Supporting Information

Organocatalytic Enantio- and Diastereoselective Assembly of Cyclopropane-Incorporated Polycyclic Molecules via Isobenzopyrylium Ions

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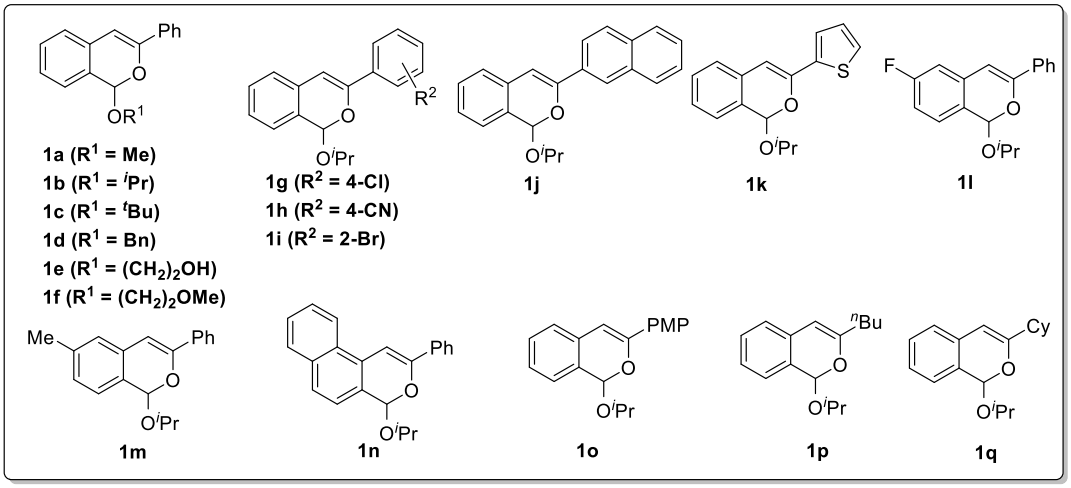
I. General Information

Flash column chromatography was performed over silica gel (200-300 or 300-400 mesh) purchased from Qindao Haiyang Co., China or SiliCycle® Inc., Canada. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. TLC was visualized by UV fluorescence (254 nm) then phosphomolybdic acid. Tetrahydrofuran was distilled from sodium/benzophenone. Anhydrous *N*,*N*-dimethyl formamide, dichloromethane, methanol, toluene, diethyl ether, acetonitrile, and *n*-hexane were purified by the Innovative® solvent purification system. Other anhydrous solvents were purchased from Sigma-Aldrich®, J&K® and Energy® and used as received. Chemicals were purchased from commercial suppliers, such as Sigma-Aldrich®, J&K®, Energy® and used without further purification unless otherwise stated. All the molecular sieves were purchased from Strem® Chemicals, and vacuum dry at 200 °C for 30 minutes. ^{1}H, ^{13}C, ^{31}P and ^{19}F NMR spectra were collected on a Bruker AV 400 and 300 MHz NMR spectrometers using residue solvent peaks as an internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm; ^{13}C NMR: $CDCl_3$ at 77.0 ppm) Data for ^{1}H NMR were recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet; d = doublet; t = triplet; q = quarter; p = pentet; sept = septet; m = multiplet; br = broad), coupling constant (Hz), integration. Mass spectra were collected on an Agilent GC/MS 5975C system, or a MALDI Micro MX mass spectrometer, or an API QSTAR XL System. Optical rotations were measured on Rudolph Research Analytical Autopol I automatic polarimeter with $[\alpha]_D$ values reported in degrees; concentration (c) is in 10 mg/mL. The enantiomeric excess values were determined by chiral HPLC using an Agilent 1200 LC instrument or Agilent 1260 LC instrument with Daicel CHIRALPAK® AD-H, IC, IC-3 or CHIRALCEL® OD-H, OD-3 columns. Unless otherwise noted, the racemic

samples in this study were prepared using the racemic phosphoric acid catalyst 1,1'-binaphthyl-2,2'-diyl hydrogenphosphate.

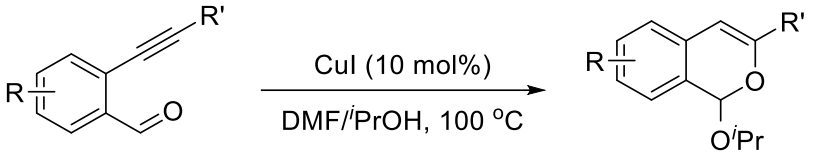
II. Preparation of Substrates

The isochromene substrates **1a, 1b, 1c, 1d, 1e, 1f, 1j, 1p** are known compounds.[1] The procedure for the synthesis of other substrates is shown below. All vinylboronic acids used here are known compounds.[2]



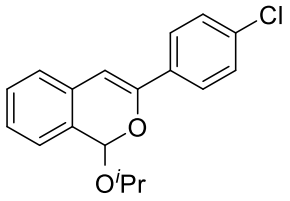
1. (a) H. Qian, W. Zhao, Z. Wang and J. Sun, *J. Am. Chem. Soc.*, 2015, **137**, 560–563. (b) Y. Liu and K. Jørgensen, *J. Am. Chem. Soc.*, 2021**, 143**, 8208–8220. (c) M. Dell'Acqua, B. Castano, C. Cecchini, T. Pedrazzini, V. Pirovano, E. Rossi, A. Caselli and G. Abbiati, *J. Org. Chem.*, 2014, **79**, 3494–3505.
2. Y. Zhang, H. Liu, L. Tang and C. Feng, *J. Am. Chem. Soc.*, 2018, **140**, 10695–10699.

General Procedure A.



S1 **1**

To an oven-dried 4-mL vial was added the aldehyde **S1** (1.0 mmol), DMF (0.5 mL), isopropanol (0.5 mL), and CuI (19.0 mg, 10 mol%). The reaction mixture was stirred at 100 °C, and the reaction progress was monitored by thin layer chromatography. Upon completion (~72 h), water (3 mL) was added. The mixture was extracted with ethyl acetate (3 × 5 mL). The combined organic layers were washed with water (10 mL) and then brine (10 mL), dried with $NaSO_4$, filtered, and concentrated. The residue was purified by silica gel (pre-treated with Et_3N) flash chromatography to afford the acetal (eluent for all the cases: *n*-hexane/EtOAc = 100:1).



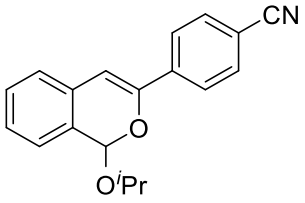
1g

3-(4-Chlorophenyl)-1-isopropoxy-1*H*-isochromene (1g) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 49% yield (0.7 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.4 Hz, 1H), 7.38 – 7.32 (m, 3H), 7.28 – 7.19 (m, 3H), 6.58 (s, 1H), 6.29 (s, 1H), 4.34 (hept, *J* = 6.0 Hz, 1H), 1.31 (d, *J* = 6.0 Hz, 3H), 1.16 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.3, 134.3, 133.2, 130.0, 129.2, 128.6, 127.5, 126.9, 126.0, 125.5, 124.6, 100.7, 96.9, 70.0, 23.5, 21.9.

HRMS (CI+) Calcd for $C_{18}H_{17}ClO_2$ [M]: 300.0917, Found: 300.0918.



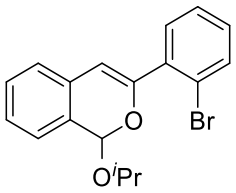
1h

4-(1-Isopropoxy-1*H*-isochromen-3-yl)benzonitrile (1h) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 62% yield (0.9 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.38 – 7.28 (m, 2H), 7.25 – 7.21 (m, 2H), 6.71 (s, 1H), 6.30 (s, 1H), 4.32 (hept, *J* = 6.0 Hz, 1H), 1.30 (d, *J* = 6.0 Hz, 3H), 1.14 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.3, 138.9, 132.2, 129.4, 129.3, 127.8, 127.6, 125.6, 125.0, 124.9, 118.8, 111.5, 103.3, 97.0, 70.2, 23.5, 21.9.

HRMS (CI+) Calcd for $C_{19}H_{17}NO_2^+$ $[M]^+$: 291.1254, Found: 291.1251.



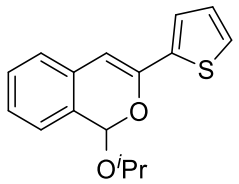
1i

3-(2-Bromophenyl)-1-isopropoxy-1*H*-isochromene (1i) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 67% yield (2.3 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.51 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.32 – 7.20 (m, 4H), 7.17 – 7.13 (m, 2H), 6.33 (s, 1H), 6.28 (s, 1H), 4.30 (hept, *J* = 6.0 Hz, 1H), 1.27 (d, *J* = 6.0 Hz, 3H), 1.21 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.5, 136.6, 133.4, 130.5, 129.8, 129.7, 129.0, 127.2, 127.1, 126.9, 125.4, 124.4, 121.8, 105.5, 97.1, 69.8, 23.4, 21.7.

HRMS (CI+) Calcd for $C_{18}H_{17}BrO_2$ [M]: 344.0412, Found: 344.0414.



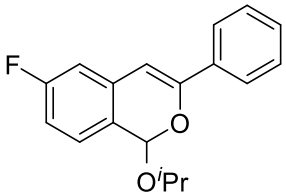
1k

1-Isopropoxy-3-(thiophen-2-yl)-1*H*-isochromene (1k) was prepared according to the General Procedure A as a brown solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 40% yield (1.1 g).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 (dd, J_1 = 3.6 Hz, J_2 = 1.2 Hz, 1H), 7.34 – 7.15 (m, 5H), 7.06 – 7.03 (m, 1H), 6.46 (s, 1H), 6.24 (s, 1H), 4.36 (hept, J = 6.3 Hz, 1H), 1.30 (d, J = 6.0 Hz, 3H), 1.21 (d, J = 6.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 139.2, 130.0, 129.1, 127.6, 127.5, 126.4, 125.53, 125.48, 124.3, 123.9, 99.6, 97.1, 70.0, 23.6, 21.9.

HRMS (CI+) Calcd for $C_{16}H_{16}O_2S$ [M]: 272.0871, Found: 272.0872.



1l

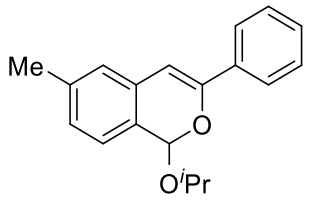
6-Fluoro-1-isopropoxy-3-phenyl-1*H*-isochromene (1l) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 65% yield (0.9 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 7.6 Hz, 2H), 7.43 – 7.34 (m, 3H), 7.21 – 7.18 (m, 1H), 6.95 – 6.87 (m, 2H), 6.54 (s, 1H), 6.29 (s, 1H), 4.36 (hept, J = 6.4 Hz, 1H), 1.31 (d, J = 6.0 Hz, 3H), 1.17 (d, J = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2 (d, *J* = 244.3 Hz), 150.4, 134.3, 132.6 (d, *J* = 9.2 Hz), 129.0, 128.4, 127.4 (d, *J* = 9.2 Hz), 125.0, 123.5 (d, *J* = 2.6 Hz), 113.4 (d, *J* = 22.4 Hz), 110.7 (d, *J* = 22.3 Hz), 99.7 (d, *J* = 2.5 Hz), 96.5, 69.9, 23.5, 21.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -112.9.

HRMS (CI+) Calcd for $C_{18}H_{17}FO_2$ [M]: 284.1213, Found: 284.1218.



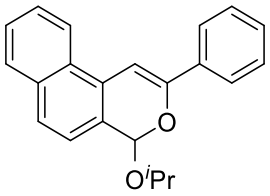
1m

1-Isopropoxy-6-methyl-3-phenyl-1*H*-isochromene (1m) was prepared according to the General Procedure A as a white solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 75% yield (2.1 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.76 (m, 2H), 7.39 – 7.29 (m, 3H), 7.11 – 7.00 (m, 3H), 6.54 (s, 1H), 6.26 (s, 1H), 4.33 (hept, *J* = 6.4 Hz, 1H), 2.33 (s, 3H), 1.28 (d, *J* = 6.0 Hz, 3H), 1.15 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 138.8, 134.8, 130.2, 128.5, 128.3, 127.4, 125.3, 124.98, 124.96, 124.8, 100.3, 96.8, 69.6, 23.5, 21.9, 21.3.

HRMS (CI+) Calcd for $C_{19}H_{20}O_2$ [M]: 280.1463, Found: 280.1467.



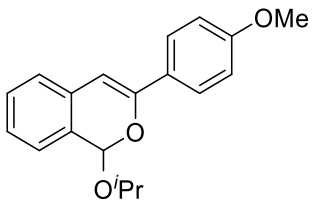
1n

4-Isopropoxy-2-phenyl-4*H*-benzo[*f*]isochromene (1n) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 66% yield (1.8 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.4 Hz, 1H), 7.91 – 7.89 (m, 2H), 7.81 – 7.79 (m, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.55 – 7.27 (m, 7H), 6.42 (s, 1H), 4.39 (hept, *J* = 6.0 Hz, 1H), 1.31 (d, *J* = 6.0 Hz, 3H), 1.18 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.3, 134.9, 133.9, 128.7, 128.5, 128.4, 128.0, 126.8, 126.5, 126.2, 126.1, 125.0, 123.6, 123.4, 122.9, 97.4, 96.0, 69.8, 23.6, 22.0.

HRMS (CI+) Calcd for $C_{22}H_{20}O_2$ [M]: 316.1463, Found: 316.1463.



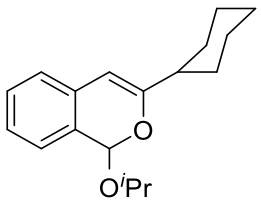
1o

1-Isopropoxy-3-(4-methoxyphenyl)-1*H*-isochromene (1o) was prepared according to the General Procedure A as a white solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 52% yield (0.4 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 6.90 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 6.78 (d, *J* = 2.4 Hz, 1H), 6.57 (s, 1H), 6.25 (s, 1H), 4.36 (hept, *J* = 6.0 Hz, 1H), 3.83 (s, 3H), 1.32 (d, *J* = 6.4 Hz, 3H), 1.17 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 134.9, 129.0, 128.4 (2C), 128.2, 125.9, 124.5, 123.5, 115.2, 110.8, 100.1, 96.8, 69.7, 55.5, 23.5, 21.9.

HRMS (CI+) Calcd for $C_{22}H_{20}O_2$ [M]: 296.1412, Found: 296.1407.



1q

3-Cyclohexyl-1-isopropoxy-1*H*-isochromene (1q) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 50:1) in 88% yield (1.2 g).

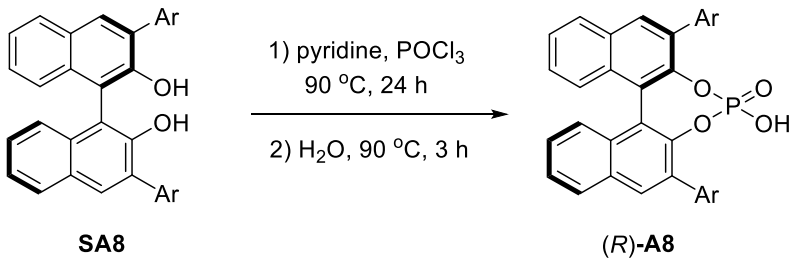
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.23 (m, 1H), 7.18 – 7.11 (m, 2H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.10 (s, 1H), 5.74 (s, 1H), 4.26 (hept, *J* = 6.4 Hz, 1H), 2.19 – 2.13 (m, 1H), 1.97 – 1.94 (m, 2H), 1.82 – 1.80 (m, 2H), 1.72 – 1.69 (m, 1H), 1.40 – 1.27 (m, 8H), 1.20 (d, *J* = 6.4 Hz, 3H).

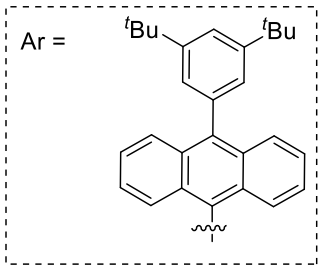
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4, 130.5, 128.9, 126.8, 125.7, 125.5, 123.7, 97.9, 96.1, 68.8, 42.3, 30.8, 30.5, 26.23, 26.16, 23.4, 21.6.

HRMS (CI+) Calcd for $C_{18}H_{24}O_2$ [M]: 272.1776, Found: 272.1773.

III. Synthesis of Catalyst (*R*)-A8

The CPA catalyst (*R*)-**A8** was prepared by following the literature procedure.[3]





(*R*)-2,6-Bis(10-(3,5-di-*tert*-butylphenyl)anthracen-9-yl)-4-hydroxydinaphtho [2,1-d:1',2'-f][1,3,2]dioxaphosphepine 4-oxide (A8). At room temperature, to a 100-mL round-bottom flask charged with the substituted binaphthol **SA8** (1.2 g, 1.2 mmol) was added anhydrous pyridine (20 mL). The flask was cooled to 0 °C, and $POCl_3$ (1.8 g, 12.0 mmol, 10.0 equiv) was slowly added. The mixture was heated at 90 °C for 24 h and then cooled to room temperature. Water (5.0 mL) was cautiously added and then the mixture was heated again at 90 °C for 3 h. The mixture was cooled to room temperature and then poured into an aqueous HCl solution (1 N, 50 mL) and extracted with DCM (50 mL × 3). The combined organic layers were sequentially washed with an aqueous HCl solution (1 N, 50 mL × 3), brine (50 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by silica gel column

3. W. Guo, Y. Luo, H. Sung, I. D. Williams, P. Li and J. Sun, *J. Am. Chem. Soc.*, 2020, **142**, 14384–14390.

chromatography (eluent: DCM/MeOH = 50:1 → 20:1) to afford the desired product. The pure product was redissolved in DCM (50 mL), and vigorously washed with an aqueous HCl solution (4 N, 50 mL × 3) to acidify the phosphoric acid and remove salt impurities. Finally, the organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo* to furnish the phosphoric acid **A8** as a light yellow solid (1.5 g, 85% yield).

$[\alpha]_D^{23}$: +0.9 (c = 1.0, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 2H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.80 – 7.74 (m, 4H), 7.69 – 7.60 (m, 8H), 7.54 – 7.50 (m, 4H), 7.28 – 7.23 (m, 8H), 7.17 – 7.10 (m, 4H), 4.09 (s, 6H), 1.38 (s, 18H), 1.26 (s, 18H).

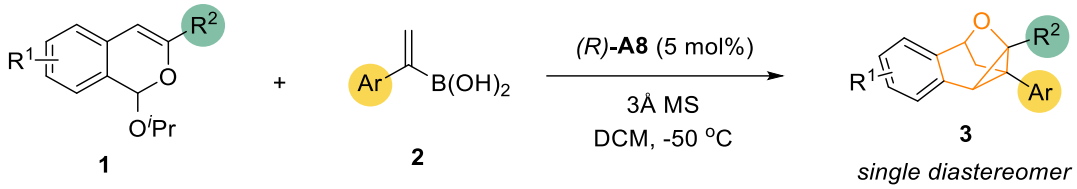
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.7, 150.6, 146.8, 146.7, 139.6, 138.0, 134.3, 132.9, 131.7, 131.44, 131.41, 131.1, 130.8, 130.3, 130.1, 129.8, 128.7, 128.1, 127.63, 127.55, 127.1, 126.9, 126.4, 126.3, 125.8, 124.9, 124.7, 122.6, 121.0, 35.1, 35.0, 31.8, 31.7.

^{31}P NMR (162 MHz, $CDCl_3$) δ 2.2.

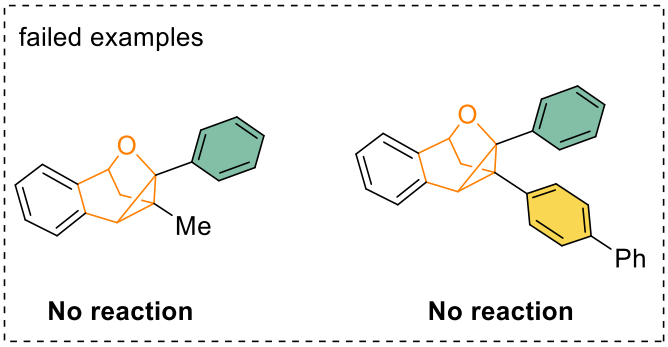
HRMS (ES-) Calcd for $C_{76}H_{68}O_4P^-$ [M - H]$^-$: 1075.4860, Found: 1075.4854.

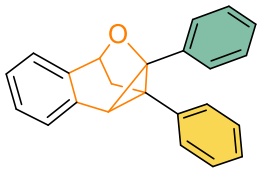
IV. CPA-Catalyzed Synthesis of Bridged Cyclopropanes

General Procedure B.



At –50 °C, to a solution of 3Å molecular sieves (30.0 mg), (*R*)-**A8** (16.1 mg, 0.015 mmol, 5 mol%) and vinylboronic acid **2** (0.75 mmol) in DCM (1.5 mL) in a 4-mL vial was added acetal **1** (0.30 mmol). The reaction mixture was stirred at –50 °C under N_2 atmosphere for 96 h. The reaction mixture was quenched by Et_3N (1 drop) and transferred to a flask with DCM (10 mL) and concentrated. Then the residue was directly purified by silica gel column chromatography to afford the desired product **3**.





3a

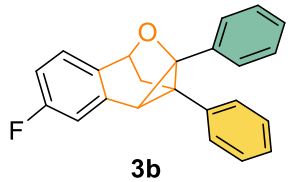
(1*S*,3*S*,7b*S*)-1,1a-Diphenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3a) was prepared according to the General Procedure B as a white solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 78% yield (72.3 mg, 96% ee).

$[\alpha]_D^{23}$: +129.2 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.1 min (major), 7.0 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.2 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.27 – 7.16 (m, 12H), 5.32 (d, *J* = 6.0 Hz, 1H), 3.22 (s, 1H), 2.66 – 2.61 (m, 1H), 1.73 (d, *J* = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.4, 135.6, 135.3, 132.2, 128.9, 128.4, 127.91, 127.85, 126.9, 126.8, 126.7, 126.3, 125.3, 122.3, 74.8, 68.5, 37.1, 35.7, 31.8.

HRMS (CI+) Calcd for $C_{23}H_{18}O$ [M]: 310.1358, Found: 310.1362.



3b

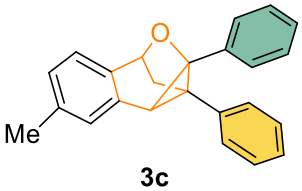
(1*S*,1a*R*,3*R*)-6-Fluoro-1,1a-diphenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3b) was prepared according to the General Procedure B as a white solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 64% yield (61.5 mg, 96% ee).

$[\alpha]_D^{23}$: +45.0 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 6.3 min (major), 5.8 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.15 (m, 12H), 6.95 – 6.90 (m, 1H), 5.31 (d, *J* = 6.0 Hz, 1H), 3.18 (s, 1H), 2.65 (dd, J_1 = 11.6 Hz, J_2 = 6.0 Hz, 1H), 1.72 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6 (d, *J* = 243.0 Hz), 136.9, 134.9, 134.4 (d, *J* = 9.0 Hz), 131.5 (d, *J* = 3.0 Hz), 128.8, 128.4, 127.9, 127.1, 126.8, 126.3, 123.9 (d, *J* = 8.0 Hz), 113.8 (d, *J* = 22.4 Hz), 111.9 (d, *J* = 21.0 Hz), 74.2, 68.5, 37.3, 35.9, 31.9 (d, *J* = 2.0 Hz).

HRMS (CI+) Calcd for $C_{23}H_{17}FO$ [M]: 328.1263, Found: 328.1264.



3c

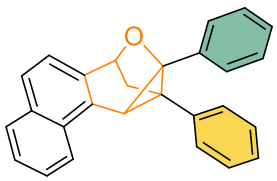
(1*S*,3*S*,7b*S*)-6-Methyl-1,1a-diphenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3c) was prepared according to the General Procedure B as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 48% yield (40.3 mg, 99% ee).

$[\alpha]_D^{23}$: +78.8 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.6 min (major), 8.0 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (s, 1H), 7.26 – 7.13 (m, 11H), 7.06 – 7.04 (m, 1H), 5.29 (d, *J* = 6.0 Hz, 1H), 3.16 (s, 1H), 2.64 – 2.60 (m, 1H), 2.39 (s, 1H), 1.73 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.6, 137.5, 135.4, 132.9, 132.1, 128.9, 128.4, 127.8, 127.4, 126.8, 126.6, 126.3, 125.9, 122.2, 74.6, 68.5, 37.5, 35.8, 31.8, 21.5.

HRMS (CI+) Calcd for $C_{24}H_{20}O$ [M]: 324.1514, Found: 324.1507.



3d

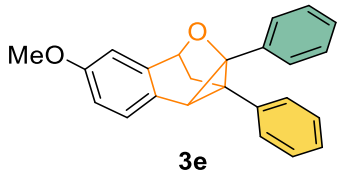
1,1a-Diphenyl-1a,2,3,9c-tetrahydro-1*H*-1,3-epoxycyclopropa[*c*]phenanthrene (3d) was prepared according to the General Procedure B as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 67% yield (72.4 mg, 97% ee).

$[\alpha]_D^{23}$: -4.9 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.5 min (major), 6.0 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.29 – 7.16 (m, 10H), 5.46 (d, *J* = 6.0 Hz, 1H), 3.92 (s, 1H), 2.68 (dd, J_1 = 12.0 Hz, J_2 = 6.0 Hz, 1H), 1.73 (d, *J* = 11.6 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 137.4, 135.3, 133.5, 132.4, 130.9, 129.0 (2C), 128.5, 127.9, 127.8, 127.0, 126.8, 126.5, 126.1, 125.4, 125.2, 122.1, 121.6, 75.1, 68.7, 36.9, 35.7, 28.2.

HRMS (CI+) Calcd for $C_{27}H_{20}NaO^+$ $[M + Na]^+$: 383.1406, Found: 383.1411.



3e

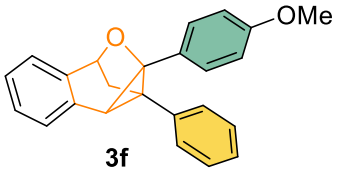
(1*S*,3*S*,7b*S*)-5-Methoxy-1,1a-diphenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3e) was prepared according to the General Procedure B as a white solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 66% yield (58.4 mg, 99% ee).

$[\alpha]_D^{23}$: +8.9 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 14.2 min (major).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.0 Hz, 1H), 7.25 – 7.15 (m, 10H), 6.90 – 6.88 (m, 1H), 6.83 (d, *J* = 2.4 Hz, 1H), 5.26 (d, *J* = 6.0 Hz, 1H), 3.81 (s, 3H), 3.16 (s, 1H), 2.62 (ddd, J_1 = 12.0 Hz, J_2 = 6.4 Hz, J_3 = 0.8 Hz, 1H), 1.73 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.8, 137.5, 136.7, 135.4, 128.9, 128.3, 127.8, 127.6, 126.8, 126.6, 126.2, 124.3, 113.3, 108.6, 74.9, 68.4, 55.5, 37.2, 35.6, 31.0.

HRMS (CI+) Calcd for $C_{24}H_{20}NaO_2^+$ [M + Na]$^+$: 363.1356, Found: 363.1362.



3f

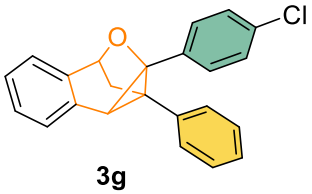
(1*S*,3*S*,7b*S*)-1-(4-Methoxyphenyl)-1a-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3f) was prepared according to the General Procedure B as a white solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 87% yield (77.1 mg, 99% ee).

$[\alpha]_D^{23}$: +138.6 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 26.1 min (major), 16.0 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.43 (m, 1H), 7.35 – 7.30 (m, 1H), 7.25 – 7.20 (m, 4H), 7.18 – 7.14 (m, 5H), 6.76 – 6.73 (m, 2H), 5.28 (d, J = 6.0 Hz, 1H), 3.71 (s, 3H), 3.16 (s, 1H), 2.66 (ddd, J_1 = 12.0 Hz, J_2 = 6.0 Hz, J_3 = 0.8 Hz, 1H), 1.71 (d, J = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 137.7, 135.7, 134.0, 132.3, 128.5, 128.3, 127.8, 126.9, 126.7, 126.4, 125.2, 122.3, 113.4, 74.7, 68.7, 55.1, 36.5, 34.7, 31.3.

HRMS (CI+) Calcd for $C_{24}H_{20}O_2$ [M]: 340.1463, Found: 340.1463.



3g

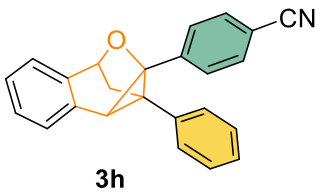
(1*S*,3*S*,7b*S*)-1-(4-Chlorophenyl)-1a-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3g) was prepared according to the General Procedure B as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 84% yield (75.7 mg, 99% ee).

$[\alpha]_D^{23}$: +147.4 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 6.1 min (major), 5.8 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 7.6 Hz, 1H), 7.36 – 7.33 (m, 1H), 7.28 – 7.23 (m, 4H), 7.22 – 7.14 (m, 5H), 7.11 – 7.08 (m, 2H), 5.31 (d, J = 6.0 Hz, 1H), 3.18 (s, 1H), 2.61 (ddd, J_1 = 12.0 Hz, J_2 = 6.0 Hz, J_3 = 0.8 Hz, 1H), 1.73 (d, J = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.9, 135.5, 134.1, 132.6, 131.9, 129.0, 128.5, 128.0 (2C), 127.4, 126.9, 126.8, 125.5, 122.4, 74.9, 68.0, 37.2, 36.0, 31.8.

HRMS (CI+) Calcd for $C_{23}H_{17}ClO$ [M]: 344.0968, Found: 344.0965.



3h

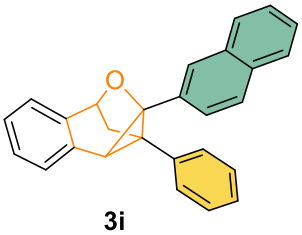
4-((1*S*,3*S*,7b*S*)-1a-Phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalen-1-yl)benzonitrile (3h) was prepared according to the General Procedure B (temperature: –35 °C, catalyst loading: 10 mol%) as a white solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 71% yield (71.1 mg, 93% ee).

$[\alpha]_D^{23}$: +252.0 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 42.5 min (major), 19.9 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.43 (m, 3H), 7.37 (td, J_1 = 6.8 Hz, J_2 = 2.4 Hz, 1H), 7.31 – 7.25 (m, 5H), 7.21 – 7.18 (m, 4H), 5.37 (d, J = 6.0 Hz, 1H), 3.26 (s, 1H), 2.61 (ddd, J_1 = 12.0 Hz, J_2 = 6.0 Hz, J_3 = 0.4 Hz, 1H), 1.77 (d, J = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9, 136.2, 135.3, 131.5, 131.4, 129.3, 128.7, 128.2, 127.3, 126.9, 125.8 (2C), 122.5, 119.0, 110.0, 75.1, 67.8, 37.8, 37.6, 33.0.

HRMS (CI+) Calcd for $C_{24}H_{18}NO^+$ $[M + H]^+$: 336.1383, Found: 336.1397.



3i

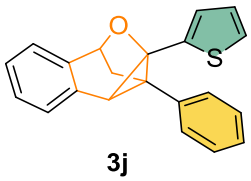
(1*S*,1a*R*,3*R*)-1-(Naphthalen-2-yl)-1a-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3i) was prepared according to the General Procedure B (temperature: –35 °C, catalyst loading: 10 mol%) as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 69% yield (75.0 mg, 94% ee).

$[\alpha]_D^{23}$: +139.9 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.5 min (major), 11.4 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 0.8 Hz, 1H), 7.74 – 7.70 (m, 2H), 7.63 (d, *J* = 8.8 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.43 – 7.34 (m, 3H), 7.29 – 7.26 (m, 2H), 7.24 – 7.21 (m, 4H), 7.20 – 7.16 (m, 1H), 7.10 (dd, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 5.39 (d, *J* = 6.0 Hz, 1H), 3.36 (s, 1H), 2.70 (ddd, J_1 = 12.0 Hz, J_2 = 6.0 Hz, J_3 = 0.8 Hz, 1H), 1.79 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.3, 135.7, 133.0, 132.9, 132.4, 132.2, 128.9, 128.4, 128.0, 127.8, 127.5, 127.4, 126.9, 126.7, 125.9, 125.6, 125.4 (2C), 124.2, 122.4, 75.0, 68.8, 37.3, 35.9, 32.0.

HRMS (CI+) Calcd for $C_{27}H_{20}O$ [M]: 360.1514, Found: 360.1527.



3j

(1*R*,1a*R*,3*R*)-1a-Phenyl-1-(thiophen-2-yl)-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3j) was prepared according to the General

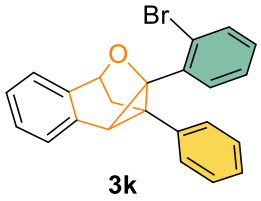
Procedure B (temperature: –35 °C, catalyst loading: 10 mol%) as a yellow solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 52% yield (49.7 mg, 93% ee).

$[\alpha]_D^{23}$: +132.9 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.3 min (major), 8.7 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 7.2 Hz, 1H), 7.36 (td, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 7.28 – 7.20 (m, 7H), 7.15 (d, J = 5.2 Hz, 1H), 6.84 (dd, J_1 = 4.8 Hz, J_2 = 3.6 Hz, 1H), 6.68 – 6.67 (m, 1H), 5.31 (d, J = 6.0 Hz, 1H), 3.22 (s, 1H), 2.69 (dd, J_1 = 12.0 Hz, J_2 = 6.0 Hz, 1H), 1.72 (d, J = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4, 136.9, 135.4, 131.7, 128.8, 128.4 (2C), 128.0, 126.9, 126.5, 125.5, 124.8, 124.3, 122.5, 75.3, 66.6, 36.5, 35.8, 32.4.

HRMS (CI+) Calcd for $C_{21}H_{16}OS$ [M]: 316.0922, Found: 316.0924.



3k

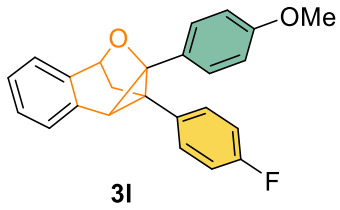
(1*R*,1a*R*,3*R*)-1-(2-Bromophenyl)-1a-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3k) was prepared according to the General Procedure B as a yellow oil (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 57% yield (67.0 mg, 96% ee).

$[\alpha]_D^{23}$: -41.9 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 14.5 min (major), 9.2 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.47 – 7.44 (m, 2H), 7.34 (td, J_1 = 7.2 Hz, J_2 = 2.0 Hz, 1H), 7.29 – 7.13 (m, 7H), 6.98 – 6.96 (m, 2H), 5.32 (d, J = 6.0 Hz, 1H), 3.17 (s, 1H), 3.05 – 3.01 (m, 1H), 1.78 (d, J = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4, 135.8, 133.53, 133.46, 132.9, 132.2, 130.4, 128.0, 127.9, 127.4, 127.2, 126.8, 125.8, 125.6, 125.4, 122.3, 75.3, 71.2, 33.1, 33.0, 32.4.

HRMS (CI+) Calcd for $C_{23}H_{17}BrO$ [M]: 388.0463, Found: 388.0367.



3l

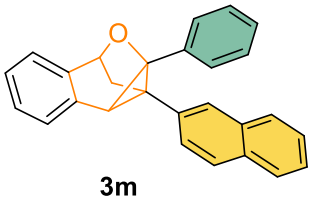
(1*S*,3*S*,7b*S*)-1a-(4-Fluorophenyl)-1-(4-methoxyphenyl)-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3l) was prepared according to the General Procedure B as a white solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 72% yield (77.5 mg, 95% ee).

$[\alpha]_D^{23}$: -0.2 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 25.6 min (major), 16.7 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 7.2 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.27 – 7.22 (m, 2H), 7.17 – 7.11 (m, 4H), 6.94 – 6.90 (m, 2H), 6.79 – 6.75 (m, 2H), 5.28 (d, *J* = 6.0 Hz, 1H), 3.75 (s, 3H), 3.12 (s, 1H), 2.63 – 2.58 (m, 1H), 1.70 (d, *J* = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.5 (d, *J* = 244.0 Hz), 158.8, 135.6, 133.5 (d, *J* = 3.0 Hz), 132.1, 130.2 (d, *J* = 7.0 Hz), 128.1, 127.9, 126.7, 125.3, 122.4, 115.4, 115.1, 113.5, 74.7, 68.5, 55.2, 36.8, 34.3, 31.2.

HRMS (ES+) Calcd for $C_{24}H_{19}FNaO_2^+$ $[M + Na]^+$: 381.1261, Found: 381.1269.



3m

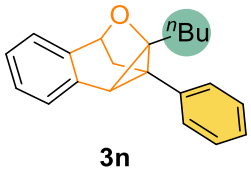
(1*S*,3*S*,7b*S*)-1a-(Naphthalen-2-yl)-1-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3m) was prepared according to the General Procedure B as a white solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 64% yield (68.8 mg, 89% ee).

$[\alpha]_D^{23}$: +216.5 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 9.6 min (major), 8.0 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.64 (m, 4H), 7.49 (d, *J* = 7.2 Hz, 1H), 7.43 – 7.32 (m, 3H), 7.27 – 7.20 (m, 5H), 7.16 – 7.11 (m, 3H), 5.34 (d, *J* = 6.0 Hz, 1H), 3.34 (s, 1H), 2.73 – 2.67 (m, 1H), 1.75 (d, *J* = 12.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.6, 135.3, 135.0, 133.3, 132.2, 132.1, 128.0, 127.93, 127.87, 127.6, 127.5, 127.0, 126.9, 126.8, 126.2, 126.0, 125.7, 125.4, 122.3, 74.9, 68.6, 37.3, 36.0, 31.9.

HRMS (ES+) Calcd for $C_{27}H_{20}NaO^+$ $[M + Na]^+$: 383.1406, Found: 383.1411.



3n

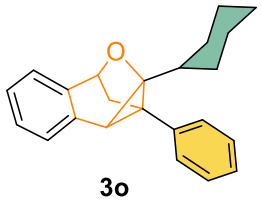
(1*R*,3*S*,7b*S*)-1-Butyl-1a-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3n) was prepared according to the General Procedure B (room temperature, catalyst loading: 10 mol%, reaction time: 48 h) as a colorless oil (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 53% yield (46.0 mg, 90% ee).

$[\alpha]_D^{23}$: -9.4 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 3% ^{i}PrOH in *n*-hexane; 0.5 mL/min; retention times: 12.9 min (major), 10.0 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.29 (m, 6H), 7.26 – 7.15 (m, 3H), 5.12 (d, *J* = 6.0 Hz, 1H), 2.61 (s, 1H), 2.52 (ddd, J_1 = 11.6 Hz, J_2 = 6.0 Hz, J_3 = 0.8 Hz, 1H), 2.03 – 1.96 (m, 1H), 1.53 – 1.36 (m, 4H), 1.26 – 1.18 (m, 2H), 0.78 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.6, 135.4, 133.0, 128.48, 128.45, 127.7, 126.5, 126.4, 124.8, 122.2, 74.7, 67.5, 36.3, 32.2, 29.0, 28.52, 28.47, 22.6, 13.9.

HRMS (ES+) Calcd for $C_{21}H_{22}NaO^+$ $[M + H]^+$: 313.1563, Found: 313.1568



3o

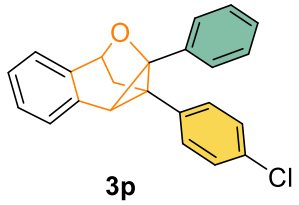
(1*R*,3*S*,7b*S*)-1-Cyclohexyl-1a-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3o) was prepared according to the General Procedure B (room temperature, catalyst loading: 10 mol%, reaction time: 48 h) as a white solid (chromatography eluent: *n*-hexane/EtOAc = 100:1) in 59% yield (55.6 mg, 92% ee).

$[\alpha]_D^{23}$: -3.0 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 5.3 min (major), 4.6 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.40 (m, 2H), 7.38 – 7.20 (m, 5H), 7.18 – 7.14 (m, 2H), 5.11 (d, *J* = 6.0 Hz, 1H), 2.66 (s, 1H), 2.60 – 2.55 (m, 1H), 1.75 (d, *J* = 12.4 Hz, 1H), 1.67 – 1.56 (m, 4H), 1.49 – 1.41 (m, 2H), 1.36 – 1.21 (m, 2H), 1.16 – 1.01 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.3, 135.6, 133.0, 128.4, 128.3, 127.6, 126.34, 126.27, 124.7, 122.1, 74.3, 71.2, 37.9, 36.1, 33.0, 30.0, 28.9, 27.6, 26.4, 26.3, 26.2.

HRMS (ES+) Calcd for $C_{23}H_{24}NaO^+$ [M + Na]$^+$: 339.1719, Found: 339.1725.



3p

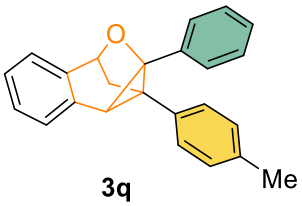
(1*S*,3*R*,7b*R*)-1a-(4-Chlorophenyl)-1-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3p) was prepared according to the General Procedure B (room temperature, catalyst loading: 5 mol%, reaction time: 4 h) as a white solid (chromatography eluent: *n*-hexane/DCM/EtOAc = 100:25:1) in 76% yield (78.6 mg, 86% ee).

$[\alpha]_D^{23}$: +178.9 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC-3 column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 9.1 min (major), 7.6 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.43 (m, 1H), 7.36 – 7.32 (m, 1H), 7.25 – 7.18 (m, 9H), 7.12 – 7.10 (m, 2H), 5.31 (d, *J* = 6.0 Hz, 1H), 3.19 (s, 1H), 2.61 – 2.56 (m, 1H), 1.71 (d, *J* = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.2, 135.7, 135.0, 132.6, 132.0, 130.3, 128.7,128.1(2C), 127.3, 126.9, 126.5, 125.6, 122.5, 77.5, 68.8, 37.2, 35.3, 31.7.

HRMS (ES+) Calcd for $C_{23}H_{18}ClO^+$ [M + H]$^+$: 345.1041, Found: 345.1025.



3q

(1*S*,3*R*,7b*R*)-1-Phenyl-1a-(*p*-tolyl)-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclo propa[*a*]naphthalene (3q) was prepared according to the General Procedure B (room temperature, catalyst loading: 5 mol%, reaction time: 12 h) as a white

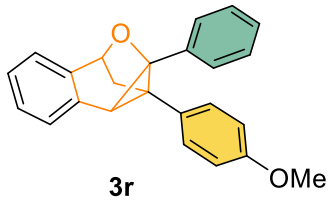
solid (chromatography eluent: *n*-hexane/DCM/EtOAc = 100:25:1) in 58% yield (52.8 mg, 79% ee).

$[\alpha]_D^{23}$: +101.8 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC-3 column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.9 min (major), 7.6 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 7.6 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.25 – 7.24 (m, 2H), 7.21 – 7.17 (m, 5H), 7.10 – 7.04 (m, 4H), 5.31 (d, J = 6.0 Hz, 1H), 3.18 (s, 1H), 2.62 (ddd, J_1 = 11.6 Hz, J_2 = 6.0 Hz, J_3 = 0.8 Hz, 1H), 2.29 (s, 3H), 1.71 (d, J = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.4, 135.8, 135.6, 134.3, 132.4, 129.3, 128.9, 128.03, 127.98, 127.0, 126.9, 126.5, 125.4, 122.5, 75.0, 68.6, 37.4, 35.5, 31.9, 21.2.

HRMS (ES+) Calcd for $C_{24}H_{21}O^+$ $[M + H]^+$: 325.1587, Found: 325.1581.



3r

(1*S*,3*R*,7b*R*)-1a-(4-Methoxyphenyl)-1-phenyl-1a,2,3,7b-tetrahydro-1*H*-1,3-epoxycyclopropa[*a*]naphthalene (3r) was prepared according to the General Procedure B as a white solid (chromatography eluent: *n*-hexane/DCM/EtOAc = 100:25:1) in 50% yield (51.0 mg, 44% ee).

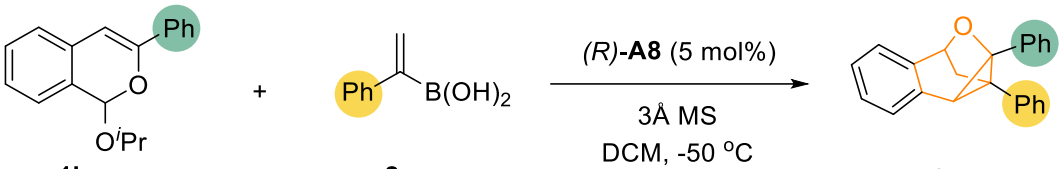
$[\alpha]_D^{23}$: +43.1 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC-3 column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.4 min (major), 11.3 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, J = 7.6 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.27 – 7.16 (m, 7H), 7.15 – 7.10 (m, 2H), 6.81 – 6.77 (m, 2H), 5.30 (d, J = 6.0 Hz, 1H), 3.76 (s, 3H), 3.15 (s, 1H), 2.61 – 2.56 (m, 1H), 1.70 (d, J = 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 135.8, 135.7, 132.5, 130.2, 129.3, 128.03, 127.99, 126.93, 126.91, 126.3, 125.4, 122.5, 114.0, 75.0, 68.4, 55.3, 37.5, 35.3, 32.0.

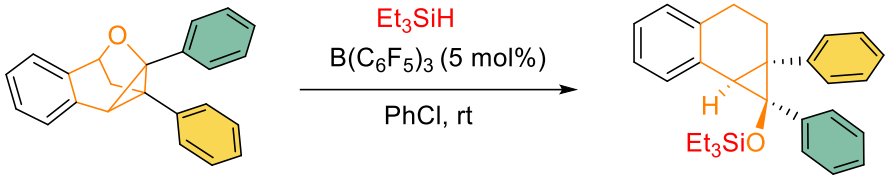
HRMS (ES+) Calcd for $C_{24}H_{21}O_2^+$ $[M + H]^+$: 341.1537, Found: 341.1531.

IV Large-Scale Reaction



At –50 °C, to a solution of 3Å molecular sieves (300.0 mg), (*R*)-**A8** (0.15 mmol, 5 mol%) and vinylboronic acid **2a** (7.5 mmol) in DCM (15 mL) in a 50-mL flask was added acetal **1a** (3.0 mmol). The reaction mixture was stirred at –50 °C under N_2 atmosphere for 168 h before it was quenched by Et_3N (1 drop), transferred to a flask with DCM (50 mL) and concentrated. Then the residue was directly purified by silica gel column chromatography to afford the desired product **3a** (706.4 mg) in 76% yield and 98% ee.

V. Product Derivatizations



3a **4**

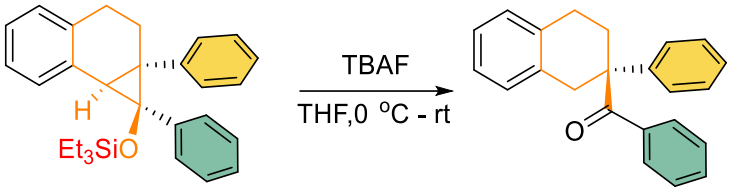
(((1*S*,1a*R*)-1,1a-Diphenyl-1a,2,3,7b-tetrahydro-1*H*-cyclopropa[*a*]naphthalen-1-yl)oxy)triethylsilane (4). At room temperature, to a solution of **3a** (31.0 mg, 0.1 mmol) and $B(C_6F_5)_3$ (2.5 mg, 5 μmol) in anhydrous DCM (1.0 mL) was added triethylsilane (14.0 mg, 0.12 mmol). The mixture was kept stirring at room temperature for 1 h before it was quenched by Et_3N (1 drop). The mixture was concentrated under reduced pressure, and the residue was directly purified by silica gel column chromatography (eluent: *n*-hexane) to afford the desired product **4** in 93% yield, 99% ee (39.7 mg).

$[\alpha]_D^{23}$: +128.4 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALDICEL® OD-H column; 0.5 % ^{i}PrOH in *n*-hexane; 0.5 mL/min; retention times: 14.8 min (major), 12.7 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.2 Hz, 1H), 7.30 – 7.28 (m, 2H), 7.24 – 6.99 (m, 10H), 6.96 – 6.92 (m, 1H), 3.22 (s, 1H), 3.07 – 3.01 (m, 1H), 2.85 – 2.74 (m, 2H), 2.07 – 2.00 (m, 1H), 0.61 (t, *J* = 8.0 Hz, 9H), 0.04 (q, *J* = 8.0 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 141.5, 137.9, 133.2, 130.7, 128.7, 128.5, 128.4, 127.7, 127.4, 126.7, 125.9, 125.5, 125.4, 73.0, 38.0, 28.7, 28.6, 27.6, 6.8, 5.3.

HRMS (CI+) Calcd for $C_{29}H_{34}OSi$ [M]: 426.2379, Found: 426.2389.



4 **5**

(*R*)-Phenyl(2-phenyl-1,2,3,4-tetrahydronaphthalen-2-yl)methanone (5). At 0 °C, to a solution of **4** (85.3 mg, 0.2 mmol) in THF (2.0 mL) was added TBAF (0.4 mL, 0.4 mmol, 1 M in THF). The mixture was kept stirring at room temperature for 1 h. The mixture was directly purified by silica gel column chromatography (eluent: *n*-hexane/EtOAc = 20:1) to afford the desired product **5** in 98% yield, 95% ee (61.2 mg).

$[\alpha]_D^{23}$: -3.3 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC-3 column; 2% ^{i}PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.4 min (major), 7.4 min (minor).

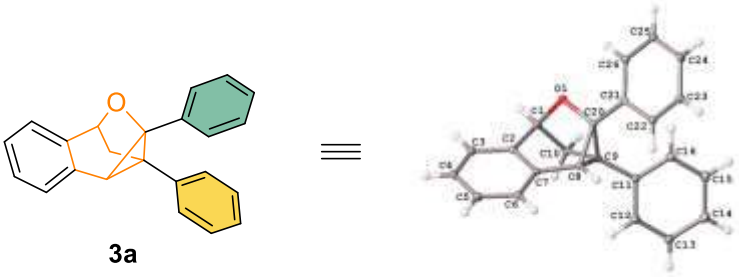
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.45 (m, 2H), 7.41 – 7.21 (m, 8H), 7.14 – 7.08 (m, 3H), 7.02 (d, *J* = 6.4 Hz, 1H), 3.42 (d, *J* = 16.8 Hz, 1H), 3.23 (d, *J* = 16.8 Hz, 1H), 2.69 – 2.63 (m, 1H), 2.57 – 2.45 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 202.4, 142.9, 136.8, 135.6, 135.2, 131.9, 129.5, 129.3 (2C), 128.8, 128.2, 127.3, 126.4, 126.2, 126.0, 54.5, 39.6, 32.0, 26.2.

HRMS (ES+) Calcd for $C_{23}H_{20}NaO^+$ $[M + Na]^+$: 335.1407, Found: 335.1417.

VI. Product Structure Determination

The structure of product **3a** was determined by X-ray crystallography. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2356608). The structures of other products were assumed by analogy.



3a

Table S1. Crystal Data and Structure Refinement for 3a.

Identification code	**3a**
Empirical formula	$C_{23}H_{18}O$
Formula weight	310.37
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	10.33817(7)
b/Å	10.45428(8)
c/Å	14.51868(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1569.15(2)
Z	4
ρ_{calc}g/cm^3	1.314
μ/mm^{-1}	0.608
F(000)	656.0
Crystal size/mm^3	0.2 ×0.18 ×0.18

Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	10.428 to 153.808
Index ranges	$-13 \leq h \leq 11$, $-12 \leq k \leq 12$, $-18 \leq l \leq 13$
Reflections collected	10133
Independent reflections	3252 [R_{int} = 0.0139, R_{sigma} = 0.0135]
Data/restraints/parameters	3252/0/218
Goodness-of-fit on F^2	1.174
Final R indexes [I>=2σ (I)]	R_1 = 0.0258, wR_2 = 0.0720
Final R indexes [all data]	R_1 = 0.0273, wR_2 = 0.0865
Largest diff. peak/hole / e $Å^{-3}$	0.24/-0.14
Flack parameter	0.01(6)

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 3a. U_{eq} is Defined as 1/3 of the Trace of the Orthogonalised U_{IJ} Tensor.

Atom	*x*	*y*	*z*	U(eq)
O(1)	2270.1(11)	2588.2(11)	2858.8(8)	14.3(3)
C(1)	1417.8(16)	2320.2(16)	3638.2(11)	15.7(3)
C(2)	189.1(17)	3046.2(16)	3469.7(11)	15.5(3)
C(3)	-1048.4(16)	2528.6(17)	3402.7(11)	17.9(3)
C(4)	-2087.8(17)	3336.5(18)	3207.7(12)	20.0(4)
C(5)	-1891.0(17)	4644.0(18)	3084.3(12)	19.4(4)
C(6)	-654.0(16)	5159.8(17)	3155.0(11)	16.7(3)
C(7)	391.8(16)	4359.0(16)	3344.8(11)	14.2(3)
C(8)	1749.4(16)	4789.0(16)	3380.2(11)	14.1(3)
C(9)	2701.6(16)	4114.5(16)	4035.1(11)	14.6(3)
C(10)	2143.8(17)	2901.2(16)	4458.7(11)	16.3(3)
C(11)	3658.3(16)	4873.7(16)	4577.0(11)	15.3(3)
C(12)	3213.0(18)	5634.1(17)	5301.0(12)	19.1(4)
C(13)	4077.9(19)	6289.8(18)	5859.4(12)	22.2(4)
C(14)	5401.3(19)	6214.1(19)	5694.3(13)	22.8(4)
C(15)	5847.6(18)	5481.5(18)	4967.4(13)	22.6(4)
C(16)	4989.0(17)	4797.4(18)	4416.7(12)	19.1(4)
C(20)	2763.4(15)	3832.9(16)	3010.8(11)	13.5(3)
C(21)	3769.8(16)	4193.6(16)	2330.5(11)	14.2(3)
C(22)	4163.2(17)	5463.3(16)	2223.0(12)	16.6(3)
C(23)	5066.3(17)	5792.8(18)	1553.7(13)	19.6(4)
C(24)	5595.8(18)	4861.9(19)	985.6(13)	22.1(4)
C(25)	5232.3(17)	3589.7(18)	1101.4(13)	20.7(4)
C(26)	4319.6(17)	3259.9(16)	1763.8(12)	17.0(3)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3a. The Anisotropic Displacement Factor Exponent Takes the Form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	17.3(6)	11.7(5)	13.9(5)	-0.3(4)	1.3(4)	-0.5(4)
C(1)	18.8(8)	14.1(7)	14.1(7)	0.7(6)	2.7(6)	0.7(6)
C(2)	18.1(8)	16.4(8)	12.0(7)	0.0(6)	2.3(6)	0.0(6)
C(3)	20.6(8)	16.5(8)	16.8(7)	-1.0(6)	3.5(6)	-2.7(7)
C(4)	14.9(7)	23.7(9)	21.6(8)	-2.0(7)	3.1(7)	-2.6(7)
C(5)	15.8(8)	22.6(9)	19.8(8)	-0.1(7)	1.6(6)	3.7(7)
C(6)	18.3(8)	16.2(8)	15.7(7)	1.1(6)	2.1(6)	1.0(6)
C(7)	15.2(8)	16.8(8)	10.6(7)	-0.2(6)	1.1(6)	-0.3(6)
C(8)	15.7(7)	11.9(7)	14.7(7)	0.0(6)	0.3(6)	1.3(6)
C(9)	16.2(8)	15.4(8)	12.1(7)	-0.5(6)	0.0(6)	1.3(6)
C(10)	19.5(8)	15.6(8)	13.7(7)	1.2(6)	-0.6(6)	1.3(6)
C(11)	18.7(8)	14.0(7)	13.3(7)	1.3(6)	-1.1(6)	-0.4(6)
C(12)	21.2(8)	19.3(8)	16.7(7)	-0.7(6)	2.7(7)	-1.5(7)
C(13)	33.0(10)	18.6(8)	15.0(8)	-3.0(6)	3.1(7)	-4.6(7)
C(14)	28.4(9)	21.8(9)	18.2(8)	1.0(7)	-7.1(7)	-4.3(7)
C(15)	19.0(8)	25.8(9)	23.1(9)	2.4(7)	-4.9(7)	1.2(7)
C(16)	18.4(8)	21.7(8)	17.3(8)	-1.1(7)	-2.1(6)	4.8(7)
C(20)	14.4(7)	12.6(8)	13.5(7)	-1.3(6)	-1.1(6)	-0.1(6)
C(21)	13.2(7)	17.7(8)	11.8(7)	-0.4(6)	-2.8(6)	1.3(6)
C(22)	15.3(7)	17.0(8)	17.6(8)	-2.3(6)	-0.2(6)	0.7(6)
C(23)	17.4(8)	20.0(8)	21.3(8)	-0.3(7)	0.1(7)	-2.5(6)
C(24)	16.8(8)	27.9(10)	21.5(8)	-0.9(7)	5.7(6)	-3.2(7)
C(25)	18.6(8)	22.7(9)	20.8(8)	-4.8(7)	3.8(7)	1.4(7)
C(26)	17.1(7)	16.6(8)	17.4(8)	-1.7(7)	-0.5(6)	1.4(6)

Table S4. Bond Lengths for 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O(1)	C(1)	1.4613(19)	C(9)	C(20)	1.517(2)
O(1)	C(20)	1.415(2)	C(11)	C(12)	1.396(2)
C(1)	C(2)	1.500(2)	C(11)	C(16)	1.397(2)
C(1)	C(10)	1.533(2)	C(12)	C(13)	1.388(3)
C(2)	C(3)	1.392(2)	C(13)	C(14)	1.391(3)
C(2)	C(7)	1.400(2)	C(14)	C(15)	1.383(3)
C(3)	C(4)	1.396(3)	C(15)	C(16)	1.392(3)
C(4)	C(5)	1.394(3)	C(20)	C(21)	1.483(2)
C(5)	C(6)	1.392(2)	C(21)	C(22)	1.397(2)
C(6)	C(7)	1.395(2)	C(21)	C(26)	1.397(2)
C(7)	C(8)	1.475(2)	C(22)	C(23)	1.391(3)
C(8)	C(9)	1.540(2)	C(23)	C(24)	1.388(3)
C(8)	C(20)	1.545(2)	C(24)	C(25)	1.392(3)
C(9)	C(10)	1.523(2)	C(25)	C(26)	1.391(3)
C(9)	C(11)	1.492(2)			

Table S5. Bond Angles for 3a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(20)	O(1)	C(1)	105.84(12)	C(9)	C(10)	C(1)	101.62(13)
O(1)	C(1)	C(2)	106.70(13)	C(12)	C(11)	C(9)	118.77(15)
O(1)	C(1)	C(10)	103.33(13)	C(12)	C(11)	C(16)	118.85(16)
C(2)	C(1)	C(10)	109.93(13)	C(16)	C(11)	C(9)	122.30(15)
C(3)	C(2)	C(1)	126.36(15)	C(13)	C(12)	C(11)	120.57(16)
C(3)	C(2)	C(7)	120.62(16)	C(12)	C(13)	C(14)	120.31(17)
C(7)	C(2)	C(1)	112.98(15)	C(15)	C(14)	C(13)	119.40(17)
C(2)	C(3)	C(4)	119.10(16)	C(14)	C(15)	C(16)	120.66(17)
C(5)	C(4)	C(3)	120.48(16)	C(15)	C(16)	C(11)	120.18(17)
C(6)	C(5)	C(4)	120.32(16)	O(1)	C(20)	C(8)	113.87(13)
C(5)	C(6)	C(7)	119.62(16)	O(1)	C(20)	C(9)	108.43(13)
C(2)	C(7)	C(8)	115.90(15)	O(1)	C(20)	C(21)	112.50(13)
C(6)	C(7)	C(2)	119.86(16)	C(9)	C(20)	C(8)	60.37(10)
C(6)	C(7)	C(8)	124.16(16)	C(21)	C(20)	C(8)	122.87(14)
C(7)	C(8)	C(9)	119.37(14)	C(21)	C(20)	C(9)	129.26(14)
C(7)	C(8)	C(20)	115.88(14)	C(22)	C(21)	C(20)	121.34(15)
C(9)	C(8)	C(20)	58.94(10)	C(22)	C(21)	C(26)	118.65(15)
C(10)	C(9)	C(8)	112.88(14)	C(26)	C(21)	C(20)	119.99(15)
C(11)	C(9)	C(8)	120.38(14)	C(23)	C(22)	C(21)	120.58(16)
C(11)	C(9)	C(10)	118.75(14)	C(24)	C(23)	C(22)	120.40(17)
C(11)	C(9)	C(20)	126.30(14)	C(23)	C(24)	C(25)	119.44(17)
C(20)	C(9)	C(8)	60.69(10)	C(26)	C(25)	C(24)	120.22(17)
C(20)	C(9)	C(10)	104.49(13)	C(25)	C(26)	C(21)	120.67(16)

Table S6. Torsion Angles for 3a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(1)	C(1)	C(2)	C(3)	121.59(17)	C(9)	C(8)	C(20)	C(21)	-119.95(17)
O(1)	C(1)	C(2)	C(7)	-56.19(18)	C(9)	C(11)	C(12)	C(13)	175.81(16)
O(1)	C(1)	C(10)	C(9)	38.38(15)	C(9)	C(11)	C(16)	C(15)	-177.15(16)
O(1)	C(20)	C(21)	C(22)	165.02(14)	C(9)	C(20)	C(21)	C(22)	-53.7(2)
O(1)	C(20)	C(21)	C(26)	-13.3(2)	C(9)	C(20)	C(21)	C(26)	128.06(18)
C(1)	O(1)	C(20)	C(8)	-40.95(16)	C(10)	C(1)	C(2)	C(3)	-127.01(17)
C(1)	O(1)	C(20)	C(9)	24.06(16)	C(10)	C(1)	C(2)	C(7)	55.20(18)
C(1)	O(1)	C(20)	C(21)	173.39(13)	C(10)	C(9)	C(11)	C(12)	-76.0(2)
C(1)	C(2)	C(3)	C(4)	-177.54(15)	C(10)	C(9)	C(11)	C(16)	100.53(19)
C(1)	C(2)	C(7)	C(6)	178.18(15)	C(10)	C(9)	C(20)	O(1)	0.86(17)
C(1)	C(2)	C(7)	C(8)	1.2(2)	C(10)	C(9)	C(20)	C(8)	108.39(14)
C(2)	C(1)	C(10)	C(9)	-75.20(16)	C(10)	C(9)	C(20)	C(21)	-141.65(17)
C(2)	C(3)	C(4)	C(5)	-0.2(3)	C(11)	C(9)	C(10)	C(1)	-170.79(14)
C(2)	C(7)	C(8)	C(9)	-34.3(2)	C(11)	C(9)	C(20)	O(1)	144.57(15)
C(2)	C(7)	C(8)	C(20)	33.0(2)	C(11)	C(9)	C(20)	C(8)	-107.90(18)
C(3)	C(2)	C(7)	C(6)	0.3(2)	C(11)	C(9)	C(20)	C(21)	2.1(3)
C(3)	C(2)	C(7)	C(8)	-176.72(15)	C(11)	C(12)	C(13)	C(14)	1.1(3)
C(3)	C(4)	C(5)	C(6)	-0.1(3)	C(12)	C(11)	C(16)	C(15)	-0.6(3)
C(4)	C(5)	C(6)	C(7)	0.4(3)	C(12)	C(13)	C(14)	C(15)	0.1(3)
C(5)	C(6)	C(7)	C(2)	-0.5(2)	C(13)	C(14)	C(15)	C(16)	-1.6(3)
C(5)	C(6)	C(7)	C(8)	176.22(16)	C(14)	C(15)	C(16)	C(11)	1.9(3)
C(6)	C(7)	C(8)	C(9)	148.84(16)	C(16)	C(11)	C(12)	C(13)	-0.8(3)
C(6)	C(7)	C(8)	C(20)	-143.80(16)	C(20)	O(1)	C(1)	C(2)	76.63(15)
C(7)	C(2)	C(3)	C(4)	0.1(2)	C(20)	O(1)	C(1)	C(10)	-39.27(15)
C(7)	C(8)	C(9)	C(10)	10.0(2)	C(20)	C(8)	C(9)	C(10)	-94.27(15)
C(7)	C(8)	C(9)	C(11)	-138.52(16)	C(20)	C(8)	C(9)	C(11)	117.25(17)
C(7)	C(8)	C(9)	C(20)	104.23(17)	C(20)	C(9)	C(10)	C(1)	-23.75(16)
C(7)	C(8)	C(20)	O(1)	-11.7(2)	C(20)	C(9)	C(11)	C(12)	144.83(17)
C(7)	C(8)	C(20)	C(9)	-110.12(16)	C(20)	C(9)	C(11)	C(16)	-38.7(3)

C(7)	C(8)	C(20)	C(21)	129.92(16)	C(20)	C(21)	C(22)	C(23)	-177.12(15)
C(8)	C(9)	C(10)	C(1)	40.17(17)	C(20)	C(21)	C(26)	C(25)	177.81(16)
C(8)	C(9)	C(11)	C(12)	70.7(2)	C(21)	C(22)	C(23)	C(24)	-0.4(3)
C(8)	C(9)	C(11)	C(16)	-112.80(19)	C(22)	C(21)	C(26)	C(25)	-0.5(2)
C(8)	C(9)	C(20)	O(1)	-107.53(14)	C(22)	C(23)	C(24)	C(25)	-1.1(3)
C(8)	C(9)	C(20)	C(21)	109.97(19)	C(23)	C(24)	C(25)	C(26)	1.8(3)
C(8)	C(20)	C(21)	C(22)	22.9(2)	C(24)	C(25)	C(26)	C(21)	-1.0(3)
C(8)	C(20)	C(21)	C(26)	-155.37(15)	C(26)	C(21)	C(22)	C(23)	1.2(3)
C(9)	C(8)	C(20)	O(1)	98.40(15)					

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3a.

Atom	*x*	*y*	*z*	U(eq)
H(1)	1260	1383	3719	19
H(3)	-1183	1638	3489	22
H(4)	-2936	2993	3159	24
H(5)	-2605	5186	2951	23
H(6)	-523	6052	3074	20
H(8)	1912	5716	3254	17
H(10A)	1549	3100	4974	20
H(10B)	2836	2324	4681	20
H(12)	2310	5703	5413	23
H(13)	3765	6793	6357	27
H(14)	5993	6661	6077	27
H(15)	6749	5445	4843	27
H(16)	5309	4277	3931	23
H(22)	3811	6107	2611	20
H(23)	5322	6660	1485	23
H(24)	6201	5091	522	26
H(25)	5609	2945	727	25
H(26)	4067	2391	1832	20

VII. Computational Details

All structures were optimized and characterized in dichloromethane with the SMD[4] solvent model (SCRF = SMD) at M06-2X[5]/6-31G(d) level. Harmonic frequency analysis calculations at the same level were performed to verify the optimized transition states (TSs, having unique one imaginary frequency). The energies were further improved by M06-2X/6-311+G(d,p) //M06-2X/6-31G(d) single-point calculations with solvent effects accounted by the SMD solvent model, using the experimental solvent (dichloromethane). Intrinsic reaction coordinate (IRC) calculations for cycloaddition transition states were carried out at the M06-2X/6-31G(d) level to verify the transition state correctly connecting with its nearby minima.[6] All DFT calculations were carried out using Gaussian 09 program.[7] Computed structures are illustrated using the CYLview.[8]

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4. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* 2009, **113**, 6378–6396.
5. (a) Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215–241. (b) Y. Zhao, D. G. Truhlar, *Acc. Chem. Res.* 2008, **41**, 157–167. (c) Y. Zhao, D. G. Truhlar, *J. Chem. Theory Comput.* 2009, **5**, 324–333.

6 K. Fukui, Acc. *Chem. Res.* 1981, **14**, 363.

7 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, , M. Ishida, T.Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.; J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Rev. A.01; Gaussian, Inc.: Wallingford, CT, 2010.

8 C. Y. Legault, *CYLView, version 1.0 b*; Université de Sherbrooke: Sherbrooke,

Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K and 1 atm for the Optimized Structures [BSI= 6-31G(d), BSII = 6-311+G(d,p)

TSA-major

M06-2X/BSI SCF energy in dichloromethane: -4205.974053 a.u.

M06-2X/BSII SCF energy in dichloromethane: -4207.035873 a.u.

M06-2X/BSII free energy in dichloromethane: -4205.885975 a.u.

P	-0.54789000	1.04013600	0.90925600
O	-1.82968000	1.48518000	-0.02031300
O	0.26954000	2.45399500	0.99916900
O	0.26497800	0.14163000	-0.02141100
O	-0.93916100	0.63247900	2.27178500
C	0.14044100	3.43686900	0.04812300
C	-1.04449700	4.14058100	-0.05484500
C	-1.14090700	5.18719700	-1.03291900
C	0.01412400	5.52661300	-1.79367800
C	1.20396300	4.77500700	-1.63092500
C	1.27887400	3.72129500	-0.75216900
H	-3.25679200	5.61404800	-0.78027700
C	-2.34993400	5.88599100	-1.30817300
C	-0.05313000	6.57976300	-2.74549700
H	2.06494700	5.02030900	-2.24808900
C	-1.22531100	7.25623400	-2.96238400
C	-2.38784200	6.89202100	-2.24151700
H	0.84463300	6.82669600	-3.30612900
H	-1.27146000	8.05731900	-3.69366700
H	-3.32315300	7.40843200	-2.43524800

Quebec, Canada, 2009. http://www.cylview.org.

