

Supporting information

Brønsted Acid-Catalyzed (4+2) Cyclocondensation of 3-Substituted Indoles with Donor-Acceptor Cyclopropanes

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1 General methods and materials ¹

NMR: Monodimensional and/or bidimensional nuclear magnetic resonance proton and carbon spectra (¹H NMR and ¹³C NMR) were acquired at 25 °C on a Bruker AC-300 spectrometer (300 MHz for ¹H and 75.5 MHz for ¹³C) and a Bruker AC-500 spectrometer (500 MHz for ¹H and 125.7 MHz for ¹³C) at the indicated temperature. Chemical shifts (δ) are reported in ppm relative to residual solvent signals (CHCl₃, 7.26 ppm for ¹H NMR, CDCl₃, 77.16 ppm for ¹³C NMR) and coupling constants (J) in hertz (Hz). The following abbreviations are used to indicate the multiplicity in NMR spectra: s, singlet; d, doublet; t, triplet; q, quartet; app, apparent; m, multiplet; bs, broad signal. ¹³C NMR spectra were acquired on a broad band decoupled mode using DEPT experiments (Distorsionless Enhancement by Polarization Transfer) for assigning different types of carbon environment. Selective n.O.e., NOESY, COSY, HSQC and HMBC experiments were acquired to confirm precise molecular configuration and to assist in deconvoluting complex multiplet signals.²

IR: Infrared spectra (IR) were measured in a Jasco FT/IR 4100 (ATR), in the interval between 4000 and 400 cm⁻¹ with a 4 cm⁻¹ resolution. Only characteristic bands are given in each case.

MS: Mass spectra (MS) were recorded on an Agilent 7890A gas chromatograph coupled to an Agilent 5975C quadrupole mass spectrometer under electronic impact ionization (EI) at 70 eV. The obtained data is presented in mass units (m/z) and the values found in brackets belong to the relative intensities comparing to the base peak (100%).

HRMS (ESI): High-resolution mass spectra were recorded on an Acquity UPLC coupled to a QTOF mass spectrometer (SYNAPT G2 HDMS) using electrospray ionization (ESI⁺).

HPLC: The enantiomeric ratio (er) of the products was determined by High Performance Liquid Chromatography on a chiral stationary phase in a Waters 2695 chromatograph coupled to a Waters 2998 photodiode array detector. Daicel *Chiralpak IA, IC, AD-H, AS-H, AZ-3* and *Chiralcel OZ-3* columns (0.46 × 25 cm) were used; specific conditions are indicated for each case.

M.p.: Melting points were measured in a Buchi B-540 apparatus in open capillary tubes and are uncorrected.

Optical rotations [α]_D²⁰ were measured at 20 °C on a Jasco P-2000 polarimeter with a sodium lamp at 589 nm and a path of length of 1 dm. Solvent and concentration are specified in each case.

X-ray: Data collections were performed using an Agilent Supernova diffractometer equipped with an Atlas CCD area detector, and a CuK α micro-focus source with multilayer optics ($\lambda = 1.54184\text{\AA}$, 250 μm FWHM beam size). The sample was kept at 150 K with an Oxford Cryosystems Cryostream 700 cooler.

¹ SGIker technical support (MEC, GV/EJ and European Social Fund) is gratefully acknowledged (NMR, HRMS and X-ray analysis)

² M. Kinss, J. K. M. Sanders, *J. Mag. Res.* **1984**, *56*, 518.

The quality of the crystals was checked under a polarizing microscope, and a suitable crystal or fragment was mounted on a Mitegen Micromount™ using Paratone N inert oil and transferred to the diffractometer.

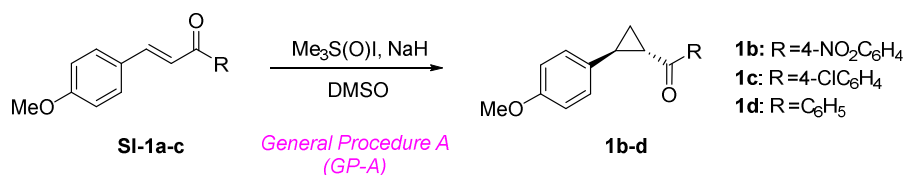
Miscellaneous: Analytical grade solvents and commercially available reagents were used without further purification. Anhydrous solvents were purified and dried with activated molecular sieves prior to use.³ For reactions carried out under inert conditions, the argon was previously dried through a column of P₂O₅ and a column of KOH and CaCl₂. All the glassware was dried for 12 hours prior to use in an oven at 140 °C, and allowed to cool under a dehumidified atmosphere.⁴ Reactions at reduced temperatures were carried out using a Thermo Haake EK90 refrigerator. Reactions were monitored using analytical thin layer chromatography (TLC), in pre-coated silica-backed plates (Merck Kiesegel 60 F254). These were visualized by ultraviolet irradiation, *p*-anisaldehyde, phosphomolybdic acid or potassium permanganate dips.⁵ For flash chromatography Silicycle 40-63, 230-400 mesh silica gel was used.⁶ For the removal of the solvents under reduced pressure Büchi R-2 series rotatory evaporators were used.

