Stereochemical Modulation of Ketyl Radical Cyclization Enabled by Pyridine-Boryl Radical: Catalytic Diastereoselective Synthesis of *trans*-2-Alkyl-1-Indanols

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Electronic Supplementary Information

1. General experimental

All the reactions were carried out under an atmosphere of argon using oven-dried (140 °C) or flame-dried glassware unless otherwise noted. Tetrahydrofuran (THF), diethyl ether (Et_2O), 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 argon. α,α,α-Trifluorotoluene (Acros, 99+%) was dried with CaH_2 (Alfa, 90~95%), distilled under argon, and degassed by freeze-pump-thaw. γ-Terpinene (**H4**, Aldrich, 97%) was dried with $MgSO_4$ (Daejung, 99%), distilled under reduced pressure, and degassed by freeze-pump-thaw. The following reagents were distilled from the indicated drying agents under argon or under reduced pressure: 1,4-cyclohexadiene (**H1**, Acros, 97%, $MgSO_4$), α-terpinene (**H3**, Alfa, 90+%, $MgSO_4$), Et_3SiH (Alfa, 98+%, 4 Å MS), and methyl isonicotinate (TCI, >99%, CaH_2). 9,10-Dihydroanthracene (**H2**, TCI, >98%) was recrystallized from EtOH. The following reagents were used without further purification: B_2pin_2 (**B1**, Alfa, 98+%), B_2neop_2 (**B2**, TCI, >98%), bis(hexyleneglycolato)diboron (**B3**, TCI, >98%), bis(2,4-dimethylpentane-2,4-glycolato)diboron (**B4**, Combi-Blocks, 98%), bis[(–)-pinanediolato]diboron (**B5**, Ambeed, 95%), and *p*-thiocresol (Alfa, 98%).

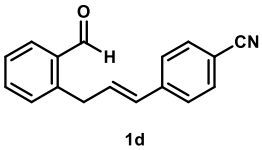
Solvents and reagents for recrystallization, work-up and chromatography were EtOH (Duksan, Extra Pure Grade), Et_2O (Samchun, Extra Pure Grade), CH_2Cl_2 (Duksan, Extra Pure Grade), EtOAc (Duksan, Extra Pure Grade), hexanes (Duksan, Extra Pure Grade), Na_2SO_4 (Duksan, 99.0%), $MgSO_4$ (Daejung, 99.0%), NaCl (Duksan, Extra Pure Grade), NH_4Cl (Daejung, Extra Pure Grade), and $NaHCO_3$ (Daejung, Extra Pure Grade). 4 Å molecular sieves (Alfa) was activated by flame-dry under reduced pressure before use. Filtration and column chromatography were performed using Merck 230–400-mesh silica gel 60 Å (0.040–0.063 mm). ^1H, ^{13}C and ^{19}F NMR spectra were recorded on a JEOL ECS400 spectrometer (400 MHz, ^1H; 100 MHz, ^{13}C; 376 MHz, ^{19}F). Chemical shifts are referenced to residual acetonitrile (1.94 ppm, ^1H), chloroform (7.26 ppm, ^1H; 77.23 ppm, ^{13}C), and hexafluorobenzene (–164.90 ppm, ^{19}F). Chemical shifts are reported in ppm, and multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and br (broad). Coupling constants, *J*, are reported in Hertz. Analytical thin-layer chromatography was conducted on Merck silica gel 60 F_{254} TLC plates and visualized with UV (254 nm) as well as *p*-anisaldehyde and potassium permanganate ($KMnO_4$) staining solutions. ESI-HRMS was performed on a Bruker Impact II quadrupole-time-of-flight (Q-TOF) spectrometer at GIST Central Research Facilities (GCRF).

2. Experimental procedures

2.1. Preparation of substrates

2.1.1. Preparation of 2-cinnmaylbenzaldehyes

1a[1] and **1b–1m**[2] were prepared following reported procedures and fully characterized in the literature except **1d** and **1e**.



1d

Column chromatographed (SiO_2, ϕ = 3.5 cm, l = 18 cm, EtOAc:hexanes = 1:20→1:7) to afford **1d** (R_f = 0.41 in EtOAc:hexanes = 1:5, off-white solid, 726 mg, 57%).

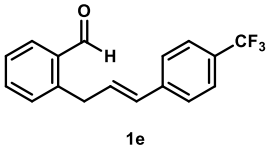
Data for **1d**:

^1H NMR: (400 MHz, $CDCl_3$) δ 10.23 (s, 1H), 7.87–7.85 (m, 1H), 7.59–7.54 (m, 3H), 7.48–7.45 (m, 1H), 7.40–7.38 (m, 2H), 7.36–7.34 (m, 1H), 6.55 (dt, J = 15.9, 6.4, 1H), 6.39 (d, J = 15.9, 1H), 4.02 (d, J = 6.4, 1H).

$^{13}C\{^1H\}$ NMR: (100 MHz, $CDCl_3$) δ 192.8, 141.9, 141.4, 134.2, 133.9, 133.5, 133.1, 132.4, 131.4, 130.0, 127.4, 126.7,

119.1, 110.5, 36.2.

HRMS (ESI): $[M+Na]^+$ calcd for $C_{17}H_{13}NNaO$: 270.0889; found: 270.0892.



1e

Column chromatographed (SiO_2, ϕ = 4.5 cm, l = 16 cm, EtOAc:hexanes = 1:20) to afford **1e** (R_f = 0.19 in EtOAc:hexanes = 1:20, off-white solid, 2.15 g, 61%).

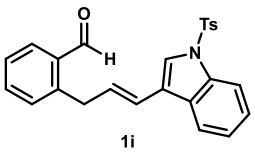
Data for **1e**:

^{1}H NMR: (400 MHz, $CDCl_3$) δ 10.26 (s, 1H), 7.87–7.86 (m, 1H), 7.59–7.51 (m, 3H), 7.47–7.43 (m, 1H), 7.42–7.40 (m, 2H), 7.37–7.35 (m, 1H), 6.51 (dt, J = 15.9, 6.4, 1H), 6.41 (d, J = 15.9, 1H), 4.02 (d, J = 6.4, 2H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 192.6, 141.8, 140.9, 134.1, 133.9, 133.0, 131.7, 131.3, 130.2, 129.0 (q, J = 32.4), 127.3, 126.4, 125.5 (q, J = 3.9), 124.4 (q, J = 271.7), 36.1.

^{19}F NMR: (376 MHz, $CDCl_3$) δ –65.7.

HRMS (ESI): $[M+H]^+$ calcd for $C_{17}H_{14}F_3O$: 291.0991; found: 291.0968.



1i

Column chromatographed (SiO_2, ϕ = 3.5 cm, l = 16 cm, EtOAc:hexanes = 1:10→1:3) to afford **1i** (R_f = 0.19 in EtOAc:hexanes = 1:10, off-white solid, 3.56 g, 57%).

Data for **1i**:

^{1}H NMR: (400 MHz, $CDCl_3$) δ 10.30 (s, 1H), 7.97–7.95 (m, 1H), 7.89–7.87 (m, 1H), 7.78–7.76 (m, 2H), 7.71–7.69 (m, 1H), 7.63–7.59 (m, 2H), 7.48–7.43 (m, 2H), 7.37–7.32 (m, 1H), 7.30–7.25 (m, 3H), 6.56–6.48 (m, 2H), 4.01 (d, J = 5.8, 2H), 2.31 (s, 3H).

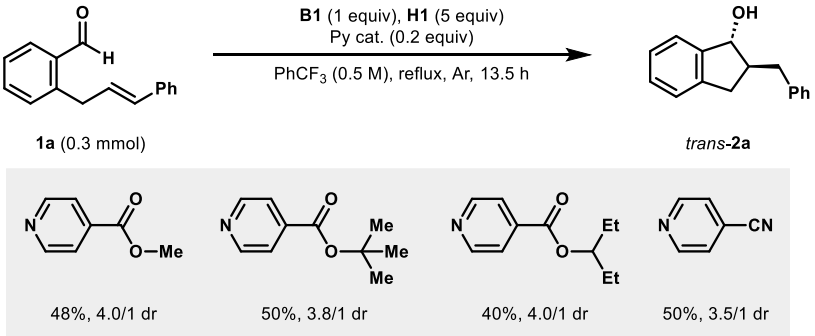
^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 192.6, 145.0, 142.2, 135.5, 135.1, 134.2, 133.9, 132.6, 131.2, 130.3, 129.9, 129.1, 127.1, 126.8, 124.9, 123.5, 123.4, 122.1, 120.6, 120.5, 113.8, 36.4, 21.6.

HRMS (ESI): $[M+Na]^+$ calcd for $C_{25}H_{21}NNaO_3S$: 438.1134; found: 438.1131.

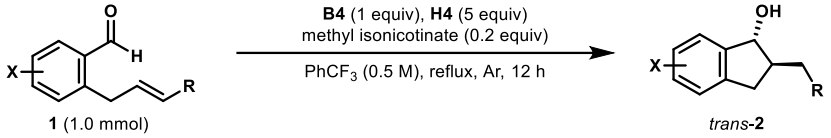
2.1.2. Preparation of other 2-allylic benzaldehydes

1n[3,4] and **1o**[5,6] were prepared following reported procedures and fully characterized in the literature.

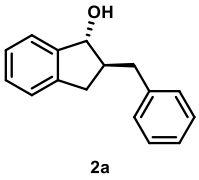
2.2. Pyridine catalyst survey



2.3. Pyridine-boryl radical-promoted cyclization of 2-allylic benzaldehydes



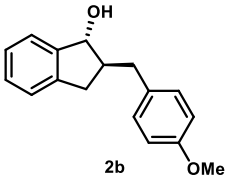
To a solution of aldehyde (**1**, 1.00 mmol), **B4** (282 mg, 1.00 mmol), and **H4** (0.80 mL, 5.0 mmol) in $PhCF_3$ (2 mL) was added methyl isonicotinate (24 μL, 0.20 mmol) at room temperature under argon, and the mixture was refluxed for 12 hours. The reaction mixture was cooled to room temperature, transferred to a round-bottomed flask with CH_2Cl_2, and stirred in the presence of 2 M aq. Na_2CO_3 (2 mL) under air for 5 minutes. The mixture was poured into water (20 mL) and extracted with CH_2Cl_2 (20 mL) four times. The combined organic layers were dried over Na_2SO_4 (6 g), filtered, and concentrated under reduced pressure. The crude material was adsorbed to silica gel and purified by column chromatography to afford the 2-alkyl-1-indanol (**2**). The diastereomeric ratio was measured by ^{1}H NMR analysis of **2** on the basis of the integral value of the proton at the hydroxyl-bearing carbon. The copies of ^{1}H NMR spectra are attached at the end of the ESI.



Column chromatographed (1st: SiO_2, ϕ = 3 cm, l = 16 cm, EtOAc:hexanes = 1:6, 2nd: ϕ = 3 cm, l = 14 cm, acetone:hexanes = 1:10) to afford **2a** (R_f = 0.28 in EtOAc:hexanes = 1:6, white solid, 120 mg, 54%, >20/1 *dr*).

Data for **2a**:[7]

^{1}H NMR: (400 MHz, CD_3CN) δ 7.32–7.15 (m, 9H), 4.83–4.80 (m, 1H), 3.40–3.36 (m, 1H), 3.11 (dd, J = 13.4, 5.2, 1H), 2.86 (dd, J = 15.3, 7.6, 1H), 2.69 (dd, J = 13.3, 9.6, 1H), 2.55–2.40 (m, 2H).



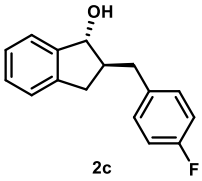
Column chromatographed (1st: SiO_2, ϕ = 3.5 cm, l = 16 cm, EtOAc:hexanes = 1:4, 2nd: ϕ = 2.5 cm, l = 16 cm, Et_2O:hexanes = 1:5→1:10) to afford **2b** (R_f = 0.34 in EtOAc:hexanes = 1:3, white solid, 146 mg, 54%, 15.7/1 *dr*).

Data for **2b**:

^{1}H NMR: (400 MHz, $CDCl_3$) δ 7.38–7.36 (m, 1H), 7.24–7.21 (m, 2H), 7.19–7.17 (m, 3H), 6.89–6.86 (m, 2H), 4.94 (d, J = 6.7, 1H), 3.81 (s, 3H), 3.04–2.98 (m, 2H), 2.75 (dd, J = 13.7,8.5, 1H), 2.60–2.45 (m, 2H).

$^{13}C\{^1H\}$ NMR: (100 MHz, $CDCl_3$) δ 158.2, 144.7, 141.8, 132.8, 130.0, 128.3, 126.9, 125.0, 124.1, 114.2, 81.0, 55.5, 52.6, 38.5, 35.9.

HRMS (ESI): $[M+H]^+$ calcd for $C_{17}H_{19}O_2$: 255.1380; found: 255.1369.



Column chromatographed (1st: SiO_2, ϕ = 3 cm, l = 14 cm, EtOAc:hexanes = 1:5, 2nd: acetone:hexanes = 1:10) to afford **2c** (R_f = 0.25 in EtOAc:hexanes = 1:5, white solid, 136 mg, 56%, >20/1 *dr*).

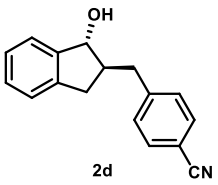
Data for **2c**:

^{1}H NMR: (400 MHz, CD_3CN) δ 7.33–7.26 (m, 3H), 7.21–7.14 (m, 3H), 7.08–7.03 (m, 2H), 4.82–4.78 (m, 1H), 3.39 (dd, *J* = 6.4, 4.3, 1H), 3.09 (dd, *J* = 13.7, 5.2, 1H), 2.86 (dd, *J* = 15.6, 7.6, 1H), 2.69 (dd, *J* = 13.6, 9.6, 1H), 2.50 (dd, *J* = 15.4, 8.7, 1H), 2.44–2.39 (m, 1H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 161.5 (d, *J* = 243.9), 144.6, 141.5, 136.4 (d, *J* = 3.5), 130.3 (d, *J* = 6.9), 128.3, 126.9, 124.9, 124.1, 115.3 (d, *J* = 20.8), 80.6, 52.1, 38.4, 35.6.

^{19}F NMR: (376 MHz, $CDCl_3$) δ –120.3.

HRMS (ESI): $[M+Na]^+$ calcd for $C_{16}H_{15}FNaO$: 265.0999; found: 265.0991.



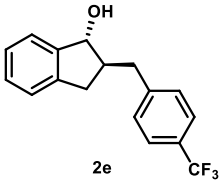
Column chromatographed (1st: SiO_2, ϕ = 2.5 cm, *l* = 16 cm, EtOAc:hexanes = 1:4→1:2, 2nd: SiO_2, ϕ = 2.5 cm, *l* = 14 cm, CH_2Cl_2) to afford **2d** (R_f = 0.11 in EtOAc:hexanes = 1:5, off-white solid, 153 mg, 61%, >20/1 *dr*).

Data for **2d**:

^{1}H NMR: (400 MHz, CD_3CN) δ 7.68–7.65 (m, 2H), 7.46–7.44 (m, 2H), 7.31–7.30 (m, 1H), 7.22–7.15 (m, 3H), 4.81–4.80 (m, 1H), 3.49 (brs, 1H), 3.18 (dd, *J* = 13.4, 5.2, 1H), 2.88–2.77 (m, 2H), 2.54–2.40 (m, 2H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 146.6, 144.4, 141.1, 132.4, 129.8, 128.5, 127.1, 124.9, 124.1, 119.1, 110.0, 80.7, 51.7, 39.4, 35.6.

HRMS (ESI): $[M+Na]^+$ calcd for $C_{17}H_{15}NNaO$: 272.1046; found: 272.1048.



Column chromatographed (SiO_2, ϕ = 3 cm, *l* = 14 cm, EtOAc:hexanes = 1:5) to afford **2e** (R_f = 0.19 in EtOAc:hexanes = 1:5, white solid, 182 mg, 62%, >20/1 *dr*).

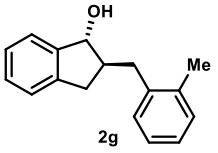
Data for **2e**:

^{1}H NMR: (400 MHz, CD_3CN) δ 7.64–7.62 (m, 2H), 7.48–7.46 (m, 2H), 7.33–7.31 (m, 1H), 7.23–7.19 (m, 2H), 7.18–7.15 (m, 1H), 4.84–4.81 (m, 1H), 3.43 (d, *J* = 6.7, 1H), 3.19 (dd, *J* = 13.4, 5.2, 1H), 2.89–2.78 (m, 2H), 2.52 (dd, *J* = 15.3, 8.9, 1H), 2.48–2.42 (m, 1H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 145.0, 144.6, 141.5, 129.4, 128.9 (q, *J* = 32.4), 128.6, 127.2, 125.7 (q, *J* = 3.8), 125.1, 124.6 (q, *J* = 271.8), 124.2, 81.0, 52.0, 39.3, 35.8.

^{19}F NMR: (376 MHz, $CDCl_3$) δ –65.5.

HRMS (ESI): $[M+Na]^+$ calcd for $C_{17}H_{15}F_3NaO$: 315.0967; found: 315.0947.



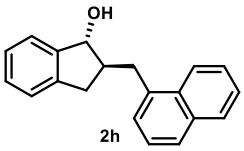
Column chromatographed (1st: SiO_2, ϕ = 3.5 cm, *l* = 20 cm, EtOAc:hexanes = 1:5, 2nd: ϕ = 2.5 cm, *l* = 12 cm, Et_2O:hexanes = 1:5→1:2) to afford **2g** (R_f = 0.15 in EtOAc:hexanes = 1:5, white solid, 135 mg, 57%, >20/1 *dr*).

Data for **2g**:

^{1}H NMR: (400 MHz, $CDCl_3$) δ 7.39–7.37 (m, 1H), 7.25–7.22 (m, 3H), 7.19–7.14 (m, 4H), 4.97 (d, *J* = 6.7, 1H), 3.09 (dd, *J* = 13.7, 6.4, 1H), 3.03 (dd, *J* = 15.4, 7.3, 1H), 2.81 (dd, *J* = 13.7, 8.5, 1H), 2.63–2.51 (m, 2H), 2.36 (s, 3H).

$^{13}C\{^1H\}$ NMR: (100 MHz, $CDCl_3$) δ 144.7, 141.8, 139.0, 136.4, 130.7, 129.6, 128.3, 127.0, 126.5, 126.2, 124.9, 124.1, 81.2, 51.1, 36.7, 36.1, 19.7.

HRMS (ESI): $[M+H]^+$ calcd for $C_{17}H_{19}O$: 239.1430; found: 239.1432.



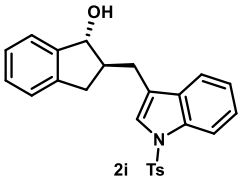
Column chromatographed (1st: SiO_2, ϕ = 2.5 cm, *l* = 16 cm, EtOAc:hexanes = 1:6, 2nd: ϕ = 2.5 cm, *l* = 13 cm, Et_2O:hexanes = 1:4→1:3) to afford **2h** (R_f = 0.28 in EtOAc:hexanes = 1:6, white solid, 142 mg, 52%, 5.3/1 *dr*).

Data for **2h**:

^{1}H NMR: (400 MHz, $CDCl_3$) δ 8.21–8.17 (m, 1H), 7.92–7.90 (m, 1H), 7.81–7.77 (m, 1H), 7.58–7.49 (m, 2H), 7.47–7.45 (m, 2H), 7.38–7.33 (m, 1H), 7.23–7.12 (m, 3H), 4.95–4.92 (m, 1H), 3.64 (dd, *J* = 13.9, 4.7, 1H), 3.46 (d, *J* = 6.7, 1H), 3.12 (dd, *J* = 13.4, 8.9, 1H), 2.84–2.76 (m, 1H), 2.67–2.56 (m, 1H).

$^{13}C\{^1H\}$ NMR: (100 MHz, $CDCl_3$) δ 144.7, 141.6, 136.9, 134.1, 132.1, 129.0, 128.3, 127.2, 126.9, 126.7, 126.1, 125.8, 125.6, 124.9, 124.1, 124.0, 81.2, 51.5, 36.4, 36.1.

HRMS (ESI): $[M+H]^+$ calcd for $C_{20}H_{19}O$: 275.1430; found: 275.1422.



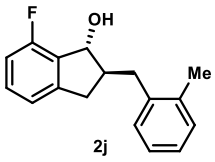
Column chromatographed (1st: SiO_2, ϕ = 2.5 cm, *l* = 16 cm, EtOAc:hexanes = 1:4, 2nd: ϕ = 2.5 cm, *l* = 8 cm, CH_2Cl_2) to afford **2i** (R_f = 0.19 in EtOAc:hexanes = 1:4, off-white solid, 160 mg, 38%, 7.4/1 *dr*).

Data for **2i**:

^{1}H NMR: (400 MHz, CD_3CN) δ 7.98–7.95 (m, 1H), 7.80–7.74 (m, 2H), 7.60–7.56 (m, 1H), 7.53–7.52 (m, 1H), 7.38–7.15 (m, 8H), 4.84–4.79 (m, 1H), 3.43 (d, *J* = 6.7, 1H), 3.12–3.05 (m, 1H), 2.91–2.79 (m, 2H), 2.55–2.45 (m, 2H), 2.31 (s, 3H).

$^{13}C\{^1H\}$ NMR: (100 MHz, $CDCl_3$) δ 145.0, 144.5, 141.5, 135.5, 135.3, 131.3, 130.0, 128.4, 127.0, 126.9, 125.0, 124.9, 124.1, 123.6, 123.3, 121.9, 119.7, 114.0, 81.1, 50.2, 36.1, 28.2, 21.7.

HRMS (ESI): $[M+Na]^+$ calcd for $C_{25}H_{23}NNaO_3S$: 440.1291; found: 440.1295.



Column chromatographed (1st: SiO_2, ϕ = 3.5 cm, *l* = 16 cm, EtOAc:hexanes = 1:8, 2nd: ϕ = 2.5 cm, *l* = 13 cm, Et_2O:hexanes = 1:4→1:3) to afford **2j** (R_f = 0.25 in EtOAc:hexanes = 1:8, white solid, 116 mg, 45%, >20/1 *dr*).

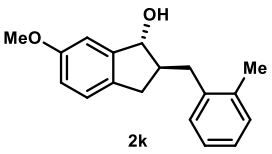
Data for **2j**:

^{1}H NMR: (400 MHz, CD_3CN) δ 7.28–7.13 (m, 5H), 7.04–7.02 (m, 1H), 6.93–6.89 (m, 1H), 5.06–5.03 (m, 1H), 3.41 (dd, *J* = 6.1, 1.8, 1H), 3.05 (dd, *J* = 17.6, 8.7, 1H), 2.93 (dd, *J* = 12.7, 4.7, 1H), 2.64–2.53 (m, 3H), 2.30 (s, 3H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 160.2 (d, *J* = 248.5), 146.0 (d, *J* = 5.8), 138.6, 136.4, 130.54, 130.47, 130.3 (d, *J* = 15.0), 129.5, 126.4, 126.1, 120.9 (d, *J* = 3.5), 113.6 (d, *J* = 20.8), 78.4, 49.3, 36.4, 36.3, 19.6.

^{19}F NMR: (376 MHz, $CDCl_3$) δ –124.2.

HRMS (ESI): $[M+H]^+$ calcd for $C_{17}H_{18}FO$: 257.1336; found: 257.1311.



2k

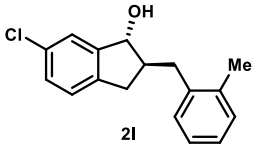
Column chromatographed (1st: SiO_2, ϕ = 3.5 cm, *l* = 16 cm, EtOAc:hexanes = 1:5, 2nd: ϕ = 2.5 cm, *l* = 12 cm, Et_2O:hexanes = 1:4→1:3→1:2) to afford **2k** (R_f = 0.22 in EtOAc:hexanes = 1:5, white solid, 174 mg, 65%, 12.5/1 *dr*).

Data for **2k**:

^{1}H NMR: (400 MHz, $CDCl_3$) δ 7.23–7.14 (m, 4H), 7.08–7.06 (m, 1H), 6.93–6.91 (m, 1H), 6.80–6.78 (m, 1H), 4.94–4.92 (m, 1H), 3.80 (s, 3H), 3.08 (dd, *J* = 13.7, 5.8, 1H), 2.96 (dd, *J* = 18.2, 10.8, 1H), 2.82 (dd, *J* = 13.6, 8.1, 1H), 2.56–2.50 (m, 2H), 2.36 (s, 3H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 159.3, 146.1, 139.0, 136.4, 133.5, 130.7, 129.6, 126.5, 126.2, 125.6, 114.9, 108.8, 81.3, 55.7, 51.7, 36.8, 35.3, 19.7.

HRMS (ESI): $[M+Na]^+$ calcd for $C_{18}H_{20}NaO_2$: 291.1356; found: 291.1339.



2l

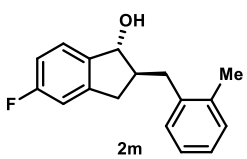
Column chromatographed (1st: SiO_2, ϕ = 3.5 cm, *l* = 16 cm, EtOAc:hexanes = 1:5, 2nd: ϕ = 3.5 cm, *l* = 16 cm, Et_2O:hexanes = 1:6→1:4) to afford **2l** (R_f = 0.31 in EtOAc:hexanes = 1:5, white solid, 155 mg, 57%, >20/1 *dr*).

Data for **2l**:

^{1}H NMR: (400 MHz, $CDCl_3$) δ 7.35–7.33 (m, 1H), 7.22–7.15 (m, 5H), 7.10–7.08 (m, 1H), 4.94–4.93 (m, 1H), 3.07 (dd, *J* = 13.9, 6.0, 1H), 2.98 (dd, *J* = 19.1, 10.8, 1H), 2.82 (dd, *J* = 13.9, 8.1, 1H), 2.59–2.51 (m, 2H), 2.36 (s, 3H), 1.64 (br, 1H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 146.6, 140.0, 138.7, 136.4, 132.7, 130.8, 129.5, 128.5, 126.7, 126.3, 126.1, 124.4, 80.8, 51.5, 36.6, 35.6, 19.7.

HRMS (ESI): $[M+Na]^+$ calcd for $C_{17}H_{17}{}^{35}ClNaO$, $C_{17}H_{17}{}^{37}ClNaO$: 295.0860, 297.0836; found: 295.0843, 297.0814.



2m

Column chromatographed (1st: SiO_2, ϕ = 3.5 cm, *l* = 16 cm, EtOAc:hexanes = 1:7→1:5, 2nd: ϕ = 2.5 cm, *l* = 14 cm, acetone:hexanes = 1:10) to afford **2m** (R_f = 0.25 in EtOAc:hexanes = 1:7, white solid, 150 mg, 59%, 16.8/1 *dr*).

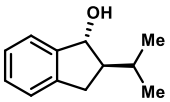
Data for **2m**:

^{1}H NMR: (400 MHz, CD_3CN) δ 7.32–7.28 (m, 1H), 7.22–7.12 (m, 4H), 6.96–6.89 (m, 2H), 4.81–4.77 (m, 1H), 3.41 (dd, *J* = 6.4, 1.8, 1H), 3.11 (dd, *J* = 13.7, 5.2, 1H), 2.86 (dd, *J* = 15.7, 7.5, 1H), 2.68 (dd, *J* = 13.7, 9.5, 1H), 2.57–2.43 (m, 2H), 2.33 (s, 3H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 163.2 (d, *J* = 245.1), 144.1 (d, *J* = 8.1), 140.2, 138.7, 136.3, 130.7, 129.5, 126.6, 126.2, 125.4 (d, *J* = 8.1), 114.0 (d, *J* = 23.1), 111.9 (d, *J* = 22.0), 80.3, 51.3, 36.6, 36.0, 19.6.

^{19}F NMR: (376 MHz, $CDCl_3$) δ –117.8.

HRMS (ESI): $[M+H]^+$ calcd for $C_{17}H_{18}FO$: 257.1336; found: 257.1309.



2n

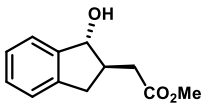
Column chromatographed (1st: SiO_2, ϕ = 3.5 cm, *l* = 17 cm, EtOAc:hexanes = 1:10, 2nd: ϕ = 2.5 cm, *l* = 16 cm, acetone:hexanes = 1:15) to afford **2n** (R_f = 0.19 in EtOAc:hexanes = 1:8, white solid, 55 mg, 31%, 2.9/1 *dr*).

