# Buchwald-Hartwig Amination Using Pd(I) Dimer Precatalysts Supported by Biaryl Phosphine Ligands

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# SUPPLEMENTARY INFORMATION

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**Table of Contents**

## 1. General Considerations

3,5-Dimethoxyaniline (Oakwood Chemical) was sublimed prior to use. Morpholine (Sigma-Aldrich), cyclohexylamine (Oakwood Chemical), 3-bromopyridine (Oakwood Chemical), 1-bromo-3,5-dimethylbenzene (Sigma-Aldrich, 97%) and 4-bromobenzotrifluoride (Sigma-Aldrich, 99%) were filtered through alumina, dried over 4Å molecular sieves and deoxygenated by sparging with $N_2$ for 30 minutes. 4-Bromotoluene (Sigma-Aldrich, 98%), 4-chlorotoluene (Sigma-Aldrich, 98%), 4-iodotoluene (Sigma-Aldrich, 99%), 2-bromotoluene (Sigma-Aldrich, 99%), 1-bromo-4-chlorobenzene (Sigma-Aldrich), and 5-chloro-2-bromopyridine (Oakwood Chemical) were used as received.

2-(Di-*tert*-butylphosphino)biphenyl (JohnPhos, **L1**, Sigma-Aldrich, 97%), 2-Dicyclohexylphosphino-2′-(*N,N*-dimethylamino)biphenyl (DavePhos, **L2**, Sigma-Aldrich, 97%), 2-Di-*tert*-butylphosphino-2′,4′,6′-triisopropylbiphenyl ($^t$BuXPhos, **L3**, Sigma-Aldrich, 97%), 2-Dicyclohexylphosphino-2′,4′,6′-triisopropylbiphenyl (XPhos, **L4**, Sigma-Aldrich, 97%), 2-Dicyclohexylphosphino-2′,6′-dimethoxybiphenyl (SPhos, **L5**, Sigma-Aldrich, 95%), and 2-Dicyclohexylphosphino-2′,6′-diisopropoxybiphenyl (RuPhos, **L6**, Sigma-Aldrich, 95%) were used as received.

Tris(dibenzylideneacetone)dipalladium(0) (Sigma-Aldrich, 97%), tetrakis(acetonitrile) palladium(II) tetrafluoroborate, KO$^t$Bu (Sigma-Aldrich, reagent grade, >98%) and NaO$^t$Bu (Sigma-Aldrich, reagent grade, 97%) were stored in a $N_2$ filled glovebox and used as received. Small portions of KO$^t$Bu and NaO$^t$Bu were removed from the glovebox and stored in a desiccator for up to two weeks (all reactions were set up outside of the glovebox).

Acetonitrile (Sigma-Aldrich, anhydrous, 99.8%) and 1,4-dioxane (Sigma-Aldrich, anhydrous, 99.8%) were used as received, dry dichloromethane was obtained from a Grubbs column with an activated alumina and copper catalyst.

Silica Gel (Fisher, Grade 60, 230-400 Mesh), alumina (Alfa Aesar, activated, basic Brockmann Grade I, 58 Å, 60 mesh powder), and Celite (Fisher, 545 filter aid, not acid washed, powder) were used as received. Deuterated chloroform (Cambridge Isotope Laboratories) and deuterated dichloromethane (Cambridge Isotope Laboratories) were used as received.

All cross-coupling reactions were performed in an oven dried 16 mL reaction tube (Fisher, 16 mm diameter, borosilicate glass) fitted with a PTFE lined magnetic stir bar and PTFE lined septum cap.

## 2. Instrumentation

$^1$H, $^{13}$C{1H}, $^{19}$F NMR spectra were recorded on DRX500 and AV400 spectrometers in ambient conditions unless stated otherwise. Bruker Topspin V3.2 software was used to process the FID data and visualize the spectra. $^1$H and $^{13}$C{1H} NMR spectra were referenced to residual solvent resonances in deuterated solvents (CDCl3: $^1$H, 7.26 ppm; $^{13}$C, 77.16 ppm; Note: due to high humidity $H_2O$ resonances are often present) and are reported relative to tetramethylsilane ($\delta$ = 0 ppm). $^{19}$F and $^{19}$F{$^1$H} NMR spectra were referenced to fluorobenzene ($\delta$ = -113.15 ppm).

Gas Chromatography Mass Spectrometry (GC-MS) data were collected on a Shimadzu GCMS-QP2010 equipped with a Restek XTI-5 column (0.25 mm diameter) with He carrier gas.

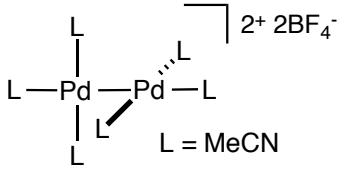
Electrospray ionization mass spectrometry (ESI-MS) data were collected on an Agilent 6530 Q-TOF LC-MS with 1260 Infinity LC (compounds **1-6**). High-resolution mass spectrometry (HRMS) data for organic substrates were collected on a Thermo Fisher Scientific Exactive Plus with IonSense ID-CUBE DART (Direct Analysis in Real Time) source (compounds **7-20**).

X-ray photoelectron spectroscopy (XPS) data was acquired using an AXIS Ultra DLD instrument (Kratos Analytical Inc., Chestnut Ridge, NY, USA) with a monochromatic Al Kα X-ray source (10 mA for survey and high-resolution scans). A 300 x 700 nm oval spot size and ultrahigh vacuum ($10^{-9}$ Torr) were used, with 160 eV pass energy for survey spectra and 20 eV for high-resolution spectra of Pd 3s using a 200 ms dwell time and 20 scans. All XPS peaks were externally referenced to the C 1s signal at 284.6 eV.

Elemental analyses were performed by Atlantic Microlab, Inc. (Norcross, GA).

## 3. Precatalyst Synthesis

**$[Pd_2MeCN_6][BF_4]_2$**

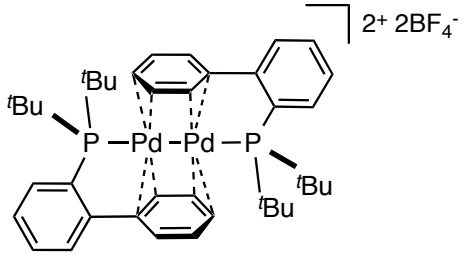



In a glovebox, $[Pd(MeCN)_4][BF_4]_2$ (0.300 g, 0.675 mmol) and $Pd_2(dba)_3$ (0.308 g, 0.336 mmol) were added to a 50 mL Schlenk flask. The flask was brought out of the box and placed under $N_2$ on a Schlenk line, then dry MeCN (7.5 mL) and dry, stabilizer-free $CH_2Cl_2$ (7.5 mL) were added *via* syringe. The mixture was stirred at room temperature for 1 hour to yield a deep red solution. The reaction mixture was filtered and washed with $CH_2Cl_2$. The volume of the filtrate was reduced to ~7-8 mL by rotary evaporation (all $CH_2Cl_2$ removed, only MeCN remaining). Diethyl ether (20 mL) was added and an orange precipitate immediately crashed out. The precipitate was filtered and washed with diethyl ether (5 x 3 mL), then isolated and dried under vacuum for 1-2 hours (0.385 g, 90%). This procedure is adapted from a reported procedure.[1]

*General Procedure for* ***$[Pd\text{-}LX]_2[BF_4]_2$ (1-6)*** *Precatalysts*

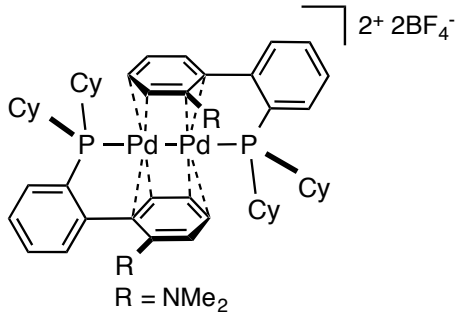
In a 20 mL scintillation vial in air, **$[Pd_2MeCN_6][BF_4]_2$** (0.055-0.316 mmol), a magnetic stir bar, and stabilizer-free $CH_2Cl_2$ (1-2 mL) were combined. In a separate vial, **L1-L6** (0.11-0.632 mmol) was dissolved in stabilizer-free $CH_2Cl_2$ (1-2 mL). The solution of **L1-L6** was added to the Pd-containing vial *via* syringe, and the reaction mixture was stirred at room temperature for 5-30 minutes. The reaction mixture was passed through a pad of Celite and the solvent was removed *in vacuo*. The isolated compounds **1-6** were used for cross-coupling reactions without further purification.

**[Pd-L1]$_2$[BF$_4$]$_2$ (1)**




Following the general procedure for synthesis of precatalysts, a solution of **L1** (JohnPhos, 32 mg, 0.11 mmol, JohnPhos) in $CH_2Cl_2$ (1 mL) was added to **[Pd$_2$MeCN$_6$][BF$_4$]$_2$** (35 mg, 0.055 mmol) in $CH_2Cl_2$ (1 mL), and the reaction mixture was stirred for 20 minutes at room temperature. Upon completion, the reaction mixture was passed through a pad of Celite and the solvent was removed *in vacuo* to yield a red-orange solid (53 mg, 99%). **1** was used in cross-coupling reactions without further purification. **$^1$H NMR (400 MHz, CD$_2$Cl$_2$)**: δ 8.45-8.38 (m, 2H), 8.02-7.97 (m, 2H), 7.97-7.88 (m, 2H), 7.73-7.69 (m, 2H), 7.30-7.24 (m, 2H), 6.44-6.38 (m, 4H), 6.48-6.33 (m, 4H), 1.56 (t, 36H, $J$ = 7.8 Hz); **$^{13}$C NMR**: *Complex too insoluble for $^{13}$C NMR characterization*; **$^{31}$P{$^1$H} NMR (162 MHz, CD$_2$Cl$_2$)**: δ 82.65 (s, 2P). Elemental Analysis found (calculated for $C_{40}H_{54}B_2F_8P_2Pd_2$): C, 49.09 (48.86); H, 5.67 (5.54). ESI-MS *m/z* [Pd**L1**]$^+$ calculated: 404.09, found: 404.04. Note: this compound was observed as a monomer species under electrospray ionization.

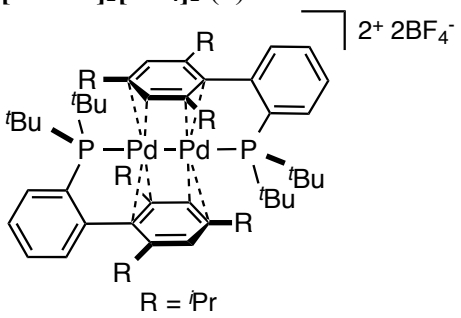
**[Pd-L2]$_2$[BF$_4$]$_2$ (2)**




Following the general procedure for synthesis of precatalysts, a solution of **L2** (DavePhos, 43 mg, 0.11 mmol, DavePhos) in $CH_2Cl_2$ (1 mL) was added to **[Pd$_2$MeCN$_6$][BF$_4$]$_2$** (35 mg, 0.055 mmol) in $CH_2Cl_2$ (1 mL), and the reaction mixture was stirred for 30 minutes at room temperature. Upon completion, the reaction mixture was passed through a pad of Celite and the solvent was removed *in vacuo* to yield a yellow-brown solid (47 mg, 72%). **2** was used in cross-coupling reactions without further purification. Single crystals suitable for X-ray diffraction studies were obtained *via* slow diffusion of pentane into a concentrated solution of 1,2-dichloroethane (there are two molecules of 1,2-dichloroethane per molecule of **2**, but the SQUEEZE method was used to render them due to disorder). *Note for Alert Level B: there were no high-angle data available and the data cut off at high angles was used as a limit in data collection.* **$^1$H NMR (400 MHz, CD$_2$Cl$_2$)**: δ 8.03-7.95 (m, 2H), 7.78-7.72 (m, 2H), 7.62-7.58 (m, 4H), 7.24-7.19 (m, 2H), 5.76 (dd, 2H, $J$ = 6.8, 1.2 Hz), 5.3-5.24 (m, 4H), 2.98-2.88 (m, 2H), 2.59 (br. s, 12H), 2.44-2.35 (m, 2H), 2.16-2.08 (4H), 2.05-1.96 (m, 6H), 1.89-1.80 (m, 6H), 1.79-1.65 (m, 8H), 1.62-1.52 (m, 8H), 1.45-1.32 (m, 8H), 1.26-1.10 (m, 8H); **$^{13}$C NMR**: *Complex too insoluble for $^{13}$C NMR characterization*; **$^{31}$P{$^1$H} NMR (162 MHz, CD$_2$Cl$_2$)**: δ 53.46 (s, 2P).

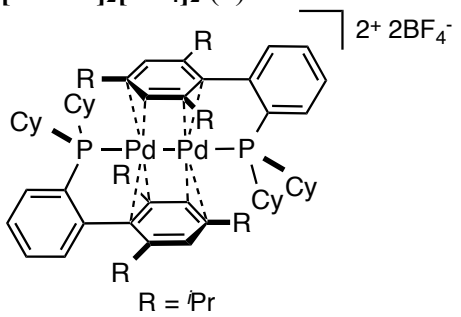
Elemental Analysis found (calculated for $C_{52}H_{72}B_2F_8N_2P_2Pd_2$): C, 53.29 (53.22); H, 6.34 (6.18); N, 2.42 (2.39). ESI-MS *m/z* $[Pd\mathbf{L2}]_2^{2+}$ calculated: 500.16, found: 500.16. Note: this compound was observed as a dimer species under electrospray ionization.

**$[Pd\text{-}L3]_2[BF_4]_2$ (3)**




Following the general procedure for synthesis of precatalysts, a solution of **L3** ($^t$BuXPhos, 46 mg, 0.11 mmol, $^t$BuXPhos) in $CH_2Cl_2$ (1 mL) was added to **$[Pd_2MeCN_6][BF_4]_2$** (35 mg, 0.055 mmol) in $CH_2Cl_2$ (1 mL), and the reaction mixture was stirred for 20 minutes at room temperature. Upon completion, the reaction mixture was passed through a pad of Celite and the solvent was removed *in vacuo* to yield a yellow-orange solid (67 mg, 99%). Attempts to purify **3** by recrystallization yielded metallic Pd, so **3** was used in cross-coupling reactions without further purification. **$^1$H NMR (400 MHz, $CD_2Cl_2$)**: δ 7.86-7.75 (m, 2H), 7.74-7.67 (m, 2H), 7.60-7.54 (m, 2H), 7.53-7.43 (m, 2H), 7.43-7.32 (m, 1H), 7.26-7.11 (m, 1H), 7.01 (s, 2H), 2.96-2.88 (m, 1H), 2.55-2.38 (m, 5H), 1.59-1.51 (m, 9H), 1.51-1.44 (m, 9H), 1.36-1.22 (m, 36H), 1.22-1.16 (m, 12H), 0.92 (d, 6H, $J$ = 6.8 Hz); **$^{13}$C NMR**: *Complex too insoluble for $^{13}$C NMR characterization*; **$^{31}$P{$^1$H} NMR (162 MHz, $CD_2Cl_2$)**: δ 71.38, 32.45, –49.30. *Note: multiple $^{31}$P resonances observed due to fluctionality of bulky ligand **L3** in solution.* Elemental Analysis found (calculated for $C_{58}H_{90}B_2F_8P_2Pd_2$): C, 53.86 (56.37); H, 7.18 (7.34). ESI-MS *m/z* $[Pd\mathbf{L3}]^+$ calculated: 530.23, found: 530.18. Note: this compound was observed as a monomer species under electrospray ionization.

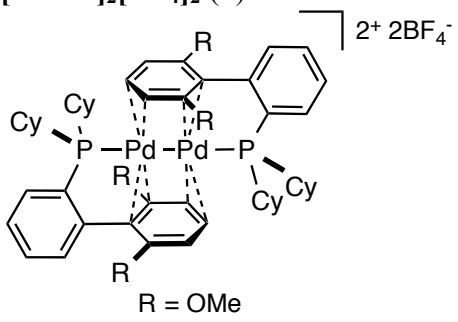
**$[Pd\text{-}L4]_2[BF_4]_2$ (4)**




Following the general procedure for synthesis of precatalysts, a solution of **L4** (XPhos, 226 mg, 0.474 mmol, XPhos) in $CH_2Cl_2$ (2 mL) was added to **$[Pd_2MeCN_6][BF_4]_2$** (150 mg, 0.237 mmol) in $CH_2Cl_2$ (2 mL), and the reaction mixture was stirred for 30 minutes at room temperature. Upon completion, the reaction mixture was passed through a pad of Celite and the solvent was removed *in vacuo* to yield a red-purple solid (302 mg, 95%). Attempts to purify **4** by recrystallization yielded metallic Pd, so **4** was used in cross-coupling reactions without further purification. **$^1$H NMR (400 MHz, $CD_2Cl_2$)**: δ 7.65-7.57 (m, 3H), 7.55-7.47 (m, 3H), 7.27-7.22

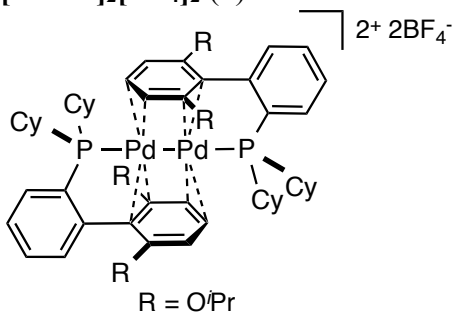
(m, 2H), 7.07 (t, 4H, $J$ = 10.0 Hz), 3.01-2.82 (m, 3H), 2.41-4.30 (m, 12H), 2.05-1.81 (m, 16H), 1.81-1.64 (m, 16H), 1.55 (d, 4H, $J$ = 6.8 Hz), 1.49 (d, 4H, $J$ = 6.8 Hz), 1.40-1.36 (m, 8H), 1.29-1.26 (m, 16H), 1.21-1.05 (m, 16H), 0.97-0.91 (m, 16 H); **$^{13}$C NMR**: *Complex too insoluble for $^{13}$C NMR characterization*; **$^{31}$P{$^{1}$H} NMR (162 MHz, $CD_2Cl_2$)**: δ 39.26 (d, 1P, $^{3}J_{P\text{-}P}$ = 84 Hz), 23.15 (d, 1P, $^{3}J_{P\text{-}P}$ = 84 Hz). *Note: multiple $^{31}$P resonances observed due to fluctionality of bulky ligand **L4** in solution.* Elemental Analysis found (calculated for $C_{66}H_{98}B_2F_8P_2Pd_2$): C, 57.60 (59.16); H, 7.30 (7.37). This compound is not stable to ESI-MS conditions.

**[Pd-L5]$_2$[BF$_4$]$_2$ (5)**




Following the general procedure for synthesis of precatalysts, a solution of **L5** (SPhos, 35 mg, 0.11 mmol, SPhos) in $CH_2Cl_2$ (1 mL) was added to **[Pd$_2$MeCN$_6$][BF$_4$]$_2$** (35 mg, 0.055 mmol) in $CH_2Cl_2$ (1 mL), and the reaction mixture was stirred for ~1 minute at room temperature. Upon completion, the reaction mixture was passed through a pad of Celite and the solvent was removed *in vacuo* to yield a red-orange solid (61 mg, 91%). *Note: The reaction mixture is initially completely in solution, but Pd-black beings to form after stirring for a few minutes. When the reaction runs for 10 minutes, the isolated yield drops significantly (21 mg, 32%)*. **5** was used in cross-coupling reactions without further purification. Single crystals suitable for X-ray diffraction studies were obtained *via* slow diffusion of diethyl ether into a concentrated solution of $CH_2Cl_2$ (there are two molecules of $CH_2Cl_2$ per molecule of **5**, but the SQUEEZE method was used to render them due to disorder). **$^{1}$H NMR (400 MHz, $CD_2Cl_2$)**: δ 8.30-8.17 (m, 2H), 7.66-7.56 (m, 4H), 7.43-7.30 (m, 2H), 6.82-6.74 (m, 2H), 6.72-6.65 (m, 4H), 5.31 (d, 2H, $J$ = 7.0 Hz), 3.91 (s, 9H), 3.14 (s, 3H), 2.33-2.23 (m, 8H), 1.97-1.89 (m, 8H), 1.89-1.81 (m, 12H), 1.79-1.71 (m, 12H), 1.48-1.39 (m, 8H), 1.36-1.24 (m, 12H); **$^{13}$C NMR**: *Complex too insoluble for $^{13}$C NMR characterization*; **$^{31}$P NMR (162 MHz, $CD_2Cl_2$)**: δ 86.16 (br. s, 2P), 60.60 (s, 1P). *Note: This compound is reported[2] to have one singlet in $^{31}$P NMR (δ = 85.7 ppm), but no NMR spectra are provided. We observed a broad singlet in that range in addition to a sharper singlet singlet upfield (~2:1 ratio), suggesting fluctional behavior in solution.* Elemental Analysis found (calculated for $C_{52}H_{70}B_2F_8P_2Pd_2$): C, 56.97 (51.72); H, 6.70 (5.84). ESI-MS $m/z$ [Pd**L5**]$_2^{2+}$ calculated: 517.14, found: 517.14. Note: this compound was observed as a dimer species under electrospray ionization.

**[Pd-L6]$_2$[BF$_4$]$_2$ (6)**




Following the general procedure for synthesis of precatalysts, a solution of **L6** (RuPhos, 295 mg, 0.632 mmol, RuPhos) in $CH_2Cl_2$ (2 mL) was added to **[Pd$_2$MeCN$_6$][BF$_4$]$_2$** (200 mg, 0.316 mmol) in $CH_2Cl_2$ (2 mL), and the reaction mixture was stirred for 30 minutes at room temperature. Upon completion, the reaction mixture was passed through a pad of Celite and the solvent was removed *in vacuo* to yield an orange solid (415 mg, 99%). **6** was used in cross-coupling reactions without further purification. Single crystals suitable for X-ray diffraction studies were obtained *via* slow diffusion of pentane into a concentrated solution of 1,2-dichloroethane. **$^1$H NMR (400 MHz, CD$_2$Cl$_2$)**: δ 8.38-8.32 (m, 2H), 7.82-7.77 (m, 2H), 7.75-7.69 (m, 2H), 7.67-7.62 (m, 2H), 7.29 (d, 2H, *J* = 7.9 Hz), 5.24 (d, 2H, *J* = 7.0 Hz), 4.22-4.12 (m, 4H), 3.02-2.91 (m, 4H), 2.07-1.95 (m, 8H), 1.90-1.77 (m, 12H), 1.63-1.47 (m, 8H), 1.33-1.22 (m, 12H), 0.94 (d, 12H, *J* = 5.9 Hz), 0.69 (d, 12H, *J* = 5.9 Hz); **$^{13}$C NMR (100 MHz, CD$_2$Cl$_2$)**: δ 151.68, 144.72, 133.76, 132.73, 131.91, 129.69, 94.41, 86.89, 80.98, 73.91, 36.79, 30.33, 29.93, 26.56, 21.50, 20.69; **$^{31}$P{$^1$H} NMR (162 MHz, CD$_2$Cl$_2$)**: δ 61.69 (s, 2P). *Note: The $^{31}$P NMR data reported here are consistent with those reported for the analogous complex* ***[Pd-L6]$_2$[CF$_3$CO$_2$]$_2$***. [3] Elemental Analysis found (calculated for $C_{60}H_{86}B_2F_8P_2Pd_2$): C, 54.54 (54.61); H, 6.63 (6.57). ESI-MS *m/z* [Pd**L6**]$_2^{2+}$ calculated: 573.20, found: 573.20. Note: this compound was observed as a dimer species under electrospray ionization.

Table S1. X-ray photoelectron spectroscopy (XPS) binding energies for **Pd(0)**, **Pd(II)**, and **1**-**6**.

| Compound | Pd 3d$_{3/2}$ (eV) | Pd 3d$_{5/2}$ (eV) |
|---|---|---|
| **Pd(0)**[a] | 344.2 | 338.9 |
| **1** | 342.7 | 337.5 |
| **2** | 342.7 | 337.4 |
| **3** | 342.8 | 337.6 |
| **4** | 342.4 | 337.1 |
| **5** | 342.9 | 337.8 |
| **6** | 342.6 | 337.3 |
| **Pd(II)**[b] | 341.8 | 336.5 |

[a]The Pd(0) source is $Pd_2dba_3$. [b]The Pd(II) source is $[PdMeCN_4][BF_4]_2$.

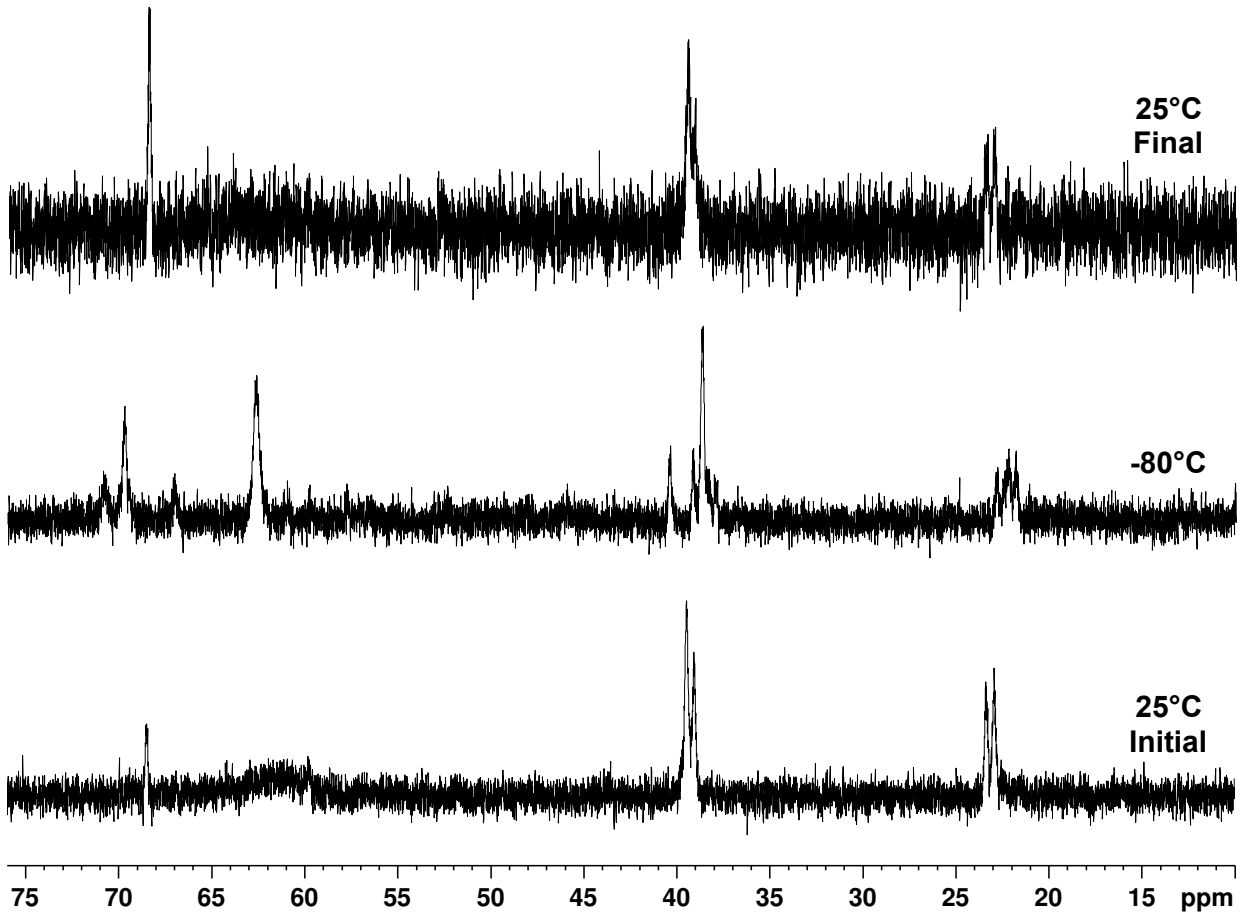



**Figure S1**. Variable temperature (VT) $^{31}$P NMR study on compound **4**. Cooling a solution of **4** in $CD_2Cl_2$ to -80°C shows the formation of new $^{31}$P resonances (middle spectrum), suggesting the limited fluctionality of the biaryl phosphine ligand at lower temperatures. Warming this sample to 25°C produces a $^{31}$P NMR spectrum that is comparable to the initial $^{31}$P NMR spectrum taken before cooling (top and bottom spectra, respectively).

## 4. Optimization of Amination Protocol

Amination of 4-bromotoluene with morpholine was optimized to identify a suitable Pd(I) dimer precatalyst (**1**-**6**), base, temperature, and reaction time to achieve optimal conversion to **7**. An oven-dried reaction tube was equipped with a magnetic stir bar and charged with Pd(I) dimer precatalyst (**1**-**6**, 0.5-1.0 mol%), ligand (**L1**-**L6**, 0.0-0.5 mol%), base (KO$^t$Bu or NaO$^t$Bu, 1.4 mmol), and 4-bromotoluene (1.0 mmol). The vial was sealed with a PTFE septum cap and the reaction tube was evacuated and backfilled with $N_2$ three times. Morpholine (1.4 mmol) and anhydrous 1,4-dioxane (1.0 mL) were added to the reaction tube *via* syringe. The rapidly stirring reaction mixture was heated at 80-100°C for 30-60 minutes in an oil bath. Upon completion, GC-MS samples were prepared by diluting an aliquot of the reaction mixture with ethyl acetate and filtered through a Celite plug. See Table S1 for detailed stoichiometry used in each cross-coupling reaction (below).

**Table S2**. Synthetic details for optimization studies of **7**.

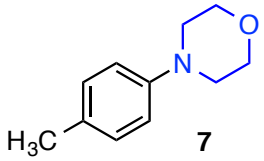
| Reaction Entry | Pd(I) Precat. | L (mol %) | 4-Br-toluene | Morpholine | Base | 1,4-dioxane | Time / Temp. |
|---|---|---|---|---|---|---|---|
| 1 | **1**, 0.5 mol%, 4.9 mg | **L1**, 0.5 mol%, 1.5 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 30 min / 100°C |
| 2 | **2**, 0.5 mol%, 5.9 mg | **L2**, 0.5 mol%, 2.0 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 30 min / 100°C |
| 3 | **3**, 0.5 mol%, 6.2 mg | **L3**, 0.5 mol%, 2.1 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 30 min / 100°C |
| 4 | **4**, 0.5 mol%, 6.7 mg | **L4**, 0.5 mol%, 2.4 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 30 min / 100°C |
| 5 | **5**, 0.5 mol%, 6.0 mg | **L5**, 0.5 mol%, 2.1 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 30 min / 100°C |
| 6 | **6**, 0.5 mol%, 6.6 mg | **L6**, 0.5 mol%, 2.3 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 30 min / 100°C |
| 7 | **6**, 1.0 mol%, 13.2 mg | **L6**, 0.5 mol%, 2.3 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 30 min / 100°C |
| 8 | **6**, 0.5 mol%, 6.6 mg | **L6**, 0.5 mol%, 2.3 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 60 min / 100°C |
| 9 | **6**, 0.5 mol%, 6.6 mg | **L6**, 0.5 mol%, 2.3 mg | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 60 min / 80°C |
| 10 | **6**, 0.5 mol%, 6.6 mg | – | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | KO$^t$Bu, 1.4 mmol, 157 mg | 1.0 mL | 60 min / 80°C |
| 11 | **6**, 0.5 mol%, 6.6 mg | – | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | NaO$^t$Bu, 1.4 mmol, 135 mg | 1.0 mL | 60 min / 80°C |
| 12 | **6**, 0.5 mol%, 6.6 mg | – | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | NaO$^t$Bu, 1.4 mmol, 135 mg | 1.0 mL | 60 min / 80°C |
| 13 | **6**, 0.5 mol%, 6.6 mg | – | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | NaO$^t$Bu, 1.4 mmol, 135 mg | 1.0 mL | 60 min / 80°C |
| 14 | **5**, 0.5 mol%, 6.0 mg | – | 1.0 mmol, 171 mg | 1.4 mmol, 122 μL | NaO$^t$Bu, 1.4 mmol, 135 mg | 1.0 mL | 60 min / 80°C |

## 5. General Amination Procedure

An oven-dried reaction tube was equipped with a magnetic stir bar and charged with Pd(I) dimer precatalyst (**4** or **6**, 0.5-1.0 mol%) and NaOtBu (336 mg, 3.5 mmol). Amine derivatives (3.5 mmol) and aryl halides (2.5 mmol) that are solid at room temperature were also added at this point. The vial was sealed with a PTFE septum cap and the reaction tube was evacuated and backfilled with $N_2$ three times. The amine derivative (if liquid, 3.5 mmol), aryl halide (if liquid, 2.5 mmol), and anhydrous 1,4-dioxane (2.5 mL) were added to the reaction tube *via* syringe. The rapidly stirring reaction mixture was heated at 80-100°C for 1-3 hours in an oil bath. Upon completion, each reaction was diluted with ethyl acetate (~4 mL) and passed through a Celite plug, then concentrated *in vacuo*. The crude product was purified *via* silica gel chromatography.

## 6. Experimental Details and Characterization Data

***N*-(4-tolyl)morpholine (7)**




**7**

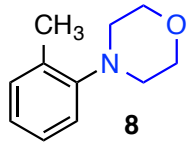
*From 4-bromotoluene*:
Following the general amination procedure, a mixture of morpholine (306 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 4-bromotoluene (428 mg, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a white solid (407 mg, 92%).

*From 4-chlorotoluene*:
Following the general amination procedure, a mixture of morpholine (306 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 4-chlorotoluene (296 μL, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a white solid (418 mg, 94%).

*From 4-iodotoluene*:
Following the general amination procedure, a mixture of morpholine (306 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 4-iodotoluene (545 mg, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a white solid (100 mg, 24%).