C	-2.23562600	3.71006800	0.72853500
C	-3.01035300	4.59552900	1.54883800
C	-2.64885700	2.39835400	0.61785400
C	-2.58784900	5.91718100	1.85539300
C	-4.23198300	4.12554100	2.10965600
C	-3.90100800	1.93378200	1.10413500
C	-3.34965300	6.72980100	2.65872000
H	-1.64335400	6.27618100	1.45858700
C	-5.00547000	4.99516800	2.92343700
C	-4.67288100	2.80408400	1.83073700
C	-4.57743200	6.27000900	3.19263600
H	-3.00651300	7.73341400	2.89105500
H	-5.94084900	4.62327600	3.33319800
H	-5.64385200	2.48405300	2.20116600
H	-5.17240100	6.92590500	3.82051500
C	-3.66275100	-1.52422000	3.65070800
C	-3.75401500	-0.43066300	2.84165700
C	-4.33437300	-0.52388100	1.53392900
C	-4.83015800	-1.79904700	1.08375300
C	-4.69271600	-2.92402900	1.96328400
C	-4.13519600	-2.79145200	3.20160300
C	-4.40270000	0.59127900	0.68367400
C	-5.40858900	-1.92085100	-0.19576100
C	-5.49320700	-0.79351300	-1.03885000
C	-4.96950600	0.47147800	-0.60052600
C	-5.04452900	1.58991300	-1.49598700
H	-4.64816100	2.54762900	-1.17510600
C	-5.60590300	1.47242100	-2.73335300
C	-6.14938600	0.22694200	-3.15828500

C	-6.09972900	-0.86189900	-2.33766700
H	-3.21238800	-1.43663200	4.63458800
H	-3.35546000	0.52424400	3.16354400
H	-5.03669200	-3.89530800	1.62517000
H	-4.04225900	-3.65813600	3.84990700
H	-5.64762900	2.33207800	-3.39510200
H	-6.61313100	0.14827000	-4.13687900
H	-6.52959400	-1.80108000	-2.66687300
C	2.10202200	0.99041400	-3.89642900
C	1.82507100	1.80000100	-2.83422300
C	2.79809200	2.04534100	-1.80860900
C	4.07948700	1.40142600	-1.90826300
C	4.32868300	0.56529700	-3.04887200
C	3.37978800	0.36923800	-4.00929300
C	2.51494100	2.88375800	-0.71411900
C	5.04088600	1.58492900	-0.89263300
C	4.71588100	2.34585300	0.25048600
C	3.43710300	2.99972800	0.33974400
C	3.14597200	3.78843500	1.50043100
H	2.18143100	4.28137500	1.56896000
C	4.05008400	3.91812300	2.51260400
C	5.32495100	3.28934400	2.41803300
C	5.64758100	2.54113400	1.32419700
H	1.34546700	0.81053900	-4.65425400
H	0.84502100	2.25567800	-2.74066200
H	5.28766500	0.06541200	-3.13171900
H	3.59115600	-0.27467800	-4.85798100
H	3.80523900	4.50914900	3.38963800
H	6.04663400	3.41644700	3.21912100

H	6.62808200	2.08361300	1.25742700
C	-5.91685200	-3.24029300	-0.67404500
C	-7.02069400	-3.85028400	-0.06644800
C	-5.30536100	-3.88110200	-1.75846700
C	-7.50191400	-5.07198900	-0.53215500
H	-7.50536600	-3.35939400	0.77358100
C	-5.79116000	-5.09904500	-2.22997600
H	-4.44365400	-3.41804300	-2.23337100
C	-6.88998400	-5.69860600	-1.61685900
H	-8.36062300	-5.53117800	-0.05149400
H	-5.30729700	-5.58115100	-3.07471700
H	-7.26896800	-6.64776100	-1.98357900
C	6.39972500	0.98642100	-1.04943900
C	7.23787700	1.40861600	-2.08921500
C	6.86103400	-0.00839100	-0.17982300
C	8.49900500	0.84310700	-2.26108600
H	6.89212900	2.18362200	-2.76830300
C	8.12180300	-0.57684100	-0.35166200
H	6.22650100	-0.32348200	0.64288600
C	8.94335800	-0.15483500	-1.39496300
H	9.13556100	1.18340600	-3.07250200
H	8.46234200	-1.34772100	0.33369500
H	9.92576700	-0.59730100	-1.52983500
C	1.38689600	-4.57938700	0.05500600
C	2.12516200	-4.67302400	1.19530100
C	3.54641700	-4.55181000	1.15060800
C	4.13387800	-4.15761300	-0.07364000
H	3.94738100	-5.13783500	3.19169200
H	1.63841600	-4.94190600	2.12537900

C	4.38880900	-4.83961300	2.24572000
C	5.53437000	-4.03567000	-0.20514200
C	6.33449200	-4.34009800	0.87317600
C	5.75583100	-4.74183100	2.09904600
H	5.95802800	-3.70928100	-1.15102700
H	7.41391200	-4.27071800	0.78737700
H	6.40218000	-4.97067900	2.94069300
O	1.99750400	-4.26035300	-1.11624000
C	-0.03074600	-4.93066000	-0.09751800
C	-0.87546000	-4.93771000	1.01956000
C	-0.53444500	-5.31208400	-1.34541900
C	-2.19836000	-5.34082700	0.88956500
H	-0.50814900	-4.59250400	1.97969000
C	-1.86209300	-5.71346400	-1.46979500
H	0.11315500	-5.30453100	-2.21573900
C	-2.69578300	-5.73555300	-0.35291700
H	-2.84524400	-5.34056300	1.76072100
H	-2.24192000	-6.01444800	-2.44178000
H	-3.72983000	-6.05324900	-0.44794600
C	2.82927500	-1.24349900	1.60885400
C	2.05363200	-0.76071700	2.68020000
C	2.62930900	-0.50260000	3.92052400
C	3.98464300	-0.74611600	4.14005300
C	4.76308100	-1.25262400	3.10121600
C	4.19140200	-1.49091600	1.85549800
H	0.99151700	-0.59419200	2.54080800
H	2.01038400	-0.11235600	4.72348500
H	4.42889300	-0.54812500	5.11131400
H	5.81808100	-1.46274300	3.25759900

H	4.81971900	-1.88262700	1.06315000
C	2.22214900	-1.45502100	0.27763100
C	3.01690600	-1.57383700	-0.82947500
H	4.09403400	-1.40604700	-0.81283100
H	2.53733700	-1.54702600	-1.80452500
B	0.59818400	-1.42006700	0.03949800
O	-0.09633000	-2.03674600	1.13024500
H	-1.02446800	-2.18944700	0.90019200
O	0.30550700	-1.93999200	-1.27212000
C	-0.76949700	-1.45986500	-2.04329400
H	-0.65624600	-0.37539700	-2.19583700
C	-0.70211800	-2.15174100	-3.39832200
H	-0.88633900	-3.22634600	-3.28322400
H	-1.45002500	-1.74432000	-4.08678900
H	0.28985600	-2.01927700	-3.84352500
C	-2.12271800	-1.70508800	-1.37766200
H	-2.22433200	-2.76624100	-1.10986300
H	-2.24574300	-1.09817000	-0.47288100
H	-2.93873300	-1.43588600	-2.05850400
C	3.24940500	-3.84156400	-1.13392600
H	3.60136000	-3.62904000	-2.13754300

TSA-minor

M06-2X/BSI SCF energy in dichloromethane: -4205.97731 a.u.

M06-2X/BSII SCF energy in dichloromethane: -4207.038216a.u.

M06-2X/BSII free energy in dichloromethane: -4205.884514 a.u.

P	0.00586600	1.10938700	-0.81365800
O	1.44404500	1.58281000	-0.19034100

O	-0.77315000	2.52990400	-0.95821000
O	-0.68327500	0.34798600	0.32949300
O	0.09010200	0.50059000	-2.15953300
C	-0.61713900	3.50736400	-0.00107300
C	0.56595300	4.21177700	0.04745300
C	0.72056500	5.21374800	1.06320600
C	-0.38957900	5.51958600	1.90203700
C	-1.59974200	4.79113000	1.76329600
C	-1.72381400	3.77528400	0.84807900
H	2.81681100	5.64520600	0.69699000
C	1.94679300	5.89607100	1.29428700
C	-0.25768800	6.52407600	2.89848200
H	-2.43306300	5.02929400	2.42007800
C	0.93111200	7.18289400	3.07933500
C	2.04784300	6.85131200	2.27520700
H	-1.11984500	6.75060200	3.52030800
H	1.02550500	7.94582200	3.84572900
H	2.99598200	7.35419200	2.43951400
C	1.67674700	3.85190900	-0.87636800
C	2.31797600	4.81309200	-1.72529500
C	2.13367500	2.54935800	-0.89816500
C	1.82615000	6.13706400	-1.88377700
C	3.47013800	4.42360800	-2.46493300
C	3.34108600	2.16853100	-1.54914900
C	2.45944500	7.02646400	-2.71612600
H	0.93008200	6.43638800	-1.34981300
C	4.10921600	5.36931300	-3.31002500
C	3.98320800	3.10736500	-2.31719900
C	3.61866200	6.64454000	-3.43290500

H	2.06361500	8.03083700	-2.83112800
H	4.99270100	5.05848700	-3.86136100
H	4.91857300	2.84969600	-2.80848200
H	4.10987500	7.36045000	-4.08460500
C	2.49190100	-1.45345600	-3.72297500
C	2.80995300	-0.30378300	-3.06197800
C	3.69233000	-0.31707900	-1.93404000
C	4.27608300	-1.56818900	-1.52479400
C	3.88570500	-2.75560400	-2.22950100
C	3.02659100	-2.70053700	-3.28899300
C	3.98106500	0.85750600	-1.22073700
C	5.18427300	-1.60235300	-0.44701800
C	5.50961300	-0.41262300	0.23566400
C	4.88287100	0.82648500	-0.13960900
C	5.18633700	2.00279800	0.62538600
H	4.69943800	2.93729900	0.36812500
C	6.06741100	1.96618000	1.66596000
C	6.72599200	0.75033500	2.00569200
C	6.45677600	-0.39388600	1.31388700
H	1.81566900	-1.42384300	-4.57193700
H	2.37676000	0.64114300	-3.36914200
H	4.28184800	-3.71174600	-1.90554500
H	2.74803000	-3.61303000	-3.80859100
H	6.27855400	2.86852800	2.23169900
H	7.44677200	0.73798900	2.81780600
H	6.97114300	-1.31196000	1.57442600
C	-2.67914100	0.85385700	3.81010900
C	-2.37411500	1.76843200	2.84573300
C	-3.24936200	1.99418600	1.73118000

C	-4.44248000	1.19642800	1.62977300
C	-4.71477600	0.23500500	2.65964400
C	-3.87176900	0.07863700	3.71980900
C	-2.96061400	2.94922700	0.73926600
C	-5.30079100	1.35644800	0.52815900
C	-5.01235900	2.31596700	-0.46040800
C	-3.82899200	3.12335300	-0.35372100
C	-3.57189600	4.09626300	-1.37511100
H	-2.68251800	4.71418100	-1.29859200
C	-4.42419000	4.25851700	-2.42786200
C	-5.60166600	3.46268800	-2.52988300
C	-5.88464900	2.52687900	-1.57916400
H	-2.00859300	0.70763200	4.65136900
H	-1.45522400	2.34104600	2.91359900
H	-5.61058600	-0.37221100	2.58153200
H	-4.09588400	-0.65053000	4.49315300
H	-4.21190300	5.00068500	-3.19139700
H	-6.27705500	3.60875000	-3.36739000
H	-6.78682900	1.92943300	-1.65608300
C	5.77796200	-2.89751600	-0.00348200
C	6.63379500	-3.63176300	-0.83230100
C	5.47948700	-3.40001900	1.26925200
C	7.16814300	-4.84502400	-0.40209200
H	6.87936200	-3.24823500	-1.81936600
C	6.01005800	-4.61376800	1.69891700
H	4.82248700	-2.82635200	1.91945800
C	6.85552700	-5.34065000	0.86217200
H	7.83122500	-5.40323200	-1.05640900
H	5.76421200	-4.99139700	2.68755500

H	7.26979700	-6.28731900	1.19577400
C	-6.49982800	0.48121600	0.37461000
C	-7.66960800	0.70909500	1.10566900
C	-6.45697200	-0.58617700	-0.52826200
C	-8.77914300	-0.11692000	0.93505400
H	-7.70858700	1.53754100	1.80826200
C	-7.56526200	-1.41248200	-0.69700500
H	-5.54760600	-0.76232700	-1.09806700
C	-8.72982400	-1.17842700	0.03303200
H	-9.68435000	0.07280700	1.50449300
H	-7.51782900	-2.23726300	-1.40278300
H	-9.59597000	-1.81978000	-0.10120500
C	0.76037600	-4.32477500	1.47700700
C	0.33346900	-4.47593600	0.11980600
C	-0.94535600	-4.81897500	-0.16287700
H	1.05746600	-4.39777700	-0.68175900
C	-2.70316400	-2.16625100	-0.39088100
C	-2.44011700	-1.53832300	-1.62238000
C	-3.21605200	-1.79480700	-2.74863500
C	-4.26393900	-2.71245700	-2.69007500
C	-4.54896300	-3.34140700	-1.47919200
C	-3.79241400	-3.06054400	-0.34701100
H	-1.62345700	-0.83273000	-1.71127100
H	-2.98617100	-1.28638400	-3.68064200
H	-4.85226600	-2.93423800	-3.57591500
H	-5.36114300	-4.06062200	-1.41502100
H	-4.04027900	-3.57518700	0.57504800
C	-1.83286200	-1.92648100	0.78244700
C	-2.26843800	-2.35559600	2.01399800

H	-3.30028600	-2.65218400	2.19142000
H	-1.69094400	-2.08091600	2.89054000
B	-0.34841400	-1.16482900	0.71175900
O	0.58941200	-1.67447400	-0.26293500
H	0.30400000	-1.51572600	-1.17523900
O	0.18665800	-1.18739000	2.03855700
C	1.16492800	-0.26025400	2.45713700
H	0.87796800	0.74499500	2.11516500
C	1.17360500	-0.26794900	3.98042900
H	1.44218300	-1.26574600	4.34785900
H	1.89702300	0.45351400	4.37509100
H	0.18210400	-0.01498800	4.37004700
C	2.55061000	-0.57622700	1.90112700
H	2.90101000	-1.53961700	2.29080200
H	2.52221100	-0.63007900	0.81004800
H	3.26661100	0.19973200	2.20030400
C	-1.58271400	-4.47033600	2.05554100
H	-2.37692300	-4.67762900	2.76485200
C	-1.48433000	-5.15177600	-1.48737600
C	-0.95341400	-4.53024600	-2.62303500
C	-2.52369200	-6.07985200	-1.62453100
C	-1.44592900	-4.84835400	-3.88451000
H	-0.18130900	-3.77373700	-2.51156600
C	-3.00952500	-6.39549100	-2.88830000
H	-2.94511500	-6.55384700	-0.74309300
C	-2.47222900	-5.78194200	-4.01996500
H	-1.03680400	-4.35437300	-4.76051000
H	-3.80970500	-7.12194200	-2.99090200
H	-2.85635400	-6.02776500	-5.00540400

O	-1.86136600	-4.94013700	0.84680700
C	-0.22782400	-4.34478800	2.48055800
C	0.11617600	-4.23495700	3.84011600
H	-0.66444200	-4.24042700	4.59603200
C	1.44751800	-4.14739600	4.18785400
C	2.44211700	-4.12846100	3.18741400
H	1.73442300	-4.08504900	5.23258500
C	2.10927100	-4.20241100	1.84946900
H	2.87333600	-4.16752800	1.07769100
H	3.48601600	-4.04593100	3.47802700

TSB-major

M06-2X/BSI SCF energy in dichloromethane: -4205.982433 a.u.

M06-2X/BSII SCF energy in dichloromethane: -4207.04699 a.u.

M06-2X/BSII free energy in dichloromethane: -4205.895196 a.u.

P	0.08882200	1.21610600	0.14559900
O	-0.86559200	2.40304400	-0.51464200
O	1.38613400	2.14216700	0.59700200
O	0.41202600	0.29989800	-0.97976200
O	-0.49051500	0.73938900	1.44261900
C	1.81819100	3.14472800	-0.22675700
C	1.10248400	4.32686300	-0.30750700
C	1.57680000	5.35846600	-1.18416000
C	2.81928000	5.17692900	-1.85713200
C	3.53061800	3.96070700	-1.69935300
C	3.03997100	2.94004400	-0.92399000
H	-0.12659500	6.68883800	-0.97993900
C	0.84409400	6.55051500	-1.44380000

C	3.31402600	6.20063100	-2.70887900
H	4.47074700	3.83051900	-2.23032100
C	2.59724600	7.35065800	-2.91503200
C	1.34095000	7.51690800	-2.28315000
H	4.26988200	6.04390600	-3.20229500
H	2.97966100	8.12608600	-3.57153100
H	0.76155100	8.41580000	-2.47166600
C	-0.17031400	4.45287200	0.45596300
C	-0.42999100	5.52039300	1.37648700
C	-1.13028000	3.47186500	0.29851600
C	0.54634400	6.49790300	1.71209500
C	-1.70183200	5.58896300	2.01460100
C	-2.40876900	3.53085100	0.92044600
C	0.26186900	7.50209000	2.60427200
H	1.53275700	6.43551300	1.26434700
C	-1.96952900	6.64649600	2.92495900
C	-2.67772800	4.59098700	1.75014600
C	-1.01369700	7.58724200	3.21199300
H	1.02469300	8.23455300	2.85088700
H	-2.94831900	6.68828800	3.39612300
H	-3.64911900	4.66764700	2.23347500
H	-1.22572200	8.38939800	3.91213900
C	-3.31664100	0.48745700	3.78048800
C	-3.04454900	1.45385700	2.85954200
C	-3.72458500	1.49368400	1.59738000
C	-4.71566400	0.48722200	1.31769400
C	-4.94865600	-0.52664500	2.30760100
C	-4.27940200	-0.52436000	3.49594700
C	-3.42119800	2.47053700	0.63311600

C	-5.40472600	0.49944600	0.08839500
C	-5.09598400	1.47792900	-0.87891000
C	-4.07954200	2.45987900	-0.61140200
C	-3.77423800	3.42333500	-1.62833200
H	-3.00407700	4.16300700	-1.43465100
C	-4.43071500	3.42627700	-2.82393100
C	-5.46258200	2.47763800	-3.07632300
C	-5.78730600	1.54516400	-2.13493100
H	-2.78283500	0.47126400	4.72586300
H	-2.27865700	2.19451600	3.05649100
H	-5.66493600	-1.31254800	2.09402300
H	-4.46951100	-1.30372200	4.22808500
H	-4.17885600	4.16111800	-3.58255500
H	-5.99850400	2.50561800	-4.02031000
H	-6.58663900	0.83960400	-2.33170000
C	2.56012000	-0.05806600	-3.91208000
C	2.70061400	0.87381200	-2.92758300
C	3.63719400	0.69090400	-1.85759200
C	4.43502300	-0.50576800	-1.83813400
C	4.24243000	-1.46692200	-2.88718100
C	3.34323400	-1.24863500	-3.89001600
C	3.77786400	1.64413800	-0.83334800
C	5.36003300	-0.71776400	-0.79644900
C	5.48993400	0.23339000	0.23548400
C	4.67233200	1.41639300	0.22713700
C	4.80574900	2.34975400	1.30673800
H	4.17673700	3.23439900	1.31161600
C	5.70137100	2.14306500	2.31482700
C	6.54414500	0.99372400	2.30150200

C	6.44192000	0.07445200	1.29769400
H	1.83555300	0.09398400	-4.70592100
H	2.08039500	1.76287800	-2.92652100
H	4.82468100	-2.38201600	-2.87363600
H	3.21404800	-1.98995700	-4.67309500
H	5.78386900	2.86025600	3.12566400
H	7.27428100	0.85430600	3.09293700
H	7.09276300	-0.79314900	1.29250200
C	-6.46775800	-0.51273000	-0.18301600
C	-7.63883900	-0.53273200	0.58500600
C	-6.32060600	-1.45671700	-1.20628300
C	-8.63086400	-1.48023600	0.34536900
H	-7.76700100	0.20130400	1.37616900
C	-7.31399000	-2.40335500	-1.45016600
H	-5.41948400	-1.44426300	-1.81403700
C	-8.47000200	-2.42086900	-0.67128700
H	-9.53196400	-1.48137200	0.95125100
H	-7.17940900	-3.12960100	-2.24685800
H	-9.24338600	-3.15998300	-0.85725500
C	6.18596000	-1.95966800	-0.77297400
C	7.18899200	-2.16727600	-1.72661900
C	5.96803500	-2.93921300	0.20371900
C	7.95844400	-3.32819300	-1.70601500
H	7.36324400	-1.41114300	-2.48749900
C	6.73868100	-4.10069700	0.22482000
H	5.18944500	-2.78443300	0.94904700
C	7.73560300	-4.29801100	-0.72995800
H	8.73423600	-3.47268200	-2.45179700
H	6.56259300	-4.85163300	0.99021600

H	8.33663900	-5.20198900	-0.71248100
C	-0.94085500	-5.18571000	0.12487200
C	-0.53461600	-5.10748600	1.41693400
C	0.85894300	-5.16517400	1.74781900
C	1.78360700	-5.12661100	0.68119200
H	0.63386900	-5.28397300	3.89018700
H	-1.28355400	-5.08920300	2.20195400
C	1.34076300	-5.25531600	3.06641500
C	3.17033000	-5.14405100	0.92544100
C	3.62018900	-5.23093200	2.22612900
C	2.70214300	-5.28804100	3.29514700
H	3.86577000	-5.09258500	0.09166100
H	4.68552600	-5.25289900	2.43315000
H	3.07442200	-5.35048200	4.31276400
O	-0.02497600	-5.25561200	-0.88062100
C	-2.33333300	-5.30769500	-0.33230900
C	-3.32112400	-4.49763200	0.23581700
C	-2.67333700	-6.25239200	-1.30690700
C	-4.64654200	-4.64061000	-0.16478100
H	-3.04412200	-3.72799600	0.95292800
C	-4.00217500	-6.39768400	-1.69335500
H	-1.90283100	-6.87805300	-1.74795400
C	-4.98915600	-5.59286800	-1.12375400
H	-5.40881900	-3.99812000	0.26593500
H	-4.26679900	-7.13837500	-2.44173300
H	-6.02482900	-5.70496300	-1.43068400
C	1.21624900	-1.94929200	1.24971600
C	0.50002900	-2.08850600	2.45119800
C	1.06679800	-1.72143300	3.66552100

C	2.35086900	-1.18045400	3.70130200
C	3.06585600	-1.00693000	2.51559200
C	2.50785200	-1.39684500	1.30315100
H	-0.50945400	-2.48899000	2.42506700
H	0.50185100	-1.84589700	4.58473600
H	2.78682800	-0.87473900	4.64796900
H	4.05377000	-0.55349700	2.53460900
H	3.04836600	-1.21675800	0.37782300
C	0.61353500	-2.30836900	-0.04121000
C	1.39186800	-2.83238700	-1.04023000
H	2.47801300	-2.87193100	-0.95105300
H	0.97918500	-2.92777500	-2.04146300
B	-0.92674100	-2.00944400	-0.34200300
O	-1.76336200	-1.38239500	0.52314400
H	-1.31285700	-0.69603500	1.08308900
O	-1.40122700	-2.49900500	-1.52691500
C	-2.68307400	-2.04281600	-1.98054200
H	-3.38886400	-2.10440200	-1.14332300
C	-2.58101200	-0.59784300	-2.44899300
H	-1.82963200	-0.51628100	-3.24264800
H	-3.54356900	-0.25344100	-2.84562000
H	-2.28631700	0.06257700	-1.62825500
C	-3.12703600	-2.97438200	-3.09256000
H	-2.44086700	-2.89980700	-3.94414000
H	-3.13751300	-4.01117900	-2.74609700
H	-4.13287500	-2.71029000	-3.43704400
C	1.25367100	-4.99075400	-0.63557500
H	1.87397100	-5.14205200	-1.51324100

TSB-minor

M06-2X/BSI SCF energy in dichloromethane: -4205.978583 a.u.

M06-2X/BSII SCF energy in dichloromethane: -4207.043656 a.u.

M06-2X/BSII free energy in dichloromethane: -4205.893742 a.u.

P	1.37472100	-0.29185900	-0.01865000
O	2.79805700	0.27766700	-0.65333800
O	1.93149300	-1.74117900	0.57145400
O	0.47557700	-0.48285100	-1.18535400
O	1.00887100	0.49828700	1.19930000
C	2.73920700	-2.48385900	-0.24537100
C	4.07445700	-2.14105000	-0.38295000
C	4.89428700	-2.92055300	-1.26453600
C	4.33765700	-4.07330000	-1.88978100
C	2.97283200	-4.39684000	-1.67825900
C	2.16321600	-3.61204800	-0.89480900
H	6.66605300	-1.67193500	-1.14993600
C	6.23779200	-2.57152100	-1.57871400
C	5.14538600	-4.86377200	-2.75146100
H	2.55854900	-5.27065600	-2.17620100
C	6.44548700	-4.51545600	-3.01128700
C	6.98959900	-3.34661500	-2.42642300
H	4.70279100	-5.74497200	-3.20889900
H	7.05503000	-5.12222100	-3.67371700
H	8.01075300	-3.05765300	-2.65665300
C	4.57953900	-0.93156400	0.32806000
C	5.70786000	-0.95124000	1.21214200
C	3.88909000	0.25545700	0.16842800
C	6.40586200	-2.14478700	1.54508500

C	6.13469500	0.26814800	1.81350800
C	4.27041500	1.47107500	0.80632300
C	7.48653600	-2.11893800	2.39158300
H	6.06497100	-3.08852300	1.13245900
C	7.26574200	0.26493900	2.67375400
C	5.40019300	1.46215000	1.58655800
C	7.93471300	-0.89924600	2.95315700
H	8.00124200	-3.04342000	2.63571800
H	7.58288700	1.20739700	3.11317200
H	5.72348900	2.37525400	2.08143600
H	8.79617300	-0.89254700	3.61373800
C	1.91035900	2.85970200	4.07603400
C	2.64975500	2.42482600	3.01706400
C	2.63015300	3.11184500	1.75757000
C	1.75971300	4.24780900	1.61736400
C	1.01422100	4.68243500	2.76489100
C	1.09002700	4.01819200	3.95328600
C	3.40303600	2.67854600	0.66266100
C	1.64609700	4.90026900	0.37519900
C	2.41909800	4.46651000	-0.71939300
C	3.31623300	3.35263500	-0.56884800
C	4.10199200	2.95125700	-1.69889800
H	4.79603800	2.12462200	-1.58253000
C	3.99596700	3.58779200	-2.90023300
C	3.08171000	4.66908700	-3.06025000
C	2.31986300	5.08909200	-2.00920600
H	1.93764200	2.31742000	5.01631400
H	3.25157800	1.52833300	3.11098200
H	0.38537900	5.56180400	2.67637500

H	0.51891800	4.36555600	4.80928500
H	4.60224300	3.26845300	-3.74238300
H	2.98894500	5.15518800	-4.02710700
H	1.61786700	5.90556500	-2.14280500
C	-0.58995900	-2.75262200	-4.03929500
C	0.26855400	-2.99951200	-3.01007700
C	-0.17311200	-3.64890800	-1.80934500
C	-1.56398000	-3.99818000	-1.69506300
C	-2.43201800	-3.72542200	-2.80692400
C	-1.96110200	-3.13139100	-3.94068900
C	0.70833900	-3.92166700	-0.74655600
C	-2.04699900	-4.58994600	-0.51400600
C	-1.16425100	-4.87274600	0.54533500
C	0.22690400	-4.52606500	0.43024600
C	1.09267700	-4.80826900	1.53716500
H	2.14306800	-4.54567600	1.45848600
C	0.62065200	-5.39870900	2.67314200
C	-0.75641500	-5.74831500	2.78445500
C	-1.61861900	-5.48745900	1.75921800
H	-0.23365700	-2.25679400	-4.93704900
H	1.30498700	-2.69075900	-3.08186600
H	-3.47643100	-4.01248800	-2.73657400
H	-2.63122400	-2.94149300	-4.77427500
H	1.29427300	-5.60357500	3.49958100
H	-1.11890300	-6.21685700	3.69455600
H	-2.66858800	-5.74603700	1.85156800
C	0.67636400	6.02341800	0.21150000
C	1.11215500	7.33851600	0.01708700
C	-0.70011700	5.76455800	0.24877400

C	0.19219200	8.37353500	-0.14270700
H	2.17835100	7.54864700	-0.00930800
C	-1.61870100	6.79918600	0.08593500
H	-1.03379800	4.74090600	0.40324000
C	-1.17523200	8.10631400	-0.11089900
H	0.54551300	9.38987800	-0.29031100
H	-2.68330100	6.58306200	0.11260500
H	-1.89204400	8.91226100	-0.23679300
C	-3.51204400	-4.83710200	-0.36277100
C	-4.07526300	-6.10333300	-0.54186100
C	-4.34986200	-3.76068700	-0.04779300
C	-5.45158200	-6.28678800	-0.40869300
H	-3.43250600	-6.94428500	-0.78838200
C	-5.72387200	-3.94185400	0.08535600
H	-3.90757900	-2.77680800	0.09799800
C	-6.27799200	-5.20890700	-0.09638400
H	-5.87899400	-7.27491200	-0.55047600
H	-6.35765000	-3.09476000	0.33436500
H	-7.34887900	-5.35606300	0.00634200
C	-5.12875200	0.82196600	0.70877600
C	-5.04154600	2.07962700	0.19318800
C	-5.05026700	2.28905300	-1.22010200
C	-4.93039300	1.15272500	-2.05077300
H	-5.27419900	4.43736200	-1.18861600
H	-5.04395800	2.93408600	0.86024800
C	-5.18544900	3.55658600	-1.81754100
C	-4.92621200	1.27235300	-3.45541800
C	-5.08103500	2.51892300	-4.01727100
C	-5.21265700	3.65903800	-3.19283200

H	-4.81548100	0.38240900	-4.06852000
H	-5.09754500	2.63355400	-5.09583400
H	-5.32539800	4.63502100	-3.65495900
O	-5.09628700	-0.24978000	-0.13202400
C	-5.29508000	0.43889600	2.11556400
C	-5.63168400	1.39976800	3.07811400
C	-5.08855600	-0.88886300	2.51107600
C	-5.74320000	1.03752800	4.41504100
H	-5.81924300	2.42887900	2.78891700
C	-5.21008000	-1.24609000	3.84860800
H	-4.80676800	-1.63917600	1.78096400
C	-5.53223800	-0.28486100	4.80463200
H	-6.00229800	1.78952700	5.15367100
H	-5.03585300	-2.27619700	4.14372900
H	-5.61946500	-0.56398800	5.85019300
C	-2.01554100	-0.10097700	1.05503300
C	-2.12474700	0.75512300	2.16281200
C	-1.94537100	0.27799800	3.45464400
C	-1.63145700	-1.06590500	3.66282800
C	-1.49795100	-1.92497200	2.57305100
C	-1.68570700	-1.44589200	1.27982200
H	-2.35788000	1.80516100	2.00018300
H	-2.04260700	0.95402100	4.29930100
H	-1.47639200	-1.43865300	4.67121900
H	-1.21560800	-2.96300500	2.72663700
H	-1.50192700	-2.09809600	0.42948900
C	-2.12464800	0.42714700	-0.31536200
C	-2.53392400	-0.36466700	-1.34801700
H	-2.70269400	-1.43205800	-1.20772100

H	-2.40293300	-0.02714200	-2.37270800
B	-1.46613100	1.83105600	-0.67312400
O	-0.49467400	2.39196400	0.08695900
H	-0.02617400	1.75447900	0.69001500
O	-1.88299800	2.44286100	-1.82518300
C	-0.97288200	3.35021900	-2.46827800
H	-0.40717600	3.89081900	-1.70160300
C	-0.00840800	2.52957100	-3.31106000
H	-0.56737400	1.92820600	-4.03827200
H	0.68461100	3.17961100	-3.85427600
H	0.57240500	1.85210600	-2.67451000
C	-1.77681800	4.33995000	-3.28847400
H	-2.35081500	3.82337000	-4.06598400
H	-2.47283800	4.89689300	-2.65307800
H	-1.10316800	5.05686600	-3.76989600
C	-4.78423700	-0.10139600	-1.40947600
H	-4.82688700	-1.03796100	-1.95657100

TSC-major

M06-2X/BSI SCF energy in dichloromethane: -4205.987003 a.u.

M06-2X/BSII SCF energy in dichloromethane: -4207.05046 a.u.

M06-2X/BSII free energy in dichloromethane: -4205.900742 a.u.

P	-0.55880900	1.07624500	-0.57469700
O	-1.79603100	2.14796500	-0.78827000
O	0.40912700	1.95050400	0.45257200
O	0.10999400	0.89530900	-1.88964800
O	-1.04087000	-0.07152800	0.25808300
C	0.67096300	3.25887100	0.12988100

C	-0.31624300	4.20771900	0.32447300
C	-0.06922100	5.56182300	-0.07166900
C	1.22382800	5.91319000	-0.54923800
C	2.22524100	4.91572100	-0.64228700
C	1.97556000	3.60083000	-0.32283600
H	-2.07262300	6.31342300	0.29354100
C	-1.07053000	6.57175800	-0.03220600
C	1.49089100	7.25597000	-0.93086100
H	3.21746100	5.20414200	-0.98142200
C	0.51036000	8.21146700	-0.86216600
C	-0.78703000	7.85821600	-0.41771400
H	2.48864400	7.50519100	-1.28285700
H	0.71984300	9.23523100	-1.15650800
H	-1.56696600	8.61326300	-0.38593600
C	-1.61031200	3.78437100	0.92184300
C	-2.11815700	4.37817100	2.12404100
C	-2.31279800	2.74906400	0.33508700
C	-1.39817600	5.35056300	2.87301900
C	-3.38331700	3.95327100	2.61684300
C	-3.57718300	2.31351500	0.81903700
C	-1.92688200	5.88899100	4.02018200
H	-0.41314500	5.65910200	2.53962800
C	-3.91025900	4.53703600	3.80027500
C	-4.09147300	2.93550700	1.93246300
C	-3.20217900	5.48871400	4.48719900
H	-1.35811900	6.62572400	4.57951500
H	-4.88255600	4.20298400	4.15273300
H	-5.06077400	2.62642300	2.31651700
H	-3.60825700	5.92692400	5.39359300

C	-4.30520900	-1.38756900	2.81069700
C	-4.00859600	-0.25113200	2.11740800
C	-4.66027200	0.05748200	0.87675700
C	-5.60985400	-0.88628900	0.35318100
C	-5.90959900	-2.05685900	1.12940500
C	-5.28406200	-2.29798200	2.31677400
C	-4.37499700	1.23813300	0.16255000
C	-6.19028900	-0.67078800	-0.91115000
C	-5.85804300	0.47949900	-1.65274000
C	-4.95466300	1.45394200	-1.10287000
C	-4.69399000	2.64343300	-1.85968800
H	-4.02956300	3.39490100	-1.44678900
C	-5.26410300	2.84518400	-3.08213900
C	-6.15087700	1.87476900	-3.63181000
C	-6.43996300	0.73639500	-2.93849900
H	-3.78863900	-1.60606100	3.74042300
H	-3.24690000	0.42599400	2.48698100
H	-6.62991500	-2.76986100	0.74178500
H	-5.51638100	-3.19578700	2.88183600
H	-5.04707100	3.75122200	-3.63956600
H	-6.60416300	2.04987000	-4.60283000
H	-7.12847900	0.00863500	-3.35427800
C	3.71629700	2.55691200	-4.08352500
C	3.11813200	2.80528100	-2.88335300
C	3.70857500	2.36575000	-1.65106200
C	4.94971400	1.64040400	-1.70776900
C	5.54617000	1.40956900	-2.99343100
C	4.95359800	1.85315500	-4.13898500
C	3.09604700	2.61796200	-0.40684900

C	5.53425800	1.14629500	-0.52495800
C	4.86626800	1.30618100	0.70627300
C	3.63993100	2.05907800	0.76776100
C	3.02124100	2.24538200	2.04865400
H	2.11331700	2.83386500	2.11480100
C	3.54686900	1.69315200	3.17934100
C	4.75481400	0.94173100	3.11830800
C	5.39959100	0.77204300	1.92810200
H	3.24286700	2.88387800	-5.00412300
H	2.16284700	3.31695600	-2.84827300
H	6.47791600	0.85610200	-3.04483000
H	5.41752900	1.65846700	-5.10118600
H	3.05103500	1.83623300	4.13434400
H	5.17075000	0.51835300	4.02746100
H	6.33297000	0.22033700	1.89431500
C	-7.14375400	-1.67555700	-1.46902900
C	-8.45459100	-1.75990100	-0.98789300
C	-6.73199200	-2.55744800	-2.47477300
C	-9.33573200	-2.71076500	-1.49868400
H	-8.78017200	-1.07729500	-0.20714700
C	-7.61308700	-3.50948200	-2.98462900
H	-5.71585100	-2.49347000	-2.85605300
C	-8.91653600	-3.58805000	-2.49748500
H	-10.35077800	-2.76543200	-1.11648200
H	-7.27926200	-4.18875700	-3.76346700
H	-9.60375400	-4.32885700	-2.89492100
C	6.87213700	0.48602600	-0.58137900
C	8.01616900	1.23777200	-0.87510200
C	7.01104300	-0.88576200	-0.35192800

C	9.26758700	0.62884200	-0.93535100
H	7.91945600	2.30508700	-1.05691500
C	8.26104000	-1.49812900	-0.41612600
H	6.12725500	-1.47732000	-0.13383900
C	9.39392700	-0.74076900	-0.70741500
H	10.14563300	1.22563000	-1.16339600
H	8.34547500	-2.56799600	-0.24480400
H	10.36960600	-1.21442400	-0.75921700
C	0.28103600	-3.62395200	-1.05955800
C	1.37687700	-4.43188100	-1.06527200
C	2.65865700	-3.91729200	-1.44597400
C	2.78275700	-2.51905100	-1.58132300
H	3.68530800	-5.81073400	-1.58996200
H	1.26443100	-5.49420300	-0.88223400
C	3.77164400	-4.73519800	-1.71447200
C	3.98772000	-1.94359700	-2.01312000
C	5.05633900	-2.76665600	-2.31645100
C	4.95220300	-4.16037200	-2.14561000
H	4.06091200	-0.86399900	-2.12006900
H	5.98672500	-2.33575000	-2.67249500
H	5.80877200	-4.78979000	-2.36651900
O	0.42352000	-2.28757100	-1.24178900
C	-1.12407600	-4.04555100	-0.97374000
C	-1.46888300	-5.40403800	-1.02126700
C	-2.13354300	-3.07915700	-0.87575200
C	-2.80211800	-5.79038200	-0.95437200
H	-0.70281600	-6.16585400	-1.12292700
C	-3.46537900	-3.47523200	-0.83456000
H	-1.87803500	-2.02451900	-0.82386600

C	-3.80569800	-4.82596200	-0.86403400
H	-3.05704800	-6.84512200	-0.98714900
H	-4.24011900	-2.71988000	-0.77214200
H	-4.84996800	-5.12356300	-0.82509000
C	3.07598300	-3.36929400	1.54808200
C	2.97230000	-4.76160700	1.75571600
C	4.10505200	-5.55756000	1.84201100
C	5.37519800	-4.98680700	1.73405000
C	5.50120800	-3.61210700	1.54714900
C	4.36611100	-2.81437000	1.45198900
H	1.98906100	-5.21188600	1.82462900
H	4.00053500	-6.62813500	1.98900100
H	6.26129100	-5.61052300	1.80454200
H	6.48530100	-3.15516500	1.48885500
H	4.48883700	-1.74006200	1.35141400
C	1.87925200	-2.54007200	1.38560200
C	1.96718300	-1.31319800	0.73132900
H	2.93449300	-0.84545100	0.55066600
H	1.14502800	-0.60915900	0.83563900
B	0.44116700	-2.93750800	1.97419900
O	-0.67517400	-2.23778700	1.69972600
H	-0.67550100	-1.44705700	1.10627700
O	0.38138900	-3.98569700	2.84639800
C	-0.85200800	-4.30154700	3.50904900
H	-1.30934900	-3.36389000	3.84569600
C	-1.80279400	-5.00771000	2.55417600
H	-1.32936600	-5.91142600	2.15246400
H	-2.71511700	-5.30417300	3.08313400
H	-2.08272300	-4.35042900	1.72578100

C	-0.49424900	-5.16160500	4.70817800
H	-0.03084400	-6.09771600	4.37691300
H	0.21024000	-4.63943400	5.36222400
H	-1.39116900	-5.40454000	5.28578700
C	1.64693400	-1.72383200	-1.18271700
H	1.57862600	-0.67366000	-1.46669600

TSC-minor

M06-2X/BSI SCF energy in dichloromethane: -4205.983129 a.u.

M06-2X/BSII SCF energy in dichloromethane: -4207.047277a.u.

M06-2X/BSII free energy in dichloromethane: -4205.898863 a.u.

P	-1.20184600	0.82095500	-0.31977400
O	-2.76221500	1.29796300	-0.57441200
O	-0.67049500	2.09756900	0.58965700
O	-0.52538300	0.78615900	-1.64429500
O	-1.18097900	-0.34445000	0.62214600
C	-1.03886000	3.36539100	0.22348500
C	-2.31878900	3.80546800	0.50376800
C	-2.69523600	5.12967100	0.10219500
C	-1.71176900	5.98065900	-0.47822300
C	-0.40262600	5.48502500	-0.70590300
C	-0.05942600	4.19269900	-0.39172700
H	-4.79763000	4.97533800	0.61879200
C	-4.02368500	5.62445600	0.22375000
C	-2.06550100	7.30343100	-0.85916700
H	0.33194100	6.14047200	-1.16846100
C	-3.34849200	7.76018100	-0.70187700
C	-4.33925600	6.90194500	-0.16723000

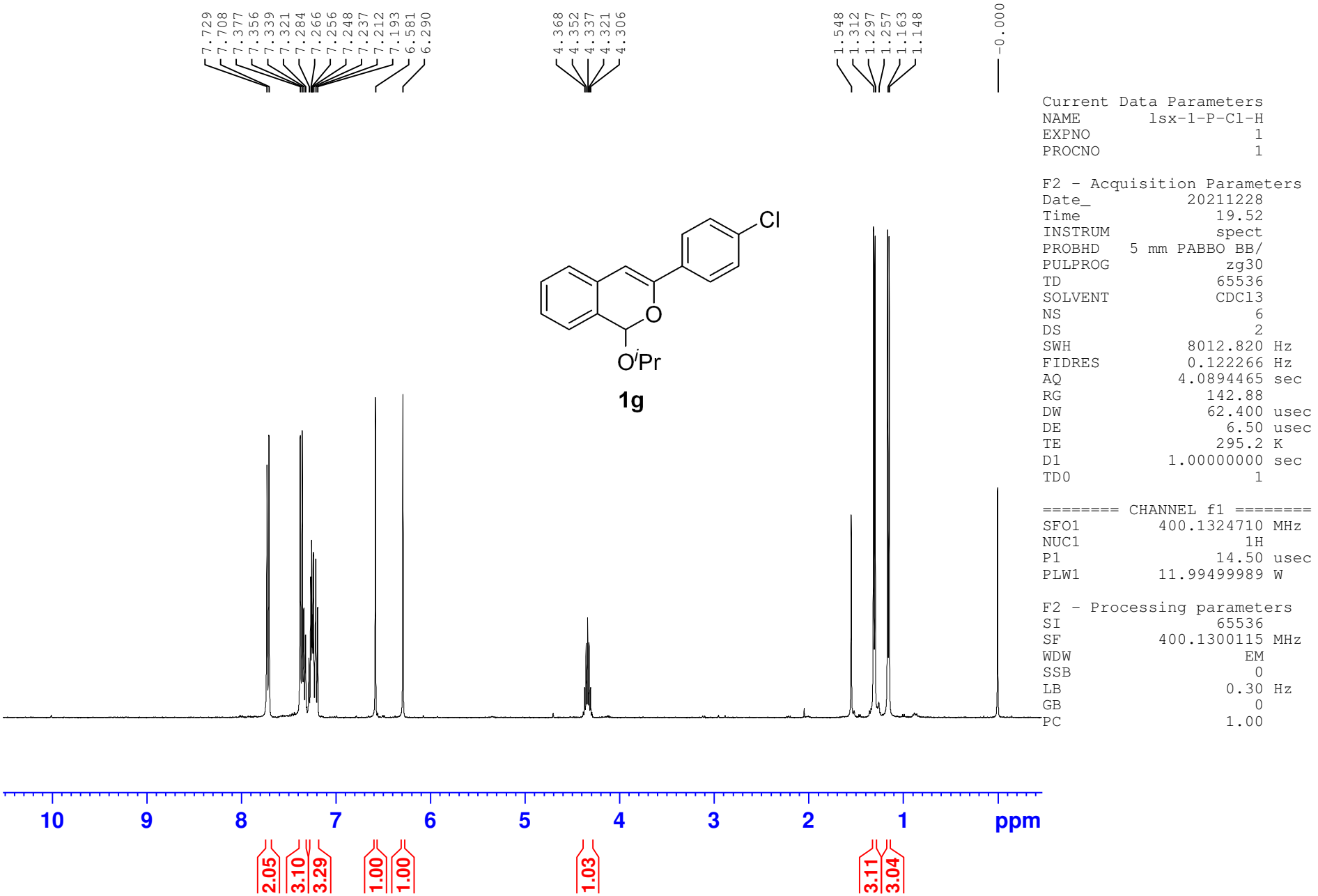
H	-1.29674000	7.94031800	-1.28920100
H	-3.61227700	8.77052900	-0.99869500
H	-5.36092100	7.25686600	-0.07114800
C	-3.28062000	2.86210500	1.13703900
C	-3.97888900	3.16346800	2.35174700
C	-3.48104300	1.62832700	0.54870200
C	-3.72725200	4.34141300	3.10718200
C	-4.93292300	2.23178000	2.85079000
C	-4.43519500	0.68860000	1.03119100
C	-4.41358600	4.59336600	4.26934200
H	-2.97156700	5.03994100	2.76322800
C	-5.63813100	2.52739900	4.04819800
C	-5.15364800	1.01403200	2.15575900
C	-5.39027100	3.68421500	4.74229100
H	-4.20047600	5.49553700	4.83477200
H	-6.37073900	1.80965700	4.40816300
H	-5.89604000	0.31869200	2.54085900
H	-5.93011300	3.90025600	5.65905900
C	-3.16270200	-3.06036700	2.66382200
C	-3.55814000	-1.87187300	2.12559300
C	-4.26417600	-1.81722000	0.87817300
C	-4.53643000	-3.05245000	0.19231000
C	-4.09999700	-4.27943000	0.79594000
C	-3.44024500	-4.28475500	1.98977400
C	-4.66256200	-0.59551200	0.30566300
C	-5.18027300	-3.03659400	-1.05908100
C	-5.56145700	-1.81198700	-1.64033200
C	-5.30363300	-0.57855500	-0.94814200
C	-5.72710900	0.64696600	-1.56038600

H	-5.54696100	1.58287400	-1.04158700
C	-6.35325100	0.65517500	-2.77205100
C	-6.61062900	-0.56718800	-3.45682700
C	-6.23158100	-1.75672500	-2.90776200
H	-2.61660900	-3.07683800	3.60196000
H	-3.31437500	-0.94133000	2.62533000
H	-4.29511700	-5.21369300	0.27973300
H	-3.11030100	-5.22368700	2.42519100
H	-6.66457200	1.59547200	-3.21685400
H	-7.11806400	-0.54767500	-4.41660900
H	-6.44156500	-2.68519000	-3.42817300
C	1.02722900	3.32467000	-4.41004700
C	0.68154100	3.53602800	-3.10902800
C	1.64098200	3.39992000	-2.05030400
C	2.97498900	2.97284900	-2.38110800
C	3.30083200	2.79776700	-3.76939800
C	2.36560800	2.97047500	-4.74669300
C	1.29789500	3.66123000	-0.71149400
C	3.92751600	2.77487100	-1.35826200
C	3.56853700	3.00794600	-0.01212400
C	2.24196700	3.46116900	0.31142800
C	1.90970000	3.69149600	1.68675600
H	0.91299400	4.04525500	1.93061700
C	2.81448300	3.46693000	2.68205900
C	4.12193100	2.99944400	2.36752800
C	4.48461800	2.78503300	1.07000100
H	0.28359700	3.42723800	-5.19431000
H	-0.33926300	3.79619900	-2.85342100
H	4.31679300	2.53451200	-4.04065100

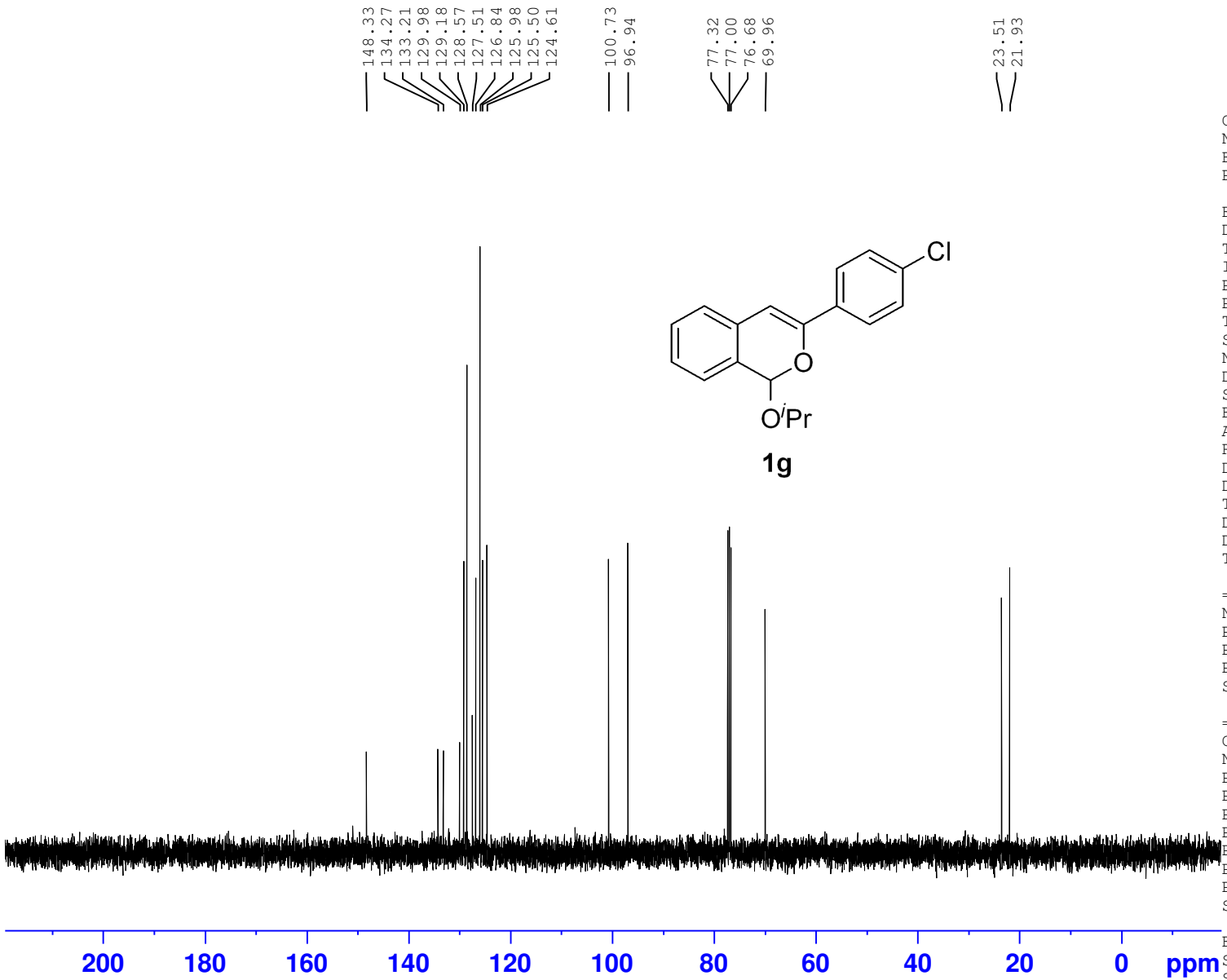
H	2.63935500	2.83606100	-5.78896200
H	2.53919400	3.63975300	3.71798600
H	4.83262700	2.80685900	3.16587600
H	5.48096100	2.42387000	0.84635900
C	-5.44480100	-4.31975400	-1.77561800
C	-6.47338500	-5.16959000	-1.35508400
C	-4.66711300	-4.69097900	-2.87841300
C	-6.72148300	-6.36589200	-2.02447400
H	-7.07961600	-4.88744300	-0.49828100
C	-4.91377400	-5.88863600	-3.54685400
H	-3.87108700	-4.03142600	-3.21549400
C	-5.94180800	-6.72814500	-3.12182500
H	-7.52570300	-7.01429000	-1.68940800
H	-4.30351800	-6.16418200	-4.40178700
H	-6.13561100	-7.66021200	-3.64416300
C	5.30530500	2.31185600	-1.69958700
C	6.42210300	3.10651400	-1.41305700
C	5.50864200	1.07116000	-2.31941000
C	7.70693600	2.67121400	-1.73059200
H	6.27786000	4.07369100	-0.93884500
C	6.79185900	0.63831900	-2.64583400
H	4.64935400	0.44384500	-2.54914900
C	7.89607900	1.43654400	-2.34954300
H	8.56061300	3.30142000	-1.49979200
H	6.92847900	-0.32191300	-3.13469900
H	8.89696800	1.10054000	-2.60356800
C	3.72506600	-3.12846000	-0.70811600
C	2.80081400	-4.02133300	-0.26406700
C	1.41695600	-3.86109400	-0.60185000

C	1.02861900	-2.62917900	-1.17018400
H	0.74920900	-5.81714700	0.01488300
H	3.13262700	-4.90960500	0.26247600
C	0.44973500	-4.86100400	-0.40388500
C	-0.31262300	-2.38014600	-1.50523200
C	-1.25009300	-3.37099200	-1.28751000
C	-0.86691200	-4.61119500	-0.74519500
H	-0.58702400	-1.41505800	-1.92092700
H	-2.29185100	-3.19053100	-1.53489100
H	-1.61912900	-5.37910900	-0.59134000
O	3.33531500	-2.03050900	-1.41407100
C	5.17961000	-3.23005300	-0.54401200
C	5.70482200	-3.82834700	0.60726200
C	6.03991700	-2.67341100	-1.49700100
C	7.08163500	-3.87491900	0.79551500
H	5.03548600	-4.20898400	1.37404800
C	7.41586900	-2.72932100	-1.30488000
H	5.62917800	-2.20209700	-2.38490600
C	7.93890600	-3.32682300	-0.15884800
H	7.48569000	-4.32109200	1.69885300
H	8.08225600	-2.30025300	-2.04710600
H	9.01315200	-3.35945100	-0.00524500
C	4.01372800	-1.00116400	1.69546800
C	4.50669600	-1.35513600	2.96718000
C	5.84073100	-1.14646300	3.29709700
C	6.72435500	-0.60490600	2.36243400
C	6.25800000	-0.25535400	1.09611800
C	4.91896800	-0.43809400	0.77496300
H	3.83223500	-1.78057500	3.69907300

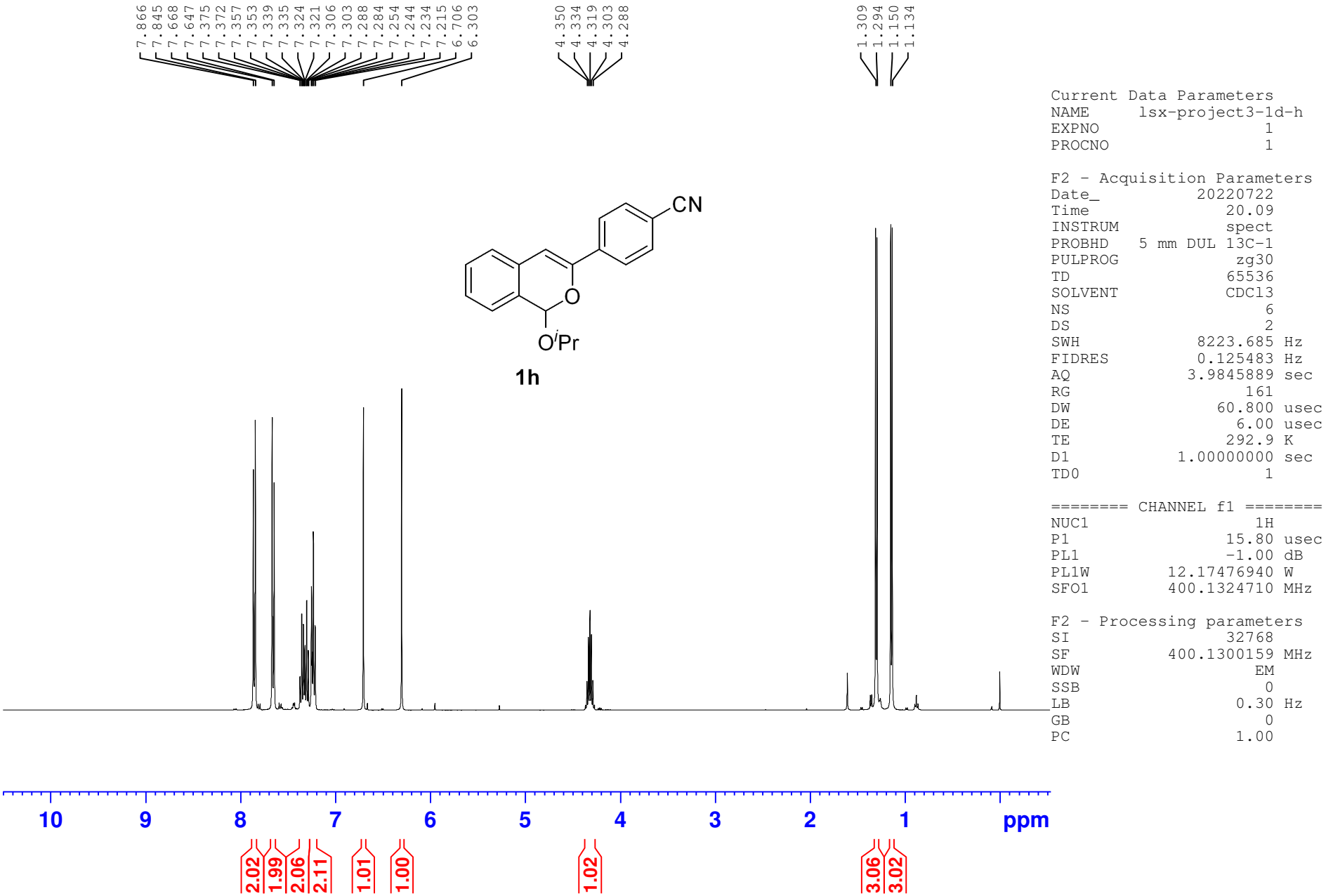
H	6.19398000	-1.41281400	4.28876400
H	7.76879000	-0.45545400	2.62036800
H	6.93315400	0.16349700	0.35320700
H	4.58190600	-0.15447700	-0.21671800
C	2.59696700	-1.17860400	1.34590300
C	2.04143400	-0.44523000	0.30942600
H	2.58297600	0.39013300	-0.13193700
H	0.96248000	-0.36241600	0.26349600
B	1.60573100	-2.17863700	2.12210900
O	0.27200500	-2.18191400	1.92640400
H	-0.18048500	-1.48601800	1.38957800
O	2.16064000	-3.07529300	2.98942300
C	1.33503900	-3.86991000	3.85104900
H	0.47206700	-3.26716600	4.15619200
C	0.84394500	-5.10303200	3.11178200
H	1.69648700	-5.69088200	2.75107900
H	0.24801900	-5.73461600	3.77921400
H	0.22115500	-4.81429800	2.26116100
C	2.17552300	-4.21921800	5.06715700
H	3.06044700	-4.79006000	4.76453100
H	2.50673000	-3.31224100	5.58246900
H	1.59596400	-4.82422800	5.77107900
C	2.05189000	-1.63403700	-1.349668000
H	1.85896000	-0.77849600	-1.992442000




```
Current Data Parameters
NAME       lsx-1-P-Cl-H
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20211228
Time              19.52
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    6
DS                    2
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ           4.0894465 sec
RG               142.88
DW               62.400 usec
DE                6.50 usec
TE               295.2 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1               14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300115 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME      lsx-project3-1c-c
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220722
Time               20.04
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   20
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE                293.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127795 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

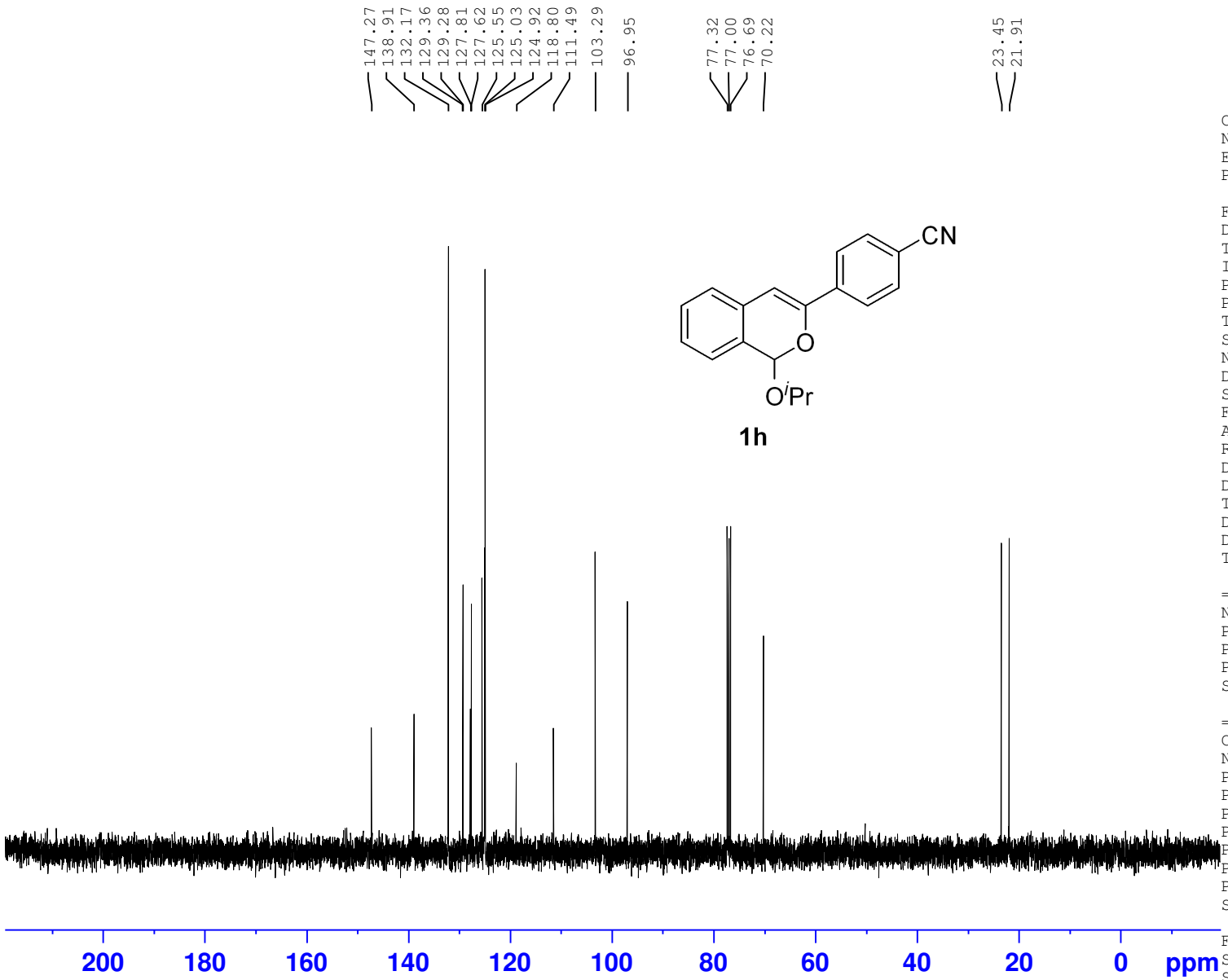


Current Data Parameters
NAME lsx-project3-1d-h
EXPNO 1
PROCNO 1

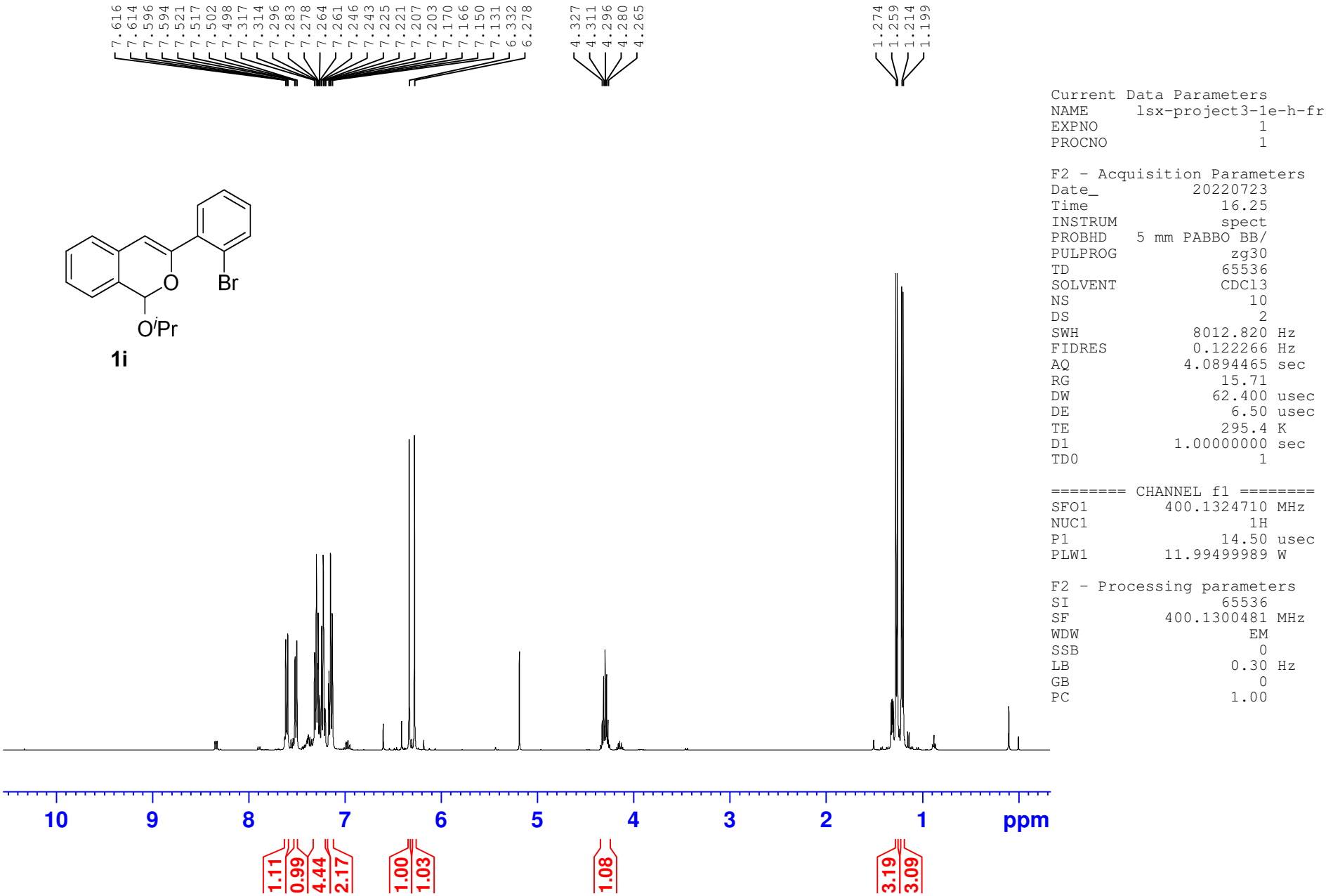
F2 - Acquisition Parameters
Date_ 20220722
Time 20.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.80 usec
PL1 -1.00 dB
PL1W 12.17476940 W
SFO1 400.1324710 MHz

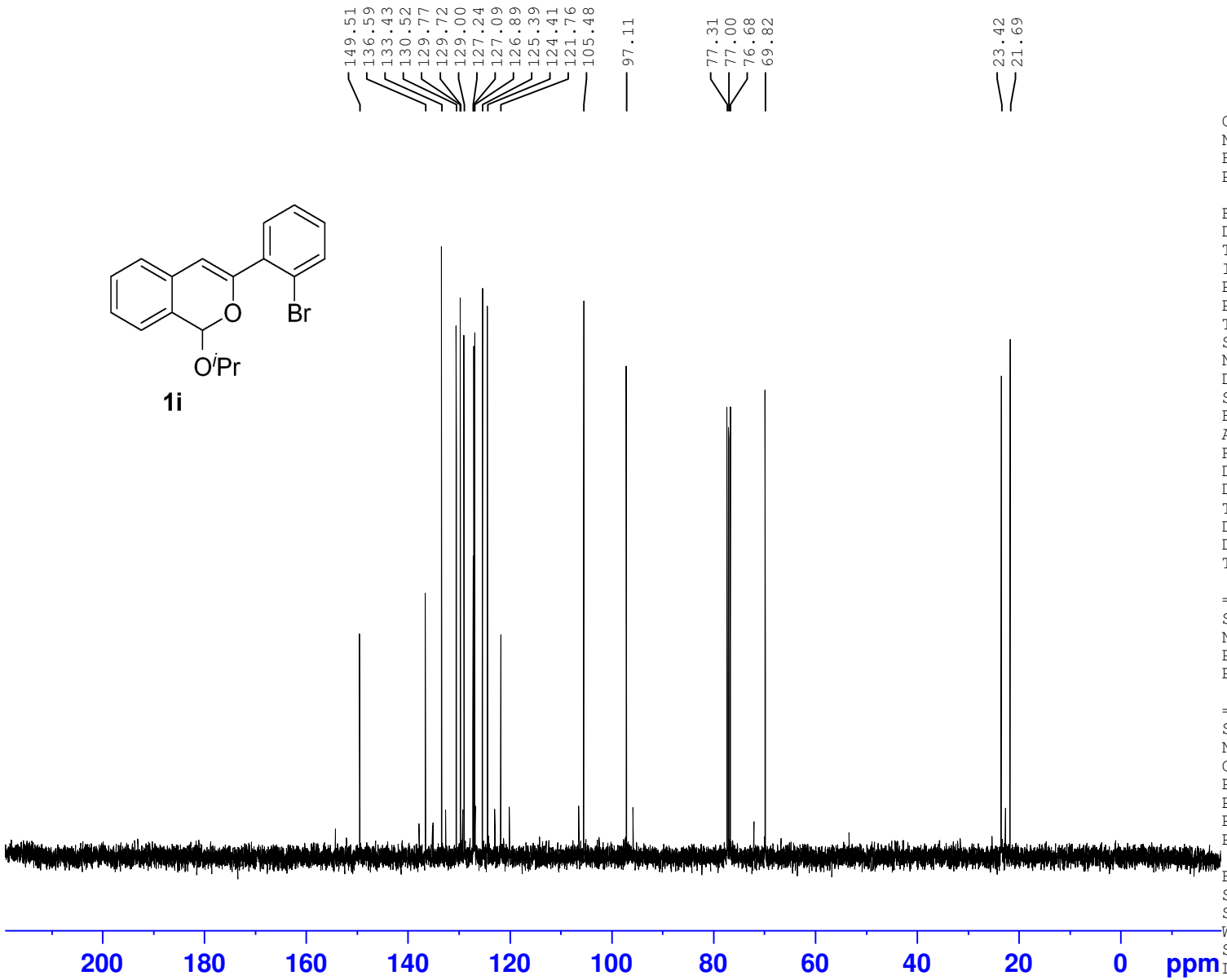
F2 - Processing parameters
SI 32768
SF 400.1300159 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
Current Data Parameters
NAME      lsx-project3-1d-c
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20220722
Time              20.07
INSTRUM           spect
PROBHD    5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   25
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE               293.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127810 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

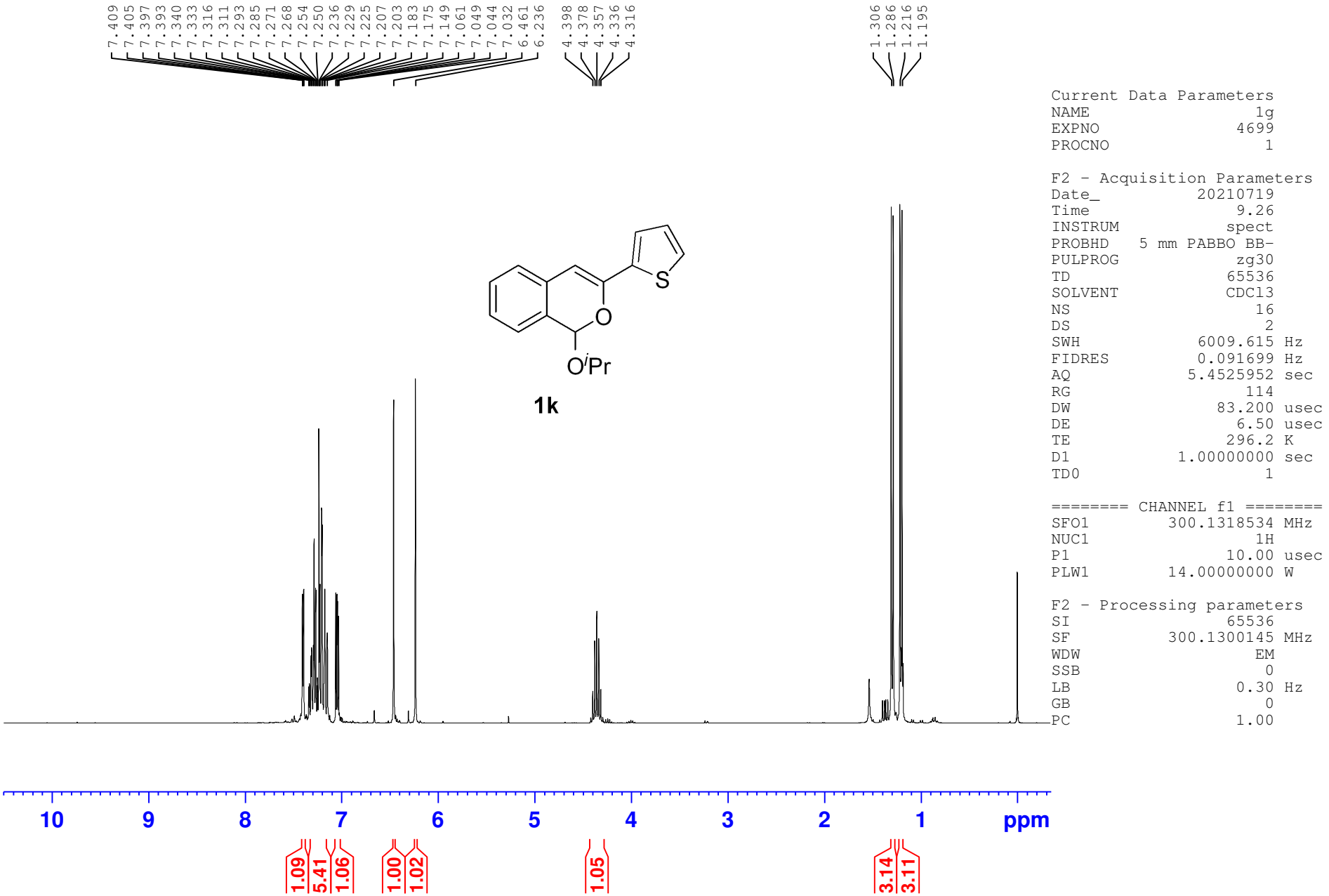



