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*Supporting Information*

# A Simple protocol for determination of enantiopurity of amines using BINOL derivatives as chiral solvating agents *via* $^{1}$H- and $^{19}$F-NMR spectroscopic analysis

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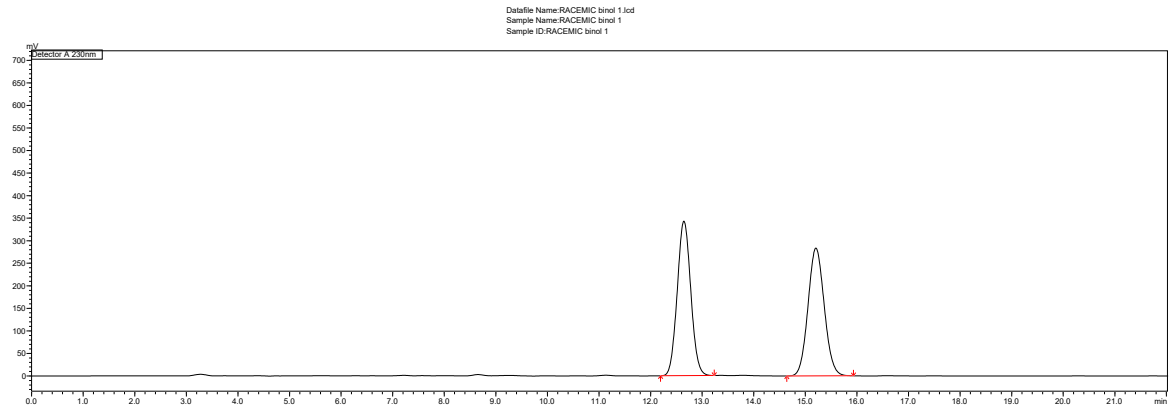
## Experimental

All solvents used in the reaction were analytical grade. (*S*)-BINOL (**1**), (*R*)-1,1'-binaphthyl-2,2'-diyl hydrogenphosphate (**4**), (1*R*,2*R*)-**5**, and (1*S*,2*S*)- **5** were gifted by Synthesis with Catalyst Pvt. Ltd., India. The enantiopurity of (*S*)-BINOL (**1**) was confirmed by high performance liquid chromatography (HPLC) analysis (Shimadzu LC-2010HT) using the Chiralpak AD-H column, before using it for the synthesis of chiral solvating agents (*S*)-**2**, (*S*)-**3a**, (*S*)-**3b**, (*S*)-**3c**, (*S*)-**3d**. The (*R*)- and (*S*)- 2-amino-3-phenylpropan-1-ol (**6**) were synthesized from D-phenylalanine and L-phenylalanine respectively by following the reported procedure.[1] The (*R*)- and (*S*)-secondary amines (**7**-**11**) were synthesized from (*R*)-(+)-1-phenylethylamine and (*S*)-(-)-1-phenylethylamine respectively by treating with their corresponding aldehydes following the reported procedure.[2] The D-phenylalanine, L-phenylalanine, (*R*)-(+)-1-phenylethylamine and (*S*)-(-)-1-phenylethylamine were purchased from sigma Aldrich. $^{1}$H and $^{13}$C-NMR, spectra were recorded on Bruker AVANCE NEO 400MHz FT-NMR spectrometers. Tetramethylsilane as an internal reference in the NMR solvent at ambient temperature was used. The reference value used for TMS in deuterated chloroform ($CDCl_3$) was 0.00 ppm for $^{1}$H-NMR and $^{13}$C-NMR spectra. The reference values used for residual chloroform in deuterated chloroform ($CDCl_3$) were 7.26 ppm and 77.0 ppm for $^{1}$H- and $^{13}$C-NMR spectra, respectively. The optical rotation was taken using Rudolph digipol polarimeter. HRMS analysis of secondary amines (**7**-**11**) was performed on Agilent 6520 Q-TOF Mass spectrometer. UV-vis spectra were recorded on Shimadzu spectrophotometer (UV-2600). The compounds were purified by column chromatography using silica gel (230-400 mesh). All the known compounds (*S*)-**2**, (*S*)-**3a**, (*S*)-**3b**, (*S*)-**3c**, (*S*)-**3d**, (*R*/*S*)-**6**, (*R*/*S*)-**7**, (*R*/*S*)-**8**, (*R*/*S*)-**9**, (*R*/*S*)-**10**, (*R*/*S*)-**11**, (*S*)-1**2**, (*S*)-**13**, (*S*)-**14a**, (*S*)-**14b**, (*S*)-**14c**, (*S*)-**14d** were characterized by $^{1}$H- and $^{13}$C-NMR spectroscopy.

## HPLC Chromatograms

### (±)-BINOL (1)

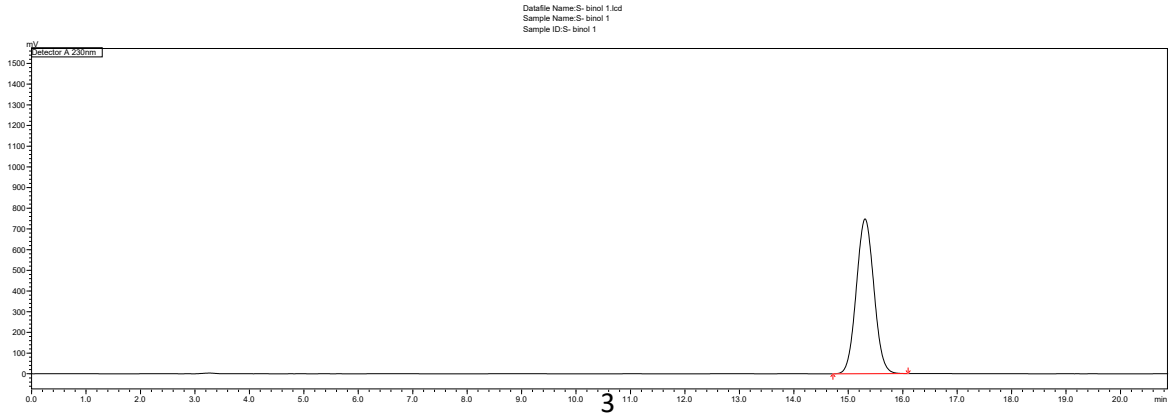
HPLC conditions: Chiralpak AD-H column, hexane/isopropyl alcohol = 80/20, flow rate = 1.0 mL/min, wavelength = 230 nm, temperature = 25 °C.




| Peak | Ret. Time | Area | Height | Conc. | Area% |
|---|---|---|---|---|---|
| 1 | 12.645 | 6260074 | 342745 | 50.188 | 50.188 |
| 2 | 15.204 | 6213293 | 283388 | 49.812 | 49.812 |
| Total | | 12473366 | 626133 | 100.000 | 100.000 |

### (*S*)-BINOL (1)

HPLC conditions: Chiralpak AD-H column, hexane/isopropyl alcohol = 80/20, flow rate = 1.0 mL/min, wavelength = 230 nm, temperature = 25 °C. Enantiomeric excess = >99.99 %: $t_R$ = 15.30 min (major).



| Peak | Ret. Time | Area | Height | Conc. | Area% |
|---|---|---|---|---|---|
| 1 | 15.308 | 16776975 | 748223 | 100.000 | 100.000 |
| Total | | 16776975 | 748223 | 100.000 | 100.000 |

## General procedure for all the experiments

The analyte (0.0125-0.2 mmol) and chiral solvating agent (0.0125-0.1 mmol) were directly mixed in an NMR tube and dissolved in 0.6 mL chloroform-*d*. After shaking the NMR tube for 30 seconds, $^{1}$H-, $^{13}$C-, and $^{19}$F-NMR spectra were recorded on a 400 MHz NMR spectrometer at 25 °C and well-resolved resonance peaks were observed for both the enantiomers present in an analyte. The enantiopurity was calculated by integrating the resonance peaks observed for each of the enantiomers of an analyte from their respective $^{1}$H-, $^{13}$C-, and $^{19}$F-NMR spectra.

## Primary amines

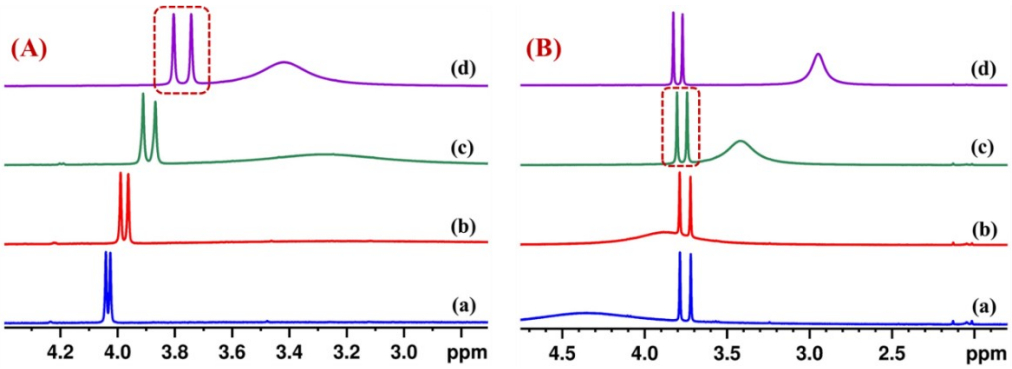



**Figure 1.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) for the different experiments performed using variable concentrations (A) [0.0125 mmol (a), 0.025 mmol (b), 0.05 mmol (c), and 0.1 mmol (d)] of (*S*)-**3a** with 0.05 mmol of *rac*-**5** and (B) [0.0125 mmol (a), 0.025 mmol (b), 0.05 mmol (c), and 0.1 mmol (d)] of *rac*-**5** with 0.1 mmol of (*S*)-**3a** in 0.6 mL chloroform-*d* at 25 ℃. Best results for separation of C<u>H</u> resonances of *rac*-**5** are highlighted in wine red colour box.

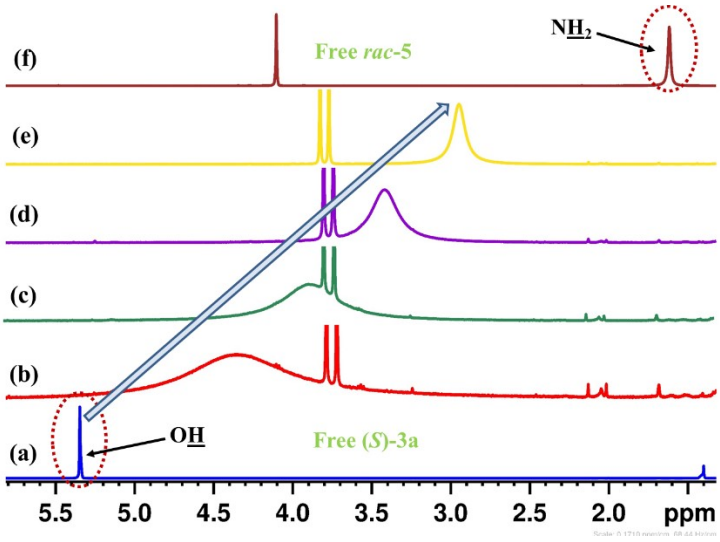



**Figure 2.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) for free (*S*)-**3a** (a), [0.0125 mmol (b), 0.025 mmol (c), 0.05 mmol (d), and 0.1 mmol (e)] of *rac*-**5** with 0.1 mmol of (*S*)-**3a** and free *rac*-**5** (f) in 0.6 mL chloroform-*d* at 25℃.

Initially, the UV-vis spectra of free (*S*)-**3a** ($A_o$) was recorded at concentration of 5 X $10^{-5}$ M in $CHCl_3$ at 25 °C. After then in this fixed concentration of (*S*)-**3a**, the (*R*)-1,2-diphenylethylenediamine (**5**) was added by increasing concentration from 1.25 X $10^{-5}$ M to 10 X $10^{-5}$ M and UV-vis spectra (A) were recorded at 25 °C (Figure 3).

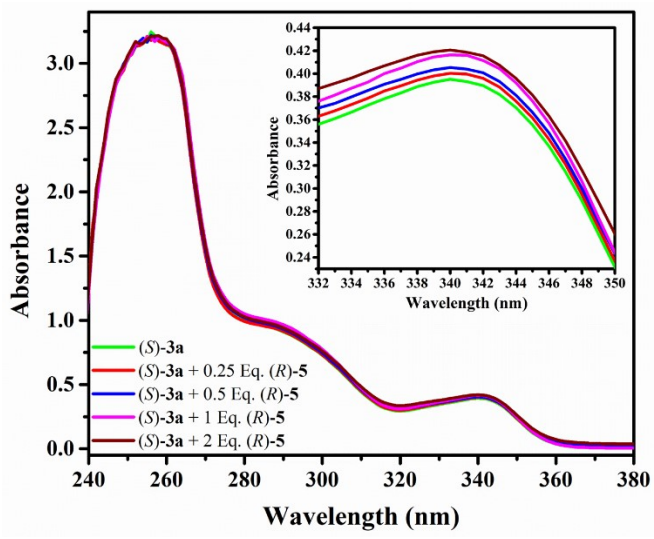



**Figure 3.** UV-vis titration curve for (*S*)-**3a** at 5 X $10^{-5}$ M concentration with increasing concentrations of (*R*)-1,2-diphenylethylenediamine (**5**), 1.25 X $10^{-5}$ M; 2.5 X $10^{-5}$ M; 5 X $10^{-5}$ M; 10 X $10^{-5}$ M in $CHCl_3$ at 25 °C.

Initially, the UV-vis spectra of free (*S*)-**3a** ($A_o$) was recorded at concentration of 5 X $10^{-5}$ M in $CHCl_3$ at 25 °C. After then in this fixed concentration of (*S*)-**3a**, the (*S*)-1,2-diphenylethylenediamine (**5**) was added by increasing concentration from 1.25 X $10^{-5}$ M to 10 X $10^{-5}$ M and UV-vis spectra (A) were recorded at 25 °C (Figure 4).

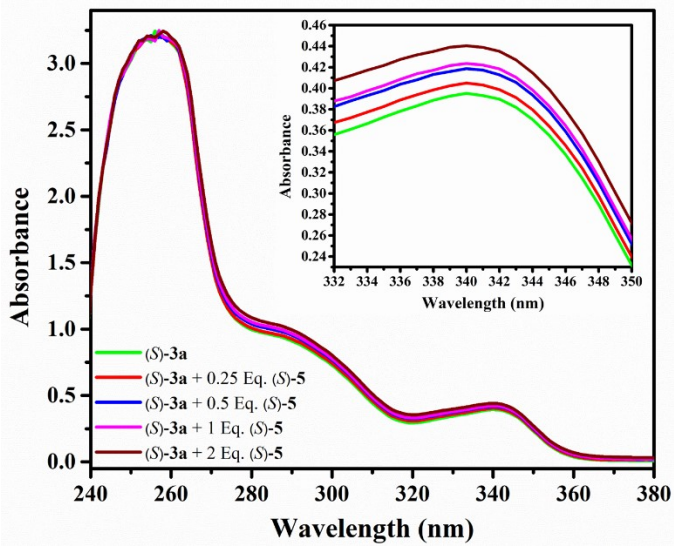



**Figure 4.** UV-vis titration curve for (*S*)-**3a** at 5 X $10^{-5}$ M concentration with increasing concentrations of (*S*)-1,2-diphenylethylenediamine (**5**), 1.25 X $10^{-5}$ M; 2.5 X $10^{-5}$ M; 5 X $10^{-5}$ M; 10 X $10^{-5}$ M in $CHCl_3$ at 25 °C.

With the increase in concentration of (*R*)/(*S*)-1,2-diphenylethylenediamine (**5**), the absorbance was also increased. At λ 341 nm, the difference in absorbance ($A-A_o = \Delta A$) was plotted as double reciprocal plot with increase in concentration [C] of 1,2-diphenylethylenediamine (**5**). The slope of the plot gives the association constant (K) value (Figure 5).

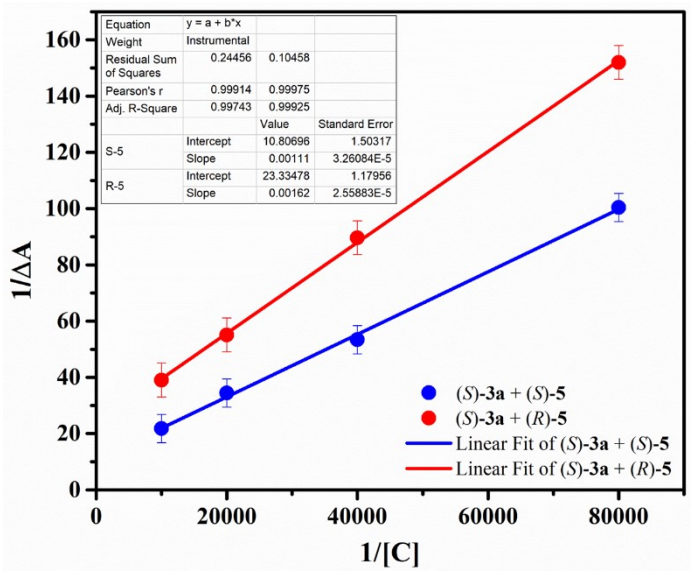



**Figure 5.** Benesi-Hildebrand plot for (*S*)-**3a** with (*R*) and (*S*)-1,2-diphenylethylenediamine (**5**) at $\lambda_{abs}$ 341 nm, linear relationship observed for 1/ΔA *versus* 1/[C] plot.

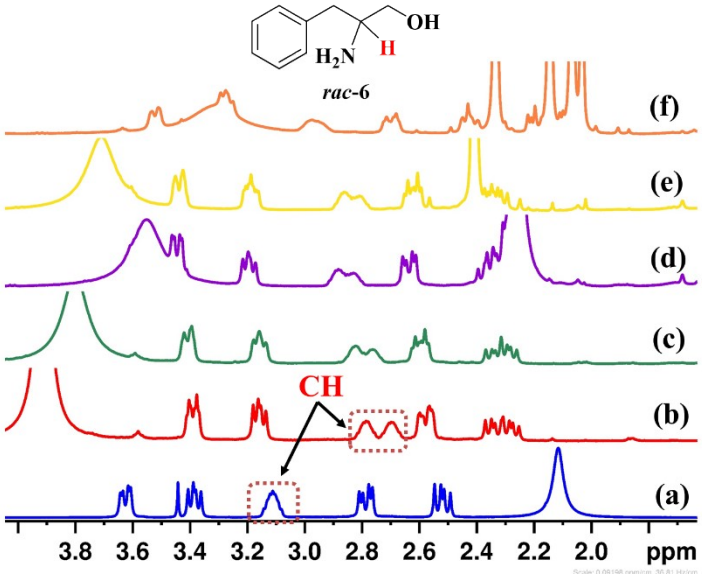



**Figure 6.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) of the (a) neat *rac*-**6** (b) *rac*-**6** with (*S*)-**1** (c) *rac*-**6** with (*S*)-**3a** (d) *rac*-**6** with (*S*)-**3b** (e) *rac*-**6** with (*S*)-**3c** (f) *rac*-**6** with (*S*)-**3d** in 0.6 mL chloroform-*d* at 25 ℃. C<u>H</u> resonances of *rac*-**6** are highlighted in wine red colour box.

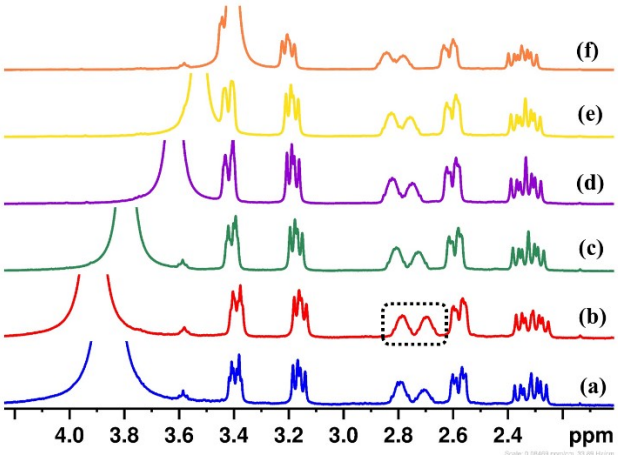



**Figure 7.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) for different experiments performed using variable concentrations of *rac*-**6** [0.0125 mmol (a), 0.025 mmol (b), 0.05 mmol (c), 0.075 mmol (d), 0.1 mmol (e), and 0.125 mmol (f)] with 0.1 mmol of (*S*)-**1** in 0.6 mL chloroform-*d* at 25 ℃. Best results for separation of C<u>H</u> resonances of *rac*-**6** are highlighted in black colour box.

## Secondary amines

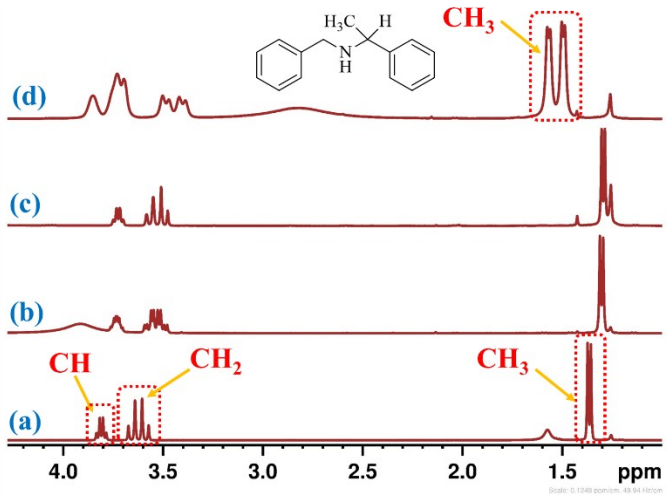



**Figure 8.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) for the neat *rac*-**7** (a) and the different experiments performed using 0.1 mmol of *rac*-**7** with 0.1 mmol of (*S*)-BINOL (b), (*S*)-**3a** (c), and (*R*)-**4** (d) as a CSA in 0.6 mL chloroform-*d* at 25 ℃. C<u>H</u>, C<u>H</u>$_2$, and C<u>H</u>$_3$ resonances of *rac*-**7** are highlighted in red colour box.

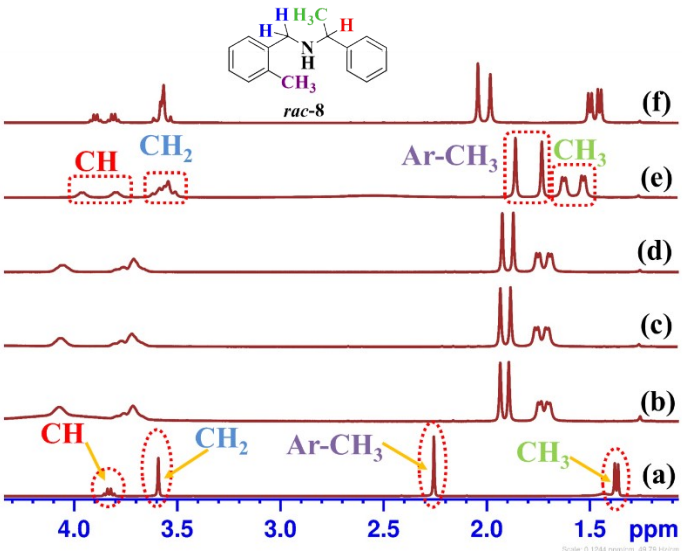
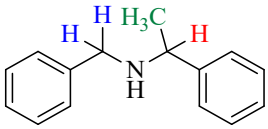
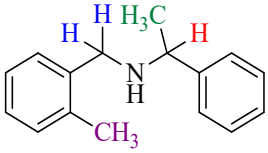
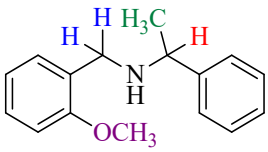
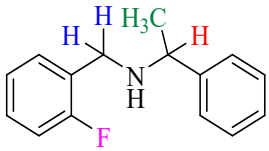
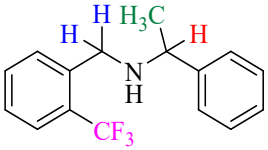



**Figure 9.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) for the neat *rac*-**8** (a) and the different experiments performed using variable concentrations [0.0125 mmol (b), 0.05 mmol (c), 0.075 mmol (d), 0.1 mmol (e), and 0.2 mmol (f)] of *rac*-**8** with 0.1 mmol of (*R*)-**4** in 0.6 mL chloroform-*d* at 25 ℃. C<u>H</u>, C<u>H</u>$_2$, C<u>H</u>$_3$, and Ar-C<u>H</u>$_3$ resonances of *rac*-**8** are highlighted in red colour box.

