

Supplementary Information

Palladaelectro-catalyzed *ortho*-C–H-monoarylation of 2-Phenylpyridines with arenediazonium salt

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Table of Contents

| | | |
|-----|--|-----|
| 1. | General Considerations | S3 |
| 2. | General procedure for preparation of starting material synthesis | S3 |
| 3. | General procedure for electrochemical C-H arylation of 2-phenylpyridine (GPEA) | S4 |
| 4. | Optimization of the Reaction Conditions | S4 |
| 5. | Control experiments | S9 |
| 6. | Characterization data of C-H arylation products | S13 |
| 7. | Characterization data of 2-phenylpyridine derivatives | S25 |
| 8. | References | S33 |
| 9. | ^1H and ^{13}C NMR data of C-H arylation products | S34 |
| 10. | ^1H and ^{13}C NMR data of 2-phenylpyridine derivatives | S80 |
| 11. | HRMS data of C-H arylation products | |

1. General Considerations:

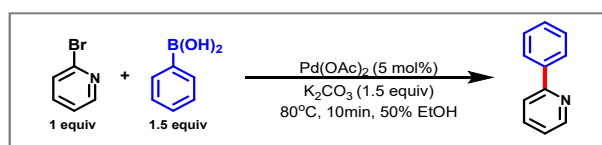
All the chemicals were purchased from Sigma Aldrich, Alfa Aesar, Spectrochem, and Sisco Research Laboratories Pvt. Ltd. Solvents were bought from Sisco Research Laboratories Pvt. Ltd. and used after distillation. Deuterated solvents were purchased from Sigma Aldrich. Silica gel (100–200 mesh) was used for column chromatography obtained from Finar. A mixture of petroleum ether and ethyl acetate was used as a gradient elution for column chromatography. Gradient elution was conducted using petroleum ether and ethyl acetate based on Merck aluminum TLC sheets (silica gel 60F254).

Catalytic reactions were performed in an undivided electrochemical cell. The electrochemical cell and platinum electrodes (5 mm × 15 mm × 0.25 mm, 99.9%) were obtained from SmartChemSynths Machine (OPC) Pvt. Ltd., Hyderabad. Graphite felt (GF) electrodes (10 mm × 15 mm × 6 mm) were connected using stainless steel 416 wire (Apex Surgined Company). Electrocatalysis and cyclic voltammetric studies were conducted using a potentiostat (PGSTAT204) from Metrohm Autolab. A divided H-cell and Nafion 117 membrane (thickness- 183 microm) both were purchased from Kanopy Techno Solutions Pvt. Ltd. Yields refer to isolated compounds. NMR spectra were recorded on a JEOL-400 spectrometer at MLSU Udaipur in CDCl₃ solvent. HRMS data were recorded using Agilent 6500 series Qtof HRMS at department of chemistry, IIT Bombay.

Chemical shifts (δ) are given in ppm, referenced to an internal TMS standard for ¹H NMR (δ 7.26). Chemical shifts of ¹³C NMR are reported relative to CDCl₃ (δ 77.00). The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

2. General procedure for preparation of starting material synthesis:

2.1. General procedure for preparation of 2-phenylpyridine and its derivatives (GPPP)



A dry, screw-cap reaction tube charged with a magnetic stir bar, 0.5 mmol of 2-bromopyridine and 0.75 mmol of benzene boronic acid, 5 mol% of Pd(OAc)₂, 1.5 equivalents of K₂CO₃, and a solvent mixture of EtOH:H₂O (1:1). The reaction mixture was heated to 80°C and stirred at 1000 rpm overnight. After cooling to ambient temperature, the reaction mixture was subjected to sequential extracted with H₂O (3 × 20 ml) and EtOAc (3 × 10 mL). The organic layer obtained was desiccated over anhydrous Na₂SO₄, filtered, and the solvent was subsequently removed via rotary evaporation. The resulting crude product underwent purification via column chromatography on silica gel to yield the final product.¹

2.2. General procedure for preparation of arene tetrafluoroborate salts (GPAT)

In a beaker, *p*-anisidine (50.0 mmol) was combined with tetrafluoroboric acid (20 mL) and deionized water (25 mL) in the presence of a magnetic stir bar. This mixture was placed in an ice bath to maintain a temperature range of 0–5°C and stirred for 15 minutes. Simultaneously, in a separate beaker, NaNO₂ (50 mmol) was dissolved in deionized water (10 mL). The NaNO₂

solution was added dropwise to *p*-anisidine solution while stirring at 700 rpm. After addition of NaNO₂, the mixture was stirred for an additional 30 minutes. The reaction mixture was then subjected to vacuum filtration. The resulting residue was dissolved in acetone (50 mL) and precipitated by the addition of diethyl ether (50 mL). The precipitate was collected via vacuum filtration to obtain the final compound.²

3. General procedure for electrochemical C-H arylation of 2-phenylpyridine (GPEA)

Electrocatalysis was conducted in a pre-dried, three-neck, undivided cell equipped with GF anode and Pt cathode. The cell was charged with substrate **1a** (0.10 mmol, 1.0 equiv.), substrate **2a** (0.25 mmol, 2.5 equiv.), Pd(OAc)₂ (2.24 mg, 10 mol %), K₂HPO₄ (43.5 mg, 2.0 equiv.), *n*Bu₄NBF₄ (33 mg, 2.0 equiv.) and in MeOH (10 mL). Electrocatalysis was performed at 80 °C with a constant current of 0.6 mA and stirring at 500 rpm for 18 h. After cooling to ambient temperature, the reaction mixture was diluted with EtOAc (5.0 mL). The GF anode was washed with EtOAc (3 × 10 mL) in an ultrasonic bath, and the washings were added to the reaction mixture. The resulting mixture was filtered through Celite to remove palladium catalysts and transferred to a separating funnel with 60 mL water. The mixture was extracted with EtOAc (3 × 10 mL), and the combined organic phases were dried over Na₂SO₄, and filtered. The solvent was removed in rotary evaporator. The crude product was purified by column chromatography on silica gel to yield the products.

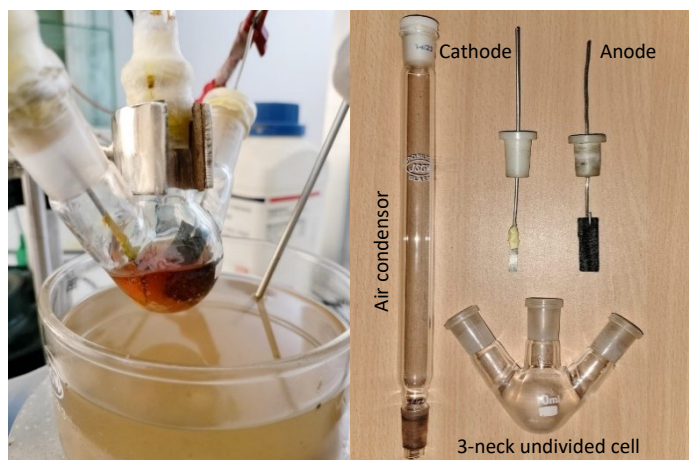
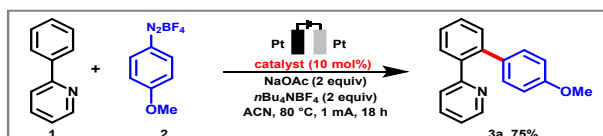


Figure 1: General reaction setup

4. Optimization of the Reaction Conditions

4.1. Optimization of catalyst



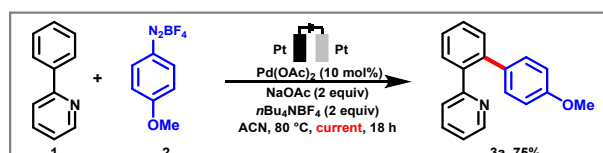
| S.No. | Catalyst | Yield(%) |
|-------|----------|----------|
| 1. | --- | n.r. |

| | | |
|----|--|------|
| 2. | Pd(OAc) ₂ | 69% |
| 3. | PdSO ₄ | n.r. |
| 4. | PdCl ₂ | n.r. |
| 5. | PdO | n.r. |
| 6. | Pd ₂ (dba) ₃ | 45% |
| 7. | Pd(TFA) ₂ | 68% |
| 8. | PdCl ₂ (PPh ₃) ₂ | n.r. |

The optimization of different catalysts in a reaction is summarized in Table S1, along with the corresponding yields. Among the catalysts tested, Pd(OAc)₂ and Pd(TFA)₂ achieved the highest yields, at 69% and 68%, respectively. In contrast, Pd₂(dba)₃ gave a lower result of 45%.

Other catalysts such as PdSO₄, PdCl₂, PdO, and PdCl₂(PPh₃)₂ showed no activity. Overall, this optimization study highlighted Pd(OAc)₂ and Pd(TFA)₂ as the most effective catalysts.

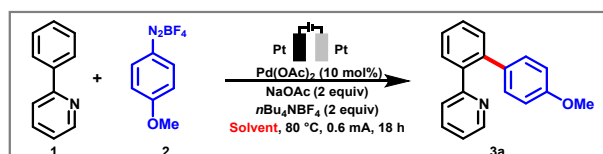
4.2. Optimization of current



| S.No. | Current | Yield (%) |
|-------|---------|-----------|
| 1. | --- | n.r. |
| 2. | 0.2mA | 20% |
| 3. | 0.4mA | 60% |
| 4. | 0.5mA | 62% |
| 5. | 0.6mA | 69% |
| 6. | 0.8mA | 60% |
| 7. | 1mA | 65% |
| 8. | 1.5mA | 64% |
| 9. | 2mA | n.r. |
| 10. | 4mA | n.r. |
| 11. | 5mA | n.r. |
| 12. | 6mA | n.r. |
| 13. | 7mA | n.r. |
| 14. | 8mA | n.r. |

The optimization of current in relation to their yields in a reaction is summarized in Table S2. The findings reveal a distinct pattern: the yield increases as the current rises from 0.2 mA to 0.6 mA, reaching a maximum of 69% at 0.6 mA. Beyond this point, the yields decline slightly, with 1.0 mA yielding 65% and 1.5 mA producing 65%. A threshold appears to exist beyond which higher current does not improve the yield, as indicated by no results (n.r.) being reported at 2 mA and above. At the lowest current of 0.2 mA, only a trace yield was observed. Overall, 0.6 mA is identified as the optimal current for achieving the highest yield.

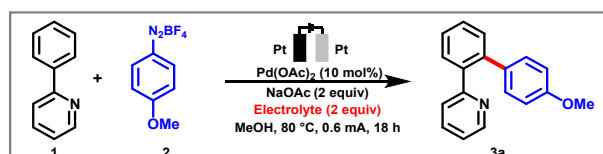
4.3. Optimization of solvent



| S.No. | Solvent | Yield(%) |
|-------|--------------------------------|----------|
| 1. | ACN | 45% |
| 2. | ACN:HFIP(9:1) | n.r. |
| 3. | ACN:HFIP(5:5) | n.r. |
| 4. | DMSO | n.r. |
| 5. | DMF | 22% |
| 6. | Acetone | n.r. |
| 7. | AcOH | n.r. |
| 8. | AcOH:(Ac) ₂ O (1:1) | n.r. |
| 9. | Isopropanol | n.r. |
| 10. | Ethanol | n.r. |
| 11. | t-Butanol | n.r. |
| 12. | C ₆ H ₆ | n.r. |
| 13. | Toluene | n.r. |
| 14. | C ₆ H ₆ | n.r. |
| 15. | Dioxane | n.r. |
| 16. | MeOH | 70% |
| 17. | MeOH:H ₂ O (1:1) | n.r. |

The optimization of various solvents and their corresponding yields in a reaction is summarized in Table S3. Methanol (MeOH) yielded the highest result among the solvents tested, achieving 70%. Dimethylformamide (DMF) produced a significantly lower yield of 22%, while acetonitrile (ACN) gave a moderate yield of 45%. Most other solvents, including combinations such as ACN:HFIP and other polar and non-polar solvents, showed no results (n.r.). These findings indicate that MeOH outperforms the other tested solvents by a substantial margin, making it as the most effective solvent for this process.

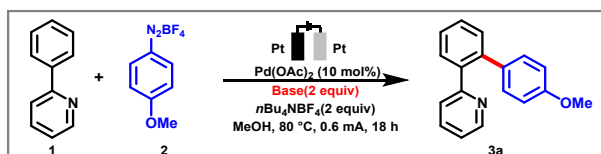
4.4. Optimization of electrolyte



| S.No. | Electrolyte | Yield (%) |
|-------|--------------------------------------|-----------|
| 1. | Lithium perchlorate | 50% |
| 2. | Tetrabutylammonium perchlorate | 63% |
| 3. | Tetrabutylhexafluorophosphate | Trace |
| 4. | Sodium perchlorate monohydrate | Trace |
| 5. | Tetrabutylammonium tetrafluoroborate | 70% |

The optimization of various electrolytes and their corresponding yield percentages is summarized in Table S4. Among the tested electrolytes, tetrabutylammonium tetrafluoroborate achieved the highest yield at 70%, followed by tetrabutylammonium perchlorate, which produced a yield of 63%. Tetrabutylhexafluorophosphate and sodium perchlorate monohydrate generated only trace amounts, indicating negligible yields. Lithium perchlorate, on the other hand, provided a moderate yield of 50%.

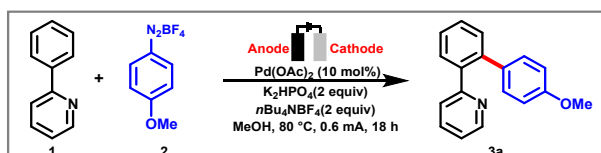
4.5. Optimization of base



| S.No. | Base | Yield(%) |
|-------|---|----------|
| 1. | NaOAc | 30% |
| 2. | C ₆ H ₅ COONa | 25% |
| 3. | NaH ₂ PO ₄ | 50% |
| 4. | NaH ₂ PO ₄ ·2H ₂ O | 55% |
| 5. | NaH ₂ PO ₄ ·H ₂ O | Trace |
| 6. | NaF | Trace |
| 7. | Na ₂ CO ₃ | 20% |
| 8. | Cs ₂ CO ₃ | n.r. |
| 9. | CH ₃ COOK | 40% |
| 10. | KH ₂ PO ₄ | 62% |
| 11. | K ₂ HPO ₄ | 69% |
| 12. | KPF ₆ | Trace |
| 13. | CsF | n.r. |
| 14. | NaOPiv | n.r. |
| 15. | KOPiv | n.r. |

The optimization of different bases and their corresponding yields is summarized in Table S5. The highest yield, 69%, was obtained using K₂HPO₄, followed by KH₂PO₄ (62%) and NaH₂PO₄·2H₂O (55%). Other bases, such as NaH₂PO₄ and CH₃COOK, yielded 50% and 40%, respectively. Bases including NaH₂PO₄·H₂O, NaF, KPF₆, and others produced only trace amounts or no yield. These results highlight the importance of carefully selecting bases to maximize yield and efficiency in chemical processes.

4.6. Optimization of electrodes

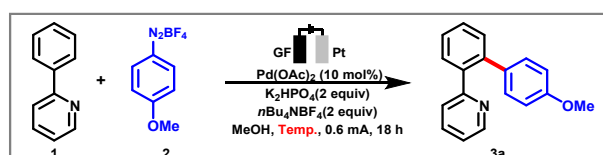


| S.No. | Anode | Cathode | Yield(%) |
|-------|---------|---------|----------|
| 1. | Pt | Pt | 69 % |
| 2. | RVC | Pt | 32% |
| 3. | RVC | RVC | n.r. |
| 4. | C cloth | Pt | trace |

| | | | |
|---|----------------|--------------|------|
| 5. | Gf rod | Pt | n.r. |
| 6. | Graphite plate | Pt | n.r. |
| 7. | GF | Pt | 75% |
| 8. | Pt | GF | 22% |
| 9. | Graphite plate | Graphite rod | n.r. |
| * Graphite felt – GF * Platinum - Pt | | | |

The optimization of electrode materials, with various anode and cathode combinations, is presented in Table S6 along with the corresponding yield percentages. Using GF felt as the anode and platinum as the cathode produced the highest yield of 75%. In contrast, platinum electrodes used as both the anode and cathode resulted 69%. The combination of RVC as the anode and platinum as the cathode produced a moderate yield of 32%. No yields were observed for other combinations, including RVC/RVC, carbon cloth/platinum, GF rod/platinum, GF plate/platinum, and GF plate/GF rod. Notably, using platinum as the anode and GF felt as the cathode yielded 22%. These findings emphasize the critical role of electrode material selection in determining reaction outcomes, with GF felt showing significant potential for enhancing product yield, whereas other materials resulted in negligible or no product formation.

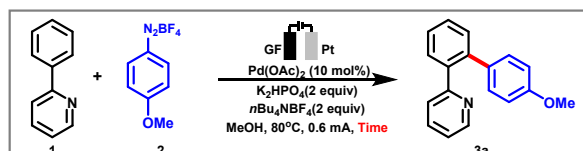
4.7. Optimization of Temperature



| Table S7. Optimization of temperature | | |
|---------------------------------------|-------------|----------|
| S.No. | Temperature | Yield(%) |
| 1. | R.T. | n.r. |
| 2. | 60°C | Trace |
| 3. | 70°C | 62% |
| 4. | 80°C | 75% |
| 5. | 90°C | 73% |
| 6. | 100°C | 72% |

In the context of Table S7, the optimization of temperature reveals that 80°C is the optimal temperature for achieving the highest yield (75%). This suggests that the reaction benefits from increased temperature but does not require excessively high heat. Temperatures above 80°C, such as 90°C and 100°C, resulted in slightly lower yields, possibly due to reduced efficiency or the occurrence of side reactions. Additionally, the reaction did not proceed at room temperature, and at 60°C the reaction produced trace amount of product. Thus, 80°C can be classified as a moderately high temperature, suitable for maximizing yield without extreme conditions.

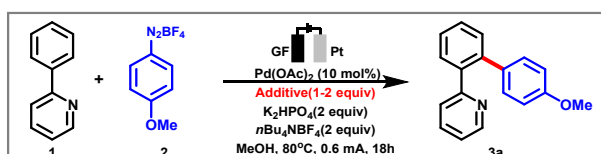
4.8. Optimization of Time



| S.No. | Time(h) | Yield(%) |
|-------|---------|----------|
| 1. | 3 h | n.r. |
| 2. | 5 h | 25% |
| 3. | 7 h | 40% |
| 4. | 10 h | 50% |
| 5. | 18 h | 75% |
| 6. | 24 h | 75% |

Table S8 summarizes optimization reaction time. This reveals that as reaction time increases, product yields increased as well: from no reaction at 3 hours to 25% at 5 hours, 40% at 7 hours, 50% at 10 hours, and a plateau of 75% at 18 and 24 hours. This indicates a time-dependent improvement in product formation, with optimal yields achieved after extended reaction periods, highlighting the importance of reaction duration in controlling the outcome of these electrochemical processes.

4.9. Optimization of additives

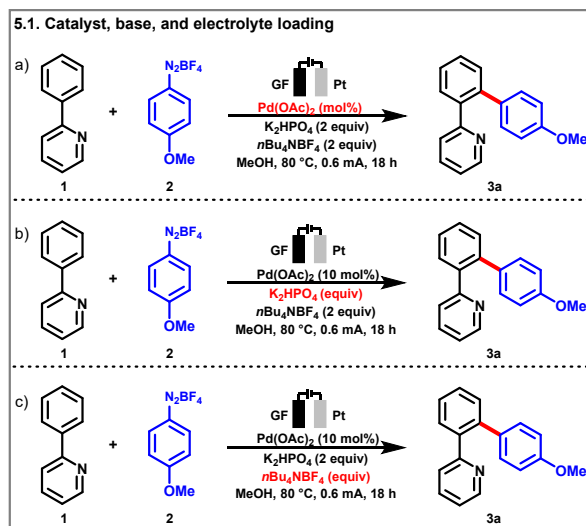


| S.No. | Additives | Result |
|-------|---|--------|
| 1. | BQ (2 equiv) | 35% |
| 2. | KI (1 equiv) | n.r. |
| 3. | I ₂ (1 equiv) | 24% |
| 4. | Pivalic acid (1 equiv) | n.r. |
| 5. | 1,4-Naphthoquinone | 30% |
| 6. | Adamantane | n.r. |
| 7. | AgF (1 equiv) | n.r. |
| 8. | AgOAc (1 equiv) | n.r. |
| 9. | Ag ₂ CO ₃ (1 equiv) | n.r. |
| 10. | --- | 75% |

The optimization of impact of various additives is presented in Table S9 along with the corresponding yield percentages. The data shows that BQ resulted in a yield of only 35%, while KI, I₂, pivalic acid, and several silver salts (AgF, AgOAc, and Ag₂CO₃) either failed to initiate a reaction or produced extremely low yields. Notably, the reaction performed best in the absence of additives, achieving a 75% yield.

5. Control experiments

5.1. Catalyst, base, and electrolyte loading

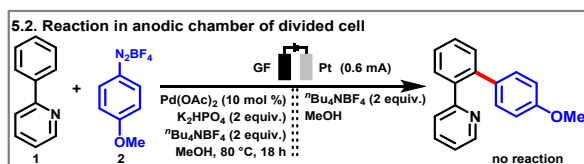


In the controlled experiments, we tested various loadings of the catalyst, base, and electrolyte individually under optimized reaction conditions. The first optimization focused on catalyst loading. Varying the amount of Pd(OAc)_2 to 5 mol% resulted in a negative impact on yield, while increasing it to 15 mol% or 20 mol% showed no significant improvement. A catalyst loading of 10 mol% Pd(OAc)_2 demonstrated evident catalytic activity under this reaction protocol.

Next, base loading was optimized. Using 0.05 mmol K_2HPO_4 resulted in no reaction, while 0.1 mmol yielded only trace amounts of the product, indicating that an increased base loading was required. Base concentrations of 0.15 mmol to 0.2 mmol K_2HPO_4 improved the isolated product yield from 50% to 75%, respectively. Thus, 0.2 mmol (2 equiv.) of base loading found to be suitable for maximizing yield.

Electrolyte loading optimization showed similar trends. Lower yields were observed with 0.05 mmol to 0.15 mmol of electrolyte. A significant improvement was achieved at 0.2 mmol of $n\text{-Bu}_4\text{NBF}_4$, yielding 75% of the isolated product. These results demonstrate that the precise amounts of catalyst, base, and electrolyte are critical for obtaining the desired product in good yield.

5.2. Reaction in anodic chamber of divided cell

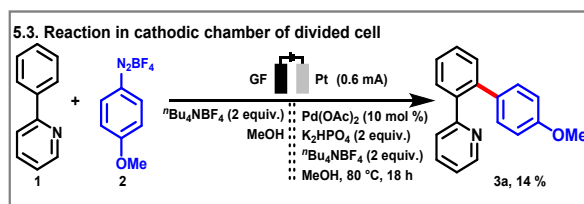


Electrocatalysis was conducted in a pre-dried H-cell separated by a Nafion membrane. The cell was equipped with a GF anode in the anodic chamber and a Pt cathode in the cathodic chamber, both attached to stainless steel wires (Figure 2a). The anodic chamber contained substrate 1a (0.10 mmol, 1.0 equiv.), substrate 2a (0.25 mmol, 2.5 equiv.), Pd(OAc)_2 (2.24 mg, 10 mol%), K_2HPO_4 (43.5 mg, 2.0 equiv.), and $n\text{-Bu}_4\text{NBF}_4$ (33 mg, 2.0 equiv.) in 10 mL of MeOH. The cathodic chamber contained $n\text{-Bu}_4\text{NBF}_4$ (33 mg, 2.0 equiv.) dissolved in 10 mL of MeOH.

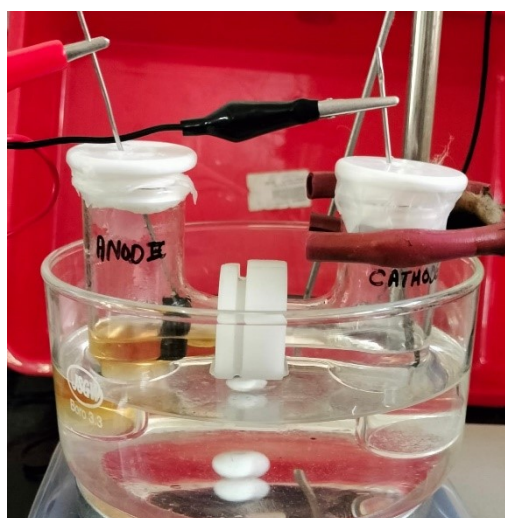
Electrocatalysis was carried out at 80 °C with a constant current of 0.6 mA and a stirring rate of 500 rpm for 18 hours. After the reaction, the crude product was purified by column chromatography on silica gel to yield the final product.

This reaction led to no product formation. This is because the reduction of arenediazonium tetrafluoroborate salts does not occur in the anodic chamber of a divided cell. This observation provides further insight into the reaction mechanism, suggesting that the cathodic reduction of arenediazonium salts generates an aryl free radical, which subsequently arylates the substrate.

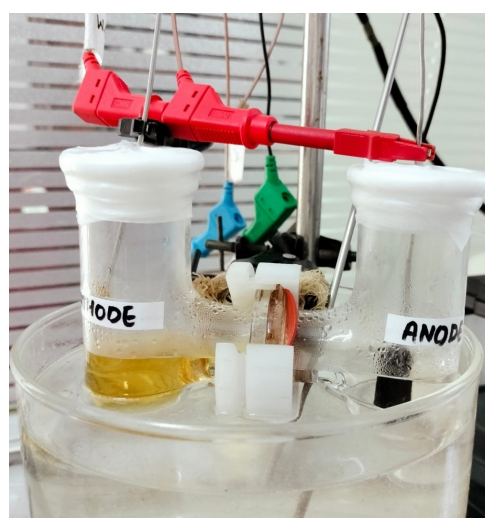
5.3. Reaction in cathodic chamber of divided cell



Electrocatalysis was conducted in a pre-dried H-cell separated by a Nafion membrane. The cell was equipped with a GF anode in the anodic chamber and a Pt cathode in the cathodic chamber, both attached to stainless steel wires (Figure 2b). The cathodic chamber contained substrate 1a (0.10 mmol, 1.0 equiv.), substrate 2a (0.25 mmol, 2.5 equiv.), $\text{Pd}(\text{OAc})_2$ (2.24 mg, 10 mol%), K_2HPO_4 (43.5 mg, 2.0 equiv.), and $n\text{-Bu}_4\text{NBF}_4$ (33 mg, 2.0 equiv.) in 10 mL of MeOH. The anodic chamber contained $n\text{-Bu}_4\text{NBF}_4$ (33 mg, 2.0 equiv.) dissolved in 10 mL of MeOH. Electrocatalysis was carried out at 80 °C with a constant current of 0.6 mA and a stirring rate of 500 rpm for 18 hours. After the reaction, the crude product was purified by column chromatography on silica gel to yield the final product. This reaction led to 14% product formation. This is because the oxidation of the palladium catalyst does not occur in the cathodic chamber of a divided cell. This observation provides further insight into the reaction mechanism, suggesting that anodic oxidation of the palladium catalyst is necessary to regenerate the active catalyst.



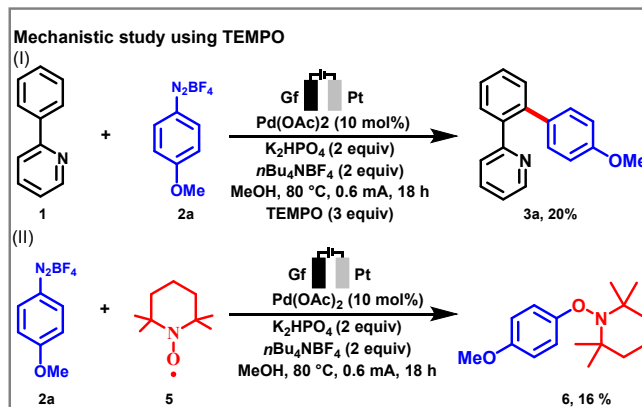
a) Reaction in anodic chamber



b) Reaction in cathodic chamber

Figure 2: Control experiment in divided cell

5.4. Mechanistic study using TEMPO



Under standard conditions, electrocatalysis was performed with TEMPO (0.3 mmol, 3 equiv.), resulting in a lower yield of approximately 20%. Similar to the first reaction, TEMPO acted as a radical scavenger, capturing the aryl radical formed from the cathodic reduction of the diazonium salt. This radical scavenging significantly reduced the product yield.³

5.5. Cyclic voltammetric studies

All cyclic voltammetric (CV) studies were performed in a pre-dried 100 mL cell equipped with a platinum disc as the working electrode, a platinum wire as the counter electrode, and an Ag/AgCl electrode as the reference electrode at a scan rate of 0.1 Vs⁻¹.

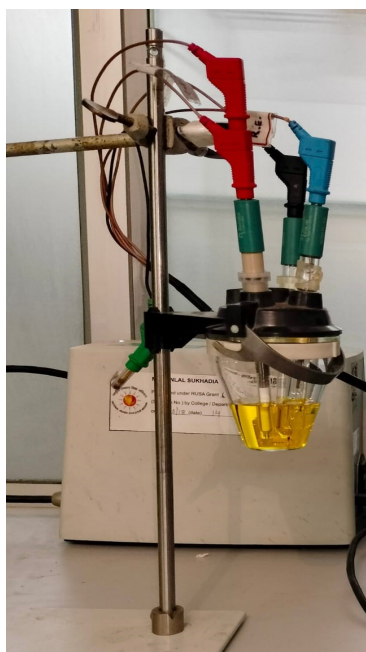


Figure 3: Cyclic Voltammetry setup

First, substrate 1a was tested, and no distinct oxidation or reduction peaks were observed (Fig. 1, blue line), indicating that this substrate is challenging to activate directly. An oxidation-reduction pair appeared at 0.1904 V and -0.6152 V in the CV of Pd(OAc)₂ with 1a (Fig. 1, red line), indicating the redox behaviour of palladium. However, Pd(OAc)₂ alone (Fig. 1, brown line) displayed only reduction peaks at -0.4565 V. Additionally, diazonium salt 2a exhibited an irreversible reduction peak at -0.3906 V (Fig. 1, yellow line), suggesting the reduction of 2a to a phenyl radical. In the presence of Pd(OAc)₂, 2a again showed two reduction peaks (Fig. 1, green line), attributed to the reduction of both 2a and Pd(OAc)₂. Finally, a CV experiment with 1a, 2a, base, and Pd(OAc)₂ revealed two reduction and one oxidation peak, suggesting the reduction of 2a and Pd(OAc)₂ and an oxidation peak corresponding to the Pd(0) to Pd(II) transition (Fig. 1, purple line). In the palladium redox system, the cathodic peak current was significantly lower than the oxidation peak, being suggestive of the current regenerating the catalytically active palladium species.

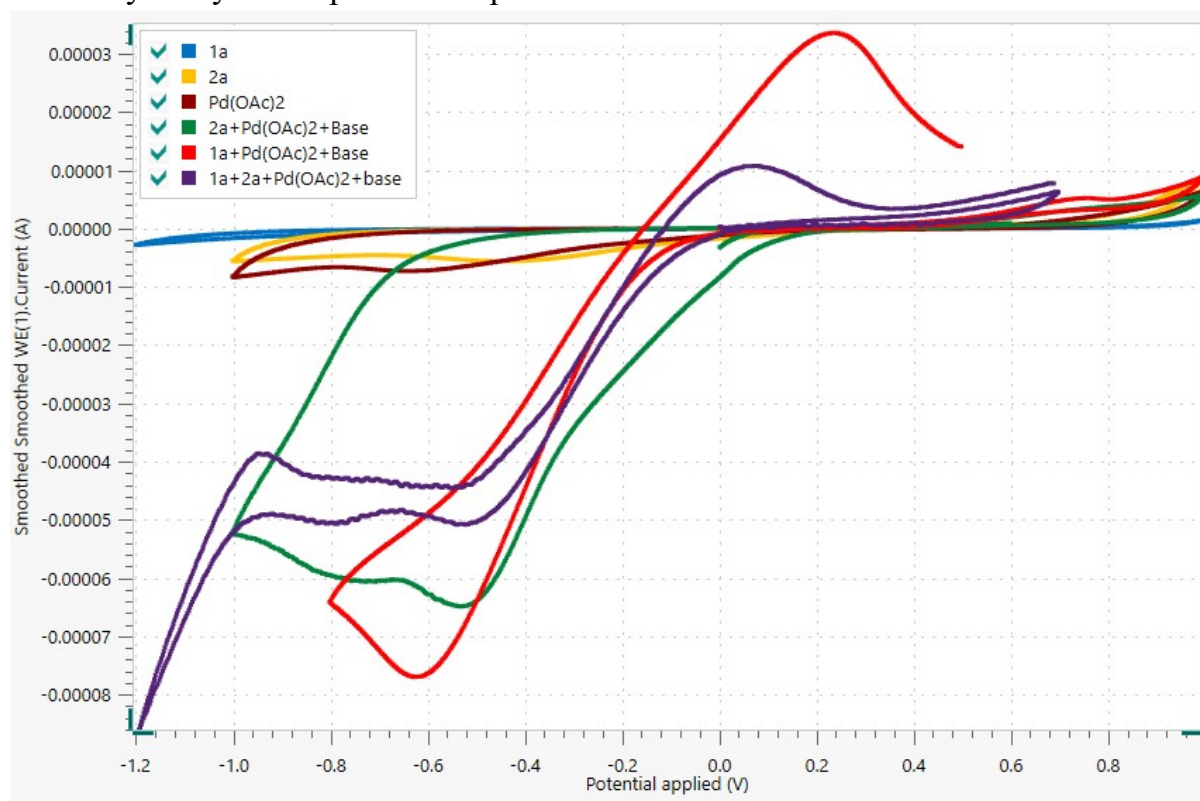
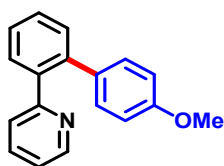


Figure 4: Cyclic Voltammetry analysis

6. Characterization data of C-H arylation products:



2-(4'-methoxy-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3a)⁴

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

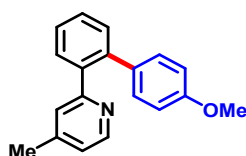
Appearance: Sticky yellow liquid.

Isolated yield: 75%

Molecular weight: 261.32 g/ mol

¹H NMR (400 MHz): δ 8.64 (d, J = 4.1 Hz), 7.67 (dd, J = 6.0, 3.5 Hz), 7.43 (dd, J = 5.4, 3.5 Hz), 7.07 (d, J = 8.8 Hz), 6.90 (d, J = 7.9 Hz), 6.77 (d, J = 8.8 Hz), 3.78 (s).

¹³C NMR (100 MHz): δ 159.51 (s), 158.58 (s), 149.50 (s), 140.26 (s), 139.40 (s), 135.36 (s), 133.76 (s), 130.85 (s), 130.54 (d, J = 5.2 Hz), 128.62 (s), 127.40 (s), 125.53 (s), 121.38 (s), 113.61 (s), 55.28 (s).



2-(4'-methoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3b)⁵

C-H arylation was carried out following the general procedure (GPEA).

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

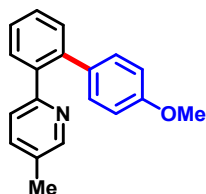
Appearance: Sticky yellow liquid.

Isolated yield: 69%

Molecular weight: 275.25 g/mol

¹H NMR (400 MHz) δ 8.47 (d, J = 5.8 Hz), 7.62 (s), 7.52 – 7.31 (m), 7.06 (d, J = 9.1 Hz), 6.96 (s), 6.77 (d, J = 9.0 Hz), 3.78 (s), 2.13 (s).

¹³C NMR (100 MHz) δ 158.54 (s), 144.75 (s), 143.90 (s), 140.26 (d, J = 8.8 Hz), 133.73 (s), 130.81 (s), 130.53 (d, J = 3.3 Hz), 128.68 (s), 127.35 (s), 126.52 (s), 122.62 (s), 113.55 (s), 55.33 (s), 29.81 (s), 21.15 (s).



2-(4'-methoxy-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3c)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: Sticky brown liquid.

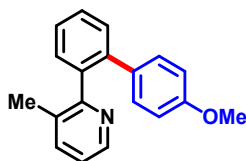
Isolated yield: 66%

Molecular weight: 275.35 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{19}H_{17}NO$: 276.1344, found: 276.1398.

1H NMR (400 MHz) δ 8.46 (dd, J = 16.6, 6.0 Hz), 7.70 – 7.63 (m), 7.51 – 7.34 (m), 7.10 – 7.02 (m), 6.91 – 6.67 (m), 3.78 (s), 2.33 – 2.28 (m).

^{13}C NMR (100 MHz) δ 158.52 (s), 156.62 (s), 149.83 (s), 140.19 (s), 139.24 (d, J = 17.9 Hz), 136.07 (s), 133.95 (s), 130.65 (dd, J = 25.9, 7.8 Hz), 129.87 (s), 128.38 (s), 127.96 (s), 127.37 (s), 124.94 (s), 113.80 (s), 113.58 (s), 55.28 (s), 18.24 (s).



2-(4'-methoxy-[1,1'-biphenyl]-2-yl)-3-methylpyridine (Scheme 2, 3d)

C-H arylation was carried out by following the general procedure GPEA.

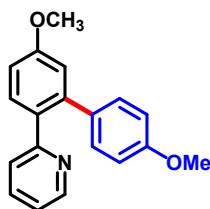
Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: Sticky brown liquid.

Isolated yield: 15%

Molecular weight: 275.35 g/ mol

1H NMR (400 MHz), δ 8.67 (d, J = 5.3 Hz), 7.66 (s), 7.60 – 7.30 (m), 7.10 (t, J = 20.4 Hz), 6.91 (d, J = 8.3 Hz), 6.76 (d, J = 9.0 Hz), 3.77 (s), 2.00 (s).



2-(4',5'-dimethoxy-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3g)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: Yellow solid.

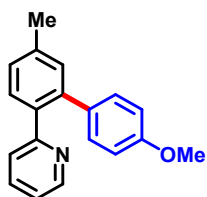
Isolated yield: 69%

Molecular weight: 291.35 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{19}H_{17}NO_2$: 291.1259, found: 291.1269.

1H NMR (400 MHz), δ 8.67 – 8.59 (m), 7.93 (d, J = 9.1 Hz), 7.64 (d, J = 1.2 Hz), 7.20 – 7.10 (m), 7.05 – 6.88 (m), 3.82 (s).

C¹³ NMR (100 MHz) δ 160.51 (s), 157.16 (s), 149.61 (s), 136.80 (s), 132.07 (s), 128.37 – 128.14 (m), 121.53 (s), 119.93 (s), 114.31 – 114.05 (m), 55.43 (s).



2-(4'-methoxy-5-methyl-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3h)⁶

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

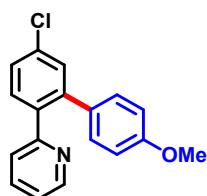
Appearance: Sticky yellow liquid.

Isolated yield: 68%

Molecular weight: 275.35 g/ mol

H¹ NMR (400 MHz) δ 8.62 (d, J = 8.1 Hz), 7.58 (d, J = 7.9 Hz), 7.39 (d, J = 2.1 Hz), 7.22 (s), 7.06 (d, J = 9.0 Hz), 6.86 (d, J = 8.0 Hz), 6.76 (d, J = 9.0 Hz), 3.77 (s), 2.42 (s).

C¹³ NMR (100 MHz) δ 158.56 (s), 155.02 (s), 149.16 (s), 140.12 (s), 139.08 (s), 138.61 (s), 135.58 (s), 133.83 (s), 131.30 (s), 130.83 (s), 130.60 (s), 128.22 (s), 125.69 (s), 121.27 (s), 113.60 (s), 55.29 (s), 21.36 (s).



2-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3i)⁸

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

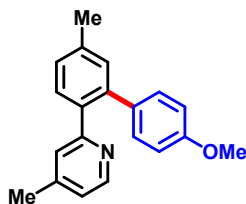
Appearance: Sticky yellow liquid.

Isolated yield: 55%

Molecular weight: 295.77 g/ mol

H¹ NMR (400 MHz) δ 8.66 (dd, J = 4.9, 3.3 Hz), 7.67 (d, J = 0.8 Hz), 7.45 (dd, J = 6.1, 4.0 Hz), 7.13 (ddd, J = 7.6, 4.9, 1.5 Hz), 7.08 (d, J = 9.0 Hz), 6.91 (d, J = 7.9 Hz), 6.78 (d, J = 9.0 Hz), 3.79 (s).

C¹³ NMR (100 MHz) δ 159.33 (s), 158.59 (s), 149.27 (s), 140.28 (s), 135.63 (s), 133.67 (s), 130.86 (s), 130.58 (d, J = 5.2 Hz), 128.74 (s), 127.44 (s), 125.67 (s), 121.49 (s), 113.62 (s), 55.29 (s).



2-(4'-methoxy-5-methyl-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3l)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: Sticky yellow liquid.

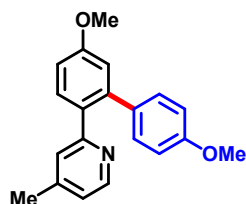
Isolated yield: 72%

Molecular weight: 289.38 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{20}H_{19}NO$: 289.1467, found: 289.1471.

1H NMR (400 MHz) δ 8.48 (d, J = 6.4 Hz), 7.63 (s), 7.43 (d, J = 7.3 Hz), 7.23 (s), 7.08 (d, J = 10.8 Hz), 6.95 (s), 6.86 – 6.66 (m), 3.79 (s), 2.44 (s), 2.13 (s).

^{13}C NMR (100 MHz) δ 158.50 (s), 131.26 (s), 130.79 (d, J = 3.2 Hz), 130.51 (d, J = 4.7 Hz), 128.12 (s), 127.32 (s), 126.41 (s), 124.09 (s), 122.46 (d, J = 14.1 Hz), 113.53 (s), 55.54 (d, J = 41.4 Hz), 55.30 – 55.23 (m), 45.40 (s), 42.55 (s), 21.36 (s), 21.14 (s).



2-(4',5'-dimethoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3m)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

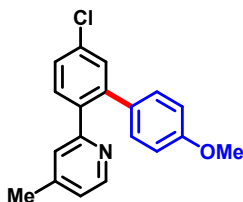
Appearance: Sticky brown liquid.

Isolated yield: 20%

Molecular weight: 305.38 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{20}H_{19}NO_2$: 306.1486, found: 306.1486.

1H NMR (400 MHz) δ 8.27 (s), 7.06 (d, J = 9.0 Hz), 6.92 (s), 6.70 (d, J = 9.0 Hz), 3.74 (s), 2.18 (s).



2-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3n)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: Sticky white liquid.

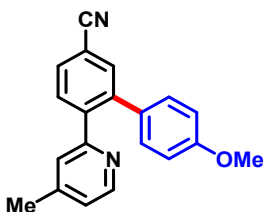
Isolated yield: 57%

Molecular weight: 309.79 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{19}H_{16}ClNO$: 309.0934, found: 309.0920.

1H NMR (400 MHz) δ 8.45 (s), 7.57 (s), 7.38 (d, $J = 7.7$ Hz), 7.04 (d, $J = 8.9$ Hz), 6.95 (s), 6.77 (d, $J = 8.9$ Hz), 6.71 (d, $J = 1.9$ Hz), 3.78 (s), 2.13 (s).

^{13}C NMR (100 MHz) δ 158.98 (s), 158.23 (s), 149.40 (s), 141.91 (s), 135.75 (s), 134.49 (s), 132.37 (s), 132.02 (s), 130.74 (s), 130.37 (s), 127.45 (s), 125.56 (s), 121.76 (s), 120.50 (s), 113.79 (s), 95.76 (s), 55.32 (s).



4'-methoxy-6-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-3-carbonitrile (Scheme 2, 3o)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: white solid.

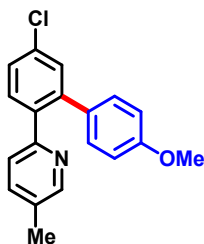
Isolated yield: 70%

Molecular weight: 300.36 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{20}H_{16}N_2O$: 323.1151, found: 323.1151.

1H NMR (400 MHz) δ 8.49 (d, $J = 6.0$ Hz), 7.72 (dd, $J = 18.9, 1.1$ Hz), 7.03 (d, $J = 9.0$ Hz), 6.79 (d, $J = 9.0$ Hz), 3.79 (s), 2.15 (s).

^{13}C NMR (100 MHz) δ 159.26 (s), 149.17 (s), 141.49 (s), 136.73 (s), 134.12 (s), 131.47 (d, $J = 5.7$ Hz), 130.64 (d, $J = 3.6$ Hz), 126.28 (s), 123.51 (s), 118.86 (s), 113.95 (s), 112.38 (s), 55.38 (s), 21.16 (s).



2-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3p)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: Sticky brown liquid.

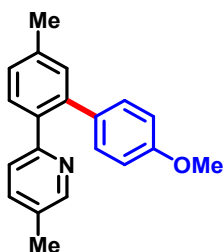
Isolated yield: 56%

Molecular weight: 309.79 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{19}H_{16}ClNO$: 310.9986, found: 310.9986.

1H NMR (400 MHz) δ 8.45 (s), 7.58 (d, $J = 8.9$ Hz), 7.42 – 7.34 (m), 7.24 – 7.18 (m), 7.04 (d, $J = 9.0$ Hz), 6.75 (dd, $J = 15.7, 8.5$ Hz), 3.77 (s), 2.28 (s).

^{13}C NMR (100 MHz) δ 158.92 (s), 155.43 (s), 149.84 (s), 141.82 (s), 137.61 (s), 136.30 (s), 134.15 (s), 132.59 (s), 131.97 (s), 131.19 (s), 130.71 (s), 130.31 (s), 127.37 (s), 124.91 (s), 113.76 (s), 55.30 (s), 18.25 (s).



2-(4'-methoxy-5-methyl-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3q)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

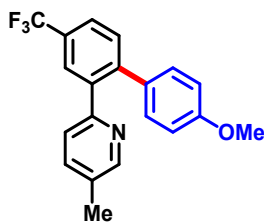
Appearance: Sticky brown liquid.

Isolated yield: 58%

Molecular weight: 289.38 g/ mol

1H NMR (400 MHz) δ 8.52 (d, $J = 4.0$ Hz), 7.68 (s), 7.60 (s), 7.54 (s), 7.19 (s), 7.05 (d, $J = 9.0$ Hz), 6.94 – 6.83 (m), 6.82 – 6.62 (m), 3.83 (s), 2.39 (s), 2.35 (s).

^{13}C NMR (100 MHz) δ 142.56 (s), 141.35 (s), 131.27 (s), 130.83 (d, $J = 5.8$ Hz), 129.45 (s), 128.19 (s), 124.73 (s), 123.48 (s), 121.89 (s), 121.13 (s), 116.83 (s), 116.35 (s), 113.57 (s), 112.26 (s), 103.39 (s), 100.32 (s), 55.67 (s), 21.82 (s), 18.31 (s).



2-(4'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3r)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: Sticky brown liquid.

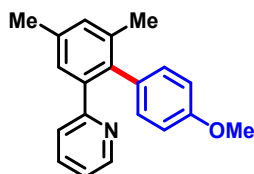
Isolated yield: 28%

Molecular weight: 343.35 g/mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{20}H_{16}F_3NO$: 343.1184, found: 343.1231.

1H NMR (400 MHz) δ 8.48 (d, $J = 2.5$ Hz), 7.92 (d, $J = 2.2$ Hz), 7.71 – 7.62 (m), 7.49 (d, $J = 8.2$ Hz), 7.25 – 7.15 (m), 7.07 (d, $J = 9.0$ Hz), 6.79 (d, $J = 9.0$ Hz), 3.79 (s), 2.31 (s).

^{13}C NMR (100 MHz) δ 159.10 (s), 155.11 (s), 149.95 (s), 143.68 (s), 136.50 (s), 132.46 (s), 131.65 (s), 130.98 (s), 130.76 (s), 127.73 (d, $J = 18.7$ Hz), 125.33 – 124.68 (m), 114.22 (s), 113.85 (s), 55.32 (s), 29.80 (s), 18.27 (s).



2-(4'-methoxy-4,6-dimethyl-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3s)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: Sticky brown liquid.

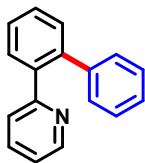
Isolated yield: 30 %

Molecular weight: 289.37 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{20}H_{19}NO$: 289.1467, found: 289.1479.

1H NMR (400 MHz) δ 8.56 (d, $J = 7.7$ Hz, 4H), 7.32 (dd, $J = 10.0, 2.6$ Hz, 10H), 7.16 (s, 5H), 7.05 – 6.93 (m, 13H), 6.78 (dd, $J = 14.2, 8.1$ Hz, 14H), 3.77 (s, 22H), 2.40 (s, 20H), 2.16 (s, 20H).

^{13}C NMR (100 MHz) δ 159.75 (s), 158.07 (s), 148.87 (s), 136.74 (d, $J = 19.3$ Hz), 134.97 (s), 131.54 (s), 131.09 (s), 128.25 (s), 125.30 (s), 120.88 (s), 113.28 (s), 55.12 (s), 21.11 – 20.90 (m).



2-([1,1'-biphenyl]-2-yl)pyridine (M.W.= 231.30 g/mol) (Scheme 3, 4a)⁷

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

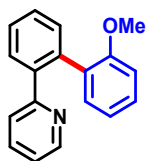
Appearance: Sticky yellow solid.

Isolated yield: 69%

Molecular weight: 231.30 g/ mol

¹H NMR (400 MHz) δ 8.67 (d, J = 7.2 Hz), 7.82 – 7.69 (m), 7.69 – 7.38 (m), 7.30 (s), 7.19 (d, J = 11.3 Hz), 7.14 (s), 6.92 (d, J = 9.4 Hz).

¹³C NMR (100 MHz) δ 159.24 (s), 149.42 (s), 141.36 (s), 140.69 (s), 139.38 (s), 135.43 (s), 130.60 (d, J = 2.8 Hz), 129.81 (s), 129.19 (s), 128.69 (s), 128.17 (s), 127.77 (s), 126.82 (s), 125.59 (s), 121.51 (s).



2-(2'-methoxy-[1,1'-biphenyl]-2-yl)pyridine (M.W.= 261.32 g/mol) (Scheme 3, 4b)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: White solid.

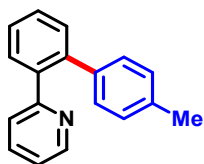
Isolated yield: 70%

Molecular weight: 261.32 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{18}H_{24}N_2NaO_5$: 262.1187, found: 262.1245.

¹H NMR (400 MHz) δ 8.60 (s), 7.72 (s), 7.45 (d, J = 5.2 Hz), 7.37 (d, J = 18.1 Hz), 7.22 (d, J = 2.0 Hz), 7.07 (s), 6.94 (d, J = 1.5 Hz), 6.71 (s), 3.33 (s).

¹³C NMR (100 MHz) δ 159.59 (s), 156.12 (s), 149.07 (s), 137.07 (s), 135.21 (s), 131.55 (s), 131.10 (s), 130.43 (s), 129.72 (s), 128.84 (s), 128.47 (s), 127.84 (s), 123.75 (s), 121.25 (s), 120.76 (s), 110.70 (s), 54.98 (s).



2-(4'-methyl-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4c)⁷

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

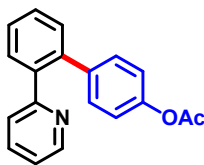
Appearance: Sticky yellow liquid.

Isolated yield: 64%

Molecular weight: 245.33 g/ mol

¹H NMR (400 MHz) δ 8.86 (d, J = 8.2 Hz), 7.93 – 7.87 (m), 7.69 – 7.59 (m), 7.48 (s), 7.36 – 7.26 (m), 7.12 (d, J = 8.0 Hz), 2.53 (s).

¹³C NMR (100 MHz) δ 159.45 (s), 149.46 (s), 140.61 (s), 139.41 (s), 138.39 (s), 136.47 (s), 135.35 (s), 130.58 (d, J = 4.1 Hz), 129.65 (s), 128.90 (s), 128.61 (s), 127.53 (s), 125.55 (s), 121.41 (s), 21.22 (s).



2'-(pyridin-2-yl)-[1,1'-biphenyl]-4-yl acetate (Scheme 3, 4d)

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

Appearance: White solid.

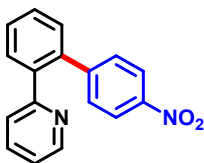
Isolated yield: 65%

Molecular weight: 289.33 g/ mol

HRMS (m/z): $[M + Na]^+$ calcd for $C_{19}H_{15}NO_2$: 289.1103, found: 289.1080.

¹H NMR (400 MHz) δ 8.61 (d, J = 6.6 Hz), 7.83 (d, J = 8.7 Hz), 7.76 – 7.62 (m), 7.47 (dd, J = 25.1, 9.7 Hz), 7.24 (s), 7.13 (dd, J = 8.0, 5.3 Hz), 6.92 (d, J = 8.4 Hz), 2.58 (s).

¹³C NMR (100 MHz) δ 198.08 (s), 158.89 (s), 149.59 (s), 146.51 (s), 139.57 (d, J = 5.7 Hz), 135.73 (s), 135.36 (s), 130.73 (s), 130.42 (s), 129.97 (s), 128.80 (s), 128.35 (d, J = 17.2 Hz), 125.36 (s), 121.76 (s), 26.75 (s).



2-(4'-nitro-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4e)⁶

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

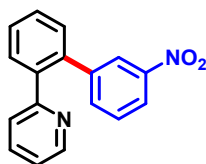
Appearance: Yellow solid.

Isolated yield: 75%

Molecular weight: 276.30 g/ mol

¹H NMR (400 MHz) δ 8.61 – 8.55 (m), 8.08 (d, J = 9.0 Hz), 7.69 (d, J = 9.7 Hz), 7.61 – 7.47 (m), 7.43 (d, J = 9.3 Hz), 7.29 (d, J = 9.0 Hz), 7.17 (ddd, J = 7.8, 5.0, 1.3 Hz), 6.99 (d, J = 7.9 Hz).

¹³C NMR (100 MHz) δ 179.02 (s), 158.43 (s), 149.49 (s), 148.44 (s), 146.66 (s), 138.50 (s), 136.24 (s), 130.87 (s), 130.46 (d, J = 13.0 Hz), 129.04 (d, J = 2.5 Hz), 125.24 (s), 123.46 (s), 122.08 (s).



2-(3'-nitro-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4f)^{4,5}

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

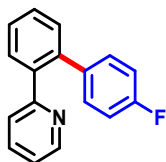
Appearance: White solid.

Isolated yield: 57%

Molecular weight: 276.30 g/ mol

¹H NMR (400 MHz) δ 8.58 (d, J = 7.5 Hz), 8.09 (d, J = 2.0 Hz), 7.68 (s), 7.53 (dd, J = 9.9, 4.9 Hz), 7.48 (s), 7.43 – 7.33 (m), 7.14 (s), 7.04 (s).

¹³C NMR (100 MHz) δ 149.51 (s), 143.12 (s), 138.24 (s), 135.97 (s), 130.81 (s), 130.49 (s), 129.24 – 128.71 (m), 125.25 (s), 124.40 (s), 122.03 (s), 121.78 (s).



2-(4'-fluoro-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4g)⁷

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

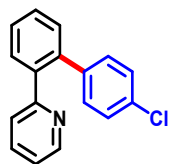
Appearance: White solid.

