

## Electronic Supporting Information

# Synthesis of 1,2-Oxaborole *via* Base-Mediated Borylation of Propynols

Sumit Ghosh,<sup>a</sup> Sudip Laru,<sup>a</sup> Mukta Singsardar,<sup>a</sup> and Alakananda Hajra<sup>\*a</sup>

<sup>a</sup>Department of Chemistry, Visva-Bharati (A Central University), Santiniketan 731235, India

Email: *alakananda.hajra@visva-bharati.ac.in*

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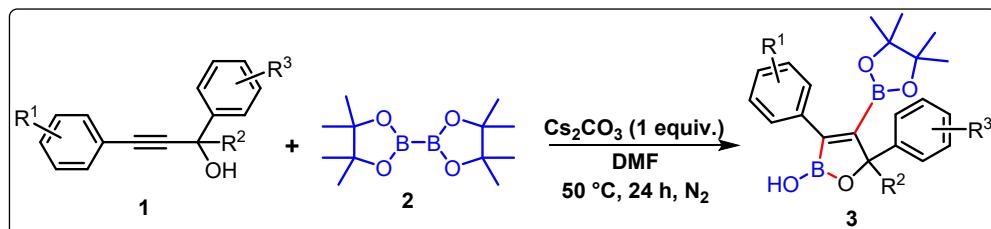
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## **1. General information:**

All reagents were purchased from commercial sources and used without further purification.  $^1\text{H}$  NMR spectra were determined on 400 MHz spectrometer as solutions in  $\text{CDCl}_3$  or  $\text{DMSO}-d_6$ . Chemical shifts were expressed in parts per million ( $\delta$ ) and the signals were reported as s (singlet), d (doublet), dd (doublet of doublet), t (triplet), m (multiplet), q (quartet), and coupling constants ( $J$ ) were given in Hz.  $^{13}\text{C}\{\text{H}\}$  NMR spectra were recorded at 100 MHz in  $\text{CDCl}_3$  or  $\text{DMSO}-d_6$  solution. Chemical shifts were referenced to  $\text{CDCl}_3$  ( $\delta = 7.26$  for  $^1\text{H}$  and  $\delta = 77.16$  for  $^{13}\text{C}\{\text{H}\}$  NMR) or  $\text{DMSO}-d_6$  ( $^1\text{H}$ ,  $\delta = 2.50$  ppm). as internal standard. TLC was done on silica gel-coated glass slide. All solvents were dried and distilled before use. Commercially available solvents were freshly distilled before the reaction. All reactions involving moisture-sensitive reactants were executed using oven-dried glassware. High-resolution mass spectra (HRMS) were collected using electrospray ionization (ESI) on a time-of-flight (TOF) mass spectrometer. The SCXRD-BRUKER D8QUEST collected the crystallographic data for the compounds **3j** and the crystal data was solved by Olex2 1.3-ac4 software. Melting points (mp.) were determined after the recrystallization of solid compounds from a solution of dichloromethane/petroleum ether (1:3). All the propargylic alcohols were prepared by this reported method.<sup>1</sup>

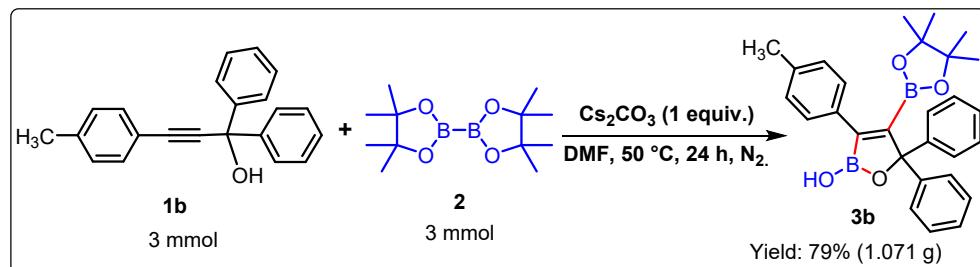
## 2. Experimental procedures:

### 2.1. Typical experimental procedure for the synthesized compounds 3a-3z:



Propargylic alcohols **1** (0.2 mmol, 1 equiv.),  $\text{B}_2\text{pin}_2$  **2** (0.2 mmol, 1 equiv., 50.8 mg) and  $\text{Cs}_2\text{CO}_3$  (0.2 mmol, 1 equiv., 65.2 mg) were loaded in an oven-dried reaction tube which was subjected to flushing with nitrogen three times. Then, DMF (2.0 mL) was added to the mixture *via* syringe, and the reaction mixture was stirred at  $50^\circ\text{C}$  for 24 h. After completion of the reaction (TLC), the reaction mixture was extracted with ethyl acetate. The organic phase was dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate as an eluting solvent to afford the pure products **3a-3z**.

### 3. Gram-scale synthesis of **3b**:

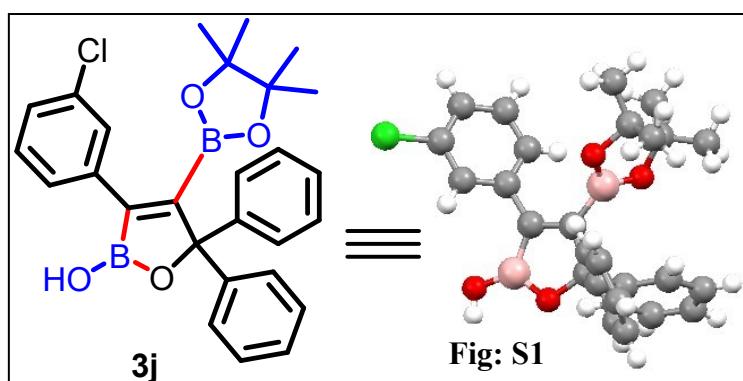


1,1-diphenyl-3-(*p*-tolyl)prop-2-yn-1-ol (**1b**, 3 mmol, 1.0 equiv., 895.15 mg),  $\text{B}_2\text{pin}_2$  (**2**, 3 mmol, 1.0 equiv., 761.82 mg) and  $\text{Cs}_2\text{CO}_3$  (3 mmol, 1.0 equiv., 977.46 mg) were loaded in an oven-dried 25 mL round bottom flask (RB) which was subjected to flushing with nitrogen for

three times. Then, DMF (12 mL) was added to the mixture *via* syringe, and the reaction mixture was stirred at 50 °C for 24 h under N<sub>2</sub> atmosphere. After completion of the reaction (TLC), the reaction mixture was extracted with ethyl acetate. The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture of petroleum ether and ethyl acetate as an eluting solvent to afford the pure product **3b** (1.071 g, 79%) as a yellow solid.

#### **4. Structure determination (X-ray crystallographic data for **3j**):**

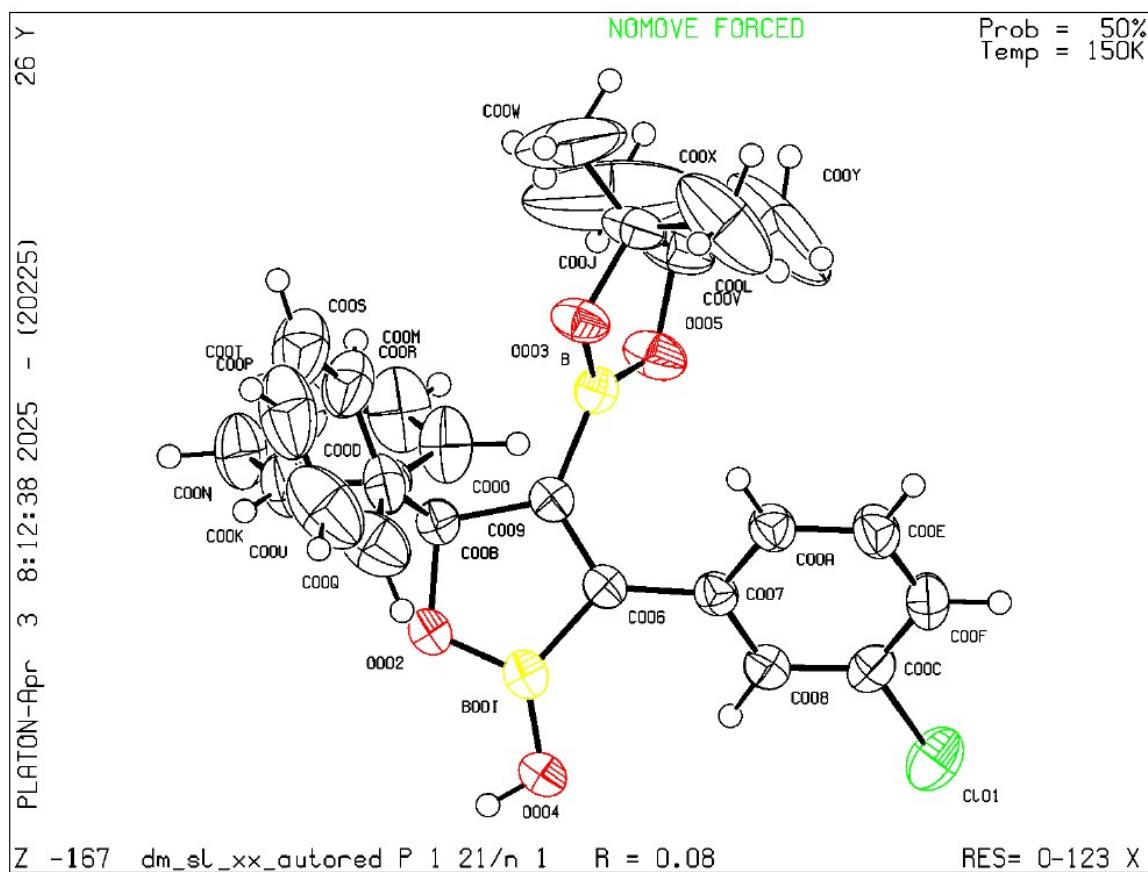
The White crystal of **3j** was obtained by crystallization from a solution in dichloromethane/petroleum ether after purification by column chromatography. Chemical formula: C<sub>27</sub>H<sub>27</sub>B<sub>2</sub>ClO<sub>4</sub>. This data was collected on a RIGAKU SATURN724+ diffractometer using Mo-K $\alpha$  radiation. The data collection was carried out by standard  $\omega$ -scan technique and was evaluated and reduced by using Crystal Clear-SM Expert software. Absorption correction (numerical) was applied to the collected reflections. The structures were solved by direct method using SHELXS-97 and refined by full-matrix least-squares with SHELXL-2012, refining on F2.



<b>Wavelength</b>	0.71073 Å
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<b>Formula</b>	C <sub>27</sub> H <sub>27</sub> B <sub>2</sub> ClO <sub>4</sub>	
<b>Crystal system</b>	monoclinic	
<b>Space group</b>	P 1 21/n 1	
<b>Unit cell dimensions</b>	a = 13.4401(4) Å	α = 90 °
	b = 10.9000 (3) Å	β = 97.099 (3) °
	c = 17.4319 (5) Å	γ = 90 °
<b>Volume</b>	2534.15(13) Å <sup>3</sup>	
<b>Z</b>	4	
<b>R-factor (%)</b>	7.73	

The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication with a CCDC reference number **CCDC 2441373**.

**Fig: S2**

View of ORTEP diagram for the crystal structure of the compound **3-(3-chlorophenyl)-5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3j)**  
(Thermal ellipsoid contour at 50% probability level).

### Alert level B

PLAT220\_ALERT\_2\_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 7.1 Ratio.

Explanation of Alert B:

This particular alert is related to the anisotropic displacement parameters (ADPs) of a non-solvent residue. Specifically, it indicates that for residue 1 (likely a solvent or impurity molecule), the ratio of the maximum to minimum atomic displacement parameter ( $U_{\text{eq}}(\text{max})/U_{\text{eq}}(\text{min})$ ) is unusually large 7.1 in this case. Typically, for well-ordered atoms in a crystal structure, the ratio of these parameters should not deviate significantly from 1. If the

ratio is much larger, it can indicate that the atom's motion is highly anisotropic or that there is some disorder in the structure.

PLAT242\_ALERT\_2\_B Low 'MainMol' Ueq as Compared to Neighbors of C00J Check

PLAT242\_ALERT\_2\_B Low 'MainMol' Ueq as Compared to Neighbors of C00L Check

Explanation of Alert B:

This alert appears in crystallographic refinement reports, typically from software like **PLATON**, and highlights that the **Ueq** (which describes the thermal motion or disorder of an atom) of the **MainMol** atoms is unusually low compared to the neighboring atoms **C00J** and **C00L**.

PLAT412\_ALERT\_2\_B Short Intra XH3 .. XHn H00G ..H00V . 1.76 Ang. x,y,z = 1\_555 Check

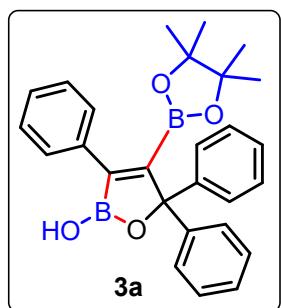
Explanation of Alert B:

The **PLAT412\_ALERT\_2\_B** is a warning from a crystallographic refinement check (typically using **PLATON** or similar tools) that points to a **short intra-molecular hydrogen bond** between two hydrogen atoms, **H00G** and **H00V**, with a distance of **1.76 Å**, which is shorter than expected.

The alert is flagging a **hydrogen–hydrogen distance** of **1.76 Å**, which is unusually short for a hydrogen bond, as typical hydrogen–hydrogen distances in molecular crystals tend to be larger. In most well-refined structures, **hydrogen-hydrogen distances** are expected to be longer than **1.76 Å**.

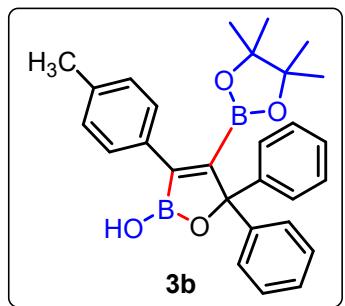
The specific **intra XH3 .. XHn** part of the message suggests that this involves a hydrogen atom (designated by **XH3**) interacting with another hydrogen atom (**XHn**), and the software has detected that the distance between these atoms is shorter than expected based on typical structural parameters.

## 5. Physical data of the compounds 3a-3z:



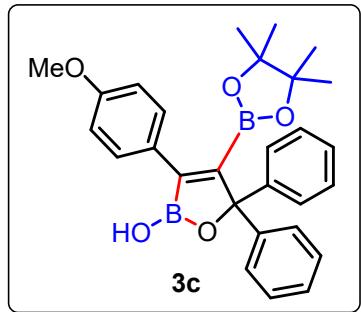
### *3,5,5-triphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3a):*

Brown yellow solid (80.7 mg, 92%); mp. 109–110 °C;  $R_f$  0.45 (PET:EtOAc = 85:15);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.50 (d,  $J$  = 7.6 Hz, 2H), 7.46–7.44 (m, 3H), 7.35–7.24 (m, 10H), 1.08 (m, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  43.4, 137.5, 128.3, 128.2, 128.0, 127.9, 127.6, 127.5, 94.5, 84.1, 24.8; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{27}\text{H}_{29}\text{B}_2\text{O}_4]^{+}$ : 439.2246; Found 439.2272.



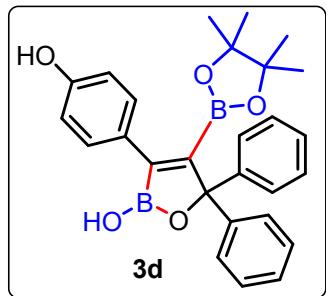
### *5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(p-tolyl)-1,2-oxaborol-2(5H)-ol (3b):*

Yellow solid (85.9 mg, 95%); mp. 140–141 °C;  $R_f$  0.45 (PET:EtOAc = 4:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.46–7.41 (m, 6H), 7.34–7.28 (m, 6H), 7.14 (d,  $J$  = 8 Hz, 2H), 5.04 (s, 1H), 2.35 (s, 3H), 1.10 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  167.9, 143.5, 137.3, 134.5, 131.1, 128.9, 128.3, 128.0, 127.9, 127.5, 94.4, 84.1, 24.8, 21.3; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{28}\text{H}_{31}\text{B}_2\text{O}_4]^{+}$ : 453.2403; Found 453.2412.



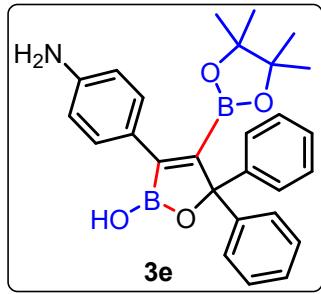
**3-(4-methoxyphenyl)-5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3c):**

Reddish yellow solid (85.3 mg, 91%); mp. 138–139 °C;  $R_f$  0.35 (PET:EtOAc = 85:15);  **$^1\text{H}$  NMR** ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.30 (d,  $J$  = 8.8, 2H), 7.26–7.24 (m, 3H), 7.14–7.06 (m, 7H), 6.67 (d,  $J$  = 8.8, 2H), 3.61 (s, 3H), 0.90 (s, 12H);  **$^{13}\text{C}\{\text{H}\}$  NMR** ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  159.2, 143.4, 130.0, 129.7, 128.0, 127.8, 127.7, 127.5, 113.5, 94.4, 84.0, 55.3, 24.8; **HRMS** (ESI–TOF) m/z: [M + Na]<sup>+</sup> Calcd for  $[\text{C}_{28}\text{H}_{30}\text{B}_2\text{O}_5\text{Na}]^+$ : 491.2172; Found 491.2162.



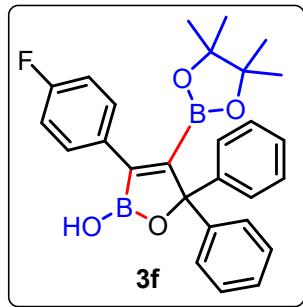
**3-(4-hydroxyphenyl)-5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3d):**

Brown solid (77.3 mg, 85%); mp. 156–157 °C;  $R_f$  0.4 (PET:EtOAc = 7:3);  **$^1\text{H}$  NMR** ( $\text{DMSO}-d_6$ , 400 MHz):  $\delta$  9.49 (s, 1H), 9.18 (s, 1H), 7.34–7.26 (m, 12H), 6.71 (d,  $J$  = 8.4 Hz, 2H), 1.04 (s, 12H);  **$^{13}\text{C}\{\text{H}\}$  NMR** ( $\text{DMSO}-d_6$ , 100 MHz):  $\delta$  157.0, 144.0, 129.5, 128.3, 127.7, 127.4, 127.3, 114.7, 92.7, 83.5, 24.5; **HRMS** (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{27}\text{H}_{29}\text{B}_2\text{O}_5]^+$ : 455.2196; Found 455.2207.



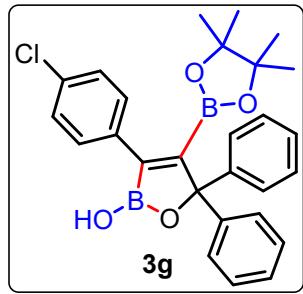
**3-(4-aminophenyl)-5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3e):**

Brown solid (77.97 mg, 86%); mp. 158–159 °C;  $R_f$  0.4 (PET:EtOAc = 7:3);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.43–7.41 (m, 4H), 7.36 (d,  $J$  = 8.4 Hz, 2H), 7.31–7.25 (m, 6H), 6.70 (d,  $J$  = 8.0 Hz, 2H), 1.08 (s, 12H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  144.7, 143.6, 129.7, 128.8, 128.1, 127.8, 127.5, 115.5, 94.3, 84.0, 24.8; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{27}\text{H}_{30}\text{B}_2\text{NO}_4]^{+}$ : 454.2355; Found 454.2362.

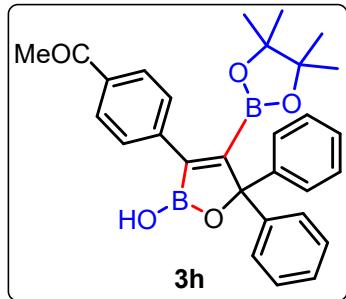


**3-(4-fluorophenyl)-5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3f):**

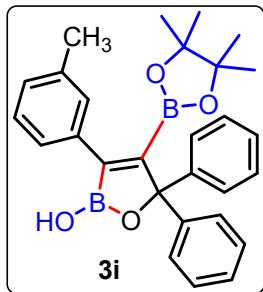
White solid (74.9 mg, 82%); mp. 154–155 °C;  $R_f$  0.4 (PET:EtOAc = 9:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.51–7.48 (m, 2H), 7.44–7.41 (m, 4H), 7.34–7.28 (m, 6H), 7.03–6.99 (m, 2H), 5.10 (s, 1H), 1.08 (s, 12H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  162.5 ( $J_{\text{C}-\text{F}} = 245$  Hz), 143.2, 133.4 ( $J_{\text{C}-\text{F}} = 3.0$  Hz), 130.2, 130.1, 128.0, 127.9, 127.8, 127.7, 127.5, 115.1, 114.9, 114.8 ( $J_{\text{C}-\text{F}} = 14.0$  Hz), 94.6, 84.2, 24.8;  $^{19}\text{F}$  NMR (376.5 MHz,  $\text{CDCl}_3$ ):  $\delta$  -114.93; HRMS (ESI–TOF) m/z: [M + Na]<sup>+</sup> Calcd for  $[\text{C}_{27}\text{H}_{27}\text{B}_2\text{FO}_4\text{Na}]^{+}$ : 479.1972; Found 479.1982.



**3-(4-chlorophenyl)-5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3g):** White solid (76.58 mg, 81%); mp. 180–181 °C;  $R_f$  0.45 (PET:EtOAc = 4:1); **1H NMR** ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.46–7.44 (m, 2H), 7.43–7.40 (m, 4H), 7.33–7.28 (m, 8H), 4.89 (s, 1H), 1.08 (s, 12H);  **$^{13}\text{C}\{\text{H}\}$  NMR** ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  143.1, 135.9, 133.4, 129.8, 128.2, 128.0, 127.9, 127.7, 94.6, 84.3, 24.8; **HRMS** (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{27}\text{H}_{28}\text{B}_2\text{ClO}_4]^{+}$ : 473.1857; Found 473.1880.

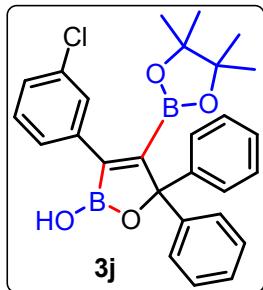


**1-(4-(2-hydroxy-5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)ethan-1-one (3h):** White solid (80.67 mg, 84%); mp. 168–169 °C;  $R_f$  0.4 (PET:EtOAc = 85:15); **1H NMR** ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.92–7.90 (m, 2H), 7.60–7.58 (m, 2H), 7.44–7.42 (m, 4H), 7.33–7.30 (m, 6H), 5.68 (s, 1H), 2.59 (s, 3H), 1.07 (s, 12H);  **$^{13}\text{C}\{\text{H}\}$  NMR** ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  198.2, 142.9, 142.6, 135.8, 128.6, 128.2, 128.0, 127.9, 127.7, 94.7, 84.3, 26.7, 24.7; **HRMS** (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{29}\text{H}_{31}\text{B}_2\text{O}_5]^{+}$ : 481.2352; Found 481.2362.



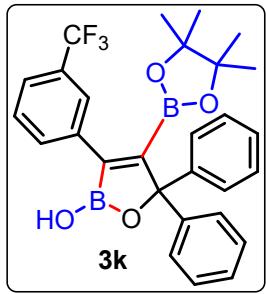
**5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(*m*-tolyl)-1,2-oxaborol-2(5*H*)-ol (3i):**

Pale yellow solid (75.10 mg, 83%); mp. 119–120 °C;  $R_f$  0.4 (PET:EtOAc = 9:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.44–7.41 (m, 4H), 7.31–7.24 (m, 8H), 7.20 (t,  $J$  = 8.4 Hz, 1H), 7.06 (d,  $J$  = 7.6 Hz, 1H), 5.21 (s, 1H), 2.33 (s, 3H), 1.06 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  143.3, 137.5, 137.3, 128.8, 128.3, 128.1, 128.0, 127.9, 127.7, 127.5, 125.4, 94.5, 84.0, 24.8, 21.5; HRMS (ESI–TOF) m/z: [M + K]<sup>+</sup> Calcd for  $[\text{C}_{28}\text{H}_{30}\text{B}_2\text{O}_4\text{K}]^+$ : 491.1962; Found 491.1956.



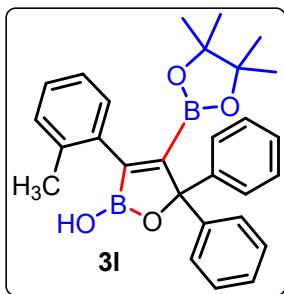
**3-(3-chlorophenyl)-5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5*H*)-ol (3j):**

White solid (75.7 mg, 80%); mp. 152–153 °C;  $R_f$  0.45 (PET:EtOAc = 4:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.41 (s, 1H), 7.33–7.31 (m, 4H), 7.23–7.16 (m, 7H), 7.14–7.12 (m, 2H), 5.56 (s, 1H), 0.99 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  142.9, 139.2, 133.8, 129.4, 128.2, 128.0, 127.9, 127.7, 127.4, 126.8, 94.7, 84.3, 24.8; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{27}\text{H}_{28}\text{B}_2\text{ClO}_4]^+$ : 473.1857; Found 473.1880.



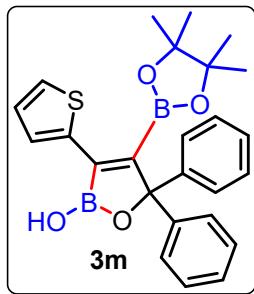
**5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(3-(trifluoromethyl)phenyl)-1,2-oxaborol-2(5H)-ol (3k):**

White solid (87.1 mg, 86%); mp. 148–149 °C;  $R_f$  0.45 (PET:EtOAc = 85:15);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.82 (s, 1H), 7.74 (d,  $J$  = 7.6 Hz, 1H), 7.55 (d,  $J$  = 7.6 Hz, 1H), 7.48–7.44 (m, 5H), 7.38–7.33 (m, 6H), 5.88 (s, 1H), 1.10 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  144.6 ( $J$  = 366 Hz), 138.1, 132.0, 130.7, 130.4, 130.1, 129.8, 128.5, 128.0 ( $J$  = 7 Hz), 127.9, 127.8, 125.7, 125.0 ( $J$  = 3 Hz), 125.03, 124.24, 124.1 ( $J$  = 6 Hz), 123.0, 120.3, 94.9, 84.3, 24.7;  $^{19}\text{F}$  NMR (376.5 MHz,  $\text{CDCl}_3$ ):  $\delta$  -62.27; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{28}\text{H}_{28}\text{B}_2\text{F}_3\text{O}_4]^+$ : 507.2120; Found 507.2143.

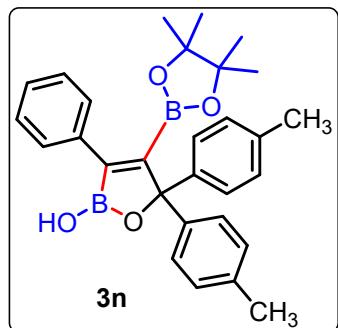


**5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(o-tolyl)-1,2-oxaborol-2(5H)-ol (3l):**

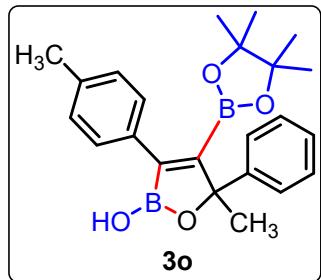
White solid (76.87 mg, 85%); mp. 111–112 °C;  $R_f$  0.4 (PET:EtOAc = 9:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.46–7.44 (m, 4H), 7.35–7.29 (m, 6H), 7.15–7.09 (m, 4H), 5.08 (s, 1H), 2.28 (s, 3H), 0.94 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  143.6, 137.9, 135.4, 129.5, 128.4, 127.9, 127.8, 127.5, 126.9, 125.2, 94.7, 83.8, 24.4, 20.5; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{28}\text{H}_{31}\text{B}_2\text{O}_4]^+$ : 453.2403; Found 453.2438.



**5,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(thiophen-2-yl)-1,2-oxaborol-2(5H)-ol (3m):** Brown solid (70.18 mg, 79%); mp. 132–133 °C;  $R_f$  0.35 (PET:EtOAc = 9:1);  **$^1\text{H}$  NMR** ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.54 (d,  $J$  = 3.6 Hz, 1H), 7.42–7.40 (m, 4H), 7.33–7.28 (m, 7H), 7.03–7.01 (m, 1H), 5.23 (s, 1H), 1.16 (s, 12H);  **$^{13}\text{C}\{\text{H}\}$  NMR** ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  143.1, 139.6, 128.8, 128.1, 127.8, 127.6, 127.4, 126.2, 94.9, 84.3, 25.0; **HRMS** (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{25}\text{H}_{27}\text{B}_2\text{O}_4\text{S}]^+$ : 445.1811; Found 445.1820.

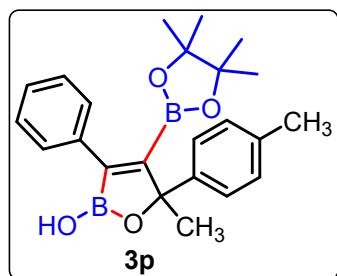


**3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5,5-di-p-tolyl-1,2-oxaborol-2(5H)-ol (3n):** White solid (82.98 mg, 89%); mp. 152–153 °C;  $R_f$  0.35 (PET:EtOAc = 9:1);  **$^1\text{H}$  NMR** ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.52–7.50 (m, 2H), 7.36–7.30 (m, 6H), 7.28–7.22 (m, 1H), 7.14–7.12 (m, 4H), 5.53 (s, 1H), 2.36 (s, 6H), 1.10 (s, 12H);  **$^{13}\text{C}\{\text{H}\}$  NMR** ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  140.4, 137.6, 137.1, 128.5, 128.4, 128.3, 128.2, 128.0, 127.9, 127.3, 94.4, 84.0, 24.8, 21.2; **HRMS** (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{29}\text{H}_{33}\text{B}_2\text{O}_4]^+$ : 467.2559; Found 467.2602.



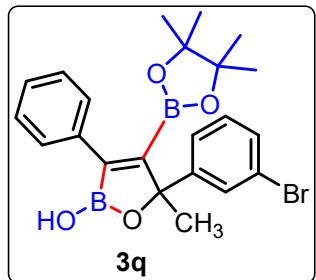
**5-methyl-5-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(p-tolyl)-1,2-oxaborol-2(5H)-ol (3o):**

White solid (56.28 mg, 72%); mp. 158–159 °C;  $R_f$  0.4 (PET:EtOAc = 9:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.45–7.42 (m, 2H), 7.36 (d,  $J$  = 8.4 Hz, 2H), 7.31–7.27 (m, 2H), 7.24–7.20 (m, 1H), 7.12 (d,  $J$  = 8 Hz, 2H), 4.81 (s, 1H), 2.33 (s, 3H), 1.93 (s, 3H), 1.10 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  142.3, 137.2, 134.4, 128.8, 128.4, 128.2, 127.4, 125.8, 89.7, 83.9, 26.5, 24.8, 24.5, 21.3; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{23}\text{H}_{29}\text{B}_2\text{O}_4]^{+}$ : 391.2246 Found 391.2234.



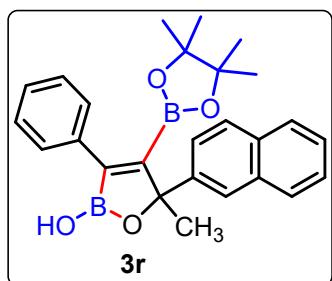
**5-methyl-3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5-(p-tolyl)-1,2-oxaborol-2(5H)-ol (3p):**

White solid (61.83 mg, 79%); mp. 168–169 °C;  $R_f$  0.45 (PET:EtOAc = 9:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.47–7.45 (m, 2H), 7.35–7.28 (m, 4H), 7.25–7.22 (m, 1H), 7.11 (d,  $J$  = 8.0 Hz, 2H), 5.31 (s, 1H), 2.31 (s, 3H), 1.93 (s, 3H), 1.12 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  139.2, 137.4, 137.0, 128.9, 128.3, 128.0, 127.3, 125.7, 89.8, 83.9, 26.6, 24.8, 24.5, 21.1; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{23}\text{H}_{29}\text{B}_2\text{O}_4]^{+}$ : 391.2246; Found 391.2255.



