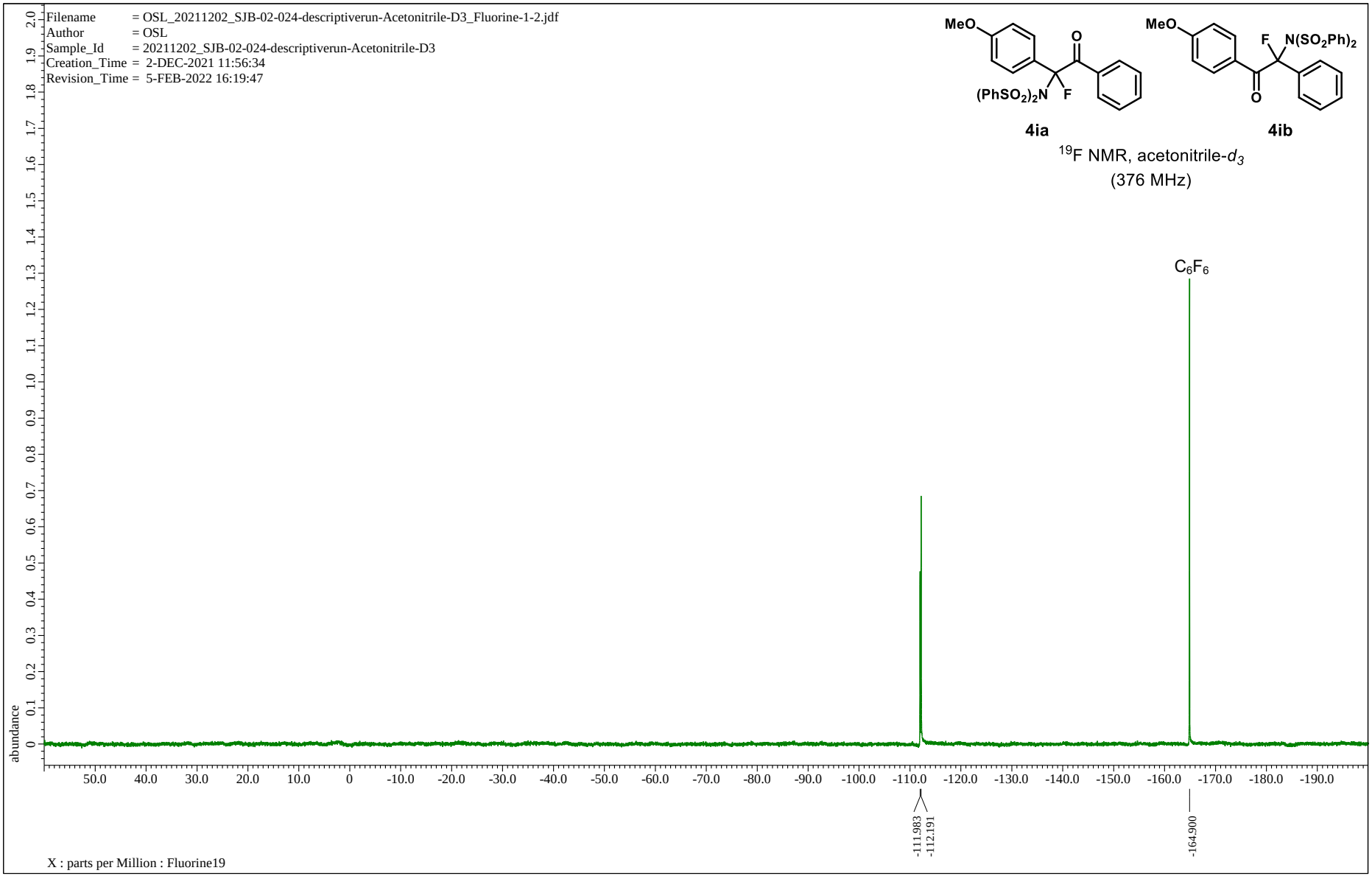

Filename = OSL_20210821_YRS-03-053 freeze-drying_Proton-1-2.jdf
Author = OSL
Sample_Id = 20210821_YRS-03-053 freeze-drying
Creation_Time = 21-AUG-2021 20:46:36
Revision_Time = 4-FEB-2022 23:47:47
MeO
O
(PhSO2)2N
F
CF3
4h
1H NMR, CDCl3
(400 MHz)
3.77
2.49
2.87
1.97
3.91
1.81
2.14
3.00
CHCl3
acetonitrile
H2O
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.884
7.779
7.759
7.684
7.666
7.643
7.624
7.606
7.578
7.556
7.510
7.493
7.260
7.129
6.594
3.837
3.775
2.008
2.006
1.567
X : parts per Million : Proton

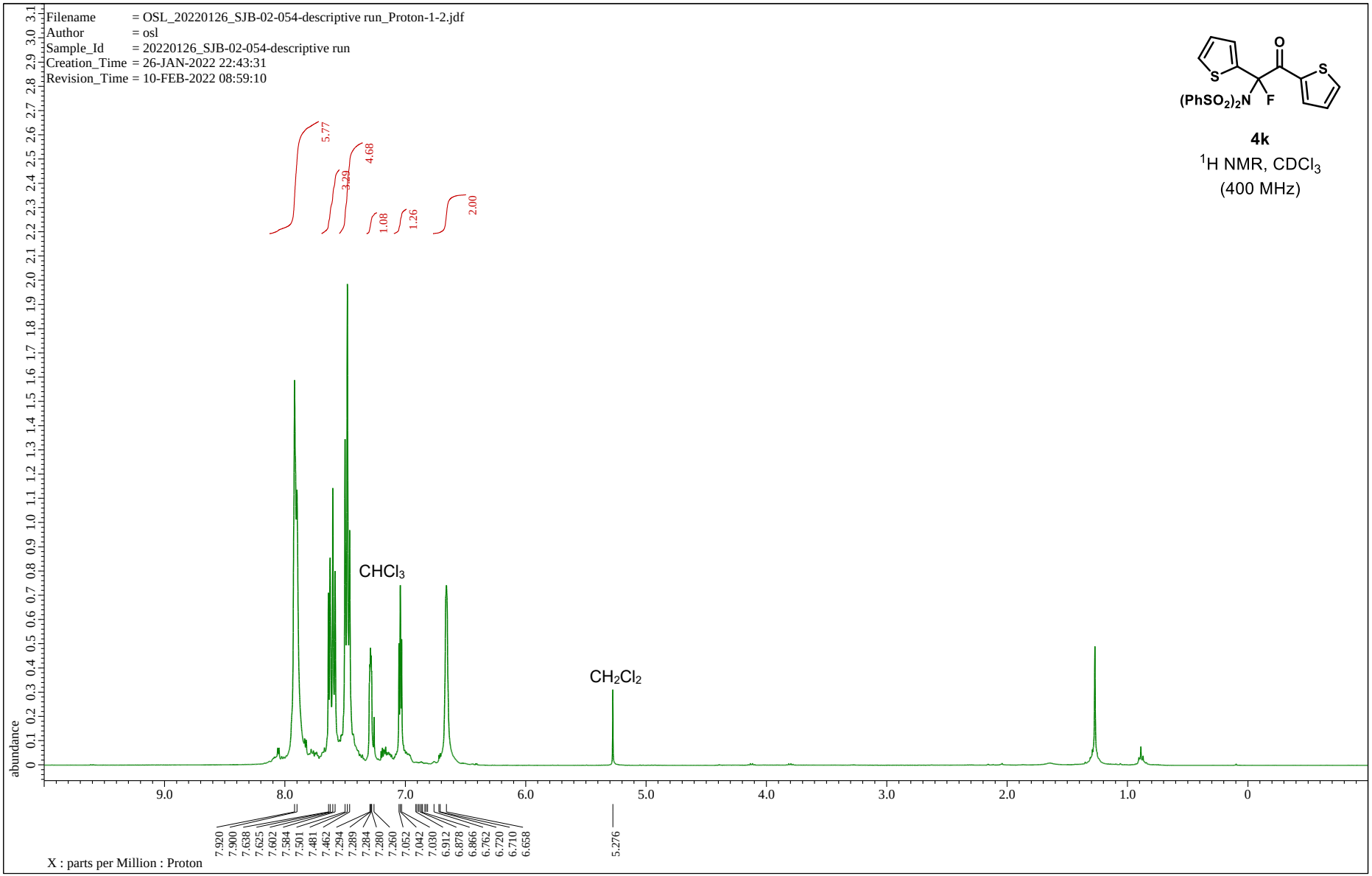

Filename = OSL_20210828_YRS-03-053 CD2Cl2_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20210828_YRS-03-053 CD2Cl2
Creation_Time = 30-AUG-2021 01:17:35
Revision_Time = 5-FEB-2022 16:25:17
MeO
O
(PhSO2)2N
F
CF3
4h
13C NMR, CD2Cl2
(100 MHz)
CD2Cl2
abundance
X : parts per Million : Carbon13
191.704
191.380
161.365
140.198
134.182
134.086
131.121
131.026
130.272
130.215
129.777
129.605
129.233
128.938
128.289
127.736
125.124
125.086
119.212
118.964
113.492
106.655
104.357
55.836
55.455
54.043
53.767
53.500
53.233
52.957