Isolated yield: 72%

Molecular weight: 249.29 g/ mol

¹H NMR (400 MHz) δ 8.61 (d, J = 4.9 Hz), 7.66 (d, J = 5.8 Hz), 7.49 – 7.36 (m), 7.10 (dd, J = 8.9, 5.4 Hz), 6.91 (t, J = 8.9 Hz).

¹³C NMR (100 MHz) δ 159.11 (s), 149.48 (s), 139.62 (s), 135.61 (s), 131.29 (d, J = 8.1 Hz), 130.56 (d, J = 11.1 Hz), 129.80 (s), 128.74 (s), 128.17 (s), 127.89 (s), 125.46 (s), 121.59 (s), 115.23 (s), 115.02 (s).



2-(4'-chloro-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4h)⁷

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

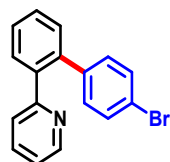
Appearance: Sticky yellow liquid.

Isolated yield: 64%

Molecular weight: 265.74 g/ mol

¹H NMR (400 MHz) δ 8.62 (d, J = 7.4 Hz), 7.74 – 7.60 (m), 7.47 (d, J = 10.4 Hz), 7.35 (d, J = 8.4 Hz), 7.15 (dd, J = 31.9, 19.0 Hz), 6.96 (dd, J = 39.1, 7.7 Hz).

¹³C NMR (100 MHz) δ 149.43 (s), 142.80 (s), 141.10 (s), 140.30 (s), 139.43 (s), 135.87 (s), 131.36 (d, J = 4.9 Hz), 131.04 (s), 130.72 (s), 130.40 (s), 128.87 (s), 128.39 (s), 128.12 (s), 125.50 (s), 121.71 (d, J = 1.5 Hz), 121.16 (s).



2-(4'-bromo-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4i)⁴

C-H arylation was carried out by following the general procedure GPEA.

Eluent: ethyl acetate/ petroleum ether (5% EA-PE).

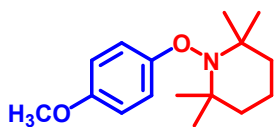
Appearance: Brown solid.

Isolated yield: 59%

Molecular weight: 310.19 g/ mol

¹H NMR (400 MHz) δ 8.64 – 8.59 (m), 7.69 – 7.64 (m), 7.46 (dd, J = 10.8, 4.3 Hz), 7.19 (d, J = 8.8 Hz), 7.15 – 7.10 (m), 7.07 (d, J = 8.8 Hz), 6.91 (d, J = 7.9 Hz).

¹³C NMR (100 MHz) δ 159.03 (s), 149.60 (s), 139.88 (s), 139.45 (d, J = 9.7 Hz), 135.64 (s), 132.90 (s), 131.04 (s), 130.67 (s), 130.44 (s), 128.75 (d, J = 1.4 Hz), 128.38 (s), 128.07 (s), 125.40 (s), 121.64 (s).



1-(4-methoxyphenoxy)-2,2,6,6-tetramethylpiperidine (Scheme 4, 6)

Eluent: ethyl acetate/ petroleum ether (3-5% EA-PE).

Appearance: colourless liquid

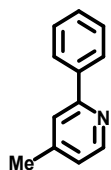
Isolated yield: 16 %

Molecular weight: 263.38 g/mol

^1H NMR (400 MHz) δ 6.77 (s, 4H), 3.75 (s, 3H), 2.04 (s, 12H), 1.24 (dd, $J = 9.2, 5.3$ Hz, 2H), 0.87 (s, 1H).

^{13}C NMR (100 MHz) δ 149.45 (s), 130.86 (s), 130.51 (s), 113.65 (s), 55.28 (s), 29.80 (s), 22.80 (s), 14.24 (s).

7. Characterization data of 2-phenylpyridine derivatives



4-methyl-2-phenylpyridine (1b)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

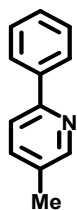
Appearance: White solid

Isolated yield: 80%

Molecular weight: 169.23 g/mol

^1H NMR (400 MHz) δ 8.55 (d, $J = 5.0$ Hz), 7.98 (d, $J = 7.0$ Hz), 7.55 (s), 7.46 (d, $J = 7.5$ Hz), 7.41 (s), 7.07 (d, $J = 5.0$ Hz), 2.42 (s).

^{13}C NMR (100 MHz) δ 157.43 (s), 149.48 (s), 147.91 (s), 139.58 (s), 128.86 (d, $J = 13.4$ Hz), 127.04 (s), 123.26 (s), 121.69 (s), 21.34 (s).



5-methyl-2-phenylpyridine (1c)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

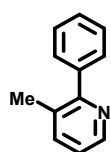
Appearance: White solid

Isolated yield: 85%

Molecular weight: 169.23 g/mol

¹H NMR (400 MHz) δ 8.62 – 8.46 (m), 8.02 – 7.92 (m), 7.67 – 7.54 (m), 7.44 (dd, J = 26.1, 4.1 Hz), 2.38 (s).

¹³C NMR (100 MHz) δ 154.91 (s), 150.14 (s), 139.48 (s), 137.46 (s), 131.72 (s), 128.74 (d, J = 10.4 Hz), 126.80 (s), 120.21 (s), 18.26 (s).



3-methyl-2-phenylpyridine (1d)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

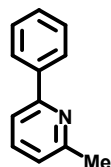
Appearance: White solid

Isolated yield: 78%

Molecular weight: 169.23 g/mol

¹H NMR (400 MHz) δ 7.96 (d, J = 8.4 Hz), 7.63 (t, J = 7.8 Hz), 7.55 – 7.49 (m), 7.45 (t, J = 4.1 Hz), 7.40 (d, J = 7.4 Hz), 7.13 – 7.05 (m), 2.63 (s).

¹³C NMR (100 MHz) δ 158.45 (s), 157.08 (s), 139.84 (s), 137.02 (s), 128.79 (d, J = 1.9 Hz), 127.11 (s), 121.72 (s), 117.78 (s), 24.86 (s).



2-methyl-6-phenylpyridine (1e)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

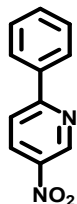
Appearance: White solid

Isolated yield: 86%

Molecular weight: 169.23 g/mol

¹H NMR (400 MHz) δ 8.02 – 7.92 (m), 7.62 (d, J = 7.7 Hz), 7.55 – 7.33 (m), 7.12 – 7.06 (m), 2.62 (s).

C¹³ NMR (100 MHz) δ 158.45 (s), 157.08 (s), 139.84 (s), 137.02 (s), 128.80 (d, J = 2.2 Hz), 127.11 (s), 121.73 (s), 117.79 (s), 24.86 (s).



5-nitro-2-phenylpyridine (1f)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

Appearance: Yellow solid

Isolated yield: 86%

Molecular weight: 200.20 g/mol

H¹ NMR (400 MHz) δ 9.49 (d, J = 3.6 Hz), 8.63 – 8.46 (m), 8.19 – 8.06 (m), 7.91 (dd, J = 8.8, 0.8 Hz), 7.61 – 7.43 (m).

C¹³ NMR (100 MHz) δ 162.57 (s), 145.35 (s), 142.94 (s), 137.12 (s), 132.07 (s), 131.00 (s), 129.24 (s), 127.78 (s), 120.19 (s).



2-(4-methoxyphenyl)pyridine (1g)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

Appearance: White solid

Isolated yield: 88%

Molecular weight: 185.23 g/mol

H¹ NMR (400 MHz) δ 8.65 (d, J = 6.2 Hz), 7.94 (d, J = 9.1 Hz), 7.69 (dd, J = 12.3, 4.3 Hz), 7.21 – 7.14 (m), 7.00 (d, J = 9.0 Hz), 3.86 (s).

C¹³ NMR (100 MHz) δ 160.52 (s), 157.16 (s), 149.57 (s), 136.87 (s), 132.01 (s), 128.28 (s), 121.55 (s), 120.00 (s), 114.20 (s), 55.45 (s).



2-(p-tolyl)pyridine (1h)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

Appearance: White solid

Isolated yield: 80%

Molecular weight: 169.23 g/mol

¹H NMR (400 MHz) δ 8.67 (d, J = 6.5 Hz), 7.89 (d, J = 8.6 Hz), 7.73 – 7.59 (m), 7.29 (d, J = 0.8 Hz), 7.17 (dd, J = 8.8, 4.9 Hz), 6.83 (dd, J = 92.9, 4.7 Hz), 2.39 (s).

¹³C NMR (100 MHz) δ 157.55 (s), 149.61 (s), 139.09 (s), 136.93 (s), 136.61 (s), 129.98 (s), 129.63 (s), 126.93 (s), 121.98 (s), 120.52 (s), 115.54 (s), 21.39 (s).



2-(4-chlorophenyl)pyridine (1i)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

Appearance: white liquid

Isolated yield: 89%

Molecular weight: 189.64 g/mol

¹H NMR (400 MHz) δ 8.69 (d, J = 8.0 Hz), 7.94 (d, J = 9.0 Hz), 7.81 – 7.67 (m), 7.45 (d, J = 8.9 Hz), 7.24 (d, J = 1.3 Hz).

¹³C NMR (100 MHz) δ 156.30 (s), 149.83 (s), 137.86 (s), 137.02 (s), 135.20 (s), 129.03 (s), 128.27 (s), 122.49 (s), 120.47 (s).



2-(4-bromophenyl)pyridine (1j)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

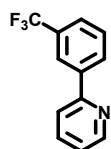
Appearance: White solid

Isolated yield: 87%

Molecular weight: 234.10 g/mol

¹H NMR (400 MHz) δ 8.66 (d, J = 8.1 Hz), 7.84 (d, J = 8.8 Hz), 7.74 – 7.63 (m), 7.57 (d, J = 8.8 Hz), 7.22 (d, J = 14.1 Hz).

¹³C NMR (100 MHz) δ 156.29 (s), 149.84 (s), 138.29 (s), 137.03 (s), 131.97 (s), 128.57 (s), 123.54 (s), 122.55 (s), 120.44 (s).



2-(3-(trifluoromethyl)phenyl)pyridine (1k)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

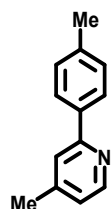
Appearance: White liquid

Isolated yield: 89%

Molecular weight: 223.20 g/mol

¹H NMR (400 MHz) δ 8.71 (d, J = 8.1 Hz), 8.27 (d, J = 0.8 Hz), 8.15 (s), 7.75 (dd, J = 3.9, 3.1 Hz), 7.68 – 7.63 (m), 7.59 (dd, J = 7.8, 0.8 Hz), 7.30 – 7.24 (m).

¹³C NMR (100 MHz) δ 155.90 (s), 149.97 (s), 140.17 (s), 137.13 (s), 130.15 (d, J = 1.4 Hz), 129.32 (s), 125.66 (s), 123.86 (s), 122.94 (s), 120.72 (s).



4-methyl-2-(p-tolyl)pyridine (1l)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

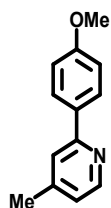
Appearance: White liquid

Isolated yield: 90%

Molecular weight: 183.25 g/mol

¹H NMR (400 MHz) δ 8.50 (d, J = 5.8 Hz), 7.85 (d, J = 8.5 Hz), 7.54 – 7.47 (m), 7.26 – 7.19 (m), 7.07 – 6.95 (m), 2.38 (s).

¹³C NMR (100 MHz) δ 157.36 (s), 149.34 (s), 138.93 (s), 136.67 (s), 129.53 (s), 126.88 (s), 122.99 (s), 121.37 (s), 21.37 (d, J = 1.3 Hz), 1.13 (s).



2-(4-methoxyphenyl)-4-methylpyridine (1m)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

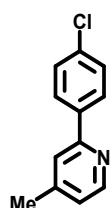
Appearance: White liquid

Isolated yield: 87%

Molecular weight: 199.25 g/mol

¹H NMR (400 MHz) δ 8.50 (d, J = 5.8 Hz), 7.93 (d, J = 9.1 Hz), 7.48 (d, J = 0.8 Hz), 7.09 – 6.93 (m), 3.85 (s), 2.39 (s).

¹³C NMR (100 MHz) δ 160.44 (s), 156.99 (s), 149.22 (s), 147.92 (s), 132.04 (s), 128.29 (s), 122.63 (s), 120.96 (s), 114.14 (s), 55.43 (s), 21.36 (s).



2-(4-chlorophenyl)-4-methylpyridine (1n)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

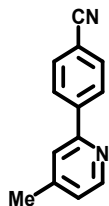
Appearance: White solid

Isolated yield: 86%

Molecular weight: 203.67 g/mol

¹H NMR (400 MHz) δ 8.53 (d, J = 5.0 Hz), 7.92 (d, J = 8.7 Hz), 7.51 (s), 7.43 (d, J = 8.7 Hz), 7.07 (dd, J = 5.0, 0.8 Hz), 2.41 (s).

C¹³ NMR (100 MHz) δ 156.16 (s), 149.49 (s), 148.16 (s), 137.92 (s), 135.06 (s), 128.96 (q, J = 1.2 Hz), 128.29 (d, J = 1.5 Hz), 123.51 (s), 121.48 (s), 21.34 (s).



4-(4-methylpyridin-2-yl)benzonitrile (1o)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

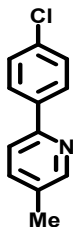
Appearance: White solid

Isolated yield: 88%

Molecular weight: 194.24 g/mol

H¹ NMR (400 MHz) δ 8.57 (d, J = 4.3 Hz), 8.09 (d, J = 8.0 Hz), 7.75 (d, J = 8.1 Hz), 7.58 (s), 7.14 (d, J = 3.8 Hz), 2.44 (s).

C¹³ NMR (100 MHz) δ 155.19 (s), 149.80 (s), 148.47 (s), 143.67 (s), 132.61 (s), 127.58 (s), 124.44 (s), 122.15 (s), 118.95 (s), 112.38 (s), 21.35 (s).



2-(4-chlorophenyl)-5-methylpyridine (1p)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

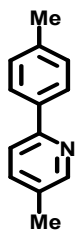
Appearance: White solid

Isolated yield: 92%

Molecular weight: 203.67 g/mol

H¹ NMR (400 MHz) δ 8.51 (s), 7.89 (d, J = 8.9 Hz), 7.67 – 7.51 (m), 7.42 (d, J = 8.9 Hz), 2.37 (s).

C¹³ NMR (100 MHz) δ 153.60 (s), 150.13 (s), 137.72 (d, J = 8.1 Hz), 134.82 (s), 132.16 (s), 129.46 (s), 128.98 (s), 128.07 (s), 120.04 (s), 116.86 (s), 18.30 (s).



5-methyl-2-(p-tolyl)pyridine (1q)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

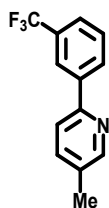
Appearance: White solid

Isolated yield: 95%

Molecular weight: 183.25g/mol

¹H NMR (400 MHz) δ 8.50 (s), 7.85 (d, J = 7.8 Hz), 7.57 (d, J = 17.7 Hz), 7.28 (s), 2.40 (s), 2.36 (s).

¹³C NMR (100 MHz) δ 154.92 (s), 150.02 (s), 138.62 (s), 137.41 (s), 136.67 (s), 131.37 (s), 130.04 (s), 129.51 (s), 126.65 (s), 119.92 (s), 21.33 (s), 18.24 (s).



5-methyl-2-(3-(trifluoromethyl)phenyl)pyridine (1r)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

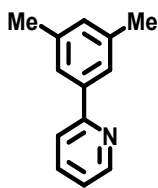
Appearance: White solid

Isolated yield: 90%

Molecular weight: 237.23g/mol

¹H NMR (400 MHz) δ 8.55 (d, J = 2.4 Hz), 8.24 (d, J = 0.7 Hz), 8.15 (d, J = 7.8 Hz), 7.82 – 7.43 (m), 2.40 (s).

¹³C NMR (100 MHz) δ 153.22 (s), 150.28 (s), 140.06 (s), 137.77 (s), 132.70 (s), 131.38 (s), 131.06 (s), 129.97 (s), 129.29 (s), 125.33 (d, J = 3.8 Hz), 123.65 (d, J = 4.0 Hz), 120.31 (s), 18.31 (s).



5-methyl-2-(3-(trifluoromethyl)phenyl)pyridine (1s)

C-H arylation was carried out by following the general procedure GPPP.

Eluent: ethyl acetate/ petroleum ether (2% EA-PE).

Appearance: Yellow liquid

Isolated yield: 87%

Molecular weight: 183.25 g/mol

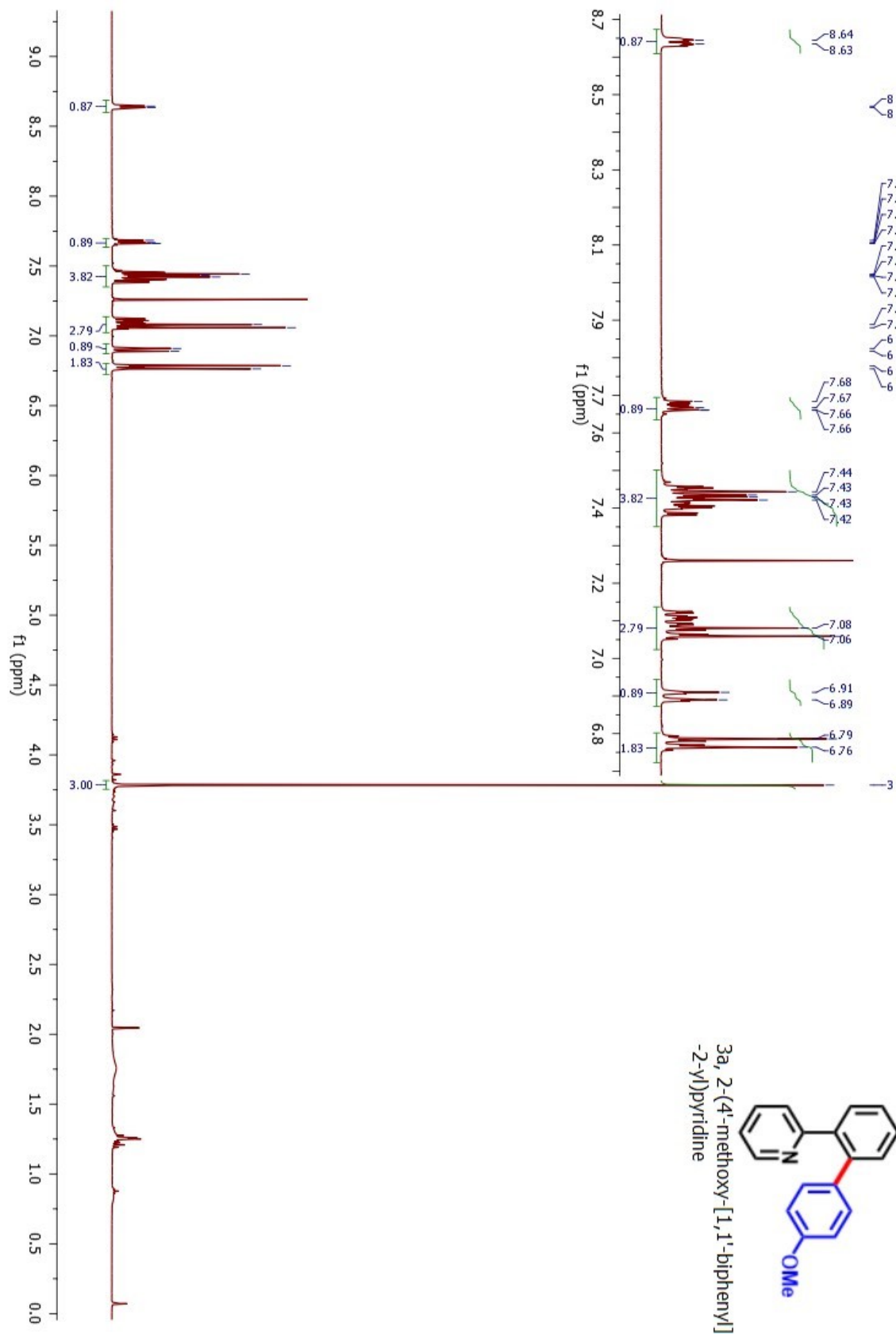
¹H NMR (400 MHz) δ 8.69 (d, J = 4.7 Hz, 1H), 7.71 (s, 2H), 7.61 (s, 2H), 7.23 – 7.17 (m, 1H), 7.07 (s, 1H), 2.40 (s, 6H).

¹³C NMR (100 MHz) δ 157.78 (s), 149.53 (s), 139.33 (s), 138.31 (s), 136.71 (s), 130.66 (s), 124.80 (s), 121.97 (s), 120.72 (s), 21.42 (s).

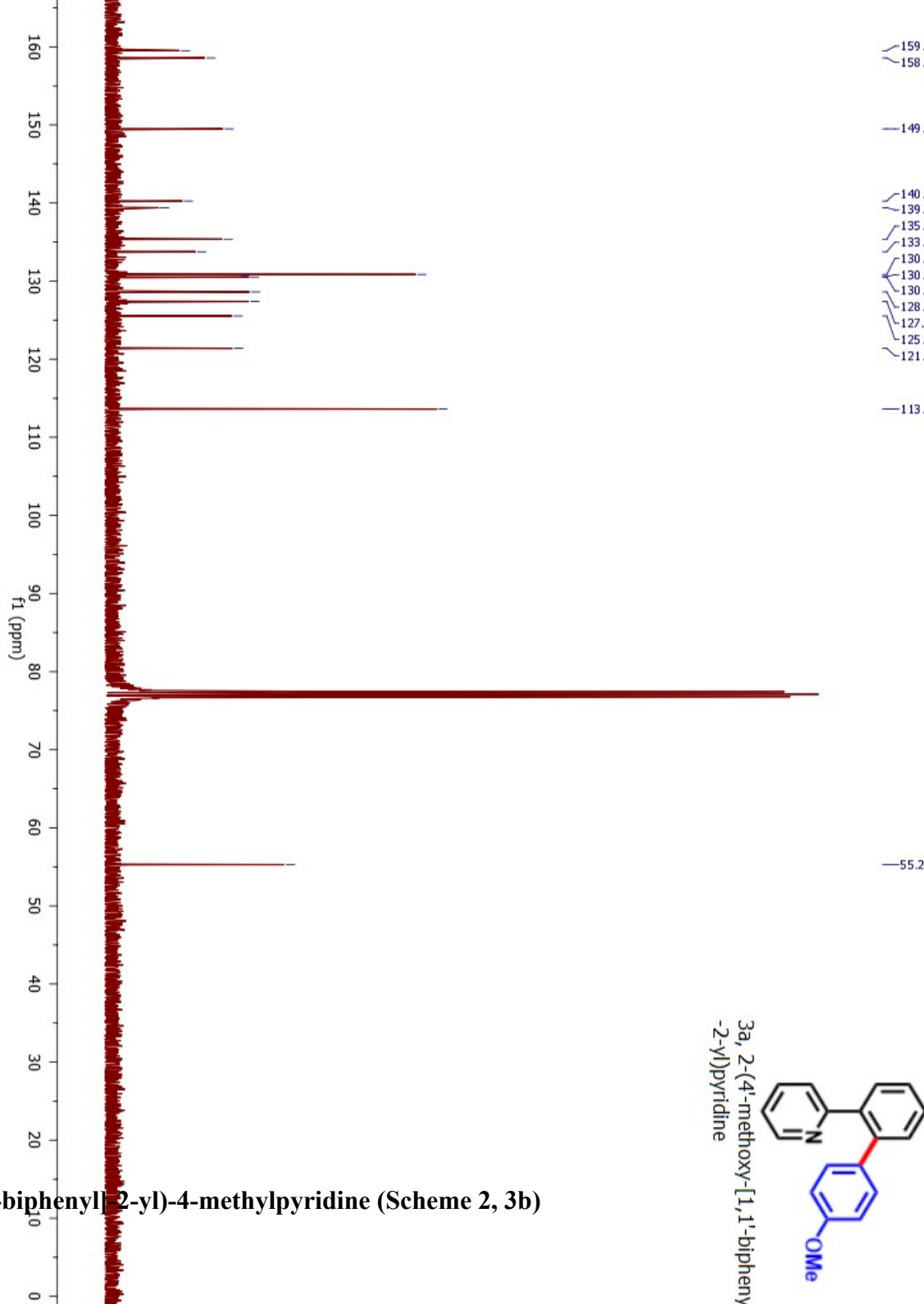
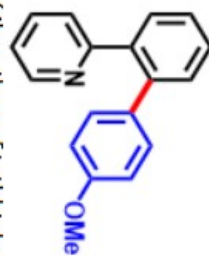
8. References

1. C. Liu, Q. Ni, P. Hu, and J. Qiu, *Org. Biomol. Chem.*, 2011, **9**(4), 1054-1060.
2. S. Shaaban, A. Jolit, D. Petkova, and N. Maulide, *Chem. Commun.*, 2015, **51**(73), 13902-13905.
3. N. Zhang, Z.-J. Quan, Z. Zhang, Y.-X. Da and X.-C. Wang, *Chem. Commun.*, 2016, **52**, 14234–14237.
4. J. Feng, G. Lu, M. Lv, and C. Cai, *Synlett*, 2013, **24**(16), 2153-2159.
5. G. M. Reddy, N. S. S. Rao, P. Satyanarayana, and H. Maheswaran, *RSC Adv.*, 2015, **5**(127), 105347-105352.
6. L. Su, D. D. Guo, B. Li, S. H. Guo, G. F. Pan, Y. R. Gao, and Y. Q. Wang, *ChemCatChem*, 2017, **9**(11), 2001-2008.
7. D. Kalyani, N. R. Deprez, L. V. Desai, and M. S. Sanford, *J. Am. Chem. Soc.*, 2005, **127**(20), 7330-7331.
8. C. Binnani, R. K. Rai, D. Tyagi, S. M. Mobin, and S. K. Singh, CH bond Activation/Arylation over Pyridine based Arene-Ruthenium (II) Complexes: Synthesis, Structure and Catalytic Activity.

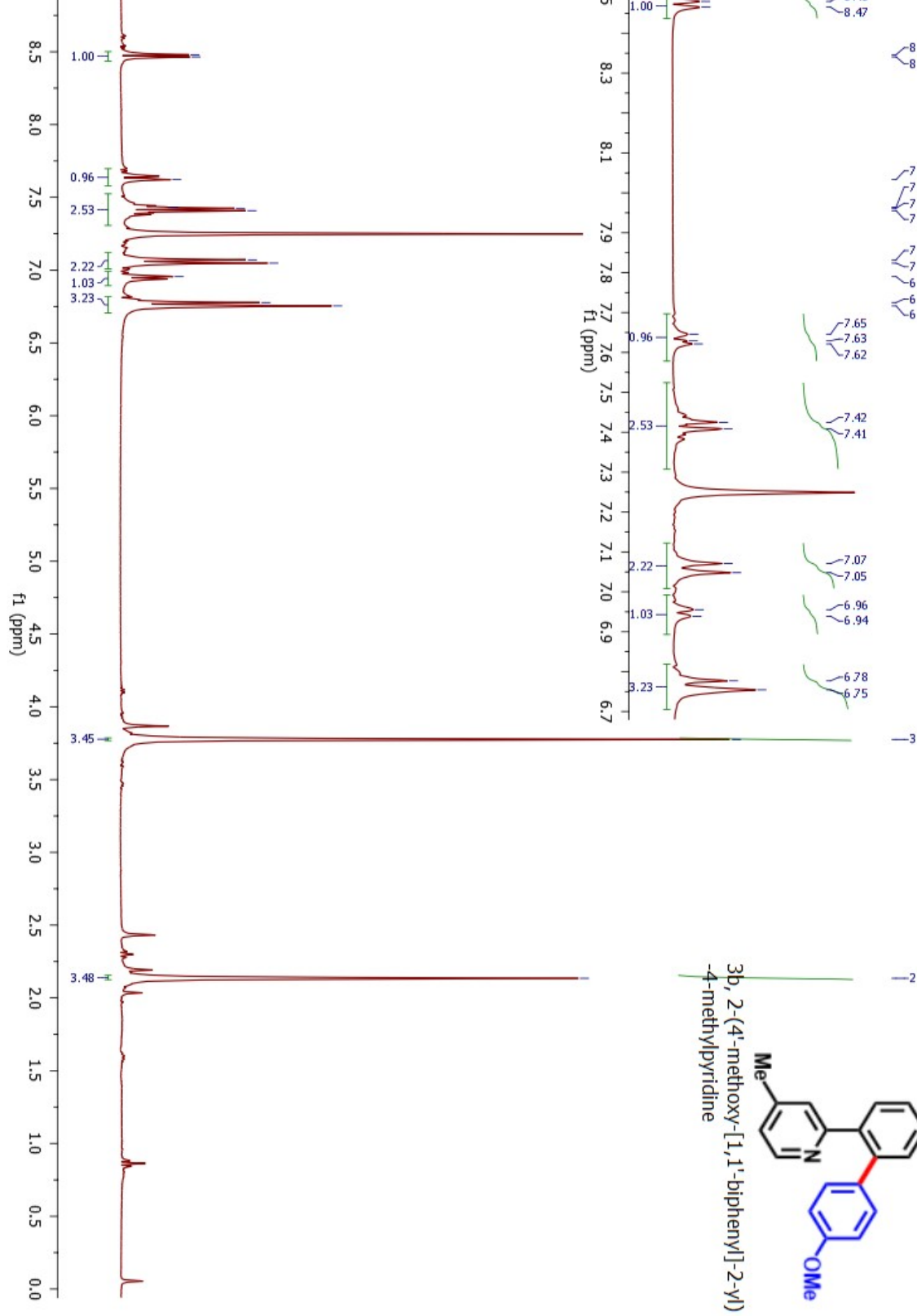
9. NMR spectra of 3a, 2-(4'-methoxy-[1,1'-biphenyl]-2-yl)pyridine

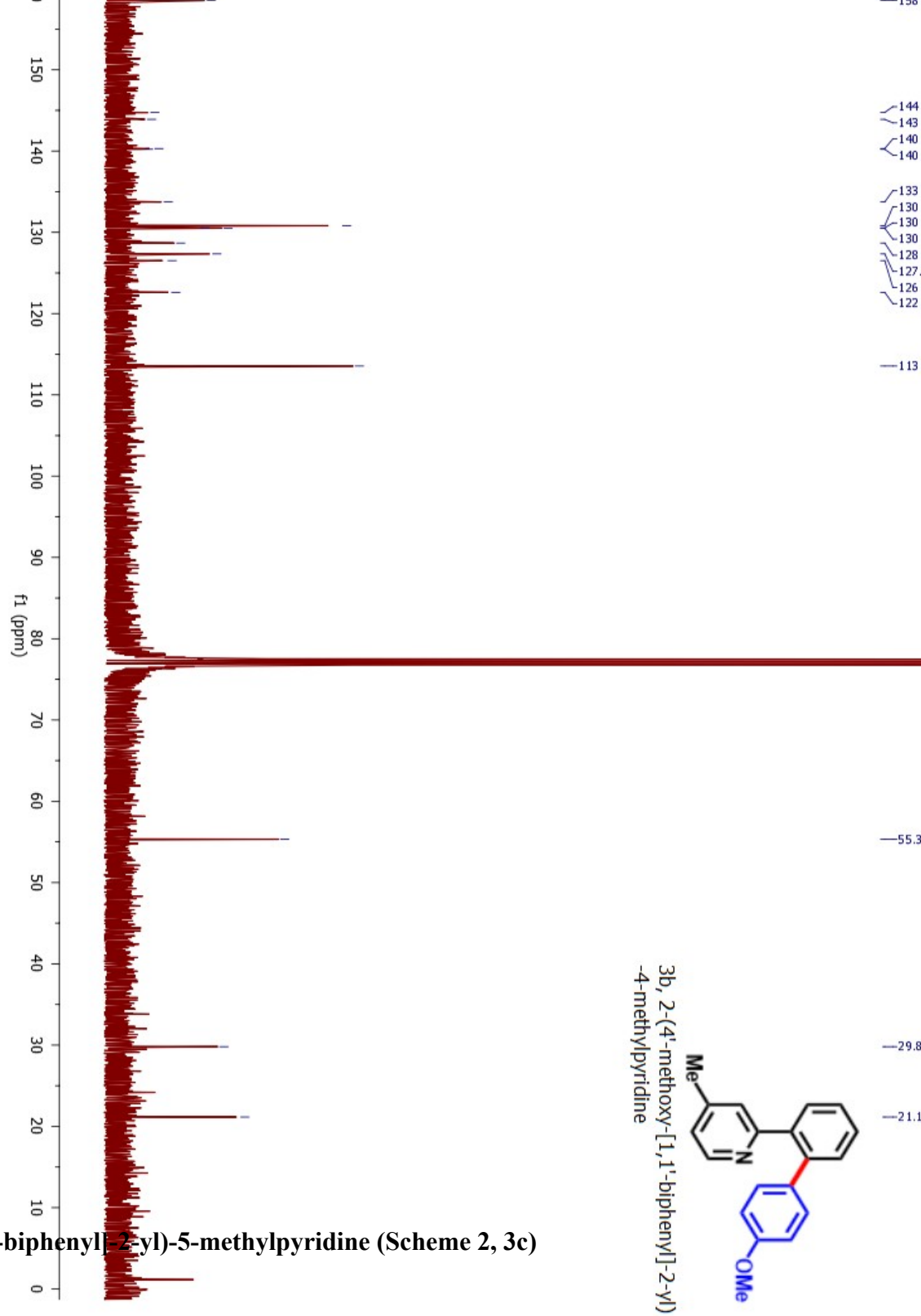


3a, 2-(4'-methoxy-[1,1'-biphenyl]-2-yl)pyridine

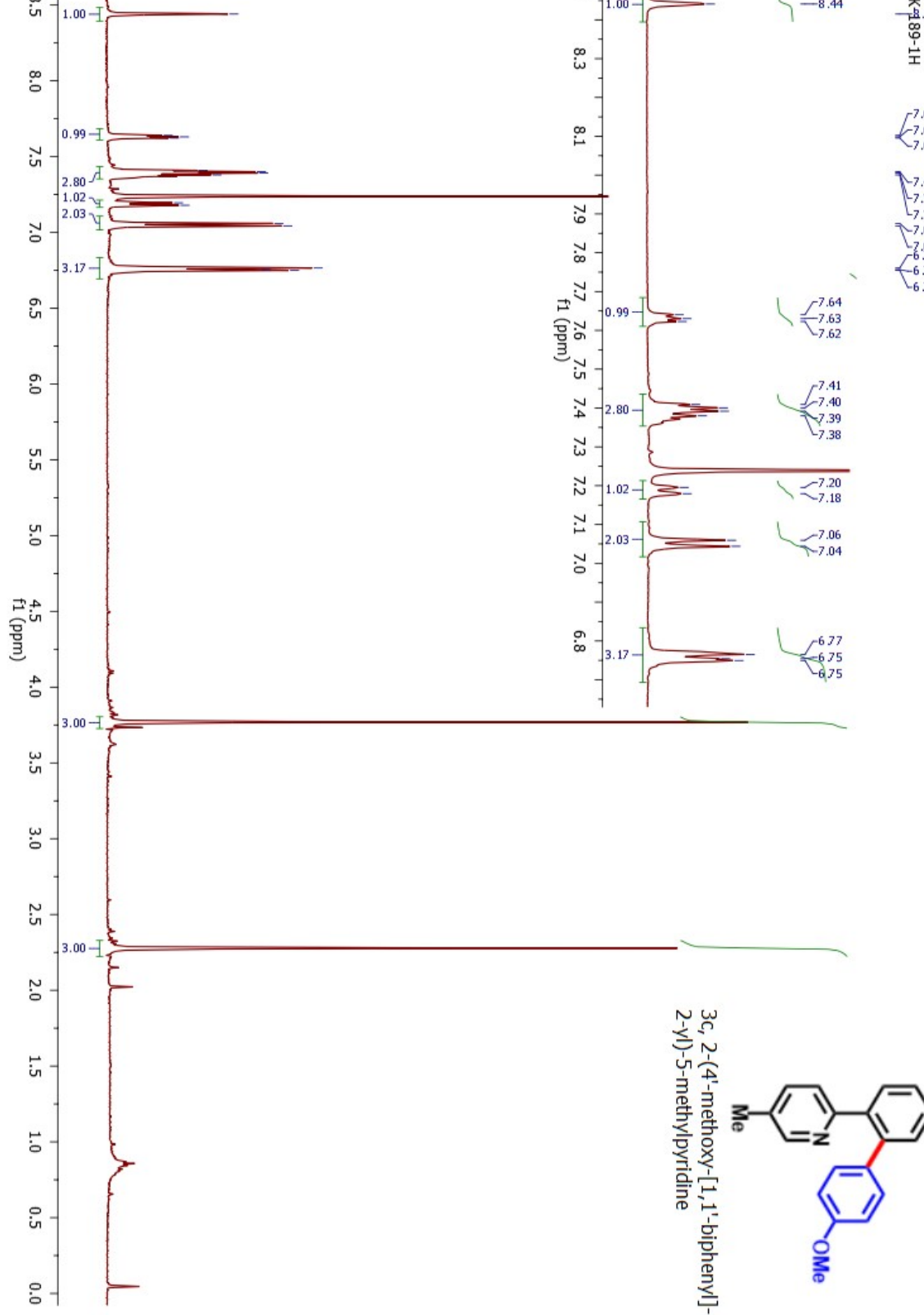


2-(4'-methoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3b)

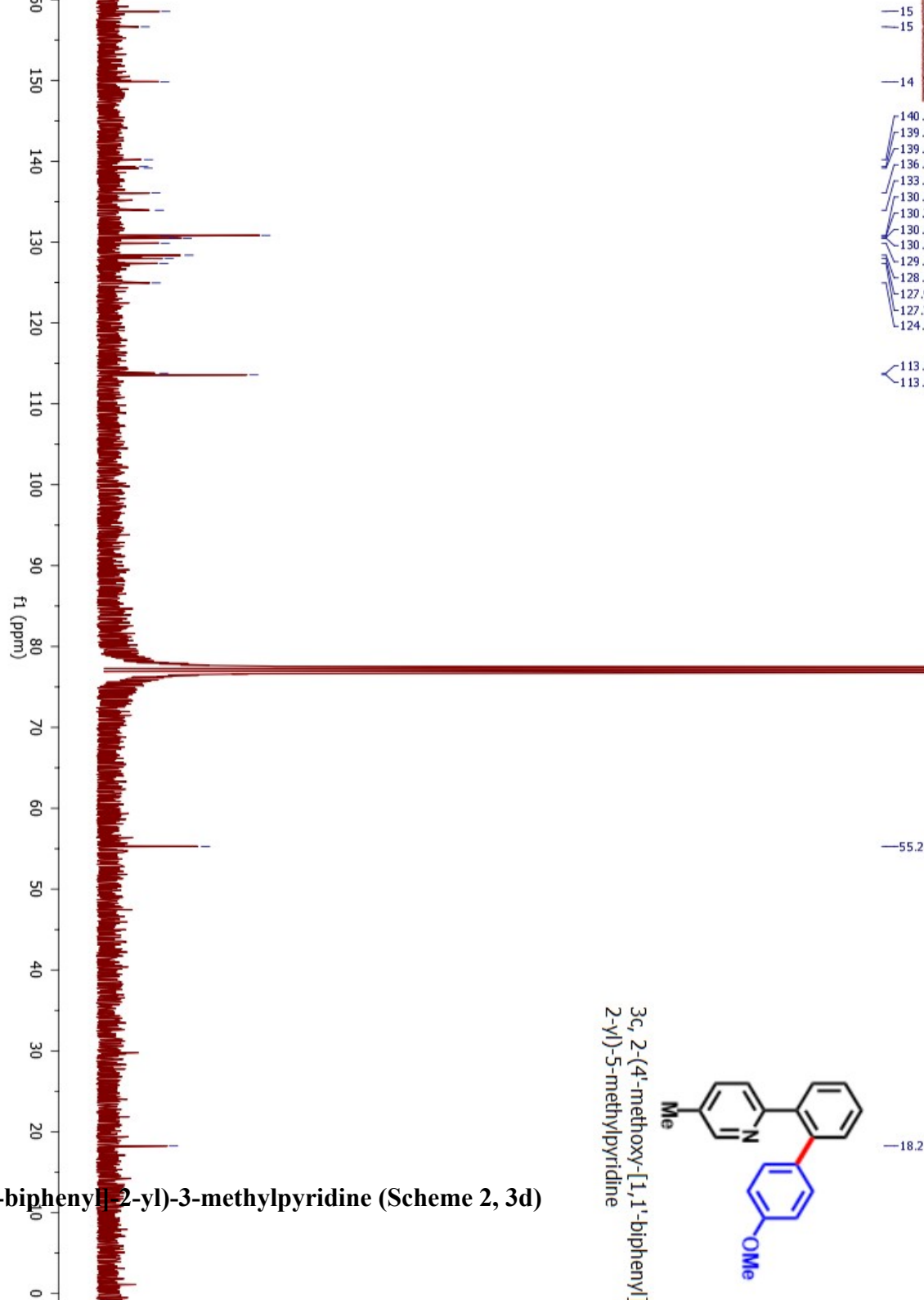
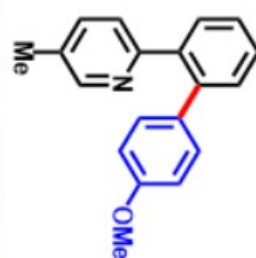




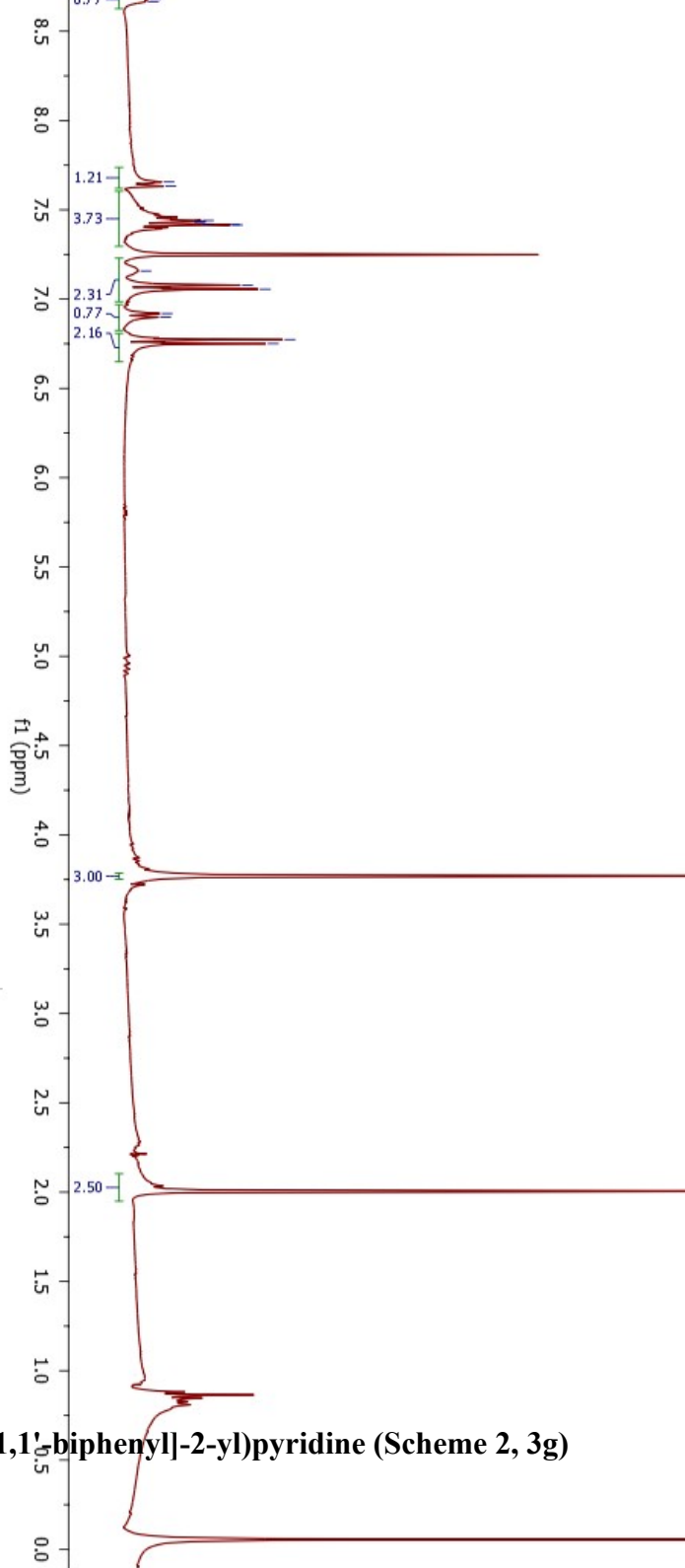
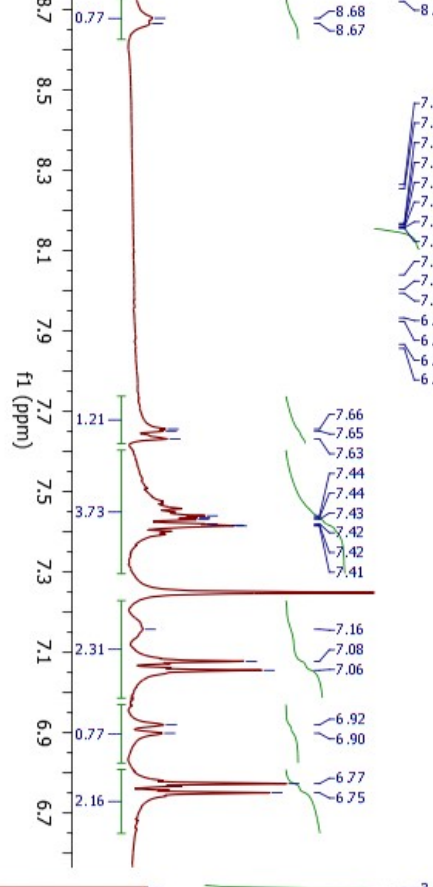
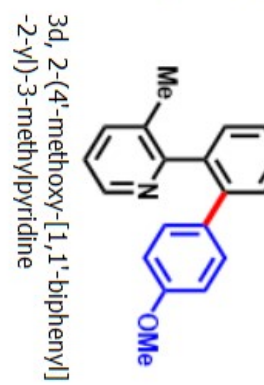
2-(4'-methoxy-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3c)



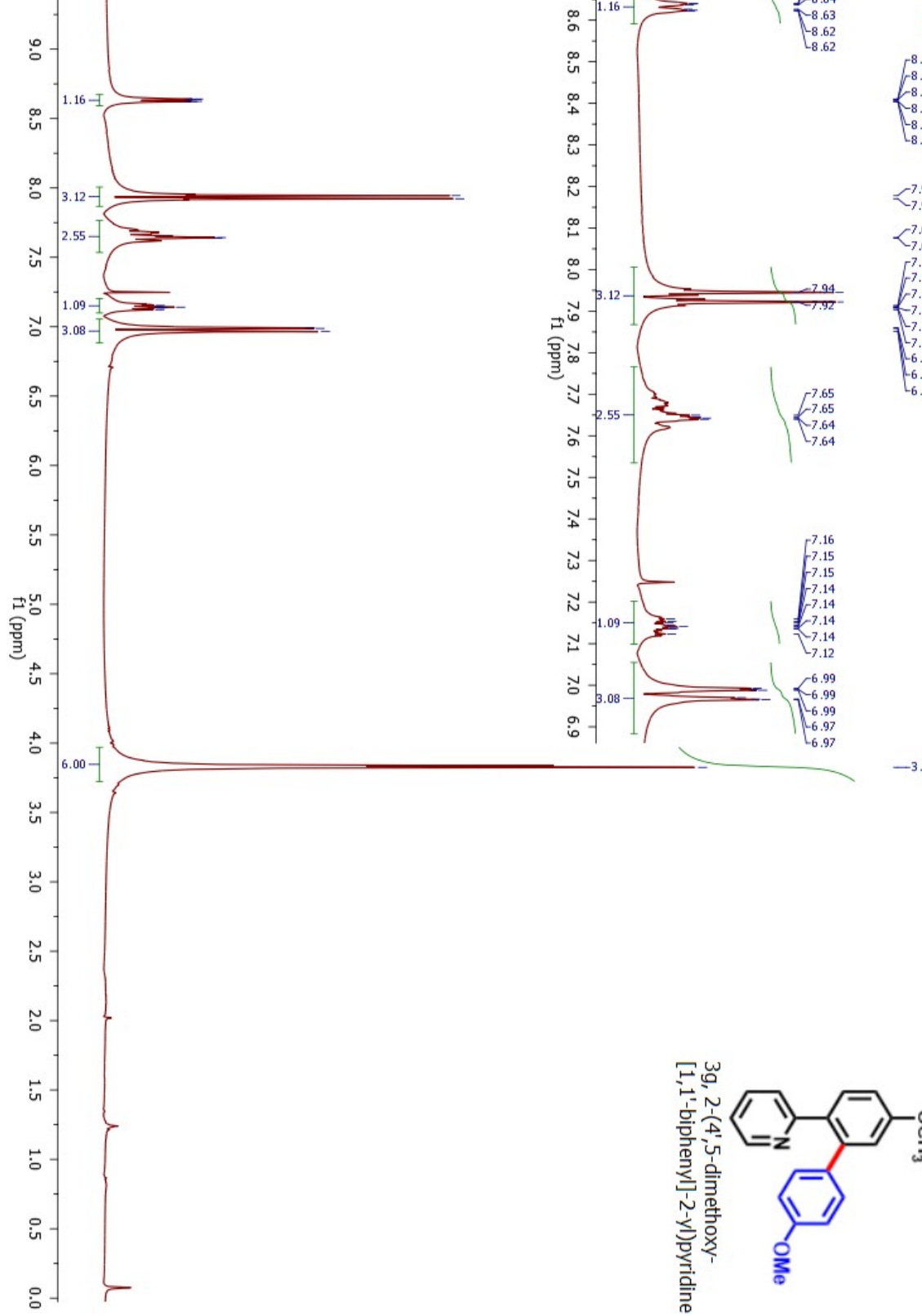
3c, 2-(4'-methoxy-[1,1'-biphenyl]-2-yl)-5-methylpyridine

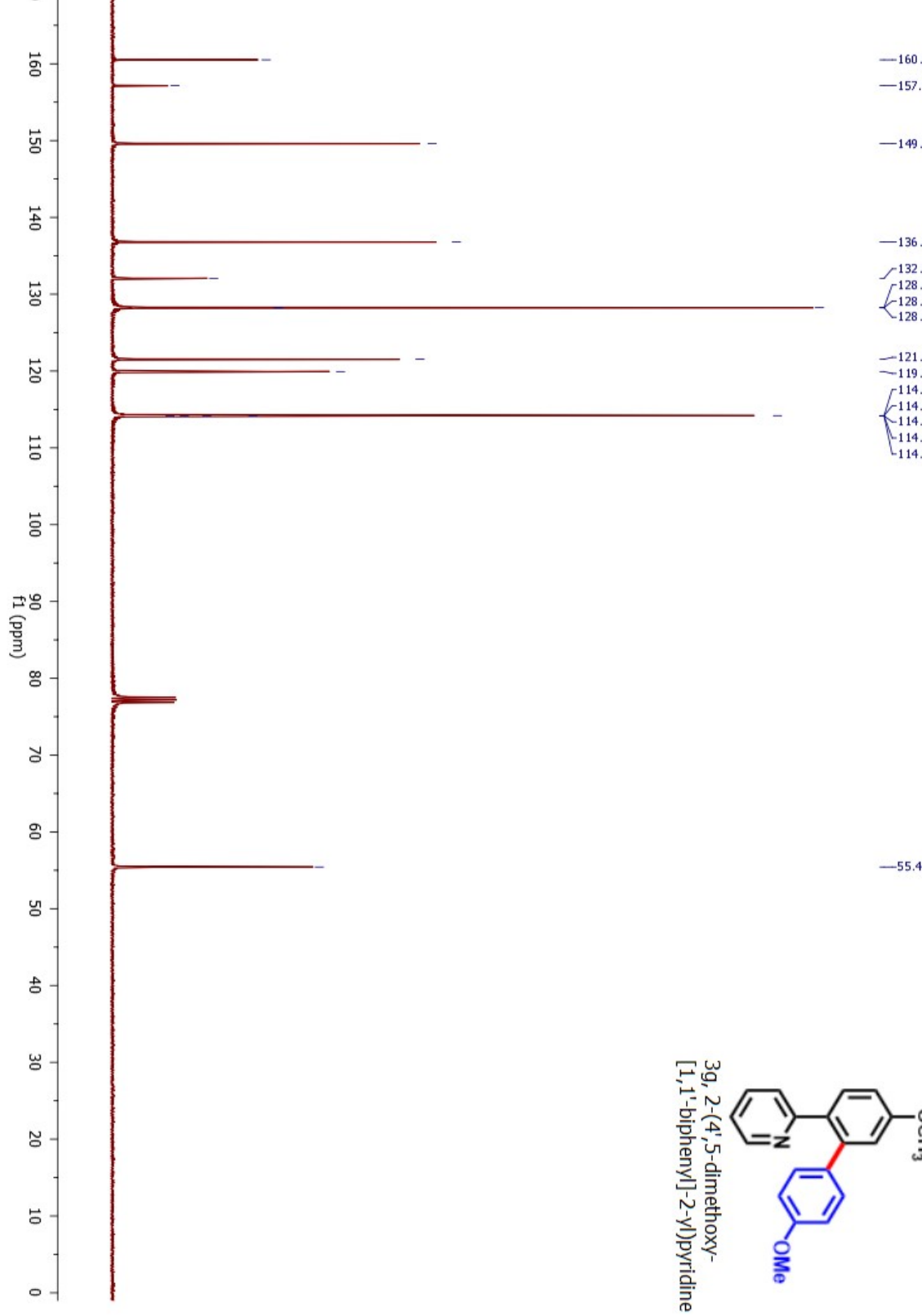


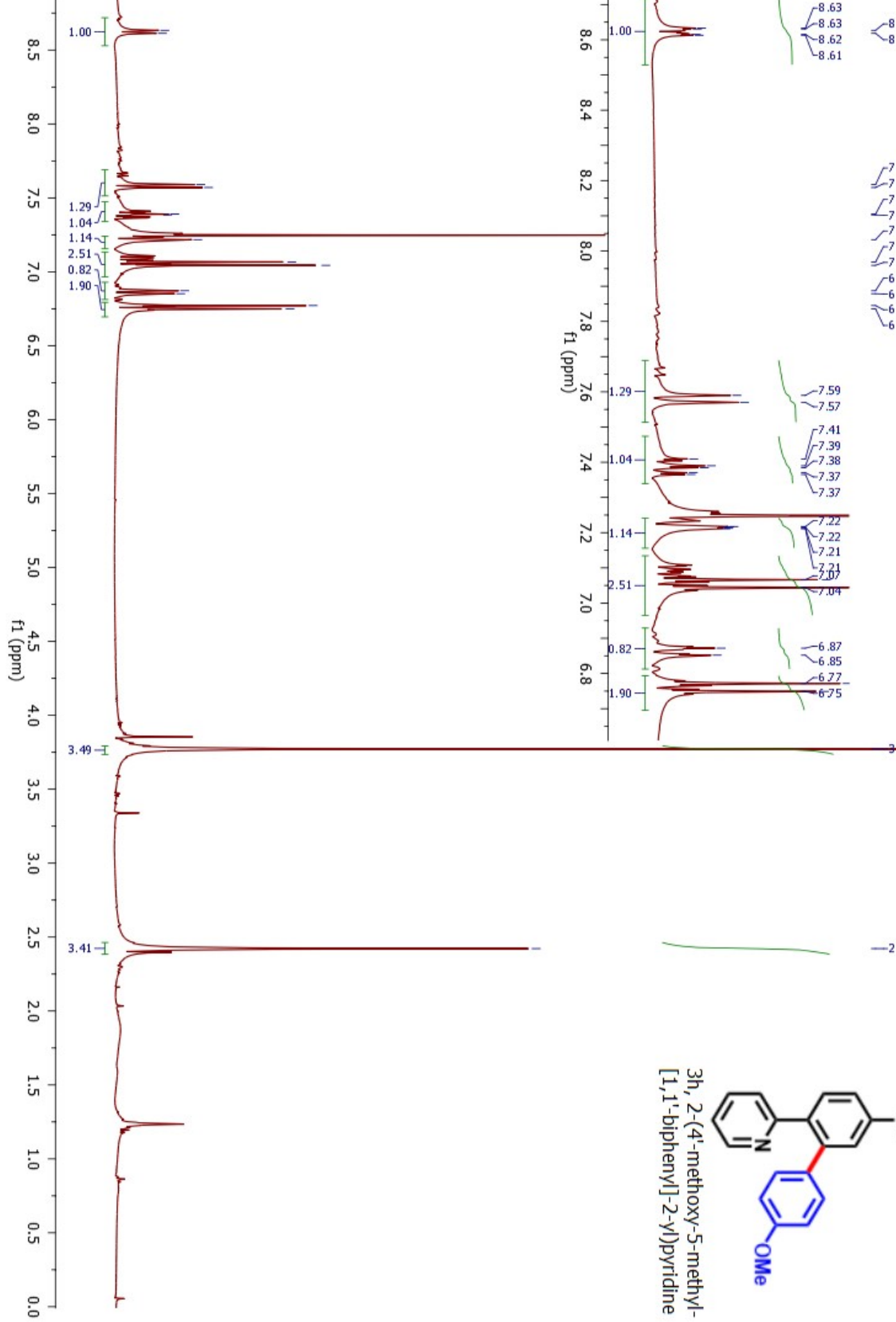
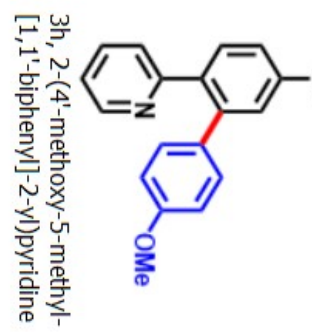
2-(4'-methoxy-[1,1'-biphenyl]-2-yl)-3-methylpyridine (Scheme 2, 3d)