**$^1$H NMR (400 MHz, $CDCl_3$)**: δ 7.13 (d, 2H, $J$ = 8.8 Hz, Ar-H), 6.87 (d, 2H, $J$ = 8.6 Hz, Ar-H), 3.89 (t, 4H, $J$ = 4.8 Hz, $CH_2$), 3.13 (t, 4H, $J$ = 4.8 Hz, $CH_2$), 2.32 (s, 3H, $CH_3$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 149.27, 129.77, 129.56, 116.09, 67.02, 49.98, 20.49.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 178.1232, found: 178.1225
These data are consistent with those reported in literature.[4]

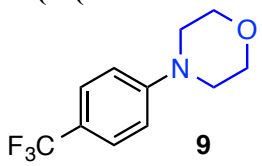
***N*-(2-tolyl)morpholine (8)**




**8**

Following the general amination procedure, a mixture of morpholine (306 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 2-bromotoluene (300 μL, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a clear-yellow oil (341 mg, 77%). **$^1$H NMR (400 MHz, $CDCl_3$)**: δ 7.28 (t, 2H, $J$ = 7.1 Hz, Ar-H), 7.13–7.09 (m, 2H, Ar-H), 3.93 (t, 2H, $J$ = 4.5 Hz, $CH_2$), 2.97 (t, 2H, $J$ = 4.5 Hz, $CH_2$), 2.43 (s, 3H, $CH_3$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 151.45, 132.65, 131.29, 126.82, 123.53, 119.08, 67.51, 52.42, 18.01.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 178.1232, found: 178.1225
These data are consistent with those reported in literature.[5]

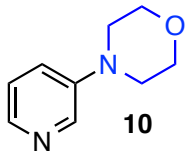
***N*-(4-(trifluoromethyl)phenyl)morpholine (9)**



**9**

Following the general amination procedure, a mixture of morpholine (306 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 4-bromobenzotrifluoride (350 μL, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a white solid (403 mg, 70%). **$^1$H NMR (400 MHz, $CDCl_3$)**: δ 7.50 (d, 2H, $J$ = 9.2 Hz, Ar-H), 6.92 (d, 2H, $J$ = 8.8 Hz, Ar-H), 3.86 (t, 4H, $J$ = 4.9 Hz, $CH_2$), 3.24 (t, 4H, $J$ = 4.9 Hz, $CH_2$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 153.38, 126.45 (q, $^3J_{C\text{-}F}$ = 3.75 Hz), 123.36 (q, $^1J_{C\text{-}F}$ = 270 Hz), 121.00 (q, $^2J_{C\text{-}F}$ = 32.5 Hz), 114.32, 66.65, 48.27; **$^{19}$F{$^1$H} NMR (376 MHz, $CDCl_3$)**: δ –61.4 (s, 3F, $CF_3$).
HRMS (DART) *m/z* $[M+H]^+$ calculated: 232.0949, found: 232.0956
These data are consistent with those reported in literature.[6]

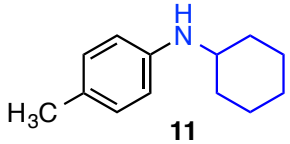
***N*-(3-pyridyl)morpholine (10)**



**10**

Following the general amination procedure, a mixture of morpholine (306 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 3-bromopyridine (240 μL, 2.5 mmol), **4** (16.7 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 100°C for 1 hour. The crude product was purified *via* silica gel chromatography (hexanes/acetone, 3:1) to provide the title compound as an orange solid (403 mg, 70%). **$^1$H NMR (400 MHz, $CDCl_3$)**: δ 8.26 (t, 1H, $J$ = 1.8 Hz, Ar-H), 8.08 (t, 1H, $J$ = 3.0 Hz, Ar-H), 7.15-7.12 (m, 2H, Ar-H), 3.83 (t, 4H, $J$ = 4.8 Hz, $CH_2$), 3.14 (t, 4H, $J$ = 4.8 Hz, $CH_2$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 146.91, 140.99, 138.20, 123.52, 122.11, 66.64, 48.56.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 165.1028, found: 165.1023
These data are consistent with those reported in literature.[1]

***N*-cyclohexyl-4-methylaniline (11)**

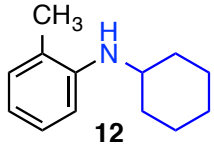


**11**

Following the general amination procedure, a mixture of cyclohexylamine (400 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 4-bromotoluene (428 mg, 2.5 mmol), **6** (33 mg, 1.0 mol%) and dioxane (2.5 mL) was heated to 100°C for 3 hours. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a white solid (404 mg, 86%). **$^1$H NMR (400 MHz, $CDCl_3$)**: δ 6.98 (d, 2H, $J$ = 8.4 Hz, Ar-H), 6.53 (d, 2H, $J$ = 8.4 Hz, Ar-H), 3.37 (br. s, 1H, NH), 3.23 (t, 1H, $J$ = 10 Hz, CH), 2.24 (s, 3H, $CH_3$), 2.06 (d, 2H, $J$ = 12.5 Hz, $CH_2$), 1.82-1.72 (m, 2H, $CH_2$), 1.70-1.62 (m, 1H, $CH_2$), 1.45-1.31 (m, 2H, $CH_2$), 1.29-1.20 (m, 1H,

$CH_2$), 1.20-1.09 (m, 2H, $CH_2$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 145.26, 129.86, 126.21, 113.60, 52.17, 33.69, 26.11, 25.18, 20.48.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 190.1596, found: 190.1591
These data are consistent with those reported in literature.[7]

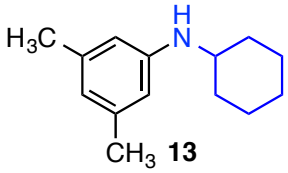
***N*-cyclohexyl-2-methylaniline (12)**



**12**

Following the general amination procedure, a mixture of cyclohexylamine (400 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 2-bromotoluene (300 μL, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a clear-yellow oil (445 mg, 94%). **$^1$H NMR (400 MHz, $CDCl_3$)**: δ 7.13 (t, 1H, $J$ = 7.9 Hz, Ar-H), 7.07 (d, 2H, $J$ = 7.2 Hz, Ar-H), 6.68-6.61 (m, 2H, Ar-H), 3.45-3.29 (m, 2H, NH and CH), 2.15 (s, 3H, $CH_3$), 2.12 (d, 2H, $J$ = 12.5 Hz, $CH_2$), 1.85-1.77 (m, 2H, $CH_2$), 1.74-1.66 (m, 1H, $CH_2$), 1.49-1.37 (m, 2H, $CH_2$), 1.34-1.18 (m, 3H, $CH_2$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 145.41, 130.37, 127.17, 121.71, 116.37, 110.29, 51.61, 33.76, 26.14, 25.16, 17.68.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 190.1596, found 190.1590
These data are consistent with those reported in literature.[6]

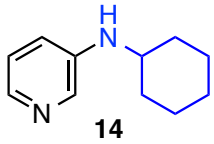
***N*-cyclohexyl-3,5-dimethylaniline (13)**



**13**

Following the general amination procedure, a mixture of cyclohexylamine (400 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 1-bromo-3,5-dimethylbenzene (340 μL, 2.5 mmol), **6** (33 mg, 1.0 mol%) and dioxane (2.5 mL) was heated to 100°C for 3 hours. The crude product was purified *via* silica gel chromatography (hexanes/$CH_2Cl_2$, 1:1) to provide the title compound as a white/tan solid (497 mg, 98%). **$^1$H NMR (400 MHz, $CDCl_3$)**: δ 6.36 (s, 1H, Ar-H), 6.26 (s, 2H, Ar-H), 3.44 (br. s, 1H, NH), 3.31-3.23 (m, 1H, CH), 2.26 (s, 6H, $CH_3$), 2.08 (d, 2H, $J$ = 12.5 Hz, $CH_2$), 1.83-1.75 (m, 2H, $CH_2$), 1.72-1.64 (m, 1H, $CH_2$), 1.47-1.35 (m, 2H, $CH_2$), 1.31-1.11 (m, 3H, $CH_2$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 147.60, 138.98, 118.97, 111.16, 51.70, 33.71, 26.10, 25.17, 21.63.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 204.1752, found: 204.1746
These data are consistent with those reported in literature.[8]

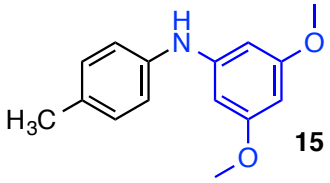
**3-(cyclohexylamino)pyridine (14)**



**14**

Following the general amination procedure, a mixture of cyclohexylamine (400 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 3-bromopyridine (240 μL, 2.5 mmol), **4** (33.4 mg, 1.0 mol%) and dioxane (2.5 mL) was heated to 100°C for 3 hours. The crude product was purified *via* silica gel chromatography (hexanes/acetone, 3:1) to provide the title compound as a clear-yellow oil (181 mg, 41%). **$^1$H NMR (400 MHz, CDCl$_3$)**: δ 7.99 (d, 1H, *J* = 2.2 Hz, Ar-H), 7.90 (d, 1H, *J* = 4.1 Hz, Ar-H), 7.04 (dd, 1H, *J* = 8.2, 4.6 Hz, Ar-H), 6.85-6.81 (m, 1H), 3.57 (br. s, 1H, NH), 3.28-3.15 (m, 1H, CH), 2.04 (d, 2H, *J* = 12.5 Hz, $CH_2$), 1.80-1.72 (m, 2H, $CH_2$), 1.69-1.61 (m, 1H, $CH_2$), 1.43-1.31 (m, 2H, $CH_2$), 1.28-1.11 (m, 3H, $CH_2$); **$^{13}$C NMR (100 MHz, CDCl$_3$)**: δ 143.46, 138.36, 136.55, 123.81, 118.81, 51.56, 33.35, 25.92, 24.99.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 177.1392, found: 177.1386
These data are consistent with those reported in literature.[9]

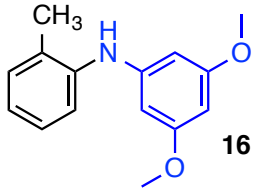
***N*-(4-tolyl)-3,5-dimethoxyaniline (15)**



**15**

Following the general amination procedure, a mixture of 3,5-dimethoxyaniline (536 mg, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 4-bromotoluene (428 mg, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a green oil (600 mg, 98%). **$^1$H NMR (400 MHz, CDCl$_3$)**: δ 7.11 (d, 2H, *J* = 8.3 Hz, Ar-H), 7.04 (d, 2H, *J* = 8.3 Hz, Ar-H), 6.19 (d, 2H, *J* = 2.2 Hz, Ar-H), 6.05 (t, 1H, *J* = 2.2 Hz, Ar-H), 5.64 (br. s, 1H, NH), 3.76 (s, 6H, O–$CH_3$), 2.32 (s, 3H, Ar-$CH_3$); **$^{13}$C NMR (100 MHz, CDCl$_3$)**: δ 161.76, 146.24, 139.88, 131.51, 129.96, 119.95, 95.08, 92.52, 55.35, 20.81.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 244.1338, found: 244.1331
These data are consistent with those reported in literature.[1]

***N*-(2-tolyl)-3,5-dimethoxyaniline (16)**

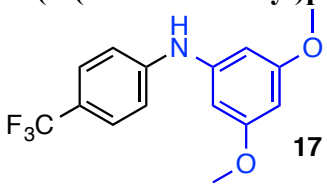


**16**

Following the general amination procedure, a mixture of 3,5-dimethoxyaniline (536 mg, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 2-bromotoluene (300 μL, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a clear oil (601 mg, 98%). **$^1$H NMR (400 MHz, CDCl$_3$)**: δ 7.29 (d, 1H, *J* = 7.9 Hz, Ar-H), 7.22 (d, 1H, *J* = 7.4 Hz, Ar-H),

7.17 (t, 1H, $J$ = 7.6 Hz, Ar-H), 6.98 (t, 1H, $J$ = 7.4 Hz, Ar-H), 6.12 (d, 2H, $J$ = 2.2 Hz, Ar-H), 6.06 (t, 1H, $J$ = 2.2 Hz, Ar-H), 5.39 (br. s, 1H, NH), 3.76 (s, 6H, O–$CH_3$), 2.27 (s, 3H, Ar-$CH_3$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 161.78, 146.46, 140.74, 131.07, 129.52, 126.89, 122.81, 120.69, 95.44, 92.54, 55.36, 18.00.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 244.1338, found: 244.1331
These data are consistent with those reported in literature.[10]

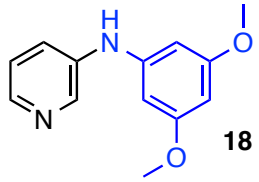
***N*-(4-(trifluoromethyl)phenyl)-3,5-dimethoxyaniline (17)**



**17**

Following the general amination procedure, a mixture of 3,5-dimethoxyaniline (536 mg, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 4-bromobenzotrifluoride (350 μL, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography ($CH_2Cl_2$) to provide the title compound as a clear oil (312 mg, 42%). **$^1$H NMR (400 MHz, $CDCl_3$)**: δ 7.48 (d, 2H, $J$ = 8.5 Hz, Ar-H), 7.08 (d, 2H, $J$ = 8.4 Hz, Ar-H), 6.30 (d, 2H, $J$ = 2.2 Hz, Ar-H), 6.18 (t, 1H, $J$ = 2.2 Hz, Ar-H), 5.91 (br. s, 1H, NH), 3.78 (s, 6H, O–$CH_3$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 161.85, 146.42, 143.32, 126.82 (q, $^3J_{C\text{-}F}$ = 3.75 Hz), 123.35 (q, $^1J_{C\text{-}F}$ = 270 Hz), 122.20 (q, $^2J_{C\text{-}F}$ = 32.5 Hz), 116.34, 98.05, 94.86, 55.50; **$^{19}$F{$^1$H} NMR (376 MHz, $CDCl_3$)**: δ –61.5 (s, 3F, $CF_3$).
HRMS (DART) *m/z* $[M+H]^+$ calculated: 298.1055, found: 298.1045

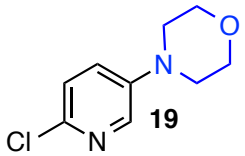
***N*-(3-pyridyl)-3,5-dimethoxyaniline (18)**



**18**

Following the general amination procedure, a mixture of 3,5-dimethoxyaniline (536 mg, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 3-bromopyridine (240 μL, 2.5 mmol), **4** (16.7 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 100°C for 1.5 hours. The crude product was purified *via* silica gel chromatography (hexanes/acetone, 3:1) to provide the title compound as a brown solid (230 mg, 40%). **$^1$H NMR (400 MHz, $CDCl_3$)**: δ 8.38 (d, 1H, $J$ = 2.6 Hz, Ar-H), 8.17 (dd, 1H, $J$ = 4.7 Hz, 1.4 Hz, Ar-H), 7.47-7.43 (m, 1H, Ar-H), 7.17 (dd, 1H, J = 8.4 Hz, 4.6 Hz, Ar-H), 6.22 (d, 2H, $J$ = 2.2 Hz, Ar-H), 6.11 (t, 1H, $J$ = 2.2 Hz, Ar-H), 5.99 (br. s, 1H, NH), 3.75 (s, 6H, O–$CH_3$); **$^{13}$C NMR (100 MHz, $CDCl_3$)**: δ 161.86, 144.28, 142.38, 140.97, 139.53, 124.65, 123.82, 96.42, 93.93, 55.43.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 231.1134, found: 231.1126

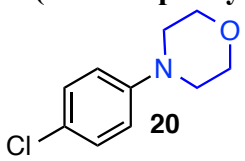
***N*-(3-(2-chloro)pyridyl)morpholine (19)**



**19**

Following the general amination procedure, a mixture of morpholine (306 μL, 3.5 mmol), NaO$^t$Bu (336 mg, 3.5 mmol), 5-bromo-2-chloropyridine (340 μL, 2.5 mmol), **4** (16.7 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 100°C for 1 hour. The crude product was purified *via* silica gel chromatography (hexanes/acetone, 3:1) to provide the title compound as a white solid (361 mg, 73%). **$^1$H NMR (400 MHz, CDCl$_3$)**: δ 7.97 (dd, 1H, $J$ = 2.7, 0.9 Hz, Ar-H), 7.17-7.11 (m, 2H, Ar-H), 3.83 (t, 4H, $J$ = 4.8 Hz, $CH_2$), 3.12 (t, 4H, $J$ = 4.8 Hz, $CH_2$); **$^{13}$C NMR (100 MHz, CDCl$_3$)**: δ 146.13, 141.59, 137.13, 125.44, 124.00, 66.54, 48.57.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 199.0638, found: 199.0631
These data are consistent with those reported in literature.[11]

***N*-(4-chlorophenyl)morpholine (20)**



**20**

Following the general amination procedure, a mixture of morpholine (260 μL, 3.0 mmol), NaO$^t$Bu (288 mg, 3.0 mmol), 1-bromo-4-chlorobenzene (479 mg, 2.5 mmol), **6** (16.5 mg, 0.5 mol%) and dioxane (2.5 mL) was heated to 80°C for 1 hour. The crude product was purified *via* silica gel chromatography (hexanes/acetone, 3:1) to provide the title compound as a white solid (454 mg, 92%). **$^1$H NMR (400 MHz, CDCl$_3$)**: δ 7.22 (d, 2H, $J$ = 9.0 Hz, Ar-H), 6.82 (d, 2H, $J$ = 9.0 Hz, Ar-H), 3.85 (t, 4H, $J$ = 4.8 Hz, $CH_2$), 3.11 (t, 4H, $J$ = 4.8 Hz, $CH_2$); **$^{13}$C NMR (100 MHz, CDCl$_3$)**: δ 150.02, 129.13, 124.97, 117.00, 66.88, 49.42.
HRMS (DART) *m/z* $[M+H]^+$ calculated: 198.0686, found: 198.0666
These data are consistent with those reported in literature.[12]

## 7. X-ray Data Collection and Processing Parameters

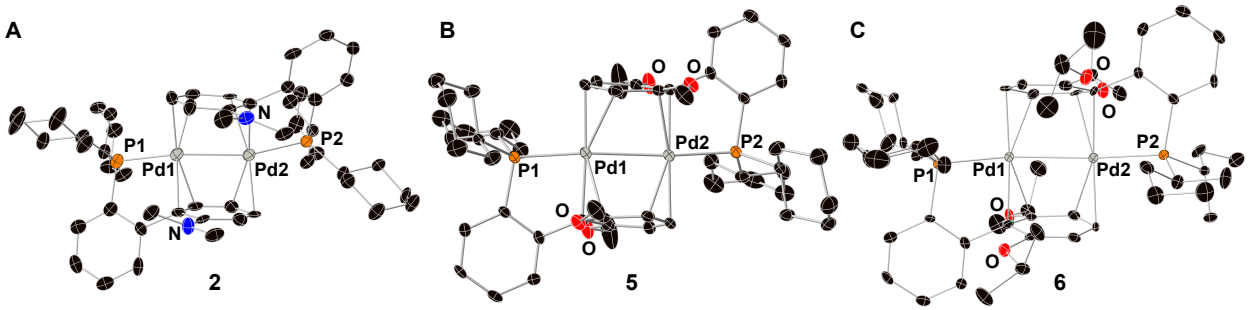



**Figure S2**. Single crystal X-Ray structures for **2** (CCDC 1812501), **5** (CCDC 1812502), and **6** (CCDC 1812500). H atoms, solvent molecules, and $BF_4^-$ counterions are omitted for clarity.

Table S3. Selected Pd–P and Pd–Pd bond distances for **2**, **5**, and **6**.

| Compound | P1–Pd1 (Å) | Pd1–Pd2 (Å) | Pd2–P2 (Å) |
|---|---|---|---|
| **2** | 2.308(2) | 2.702(1) | 2.315(2) |
| **5** | 2.3084(8) | 2.7155(4) | 2.3084(8) |
| **6** | 2.314(2) | 2.7184(9) | 2.306(2) |

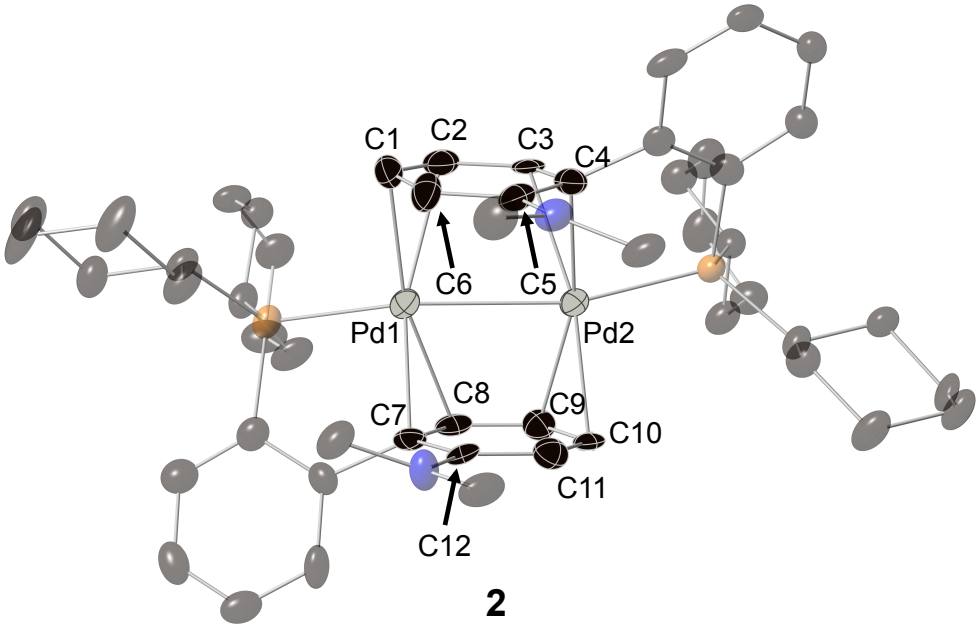



**Figure S3**. Single crystal X-ray structure of **2** highlighting the benzene rings coordinated to Pd. See Table S4 for selected C–C and C–Pd bond distances. H atoms, solvent molecules, and $BF_4^-$ counterions are omitted for clarity.

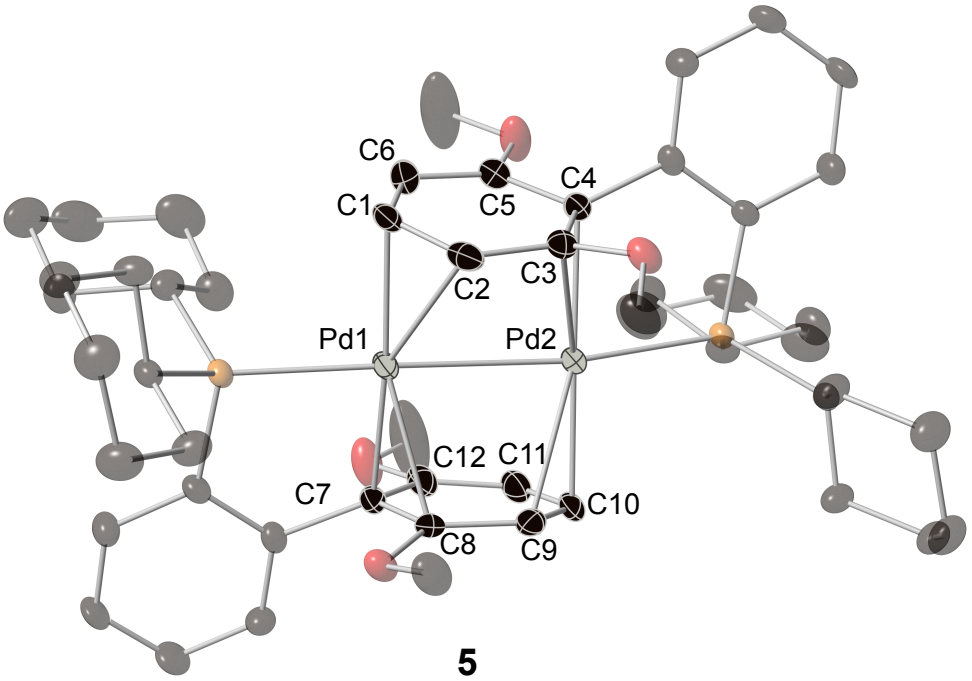



**Figure S4**. Single crystal X-ray structure of **5** highlighting the benzene rings coordinated to Pd. See Table S4 for selected C–C and C–Pd bond distances. H atoms, solvent molecules, and $BF_4^-$ counterions are omitted for clarity.

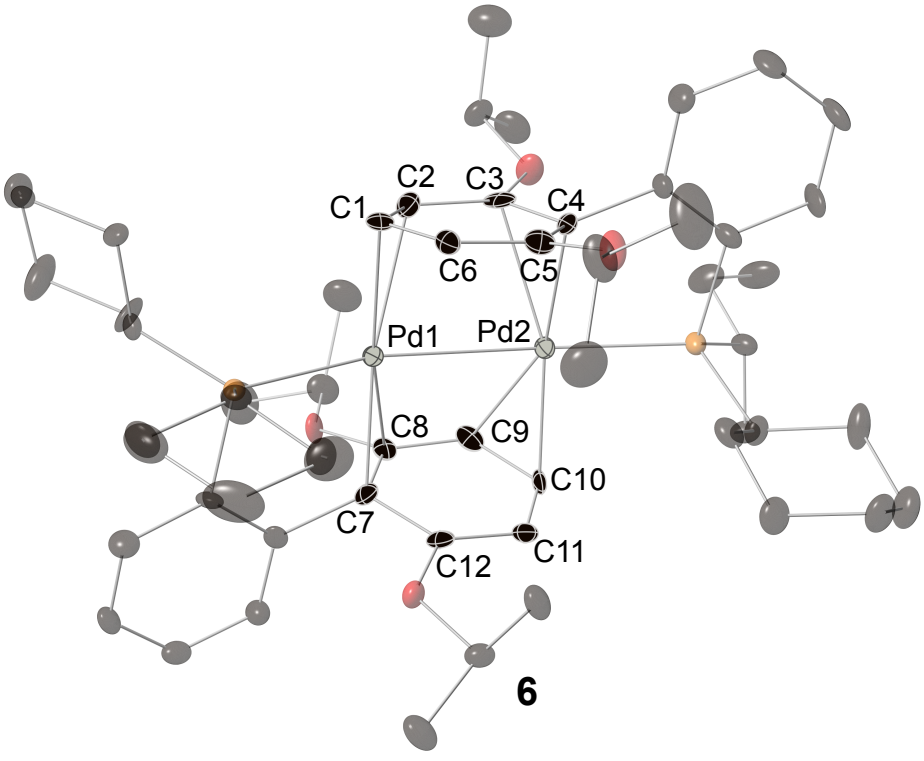



**Figure S5**. Single crystal X-ray structure of **6** highlighting the benzene rings coordinated to Pd. See Table S4 for selected C–C and C–Pd bond distances. H atoms, solvent molecules, and $BF_4^-$ counterions are omitted for clarity.

Table S4. Selected bond distances for benzene rings coordinated to Pd in complexes **2**, **5**, and **6**.

| | Bond Distance (Å) | | |
|---|---|---|---|
| Selected bond | **2** | **5** | **6** |
| C1–C2 | 1.410(1) | 1.408(5) | 1.402(1) |
| C2–C3 | 1.403(1) | 1.416(4) | 1.418(1) |
| C3–C4 | 1.434(1) | 1.437(4) | 1.435(1) |
| C4–C5 | 1.457(1) | 1.455(5) | 1.437(1) |
| C5–C6 | 1.399(1) | 1.377(5) | 1.373(1) |
| C6–C1 | 1.410(1) | 1.407(4) | 1.437(1) |
| C7–C8 | 1.434(1) | 1.437(4) | 1.425(1) |
| C8–C9 | 1.392(1) | 1.416(5) | 1.408(1) |
| C9–C10 | 1.391(1) | 1.409(5) | 1.420(1) |
| C10–C11 | 1.441(1) | 1.407(4) | 1.423(1) |
| C11–C12 | 1.373(1) | 1.377(5) | 1.365(1) |
| C12–C7 | 1.487(1) | 1.455(5) | 1.453(1) |
| Pd1–C1 | 2.235(9) | 2.196(3) | 2.224(8) |
| Pd1–C2 | 2.360(8) | 2.414(3) | 2.344(9) |
| Pd2–C3 | 2.305(7) | 2.317(3) | 2.340(9) |
| Pd2–C4 | 2.167(8) | 2.192(3) | 2.200(9) |
| Pd1–C7 | 2.163(7) | 2.192(3) | 2.182(9) |
| Pd1–C8 | 2.346(8) | 2.317(3) | 2.380(9) |
| Pd2–C9 | 2.340(8) | 2.414(3) | 2.355(8) |
| Pd2–C10 | 2.225(8) | 2.196(3) | 2.220(8) |

The single crystal X-ray structures for **2**, **5**, and **6** all exhibit distorted bond distances for the benzene rings coordinated to Pd (Figures S3-S5 and Table S4). The shortest C–C bond distances range from 1.365(1) to 1.399(1) Å, and the longest C–C bond distances range from 1.453(1) to 1.487(1) Å. For all three structures, the Pd–C bond distances range from 2.163(7) to 2.414(3) Å.

Table S5. Crystal data and structure refinement for **2**, **5** and **6**.

| Compound | **2** | **5** | **6** |
|---|---|---|---|
| Empirical formula | C52 H72 B2 F8 N2 P2 Pd2 | C52 H70 B2 F8 O4 P2 Pd2 | C66 H98 B2 Cl6 F8 O4 P2 Pd2 (3 DCE) |
| Formula weight | 1173.47 | 1207.44 | 1616.5 |
| Temperature | 100.0 K | 180 K | 100.0 K |
| Wavelength | 1.54178 Å | 0.71073 Å | 0.71073 Å |
| Crystal system | Monoclinic | Monoclinic | Orthorhombic |
| Space group | P 21/n | C 2/c | $Pna2_1$ |
| Unit cell dimensions | a = 9.2989(4) Å (α= 90°) | a = 19.9242(6) Å (α= 90°) | a = 21.0268(14) Å (α= 90°) |
| | b = 42.0772(15) Å (β= 96.141(3)°) | b = 15.4346(4) Å (β= 106.142(2)°) | b = 16.0162(9) Å (β = 90°) |
| | c = 14.9666(7) Å (γ = 90°) | c = 19.9878(7) Å (γ = 90°) | c = 21.3417(12) Å (γ= 90°) |
| Volume | 5822.4(4) $Å^3$ | 5904.4(3) $Å^3$ | 7187.2(7) $Å^3$ |
| Z | 4 | 4 | 4 |
| Density (calculated) | 1.339 $Mg/m^3$ | 1.358 $Mg/m^3$ | 1.494 $Mg/m^3$ |
| Absorption coefficient | 5.997 $mm^{-1}$ | 0.727 $mm^{-1}$ | 0.834 $mm^{-1}$ |
| F(000) | 2408 | 2472 | 3328 |
| Crystal size | 0.18 x 0.07 x 0.03 $mm^3$ | 0.26 x 0.12 x 0.08 $mm^3$ | 0.28 x 0.16 x 0.12 $mm^3$ |
| Theta range for data collection | 2.100 to 59.033°. | 1.695 to 28.329°. | 1.590 to 26.376°. |
| Index ranges | -8<=h<=10, -46<=k<=45, -16<=l<=16 | -26<=h<=26, -19<=k<=20, -26<=l<=26 | -22<=h<=26, -20<=k<=11, -26<=l<=25 |
| Reflections collected | 24734 | 22573 | 32553 |
| Independent reflections | 8381 [R(int) = 0.1125] | 7260 [R(int) = 0.0398] | 13353 [R(int) = 0.0873] |
| Completeness to theta | 99.9% (theta = 59.034°) | 99.5% (theta = 25.242°) | 100% (theta = 25.242°) |
| Absorption correction | Semi-empirical from equivalents | Semi-empirical from equivalents | Semi-empirical from equivalents |
| Max. and min. transmission | 0.5152 and 0.3329 | 0.7457 and 0.6869 | 0.2602 and 0.2101 |
| Refinement method | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 8381 / 0 / 617 | 7260 / 0 / 318 | 13353 / 1 / 833 |
| Goodness-of-fit on $F^2$ | 1.026 | 1.073 | 1.039 |
| Final R indices [I>2sigma(I)] | R1 = 0.0587, wR2 = 0.1283 | R1 = 0.0418, wR2 = 0.0949 | R1 = 0.0573, wR2 = 0.1259 |
| R indices (all data) | R1 = 0.0926, wR2 = 0.1419 | R1 = 0.0559, wR2 = 0.1005 | R1 = 0.0697, wR2 = 0.1350 |
| Absolute structure parameter | n/a | n/a | 0.29(4) |
| Extinction coefficient | n/a | n/a | n/a |
| Largest diff. peak and hole | 0.877 and -1.113 $e.Å^{-3}$ | 0.827 and -0.996 $e.Å^{-3}$ | 0.720 and -0.679 $e.Å^{-3}$ |
| SQUEEZE | Found: 383e/uc. Calc. for 8 DCE, 400e/uc | 378e/uc; probably eight DCM | n/a |

Table S6. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for **2**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Pd(2) | 4699(1) | 6000(1) | 2766(1) | 23(1) |
| Pd(1) | 3361(1) | 6516(1) | 3365(1) | 23(1) |
| P(2) | 5775(2) | 5511(1) | 2633(1) | 24(1) |
| P(1) | 2891(2) | 6988(1) | 4074(1) | 23(1) |
| F(5) | 8529(5) | 6684(1) | 1375(4) | 52(1) |
| F(8) | 6795(6) | 6894(1) | 359(5) | 70(2) |
| F(7) | 9018(6) | 6768(1) | -47(4) | 62(2) |
| N(1) | 3347(7) | 6788(2) | 1022(4) | 30(2) |
| F(6) | 8710(7) | 7197(2) | 885(5) | 74(2) |
| N(2) | 1278(7) | 5867(2) | 1346(4) | 29(2) |
| C(34) | 4415(7) | 7159(2) | 2685(5) | 21(2) |

| | | | | |
|---|---|---|---|---|
| C(10) | 4633(8) | 6805(2) | 2545(5) | 25(2) |
| C(6) | 2692(7) | 5742(2) | 2795(5) | 23(2) |
| C(33) | 5061(7) | 7370(2) | 2106(5) | 29(2) |
| C(5) | 3002(8) | 5833(2) | 3719(5) | 29(2) |
| C(28) | 5365(8) | 7004(2) | 5362(5) | 34(2) |
| C(40) | 4220(8) | 5245(2) | 2558(5) | 27(2) |
| C(11) | 5703(7) | 6657(2) | 3170(5) | 25(2) |
| C(38) | 3047(9) | 4732(2) | 2413(5) | 31(2) |
| C(7) | 176(8) | 6060(2) | 824(6) | 36(2) |
| C(1) | 1628(8) | 5940(2) | 2228(6) | 28(2) |
| F(3) | 9867(9) | 6219(2) | 5405(6) | 105(3) |
| C(36) | 1623(8) | 5203(2) | 2520(5) | 28(2) |
| C(12) | 6515(8) | 6394(2) | 2941(6) | 35(2) |
| C(4) | 2344(8) | 6092(2) | 4089(5) | 29(2) |
| C(3) | 1308(8) | 6267(2) | 3561(6) | 29(2) |
| C(22) | 733(8) | 7400(2) | 4694(6) | 29(2) |
| C(17) | 983(8) | 7109(2) | 4112(5) | 26(2) |
| C(31) | 4419(8) | 7810(2) | 2993(5) | 28(2) |
| C(52) | 8334(8) | 5587(2) | 3773(5) | 29(2) |
| C(32) | 5016(7) | 7692(2) | 2258(6) | 29(2) |
| C(9) | 4365(8) | 6662(2) | 1656(5) | 29(2) |
| C(35) | 2884(8) | 5390(2) | 2606(5) | 24(2) |
| C(18) | 185(8) | 7146(2) | 3160(5) | 29(2) |
| C(24) | 3055(8) | 6817(2) | 5892(5) | 32(2) |
| C(39) | 4305(9) | 4916(2) | 2478(5) | 33(2) |
| C(8) | 2219(8) | 5694(2) | 808(5) | 33(2) |
| C(23) | 3731(8) | 7042(2) | 5237(5) | 26(2) |
| C(37) | 1731(8) | 4878(2) | 2413(5) | 31(2) |
| C(15) | 2135(8) | 6980(2) | 1227(5) | 34(2) |
| C(29) | 3776(8) | 7278(2) | 3407(5) | 26(2) |
| C(13) | 6305(9) | 6272(2) | 2059(6) | 34(2) |
| C(47) | 7020(8) | 5372(2) | 3599(5) | 26(2) |
| C(21) | -894(8) | 7457(2) | 4722(6) | 33(2) |
| C(48) | 6250(8) | 5344(2) | 4462(5) | 37(2) |
| C(41) | 6819(8) | 5440(2) | 1656(5) | 29(2) |
| C(46) | 7568(9) | 5112(2) | 1628(6) | 36(2) |

| | | | | |
|---|---|---|---|---|
| C(19) | -1422(8) | 7213(2) | 3203(5) | 34(2) |
| C(51) | 9395(8) | 5454(2) | 4522(5) | 32(2) |
| C(30) | 3811(8) | 7603(2) | 3572(5) | 28(2) |
| C(50) | 8698(9) | 5412(2) | 5385(5) | 38(2) |
| C(16) | 3254(10) | 6672(2) | 90(5) | 41(2) |
| F(2) | 8454(9) | 6583(2) | 4892(7) | 130(4) |
| C(2) | 1002(8) | 6193(2) | 2620(5) | 29(2) |
| C(42) | 5904(9) | 5502(2) | 770(5) | 37(2) |
| C(20) | -1670(8) | 7497(2) | 3794(6) | 36(2) |
| C(45) | 8493(9) | 5102(2) | 852(5) | 39(2) |
| C(26) | 5276(10) | 6874(2) | 6986(6) | 45(2) |
| C(25) | 3616(9) | 6896(2) | 6859(6) | 37(2) |
| C(27) | 5945(9) | 7087(2) | 6316(6) | 45(2) |
| C(14) | 5201(9) | 6402(2) | 1448(6) | 34(2) |
| C(49) | 7337(9) | 5204(2) | 5216(6) | 43(2) |
| F(1) | 7685(10) | 6252(2) | 5863(8) | 146(4) |
| F(4) | 9325(12) | 6608(3) | 6260(8) | 169(5) |
| B(1) | 8863(11) | 6432(3) | 5536(8) | 43(3) |
| C(43) | 6827(10) | 5481(3) | -16(5) | 48(3) |
| C(44) | 7591(10) | 5158(3) | -36(6) | 51(3) |
| B(2) | 8205(13) | 6877(3) | 662(9) | 55(3) |

Table S7. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for **5**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Pd(1) | 4451(1) | 5824(1) | 7779(1) | 16(1) |
| P(1) | 3473(1) | 6068(1) | 8156(1) | 17(1) |
| O(2) | 3578(1) | 4557(1) | 6803(1) | 23(1) |
| F(4) | 5189(1) | 7679(2) | 10256(2) | 56(1) |
| F(3) | 5038(2) | 6231(2) | 10334(2) | 55(1) |
| O(1) | 3775(1) | 7549(2) | 6514(2) | 34(1) |
| F(2) | 4221(1) | 7142(2) | 10498(2) | 57(1) |
| F(1) | 5266(1) | 7056(2) | 11306(1) | 56(1) |

| | | | | |
|---|---|---|---|---|
| C(26) | 2776(2) | 6170(2) | 7355(2) | 18(1) |
| C(25) | 2066(2) | 6239(2) | 7324(2) | 25(1) |
| C(13) | 3730(2) | 6067(2) | 6748(2) | 18(1) |
| C(14) | 3987(2) | 5208(2) | 6691(2) | 18(1) |
| C(6) | 3547(2) | 5154(2) | 9414(2) | 23(1) |
| C(21) | 2974(2) | 6190(2) | 6742(2) | 18(1) |
| C(22) | 2474(2) | 6311(2) | 6110(2) | 22(1) |
| C(1) | 3149(2) | 5233(2) | 8641(2) | 18(1) |
| C(18) | 4059(2) | 6770(2) | 6471(2) | 23(1) |
| C(5) | 3175(2) | 4498(2) | 9757(2) | 27(1) |
| C(15) | 4578(2) | 5075(2) | 6442(2) | 22(1) |
| C(23) | 1777(2) | 6394(2) | 6085(2) | 26(1) |
| C(7) | 3517(2) | 7096(2) | 8639(2) | 22(1) |
| C(24) | 1573(2) | 6362(2) | 6692(2) | 26(1) |
| C(12) | 3705(2) | 7844(2) | 8220(2) | 30(1) |
| C(16) | 4856(2) | 5775(2) | 6154(2) | 25(1) |
| C(17) | 4593(2) | 6618(2) | 6172(2) | 26(1) |
| C(20) | 3879(2) | 3697(2) | 6915(2) | 33(1) |
| C(2) | 3118(2) | 4357(2) | 8278(2) | 26(1) |
| C(4) | 3106(2) | 3617(2) | 9402(2) | 32(1) |
| C(3) | 2753(2) | 3694(2) | 8623(2) | 32(1) |
| C(9) | 2951(2) | 8166(3) | 9263(2) | 40(1) |
| C(8) | 2847(2) | 7320(2) | 8845(2) | 31(1) |
| C(11) | 3820(2) | 8676(3) | 8645(3) | 44(1) |
| C(10) | 3168(2) | 8908(3) | 8871(3) | 46(1) |
| B(1) | 4928(2) | 7035(3) | 10599(2) | 32(1) |
| C(19) | 4094(3) | 8278(3) | 6279(4) | 79(2) |