2 Experimental procedures and characterization

2.1 Synthesis of donor-acceptor cyclopropanes 1a-o

Compounds **1a**⁷, **1e**⁷, **1g**⁷ and **1l**⁷ were prepared following procedures previously described in the literature.

2.1.1 Synthesis of acyl-substituted donor-acceptor cyclopropanes (1b-d)



Scheme S1. General Procedure A for the synthesis of ketone substituted cyclopropanes 1b-d

³ (a) W. L. F. Armarego, C. L. L. Chai, *Purification of Laboratory Chemicals*, 7th ed.; Elsevier: Oxford, 2012. (b) D. B. G. Williams, M. Lawton, *J. Org. Chem.* **2010**, *75*, 8351.

⁴ G. W. Kramer, A. B. Levy, M. M. Midland, *Organic Synthesis via Boranes*, John Wiley & Sons, New York, 1975.

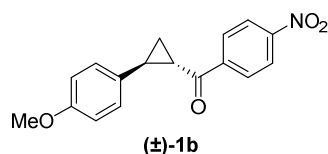
⁵ E. Stahl, *Thin Layer Chromatography*, Springer Verlag: Berlin, 1969.

⁶ W. C. Still, H. Kahn, A. J. Mitra, *J. Org. Chem.* **1978**, *43*, 2923.

⁷ Ortega, A.; Manzano, R.; Uria, U.; Carrillo, L.; Reyes, E.; Tejero, T.; Merino, P.; Vicario, J. L., *Angew. Chem. Int. Ed.*, **2018**, *57*, 8225.

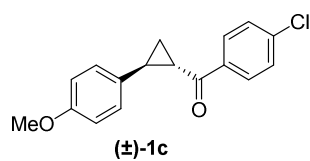
Alkenes **SI-1a**⁸, **SI-1b**,⁹ and **SI-1c**,¹⁰ were reported compounds and were prepared following the procedures described in the literature.

General Procedure A (GP-A) for the synthesis of ketone substituted cyclopropanes 1b-d. DMSO (0.24M) was added to a mixture of trimethylsulfoxonium iodide (1.2 eq.) and sodium hydride (1.2 eq.) and the mixture was stirred at room temperature for 30 minutes. Then, the corresponding alkene (1.0 eq.) in DMSO (0.5M) was added to the solution at 0 °C and the solution was stirred for 2h at 60 °C in an oil bath. The reaction was quenched by adding saturated aqueous NH₄Cl solution and was extracted with ethyl acetate (3 x 20 mL). The combined organic phases were washed with saturated aqueous solution of NaCl and dried over Na₂SO₄. Removal of the volatile substances under reduced pressure followed by purification by column chromatography on silica gel gave the corresponding cyclopropanes **1b-d**.



(±)-**trans**-[2-(4-Methoxyphenyl)cyclopropyl](4-nitrophenyl)methanone

(1b). Following *GP-A*, **1b** (416 mg, 1.4 mmol, 40%) was isolated by FC (petroleum ether/EtOAc, 19:1) on silica gel as a yellow solid, starting from **SI-1a** (1.0 g, 3.5 mmol, 1.0 eq.) in DMSO (7.0 mL) and the mixture of trimethylsulfoxonium iodide (0.92 g, 4.2 mmol, 1.2 eq.) and NaH (100 mg, 4.2 mmol, 1.2 eq.) in DMSO (17.5 mL). $R_f = 0.50$ (petroleum ether/EtOAc, 19:1). ¹H NMR (300 MHz, CDCl₃) δ 8.26 (d, $J = 9.0$ Hz, 2H, C_{arom}-H), 8.10 (d, $J = 9.0$ Hz, 2H, C_{arom}-H), 7.11 (d, $J = 8.7$ Hz, 2H, C_{arom}-H), 6.85 (d, $J = 8.7$ Hz, 2H, C_{arom}-H), 3.78 (s, 3H, OCH₃), 2.82 (ddd, $J = 7.9, 5.2, 3.9$ Hz, 1H, CH-PMP), 2.72 (ddd, $J = 8.8, 6.8, 3.9$ Hz, 1H, CHC=O), 1.95 (ddd, $J = 8.8, 5.2, 4.1$ Hz, 1H, CH_aCH_b), 1.67-1.56 (m, 1H, CH_aCH_b). ¹³C NMR (75 MHz, CDCl₃) δ 197.2 (C=O), 158.7 (C_{arom}-OCH₃), 150.2 (C_{arom}-NO₂), 142.3 (C_{arom}-C), 131.7 (C_{arom}-C), 129.1 (2×C_{arom}-H), 127.4 (2×C_{arom}-H), 123.8 (2×C_{arom}-H), 114.2 (2×C_{arom}-H), 55.4 (OCH₃), 31.0 (CHC=O), 30.1 (C_{arom}CHCH₂), 19.8 (CH₂). IR (ATR): 2934 (C-H st), 1671 (C=O st), 1515 (NO₂ st as), 1341 (NO₂ st sim) cm⁻¹. HRMS (ESI) m/z : [M+H]⁺ Calcd for C₁₇H₁₆NO₄ 298.1079; Found 298.1084. **M.p.**: 61-63 °C (petroleum ether/EtOAc).



