

Supporting Information

Furan-2-Carboxamides as Dienes in Cascade S_N2' /Intramolecular Diels-Alder Reaction with MBH Carbonates

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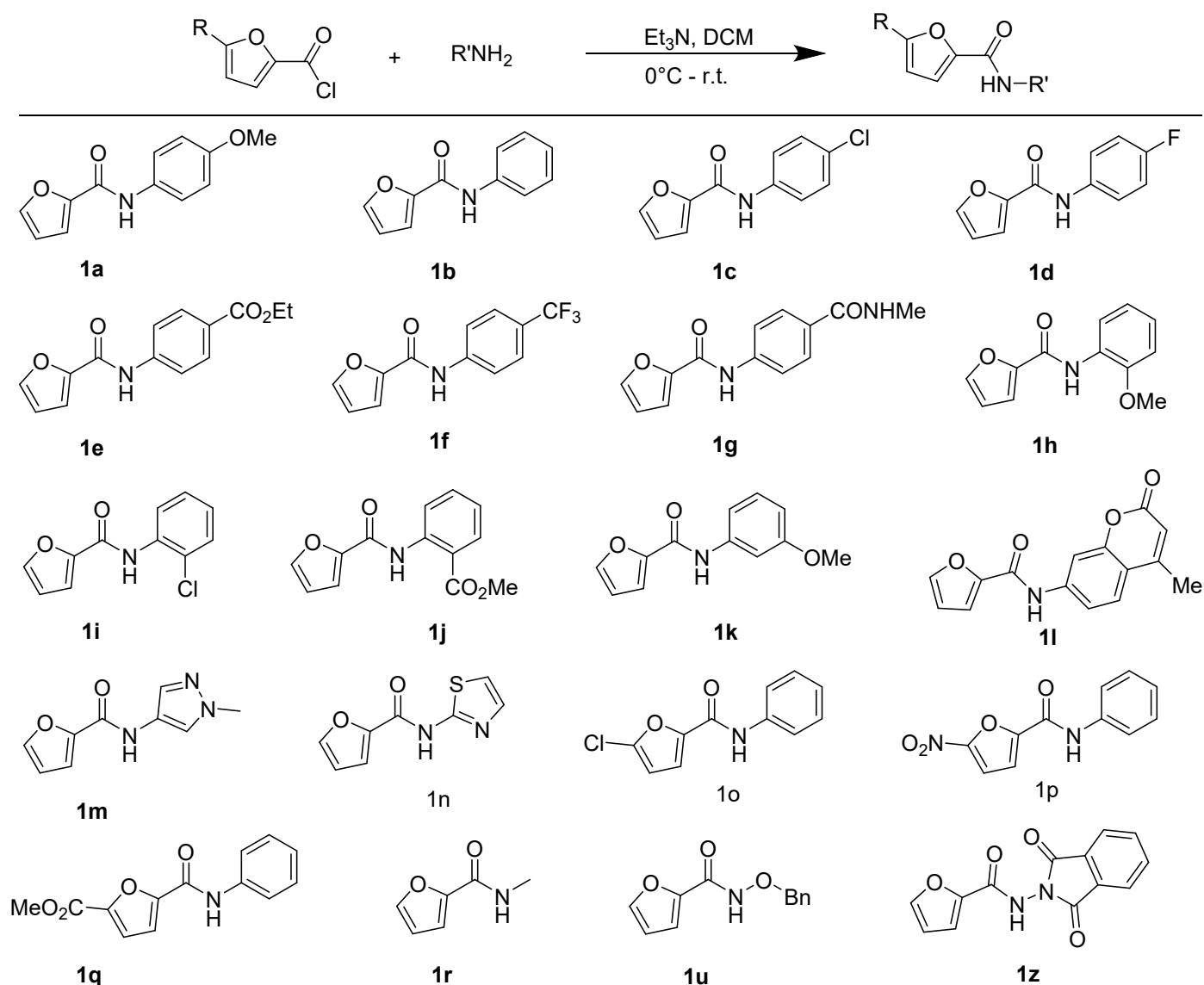
Table of Contents

I. General Information.....	2
II. Preparation of Starting Materials.....	3
III. Experimental Procedure and Characterization Data of Products.....	10
IV. Control experiments.....	30
V. Gram-scale synthesis and chemical transformations.....	32
VI. X-ray crystallographic data for compound 4c (CCDC:2516694).....	36
VII. Computational Details.....	38
VIII. References.....	55
IX. NMR Spectra.....	58

I. General Information.

Unless otherwise noted, all reagents and solvents were used as supplied by commercial sources without further purification. Chromatography was carried on flash silica gel (200–300 mesh). All reactions were monitored by TLC on silica gel 60 (F₂₅₄) aluminum plates, visualized under UV light (254 or 365 nm). Melting points were measured using a SGW X-4 apparatus and were uncorrected. NMR spectra were recorded on a Varian spectrometer operating at 400 MHz for ¹H NMR and 101 MHz for ¹³C NMR using CDCl₃ or DMSO-*d*₆ as solvents. Chemical shifts (δ) are reported in parts per million (ppm) relative to tetramethylsilane (TMS) as an internal standard. Multiplicities are indicated as follows: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; dd = doublet of doublets; dt = doublet of triplets; brs = broad singlet. Coupling constant (Hz) (*J* values) are reported in Hertz (Hz). High-resolution mass spectra (HRMS) were acquired on a quadrupole time-of-flight (Q-TQF) mass spectrometer using electrospray ionization (ESI) positive ionization source.

II. Preparation of Starting Materials



General Procedure A:^[1] A solution of the appropriate amine (10 mmol) and Et₃N (1.52 mL, 11 mmol) in dichloromethane (10 mL) was cooled in an ice-water bath and stirred vigorously. 2-Furoyl chloride (11 mmol) in dichloromethane (5 mL) was added dropwise over 1 h. The reaction mixture was then allowed to warm to room temperature and stirred for 4 h. After quenching with water (50 mL), the organic layer was separated and the aqueous phase was extracted with dichloromethane (3 × 5 mL). The combined extracts were washed with saturated NaHCO₃ (2 × 15 mL) and brine (2 × 15 mL), dried over Na₂SO₄ and concentrated to dryness. The crude product was recrystallized or purified by column chromatography on silica gel to afford the pure amide.

Substrates **1a** – **1r**, **1u** and **1z** were prepared according to General Procedure A.

N-(4-Methoxyphenyl)furan-2-carboxamide (**1a**) [2]

White solid (1.74 g, 80%), m.p.: 108.3–109.0 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.99 (s, 1H), 7.59 – 7.52 (m, 2H), 7.50 (s, 1H), 7.22 (d, *J* = 3.5 Hz, 1H), 6.94 – 6.86 (m, 2H), 6.55 (dd, *J* = 3.6, 1.7 Hz, 1H), 3.81 (s, 3H).

N-Phenylfuran-2-carboxamide (**1b**) [2]

White solid (1.57 g, 84%), m.p.: 124.7–125.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.08 (s, 1H), 7.65 (d, *J* = 7.9 Hz, 2H), 7.51 (d, *J* = 1.8 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.24 (d, *J* = 3.6 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 6.56 (dd, *J* = 3.7, 1.7 Hz, 1H).

N-(4-Chlorophenyl)furan-2-carboxamide (**1c**) [2]

White solid (1.81 g, 82%), m.p.: 150.8–151.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.08 (s, 1H), 7.65 – 7.57 (m, 2H), 7.52 (d, *J* = 1.8 Hz, 1H), 7.36 – 7.29 (m, 2H), 7.25 (d, *J* = 3.5 Hz, 1H), 6.57 (dd, *J* = 3.6, 1.9 Hz, 1H).

N-(4-Fluorophenyl)furan-2-carboxamide (**1d**) [3]

White solid (1.62 g, 79%), m.p.: 102.9–103.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.06 (s, 1H), 7.65 – 7.58 (m, 2H), 7.54 – 7.49 (m, 1H), 7.24 (d, *J* = 3.3 Hz, 1H), 7.06 (t, *J* = 8.7 Hz, 2H), 6.57 (dd, *J* = 3.4, 1.7 Hz, 1H).

Ethyl 4-(furan-2-carboxamido)benzoate (**1e**) [1]

White solid (2.05 g, 79%), m.p.: 130.7–131.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.23 (s, 1H), 8.06 (d, *J* = 8.7 Hz, 2H), 7.74 (d, *J* = 8.7 Hz, 2H), 7.55 – 7.52 (m, 1H), 7.28 (d, *J* = 3.5 Hz, 1H), 6.59 (dd, *J* = 3.4, 1.7 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H).

N-(4-(Trifluoromethyl)phenyl)furan-2-carboxamide (**1f**) [4]

White solid (2.01 g, 79%), m.p.: 152.3–153.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.20 (s, 1H), 7.79 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 8.6 Hz, 2H), 7.56 – 7.52 (m, 1H), 7.29 (d, *J* = 3.5 Hz, 1H), 6.59 (dd, *J* = 3.5, 1.7 Hz, 1H).

N-(4-(Methylcarbamoyl)phenyl)furan-2-carboxamide (**1g**)

White solid (1.61 g, 66%), m.p.:223.3-223.7 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.38 (s, 1H), 8.40 – 8.31 (m, 1H), 7.97 (s, 1H), 7.83 (m, 4H), 7.38 (d, *J* = 3.2 Hz, 1H), 6.76 – 6.69 (m, 1H), 2.78 (d, *J* = 4.1 Hz, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.6, 156.8, 147.8, 146.5, 141.6, 130.0, 128.3, 119.9, 115.7, 112.8, 26.7. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₃H₁₃N₂O₃⁺ 245.0921, found 245.0934.

N-(2-Methoxyphenyl)furan-2-carboxamide (**1h**) [5]

White solid (1.61 g, 74%), m.p.: 122.3-123.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.78 (s, 1H), 8.49 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.56 – 7.50 (m, 1H), 7.22 (d, *J* = 3.4 Hz, 1H), 7.08 (td, *J* = 7.8, 1.5 Hz, 1H), 7.00 (td, *J* = 7.8, 1.5 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.55 (dd, *J* = 3.4, 1.7 Hz, 1H), 3.95 (s, 3H).

N-(2-Chlorophenyl)furan-2-carboxamide (**1i**) [6]

White solid (2.21 g, 77%), m.p.: 90.6-91.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.71 (s, 1H), 8.53 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.56 (d, *J* = 1.8 Hz, 1H), 7.41 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.27 (d, *J* = 3.4 Hz, 1H), 7.08 (td, *J* = 7.7, 1.6 Hz, 1H), 6.58 (dd, *J* = 3.5, 1.8 Hz, 1H).

Methyl 2-(furan-2-carboxamido)benzoate (**1j**) [7]

White solid (2.21 g, 90%), m.p.:114.0-114.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.02 (s, 1H), 8.86 (d, *J* = 8.4 Hz, 1H), 8.08 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.65 – 7.55 (m, 2H), 7.27 (s, 1H), 7.12 (t, *J* = 7.7 Hz, 1H), 6.56 (dd, *J* = 3.4, 1.7 Hz, 1H), 3.98 (s, 3H).

N-(3-Methoxyphenyl)furan-2-carboxamide (**1k**) [8]

Yellow solid (2.21 g, 77%), m.p.: 82.3-83.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.08 (s, 1H), 7.51 (dd, *J* = 1.8, 0.9 Hz, 1H), 7.45 (t, *J* = 2.3 Hz, 1H), 7.25 (dd, *J* = 7.7, 3.8 Hz, 2H), 7.10 (ddd, *J* = 8.0, 2.1, 0.9 Hz, 1H), 6.70 (ddd, *J* = 8.3, 2.5, 0.9 Hz, 1H), 6.56 (dd, *J* = 3.5, 1.8 Hz, 1H), 3.83 (s, 3H).

N-(4-Methyl-2-oxo-2H-chromen-7-yl)furan-2-carboxamide (**1l**) [9]

White solid (2.21 g, 82%), m.p.: 254.7-255.4 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.60 (s, 1H), 8.00 (d, *J* = 1.7 Hz, 1H), 7.91 (s, 1H), 7.76 (s, 2H), 7.42 (d, *J* = 3.5 Hz, 1H), 6.75 (dd, *J* = 3.6, 1.7 Hz, 1H), 6.29 (d, *J* = 1.6 Hz, 1H), 2.42 (s, 3H).

N-(1-Methyl-1H-pyrazol-4-yl)furan-2-carboxamide (**1m**)^[10]

Yellow solid (1.53 g, 80%), m.p.: 119-120 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.42 (s, 1H), 7.97 (s, 1H), 7.90 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.56 (s, 1H), 7.21 (dd, *J* = 3.5, 0.8 Hz, 1H), 6.68 (dd, *J* = 3.5, 1.7 Hz, 1H), 3.81 (s, 3H).

N-(Thiazol-2-yl)furan-2-carboxamide (**1n**)^[11]

White solid (1.75 g, 90%), m.p.: 143.7-144.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 11.21 (s, 1H), 7.57 (s, 1H), 7.52 (d, *J* = 3.6 Hz, 1H), 7.36 (d, *J* = 3.6 Hz, 1H), 7.04 (d, *J* = 3.6 Hz, 1H), 6.65 – 6.58 (m, 1H).

5-Chloro-*N*-phenylfuran-2-carboxamide (**1o**)^[12]

Yellow solid (2.21 g, 56%), m.p.: 107.3-108.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.93 (s, 1H), 7.64 (d, *J* = 7.9 Hz, 2H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.22 (d, *J* = 3.6 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 6.37 (d, *J* = 3.6 Hz, 1H).

5-Nitro-*N*-phenylfuran-2-carboxamide (**1p**)^[13]

Yellow solid (1.18 g, 51%), m.p.: 174.0-175.0 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.20 (s, 1H), 7.68 (d, *J* = 7.9 Hz, 2H), 7.46 – 7.35 (m, 4H), 7.22 (t, *J* = 7.5 Hz, 1H).

Methyl 5-(phenylcarbamoyl)furan-2-carboxylate (**1q**)^[14]

White solid (1.22 g, 49.6%), m.p.: 114.5-115.0 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.25 (s, 1H), 7.68 (d, *J* = 7.9 Hz, 2H), 7.39 (t, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 3.6 Hz, 1H), 7.25 (d, *J* = 2.9 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 3.96 (s, 3H).

N-Methylfuran-2-carboxamide (**1r**)^[15]

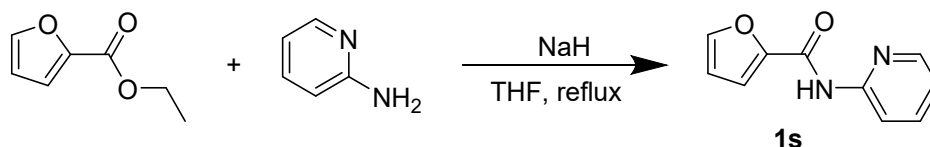
White solid (1.74 g, 81.3%), m.p.: 61.2-62.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.42 (d, *J* = 1.7 Hz, 1H), 7.11 (d, *J* = 3.5 Hz, 1H), 6.49 (dd, *J* = 3.5, 1.8 Hz, 1H), 6.42 (s, 1H), 2.99 (d, *J* = 5.0 Hz, 3H).

N-(Benzyloxy)furan-2-carboxamide (**1u**): [16]

White solid (1.89 g, 87%), m.p.: 82.3-82.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.72 (s, 1H), 7.50 – 7.35 (m, 6H), 7.23 – 7.17 (m, 1H), 6.51 (q, *J* = 1.8 Hz, 1H), 5.03 (s, 2H).

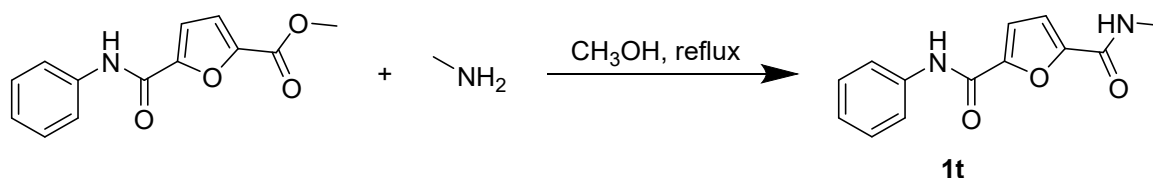
N-(1,3-Dioxoisindolin-2-yl)furan-2-carboxamide (**1z**) [17]

White solid (1.74 g, 68%), m.p.: 163.7-164.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.33 (s, 1H), 7.95 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.82 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.58 – 7.54 (m, 1H), 7.29 (d, *J* = 3.6 Hz, 1H), 6.58 (dd, *J* = 3.6, 1.8 Hz, 1H).



Procedure for synthesis of substrate 1s:[18-19] To a stirred suspension of pyridin-2-amine (510 mg, 5.4 mmol, 2.7 equiv) in anhydrous THF (20 mL) was added NaH (60% dispersion in mineral oil, 1.04 g, 26 mmol, 13 equiv). The mixture was heated at reflux for 3 h, then ethyl 2-furancarboxylate (280 mg, 2 mmol) was added. Reflux was continued for a further 3 h. After cooling, the solvent was removed in vacuo and the residue purified by silica gel column chromatography (petroleum ether/EtOAc = 1:1, v/v) to afford the product **1s**.

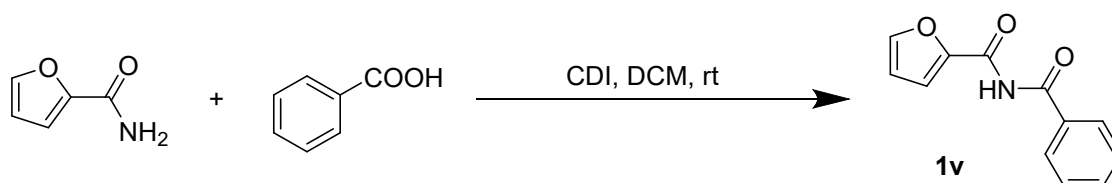
Yellow solid (300 mg, 80%), m.p.: 72.0-72.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.76 (s, 1H), 8.33 (d, *J* = 7.1 Hz, 2H), 7.75 (t, *J* = 8.0 Hz, 1H), 7.54 (s, 1H), 7.28 (d, *J* = 3.5 Hz, 1H), 7.08 (t, *J* = 6.2 Hz, 1H), 6.58 (dd, *J* = 3.7, 1.8 Hz, 1H).



Procedure for the synthesis of substrate 1t:[18] To a solution (10 mL) of methyl 5-(phenylaminocarbonyl)furan-2-carboxylate (245 mg, 2 mmol) in methanol was added 40%

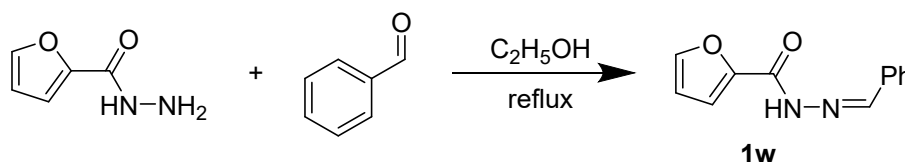
aqueous methylamine (13.8 mL, 4 mmol). The mixture was heated at reflux for 2 h, then concentrated under reduced pressure. Purification by silica gel column chromatography (petroleum ether/EtOAc = 1:1, v/v) afforded product **1t**.

White solid (214 mg, 96%), m.p.:196.7-197.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.20 (s, 1H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.36 (t, *J* = 7.9 Hz, 2H), 7.25 (d, *J* = 1.7 Hz, 1H), 7.20 – 7.14 (m, 2H), 6.60 (s, 1H), 3.00 (d, *J* = 5.0, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 158.1, 156.0, 149.3, 148.0, 138.4, 129.2, 124.7, 121.1, 116.1, 114.8, 79.7, 79.4, 79.1, 25.9. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₃H₁₃N₂O₃⁺ 245.0921, found 245.0934.



Procedure for the synthesis of substrate 1v:^[20] A solution of benzoic acid (244 mg, 2 mmol) and 1,1'-carbonyldiimidazole (CDI, 356 mg, 2.2 mmol, 1.1 equiv) in anhydrous DCM was stirred at room temperature for 5 min. Furan-2-carboxamide (222 mg, 2 mmol, 1.0 equiv) and NaH (60% dispersion in mineral oil, 72 mg, 3 mmol, 1.5 equiv) were added, and the mixture was stirred at room temperature for 4 h while the reaction was monitored by TLC. Upon completion, the reaction was quenched with water, and the mixture was extracted with DCM. The combined organic layers were washed with brine, dried (Na₂SO₄), and concentrated in vacuo. The crude product was purified by column chromatography to afford the product **1v**.

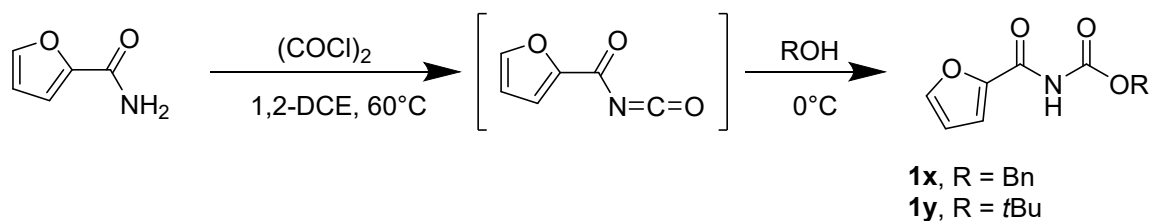
White solid (234 mg, 54.4%), m.p.:196.7-197.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.32 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 2H), 7.67 – 7.48 (m, 4H), 7.41 (d, *J* = 3.6 Hz, 1H), 6.63 (d, *J* = 3.7 Hz, 1H).



Procedure for the synthesis of substrate 1w:^[21] Benzaldehyde (530 mg, 5 mmol) and furan-2-carbohydrazide (630 mg, 5 mmol, 1 equiv) were dissolved in ethanol. The mixture was stirred and heated at reflux for 6 h, during which the product precipitated. After cooling,

the solid was collected by filtration and purified by recrystallization from ethanol to afford the product **1w**.

White solid (931 mg, 87%), m.p.: 222.7-223.6 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.87 (s, 1H), 8.47 (s, 1H), 7.97 (s, 1H), 7.73 (d, *J* = 6.8 Hz, 2H), 7.48 (d, *J* = 6.7 Hz, 3H), 7.32 (s, 1H), 6.73 (s, 1H).



General Procedure B:^[22] Oxalyl chloride (0.43 mL, 4.94 mmol, 1.2 equiv) was added dropwise to a stirred solution of furan-2-carboxamide (455 mg, 4.1 mmol) in 1,2-dichloroethane (10 mL) at 0 °C. The mixture was warmed to 60 °C and stirred for 1 h, then cooled back to 0 °C. A solution of the appropriate alcohol (8.2 mmol, 2 equiv) in 1,2-dichloroethane was introduced, and stirring was continued at 0 °C for 2 h. The reaction was quenched with saturated aqueous NaHCO₃, extracted with DCM, and the combined organic phases were washed with brine, dried over Na₂SO₄, and concentrated. The crude product was purified by silica gel column chromatography (DCM to DCM/EtOAc 9:1, v/v) to afford the desired product.

Substrates **1x** and **1y** were prepared according to General Procedure B.

N-(Benzyloxy)furan-2-carboxamide (**1x**)

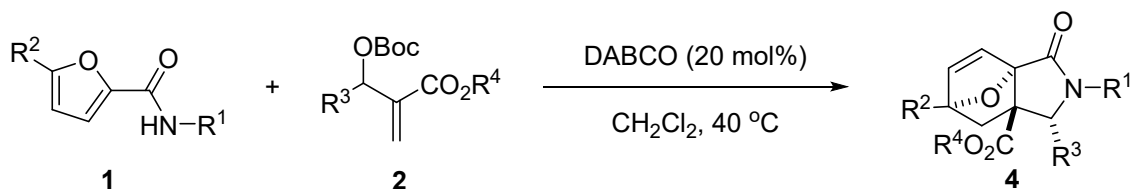
White solid (944 mg, 94%), m.p.: 130.1-131.0 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.35 (s, 1H), 7.50 (s, 1H), 7.46 – 7.31 (m, 6H), 6.58 (dd, *J* = 3.7, 1.7 Hz, 1H), 5.27 (s, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 154.7, 150.4, 146.2, 145.4, 135.0, 128.7, 128.7, 117.8, 113.1, 68.0. HRMS (ESI) *m/z*: [M + Na]⁺ Calcd for C₁₃H₁₁NNaO₄⁺ 268.0580, found 268.0560.

tert-Butyl(furan-2-carbonyl)carbamate (**1y**)

White solid (486 mg, 56%), m.p.: 142.3-142.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 7.51 (s, 1H), 7.31 (d, *J* = 3.7 Hz, 1H), 6.57 (dd, *J* = 3.6, 1.8 Hz, 1H), 1.54 (s, 9H). ¹³C

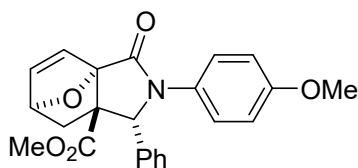
NMR (101 MHz, CDCl₃) δ 155.1, 149.1, 146.5, 145.1, 117.3, 113.0, 82.8, 28.0. HRMS (ESI)
m/z: [M + Na]⁺ Calcd for C₁₀H₁₃NNaO₄⁺ 234.0737, found 234.0754.

III. Experimental Procedure and Characterization Data of Products



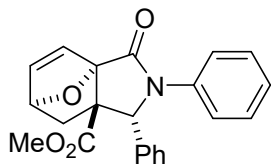
General experimental procedure: A mixture of furan-2-carboxamide **1** (0.2 mmol), MBH carbonate **2** (0.24 mmol, 1.2 equiv), and DABCO (4.5 mg, 0.04 mmol, 20 mol%) in CH₂Cl₂ (2.0 mL) was stirred in a sealed tube at 40 °C (oil bath) until TLC analysis indicated the complete consumption of **1**. The solvent was removed under reduced pressure, and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether/EtOAc) to afford the corresponding product.

Methyl 2-(4-methoxyphenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4a)



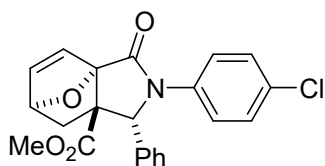
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (77 mg, 99% yield, dr > 20:1), m.p.: 96.3–97.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.49 (brs, 1H), 7.39 – 7.27 (m, 5H), 7.08 (brs, 1H), 6.81 (d, *J* = 8.9 Hz, 2H), 6.64 (d, *J* = 5.7 Hz, 1H), 6.57 (d, *J* = 5.7 Hz, 1H), 5.32 (s, 1H), 4.98 (d, *J* = 4.1 Hz, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 1.97 (d, *J* = 12.3 Hz, 1H), 1.65 (dd, *J* = 12.2, 4.4 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 173.0, 167.2, 157.8, 140.0, 137.0, 132.9, 131.0, 128.9, 128.3, 125.2, 114.3, 94.1, 82.3, 70.1, 59.6, 55.4, 53.0, 33.9. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₃H₂₂NO₅⁺ 392.1492, found 392.1499.

Methyl 3-oxo-1,2-diphenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4b)



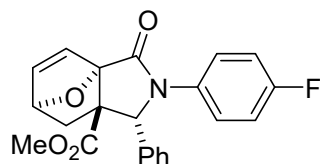
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (64 mg, 89% yield, dr > 20:1), m.p.: 183.5–185.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.49 (d, *J* = 8.4 Hz, 2H), 7.44 (brs, 1H), 7.34 – 7.26 (m, 5H), 7.14 (t, *J* = 7.4 Hz, 2H), 6.65 (d, *J* = 5.8 Hz, 1H), 6.58 (dd, *J* = 5.8, 1.6 Hz, 1H), 5.43 (s, 1H), 4.97 (dd, *J* = 4.5, 1.5 Hz, 1H), 3.77 (s, 3H), 1.98 (d, *J* = 12.3 Hz, 1H), 1.68 (dd, *J* = 12.3, 4.6 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.9, 167.3, 140.1, 138.2, 136.9, 132.9, 129.0, 128.8, 128.3, 126.1, 123.1, 94.1, 82.3, 69.4, 59.5, 53.1, 34.0. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₂H₂₀NO₄⁺ 362.1387, found 362.1378.

Methyl 2-(4-chlorophenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4c)



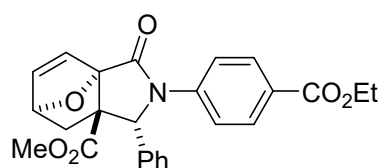
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (70 mg, 89% yield, dr > 20:1), m.p.: 138.9-139.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.46 (d, *J* = 8.9 Hz, 2H), 7.42 – 7.27 (m, 4H), 7.24 (d, *J* = 8.9 Hz, 1H), 7.13 (brs, 1H), 6.63 (d, *J* = 5.8 Hz, 1H), 6.58 (dd, *J* = 5.8, 1.5 Hz, 1H), 5.39 (s, 1H), 4.97 (dd, *J* = 4.5, 1.5 Hz, 1H), 3.77 (s, 3H), 1.98 (d, *J* = 12.3 Hz, 1H), 1.68 (dd, *J* = 12.3, 4.6 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.8, 167.3, 140.2, 136.7, 136.5, 132.7, 131.3, 129.1, 128.8, 128.5, 128.1, 124.0, 94.0, 82.4, 69.3, 59.4, 53.1, 34.0. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₂H₁₉ClNO₄⁺ 396.0997, found 396.1002.

Methyl 2-(4-fluorophenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4d)



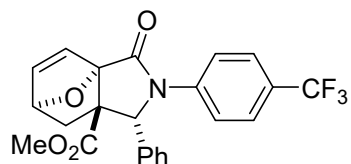
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (60 mg, 79% yield, dr > 20:1), m.p.: 137.2-139.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.45 – 7.41 (m, 3H), 7.35 – 7.28 (m, 3H), 7.10 (brs, 1H), 6.97 (t, *J* = 8.7 Hz, 2H), 6.63 (d, *J* = 5.8 Hz, 1H), 6.58 (dd, *J* = 5.8, 1.5 Hz, 1H), 5.35 (s, 1H), 4.98 (dd, *J* = 4.5, 1.5 Hz, 1H), 3.78 (s, 3H), 1.98 (d, *J* = 12.3 Hz, 1H), 1.67 (dd, *J* = 12.3, 4.6 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.8, 160.5 (d, *J*_{C-F} = 251.5 Hz), 167.3, 140.1, 136.6, 134.1, 132.8, 128.9, 128.5, 125.2 (d, *J*_{C-F} = 8.3 Hz), 115.9 (d, *J*_{C-F} = 22.6 Hz), 94.0, 82.4, 69.9, 59.5, 53.1, 34.0. ¹⁹F NMR (376 MHz, CDCl₃) δ -115.25. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₂H₁₉FNO₄⁺ 380.1293, found 380.1282.

Methyl 2-(4-(ethoxycarbonyl)phenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (**4e**)



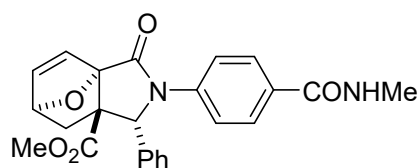
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (85 mg, yield 98%, dr > 20:1), m.p.: 157.3-158.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.95 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.42 – 7.26 (m, 4H), 7.18 (brs, 1H), 6.64 (d, *J* = 5.8 Hz, 1H), 6.59 (dd, *J* = 5.8, 1.5 Hz, 1H), 5.51 (s, 1H), 4.97 (dd, *J* = 4.4, 1.4 Hz, 1H), 4.32 (q, *J* = 7.1 Hz, 2H), 3.76 (s, 3H), 1.99 (d, *J* = 12.3 Hz, 1H), 1.72 (dd, *J* = 12.3, 4.6 Hz, 1H), 1.34 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 172.7, 167.5, 165.9, 142.1, 140.2, 136.5, 132.7, 130.4, 129.1, 128.5, 127.9, 127.1, 121.3, 94.0, 82.4, 68.8, 60.9, 59.2, 53.1, 34.1, 14.3. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₅H₂₄NO₆⁺ 434.1598, found 434.1629.

Methyl 3-oxo-1-phenyl-2-(4-(trifluoromethyl)phenyl)-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (**4f**)



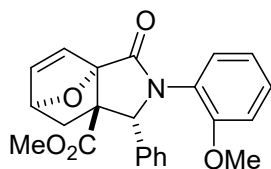
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (84.6 mg, 99% yield, dr > 20:1), m.p.: 139.2-140.3 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.70 (d, J = 8.6 Hz, 2H), 7.53 (d, J = 8.7 Hz, 2H), 7.41 – 7.27 (m, 4H), 7.19 (brs, 1H), 6.64 (d, J = 5.8 Hz, 1H), 6.60 (dd, J = 5.8, 1.4 Hz, 1H), 5.48 (s, 1H), 4.98 (dd, J = 4.5, 1.3 Hz, 1H), 3.76 (s, 3H), 2.00 (d, J = 12.3 Hz, 1H), 1.71 (dd, J = 12.3, 4.6 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 172.7, 167.6, 141.3, 140.3, 136.4, 132.7, 129.2, 128.6, 127.9, 126.2 (q, $J_{\text{C-F}}$ = 3.7 Hz), 121.9, 94.0, 82.5, 69.0, 59.4, 53.2, 34.1. ^{19}F NMR (376 MHz, CDCl_3) δ -62.43. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{23}\text{H}_{19}\text{F}_3\text{NO}_4^+$ 430.1261, found 430.1240.

Methyl 2-(4-(methylcarbamoyl)phenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (**4g**)



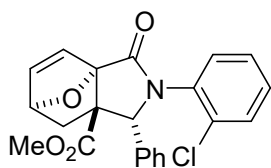
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (73 mg, 87% yield, dr > 20:1), m.p.: 131.5-132.4 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.67 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.4 Hz, 4H), 7.39 – 7.27 (m, 3H), 7.17 (brs, 1H), 6.64 (d, J = 5.7 Hz, 1H), 6.59 (d, J = 5.6 Hz, 1H), 6.13 (brs, 1H), 5.50 (s, 1H), 5.30 (s, 1H), 4.97 (d, J = 3.7 Hz, 1H), 3.76 (s, 3H), 2.97 (d, J = 4.6 Hz, 3H), 1.99 (d, J = 12.3 Hz, 1H), 1.71 (dd, J = 12.2, 4.4 Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 172.7, 167.6, 167.4, 140.5, 140.4, 136.3, 132.7, 131.6, 129.1, 128.7, 128.5, 127.8, 122.0, 94.1, 82.4, 68.9, 59.2, 53.2, 34.1, 26.8. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{24}\text{H}_{23}\text{N}_2\text{O}_5^+$ 419.1601, found 419.1604.

Methyl 2-(2-methoxyphenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (**4h**)



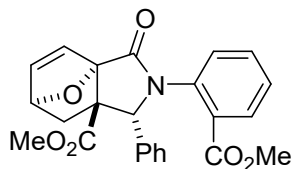
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (76.6 mg, 98% yield, dr > 20:1), m.p.: 141.1-142.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.66 (brs, 1H), 7.33 – 7.16 (m, 5H), 7.00 (brs, 1H), 6.91 – 6.87 (m, 2H), 6.69 (d, *J* = 5.8 Hz, 1H), 6.54 (d, *J* = 5.6 Hz, 1H), 5.55 (s, 1H), 4.97 (d, *J* = 4.1 Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H), 1.91 (d, *J* = 12.3 Hz, 1H), 1.67 (dd, *J* = 12.2, 4.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 173.4, 167.3, 155.1, 139.5, 136.9, 133.6, 129.2, 129.1, 128.7, 128.2, 125.5, 120.9, 112.5, 93.0, 81.9, 69.2, 59.8, 55.9, 52.7, 34.5. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₃H₂₂NO₅⁺ 392.1492, found 392.1499.

Methyl 2-(2-chlorophenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4i)



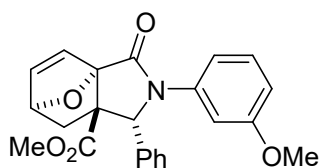
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (66.5 mg, 84% yield, dr > 20:1), m.p.: 141.8-142.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.76 (brs, 1H), 7.42 – 7.27 (m, 3H), 7.25 – 7.16 (m, 4H), 7.02 (brs, 1H), 6.71 (d, *J* = 5.1 Hz, 1H), 6.57 (d, *J* = 4.9 Hz, 1H), 5.57 (s, 1H), 5.03 (s, 1H), 3.82 (s, 3H), 1.93 (d, *J* = 12.2 Hz, 1H), 1.71 (d, *J* = 12.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 173.1, 167.8, 139.7, 136.0, 134.4, 133.3, 132.0, 130.9, 129.5, 129.3, 128.9, 128.6, 128.3, 127.6, 100.0, 82.0, 69.6, 59.8, 52.8, 34.7. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₂H₁₉ClNO₄⁺ 396.0997, found 396.1002.

Methyl 2-(2-(methoxycarbonyl)phenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4j)



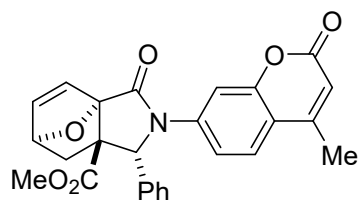
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (81.2 mg, 97% yield, dr = 12:1), m.p.: 144.4-145.9 °C; Data for major isomer: ¹H NMR (400 MHz, CDCl₃) δ 7.97 (brs, 1H), 7.83 (d, *J* = 6.7 Hz, 1H), 7.42 (t, *J* = 7.1 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.26 – 7.19 (m, 3H), 7.08 (brs, 1H), 6.64 (d, *J* = 5.8 Hz, 1H), 6.56 (dd, *J* = 5.8, 1.6 Hz, 1H), 5.74 (s, 1H), 5.03 (d, *J* = 3.1 Hz, 1H), 3.91 (s, 3H), 3.81 (s, 3H), 1.93 (d, *J* = 12.2 Hz, 1H), 1.72 (dd, *J* = 12.3, 4.5 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 173.2, 167.3, 166.6, 139.8, 136.4, 136.0, 132.7, 132.4, 131.3, 129.2, 128.4, 128.3, 126.8, 124.7, 93.5, 81.9, 69.7, 59.2, 53.0, 52.5, 34.6. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₄H₂₂NO₆⁺ 420.1442, found 420.1454.

Methyl 2-(3-methoxyphenyl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4k)



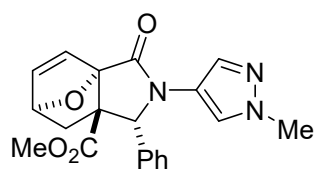
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (75 mg, 96% yield, dr > 20:1), m.p.: 127.3-128.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.42 (brs, 1H), 7.34 – 7.26 (m, 2H), 7.20 – 7.09 (m, 3H), 7.01 (d, *J* = 8.1 Hz, 1H), 6.68 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.64 (d, *J* = 5.8 Hz, 1H), 6.57 (dd, *J* = 5.8, 1.5 Hz, 1H), 5.41 (s, 1H), 4.97 (dd, *J* = 4.4, 1.4 Hz, 1H), 3.77 (s, 3H), 3.72 (s, 3H), 1.97 (d, *J* = 12.3 Hz, 1H), 1.68 (dd, *J* = 12.3, 4.7 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.9, 167.3, 159.9, 140.1, 139.4, 137.0, 132.9, 129.6, 128.7, 128.3, 128.2, 115.0, 111.6, 109.0, 94.2, 82.3, 69.4, 59.4, 55.3, 53.1, 34.0. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₃H₂₂NO₅⁺ 392.1492, found 392.1499.

Methyl 2-(4-methyl-2-oxo-2H-chromen-7-yl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4l)



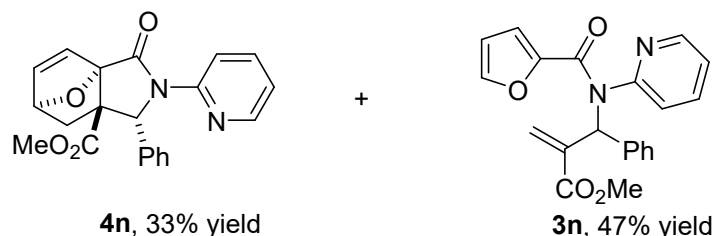
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (55.8 mg, 63% yield, dr > 20:1), m.p.: 183.2-184.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.84 (d, *J* = 8.8 Hz, 1H), 7.52 (d, *J* = 8.7 Hz, 1H), 7.36 (brs, 2H), 7.30 (brs, 3H), 7.21 (brs, 1H), 6.64 (d, *J* = 5.6 Hz, 1H), 6.60 (d, *J* = 6.0 Hz, 1H), 6.19 (s, 1H), 5.48 (s, 1H), 4.98 (d, *J* = 4.0 Hz, 1H), 3.76 (s, 3H), 2.37 (s, 3H), 2.00 (d, *J* = 12.3 Hz, 1H), 1.72 (dd, *J* = 12.2, 4.1 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.6, 160.7, 167.6, 153.8, 151.9, 141.4, 140.4, 136.2, 132.9, 132.6, 129.2, 128.7, 127.7, 125.1, 117.8, 117.3, 117.1, 114.3, 109.3, 94.0, 82.5, 68.9, 59.3, 53.2, 34.1, 18.6. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₆H₂₂NO₆⁺ 444.1442, found 444.1408.

Methyl 2-(1-methyl-1H-pyrazol-4-yl)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4m)



Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (72 mg, 99% yield, dr > 20:1), m.p.: 140.0-140.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.0 (s, 1H), 7.40 (brs, 1H), 7.33 – 7.30 (m, 2H), 7.26 – 7.00 (m, 2H), 7.12 (brs, 1H), 6.63 (d, *J* = 5.4 Hz, 1H), 6.57 (d, *J* = 5.7 Hz, 1H), 5.19 (s, 1H), 4.95 (d, *J* = 4.1 Hz, 1H), 3.83 (s, 3H), 3.72 (s, 3H), 1.96 (d, *J* = 12.3 Hz, 1H), 1.68 (dd, *J* = 12.1, 4.0 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.8, 165.2, 140.1, 136.2, 132.8, 130.2, 129.2, 128.5, 127.8, 122.2, 121.9, 93.5, 82.3, 68.6, 60.4, 53.1, 39.3, 33.8. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₀H₂₀N₃O₄⁺ 366.1448, found 366.1437.

Methyl 3-oxo-1-phenyl-2-(pyridin-2-yl)-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4n)

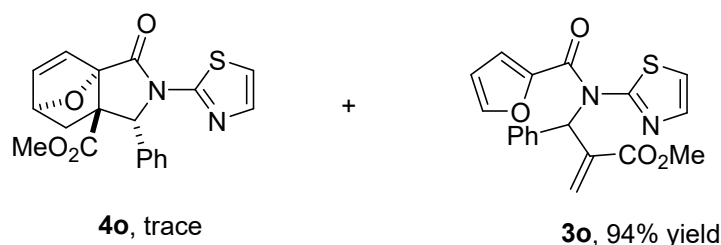


Under standard conditions, the reaction afforded a mixture of **4n** and intermediate **3n**, which could not be fully converted even upon prolonged reaction. The two components were separated by column chromatography (eluent: petroleum ether/EtOAc = 4:1).

Characterization data for product **4n**: White solid (24 mg, 33% yield, dr > 20:1), m.p.: 149.6–150.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.39 (d, *J* = 8.3 Hz, 1H), 8.17 (d, *J* = 4.4 Hz, 1H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.36 – 7.12 (m, 5H), 7.01 – 6.94 (m, 1H), 6.65 (d, *J* = 5.7 Hz, 1H), 6.57 (d, *J* = 5.5 Hz, 1H), 6.26 (s, 1H), 4.95 (d, *J* = 3.9 Hz, 1H), 3.73 (s, 3H), 1.98 (d, *J* = 12.2 Hz, 1H), 1.75 (dd, *J* = 12.1, 4.4 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 173.0, 167.7, 150.5, 147.7, 140.0, 137.9, 137.7, 132.9, 127.6, 120.3, 116.7, 94.7, 82.4, 65.8, 58.5, 53.0, 34.1. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₁H₁₉N₂O₄⁺ 363.1339, found 363.1353.

Characterization data for intermediate **3n**: Colorless oil (34 mg, 47% yield); ¹H NMR (400 MHz, CDCl₃) δ 8.39 (d, *J* = 4.6 Hz, 1H), 7.74 (s, 1H), 7.57 (t, *J* = 7.7 Hz, 1H), 7.31 (d, *J* = 31.9 Hz, 5H), 7.21 – 7.04 (m, 2H), 6.90 (d, *J* = 7.9 Hz, 1H), 6.40 – 6.06 (m, 2H), 5.18 (s, 2H), 3.70 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 167.9, 159.5, 154.8, 148.9, 147.5, 144.2, 143.2, 137.6, 134.6, 129.4, 128.9, 128.5, 128.0, 123.0, 122.4, 116.5, 111.1, 52.1, 44.4. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₁H₁₉N₂O₄⁺ 363.1339, found 363.1353.

Methyl (1*R*,3*aS*,6*S*,7*aR*)-3-oxo-1-phenyl-2-(thiazol-2-yl)-2,3,6,7-tetrahydro-3*a*,6-epoxyisoindole-7*a*(1*H*)-carboxylate (**4o**)

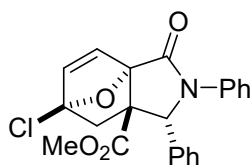


Under standard conditions, the reaction afforded product **4o** in trace amount; while intermediate **3o** was isolated as the major product by column chromatography (eluent:

petroleum ether/EtOAc = 4:1). The intermediate failed to convert even upon prolonged reaction times or at elevated temperature (toluene, reflux).

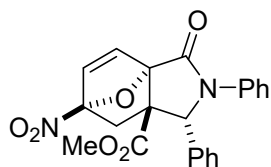
Characterization data for **3o**: Colorless oil (69.2 mg, 94% yield). ¹H NMR (400 MHz, CDCl₃) δ 7.60 (brs, 1H), 7.47 – 7.41 (m, 3H), 7.37 – 7.31 (m, 3H), 7.23 (d, *J* = 3.4 Hz, 1H), 6.84 (d, *J* = 4.7 Hz, 1H), 6.61 (d, *J* = 6.6 Hz, 1H), 6.60 (s, 1H), 6.52 (brs, 1H), 5.45 (s, 1H), 3.79 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 166.9, 165.8, 165.5, 151.8, 145.4, 138.5, 136.0, 129.2, 128.9, 128.5, 128.4, 124.6, 115.7, 111.6, 108.6, 61.4, 52.5. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₉H₁₇N₂O₄S⁺ 369.0904, found 369.0894.

Methyl 6-chloro-3-oxo-1,2-diphenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4p)



Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (65.6 mg, 83% yield, dr > 20:1), m.p.: 170.7-172.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.46 (d, *J* = 8.1 Hz, 3H), 7.37 – 7.26 (m, 5H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.12 – 7.07 (m, 1H), 6.75 (d, *J* = 5.6 Hz, 1H), 6.53 (d, *J* = 5.6 Hz, 1H), 5.42 (s, 1H), 3.79 (s, 3H), 2.54 (d, *J* = 12.3 Hz, 1H), 1.85 (d, *J* = 12.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 171.8, 165.3, 142.2, 137.8, 136.0, 134.2, 129.1, 128.9, 128.6, 125.9, 126.4, 123.2, 101.0, 91.4, 69.5, 61.9, 53.4, 43.2. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₂H₁₉ClNO₄⁺ 396.0997, found 396.1002.

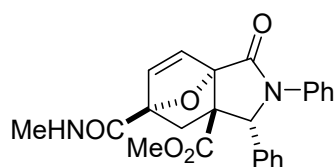
Methyl 6-nitro-3-oxo-1,2-diphenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4q)



Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (78.8 mg, 97% yield, dr > 20:1), m.p.: 177.6-178.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.56 – 7.51 (m, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.43 – 7.38 (m, 1H), 7.19 (t, *J* = 7.3 Hz, 1H), 7.10 (brs, 1H), 6.92 (d, *J* = 5.7 Hz, 1H), 6.87 (d, *J* = 5.6 Hz, 1H), 5.48 (s, 1H), 3.84 (s, 3H), 2.71

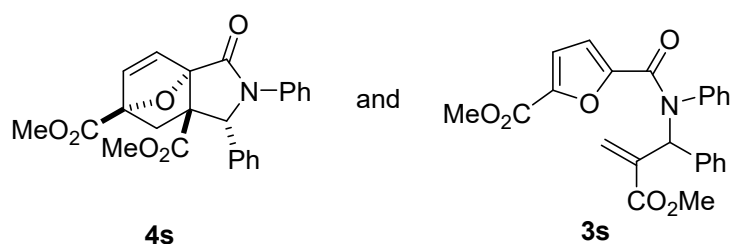
(d, $J = 12.1$ Hz, 1H), 1.99 (d, $J = 12.1$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 171.1, 164.1, 137.5, 137.0, 136.1, 135.2, 129.5, 129.2, 128.8, 128.6, 128.0, 126.8, 123.3, 112.7, 91.5, 69.4, 60.9, 53.7, 39.0. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_6^+$ 407.1238, found 407.1227.

Methyl 6-(methylcarbamoyl)-3-oxo-1,2-diphenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4r)



Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (52 mg, 62% yield, dr > 20:1), m.p.: 156.3–157.6 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.51 (d, $J = 7.8$ Hz, 2H), 7.42 – 7.28 (m, 6H), 7.16 (t, $J = 7.2$ Hz, 2H), 6.76 (d, $J = 5.6$ Hz, 1H), 6.69 (d, $J = 5.6$ Hz, 1H), 5.86 (brs, 1H), 5.47 (s, 1H), 3.78 (s, 3H), 2.70 (d, $J = 4.9$ Hz, 3H), 2.38 (d, $J = 12.4$ Hz, 1H), 1.70 (d, $J = 12.5$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 172.1, 168.2, 166.2, 140.4, 137.9, 136.6, 132.9, 129.1, 128.7, 128.5, 126.3, 122.9, 94.2, 91.8, 69.5, 60.8, 53.3, 37.8, 25.6. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{24}\text{H}_{23}\text{N}_2\text{O}_5^+$ 419.1601, found 419.1604.

Dimethyl 3-oxo-1,2-diphenyl-2,3-dihydro-3a,6-epoxyisoindole-6,7a(1H,7H)-dicarboxylate (4s)

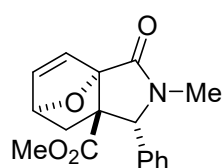


Under standard conditions, the reaction furnished an inseparable mixture of product **4s** and intermediate **3s** (**4s**:**3s** = 5:4), which could not be driven to completion even with extended reaction times. Column chromatography (petroleum ether/EtOAc = 4:1) afforded 75.4 mg of a colorless oil (90% total yield). Characterization for the inseparable mixture was limited to ^1H NMR spectroscopy.

^1H NMR (400 MHz, CDCl_3) for **4s**: δ 7.46 (d, $J = 7.9$ Hz, 2H), 7.38 – 7.21 (m, 7H, overlapped), 7.15 (t, $J = 7.2$ Hz, 1H), 6.74 (d, $J = 5.5$ Hz, 1H), 6.70 (d, $J = 5.6$ Hz, 1H), 5.45 (s, 1H), 3.80 (s, 3H, overlapped), 3.73 (s, 3H), 2.33 (d, $J = 12.1$ Hz, 1H), 1.78 (d, $J = 12.1$ Hz, 1H).

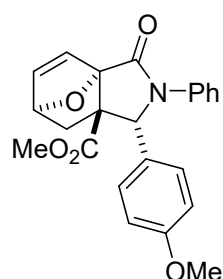
^1H NMR (400 MHz, CDCl_3) for **3s**: δ 7.54 (brs, 1H), 7.38 – 7.21 (m, 5H, overlapped), 7.11 – 7.05 (m, 4H), 6.90 (d, $J = 3.0$ Hz, 1H), 6.61 (s, 1H), 6.45 (s, 1H), 5.99 (d, $J = 3.2$ Hz, 1H), 5.65 (s, 1H), 3.80 (s, 3H, overlapped), 3.71 (s, 3H).

Methyl 2-methyl-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4t)



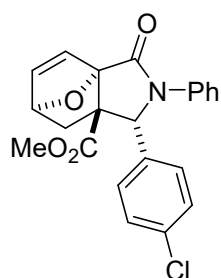
Under standard conditions, no reaction was observed.

Methyl 1-(4-methoxyphenyl)-3-oxo-2-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4u)



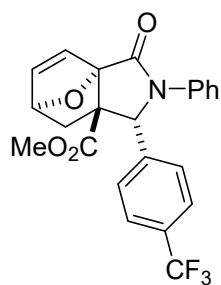
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (77.4 mg, 99% yield, dr > 20:1), m.p.: 152.2-153.4 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.47 (d, $J = 7.9$ Hz, 2H), 7.37 (brs, 1H), 7.30 (d, $J = 7.6$ Hz, 2H), 7.14 (t, $J = 7.3$ Hz, 1H), 7.02 (brs, 1H), 6.84 (d, $J = 8.2$ Hz, 2H), 6.64 (d, $J = 5.8$ Hz, 1H), 6.58 (d, $J = 5.7$ Hz, 1H), 5.37 (s, 1H), 4.99 (d, $J = 3.9$ Hz, 1H), 3.78 (s, 3H), 3.77 (s, 3H), 1.97 (d, $J = 12.2$ Hz, 1H), 1.72 (dd, $J = 12.1, 4.4$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 173.0, 167.2, 159.4, 140.1, 138.2, 133.0, 129.9, 129.0, 128.8, 126.1, 123.2, 114.3, 113.7, 94.1, 82.3, 69.1, 59.6, 55.3, 53.0, 34.0. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{23}\text{H}_{22}\text{NO}_5^+$ 392.1492, found 392.1499.

Methyl 1-(4-chlorophenyl)-3-oxo-2-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4v)



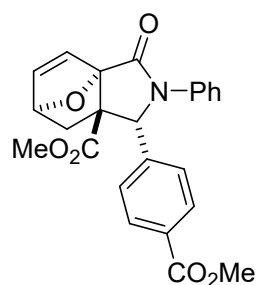
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (74.2 mg, 94% yield, dr > 20:1), m.p.: 172.1-173.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.45 (d, *J* = 8.0 Hz, 2H), 7.38 (brs, 1H), 7.33 – 7.27 (m, 4H), 7.16 (t, *J* = 7.3 Hz, 1H), 7.07 (brs, 1H), 6.64 (d, *J* = 5.7 Hz, 1H), 6.59 (d, *J* = 5.7 Hz, 1H), 5.41 (s, 1H), 4.99 (d, *J* = 2.9 Hz, 1H), 3.77 (s, 3H), 1.99 (d, *J* = 12.3 Hz, 1H), 1.68 (dd, *J* = 12.2, 4.5 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.7, 167.1, 140.2, 137.9, 135.5, 134.2, 132.8, 130.1, 129.6, 129.3, 129.1, 128.6, 126.3, 123.1, 94.1, 82.4, 68.8, 59.3, 53.1, 34.1. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₂H₁₉ClNO₄⁺ 396.0997, found 396.1002.

Methyl 3-oxo-2-phenyl-1-(4-(trifluoromethyl)phenyl)-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4w)



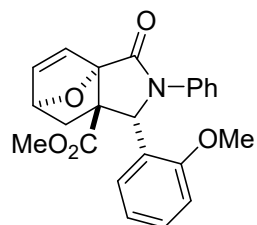
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (70.4 mg, 82% yield, dr > 20:1), m.p.: 155.1-156.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.58 (brs, 3H), 7.46 (d, *J* = 7.9 Hz, 2H), 7.31 (t, *J* = 7.7 Hz, 2H), 7.25 (brs, 1H), 7.17 (t, *J* = 7.2 Hz, 1H), 6.65 (d, *J* = 5.8 Hz, 1H), 6.60 (d, *J* = 5.7 Hz, 1H), 5.51 (s, 1H), 4.99 (d, *J* = 4.0 Hz, 1H), 3.79 (s, 3H), 2.01 (d, *J* = 12.4 Hz, 1H), 1.62 (dd, *J* = 12.1, 4.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.5, 167.1, 141.1, 140.2, 137.8, 132.7, 129.2, 126.4, 125.4, 123.0, 94.1, 82.4, 68.8, 59.3, 53.2, 34.1. ¹⁹F NMR (376 MHz, CDCl₃) δ -62.60. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₃H₁₉F₃NO₄⁺ 430.1261, found 430.1240.

Methyl *1-(4-(methoxycarbonyl)phenyl)-3-oxo-2-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4x)*



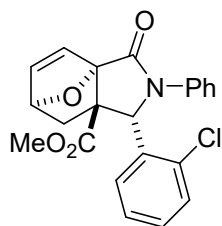
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (80.5 mg, 96% yield, dr > 20:1), m.p.: 186.4-187.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.00 (brs, 2H), 7.52 (s, 1H), 7.47 (d, *J* = 7.8 Hz, 2H), 7.30 (d, *J* = 7.5 Hz, 2H), 7.23 (brs, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.64 (d, *J* = 5.8 Hz, 1H), 6.59 (d, *J* = 5.7 Hz, 1H), 5.49 (s, 1H), 4.96 (d, *J* = 3.3 Hz, 1H), 3.90 (s, 3H), 3.78 (s, 3H), 1.99 (d, *J* = 12.3 Hz, 1H), 1.64 (dd, *J* = 12.3, 4.4 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.6, 167.1, 166.6, 142.1, 140.2, 137.9, 132.7, 130.2, 129.7, 129.1, 128.8, 128.4, 126.3, 123.0, 94.1, 82.3, 69.0, 59.3, 53.2, 52.3, 34.0. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₄H₂₂NO₆⁺ 420.1442, found 420.1454.

Methyl *1-(2-methoxyphenyl)-3-oxo-2-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4y)*



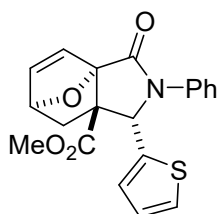
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (75.1 mg, 96% yield, dr > 20:1), m.p.: 214.5-215.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, *J* = 7.8 Hz, 2H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 2H), 7.13 (t, *J* = 7.2 Hz, 1H), 6.89 – 6.86 (m, 2H), 6.60 – 6.56 (m, 2H), 5.84 (s, 1H), 4.90 (d, *J* = 3.5 Hz, 1H), 3.85 (s, 3H), 3.76 (s, 3H), 2.08 (d, *J* = 12.2 Hz, 1H), 1.54 (dd, *J* = 12.2, 4.4 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.7, 167.6, 156.3, 140.2, 138.4, 132.4, 129.1, 128.9, 128.8, 125.6, 125.0, 122.3, 120.8, 109.7, 94.5, 82.1, 62.9, 58.6, 55.5, 52.9, 33.7. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₃H₂₂NO₅⁺ 392.1492, found 392.1499.

Methyl 1-(2-chlorophenyl)-3-oxo-2-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4z)



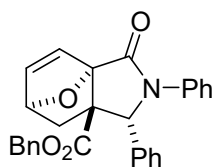
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (77.4 mg, 98% yield, dr > 20:1), m.p.: 165.7-166.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.54 (d, *J* = 7.7 Hz, 2H), 7.41 – 7.28 (m, 4H), 7.21 (t, *J* = 6.0 Hz, 2H), 7.15 (t, *J* = 7.2 Hz, 2H), 6.63 – 6.56 (m, 2H), 5.92 (s, 1H), 4.93 (d, *J* = 3.6 Hz, 1H), 3.77 (s, 3H), 2.19 (d, *J* = 12.4 Hz, 1H), 1.58 (dd, *J* = 12.4, 4.8 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.2, 167.4, 140.4, 138.0, 134.5, 133.5, 132.1, 130.0, 129.4, 129.2, 129.1, 127.2, 125.9, 122.2, 94.7, 82.3, 65.4, 58.5, 53.1, 33.7. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₂H₁₉ClNO₄⁺ 396.0997, found 396.1002.

Methyl 3-oxo-2-phenyl-1-(thiophen-2-yl)-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4aa)



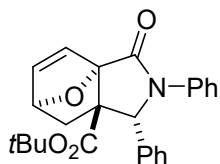
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (69.7 mg, 95% yield, dr > 20:1), m.p.: 166.6-167.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.40 (d, *J* = 7.9 Hz, 2H), 7.36 – 7.27 (m, 3H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.01 (d, *J* = 3.6 Hz, 1H), 6.93 (t, *J* = 4.1 Hz, 1H), 6.65 – 6.60 (m, 2H), 5.65 (s, 1H), 5.13 (d, *J* = 4.1 Hz, 1H), 3.78 (s, 3H), 2.06 (d, *J* = 12.2 Hz, 1H), 1.98 (dd, *J* = 12.2, 4.2 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.5, 166.6, 140.3, 137.7, 132.3, 129.1, 128.6, 127.1, 126.8, 126.7, 124.1, 93.9, 82.4, 65.8, 59.5, 53.1, 34.1. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₀H₁₈NO₄S⁺ 368.0951, found 368.0987.

Benzyl 3-oxo-1,2-diphenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4ab)



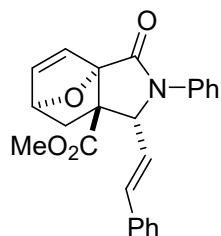
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (80.4 mg, 92% yield, dr > 20:1), m.p.: 133.7-134.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.43 (brs, 1H), 7.35 – 7.25 (m, 10H), 7.22 (t, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.2 Hz, 1H), 7.06 – 7.02 (m, 1H), 6.55 – 6.50 (m, 2H), 5.32 (s, 1H), 5.27 (d, *J* = 12.0 Hz, 1H), 5.13 (d, *J* = 12.0 Hz, 1H), 4.96 (d, *J* = 4.0 Hz, 1H), 1.98 (d, *J* = 12.2 Hz, 1H), 1.67 (dd, *J* = 12.2, 4.2 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 182.3, 172.0, 140.0, 138.1, 136.9, 135.0, 132.9, 132.8, 128.9, 128.8, 128.7, 128.6, 128.3, 127.5, 126.0, 123.6, 123.1, 94.1, 82.4, 69.4, 67.5, 59.6, 34.0. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₈H₂₄NO₄⁺ 438.1700, found 438.1715.

tert-Butyl 3-oxo-1,2-diphenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4ac)



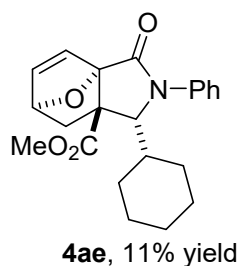
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (75.8 mg, 94% yield, dr > 20:1), m.p.: 182.4-183.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.50 (d, *J* = 7.8 Hz, 2H), 7.43 (brs, 1H), 7.34 – 7.26 (m, 5H), 7.12 (t, *J* = 7.2 Hz, 2H), 6.67 (d, *J* = 5.7 Hz, 1H), 6.59 (d, *J* = 5.9 Hz, 1H), 5.37 (s, 1H), 4.94 (d, *J* = 4.0 Hz, 1H), 1.94 (d, *J* = 12.2 Hz, 1H), 1.62 (dd, *J* = 12.1, 4.6 Hz, 1H), 1.46 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ 171.2, 167.5, 140.0, 138.3, 137.2, 135.5, 132.8, 129.0, 128.3, 128.2, 125.8, 122.7, 94.0, 82.4, 69.7, 60.2, 33.7, 28.0. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₅H₂₆NO₄⁺ 404.1856, found 404.1859.

Methyl (E)-3-oxo-2-phenyl-1-styryl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4ad)

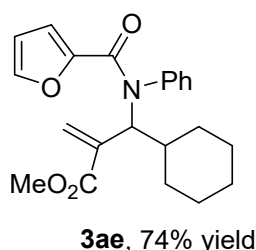


Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (48 mg, 62% yield, dr = 5:1), m.p.: 141.4-142.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.49 (d, *J* = 8.0 Hz, 2H), 7.39 – 7.27 (m, 7H), 7.22 (t, *J* = 7.6 Hz, 1H), 6.65 – 6.62 (m, 2H), 6.46 (d, *J* = 16.1 Hz, 1H), 6.32 (dd, *J* = 16.0, 9.1 Hz, 1H), 5.26 (d, *J* = 4.5 Hz, 1H), 4.84 (d, *J* = 9.1 Hz, 1H), 3.76 (s, 3H), 2.53 (dd, *J* = 12.3, 4.6 Hz, 1H), 2.08 (d, *J* = 12.4 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 172.6, 166.4, 139.8, 137.8, 135.6, 135.6, 132.3, 129.2, 128.8, 128.5, 127.4, 126.8, 126.8, 124.5, 93.9, 82.6, 69.2, 59.5, 53.0, 33.9. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₄H₂₂NO₄⁺ 388.1543, found 388.1579.

Methyl 1-cyclohexyl-3-oxo-2-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4ae)



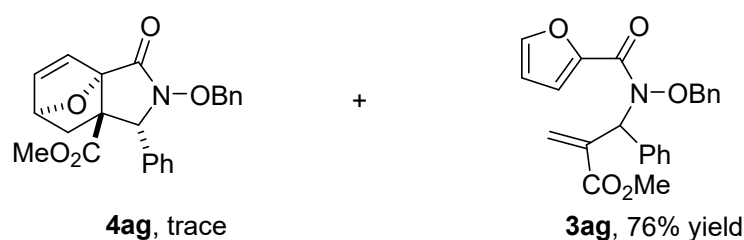
+



Under standard conditions, the reaction afforded a mixture of **4ae** and intermediate **3ae**, which could not be fully converted even upon prolonged reaction. The two components were separated by column chromatography (eluent: petroleum ether/EtOAc = 4:1).

Characterization data for **4ae**: White solid (8.1 mg, 11% yield, dr > 20:1), m.p.: 133.4-134.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.43 – 7.36 (m, 4H), 7.26 – 7.22 (m, 1H), 6.60 (d, *J* = 5.5 Hz, 1H), 6.52 (d, *J* = 5.7 Hz, 1H), 5.25 (d, *J* = 4.0 Hz, 1H), 4.14 (d, *J* = 7.6 Hz, 1H), 3.72 (s, 3H), 2.45 (dd, *J* = 12.4, 4.8 Hz, 1H), 2.26 (d, *J* = 12.4 Hz, 1H), 1.87 – 1.78 (m, 1H), 1.75 – 1.61 (m, 4H), 1.22 – 1.06 (m, 2H), 1.02 – 0.95 (m, 1H), 0.92 – 0.76 (m, 2H), 0.71 – 0.61 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 173.5, 166.8, 139.5, 139.3, 133.0, 129.0, 126.5, 124.8,

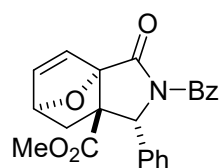
Methyl (1*R*,3*aS*,6*S*,7*aR*)-2-(benzyloxy)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3*a*,6-epoxyisoindole-7*a*(1*H*)-carboxylate (**4ag**)



Under standard conditions, the reaction afforded product **4ag** in trace amount; while intermediate **3ag** was isolated as the major product by column chromatography (eluent: petroleum ether/EtOAc = 4:1). The intermediate failed to convert even upon prolonged reaction times or at elevated temperature (toluene, reflux).

Characterization data for **3ag**: Colorless oil (59 mg, 76% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, $J = 1.7$ Hz, 1H), 7.53 (d, $J = 8.0$ Hz, 2H), 7.43 – 7.33 (m, 3H), 7.32 – 7.27 (m, 3H), 7.21 (dd, $J = 3.5, 0.8$ Hz, 1H), 7.09 – 7.04 (m, 2H), 6.82 (s, 1H), 6.50 (s, 1H), 6.49 (dd, $J = 3.6, 1.6$ Hz, 1H), 5.95 (d, $J = 1.6$ Hz, 1H), 4.60 (d, $J = 9.1$ Hz, 1H), 4.05 (d, $J = 9.1$ Hz, 1H), 3.67 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 166.1, 160.2, 146.0, 145.6, 138.3, 135.9, 134.0, 129.7, 129.2, 128.8, 128.7, 128.5, 128.5, 127.6, 118.4, 111.7, 78.8, 62.1, 52.2. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{23}\text{H}_{22}\text{NO}_5^+$ 392.1492, found 392.1499.