Data for **2n**:

^{1}H NMR:[8] (400 MHz, CD_3CN) δ 7.35–7.18 (m, 5H), 4.88–4.85 (m, 1H), 3.26 (d, *J* = 7.3, 1H), 2.99 (dd, *J* = 15.7, 8.4, 1H), 2.54 (dd, *J* = 15.7, 9.0, 1H), 1.89–1.81 (m, 1H), 1.07 (d, *J* = 6.7, 3H), 0.97 (d, *J* = 6.7, 3H).

^{13}C{^{1}H} NMR: (100 MHz, $CDCl_3$) δ 145.5, 141.8, 128.1, 126.8, 124.8, 124.1, 79.9, 57.7, 34.0, 31.5, 21.7, 20.8.

HRMS (ESI): $[M+H]^+$ calcd for $C_{12}H_{17}O$: 177.1274; found: 177.1260.



2o

Column chromatographed (1st: SiO_2, ϕ = 2.5 cm, *l* = 18 cm, EtOAc:hexanes = 1:4, 2nd: SiO_2, ϕ = 2.5 cm, *l* = 16 cm, acetone:hexanes = 1:10→1:5, 3rd: SiO_2, ϕ = 2.5 cm, *l* = 14 cm, EtOAc:hexanes = 1:3) to afford **2o** (R_f = 0.19 in EtOAc:hexanes = 1:3, white solid, 90 mg, 44%, >20/1 *dr*).

Data for **2o**:[5]

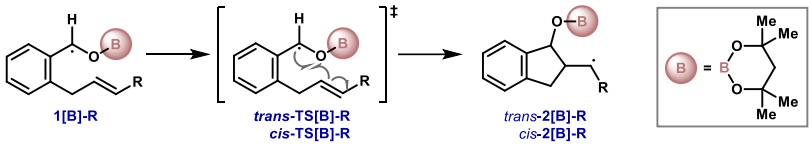
^{1}H NMR: (400 MHz, CD_3CN) δ 7.32–7.30 (m, 1H), 7.23–7.20 (m, 3H), 4.81–4.78 (m, 1H), 3.66 (s, 3H), 3.61 (d, *J* = 6.1, 1H), 3.12 (dd, *J* = 15.3, 7.3, 1H), 2.73 (dd, *J* = 15.3, 5.5, 1H), 2.56–2.41 (m, 3H).

3. DFT calculation

3.1. Method

The transition structures were obtained at the UM06-2X[9]/6-31++G(d,p) level of theory using the Gaussian 16 suite of programs.[10] To account for the solvent effect, the polarizable continuum model (PCM) was employed with the default parameters for 1,2-DCE.[11,12] For thermal energy correction, the calculations were conducted at 375.15 K. The optimized saddle points were validated by the presence of a single negative vibrational frequency and the intrinsic reaction coordinate (IRC) calculation at the same level of theory. The NCI plot analysis[13] was performed using the Multiwfn software[14] and visualized by VMD[15].

3.2. Computational data (Figure 2)



3.2.1. 2-Allylbenzaldehyde

- computed data for **1[B]-H**

: total free energy = –912.239933 Hartree

: relative free energy = 0.00 kcal/mol

: no imaginary frequency

: Cartesian coordinates

Atom	X	Y	Z
B	1.16902800	-0.60125200	0.03173900
O	-0.14843100	-1.03300200	0.04152800
C	-1.17151000	-0.17134400	-0.17126700
C	-2.98431600	2.47408300	0.59880500
C	-2.49617600	-0.65331800	-0.11268300
O	2.10324300	-1.54081200	0.34080000
O	1.44181900	0.69362000	-0.28144600
C	3.49012400	-1.19972500	0.13433900
C	4.29748300	-2.11788300	1.04314200
C	2.74324600	1.28760500	-0.07221800
C	2.52835800	2.45362100	0.88970700
C	-2.75661100	-2.02096500	0.17118700
C	-3.60377200	0.22171400	-0.34327600
C	-4.89208600	-0.29484500	-0.28027900
C	-5.13561900	-1.64405900	0.00289300
C	-4.05492500	-2.50255400	0.22817400
H	-4.22994800	-3.55157900	0.44741400
H	-1.91626300	-2.68486200	0.34319200
H	-5.73108600	0.37329800	-0.46013700
H	-6.15379200	-2.01671100	0.04355500
H	-0.90873000	0.85949400	-0.36488900
C	-3.39282300	1.69399500	-0.62730600
C	-1.91173200	3.26144800	0.67588100
H	-2.64550100	1.83830200	-1.41740700
H	-4.33672700	2.10443200	-1.00500800
H	1.86276700	3.19570100	0.43962600
H	3.48412200	2.93349400	1.12108400
H	2.08020600	2.09823300	1.82191600
H	4.03195900	-1.95042100	2.09041600
H	5.36778800	-1.93098800	0.91627800
H	4.09275300	-3.16227200	0.79216300
C	3.22805600	1.82313200	-1.41719900
C	3.82563600	-1.48427400	-1.33009000

H	2.47994200	2.50845300	-1.82551400
H	3.40101600	1.02868200	-2.14355600
H	4.16331800	2.37339200	-1.27901900
H	3.77078100	-2.56120900	-1.51191200
H	4.83521800	-1.13910700	-1.57198600
H	3.11745000	-0.99596900	-2.00356000
C	3.69818500	0.26051200	0.56242300
H	4.73248100	0.55815600	0.36033600
H	3.56151300	0.29022200	1.65051800
H	-3.63770200	2.36647400	1.46488100
H	-1.23758100	3.38239600	-0.17030500
H	-1.67128800	3.80735800	1.58275300

- computed data for ***trans*-TS[B]-H**

: total free energy = –912.209780 Hartree

: relative free energy = 18.92 kcal/mol

: a single imaginary frequency at –539.06 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
B	-1.00868900	-0.46814000	-0.15884600
O	0.33631600	-0.75061200	-0.32593300
C	1.29311900	0.08549900	0.16891400
C	1.85839000	1.69064300	-1.16757200
C	2.65715100	-0.44373800	0.24112200
O	-1.87294700	-1.24379000	-0.87226600
O	-1.38529000	0.51644800	0.70209000
C	-3.27547900	-1.15453400	-0.54882600
C	-4.03232500	-1.63928400	-1.77896900
C	-2.73347300	1.03164800	0.75716300
C	-2.63776800	2.51734400	0.41875400
C	2.99868500	-1.78199200	0.45391400
C	3.65771200	0.52192400	0.03582600
C	4.99688200	0.15472400	0.10719200
C	5.34113800	-1.17759700	0.35829200
C	4.34522000	-2.14309000	0.51766200
H	4.61848400	-3.17948400	0.69064700
H	2.21680300	-2.52505200	0.58071000
H	5.77330700	0.89601000	-0.06399100
H	6.38683100	-1.46560300	0.40359700
H	0.95700700	0.76727000	0.94798900
C	3.13074000	1.88265700	-0.35196300
C	0.86339700	2.62669800	-1.23516800
H	2.89810700	2.48939900	0.53489600
H	3.88020400	2.43571900	-0.92915500
H	-2.01191500	3.03118100	1.15430200
H	-3.63326700	2.97179100	0.42423000
H	-2.19507900	2.65169300	-0.57210400
H	-3.81314000	-1.00132400	-2.63945300

H	-5.11001500	-1.62147500	-1.59217900
H	-3.73574000	-2.66431300	-2.01793500
C	-3.23049600	0.87116000	2.19214500
C	-3.54219100	-2.08890400	0.63193500
H	-2.53004200	1.36005800	2.87509200
H	-3.32490400	-0.17474900	2.48525000
H	-4.20891300	1.34856100	2.29900800
H	-3.39279100	-3.12494200	0.31531300
H	-4.56921600	-1.97753800	0.99214900
H	-2.85700600	-1.89068300	1.45951300
C	-3.61719300	0.31872900	-0.28241600
H	-4.66723900	0.40407200	0.01688400
H	-3.51196700	0.84220600	-1.24092500
H	1.95242200	0.99062400	-1.99998000
H	0.78496100	3.42096000	-0.49690500
H	0.07085100	2.54862400	-1.97187000

- computed data for ***cis*-TS[B]-H**

: total free energy = –912.209019 Hartree

: relative free energy = 19.40 kcal/mol

: a single imaginary frequency at –547.18 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
B	0.89024700	0.13390000	-0.39843400
O	-0.47145000	0.08341000	-0.63771100
C	-1.34102300	0.63538000	0.26473500
C	-1.51906700	-0.95397600	1.76593200
C	-2.76529100	0.54938100	-0.12437700
O	1.66728100	-0.62945800	-1.21829700
O	1.37217100	0.95827400	0.57676900
C	3.05189100	-0.90515600	-0.92570400
C	3.16424100	-2.42197100	-0.78266400
C	2.79958000	1.11731100	0.69551700
C	3.06785400	1.50782300	2.14388700
C	-3.47024600	1.58324600	-0.74598900
C	-3.40796500	-0.65758300	0.18483800
C	-4.74812400	-0.83381900	-0.15451000
C	-5.44665600	0.19325900	-0.79217900
C	-4.81262800	1.40259500	-1.08165400
H	-5.36314300	2.20336400	-1.56537300
H	-2.96911000	2.52087400	-0.97072600
H	-5.25249000	-1.76405900	0.09403200
H	-6.49238200	0.05554500	-1.04963600
H	-0.97043900	1.51259100	0.79174400
C	-2.56441500	-1.66534300	0.92512200
C	-0.27854200	-1.48605800	1.98040000
H	-3.19816800	-2.29364300	1.56154400
H	-2.05698500	-2.33458100	0.21797200

H	-1.91159400	-0.24628100	2.49741400
H	2.53650000	2.43285100	2.38451700
H	4.13842400	1.66774000	2.30243500
H	2.72473300	0.72037000	2.82083200
H	2.49912000	-2.77609000	0.01041300
H	4.19088200	-2.70541100	-0.53114500
H	2.88425500	-2.91024800	-1.72031000
C	3.22232200	2.25015100	-0.24033000
C	3.88341700	-0.44958300	-2.12307600
H	2.81034400	3.19516900	0.12495700
H	2.84463000	2.09072400	-1.25270000
H	4.31230000	2.33607000	-0.28032100
H	3.51159500	-0.93823300	-3.02806200
H	4.92912200	-0.73679000	-1.97862200
H	3.84078900	0.62939700	-2.27305000
C	3.46087300	-0.23559900	0.39868700
H	3.17948200	-0.90601900	1.22135600
H	4.55037500	-0.12784300	0.42903800
H	0.09379800	-2.30227400	1.36553200
H	0.39539500	-1.07086600	2.72240600

- computed data for ***trans*-2[B]-H**

: total free energy = –912.244490 Hartree

: relative free energy = –2.86 kcal/mol

: no imaginary frequency

: Cartesian coordinates

Atom	X	Y	Z
B	-0.97537100	-0.36765500	-0.28812400
O	0.35545700	-0.55471300	-0.56184700
C	1.33752900	0.30981700	-0.02461000
C	1.69461000	1.47159700	-0.98809500
C	2.66258600	-0.38284900	0.17445900
O	-1.85332800	-1.13337200	-1.00737100
O	-1.36499000	0.51491700	0.68022100
C	-3.22435100	-1.16144200	-0.56910600
C	-4.04791400	-1.64352700	-1.75679900
C	-2.72384000	0.97847000	0.81566200
C	-2.69874100	2.47776700	0.52588700
C	2.91409100	-1.68090600	0.60165200
C	3.70519300	0.49850500	-0.12223700
C	5.02813700	0.08823800	0.01225000
C	5.28985900	-1.21653700	0.44144100
C	4.24269500	-2.09529800	0.73173200
H	4.46408100	-3.10791900	1.05460000
H	2.09425400	-2.36038800	0.81690200
H	5.84601700	0.76389200	-0.22316400
H	6.31703300	-1.55388200	0.54177100
H	0.98135700	0.72401000	0.92956900

C	3.14791000	1.83095800	-0.56898400
C	0.72865200	2.59915700	-0.96879000
H	3.12836100	2.54063000	0.26919700
H	3.71519200	2.29388300	-1.38073400
H	-2.06026800	2.99162900	1.25073000
H	-3.70925200	2.89347700	0.58879600
H	-2.30425100	2.65966500	-0.47829400
H	-3.94341700	-0.95428700	-2.59926500
H	-5.10536000	-1.70951500	-1.48428200
H	-3.70490300	-2.63360500	-2.07003600
C	-3.14535700	0.74900500	2.26551400
C	-3.33119000	-2.16168000	0.58318800
H	-2.42305900	1.22663000	2.93368100
H	-3.20128200	-0.31082800	2.51713200
H	-4.12815600	1.19682500	2.43998300
H	-3.12451400	-3.16853400	0.20935400
H	-4.33473600	-2.14930400	1.01914400
H	-2.60521400	-1.93988100	1.36932300
C	-3.63841100	0.26987000	-0.20109900
H	-4.66787400	0.27323200	0.17301800
H	-3.63261100	0.84580500	-1.13491300
H	1.73500900	1.02487600	-1.98953400
H	0.54980300	3.13650400	-0.04310400
H	0.24479500	2.95384900	-1.86966100

- computed data for ***cis*-2[B]-H**

: total free energy = –912.245073 Hartree

: relative free energy = –3.23 kcal/mol

: no imaginary frequency

: Cartesian coordinates

Atom	X	Y	Z
B	-0.87581900	-0.08815200	-0.28743600
O	0.47802500	0.02015300	-0.47827400
C	1.36233600	-0.18391000	0.62104000
C	1.59887300	1.15125400	1.40378700
C	2.73707700	-0.49202600	0.07926500
O	-1.66846300	0.30841300	-1.32949600
O	-1.36680500	-0.60372500	0.88319500
C	-3.07715900	0.56587200	-1.17571400
C	-3.27926900	2.04921800	-1.48170600
C	-2.77968400	-0.86545200	0.97374100
C	-3.12277600	-0.85981600	2.45847200
C	3.22391100	-1.70326700	-0.40115200
C	3.52781400	0.65976000	0.07048100
C	4.83024800	0.61058200	-0.41989900
C	5.32610300	-0.60461700	-0.89982200
C	4.53083300	-1.75430100	-0.89149300

H	4.93400800	-2.69101900	-1.26363100
H	2.60101700	-2.59380100	-0.39196500
H	5.45519200	1.49946900	-0.42665100
H	6.34216500	-0.65836700	-1.27903900
H	0.96295700	-0.96730100	1.27154200
C	2.75844400	1.82991900	0.63423000
C	0.39298100	2.00063500	1.58570500
H	3.36173000	2.47407400	1.27995800
H	2.36274000	2.45313700	-0.17826600
H	1.98179000	0.84409600	2.38558400
H	-2.53685300	-1.62255300	2.97909100
H	-4.18542100	-1.07495900	2.60450300
H	-2.89688000	0.11585800	2.89813800
H	-2.67076700	2.65847400	-0.80657100
H	-4.33015700	2.32571600	-1.35115900
H	-2.98422700	2.26553100	-2.51238700
C	-3.04048500	-2.25024500	0.37987900
C	-3.82109100	-0.26887000	-2.21638400
H	-2.57368100	-3.01015000	1.01311400
H	-2.61188200	-2.33890100	-0.62103300
H	-4.11392300	-2.45434900	0.32250100
H	-3.42143000	-0.04771100	-3.21012900
H	-4.88477800	-0.01319400	-2.20552500
H	-3.72324600	-1.33990000	-2.03643400
C	-3.52264100	0.27743100	0.26971100
H	-3.34558800	1.17873000	0.87118100
H	-4.60089700	0.08525600	0.28646200
H	0.06136900	2.65724700	0.78828300
H	-0.21929100	1.92365000	2.47536800

3.2.2. 2-Crotylbenzaldehyde

- computed data for **1[B]-Me**

: total free energy = –951.515747 Hartree

: relative free energy = 0.00 kcal/mol

: no imaginary frequency

: Cartesian coordinates

Atom	X	Y	Z
B	-1.24198500	-0.70244700	0.07173100
O	0.04036300	-1.22984000	0.09388900
C	1.11180100	-0.43508500	0.33197200
C	2.97429500	2.18973400	-0.27071500
C	2.41013500	-0.96580200	0.18491800
O	-2.24911600	-1.60223400	-0.07244200
O	-1.40801200	0.64418800	0.19208100
C	-3.60943100	-1.20198900	-0.34565000
C	-4.00062100	-1.88408500	-1.65473600
C	-2.74778700	1.15528700	0.36167000

C	-2.72053500	2.59645300	-0.13148300
C	2.60142800	-2.31396700	-0.22045400
C	3.56109000	-0.15631000	0.44378200
C	4.82281600	-0.71624200	0.28661000
C	4.99860700	-2.04550000	-0.11722500
C	3.87539700	-2.83940600	-0.36927900
H	3.99785200	-3.87220500	-0.68160100
H	1.72781800	-2.92742600	-0.41320600
H	5.69559100	-0.09912700	0.48714600
H	5.99805300	-2.45244400	-0.23024900
H	0.90691600	0.58976700	0.60792200
C	3.42176200	1.29364500	0.85939300
C	1.91344000	2.99801000	-0.22878100
H	2.72202900	1.39063600	1.69933100
H	4.39838200	1.63568700	1.22187700
H	-1.98297400	3.16976900	0.43757000
H	-3.70238300	3.06015300	0.00091300
H	-2.45214500	2.63420300	-1.19071400
H	-3.31876800	-1.58611700	-2.45606800
H	-5.01911200	-1.60197800	-1.93849500
H	-3.95652700	-2.97076000	-1.54053200
C	-3.07116200	1.11790500	1.85531100
C	-4.48633200	-1.73855900	0.78369800
H	-2.43543200	1.83478100	2.38261600
H	-2.88187600	0.12937000	2.27965900
H	-4.11779200	1.38202100	2.03289600
H	-4.34958100	-2.82051400	0.86471300
H	-5.53849200	-1.53760300	0.56188600
H	-4.24616000	-1.28883500	1.74734800
C	-3.69327400	0.32585900	-0.51856300
H	-4.72610100	0.65072400	-0.35439900
H	-3.44247400	0.56600900	-1.55926000
H	3.58065400	2.15060400	-1.17765100
H	1.30883000	3.02115100	0.68091500
C	1.46447400	3.88635800	-1.35151100
H	2.12849700	3.79623300	-2.21531200
H	1.44421700	4.93585000	-1.03925600
H	0.44840900	3.62754200	-1.66868500

- computed data for ***trans*-TS[B]-Me**

: total free energy = –951.484823 Hartree

: relative free energy = 19.41 kcal/mol

: a single imaginary frequency at –550.79 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
B	-0.96324900	-0.56520000	-0.04621900
O	0.37327000	-0.83444900	-0.27565400
C	1.34281400	-0.07765800	0.32260400

C	1.82499300	1.74967900	-0.73797800
C	2.71556500	-0.57924600	0.24214400
O	-1.85190300	-1.29580200	-0.77396300
O	-1.31406900	0.37451000	0.87874500
C	-3.25147000	-0.95410300	-0.85666000
C	-3.53007400	-0.64706600	-2.32666200
C	-2.70322900	0.46081800	1.25849300
C	-2.90285200	1.85700000	1.83437000
C	3.08888100	-1.92561100	0.19825000
C	3.69155600	0.43102900	0.16622100
C	5.03810800	0.08740200	0.11528400
C	5.41493500	-1.25971200	0.11233400
C	4.44225100	-2.26098100	0.13949600
H	4.73895700	-3.30510000	0.11402600
H	2.32559300	-2.69788900	0.22414100
H	5.79420000	0.86531600	0.04374800
H	6.46606200	-1.52642800	0.06200500
H	1.03194200	0.44313100	1.22640700
C	3.13076700	1.82852700	0.04130400
C	0.80350200	2.64955500	-0.60447600
H	2.93167100	2.26844300	1.02908200
H	3.84997400	2.48517200	-0.46124400
H	-2.23978500	2.00368100	2.69154900
H	-3.93742800	1.98714300	2.16507000
H	-2.67560800	2.61832600	1.08251800
H	-2.88960900	0.17171000	-2.66832400
H	-4.57555400	-0.35300200	-2.46125200
H	-3.33096800	-1.52978300	-2.94079900
C	-2.95858100	-0.59427900	2.33516900
C	-4.05185700	-2.18399200	-0.43394100
H	-2.39684800	-0.33592900	3.23723000
H	-2.63044000	-1.58378200	2.00793200
H	-4.02212100	-0.64316700	2.58708200
H	-3.74780600	-3.04069900	-1.04182000
H	-5.11880900	-2.00458400	-0.59540500
H	-3.90094500	-2.43524200	0.61654900
C	-3.55718700	0.29335900	-0.00532400
H	-4.61841300	0.29413900	0.26549400
H	-3.38431000	1.18416100	-0.62245500
H	1.88792900	1.20166500	-1.68184600
H	0.78465200	3.29801500	0.27199600
C	-0.38378400	2.69169100	-1.51620500
H	-0.25459000	2.00794500	-2.36126600
H	-0.55585200	3.69867500	-1.91433100
H	-1.30005800	2.40154900	-0.98453800

- computed data for ***cis*-TS[B]-Me**

: total free energy = –951.483559 Hartree

: relative free energy = 20.20 kcal/mol

: a single imaginary frequency at –555.77 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
B	-0.86465800	-0.43685200	-0.27030400
O	0.49696200	-0.52119800	-0.47953100
C	1.36676100	-0.32284000	0.56365600
C	1.62439400	1.85865800	0.50589000
C	2.78411000	-0.58250200	0.23533700
O	-1.64632900	-0.45834700	-1.38786900
O	-1.35772800	-0.39853600	1.00409100
C	-3.04475500	-0.10766800	-1.35966700
C	-3.18462400	1.16649800	-2.19036900
C	-2.77295100	-0.62100800	1.17337400
C	-3.13615900	-0.07329200	2.54747600
C	3.45472300	-1.76941400	0.54234000
C	3.46148100	0.46482900	-0.40572600
C	4.79874300	0.30640200	-0.76436800
C	5.46188400	-0.88805300	-0.47503300
C	4.79503800	-1.92176200	0.18451100
H	5.31820600	-2.84311100	0.42080300
H	2.92792400	-2.57155600	1.05227100
H	5.32952300	1.12052900	-1.25135000
H	6.50566600	-1.00594100	-0.74981600
H	0.97878300	-0.58538900	1.54619900
C	2.65711900	1.72627300	-0.59926000
C	0.40096400	2.43124600	0.29293600
H	3.32141400	2.59820900	-0.60908800
H	2.14025300	1.70653300	-1.56774300
H	2.02384400	1.87039200	1.52254600
H	-2.54810900	-0.58146400	3.31691200
H	-4.19788700	-0.23856000	2.75245800
H	-2.93030100	0.99923600	2.60261100
H	-2.55773900	1.95894800	-1.76960700
H	-4.22445400	1.50775800	-2.19171000
H	-2.87308400	0.98151600	-3.22224200
C	-3.01867600	-2.12982500	1.12892900
C	-3.81521400	-1.24224000	-2.03145200
H	-2.54152500	-2.60106200	1.99290200
H	-2.59457000	-2.57520500	0.22560400
H	-4.09005800	-2.34974800	1.15794000
H	-3.39976900	-1.42400500	-3.02663400
H	-4.86731800	-0.96263900	-2.13956800
H	-3.76328500	-2.17034900	-1.46035600
C	-3.51141400	0.16655300	0.08391200
H	-3.35666100	1.23024500	0.30462000
H	-4.58797000	-0.02120000	0.15835400
H	0.06247000	2.56703800	-0.73498400
C	-0.54060100	2.83399700	1.38566400
H	-1.52201800	2.36235500	1.26066900

H	-0.70615200	3.91851200	1.39191000
H	-0.15208200	2.54275100	2.36638400

- computed data for ***trans*-2[B]-Me**

: total free energy = –951.520328 Hartree

: relative free energy = –2.87 kcal/mol

: no imaginary frequency

: Cartesian coordinates

Atom	X	Y	Z
B	-0.93722600	-0.41593500	-0.21541700
O	0.37970800	-0.51549000	-0.58532100
C	1.38279100	0.19588800	0.11518000
C	1.73596700	1.55199000	-0.56049300
C	2.70639100	-0.52770900	0.12173200
O	-1.83304200	-1.10484500	-0.98305400
O	-1.28876900	0.33663400	0.87229700
C	-3.25480500	-0.88483500	-0.90860900
C	-3.69213000	-0.42684400	-2.29900900
C	-2.65037400	0.28457700	1.33827600
C	-2.89107900	1.58803000	2.09046700
C	2.95791800	-1.89017200	0.22652100
C	3.74890300	0.39799400	0.02533600
C	5.07142800	-0.03433800	0.03901400
C	5.33333300	-1.40400400	0.14344300
C	4.28642400	-2.32526800	0.23356500
H	4.50768900	-3.38582400	0.30408800
H	2.13817400	-2.60045900	0.28790000
H	5.88899800	0.67684800	-0.04309700
H	6.36023200	-1.75676300	0.14511700
H	1.05026300	0.38003000	1.14652400
C	3.19031500	1.79806300	-0.09092400
C	0.77855700	2.65866100	-0.29246800
H	3.18556700	2.29268300	0.89035900
H	3.75165000	2.43637900	-0.77853300
H	-2.18676500	1.67235300	2.92285600
H	-3.90972100	1.61662600	2.48835600
H	-2.74805300	2.44361600	1.42372400
H	-3.15453400	0.48254200	-2.58377800
H	-4.76598600	-0.21611200	-2.30989800
H	-3.47941900	-1.20611500	-3.03627000
C	-2.77391700	-0.90431300	2.29180400
C	-3.91724000	-2.22364000	-0.58849200
H	-2.17748100	-0.71373300	3.18856300
H	-2.40099600	-1.82224000	1.83176100
H	-3.81514800	-1.05868900	2.59024100
H	-3.61416100	-2.96438300	-1.33387900
H	-5.00551200	-2.11810300	-0.62679300
H	-3.64252100	-2.59681900	0.39858200

C	-3.57792400	0.21720900	0.11727300
H	-4.61616800	0.10996700	0.44952500
H	-3.50296400	1.18915600	-0.38747300
H	1.75668200	1.33601500	-1.63903900
H	0.78618500	3.09898400	0.70287900
C	-0.38162200	2.93558400	-1.18748100
H	-0.12988200	2.73951900	-2.23528000
H	-0.72143400	3.97231700	-1.10034400
H	-1.24936000	2.30025400	-0.94121200

- computed data for ***cis*-2[B]-Me**

: total free energy = –951.519971 Hartree

: relative free energy = –2.65 kcal/mol

: no imaginary frequency

: Cartesian coordinates

Atom	X	Y	Z
B	0.83656100	-0.45784500	0.16178400
O	-0.51922700	-0.51911100	0.35836700
C	-1.38838500	0.15676300	-0.54790500
C	-1.57971500	1.64859500	-0.11575400
C	-2.77849500	-0.40958000	-0.38768600
O	1.62221600	-0.89135600	1.19539000
O	1.34271500	-0.02917500	-1.03814900
C	3.02277100	-0.56735900	1.28655400
C	3.17542000	0.34537000	2.50252000
C	2.75437900	-0.19712300	-1.26802900
C	3.13300000	0.77475700	-2.37850800
C	-3.30609000	-1.57506500	-0.93324900
C	-3.53614600	0.39685500	0.46614400
C	-4.84558400	0.04396000	0.78225500
C	-5.38229700	-1.12383200	0.23329000
C	-4.62048000	-1.92883000	-0.61847800
H	-5.05519200	-2.82985000	-1.03998900
H	-2.70891900	-2.19714400	-1.59472300
H	-5.44520100	0.66640100	1.44090600
H	-6.40437400	-1.40689300	0.46645500
H	-0.99487600	0.07344900	-1.56556100
C	-2.72645700	1.58772400	0.91989500
C	-0.34100400	2.33708600	0.34192500
H	-3.30405300	2.51580300	0.95434300
H	-2.32167400	1.41223300	1.92521800
H	-1.96391800	2.15944000	-1.01171200
H	2.53050100	0.57383700	-3.26913900
H	4.18975800	0.66118900	-2.63790500
H	2.95756300	1.80668000	-2.06216000
H	2.55192500	1.23696000	2.38149600
H	4.21759900	0.66016000	2.61550400
H	2.86549200	-0.17965200	3.41053400

C	2.98947500	-1.63624800	-1.72934000
C	3.78502900	-1.86829800	1.52958600
H	2.52141100	-1.78472700	-2.70678300
H	2.54800100	-2.35255300	-1.03230000
H	4.05949600	-1.84682100	-1.81867800
H	3.36719000	-2.37523600	2.40399300
H	4.83893700	-1.64957700	1.72555900
H	3.72756200	-2.54623900	0.67696400
C	3.48973800	0.18059300	0.02340700
H	3.31978400	1.25503000	0.17231000
H	4.56816700	0.03908200	-0.10660200
H	-0.09135100	2.31821300	1.39877400
C	0.50505600	3.10914800	-0.61266200
H	1.49476700	3.32305700	-0.19925700
H	0.04088800	4.07238800	-0.87562300
H	0.64080500	2.55403500	-1.54920700