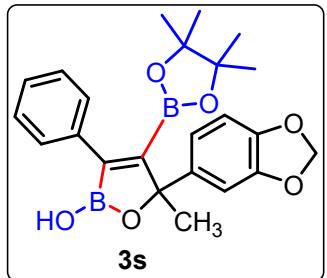
**5-(3-bromophenyl)-5-methyl-3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3q):**

White solid (68.54 mg, 75%); mp. 156–157 °C;  $R_f$  0.4 (PET:EtOAc = 9:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.51 (s, 1H), 7.35–7.33 (m, 2H), 7.29–7.25 (m, 2H), 7.20 (t,  $J$  = 7.2 Hz, 2H), 7.16–7.12 (m, 1H), 7.09–7.05 (m, 1H), 5.54 (s, 1H), 1.82 (s, 3H), 1.04 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  144.9, 137.0, 130.4, 129.9, 128.9, 128.3, 128.1, 127.5, 124.3, 122.4, 89.5, 84.1, 26.8, 24.9, 24.6; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{22}\text{H}_{26}\text{B}_2\text{BrO}_4]^+$ : 455.1195; Found 455.1230.

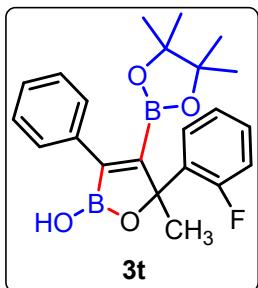


**5-methyl-5-(naphthalen-2-yl)-3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3r):**

White solid (67.59 mg, 79%); mp. 138–139 °C;  $R_f$  0.4 (PET:EtOAc = 85:15);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  8.00 (s, 1H), 7.88–7.83 (m, 3H), 7.61–7.59 (m, 1H), 7.56–7.54 (m, 2H), 7.51–7.49 (m, 2H), 7.36 (t,  $J$  = 7.6 Hz, 2H), 7.31–7.27 (m, 1H), 5.95 (s, 1H), 2.14 (s, 3H), 1.11 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  139.7, 137.3, 133.2, 132.7, 128.3, 128.2, 128.09, 128.06, 127.6, 127.4, 126.0, 125.9, 124.5, 124.1, 90.0, 84.0, 26.6, 24.8, 24.4; HRMS (ESI–TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{26}\text{H}_{29}\text{B}_2\text{O}_4]^+$ : 427.2246; Found 427.2274.

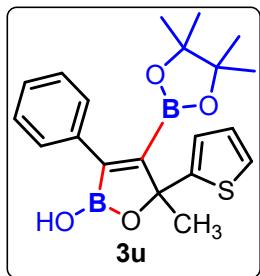


**5-(benzo[d][1,3]dioxol-5-yl)-5-methyl-3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3s):** Brown solid (62.50 mg, 74%); mp. 179–180 °C;  $R_f$  0.4 (PET:EtOAc = 85:15);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.51–7.48 (m, 2H), 7.36–7.32 (m, 2H), 7.30–7.25 (m, 1H), 6.99–6.96 (m, 2H), 6.78–6.76 (m, 1H), 5.95–5.94 (m, 2H), 1.95 (s, 3H), 1.17 (s, 12H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  147.6, 146.8, 137.3, 136.3, 128.3, 128.0, 127.3, 119.2, 107.8, 106.8, 101.0, 89.6, 84.0, 26.7, 24.8, 24.5; HRMS (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for  $[\text{C}_{23}\text{H}_{27}\text{B}_2\text{O}_6]^+$ : 421.1988; Found 421.2016.

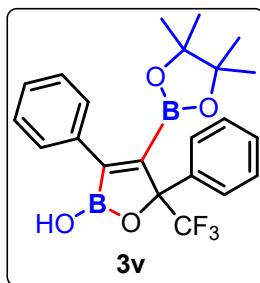


**5-(2-fluorophenyl)-5-methyl-3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol (3t):** Green solid (59.11 mg, 75%); mp. 148–149 °C;  $R_f$  0.5 (PET:EtOAc = 9:1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  7.37–7.33 (m, 3H), 7.19–7.15 (m, 2H), 7.12–7.08 (m, 2H), 6.95 (t,  $J$  = 7.6 Hz, 1H), 6.88–6.83 (m, 1H), 5.37 (s, 1H), 1.84 (s, 3H), 1.00 (s, 6H), 0.97 (s, 6H);  $^{13}\text{C}\{\text{H}\}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  160.9 ( $J_{\text{C}-\text{F}} = 247.0$  Hz), 137.4, 129.5 ( $J_{\text{C}-\text{F}} = 9.0$  Hz), 129.4, 129.3, 128.2, 128.1, 127.9, 127.3, 123.9 ( $J_{\text{C}-\text{F}} = 3.0$  Hz), 116.3 ( $J_{\text{C}-\text{F}} = 23.0$  Hz),

88.6, 84.1, 26.9, 26.8, 24.9, 24.6; **<sup>19</sup>F NMR** (376.5 MHz, CDCl<sub>3</sub>):  $\delta$  -109.53; **HRMS** (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for [C<sub>22</sub>H<sub>26</sub>B<sub>2</sub>FO<sub>4</sub>]<sup>+</sup>: 395.1996; Found 395.2014.

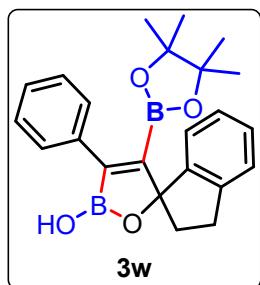


**5-methyl-3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5-(thiophen-2-yl)-1,2-oxaborol-2(5H)-ol (3u):** Brown solid (61.90 mg, 81%); mp. 130–131 °C; R<sub>f</sub> 0.4 (PET:EtOAc = 9:1); **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 400 MHz):  $\delta$  7.51–7.48 (m, 2H), 7.34–7.30 (m, 2H), 7.28–7.24 (m, 1H), 7.21–7.19 (m, 1H), 7.07–7.06 (m, 1H), 6.93–6.91 (m, 1H), 5.78 (s, 1H), 2.01 (s, 3H), 1.16 (s, 6H), 1.13 (s, 6H); **<sup>13</sup>C{<sup>1</sup>H} NMR** (CDCl<sub>3</sub>, 100 MHz):  $\delta$  147.3, 137.0, 128.4, 128.0, 127.5, 126.6, 125.0, 124.6, 87.7, 84.0, 27.7, 24.7, 24.4; **HRMS** (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for [C<sub>20</sub>H<sub>25</sub>B<sub>2</sub>O<sub>4</sub>S]<sup>+</sup>: 383.1654; Found 383.1650.

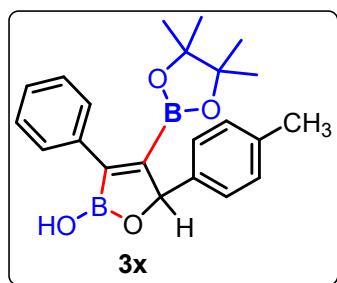


**3,5-diphenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5-(trifluoromethyl)-1,2-oxaborol-2(5H)-ol (3v):** White solid (67.09 mg, 78%); mp. 182–183 °C; R<sub>f</sub> 0.4 (PET:EtOAc = 85:15); **<sup>1</sup>H NMR** (DMSO-d<sub>6</sub>, 400 MHz):  $\delta$  9.95 (s, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.47–7.37 (m, 6H), 7.36–7.29 (m, 3H), 1.16 (s, 6H), 1.14 (s, 6H); **<sup>13</sup>C{<sup>1</sup>H} NMR** (DMSO-d<sub>6</sub>, 100 MHz):  $\delta$  152.6 (*J*<sub>C-F</sub> = 250.0 Hz), 151.3 (*J*<sub>C-F</sub> = 3.0 Hz), 151.2, 136.3, 134.9, 128.9, 128.4, 128.1 (*J*<sub>C-F</sub> = 9.0 Hz), 127.8, 126.2, 125.8, 123.0, 88.8 (t, *J*<sub>C-F</sub> = 29.0 Hz), 84.2, 24.5, 24.4; **<sup>19</sup>F NMR**

(376.5 MHz, DMSO-d<sub>6</sub>): δ -74.0; **HRMS** (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for [C<sub>22</sub>H<sub>24</sub>B<sub>2</sub>F<sub>3</sub>O<sub>4</sub>]<sup>+</sup>: 431.1807; Found 431.1811.

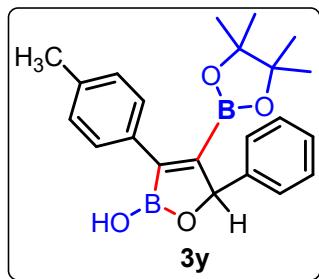


**3'-phenyl-4'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-2,3-dihydro-2'H-spiro[indene-1,5'-[1,2]oxaborol]-2'-ol (3w):** White solid (55.04 mg, 71%); mp. 170–171 °C; R<sub>f</sub> 0.4 (PET:EtOAc = 85:15); **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 400 MHz): δ 7.56–7.53 (m, 2H), 7.35–7.30 (m, 2H), 7.28–7.22 (m, 3H), 7.17–7.15 (m, 1H), 7.14–7.09 (m, 1H), 5.19 (s, 1H), 3.27–3.19 (m, 1H), 3.10–3.03 (m, 1H), 2.88–2.80 (m, 1H), 2.33–2.27 (m, 1H), 1.02 (s, 6H), 0.97 (s, 6H); **<sup>13</sup>C{<sup>1</sup>H} NMR** (CDCl<sub>3</sub>, 100 MHz): δ 144.7, 142.7, 137.3, 128.8, 128.3, 128.2, 127.4, 126.6, 124.9, 124.0, 98.2, 83.9, 37.4, 30.6, 24.5, 24.2; **HRMS** (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for [C<sub>23</sub>H<sub>27</sub>B<sub>2</sub>O<sub>4</sub>]<sup>+</sup>: 389.2090; Found 389.2115.



**3-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5-(p-tolyl)-1,2-oxaborol-2(5H)-ol (3x):** Brown oil (55.09 mg, 73%); R<sub>f</sub> 0.5 (PET:EtOAc = 9:1); **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 400 MHz): δ 7.57–7.55 (m, 2H), 7.35–7.31 (m, 2H), 7.28–7.24 (m, 1H), 7.20 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 7.6 Hz, 2H), 5.86 (s, 1H), 2.32 (s, 3H), 1.08 (s, 6H), 1.03 (s, 6H); **<sup>13</sup>C{<sup>1</sup>H} NMR** (CDCl<sub>3</sub>, 100 MHz): δ 138.0, 137.1, 135.5, 129.1, 128.4, 128.1, 127.5, 127.3, 87.0, 84.1, 24.7, 24.2,

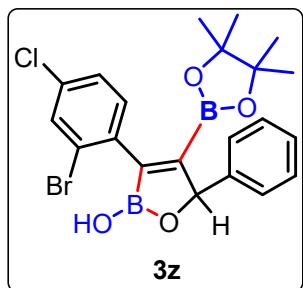
21.3; **HRMS** (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for [C<sub>22</sub>H<sub>27</sub>B<sub>2</sub>O<sub>4</sub>]<sup>+</sup>: 377.2090; Found 377.2109.



**5-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-3-(p-tolyl)-1,2-oxaborol-2(5H)-ol**

(3y): Yellow solid (55.66 mg, 74%); mp. 135–136 °C; R<sub>f</sub> 0.5 (PET:EtOAc = 9:1); **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 400 MHz): δ 7.48 (d, J = 8.0 Hz, 2H), 7.32–7.25 (m, 5H), 7.14 (d, J = 8.0 Hz, 2H), 5.88 (s, 1H), 5.28 (s, 1H), 2.35 (s, 3H), 1.07 (s, 6H), 1.03 (s, 6H); **<sup>13</sup>C{<sup>1</sup>H} NMR** (CDCl<sub>3</sub>, 100 MHz): δ 138.6, 137.4, 134.0, 128.9, 128.4, 128.3, 127.4, 87.1, 84.0, 24.7, 24.2, 21.4;

**HRMS** (ESI-TOF) m/z: [M + K]<sup>+</sup> Calcd for [C<sub>22</sub>H<sub>26</sub>B<sub>2</sub>O<sub>4</sub>K]<sup>+</sup>: 415.1649; Found 415.1660.

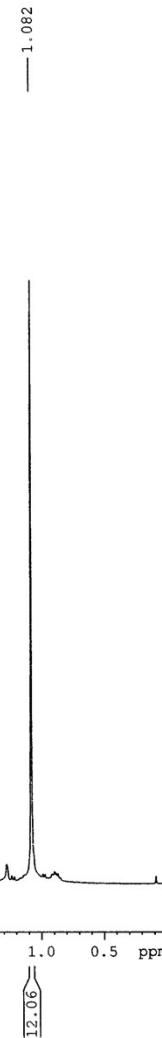
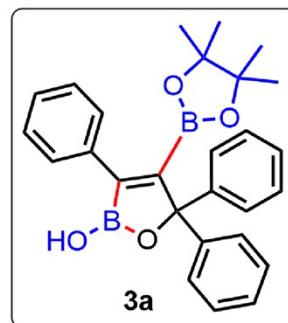
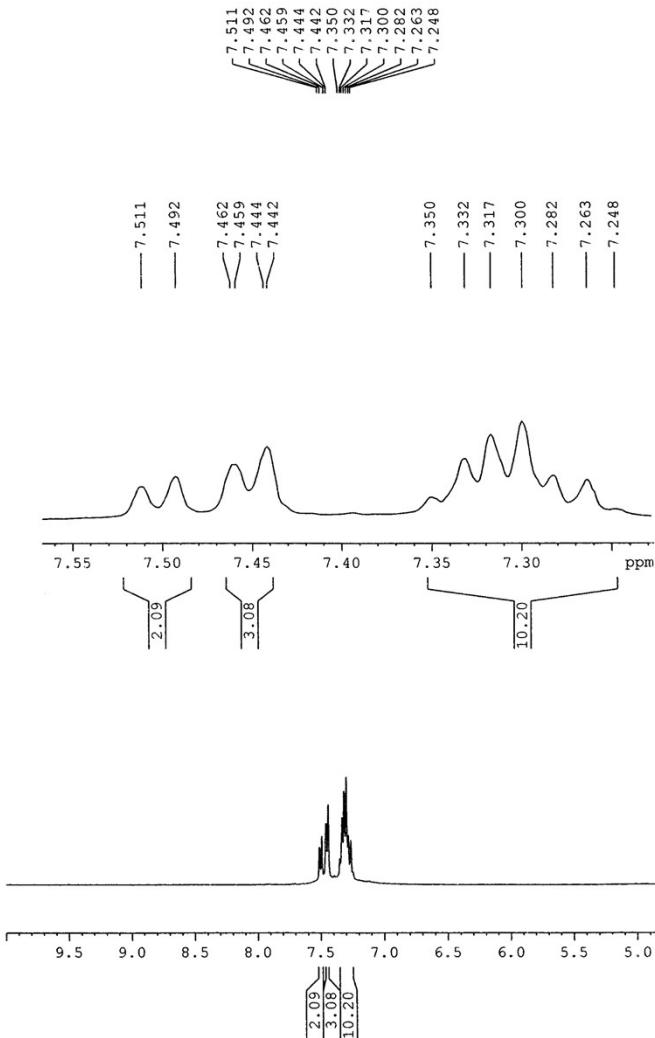


**3-(2-bromo-4-chlorophenyl)-5-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2-oxaborol-2(5H)-ol** (3z): Yellow solid (66.70 mg, 70%); mp. 185–186 °C; R<sub>f</sub> 0.45 (PET:EtOAc = 9:1); **<sup>1</sup>H NMR** (CDCl<sub>3</sub>, 400 MHz): δ 7.60–7.56 (m, 3H), 7.37–7.32 (m, 2H), 7.31–7.27 (m, 1H), 7.24–7.21 (m, 1H), 7.07 (d, J = 8.0 Hz, 1H), 6.35 (s, 1H), 5.11 (s, 1H), 1.11 (s, 6H), 1.05 (s, 6H); **<sup>13</sup>C{<sup>1</sup>H} NMR** (CDCl<sub>3</sub>, 100 MHz): δ 136.7, 136.5, 134.8, 132.5, 129.8, 128.39, 128.31, 128.0, 127.9, 125.0, 84.7, 84.3, 24.7, 24.3; **HRMS** (ESI-TOF) m/z: [M + H]<sup>+</sup> Calcd for [C<sub>21</sub>H<sub>23</sub>B<sub>2</sub>BrClO<sub>4</sub>]<sup>+</sup>: 475.0649; Found 475.0673.

## **6. References:**

- (1) (a) Zhu, W.-R.; Su, Q.; Deng, X.-Y.; Ouyang, Z.-L.; Weng, J.; Lu, G. Organocatalytic asymmetric cascade bicyclization: access to chiral polycyclic bisindoles from 2-indolylmethanols and propargylic alcohols. *Org. Chem. Front.* **2024**, *11* (7), 2040-2046. (b) He, W.; Zheng, W.-F.; Qian, H. Rh-Catalyzed Carbonylative Cyclization of Propargylic Alcohols with Aryl Boronic Acids. *Org. Lett.* **2024**, *26* (29), 6279-6283. (c) Yan, W.; Wang, Q.; Chen, Y.; Petersen, J. L.; Shi, X. Iron-Catalyzed C–O Bond Activation for the Synthesis of Propargyl-1,2,3-triazoles and 1,1-Bis-triazoles. *Org. Lett.* **2010**, *12* (15), 3308-3311.

## **7. NMR spectra [ $^1\text{H}$ , $^{13}\text{C}$ { $^1\text{H}$ }, and $^{19}\text{F}$ ] of synthesized products**



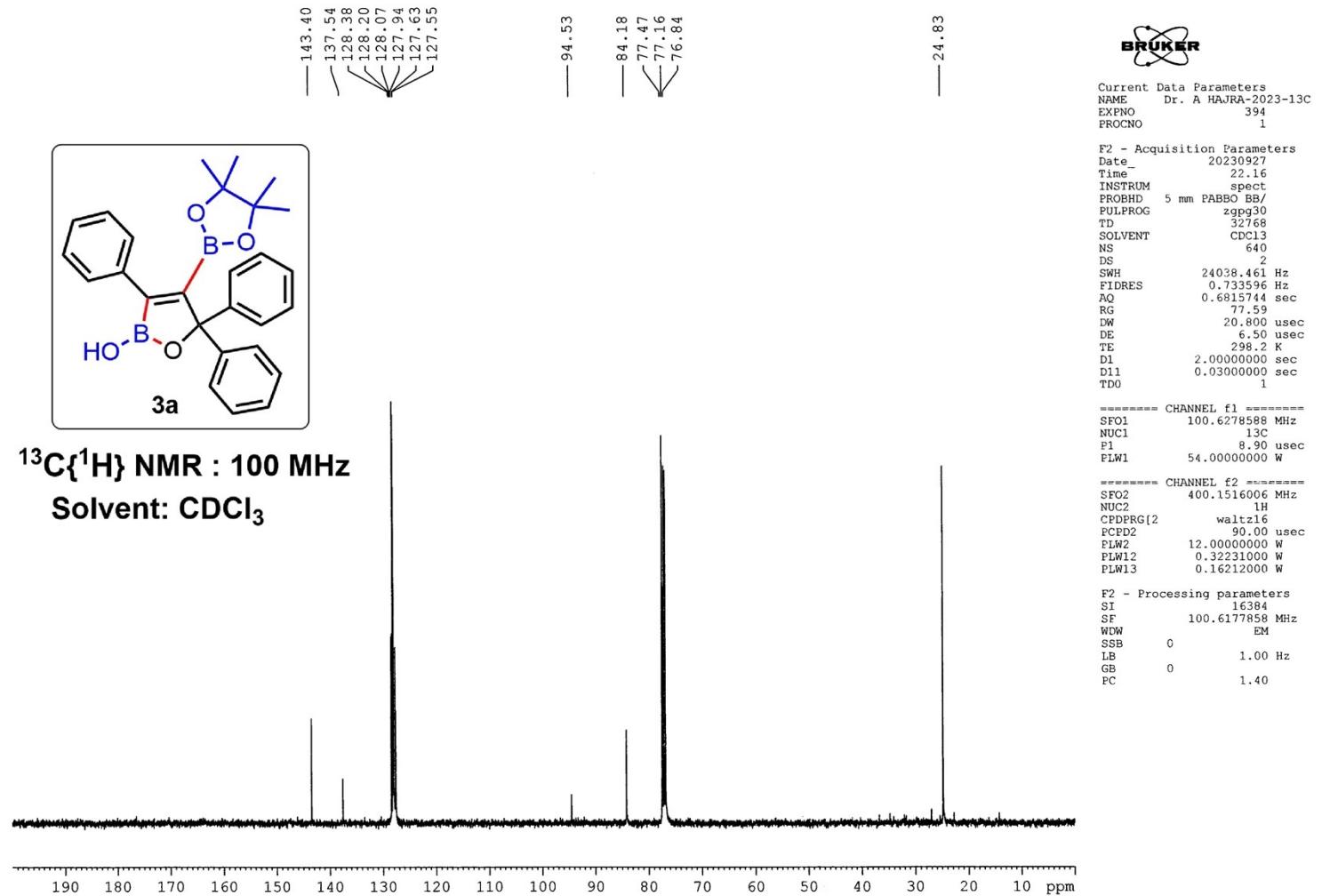
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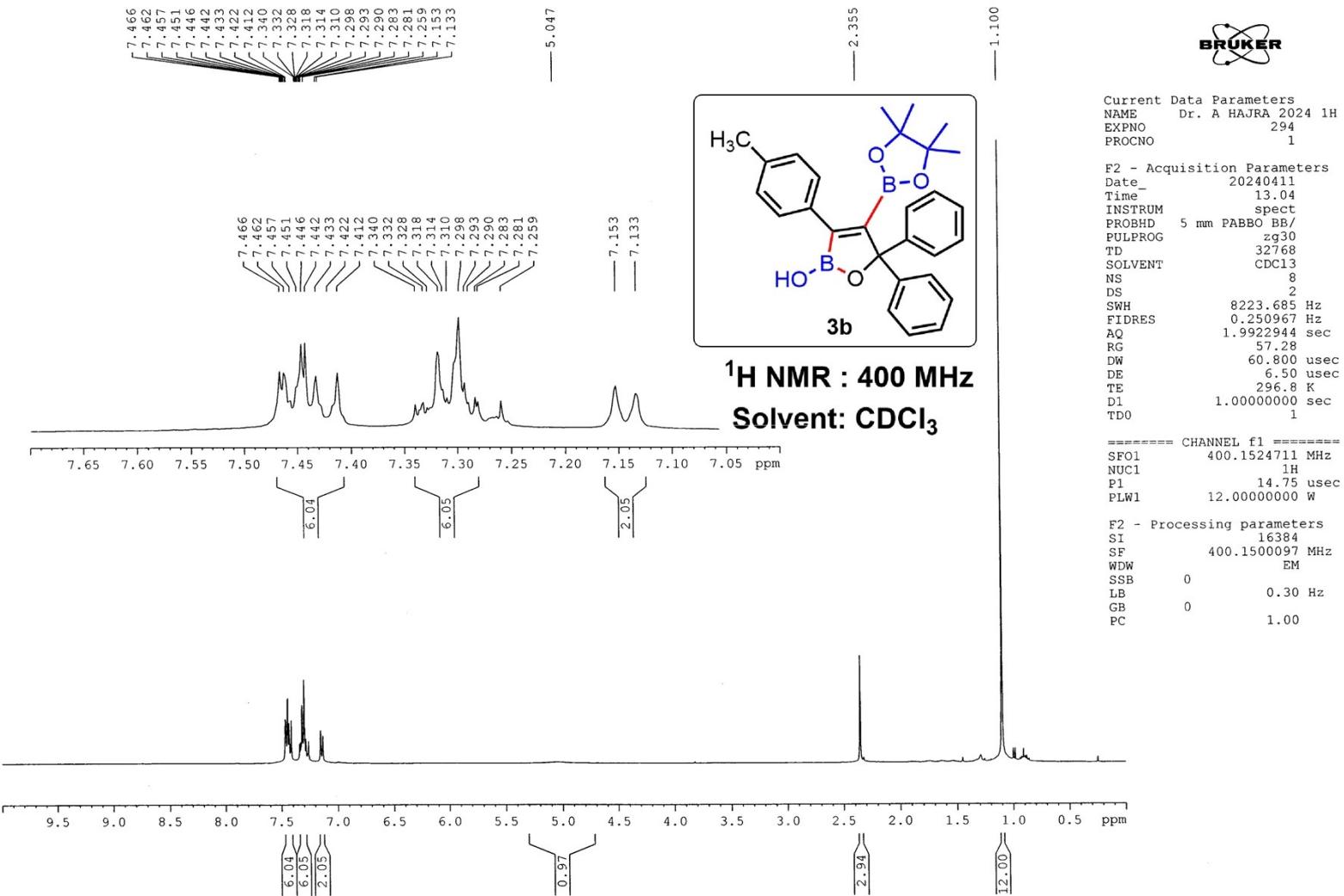
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EXPNO 1142  
PROCNO 1

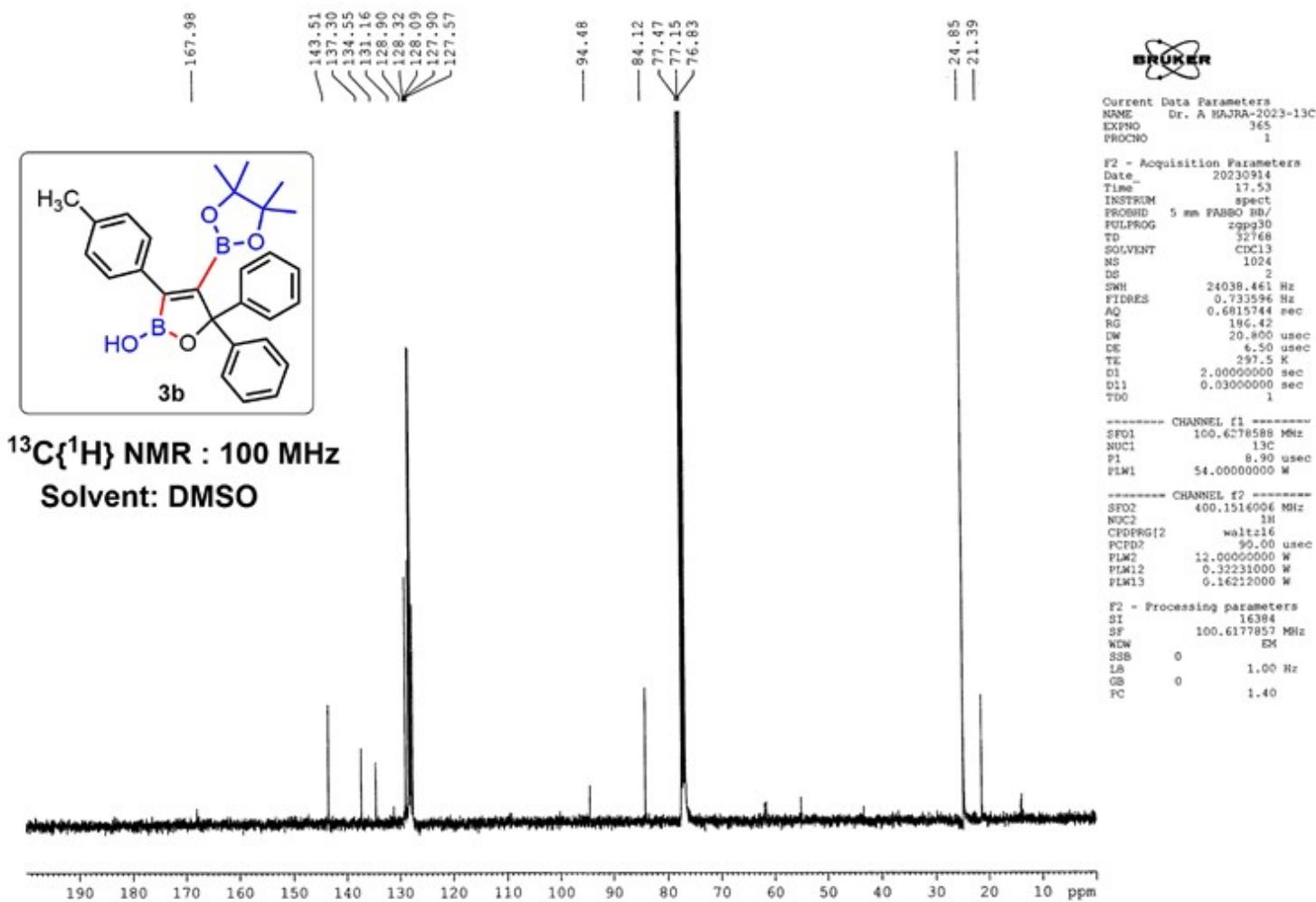
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NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
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RG 67.81  
DW 60.800 usec  
DE 6.50 usec  
TE 297.8 K  
D1 1.0000000 sec  
TDO 1

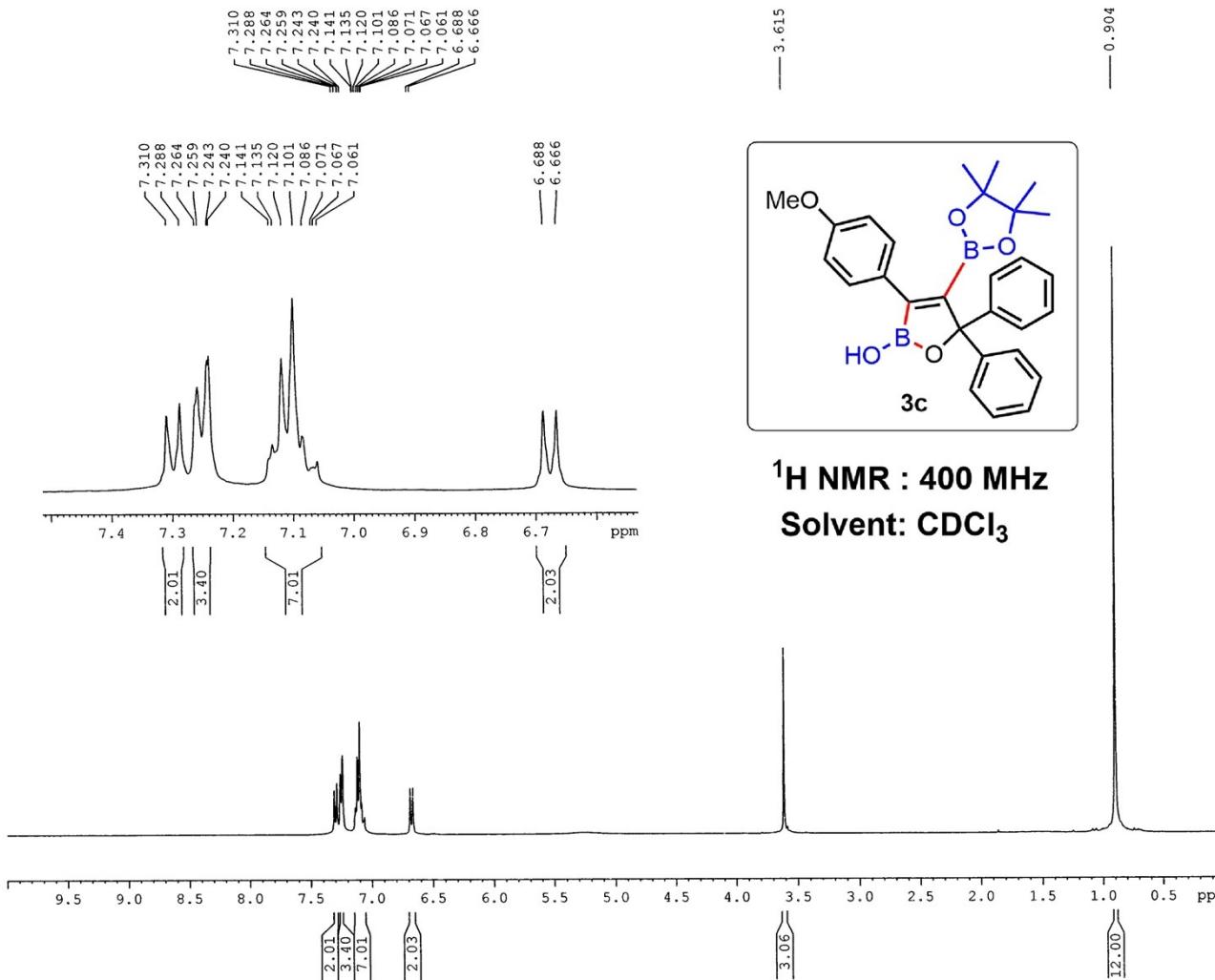
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**BRUKER**