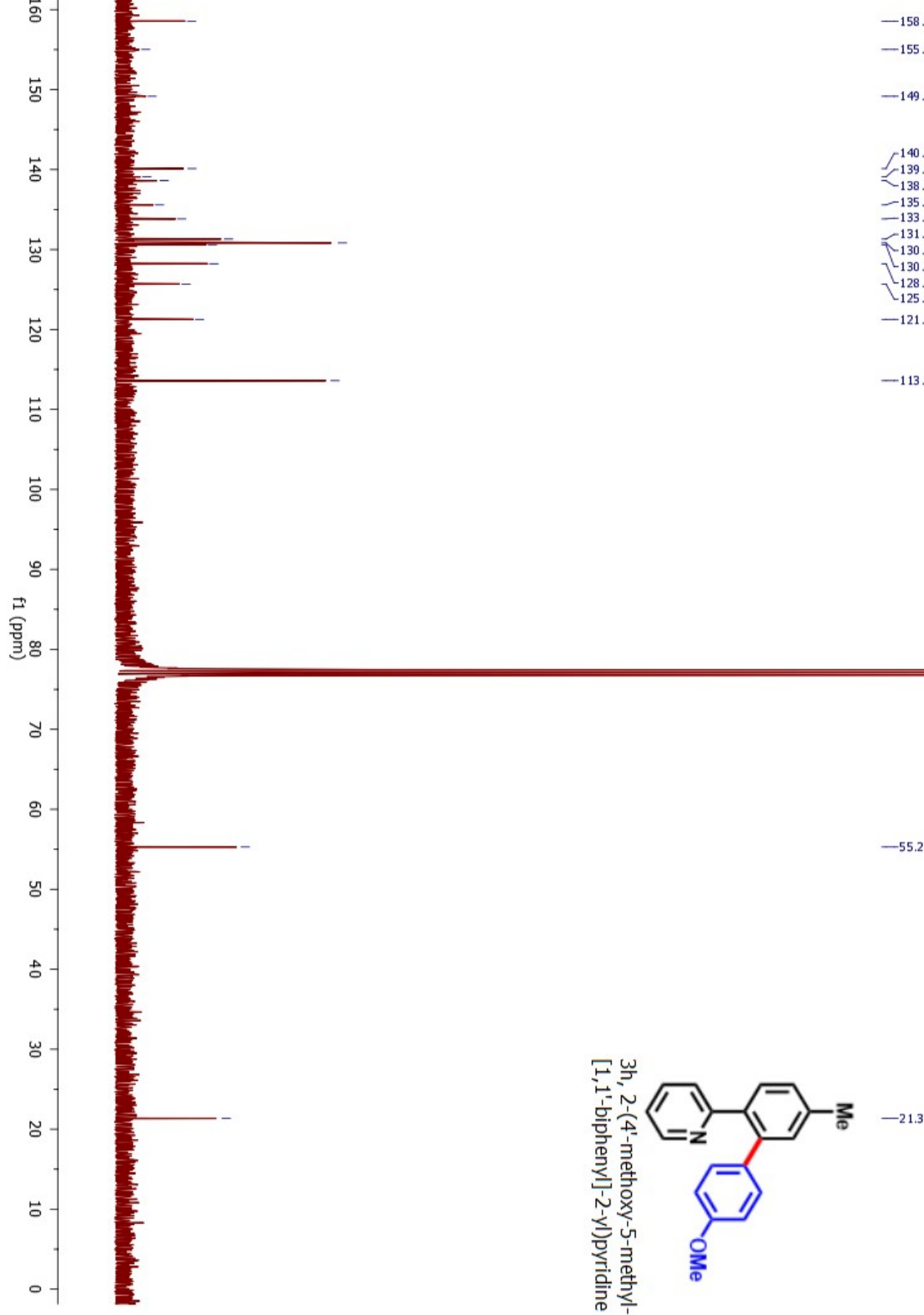
2-(4',5-dimethoxy-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3g)



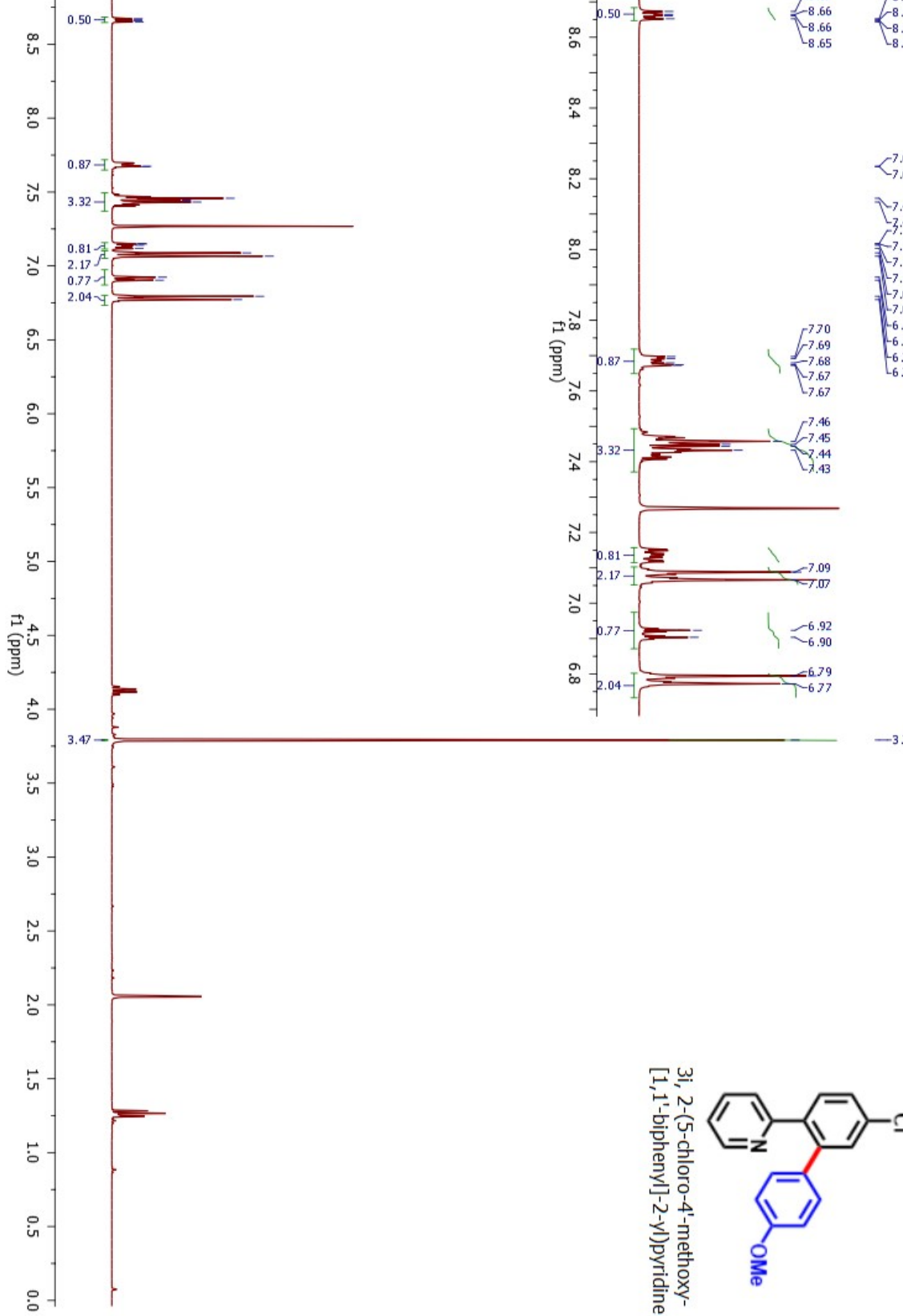




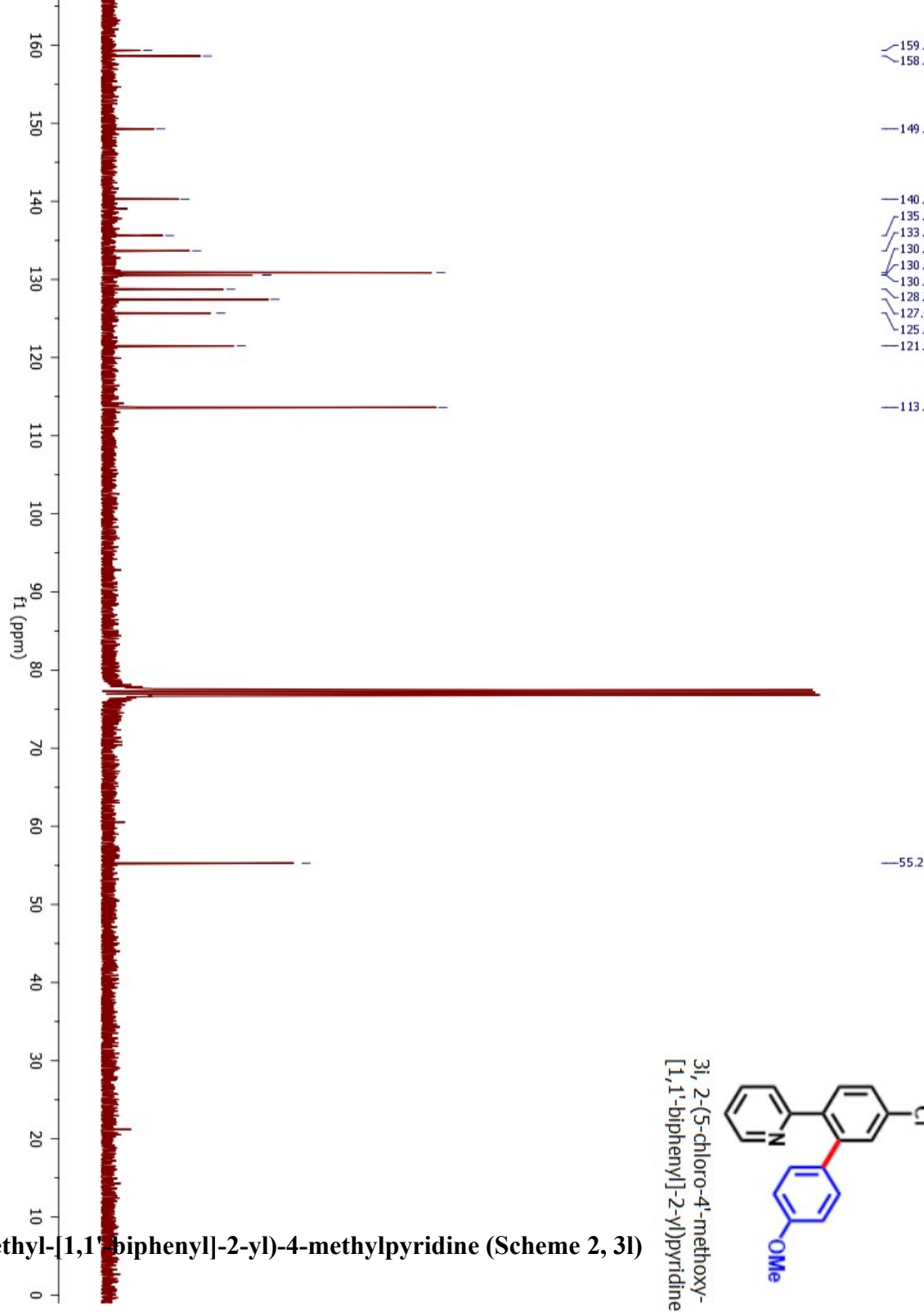
2-(4'-methoxy-5-me

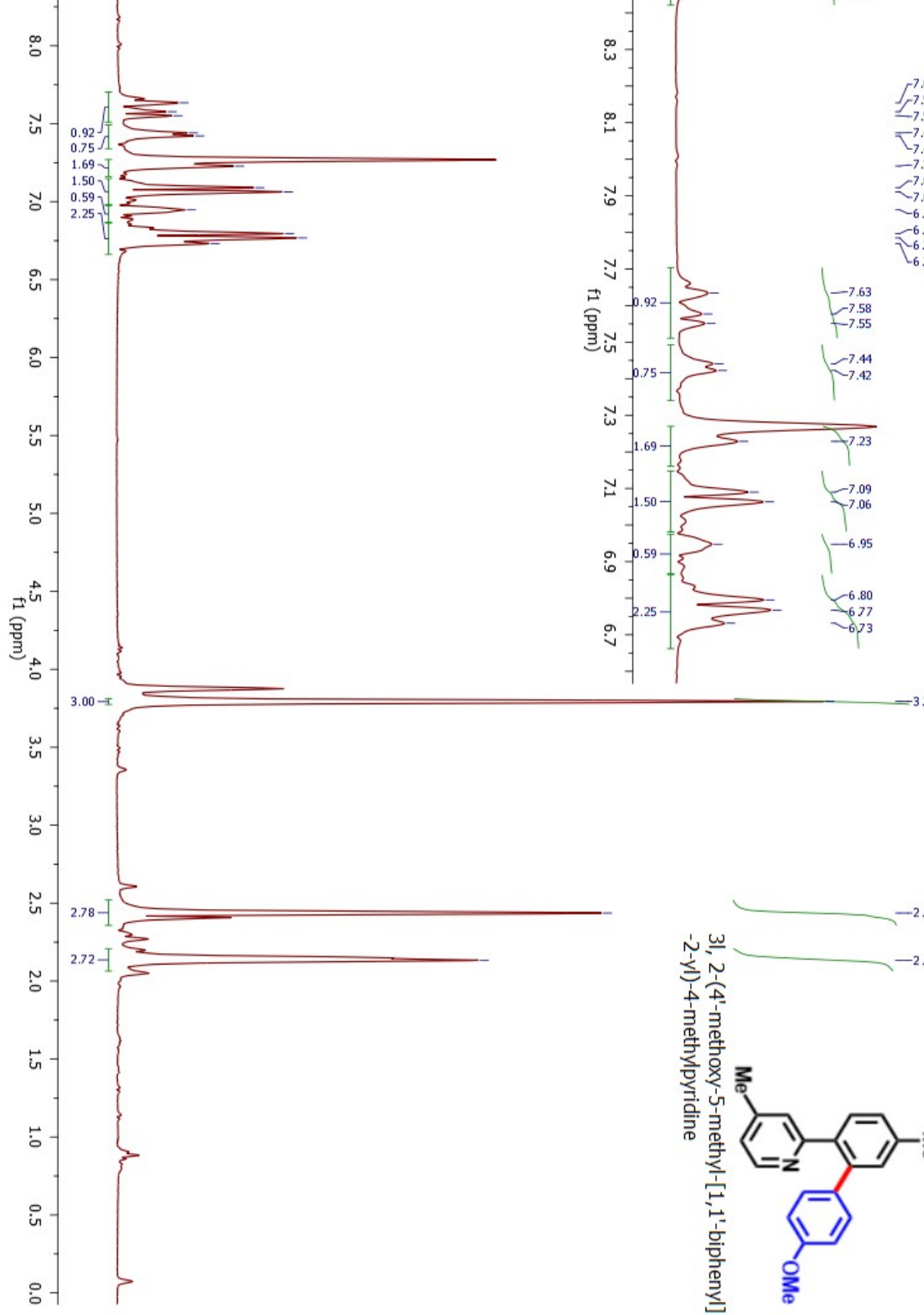


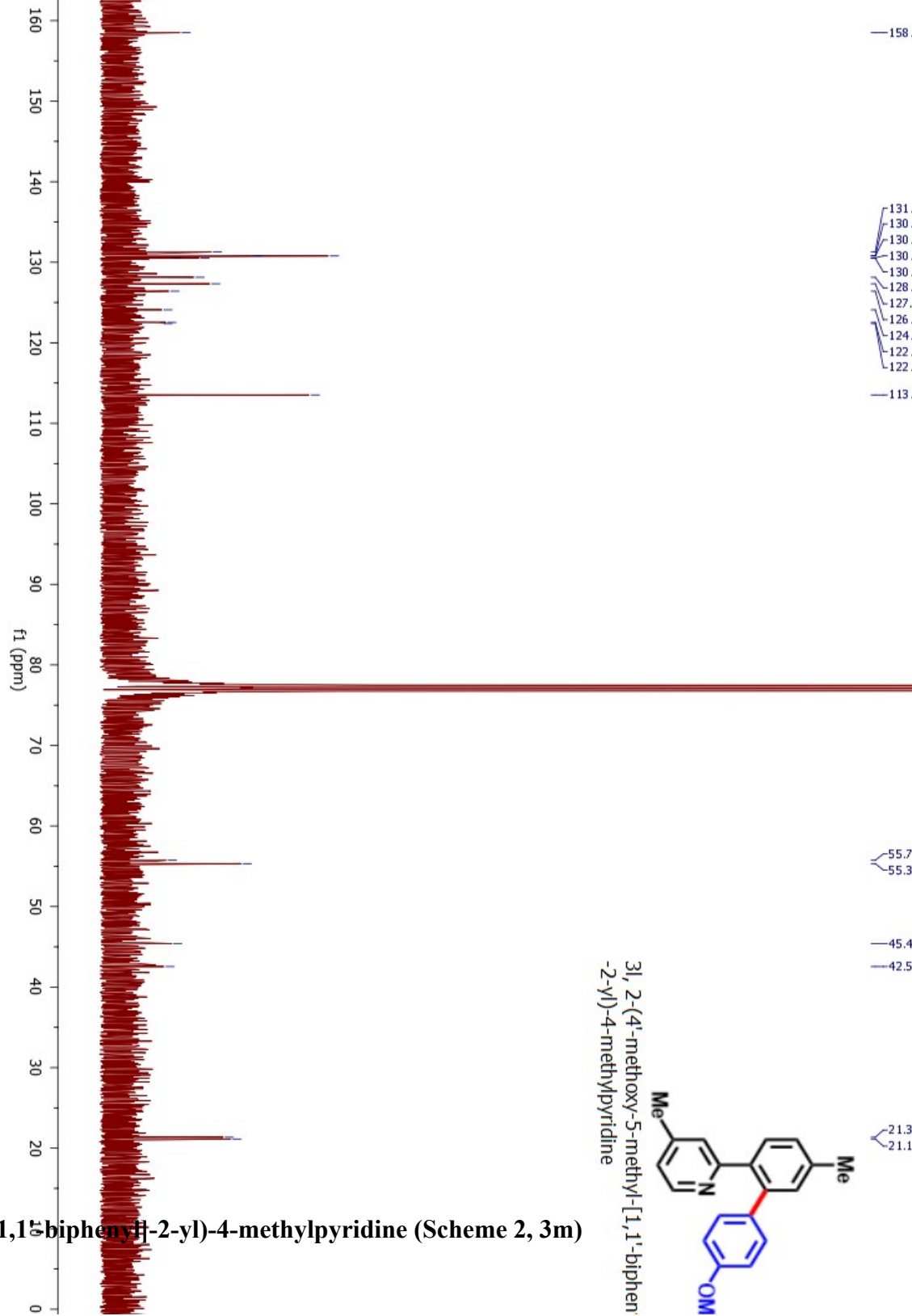
2-(5-chloro-4'-methoxy-2-pyridyl)-4-chlorobiphenyl



2-(4'-methoxy-5-methyl-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3l)

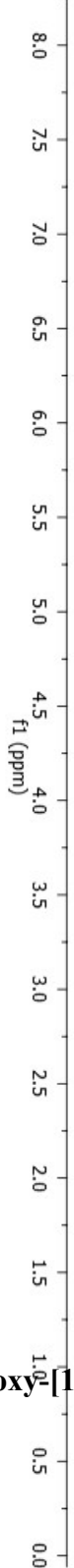
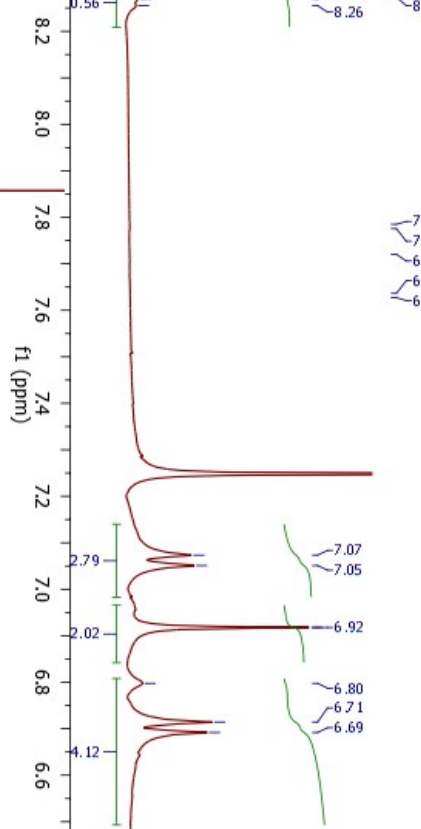
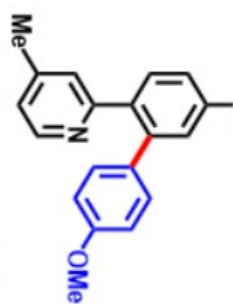




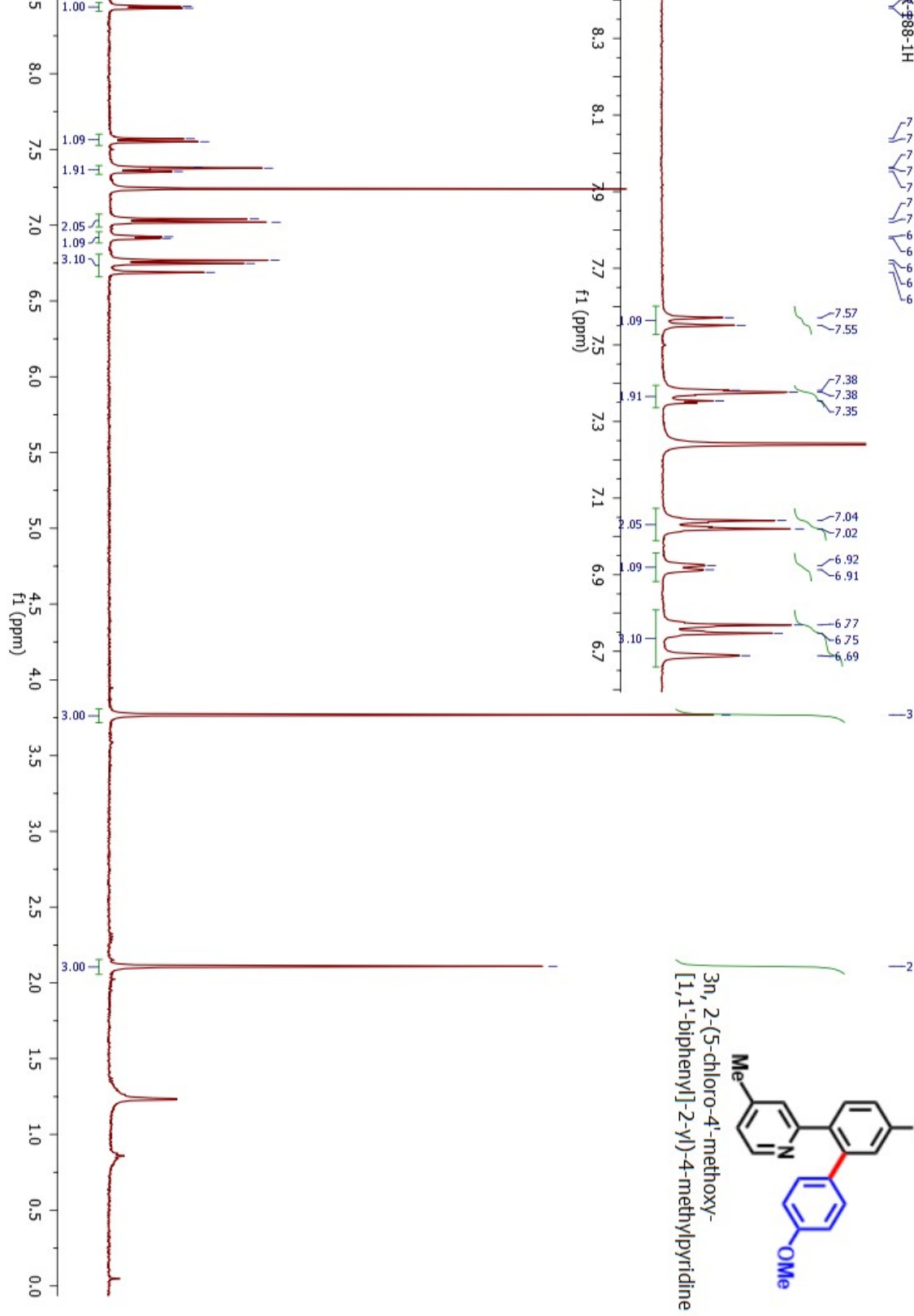


2-(4',5-dimethoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3m)

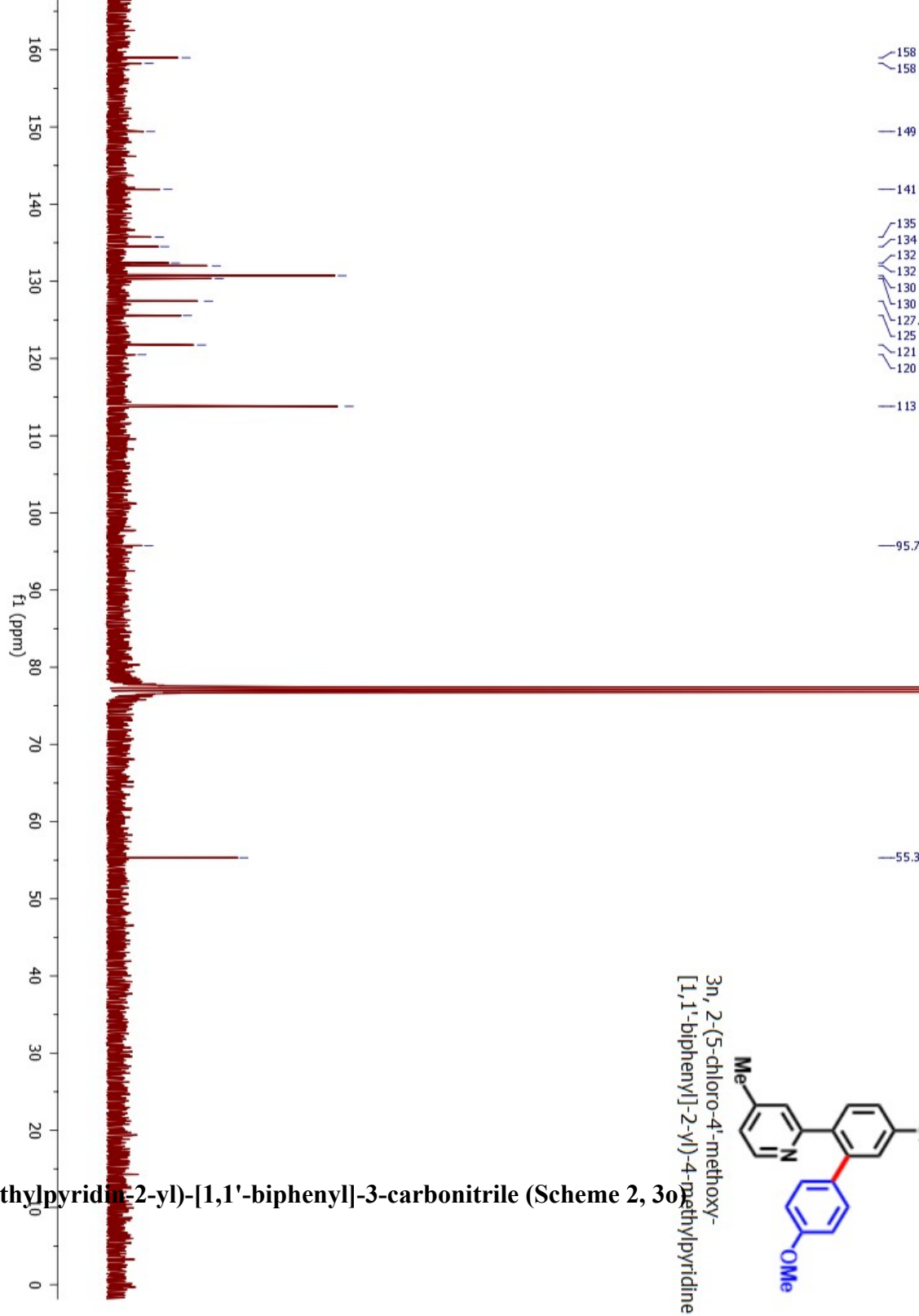
3m, 2-(4',5'-dimethoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine



2-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3n)

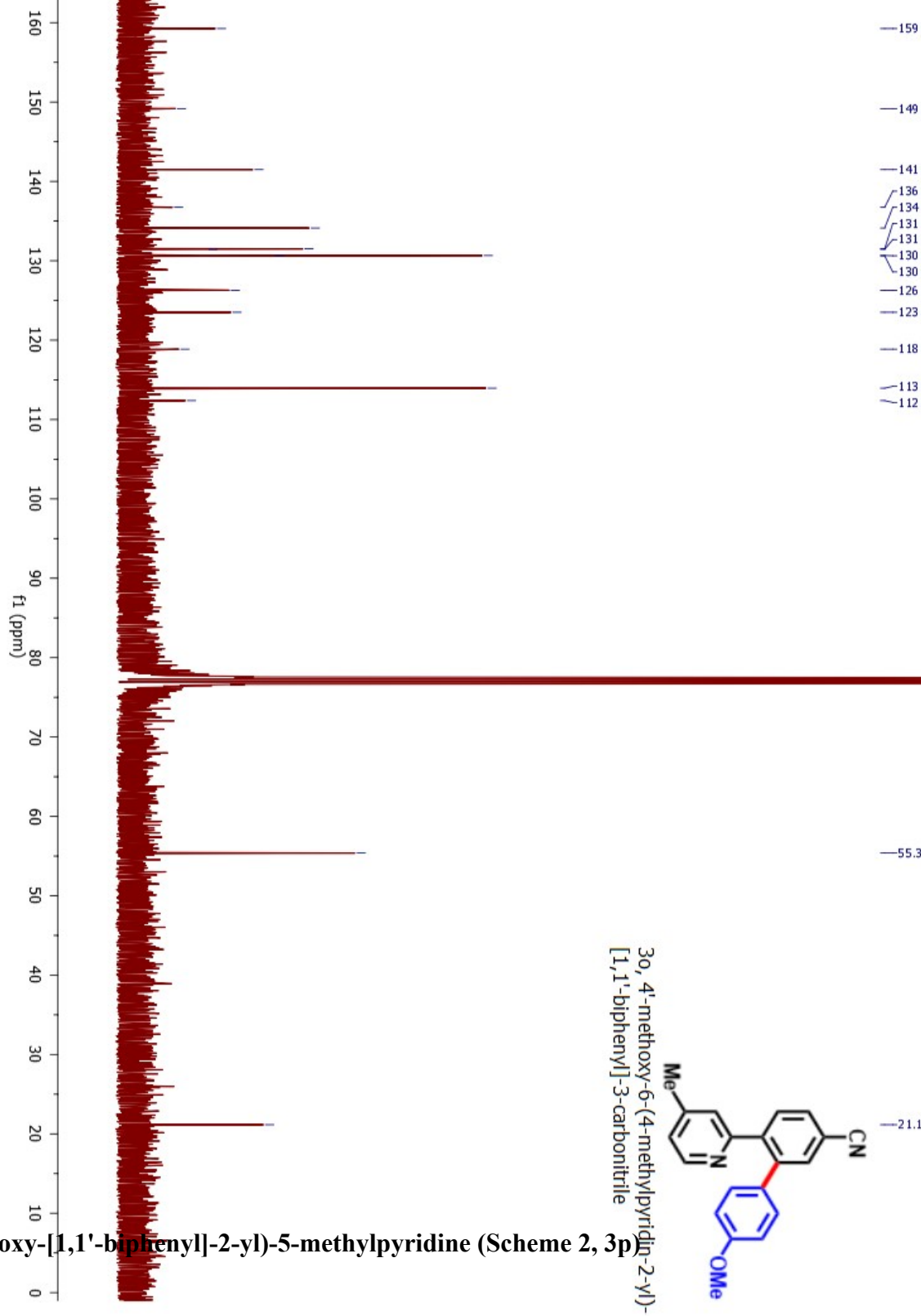


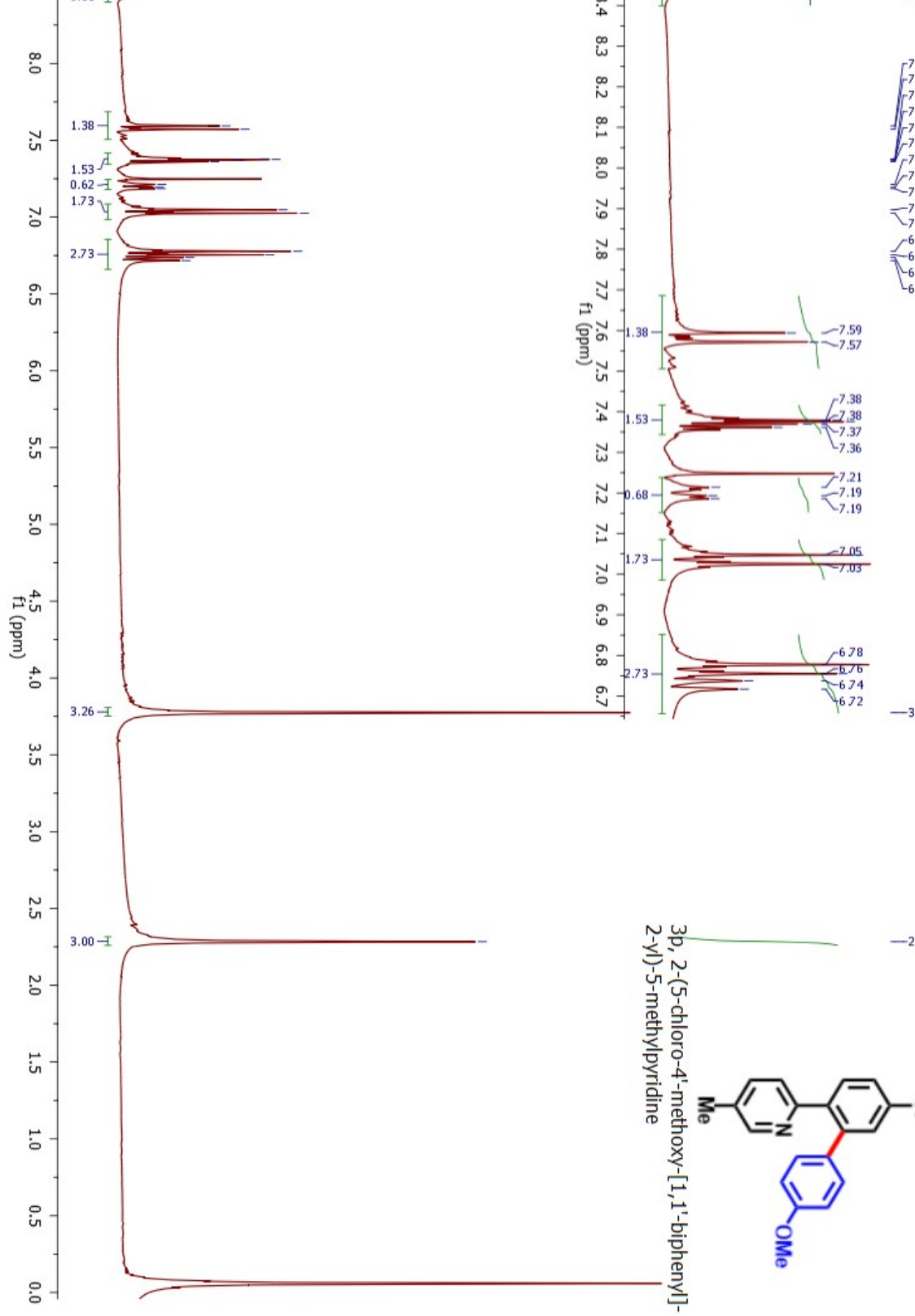
4'-methoxy-6-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-3-carbonitrile (Scheme 2, 30)



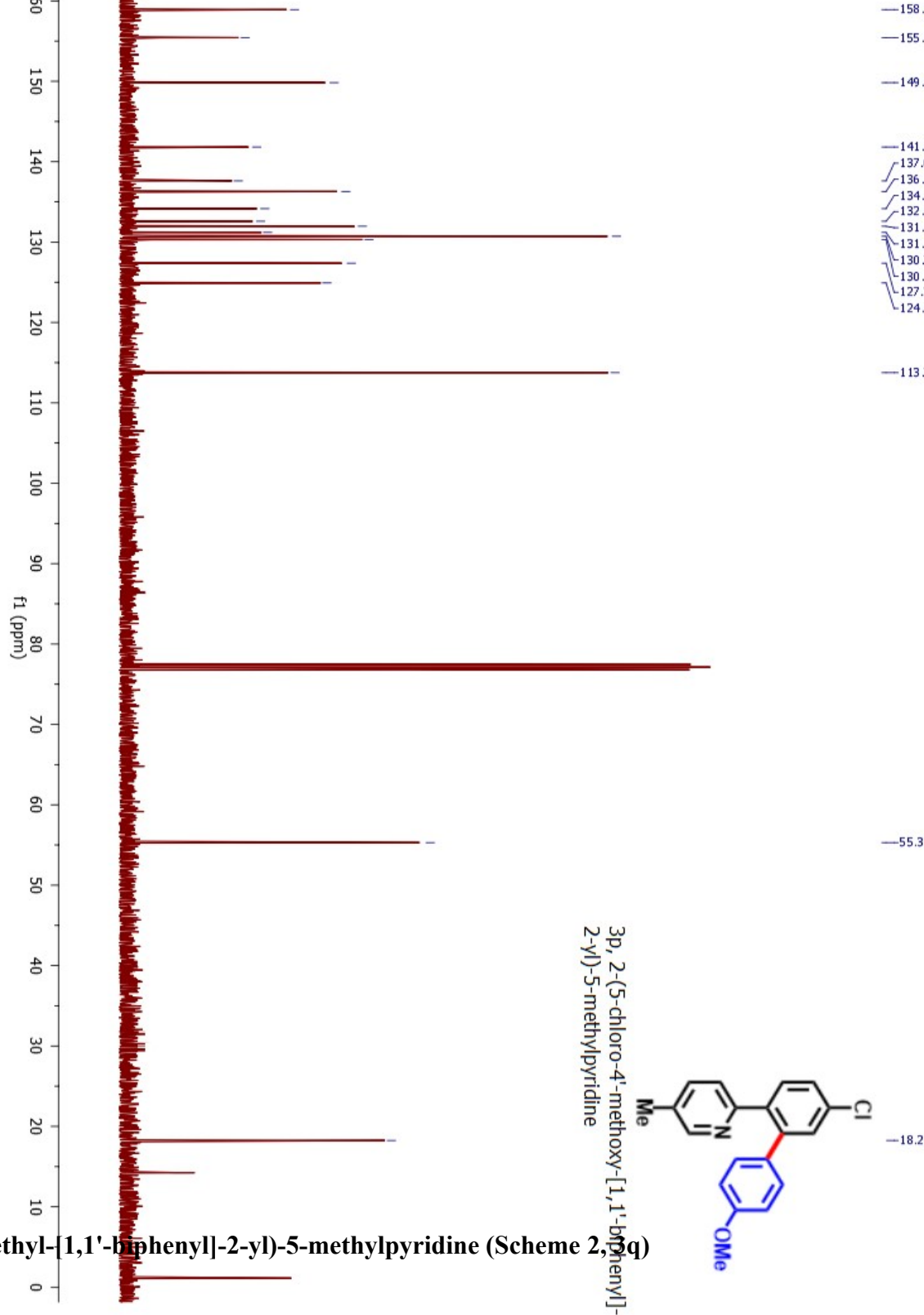


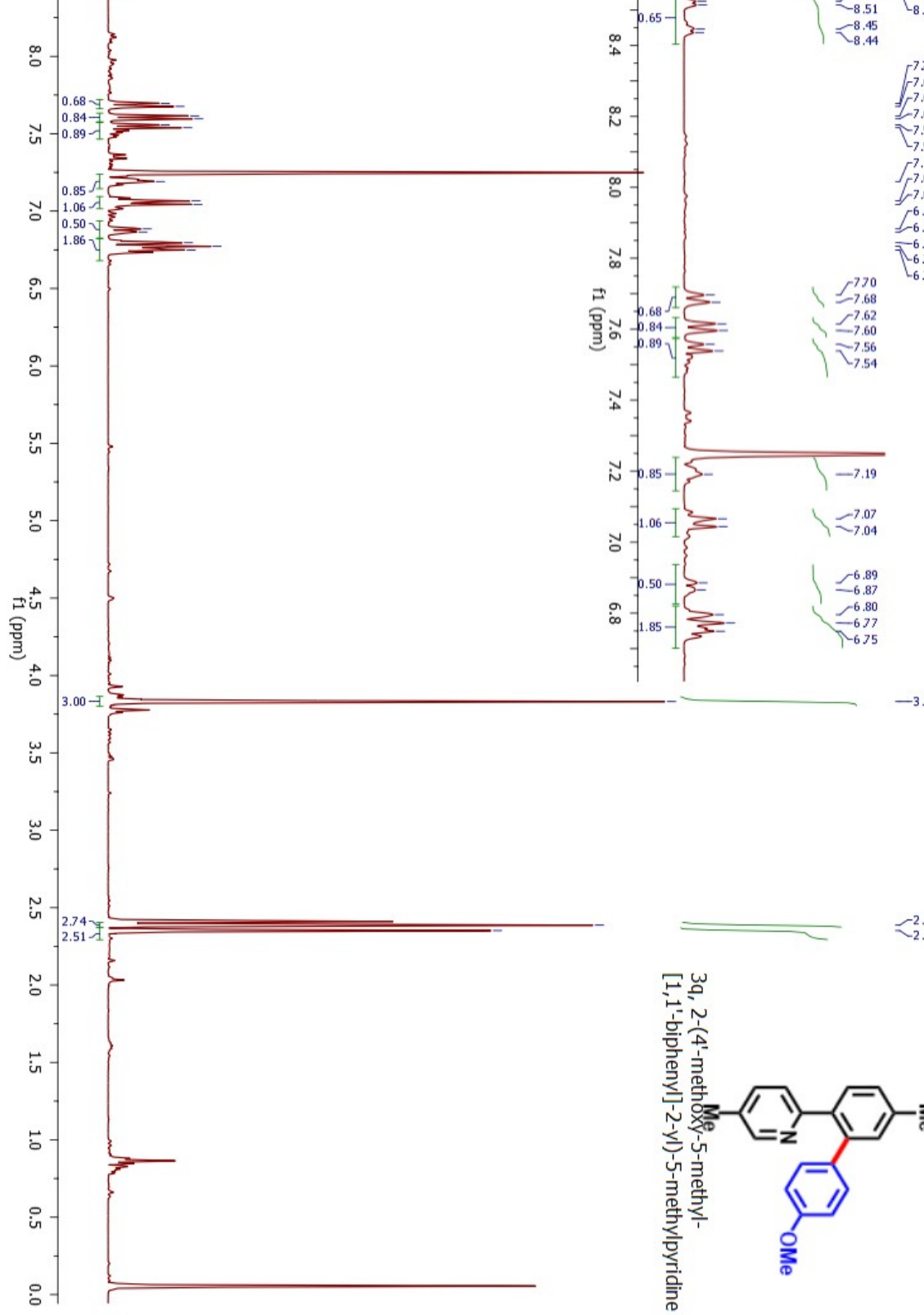
2-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3p)

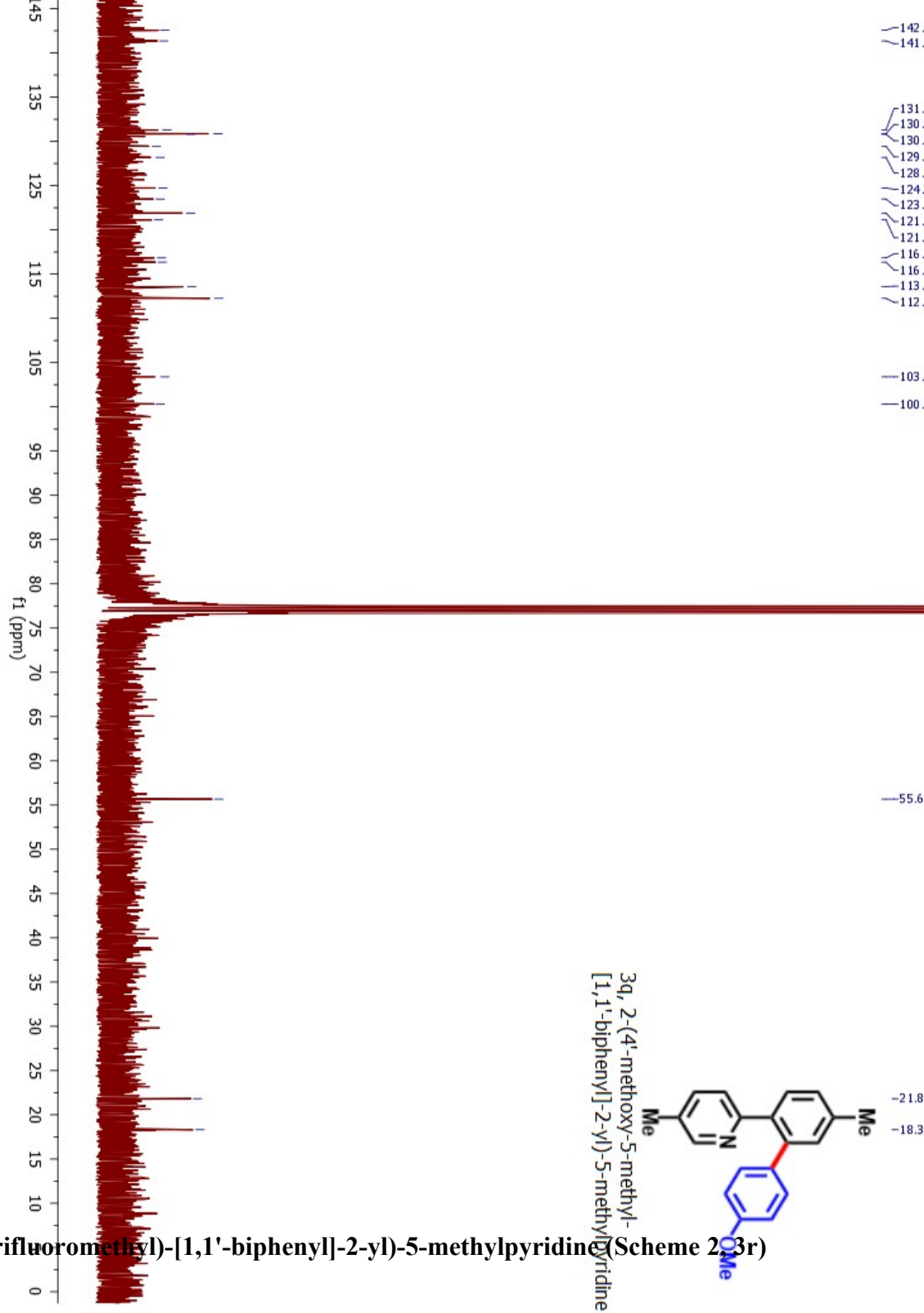




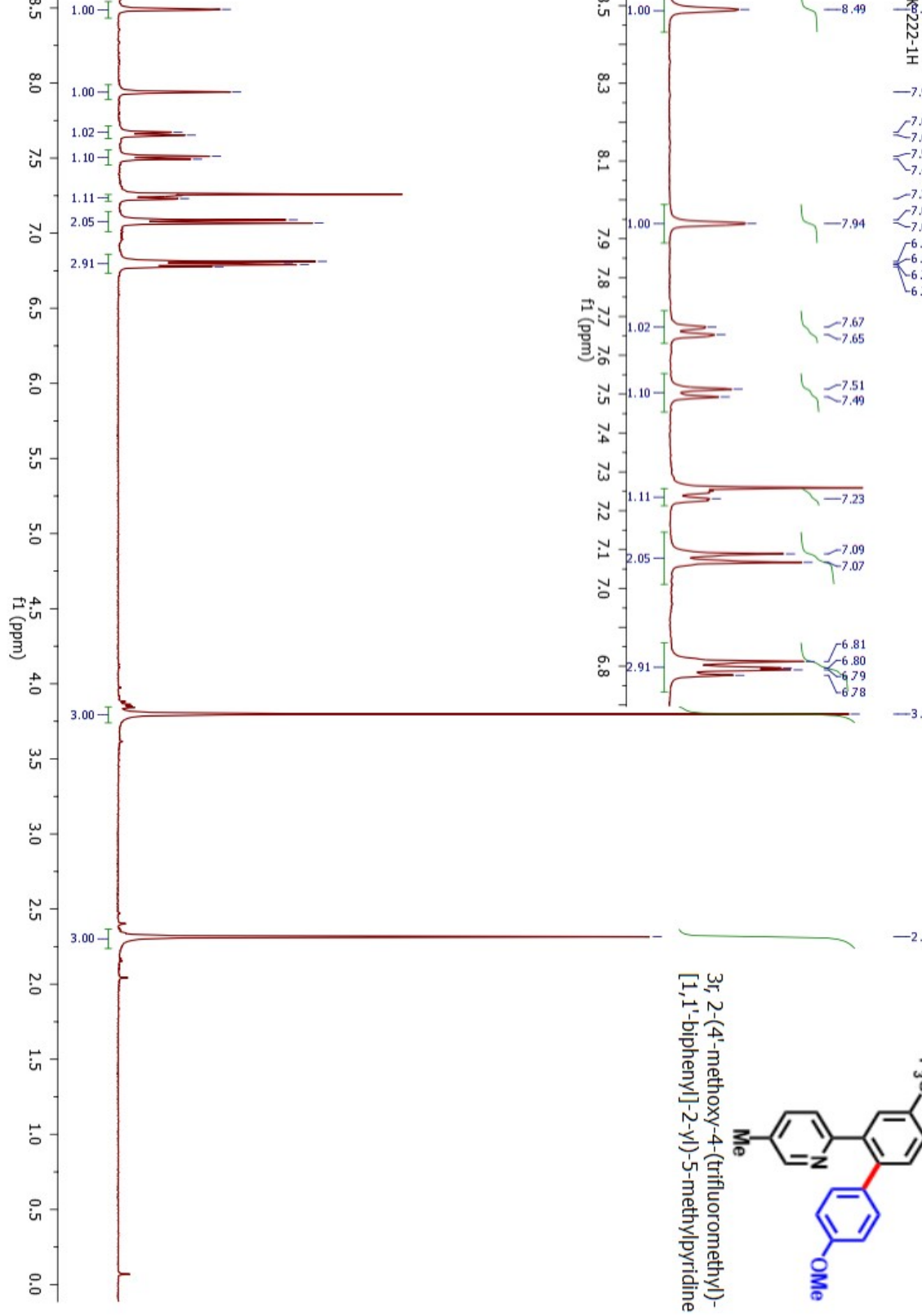
2-(4'-methoxy-5-methyl-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 6q)