3.2.3. 2-Cinnamylbenzaldehyde

- computed data for **1[B]-Ph**

: total free energy = –1143.143066 Hartree

: relative free energy = 0.00 kcal/mol

: no imaginary frequency

: Cartesian coordinates

Atom	X	Y	Z
B	-0.80181500	-1.88589100	0.03138400
O	0.56150500	-2.14173300	0.07144300
C	1.43048800	-1.16810800	0.43696000
C	2.39633000	1.85519700	0.51784100
C	2.79403500	-1.28990500	0.09739600
O	-1.60220000	-2.95198700	-0.24169500
O	-1.24438700	-0.62088200	0.26080800
C	-3.02388600	-2.77613200	-0.06369300
C	-3.69846800	-3.85063400	-0.90637700
C	-2.60034200	-0.20568800	-0.02467700
C	-2.50097800	0.89834300	-1.07486200
C	3.25773800	-2.40907500	-0.64512200
C	3.73759200	-0.28690800	0.48808300
C	5.06901500	-0.44104300	0.12270500
C	5.51280800	-1.54772700	-0.61153900
C	4.59419400	-2.53110200	-0.99146400
H	4.92554300	-3.39500100	-1.55979500
H	2.54200400	-3.16964100	-0.93828400
H	5.78349400	0.32228600	0.42153700
H	6.56024000	-1.63817800	-0.87963000
H	1.01586400	-0.32206800	0.96578200
C	3.30897300	0.93004400	1.28348600
C	1.22522300	2.29686900	0.99053500

H	0.92569100	1.98632200	1.99347200
C	0.25123500	3.15457300	0.29219300
H	2.81299800	0.62504300	2.21428800
H	4.21432300	1.47750400	1.57185000
H	2.74123100	2.14817400	-0.47374900
H	-1.95288300	1.75663100	-0.67513700
H	-3.50296400	1.22748900	-1.36849800
H	-1.98015200	0.52985800	-1.96369400
H	-3.44098600	-3.72716000	-1.96176200
H	-4.78527100	-3.78893300	-0.79885100
H	-3.37018100	-4.84084700	-0.57870400
C	-3.17976400	0.37486600	1.26262300
C	-3.33803100	-2.99476100	1.41662300
H	-2.52343800	1.17344300	1.62216600
H	-3.28107100	-0.37398400	2.04918500
H	-4.16692600	0.80229500	1.06295400
H	-3.13876200	-4.03720400	1.68032000
H	-4.38894300	-2.77473400	1.62657700
H	-2.71430500	-2.36310000	2.05378100
C	0.32769900	3.43209500	-1.08186700
C	-0.63718800	4.21963000	-1.70218700
C	-1.70378300	4.74275500	-0.96649600
C	-1.79412700	4.47188600	0.39796000
C	-0.82531300	3.68434500	1.01806600
H	1.13414200	3.01310000	-1.67598900
H	-0.56441100	4.41731500	-2.76725600
H	-2.45834500	5.35060400	-1.45554300
H	-2.62016600	4.86879400	0.98012400
H	-0.90348900	3.46979500	2.08109800
C	-3.40923100	-1.38724700	-0.59179900
H	-4.47568600	-1.21132100	-0.41522000
H	-3.26312700	-1.41384800	-1.67873200

- computed data for ***trans*-TS[B]-Ph**

: total free energy = –1143.122373 Hartree

: relative free energy = 12.99 kcal/mol

: a single imaginary frequency at –488.51 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
B	-0.48680800	-1.21434300	-0.11463900
O	0.85132700	-1.05056100	-0.44160000
C	1.71948000	-0.38361900	0.36890800
C	1.93592900	1.81445400	-0.05864700
C	3.14215900	-0.61919800	0.10623300
O	-1.26387700	-1.74946800	-1.09748100
O	-0.92201500	-0.87378200	1.12662600
C	-2.59343200	-2.18346700	-0.74650100
C	-3.40506400	-2.16758400	-2.03578600

C	-2.32474500	-0.85240500	1.47877100
C	-2.62821100	0.56755400	1.94618700
C	3.66086900	-1.84422100	-0.32876000
C	3.99313800	0.48675200	0.27390700
C	5.36191400	0.34070100	0.06745200
C	5.88437200	-0.89345700	-0.32795500
C	5.03255400	-1.97963600	-0.53812800
H	5.43756300	-2.93173700	-0.86686000
H	2.99039600	-2.68377100	-0.48719500
H	6.01946900	1.19849200	0.18381700
H	6.95137700	-0.99945300	-0.49718900
H	1.37477500	-0.20097400	1.38388400
C	3.30863000	1.79663200	0.58592600
C	0.89059100	2.51891800	0.47082900
H	1.00385000	2.95019300	1.46540200
C	-0.42046000	2.67303200	-0.14874800
H	3.19688600	1.93606600	1.67001500
H	3.91788800	2.63146600	0.21969800
H	1.91352300	1.55386400	-1.11800100
H	-2.00217400	0.82409900	2.80648300
H	-3.67976900	0.65069800	2.23883600
H	-2.43004400	1.27872100	1.13995400
H	-3.45189900	-1.15486100	-2.44556100
H	-4.42395400	-2.51827600	-1.84701000
H	-2.94015600	-2.82422500	-2.77636700
C	-2.52108700	-1.82575700	2.63883900
C	-2.48981300	-3.61252100	-0.21152200
H	-1.86131100	-1.54315800	3.46417100
H	-2.30059200	-2.85658700	2.36019500
H	-3.55575400	-1.77719500	2.99060400
H	-2.18610200	-4.28267900	-1.02068900
H	-3.45285800	-3.95189900	0.18146000
H	-1.74206700	-3.68793300	0.58135900
C	-0.84822800	1.86210900	-1.21848200
C	-2.12411000	2.00464100	-1.75609800
C	-3.00783200	2.95790800	-1.24403000
C	-2.59702300	3.77180000	-0.18587900
C	-1.32350900	3.62731000	0.35604700
H	-0.18343200	1.10138200	-1.61956400
H	-2.43321300	1.36100500	-2.57481600
H	-4.00391200	3.06213100	-1.66217800
H	-3.27447900	4.51583300	0.22233200
H	-1.01551100	4.25515500	1.18845900
C	-3.18718900	-1.17399000	0.24543600
H	-4.17289100	-1.51926400	0.57543200
H	-3.33863700	-0.24060700	-0.31183600

- computed data for ***cis*-TS[B]-Ph**

: total free energy = –1143.120289 Hartree

: relative free energy = 14.29 kcal/mol

: a single imaginary frequency at –527.57 cm^{-1}

: Cartesian coordinates

Atom	X	Y	Z
B	-0.25027800	-1.37335500	0.08708000
O	1.12371600	-1.23192200	-0.02472200
C	1.77522800	-0.26106100	0.67962500
C	1.55362200	1.45057000	-0.77714400
C	3.24066800	-0.26197400	0.51660200
O	-0.83179200	-2.20968700	-0.81772100
O	-0.91048300	-0.73117000	1.08992000
C	-2.26185400	-2.27523400	-0.99346300
C	-2.52884500	-1.89903800	-2.44957100
C	-2.30422900	-1.03736900	1.29995100
C	-2.91832300	0.19188100	1.95674000
C	4.13201500	-0.73157900	1.48453900
C	3.72269100	0.26584200	-0.69166600
C	5.09304900	0.28476200	-0.93828000
C	5.98211300	-0.20814200	0.02013800
C	5.50480500	-0.70563600	1.23313300
H	6.19969000	-1.07233700	1.98204600
H	3.75269800	-1.12435500	2.42394200
H	5.47050000	0.70457200	-1.86712900
H	7.05023700	-0.18529700	-0.17283200
H	1.31422900	0.03579900	1.61929400
C	2.67354400	0.85226400	-1.60469300
C	0.25634100	1.46652500	-1.20969100
H	-0.00624400	0.85380300	-2.07331900
C	-0.83720500	2.22541000	-0.60992100
H	3.12190200	1.62060700	-2.24542400
H	2.25866700	0.08107900	-2.26633100
H	1.87286200	2.17550400	-0.02805200
H	-2.39969400	0.41061000	2.89506200
H	-3.97645700	0.01594100	2.17396800
H	-2.82769000	1.05912900	1.29669300
H	-2.13027900	-0.90179100	-2.65912000
H	-3.60454900	-1.89498200	-2.65074400
H	-2.04791500	-2.61701600	-3.11983300
C	-2.37714100	-2.23656600	2.24550900
C	-2.69577800	-3.72056000	-0.75828200
H	-2.00849000	-1.94325700	3.23267200
H	-1.75766500	-3.06323800	1.89010700
H	-3.40812800	-2.58831400	2.34802700
H	-2.13214500	-4.38080300	-1.42354200
H	-3.76090400	-3.82883300	-0.98330100
H	-2.52708600	-4.04278500	0.26955300
C	-2.08189900	2.27579800	-1.26442100
C	-3.14229900	3.01627400	-0.74837000
C	-2.98766300	3.72598400	0.44350700

C	-1.76260800	3.67585900	1.11411400
C	-0.70425300	2.93398100	0.59997100
H	-2.20798000	1.73316700	-2.19873100
H	-4.08992700	3.04047300	-1.27818900
H	-3.81125900	4.30516400	0.84860100
H	-1.63475900	4.21319100	2.04917200
H	0.23244000	2.89685800	1.14820000
C	-2.96056800	-1.26259000	-0.06905300
H	-2.96498100	-0.28622400	-0.57086600
H	-4.00566100	-1.56007100	0.06921400

- computed data for ***trans*-2[B]-Ph**

: total free energy = –1143.162350 Hartree

: relative free energy = –12.10 kcal/mol

: no imaginary frequency

: Cartesian coordinates

Atom	X	Y	Z
B	-0.42333200	-1.05475400	-0.23942000
O	0.83957000	-0.68856300	-0.63551600
C	1.71436100	0.03529400	0.20798400
C	1.80426300	1.54039000	-0.19506300
C	3.14117400	-0.43696200	0.06047300
O	-1.20851400	-1.61155500	-1.21210300
O	-0.81794700	-0.88357300	1.05589900
C	-2.44822900	-2.22447400	-0.81462800
C	-3.34172700	-2.22877500	-2.04910200
C	-2.19057700	-1.02306700	1.47987000
C	-2.60159000	0.32933400	2.05488000
C	3.60954200	-1.74192300	-0.04402200
C	4.01692400	0.64926400	0.05092000
C	5.38919000	0.44244000	-0.06080300
C	5.86797900	-0.86610400	-0.16640900
C	4.98591800	-1.95077800	-0.16001800
H	5.37395600	-2.96050400	-0.25178600
H	2.91673000	-2.57882700	-0.04867700
H	6.07759200	1.28305900	-0.07652900
H	6.93494900	-1.04256600	-0.26276600
H	1.38159800	-0.05565700	1.25055500
C	3.24947600	1.94318500	0.18048100
C	0.76135100	2.42055000	0.40440200
H	1.02676800	2.95815000	1.31248200
C	-0.56107100	2.59328800	-0.08475000
H	3.28247700	2.30168600	1.21811300
H	3.63837600	2.74385400	-0.45455400
H	1.72364700	1.54046100	-1.29145900
H	-1.95517200	0.59359700	2.89768400
H	-3.63867300	0.29368500	2.40369900
H	-2.51463200	1.10358700	1.28762900

H	-3.53033000	-1.20548100	-2.38618600
H	-4.29931500	-2.70780200	-1.82424100
H	-2.85557500	-2.78034000	-2.85871600
C	-2.22800900	-2.07875600	2.58291100
C	-2.14513700	-3.66055000	-0.38387300
H	-1.54430500	-1.78814700	3.38578700
H	-1.93696500	-3.06637900	2.22375300
H	-3.23866800	-2.14614200	2.99637000
H	-1.81471400	-4.23792600	-1.25207700
H	-3.03498800	-4.13851900	0.03682100
H	-1.34588700	-3.69103100	0.36040100
C	-1.07051200	1.88230400	-1.20400600
C	-2.38769400	2.04701600	-1.61233900
C	-3.23908600	2.93182700	-0.94247300
C	-2.74972100	3.66249100	0.14835500
C	-1.44104800	3.49645000	0.57190500
H	-0.42786100	1.19139200	-1.74074600
H	-2.75583000	1.48018500	-2.46278400
H	-4.26695300	3.05474900	-1.26765800
H	-3.40045300	4.35696300	0.67114600
H	-1.07188800	4.05548700	1.42790300
C	-3.09003000	-1.35712900	0.27669500
H	-4.01009500	-1.83315000	0.63299900
H	-3.37648500	-0.41299000	-0.20464300

- computed data for ***cis*-2[B]-Ph**

: total free energy = –1143.160776 Hartree

: relative free energy = –11.11 kcal/mol

: no imaginary frequency

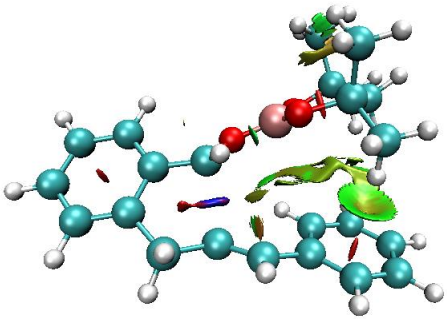
: Cartesian coordinates

Atom	X	Y	Z
B	-0.21992300	-1.32021400	0.00196000
O	1.11758100	-1.07328000	-0.18985600
C	1.72510400	0.04541900	0.45160600
C	1.57031200	1.32993300	-0.42559400
C	3.22037400	-0.16148300	0.45809800
O	-0.78907800	-2.23844500	-0.83700600
O	-0.89585200	-0.68508300	1.00661700
C	-2.21599100	-2.36872300	-0.98368100
C	-2.52757900	-2.03747300	-2.44243400
C	-2.25716000	-1.07175300	1.27202100
C	-2.92656700	0.13083300	1.92521400
C	3.98401700	-0.92277500	1.33630300
C	3.80810400	0.50897100	-0.61781600
C	5.18227700	0.42820900	-0.82636800
C	5.95535700	-0.33185500	0.05555000
C	5.36330100	-1.00276700	1.12938200
H	5.98012600	-1.58426200	1.80744400

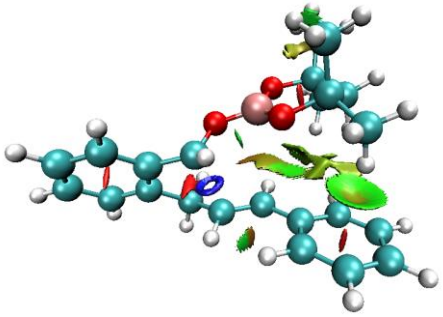
H	3.51821000	-1.44214600	2.16952300
H	5.65000500	0.94993000	-1.65679900
H	7.02916000	-0.39799400	-0.09138600
H	1.29360400	0.17935000	1.44821500
C	2.75914200	1.24882000	-1.41316800
C	0.23857900	1.48024500	-1.07594600
H	0.08457800	0.95749100	-2.01826000
C	-0.85897400	2.22291800	-0.55851800
H	3.08582500	2.23688000	-1.74862100
H	2.47921200	0.67115900	-2.30344900
H	1.76394500	2.17363600	0.24765900
H	-2.38554800	0.40945400	2.83468700
H	-3.96059200	-0.10925000	2.19173600
H	-2.92231600	0.98550000	1.24239000
H	-2.17434500	-1.02936400	-2.68092400
H	-3.60625000	-2.08209100	-2.62233900
H	-2.03003700	-2.75001200	-3.10650600
C	-2.22683500	-2.25250600	2.24330600
C	-2.58445600	-3.82516500	-0.70761800
H	-1.84142000	-1.91653600	3.21038800
H	-1.57246000	-3.04869900	1.88077800
H	-3.23085400	-2.66189500	2.39082300
H	-1.99823200	-4.47676800	-1.36187500
H	-3.64590600	-3.98645300	-0.91833000
H	-2.39177500	-4.11263700	0.32644000
C	-2.07380800	2.28176300	-1.29222900
C	-3.16275600	3.00391300	-0.82817900
C	-3.08542300	3.69738100	0.38590600
C	-1.90224400	3.64693200	1.13010800
C	-0.80945000	2.92140900	0.67576200
H	-2.13850800	1.74978100	-2.23851300
H	-4.07796600	3.03171500	-1.41189400
H	-3.93654600	4.26483700	0.74775400
H	-1.83725500	4.17315800	2.07775400
H	0.09037000	2.88560500	1.28144200
C	-2.94305400	-1.36778200	-0.06831200
H	-3.01343100	-0.40676400	-0.59542900
H	-3.96682500	-1.71489400	0.10907500

3.3. NCI plot analysis

In each transition structures, broad green isosurface is shown between the C–H bond and the aromatic ring, indicating the presence of attractive van der Waals interaction.



***trans*-TS[B]-Ph**



***cis*-TS[B]-Ph**

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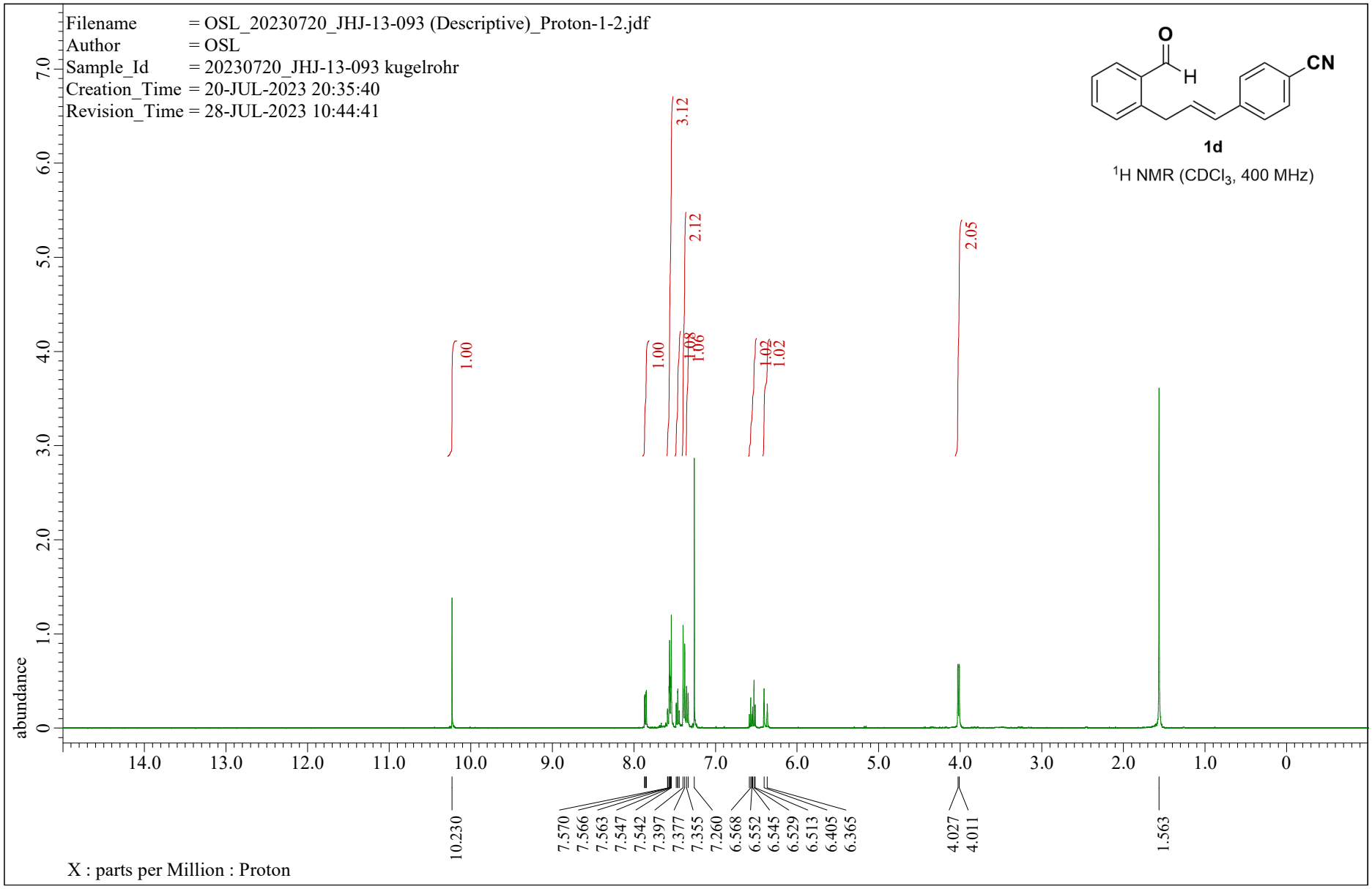
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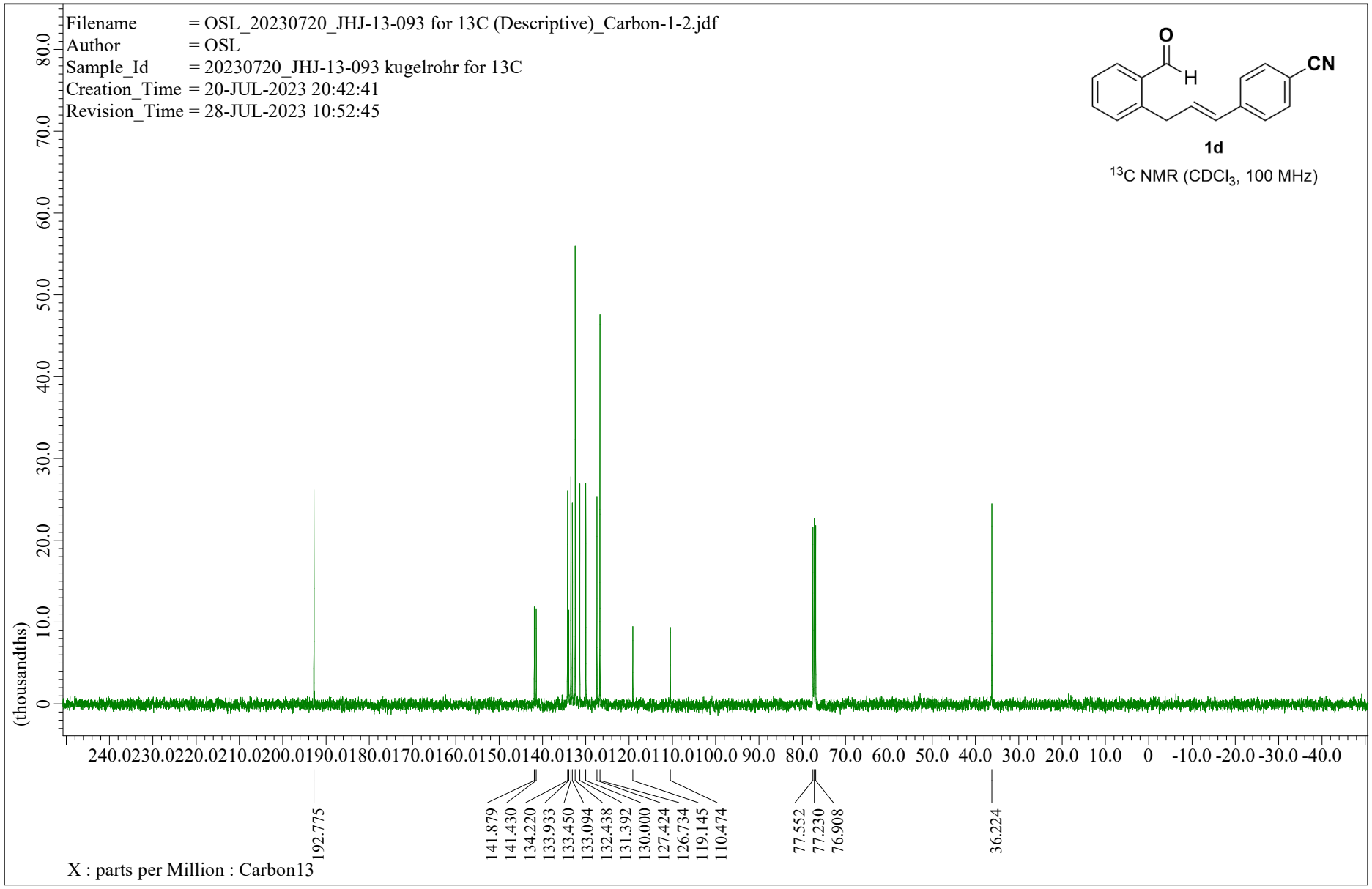
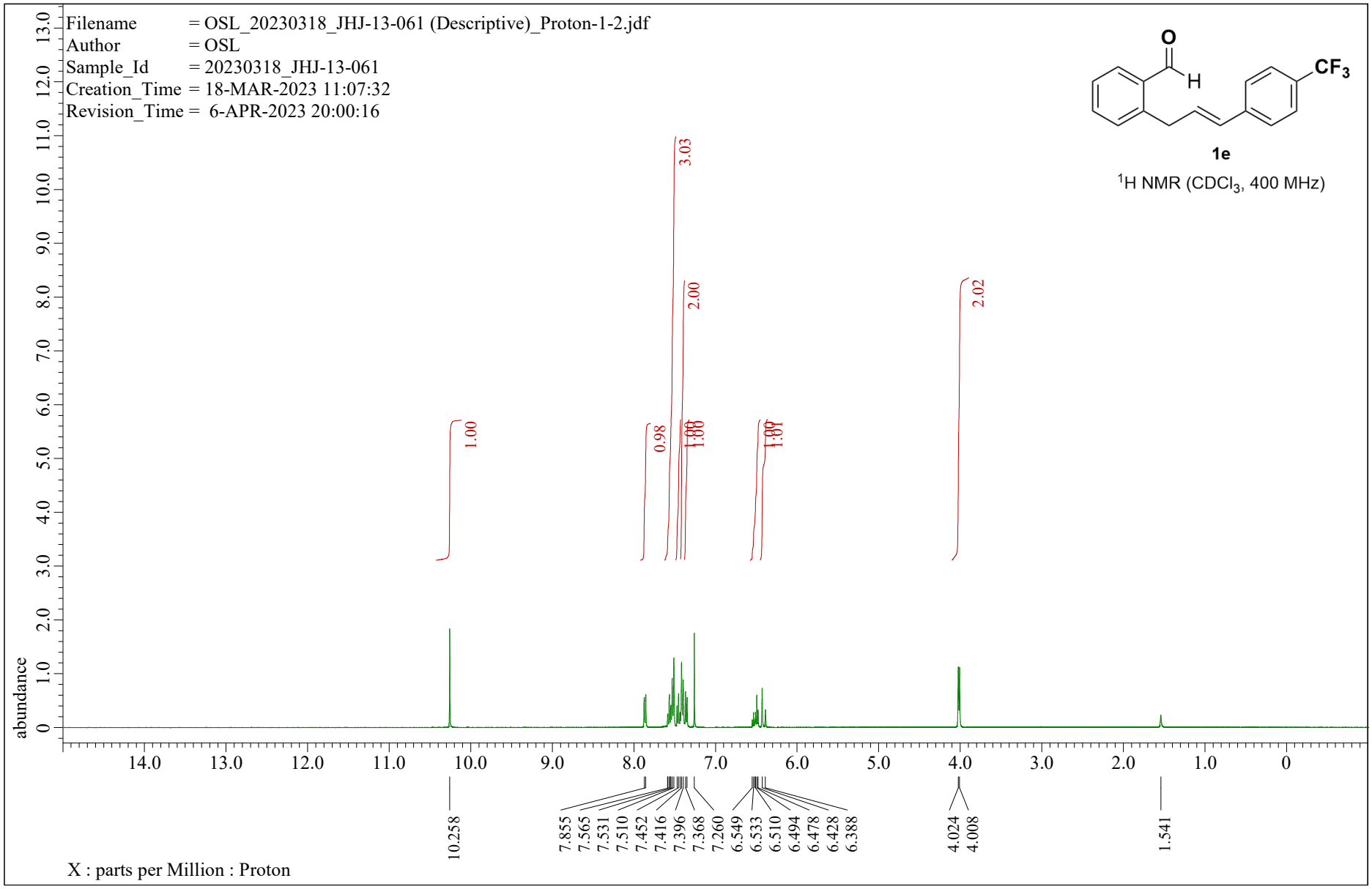
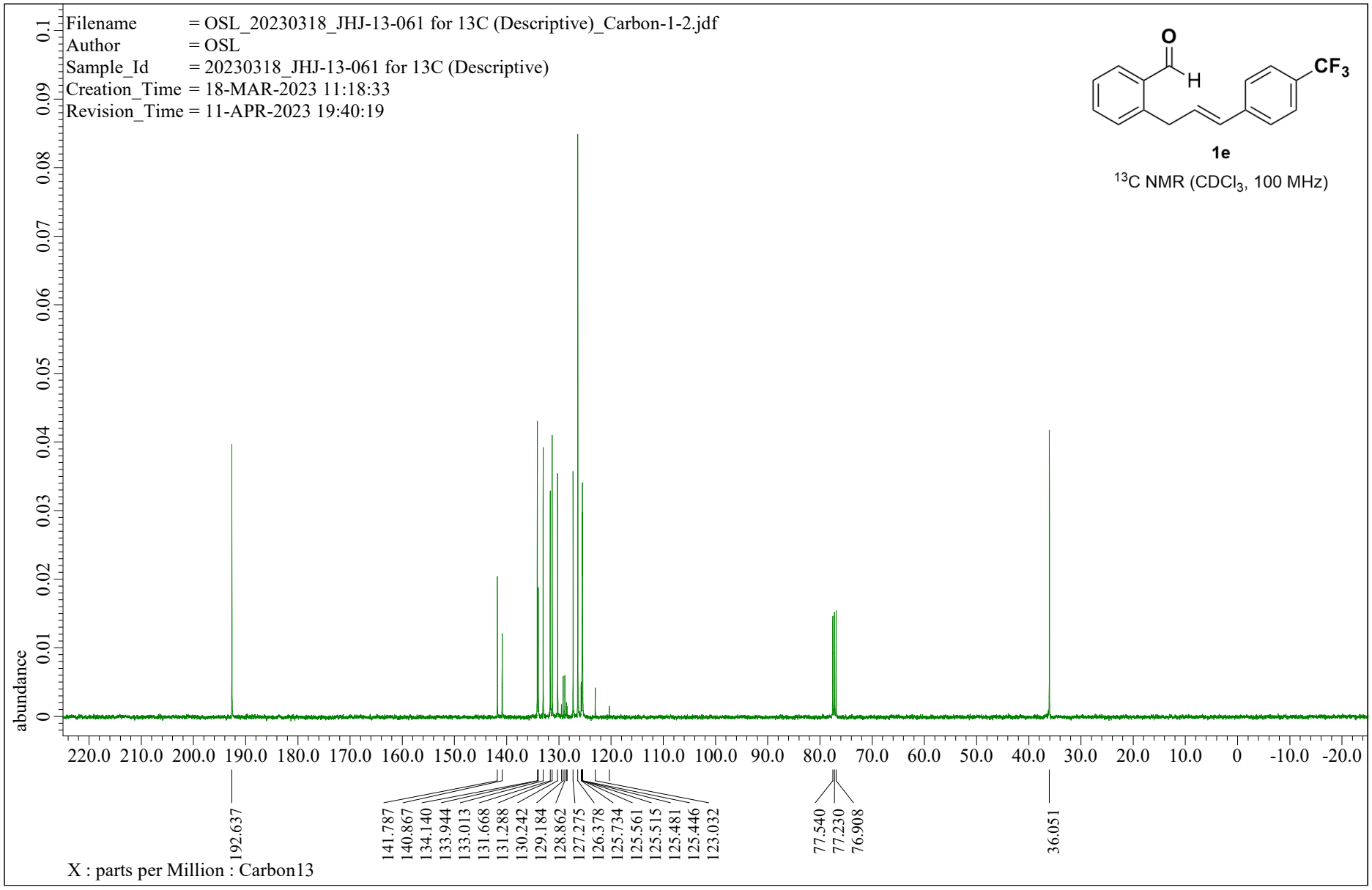
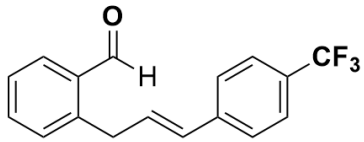
O
H
CN
1d
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton
10.230
7.570
7.566
7.563
7.547
7.542
7.397
7.377
7.355
7.260
6.568
6.552
6.545
6.529
6.513
6.405
6.365
4.027
4.011
1.563