Current Data Parameters  
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EXPNO 1146  
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TD             32768
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NS              8
DS              2
SWH             8223.685 Hz
FIDRES        0.250967 Hz
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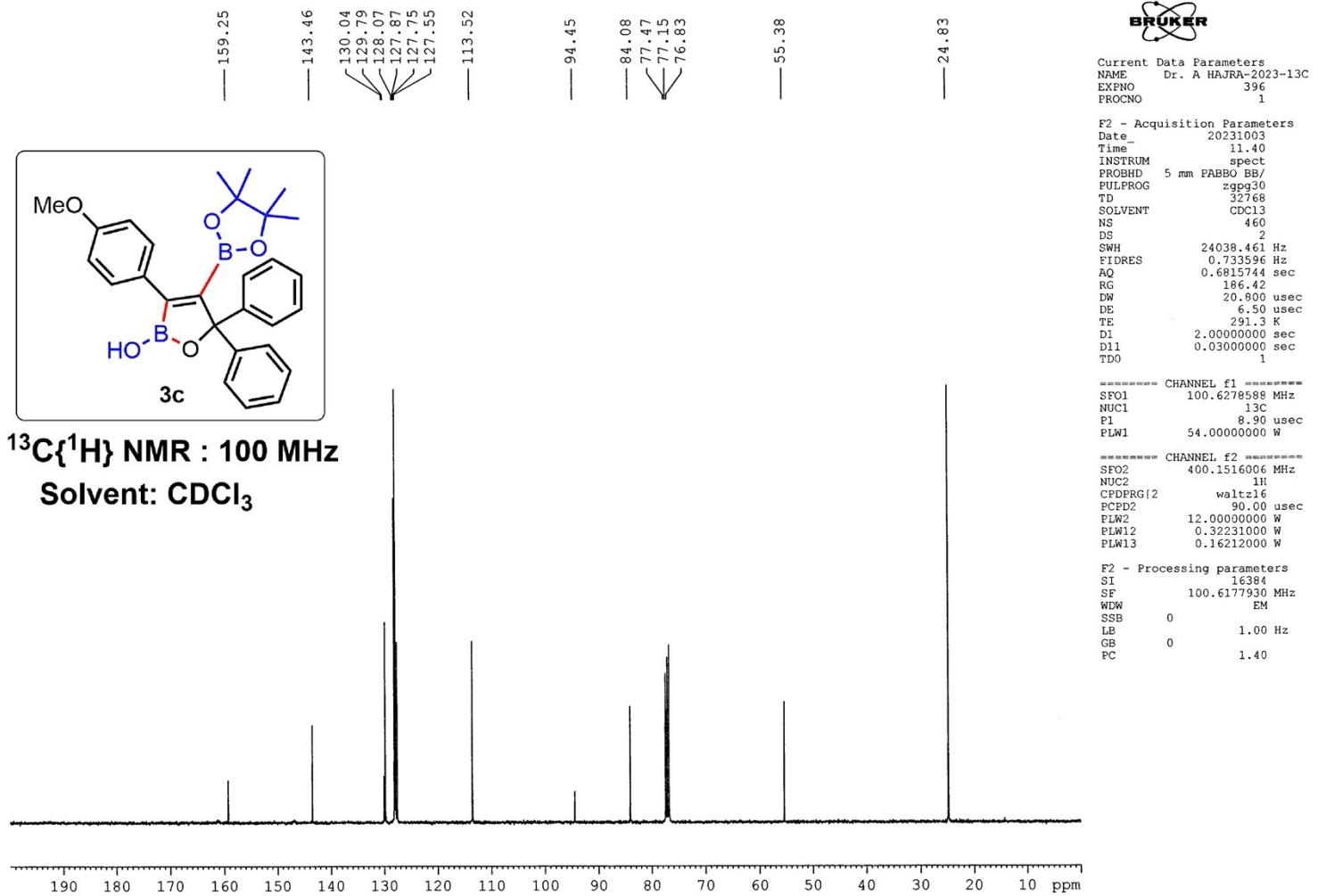
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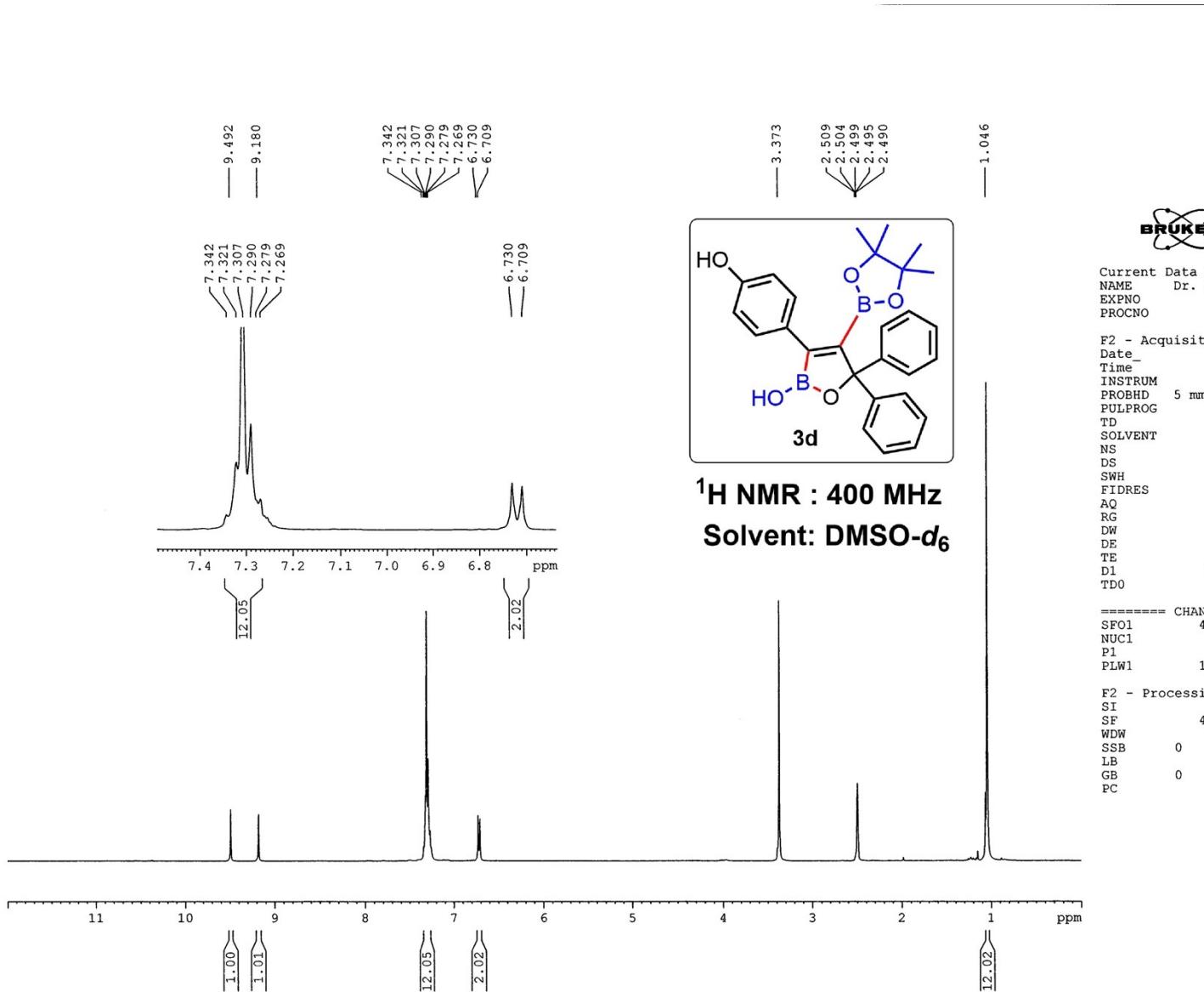
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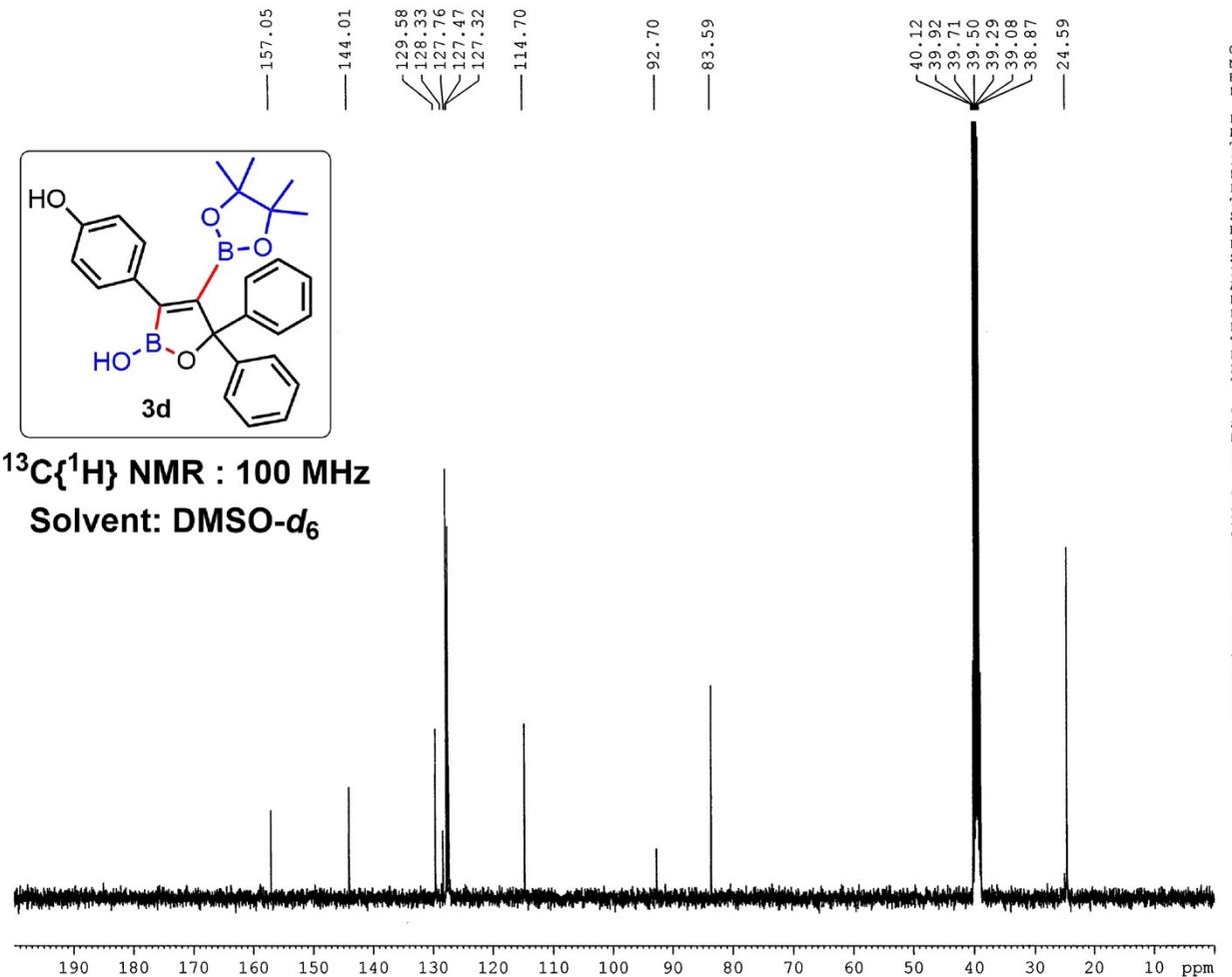
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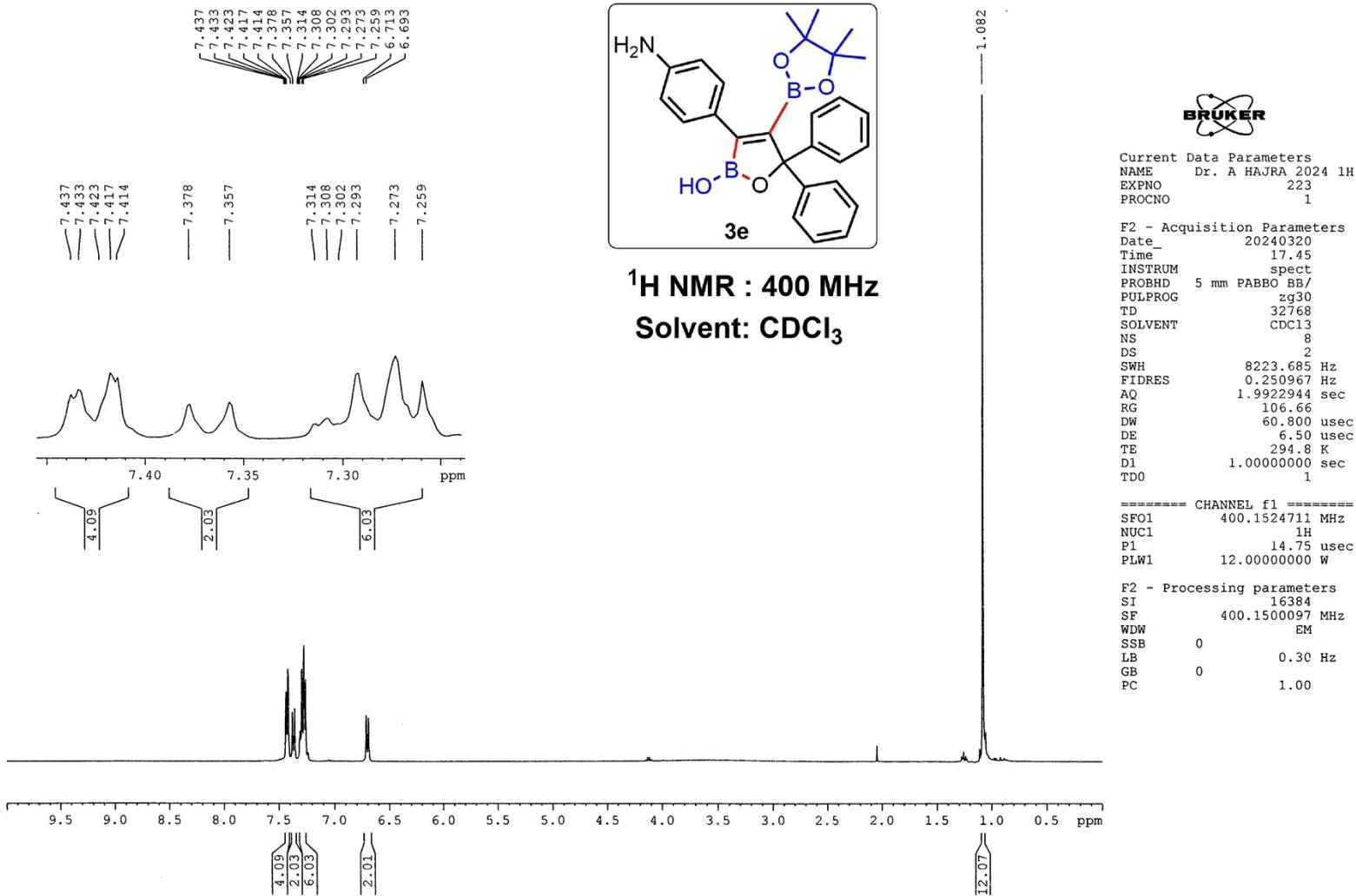
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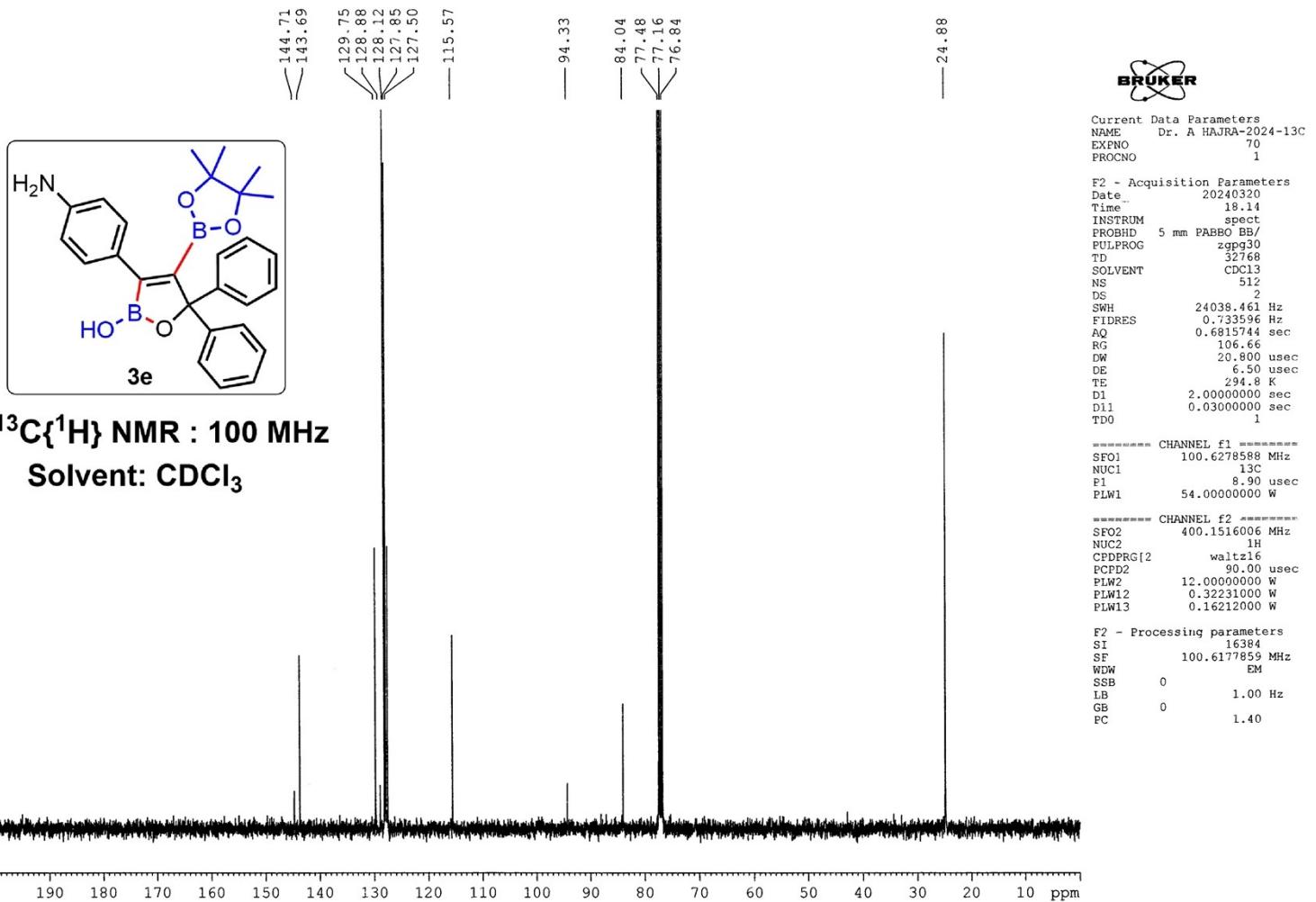
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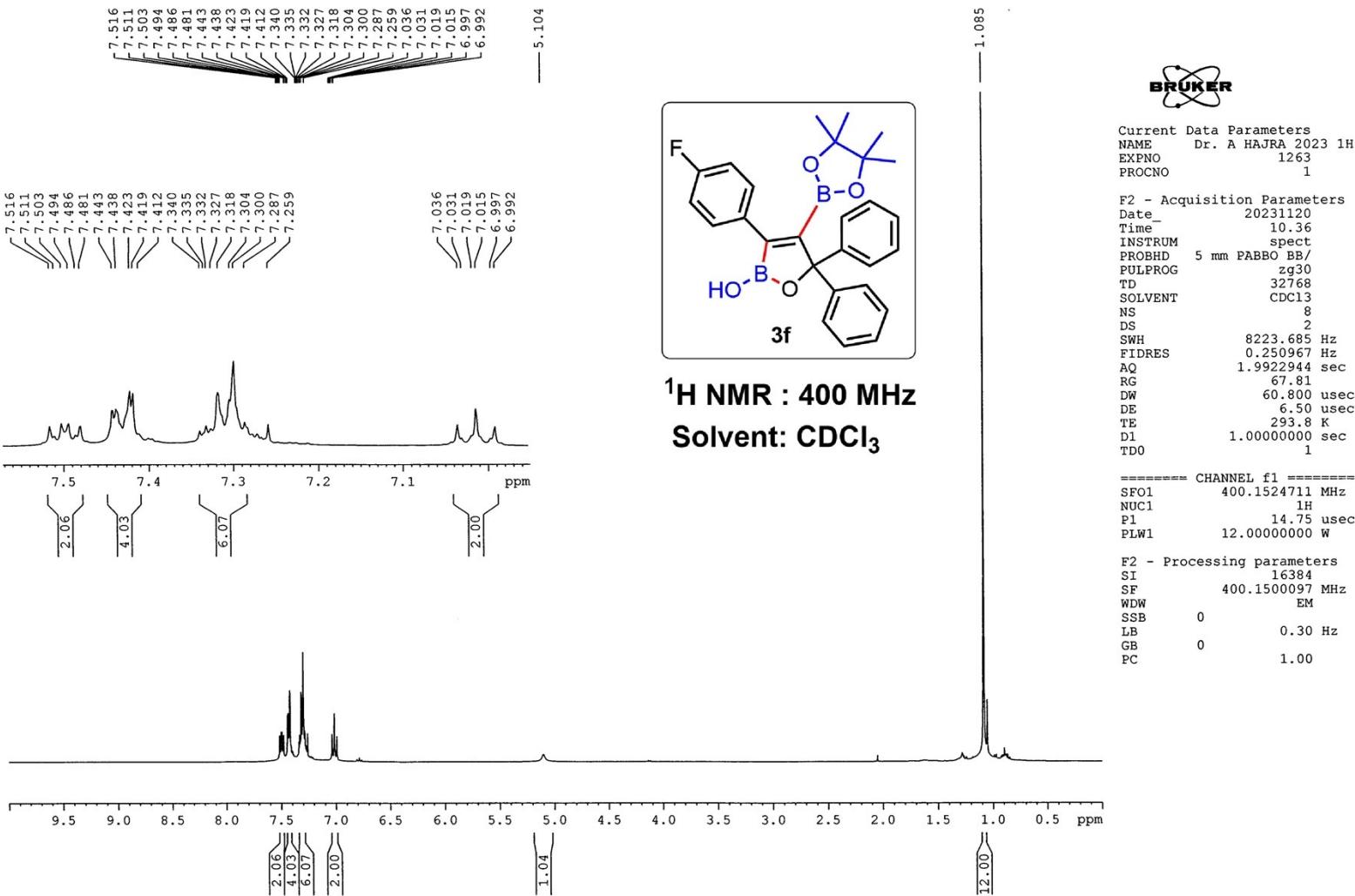