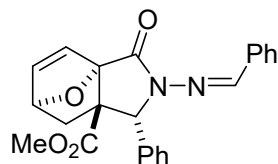
Methyl 2-benzoyl-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3*a*,6-epoxyisoindole-7*a*(1*H*)-carboxylate (**4ah**)



Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (59 mg, 76% yield, dr > 20:1), m.p.: 126.3–127.6 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.74 (dd, $J = 8.8, 1.3$ Hz, 2H), 7.57 – 7.51 (m, 1H), 7.46 – 7.41 (m, 3H), 7.38 – 7.34 (m, 3H), 7.31 – 7.27 (m, 1H), 6.58 (dd, $J = 5.9, 1.6$ Hz, 1H), 6.52 (d, $J = 5.9$ Hz, 1H), 5.89 (s, 1H), 5.04 (dd, $J = 4.5, 1.6$ Hz, 1H), 3.77 (s, 3H), 1.98 (d, $J = 12.3$ Hz, 1H), 1.78 (dd, $J = 12.3, 4.6$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 172.4, 169.8, 167.9, 140.4, 137.2, 133.8, 132.7, 131.7,

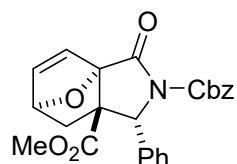
129.1, 128.8, 128.4, 128.2, 94.1, 82.7, 65.1, 58.3, 53.2, 34.2. HRMS (ESI) m/z : $[M + H]^+$
Calcd for $C_{23}H_{20}NO_5^+$ 390.1336, found 390.1320.

Methyl 2-(benzylideneamino)-3-oxo-1-phenyl-2,3,6,7-tetrahydro-3a,6-epoxyisoindole-7a(1H)-carboxylate (4ai)



Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (69.9 mg, 90% yield, dr > 20:1), m.p.: 162.6-163.7 °C; 1H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.62 (d, $J = 7.3$ Hz, 2H), 7.45 – 7.29 (m, 6H), 7.24 (d, $J = 7.8$ Hz, 2H), 6.63 (d, $J = 5.8$ Hz, 1H), 6.57 (d, $J = 5.8$ Hz, 1H), 5.38 (s, 1H), 4.96 (d, $J = 4.4$ Hz, 1H), 3.75 (s, 3H), 1.98 (d, $J = 12.2$ Hz, 1H), 1.70 (dd, $J = 12.2, 4.4$ Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.6, 164.6, 148.6, 140.1, 135.3, 133.9, 132.7, 130.6, 128.6, 127.9, 92.5, 82.3, 67.5, 59.2, 53.2, 33.4. HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{23}H_{21}N_2O_4^+$ 389.1496, found 389.1520.

2-Benzyl 7a-methyl 3-oxo-1-phenyl-6,7-dihydro-3a,6-epoxyisoindole-2,7a(1H,3H)-dicarboxylate (4aj)



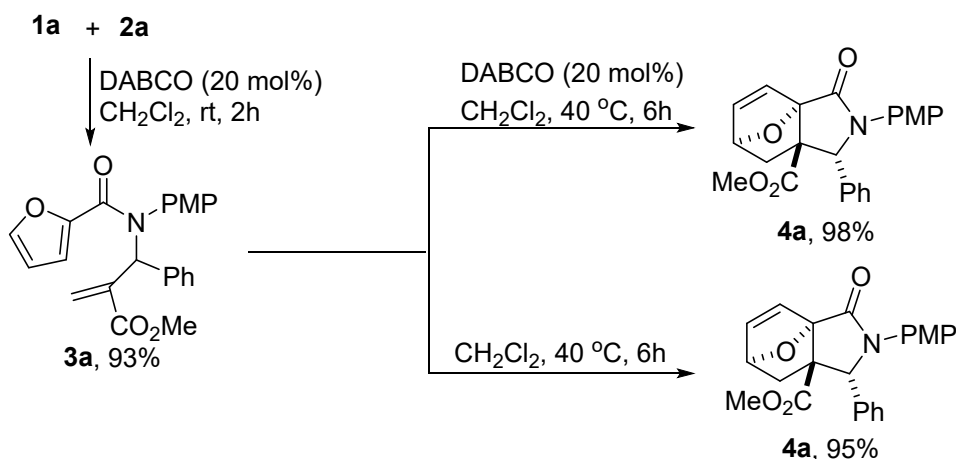
Purification by column chromatography (eluent: petroleum ether/EtOAc = 4:1). White solid (77 mg, 92% yield, dr > 20:1), m.p.: 126.3–127.6 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.30 (m, 4H), 7.26 – 7.10 (m, 4H), 7.08 – 7.02 (m, 2H), 6.56 (s, 2H), 5.49 (s, 1H), 5.24 (d, $J = 12.5$ Hz, 1H), 5.10 (d, $J = 12.5$ Hz, 1H), 4.94 (d, $J = 4.4$ Hz, 1H), 3.74 (s, 3H), 1.93 (d, $J = 12.3$ Hz, 1H), 1.70 (dd, $J = 12.3, 4.5$ Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3, 166.7, 151.1, 140.4, 137.6, 134.8, 132.2, 128.5, 128.3, 128.2, 127.7, 93.3, 82.6, 68.4, 66.5, 58.4, 53.2, 34.2. HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{24}H_{22}NO_6^+$ 420.1442, found 420.1454.

2-(tert-Butyl) 7a-methyl (1R,3aS,6S,7aR)-3-oxo-1-phenyl-6,7-dihydro-3a,6-epoxyisoindole-2,7a(1H,3H)-dicarboxylate (4ak)

137.5, 134.74, 134.67, 133.2, 133.1, 130.4, 129.4, 128.8, 128.7, 128.2, 126.7, 123.8, 123.7, 119.5, 111.8, 64.3, 52.0. HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{24}H_{19}N_2O_6^+$ 431.1238, found 431.1218.

IV. Control experiments

a.



Step 1: Preparation of Intermediate **3a**

To a sealed tube containing compound **1a** (108.5 mg, 0.5 mmol), and **2a** (175.4 mg, 0.6 mmol, 1.2 equiv) in CH₂Cl₂ (5.0 mL) was added DABCO (11.2 mg, 0.1 mmol, 20 mol%). The reaction mixture was stirred at room temperature for 2 h. Upon completion, the solvent was removed in *vacuo*, and the crude product was purified by flash chromatography on silica gel (petroleum ether/EtOAc= 4:1) to afford intermediate **3a** (181.9 mg, 93%). Due to its instability at ambient temperature, **3a** used immediately in subsequent reactions.

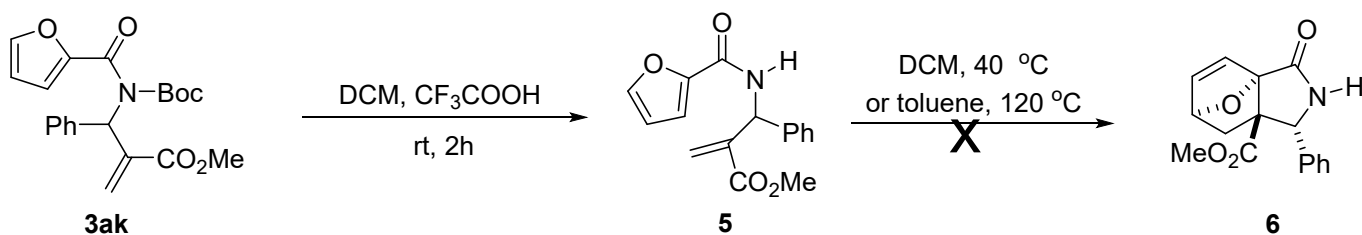
Step 2: Conversion to Product **4a**

Intermediate **3a** (78.2 mg, 0.2 mmol) and DABCO (4.5 mg, 0.04 mmol, 20 mol%) were dissolved in CH₂Cl₂ (2 mL) in a sealed tube and heated to 40 °C for 6 h. Standard workup and purification afforded product **4a** in 98% yield (76.7 mg).

Control Experiment:

As a control, the reaction was performed under identical conditions without DABCO, product **4a** was isolated in 95% yield.

b.



Step 1: Preparation of Intermediate **5**

Compound **3ak** (115.5 mg, 0.3 mmol) was treated trifluoroacetic acid (0.07 mL, 0.9 mmol, 3 equiv) in CH₂Cl₂ (3 mL) at room temperature for 2 h. Standard workup and purification by flash chromatography on silica gel (petroleum ether/EtOAc = 4:1) afforded compound **5** as a colorless oil (84.7 mg, 99%). ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, *J* = 9.0 Hz, 1H), 7.47 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.34 (d, *J* = 4.4 Hz, 4H), 7.28 (dd, *J* = 4.9, 3.7 Hz, 1H), 7.18 (dd, *J* = 3.6, 0.8 Hz, 1H), 6.52 (dd, *J* = 3.5, 1.8 Hz, 1H), 6.42 (d, *J* = 0.8 Hz, 1H), 6.19 (d, *J* = 9.0 Hz, 1H), 6.01 (d, *J* = 0.9 Hz, 1H), 3.72 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 166.3, 157.7, 147.5, 144.4, 139.2, 138.9, 128.8, 128.0, 127.7, 126.5, 115.2, 112.4, 54.5, 52.2.

Step 2: IMDA reaction attempts

Subsequent IMDA attempts proved unsuccessful: No formation of the desired product **6** was detected by LC-MS after stirring compound **5** (57.0 mg, 0.2 mmol) in CH₂Cl₂ at 40 °C for 24 h. Similarly, heating in toluene at 110°C for 24 h also failed to product **6**.

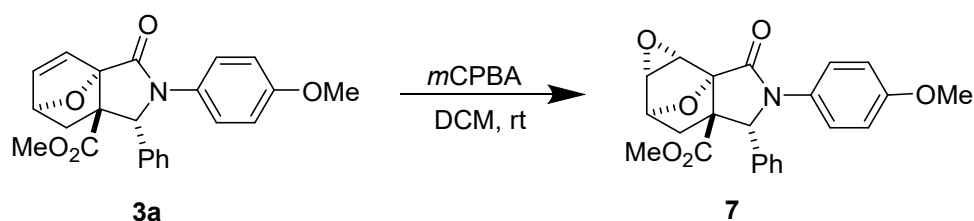
V. Gram-scale synthesis and chemical transformations

a. Gram-scale reaction of 4a

A mixture of **1a** (1.08 g, 5.0 mmol), MBH carbonate **2a** (1.75 mg, 6.0 mmol, 1.2 equiv), and DABCO (112 mg, 1.0 mmol, 20 mol%) was dissolved in DCM (40.0 mL). The reaction mixture was stirred at 40 °C until completion, as monitored by TLC. After removing the solvent under reduced pressure, the residue was purified by flash column chromatography on silica gel (eluent: petroleum ether/EtOAc = 4:1), to afford product **4a** (1.9 g, 97% yield).

b. Chemical transformations

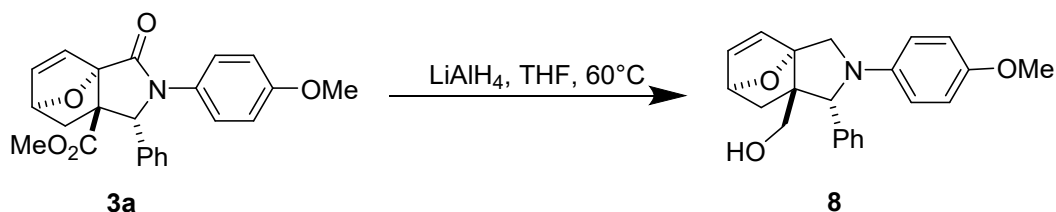
Synthesis of compound **7**:



A solution of **3a** (78 mg, 0.2 mmol) in dichloromethane (2.0 mL) was cooled to 0 °C. *m*-CPBA (104 mg, 0.6 mmol, 3.0 equiv) was added, and the mixture was warmed to room temperature and stirred for 3 h. Upon completion, the reaction mixture was diluted with additional dichloromethane and washed sequentially with saturated aqueous NaHCO₃ and brine. The organic phase was dried over Na₂SO₄, filtered and concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5/1) to afford the desired product **7** (70 mg, 86% yield) as a single isomer. White solid, m.p.: 129.7-130.7 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.52 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.27 (m, 5H), 7.01 (d, *J* = 6.9 Hz, 1H), 6.80 (d, *J* = 9.0 Hz, 2H), 5.26 (s, 1H), 4.48 (d, *J* = 5.0 Hz, 1H), 3.89 (s, 3H), 3.72 (s, 3H), 3.65 (d, *J* = 3.2 Hz, 1H), 3.41 (d, *J* = 3.2 Hz, 1H), 2.20 (d, *J* = 13.2 Hz, 1H), 1.62 (dd, *J* = 13.2, 5.1 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 171.9, 165.9, 157.8, 136.2, 130.7, 129.2, 128.6, 128.5, 128.3, 125.1,

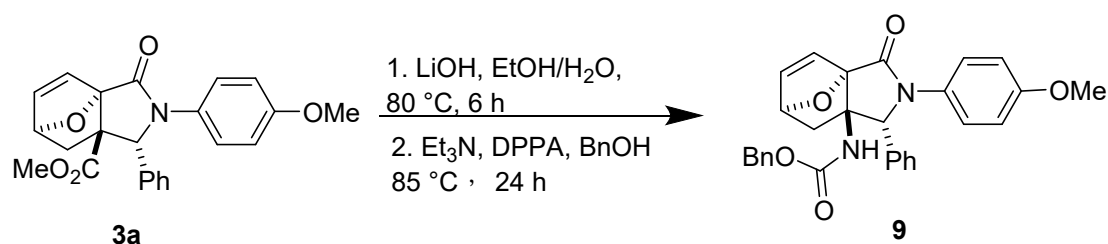
114.3, 89.5, 78.3, 70.4, 61.6, 55.4, 53.5, 48.9, 47.6, 34.7. HRMS (ESI) m/z : $[M + Na]^+$ Calcd for $C_{23}H_{21}NNaO_6^+$ 430.1261, found 430.1240.

Synthesis of compound **8**:



$LiAlH_4$ (30 mg, 0.8 mmol, 4.0 equiv) was slowly added to a suspension of **3a** (78 mg, 0.2 mmol) in anhydrous THF (2.0 mL) at room temperature under N_2 atmosphere. After addition, the mixture was heated to $60\text{ }^\circ\text{C}$ and stirred for 12 h. The reaction was carefully quenched at $0\text{ }^\circ\text{C}$ by sequential dropwise addition of H_2O (2.0 mL), 15% aqueous NaOH (2.0 mL) and H_2O (2.0 mL) again. The resulting mixture was stirred at room temperature for 30 min, then filtered through a pad of Celite. The filtrate was extracted with diethyl ether, and the combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4 , filtered, and concentrated in *vacuo*. The crude residue was purified by flash column chromatography on silica gel (eluent: petroleum ether/EtOAc = 10:1) to afford product **8** (31 mg, 67% yield) as a white solid, m.p.: $90.2\text{--}91.1\text{ }^\circ\text{C}$. 1H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.26 (m, 5H), 6.79 – 6.71 (m, 4H), 5.71 – 5.58 (m, 2H), 5.46 (s, 1H), 4.36 (s, 1H), 4.01 (dd, $J = 7.5, 0.9$ Hz, 1H), 3.72 (s, 3H), 3.61 (d, $J = 7.5$ Hz, 1H), 2.76 (d, $J = 19.7$ Hz, 1H), 2.33 – 2.24 (m, 2H), 2.17 (ddt, $J = 18.0, 4.5, 2.5$ Hz, 1H), 2.04 (t, $J = 10.8$ Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.6, 140.1, 138.9, 129.0, 127.6, 126.8, 123.4, 122.6, 117.0, 114.7, 90.3, 78.4, 76.4, 73.1, 55.6, 49.7, 30.7, 22.4. HRMS (ESI) m/z : $[M + Na]^+$ Calcd for $C_{22}H_{23}NNaO_3^+$ 372.1570, found 372.1599.

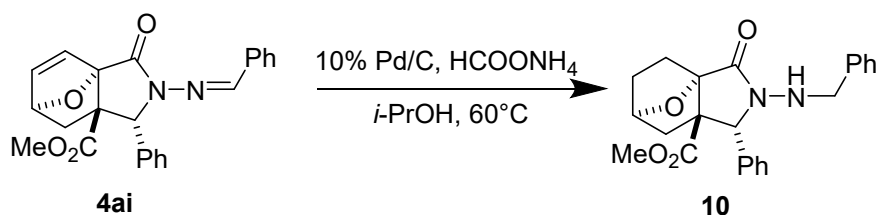
Synthesis of compound **9**:



A solution of compound **3a** (78 mg, 0.2 mmol) in EtOH/H₂O (2:1 v/v, 3.0 mL) was treated with LiOH (5.7 mg, 0.24 mmol, 1.2 equiv) and stirred at 80 °C for 6 h. After cooling, the mixture was neutralized with 1N HCl and extracted with dichloromethane. The combined organics were dried over anhydrous Na₂SO₄ and concentrated in *vacuo* to afford the crude carboxylic acid, which was used directly in the next step without further purification.

To a solution of the crude carboxylic acid and Et₃N (22 mg, 0.22 mmol, 1.1 equiv) in dry toluene (2.0 mL) was added dropwise diphenylphosphoryl azide (DPPA, 61 mg, 0.22 mmol, 1.1 equiv). The reaction mixture was stirred at room temperature for 4 h, then BnOH (65 mg, 0.6 mmol, 3.0 equiv) was added. The mixture was heated to 85 °C and stirred for 24 h. After cooling to room temperature, the reaction was quenched with H₂O and extracted with EtOAc. The combined organics were dried over anhydrous Na₂SO₄, filtered, and concentrated. The crude residue was purified by flash column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1) to yield the desired product **6** (56 mg, 58% yield) as a white solid, m.p.: 188.7-189.7 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.67 – 7.24 (m, 10H), 7.21 (s, 2H), 6.70 (d, *J* = 8.7 Hz, 4H), 5.61 – 5.44 (m, 2H), 5.18 – 5.08 (m, 2H), 4.87 (d, *J* = 4.1 Hz, 1H), 3.68 (s, 3H), 2.14 (d, *J* = 8.1 Hz, 1H), 1.37 (d, *J* = 12.5 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 166.6, 157.2, 156.0, 142.5, 137.4, 135.9, 131.1, 131.0, 128.7, 128.5, 128.3, 127.9, 124.1, 114.1, 93.6, 82.7, 80.0, 67.2, 66.3, 55.4, 39.6, 29.8. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₉H₂₇N₂O₅⁺ 483.1914, found 483.1904.

Synthesis of compound **10**:



A sealed tube was charged with compound **4ai** (78 mg, 0.2 mmol), 10% Pd/C (21 mg), and isopropyl alcohol (5.0 mL). To the stirring mixture were added ammonium formate (4.2 mg, 5.0 mmol) and H₂O (96 μL, 6 mmol). The tube was then sealed with a Teflon cap and immersed in a preheated oil bath at 60 °C for 4 hours. After completion, the mixture was cooled to room temperature and filtered through a short pad of Celite, and the filtrate was concentrated under reduced pressure. The crude residue was purified by flash column

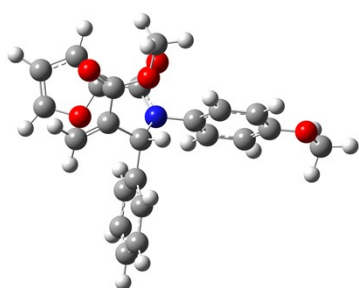
chromatography on silica gel (gradient elution: petroleum ether/EtOAc from 100:1 to 5:1) to afford product **10** (72 mg, 92% yield) as a white solid, m.p.:110.7-111.3°C. ¹H NMR (400 MHz, CDCl₃) δ 7.36 (brs, 2H), 7.32 – 7.21 (m, 7H), 6.92 (brs, 1H), 4.88 (t, *J* = 5.2 Hz, 1H), 4.81 (s, 1H), 4.51 (t, *J* = 5.2 Hz, 1H), 4.18 (dd, *J* = 12.7, 4.8 Hz, 1H), 4.09 (dd, *J* = 12.7, 4.7 Hz, 1H), 3.66 (s, 3H), 2.21 (d, *J* = 12.7 Hz, 1H), 2.13 – 2.02 (m, 1H), 1.97 – 1.88 (m, 1H), 1.65 – 1.56 (m, 2H), 1.40 (ddd, *J* = 12.7, 5.1, 2.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 173.4, 167.8, 137.7, 136.6, 129.9, 129.0, 128.8, 128.53, 128.50, 127.8, 90.1, 80.6, 68.8, 59.8, 53.9, 53.0, 38.5, 29.1, 27.0. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₃H₂₅N₂O₄⁺ 393.1809, found 393.1802.

Hall group	C -2yc	C -2yc
Moiety formula	C22 H18 Cl N O4	?
Sum formula	C22 H18 Cl N O4	C22 H18 Cl N O4
Mr	395.82	395.82
Dx,g cm-3	1.365	1.365
Z	4	4
Mu (mm-1)	0.227	0.227
F000	824.0	824.0
F000'	824.98	
h,k,lmax	17,22,11	17,22,11
Nref	4431[2221]	4403
Tmin,Tmax	0.976,0.984	
Tmin'	0.967	
Correction method=	Not given	
Data completeness=	1.98/0.99	Theta(max)= 27.505
R(reflections)=	0.0450(4037)	wR2(reflections)= 0.1411(4403)
S =	1.106	Npar= 255

VII. Computational Details

Density functional theory (DFT) calculations were performed using Gaussian 16.^[23] Geometry optimizations were performed at the B3LYP level of theory with the 6-311G(d, p) basis set, without any symmetry constraints. Frequency calculations at the same level were conducted to verify the nature of all stationary points: all intermediates were confirmed to be true minima on the potential energy surface with no imaginary frequencies, while transition states were identified as first-order saddle points with one and only one imaginary frequency. Thermal corrections were obtained from these frequency analyses. To account for solvent effects, the SMD implicit solvation model was employed using dichloromethane (DCM) as the solvent.

Compound 3a



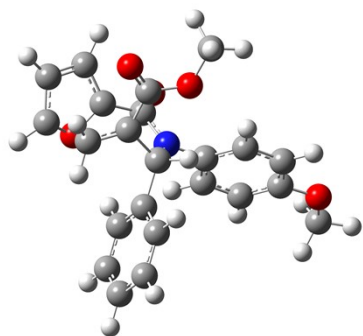
Zero-point correction=	0.393466 (Hartree/Particle)
Thermal correction to Energy=	0.419857
Thermal correction to Enthalpy=	0.420801
Thermal correction to Gibbs Free Energy=	0.334440
Sum of electronic and zero-point Energies=	-1319.880699
Sum of electronic and thermal Energies=	-1319.854308
Sum of electronic and thermal Enthalpies=	-1319.853364
Sum of electronic and thermal Free Energies=	-1319.939725

Center	Atomic	Forces (Hartrees/Bohr)		
Number	Number	X	Y	Z

1	8	0.000001355	-0.000003405	0.000003981
2	8	0.000005428	-0.000011270	0.000009276
3	8	-0.000002683	0.000003418	0.000002491
4	8	-0.000001001	-0.000000636	0.000004394
5	7	-0.000003659	-0.000000127	0.000002234
6	6	0.000000148	-0.000000408	-0.000000213
7	6	-0.000000079	0.000000361	0.000000337
8	1	-0.000000257	0.000000912	0.000000588
9	6	-0.000000256	0.000000466	0.000000746
10	1	-0.000000144	0.000000472	0.000001311
11	6	0.000001896	-0.000000469	-0.000000530
12	6	0.000000180	-0.000001627	-0.000000654
13	1	0.000000415	-0.000001558	-0.000000657
14	6	0.000000351	-0.000001228	-0.000000874
15	1	-0.000000037	-0.000001836	-0.000001473
16	6	0.000008708	0.000011218	-0.000005134
17	6	0.000002262	-0.000011500	0.000002004
18	1	-0.000000217	0.000002388	0.000000332
19	6	-0.000021242	-0.000013655	0.000010112
20	6	0.000004570	-0.000004699	-0.000013291
21	6	0.000026439	0.000011691	0.000004731
22	1	-0.000007118	0.000003994	-0.000002276
23	1	-0.000001509	0.000004710	-0.000008112
24	6	0.000000816	-0.000004670	-0.000013241
25	1	0.000001141	-0.000005867	0.000004550
26	6	-0.000005072	0.000010640	0.000006113
27	1	0.000000721	-0.000001049	0.000003944
28	6	-0.000011012	0.000007708	0.000007101
29	1	0.000001341	-0.000001465	0.000003991
30	6	0.000002394	0.000001292	-0.000003186

31	6	-0.000002364	-0.000002338	-0.000002058
32	1	0.000000110	-0.000000435	-0.000000748
33	6	-0.000000292	0.000000078	-0.000002705
34	1	-0.000000290	-0.000001206	-0.000003117
35	6	0.000000255	0.000000551	-0.000003631
36	1	-0.000000848	0.000000309	-0.000004279
37	6	-0.000001164	0.000001132	-0.000002625
38	1	-0.000001090	0.000001998	-0.000003477
39	6	-0.000000537	0.000002799	-0.000002224
40	1	-0.000001187	0.000001809	-0.000002045
41	6	0.000000273	-0.000000397	0.000001174
42	6	0.000000098	0.000002875	0.000003297
43	1	0.000000484	0.000001594	0.000002997
44	1	-0.000000192	0.000002430	0.000003444
45	1	0.000000779	0.000000960	0.000003600
46	8	0.000000380	-0.000000642	-0.000000611
47	6	0.000000670	-0.000000863	-0.000001403
48	1	0.000000275	-0.000001104	-0.000001368
49	1	0.000000325	-0.000001325	-0.000002030
50	1	0.000000438	-0.000002025	-0.000000786

TS



Zero-point correction=

0.393750 (Hartree/Particle)

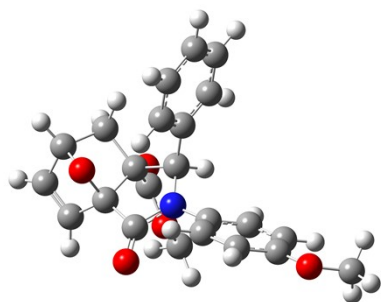
Thermal correction to Energy=	0.418701
Thermal correction to Enthalpy=	0.419645
Thermal correction to Gibbs Free Energy=	0.337642
Sum of electronic and zero-point Energies=	-1319.847965
Sum of electronic and thermal Energies=	-1319.823014
Sum of electronic and thermal Enthalpies=	-1319.822070
Sum of electronic and thermal Free Energies=	-1319.904073

Center	Atomic	Forces (Hartrees/Bohr)			
Number	Number	X	Y	Z	

1	8	-0.000000408	-0.000000393	-0.000000653	
2	8	-0.000000620	0.000001424	-0.000000662	
3	8	0.000000732	0.000000472	-0.000000702	
4	8	0.000000965	0.000001118	-0.000001375	
5	7	0.000000349	0.000000059	-0.000000031	
6	6	0.000000385	-0.000001390	0.000001217	
7	6	0.000000617	-0.000001159	0.000000759	
8	1	0.000001233	-0.000001333	0.000000752	
9	6	0.000000193	-0.000000794	0.000000484	
10	1	0.000000944	-0.000000816	0.000000020	
11	6	0.000000293	-0.000000395	0.000000402	
12	6	-0.000000630	-0.000000063	0.000000671	
13	1	-0.000000572	-0.000000258	0.000000699	
14	6	-0.000000061	-0.000000683	0.000001157	
15	1	-0.000000257	-0.000001187	0.000001254	
16	6	0.000000125	0.000000310	-0.000000140	
17	6	0.000000055	0.000000196	-0.000000283	
18	1	0.000001011	-0.000000300	0.000000038	
19	6	0.000000177	0.000000569	-0.000000773	

20	6	-0.000000236	0.000000635	-0.000000698
21	6	-0.000000179	0.000000908	-0.000000887
22	1	0.000000290	0.000001157	-0.000001239
23	1	-0.000000433	0.000001061	-0.000000767
24	6	-0.000000798	0.000001425	-0.000001179
25	1	-0.000000905	0.000001608	-0.000001077
26	6	-0.000000170	0.000001546	-0.000001465
27	1	-0.000000180	0.000001911	-0.000001726
28	6	-0.000000019	0.000001338	-0.000001177
29	1	0.000000323	0.000001331	-0.000001381
30	6	-0.000000476	0.000000059	0.000000064
31	6	-0.000000920	0.000000191	0.000000249
32	1	-0.000001219	0.000000437	0.000000254
33	6	-0.000001443	0.000000303	0.000000409
34	1	-0.000001857	0.000000144	0.000000654
35	6	-0.000001183	-0.000000033	0.000000560
36	1	-0.000001606	-0.000000108	0.000000798
37	6	-0.000000930	-0.000000028	0.000000322
38	1	-0.000000551	-0.000000282	0.000000509
39	6	-0.000000239	-0.000000364	0.000000335
40	1	0.000000173	-0.000000057	0.000000062
41	6	0.000001168	0.000000801	-0.000001027
42	6	0.000001850	0.000000152	-0.000000832
43	1	0.000001961	-0.000000099	-0.000000756
44	1	0.000002057	0.000000267	-0.000001211
45	1	0.000001700	0.000000470	-0.000001191
46	8	0.000000353	-0.000001805	0.000001525
47	6	-0.000000801	-0.000001923	0.000001839
48	1	0.000000248	-0.000002338	0.000002127
49	1	-0.000000362	-0.000002191	0.000002183
50	1	-0.000000145	-0.000001892	0.000001890

Compound **4a**



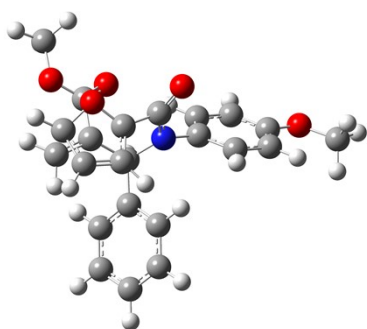
Zero-point correction=	0.396783 (Hartree/Particle)
Thermal correction to Energy=	0.421422
Thermal correction to Enthalpy=	0.422366
Thermal correction to Gibbs Free Energy=	0.340712
Sum of electronic and zero-point Energies=	-1319.881924
Sum of electronic and thermal Energies=	-1319.857285
Sum of electronic and thermal Enthalpies=	-1319.856340
Sum of electronic and thermal Free Energies=	-1319.937994

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	8	-0.000001339	0.000000134	-0.000000305
2	8	0.000000491	0.000000272	-0.000000739
3	8	0.000000745	-0.000000987	0.000000412
4	8	-0.000001667	-0.000000361	-0.000000306
5	7	-0.000004486	0.000008101	0.000006427
6	6	0.000006875	-0.000005837	0.000026978
7	6	0.000002934	0.000006098	-0.000009721
8	1	0.000003427	-0.000000190	0.000008287
9	6	0.000004217	0.000004274	-0.000000012

10	1	0.000001877	0.000000292	-0.000000026
11	6	0.000003878	-0.000005572	-0.000002992
12	6	-0.000002543	-0.000000457	-0.000008476
13	1	-0.000004054	-0.000004543	0.000010719
14	6	-0.000005887	-0.000003000	-0.000004049
15	1	0.000005760	0.000002443	0.000009719
16	6	0.000001152	0.000000764	-0.000001039
17	6	-0.000000005	-0.000003790	-0.000005140
18	1	0.000003965	0.000002794	0.000002865
19	6	0.000000969	-0.000000718	-0.000000885
20	6	-0.000001228	0.000000131	-0.000001695
21	6	0.000000426	-0.000004856	0.000001300
22	1	0.000000345	0.000000653	-0.000005348
23	1	-0.000002647	0.000003046	-0.000000011
24	6	-0.000001487	-0.000002136	-0.000003143
25	1	0.000001011	0.000002536	-0.000001066
26	6	0.000002030	0.000000656	-0.000002924
27	1	-0.000002255	-0.000000832	-0.000001750
28	6	0.000000438	-0.000002544	-0.000002992
29	1	-0.000001033	0.000001535	-0.000000359
30	6	-0.000000640	-0.000000002	0.000000236
31	6	0.000001986	-0.000000910	-0.000000115
32	1	-0.000000832	0.000001546	-0.000001539
33	6	0.000001063	0.000001415	0.000001668
34	1	0.000000786	0.000000426	-0.000003376
35	6	-0.000000788	0.000001863	0.000000777
36	1	0.000001674	-0.000001248	-0.000001674
37	6	-0.000001883	0.000001365	-0.000002720
38	1	0.000001533	-0.000001755	0.000001229
39	6	0.000000818	0.000000040	-0.000003645
40	1	-0.000000379	0.000000126	0.000003246

41	6	-0.000001083	0.000003287	-0.000002664
42	6	-0.000001835	-0.000001995	0.000000541
43	1	-0.000002537	-0.000003968	-0.000000022
44	1	-0.000002304	-0.000000173	-0.000000215
45	1	0.000000102	-0.000002165	0.000000055
46	8	-0.000000547	0.000007709	-0.000020402
47	6	-0.000003015	-0.000002346	0.000003654
48	1	-0.000000596	-0.000000263	0.000002417
49	1	0.000000656	-0.000000039	0.000003862
50	1	-0.000004086	-0.000000817	0.000004956

TS'



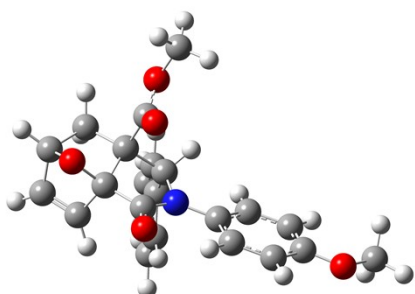
Zero-point correction=	0.393784 (Hartree/Particle)
Thermal correction to Energy=	0.418528
Thermal correction to Enthalpy=	0.419473
Thermal correction to Gibbs Free Energy=	0.338792
Sum of electronic and zero-point Energies=	-1319.823256
Sum of electronic and thermal Energies=	-1319.798512
Sum of electronic and thermal Enthalpies=	-1319.797568
Sum of electronic and thermal Free Energies=	-1319.878248

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z

1	6	-0.000000170	-0.000000381	0.000000300
2	8	0.000000429	0.000001035	0.000001022
3	8	0.000000595	0.000001677	0.000000841
4	6	0.000000329	0.000001532	0.000000451
5	7	-0.000000271	0.000000084	0.000000077
6	6	-0.000000175	-0.000000074	0.000000155
7	6	0.000000345	0.000001864	-0.000000547
8	6	0.000000339	0.000001275	0.000000321
9	6	0.000000259	0.000000263	0.000000316
10	6	-0.000000260	0.000000658	-0.000000349
11	6	0.000000145	0.000001704	0.000000094
12	6	0.000000026	0.000002039	-0.000000604
13	6	0.000000164	-0.000000906	0.000001144
14	6	0.000000433	-0.000001584	0.000001116
15	6	0.000000329	-0.000001114	0.000000936
16	6	0.000000151	-0.000000487	0.000000448
17	6	0.000000974	0.000000427	0.000000763
18	8	0.000000054	-0.000001615	0.000000966
19	6	-0.000000176	-0.000001425	0.000000859
20	6	-0.000000389	-0.000000400	-0.000001075
21	6	-0.000000621	-0.000000471	-0.000001378
22	6	-0.000001290	-0.000000665	-0.000002422
23	6	-0.000001206	-0.000000391	-0.000002703
24	6	-0.000001013	0.000000144	-0.000002417
25	6	-0.000000616	0.000000190	-0.000001263
26	6	0.000000823	-0.000000203	0.000001061
27	8	0.000000635	-0.000001057	0.000000947
28	8	0.000000535	0.000000241	0.000001124
29	6	0.000000812	-0.000000158	0.000001927
30	1	-0.000000253	-0.000000676	-0.000000013

31	1	-0.000000112	0.000001890	-0.000001043
32	1	-0.000000029	0.000000391	-0.000000162
33	1	-0.000000292	0.000000731	-0.000000961
34	1	0.000000417	0.000002077	0.000000158
35	1	-0.000000132	0.000002363	-0.000001258
36	1	0.000000224	-0.000001193	0.000001227
37	1	0.000000305	-0.000002063	0.000001475
38	1	0.000000120	-0.000000112	0.000000373
39	1	0.000000128	0.000000522	-0.000000093
40	1	0.000000204	-0.000001936	0.000001063
41	1	0.000000453	-0.000001011	0.000001036
42	1	-0.000000076	-0.000001393	0.000000142
43	1	-0.000000684	-0.000001126	-0.000001197
44	1	-0.000001309	-0.000001123	-0.000002590
45	1	-0.000001517	-0.000000234	-0.000003269
46	1	-0.000001060	0.000000583	-0.000002591
47	1	-0.000000409	0.000000556	-0.000001007
48	1	0.000000811	0.000000222	0.000002032
49	1	0.000001142	0.000000068	0.000002428
50	1	0.000000880	-0.000000736	0.000002141

Compound **4a'**



Zero-point correction=

0.396979 (Hartree/Particle)

Thermal correction to Energy=	0.421304
Thermal correction to Enthalpy=	0.422248
Thermal correction to Gibbs Free Energy=	0.342369
Sum of electronic and zero-point Energies=	-1319.851482
Sum of electronic and thermal Energies=	-1319.827157
Sum of electronic and thermal Enthalpies=	-1319.826213
Sum of electronic and thermal Free Energies=	-1319.906092

Center	Atomic	Forces (Hartrees/Bohr)		
Number	Number	X	Y	Z

1	6	0.000001788	-0.000000618	0.000001449
2	8	0.000000541	-0.000000856	-0.000000133
3	8	0.000000908	0.000000101	0.000003458
4	6	0.000001897	-0.000002452	0.000001485
5	7	0.000001573	-0.000001557	0.000000708
6	6	-0.000001610	-0.000002495	0.000001642
7	6	-0.000004229	0.000000072	-0.000005640
8	6	-0.000000712	-0.000000051	-0.000001233
9	6	-0.000002186	0.000000518	-0.000002828
10	6	0.000000391	0.000004445	-0.000002826
11	6	0.000001326	0.000000497	-0.000002707
12	6	0.000000870	0.000001427	-0.000002131
13	6	0.000000246	-0.000000147	0.000002102
14	6	0.000000136	-0.000004458	0.000004122
15	6	-0.000000203	-0.000002421	0.000003031
16	6	-0.000000225	-0.000004144	0.000002871
17	6	0.000001674	-0.000000742	0.000001275
18	8	0.000000615	-0.000002975	0.000004091
19	6	-0.000000015	-0.000001211	0.000005309

20	6	0.000002418	0.000000075	0.000000158
21	6	-0.000001508	0.000001568	-0.000002617
22	6	0.000001745	0.000001348	-0.000002905
23	6	0.000002390	0.000001461	-0.000003093
24	6	0.000003752	0.000000160	-0.000002370
25	6	0.000001996	-0.000000720	-0.000000555
26	6	0.000002302	0.000002911	0.000002599
27	8	-0.000004121	-0.000000061	-0.000001422
28	8	-0.000002619	0.000001919	-0.000001476
29	6	-0.000004000	0.000002369	0.000000898
30	1	-0.000001190	0.000003580	-0.000001121
31	1	0.000002377	-0.000000699	-0.000001484
32	1	-0.000000877	0.000003278	-0.000001784
33	1	-0.000001215	0.000001043	-0.000003317
34	1	-0.000000388	0.000002449	-0.000002381
35	1	0.000002699	0.000000309	-0.000003915
36	1	0.000000730	-0.000003434	0.000002497
37	1	0.000000155	-0.000003721	0.000004084
38	1	-0.000001426	-0.000003060	0.000002203
39	1	-0.000001994	0.000002851	-0.000001177
40	1	-0.000000587	-0.000003244	0.000004968
41	1	-0.000000227	-0.000003379	0.000003703
42	1	-0.000001007	-0.000001142	0.000003365
43	1	-0.000000354	0.000002014	-0.000001914
44	1	0.000000719	0.000002244	-0.000003786
45	1	0.000002401	0.000000058	-0.000003970
46	1	0.000003013	-0.000001031	-0.000002874
47	1	0.000004289	0.000000219	-0.000000274
48	1	-0.000003940	0.000003057	0.000000727
49	1	-0.000004037	0.000002329	0.000001038
50	1	-0.000004281	0.000002318	0.000002151

VIII. References

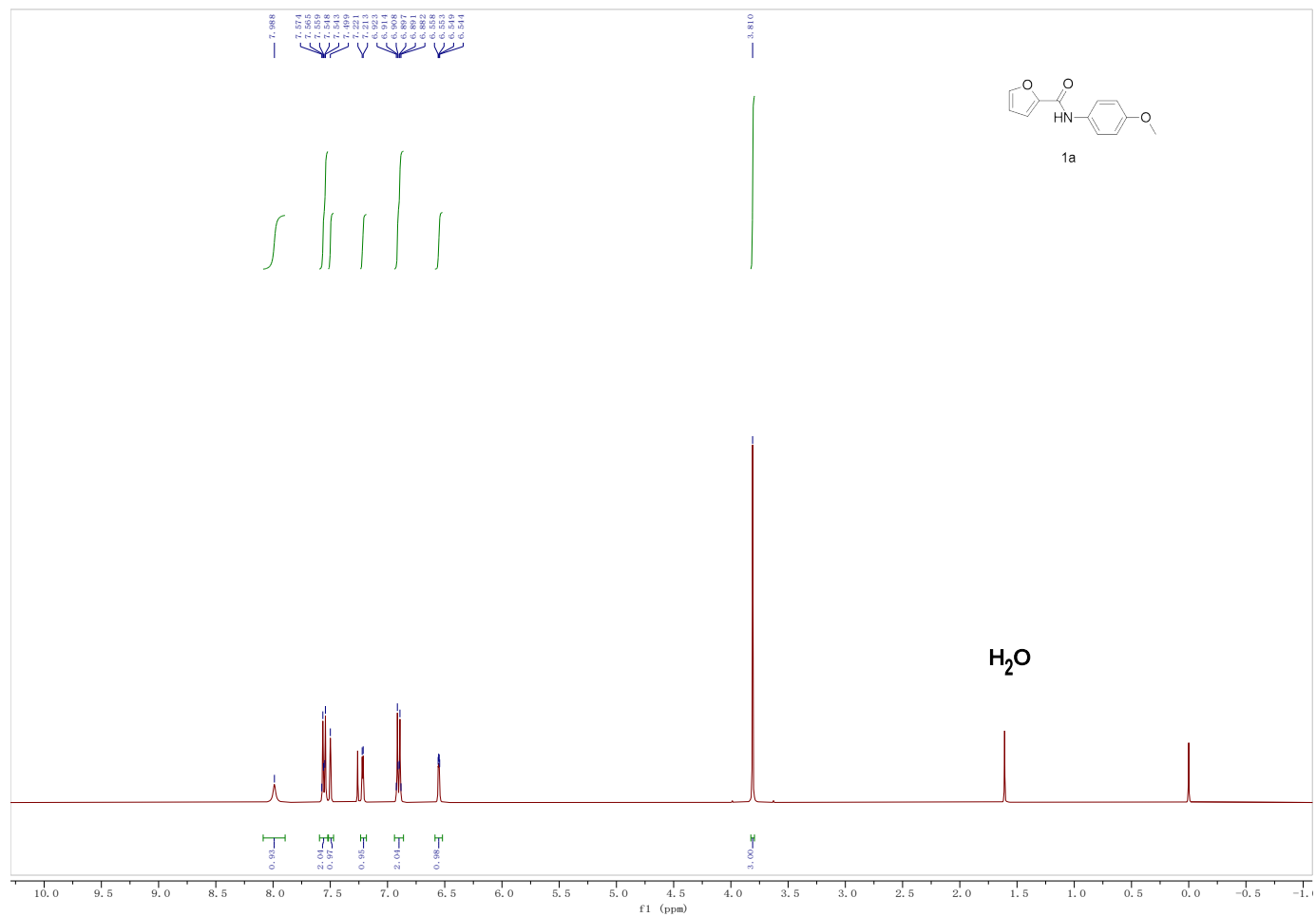
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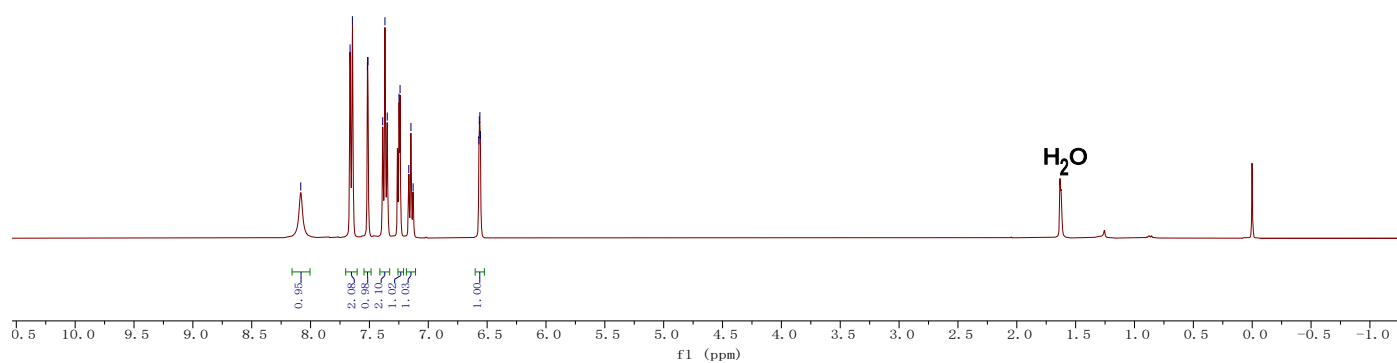
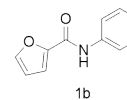
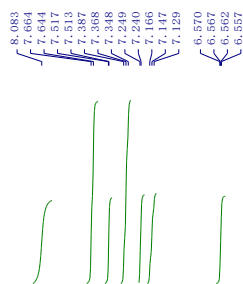
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IX. NMR Spectra