Filename = OSL_20230720_JHJ-13-093 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230720_JHJ-13-093 kugelrohr for 13C
Creation_Time = 20-JUL-2023 20:42:41
Revision_Time = 28-JUL-2023 10:52:45
O
H
CN
1d
13C NMR (CDCl3, 100 MHz)
(thousandths)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
240.0 230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0
192.775
141.879
141.430
134.220
133.933
133.450
133.094
132.438
131.392
130.000
127.424
126.734
119.145
110.474
77.552
77.230
76.908
36.224
X : parts per Million : Carbon13


Filename = OSL_20230318_JHJ-13-061 (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230318_JHJ-13-061
Creation_Time = 18-MAR-2023 11:07:32
Revision_Time = 6-APR-2023 20:00:16
O
H
CF3
1e
1H NMR (CDCl3, 400 MHz)
3.03
2.00
2.02
1.00
0.98
abundance
X : parts per Million : Proton
10.258
7.855
7.565
7.531
7.510
7.452
7.416
7.396
7.368
7.260
6.549
6.533
6.510
6.494
6.478
6.428
6.388
4.024
4.008
1.541

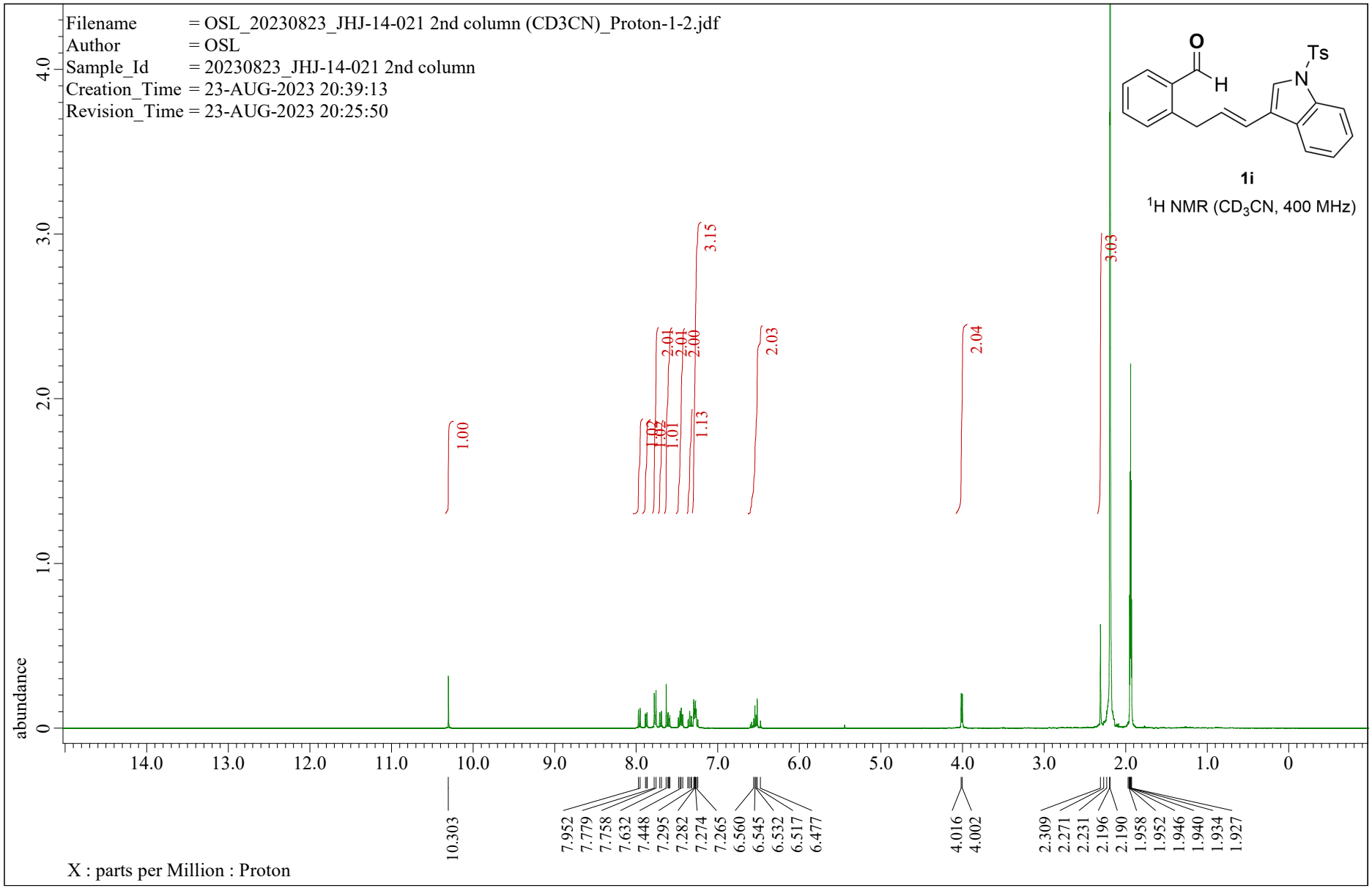

Filename = OSL_20230318_JHJ-13-061 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230318_JHJ-13-061 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 11:18:33
Revision_Time = 11-APR-2023 19:40:19
O
H
CF3
1e
13C NMR (CDCl3, 100 MHz)
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
192.637
141.787
140.867
134.140
133.944
133.013
131.668
131.288
130.242
129.184
128.862
127.275
126.378
125.734
125.561
125.515
125.481
125.446
123.032
77.540
77.230
76.908
36.051
X : parts per Million : Carbon13

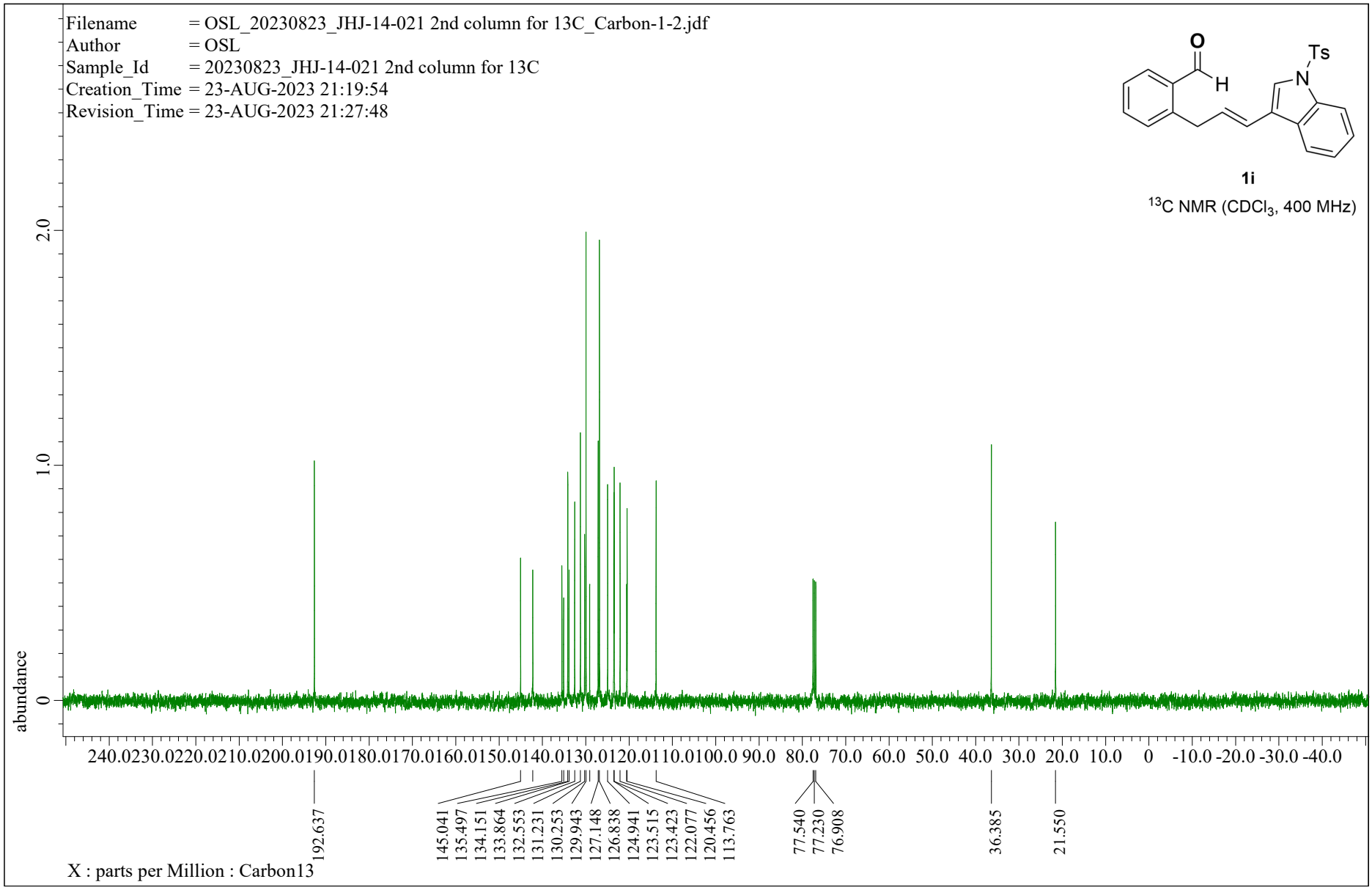
Filename = OSL_20230318_JHJ-13-061 (Descriptive)_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20230318_JHJ-13-061 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 11:11:16
Revision_Time = 13-APR-2023 16:24:51

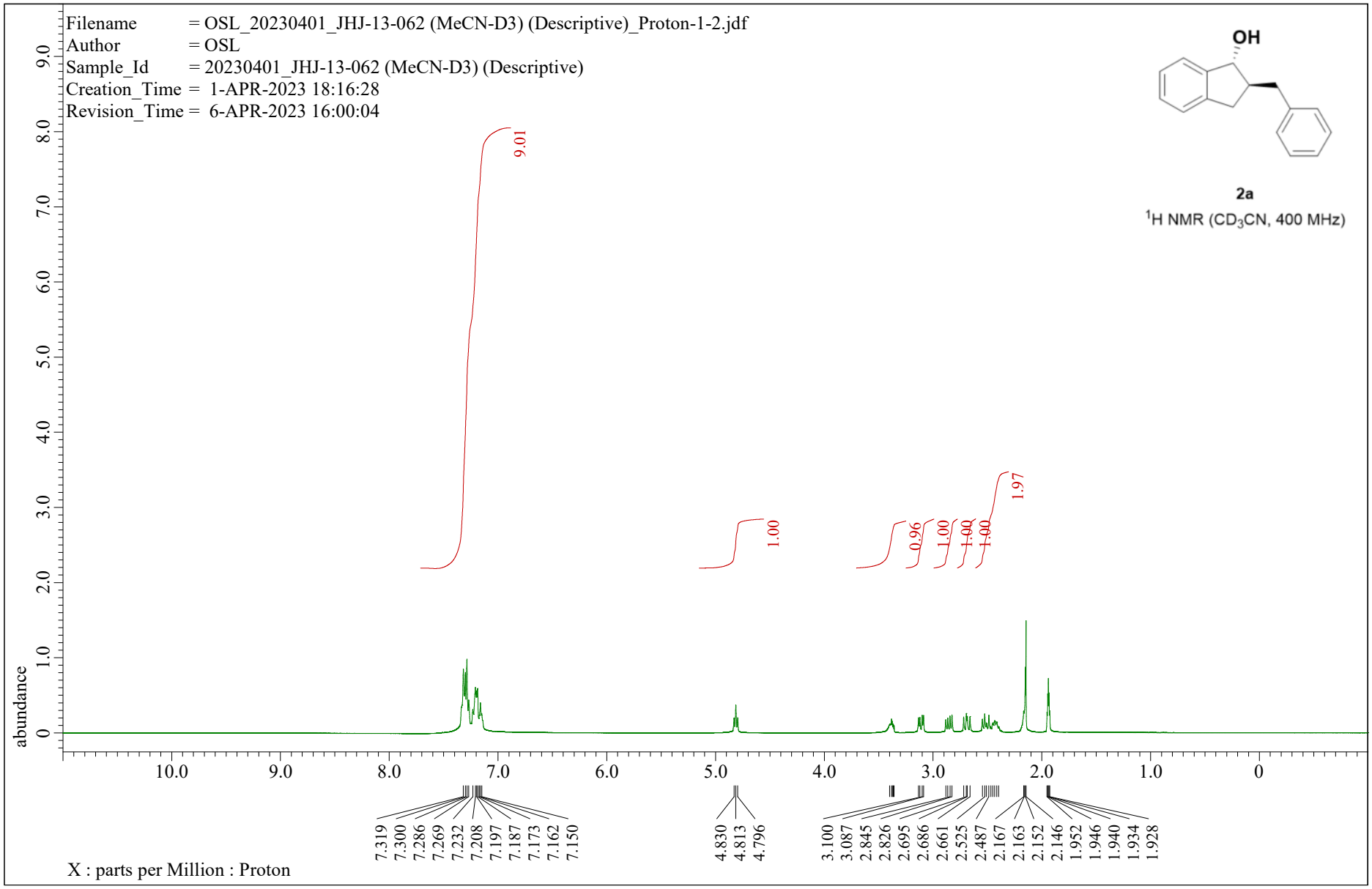


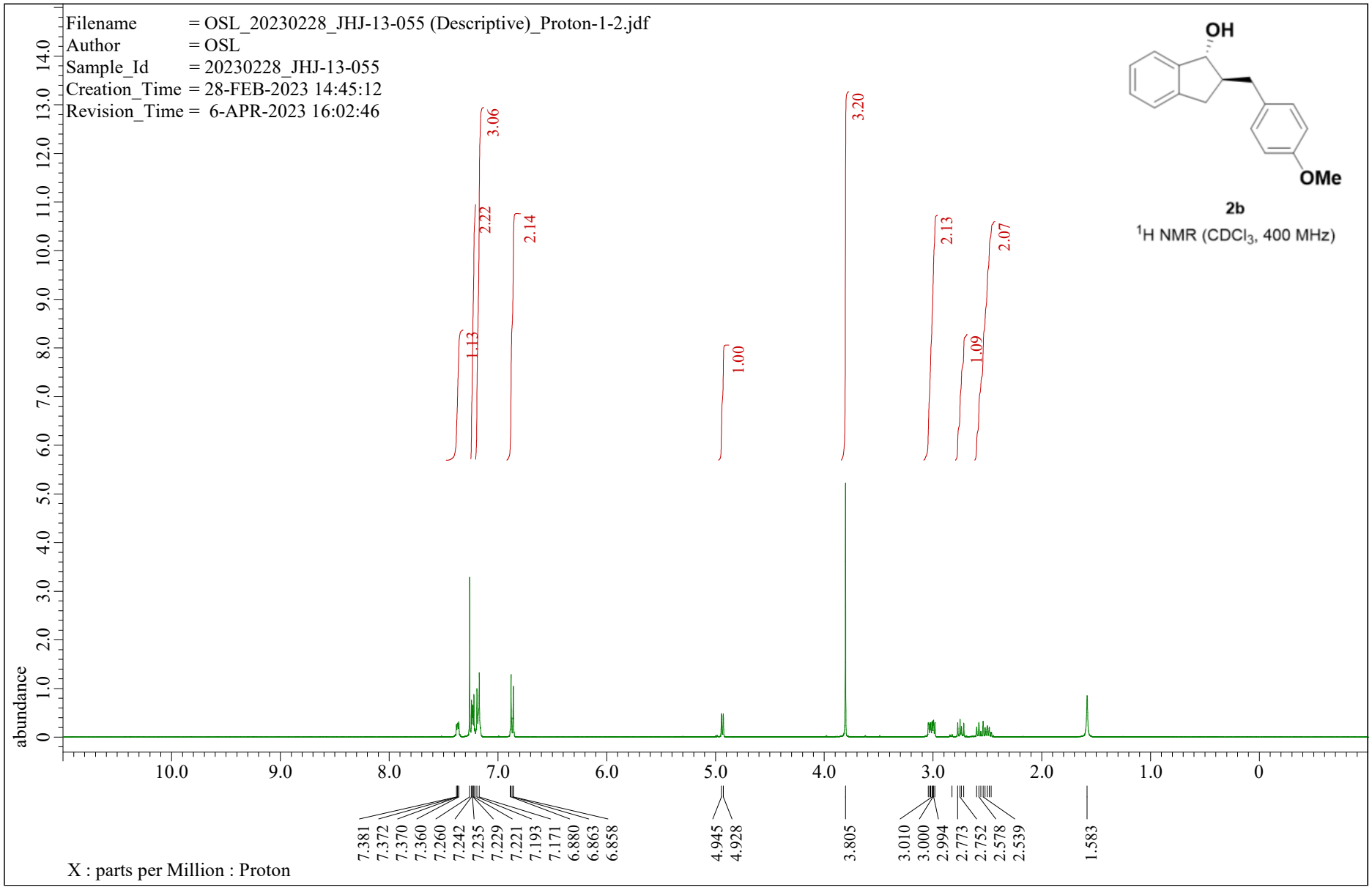
1e

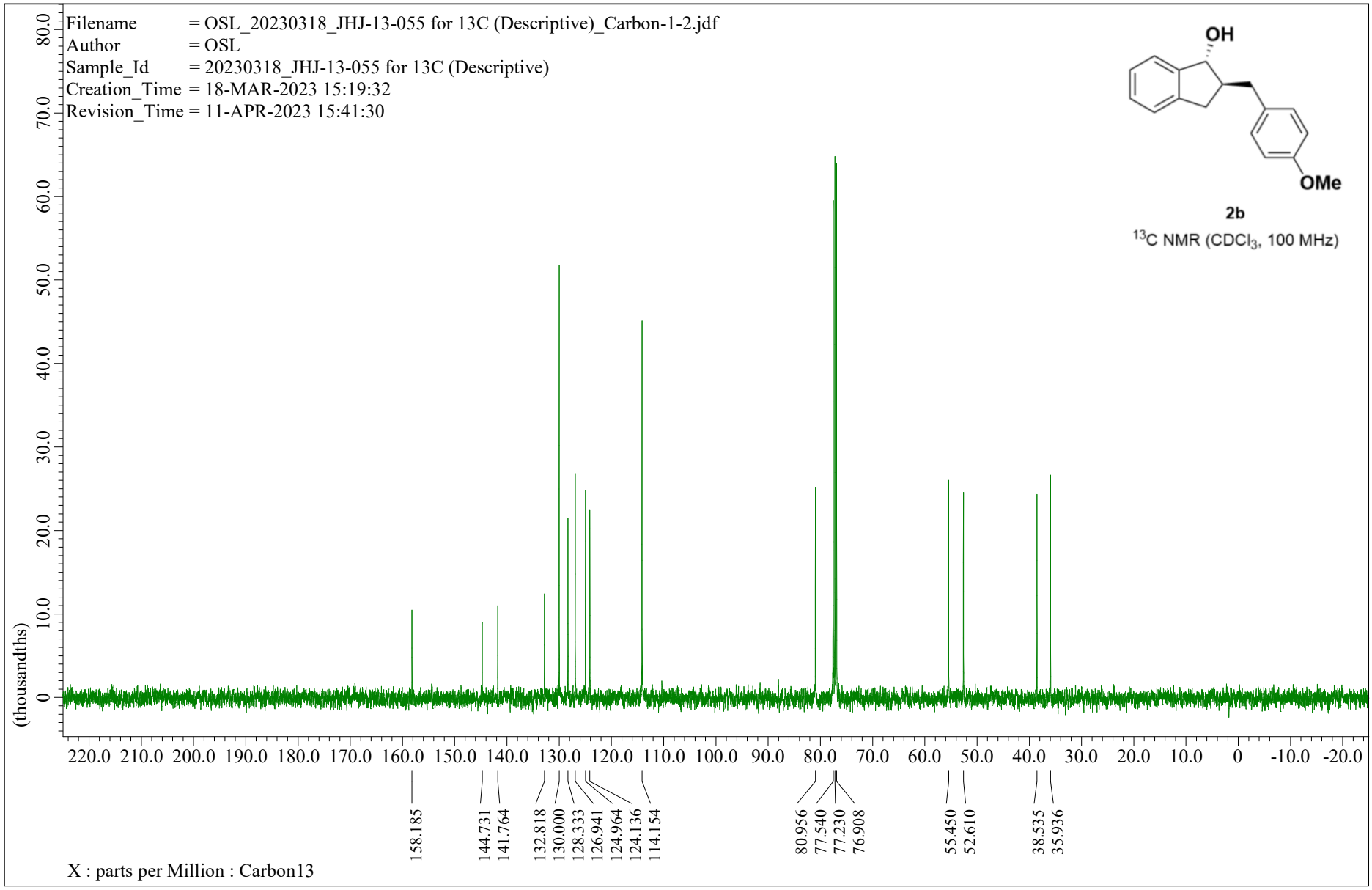
^{19}F NMR ($CDCl_3$, 376 MHz)

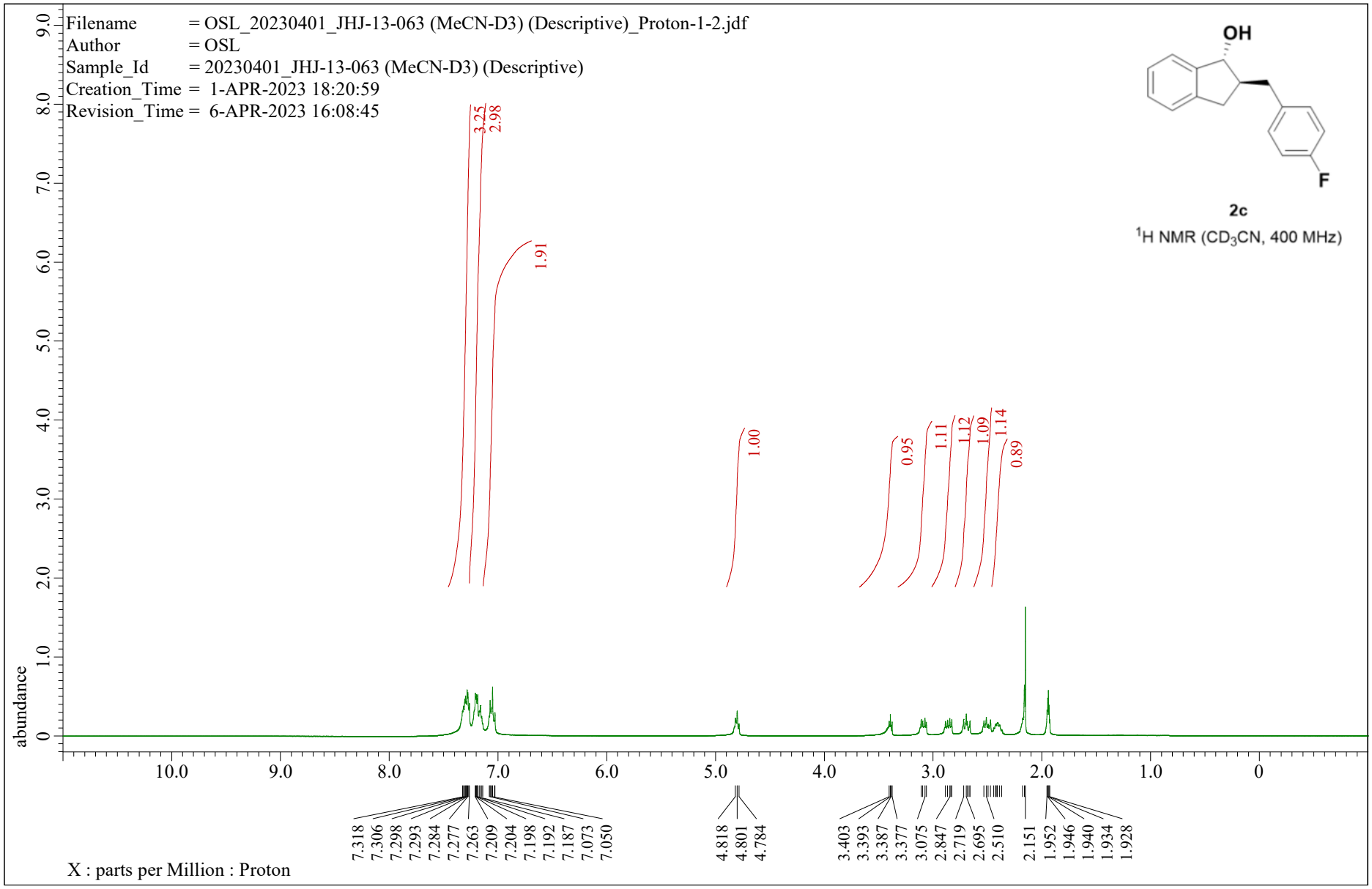

Filename = OSL_20230823_JHJ-14-021 2nd column (CD3CN)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230823_JHJ-14-021 2nd column
Creation_Time = 23-AUG-2023 20:39:13
Revision_Time = 23-AUG-2023 20:25:50
O
H
N
Ts
1i
1H NMR (CD3CN, 400 MHz)
abundance
X : parts per Million : Proton
10.303
7.952
7.779
7.758
7.632
7.448
7.295
7.282
7.274
7.265
6.560
6.545
6.532
6.517
6.477
4.016
4.002
2.309
2.271
2.231
2.196
2.190
1.958
1.952
1.946
1.940
1.934
1.927