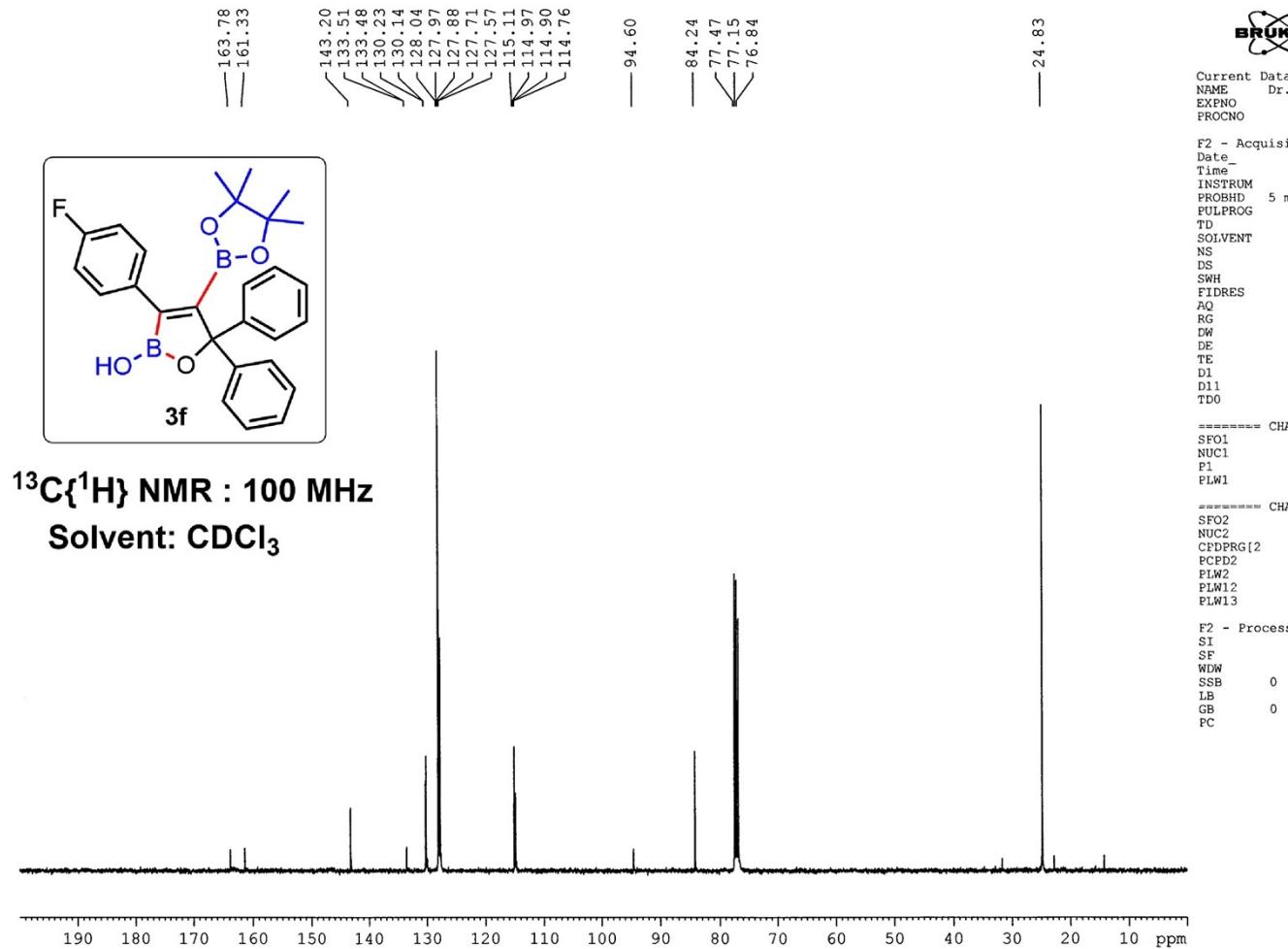


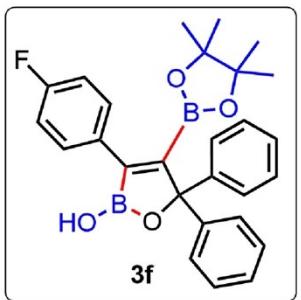






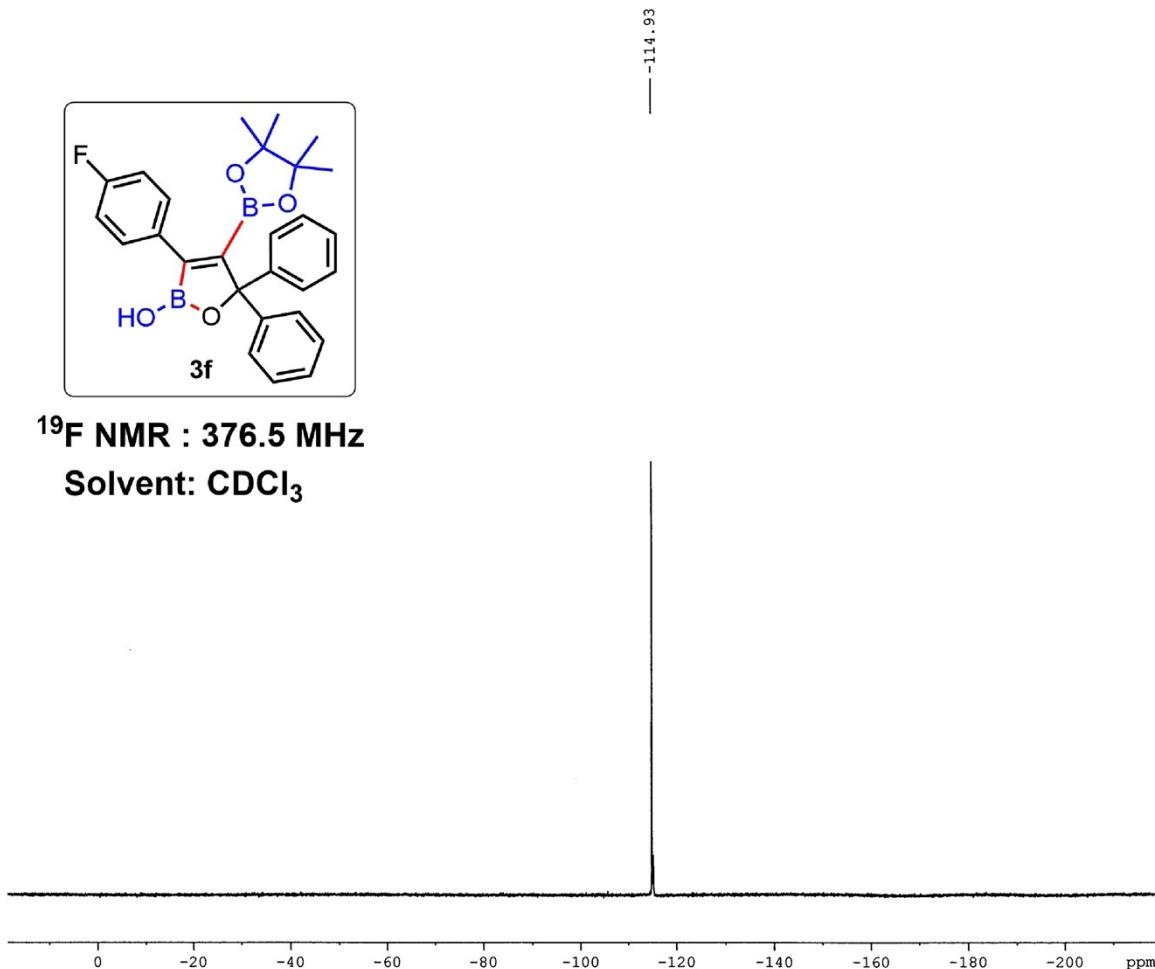






**<sup>19</sup>F NMR : 376.5 MHz**

**Solvent: CDCl<sub>3</sub>**



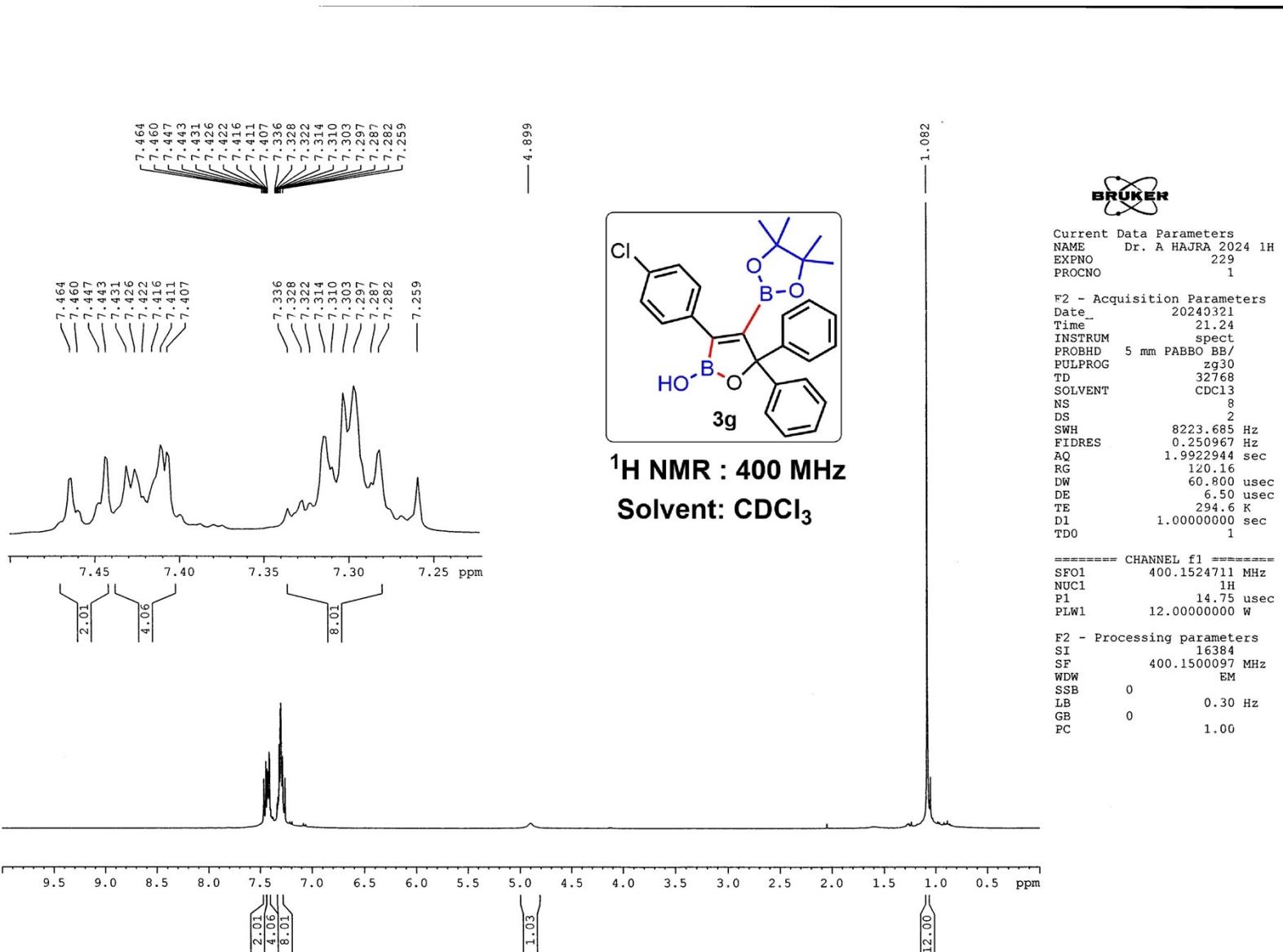
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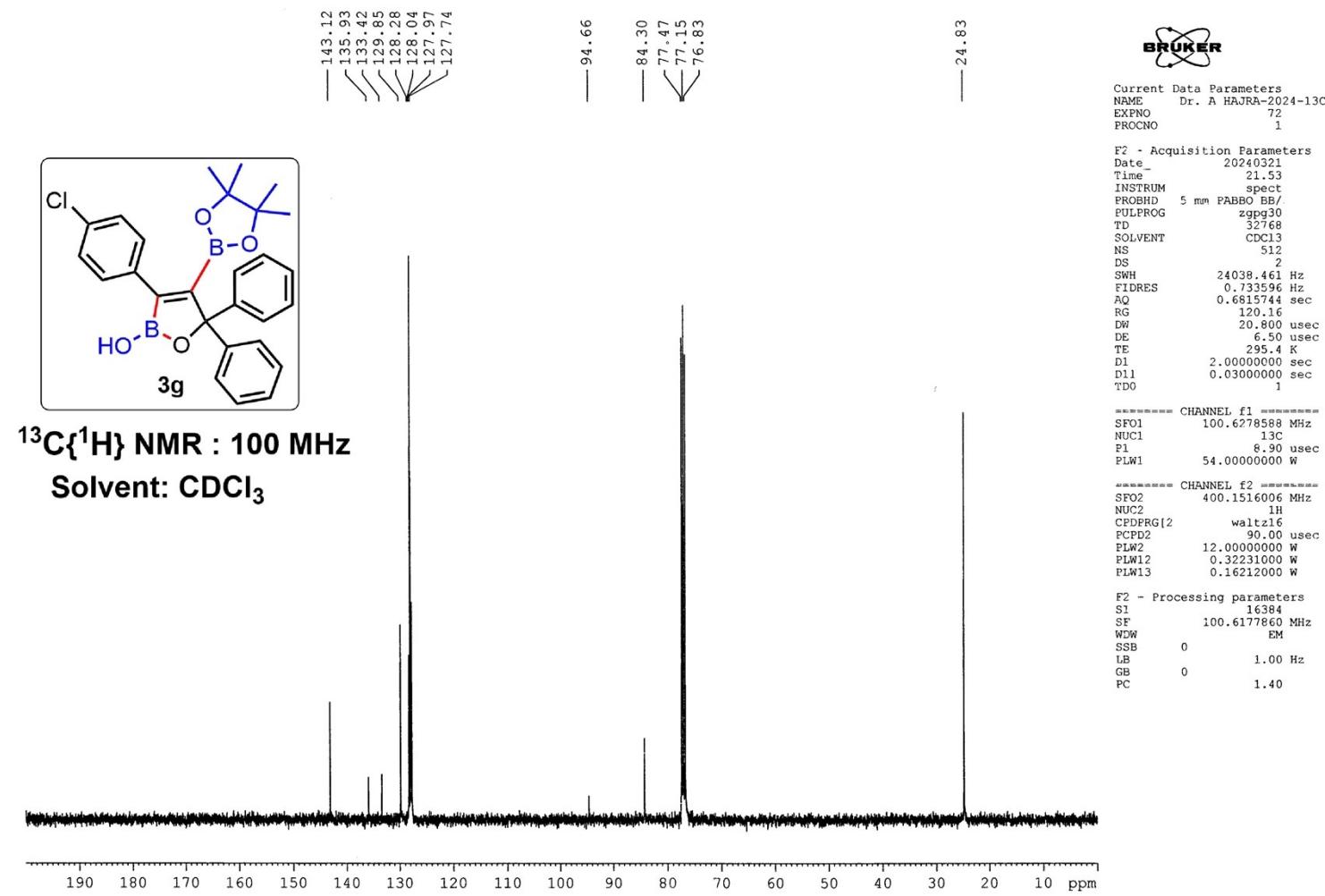
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TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 89285.711 Hz  
FIDRES 2.724784 Hz  
AQ 0.1835008 sec  
RG 67.81  
DW 5.600 usec  
DE 6.50 usec  
TE 293.5 K  
D1 1.0000000 sec  
TDO 1

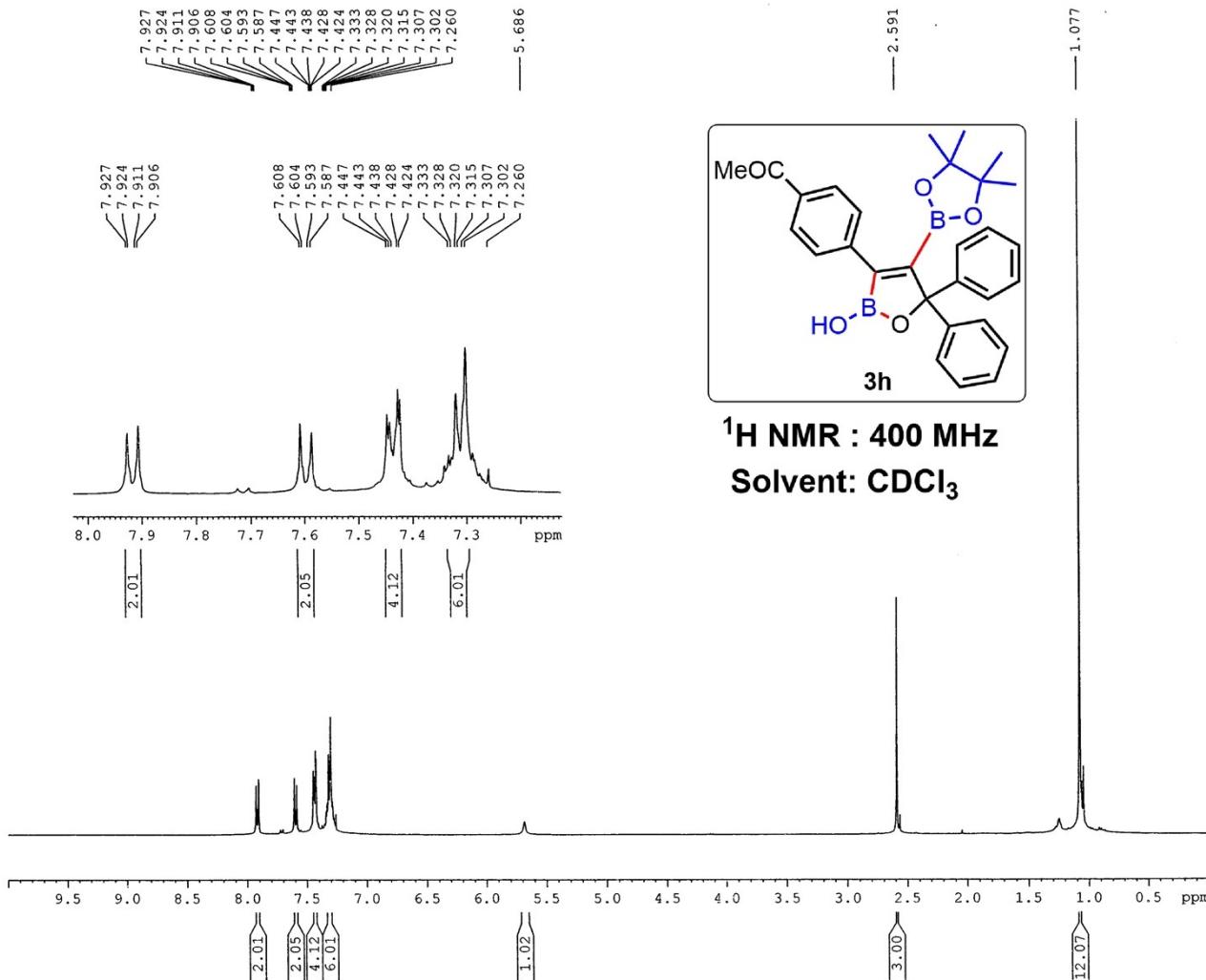
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GB 0  
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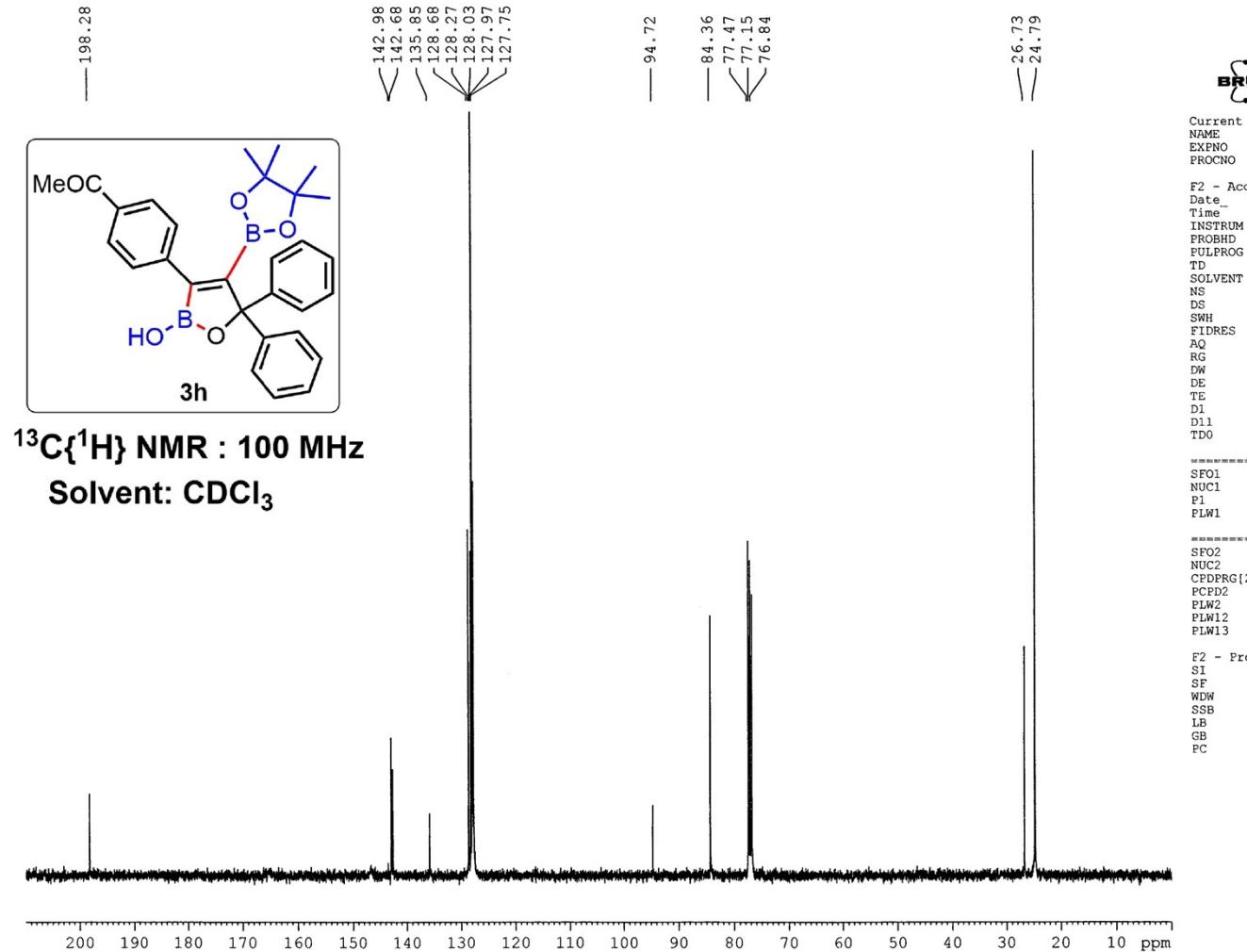
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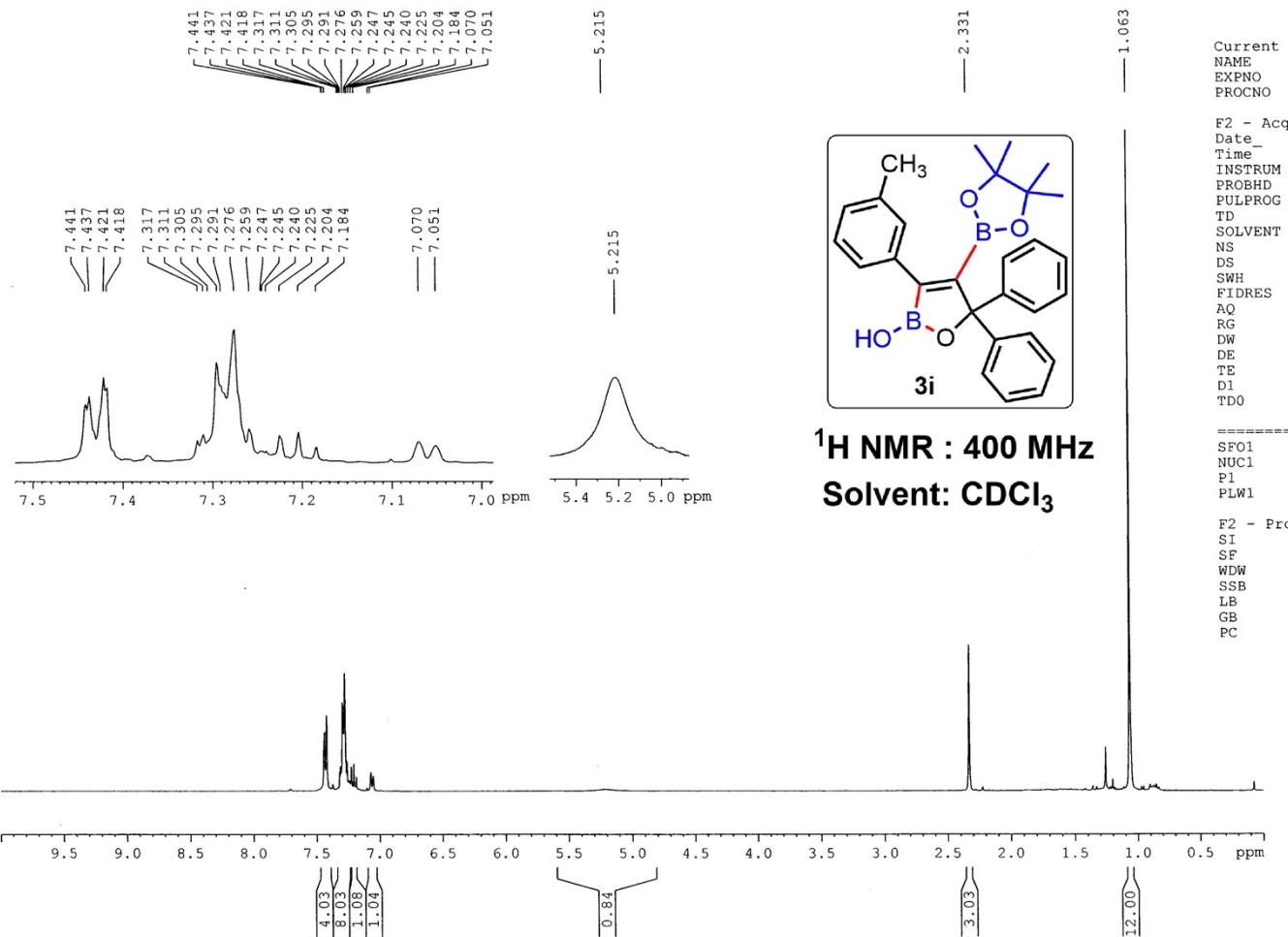
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EXPNO 139  
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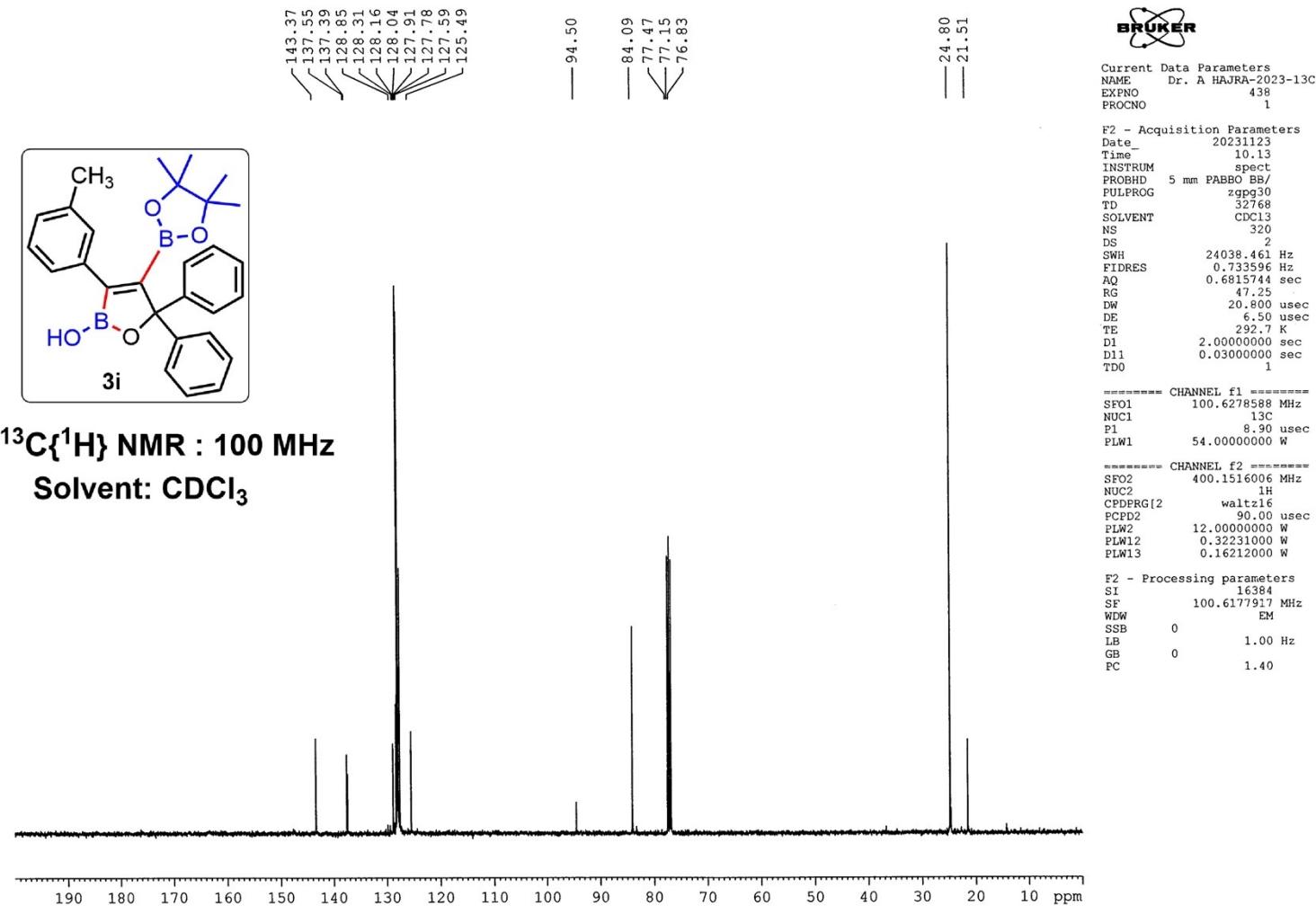
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NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 47.25  
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DE 6.50 usec  
TE 296.3 K  
D1 1.0000000 sec  
TDO 1

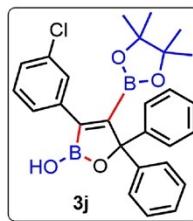
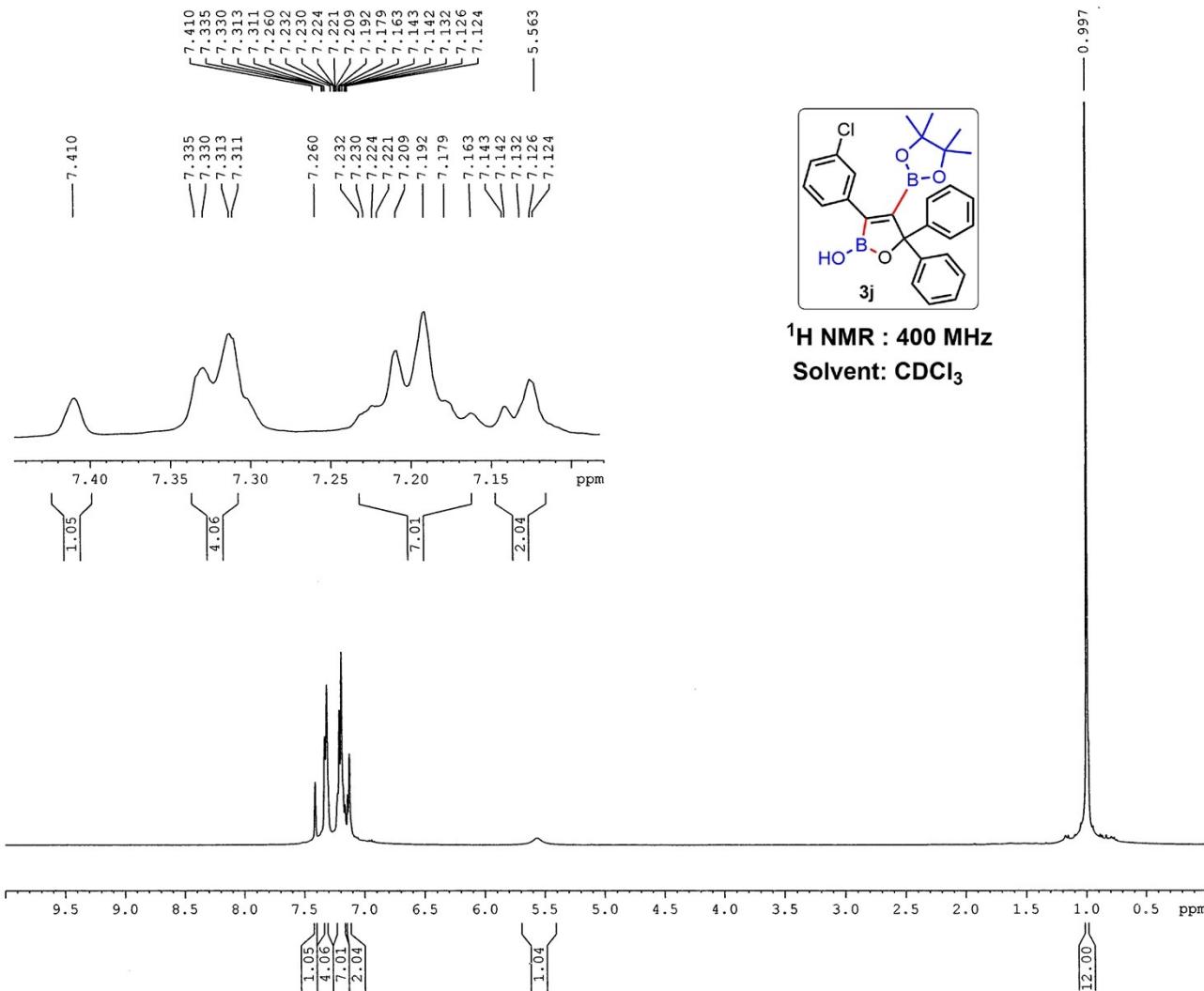
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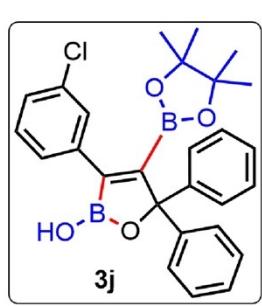




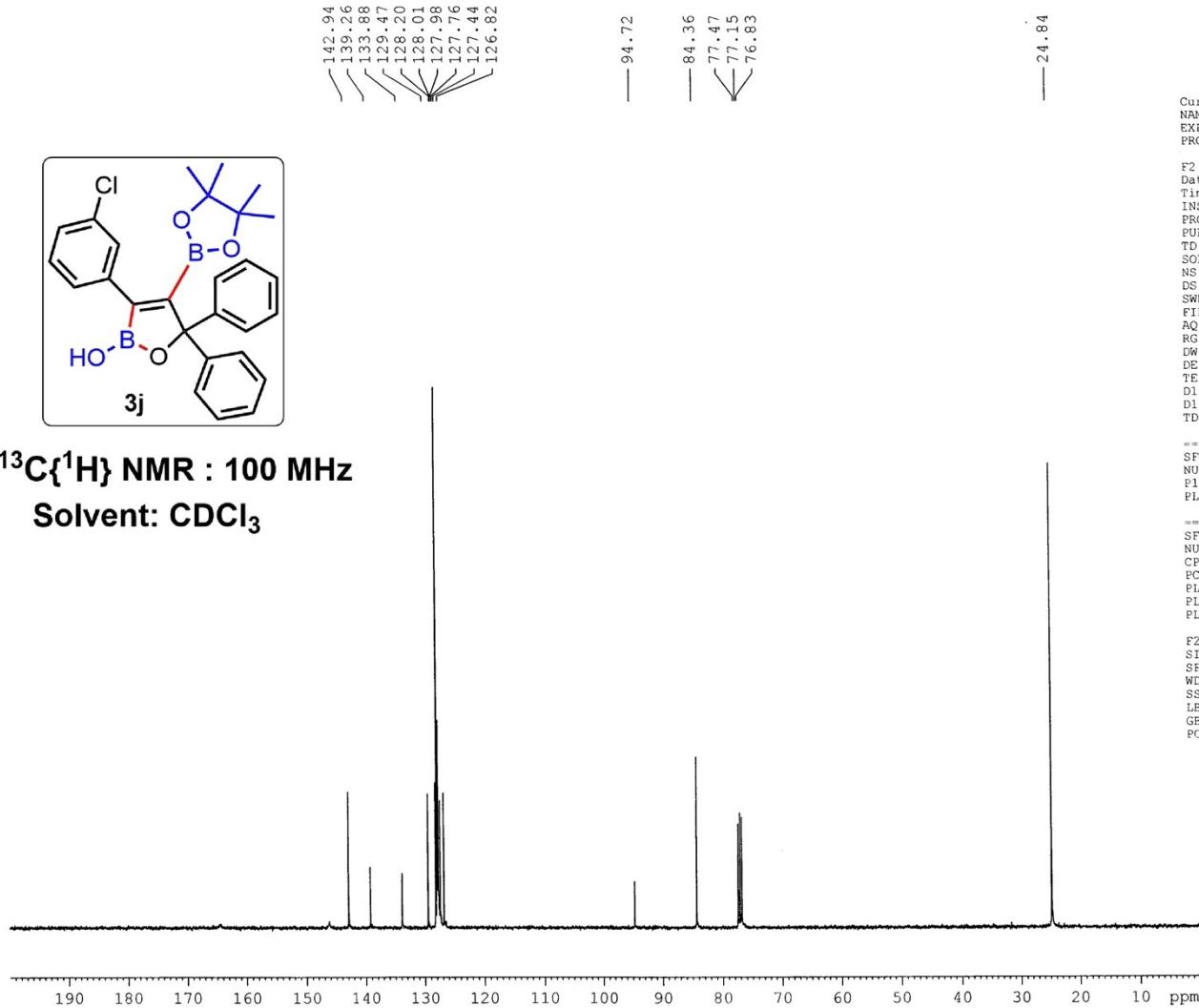




**<sup>1</sup>H NMR : 400 MHz**  
**Solvent: CDCl<sub>3</sub>**



**$^{13}\text{C}\{\text{H}\}$  NMR : 100 MHz**  
**Solvent:  $\text{CDCl}_3$**



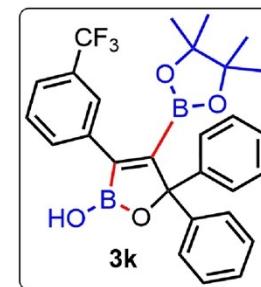
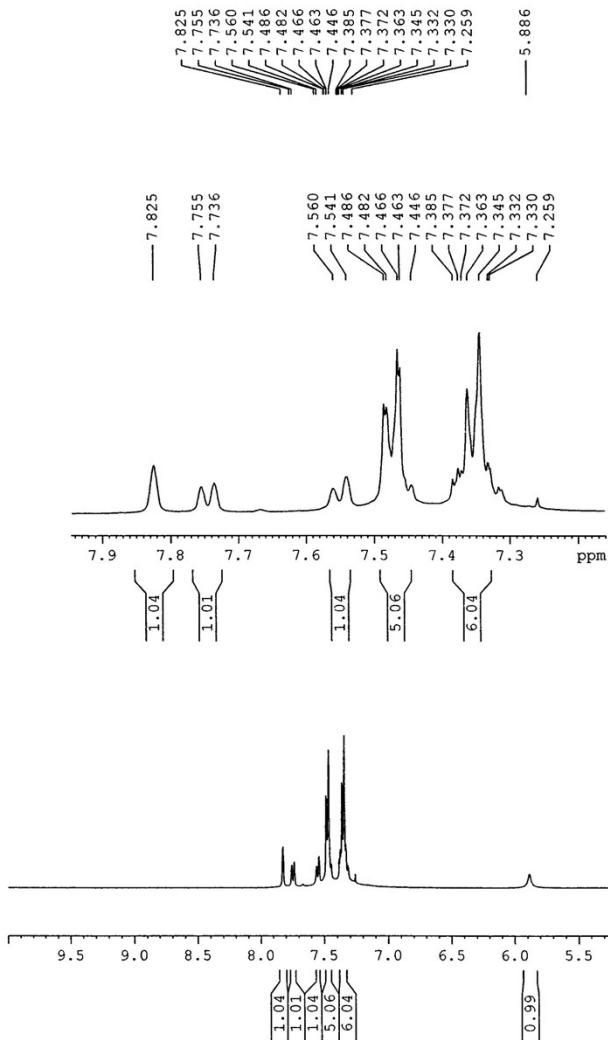
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 TD 32768  
 SOLVENT CDCl3  
 NS 256  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
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 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
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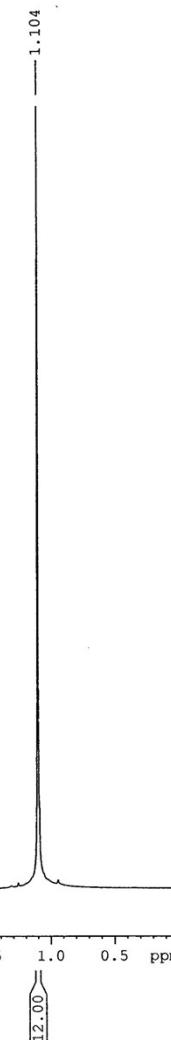
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 NUC2 1H  
 CPDPRG12 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

F2 - Processing parameters  
 SI 16384  
 SF 100.6177946 MHz  
 WDW EM  
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 LB 1.00 Hz  
 GB 0  
 PC 1.40