Table S8. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for **6**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Pd(1) | 7255(1) | 2039(1) | 5470(1) | 10(1) |
| Pd(2) | 6407(1) | 2019(1) | 4509(1) | 11(1) |

| | | | | |
|---|---|---|---|---|
| P(1) | 7885(1) | 1751(2) | 6333(1) | 13(1) |
| P(2) | 5769(1) | 1705(1) | 3662(1) | 13(1) |
| Cl(2) | 4765(1) | 7824(2) | 5976(2) | 50(1) |
| Cl(5) | 6061(2) | 6955(2) | 3614(2) | 55(1) |
| Cl(3) | 3788(2) | 7344(2) | 4560(2) | 51(1) |
| Cl(1) | 6191(2) | 7005(2) | 6272(2) | 55(1) |
| Cl(4) | 2294(2) | 8196(2) | 4768(2) | 59(1) |
| Cl(6) | 4803(2) | 6306(2) | 2783(2) | 68(1) |
| F(7) | 4356(3) | 5182(4) | 4724(3) | 45(2) |
| F(8) | 4469(3) | 3845(4) | 5050(3) | 41(2) |
| O(3) | 6523(3) | 3334(4) | 6182(3) | 17(1) |
| F(5) | 4891(3) | 4884(4) | 5619(3) | 51(2) |
| O(1) | 6272(3) | 459(4) | 6276(3) | 17(1) |
| F(4) | 4096(4) | 1318(4) | 4998(3) | 49(2) |
| F(1) | 4425(3) | -12(4) | 5149(3) | 40(2) |
| O(4) | 7086(3) | 3259(4) | 3774(3) | 21(1) |
| F(6) | 5318(3) | 4537(4) | 4678(3) | 40(2) |
| O(2) | 7428(3) | 395(4) | 3746(3) | 22(2) |
| C(28) | 7051(5) | 1837(5) | 8073(4) | 19(2) |
| C(60) | 4524(4) | 2406(5) | 3762(4) | 16(2) |
| C(29) | 7499(5) | 1738(6) | 7615(4) | 21(2) |
| F(2) | 3417(3) | 374(5) | 5387(4) | 73(3) |
| C(48) | 6324(4) | 1657(6) | 3014(4) | 17(2) |
| F(3) | 3715(4) | 276(5) | 4384(4) | 72(3) |
| C(12) | 6142(4) | 1141(5) | 5921(4) | 14(2) |
| C(6) | 7752(4) | 2669(6) | 4609(4) | 16(2) |
| C(2) | 7962(4) | 1164(5) | 4559(4) | 13(2) |
| C(43) | 6959(4) | 1727(6) | 3161(4) | 17(2) |
| C(32) | 7797(5) | 50(5) | 6094(4) | 22(2) |
| C(49) | 5389(4) | 674(5) | 3738(4) | 16(2) |
| C(11) | 5710(4) | 1174(5) | 5444(4) | 15(2) |
| C(22) | 6219(5) | -793(6) | 5621(4) | 24(2) |
| C(44) | 7420(5) | 1706(6) | 2691(4) | 22(2) |
| C(59) | 4015(4) | 2889(6) | 3397(4) | 20(2) |
| C(5) | 7334(4) | 2605(6) | 4090(4) | 17(2) |
| C(33) | 8131(5) | -791(6) | 6020(5) | 33(3) |

| | | | | |
|---|---|---|---|---|
| C(9) | 5893(4) | 2694(5) | 5348(4) | 16(2) |
| C(27) | 6422(4) | 1969(5) | 7903(4) | 19(2) |
| C(23) | 5929(4) | -313(5) | 6170(4) | 18(2) |
| C(8) | 6308(4) | 2660(6) | 5865(4) | 13(2) |
| C(19) | 6361(5) | 4177(6) | 5984(4) | 22(2) |
| C(38) | 9119(4) | 2486(7) | 6273(4) | 24(2) |
| C(54) | 5878(4) | -1(5) | 3911(4) | 20(2) |
| C(45) | 7235(5) | 1584(7) | 2073(4) | 26(2) |
| C(51) | 4679(5) | -454(7) | 3293(5) | 31(2) |
| C(16) | 7383(4) | 4078(6) | 3789(5) | 21(2) |
| C(14) | 7469(6) | -838(7) | 4382(6) | 39(3) |
| C(7) | 6478(4) | 1879(6) | 6138(5) | 16(2) |
| C(26) | 6240(5) | 1981(5) | 7285(4) | 19(2) |
| C(30) | 7324(4) | 1755(6) | 6973(4) | 16(2) |
| C(52) | 5160(5) | -1108(6) | 3483(5) | 27(2) |
| C(50) | 5001(5) | 403(6) | 3168(5) | 27(2) |
| C(31) | 8273(4) | 720(5) | 6294(4) | 18(2) |
| C(4) | 7186(4) | 1796(7) | 3841(4) | 15(2) |
| C(21) | 6777(5) | 4416(6) | 5425(5) | 34(2) |
| C(1) | 8086(4) | 1970(5) | 4828(4) | 14(2) |
| C(3) | 7532(4) | 1090(5) | 4078(4) | 16(2) |
| B(2) | 4755(5) | 4624(7) | 5020(5) | 21(2) |
| C(63) | 5005(6) | 6799(7) | 5792(6) | 43(3) |
| C(17) | 6848(5) | 4694(6) | 3644(5) | 28(2) |
| C(58) | 4231(5) | 3769(6) | 3262(5) | 27(2) |
| C(53) | 5546(5) | -824(6) | 4039(4) | 24(2) |
| C(55) | 5139(4) | 2402(5) | 3369(4) | 15(2) |
| C(20) | 6499(6) | 4712(6) | 6550(5) | 39(3) |
| C(10) | 5579(4) | 1954(5) | 5152(4) | 16(2) |
| C(47) | 6140(5) | 1553(6) | 2387(4) | 25(2) |
| C(62) | 3584(8) | 8386(8) | 4809(7) | 69(5) |
| C(61) | 2999(9) | 8412(9) | 5205(6) | 71(5) |
| C(13) | 7792(5) | -353(6) | 3863(5) | 26(2) |
| C(18) | 7909(5) | 4092(7) | 3309(5) | 36(3) |
| C(57) | 4846(5) | 3790(7) | 2904(5) | 32(2) |
| C(39) | 9587(5) | 3061(7) | 6609(4) | 30(3) |

| | | | | |
|---|---|---|---|---|
| C(40) | 9340(5) | 3933(7) | 6662(5) | 38(3) |
| C(56) | 5372(4) | 3283(6) | 3256(5) | 24(2) |
| C(25) | 6690(4) | 1864(5) | 6817(4) | 13(2) |
| C(37) | 8486(4) | 2485(6) | 6612(4) | 20(2) |
| C(41) | 8684(5) | 3978(8) | 6968(6) | 42(3) |
| C(42) | 8223(5) | 3379(6) | 6636(5) | 28(2) |
| C(34) | 8460(6) | -1058(7) | 6634(6) | 41(3) |
| B(1) | 3910(6) | 492(9) | 4991(6) | 36(3) |
| C(15) | 7806(6) | -806(8) | 3250(6) | 51(4) |
| C(24) | 6002(5) | -791(6) | 6783(4) | 29(2) |
| C(46) | 6598(5) | 1518(7) | 1913(4) | 27(2) |
| C(36) | 8591(5) | 462(6) | 6919(4) | 26(2) |
| C(64) | 5676(6) | 6705(8) | 5644(7) | 56(4) |
| C(35) | 8915(5) | -395(7) | 6848(5) | 37(3) |
| C(65) | 5449(17) | 6390(20) | 3953(17) | 55(1) |
| C(66) | 5229(14) | 5824(17) | 3484(12) | 35(8) |
| C(66') | 4830(30) | 6140(20) | 3521(17) | 90(20) |
| C(65') | 5526(15) | 6040(30) | 3753(16) | 48(12) |

## 8. References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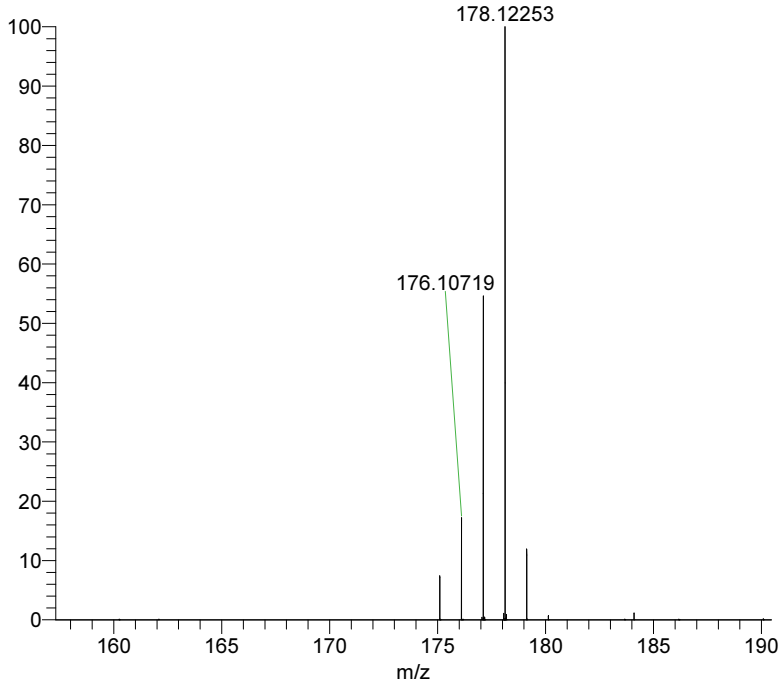
## 9. NMR Spectra and MS Data

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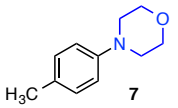


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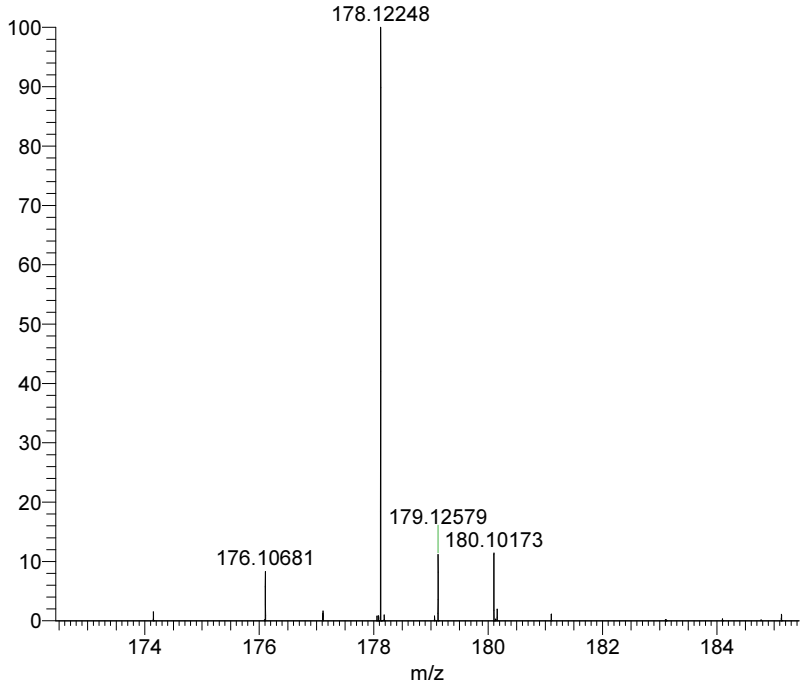


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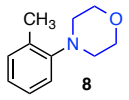


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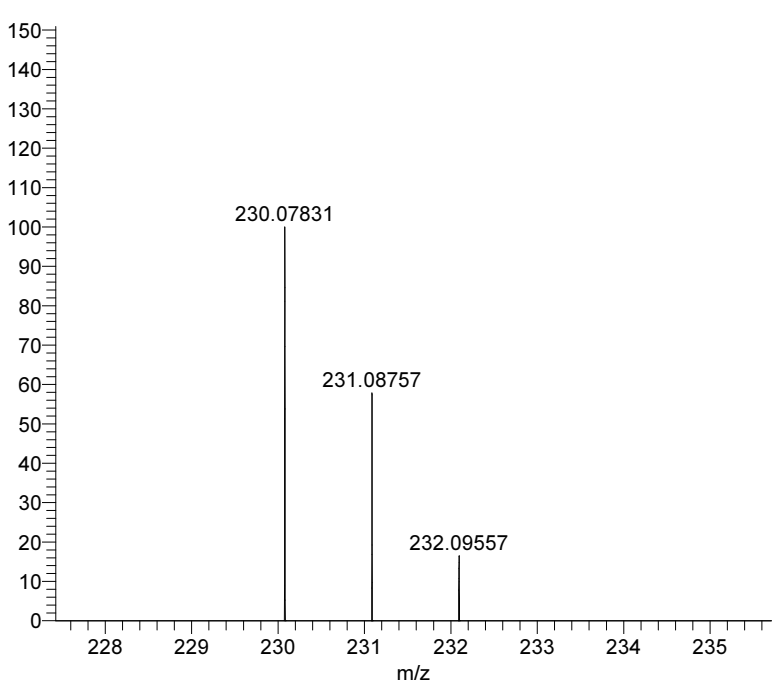


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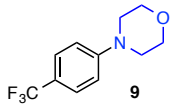


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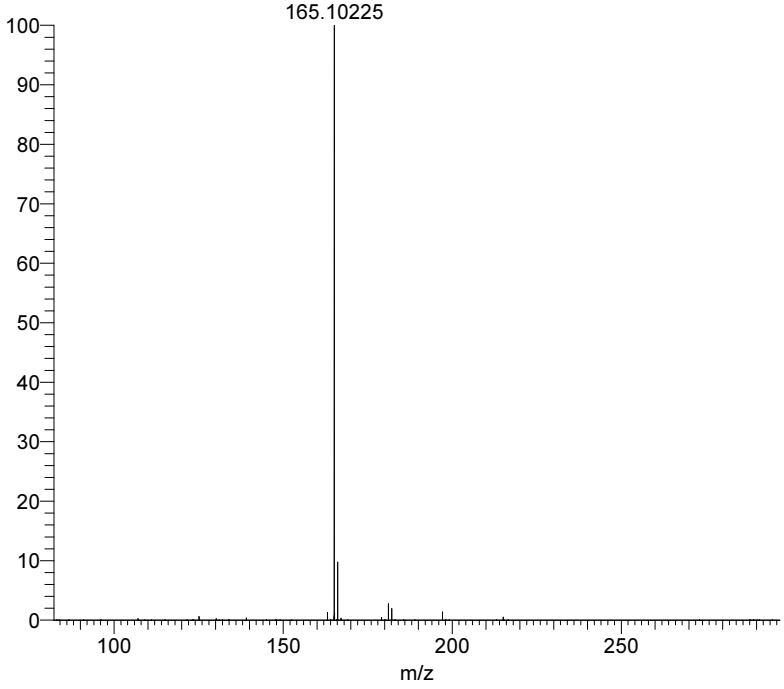


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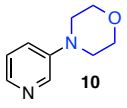


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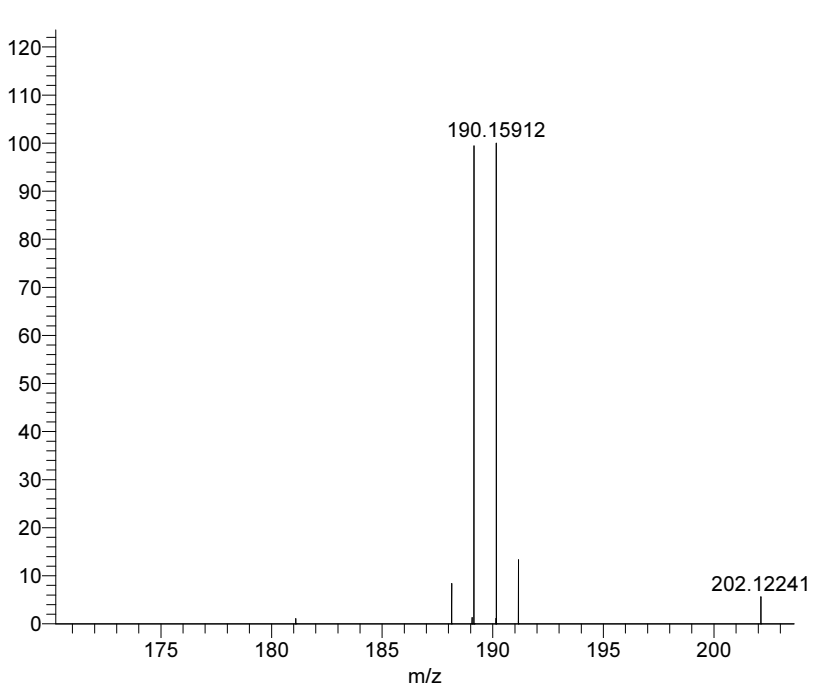


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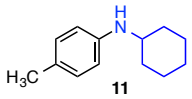


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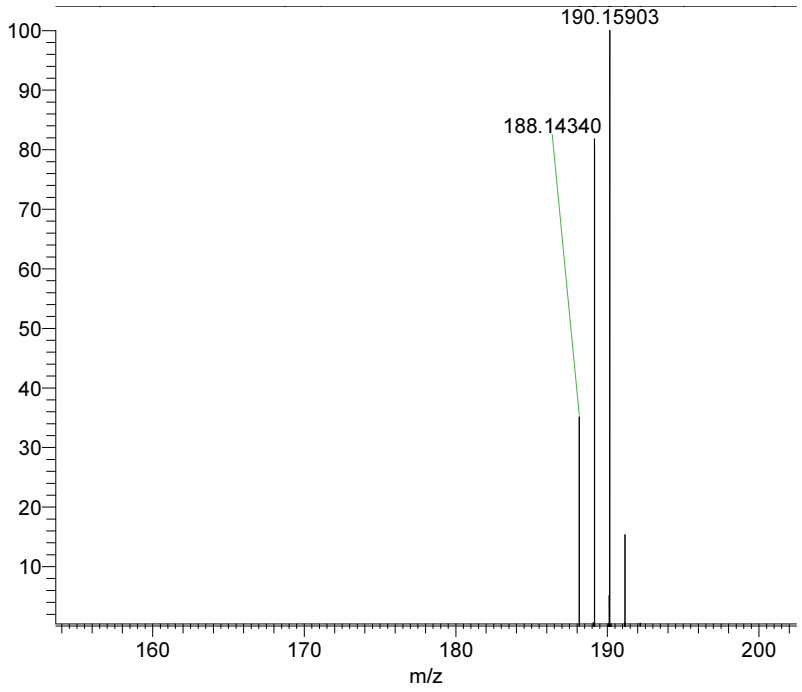


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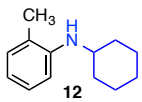


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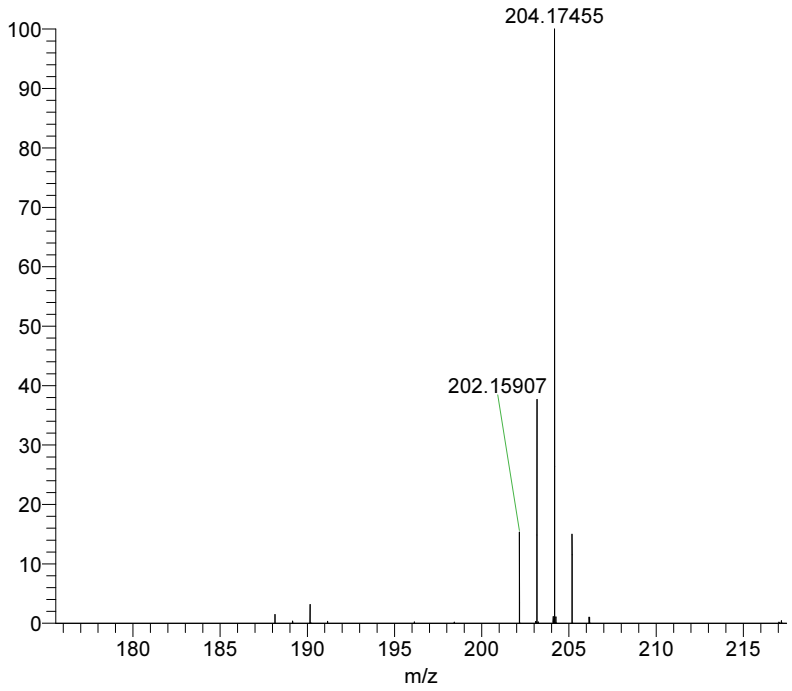


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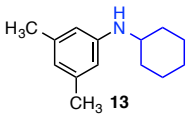


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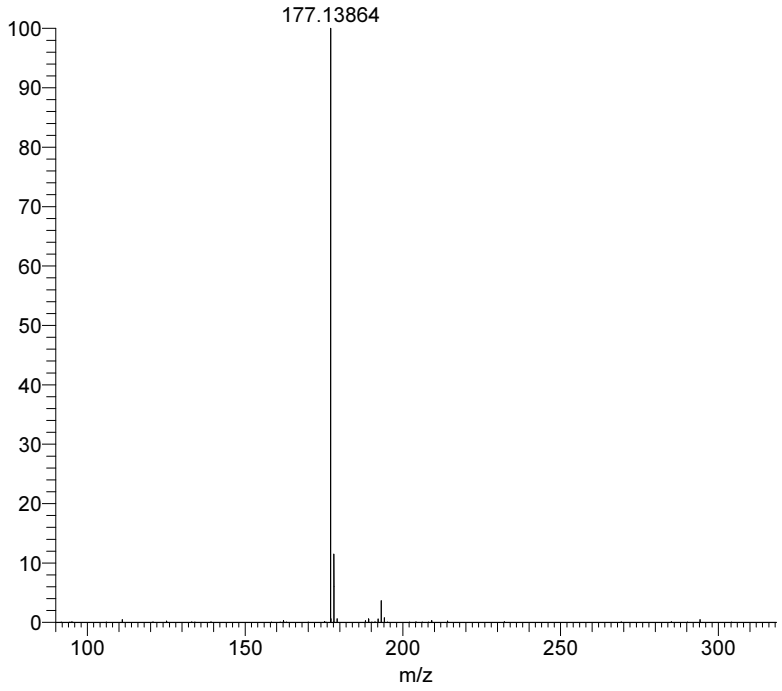


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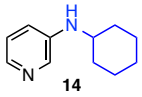


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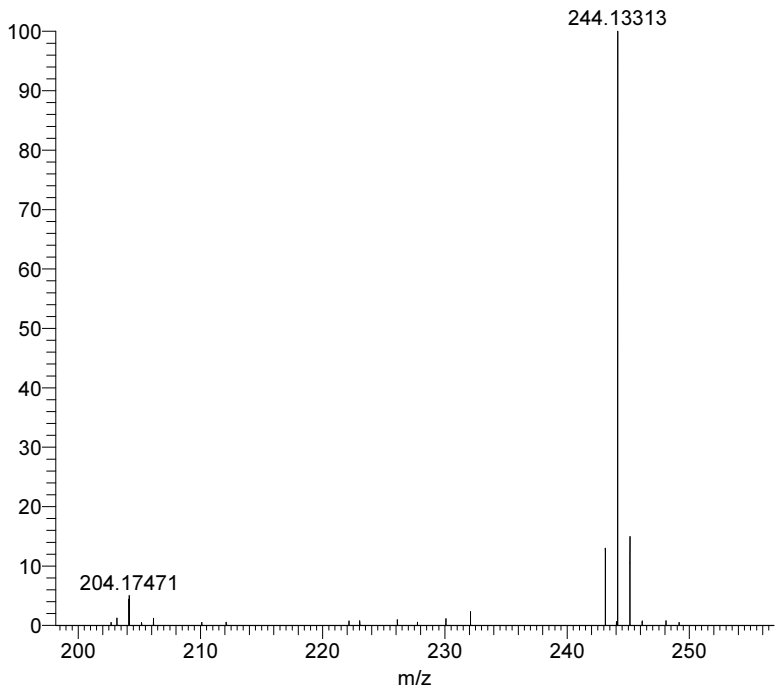


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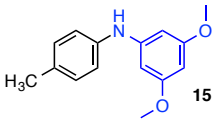


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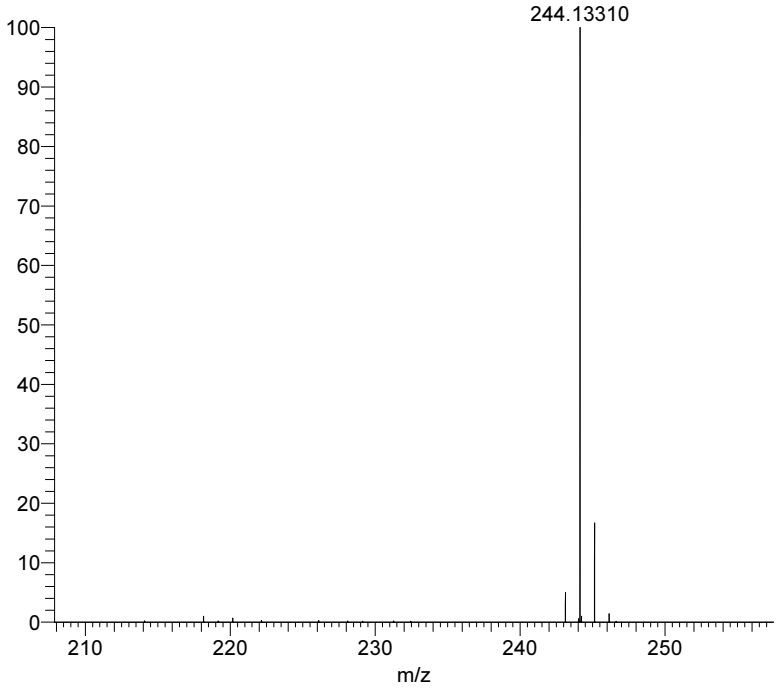


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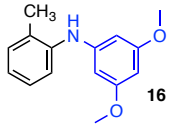


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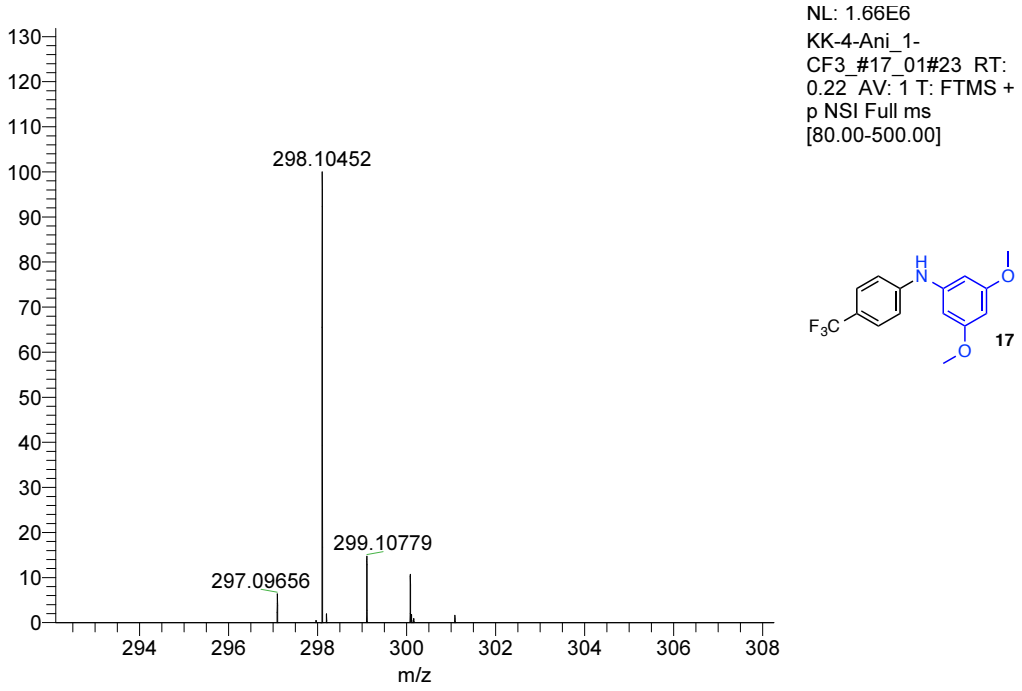
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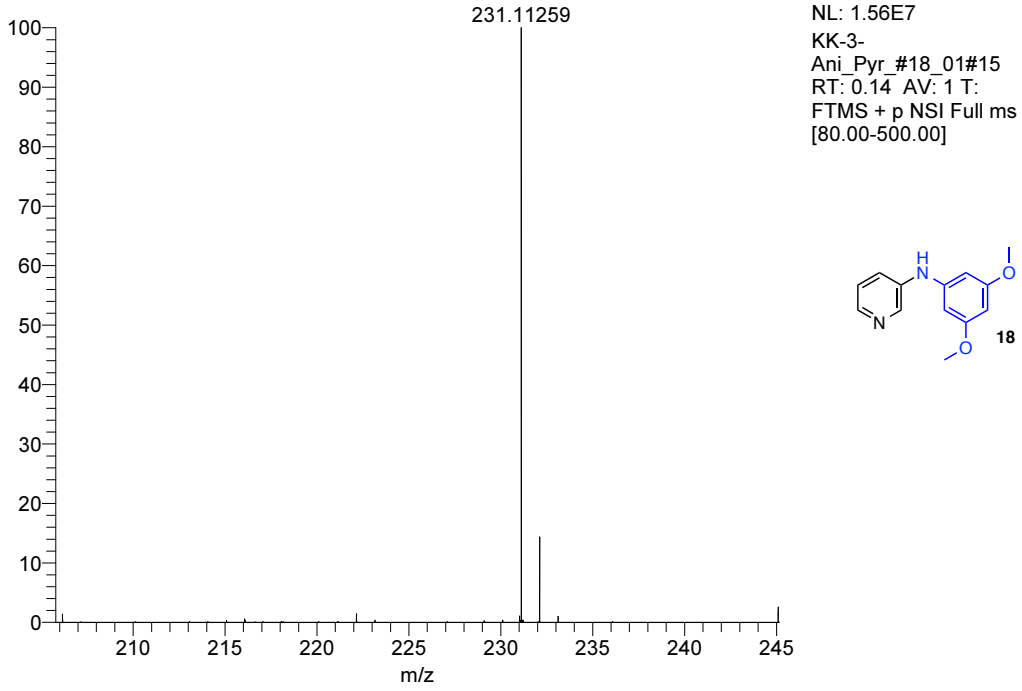
17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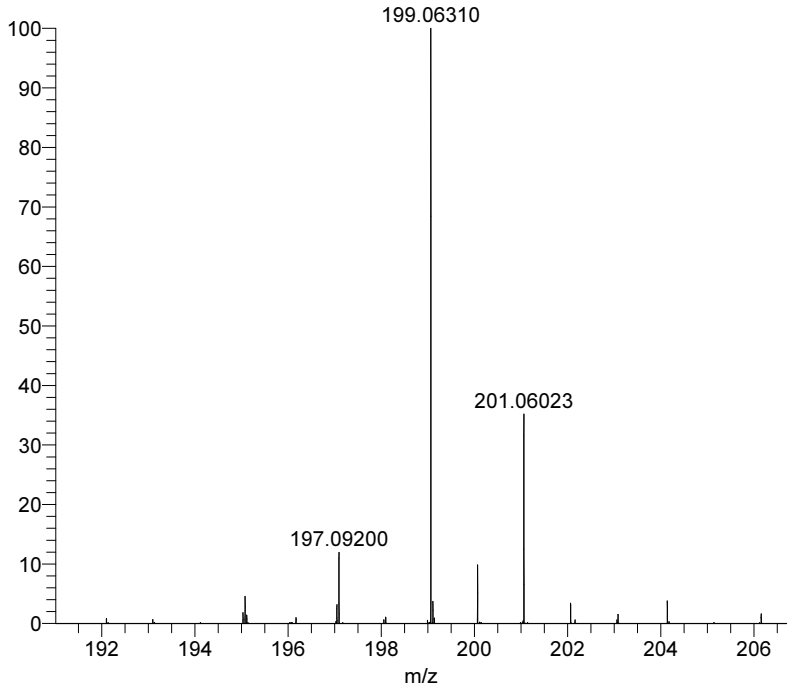


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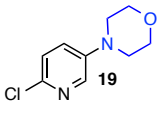


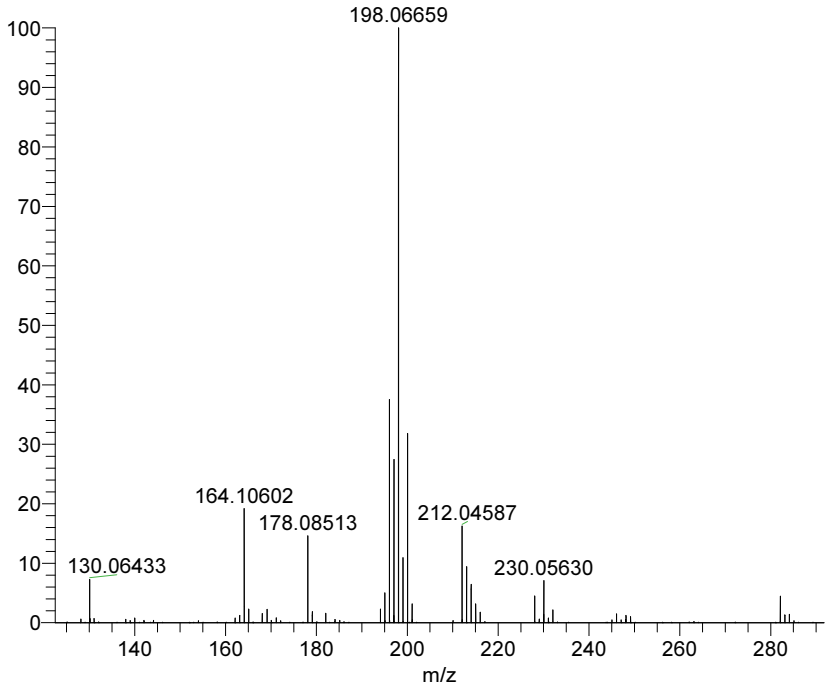


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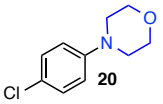