```
Current Data Parameters
NAME      lsx-project3-1e-h-fr
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_           20220723
Time               16.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    10
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 15.71
DW                62.400 usec
DE                 6.50 usec
TE                295.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300481 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

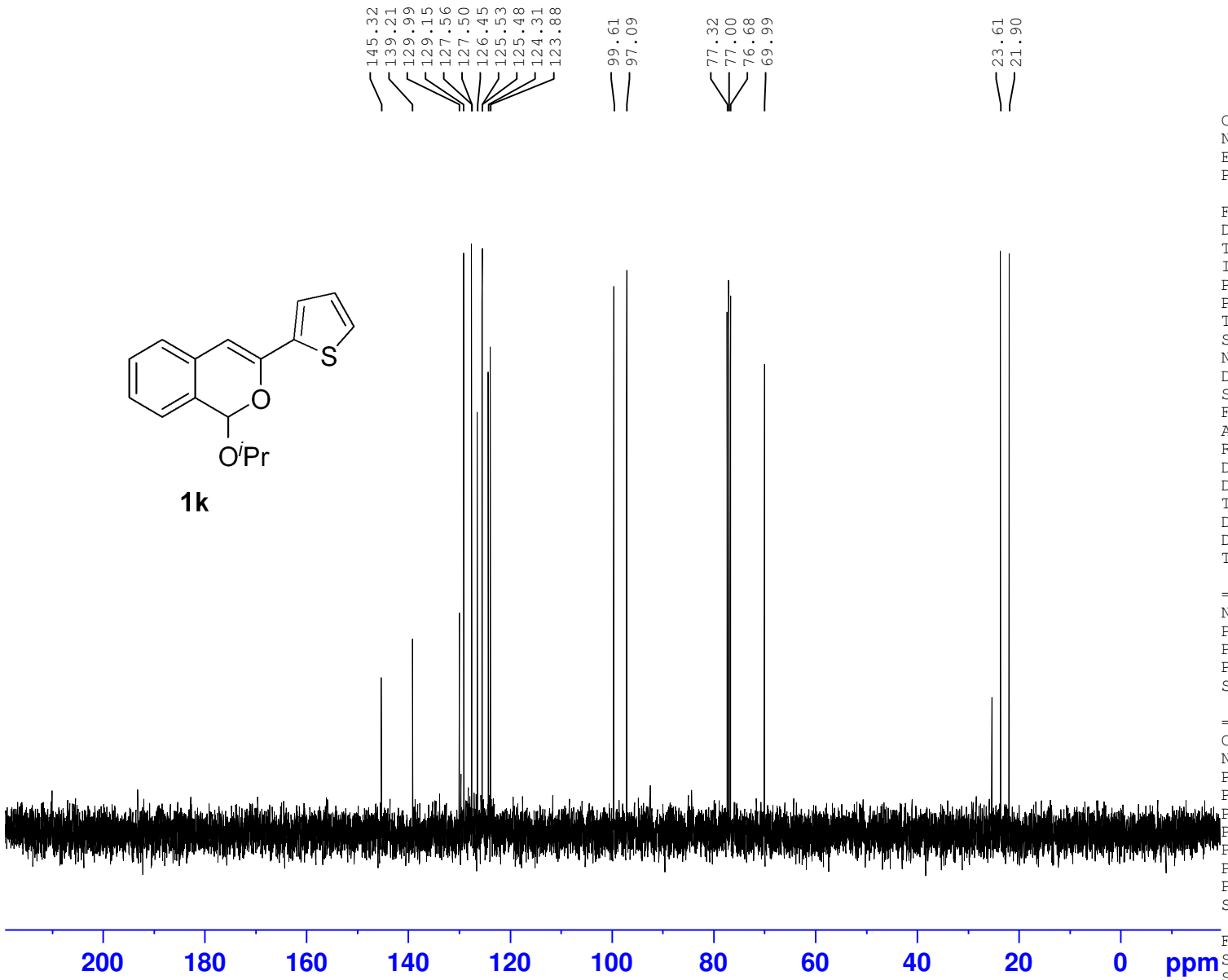



```
Current Data Parameters
NAME      lsx-project3-1e-c-fr
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220723
Time                  16.27
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       10
DS                        2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                   196.92
DW                   20.800 usec
DE                    6.50 usec
TE                   295.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            100.6228298 MHz
NUC1                    13C
P1                    9.70 usec
PLW1            46.98899841 W

======== CHANNEL f2 ========
SFO2            400.1316005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2            11.99499989 W
PLW12            0.34213999 W
PLW13            0.27713001 W

F2 - Processing parameters
SI                    32768
SF              100.6127927 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

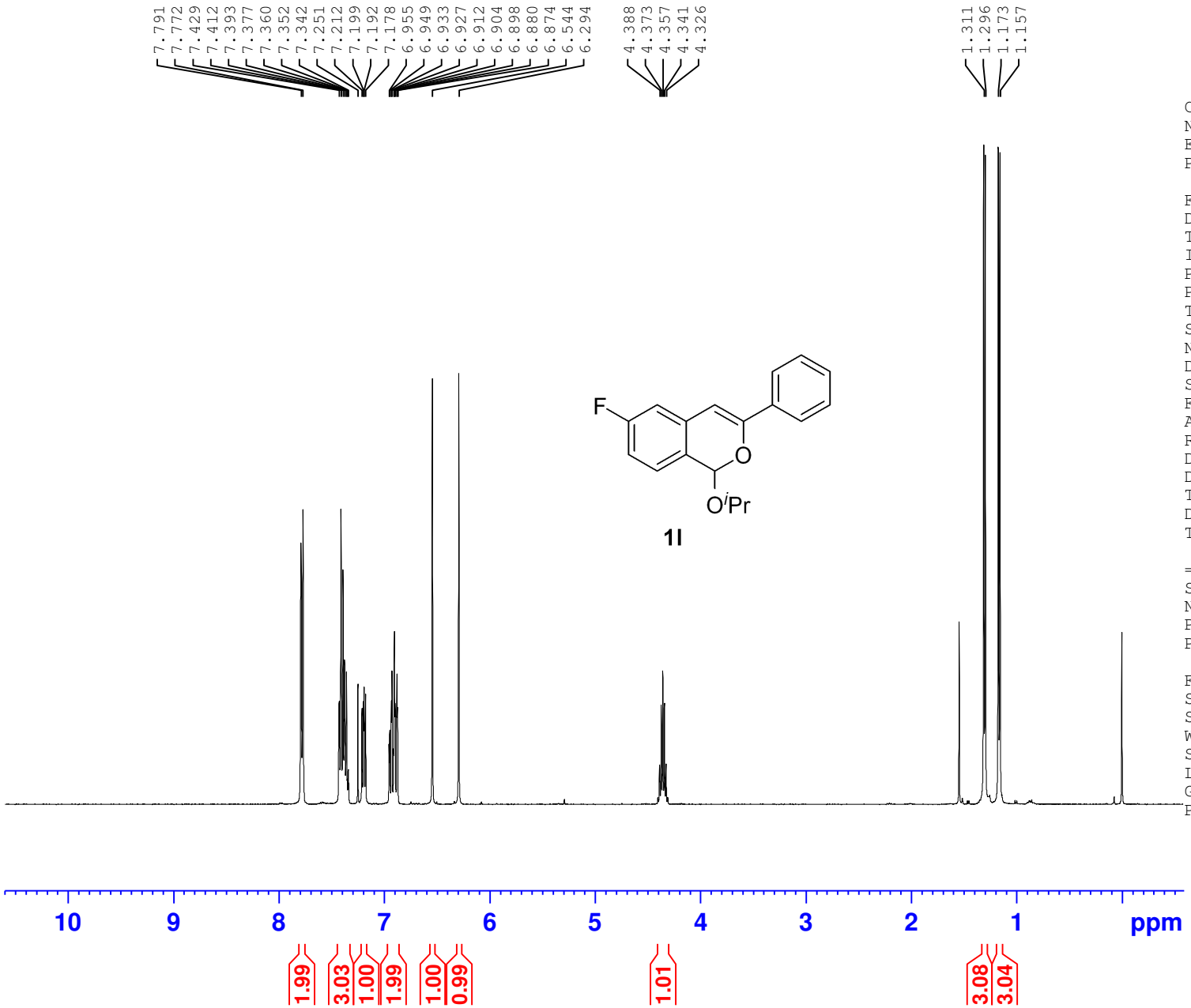
3sjwei 4699 lsx-7-84-h-fr 1h cdcl3



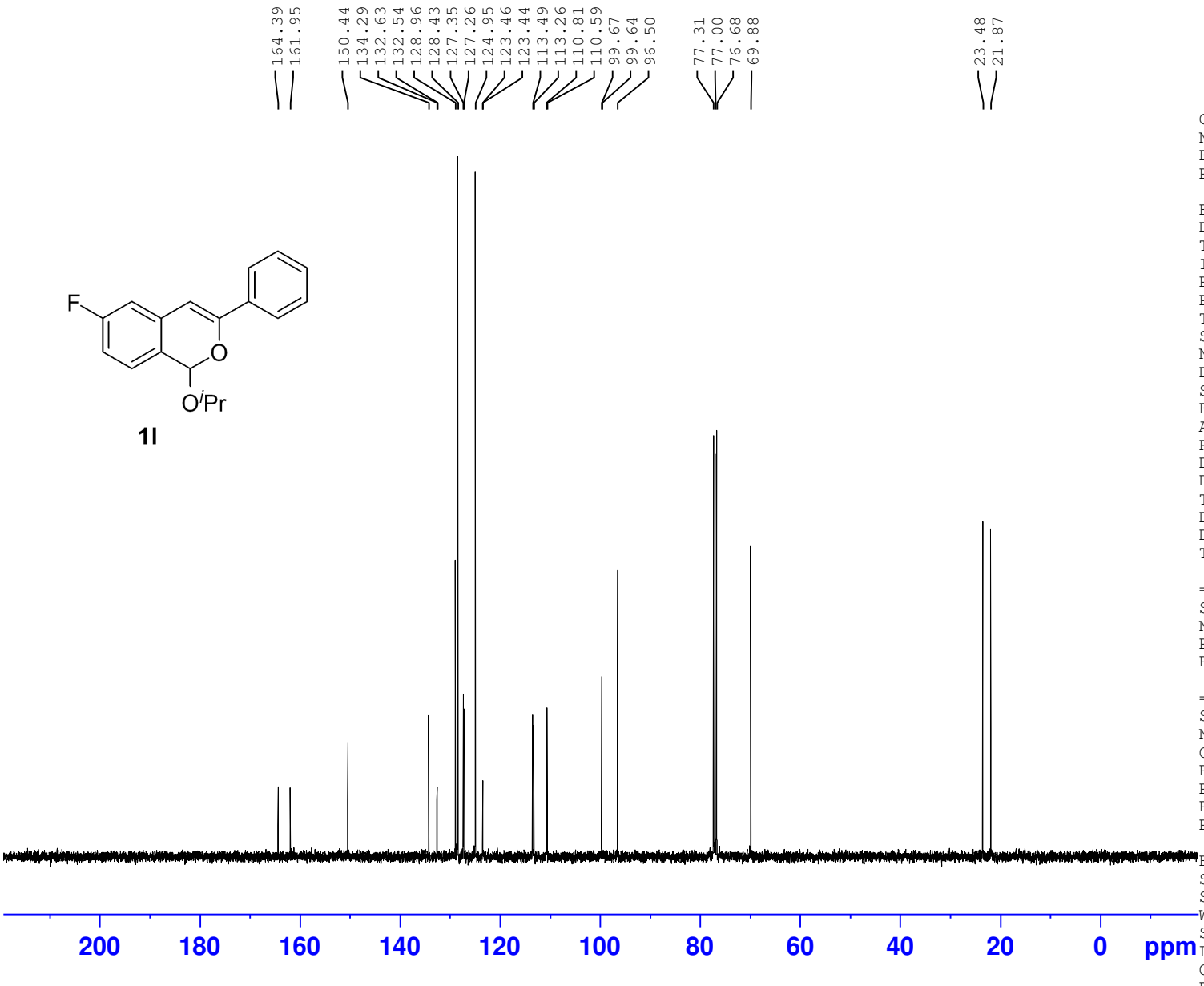

```
Current Data Parameters
NAME                  1g
EXPNO               4699
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210719
Time                9.26
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4525952 sec
RG                   114
DW                83.200 usec
DE                 6.50 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         14.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300145 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME      lsx-project3-1g-c
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20220722
Time              20.20
INSTRUM           spect
PROBHD    5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   26
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE               293.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127824 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

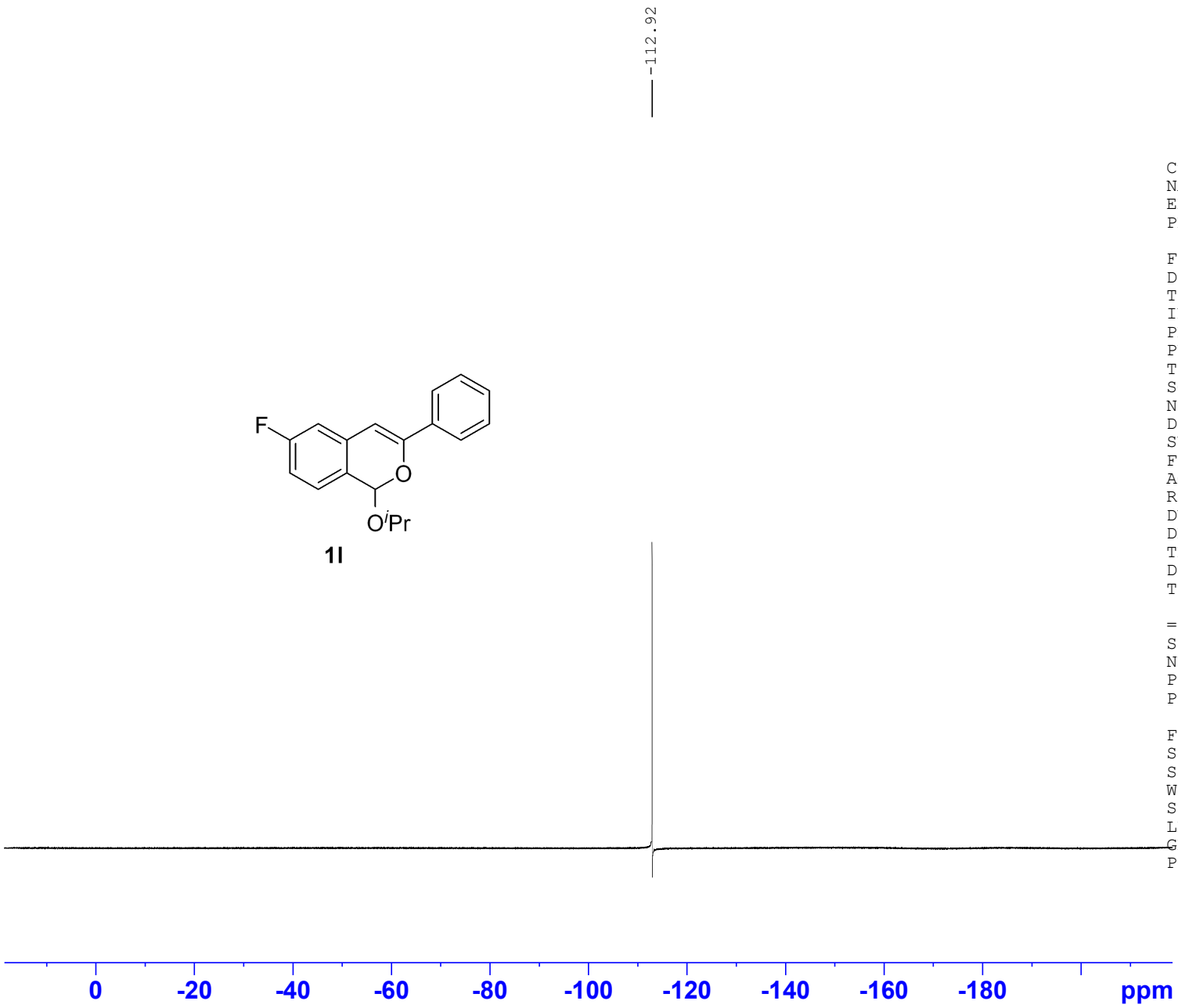



```
Current Data Parameters
NAME          lsx-1-7f-h
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211228
Time               19.37
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                112.31
DW                62.400 usec
DE                 6.50 usec
TE                294.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300135 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

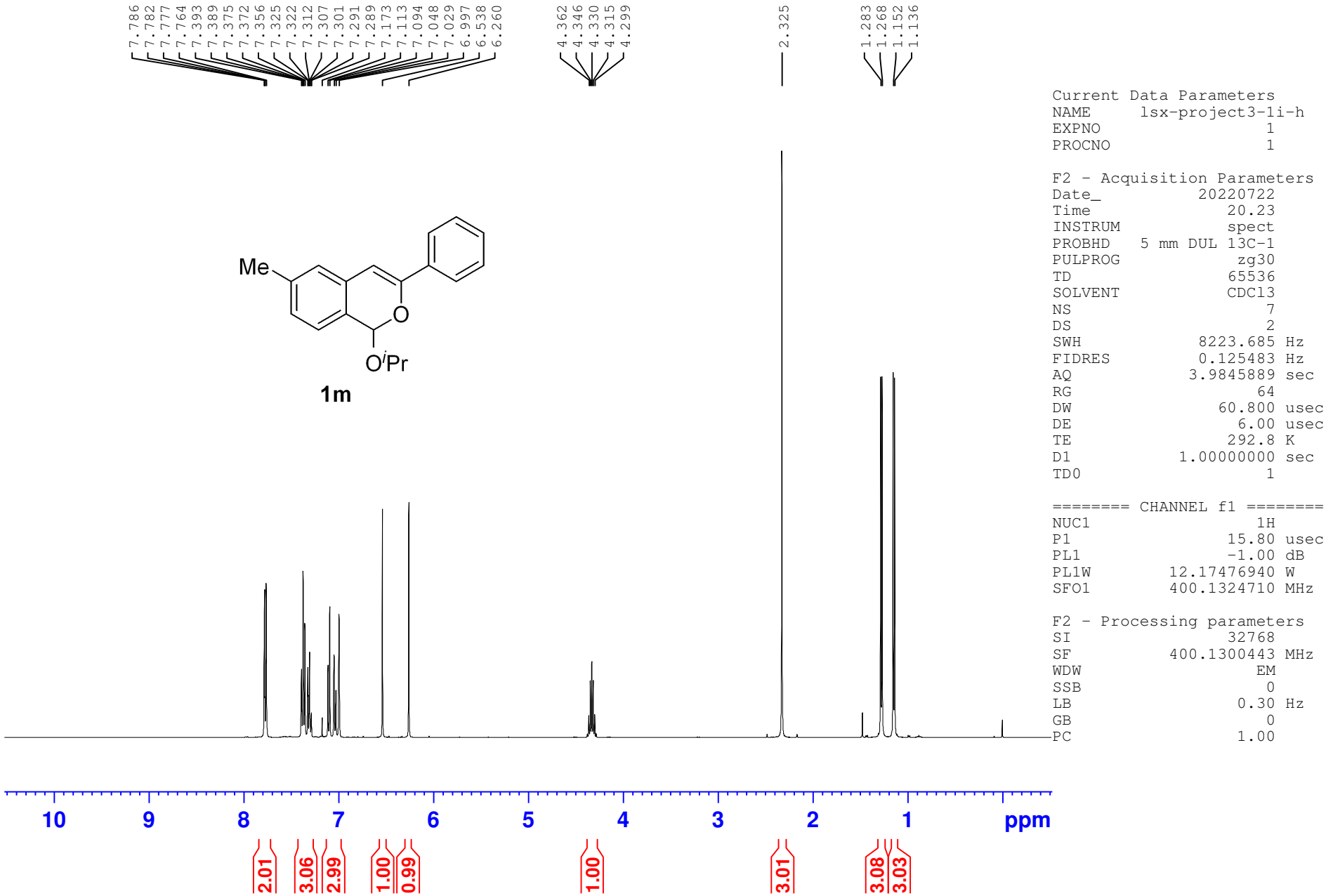


1l

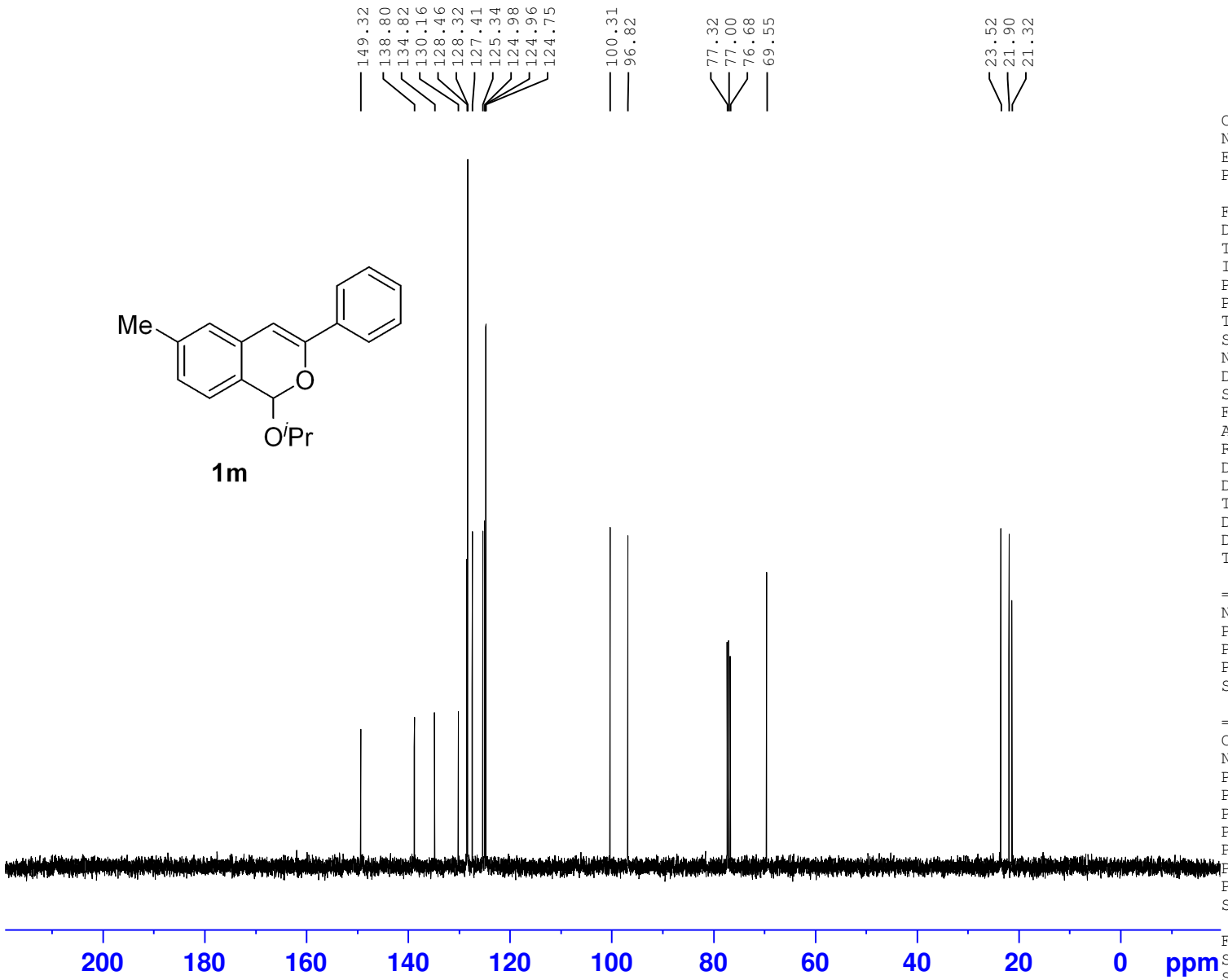
```
Current Data Parameters
NAME      lsx-project3-1h-c-fr
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220723
Time                  16.36
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       72
DS                        2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                   196.92
DW                   20.800 usec
DE                    6.50 usec
TE                   296.3 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            100.6228298 MHz
NUC1                    13C
P1                    9.70 usec
PLW1            46.98899841 W

======== CHANNEL f2 ========
SFO2            400.1316005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2            11.99499989 W
PLW12            0.34213999 W
PLW13            0.27713001 W

F2 - Processing parameters
SI                    32768
SF              100.6127787 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



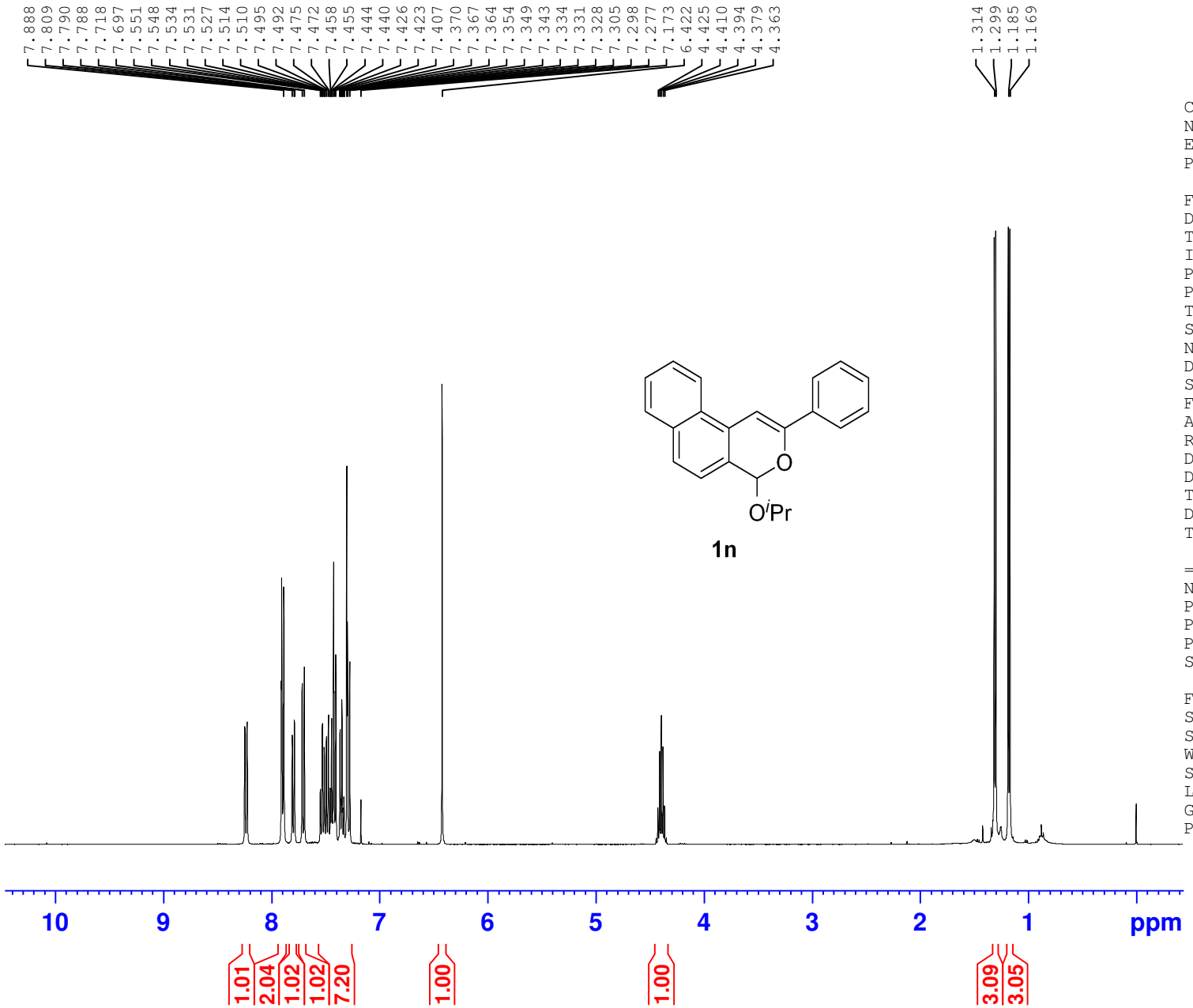

```
Current Data Parameters
NAME          lsx-1-7f-f
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211228
Time              19.39
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgflqn
TD              131072
SOLVENT           CDCl3
NS                    8
DS                    4
SWH           89285.711 Hz
FIDRES         0.681196 Hz
AQ            0.7340032 sec
RG               196.92
DW                5.600 usec
DE                6.50 usec
TE                294.9 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        376.4607164 MHz
NUC1                19F
P1                14.70 usec
PLW1        15.99600029 W

F2 - Processing parameters
SI                65536
SF          376.4983660 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



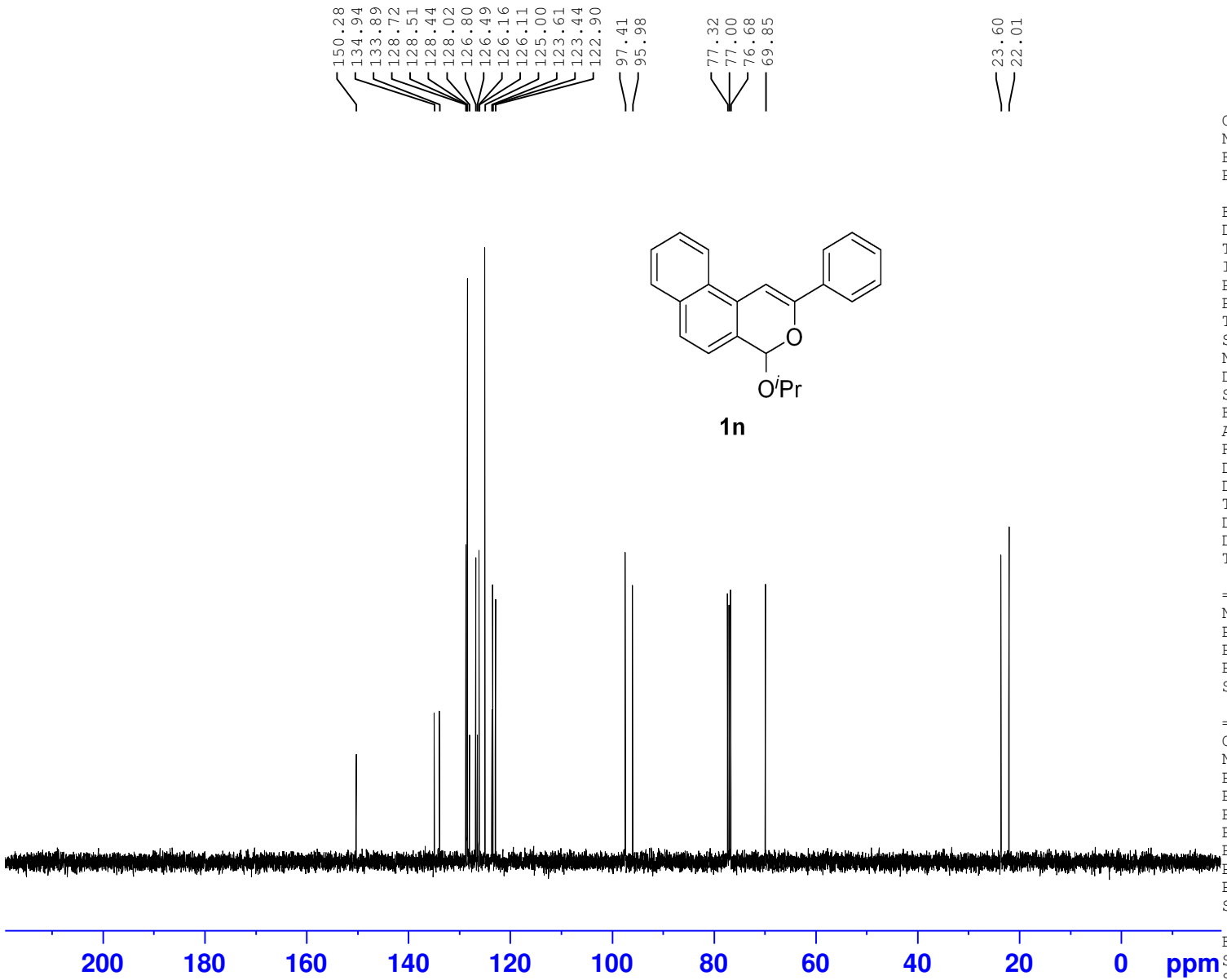

```
Current Data Parameters
NAME      lsx-project3-1i-h
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220722
Time               20.23
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                    64
DW                60.800 usec
DE                 6.00 usec
TE                292.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.80 usec
PL1                -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300443 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



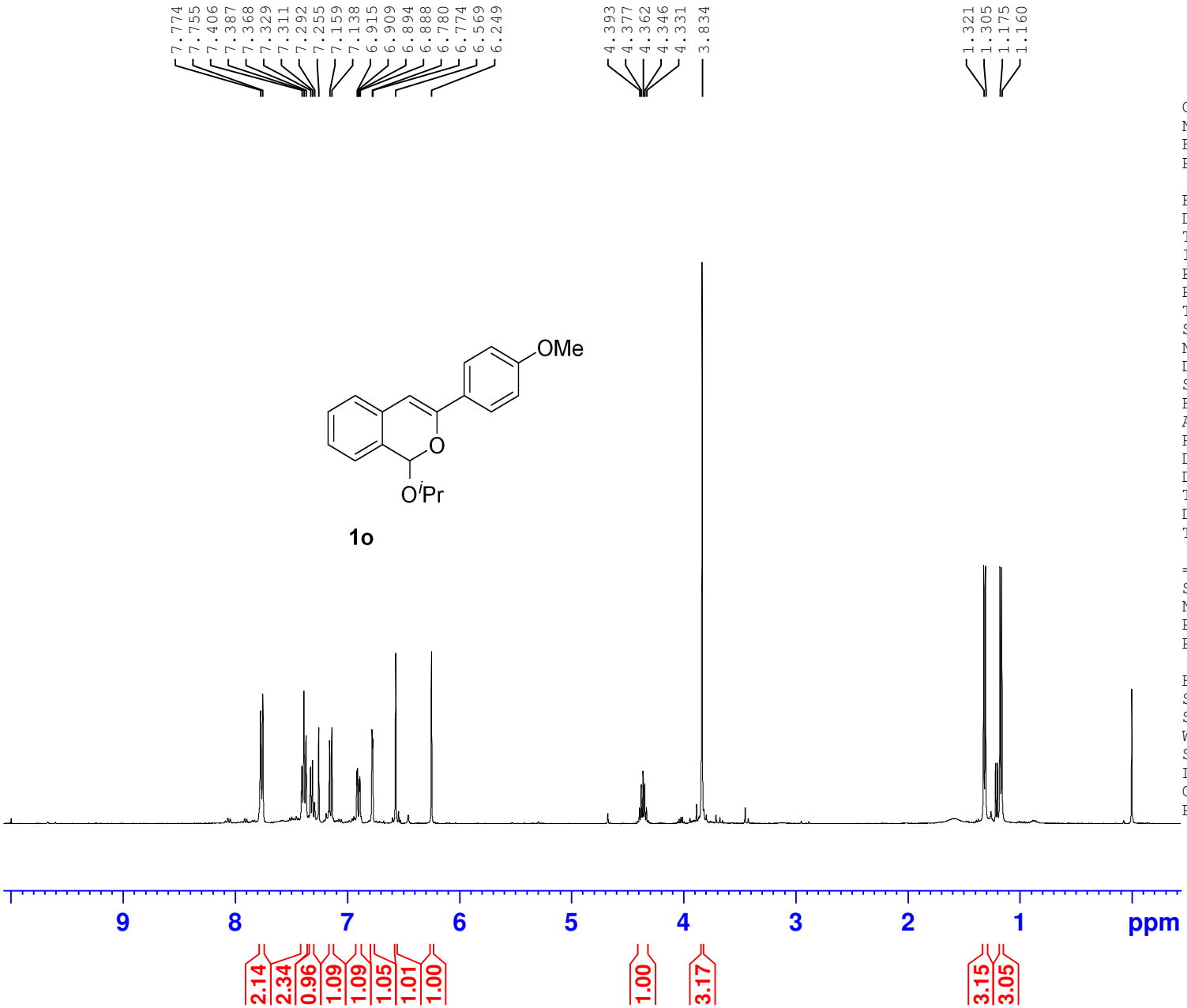

```
Current Data Parameters
NAME      lsx-project3-1i-c
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20220722
Time              20.26
INSTRUM           spect
PROBHD    5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   33
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE               293.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127854 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



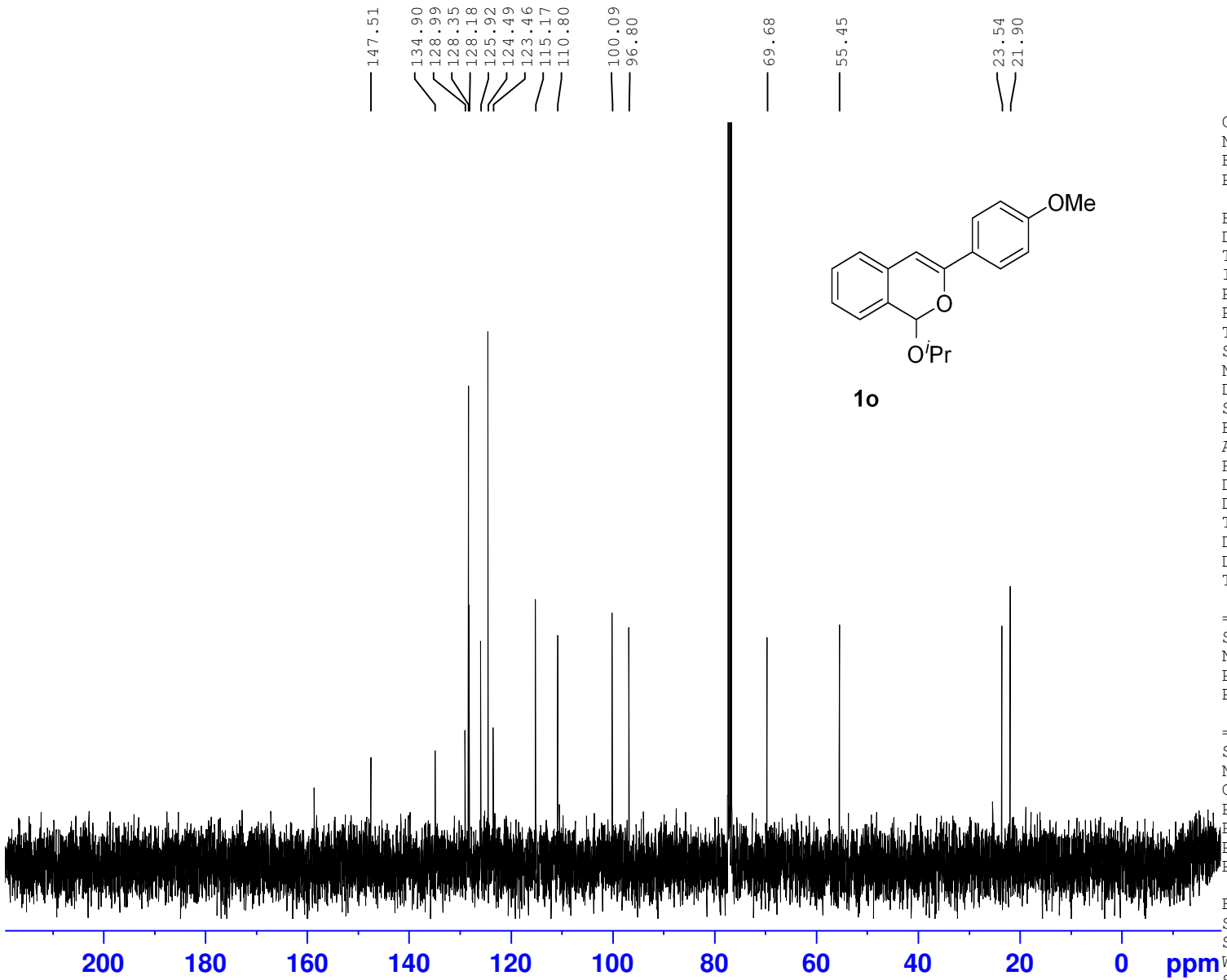

```
Current Data Parameters
NAME      lsx-project3-1j-h
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20220722
Time                20.29
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                    101
DW                 60.800 usec
DE                  6.00 usec
TE                 292.8 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.80 usec
PL1                -1.00 dB
PL1W         12.17476940 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF           400.1300444 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```



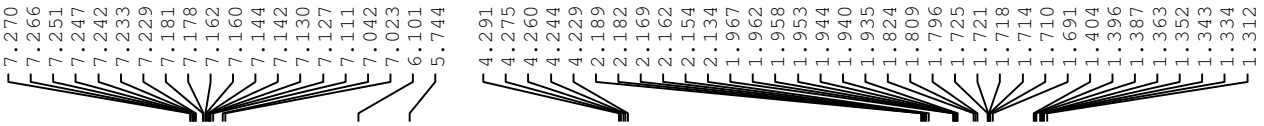

```
Current Data Parameters
NAME      lsx-project3-1j-c
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20220722
Time              20.32
INSTRUM           spect
PROBHD    5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   47
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE               293.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127847 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



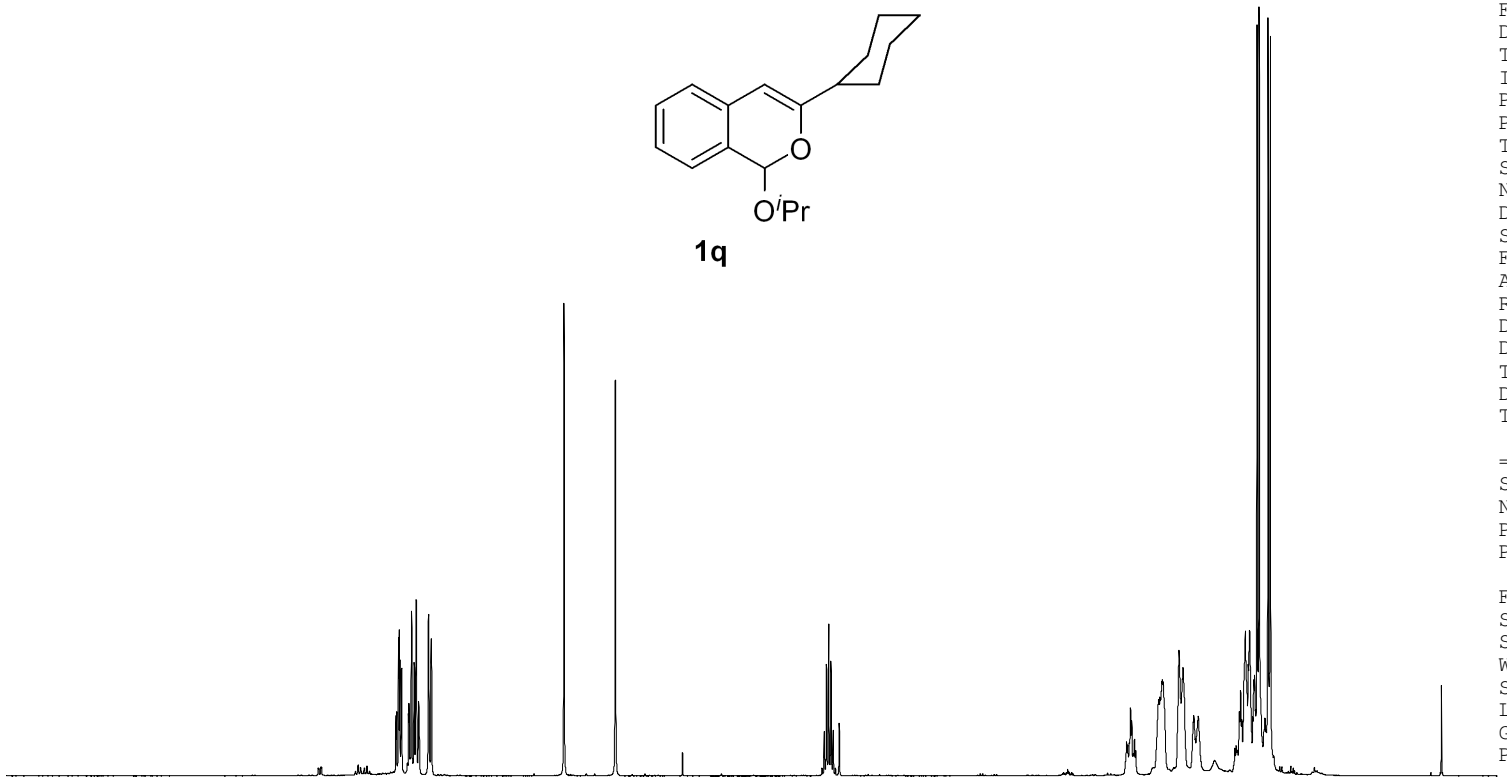

```
Current Data Parameters
NAME       lsx-1-6ome-c
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20211228
Time              19.50
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    9
DS                    2
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ           4.0894465 sec
RG              126.97
DW              62.400 usec
DE               6.50 usec
TE              295.4 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1              14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300119 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

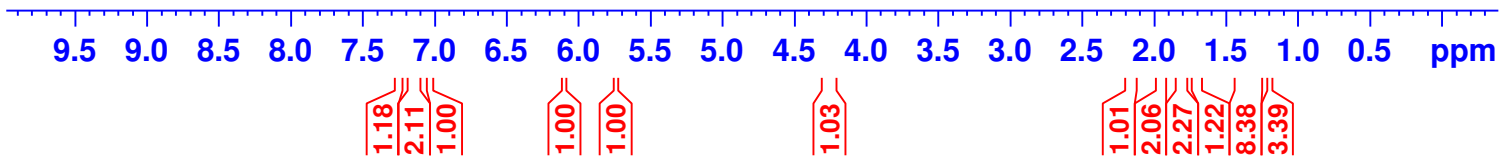



```
Current Data Parameters
NAME       lsx-1-6ome-h
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20211228
Time              19.48
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   59
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127725 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

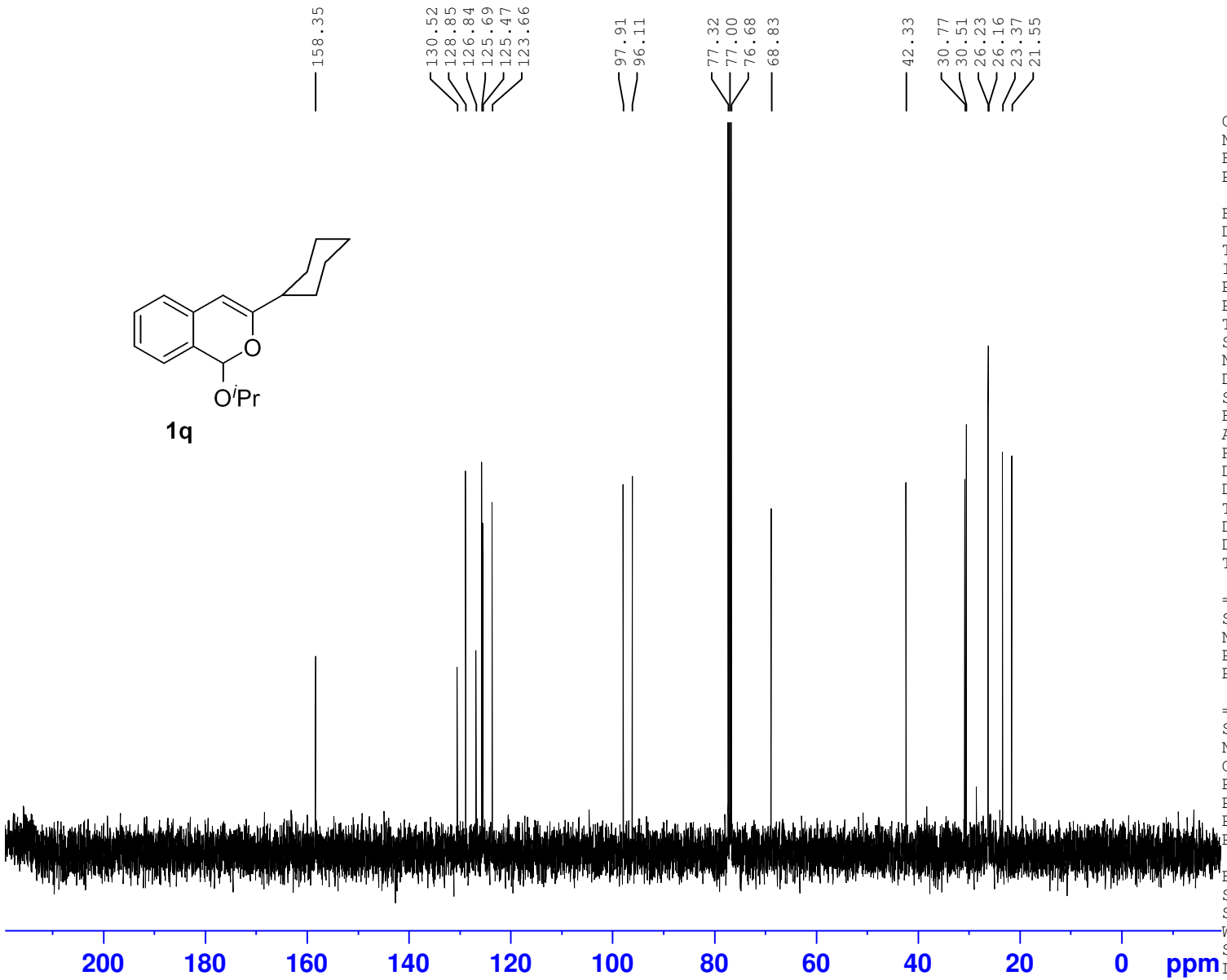


1q

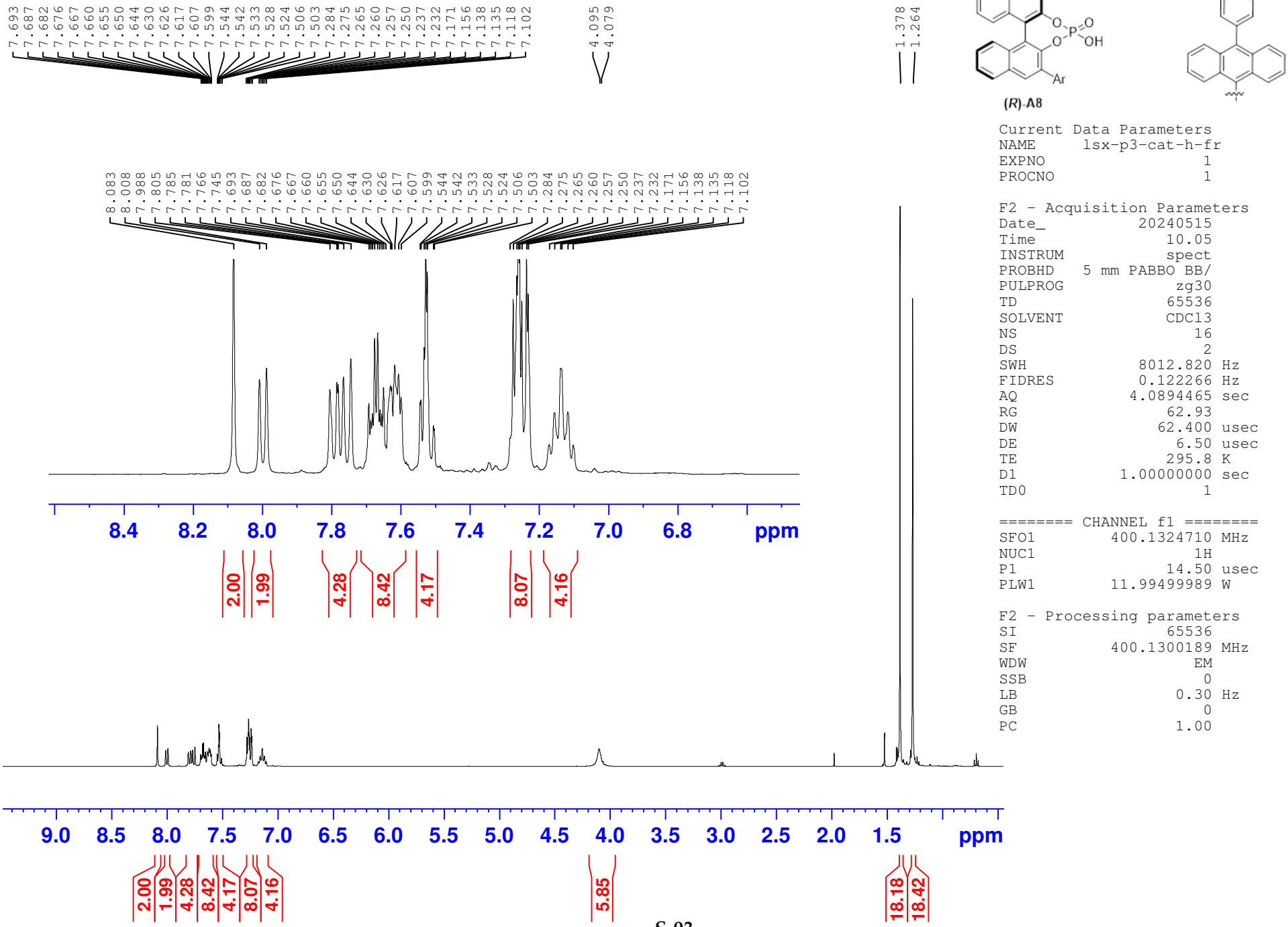




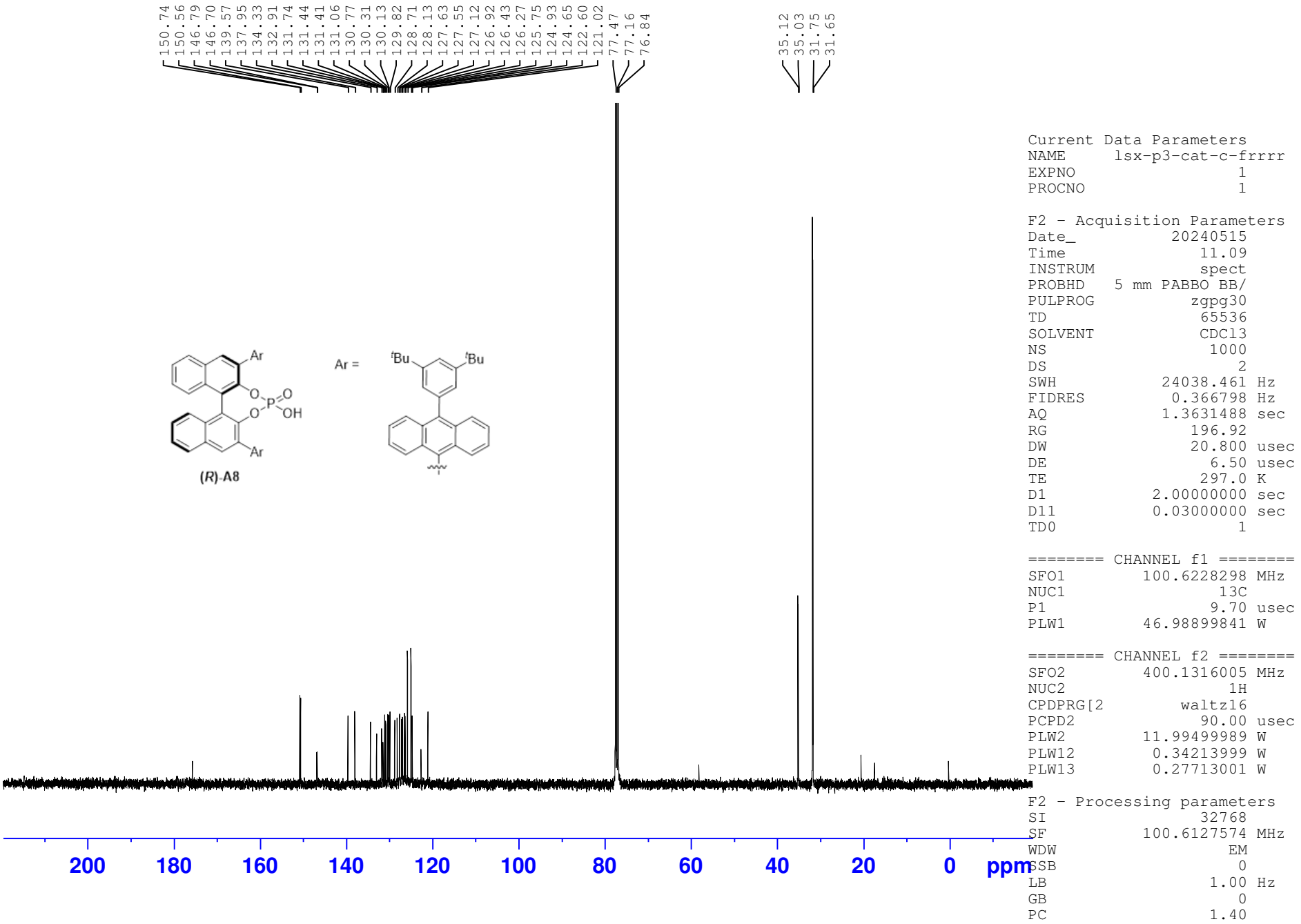

```
Current Data Parameters
NAME      lsx-project3-1l-h-fr
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220723
Time               13.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     5
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 31.55
DW                62.400 usec
DE                 6.50 usec
TE                295.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300174 MHz
WDW                  EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



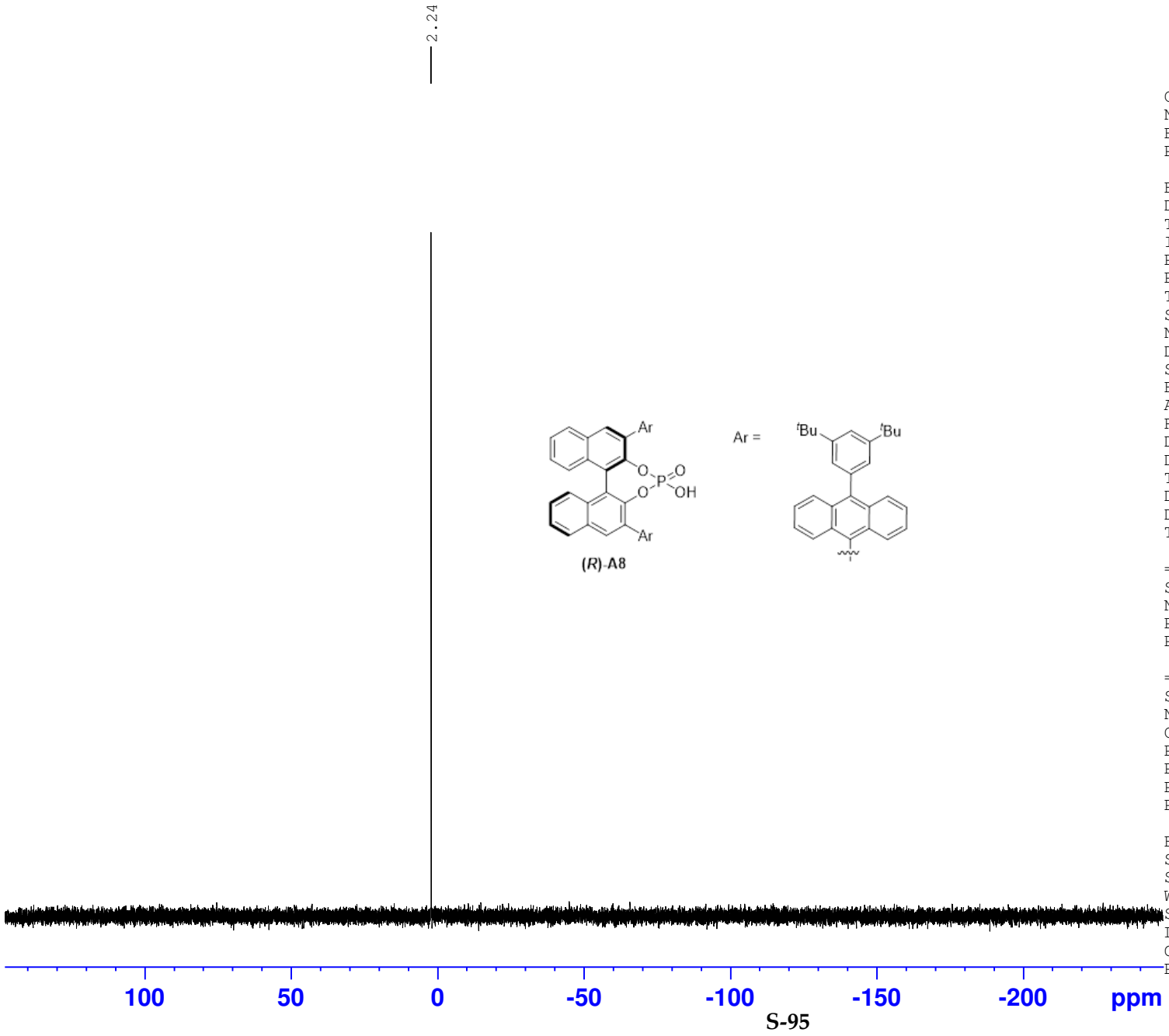

```
Current Data Parameters
NAME      lsx-project3-1l-c-fr
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20220723
Time                13.56
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                295.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127753 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



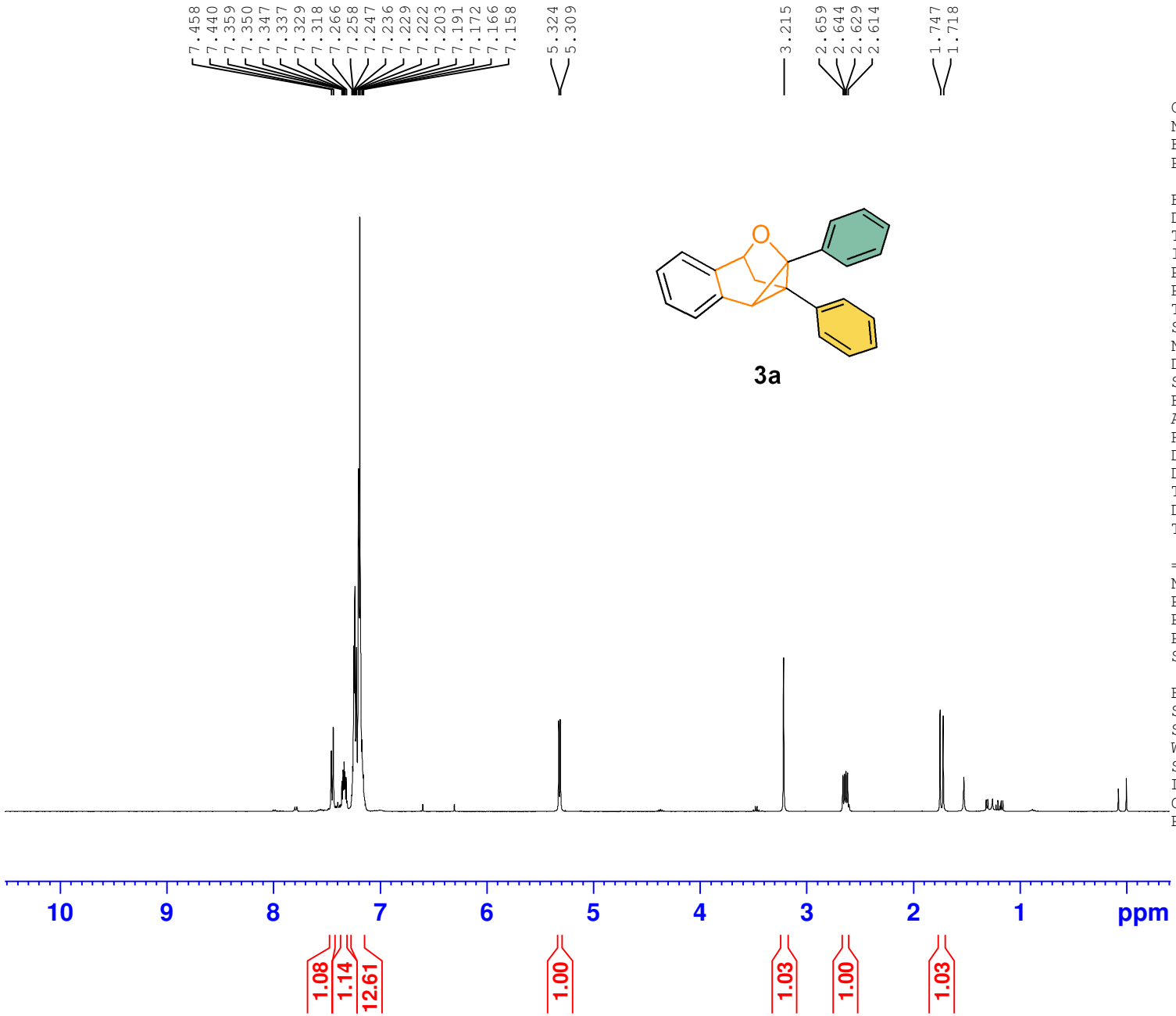