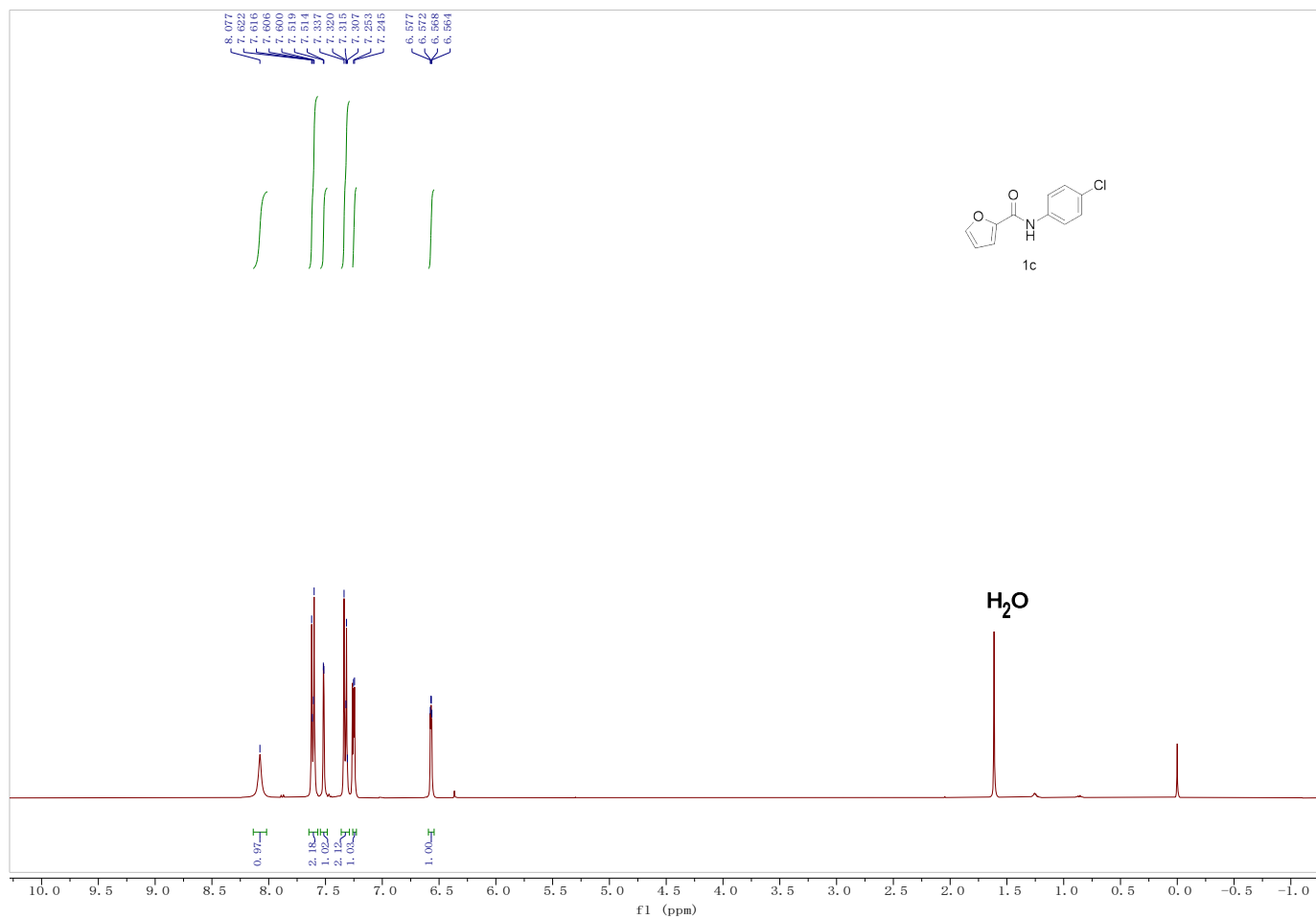
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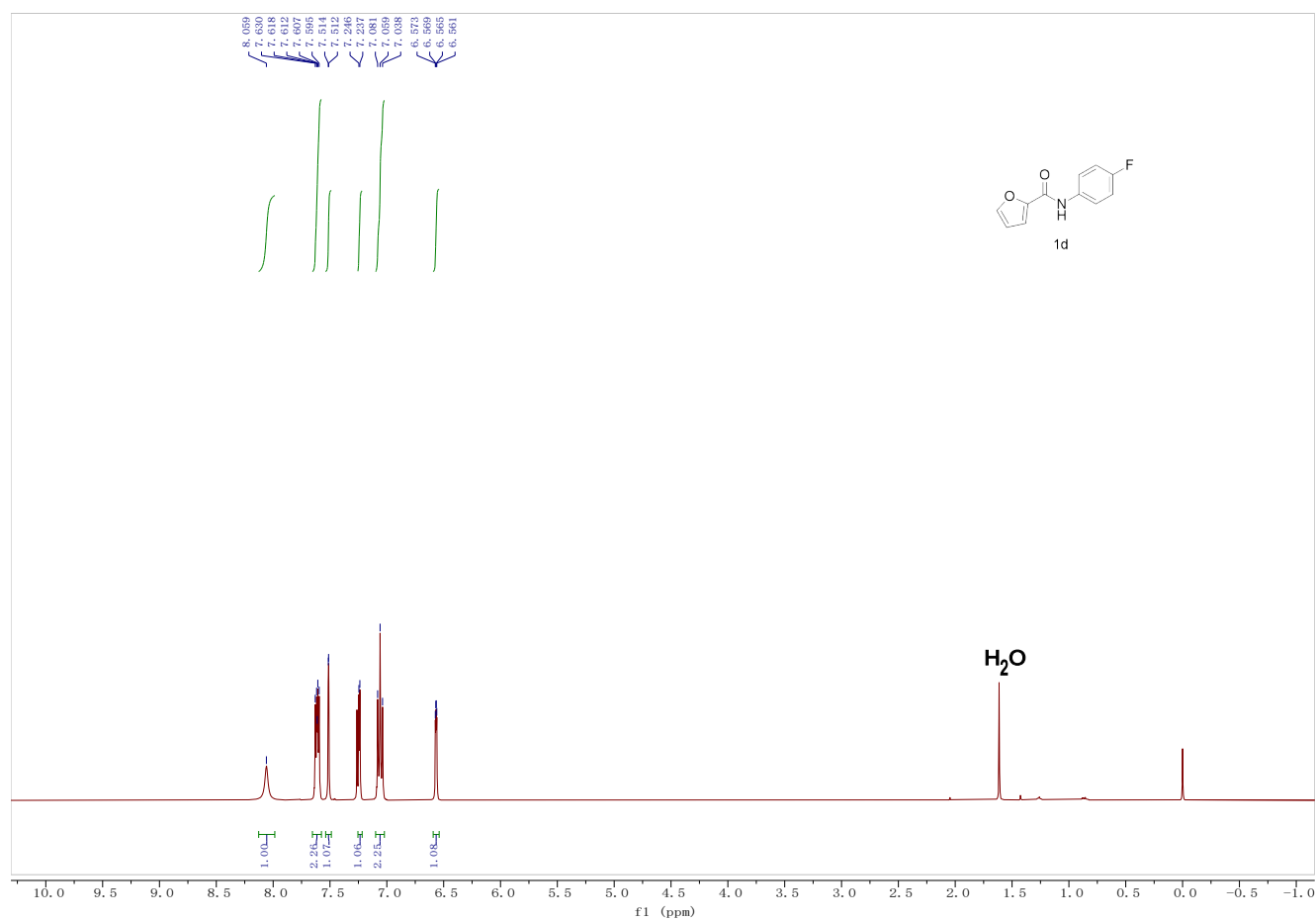
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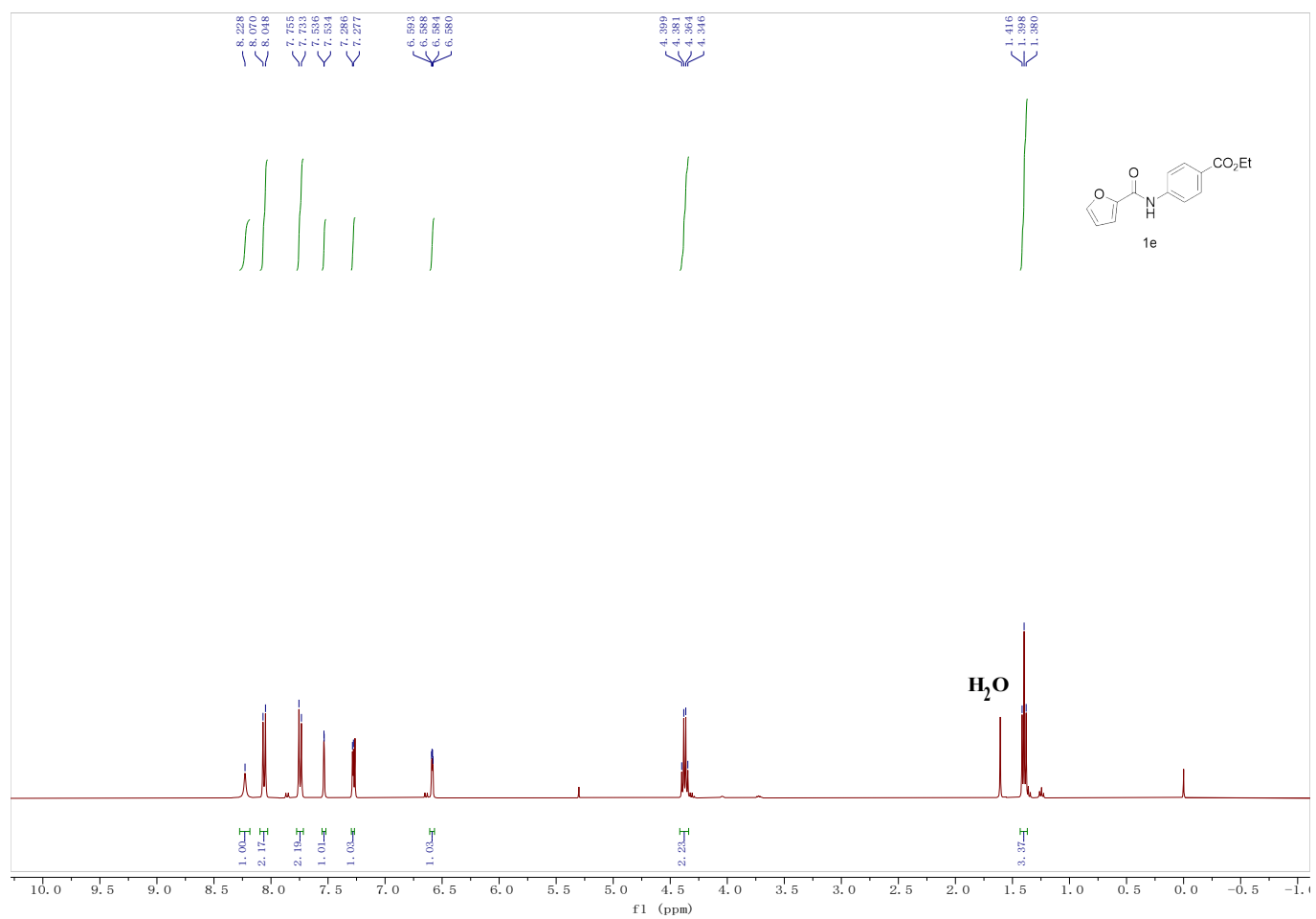
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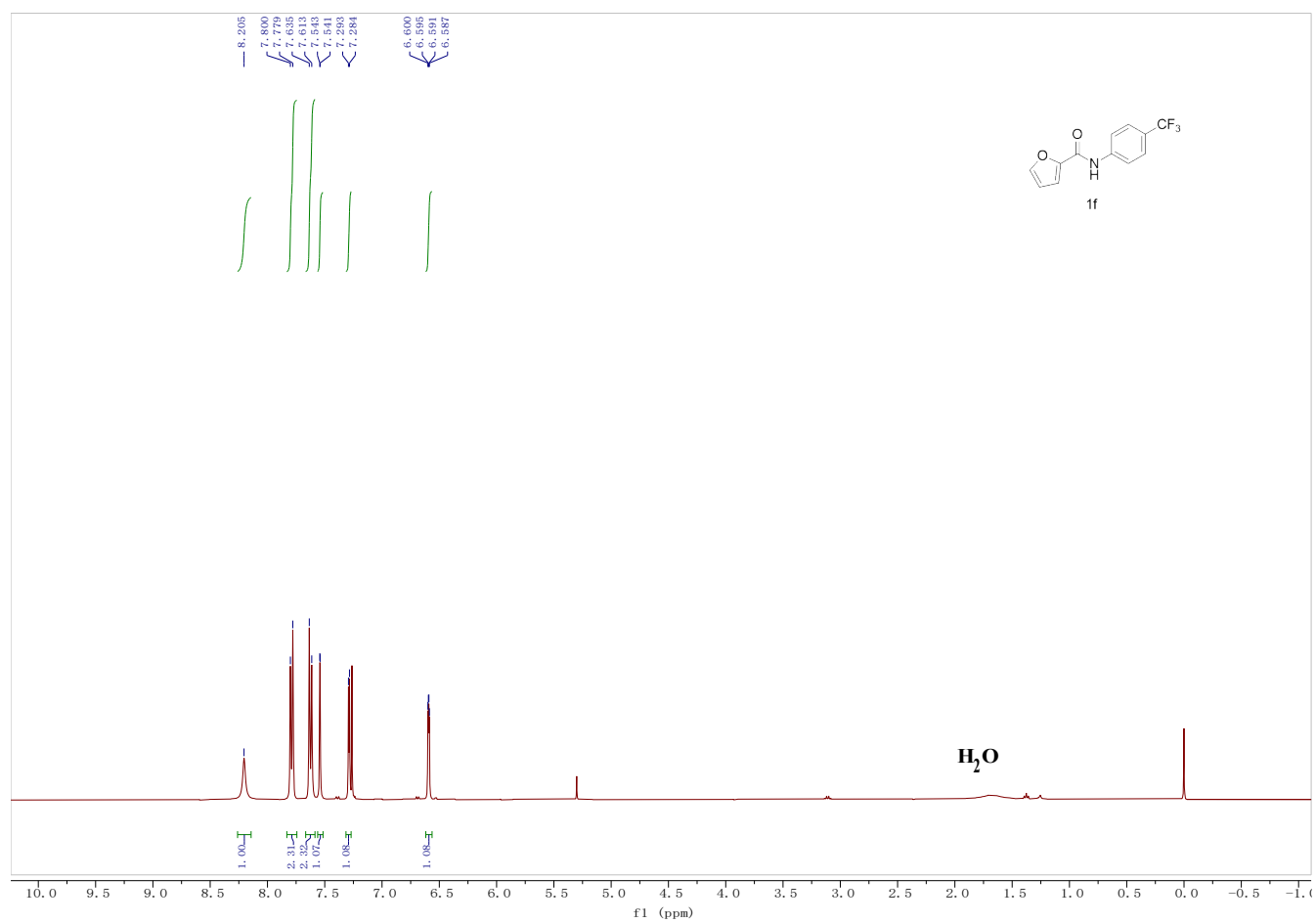
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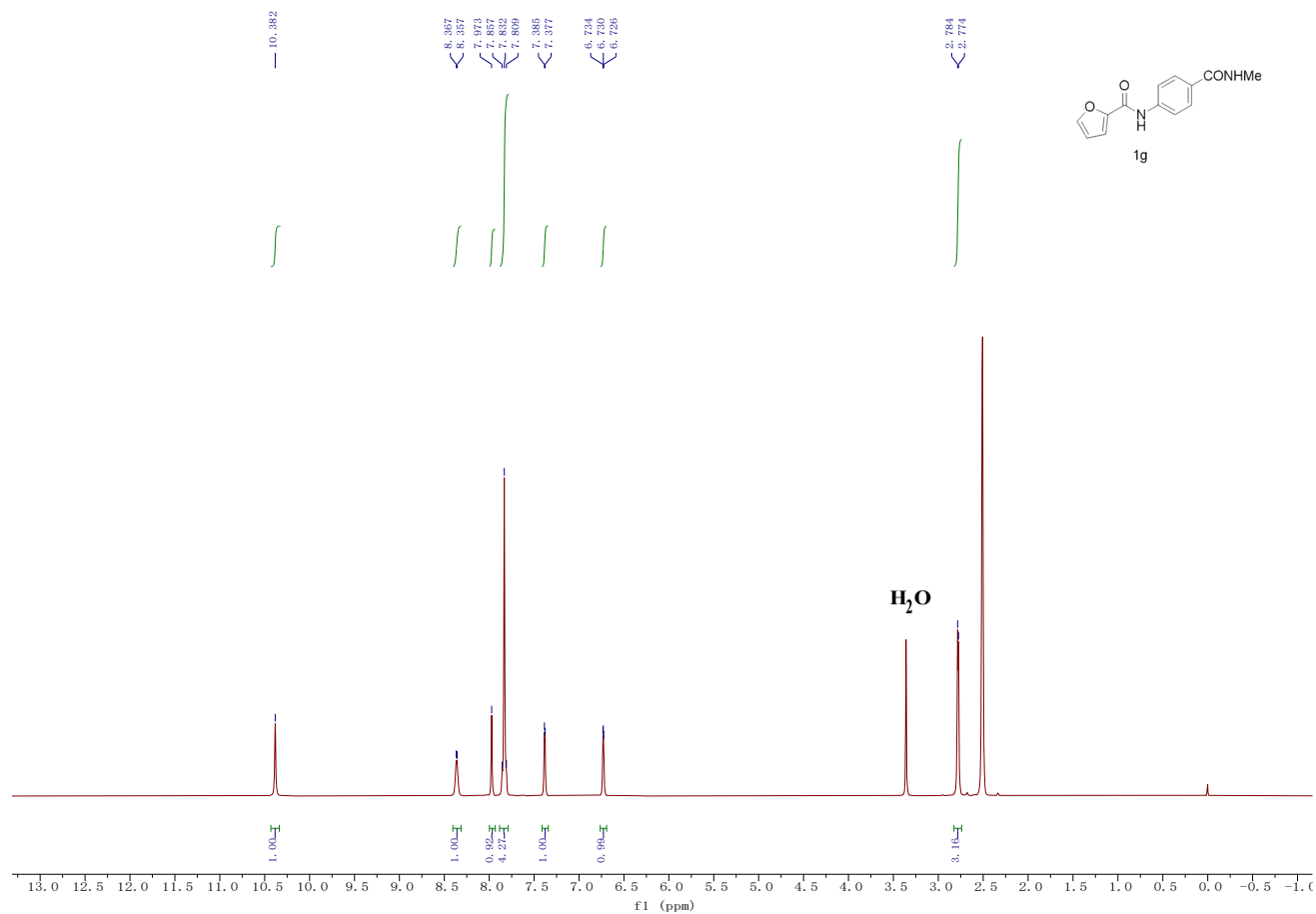
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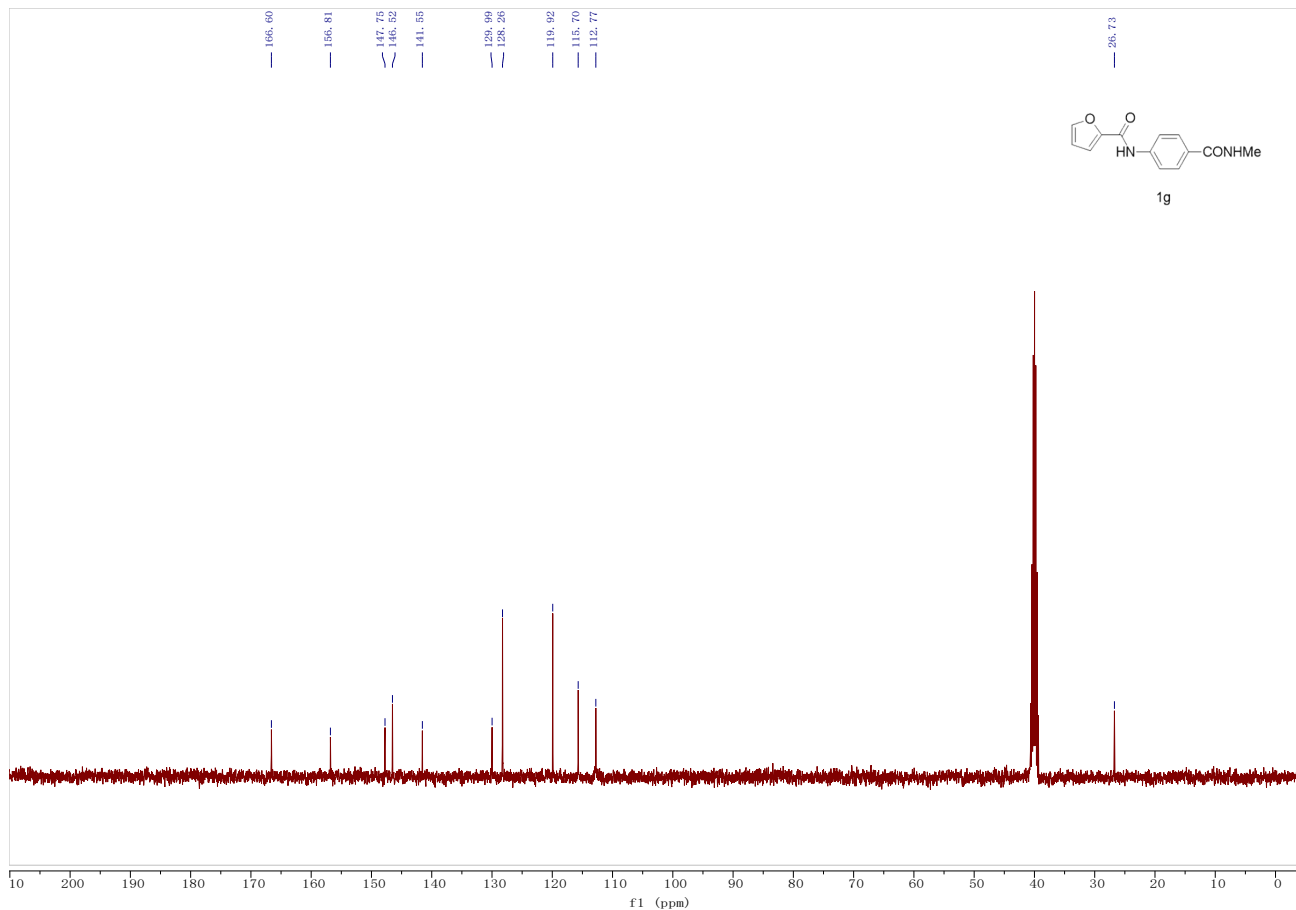
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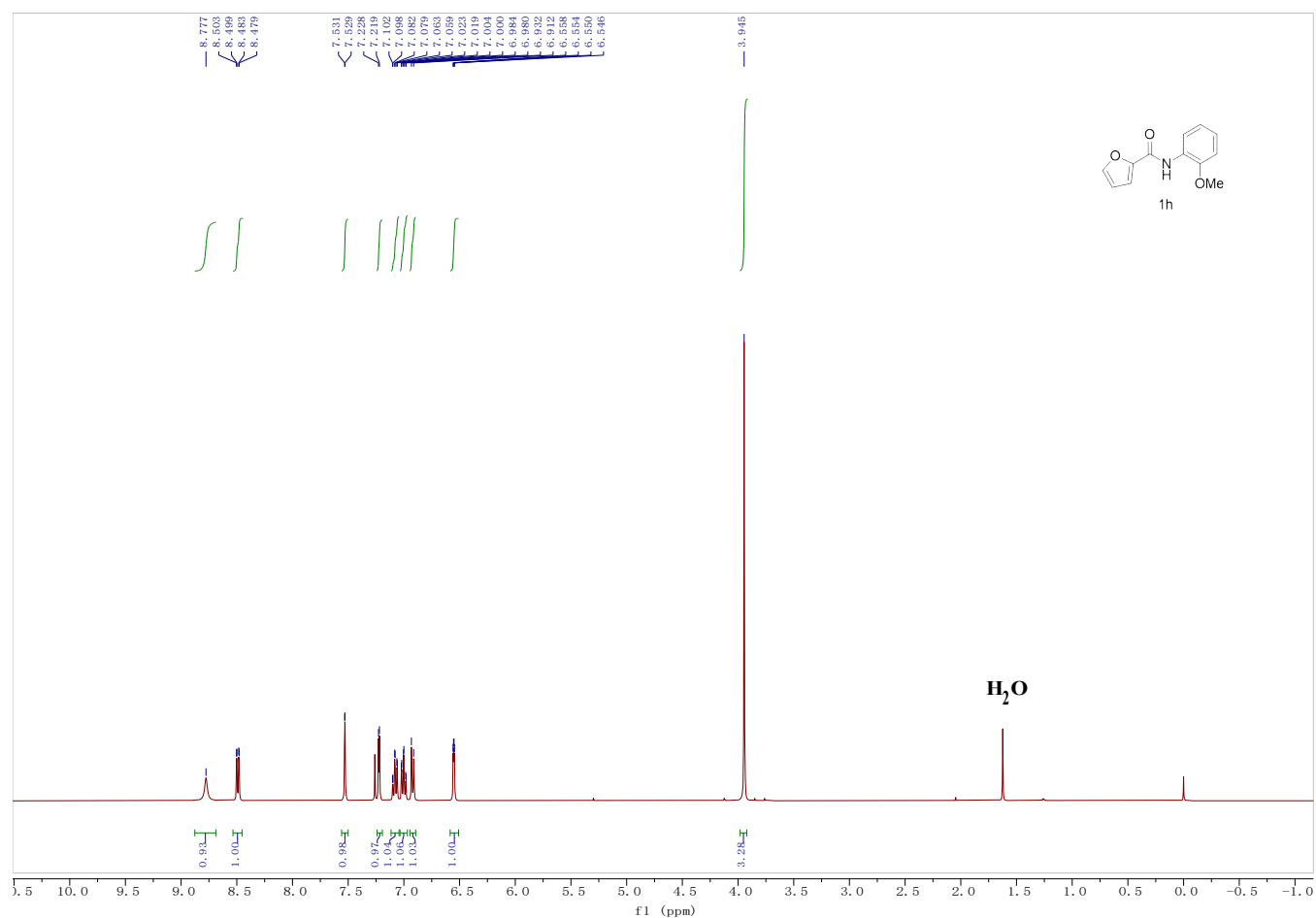
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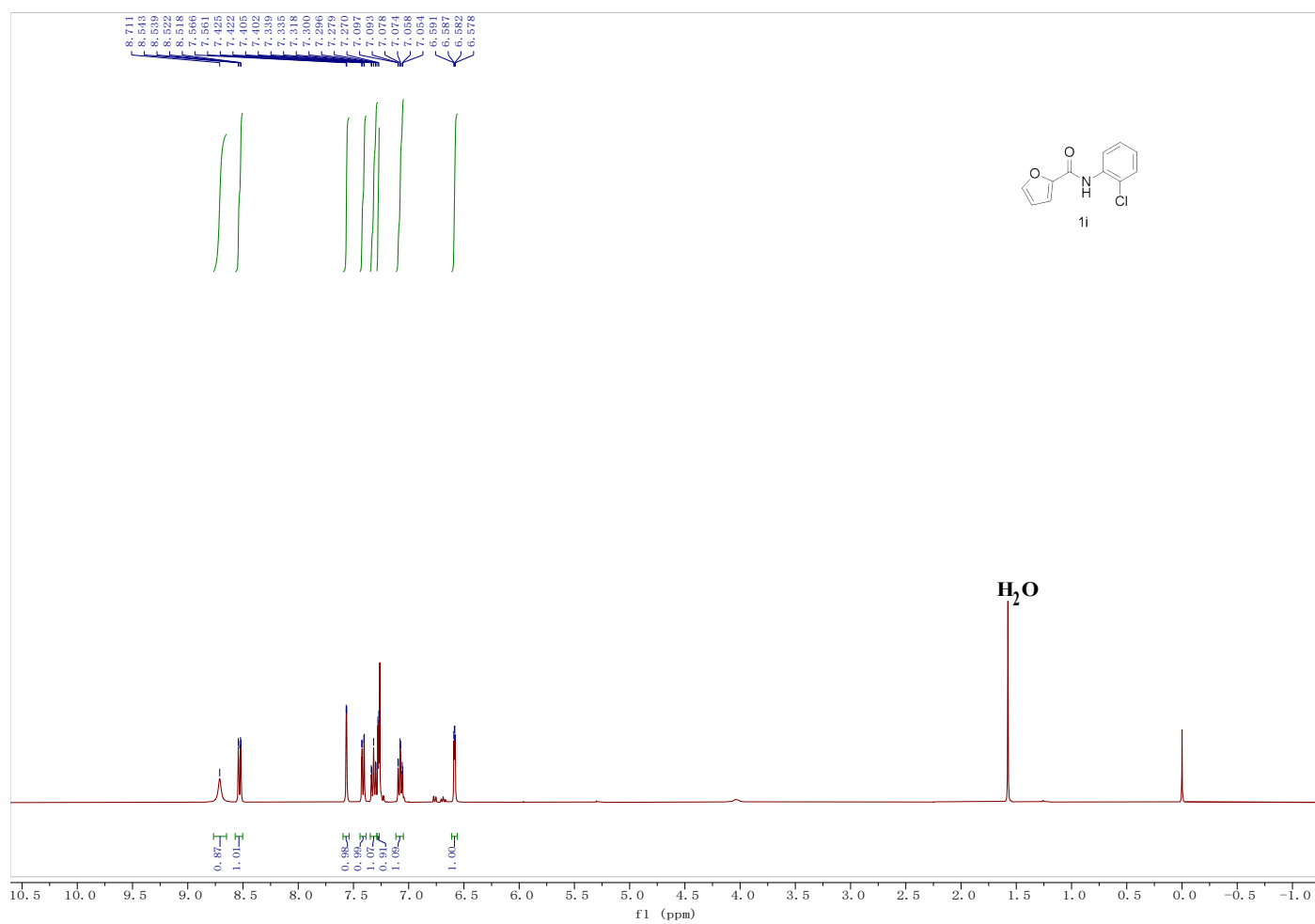
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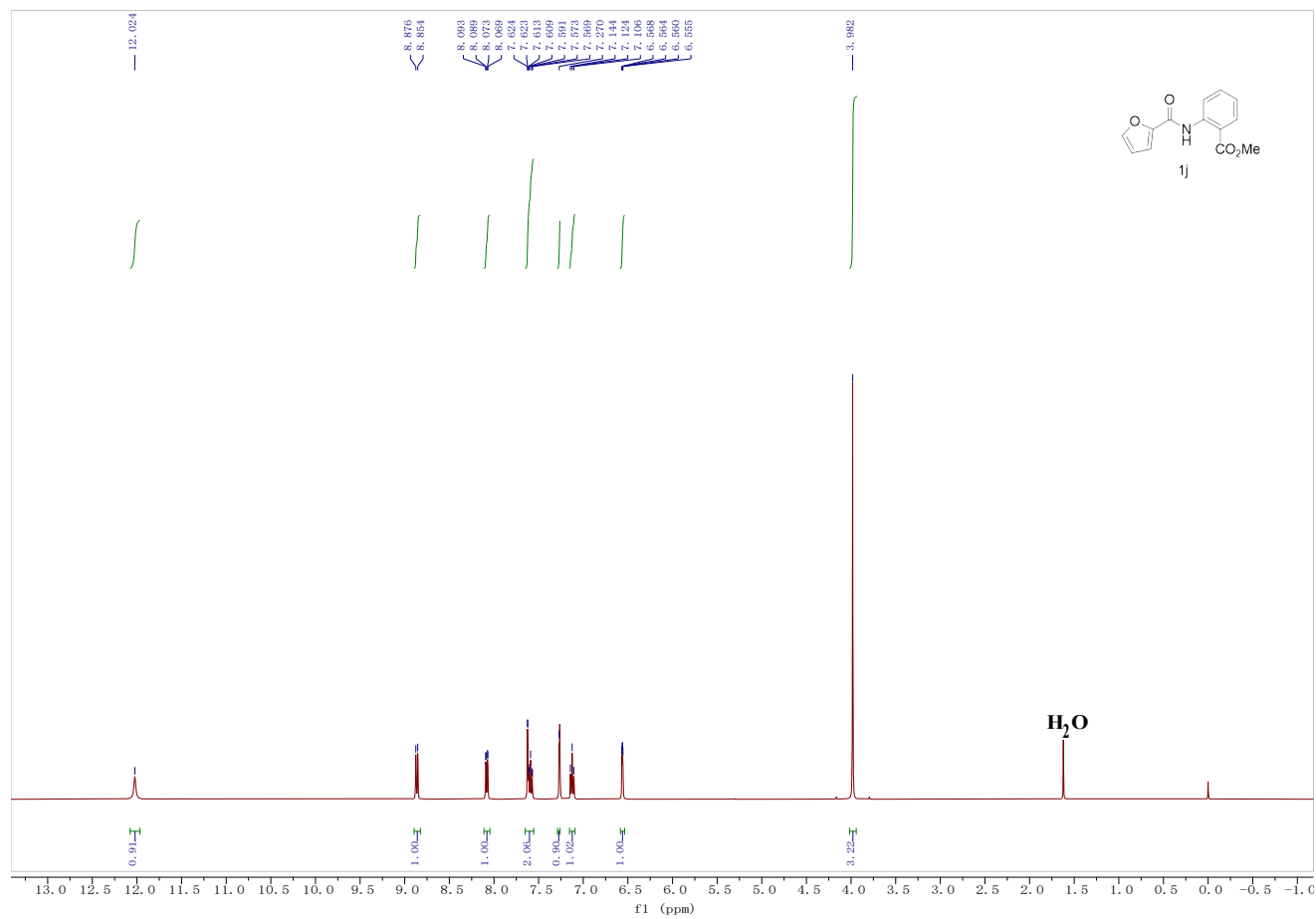
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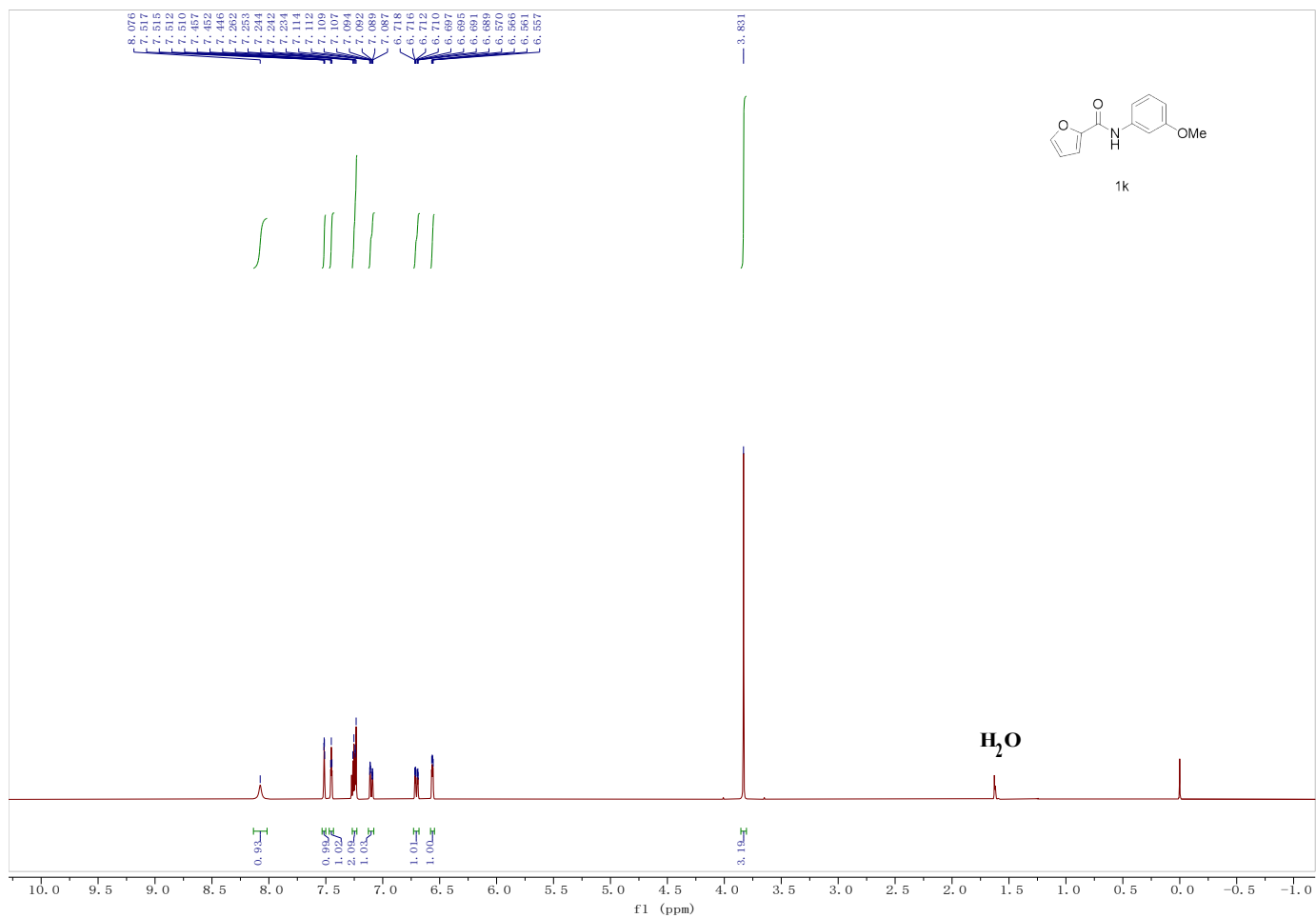
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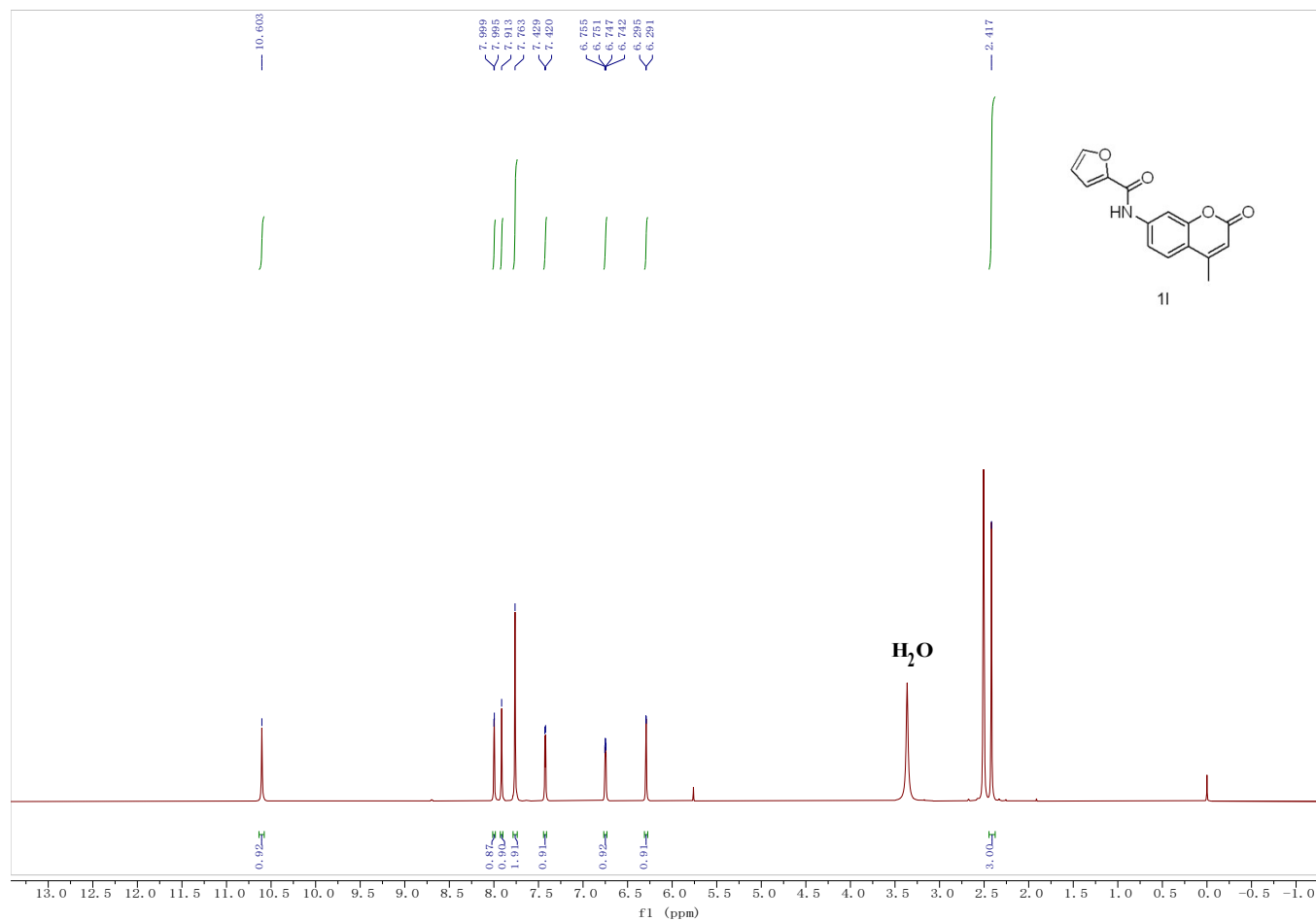
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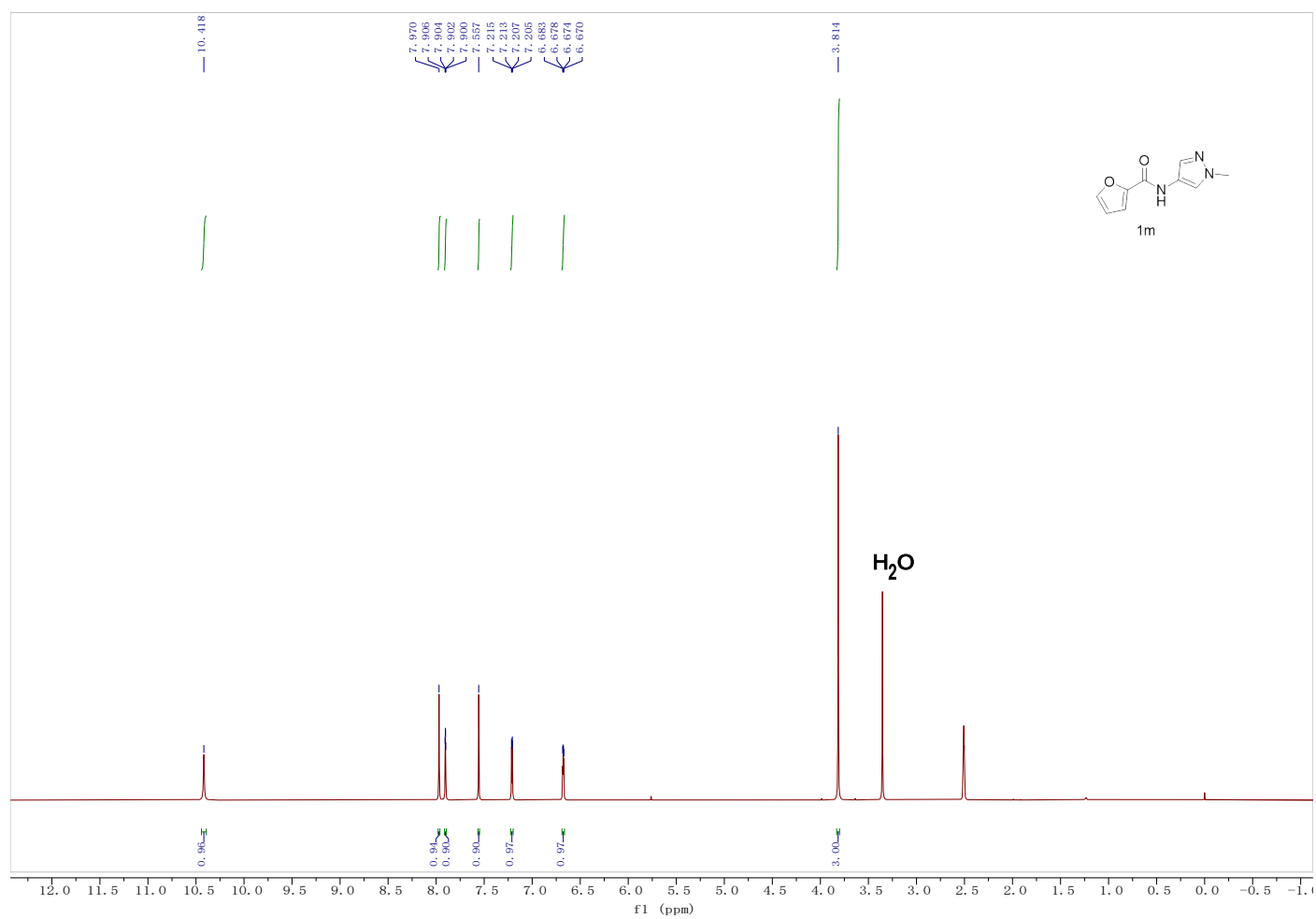
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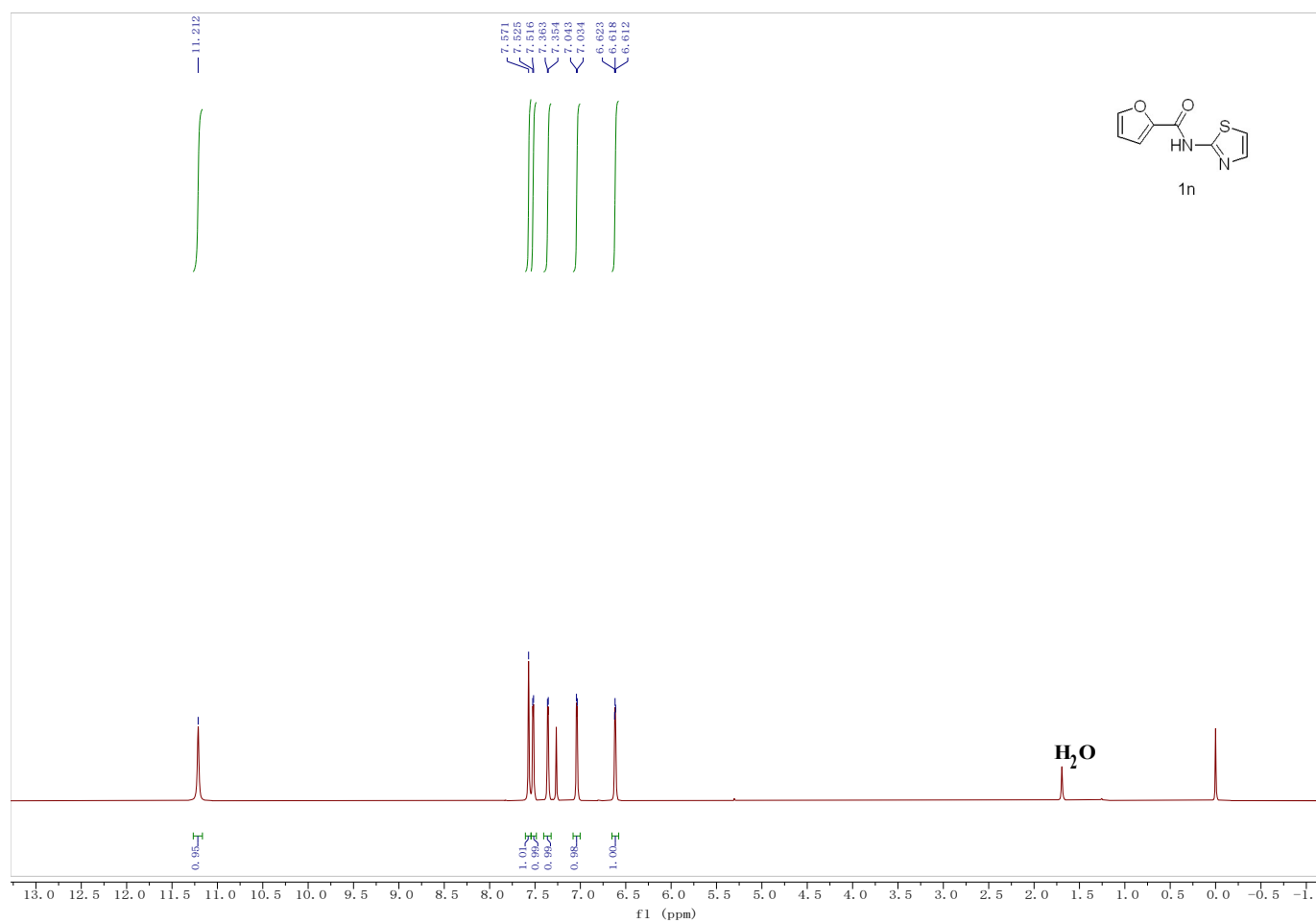
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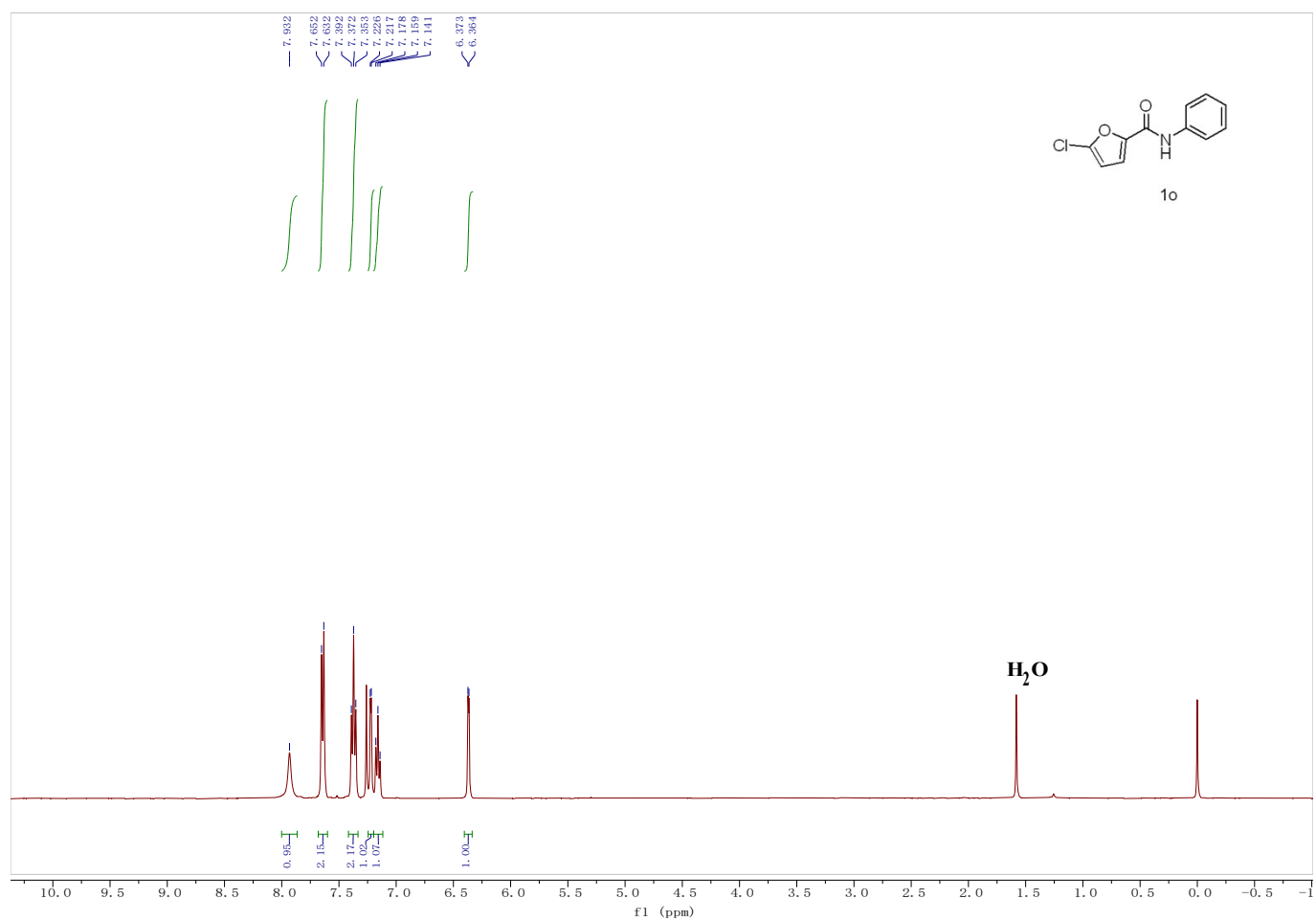
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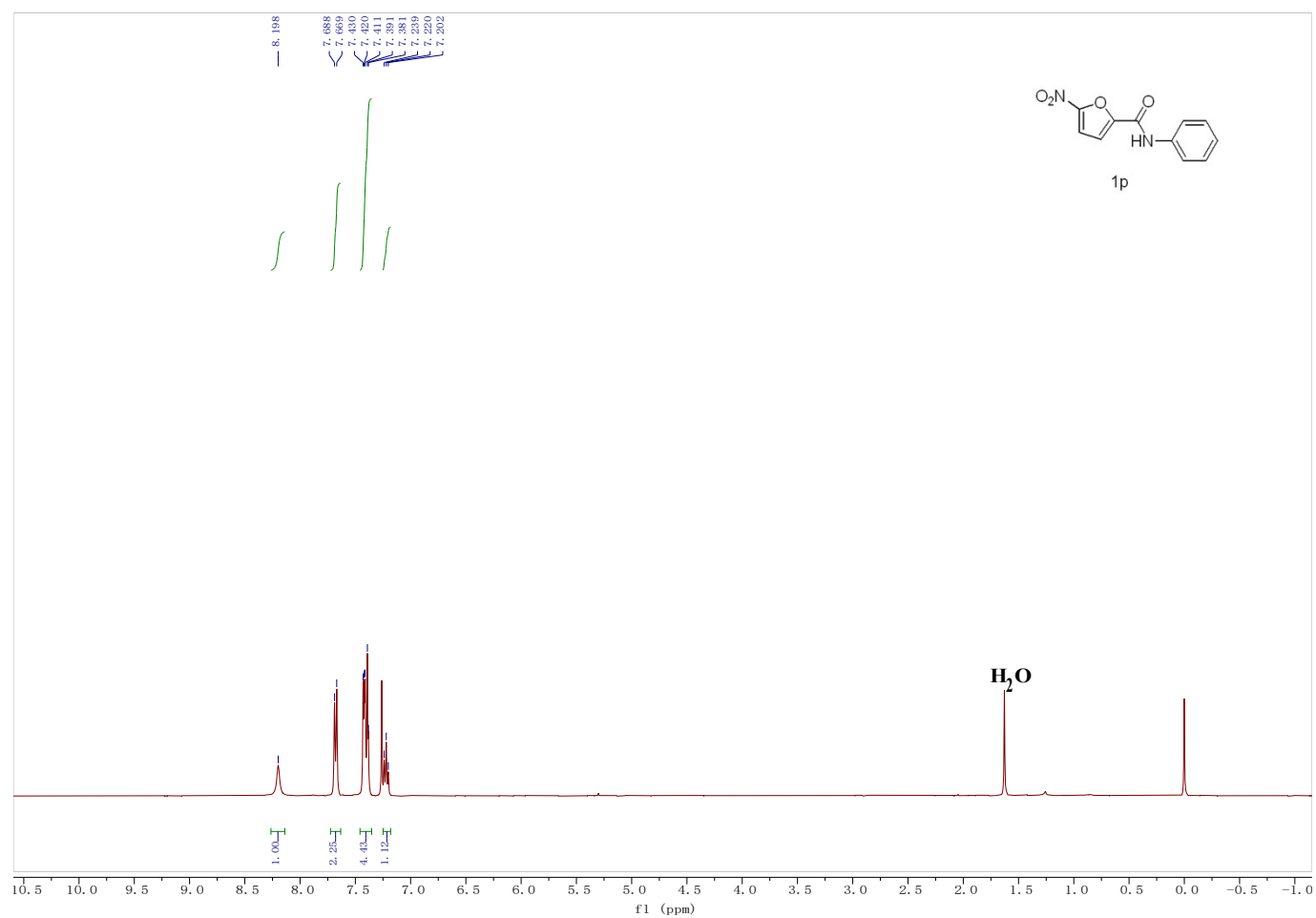
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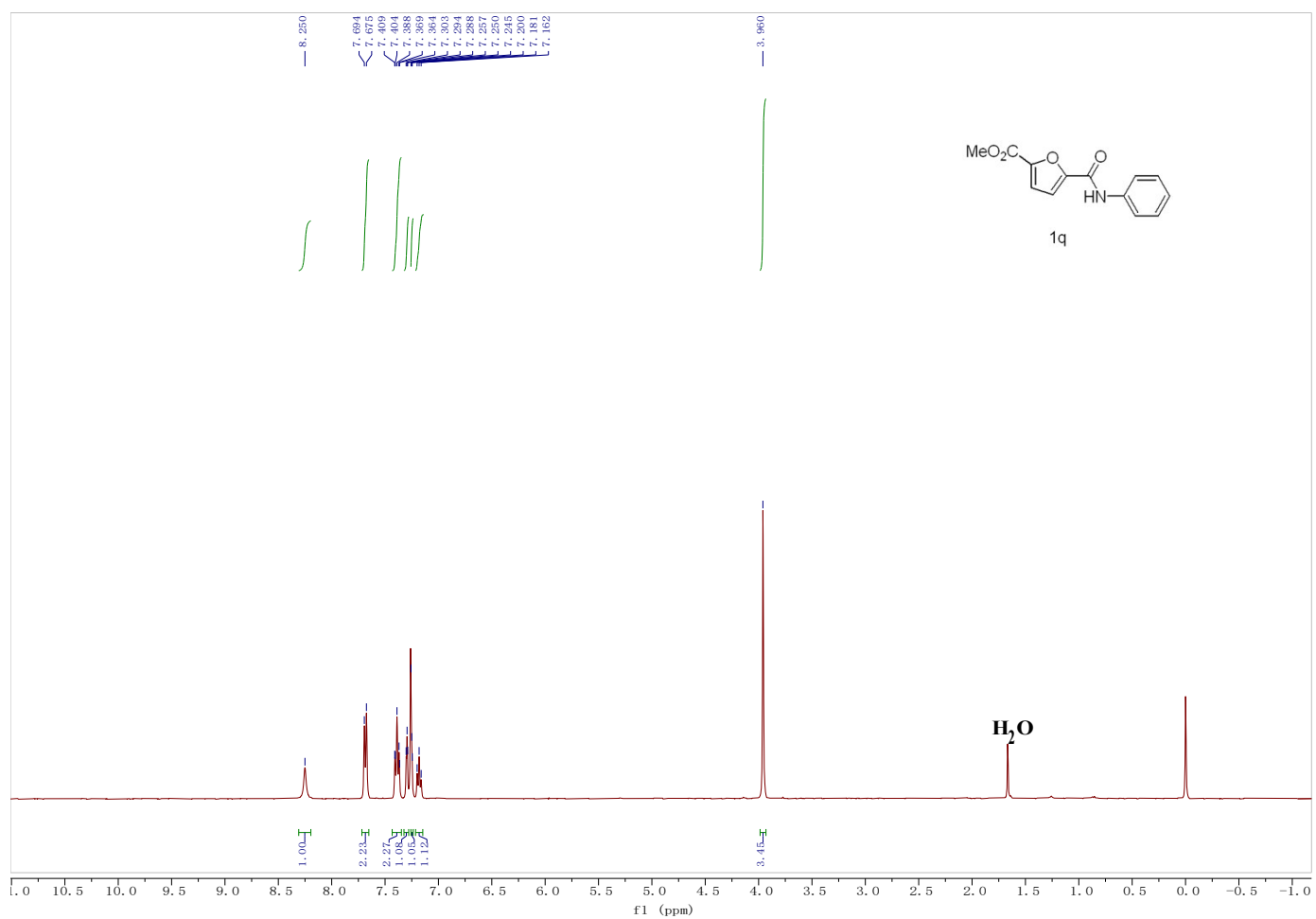
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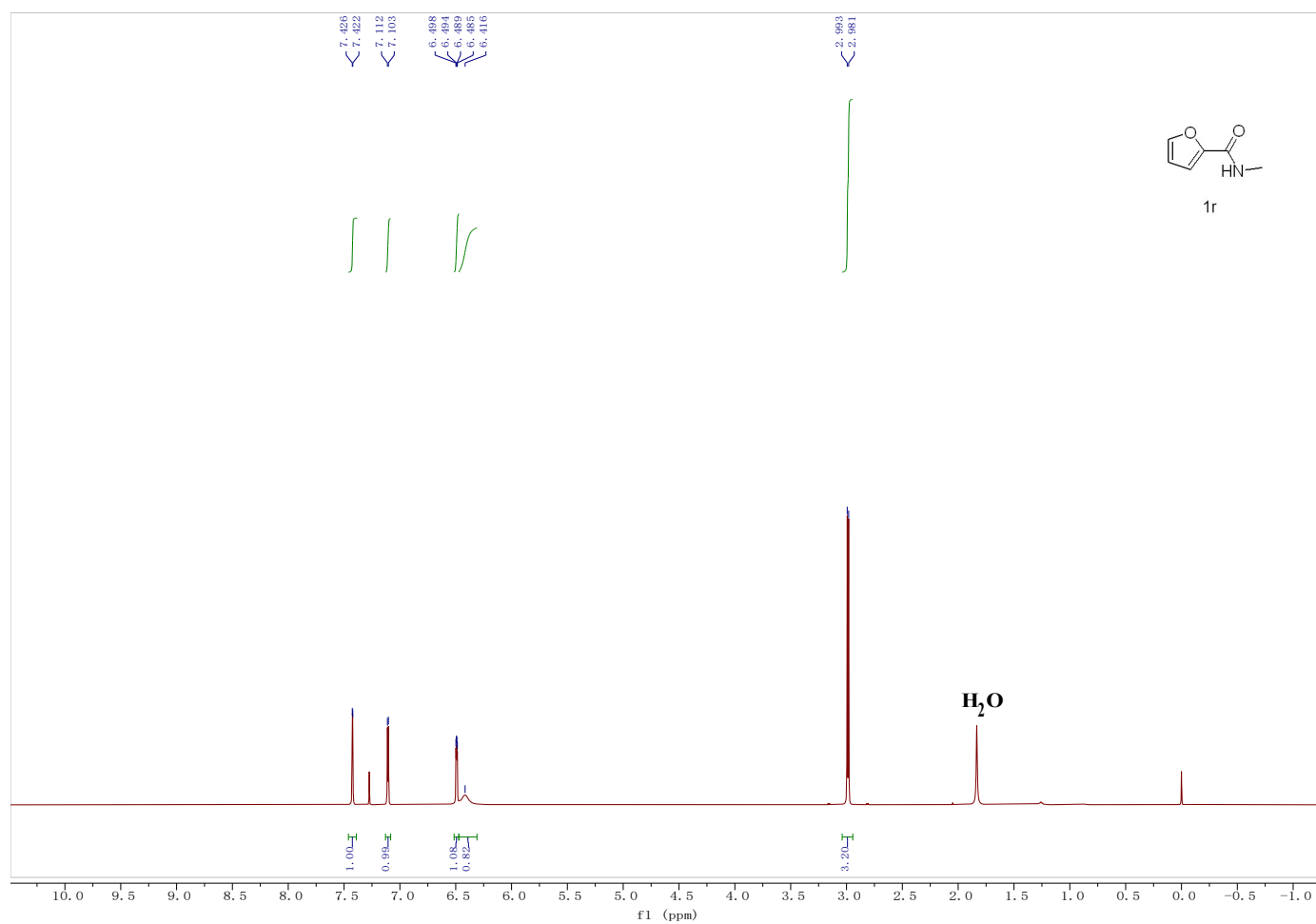
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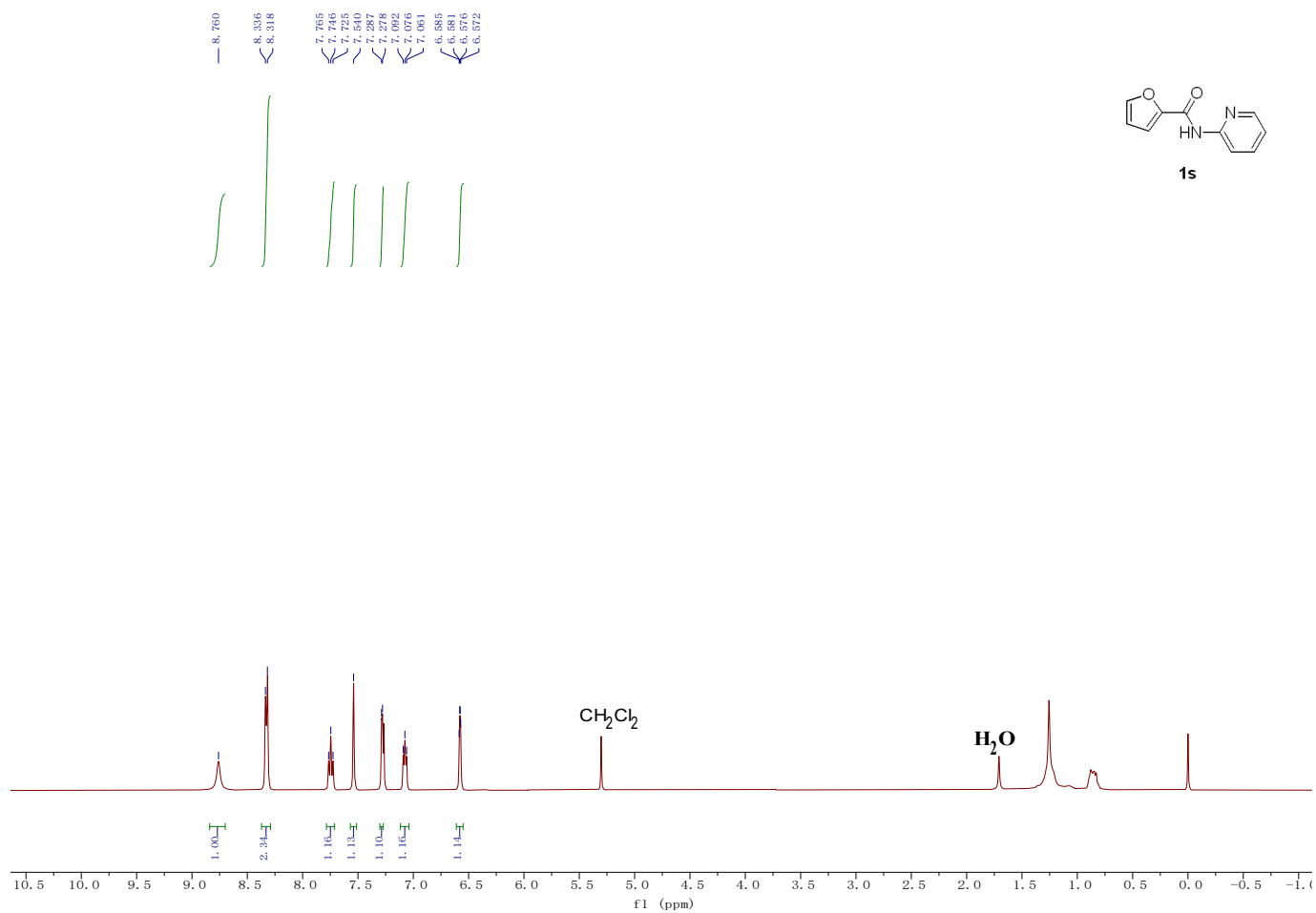
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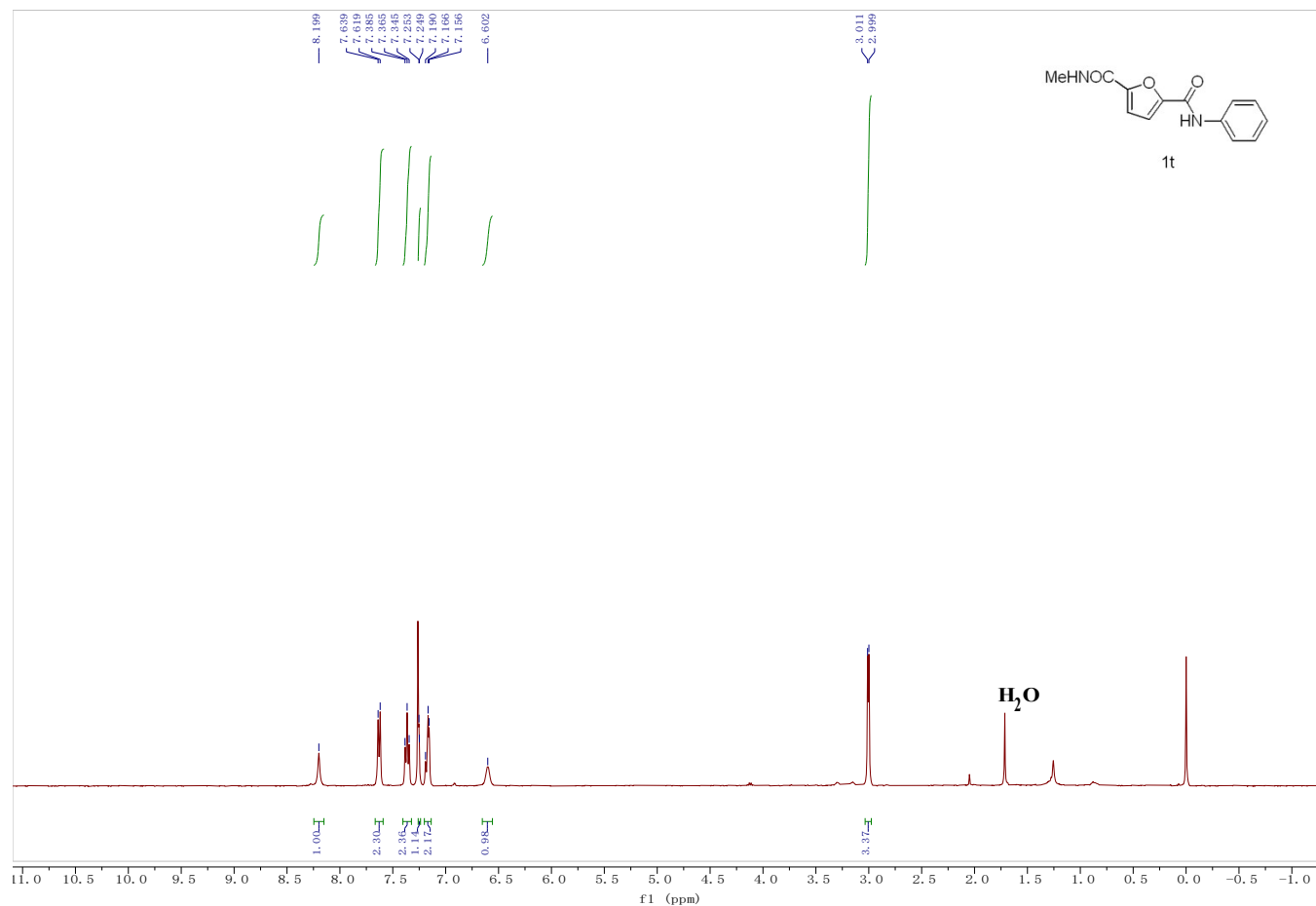
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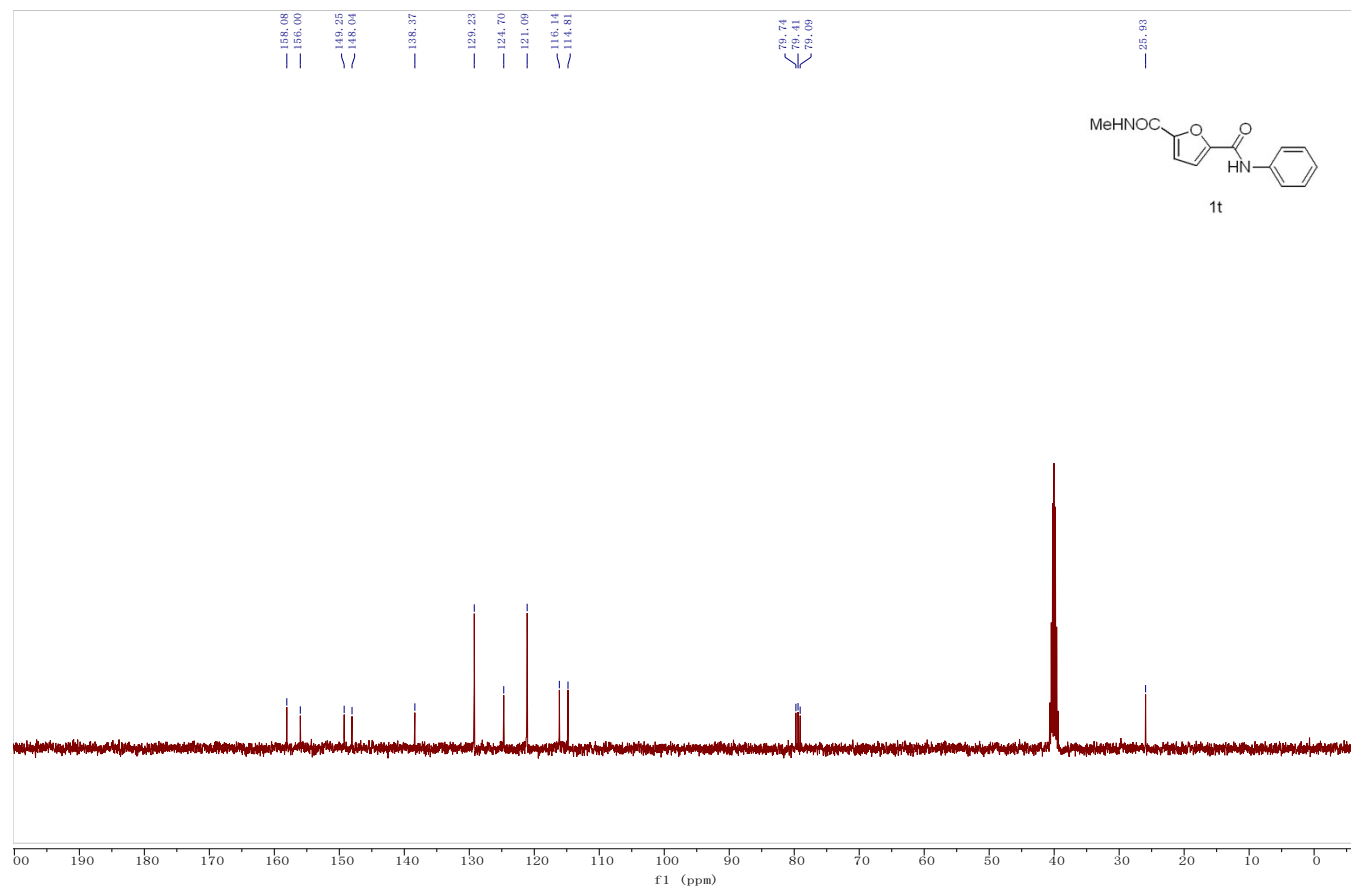
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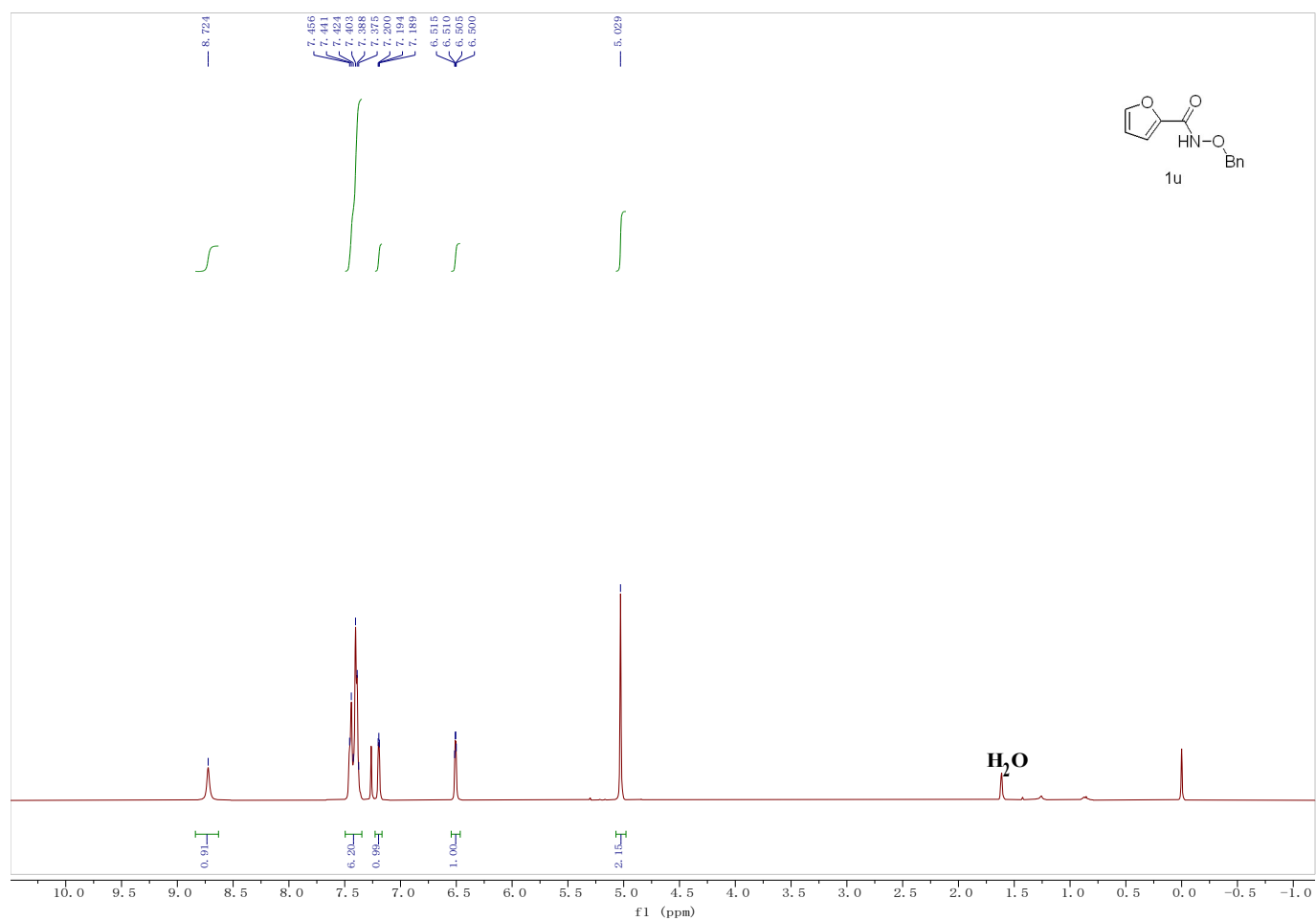
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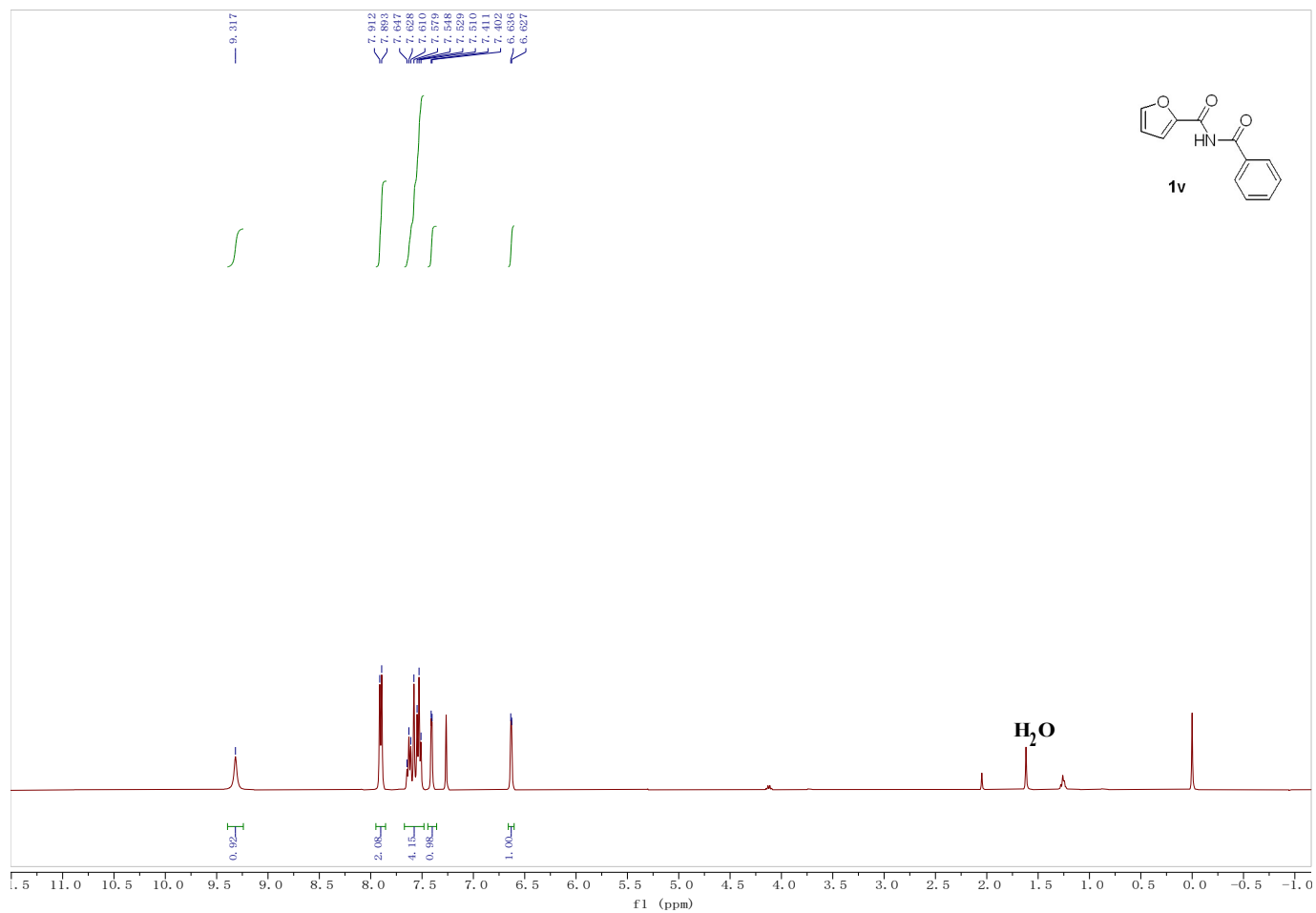
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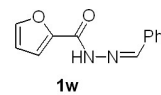
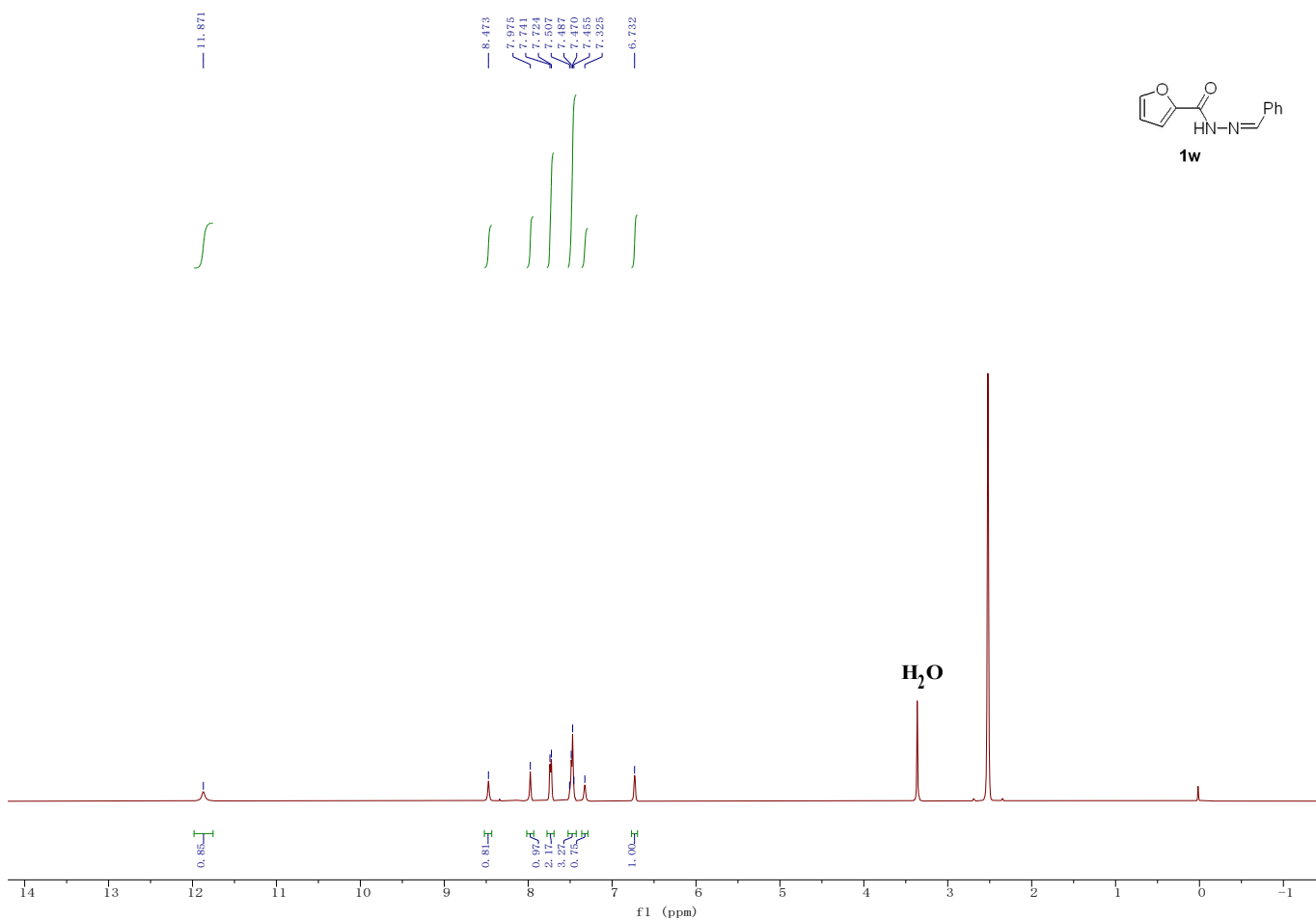
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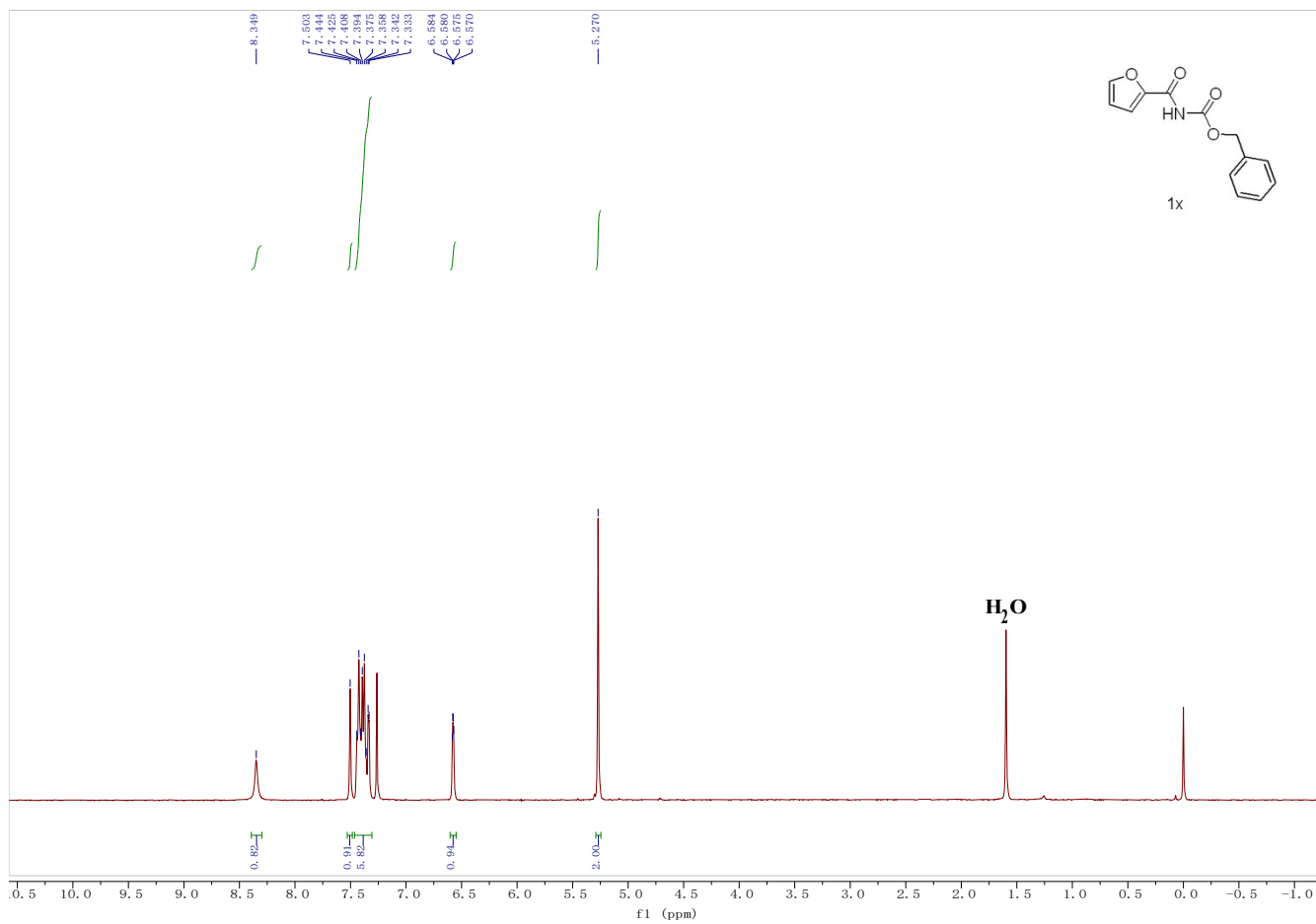
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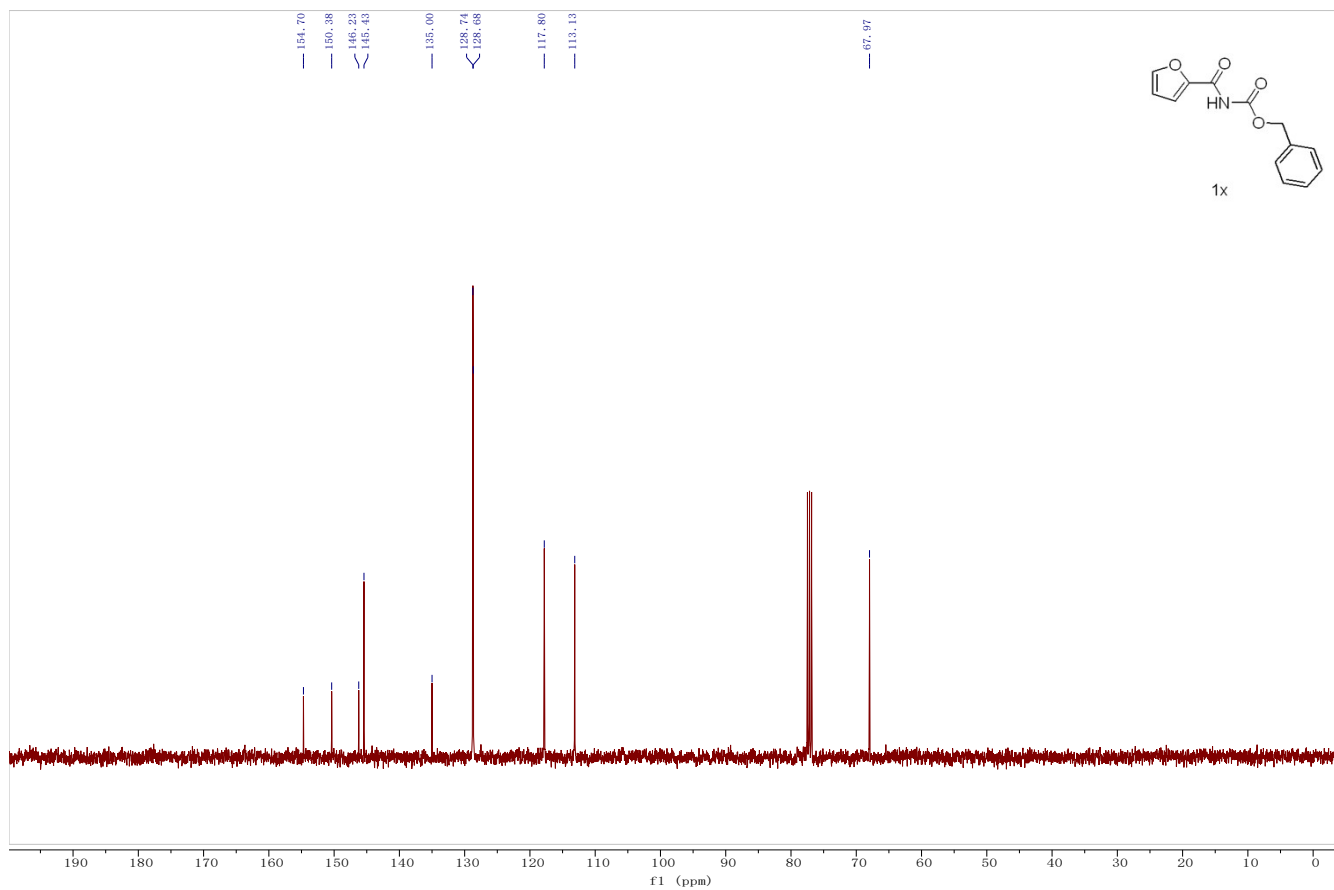
