

Pd-catalyzed dehydrogenative annulation approach for the efficient synthesis of phenanthridinones

(Electronic Supplementary Information)

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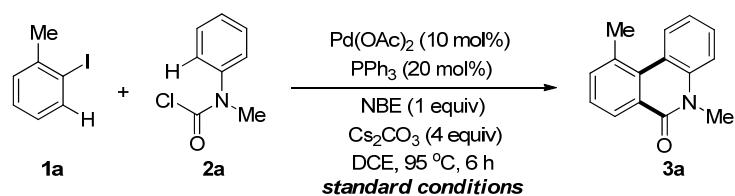
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General remarks

All manipulations were conducted with schlenk tubes. ¹H-NMR spectra were recorded on Bruker AVANCE III-400 spectrometers. Chemical shifts (in ppm) were calibrated with CDCl₃ or DMSO-d₆ (tetramethylsilane, δ = 0 ppm). ¹³C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with CDCl₃ (δ = 77.00 ppm) or DMSO-d₆ (δ = 39.50 ppm). NMR yields were determined using standard curves with 1,1,2,2-tetrachloroethane as internal standard. EI-MS data was obtained from Agilent 7890A-5975C GCMS system. High Resolution Mass spectra were recorded using a Fourier Transform Ion Cyclotron Resonance Mass spectrometer (APEX IV, Bruker). Unless otherwise noted, materials obtained from commercial suppliers were used without further purification.

Optimization of reaction conditions

Table S1: Control experiments for acylation and annulation.^[a]



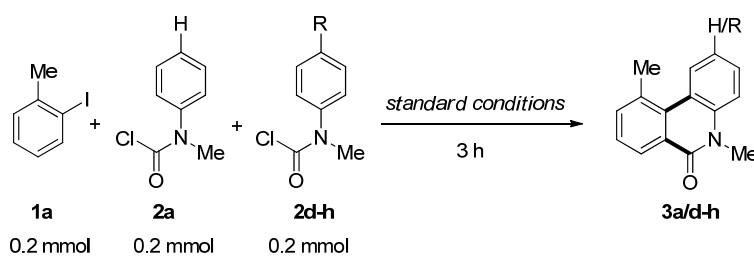
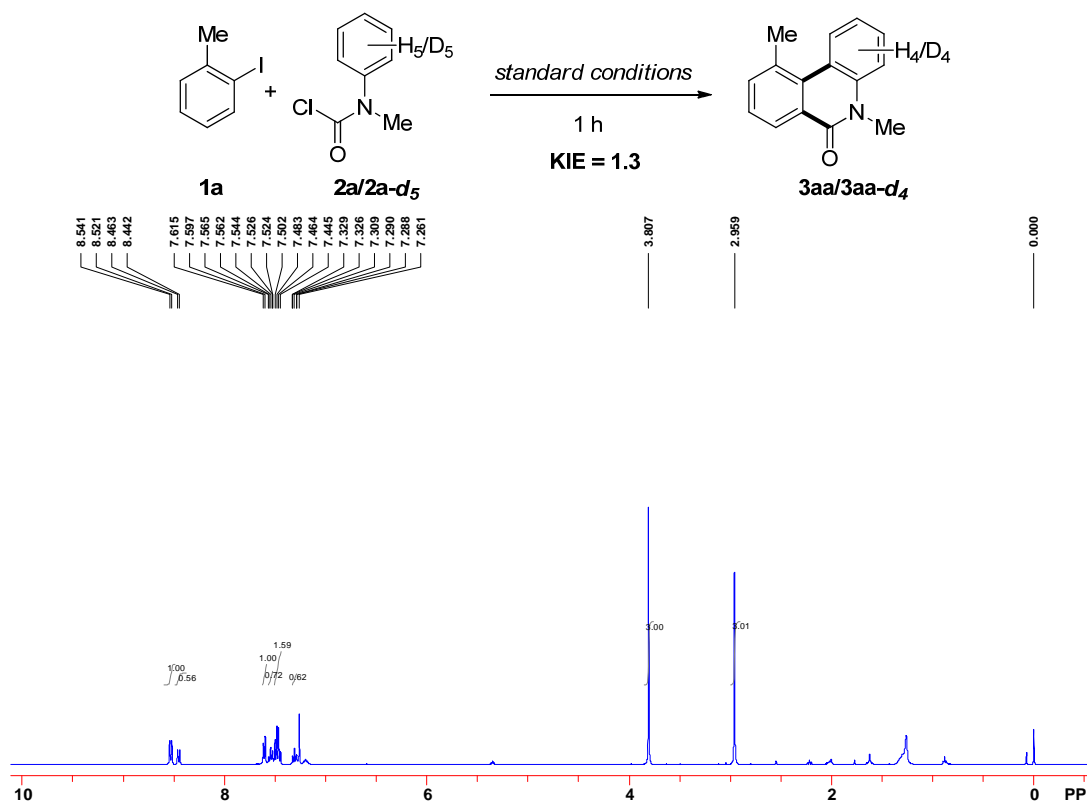
Entry	Change from the standard conditions	Yield [%] ^[b]
1	none	99 (98) ^c
2	no Pd(OAc) ₂	0
3	no PPh ₃	0
4	no NBE	0
5	no Cs ₂ CO ₃	0
6	PdCl ₂ instead of Pd(OAc) ₂	54
7	TFP instead of PPh ₃	83
8	K ₂ CO ₃ instead of Cs ₂ CO ₃	31
9	dioxane instead of DCE	5
10	MeCN instead of DCE	12
11	toluene instead of DCE	96
12	80°C	45

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), Pd catalyst (0.02 mmol), ligand (0.04 mmol), NBE (0.2 mmol), and base (0.8 mmol) in solvent (2 mL) at 95 °C for 6 h. [b] Determined by ¹H NMR of crude product using internal standard. [c] Isolated yield.

Initially, we endeavoured to realize Pd-catalyzed dehydrogenative acylation and annulation reaction using iodobenzenes and anilines with norbornene under CO, however, only the ipso position of iodobenzenes was carbonylated, providing linear amides without cyclization. We hypothesized that properly pre-functionalized carbonyl anilines may inhibit the carbonylation at ipso position in order to preclude the byproducts. As our expected, when 1-iodo-2-methylbenzene (**1a**) was reacted with methyl(phenyl)carbamic chloride (**2a**), the intermolecular acylation and

annulation was carried out, successfully affording phenanthridinone **3a** (Table S1). The desired product **3a** could be obtained up to 99% yield when using Pd(OAc)₂/PPh₃ as the metal/ligand combination, NBE, and Cs₂CO₃ as the base in DCE at 95 °C (entry 1). A series of control experiments indicated that the palladium, phosphine ligand, NBE, and base were all essential for this transformation (entries 2–5). PdCl₂ catalyst diminished the yield indicating that acetate anion is more helpful to the C–H activation (entry 6). In contrast, when more-electron-deficient tri(2-furyl)phosphine ligand was tested, the yield was inferior slightly (entry 7). When using potassium carbonate as a base, the yield was dramatically decreased (entry 8). Among the solvents tested, the polar solvents such as dioxane and MeCN suppressed this reaction (entries 9–10), while non-polar solvents such as DCE and toluene showed the optimal conditions (entries 1 and 11). Finally, the reaction could still proceed even at 80 °C albeit giving lower yield (entry 12).

Preliminary mechanistic studies



3a(H) : 3d-h(Me, F, Cl, OCF₃, CN)

3a:3d	3a:3e	3a:3f	3a:3g	3a:3h
1:1.12	1:0.90	1:0.78	1:0.68	1:0.47

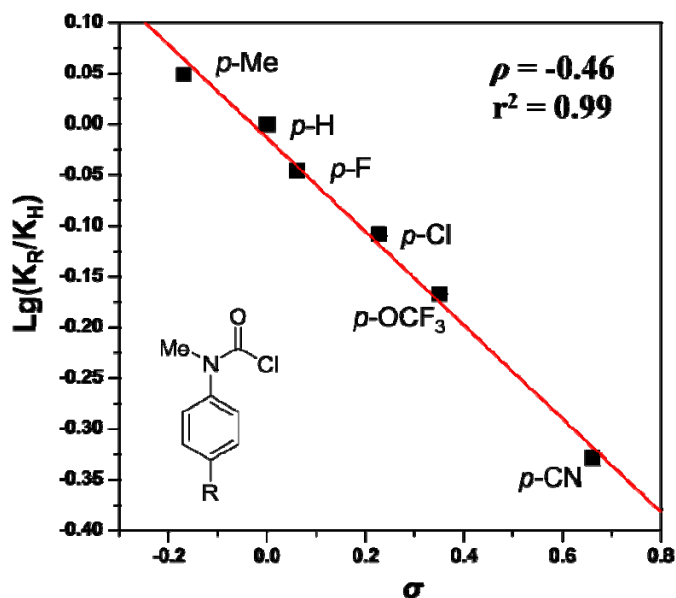


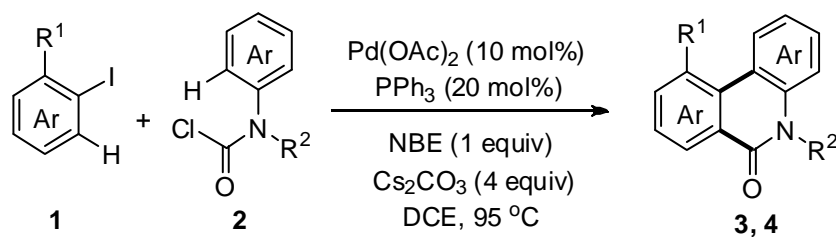
Fig. S1. Hammett plot of the acylation and annulation of substituted aryl carbamic chlorides **2**

Experimental procedure and characterization data

Preparation of aryl iodides **1** and aryl carbamic chlorides **2**

Aryl iodides **1a-g** and **1i-l** were purchased from commercial sources. **1h** was prepared according to literature methods.¹ For the preparation of **1m**, see the reference.² Aryl carbamic chlorides **2** were prepared following the known procedures.³

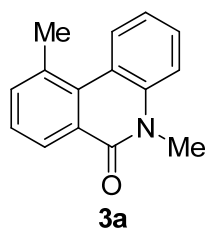
Typical procedure for Pd-catalyzed acylation and annulation of aryl iodides and aryl carbamic chlorides:



Aryl iodides **1** (0.2 mmol), aryl carbamic chlorides **2** (0.4 mmol), Pd(OAc)₂ (0.02 mmol), PPh₃ (0.04 mmol), NBE (0.2 mmol), Cs₂CO₃ (0.8 mmol), and DCE (2 mL) were added to a 20 mL Schlenk flask with a magnetic stir bar and the mixture was heated at 95 °C. Monitor the reaction by TLC to confirm whether the aryl iodides disappeared. After cooling to room temperature, the reaction mixture was diluted with AcOEt (5.0 mL) and the solution was concentrated under vacuum. Finally, the mixture was purified through column chromatography to afford the pure product.

Phenanthridinones

5,10-dimethylphenanthridin-6(5H)-one (**3a**)⁴



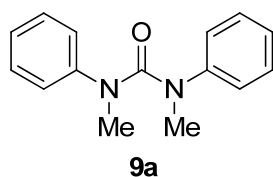
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 12/1), affords 43.8 mg (98%) of **3a** as white solid, along with 16.7 mg (0.07 mmol) of byproduct **9a** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.49 (d, *J* = 7.6 Hz, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 7.54 (d, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.24 (d, *J* = 7.6 Hz, 1H), 3.75 (s, 3H), 2.88 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.8, 138.1, 136.7(2C), 134.3, 132.8, 128.5, 127.7, 127.2, 127.1, 121.4, 120.6, 114.6, 30.2, 25.9.

EI-MS: *m/z* 223.1.

1,3-dimethyl-1,3-diphenylurea (**9a**)⁵

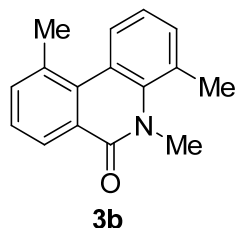


¹H NMR (400 MHz, CDCl₃): δ 7.04 (t, *J* = 7.6 Hz, 4H), 6.92 (t, *J* = 7.2 Hz, 2H), 6.77-6.80 (m, 4H), 3.19 (s, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 161.2, 145.5, 128.5, 125.6, 124.7, 39.2.

EI-MS: *m/z* 240.1.

4,5,10-trimethylphenanthridin-6(5*H*)-one (**3b**)



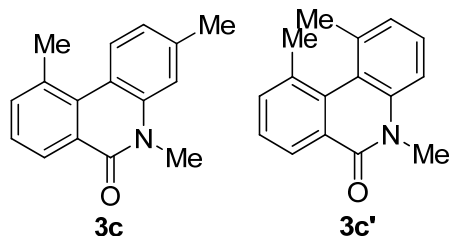
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), methyl(*o*-tolyl)carbamic chloride (**2b**) (73.5 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 12/1), affords 45.6 mg (96%) of **3b** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.41 (dd, *J* = 7.6, 0.8 Hz, 1H), 8.19 (d, *J* = 7.6 Hz, 1H), 7.57 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.29 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.19 (t, *J* = 8.0 Hz, 1H), 3.74 (s, 3H), 2.91 (s, 3H), 2.64 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.7, 139.3, 136.7, 134.1, 133.8, 132.9, 127.6, 127.1, 126.7, 126.4, 125.3, 123.2, 122.2, 38.9, 25.5, 23.4.

HRMS *m/z* (ESI) calcd for C₁₆H₁₆NO [M+H]⁺ 238.1226, found: 238.1230; calcd for C₁₆H₁₅NNaO [M+Na]⁺ 260.1046, found: 260.1049.

3,5,10-trimethylphenanthridin-6(5*H*)-one (**3c**) and 1,5,10-trimethylphenanthridin-6(5*H*)-one (**3c'**)



The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), methyl(*m*-tolyl)carbamic chloride (**2c**) (73.5 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 43.2 mg (91%) of **3c** and 3.6 mg (8%) of **3c'** as white solids.

3c:

¹H NMR (400 MHz, CDCl₃): δ 8.48 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.24 (d, *J* = 8.4 Hz, 1H), 7.52 (dd, *J* = 7.2, 0.4 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.17 (s, 1H), 7.05 (dd, *J* = 8.0, 1.2 Hz, 1H), 3.74 (s, 3H), 2.87 (s, 3H), 2.47 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.0, 138.8, 138.2, 136.6, 134.0, 132.9, 127.5, 127.1, 126.8, 126.6, 122.5, 118.2, 115.1, 30.2, 25.9, 21.6.

HRMS *m/z* (ESI) calcd for C₁₆H₁₆NO [M+H]⁺ 238.1226, found: 238.1230.

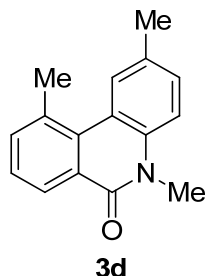
3c':

¹H NMR (400 MHz, CDCl₃): δ 8.31 (d, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 6.8 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.14 (d, *J* = 7.2 Hz, 1H), 3.67 (s, 3H), 2.45 (s, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 162.4, 138.5, 136.5, 135.2, 134.1, 133.6, 128.7, 128.0, 127.0, 125.3, 124.9, 119.7, 110.9, 30.4, 22.1, 21.7.

HRMS *m/z* (ESI) calcd for C₁₆H₁₆NO [M+H]⁺ 238.1226, found: 238.1229.

2,5,10-trimethylphenanthridin-6(5*H*)-one (**3d**)



The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), methyl(*p*-tolyl)carbamic chloride (**2d**) (73.5 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 15/1), affords 46.5 mg

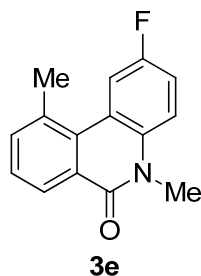
(98%) of **3d** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.52 (d, *J* = 8.0 Hz, 1H), 8.25 (s, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.35 (s, 2H), 3.78 (s, 3H), 2.96 (s, 3H), 2.49 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.8, 136.6, 136.0, 134.3, 132.9, 130.7, 129.4, 128.0, 127.3, 127.2, 127.0, 120.6, 114.5, 30.3, 26.0, 21.2.

HRMS *m/z* (ESI) calcd for C₁₆H₁₆NO [M+H]⁺ 238.1226, found: 238.1230; calcd for C₁₆H₁₅NNaO [M+Na]⁺ 260.1046, found: 260.1049.

2-fluoro-5,10-dimethylphenanthridin-6(5*H*)-one (**3e**)



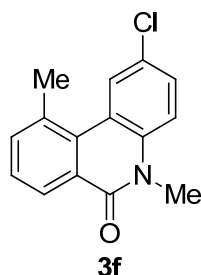
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), (4-fluorophenyl)(methyl)carbamic chloride (**2e**) (75.0 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 7/1), affords 44.8 mg (93%) of **3e** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.48 (d, *J* = 7.6 Hz, 1H), 8.08 (d, *J* = 7.2 Hz, 1H), 7.56 (d, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.33 (dd, *J* = 8.8, 5.2 Hz, 1H), 7.21 (t, *J* = 7.8 Hz, 1H), 3.74 (s, 3H), 2.88 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.4, 157.5 (d, *J* = 237.1 Hz), 136.9, 134.8, 134.5, 131.9, 127.8, 127.5, 121.9 (d, *J* = 8.2 Hz), 115.8 (d, *J* = 8.9 Hz), 115.5 (d, *J* = 23.0 Hz), 114.1, 113.8, 30.5, 25.7.

HRMS *m/z* (ESI) calcd for C₁₅H₁₃FNO [M+H]⁺ 242.0976, found: 242.0973.

2-chloro-5,10-dimethylphenanthridin-6(5*H*)-one (**3f**)



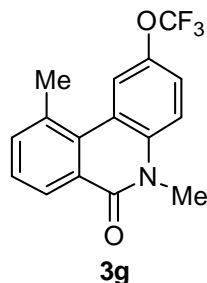
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), (4-chlorophenyl)(methyl)carbamic chloride (**2f**) (81.6 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 47.9 mg (93%) of **3f** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.46 (d, *J* = 7.6 Hz, 1H), 8.31 (s, 1H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.43 (dd, *J* = 9.2, 1.6 Hz, 1H), 7.30 (d, *J* = 8.8 Hz, 1H), 3.73 (s, 3H), 2.87 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.5, 137.0, 136.7, 134.5, 131.7, 128.3, 127.8, 127.4, 127.33, 127.26, 127.0, 121.9, 115.9, 30.4, 25.8.

HRMS *m/z* (ESI) calcd for C₁₅H₁₃ClNO [M+H]⁺ 258.0680, found: 258.0683.

5,10-dimethyl-2-(trifluoromethoxy)phenanthridin-6(5*H*)-one (**3g**)



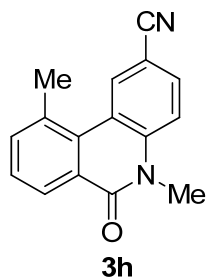
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), methyl(4-(trifluoromethoxy)phenyl)carbamic chloride (**2g**) (101.5 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 51.6 mg (84%) of **3g** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.48 (dd, *J* = 7.6, 0.8 Hz, 1H), 8.28 (s, 1H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.37 (dd, *J* = 9.2, 1.6 Hz, 1H), 3.76 (s, 3H), 2.89 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.6, 143.3 (d, *J* = 2.6 Hz), 137.1, 136.8, 134.5, 131.8, 128.0, 127.5, 127.4, 121.6, 121.2, 120.7 (q, *J* = 255.4 Hz), 120.4, 115.7, 30.5, 25.6.

HRMS *m/z* (ESI) calcd for C₁₆H₁₃F₃NO₂ [M+H]⁺ 308.0893, found: 308.0895.

5,10-dimethyl-6-oxo-5,6-dihydrophenanthridine-2-carbonitrile (**3h**)



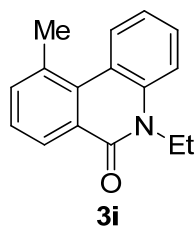
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), (4-cyanophenyl)(methyl)carbamic chloride (**2h**) (77.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 12 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 4/1), affords 14.8 mg (30%) of **3h** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.65 (s, 1H), 8.47 (d, *J* = 7.6 Hz, 1H), 7.77 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 8.4 Hz, 1H), 3.78 (s, 3H), 2.92 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.7, 141.2, 137.5, 134.6, 131.8, 131.6, 131.2, 128.5, 127.5, 127.3, 121.2, 119.0, 115.5, 105.0, 30.6, 25.7.

HRMS *m/z* (ESI) calcd for C₁₆H₁₃N₂O [M+H]⁺ 249.1022, found: 249.1020.

5-ethyl-10-methylphenanthridin-6(5H)-one (**3i**)



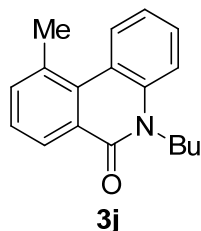
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), ethyl(phenyl)carbamic chloride (**2i**) (73.5 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 20/1), affords 46.6 mg (98%) of **3i** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.52 (d, *J* = 7.6 Hz, 1H), 8.43 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.52 (td, *J* = 7.8, 1.2 Hz, 1H), 7.44-7.48 (m, 2H), 7.27 (td, *J* = 7.6, 1.2 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 2.92 (s, 3H), 1.43 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.4, 137.1, 136.8, 134.3, 133.0, 128.6, 128.0, 127.3, 127.1, 121.3, 121.0, 114.6, 38.0, 26.0, 12.6.

HRMS *m/z* (ESI) calcd for C₁₆H₁₆NO [M+H]⁺ 238.1226, found: 238.1229.

5-butyl-10-methylphenanthridin-6(5H)-one (**3j**)



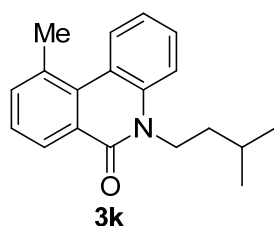
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), butyl(phenyl)carbamic chloride (**2j**) (84.7 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 40/1), affords 49.4 mg (93%) of **3j** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.53 (dd, *J* = 7.8, 1.0 Hz, 1H), 8.45 (d, *J* = 8.0 Hz, 1H), 7.59 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.53 (ddd, *J* = 8.4, 7.6, 1.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.44 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.28 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 4.38 (t, *J* = 8.0 Hz, 2H), 2.94 (s, 3H), 1.81 (tt, *J* = 7.6, 7.6 Hz, 2H), 1.52 (tq, *J* = 7.6, 7.6 Hz, 2H), 1.02 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.7, 137.4, 136.9, 134.4, 133.1, 128.7, 128.1, 127.4, 127.32, 127.26, 121.4, 121.1, 114.9, 42.9, 29.4, 26.1, 20.4, 13.9.

HRMS *m/z* (ESI) calcd for C₁₈H₂₀NO [M+H]⁺ 266.1539, found: 266.1542.

5-isopentyl-10-methylphenanthridin-6(5H)-one (**3k**)



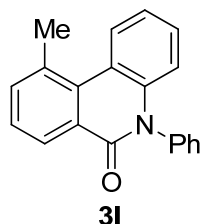
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), isopentyl(phenyl)carbamic chloride (**2k**) (90.3 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 40/1), affords 54.2 mg (97%) of **3k** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.52 (dd, *J* = 7.8, 1.0 Hz, 1H), 8.45 (d, *J* = 7.6 Hz, 1H), 7.59 (dd, *J* = 7.4, 0.6 Hz, 1H), 7.53 (ddd, *J* = 8.4, 7.6, 1.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.44 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.28 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 4.40 (t, *J* = 8.0 Hz, 2H), 2.95 (s, 3H), 1.83 (heptet, *J* = 6.6 Hz, 1H), 1.71 (dt, *J* = 9.2, 7.2 Hz, 2H), 1.06 (d, *J* = 6.4 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃): δ 161.5, 137.3, 136.7, 134.2, 133.0, 128.6, 128.0, 127.3, 127.1 (2C), 121.2, 121.0, 114.7, 41.6, 35.8, 26.6, 26.0, 22.5 (2C).

HRMS *m/z* (ESI) calcd for C₁₉H₂₂NO [M+H]⁺ 280.1696, found: 280.1702; calcd for C₁₉H₂₁NNaO [M+Na]⁺ 302.1515, found: 302.1522.

10-methyl-5-phenylphenanthridin-6(5H)-one (**3l**)



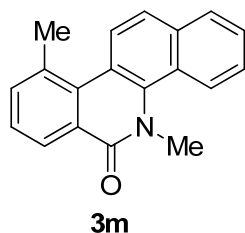
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), diphenylcarbonyl chloride (**2l**) (92.7 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 54.2 mg (95%) of **3l** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.53 (d, *J* = 8.0 Hz, 1H), 8.45 (dd, *J* = 7.8, 0.8 Hz, 1H), 7.58-7.64 (m, 3H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 2H), 7.26 (tt, *J* = 5.2, 5.2 Hz, 2H), 6.73 (dd, *J* = 7.2, 1.6 Hz, 1H), 2.98 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.8, 139.3, 138.4, 137.2, 134.5, 133.3, 130.1, 129.0, 128.6, 128.1, 127.54, 127.46, 127.36, 127.35, 121.7, 120.5, 116.8, 26.0.

HRMS *m/z* (ESI) calcd for C₂₀H₁₆NO [M+H]⁺ 286.1226, found: 286.1232.

5,10-dimethylbenzo[*c*]phenanthridin-6(5H)-one (**3m**)



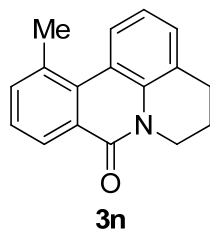
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), methyl(naphthalen-1-yl)carbamic chloride (**2m**) (87.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 20/1), affords 36.0 mg (66%) of **3m** as white solid. The reaction in toluene (2 mL) affords 39.2 mg (72%) of **3m**.

¹H NMR (400 MHz, CDCl₃): δ 8.50 (d, *J* = 7.6 Hz, 1H), 8.38 (d, *J* = 8.8 Hz, 1H), 8.26 (d, *J* = 8.4 Hz, 1H), 7.86 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.45-7.53 (m, 3H), 3.98 (s, 3H), 2.94 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.7, 137.0, 136.8, 134.2, 133.8, 133.5, 127.9, 127.3, 127.0, 126.9, 126.4, 125.5, 124.5, 124.3, 124.0, 122.2, 118.8, 41.2, 25.8.

HRMS *m/z* (ESI) calcd for C₁₉H₁₆NO [M+H]⁺ 274.1226, found: 274.1229.

12-methyl-5,6-dihydro-4H-phenanthridin-8(4H)-one (**3n**)



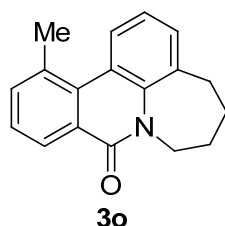
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), 3,4-dihydroquinoline-1(2H)-carbonyl chloride (**2n**) (78.3 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in toluene (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 15.9 mg (32%) of **3n** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.51 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.27 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 6.8 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.30 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.19 (t, *J* = 8.0 Hz, 1H), 4.29 (t, *J* = 7.2 Hz, 2H), 3.05 (t, *J* = 6.2 Hz, 2H), 2.94 (s, 3H), 2.14 (tt, *J* = 7.2, 6.0 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃): δ 161.5, 136.7, 134.8, 134.4, 133.3, 128.8, 127.2, 127.1, 126.9, 126.1, 125.2, 120.9, 120.7, 43.3, 28.6, 26.0, 20.7.

HRMS *m/z* (ESI) calcd for C₁₇H₁₆NO [M+H]⁺ 250.1226, found: 250.1230.

13-methyl-6,7-dihydro-4H-azepino[3,2,1-*de*]phenanthridin-9(5H)-one (**3o**)



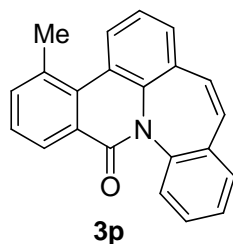
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), 2,3,4,5-tetrahydro-1*H*-benzo[*b*]azepine-1-carbonyl chloride (**2o**) (83.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in toluene (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 48.9 mg (93%) of **3o** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.44 (d, *J* = 7.6 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.55 (d, *J* = 7.2 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.13 (t, *J* = 7.8 Hz, 1H), 4.38 (t, *J* = 5.6 Hz, 2H), 3.16 (t, *J* = 5.6 Hz, 2H), 2.89 (s, 3H), 2.15 (tt, *J* = 6.8, 6.4 Hz, 2H), 2.00 (tt, *J* = 6.8, 6.4 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃): δ 163.1, 138.9, 136.6, 134.1, 133.8, 131.6, 130.7, 127.5, 126.9, 126.6, 125.4, 122.4, 121.6, 46.2, 33.5, 25.7, 25.6, 23.7.

HRMS *m/z* (ESI) calcd for C₁₈H₁₈NO [M+H]⁺ 264.1383, found: 264.1387.

15-methyl-11*H*-benzo[6,7]azepino[3,2,1-*de*]phenanthridin-11-one (**3p**)



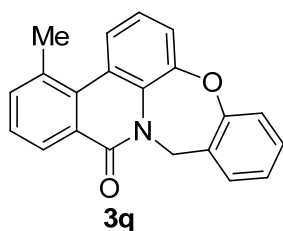
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), 5*H*-dibenzo[*b,f*]azepine-5-carbonyl chloride (**2p**) (102.3 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in toluene (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 25.4 mg (41%) of **3p** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.37 (d, *J* = 7.6 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.20-7.26 (m, 4H), 7.15 (d, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 11.6 Hz, 1H), 6.75 (d, *J* = 6.8 Hz, 1H), 6.62 (d, *J* = 11.2 Hz, 1H), 2.90 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 167.5, 142.9, 142.8, 137.1, 134.8, 134.4, 134.2, 132.7, 131.3, 131.1, 130.7, 130.0, 129.9, 129.4, 129.0, 127.4, 127.2 (2C), 126.0, 124.9, 124.3, 24.1.

HRMS *m/z* (ESI) calcd for C₂₂H₁₆NO [M+H]⁺ 310.1226, found: 310.1230.

4-methylbenzo[6,7][1,4]oxazepino[2,3,4-*de*]phenanthridin-8(10*H*)-one (**3q**)



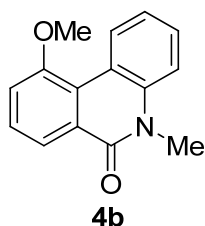
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), dibenzo[*b,f*][1,4]oxazepine-10(11*H*)-carbonyl chloride (**2q**) (103.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in toluene (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 20/1), affords 39.5 mg (69%) of **3q** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.43 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.03 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.57 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.53 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.43 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.32 (td, *J* = 8.0, 1.6 Hz, 1H), 7.24 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.17 (td, *J* = 7.2, 1.2 Hz, 1H), 5.76 (s, 2H), 2.84 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 158.9, 145.6, 136.8, 134.3, 133.5, 130.1, 129.9, 129.8, 129.1, 127.4, 127.1, 126.9, 125.4, 124.1, 123.3, 122.00, 121.95, 119.3, 44.0, 25.4.

HRMS *m/z* (ESI) calcd for C₂₁H₁₆NO₂ [M+H]⁺ 314.1176, found: 314.1178.

10-methoxy-5-methylphenanthridin-6(5*H*)-one (**4b**)⁶

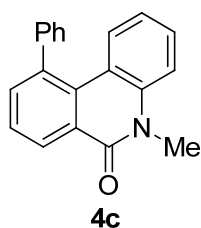


The reaction of 1-iodo-2-methoxybenzene (**1b**) (46.8 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 20/1), affords 27.9 mg (58%) of **4b** as white solid. The reaction in toluene (2 mL) affords 40.2 mg (84%) of **4b**.

¹H NMR (400 MHz, CDCl₃): δ 9.27 (d, *J* = 8.4 Hz, 1H), 8.26 (d, *J* = 8.0 Hz, 1H), 7.49-7.54 (m, 2H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.28 (t, *J* = 8.4 Hz, 2H), 4.06 (s, 3H), 3.80 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.4, 157.4, 137.6, 128.9, 128.6, 128.0, 127.7, 123.2, 122.2, 121.1, 119.2, 114.4, 114.3, 55.9, 30.3.

5-methyl-10-phenylphenanthridin-6(5*H*)-one (**4c**)



The reaction of 2-iodo-1,1'-biphenyl (**1c**) (56.0 mg, 0.2 mmol), methyl(phenyl)carbamic chloride

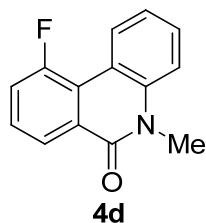
(**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 46.2 mg (81%) of **4c** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.62 (t, *J* = 7.6 Hz, 1H), 7.57 (d, *J* = 4.8 Hz, 2H), 7.42-7.47 (m, 3H), 7.34-7.38 (m, 5H), 6.77 (dt, *J* = 8.4, 4.0 Hz, 1H), 3.80 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.7, 143.4, 139.4, 138.3, 136.2, 131.6, 129.1, 128.9, 128.8, 128.3, 127.4, 127.2, 127.1, 121.0, 119.4, 114.6, 30.3.

HRMS *m/z* (ESI) calcd for C₂₀H₁₆NO [M+H]⁺ 286.1226, found: 286.1229.

10-fluoro-5-methylphenanthridin-6(5*H*)-one (**4d**)



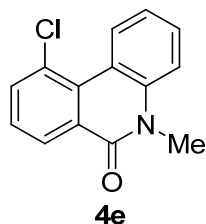
The reaction of 1-fluoro-2-iodobenzene (**1d**) (44.4 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 27.2 mg (60%) of **4d** as white solid. The reaction in toluene (2 mL) affords 39.5 mg (87%) of **4d**.

¹H NMR (400 MHz, CDCl₃): δ 8.71 (ddd, *J* = 8.4, 3.6, 1.2 Hz, 1H), 8.41 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.44-7.58 (m, 3H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.32 (tt, *J* = 7.6, 0.8 Hz, 1H), 3.80 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 160.6 (d, *J* = 3.4 Hz), 159.9 (d, *J* = 252.4 Hz), 137.8, 129.7 (d, *J* = 2.1 Hz), 128.2, 128.0 (d, *J* = 15.4 Hz), 127.9 (d, *J* = 3.1 Hz), 124.9 (d, *J* = 2.7 Hz), 122.8 (d, *J* = 1.8 Hz), 122.4 (d, *J* = 9.0 Hz), 119.8 (d, *J* = 24.8 Hz), 117.0 (d, *J* = 5.2 Hz), 114.7, 30.3.

HRMS *m/z* (ESI) calcd for C₁₄H₁₁FN O [M+H]⁺ 228.0819, found: 228.0820.

10-chloro-5-methylphenanthridin-6(5*H*)-one (**4e**)



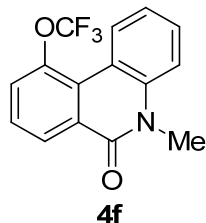
The reaction of 1-chloro-2-iodobenzene (**1e**) (47.7 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 42.5 mg (87%) of **4e** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 9.43 (d, *J* = 8.4 Hz, 1H), 8.58 (d, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 3.78 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 160.8, 138.2, 136.3, 130.8, 130.3, 129.9, 128.7, 128.3, 127.7 (2C), 121.8, 118.5, 114.7, 30.5.

HRMS m/z (ESI) calcd for $\text{C}_{14}\text{H}_{11}\text{ClNO}$ $[\text{M}+\text{H}]^+$ 244.0524, found: 244.0524.

5-methyl-10-(trifluoromethoxy)phenanthridin-6(5H)-one (**4f**)



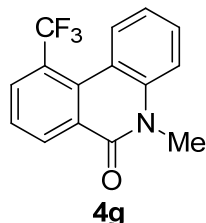
The reaction of 1-iodo-2-(trifluoromethoxy)benzene (**1f**) (57.6 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), $\text{Pd}(\text{OAc})_2$ (4.5 mg, 0.02 mmol), PPh_3 (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs_2CO_3 (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 15/1), affords 50.3 mg (86%) of **4f** as white solid.

^1H NMR (400 MHz, CDCl_3): δ 8.87 (d, $J = 8.4$ Hz, 1H), 8.60 (d, $J = 8.0$ Hz, 1H), 7.67 (d, $J = 8.0$ Hz, 2H), 7.57 (t, $J = 7.6$ Hz, 1H), 7.43 (d, $J = 8.4$ Hz, 1H), 7.32 (t, $J = 7.6$ Hz, 1H), 3.80 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 160.4, 145.6 (d, $J = 1.9$ Hz), 138.2, 130.1, 128.3, 128.1, 127.82, 127.78, 126.9, 126.0, 122.8, 120.6 (q, $J = 257.3$ Hz), 117.1, 114.9, 30.4.

HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{11}\text{F}_3\text{NO}_2$ $[\text{M}+\text{H}]^+$ 294.0736, found: 294.0737.

5-methyl-10-(trifluoromethyl)phenanthridin-6(5H)-one (**4g**)



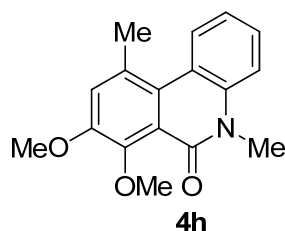
The reaction of 1-iodo-2-(trifluoromethyl)benzene (**1g**) (54.4 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), $\text{Pd}(\text{OAc})_2$ (4.5 mg, 0.02 mmol), PPh_3 (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs_2CO_3 (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 12/1), affords 39.8 mg (72%) of **4g** as white solid.

^1H NMR (400 MHz, CDCl_3): δ 8.82 (d, $J = 8.0$ Hz, 1H), 8.36 (d, $J = 8.4$ Hz, 1H), 8.16 (d, $J = 7.6$ Hz, 1H), 7.67 (t, $J = 7.6$ Hz, 1H), 7.59 (t, $J = 7.6$ Hz, 1H), 7.43 (d, $J = 8.4$ Hz, 1H), 7.31 (t, $J = 7.6$ Hz, 1H), 3.79 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 160.8, 138.3, 133.2, 132.9, 132.5 (q, $J = 6.7$ Hz), 130.4, 129.0 (q, $J = 7.5$ Hz), 128.4, 127.0, 125.4 (q, $J = 28.4$ Hz), 124.8 (q, $J = 271.5$ Hz), 122.1, 117.6, 114.6, 30.5.

HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{11}\text{F}_3\text{NO}$ $[\text{M}+\text{H}]^+$ 278.0787, found: 278.0785.

7,8-dimethoxy-5,10-dimethylphenanthridin-6(5H)-one (**4h**)



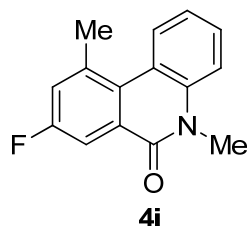
The reaction of 1-iodo-4,5-dimethoxy-2-methylbenzene (**1h**) (55.6 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 3/1), affords 27.3 mg (48%) of **4h** as white solid. The reaction in toluene (2 mL) affords 43.6 mg (77%) of **4h**.

¹H NMR (400 MHz, CDCl₃): δ 8.13 (d, *J* = 8.4 Hz, 1H), 7.43 (td, *J* = 7.8, 1.2 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.20 (td, *J* = 7.6, 0.8 Hz, 1H), 7.19 (s, 1H), 4.01 (s, 3H), 3.96 (s, 3H), 3.69 (s, 3H), 2.84 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 160.3, 151.7, 148.4, 137.5, 130.2, 127.8, 127.6, 127.3, 121.4, 121.2, 121.0, 120.2, 114.0, 61.5, 56.3, 30.1, 25.6.

HRMS *m/z* (ESI) calcd for C₁₇H₁₈NO₃ [M+H]⁺ 284.1281, found: 284.1280.

8-fluoro-5,10-dimethylphenanthridin-6(5*H*)-one (**4i**)



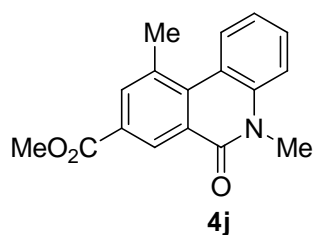
The reaction of 4-fluoro-1-iodo-2-methylbenzene (**1i**) (47.2 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 20/1), affords 46.5 mg (96%) of **4i** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.29 (d, *J* = 8.4 Hz, 1H), 8.10 (dd, *J* = 8.8, 2.8 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.24-7.28 (m, 2H), 3.73 (s, 3H), 2.87 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 160.9 (d, *J* = 3.4 Hz), 160.8 (d, *J* = 246.8 Hz), 137.7 (d, *J* = 6.9 Hz), 137.5, 129.4 (d, *J* = 2.0 Hz), 129.1 (d, *J* = 8.3 Hz), 128.4, 127.1, 124.1 (d, *J* = 22.1 Hz), 121.7, 120.0, 114.8, 112.5 (d, *J* = 22.0 Hz), 30.4, 26.0.

HRMS *m/z* (ESI) calcd for C₁₅H₁₃FNO [M+H]⁺ 242.0976, found: 242.0977.

methyl 5,10-dimethyl-6-oxo-5,6-dihydrophenanthridine-8-carboxylate (**4j**)



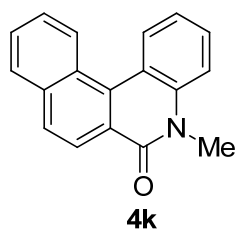
The reaction of methyl 4-iodo-3-methylbenzoate (**1j**) (55.2 mg, 0.2 mmol), methyl(phenyl)carbamoyl chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 5/1), affords 54.1 mg (96%) of **4j** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 9.00 (s, 1H), 8.35 (*J* = 8.0 Hz, 1H), 8.11 (s, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 3.95 (s, 3H), 3.72 (s, 3H), 2.90 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 166.2, 161.2, 138.8, 136.5, 136.4, 134.8, 129.6, 128.7, 128.1 (2C), 127.1, 121.7, 119.8, 114.8, 52.1, 30.3, 25.9.

HRMS *m/z* (ESI) calcd for C₁₇H₁₆NO₃ [M+H]⁺ 282.1125, found: 282.1122.

5-methylbenzo[*k*]phenanthridin-6(5*H*)-one (**4k**)^{4,7}

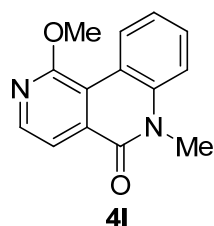


The reaction of 1-iodonaphthalene (**1k**) (50.8 mg, 0.2 mmol), methyl(phenyl)carbamoyl chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 46.7 mg (90%) of **4k** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.79 (d, *J* = 8.0 Hz, 1H), 8.55 (d, *J* = 8.0 Hz, 1H), 8.46 (d, *J* = 8.4 Hz, 1H), 7.95 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.62 (ttd, *J* = 6.8, 6.8, 1.2 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 3.80 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.7, 138.3, 136.1, 132.5, 129.0, 128.74, 128.72, 128.45, 128.41, 127.7, 127.6, 126.6, 124.4, 123.8, 121.8, 119.4, 114.7, 30.3.

1-methoxy-6-methylbenzo[*c*][2,6]naphthyridin-5(6*H*)-one (**4l**)



The reaction of 3-iodo-2-methoxypyridine (**1l**) (47.0 mg, 0.2 mmol), methyl(phenyl)carbamoyl chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol),

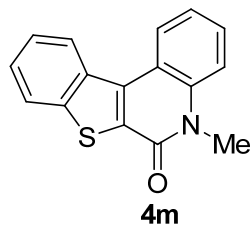
NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 15/1), affords 38.0 mg (79%) of **4l** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 9.17 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.29 (d, *J* = 5.2 Hz, 1H), 7.98 (d, *J* = 5.2 Hz, 1H), 7.56 (ddd, *J* = 8.4, 7.2, 1.6 Hz, 1H), 7.43 (d, *J* = 7.6 Hz, 1H), 7.34 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 4.22 (s, 3H), 3.82 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.0, 144.0, 138.0, 134.1, 129.4, 128.6, 122.8, 117.9, 117.5, 114.7, 114.4, 54.2, 30.4.

HRMS *m/z* (ESI) calcd for C₁₄H₁₃N₂O₂ [M+H]⁺ 241.0972, found: 241.0974.

5-methylbenzo[4,5]thieno[2,3-*c*]quinolin-6(5*H*)-one (**4m**)



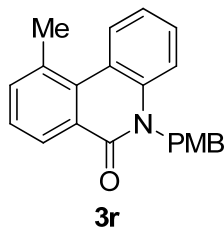
The reaction of 3-iodobenzo[*b*]thiophene (**1m**) (52.0 mg, 0.2 mmol), methyl(phenyl)carbamic chloride (**2a**) (67.9 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in toluene (2 mL) at 110 °C for 12 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 6/1), further purified by recrystallization, affords 29.6 mg (56%) of **4m** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.57-8.60 (m, 2H), 7.96-7.98 (m, 1H), 7.50-7.57 (m, 3H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.36 (td, *J* = 7.6, 1.0 Hz, 1H), 3.84 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 158.4, 142.6, 138.5, 135.8, 135.0, 132.8, 128.5, 126.9, 125.4, 125.2, 123.9, 123.7, 122.4, 119.4, 115.3, 29.9.

HRMS *m/z* (ESI) calcd for C₁₆H₁₂NOS [M+H]⁺ 266.0634, found: 266.0637.

5-(4-methoxybenzyl)-10-methylphenanthridin-6(5*H*)-one (**3r**)



The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), (4-methoxybenzyl)(phenyl)carbamic chloride (**2r**) (110.3 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in toluene (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 8/1), affords 60.4 mg (92%) of **3r** as white solid.