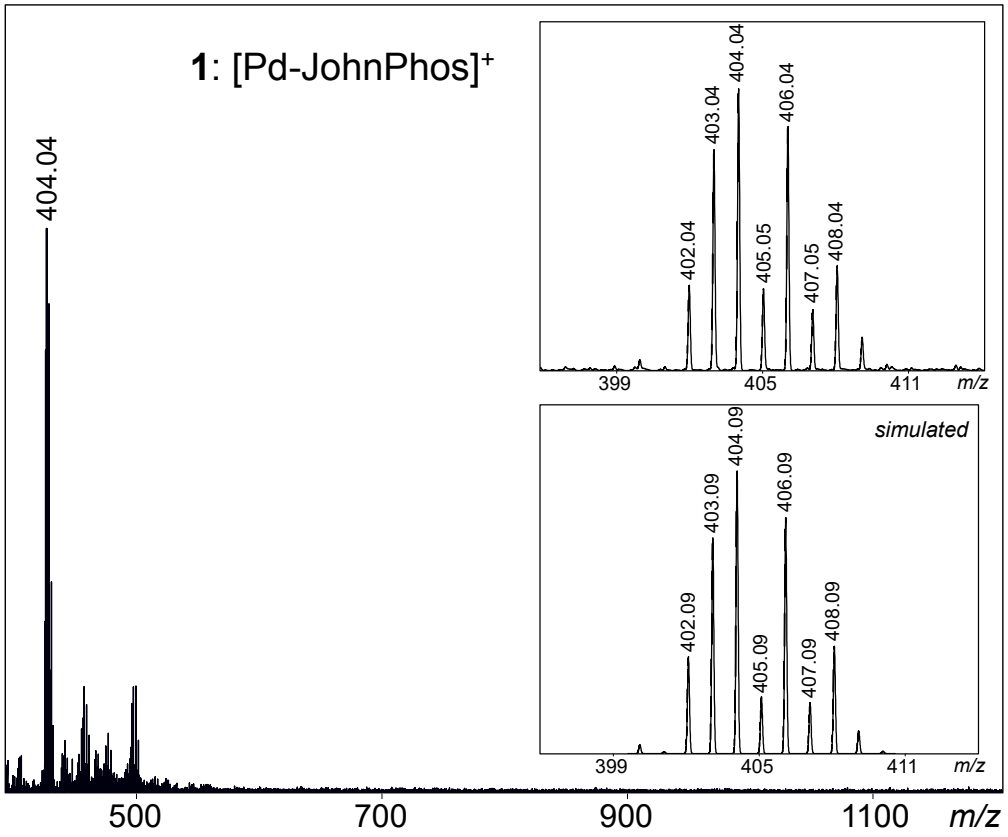
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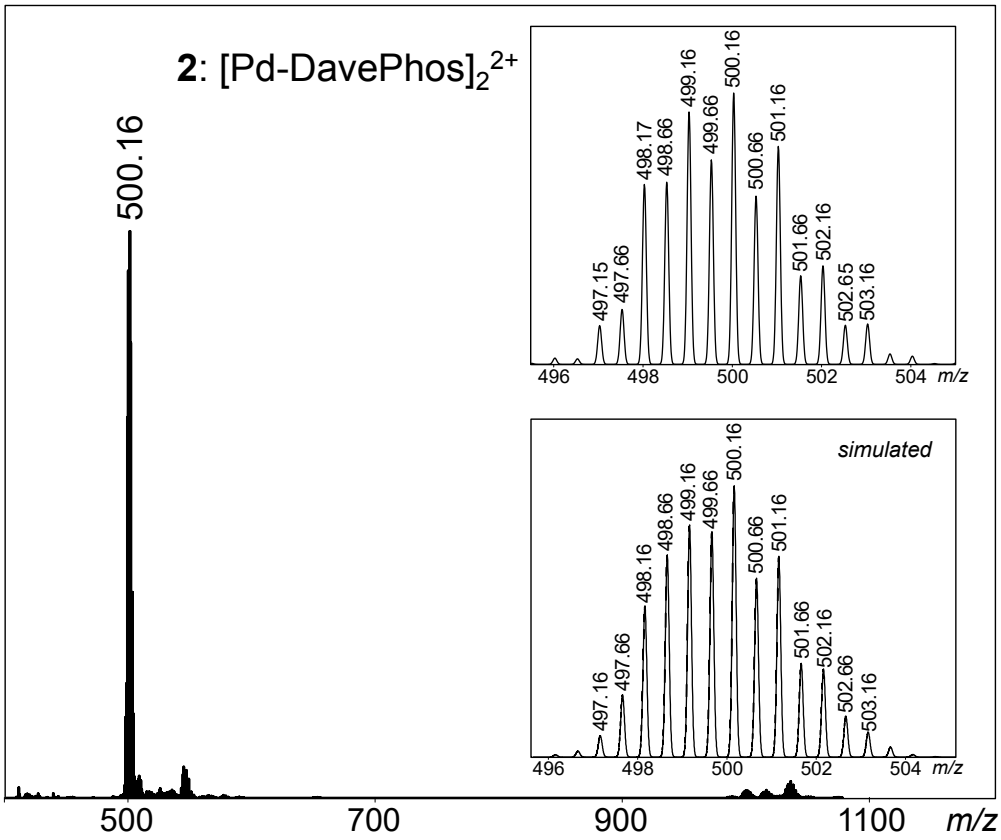
411
m/z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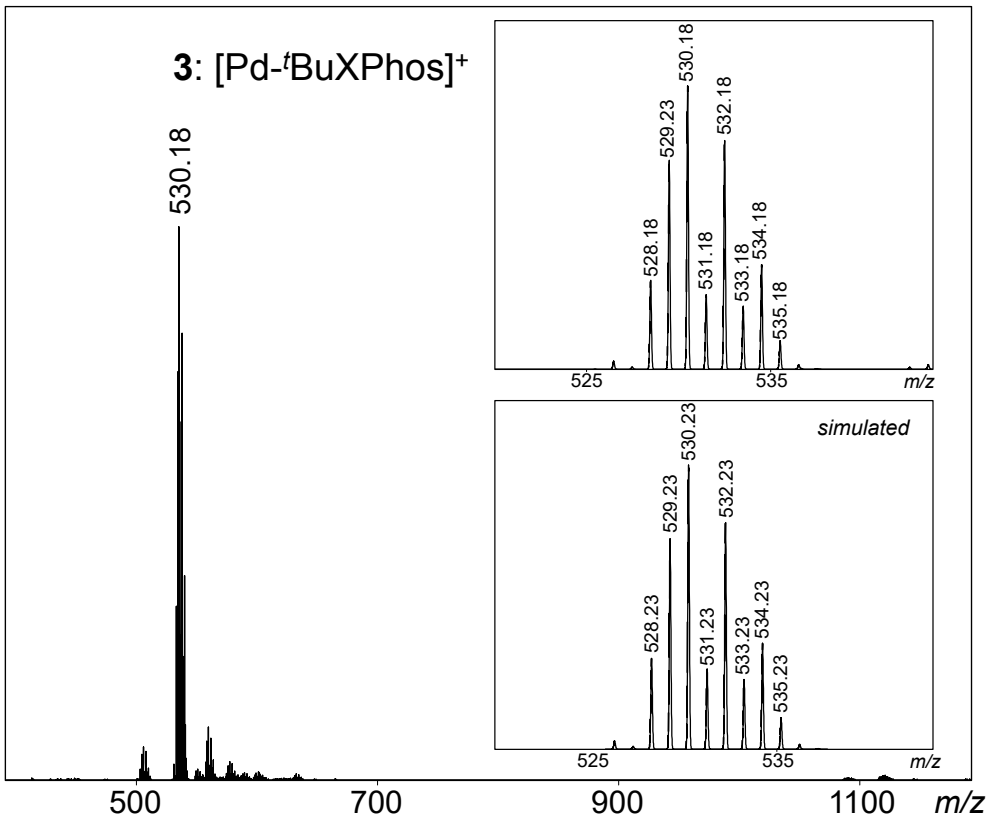
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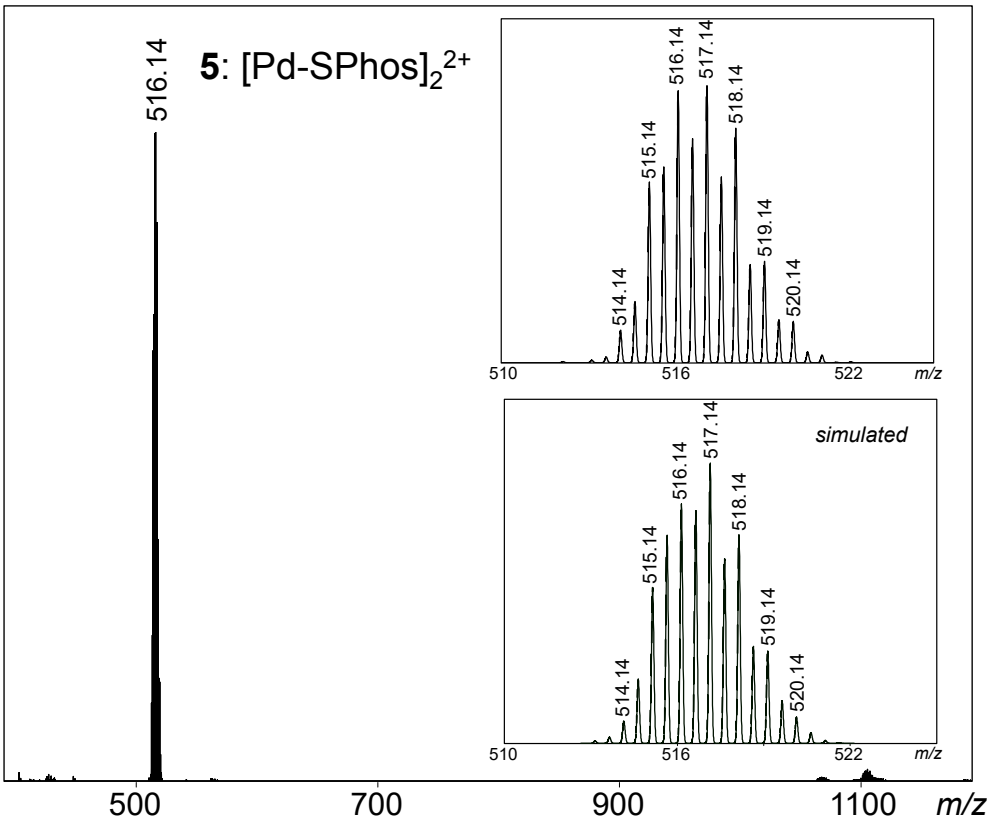
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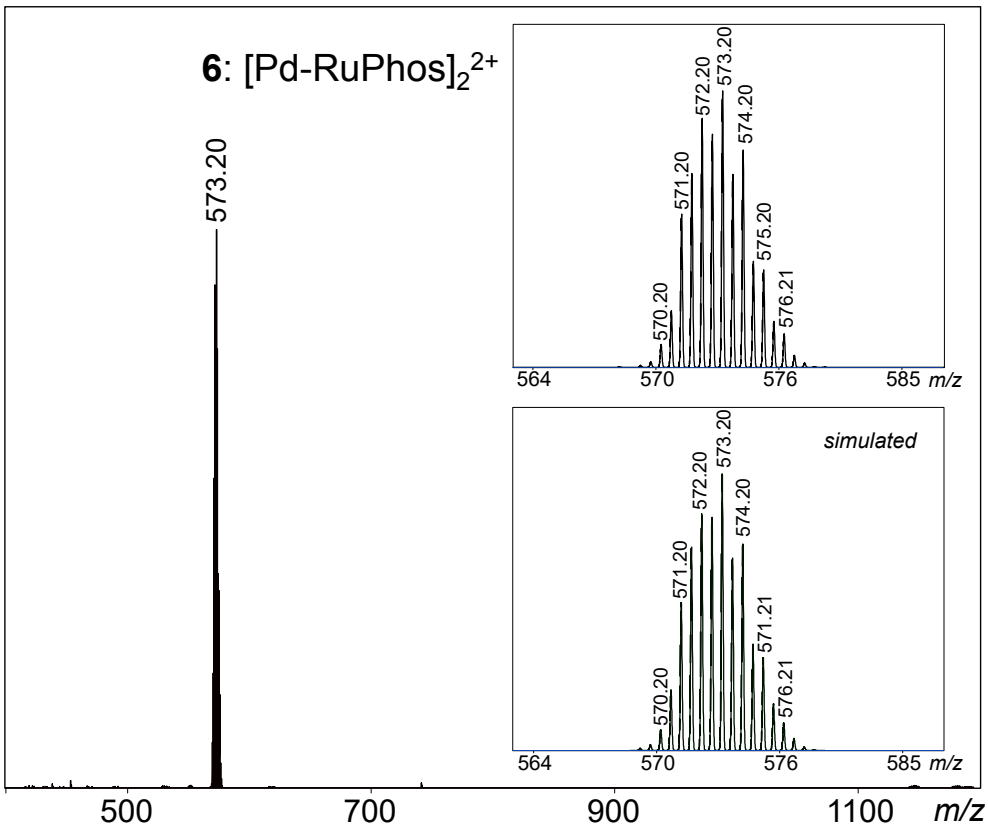
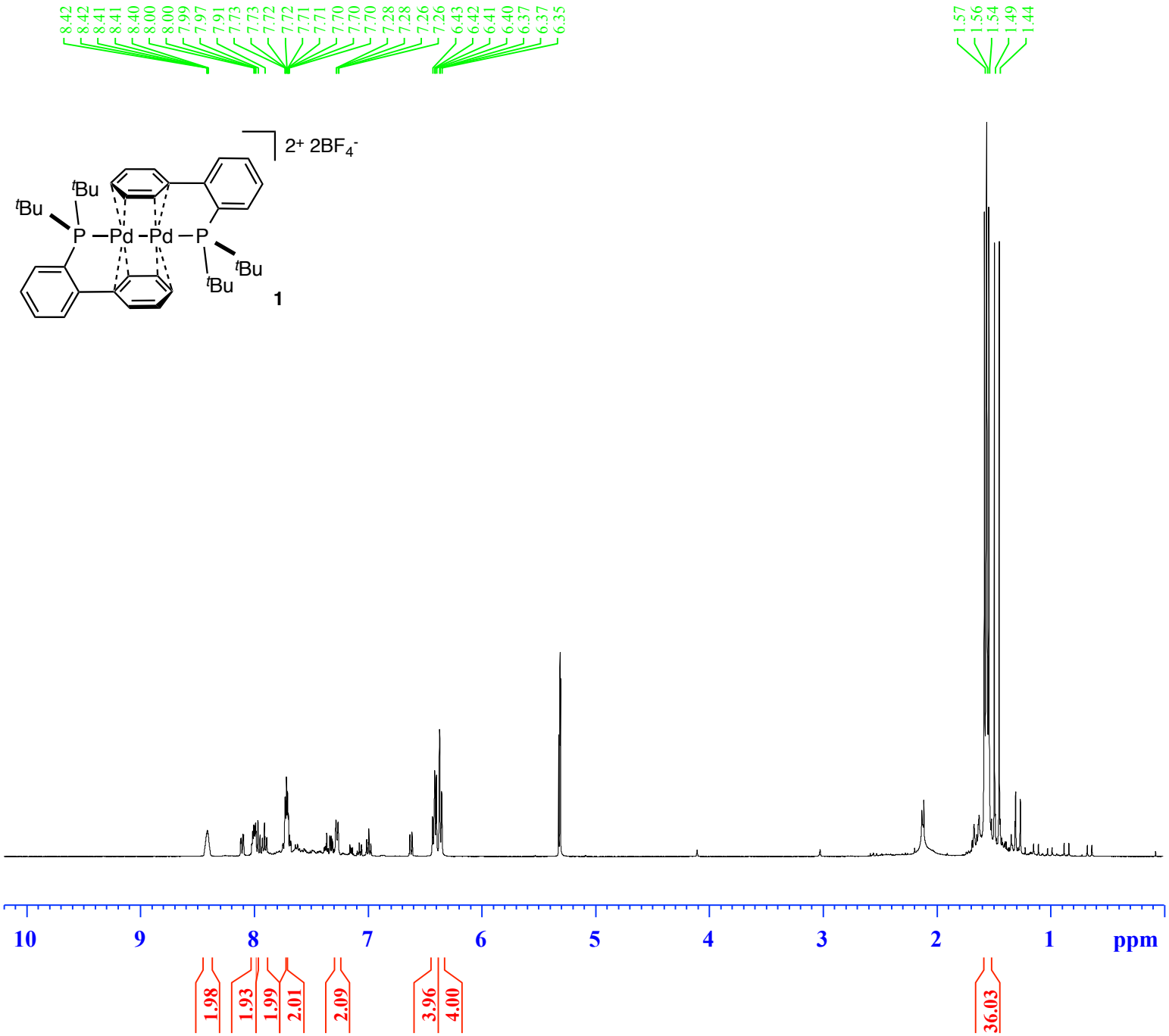
514.14
515.14
516.14
517.14
518.14
519.14
520.14
510
516
522
m/z
simulated
514.14
515.14
516.14
517.14
518.14
519.14
520.14
510
516
522
m/z
500
700
900
1100
m/z


6: [Pd-RuPhos]2 2+
573.20
500
700
900
1100
m/z
570.20
571.20
572.20
573.20
574.20
575.20
576.21
564
570
576
585 m/z
simulated
570.20
571.20
571.21
572.20
573.20
574.20
576.21
564
570
576
585 m/z

# $^1$H NMR, **1**



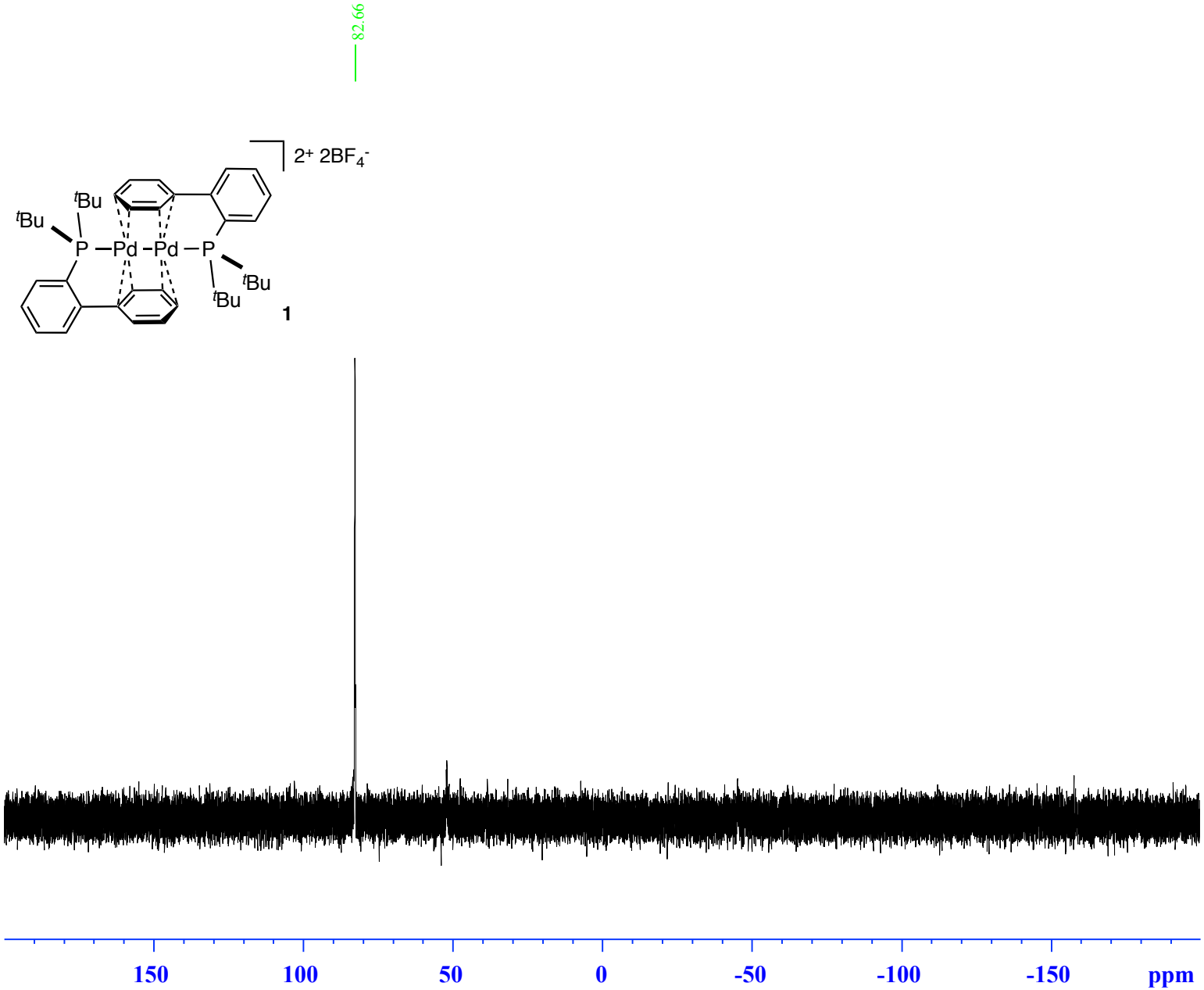

Current Data Parameters
NAME Oct21-2017-spokoyny
EXPNO 100
PROCN O 1

F2 - Acquisition Parameters
Date_ 20171021
Time 17.15
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPRO zg30
G TD 52882
SOLVEN CD2Cl2
T NS 32
DS 0
SW 8012.820 Hz
H 0.151523 Hz
FIDRES 3.2998369 sec
AQ 155.85
RG 62.400 usec
DW 6.50 usec
DE 298.1 K
TE 2.00000000 sec
D1 1
TD0 1

CHANNEL f1
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300203 MHz
WD EM
W 0
SSB 0
LB 0.30 Hz
GB
PC 1.00

# $^{31}$P NMR, **1**




Current Data Parameters
NAME KK-3-049 Pd-JohnPhos, CD2Cl2, 31P
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171021
Time 15.21
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG z g d c 3 0
TD 1 3 1 0 7 2
SOLVENT CD2Cl2
NS 128
DS 0
SW 100000.000 Hz
H 0.762939 Hz
FIDRES 0.6553600 sec
AQ 13004
RG 5.000 usec
D 6.00 usec
W 296.9 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
d11
TD0

======== CHANNEL f1 ========
NUC1 31P
P1 9.00 usec
PL1 0 dB
SFO1 202.5370460 MHz

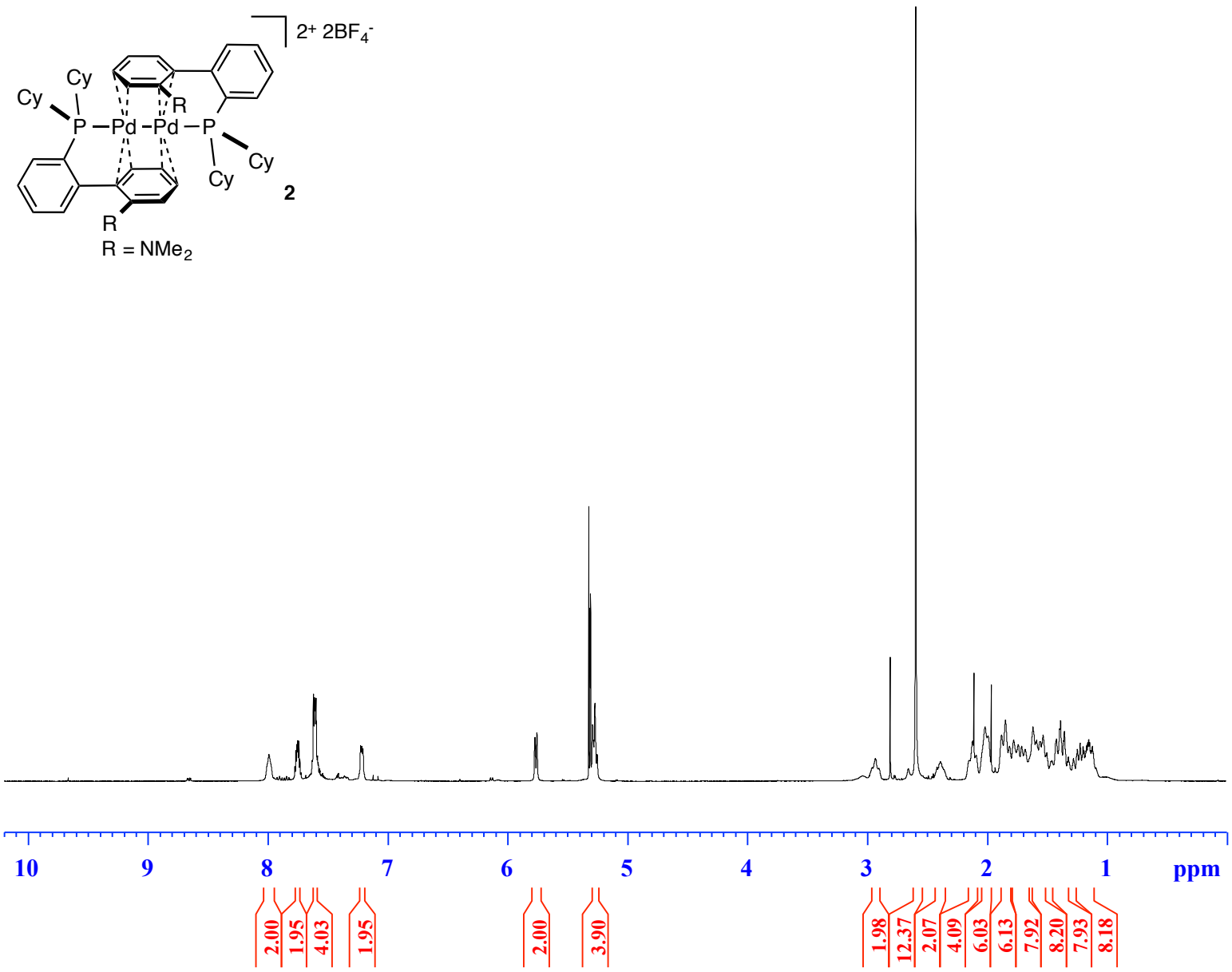
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 off
PCPD2 PL2 100.00 usec
PL12 0 dB
SFO2 17.52 dB
500.3300000 MHz

F2 - Processing parameters
SI 131072
SF 202.5371639 MHz
WD EM
W 0
SSB 1.00 Hz
LB 0
GB 1.40
PC

# $^1$H NMR, **2**




**2**

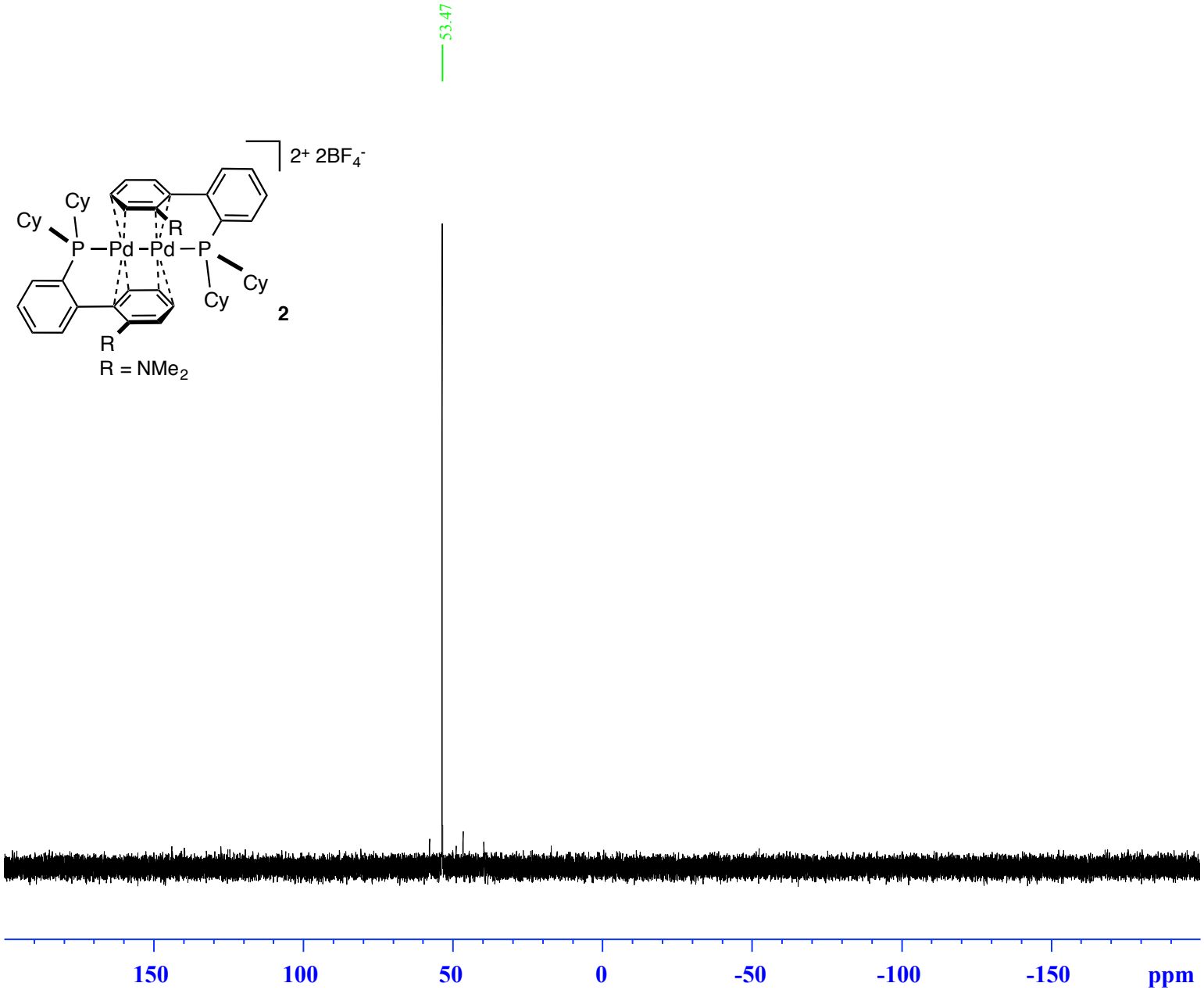



Current Data Parameters
NAME Oct21-2017-spokoyny
EXPNO 90
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171021
Time 16.59
INSTRU av400
M 5 mm PABBO BB/
PROBHD zg30
PULPRO 52882
G TD CD2Cl2
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 155.85
AQ 62.400 usec
RG 6.50 usec
DW 298.1 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300203 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{31}$P NMR, **2**




Current Data Parameters
NAME KK-3-048 Pd-DavePhos, CD2Cl2, 31P
EXPNO 2
PROCN 1
O

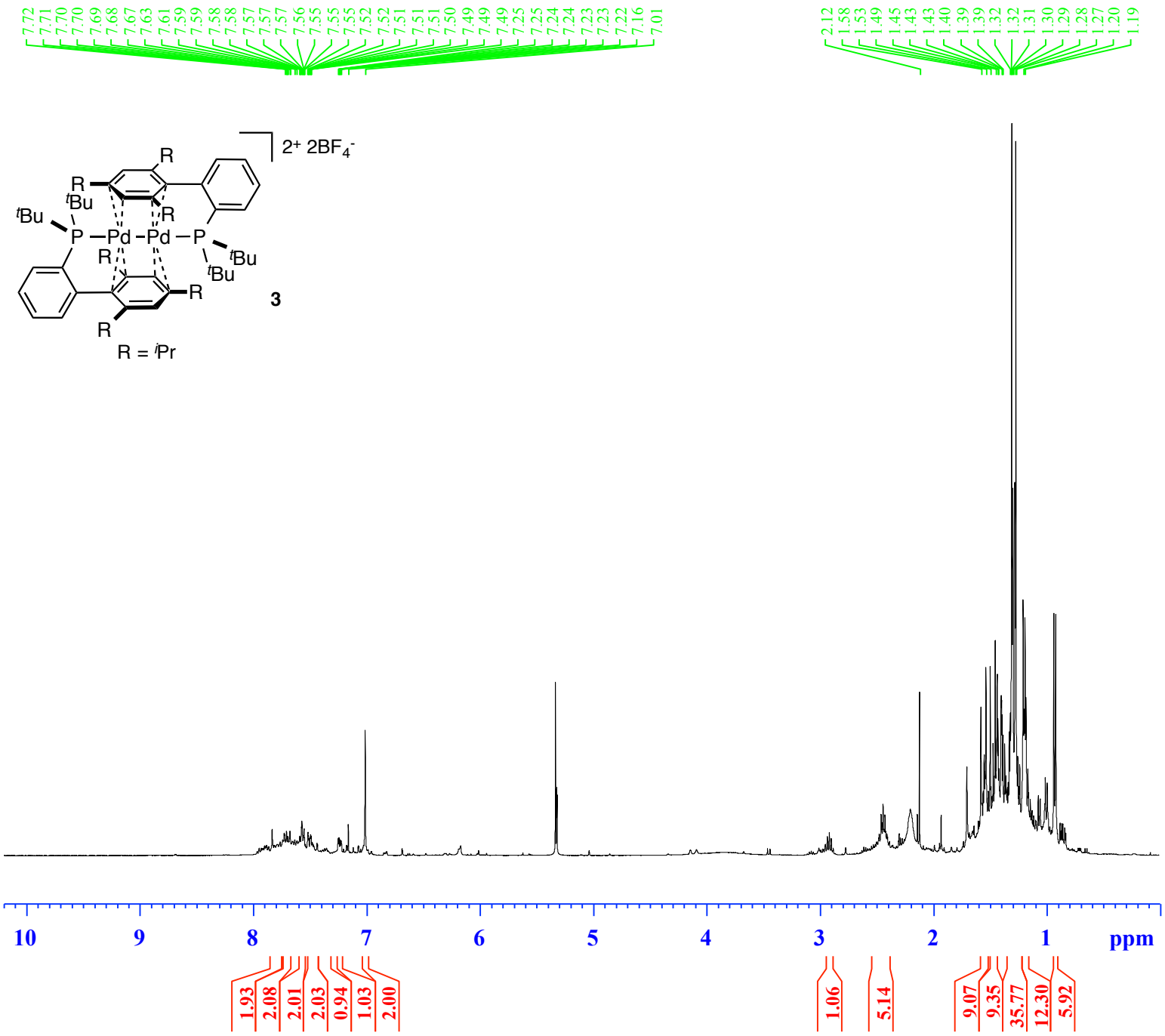
F2 - Acquisition Parameters
Date_ 20171021
Time 15.13
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG z g d c 3 0
TD 1 3 1 0 7 2
SOLVENT CD2Cl2
NS 80
DS 0
SW 100000.000 Hz
H 0.762939 Hz
FIDRES 0.6553600 sec
AQ 13004
RG 5.000 usec
D 6.00 usec
W 296.9 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
d11
TD0 ======== CHANNEL f1 ========
NUC1 31P
P1 9.00 usec
PL1 0 dB
SFO1 202.5370460 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 off
PCPD2 PL2 100.00 usec
PL12 0 dB
SFO2 17.52 dB
500.3300000 MHz

F2 - Processing parameters
SI 131072
SF 202.5371639 MHz
WD EM
W 0
SSB 1.00 Hz
LB 0
GB 1.40
PC

# $^1$H NMR, **3**




Current Data Parameters
NAME Oct21-2017-spokoyny
EXPNO 80
PROCN O 1

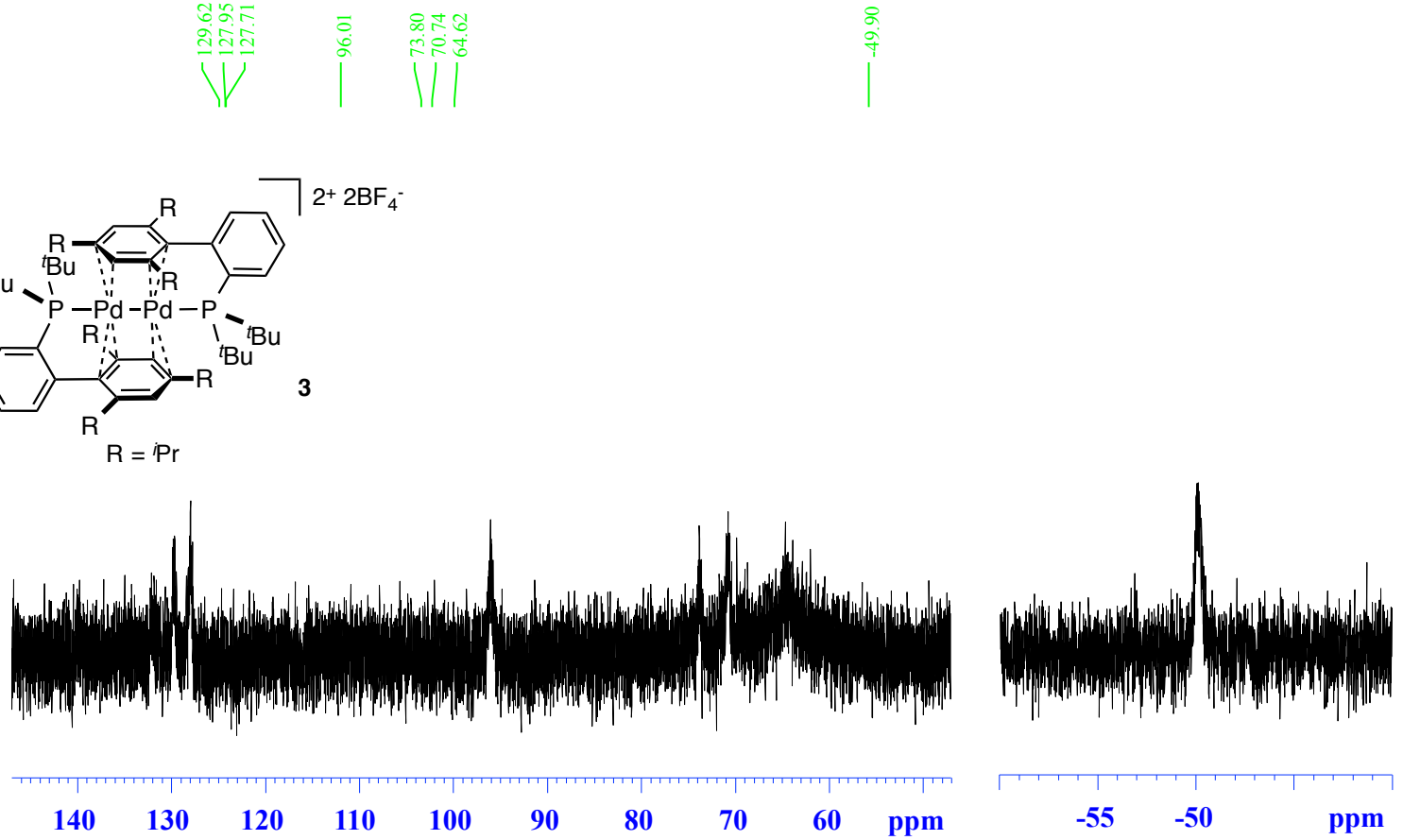
F2 - Acquisition Parameters
Date_ 20171021
Time 16.44
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CD2Cl2
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 94.6
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300153 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB
PC 1.00