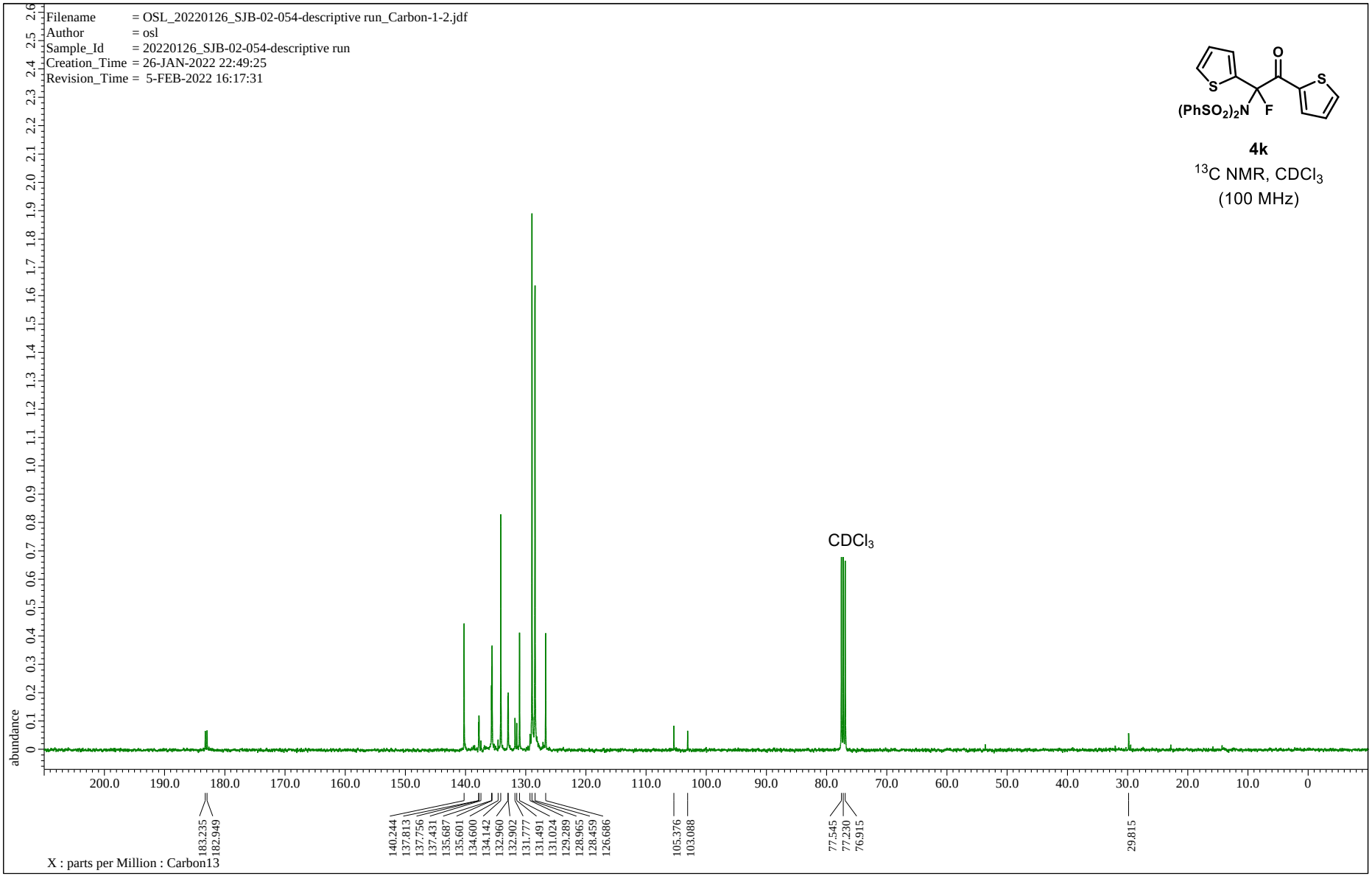

Filename = OSL_20210826_YRS-03-053 fr 4-6 freeze drying_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20210826_YRS-03-053 fr 4-6 freeze drying
Creation_Time = 27-AUG-2021 00:07:34
Revision_Time = 5-FEB-2022 16:22:19
MeO
O
(PhSO2)2N
F
CF3
4h
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
-66.511
-115.287
-164.900
X : parts per Million : Fluorine19