(±)-**trans**-(4-Chlorophenyl)[2-(4-methoxyphenyl)cyclopropyl]methanone

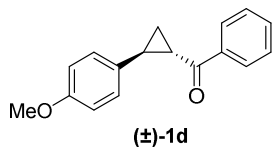
(1c). Following *GP-A*, **1c** (889 mg, 3.1 mmol, 56%) was isolated by FC (petroleum ether/EtOAc, 19:1) on silica gel as a white solid, starting from **SI-1b** (1.5 g, 5.5 mmol, 1.0 eq.) in DMSO (11.0 mL) and the mixture of trimethylsulfoxonium iodide (1.4 g, 6.6 mmol, 1.2 eq.) and NaH (158 mg, 6.6 mmol, 1.2 eq.) in DMSO (27.5 mL). $R_f = 0.50$ (petroleum ether/EtOAc, 19:1). ¹H NMR (300 MHz, CDCl₃) δ 7.93 (d, $J = 8.6$ Hz, 2H, C_{arom}-H), 7.42 (d, $J = 8.6$ Hz, 2H, C_{arom}-H), 7.11 (d, $J = 8.6$ Hz, 2H, C_{arom}-H), 6.86 (d, $J = 8.6$ Hz, 2H, C_{arom}-H), 3.80 (s, 3H, OCH₃), 2.77 (ddd, $J = 7.9, 5.2, 4.0$ Hz, 1H, CH-PMP), 2.67 (ddd, $J = 9.0, 6.7, 4.0$ Hz, 1H, CHC=O), 1.91 (ddd, $J = 9.0, 5.2, 4.1$ Hz, 1H, CH_aCH_b), 1.54 (ddd, $J = 7.9, 6.7, 4.1$

⁸ Gaikwad, S.; Goswami, A.; De, S.; Schmittel, M. *Angew. Chem Int. Ed.* **2016**, *55*, 10512.

⁹ Kumar, R.; Mohanakrishnan, D.; Sharma, A.; Kaushik, N. K.; Kalia, K.; Sinha, A. K.; Sahal, D. *Eur. J. Med. Chem.* **2010**, *45*, 5292.

¹⁰ Downey, C. W.; Glist, H. M.; Takashima, A.; Bottum, R. S.; Dixon, G. J. *Tetrahedron Lett.* **2018**, *59*, 3080.

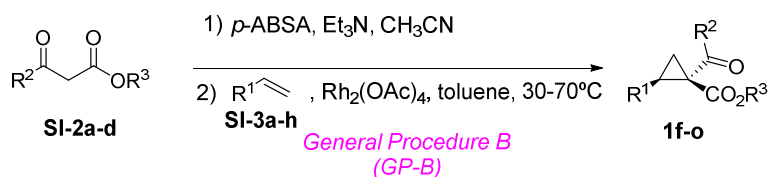
Hz, 1H, CH_aCH_b). ¹³C NMR (75 MHz, CDCl₃) δ 197.5 (C=O), 158.6 (C_{arom}-OCH₃), 139.4 (C_{arom}-C), 136.2 (C_{arom}-C), 132.3 (C_{arom}-C), 129.6 (2×C_{arom}-H), 129.0 (2×C_{arom}-H), 127.5 (2×C_{arom}-H), 114.2 (2×C_{arom}-H), 55.4 (OCH₃), 30.0 (C_{arom}CHCH₂), 29.3 (CHC=O), 19. (CH₂). IR (ATR): 2937 (C-H st), 1664 (C=O st), 1032 (C-Cl st) cm⁻¹. MS (EI) m/z (%): 286.0 (M⁺, 17), 147.0 (100), 138.9 (60), 115.0 (30), 113.0 (18), 111.0 (48), 103.0 (22), 91.0 (35), 78.0 (35), 78.0 (20), 77.0 (22), 75.0 (27). HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₇H₁₆O₂Cl 287.0839; Found 287.0839. M.p.: 71-74 °C (petroleum ether/EtOAc).



(±)-*trans*-[2-(4-Methoxyphenyl)cyclopropyl](phenyl)methanone (1d).

Following GP-A, **1d** (378 mg, 1.5 mmol, 71%) was isolated by FC (petroleum ether/EtOAc, from 19:1 to 9:1) on silica gel as a colorless oil, starting from **SI-1c** (0.50 g, 2.1 mmol, 1.0 eq.) in DMSO (4.2 mL) and the mixture of trimethylsulfoxonium iodide (0.55 g, 2.5 mmol, 1.2 eq.) and NaH (60 mg, 2.5 mmol, 1.2 eq.) in DMSO (10.4 mL). R_f = 0.60 (petroleum ether/EtOAc, 19:1). ¹H NMR (300 MHz, CDCl₃) δ 8.01 (dd, *J* = 8.2, 1.4 Hz, 2H, C_{arom}-H), 7.63-7.53 (m, 1H, C_{arom}-H), 7.51-7.40 (m, 2H, C_{arom}-H), 7.13 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.87 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 3.81 (s, 3H, OCH₃), 2.85 (ddd, *J* = 7.8, 5.2, 4.0 Hz, 1H, CH-PMP), 2.68 (ddd, *J* = 8.9, 6.6, 4.0 Hz, 1H, CHC=O), 1.92 (ddd, *J* = 8.9, 5.2, 4.0 Hz, 1H, CH_aCH_b), 1.53 (ddd, *J* = 7.8, 6.6, 4.0 Hz, 1H, CH_aCH_b). ¹³C NMR (75 MHz, CDCl₃) δ 198.7 (C=O), 158.6 (C_{arom}-OCH₃), 137.9 (C_{arom}-C), 132.9 (C_{arom}-H), 132.6 (C_{arom}-C), 128.7 (2×C_{arom}-H), 128.2 (2×C_{arom}-H), 127.5 (2×C_{arom}-H), 114.1 (2×C_{arom}-H), 55.4 (OCH₃), 29.8 (C_{arom}CHCH₂), 29.3 (CHC=O), 19.0 (CH₂). IR (ATR): 2934 (C-H st), 1664 (C=O st) cm⁻¹. MS (EI) m/z (%): 252.1 (M⁺, 30), 250.1 (29), 147.0 (41), 115.0 (24), 105.0 (70), 103.0 (21), 91.0 (24), 78.0 (29), 77.0 (100), 51.0 (31). HRMS (ESI) m/z: [M+H]⁺ Calcd for C₁₇H₁₇O₂ 253.1229; Found 253.1228.