**<sup>1</sup>H NMR : 400 MHz**  
**Solvent: CDCl<sub>3</sub>**

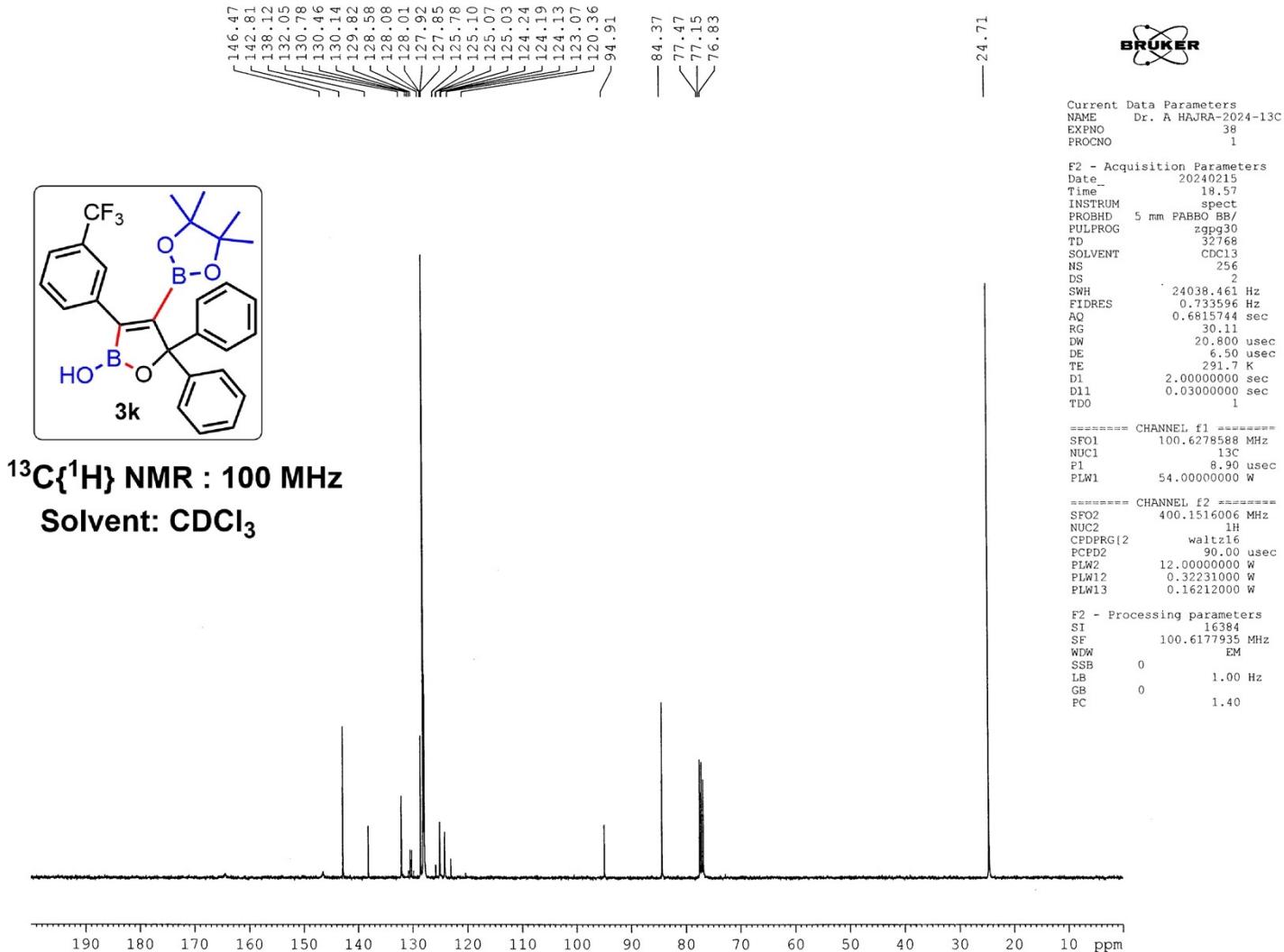


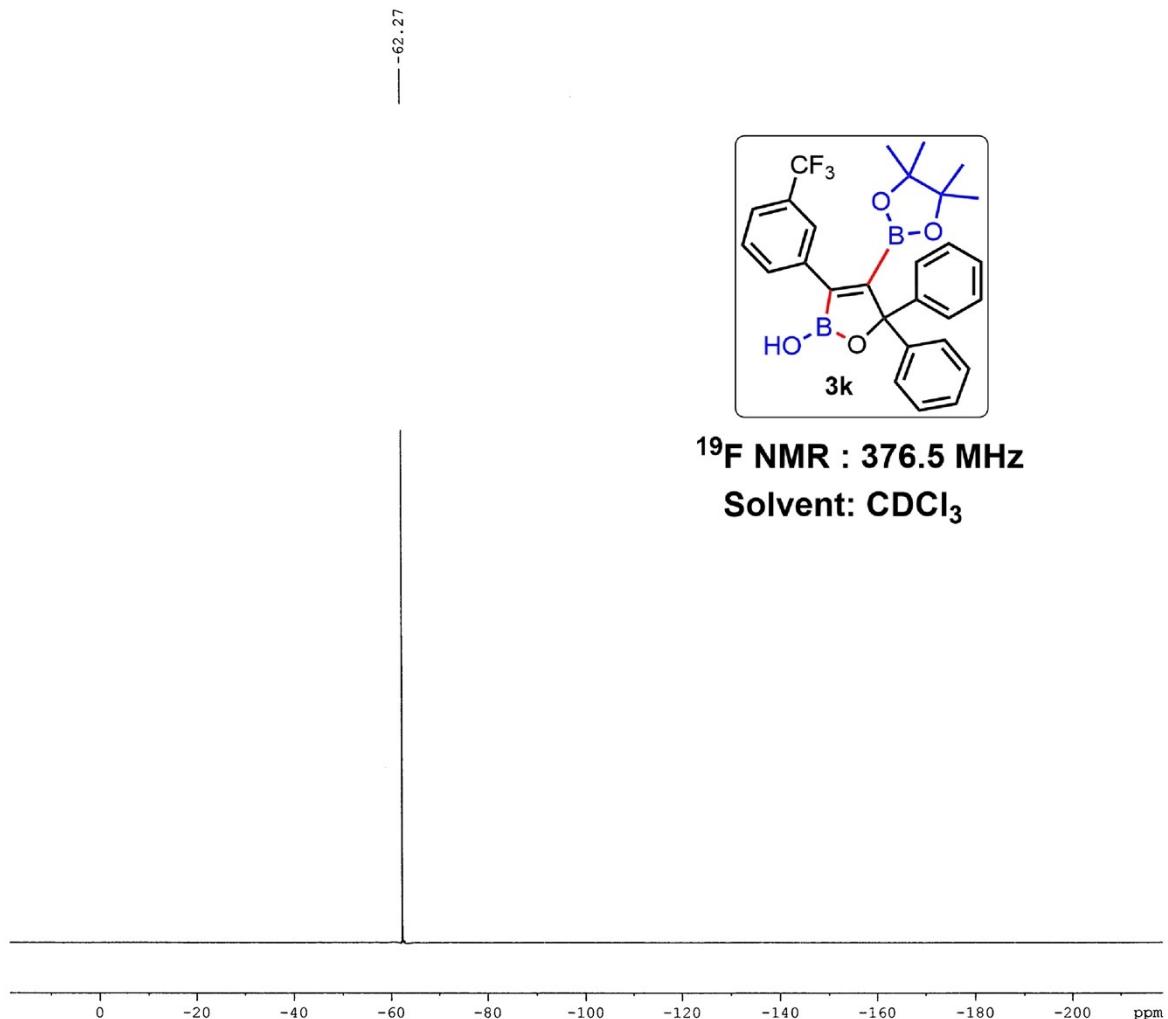
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 PULPROG zg30  
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 NS 8  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9922944 sec  
 RG 30.11  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 290.9 K  
 D1 1.0000000 sec  
 TDO 1

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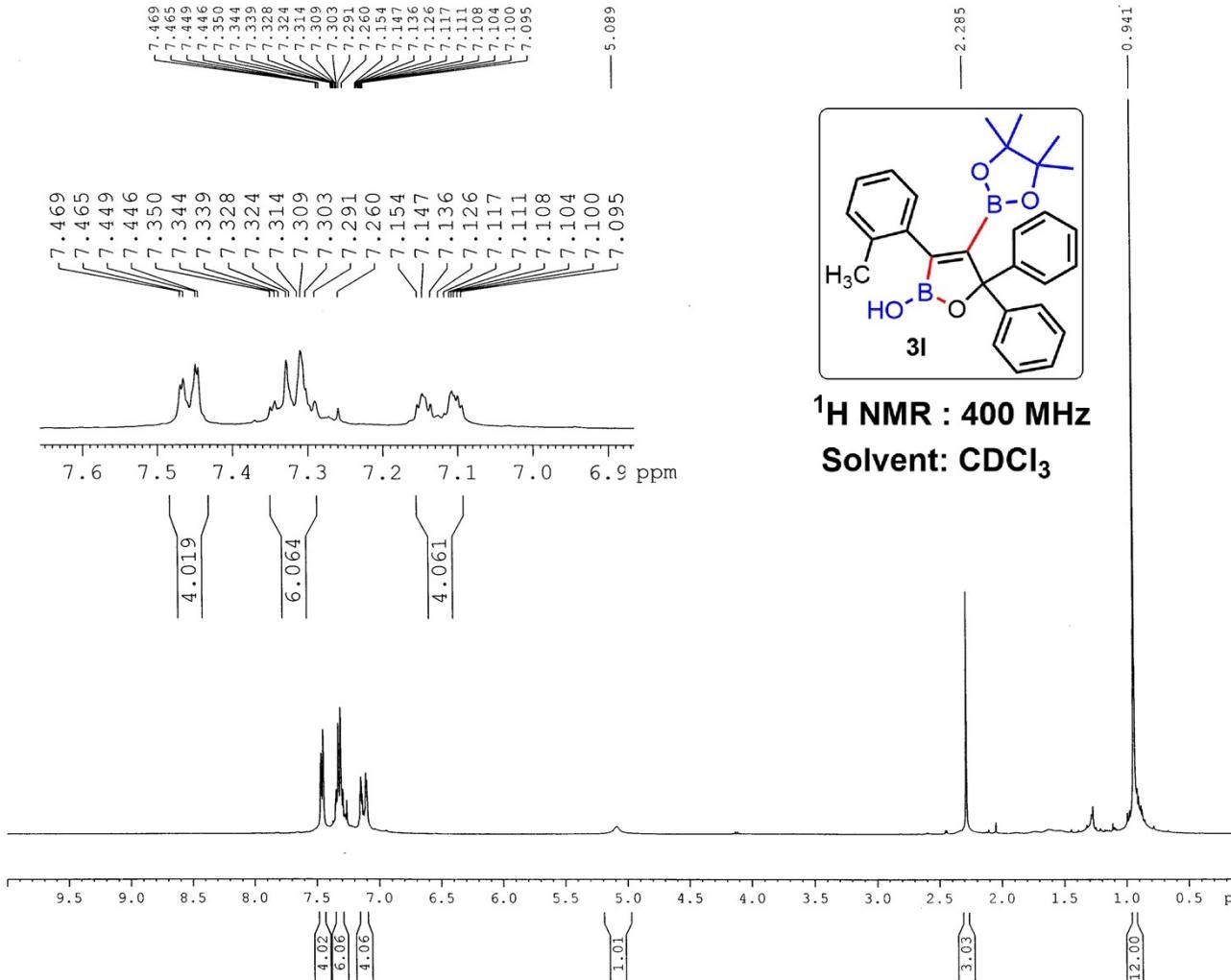


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 SOLVENT  $\text{CDCl}_3$   
 NS 8  
 DS 2  
 SWH 89285.711 Hz  
 FIDRES 2.724784 Hz  
 AQ 0.1835008 sec  
 RG 30.11  
 DW 5.600 usec  
 DE 6.50 usec  
 TE 291.0 K  
 D1 1.0000000 sec  
 TDO 1

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 NUC1 <sup>19</sup>F  
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 PLW1 20.0000000 W

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Current Data Parameters  
NAME Dr. A HAJRA 2023 1H  
EXPNO 1268  
PROCNO 1

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PULPROG_      zg30
TD_            32768
SOLVENT_       CDC13
NS_            8
DS_            2
SWH_           8223.685 Hz
FIDRES_        0.250967 Hz
AQ_            1.9992944 sec
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TDO_           1

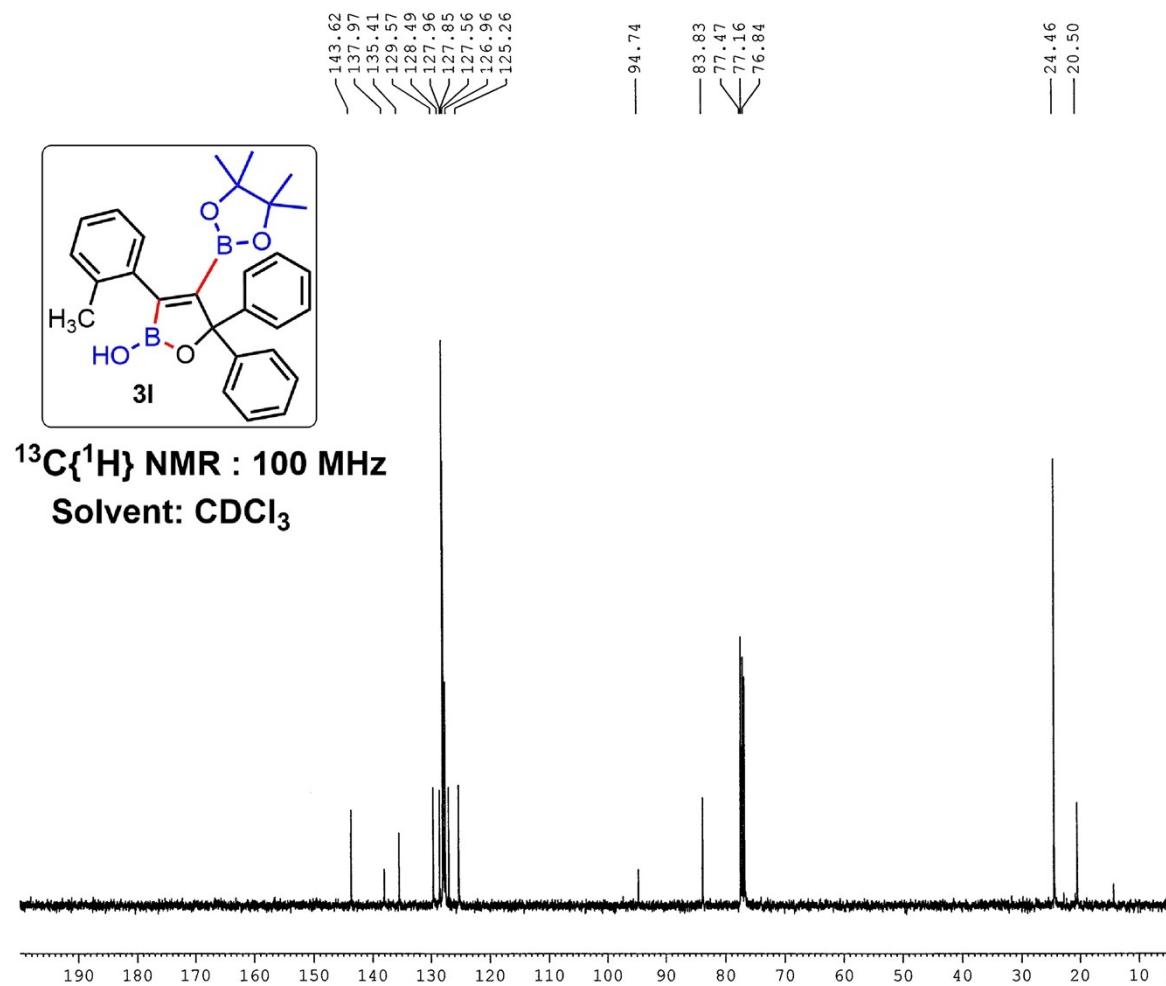
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F2 - Processing parameters
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**BRUKER**

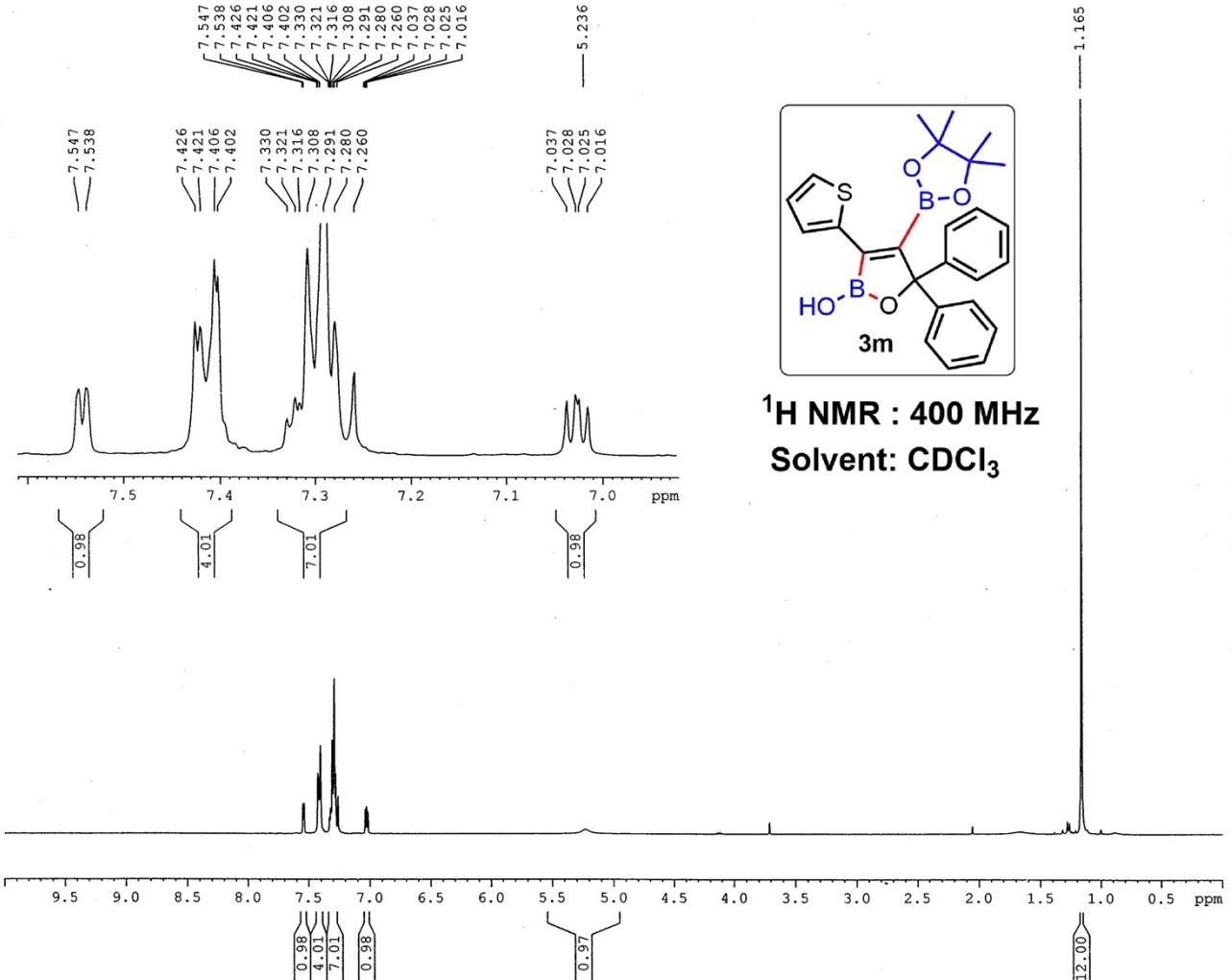
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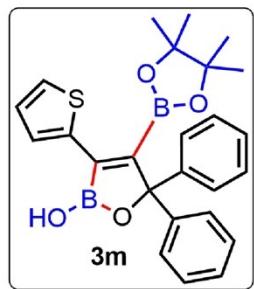
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SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 47.25  
DW 20.800 usec  
DE 6.50 usec  
TE 232.5 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
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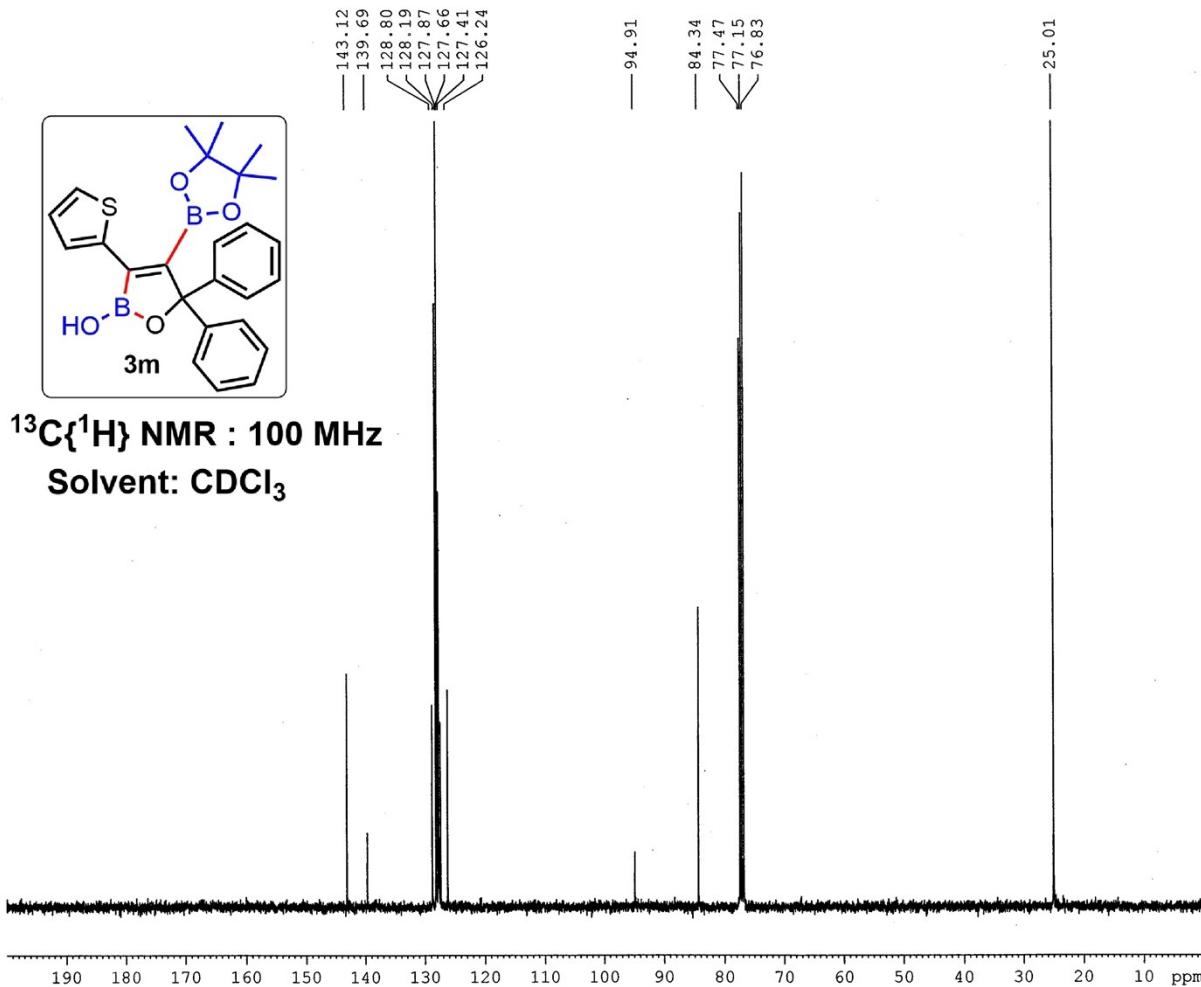
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PLW12 0.32231000 W  
PLW13 0.16212000 W

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WDW EM  
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$^{13}\text{C}\{\text{H}\}$  NMR : 100 MHz  
Solvent:  $\text{CDCl}_3$



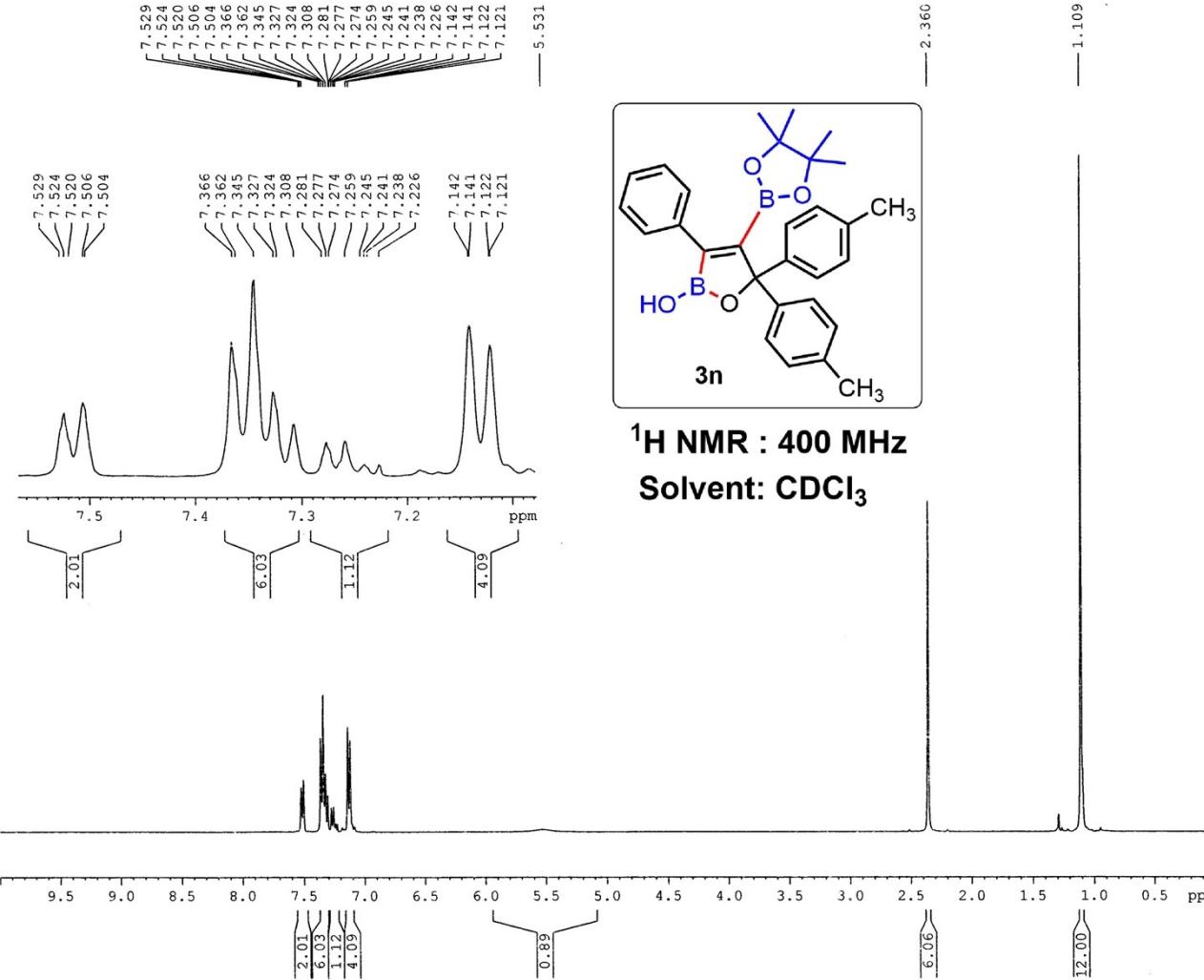
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TD 32768  
SOLVENT CDCl3  
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DS 2  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 0.6815744 sec  
RG 87.66  
DW 20.800 usec  
DE 6.50 usec  
TE 288.9 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 100.6278588 MHz  
NUC1 13C  
P1 8.90 usec  
PLW1 54.0000000 W

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NUC2 1H  
CPDPG[2] waltz16  
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PLW2 12.00000000 W  
PLW12 0.32231000 W  
PLW13 0.16212000 W

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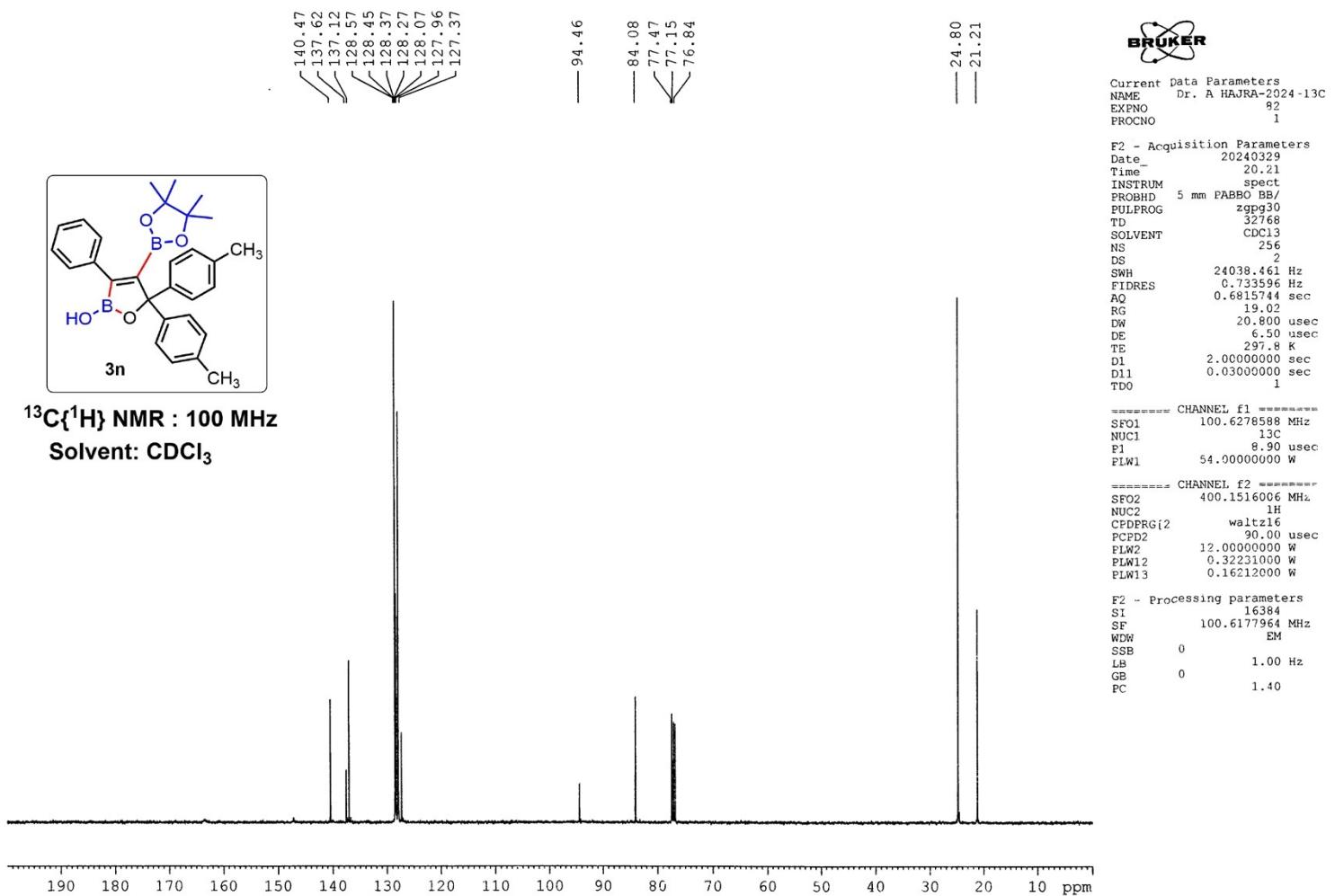
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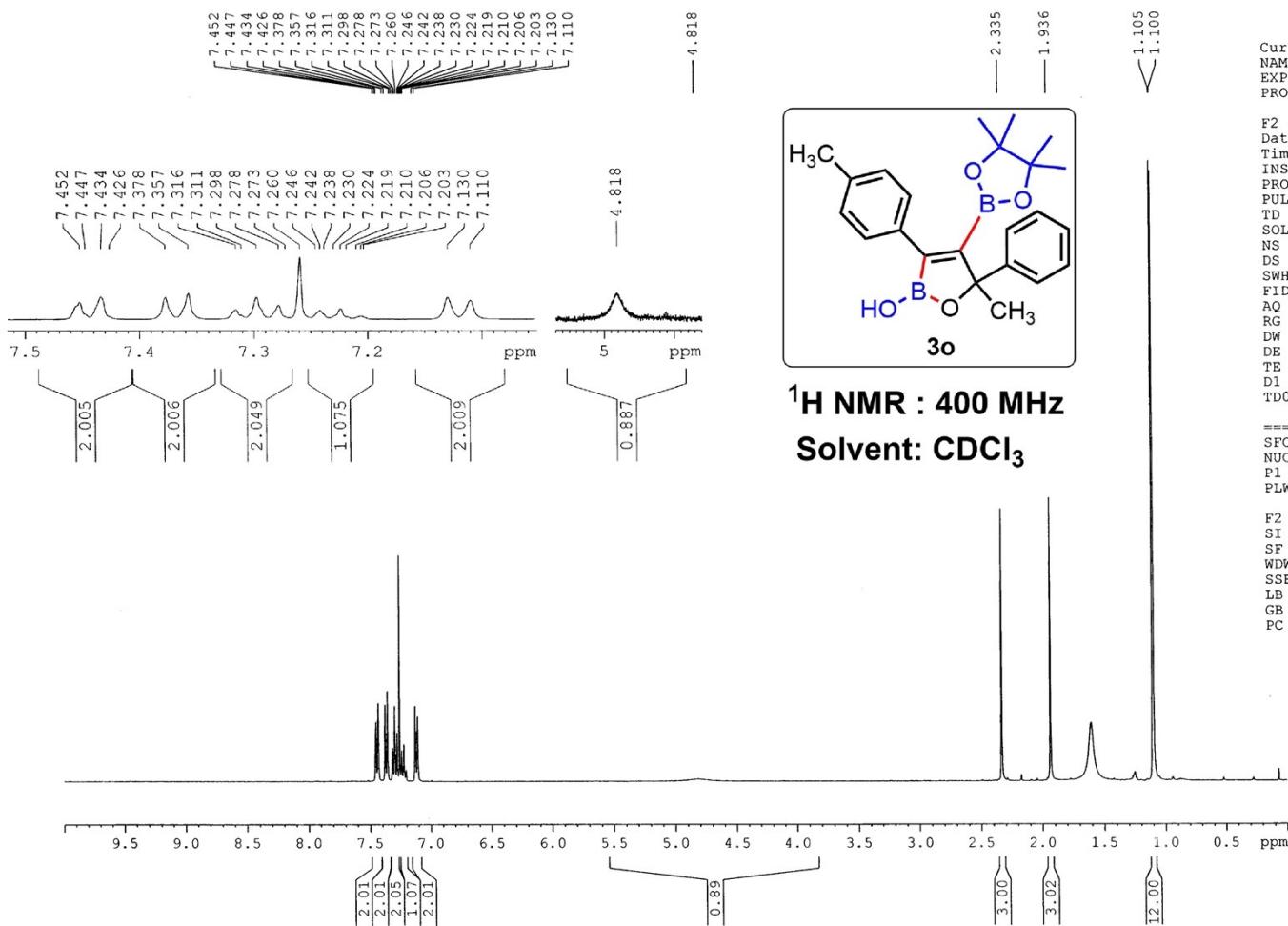
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 PULPROG zg30  
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 DS 2  
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 FIDRES 0.250967 Hz  
 AQ 1.9922944 sec  
 RG 19.02  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.5 K  
 D1 1.0000000 sec  
 TDO 1