# $^{31}$P NMR, **3**



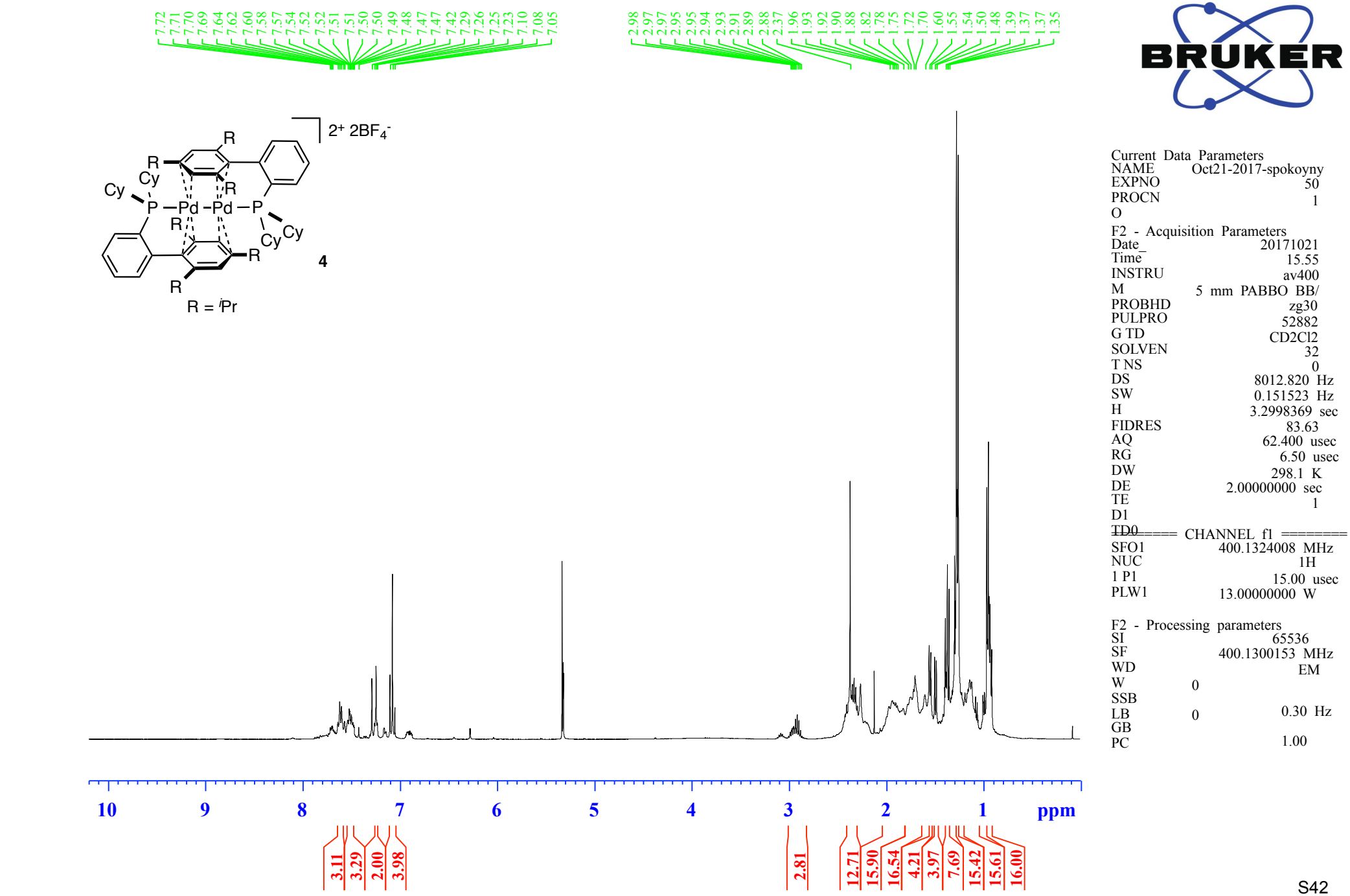

Current Data Parameters
NAME KK-3-047_2 Pd-tBuXPhos, CD2Cl2, 31P
EXPNO 4
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171219
Time 13.22
INSTRU drx500
M 5 mm bb-Z Z800
PROBHD zgdc30
PULPRO 131072
G TD CD2Cl2
SOLVEN 4096
T NS 0
DS 100000.000 Hz
SWH 0.762939 Hz
FIDRES 0.6553600 sec
AQ 14596.5
RG 5.000 usec
D 6.00 usec
W 296.9 K
DE 0.25000000 sec
T E 0.03000000 sec
D1 1
d11
TD0
======== CHANNEL f1 ========
NUC 31P
1 P1 9.00 usec
PL1 0 dB
SFO1 202.5370460 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 off
PCPD2 PL2 100.00 usec
PL12 0 dB
SFO2 17.52 dB
500.3300000 MHz

F2 - Processing parameters
SI 131072
SF 202.5373052 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **4**




BRUKER

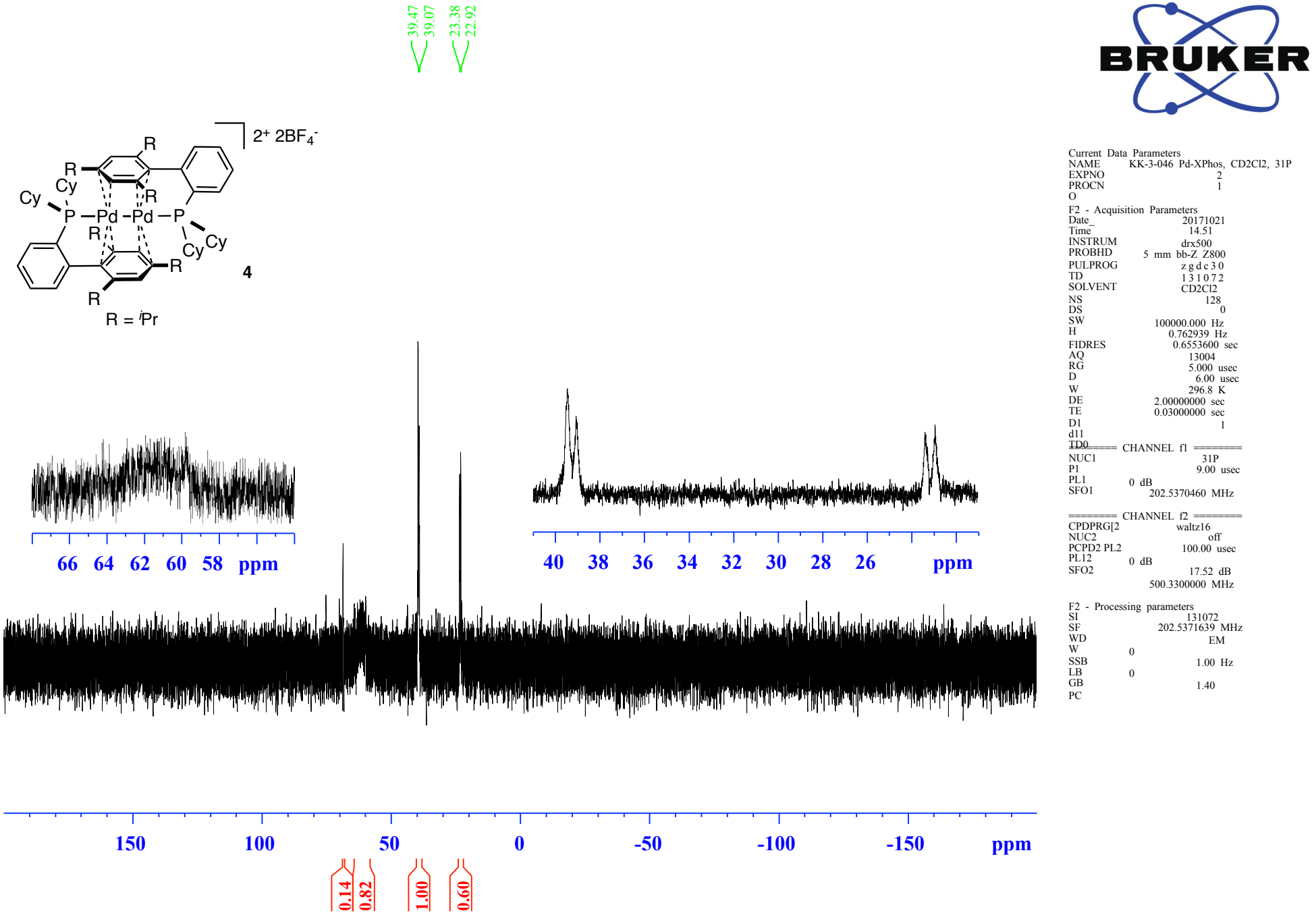
Current Data Parameters
NAME Oct21-2017-spokoyny
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171021
Time 15.55
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 52882
SOLVENT CD2Cl2
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 83.63
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300153 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

# $^{31}$P NMR, **4**




BRUKER

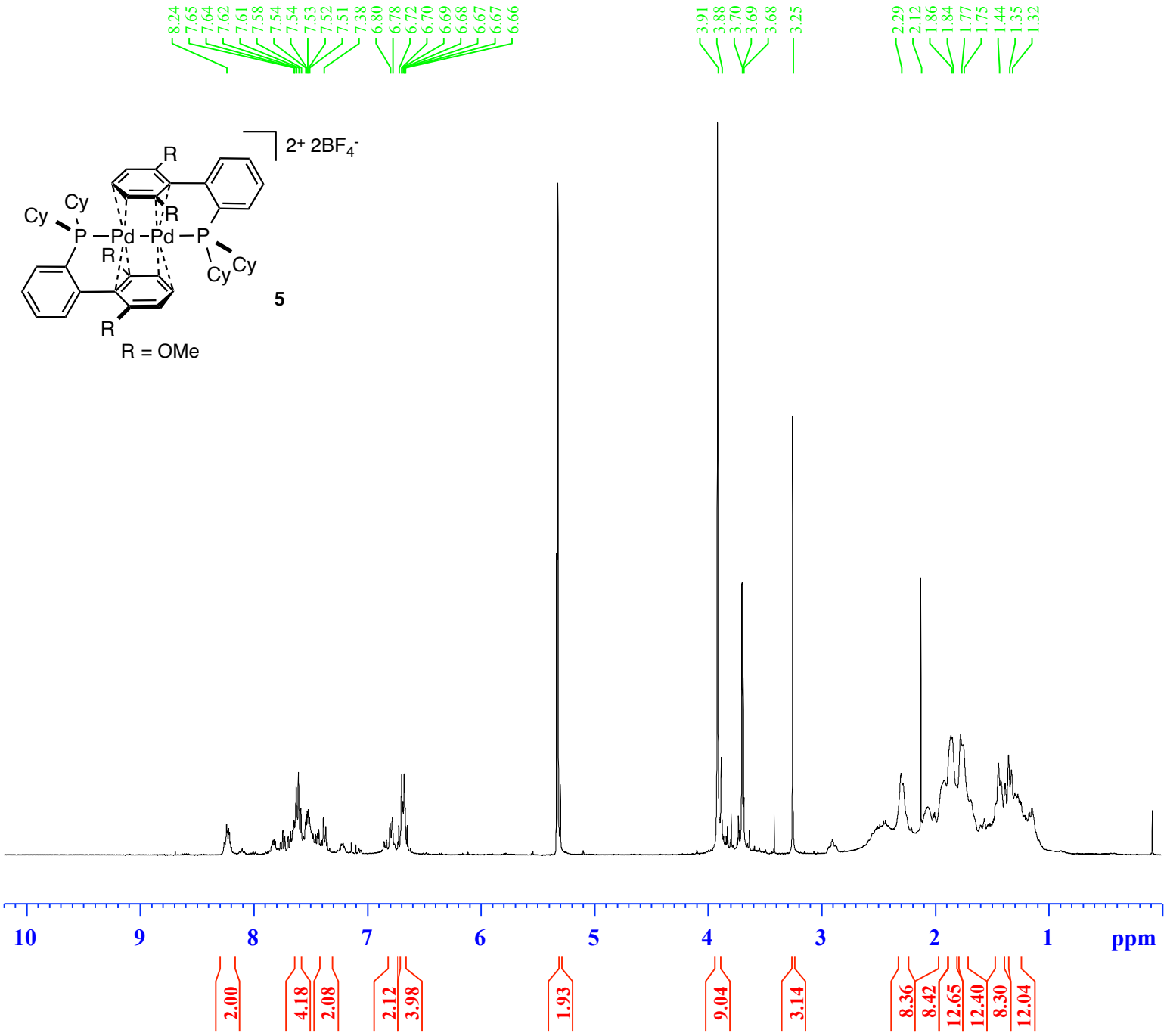
Current Data Parameters
NAME KK-3-046 Pd-XPhos, CD2Cl2, 31P
EXPNO 2
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171021
Time 14.51
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG z g d c 3 0
TD 1 3 1 0 7 2
SOLVENT CD2Cl2
NS 128
DS 0
SW 100000.000 Hz
H 0.762939 Hz
FIDRES 0.6553600 sec
AQ 13004
RG 5.000 usec
D 6.00 usec
W 296.8 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
d11
TD0
======== CHANNEL f1 ========
NUC1 31P
P1 9.00 usec
PL1 0 dB
SFO1 202.5370460 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 off
PCPD2 PL2 100.00 usec
PL12 0 dB
SFO2 17.52 dB
500.3300000 MHz

F2 - Processing parameters
SI 131072
SF 202.5371639 MHz
WD EM
W 0
SSB 1.00 Hz
LB 0
GB 1.40
PC

# $^1$H NMR, **5**

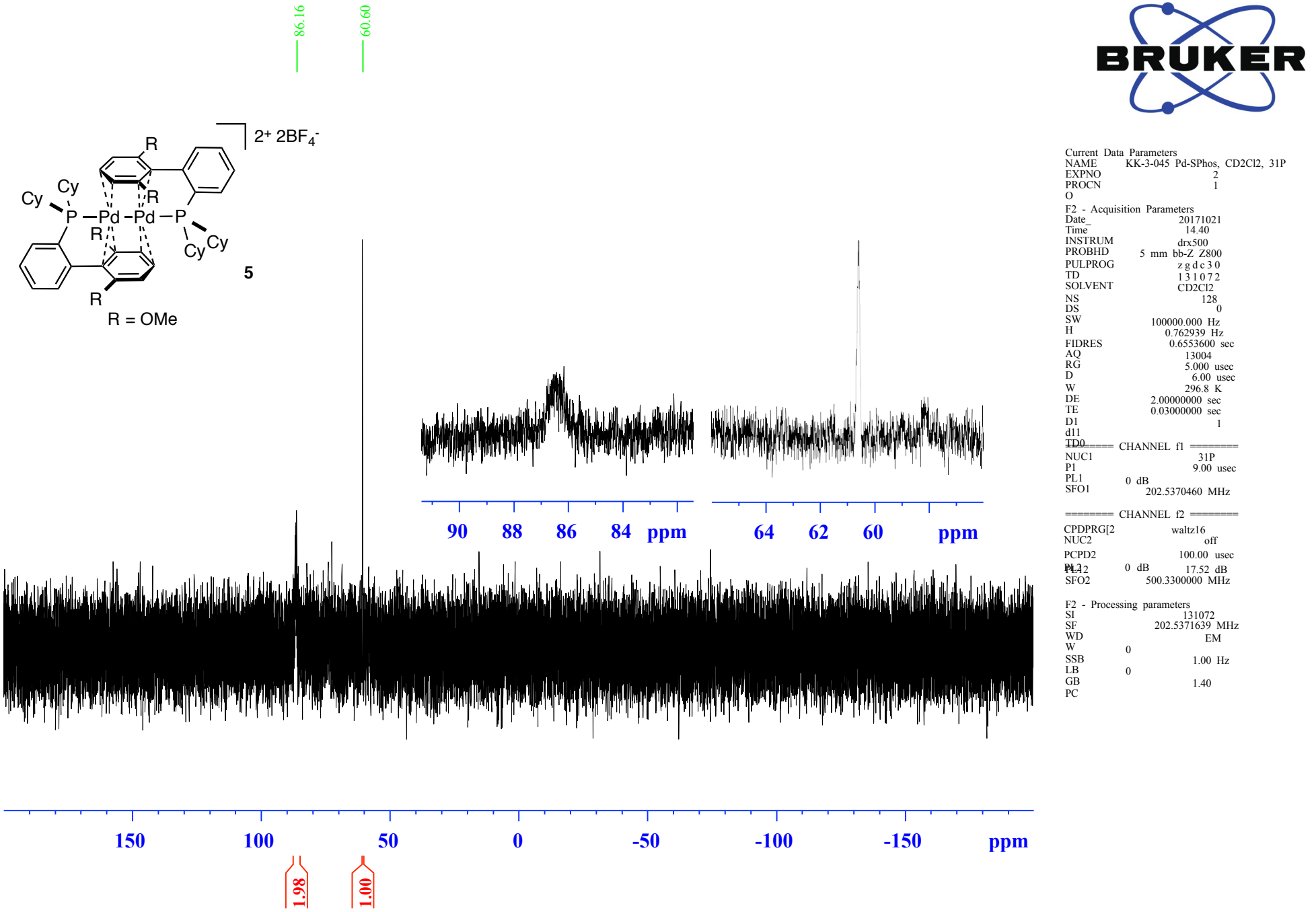



Current Data Parameters
NAME Oct21-2017-spokoyny
EXPNO 40
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171021
Time 15.39
INSTRU av400
M 5 mm PABBO BB/
PROBHD zg30
PULPRO 52882
G TD CD2Cl2
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 155.85
AQ 62.400 usec
RG 6.50 usec
DW 298.1 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300154 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{31}$P NMR, **5**



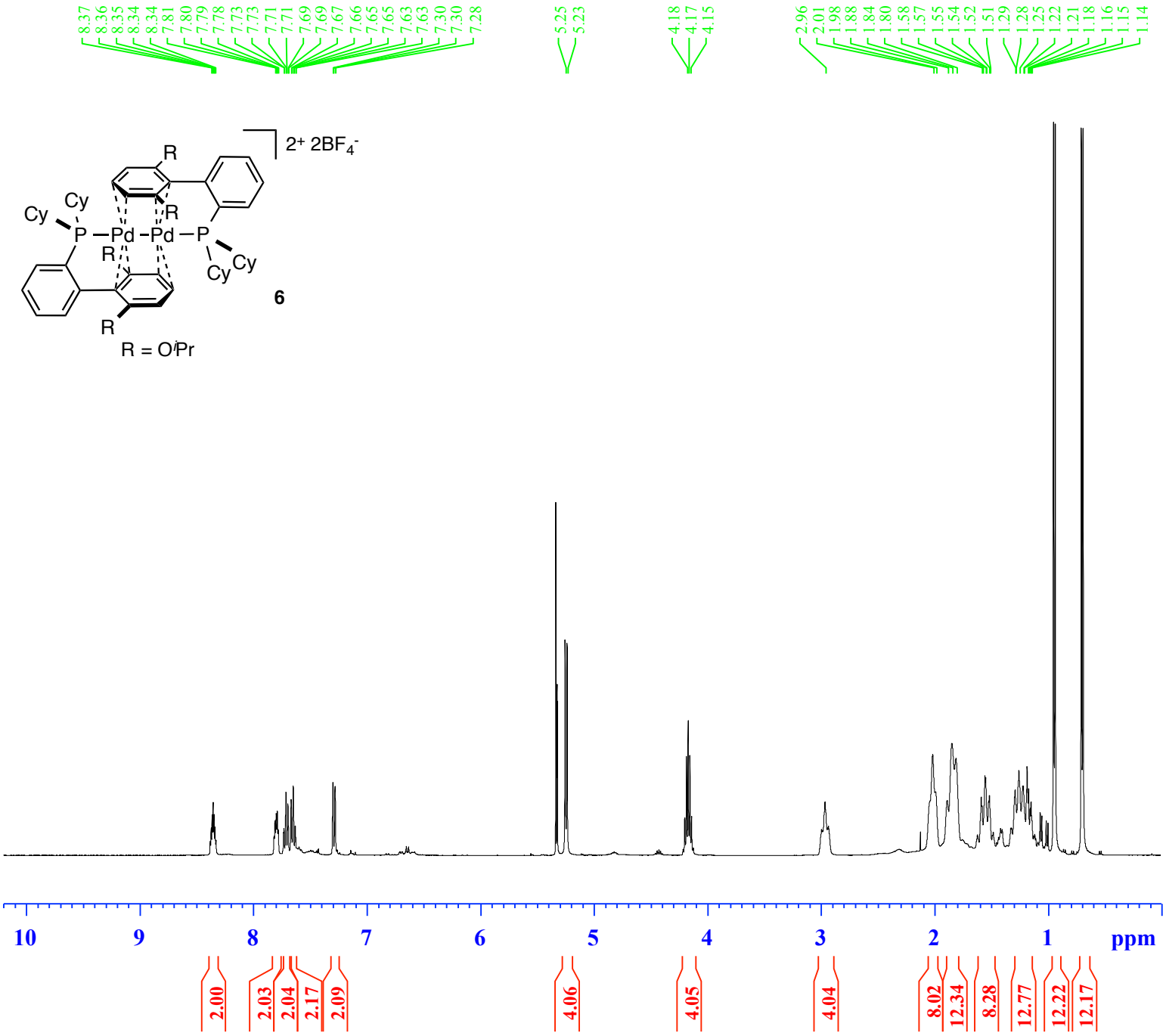

Current Data Parameters
NAME KK-3-045 Pd-SPhos, CD2Cl2, 31P
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171021
Time 14.40
INSTRUM drx500
PROBHD 5 mm bb-Z Z800
PULPROG z g d c 3 0
TD 1 3 1 0 7 2
SOLVENT CD2Cl2
NS 128
DS 0
SW 100000.000 Hz
H 0.762939 Hz
FIDRES 0.6553600 sec
AQ 13004
RG 5.000 usec
D 6.00 usec
W 296.8 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
d11
TD0
======== CHANNEL f1 ========
NUC1 31P
P1 9.00 usec
PL1 0 dB
SFO1 202.5370460 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 off
PCPD2 100.00 usec
PL2 0 dB 17.52 dB
SFO2 500.3300000 MHz

F2 - Processing parameters
SI 131072
SF 202.5371639 MHz
WD EM
W 0
SSB 1.00 Hz
LB 0
GB 1.40
PC

# $^1$H NMR, **6**



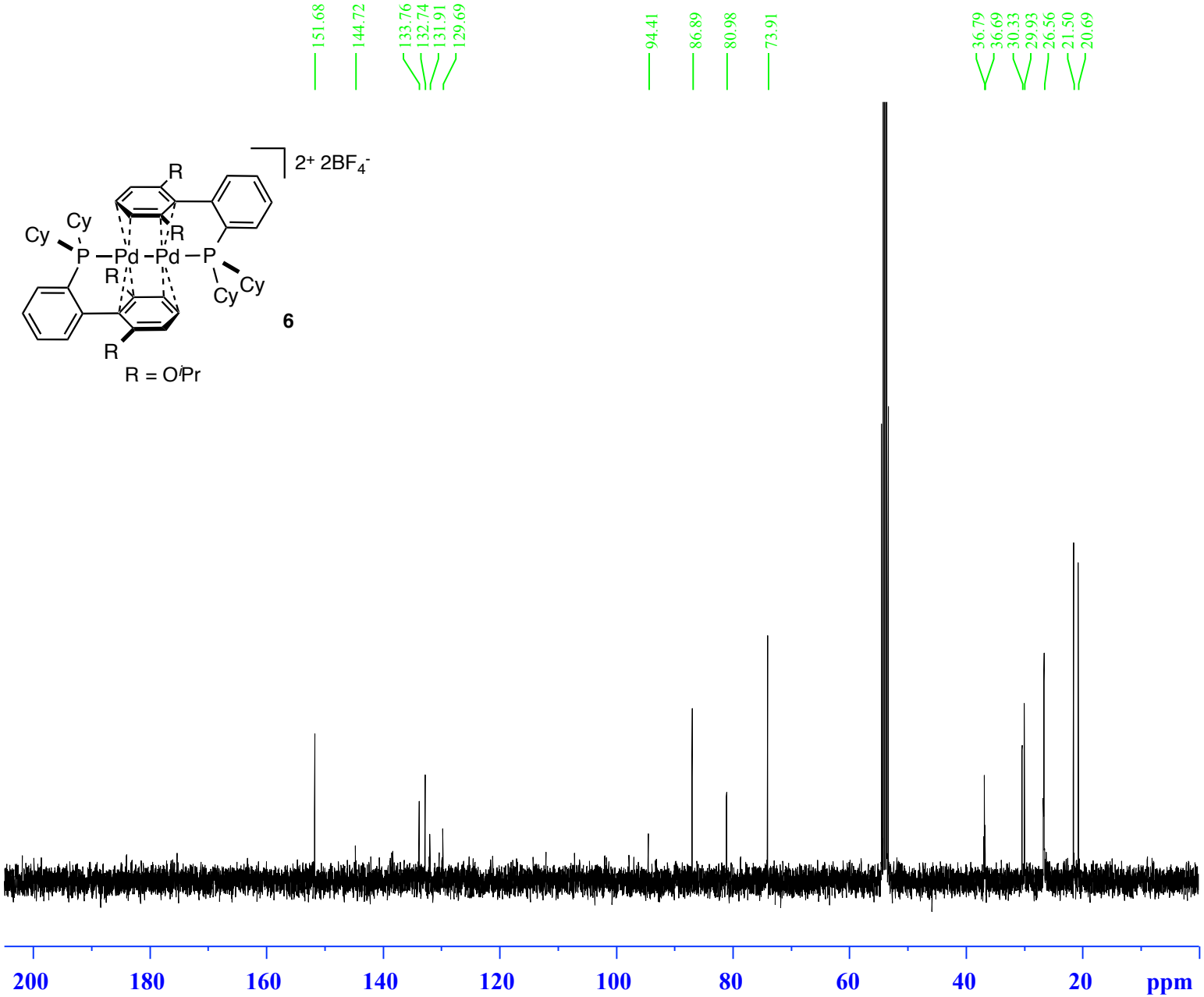

Current Data Parameters
NAME Oct21-2017-spokoyny
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171021
Time 15.23
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPRO zg30
G TD 52882
SOLVEN CD2Cl2
T NS 32
DS 0
SW 8012.820 Hz
H 0.151523 Hz
FIDRES 3.2998369 sec
AQ 83.63
RG 62.400 usec
DW 6.50 usec
DE 298.1 K
TE 2.00000000 sec
D1 1
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300153 MHz
WD EM
W 0
SSB 0
LB 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **6**




Current Data Parameters
NAME Oct21-2017-spokoyny
EXPNO 31
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171021
Time 15.32
INSTRU av400
M 5 mm PABBO BB/
PROBHD zgpg30
PULPRO 65536
G TD CD2Cl2
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 298.8 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

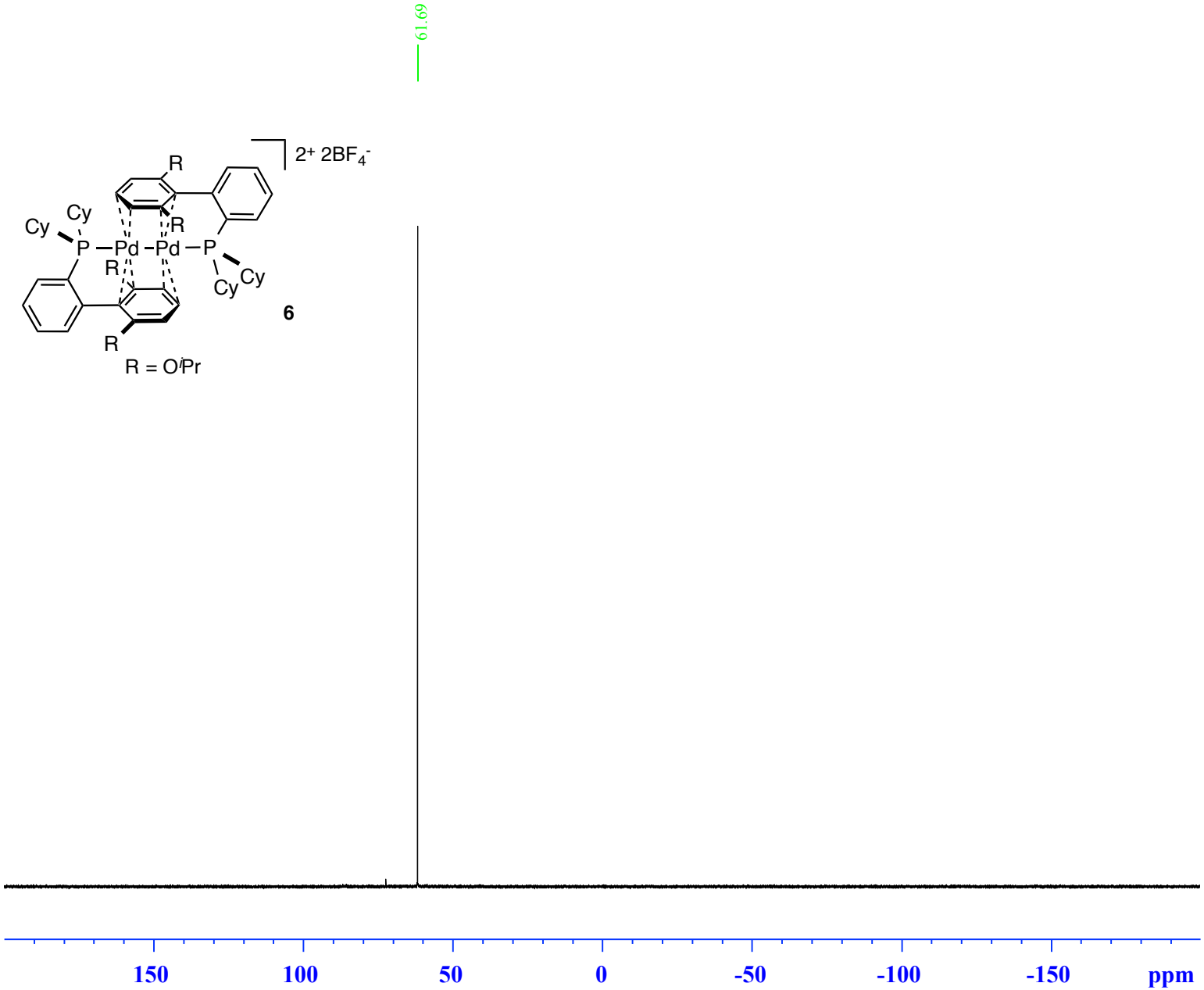
======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127277 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^{31}P\{^{1}H\}$ NMR, **6**




**6**



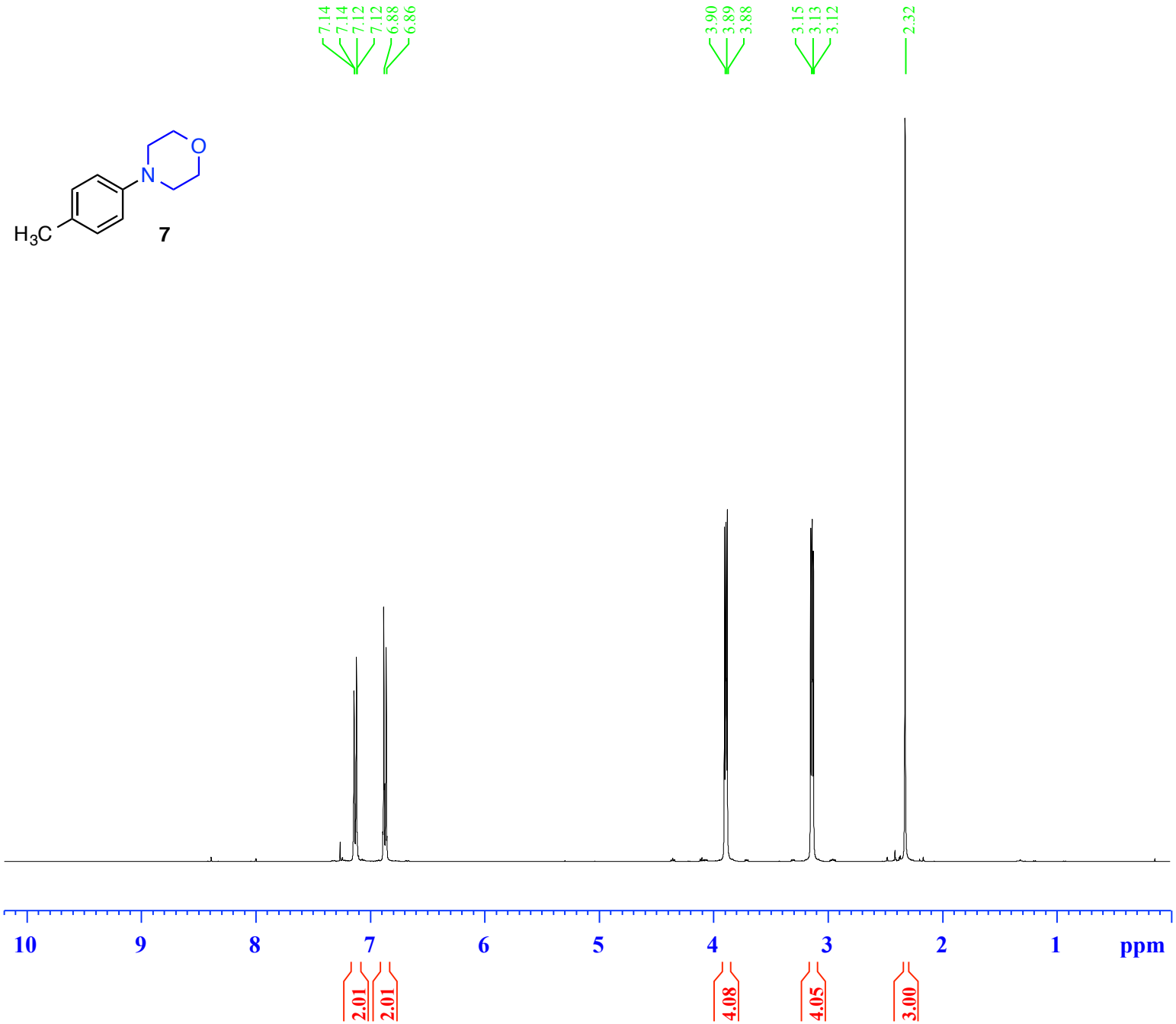

Current Data Parameters
NAME KK-3-044 Pd-RuPhos, CD2Cl2, 31P
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171021
Time 14.25
INSTRUM drx500
M 5 mm bb-Z Z800
PROBHD z g d c 3 0
PULPRO 1 3 1 0 7 2
G TD CD2Cl2
SOLVEN 64
T NS 0
DS 100000.000 Hz
SWH 0.762939 Hz
FIDRES 0.6553600 sec
AQ 13004
R 5.000 usec
G 6.00 usec
D 296.9 K
W 2.00000000 sec
DE 0.03000000 sec
T E 1
D1
d11 ======== CHANNEL f1 ========
NUC1 31P
1 P1 9.00 usec
PL1 0 dB
SFO1 202.5370460 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 PL2 100.00 usec
PL12 0 dB
SFO2 17.52 dB
500.3320013 MHz

F2 - Processing parameters
SI 131072
SF 202.5371639 MHz
WD EM
W 0
SSB 1.00 Hz
LB 0
GB 1.40
PC

# $^1$H NMR, **7**

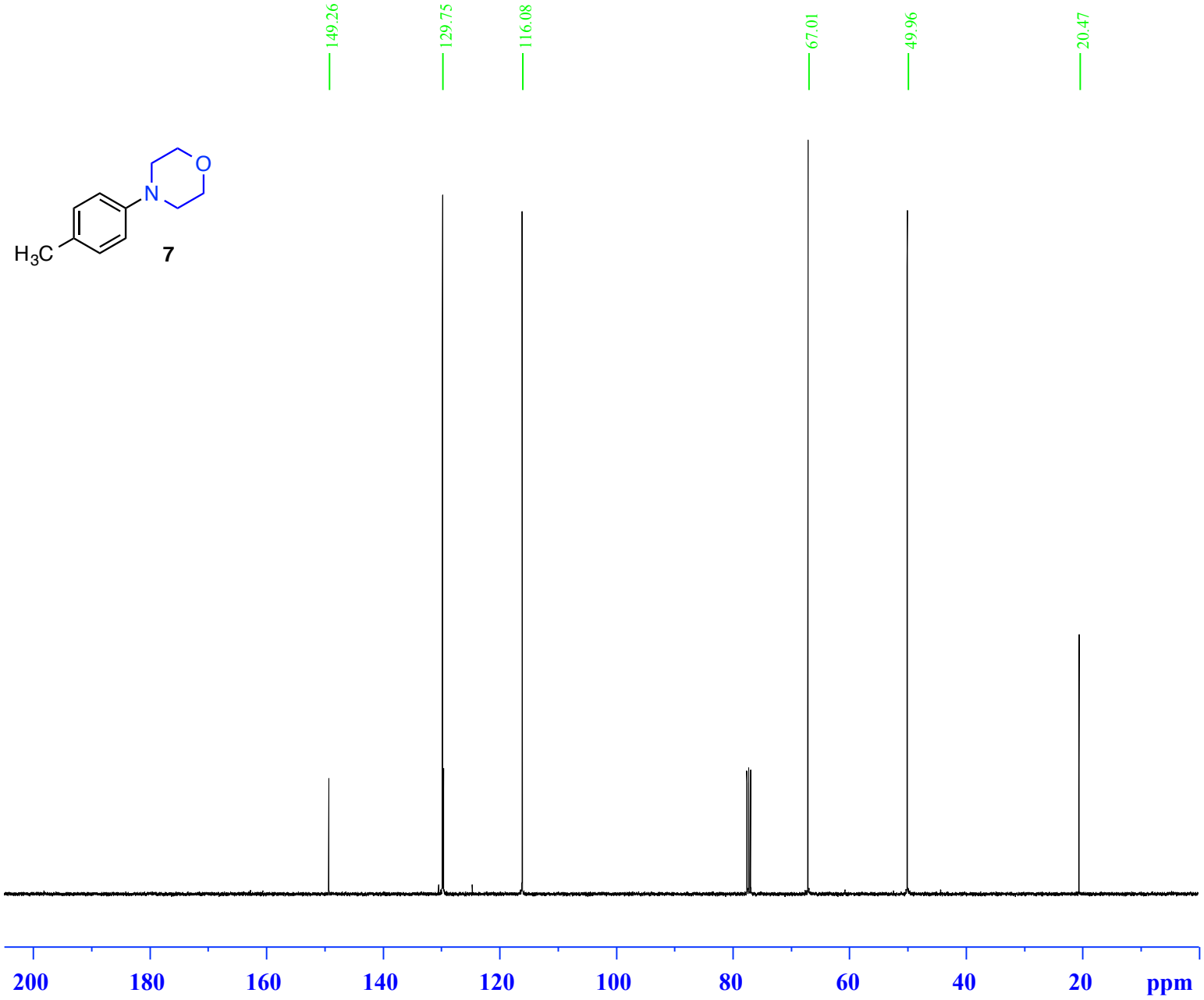



Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 120
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171013
Time 23.24
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 24
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 30.37
AQ 62.400 usec
RG 6.50 usec
DW 298.1 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300173 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **7**