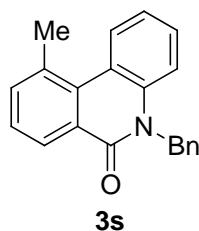
¹H NMR (400 MHz, CDCl₃): δ 8.59 (d, *J* = 7.6 Hz, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.346-7.354 (m, 2H), 7.18-7.23 (m, 3H), 6.80 (d, *J* = 8.4 Hz, 2H), 5.56 (s, 2H), 3.71 (s, 3H), 2.91 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 162.1, 158.6, 137.4, 137.0, 134.4, 133.2, 128.6, 128.5, 127.8,

127.5, 127.2, 127.1, 121.5, 120.9, 115.7, 114.1, 55.1, 46.1, 26.0.

HRMS *m/z* (ESI) calcd for C₂₂H₂₀NO₂ [M+H]⁺ 330.1489, found: 330.1496.

5-benzyl-10-methylphenanthridin-6(5*H*)-one (**3s**)



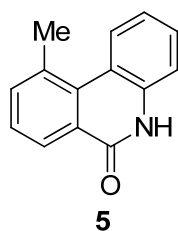
The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), benzyl(phenyl)carbamic chloride (**2s**) (98.3 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in toluene (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 10/1), affords 59.4 mg (99%) of **3s** as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.60 (d, *J* = 8.0 Hz, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.21-7.37 (m, 8H), 5.64 (s, 2H), 2.93 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 164.7, 137.4, 137.1, 136.5, 134.4, 133.2, 128.7, 128.5, 127.8, 127.5, 127.2, 127.0, 126.4, 121.6, 120.9, 115.7, 46.7, 26.0.

HRMS *m/z* (ESI) calcd for C₂₁H₁₈NO [M+H]⁺ 300.1383, found: 300.1388.

10-methylphenanthridin-6(5*H*)-one (**5**)⁸

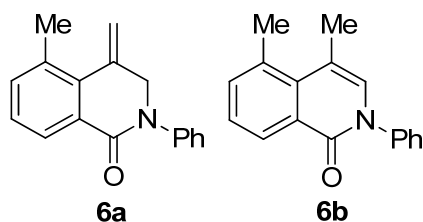


3r (65.9 mg, 0.2 mmol) and trifluoroacetic acid (2.0 mL) were added to a 5 mL screw vial with a magnetic stir bar. The vial was capped and the mixture was stirred at 90 °C for 20 h. After cooling to room temperature, the mixture was evaporated and isolated by column chromatography (silica gel, petroleum ether/AcOEt = 2/1), affords 38.2 mg (91%) of **5** as white solid.

¹H NMR (400 MHz, DMSO-*d*₆): δ 11.74 (br s, 1H), 8.45 (d, *J* = 5.6 Hz, 1H), 8.33 (d, *J* = 4.8 Hz, 1H), 7.71 (s, 1H), 7.44-7.55 (m, 3H), 7.27 (s, 1H), 2.93 (s, 3H).

¹³C NMR (100 MHz, DMSO-*d*₆): δ 160.9, 137.0 (2C), 135.2, 133.3, 128.8, 127.4, 127.3, 127.2, 126.0, 121.7, 118.8, 116.2, 25.6.

5-methyl-4-methylene-2-phenyl-3,4-dihydroisoquinolin-1(2*H*)-one (**6a**) and 4,5-dimethyl-2-phenylisoquinolin-1(2*H*)-one (**6b**)



The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), allyl(phenyl)carbamic chloride (**2t**) (78.3 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in DCE (2 mL) at 95 °C for 6 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 12/1), affords 39.8 mg (80%) of **6a** as white solid and 7.4 mg (15%) of **6b** as white solid.

6a:

¹H NMR (400 MHz, CDCl₃): δ 8.09 (d, *J* = 7.6 Hz, 1H), 7.40-7.43 (m, 5H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.23-7.27 (m, 1H), 5.60 (s, 1H), 5.43 (s, 1H), 4.45 (s, 2H), 2.53 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 163.6, 142.4, 136.4, 135.3, 135.1, 134.0, 129.9, 128.9, 127.9, 127.0, 126.3, 125.2, 118.1, 57.5, 21.3.

HRMS *m/z* (ESI) calcd for C₁₇H₁₆NO [M+H]⁺ 250.1226, found: 250.1228; calcd for C₁₇H₁₅NNaO [M+Na]⁺ 272.1046, found: 272.1047.

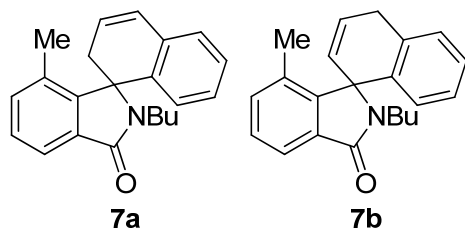
6b:

¹H NMR (400 MHz, CDCl₃): δ 8.47 (d, *J* = 7.6 Hz, 1H), 7.37-7.51 (m, 7H), 6.94 (s, 1H), 2.81 (s, 3H), 2.53 (s, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 161.8, 141.2, 136.6, 136.3, 134.6, 130.6, 129.2, 127.9, 127.4, 126.8, 113.1, 24.1, 21.7.

HRMS *m/z* (ESI) calcd for C₁₇H₁₆NO [M+H]⁺ 250.1226, found: 250.1228.

2-butyl-7-methyl-2'*H*-spiro[isindoline-1,1'-naphthalen]-3-one (**7a**) and
2-butyl-7-methyl-4'*H*-spiro[isindoline-1,1'-naphthalen]-3-one (**7b**)



The reaction of 1-iodo-2-methylbenzene (**1a**) (43.6 mg, 0.2 mmol), butyl(3,4-dihydronaphthalen-1-yl)carbamic chloride (**2u**) (105.5 mg, 0.4 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol), PPh₃ (10.5 mg, 0.04 mmol), NBE (18.8 mg, 0.2 mmol), and Cs₂CO₃ (260.6 mg, 0.8 mmol) in toluene (2 mL) at 110 °C for 12 h, isolated by column chromatography (silica gel, petroleum ether/AcOEt = 6/1), affords 47.6 mg (75%) of **7a** as white solid and 3.8 mg (6%) of **7b** as white solid.

7a:

¹H NMR (400 MHz, CDCl₃): δ 7.76 (d, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.18-7.24 (m, 3H), 7.03 (t, *J* = 7.2 Hz, 1H), 6.64 (d, *J* = 7.6 Hz, 1H), 6.38 (dt, *J* = 10.0, 3.6 Hz, 1H), 5.38 (d, *J* = 10.4 Hz, 1H), 3.70 (d, *J* = 22.8 Hz, 1H), 3.68 (d, *J* = 22.8 Hz, 1H), 3.26 (ddd, *J* = 14.4, 9.6, 5.6 Hz, 1H), 3.08 (ddd, *J* = 14.4, 9.6, 5.6 Hz, 1H), 1.84 (s, 3H), 1.26-1.42 (m, 2H), 1.19 (tq, *J* = 7.6, 7.2 Hz, 2H), 0.77 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 168.4, 148.2, 134.7, 133.7, 133.2, 132.1, 131.7, 128.9, 128.5, 128.1, 127.6, 127.1, 126.8, 125.7, 120.8, 65.7, 40.1, 30.8, 29.2, 20.3, 16.7, 13.5.

HRMS *m/z* (ESI) calcd for C₂₂H₂₄NO [M+H]⁺ 318.1852, found: 318.1856.

7b:

¹H NMR (400 MHz, CDCl₃): δ 7.74 (d, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 7.6

Hz, 1H), 7.27 (td, $J = 7.6, 1.2$ Hz, 1H), 7.18 (d, $J = 6.8$ Hz, 1H), 7.02 (td, $J = 7.4, 1.2$ Hz, 1H), 6.64 (dd, $J = 5.8, 3.0$ Hz, 1H), 6.53 (d, $J = 8.0$ Hz, 1H), 6.16 (ddd, $J = 9.8, 5.4, 2.6$ Hz, 1H), 3.25-3.35 (m, 2H), 3.16 (ddd, $J = 13.6, 9.6, 6.0$ Hz, 1H), 2.46 (dd, $J = 19.8, 5.4$ Hz, 1H), 2.02 (s, 3H), 1.09-1.33 (m, 4H), 0.75 (t, $J = 7.2$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 166.9, 149.3, 134.3, 134.0, 132.53, 132.45, 131.6, 128.7, 128.6, 128.3, 127.1, 126.9, 126.8, 125.6, 120.9, 64.2, 40.7, 34.6, 30.7, 20.4, 18.7, 13.5.

HRMS m/z (ESI) calcd for $\text{C}_{22}\text{H}_{24}\text{NO}$ $[\text{M}+\text{H}]^+$ 318.1852, found: 318.1850.

Details of Calculation

All of the DFT calculations were performed with the Gaussian 09 program package.¹¹ The geometry optimization of all the minima involved were performed at the M06 level of theory¹² with the LACVP(d) basis set¹³. It consists of the standard 6-31G(d) basis set for lighter atoms (H, C, N, O, and P) and the LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double- ζ) basis set for Pd, Cs and I. The structures of the reactants, intermediates, transition states, and products were fully optimized without any restriction. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. IRC calculations¹⁴ were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. Single-point solvent calculations (with LACVP(d) basis set) were performed at the optimized gas-phase geometries for all the intermediates and transition states, using the CPCM¹⁵ approach as implemented in Gaussian 09, employing DCE as a solvent. Through the same approach full optimization, without any restriction, was carried out for the model reactions. The reported energies are Gibbs free energies in gas-phase (ΔG). Gibbs free energies in DCE solution (ΔG_{DCE}) are also given in parenthesis.

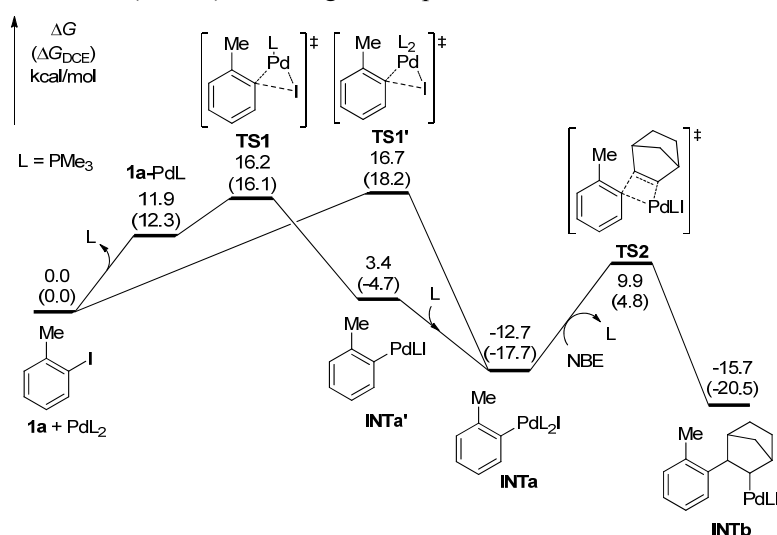


Fig. S2 DFT-computed energy profiles for the oxidative addition of **1a** with Pd^0 through the bisphosphine and monophosphine pathways

DFT-Computed Energies of All Stationary Points

Table S2. Sum of electronic and thermal enthalpies (H , in Hartree), sum of electronic and thermal

free energies (G , in Hartree), thermal correction to Gibbs free energy ($CGFE$, in Hartree), electronic energy in DCE (E_{DCE} , in Hartree), and free energies in DCE (G_{DCE} , in Hartree). For transition state structures, one imaginary frequency (IFreq) was observed and given below. For all minimum structures, no imaginary frequency was observed.

Structure	H	G	$CGFE$	E_{MeCN}	G_{MeCN}	IFreq
1a	-281.963388	-282.006774	0.082493	-282.092242	-282.009749	-
PdL₂	-1048.483740	-1048.549714	0.179943	-1048.736656	-1048.556713	-
1a-PdL	-869.601413	-869.671531	0.180636	-869.859125	-869.678489	-
TS1	-869.598387	-869.664693	0.183711	-869.856094	-869.672383	-85.1224
INTa'	-869.618510	-869.685100	0.184735	-869.890292	-869.705557	-
TS1'	-1330.447548	-1330.529885	0.289678	-1330.827086	-1330.537408	-109.4131
INTa	-1330.495152	-1330.576655	0.292714	-1330.887321	-1330.594607	-
NBE	-272.341258	-272.375916	0.124557	-272.501380	-272.376823	-
L	-460.829190	-460.865964	0.083528	-460.951951	-460.868423	-
TS2	-1141.973407	-1142.050654	0.334487	-1142.401658	-1142.067171	-253.5108
INTb	-1142.014451	-1142.091482	0.337502	-1142.445034	-1142.107532	-
CsI	-31.265187	-31.296705	-0.027250	-31.326147	-31.353397	-
Cs₂CO₃	-303.394684	-303.439990	-0.020908	-303.496145	-303.517053	-
CsHCO₃	-284.140976	-284.178831	-0.003043	-284.218001	-284.221044	-
INTb'	-1414.150573	-1414.238043	0.347055	-1414.632437	-1414.285382	-
TS3	-1414.106464	-1414.192730	0.342595	-1414.582533	-1414.239938	-1889.5607
INTc	-1590.861420	-1590.947343	0.435836	-1591.394382	-1590.958546	-
2a	-899.343758	-899.391958	0.108779	-899.507991	-899.399212	-
INTc'	-2029.367003	-2029.462178	0.463283	-2029.936917	-2029.473634	-
TS4	-2029.332682	-2029.426074	0.463133	-2029.904171	-2029.441038	-169.0784
INTd	-2029.372481	-2029.466753	0.463977	-2029.950676	-2029.486699	-

TS5	-2029.356370	-2029.452089	0.460536	-2029.930853	-2029.470317	-217.9500
INTe	-2029.411750	-2029.506199	0.465381	-2029.994227	-2029.528846	-
TS6	-2029.374964	-2029.470699	0.461267	-2029.954083	-2029.492816	-230.5861
INTf	-1757.012482	-1757.096620	0.311612	-1757.429557	-1757.117945	-
INTf'	-1580.401996	-1580.490356	0.329877	-1580.860748	-1580.530871	-
TS7	-1580.392132	-1580.480551	0.324101	-1580.844100	-1580.519999	-1747.2775
CsCl	-480.062325	-480.091514	-0.024862	-480.123943	-480.148805	-
INTg	-1757.099292	-1757.192406	0.410410	-1757.617263	-1757.206853	-
TS8	-1757.092150	-1757.183709	0.410445	-1757.607199	0.410445	-223.8556
3a	-708.651013	-708.704197	0.205400	-708.916949	-708.711549	-
TS9	-1947.826674	-1947.912590	0.317778	-1948.242706	-1947.924928	-103.8205
INTh	-1947.873113	-1947.959606	0.318347	-1948.299754	-1947.981407	-

The coordinates of all stationary points (Å)

1a				P	-2.31959200	0.00036100	0.00221000
C	-2.66578800	0.85072500	0.00007600	C	-3.16761800	0.08988400	1.63616600
C	-1.27255000	0.97586800	-0.00041900	H	-2.87151400	-0.76834900	2.25092700
C	-0.53303700	-0.21045500	-0.00039500	H	-2.85760100	1.00130400	2.16101100
C	-1.14025200	-1.46170000	-0.00027300	H	-4.26195000	0.09332700	1.52532700
C	-2.52808000	-1.54975600	0.00003800	C	-3.17620800	1.37336800	-0.88095200
C	-3.29199600	-0.38892000	0.00028300	H	-2.88198500	1.36948000	-1.93716100
H	-3.26655700	1.76059100	0.00023700	H	-4.26995600	1.27981900	-0.81104000
H	-0.53116400	-2.36318200	-0.00050900	H	-2.86930000	2.33401000	-0.45068700
H	-3.00547500	-2.52802700	0.00013400	C	-3.18926200	-1.44883500	-0.73388800
H	-4.37884800	-0.44771200	0.00079600	H	-4.28204900	-1.33981700	-0.67370400
C	-0.64148000	2.33282200	-0.00006900	H	-2.89689000	-1.55772700	-1.78502100
H	0.00026700	2.47859200	-0.87948800				
H	-1.40446200	3.11968400	-0.00188600	1a-PdL			
H	-0.00326300	2.47969500	0.88177000	Pd	-0.67413700	0.18829400	-0.05806100
I	1.60431300	-0.14700300	0.00006600	P	-2.93731900	-0.19165200	0.08634900
				I	1.93923200	-1.57210800	-0.17169700
PdL₂				C	1.19684600	1.14100300	-1.44821500
Pd	-0.00016400	-0.00624300	-0.01258800	C	1.18462800	2.53411400	-1.56208700
P	2.31939800	0.00026100	-0.00065400	C	1.43531600	3.32074000	-0.44785200

C	1.66998700	2.72496200	0.79037700	H	-3.35453400	1.57097300	-0.93321800
C	1.69024200	1.33939900	0.95807000	H	-4.72773900	0.97741100	0.05511000
C	1.45288900	0.54533100	-0.19366600	C	-3.58368300	-1.33263600	1.53551200
H	0.99691600	2.98890900	-2.53321800	H	-4.68008100	-1.25843000	1.50975800
H	1.44137600	4.40574500	-0.53380000	H	-3.29888200	-2.38813600	1.61796400
H	1.85485600	3.35009800	1.66458600	H	-3.21145000	-0.81092300	2.42506400
H	1.08851400	0.51400000	-2.33055400	C	1.93704800	-0.30161900	2.36829600
C	-4.05595100	0.74141900	-1.04137100	H	2.41524600	-0.90929700	3.14598100
H	-5.11063300	0.47779500	-0.87422800	H	2.31690400	0.72638500	2.45993900
H	-3.92364400	1.81759800	-0.87946100	H	0.86131000	-0.25903100	2.57637300
H	-3.79231700	0.52347800	-2.08307100				
C	-3.75880100	0.13614500	1.70337700	INTa'			
H	-3.63112600	1.19168200	1.97097100	Pd	-0.14740800	-0.78468300	0.00662000
H	-4.83254100	-0.09931500	1.66787000	P	2.12271400	-1.32883000	0.01060500
H	-3.28550800	-0.46877600	2.48584400	C	2.86401300	-1.33625000	-1.66408000
C	-3.51066700	-1.91282200	-0.23381600	H	2.78976200	-0.32883800	-2.09162200
H	-3.21768700	-2.21285000	-1.24694200	H	3.92125100	-1.63236900	-1.62644200
H	-3.02691700	-2.59907200	0.47130900	H	2.31571900	-2.02852400	-2.31327200
H	-4.60209600	-2.00275900	-0.13337900	C	2.53481900	-3.00034600	0.64550300
C	2.02425100	0.74460800	2.29160200	H	1.97696800	-3.75913100	0.08440800
H	1.32335300	-0.04936400	2.57515500	H	3.61036600	-3.20382900	0.55007400
H	3.02871000	0.29581900	2.28221200	H	2.24789700	-3.07665300	1.70062500
H	2.00706600	1.51257500	3.07371600	C	3.27882900	-0.24523100	0.92785000
				H	3.00817700	-0.21188600	1.98970900
				H	4.30864900	-0.61408600	0.82953100
TS1				H	3.21636400	0.77405600	0.52649100
Pd	-0.47137200	-0.44209500	-0.07682600	I	-2.72304900	-0.25955000	-0.12146500
P	-2.82531500	-0.59771200	0.02748100	C	0.56422000	1.90934200	0.97045200
I	0.78870700	1.96703400	-0.14296500	C	1.07703700	3.19962600	0.79322600
C	1.93746700	-0.87111200	-1.43157200	C	1.44375000	3.67908100	-0.46017600
C	1.58009200	-0.41022200	-0.16035100	C	1.28760600	2.87394200	-1.58234900
H	1.45879700	-0.44967400	-2.31407100	C	0.78240400	1.58070400	-1.44063700
C	2.23098500	-0.85336400	1.00553000	C	0.45509000	1.11576000	-0.17366800
C	2.91738100	-1.85390900	-1.55380400	H	1.18036000	3.83976000	1.67078200
H	3.18884700	-2.22845000	-2.53955200	H	1.84115600	4.68768200	-0.55999800
C	3.55415500	-2.33170700	-0.41497000	H	1.54916600	3.24509000	-2.57222100
H	4.32993900	-3.09074300	-0.50076400	H	0.63923700	0.94575700	-2.31441200
C	3.21073700	-1.83476800	0.83960500	C	0.14336300	1.43182900	2.32658200
H	3.71851000	-2.21355900	1.72791000	H	0.45211800	2.13524100	3.11001200
C	-3.76127000	-1.47794500	-1.29054800	H	-0.94883700	1.31711100	2.37546800
H	-3.47361100	-2.53570300	-1.30864700	H	0.56648300	0.44392600	2.55873900
H	-4.84580400	-1.40399500	-1.12753000				
H	-3.51679300	-1.04382000	-2.26707900	TS1'			
C	-3.63280800	1.05265500	-0.00751600	Pd	-0.44340400	0.20527100	-0.22342700
H	-3.25992000	1.65397300	0.83059500				

P	-2.67514500	-0.33728300	0.50508500	P	2.61800900	0.54658200	0.01594900
P	-0.02938500	2.53786600	-0.60989100	P	-0.55414200	2.39765200	-0.02630300
I	0.76191300	-2.19545100	-1.05485400	C	-0.24332500	3.13926100	-1.67584100
C	2.63632500	0.24597600	-0.37450700	H	-0.80326700	2.57093200	-2.42884200
C	3.58972300	0.92017200	0.37062300	H	-0.56131000	4.19057900	-1.71019400
C	3.57202600	0.82792500	1.76383100	H	0.82264000	3.07446900	-1.92667900
C	2.60350100	0.05050400	2.38090600	C	0.21675200	3.60578600	1.12283500
C	1.61908500	-0.64453500	1.66188300	H	1.29903100	3.65423300	0.96283000
C	1.62638700	-0.49392000	0.26177100	H	-0.20966800	4.60850700	0.98095900
H	4.35239600	1.51059700	-0.13672300	H	0.03598800	3.28518900	2.15635400
H	4.32537200	1.33861900	2.36096800	C	-2.32867800	2.78398200	0.21755300
H	2.60506100	-0.04863500	3.46782600	H	-2.63865100	2.50801100	1.23206900
H	2.64881400	0.29396400	-1.46273800	H	-2.49504000	3.86008100	0.07084600
C	1.15475900	3.21365900	-1.85606800	H	-2.94270100	2.21309900	-0.48815700
H	1.24658800	4.30697100	-1.77973600	C	3.29879100	-0.00078000	-1.59750100
H	2.14230900	2.76339900	-1.69457500	H	4.39341200	0.09109000	-1.62322700
H	0.82169200	2.95192800	-2.86766600	H	3.01041400	-1.04478900	-1.76716000
C	0.63214100	3.32658300	0.91976300	H	2.86488900	0.60707100	-2.40194700
H	1.58829500	2.85436400	1.18275400	C	3.41951800	2.20297200	0.17399500
H	0.78170500	4.40967900	0.79797000	H	4.50256400	2.12689500	0.00399500
H	-0.06860700	3.14907300	1.74601100	H	3.00478500	2.91011200	-0.55642600
C	-1.48587300	3.62548200	-0.93284200	H	3.25799800	2.60577900	1.18177100
H	-1.94258900	3.35971800	-1.89457100	C	3.61810200	-0.40768000	1.22090600
H	-2.23546000	3.45997700	-0.14720700	H	3.34767000	-1.46752900	1.15010300
H	-1.21583100	4.69171100	-0.94804500	H	4.69181700	-0.28331900	1.02348700
C	-4.06068100	0.08545300	-0.63674100	H	3.39549600	-0.06546600	2.23864800
H	-5.04273500	-0.14851700	-0.19992200	I	0.64007100	-2.48180800	-0.06720200
H	-4.01916300	1.15577000	-0.87641400	C	-2.60497900	-0.45130000	0.98062700
H	-3.94360200	-0.47094800	-1.57445300	C	-3.96769200	-0.69066700	0.77928400
C	-3.12099400	-2.07511600	0.93516700	C	-4.51295500	-0.75906600	-0.49933400
H	-4.17245600	-2.16704000	1.24418800	C	-3.68801100	-0.60280600	-1.60750000
H	-2.93996700	-2.72360800	0.06893000	C	-2.32577200	-0.36160100	-1.42476100
H	-2.47636600	-2.42489200	1.75192800	C	-1.78825300	-0.27260400	-0.14276900
C	-3.24729500	0.52660300	2.03303400	H	-4.61091500	-0.83126600	1.65025100
H	-4.28164900	0.26147100	2.29750100	H	-5.57820200	-0.94646400	-0.62781700
H	-2.58886000	0.26877000	2.87235800	H	-4.09857800	-0.67521600	-2.61447600
H	-3.18318000	1.61192000	1.88086200	H	-1.67572800	-0.25918300	-2.29593900
C	0.64792900	-1.49715600	2.43071700	C	-2.03771000	-0.39718600	2.36835200
H	-0.24761900	-0.93370800	2.72859300	H	-2.81825100	-0.51849200	3.13097500
H	0.30951200	-2.36011100	1.84410200	H	-1.28863800	-1.18879100	2.51404700
H	1.11728000	-1.87258200	3.34984600	H	-1.52027700	0.55725700	2.56128300

INTa

Pd 0.20430400 0.19694900 0.03924300

NBE

C 1.17571200 0.77449600 -0.51943000

C	-0.08459300	1.12040500	0.32377300	C	0.82432000	1.64245100	-0.43759900
C	-0.08448100	-1.12044900	0.32364300	C	-3.22600300	3.09390000	0.11796300
C	1.17581900	-0.77433100	-0.51946300	C	-4.09807700	1.81472300	0.05044900
H	1.12198900	1.20314100	-1.52756200	P	-1.19180300	-2.39312100	-0.29161800
H	2.07992000	1.17252900	-0.03877800	C	-2.86186100	-2.61889100	-1.02936700
H	1.12221600	-1.20290500	-1.52764200	C	1.09043700	1.98640500	2.08849400
H	2.08006800	-1.17230200	-0.03883000	C	-0.27521700	-3.72959200	-1.14358800
C	-0.03116300	-0.00008000	1.37129600	C	-1.42321100	-3.05472500	1.40069600
H	-0.89879500	-0.00015500	2.04261200	H	4.00039700	3.78479700	-1.05091300
H	0.89712700	-0.00009300	1.96196400	H	3.14307900	3.44668700	1.23910800
C	-1.27197800	0.66877500	-0.49808000	H	-1.08236500	2.37930100	-1.53335200
H	-1.91195600	1.32799600	-1.08024200	H	-2.45155200	0.26116500	-1.69183700
C	-1.27193700	-0.66884400	-0.49813000	H	-3.56196900	-0.24276900	0.74037500
H	-1.91194500	-1.32796200	-1.08036300	H	-1.17718400	3.33771700	0.97190600
H	-0.11158300	2.15086300	0.69370300	H	-1.43307500	0.82147400	1.88541300
H	-0.11131100	-2.15094400	0.69348400	H	-2.87639700	1.77855700	2.34944300

L = PMes

C	-1.50528100	-0.59596200	0.28648600	H	-3.16952000	3.62601700	-0.84057000
P	0.00004300	-0.00009400	-0.62302900	H	-3.61233000	3.80442600	0.86005700
C	0.23634600	1.60132300	0.28647900	H	1.88103300	2.33235700	2.76518700
C	1.26883700	-1.00529000	0.28657100	H	0.16660600	2.50511800	2.37816300
H	1.15796200	-0.91894400	1.37756400	H	0.94458400	0.91297600	2.27252700
H	1.17863400	-2.06259700	0.00841300	H	2.83308100	2.70984500	-2.98041000
H	2.27732400	-0.67364700	0.01019200	H	-0.82209100	-4.67915700	-1.06268900
H	-1.37458500	-0.54435300	1.37745200	H	-0.14835400	-3.47143200	-2.20164200
H	-2.37505600	0.01243700	0.00943600	H	0.72020600	-3.82803300	-0.69708500
H	-1.72400300	-1.63456700	0.00924300	H	-1.88797700	-4.05019100	1.37869400
H	0.21561100	1.46234800	1.37746300	H	-0.44435100	-3.11664600	1.89098000
H	1.19802300	2.05061700	0.00950400	H	-2.05611200	-2.37175300	1.98184300
H	-0.55396800	2.30968500	0.00896100	H	-3.19154000	-3.66057900	-0.91708200

TS2

Pd	-0.22034200	-0.24368300	-0.28980600	H	0.78585700	1.38520700	-2.57655900
C	1.31022100	1.83951200	-1.73266800	I	2.17300400	-1.40396500	0.43993700

C	-2.11273500	0.63014100	-0.72003800
C	-1.31888100	1.81645900	-0.63402200
C	-1.84007400	2.56452100	0.57235900
C	-2.26765400	1.42531100	1.50569000
C	-3.09512800	0.70341800	0.43826000
C	2.45642500	2.58845100	-1.96579300
C	3.10662000	3.18397900	-0.89093600
C	2.61507300	3.00030000	0.39500200
C	1.47803100	2.22779900	0.65847900

INTb

Pd	0.08874800	0.27364300	0.31481400
C	-0.45582000	-1.69799400	1.92566500
C	-1.95025300	0.53776600	0.66219300
C	-2.35561100	-0.95362200	0.53747000
C	-3.20911000	-0.95036200	-0.74388100
C	-2.59103300	0.17065400	-1.59003400
C	-2.69336800	1.21962300	-0.47966800

C	0.63588100	-2.47360000	2.29731800	Cs₂CO₃			
C	1.15402000	-3.37894900	1.38538500	C	-0.00032700	1.21757400	-0.00040000
C	0.58339100	-3.48240800	0.12395800	O	-0.00020300	-0.11184100	-0.00116900
C	-0.51079700	-2.71375900	-0.27942400	O	1.11721000	1.84305100	-0.03403000
C	-1.06571200	-1.79400800	0.64915000	O	-1.11822700	1.84260800	0.03436600
C	-4.55763900	-0.31042300	-0.37132500	Cs	2.85370600	-0.32627300	0.00203100
C	-4.19798900	1.17913200	-0.14476800	Cs	-2.85349200	-0.32638200	-0.00186600
P	0.51929700	2.51229700	0.30654700				
C	-0.65510600	3.62248600	1.17809700	CsHCO₃			
C	-1.01218500	-2.93918700	-1.67782600	C	-2.00439300	0.04371000	-0.00022500
C	2.09855000	2.99049800	1.09551400	O	-1.47856800	-1.10068100	-0.00061300
C	0.64549500	3.24084100	-1.36639800	O	-3.38368600	0.06866300	0.00065700
H	2.01539200	-3.99210500	1.64270400	O	-1.44261100	1.15507600	-0.00052600
H	1.01647800	-4.17399600	-0.59807400	Cs	1.20172000	-0.00688500	0.00007800
H	-2.99446800	-1.26750000	1.38068600	H	-3.62934400	-0.86807100	0.00093400
H	-2.12105800	0.99030500	1.64932500				
H	-2.33591900	2.22365500	-0.74187200	INTb'			
H	-3.32571300	-1.92619900	-1.22344300	Pd	-0.73057300	-0.18635900	0.12716300
H	-1.55087700	-0.00429500	-1.90401600	C	-1.97902000	-0.14177400	2.07256100
H	-3.19579200	0.41469800	-2.47509200	C	-0.84803800	1.85446500	0.41470300
H	-4.76621700	1.83655500	-0.81778700	C	-2.34411500	1.94334800	0.79790500
H	-4.39650100	1.51667800	0.88200400	C	-2.90898800	2.76314200	-0.37603900
H	-5.01266700	-0.78286500	0.50959200	C	-2.03369300	2.34458400	-1.56605700
H	-5.26802500	-0.42124800	-1.20144500	C	-0.71015100	2.65843600	-0.86104700
H	-0.26863300	-3.50597000	-2.24977900	C	-2.28562200	-1.42886300	2.55764100
H	-1.94517600	-3.51982000	-1.69405700	C	-3.34593400	-2.11839800	2.01883900
H	-1.19247000	-2.00727200	-2.22285900	C	-4.09176600	-1.53464700	0.98465100
H	1.06894500	-2.36540300	3.28947400	C	-3.81969600	-0.27293600	0.47529800
H	2.23010800	4.08105600	1.05653300	C	-2.73712700	0.47578100	1.03883000
H	2.10008600	2.66081900	2.14099600	C	-2.42601600	4.21029800	-0.16555300
H	2.92467100	2.48875200	0.57929900	C	-0.91092400	4.14024200	-0.48702100
H	0.83763700	4.32162900	-1.31515500	P	-0.68047400	-2.46784800	-0.77294100
H	1.46687500	2.74256400	-1.89556000	C	0.97728300	-3.13657400	-1.19653800
H	-0.27920200	3.06148500	-1.92818000	C	-4.70914900	0.24127800	-0.62009600
H	-0.33094400	4.66823100	1.08822400	C	-1.54663900	-4.00259600	-0.22016900
H	-1.66941800	3.52725100	0.77552400	C	-1.42215400	-2.22777300	-2.43578800
H	-0.68294700	3.34963900	2.24025700	H	-3.60651000	-3.11255300	2.38010400
H	-0.91197500	-1.03494300	2.66217000	H	-4.92917600	-2.09049100	0.55925800
I	2.59508800	-0.31611100	-0.71542800	H	-2.52882500	2.49068100	1.73995100
				H	-0.11763000	2.09054500	1.19989300
				H	0.19853600	2.43075700	-1.42642200
CsI				H	-3.99336900	2.70309100	-0.51084800
Cs	0.00000000	0.00000000	1.76344300	H	-2.10569000	1.28370300	-1.84640700
I	0.00000000	0.00000000	-1.82998800	H	-2.21112000	2.96739300	-2.45507700

H	-0.64984300	4.79708500	-1.32975300	H	1.13762100	-1.38035800	1.99850700
H	-0.28274800	4.43815900	0.36422400	H	-2.66289700	-3.21453400	1.22938000
H	-2.63564100	4.57255500	0.85083100	H	-1.49304200	-1.09228100	2.29426600
H	-2.94756300	4.88240300	-0.86096200	H	-0.95860200	-2.57909300	3.14191800
H	-5.38993400	-0.55076100	-0.95560100	H	1.25703400	-3.85766200	2.14300000
H	-5.33168300	1.08331200	-0.28858000	H	1.39253500	-3.59093100	0.39412200
H	-4.14099500	0.58293400	-1.49410100	H	-0.71430100	-4.71268400	0.14279700
H	-1.68802400	-1.85243300	3.36314100	H	-0.87393800	-4.80442000	1.90397000
H	-1.44224300	-4.80621100	-0.96322300	H	-2.73652600	2.10687100	-1.55047100
H	-1.13377900	-4.34611900	0.73686600	H	-0.84681100	0.50954400	-1.46828700
H	-2.61271900	-3.79003300	-0.07118500	C	1.37285800	1.00745800	-1.64217200
H	-1.36396100	-3.13214100	-3.05832900	O	1.48361700	1.07964900	-0.31607300
H	-2.47386000	-1.93135000	-2.31709300	O	0.20483200	0.93822200	-2.19644800
H	-0.87369600	-1.40509800	-2.91154900	O	2.43345900	0.98083300	-2.30589200
H	0.88998600	-4.01611600	-1.85073500	Cs	3.84841300	-0.60540300	-0.32955400
H	1.55503700	-2.35319000	-1.70333300	C	-4.18767200	-3.03966700	-0.83578900
H	1.50663900	-3.42167800	-0.27918700	H	-3.37988900	-3.74637600	-1.06821900
H	-1.26388900	0.46544400	2.62955400	H	-4.55271900	-3.28796300	0.17172700
C	1.84933100	-0.03992400	-0.87163500	H	-5.01368200	-3.24392400	-1.52944700
O	1.89437800	-0.06385400	0.41186100	C	-2.36868800	3.74037700	1.40253700
O	2.86865400	-0.08944700	-1.61702000	H	-2.31221000	4.83721600	1.35844200
O	0.65465900	0.01342800	-1.44979500	H	-3.14587600	3.39010400	0.71219900
Cs	4.75998400	0.26110500	0.51127100	H	-2.65981600	3.43879000	2.41612100
TS3				C	-0.29816600	3.84311200	-0.57995400
Pd	-0.47788300	0.60779800	0.59298400	H	-0.82678600	3.41654600	-1.44003400
C	-2.04396300	0.15576500	-0.95393400	H	-0.49373400	4.92181100	-0.50393600
C	-0.05892700	-1.36571100	0.14005800	H	0.76995500	3.66658400	-0.75368200
C	-1.34924700	-2.13109900	-0.23772000	C	0.37916000	3.74970700	2.16366100
C	-1.61740200	-2.93383600	1.07068700	H	0.31911600	4.84647500	2.12211800
C	-0.99769900	-2.06791000	2.16855800	H	0.14986500	3.41652800	3.18307800
C	0.36507000	-1.96237600	1.46995300	H	1.40144700	3.43617200	1.91713200
C	-3.03066800	1.07391600	-1.34702600	INTc			
C	-4.34360000	0.67938600	-1.55472300	C	-3.60424100	1.18560900	-0.74550900
C	-4.68283300	-0.65876800	-1.37452500	C	-2.38978100	0.53270900	-0.46725700
C	-3.74659500	-1.60573800	-0.95524000	C	-1.17419000	1.24577400	-0.42229200
C	-2.42630900	-1.18509600	-0.70680000	C	-1.20510500	2.62251100	-0.67182300
C	-0.65046400	-4.12559100	1.06949500	C	-2.40320500	3.27920000	-0.93944700
C	0.73262800	-3.45127000	1.26538700	C	-3.59319500	2.56207900	-0.97065500
P	-0.76350300	2.95748900	0.95805900	C	-2.30802400	-0.94066900	-0.24507800
H	-5.09694800	1.39233400	-1.88957900	C	-0.82449300	-1.41666600	-0.22923300
H	-5.70308000	-0.98916900	-1.57997700	C	-0.69397300	-2.10479300	1.14142600
H	-1.14864000	-2.86391600	-1.04403200	C	-1.49901100	-3.41965000	1.10174900
H	0.70419300	-1.36517700	-0.65119300	C	-2.97073900	-2.92833500	1.11717000

C	-2.82420800	-1.40196800	1.14325500	H	0.99235500	-2.33832700	-2.72303000
C	-1.58735600	-1.23272900	2.02756700	H	2.00107200	-0.98635600	-3.26039900
Pd	0.56557500	0.15890100	-0.28054800				
P	1.98391100	1.83591500	0.76706300	2a			
C	1.21715900	3.32395800	1.53698700	C	-2.50678600	-0.31503700	1.18490600
C	-4.89437800	0.42315800	-0.85138000	C	-1.16165900	0.03063900	1.22454300
P	2.29540600	-1.41284900	-0.88523400	C	-0.50861700	0.38851200	0.04803400
C	2.46600000	0.91876600	2.29595300	C	-1.20004000	0.42034000	-1.16016600
C	3.61714200	2.54807300	0.27588800	C	-2.54938700	0.08607300	-1.19193600
H	-1.26042200	-4.02002900	0.21133900	C	-3.20265000	-0.28479700	-0.02072600
H	-2.40859400	4.35208100	-1.13509800	H	-3.01659800	-0.60199100	2.10272900
H	-4.53352000	3.07151300	-1.18939000	H	-0.60417600	0.01871300	2.15958000
H	-2.88273900	-1.47037300	-1.02739300	H	-0.67071400	0.70199100	-2.06992100
H	-0.62070700	-2.12013700	-1.05340300	H	-3.08947400	0.10833800	-2.13663800
H	0.33726600	-2.23515000	1.49934600	H	-4.25768100	-0.55109600	-0.04640900
H	-3.72521300	-0.87000500	1.47482300	N	0.86154500	0.79802300	0.07794800
H	-1.23883900	-0.19331000	2.09946100	C	1.18047500	2.19174400	-0.23731700
H	-1.72876300	-1.64452400	3.03826000	H	0.25598000	2.77284000	-0.19527300
H	-1.27798700	-4.04190300	1.98170400	H	1.89512800	2.58617900	0.49200500
H	-3.54543100	-3.27114300	0.24520300	H	1.62535000	2.28082000	-1.23684200
H	-3.49533100	-3.28583000	2.01427100	C	1.93743900	-0.00987300	0.25476100
H	-0.27835700	3.19724900	-0.68487400	O	3.08390000	0.33473600	0.24148500
H	4.07052900	3.11049600	1.10471900	Cl	1.51156900	-1.74271000	0.51485900
H	4.30575400	1.74843600	-0.02252100				
H	3.48794400	3.22271600	-0.57891600	INTc'			
H	3.05372600	1.54411200	2.98321600	Pd	-0.05983200	-0.54631900	-0.77157500
H	1.55490600	0.57861300	2.80574900	C	0.89509000	1.25599700	-0.81420700
H	3.05054900	0.02769700	2.03196300	C	1.62544100	-1.03063900	0.32945200
H	1.84595200	3.70609100	2.35336600	C	2.52179500	0.19492900	0.68935900
H	1.08648600	4.11928800	0.79396900	C	3.90588100	-0.24336400	0.14541500
H	0.22587400	3.06197300	1.92601000	C	3.52363400	-1.03712900	-1.10805200
H	-5.72637800	1.08858600	-1.11468900	C	2.59322400	-1.99440700	-0.35918700
H	-4.83967900	-0.35901000	-1.62336600	C	0.42831000	2.34948300	-1.54891700
H	-5.16299900	-0.08653800	0.08472100	C	0.99329600	3.61333000	-1.37866000
C	4.07698100	-0.94555500	-0.99459100	C	2.02906700	3.79285100	-0.46762900
C	2.44373600	-3.06762900	-0.09105200	C	2.55401300	2.71250700	0.24701600
C	1.98802200	-1.88718600	-2.63499100	C	1.99632200	1.43797600	0.04632100
H	4.66907600	-1.73955600	-1.47116600	C	4.45351500	-1.34859400	1.05507400
H	4.17681800	-0.02768500	-1.58834200	C	3.53928300	-2.55641600	0.72344200
H	4.48849300	-0.75672600	0.00554000	P	-1.04465400	-2.75242200	-0.61417900
H	3.16666600	-3.69868900	-0.62655200	H	0.61124800	4.46187100	-1.94748600
H	2.77259200	-2.95321500	0.95004100	H	2.45595400	4.78572100	-0.31315400
H	1.46798100	-3.56855400	-0.08338100	H	2.58781100	0.31433300	1.78846300
H	2.74187700	-2.59717700	-3.00352800	H	1.16116900	-1.48032200	1.22301700

H	2.11417900	-2.77588000	-0.96480700				
H	4.59989700	0.59209000	-0.00958300	TS4			
H	3.00125800	-0.43764200	-1.86392200	Pd	-0.08718600	-0.15526700	-0.64932600
H	4.38527400	-1.54144100	-1.56943100	C	-1.94053900	-0.99641300	-0.66589300
H	4.12207800	-3.40033100	0.32717400	C	-1.09723000	1.16018700	0.59684600
H	2.98972700	-2.92664500	1.60146700	C	-2.51207100	0.67483800	1.04009400
H	4.41886700	-1.06410700	2.11643100	C	-3.38668600	1.91632100	0.74106500
H	5.50201900	-1.56968800	0.81230200	C	-2.78076000	2.40811300	-0.57545800
H	-0.38985500	2.23133900	-2.26092100	C	-1.36941300	2.54808200	-0.00362300
Cl	-2.63947100	0.46512900	-1.53940000	C	-2.22107100	-2.05403100	-1.52564500
C	-2.56738100	2.17774500	-0.85651700	C	-3.47031400	-2.66482800	-1.46318400
O	-2.75312900	3.08973000	-1.60396000	C	-4.40636000	-2.24392200	-0.52413700
N	-2.27534200	2.22660700	0.45936800	C	-4.14233400	-1.18073800	0.33936200
C	-1.87552900	3.55227400	0.94981600	C	-2.89970300	-0.52933200	0.24221000
H	-0.83584900	3.76651500	0.66155400	C	-2.99465600	3.04011100	1.71091400
H	-2.53070300	4.31050500	0.51260300	C	-1.61612500	3.50662300	1.17583400
H	-1.97575300	3.56037000	2.03798700	P	1.77044600	1.44013200	-1.30552700
C	3.69603100	2.94203500	1.19632000	H	-3.70431300	-3.49553100	-2.12885700
H	3.61681500	2.32514900	2.10223400	H	-5.36902100	-2.75331100	-0.45094800
H	4.66825800	2.70327300	0.74042700	H	-2.53188200	0.45638300	2.12443500
H	3.74063400	3.99334600	1.50921300	H	-0.38417100	1.22810000	1.43788700
C	-0.61754200	-3.94330200	-1.95100600	H	-0.61052900	2.91620900	-0.70340200
H	-0.97390700	-3.55554600	-2.91287700	H	-4.46123200	1.70209100	0.72298500
H	0.47177300	-4.05417300	-2.01730000	H	-2.85428000	1.67514400	-1.38959200
H	-1.06797600	-4.93001600	-1.77281700	H	-3.20134700	3.36690700	-0.91126200
C	-0.59029200	-3.71548500	0.88484500	H	-1.65827100	4.54768900	0.82295000
H	0.49746000	-3.84725600	0.93515600	H	-0.81782800	3.45032200	1.92994700
H	-0.90920700	-3.15658200	1.77405800	H	-2.94981400	2.68507600	2.75021400
H	-1.06943900	-4.70434900	0.88649100	H	-3.72769400	3.85731100	1.67987800
C	-2.87765100	-2.92138900	-0.57822700	H	-1.45869700	-2.42946200	-2.20838500
H	-3.27948700	-2.33693100	0.26007400	Cl	1.40144300	-2.03532300	-1.55719400
H	-3.30898200	-2.52466000	-1.50562000	C	0.48932500	-1.97620900	0.57042600
H	-3.17915400	-3.97243400	-0.46728500	O	-0.30378100	-2.84766600	0.70210400
C	-2.19929400	1.12121600	1.35988100	N	1.37342100	-1.51819400	1.50571100
C	-1.00252700	0.86196000	2.02565700	C	0.87681000	-1.74094600	2.87184400
C	-3.33540300	0.36123800	1.62941900	H	-0.09282900	-1.24304400	3.01002900
C	-0.94830100	-0.16466400	2.96300500	H	0.75020000	-2.81416200	3.05628300
H	-0.11724500	1.45239900	1.78879700	H	1.60342700	-1.32873000	3.57568100
C	-3.26644400	-0.68033400	2.54814400	C	-5.18294900	-0.77354100	1.34473700
H	-4.26686200	0.59176900	1.11396300	H	-4.73819600	-0.38113400	2.26909900
C	-2.07429400	-0.94185600	3.22029700	H	-5.85503900	0.00730300	0.95831100
H	-0.01248700	-0.36477500	3.48336100	H	-5.81467500	-1.62934500	1.61610000
H	-4.15587600	-1.27226400	2.75909000	C	1.09631500	2.02254400	-2.92082200
H	-2.02759900	-1.74370200	3.95599500	H	1.02198300	1.15514700	-3.59007200