**Table 1**. The chemical shift difference ($\Delta\delta^{R/S}$) values of clearly baseline resolved $^{1}$H, $^{13}$C, and $^{19}$F signals of secondary amines (**7**-**11**).

| Entry | Secondary amines | Chemical shift difference ($\Delta\delta^{R/S}$)(ppm) | |
|---|---|---|---|
| | | For $^{1}$H/$^{19}$F signal | For $^{13}$C signal |
| 1 |  | $CH_2$ and CH peaks mix with each other<br>$CH_3$: 0.07 | $CH_2$: 0.25<br>$CH_3$: 0.04<br>CH: 0.30 |
| 2 |  | $CH_2$: no sep<br>$CH_3$: 0.09<br>CH: 0.16<br>$CH_3$: 0.13 | $CH_2$: 0.50<br>$CH_3$: 0.10<br>CH: 0.59<br>$CH_3$: 0.18 |
| 3 |  | $CH_2$ and CH peaks mix with each other<br>$CH_3$: 0.11<br>$OCH_3$: 0.10 | $CH_2$: no sep.<br>$CH_3$: 0.06<br>CH: no sep.<br>$OCH_3$: 0.20 |
| 4 |  | $CH_2$: 0.02<br>$CH_3$: 0.06<br>CH: 0.09<br>F: 0.14 | $CH_2$: 0.26<br>$CH_3$: 0.02<br>CH: 0.30 |
| 5 |  | $CH_2$: no sep.<br>$CH_3$: 0.07<br>CH: 0.13<br>$CF_3$: 0.03 | $CH_2$: no sep.<br>$CH_3$: 0.10<br>CH: 0.02<br>$CF_3$: 0.37 |

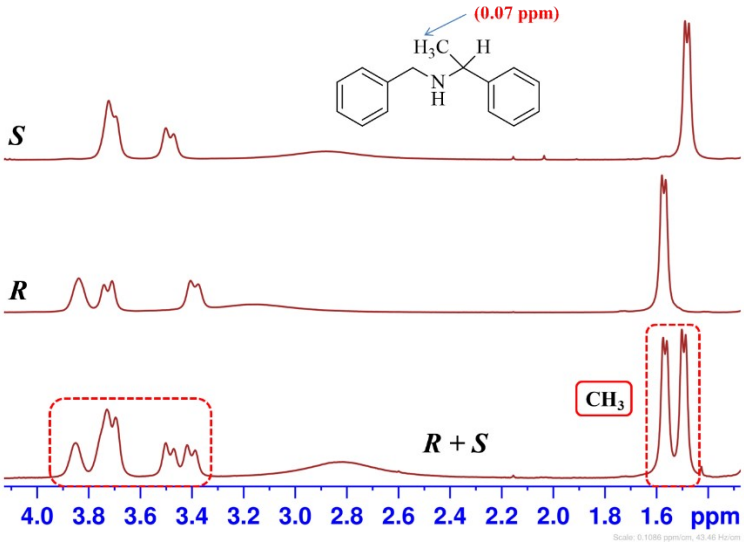



**Figure 10.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**7**/(*R*)-**7**/(*S*)-**7** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

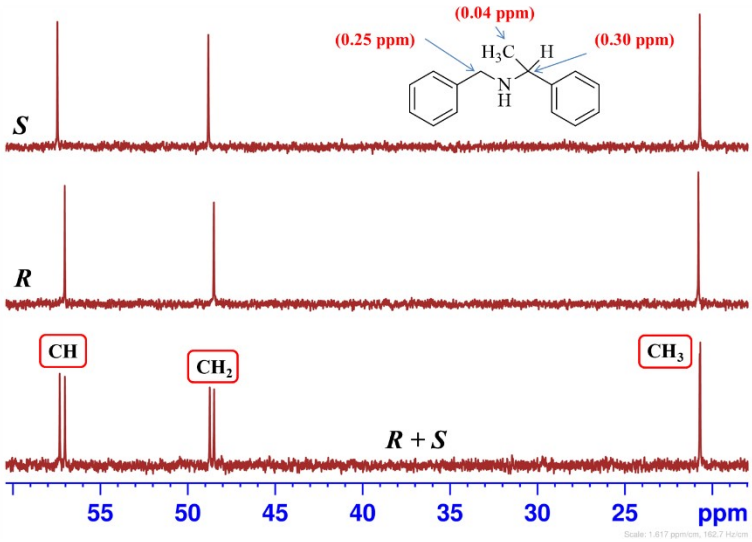



**Figure 11.** Partial stacked plot of $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**7**/(*R*)-**7**/(*S*)-**7** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

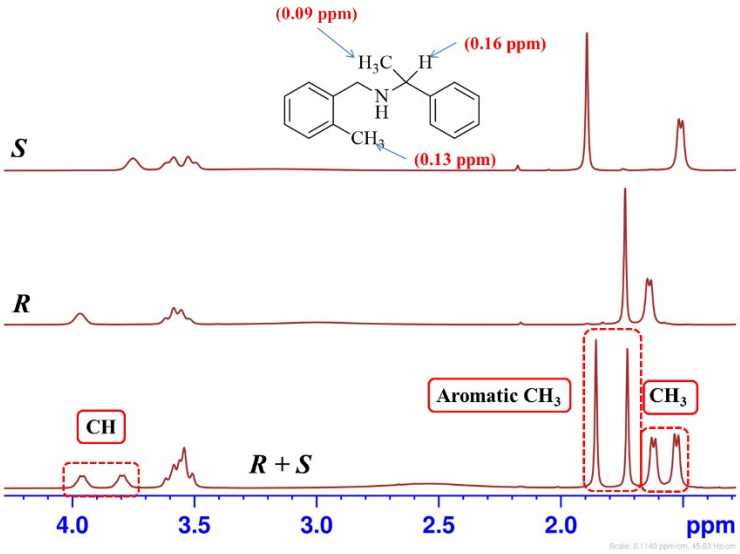



**Figure 12.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**8**/(*R*)-**8**/(*S*)-**8** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

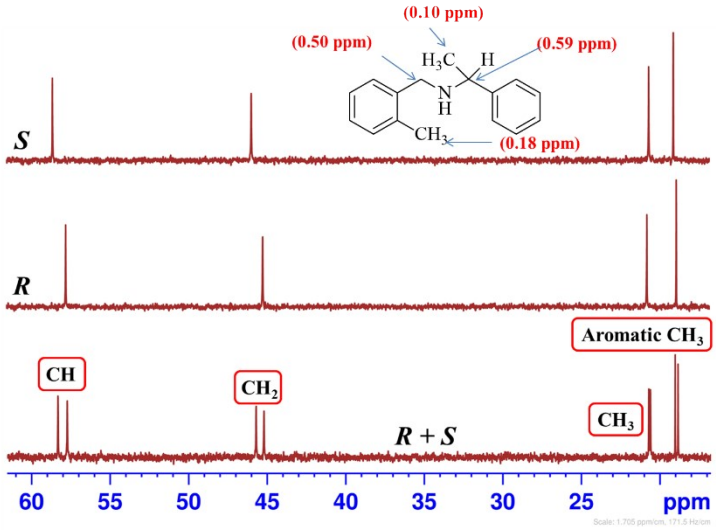



**Figure 13.** Partial stacked plot of $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**8**/(*R*)-**8**/(*S*)-**8** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

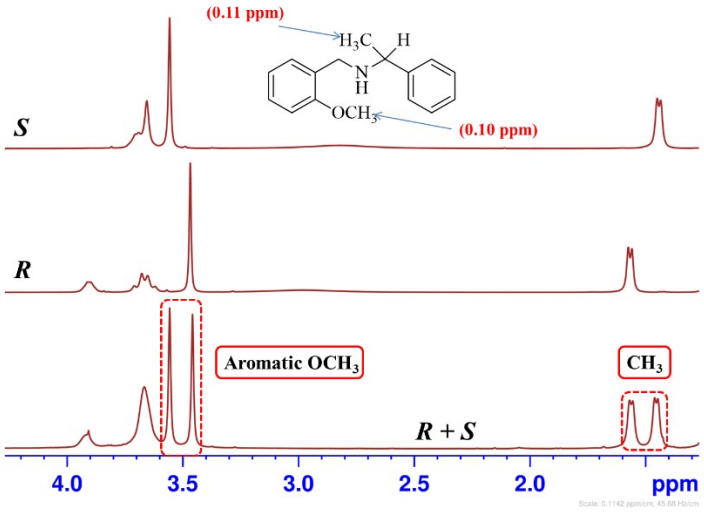



**Figure 14.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**9**/(*R*)-**9**/(*S*)-**9** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

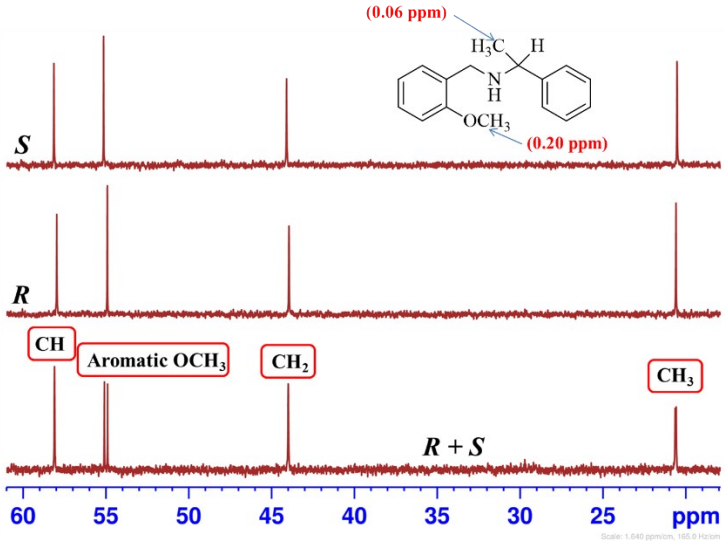



**Figure 15.** Partial stacked plot of $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**9**/(*R*)-**9**/(*S*)-**9** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

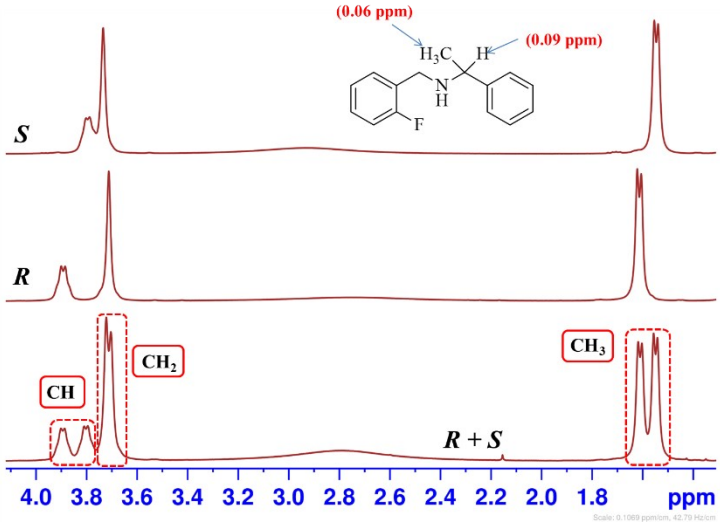



**Figure 16.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**10**/(*R*)-**10**/(*S*)-**10** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

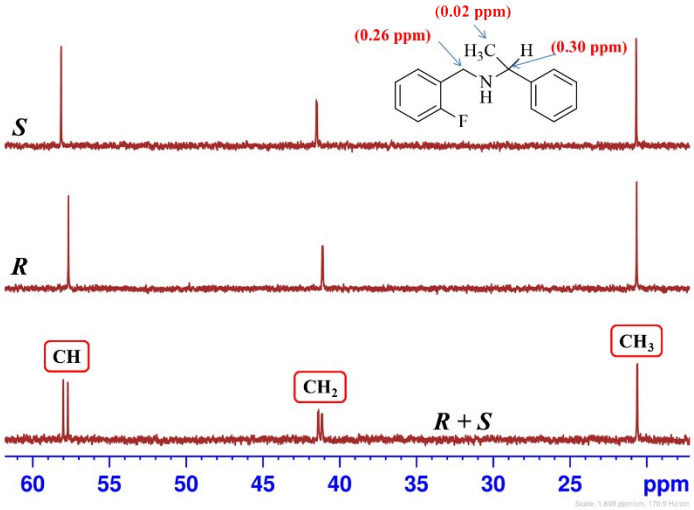



**Figure 17.** Partial stacked plot of $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**10**/(*R*)-**10**/(*S*)-**10** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

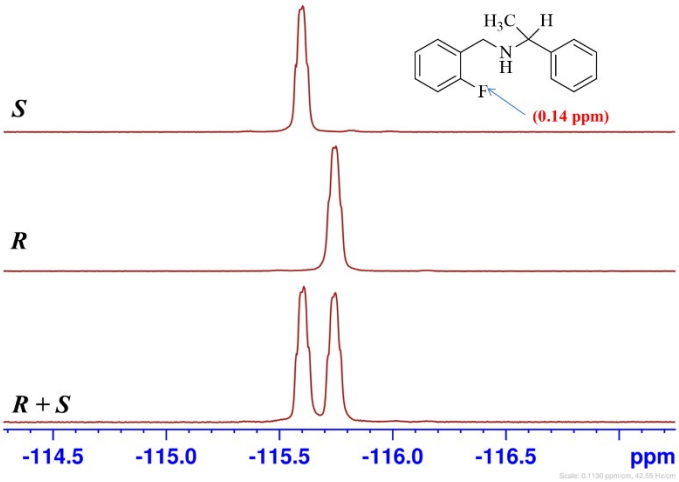



**Figure 18.** Partial stacked plot of $^{19}$F-NMR spectrum (376 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**10**/(*R*)-**10**/(*S*)-**10** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

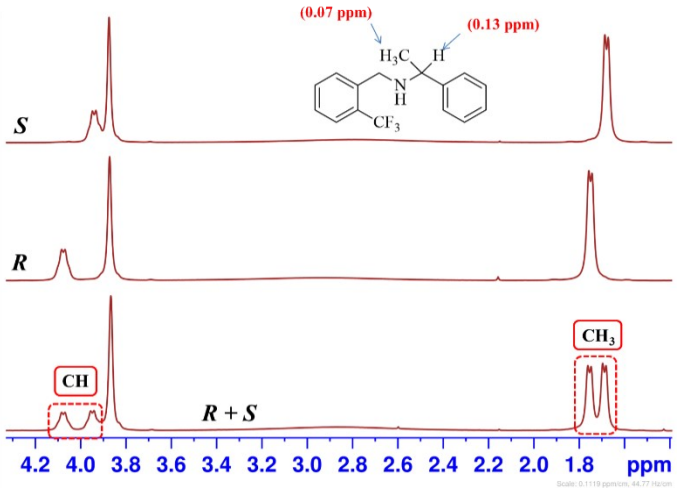



**Figure 19.** Partial stacked plot of $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**11**/(*R*)-**11**/(*S*)-**11** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

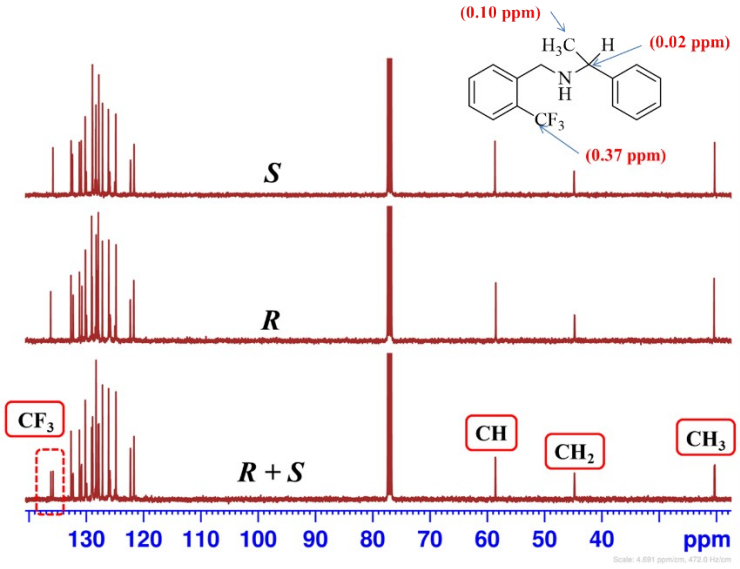



**Figure 20.** Partial stacked plot of $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**11**/(*R*)-**11**/(*S*)-**11** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

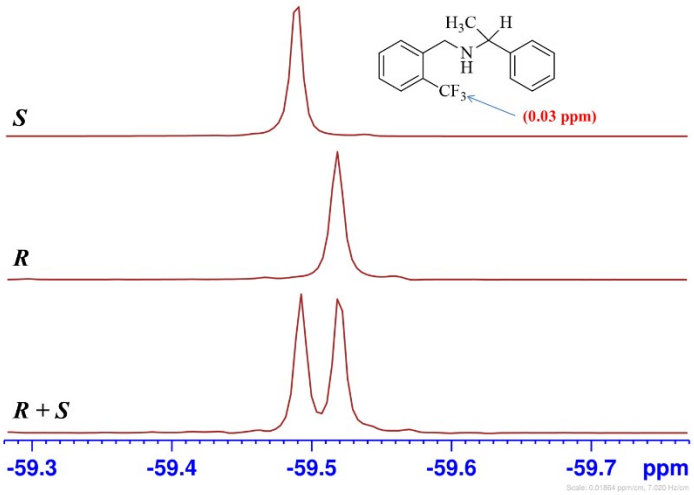
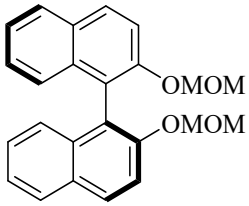



**Figure 21.** Partial stacked plot of $^{19}$F-NMR spectrum (376 MHz, $CDCl_3$) recorded for the experiment of 0.1 mmol of *rac*-**11**/(*R*)-**11**/(*S*)-**11** with 0.1 mmol of (*R*)-**4** as a CSA in 0.6 mL chloroform-*d* at 25℃.

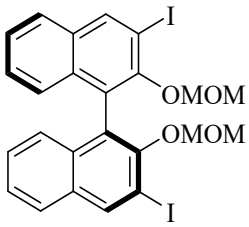
## Characterization of chiral solvating agents (CSAs) and analytes

### (*S*)-2,2'-Bis(methoxymethoxy)-1,1'-binaphthalene (12)[3]



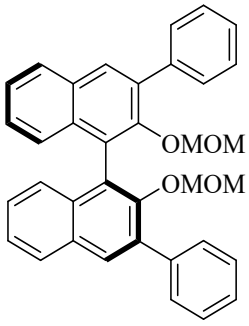
Compound **12** was synthesized by exactly following the reported literature procedure.[3] White solid, Yield (12.17 g, 98%); mp: 92-94 °C; $[\alpha]_{589}^{25}$ = -92.0° (*c* = 1.0, THF); $^{1}$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.94 (d, *J* = 9.0 Hz, 2H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 9.0 Hz, 2H), 7.34 (t, *J* = 7.9 Hz, 2H), 7.21 (t, *J* = 6.9 Hz, 2H), 7.15 (d, *J* = 8.5 Hz, 2H), 5.07 (d, *J* = 6.8 Hz, 2H), 4.97 (d, *J* = 6.8 Hz, 2H), 3.14 (s, 6H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 152.67 (2C), 134.04 (2C), 129.90 (2C), 129.41 (2C), 127.88 (2C), 126.31 (2C), 125.57 (2C), 124.08 (2C), 121.33 (2C), 117.32 (2C), 95.24 (2C), 55.84 (2C) ppm.

**(*S*)-3,3'-Diiodo-2,2'-bis(methoxymethoxy)-1,1'-binaphthalene (13)[4, 5]**



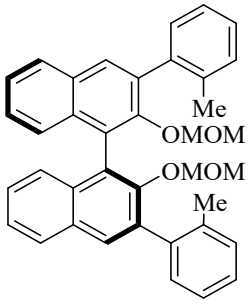

Compound **13** was synthesized by exactly following the reported literature procedure.[4] White solid, Yield (951 mg, 75%); mp: 86-88 °C; $[\alpha]_{589}^{25}$ = -9.5° (*c* = 1.0, THF); $^{1}$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 8.52 (s, 2H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.29-7.24 (m, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 4.79 (d, *J* = 5.6 Hz, 2H), 4.67 (d, *J* = 6.0 Hz, 2H), 2.57 (s, 6H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 152.13 (2C), 140.00, 139.97, 133.79 (2C), 132.18 (2C), 127.08 (2C), 126.71 (2C), 126.48 (2C), 126.21 (2C), 125.82 (2C), 99.38 (2C), 92.43 (2C), 56.50, 56.45, 29.68 (acetone impurity) ppm.

**(*S*)-2,2'-Bis(methoxymethoxy)-3,3'-diphenyl-1,1'-binaphthalene (14a)[3, 6]**



A two-necked 100 mL Schlenk flask was oven-dried for 4 h and flushed with argon. The (*S*)-3,3'-diiodo-2,2'-bis(methoxymethoxy)-1,1'-binaphthalene (**13**) (700 mg, 1.12 mmol), phenylboronic acid (272 mg, 2.23 mmol), barium hydroxide octahydrate (878 mg, 2.78 mmol) and tetrakis(triphenylphosphine)palladium(0) (129 mg, 0.11 mmol, 10 mol%) were added into it and again the flask was evacuated and backfilled with argon. 10 mL of 1,4-dioxane and 3 mL water was added by syringe to the Schlenk flask and the reaction mixture was heated to 80 °C for 24 h. The reaction progress was monitored by TLC. After cooling the reaction mixture to room temperature, the solution was concentrated under reduced pressure and the residue was extracted with dichloromethane (3 x 10 mL). The combined organic layers were washed with 1N aqueous hydrochloride solution (2 x 10 mL), brine solution, dried over anhydrous $Na_2SO_4$, and concentrated under reduced pressure. The obtained crude product **14a** was purified by column chromatography (hexane/ethyl acetate) (19:1 v/v) and foamy white solid was obtained as pure product **14a** in 85% yield.[6] Foamy white solid, Yield (499 mg, 85%); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.95 (s, 2H), 7.89 (d, $J$ = 8.1 Hz, 2H), 7.76 (d, $J$ = 7.3 Hz, 4H), 7.47 (t, $J$ = 7.7 Hz, 4H), 7.44-7.36 (m, 4H), 7.29 (s, 4H), 4.41 (d, $J$ = 5.8 Hz, 2H), 4.37 (d, $J$ = 5.7 Hz, 2H), 2.34 (s, 6H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 151.32 (2C), 139.04 (2C), 135.48 (2C), 133.62 (2C), 130.86 (2C), 130.59 (2C), 129.65 (4C), 128.35 (4C), 127.87 (2C), 127.31 (2C), 126.53 (2C), 126.44 (2C), 126.32 (2C), 125.19 (2C), 98.52 (2C), 55.85 (2C) ppm.

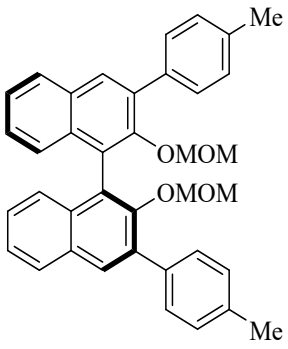
**(*S*)-2,2'-Bis(methoxymethoxy)-3,3'-di-*o*-tolyl-1,1'-binaphthalene (14b)[7]**




Compound **14b** was synthesized by following the procedure of compound **14a**. White solid, Yield (492 mg, 79%); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.88-7.83 (m, 4H), 7.49-7.25 (m, 14H), 4.44-4.17 (m, 4H), 2.35-2.21 (m, 12H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 152.13, 139.26, 138.90, 137.80, 137.07, 136.22, 135.73, 133.65, 130.81, 130.63, 130.44, 130.35, 130.23, 129.86,

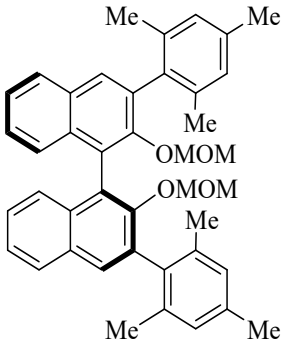
129.71, 127.88, 127.79, 127.66, 127.61, 126.36, 126.25, 126.15, 125.81, 125.59, 125.16, 125.02, 98.54, 98.14, 77.36, 77.04, 76.72, 55.67, 55.52, 20.34, 20.03 ppm.

**(*S*)-2,2'-Bis(methoxymethoxy)-3,3'-di-*p*-tolyl-1,1'-binaphthalene (14c)[8]**




Compound **14c** was synthesized by following the procedure of compound **14a**. White solid, Yield (513 mg, 83%); $^{1}$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.92 (s, 2H), 7.86 (d, $J$ = 8.4 Hz, 2H), 7.65 (d, $J$ = 8.0 Hz, 4H), 7.41-7.37 (m, 2H), 7.29-7.24 (m, 8H), 4.41 (d, $J$ = 6.0 Hz, 2H), 4.36 (d, $J$ = 6.0 Hz, 2H), 2.41 (s, 6H), 2.33 (s, 6H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 151.32 (2C), 137.05 (2C), 136.07 (2C), 135.34 (2C), 133.53 (2C), 130.89 (2C), 130.40 (2C), 129.44 (4C), 129.08 (4C), 127.79 (2C), 126.57 (2C), 126.46 (2C), 126.15 (2C), 125.10 (2C), 98.39 (2C), 55.84 (2C), 21.26 (2C) ppm.

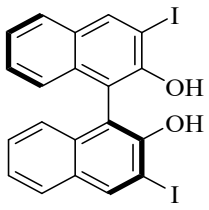
**(*S*)-3,3'-Dimesityl-2,2'-bis(methoxymethoxy)-1,1'-binaphthalene (14d)[9]**




Compound **14d** was synthesized by following the procedure of compound **14a**. White solid, Yield (522 mg, 76%); $^{1}$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.83 (d, $J$ =8.1 Hz, 2H), 7.71 (s, 2H), 7.42-7.27 (m, 6H), 6.96 (s, 4H), 4.31 (d, $J$ = 5.7 Hz, 2H), 4.27 (d, $J$ = 5.7 Hz, 2H), 2.32 (s, 6H), 2.30 (s, 6H), 2.21 (s, 6H), 2.14 (s, 6H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 151.96 (2C),

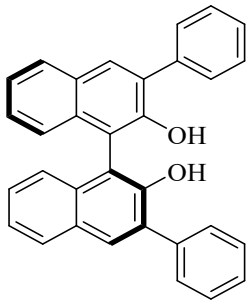
137.17 (2C), 136.86 (2C), 136.64 (2C), 135.54 (2C), 134.61 (2C), 133.59 (2C), 130.88 (2C), 130.72 (2C), 128.09 (4C), 127.76 (2C), 126.30 (2C), 126.22 (2C), 126.11 (2C), 124.92 (2C), 97.99 (2C), 55.60 (2C), 21.10 (2C), 20.99 (2C), 20.64 (2C) ppm.

**(*S*)-3,3'-diiodo-[1,1'-binaphthalene]-2,2'-diol (2)[8, 3]**



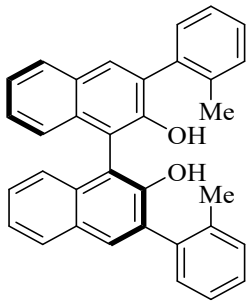

The compound **13** (500 mg, 0.798 mmol) was dissolved in 10 mL of tetrahydrofuran and 20 mL of methanol. 10 mL of hydrochloride (12 M) solution was added to the above solution and the resulting reaction mixture was stirred at room temperature for 9 h. Tetrahydrofuran and methanol was evaporated under reduced pressure and the residue was extracted with dichloromethane (3 x 30 mL). The combined organic layers were washed with 10% aqueous sodium carbonate solution, brine, dried over $Na_2SO_4$, and concentrated under reduced pressure. The obtained product was further purified by column chromatography (hexane/ethyl acetate) (19:1 v/v) and light yellow solid was obtained as pure product **2** in 98% yield.[8] Light yellow solid, Yield (421 mg, 98%); mp: 280-282 °C; $[\alpha]_{589}^{25}$ = -90.8° (*c* = 1.0, THF); $^1$H-NMR (400 MHz, DMSO-$d_6$): $\delta$ = 9.01 (s, 2H), 8.57 (s, 2H), 7.85 (d, *J* = 7.9 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 2H), 7.21 (t, *J* = 7.0 Hz, 2H), 6.76 (d, *J* = 8.3 Hz, 2H) ppm. $^{13}$C-NMR (100 MHz, DMSO-$d_6$): $\delta$ = 152.26 (2C), 139.62 (2C), 134.17 (2C), 130.50 (2C), 127.51 (2C), 127.28 (2C), 124.44 (2C), 123.86 (2C), 114.82 (2C), 90.97 (2C) ppm.

**(*S*)-3,3'-diphenyl-[1,1'-binaphthalene]-2,2'-diol (3a)[8, 10]**



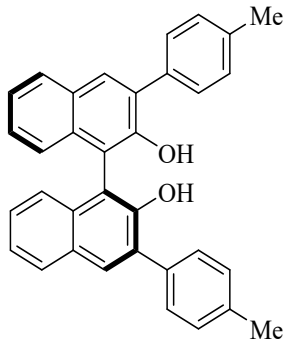
Compound **3a** was obtained after deprotection of compound **14a** under acidic conditions following the procedure of compound **2**. The product **3a** was further purified by column chromatography (hexane/ethyl acetate) (49:1 v/v) and foamy white solid was obtained as pure product **3a** in 98% yield.[8] Foamy white solid, Yield (408 mg, 98%); mp: 198-200 °C; $[\alpha]_{589}^{25}$ = -97.7° (*c* = 1, THF); $^{1}$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 8.00 (s, 2H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 7.8 Hz, 4H), 7.47 (t, *J* = 7.8 Hz, 4H), 7.40-7.34 (m, 4H), 7.29 (t, *J* = 6.8 Hz, 2H), 7.23-7.20 (m, 2H), 5.34 (s, 2H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 150.16 (2C), 137.50 (2C), 132.99 (2C), 131.40 (2C), 130.71 (2C), 129.63 (4C), 129.47 (2C), 128.50 (4C), 128.47 (2C), 127.78 (2C), 127.36 (2C), 124.35 (2C), 124.31 (2C), 112.46 (2C) ppm.