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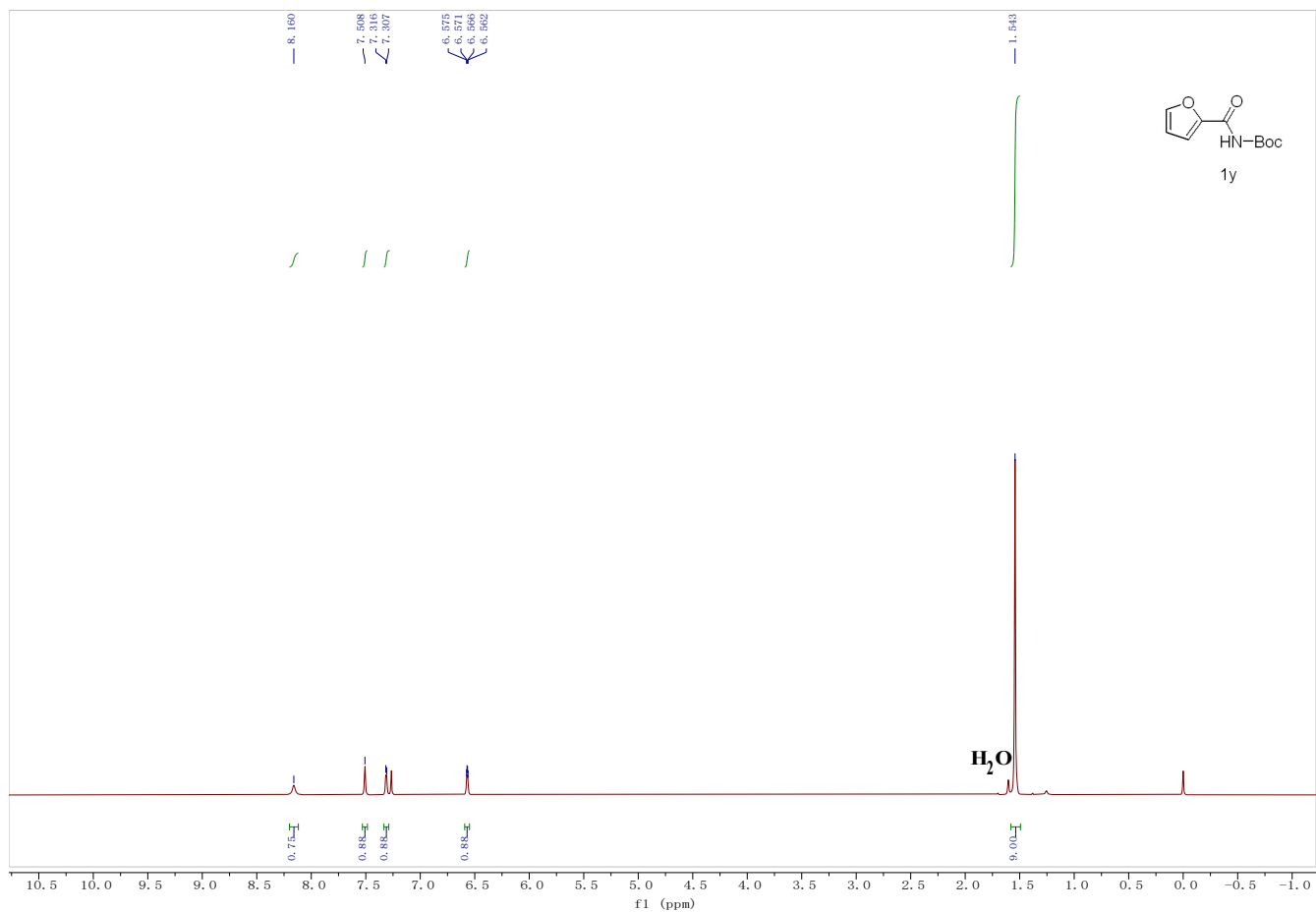
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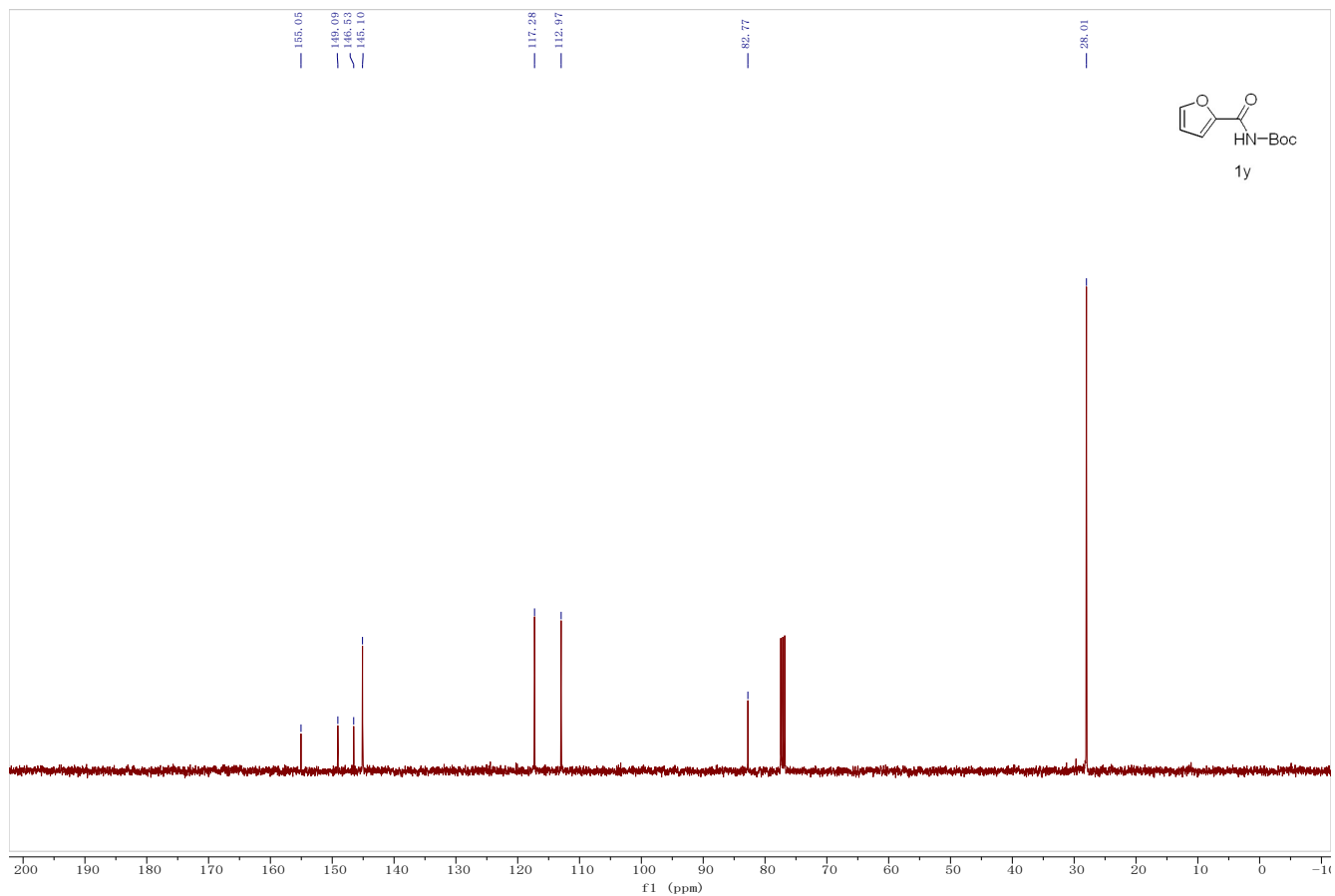
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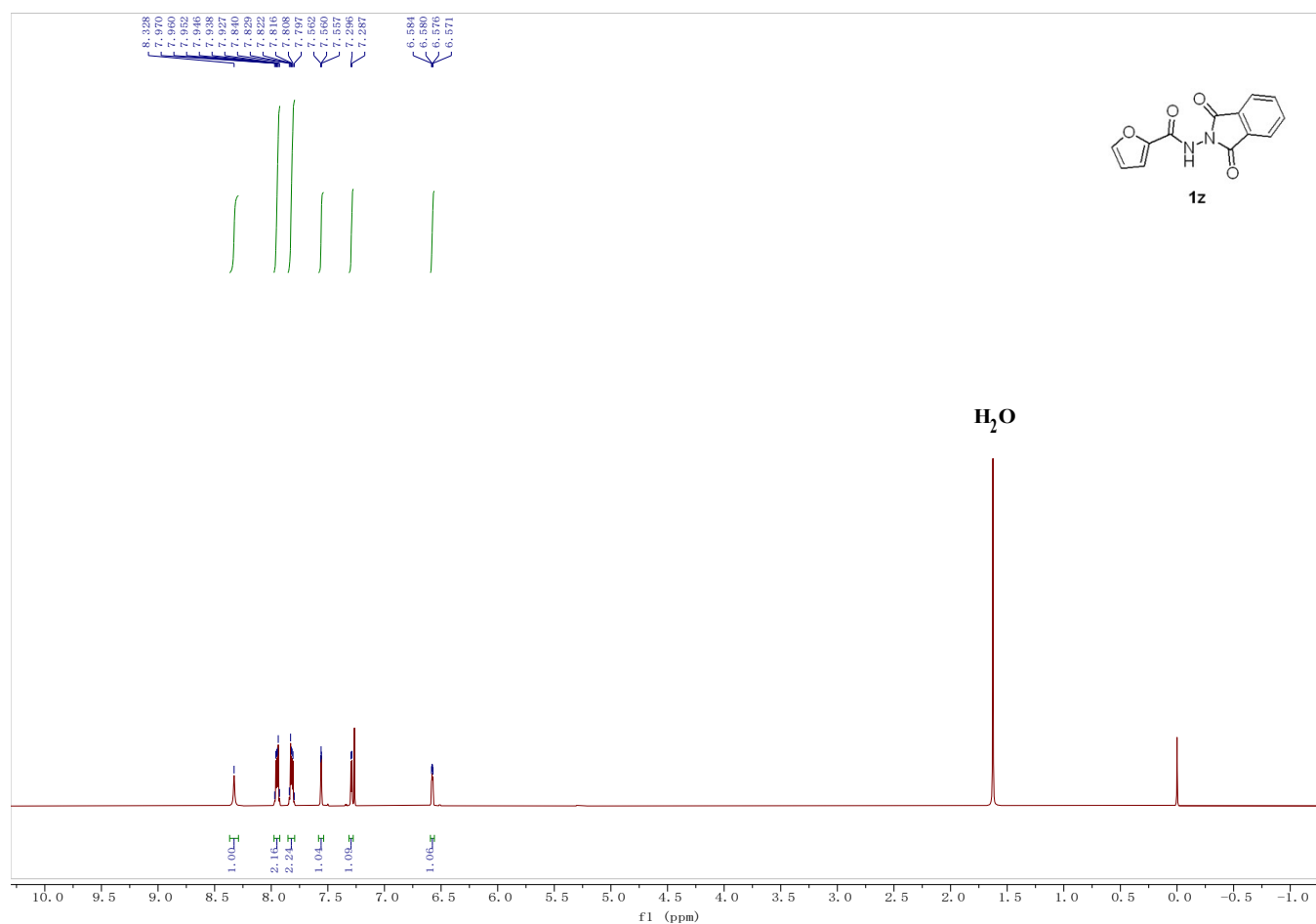
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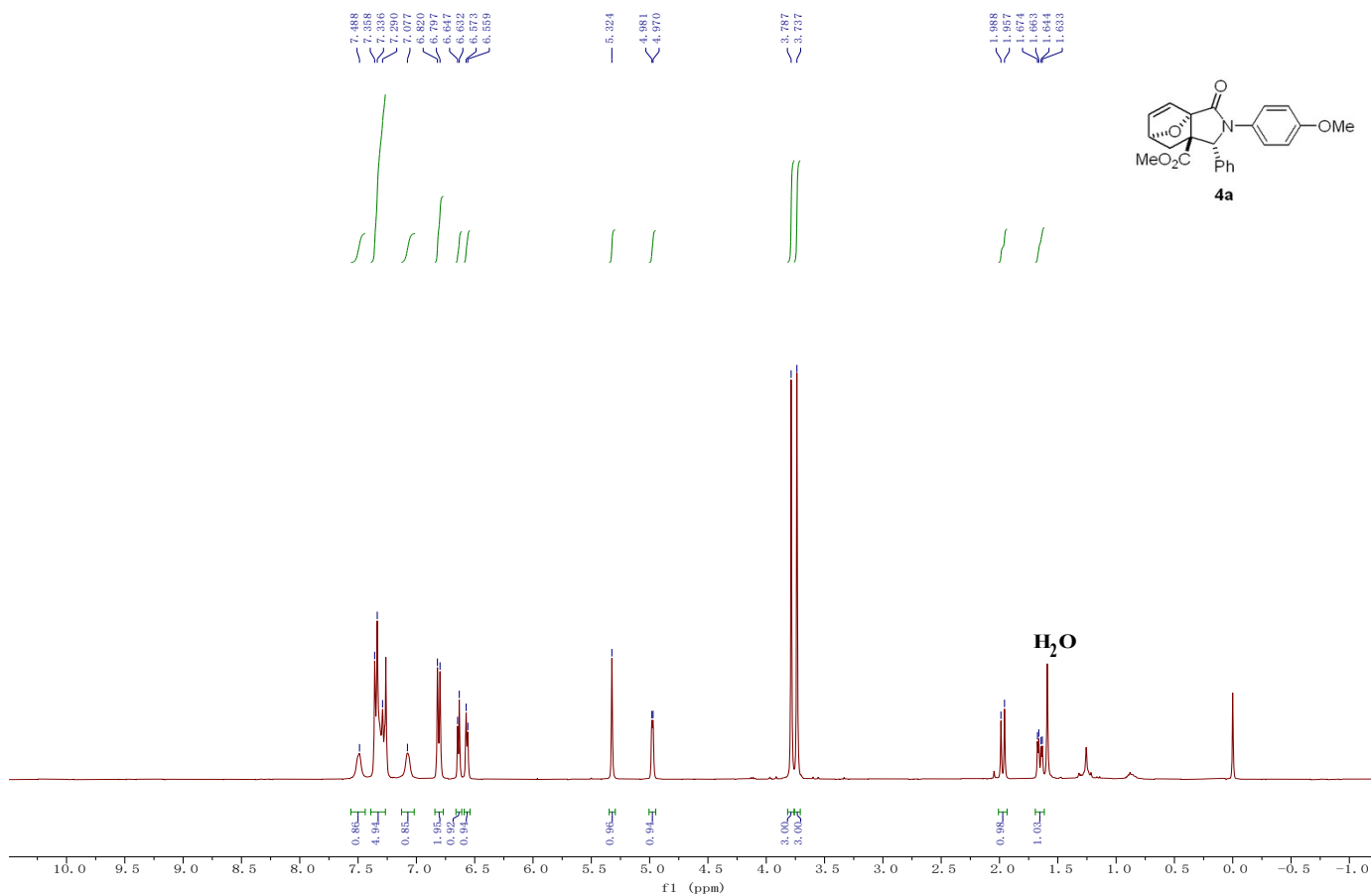
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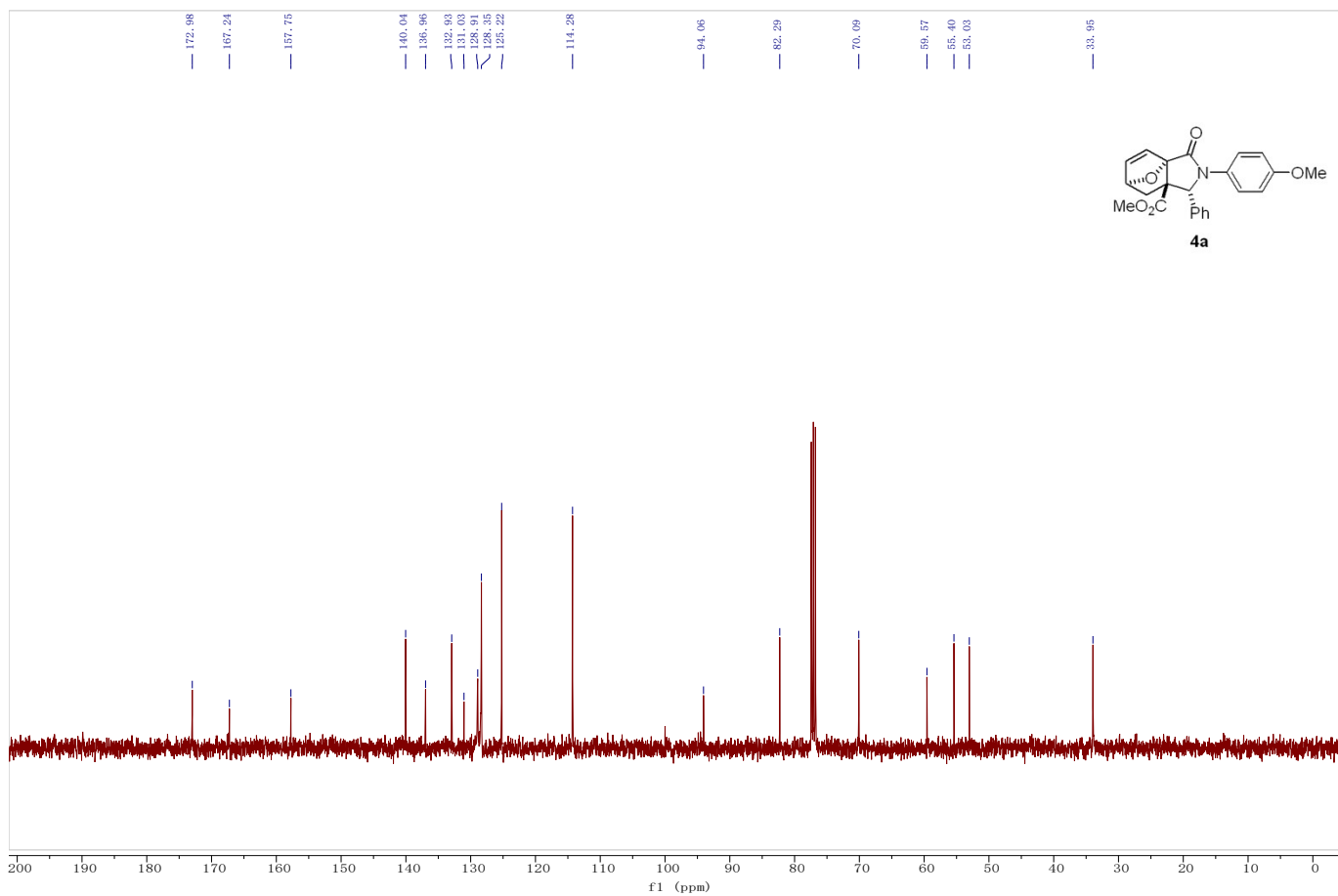
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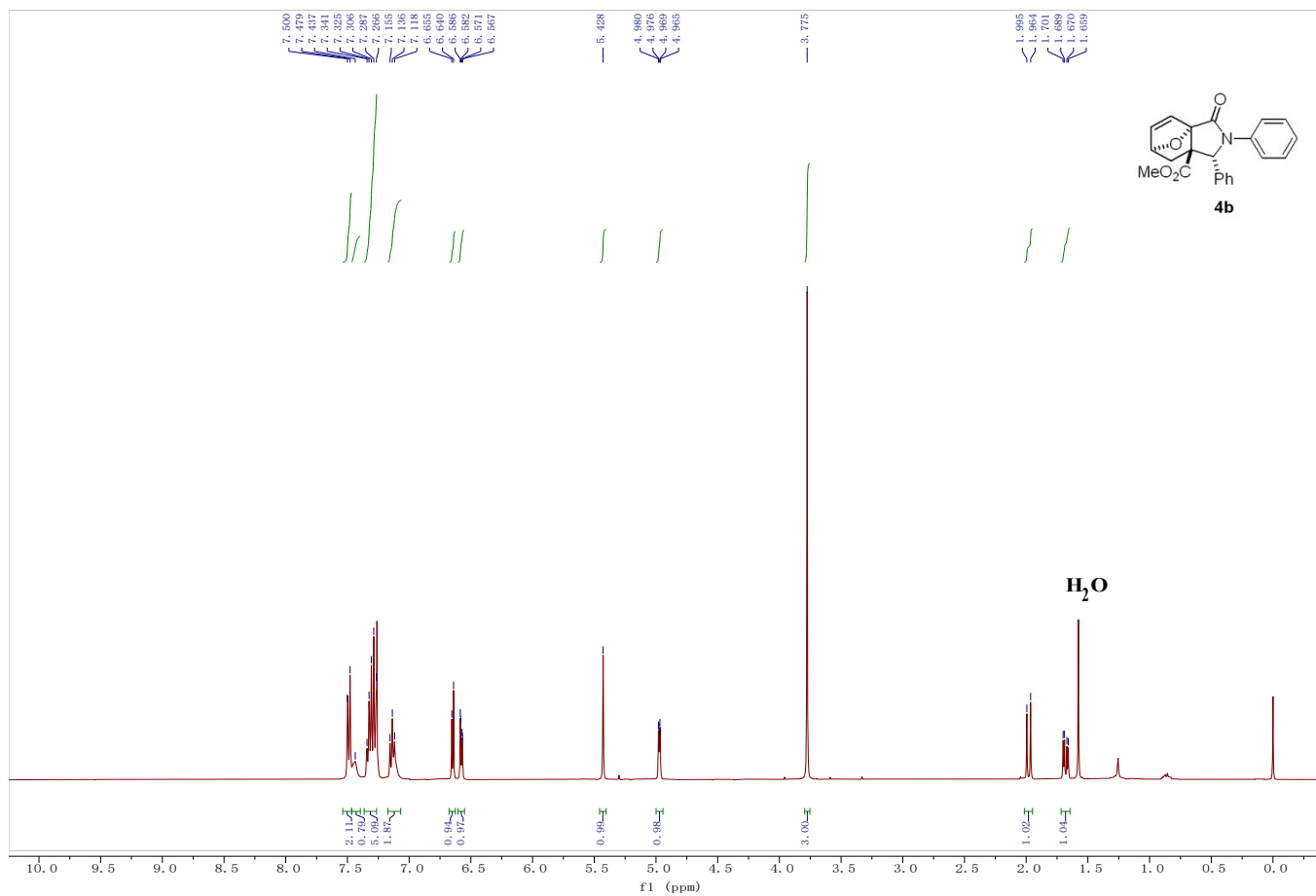
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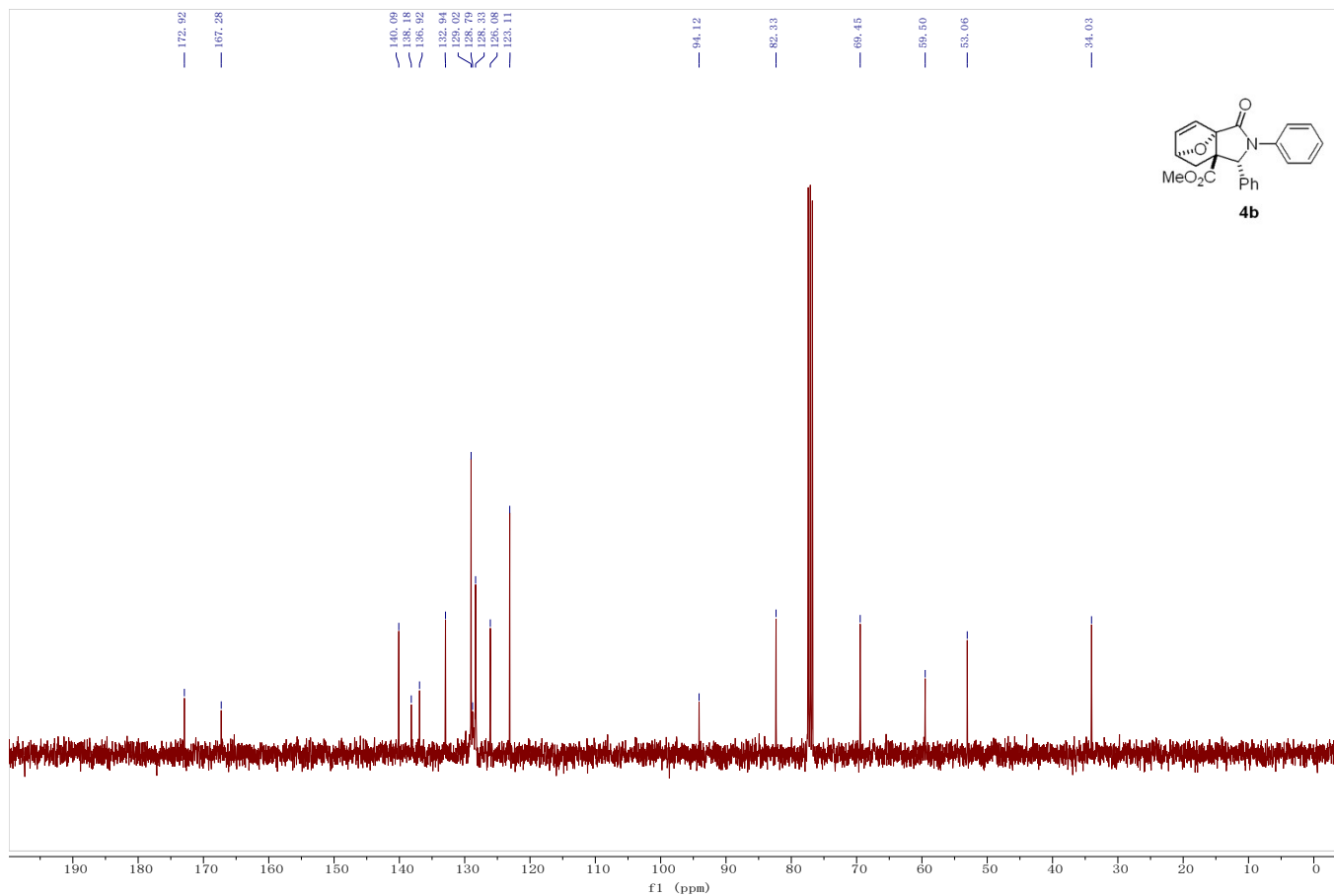
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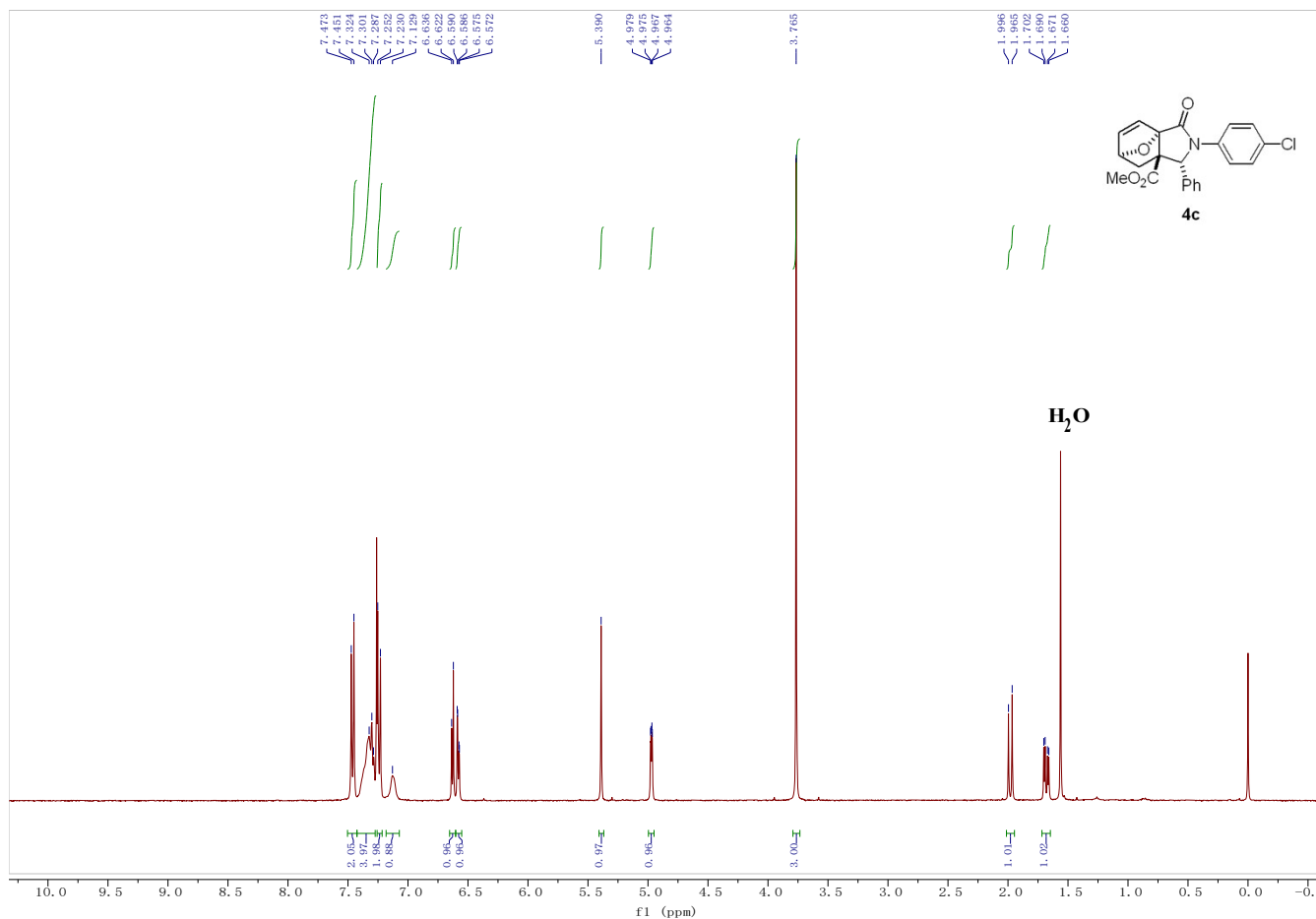
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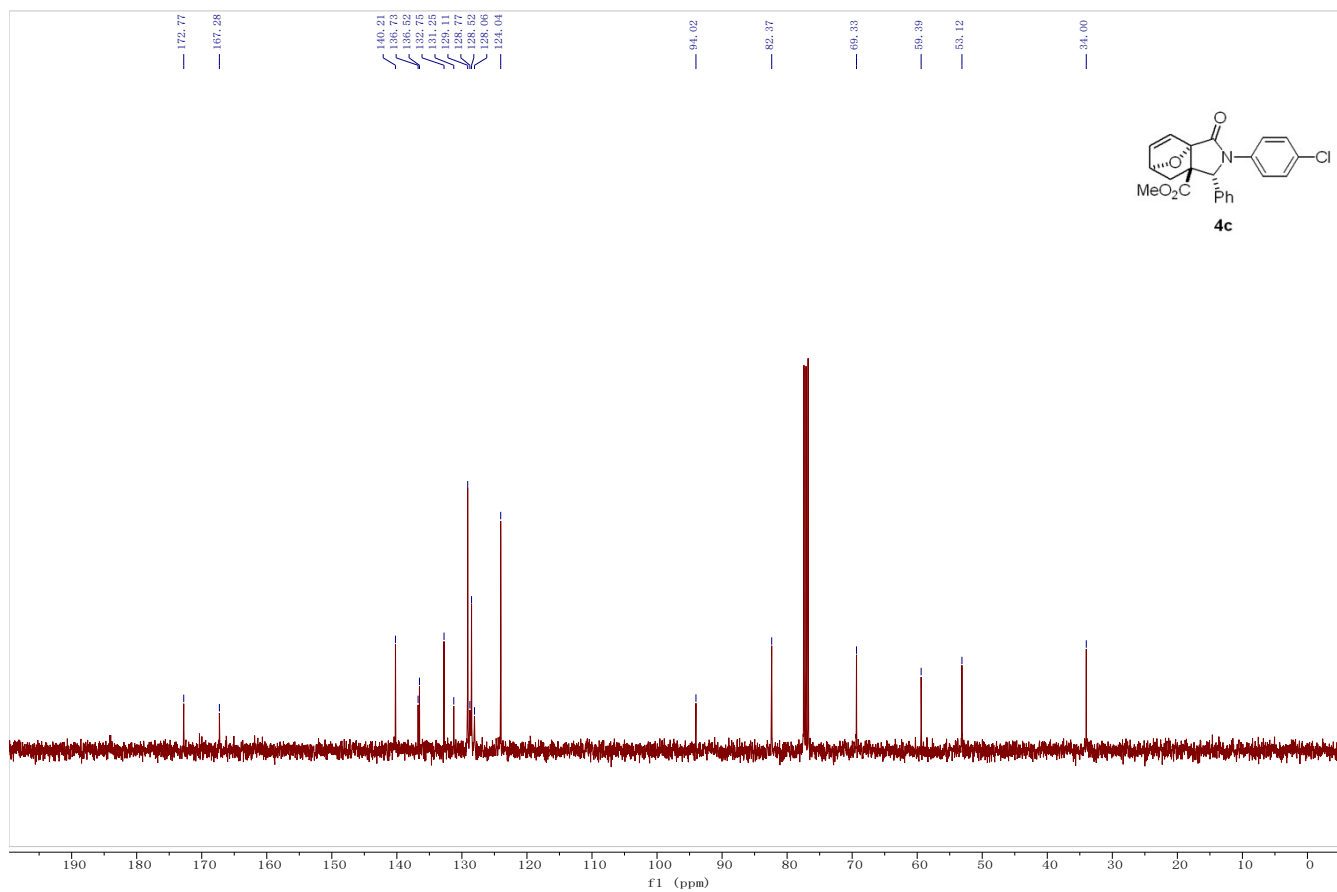
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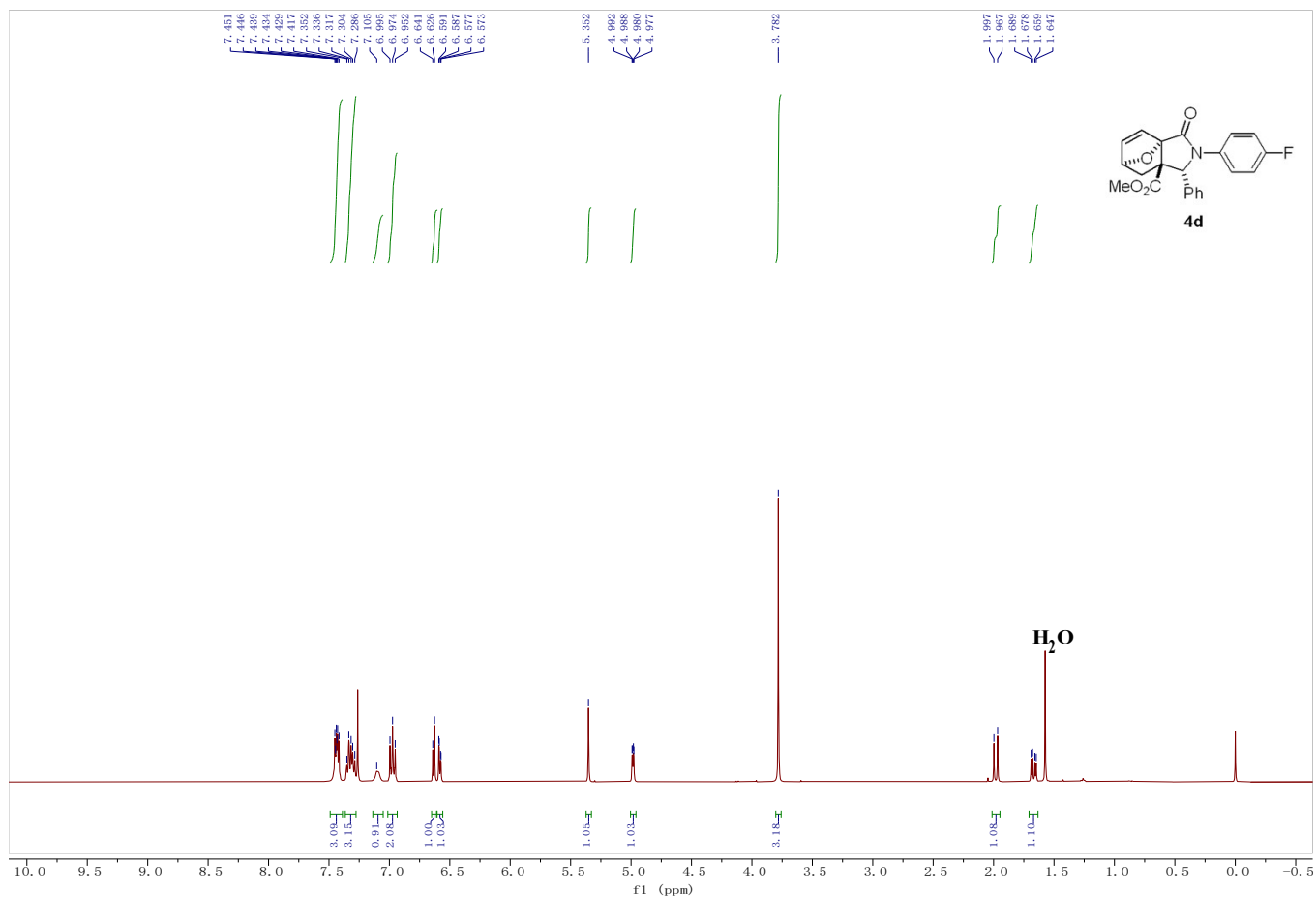
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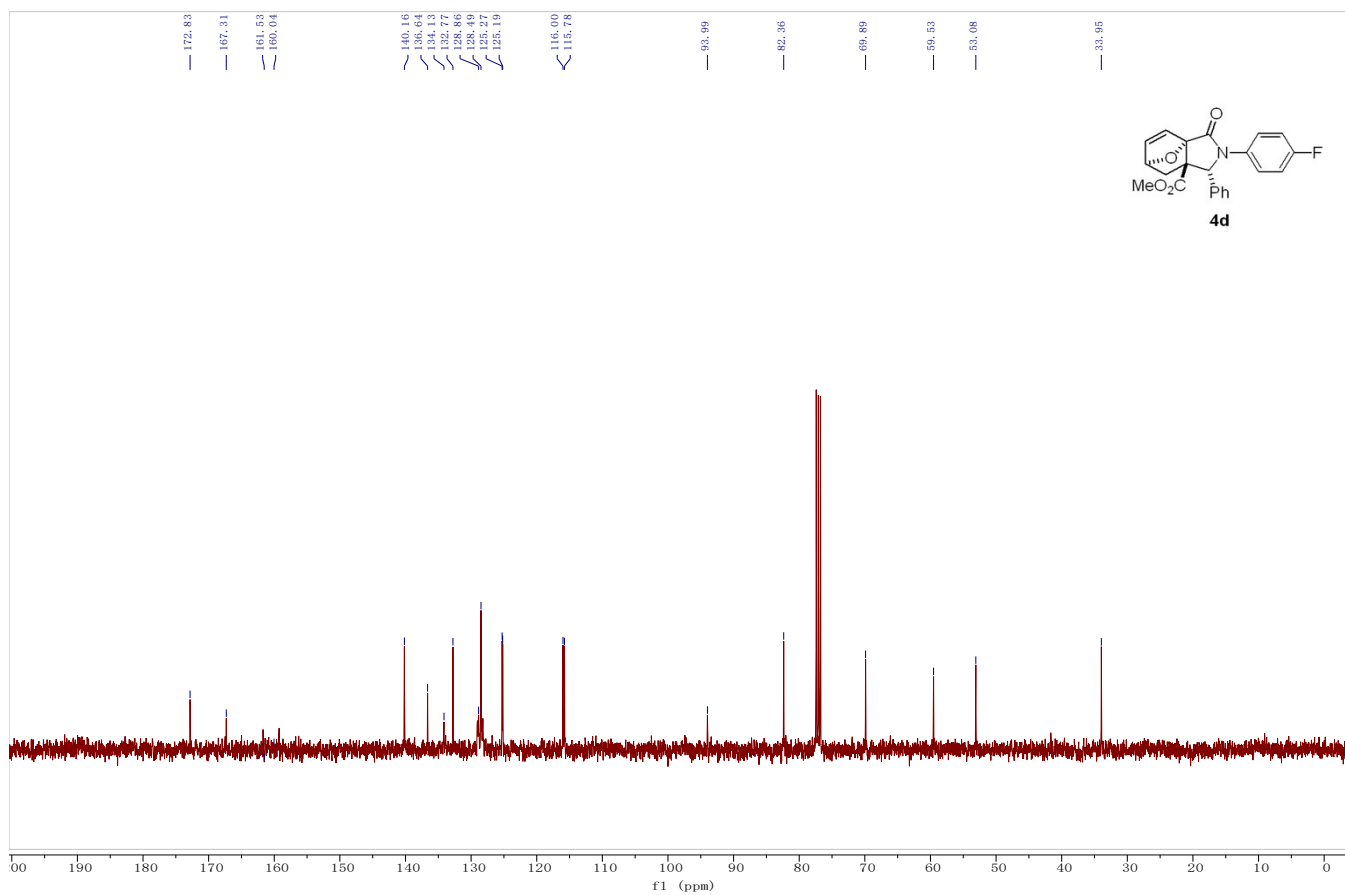
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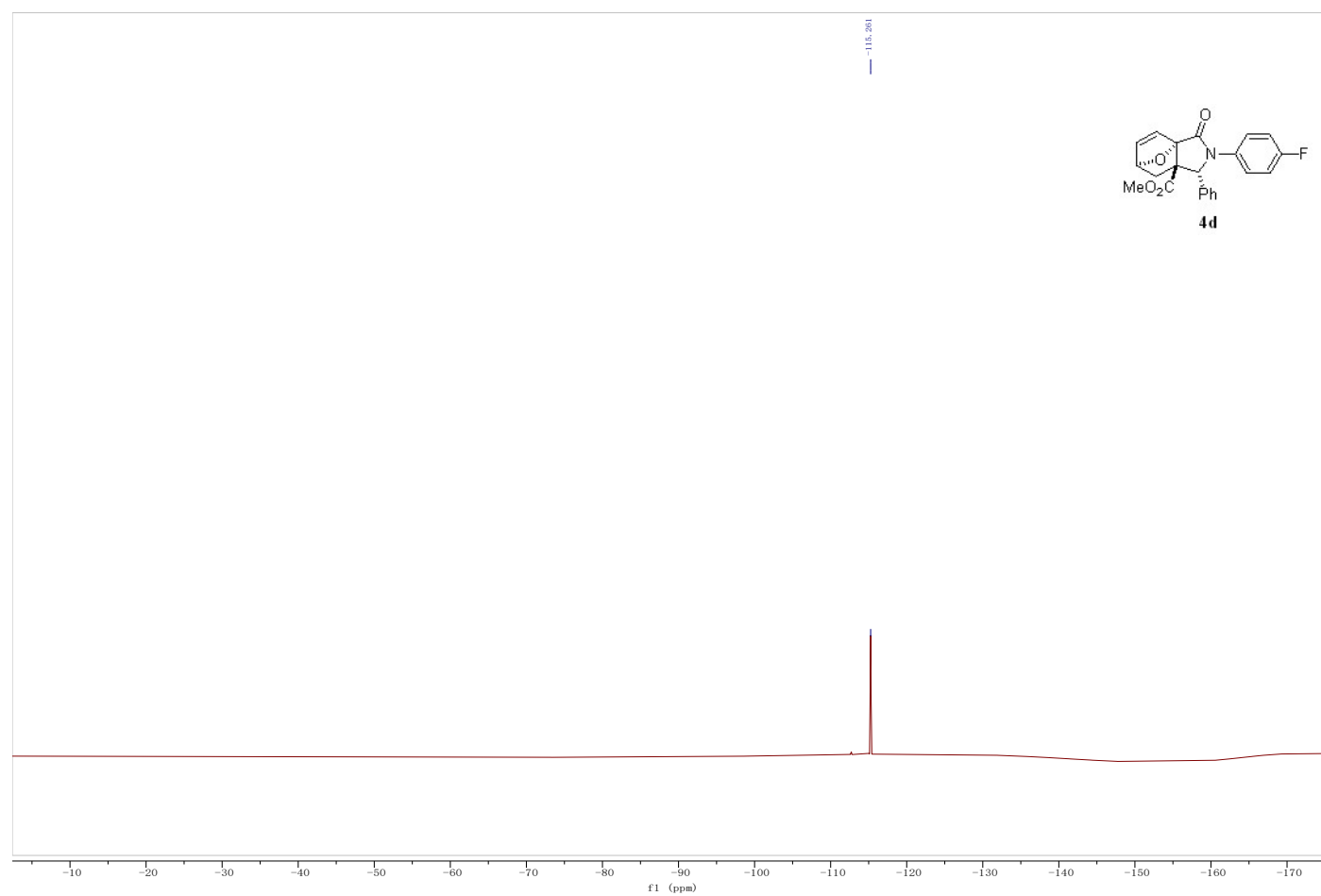
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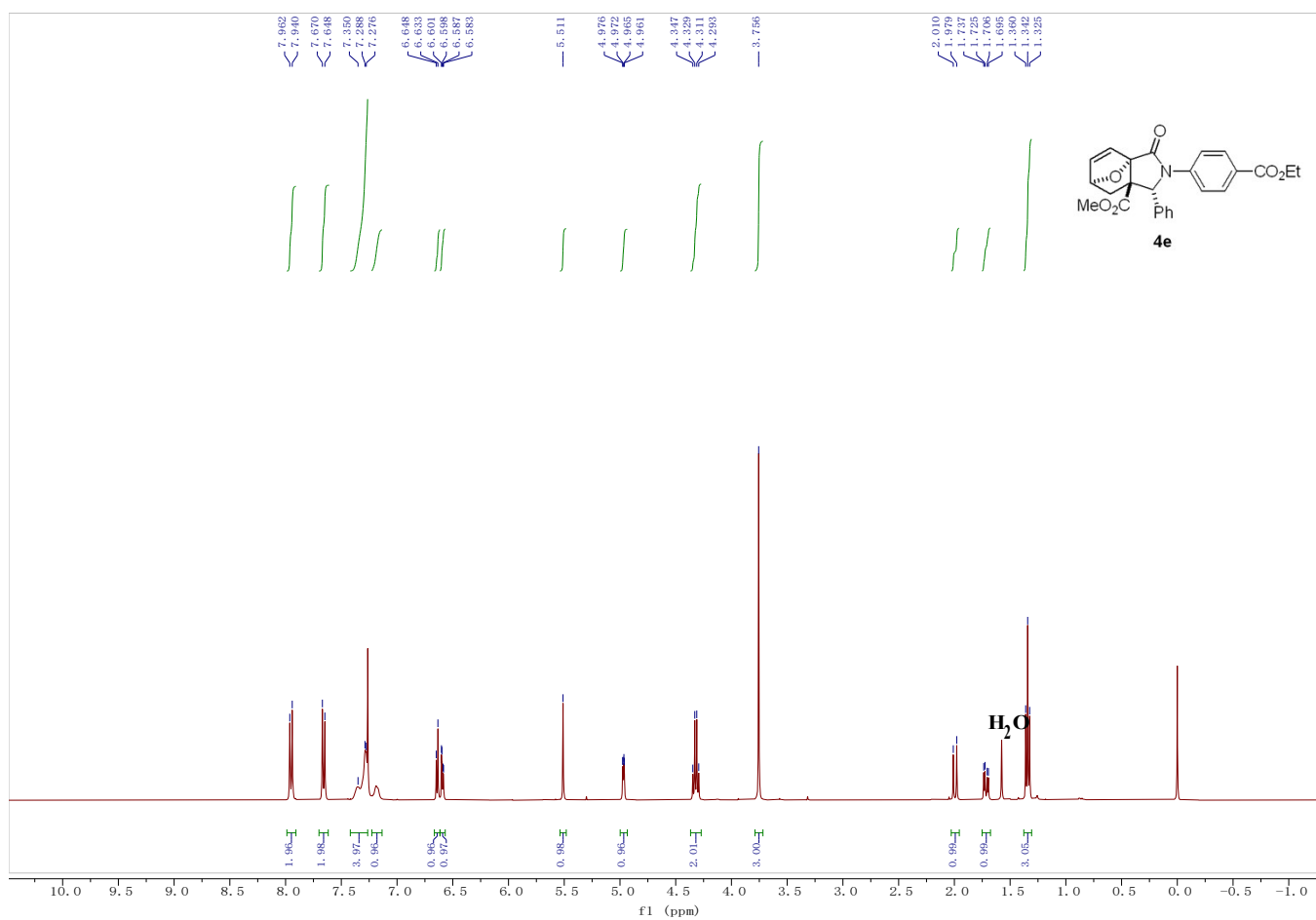
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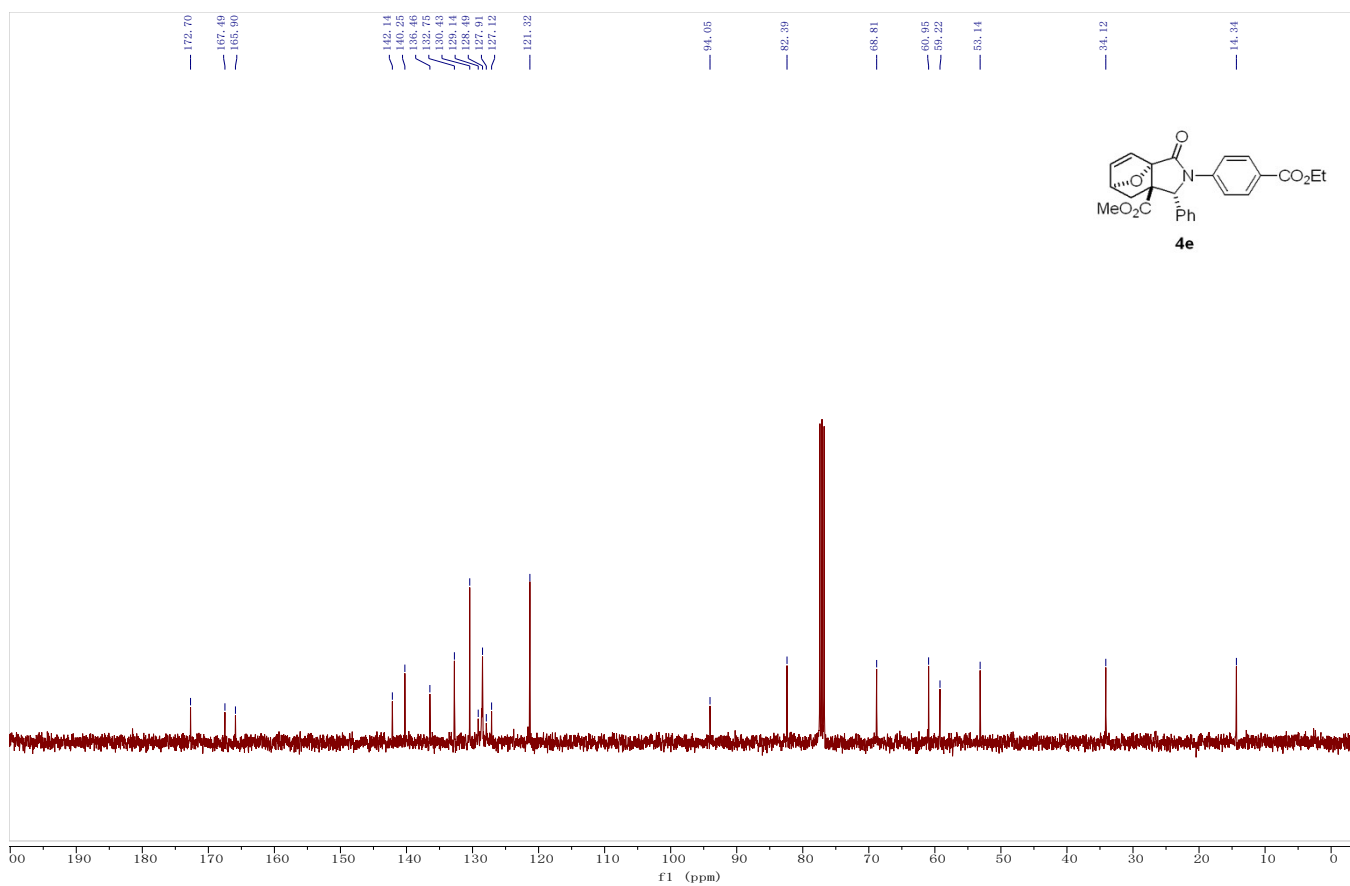
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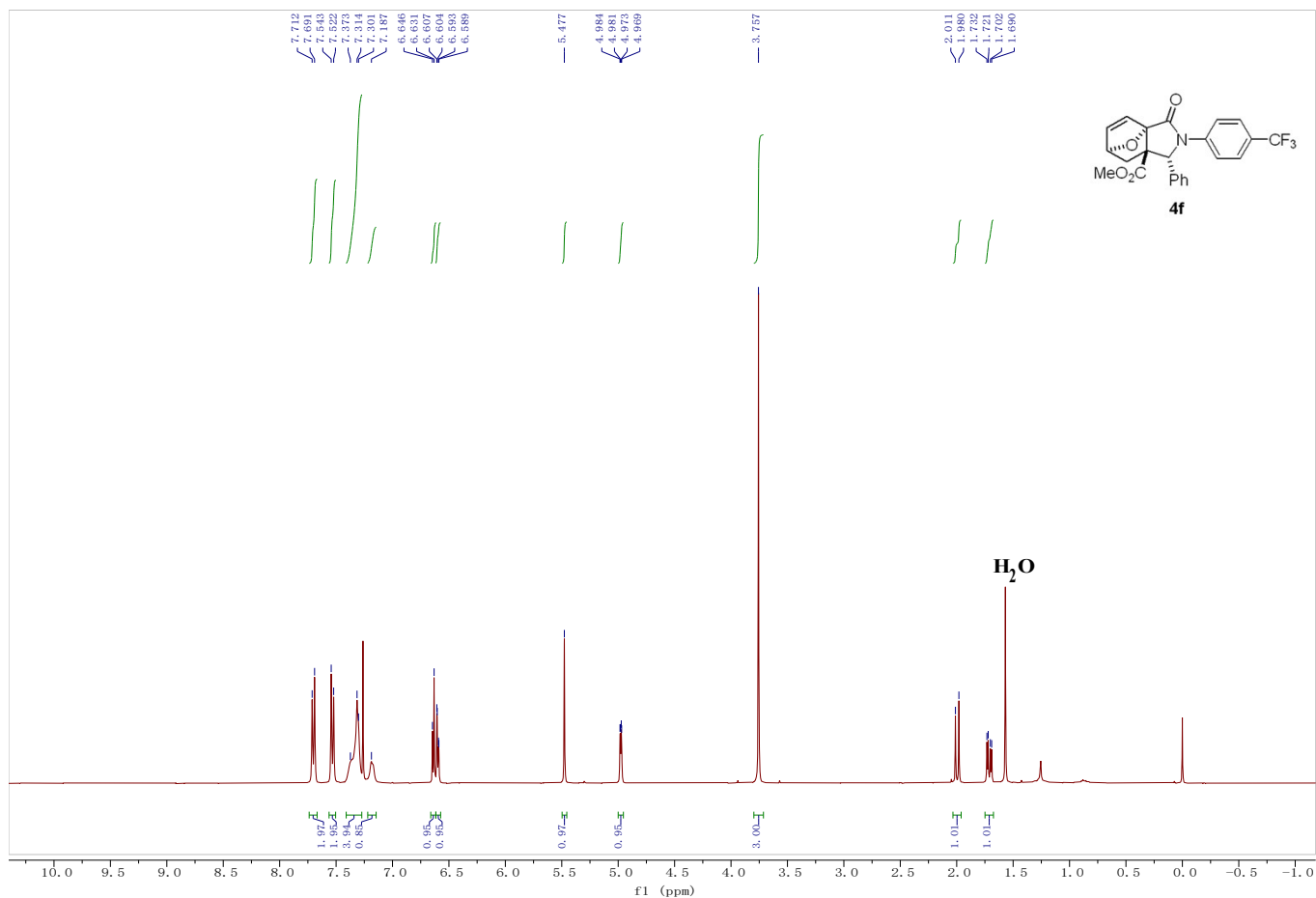
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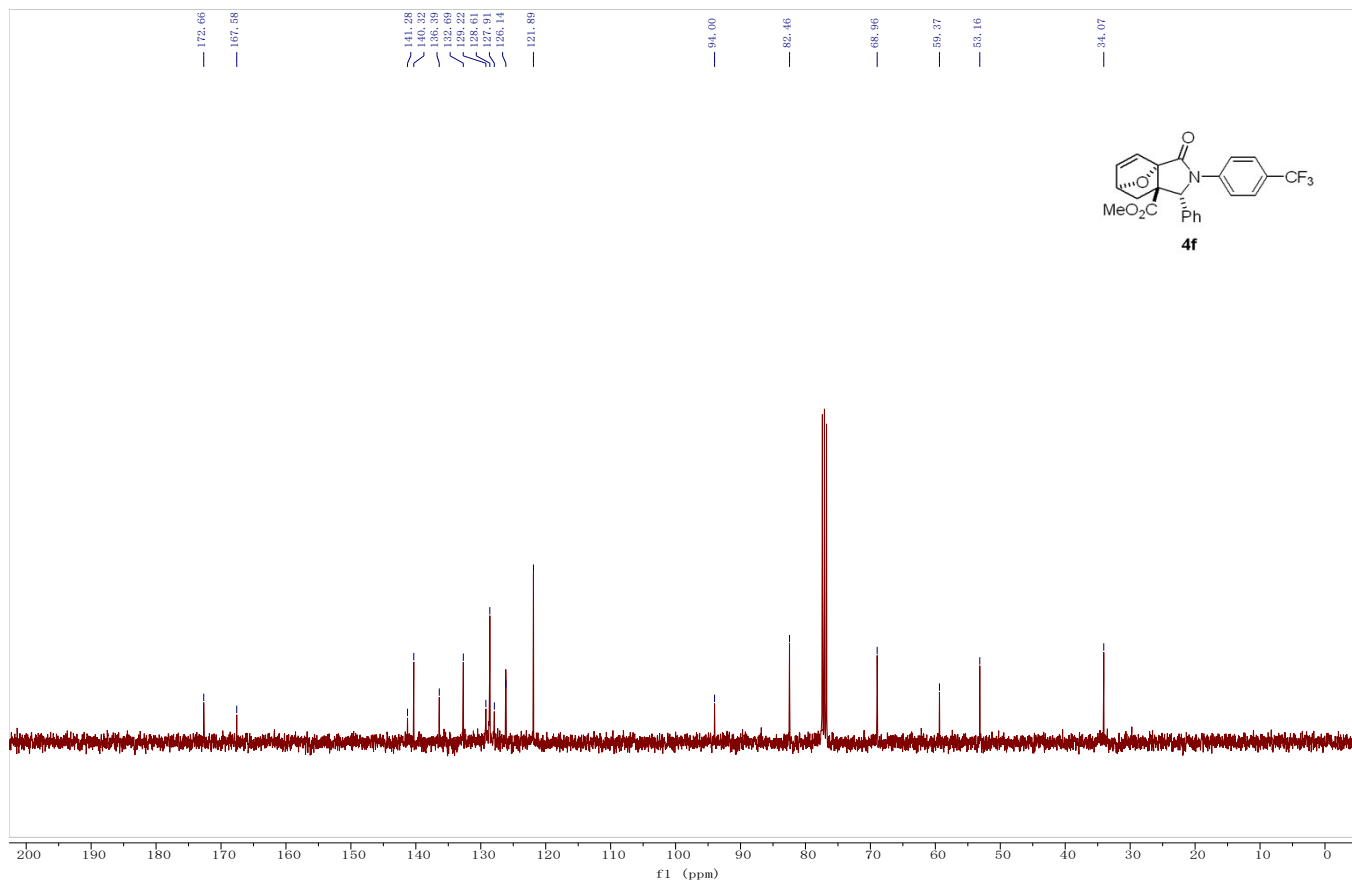
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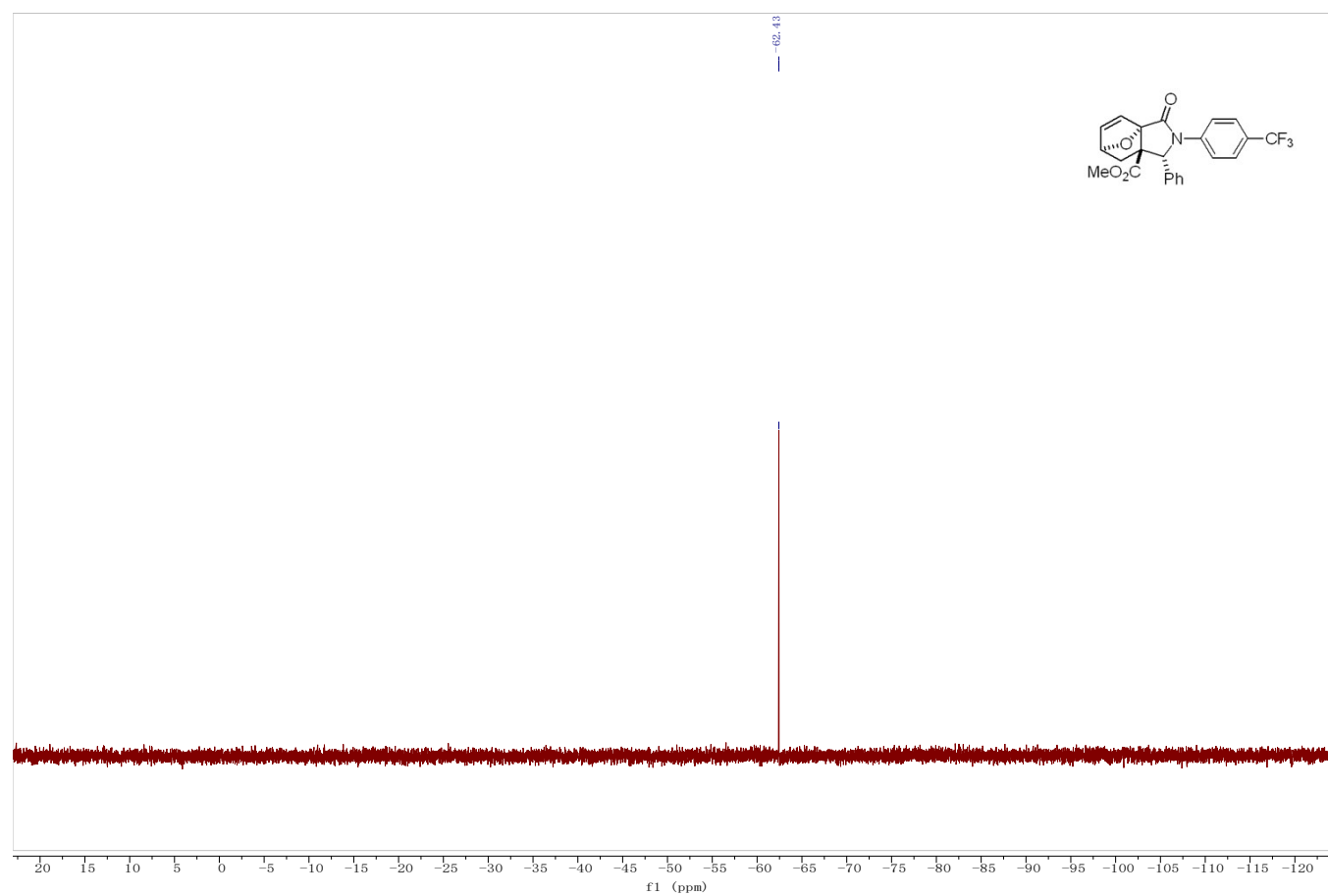
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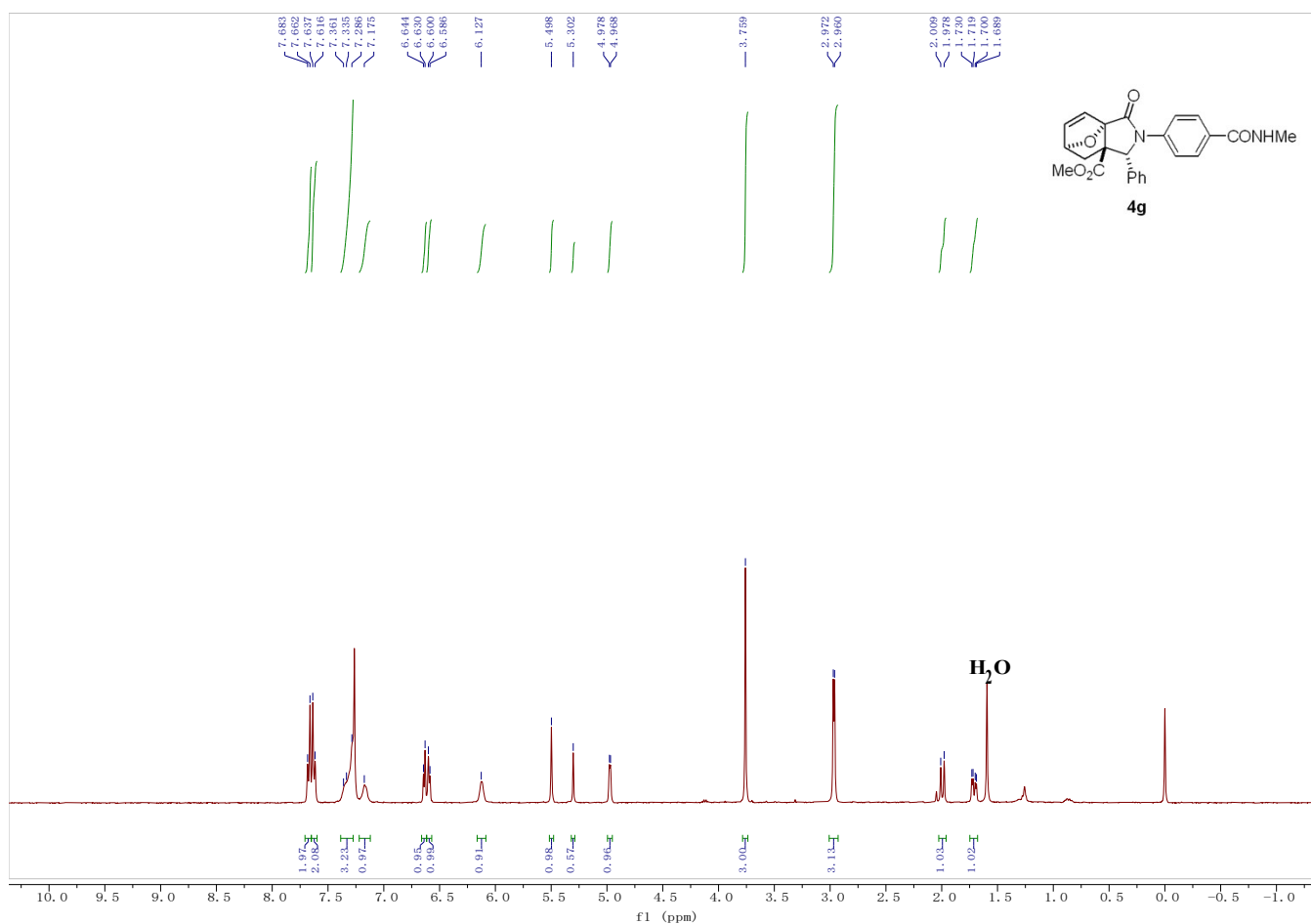
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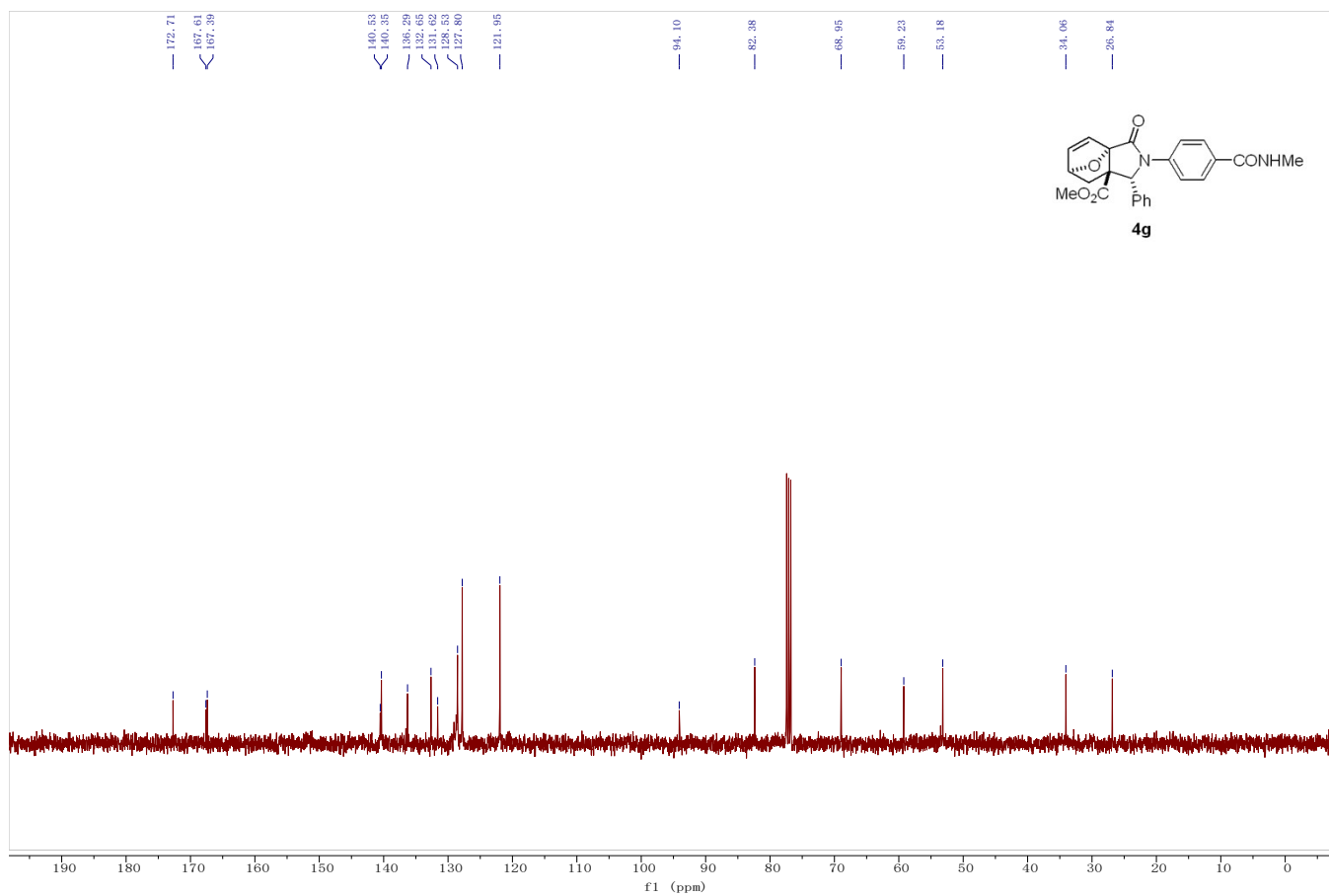
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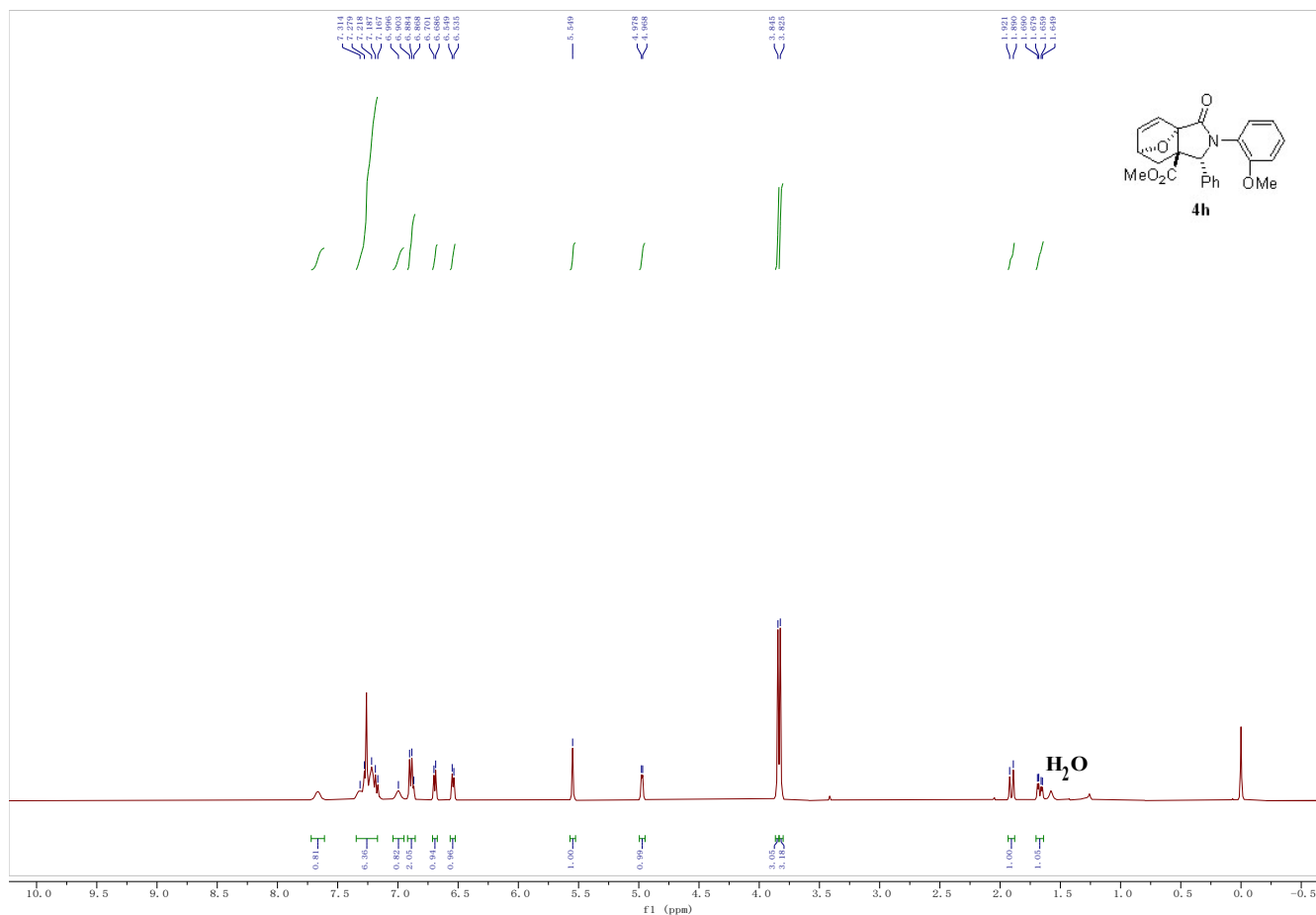
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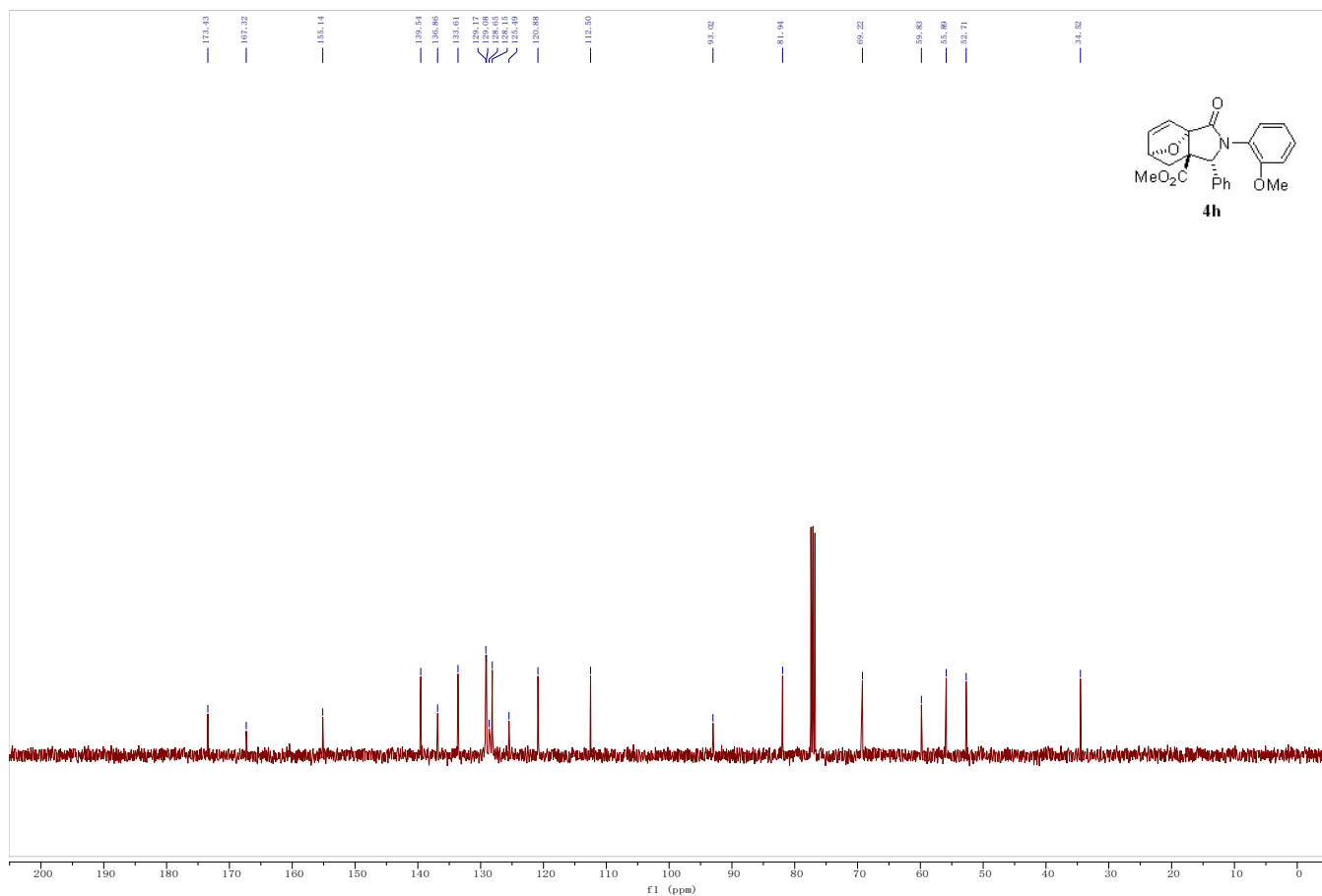
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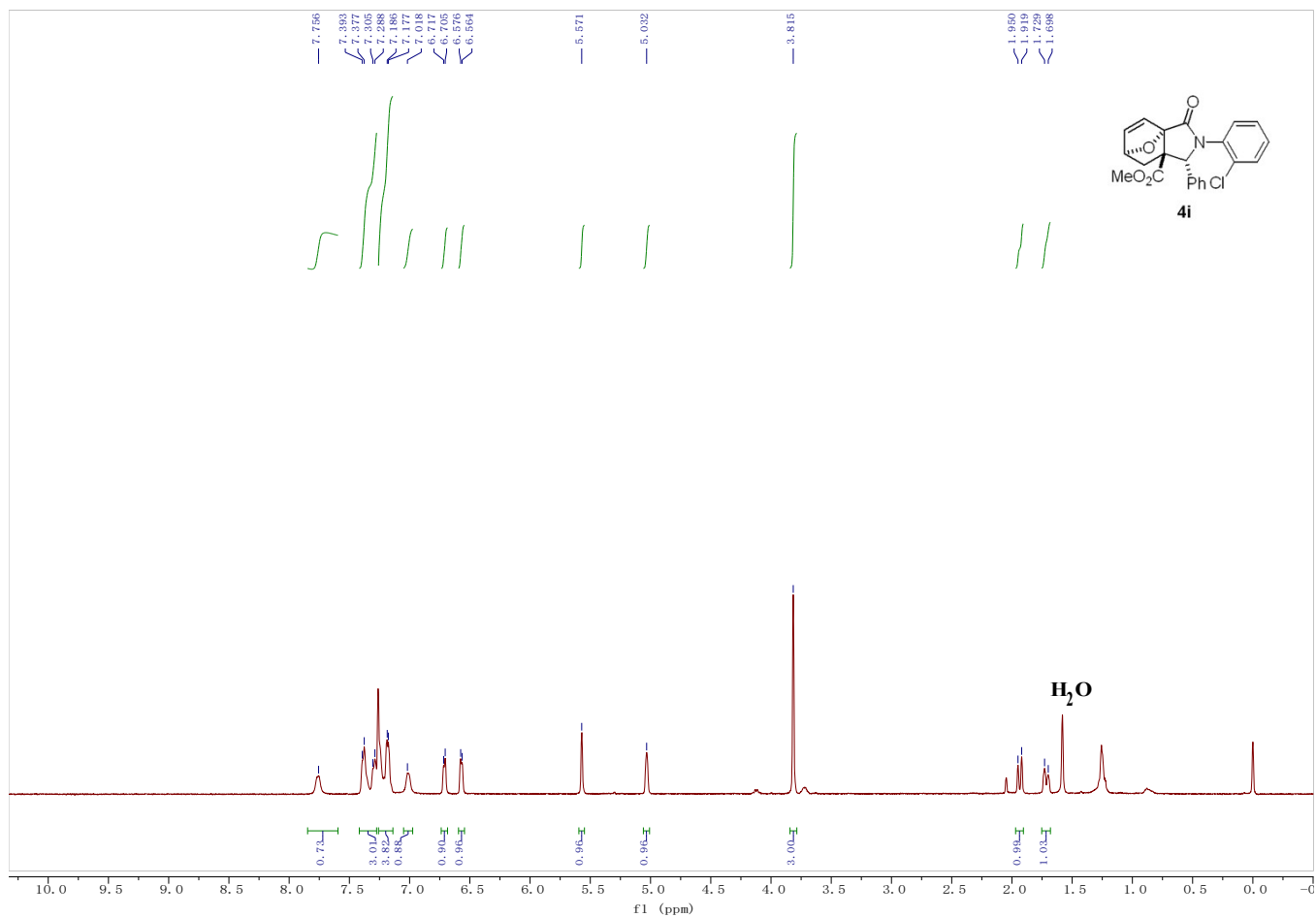
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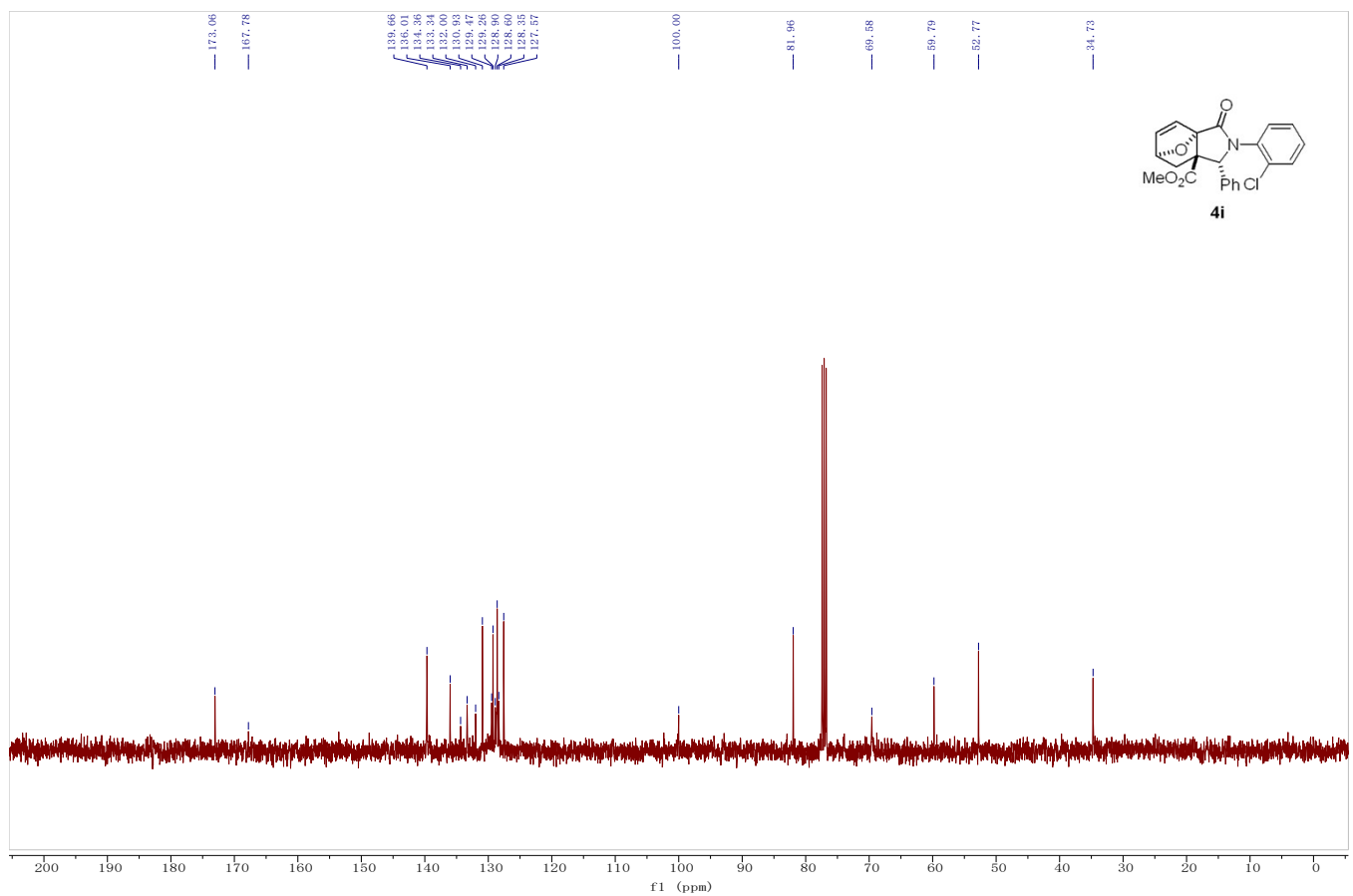
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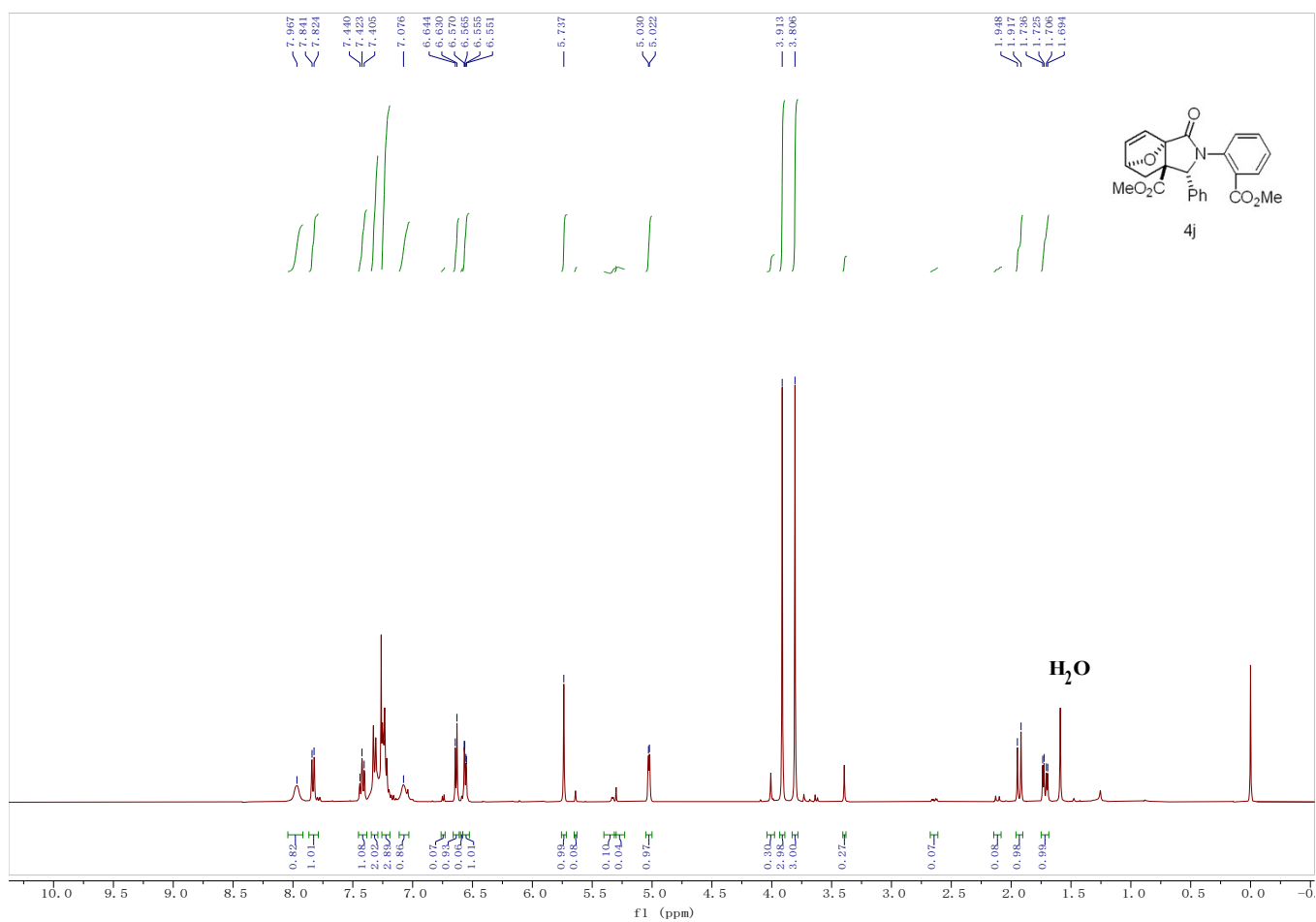
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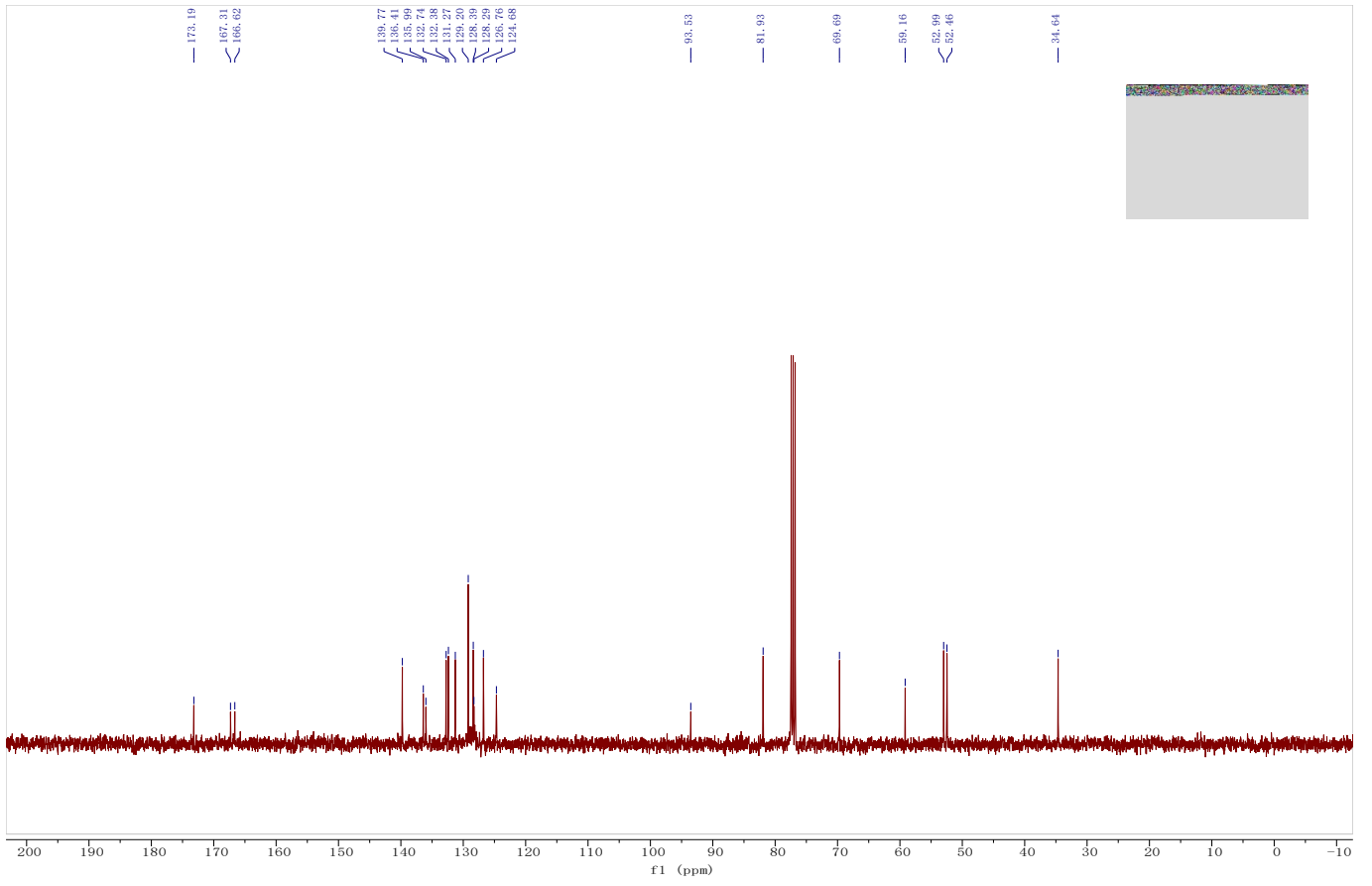