2.1.2 Synthesis of cyclopropanes derived from β-ketoesters (1f, 1h-k, 1m-o)



1f: R¹ = 4-OMe-C₆H₄, R² = 4-Cl-C₆H₄, R³ = Et **1k**: R¹ = 4-Br-C₆H₄, R² = Me, R³ = Bn
1h: R¹ = 4-OMe-C₆H₄, R² = Ph, R³ = *t*-Bu **1m**: R¹ = 2-OMe-C₆H₄, R² = Me, R³ = Bn
1i: R¹ = 4-*t*-Bu-C₆H₄, R² = Me, R³ = Bn **1n**: R¹ = 2,4,6-Me₃-C₆H₂, R² = Me, R³ = Bn
1j: R¹ = Ph, R² = Me, R³ = Bn **1o**: R¹ = 4-Me-C₆H₄, R² = Ph, R³ = Et

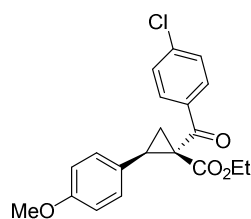
Scheme S2. General Procedure B for the synthesis of cyclopropanes derived from β-ketoesters

Acetoacetates **SI-2b-d** were obtained from commercial sources. Intermediate **SI-2a**¹¹ was prepared following the procedures described in the literature.

¹¹ Katritzky, A. R.; Wang, Z.; Wang, M.; Wilkerson, C. R.; Hall, C. D.; Akhmedov, N. G. *J. Org. Chem.* **2004**, *69*, 6617.

Vinylarenes **SI-3a-d** and **SI-3f-g** were obtained from commercial sources. Vinylarene **SI-3e**¹² was a reported compound and it was prepared following the procedure described in the literature.

General Procedure B (GP-B) for the synthesis of donor-acceptor cyclopropanes (1f, 1h-k, 1m-o): Triethylamine (1.5 eq.) was added dropwise to a solution of the corresponding β -ketoester **SI-2a-d** (1.0 eq.) and 4-acetamidobenzenesulfonyl azide (*p*-ABSA) (1.2 eq.) in acetonitrile (0.13M), at 0 °C. The resulting mixture was stirred at room temperature for 8-12 hours, time during which the corresponding sulfonamide precipitated. Volatiles were evaporated, the residue was suspended in CH₂Cl₂, silica gel was added and solvent was evaporated. The resulting solid mixture was loaded onto a pad of silica and eluted with petroleum ether/EtOAc (10:1) to provide the corresponding diazocompound. Benzyl 2-diazo-3-oxobutanoate¹³ was synthesized in 10 g-scale¹⁴ and used for the synthesis of cyclopropanes **1i-k** and **1m-n**. The rest of diazocompounds were immediately used in the next step without further purification. The catalyst Rh₂(OAc)₄ (0.3-2 mol%) was added to a solution of the corresponding crude diazocompound (1.0 eq.) and vinylarene **SI-3a-o** in dry toluene or dichloromethane (0.15-1 M) and the mixture was stirred between 30-70 °C in an oil bath. After completion of the reaction, the mixture was quenched with H₂O. The aqueous phase was extracted with EtOAc (2×20 mL) and the combined organic layers were washed with brine (2×20 mL), dried over anhydrous Na₂SO₄, and purified by flash column chromatography to obtain the pure cyclopropane.