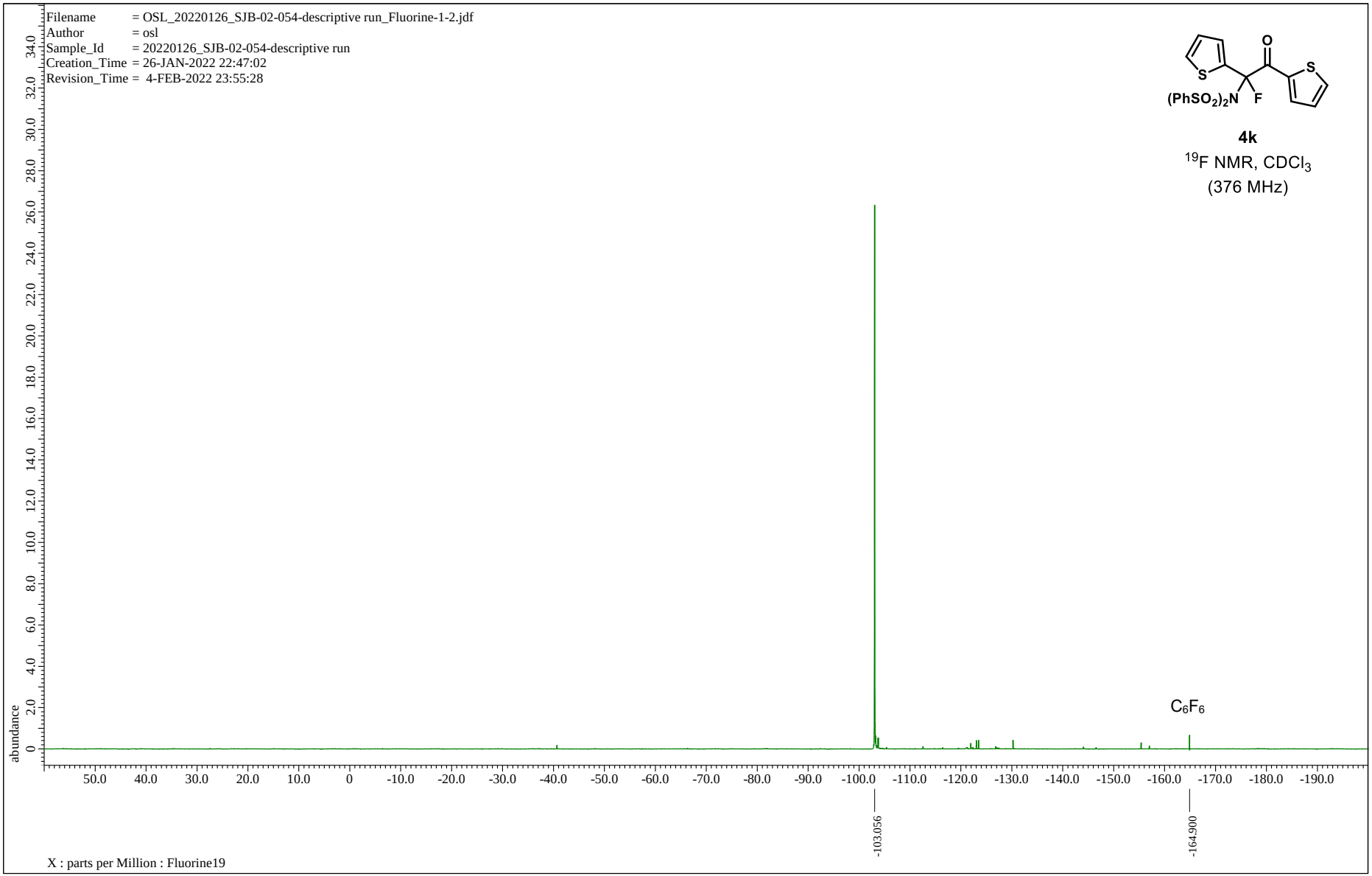

Filename = OSL_20211203_SJB-02-024-descriptiverun-Acetonitrile-D3-45C_Proton-2-2.jdf
Author = OSL
Sample_Id = 20211203_SJB-02-024-descriptiverun-Acetonitrile-D3-45C
Creation_Time = 3-DEC-2021 10:02:02
Revision_Time = 4-FEB-2022 23:27:06
MeO
O
(PhSO2)2N
F
4ia
MeO
F
N(SO2Ph)2
O
4ib
4ia:4ib = 63:37 rr
1H NMR, acetonitrile-d3
(400 MHz, 45 °C)
2.01
0.68
1.16
3.08
1.18
1.92
3.00
1.80
4ia
4ib
CHD2CN
H2O
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.783
7.778
7.773
7.761
7.756
7.730
7.709
7.689
7.683
7.579
7.572
7.560
7.541
7.522
7.394
7.374
7.354
7.097
7.078
6.890
6.867
6.628
6.606
3.797
3.794
3.758
2.070
1.952
1.946
1.940
1.934
1.928
X : parts per Million : Proton

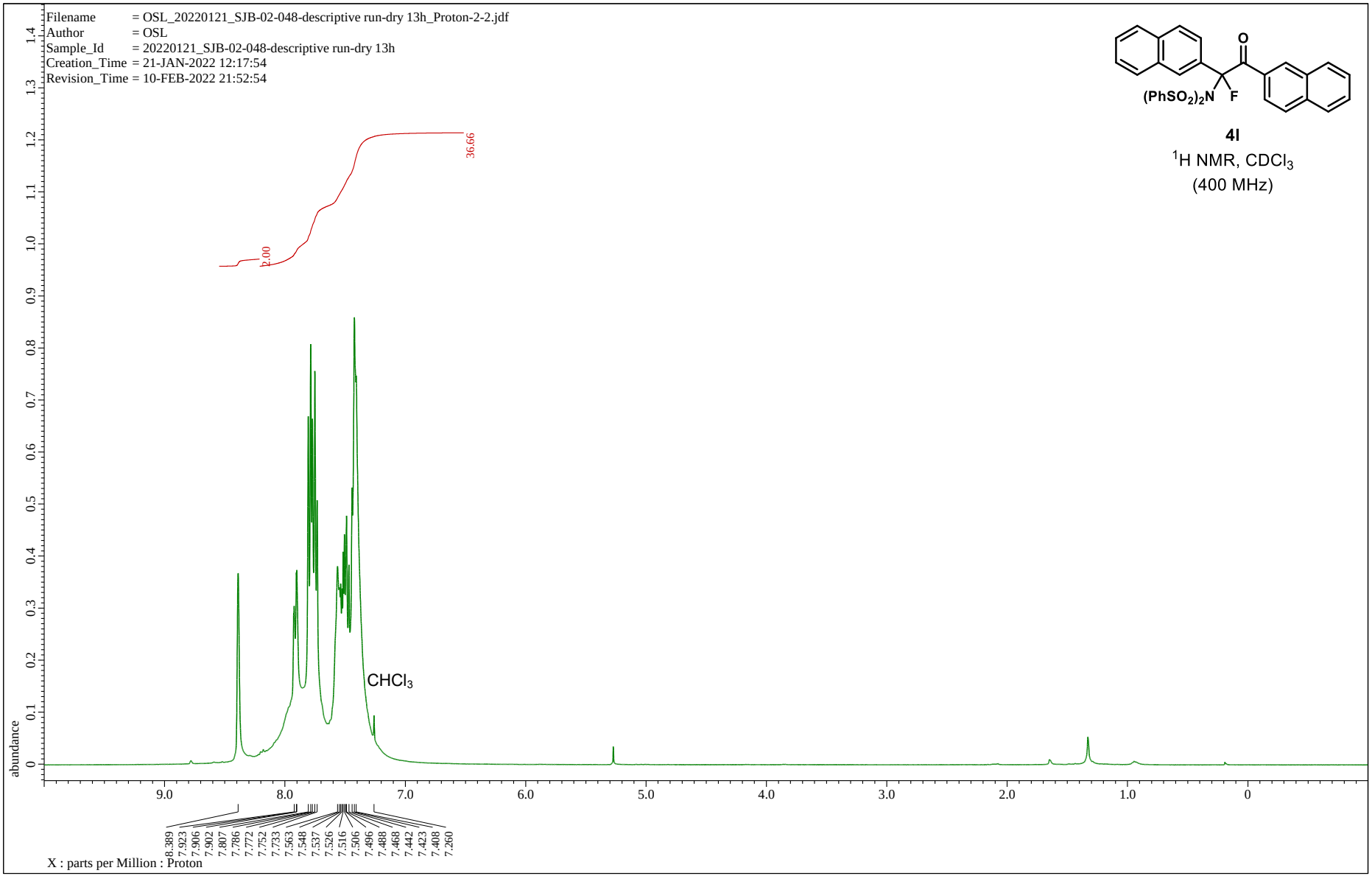

Filename = OSL_20211126_SJB-02-024-descriptiverun-CDCl3_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20211126_SJB-02-024-descriptiverun-CDCl3
Creation_Time = 26-NOV-2021 12:18:47
Revision_Time = 4-FEB-2022 23:37:09
MeO
O
(PhSO2)2N
F
4ia
MeO
F
N(SO2Ph)2
O
4ib
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
192.370
192.064
190.434
190.139
163.413
161.039
140.549
133.961
130.090
130.033
128.822
128.402
128.173
120.183
119.935
113.614
113.318
107.273
106.997
104.947
104.690
77.545
77.230
76.906
55.472
55.415