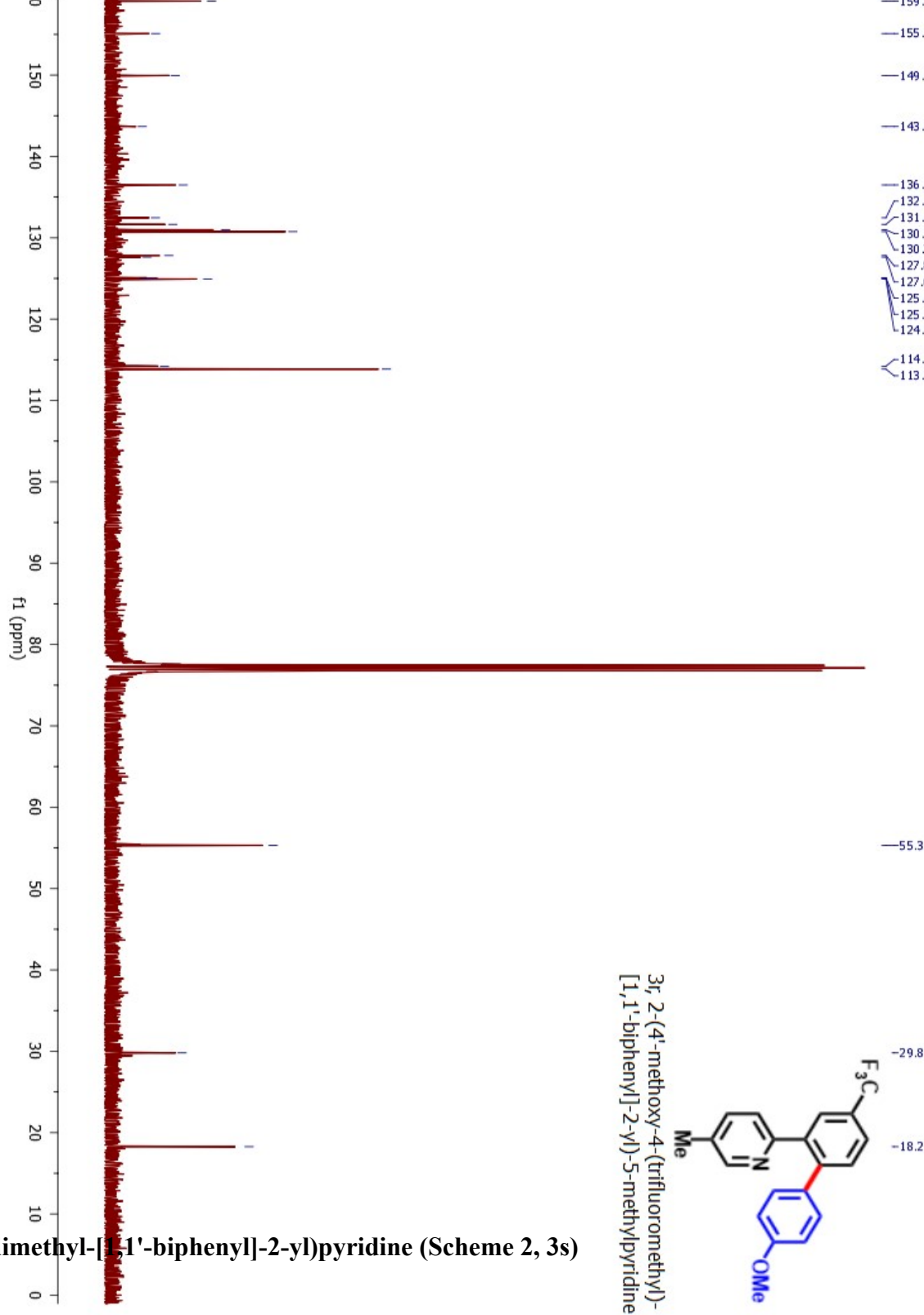




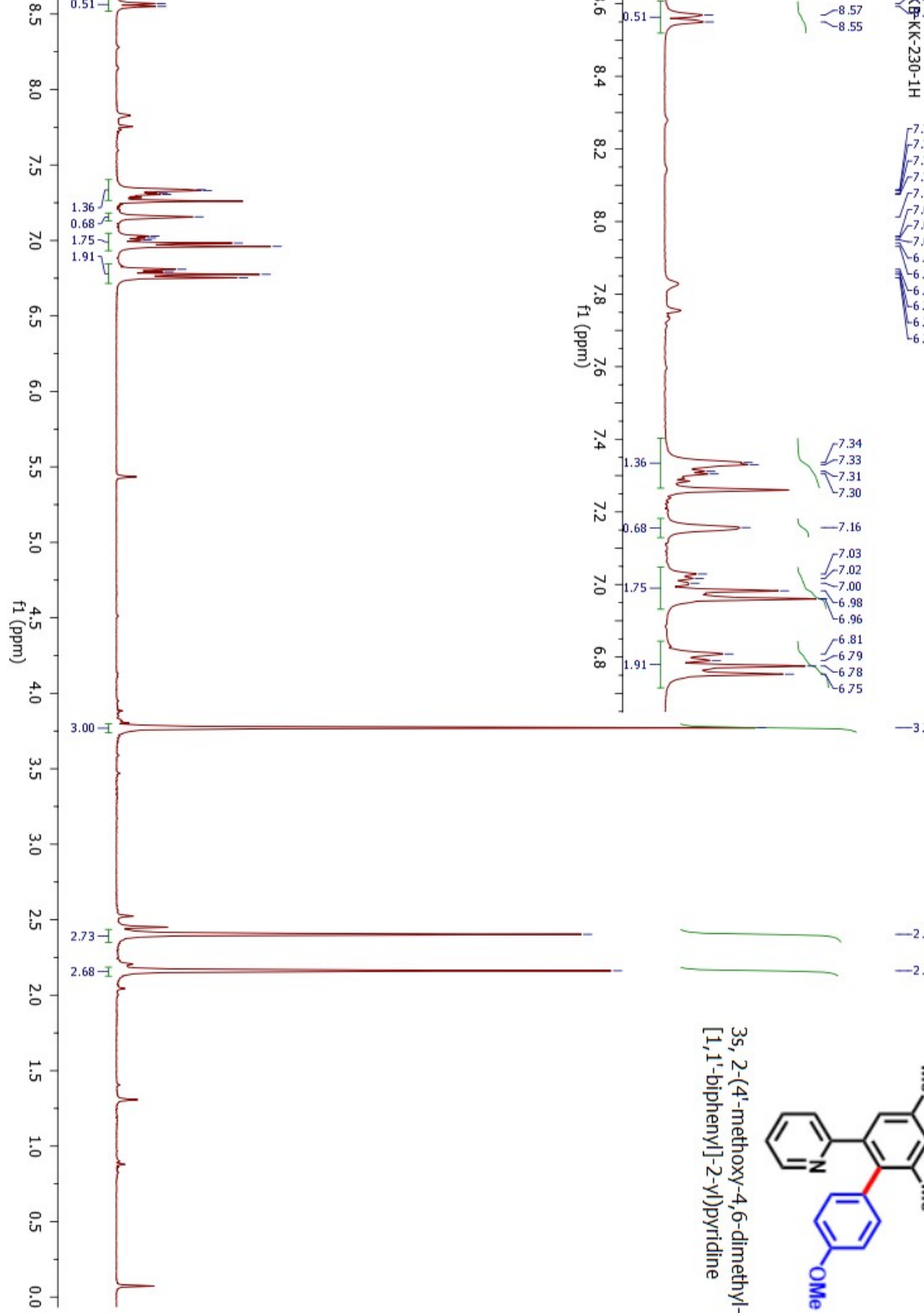


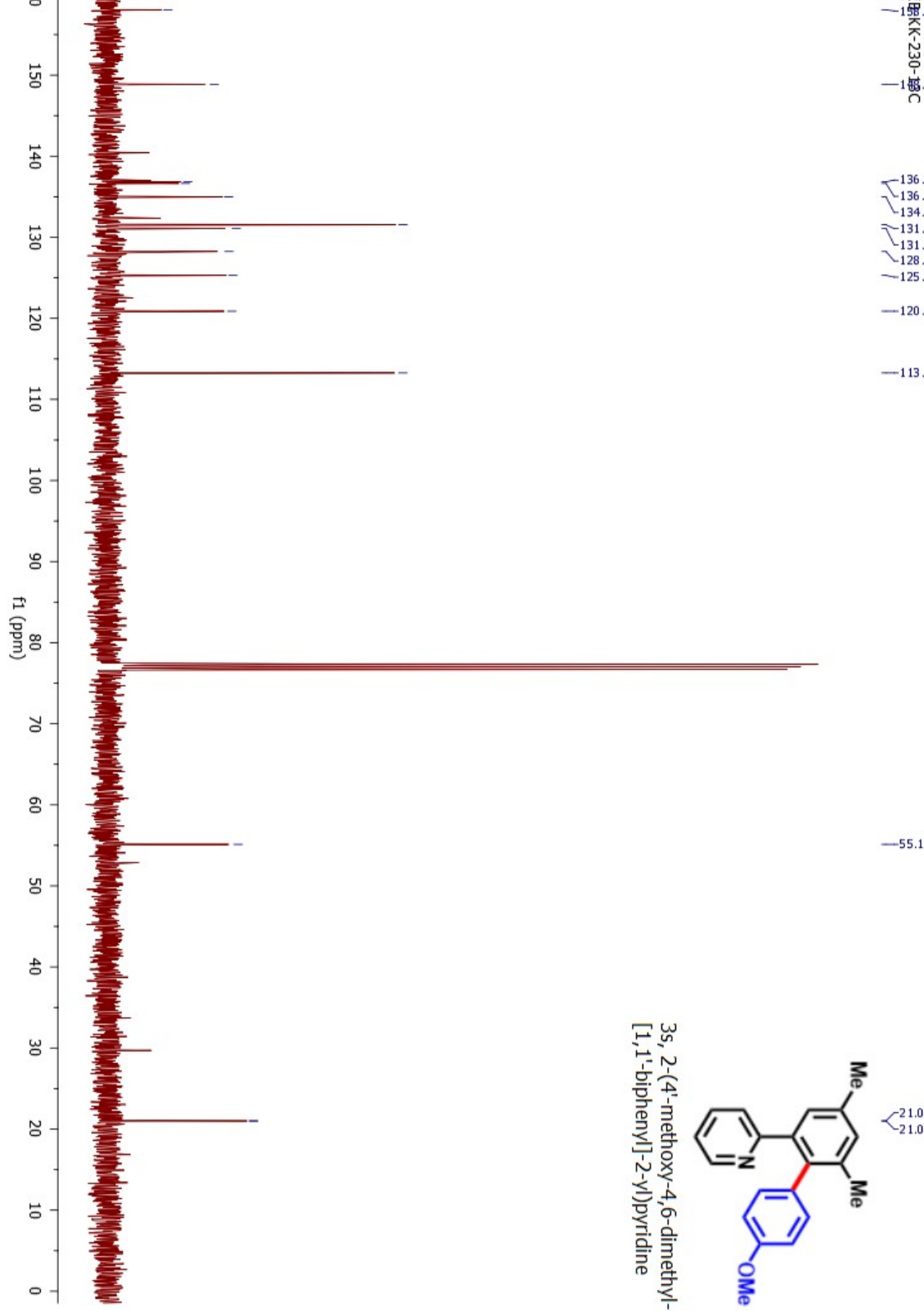
2-(4'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3r)

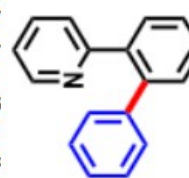




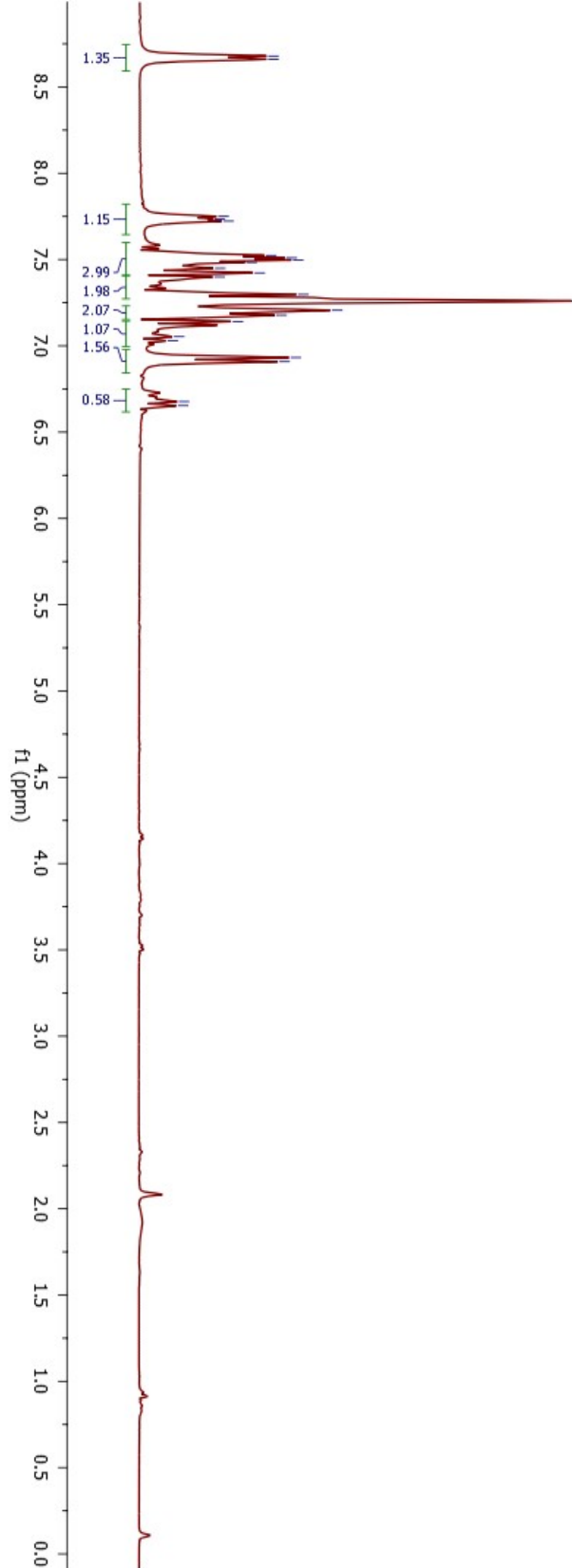
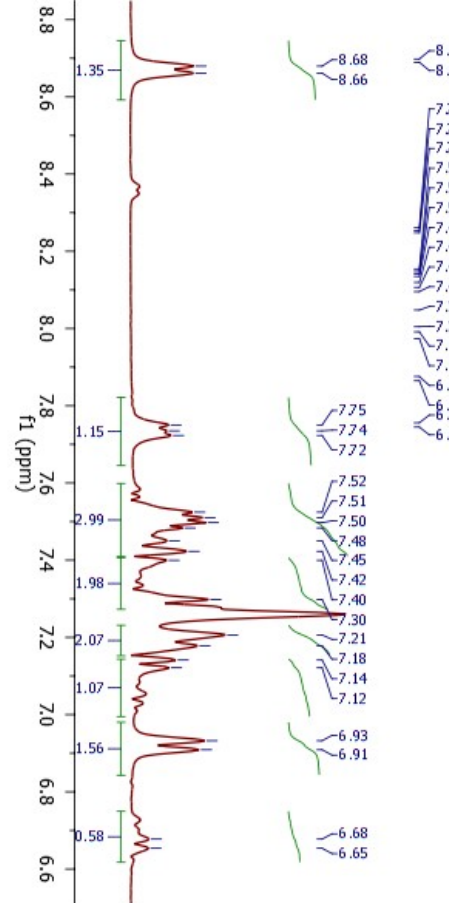
2-(4'-methoxy-4,6-dimethyl-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3s)





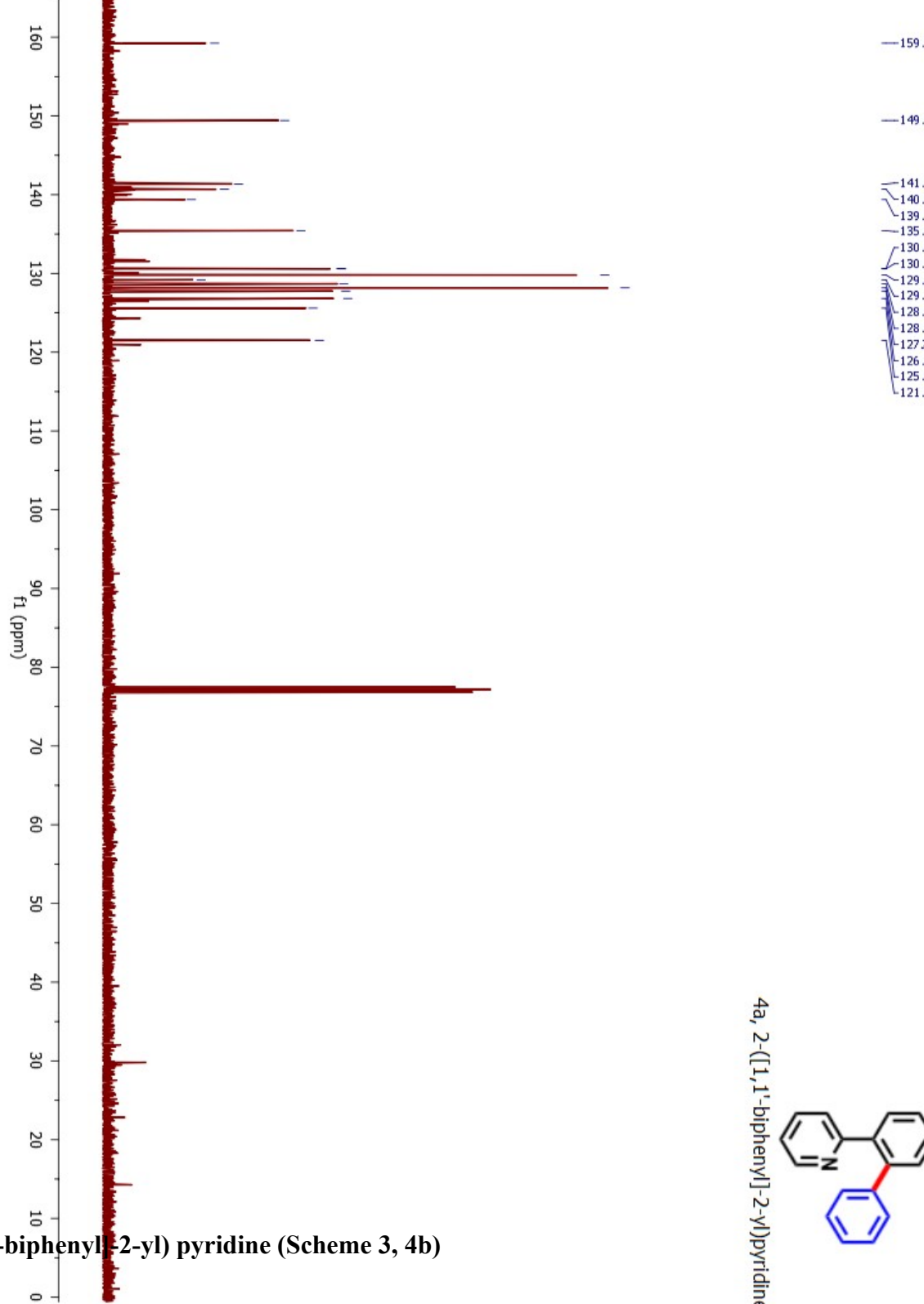
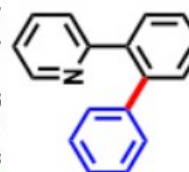


4a, 2-([1,1'-biphenyl]-2-yl)pyridine

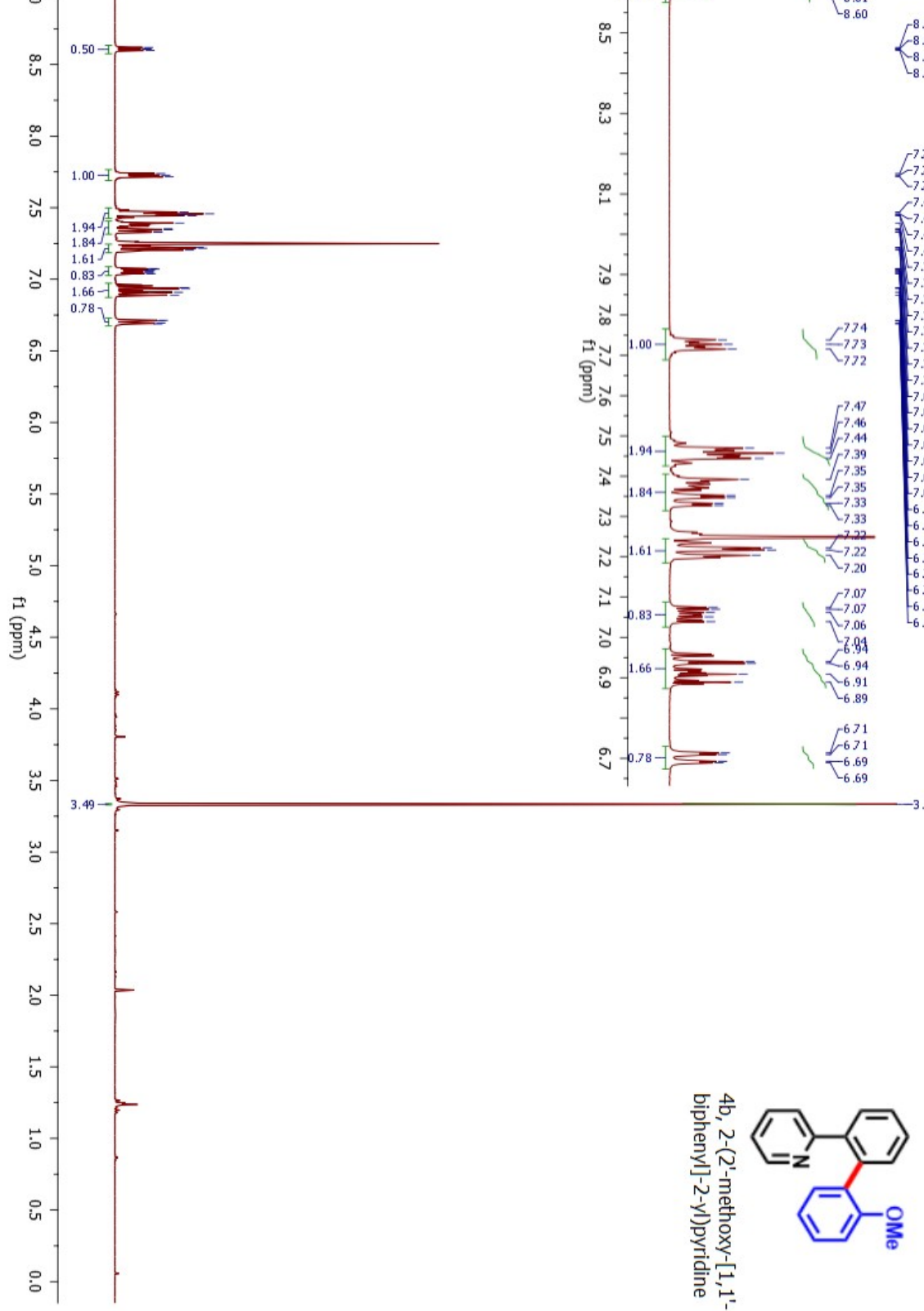


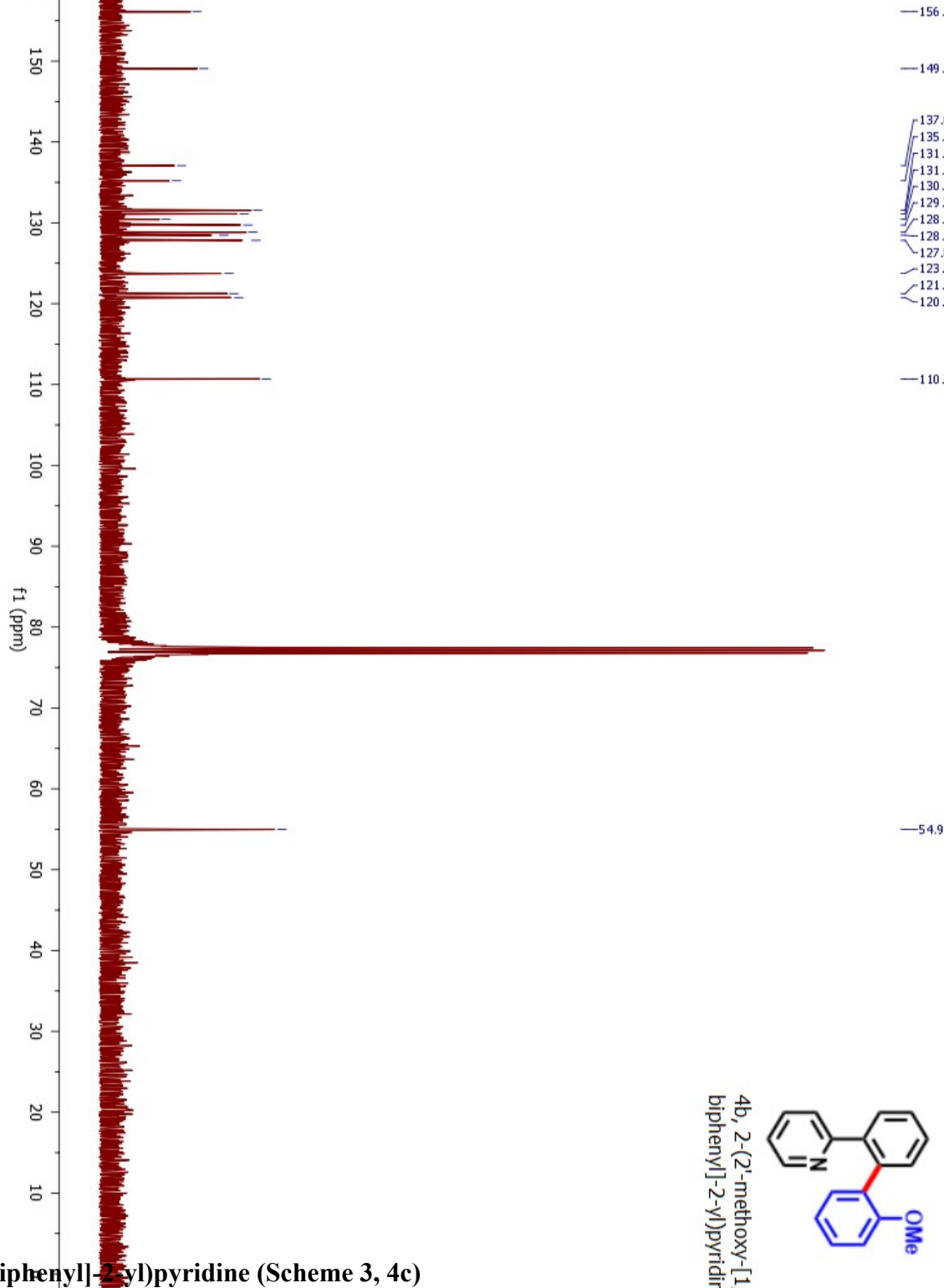
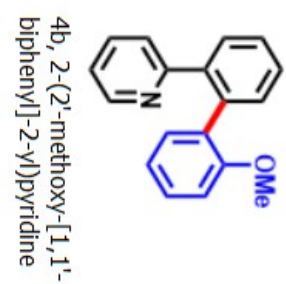
2-([1,1'-biphenyl]-2-yl)pyridine

4a, 2-([1,1'-biphenyl]-2-yl)pyridine

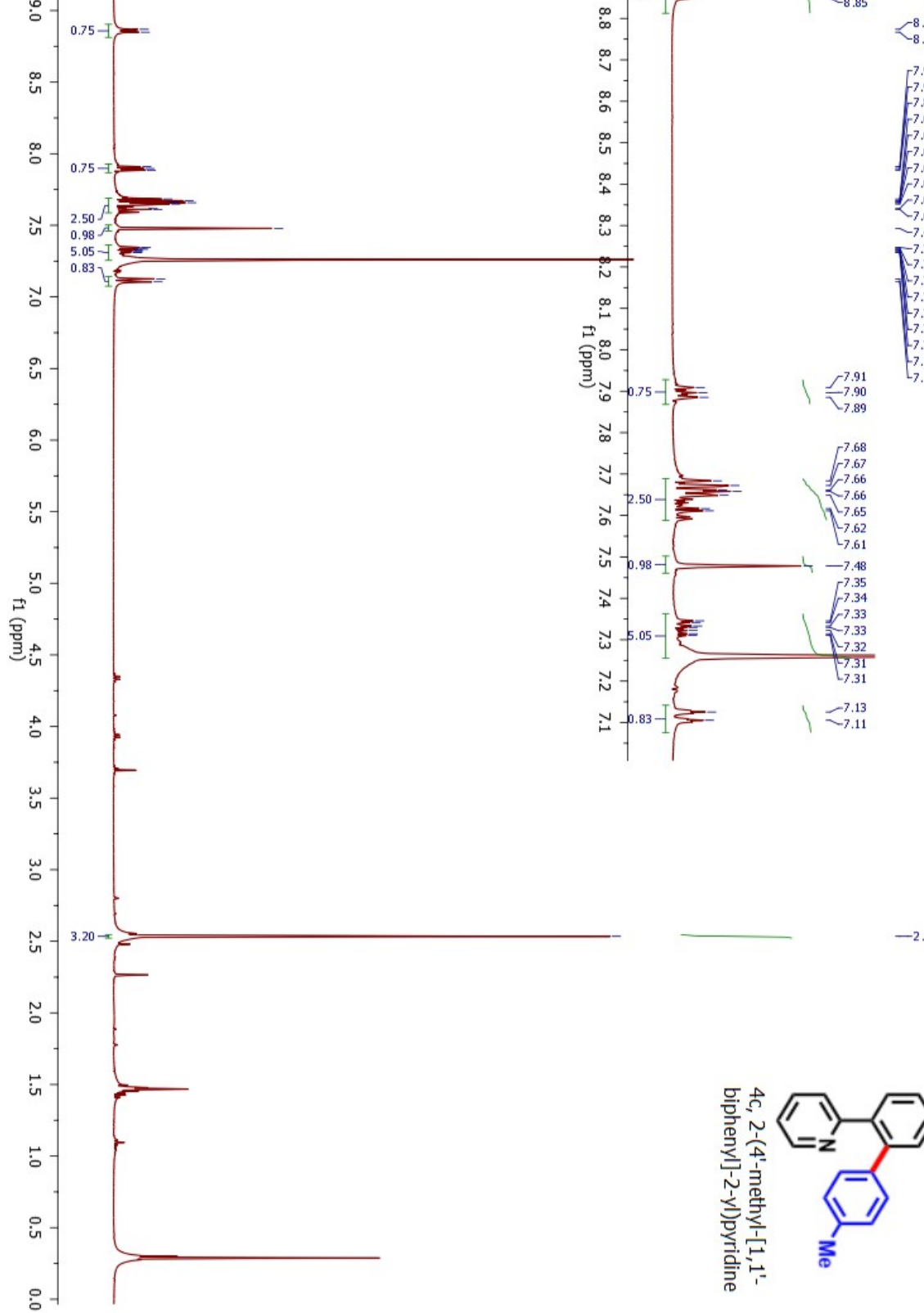


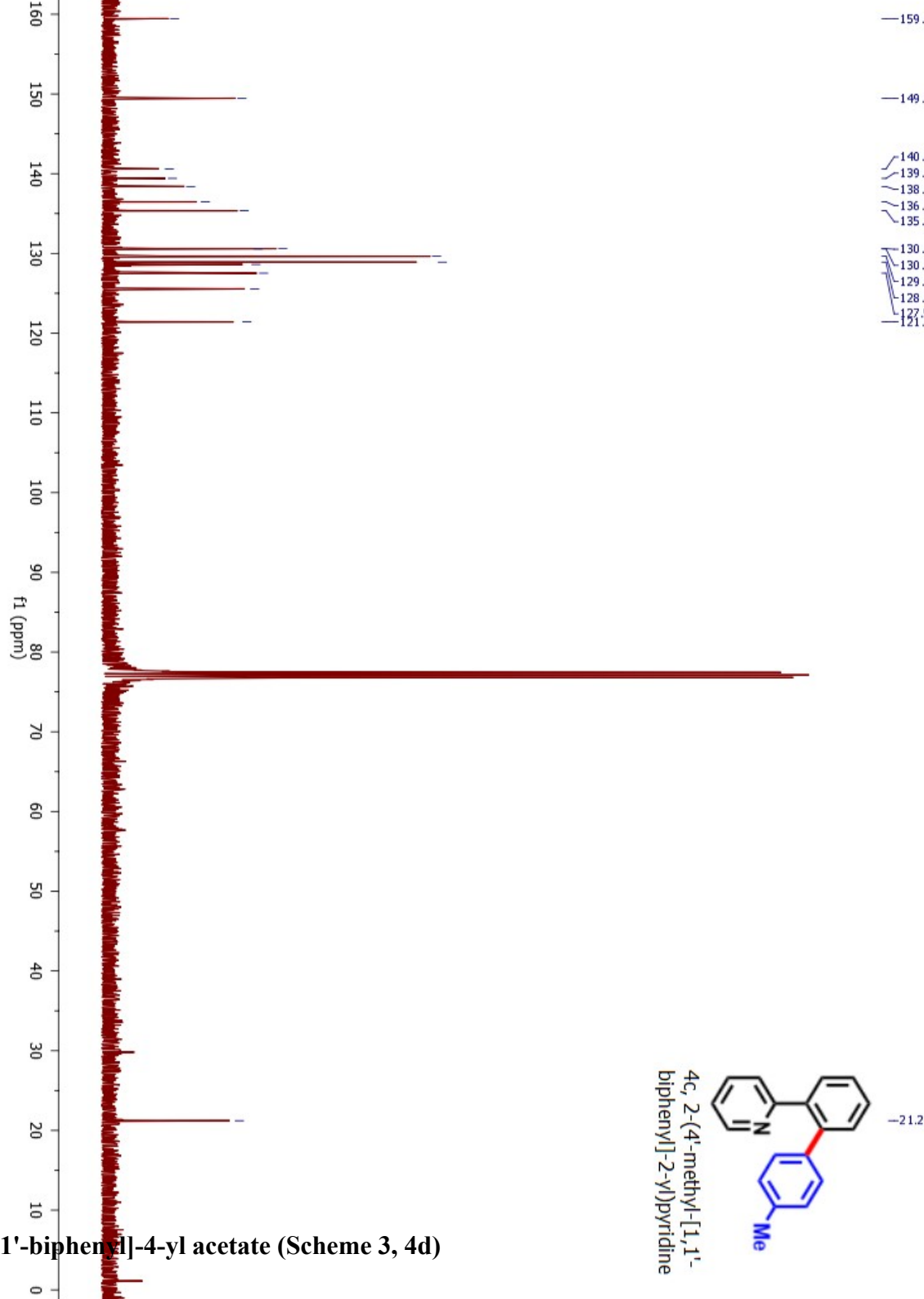
2-(2'-methoxy-[1,1'-biphenyl]-2-yl) pyridine (Scheme 3, 4b)



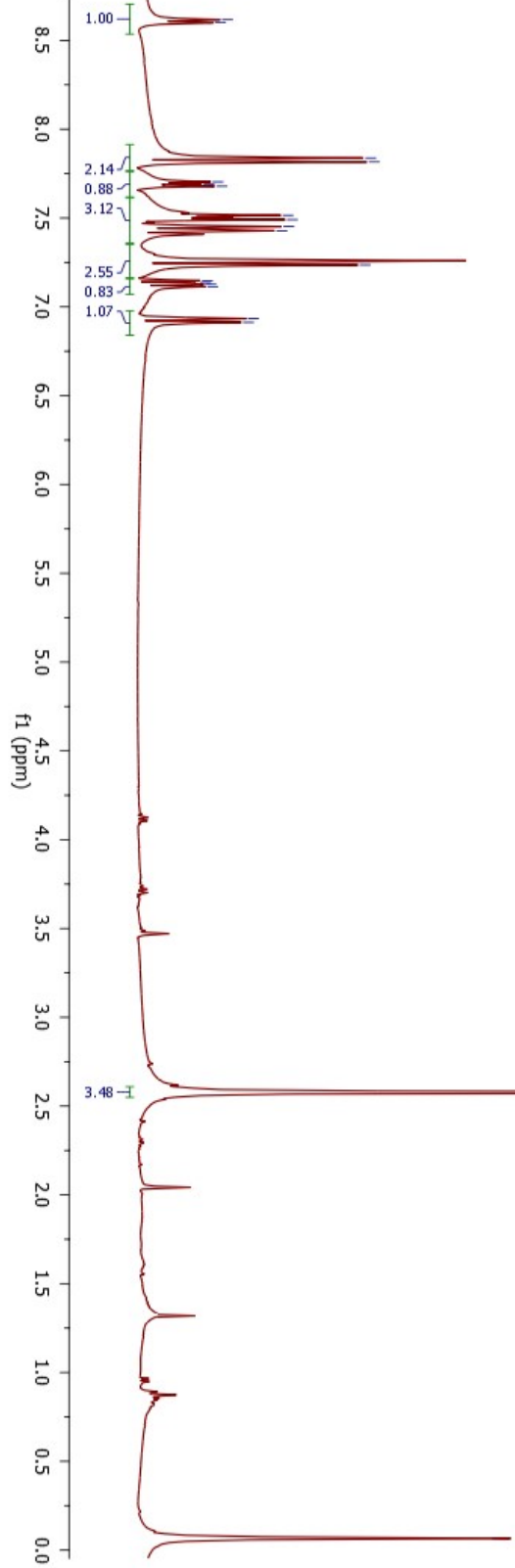
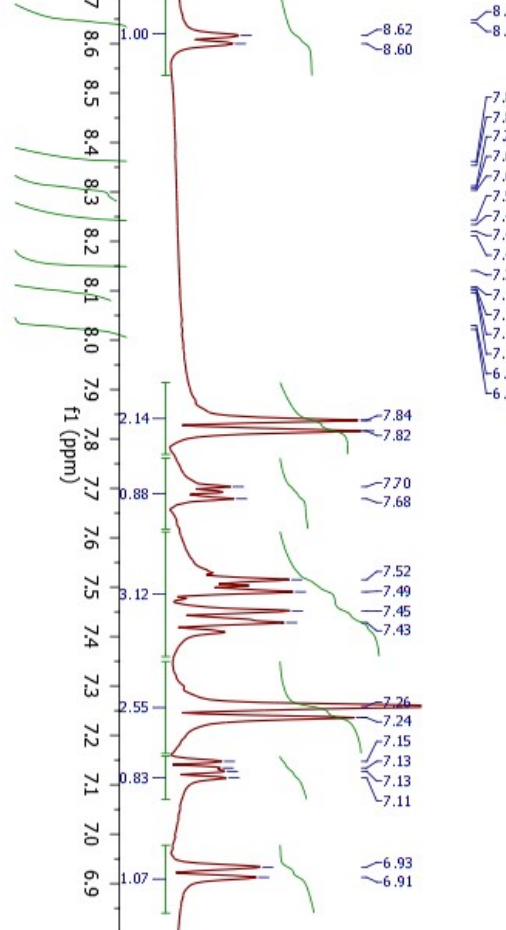
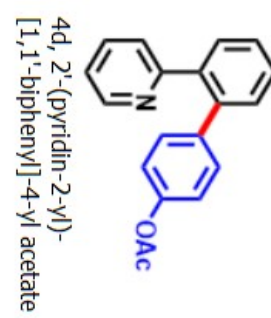


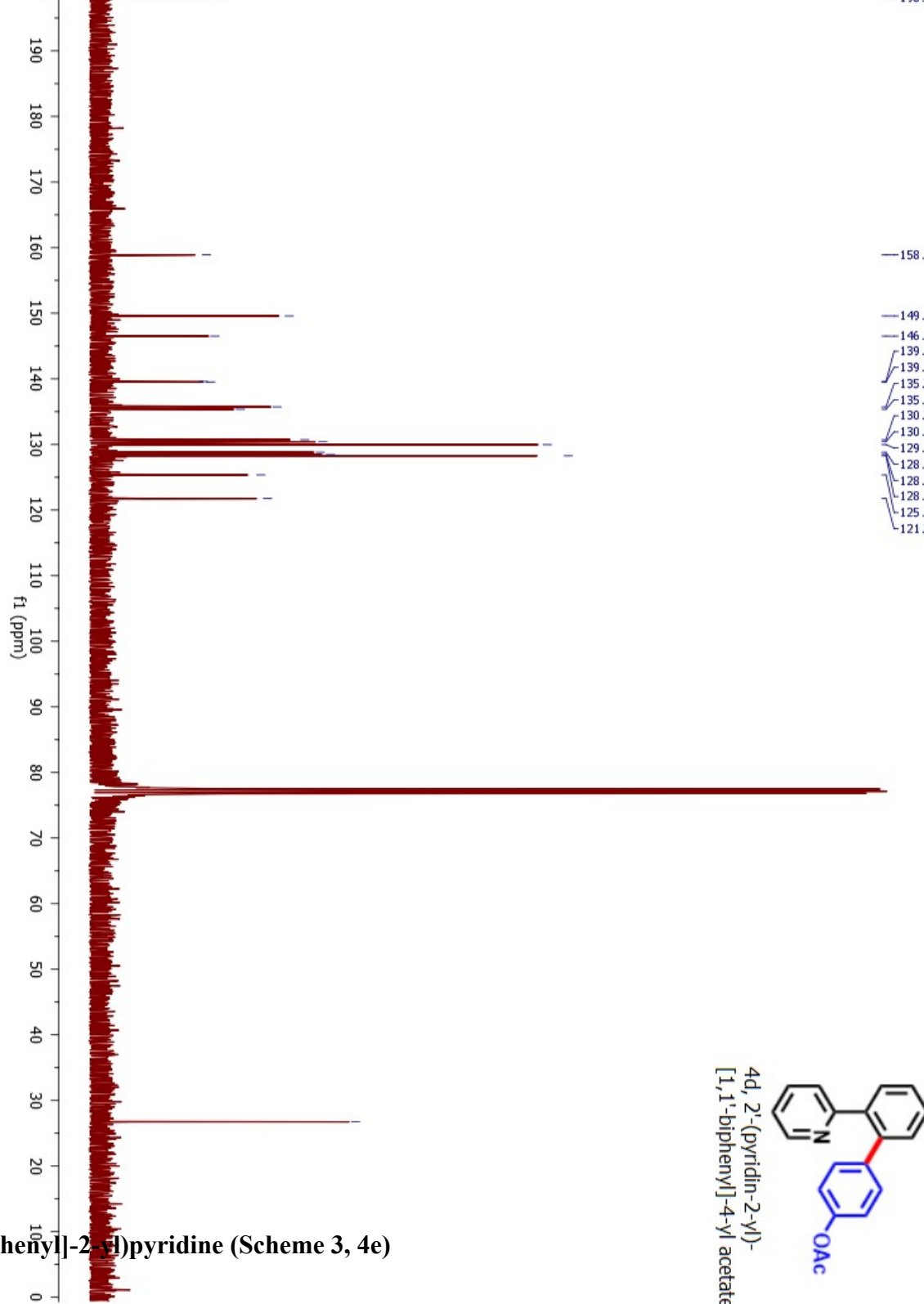
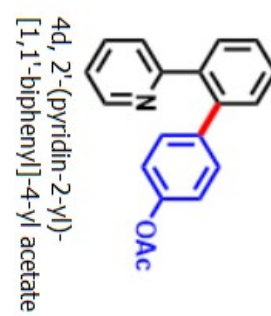
2-(4'-methyl-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4c)



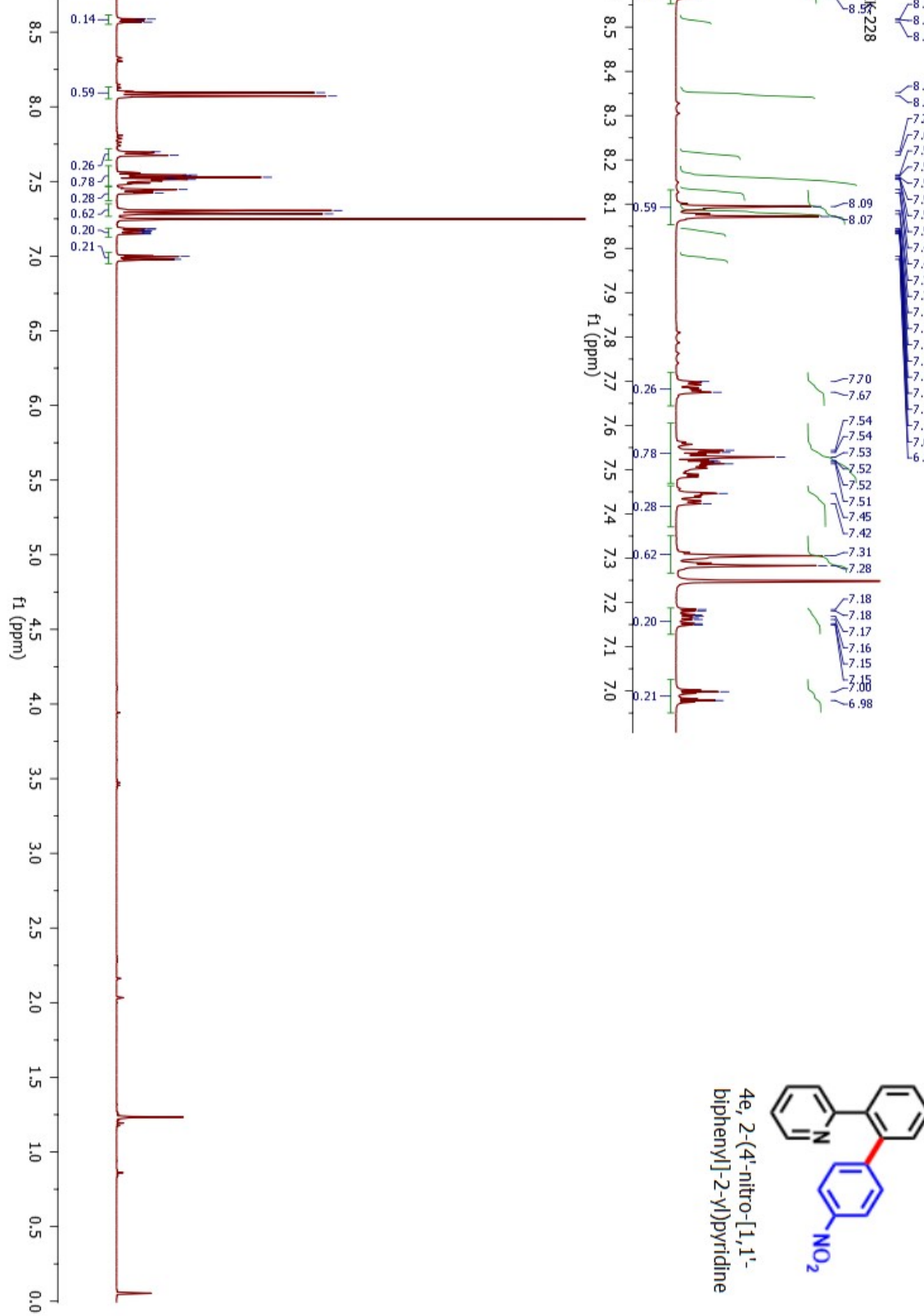


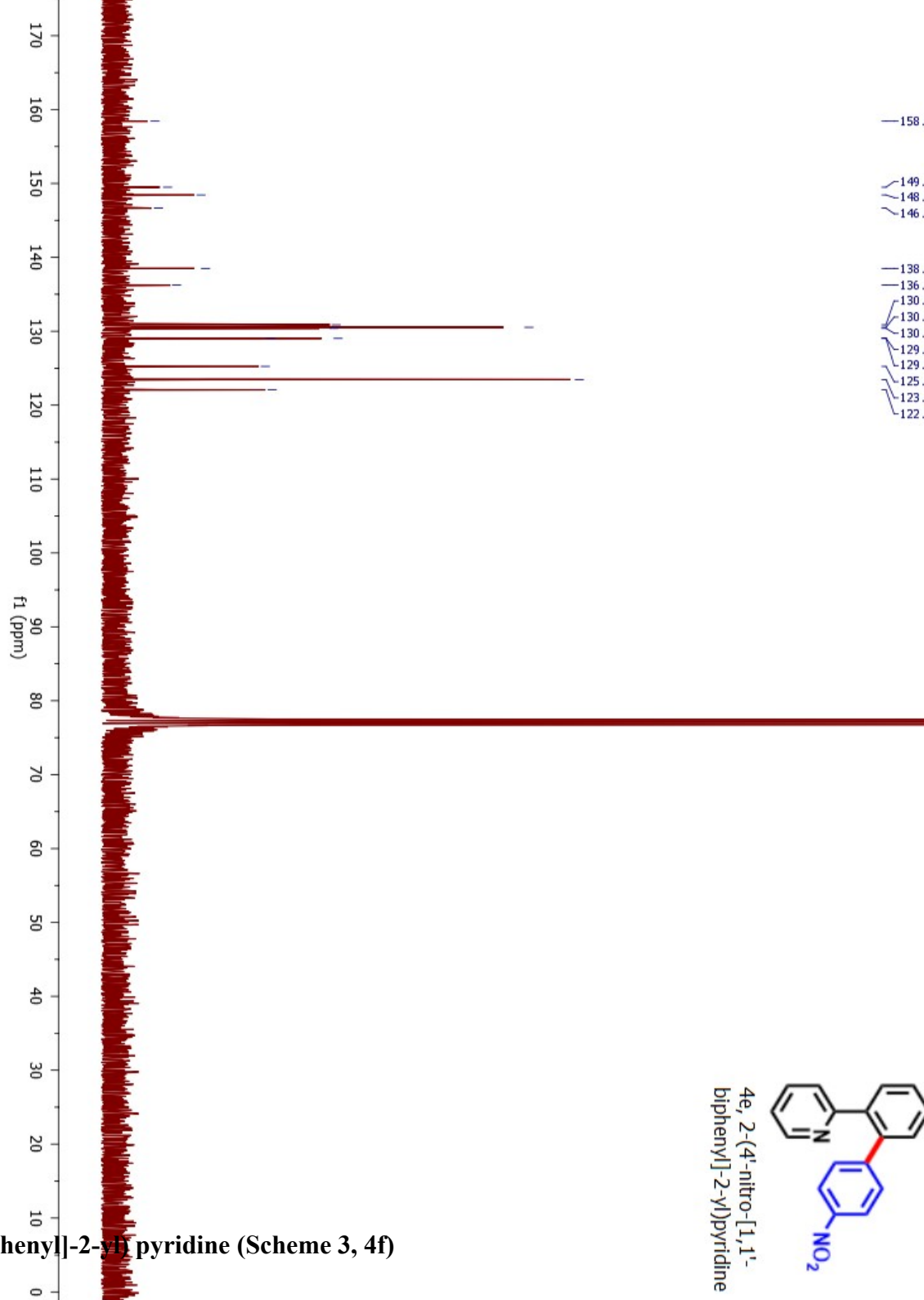
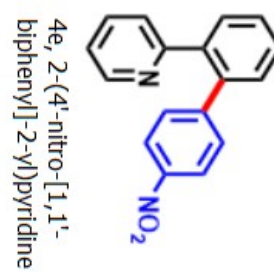
2'-(pyridin-2-yl)-[1,1'-biphenyl]-4-yl acetate (Scheme 3, 4d)



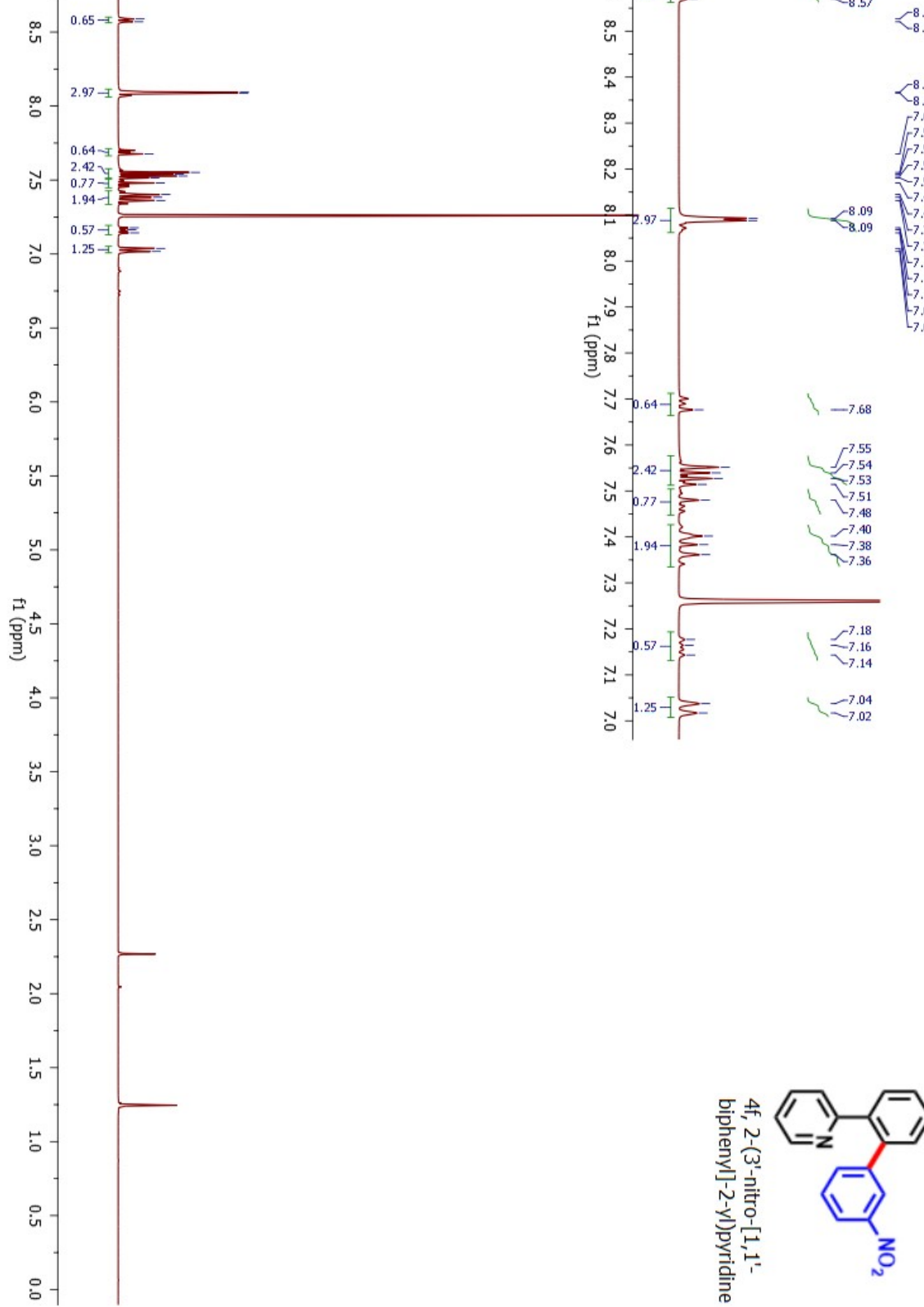


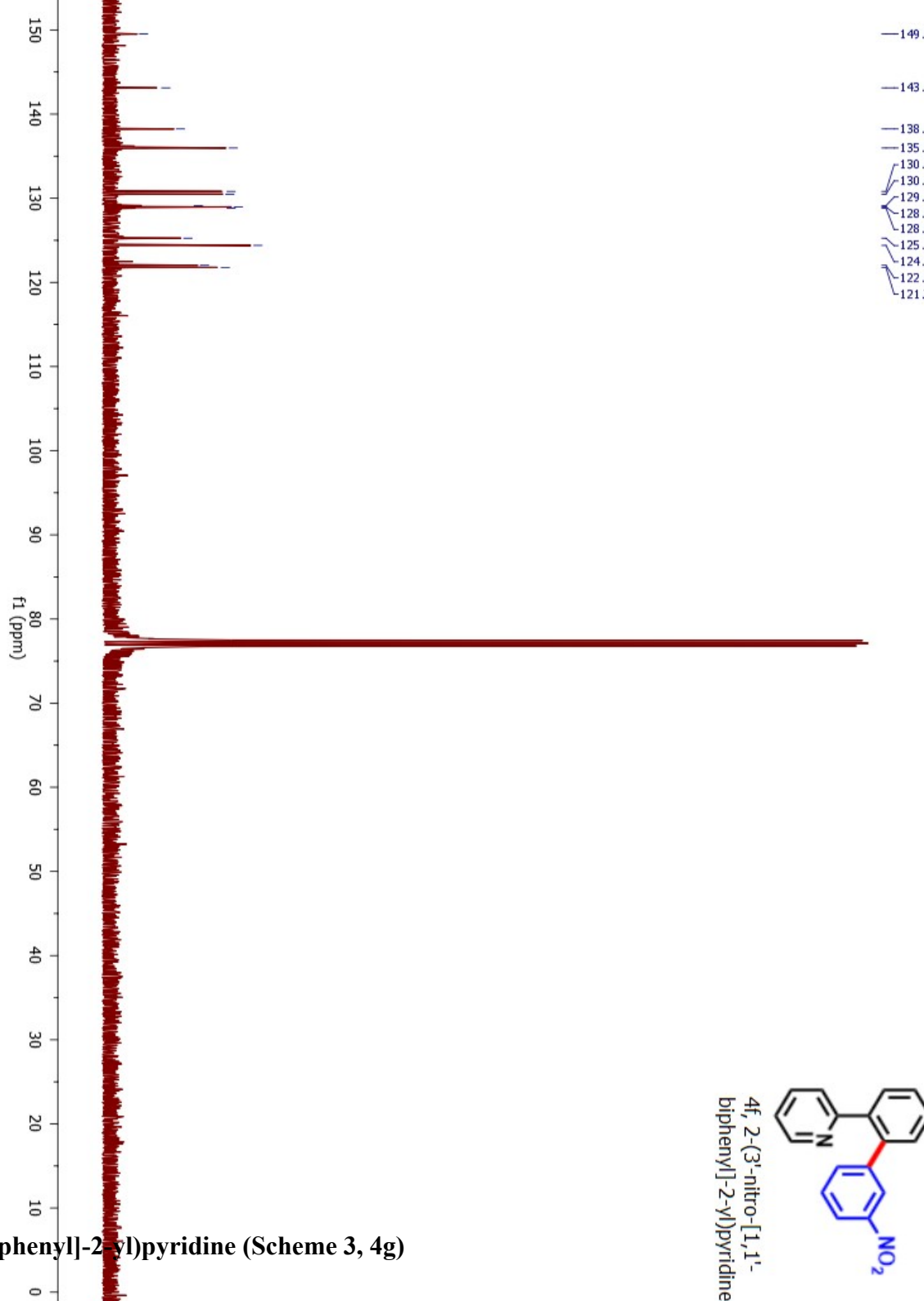
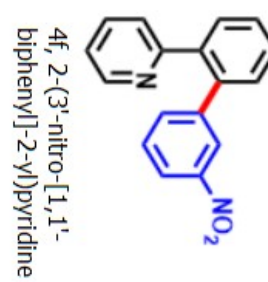
2-(4'-nitro-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4e)