```
Current Data Parameters
NAME      lsx-p3-cat-h-fr
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20240515
Time                10.05
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 62.93
DW                62.400 usec
DE                 6.50 usec
TE                295.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300189 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME      lsx-p3-cat-c-frrrr
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20240515
Time               11.09
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1000
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE                297.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127574 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```




```
Current Data Parameters
NAME      lsx-p3-cat-p-fr
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20240515
Time               10.07
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   17
DS                    4
SWH           64102.562 Hz
FIDRES         0.978127 Hz
AQ            0.5111808 sec
RG               196.92
DW                7.800 usec
DE                6.50 usec
TE                296.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        161.9674942 MHz
NUC1                31P
P1                14.70 usec
PLW1        11.99499989 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          161.9755930 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

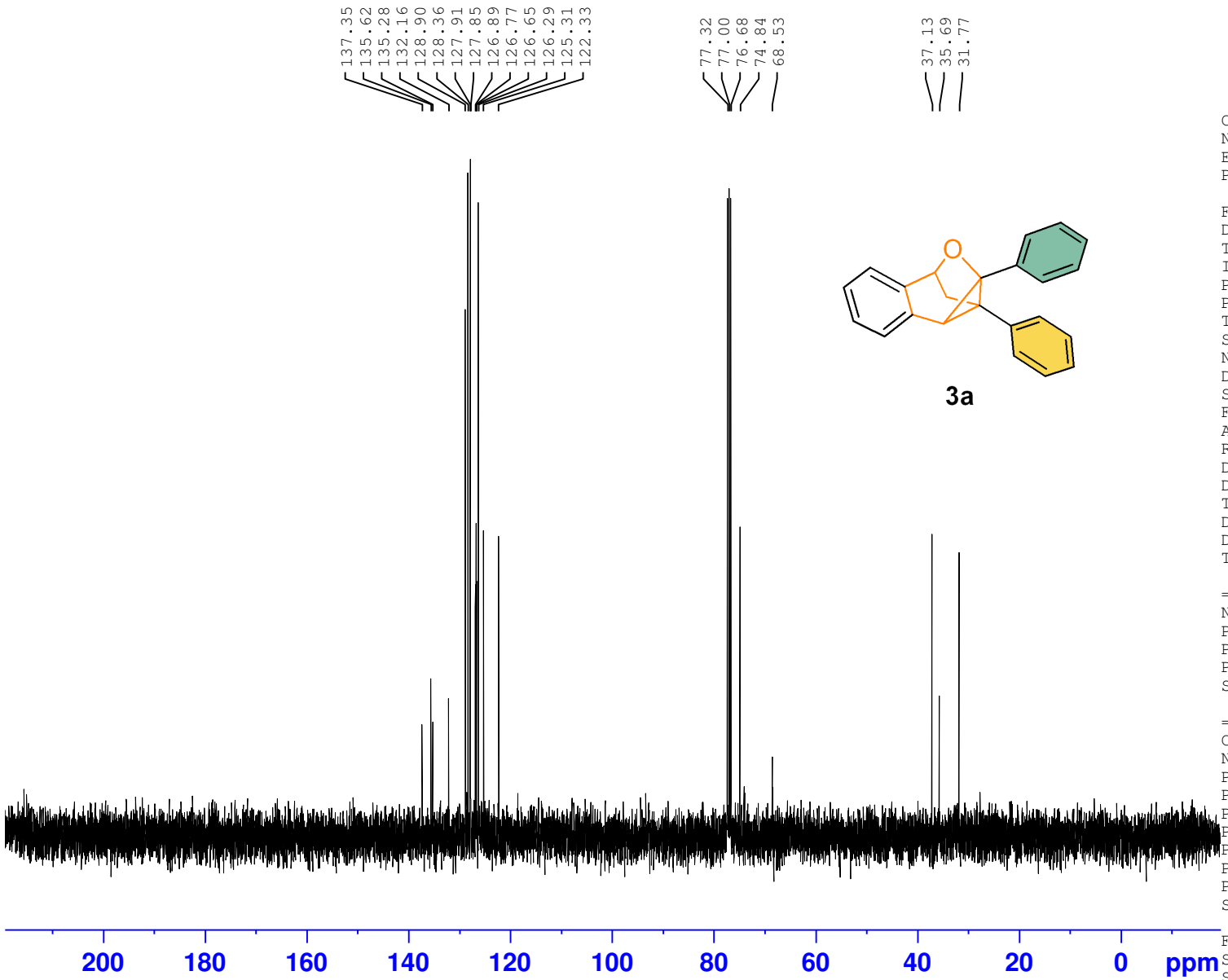


Current Data Parameters
NAME lsx-p3-3a-h-fr
EXPNO 1
PROCNO 1

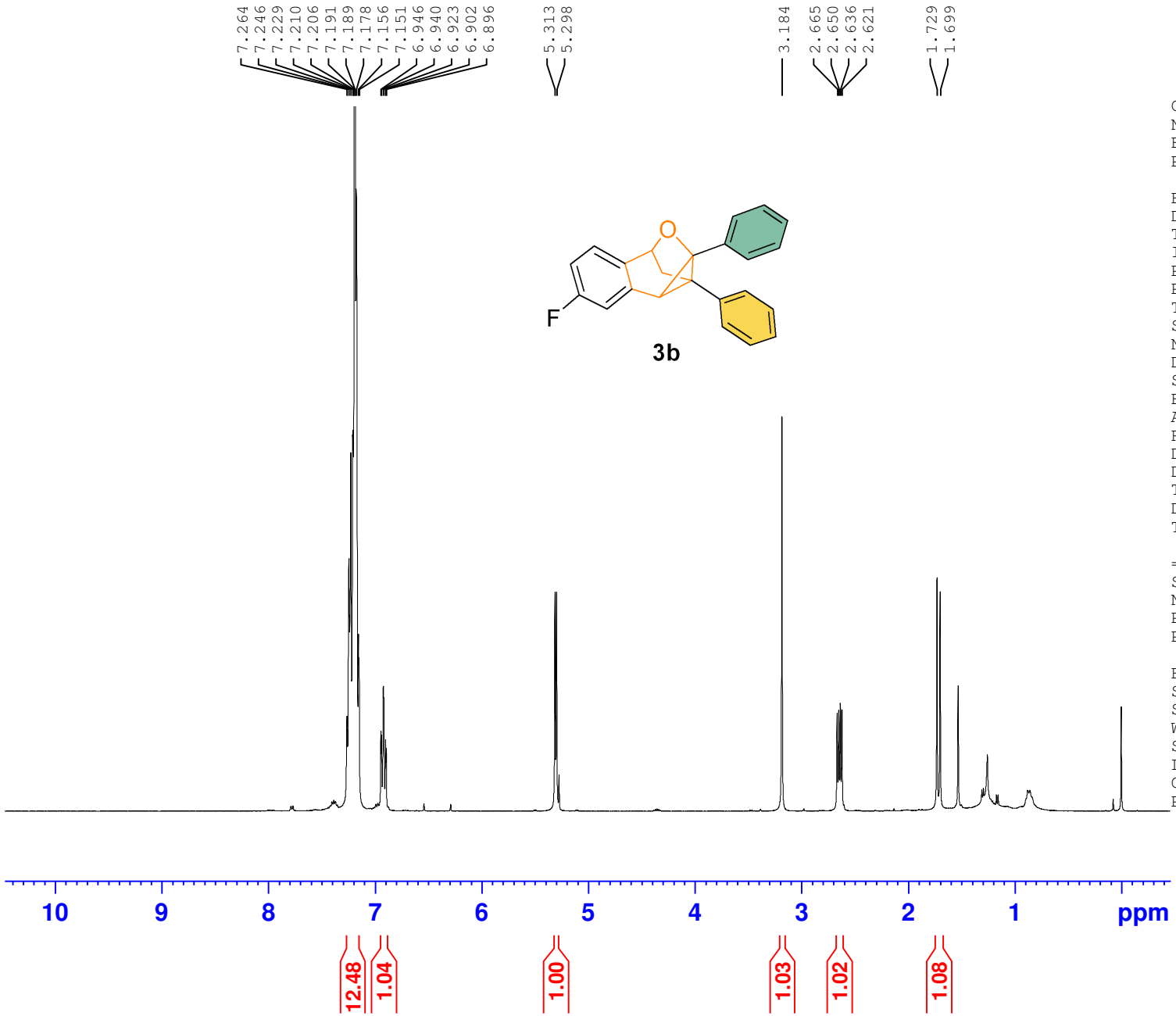
F2 - Acquisition Parameters
Date_ 20220726
Time 17.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.80 usec
PL1 -1.00 dB
PL1W 12.17476940 W
SFO1 400.1324710 MHz

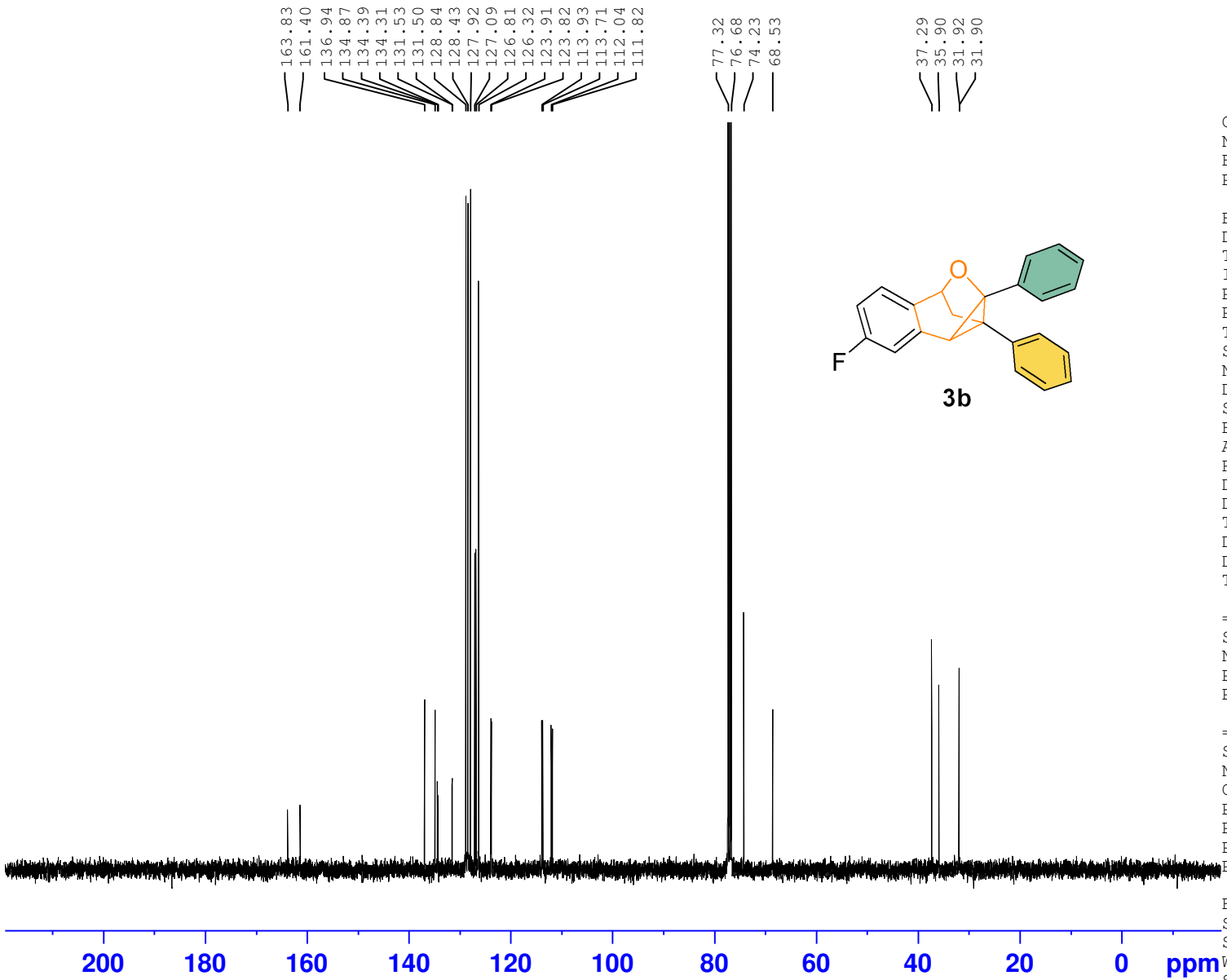
F2 - Processing parameters
SI 32768
SF 400.1300235 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



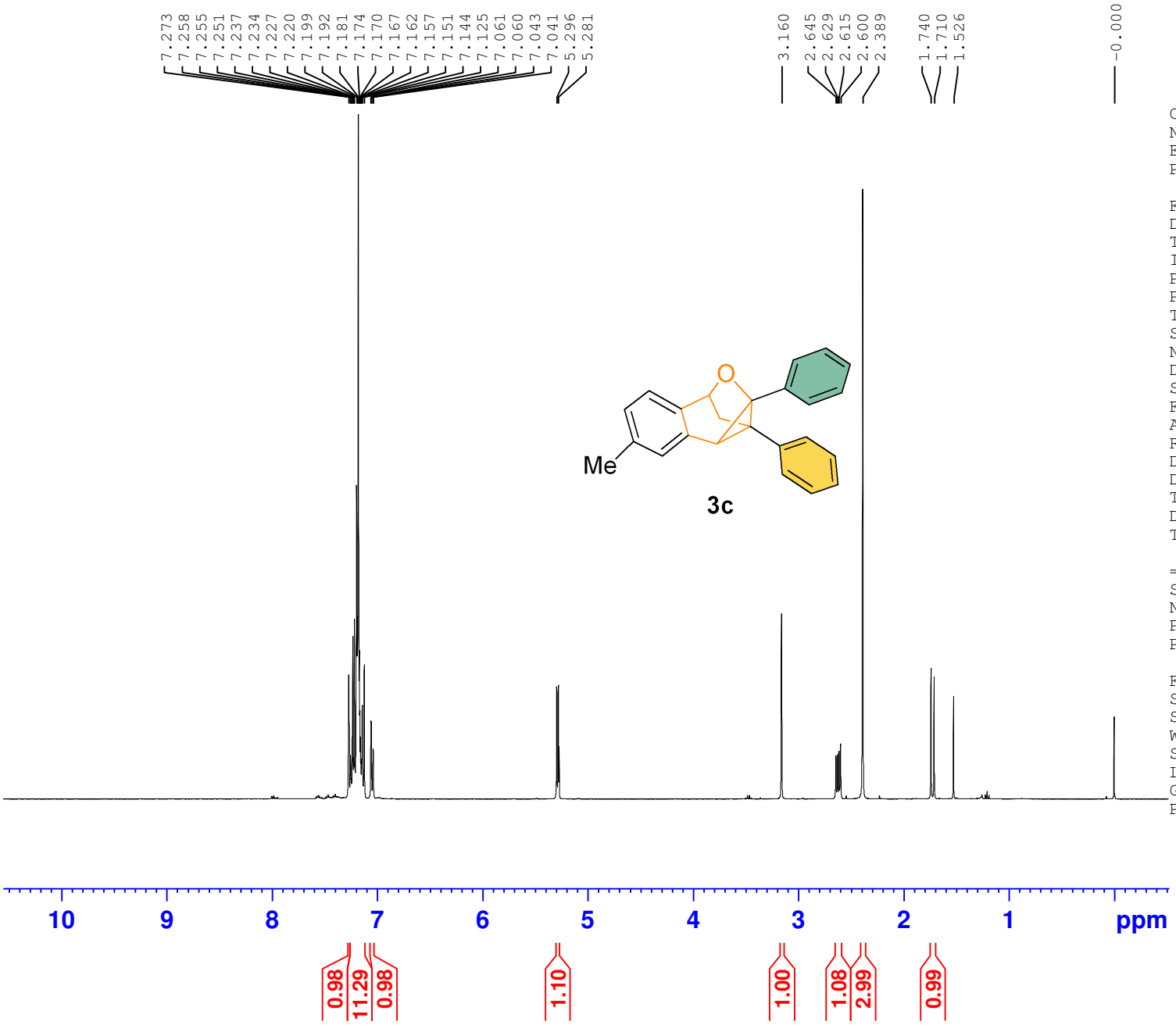

```
Current Data Parameters
NAME      lsx-p3-3a-c-fr
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220726
Time               17.21
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   46
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE                293.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127769 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



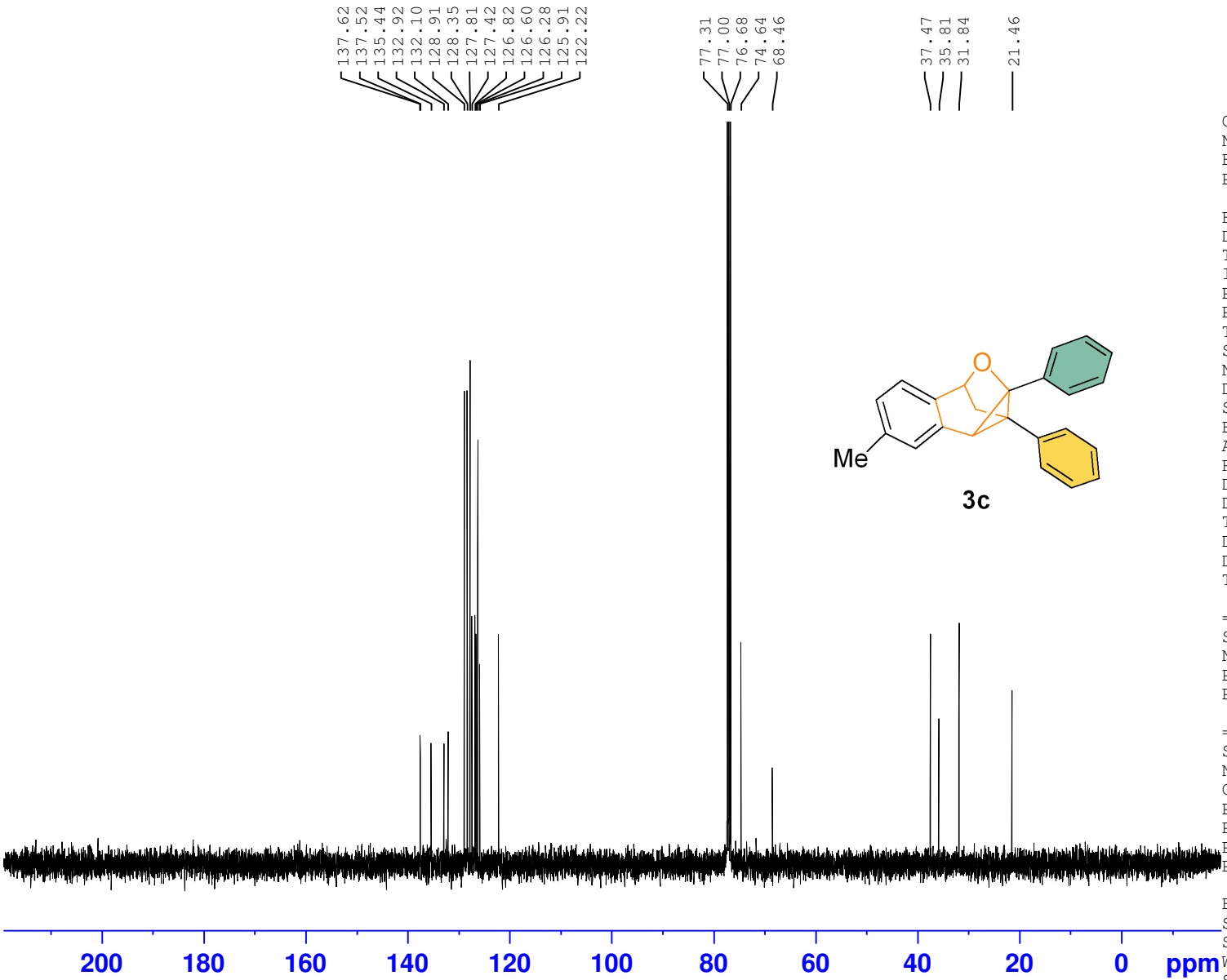

```
Current Data Parameters
NAME      lsx-1-174-h-fr
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220104
Time               15.40
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                164.33
DW                62.400 usec
DE                 6.50 usec
TE                295.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                 65536
SF          400.1300192 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



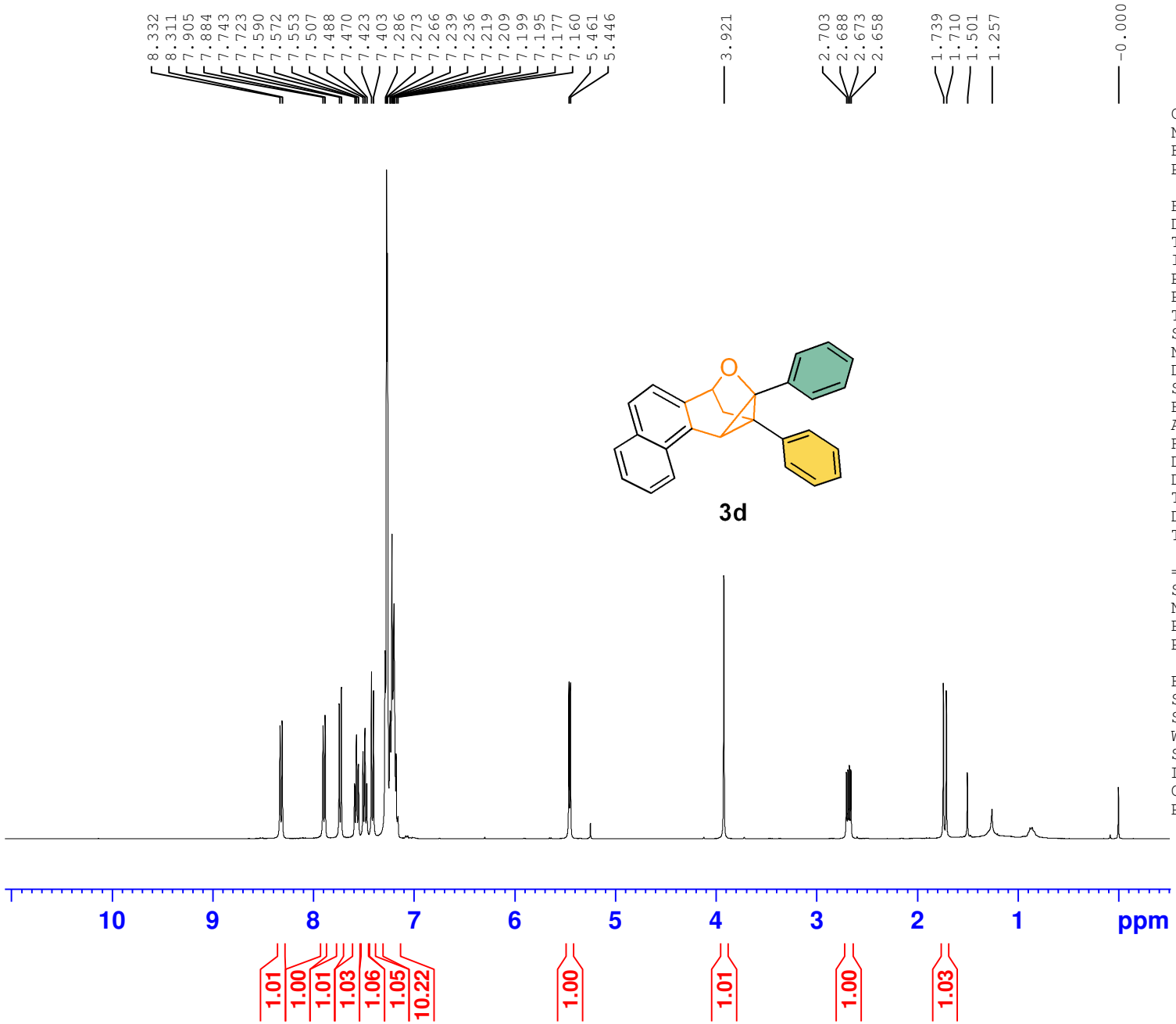

```
Current Data Parameters
NAME      lsx-1-174-c-fr
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220104
Time               15.53
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  209
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127748 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```



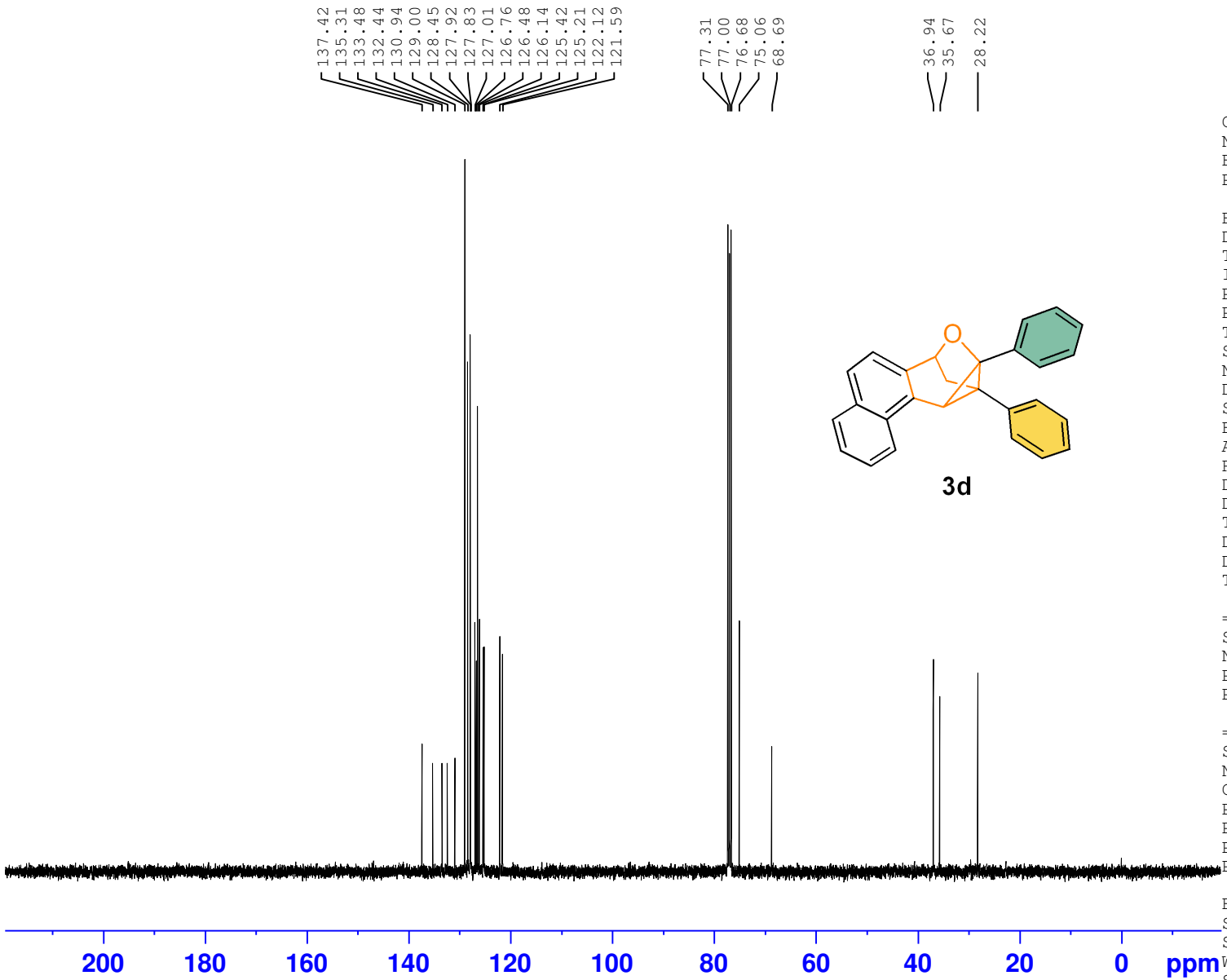

```
Current Data Parameters
NAME          lsx-2-9c-h
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220122
Time               12.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 82.92
DW                62.400 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300205 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



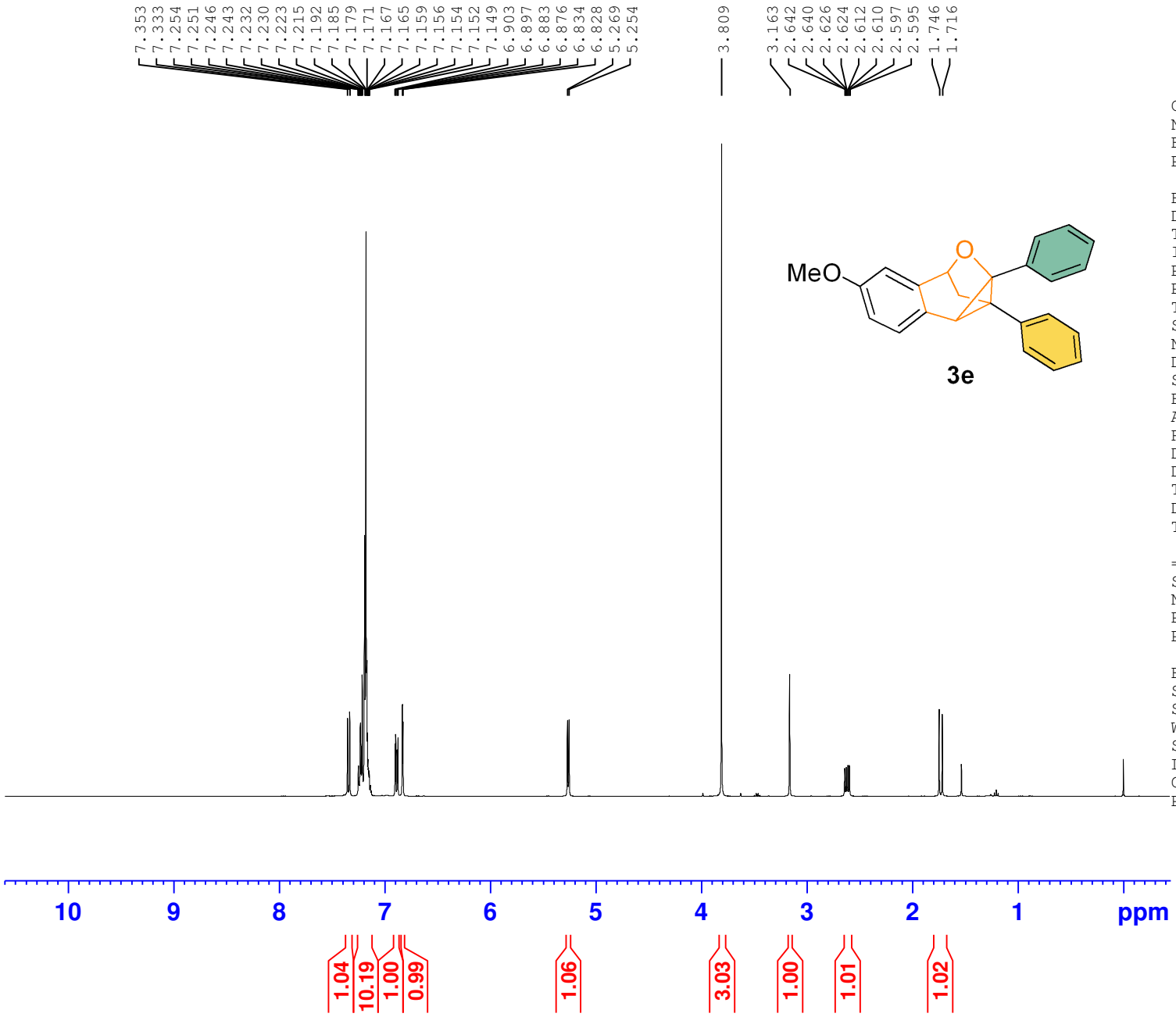

```
Current Data Parameters
NAME          lsx-2-9c-c
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220122
Time               12.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               295.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127754 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```



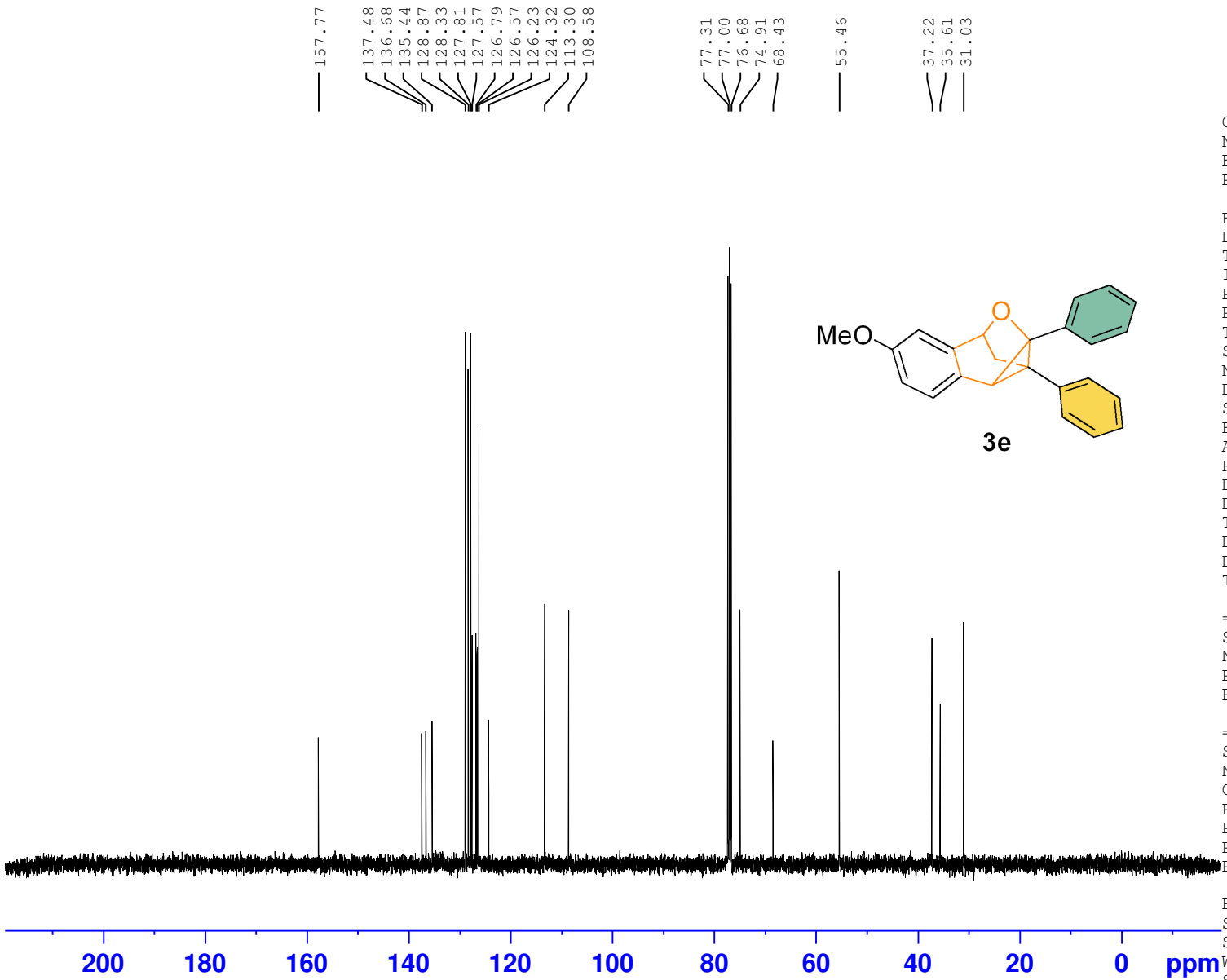

```
Current Data Parameters
NAME      lsx-1-176-h-fr
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220104
Time               15.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                112.31
DW                62.400 usec
DE                 6.50 usec
TE                295.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300303 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



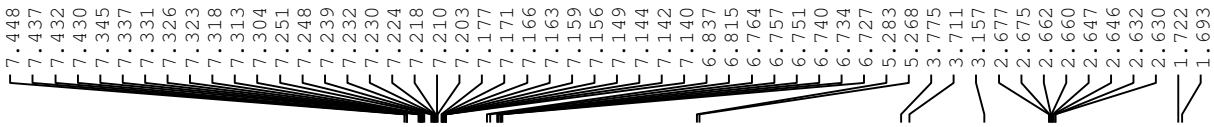

```
Current Data Parameters
NAME      lsx-1-176-c-fr
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220104
Time               16.07
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  118
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127780 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



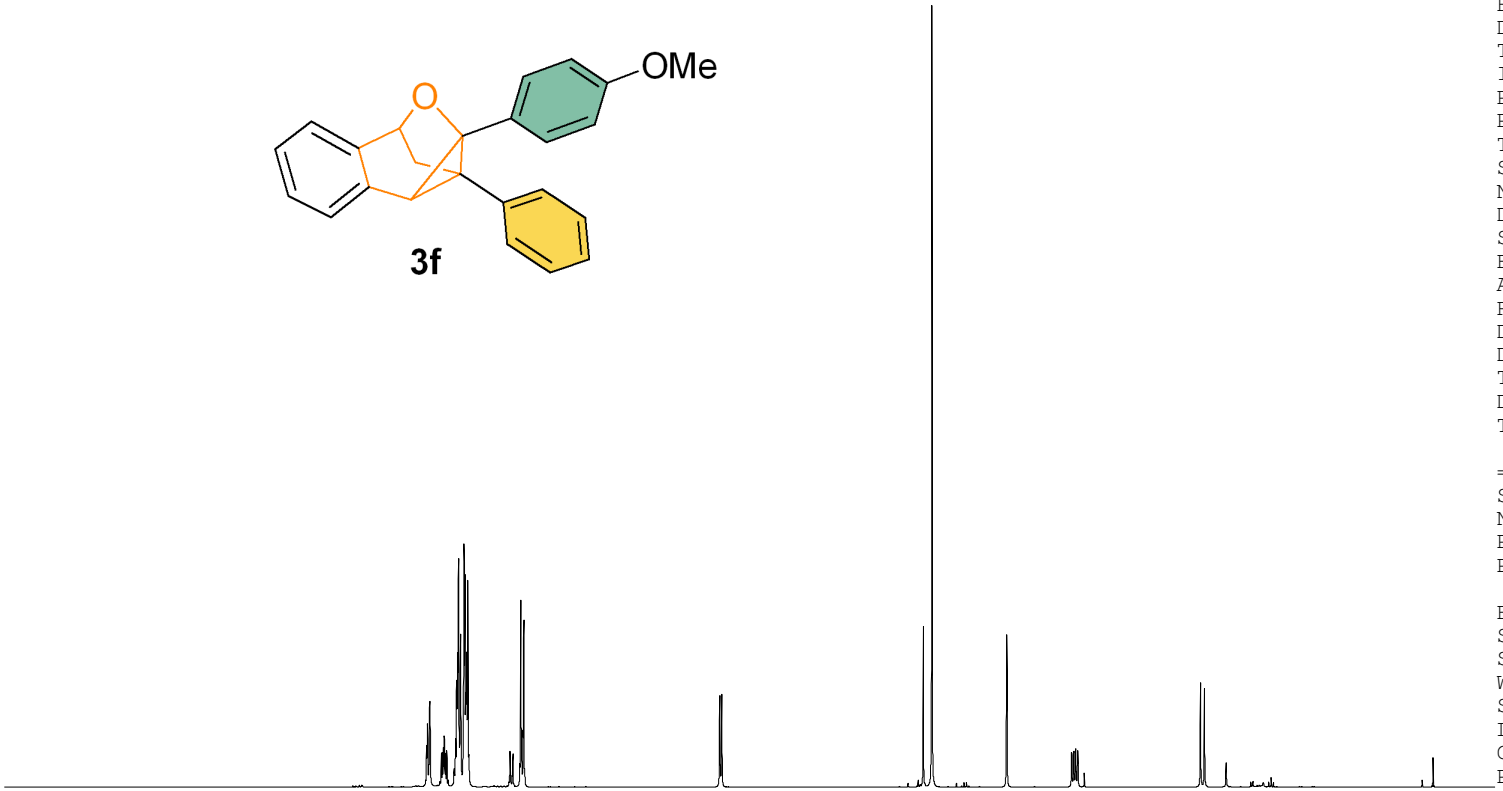

```
Current Data Parameters
NAME          lsx-2-9d-h
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220122
Time               12.31
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 54.81
DW                62.400 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300246 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

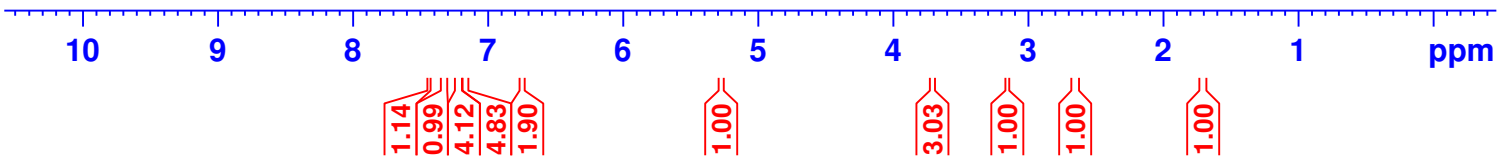



```
Current Data Parameters
NAME          lsx-2-9d-c
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220122
Time               12.35
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   59
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127777 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

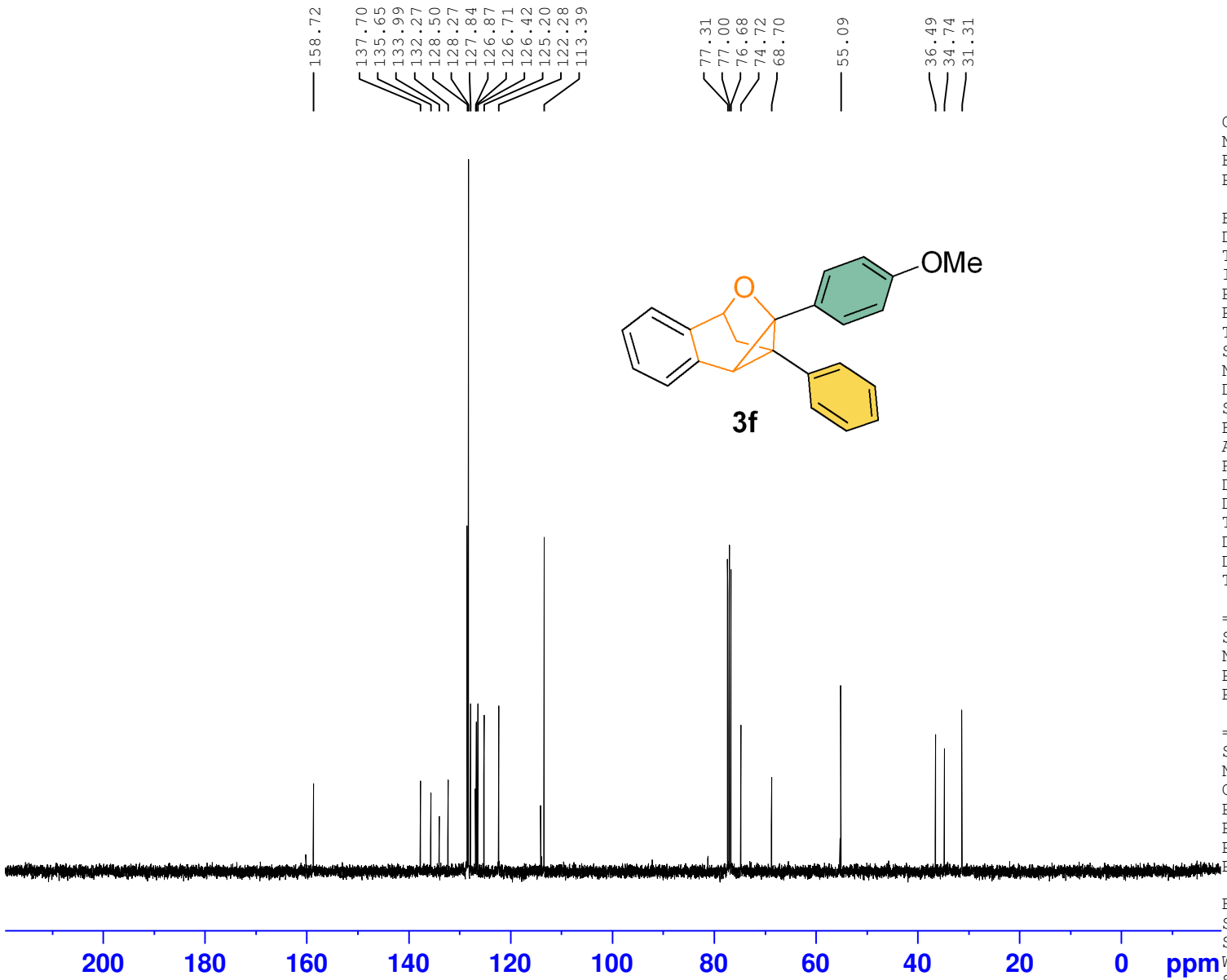


3f

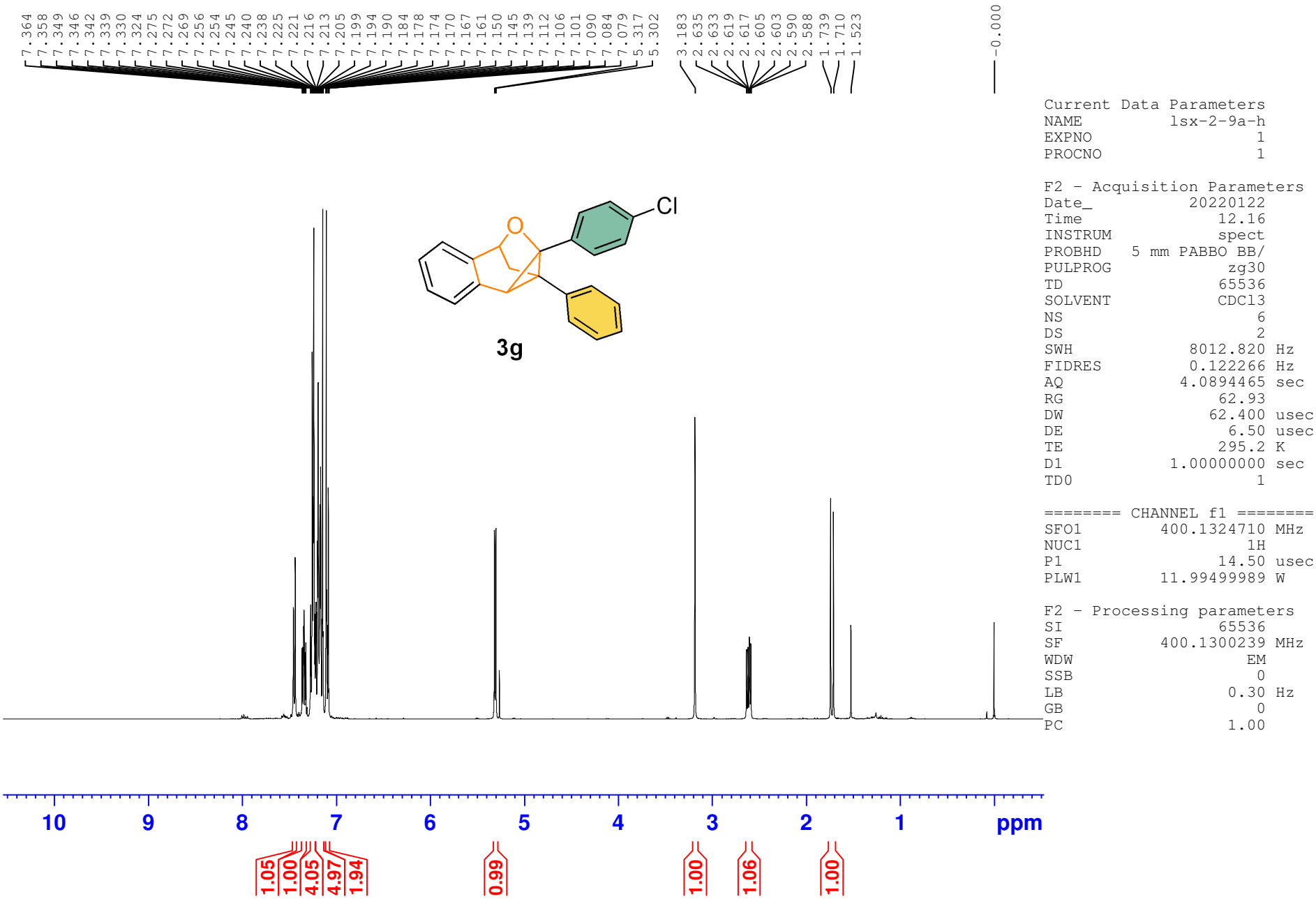




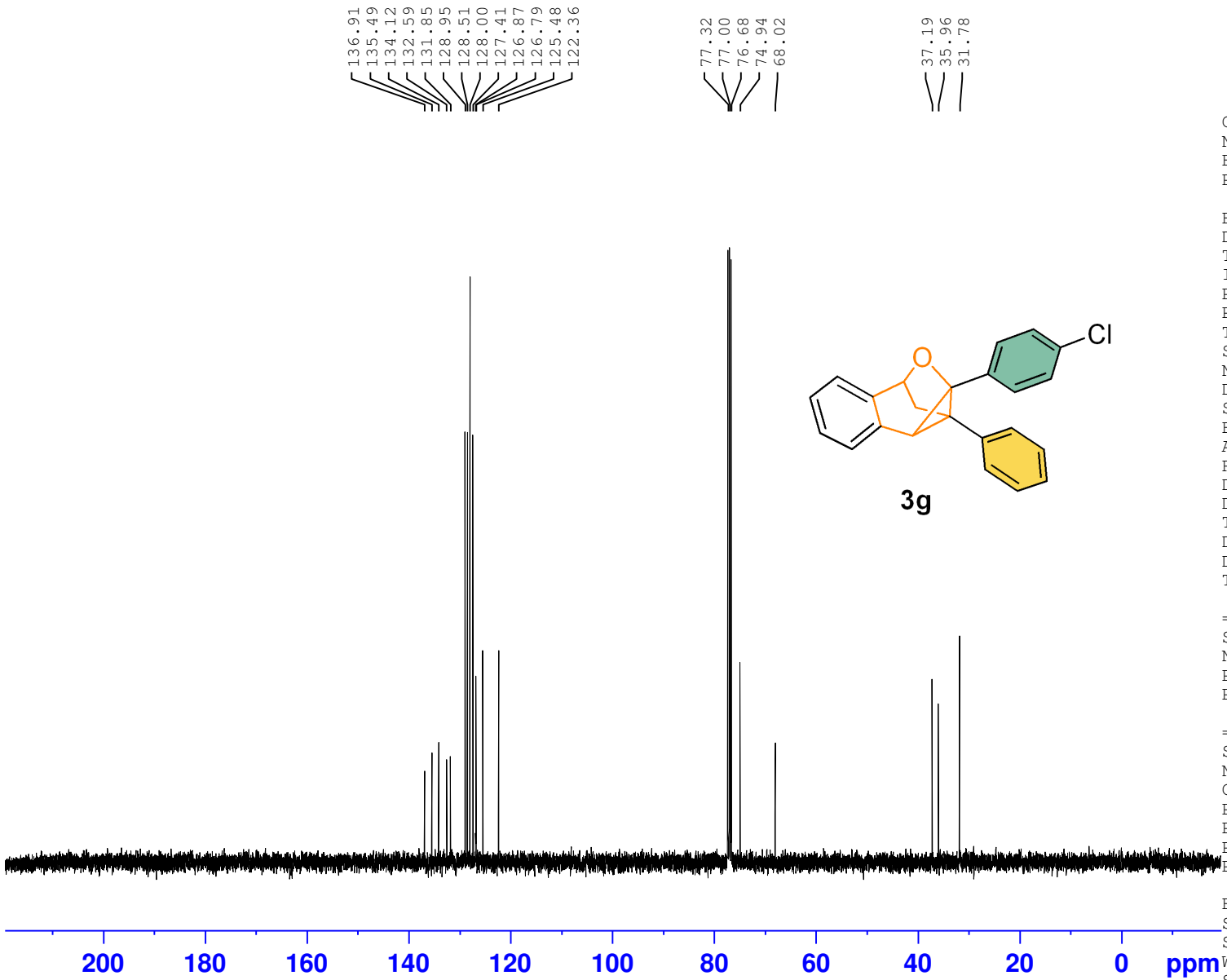

```
Current Data Parameters
NAME          lsx-2-9b-h
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220122
Time               12.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     9
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 27.78
DW                62.400 usec
DE                 6.50 usec
TE                295.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300322 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



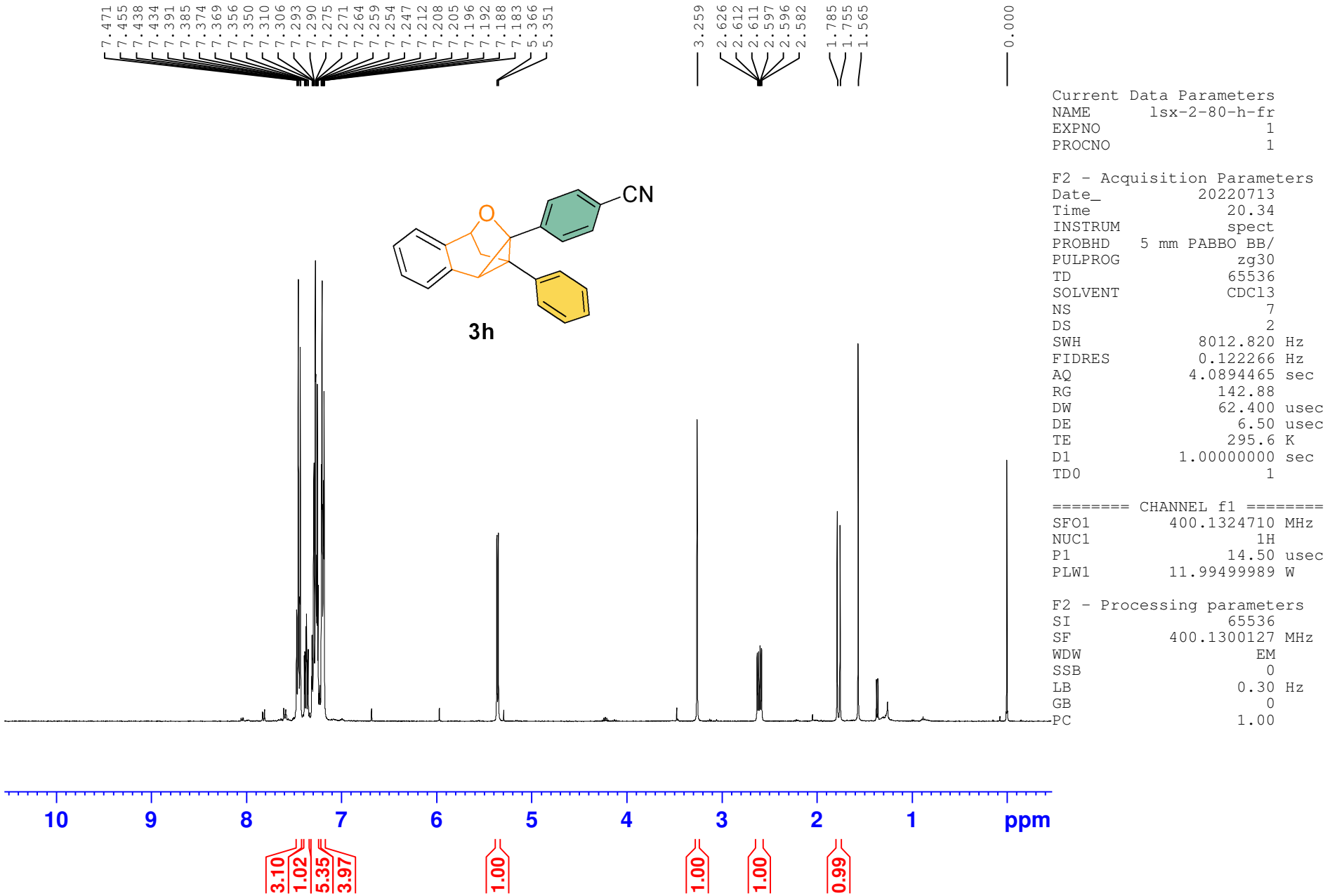

```
Current Data Parameters
NAME          lsx-2-9b-c
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220122
Time               12.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   21
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               295.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6127814 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME          lsx-2-9a-h
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220122
Time               12.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 62.93
DW                62.400 usec
DE                 6.50 usec
TE                295.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300239 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```




```
Current Data Parameters
NAME          lsx-2-9a-c
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220122
Time               12.18
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   30
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE                295.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127770 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

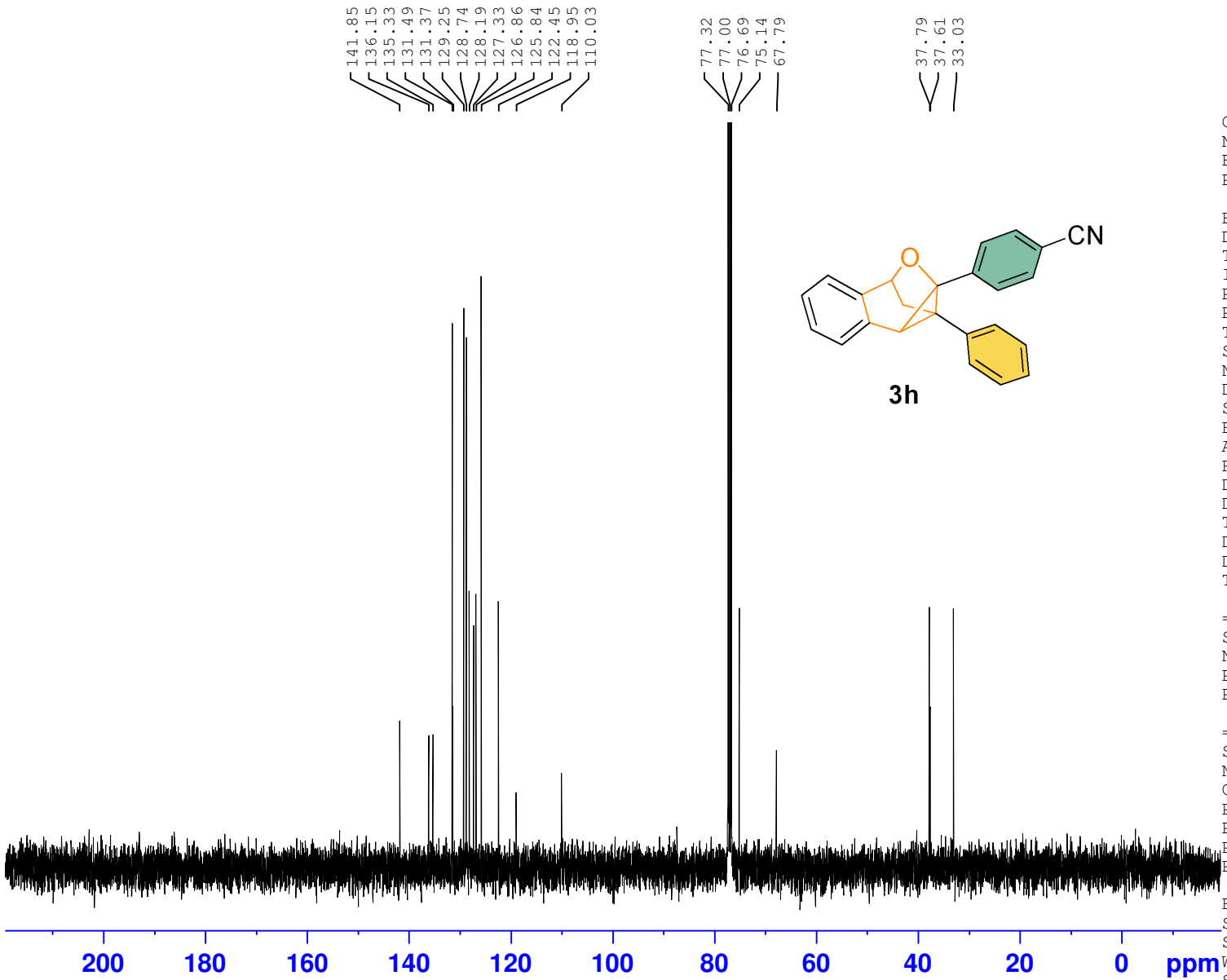


Current Data Parameters
NAME lsx-2-80-h-fr
EXPNO 1
PROCNO 1

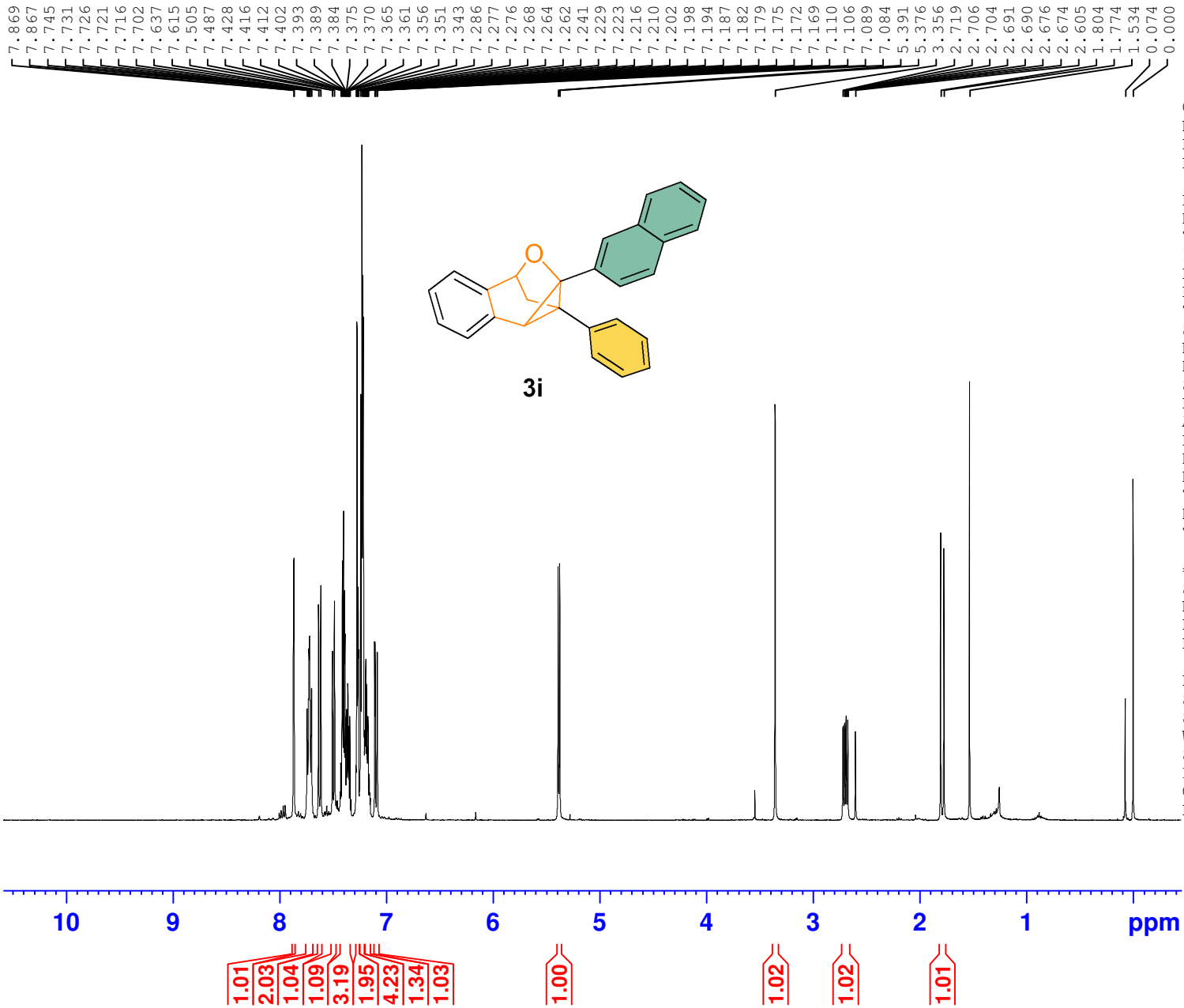
F2 - Acquisition Parameters
Date_ 20220713
Time 20.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 142.88
DW 62.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1

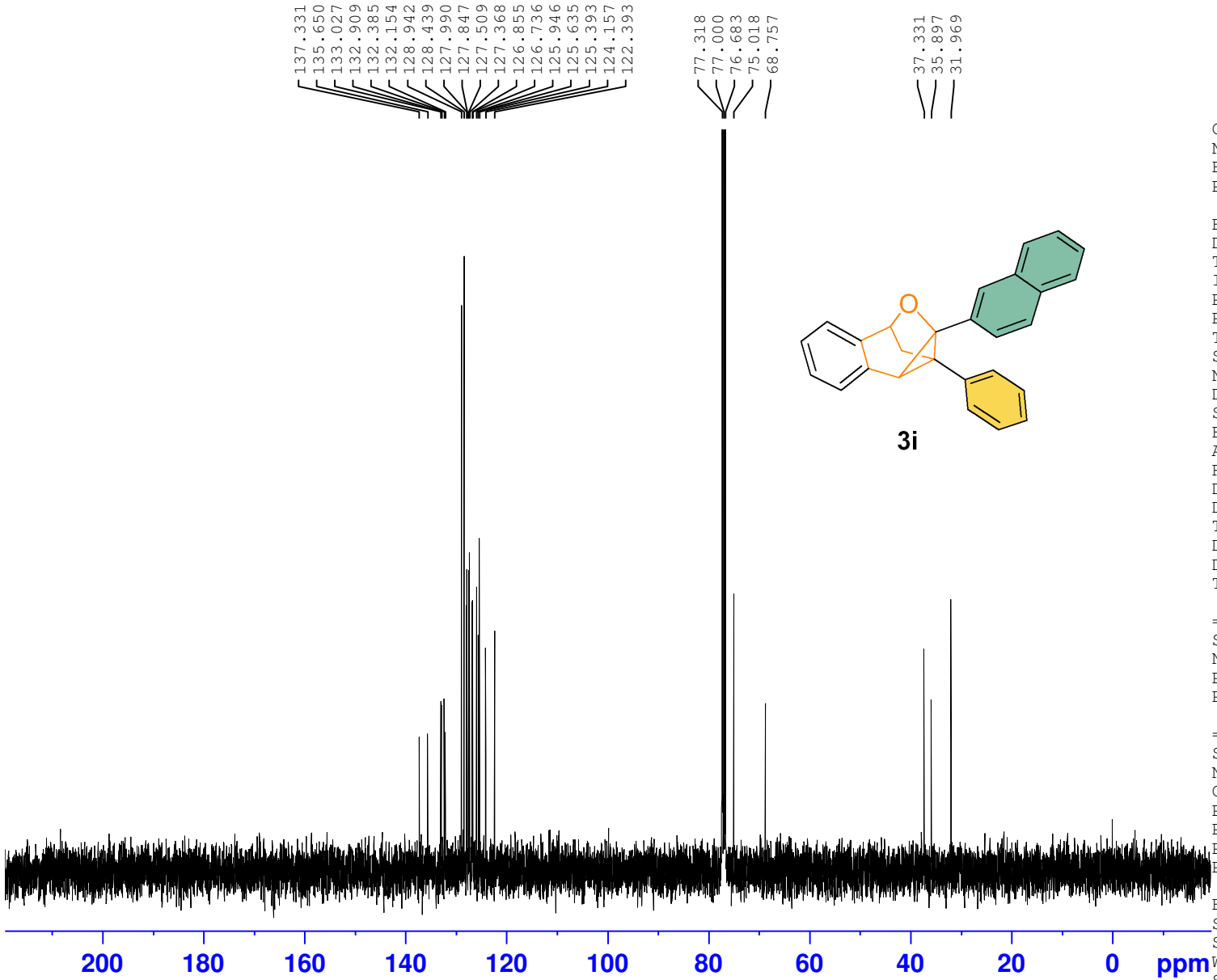
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

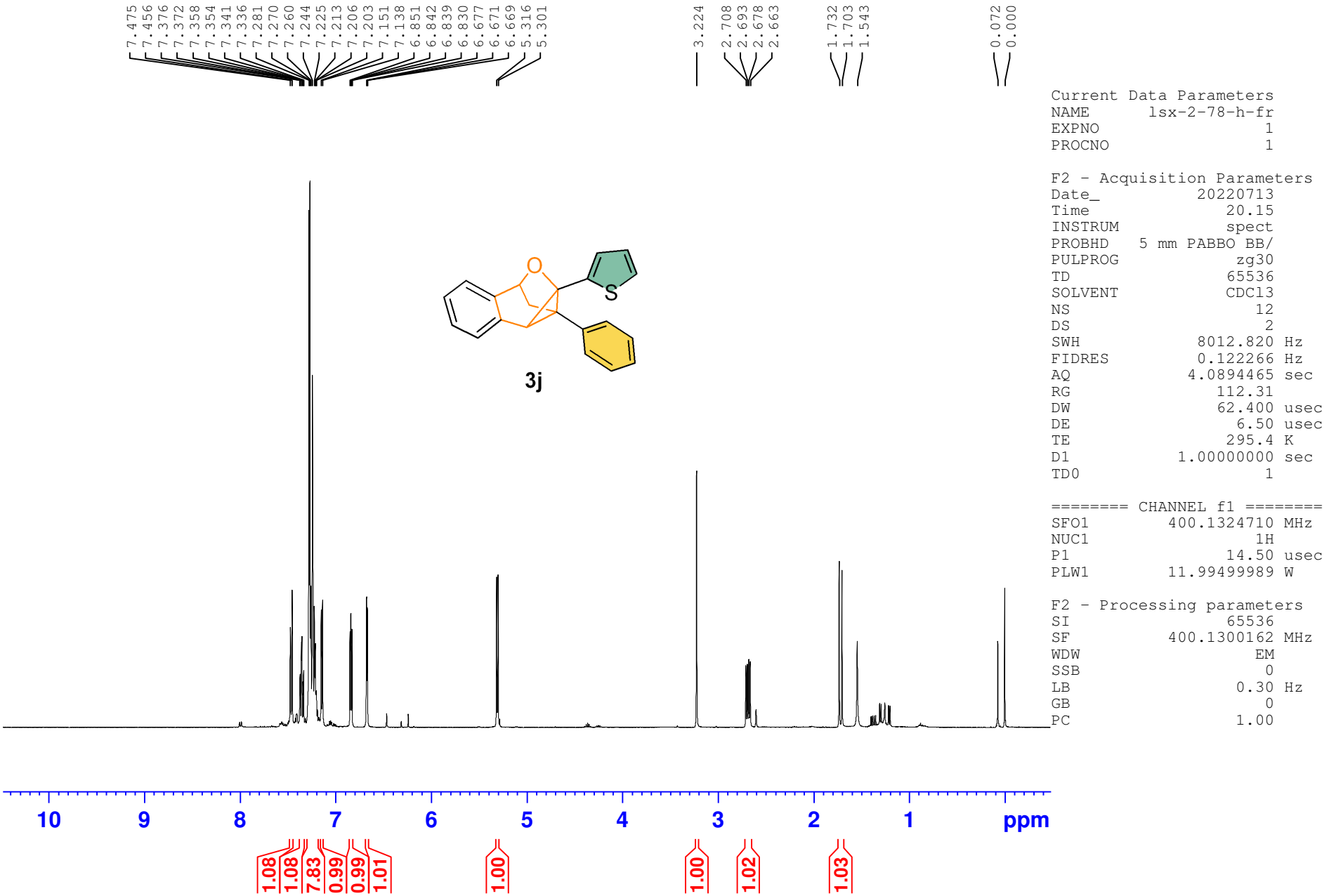