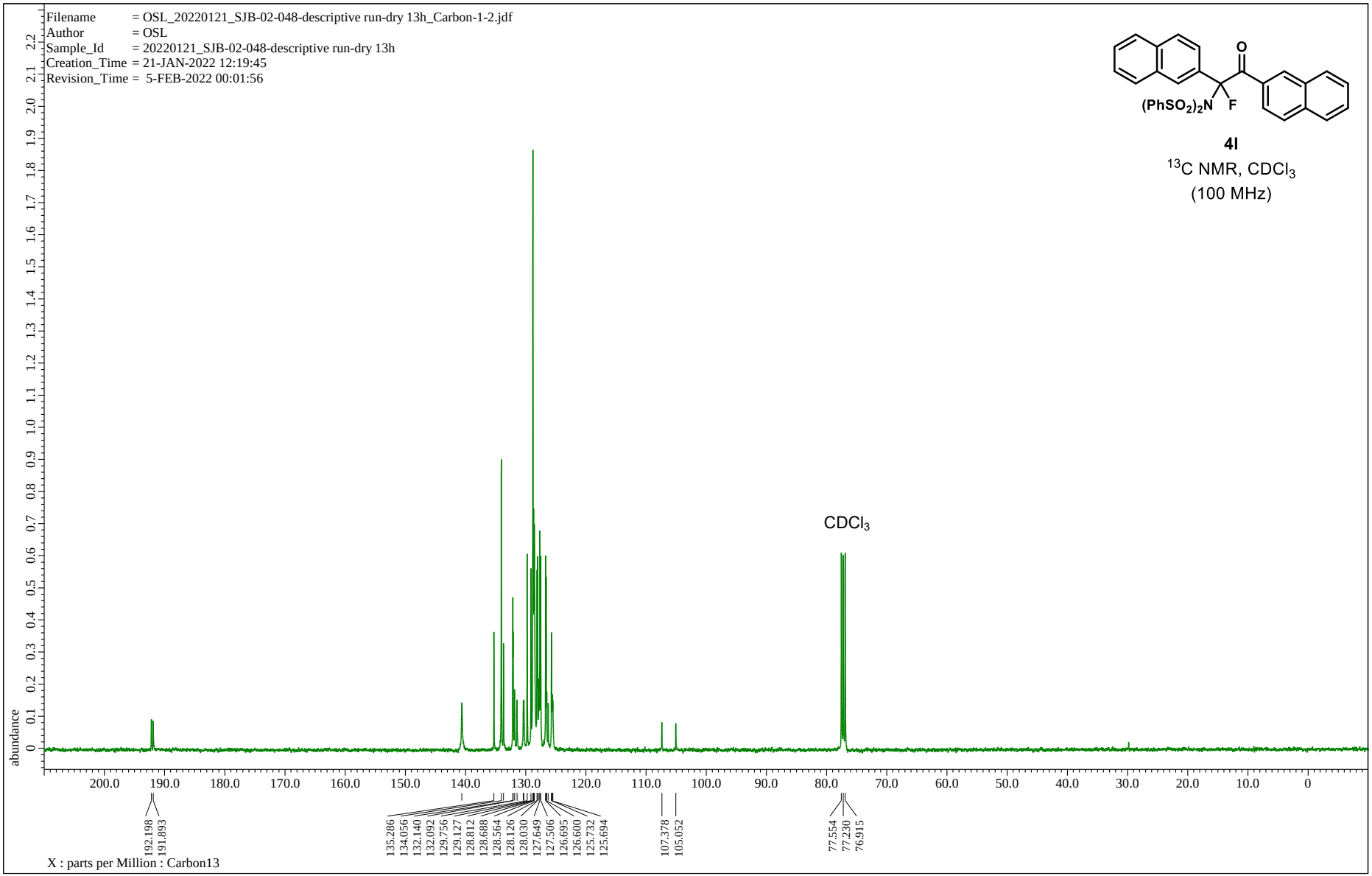

Filename = OSL_20211202_SJB-02-024-descriptiverun-Acetonitrile-D3_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20211202_SJB-02-024-descriptiverun-Acetonitrile-D3
Creation_Time = 2-DEC-2021 11:56:34
Revision_Time = 5-FEB-2022 16:19:47
MeO
O
(PhSO2)2N F
4ia
MeO
F N(SO2Ph)2
O
4ib
19F NMR, acetonitrile-d3
(376 MHz)
C6F6
abundance
-111.983
-112.191
-164.900
X : parts per Million : Fluorine19

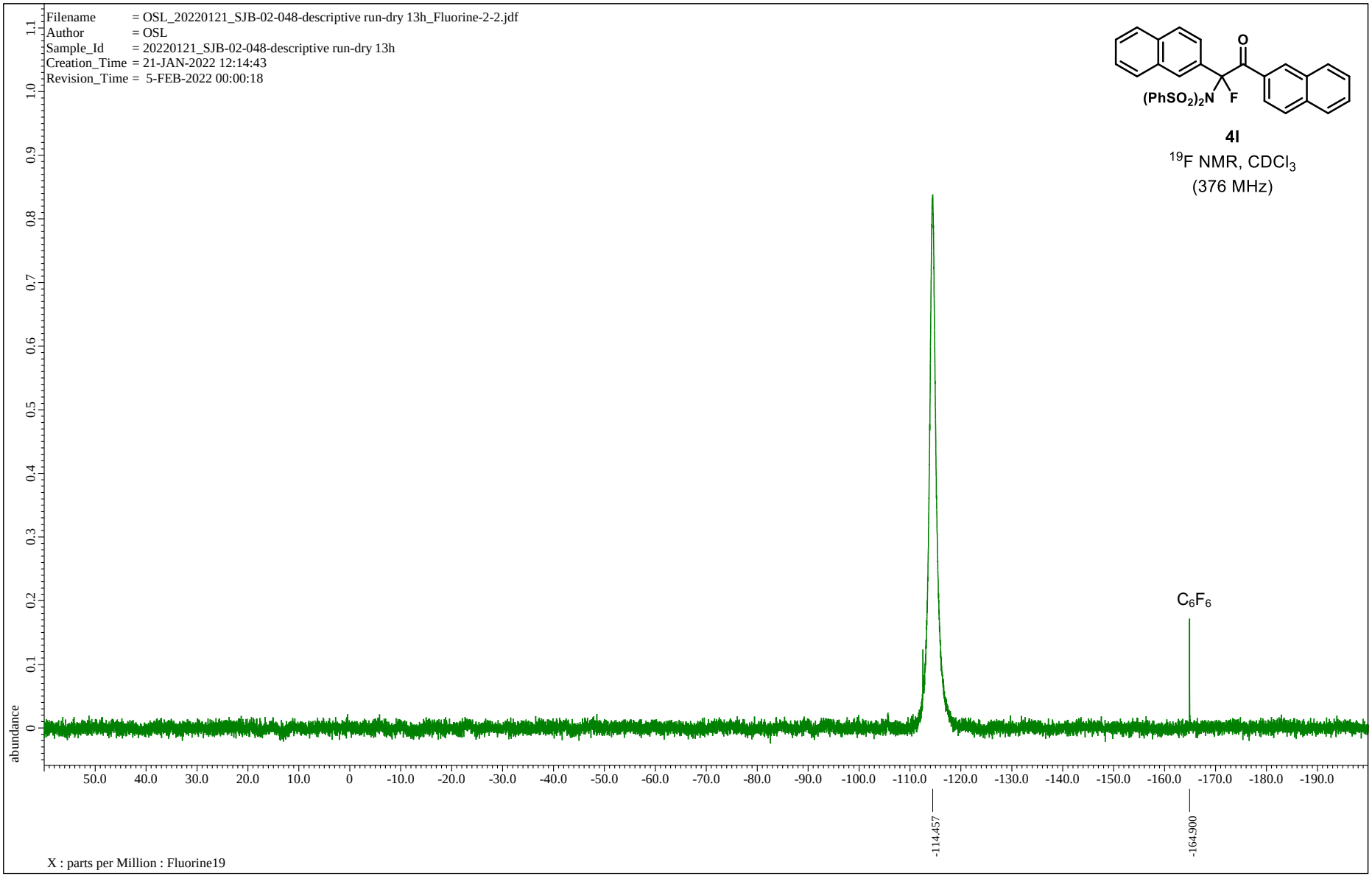

Filename = OSL_20220126_SJB-02-054-descriptive run_Proton-1-2.jdf
Author = osl
Sample_Id = 20220126_SJB-02-054-descriptive run
Creation_Time = 26-JAN-2022 22:43:31
Revision_Time = 10-FEB-2022 08:59:10
5.77
3.29
4.68
1.08
1.26
2.00
CHCl3
CH2Cl2
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.920
7.900
7.638
7.625
7.602
7.584
7.501
7.481
7.462
7.294
7.289
7.284
7.280
7.260
7.052
7.042
7.030
6.912
6.878
6.866
6.762
6.720
6.710
6.658
5.276
X : parts per Million : Proton
(PhSO2)2N
F
S
S
O
4k
1H NMR, CDCl3
(400 MHz)