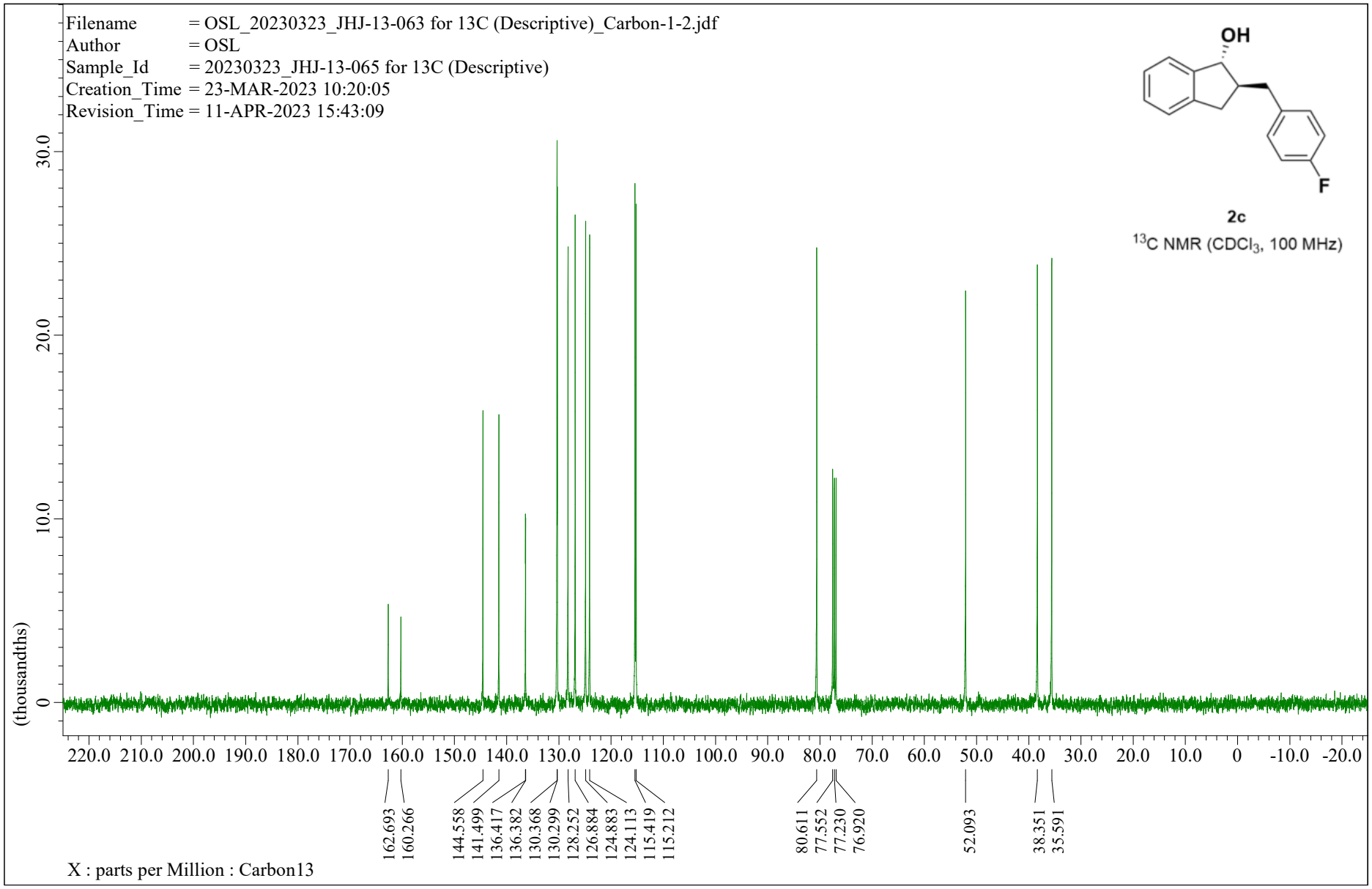

Filename = OSL_20230823_JHJ-14-021 2nd column for 13C_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230823_JHJ-14-021 2nd column for 13C
Creation_Time = 23-AUG-2023 21:19:54
Revision_Time = 23-AUG-2023 21:27:48
O
H
N
Ts
1i
13C NMR (CDCl3, 400 MHz)
abundance
2.0
1.0
0
240.0 230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0
192.637
145.041
135.497
134.151
133.864
132.553
131.231
130.253
129.943
127.148
126.838
124.941
123.515
123.423
122.077
120.456
113.763
77.540
77.230
76.908
36.385
21.550
X : parts per Million : Carbon13

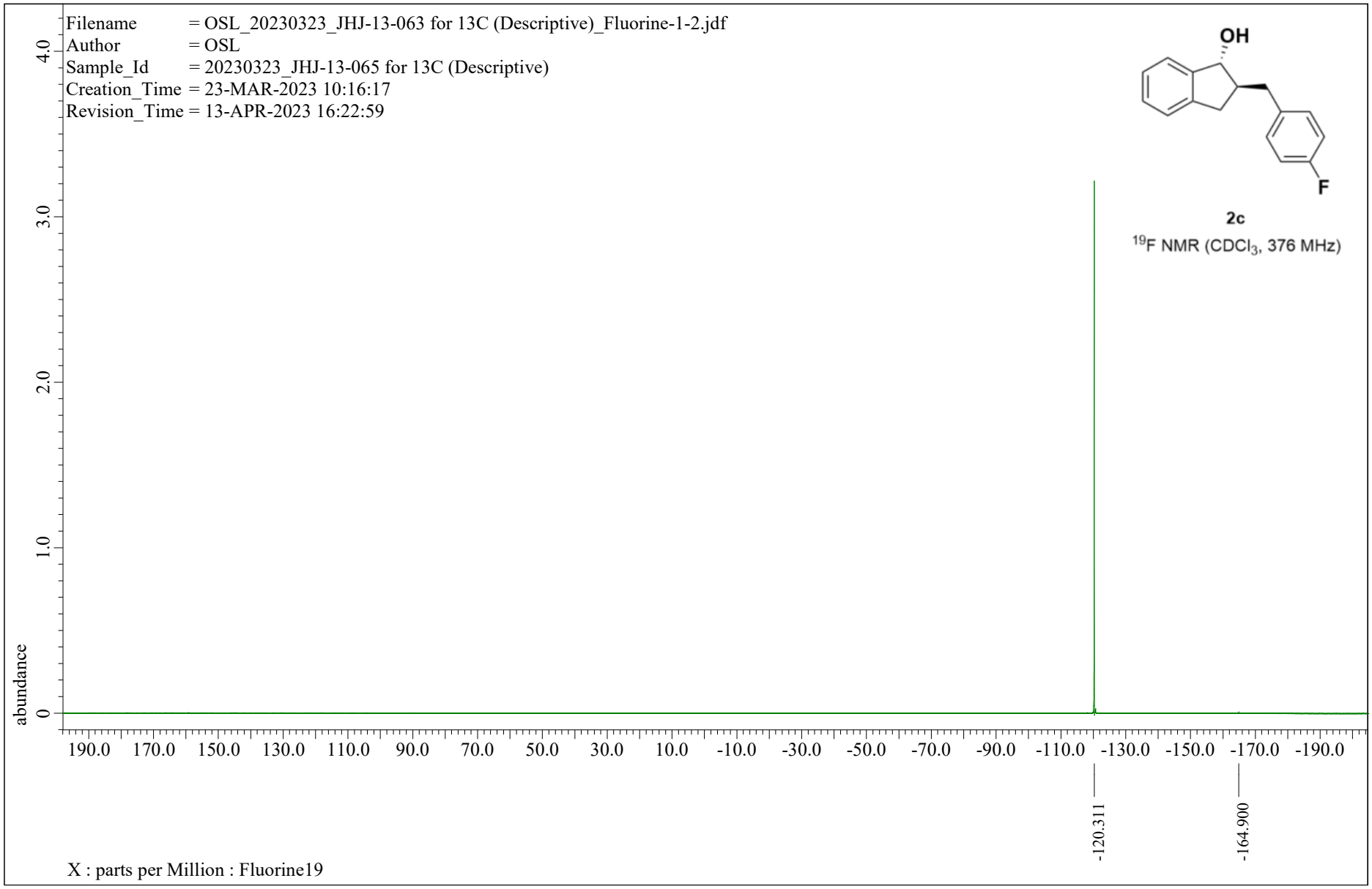

Filename = OSL_20230401_JHJ-13-062 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230401_JHJ-13-062 (MeCN-D3) (Descriptive)
Creation_Time = 1-APR-2023 18:16:28
Revision_Time = 6-APR-2023 16:00:04
OH
2a
1H NMR (CD3CN, 400 MHz)
9.01
1.00
0.96
1.00
1.00
1.00
1.97
abundance
X : parts per Million : Proton
7.319
7.300
7.286
7.269
7.232
7.208
7.197
7.187
7.173
7.162
7.150
4.830
4.813
4.796
3.100
3.087
2.845
2.826
2.695
2.686
2.661
2.525
2.487
2.167
2.163
2.152
2.146
1.952
1.946
1.940
1.934
1.928

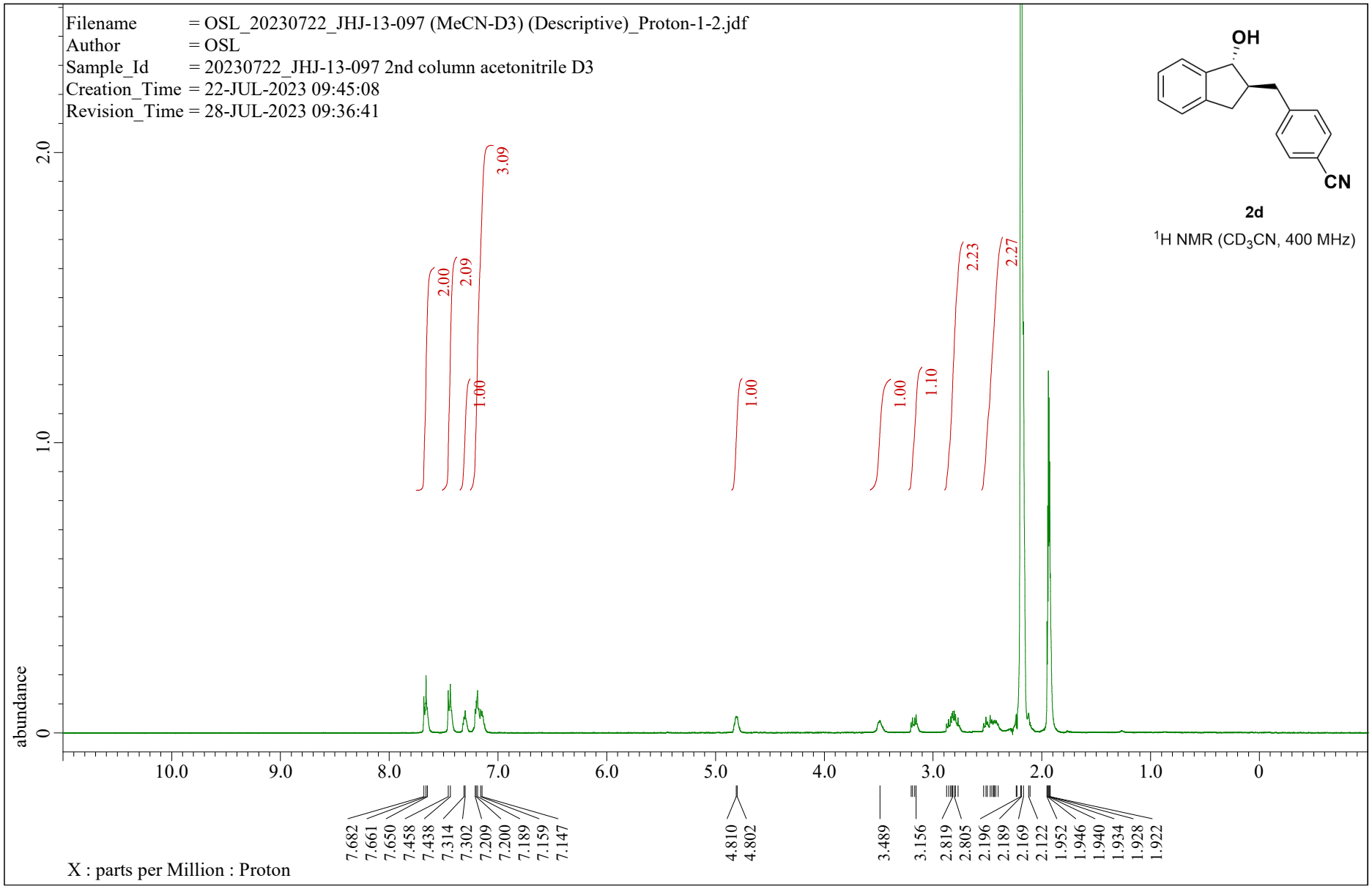

Filename = OSL_20230228_JHJ-13-055 (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230228_JHJ-13-055
Creation_Time = 28-FEB-2023 14:45:12
Revision_Time = 6-APR-2023 16:02:46
OH
OMe
2b
1H NMR (CDCl3, 400 MHz)
3.06
2.22
2.14
1.13
1.00
3.20
2.13
1.09
2.07
abundance
X : parts per Million : Proton
7.381
7.372
7.370
7.360
7.260
7.242
7.235
7.229
7.221
7.193
7.171
6.880
6.863
6.858
4.945
4.928
3.805
3.010
3.000
2.994
2.773
2.752
2.578
2.539
1.583

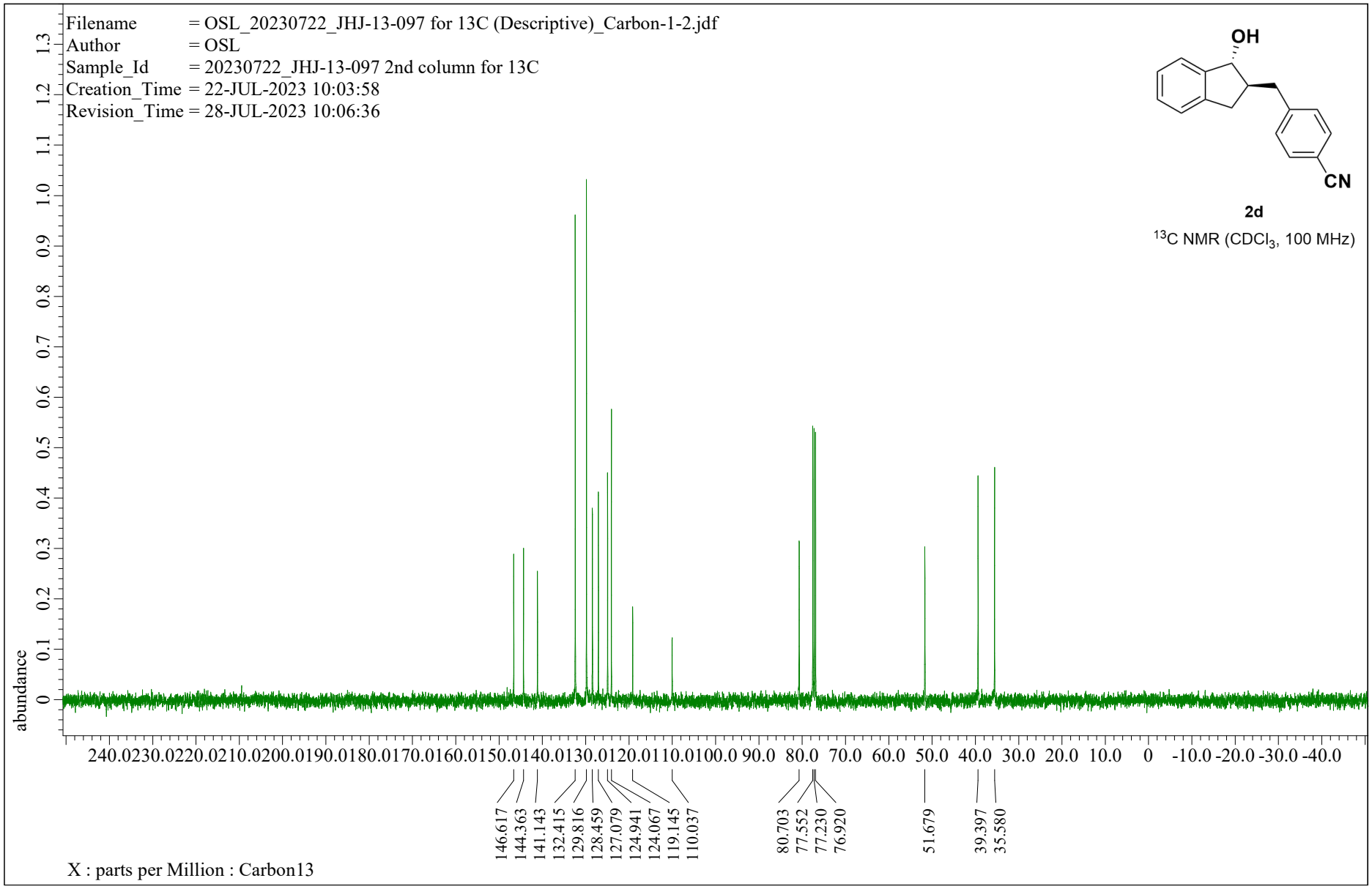

Filename = OSL_20230318_JHJ-13-055 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230318_JHJ-13-055 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 15:19:32
Revision_Time = 11-APR-2023 15:41:30
OH
OMe
2b
13C NMR (CDCl3, 100 MHz)
(thousandths)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
158.185
144.731
141.764
132.818
130.000
128.333
126.941
124.964
124.136
114.154
80.956
77.540
77.230
76.908
55.450
52.610
38.535
35.936
X : parts per Million : Carbon13

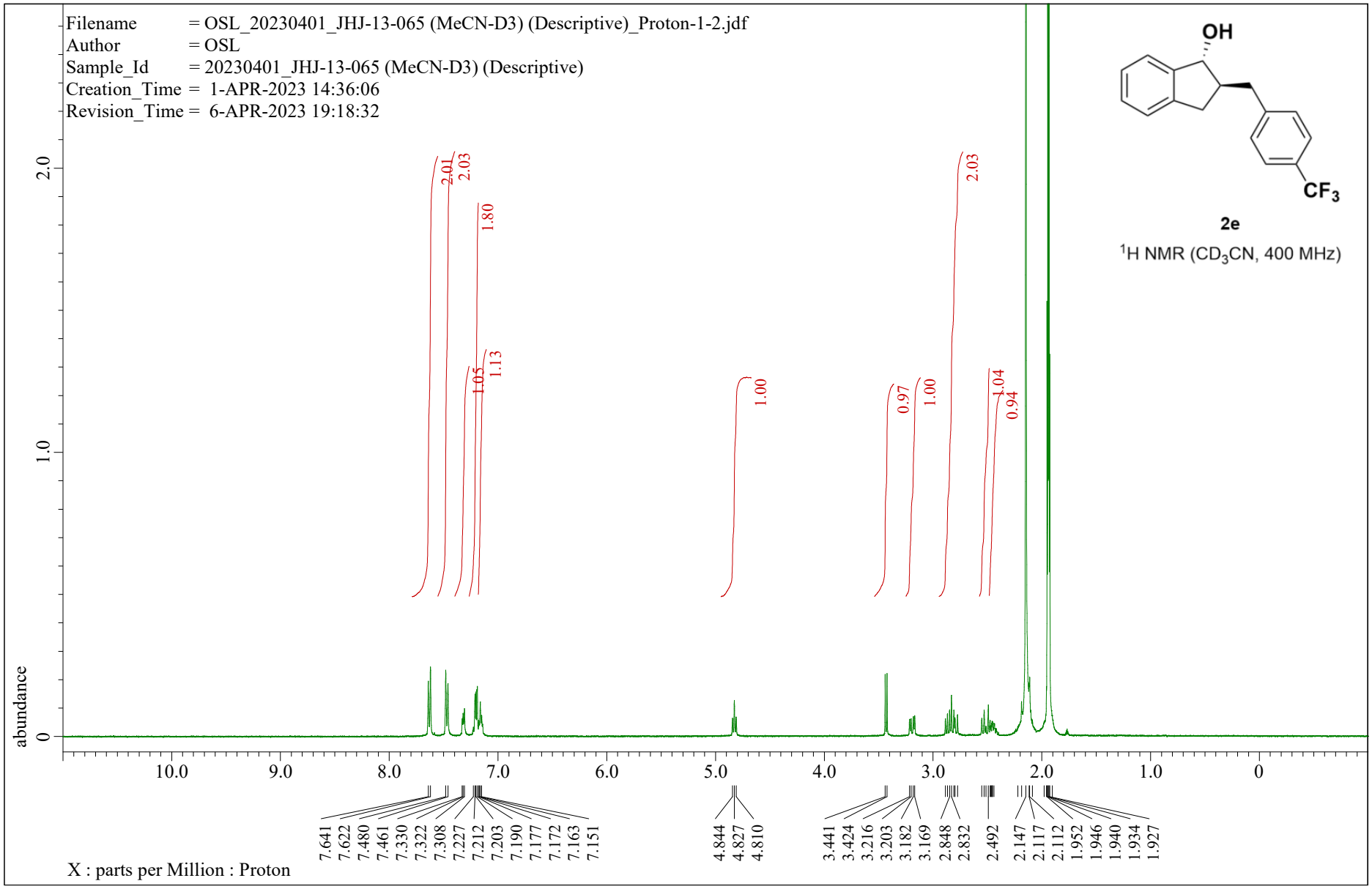

Filename = OSL_20230401_JHJ-13-063 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230401_JHJ-13-063 (MeCN-D3) (Descriptive)
Creation_Time = 1-APR-2023 18:20:59
Revision_Time = 6-APR-2023 16:08:45
OH
F
2c
1H NMR (CD3CN, 400 MHz)
3.25
2.98
1.91
1.00
0.95
1.11
1.12
1.09
1.14
0.89
abundance
X : parts per Million : Proton
7.318
7.306
7.298
7.293
7.284
7.277
7.263
7.209
7.204
7.198
7.192
7.187
7.073
7.050
4.818
4.801
4.784
3.403
3.393
3.387
3.377
3.075
2.847
2.719
2.695
2.510
2.151
1.952
1.946
1.940
1.934
1.928

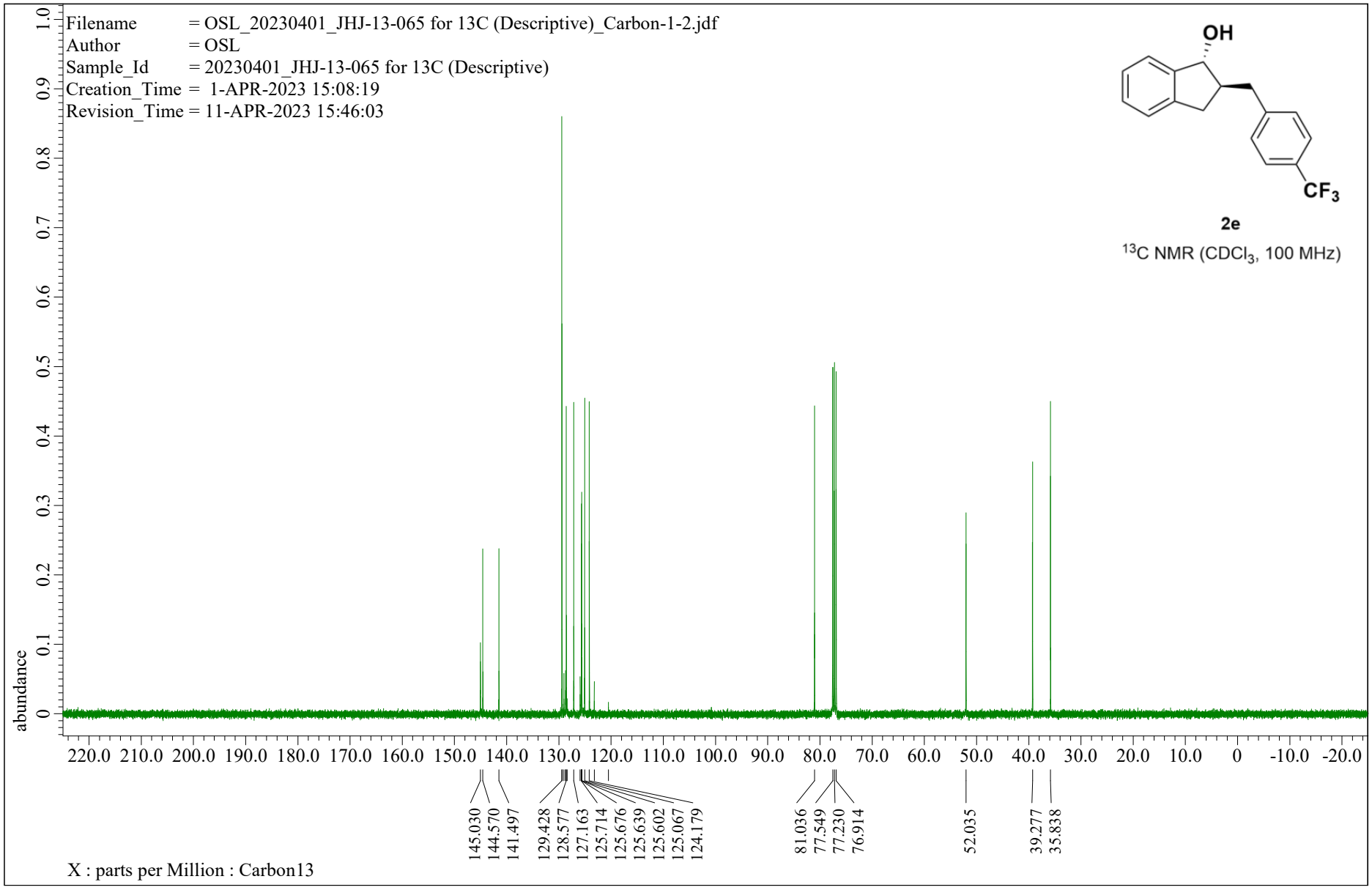

Filename = OSL_20230323_JHJ-13-063 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230323_JHJ-13-065 for 13C (Descriptive)
Creation_Time = 23-MAR-2023 10:20:05
Revision_Time = 11-APR-2023 15:43:09
OH
F
2c
13C NMR (CDCl3, 100 MHz)
(thousandths)
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
162.693
160.266
144.558
141.499
136.417
136.382
130.368
130.299
128.252
126.884
124.883
124.113
115.419
115.212
80.611
77.552
77.230
76.920
52.093
38.351
35.591
X : parts per Million : Carbon13