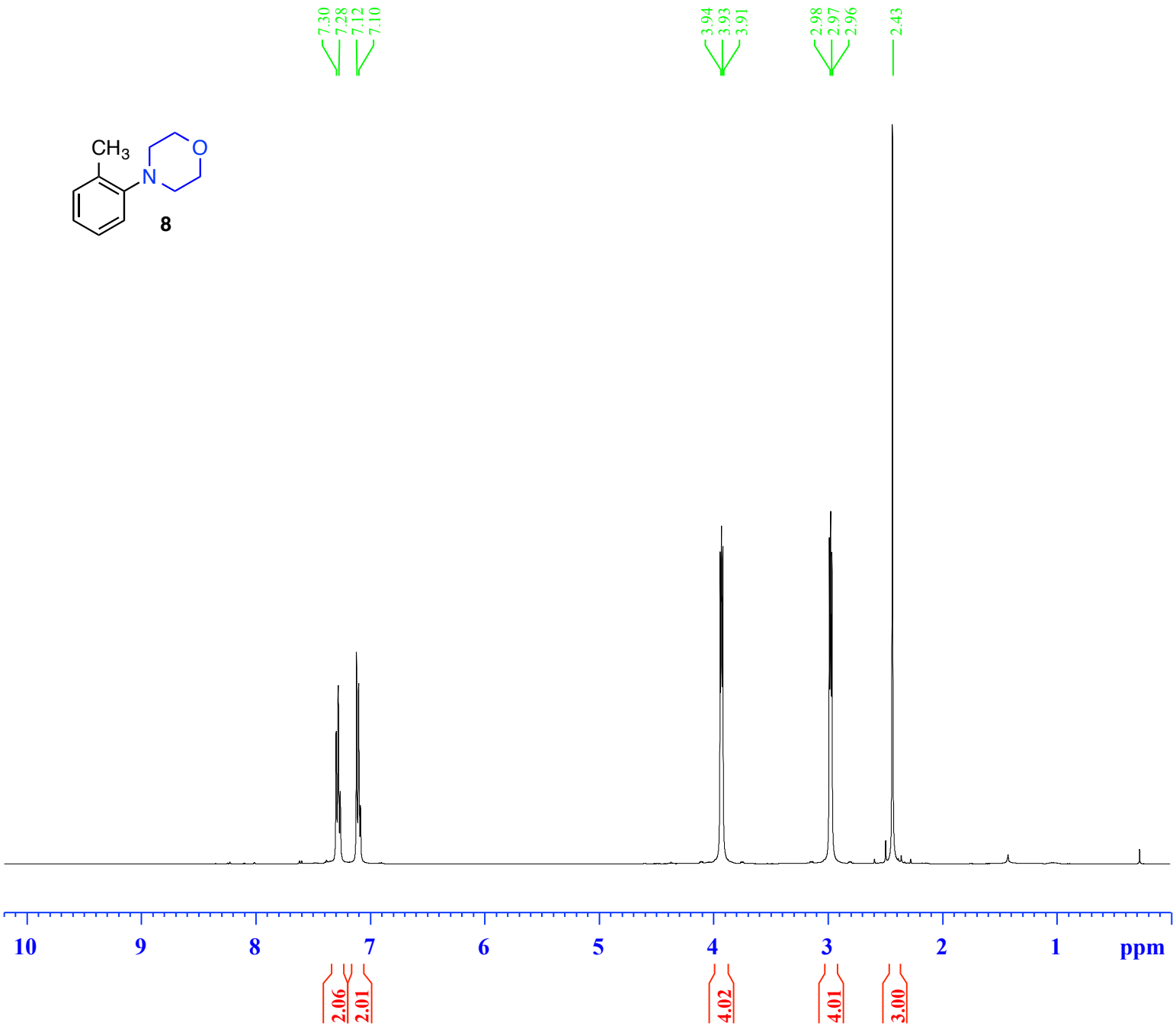

Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 121
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171013
Time 23.33
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 298.8 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127715 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **8**

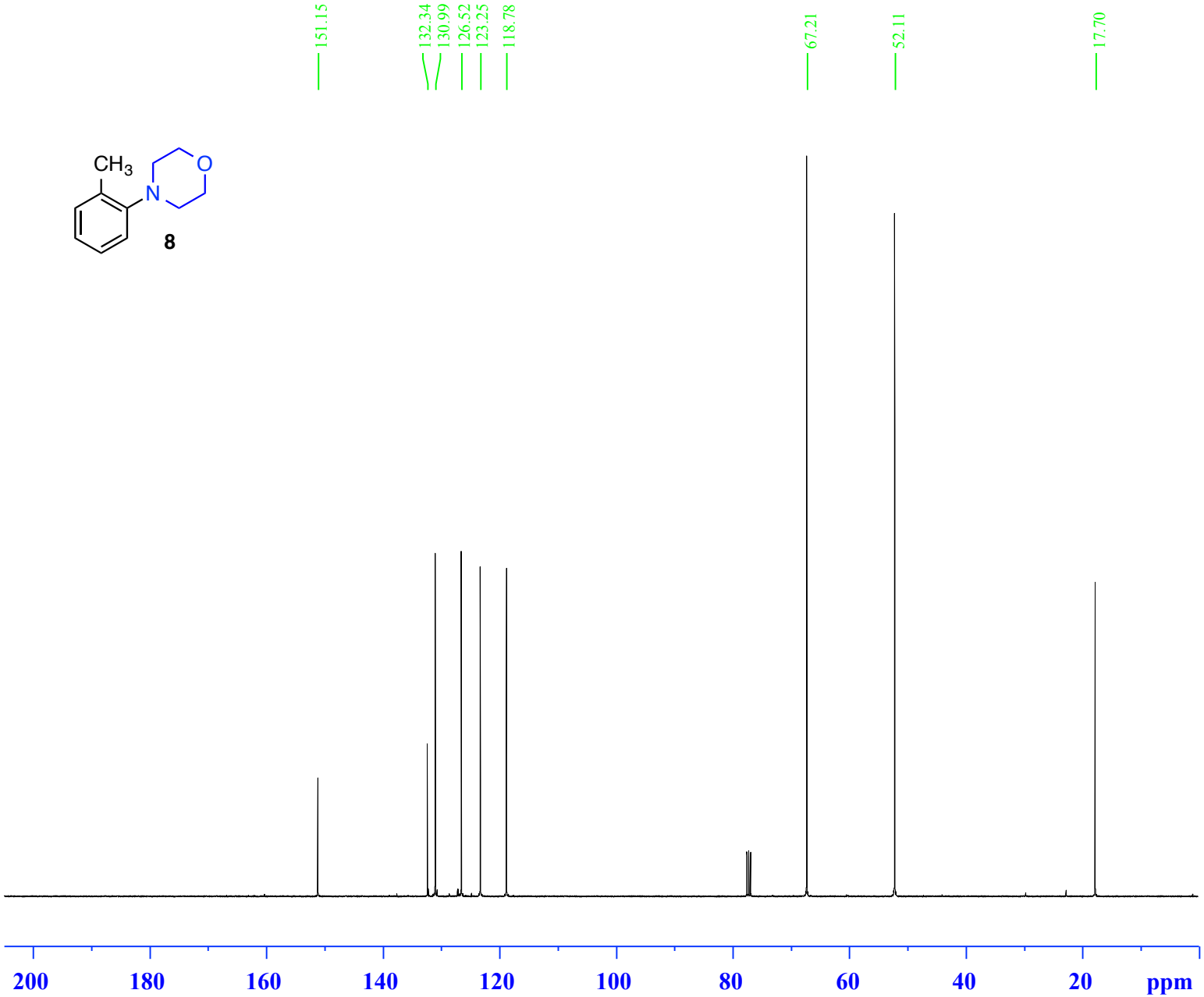



Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 130
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171013
Time 23.39
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 24
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 7.7
AQ 62.400 usec
RG 6.50 usec
DW 298.1 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300184 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **8**



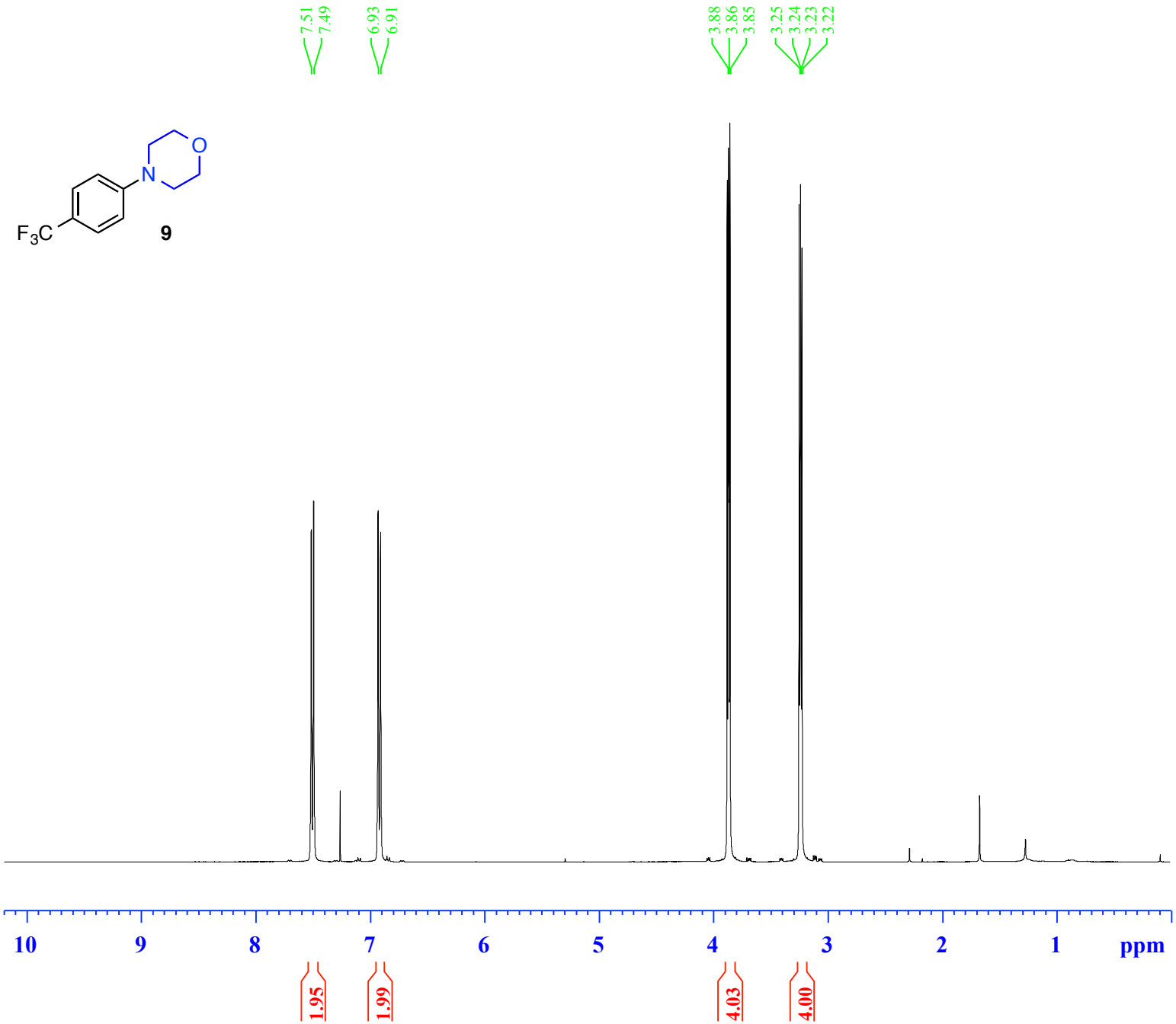

Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 131
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171013
Time 23.47
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 298.8 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6128007 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **9**

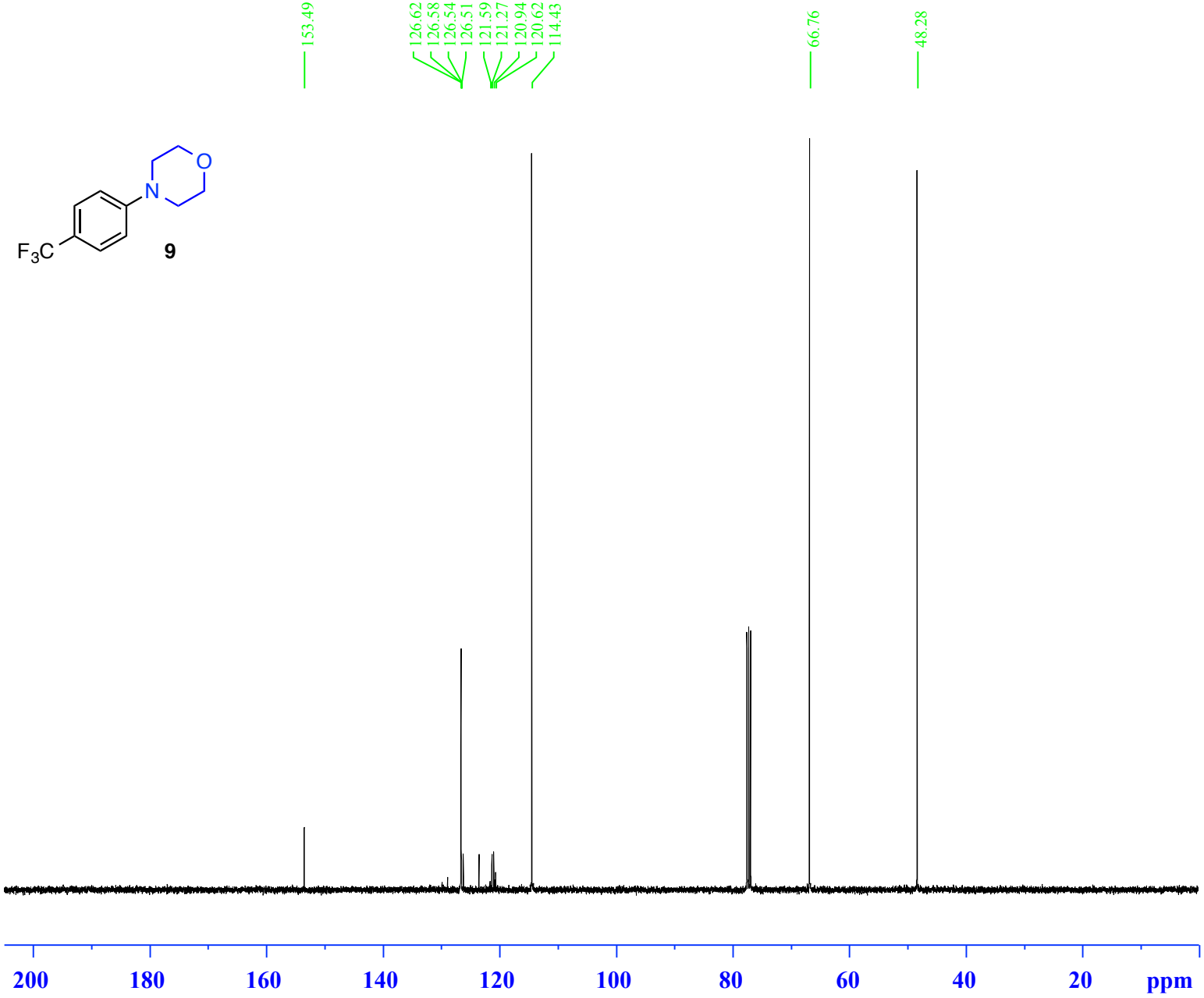



Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 140
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171013
Time 23.54
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 24
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 67.78
AQ 62.400 usec
RG 6.50 usec
DW 298.1 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300176 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **9**



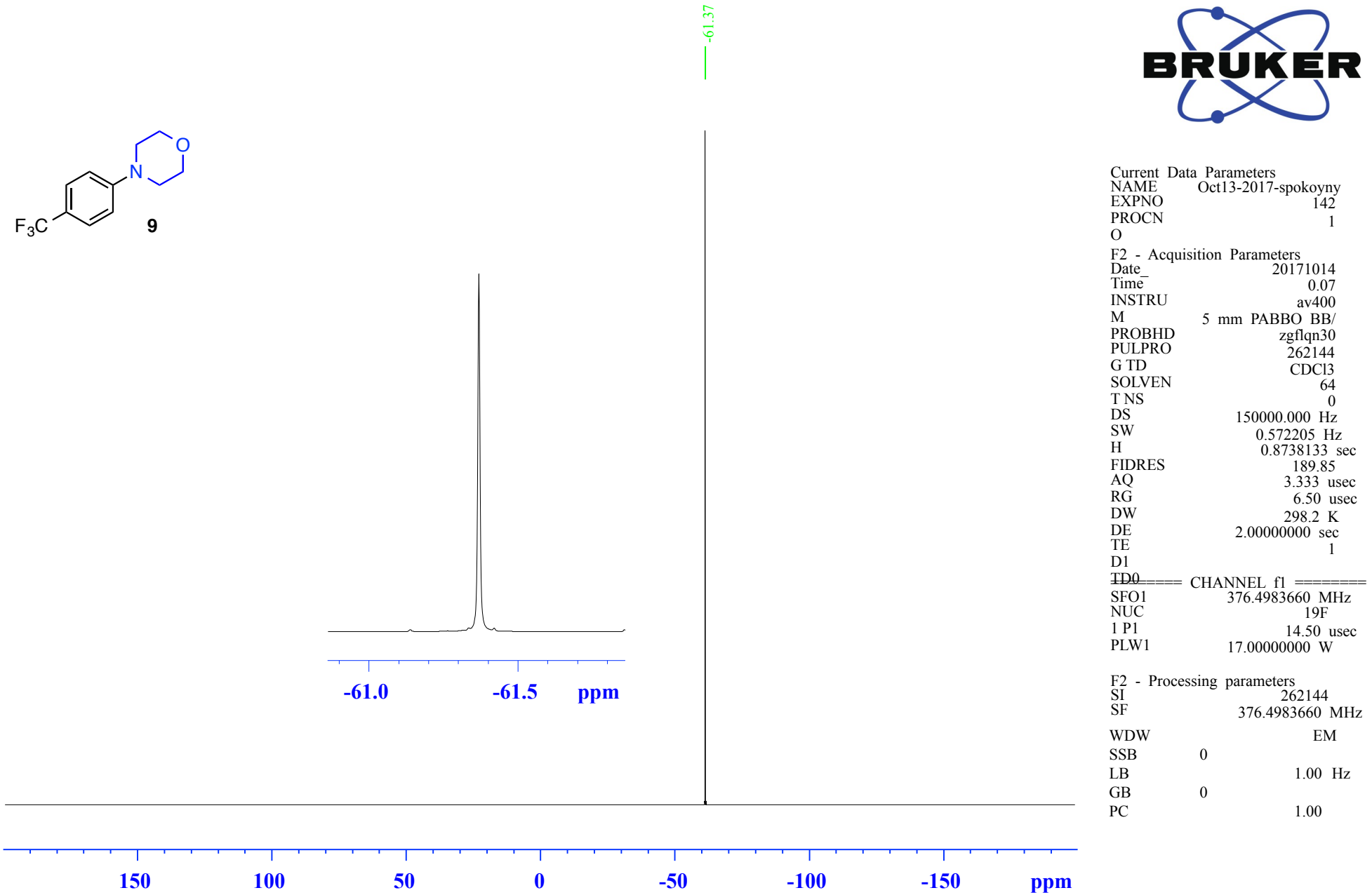

Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 141
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171014
Time 0.02
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 298.8 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127590 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^{19}$F NMR, **9**

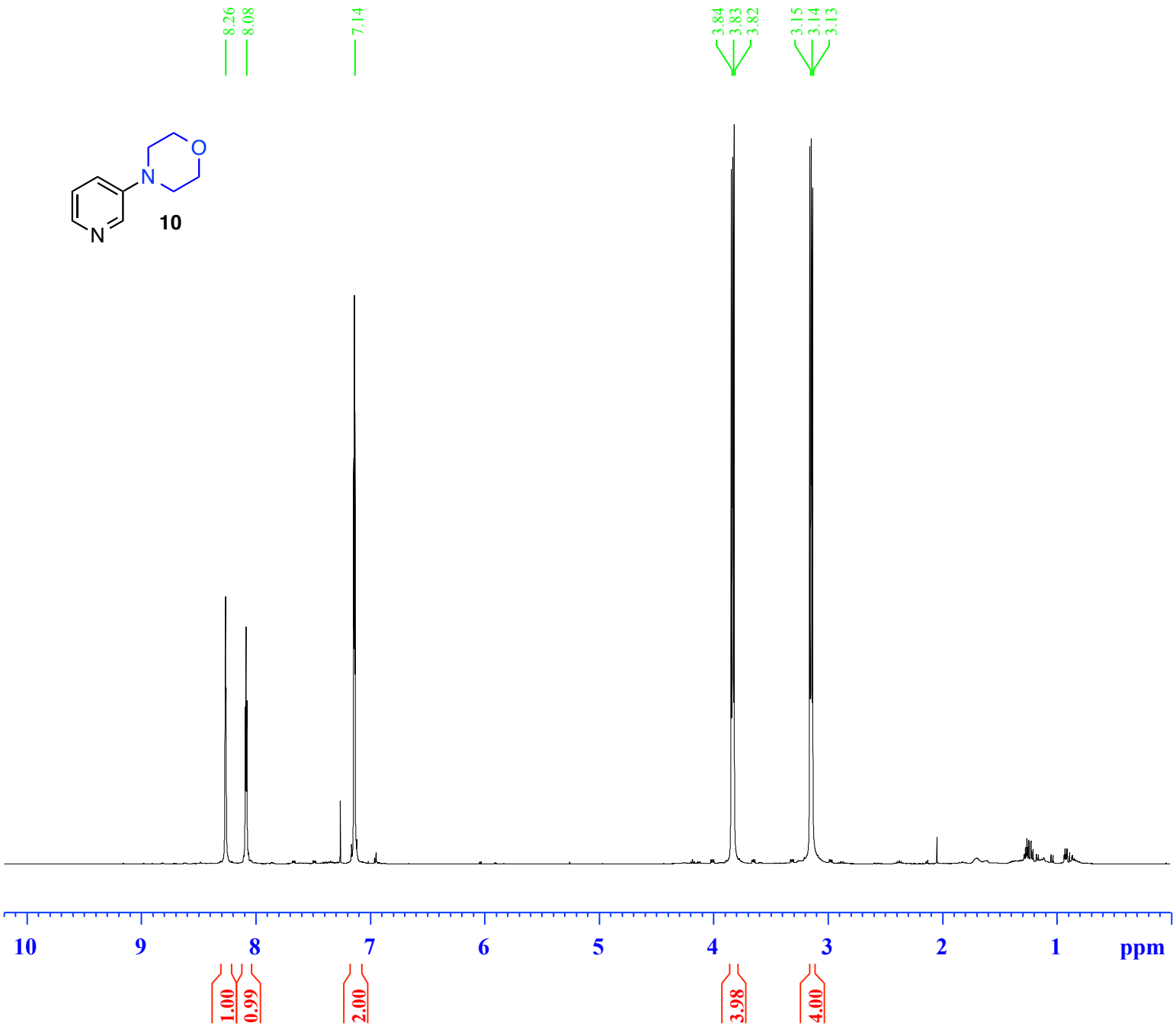



Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 142
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171014
Time 0.07
INSTRU av400
M 5 mm PABBO BB/
PROBHD zgflqn30
PULPRO 262144
G TD CDCl3
SOLVEN 64
T NS 0
DS 150000.000 Hz
SW 0.572205 Hz
H 0.8738133 sec
FIDRES 189.85
AQ 3.333 usec
RG 6.50 usec
DW 298.2 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 376.4983660 MHz
NUC 19F
1 P1 14.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 262144
SF 376.4983660 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

# $^{1}$H NMR, **10**

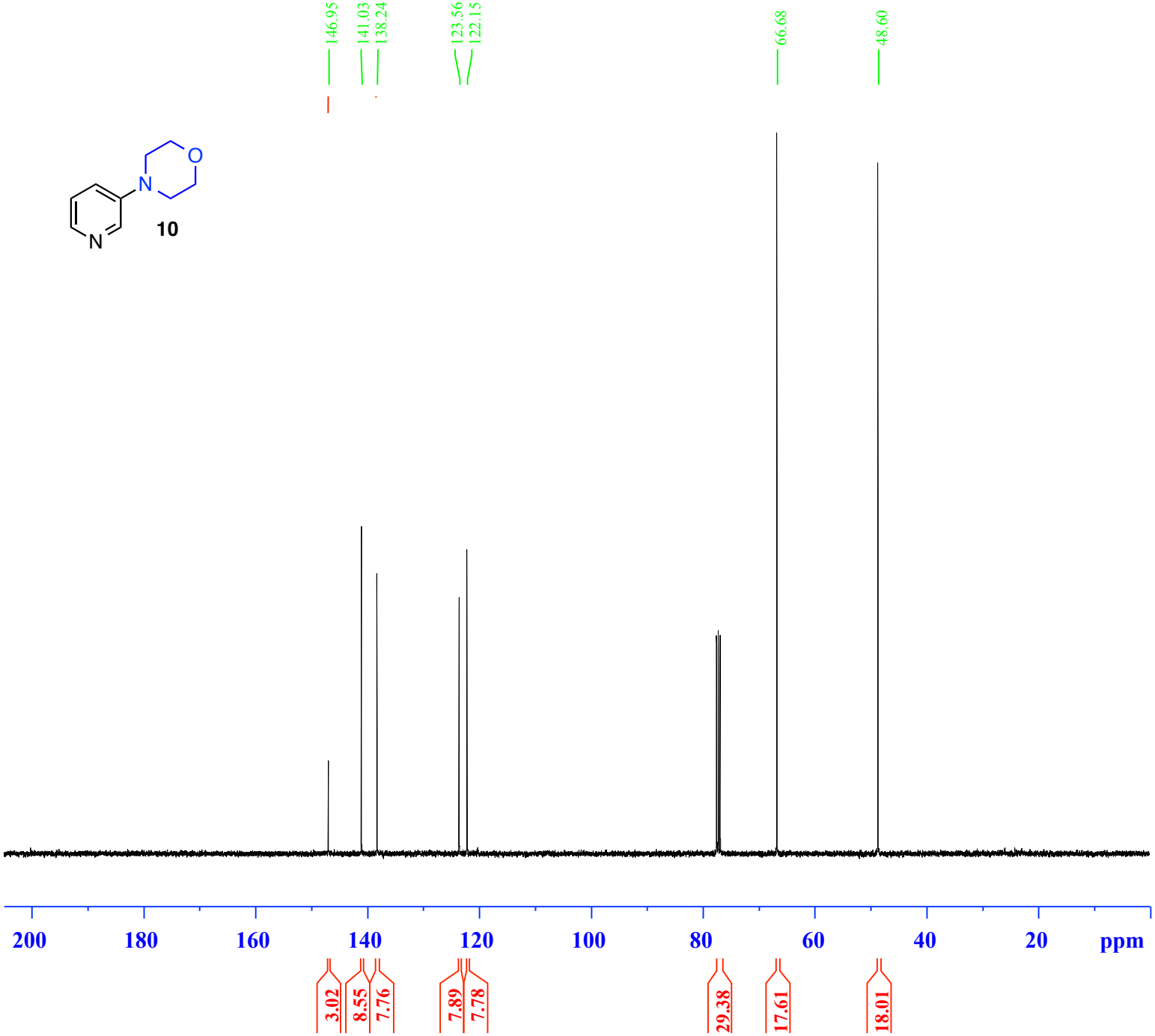



Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 160
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171014
Time 0.29
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 24
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 53.36
AQ 62.400 usec
RG 6.50 usec
DW 298.1 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300177 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **10**




BRUKER

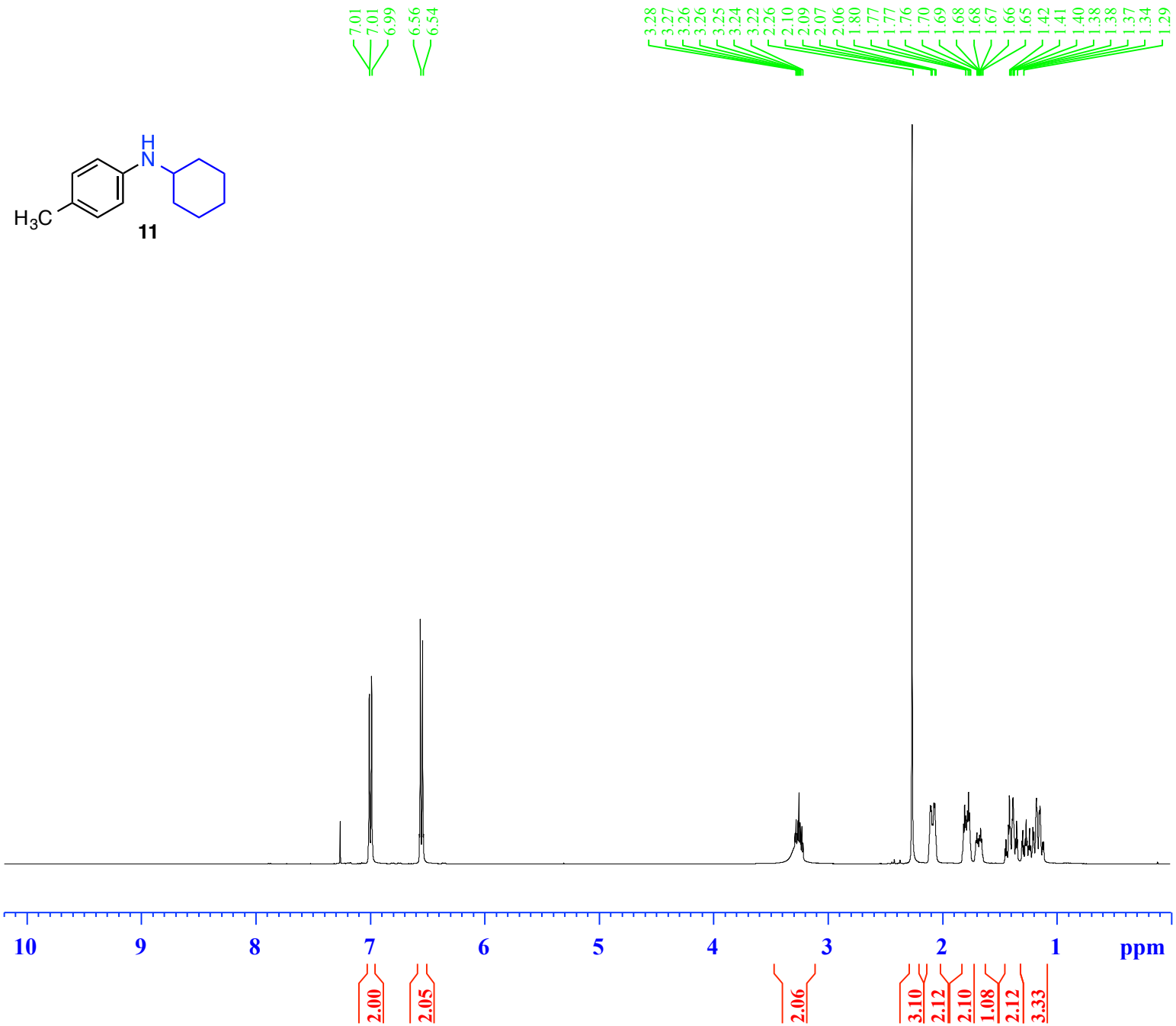
Current Data Parameters
NAME Oct13-2017-spokoyny
EXPNO 161
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171014
Time 0.37
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 298.8 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127662 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **11**



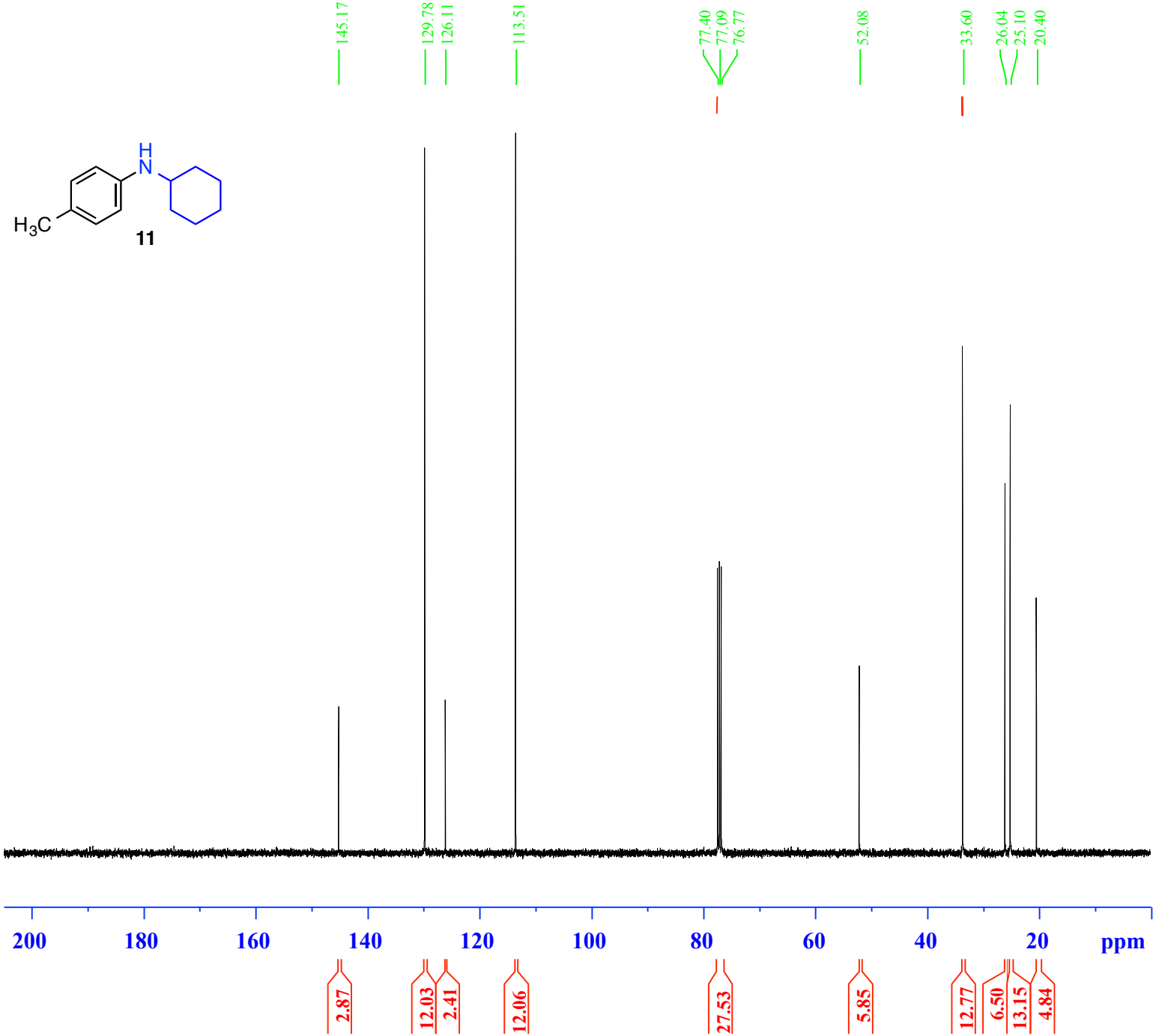

Current Data Parameters
NAME Nov20-2017-spokoyny
EXPNO 190
PROCN O 1

F2 - Acquisition Parameters
Date_ 20171120
Time 18.09
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG z g 3 0
TD 5 2 8 8 2
SOLVENT CDCl3
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.151523 Hz
AQ 3.2998369 sec
RG 48.1
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300175 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **11**




Current Data Parameters
NAME Nov20-2017-spokoyny
EXPNO 191
PROCNO 1

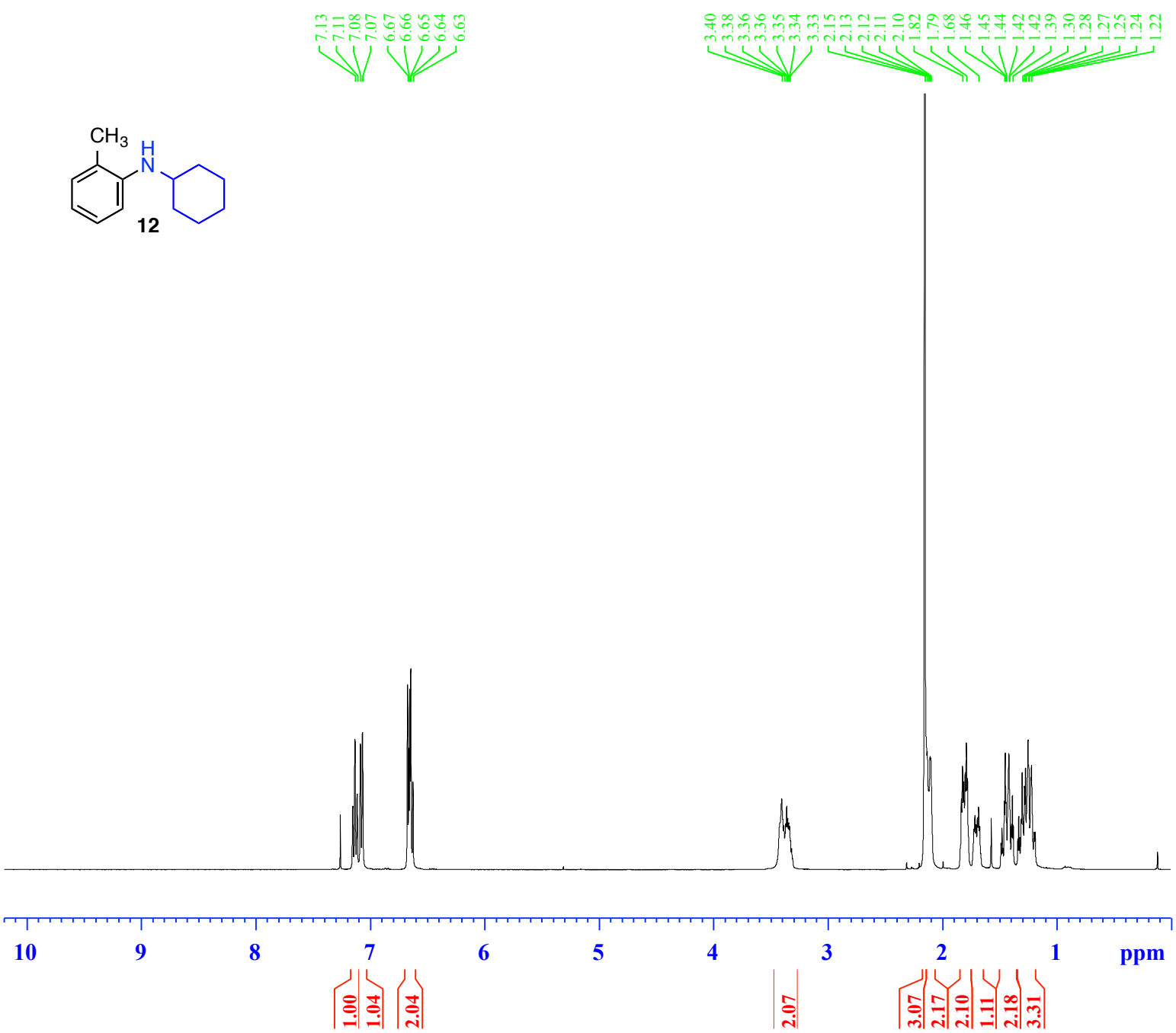
F2 - Acquisition Parameters
Date_ 20171120
Time 18.17
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 189.85
DW 19.800 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127701 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **12**