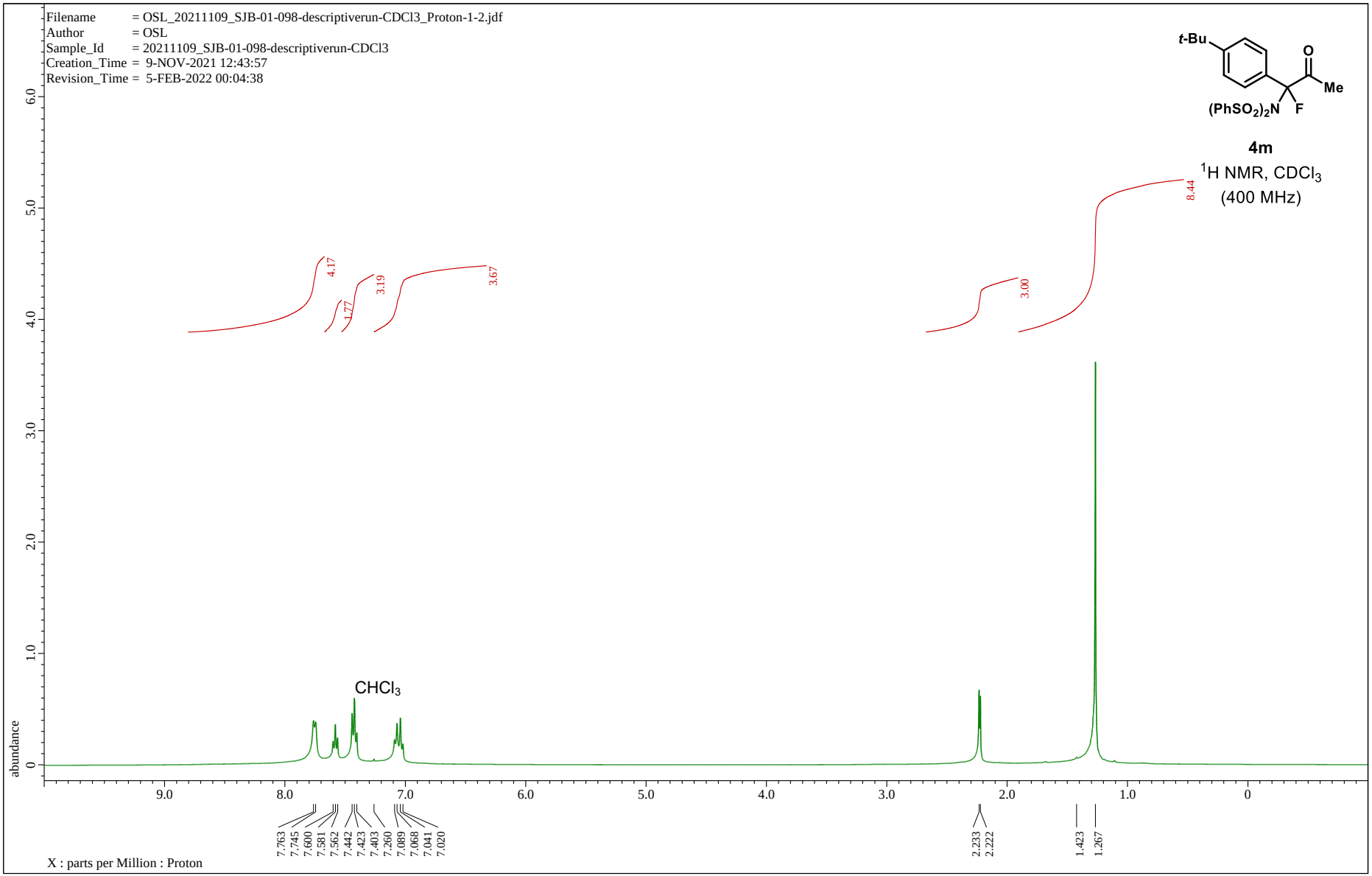

Filename = OSL_20220126_SJB-02-054-descriptive run_Carbon-1-2.jdf
Author = osl
Sample_Id = 20220126_SJB-02-054-descriptive run
Creation_Time = 26-JAN-2022 22:49:25
Revision_Time = 5-FEB-2022 16:17:31
(PhSO2)2N F
4k
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
183.235
182.949
140.244
137.813
137.756
137.431
135.687
135.601
134.600
134.142
132.960
132.902
131.777
131.491
131.024
129.289
128.965
128.459
126.686
105.376
103.088
77.545
77.230
76.915
29.815

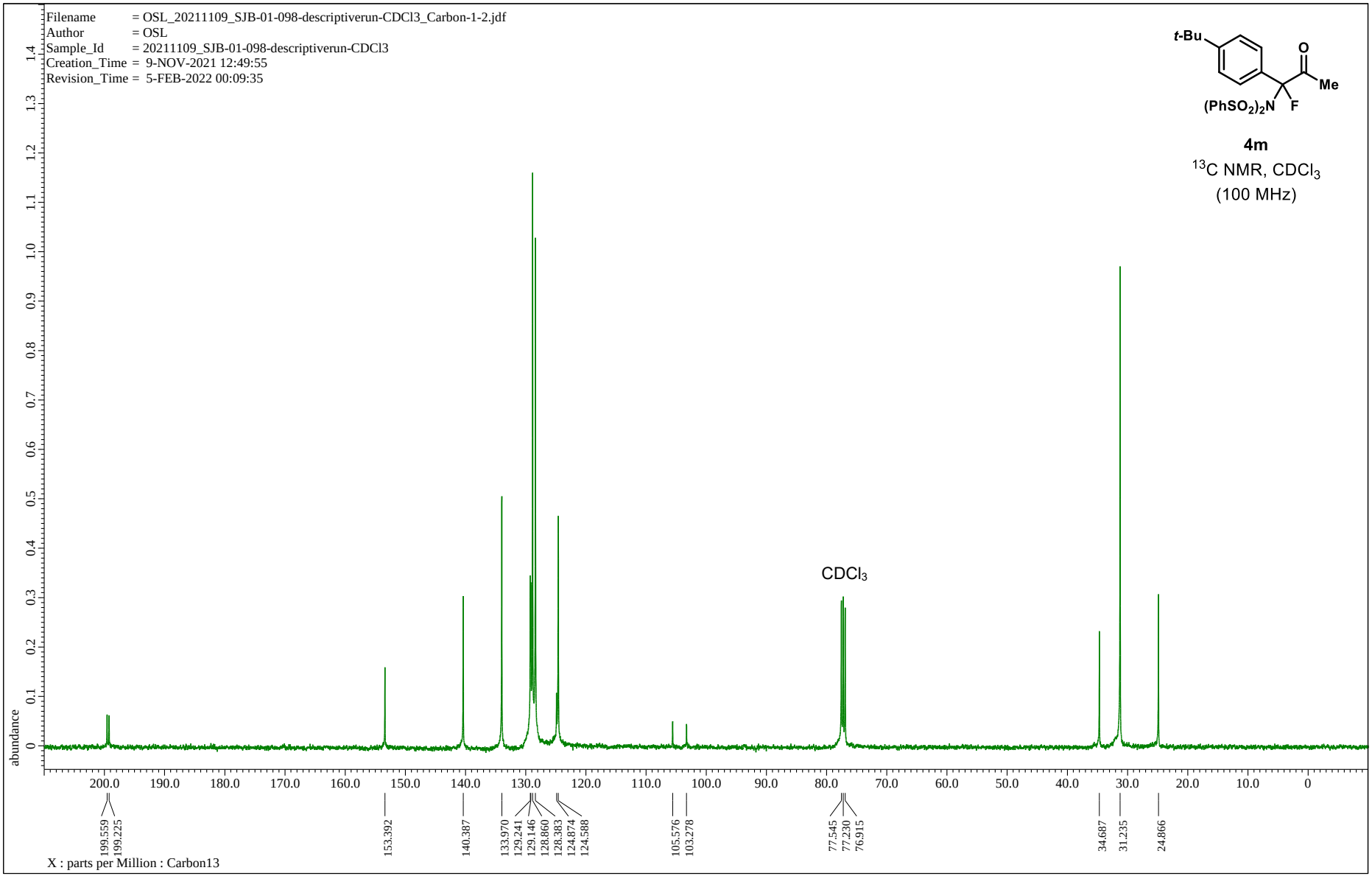

Filename = OSL_20220126_SJB-02-054-descriptive run_Fluorine-1-2.jdf
Author = osl
Sample_Id = 20220126_SJB-02-054-descriptive run
Creation_Time = 26-JAN-2022 22:47:02
Revision_Time = 4-FEB-2022 23:55:28
(PhSO2)2N F
4k
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
-103.056
-164.900
X : parts per Million : Fluorine19