H	0.08859100	2.44014400	-2.80261300	H	2.48287800	1.30497900	1.77545800
H	1.74801700	2.77676900	-3.38408100	H	1.75521200	-0.92416500	1.38126000
C	2.20931500	3.02390700	-0.46861500	H	2.59266100	-1.76366900	-1.08014900
H	1.31437100	3.55312000	-0.12064900	H	3.90757800	2.25405400	-0.32929000
H	2.83598700	2.79889900	0.40260500	H	2.43709900	0.73638900	-1.95294800
H	2.77234600	3.68211700	-1.14490400	H	4.14089300	0.19335500	-1.99228400
C	3.43300300	0.87717300	-1.84708000	H	4.92307200	-1.63555400	-0.27256300
H	4.07794000	0.70982200	-0.97653100	H	4.00963100	-1.63750400	1.24325900
H	3.33411800	-0.07275900	-2.38525300	H	4.74163200	0.61431400	1.65383900
H	3.89877300	1.62739000	-2.50123600	H	5.65699300	0.55477500	0.14102800
C	2.66450700	-0.94507700	1.33765000	H	2.17926200	5.16640000	1.27821700
C	2.93366700	0.30410700	1.89949500	H	2.75083100	3.60987200	1.90461900
C	3.69545000	-1.68655800	0.76101500	H	3.36768100	4.22879900	0.37208500
C	4.23064200	0.80603100	1.89177900	H	-1.63822500	1.80597300	-1.64503000
H	2.11678000	0.87283500	2.34620300	H	-1.61553000	-4.69836000	1.18201400
C	4.98644900	-1.17098500	0.74026400	H	-1.76410400	-3.09818500	1.96529700
H	3.47765200	-2.66577800	0.34136000	H	-2.59400600	-3.41457600	0.42356500
C	5.26052400	0.06971100	1.31109200	H	-0.17749800	-5.15719400	-1.06941000
H	4.43612300	1.77614300	2.34268000	H	-0.93350600	-3.84332900	-2.04053800
H	5.78785100	-1.75342300	0.28956300	H	0.81792500	-3.90859000	-1.89516000
H	6.27652100	0.46023900	1.30793700	H	1.00317100	-4.71511000	1.39014700
				H	2.11404300	-3.49048300	0.71670300
				H	1.11994500	-3.09276700	2.14283800
INTd				Cl	0.07464600	-0.91962900	-2.72915800
Pd	-0.06476800	-0.54851600	-0.30608000	C	-0.68308700	-0.33255300	1.66091200
C	0.12970800	1.48456200	-0.44819800	O	-0.01579400	-0.63766600	2.63199600
C	1.88732800	-0.33804600	0.46669400	N	-1.99421500	0.06591700	1.81019000
C	2.28397100	1.13432800	0.70261600	C	-2.48076100	0.20596000	3.18173700
C	3.59980300	1.22329800	-0.12222200	H	-2.10840500	1.12636300	3.65116900
C	3.26968900	0.36391400	-1.34514400	H	-3.57433800	0.21666800	3.17097300
C	2.90226900	-0.87173900	-0.52294000	H	-2.12765800	-0.64198700	3.77593800
C	-0.81569700	2.26621600	-1.09984700	C	-2.83389700	0.47203600	0.74280100
C	-0.70354000	3.65249600	-1.04182800	C	-2.94991600	-0.29821700	-0.41569300
C	0.34568400	4.24088700	-0.34407400	C	-3.57050300	1.65369400	0.85069000
C	1.33433500	3.46765700	0.26513500	C	-3.73789000	0.13678600	-1.47717800
C	1.23121400	2.06681100	0.18966100	H	-2.43660900	-1.25752100	-0.49122500
C	4.66728600	0.37901600	0.58323000	C	-4.38768900	2.06358000	-0.19493000
C	4.19004300	-1.07044700	0.31929700	H	-3.47344900	2.26790500	1.74428500
P	-0.19761700	-3.00648400	0.10792500	C	-4.46683200	1.31496200	-1.36772400
C	1.13779000	-3.64298500	1.19291400	H	-3.77641200	-0.45934600	-2.38688300
C	2.46194600	4.14595000	0.99033400	H	-4.95016600	2.99098600	-0.10095800
C	-1.68383600	-3.61711500	1.00113000	H	-5.09406800	1.65013700	-2.19126600
C	-0.11678200	-4.09828400	-1.35543100				
H	-1.45098100	4.27546200	-1.53343400				
H	0.41110300	5.32787200	-0.27401000	TS5			

Pd	0.27062600	-0.66457800	-0.27794300	Cl	-1.22289900	-1.55304000	-2.07216800
C	-0.18974900	1.36377000	-0.34070100	C	-0.57930000	0.28989600	1.46856900
C	2.07157200	-0.00305000	0.53296600	O	0.15297500	0.58186700	2.38163800
C	2.12640600	1.55056300	0.56683100	N	-1.89194800	-0.06304700	1.68076300
C	3.35559500	1.82091300	-0.35172800	C	-2.26425400	-0.13344800	3.09892600
C	3.21923100	0.73677100	-1.42114800	H	-2.38795500	0.86796600	3.53604400
C	3.20000000	-0.41094100	-0.41007400	H	-3.20926400	-0.68002500	3.17223700
C	-1.27911700	1.85387400	-1.06319000	H	-1.48543700	-0.65868700	3.65877200
C	-1.35184400	3.21568800	-1.33223500	C	-3.00936000	0.13551200	0.80468000
C	-0.35758600	4.06511500	-0.86161200	C	-3.53141200	-0.91816000	0.06711300
C	0.77645500	3.58210000	-0.20120000	C	-3.63669100	1.38339100	0.79534000
C	0.88282000	2.20021400	0.02256500	C	-4.65278900	-0.70799800	-0.73066100
C	4.61709300	1.37159700	0.39653000	H	-3.03920100	-1.88657600	0.09486700
C	4.52011300	-0.17294300	0.35525300	C	-4.76196800	1.58616800	0.00879700
P	0.81734100	-2.97884500	0.06087100	H	-3.21008400	2.19608200	1.38392500
C	2.04621300	-3.45893600	1.33952900	C	-5.26495300	0.53961900	-0.76332200
C	1.81161900	4.56848400	0.26657500	H	-5.03739300	-1.52483500	-1.33795500
C	-0.67844200	-3.88538100	0.60167000	H	-5.24178400	2.56327800	-0.01080000
C	1.35717100	-3.92406100	-1.40934800	H	-6.13993400	0.69972800	-1.39112100
H	-2.19884000	3.61567200	-1.88872500				
H	-0.44785900	5.14153900	-1.01875900	INTe			
H	2.33178200	1.90942000	1.58832700	Pd	-1.55975300	0.27367300	-0.28650800
H	2.13530800	-0.45436400	1.52878300	C	0.72697200	1.24433000	0.69566600
H	3.11802100	-1.42225500	-0.82968400	C	-0.32340600	-1.38204100	-0.32853900
H	3.40783900	2.84812400	-0.72497800	C	0.92844800	-0.67244300	-0.90913500
H	2.29819600	0.81227500	-2.01479700	C	1.01850700	-1.29618100	-2.31822100
H	4.08157200	0.69752900	-2.10144800	C	-0.43726800	-1.61836000	-2.68048400
H	5.36340500	-0.61408100	-0.19481700	C	-0.70708500	-2.40095600	-1.39147100
H	4.50448000	-0.63074000	1.35414200	C	0.54907900	2.57531700	1.06716200
H	4.65289000	1.77219200	1.41888200	C	0.44224700	3.55602200	0.09521400
H	5.51820200	1.72352500	-0.12335400	C	0.50103000	3.19338200	-1.23903400
H	1.32932300	5.50526900	0.57484700	C	0.64082200	1.86413400	-1.65329800
H	2.38886600	4.19718700	1.12240200	C	0.74882700	0.84093300	-0.67536200
H	2.53085400	4.82968900	-0.52314300	C	1.57424700	-2.71738400	-2.11576000
H	-2.04474700	1.17288600	-1.42849900	C	0.40447200	-3.46858100	-1.43068900
H	-0.46544700	-4.95018500	0.76865900	P	-3.17707800	-0.80046100	0.86434400
H	-1.06084500	-3.43903800	1.52884600	C	-2.78004900	-2.40017400	1.66107600
H	-1.43884100	-3.77493200	-0.18108700	C	0.68899500	1.63721700	-3.13933400
H	1.43544500	-4.99657200	-1.18462900	C	-3.66972500	0.24293000	2.27505700
H	0.61891900	-3.75591000	-2.20256100	C	-4.72630700	-1.12624500	-0.04574600
H	2.33029700	-3.55930900	-1.76024900	H	0.29423800	4.59691800	0.37425600
H	2.11541000	-4.55171500	1.42739700	H	0.39889700	3.96060100	-2.00535900
H	3.03828500	-3.06267000	1.08891900	H	1.84130200	-0.96323600	-0.37123200
H	1.74780900	-3.04167600	2.30952500	H	-0.18660200	-1.81376700	0.67317700

H	-1.72081600	-2.81232600	-1.28539000	C	-1.20977000	1.47835200	-0.96950700
H	1.59549800	-0.72182200	-3.04787700	C	-0.07931000	1.54776700	-0.08139900
H	-1.09615700	-0.74301900	-2.77999500	C	-0.29646900	2.80149900	0.74086700
H	-0.51879900	-2.23189800	-3.58919400	C	-1.82579800	2.88166900	0.83419200
H	0.09248300	-4.34545700	-2.01546400	C	-2.04720700	2.70811800	-0.66967200
H	0.65852900	-3.82510100	-0.42182600	C	2.43217100	-1.39993100	1.37521200
H	2.49950300	-2.71818100	-1.52238500	C	2.40354100	-1.25232700	2.75112800
H	1.81210600	-3.16800300	-3.08887300	C	1.37918600	-0.51849100	3.33395200
H	0.40542500	2.55723500	-3.66243200	C	0.35608200	0.05994900	2.57848700
H	1.69957100	1.37025300	-3.47749600	C	0.38730900	-0.09538500	1.18091400
H	0.00796500	0.85191300	-3.48007600	C	-0.01556300	3.95322500	-0.25866600
H	0.49293600	2.82358400	2.12616800	C	-1.22908700	3.89951000	-1.22160600
H	-4.45110800	-0.24240800	2.87664900	P	-3.47699800	-0.85377000	-0.93569500
H	-2.77813200	0.42706800	2.88718400	C	-4.15652100	0.16509000	-2.30539600
H	-4.02232600	1.20308800	1.88061100	C	-0.78463100	0.70257400	3.31465200
H	-5.50220000	-1.52736700	0.62108200	C	-3.19245500	-2.46031100	-1.75828700
H	-5.06481200	-0.18163100	-0.48747300	C	-4.94835700	-1.14212400	0.10823100
H	-4.53813300	-1.84139000	-0.85578300	H	3.16812000	-1.71762900	3.37013800
H	-3.64522900	-2.77150100	2.22702600	H	1.34146000	-0.41764300	4.41945500
H	-2.49015400	-3.14960300	0.91493600	H	0.91306300	1.38644300	-0.49696100
H	-1.93929300	-2.24758800	2.34924300	H	-1.06308500	1.16013400	-2.00528700
Cl	-2.97573500	2.24715200	-0.54419300	H	-3.08834800	2.67464600	-1.01110400
C	0.87847000	0.30937300	1.86948300	H	0.27930400	2.86801200	1.66995000
O	-0.04903400	0.11198100	2.64391800	H	-2.28150800	2.07884400	1.42595600
N	2.10842800	-0.26979200	2.10830200	H	-2.17122000	3.85574000	1.20789600
C	2.14696000	-1.21755500	3.21701500	H	-1.81761700	4.82597300	-1.17245900
H	3.18894900	-1.41482900	3.48174800	H	-0.93826200	3.75170500	-2.26986800
H	1.62253600	-0.79077000	4.07611600	H	0.94782500	3.82770600	-0.77213500
H	1.64812900	-2.16222600	2.95406000	H	0.02769200	4.90939700	0.27901800
C	3.27590500	-0.10431000	1.31554600	H	-0.63415100	0.62555700	4.39828200
C	3.99897200	-1.23803900	0.92807800	H	-0.90932600	1.76513100	3.07512200
C	3.72684600	1.15851800	0.92784700	H	-1.72532100	0.18901000	3.07135400
C	5.14320000	-1.11070000	0.15087600	H	3.21682000	-1.99131000	0.90741300
H	3.64168100	-2.22552100	1.22109500	H	-4.10482300	-2.82278000	-2.25215100
C	4.86248000	1.27614000	0.13390100	H	-2.38952900	-2.34835600	-2.49685100
H	3.18799700	2.04718100	1.24800100	H	-2.85933200	-3.17435200	-0.99635900
C	5.57569800	0.14754700	-0.25686800	H	-5.75748700	-1.60871600	-0.47049300
H	5.69295100	-2.00264700	-0.14501600	H	-4.64913500	-1.79539000	0.93589300
H	5.20029900	2.26649500	-0.16615800	H	-5.30139900	-0.19008700	0.52277500
H	6.46830600	0.24777800	-0.87120000	H	-4.98938300	-0.35527700	-2.79804700
				H	-4.52093800	1.12677000	-1.92443000
TS6				H	-3.37283300	0.36191500	-3.04721500
Pd	-1.51163300	-0.25530400	0.17898300	Cl	-1.93023200	-2.26929400	1.50472800
C	1.44538200	-0.80751500	0.58209900	C	1.46520300	-1.01669400	-0.89556600

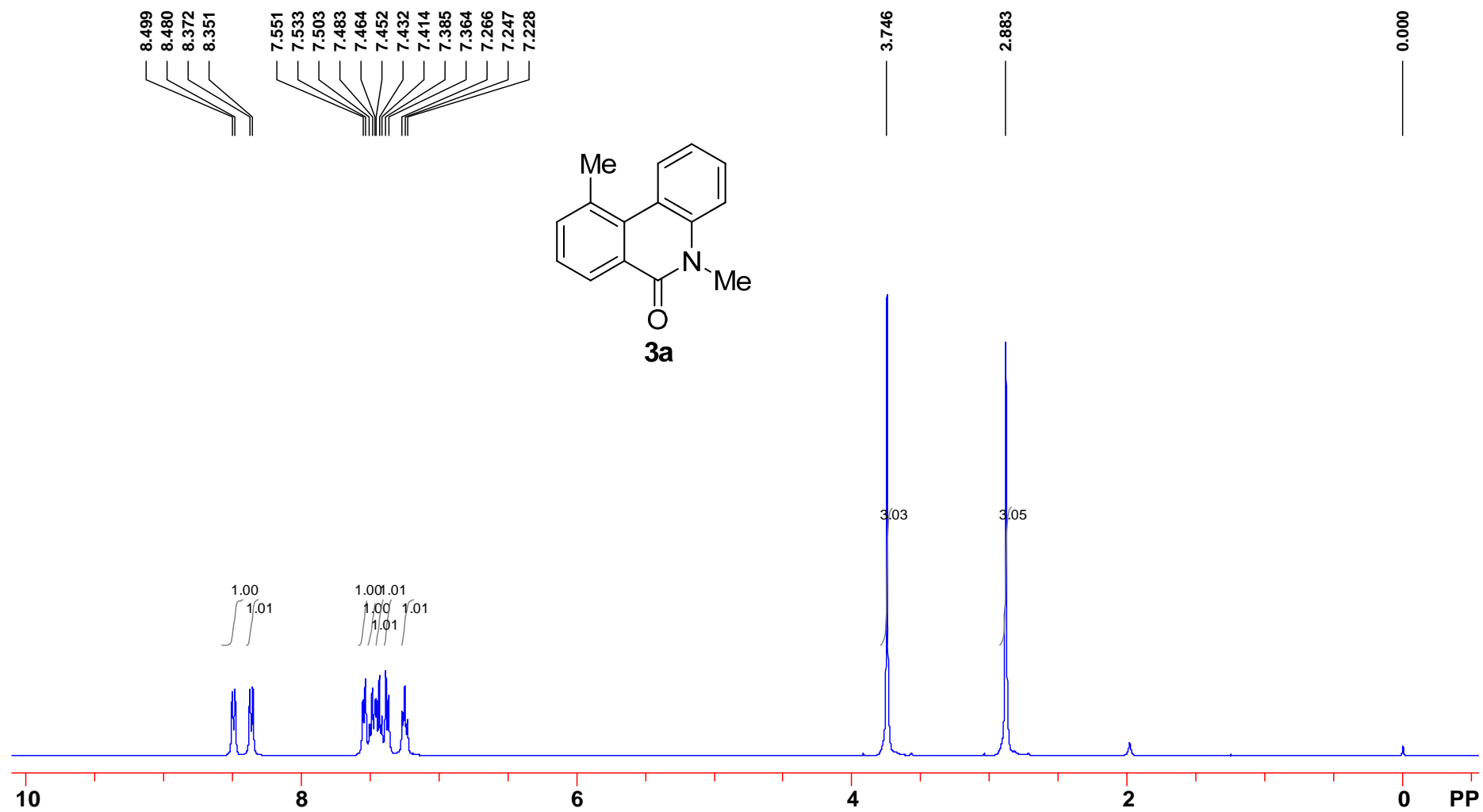
O	0.43802500	-1.16694700	-1.55131400	H	-3.96755000	1.19876600	1.69394400
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C	2.65736700	-1.44998100	-2.94512500	Cl	-0.87792500	-2.35121500	-1.08786600
H	2.35987100	-0.59612500	-3.57077000	C	1.99790400	0.92836200	-1.73615600
H	3.65073000	-1.78668100	-3.25626800	O	2.32870100	1.01139300	-2.90287400
H	1.92872400	-2.25052700	-3.09493900	N	1.31461500	1.98489200	-1.11169800
C	3.89143200	-0.47958100	-1.05582800	C	0.65121800	2.95091900	-1.96948700
C	3.91255300	0.85765100	-0.66113600	H	0.61158200	3.92658000	-1.47313900
C	5.07205500	-1.22343900	-1.02110100	H	1.23239300	3.02638900	-2.89166500
C	5.09310600	1.43361500	-0.20587200	H	-0.37074200	2.63348500	-2.23392000
H	2.99702200	1.44720500	-0.71092800	C	0.98655000	1.93698200	0.25480300
C	6.25386400	-0.64023400	-0.58182800	C	-0.36226100	1.93820400	0.67650300
H	5.04681300	-2.27114400	-1.32082300	C	2.00341300	1.89391200	1.21938000
C	6.26707800	0.68891200	-0.16744400	C	-0.65603000	1.81761400	2.05248000
H	5.09604900	2.47550100	0.10959300	H	-1.14139400	2.23960500	-0.02388200
H	7.16754000	-1.23151000	-0.55300100	C	1.69198700	1.79185500	2.56300800
H	7.19176200	1.14257700	0.18437700	H	3.03848800	1.91491700	0.88461300
				C	0.36078600	1.72588400	2.98734700
				H	-1.69801300	1.83355800	2.36955200
INTf				H	2.49578500	1.75255100	3.29581100
Pd	-0.58152600	-0.30139100	0.06340500	H	0.12563200	1.63101200	4.04511000
C	2.31484800	-0.24346000	-0.87069600				
C	3.62201400	-0.73578600	-0.97118700				
C	4.05199900	-1.72877500	-0.10636900	INTf'			
C	3.17159500	-2.23292300	0.84594200	Pd	-0.71713300	0.62456700	-0.78615600
C	1.84558200	-1.79615600	0.92886900	C	-0.98613600	-1.51242600	-1.92650000
C	1.42027300	-0.79799000	0.04643100	C	-2.04496000	-1.18359200	-2.78188500
P	-3.01292700	-0.10434500	-0.14865900	C	-3.33997400	-1.61227500	-2.50056000
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C	-3.94364800	-1.58354700	0.39670400	P	-0.21371500	2.58942600	0.22608400
H	5.07120300	-2.10677200	-0.16498300	H	-4.15953800	-1.35568300	-3.16976400
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H	1.47054600	-3.03923600	2.65125500	H	-1.83191900	-0.59734300	-3.67484100
H	0.37716900	-1.64534200	2.51087800	H	0.05876300	-1.24495700	-2.16090800
H	0.16475600	-3.03526900	1.44039900	C	1.87493400	0.68399100	-1.82898200
H	4.28615900	-0.30308400	-1.71867000	O	2.92813000	1.34500400	-1.60831100
H	-4.55800400	-0.00060200	-2.05839700	O	0.75182600	1.34126100	-2.13512800
H	-3.08762700	0.98597900	-2.32039900	O	1.81186800	-0.59011900	-1.69007500
H	-2.99188400	-0.78249300	-2.46413100	H	-2.73524600	-3.25767700	0.42533400
H	-5.00165700	-1.51263000	0.10938600	N	-0.21293900	-2.44088100	0.19719100
H	-3.48764200	-2.46610600	-0.06627400	C	-0.08471300	-1.64990900	1.31587600
H	-3.87051900	-1.68807000	1.48579200	O	0.93564600	-1.68109900	2.00684600
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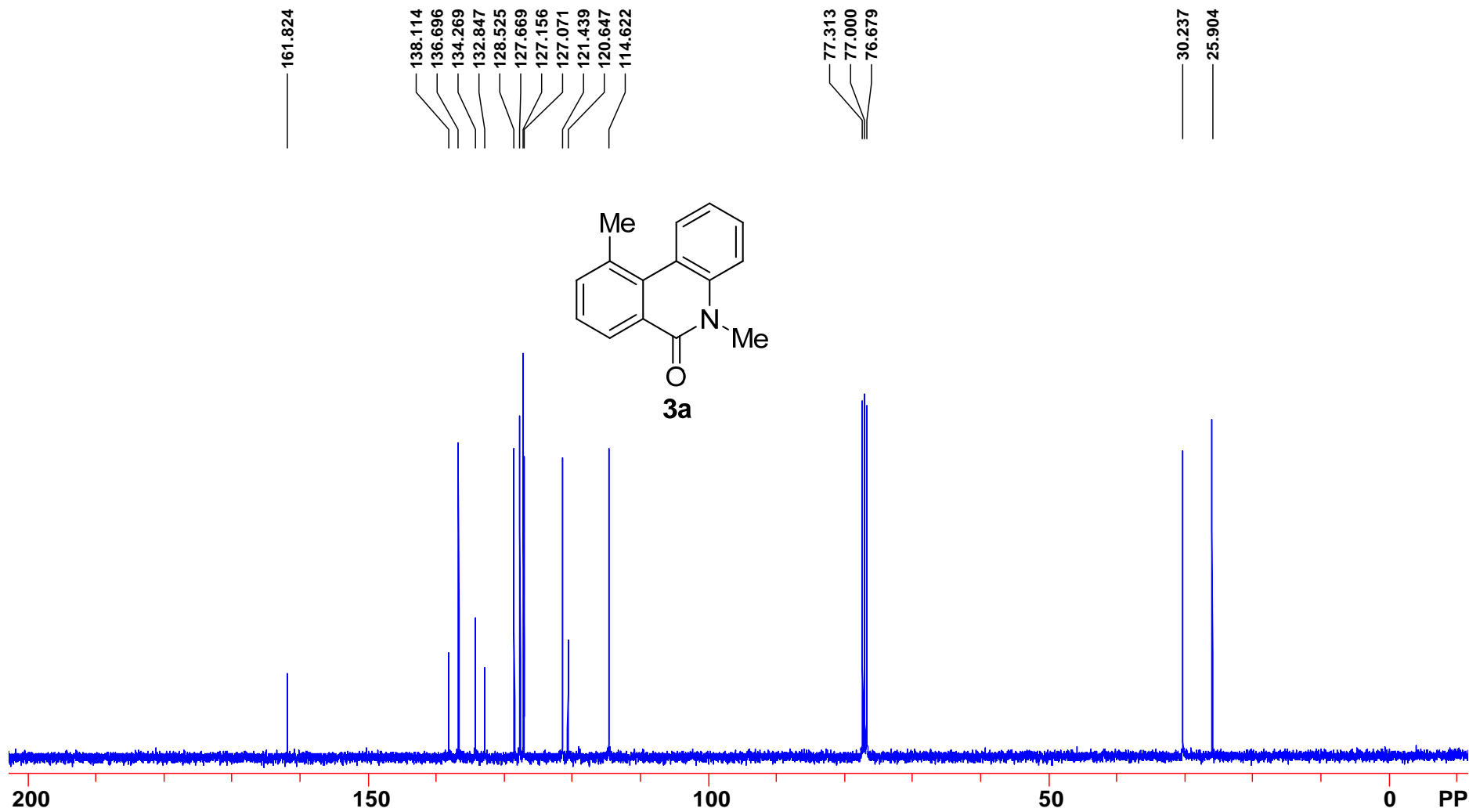
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H	3.41793300	-0.93892000	-2.52608100	C	-0.13038200	-4.20437300	-0.23076600
C	3.32197100	-2.58921900	0.11360200	H	-0.34277500	-4.33447400	-1.29910900
H	2.86918600	-3.01531900	1.01857800	H	0.95004900	-4.32117500	-0.08088100
H	3.09190600	-3.25179500	-0.73051900	H	-0.65296800	-4.98921900	0.33363200
H	4.41218100	-2.55687100	0.24852100	C	-0.37691100	-2.58026700	2.12080200
C	3.36035600	0.06072100	1.16284300	H	0.70149700	-2.57434600	2.32918300
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N	-0.13465800	1.69080900	1.75702800	P	-0.23992300	2.73244100	-0.07589400
C	0.43621500	2.30638100	0.59445700	C	-1.95178600	3.11977100	-0.62142500
C	0.75527400	3.66410600	0.65680500	H	-2.63794200	2.37296900	-0.19902800
C	0.71101000	1.55247000	-0.55673100	H	-2.26184900	4.12495600	-0.30323600
C	1.33778500	4.29997400	-0.43428400	H	-2.02193300	3.04524700	-1.71332200
H	0.52791000	4.22339200	1.56560900	C	0.66422600	4.22893900	-0.66253700
C	1.25509900	2.22225700	-1.65580500	H	1.69331800	4.21629400	-0.28134600
C	1.57771900	3.57840400	-1.59904000	H	0.71005500	4.23077100	-1.75814700
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H	2.01613500	4.07095400	-2.46696700	H	-0.82672200	4.06716100	1.91988000
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H	1.58507300	2.16683700	2.83313300	H	0.63246900	3.06574400	2.18271800
H	0.07025000	2.30567700	3.77789800	C	-0.85748100	-1.37240200	1.97913300
H	0.72134200	0.70499800	3.40446100	O	-0.55631100	-1.49142200	3.16170700
C	-2.14305100	0.93111600	0.54204500	N	-1.92152800	-0.56430700	1.59916300
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C	-2.39147100	0.17011500	-1.73629700	C	-3.76726500	-0.46693100	0.01350900
C	-3.48952200	1.30936700	0.57945900	C	-1.47359100	-0.31222900	-0.78663800
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C	-3.72114500	0.59389200	-1.70248800	C	-3.34492700	-0.25082500	-2.34578600
H	-4.33692000	0.47769000	-2.59674400	H	-5.31669300	-0.36648200	-1.47428000
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H	-0.94807100	0.10680900	-3.33612400	H	-3.70891900	-0.16657500	-3.36928500
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P	-0.66323900	-2.52549700	0.30641300	H	-3.49047400	-0.59669500	3.03897400
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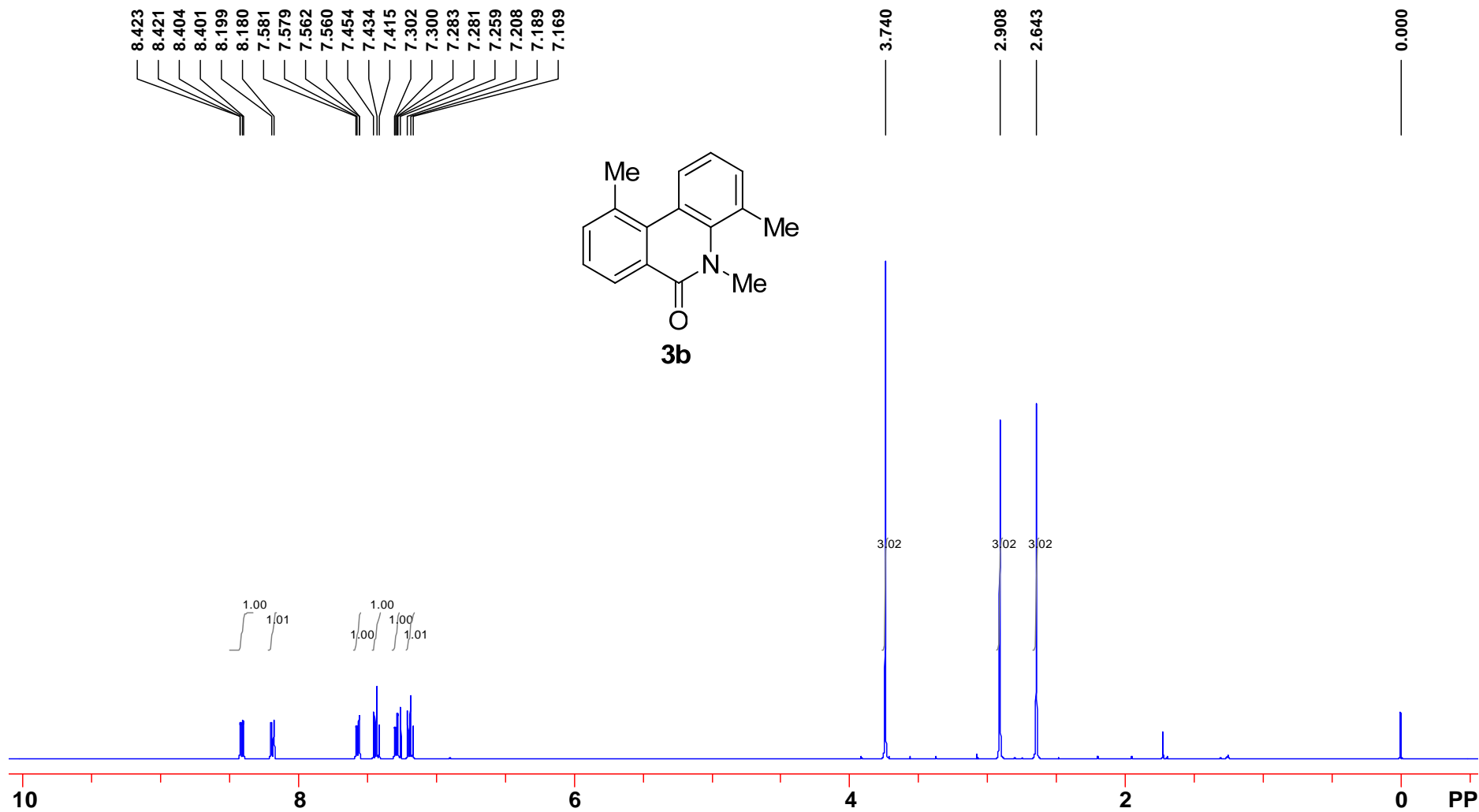
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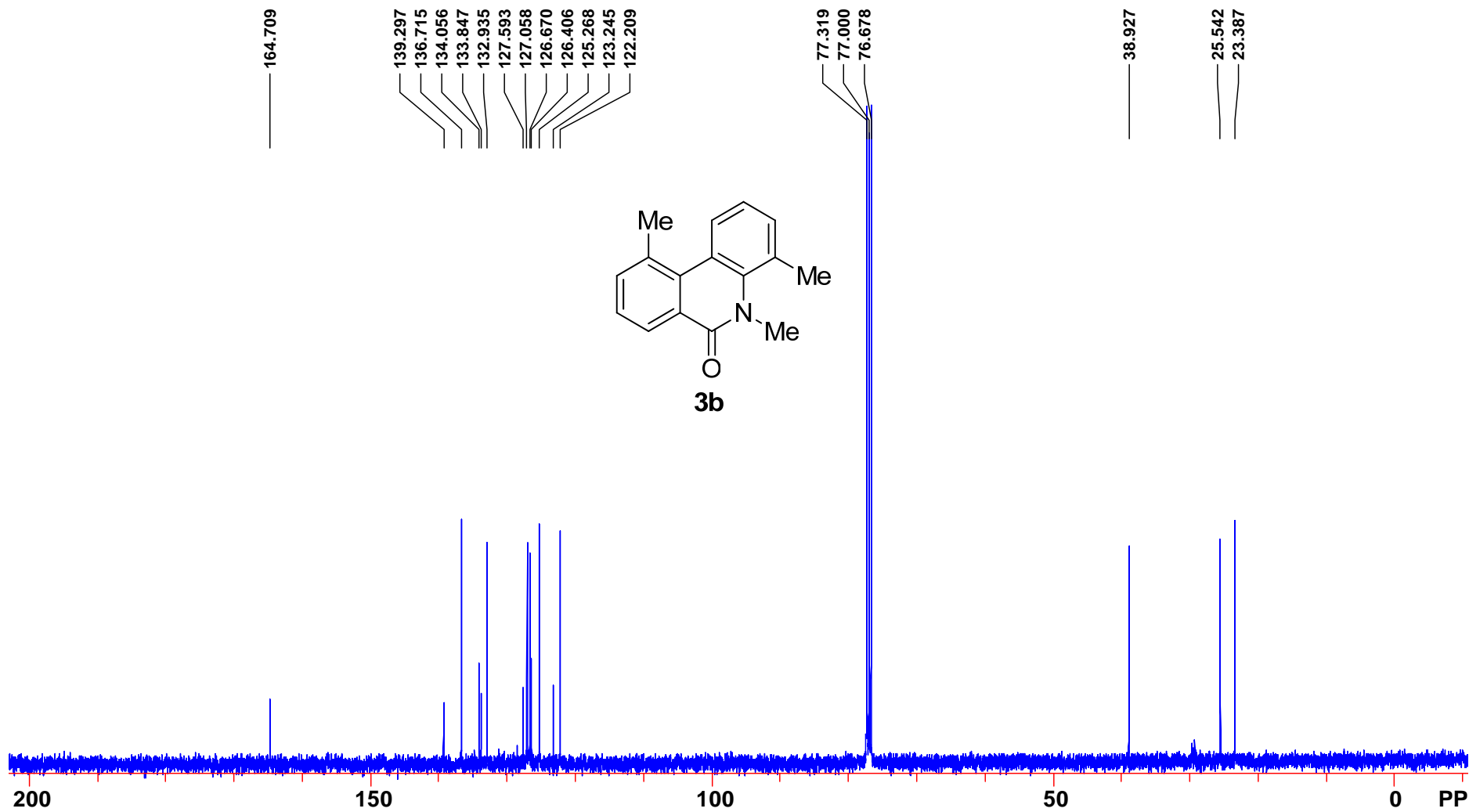
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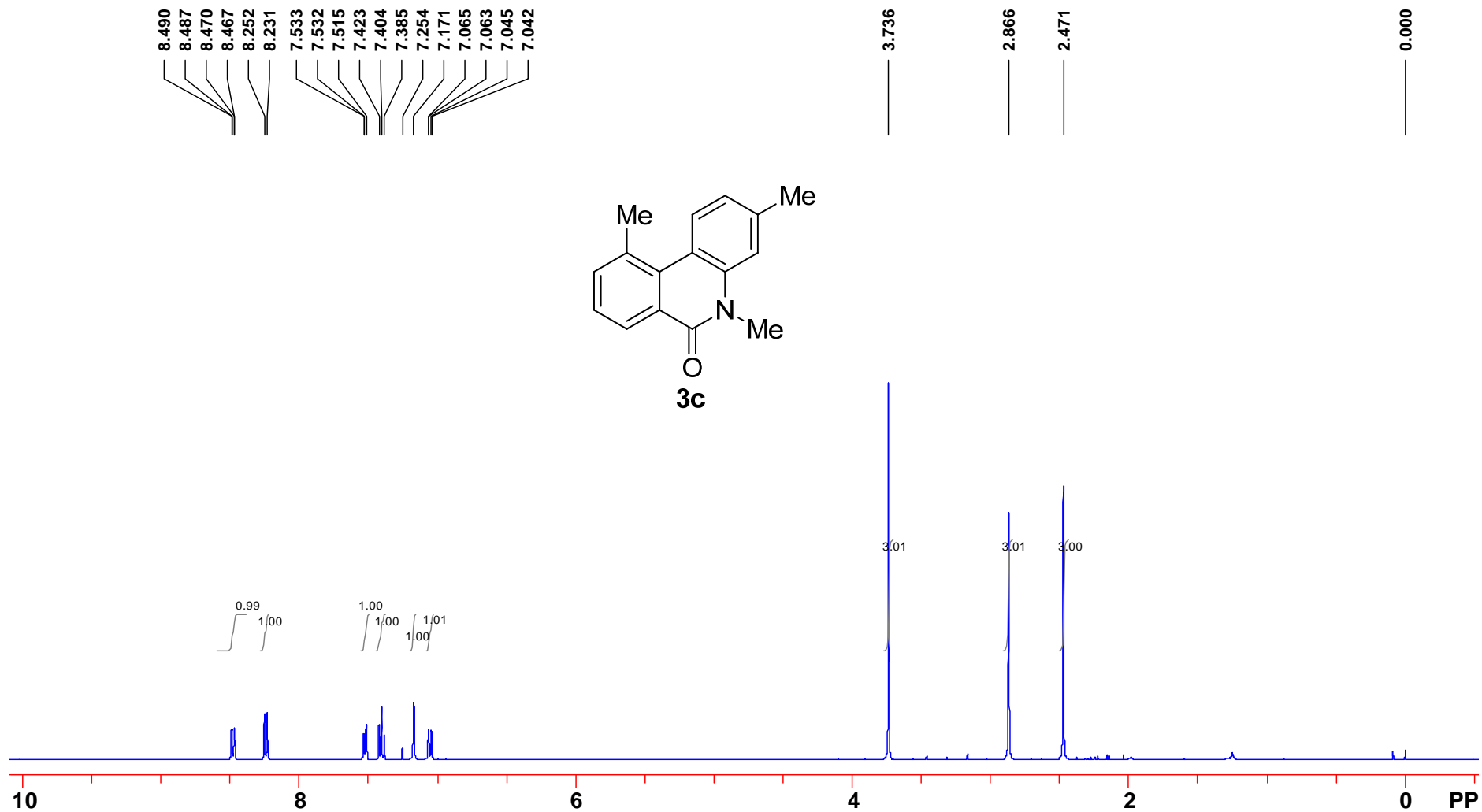
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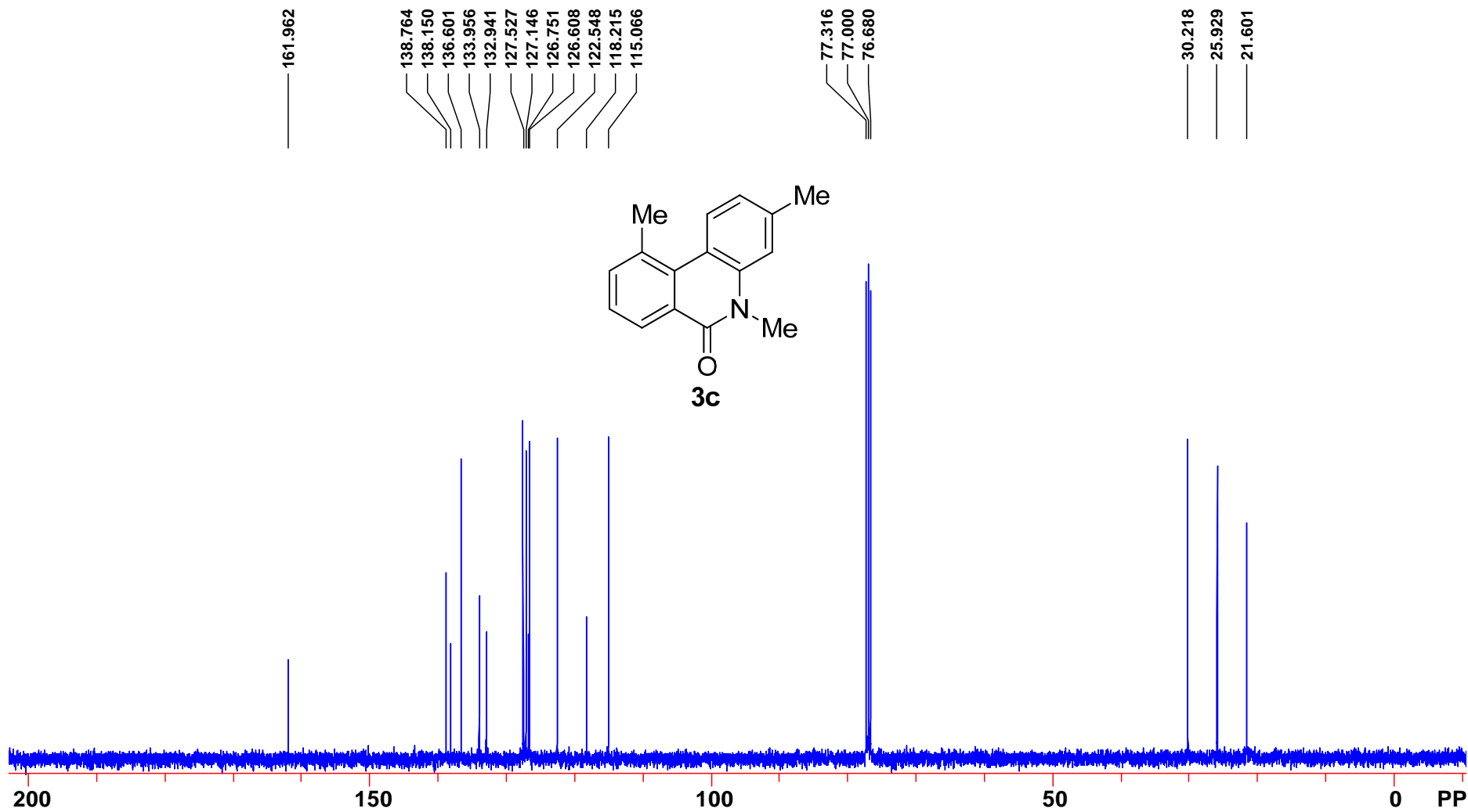


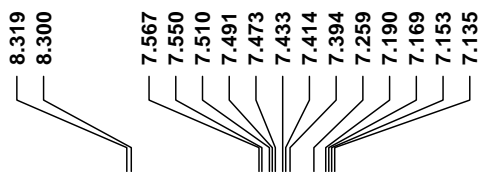








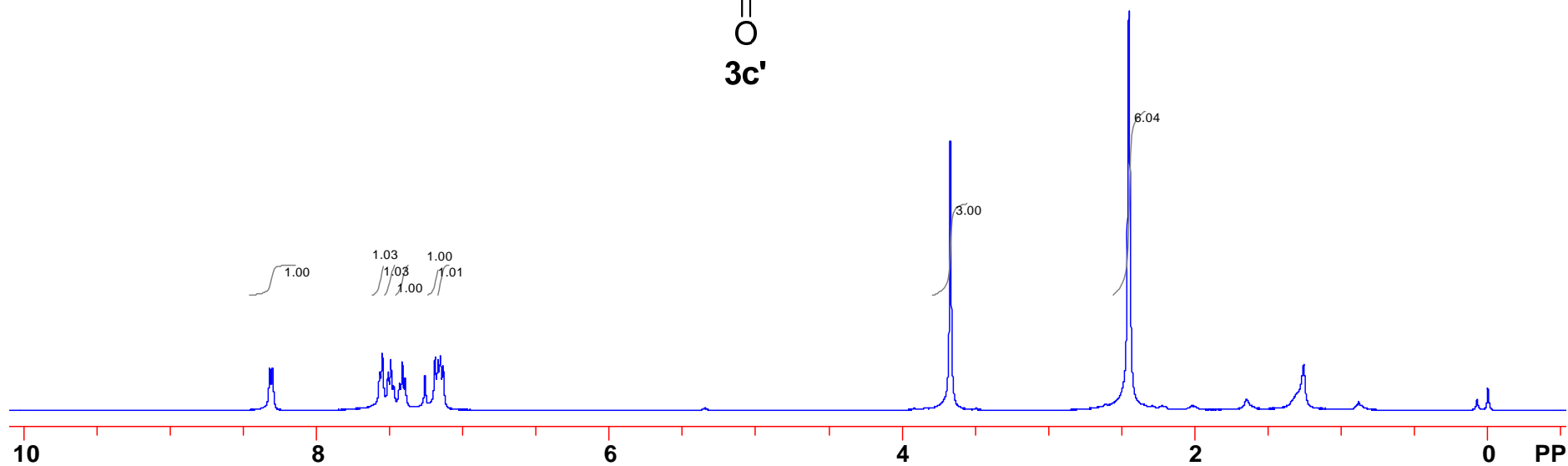
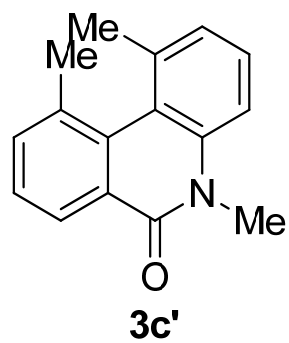