**(*S*)-3,3'-di-*o*-tolyl-[1,1'-binaphthalene]-2,2'-diol (3b)[7, 8]**



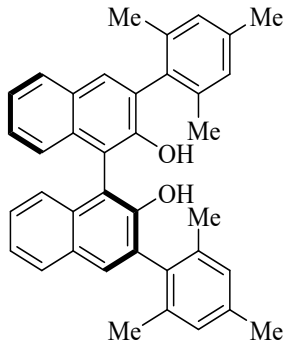

Compound **3b** was obtained after deprotection of compound **14b** under acidic conditions following the procedure of compound **2**. The product **3b** was further purified by column chromatography (hexane/ethyl acetate) (49:1 v/v) and foamy white solid was obtained as pure product **3b** in 96% yield.[8] Foamy white solid, Yield (397 mg, 96%); mp: 94-96 °C; $[\alpha]_{589}^{25}$ = -139.2° (*c* = 0.13, $CH_2Cl_2$); $^{1}$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.88 (d, *J* = 8.0 Hz, 2H), 7.85 (s, 2H), 7.40-7.25 (m, 14H), 5.12 (s, 2H), 2.26 (s, 6H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 150.19 (2C), 137.26 (2C), 136.94 (2C), 133.26 (2C), 131.07 (2C), 130.89 (2C), 130.29 (2C), 130.12 (2C), 129.23 (2C), 128.35 (2C), 128.28 (2C), 127.12 (2C), 126.01 (2C), 124.41 (2C), 124.16 (2C), 112.42 (2C), 20.00 (2C) ppm.

**(*S*)-3,3'-di-*p*-tolyl-[1,1'-binaphthalene]-2,2'-diol (3c)[8]**




Compound **3c** was obtained after deprotection of compound **14c** under acidic conditions following the procedure of compound **2**. The product **3c** was further purified by column chromatography (hexane/ethyl acetate) (49:1 v/v) and white solid was obtained as pure product **3c** in 98% yield.[8] White solid, Yield (423 mg, 98%); mp: 150-152 °C; $[\alpha]_{589}^{25}$ = -94.4° ($c$ = 0.13, $CH_2Cl_2$); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.98 (s, 2H), 7.89 (d, $J$ = 8.0 Hz, 2H), 7.61 (d, $J$ = 7.5 Hz, 4H), 7.36 (t, $J$ = 7.8 Hz, 2H), 7.30-7.28 (m, 6H), 7.22-7.20 (m, 2H), 5.35 (s, 2H), 2.41 (s, 6H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 150.22 (2C), 137.62 (2C), 134.54 (2C), 132.92 (2C), 131.11 (2C), 130.68 (2C), 129.48 (6C), 129.26 (4C), 128.39 (2C), 127.18 (2C), 124.34 (2C), 124.25 (2C), 112.51 (2C), 21.27 (2C) ppm.

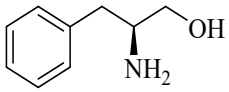
**(*S*)-3,3'-dimesityl-[1,1'-binaphthalene]-2,2'-diol (3d)[7, 8]**




Compound **3d** was obtained after deprotection of compound **14d** under acidic conditions following the procedure of compound **2**. The product **3d** was further purified by column chromatography (hexane/ethyl acetate) (49:1 v/v) and white solid was obtained as pure product **3d** in 96% yield.[8] White solid, Yield (429 mg, 96%); mp: 110-112 °C; $[\alpha]_{589}^{25}$ = -86.18° ($c$ = 1, THF); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.87 (d, $J$ = 8.0 Hz, 2H), 7.74 (s, 2H), 7.38 (t, $J$ = 7.0

Hz, 2H), 7.31 (t, *J* = 6.8 Hz, 2H), 7.25-7.23 (m, 2H), 7.01 (s, 4H), 5.01 (s, 2H), 2.34 (s, 6H), 2.14 (s, 6H), 2.07 (s, 6H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 150.03 (2C), 137.78 (2C), 137.17 (2C), 137.10 (2C), 133.44 (2C), 132.93 (2C), 130.68 (2C), 129.47 (2C), 129.45 (2C), 128.54 (2C), 128.46 (2C), 128.27 (2C), 126.84 (2C), 124.57 (2C), 123.87 (2C), 112.96 (2C), 21.17 (2C), 20.56 (2C), 20.46 (2C) ppm.

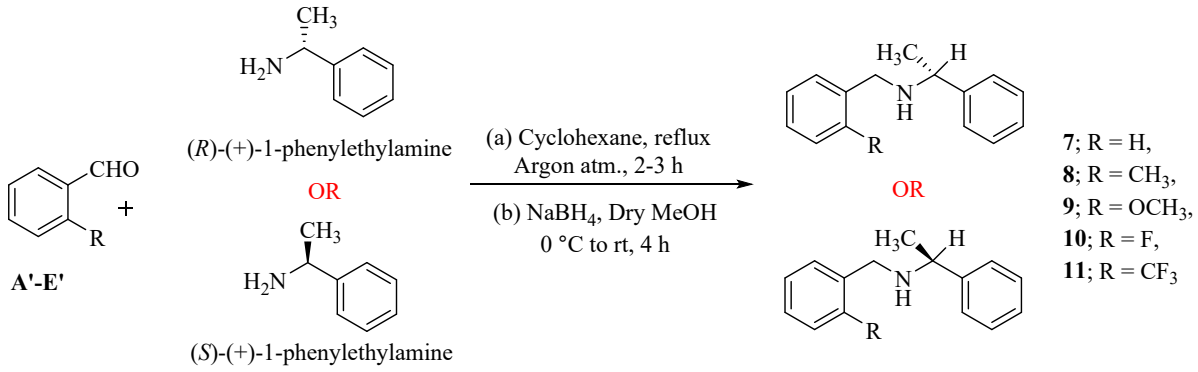
**(*S*)-2-amino-3-phenylpropan-1-ol (6)[1]**




(*S*)-2-amino-3-phenylpropan-1-ol (**6**) was prepared from L-phenyl alanine in two steps. **Step I**: To the ice-cold suspension of L-phenyl alanine (1 g, 6.0 mmol) in ethanol (30 mL), $SOCl_2$ (0.7 mL, 9.1 mmol) was added dropwise with stirring and the reaction mixture was refluxed for 4 h. Ethanol was evaporated in vacuo and the obtained solid was washed with dry diethyl ether (4 x 60 mL), filtered and dried on vaccum pump. The obtained solid was used as such in second step. **Step II**: The solution of L-phenylalanine ethyl ester hydrochloride (1.3 g, 5.6 mmol) in 50% aqueous ethanol (15 mL) was dropwise added with stirring to the solution of sodium borohydride (934 mg, 24.7 mmol) in 50% aqueous ethanol (15 mL) and the reaction mixture was refluxed for 5 h. Ethanol was evaporated in vacuo and the obtained aqueous solution was extracted with ethyl acetate (3 x 40 mL). The combined organic layer was washed with brine solution, dried over anhydrous $Na_2SO_4$, and concentrated under reduced pressure. The obtained product (*S*)-**6** was further purified by passing through a silica gel pad with ethyl acetate as an eluent. The pale yellow solid was obtained as a product (*S*)-**6** in 71% yield.[1] Pale yellow solid, Yield (605 mg, 71%); mp: 84-86 °C; $[\alpha]_{589}^{25}$ = -25.5 (*c* = 1, EtOH); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.31-7.28 (m, 2H), 7.23-7.17 (m, 3H), 3.62 (dd, *J* = 10.7, 3.5 Hz, 1H), 3.40-3.36 (m, 1H), 3.11 (quint, *J* = 8.8 Hz, 1H), 2.78 (dd, *J* = 13.3, 5.1 Hz, 1H), 2.54-2.49 (m, 1H), 2.11 (brs, 3H, OH, $NH_2$) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 138.69, 129.21 (2C), 128.58 (2C), 126.43, 66.26, 54.20, 40.84 ppm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_9H_{14}NO$): 152.1075, found: 152.1063. D-Phenylalanine was used to afford the (*R*)-**6** in 72% yield.

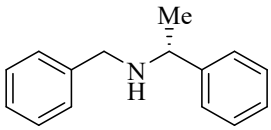
**General procedure for the synthesis of secondary amines (7-11)[2]**

In a 100 mL round bottom flask equipped with Dean-Stark apparatus, a mixture of (*R*)-(+)-1-phenylethylamine or (*S*)-(-)-1-phenylethylamine (1.9 mL, 14.9 mmol) and benzaldehydes **A'-E'** (16.5 mmol) in dry cyclohexane (40 mL) was refluxed for 2-3 h under an argon atmosphere. After cooling the reaction mixture to room temperature, it was concentrated under reduced pressure. The obtained crude imine was dissolved in dry methanol (30 mL) and sodium borohydride (0.8 g, 21.2 mmol) was added in four equal portions in 15 minutes at 0 °C. After 30 minutes, the reaction mixture was stirred at room temperature for 3-4 h. After then the solution was concentrated under reduced pressure and 30% aqueous ammonium hydroxide solution (50 mL) was added to it. The product was extracted with diethyl ether (3 x 30 mL) and the obtained organic layers were washed with brine solution (3 x 40 mL), dried over $Na_2SO_4$, filtered and concentrated under reduced pressure. The crude product was obtained as a yellow oil so it is further diluted with diethyl ether (100 mL) and 1N aqueous hydrochloride (10 mL) was added to it. The obtained white solid was filtered, washed with diethyl ether and dissolved in 4N aqueous sodium hydroxide solution (40 mL). After then the basic solution was extracted with diethyl ether (3 x 30 mL) and the obtained organic layers were washed with brine (1 x 100 mL), dried over $Na_2SO_4$, filtered and concentrated under reduced pressure. The pure product was obtained as a colorless oil in 92-98% yield.



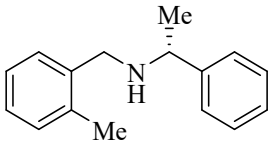

**Scheme 1.** Synthesis of secondary amines (**7**-**11**) from their corresponding aldehydes and (*R*)-(+)-1-phenylethylamine or (*S*)-(-)-1-phenylethylamine.

**(*R*)-*N*-benzyl-1-phenylethan-1-amine (7)**[2, 11]



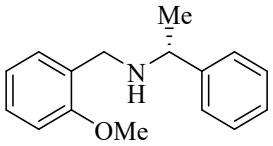
Colorless oil, Yield (3.1 g, 98%); $[\alpha]_{589}^{25}$ = +47.9° (*c* = 1.42, $CHCl_3$); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.35-7.21 (m, 10H), 3.80 (q, *J* = 6.6 Hz, 1H), 3.66 (d, *J* = 13.1 Hz, 1H), 3.59 (d, *J* = 13.2 Hz, 1H), 1.57 (s, 1H), 1.36 (d, *J* = 6.6 Hz, 3H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 145.62, 140.69, 128.51 (2C), 128.41 (2C), 128.17 (2C), 126.97, 126.88, 126.75 (2C), 57.53, 51.70, 24.58 ppm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{15}H_{18}N$): 212.1439, found: 212.1434. (*S*)-(-)-1-phenylethylamine was used to afford (*S*)-**7** in 96% yield.

**(*R*)-*N*-(2-methylbenzyl)-1-phenylethan-1-amine (8)[2]**



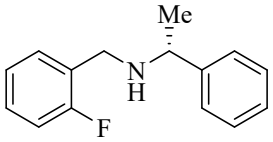

Colorless oil, Yield (3.2 g, 95%); $[\alpha]_{589}^{25}$ = +40.7° (*c* = 1.13, $CHCl_3$); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.38-7.32 (m, 4H), 7.26-7.24 (m, 2H), 7.16-7.13 (m, 3H), 3.84 (q, *J* = 6.5 Hz, 1H), 3.60 (s, 2H), 2.26 (s, 3H), 1.47 (brs, 1H, NH), 1.38 (d, *J* = 6.5 Hz, 3H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 145.72, 138.58, 136.40, 130.24, 128.53, 128.42 (2C), 126.91 (2C), 126.69 (2C), 125.85, 58.20, 49.67, 24.57, 18.90 ppm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{16}H_{20}N$): 226.1595, found: 226.1589. (*S*)-(-)-1-phenylethylamine was used to afford (*S*)-**8** in 93% yield.

**(*R*)-*N*-(2-methoxybenzyl)-1-phenylethan-1-amine (9)[2]**



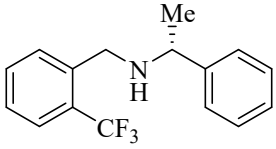

Colorless oil, Yield (3.4 g, 94%); $[\alpha]_{589}^{25}$ = +54.8° (*c* = 1.13, $CHCl_3$); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.37-7.31 (m, 4H), 7.25-7.20 (m, 2H), 7.16-7.14 (m, 1H), 6.91-6.84 (m, 2H), 3.80-3.74 (m, 4H), 3.70 (d, *J* = 13.3 Hz, 1H), 3.57 (d, *J* = 13.3 Hz, 1H), 1.91 (s, 1H), 1.34 (d, *J* = 6.6 Hz, 3H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 157.74, 145.82, 129.98, 128.58, 128.38 (2C), 128.15, 126.87 (2C), 126.83, 120.38, 110.27, 57.19, 55.22, 47.26, 24.61 ppm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{16}H_{20}NO$): 242.1544, found: 242.1537. (*S*)-(-)-1-phenylethylamine was used to afford (*S*)-**9** in 92% yield.

**(*R*)-*N*-(2-fluorobenzyl)-1-phenylethan-1-amine (10)[2]**




Colorless oil, Yield (3.3 g, 96%); $[\alpha]_{589}^{25}$ = +54.6° (*c* = 1.13, $CHCl_3$); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.36-7.31 (m, 4H), 7.28-7.18 (m, 3H), 7.07 (t, *J* = 7.4 Hz, 1H), 7.00 (t, *J* = 8.9 Hz, 1H), 3.79 (q, *J* = 6.6 Hz, 1H), 3.72 (d, *J* = 13.6 Hz, 1H), 3.64 (d, *J* = 13.6 Hz, 1H), 1.66 (s, 1H), 1.36 (d, *J* = 6.6 Hz, 3H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 161.29 (d, *J* = 244 Hz), 145.39, 130.50 (d, *J* = 5.0 Hz), 128.59 (d, *J* = 8.0 Hz), 128.51 (2C), 127.48 (d, *J* = 14 Hz), 127.02, 126.77 (2C), 124.00 (d, *J* = 3.0 Hz), 115.30 (d, *J* = 22 Hz), 57.47, 45.32 (d, *J* = 3.0 Hz), 24.56 ppm. $^{19}$F-NMR (376 MHz, $CDCl_3$): $\delta$ = -119.31 (s) ppm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{15}H_{17}FN$): 230.1345, found: 230.1340. (*S*)-(-)-1-phenylethylamine was used to afford (*S*)-**10** in 96% yield.

**(*R*)-1-phenyl-*N*-(2-(trifluoromethyl)benzyl)ethan-1-amine (11)[2, 12]**




Colorless oil, Yield (4.0 g, 96%); $[\alpha]_{589}^{25}$ = +30.3° (*c* = 1.13, $CHCl_3$); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$ = 7.59 (t, *J* = 8.2 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.38-7.29 (m, 5H), 7.25 (t, *J* = 8.8 Hz, 1H), 3.86-3.74 (m, 3H), 1.58 (s, 1H), 1.37 (d, *J* = 6.5 Hz, 3H) ppm. $^{13}$C-NMR (100 MHz, $CDCl_3$): $\delta$ = 145.39, 139.27, 131.83, 130.82, 128.51, 127.05, 126.85, 126.73, 125.85 (q, *J* = 6.0 Hz), 58.01, 48.03 (q, *J* = 2.0 Hz), 24.52 ppm. $^{19}$F-NMR (376 MHz, $CDCl_3$): $\delta$ = -59.52 (s) ppm. HRMS(ESI): *m/z* calcd. for $[M + H]^+$ ($C_{16}H_{17}F_3N$): 280.1313, found: 280.1308. (*S*)-(-)-1-phenylethylamine was used to afford (*S*)-**11** in 94% yield.

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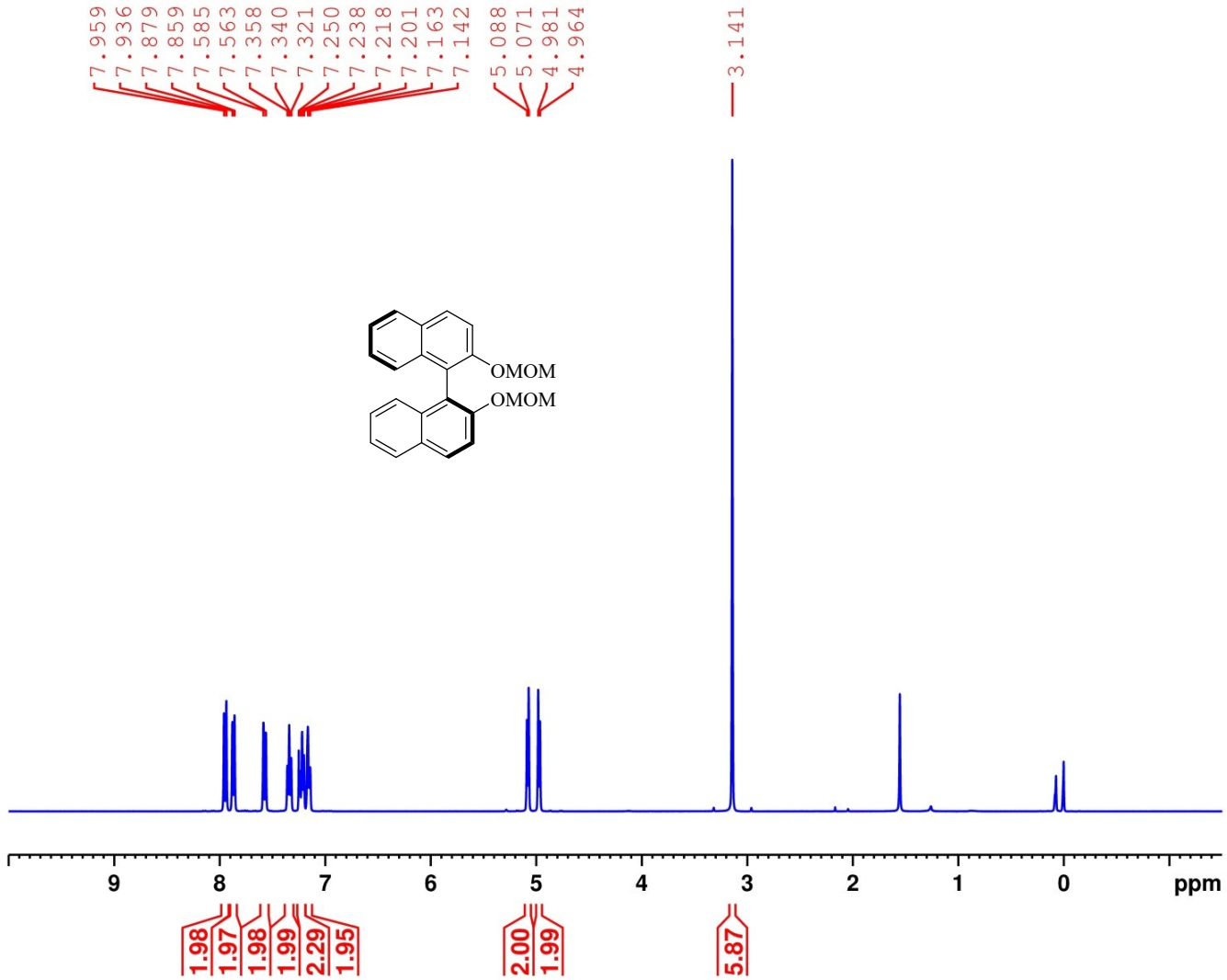


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TE                298.0 K
D1            1.00000000 sec
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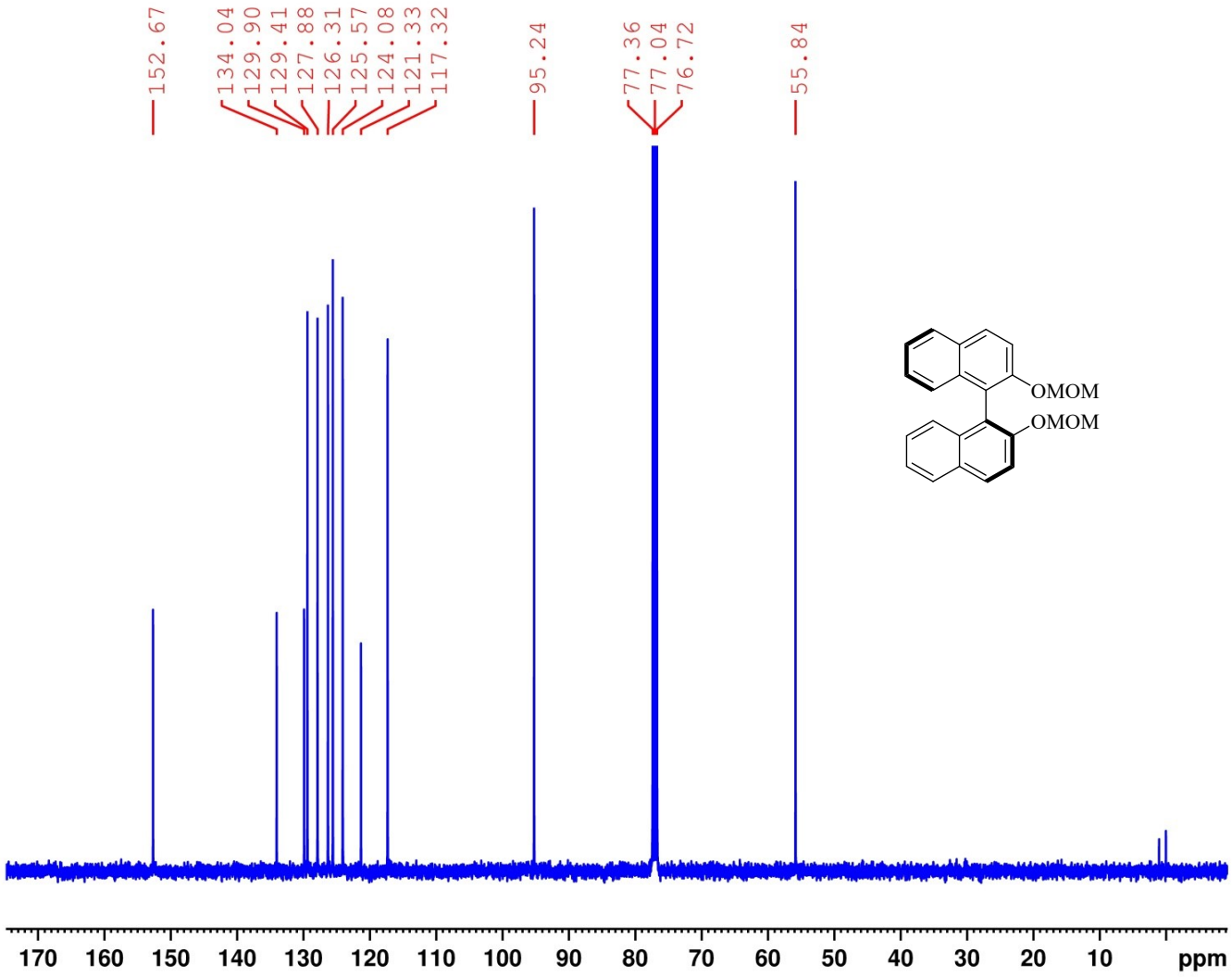