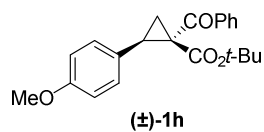
(±)-1f Ethyl (±)-cis-1-(4-chlorobenzoyl)-2-(4-methoxyphenyl)cyclopropane-1-carboxylate (1f). Following *GP-B*, **1f** (2.08 g, 5.8 mmol, 58%, dr > 20:1) was isolated by FC (petroleum ether/EtOAc, from 19:1 to 9:1) on silica gel as white solid starting from ethyl 4-chlorobenzoylacetate (2.27 g, 10.0 mmol, 1.0 eq.) and *p*-ABSA (2.64 g, 11.0 mmol, 1.1 eq.) in CH₃CN (25 mL) using Et₃N (4.2 mL, 30.0 mmol, 3.0 eq.). After dissolving the crude ethyl 2-diazo-3-oxo-3-(4-chlorophenyl)propanoate (2.09 g, 8.3 mmol, 1.0 eq.) and 4-methoxystyrene (2.8 mL, 20.7 mmol, 2.5 eq.) in toluene (8.3 mL), Rh₂(OAc)₄ (11 mg, 0.026 mmol, 2 mol%) was added. R_f = 0.60 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.84 (d, *J* = 8.6 Hz, 2H, C_{arom}-H), 7.42 (d, *J* = 8.6 Hz, 2H, C_{arom}-H), 7.22 (d, *J* = 8.5 Hz, 2H, C_{arom}-H), 6.83 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 3.78 (s, 3H, OCH₃), 3.77-3.66 (m, 2H, OCH₂), 3.50 (app t, *J* = 8.6 Hz, 1H, CHCH₂), 2.39 (dd, *J* = 8.1, 4.8 Hz, 1H, CHCH_aH_b), 1.66 (dd, *J* = 9.2, 4.8 Hz, 1H, CHCH_aH_b), 0.74 (t, *J* = 7.1 Hz, 3H, CH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 193.9 (C_{arom}C=O), 168.4 (COO), 158.9 (C_{arom}-OCH₃), 139.3 (C_{arom}-Cl), 135.9 (C_{arom}-CO), 130.3 (2×C_{arom}-H), 129.7 (2×C_{arom}-H), 128.9 (2×C_{arom}-H), 126.6 (C_{arom}-C), 113.6 (2×C_{arom}-H), 61.3 (OCH₂), 55.3 (OCH₃), 42.3 (CCH₂), 30.5 (CHCH₂), 20.4 (CHCH₂), 13.7 (CH₂CH₃). **IR** (ATR): 1726 (C=O st), 1673 (C=O st), 1176 (C-O st as), 1086 (C-Cl) cm⁻¹. **MS** (EI) *m/z* (%): 358.1 (M⁺, 15), 356.0 (16), 312.0

¹² Li, R.; Chen, X.; Song, X.-R.; Ding, H.; Wang, P.; Xiao, Q.; Liang, Y.-M. *Adv. Synth. Catal.* **2017**, 359, 3962.

¹³ Meyer, M. E.; Ferreira, E. M.; Stoltz, B. M. *Chem. Commun.* **2006**, 1316.

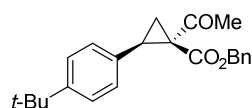
¹⁴ From benzyl acetoacetate (10.0 g, 52.0 mmol, 1.0 eq.) and *p*-ABSA (15.0 g, 62.4 mmol, 1.2 eq.) in CH₃CN (370 mL), and Et₃N (10.9 mL, 78.0 mmol, 1.5 eq.), to afford benzyl 2-diazo-3-oxobutanoate in >90% yield.

(24), 200.0 (43), 144.9 (21), 141.0 (32), 139.0 (100), 111.0 (37). **HRMS (ESI) m/z:** [M+Na]⁺ Calcd for C₂₀H₁₉O₄ClNa 381.0870; Found 381.0882. **M.p.:** 89-92 °C (petroleum ether/EtOAc).