```
Current Data Parameters
NAME      lsx-2-80-c-fr
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20220713
Time              20.38
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  88
DS                   2
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1               13C
P1                9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127729 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

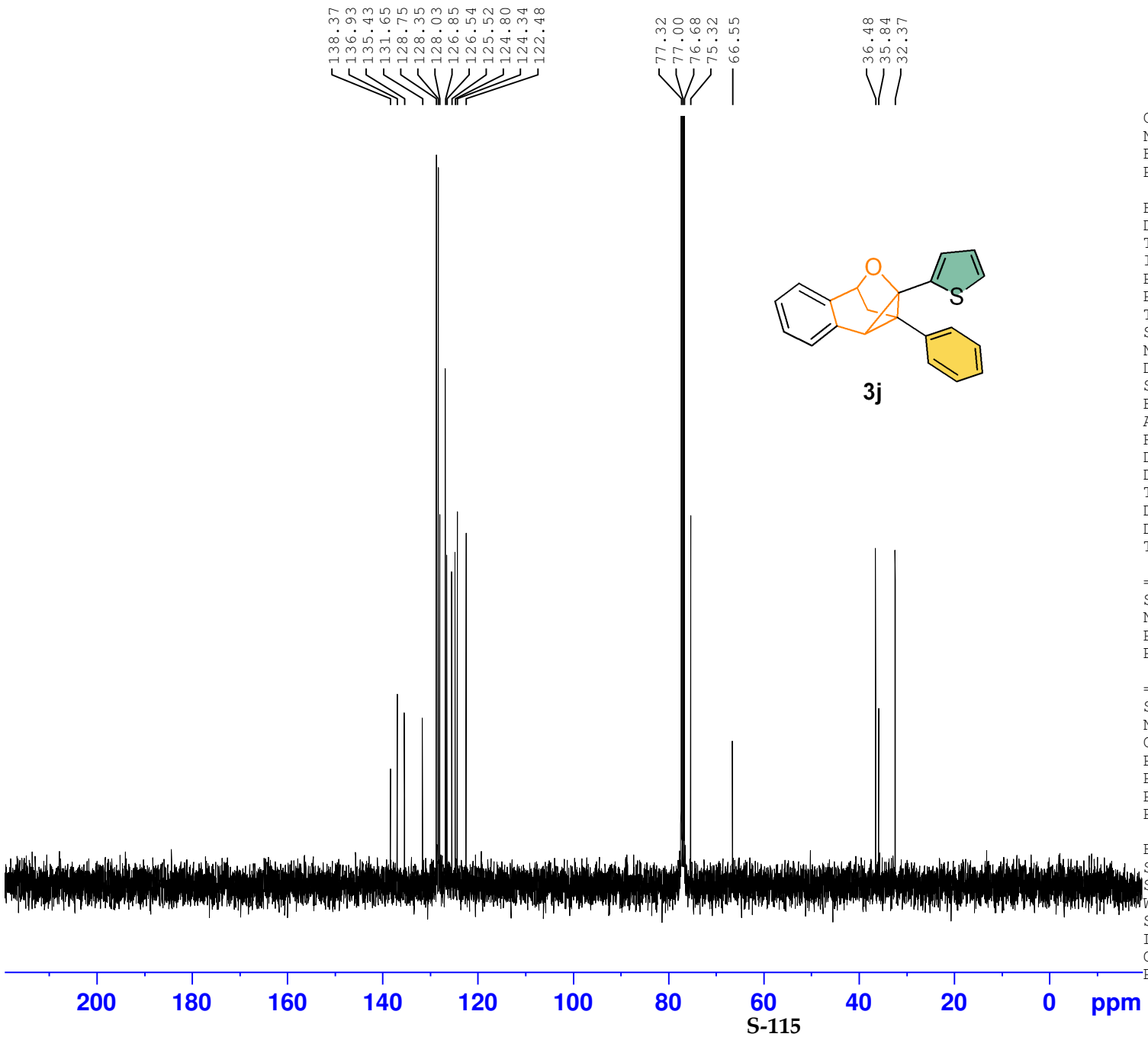

7.869
7.867
7.745
7.731
7.726
7.721
7.716
7.702
7.637
7.615
7.505
7.487
7.428
7.416
7.412
7.402
7.393
7.389
7.384
7.375
7.370
7.365
7.361
7.356
7.351
7.343
7.286
7.277
7.276
7.268
7.264
7.262
7.241
7.229
7.223
7.216
7.210
7.202
7.198
7.194
7.187
7.182
7.179
7.175
7.172
7.169
7.110
7.106
7.089
7.084
5.391
5.376
3.356
2.719
2.706
2.704
2.691
2.690
2.676
2.674
2.605
1.804
1.774
1.534
0.074
0.000
3i
Current Data Parameters
NAME lsx-2-79-h-fr
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220713
Time 20.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 112.31
DW 62.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W
F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.01
2.03
1.04
1.09
3.19
1.95
4.23
1.34
1.03
1.00
1.02
1.02
1.01



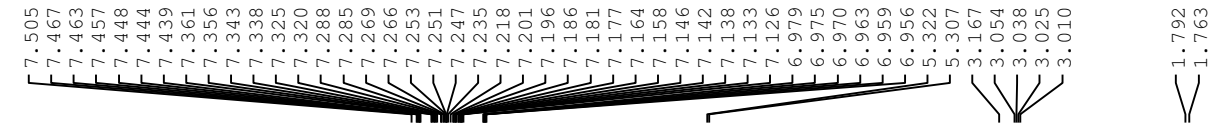

```
Current Data Parameters
NAME      lsx-2-79-c-fr
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20220713
Time              20.31
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 105
DS                   2
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1               13C
P1                9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127736 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```



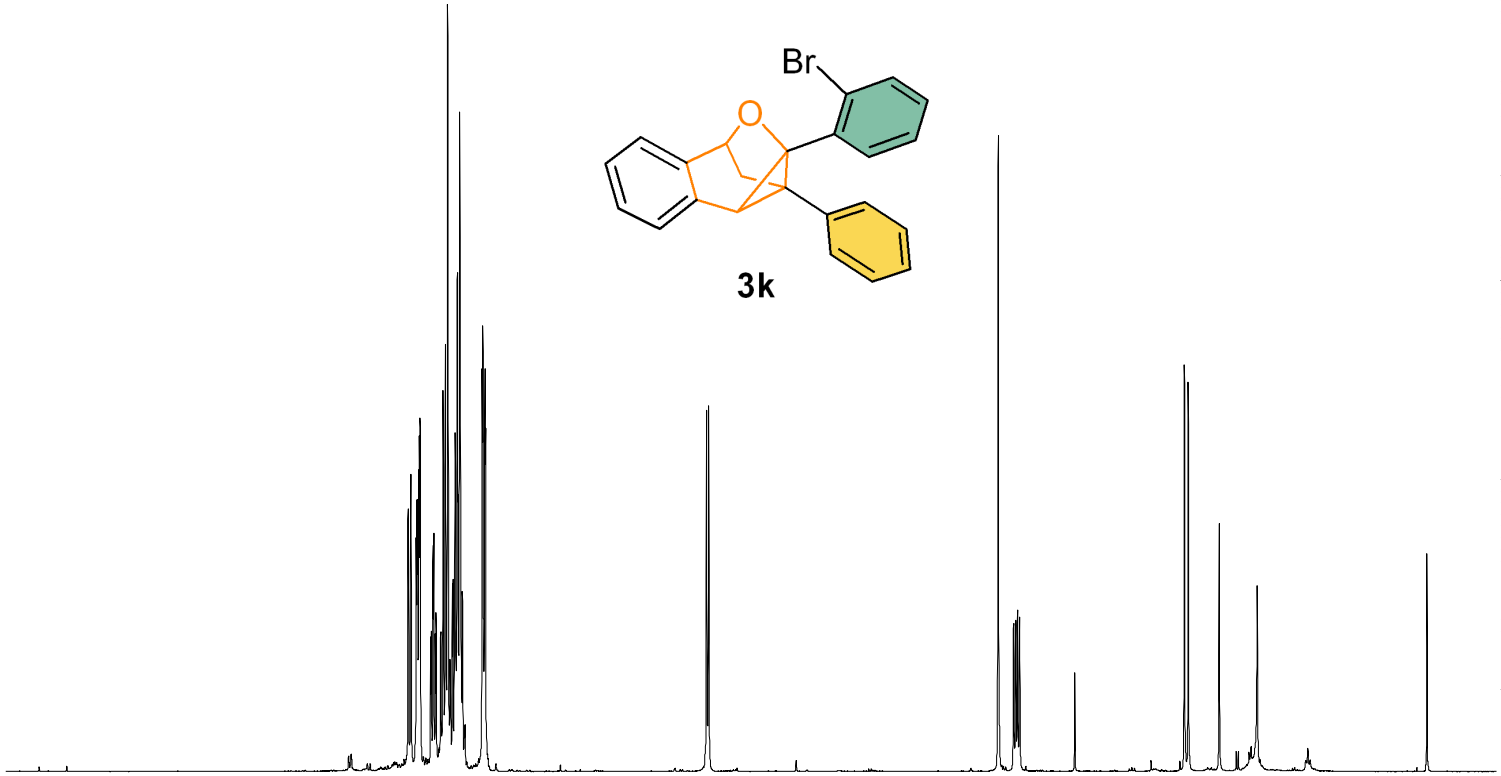

```
Current Data Parameters
NAME      lsx-2-78-h-fr
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20220713
Time              20.15
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   12
DS                    2
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG               112.31
DW               62.400 usec
DE                6.50 usec
TE               295.4 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300162 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

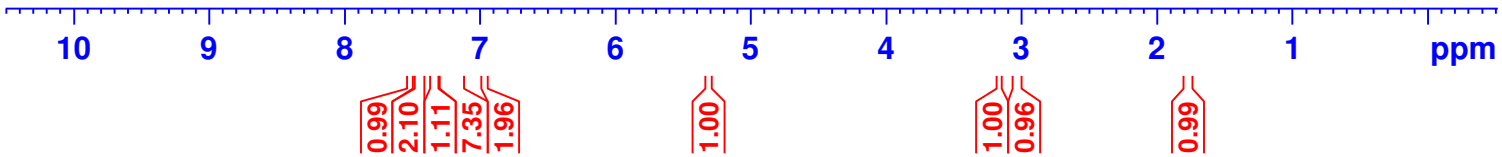



```
Current Data Parameters
NAME      lsx-2-78-c-fr
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20220713
Time              20.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 103
DS                   2
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631488 sec
RG              196.92
DW              20.800 usec
DE               6.50 usec
TE              296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1               13C
P1                9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127736 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

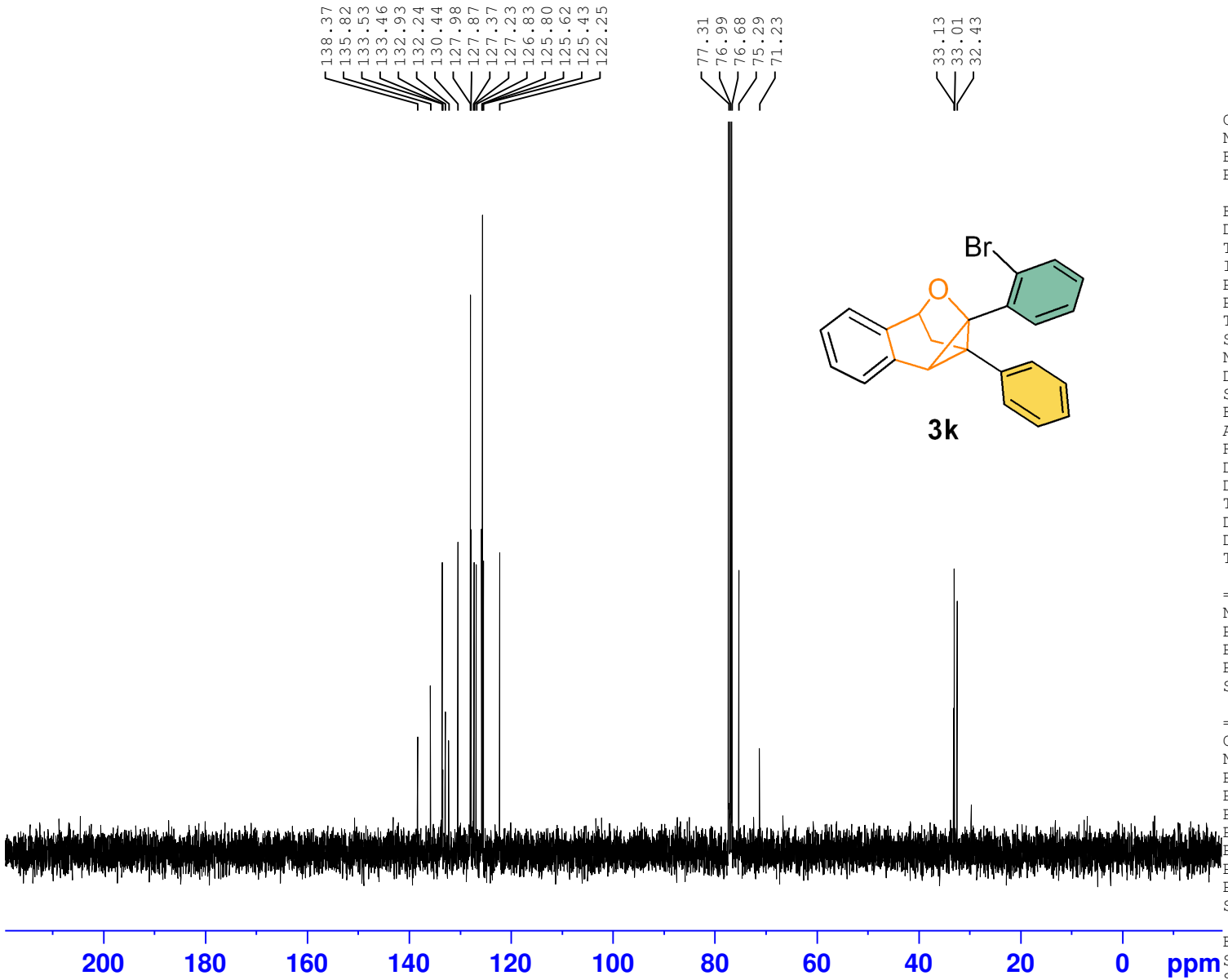


3k

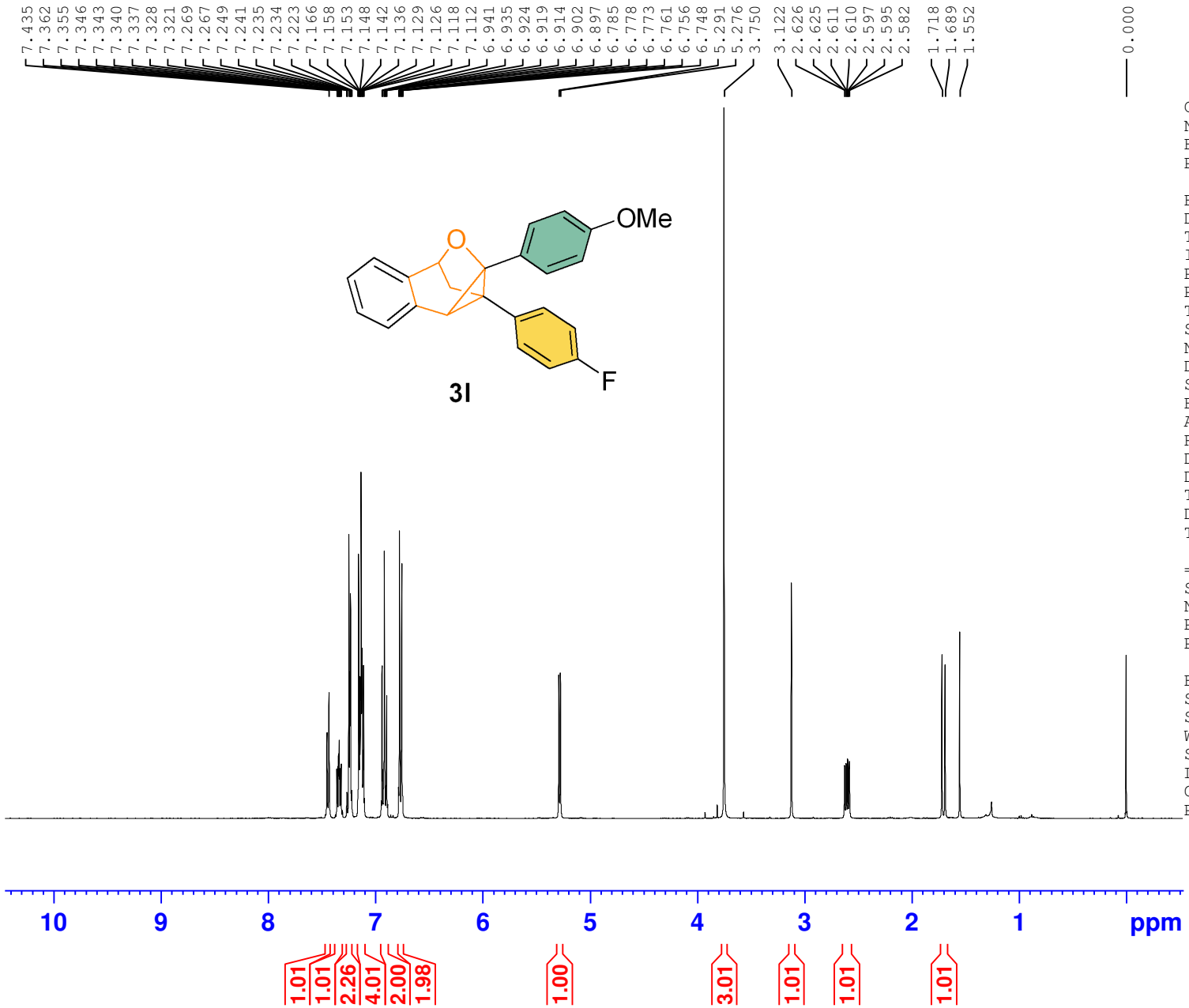




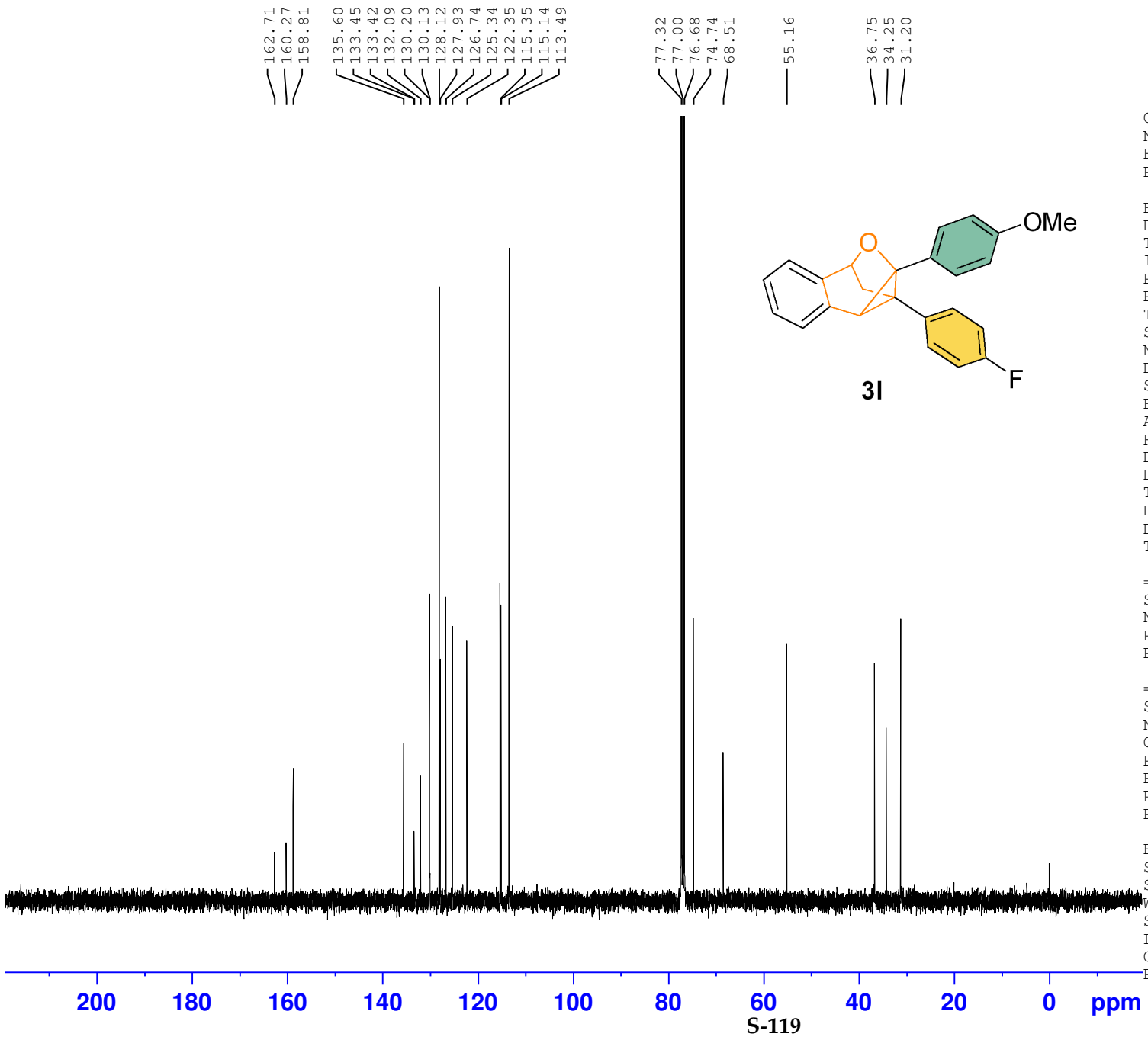

```
Current Data Parameters
NAME      lsx-p3-3e-h-fr
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220726
Time               14.30
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                   287
DW                60.800 usec
DE                 6.00 usec
TE                292.9 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.80 usec
PL1                -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300198 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME      lsx-p3-3e-h-fr-C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220726
Time               14.31
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   81
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE                293.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.39 dB
PL13               18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127769 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

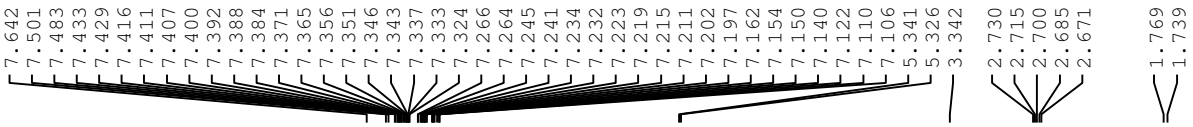



```
Current Data Parameters
NAME      lsx-2-32-h-fr
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20220712
Time              16.43
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ            4.0894465 sec
RG               103.52
DW                62.400 usec
DE                 6.50 usec
TE                295.4 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300146 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

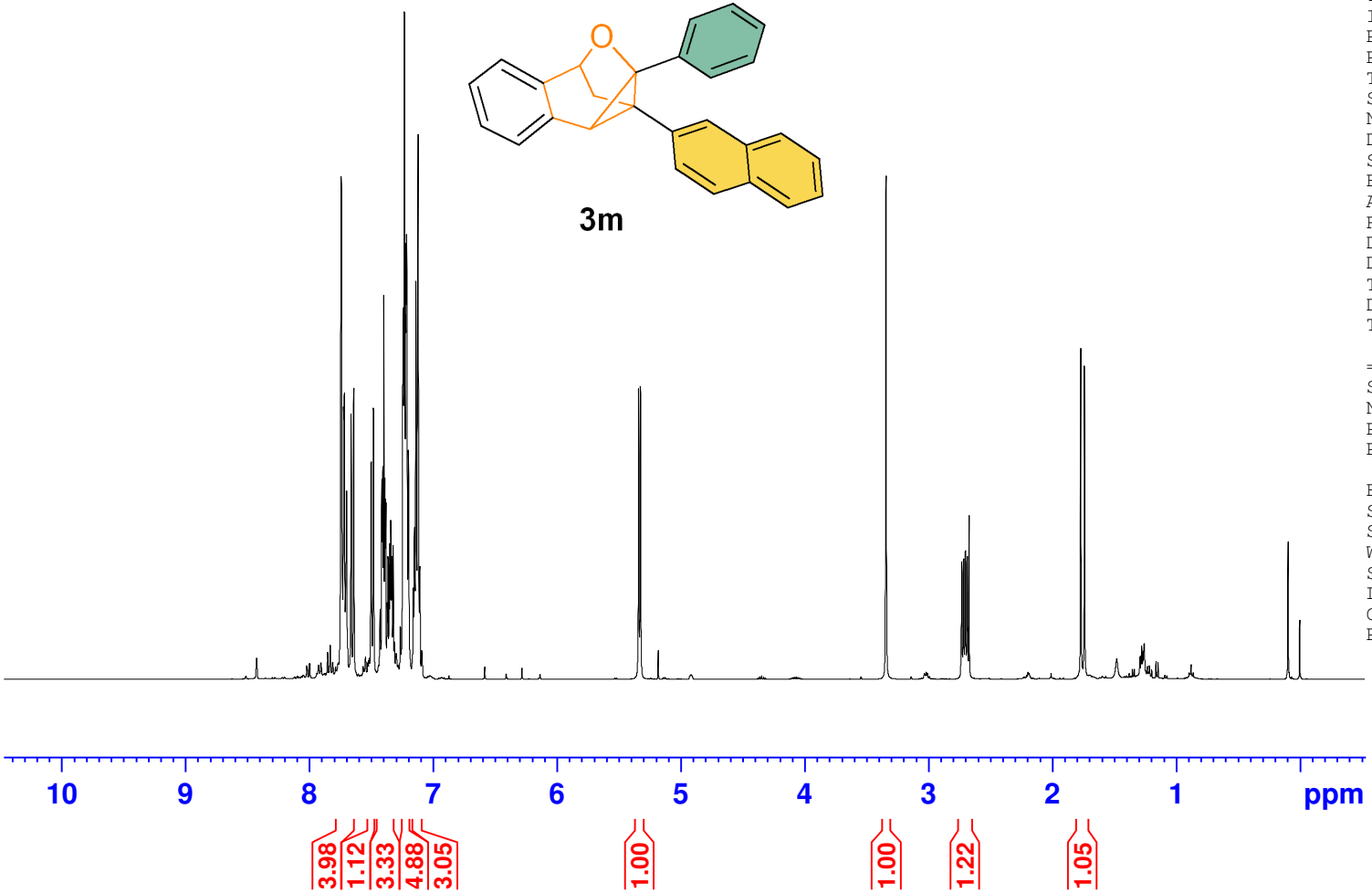


3l

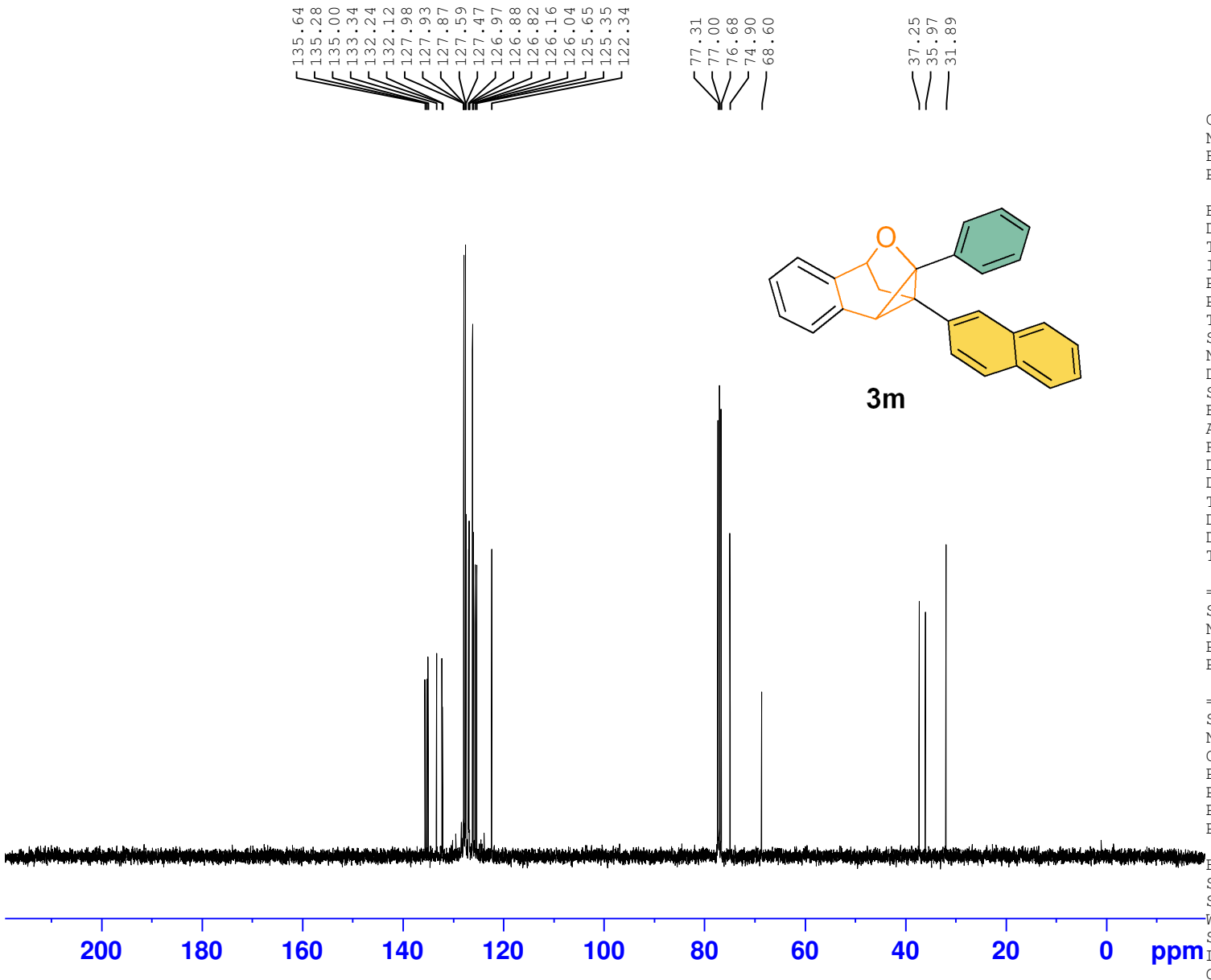
```
Current Data Parameters
NAME      lsx-2-32-c-fr
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20220712
Time              16.59
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  268
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE                296.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127729 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```



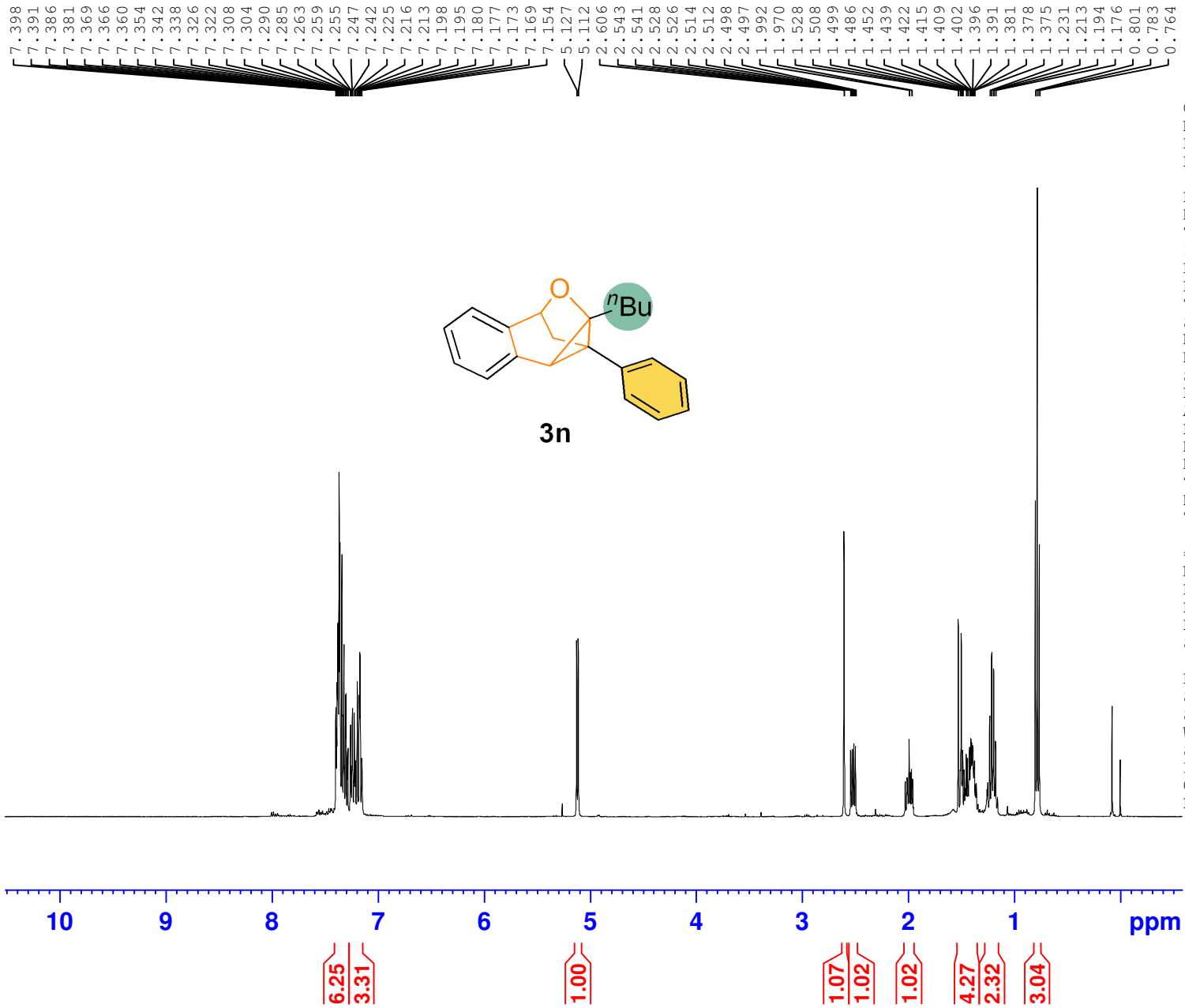
3m



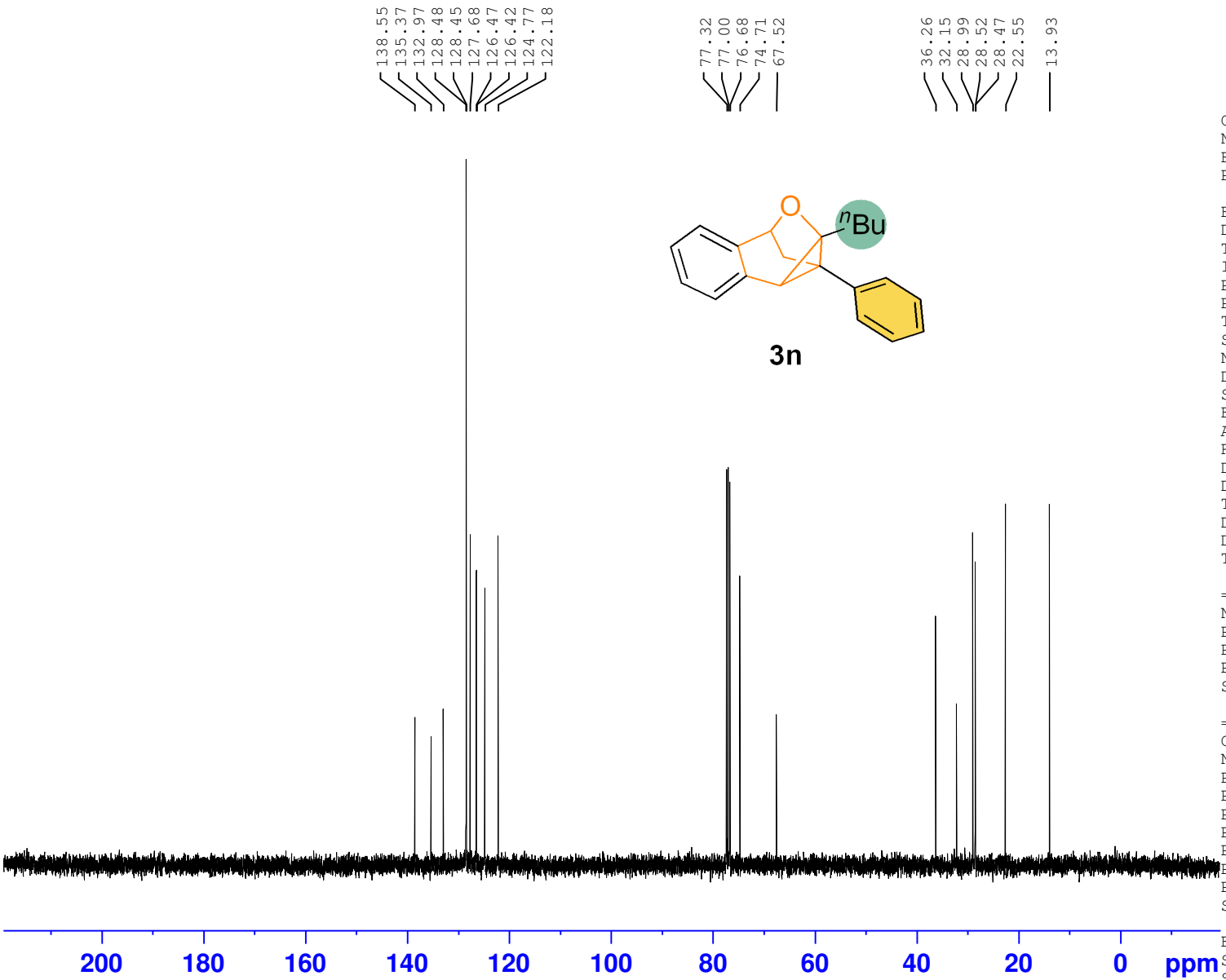

```
Current Data Parameters
NAME      lsx-project3-3m-h-fr
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220723
Time                  14.19
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894465 sec
RG                    39.46
DW                  62.400 usec
DE                   6.50 usec
TE                  295.4 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300537 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



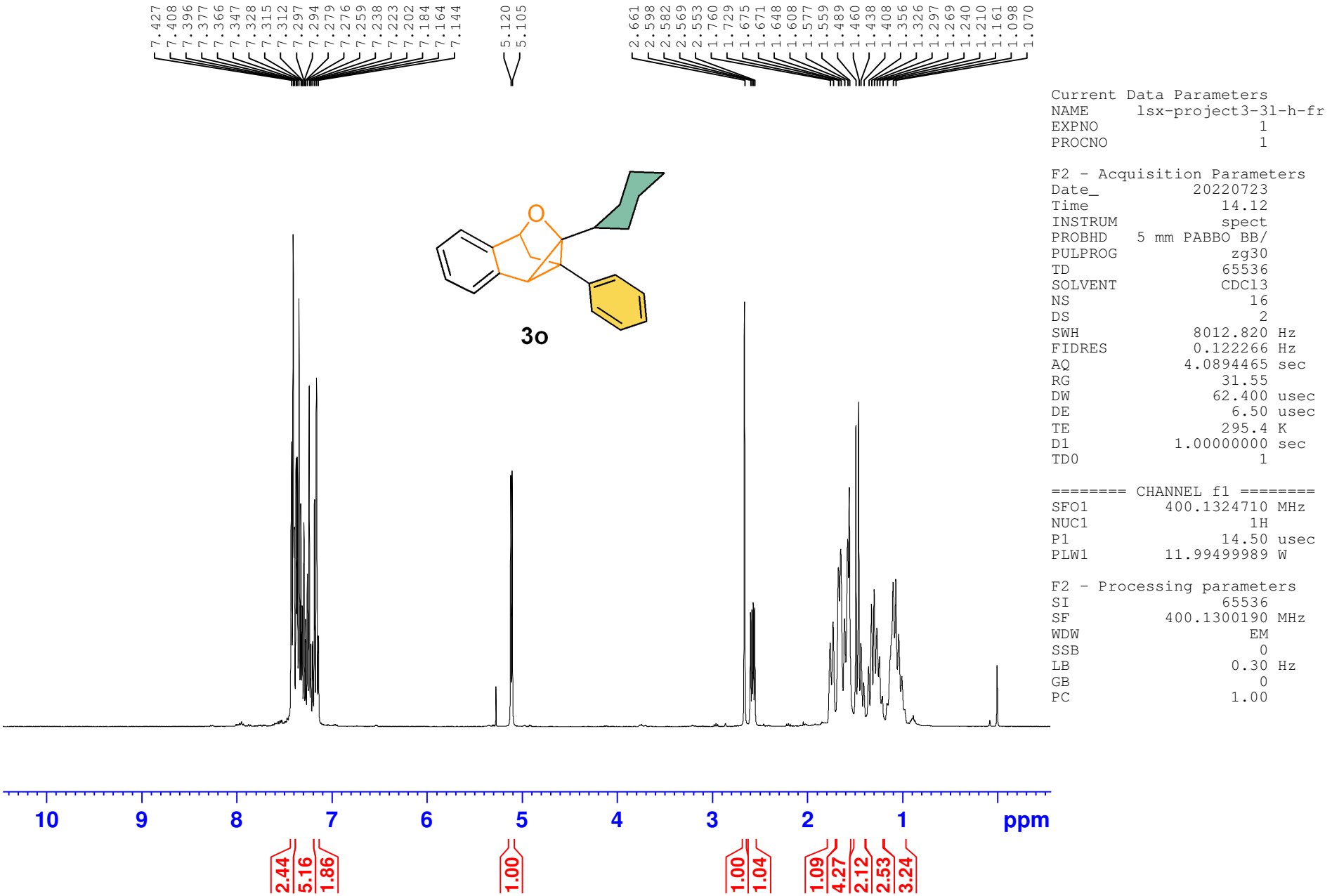

```
Current Data Parameters
NAME      lsx-project3-3m-c-fr
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220723
Time                  14.22
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      46
DS                       2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                   196.92
DW                   20.800 usec
DE                    6.50 usec
TE                   296.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                    13C
P1                    9.70 usec
PLW1          46.98899841 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2          11.99499989 W
PLW12          0.34213999 W
PLW13          0.27713001 W

F2 - Processing parameters
SI                    32768
SF            100.6127872 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```




```
Current Data Parameters
NAME      lsx-project3-3k-h-fr
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220725
Time                  20.53
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ               3.9845889 sec
RG                      144
DW                   60.800 usec
DE                    6.00 usec
TE                   292.7 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.80 usec
PL1                  -1.00 dB
PL1W           12.17476940 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF             400.1300236 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```




```
Current Data Parameters
NAME      lsx-project3-3k-c-fr
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220725
Time                  21.01
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      126
DS                        1
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                     2050
DW                   20.800 usec
DE                    6.00 usec
TE                   293.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    40.00 usec
PL1                   -3.00 dB
PL1W          60.64365387 W
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 14.39 dB
PL13                 18.00 dB
PL2W          12.17476940 W
PL12W          0.35193357 W
PL13W          0.15327126 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF           100.6127774 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```


7.427
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7.396
7.377
7.366
7.347
7.328
7.315
7.312
7.297
7.294
7.279
7.276
7.259
7.238
7.223
7.202
7.184
7.164
7.144
5.120
5.105
2.661
2.598
2.582
2.569
2.553
1.760
1.729
1.675
1.671
1.648
1.608
1.577
1.559
1.489
1.460
1.438
1.408
1.356
1.326
1.297
1.269
1.240
1.210
1.161
1.098
1.070
3o
Current Data Parameters
NAME lsx-project3-3l-h-fr
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220723
Time 14.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.55
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W
F2 - Processing parameters
SI 65536
SF 400.1300190 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
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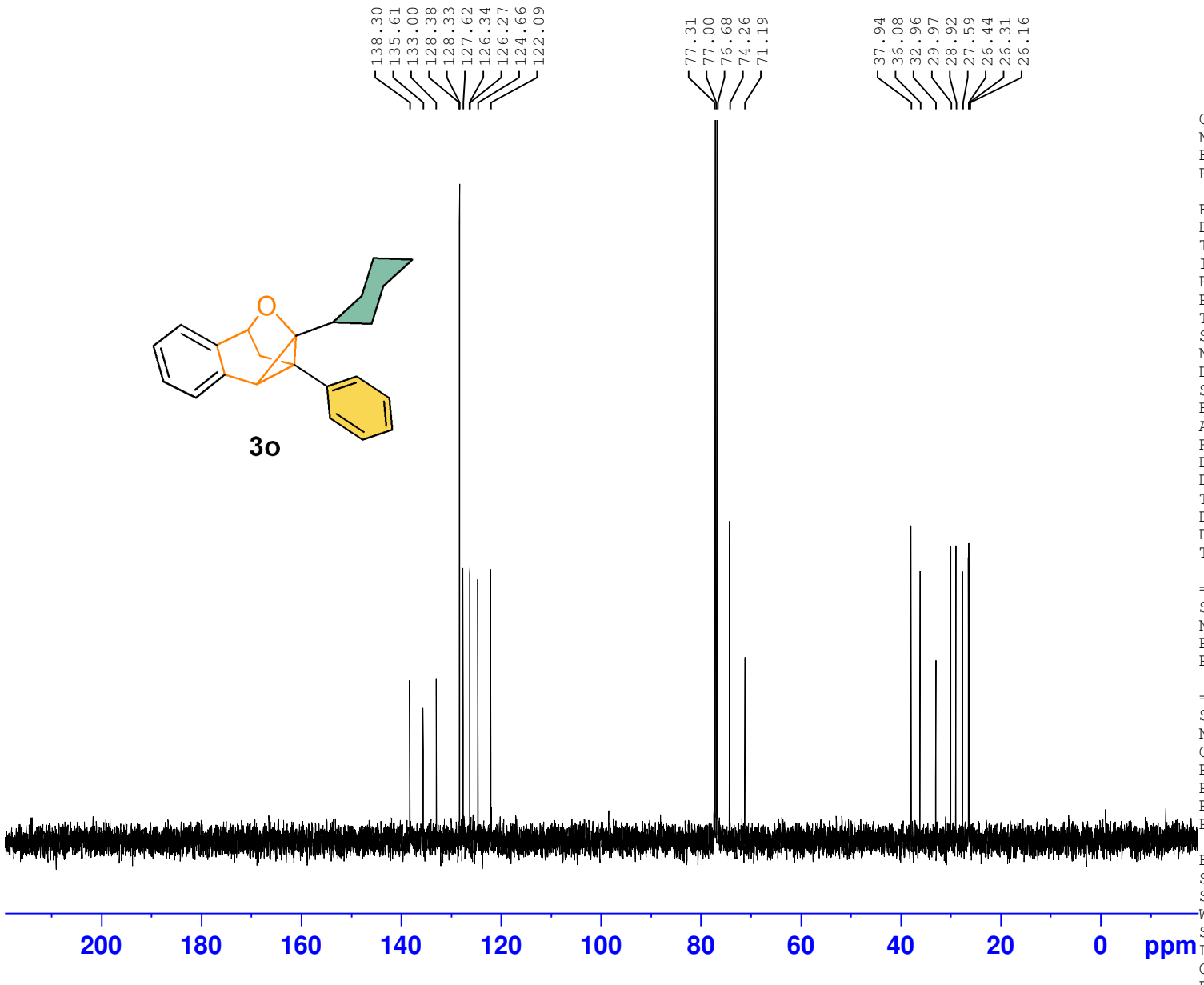
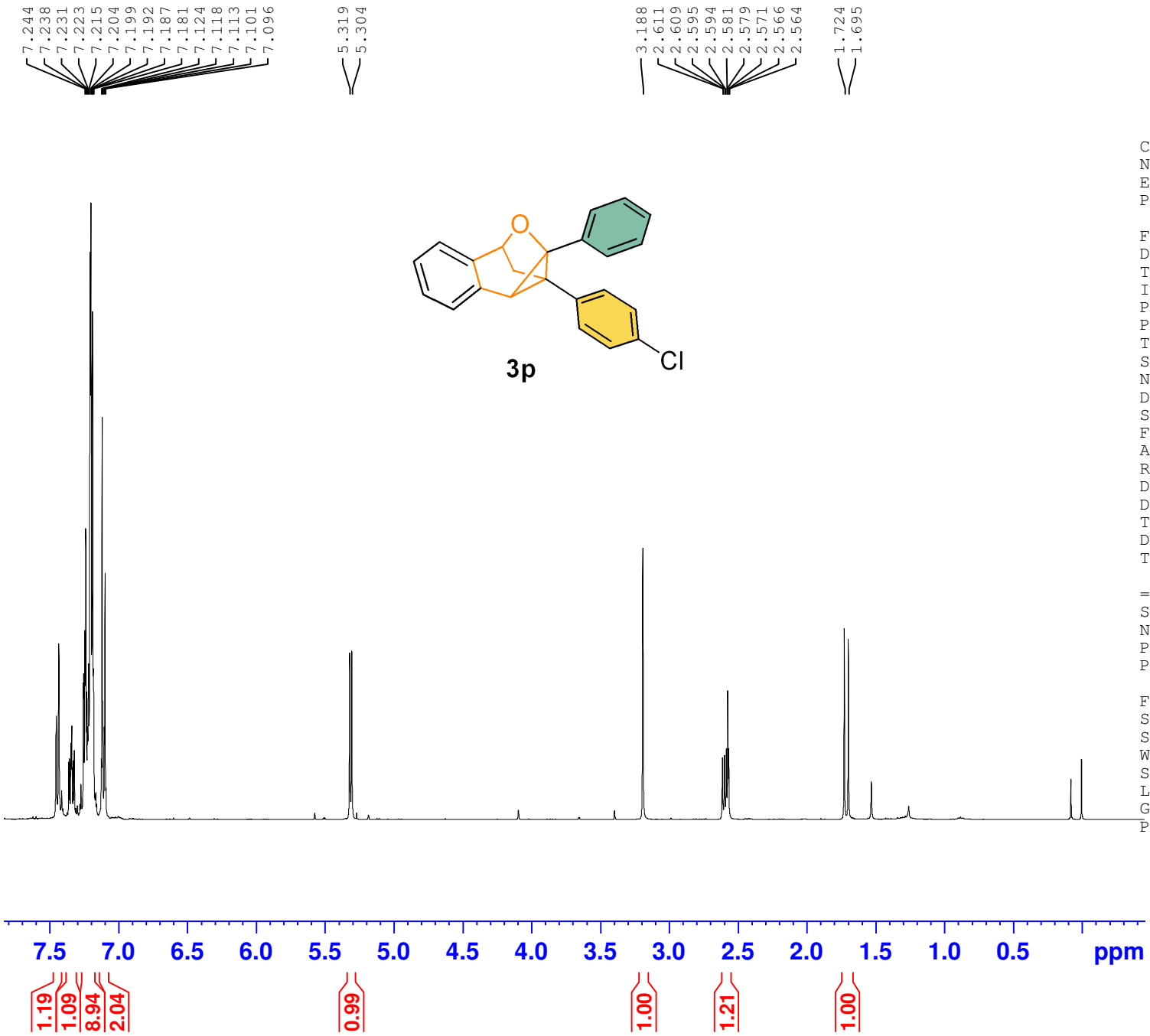
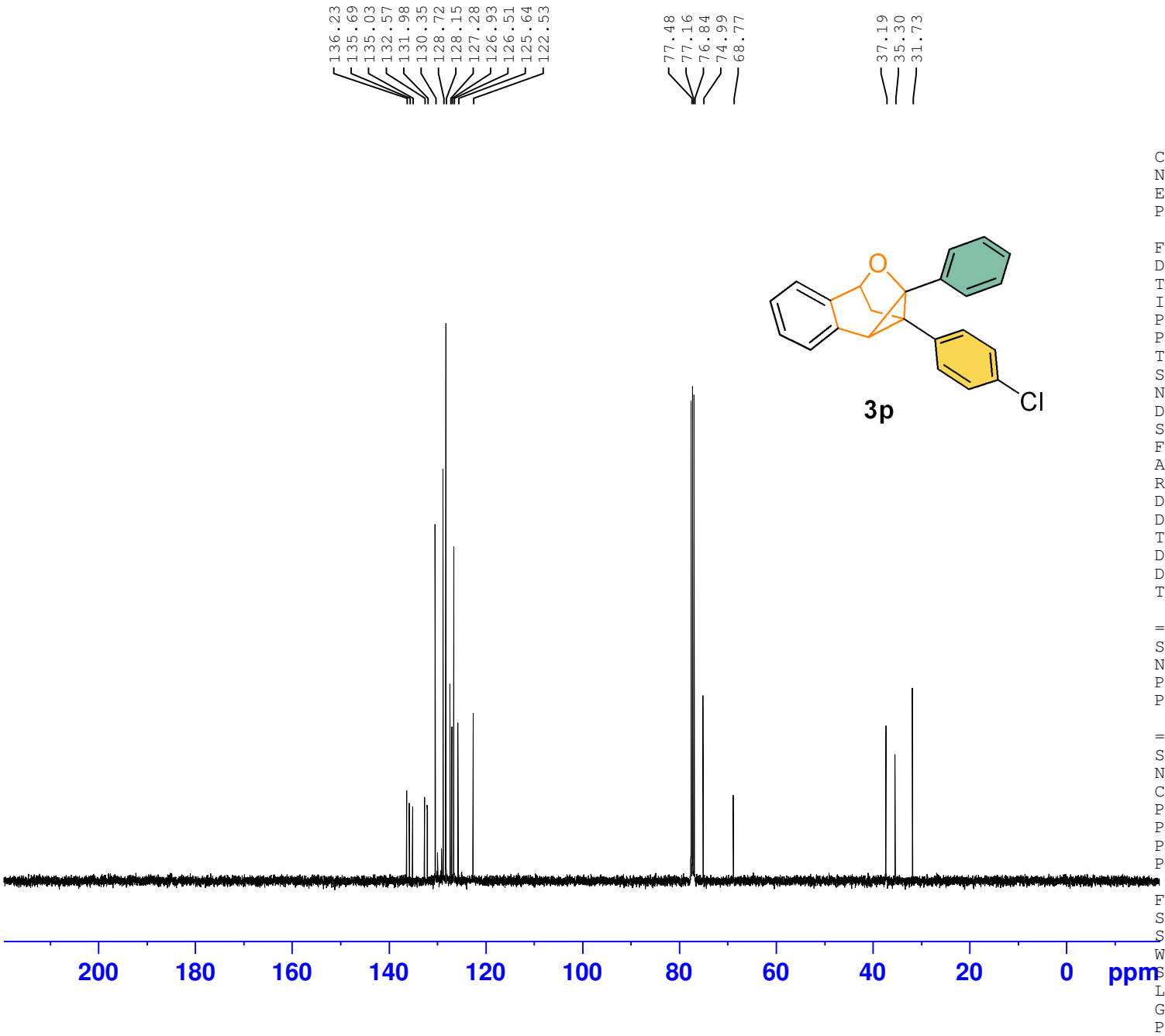
5.16
1.86
1.00
1.00
1.04
1.09
4.27
2.12
2.53
3.24



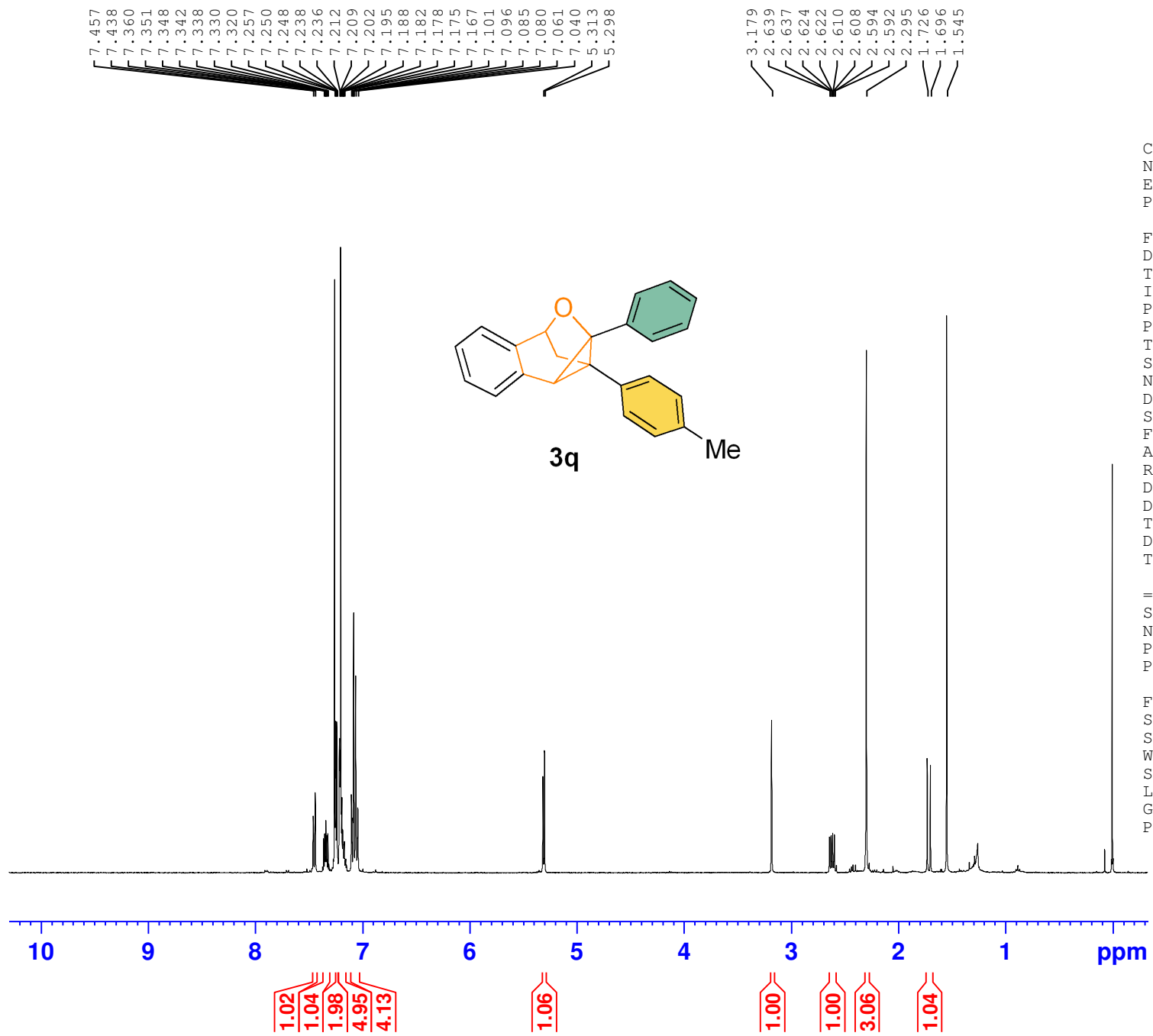

```
Current Data Parameters
NAME      lsx-project3-3l-c-fr
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20220723
Time                   14.15
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        30
DS                         2
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                 1.3631488 sec
RG                    196.92
DW                    20.800 usec
DE                     6.50 usec
TE                     296.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             100.6228298 MHz
NUC1                     13C
P1                     9.70 usec
PLW1             46.98899841 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             11.99499989 W
PLW12             0.34213999 W
PLW13             0.27713001 W

F2 - Processing parameters
SI                     32768
SF               100.6127761 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```



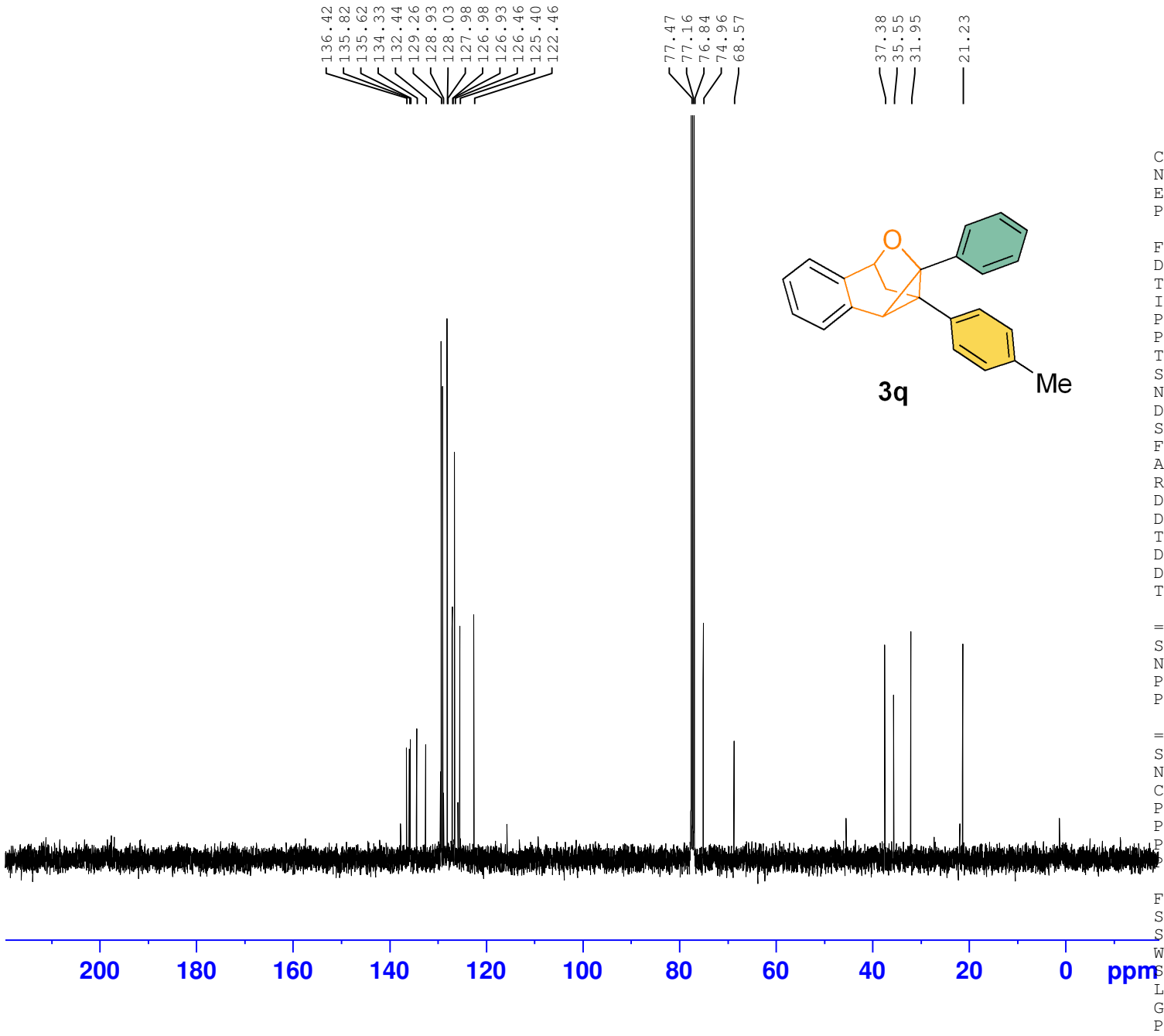

```
Current Data Parameters
NAME      lsx-8-143cc-h-fr
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20240722
Time                 19.31
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  62.93
DW                62.400 usec
DE                 6.50 usec
TE                296.1 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                  65536
SF           400.1300214 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



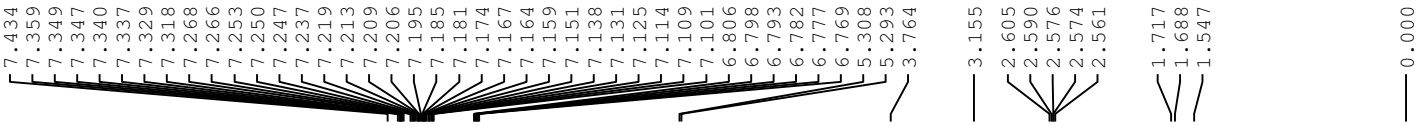

```
Current Data Parameters
NAME      lsx-8-143cc-c-fr
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20240722
Time                 19.38
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    116
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                 196.92
DW                 20.800 usec
DE                  6.50 usec
TE                 297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                   9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                   32768
SF           100.6127597 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

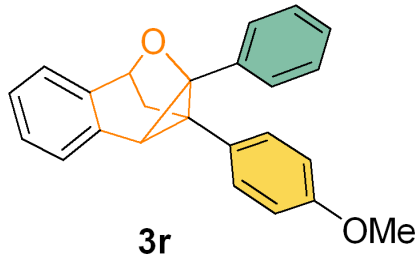



```
Current Data Parameters
NAME      lsx-8-143b-h-fr
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20240721
Time                18.22
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ              4.0894465 sec
RG                 164.33
DW                 62.400 usec
DE                  6.50 usec
TE                 296.2 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                  65536
SF           400.1300107 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