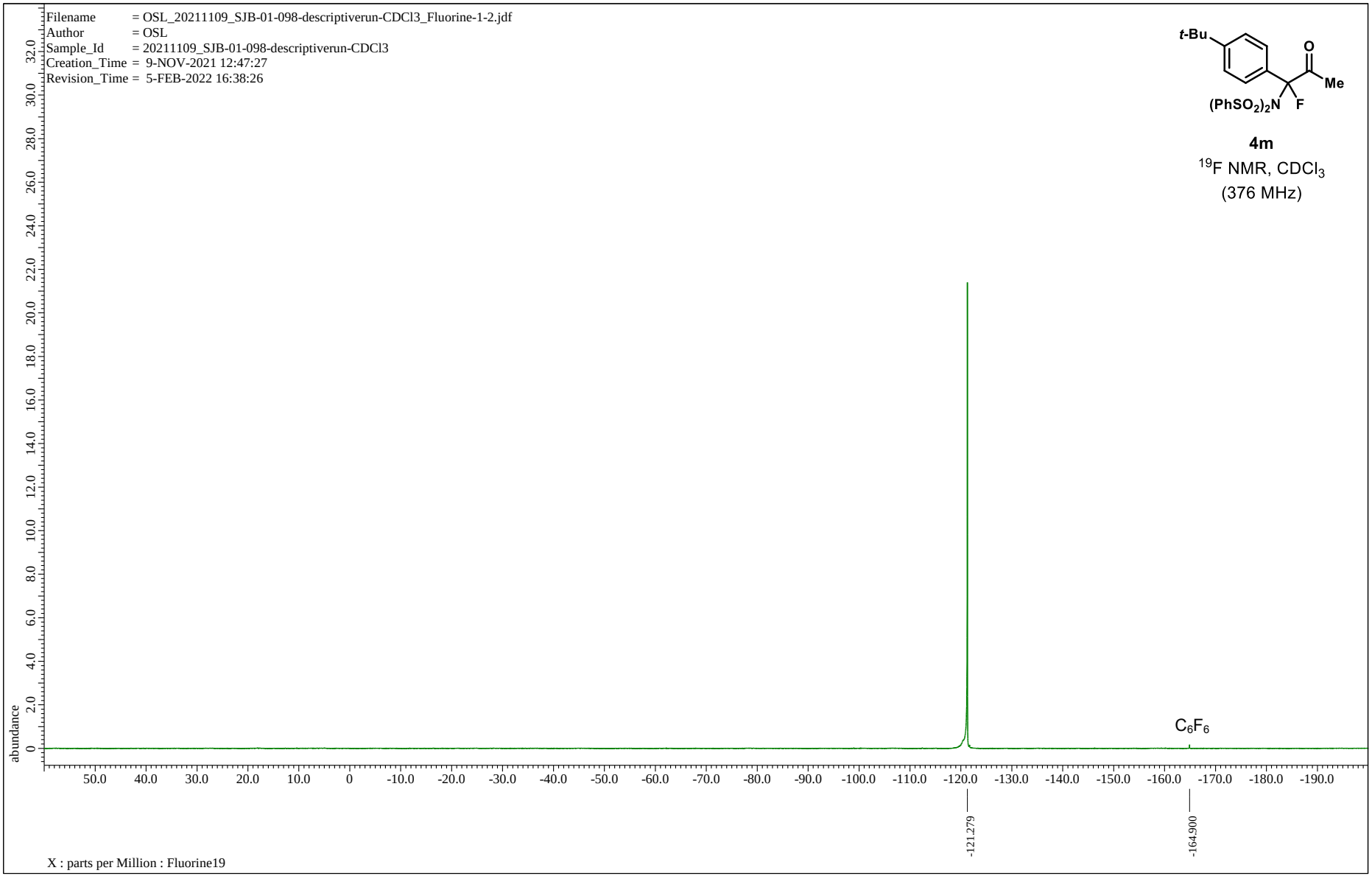

Filename = OSL_20220121_SJB-02-048-descriptive run-dry 13h_Proton-2-2.jdf
Author = OSL
Sample_Id = 20220121_SJB-02-048-descriptive run-dry 13h
Creation_Time = 21-JAN-2022 12:17:54
Revision_Time = 10-FEB-2022 21:52:54
36.66
2.00
CHCl3
abundance
X : parts per Million : Proton
8.389
7.923
7.906
7.902
7.807
7.786
7.772
7.752
7.733
7.563
7.548
7.537
7.526
7.516
7.506
7.496
7.488
7.468
7.442
7.423
7.408
7.260
(PhSO2)2N
F
O
4l
1H NMR, CDCl3
(400 MHz)

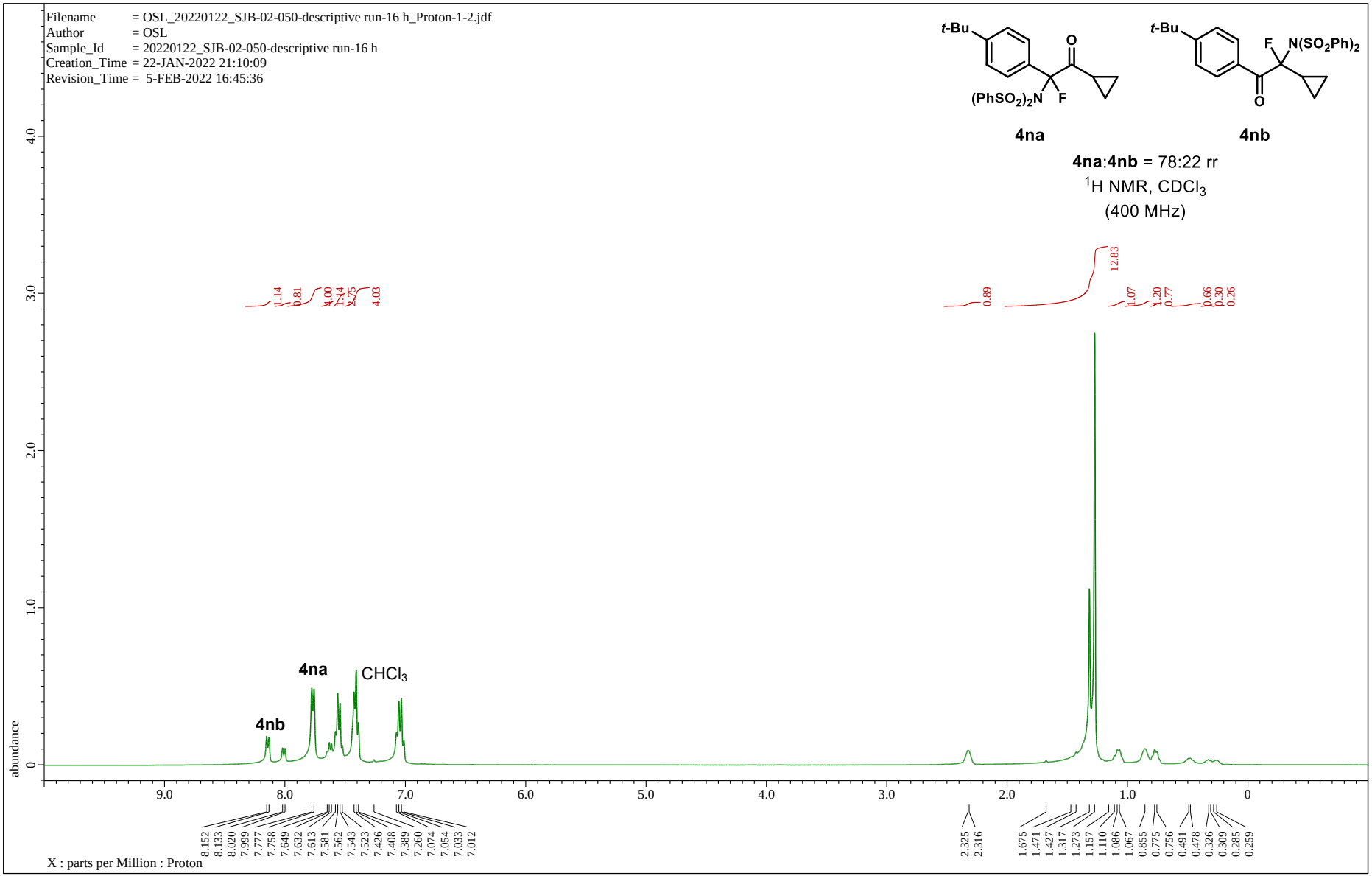

Filename = OSL_20220121_SJB-02-048-descriptive run-dry 13h_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20220121_SJB-02-048-descriptive run-dry 13h
Creation_Time = 21-JAN-2022 12:19:45
Revision_Time = 5-FEB-2022 00:01:56
(PhSO2)2N F
O
4l
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
192.198
191.893
135.286
134.056
132.140
132.092
129.756
129.127
128.812
128.688
128.564
128.126
128.030
127.649
127.506
126.695
126.600
125.732
125.694
107.378
105.052
77.554
77.230
76.915