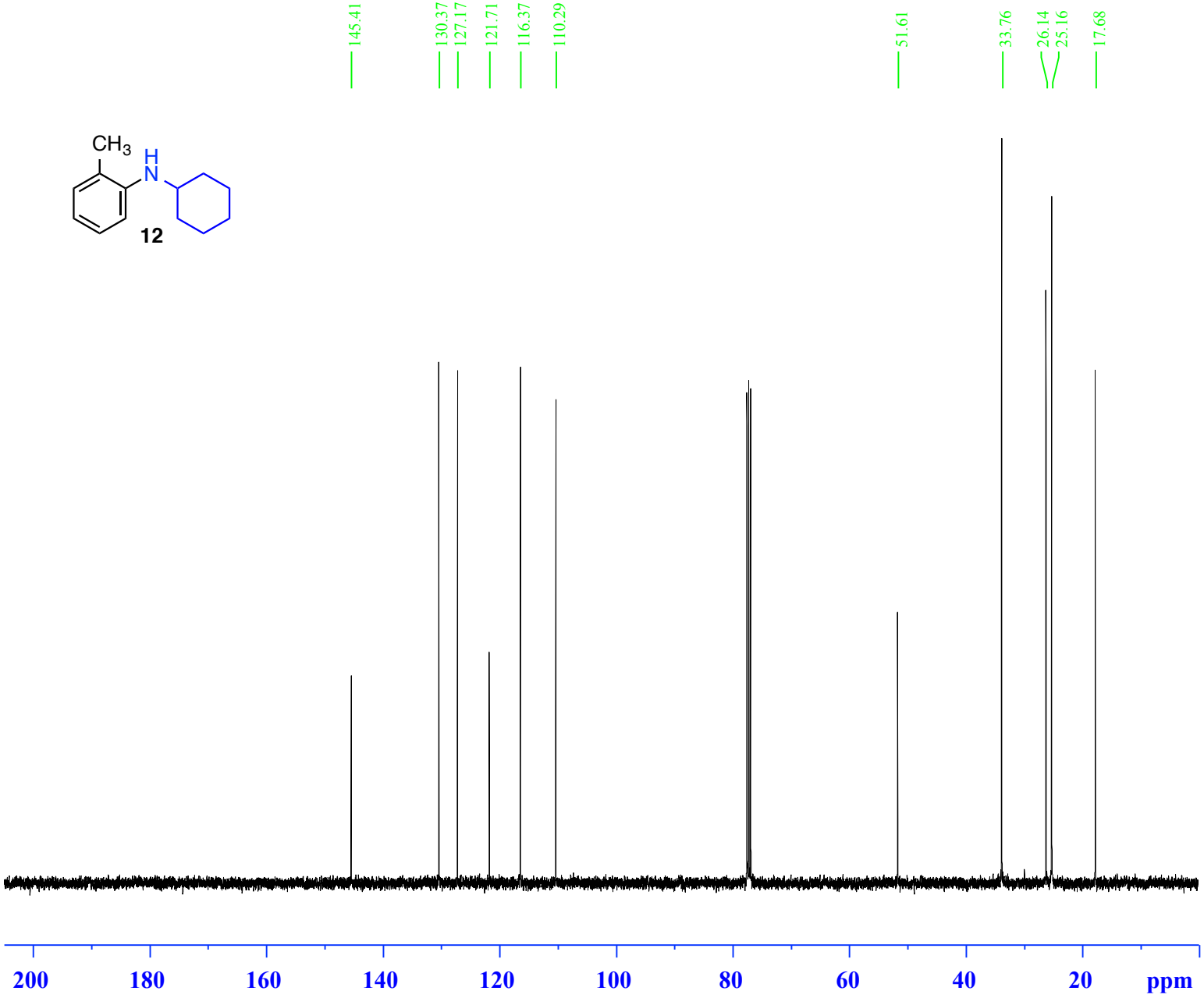


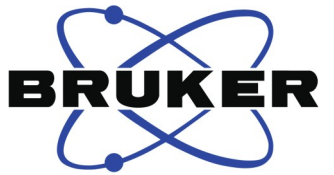

Current Data Parameters
NAME Oct26-2017-spokoyny
EXPNO 270
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171026
Time 22.07
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 53.36
AQ 62.400 usec
RG 6.50 usec
DW 298.4 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300175 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **12**




Current Data Parameters
NAME Oct26-2017-spokoyny
EXPNO 271
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171026
Time 22.15
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 189.85
DW 19.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

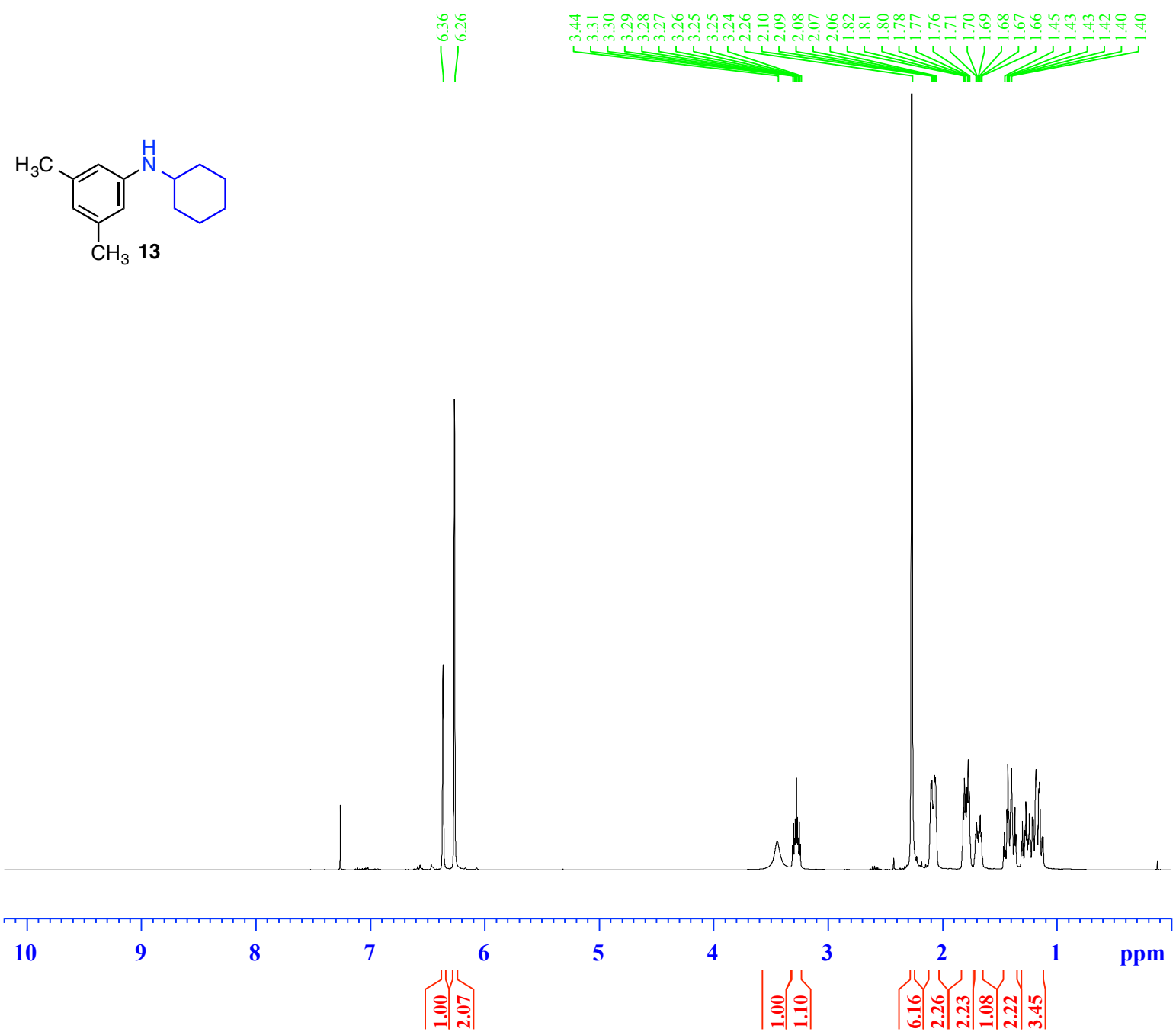
======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127623 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **13**




**13**

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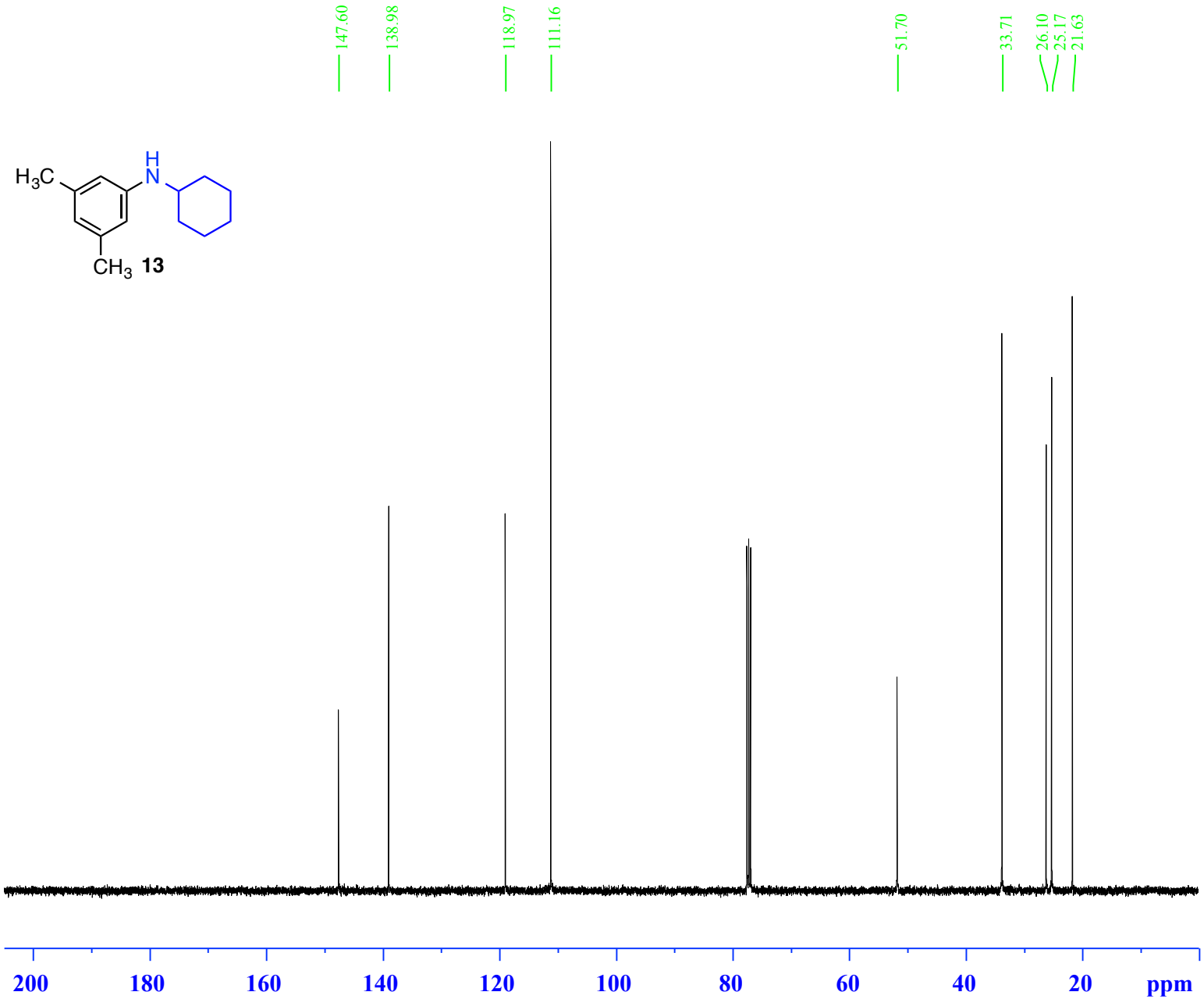
Current Data Parameters
NAME Nov20-2017-spokoyny
EXPNO 200
PROCN O 1

F2 - Acquisition Parameters
Date_ 20171120
Time 18.25
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPRO z g 3 0
G TD 5 2 8 8 2
SOLVEN CDCl3
T NS 32
DS 0
SW 8012.820 Hz
H 0.151523 Hz
FIDRES 3.2998369 sec
AQ 44.29
RG 62.400 usec
DW 6.50 usec
DE 297.9 K
TE 2.00000000 sec
D1 1
TD0

CHANNEL f1
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300175 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$NMR, **13**




**13**

BRUKER

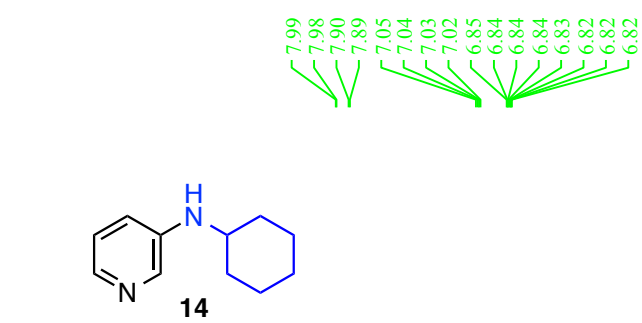
Current Data Parameters
NAME Nov20-2017-spokoyny
EXPNO 201
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171120
Time 18.33
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 298.7 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127631 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

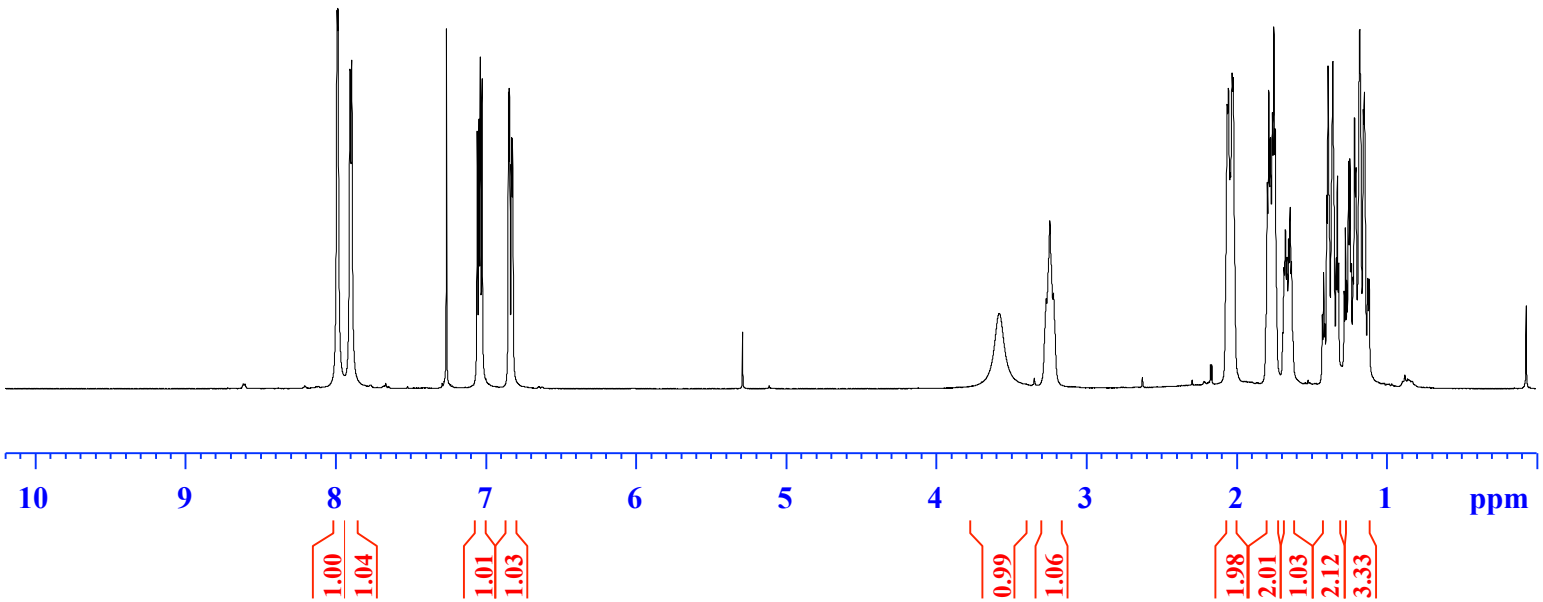
# $^1$H NMR, **14**







**14**

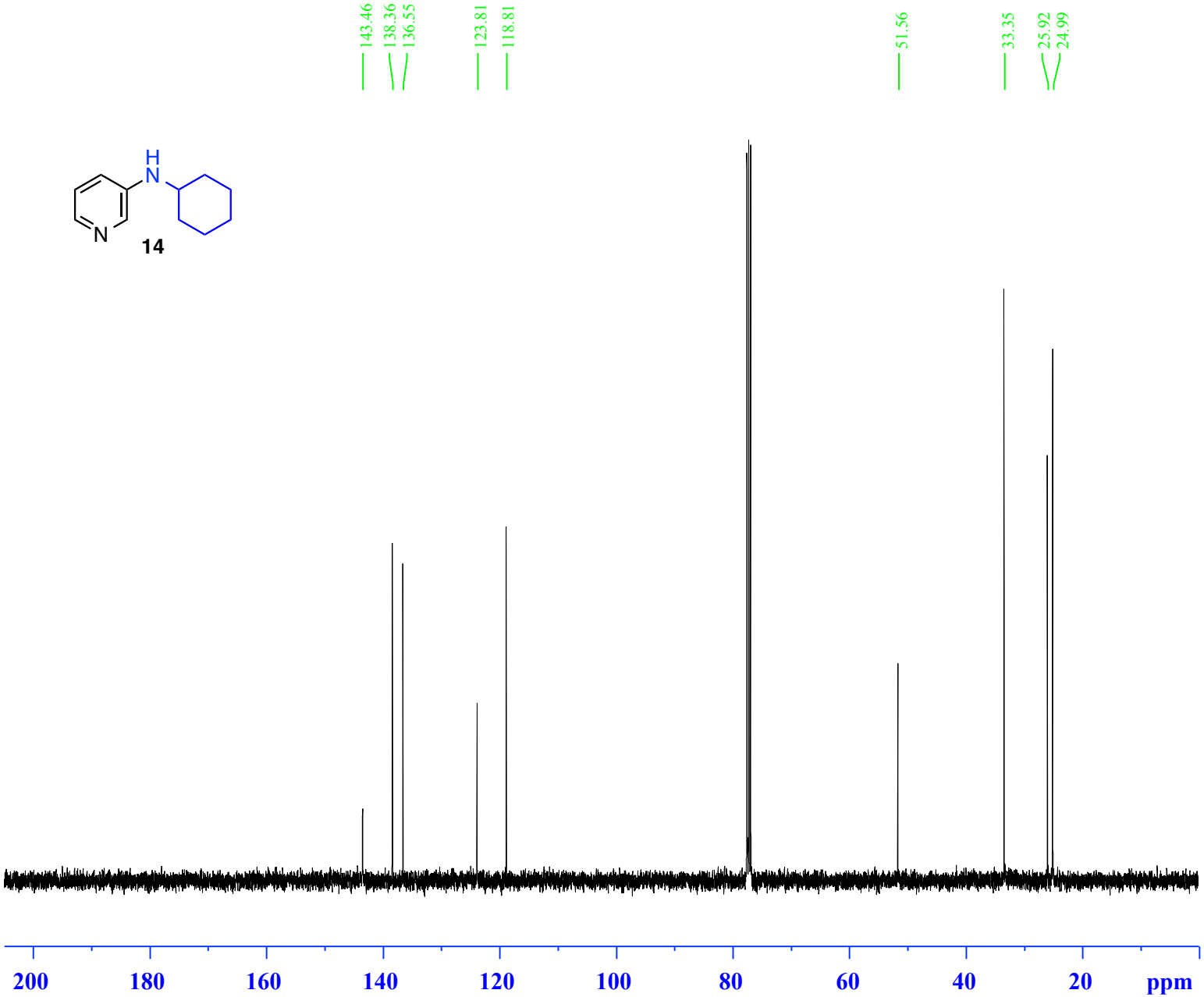



Current Data Parameters
NAME Nov22-2017-spokoyny
EXPNO 10
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171122
Time 14.02
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 107.83
AQ 62.400 usec
RG 6.50 usec
DW 298.5 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300177 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **14**







**14**

Current Data Parameters
NAME Nov22-2017-spokoyny
EXPNO 11
PROCNO 1

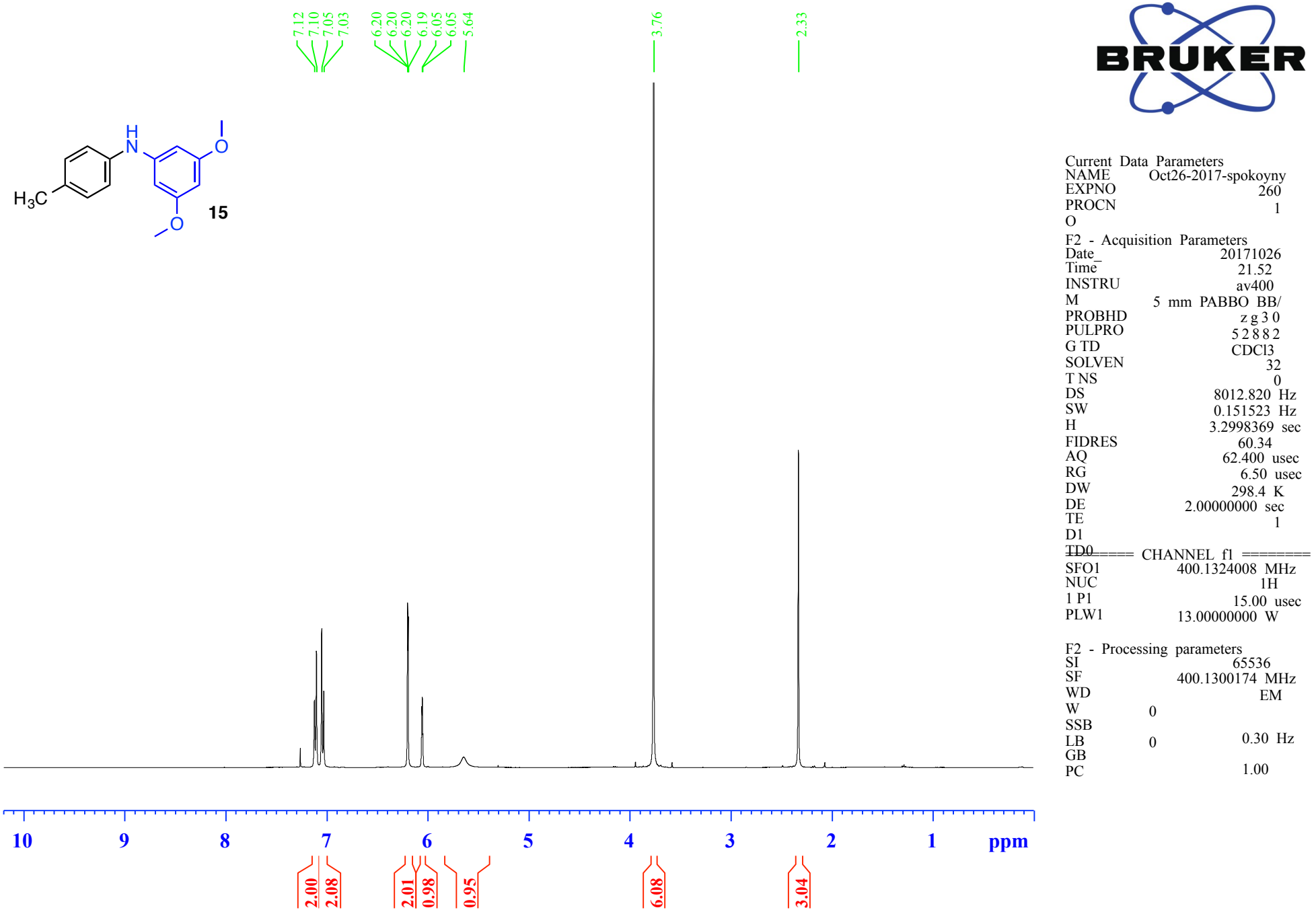
F2 - Acquisition Parameters
Date_ 20171122
Time 13.58
INSTRUM av400
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976128 sec
RG 189.85
DW 19.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127590 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **15**

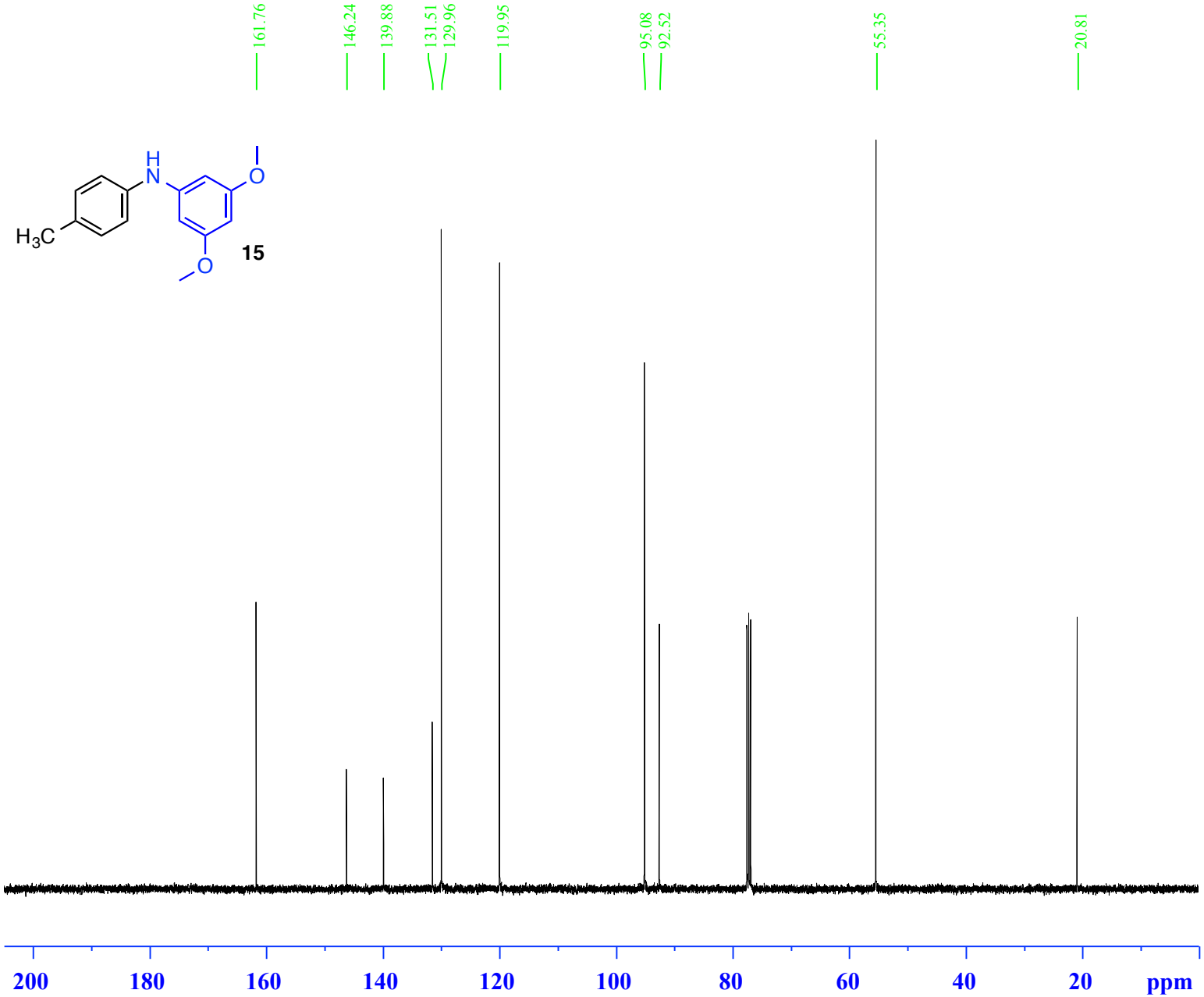



Current Data Parameters
NAME Oct26-2017-spokoyny
EXPNO 260
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171026
Time 21.52
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 60.34
AQ 62.400 usec
RG 6.50 usec
DW 298.4 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

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

# $^{13}C\{^{1}H\}$ NMR, **15**



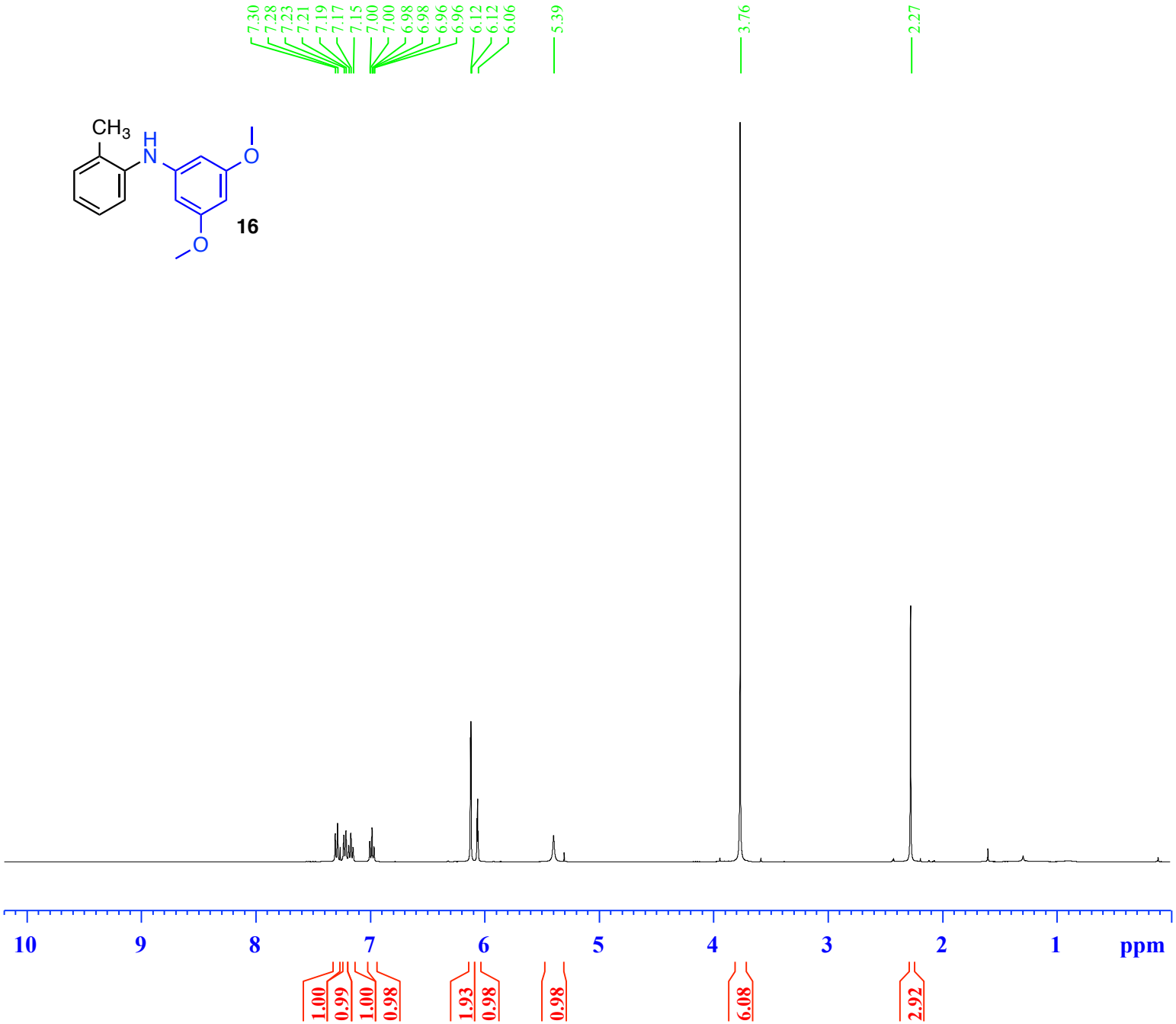

Current Data Parameters
NAME Oct26-2017-spokoyny
EXPNO 261
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171026
Time 22.00
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 299.2 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======= CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127634 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **16**

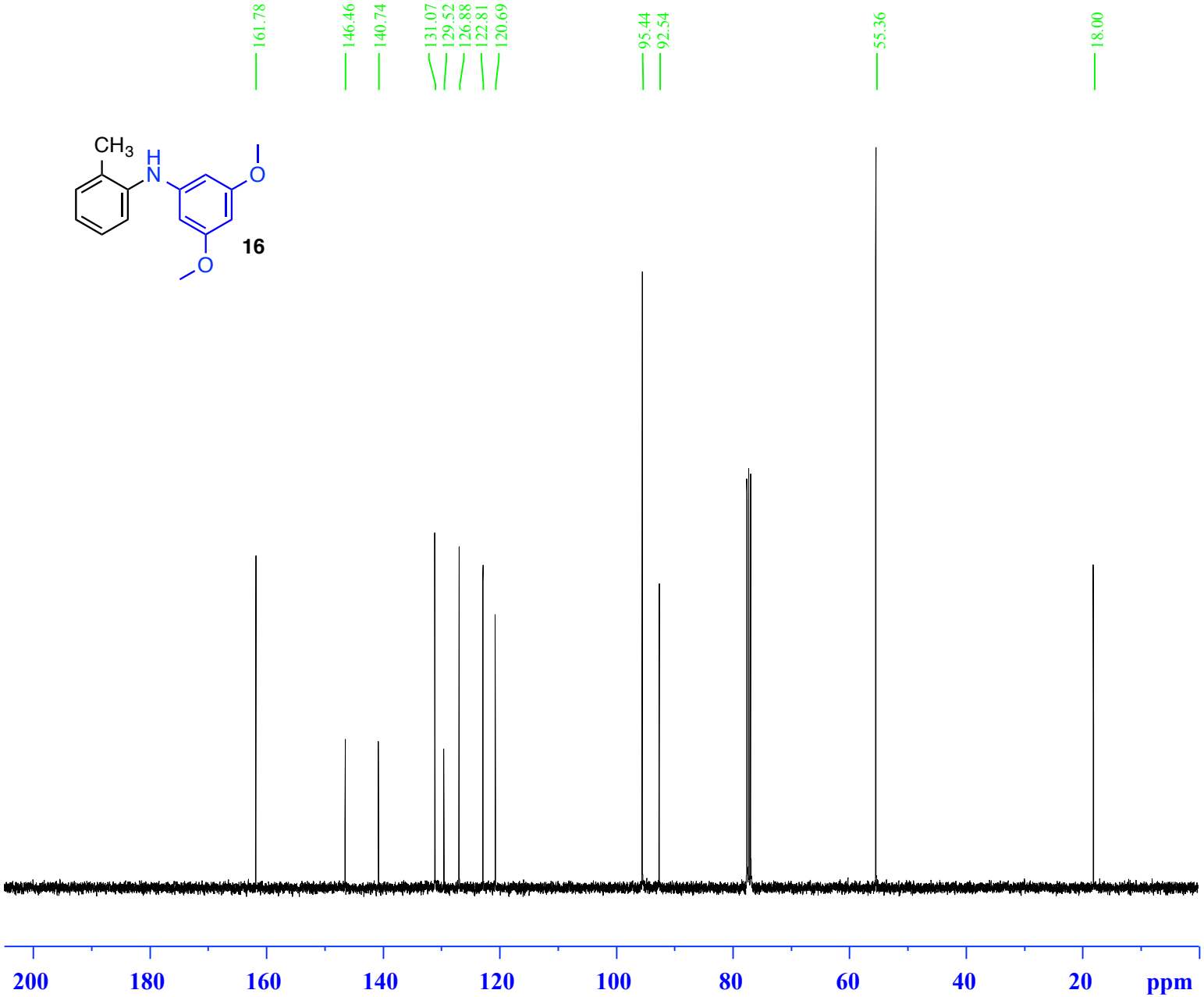



Current Data Parameters
NAME Oct23-2017-spokoyny
EXPNO 160
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171023
Time 20.15
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 67.78
AQ 62.400 usec
RG 6.50 usec
DW 298.5 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300175 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **16**