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 NUC1 1H  
 P1 14.75 usec  
 PLW1 12.00000000 W

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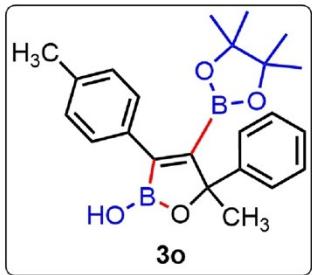
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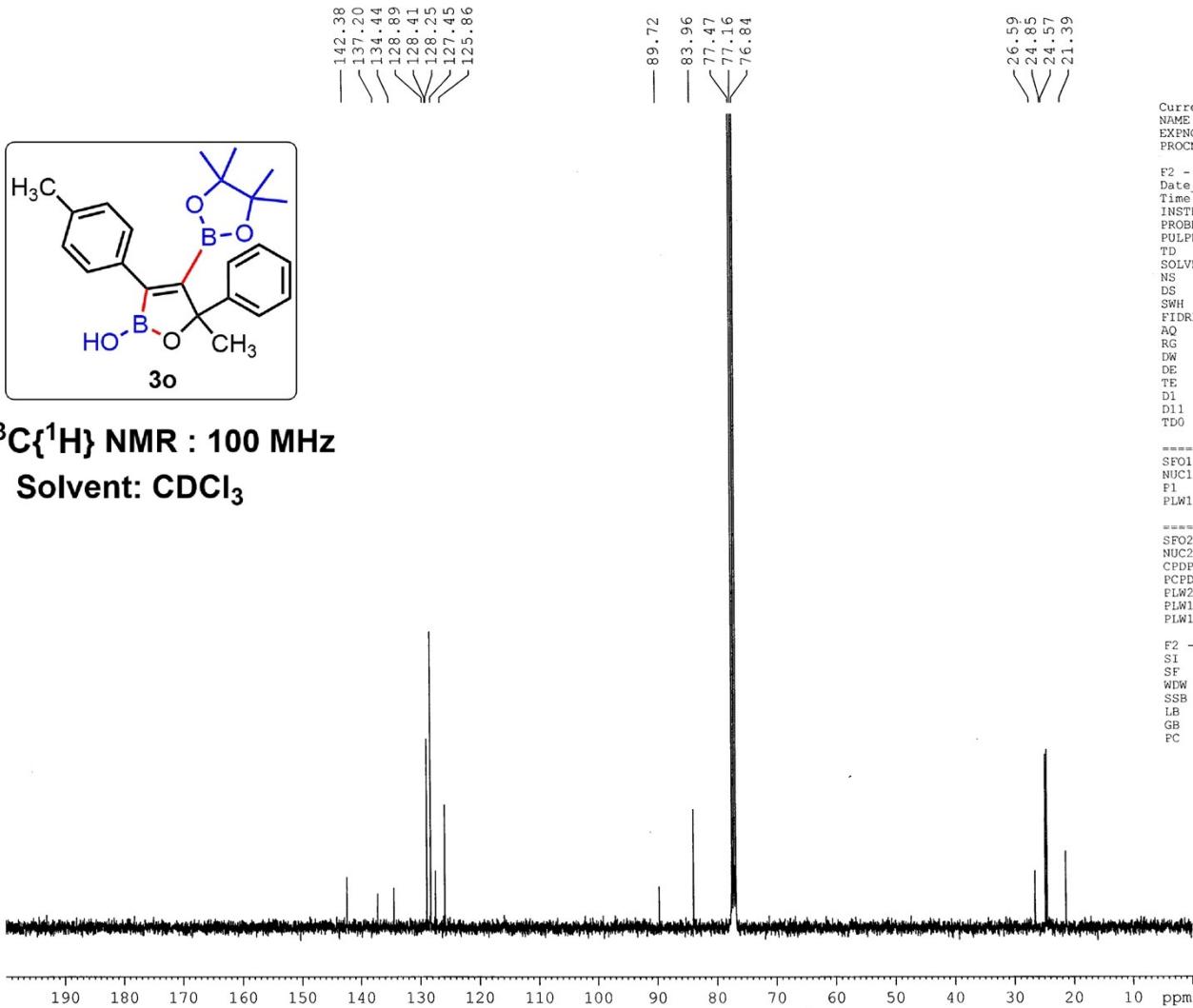
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 PULPROG zg30  
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 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9922944 sec  
 RG 148.91  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 293.4 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
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 NUC1 1H  
 P1 14.75 usec  
 PLW1 12.0000000 W

F2 - Processing parameters  
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 SF 400.1500097 MHz  
 WDW EM  
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 PC 1.00



**$^{13}\text{C}\{\text{H}\}$  NMR : 100 MHz**  
**Solvent:  $\text{CDCl}_3$**



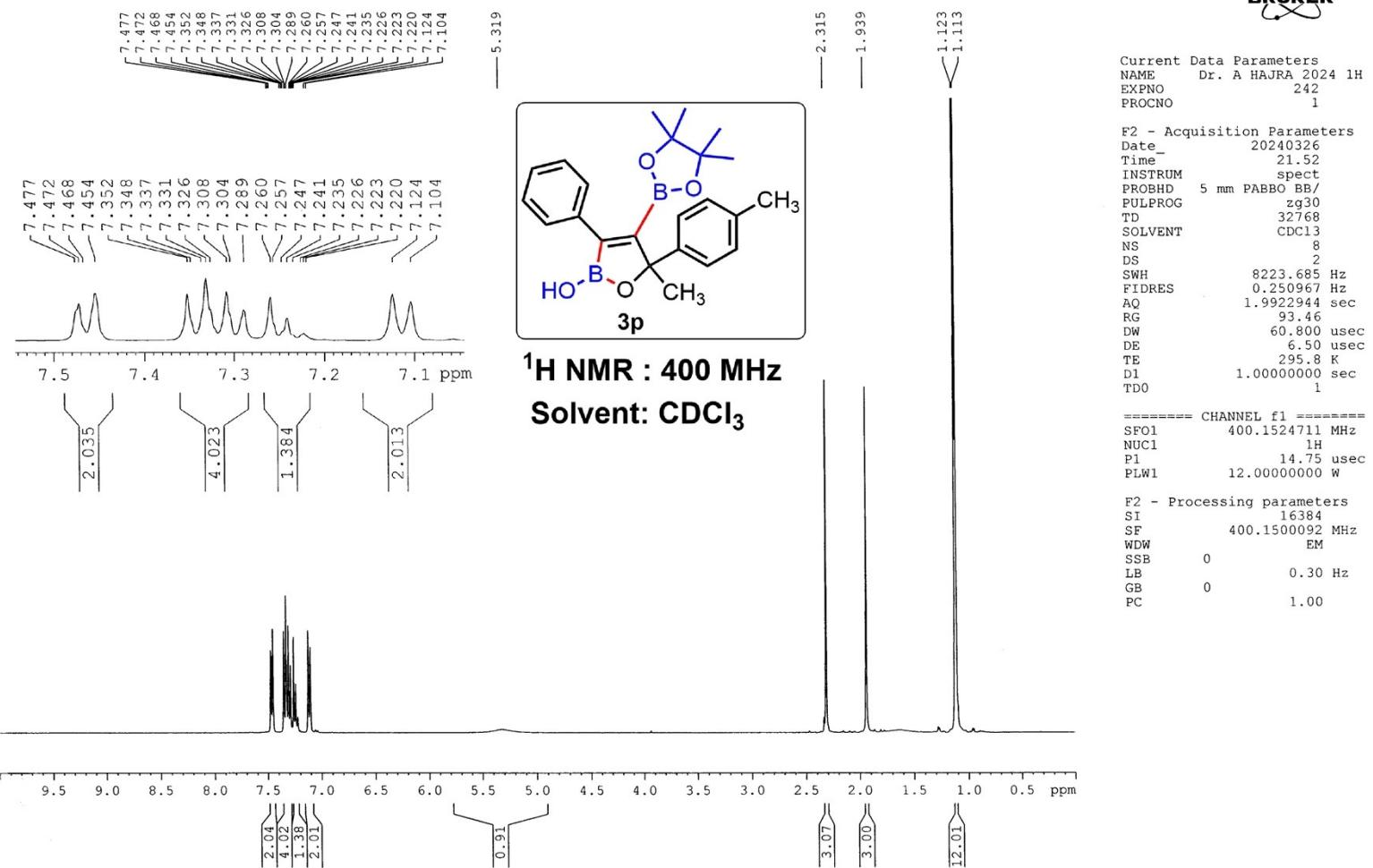
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 EXPNO 398  
 PROCNO 1

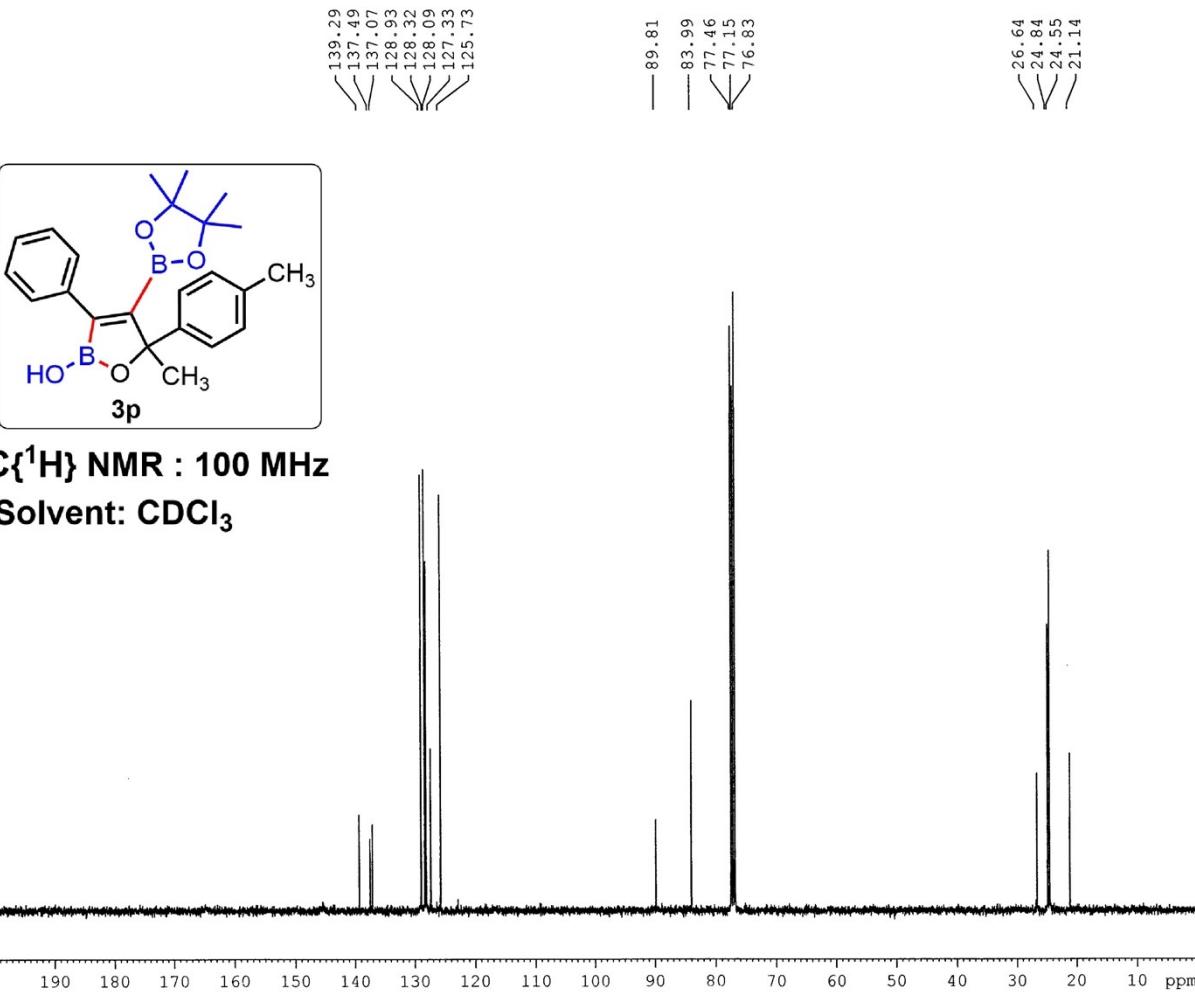
F2 - Acquisition Parameters  
 Date 20231004  
 Time 23.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB  
 PULPROG zgppg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 1024  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 0.6815744 sec  
 RG 186.42  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1 sec

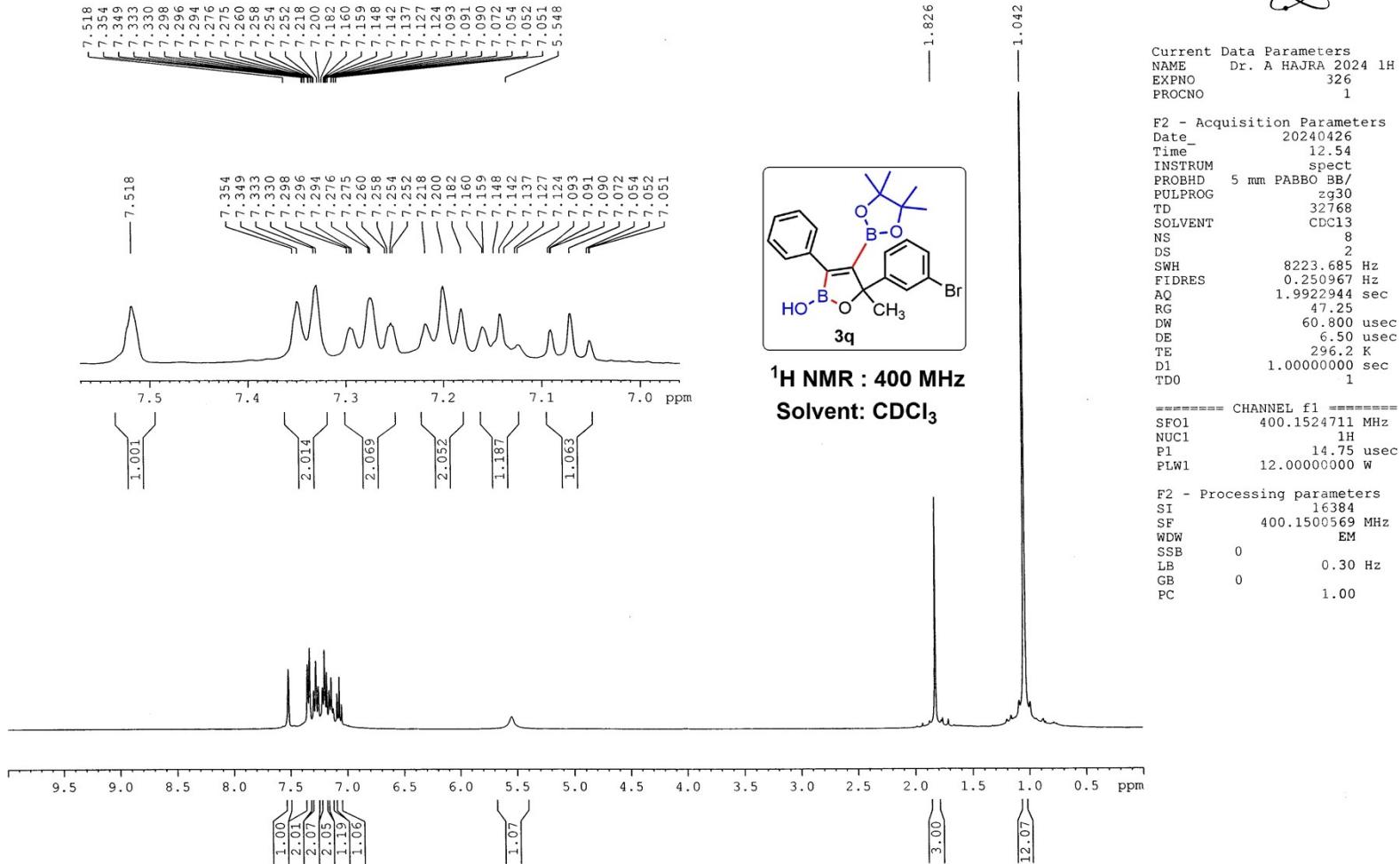
===== CHANNEL f1 =====  
 SF01 100.6278588 MHz  
 NUC1 13C  
 F1 8.90 usec  
 PLW1 54.00000000 W

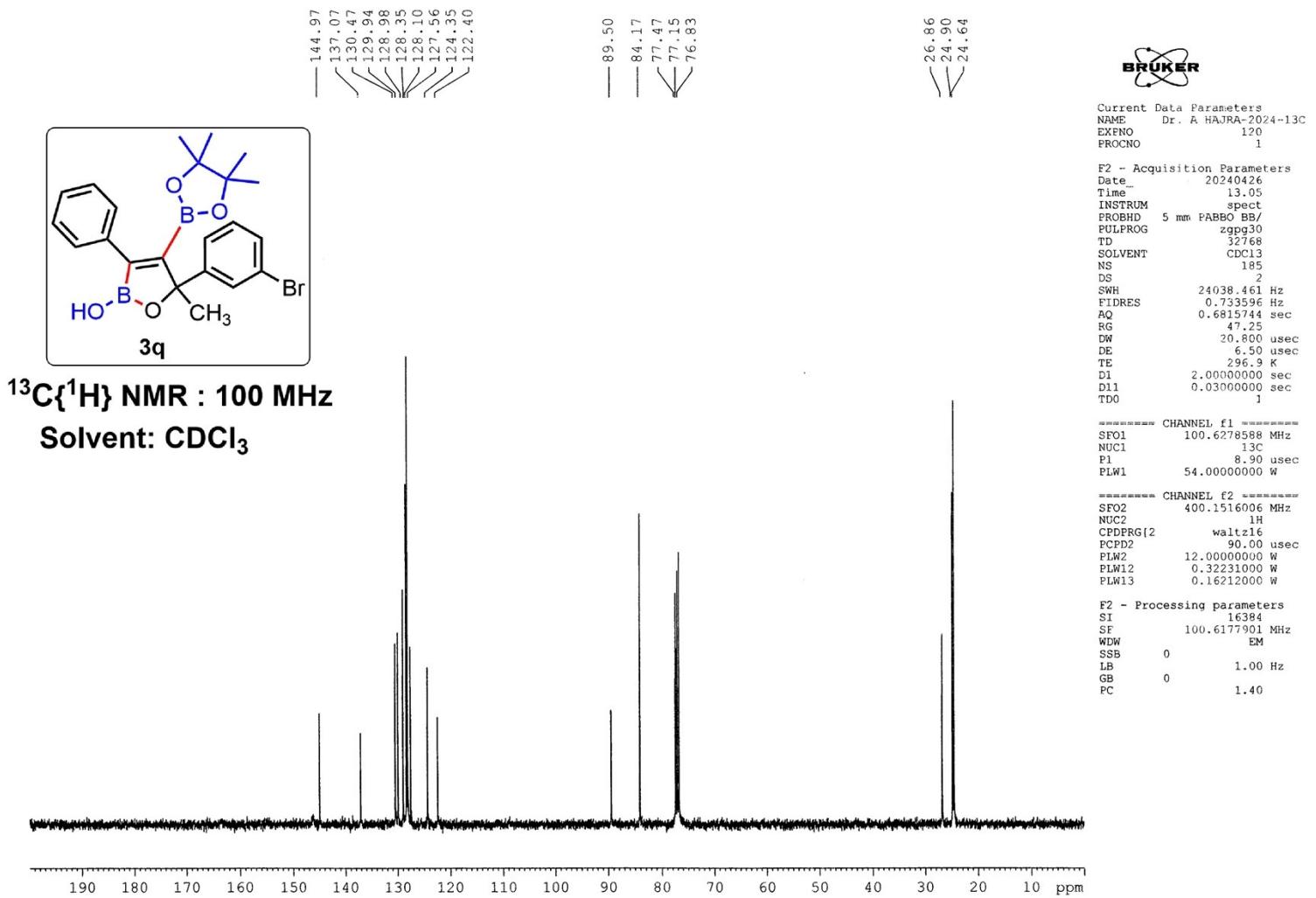
===== CHANNEL f2 =====  
 SF02 400.1516006 MHz  
 NUC2 1H  
 CPDPBG[2] waltz16  
 FCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.32231000 W  
 PLW13 0.16212000 W

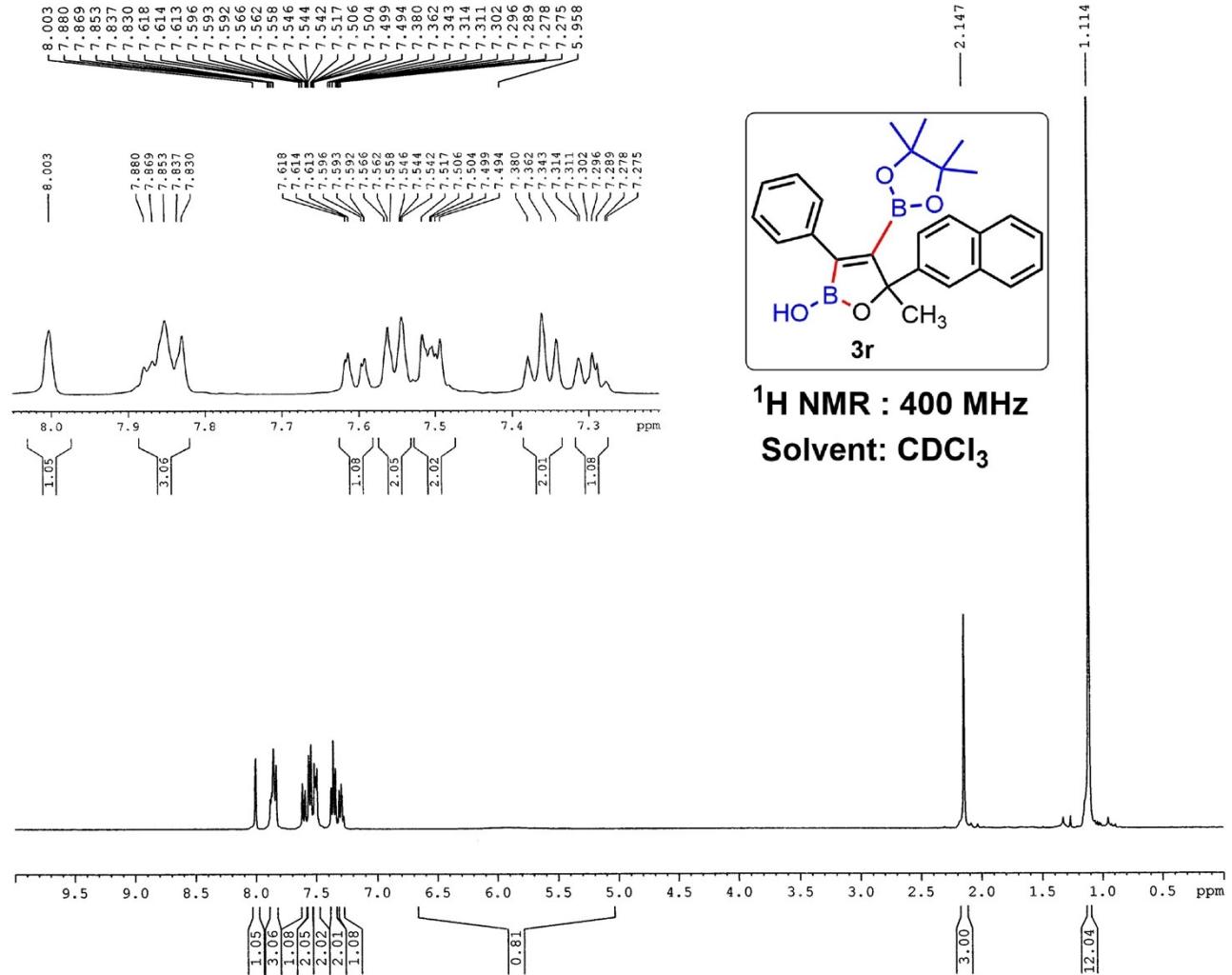
F2 - Processing parameters  
 SI 16384  
 SF 100.6177844 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