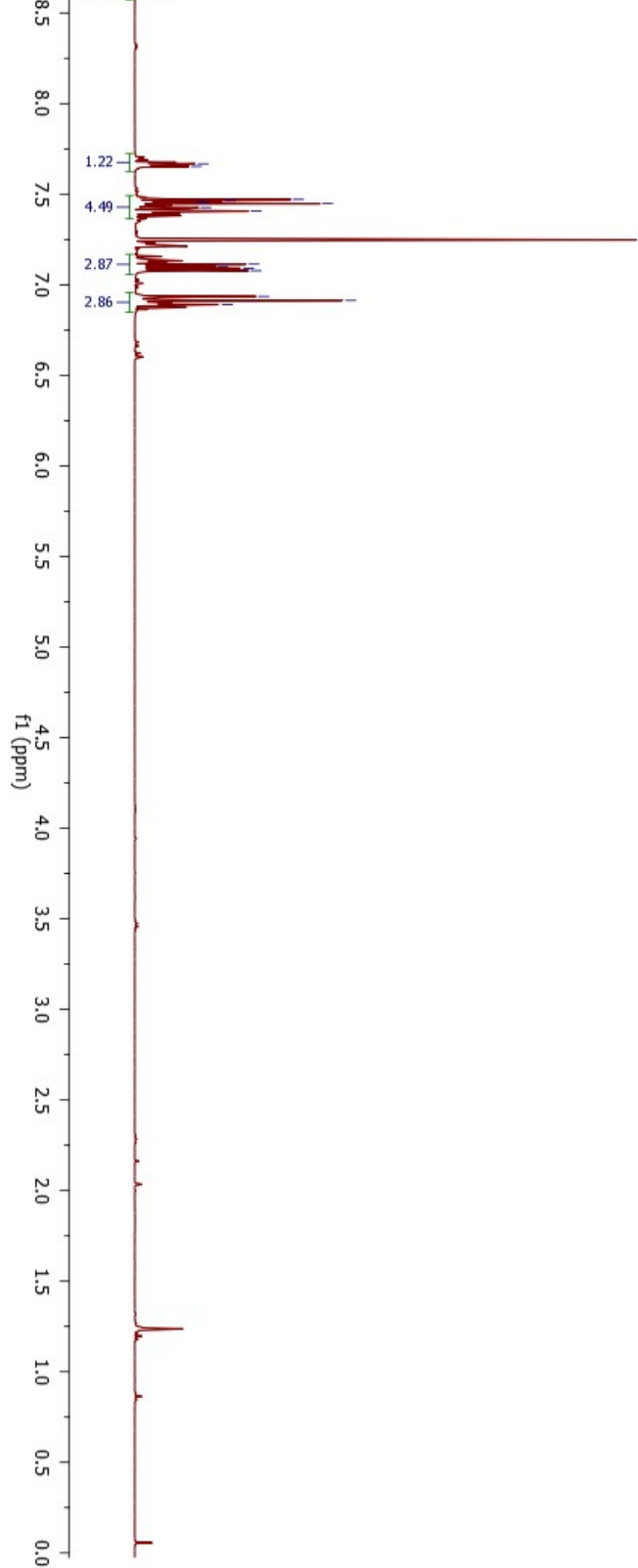
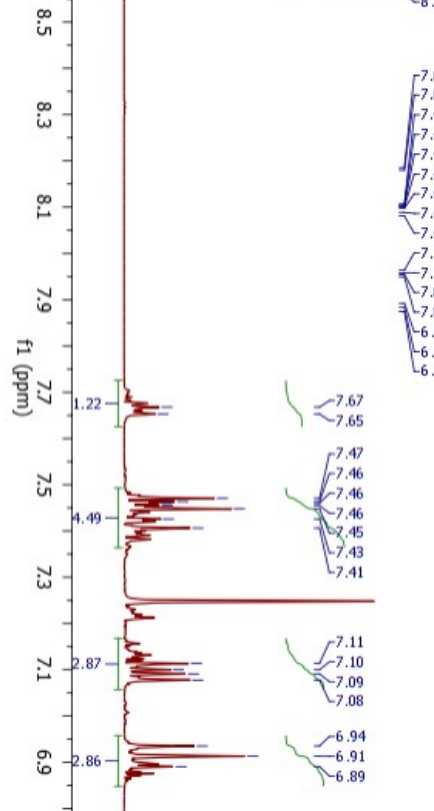
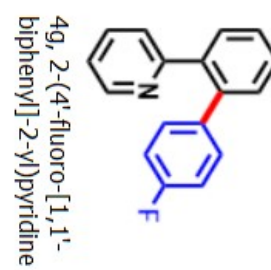


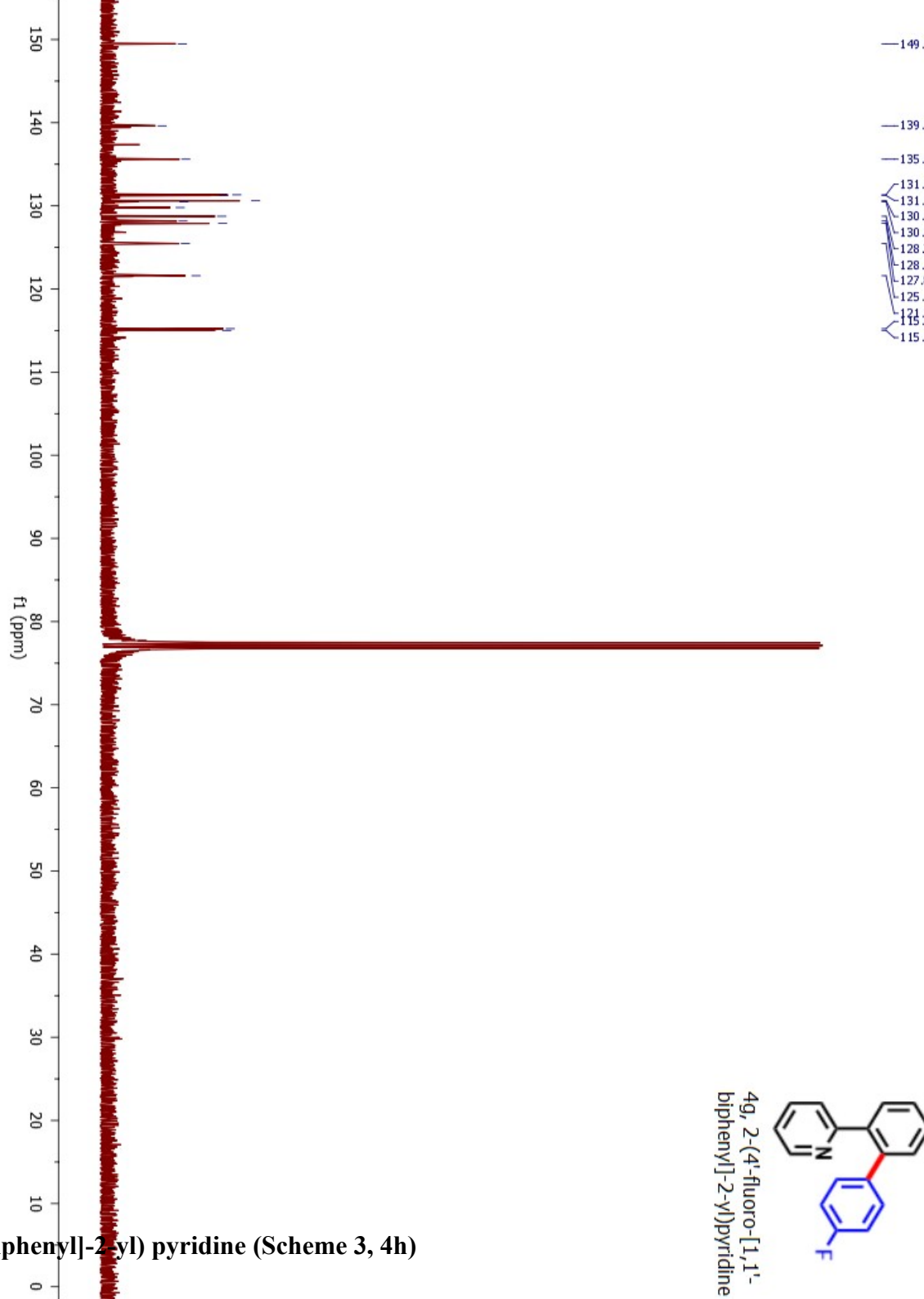
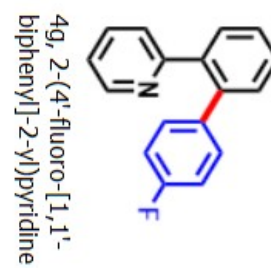
2-(3'-nitro-[1,1'-biphenyl]-2-yl) pyridine (Scheme 3, 4f)



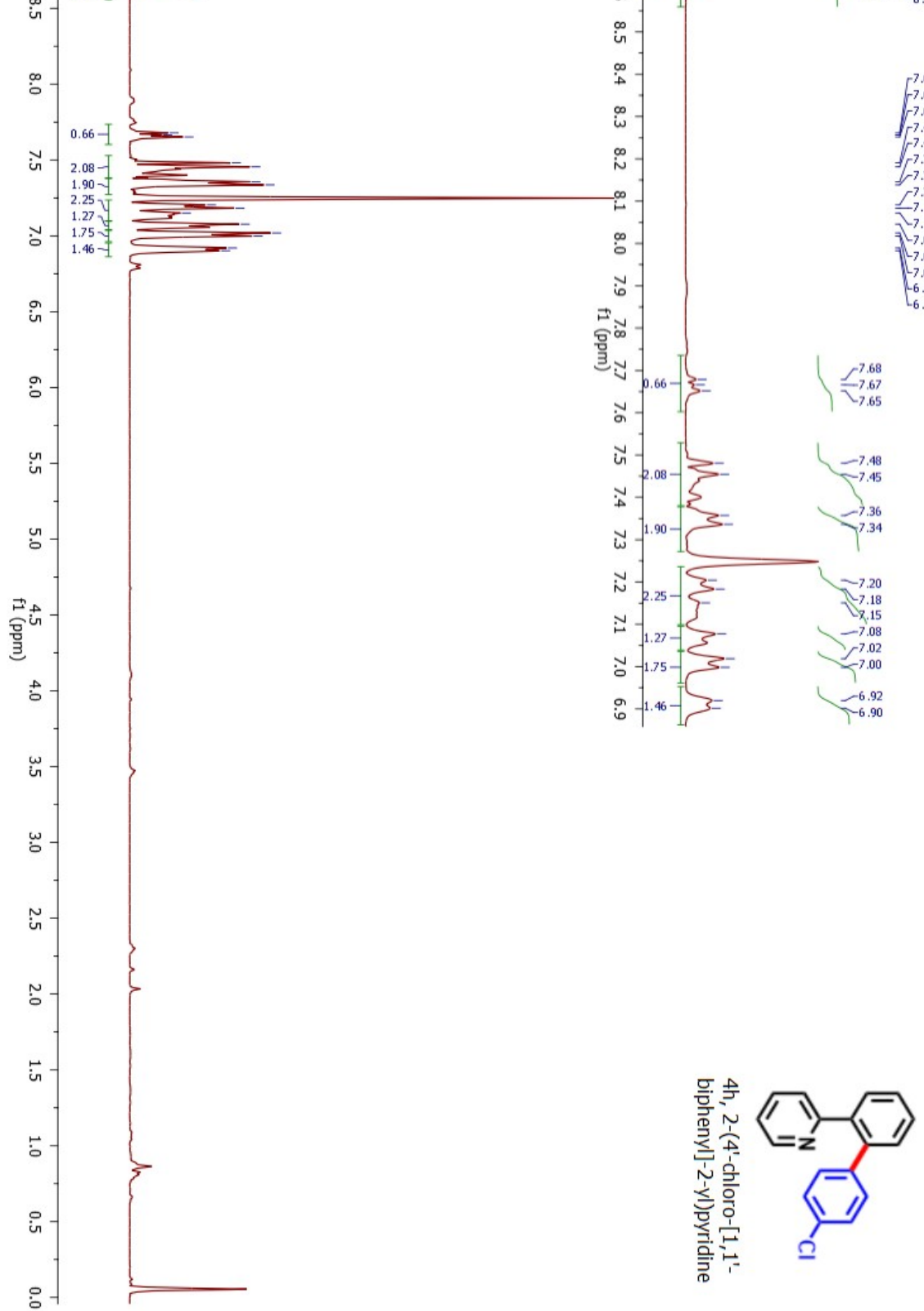


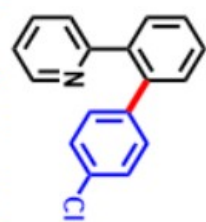
2-(4'-fluoro-[1,1'-biphenyl]-2-yl)pyridine (Scheme 3, 4g)



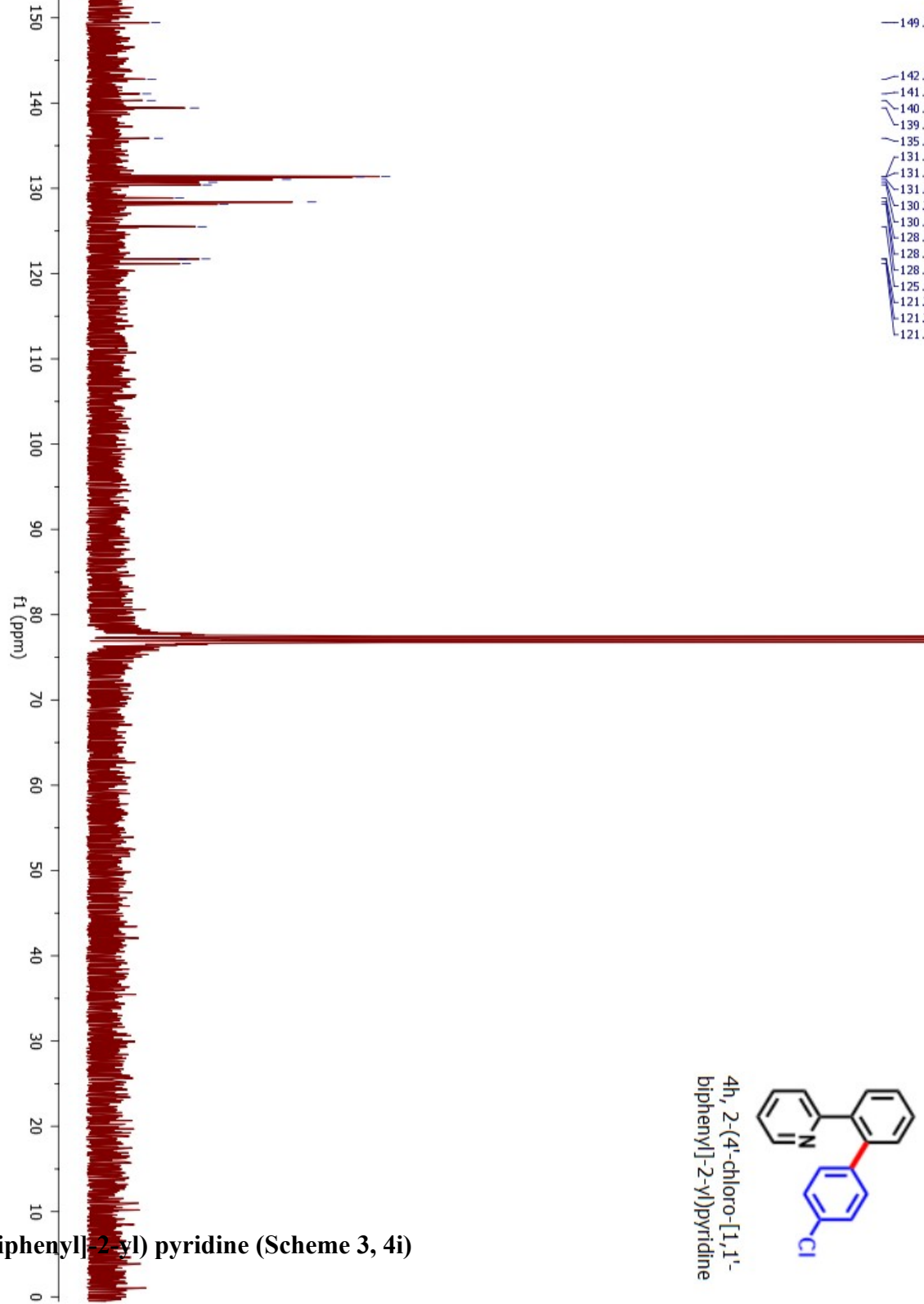


2-(4'-chloro-[1,1'-biphenyl]-2-yl) pyridine (Scheme 3, 4h)

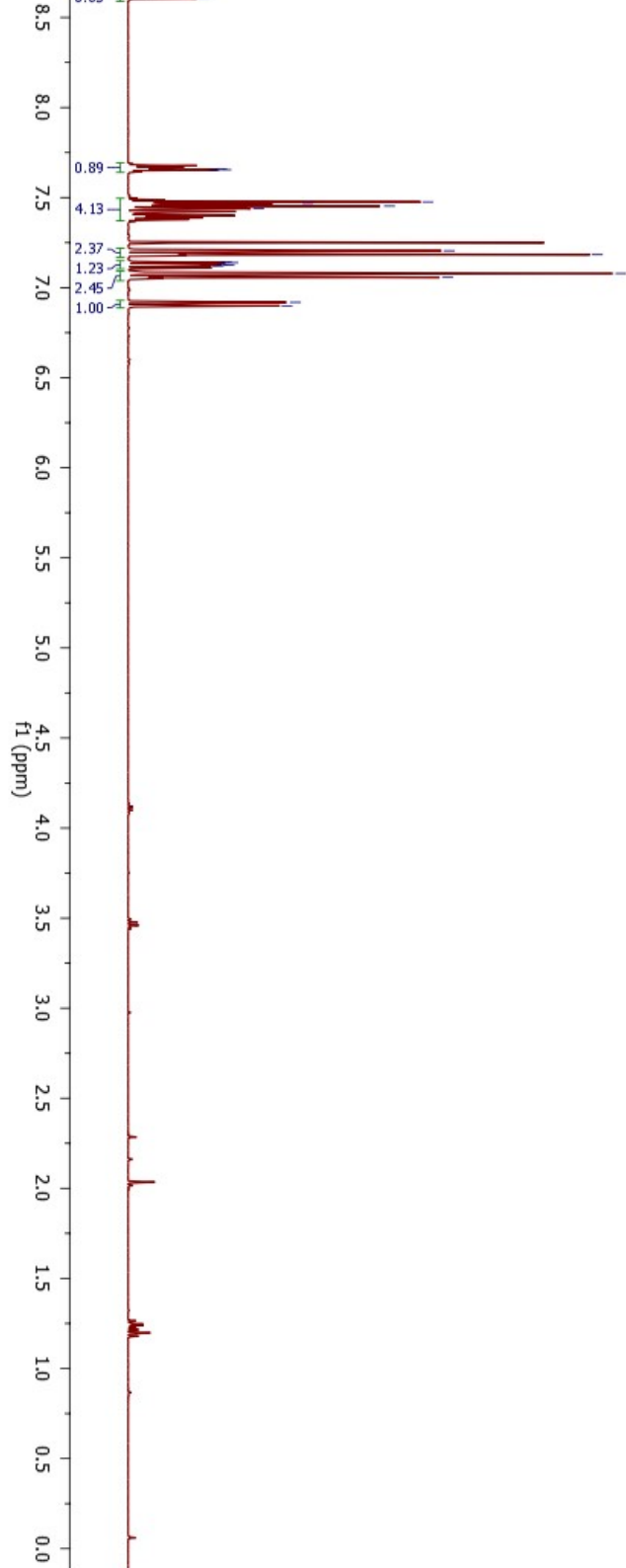
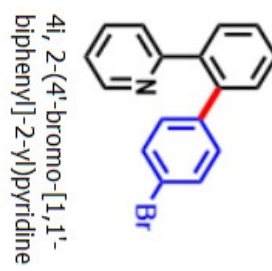
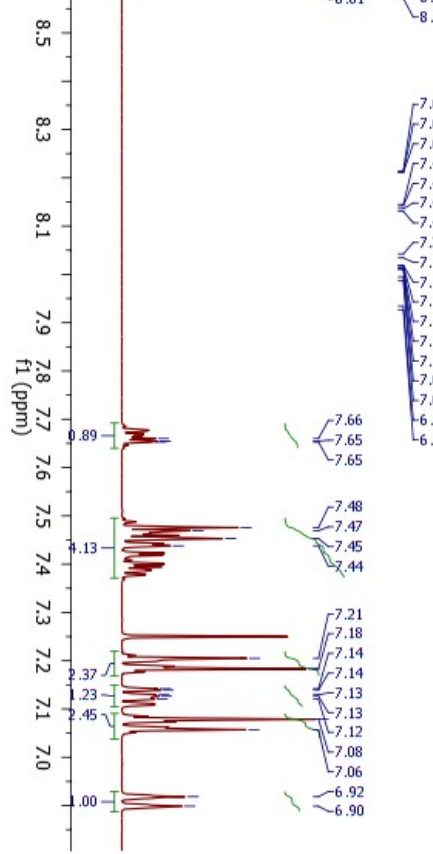


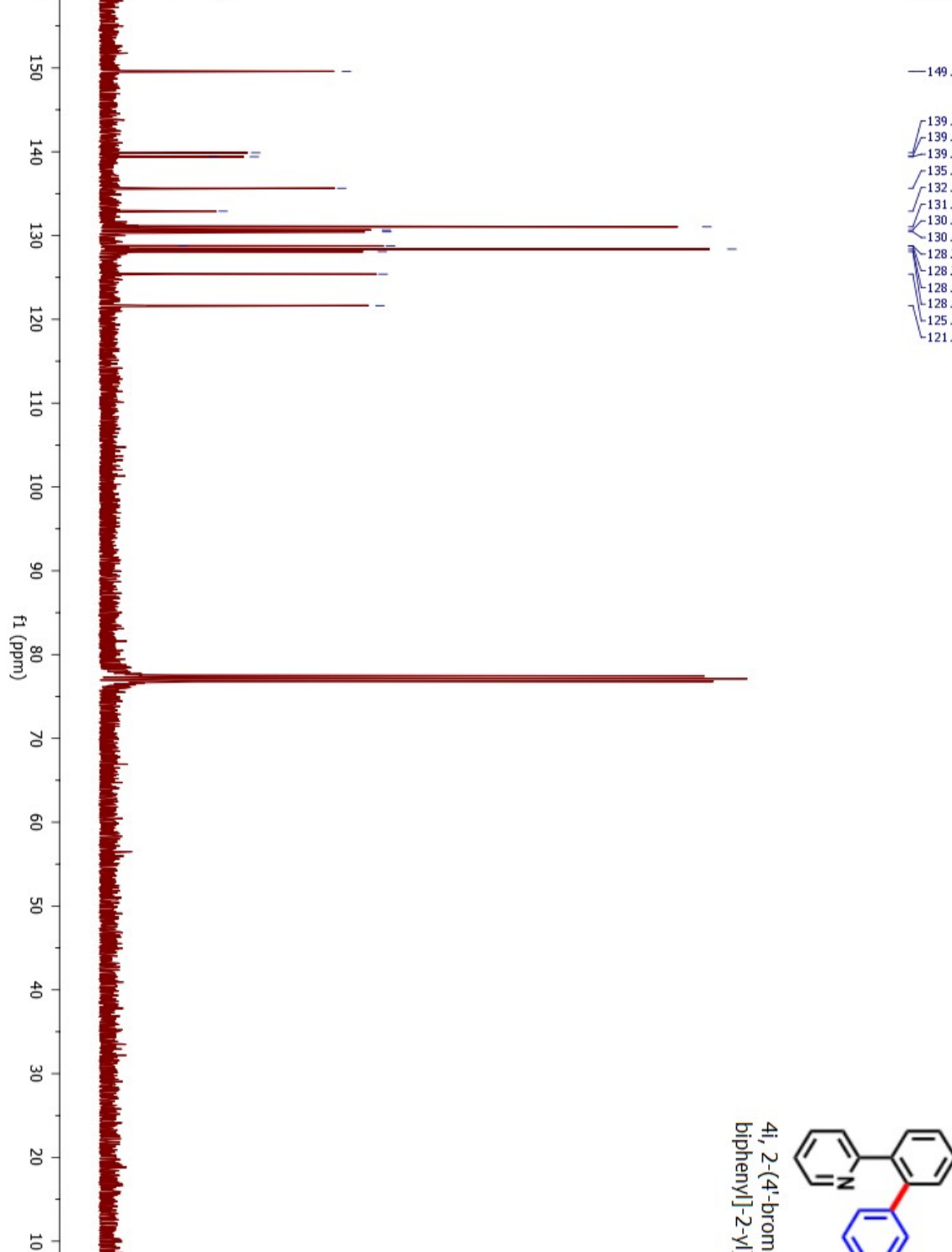


4h, 2-(4'-chloro-[1,1'-biphenyl]-2-yl)pyridine

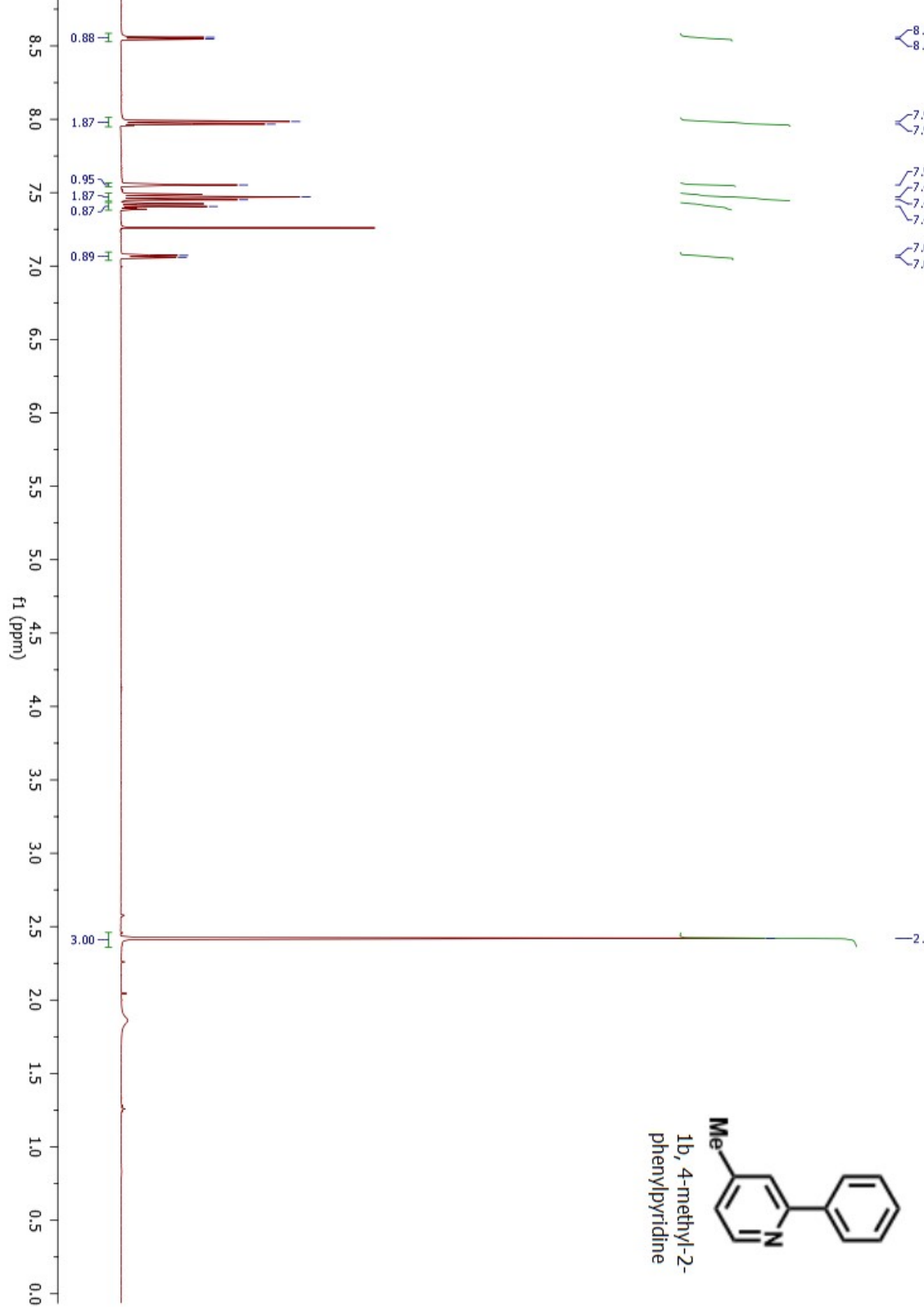
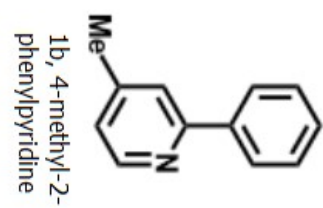


2-(4'-bromo-[1,1'-biphenyl]-2-yl) pyridine (Scheme 3, 4i)

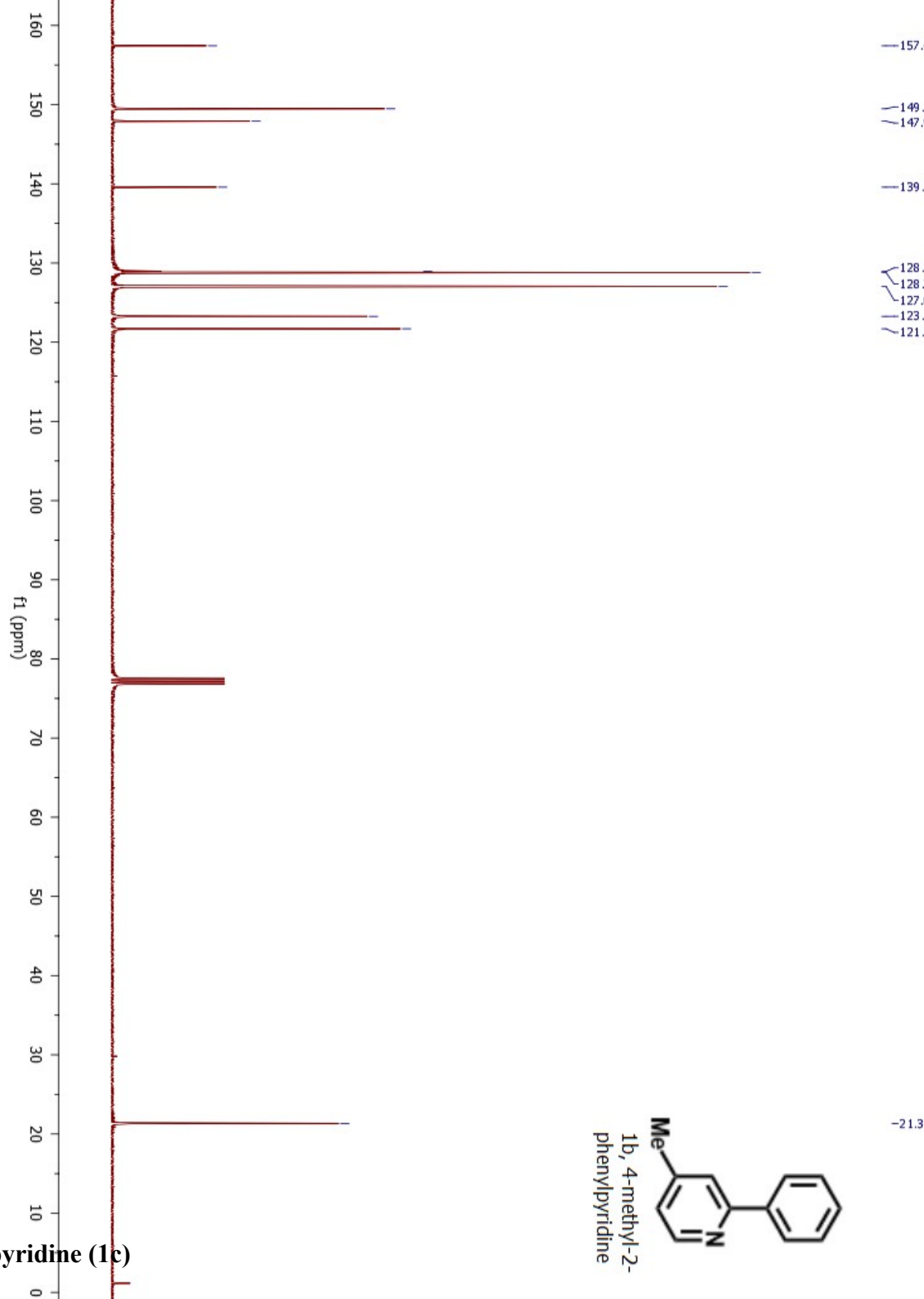


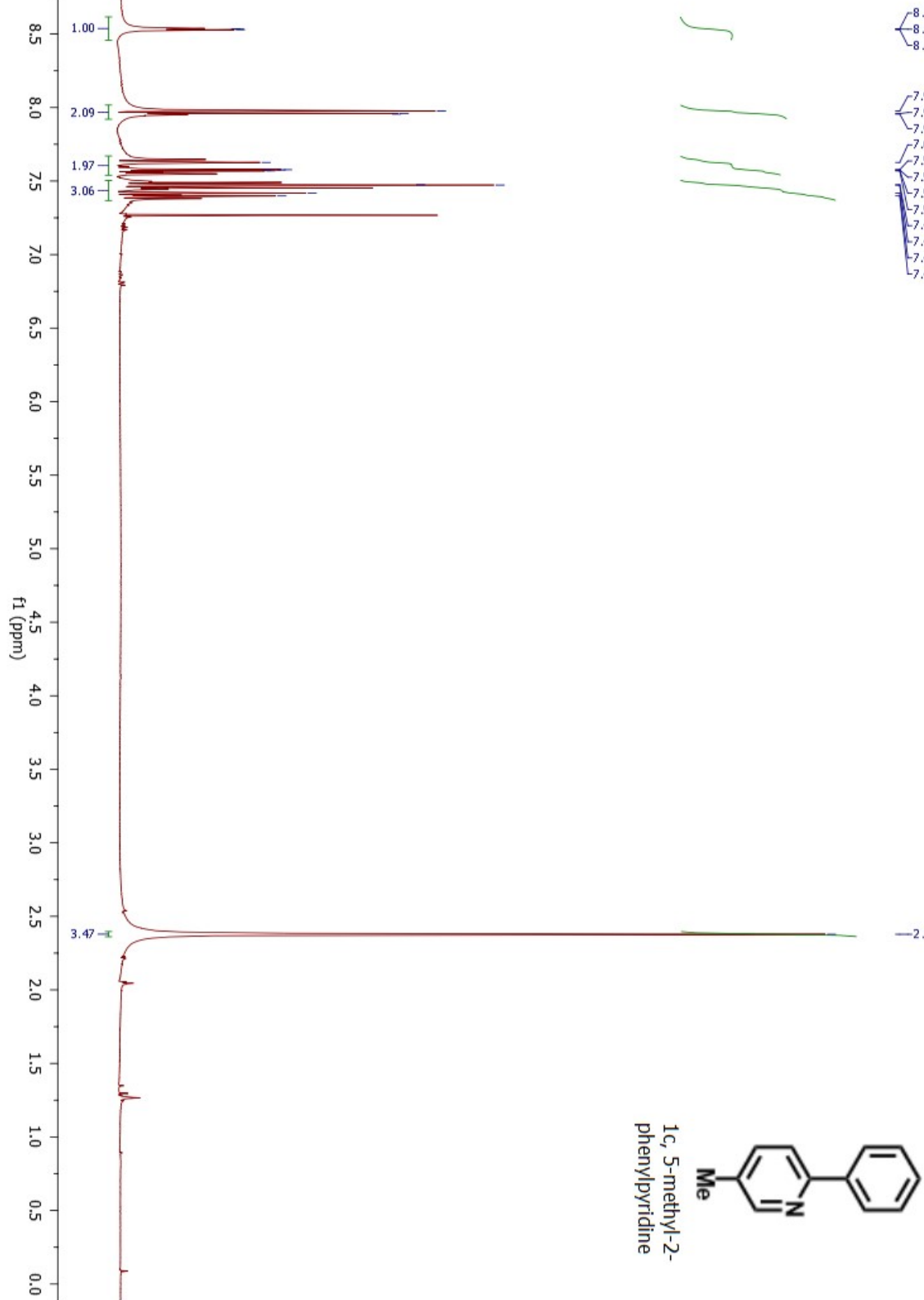


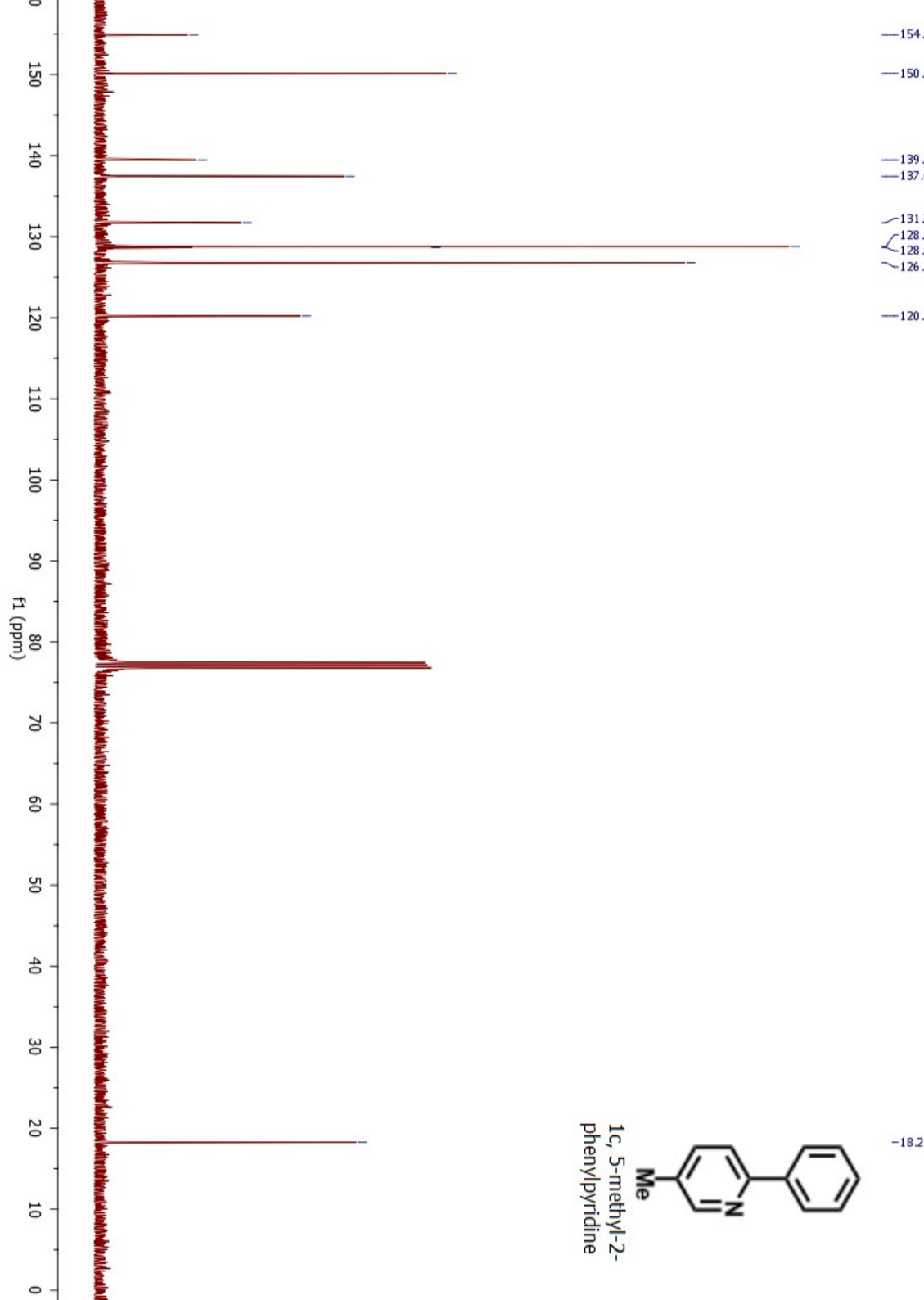
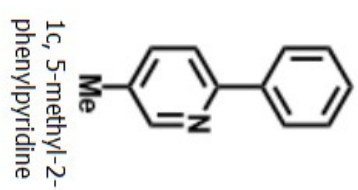
10. ¹H and ¹³C NMR data of 2-phenylpyridine derivatives
4-methyl-2-phenylpyridine (1b)



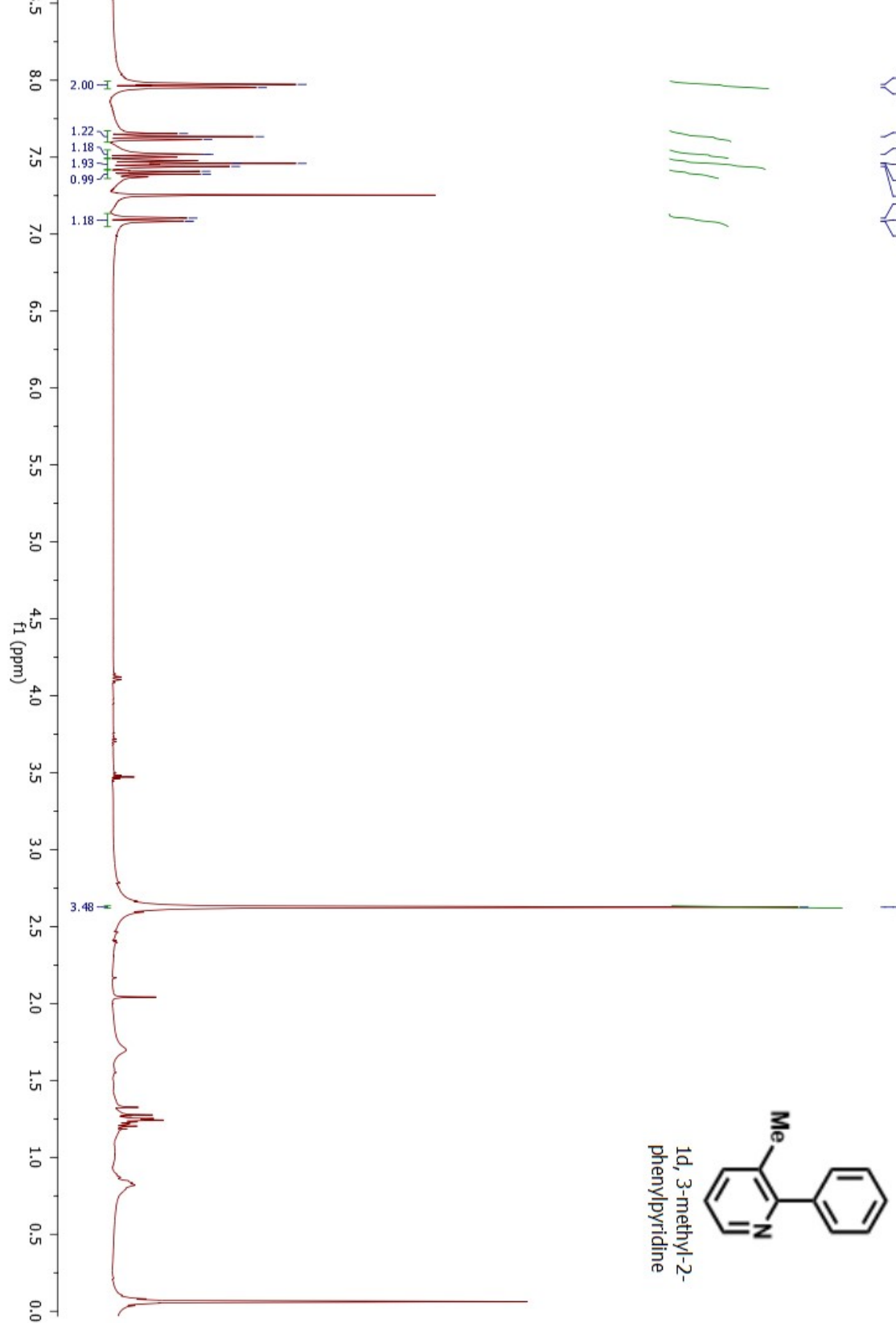
5-methyl-2-phenylpyridine (1c)

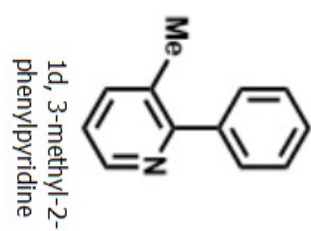




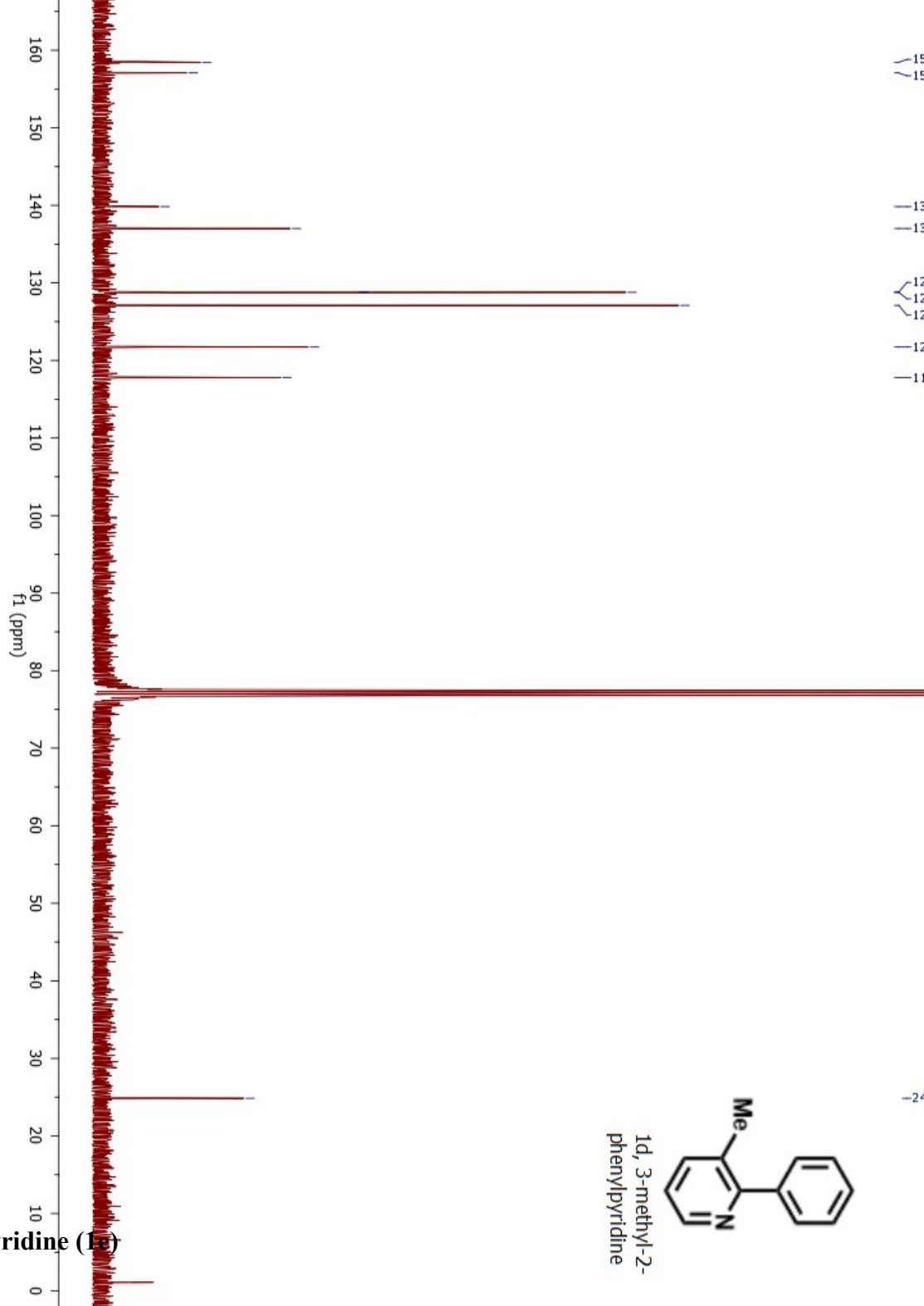


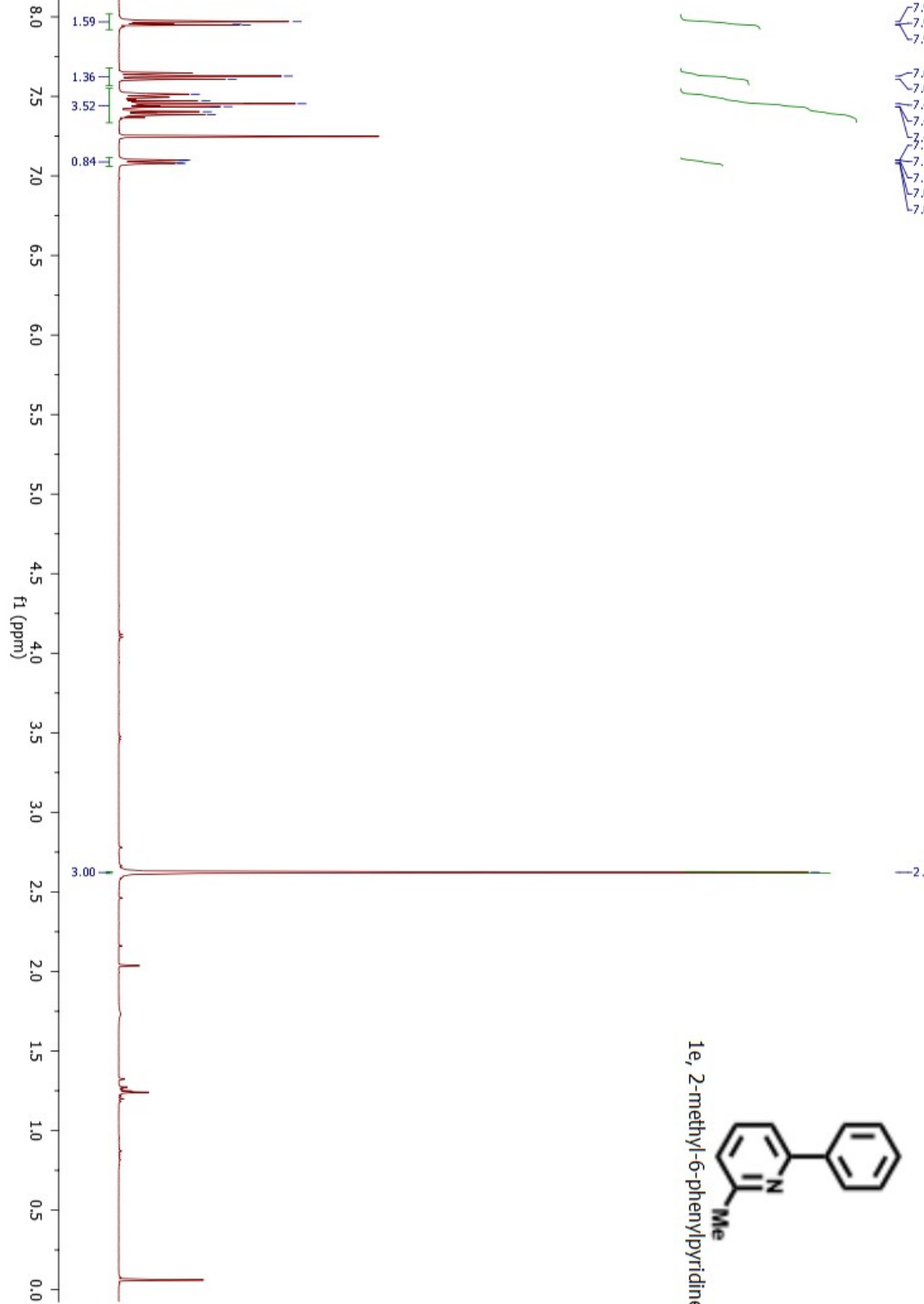
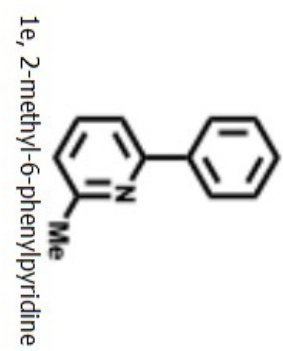
3-methyl-2-phenylpyridine



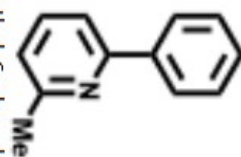


2-methyl-6-phenylpyridine (1e)