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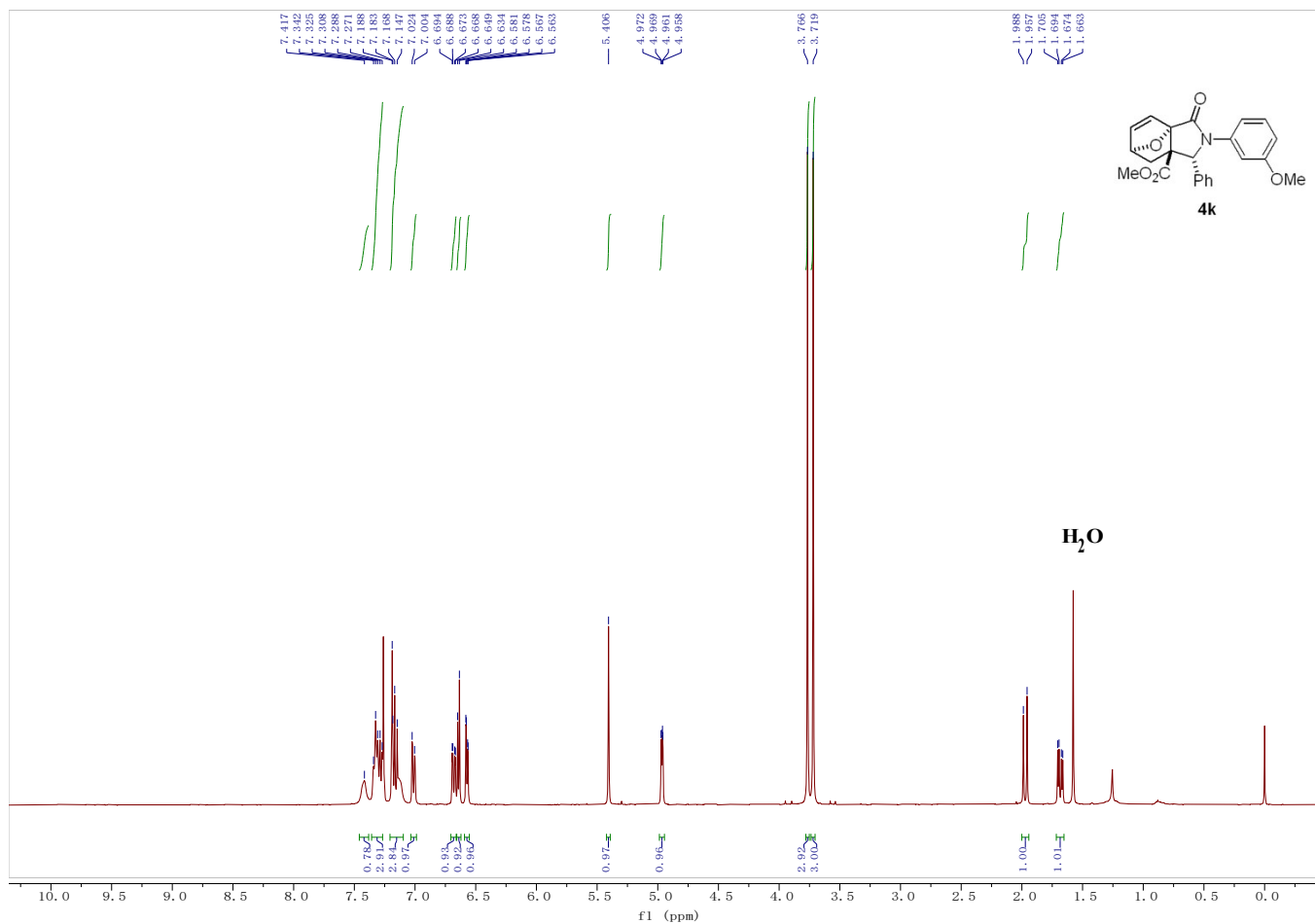
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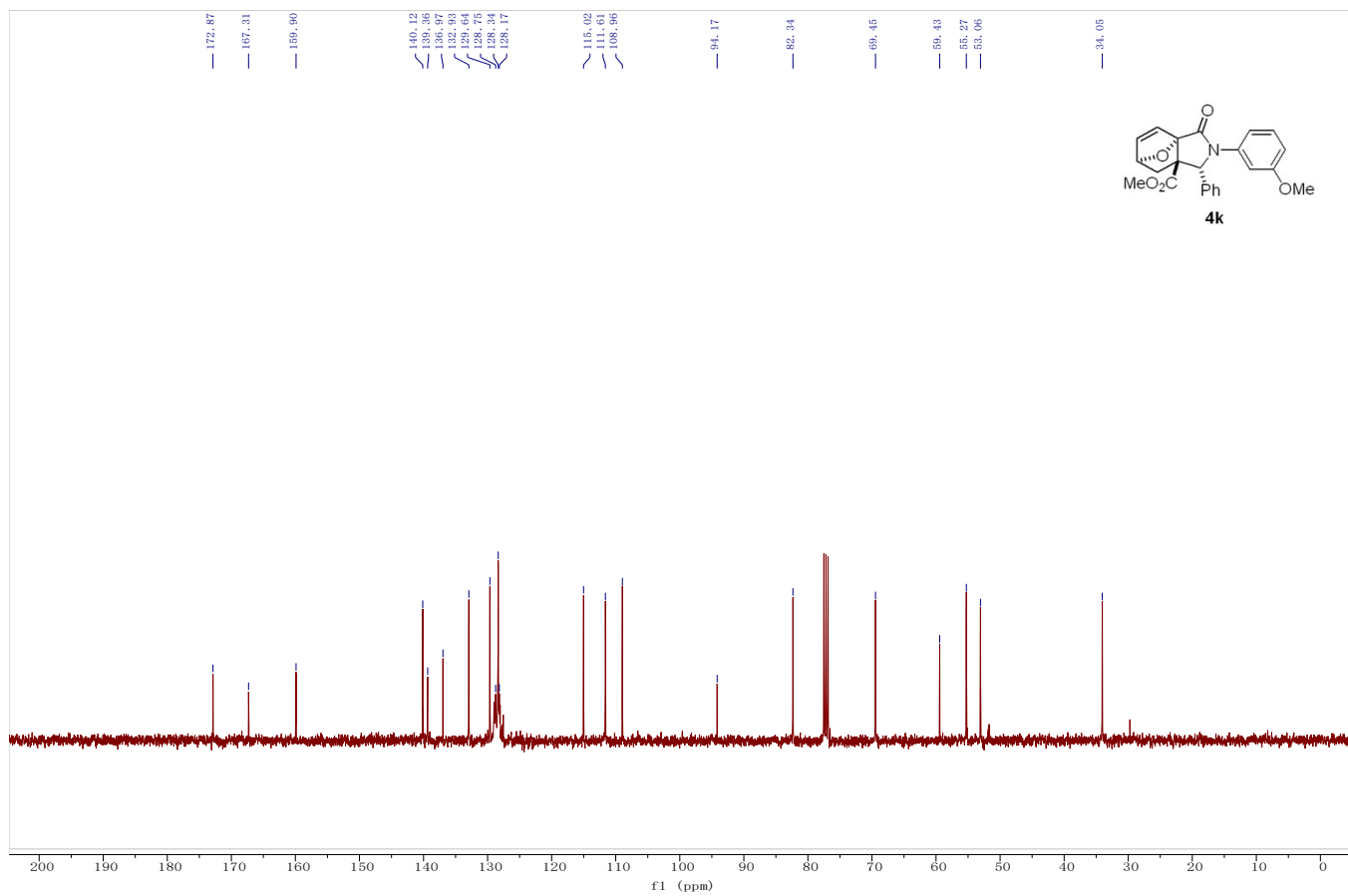
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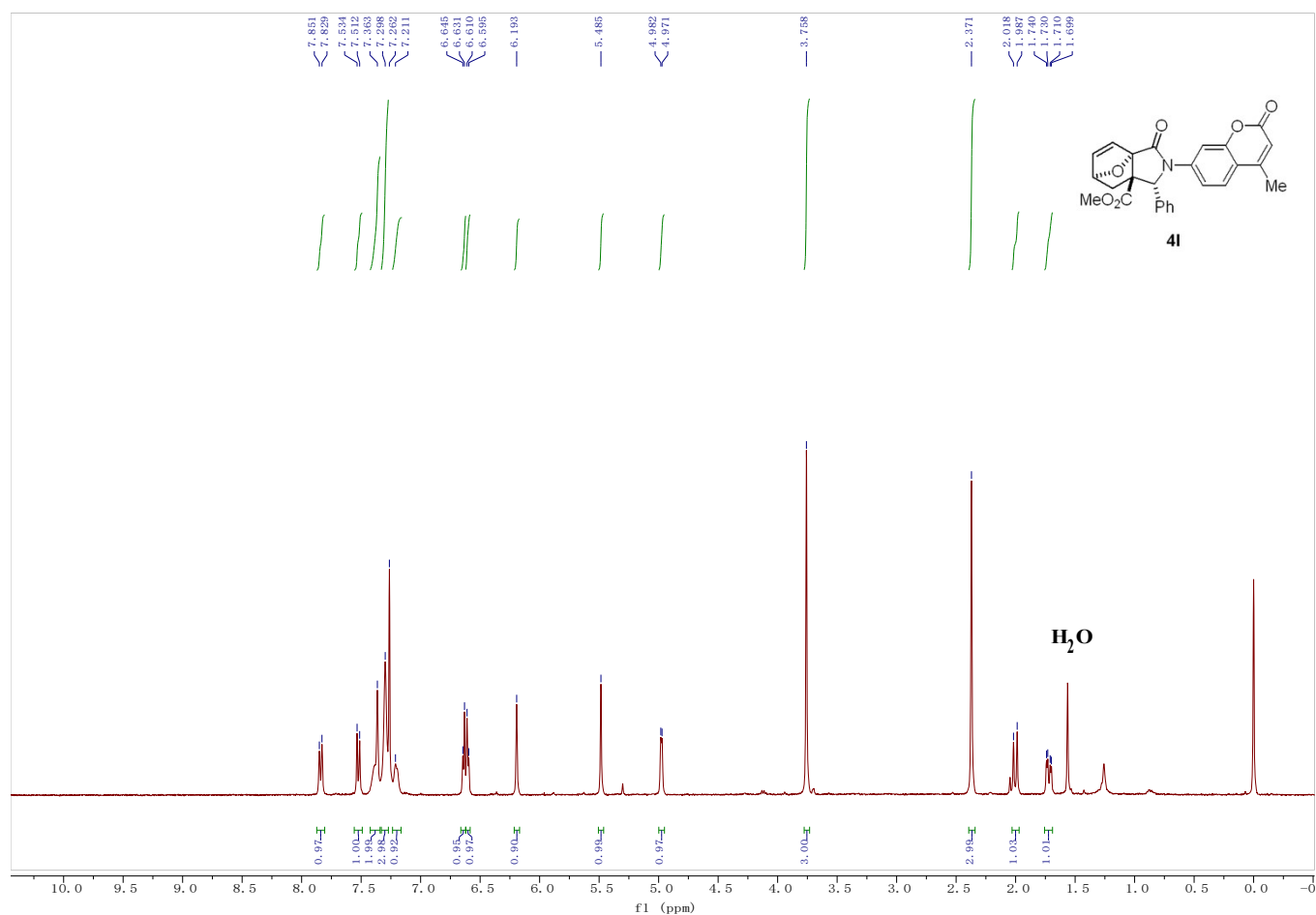
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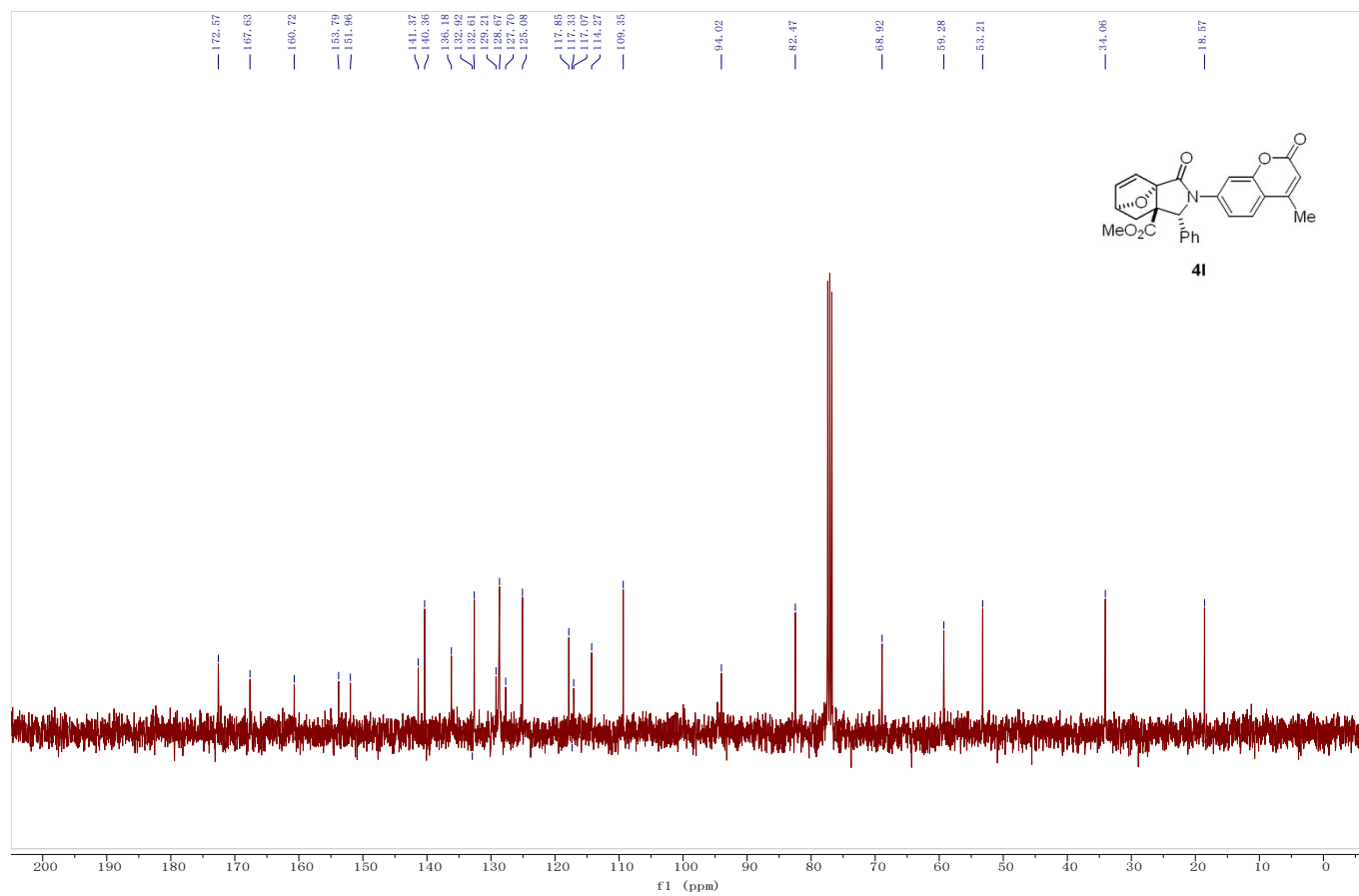
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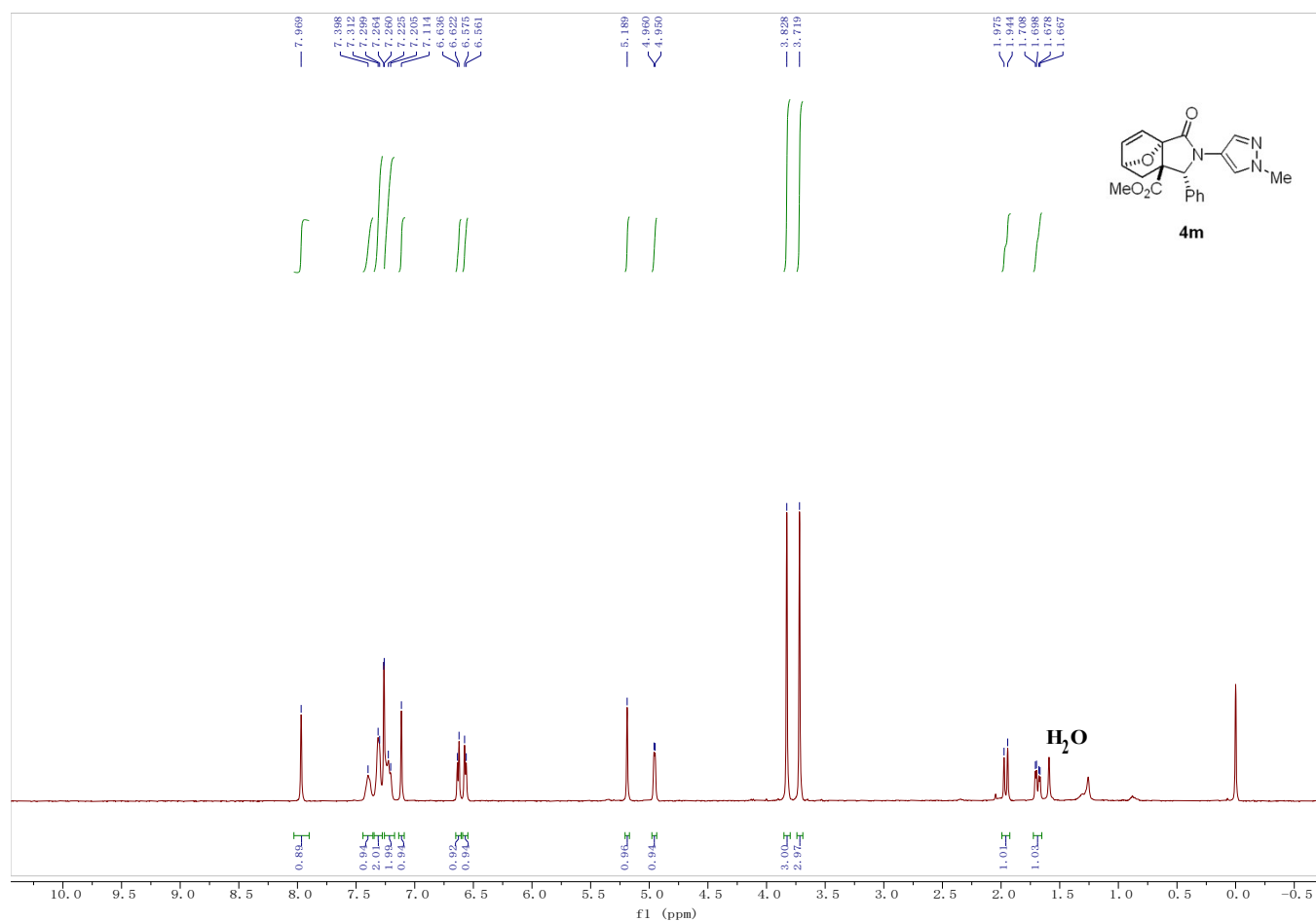
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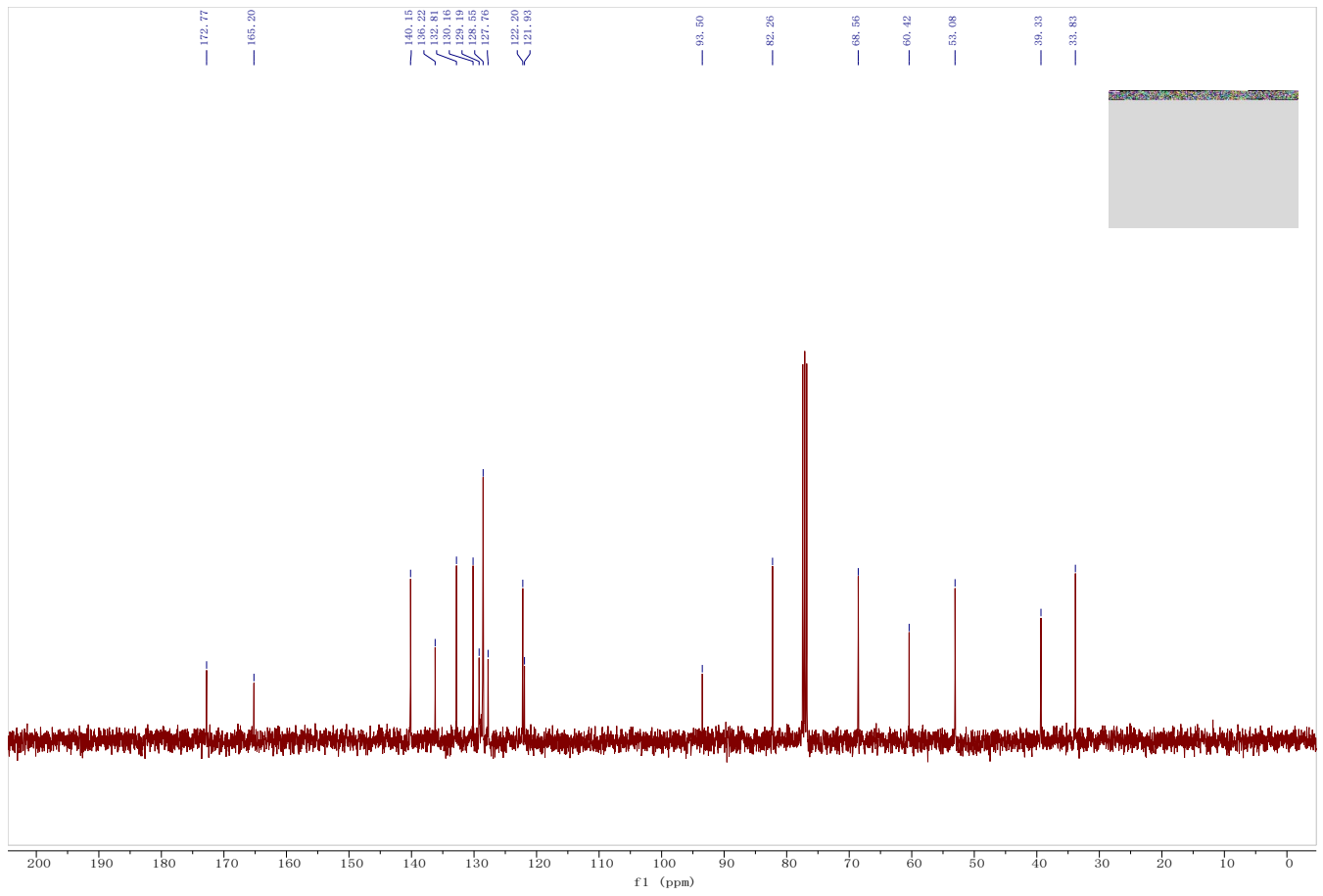
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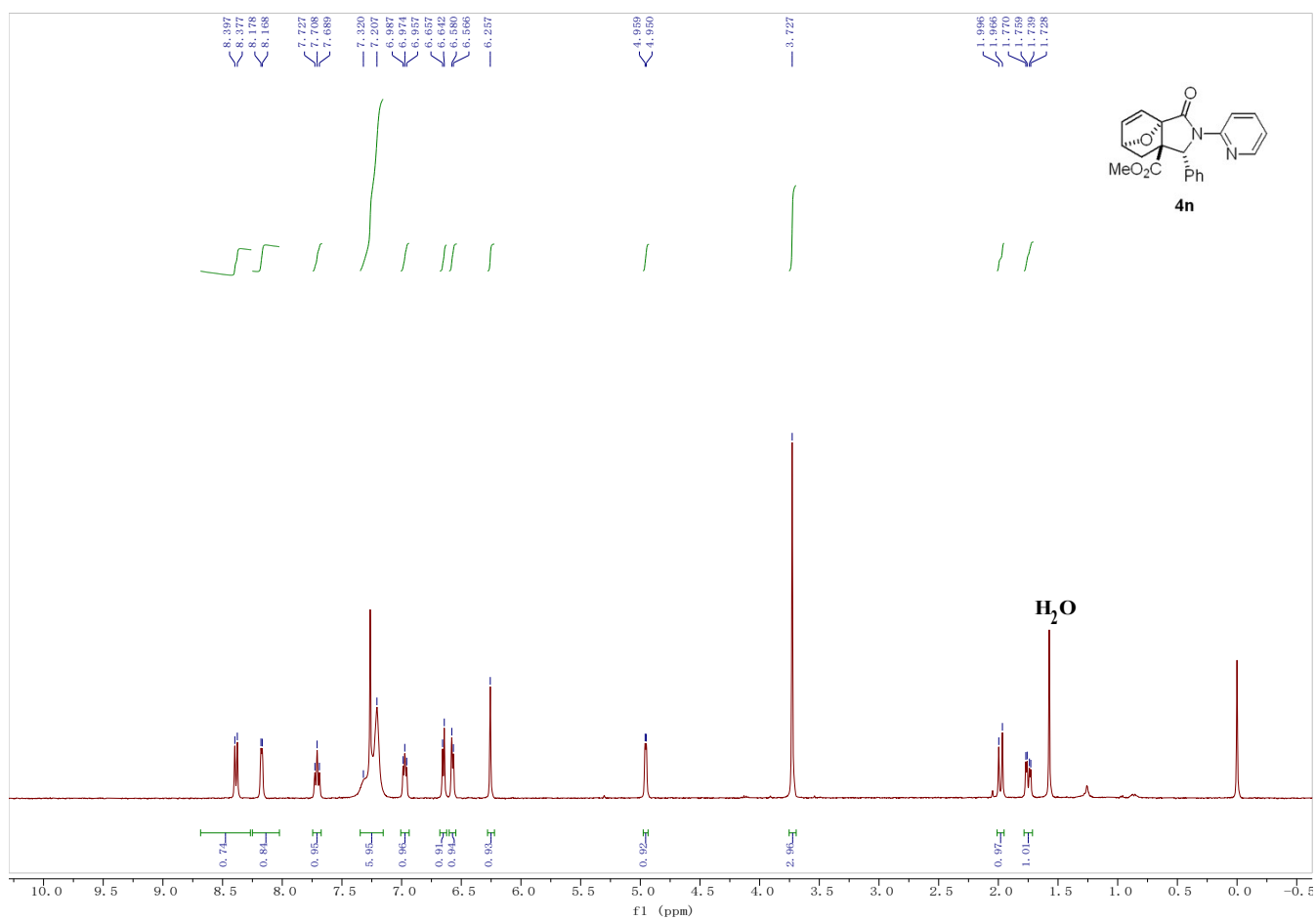
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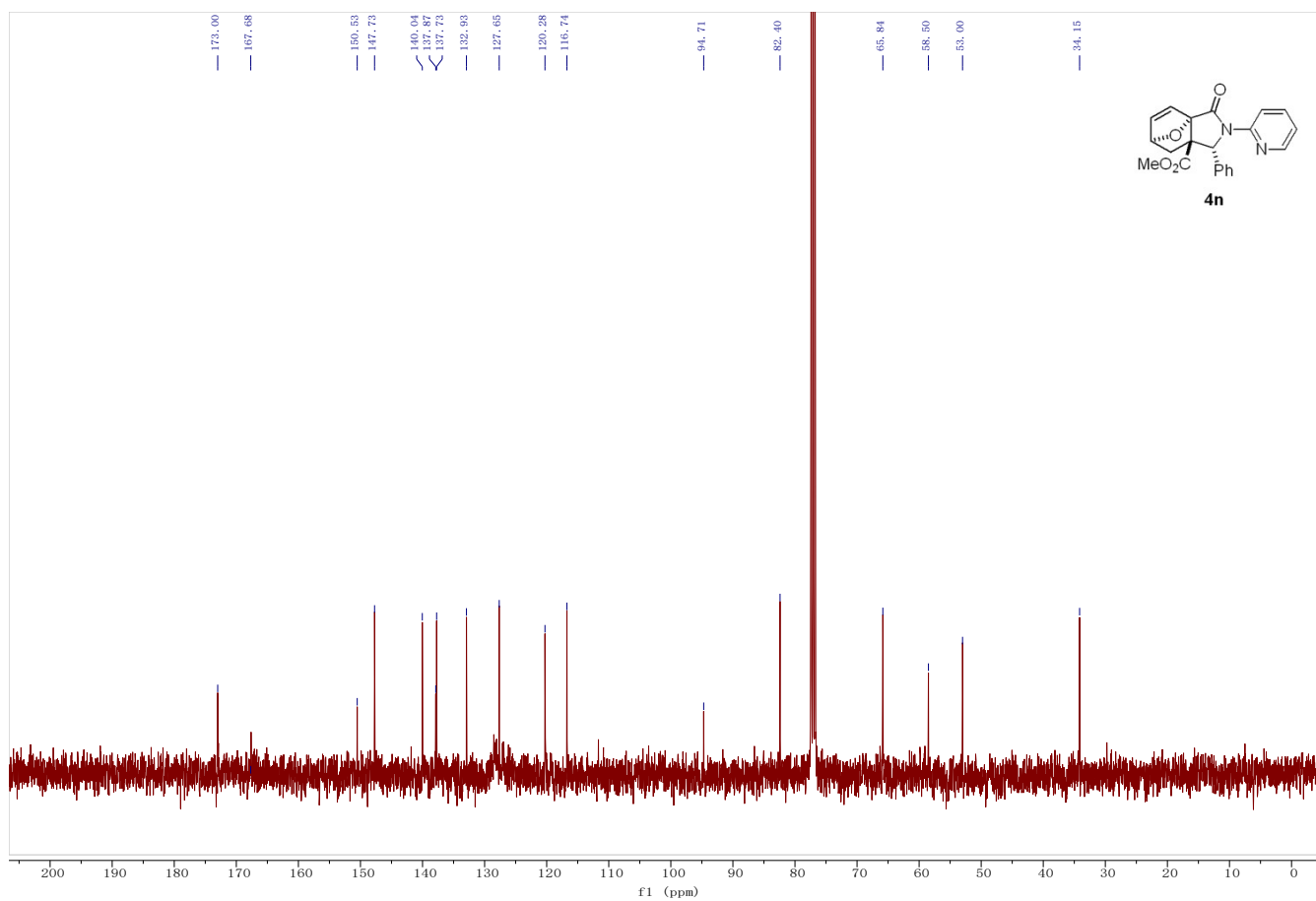
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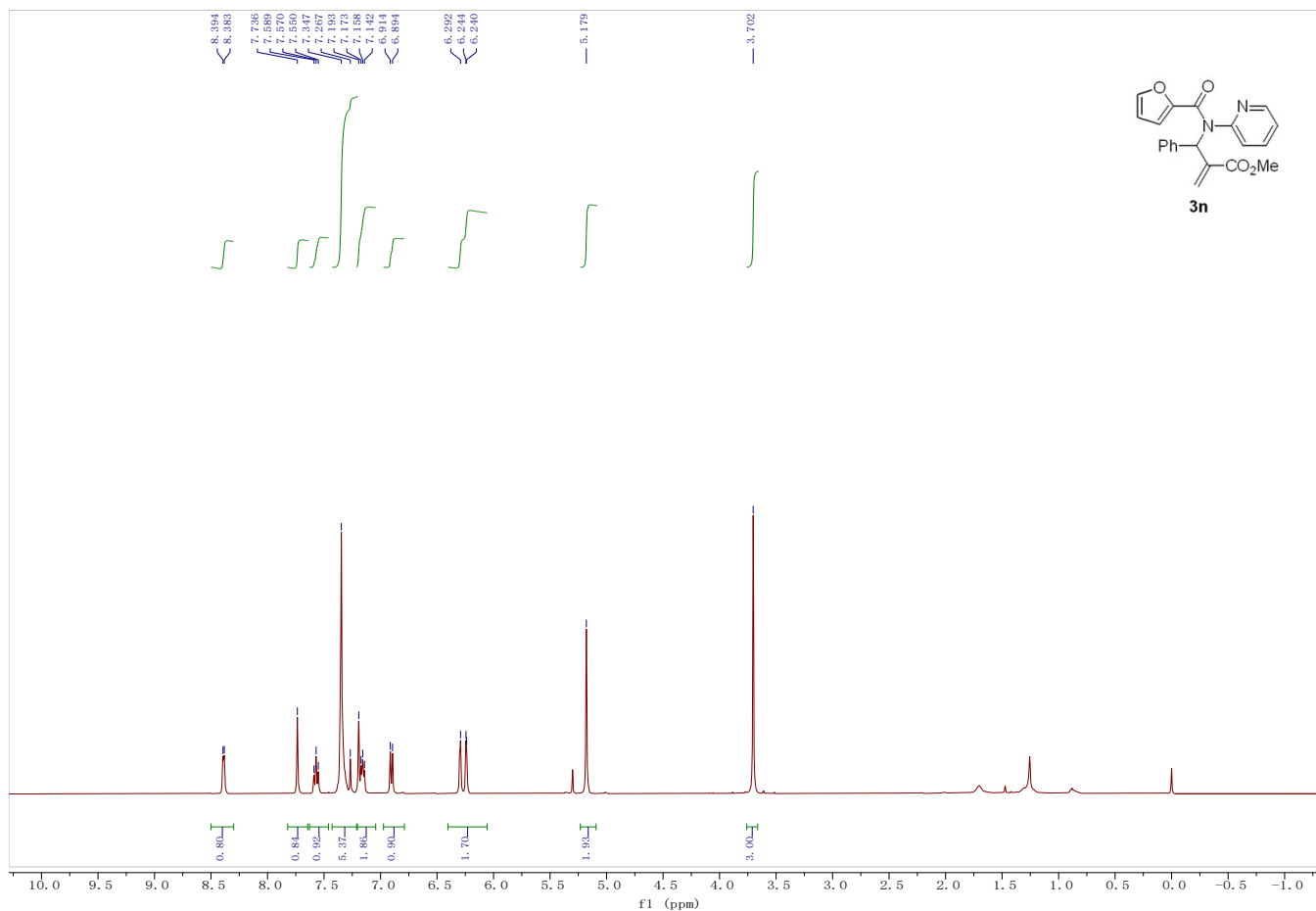
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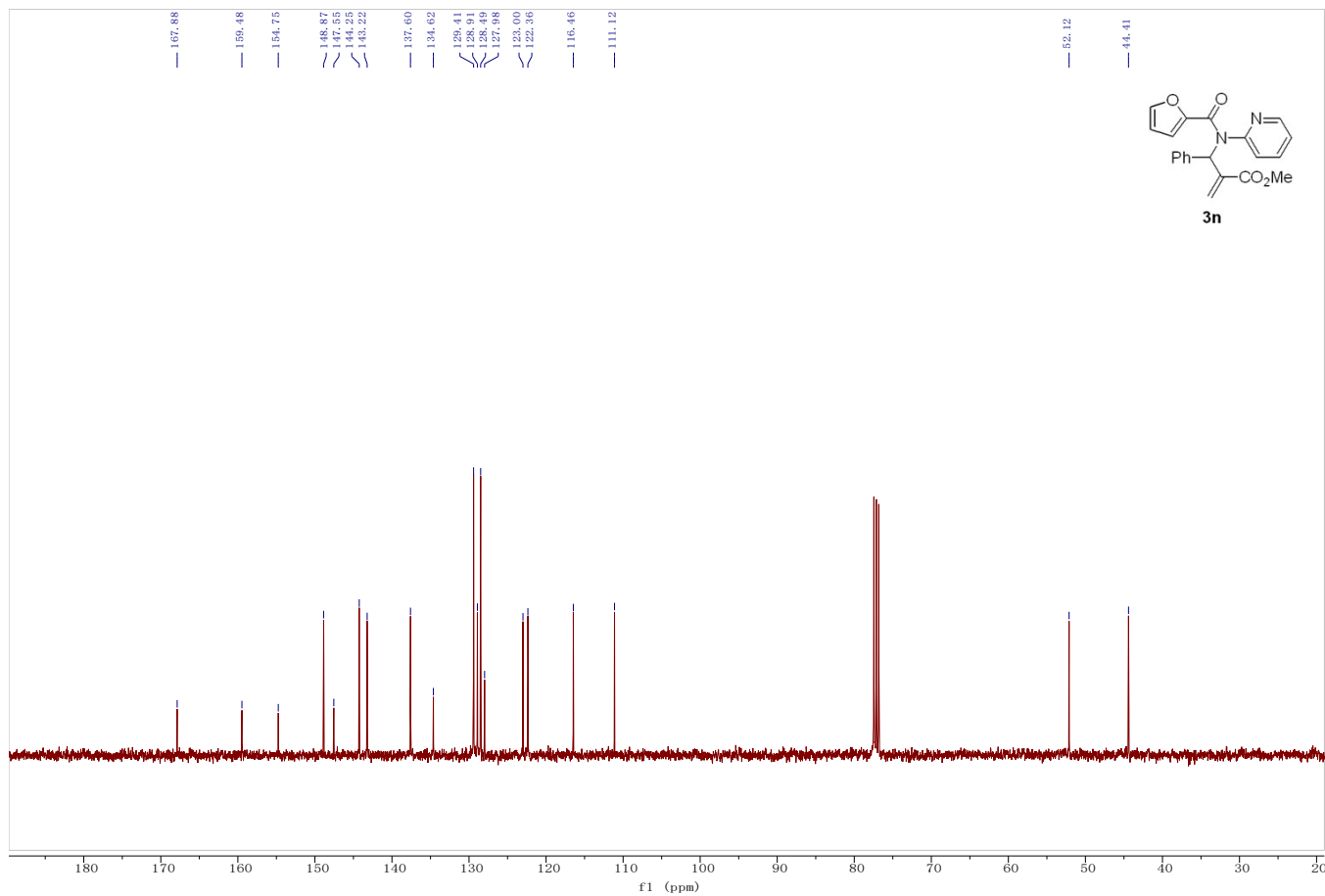
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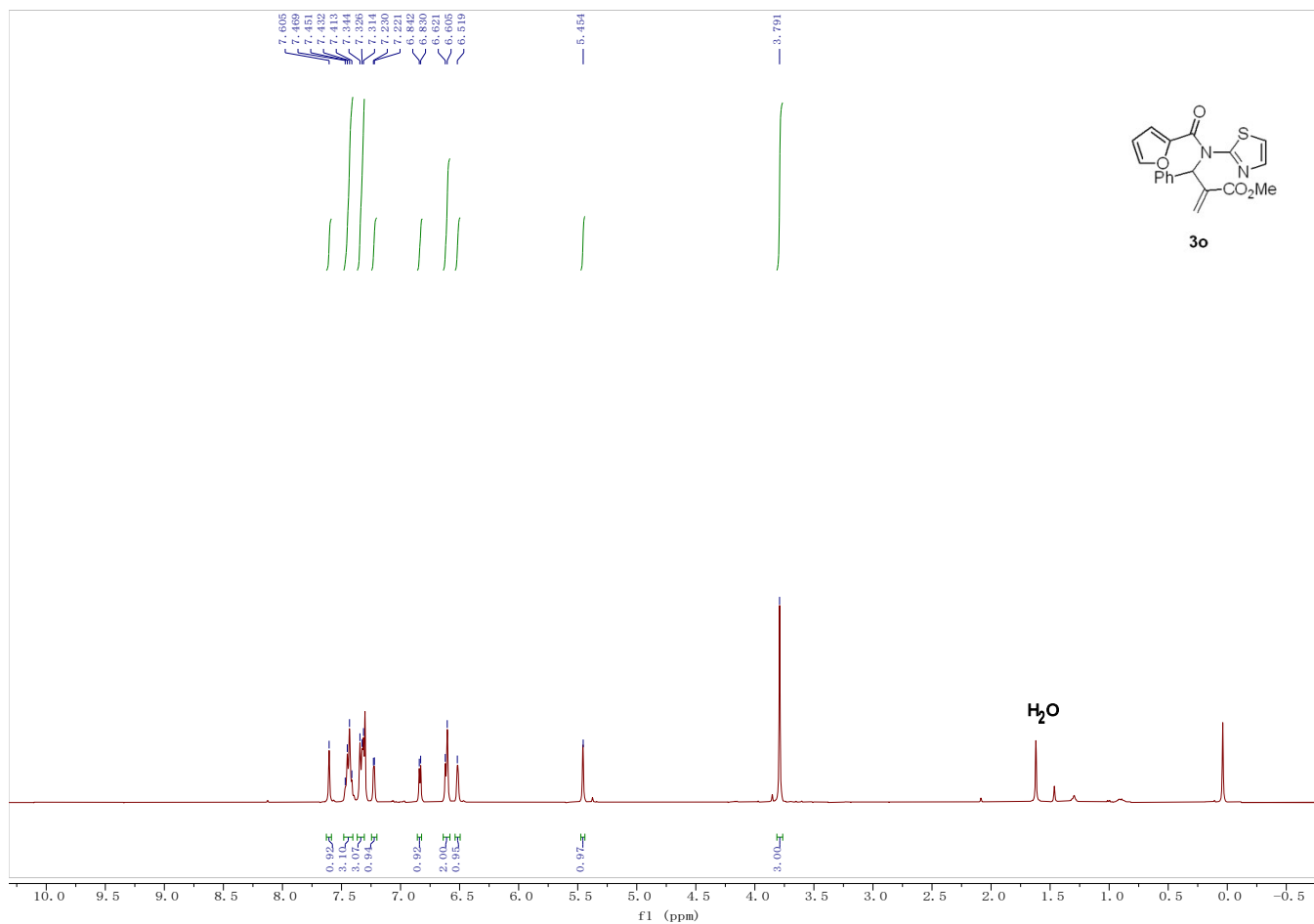
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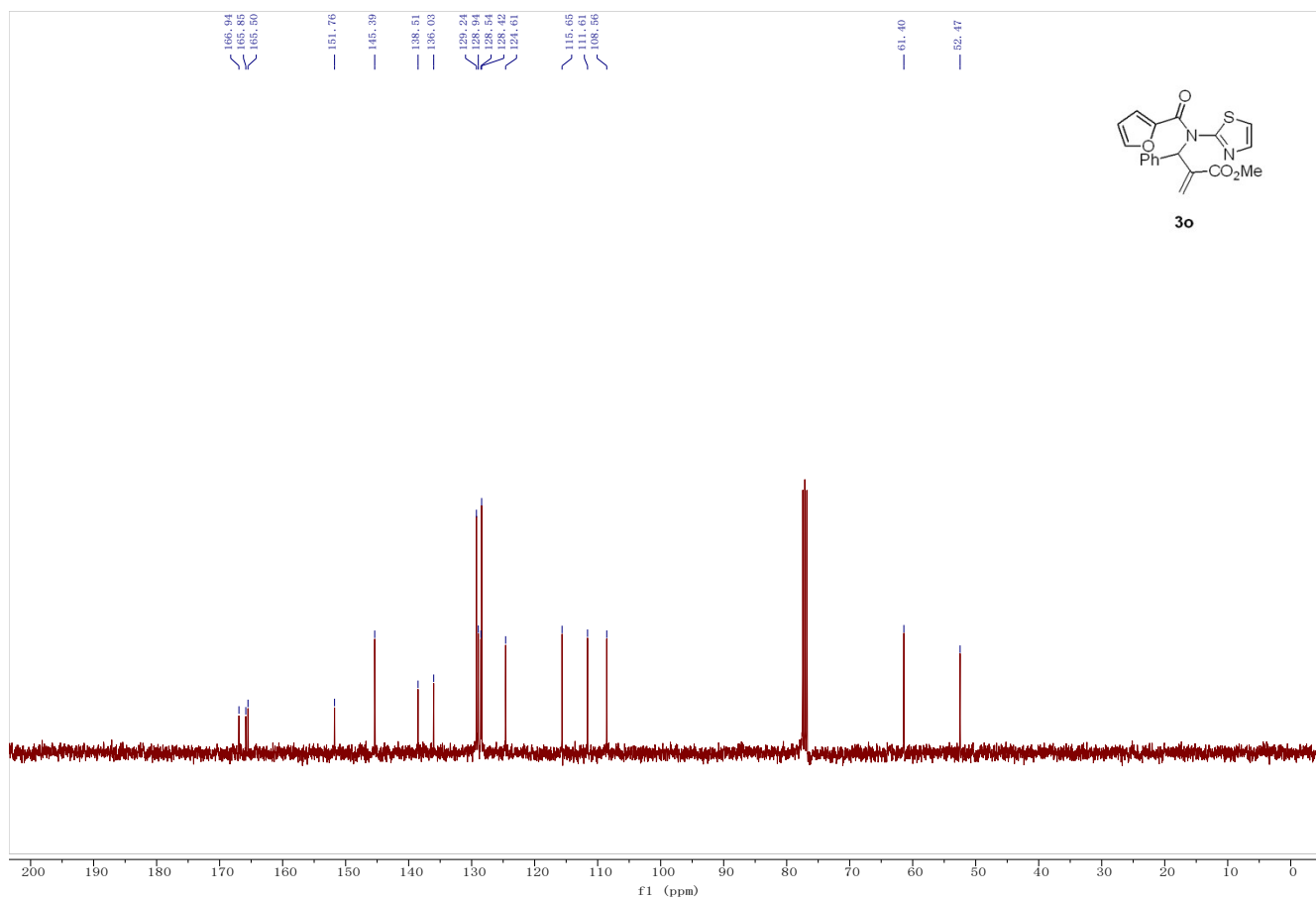
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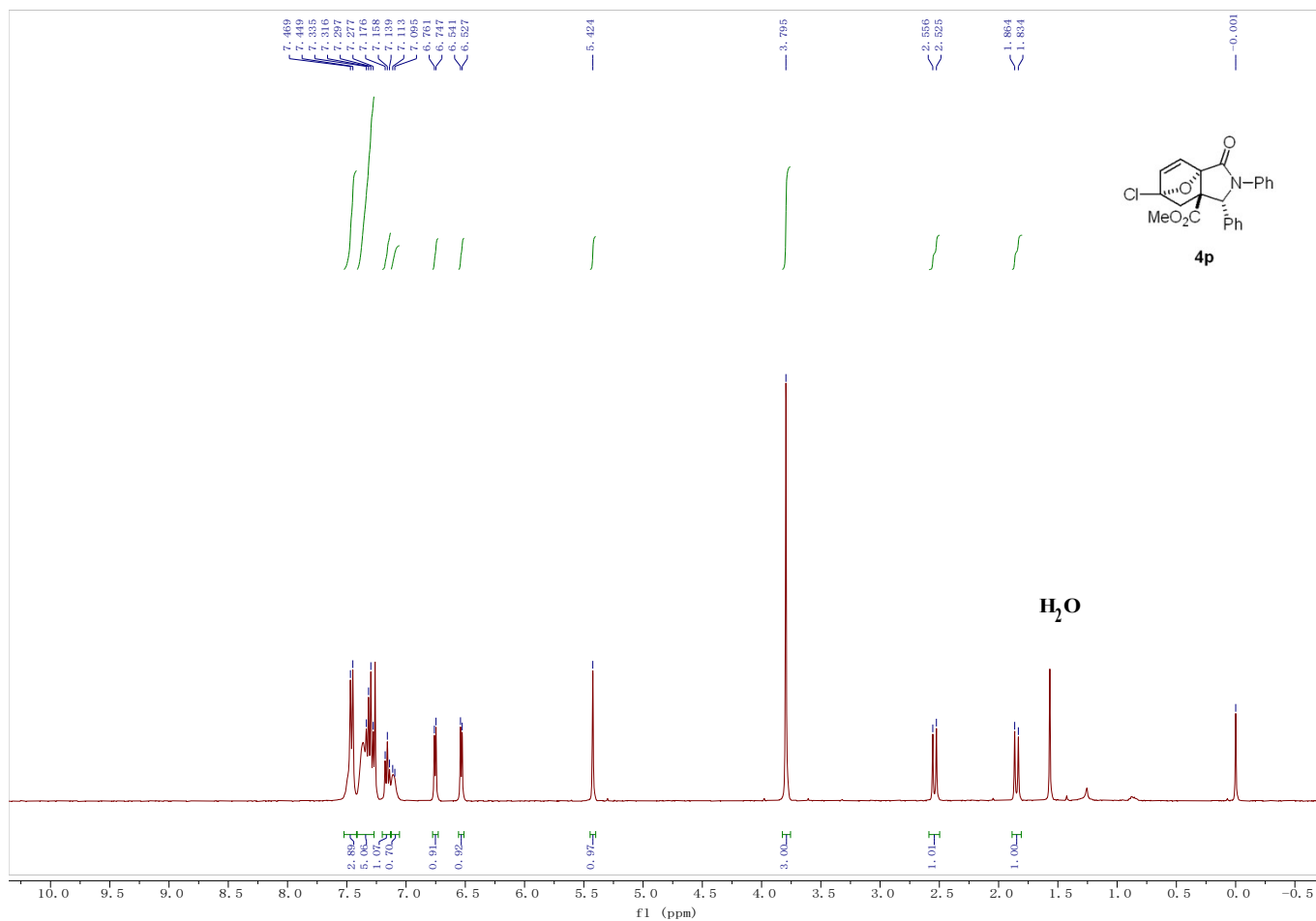
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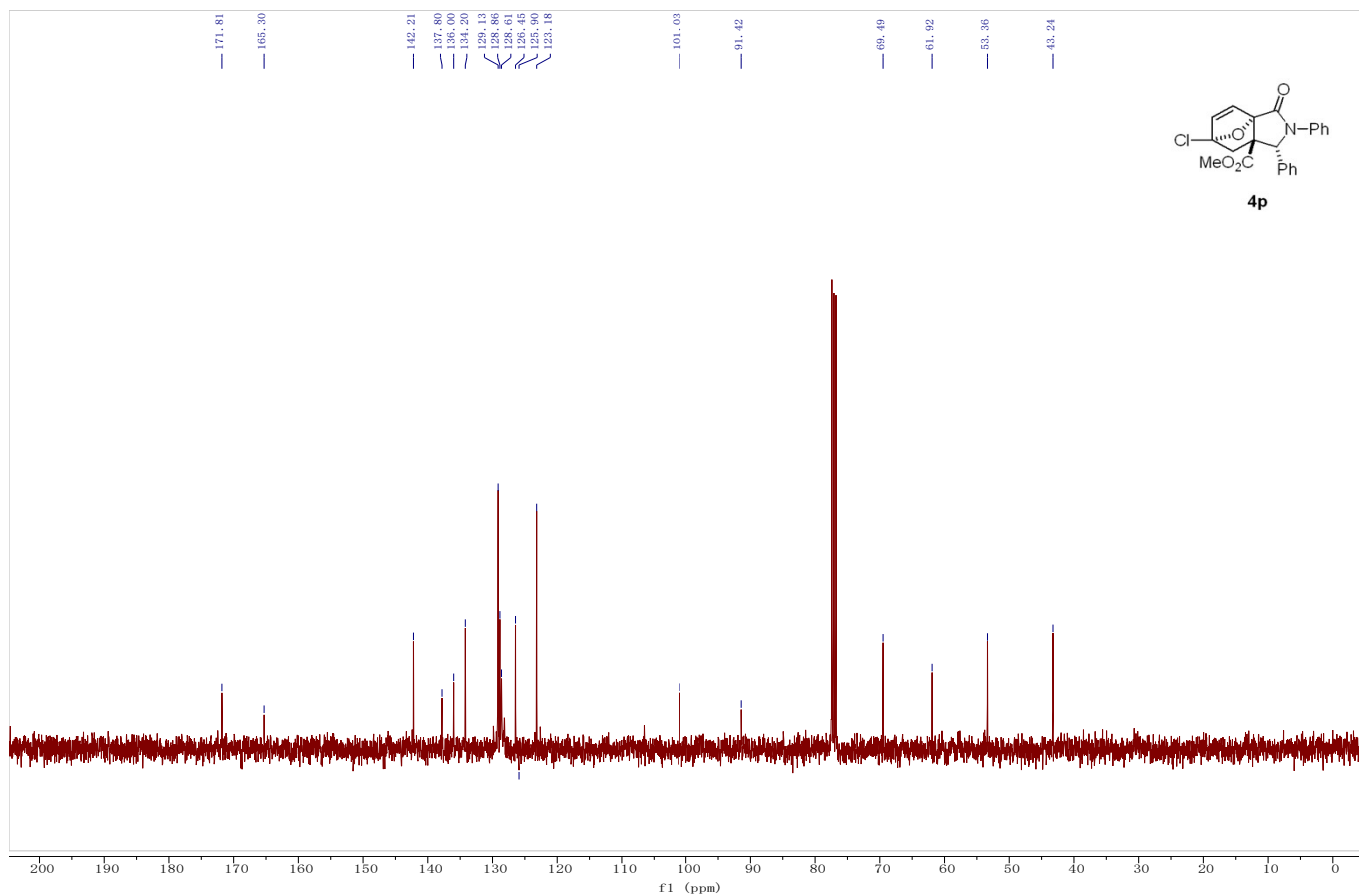
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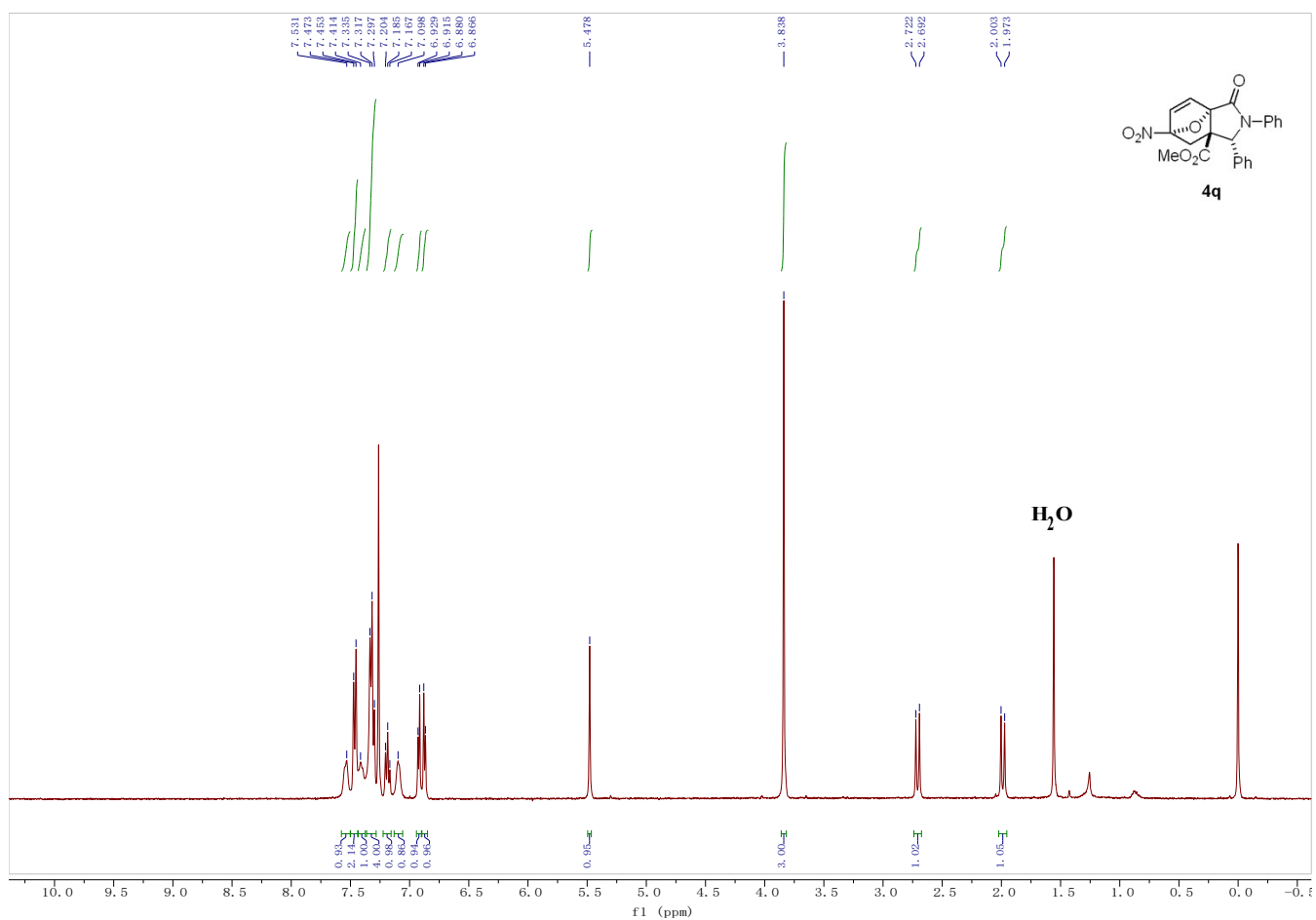
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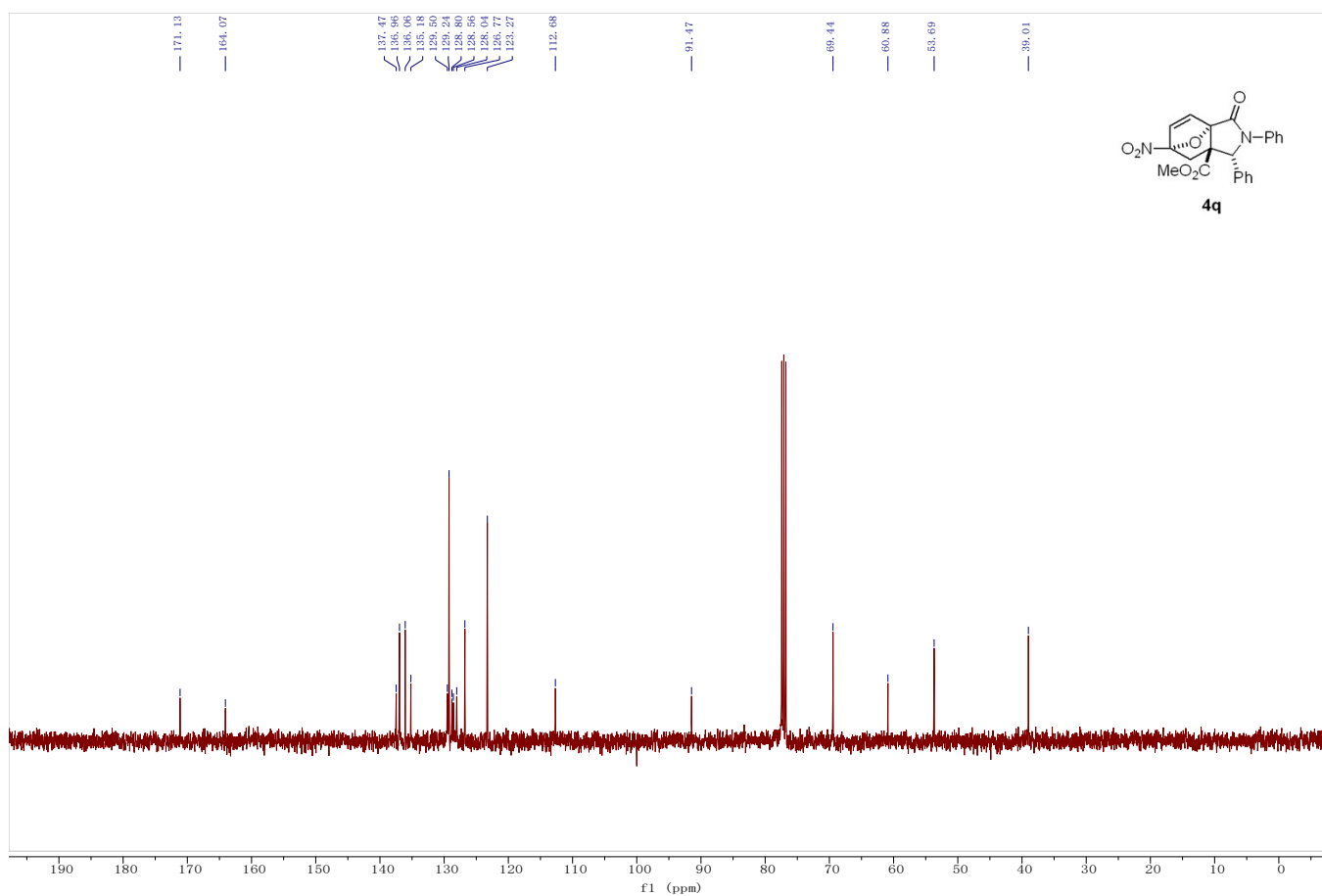
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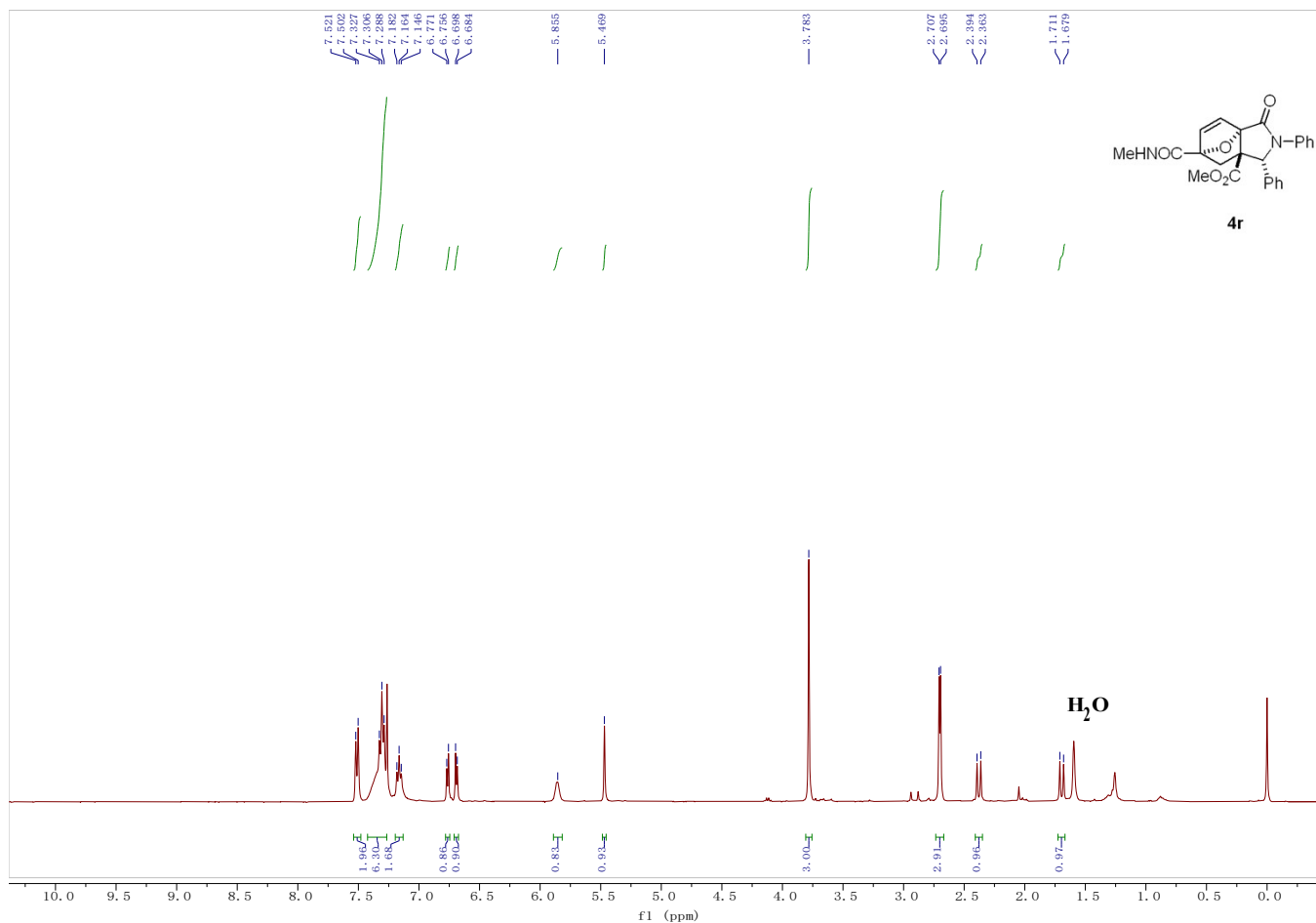
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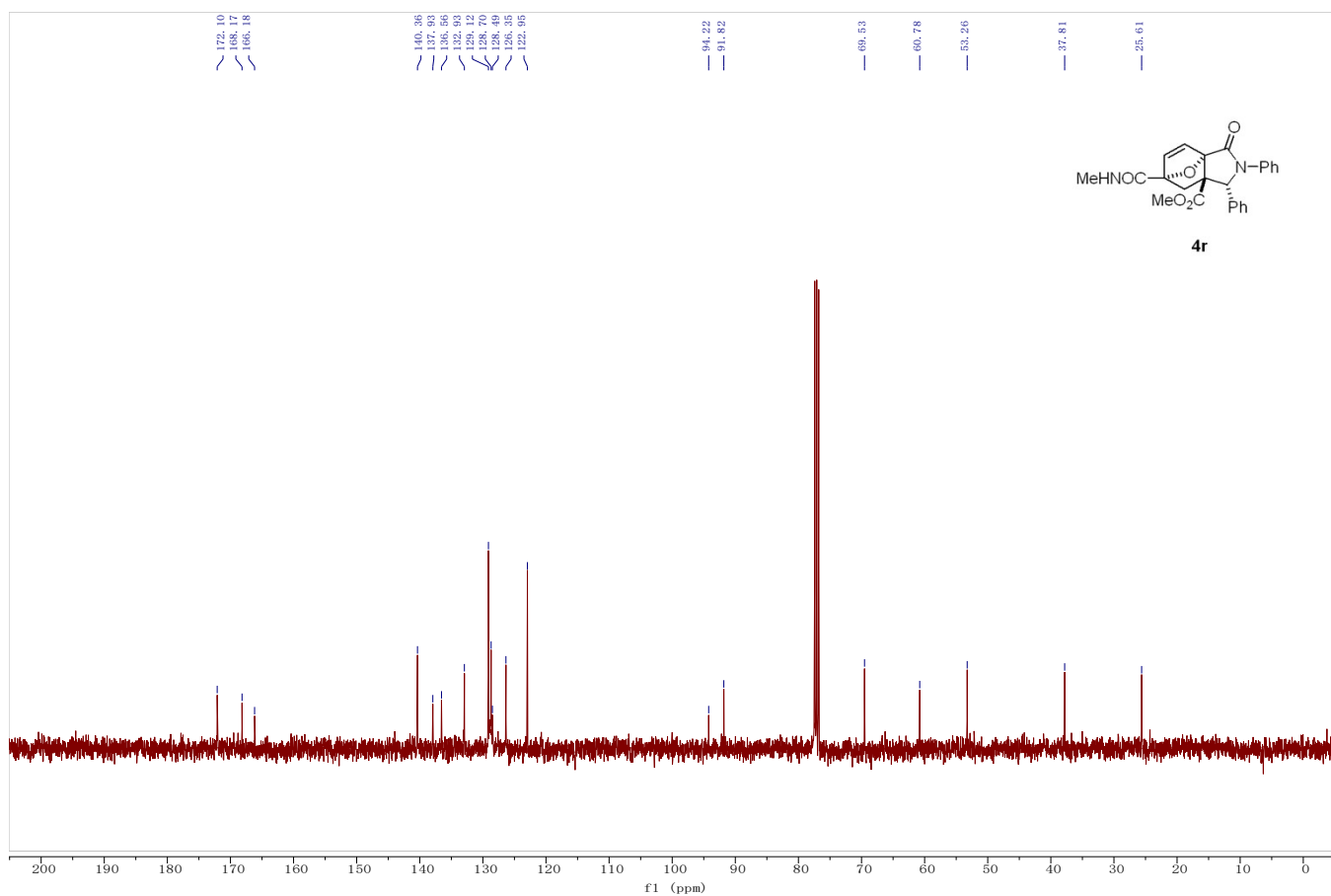
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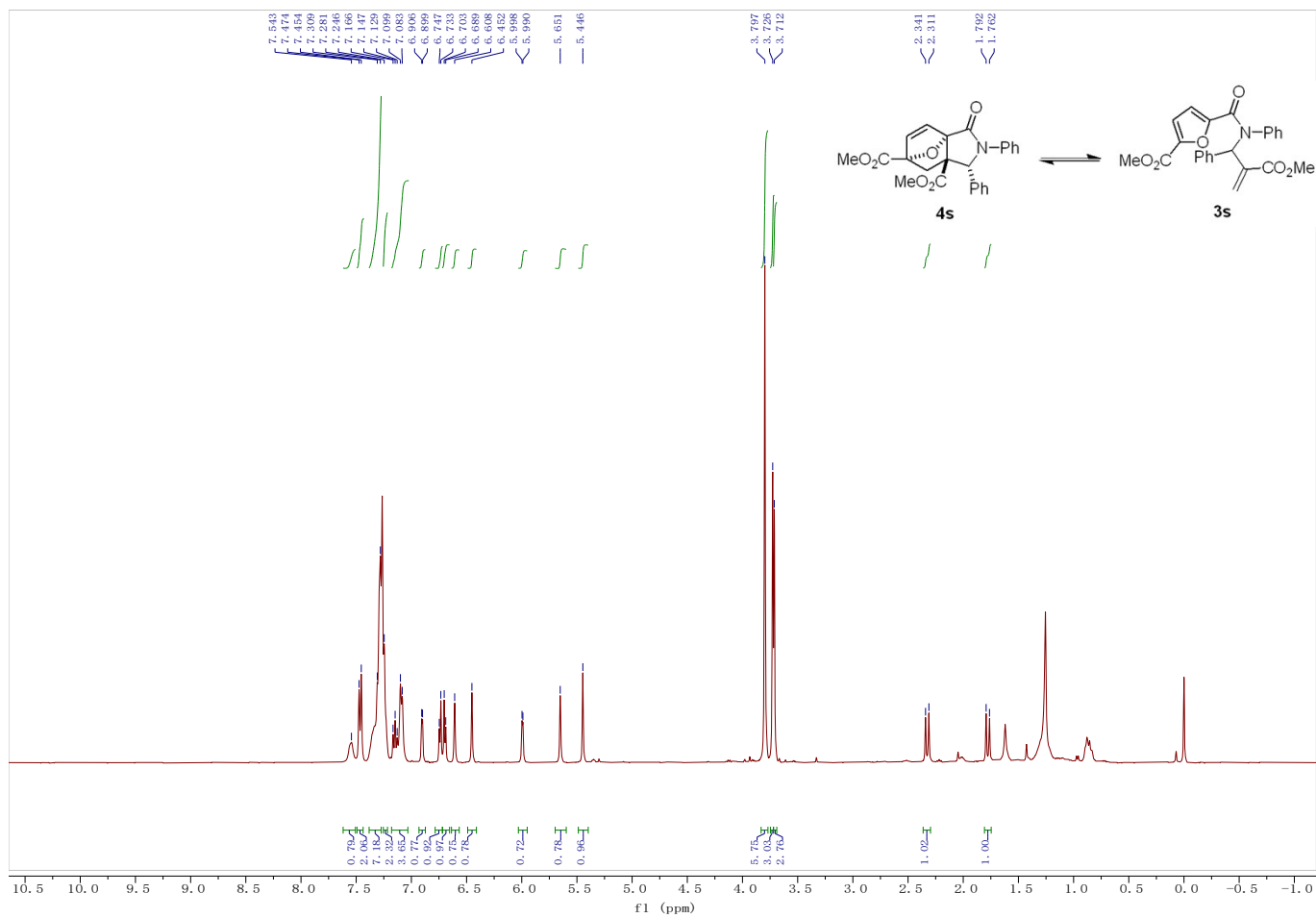
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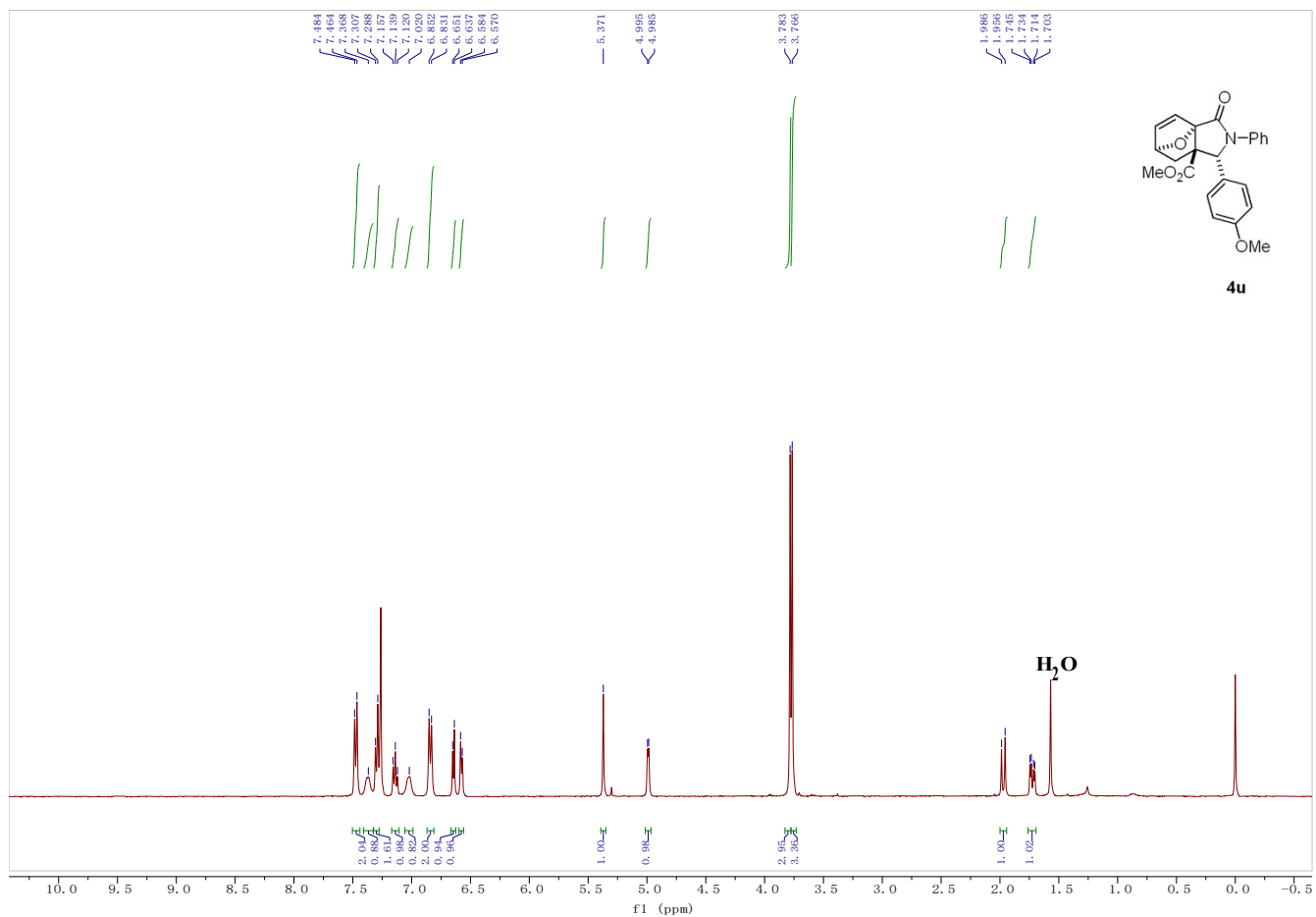
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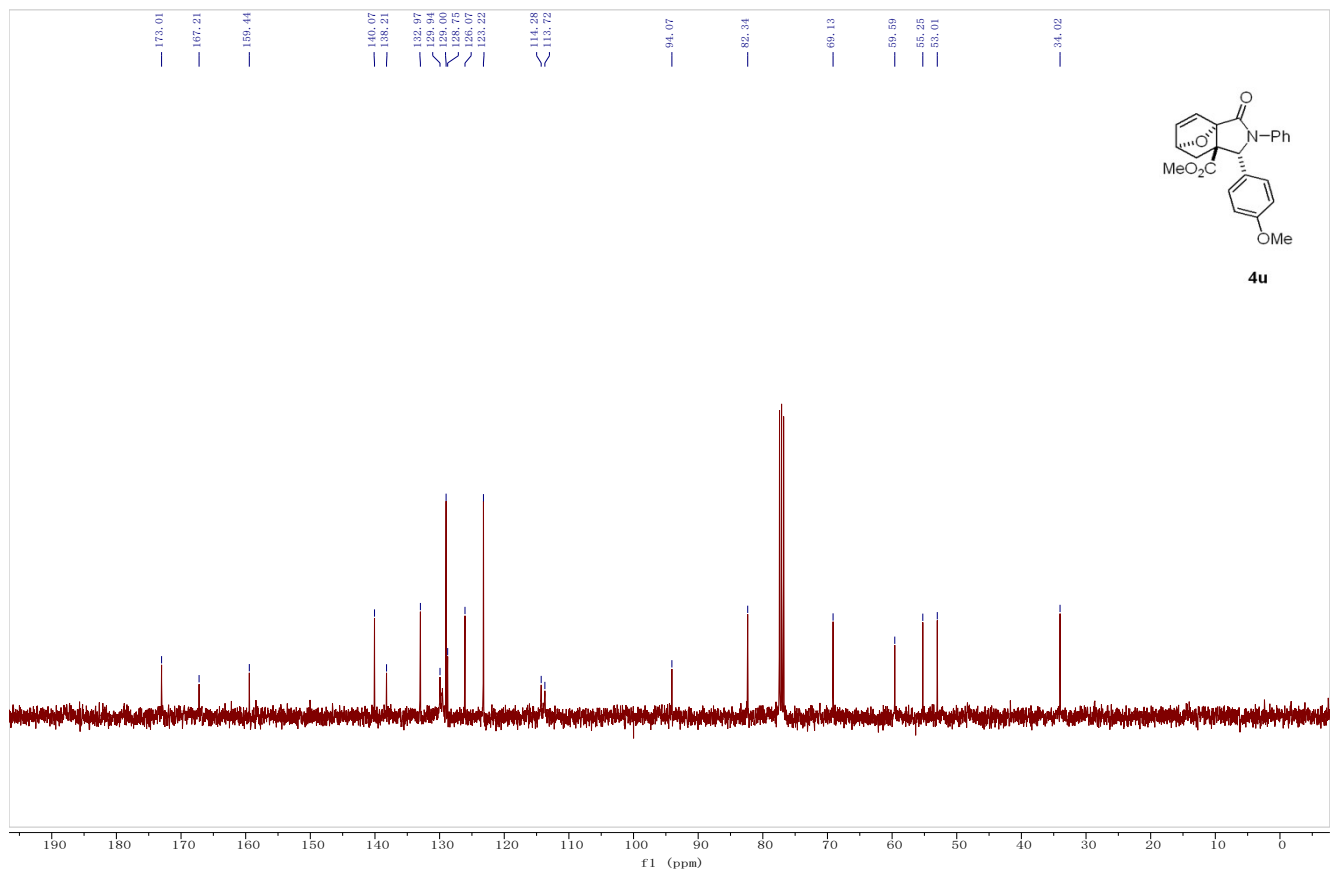
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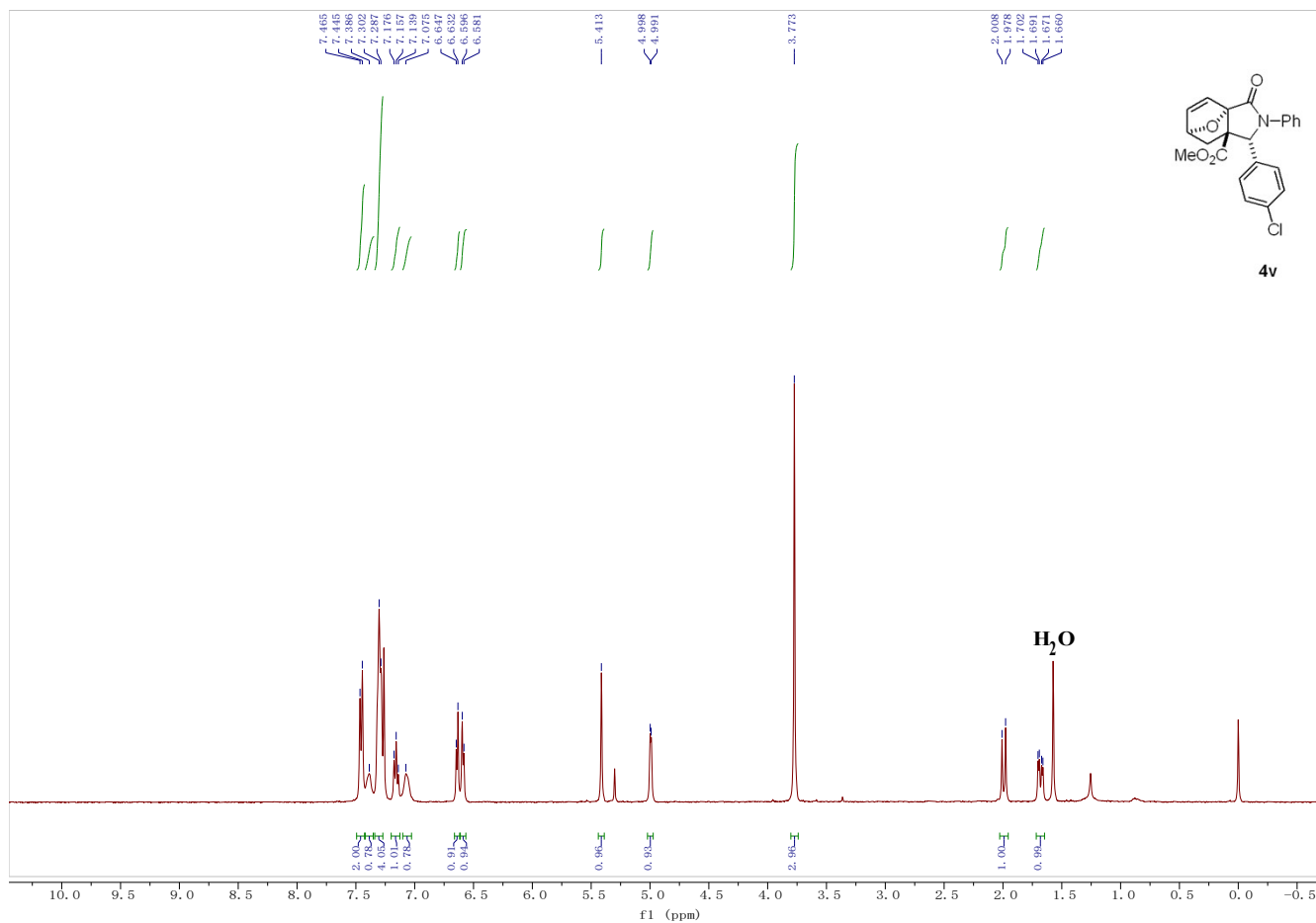
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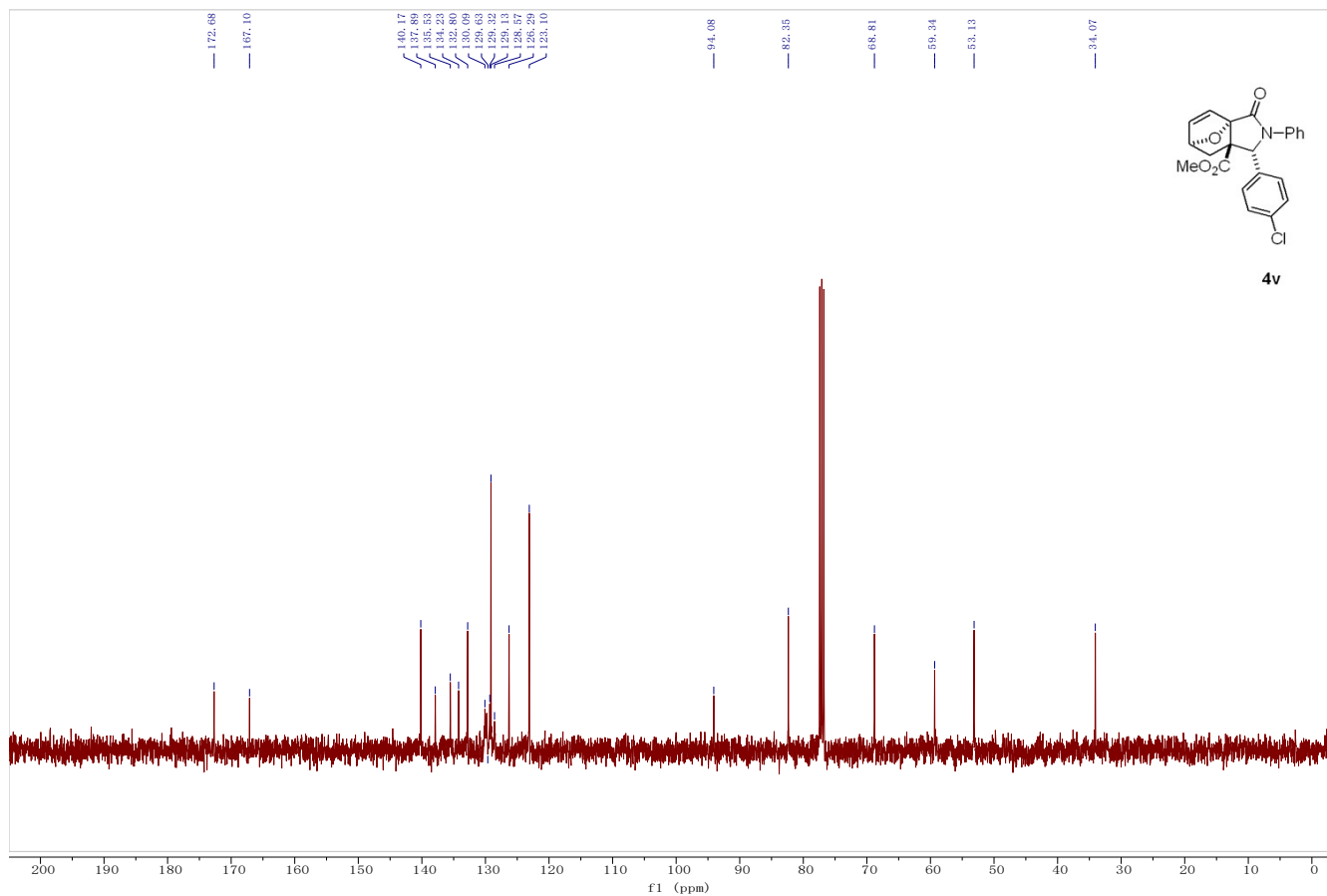
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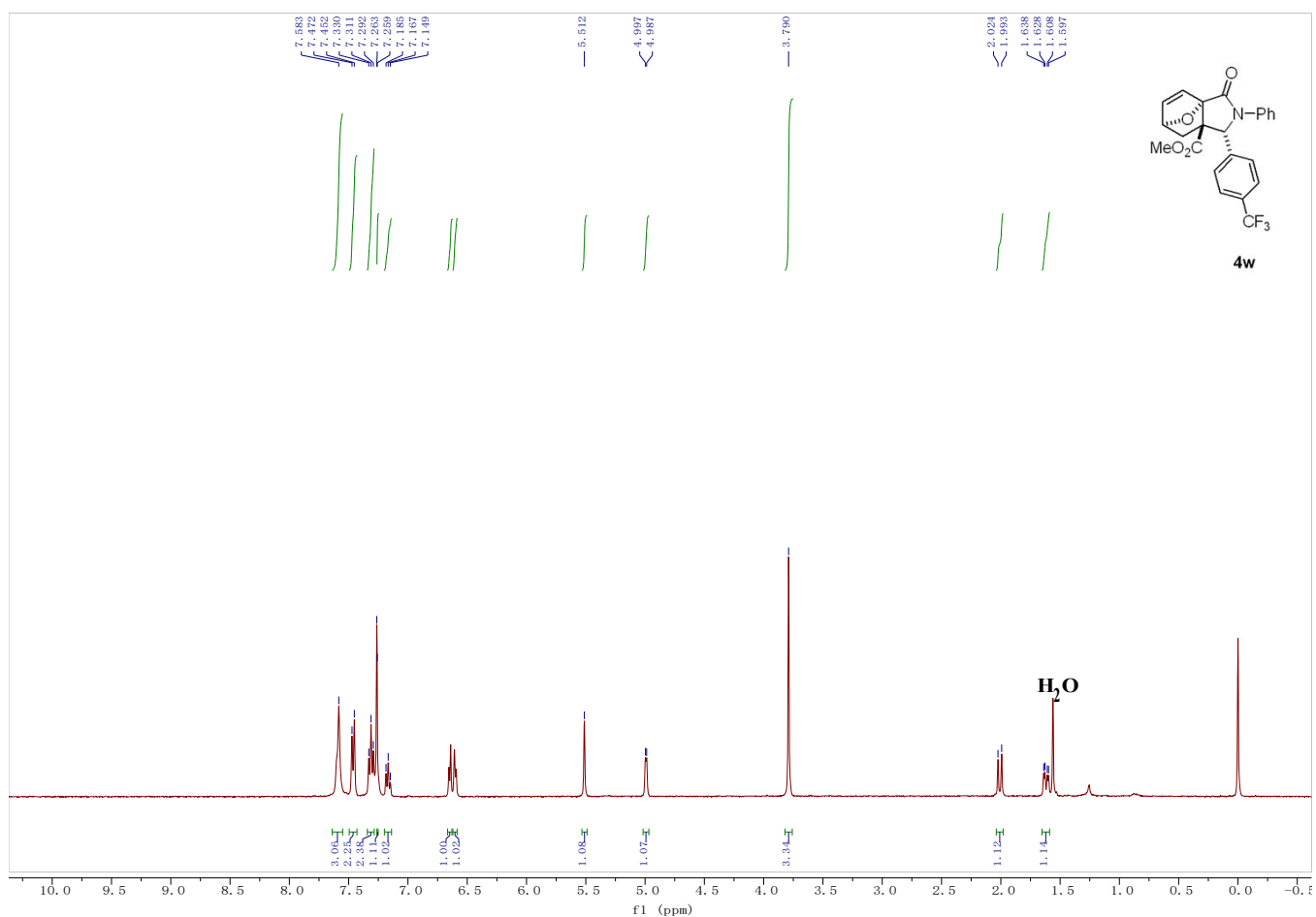
^1H NMR (400 MHz) in CDCl_3