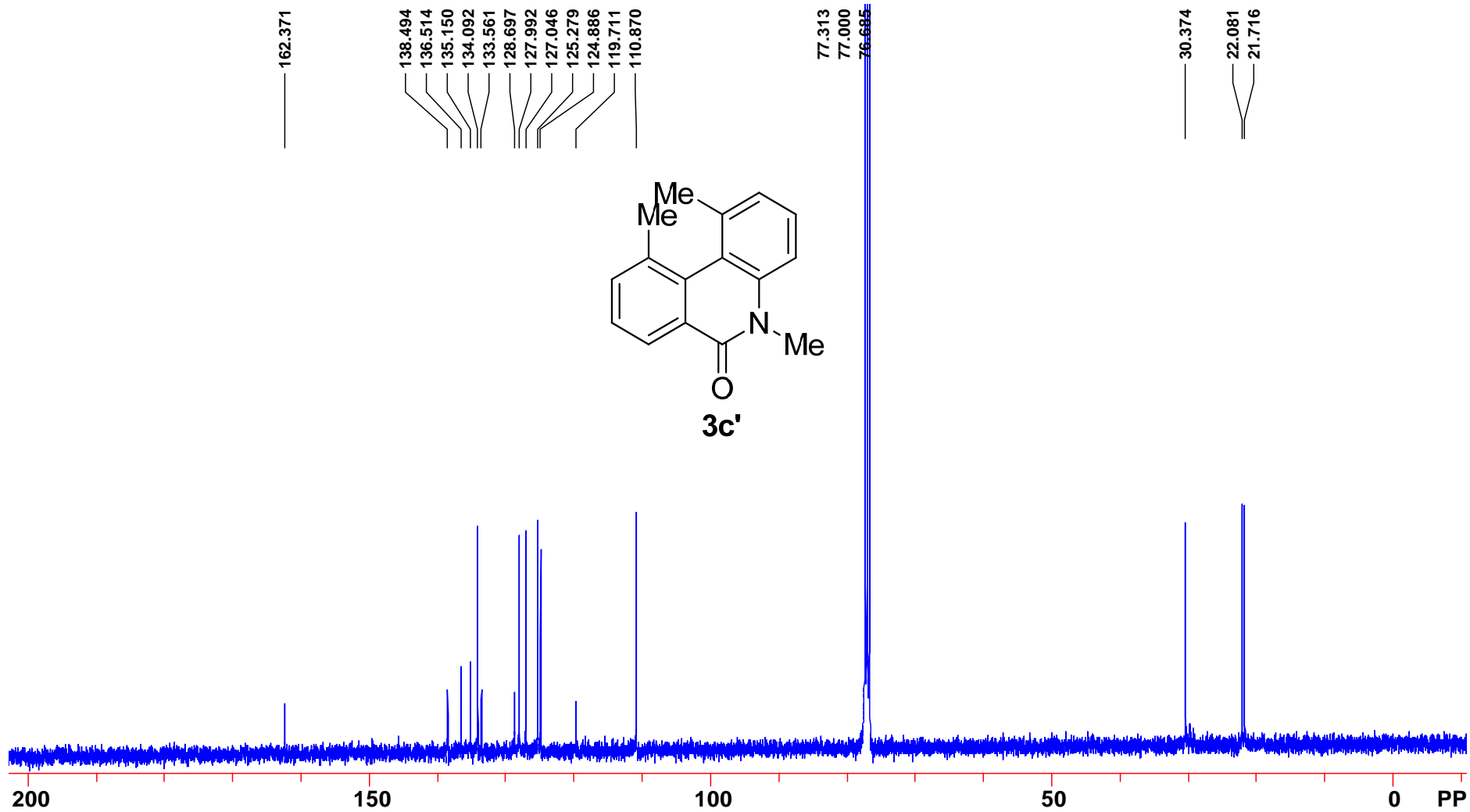


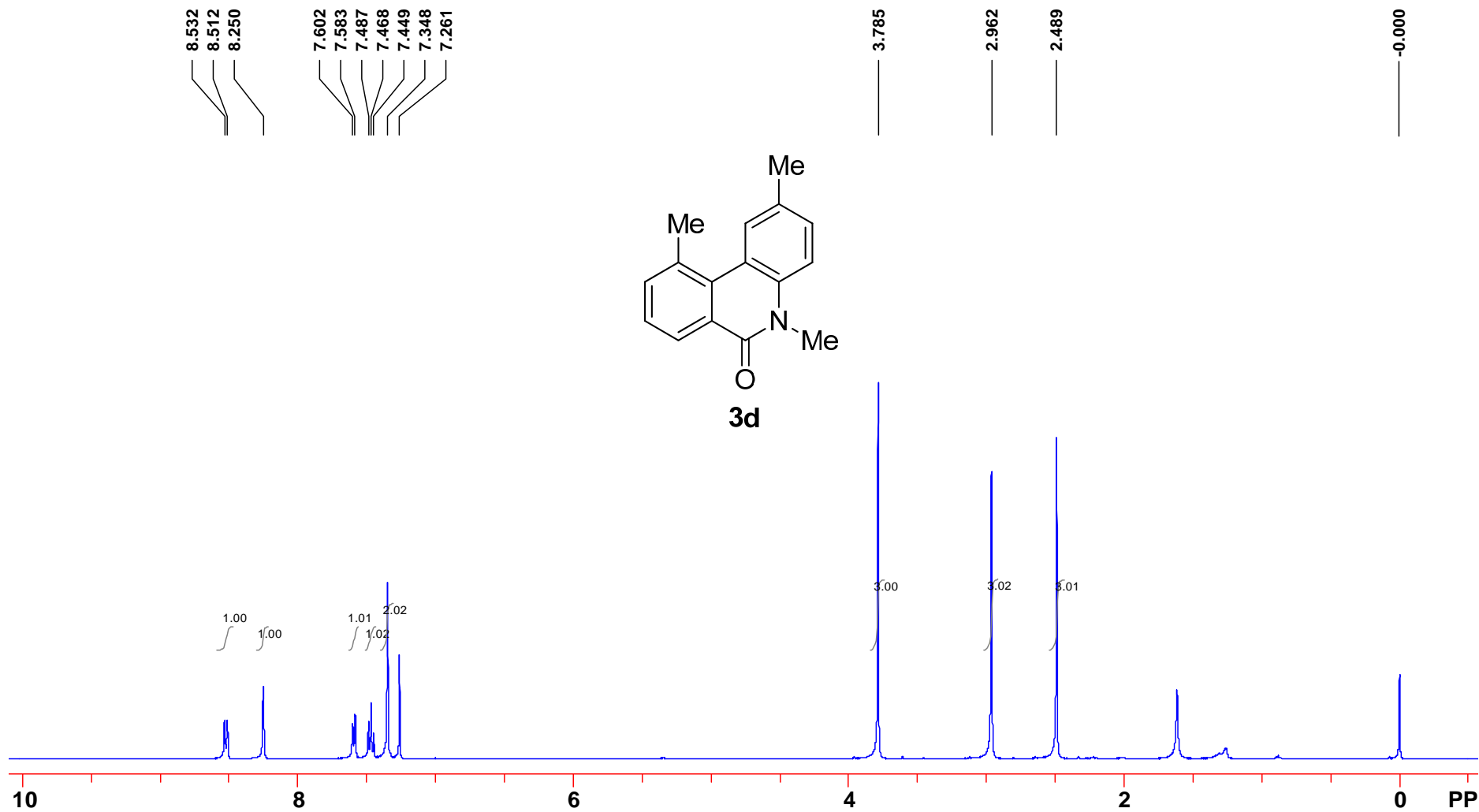
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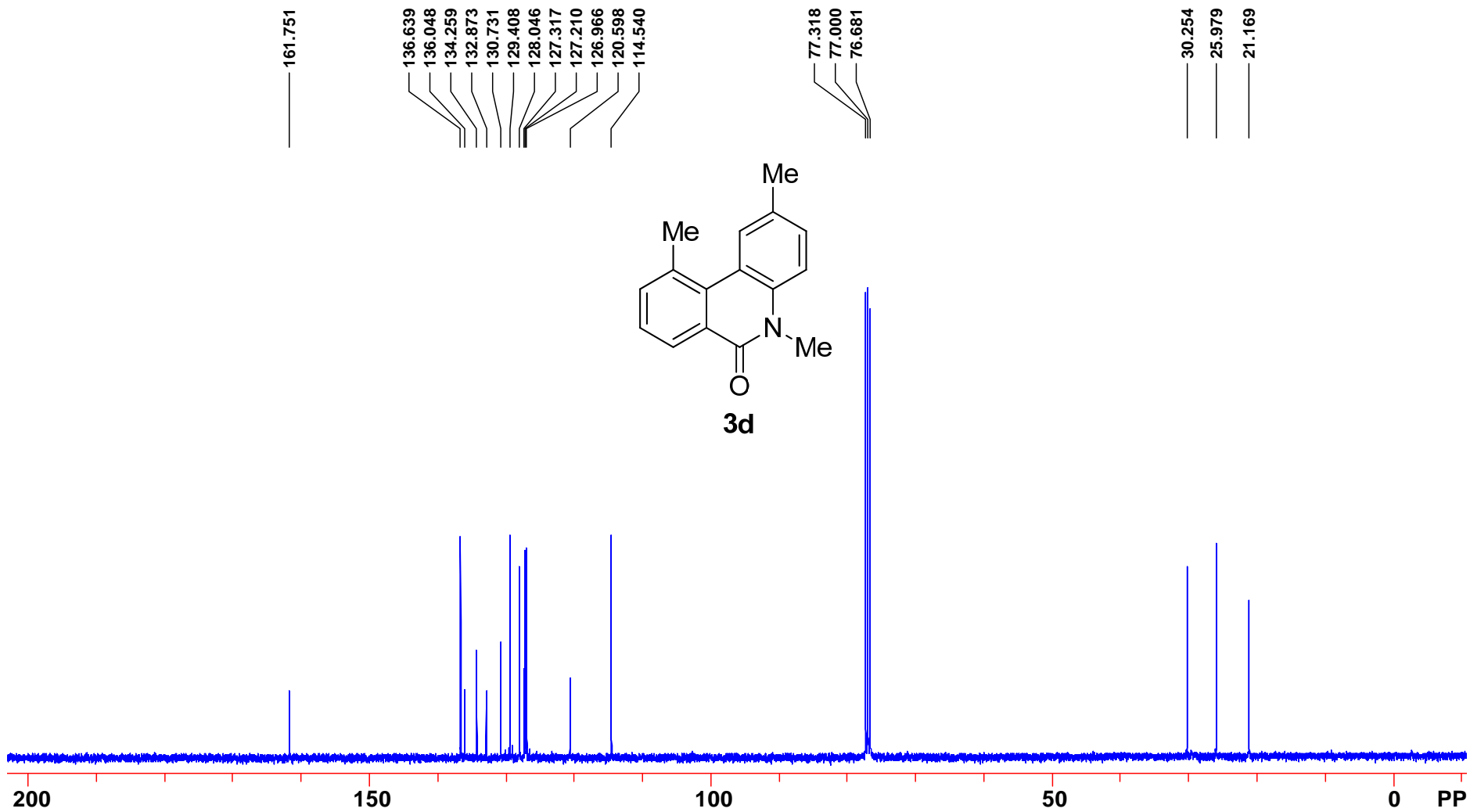
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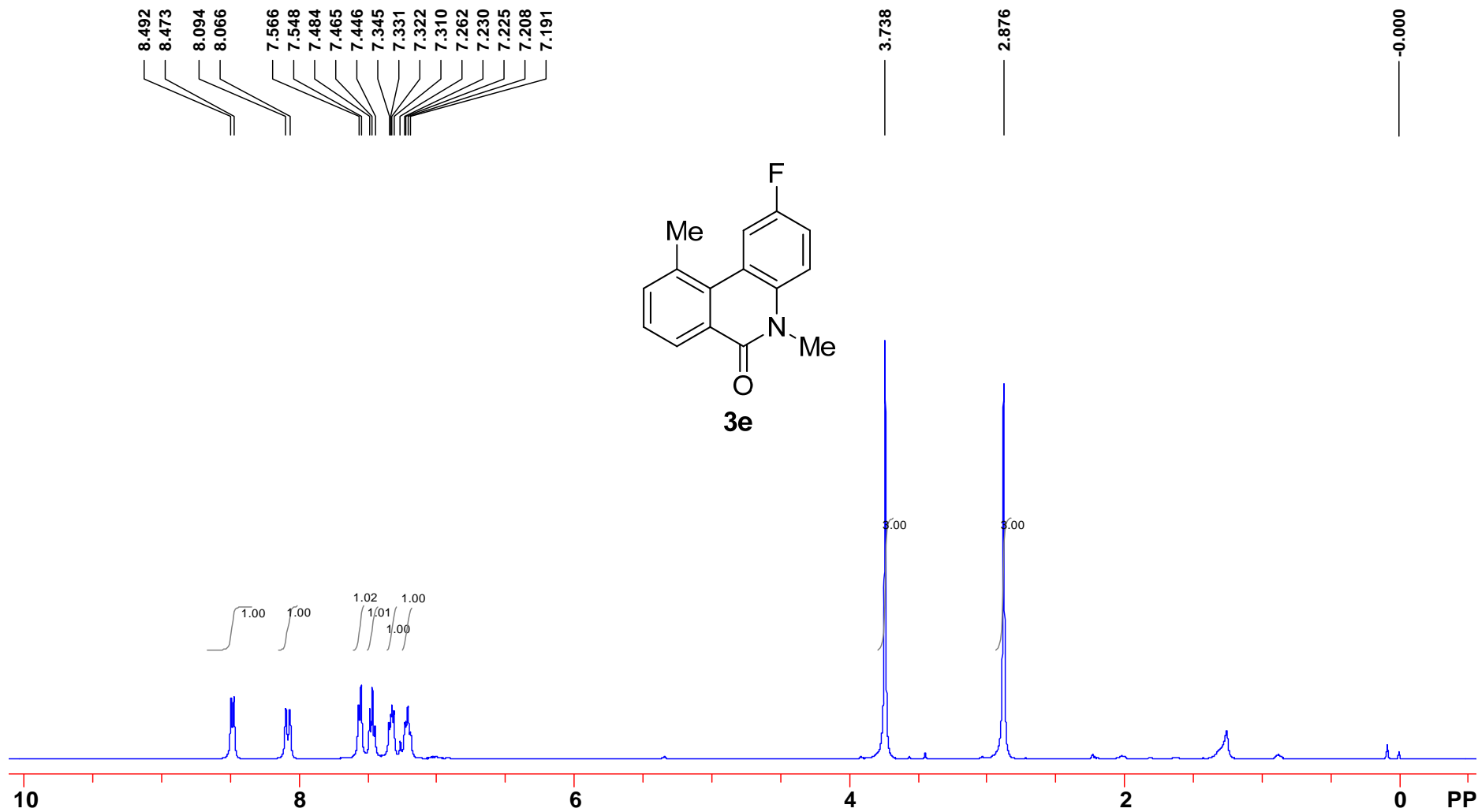
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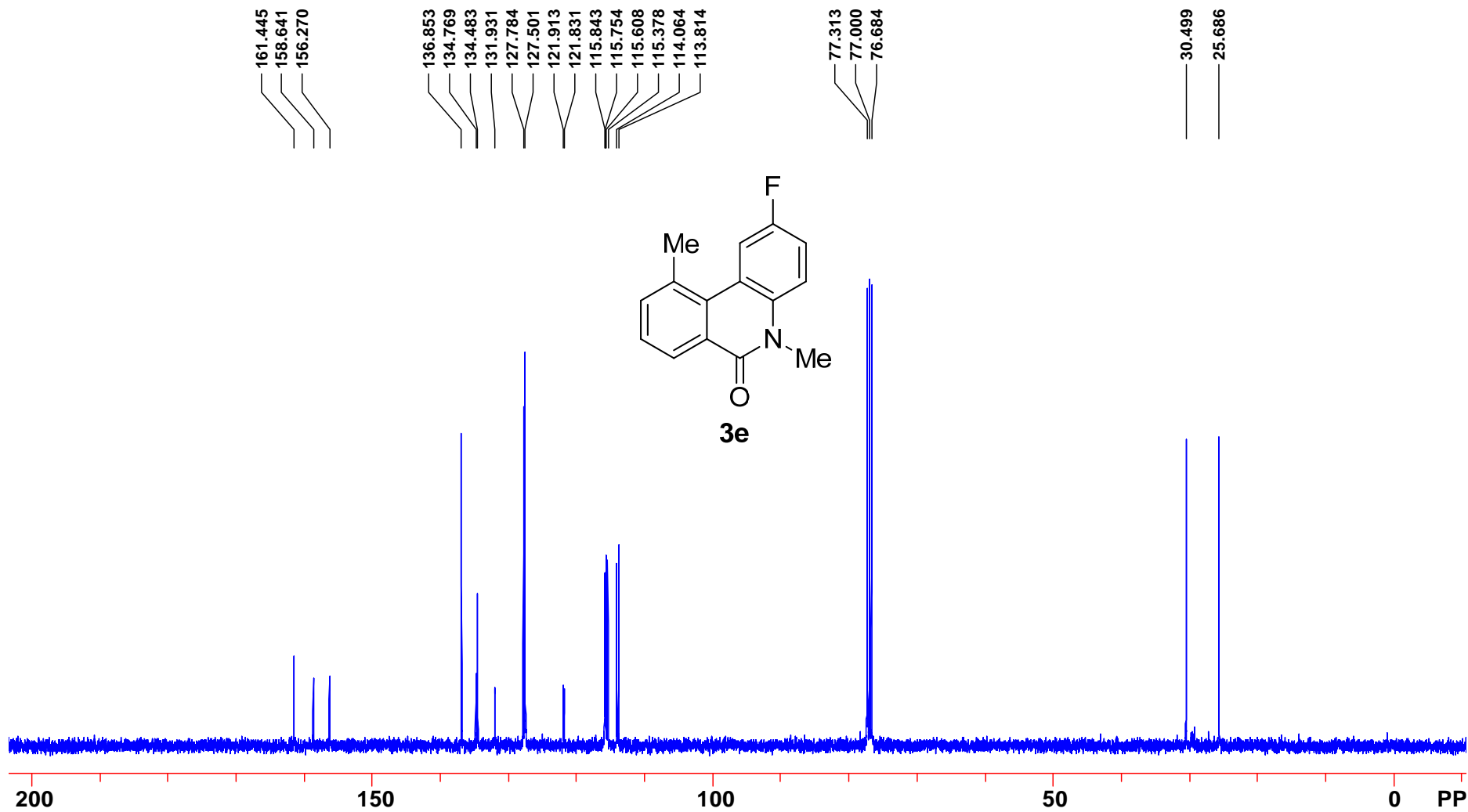