1e, 2-methyl-6-phenylpyridine

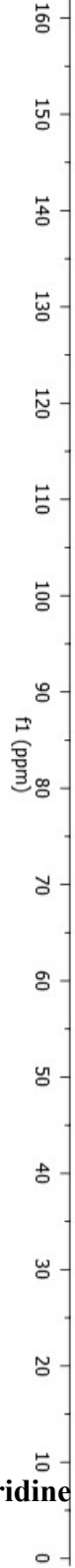


-24.8

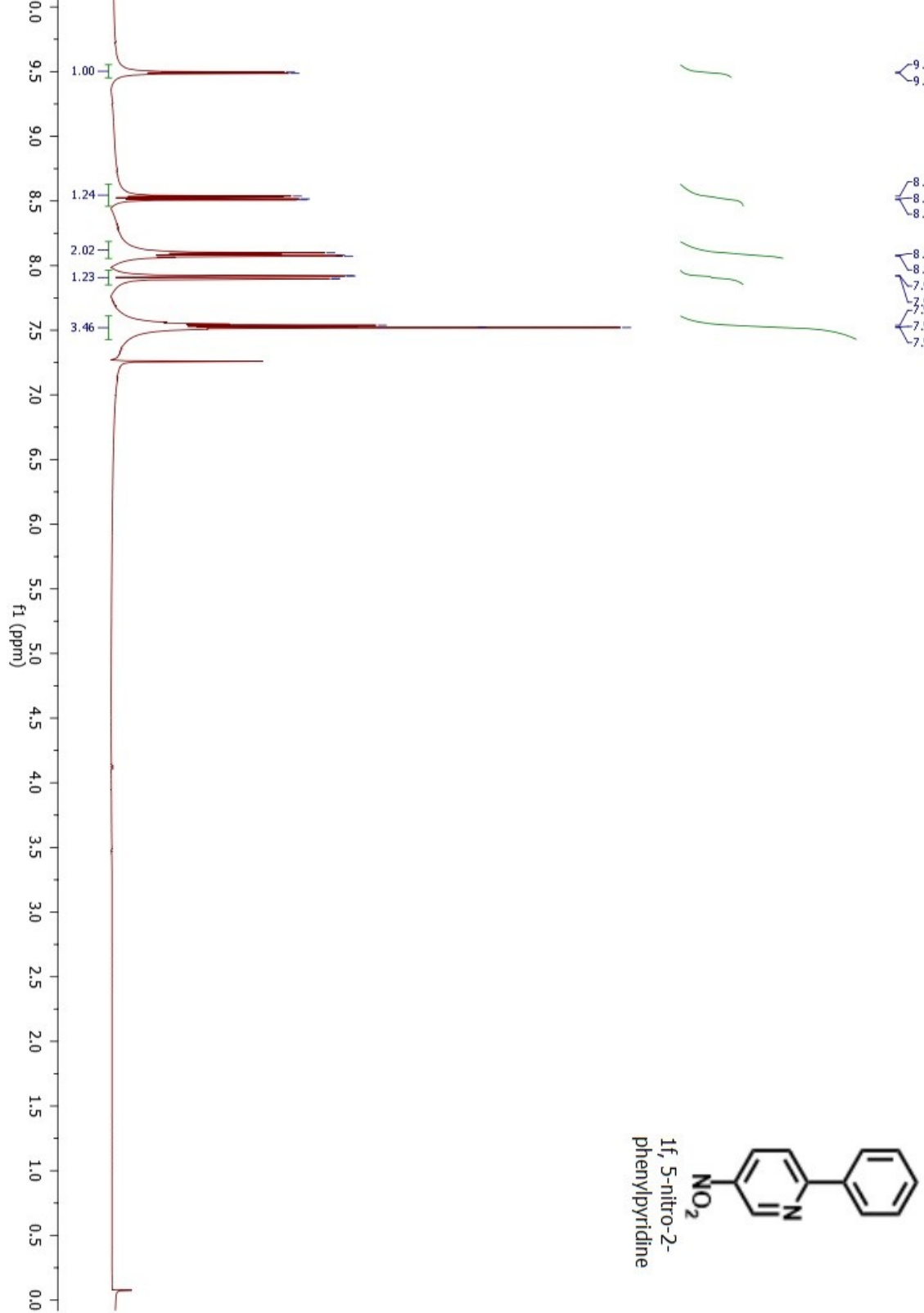
128.7
128.7
127.7
121.1
117.2

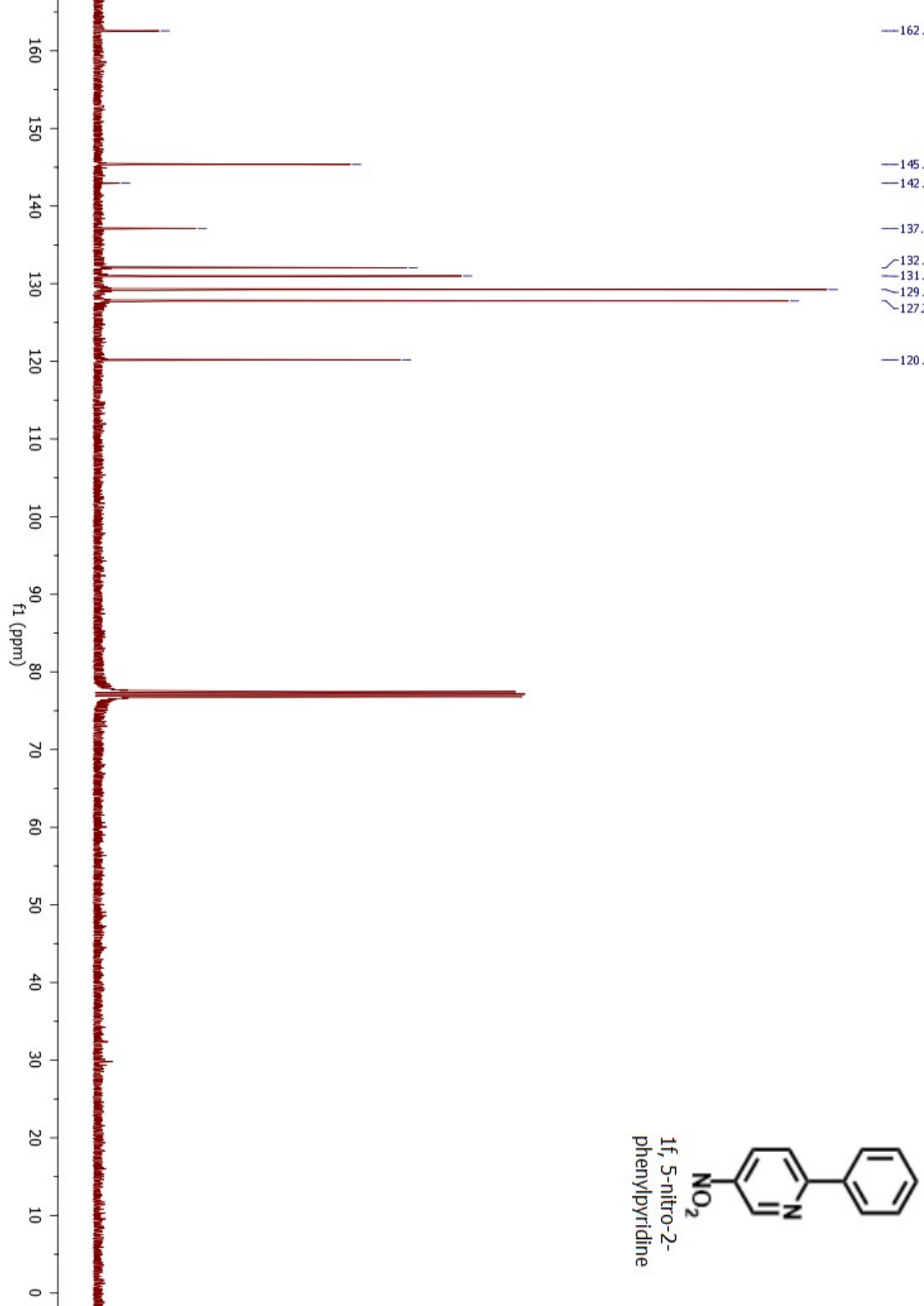
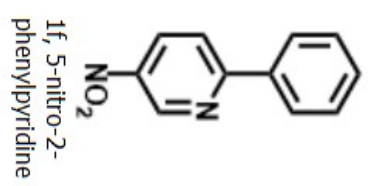
139.7
137.7

158.7
157.7



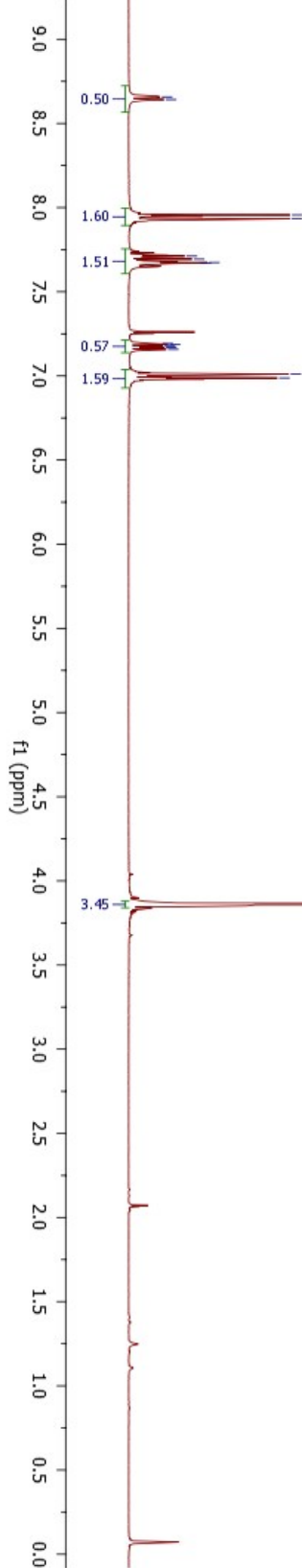
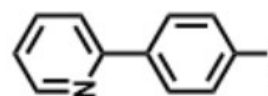
5-nitro-2-phenylpyridine (1f)



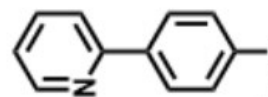


Handwritten notes: \int , \int , \int , \int

1g, 2-(4-methoxyphenyl)
pyridine



2-(4-methoxyphenyl)

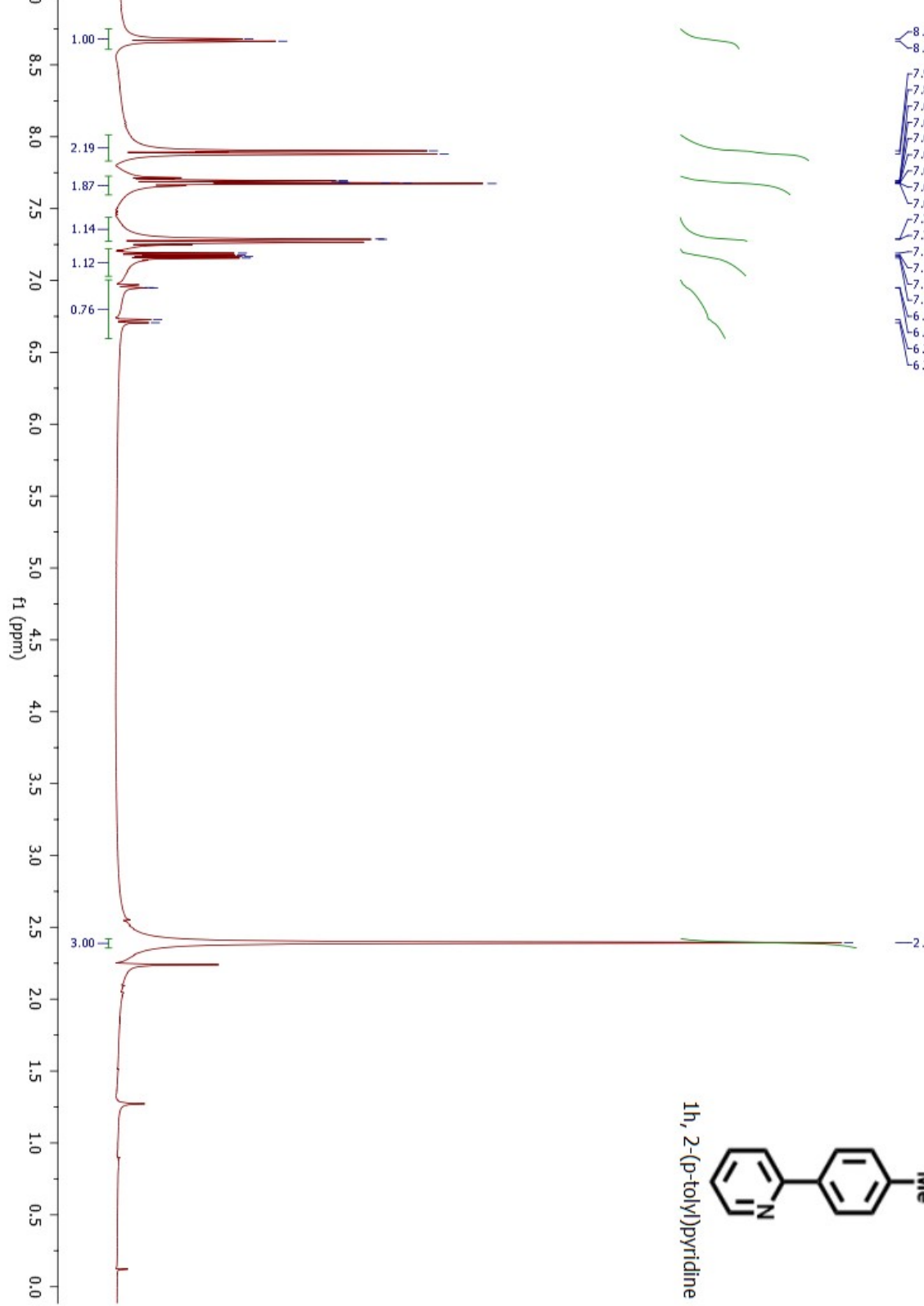


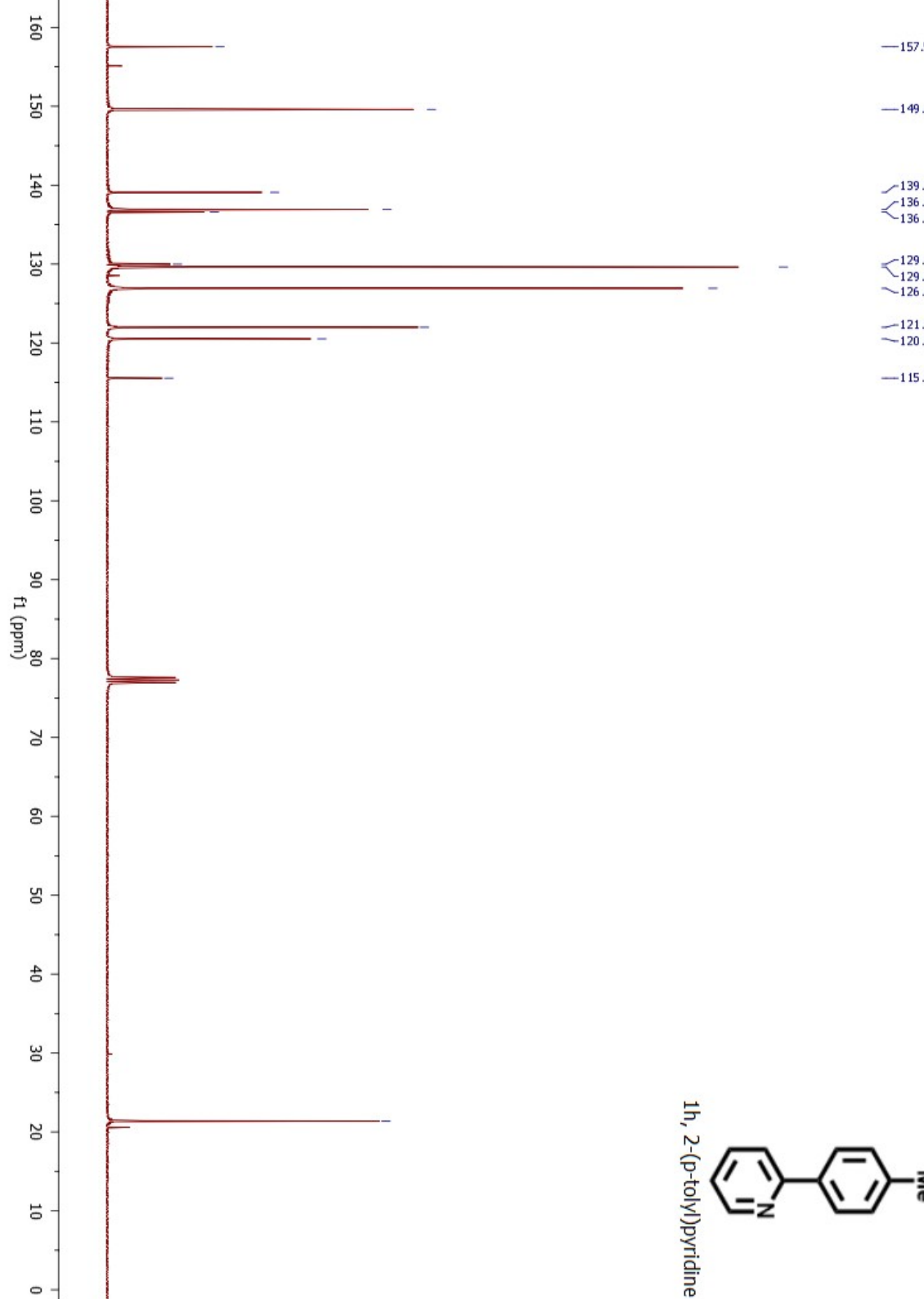
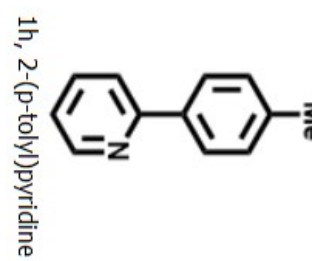
1g, 2-(4-methoxyphenyl)
pyridine

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

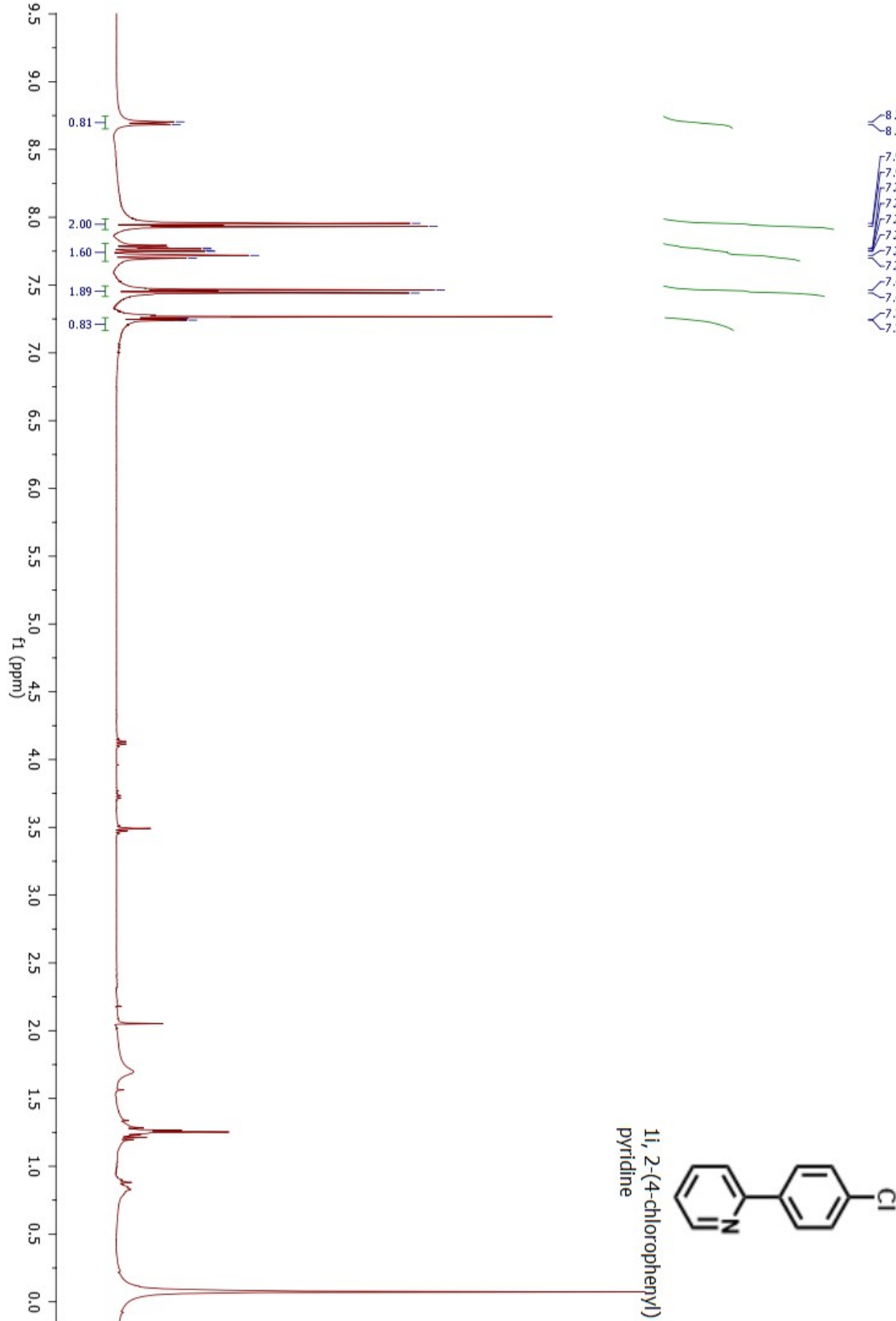
f1 (ppm)

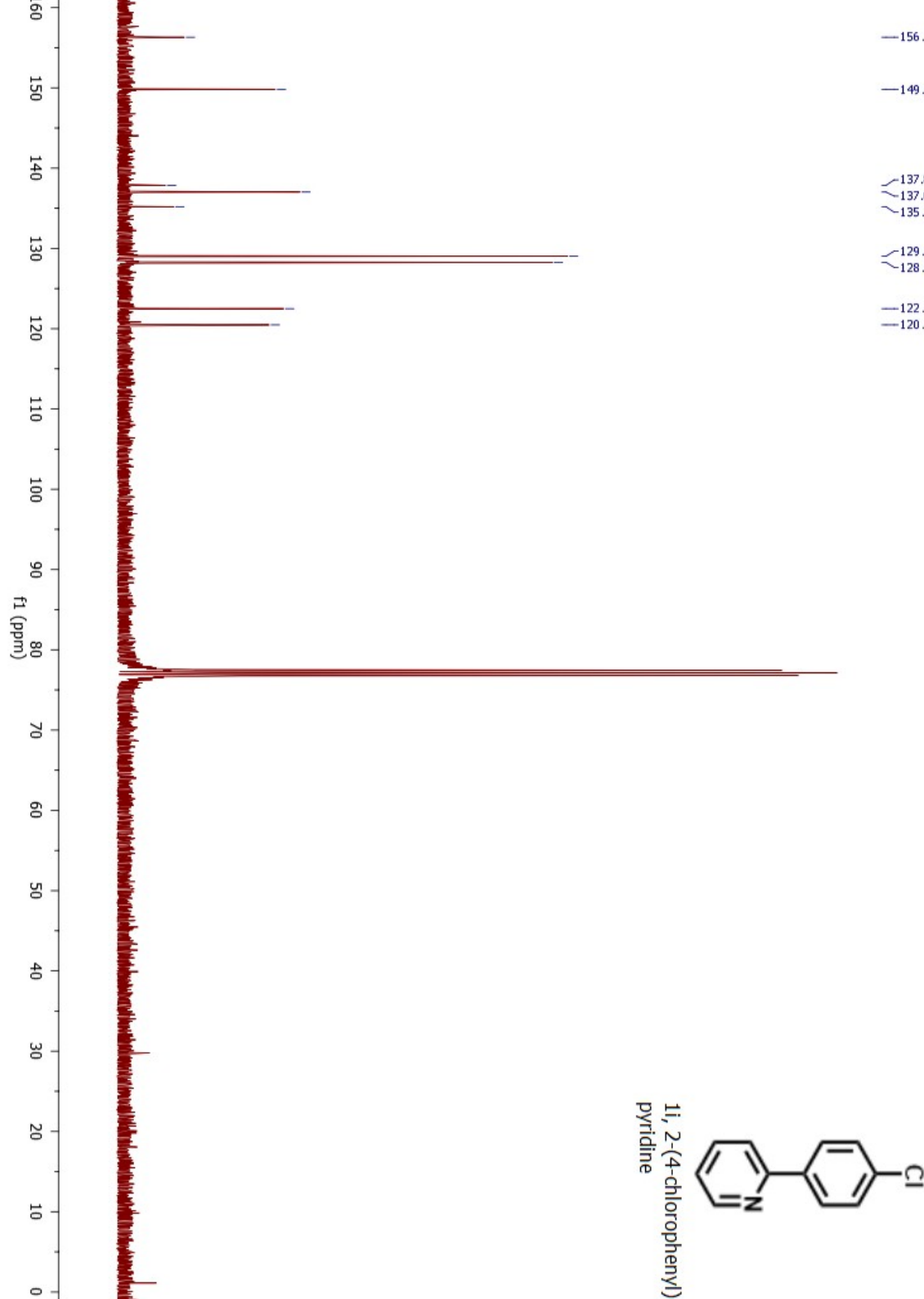
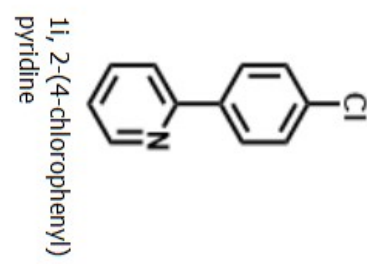
2-(p-tolyl)pyridine (1h)

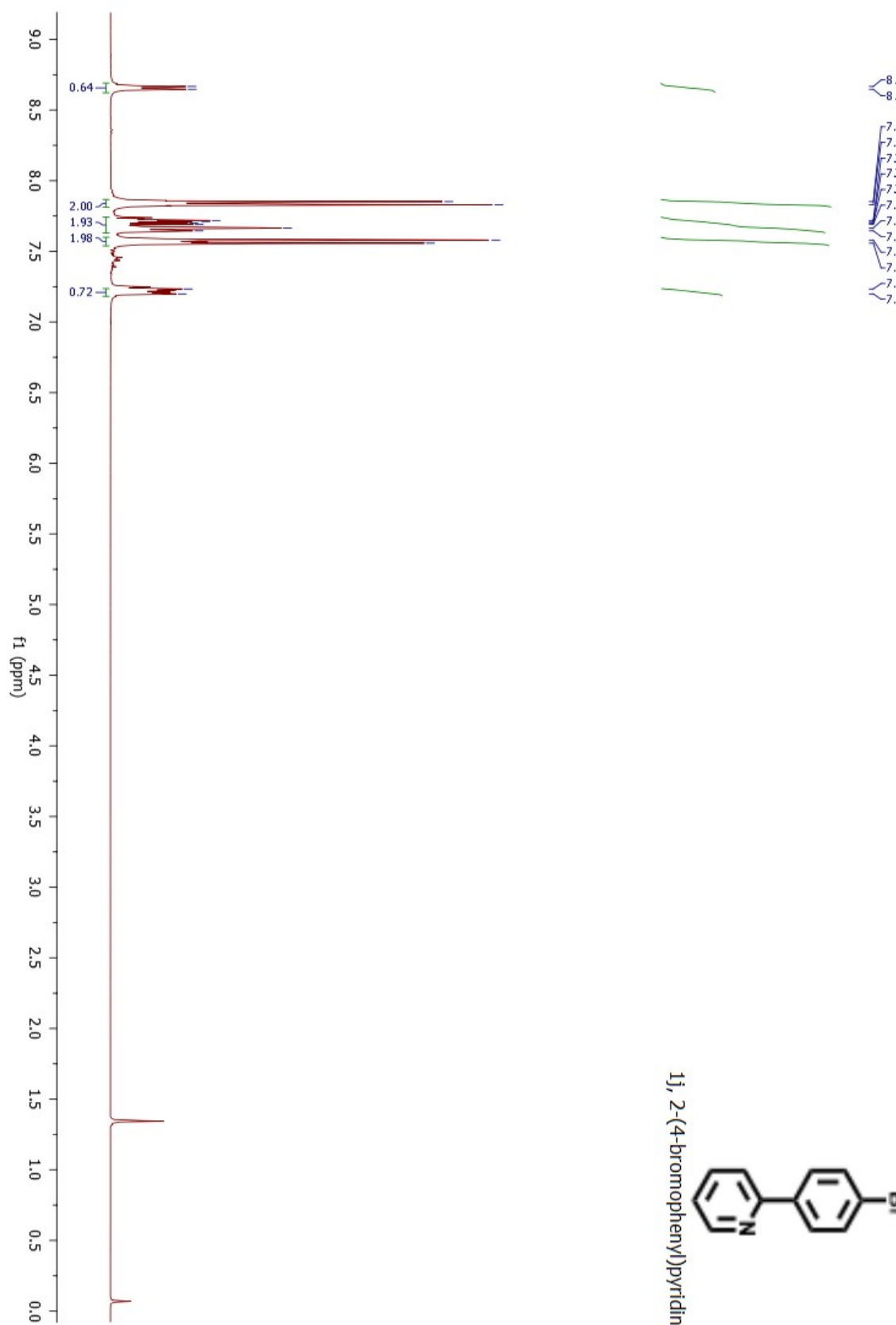
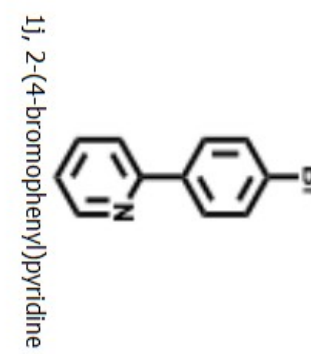




2-(4-chlorophenyl)I

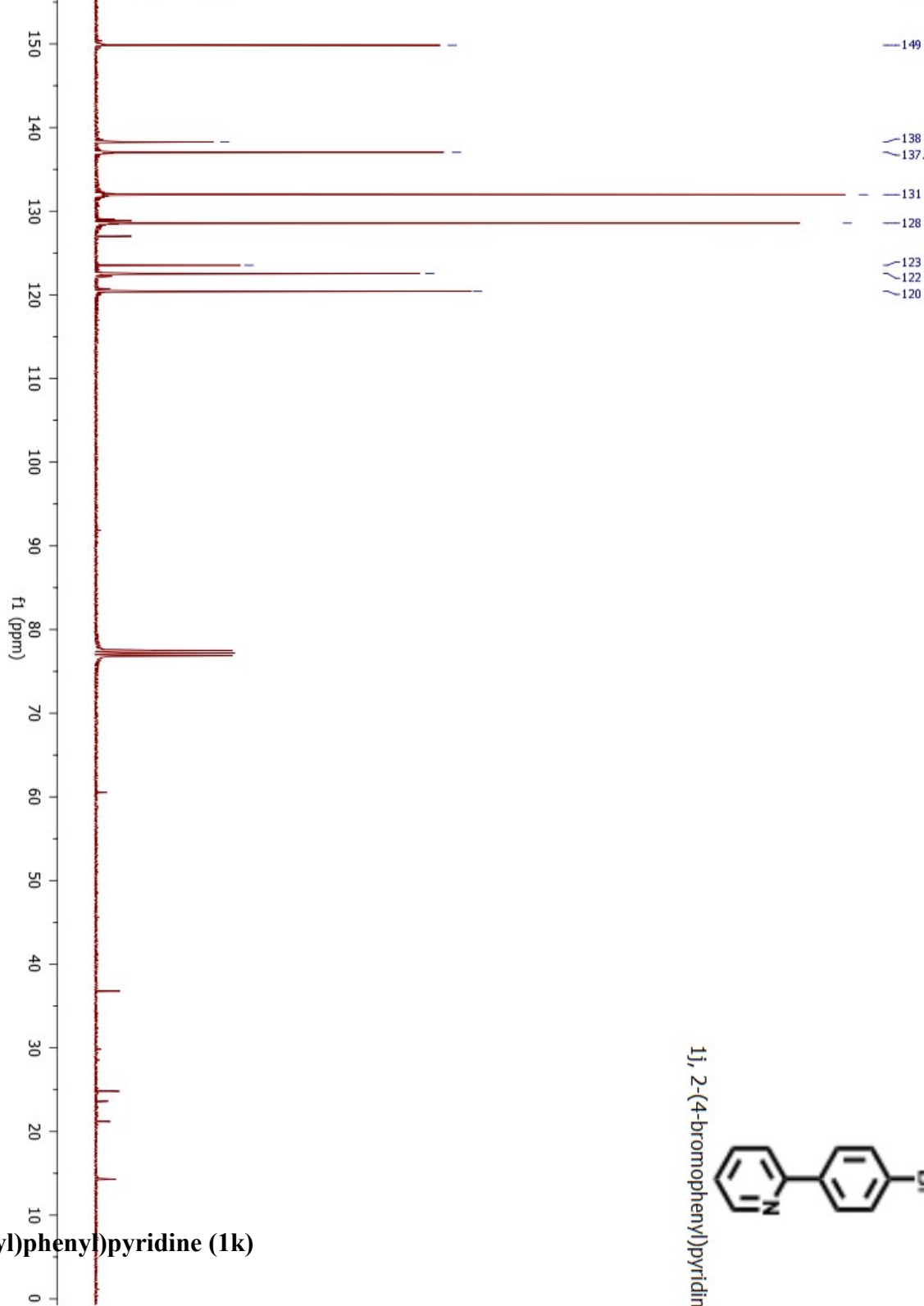
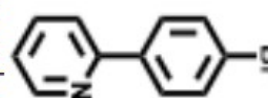




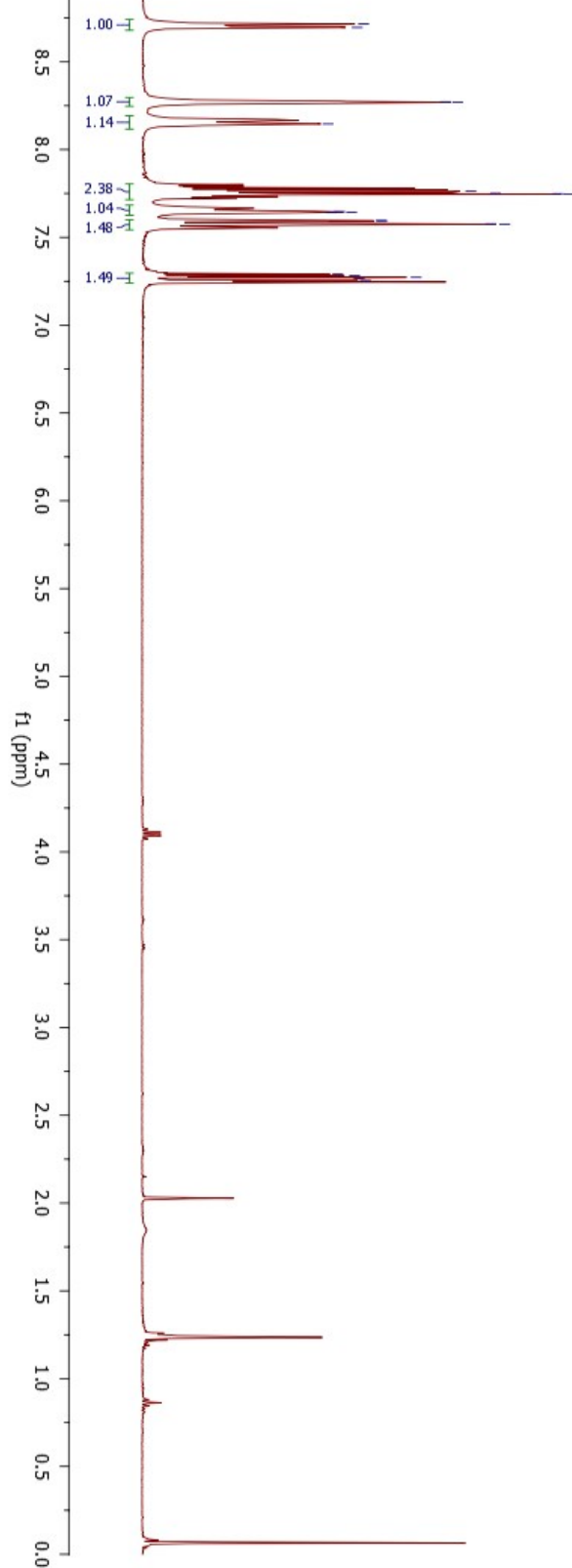
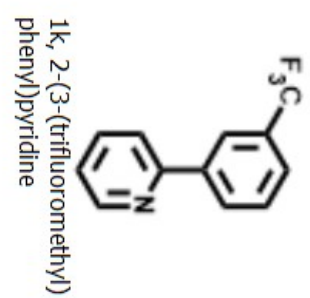


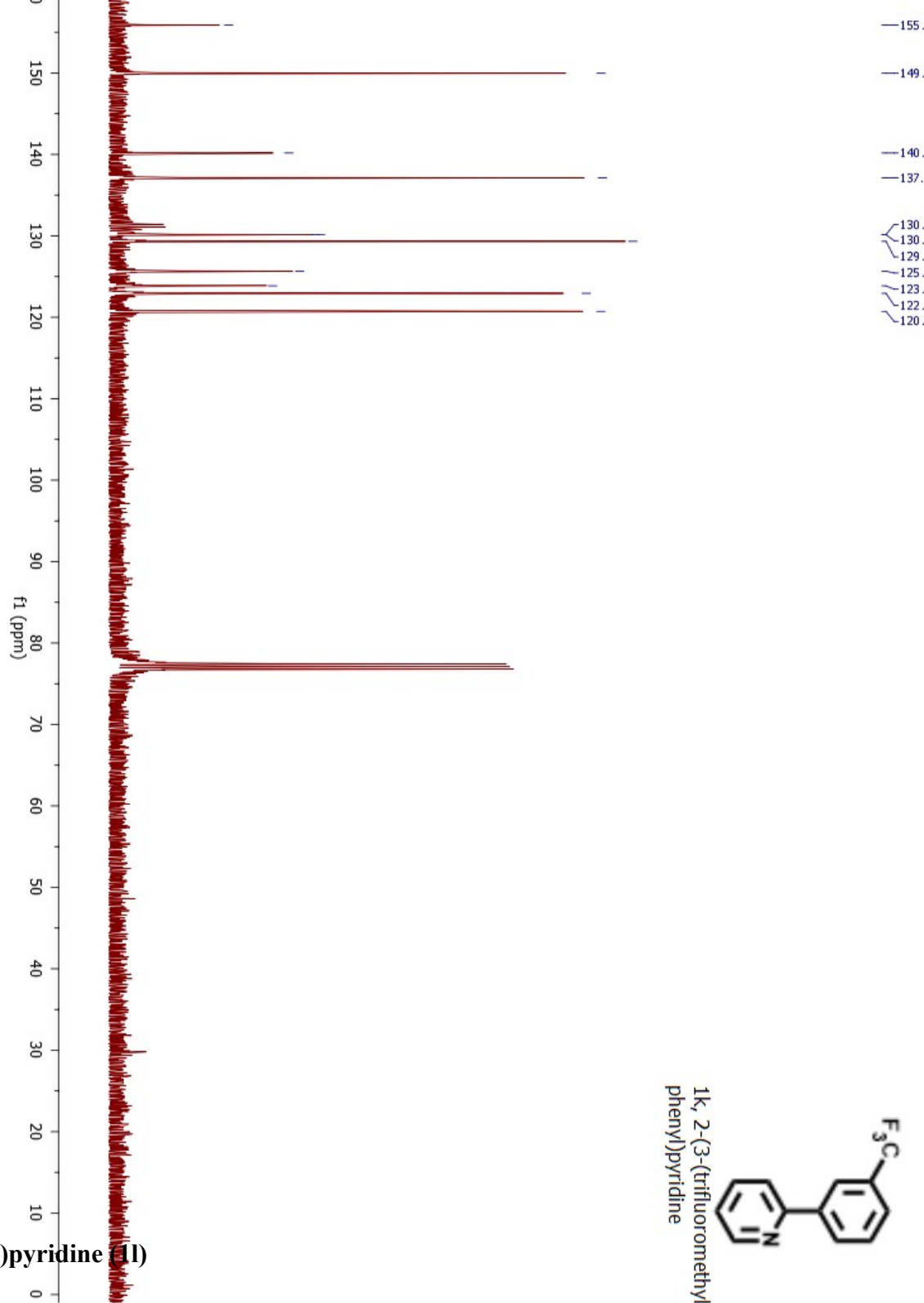
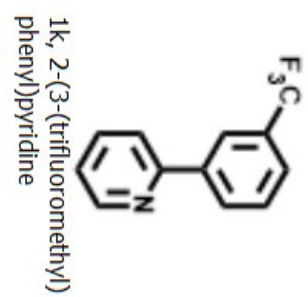
2-(4-bromophenyl)

1j, 2-(4-bromophenyl)pyridine

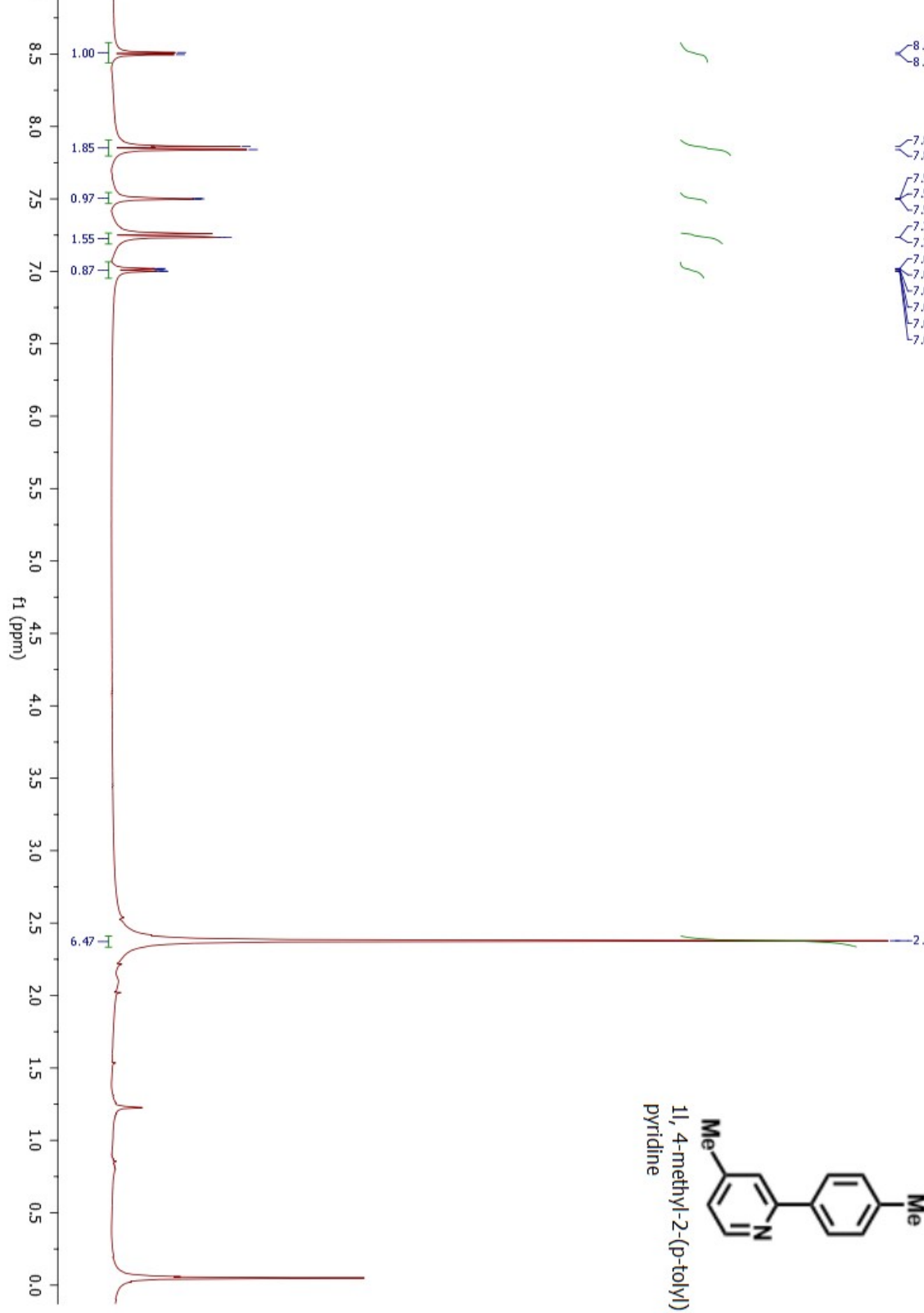


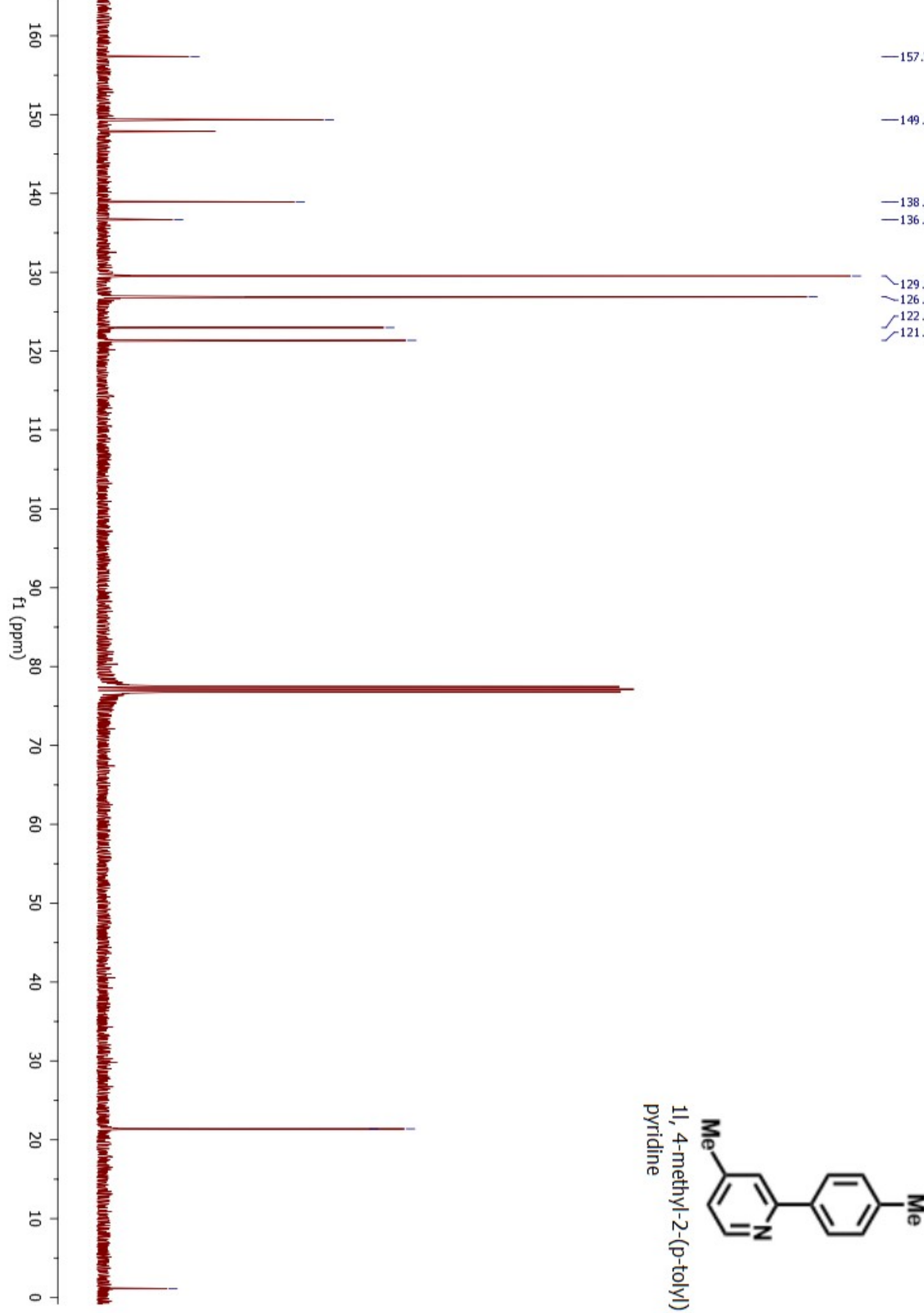
2-(3-(trifluoromethyl)phenyl)pyridine (1k)



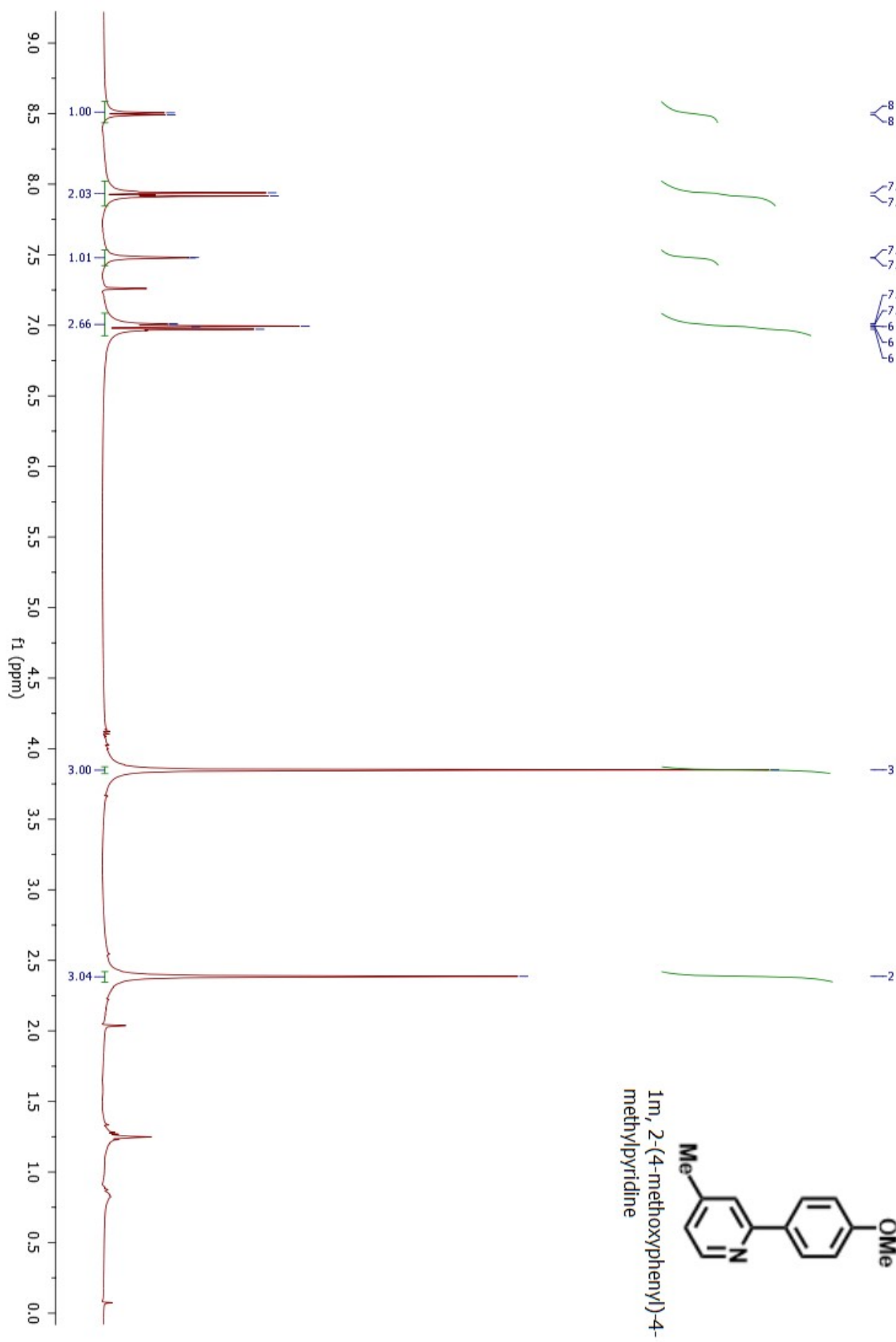


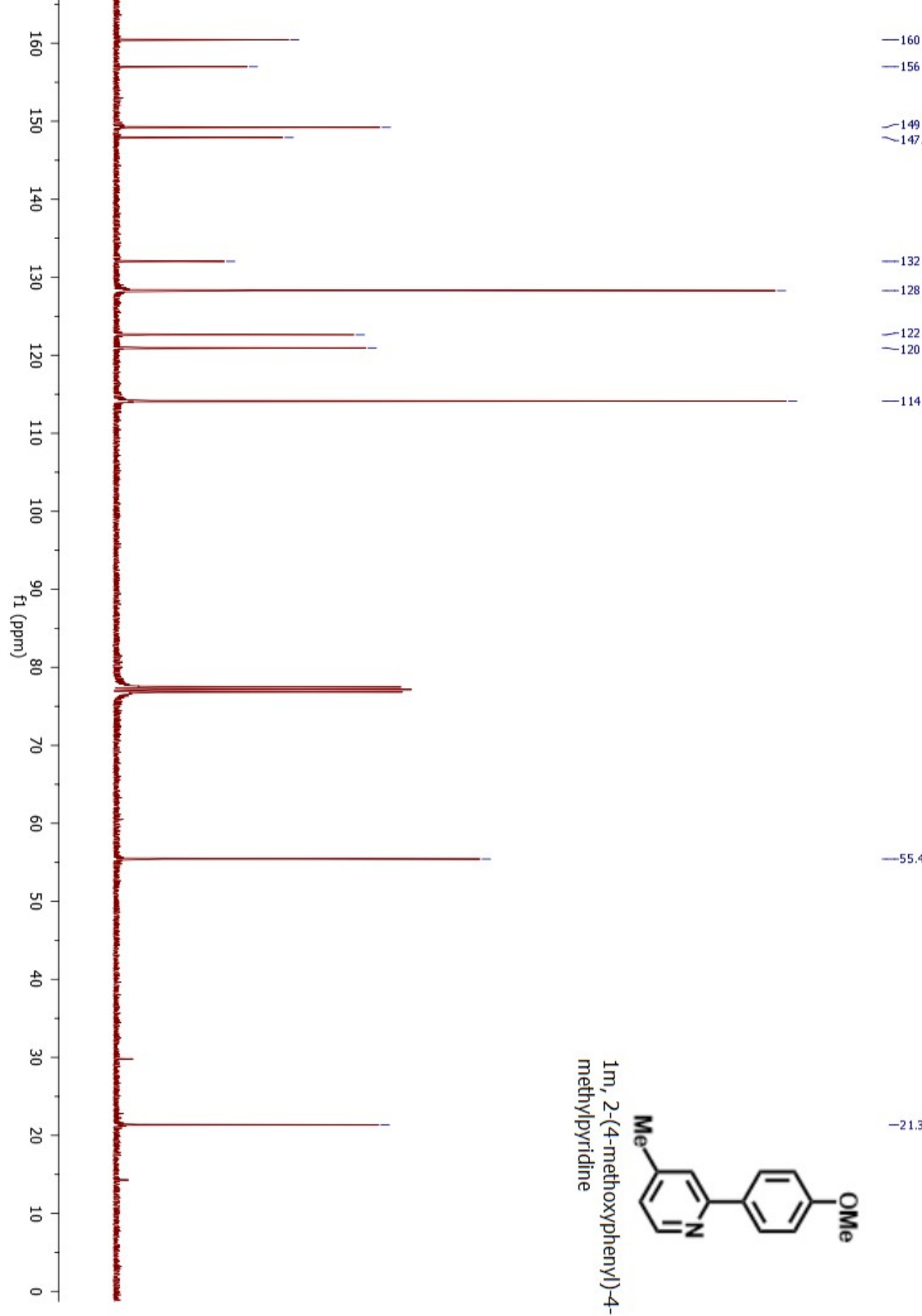
4-methyl-2-(p-tolyl)pyridine (1l)