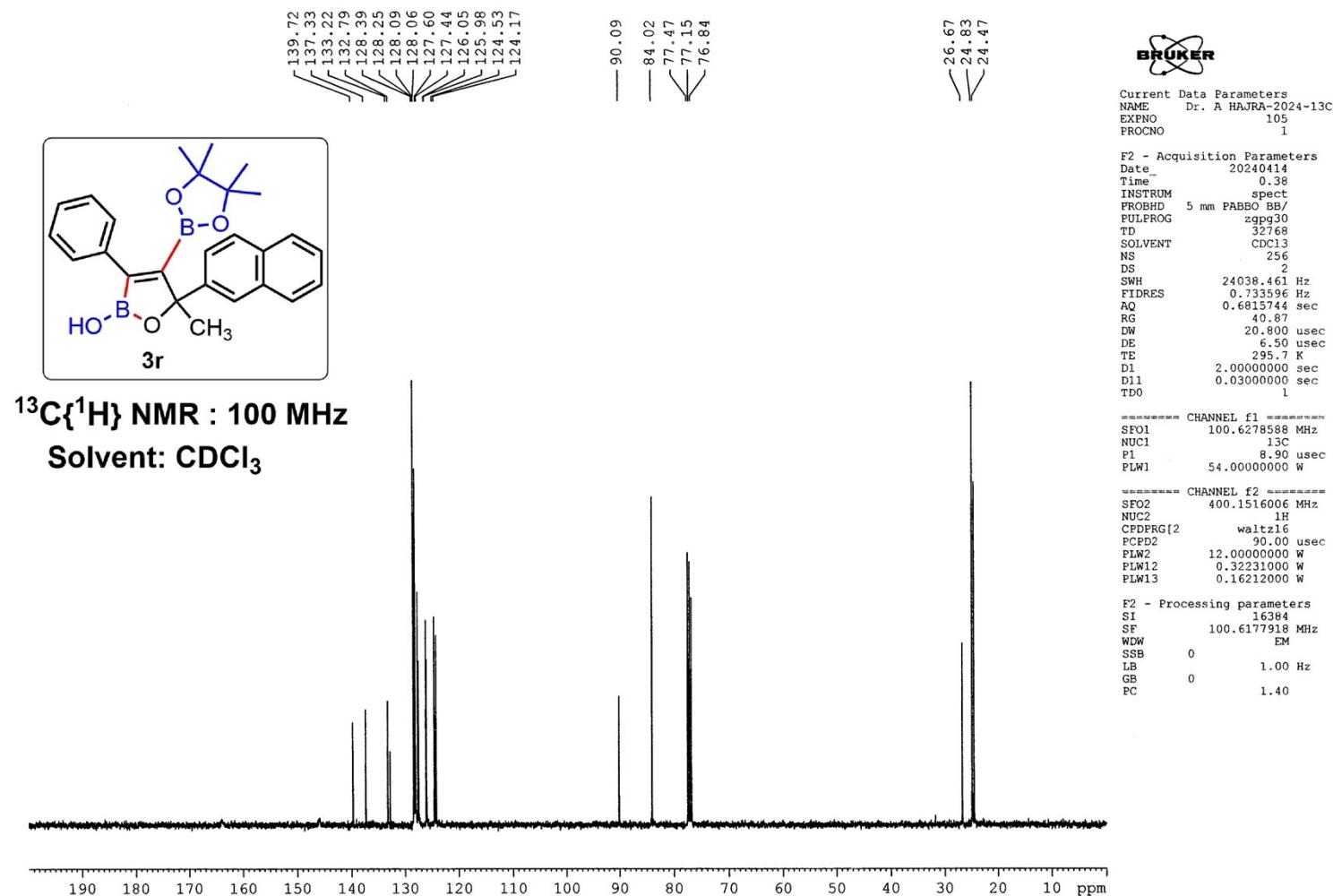


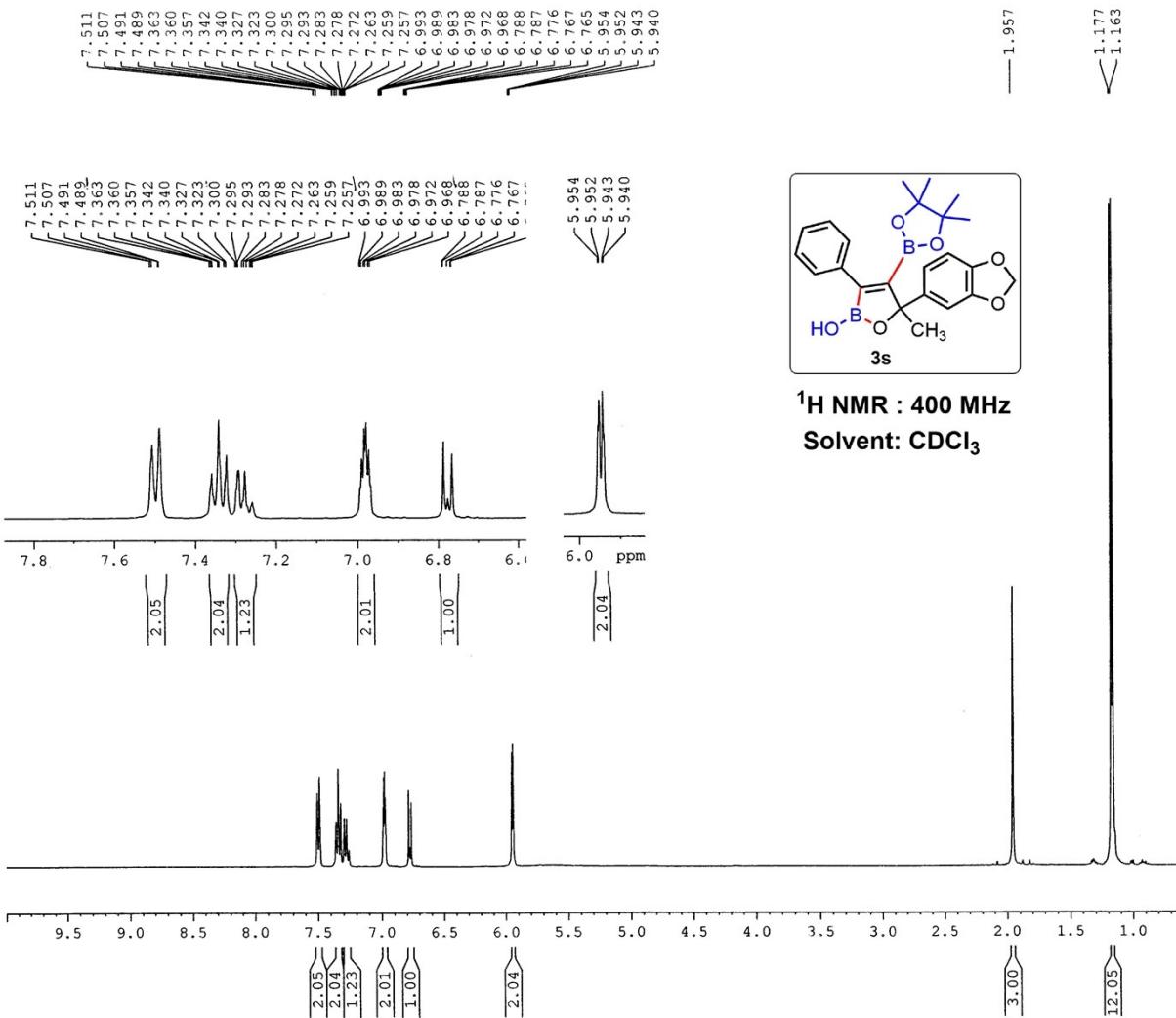












**<sup>1</sup>H NMR : 400 MHz**  
**Solvent: CDCl<sub>3</sub>**

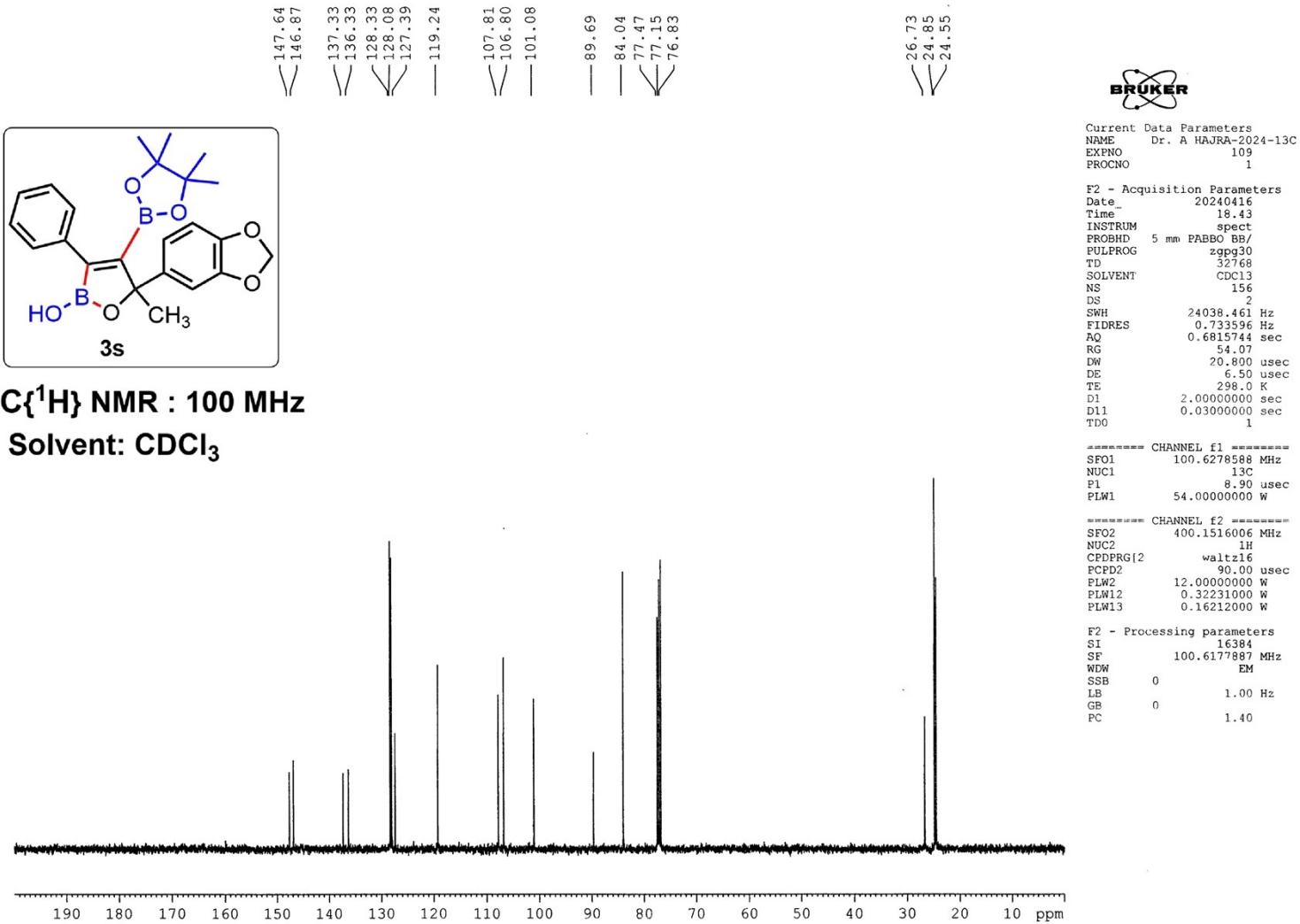


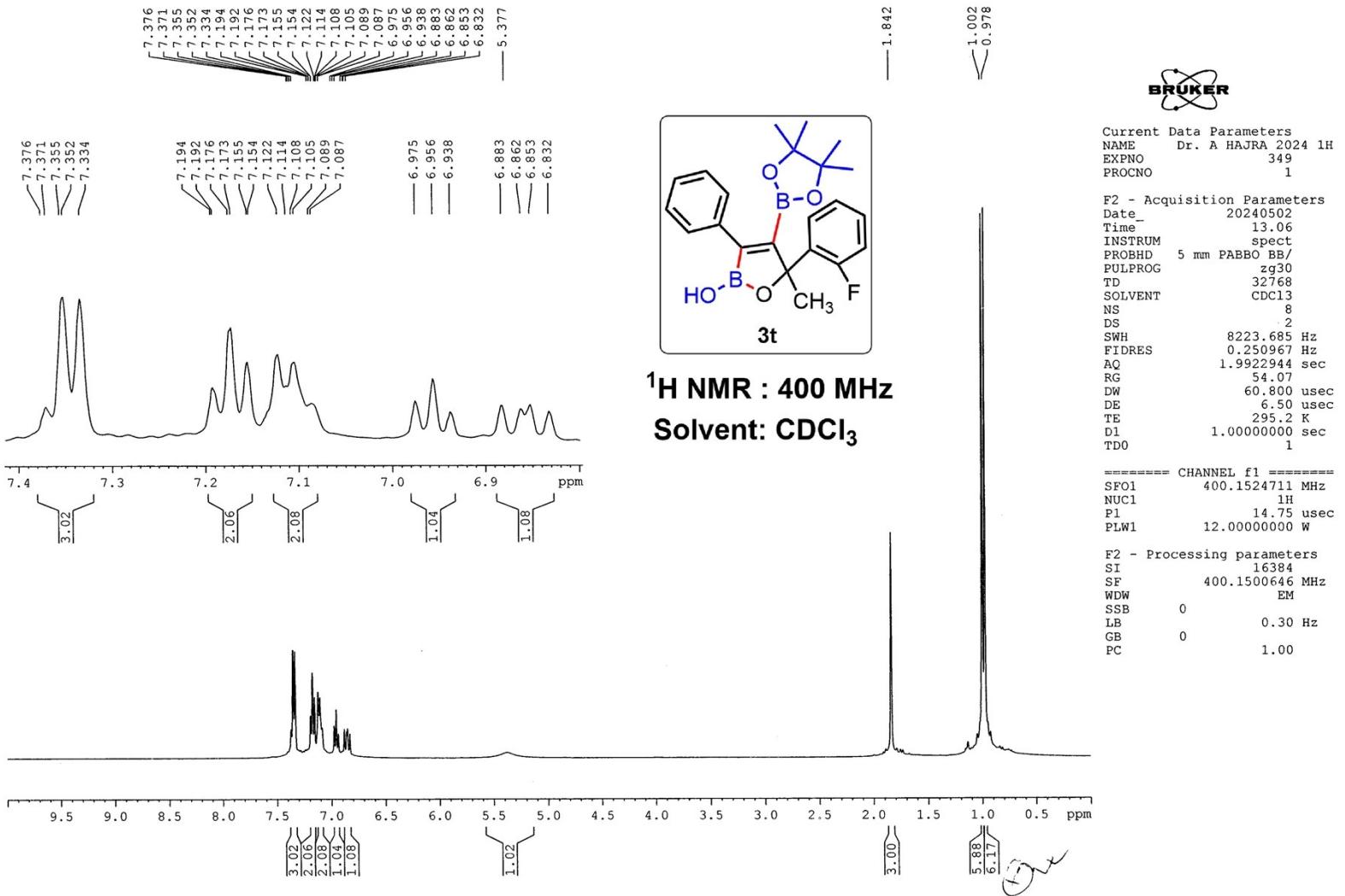
Current Data Parameters  
NAME Dr. A HAJRA 2024 1H  
EXPNO 307  
PROCNO 1

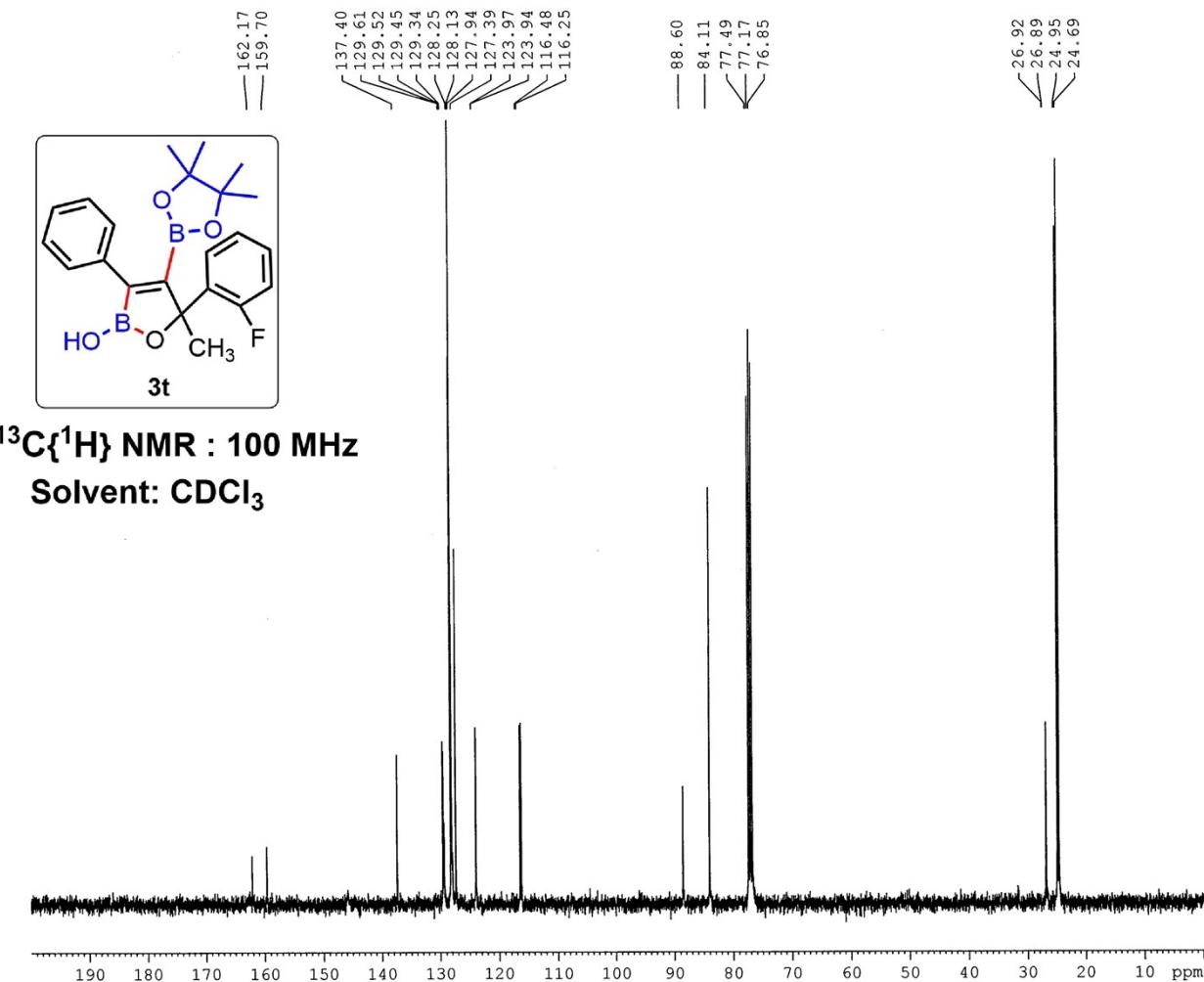
F2 - Acquisition Parameters  
Date\_ 20240416  
Time 18.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 54.07  
DW 60.800 usec  
DE 6.50 usec  
TE 297.7 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1499962 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00







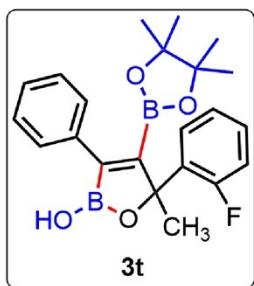


Current Data Parameters  
NAME Dr. A HAJRA 2024 1F  
EXPNO 350  
PROCNO 1

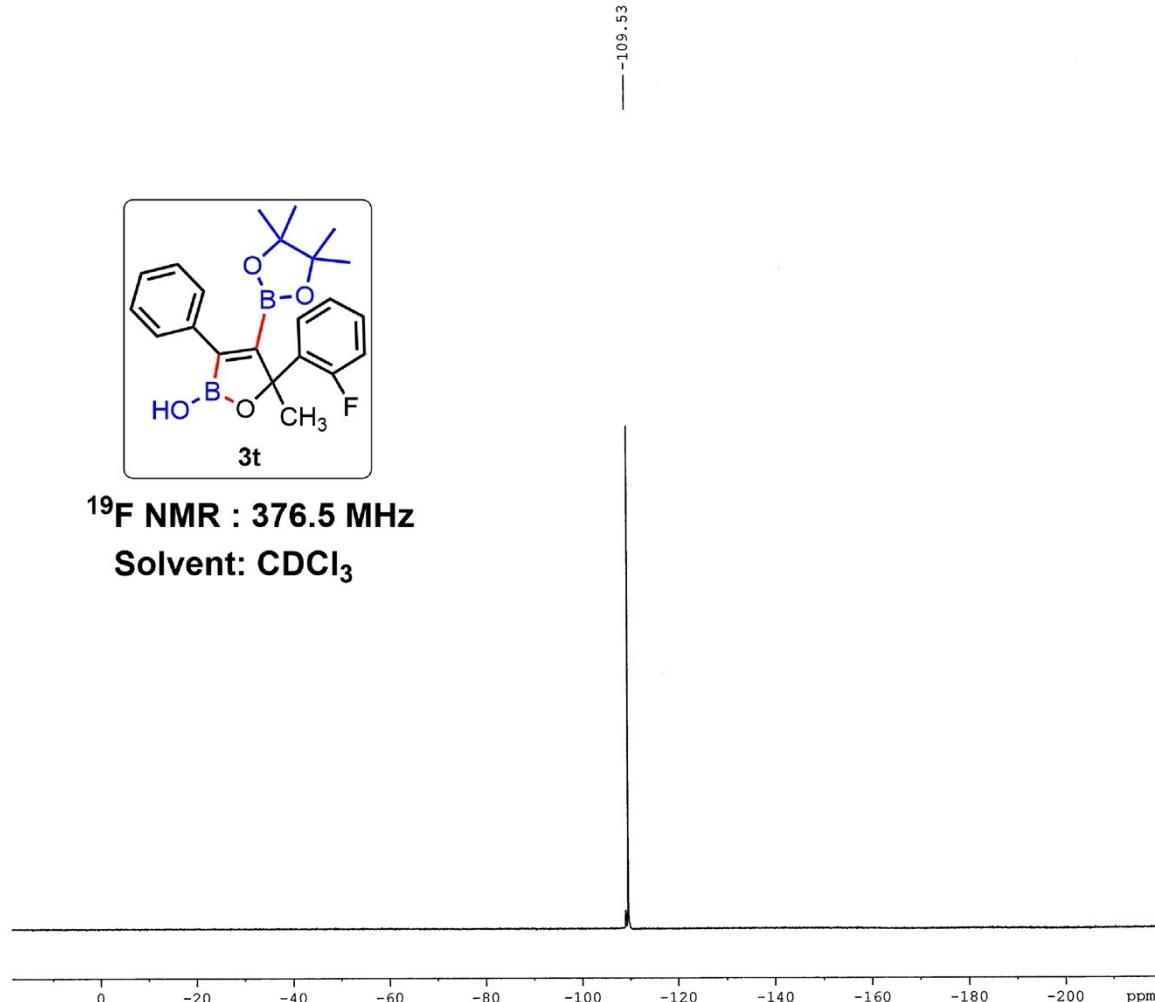
F2 - Acquisition Parameters  
Date\_ 20240502  
Time 13.09  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgflqn  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 89285.711 Hz  
FIDRES 2.724784 Hz  
AQ 0.1835008 sec  
RG 54.07  
DW 5.600 usec  
DE 6.50 usec  
TE 295.3 K  
D1 1.0000000 sec  
TDO 1

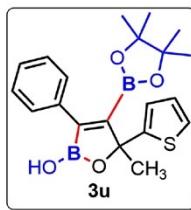
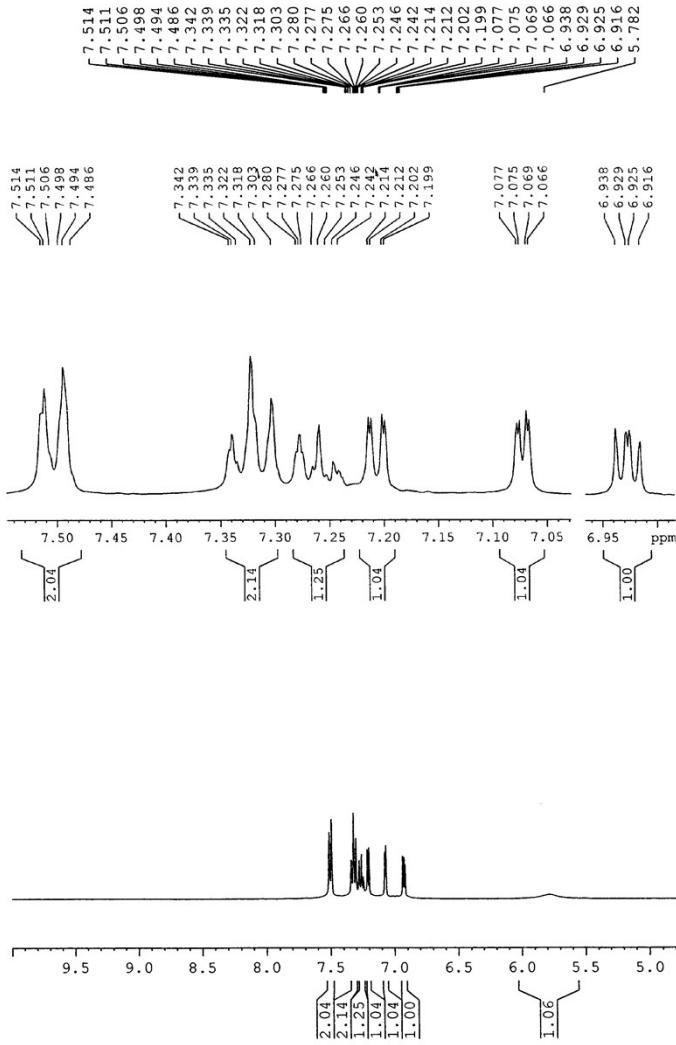
===== CHANNEL f1 =====  
SFO1 376.4795333 MHz  
NUC1 19F  
P1 12.50 usec  
PLW1 20.0000000 W

F2 - Processing parameters  
SI 16384  
SF 376.5171850 MHz  
WDW EM  
SSB 0 0.30 Hz  
LB 0  
GB 0  
PC 1.00



**<sup>19</sup>F NMR : 376.5 MHz**  
**Solvent: CDCl<sub>3</sub>**





<sup>1</sup>H NMR : 400 MHz

**Solvent: CDCl<sub>3</sub>**

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Current Data Parameters  
NAME Dr. A HAJRA 2024 1H  
EXPNO 266  
PROCNO 1

```

F2 - Acquisition Parameters
Date_      20240403
Time       19.14
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD        32768
SOLVENT    CDC13
NS         8
DS         2
SWH       8223.685 Hz
FIDRES   0.250967 Hz
AQ        1.9922944 sec
RG        40.87
DW        60.800 usec
DE        6.50  usec
TE        296.6 K
D1        1.00000000 sec
TD0           1

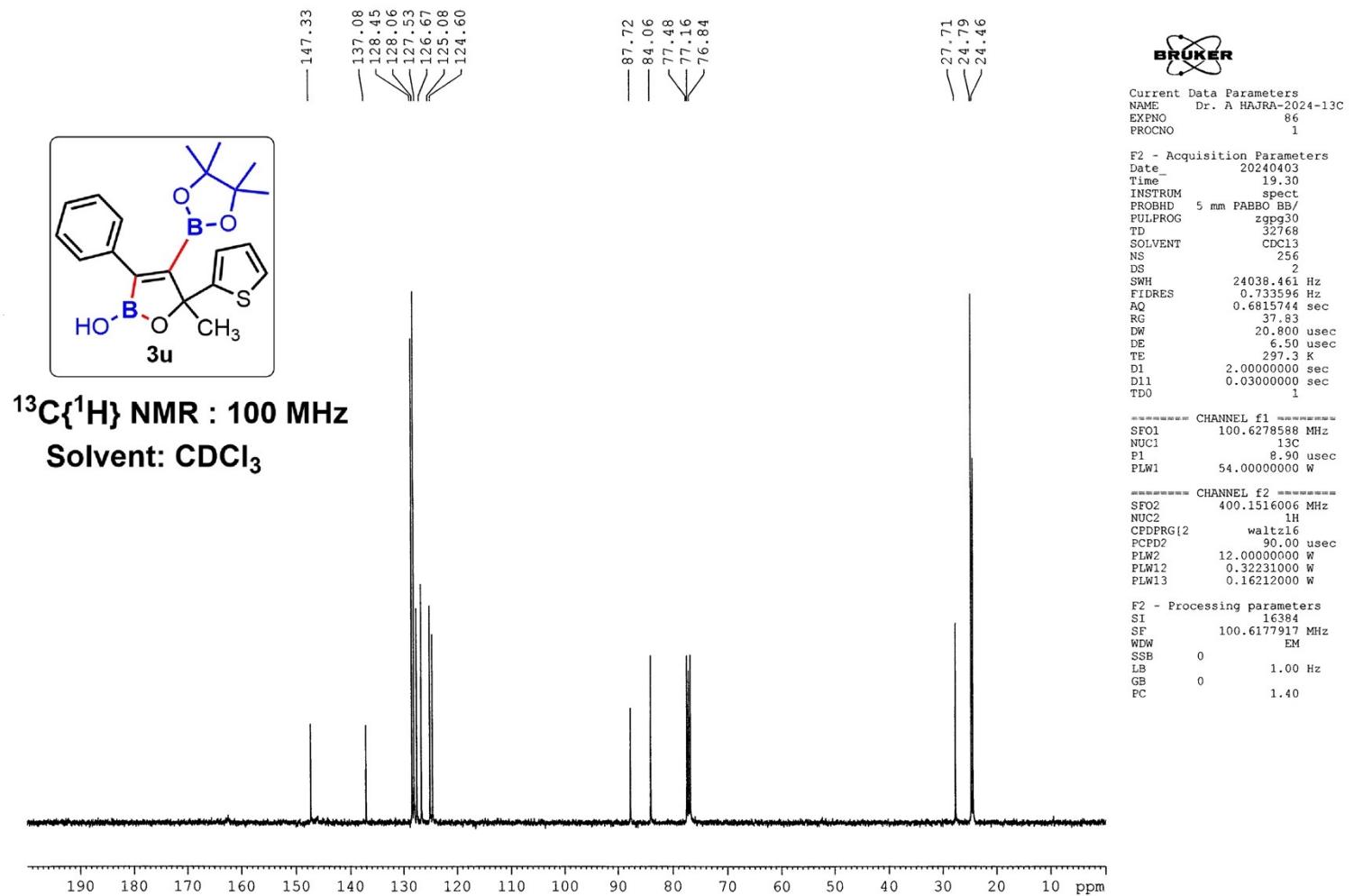
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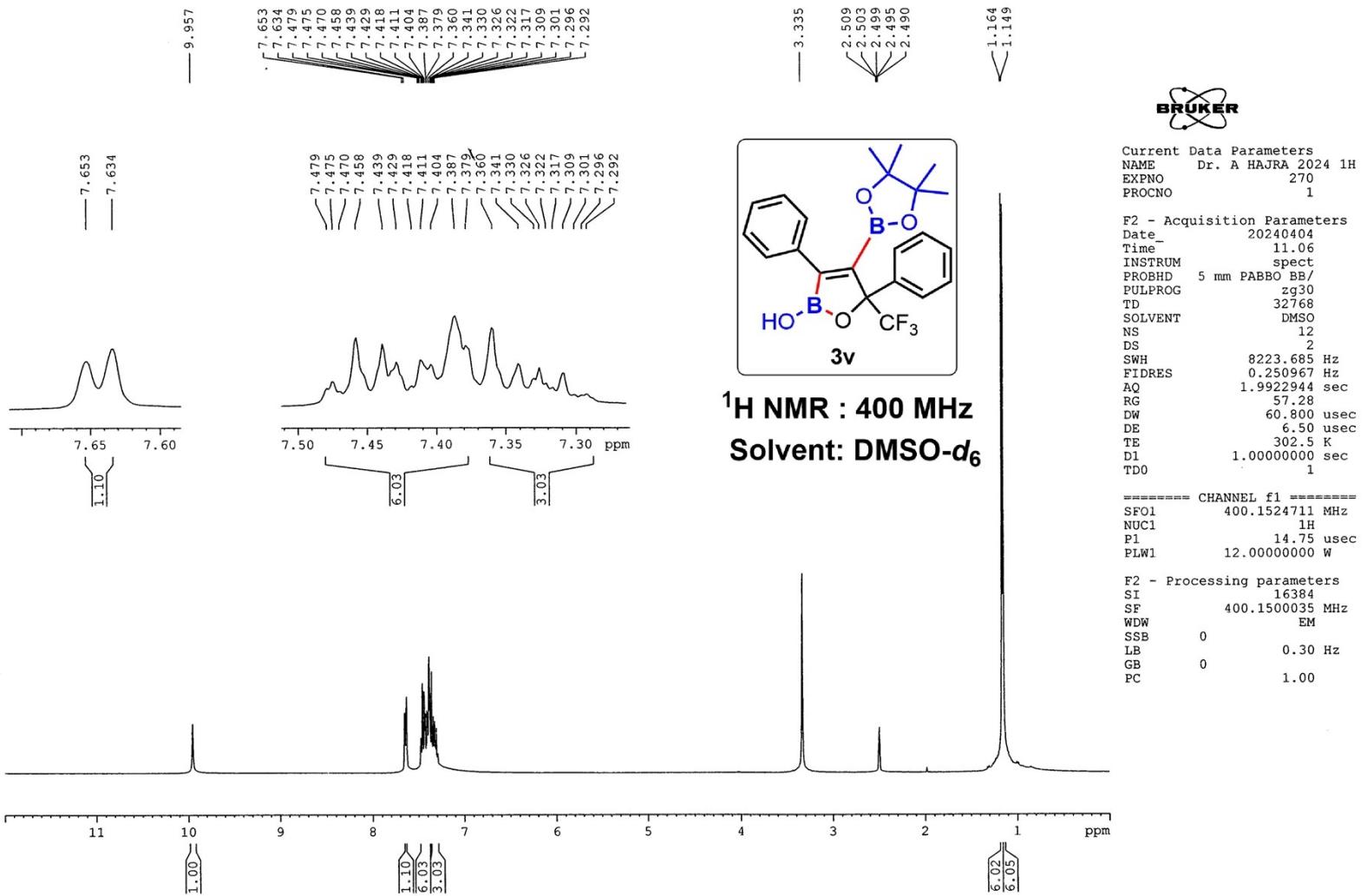
===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.00000000 W

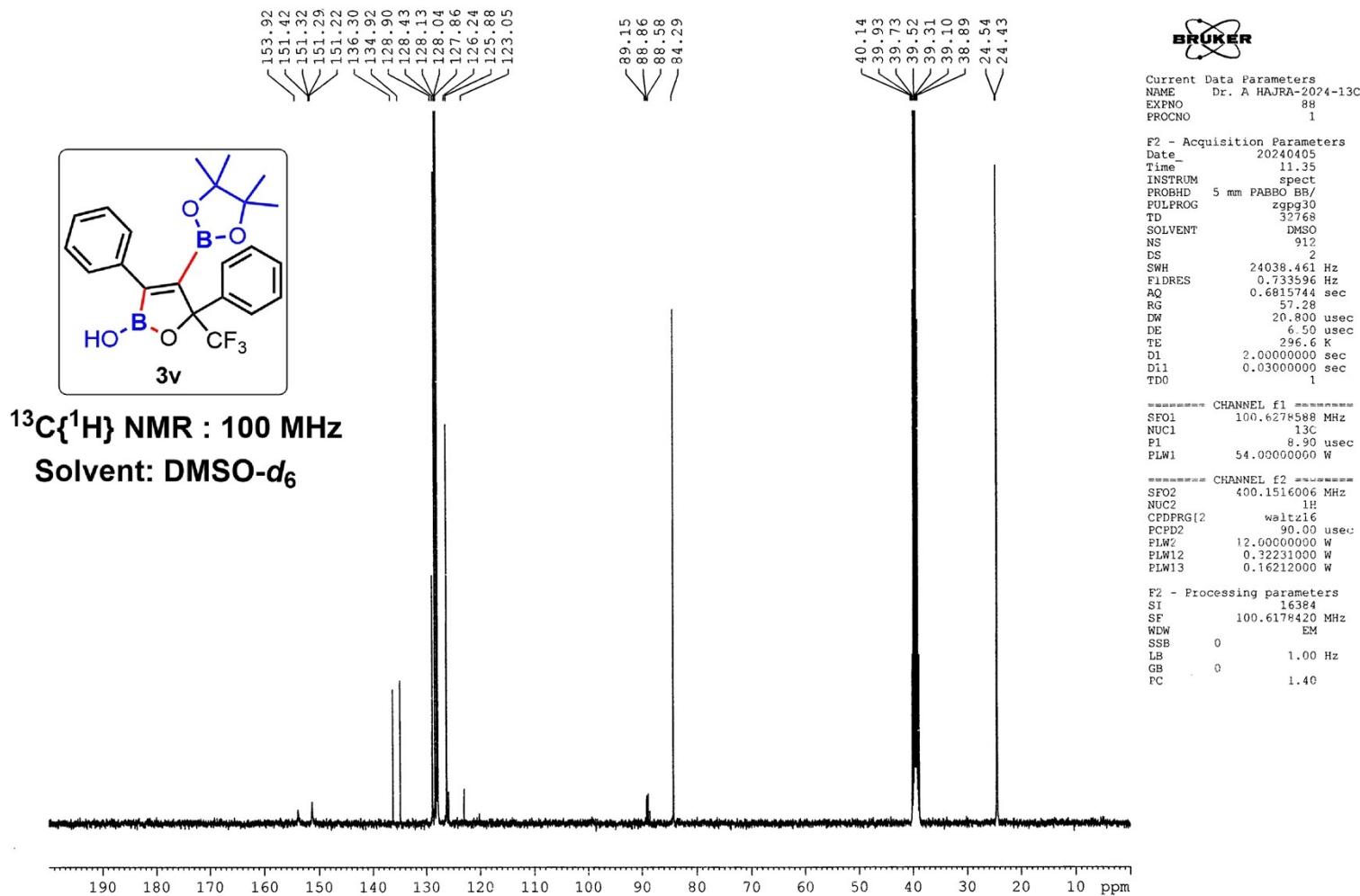
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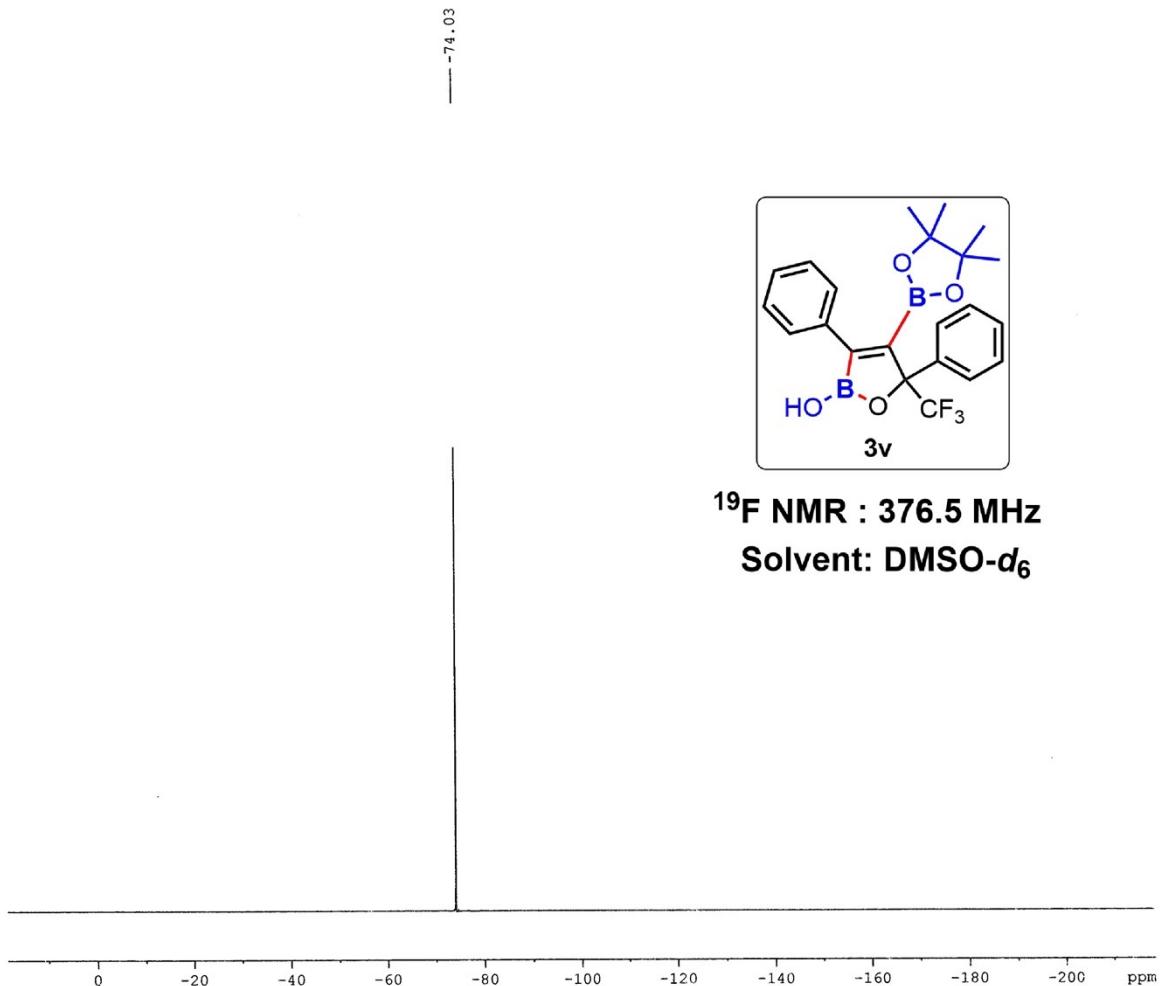
F2 - Processing parameters
SI           16384
SF          400.1500147 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB          0
PC          1.00