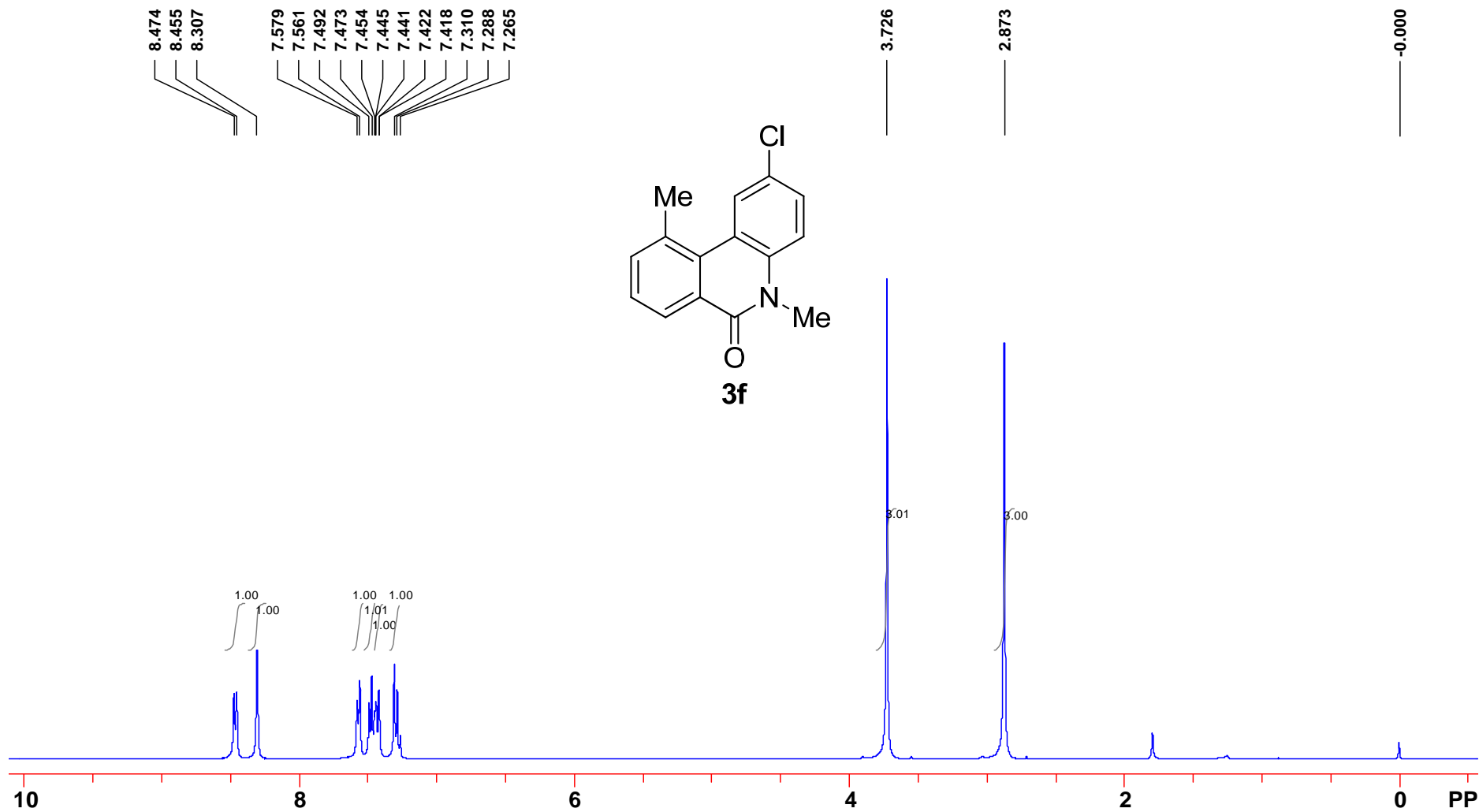


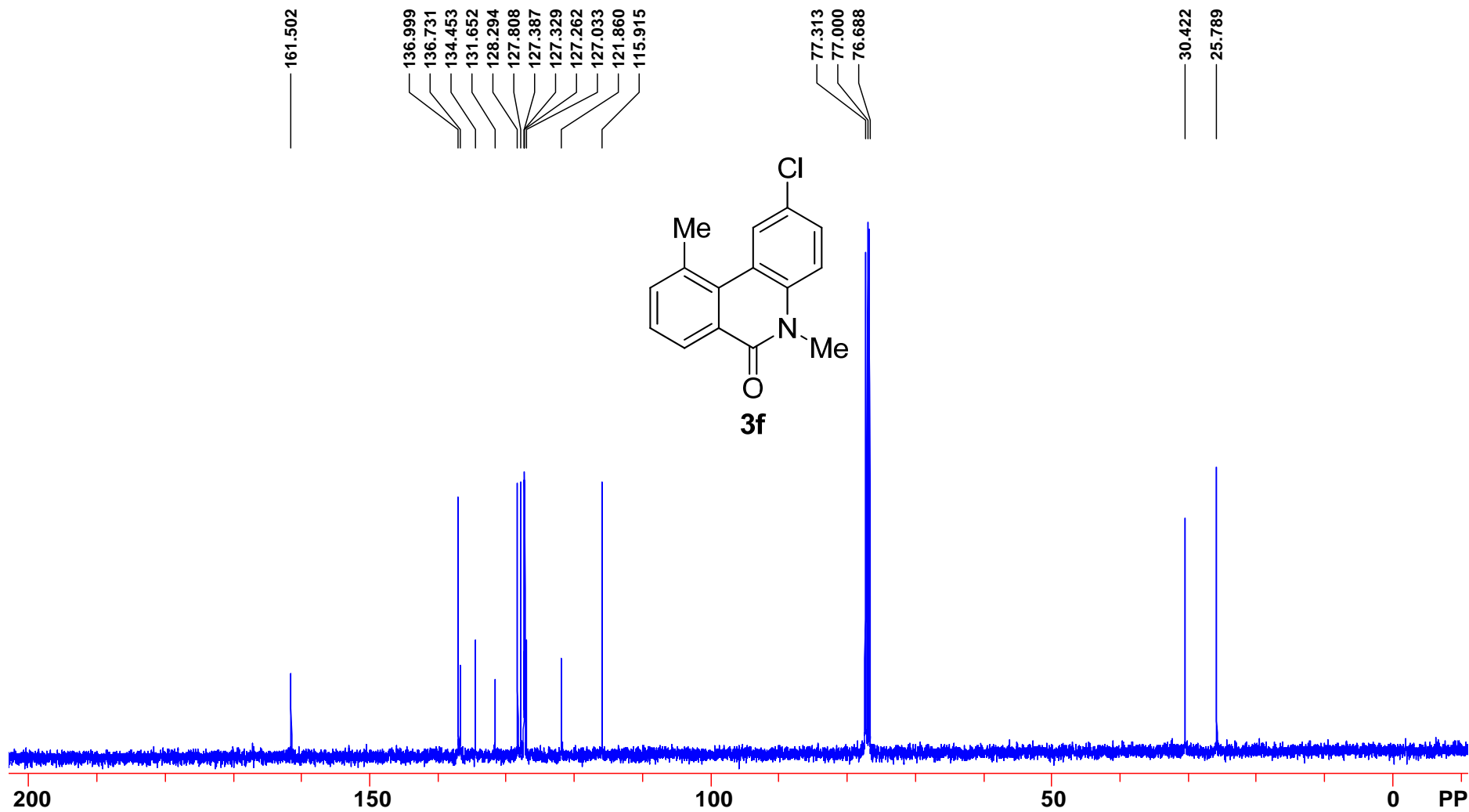


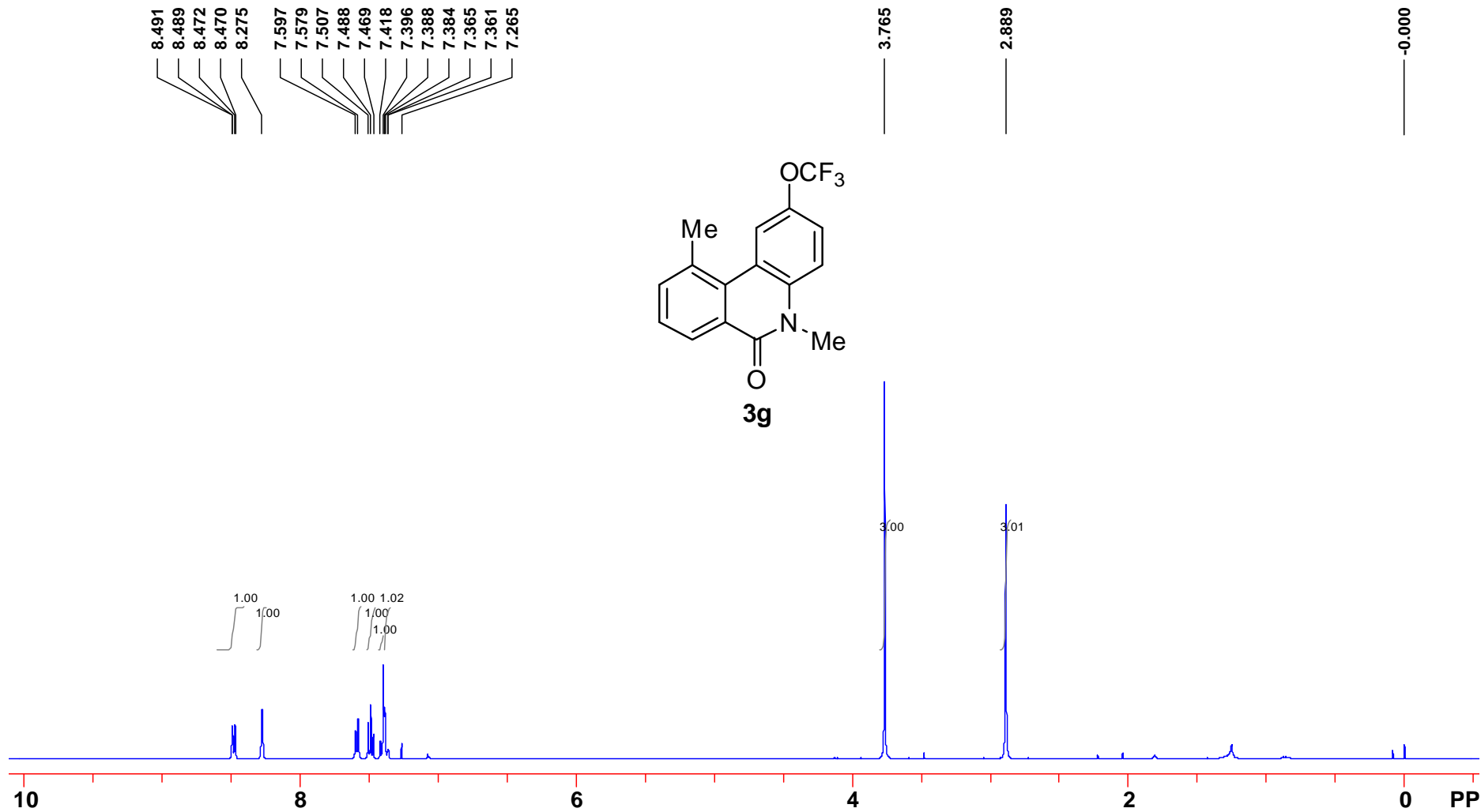


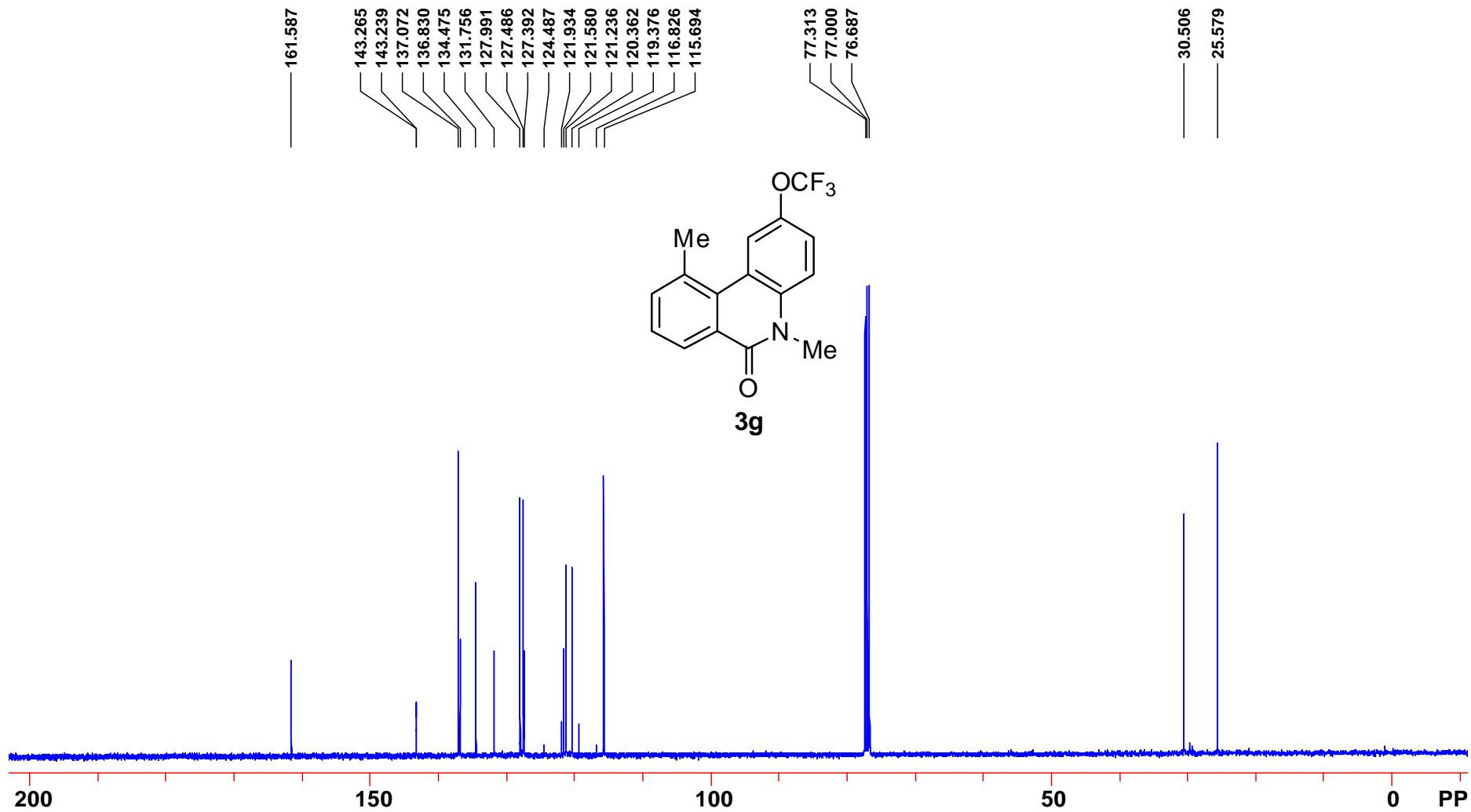


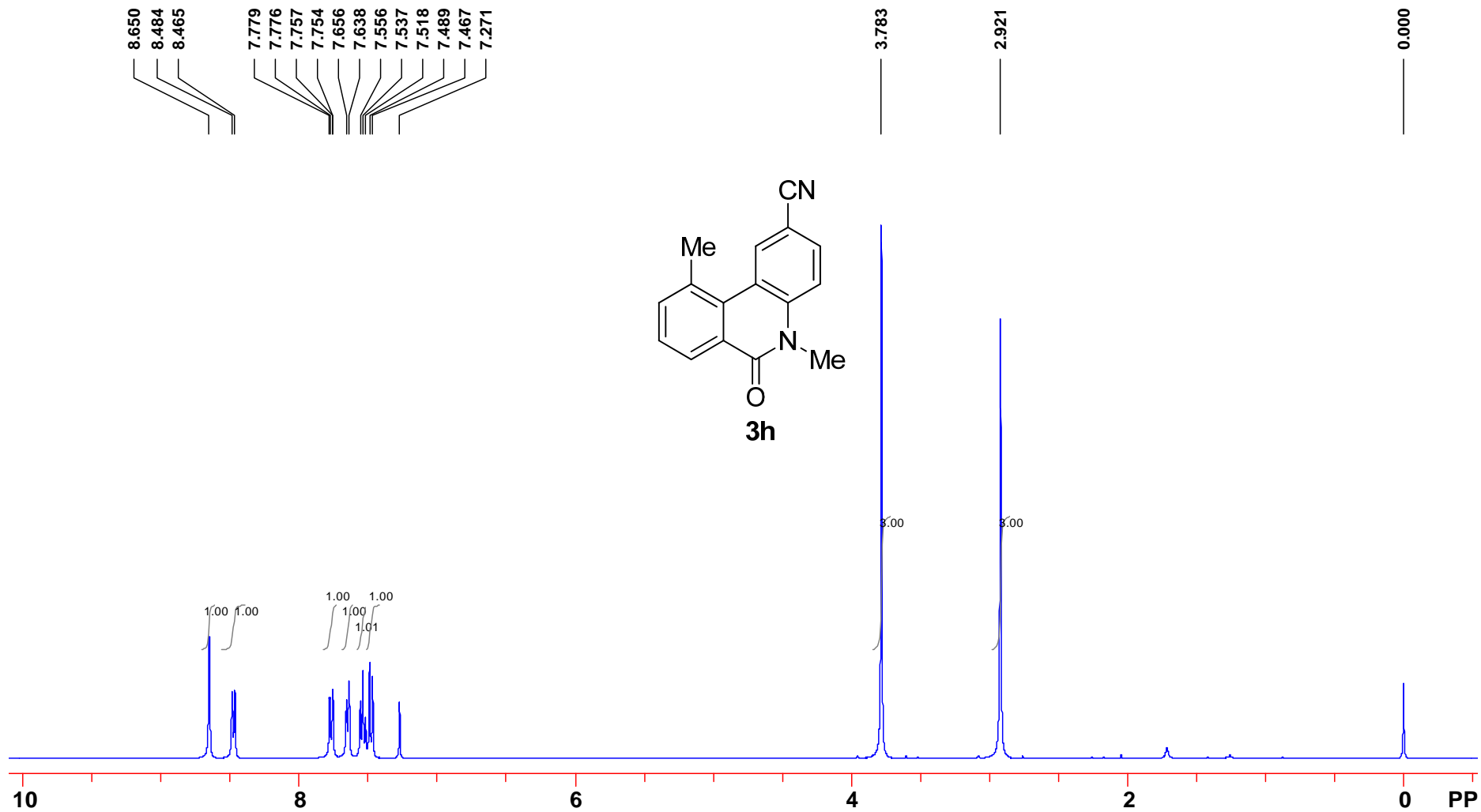


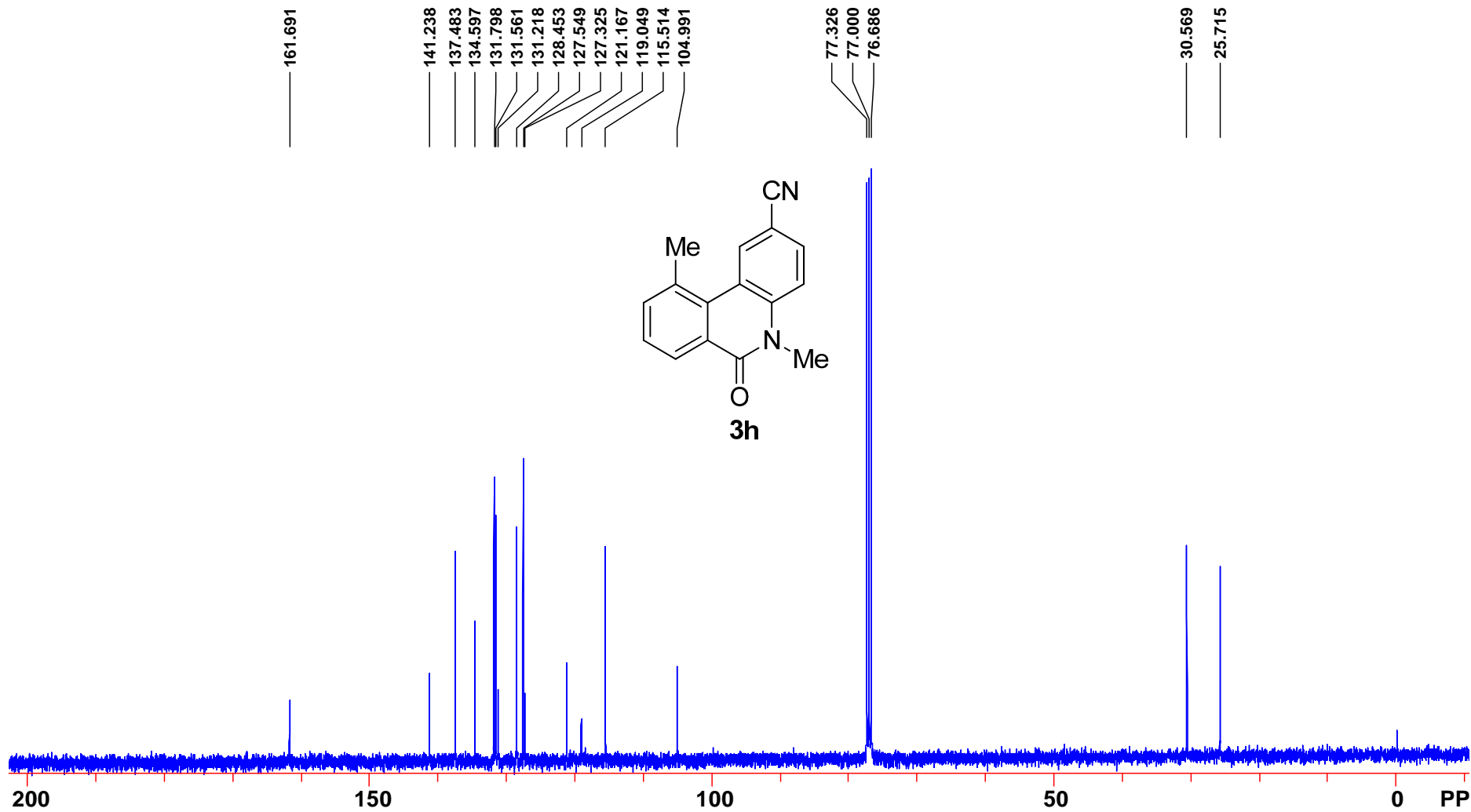


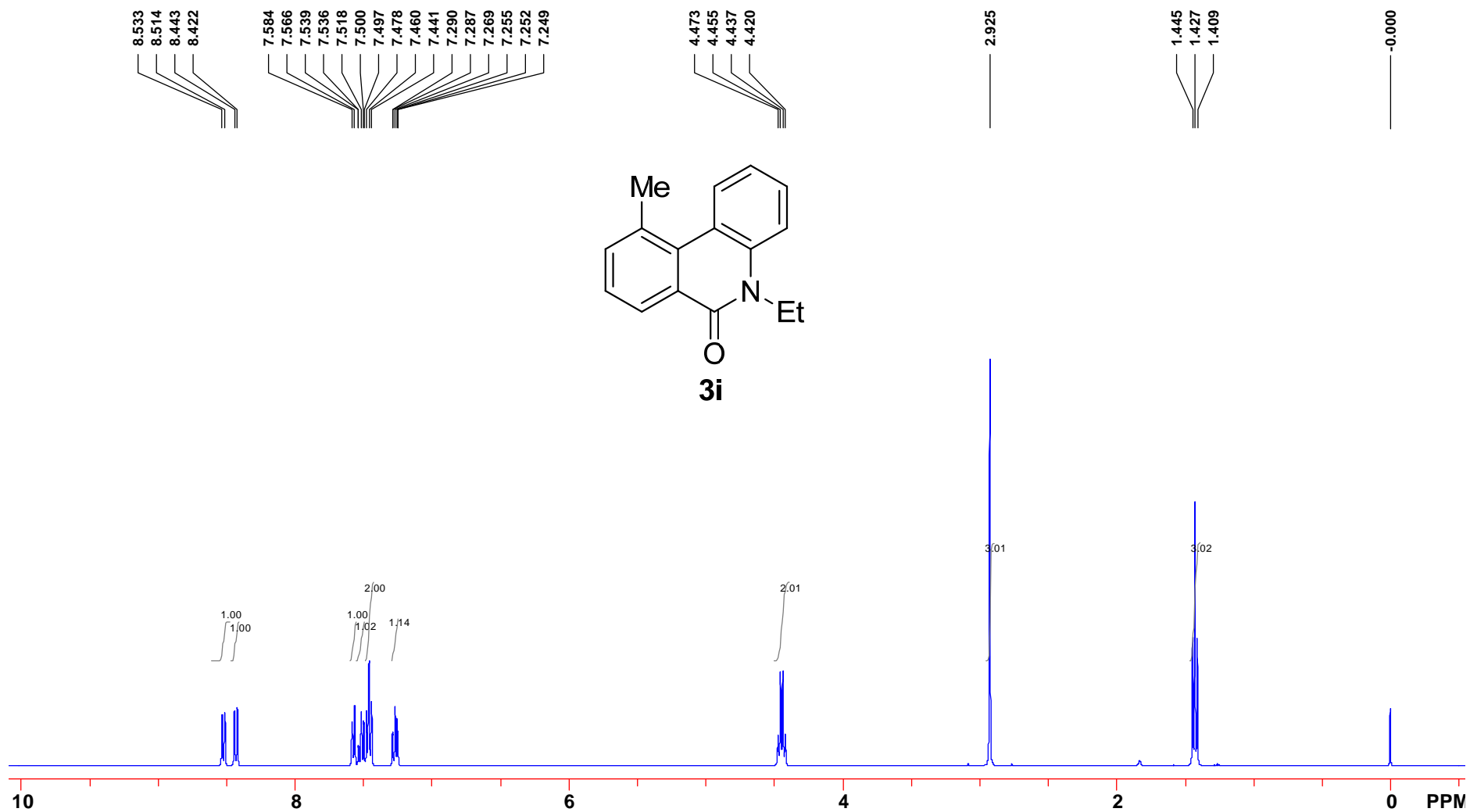


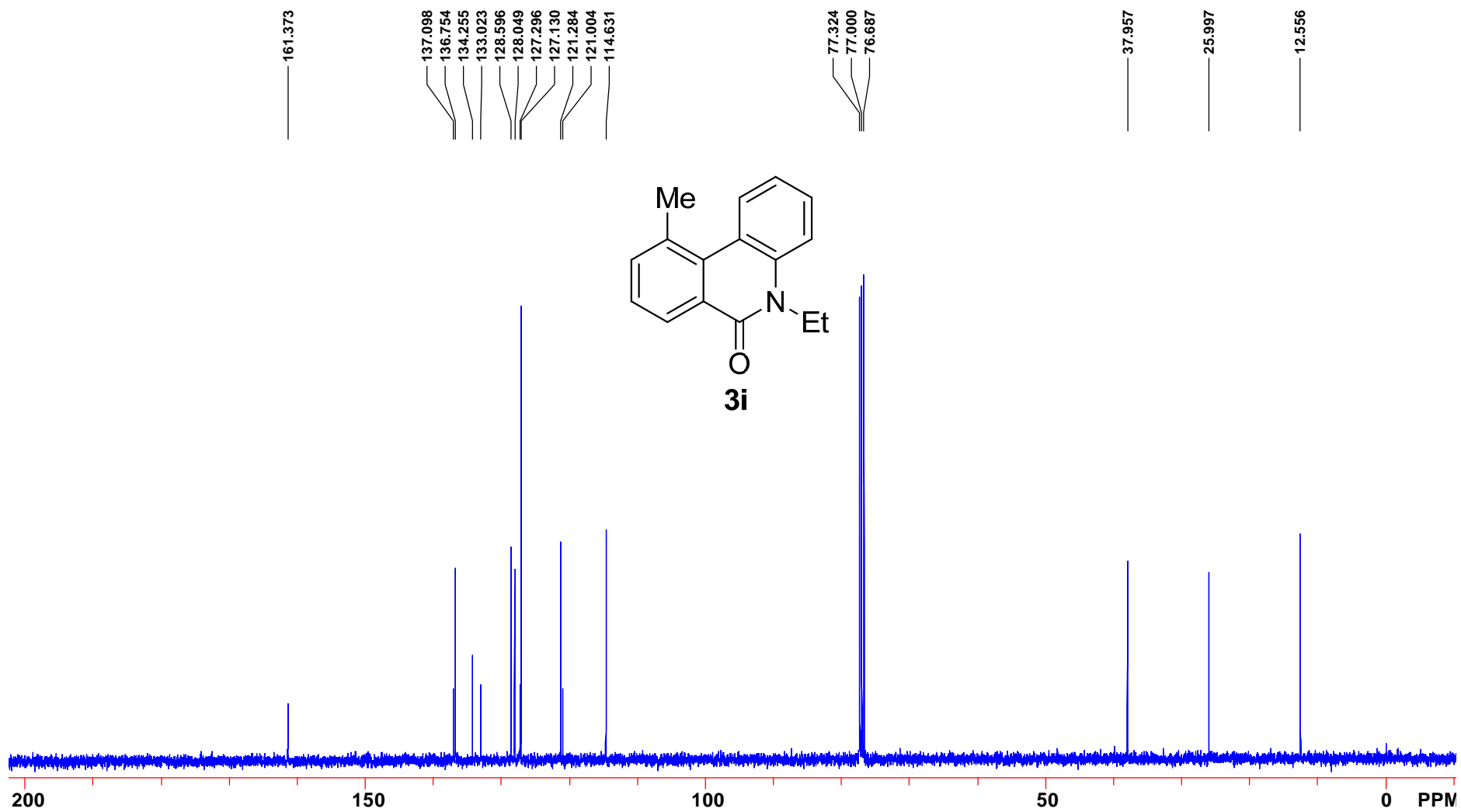


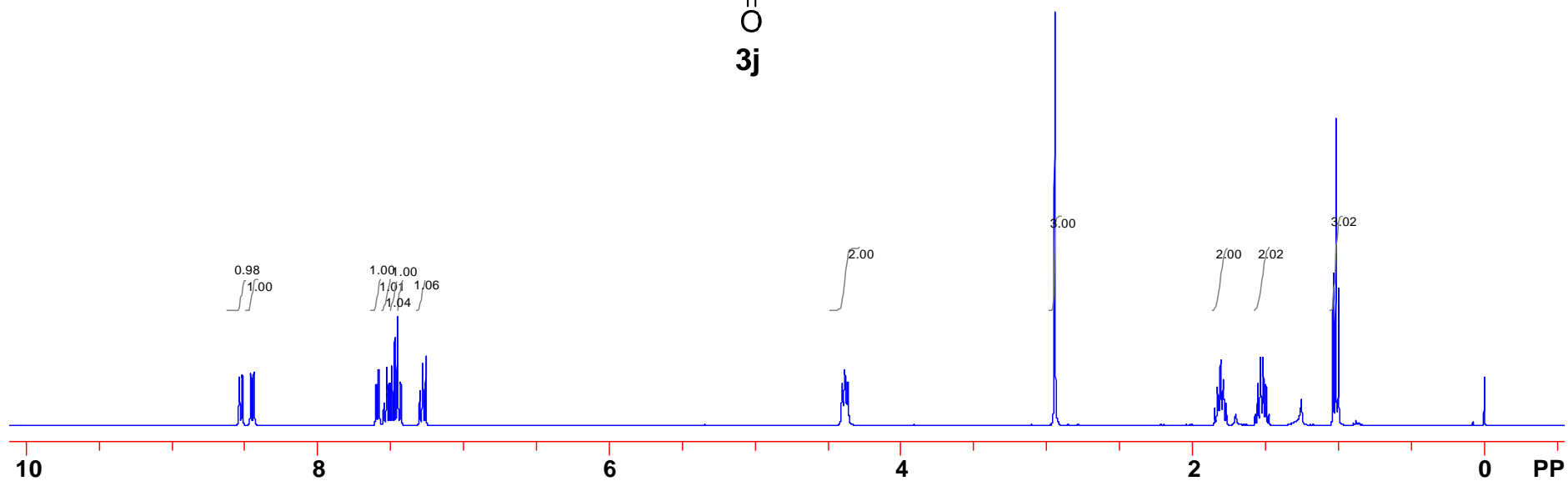
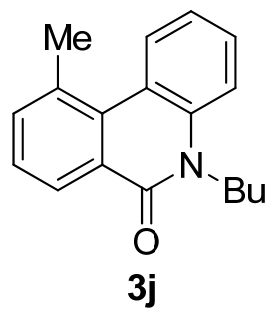
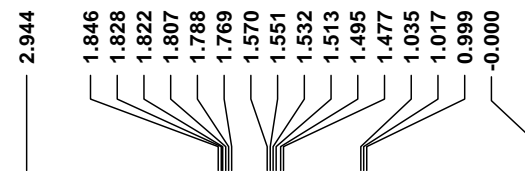
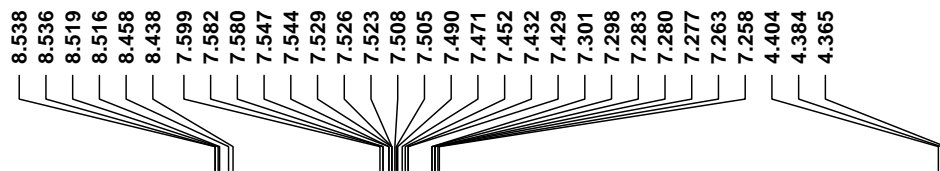


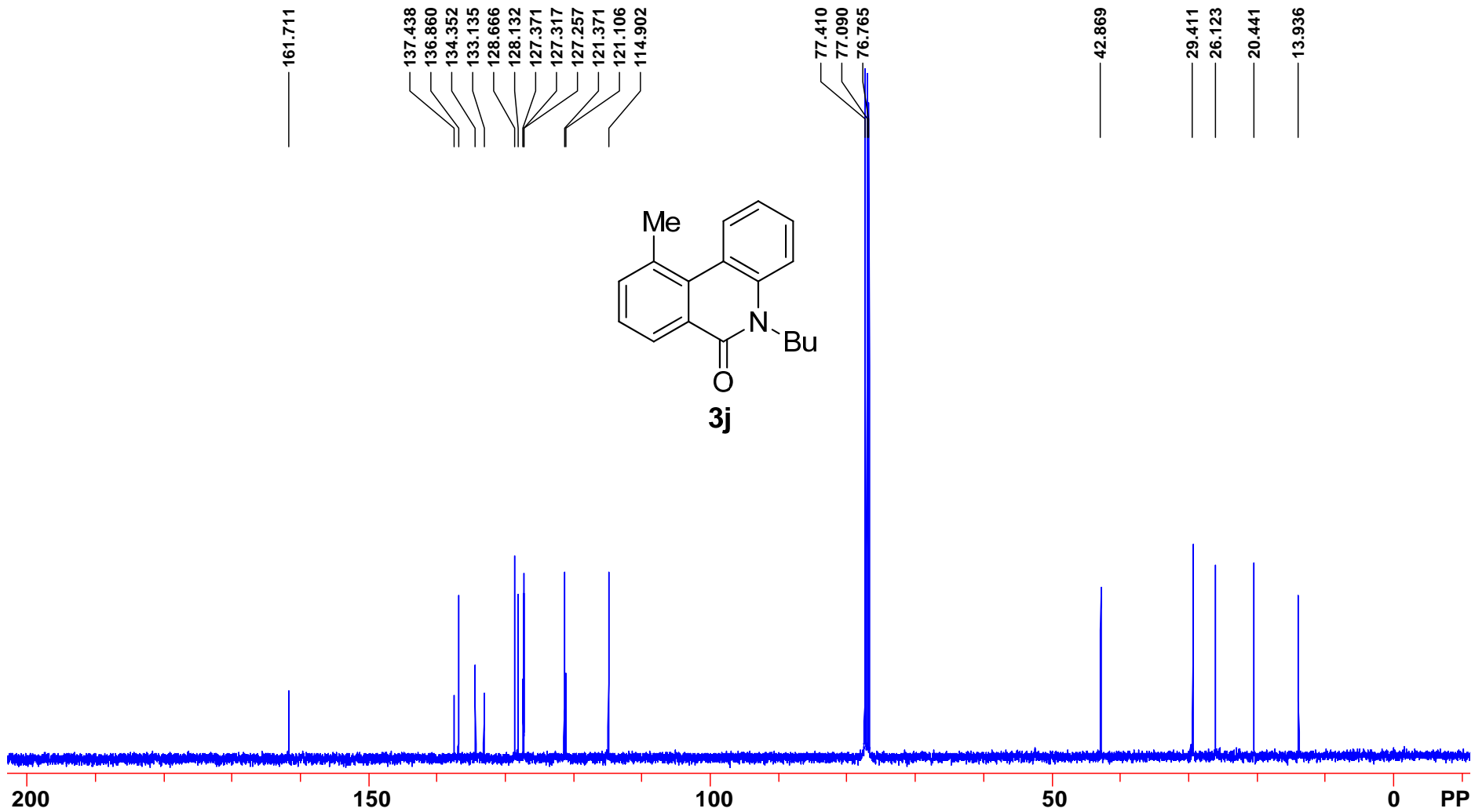


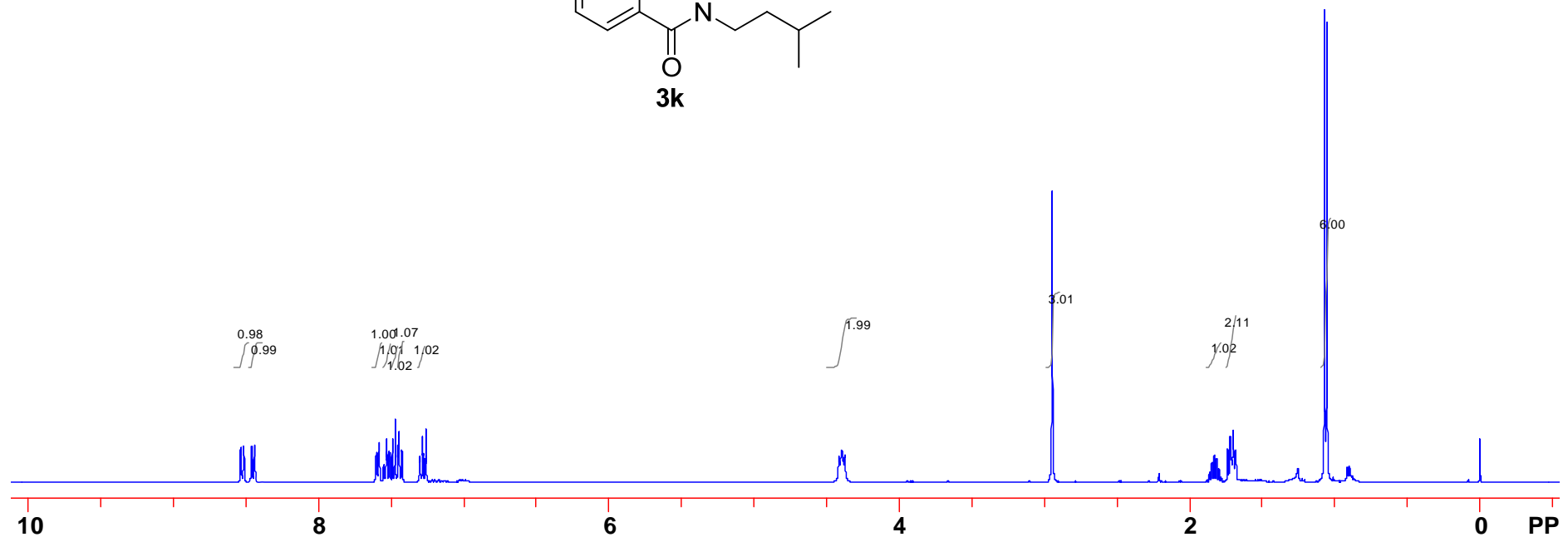
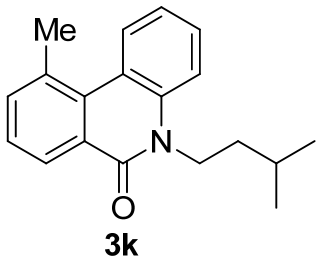
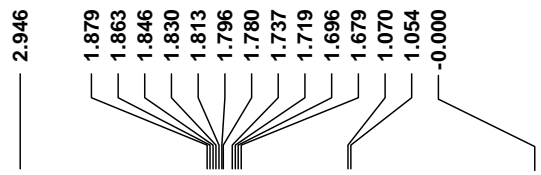
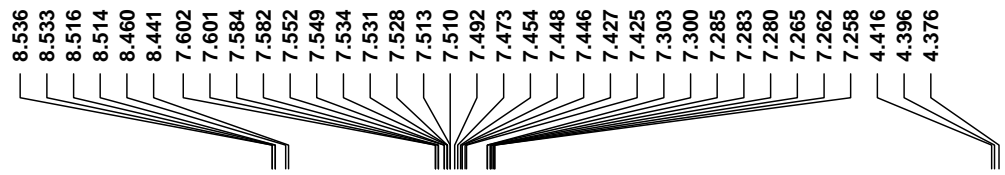


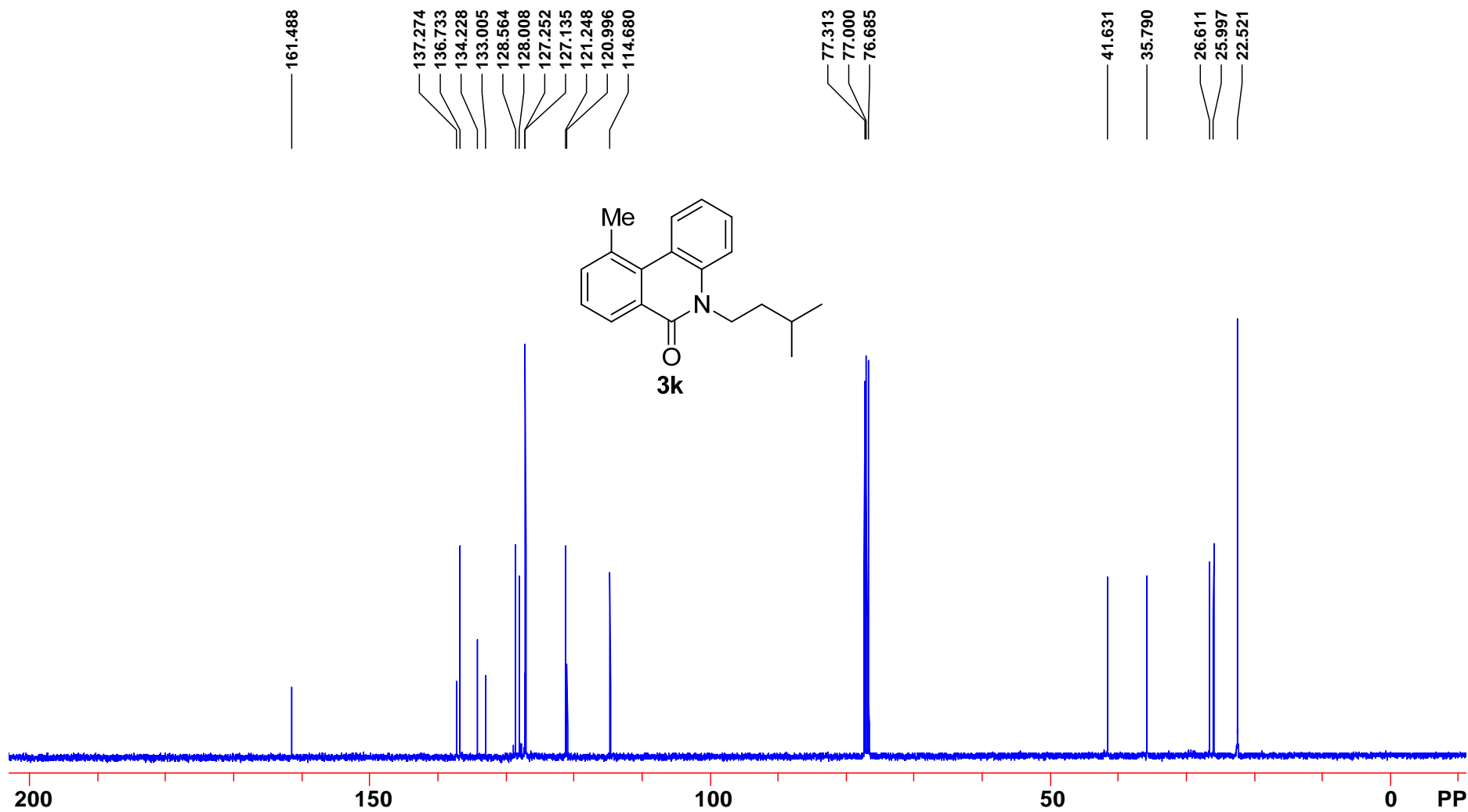








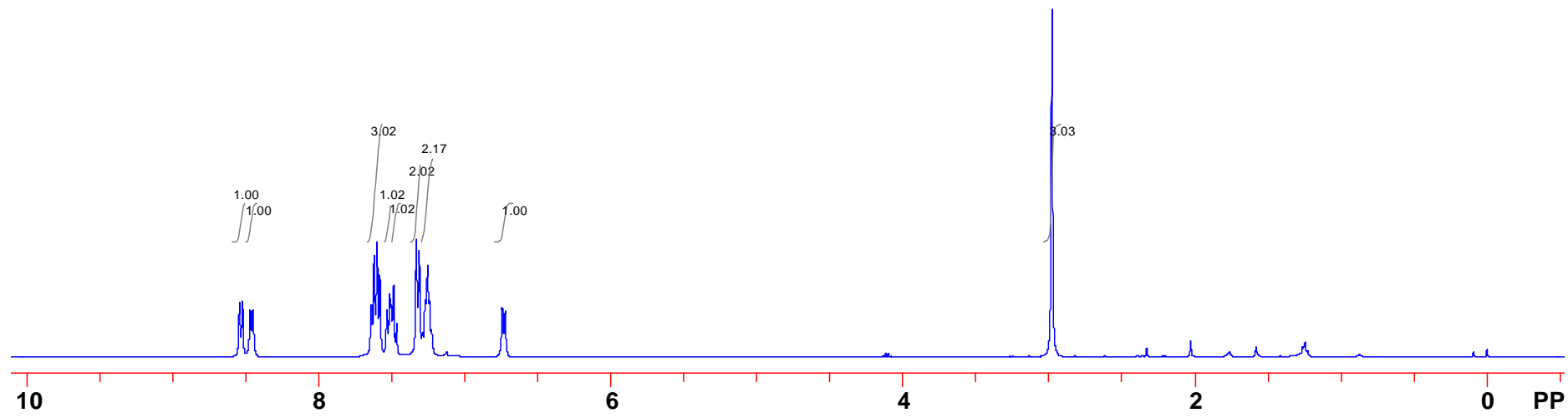
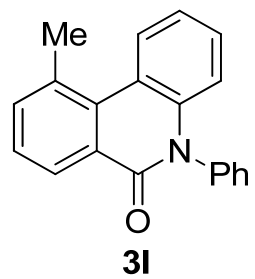


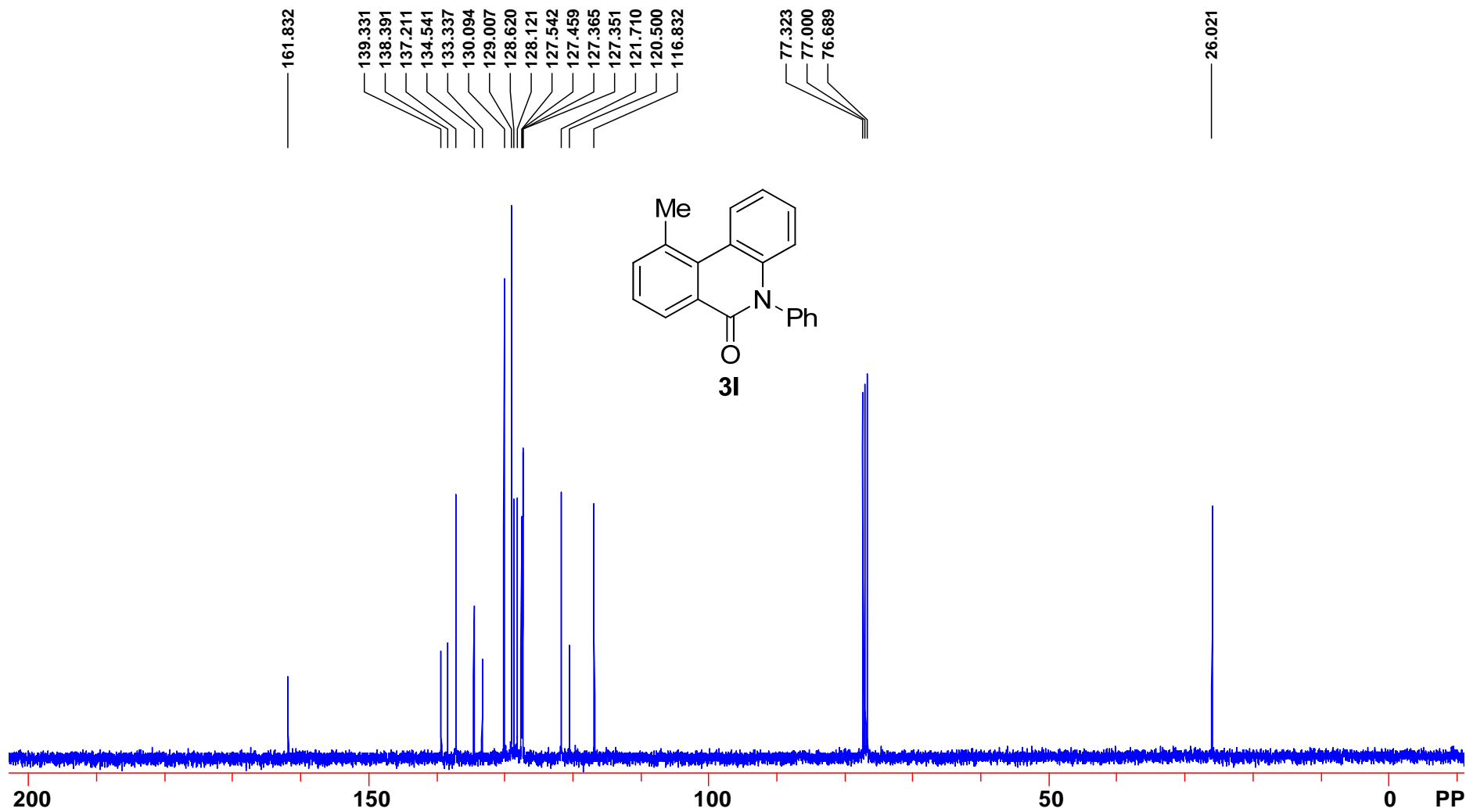


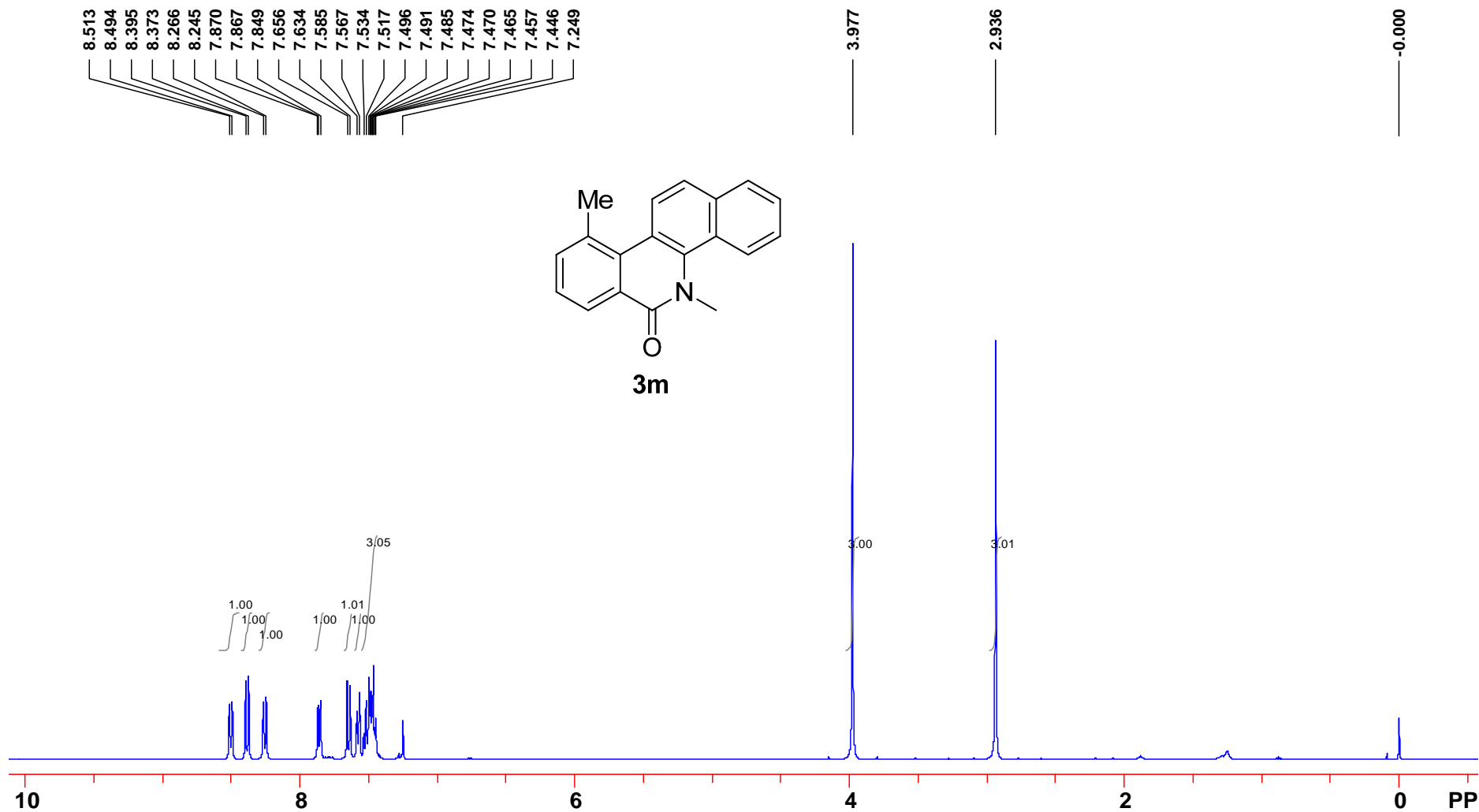
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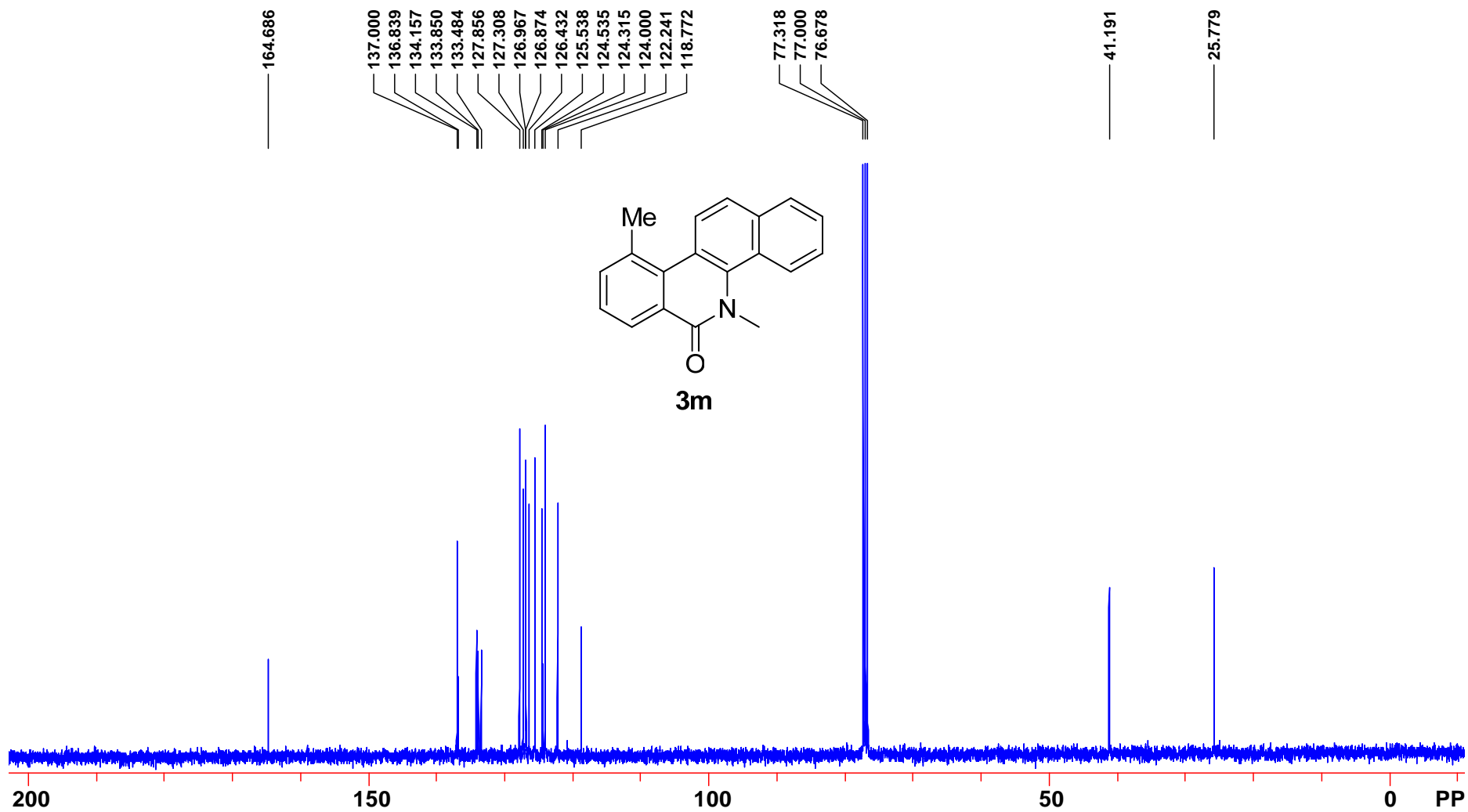
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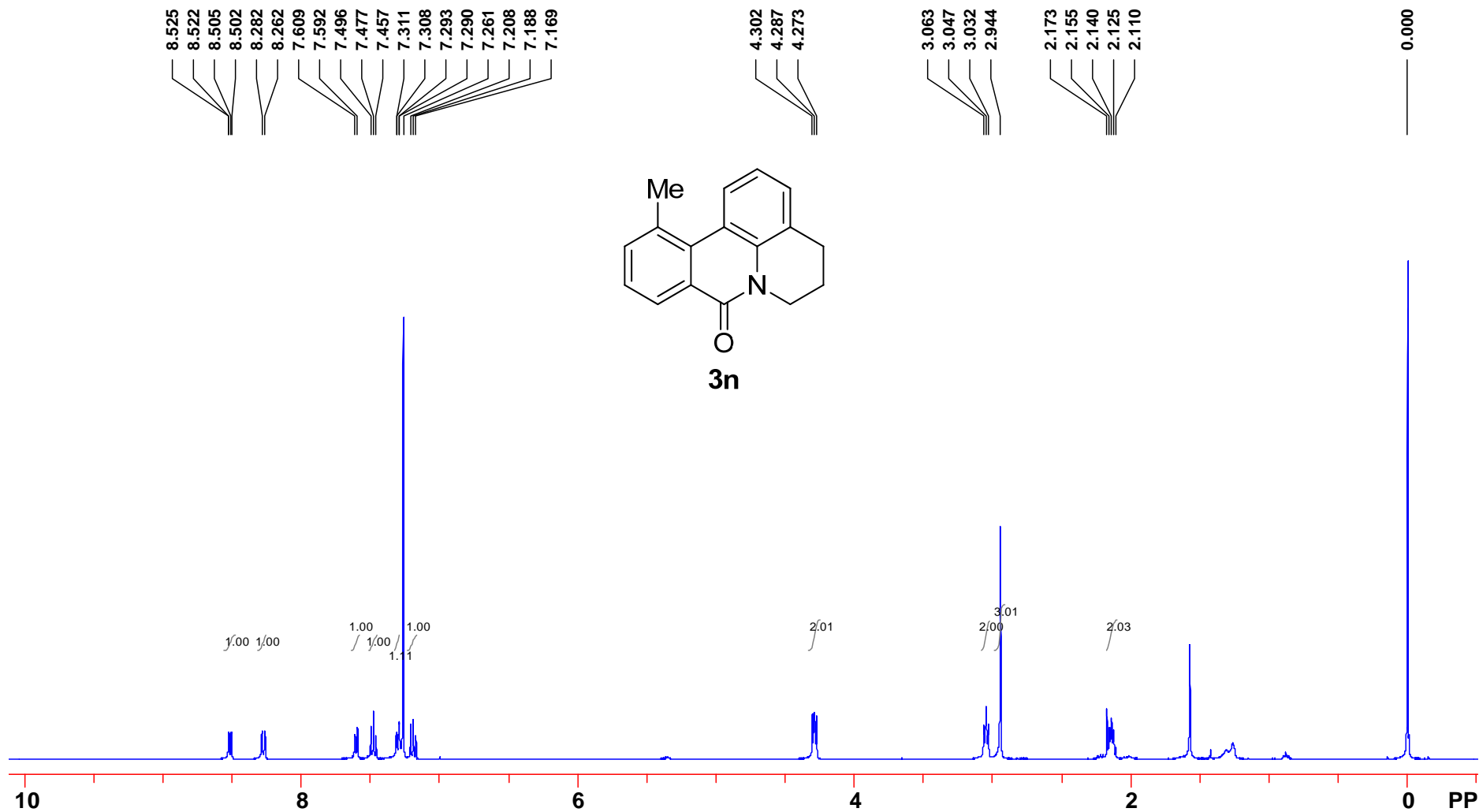
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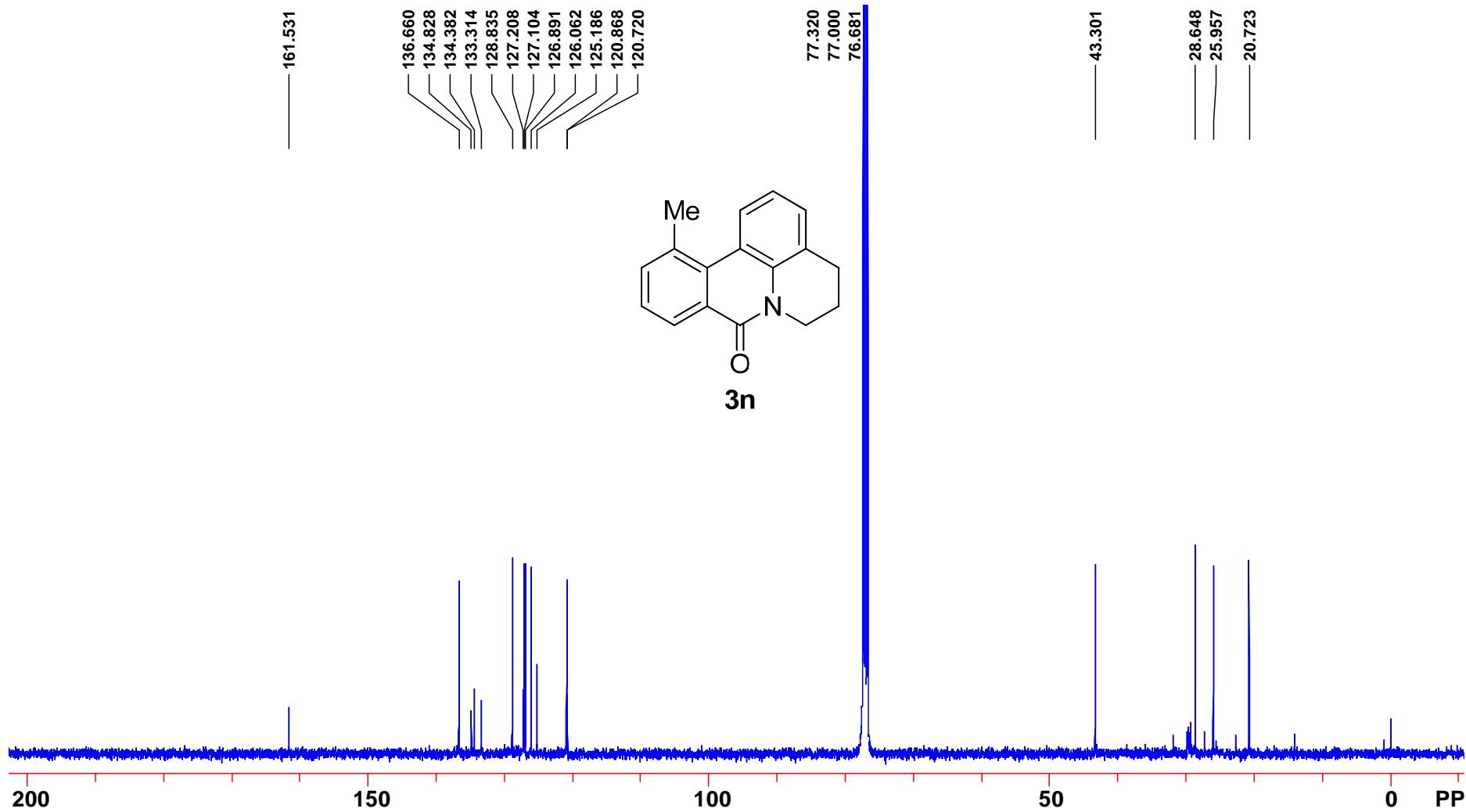