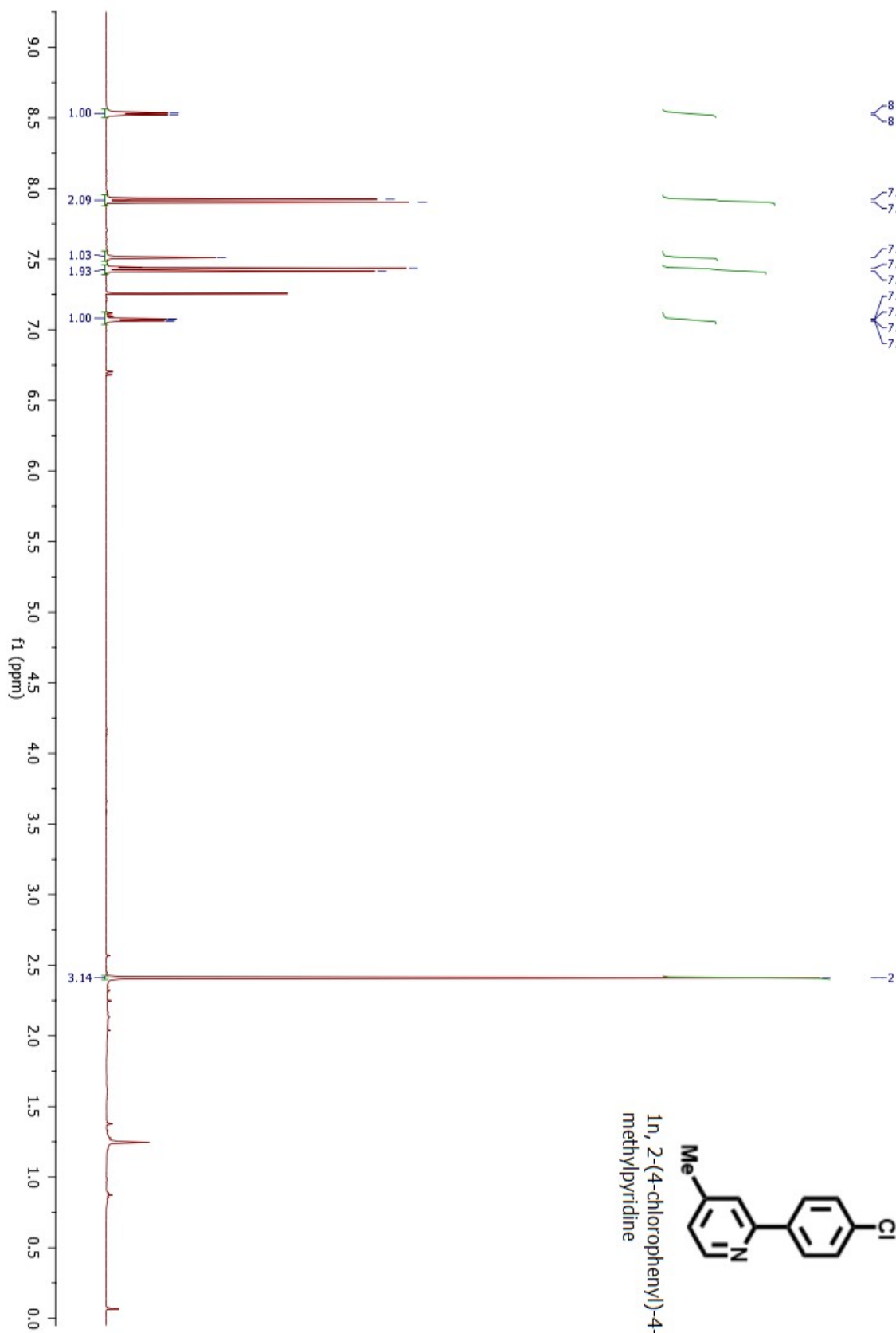


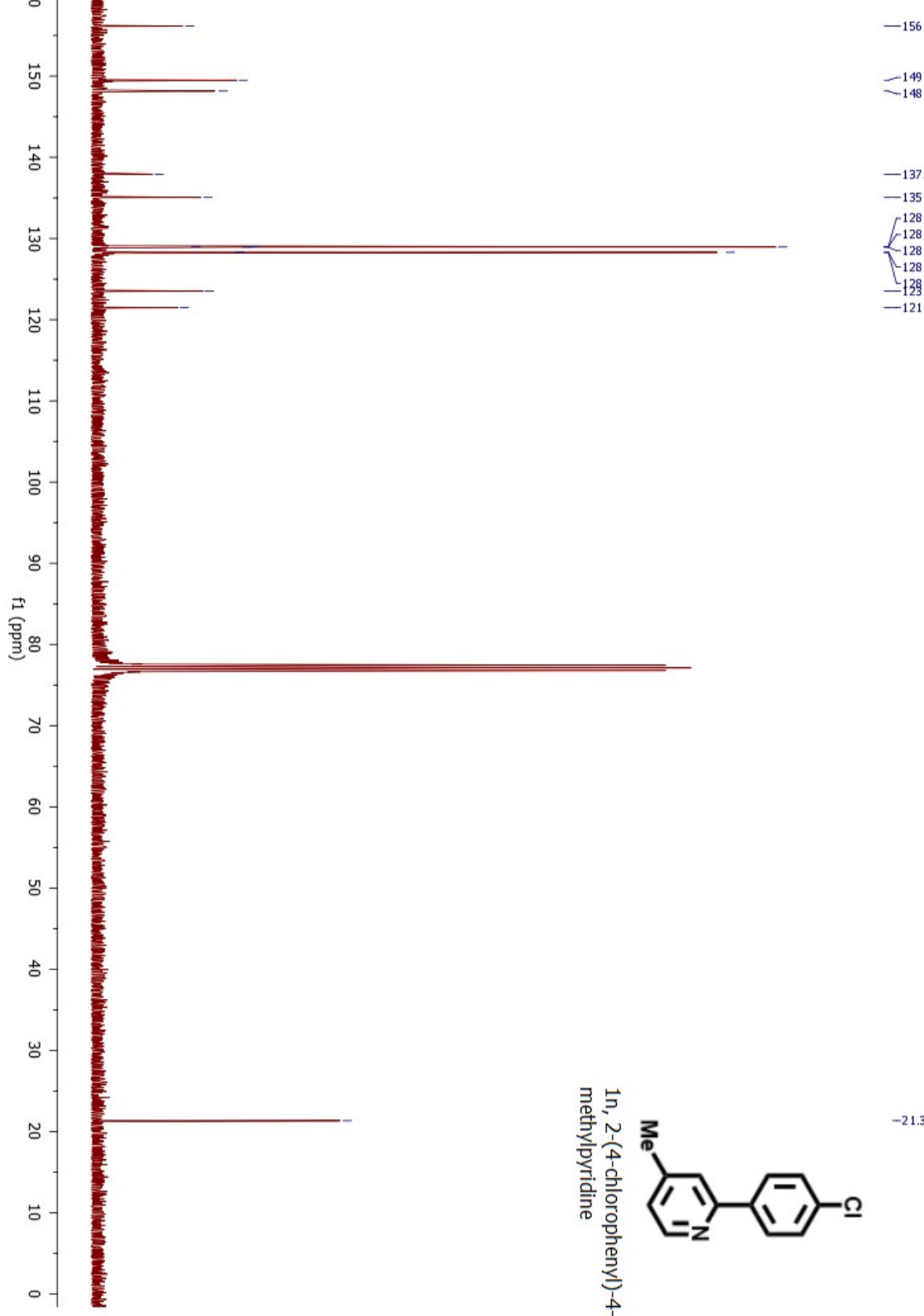
2-(4-methoxypheny

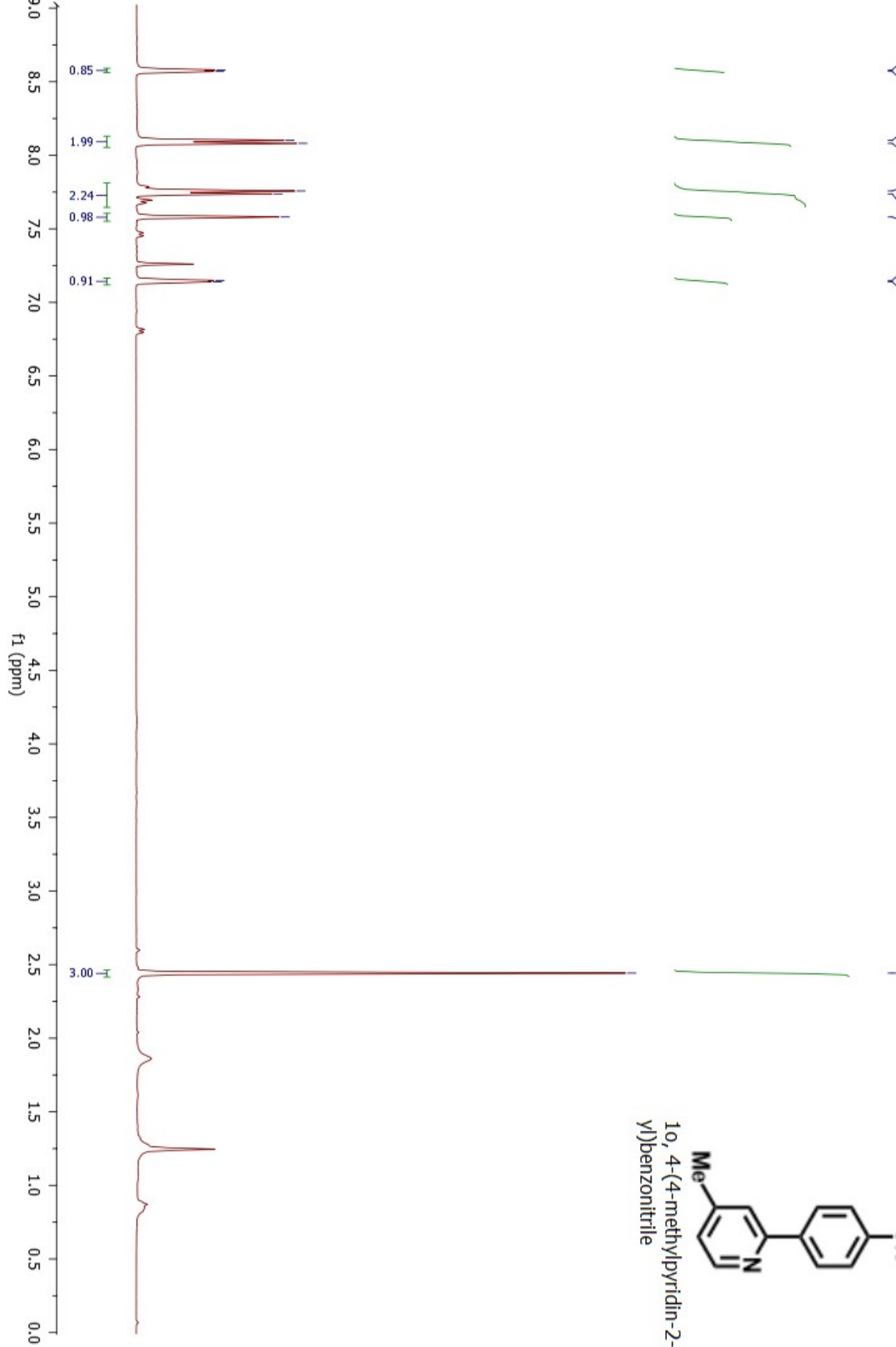
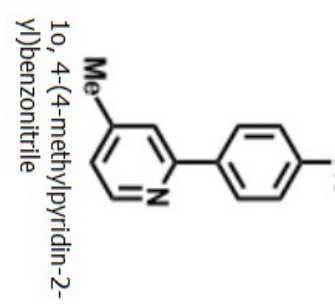




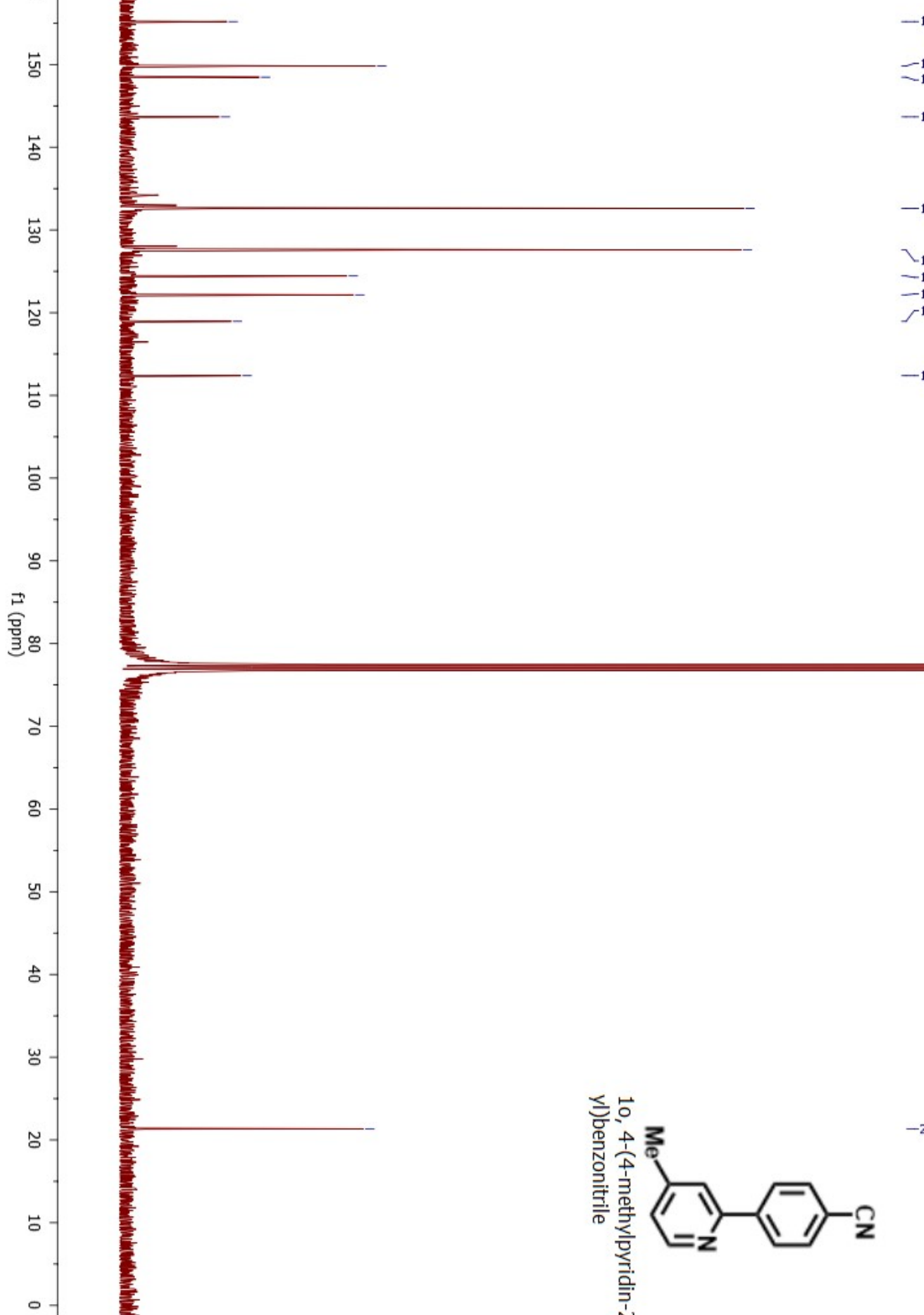
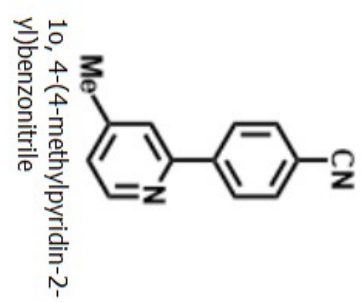
2-(4-chlorophenyl)-



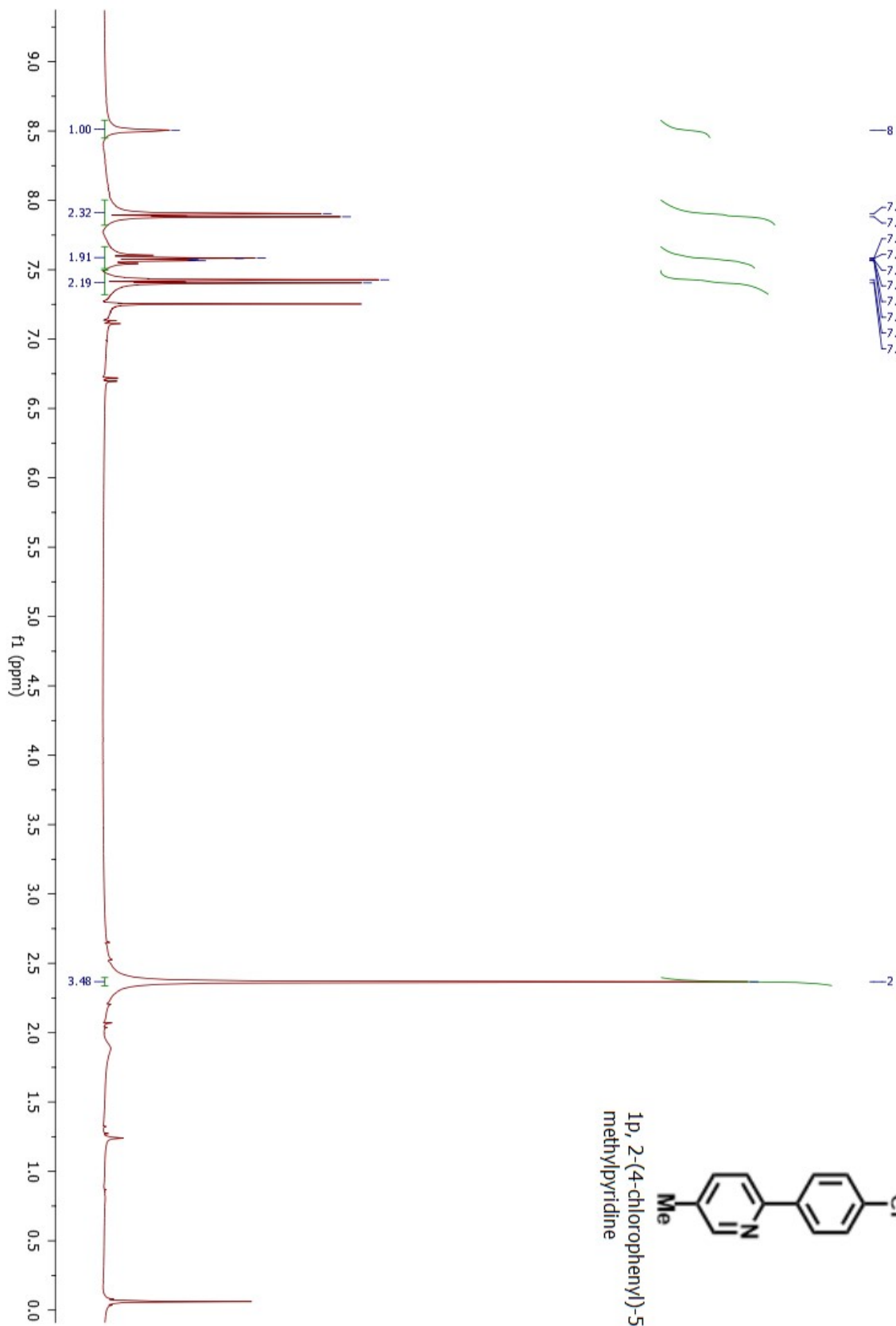


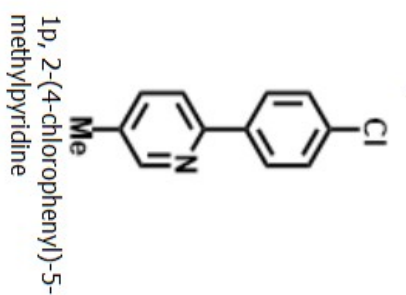


4-(4-methylpyridin-2-

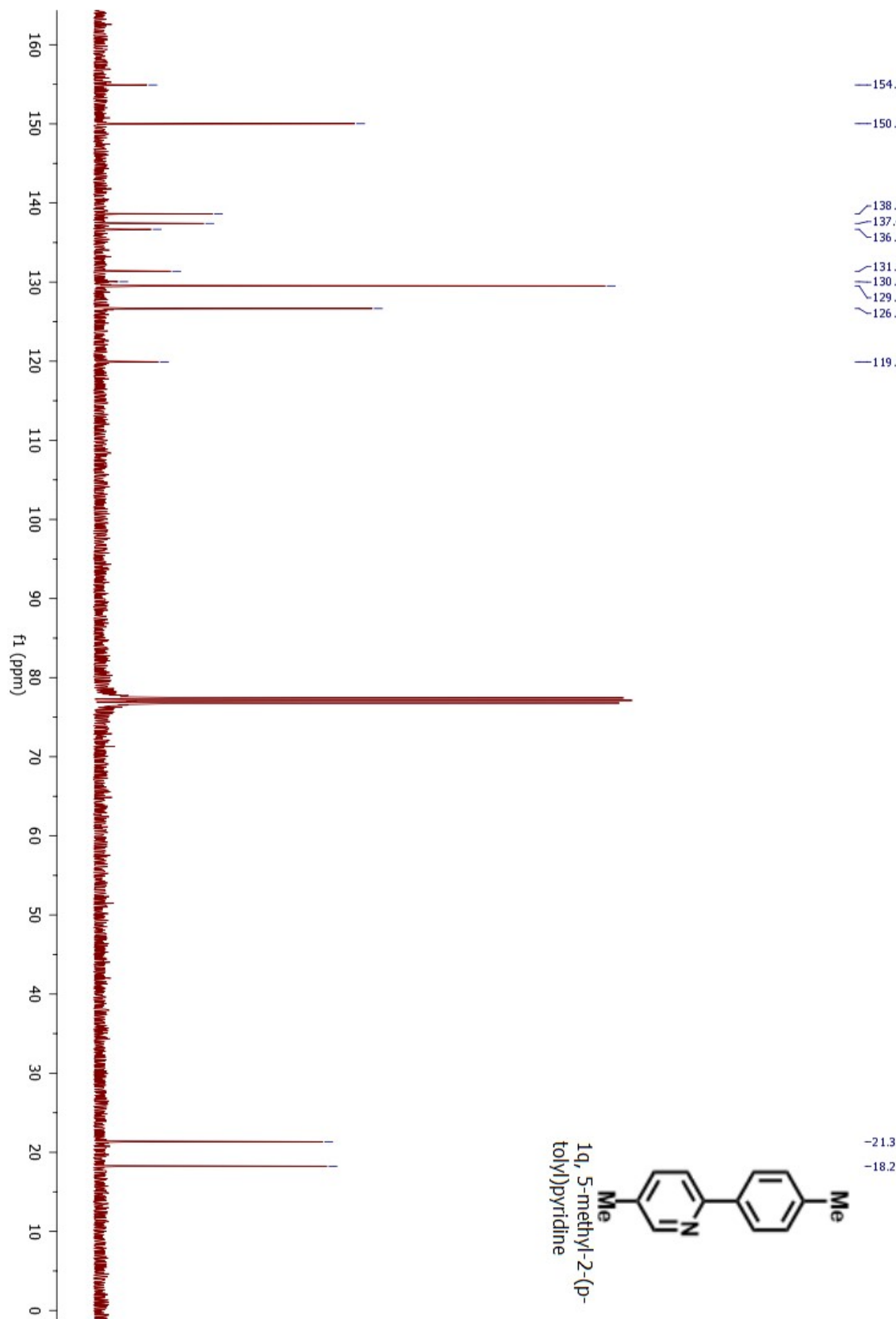


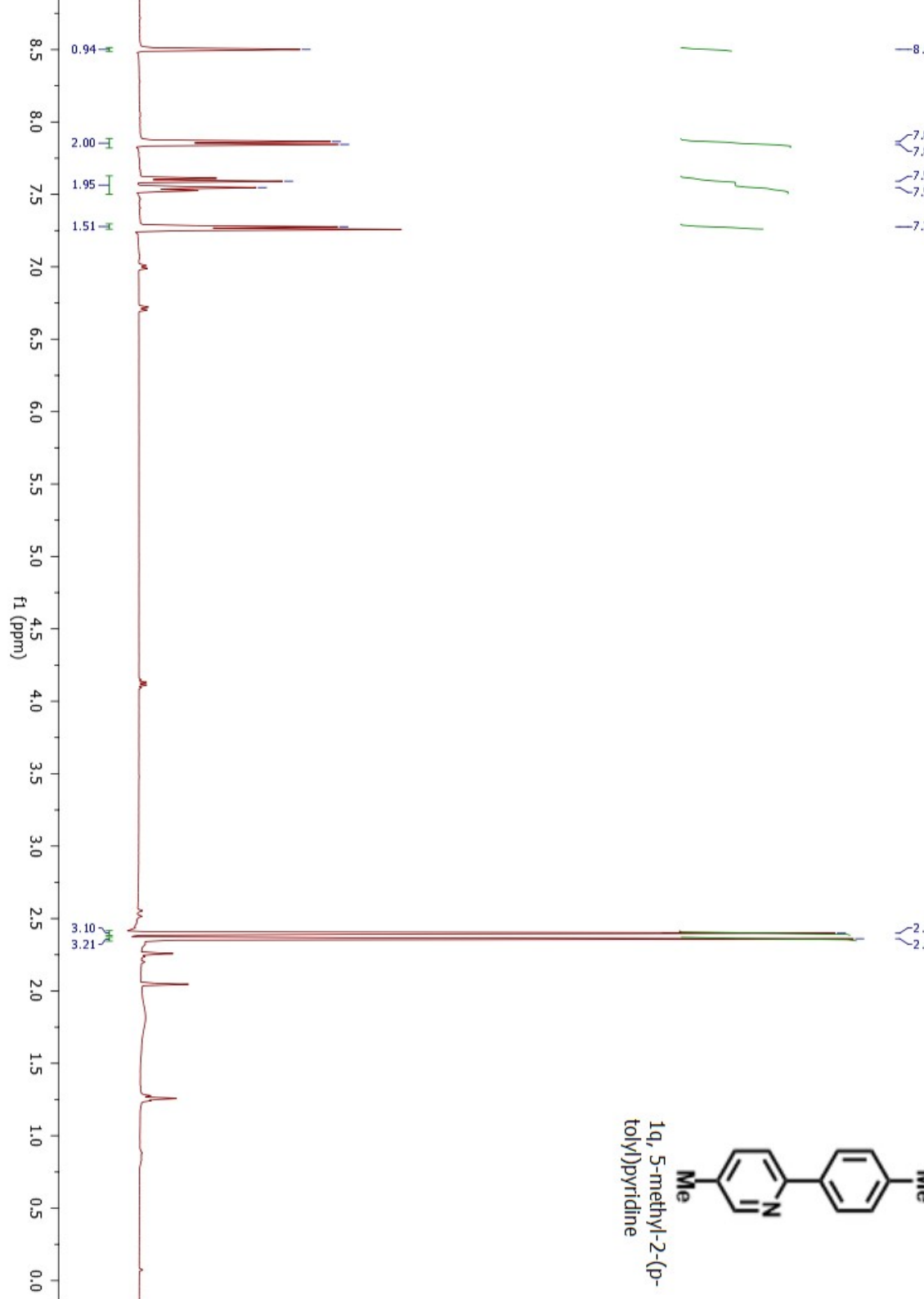
2-(4-chlorophenyl)-



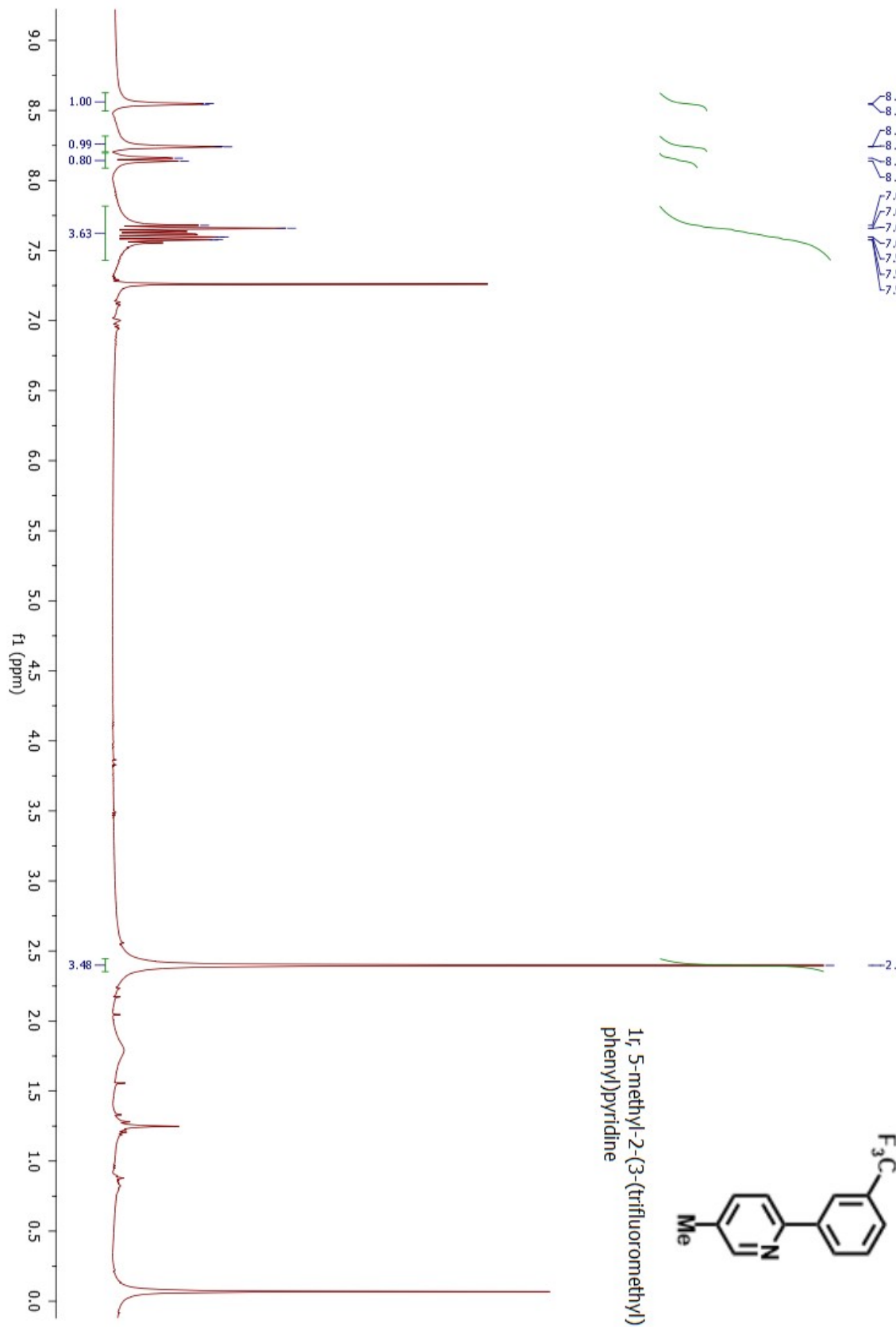


5-methyl-2-(p-tolyl)

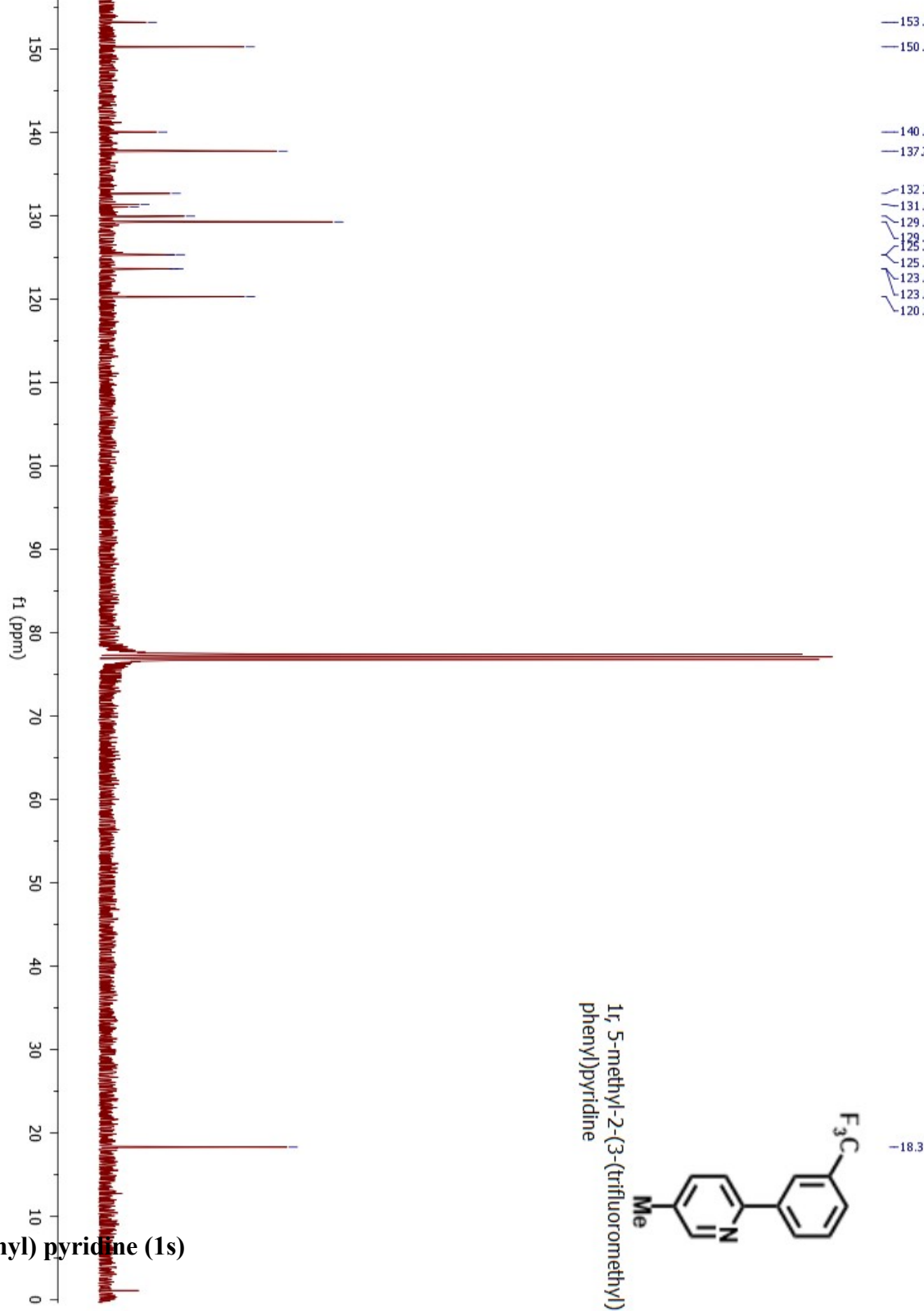


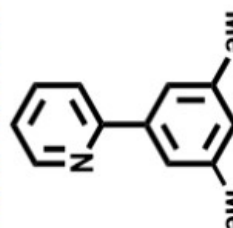
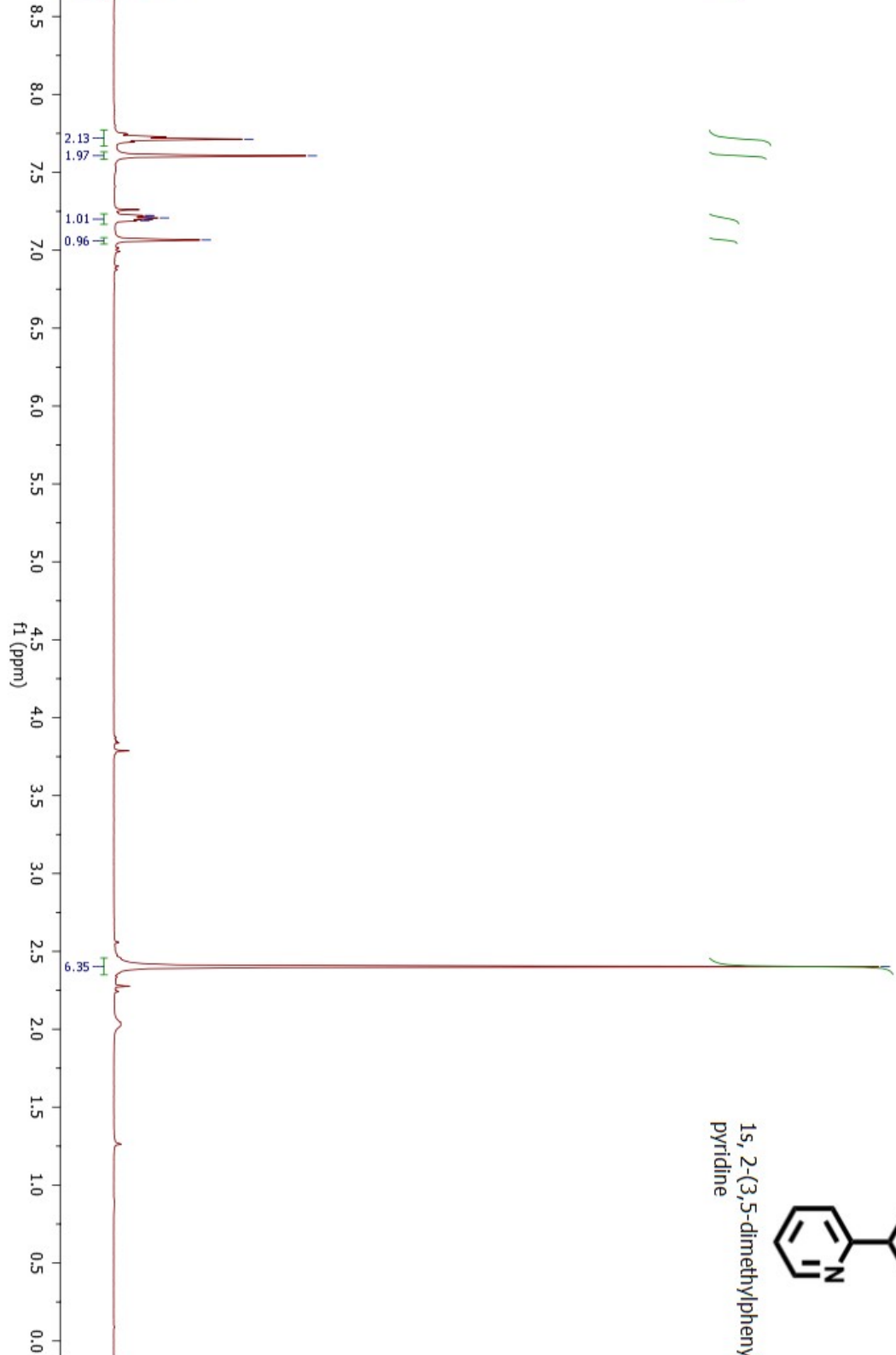


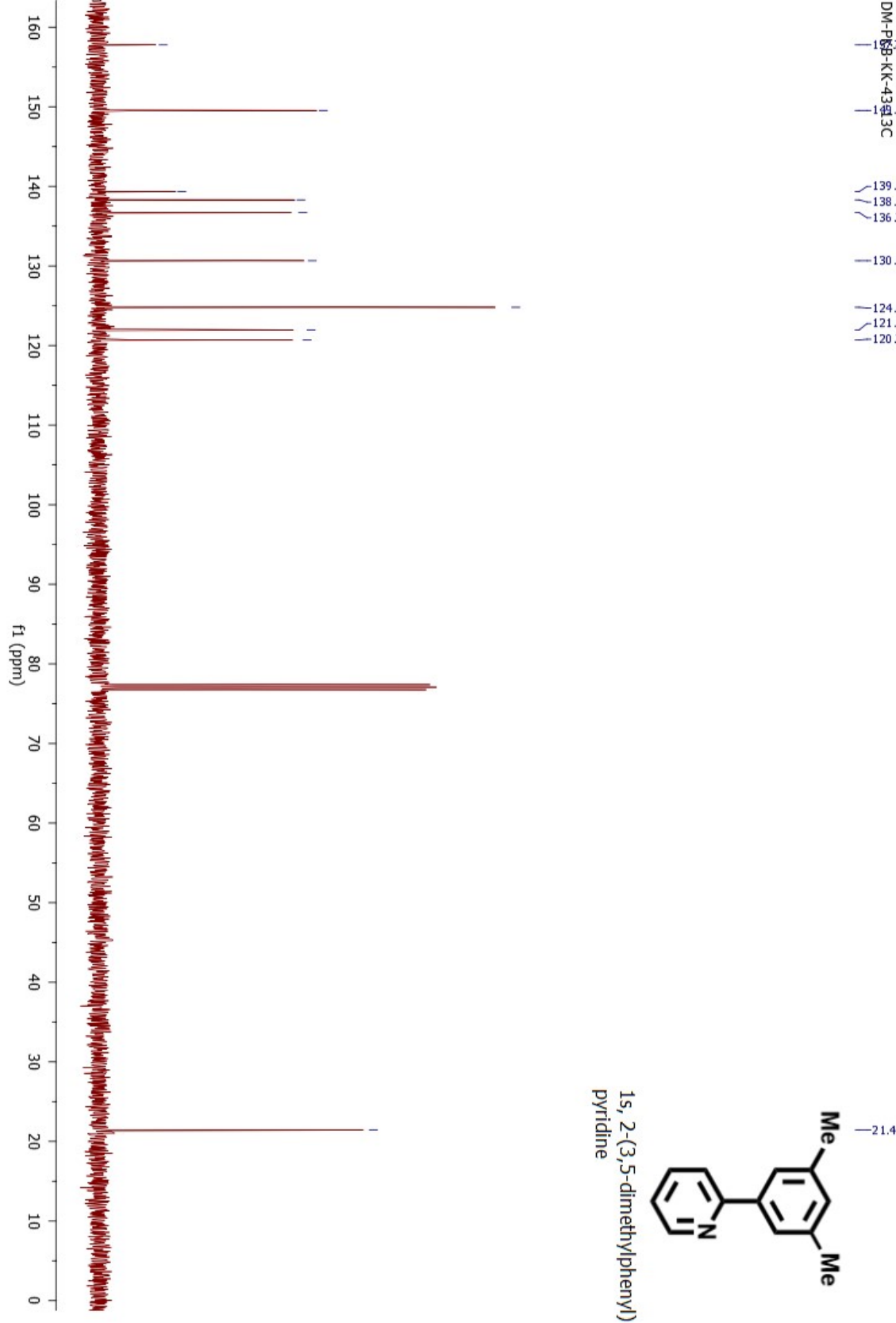
5-methyl-2-(3-(trifl

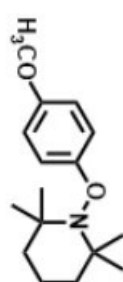


2-(3,5-dimethylphenyl) pyridine (1s)

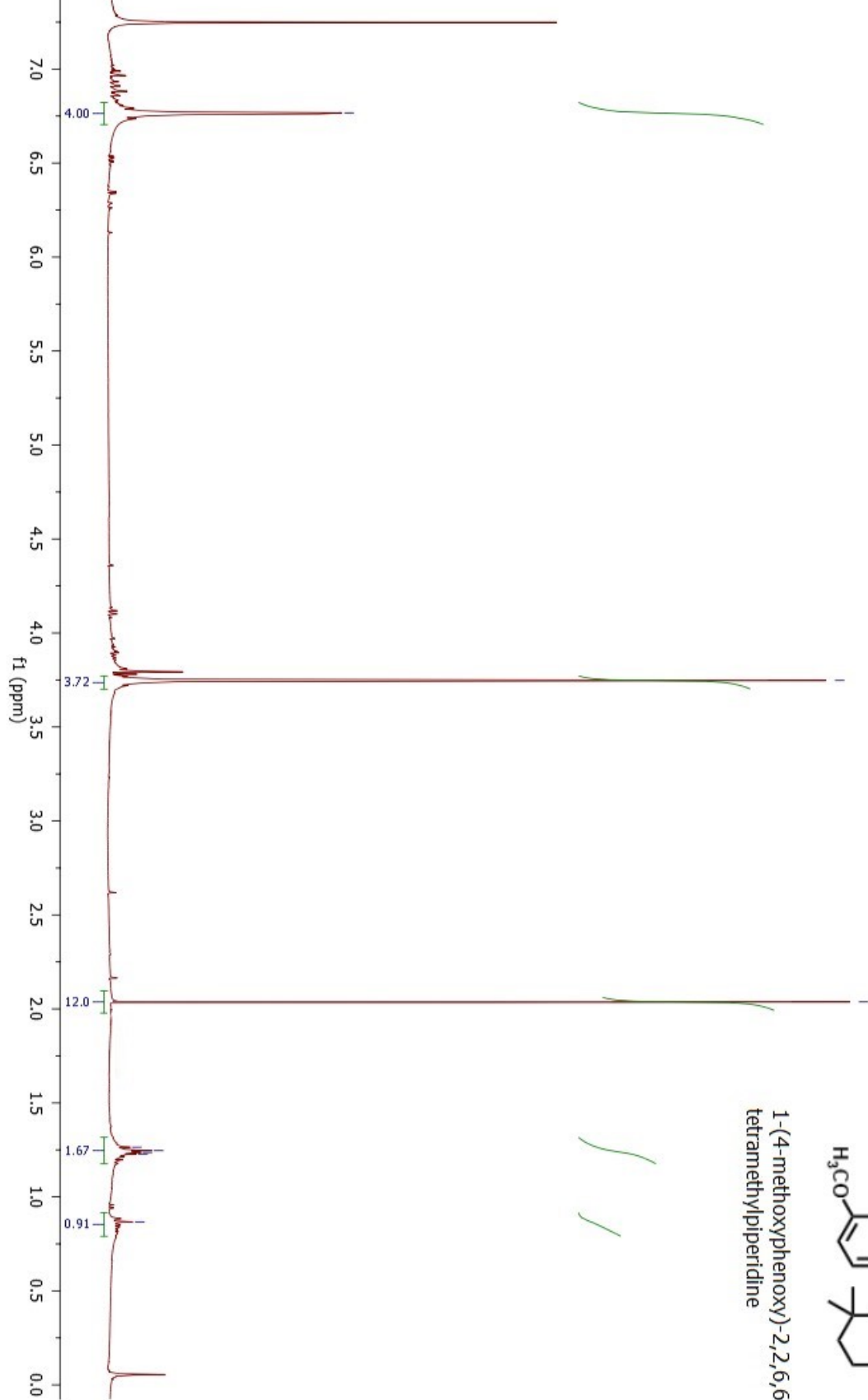


1s, 2-(3,5-dimethylphenyl)
pyridine

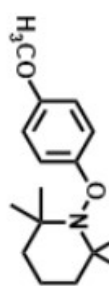




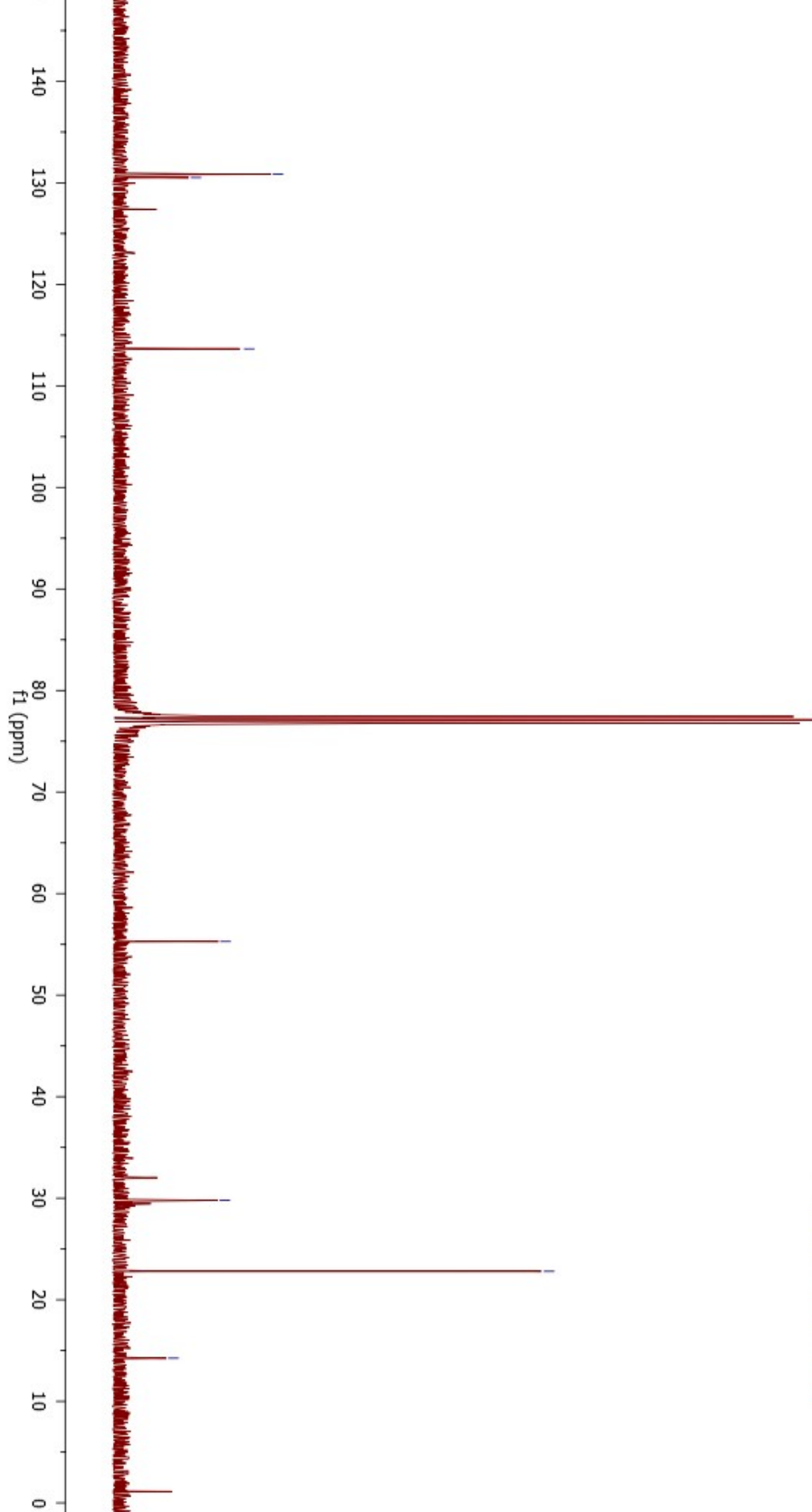
1-(4-methoxyphenoxy)-2,2,6,6-tetramethylpiperidine



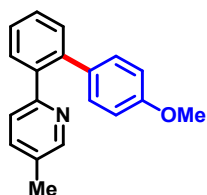
1-(4-methoxyphenoxy)



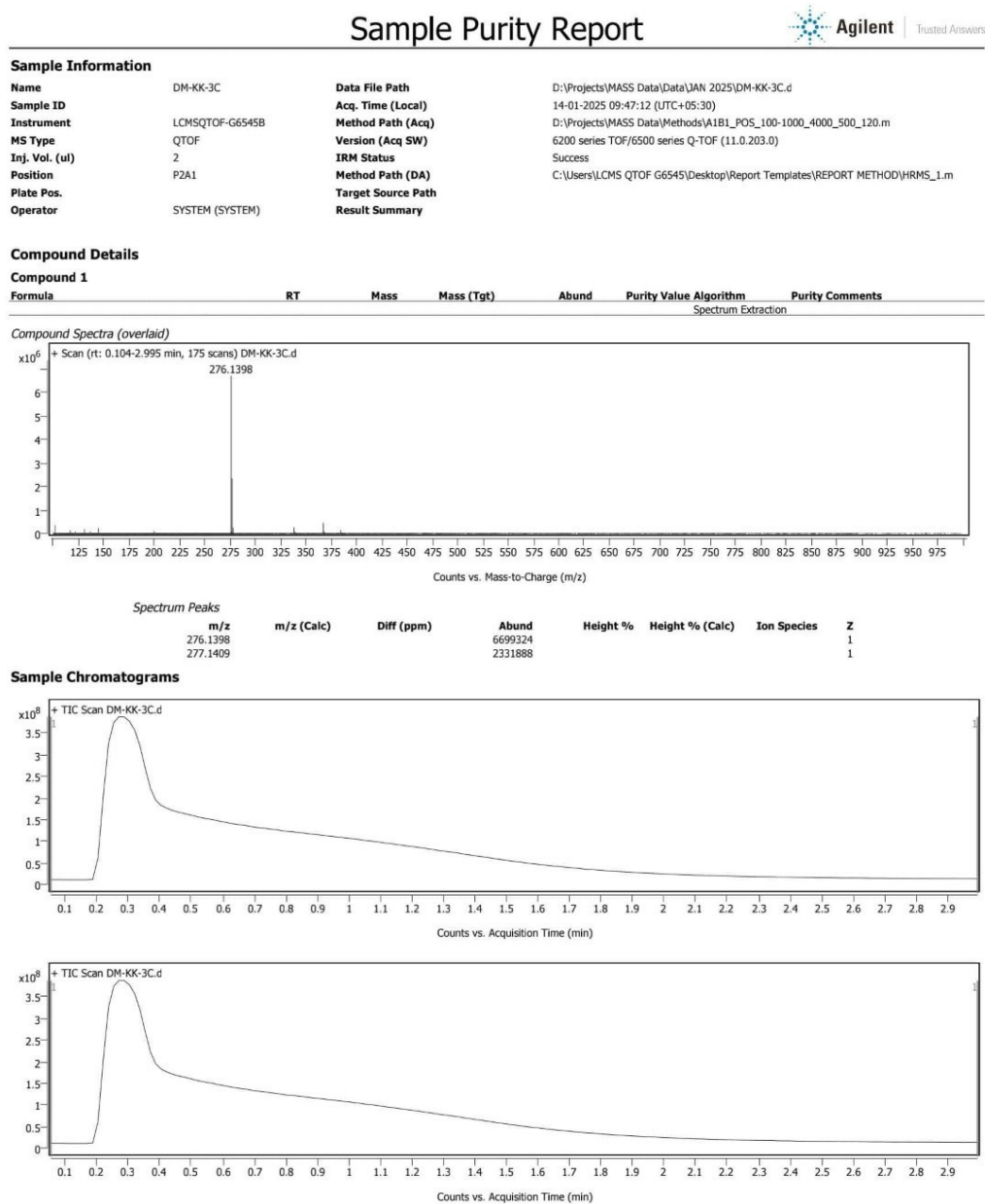
1-(4-methoxyphenoxy)-2,2,6,6-tetramethylpiperidine