BRUKER

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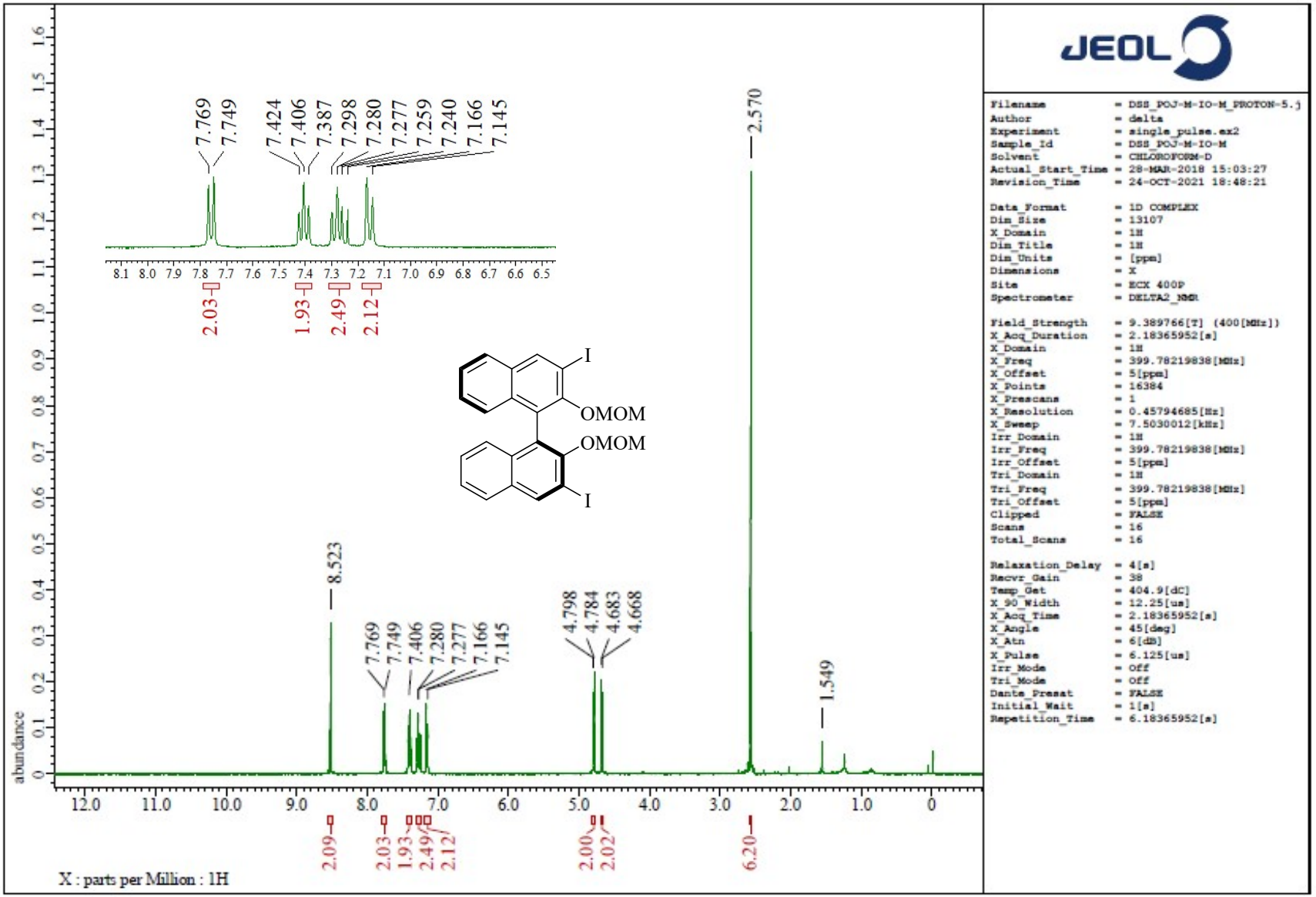
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1.93
2.49
2.12
I
OMOM
OMOM
I
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4.683
4.668
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abundance
2.09
2.03
1.93
2.49
2.12
2.00
2.02
6.20
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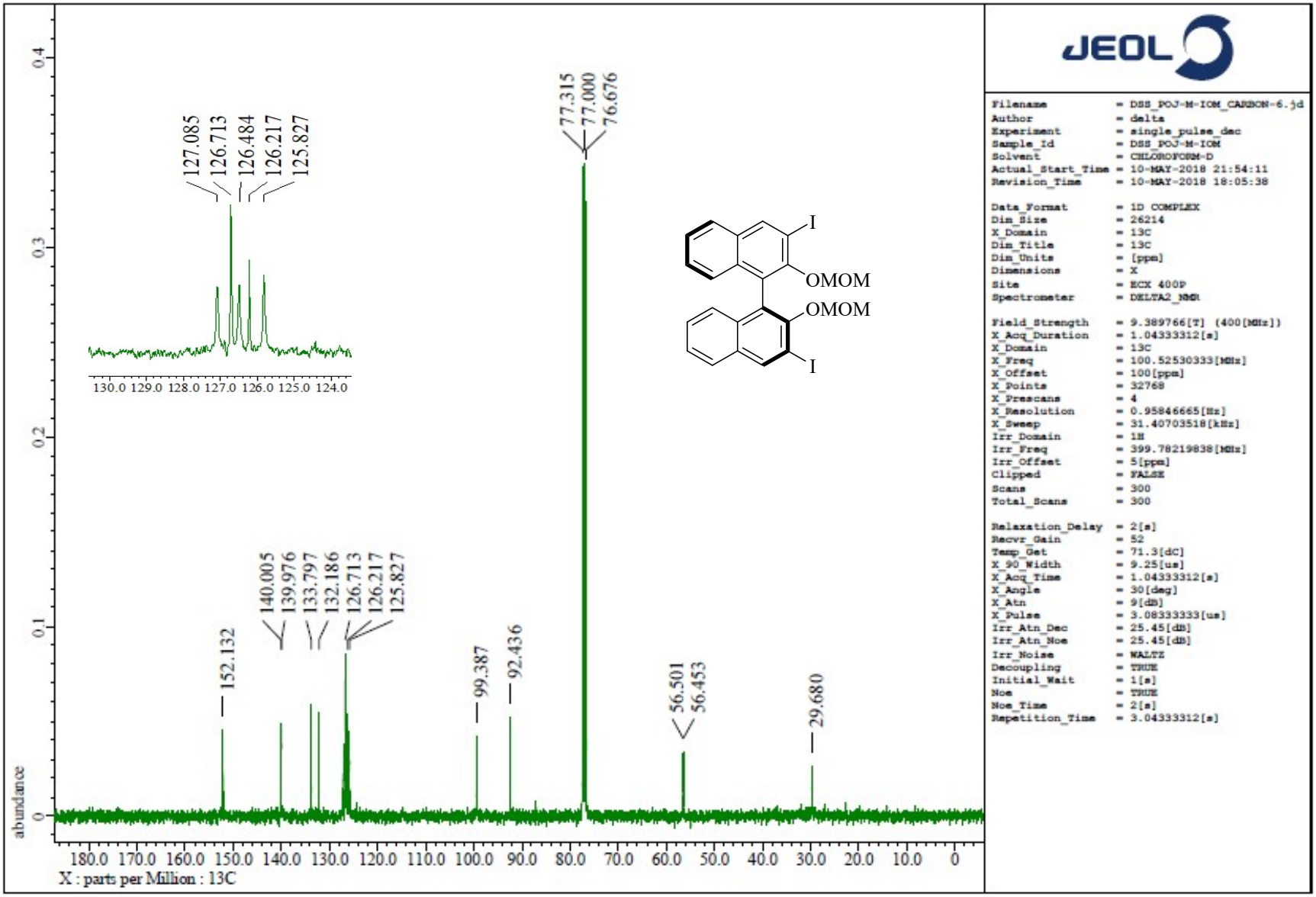


JEOL

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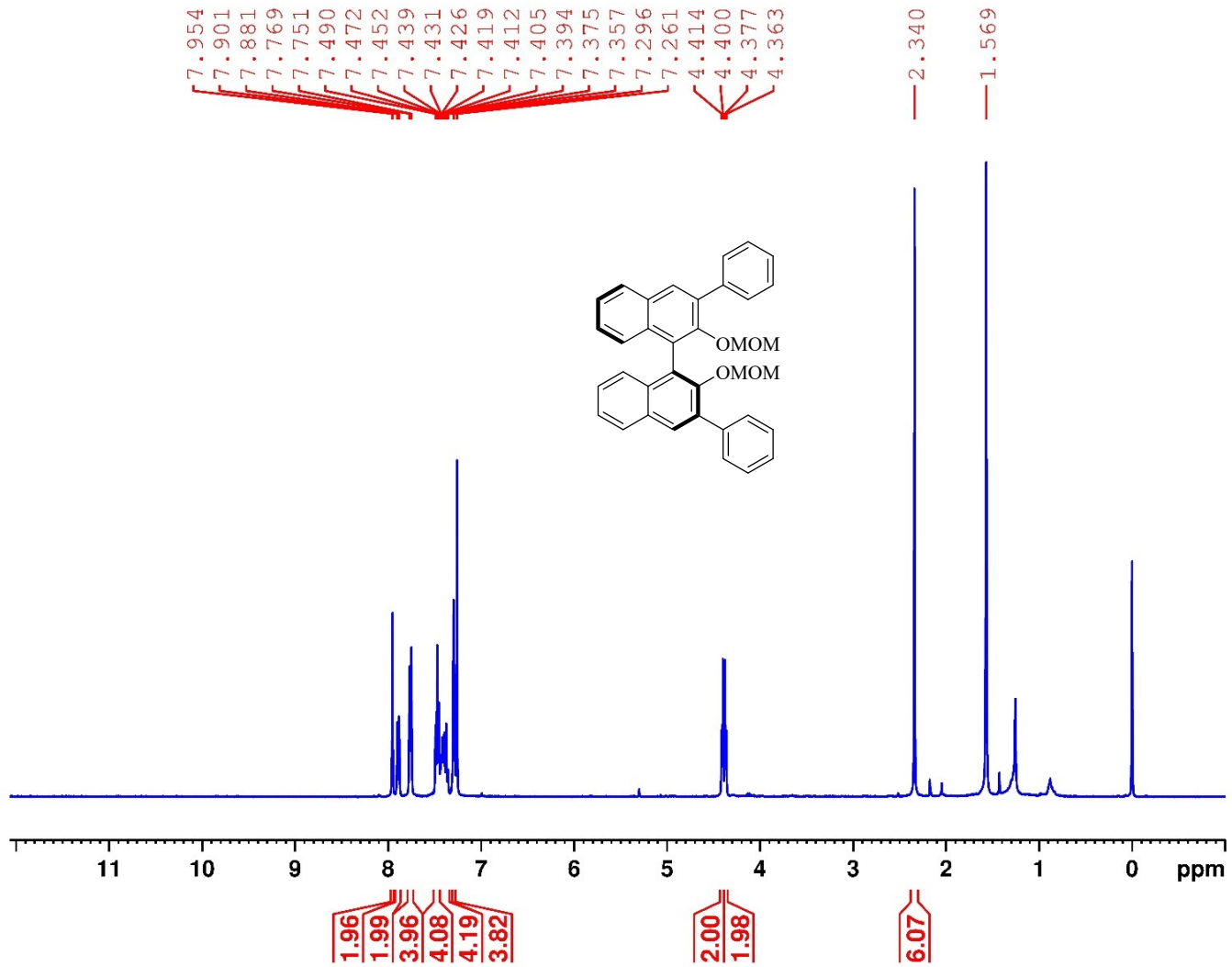


BRUKER

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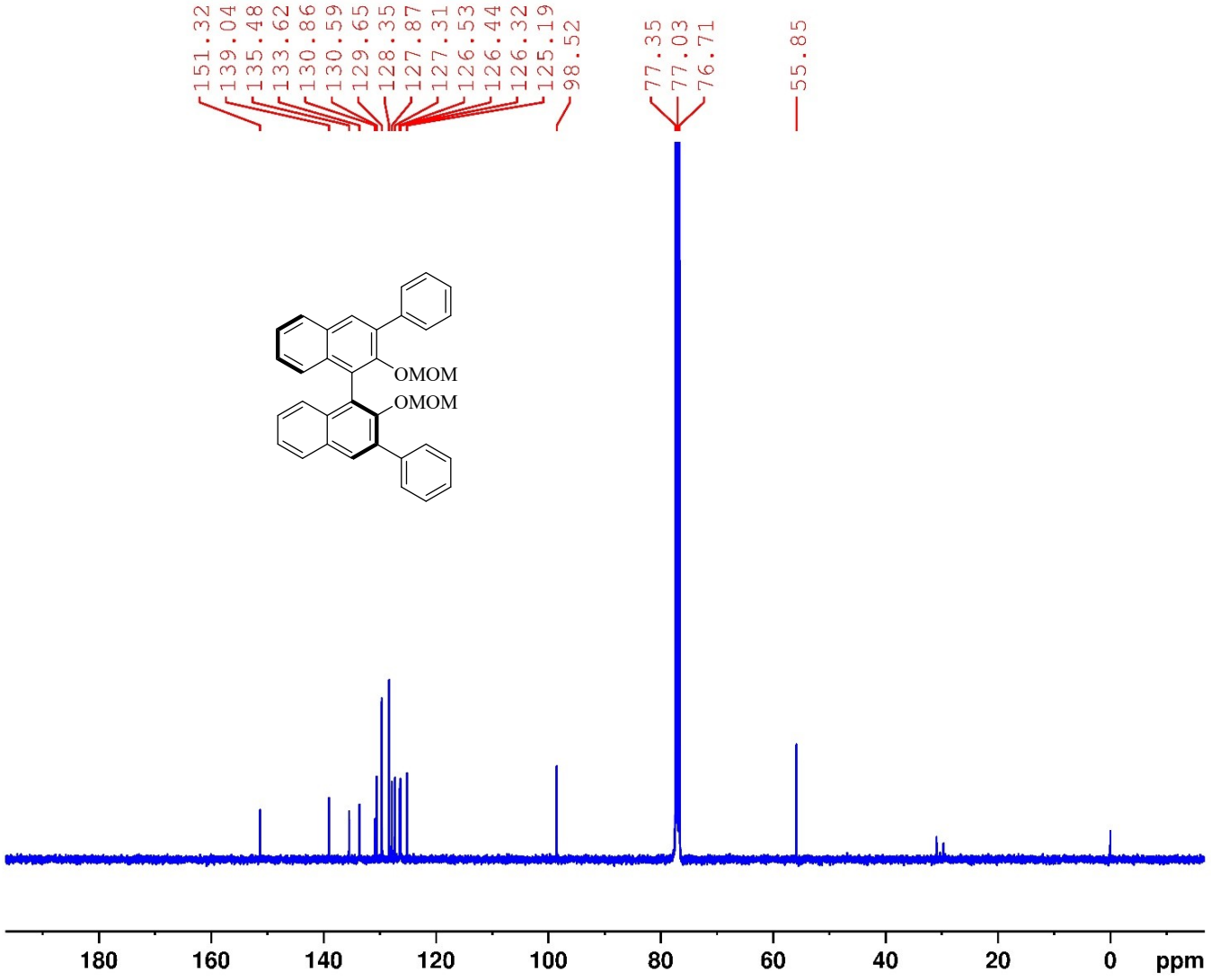


BRUKER

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DE                 6.50 usec
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D11           0.03000000 sec
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SFO2        400.1716007 MHz
NUC2               1H
CPDPRG[2        waltz65
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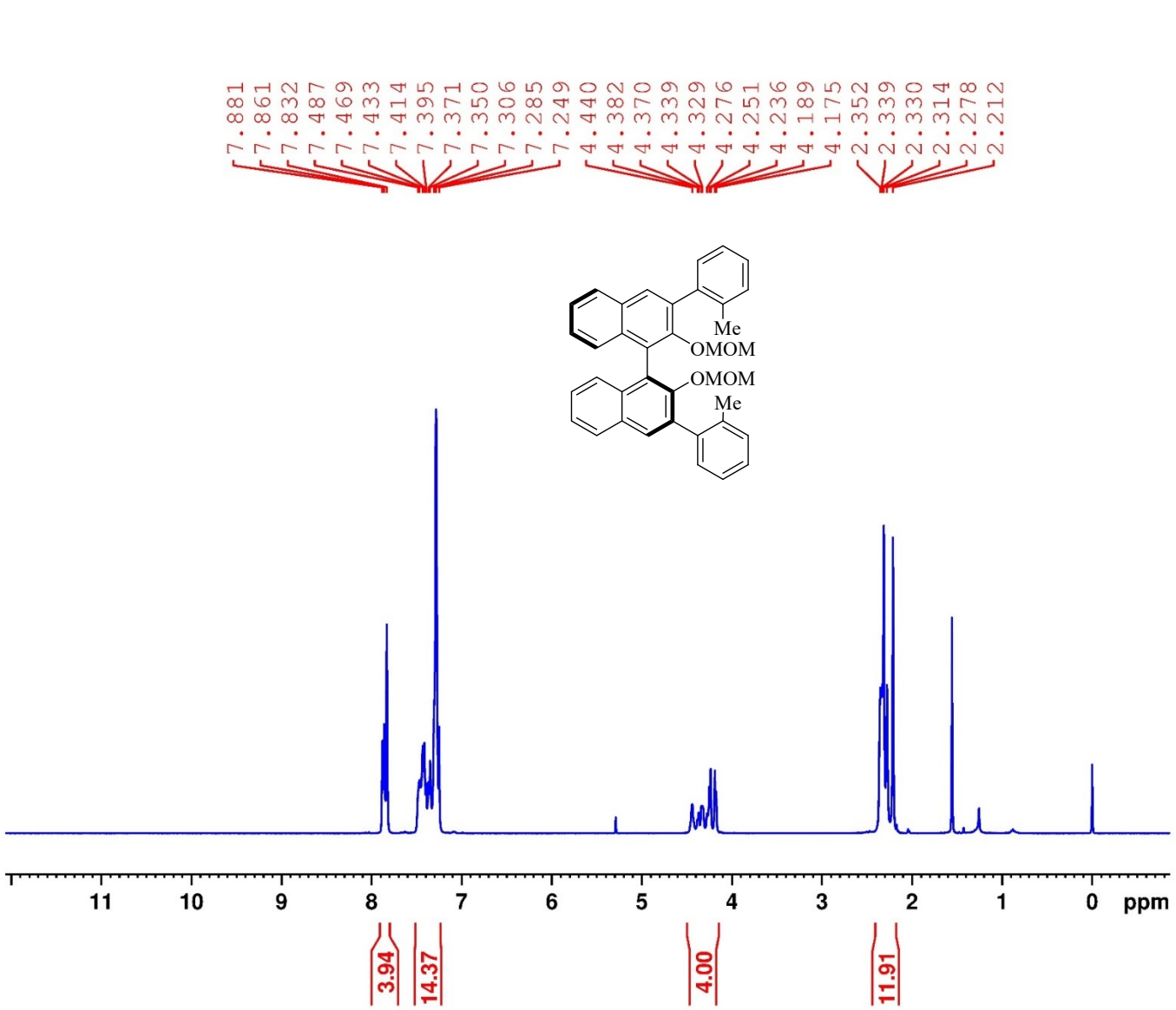


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DE 12.86 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
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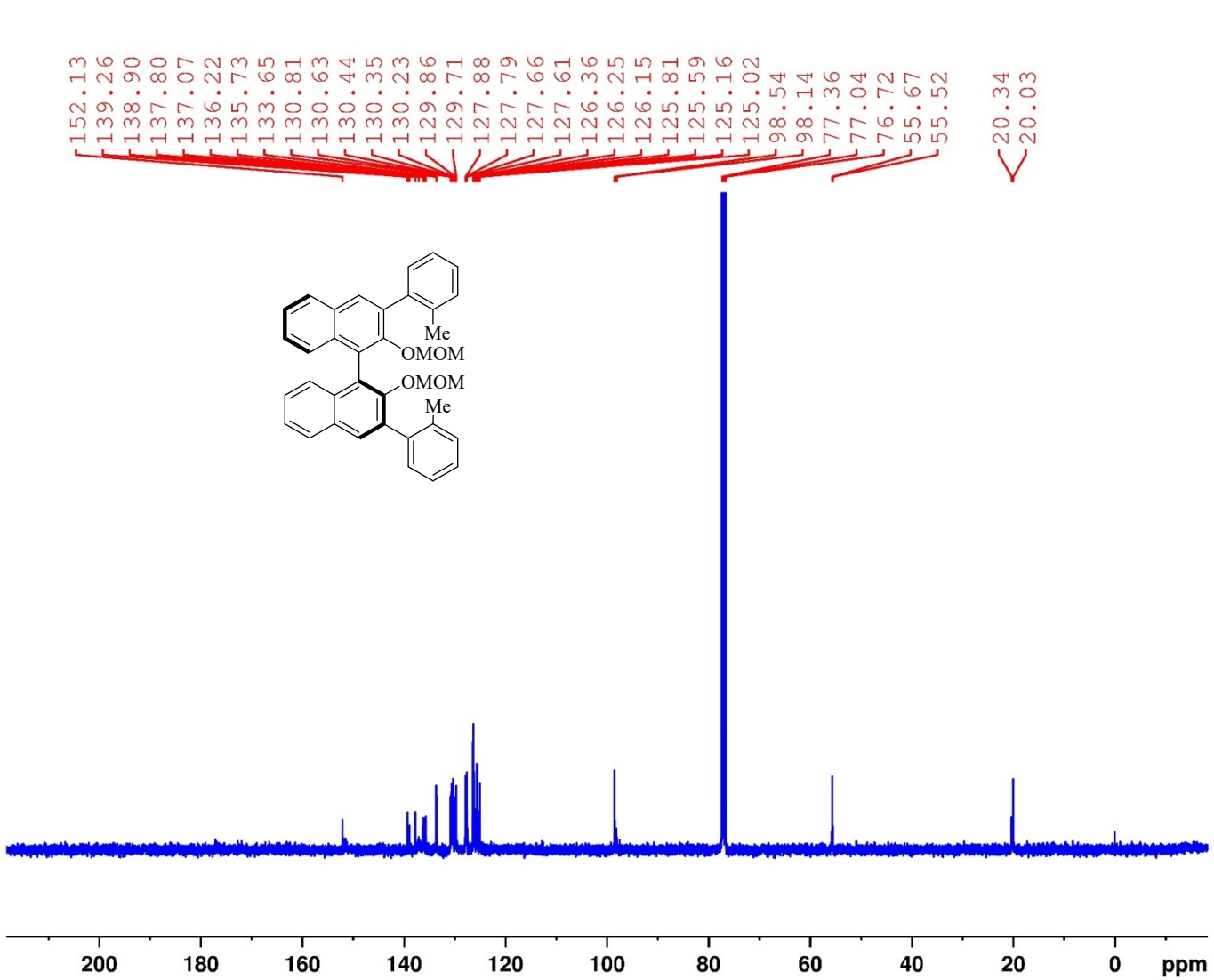


BRUKER

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NUC2                1H
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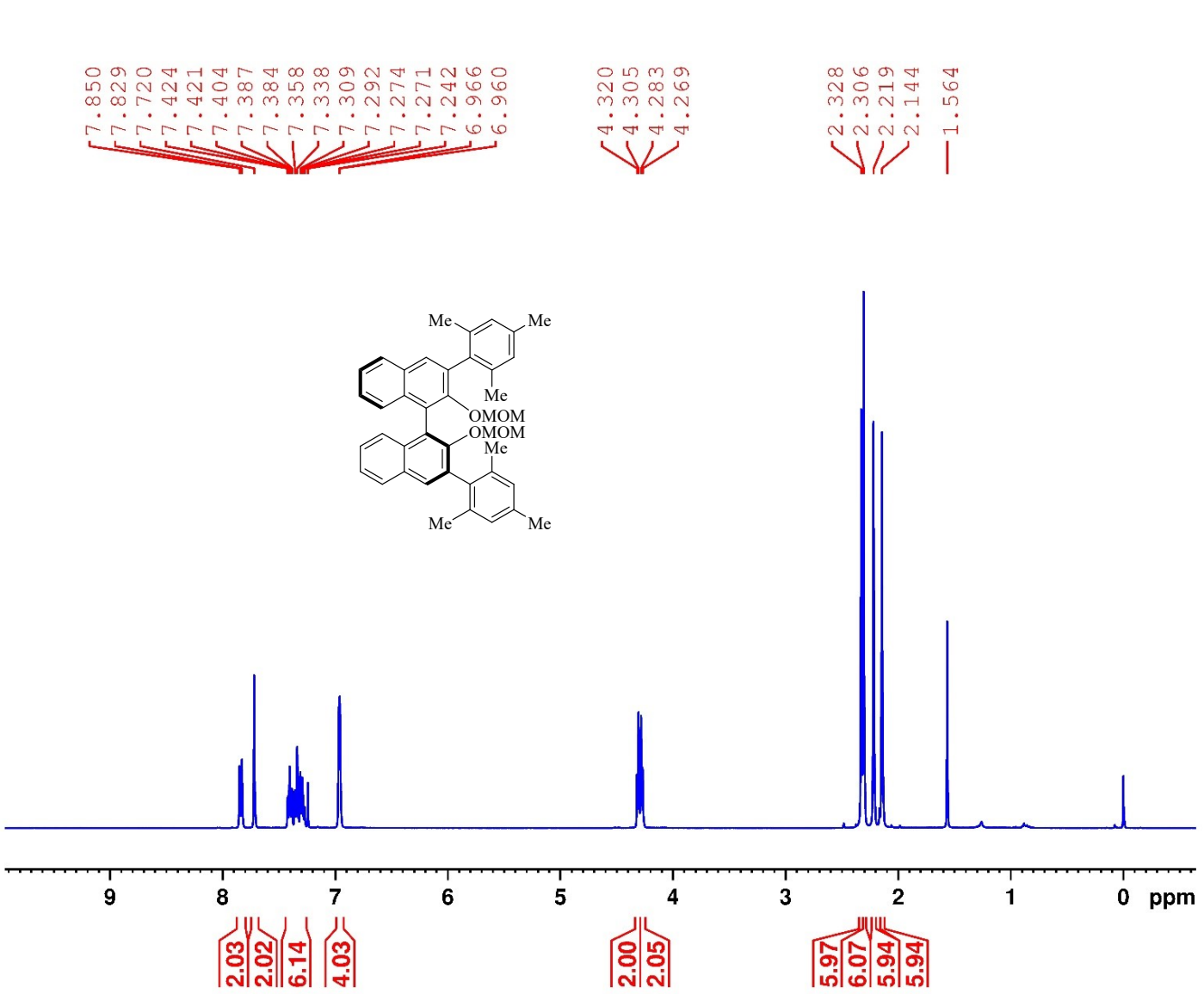