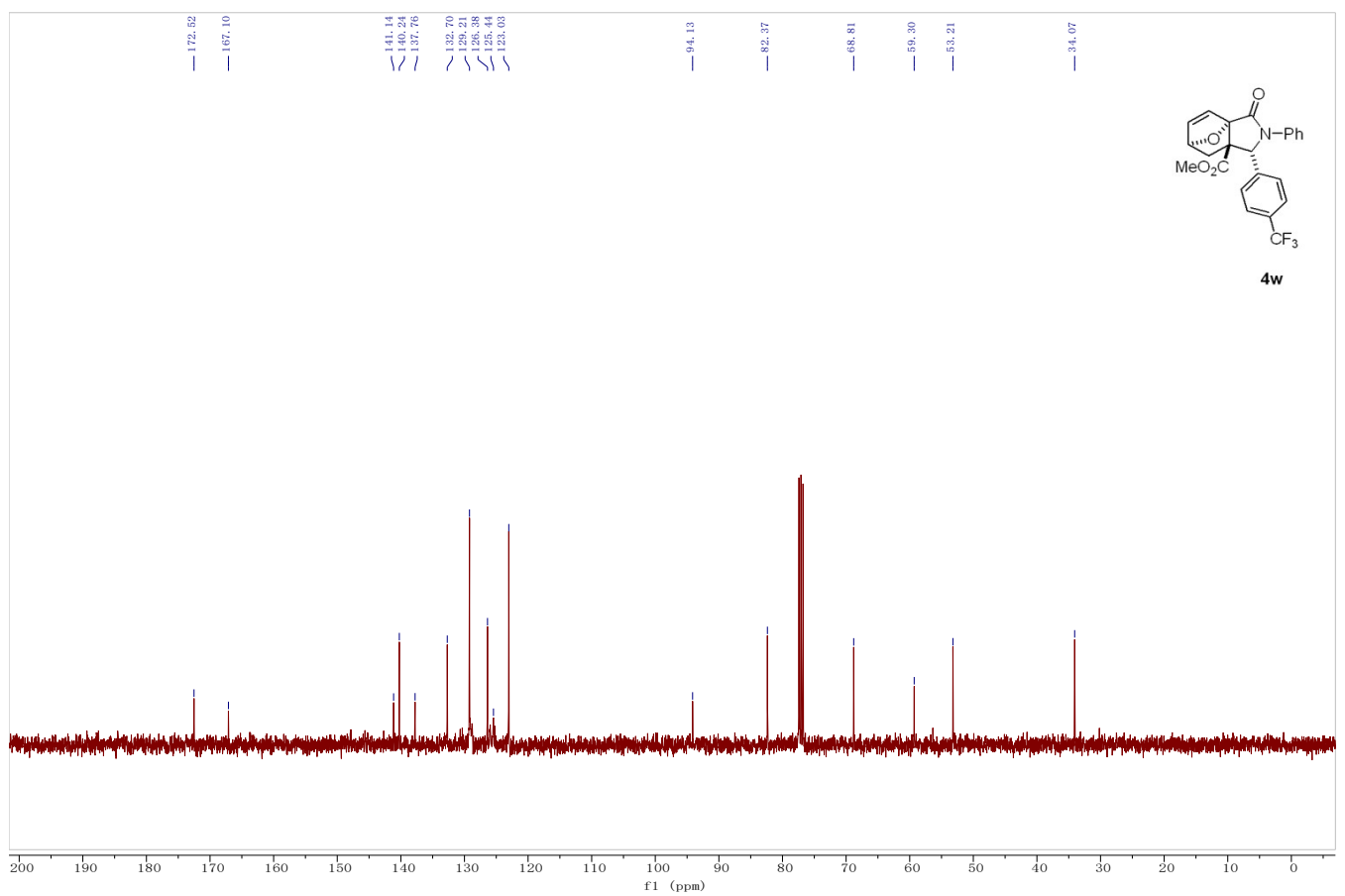
^{13}C NMR (101 MHz) in CDCl_3



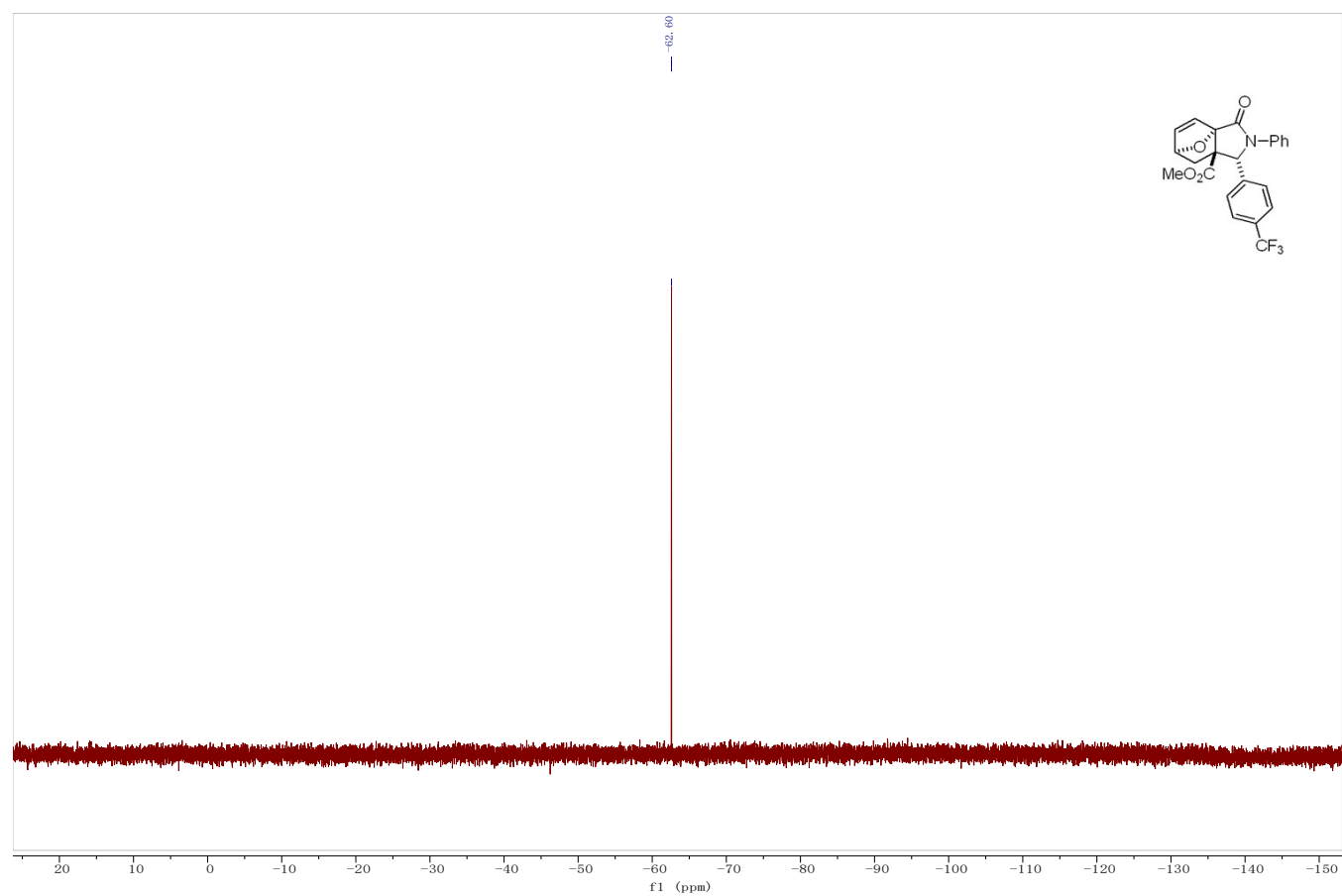
^1H NMR (400 MHz) in CDCl_3



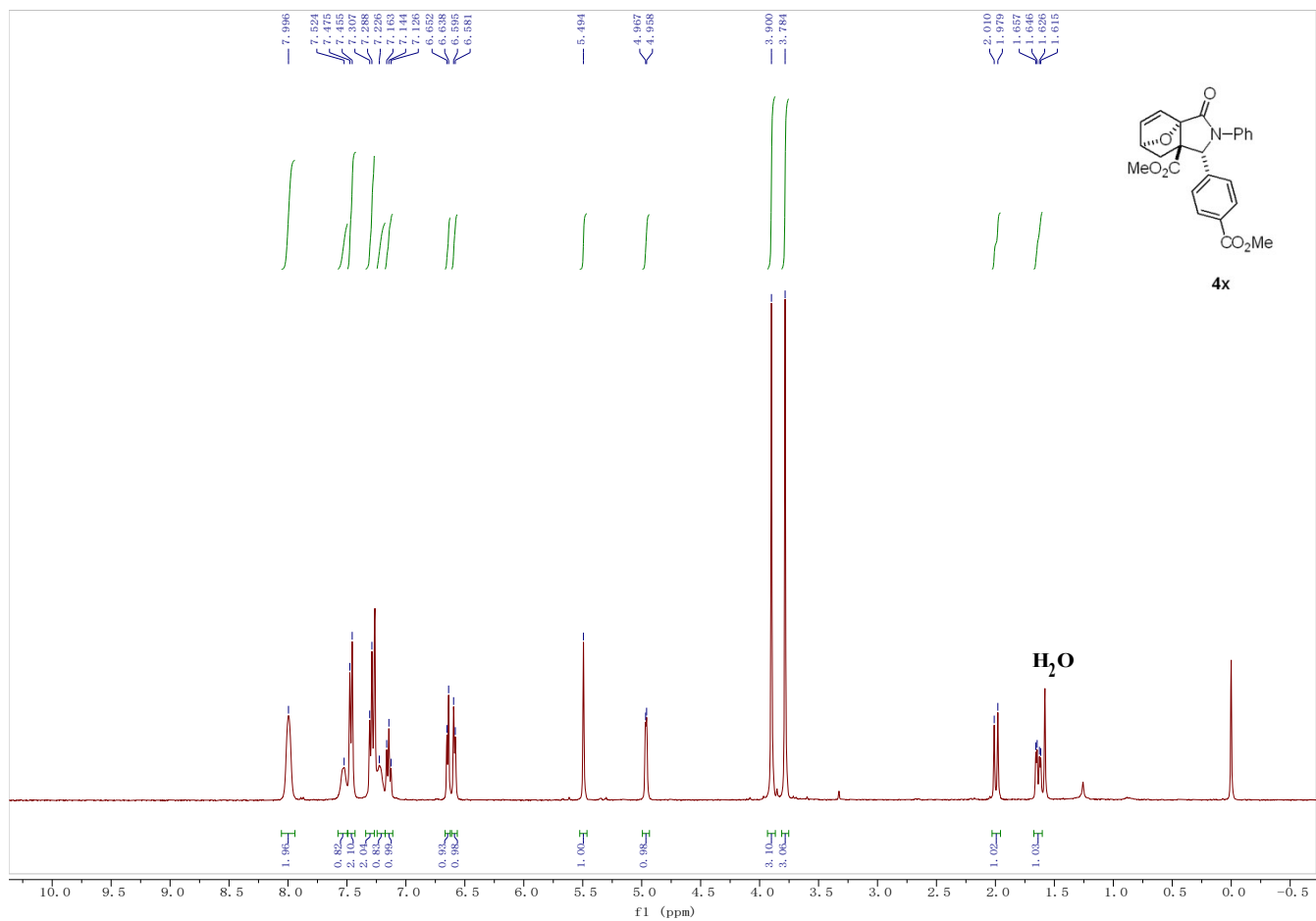
^{13}C NMR (101 MHz) in CDCl_3



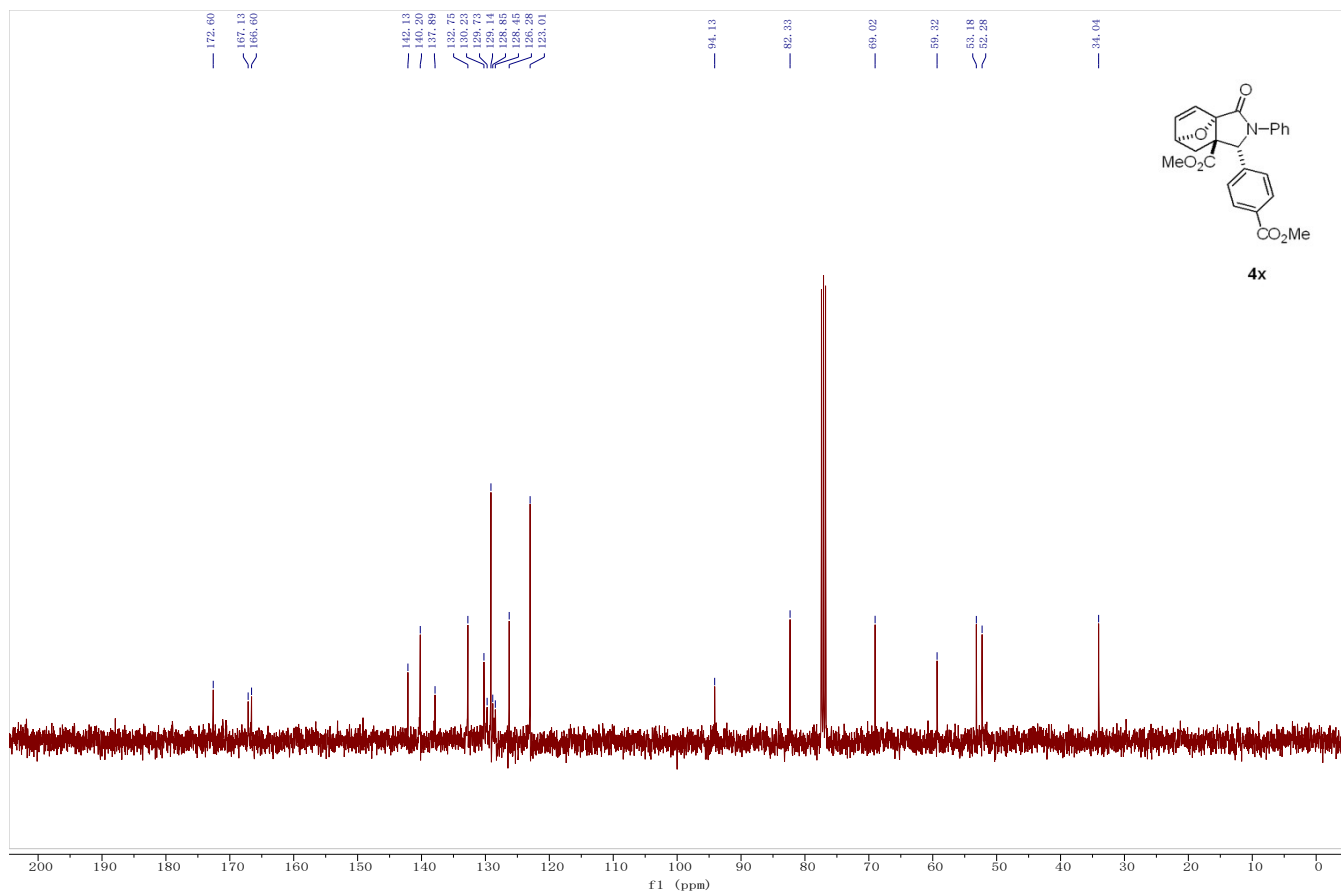
^{19}F NMR (376 MHz) in CDCl_3



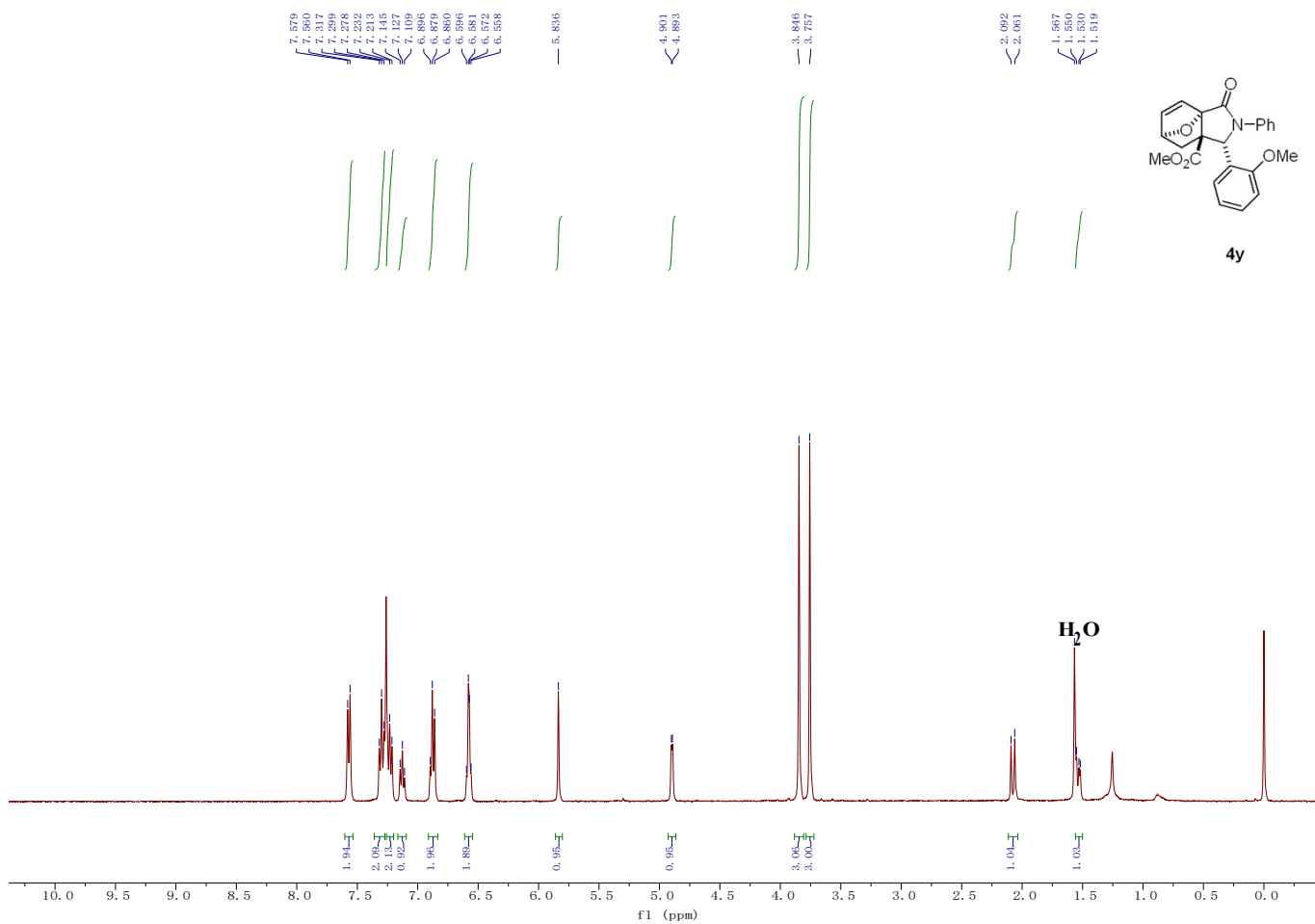
^1H NMR (400 MHz) in CDCl_3



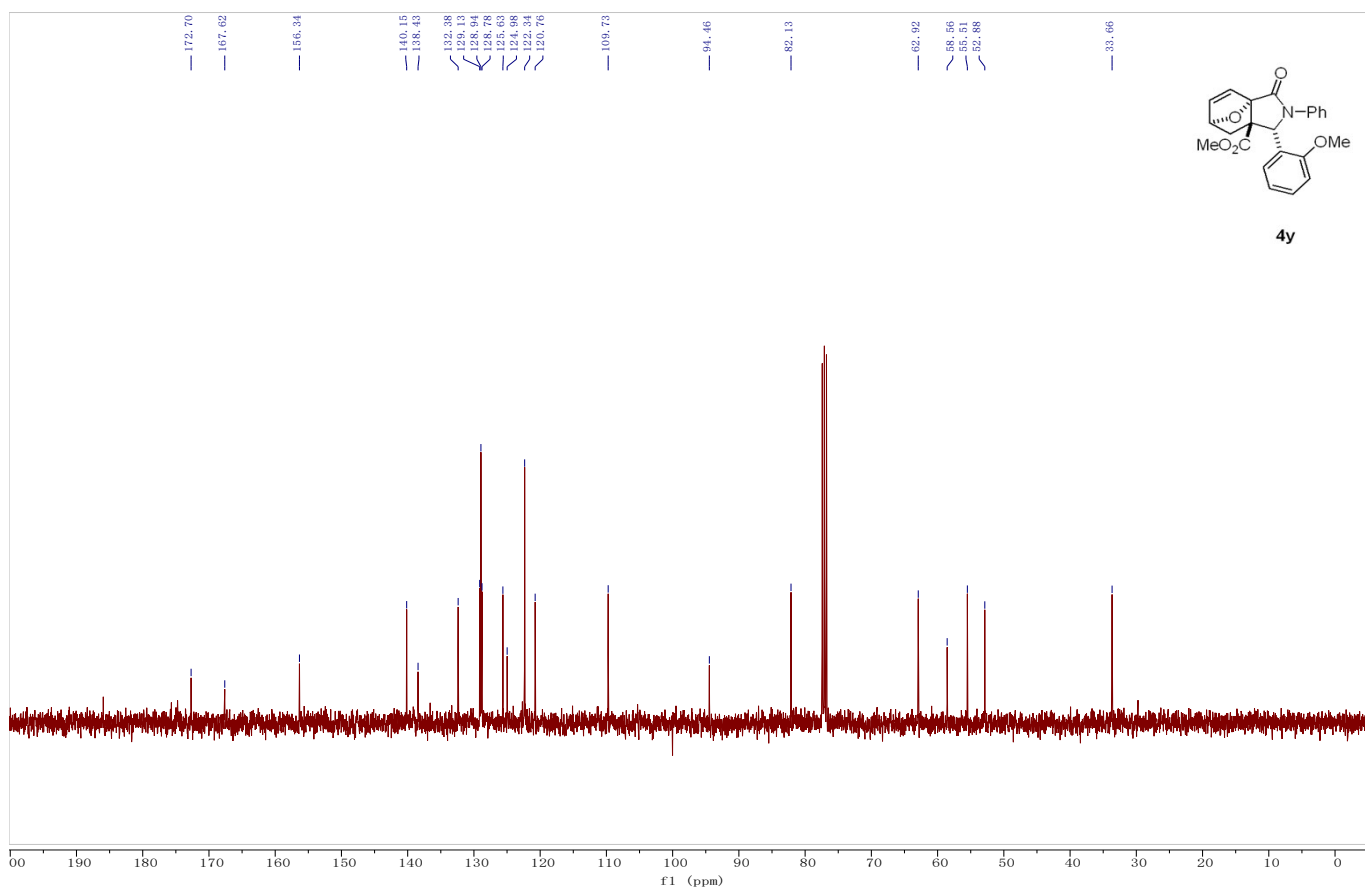
^{13}C NMR (101 MHz) in CDCl_3



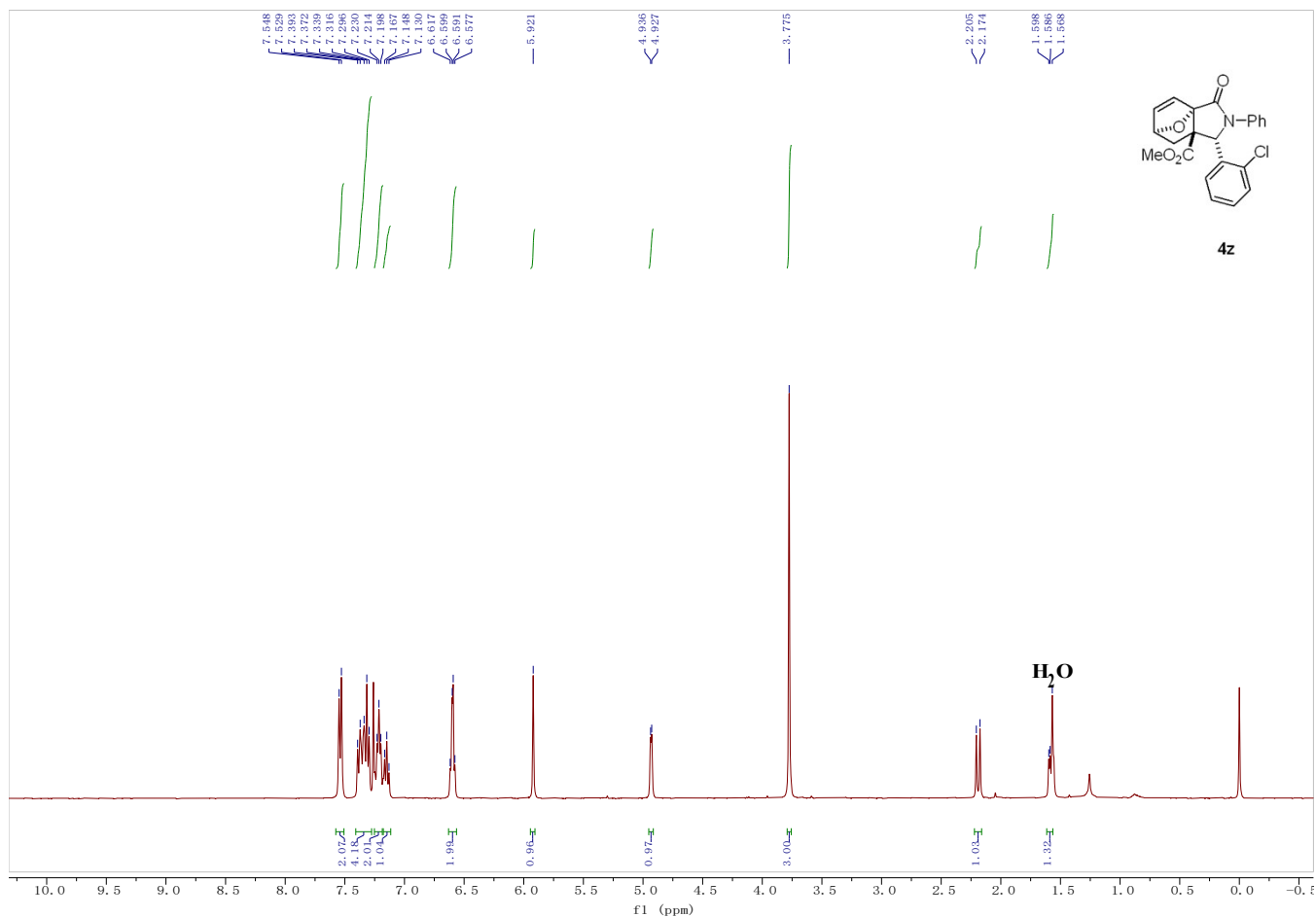
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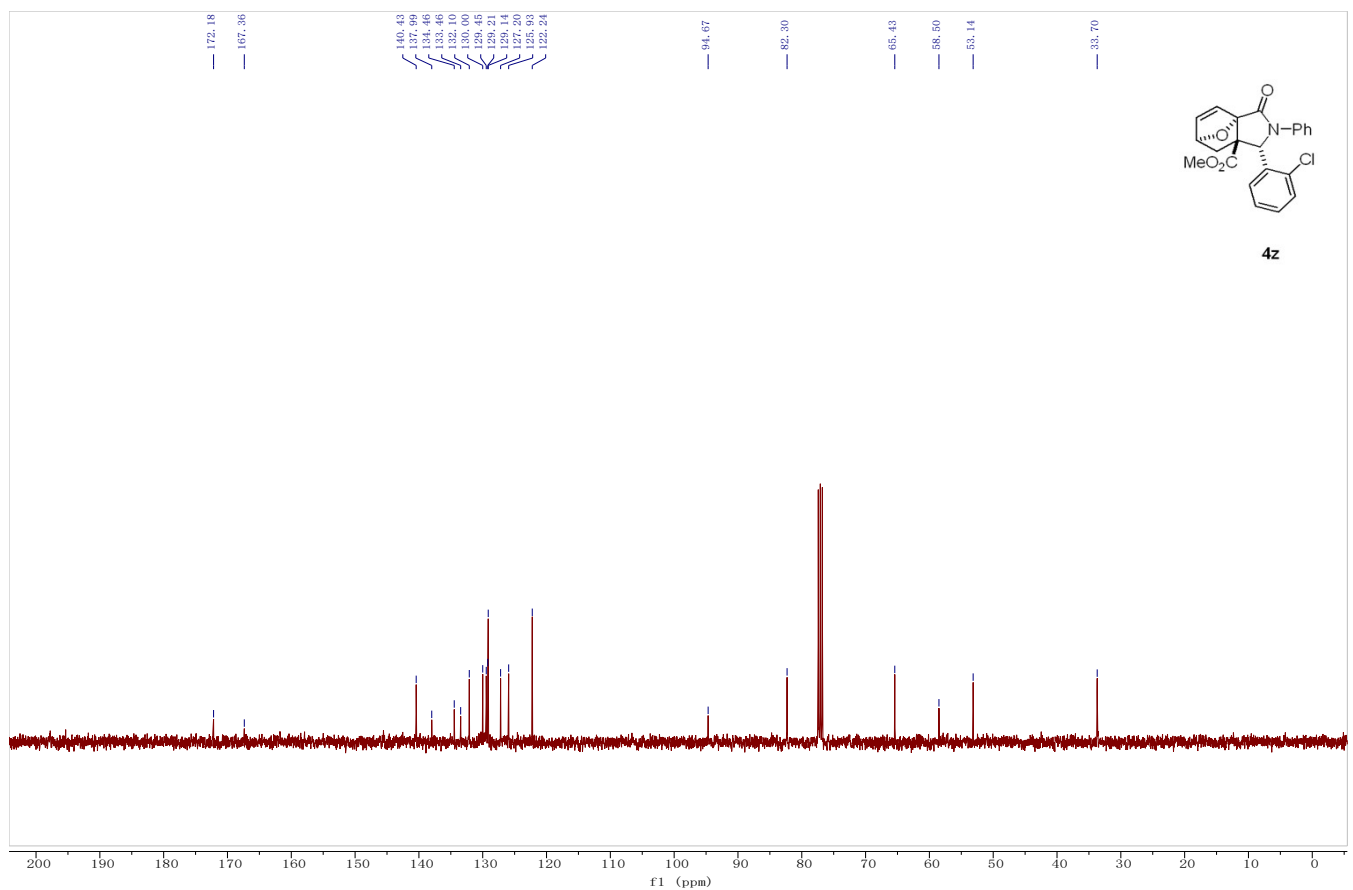
^{13}C NMR (101 MHz) in CDCl_3