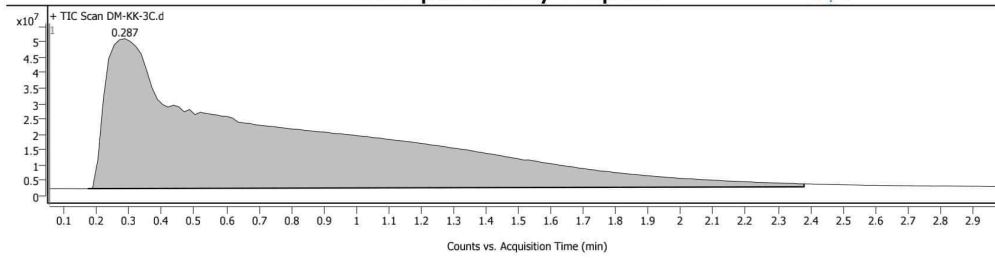
11. HRMS data of C-H arylation products:



2-(4'-methoxy-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3c)



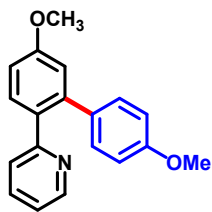
Sample Purity Report



Chromatogram Peaks

| RT | Height | Height % | Area | Area % | Base Peak m/z | Symmetry | Width Label |
|-------|----------|----------|------------|--------|------------------|----------|-------------|
| 0.287 | 48718492 | 100.00 | 1853860722 | 100.00 | 276.1392 | 16.87 | 2.207 |

MassHunter Qual 10.0
(End of Report)



2-(4',5-dimethoxy-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3g)

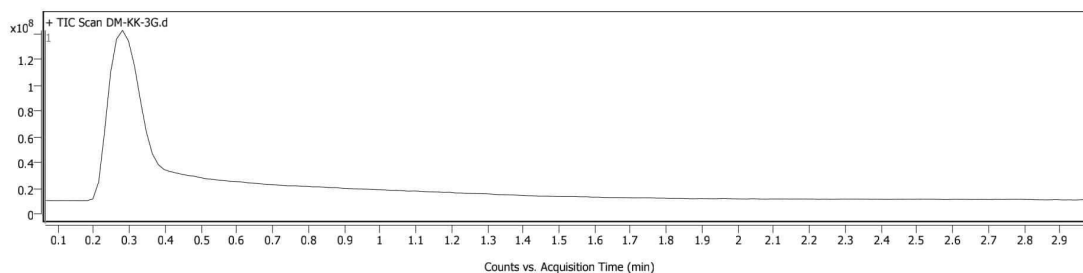
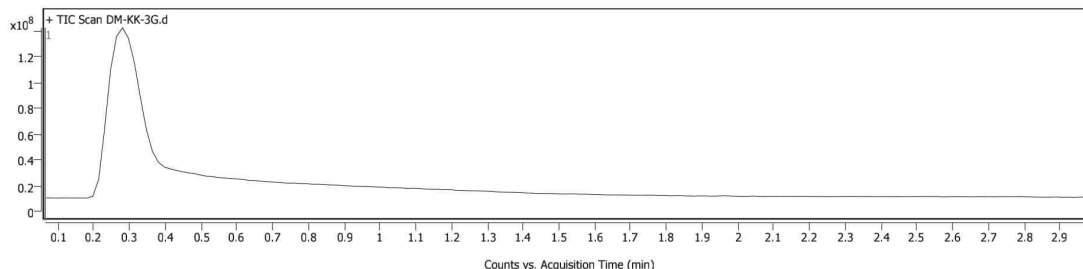
Target Screening Report



Sample Information

| | | | |
|-----------------------|-----------------|---------------------------|---|
| Name | DM-KK-3G | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-3G.d |
| Sample ID | | Acq. Time (Local) | 13-01-2025 16:05:41 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A3 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS_IITB_1.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

Sample Chromatograms



Compound Summary

| Cpd | Name | Formula | CAS | RT | Mass | Mass (Tgt) | Diff (Tgt, ppm) | Score | Algorithm |
|-----|------|--------------|-----|-------|----------|------------|-----------------|-------|-----------|
| 1 | | C19 H17 N O2 | | 0.281 | 291.1269 | 291.1259 | 3.25 | 97.35 | FBF |

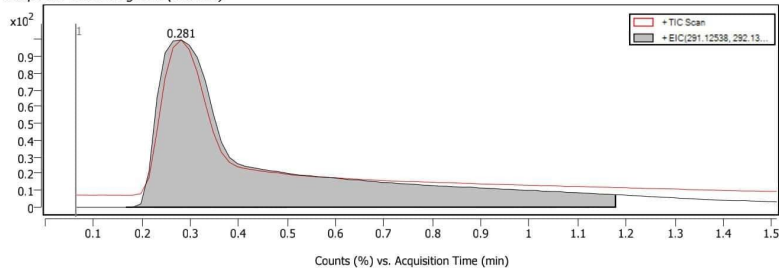
Compound Details

Cpd. 1: C19 H17 N O2

| Name | Formula | RT | RI | Mass | Diff (Tgt, ppm) | CAS | ID Source | Score | Algorithm |
|------|--------------|-------|----|----------|-----------------|-----|-----------|-------|-----------|
| | C19 H17 N O2 | 0.281 | | 291.1269 | 3.25 | | FBF | 97.35 | FBF |

| Species | m/z | Score (Tgt) | Score (Lib) | Score (DB) | Score (MFG) | Score (RT) |
|-----------|-------------------|-------------|-------------|------------|-------------|------------|
| M+ (M+H)+ | 291.1214 292.1343 | 97.35 | | | | |
| (M+Na)+ | 314.1153 | | | | | |

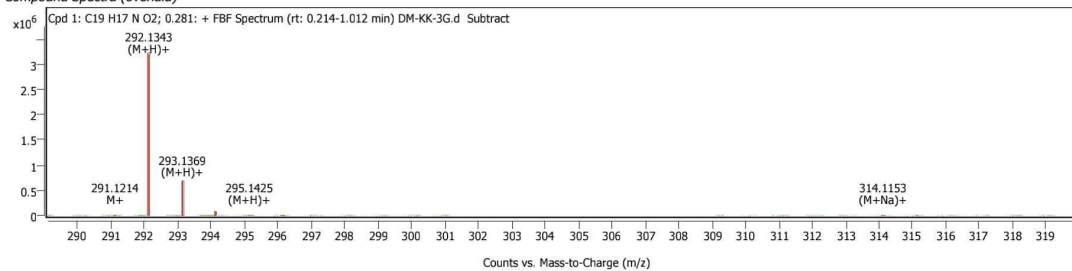
Compound Chromatograms (overlaid)



Structure

Target Screening Report

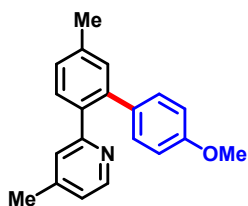
Compound Spectra (overlaid)



Compound ID Table

| Name | Formula | Species | RT | RT Diff | Mass | CAS | ID Source | Score | Score (Lib) | Score (Tgt) |
|------|--------------|----------------------|-------|---------|----------|-----|-----------|-------|-------------|-------------|
| | C19 H17 N O2 | M+ (M+H)+ (M+Na)+ | 0.281 | | 291.1269 | | FBF | 97.35 | | 97.35 |

MassHunter Qual 10.0
(End of Report)



2-(4'-methoxy-5-methyl-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3I)

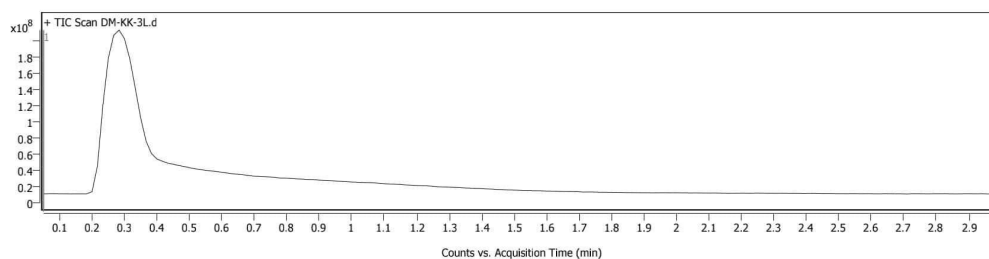
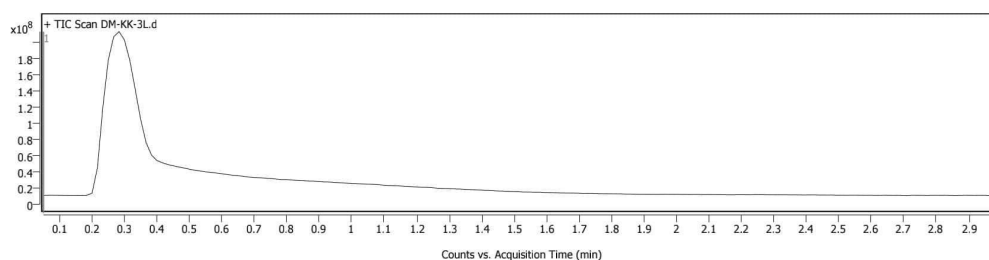
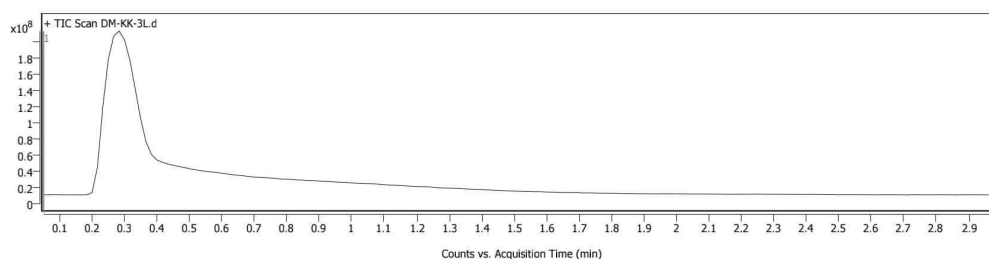
Target Screening Report



Sample Information

| | | | |
|-----------------------|-----------------|---------------------------|--|
| Name | DM-KK-3L | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-3L.d |
| Sample ID | | Acq. Time (Local) | 14-01-2025 09:51:17 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A2 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS_1.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

Sample Chromatograms



Compound Summary

| Cpd | Name | Formula | CAS | RT | Mass | Mass (Tgt) | Diff (Tgt, ppm) | Score | Algorithm |
|-----|------|-------------|-----|-------|----------|------------|-----------------|-------|-----------|
| 1 | | C20 H19 N O | | 0.284 | 289.1471 | 289.1467 | 1.44 | 79.60 | FBF |

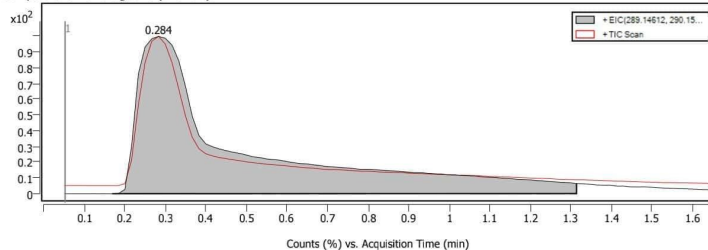
Compound Details

Cpd. 1: C20 H19 N O

| Name | Formula | RT | RI | Mass | Diff (Tgt, ppm) | CAS | ID Source | Score | Algorithm |
|------------------|-------------------|--------------------|--------------------|-------------------|--------------------|-------------------|-----------|-------|-----------|
| | C20 H19 N O | 0.284 | | 289.1471 | 1.44 | | FBF | 79.60 | FBF |
| Species | | | | | | | | | |
| | m/z | Score (Tgt) | Score (Lib) | Score (DB) | Score (MFG) | Score (RT) | | | |
| M+ (M+H)+ | 289.1327 290.1550 | 79.60 | | | | | | | |
| (M+H2O)+ (M+Na)+ | 307.1509 312.1337 | | | | | | | | |
| (M+K)+ | 328.1113 | | | | | | | | |

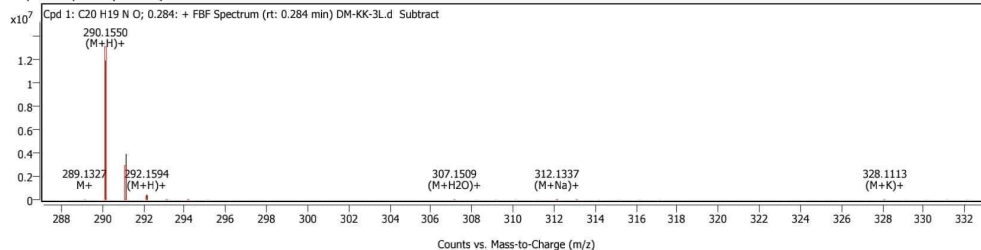
Target Screening Report

Compound Chromatograms (overlaid)



Structure

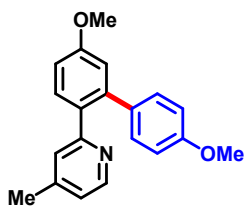
Compound Spectra (overlaid)



Compound ID Table

| Name | Formula | Species | RT | RT Diff | Mass | CAS | ID Source | Score | Score (Lib) | Score (Tgt) |
|------|-------------|--|-------|---------|----------|-----|-----------|-------|-------------|-------------|
| | C20 H19 N O | M+ (M+H)+ (M+H2O)+ (M+Na)+ (M+K)+ | 0.284 | | 289.1471 | | FBF | 79.60 | | 79.60 |

MassHunter Qual 10.0
(End of Report)



2-(4',5-dimethoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3m)

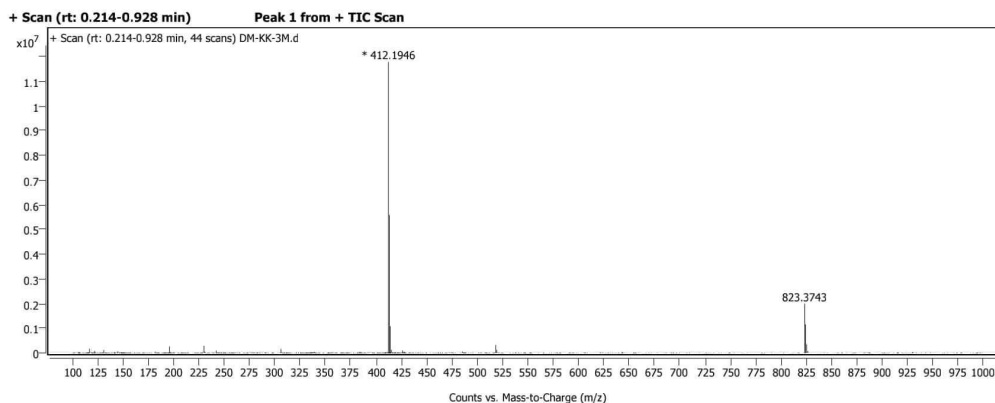
Department of Chemistry I.I.T. (B)



Sample Information

| | | | |
|----------------|-----------------|--------------------|--|
| Name | DM-KK-3M | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-3M.d |
| Sample ID | | Acq. Time (Local) | 01-01-2025 15:22:30 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A3 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

Sample Spectra

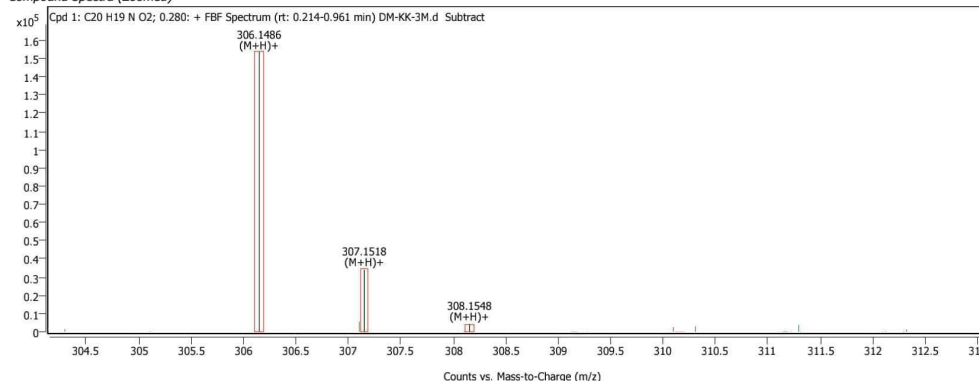


Compound Details

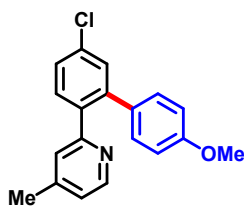
Cpd. 1: C20 H19 N O2

| Formula | m/z | Observed M/Z | Difference Da | Difference PPM | Score |
|--------------|----------|------------------|--------------------|--------------------|-------|
| C20 H19 N O2 | 306.1486 | 306.148642373801 | -0.242616304944931 | -0.795094217749182 | 99.74 |

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)



2-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)-4-methylpyridine (Scheme 2, 3n)

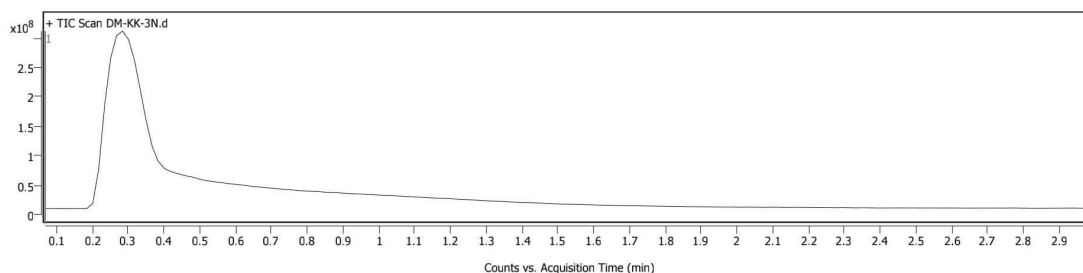
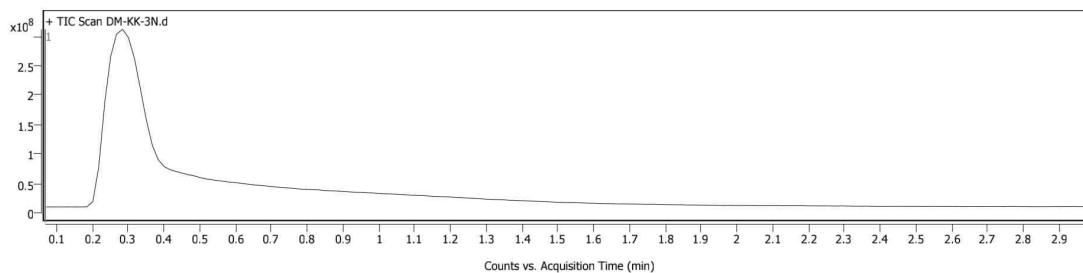
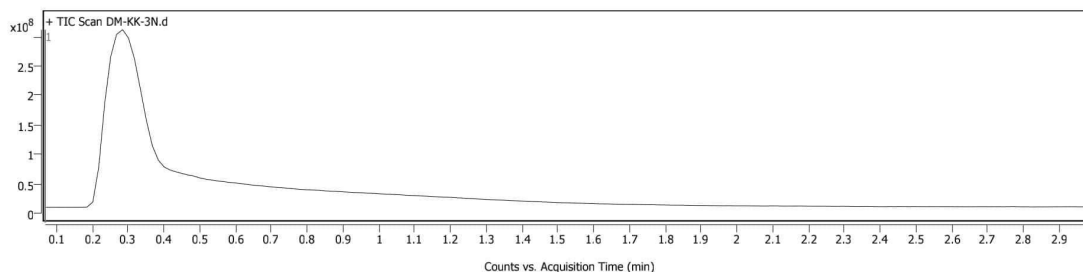
Target Screening Report



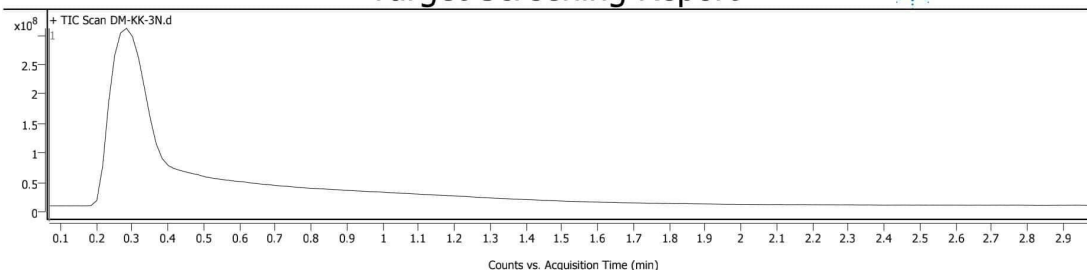
Sample Information

| | | | |
|-----------------------|-----------------|---------------------------|---|
| Name | DM-KK-3N | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-3N.d |
| Sample ID | | Acq. Time (Local) | 13-01-2025 16:09:46 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A4 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS_IITB_1.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

Sample Chromatograms



Target Screening Report



Compound Summary

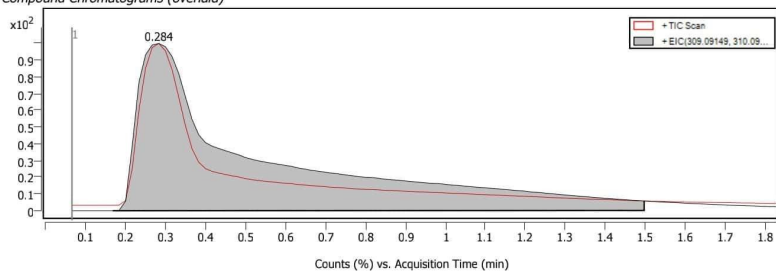
| Cpd | Name | Formula | CAS | RT | Mass | Mass (Tgt) | Diff (Tgt, ppm) | Score | Algorithm |
|-----|------|--|-----|-------|----------|------------|-----------------|-------|-----------|
| 1 | | C ₁₉ H ₁₆ ClN ₂ O | | 0.284 | 309.0934 | 309.0920 | 4.37 | 90.15 | FBF |

Compound Details

Cpd. 1: C₁₉H₁₆ClN₂O

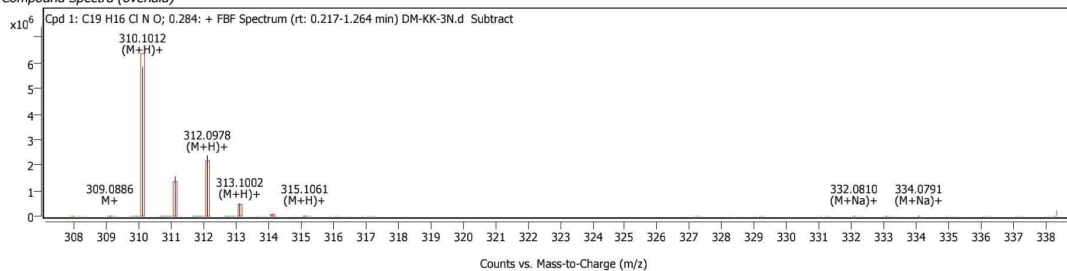
| Name | Formula | RT | RI | Mass Diff (Tgt, ppm) | CAS | ID Source | Score | Algorithm |
|-----------------------|--|-------------|-------------|----------------------|-------------|------------|-------|-----------|
| | C ₁₉ H ₁₆ ClN ₂ O | 0.284 | | 309.0934 | | FBF | 90.15 | FBF |
| | | | | | | | | |
| Species | m/z | Score (Tgt) | Score (Lib) | Score (DB) | Score (MFG) | Score (RT) | | |
| M+ (M+H) ⁺ | 309.0886 | 310.1012 | 90.15 | | | | | |
| (M+Na) ⁺ | 332.0810 | | | | | | | |

Compound Chromatograms (overlaid)



Structure

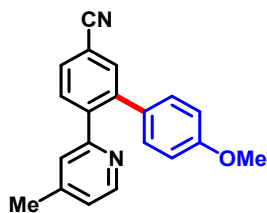
Compound Spectra (overlaid)



Compound ID Table

| Name | Formula | Species | RT | RT Diff | Mass | CAS | ID Source | Score | Score (Lib) | Score (Tgt) |
|------|--|--|-------|---------|----------|-----|-----------|-------|-------------|-------------|
| | C ₁₉ H ₁₆ ClN ₂ O | M+ (M+H) ⁺ (M+Na) ⁺ | 0.284 | | 309.0934 | | FBF | 90.15 | | 90.15 |

MassHunter Qual 10.0
(End of Report)



4'-methoxy-6-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-3-carbonitrile (Scheme 2, 3o)

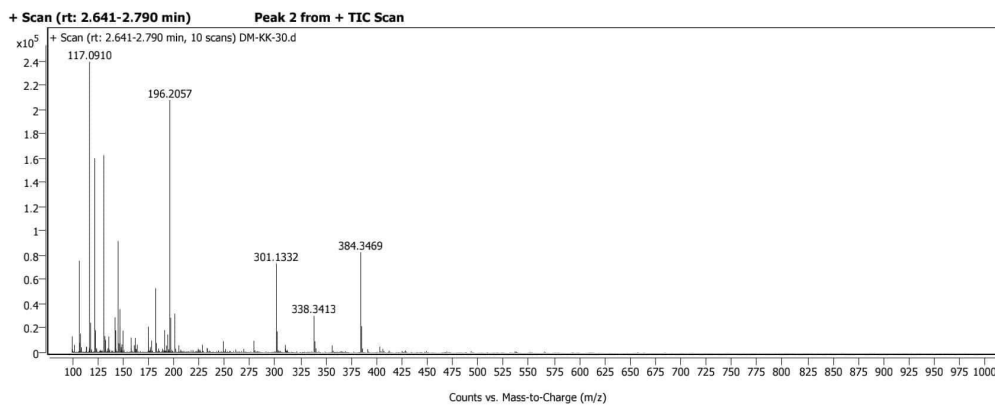
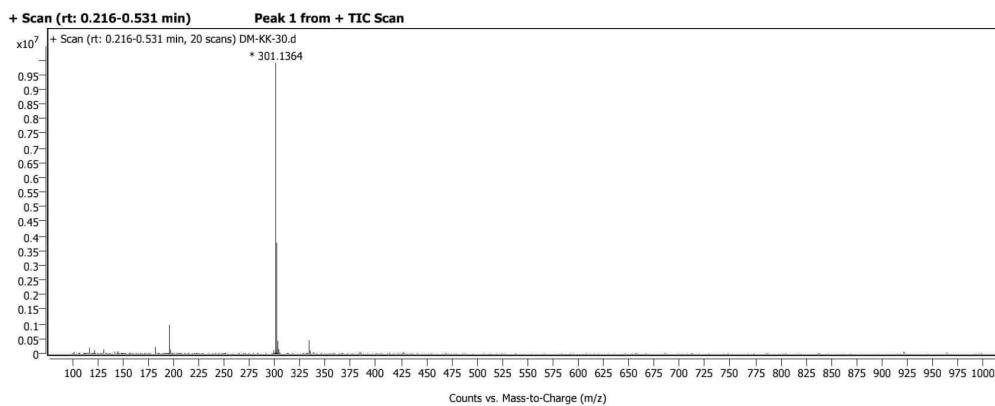
Department of Chemistry I.I.T. (B)



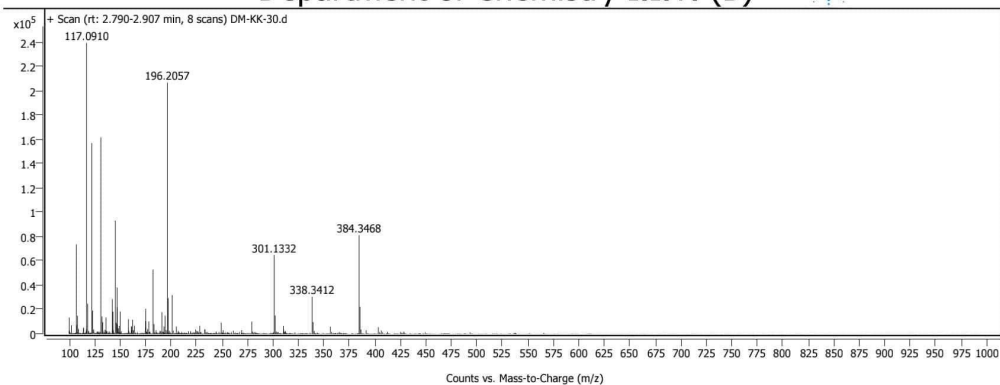
Sample Information

| | | | |
|-----------------------|-----------------|---------------------------|--|
| Name | DM-KK-30 | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-30.d |
| Sample ID | | Acq. Time (Local) | 01-01-2025 15:18:25 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A2 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

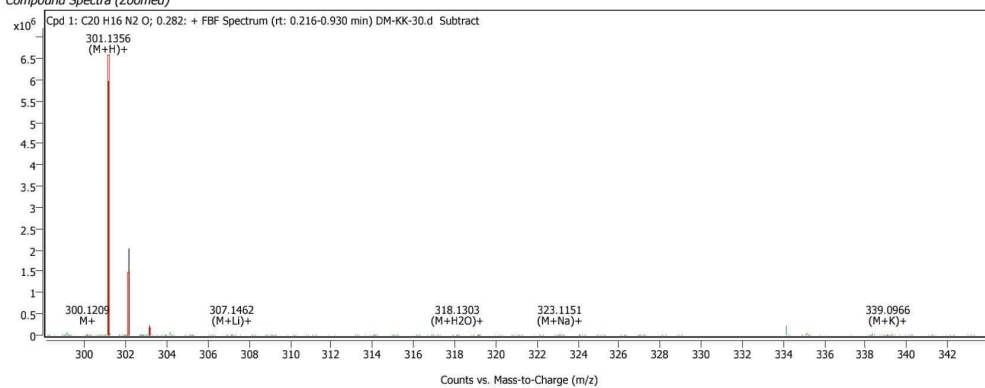
Sample Spectra

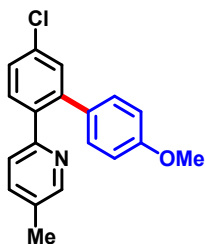


+ Scan (rt: 2.790-2.907 min) Peak 3 from + TIC Scan

**Compound Details**Cpd. 1: C₂₀H₁₆N₂O

| Formula | m/z | Observed M/Z | Difference Da | Difference PPM | Score |
|--|----------|------------------|-----------------|------------------|-------|
| C ₂₀ H ₁₆ N ₂ O | 323.1151 | 323.115108063764 | 1.6224649783112 | 5.40594135713416 | 74.95 |

Compound Spectra (Zoomed)**MassHunter Qual 10.0**
(End of Report)



2-(5-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme

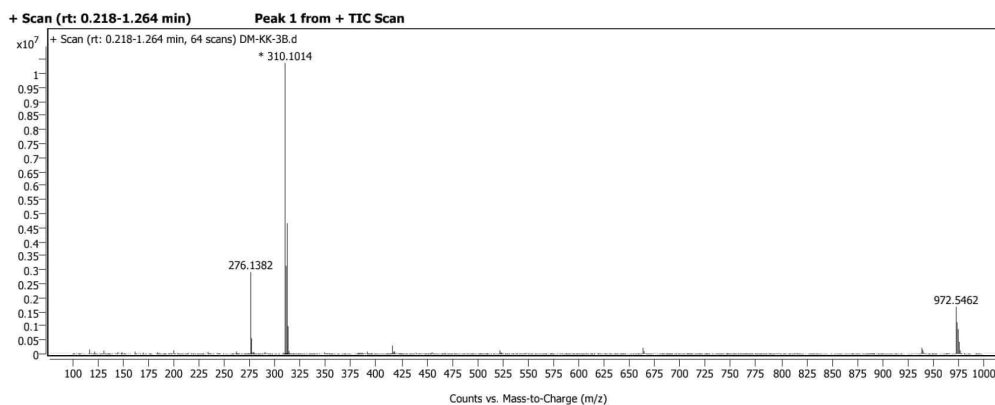
Department of Chemistry I.I.T. (B)



Sample Information

| | | | |
|----------------|-----------------|--------------------|--|
| Name | DM-KK-3B | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-3B.d |
| Sample ID | | Acq. Time (Local) | 01-01-2025 14:50:01 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A3 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

Sample Spectra

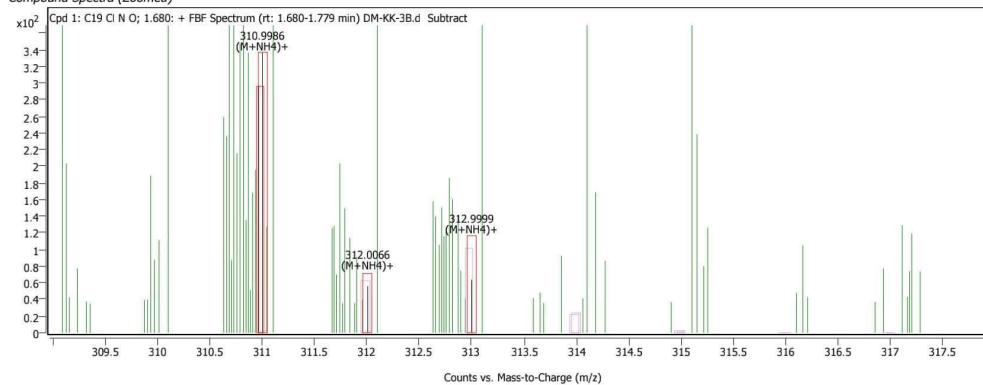


Compound Details

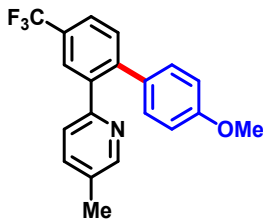
Cpd. 1: C₁₉ClN₂O

| Formula | m/z | Observed M/Z | Difference Da | Difference PPM | Score |
|------------------------------------|----------|------------------|-------------------|-------------------|-------|
| C ₁₉ ClN ₂ O | 310.9986 | 310.998630283371 | -5.49471107427735 | -18.7554026563236 | 62.04 |

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)



2-(4'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)-5-methylpyridine (Scheme 2, 3r)

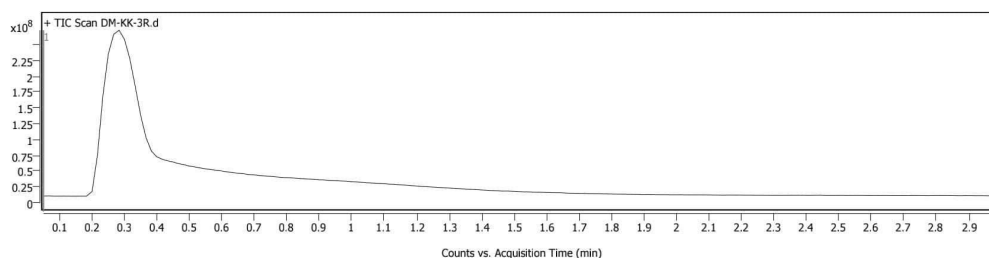
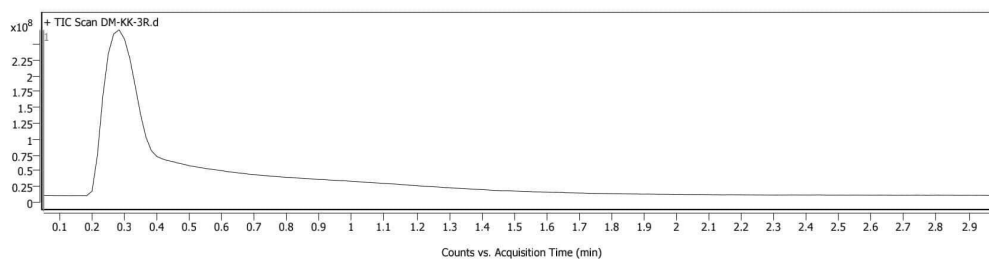
Target Screening Report



Sample Information

| | | | |
|-----------------------|-----------------|---------------------------|--|
| Name | DM-KK-3R | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-3R.d |
| Sample ID | | Acq. Time (Local) | 14-01-2025 09:55:21 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A3 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS_1.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

Sample Chromatograms



Compound Summary

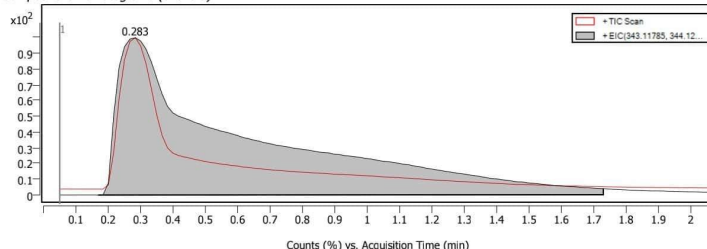
| Cpd | Name | Formula | CAS | RT | Mass | Mass (Tgt) | Diff (Tgt, ppm) | Score | Algorithm |
|-----|------|----------------|-----|-------|----------|------------|-----------------|-------|-----------|
| 1 | | C20 H16 F3 N O | | 0.283 | 343.1231 | 343.1184 | 13.71 | 75.15 | FBF |

Compound Details

Cpd. 1: C20 H16 F3 N O

| Name | Formula | RT | RI | Mass | Diff (Tgt, ppm) | CAS | ID Source | Score | Algorithm |
|----------------|-------------------|-------------|-------------|------------|-----------------|------------|-----------|-------|-----------|
| | C20 H16 F3 N O | 0.283 | | 343.1231 | 13.71 | | FBF | 75.15 | FBF |
| Species | m/z | Score (Tgt) | Score (Lib) | Score (DB) | Score (MFG) | Score (RT) | | | |
| (M+H)+ (M+Na)+ | 344.1308 366.1056 | 75.15 | | | | | | | |

Compound Chromatograms (overlaid)

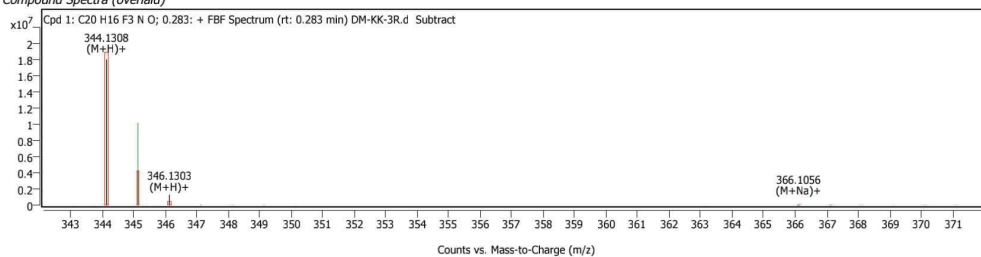


Structure

Target Screening Report



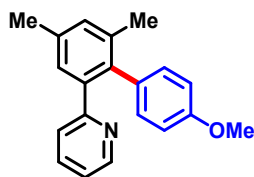
Compound Spectra (overlaid)



Compound ID Table

| Name | Formula | Species | RT | RT Diff | Mass | CAS | ID Source | Score | Score (Lib) | Score (Tgt) |
|------|--|---|-------|---------|----------|-----|-----------|-------|-------------|-------------|
| | C ₂₀ H ₁₆ F ₃ N O | (M+H) ⁺ (M+Na) ⁺ | 0.283 | | 343.1231 | | FBF | 75.15 | | 75.15 |

MassHunter Qual 10.0
(End of Report)



2-(4'-methoxy-4,6-dimethyl-[1,1'-biphenyl]-2-yl)pyridine (Scheme 2, 3s)

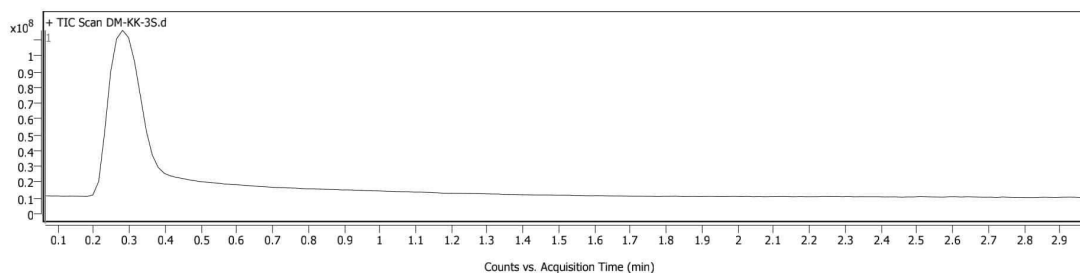
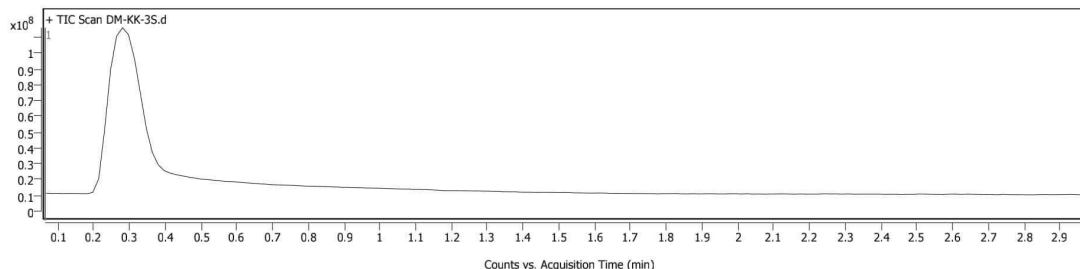
Target Screening Report



Sample Information

| | | | |
|-----------------------|-----------------|---------------------------|---|
| Name | DM-KK-3S | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-3S.d |
| Sample ID | | Acq. Time (Local) | 13-01-2025 16:01:36 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A2 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS_IITB_1.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

Sample Chromatograms



Compound Summary

| Cpd | Name | Formula | CAS | RT | Mass | Mass (Tgt) | Diff (Tgt, ppm) | Score | Algorithm |
|-----|------|-------------|-----|-------|----------|------------|-----------------|-------|-----------|
| 1 | | C20 H19 N O | | 0.281 | 289.1479 | 289.1467 | 4.38 | 93.98 | FBF |

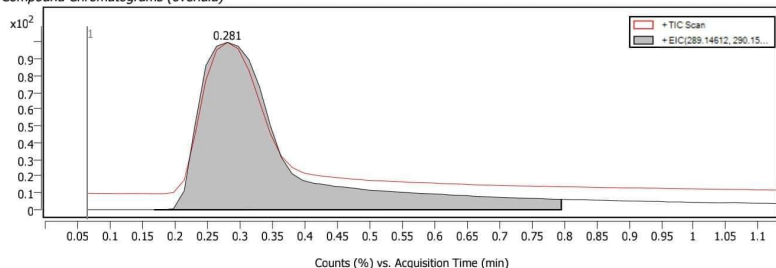
Compound Details

Cpd. 1: C20 H19 N O

| Name | Formula | RT | RI | Mass Diff (Tgt, ppm) | CAS | ID Source | Score | Algorithm |
|------|-------------|-------|----|----------------------|-----|-----------|-------|-----------|
| | C20 H19 N O | 0.281 | | 289.1479 | | FBF | 93.98 | FBF |

| Species | m/z | Score (Tgt) | Score (Lib) | Score (DB) | Score (MFG) | Score (RT) |
|--|-------------------|-------------|-------------|------------|-------------|------------|
| (M+H) ⁺ (M+Na) ⁺ | 290.1554 312.1364 | 93.98 | | | | |

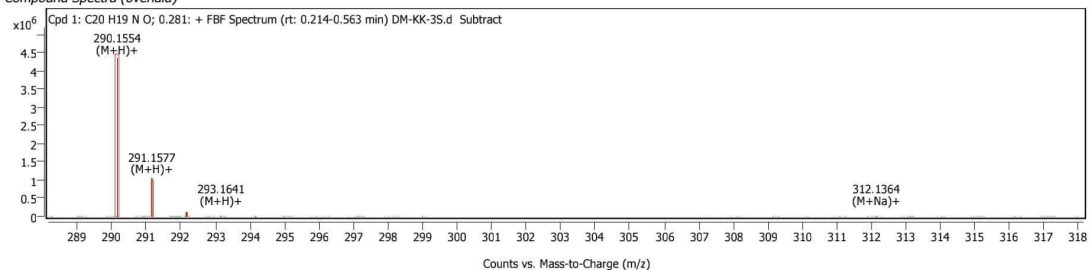
Compound Chromatograms (overlaid)



Structure

Target Screening Report

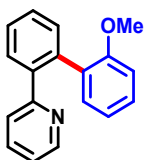
Compound Spectra (overlaid)



Compound ID Table

| Name | Formula | Species | RT | RT Diff | Mass | CAS | ID Source | Score | Score (Lib) | Score (Tgt) |
|------|-------------------------------------|---|-------|---------|----------|-----|-----------|-------|-------------|-------------|
| | C ₂₀ H ₁₉ N O | (M+H) ⁺ (M+Na) ⁺ | 0.281 | | 289.1479 | | FBF | 93.98 | | 93.98 |

MassHunter Qual 10.0
(End of Report)



2-(2'-methoxy-[1,1'-biphenyl]-2-yl)pyridine (M.W.= 261.32 g/mol) (Scheme 3, 4b)

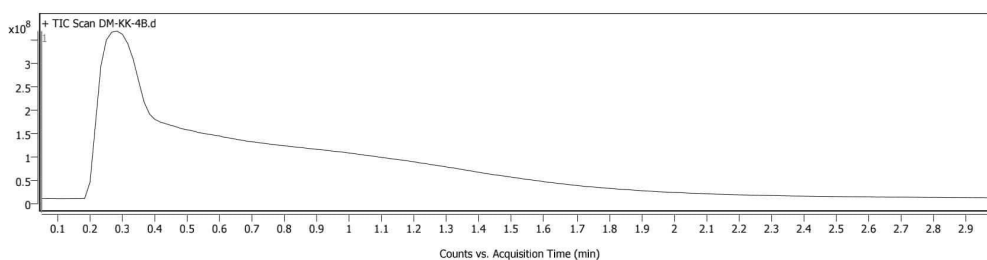
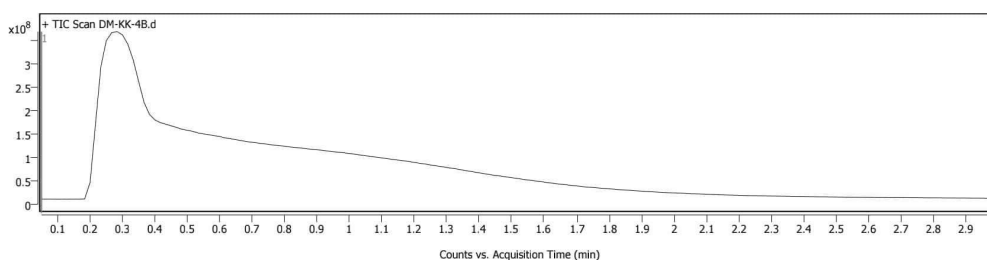
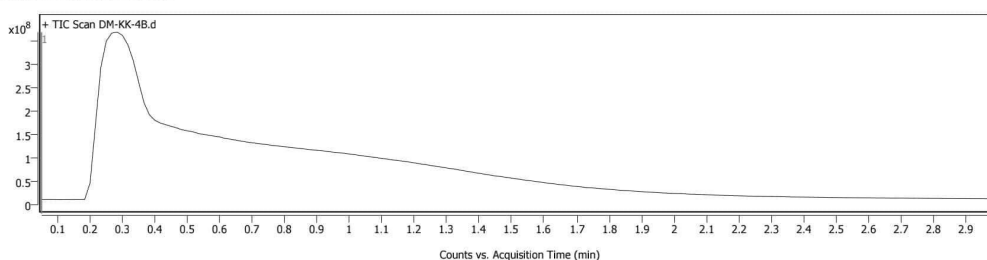
Target Screening Report



Sample Information

| | | | |
|-----------------------|-----------------|---------------------------|--|
| Name | DM-KK-4B | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-4B.d |
| Sample ID | | Acq. Time (Local) | 14-01-2025 09:59:25 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A4 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS_1.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 0 qualified (1 targets) |

Sample Chromatograms



Compound Summary

| Cpd | Name | Formula | CAS | RT | Mass | Mass (Tgt) | Diff (Tgt, ppm) | Score | Algorithm |
|-----|------|---------|-----|----|------|------------|-----------------|-------|---------------------|
| 1 | | | | | | | | | Spectrum Extraction |

Compound Details

| Compound 1 | Name | Formula | RT | RI | Mass | Diff (Tgt, ppm) | CAS | ID Source | Score | Algorithm |
|------------|------|---------|----|----|------|-----------------|-----|-----------|-------|---------------------|
| | | | | | | | | | | Spectrum Extraction |

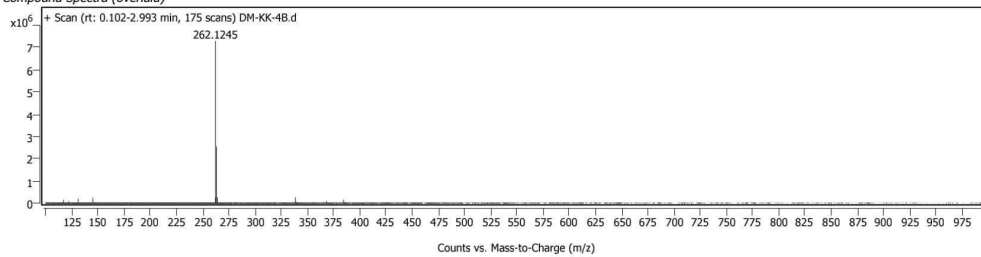
Compound Chromatograms (overlaid)

Structure

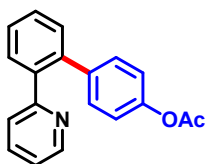
Target Screening Report



Compound Spectra (overlaid)



MassHunter Qual 10.0
(End of Report)



2'-(pyridin-2-yl)-[1,1'-biphenyl]-4-yl acetate (Scheme 3, 4d)

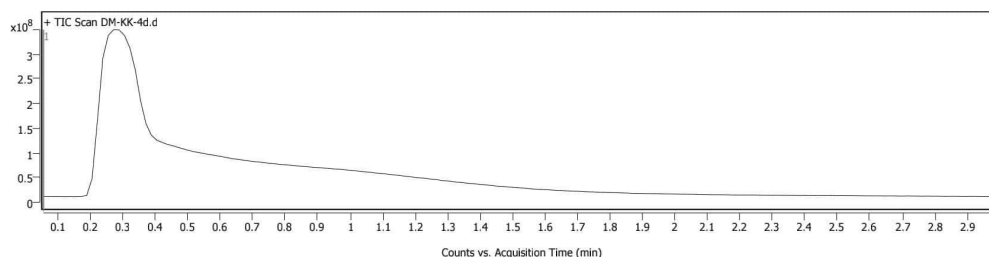
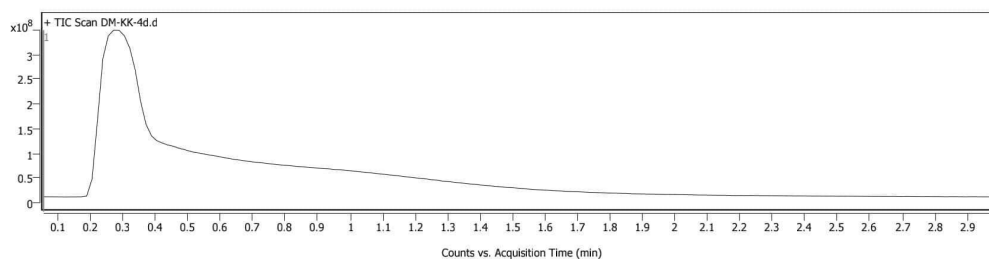
Target Screening Report



Sample Information

| | | | |
|-----------------------|-----------------|---------------------------|--|
| Name | DM-KK-4d | Data File Path | D:\Projects\MASS Data\Data\JAN 2025\DM-KK-4d.d |
| Sample ID | | Acq. Time (Local) | 14-01-2025 10:03:26 (UTC+05:30) |
| Instrument | LCMSQTOF-G6545B | Method Path (Acq) | D:\Projects\MASS Data\Methods\A1B1_POS_100-1000_4000_500_120.m |
| MS Type | QTOF | Version (Acq SW) | 6200 series TOF/6500 series Q-TOF (11.0.203.0) |
| Inj. Vol. (ul) | 2 | IRM Status | Success |
| Position | P2A5 | Method Path (DA) | C:\Users\LCMS QTOF G6545\Desktop\Report Templates\REPORT METHOD\HRMS_1.m |
| Plate Pos. | | Target Source Path | |
| Operator | SYSTEM (SYSTEM) | Result Summary | 1 qualified (1 targets) |

Sample Chromatograms



Compound Summary

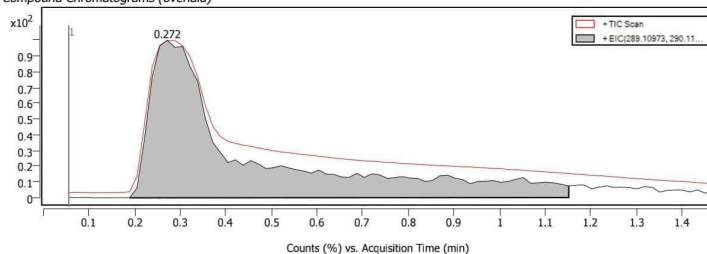
| Cpd | Name | Formula | CAS | RT | Mass | Mass (Tgt) | Diff (Tgt, ppm) | Score | Algorithm |
|-----|------|--------------|-----|-------|----------|------------|-----------------|-------|-----------|
| 1 | | C19 H15 N O2 | | 0.272 | 289.1080 | 289.1103 | -8.01 | 75.69 | FBF |

Compound Details

Cpd. 1: C19 H15 N O2

| Name | Formula | RT | RI | Mass | Diff (Tgt, ppm) | CAS | ID Source | Score | Algorithm |
|----------------|--------------|-------------------|-------------|-------------|-----------------|-------------|------------|-------|-----------|
| | C19 H15 N O2 | 0.272 | | 289.1080 | -8.01 | | FBF | 75.69 | FBF |
| Species | | m/z | Score (Tgt) | Score (Lib) | Score (DB) | Score (MFG) | Score (RT) | | |
| (M+H)+ (M+Na)+ | | 290.1157 312.0901 | 75.69 | | | | | | |

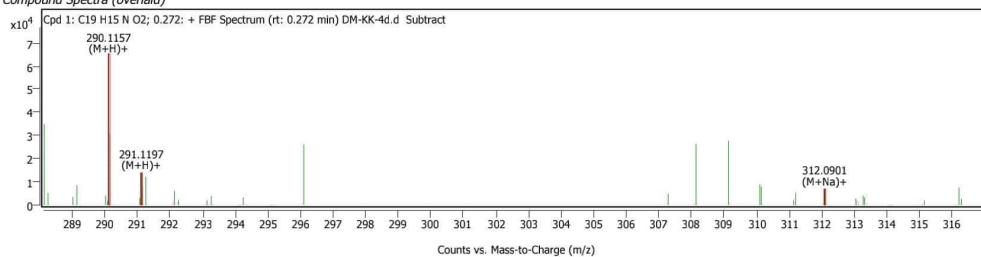
Compound Chromatograms (overlaid)



Structure

Target Screening Report

Compound Spectra (overlaid)



Compound ID Table

| Name | Formula | Species | RT | RT Diff | Mass | CAS | ID Source | Score | Score (Lib) | Score (Tgt) |
|------|--|-------------------|-------|---------|----------|-----|-----------|-------|-------------|-------------|
| | C ₁₉ H ₁₅ N O ₂ | (M+H)+ (M+Na)+ | 0.272 | | 289.1080 | | FBF | 75.69 | | 75.69 |

MassHunter Qual 10.0
(End of Report)