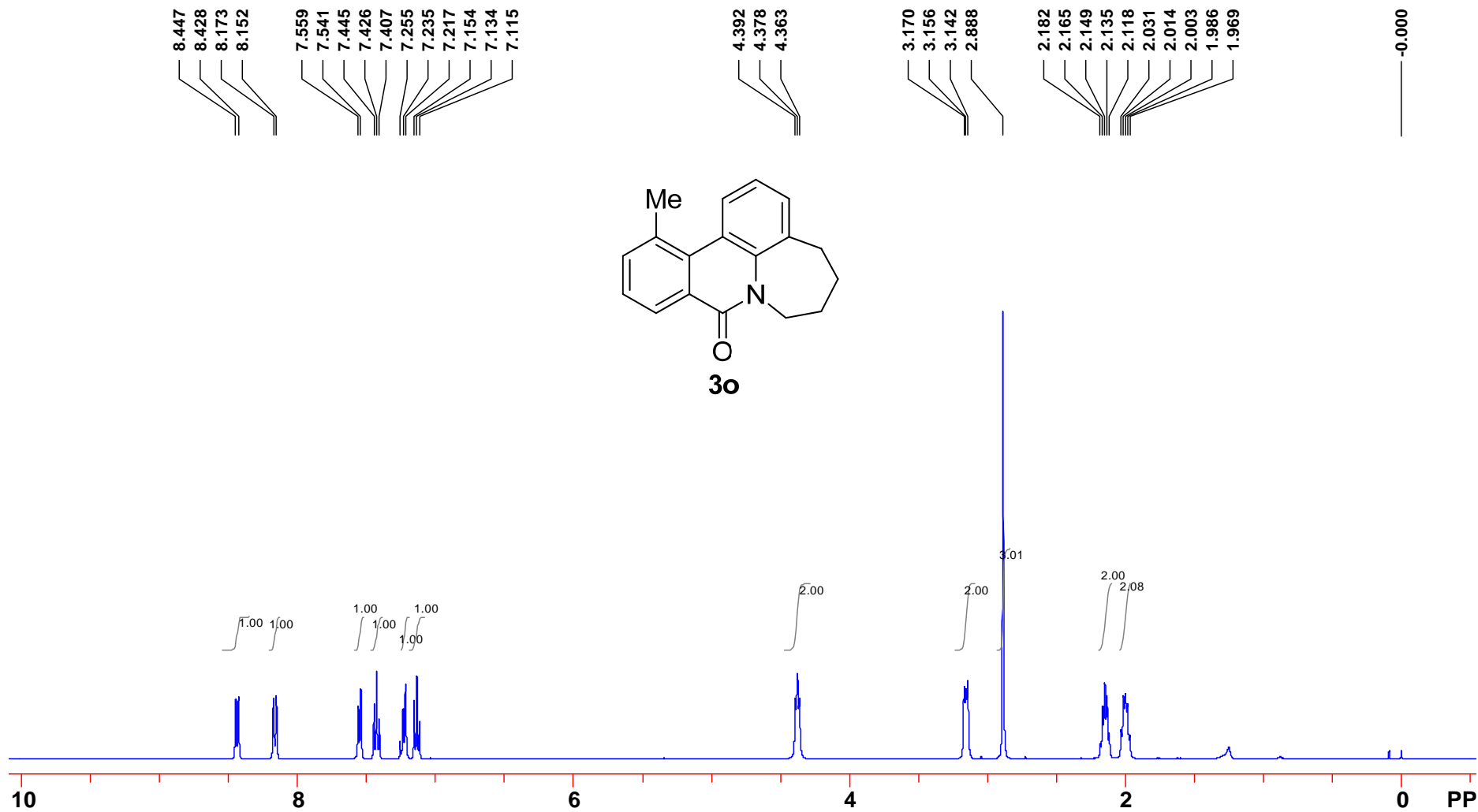


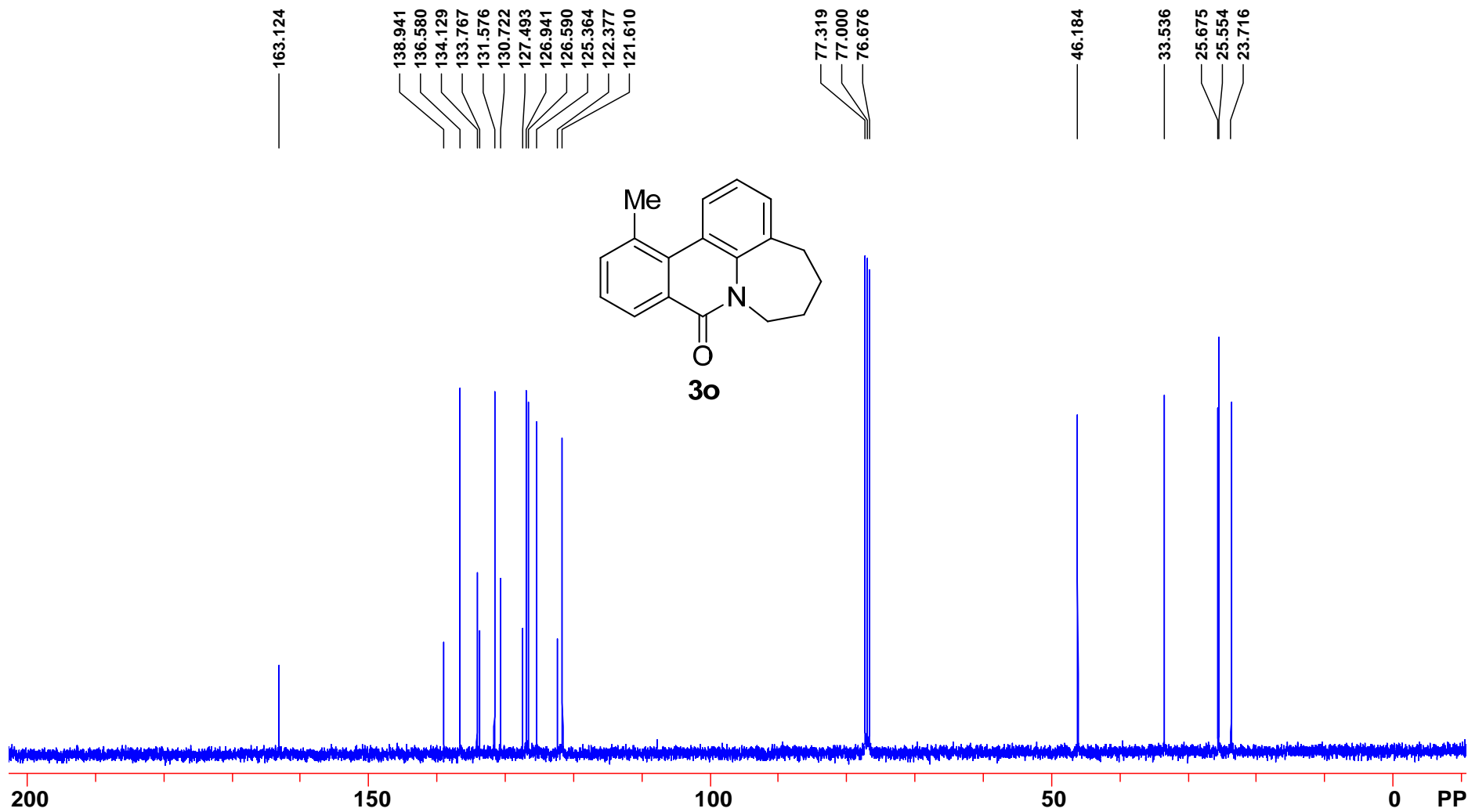


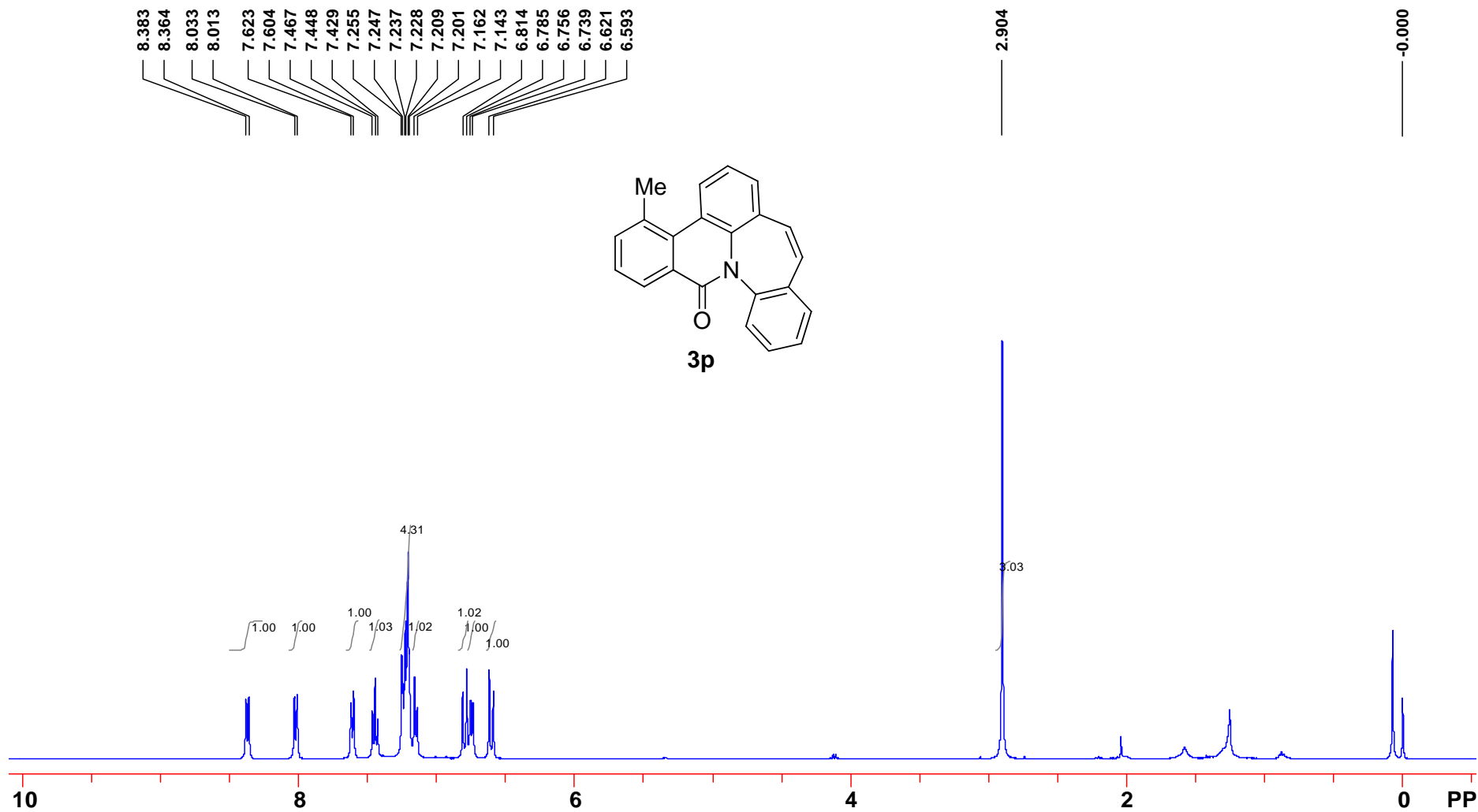


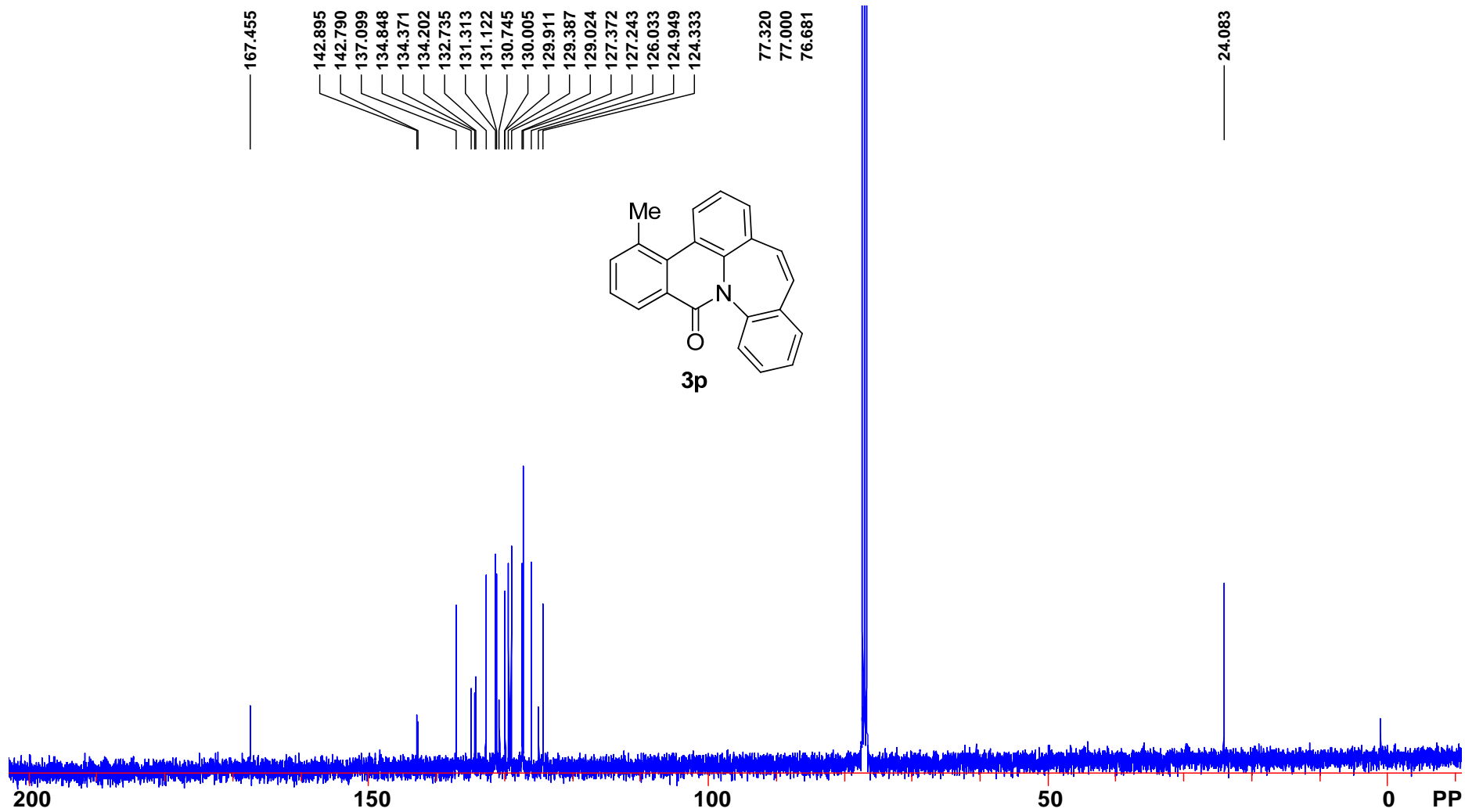


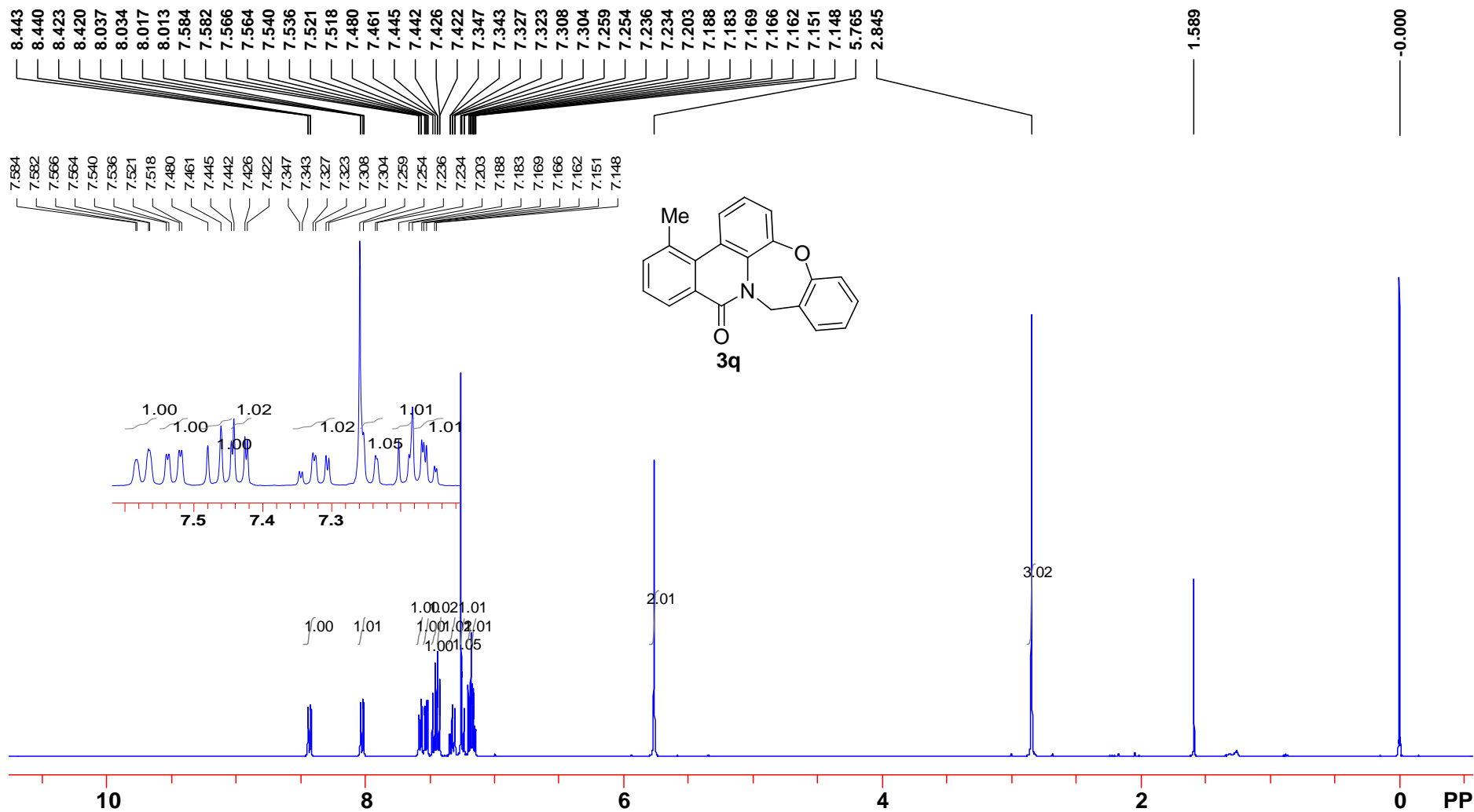


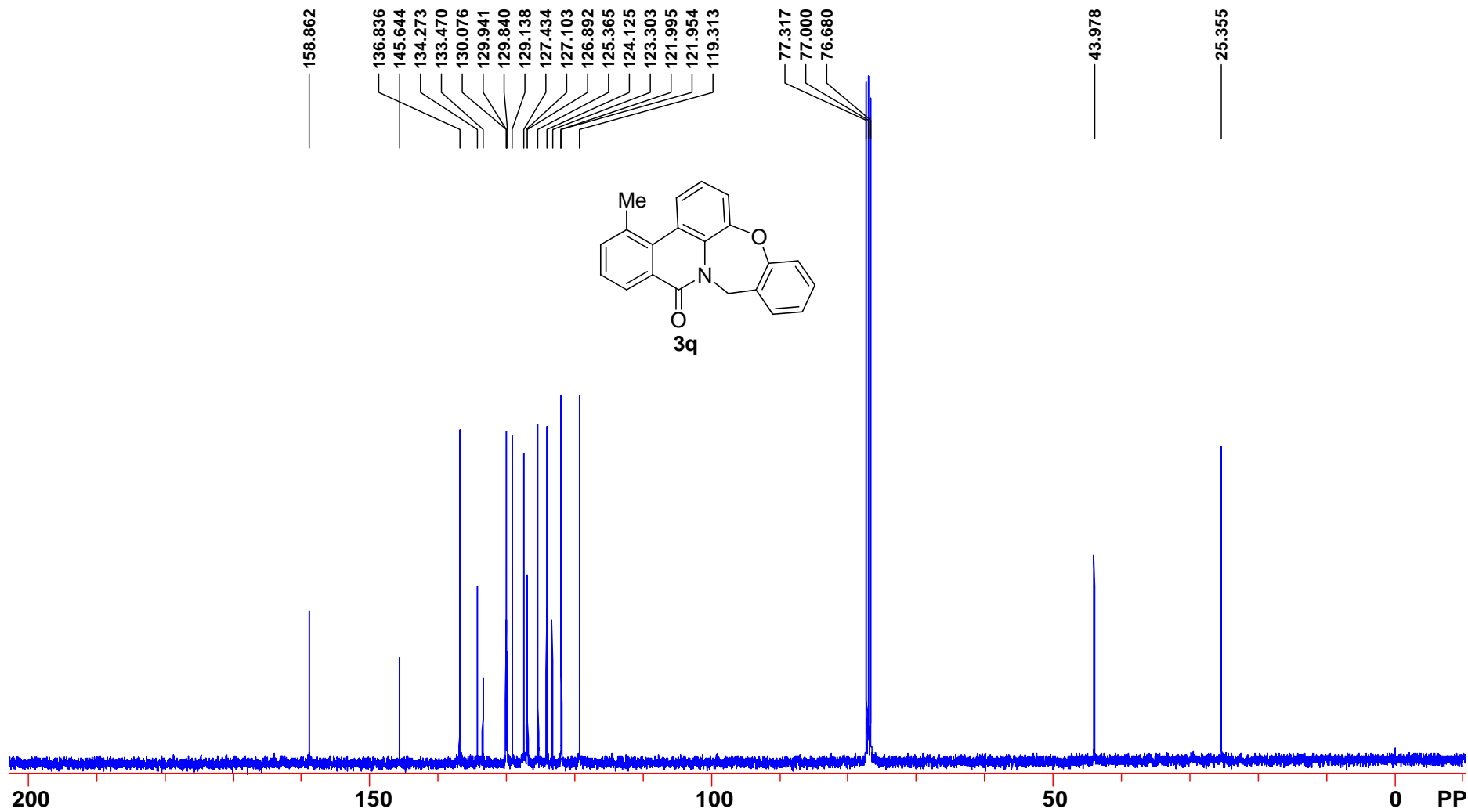


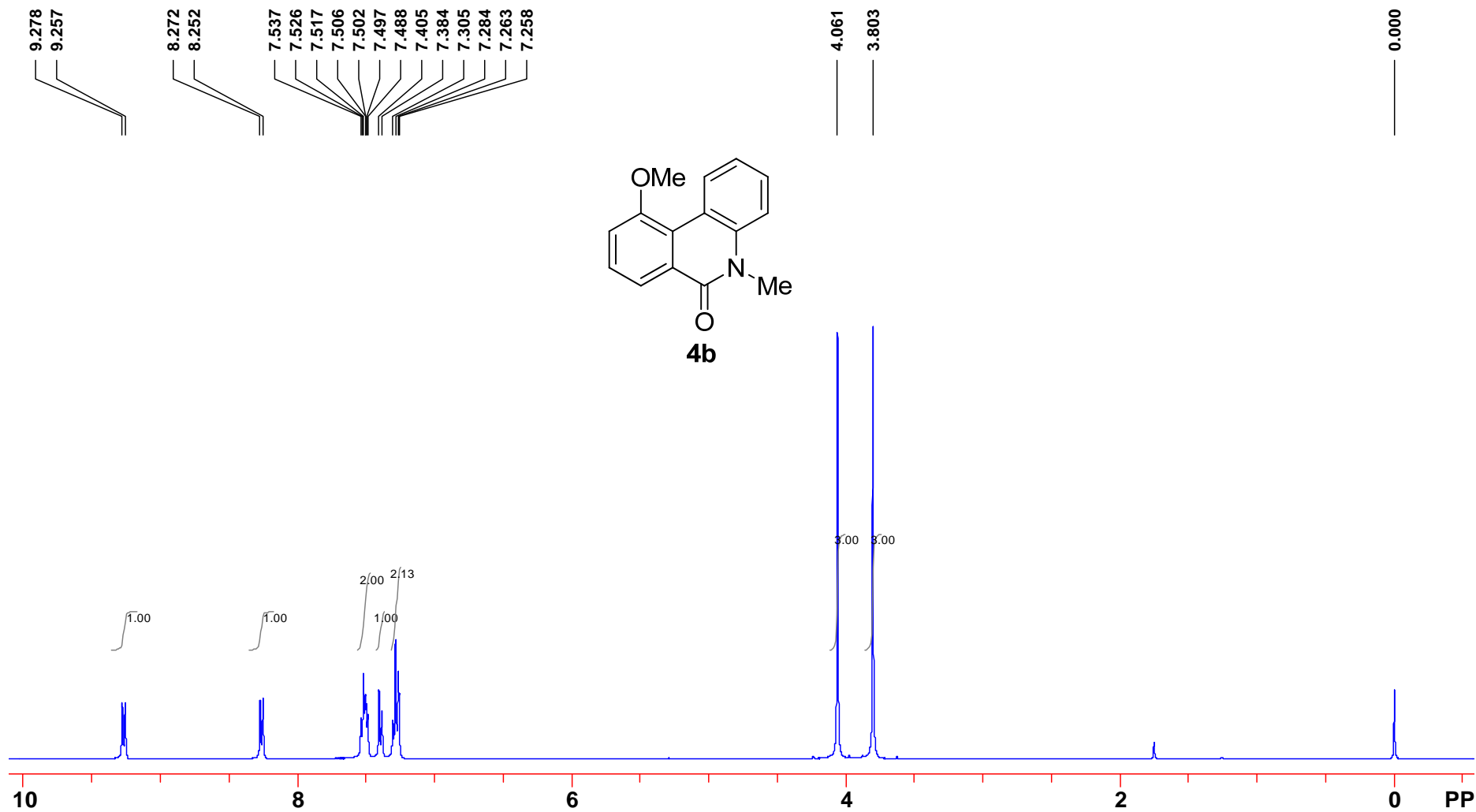


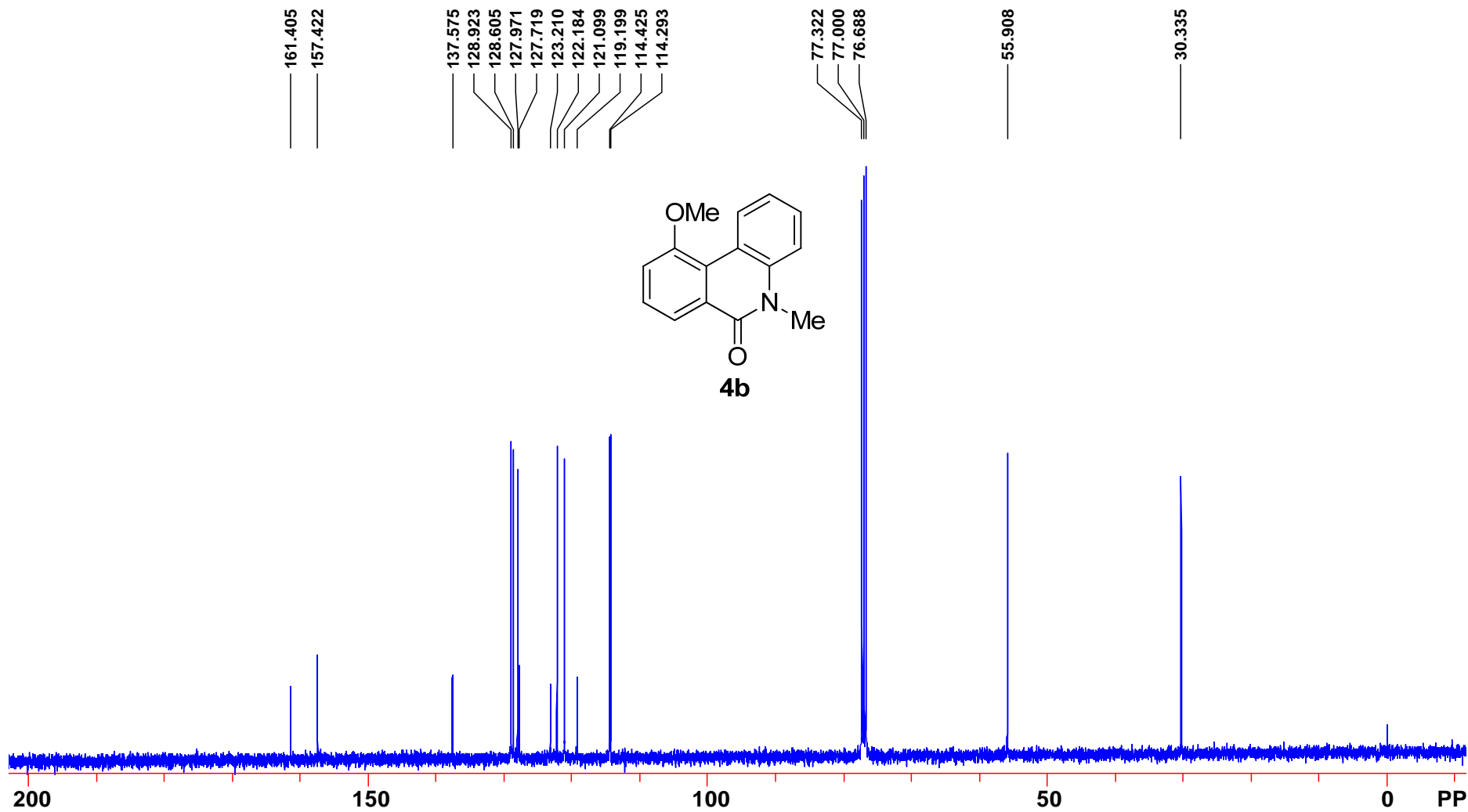








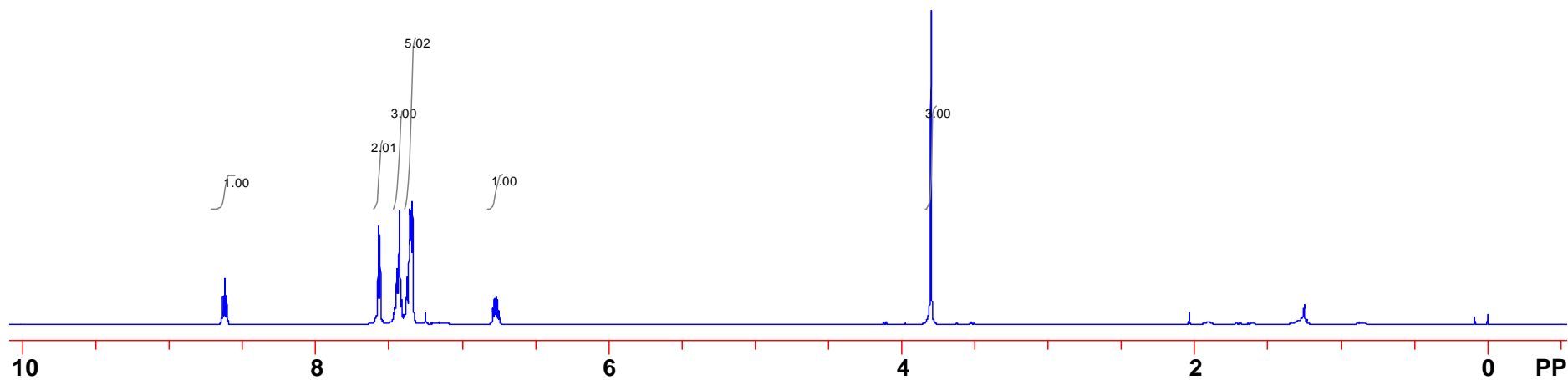
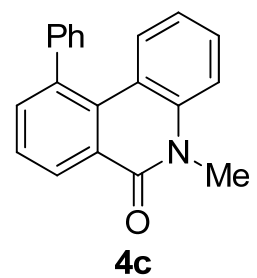


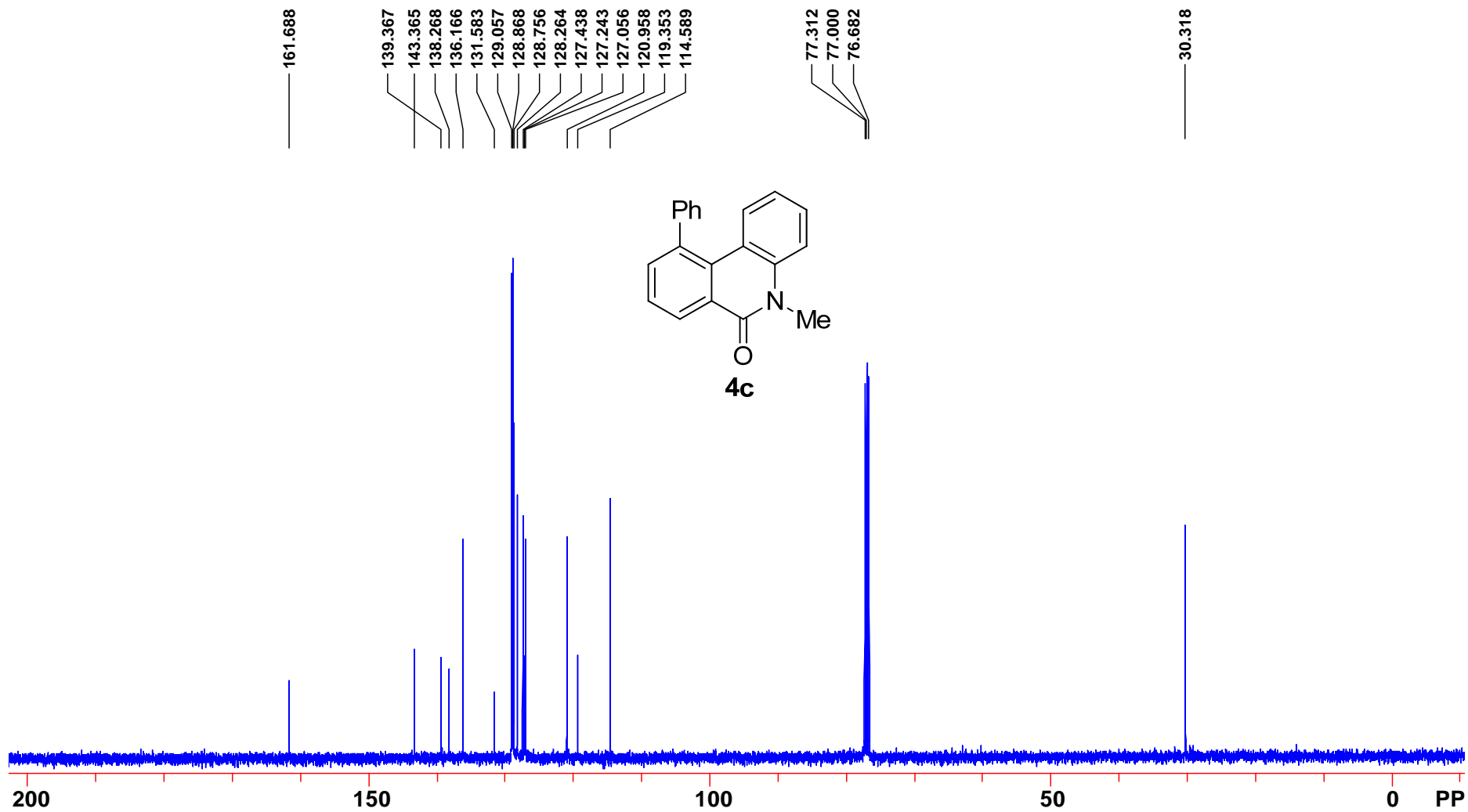


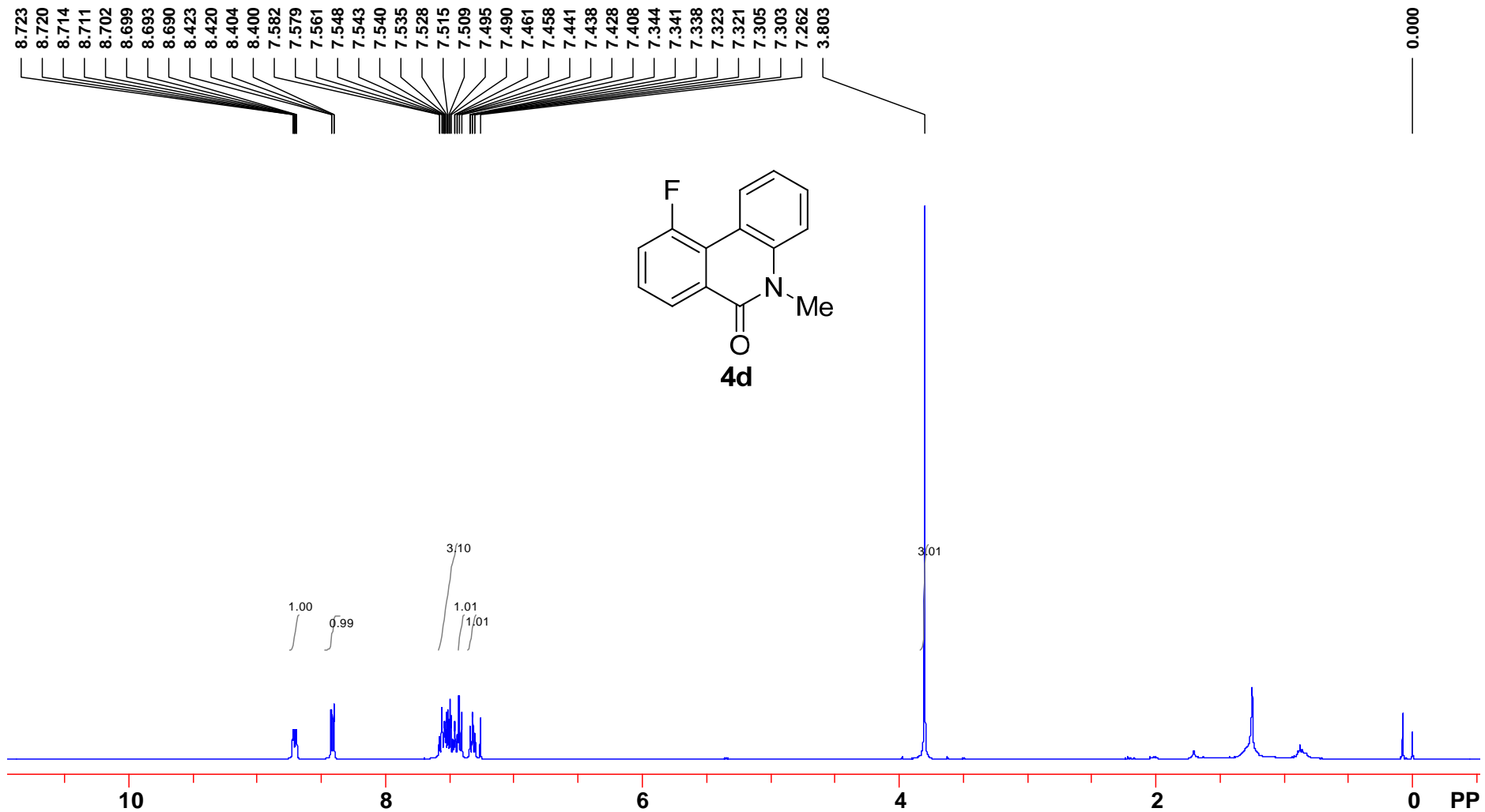
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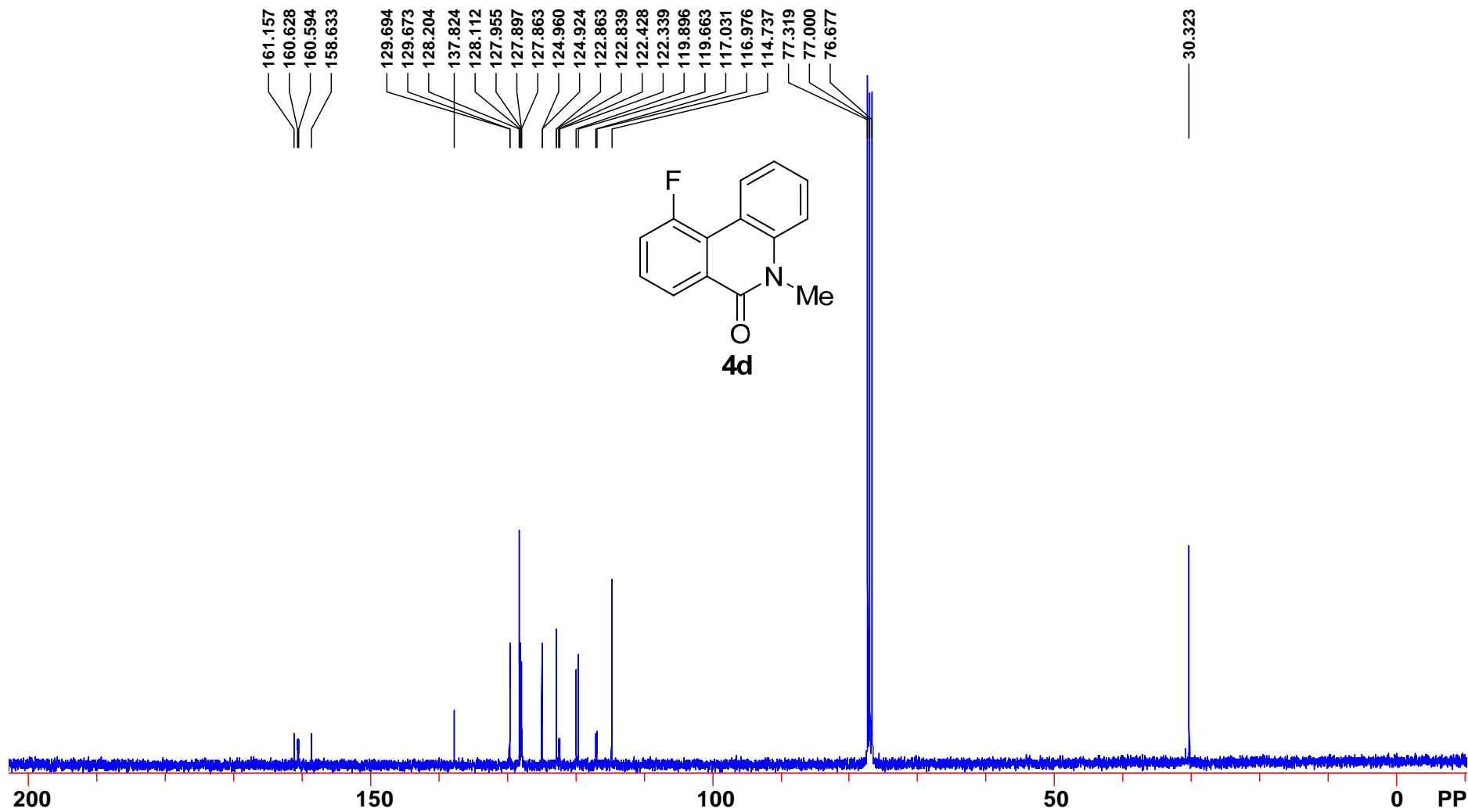
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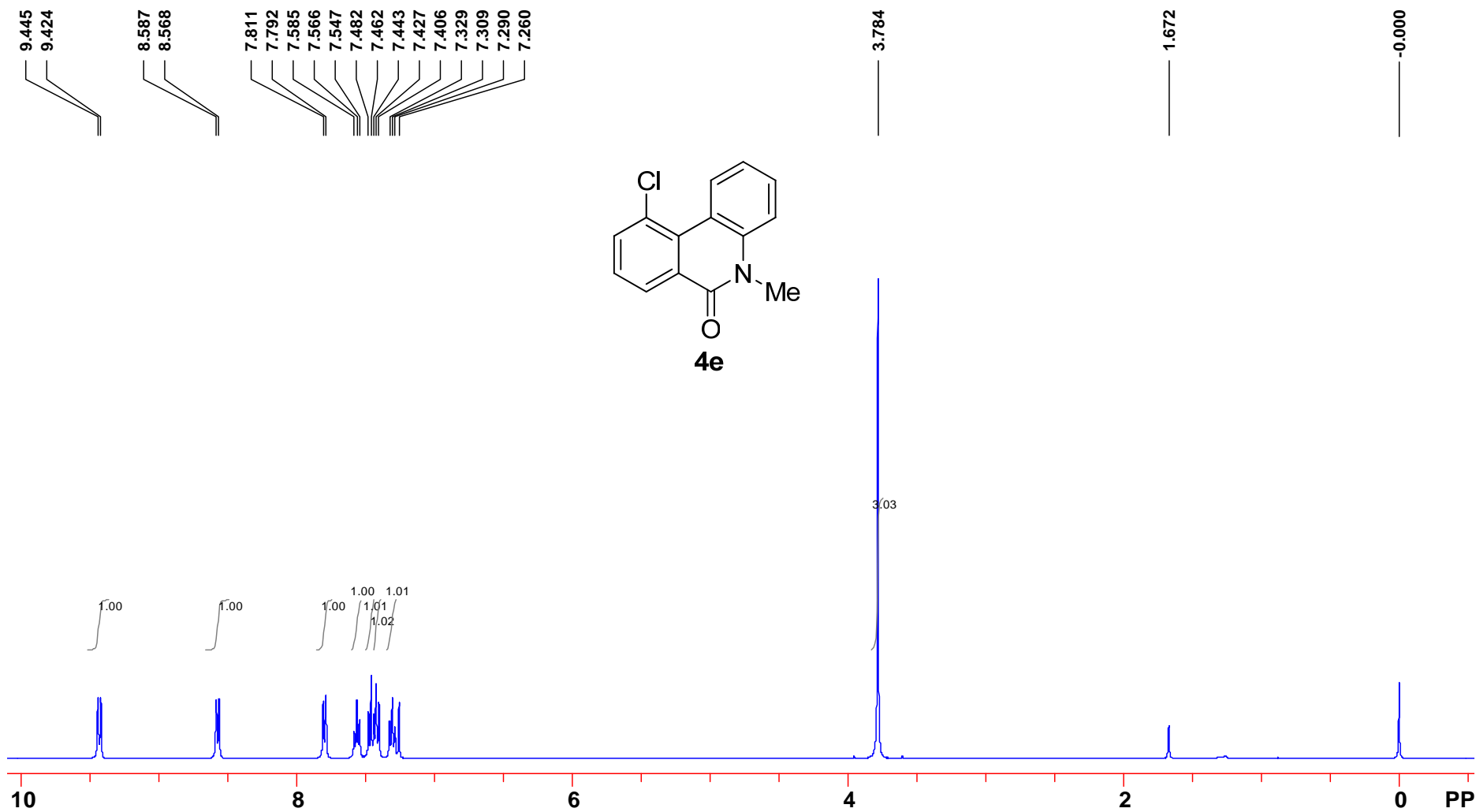
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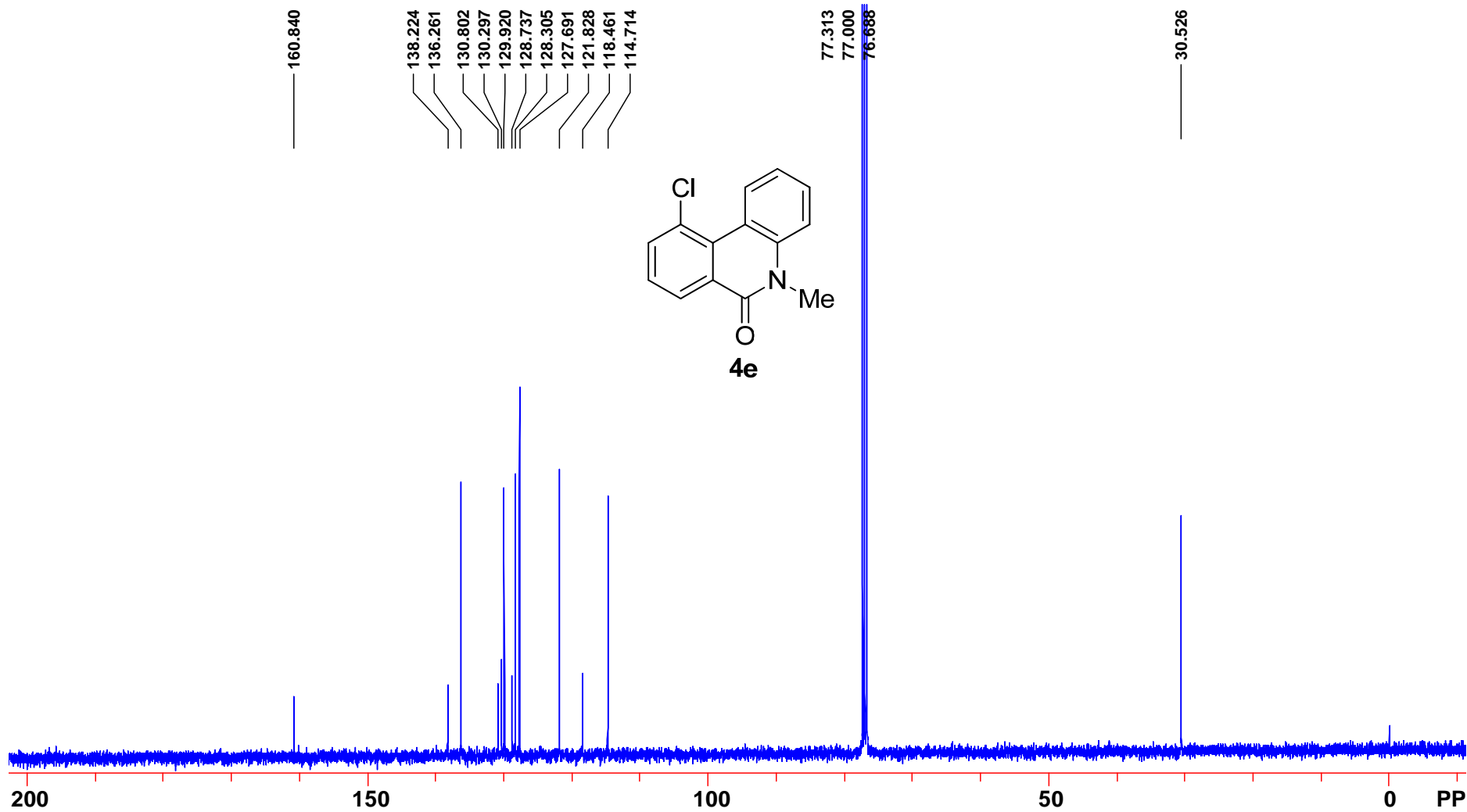