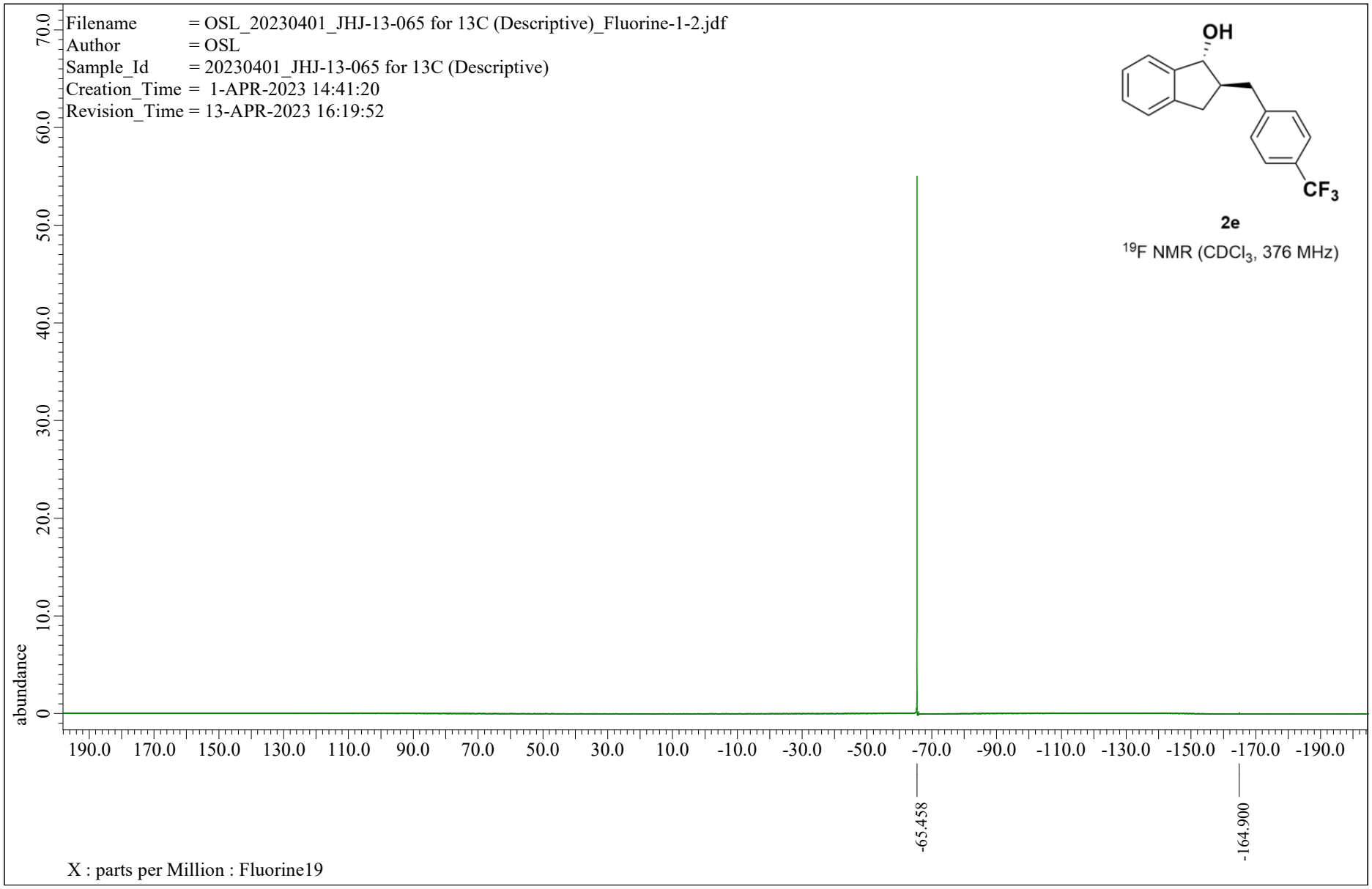

Filename = OSL_20230323_JHJ-13-063 for 13C (Descriptive)_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20230323_JHJ-13-065 for 13C (Descriptive)
Creation_Time = 23-MAR-2023 10:16:17
Revision_Time = 13-APR-2023 16:22:59
OH
F
2c
19F NMR (CDCl3, 376 MHz)
abundance
4.0
3.0
2.0
1.0
0
190.0 170.0 150.0 130.0 110.0 90.0 70.0 50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0
-120.311
-164.900
X : parts per Million : Fluorine19

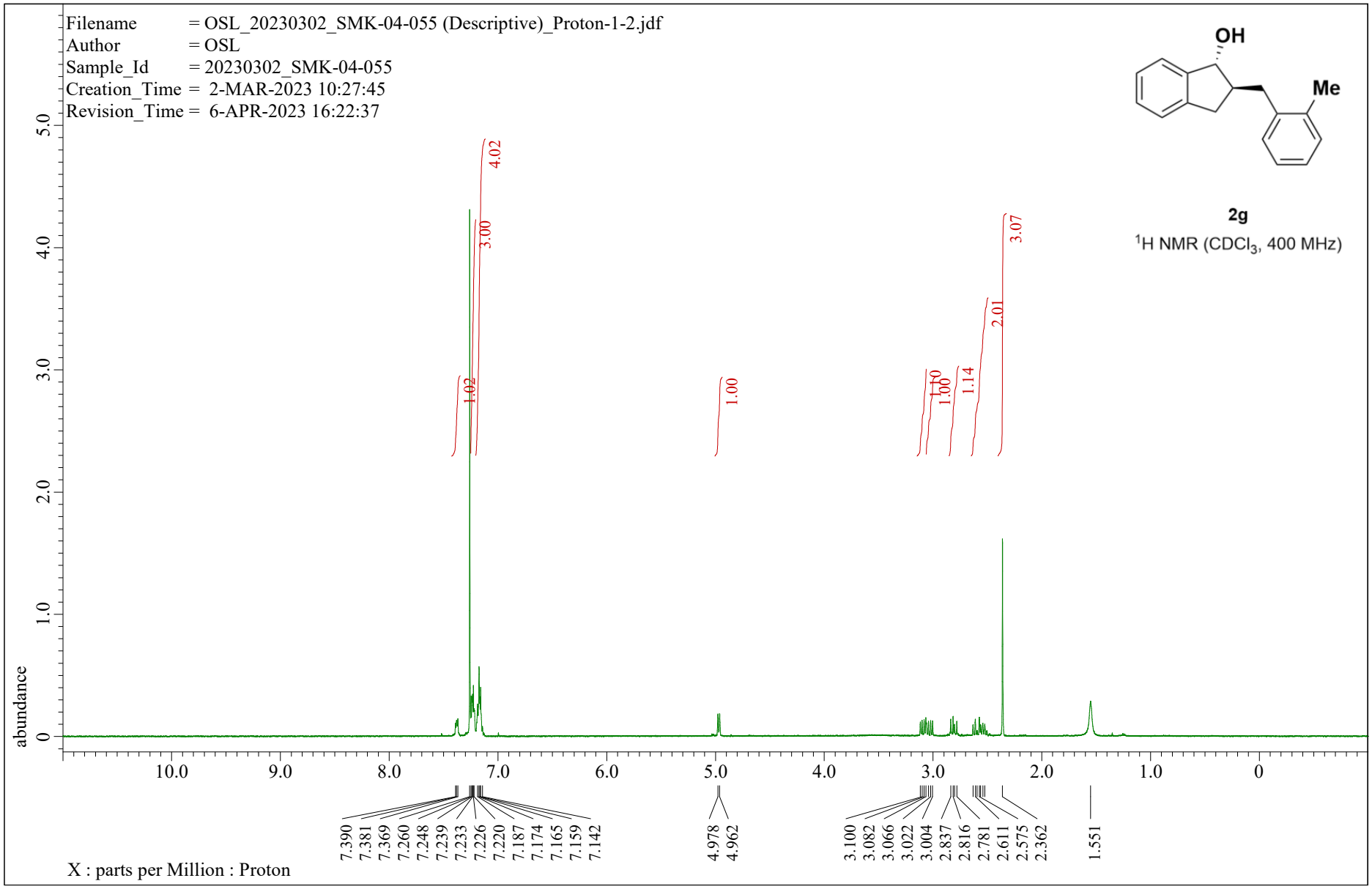

Filename = OSL_20230722_JHJ-13-097 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230722_JHJ-13-097 2nd column acetonitrile D3
Creation_Time = 22-JUL-2023 09:45:08
Revision_Time = 28-JUL-2023 09:36:41
OH
CN
2d
1H NMR (CD3CN, 400 MHz)
abundance
2.0
1.0
0
3.09
2.00
2.09
1.00
1.00
1.00
1.10
2.23
2.27
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.682
7.661
7.650
7.458
7.438
7.314
7.302
7.209
7.200
7.189
7.159
7.147
4.810
4.802
3.489
3.156
2.819
2.805
2.196
2.189
2.169
2.122
1.952
1.946
1.940
1.934
1.928
1.922
X : parts per Million : Proton

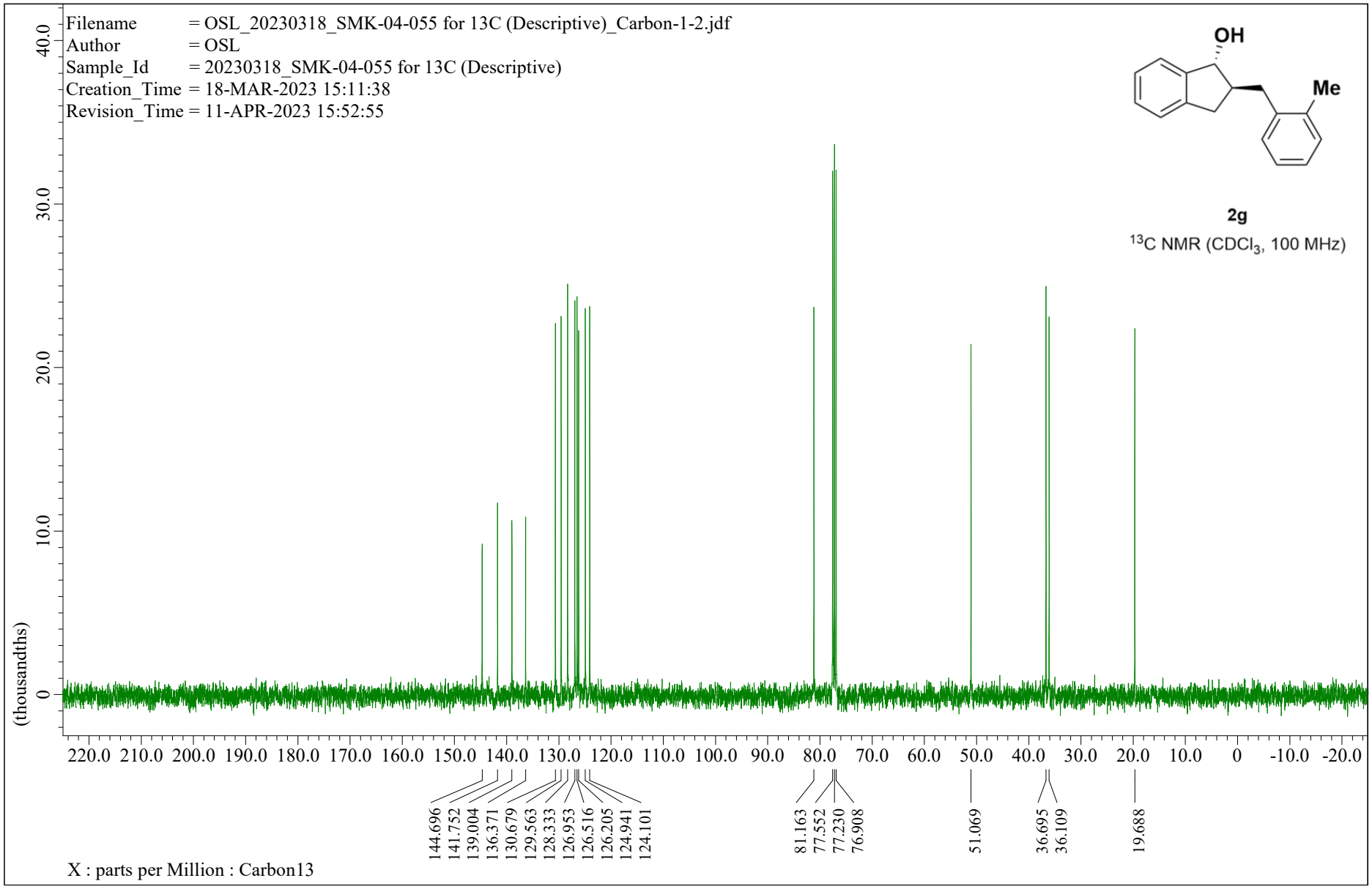

Filename = OSL_20230722_JHJ-13-097 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230722_JHJ-13-097 2nd column for 13C
Creation_Time = 22-JUL-2023 10:03:58
Revision_Time = 28-JUL-2023 10:06:36
OH
CN
2d
13C NMR (CDCl3, 100 MHz)
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3
240.0 230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0
146.617
144.363
141.143
132.415
129.816
128.459
127.079
124.941
124.067
119.145
110.037
80.703
77.552
77.230
76.920
51.679
39.397
35.580
X : parts per Million : Carbon13

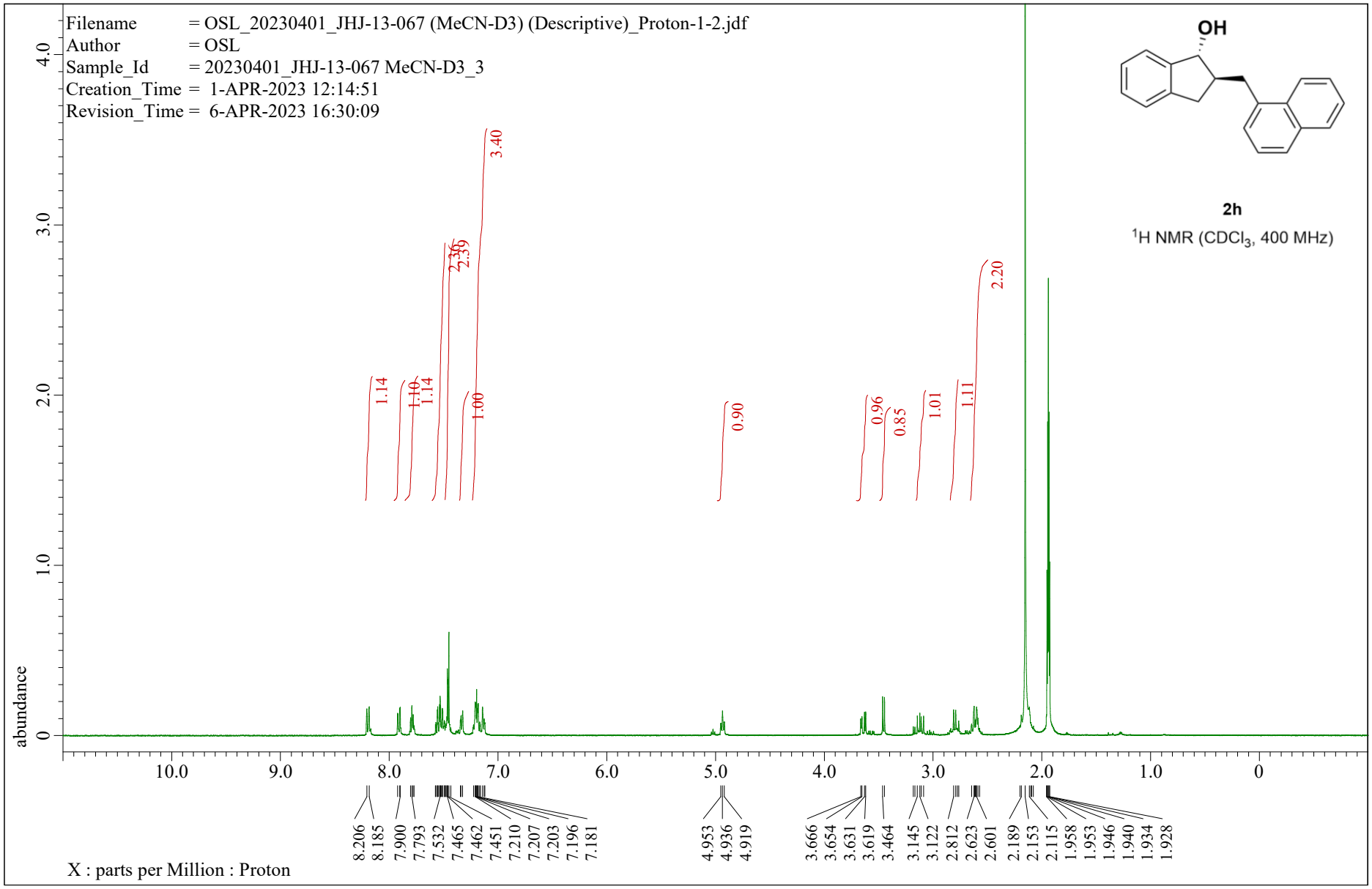

Filename = OSL_20230401_JHJ-13-065 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230401_JHJ-13-065 (MeCN-D3) (Descriptive)
Creation_Time = 1-APR-2023 14:36:06
Revision_Time = 6-APR-2023 19:18:32
OH
CF3
2e
1H NMR (CD3CN, 400 MHz)
abundance
X : parts per Million : Proton

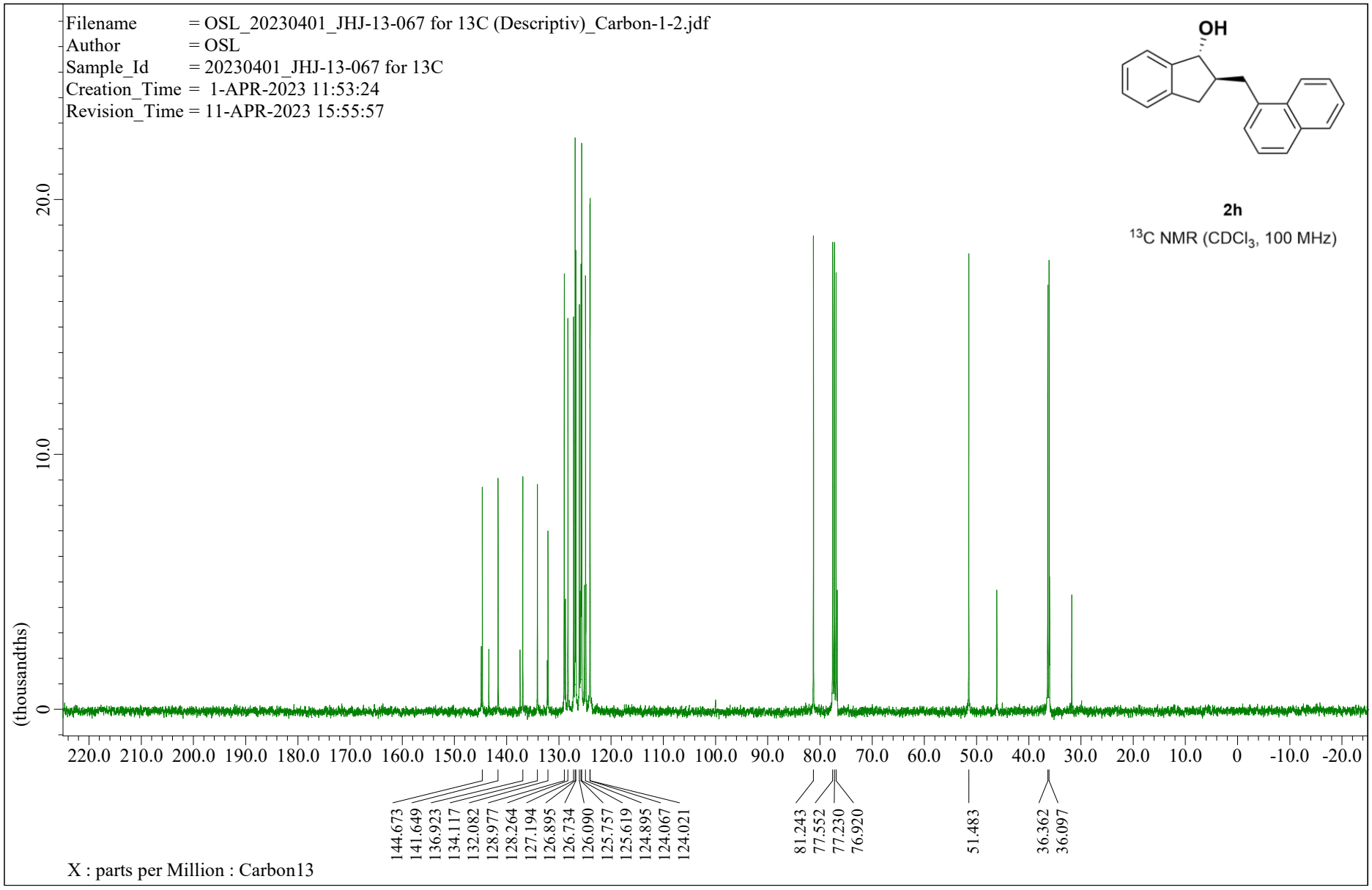

Filename = OSL_20230401_JHJ-13-065 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230401_JHJ-13-065 for 13C (Descriptive)
Creation_Time = 1-APR-2023 15:08:19
Revision_Time = 11-APR-2023 15:46:03
OH
CF3
2e
13C NMR (CDCl3, 100 MHz)
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
145.030
144.570
141.497
129.428
128.577
127.163
125.714
125.676
125.639
125.602
125.067
124.179
81.036
77.549
77.230
76.914
52.035
39.277
35.838
X : parts per Million : Carbon13

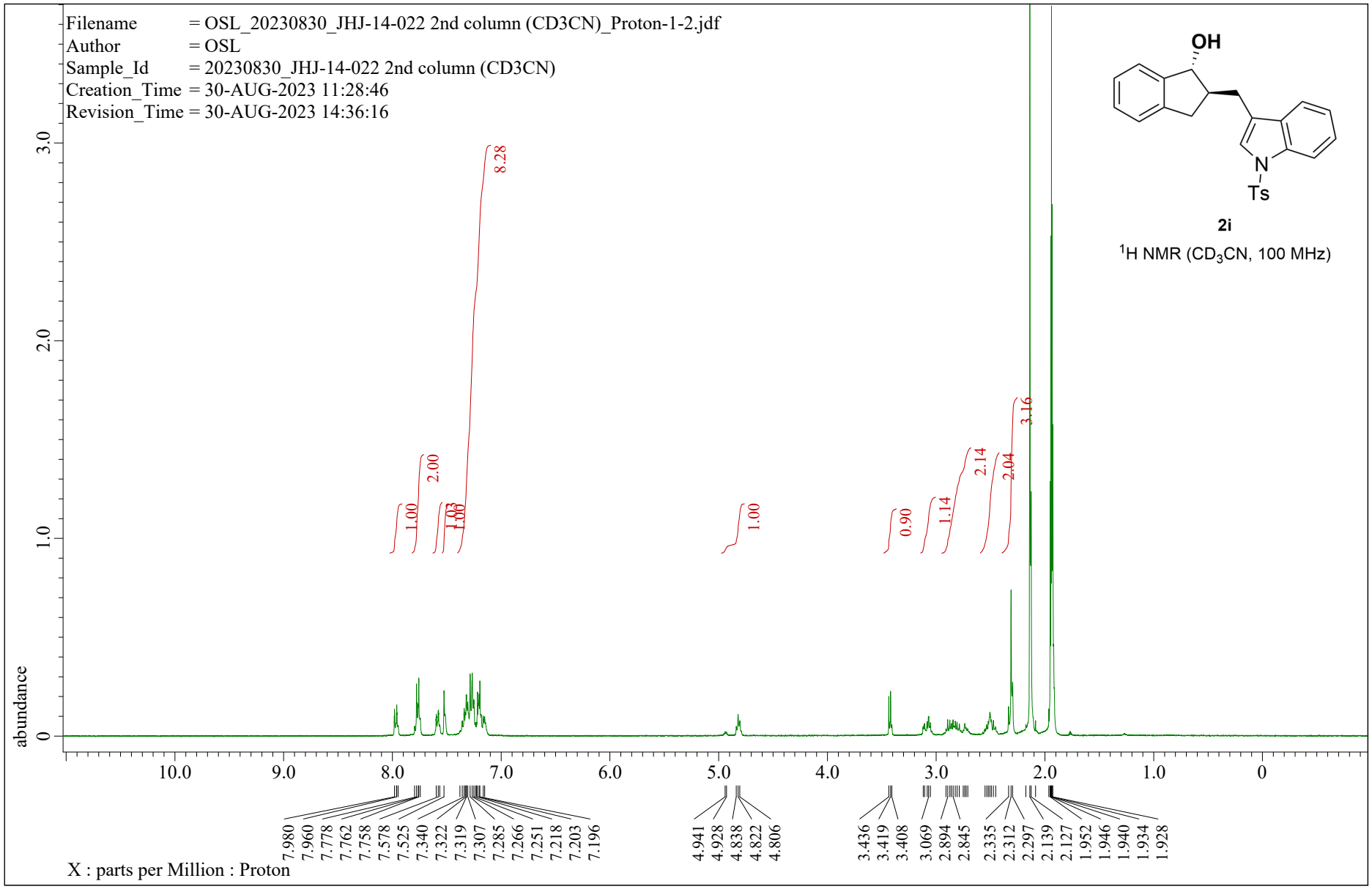

Filename = OSL_20230401_JHJ-13-065 for 13C (Descriptive)_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20230401_JHJ-13-065 for 13C (Descriptive)
Creation_Time = 1-APR-2023 14:41:20
Revision_Time = 13-APR-2023 16:19:52
OH
CF3
2e
19F NMR (CDCl3, 376 MHz)
abundance
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
190.0 170.0 150.0 130.0 110.0 90.0 70.0 50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0
-65.458
-164.900
X : parts per Million : Fluorine19

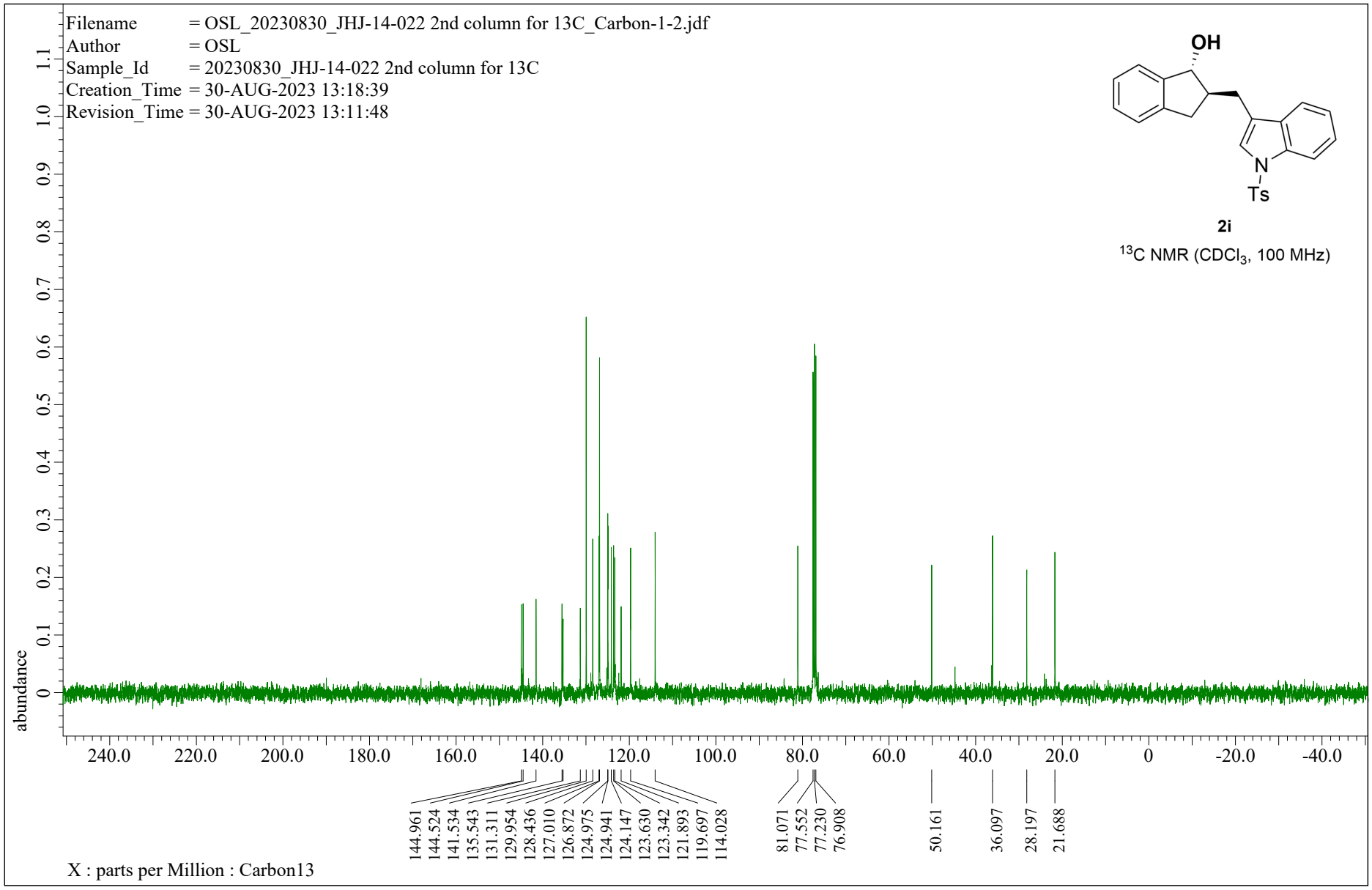

Filename = OSL_20230302_SMK-04-055 (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230302_SMK-04-055
Creation_Time = 2-MAR-2023 10:27:45
Revision_Time = 6-APR-2023 16:22:37
OH
Me
2g
^{1}H NMR ($CDCl_3$, 400 MHz)
abundance
X : parts per Million : Proton
4.02
3.00
1.02
1.00
1.10
1.00
1.14
2.01
3.07
7.390
7.381
7.369
7.260
7.248
7.239
7.233
7.226
7.220
7.187
7.174
7.165
7.159
7.142
4.978
4.962
3.100
3.082
3.066
3.022
3.004
2.837
2.816
2.781
2.611
2.575
2.362
1.551