tert-Butyl (±)-cis-1-benzoyl-2-(4-methoxyphenyl)cyclopropane-1-carboxylate

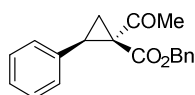
(1h). Following *GP-B*, **1h** (938 mg, 2.7 mmol, 72%, dr 2.5:1) was isolated by FC (petroleum ether/EtOAc, from 19:1 to 9:1) on silica gel as yellow oil starting from *tert*-butyl benzoylacetate (815 mg, 3.7 mmol, 1.0 eq.) and *p*-ABSA (1.1 g, 4.4 mmol, 1.2 eq.) in CH₃CN (26 mL) using Et₃N (0.8 mL, 5.5 mmol, 1.5 eq.). After dissolving the crude *tert*-butyl 2-diazo-3-oxo-3-phenylpropanoate (920 mg, 3.7 mmol, 1.0 eq.) and 4-methoxystyrene (2.5 mL, 18.5 mmol, 5.0 eq.) in toluene (3.7 mL), Rh₂(OAc)₄ (32 mg, 0.07 mmol, 2 mol%) was added. R_f = 0.50 (petroleum ether/EtOAc, 8:2). **¹H NMR** (300 MHz, CDCl₃) (* indicates minor diastereoisomer resonances) δ 8.06-7.79 (m, 2H, C_{arom}-H), 7.73-7.62* (m, 2H, C_{arom}-H), 7.59-7.48* (m, 2H, C_{arom}-H), 7.50-7.27 (m, 3H, C_{arom}-H), 7.50-7.27* (m, 1H, C_{arom}-H), 7.34-7.18 (m, 2H, C_{arom}-H), 7.07* (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.83 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.66* (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 3.77 (s, 3H, OCH₃), 3.65* (s, 3H, OCH₃), 3.52 (app t, *J* = 8.6 Hz, 1H, CHCH₂), 3.43* (app t, *J* = 8.6 Hz, 1H, CHCH₂), 2.38* (dd, *J* = 4.9, 3.1 Hz, 1H, CH_aCH_b), 2.33 (dd, *J* = 8.0, 4.7 Hz, 1H, CH_aCH_b), 1.70* (dd, *J* = 9.2, 4.9 Hz, 1H, CH_aCH_b), 1.59 (dd, *J* = 9.1, 4.7 Hz, 1H, CH_aCH_b), 1.17* (s, 9H, C(CH₃)₃), 0.90 (s, 9H, C(CH₃)₃). **¹³C NMR** (75 MHz, CDCl₃) (* indicates minor diastereoisomer resonances) δ 196.1 (C_{arom}-C=O), 193.6* (C_{arom}-C=O), 170.2* (COO), 167.3 (COO), 158.8 (C_{arom}-OCH₃), 158.8* (C_{arom}-OCH₃), 138.3 (C_{arom}-C), 138.3* (C_{arom}-C), 132.6 (C_{arom}-H), 132.3* (C_{arom}-H), 130.4 (2×C_{arom}-H), 129.2* (2×C_{arom}-H), 128.5 (2×C_{arom}-H), 128.4* (2×C_{arom}-H), 128.1 (2×C_{arom}-H), 128.1* (2×C_{arom}-H), 127.1 (C_{arom}-C), 126.2* (C_{arom}-C), 113.7* (2×C_{arom}-H), 113.5 (2×C_{arom}-H), 82.2* (C(CH₃)₃), 81.6 (C(CH₃)₃), 55.4 (OCH₃), 55.2* (OCH₃), 43.4 (CCH₂), 43.1* (CCH₂), 33.6* (CHCH₂), 29.8 (CHCH₂), 27.7* (C(CH₃)₃), 27.4 (C(CH₃)₃), 20.2 (CHCH₂), 18.2* (CHCH₂). **IR** (ATR): 1720 (C=O st), 1678 (C=O st), 1166 (C-O st as) cm⁻¹. **MS** (EI) m/z (%): 352.1 (M⁺, 1), 278.0 (33), 277.0 (16), 250.1 (26), 235 (21), 200 (21), 147 (31) 105.0 (100), 77.0 (49), 56.1 (20). **HRMS (ESI) m/z:** [M+Na]⁺ Calcd for C₂₂H₂₄O₄Na 375.1572; Found 375.1569.



Benzyl (±)-cis-1-acetyl-2-(4-(tert-butyl)phenyl)cyclopropane-1-carboxylate

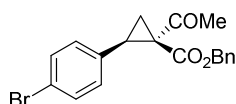
(1i). Following *GP-B*, **1i** (771 mg, 2.2 mmol, 42%, dr > 20:1) was isolated by FC (petroleum ether/EtOAc, from 19:1 to 9:1) on silica gel as a white solid starting from benzyl 2-diazo-3-oxobutanoate (1.1 g, 5.2 mmol, 1.0 eq.), 4-*tert*-butylstyrene (4.2 g, 26.0 mmol, 5.0 eq.), toluene (5.2 mL) and Rh₂(OAc)₄ (38 mg, 0.08 mmol, 2 mol%). R_f = 0.50 (petroleum ether/EtOAc, 8:2). **¹H NMR** (300 MHz, CDCl₃) δ 7.40-7.24 (m, 5H, C_{arom}-H), 7.19-7.08 (m, 2H, C_{arom}-H), 7.04-6.91 (m, 2H, C_{arom}-H), 4.86 (d, *J* = 12.1 Hz, 1H, OCH_aH_b), 4.68 (d, *J* = 12.1 Hz, 1H, OCH_aH_b), 3.29 (app t, *J* = 8.7 Hz, 1H, CHCH₂), 2.46 (s, 3H, CH₃C=O), 2.25 (dd, *J* = 8.4, 4.3 Hz, 1H, CHCH_aH_b), 1.78 (dd, *J* = 8.7, 4.2 Hz, 1H, CHCH_aH_b), 1.33 (s, 9H, C(CH₃)₃). **¹³C NMR** (75 MHz, CDCl₃) δ 202.1 (CH₃C=O), 168.3 (COO), 150.3 (C_{arom}C(CH₃)₃), 135.0 (C_{arom}-C), 131.8 (C_{arom}-C), 128.5 (4×C_{arom}-H), 128.4 (2×C_{arom}-H), 128.3 (C_{arom}-H), 125.1 (2×C_{arom}-H), 67.2 (OCH₂), 44.7 (CCH₂), 35.6 (CH₃C=O), 34.5 (C(CH₃)₃), 31.4 (C(CH₃)₃), 29.7

(CHCH₂), 21.9 (CHCH₂). **IR** (ATR): 1728 (C=O st), 1691 (C=O st) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₂₃H₂₇O₃ 351.1960; Found 351.1967. **M.p.**: 48-51 °C (petroleum ether/EtOAc).