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DW 61.000 usec
DE 12.86 usec
TE 298.0 K
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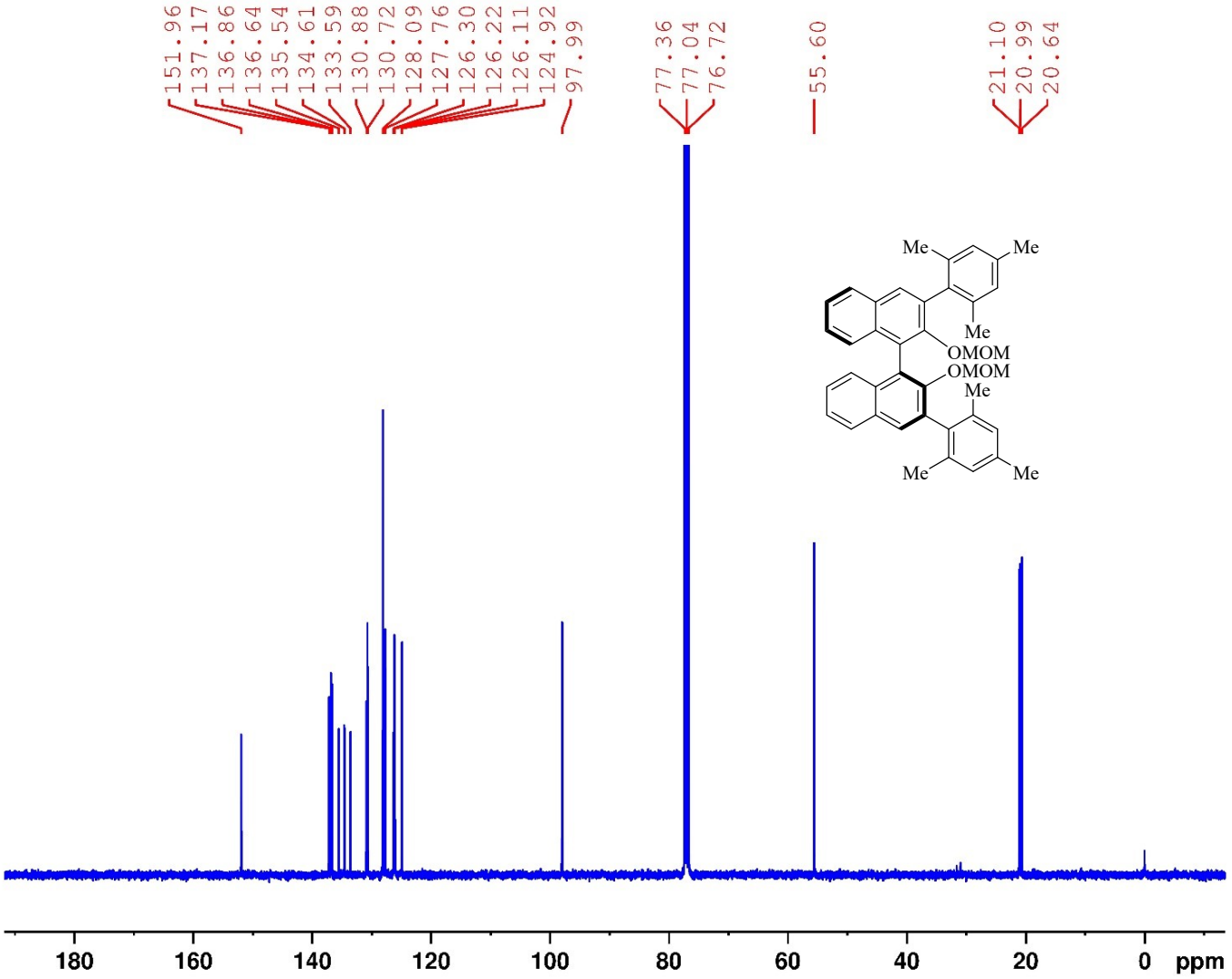
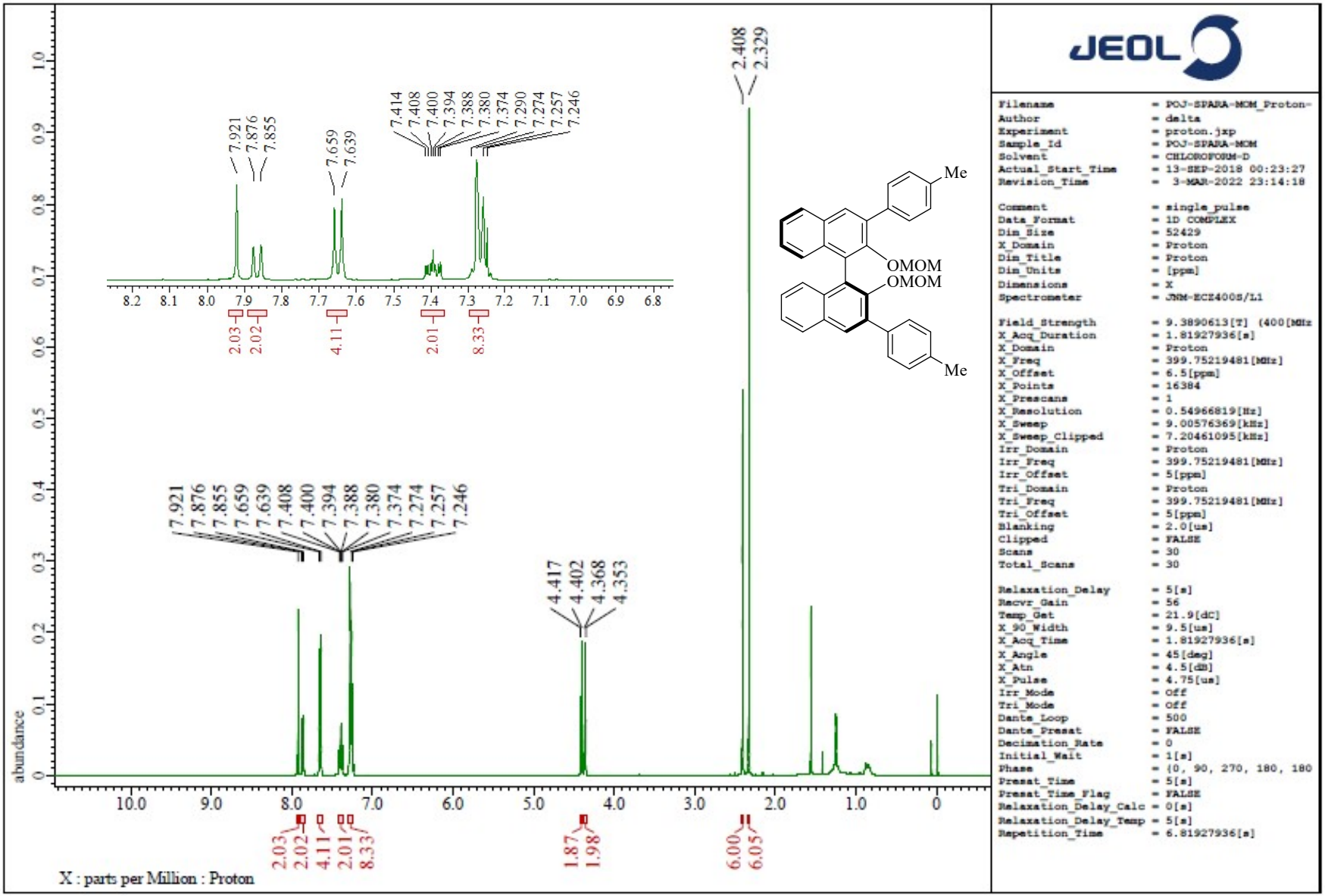
GB 0
PC 1.00



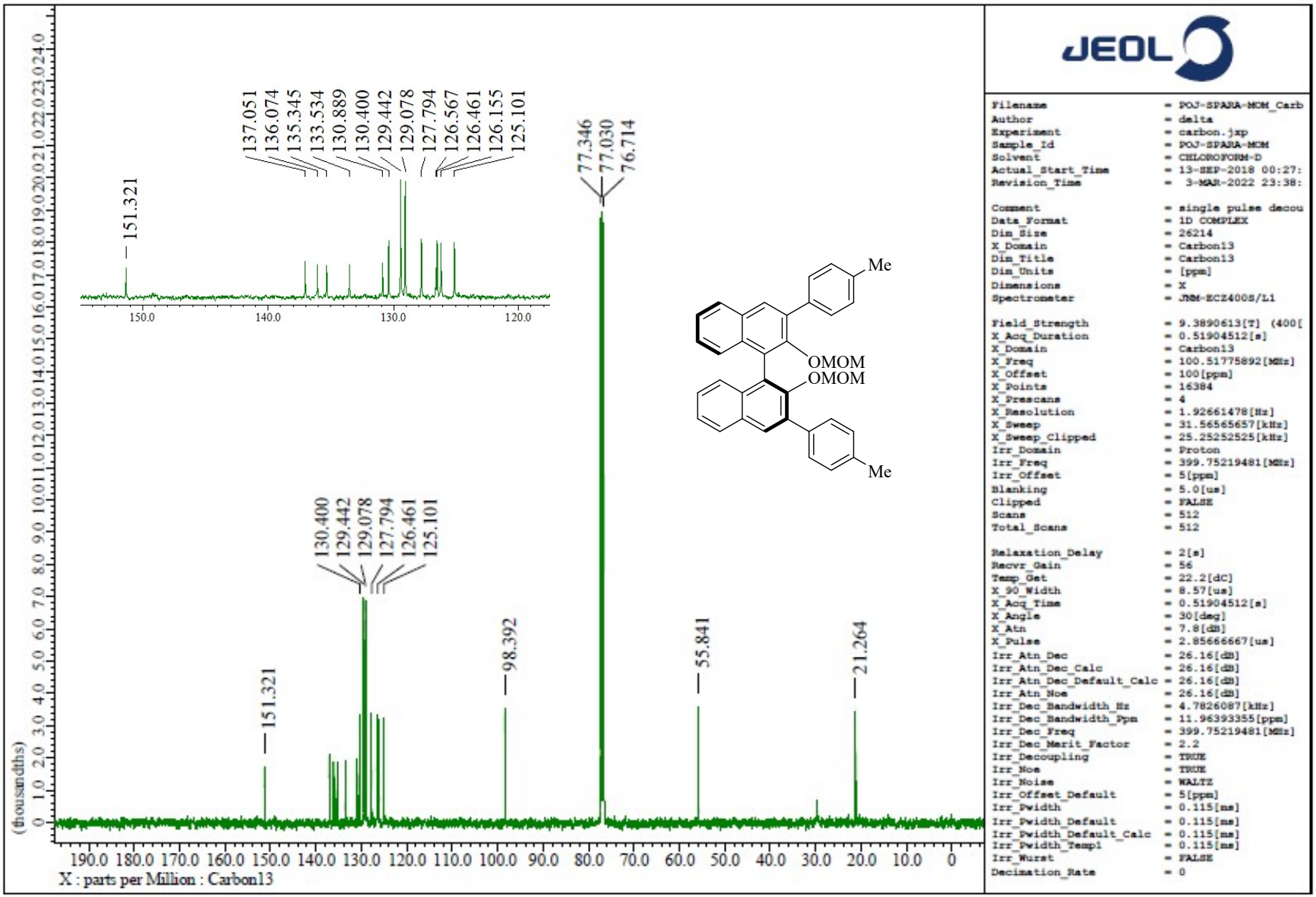

BRUKER

```
Current Data Parameters
NAME      Aug25-2020-nmr
EXPNO                 39
PROCNO                 1

F2 - Acquisition Parameters
Date_           20200826
Time                2.11 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW                21.000 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1
SFO1         100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                32768
SF           100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

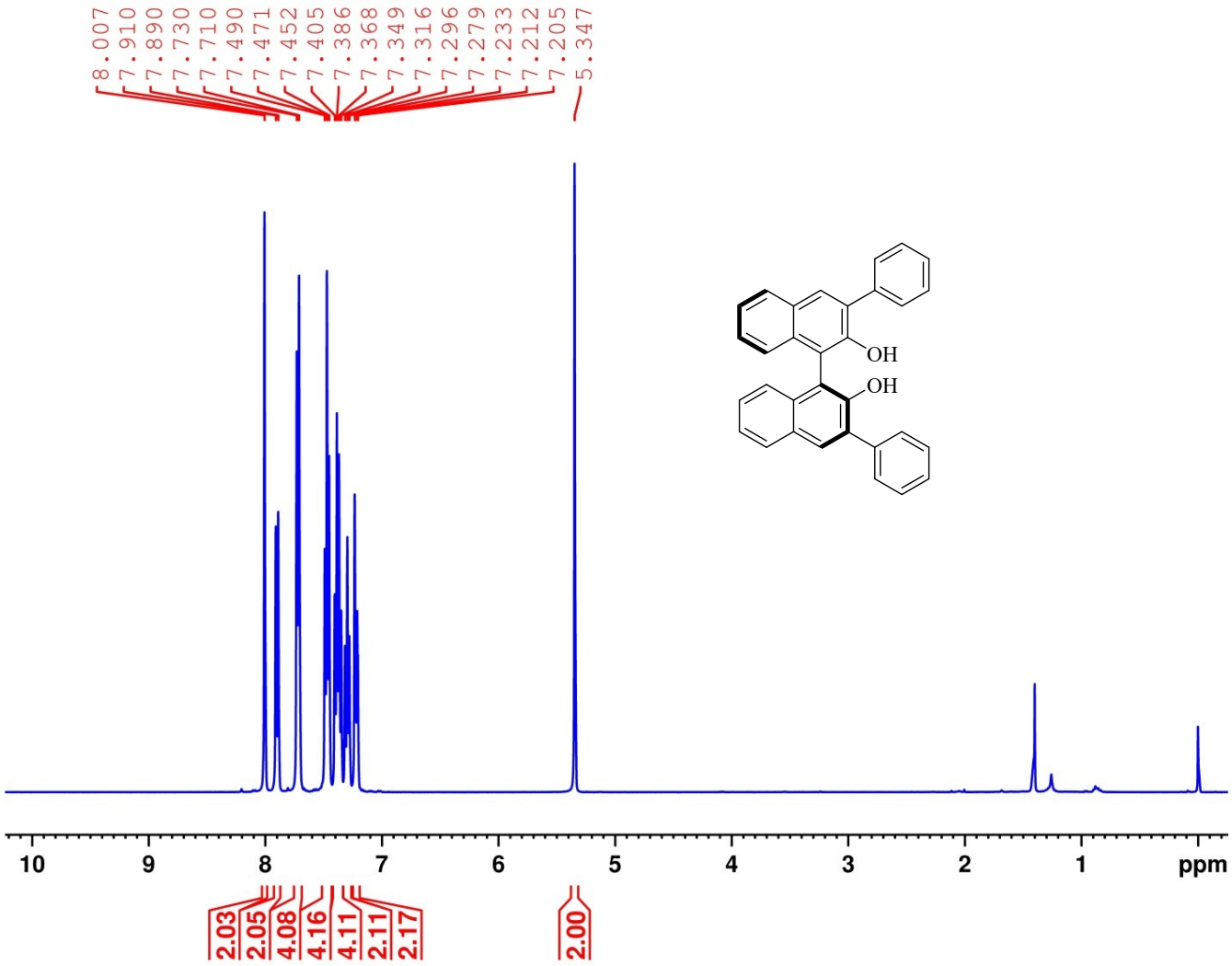



JEOL

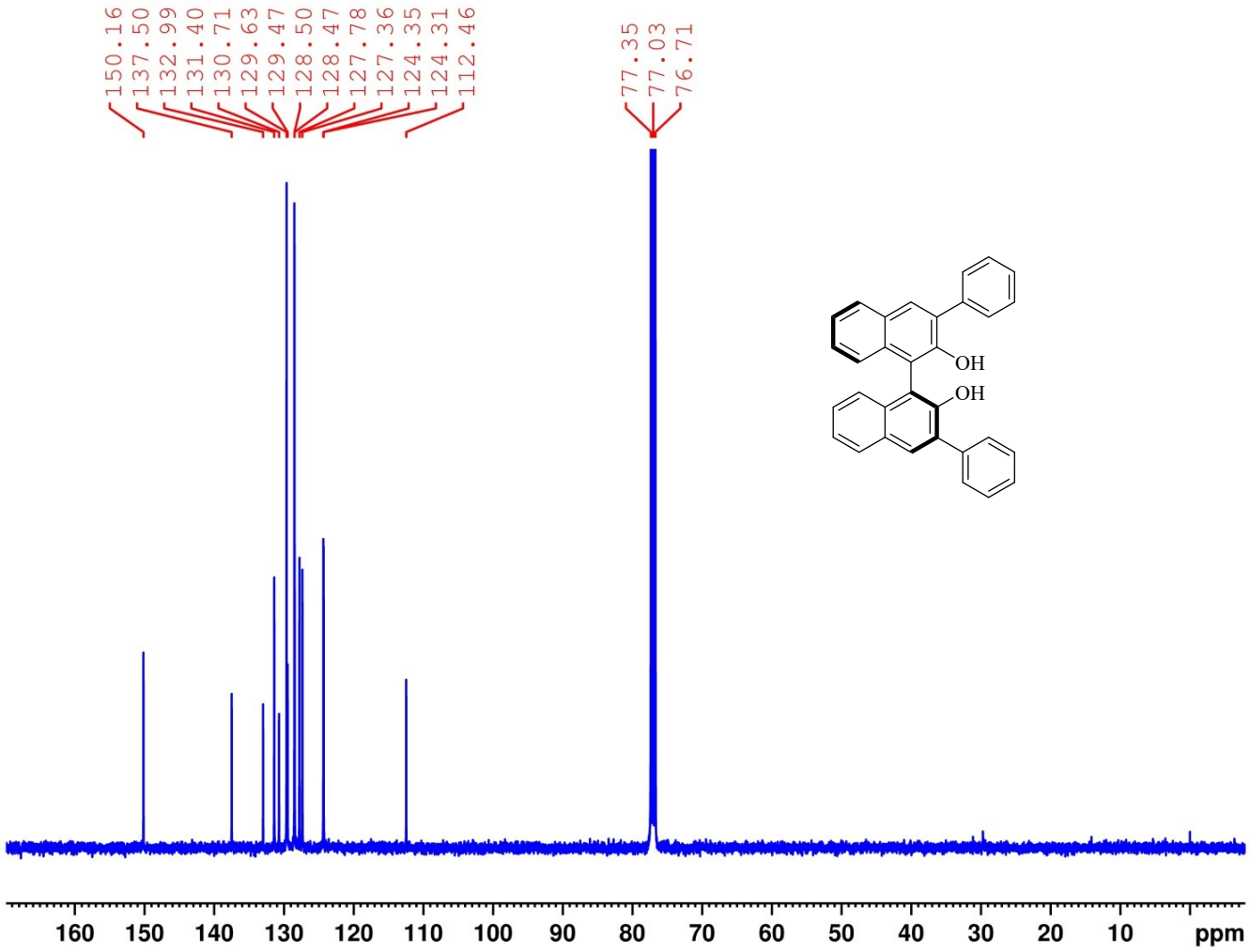
| | |
|---|---|
| Filename | = POJ-SPARA-MOM_Proton- |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = POJ-SPARA-MOM |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 13-SEP-2018 00:23:27 |
| Revision_Time | = 3-MAR-2022 23:14:18 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 52429 |
| X_Domain | = Proton |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.3890613[T] (400[MHz |
| X_Acq_Duration | = 1.81927936[s] |
| X_Domain | = Proton |
| X_Freq | = 399.75219481[MHz] |
| X_Offset | = 6.5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.54966819[Hz] |
| X_Sweep | = 9.00576369[kHz] |
| X_Sweep_Clipped | = 7.20461095[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.75219481[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 399.75219481[MHz] |
| Tri_Offset | = 5[ppm] |
| Blanking | = 2.0[us] |
| Clipped | = FALSE |
| Scans | = 30 |
| Total_Scans | = 30 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 21.9[dC] |
| X_90_Width | = 9.5[us] |
| X_Acq_Time | = 1.81927936[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 4.5[dB] |
| X_Pulse | = 4.75[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |
| Decimation_Rate | = 0 |
| Initial_Wait | = 1[s] |
| Phase | = (0, 90, 270, 180, 180 |
| Presat_Time | = 5[s] |
| Presat_Time_Flag | = FALSE |
| Relaxation_Delay_Calc | = 0[s] |
| Relaxation_Delay_Temp | = 5[s] |
| Repetition_Time | = 6.81927936[s] |



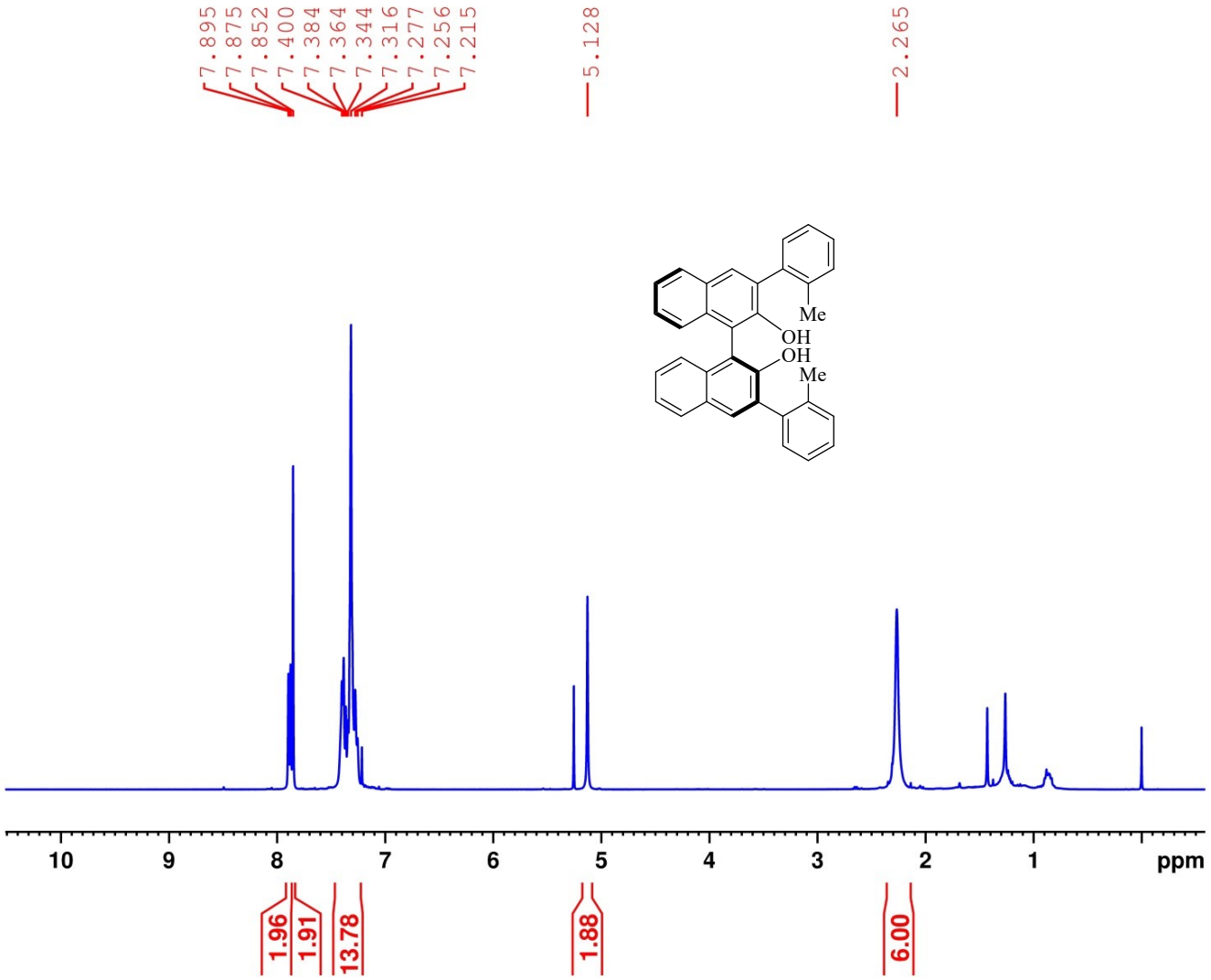

| | |
|---|---|
| Filename | = POJ-SPARA-MOM_Carb |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = POJ-SPARA-MOM |
| Solvent | = CHLOROFORM-D |
| Actual_Start_Time | = 13-SEP-2018 00:27: |
| Revision_Time | = 3-MAR-2022 23:38: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| X_Domain | = Carbon13 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ400S/L1 |
| Field_Strength | = 9.3890613[T] (400[ |
| X_Acq_Duration | = 0.51904512[s] |
| X_Domain | = Carbon13 |
| X_Freq | = 100.51775892[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 4 |
| X_Resolution | = 1.92661478[Hz] |
| X_Sweep | = 31.56565657[kHz] |
| X_Sweep_Clipped | = 25.25252525[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 399.75219481[MHz] |
| Irr_Offset | = 5[ppm] |
| Blanking | = 5.0[us] |
| Clipped | = FALSE |
| Scans | = 512 |
| Total_Scans | = 512 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 22.2[dC] |
| X_90_Width | = 8.57[us] |
| X_Acq_Time | = 0.51904512[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 7.8[dB] |
| X_Pulse | = 2.85666667[us] |
| Irr_Atn_Dec | = 26.16[dB] |
| Irr_Atn_Dec_Calc | = 26.16[dB] |
| Irr_Atn_Dec_Default_Calc | = 26.16[dB] |
| Irr_Atn_Noe | = 26.16[dB] |
| Irr_Dec_Bandwidth_Hz | = 4.7826087[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 11.96393355[ppm] |
| Irr_Dec_Freq | = 399.75219481[MHz] |
| Irr_Dec_Merit_Factor | = 2.2 |
| Irr_Decoupling | = TRUE |
| Irr_Noe | = TRUE |
| Irr_Noise | = WALTZ |
| Irr_Offset_Default | = 5[ppm] |
| Irr_Pwidth | = 0.115[ms] |
| Irr_Pwidth_Default | = 0.115[ms] |
| Irr_Pwidth_Default_Calc | = 0.115[ms] |
| Irr_Pwidth_Temp1 | = 0.115[ms] |
| Irr_Wurst | = FALSE |
| Decimation_Rate | = 0 |



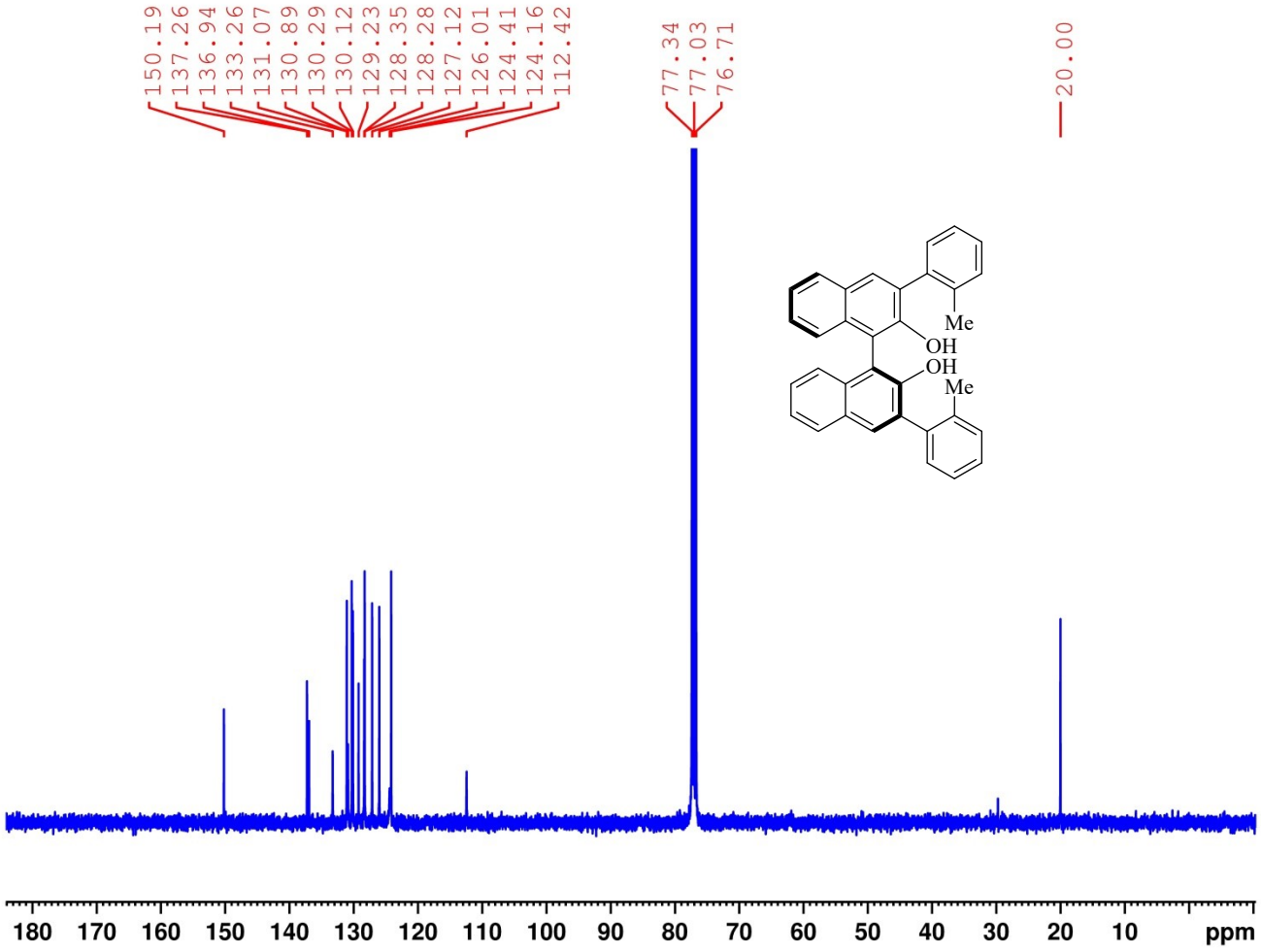

```
Current Data Parameters
NAME      Oct02-2020-nmr
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201002
Time              16.47 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8196.722 Hz
FIDRES        0.250144 Hz
AQ            3.9976959 sec
RG                  101
DW               61.000 usec
DE                12.86 usec
TE                297.3 K
D1           1.00000000 sec
TD0                   1
SFO1        400.1724710 MHz
NUC1                 1H
P0                 4.67 usec
P1                14.00 usec
PLW1        16.77000046 W