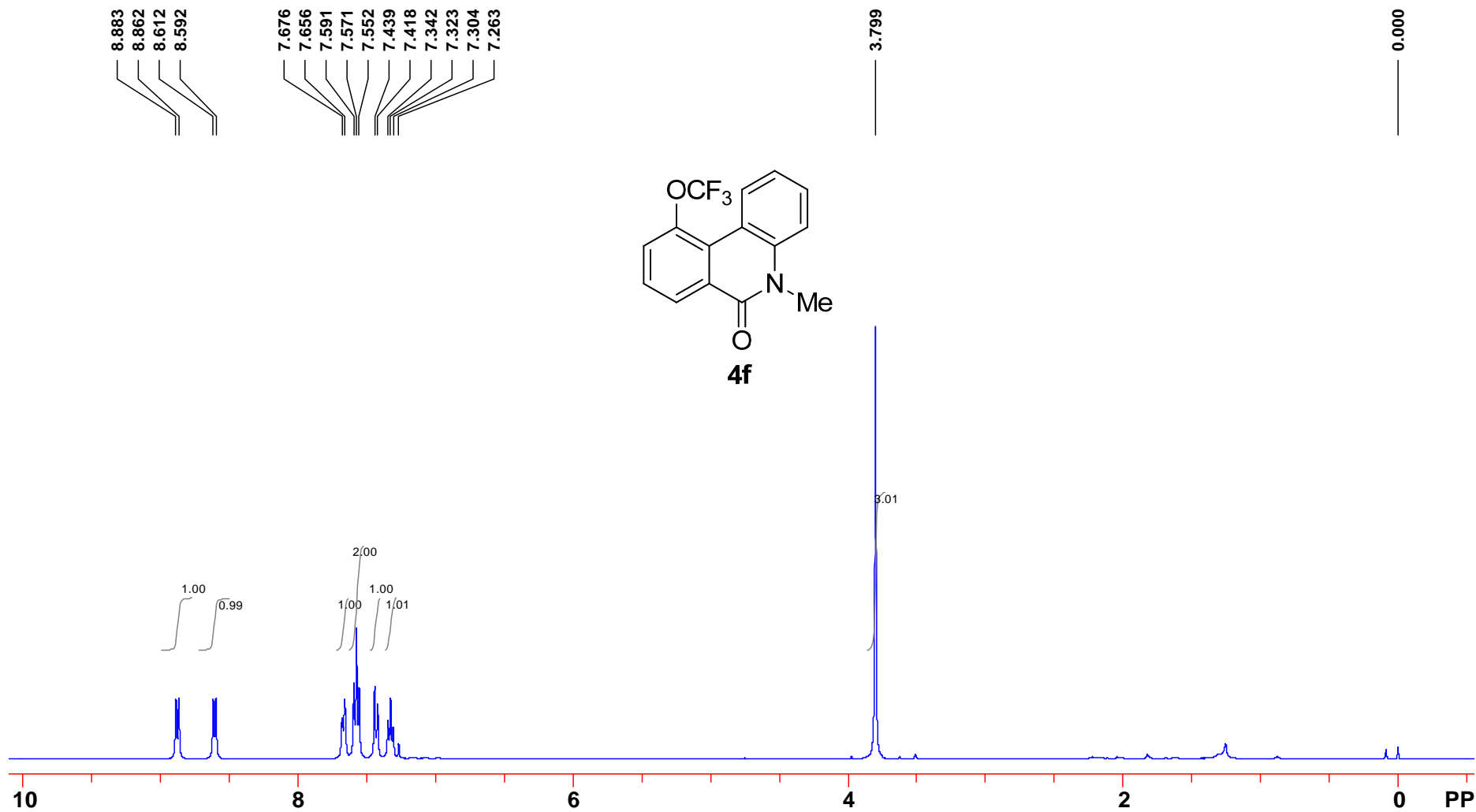


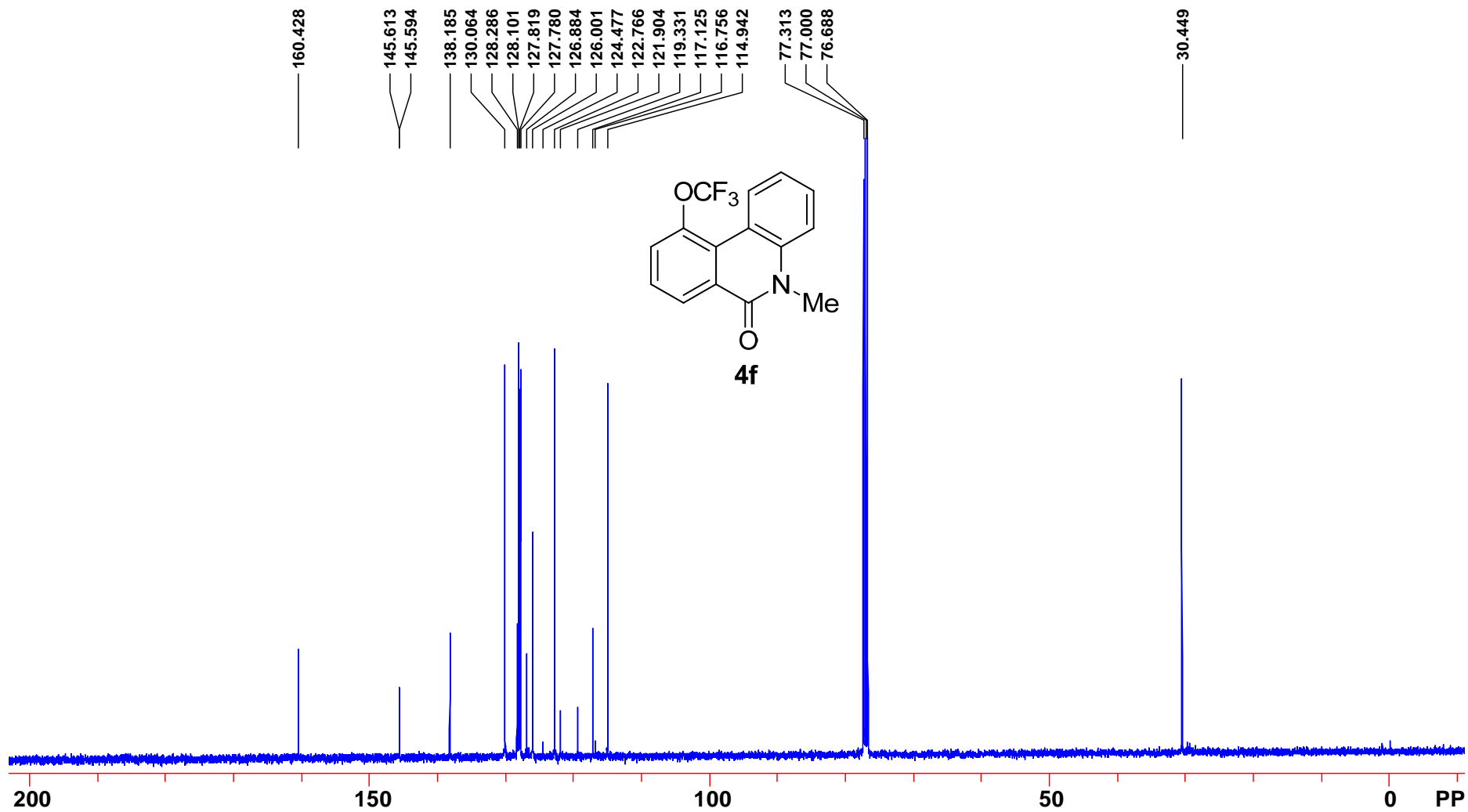


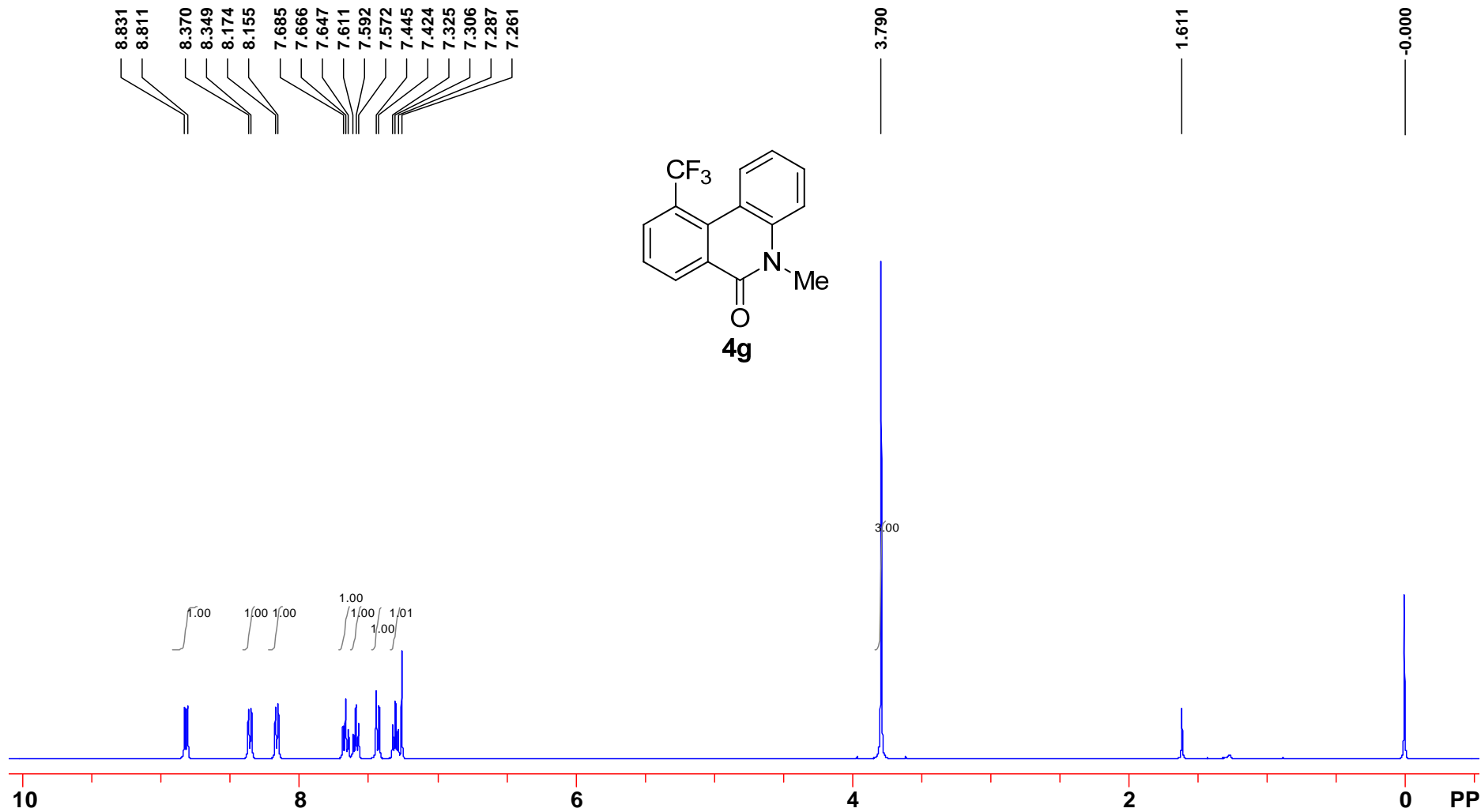


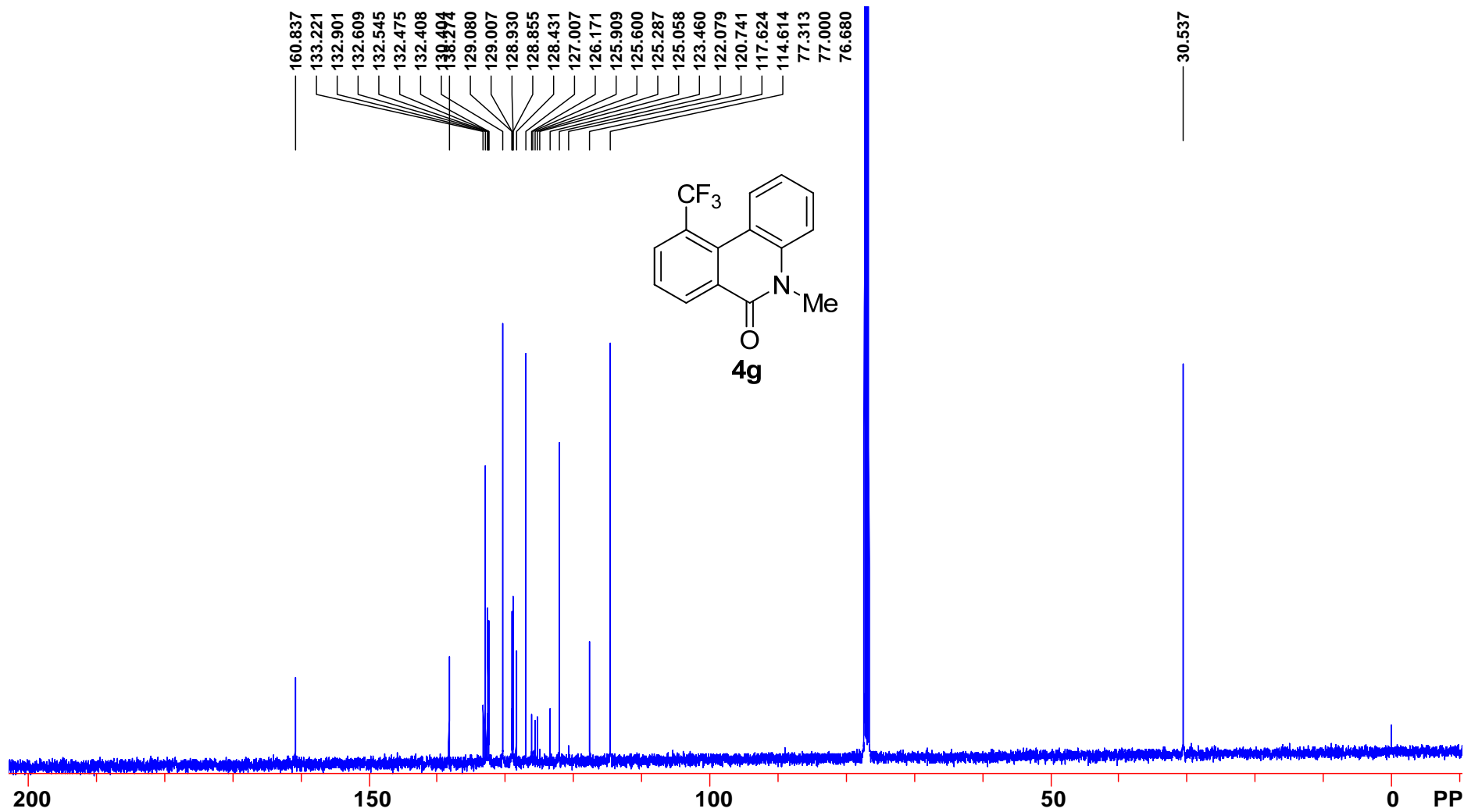


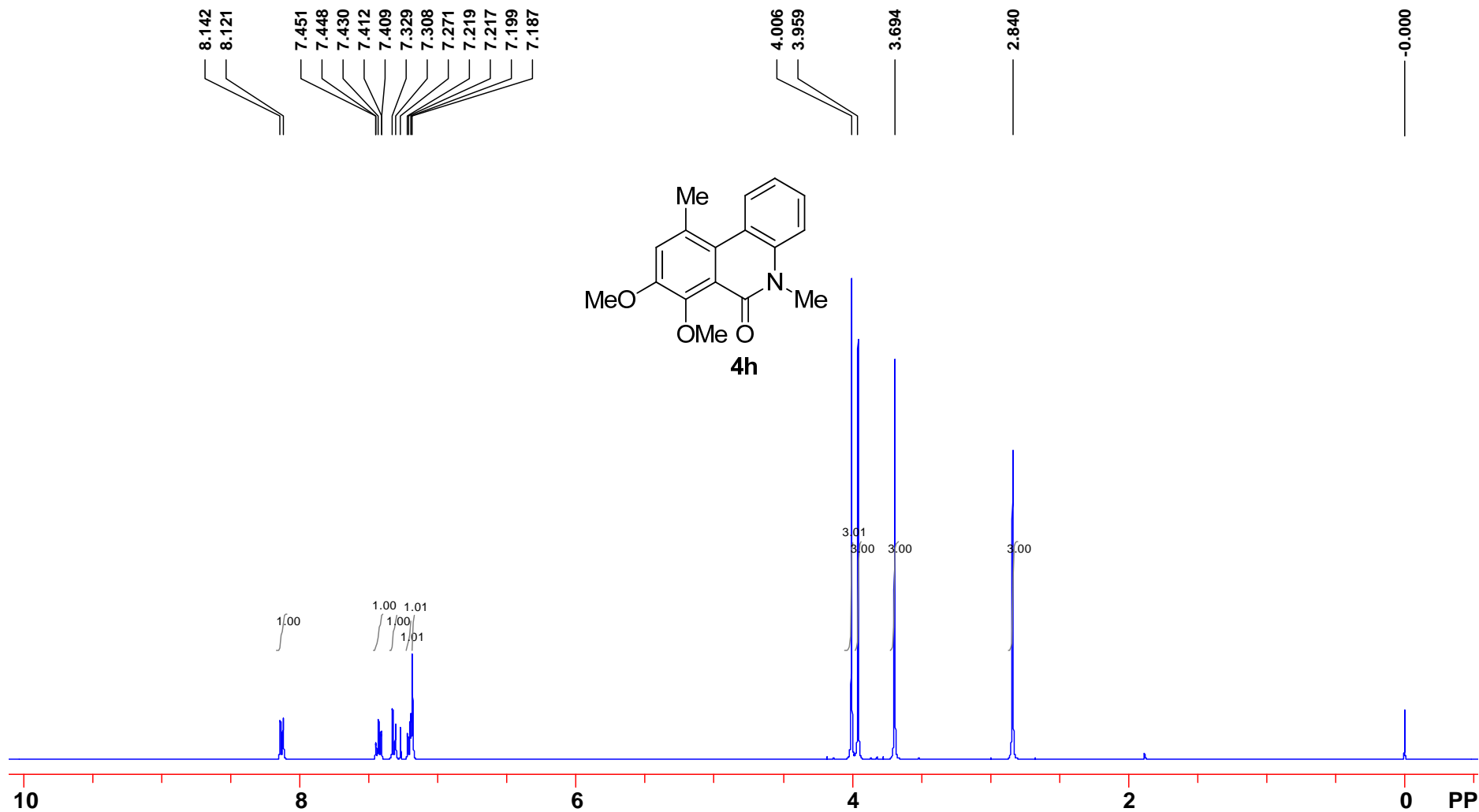


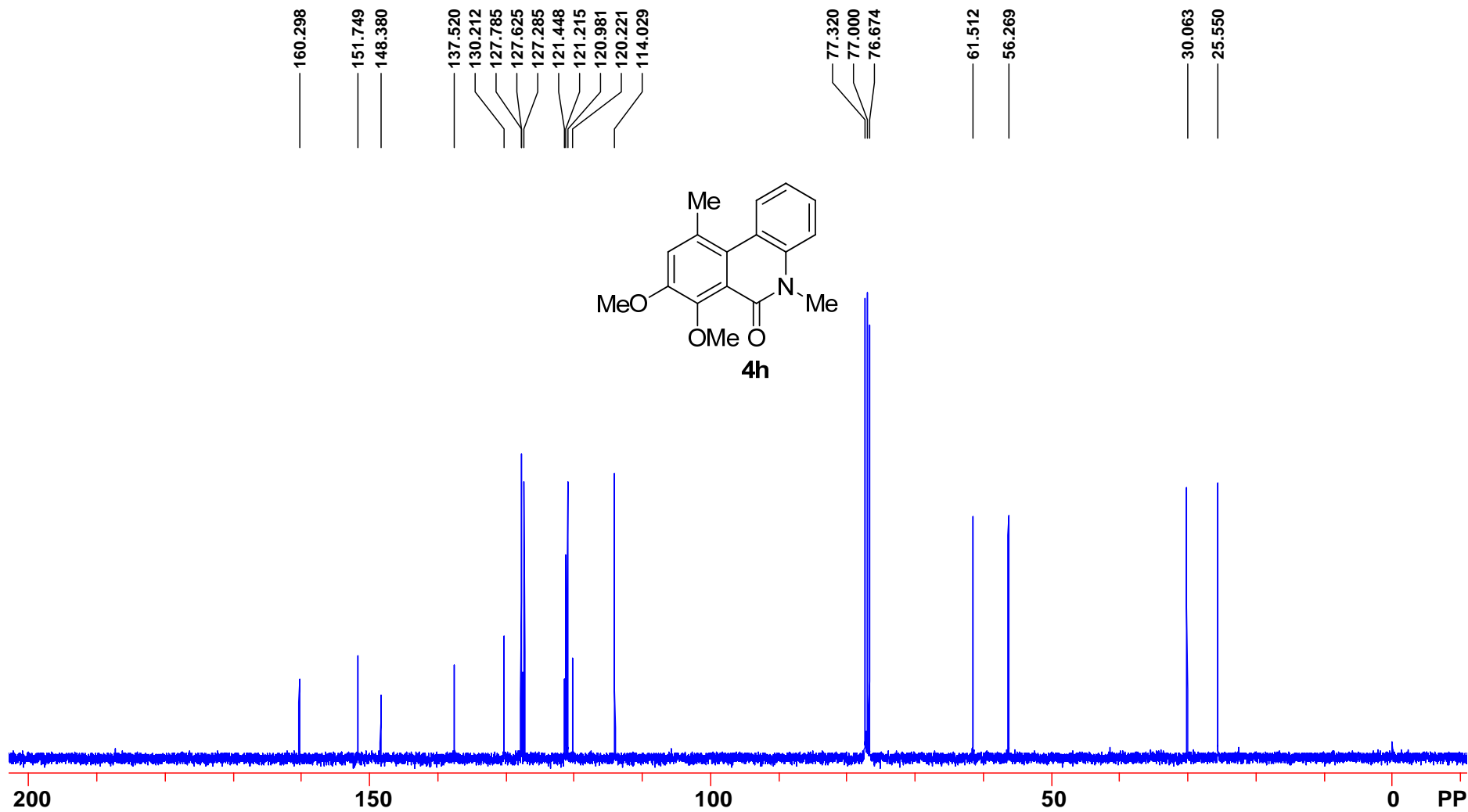










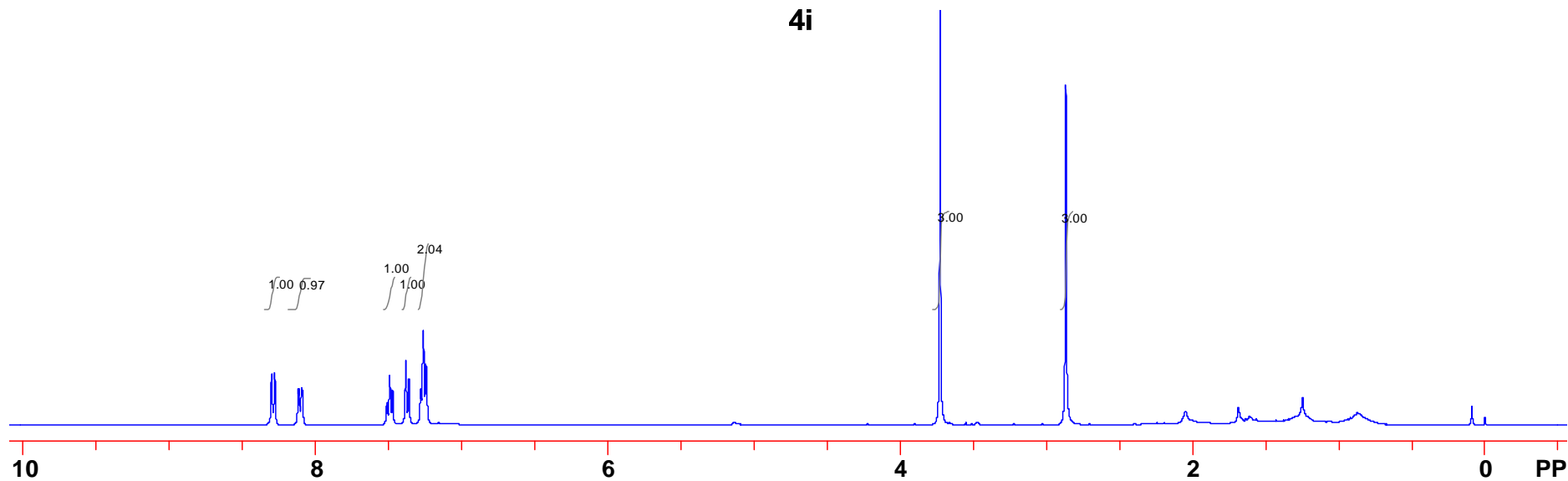
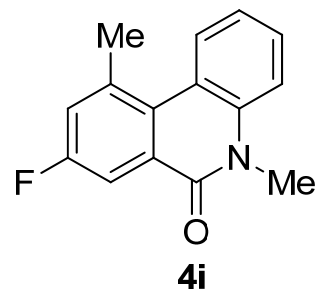


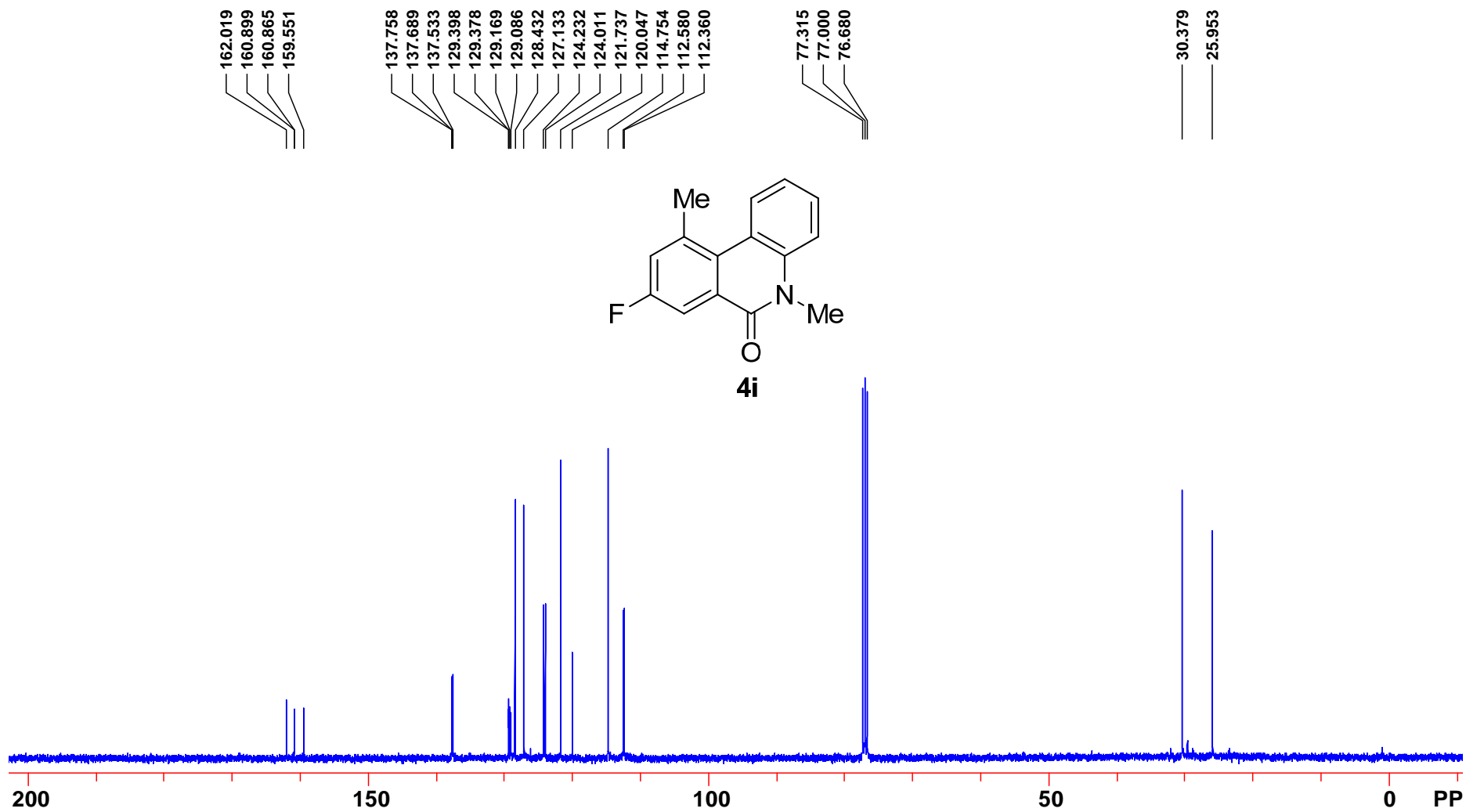
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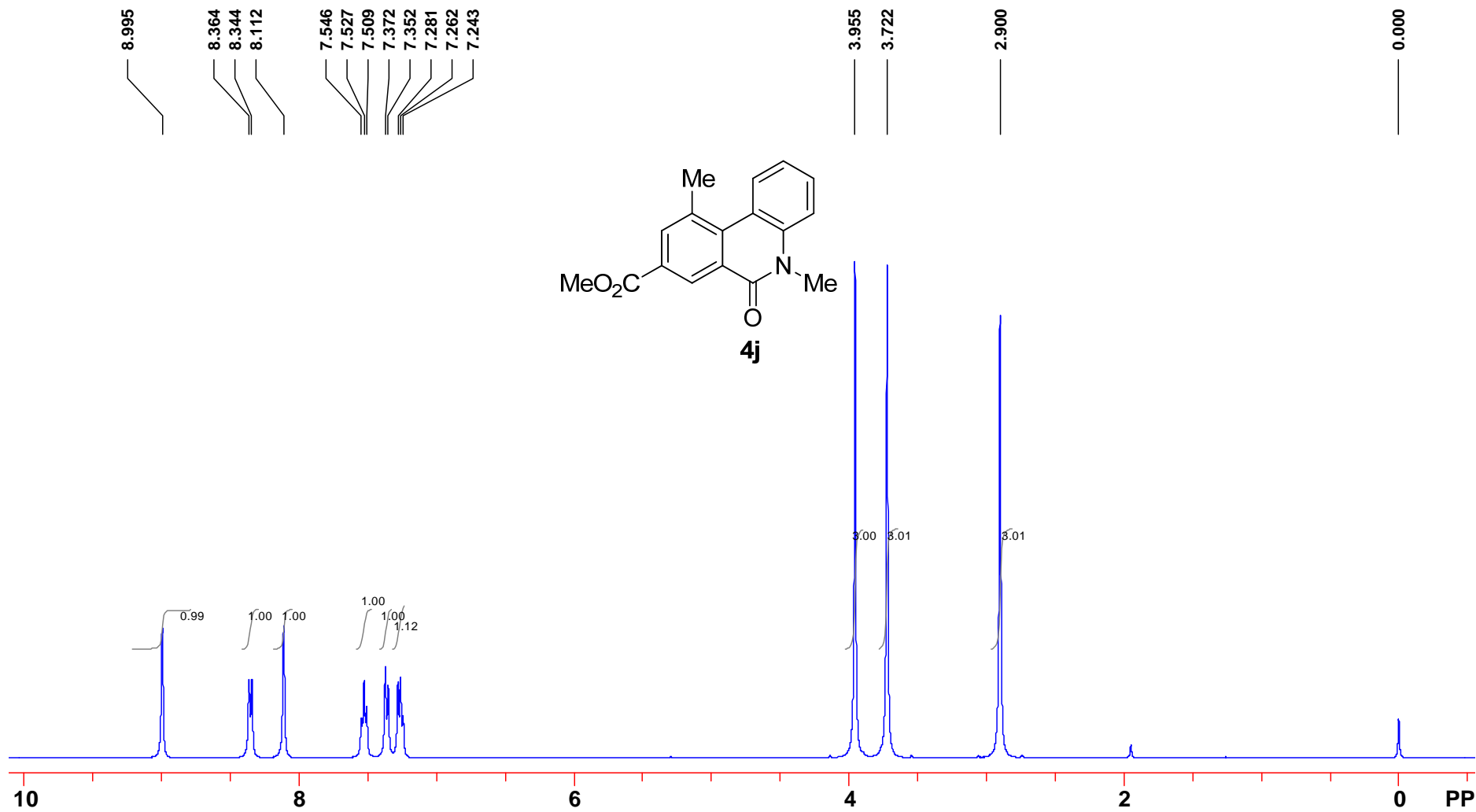
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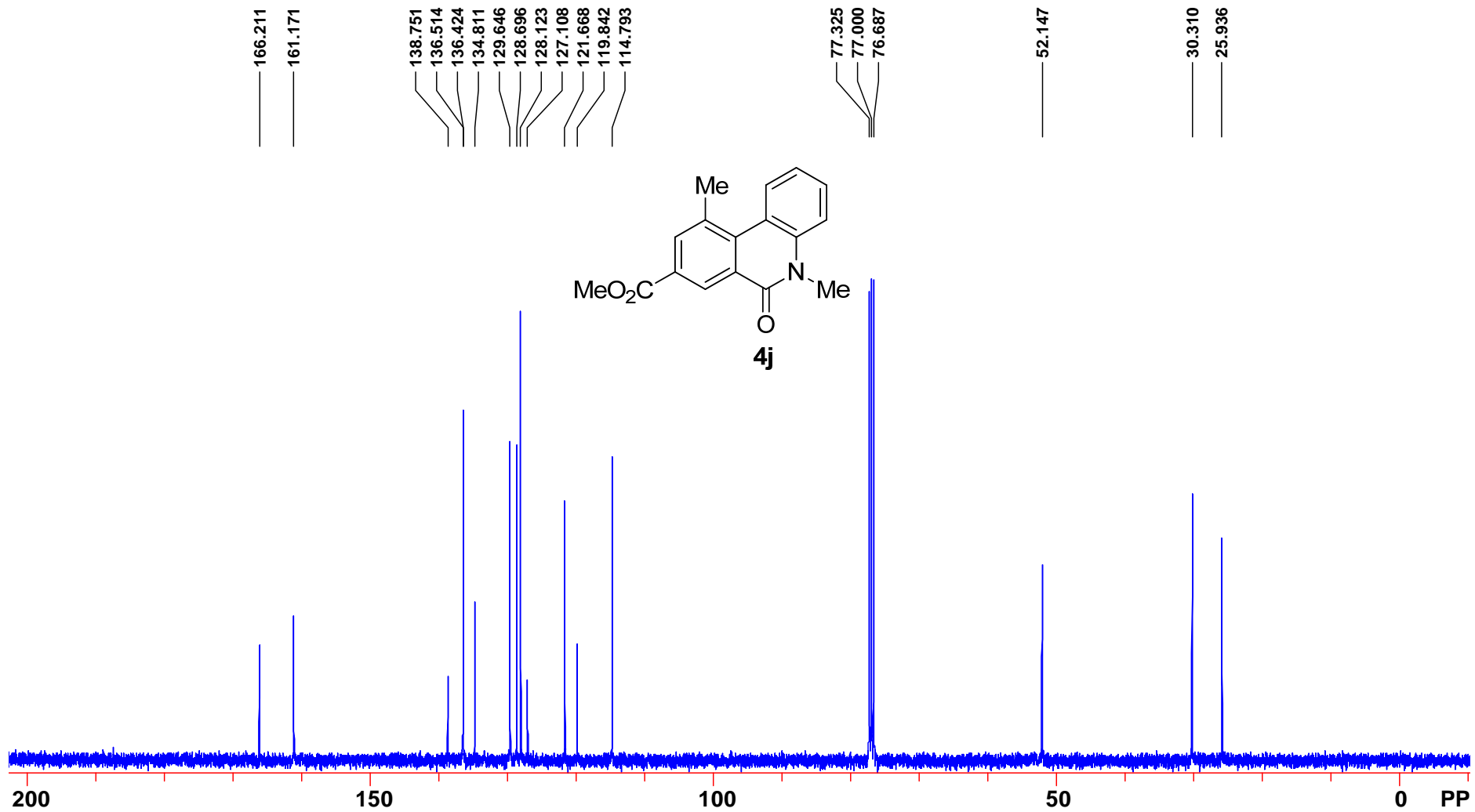
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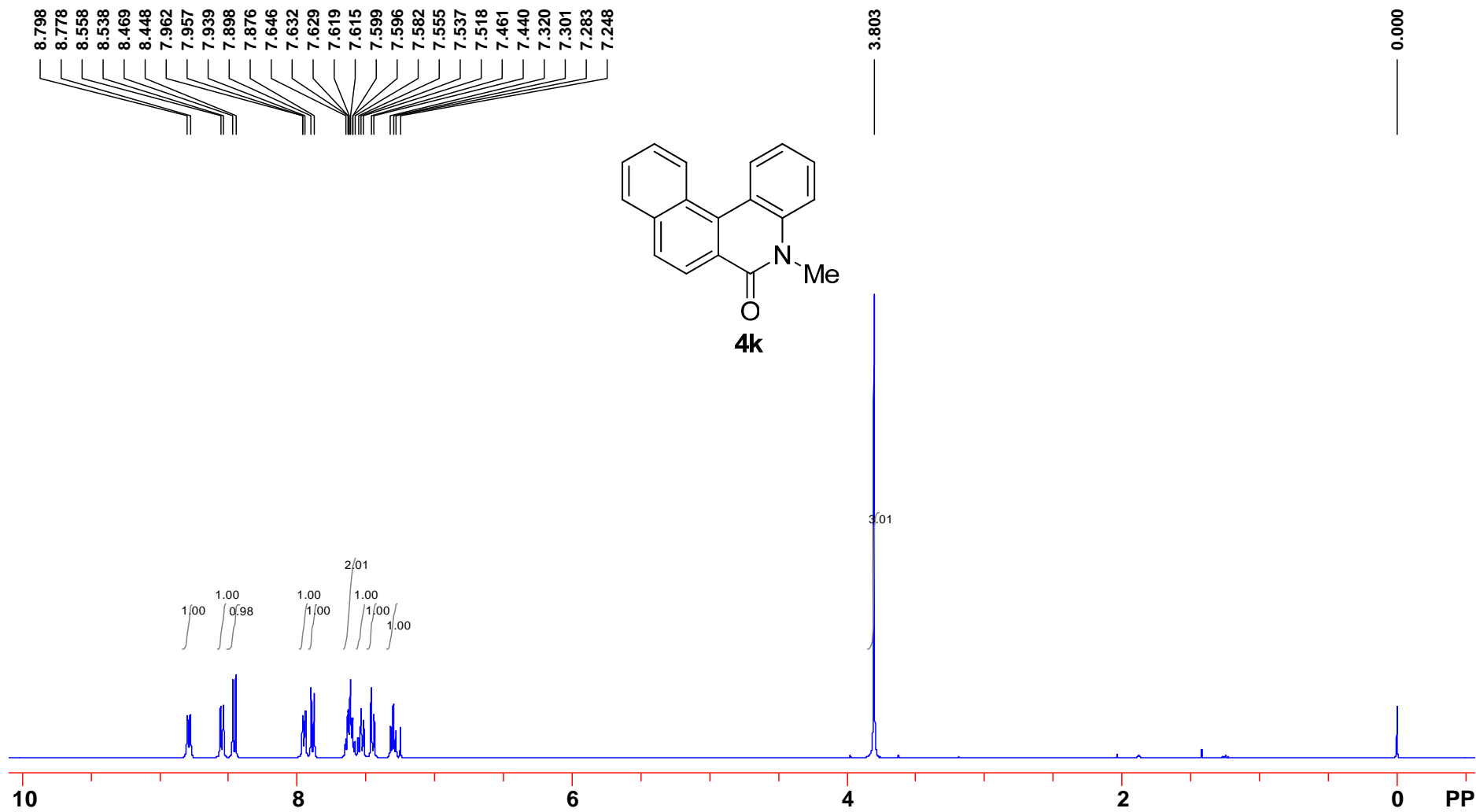
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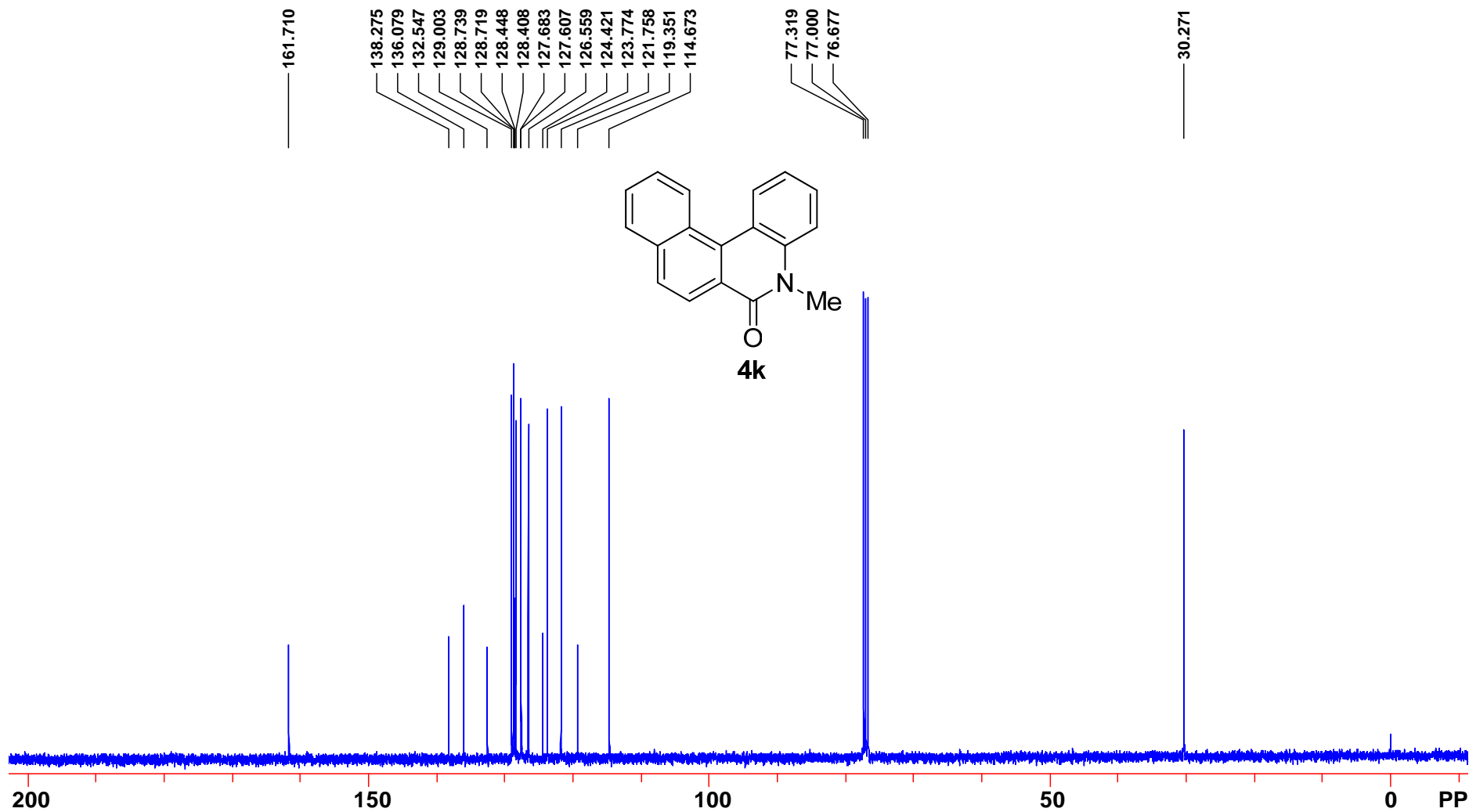