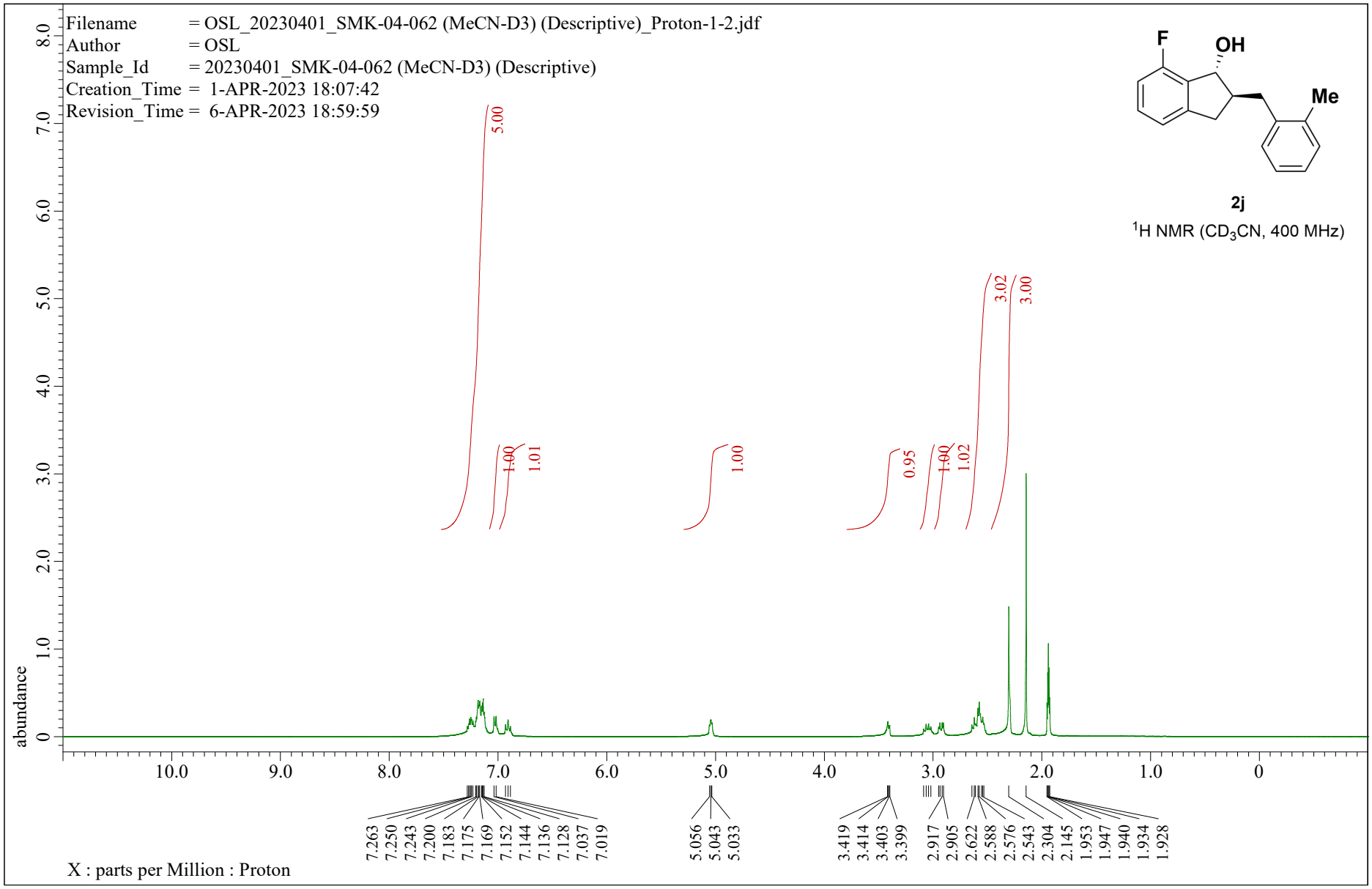

Filename = OSL_20230318_SMK-04-055 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230318_SMK-04-055 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 15:11:38
Revision_Time = 11-APR-2023 15:52:55
OH
Me
2g
13C NMR (CDCl3, 100 MHz)
(thousandths)
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
144.696
141.752
139.004
136.371
130.679
129.563
128.333
126.953
126.516
126.205
124.941
124.101
81.163
77.552
77.230
76.908
51.069
36.695
36.109
19.688
X : parts per Million : Carbon13

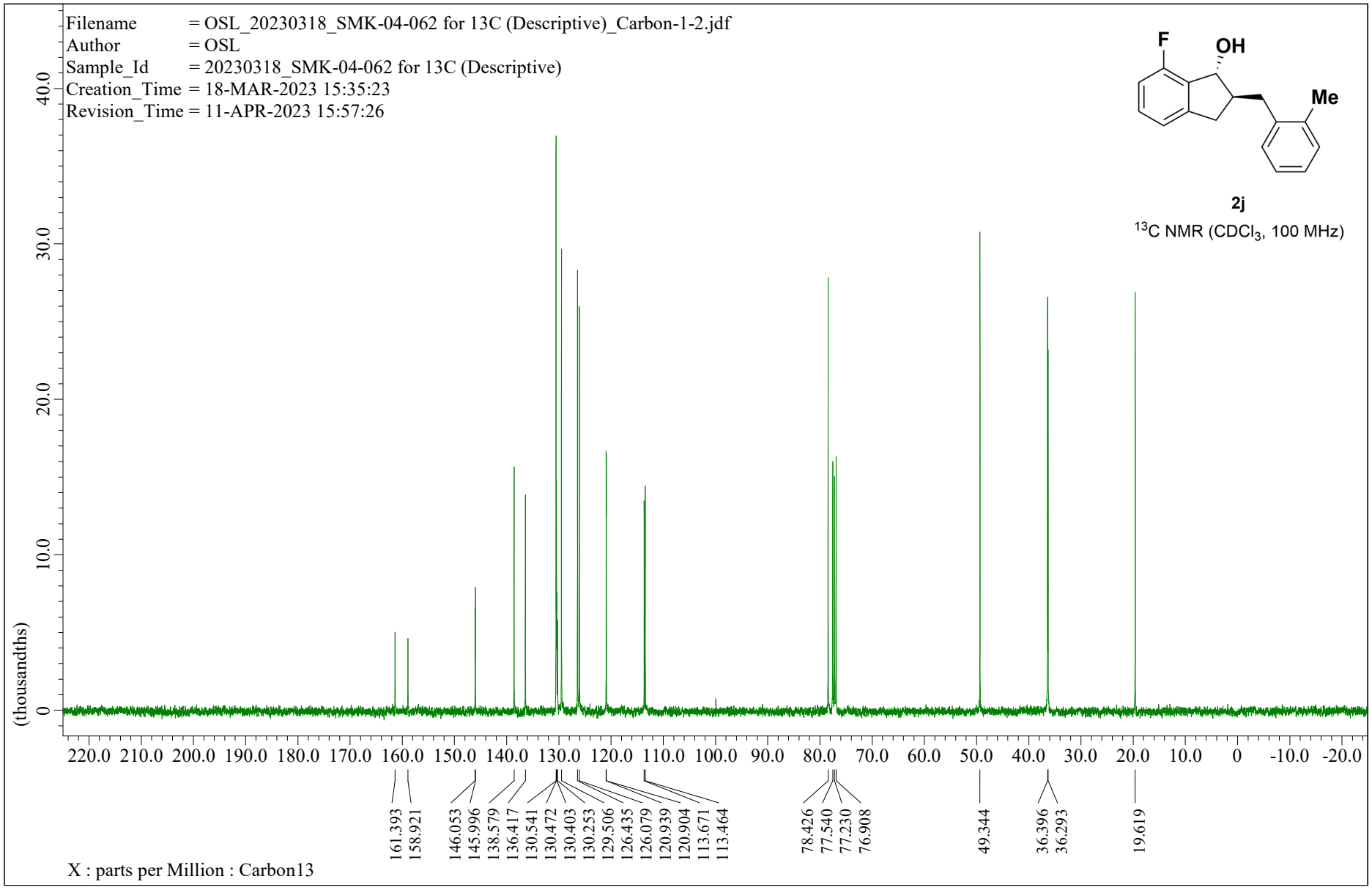

Filename = OSL_20230401_JHJ-13-067 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230401_JHJ-13-067 MeCN-D3_3
Creation_Time = 1-APR-2023 12:14:51
Revision_Time = 6-APR-2023 16:30:09
OH
2h
1H NMR (CDCl3, 400 MHz)
abundance
X : parts per Million : Proton
1.14
1.10
1.14
2.36
2.39
3.40
1.00
0.90
0.96
0.85
1.01
1.11
2.20
8.206
8.185
7.900
7.793
7.532
7.465
7.462
7.451
7.210
7.207
7.203
7.196
7.181
4.953
4.936
4.919
3.666
3.654
3.631
3.619
3.464
3.145
3.122
2.812
2.623
2.601
2.189
2.153
2.115
1.958
1.953
1.946
1.940
1.934
1.928


Filename = OSL_20230401_JHJ-13-067 for 13C (Descriptiv)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230401_JHJ-13-067 for 13C
Creation_Time = 1-APR-2023 11:53:24
Revision_Time = 11-APR-2023 15:55:57
OH
2h
13C NMR (CDCl3, 100 MHz)
(thousandths)
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
144.673
141.649
136.923
134.117
132.082
128.977
128.264
127.194
126.895
126.734
126.090
125.757
125.619
124.895
124.067
124.021
81.243
77.552
77.230
76.920
51.483
36.362
36.097
X : parts per Million : Carbon13

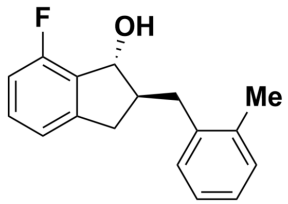

Filename = OSL_20230830_JHJ-14-022 2nd column (CD3CN)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230830_JHJ-14-022 2nd column (CD3CN)
Creation_Time = 30-AUG-2023 11:28:46
Revision_Time = 30-AUG-2023 14:36:16
OH
N
Ts
2i
1H NMR (CD3CN, 100 MHz)
abundance
X : parts per Million : Proton
8.28
2.00
1.00
1.00
0.90
1.14
2.14
2.04
3.16
7.980
7.960
7.778
7.762
7.758
7.578
7.525
7.340
7.322
7.319
7.307
7.285
7.266
7.251
7.218
7.203
7.196
4.941
4.928
4.838
4.822
4.806
3.436
3.419
3.408
3.069
2.894
2.845
2.335
2.312
2.297
2.139
2.127
1.952
1.946
1.940
1.934
1.928


Filename = OSL_20230830_JHJ-14-022 2nd column for 13C_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230830_JHJ-14-022 2nd column for 13C
Creation_Time = 30-AUG-2023 13:18:39
Revision_Time = 30-AUG-2023 13:11:48
OH
N
Ts
2i
13C NMR (CDCl3, 100 MHz)
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
240.0
220.0
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0
-20.0
-40.0
144.961
144.524
141.534
135.543
131.311
129.954
128.436
127.010
126.872
124.975
124.941
124.147
123.630
123.342
121.893
119.697
114.028
81.071
77.552
77.230
76.908
50.161
36.097
28.197
21.688
X : parts per Million : Carbon13


Filename = OSL_20230401_SMK-04-062 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230401_SMK-04-062 (MeCN-D3) (Descriptive)
Creation_Time = 1-APR-2023 18:07:42
Revision_Time = 6-APR-2023 18:59:59
F
OH
Me
2j
1H NMR (CD3CN, 400 MHz)
5.00
1.00
1.01
1.00
0.95
1.00
1.02
3.02
3.00
abundance
X : parts per Million : Proton
7.263
7.250
7.243
7.200
7.183
7.175
7.169
7.152
7.144
7.136
7.128
7.037
7.019
5.056
5.043
5.033
3.419
3.414
3.403
3.399
2.917
2.905
2.622
2.588
2.576
2.543
2.304
2.145
1.953
1.947
1.940
1.934
1.928

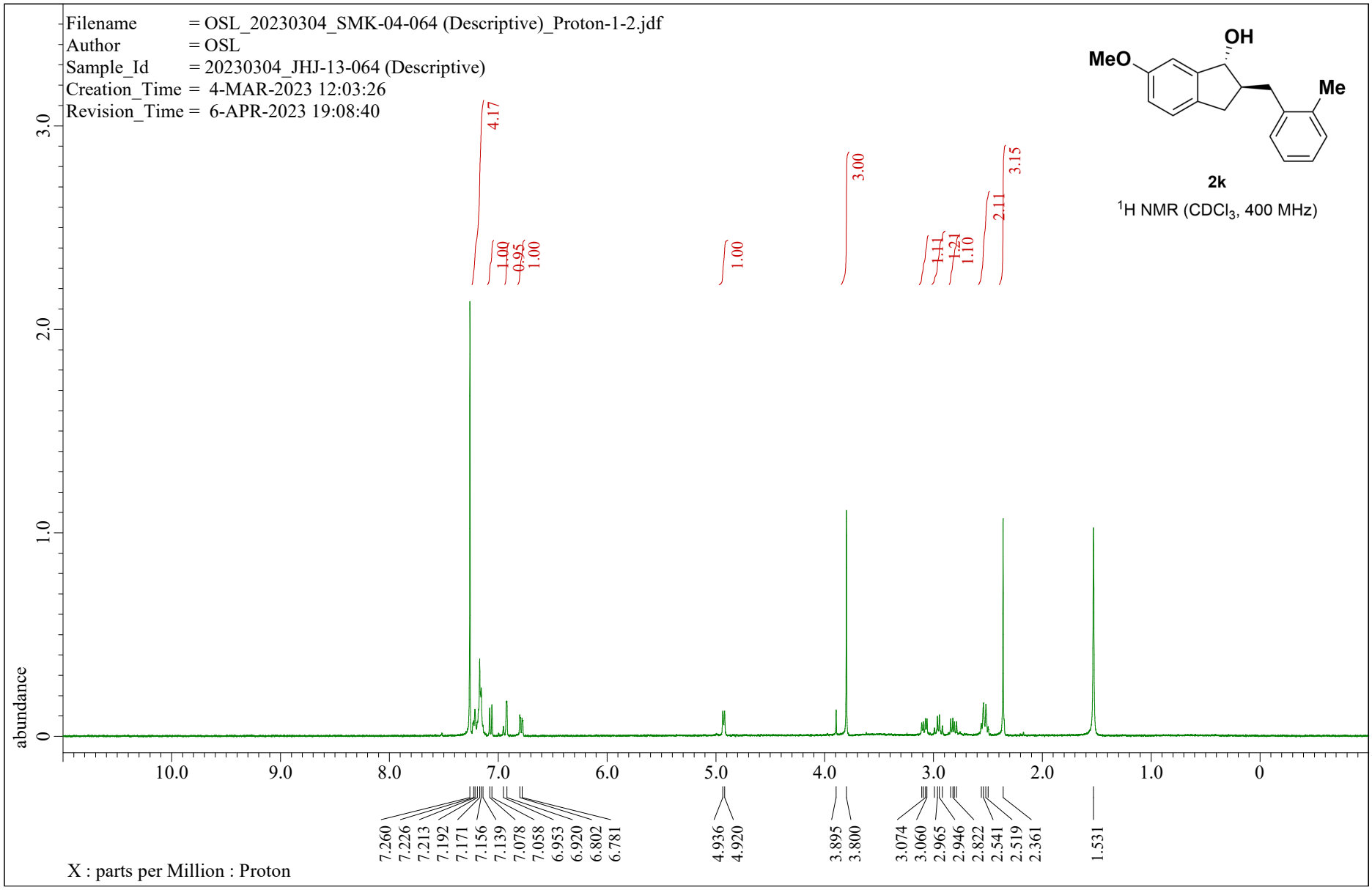

Filename = OSL_20230318_SMK-04-062 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230318_SMK-04-062 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 15:35:23
Revision_Time = 11-APR-2023 15:57:26
F
OH
Me
2j
13C NMR (CDCl3, 100 MHz)
(thousandths)
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
161.393
158.921
146.053
145.996
138.579
136.417
130.541
130.472
130.403
130.253
129.506
126.435
126.079
120.939
120.904
113.671
113.464
78.426
77.540
77.230
76.908
49.344
36.396
36.293
19.619
X : parts per Million : Carbon13

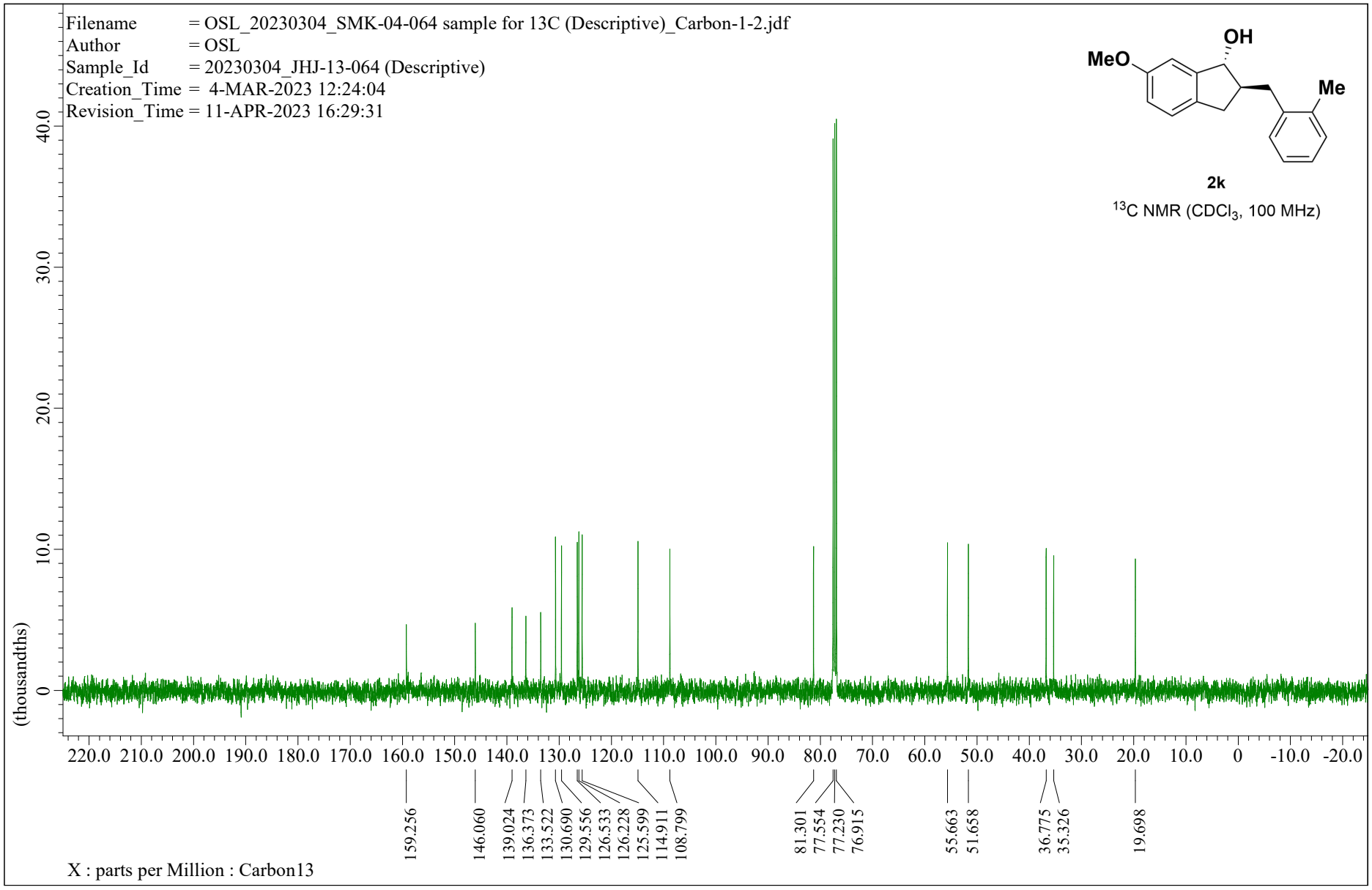
Filename = OSL_20230318_SMK-04-062 for 13C (Descriptive)_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20230318_SMK-04-062 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 15:40:23
Revision_Time = 13-APR-2023 16:28:33

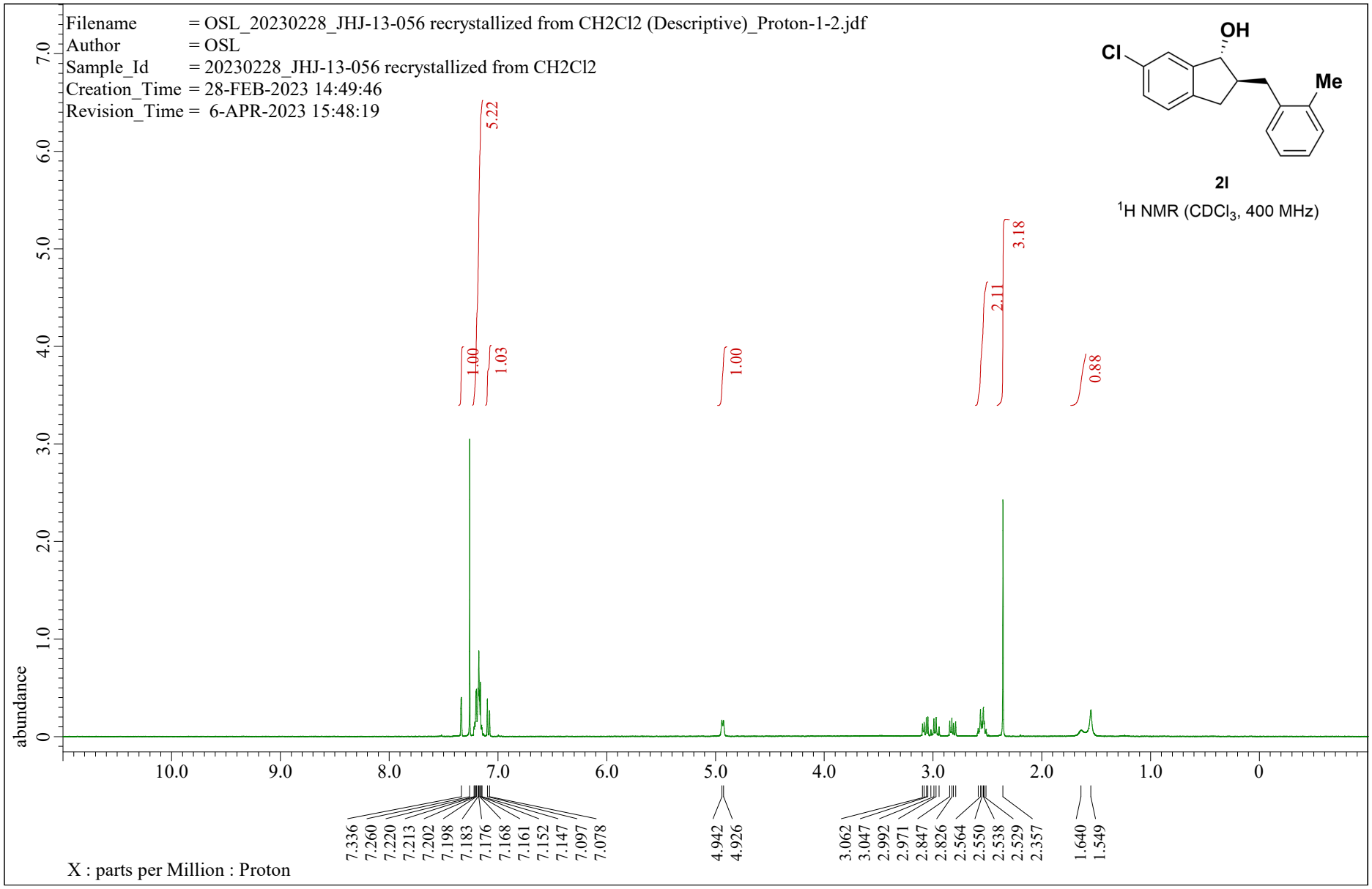


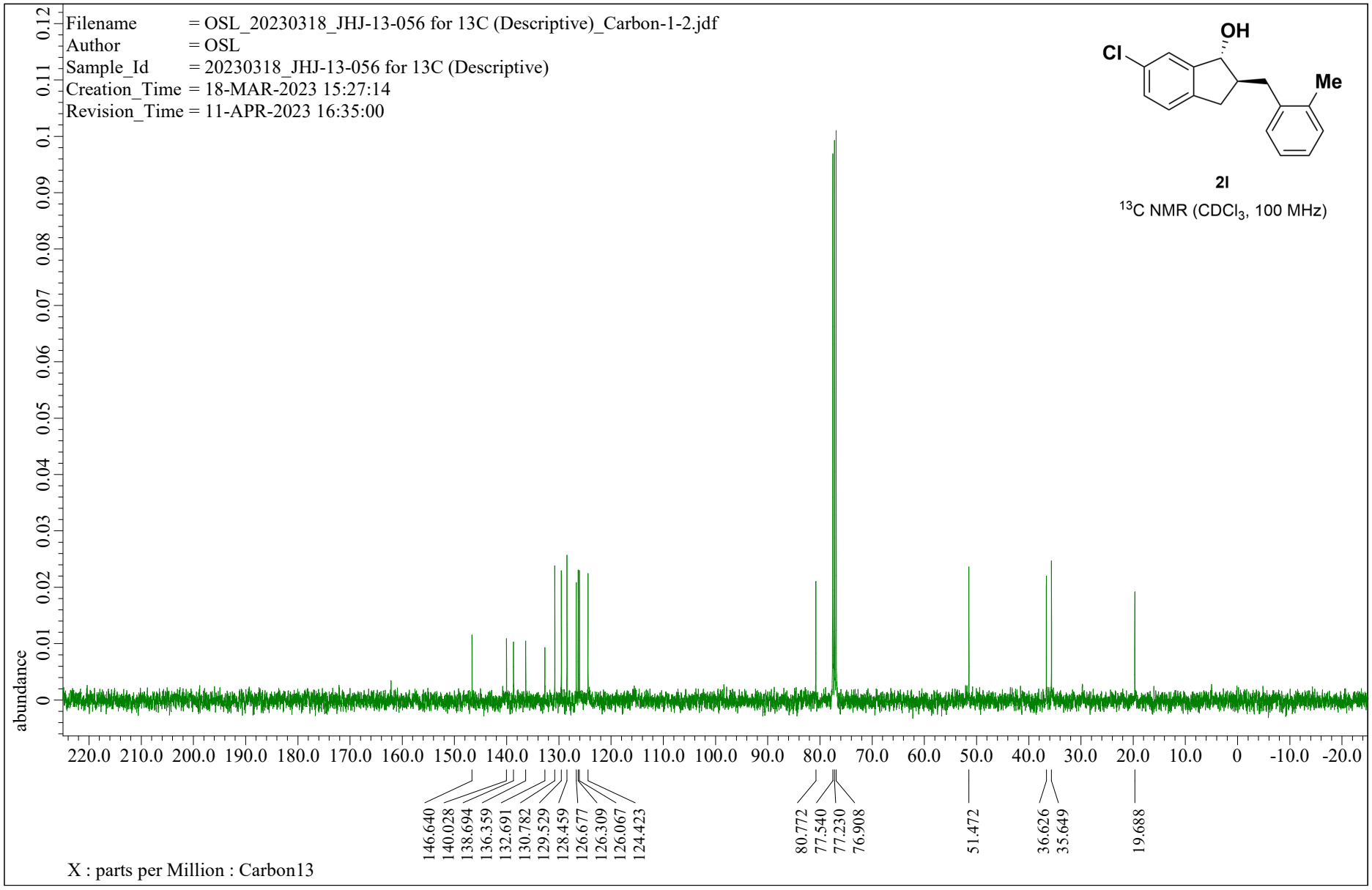
2j

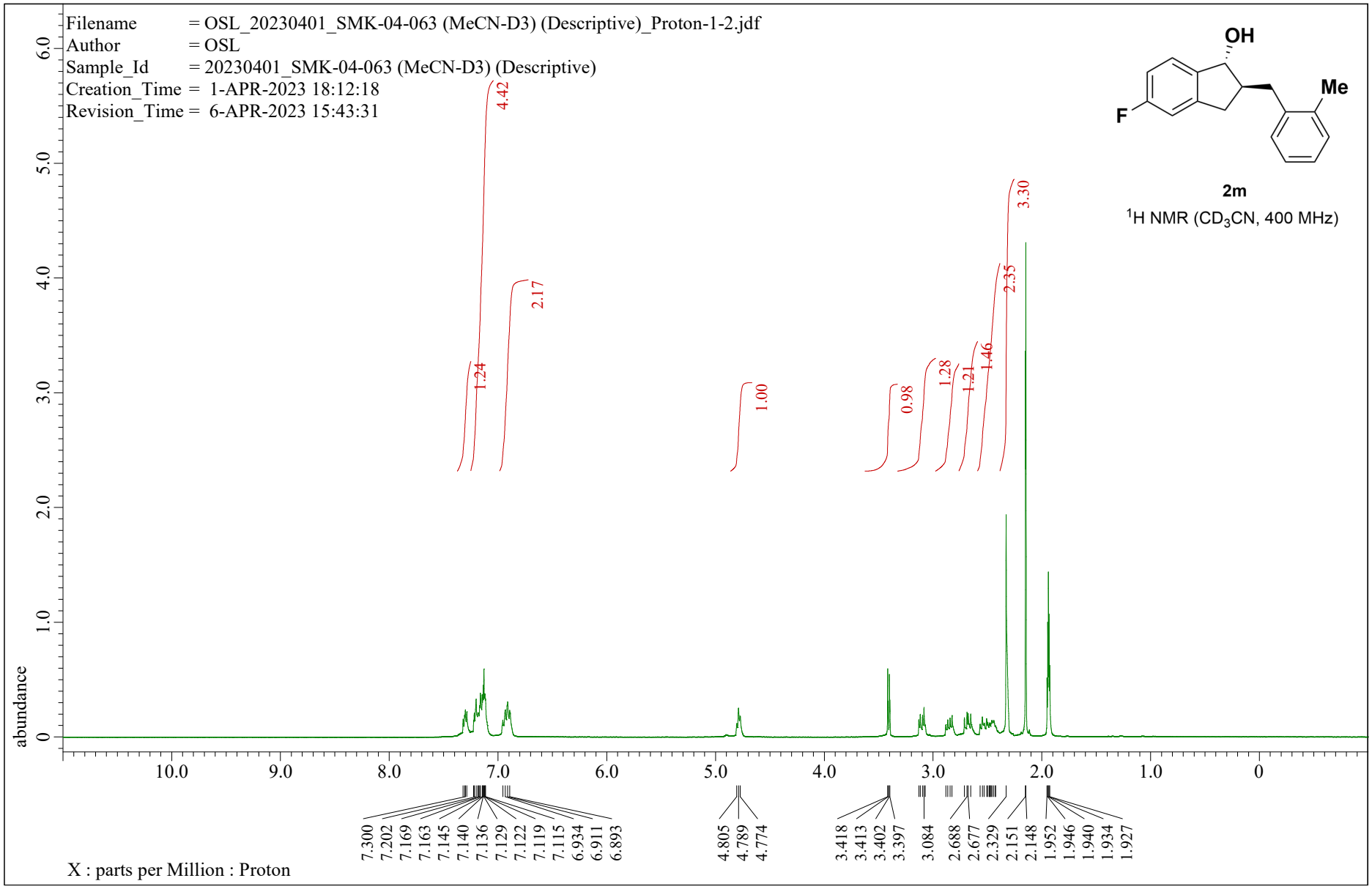
^{19}F NMR ($CDCl_3$, 376 MHz)