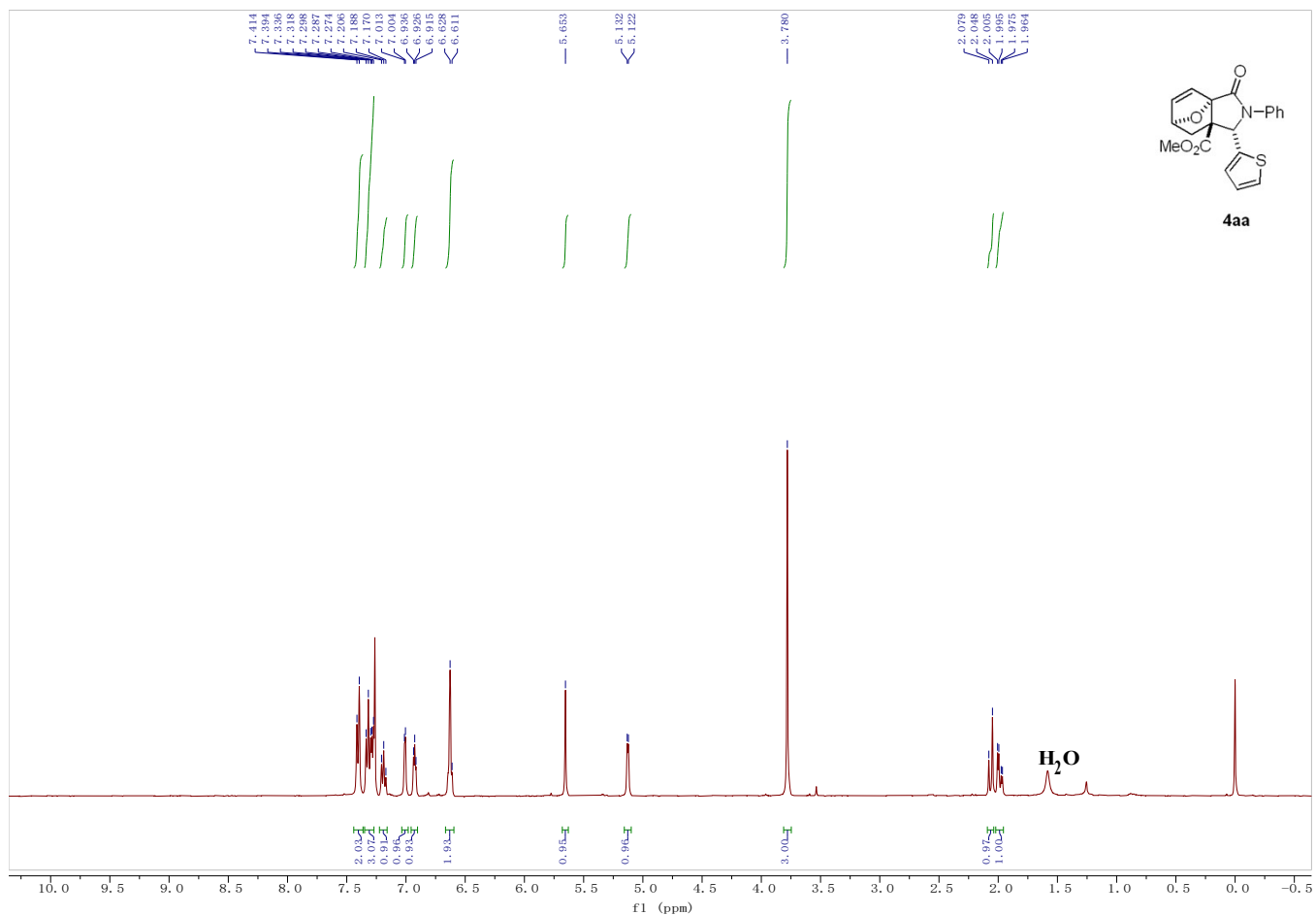
^1H NMR (400 MHz) in CDCl_3



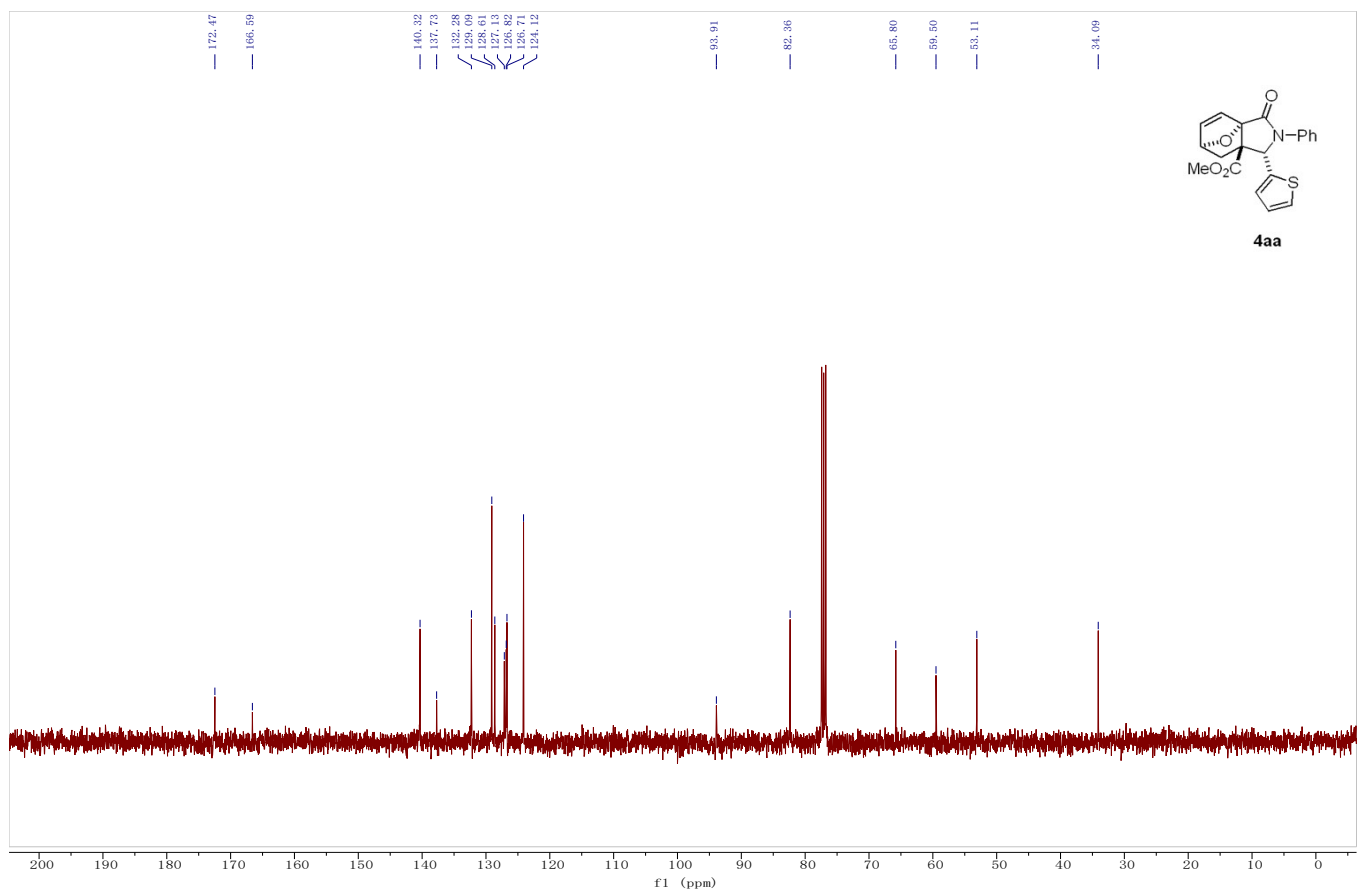
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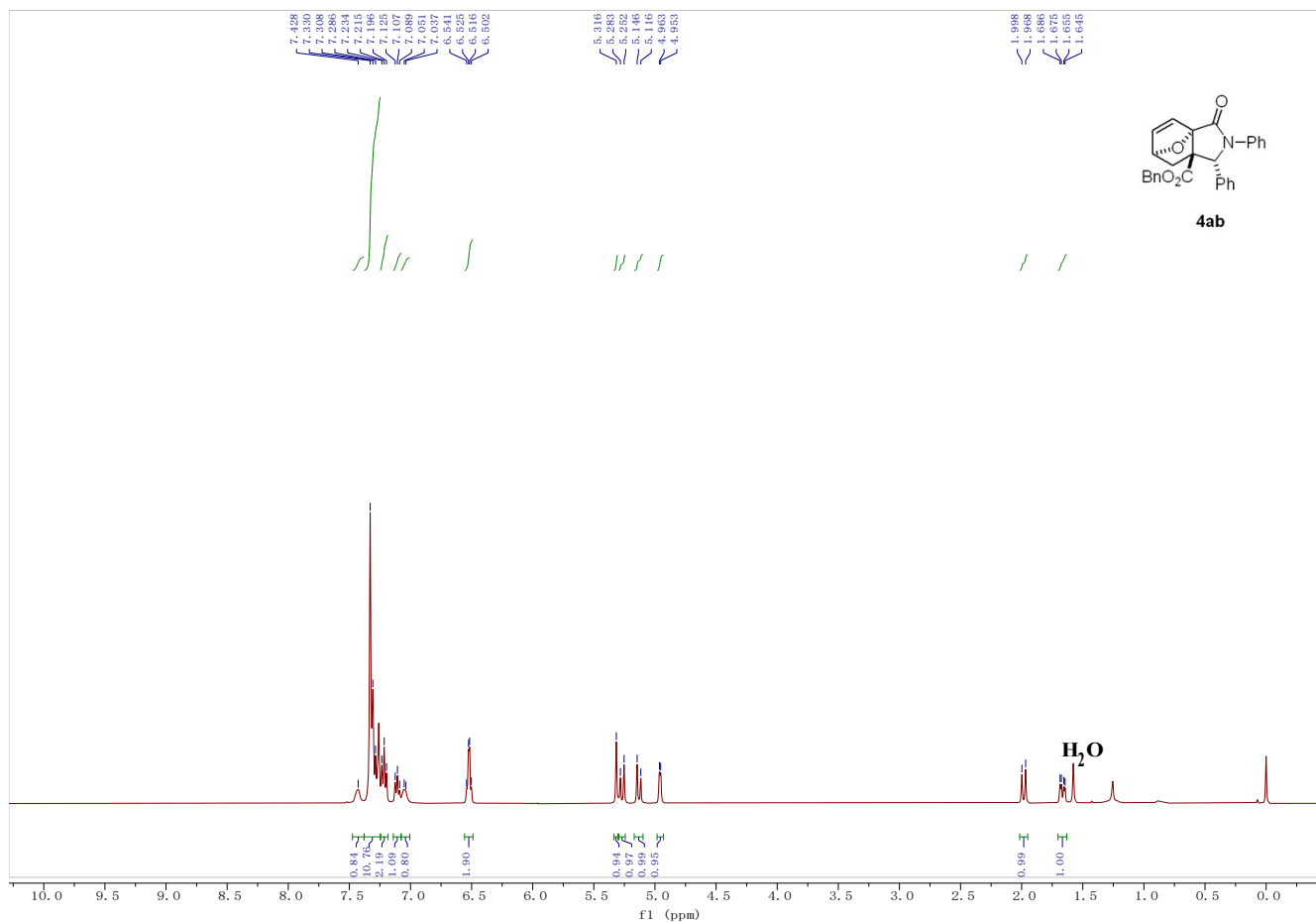
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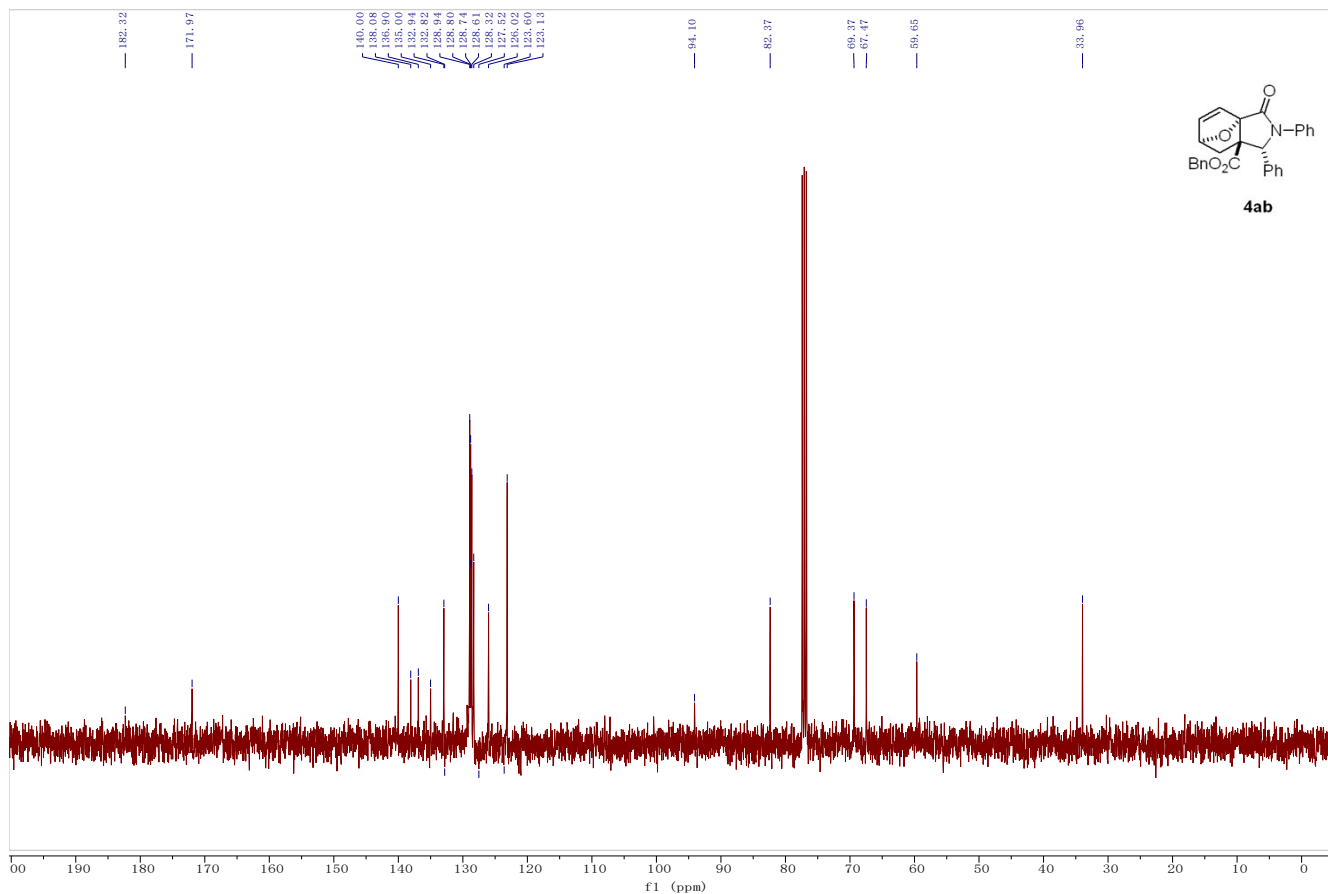
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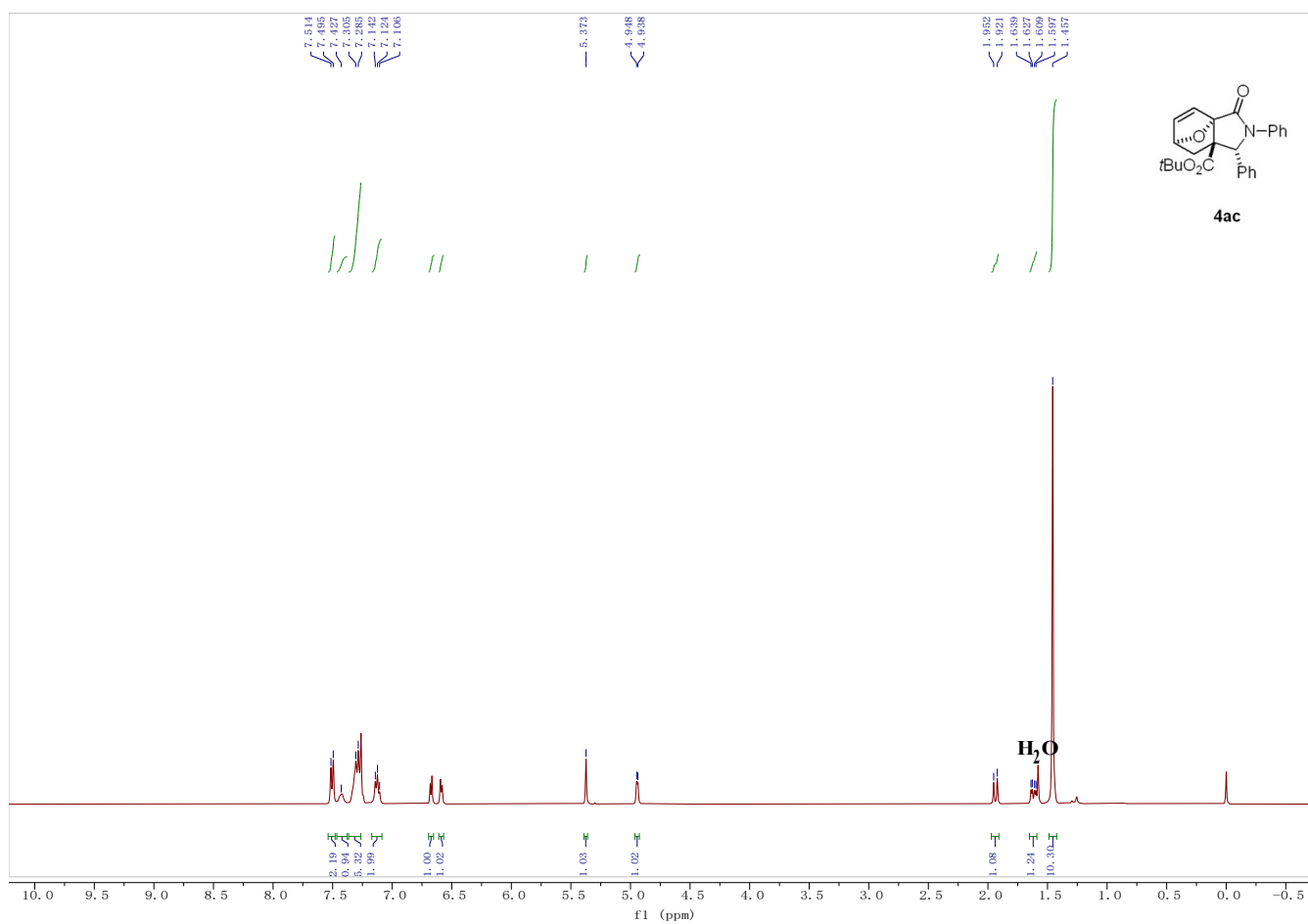
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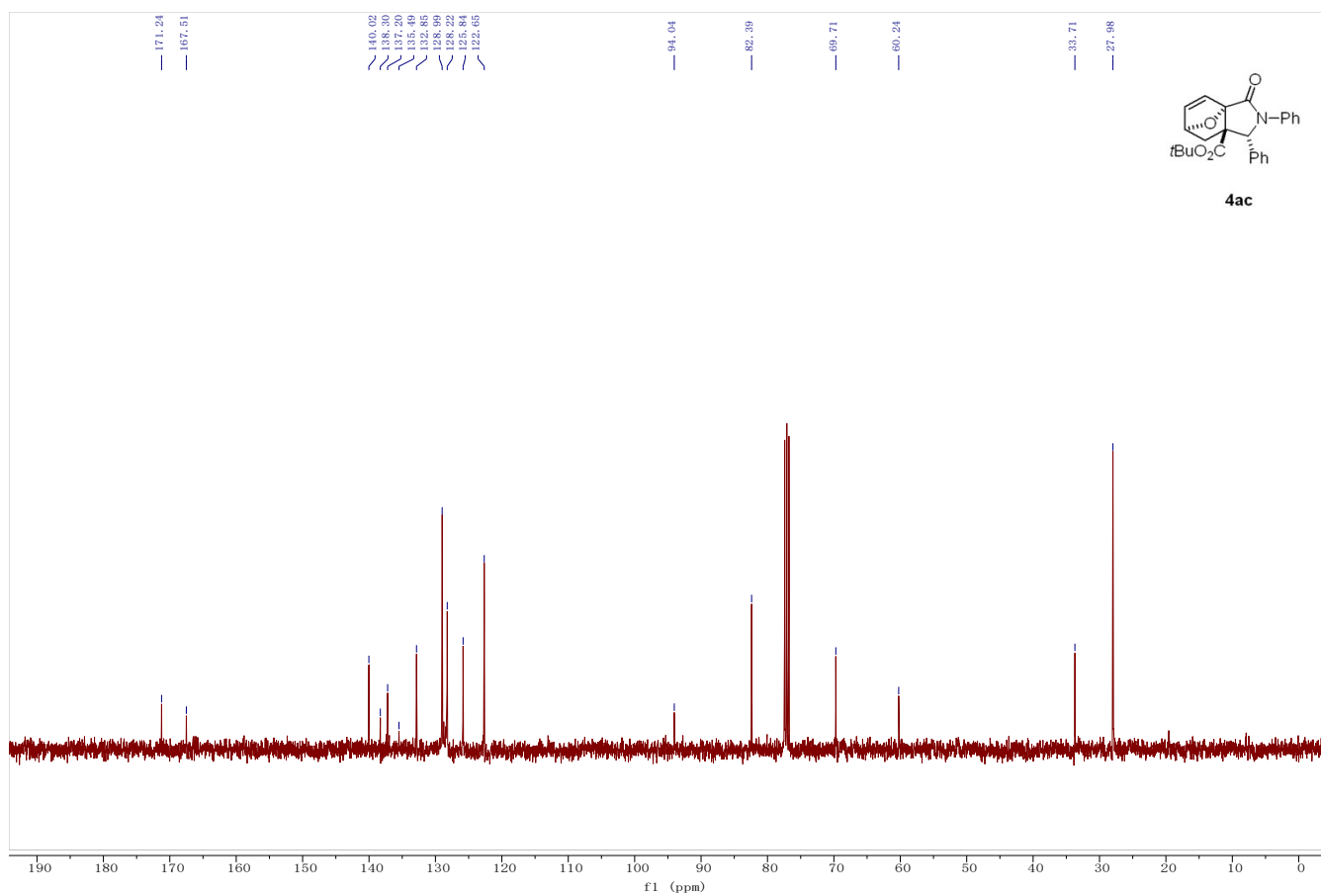
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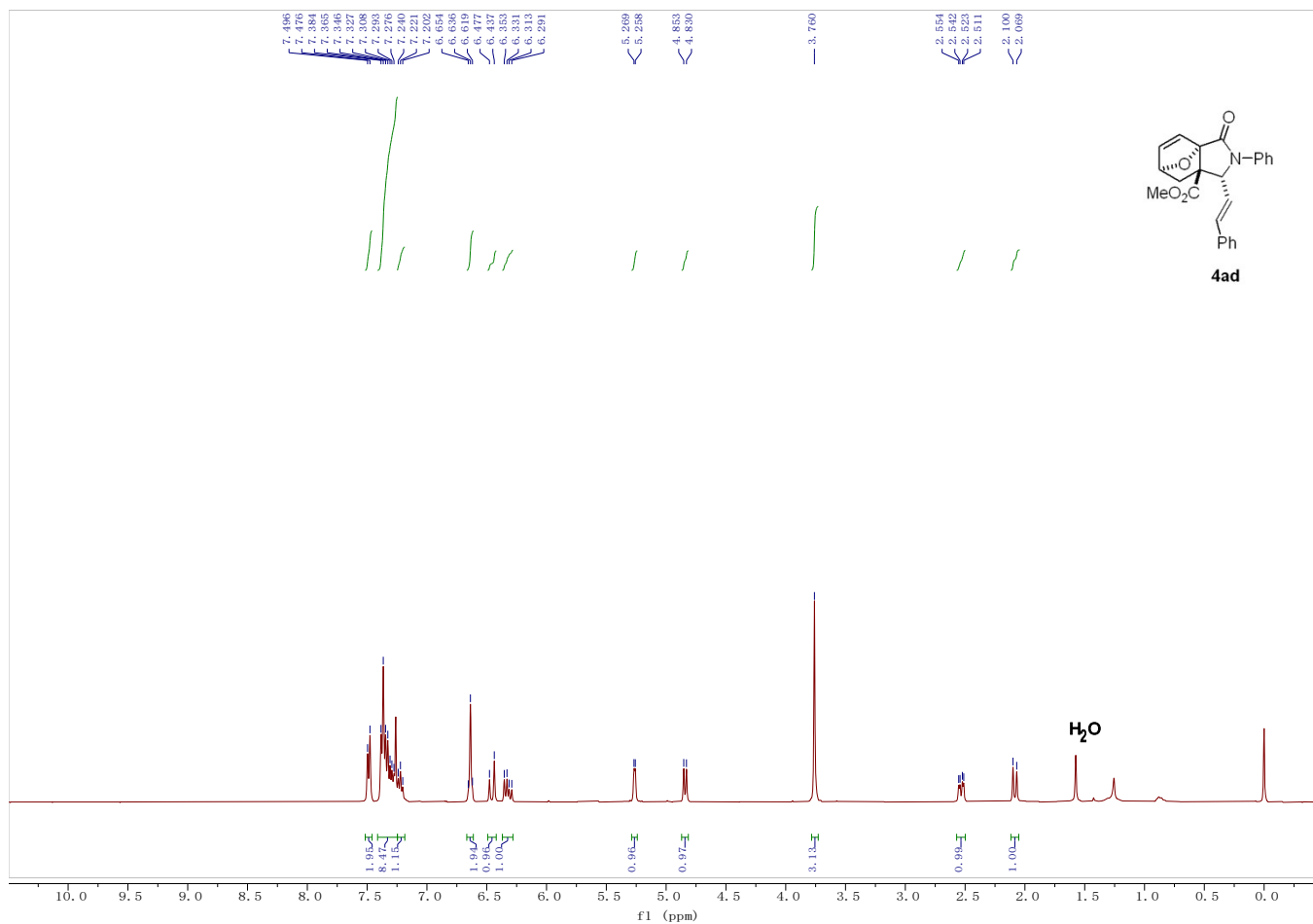
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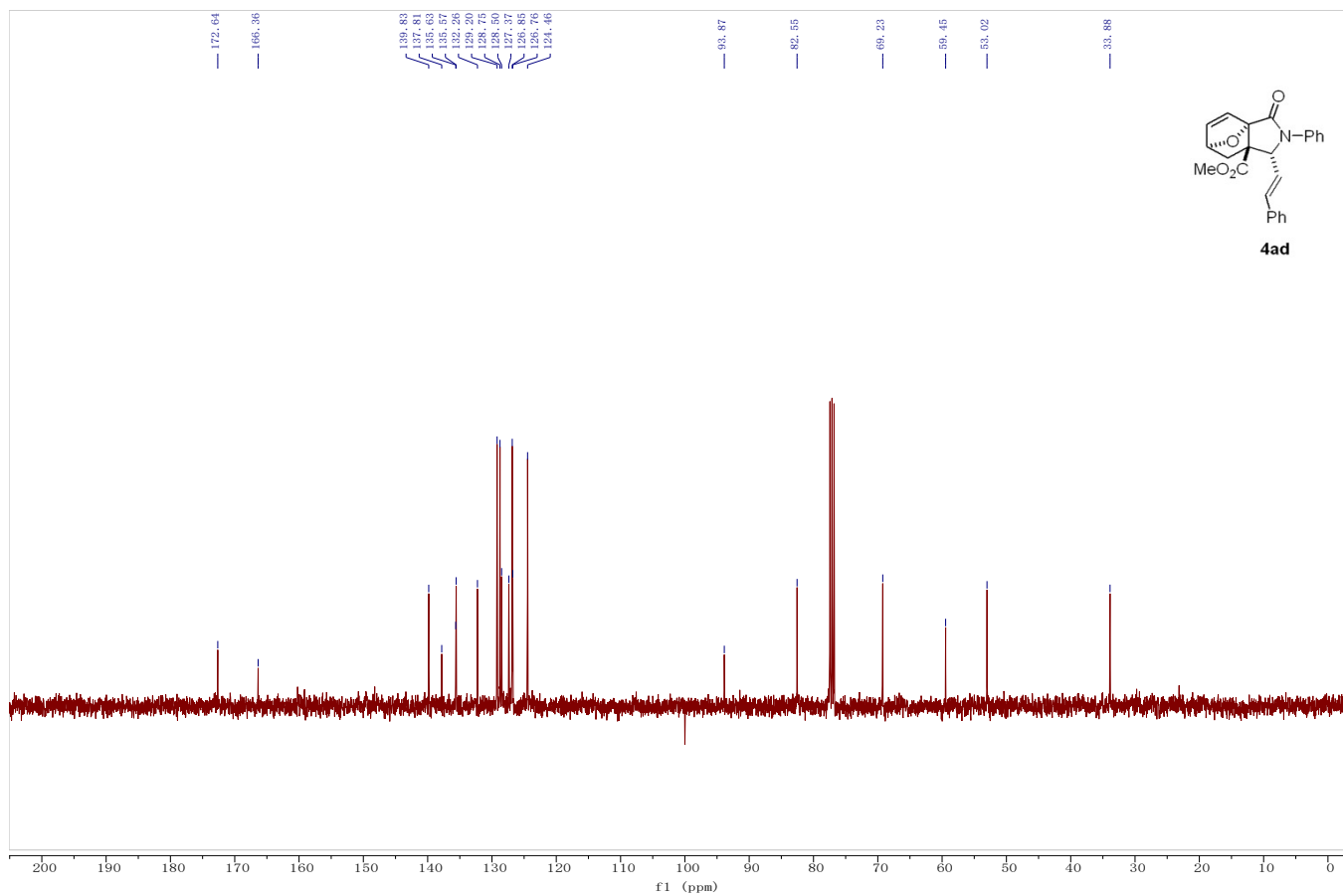
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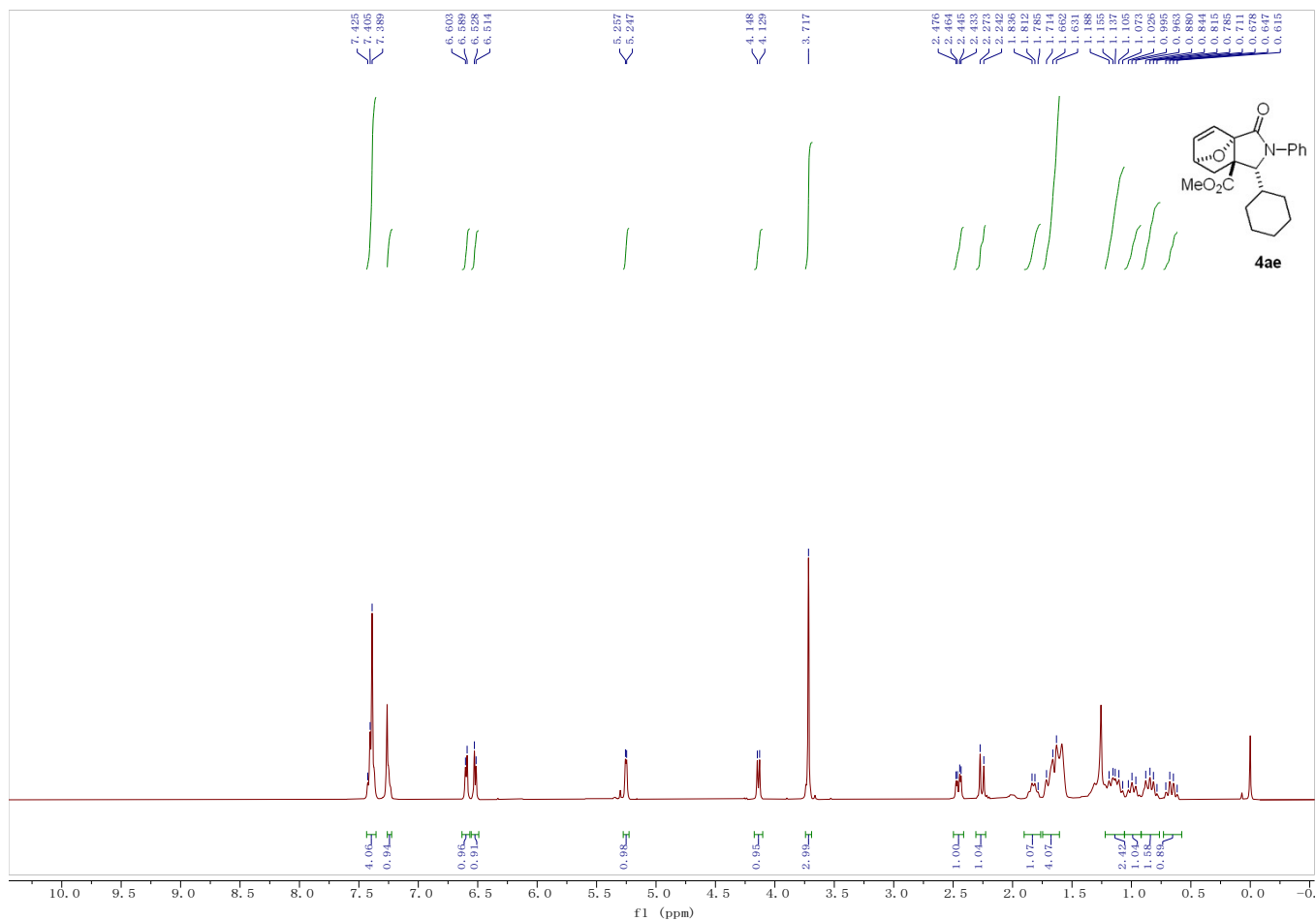
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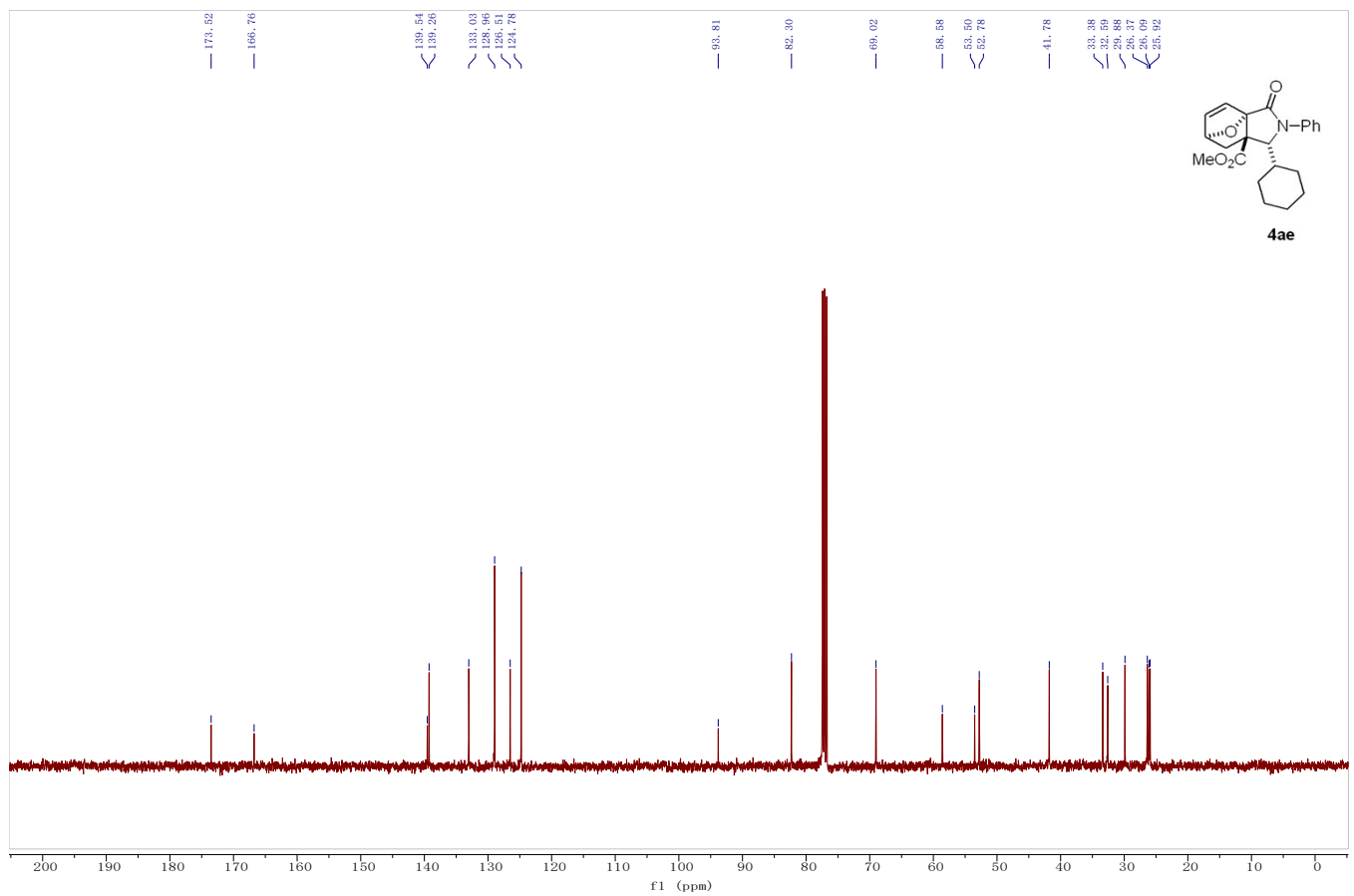
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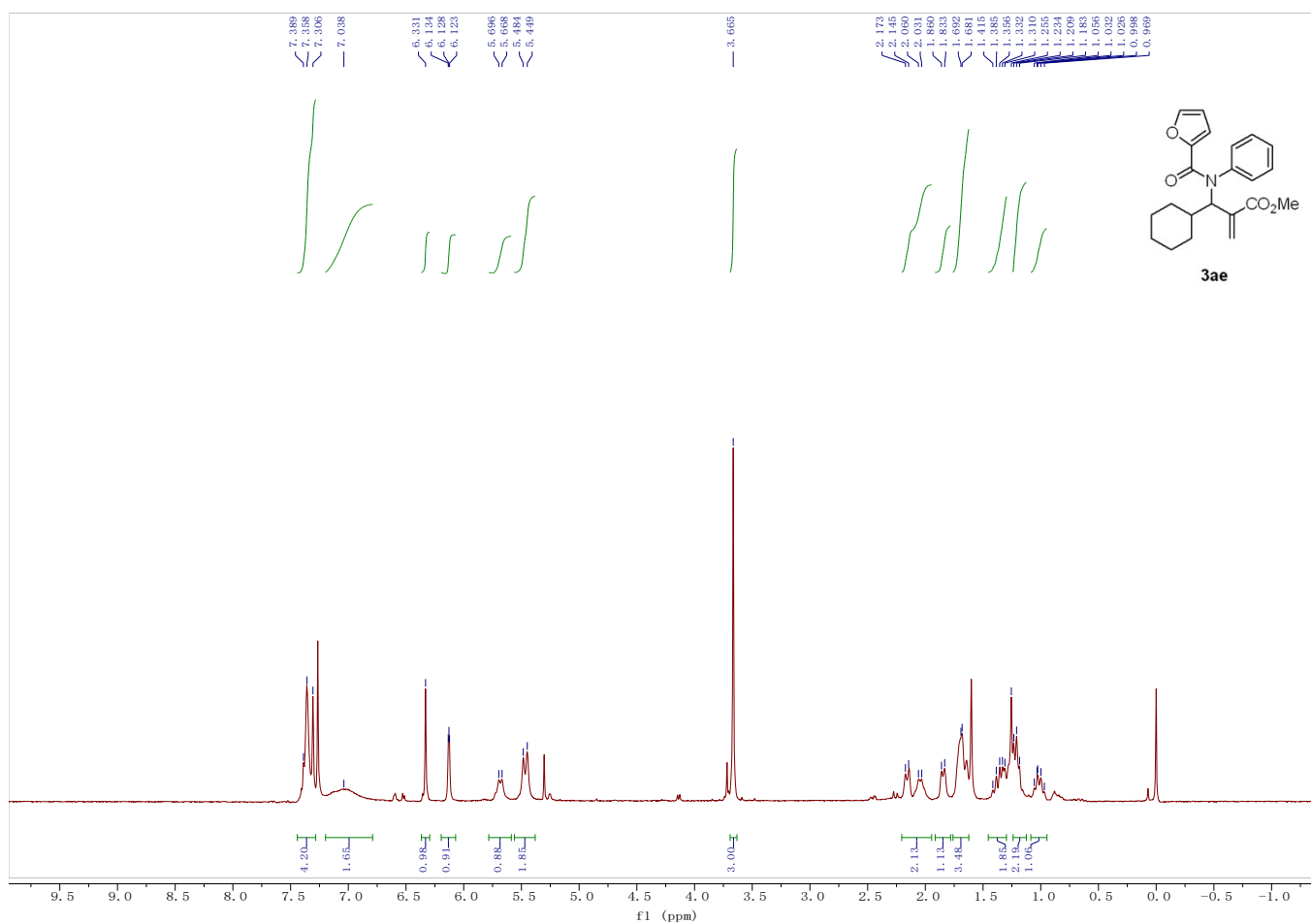
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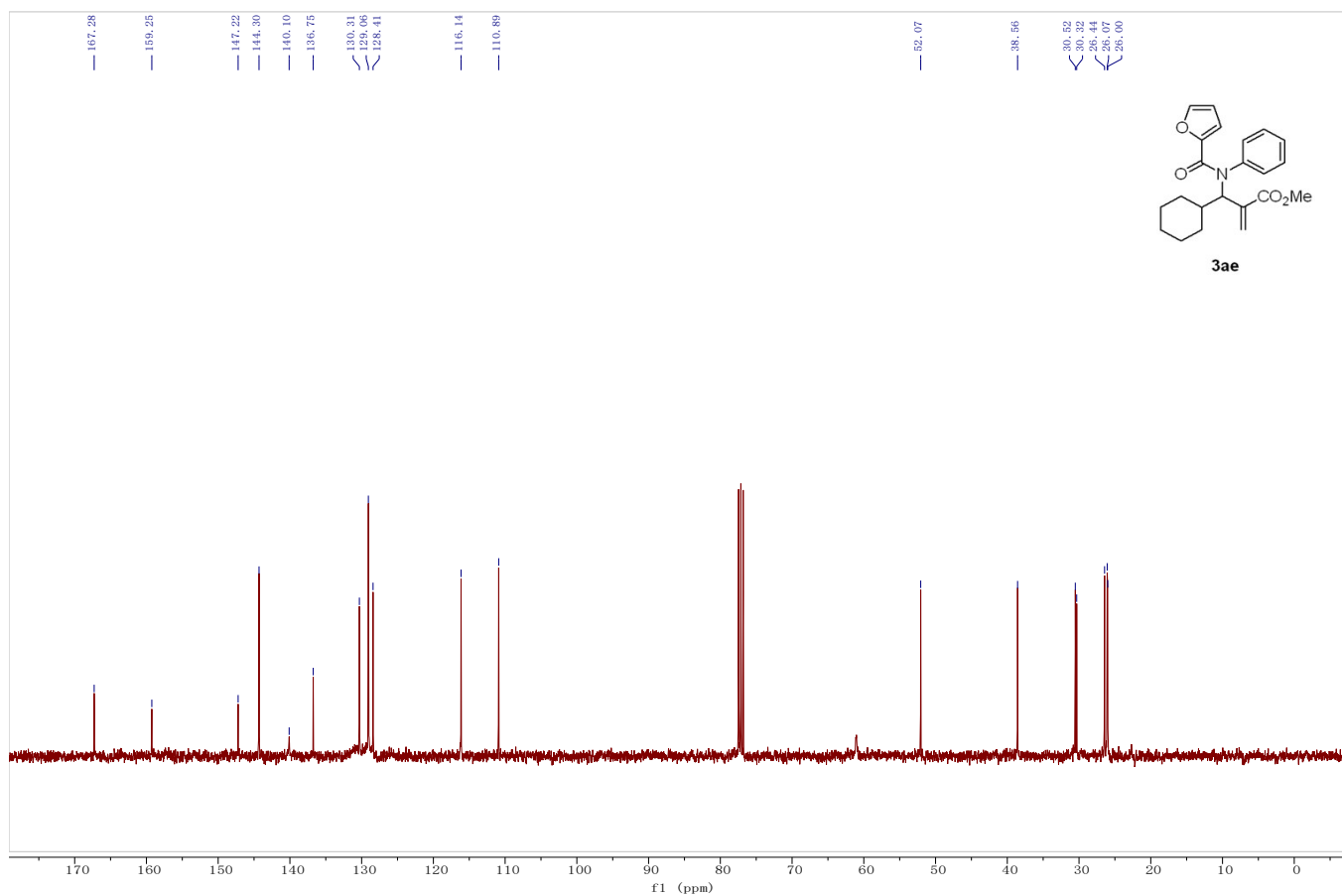
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^1H NMR (400 MHz) in CDCl_3