```







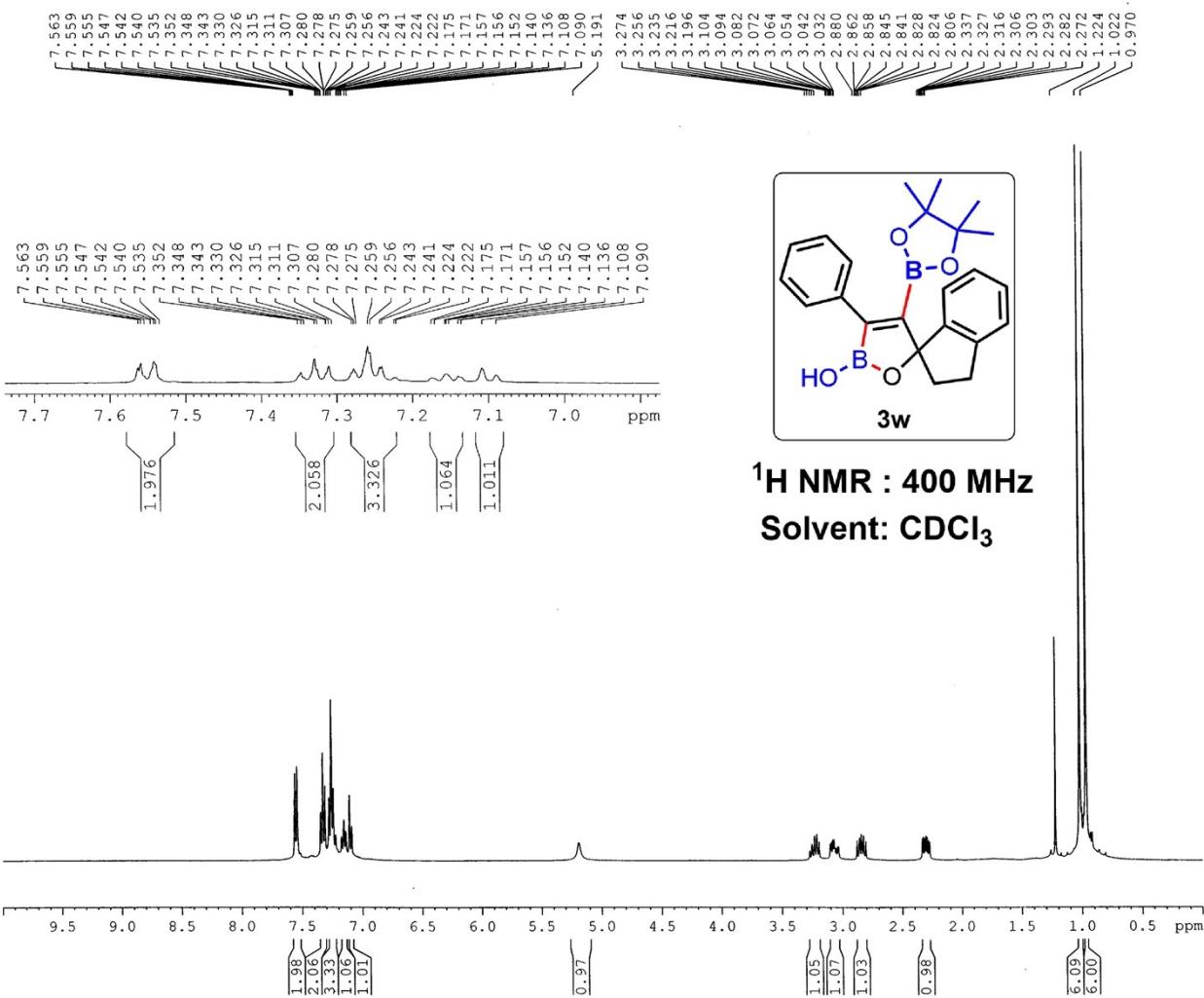


Current Data Parameters  
 NAME Dr. A HAJRA 2024 1H  
 EXPNNO 271  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20240405  
 Time 10.51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgfgn  
 TD 32768  
 SOLVENT DMSO  
 NS 8  
 DS 2  
 SWH 89285.711 Hz  
 FIDRES 2.724784 Hz  
 AQ 0.1835008 sec  
 RG 186.42  
 DW 5.600 usec  
 DE 6.50 usec  
 TE 296.0 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 376.4795333 MHz  
 NUCL 19F  
 P1 12.50 usec  
 PLW1 20.0000000 W

F2 - Processing parameters  
 SI 16384  
 SF 376.5171850 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



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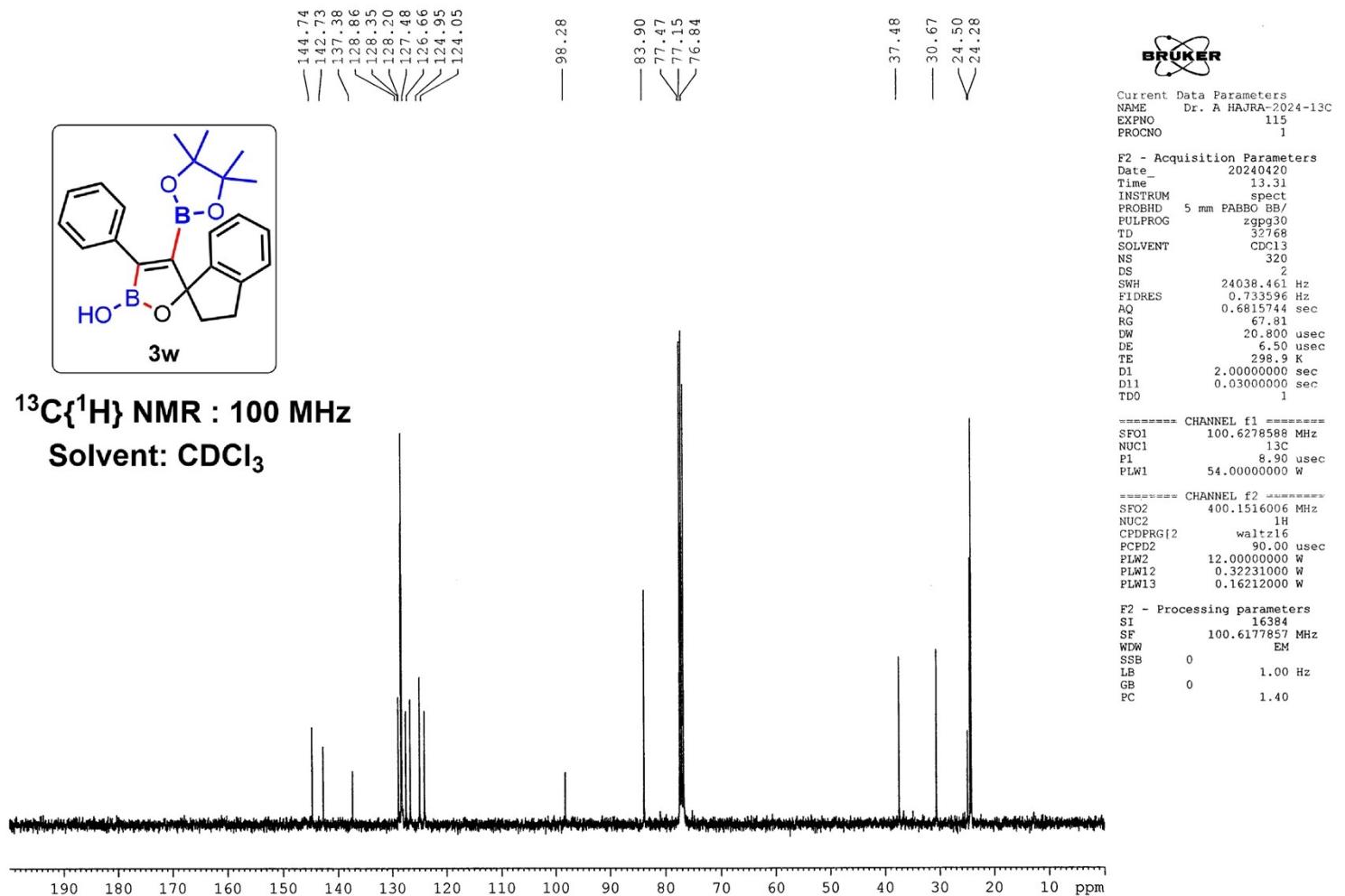
Current Data Parameters  
 NAME Dr. A HAJRA 2024 1H  
 EXPNO 319  
 PROCNO 1

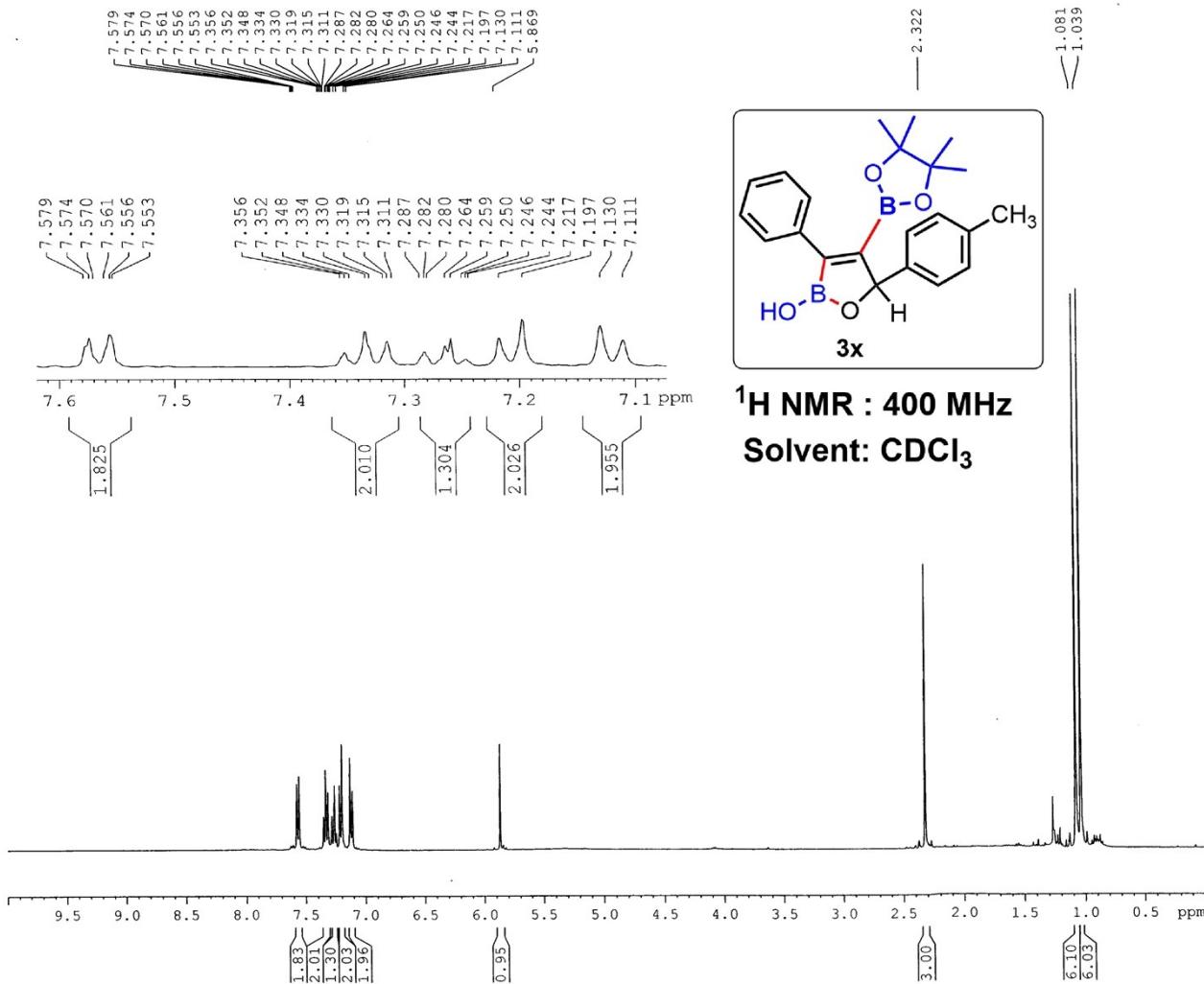
F2 - Acquisition Parameters  
 Date 20240420  
 Time 13.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 1.9922944 sec  
 RG 67.81  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 298.7 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 ======

SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 14.75 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 16384  
 SF 400.1500113 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
NAME Dr. A HAJRA 2024 1H  
EXPNO 384  
PROCNO 1

```

F2 - Acquisition Parameters
Date_          20240510
Time           16.12
INSTRUM        spect
PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD             32768
SOLVENT        CDCl3
NS              8
DS              2
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ             1.9922944 sec
RG             87.66
DW             60.800 used
DE             6.50 used
TE             292.9 K
D1             1.0000000 sec
TDO             1

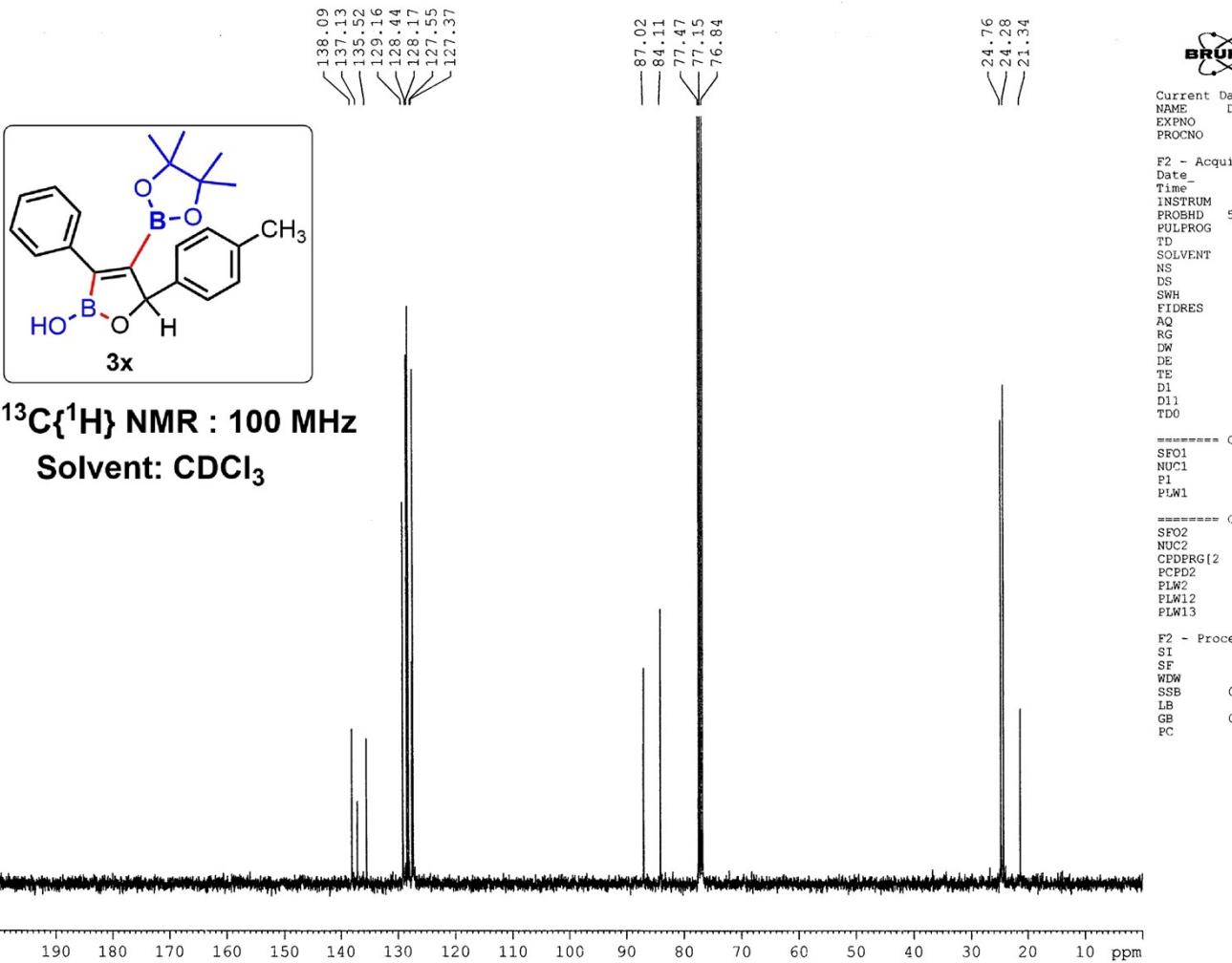
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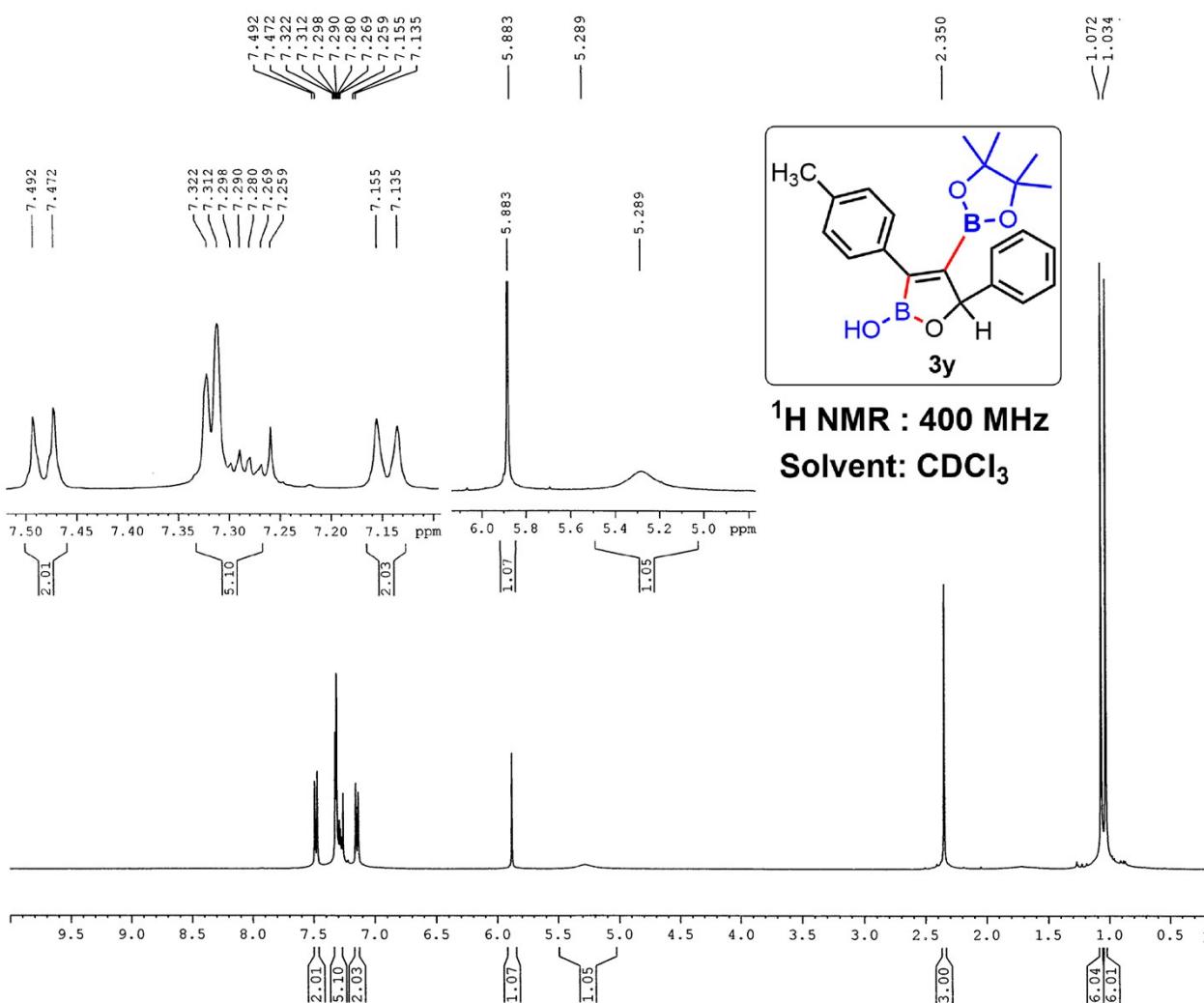
===== CHANNEL f1 =====  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 14.75 used  
PLW1 12.0000000 w

```

F2 - Processing parameters
SI          16384
SF          400.1500097 MHz
WDW          EM
SSB          0
LB          0.30 Hz
GB          0
PC          1.00

```





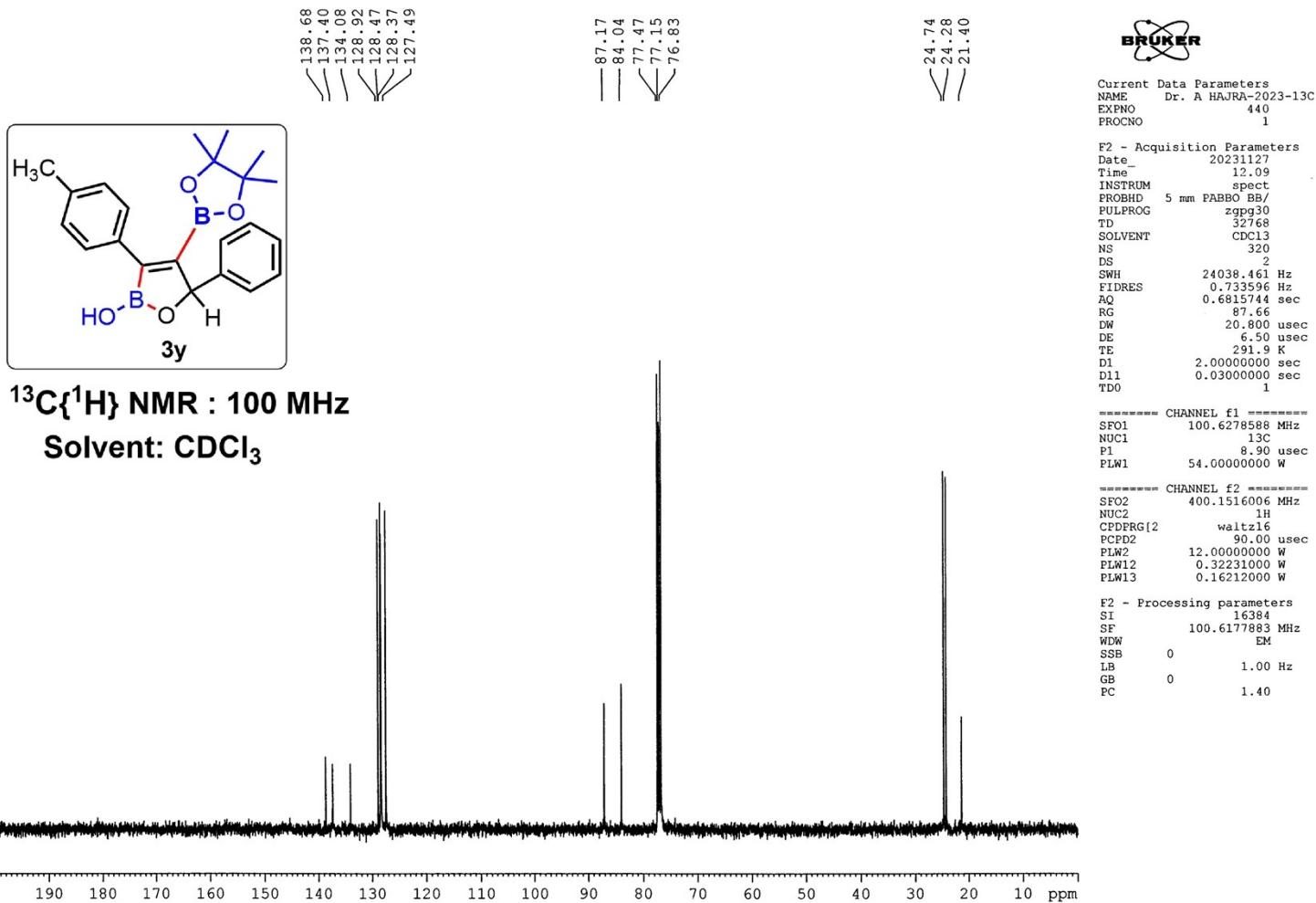
**BRUKER**

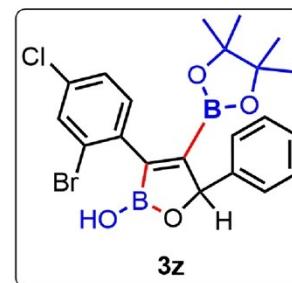
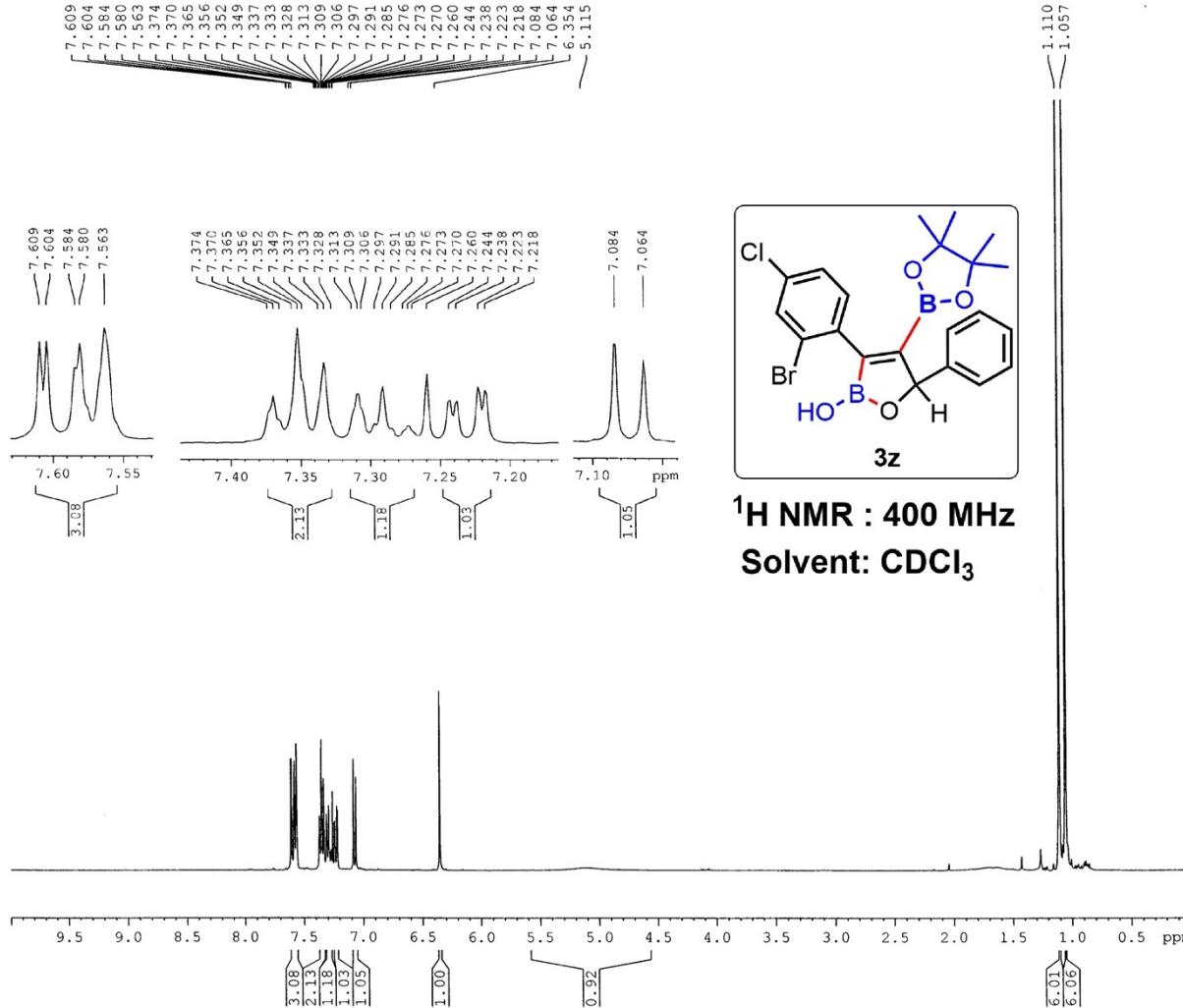
Current Data Parameters  
NAME Dr. A HAJRA 2023 1H  
EXPNO 1269  
PROCNO 1

F2 - Acquisition Parameters  
Date 20231127  
Time 11.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 87.66  
DW 60.800 usec  
DE 6.50 usec  
TE 291.4 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.0000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500097 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





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Current Data Parameters  
NAME Dr. A HAJRA 2024 1H  
EXPNO 502  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20240618  
Time\_ 13.24  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 8  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 1.9922944 sec  
RG 93.46  
DW 60.800 usec  
DE 6.50 usec  
TE 295.4 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 400.1524711 MHz  
NUC1 1H  
P1 14.75 usec  
PLW1 12.0000000 W

F2 - Processing parameters  
SI 16384  
SF 400.1500097 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