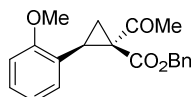
(±)-**1j** **Benzyl (±)-cis-1-acetyl-2-phenylcyclopropane-1-carboxylate (1j).** Following *GP-B*,

1j (918 mg, 3.1 mmol, 60%, dr > 20:1) was isolated by FC (petroleum ether/EtOAc, from 19:1 to 9:1) on silica gel as yellow oil starting from benzyl 2-diazo-3-oxobutanoate (1.1 g, 5.2 mmol, 1.0 eq.), styrene (1.1 g, 10.4 mmol, 2.0 eq.), toluene (5.2 mL) and Rh₂(OAc)₄ (38 mg, 0.08 mmol, 2 mol%). R_f = 0.55 (petroleum ether/EtOAc, 8:2). **¹H NMR** (300 MHz, CDCl₃) δ 7.37-7.12 (m, 8H, C_{arom}-H), 7.09-6.91 (m, 2H, C_{arom}-H), 4.85 (d, *J* = 12.1 Hz, 1H, OCH_aCH_b), 4.70 (d, *J* = 12.1 Hz, 1H, OCH_aCH_b), 3.31 (app t, *J* = 8.6 Hz, 1H, CHCH_aH_b), 2.44 (s, 3H, CH₃), 2.25 (dd, *J* = 8.2, 4.6 Hz, 1H, CHCH_aH_b), 1.75 (dd, *J* = 9.2, 4.6 Hz, 1H, CHCH_aH_b). **¹³C NMR** (75 MHz, CDCl₃) δ 202.2 (CH₃C=O), 168.3 (COO), 135.0 (C_{arom}-C), 134.9 (C_{arom}-C), 128.9 (2×C_{arom}-H), 128.6 (4×C_{arom}-H), 128.4 (C_{arom}-H), 128.3 (2×C_{arom}-H), 127.6 (C_{arom}-H), 67.3 (OCH₂), 44.8 (CC=O), 35.7 (CHCH₂), 29.8 (CH₃), 21.8 (CHCH₂). **IR** (ATR): 1728 (C=O st), 1691 (C=O st), 1166 (C-O st as) cm⁻¹. **MS** (EI) m/z (%): 203.0 (M⁺-C₇H₇, 2), 115.0 (17), 91.1 (100), 77.0 (17). **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for: C₁₉H₁₈O₃Na 317.1154; Found 317.1164.



(±)-**1k** **Benzyl (±)-cis-1-acetyl-2-(4-bromophenyl)cyclopropane-1-carboxylate (1k).**

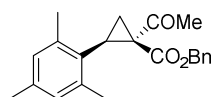
Following *GP-B*, **1k** (2.3 g, 6.1 mmol, 59%, dr > 20:1) was isolated by FC (petroleum ether/EtOAc, from 19:1 to 9:1) on silica gel as white solid starting from 2-diazo-3-oxobutanoate (1.1 g, 5.2 mmol, 1.0 eq.), 4-bromostyrene (1.9 g, 10.4 mmol, 2.0 eq.), toluene (5.2 mL) and Rh₂(OAc)₄ (38 mg, 0.08 mmol, 2 mol%). R_f = 0.40 (petroleum ether/EtOAc, 8:2). **¹H NMR** (300 MHz, CDCl₃) δ 7.61-7.15 (m, 5H, C_{arom}-H), 7.13-6.76 (m, 4H, C_{arom}-H), 4.93 (d, *J* = 11.9 Hz, 1H, OCH_aCH_b), 4.80 (d, *J* = 11.9 Hz, 1H, OCH_aCH_b), 3.24 (app t, *J* = 8.6 Hz, 1H, CHCH_aH_b), 2.44 (s, 3H, CH₃), 2.19 (dd, *J* = 8.1, 4.7 Hz, 1H, CHCH_aH_b), 1.73 (dd, *J* = 9.1, 4.7 Hz, 1H, CHCH_aH_b). **¹³C NMR** (75 MHz, CDCl₃) δ 201.9 (CH₃C=O), 168.0 (COO), 134.9 (C_{arom}-C), 133.9 (C_{arom}-C), 131.4 (2×C_{arom}-H), 130.6 (2×C_{arom}-H), 128.8 (2×C_{arom}-H), 128.7 (2×C_{arom}-H), 128.6 (C_{arom}-H), 121.6 (C_{arom}-C), 67.5 (OCH₂), 44.7 (CC=O), 34.6 (CHCH₂), 29.8 (CCH₃), 21.8 (CHCH₂). **IR** (ATR): 1725 (C=O st), 1693 (C=O st), 1166 (C-O st as) cm⁻¹. **MS** (EI) m/z (%): 371.9 (M⁺, 1), 91.1 (100). **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₁₉H₁₇BrO₃Na 395.0259; Found 395.0265. **M.p.**: 103-106 °C (petroleum ether/EtOAc).



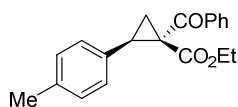
(±)-**1m** **Benzyl (±)-cis-1-acetyl-2-(2-methoxyphenyl)cyclopropane-1-carboxylate (1m).**