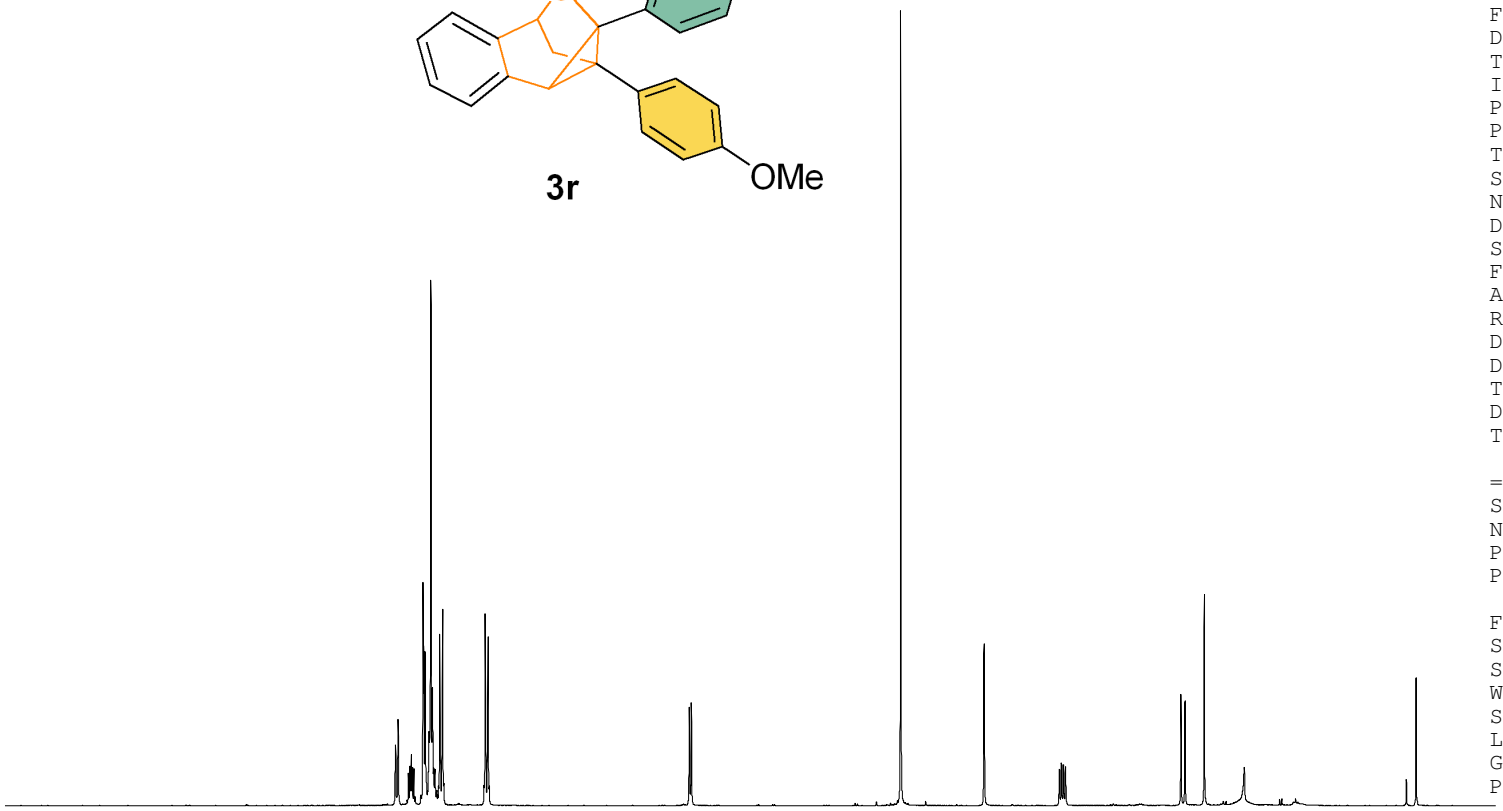


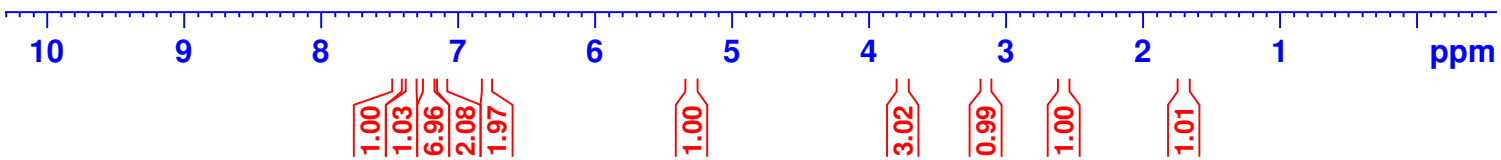

```
Current Data Parameters
NAME      lsx-8-143bb-c-fr
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20240722
Time                19.26
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    71
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                   9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127593 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



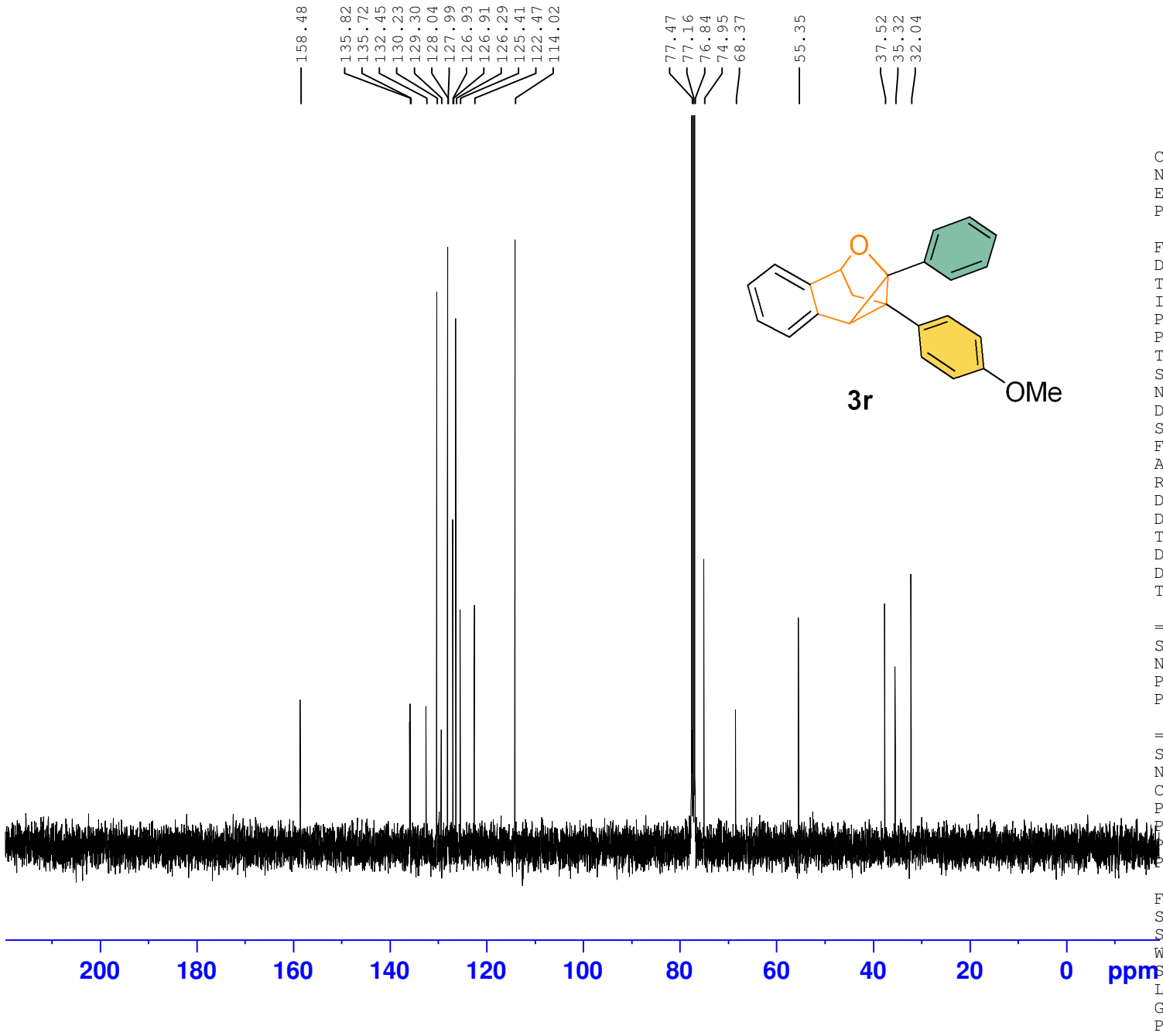


3r

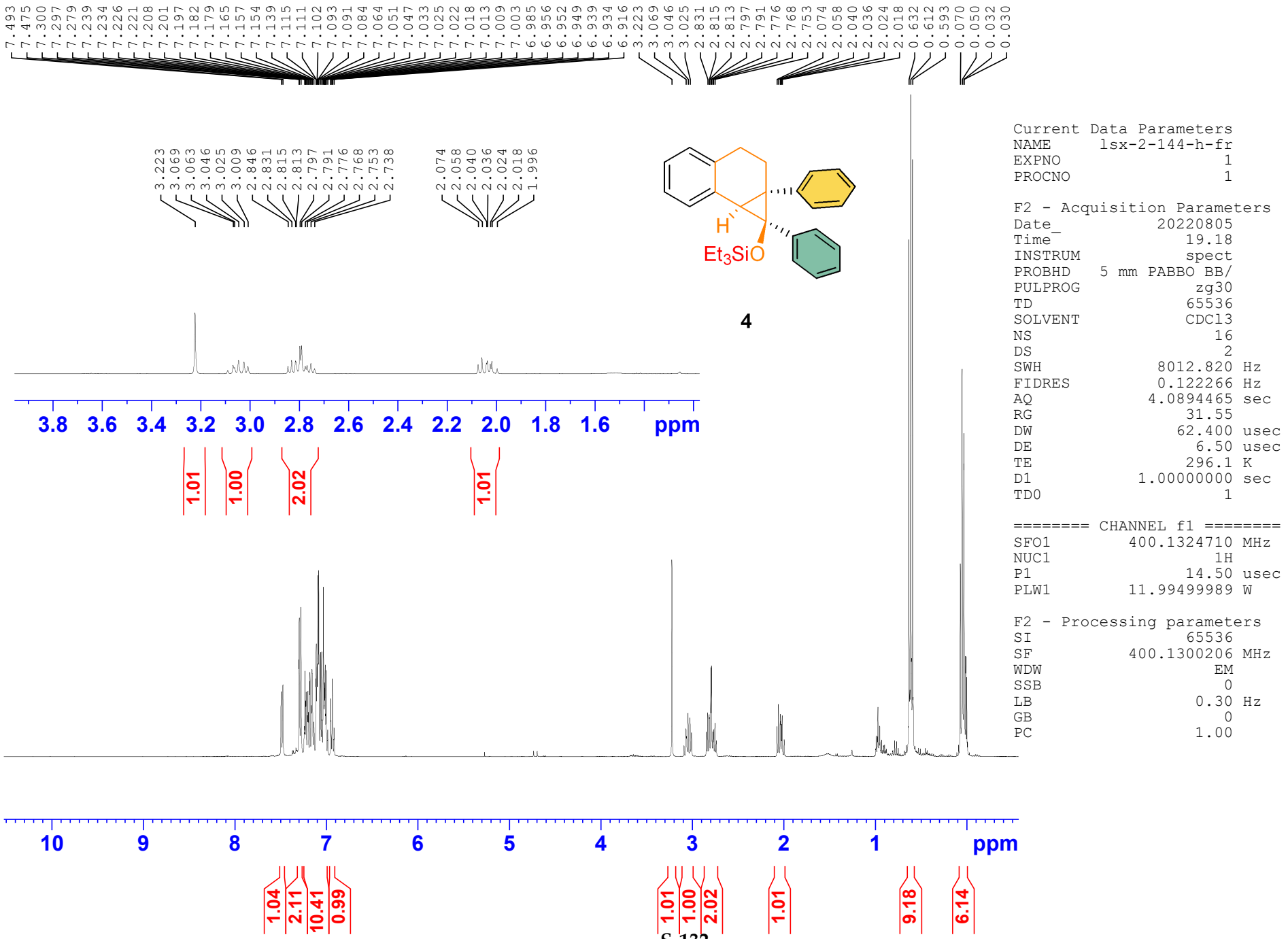


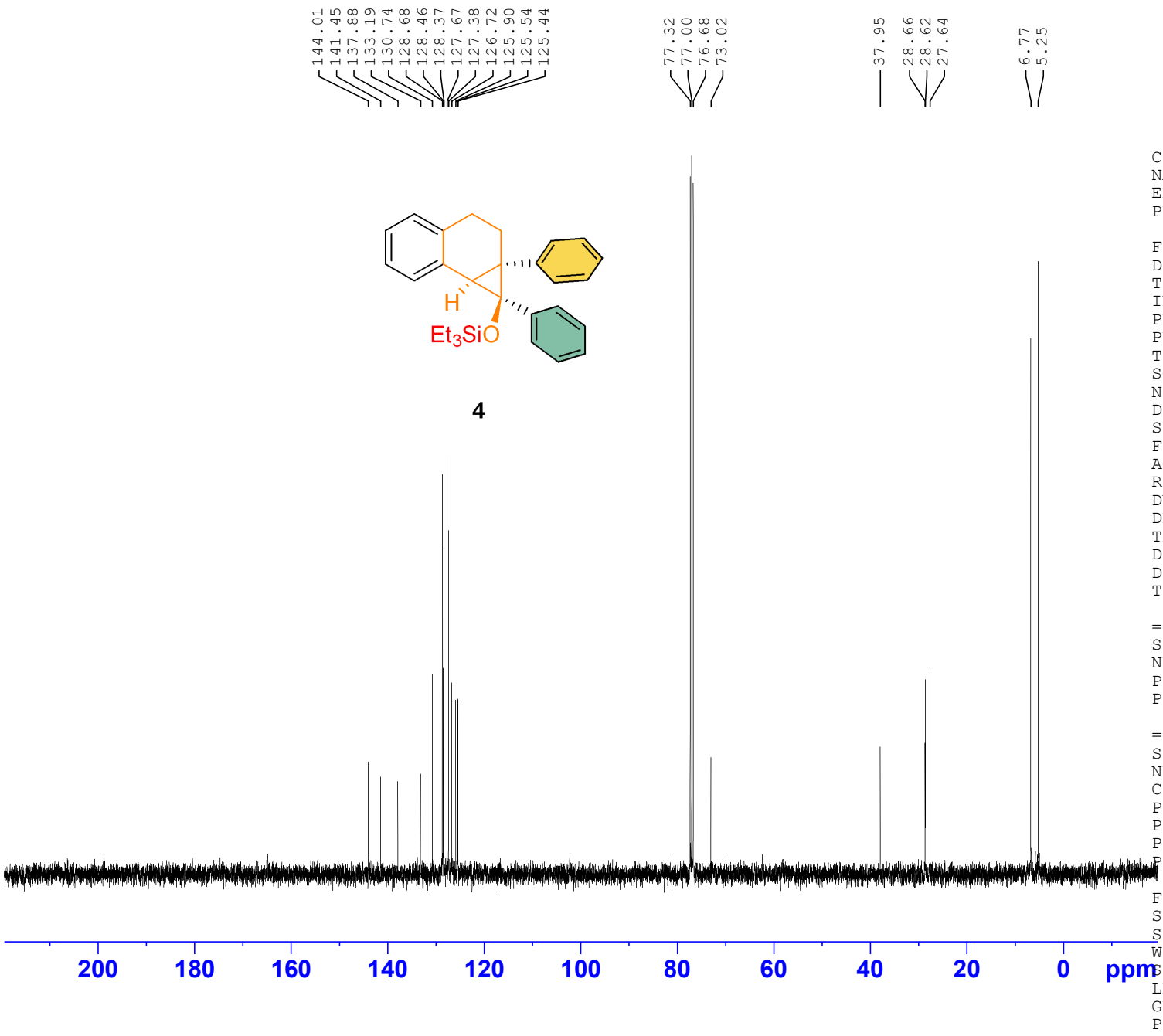



```
Current Data Parameters
NAME      lsx-8-143aa-h-fr
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20240722
Time                 19.00
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ              4.0894465 sec
RG                 164.33
DW                 62.400 usec
DE                  6.50 usec
TE                 295.9 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                  65536
SF           400.1300124 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

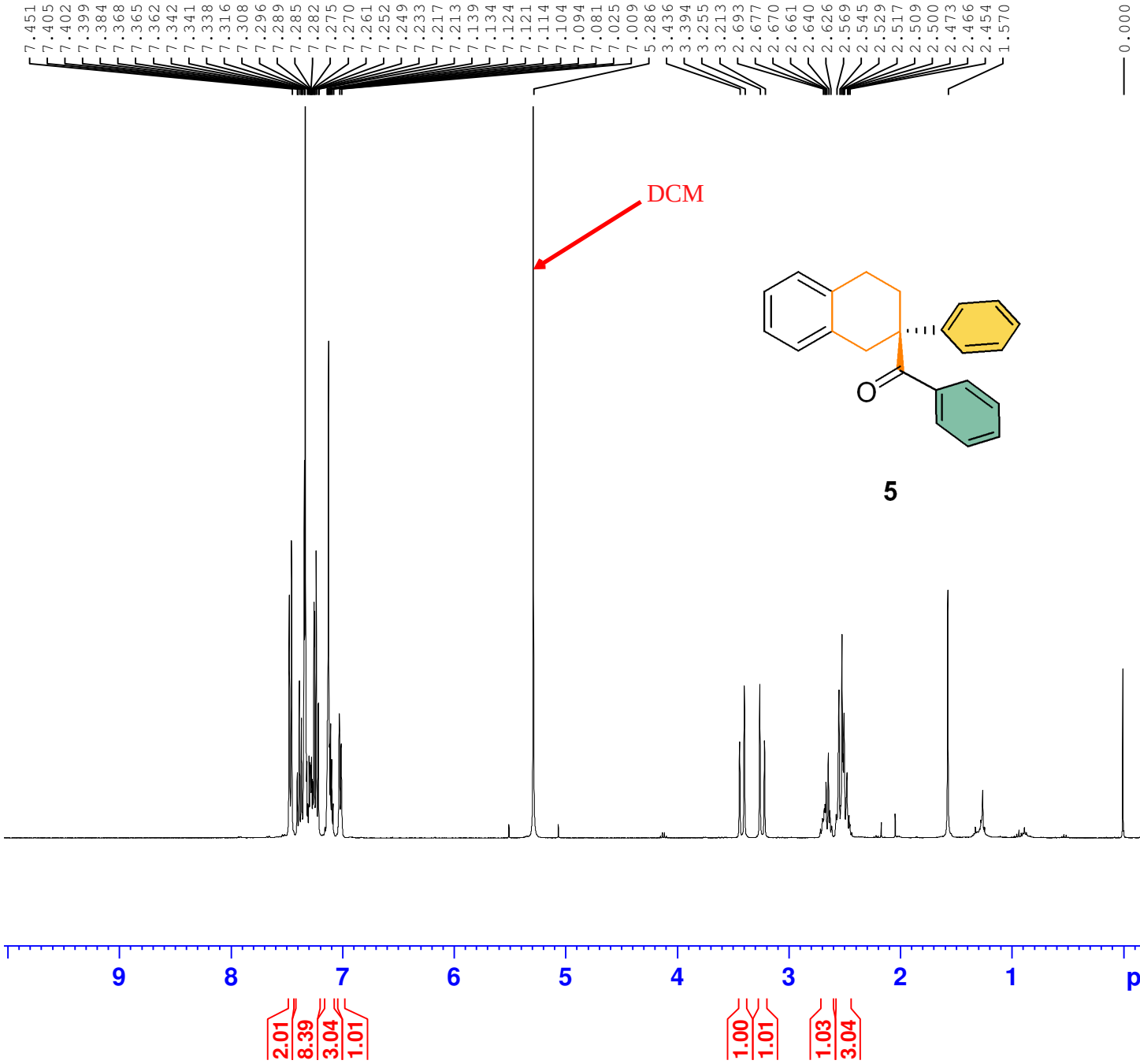



```
Current Data Parameters
NAME      lsx-8-143aa-c-fr
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20240722
Time                 19.17
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   268
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                  32768
SF           100.6127560 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

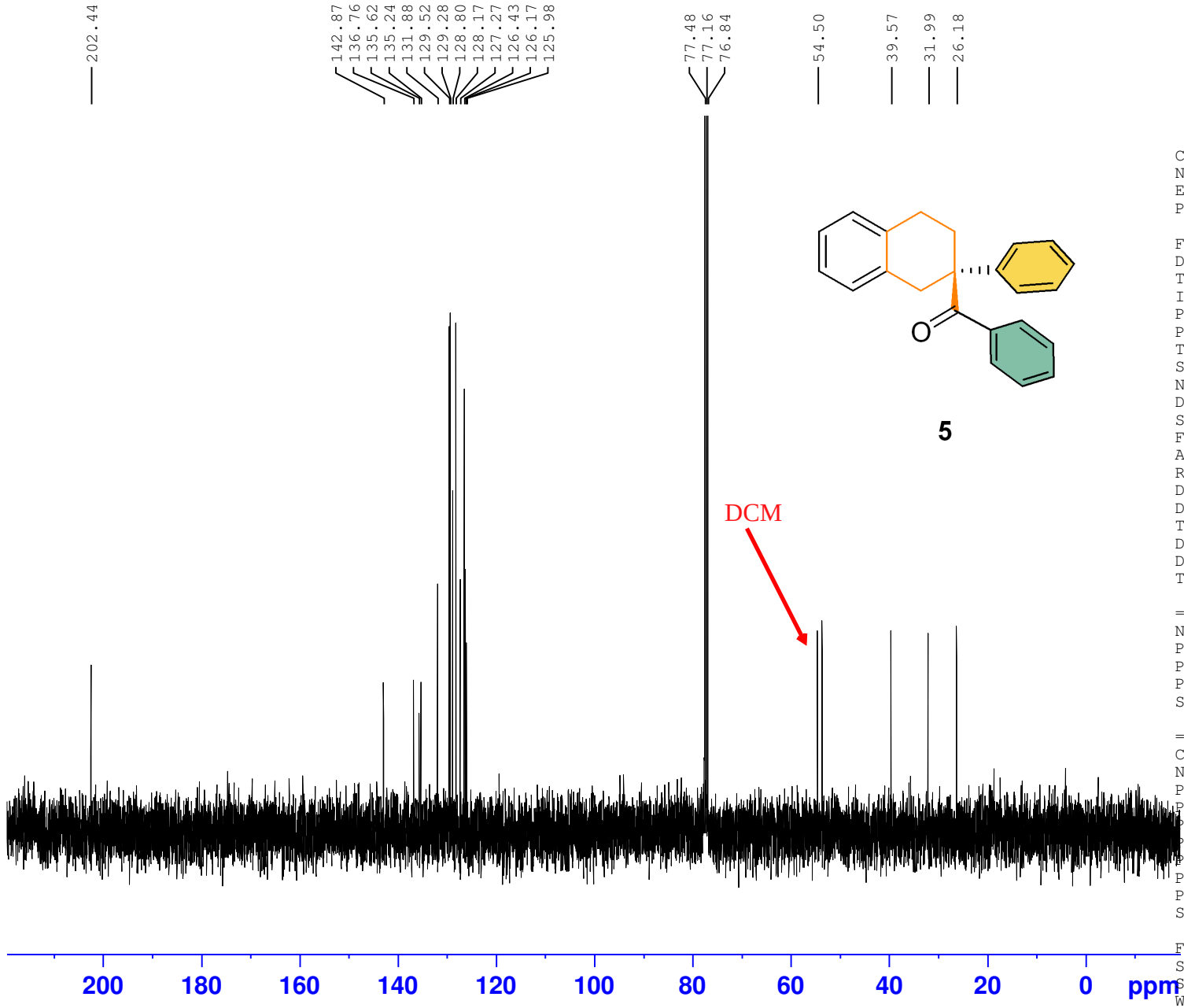

7.493 7.475 7.300 7.297 7.279 7.239 7.234 7.226 7.221 7.208 7.201 7.197 7.182 7.179 7.165 7.157 7.154 7.139 7.115 7.111 7.102 7.093 7.091 7.084 7.064 7.051 7.047 7.033 7.025 7.022 7.018 7.013 7.009 7.003 6.985 6.956 6.952 6.949 6.939 6.934 6.916
3.223 3.069 3.046 3.025 2.831 2.815 2.813 2.797 2.791 2.776 2.768 2.753 2.074 2.058 2.040 2.036 2.024 2.018 0.632 0.612 0.593 0.070 0.050 0.032 0.030
3.223 3.069 3.063 3.046 3.025 3.009 2.846 2.831 2.815 2.813 2.797 2.791 2.776 2.768 2.753 2.738
2.074 2.058 2.040 2.036 2.024 2.018 1.996
H
Et3SiO
4
3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 ppm
1.01 1.00 2.02 1.01
10 9 8 7 6 5 4 3 2 1 ppm
1.04 2.11 10.41 0.99 1.01 1.00 2.02 1.01 9.18 6.14
Current Data Parameters
NAME lsx-2-144-h-fr
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220805
Time 19.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.55
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W
F2 - Processing parameters
SI 65536
SF 400.1300206 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
Current Data Parameters
NAME      lsx-2-144-cc-fr
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20220805
Time                19.25
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    52
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                 196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                  9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                  32768
SF           100.6127737 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



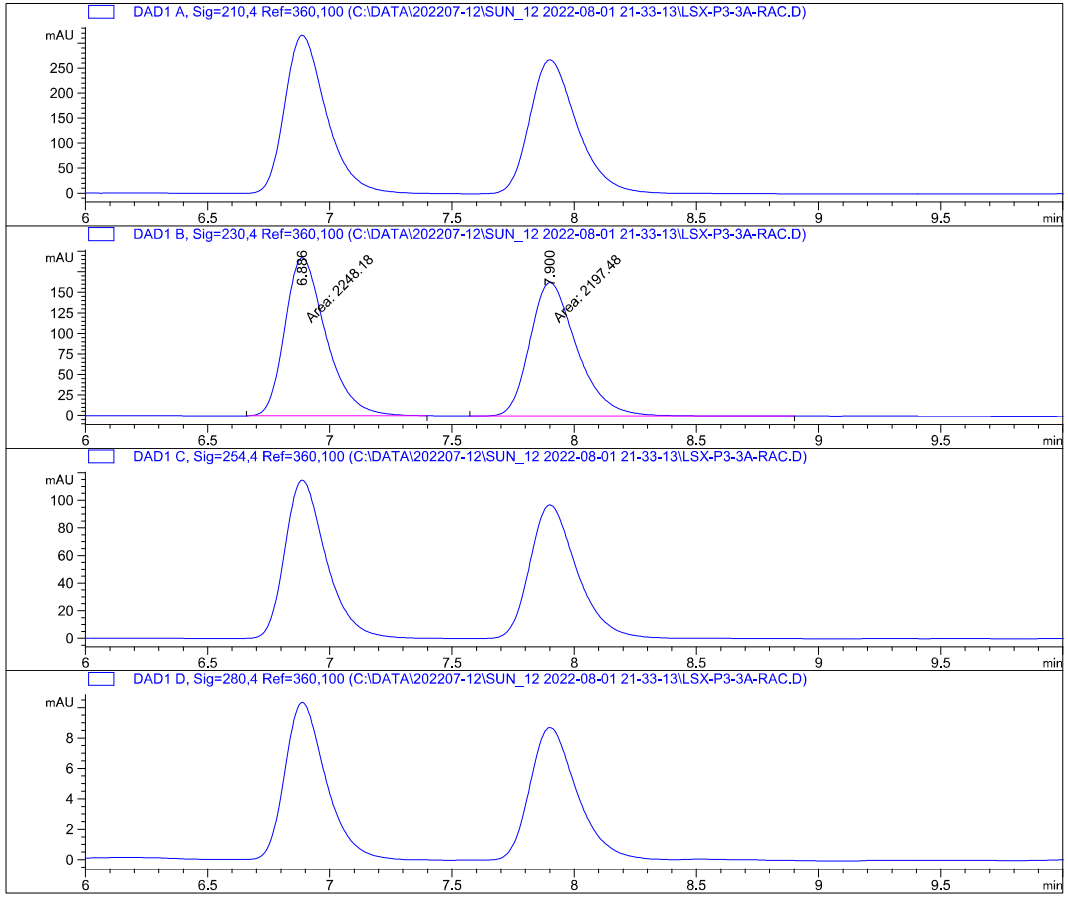

```
Current Data Parameters
NAME      lsx-8-tbaf-h-fr
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20240713
Time                19.24
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                    362
DW                60.800 usec
DE                 6.00 usec
TE                296.7 K
D1           1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.80 usec
PL1                -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF          400.1300141 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```



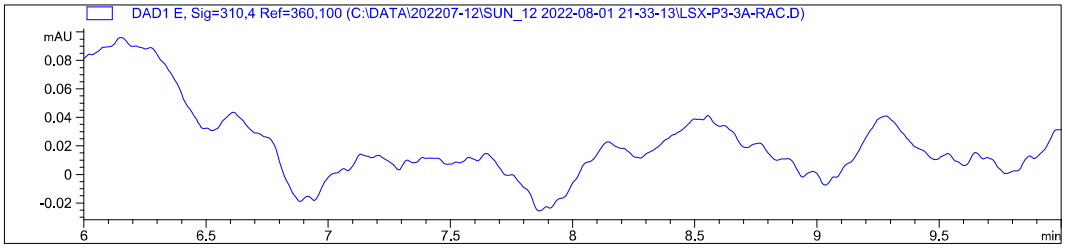

```
Current Data Parameters
NAME      lsx-8-tbaf-c-fr
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20240713
Time               19.36
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  181
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 80.6
DW                20.800 usec
DE                 6.00 usec
TE                297.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.39 dB
PL13               18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127572 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Data File C:\DATA\202207-12\SUN_12 2022-08-01 21-33-13\LSX-P3-3A-RAC.D
Sample Name:

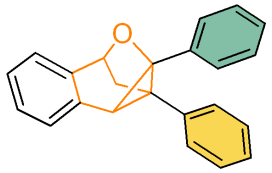
```
==========================================================================
Acq. Operator   :                              Seq. Line :   5
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 1/8/2022 7:59:55 am              Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-08-01 21-33-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 00-13-49\AD-01
                  -30-0.5.M (Sequence Method)
Last changed    : 13/3/2024 6:46:32 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-08-01 21-33-13\LSX-P3-3A-RAC.D
Sample Name:



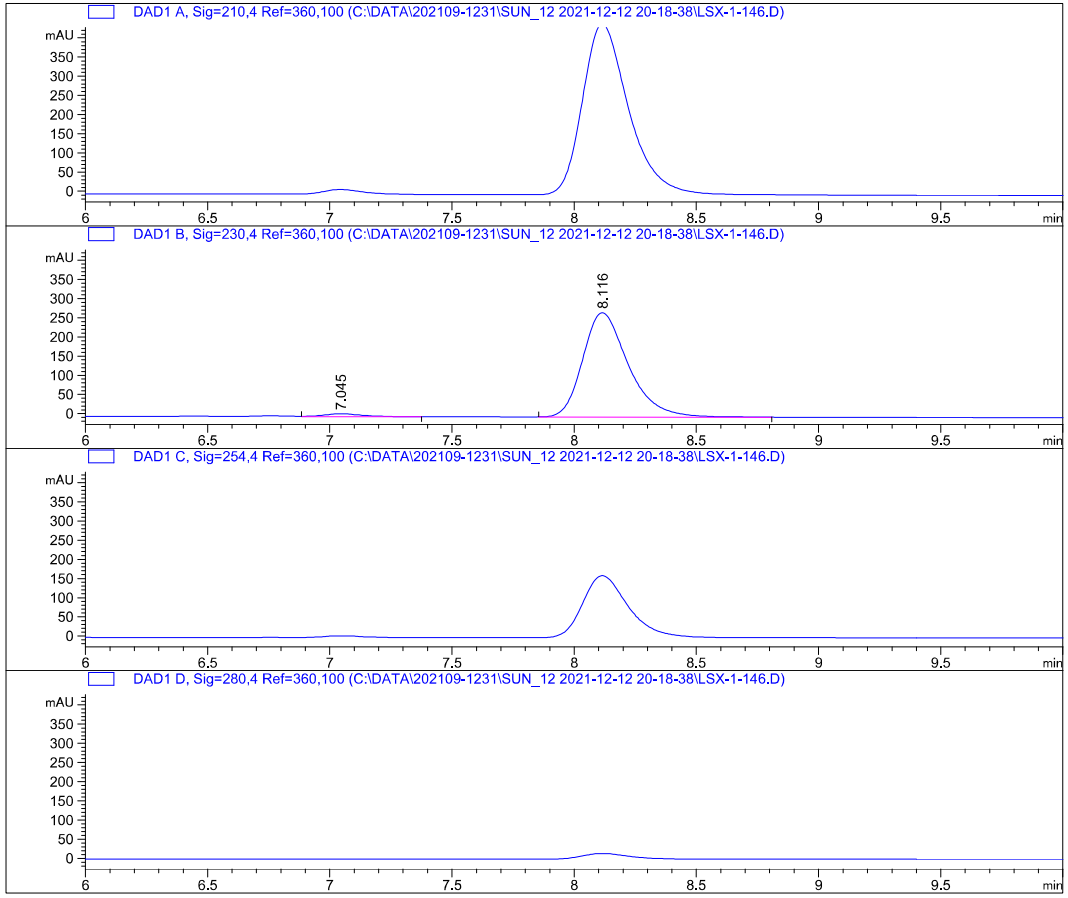

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.886 MM    0.1945 2248.17627  192.65378  50.5702
   2   7.900 MM    0.2246 2197.47681  163.04517  49.4298

Totals :                  4445.65308  355.69894


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



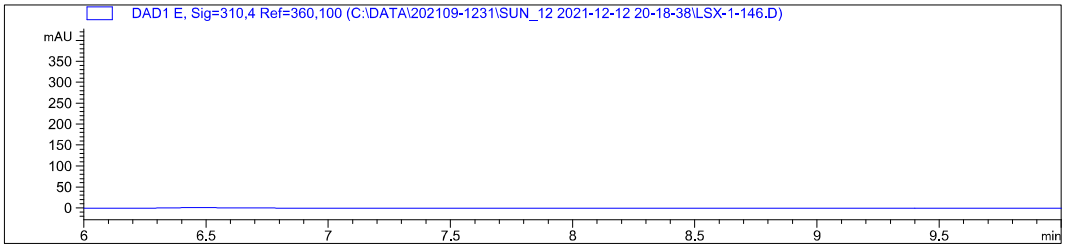
rac-3a

Data File C:\DATA\202109-1231\SUN_12 2021-12-12 20-18-38\LSX-1-146.D
Sample Name:

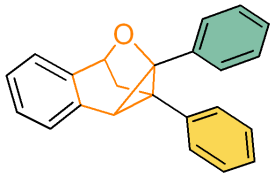
```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location :   41
Injection Date  : 12/12/2021 4:31:25 am          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2021-12-12 20-18-38\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 00-13-49\AD-01
                  -30-0.5.M (Sequence Method)
Last changed    : 13/3/2024 6:43:39 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202109-1231\SUN_12 2021-12-12 20-18-38\LSX-1-146.D
Sample Name:



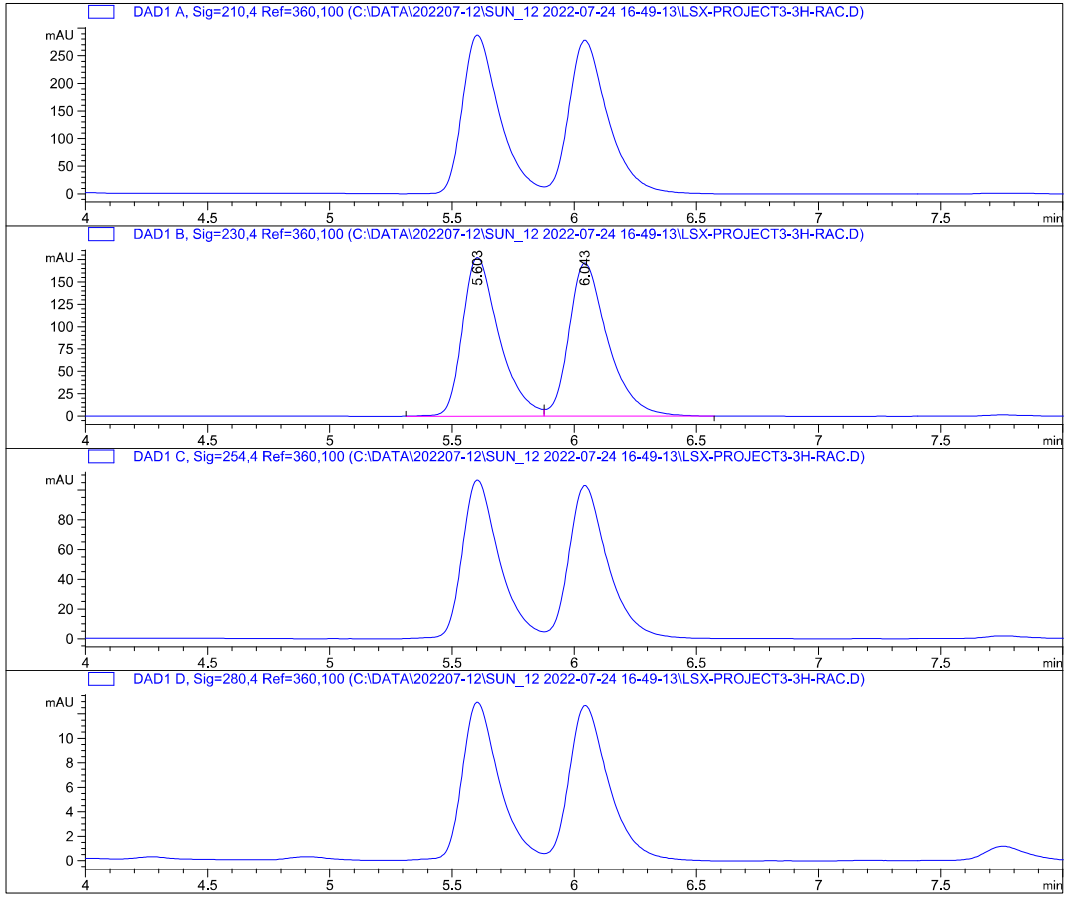

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.045 VB    0.1691   79.63106    7.19634   2.2089
   2   8.116 BB    0.1972 3525.37769  272.00723  97.7911

Totals :                   3605.00874  279.20358


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                    *** End of Report ***
```



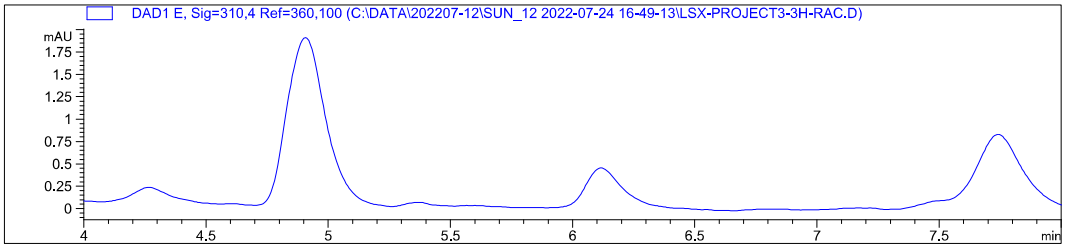
3a

Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3H-RAC.D
Sample Name:

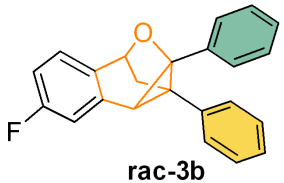
```
==================================================================
Acq. Operator   :                          Seq. Line :   6
Acq. Instrument : Instrument 1              Location :   45
Injection Date  : 24/7/2022 4:06:57 am           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-07-24 16-49-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:28:03 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3H-RAC.D
Sample Name:



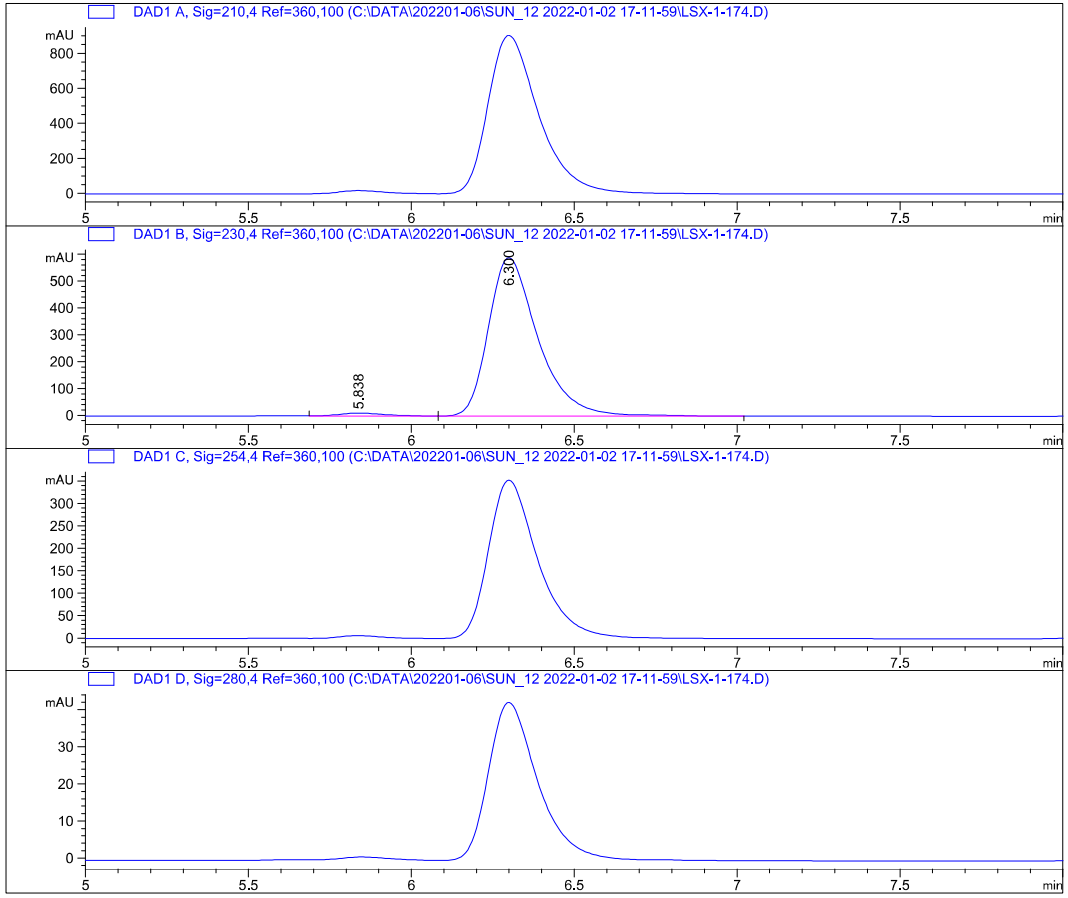

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.603 BV    0.1560 1857.32861  177.67133  49.4033
   2   6.043 VB    0.1653 1902.19141  171.62758  50.5967

Totals :                  3759.52002  349.29890


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                      *** End of Report ***
```



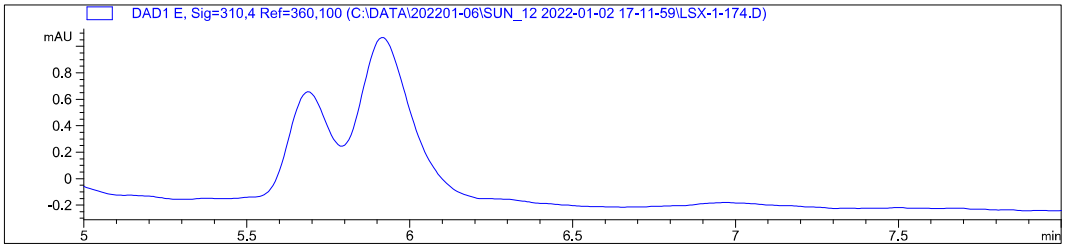
rac-3b

Data File C:\DATA\202201-06\SUN_12 2022-01-02 17-11-59\LSX-1-174.D
Sample Name:

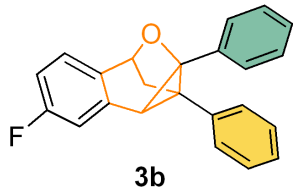
```
==========================================================================
Acq. Operator   :                              Seq. Line :  18
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 2/1/2022 6:09:32 am               Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-01-02 17-11-59\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:29:02 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-01-02 17-11-59\LSX-1-174.D
Sample Name:



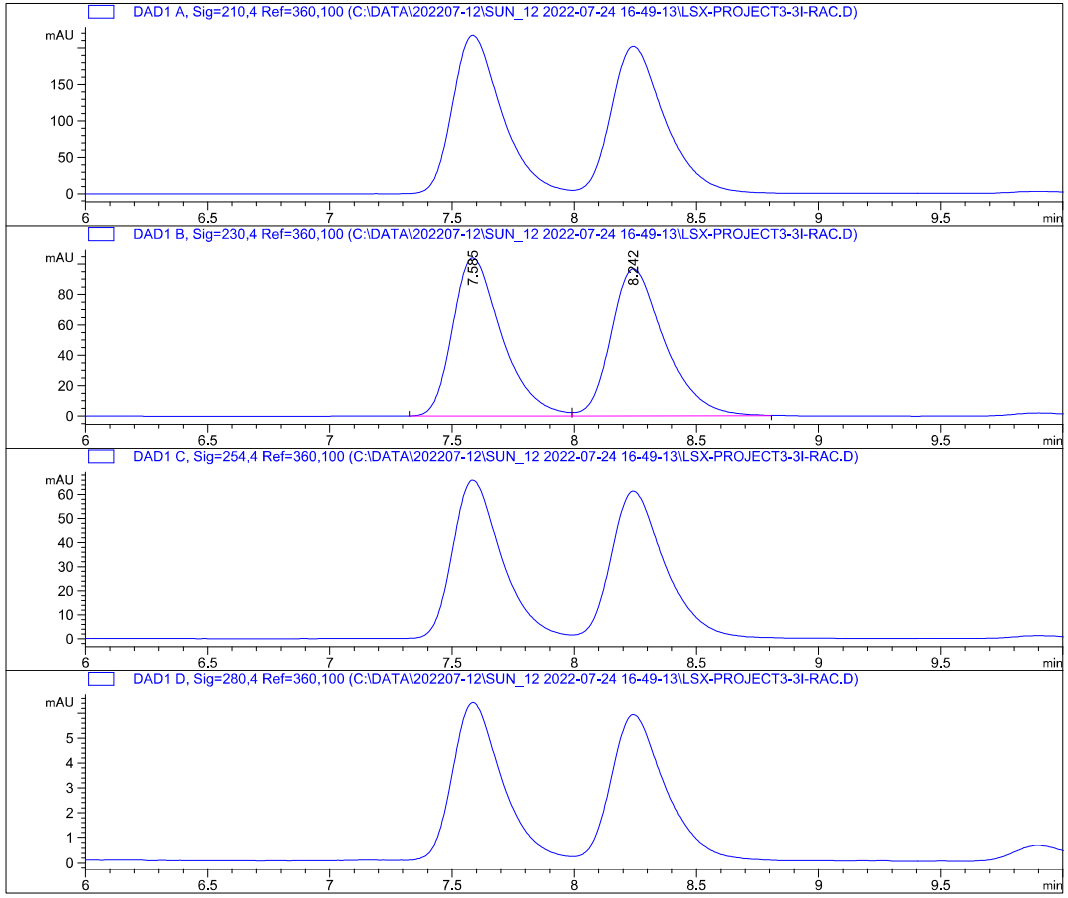

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.838 VV    0.1522  111.83696   11.04016   1.7620
   2   6.300 VB    0.1594 6235.43604  589.52393  98.2380

Totals :                   6347.27299  600.56408



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



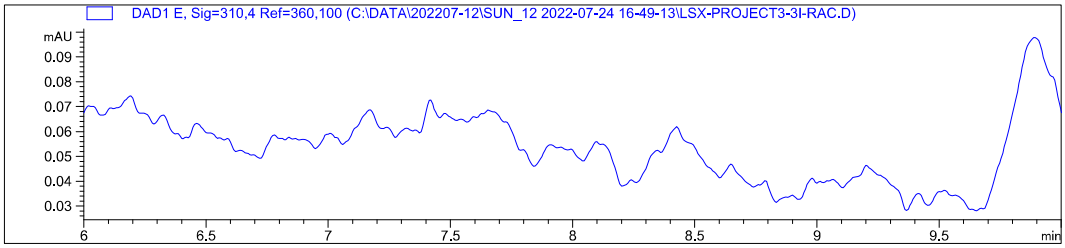
3b

Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3I-RAC.D
Sample Name:

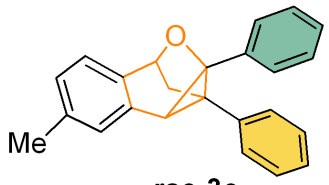
```
==========================================================================
Acq. Operator   :                              Seq. Line :   7
Acq. Instrument : Instrument 1                  Location :   46
Injection Date  : 24/7/2022 4:37:58 am             Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-07-24 16-49-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:32:00 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3I-RAC.D
Sample Name:



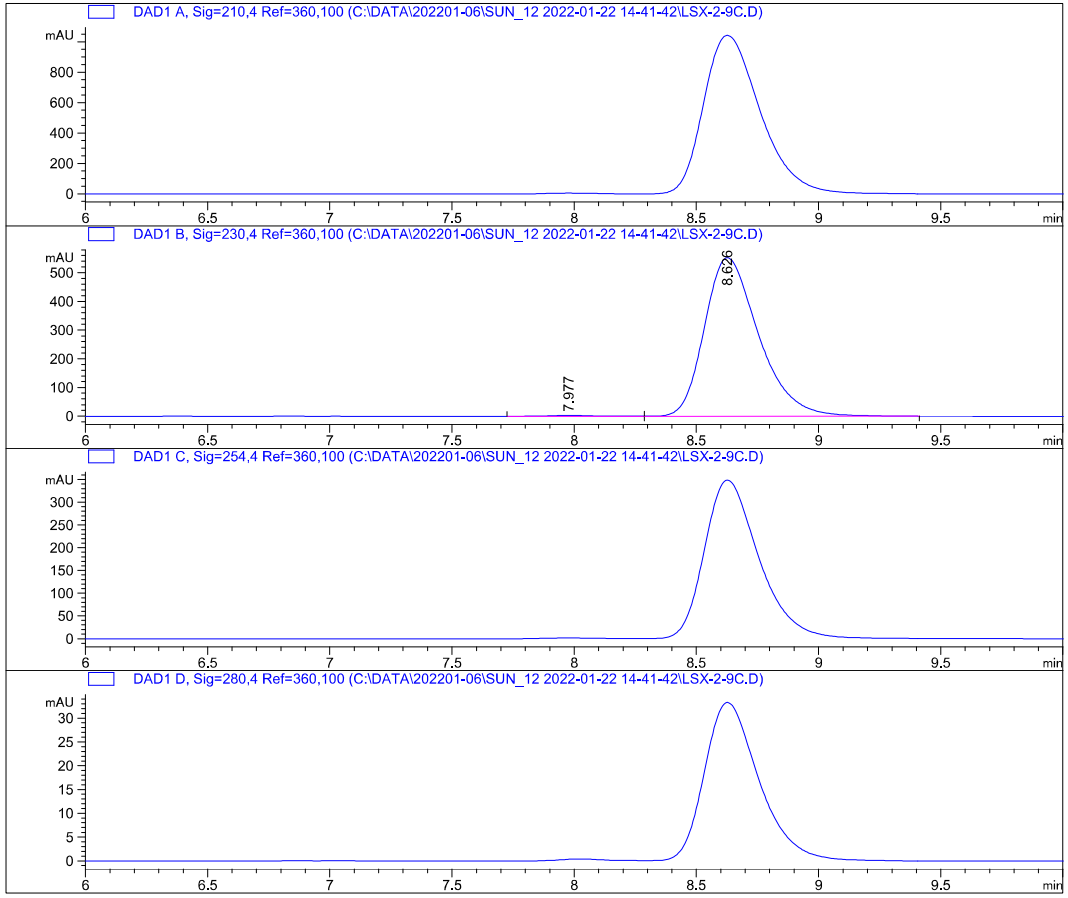

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.585 BV    0.2117 1462.05786  104.22356  49.6991
   2   8.242 VB    0.2283 1479.75928   96.82571  50.3009

Totals :                  2941.81714  201.04926



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



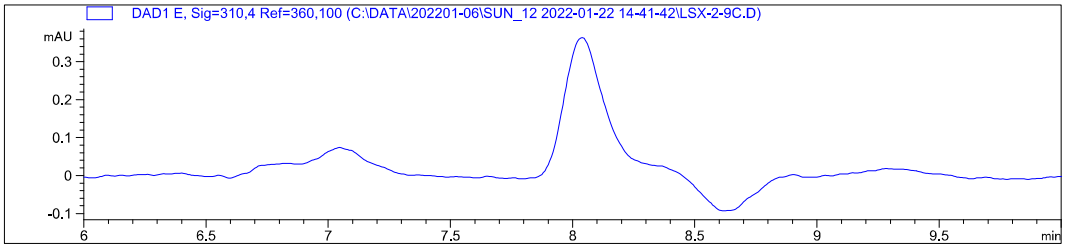
rac-3c

Data File C:\DATA\202201-06\SUN_12 2022-01-22 14-41-42\LSX-2-9C.D
Sample Name:

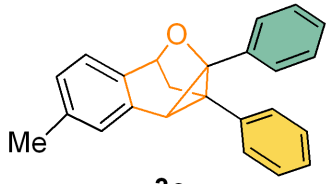
```
==========================================================================
Acq. Operator   :                              Seq. Line :   4
Acq. Instrument : Instrument 1                  Location :   43
Injection Date  : 21/1/2022 11:56:27 pm             Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-01-22 14-41-42\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:32:00 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-01-22 14-41-42\LSX-2-9C.D
Sample Name:



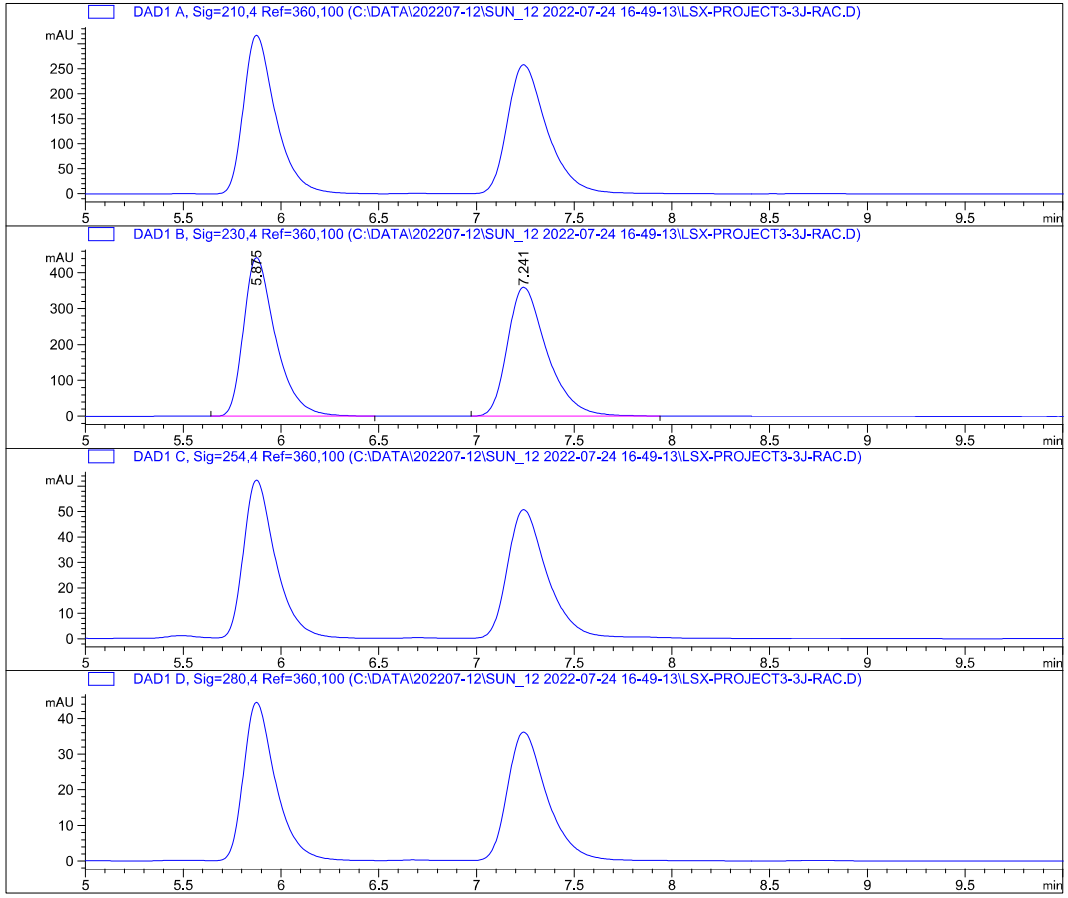

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.977 BV    0.2237   41.06731    2.79093   0.4792
   2   8.626 VB    0.2339 8529.00488  553.08282  99.5208

Totals :                   8570.07219  555.87375



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



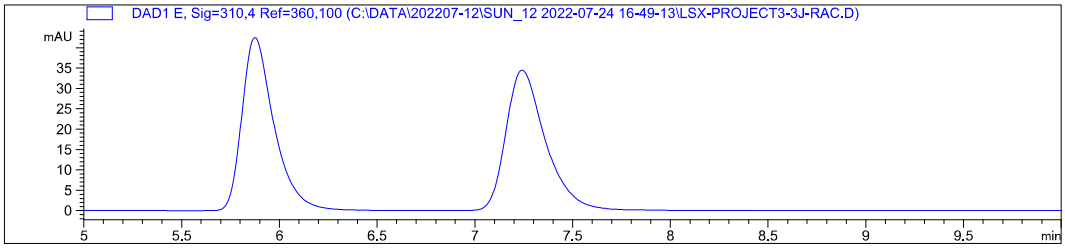
3c

Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3J-RAC.D
Sample Name:

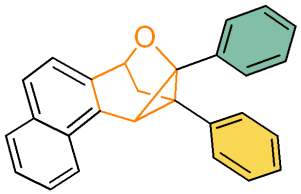
```
==================================================================
Acq. Operator   :                          Seq. Line :   8
Acq. Instrument : Instrument 1              Location :   47
Injection Date  : 24/7/2022 5:08:58 am          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-07-24 16-49-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:34:10 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3J-RAC.D
Sample Name:



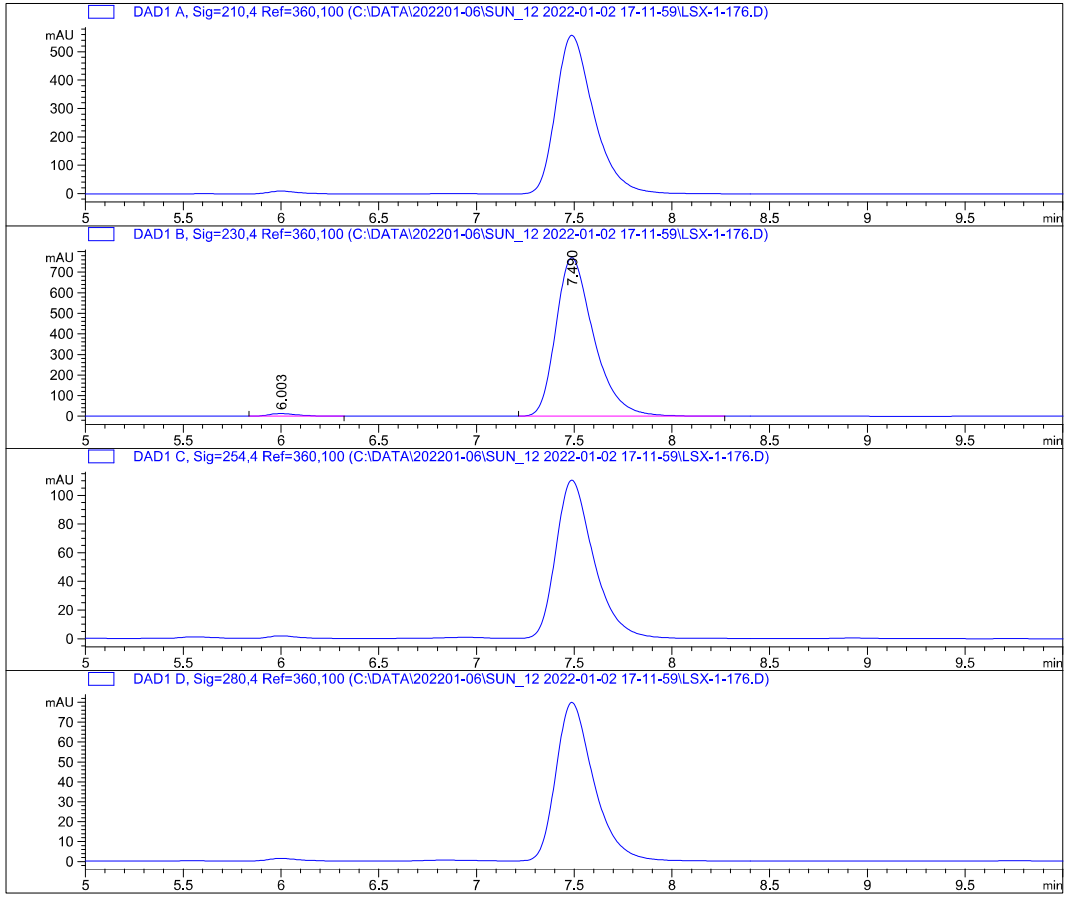

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.875 VB    0.1710 5037.94092  441.99258  49.9651
   2   7.241 BB    0.2118 5044.97656  359.28168  50.0349

Totals :                  1.00829e4   801.27426



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                     *** End of Report ***
```



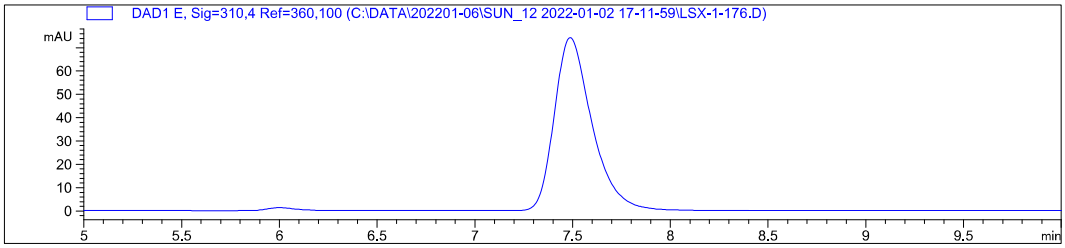
rac-3d

Data File C:\DATA\202201-06\SUN_12 2022-01-02 17-11-59\LSX-1-176.D
Sample Name:

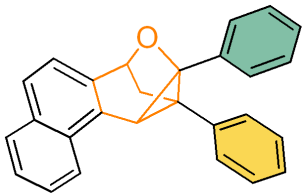
```
==========================================================================
Acq. Operator   :                              Seq. Line :  19
Acq. Instrument : Instrument 1                  Location :   42
Injection Date  : 2/1/2022 6:40:32 am               Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-01-02 17-11-59\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:37:58 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-01-02 17-11-59\LSX-1-176.D
Sample Name:



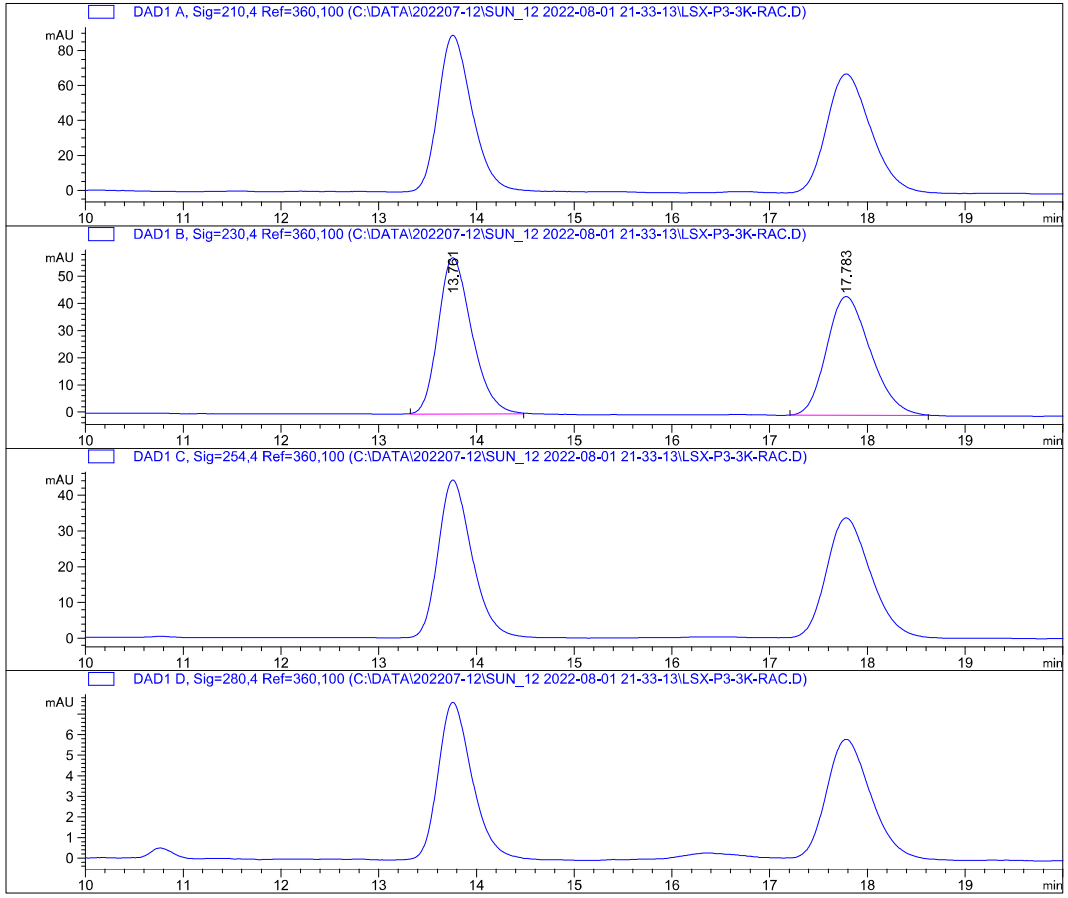

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.003 BB    0.1590  135.40482   12.83902   1.2870
   2   7.490 BB    0.2032 1.03853e4   770.76685  98.7130

Totals :                   1.05207e4   783.60586



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



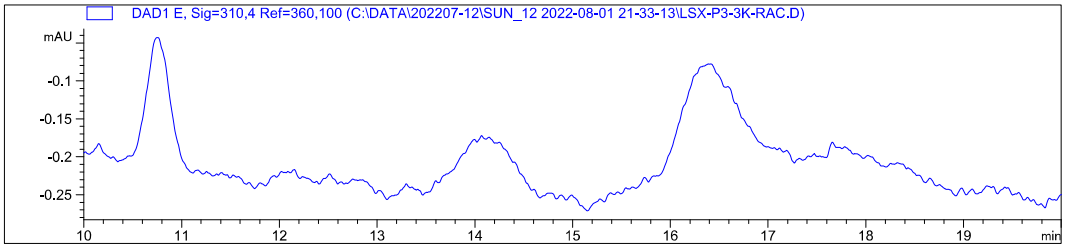
3d

Data File C:\DATA\202207-12\SUN_12 2022-08-01 21-33-13\LSX-P3-3K-RAC.D
Sample Name:

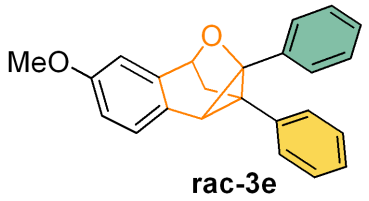
```
==========================================================================
Acq. Operator   :                              Seq. Line :   7
Acq. Instrument : Instrument 1                  Location :   44
Injection Date  : 1/8/2022 9:01:54 am              Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-08-01 21-33-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 00-13-49\AD-01
                  -30-0.5.M (Sequence Method)
Last changed    : 13/3/2024 6:50:29 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-08-01 21-33-13\LSX-P3-3K-RAC.D
Sample Name:



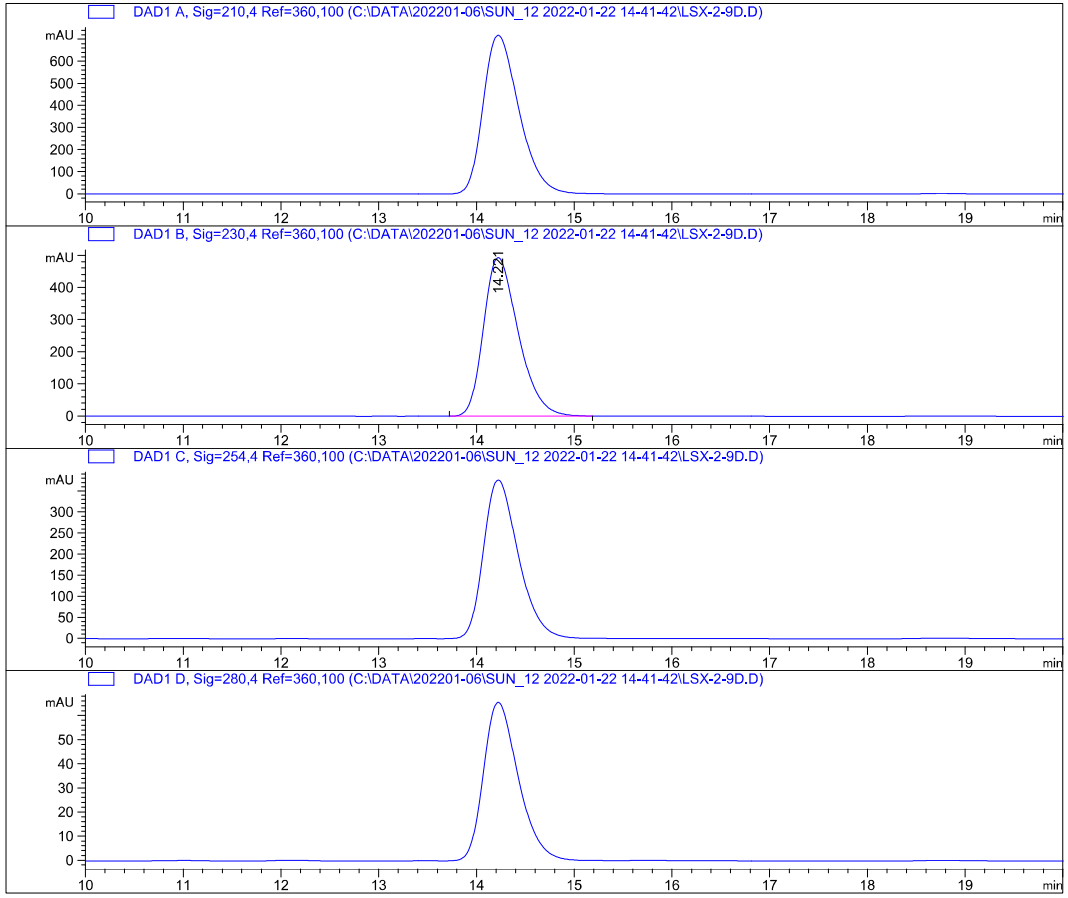

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.761 BB    0.3678 1380.30212   57.54430  50.2088
   2  17.783 BB    0.4792 1368.82336   43.72640  49.7912

Totals :                  2749.12549  101.27070



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



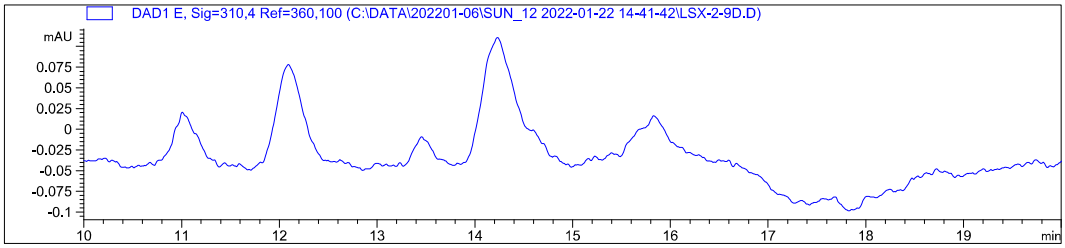
rac-3e

Data File C:\DATA\202201-06\SUN_12 2022-01-22 14-41-42\LSX-2-9D.D
Sample Name:

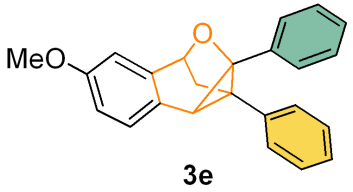
```
==========================================================================
Acq. Operator   :                              Seq. Line :   5
Acq. Instrument : Instrument 1                  Location :   44
Injection Date  : 22/1/2022 12:27:26 am            Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-01-22 14-41-42\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:39:15 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-01-22 14-41-42\LSX-2-9D.D
Sample Name:



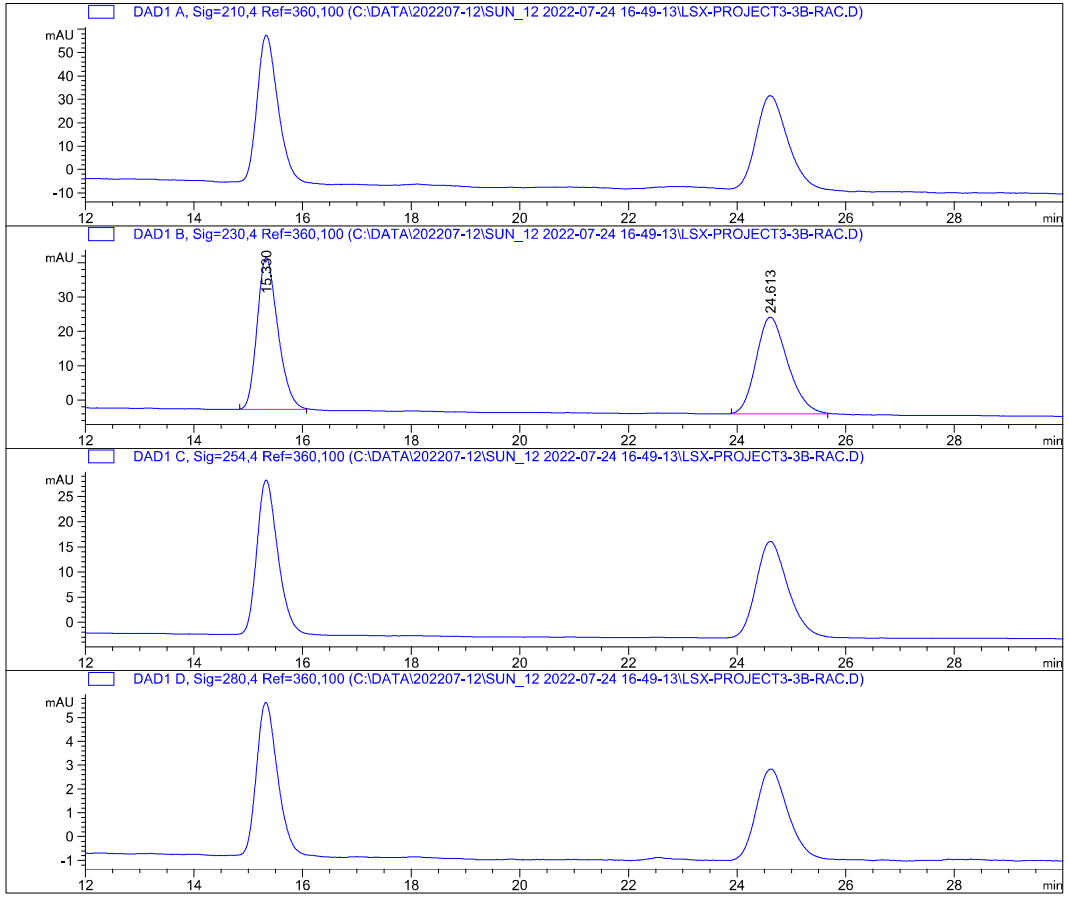

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.221 BB    0.3809 1.22079e4   493.01736 100.0000

Totals :                  1.22079e4   493.01736


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



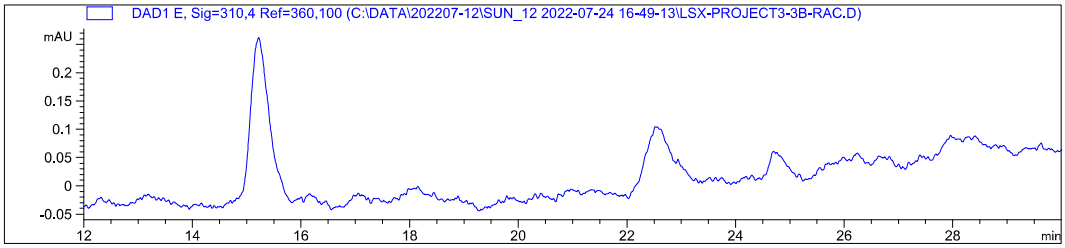
3e

Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3B-RAC.D
Sample Name:

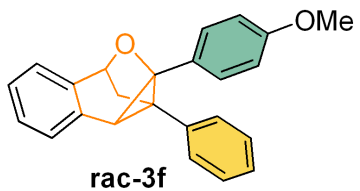
```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 24/7/2022 2:03:03 am             Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-07-24 16-49-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 00-13-49\AD-01
                  -30-0.5.M (Sequence Method)
Last changed    : 13/3/2024 6:54:01 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3B-RAC.D
Sample Name:



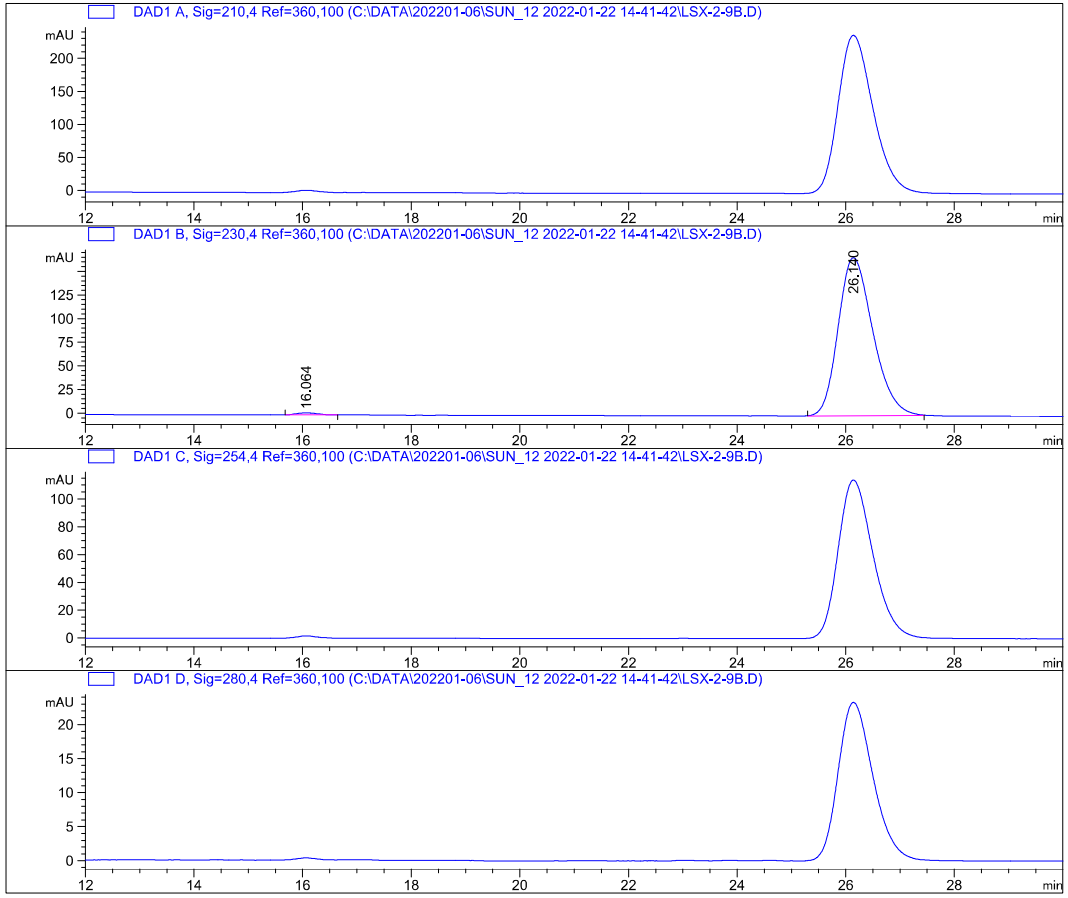

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.330 BB    0.4085 1177.19836   44.22970  50.8037
   2  24.613 BB    0.6081 1139.95337   28.17158  49.1963

Totals :                  2317.15173   72.40128


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



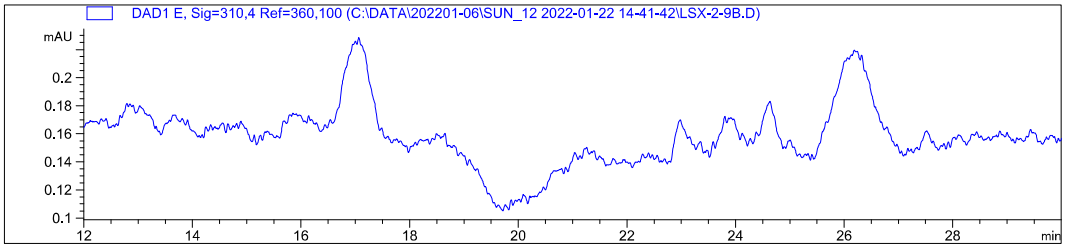
rac-3f

Data File C:\DATA\202201-06\SUN_12 2022-01-22 14-41-42\LSX-2-9B.D
Sample Name:

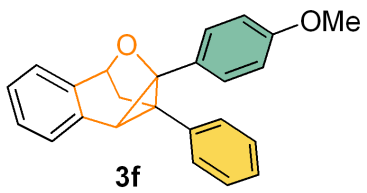
```
==========================================================================
Acq. Operator   :                              Seq. Line :   3
Acq. Instrument : Instrument 1                  Location :   42
Injection Date  : 21/1/2022 11:25:27 pm             Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-01-22 14-41-42\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 00-13-49\AD-01
                  -30-0.5.M (Sequence Method)
Last changed    : 13/3/2024 6:54:01 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-01-22 14-41-42\LSX-2-9B.D
Sample Name:



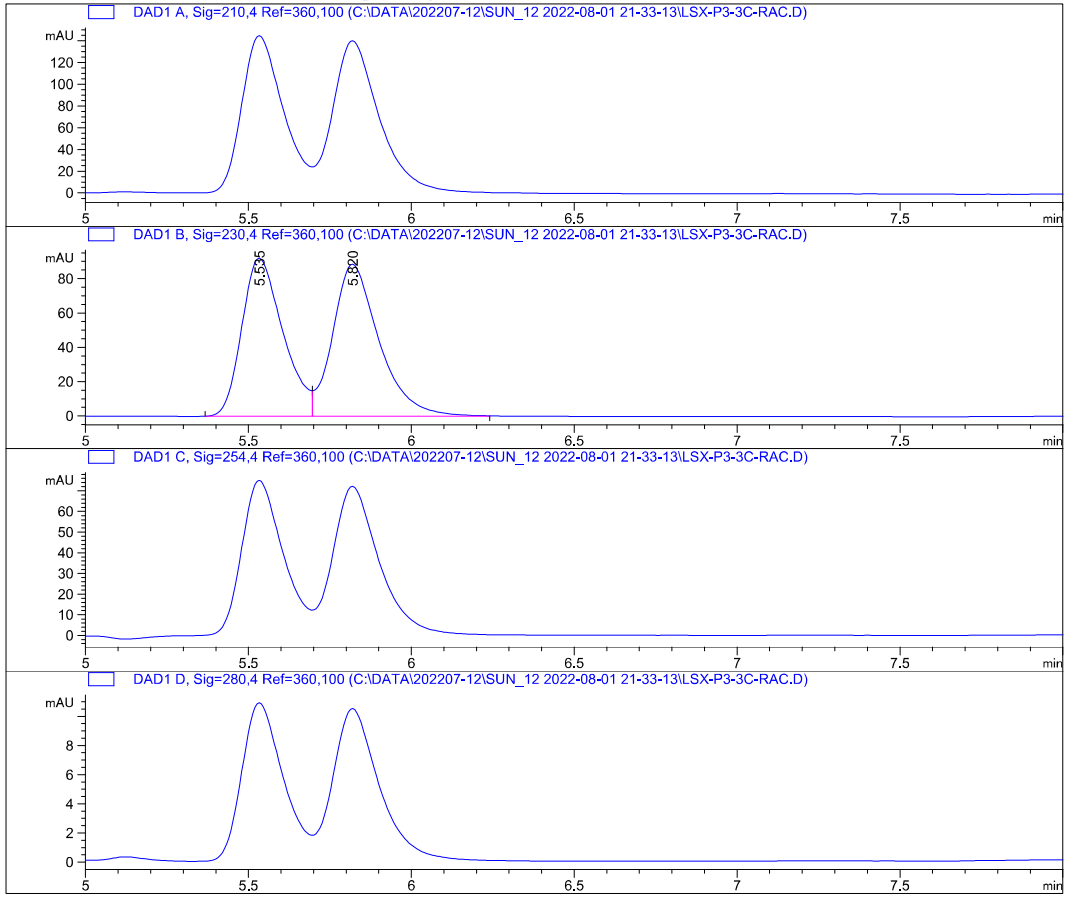

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.064 BB    0.3842   54.60185    2.13649   0.7303
   2  26.140 BB    0.6878 7422.14063  167.23262  99.2697

Totals :                  7476.74247  169.36911


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



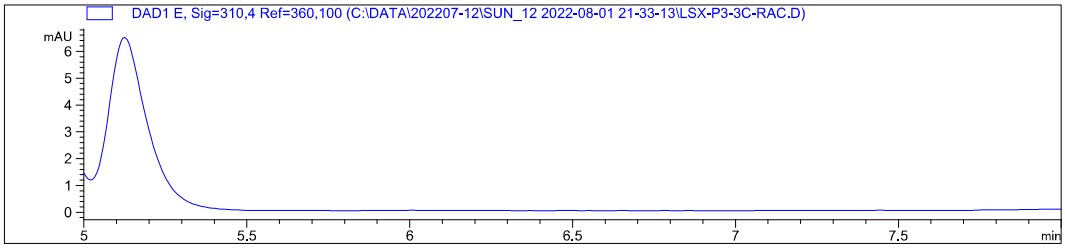
3f

Data File C:\DATA\202207-12\SUN_12 2022-08-01 21-33-13\LSX-P3-3C-RAC.D
Sample Name:

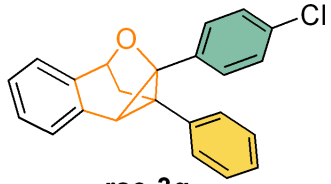
```
==========================================================================
Acq. Operator   :                                Seq. Line :   6
Acq. Instrument : Instrument 1                    Location :   43
Injection Date  : 1/8/2022 8:30:54 am                 Inj :   1
                                                Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-08-01 21-33-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 00-13-49\AD-01
                  -30-0.5.M (Sequence Method)
Last changed    : 13/3/2024 6:49:02 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-08-01 21-33-13\LSX-P3-3C-RAC.D
Sample Name:



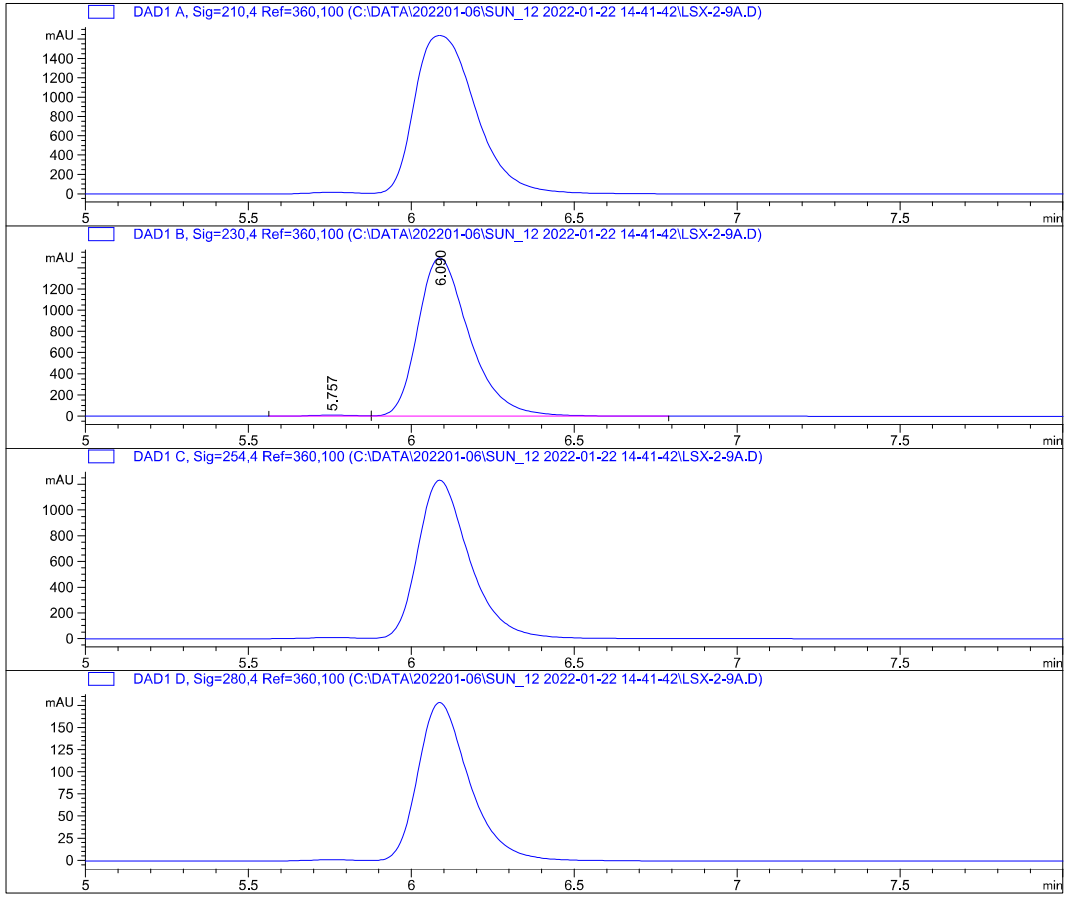

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.535 BV    0.1323  808.85852   92.28972  47.9678
   2   5.820 VB    0.1474  877.39423   88.69310  52.0322

Totals :                  1686.25275  180.98282


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



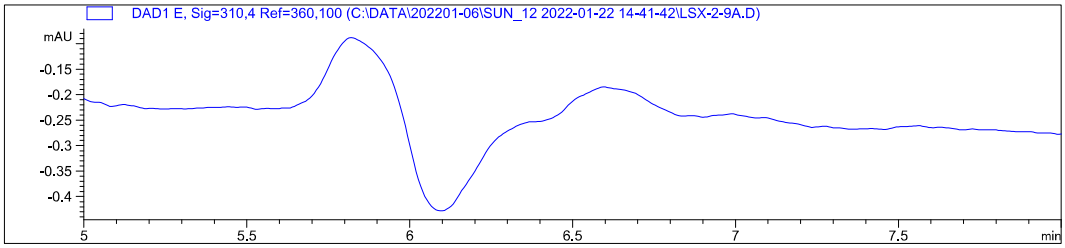
rac-3g

Data File C:\DATA\202201-06\SUN_12 2022-01-22 14-41-42\LSX-2-9A.D
Sample Name:

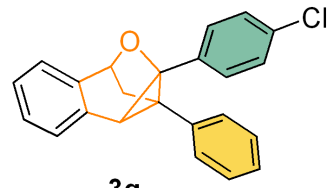
```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 21/1/2022 10:54:29 pm             Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-01-22 14-41-42\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 00-13-49\AD-01
                  -30-0.5.M (Sequence Method)
Last changed    : 13/3/2024 6:51:40 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-01-22 14-41-42\LSX-2-9A.D
Sample Name:



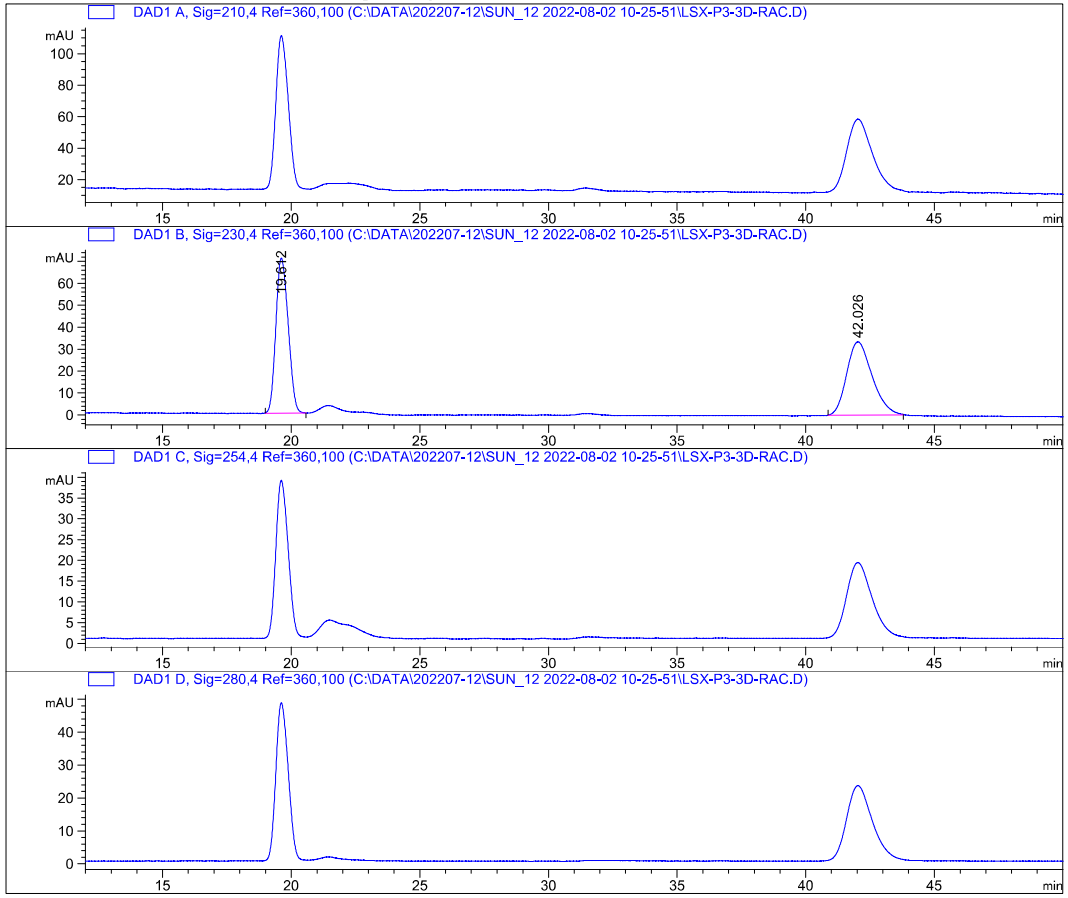

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.757 BV    0.1488  108.80631   11.45479   0.6537
   2   6.090 VB    0.1666 1.65353e4  1500.02625  99.3463

Totals :                  1.66441e4  1511.48103


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.167 BB    0.1859   18.95916    1.51598 100.0000

Totals :                    18.95916    1.51598

==========================================================================
                        *** End of Report ***
```



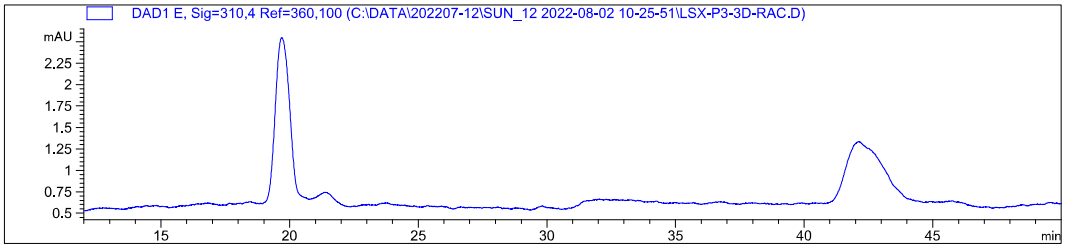
3g

Data File C:\DATA\202207-12\SUN_12 2022-08-02 10-25-51\LSX-P3-3D-RAC.D
Sample Name:

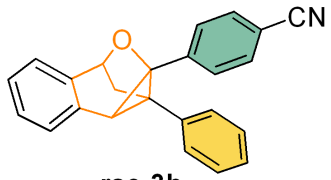
```
==========================================================================
Acq. Operator   :                              Seq. Line :   3
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 1/8/2022 8:09:45 pm               Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-08-02 10-25-51\IC-05-60.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 00-13-49\AD-01
                  -30-0.5.M (Sequence Method)
Last changed    : 13/3/2024 6:59:52 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-08-02 10-25-51\LSX-P3-3D-RAC.D
Sample Name:



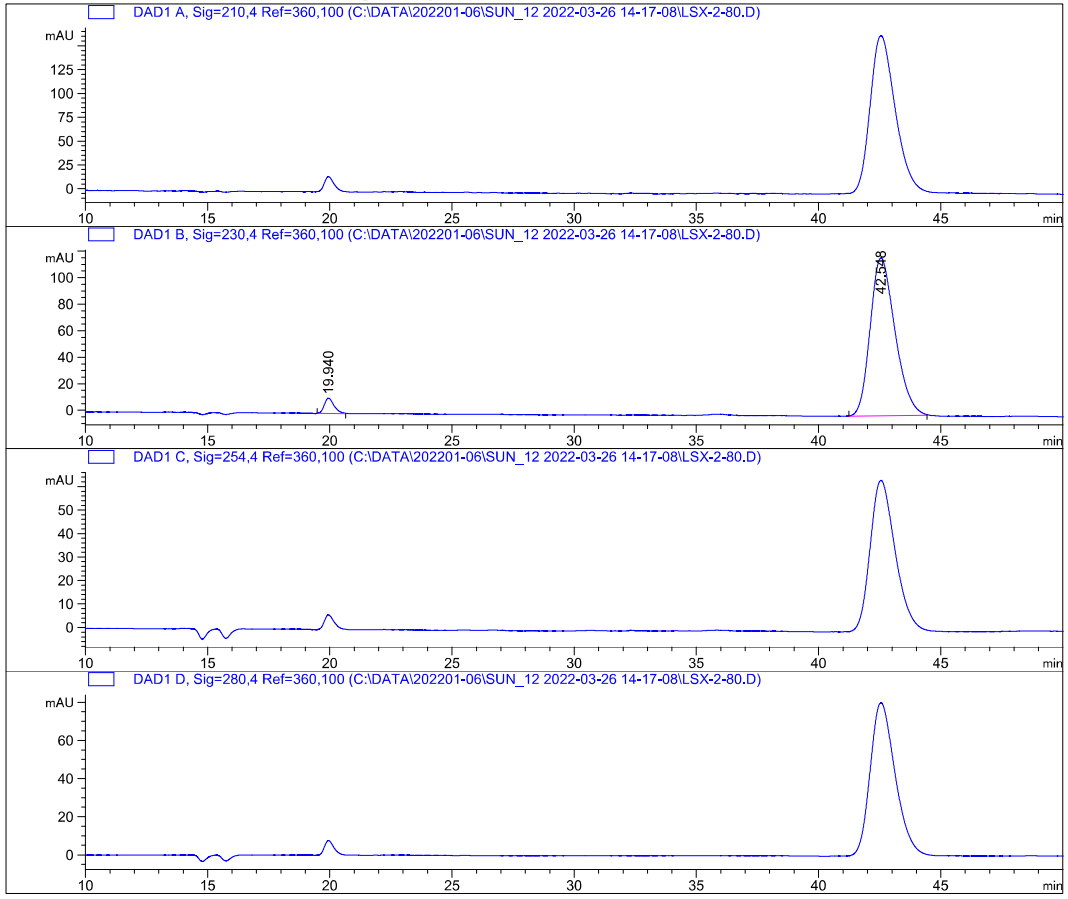

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  19.612 BB    0.5332 2361.09155   70.76770  50.6720
   2  42.026 BB    1.0080 2298.46875   33.43648  49.3280

Totals :                  4659.56030  104.20418


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



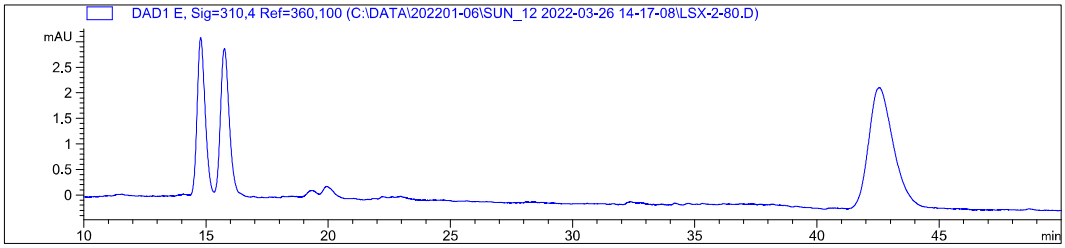
rac-3h

Data File C:\DATA\202201-06\SUN_12 2022-03-26 14-17-08\LSX-2-80.D
Sample Name:

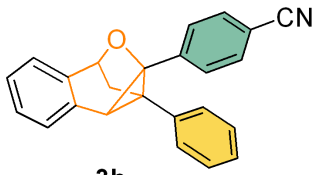
```
==================================================================
Acq. Operator   :                          Seq. Line :  17
Acq. Instrument : Instrument 1              Location :  43
Injection Date  : 26/3/2022 3:46:18 am           Inj :  1
                                        Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 8.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-03-26 14-17-08\IC-05-60.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:13:55 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-03-26 14-17-08\LSX-2-80.D
Sample Name:



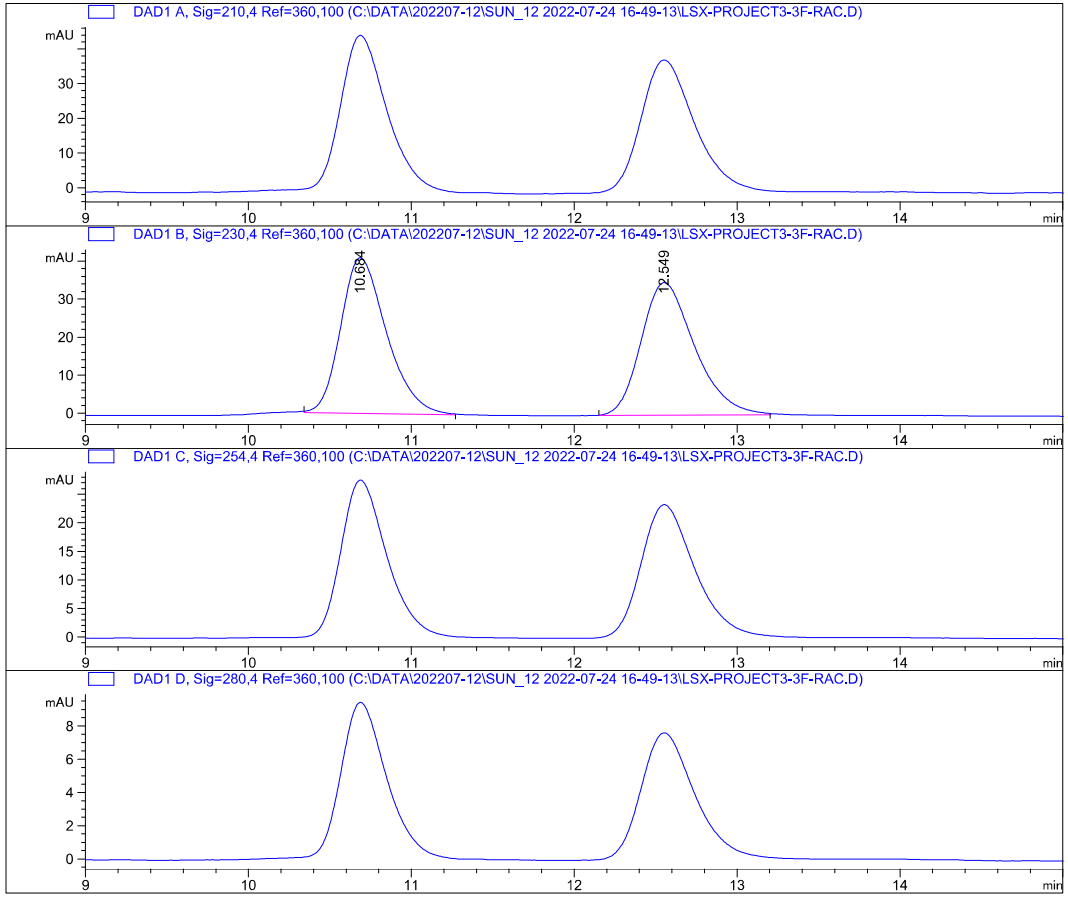

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  19.940 BB    0.4227  313.61639   11.48019   3.5907
   2  42.548 BB    1.0803 8420.54102  118.88423  96.4093

Totals :                  8734.15741  130.36442


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                      *** End of Report ***
```



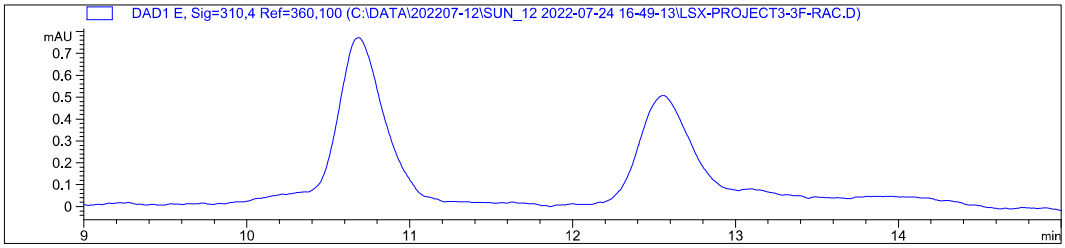
3h

Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3F-RAC.D
Sample Name:

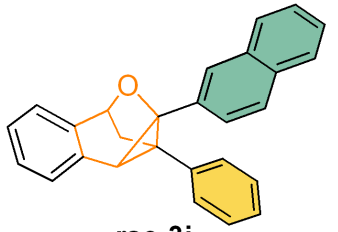
```
==========================================================================
Acq. Operator   :                              Seq. Line :   4
Acq. Instrument : Instrument 1                  Location :   43
Injection Date  : 24/7/2022 3:05:01 am             Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-07-24 16-49-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:20:12 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3F-RAC.D
Sample Name:



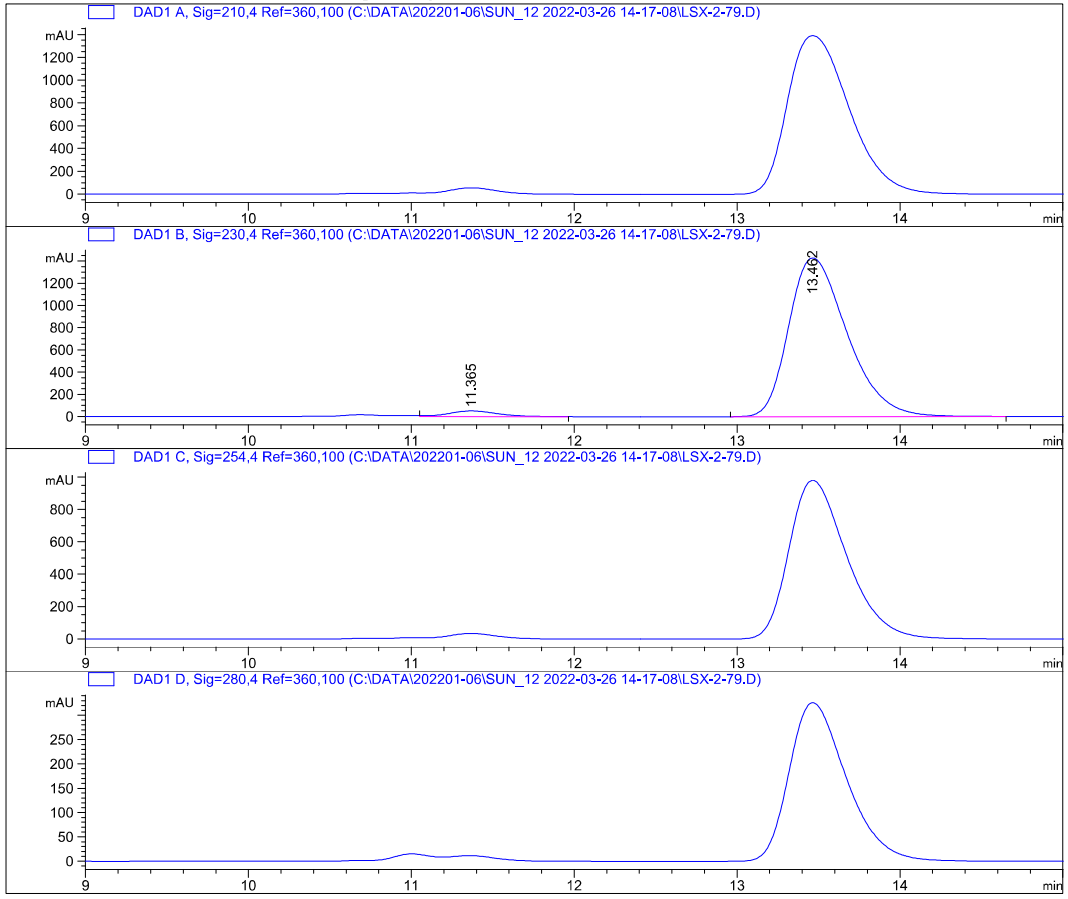

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.684 BB    0.2979  800.22064   40.97282  50.1543
   2  12.549 BB    0.3459  795.29755   34.89804  49.8457

Totals :                  1595.51819   75.87086


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



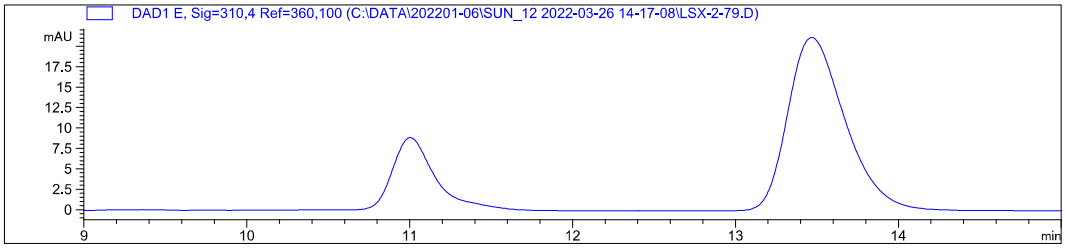
rac-3i

Data File C:\DATA\202201-06\SUN_12 2022-03-26 14-17-08\LSX-2-79.D
Sample Name:

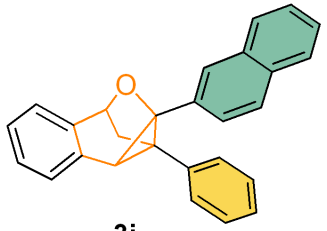
```
==========================================================================
Acq. Operator   :                              Seq. Line :  11
Acq. Instrument : Instrument 1                  Location :  42
Injection Date  : 26/3/2022 2:09:47 am             Inj :  1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 8.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-03-26 14-17-08\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:20:12 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-03-26 14-17-08\LSX-2-79.D
Sample Name:



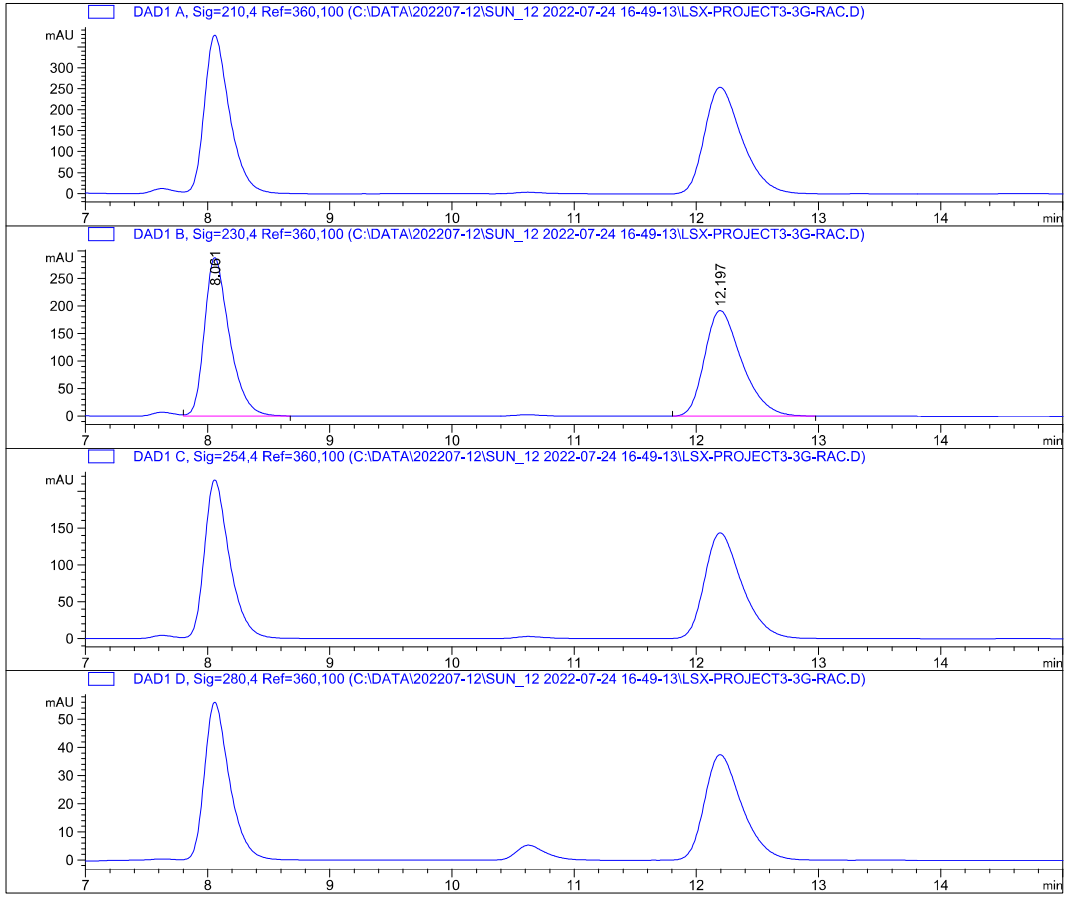

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.365 VB    0.3222 1072.72888   50.84315   2.9248
   2  13.462 BB    0.3867 3.56041e4  1428.71472  97.0752

Totals :                  3.66769e4  1479.55787


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



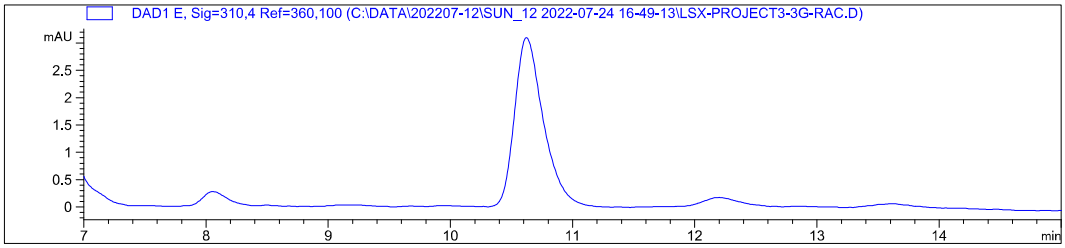
3i

Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3G-RAC.D
Sample Name:

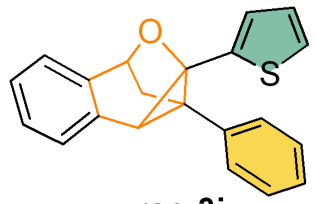
```
==========================================================================
Acq. Operator   :                              Seq. Line :   5
Acq. Instrument : Instrument 1                  Location :   44
Injection Date  : 24/7/2022 3:35:58 am             Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-07-24 16-49-13\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:25:44 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-07-24 16-49-13\LSX-PROJECT3-3G-RAC.D
Sample Name:



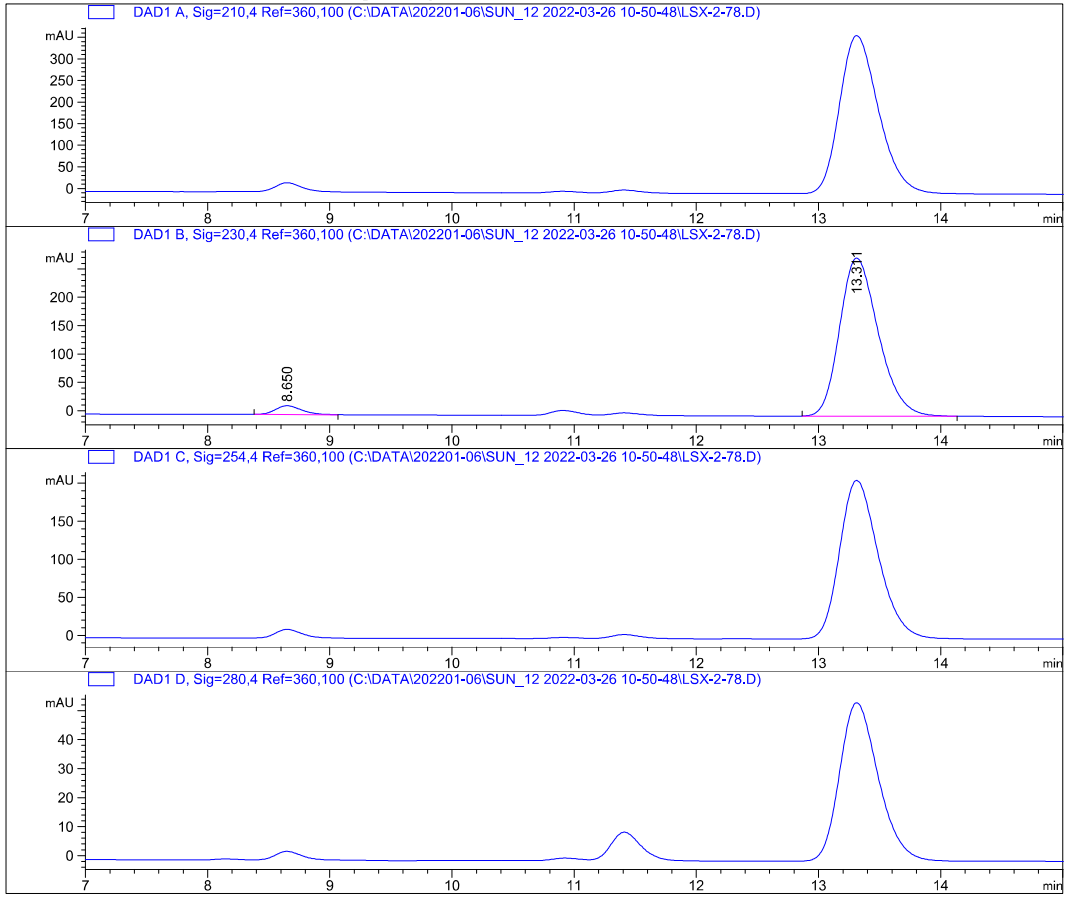

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.061 VB    0.2140 4101.22998  288.21036  50.1711
   2  12.197 BB    0.3213 4073.25879  192.12576  49.8289

Totals :                  8174.48877  480.33612


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



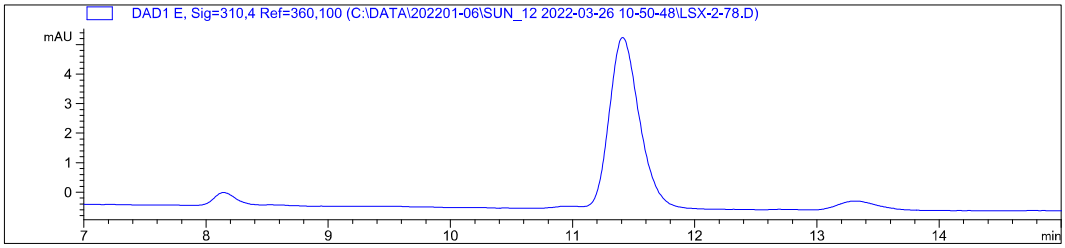
rac-3j

Data File C:\DATA\202201-06\SUN_12 2022-03-26 10-50-48\LSX-2-78.D
Sample Name:

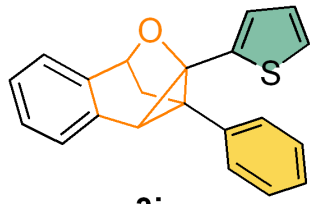
```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 25/3/2022 8:03:36 pm             Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 8.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-03-26 10-50-48\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:25:44 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-03-26 10-50-48\LSX-2-78.D
Sample Name:



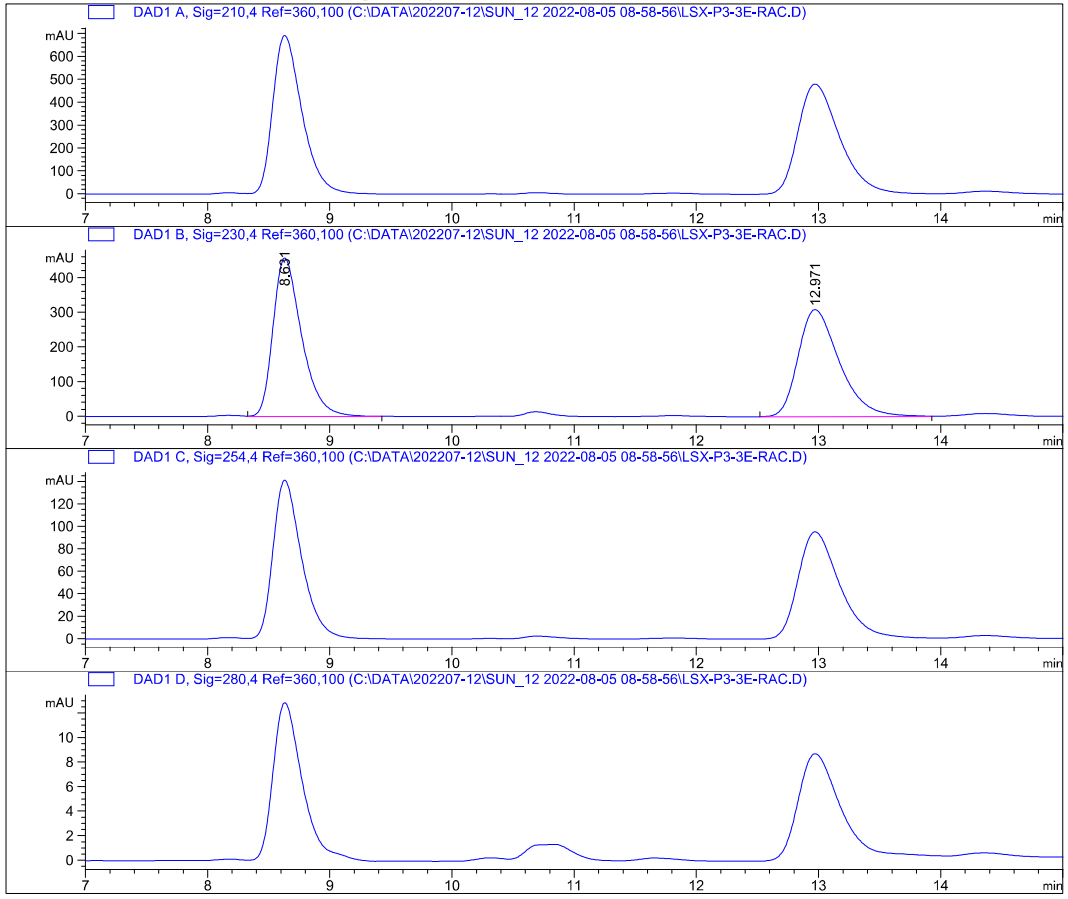

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.650 BB    0.2285  231.77061   15.49835   3.6366
   2  13.311 BB    0.3387 6141.45313  279.10840  96.3634

Totals :                  6373.22374  294.60674



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



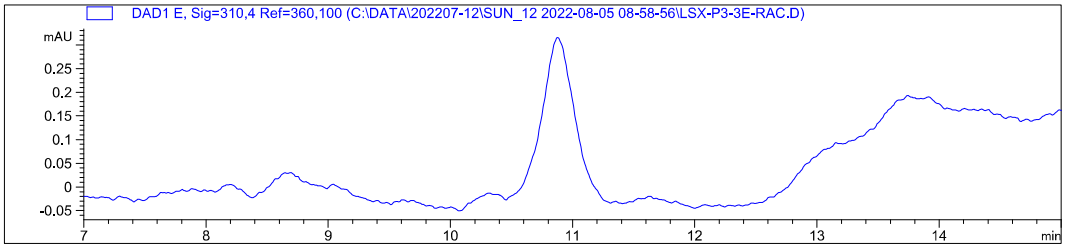
3j

Data File C:\DATA\202207-12\SUN_12 2022-08-05 08-58-56\LSX-P3-3E-RAC.D
Sample Name:

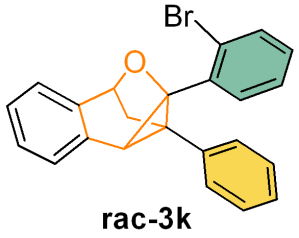
```
==========================================================================
Acq. Operator   :                              Seq. Line :   8
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 4/8/2022 9:02:18 pm               Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 8.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-08-05 08-58-56\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:16:44 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-08-05 08-58-56\LSX-P3-3E-RAC.D
Sample Name:



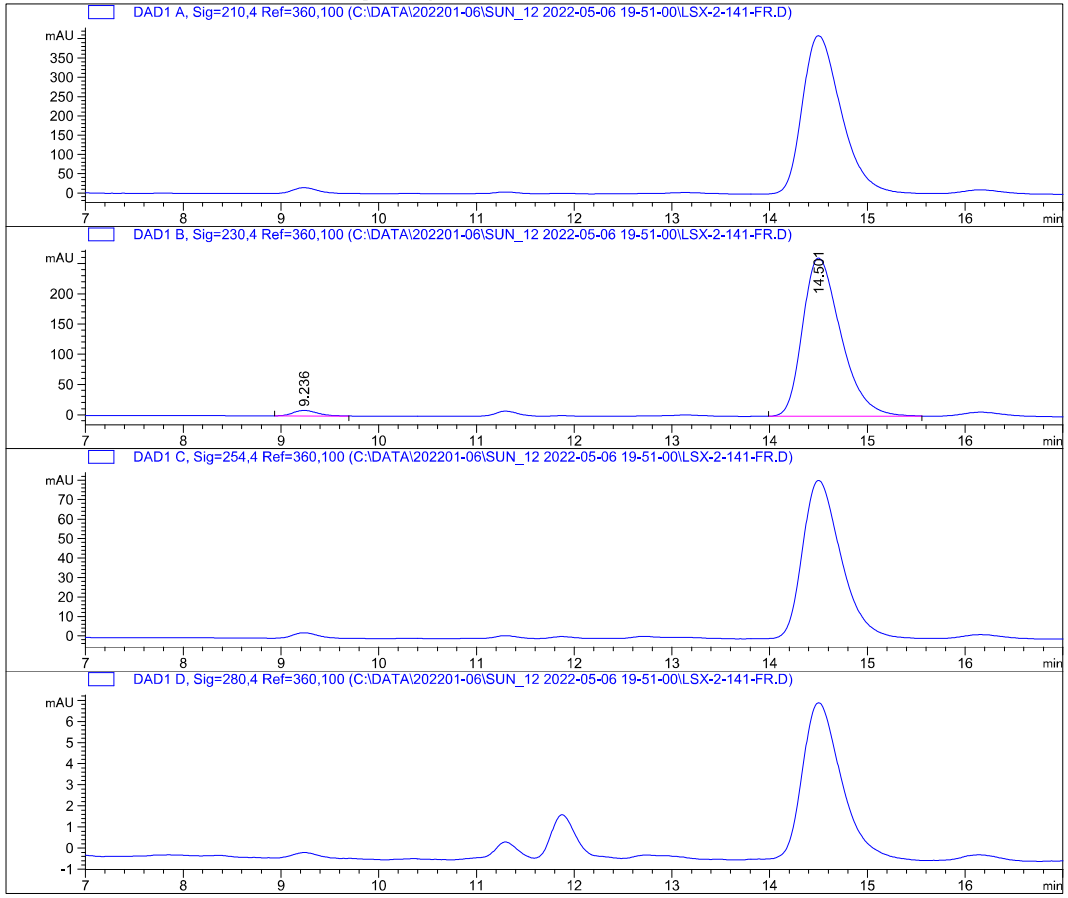

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.631 VB    0.2464 7458.77051  457.08408  50.7257
   2  12.971 BB    0.3602 7245.36279  308.31094  49.2743

Totals :                  1.47041e4   765.39502


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



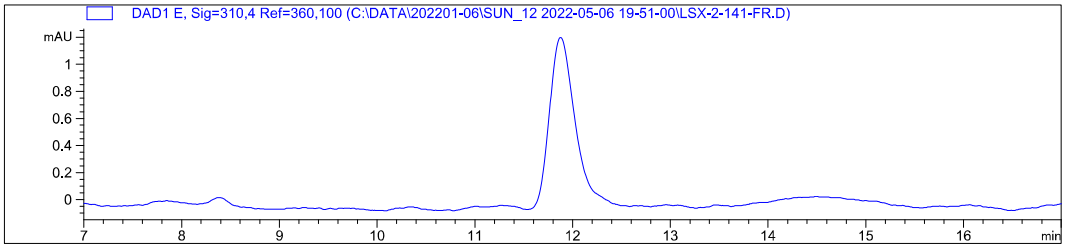
rac-3k

Data File C:\DATA\202201-06\SUN_12 2022-05-06 19-51-00\LSX-2-141-FR.D
Sample Name:

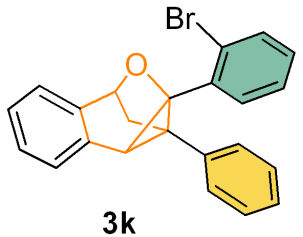
```
==========================================================================
Acq. Operator   :                                Seq. Line :   2
Acq. Instrument : Instrument 1                    Location :   41
Injection Date  : 6/5/2022 5:04:00 am                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-05-06 19-51-00\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:18:07 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-05-06 19-51-00\LSX-2-141-FR.D
Sample Name:



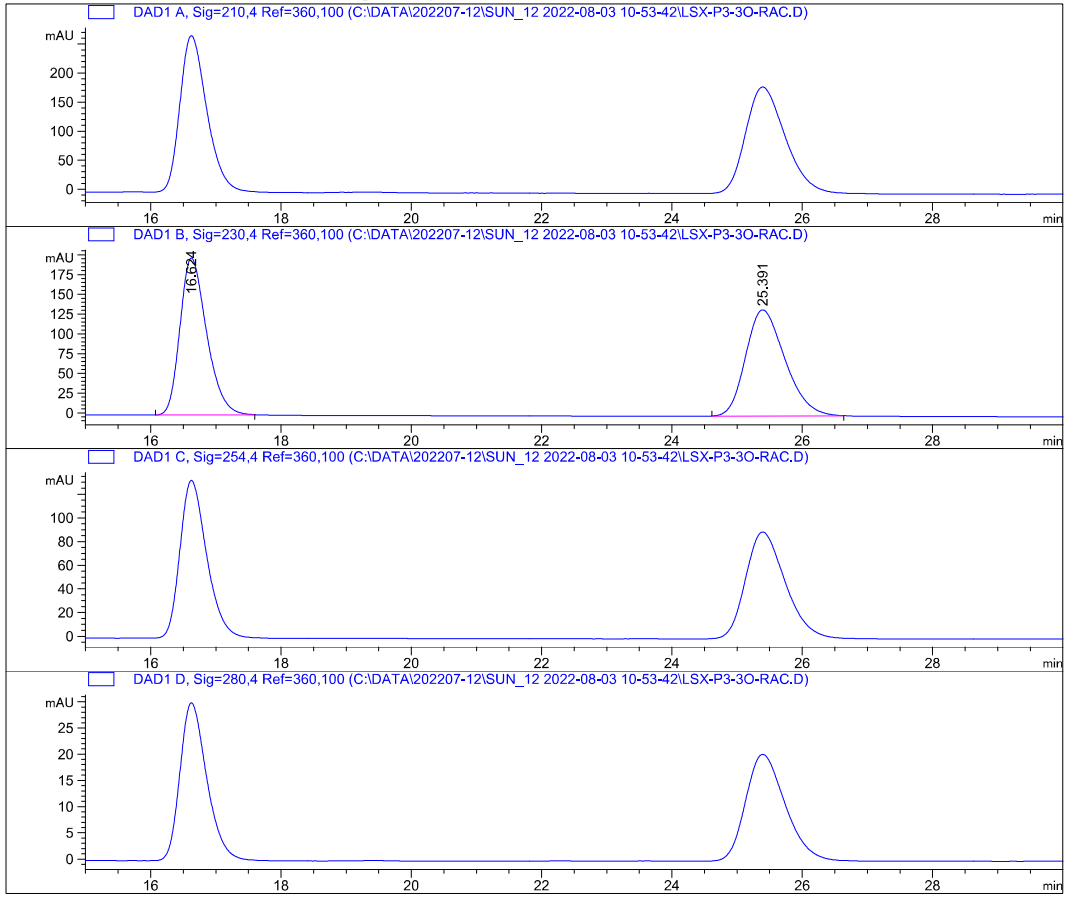

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.236 BB    0.2621  157.32568    9.08126   2.1678
   2  14.501 BB    0.4166 7100.08203  261.63687  97.8322

Totals :                  7257.40771  270.71813



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



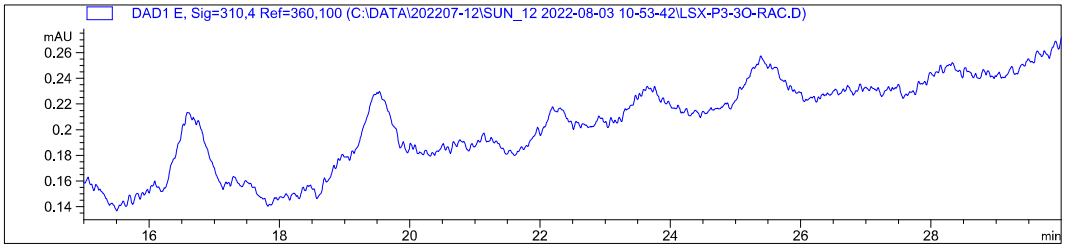
3k

Data File C:\DATA\202207-12\SUN_12 2022-08-03 10-53-42\LSX-P3-3O-RAC.D
Sample Name:

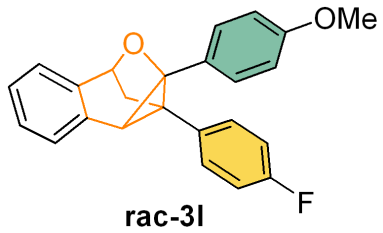
```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 2/8/2022 8:06:45 pm              Inj :   1
                                             Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 8.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-08-03 10-53-42\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:50:10 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-08-03 10-53-42\LSX-P3-3O-RAC.D
Sample Name:



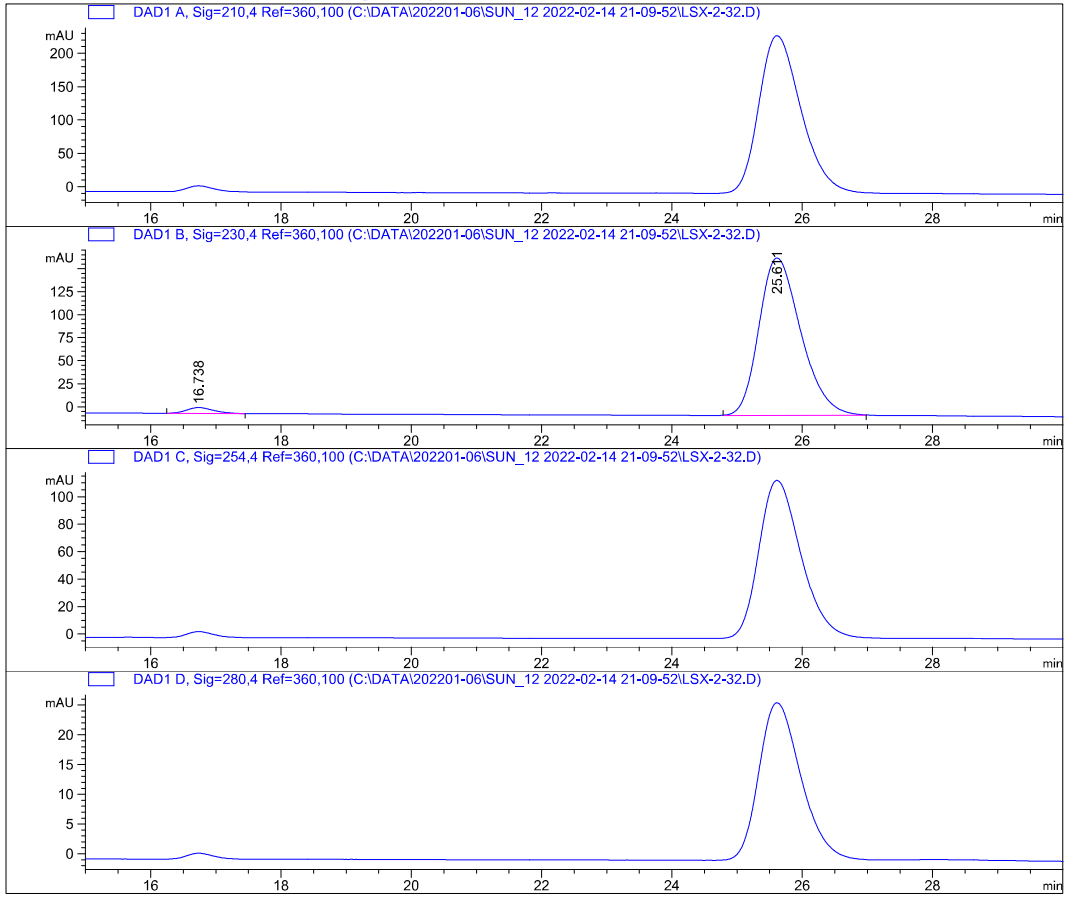

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.624 BB    0.4381 5646.89551  198.38628  50.0481
   2  25.391 BB    0.6482 5636.03174  134.14885  49.9519

Totals :                  1.12829e4   332.53513



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



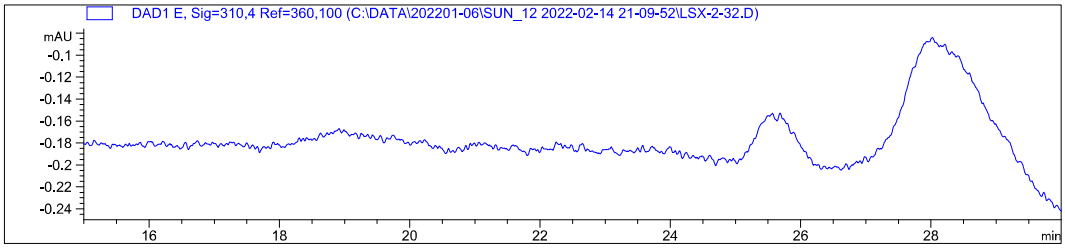
rac-3l

Data File C:\DATA\202201-06\SUN_12 2022-02-14 21-09-52\LSX-2-32.D
Sample Name:

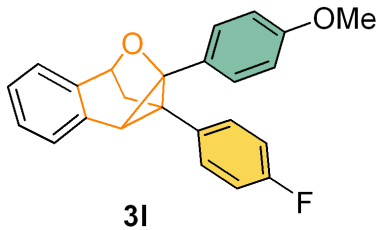
```
==========================================================================
Acq. Operator   :                              Seq. Line :  20
Acq. Instrument : Instrument 1                  Location :   44
Injection Date  : 14/2/2022 1:22:01 pm               Inj :   1
                                             Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-02-14 21-09-52\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:50:10 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-02-14 21-09-52\LSX-2-32.D
Sample Name:



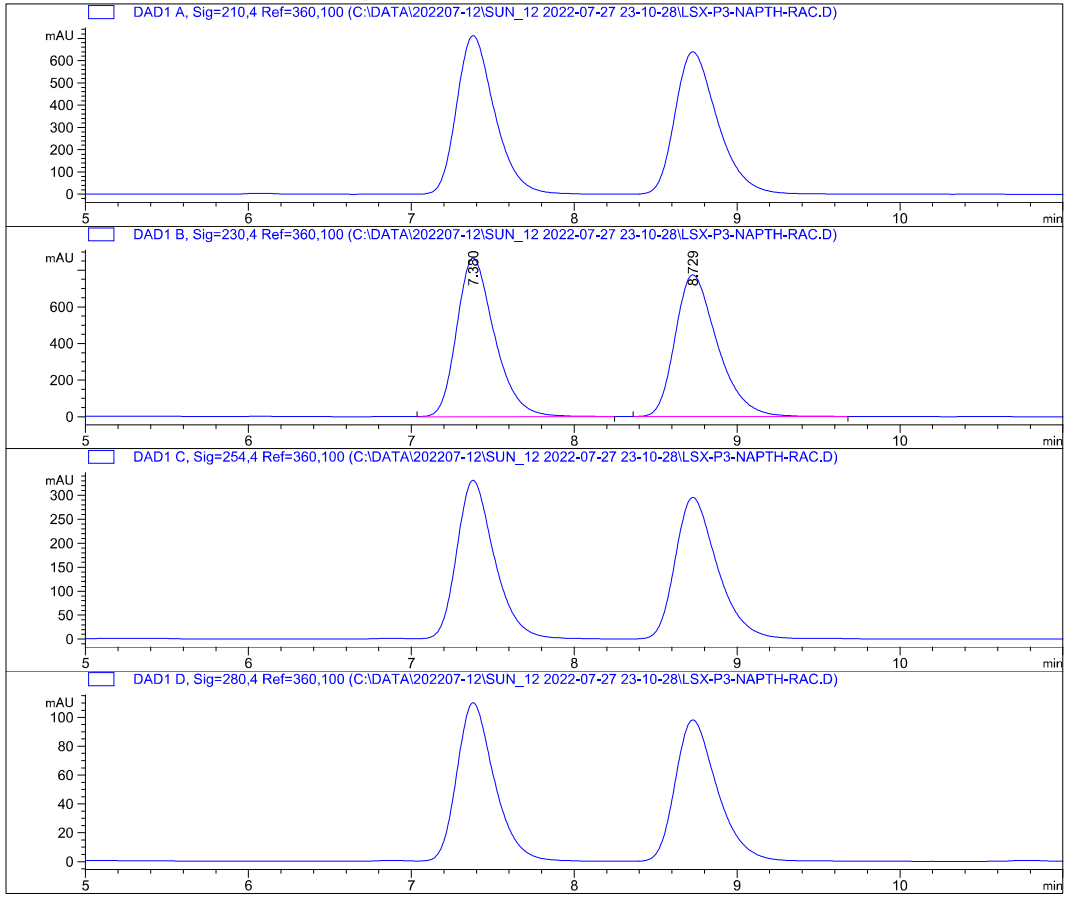

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.738 BB    0.4070  178.94763    6.30701   2.2903
   2  25.611 BB    0.6872 7634.36328  170.87814  97.7097

Totals :                  7813.31091  177.18515


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



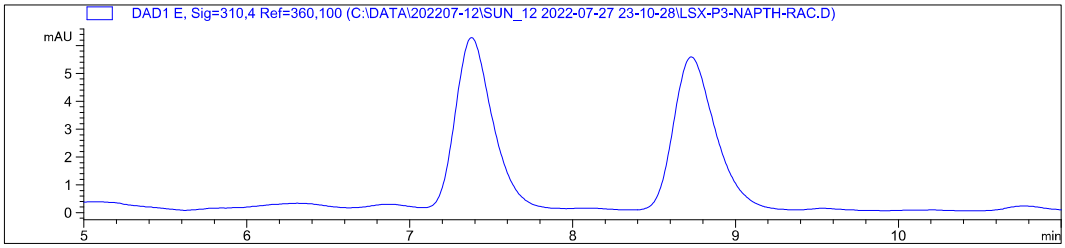
3l

Data File C:\DATA\202207-12\SUN_12 2022-07-27 23-10-28\LSX-P3-NAPTH-RAC.D
Sample Name:

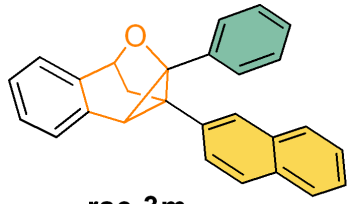
```
==========================================================================
Acq. Operator   :                              Seq. Line :   5
Acq. Instrument : Instrument 1                  Location :   74
Injection Date  : 27/7/2022 9:56:54 am             Inj :   1
                                             Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-07-27 23-10-28\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:47:51 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-07-27 23-10-28\LSX-P3-NAPTH-RAC.D
Sample Name:



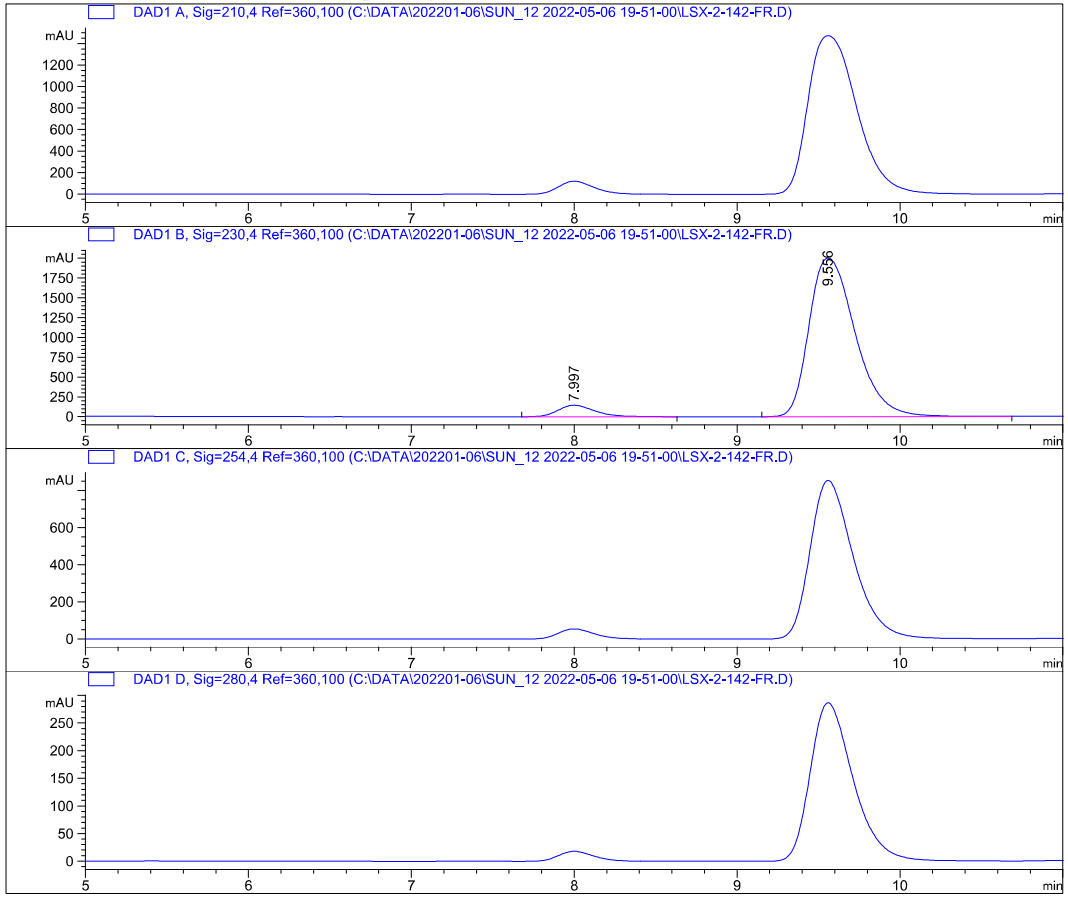

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.380 BB    0.2440 1.39588e4   866.09265  50.0258
   2   8.729 BB    0.2741 1.39444e4   774.32813  49.9742

Totals :                  2.79032e4  1640.42078


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



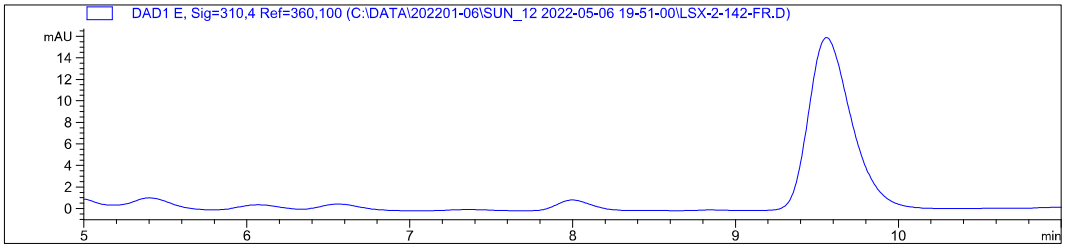
rac-3m

Data File C:\DATA\202201-06\SUN_12 2022-05-06 19-51-00\LSX-2-142-FR.D
Sample Name:

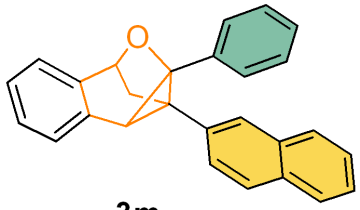
```
==========================================================================
Acq. Operator   :                              Seq. Line :   3
Acq. Instrument : Instrument 1                  Location :   42
Injection Date  : 6/5/2022 5:35:06 am               Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-05-06 19-51-00\IC-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:47:51 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-05-06 19-51-00\LSX-2-142-FR.D
Sample Name:



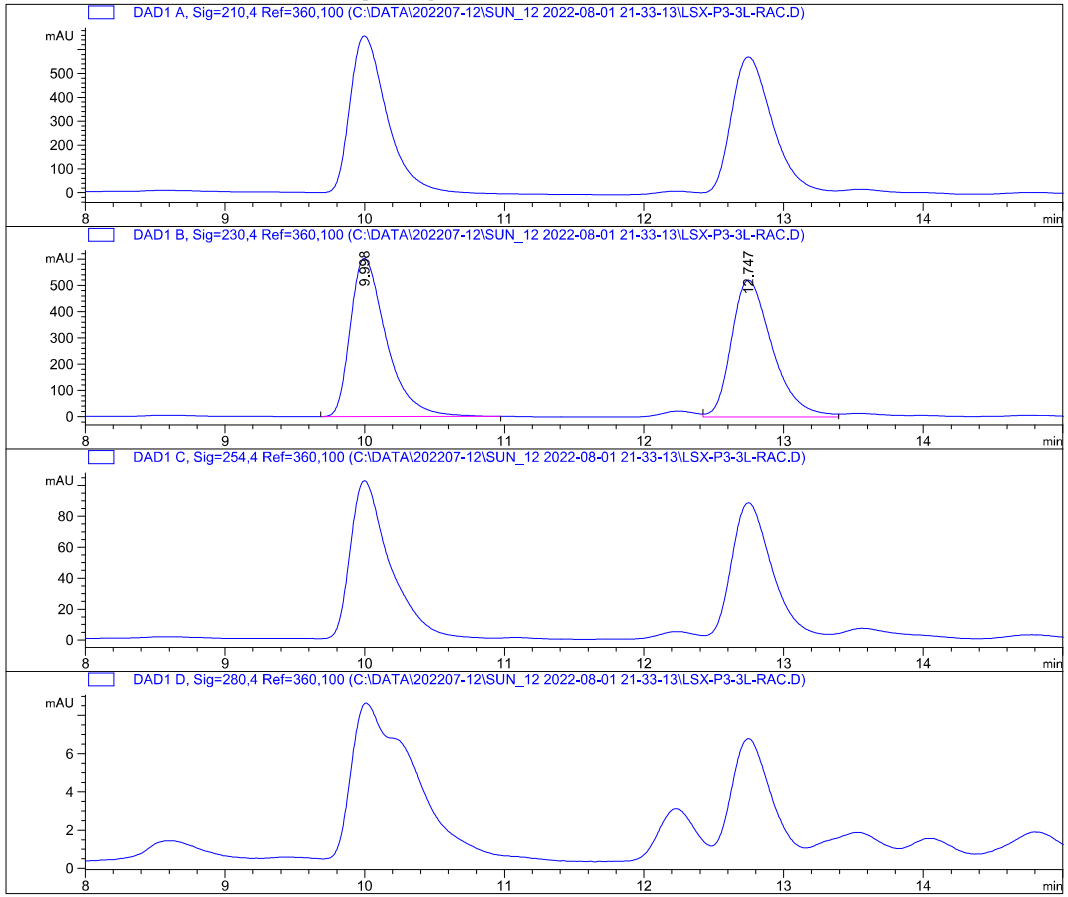

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.997 BB    0.2361 2240.99194  145.19551   5.3680
   2   9.556 BB    0.3080 3.95061e4  2004.24268  94.6320

Totals :                  4.17470e4  2149.43819


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



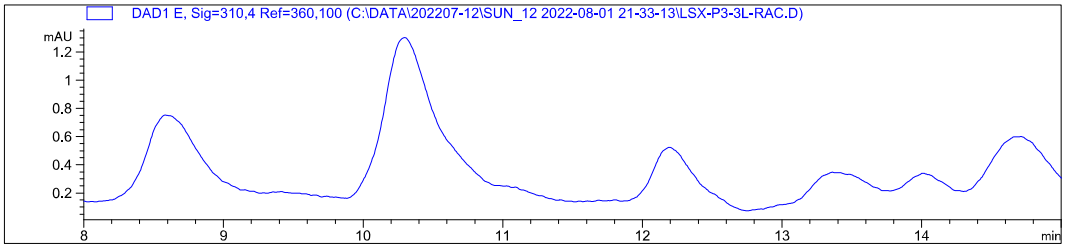
3m

Data File C:\DATA\202207-12\SUN_12 2022-08-01 21-33-13\LSX-P3-3L-RAC.D
Sample Name:

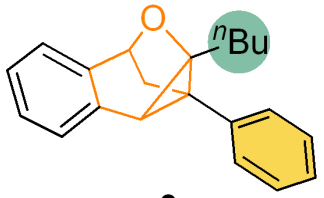
```
==========================================================================
Acq. Operator   :                          Seq. Line :  13
Acq. Instrument : Instrument 1              Location :  42
Injection Date  : 1/8/2022 11:58:09 am          Inj :  1
                                        Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-08-01 21-33-13\AD-03-30-0.5.M
Last changed    :
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:41:01 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-08-01 21-33-13\LSX-P3-3L-RAC.D
Sample Name:



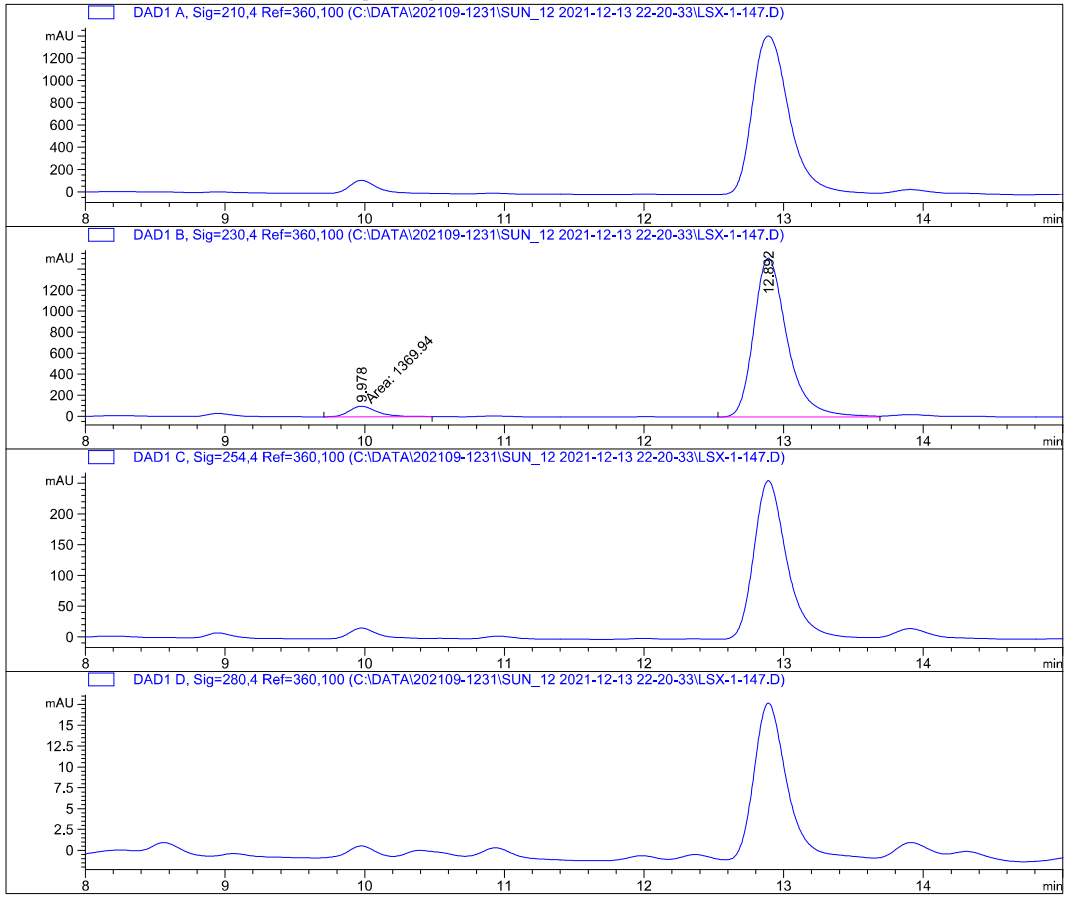

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.998 BB    0.2731 1.08005e4   602.47620  50.4473
   2  12.747 VV    0.3114 1.06090e4   521.29974  49.5527

Totals :                  2.14095e4  1123.77594


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



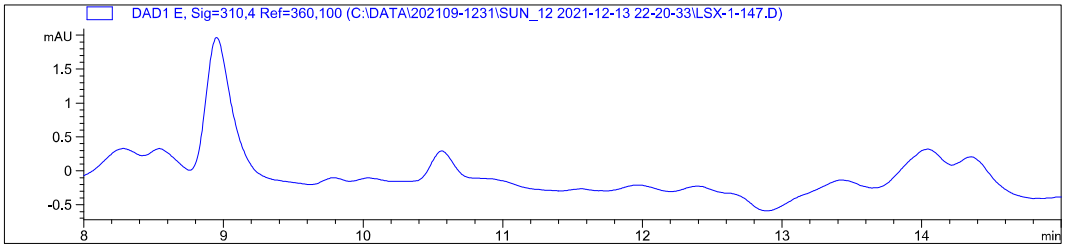
rac-3n

Data File C:\DATA\202109-1231\SUN_12 2021-12-13 22-20-33\LSX-1-147.D
Sample Name:

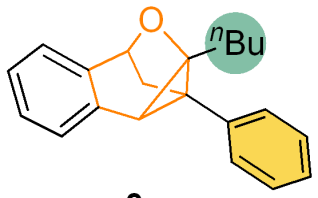
```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location :   41
Injection Date  : 13/12/2021 6:33:17 am         Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2021-12-13 22-20-33\AD-03-30-0.5.M
Last changed    :
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:41:01 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202109-1231\SUN_12 2021-12-13 22-20-33\LSX-1-147.D
Sample Name:



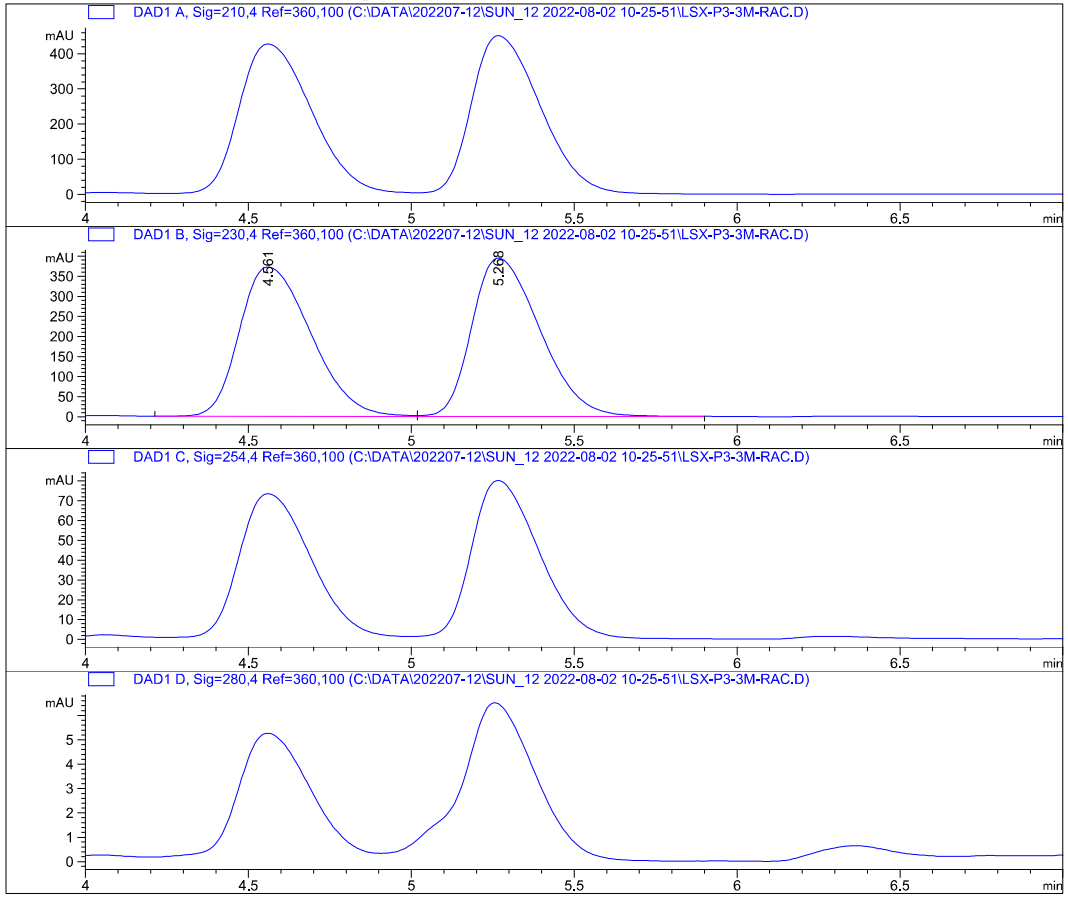

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.978 MM    0.2271 1369.93945  100.54881   5.1421
   2  12.892 BV    0.2551 2.52716e4  1510.90625  94.8579

Totals :                  2.66416e4  1611.45506



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                     *** End of Report ***
```



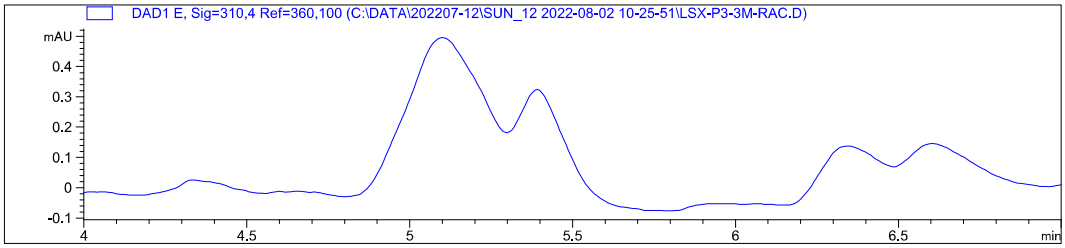
3n

Data File C:\DATA\202207-12\SUN_12 2022-08-02 10-25-51\LSX-P3-3M-RAC.D
Sample Name:

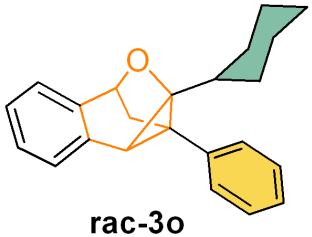
```
==========================================================================
Acq. Operator   :                              Seq. Line :   6
Acq. Instrument : Instrument 1                  Location :   42
Injection Date  : 1/8/2022 9:32:52 pm               Inj :   1
                                             Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-08-02 10-25-51\AD-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:44:59 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202207-12\SUN_12 2022-08-02 10-25-51\LSX-P3-3M-RAC.D
Sample Name:



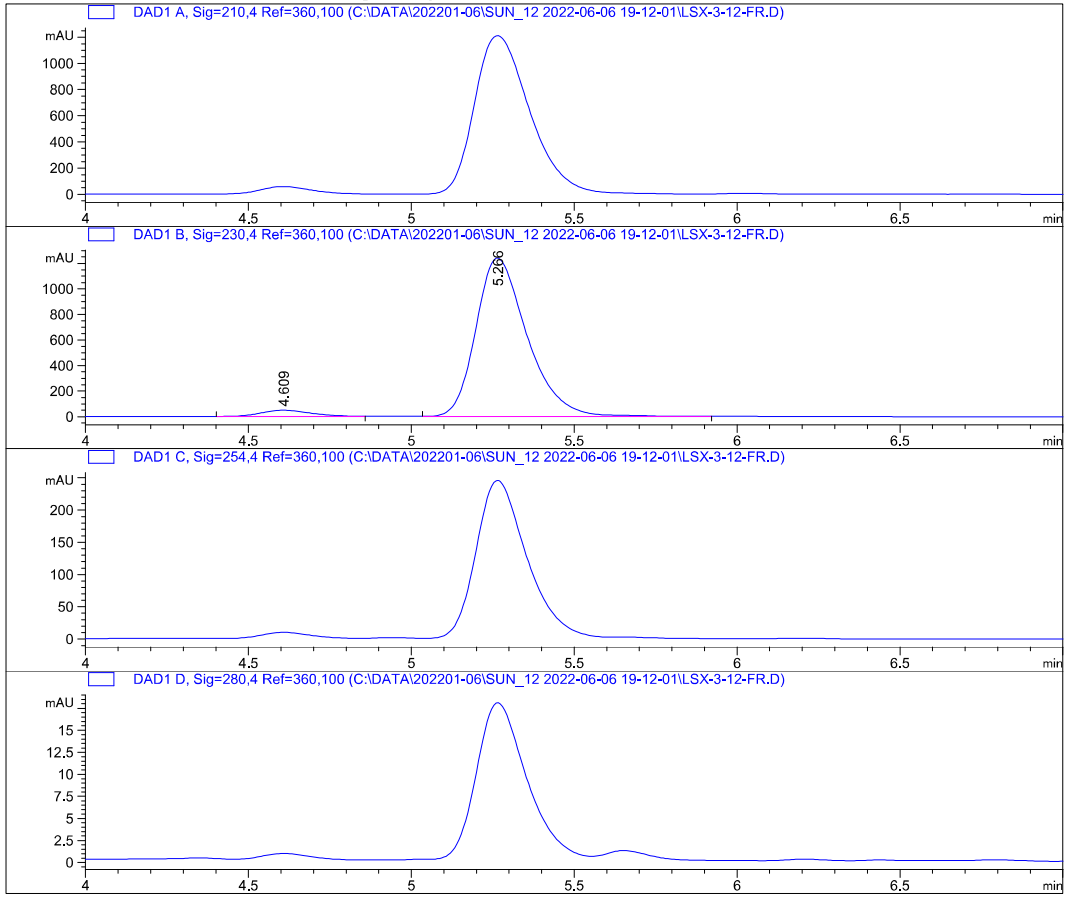

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.561 VV    0.2414 5656.20166  371.97165  49.7169
   2   5.268 VB    0.2292 5720.62207  394.34897  50.2831

Totals :                  1.13768e4   766.32062


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



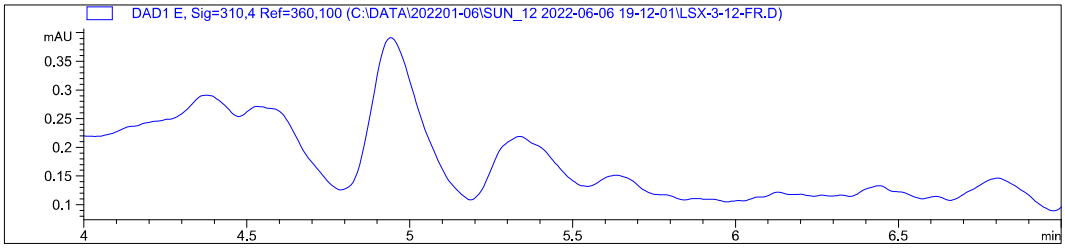
rac-3o

Data File C:\DATA\202201-06\SUN_12 2022-06-06 19-12-01\LSX-3-12-FR.D
Sample Name:

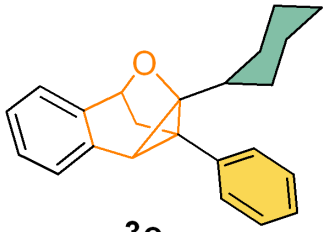
```
==========================================================================
Acq. Operator   :                              Seq. Line :  14
Acq. Instrument : Instrument 1                  Location :  41
Injection Date  : 6/6/2022 7:43:36 am               Inj :  1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 8.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2022-06-06 19-12-01\AD-02-30.M
Last changed    :
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-13 17-26-47\OD-00
                  -20.M (Sequence Method)
Last changed    : 13/3/2024 10:44:59 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202201-06\SUN_12 2022-06-06 19-12-01\LSX-3-12-FR.D
Sample Name:

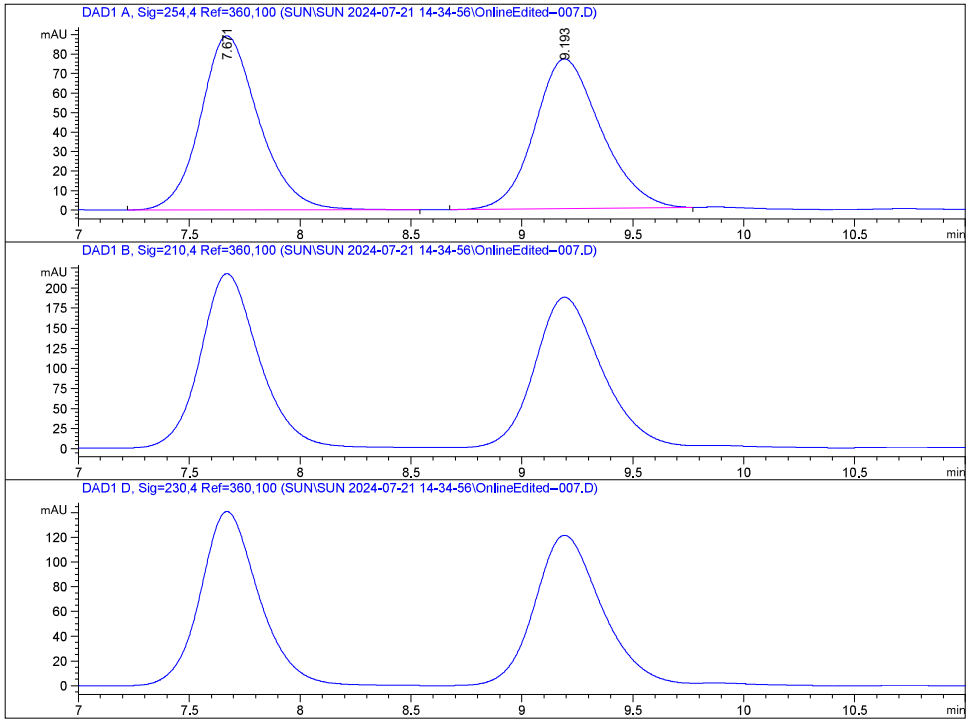



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.609 BV    0.1649  530.77295   48.80680   3.7515
   2   5.266 VB    0.1660 1.36176e4  1241.16309  96.2485

Totals :                  1.41484e4  1289.96989


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

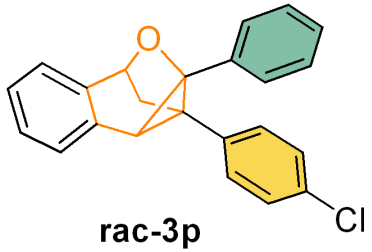


3o

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   7
Sample Operator : SYSTEM
Acq. Instrument : HPLC                           Location :   P1-D-01
Injection Date  : 21/7/2024 3:54:36 pm               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-21 14-34-56
                  \IC3-2-25.M
Last changed    : 2/7/2024 6:32:09 pm by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-21 14-34-56
                  \IC3-2-25.M (Sequence Method)
Last changed    : 22/7/2024 3:53:30 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

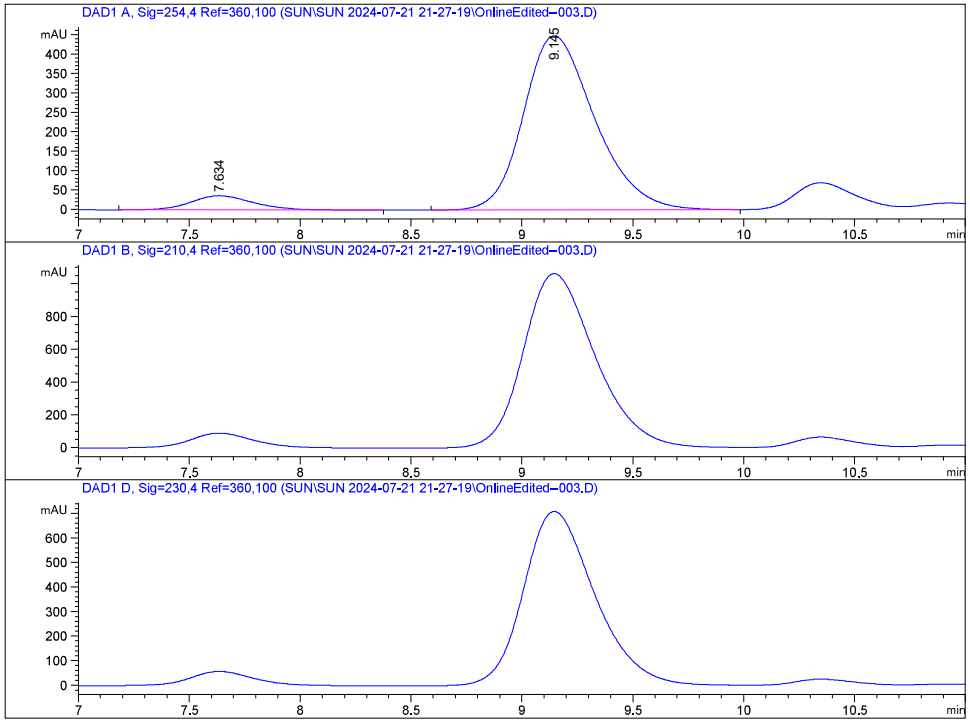



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.671 BB    0.2776 1639.43286   89.33002  50.6508
   2   9.193 BB    0.3157 1597.30408   76.77734  49.3492

Totals :                  3236.73694  166.10736



Signal 2: DAD1 B, Sig=210,4 Ref=360,100


Signal 3: DAD1 D, Sig=230,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



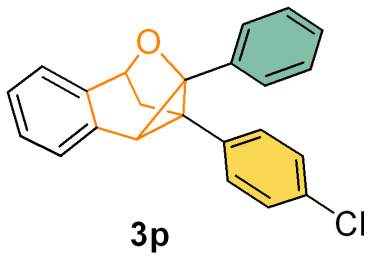
rac-3p

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Sample Operator : SYSTEM
Acq. Instrument : HPLC                          Location :   P1-D-01
Injection Date  : 21/7/2024 9:44:59 pm               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-21 21-27-19
                  \IC3-2-25.M
Last changed    : 2/7/2024 6:32:09 pm by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-21 21-27-19
                  \IC3-2-25.M (Sequence Method)
Last changed    : 22/7/2024 3:54:28 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



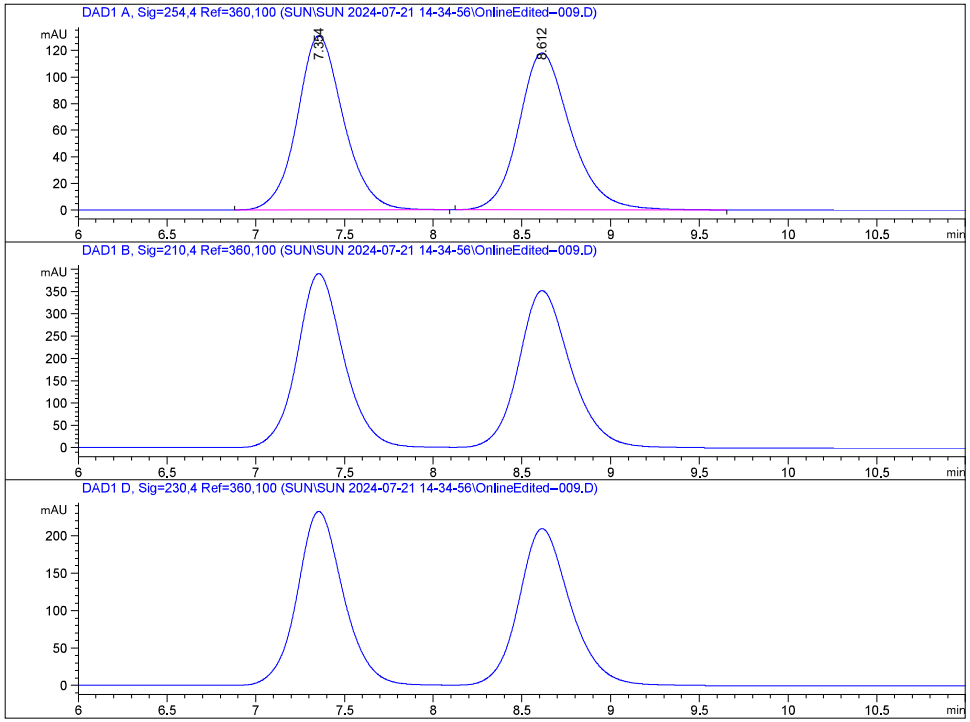
Data File C:\Users\P...\ChemStation\1\Data\SUN\SUN 2024-07-21 21-27-19\OnlineEdited--003.D
Sample Name: lsx-8-143crac

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.634 BB    0.2946  724.15308   36.62976   6.7459
   2   9.145 BB    0.3398 1.00105e4   447.76245  93.2541

Totals :                   1.07346e4   484.39222


Signal 2: DAD1 B, Sig=210,4 Ref=360,100


Signal 3: DAD1 D, Sig=230,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



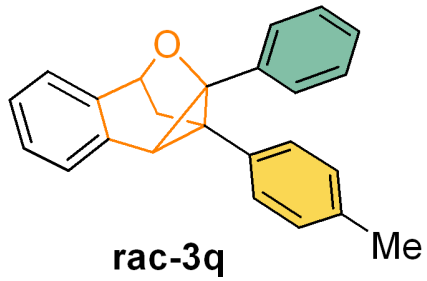
3p

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   9
Sample Operator : SYSTEM
Acq. Instrument : HPLC                          Location :   P1-D-03
Injection Date  : 21/7/2024 4:47:34 pm               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-21 14-34-56
                  \IC3-2-25.M
Last changed    : 2/7/2024 6:32:09 pm by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-21 14-34-56
                  \IC3-2-25.M (Sequence Method)
Last changed    : 22/7/2024 3:51:26 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\Users\P...\ChemStation\1\Data\SUN\SUN 2024-07-21 14-34-56\OnlineEdited--009.D
Sample Name: lsx-8-143brac

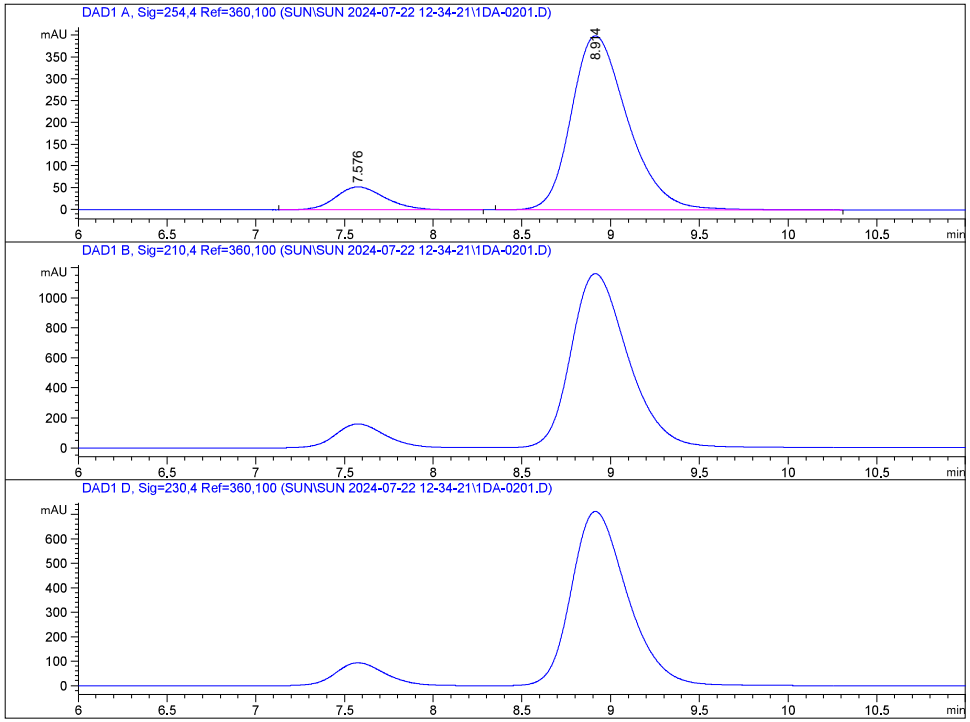
```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.354 BB    0.2712 2371.44141  130.66690  49.6549
   2   8.612 BB    0.3101 2404.39990  117.79632  50.3451

Totals :                  4775.84131  248.46322


Signal 2: DAD1 B, Sig=210,4 Ref=360,100


Signal 3: DAD1 D, Sig=230,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



rac-3q

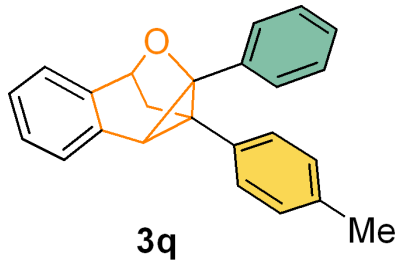
Data File C:\Users\P...Documents\ChemStation\1\Data\SUN\SUN 2024-07-22 12-34-21\1DA-0201.D
Sample Name: lsx-8-143brt

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Sample Operator : SYSTEM
Acq. Instrument : HPLC                           Location :   P1-D-01
Injection Date  : 22/7/2024 12:48:04 pm               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 8.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-22 12-34-21
                  \IC3-2-25.M
Last changed    : 2/7/2024 6:32:09 pm by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-22 12-34-21
                  \IC3-2-25.M (Sequence Method)
Last changed    : 22/7/2024 3:52:38 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



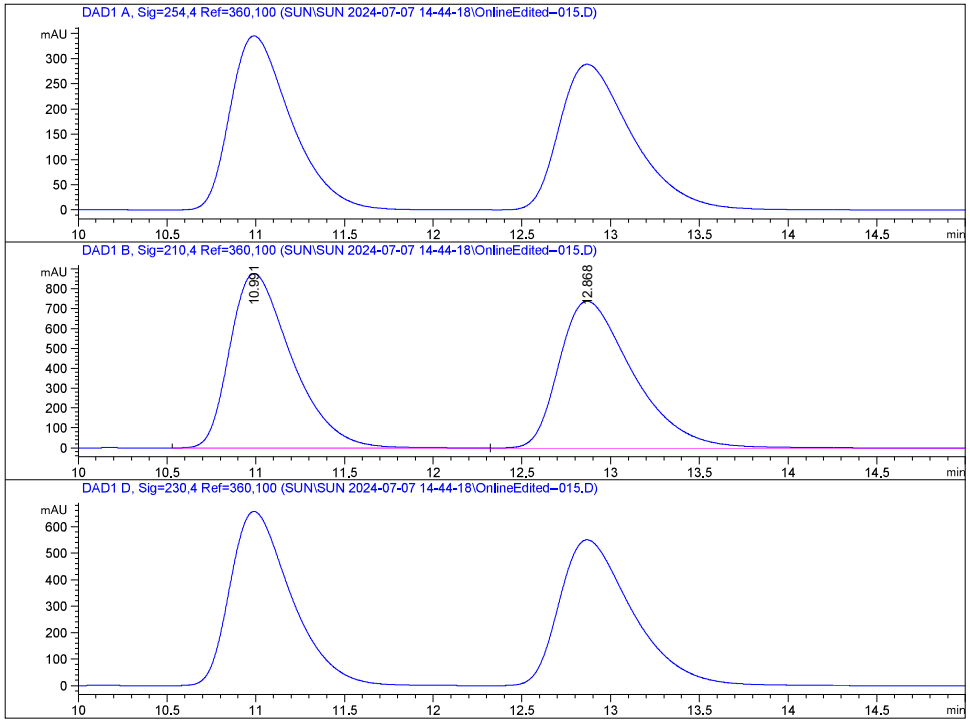
Data File C:\Users\P...Documents\ChemStation\1\Data\SUN\SUN 2024-07-22 12-34-21\1DA-0201.D
Sample Name: lsx-8-143brt

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.576 BB    0.2970 1029.88721   52.81315  10.4569
   2   8.914 BB    0.3380 8819.01270  399.61432  89.5431

Totals :                  9848.89990  452.42747


Signal 2: DAD1 B, Sig=210,4 Ref=360,100


Signal 3: DAD1 D, Sig=230,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



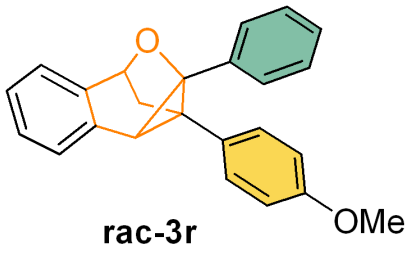
3q

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  15
Sample Operator : SYSTEM
Acq. Instrument : HPLC                           Location :   P1-D-03
Injection Date  : 7/7/2024 6:11:14 pm                 Inj :   1
                                                Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 8.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-07 14-44-18
                  \IC3-2-25.M
Last changed    : 2/7/2024 6:32:09 pm by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-07 14-44-18
                  \IC3-2-25.M (Sequence Method)
Last changed    : 22/7/2024 3:46:47 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



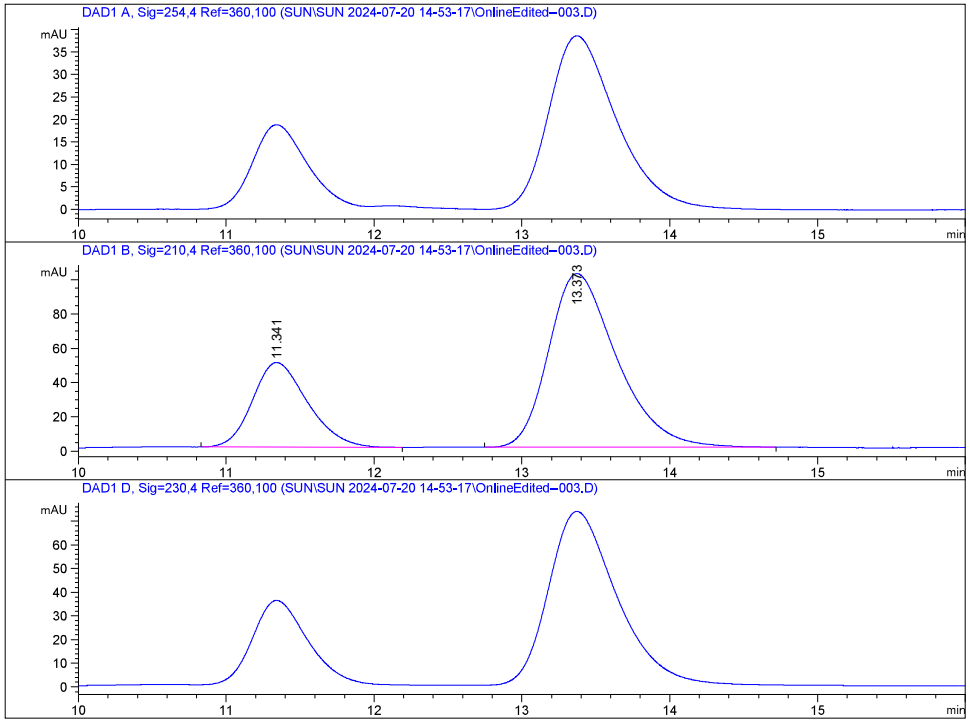
Data File C:\Users\P...\ChemStation\1\Data\SUN\SUN 2024-07-07 14-44-18\OnlineEdited--015.D
Sample Name: lsx-8-120rac

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100


Signal 2: DAD1 B, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.991 BB    0.3685 2.12142e4   876.14178  49.8608
   2  12.868 BB    0.4359 2.13327e4   737.73883  50.1392

Totals :                  4.25469e4  1613.88062


Signal 3: DAD1 D, Sig=230,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



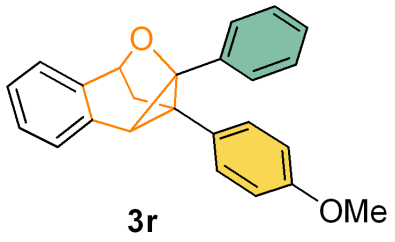
rac-3r

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :   3
Sample Operator : SYSTEM
Acq. Instrument : HPLC                        Location :   P1-D-01
Injection Date  : 20/7/2024 3:23:26 pm             Inj :   1
                                            Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 10.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-20 14-53-17
                  \IC3-2-25.M
Last changed    : 2/7/2024 6:32:09 pm by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-20 14-53-17
                  \IC3-2-25.M (Sequence Method)
Last changed    : 22/7/2024 3:39:01 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\Users\P...\ChemStation\1\Data\SUN\SUN 2024-07-20 14-53-17\OnlineEdited--003.D
Sample Name: lsx-8-143a

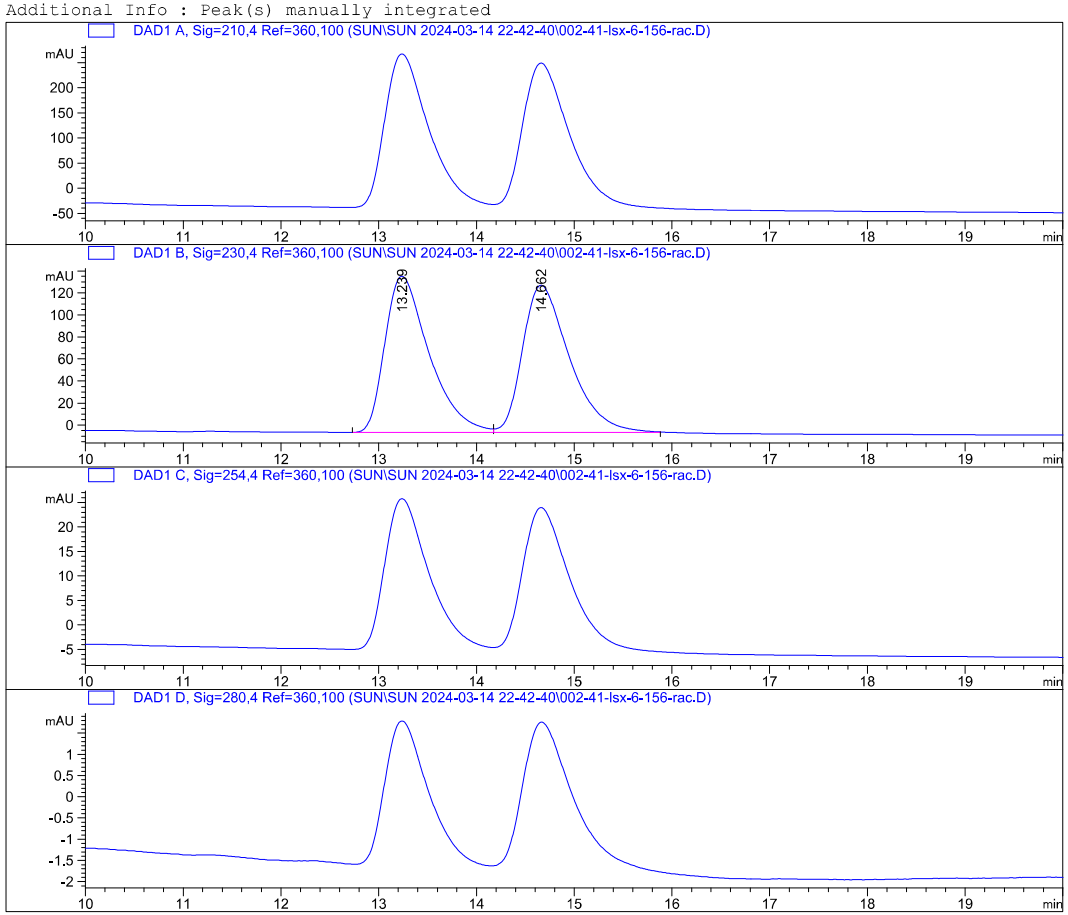
```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100


Signal 2: DAD1 B, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.341 BB    0.3718 1274.70825   49.27628  28.2194
   2  13.373 BB    0.4679 3242.43311  101.18215  71.7806

Totals :                  4517.14136  150.45843


Signal 3: DAD1 D, Sig=230,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



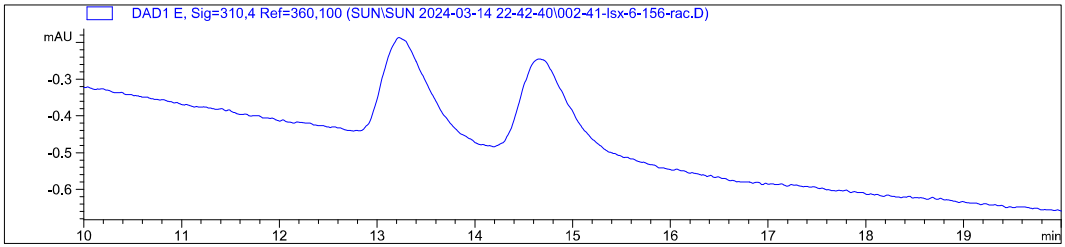
3r

Data File C:\Users\P...emStation\1\Data\SUN\SUN 2024-03-14 22-42-40\002-41-lsx-6-156-rac.D
Sample Name: lsx-6-156-rac

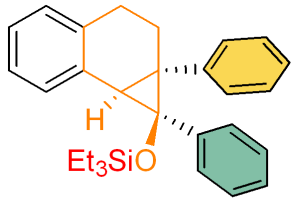
```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : LC1260                         Location :   41
Injection Date  : 14/3/2024 10:55:26 pm              Inj :   1
                                               Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-14 22-42-40\OD-
                  005-30-0.5.M
Last changed    : 14/3/2024 10:54:38 pm by SYSTEM
                  (modified after loading)
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-14 22-42-40\OD-
                  005-30-0.5.M (Sequence Method)
Last changed    : 16/3/2024 11:03:28 am by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\Users\P...emStation\1\Data\SUN\SUN 2024-03-14 22-42-40\002-41-lsx-6-156-rac.D
Sample Name: lsx-6-156-rac



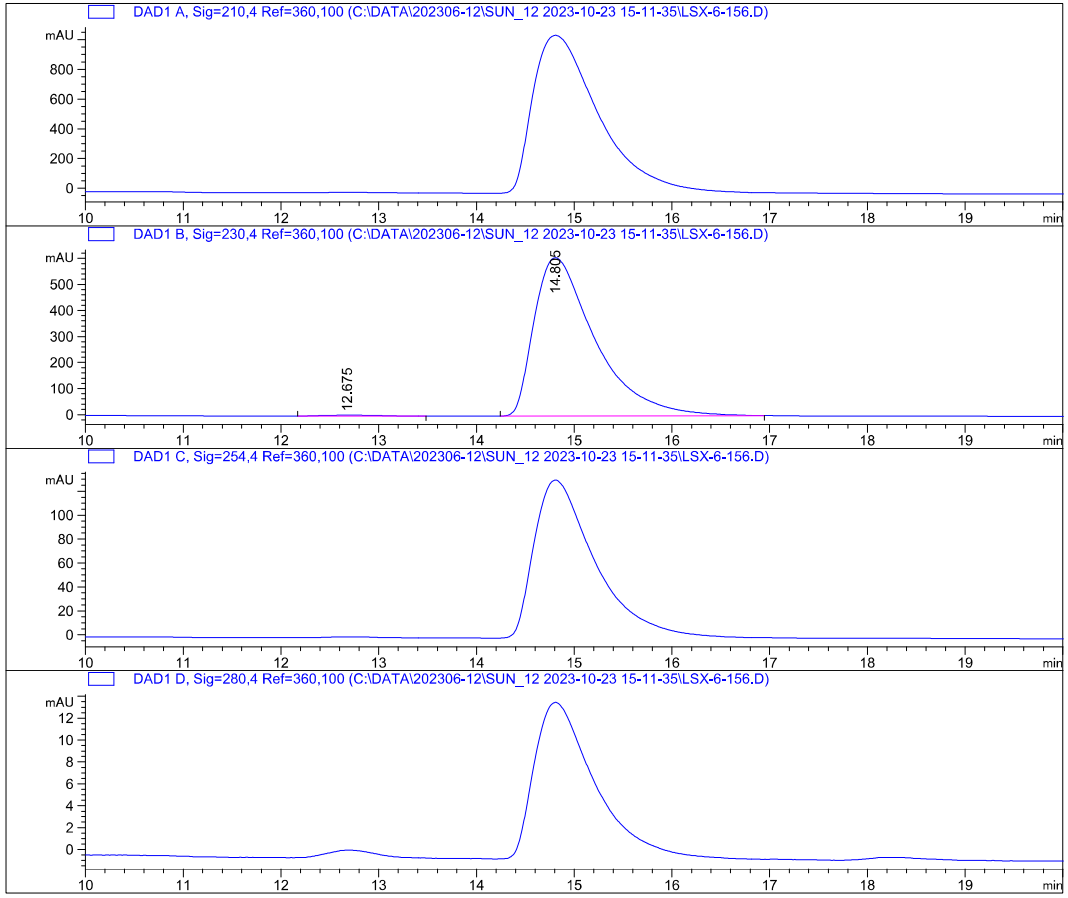

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.239 BV    0.4763 4445.55176  141.59248  49.9927
   2  14.662 VB    0.5044 4446.84326  133.58446  50.0073

Totals :                  8892.39502  275.17694



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                      *** End of Report ***
```



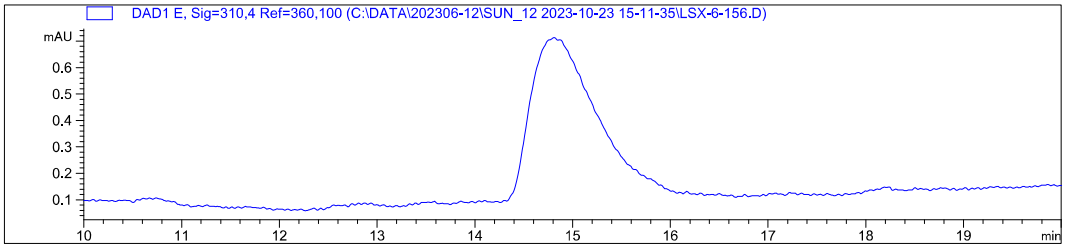
rac-4

Data File C:\DATA\202306-12\SUN_12 2023-10-23 15-11-35\LSX-6-156.D
Sample Name:

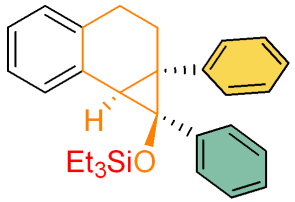
```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location :   41
Injection Date  : 23/10/2023 12:24:27 am            Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3.000 µl
Acq. Method     : C:\Chem32\1\DATA\SUN_12 2023-10-23 15-11-35\OD-005-30-0.5.M
Last changed    :
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-03-14 15-51-32\OD-00
                  -20.M (Sequence Method)
Last changed    : 14/3/2024 10:41:18 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\DATA\202306-12\SUN_12 2023-10-23 15-11-35\LSX-6-156.D
Sample Name:

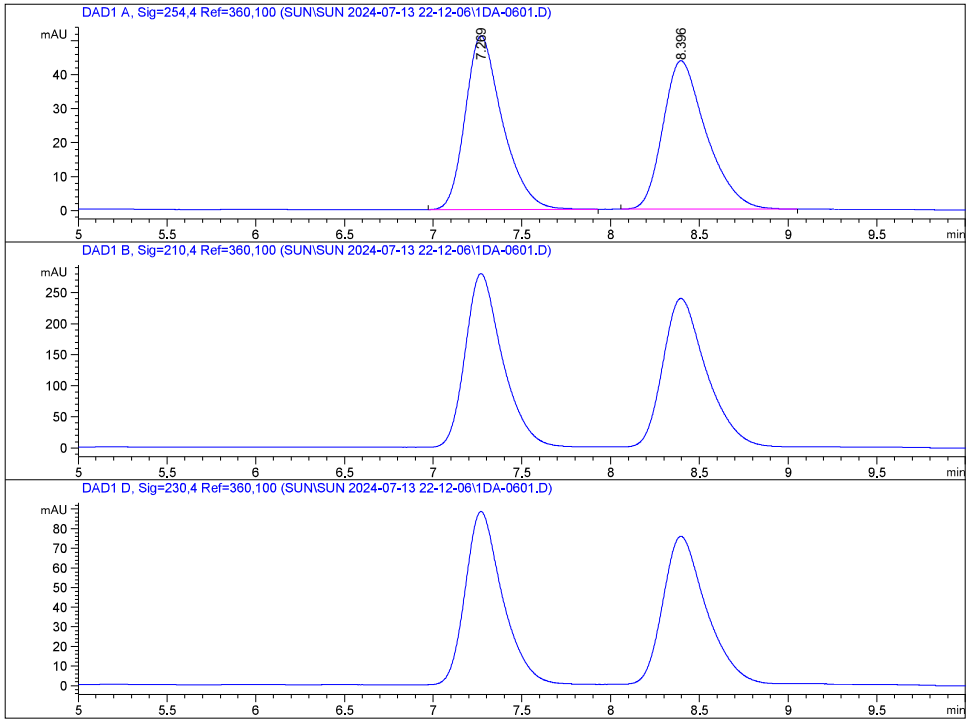



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100


Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.675 BB    0.4218  114.07614    3.41453   0.4315
   2  14.805 BB    0.6554 2.63224e4   607.67755  99.5685

Totals :                  2.64364e4   611.09208



Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



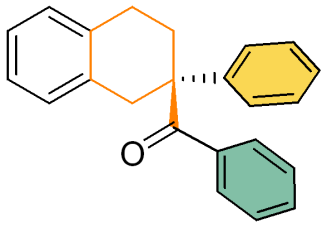
4

```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :   6
Sample Operator : SYSTEM
Acq. Instrument : HPLC                        Location :   P1-D-01
Injection Date  : 13/7/2024 11:49:44 pm            Inj :   1
                                            Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-13 22-12-06
                  \IC3-2-25.M
Last changed    : 2/7/2024 6:32:09 pm by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-13 22-12-06
                  \IC3-2-25.M (Sequence Method)
Last changed    : 22/7/2024 9:45:20 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\Users\P...Documents\ChemStation\1\Data\SUN\SUN 2024-07-13 22-12-06\1DA-0601.D
Sample Name: lsx-8-139tbafrac

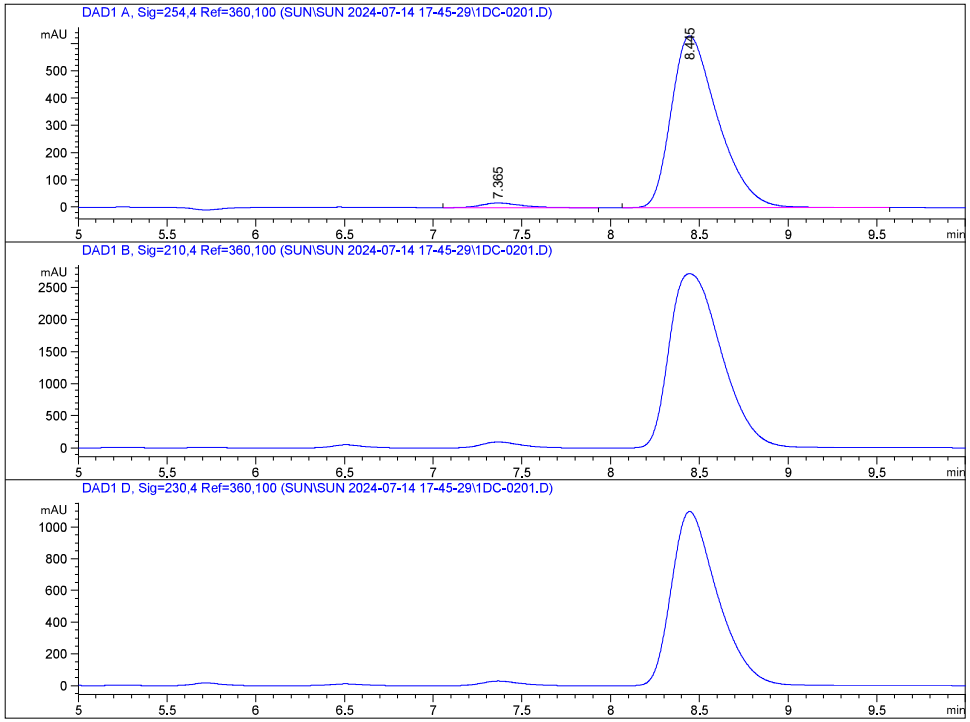
```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.269 BB    0.2164  745.83508   51.21305  50.1220
   2   8.396 BB    0.2479  742.20300   43.76320  49.8780

Totals :                   1488.03809   94.97625


Signal 2: DAD1 B, Sig=210,4 Ref=360,100


Signal 3: DAD1 D, Sig=230,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



rac-5

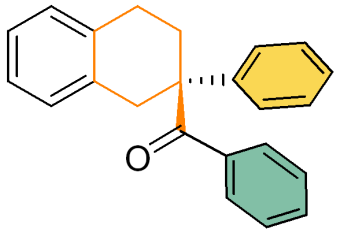
Data File C:\Users\P...Documents\ChemStation\1\Data\SUN\SUN 2024-07-14 17-45-29\1DC-0201.D
Sample Name: lsx-8-139

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Sample Operator : SYSTEM
Acq. Instrument : HPLC                           Location :   P1-D-03
Injection Date  : 14/7/2024 5:58:36 pm                Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-14 17-45-29
                  \IC3-2-25.M
Last changed    : 2/7/2024 6:32:09 pm by SYSTEM
Analysis Method : C:\Users\Public\Documents\ChemStation\1\Data\SUN\SUN 2024-07-14 17-45-29
                  \IC3-2-25.M (Sequence Method)
Last changed    : 22/7/2024 3:44:09 pm by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\Users\P...Documents\ChemStation\1\Data\SUN\SUN 2024-07-14 17-45-29\1DC-0201.D
Sample Name: lsx-8-139

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.365 BB    0.2214  254.72859   16.99403   2.1785
   2   8.445 BB    0.2745 1.14379e4   629.57275  97.8215

Totals :                   1.16926e4   646.56679


Signal 2: DAD1 B, Sig=210,4 Ref=360,100


Signal 3: DAD1 D, Sig=230,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



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