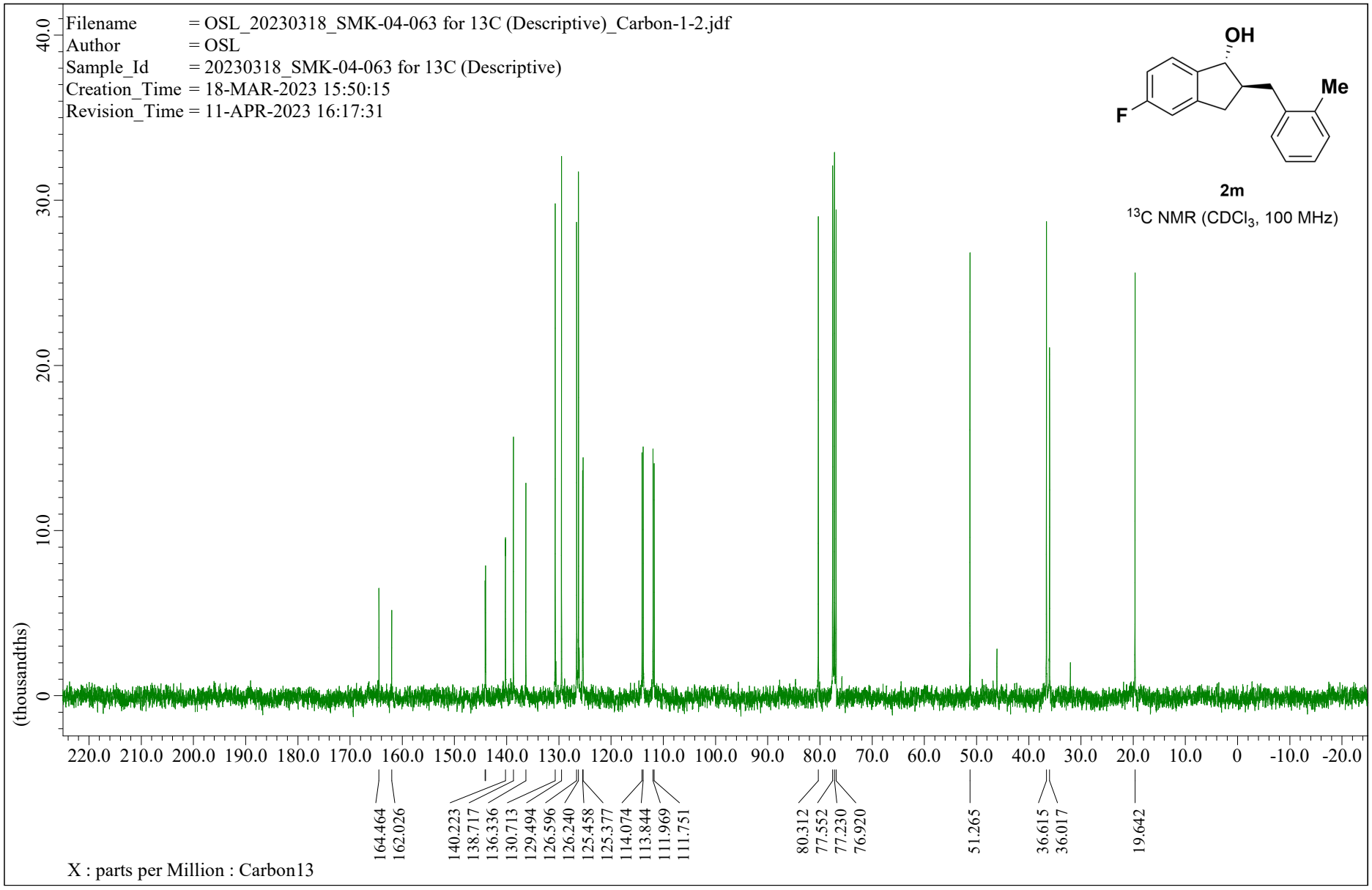

Filename = OSL_20230304_SMK-04-064 (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230304_JHJ-13-064 (Descriptive)
Creation_Time = 4-MAR-2023 12:03:26
Revision_Time = 6-APR-2023 19:08:40
MeO
OH
Me
2k
1H NMR (CDCl3, 400 MHz)
4.17
1.00
0.95
1.00
1.00
3.00
1.11
1.21
1.10
2.11
3.15
abundance
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.260
7.226
7.213
7.192
7.171
7.156
7.139
7.078
7.058
6.953
6.920
6.802
6.781
4.936
4.920
3.895
3.800
3.074
3.060
2.965
2.946
2.822
2.541
2.519
2.361
1.531
X : parts per Million : Proton

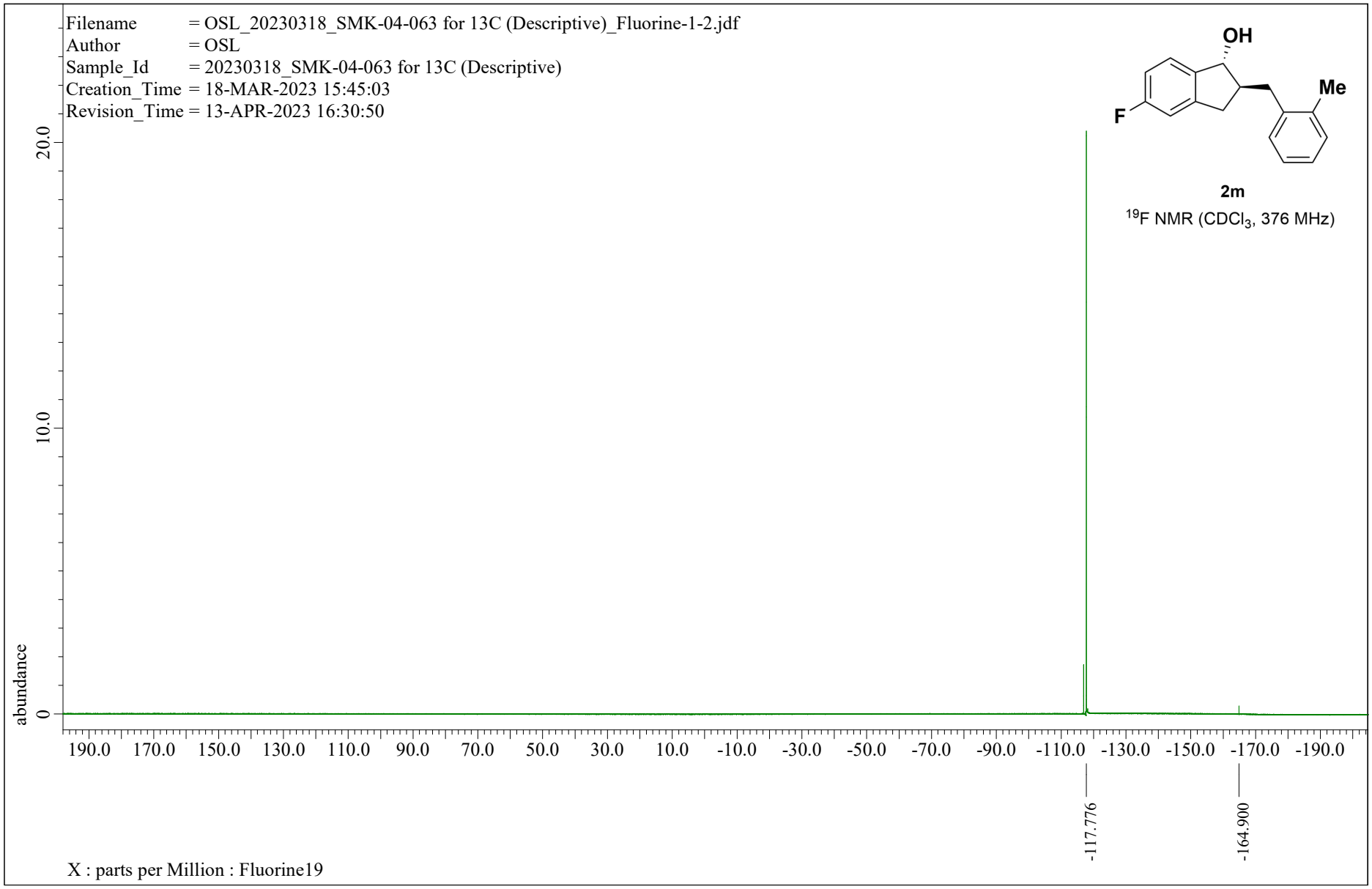

Filename = OSL_20230304_SMK-04-064 sample for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230304_JHJ-13-064 (Descriptive)
Creation_Time = 4-MAR-2023 12:24:04
Revision_Time = 11-APR-2023 16:29:31
MeO
OH
Me
2k
13C NMR (CDCl3, 100 MHz)
(thousandths)
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
159.256
146.060
139.024
136.373
133.522
130.690
129.556
126.533
126.228
125.599
114.911
108.799
81.301
77.554
77.230
76.915
55.663
51.658
36.775
35.326
19.698
X : parts per Million : Carbon13

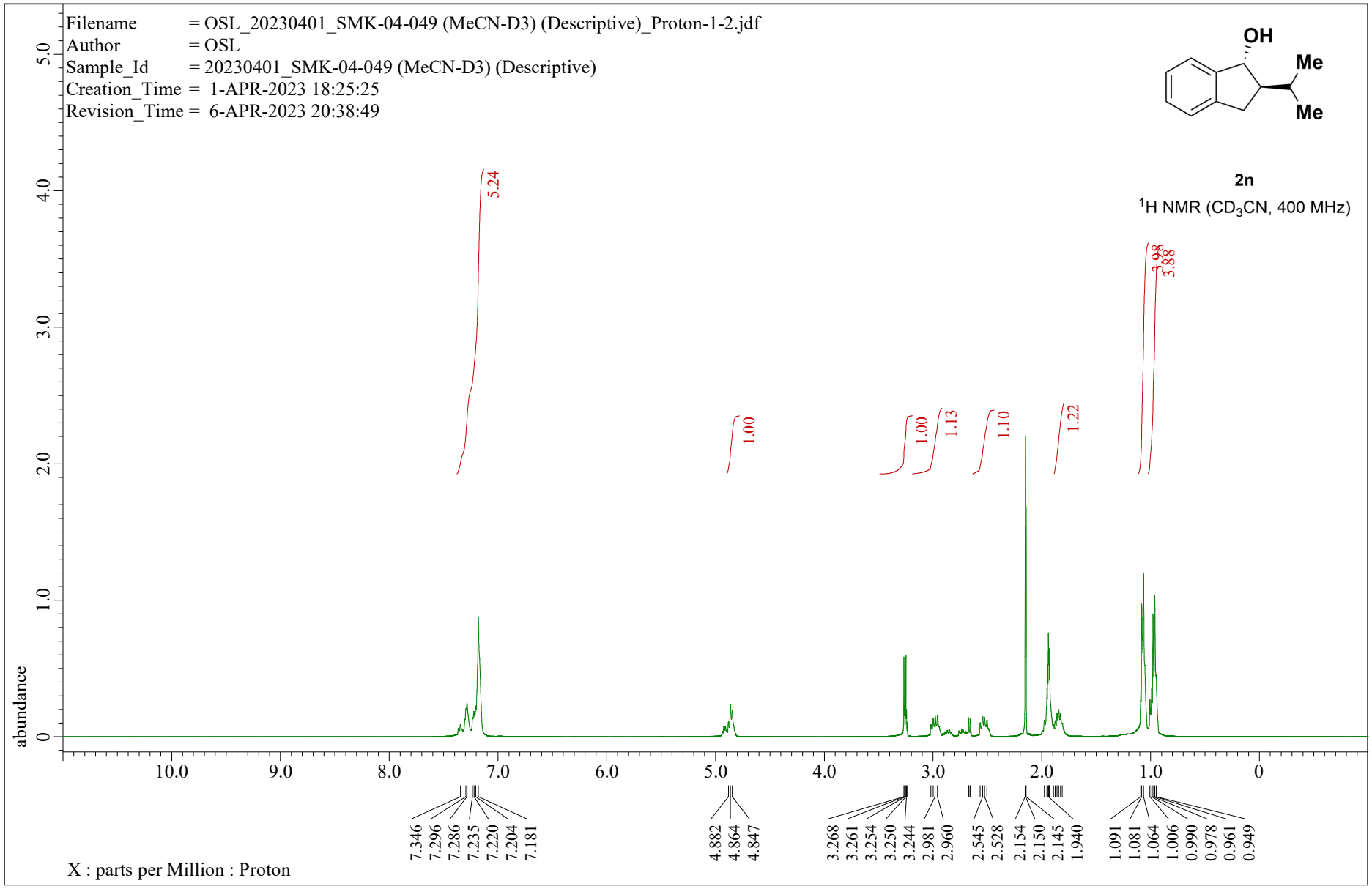

Filename = OSL_20230228_JHJ-13-056 recrystallized from CH2Cl2 (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230228_JHJ-13-056 recrystallized from CH2Cl2
Creation_Time = 28-FEB-2023 14:49:46
Revision_Time = 6-APR-2023 15:48:19
Cl
OH
Me
2l
1H NMR (CDCl3, 400 MHz)
5.22
3.18
2.11
1.00
1.03
1.00
0.88
abundance
X : parts per Million : Proton
7.336
7.260
7.220
7.213
7.202
7.198
7.183
7.176
7.168
7.161
7.152
7.147
7.097
7.078
4.942
4.926
3.062
3.047
2.992
2.971
2.847
2.826
2.564
2.550
2.538
2.529
2.357
1.640
1.549

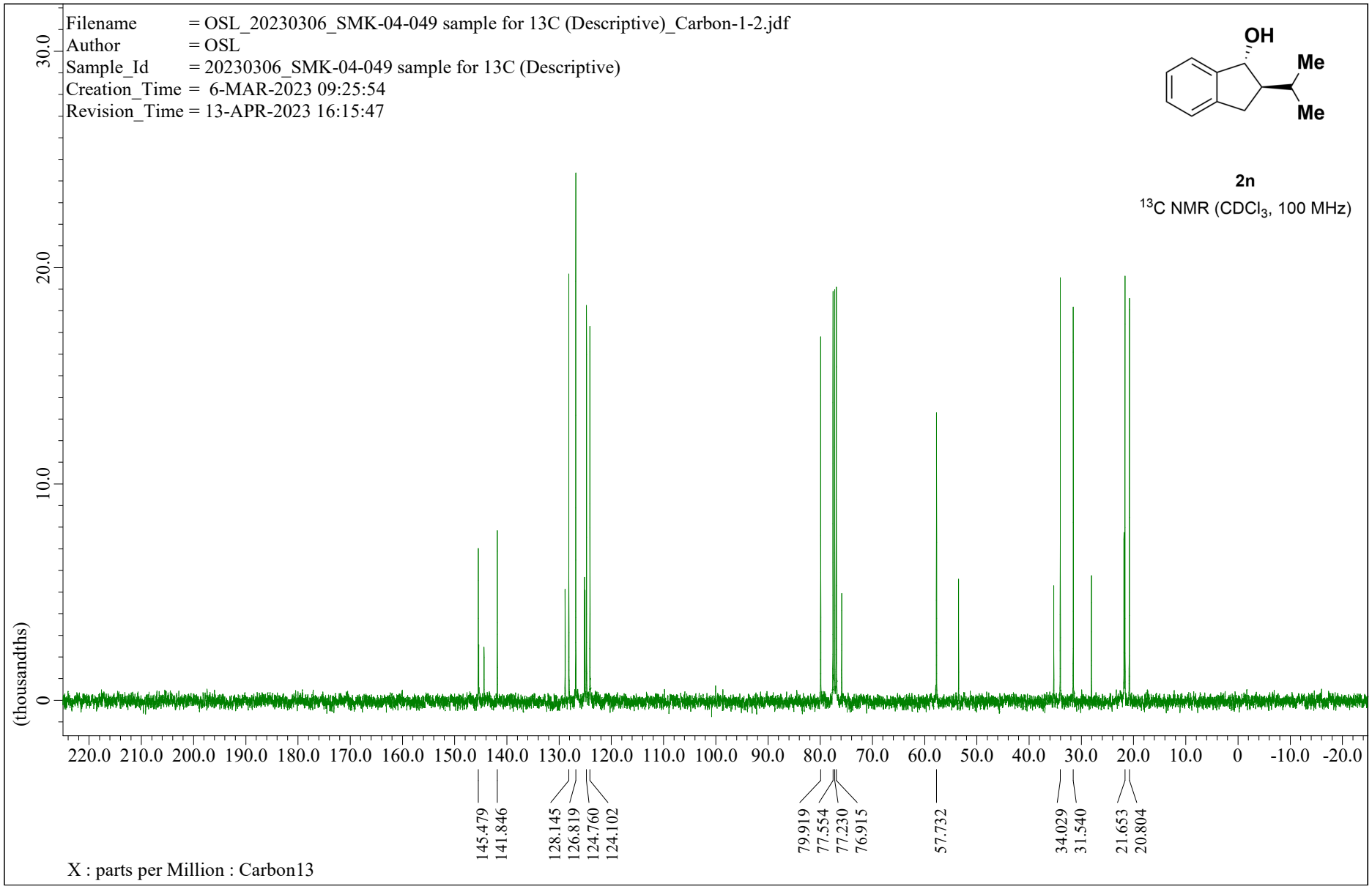

Filename = OSL_20230318_JHJ-13-056 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230318_JHJ-13-056 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 15:27:14
Revision_Time = 11-APR-2023 16:35:00
Cl
OH
Me
2l
13C NMR (CDCl3, 100 MHz)
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
146.640
140.028
138.694
136.359
132.691
130.782
129.529
128.459
126.677
126.309
126.067
124.423
80.772
77.540
77.230
76.908
51.472
36.626
35.649
19.688
X : parts per Million : Carbon13

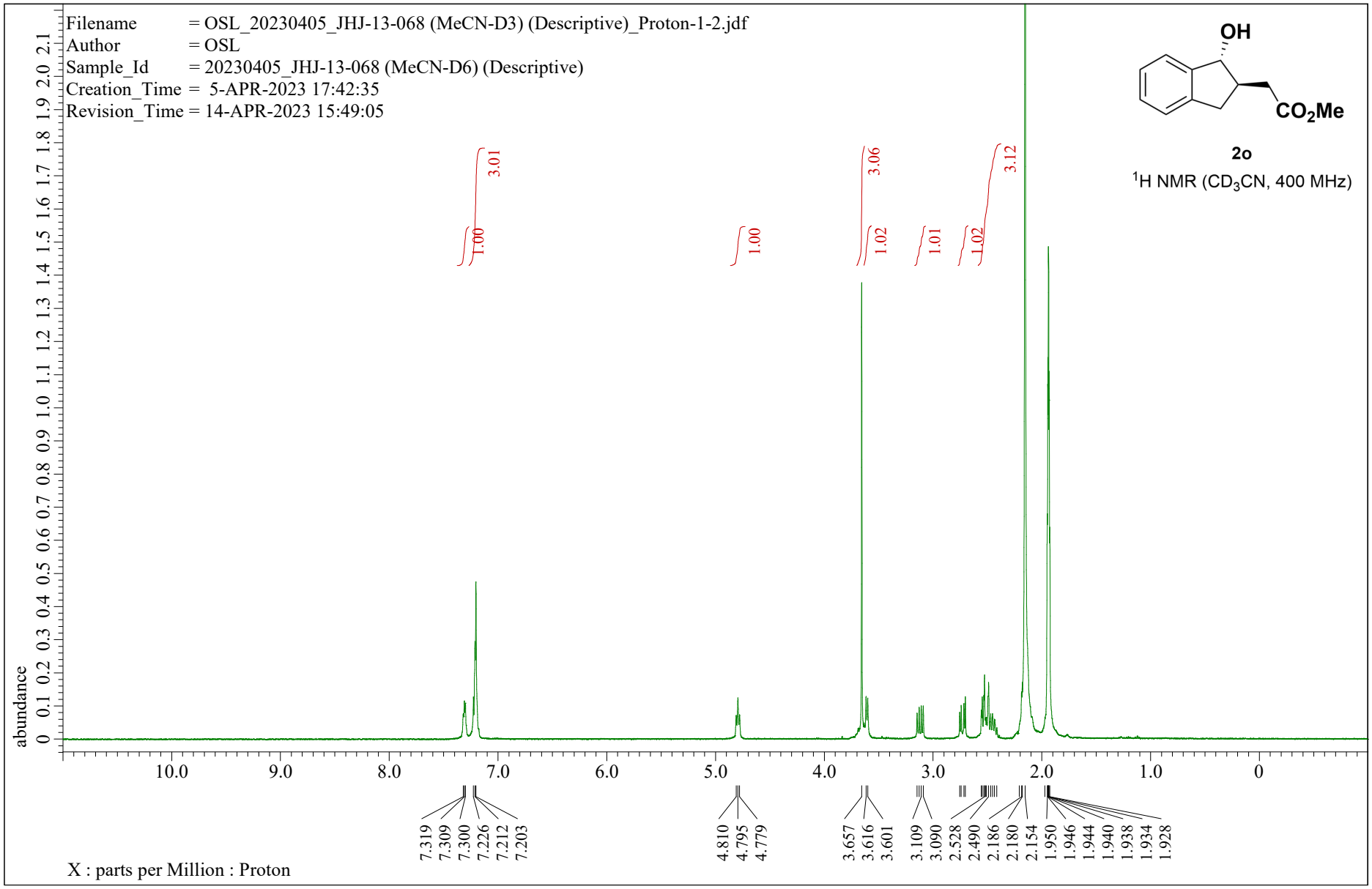

Filename = OSL_20230401_SMK-04-063 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230401_SMK-04-063 (MeCN-D3) (Descriptive)
Creation_Time = 1-APR-2023 18:12:18
Revision_Time = 6-APR-2023 15:43:31
OH
Me
F
2m
1H NMR (CD3CN, 400 MHz)
4.42
2.17
1.24
1.00
0.98
1.28
1.21
1.46
2.35
3.30
abundance
X : parts per Million : Proton
7.300
7.202
7.169
7.163
7.145
7.140
7.136
7.129
7.122
7.119
7.115
6.934
6.911
6.893
4.805
4.789
4.774
3.418
3.413
3.402
3.397
3.084
2.688
2.677
2.329
2.151
2.148
1.952
1.946
1.940
1.934
1.927


Filename = OSL_20230318_SMK-04-063 for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230318_SMK-04-063 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 15:50:15
Revision_Time = 11-APR-2023 16:17:31
OH
Me
F
2m
13C NMR (CDCl3, 100 MHz)
(thousandths)
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
164.464
162.026
140.223
138.717
136.336
130.713
129.494
126.596
126.240
125.458
125.377
114.074
113.844
111.969
111.751
80.312
77.552
77.230
76.920
51.265
36.615
36.017
19.642
X : parts per Million : Carbon13


Filename = OSL_20230318_SMK-04-063 for 13C (Descriptive)_Fluorine-1-2.jdf
Author = OSL
Sample_Id = 20230318_SMK-04-063 for 13C (Descriptive)
Creation_Time = 18-MAR-2023 15:45:03
Revision_Time = 13-APR-2023 16:30:50
OH
Me
F
2m
19F NMR (CDCl3, 376 MHz)
abundance
20.0
10.0
0
190.0 170.0 150.0 130.0 110.0 90.0 70.0 50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0
-117.776
-164.900
X : parts per Million : Fluorine19


Filename = OSL_20230401_SMK-04-049 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230401_SMK-04-049 (MeCN-D3) (Descriptive)
Creation_Time = 1-APR-2023 18:25:25
Revision_Time = 6-APR-2023 20:38:49
OH
Me
Me
2n
1H NMR (CD3CN, 400 MHz)
abundance
X : parts per Million : Proton
5.24
1.00
1.00
1.13
1.10
1.22
3.98
3.88
7.346
7.296
7.286
7.235
7.220
7.204
7.181
4.882
4.864
4.847
3.268
3.261
3.254
3.250
3.244
2.981
2.960
2.545
2.528
2.154
2.150
2.145
1.940
1.091
1.081
1.064
1.006
0.990
0.978
0.961
0.949


Filename = OSL_20230306_SMK-04-049 sample for 13C (Descriptive)_Carbon-1-2.jdf
Author = OSL
Sample_Id = 20230306_SMK-04-049 sample for 13C (Descriptive)
Creation_Time = 6-MAR-2023 09:25:54
Revision_Time = 13-APR-2023 16:15:47
OH
Me
Me
2n
13C NMR (CDCl3, 100 MHz)
(thousandths)
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
145.479
141.846
128.145
126.819
124.760
124.102
79.919
77.554
77.230
76.915
57.732
34.029
31.540
21.653
20.804
X : parts per Million : Carbon13


Filename = OSL_20230405_JHJ-13-068 (MeCN-D3) (Descriptive)_Proton-1-2.jdf
Author = OSL
Sample_Id = 20230405_JHJ-13-068 (MeCN-D6) (Descriptive)
Creation_Time = 5-APR-2023 17:42:35
Revision_Time = 14-APR-2023 15:49:05
OH
CO2Me
2o
1H NMR (CD3CN, 400 MHz)
abundance
3.01
1.00
1.00
3.06
1.02
1.01
1.02
3.12
7.319
7.309
7.300
7.226
7.212
7.203
4.810
4.795
4.779
3.657
3.616
3.601
3.109
3.090
2.528
2.490
2.186
2.180
2.154
1.950
1.946
1.944
1.940
1.938
1.934
1.928
X : parts per Million : Proton