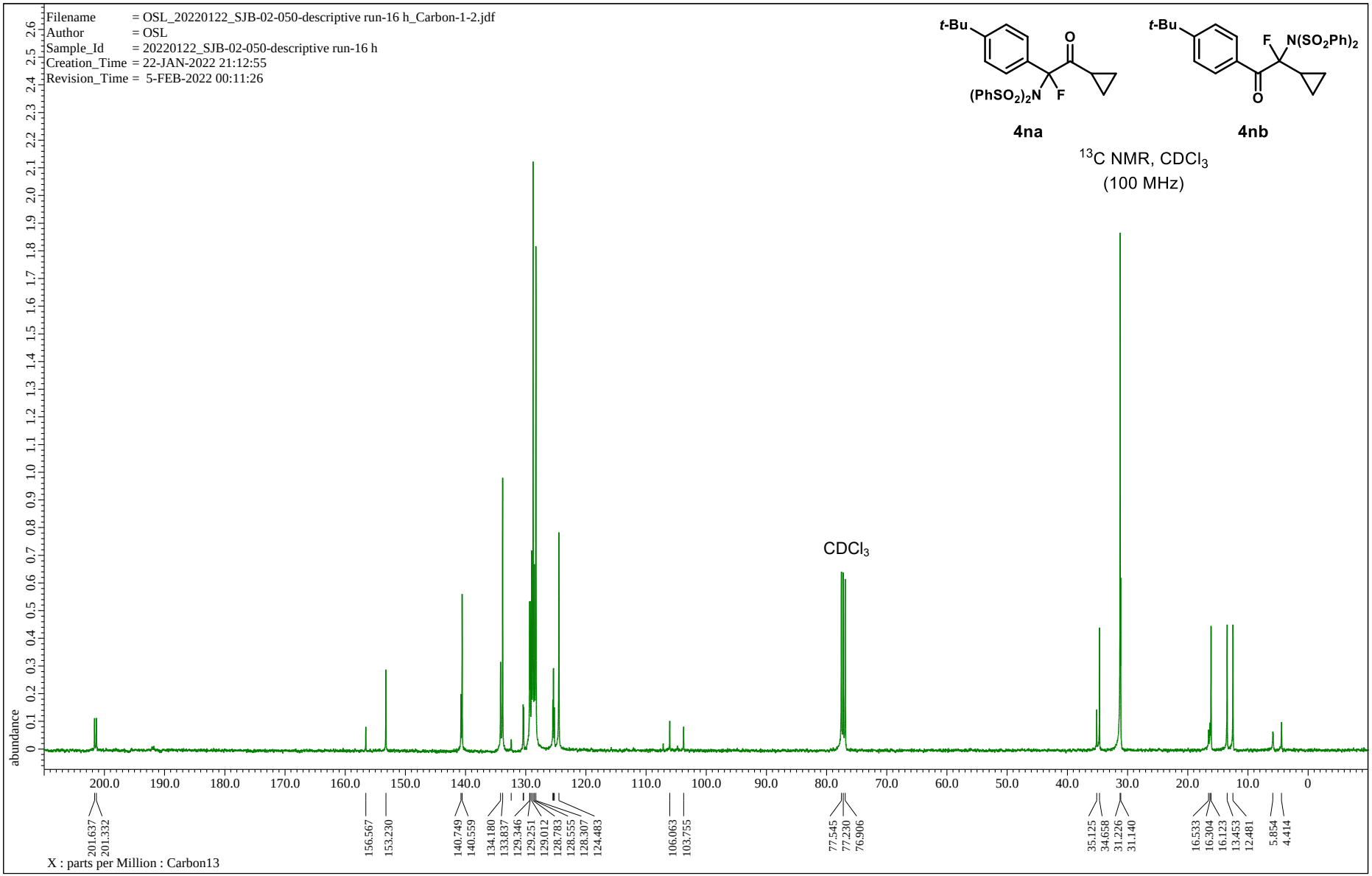

Filename = OSL_20220121_SJB-02-048-descriptive run-dry 13h_Fluorine-2-2.jdf
Author = OSL
Sample_Id = 20220121_SJB-02-048-descriptive run-dry 13h
Creation_Time = 21-JAN-2022 12:14:43
Revision_Time = 5-FEB-2022 00:00:18
(PhSO2)2N F
O
4l
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
-114.457
-164.900
X : parts per Million : Fluorine19


Filename = OSL_20211109_SJB-01-098-descriptiverun-CDCl3_Proton-1-2.jdf
Author = OSL
Sample_Id = 20211109_SJB-01-098-descriptiverun-CDCl3
Creation_Time = 9-NOV-2021 12:43:57
Revision_Time = 5-FEB-2022 00:04:38
t-Bu
O
Me
(PhSO2)2N
F
4m
1H NMR, CDCl3
(400 MHz)
8.44
4.17
1.77
3.19
3.67
3.00
CHCl3
abundance
X : parts per Million : Proton
7.763
7.745
7.600
7.581
7.562
7.442
7.423
7.403
7.260
7.089
7.068
7.041
7.020
2.233
2.222
1.423
1.267


Filename = OSL_20211109_SJB-01-098-descriptiverun-CDCl3_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20211109_SJB-01-098-descriptiverun-CDCl3
Creation_Time = 9-NOV-2021 12:49:55
Revision_Time = 5-FEB-2022 00:09:35
t-Bu
O
Me
(PhSO2)2N
F
4m
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
199.559
199.225
153.392
140.387
133.970
129.241
129.146
128.860
128.383
124.874
124.588
105.576
103.278
77.545
77.230
76.915
34.687
31.235
24.866


Filename = OSL_20211109_SJB-01-098-descriptiverun-CDCl3_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20211109_SJB-01-098-descriptiverun-CDCl3
Creation_Time = 9-NOV-2021 12:47:27
Revision_Time = 5-FEB-2022 16:38:26
t-Bu
O
Me
(PhSO2)2N
F
4m
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
-121.279
-164.900
X : parts per Million : Fluorine19