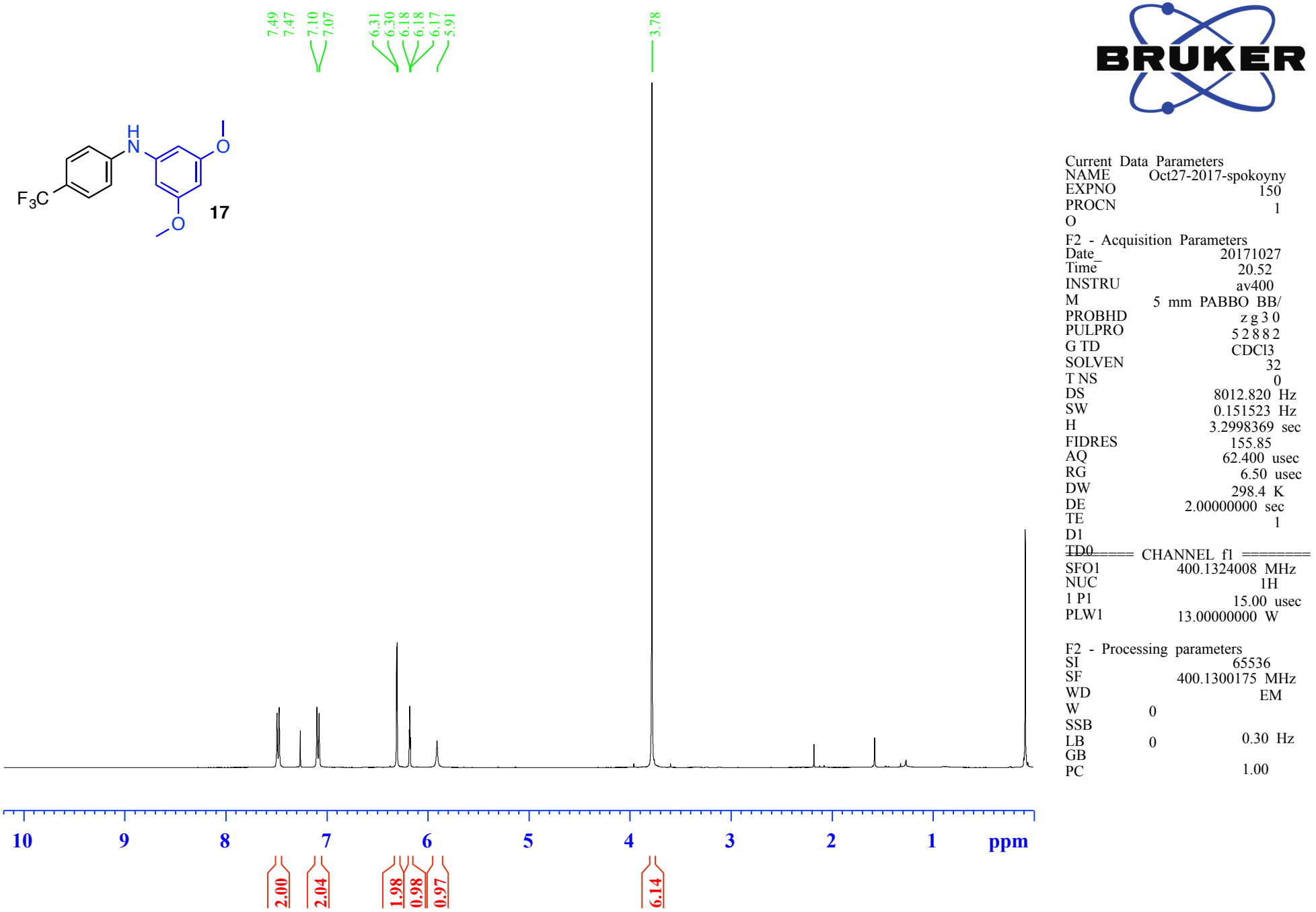

Current Data Parameters
NAME Oct23-2017-spokoyny
EXPNO 161
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171023
Time 20.24
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 299.3 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127623 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **17**

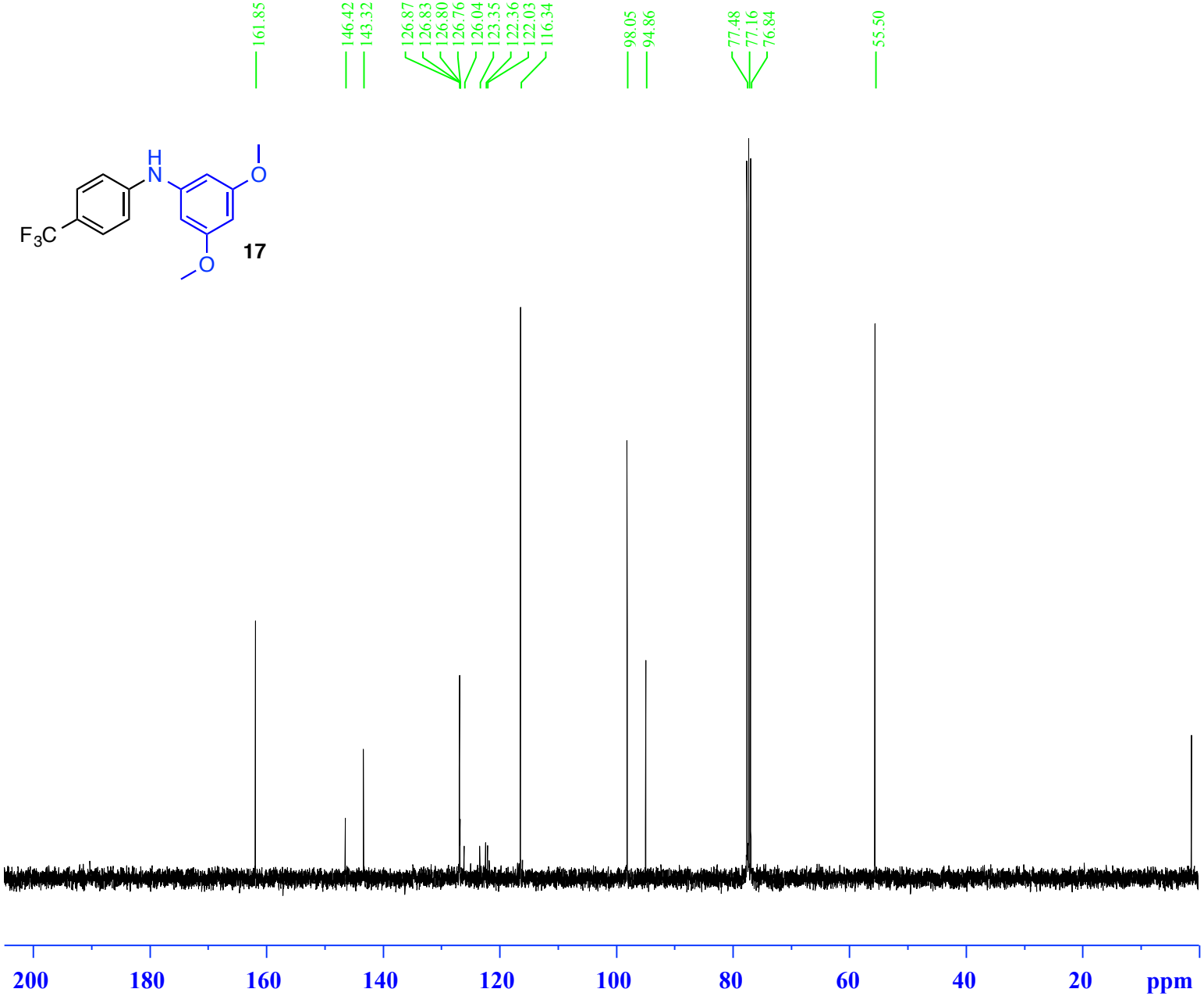



Current Data Parameters
NAME Oct27-2017-spokoyny
EXPNO 150
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171027
Time 20.52
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 155.85
AQ 62.400 usec
RG 6.50 usec
DW 298.4 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300175 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **17**



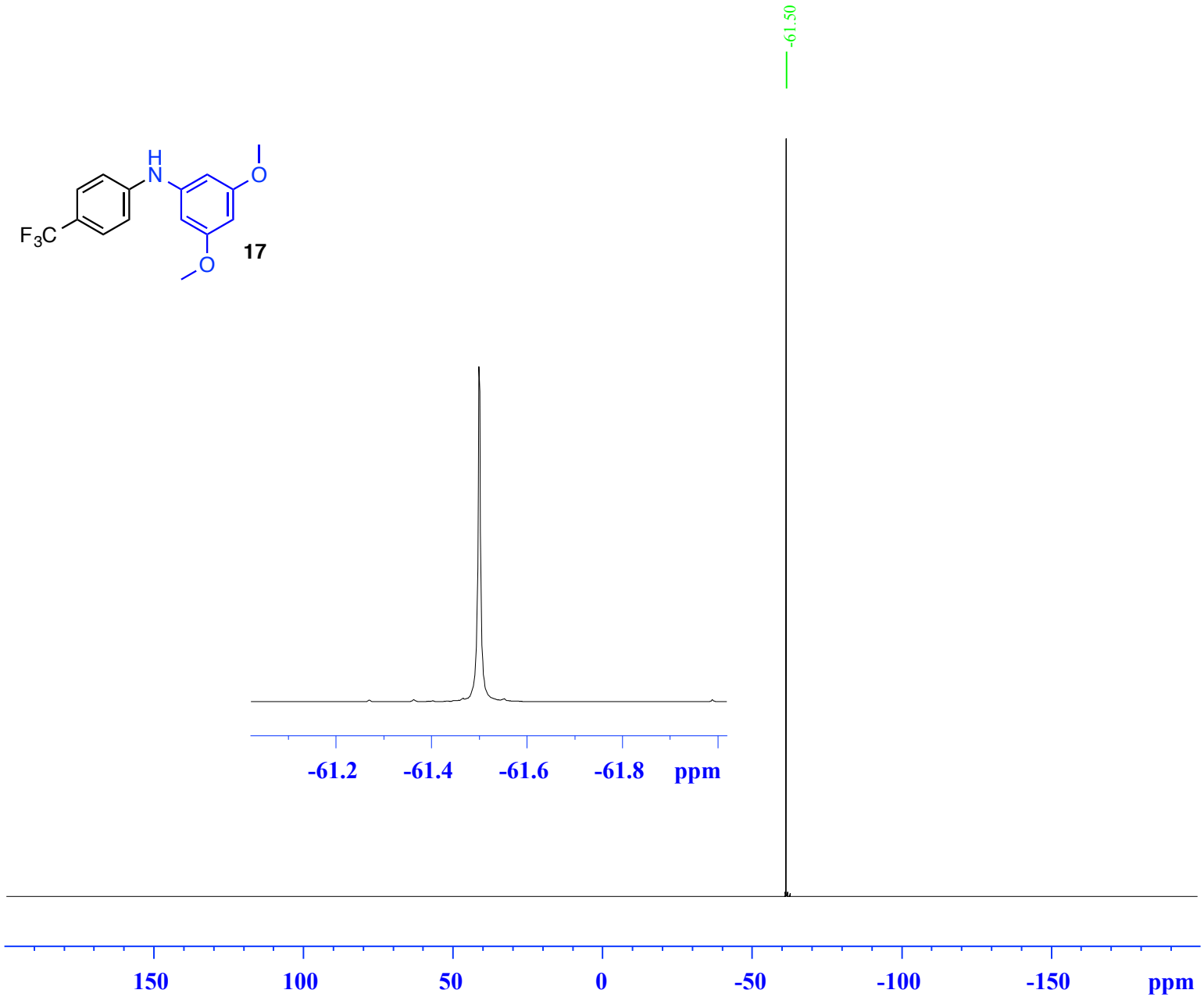

Current Data Parameters
NAME Oct27-2017-spokoyny
EXPNO 151
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171027
Time 21.00
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 299.2 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127573 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^{19}F\{^{1}H\}$ NMR, **17**



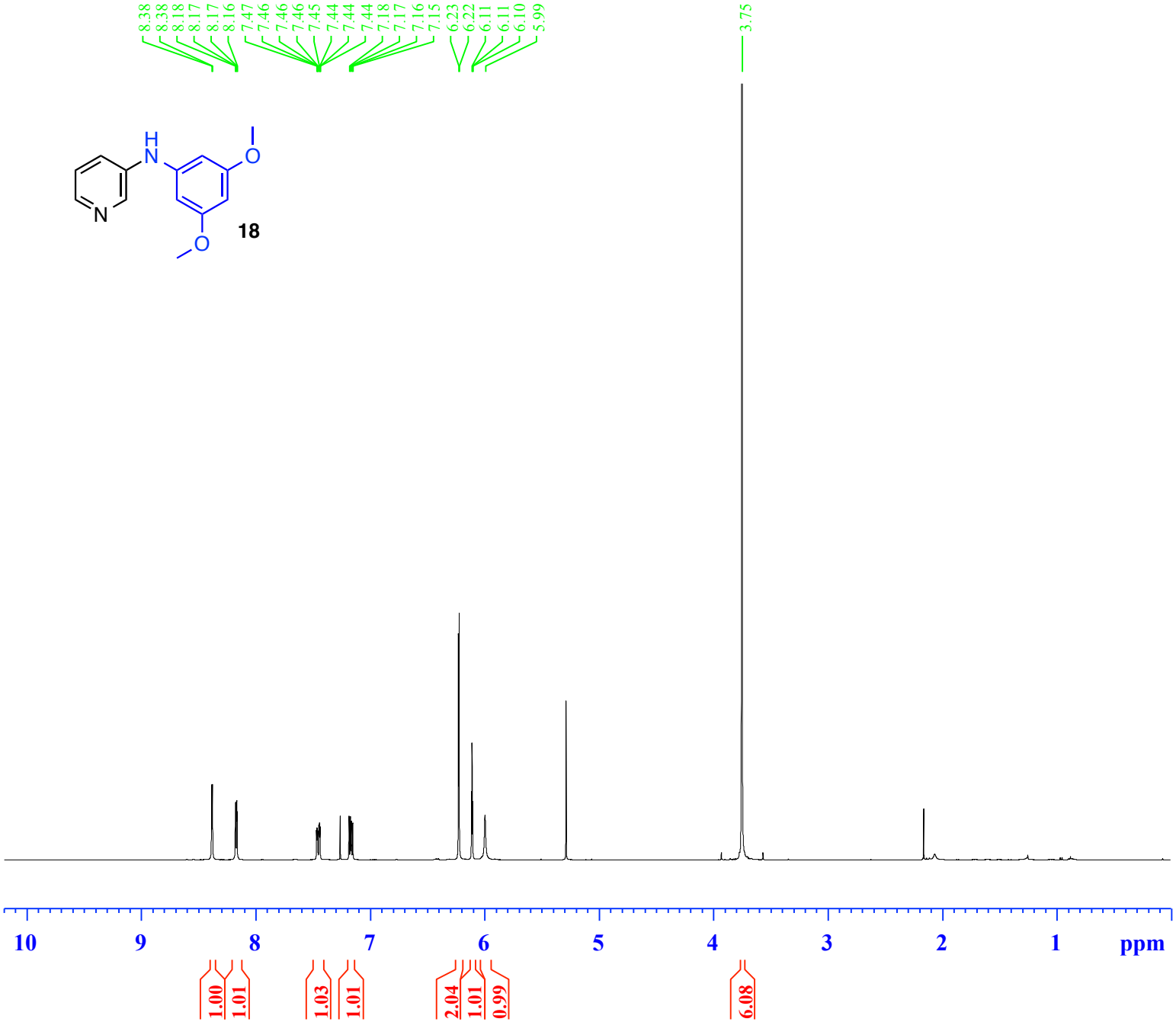

Current Data Parameters
NAME Oct27-2017-spokoyny
EXPNO 152
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171027
Time 21.03
INSTRU av400
M 5 mm PABBO BB/
PROBHD zgfhigqn.2
PULPRO 262144
G TD CDCl3
SOLVEN 32
T NS 0
DS 150000.000 Hz
SW 0.572205 Hz
H 0.8738133 sec
FIDRES 189.85
AQ 3.333 usec
RG 6.50 usec
DW 298.8 K
DE 1.00000000 sec
TE 0.03000000 sec
D1 0.00002000 sec
D11 1
D12
TD0 ======== CHANNEL f1 ========
SFO1 376.4983660 MHz
NUC 19F
1 P1 14.50 usec
PLW1 17.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W

F2 - Processing parameters
SI 262144
SF 376.4983660 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

# $^1$H NMR, **18**

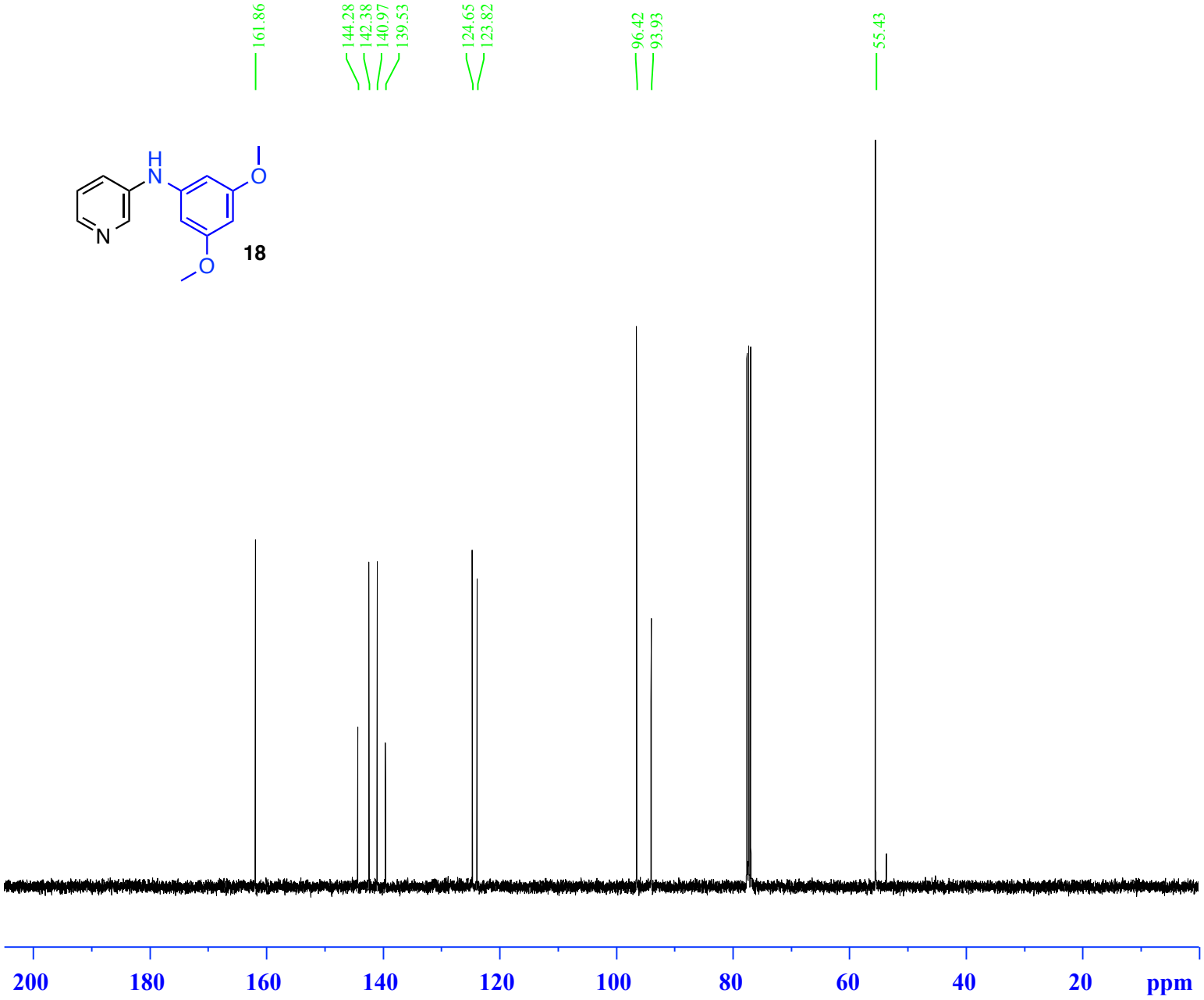



Current Data Parameters
NAME Oct27-2017-spokoyny
EXPNO 160
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171027
Time 21.09
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 94.6
AQ 62.400 usec
RG 6.50 usec
DW 298.4 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300176 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **18**



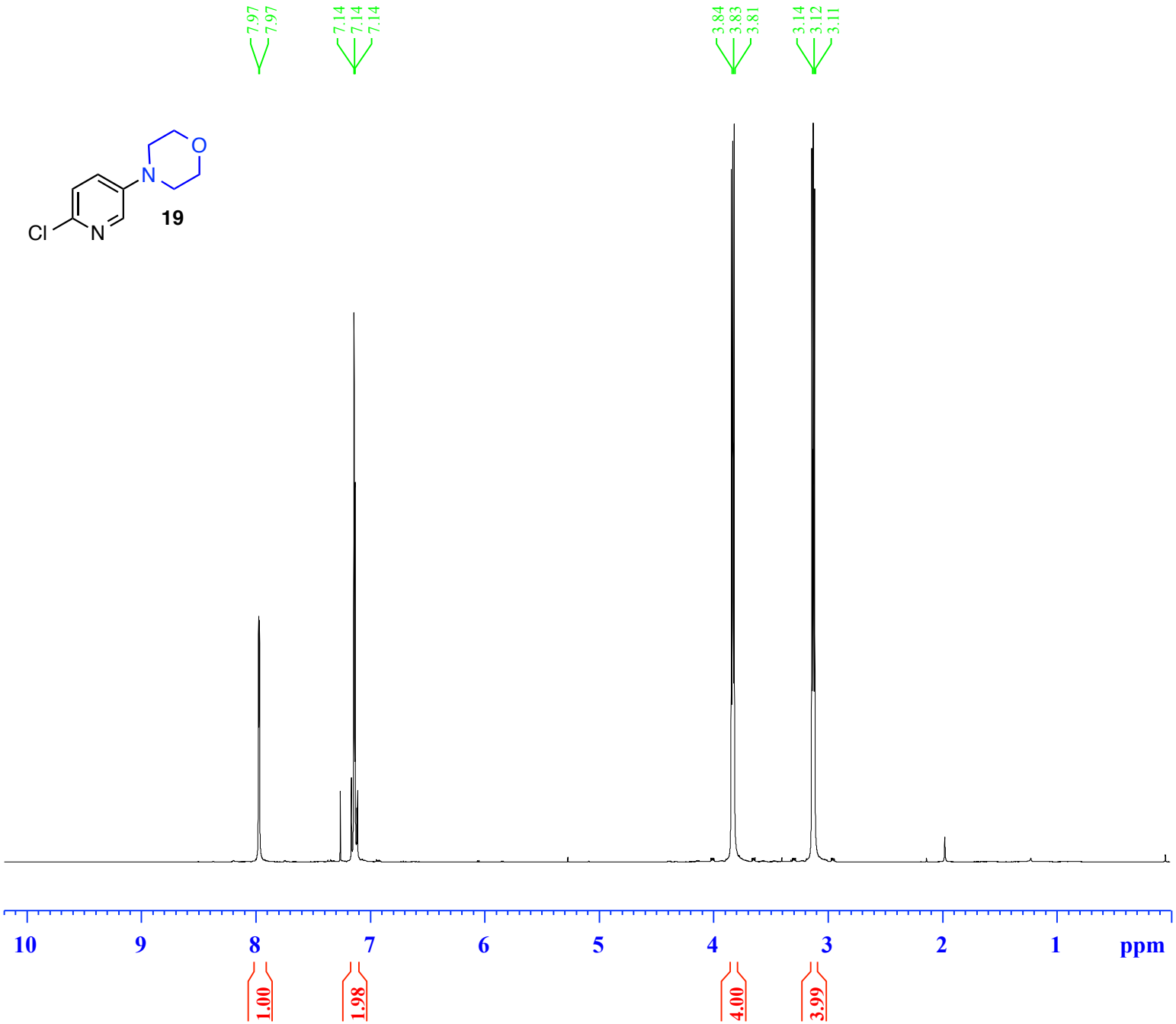

Current Data Parameters
NAME Oct27-2017-spokoyny
EXPNO 161
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171027
Time 21.18
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 299.2 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127609 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **19**

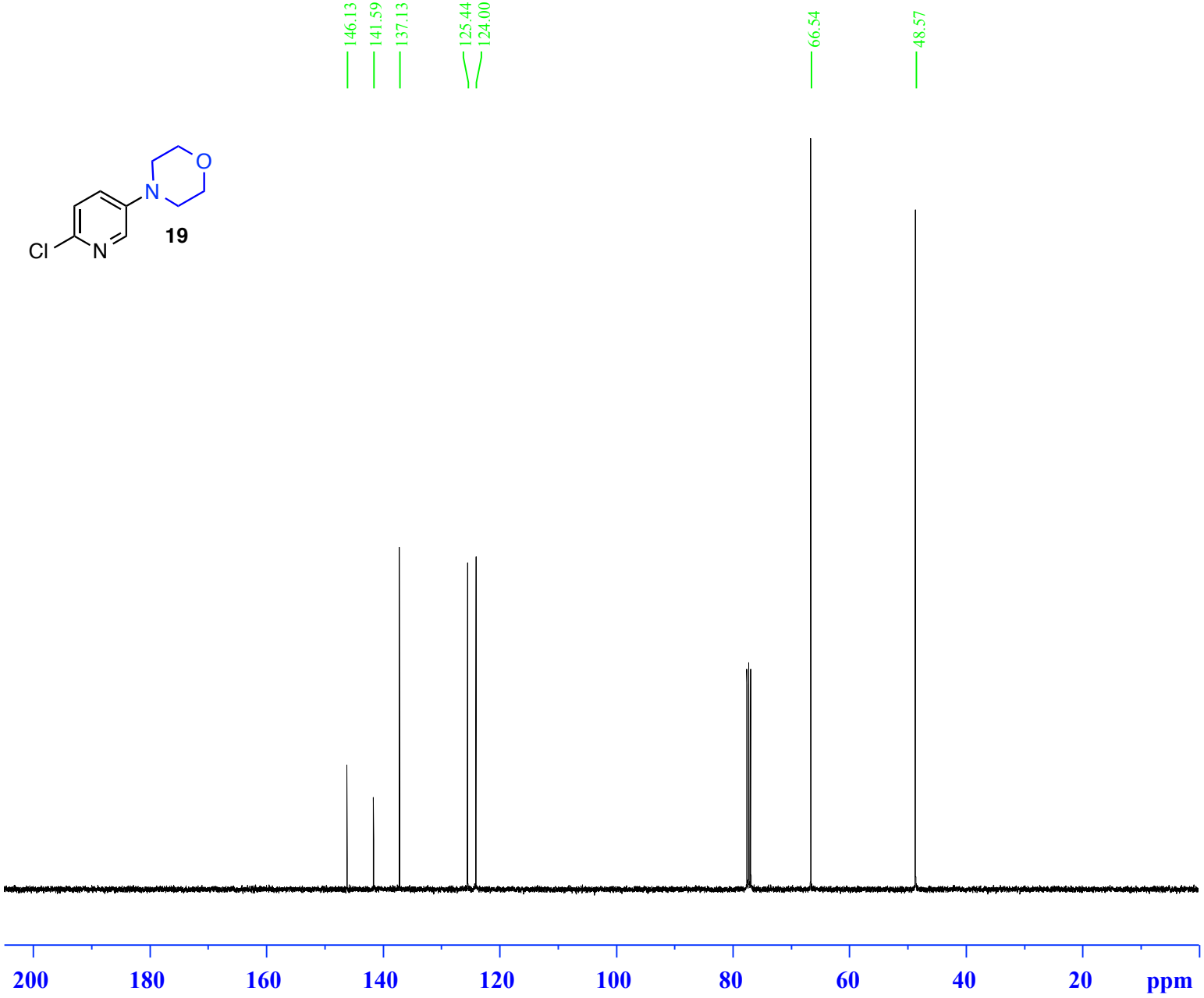



Current Data Parameters
NAME Nov20-2017-spokoyny
EXPNO 210
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171120
Time 18.40
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g 3 0
PULPRO 5 2 8 8 2
G TD CDCl3
SOLVEN 32
T NS 0
DS 8012.820 Hz
SW 0.151523 Hz
H 3.2998369 sec
FIDRES 67.78
AQ 62.400 usec
RG 6.50 usec
DW 298.0 K
DE 2.00000000 sec
TE 1
D1
TD0 ======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC 1H
1 P1 15.00 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300176 MHz
WD EM
W 0
SSB
LB 0 0.30 Hz
GB
PC 1.00

# $^{13}C\{^{1}H\}$ NMR, **19**



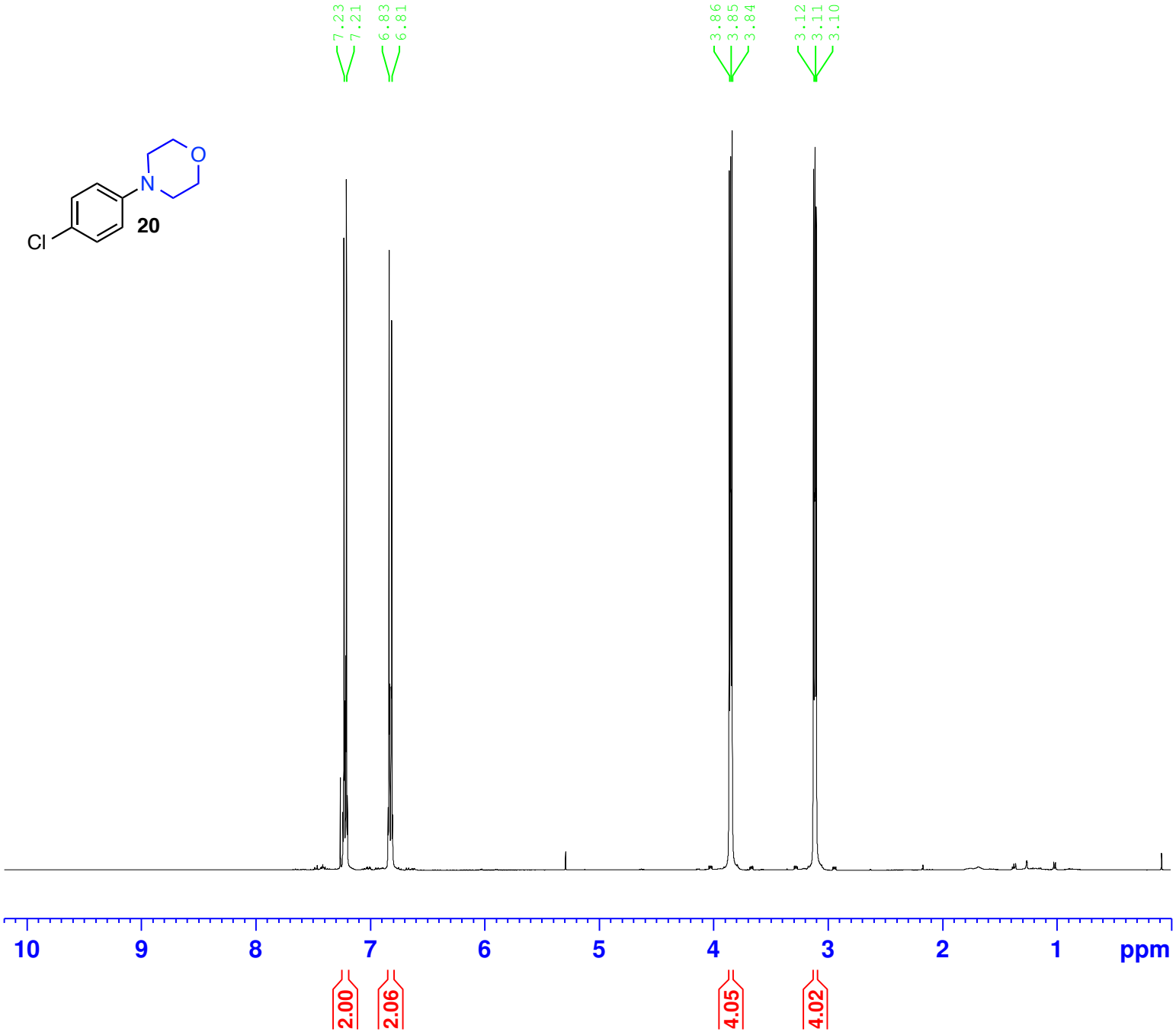

Current Data Parameters
NAME Nov20-2017-spokoyny
EXPNO 211
PROCN 1
O

F2 - Acquisition Parameters
Date_ 20171120
Time 18.49
INSTRU av400
M 5 mm PABBO BB/
PROBHD z g p g 3 0
PULPRO 6 5 5 3 6
G TD CDCl3
SOLVEN 128
T NS 0
DS 25252.525 Hz
SW 0.385323 Hz
H 1.2976128 sec
FIDRES 189.85
AQ 19.800 usec
RG 6.50 usec
DW 298.7 K
DE 2.00000000 sec
TE 0.03000000 sec
D1 1
D11
TD0 ======== CHANNEL f1 ========
SFO1 100.6243395 MHz
NUC 13C
1 P1 10.00 usec
PLW1 52.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.36111000 W
PLW13 0.29249999 W

F2 - Processing parameters
SI 65536
SF 100.6127649 MHz
WD EM
W
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

# $^1$H NMR, **20**



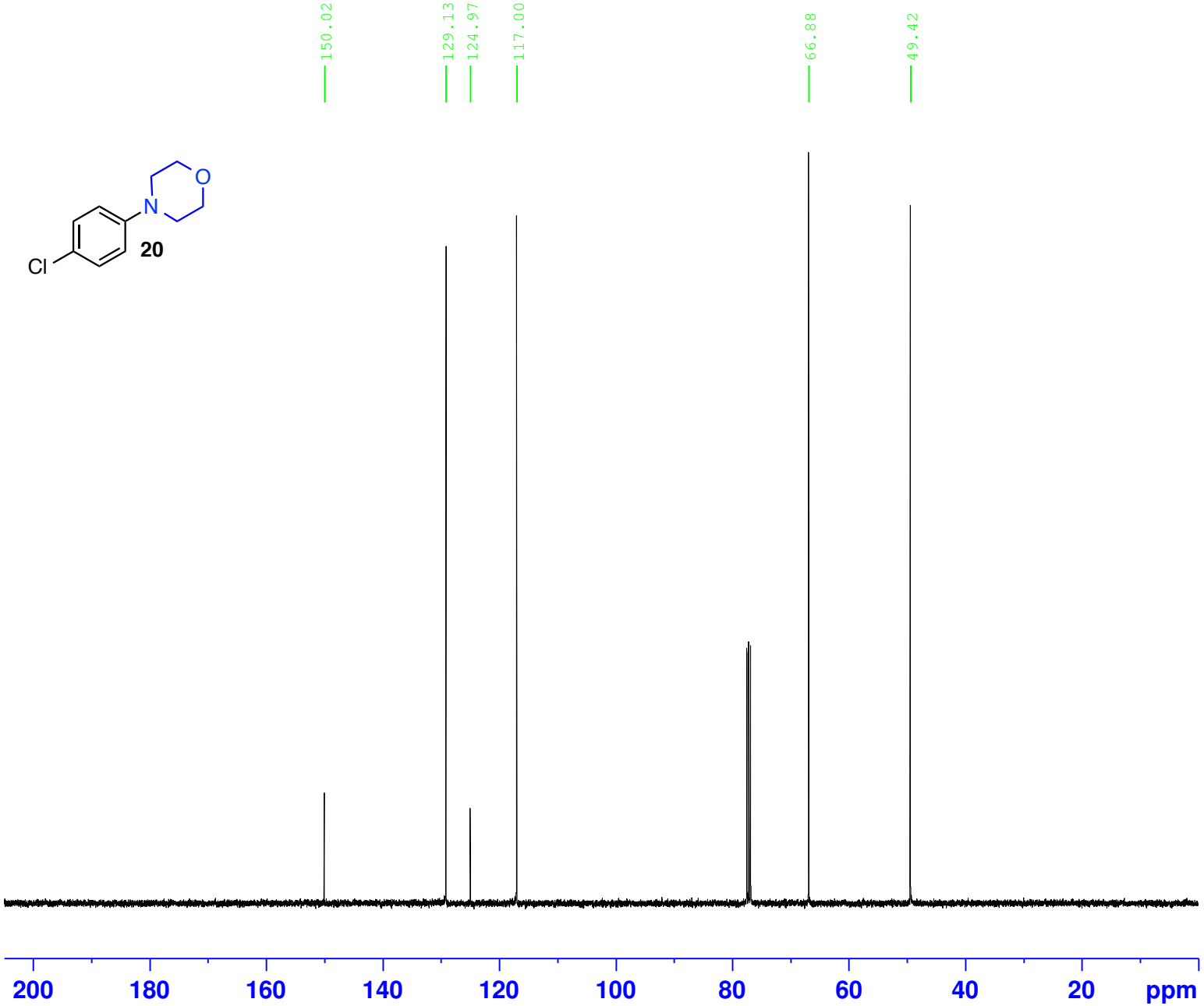

```
Current Data Parameters
NAME      Jan29-2018-spokoyny
EXPNO                  130
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180129
Time               20.56
INSTRUM            av400
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 52882
SOLVENT            CDCl3
NS                    32
DS                     0
SWH             8012.820 Hz
FIDRES          0.151523 Hz
AQ             3.2998369 sec
RG                 67.78
DW                62.400 usec
DE                 6.50 usec
TE                298.5 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                1H
P1                15.00 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300175 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

# $^{13}C\{^{1}H\}$ NMR, **20**




```
Current Data Parameters
NAME      Jan29-2018-spokoyny
EXPNO                  131
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180129
Time               21.04
INSTRUM            av400
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG               189.85
DW               19.800 usec
DE                6.50 usec
TE                299.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6243395 MHz
NUC1                13C
P1                10.00 usec
PLW1         52.00000000 W

======== CHANNEL f2 ========
SFO2         400.1324008 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.00000000 W
PLW12         0.36111000 W
PLW13         0.29249999 W

F2 - Processing parameters
SI                65536
SF           100.6127614 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```