F2 - Processing parameters
SI                65536
SF        400.1700320 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME      Jul01-2021-nmr
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210701
Time              17.26 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                81.25
DW               21.000 usec
DE                6.50 usec
TE               300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1               13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2            90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```



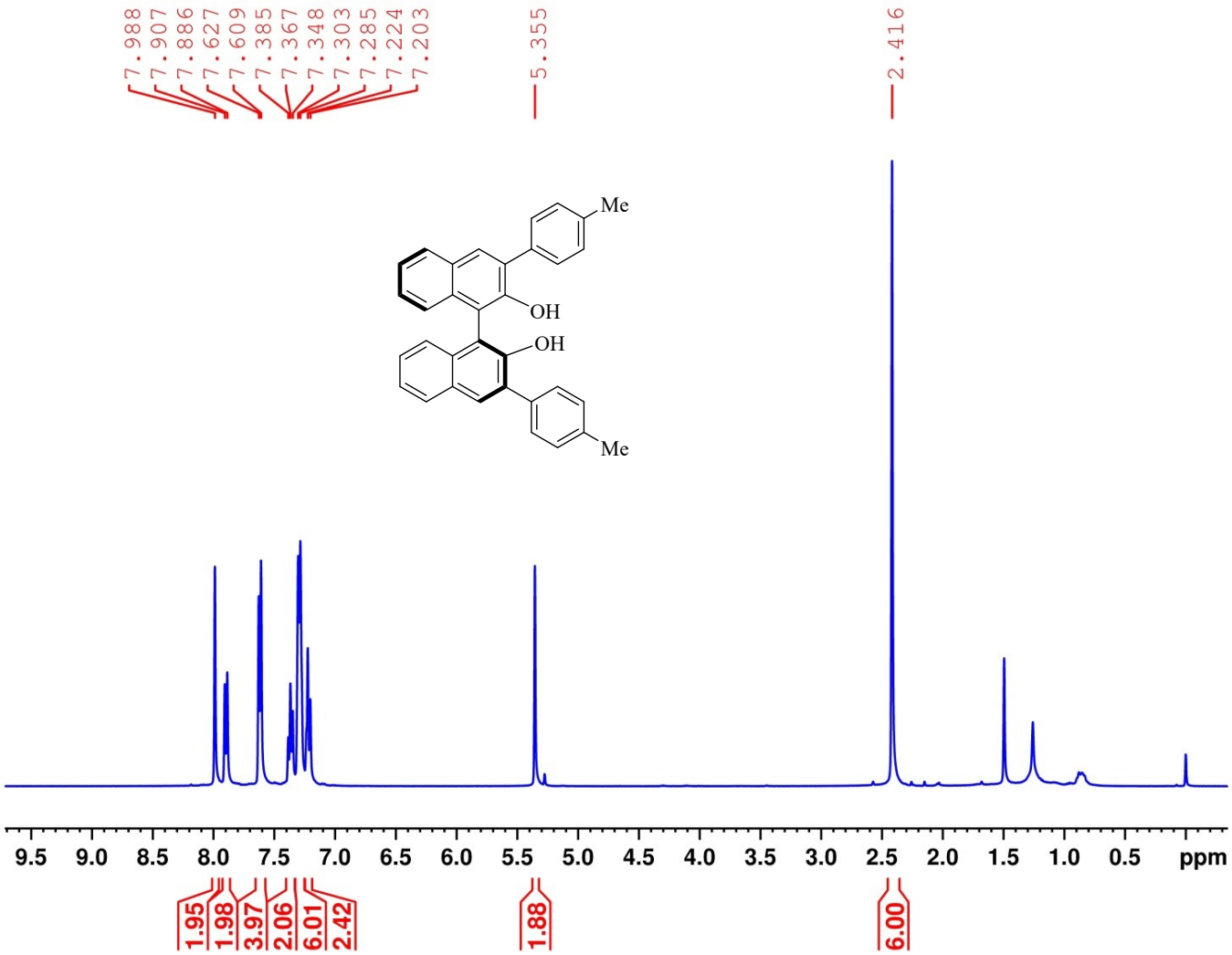

```
Current Data Parameters
NAME      Oct02-2020-nmr
EXPNO                 24
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201002
Time              16.52 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                297.4 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700280 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




Current Data Parameters
NAME Jul01-2021-nmr
EXPNO 31
PROCNO 1

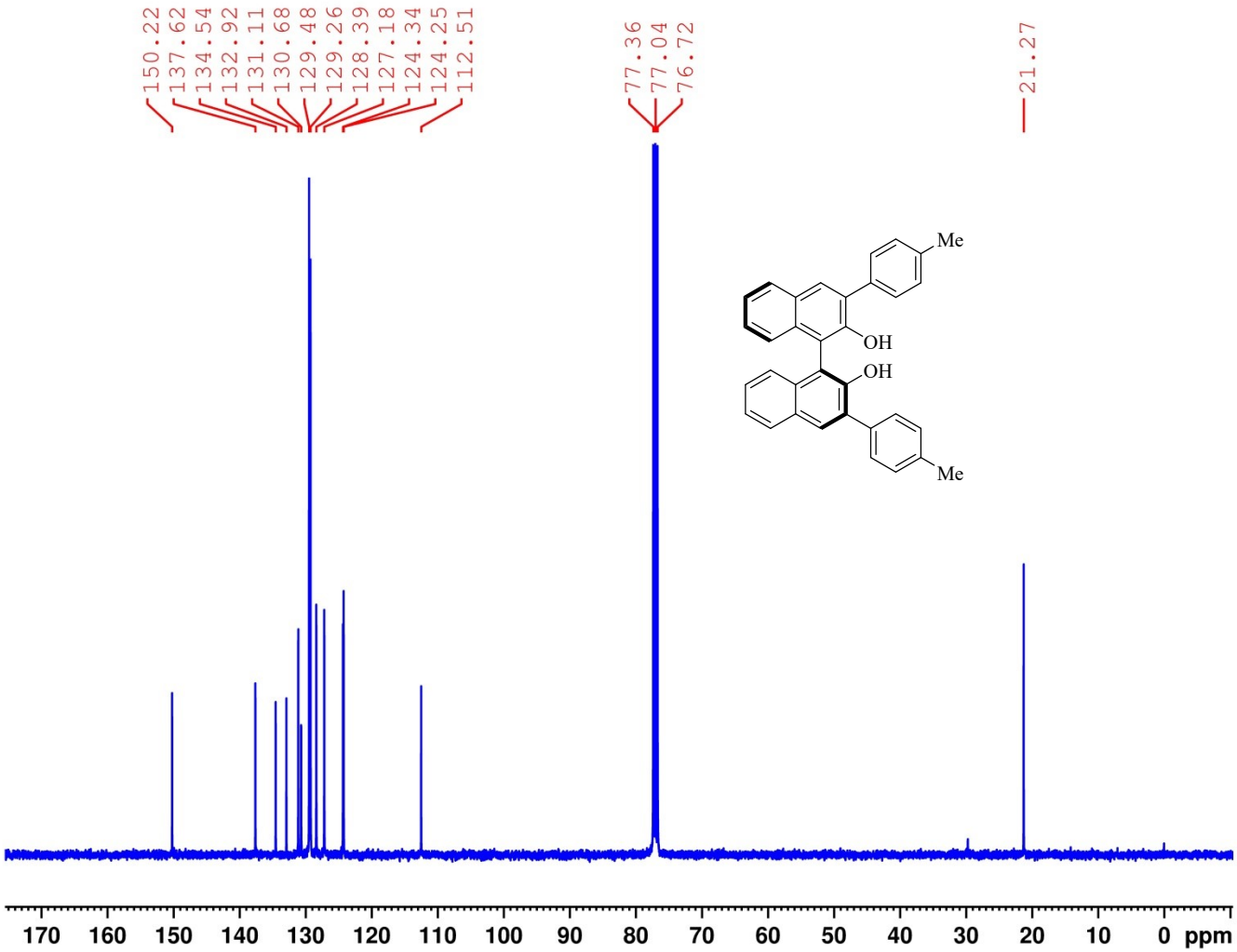
F2 - Acquisition Parameters
Date_ 20210701
Time 18.32 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 81.25
DW 21.000 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6328888 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 60.89300156 W
SFO2 400.1716007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 16.77000046 W
PLW12 0.40580001 W
PLW13 0.20411000 W

F2 - Processing parameters
SI 32768
SF 100.6228265 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




BRUKER

```
Current Data Parameters
NAME      Jul01-2021-nmr
EXPNO                 40
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210701
Time              18.37 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700198 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

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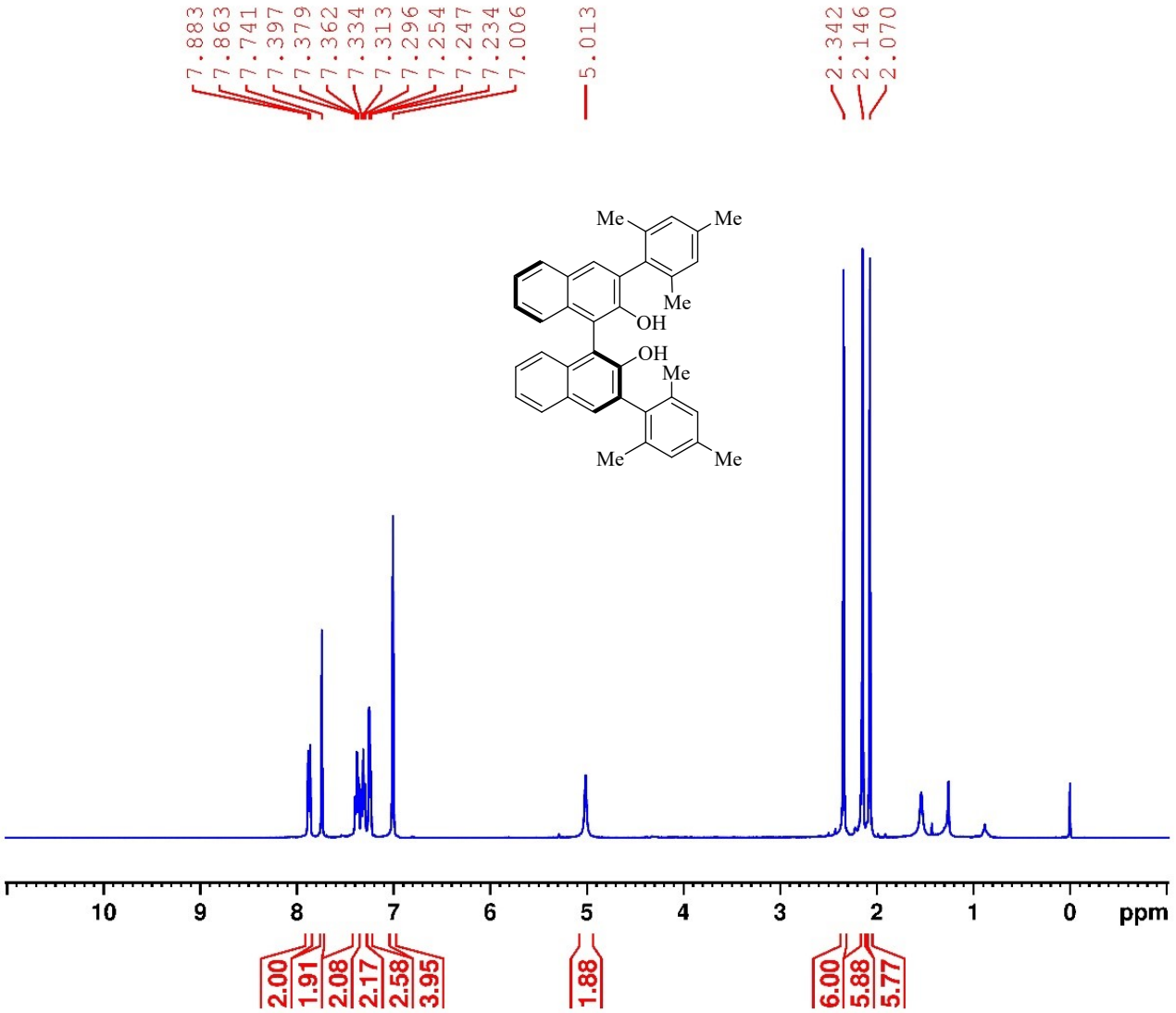
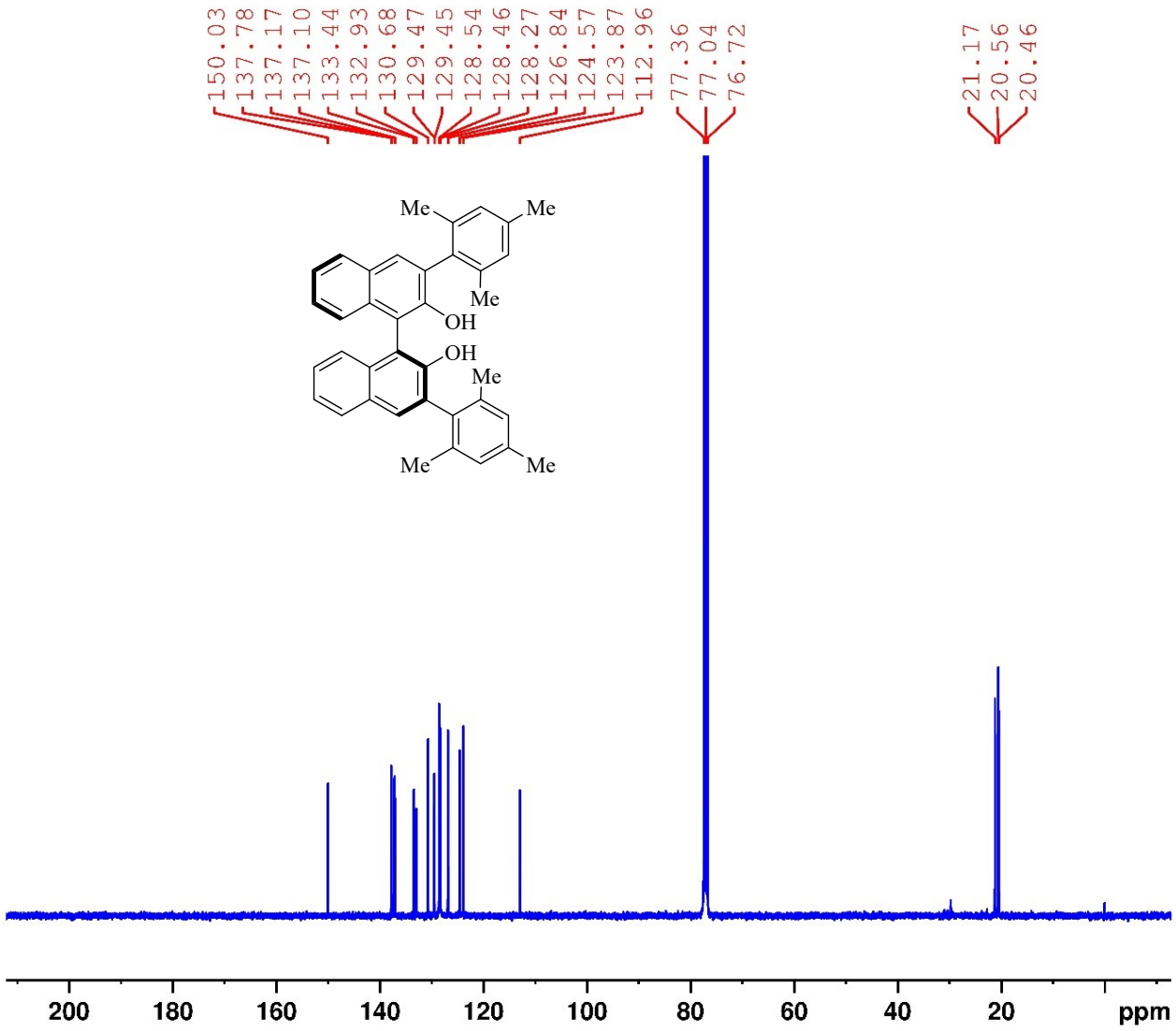
```
Current Data Parameters
NAME      Jul01-2021-nmr
EXPNO                 41
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210701
Time              19.37 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                81.25
DW               21.000 usec
DE                6.50 usec
TE               300.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1               13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2               1H
CPDPRG[2         waltz65
PCPD2            90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```



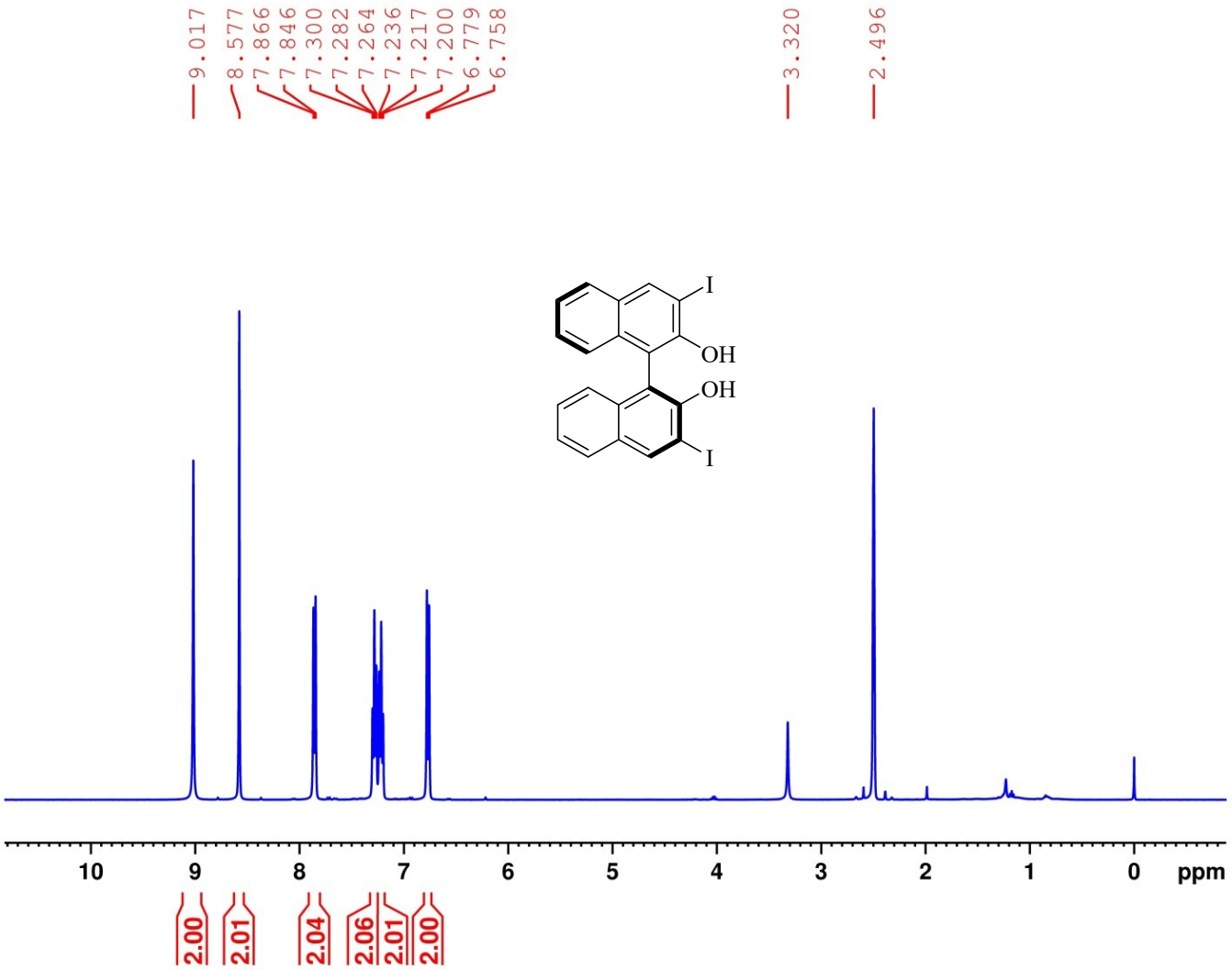

BRUKER

```
Current Data Parameters
NAME      can13-2022-nmr
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220113
Time              13.12 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                    16
DS                     2
SWH              8196.722 Hz
FIDRES           0.250144 Hz
AQ               3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 7.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700052 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



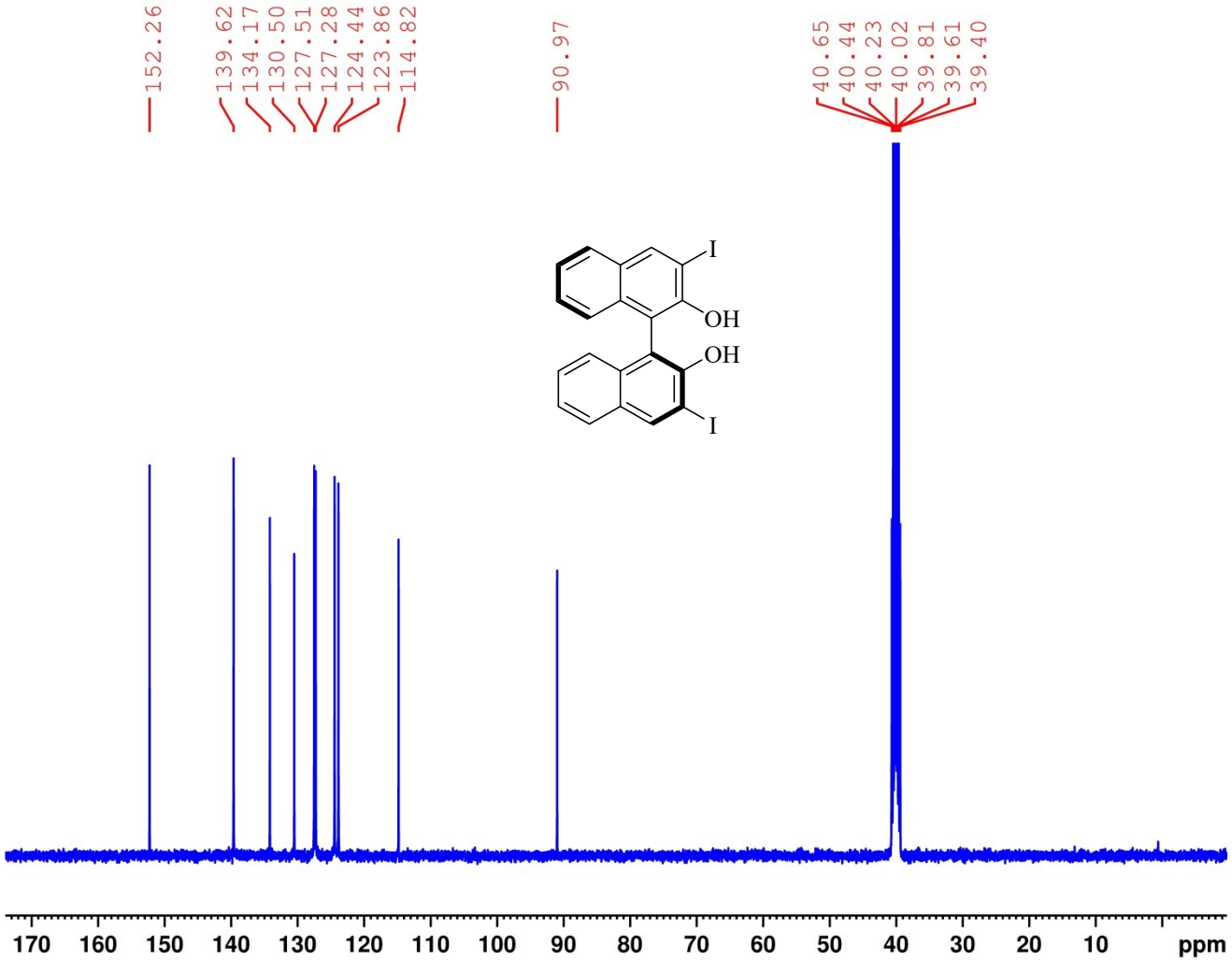

BRUKER

```
Current Data Parameters
NAME      Jan13-2022-rmr
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220113
Time              16.10 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3000
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE               296.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



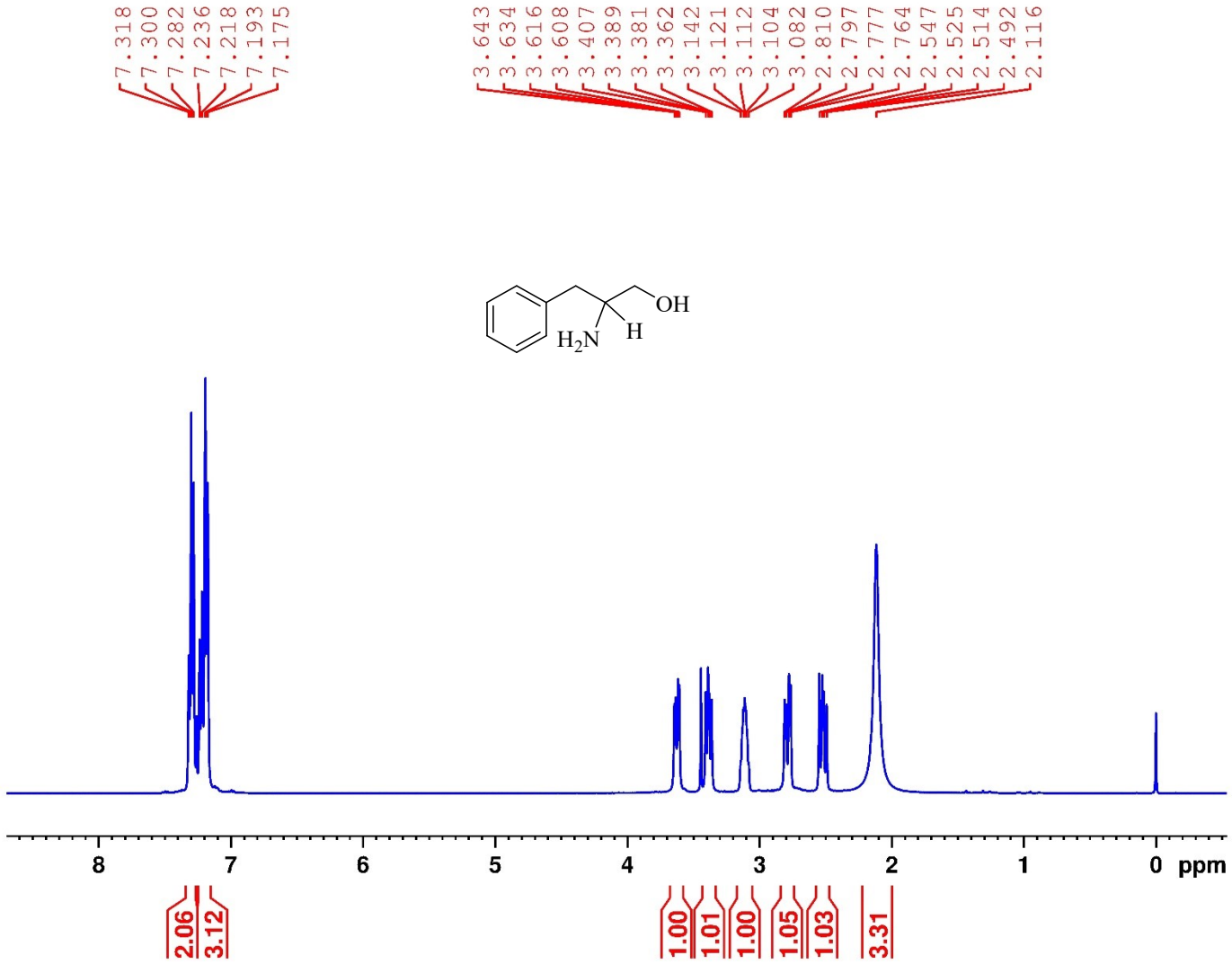