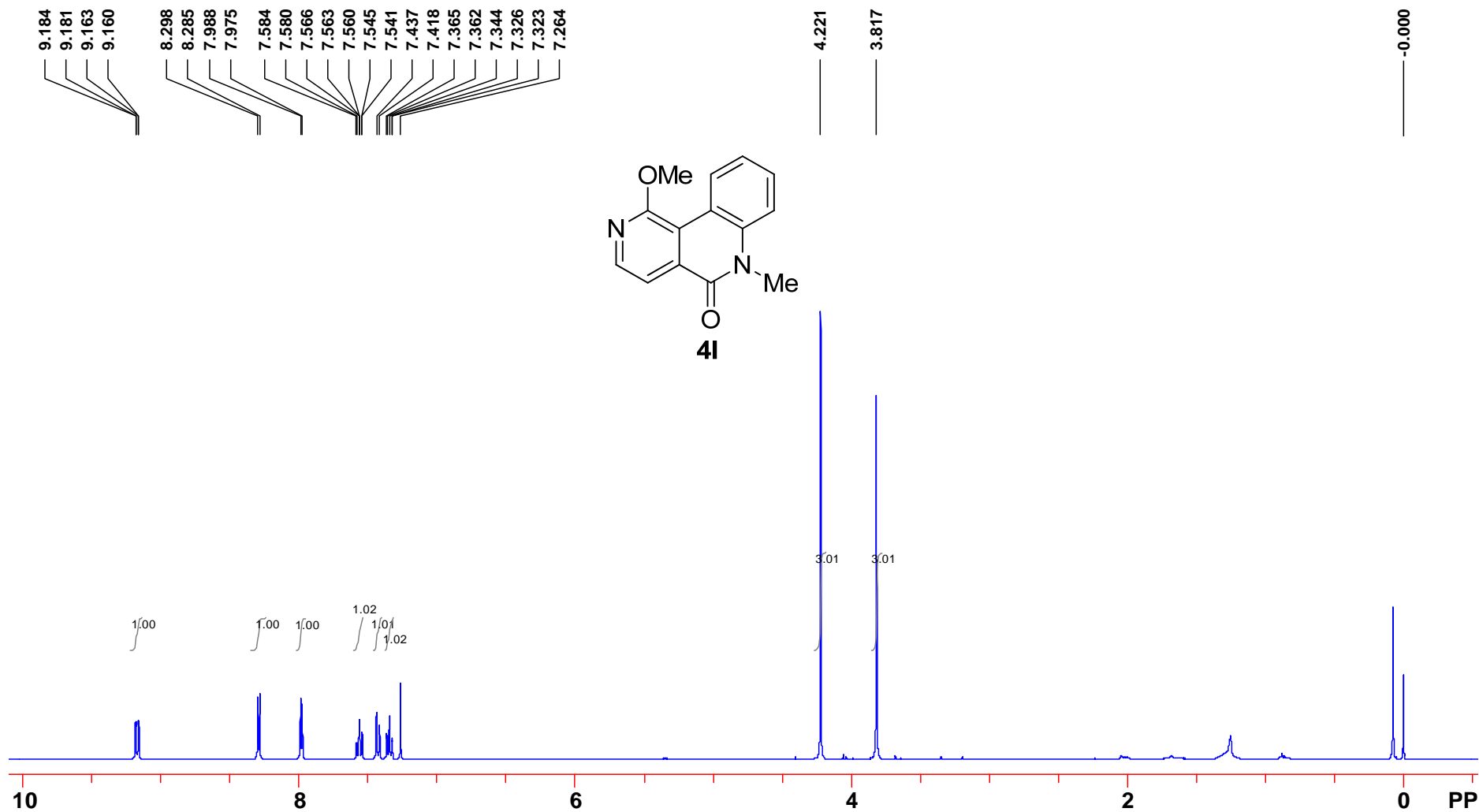


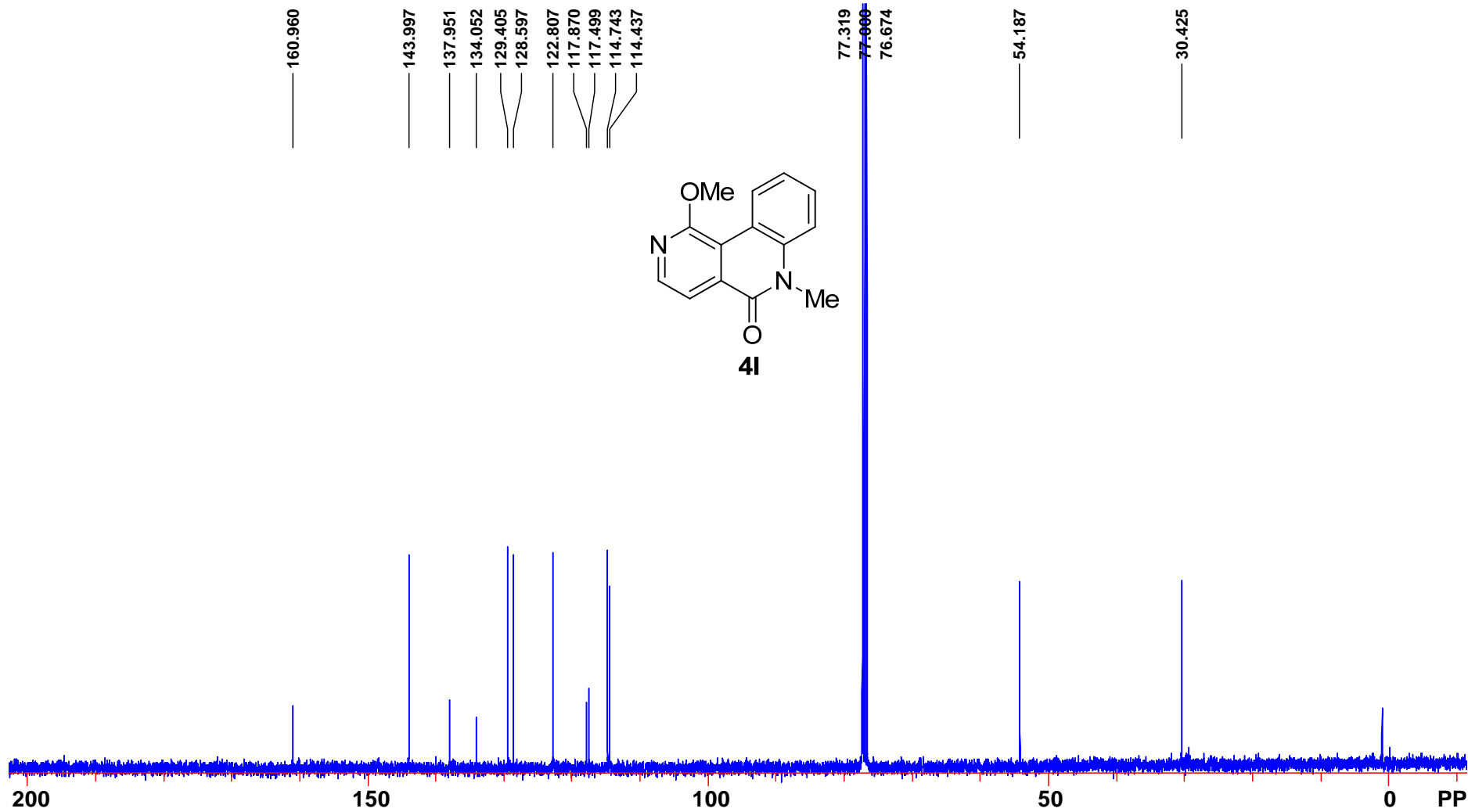


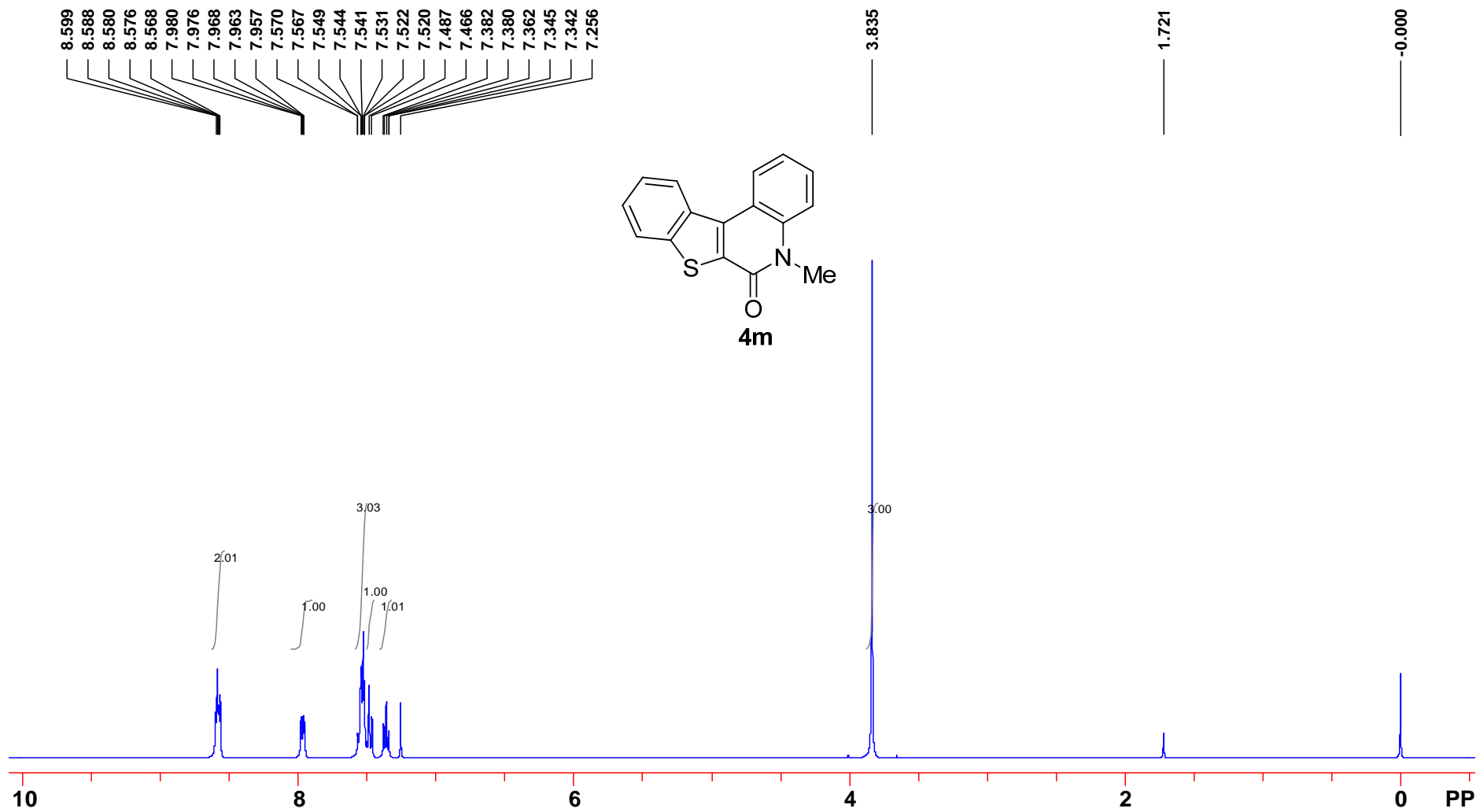


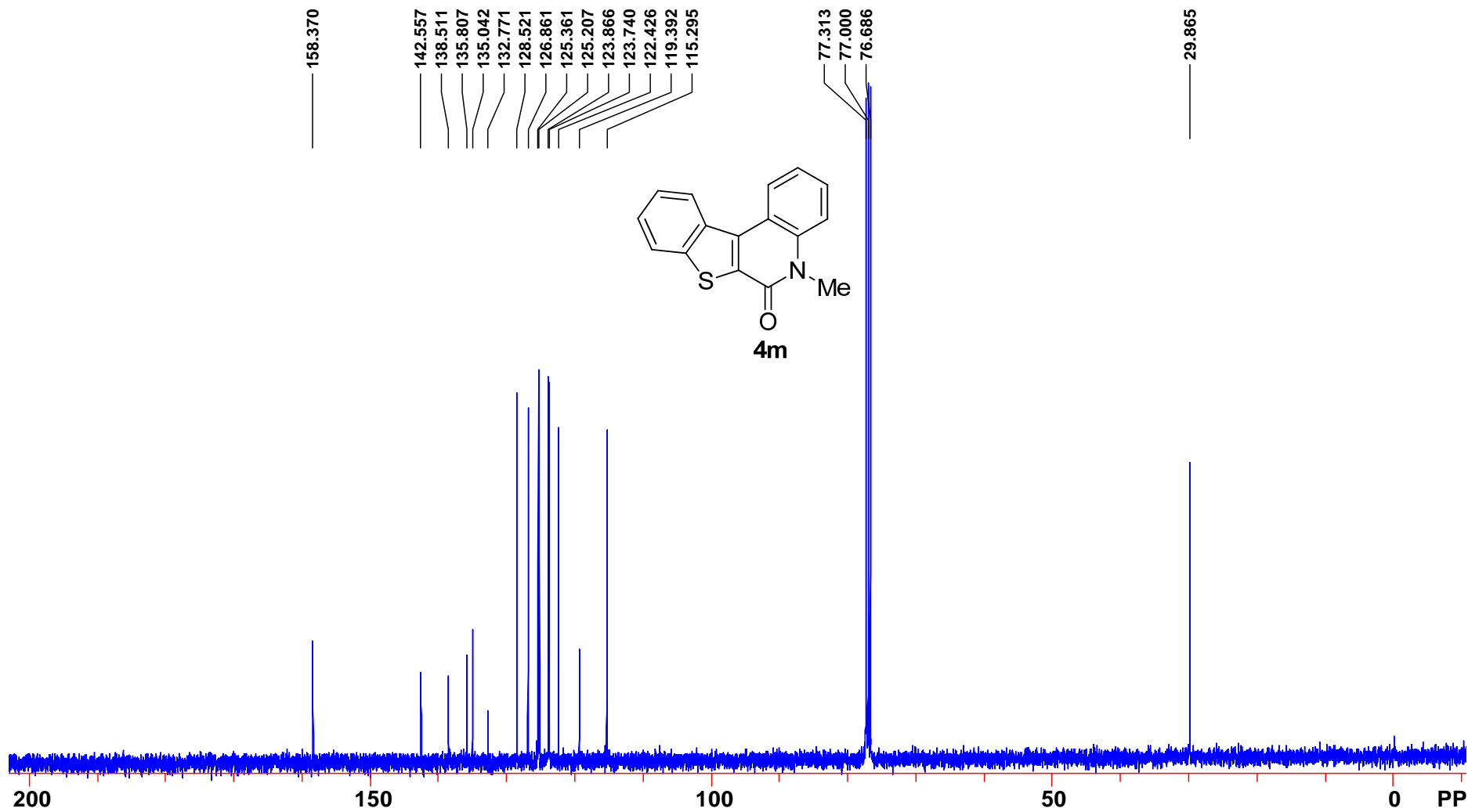


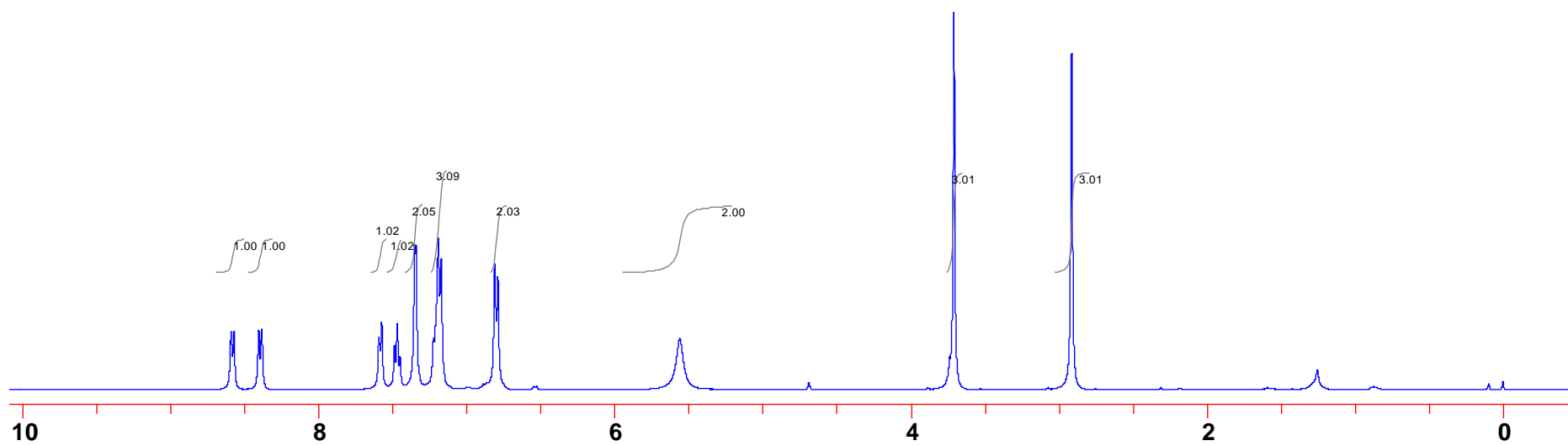
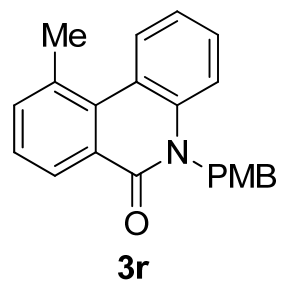


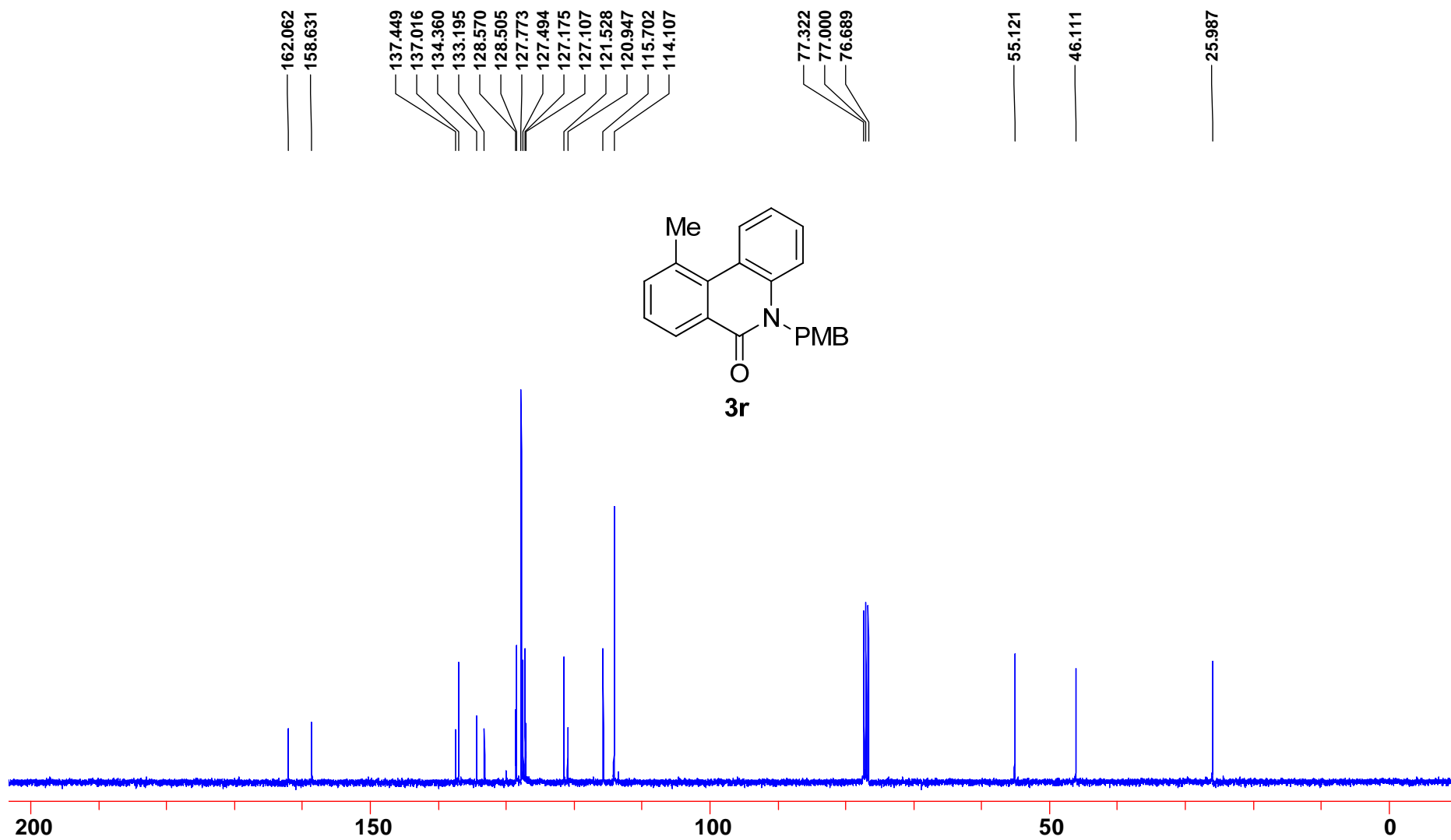


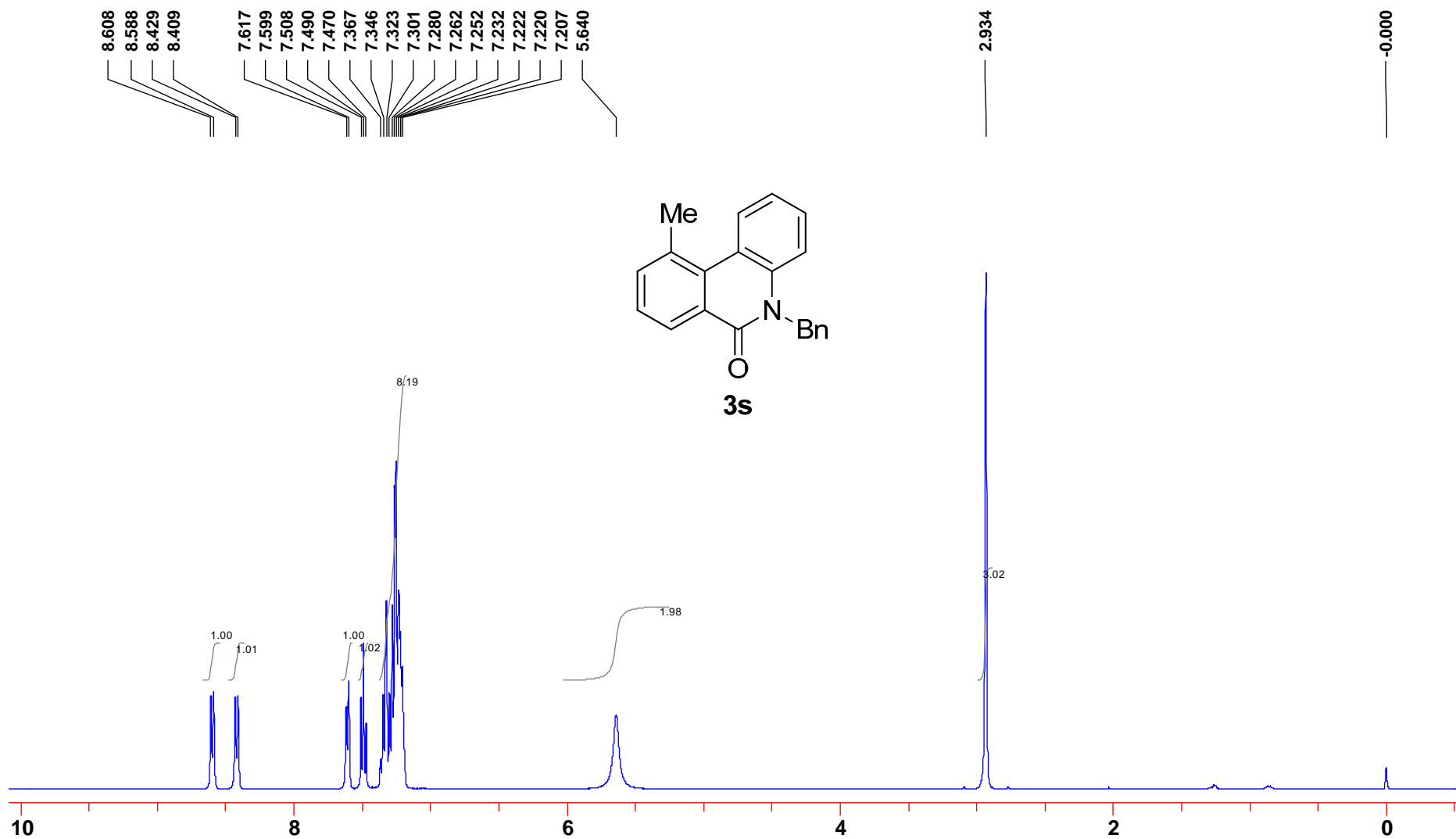


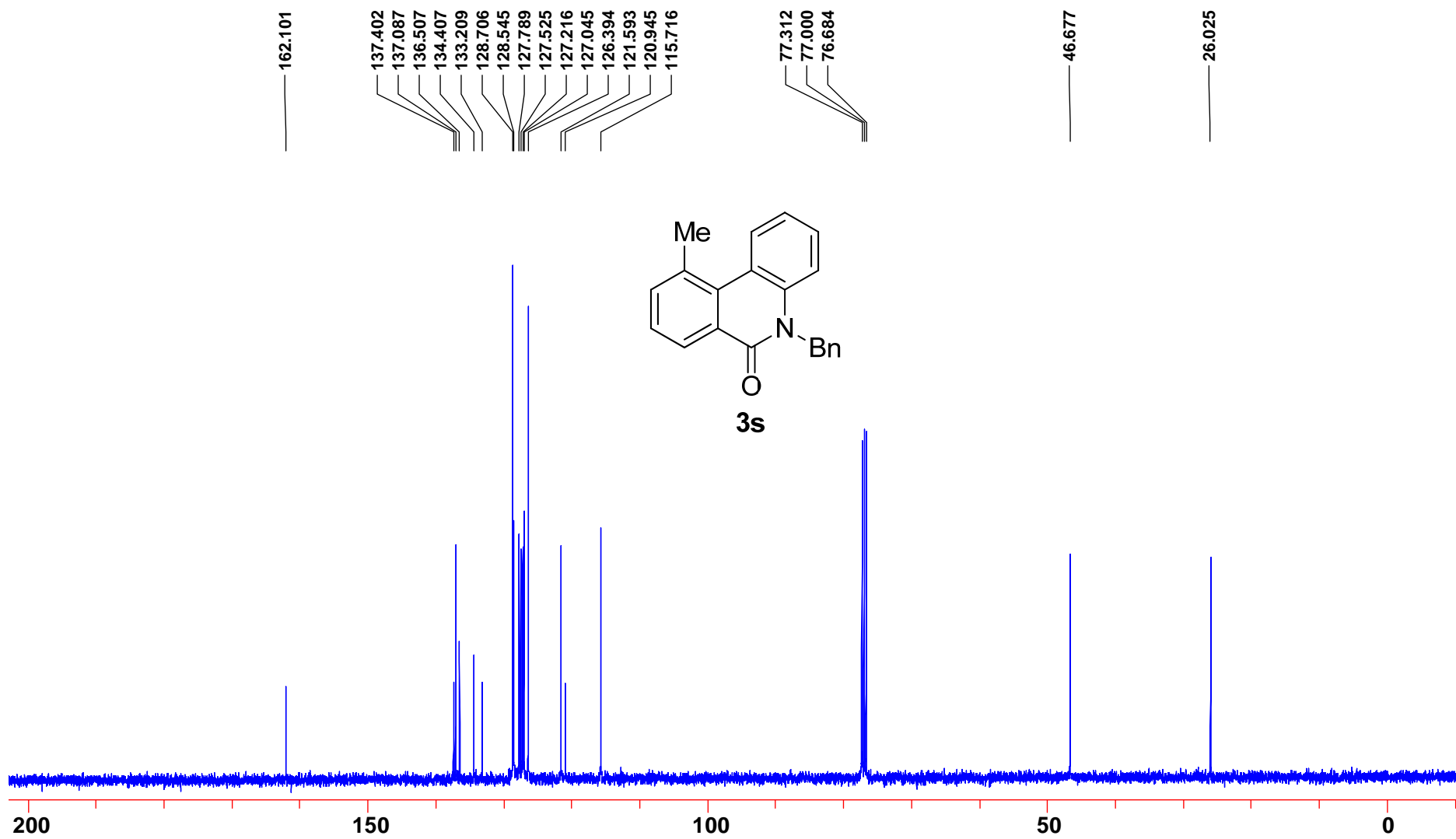


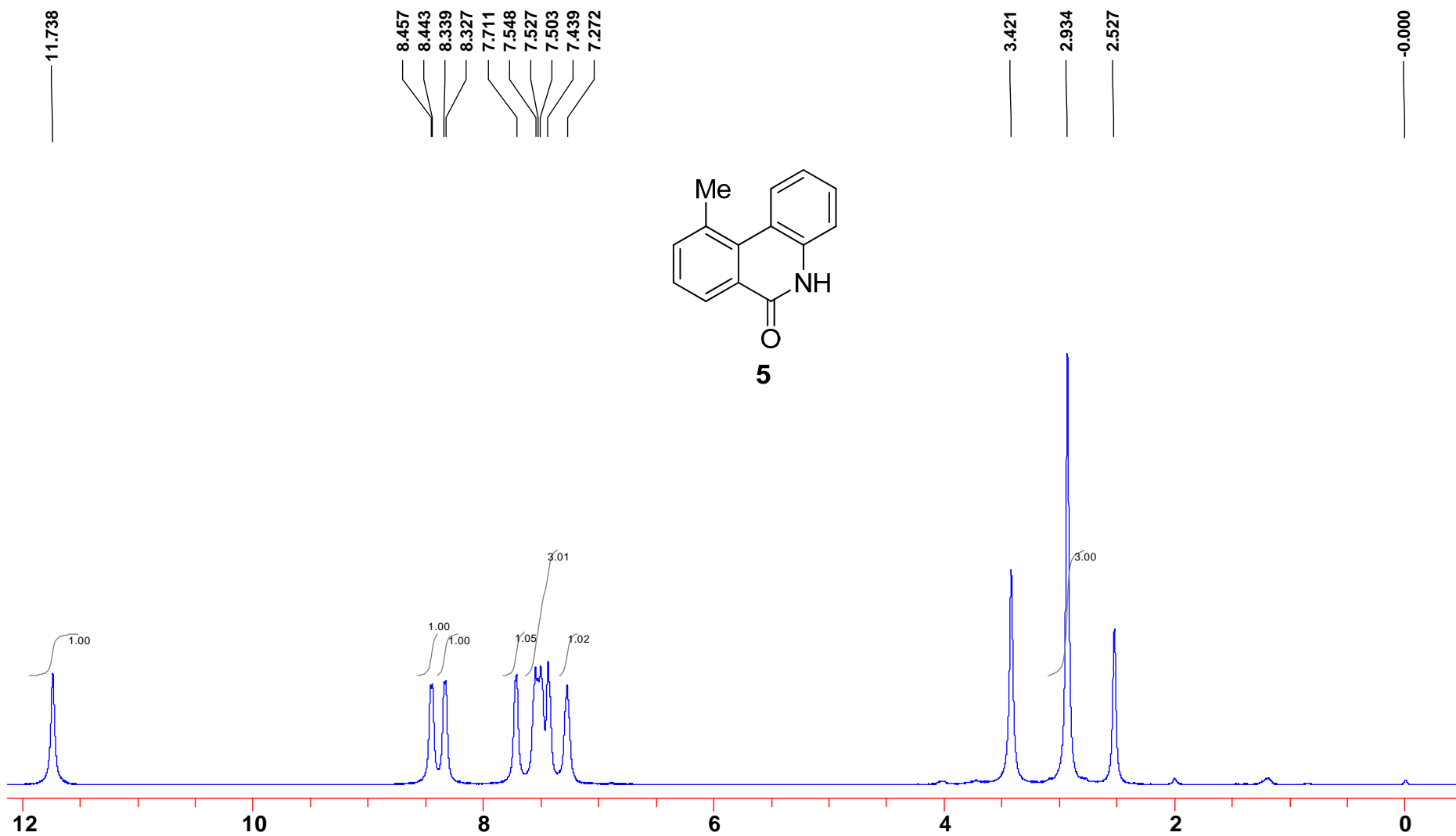


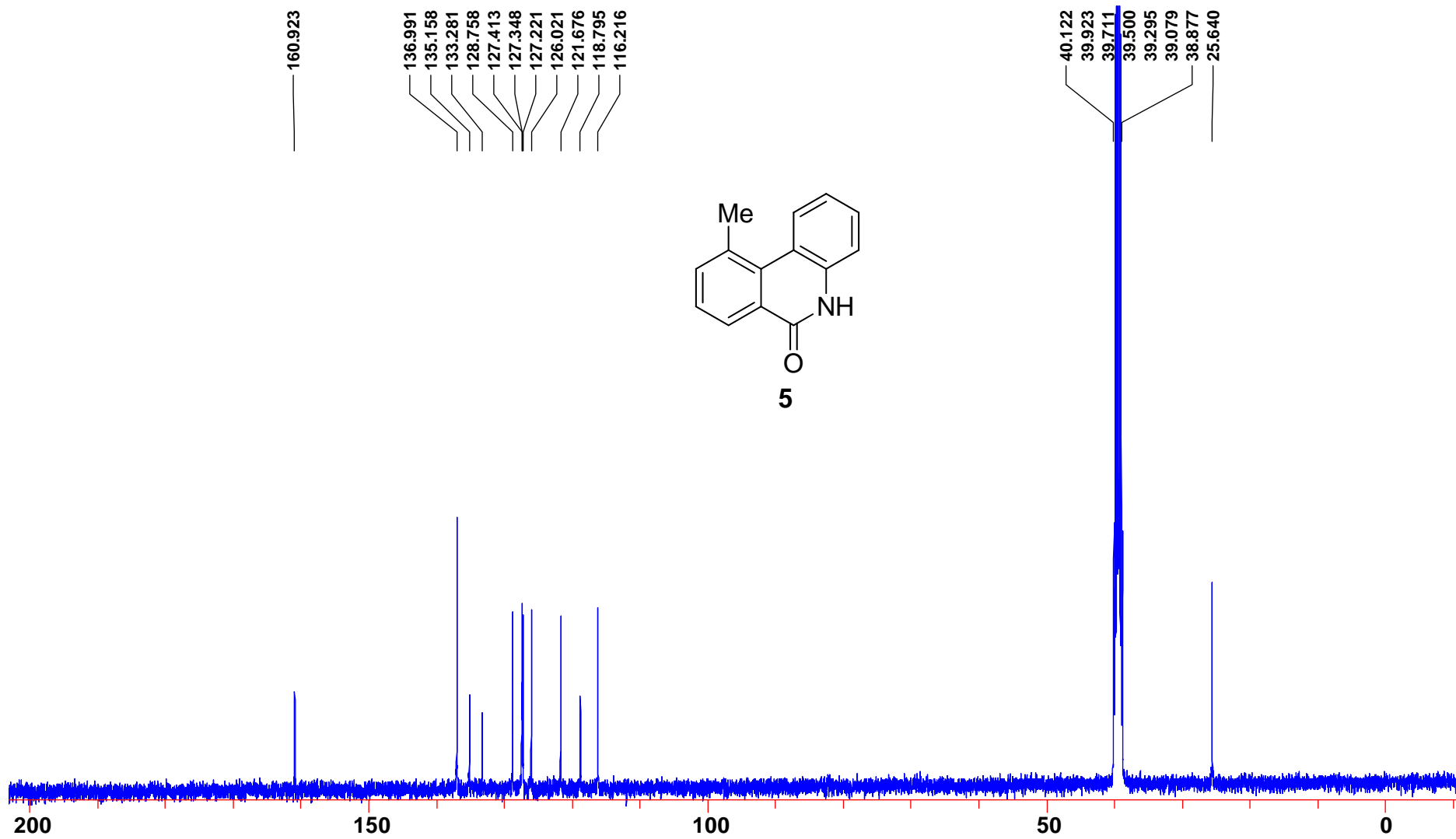


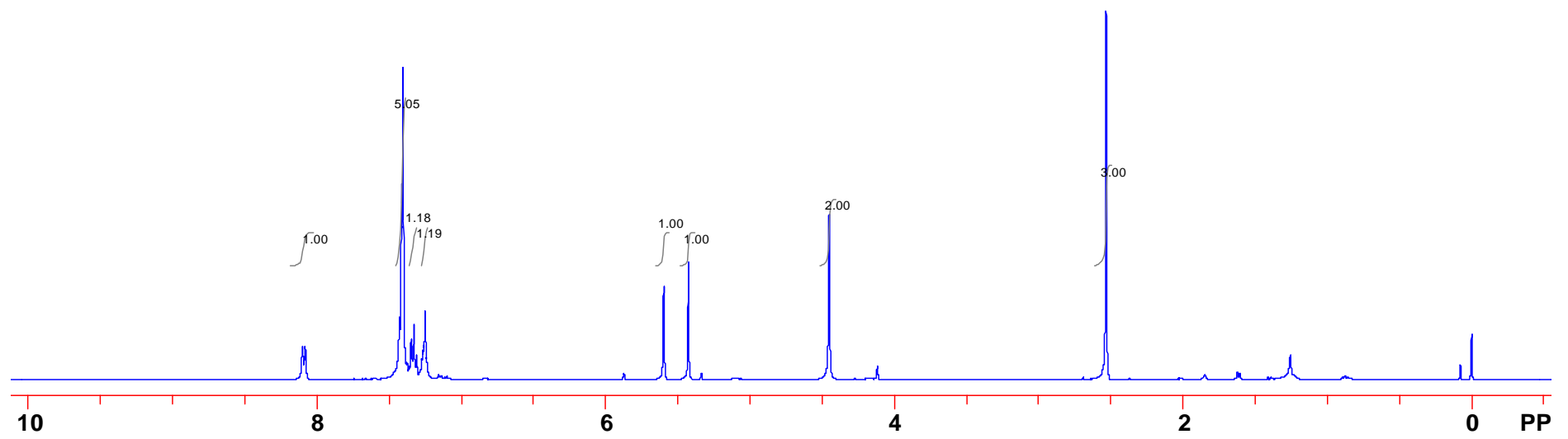
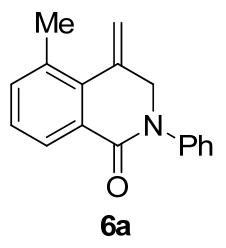
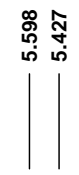
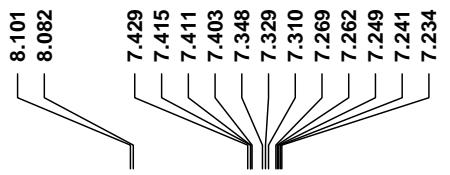


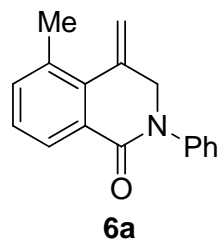
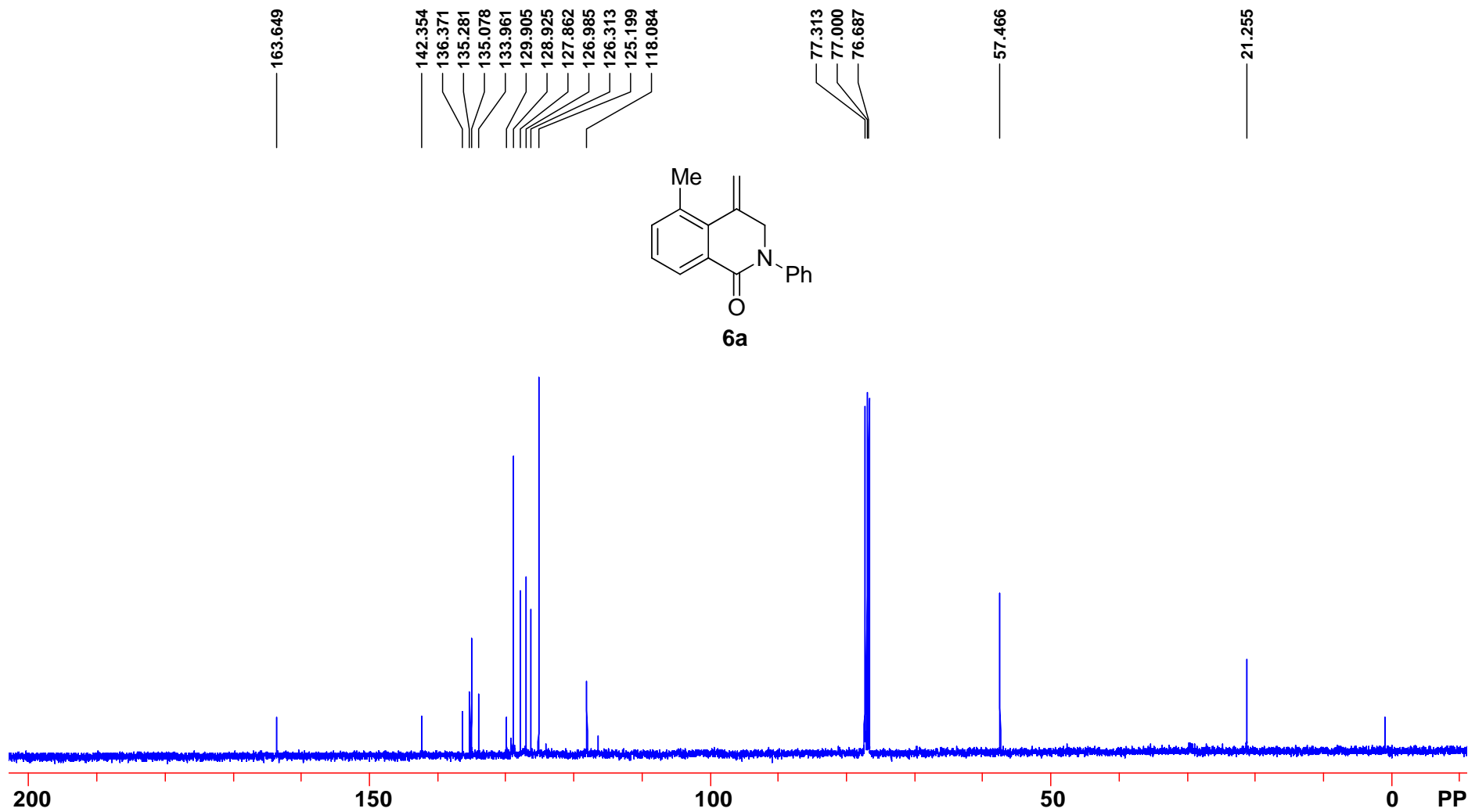


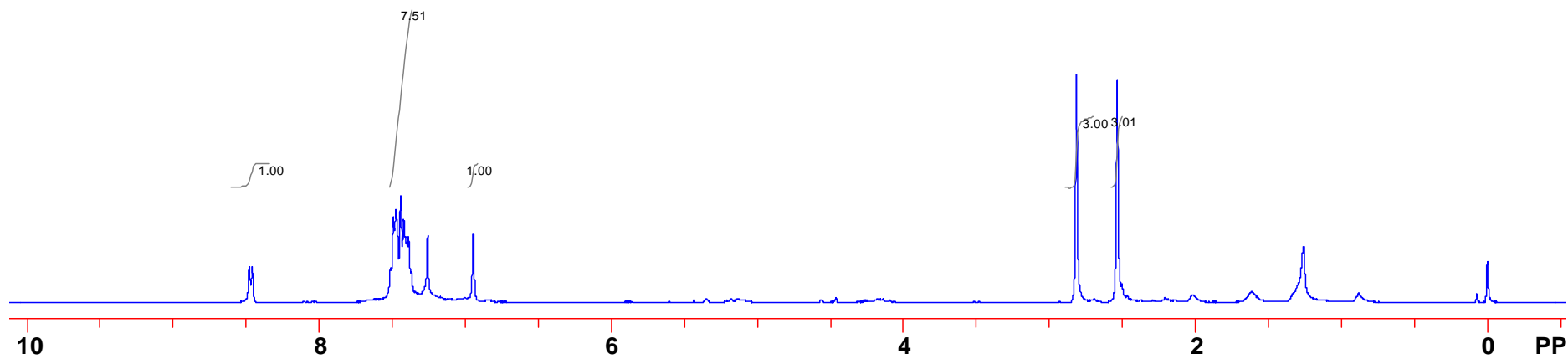
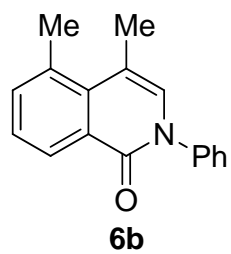
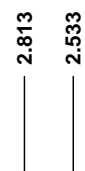
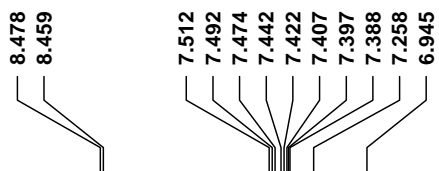


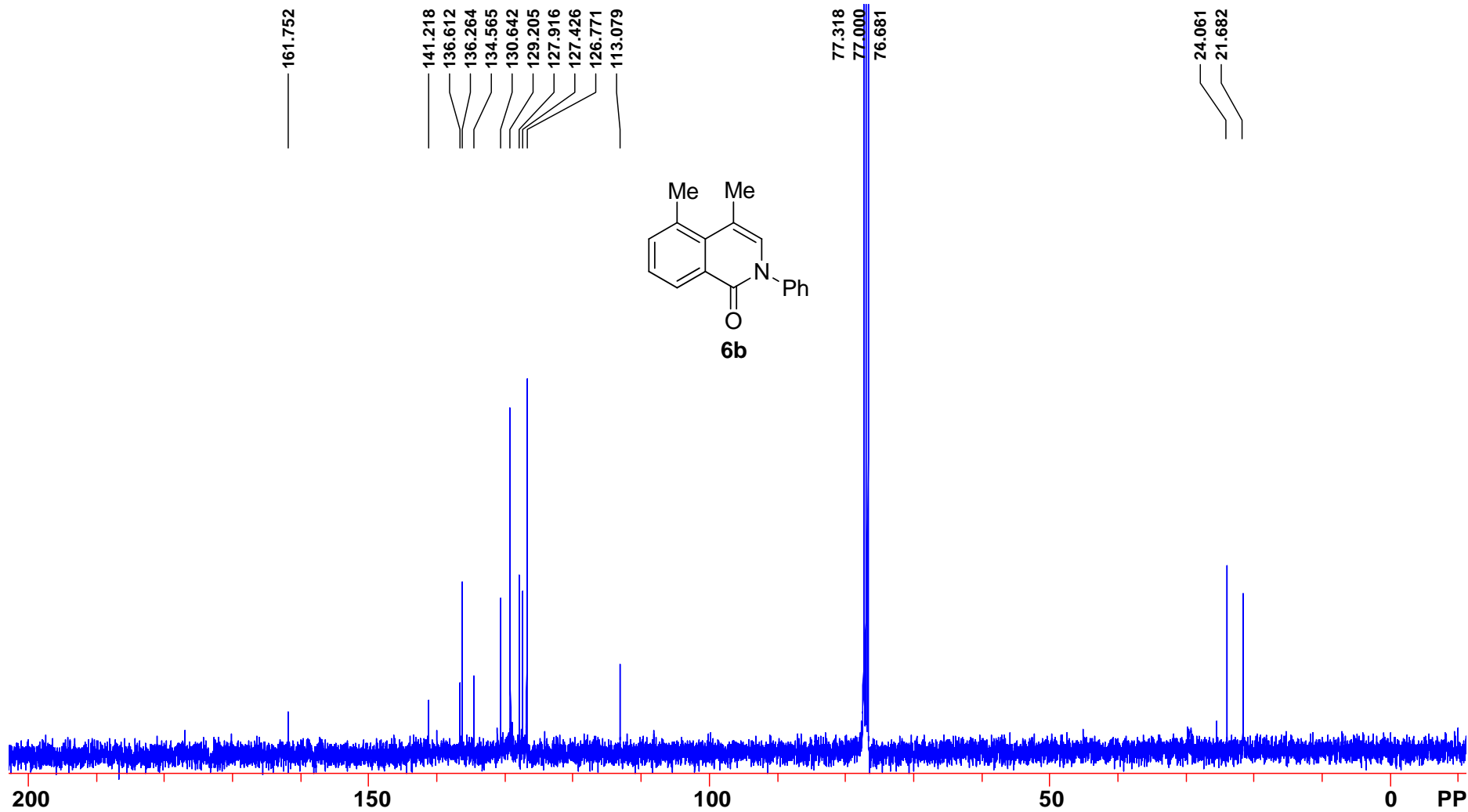












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