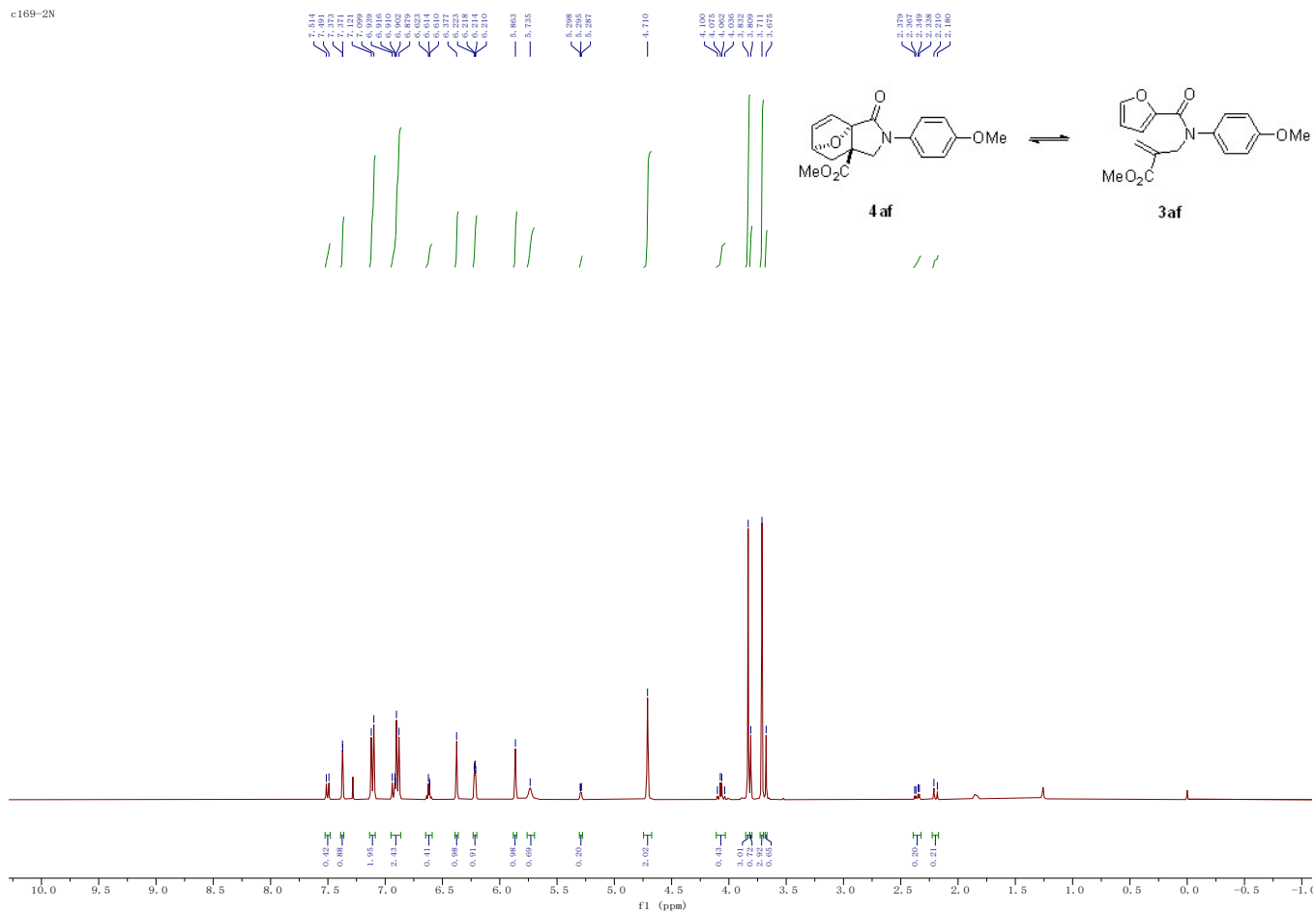


^{13}C NMR (101 MHz) in CDCl_3

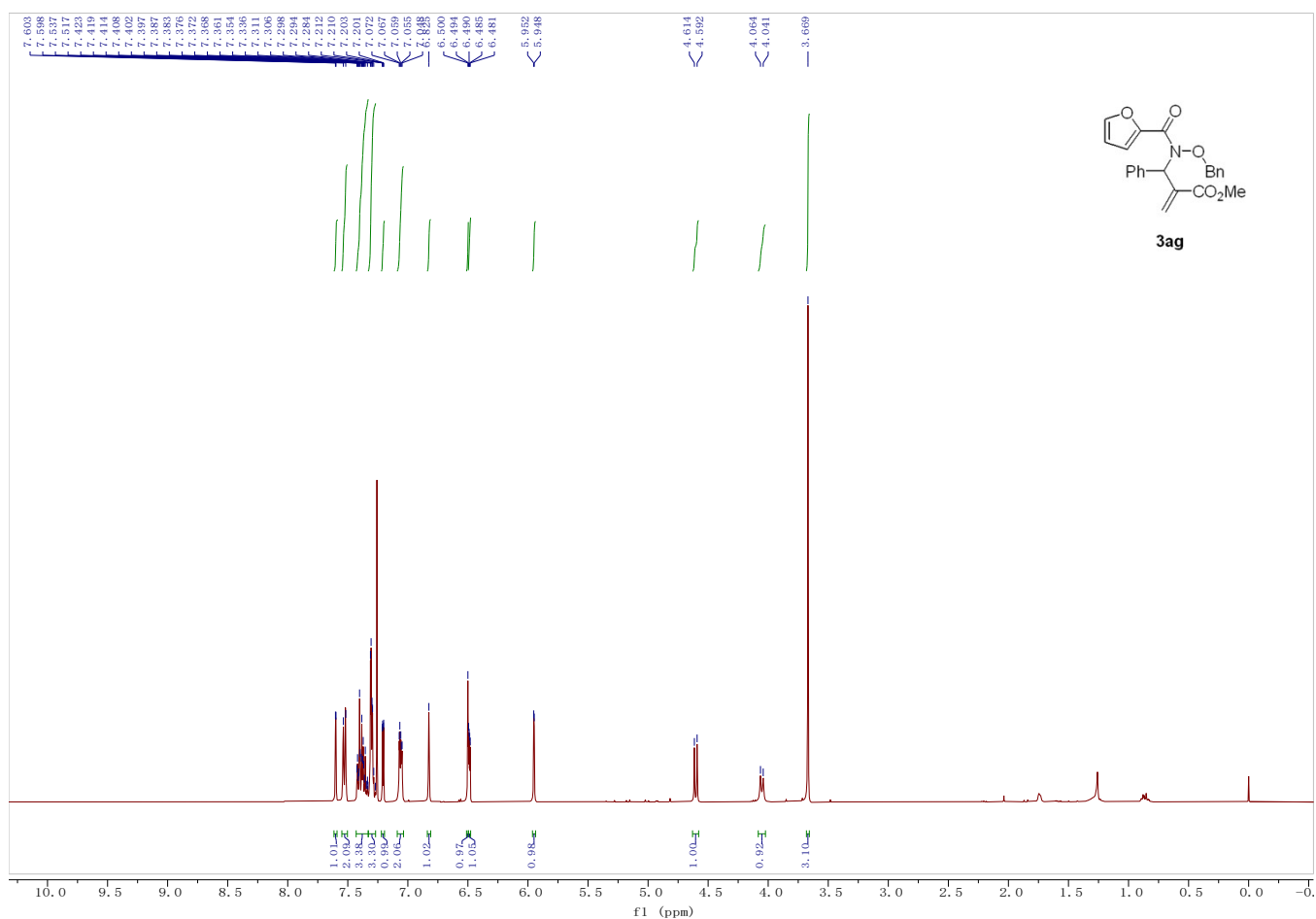


^1H NMR (400 MHz) in CDCl_3

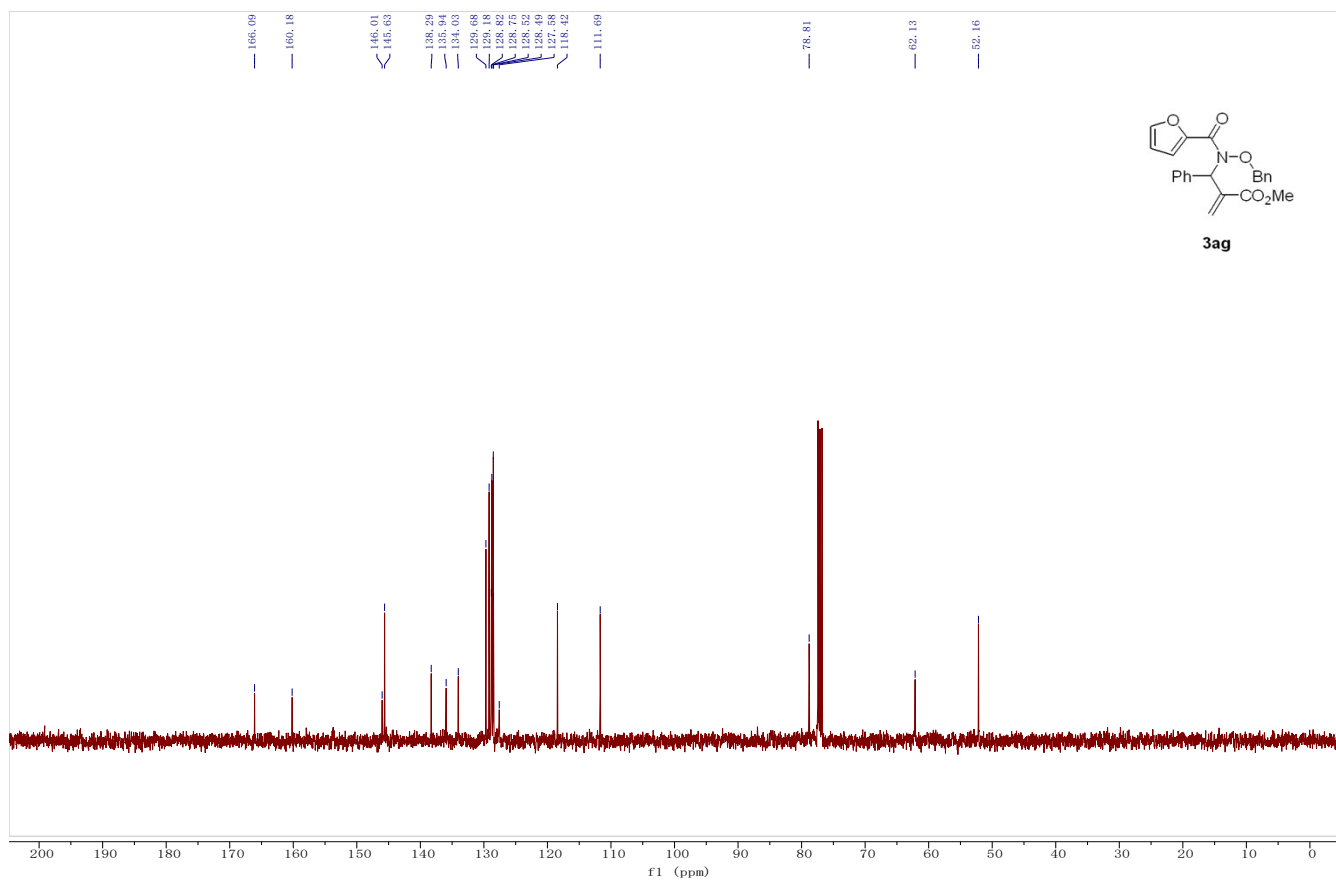
c169-2N



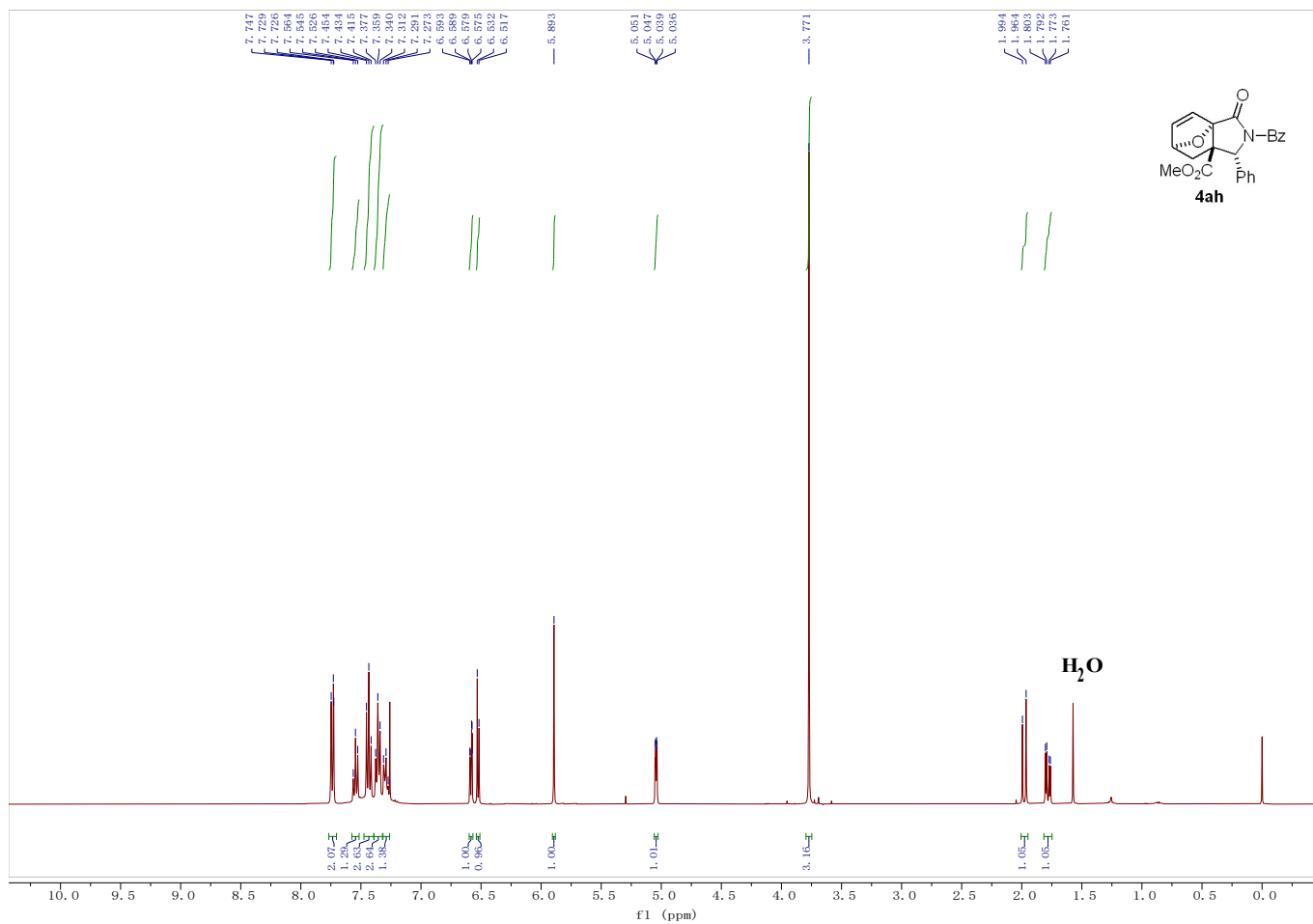
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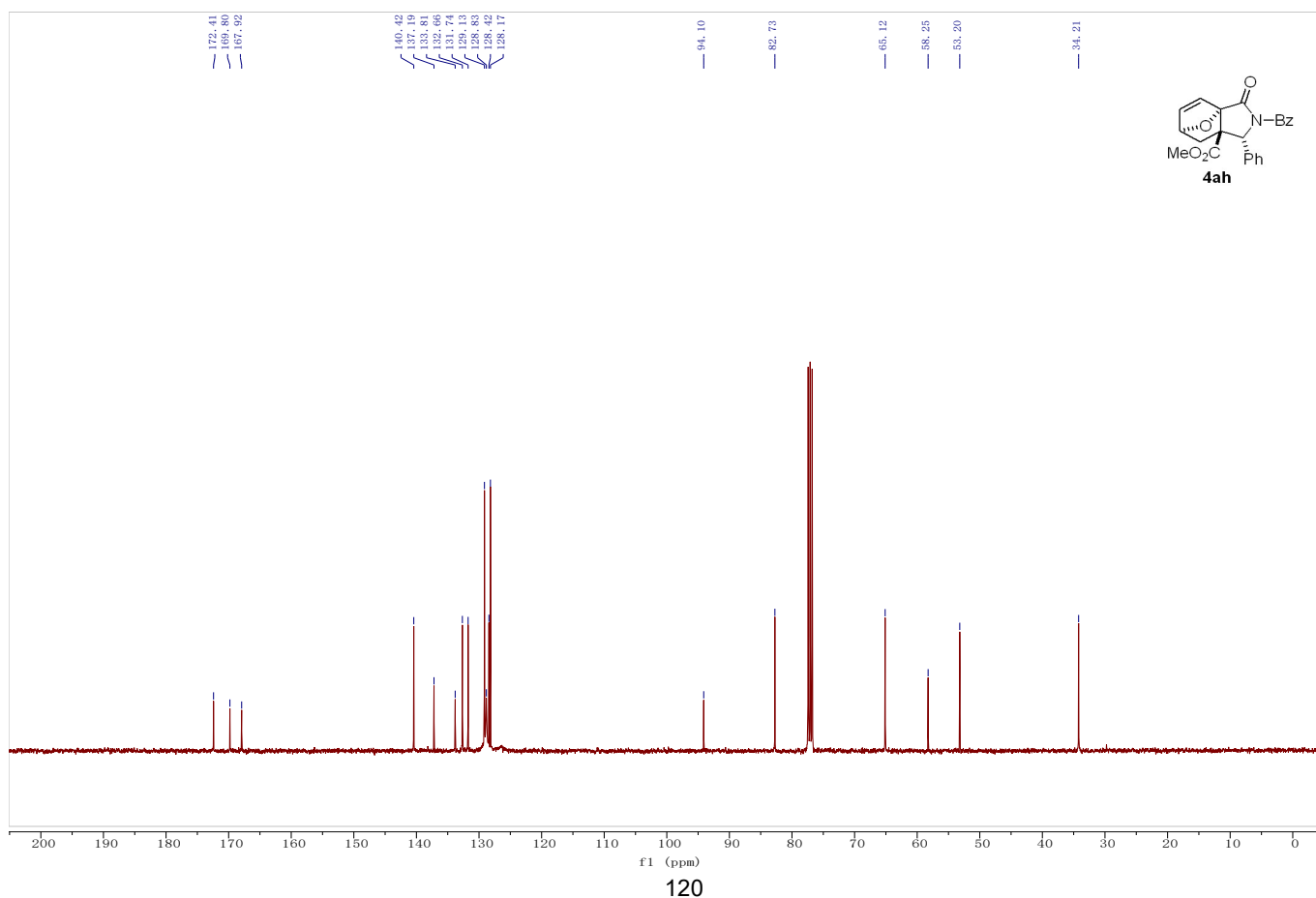
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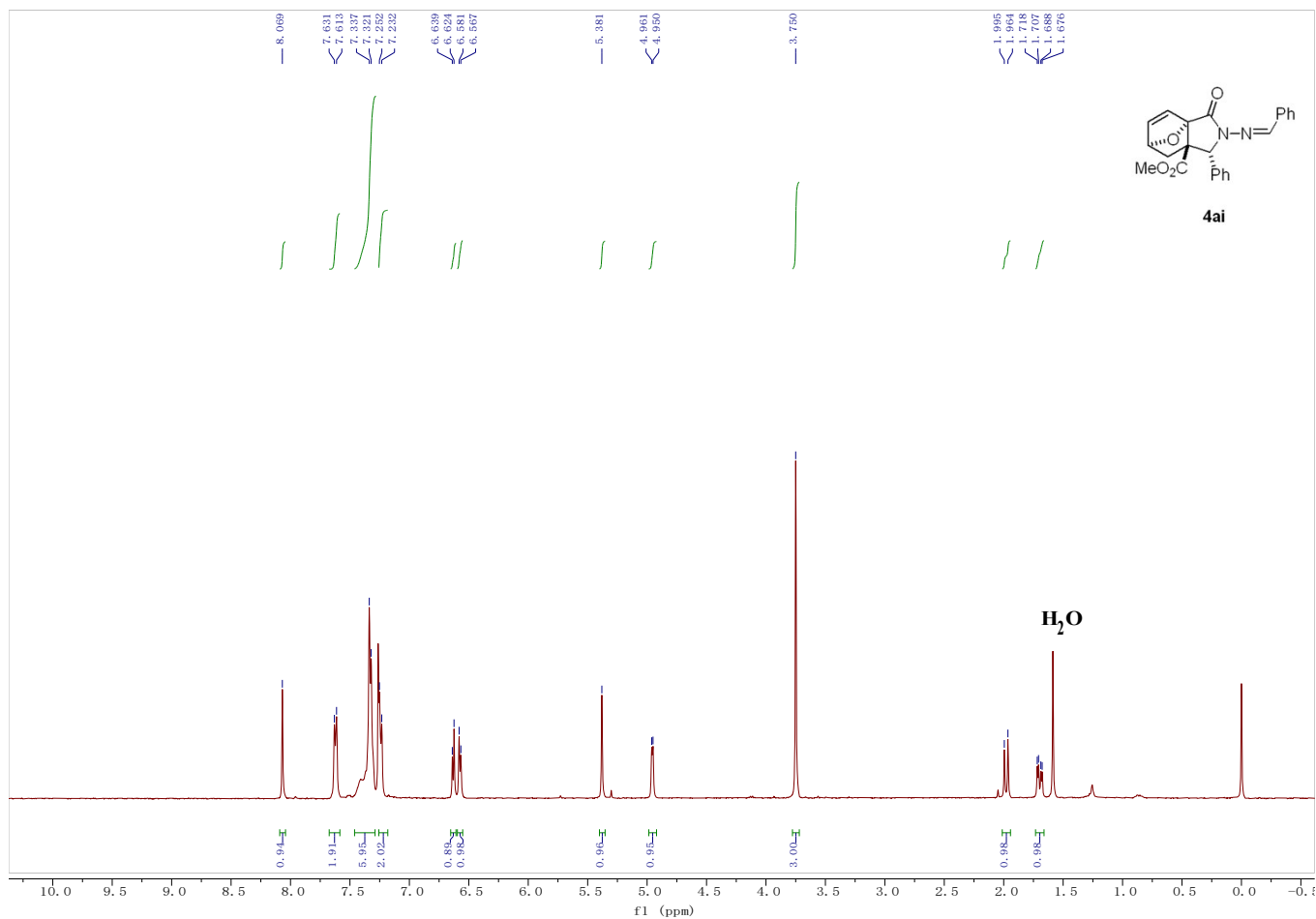
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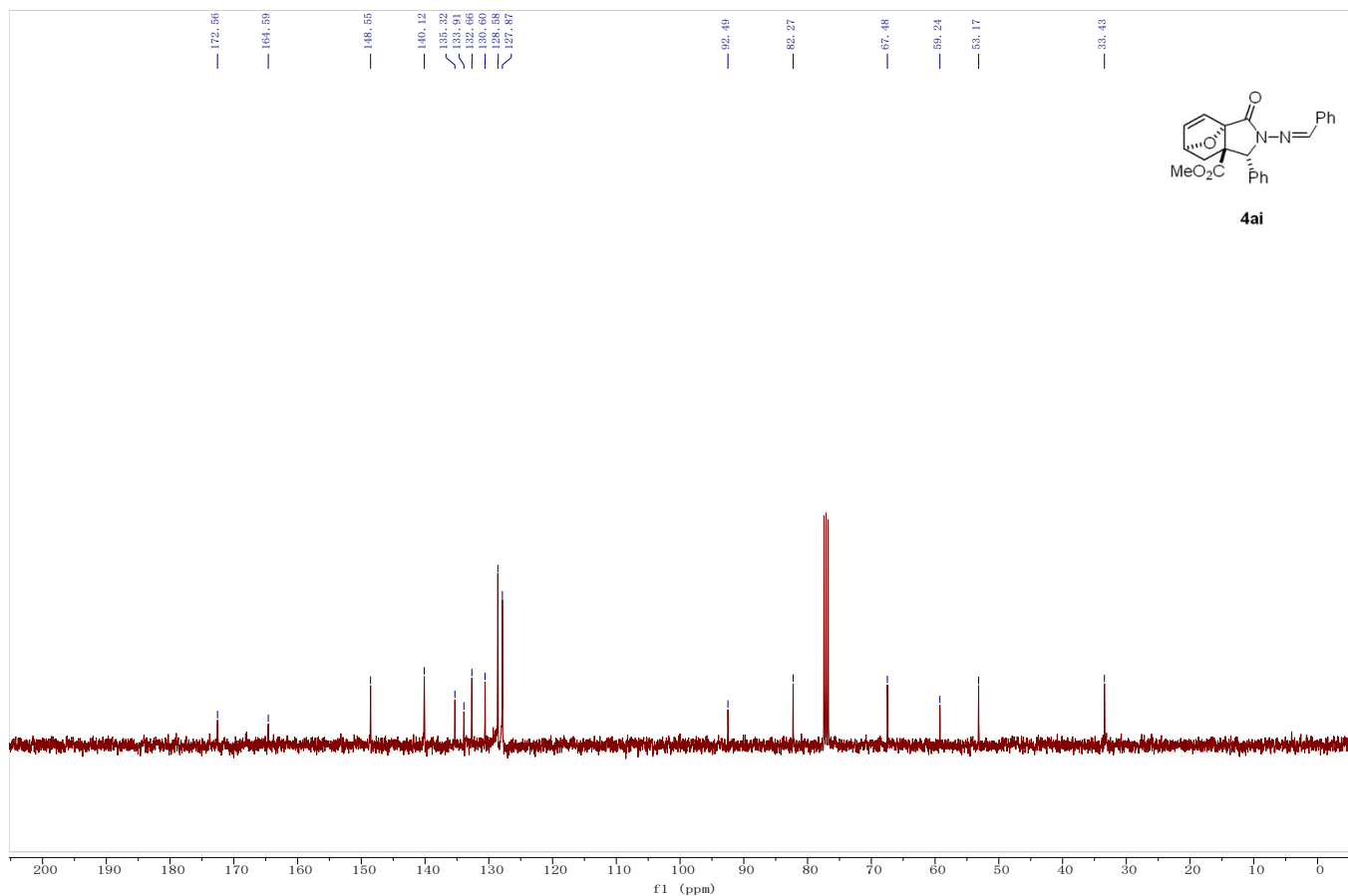
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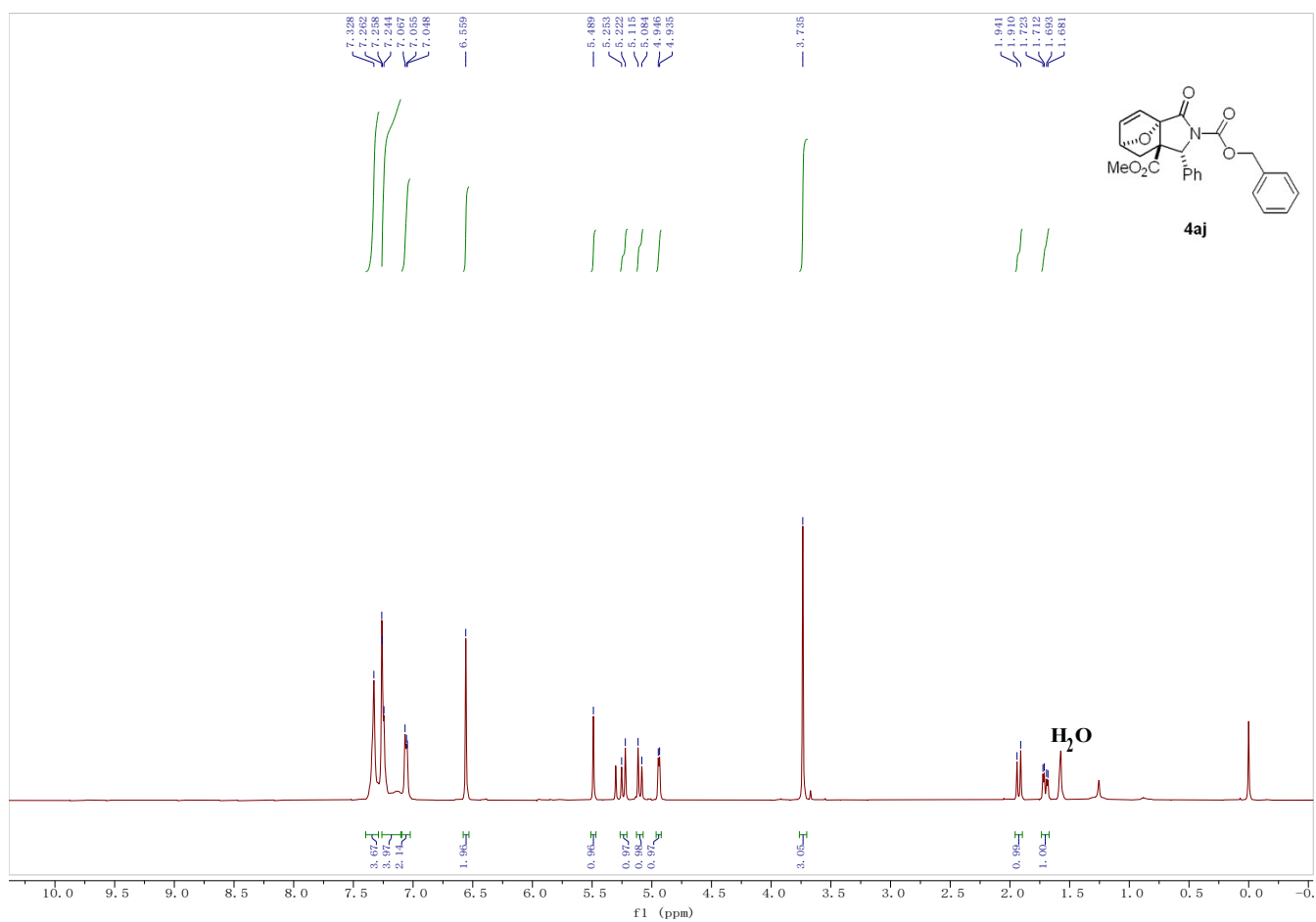
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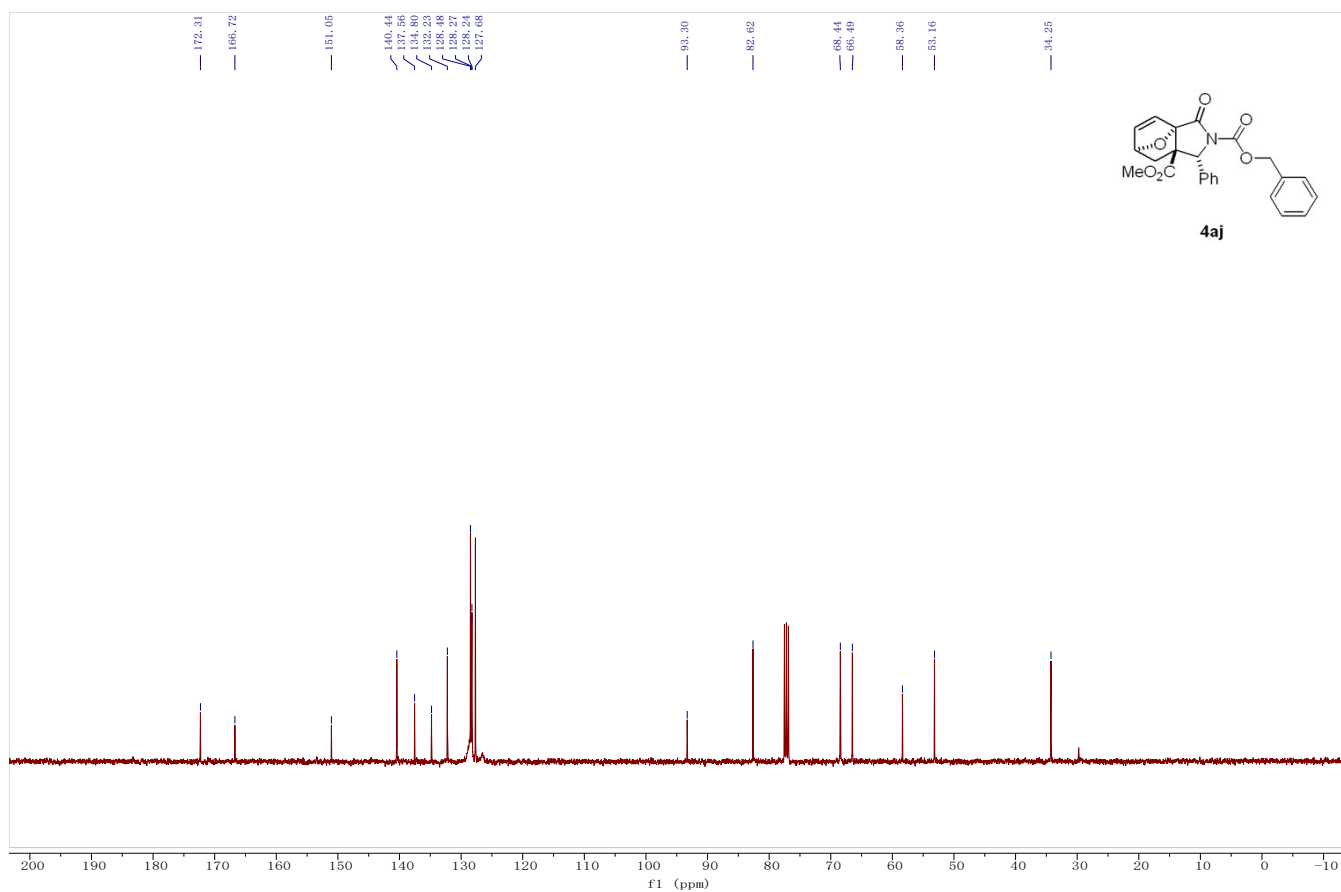
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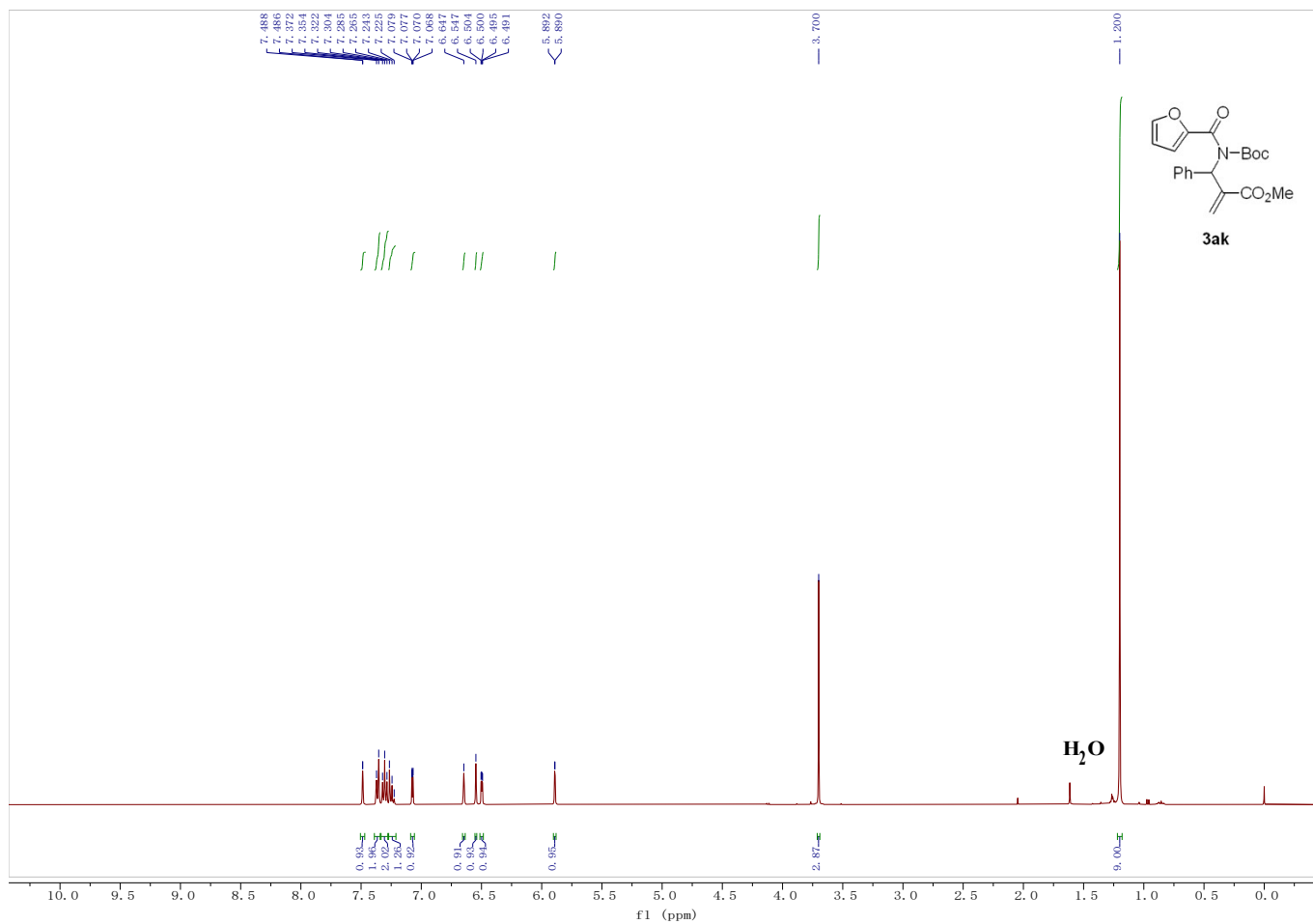
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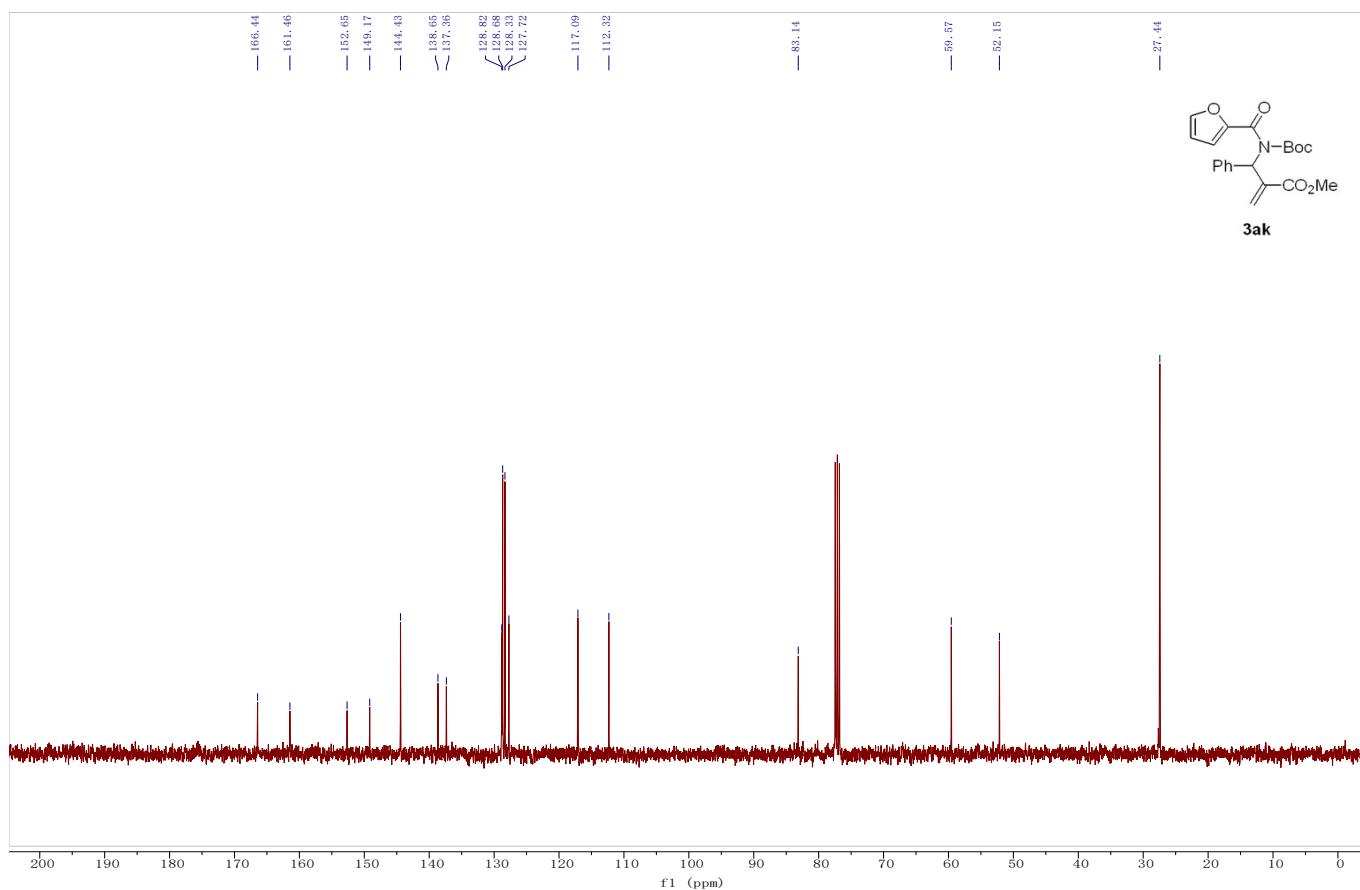
^{13}C NMR (101 MHz) in CDCl_3



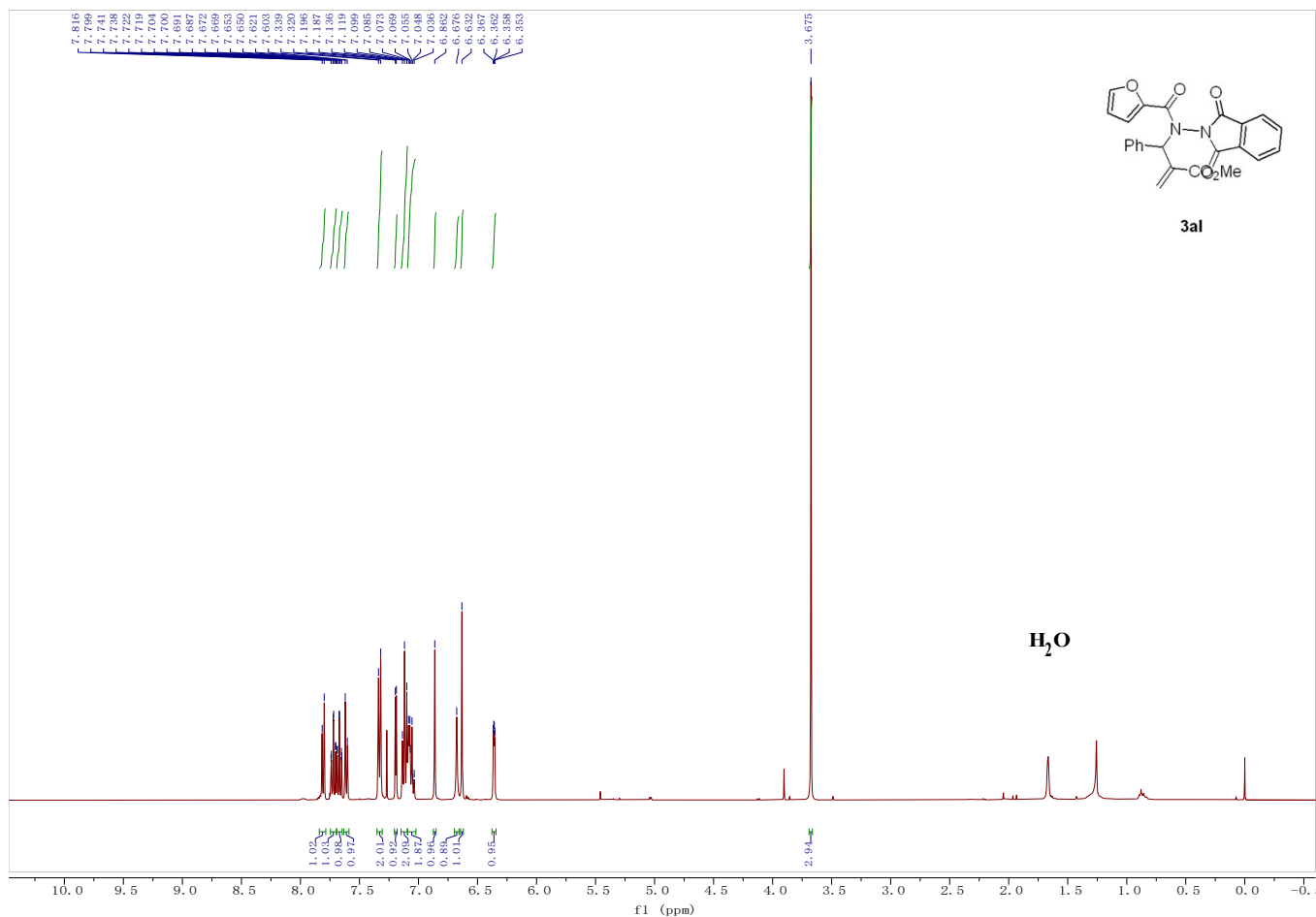
¹H NMR (400 MHz) in CDCl₃



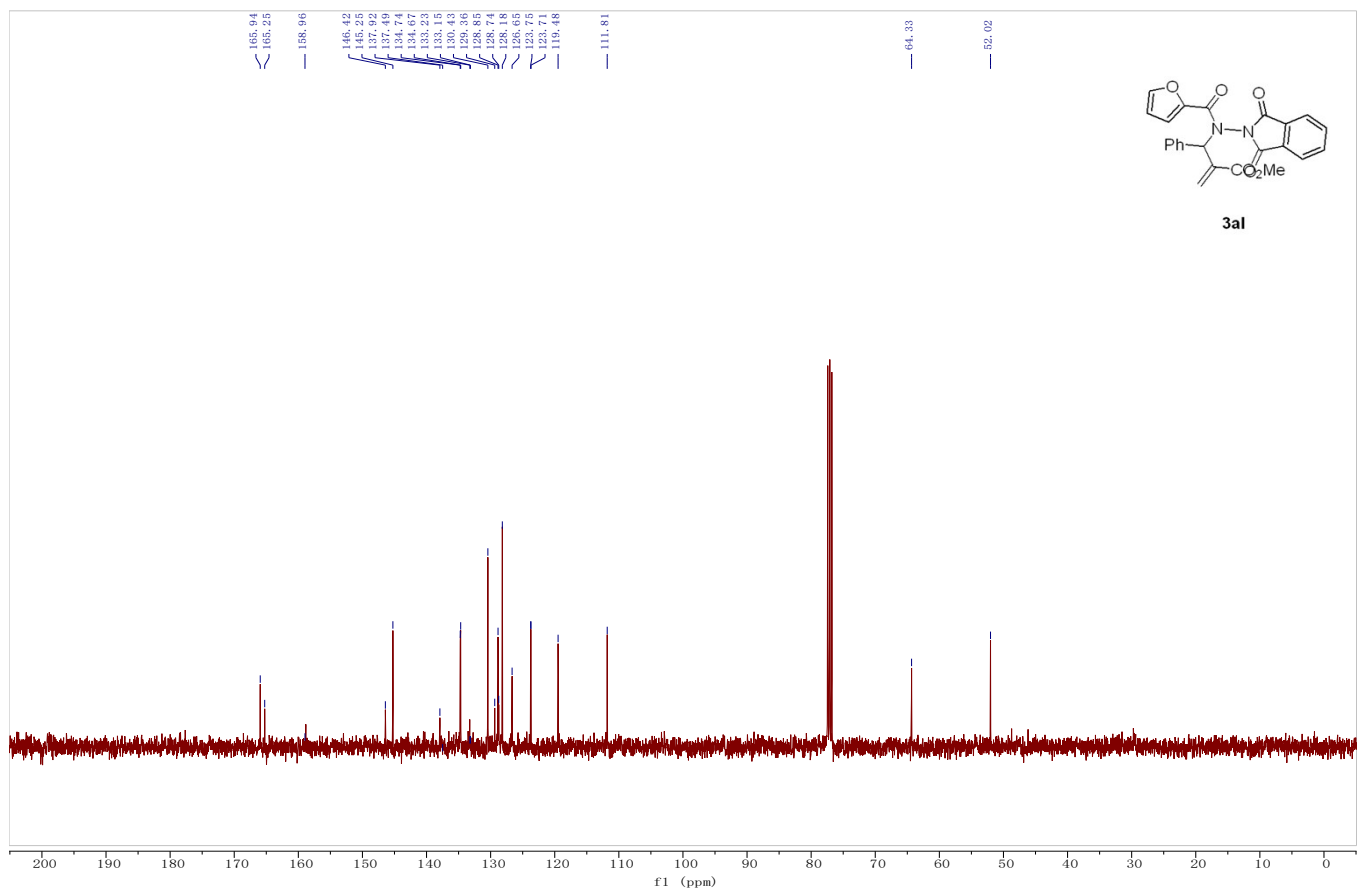
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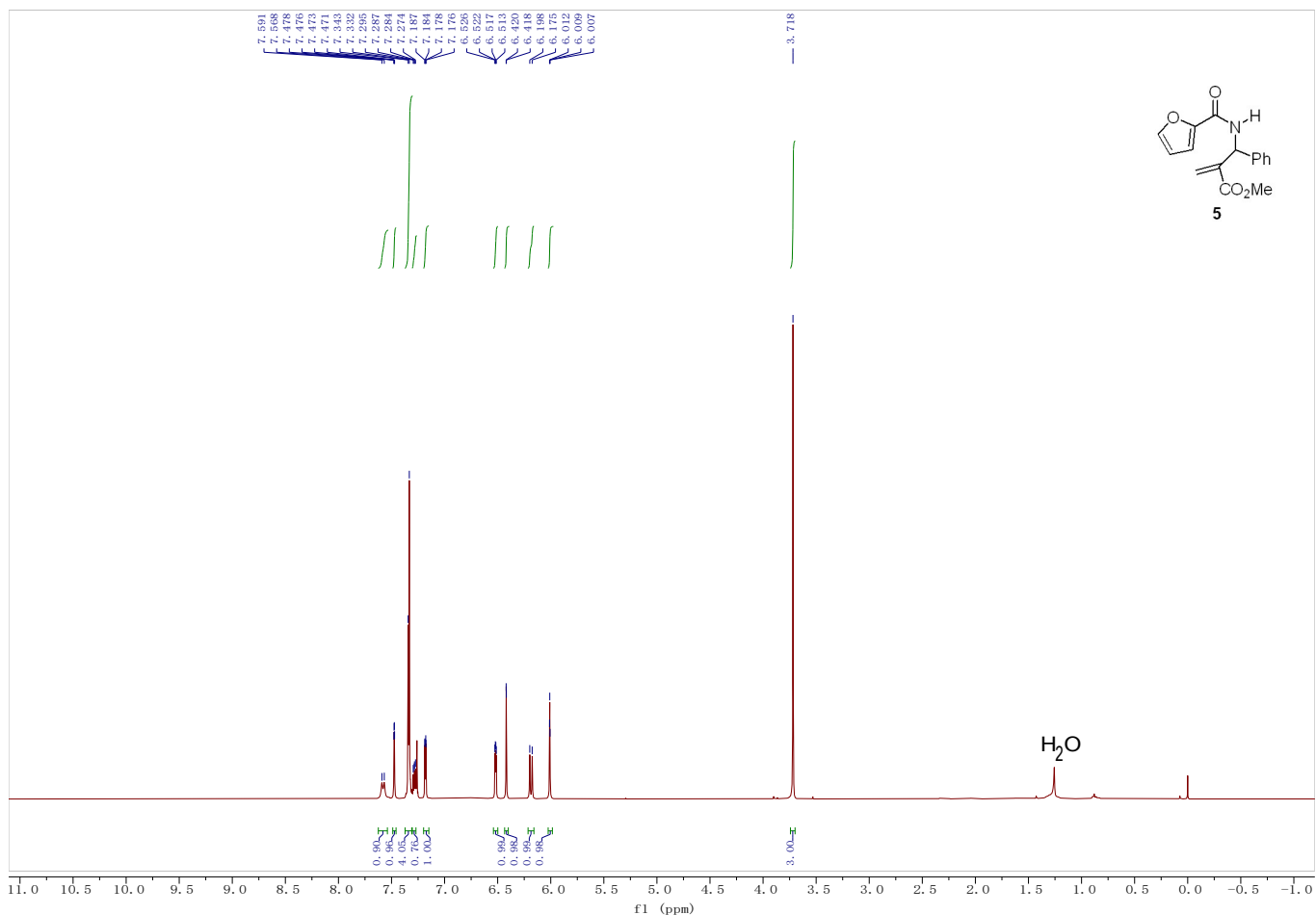
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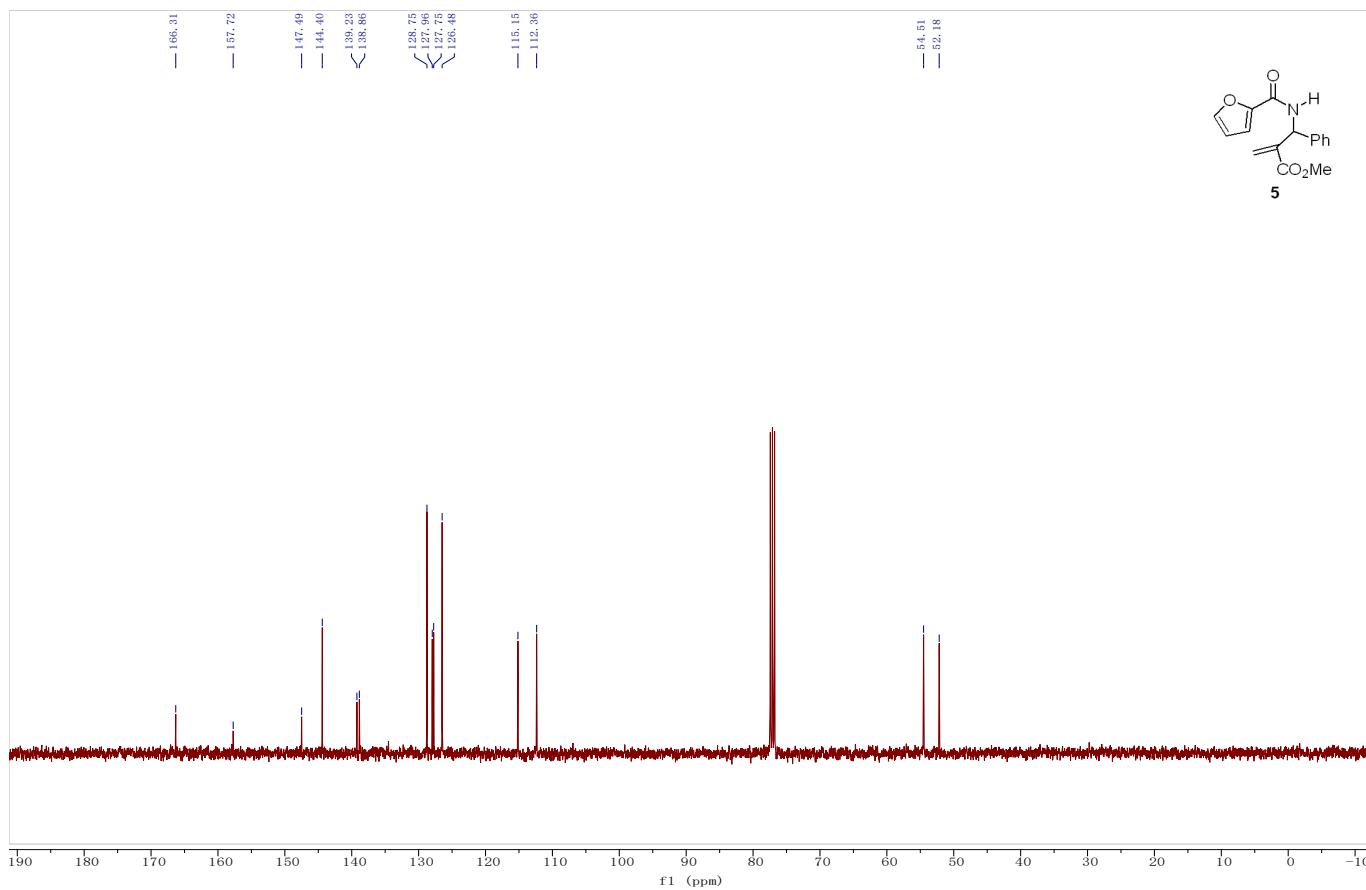
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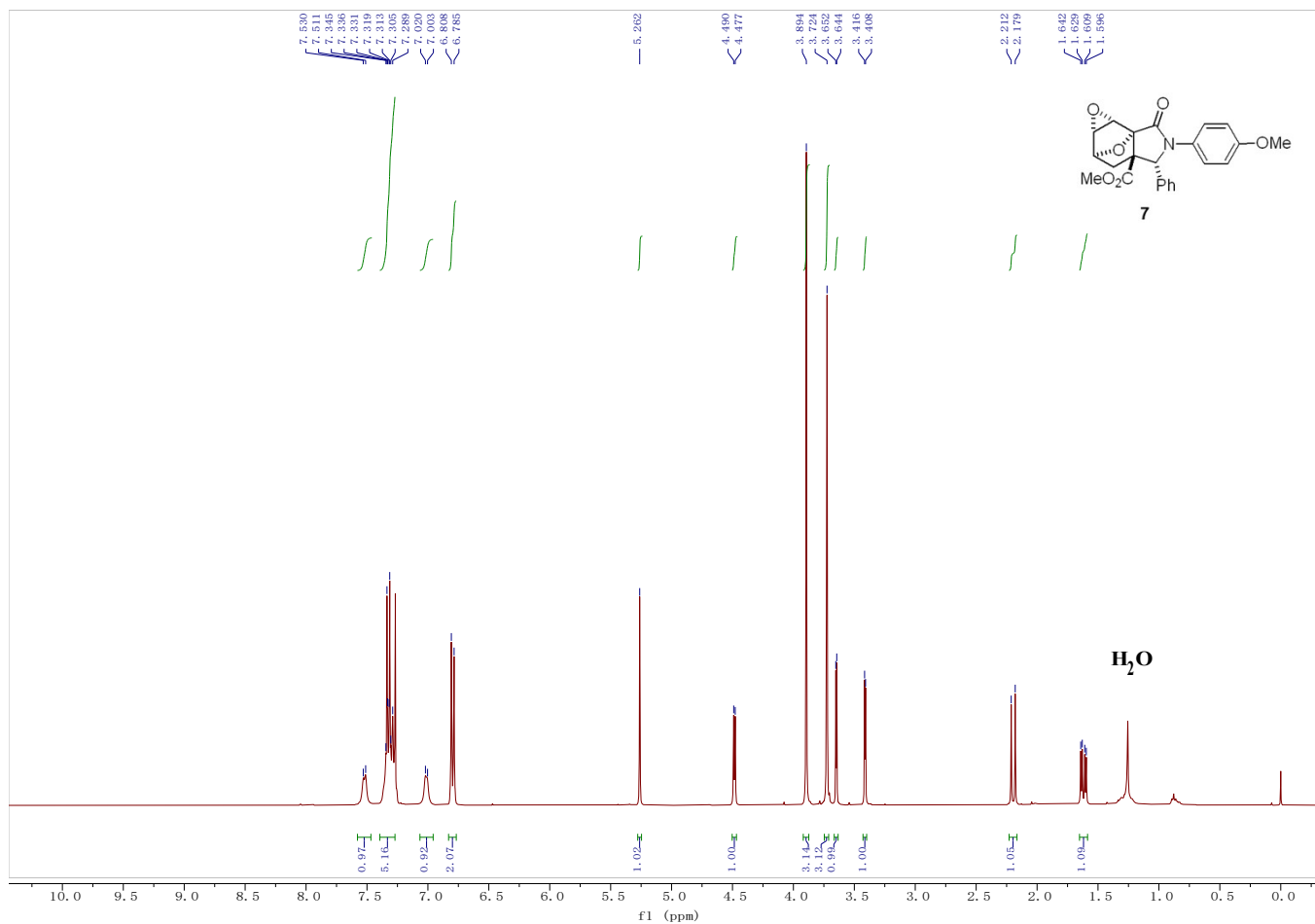
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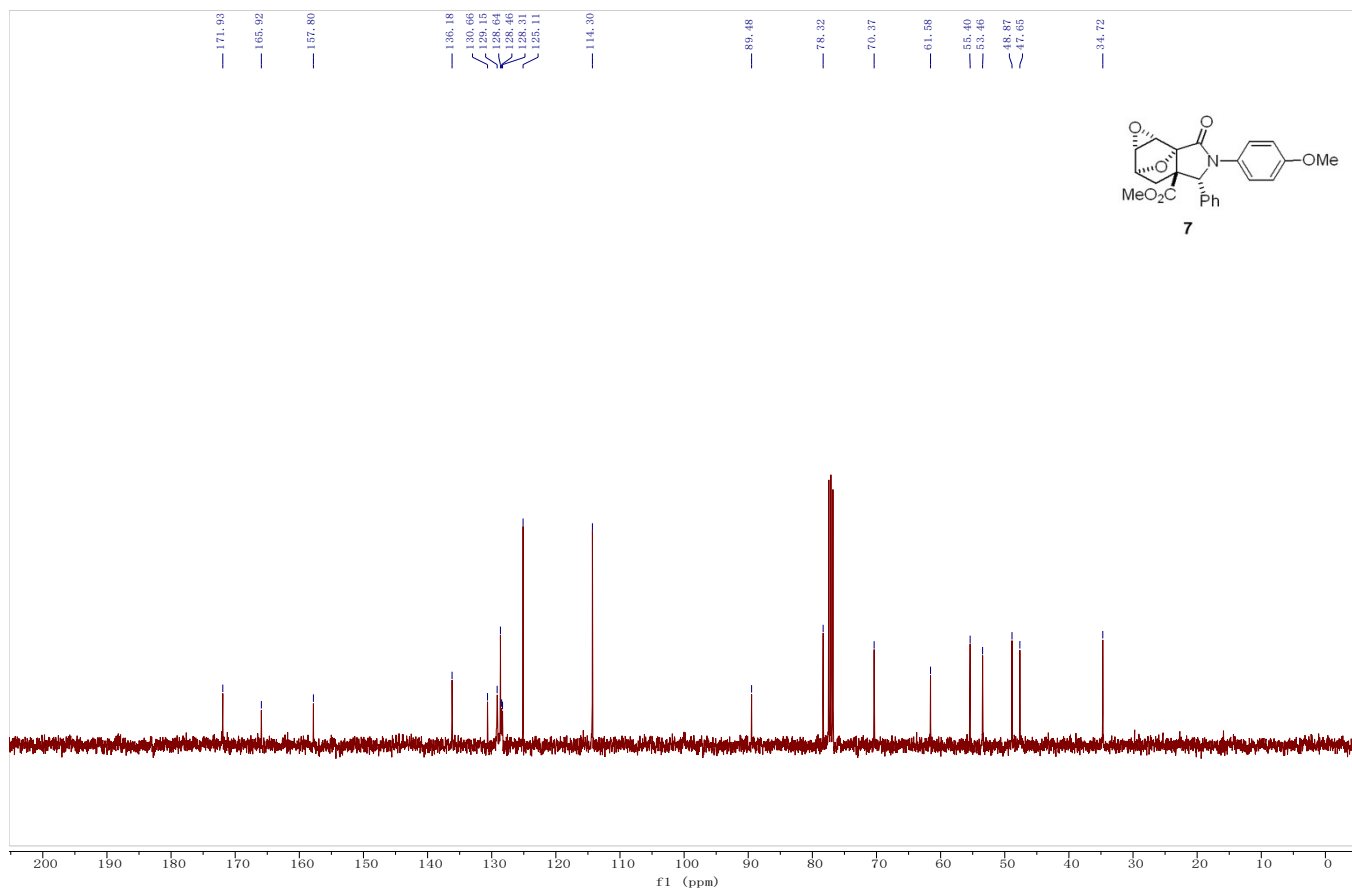
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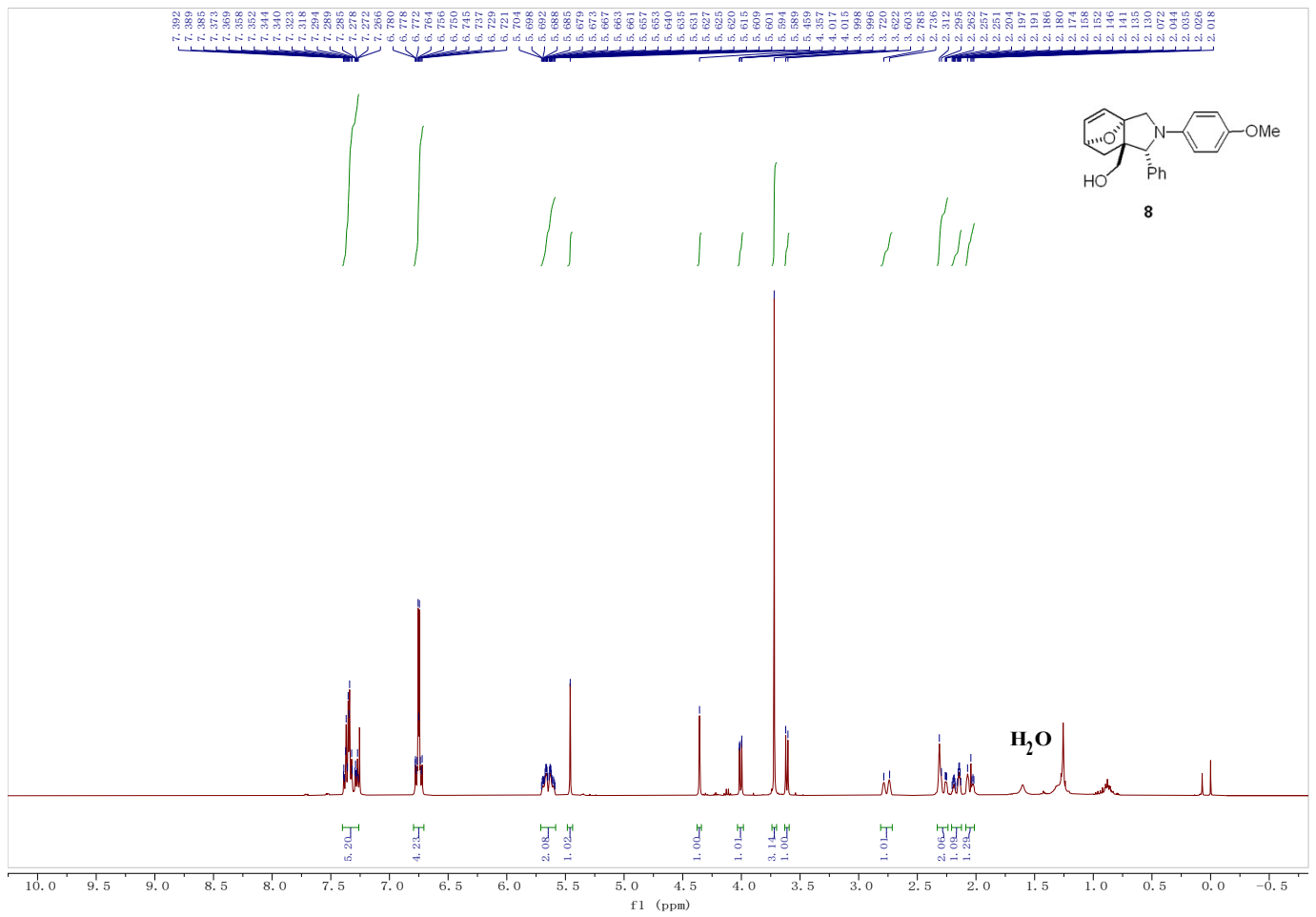
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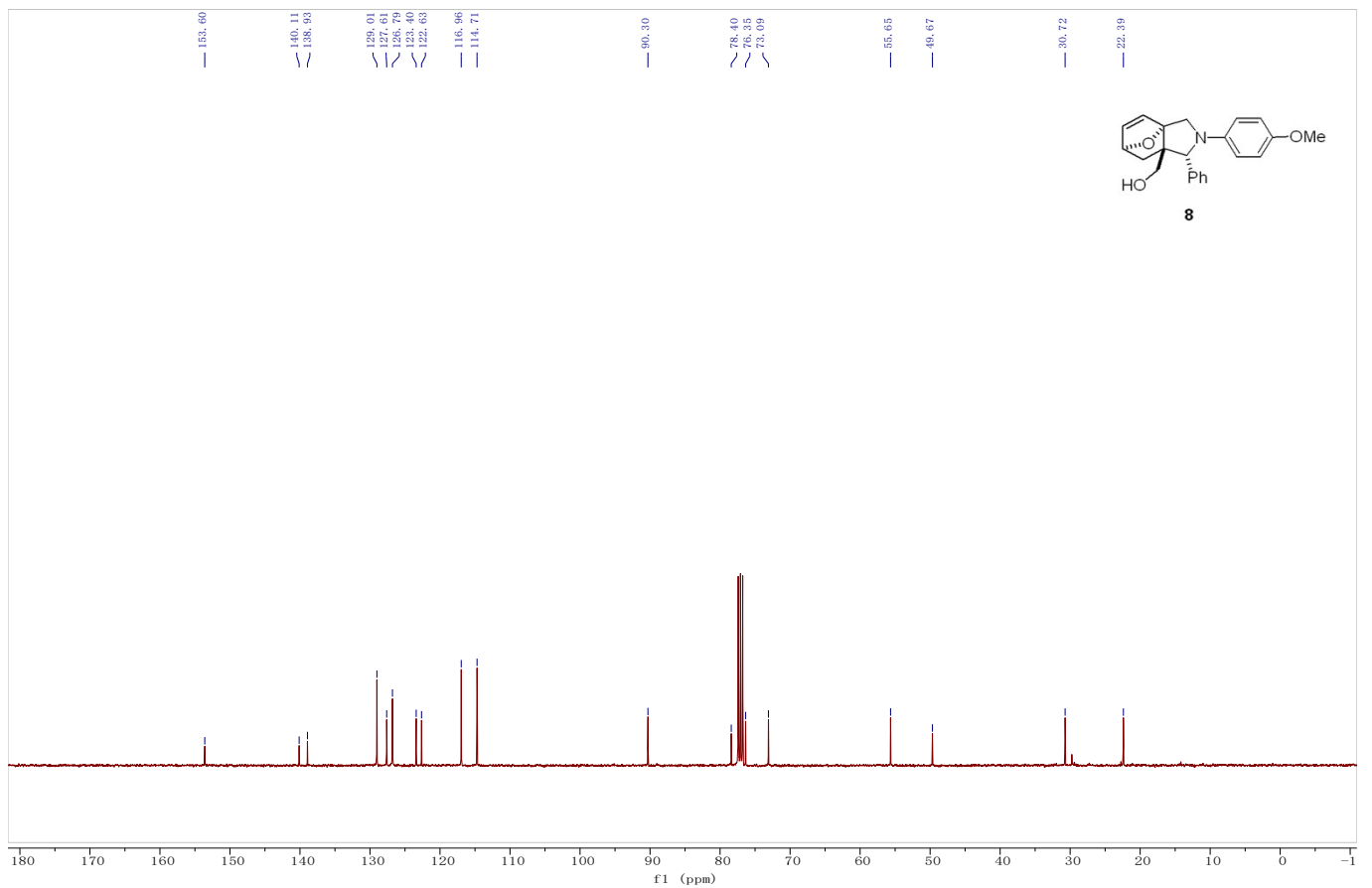
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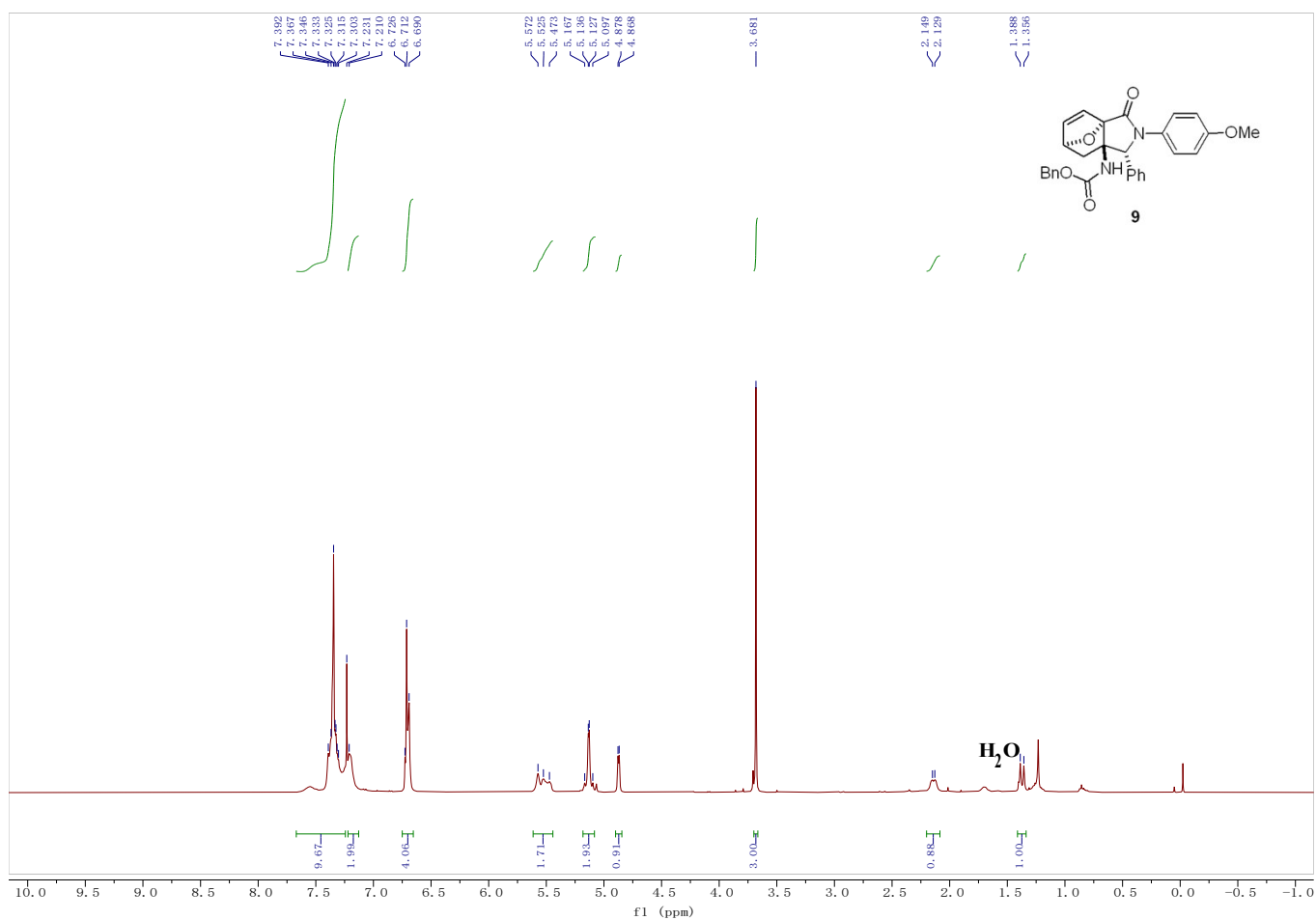
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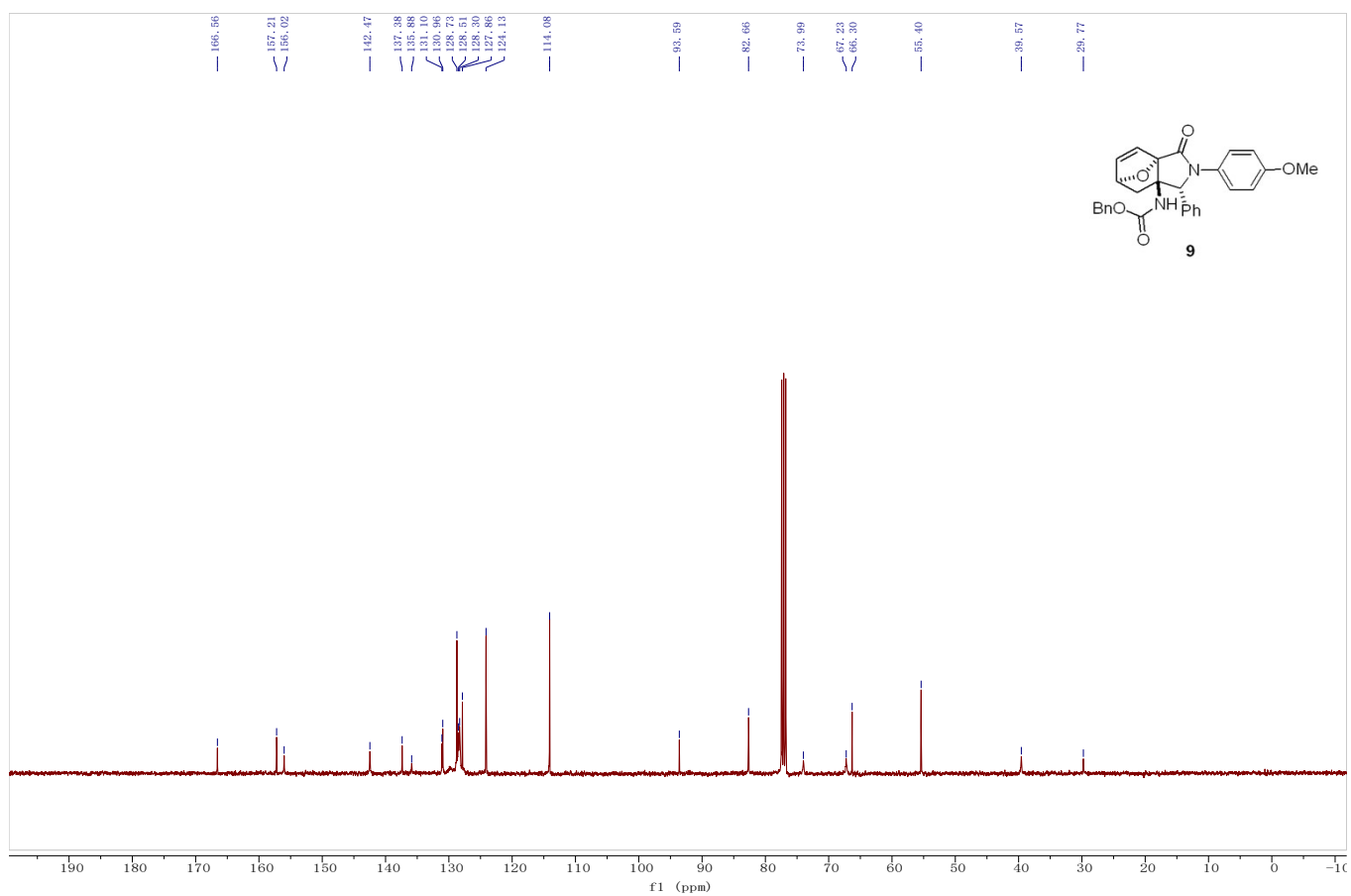
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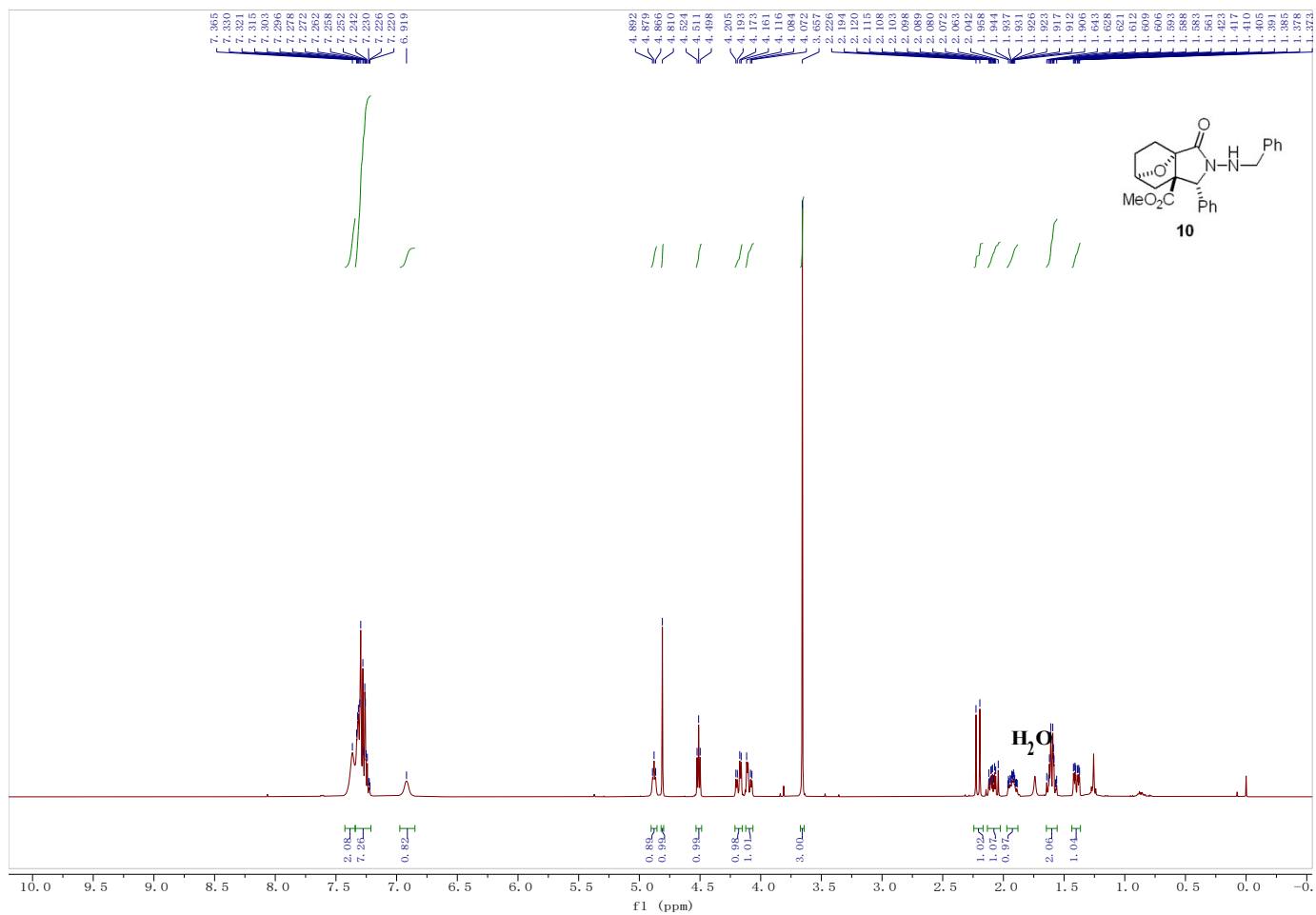
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^{13}C NMR (101 MHz) in CDCl_3



^1H NMR (400 MHz) in CDCl_3



^{13}C NMR (101 MHz) in CDCl_3