```
Current Data Parameters
NAME      Jul01-2021-nmr
EXPNO                 60
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210701
Time              20.46 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700043 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



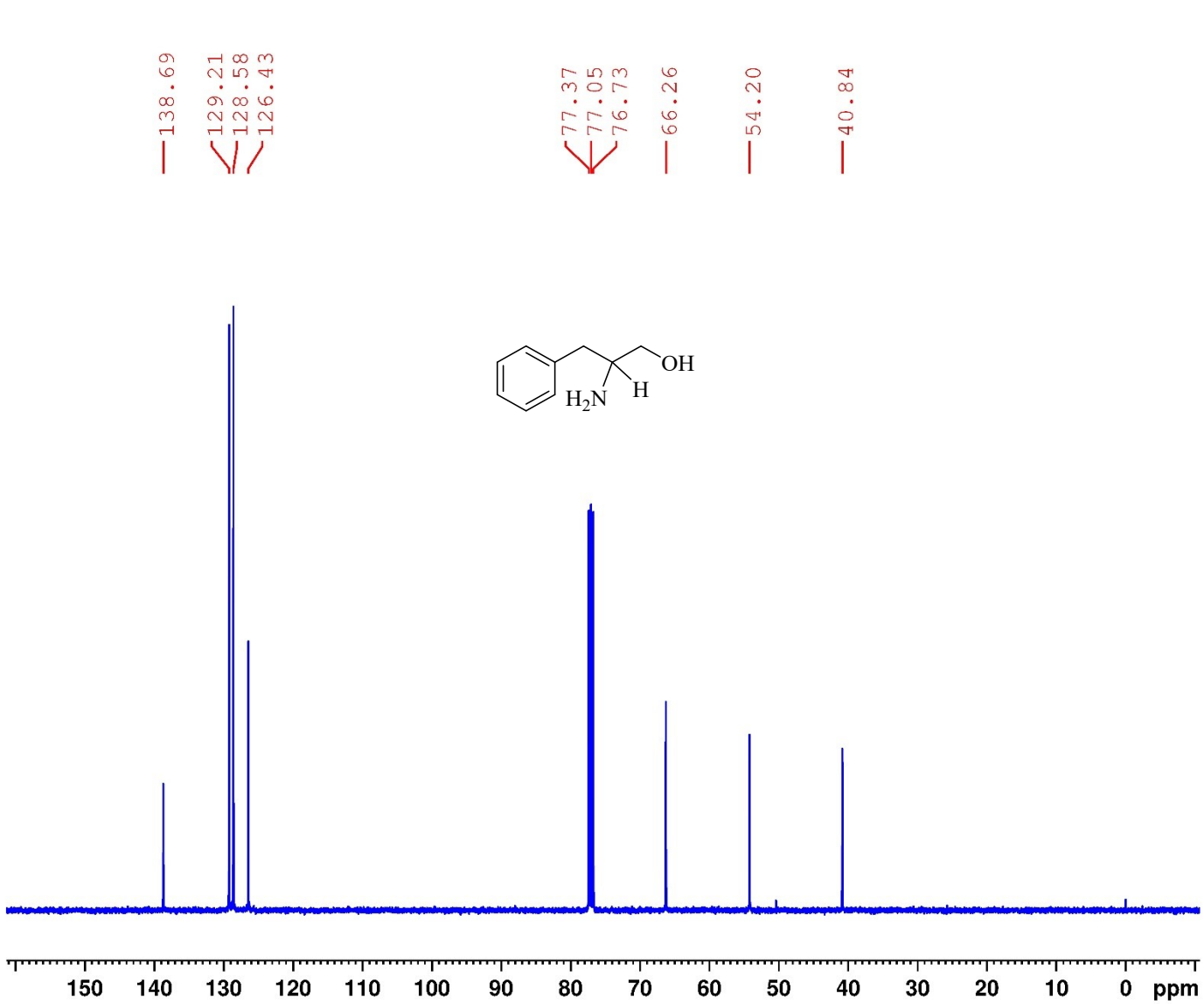

BRUKER

```
Current Data Parameters
NAME      Jul01-2021-nmr
EXPNO                 61
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210701
Time              21.46 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                   101
DW               21.000 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                  1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                 32768
SF           100.6228265 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

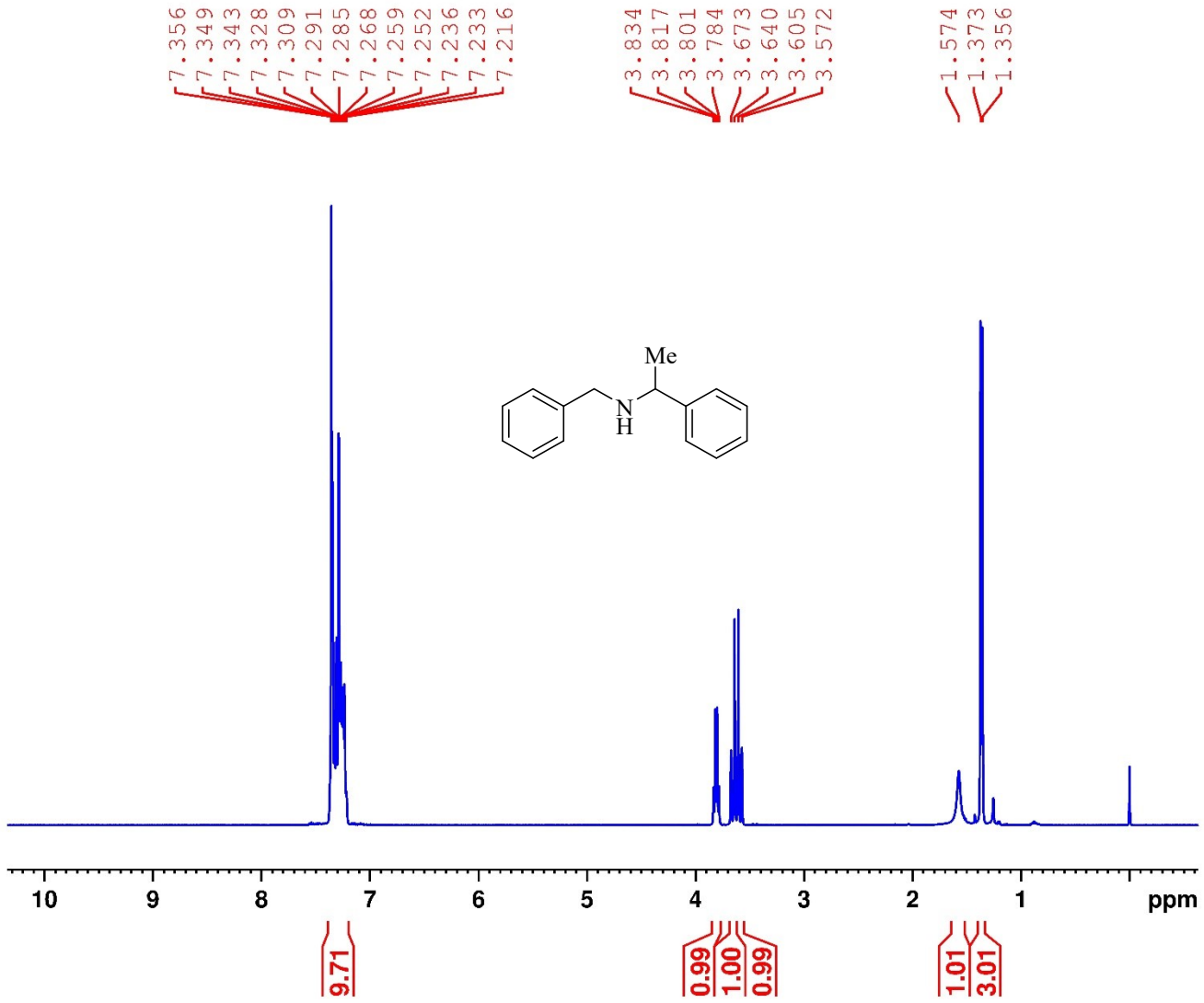



BRUKER

```
Current Data Parameters
NAME      Jan20-2021-nmr
EXPNO                 50
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210120
Time               16.31 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                303.0 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1          16.77000046 W

F2 - Processing parameters
SI                 65536
SF            400.1700102 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME      Jan20-2021-nmr
EXPNO                 51
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210120
Time              17.39 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE               303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                32768
SF           100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

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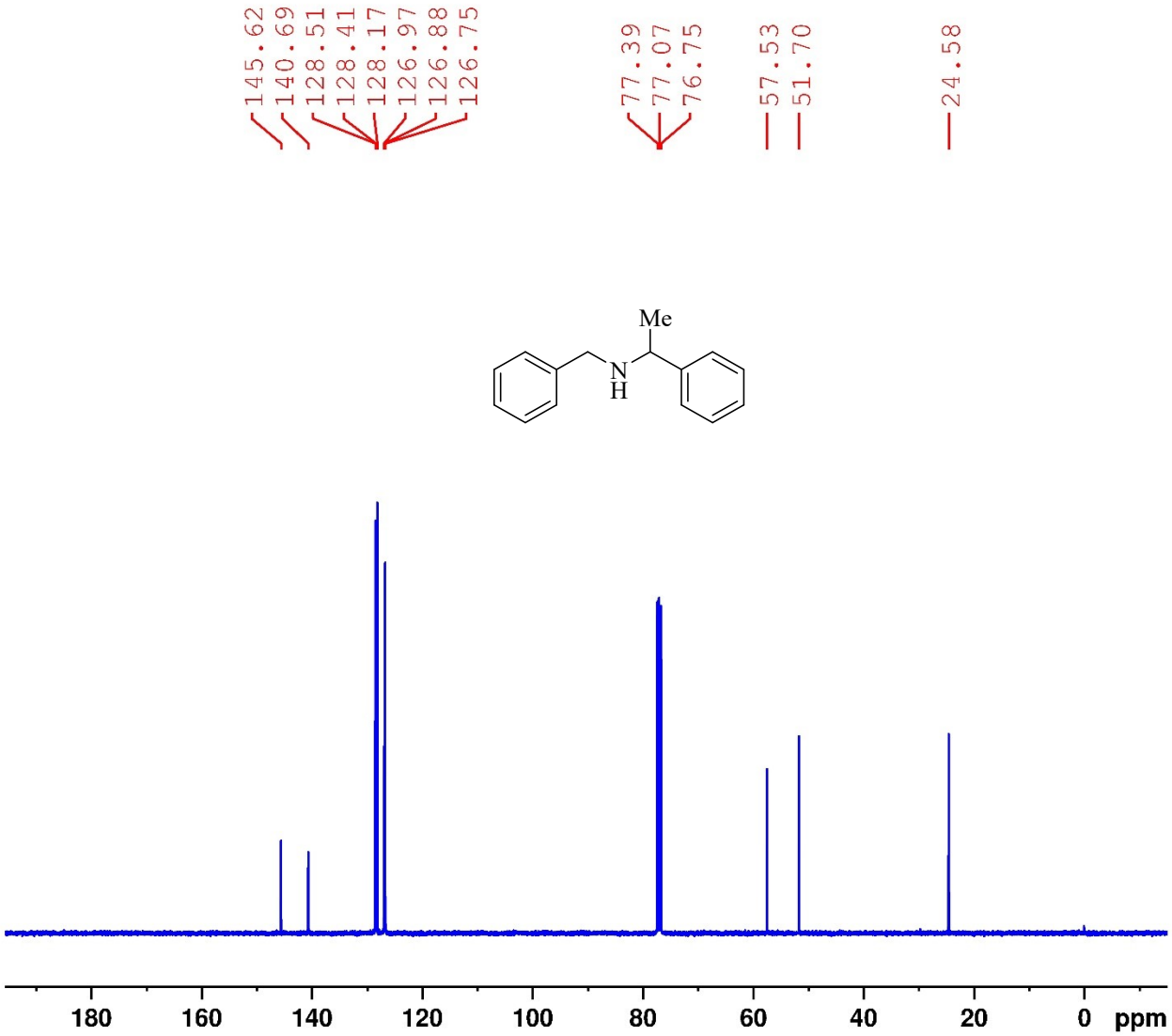
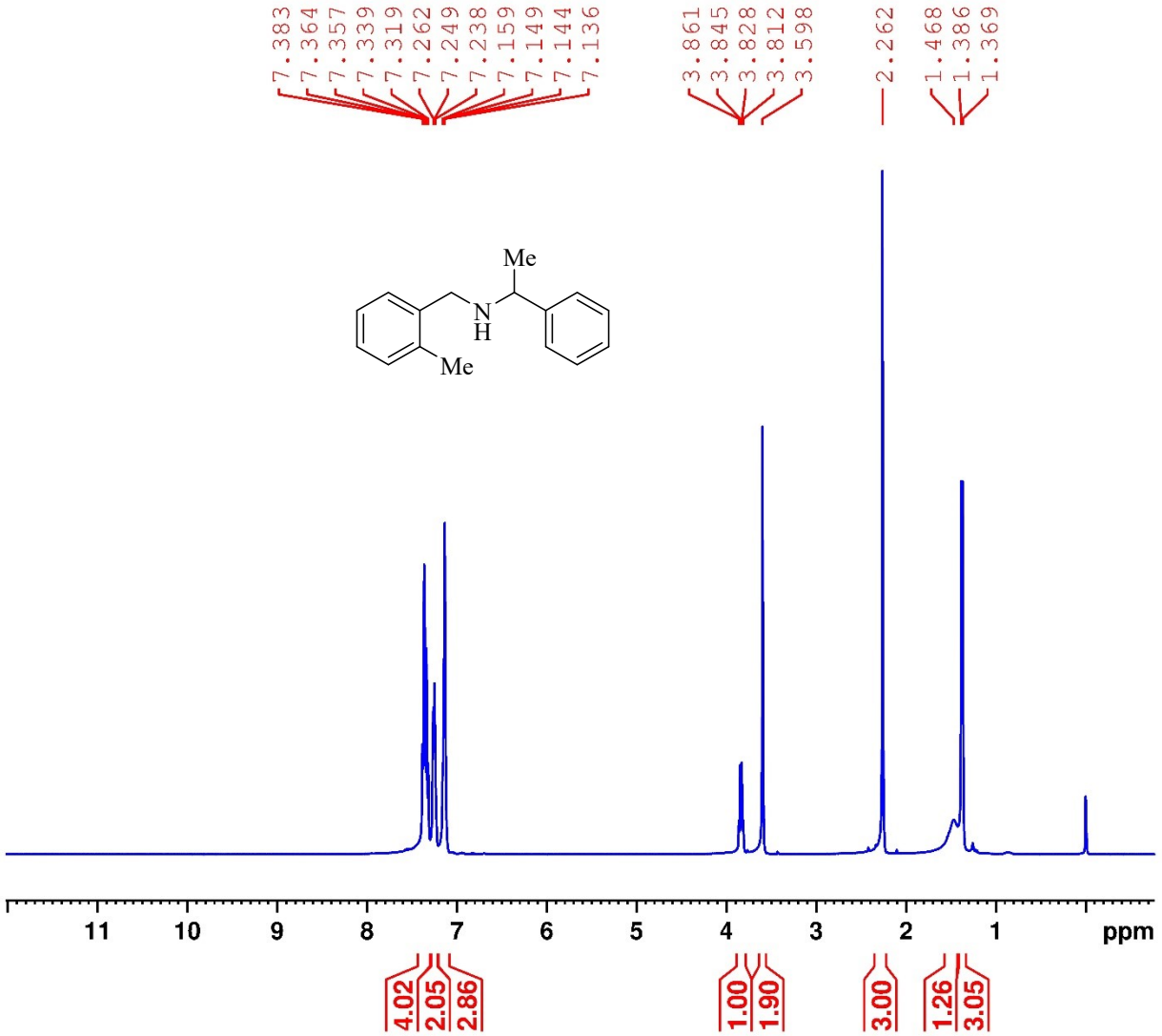
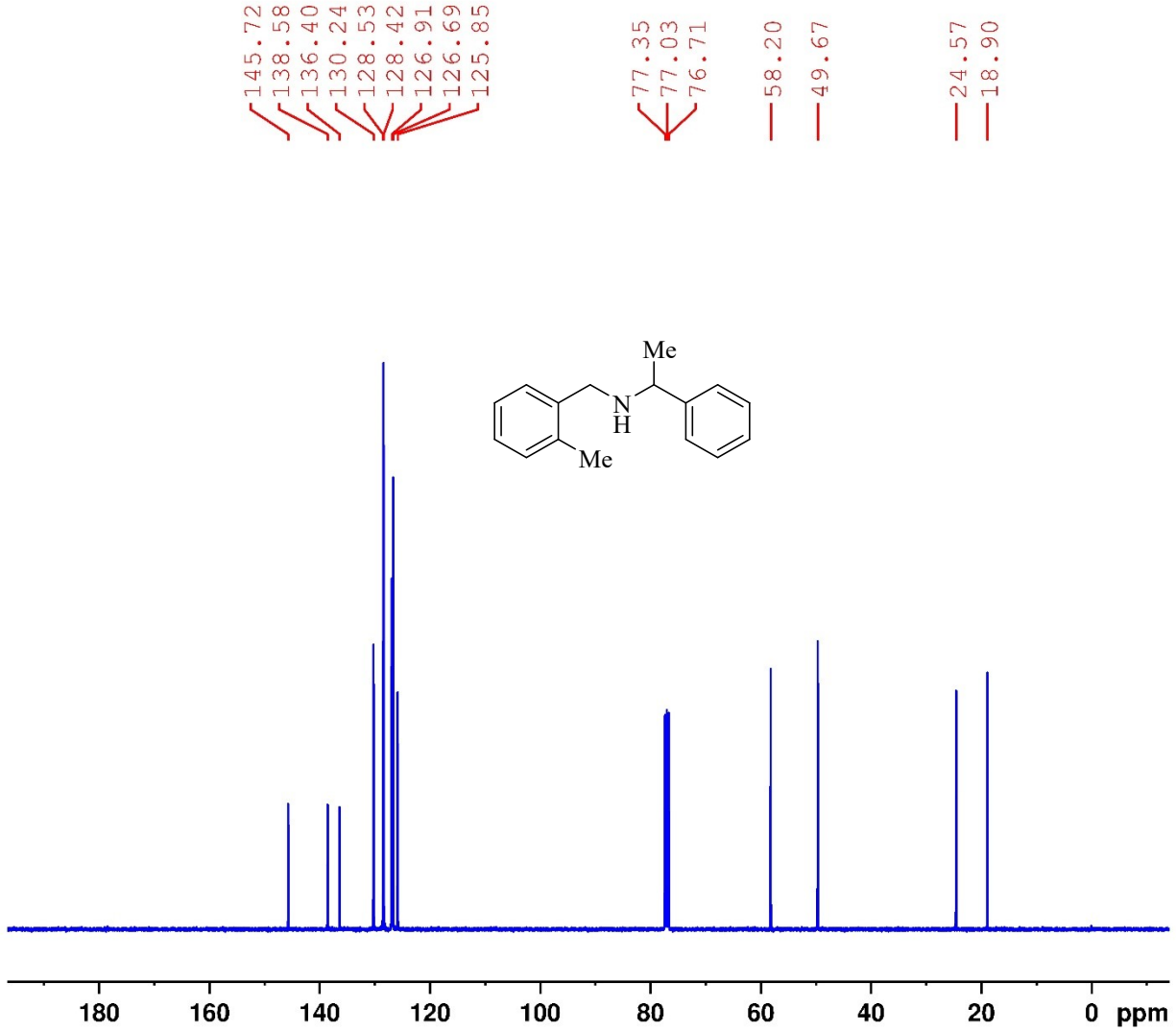
```
Current Data Parameters
NAME      Dec30-2020-nmr
EXPNO                 50
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201230
Time              15.16 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                441.3 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700196 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME      Dec30-2020-nmr
EXPNO                 51
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201230
Time              15.47 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                447.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1
SFO1         100.6328888 MHz
NUC1                13C
P0                 3.33 usec
P1                10.00 usec
PLW1         60.89300156 W
SFO2         400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                32768
SF           100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



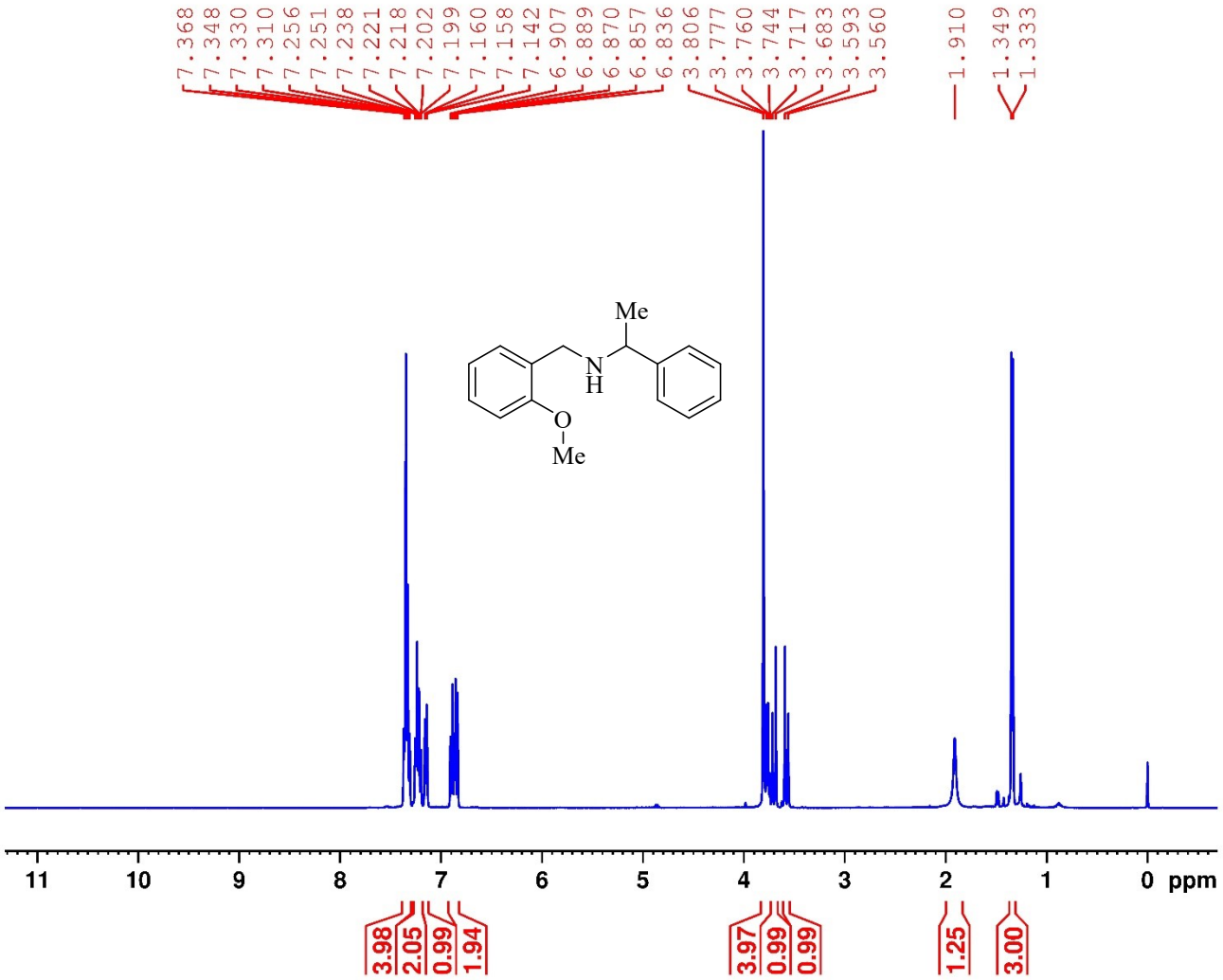

```
Current Data Parameters
NAME      Jun18-2021-nmr
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210618
Time              14.54 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                300.0 K
D1             1.00000000 sec
ID0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF          400.1700187 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




Current Data Parameters
NAME Feb04-2021-nmr
EXPNO 81
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210204
Time 19.22 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6328888 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 60.89300156 W
SFO2 400.1716007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 16.77000046 W
PLW12 0.40580001 W
PLW13 0.20411000 W