Filename = OSL_20220122_SJB-02-050-descriptive run-16 h_Proton-1-2.jdf
Author = OSL
Sample_Id = 20220122_SJB-02-050-descriptive run-16 h
Creation_Time = 22-JAN-2022 21:10:09
Revision_Time = 5-FEB-2022 16:45:36
t-Bu
O
(PhSO2)2N
F
4na
t-Bu
F
N(SO2Ph)2
O
4nb
4na:4nb = 78:22 rr
1H NMR, CDCl3
(400 MHz)
4nb
4na
CHCl3
abundance
X : parts per Million : Proton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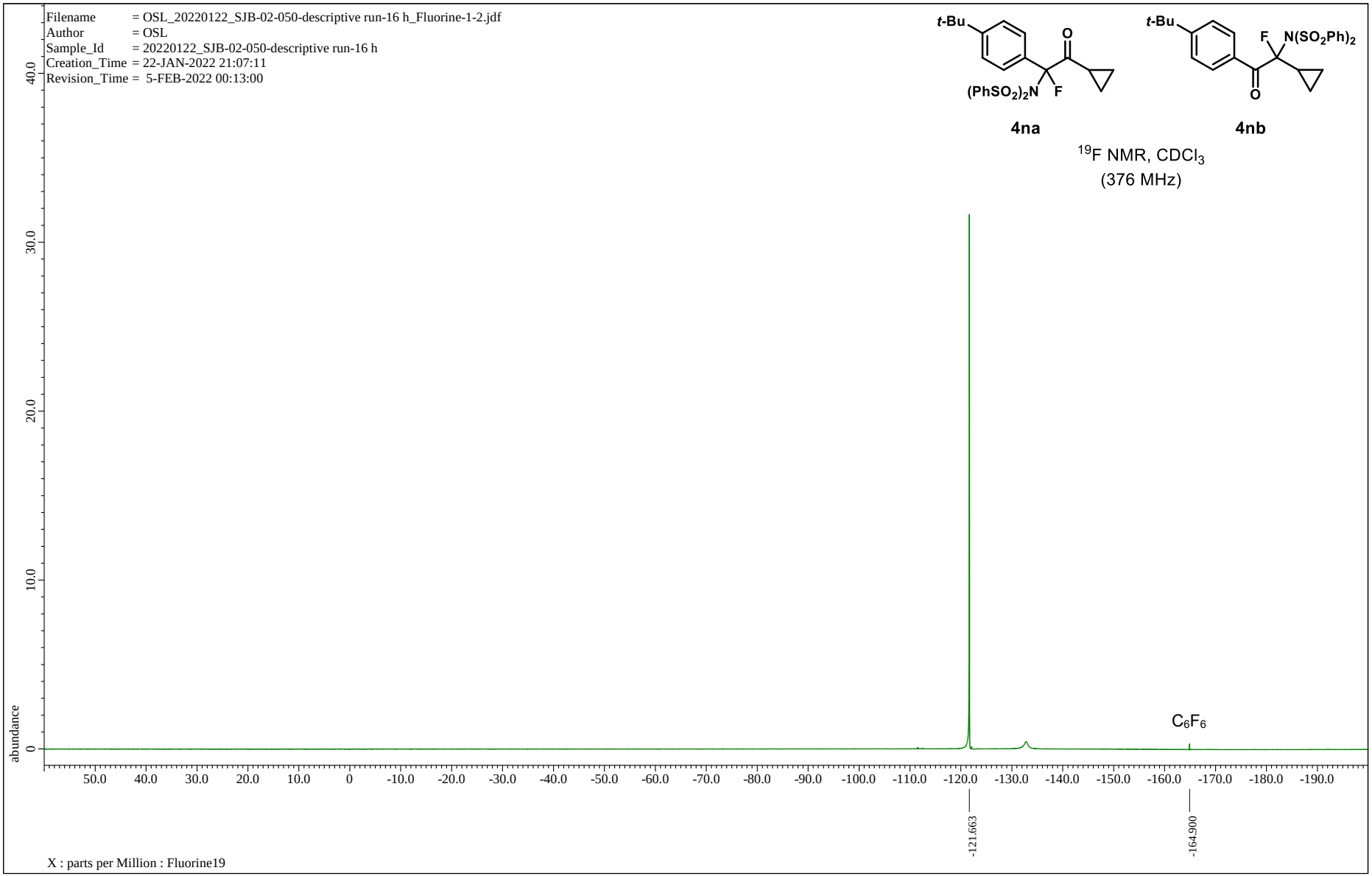
Author = OSL
Sample_Id = 20220122_SJB-02-050-descriptive run-16 h
Creation_Time = 22-JAN-2022 21:12:55
Revision_Time = 5-FEB-2022 00:11:26
t-Bu
O
(PhSO2)2N F
4na
t-Bu
F N(SO2Ph)2
O
4nb
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
201.637
201.332
156.567
153.230
140.749
140.559
134.180
133.837
129.346
129.251
129.012
128.783
128.555
128.307
124.483
106.063
103.755
77.545
77.230
76.906
35.125
34.658
31.226
31.140
16.533
16.304
16.123
13.453
12.481
5.854
4.414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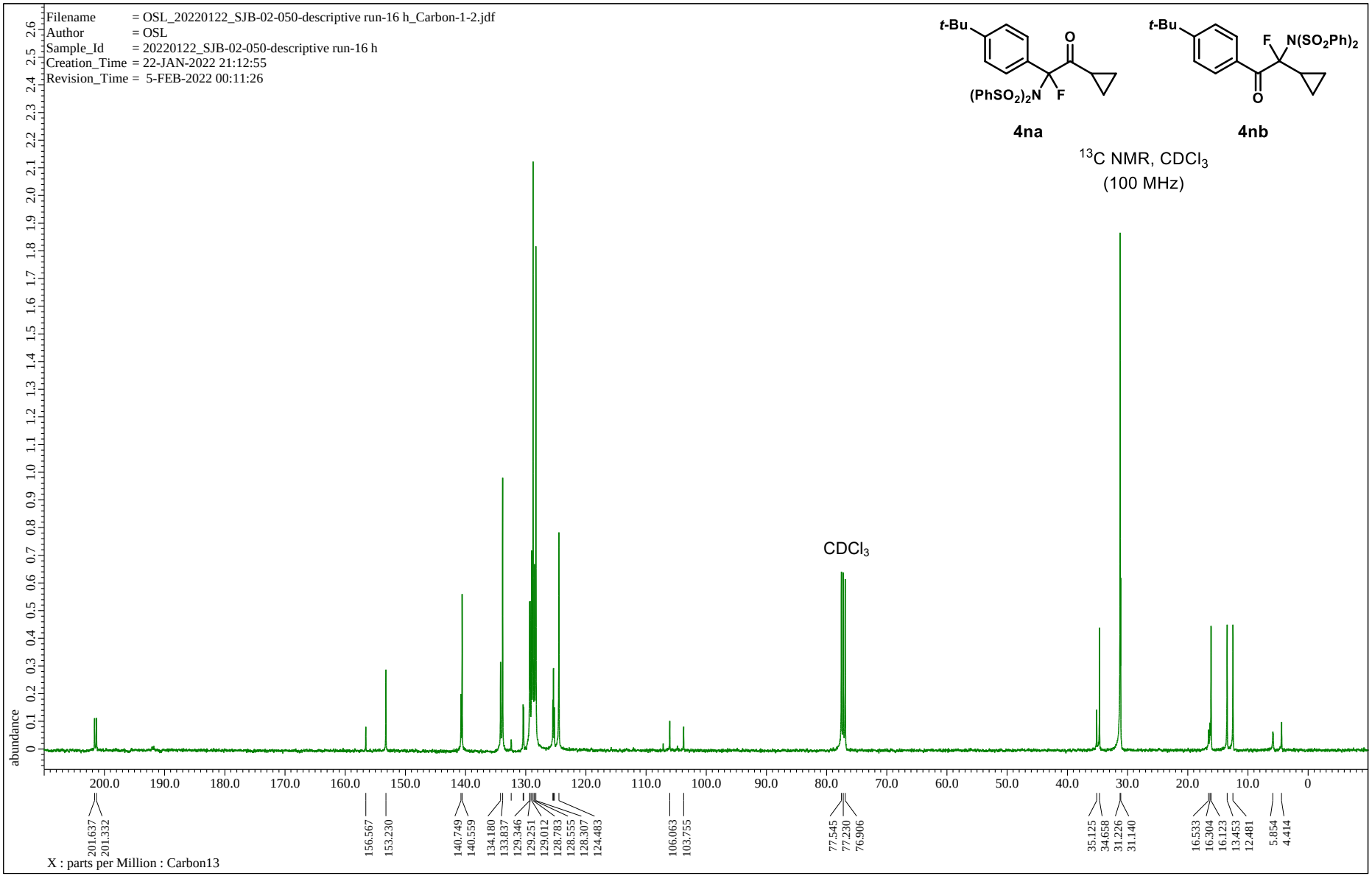
Author = OSL
Sample_Id = 20220122_SJB-02-050-descriptive run-16 h
Creation_Time = 22-JAN-2022 21:07:11
Revision_Time = 5-FEB-2022 00:13:00
t-Bu
O
(PhSO2)2N F
4na
t-Bu
F N(SO2Ph)2
O
4nb
19F NMR, CDCl3
(376 MHz)
C6F6
abundance
40.0
30.0
20.0
10.0
0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
-121.663
-164.900
X : parts per Million : Fluorine19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Author = OSL
Sample_Id = 20220122_SJB-02-050-descriptive run-16 h
Creation_Time = 22-JAN-2022 21:12:55
Revision_Time = 5-FEB-2022 00:11:26
t-Bu
O
(PhSO2)2N F
4na
t-Bu
F N(SO2Ph)2
O
4nb
13C NMR, CDCl3
(100 MHz)
CDCl3
abundance
X : parts per Million : Carbon13
201.637
201.332
156.567
153.230
140.749
140.559
134.180
133.837
129.346
129.251
129.012
128.783
128.555
128.307
124.483
106.063
103.755
77.545
77.230
76.906
35.125
34.658
31.226
31.140
16.533
16.304
16.123
13.453
12.481
5.854
4.414