F2 - Processing parameters
SI 32768
SF 100.6228338 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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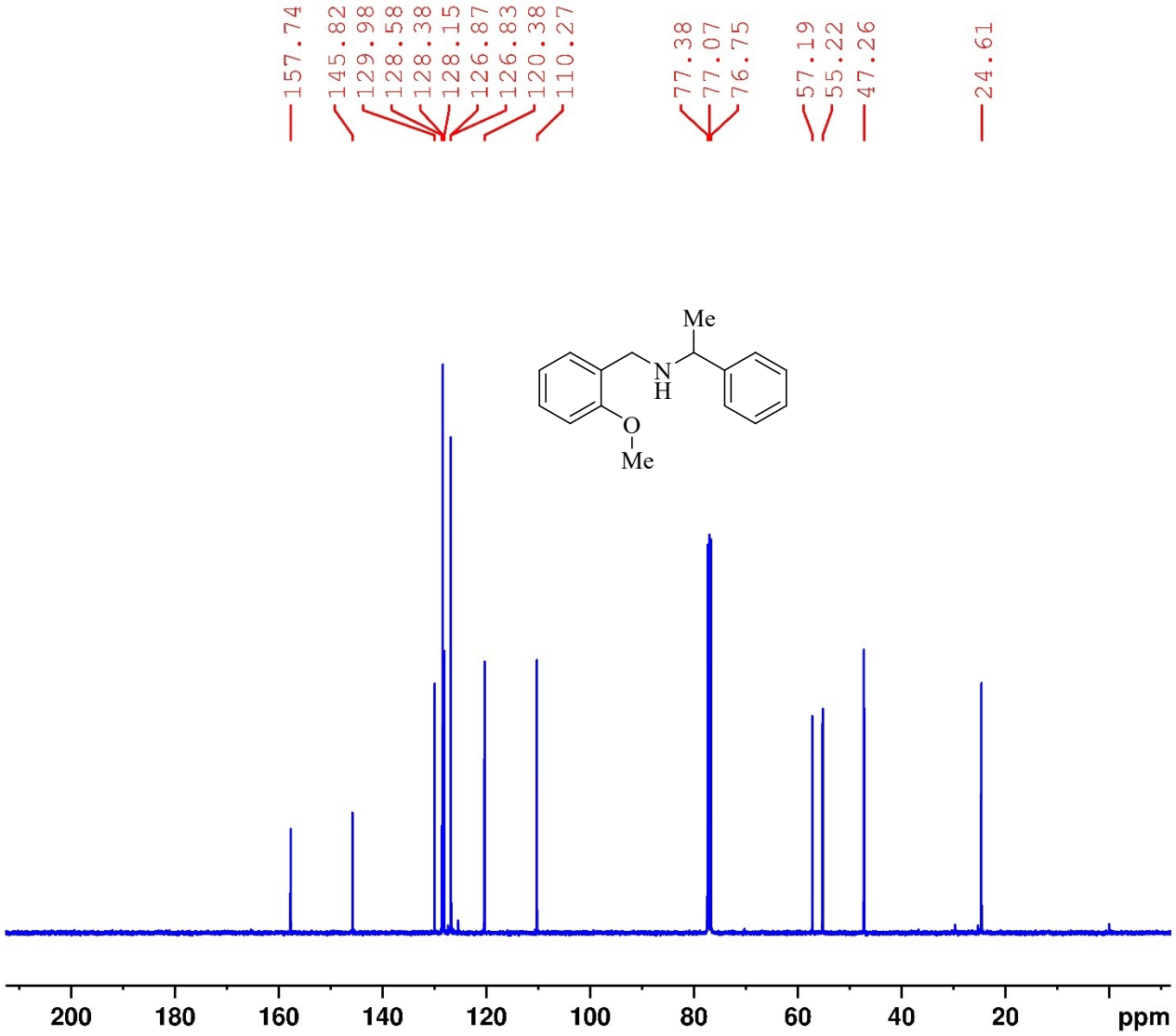
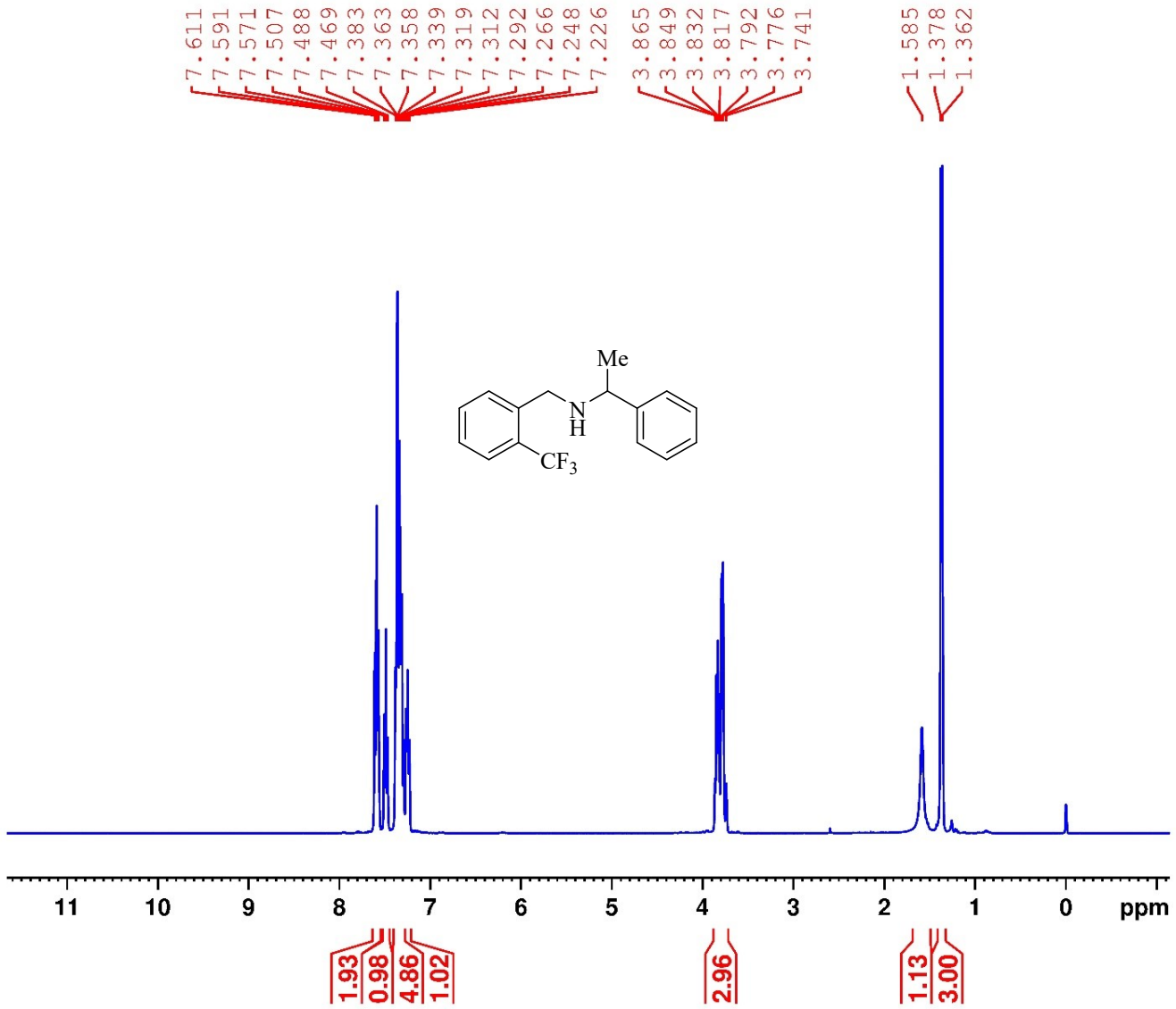
```
Current Data Parameters
NAME      Feb04-2021-nmr
EXPNO                 90
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210204
Time               19.28 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ             3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700189 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



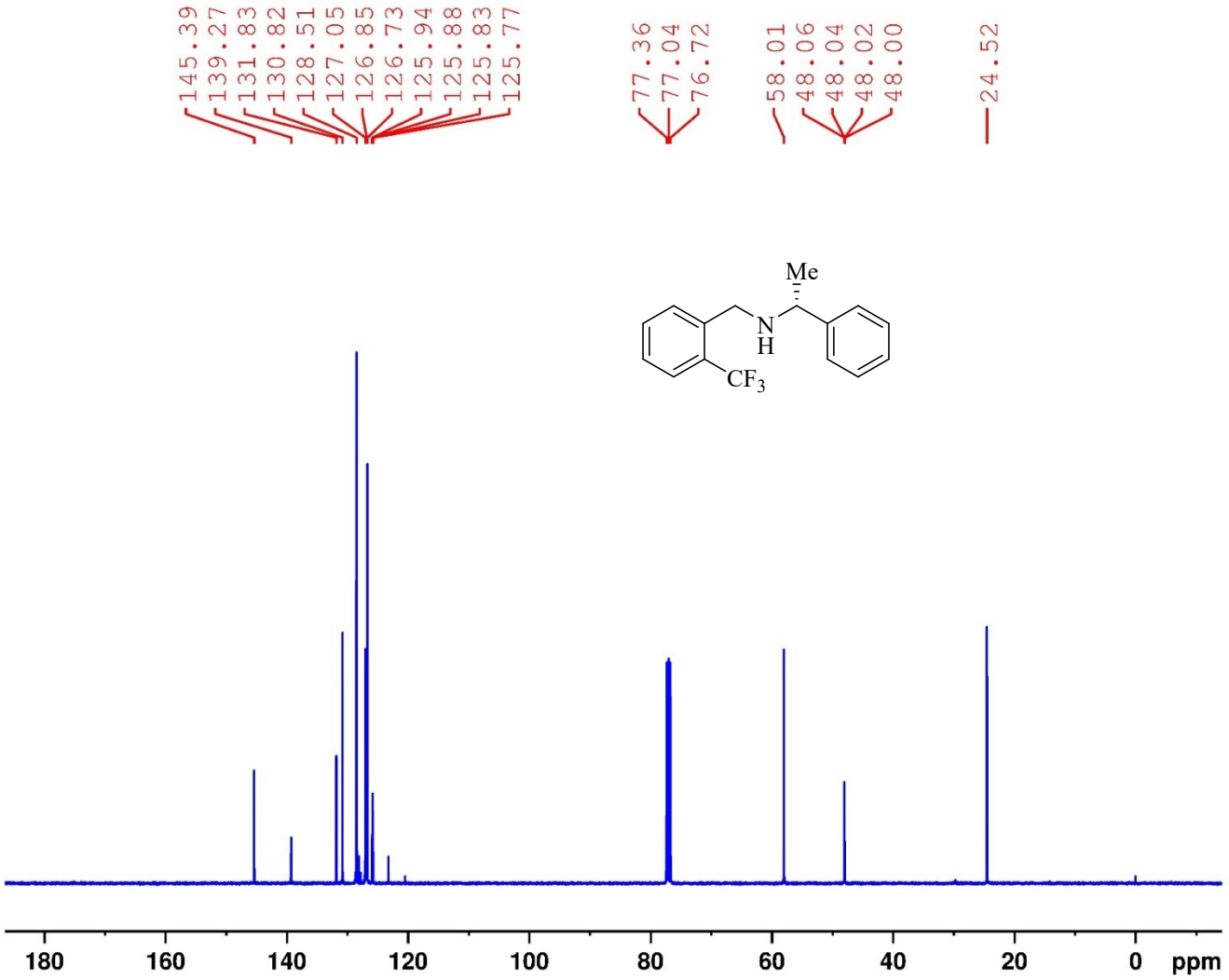

```
Current Data Parameters
NAME      Feb04-2021-nmr
EXPNO                 91
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210204
Time                20.27 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1         60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             90.00 usec
PLW2         16.77000046 W
PLW12         0.40580001 W
PLW13         0.20411000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




Current Data Parameters
NAME Feb04-2021-nmr
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210204
Time 20.32 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RC 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W

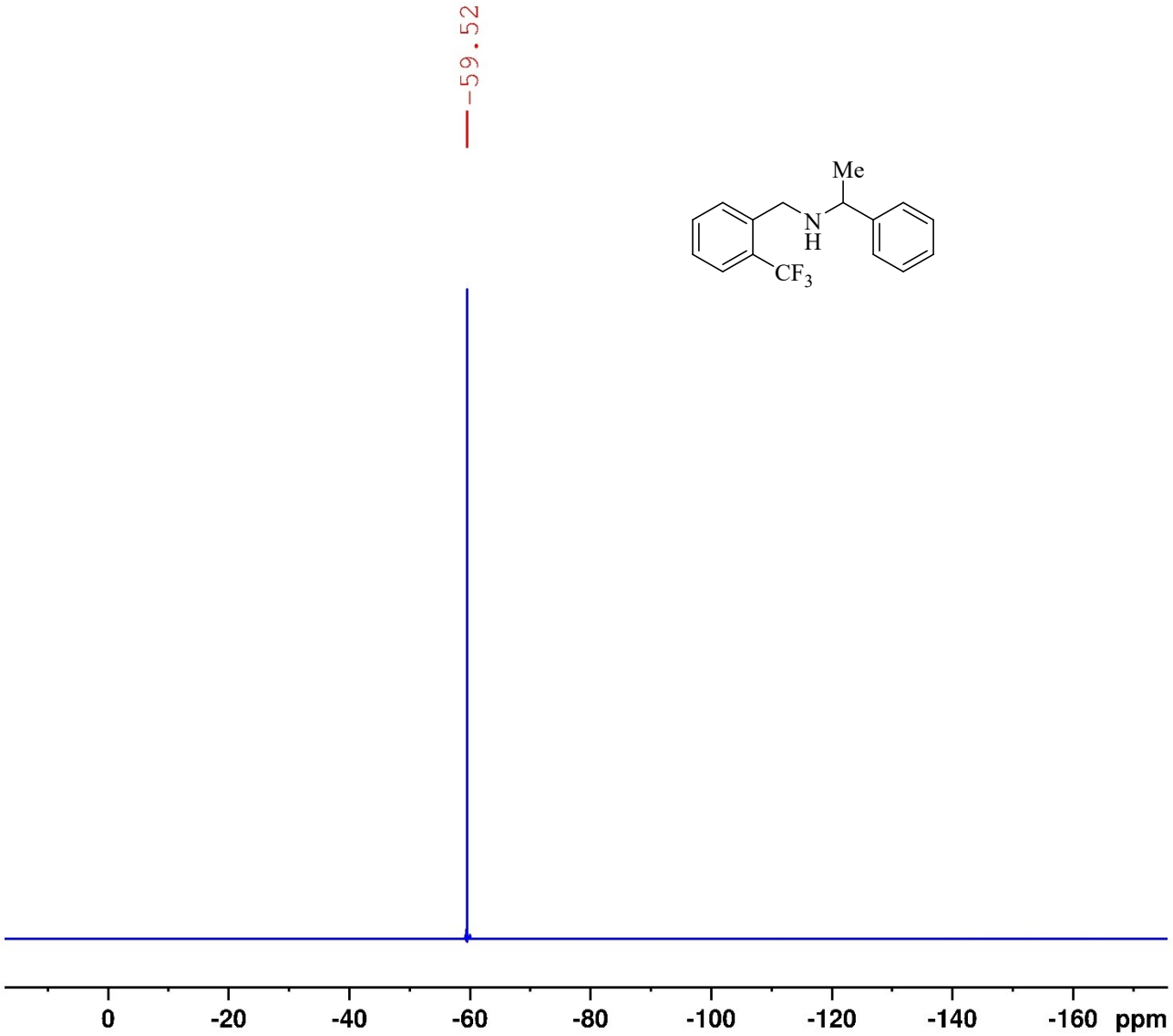
F2 - Processing parameters
SI 65536
SF 400.1700237 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



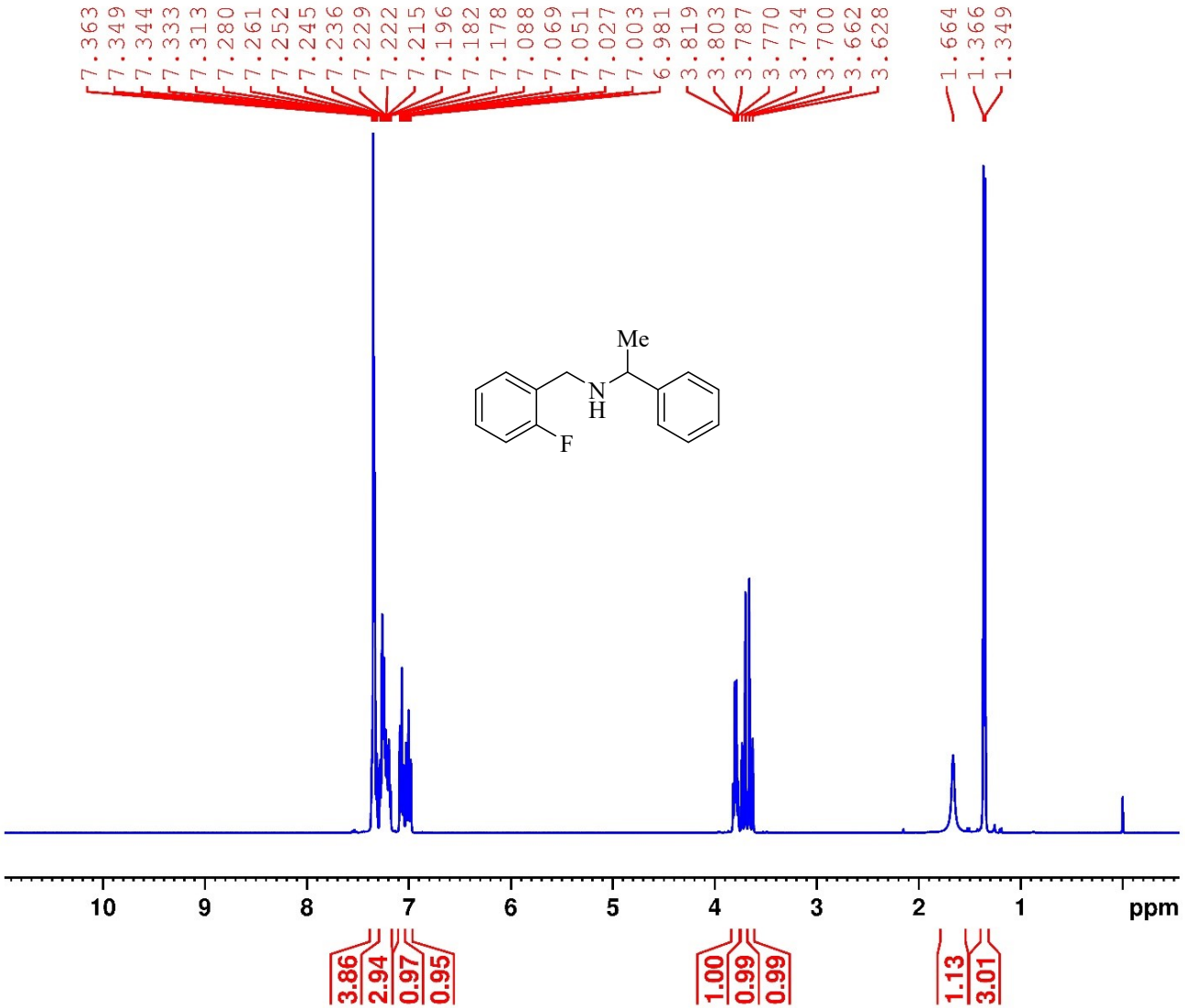

Current Data Parameters
NAME May02-2022-nmr
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220503
Time 6.35 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 101
DW 21.000 usec
DE 6.50 usec
TE 302.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6328888 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 60.89300156 W
SFO2 400.1716007 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 16.77000046 W
PLW12 0.40580001 W
PLW13 0.20411000 W

F2 - Processing parameters
SI 32768
SF 100.6228265 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
NAME      Mar22-2022-nmr
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220322
Time              11.02 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG               zg
TD                131072
SOLVENT             CDCl3
NS                    16
DS                     4
SWH            90909.094 Hz
FIDRES          1.387163 Hz
AQ             0.7208960 sec
RG                   101
DW                 5.500 usec
DE                 6.50 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1
SFO1         376.4983502 MHz
NUC1                 19F
P1                15.00 usec
PLW1         19.22800064 W

F2 - Processing parameters
SI                 65536
SF           376.5360038 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

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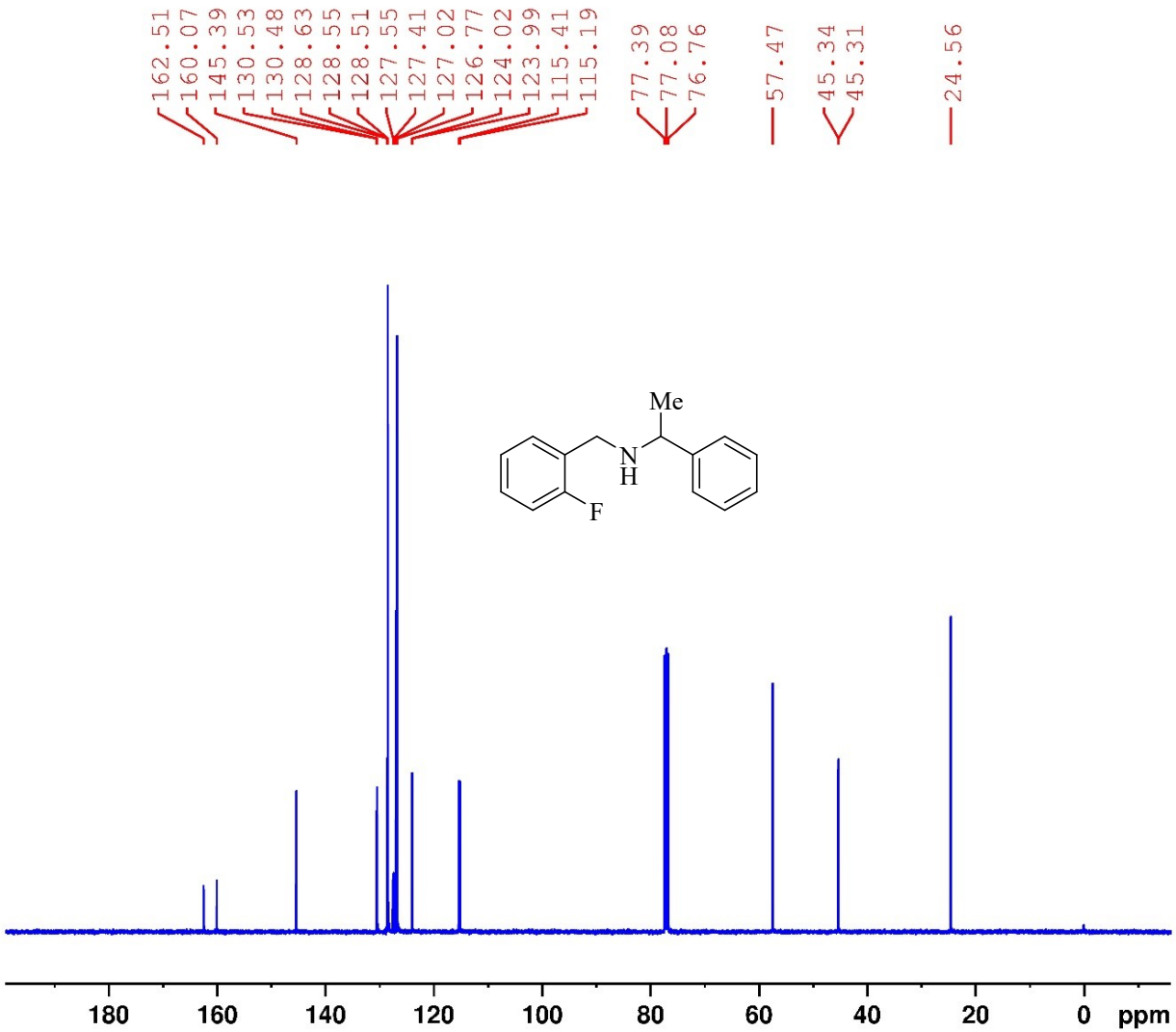
```
Current Data Parameters
NAME      Feb04-2021-nmr
EXPNO                110
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210204
Time              21.08 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ              3.9976959 sec
RG                   101
DW                61.000 usec
DE                12.86 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                 4.67 usec
P1                14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF           400.1700228 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

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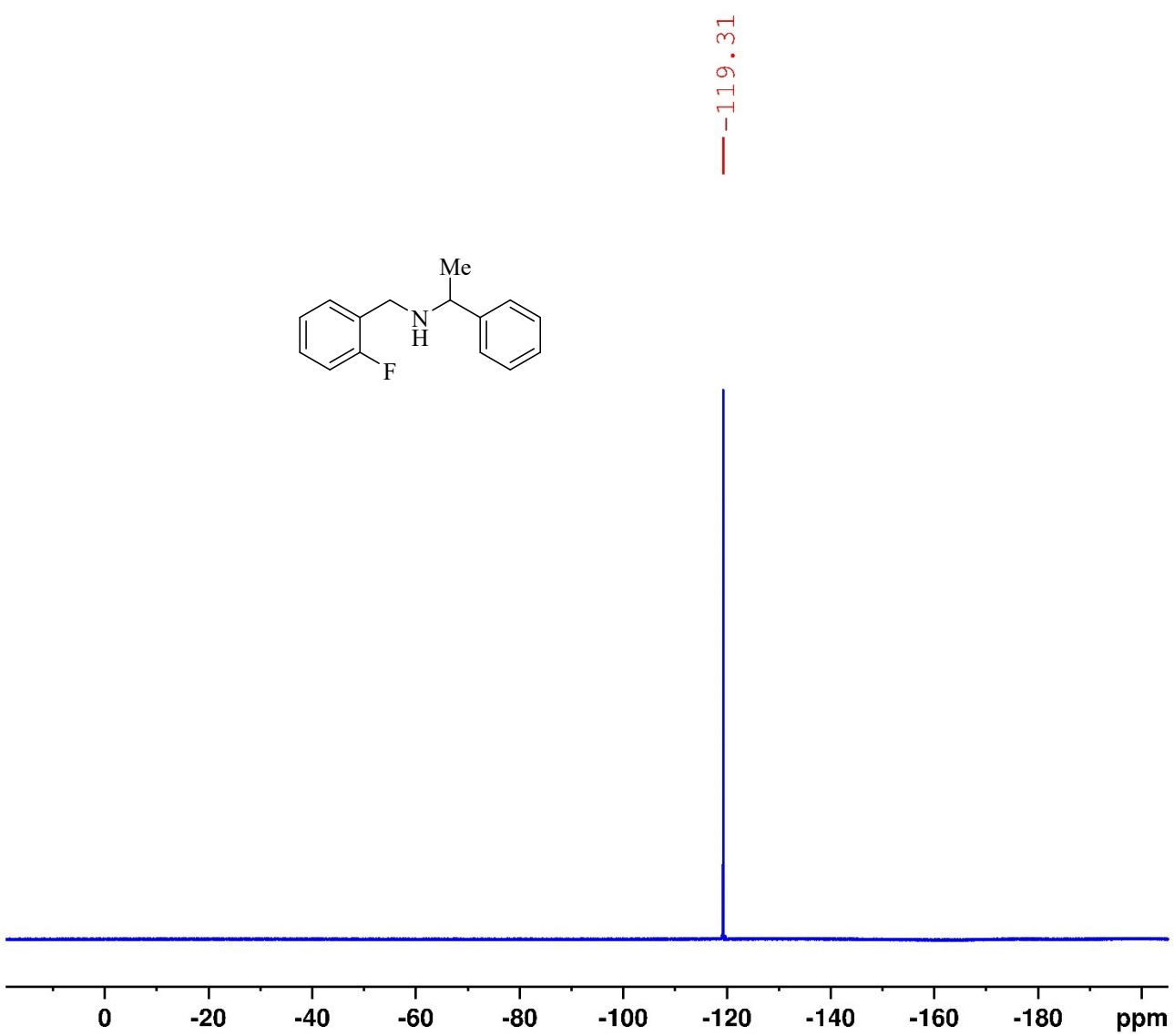
```
Current Data Parameters
NAME      Feb04-2021-nmr
EXPNO              111
PROCNO               1

F2 - Acquisition Parameters
Date_          20210204
Time              21.38 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           23809.523 Hz
FIDRES        0.726609 Hz
AQ            1.3762560 sec
RG                  101
DW               21.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6328888 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        60.89300156 W
SFO2        400.1716007 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            90.00 usec
PLW2        16.77000046 W
PLW12        0.40580001 W
PLW13        0.20111000 W

F2 - Processing parameters
SI                32768
SF          100.6228265 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME      Mar22-2022-nmr
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220322
Time              11.06 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG               zg
TD              131072
SOLVENT           CDCl3
NS                   16
DS                    4
SWH           90909.094 Hz
FIDRES         1.387163 Hz
AQ            0.7208960 sec
RG                  101
DW                5.500 usec
DE                6.50 usec
TE                300.0 K
D1           1.00000000 sec
TD0                   1
SFO1        376.4983502 MHz
NUC1               19F
P1                15.00 usec
PLW1        19.22800064 W

F2 - Processing parameters
SI                65536
SF          376.5360038 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```