Following *GP-B*, **1m** (1.3 g, 4.1 mmol, 78%, dr 5:1) was isolated by FC (petroleum ether/EtOAc, from 19:1 to 9:1) on silica gel as a colorless oil starting from benzyl 2-diazo-3-oxobutanoate (1.1 g, 5.2 mmol, 1.0 eq.), 2-methoxystyrene (3.6 mL, 26.0 mmol, 5.0 eq.), toluene (5.2 mL) and Rh₂(OAc)₄ (38 mg, 0.08 mmol, 2 mol%). R_f = 0.50 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) (* indicates minor diastereoisomer resonances) δ 7.61-7.747* (m, 1H, C_{arom}-H), 7.42-7.36 (m, 1H, C_{arom}-H), 7.33-7.20 (m, 3H, C_{arom}-H), 7.10-6.98 (m, 3H, C_{arom}-H), 6.90-6.82 (m, 1H, C_{arom}-H), 6.76 (d, *J* = 8.2 Hz, 1H, C_{arom}-H), 5.31* (d, *J* = 12.5 Hz, 1H, OCH_aH_b), 5.25* (d, *J* = 12.4 Hz, 1H, OCH_aH_b), 4.85 (d, *J* = 12.1 Hz, 1H,

OCH_aH_b), 4.65 (d, $J = 12.1$ Hz, 1H, OCH_aH_b), 3.82* (s, 3H, OCH₃), 3.69 (s, 3H, OCH₃), 3.40* (app t, $J = 8.7$ Hz, 1H, CHCH₂), 3.13 (app t, $J = 8.8$ Hz, 1H, CHCH₂), 2.52 (s, 3H, CH₃C=O), 2.35* (dd, $J = 8.6, 4.7$ Hz, 1H, CHCH_aH_b), 2.20 (dd, $J = 8.4, 4.5$ Hz, 1H, CHCH_aH_b), 2.02* (s, 3H, CH₃C=O), 1.90 (dd, $J = 9.1, 4.5$ Hz, 1H, CHCH_aH_b), 1.72* (dd, $J = 8.9, 4.7$ Hz, 1H, CHCH_aH_b). ¹³C NMR (75 MHz, CDCl₃) (* indicates minor diastereoisomer resonances) δ 202.7 (CH₃C=O), 200.1* (CH₃C=O), 170.1* (COO), 168.5 (COO), 159.0 (C_{arom}-OCH₃), 158.6* (C_{arom}-OCH₃), 135.7* (C_{arom}-C), 135.3 (C_{arom}-C), 128.90 (C_{arom}-H), 128.86* (C_{arom}-H), 128.7 (C_{arom}-H), 128.6* (C_{arom}-H), 128.41 (2×C_{arom}-H), 128.39 (2×C_{arom}-H), 128.2 (C_{arom}-H), 128.0* (C_{arom}-H), 123.5 (C_{arom}-C), 122.4* (C_{arom}-C), 120.3* (C_{arom}-H), 120.0 (C_{arom}-H), 110.0 (C_{arom}-H), 109.7* (C_{arom}-H), 66.9* (OCH₂), 66.8 (OCH₂), 55.3 (OCH₃), 55.2* (OCH₃), 43.3 (CCH₂), 43.0* (CCH₂), 32.8 (CH₃C=O), 31.5* (CH₃C=O), 29.8 (CHCH₂), 29.6* (CHCH₂), 20.5 (CHCH₂), 17.5* (CHCH₂). IR (ATR): 1721 (C=O st), 1693 (C=O st), 1170 (C-O st as) cm⁻¹. MS (EI) m/z (%): 324.1 (M⁺, 2), 91.1 (100), 77.0 (11), 65.1 (11). HRMS (ESI) m/z: [M+H]⁺ Calcd for C₂₀H₂₁O₄ 325.1440; Found 325.1449.



(±)-**1n** **Benzyl (±)-cis-1-acetyl-2-mesitylcyclopropane-1-carboxylate (1n)**. Following *GP-B*, **1n** (523 mg, 1.5 mmol, 42%, dr > 20:1) was isolated by FC (petroleum ether/EtOAc, from 19:1 to 9:1) on silica gel as yellow oil starting from benzyl 2-diazo-3-oxobutanoate (0.8 g, 3.7 mmol, 1.0 eq.), 1,3,5-trimethyl-2-vinylbenzene (1.1 g, 7.4 mmol, 2.0 eq.), toluene (5.2 mL) and Rh₂(OAc)₄ (31 mg, 0.07 mmol, 2 mol%). R_f = 0.50 (petroleum ether/EtOAc, 8:2). ¹H NMR (300 MHz, CDCl₃) δ 7.37-7.16 (m, 3H, C_{arom}-H), 7.09-6.88 (m, 2H, C_{arom}-H), 6.75 (s, 2H, C_{arom}-H), 4.84 (d, $J = 12.0$ Hz, 1H, OCH_aCH_b), 4.59 (d, $J = 12.0$ Hz, 1H, OCH_aCH_b), 3.16 (app t, $J = 9.3$ Hz, 1H, CHCH_aH_b), 2.59 (s, 3H, COCH₃), 2.45 (dd, $J = 9.1, 4.3$ Hz, 1H, CHCH_aH_b), 2.36-2.05 (m, 9H, 3×C_{arom}-CH₃), 1.99 (dd, $J = 9.5, 4.3$ Hz, 1H, CHCH_aH_b). ¹³C NMR (75 MHz, CDCl₃) δ 203.4 (CH₃C=O), 169.2 (COO), 136.5 (C_{arom}-C), 135.0 (C_{arom}-C), 129.3 (C_{arom}-H), 129.0 (C_{arom}-C), 128.8 (C_{arom}-C), 128.7 (2×C_{arom}-H), 128.6 (C_{arom}-H), 128.43 (2×C_{arom}-H), 128.40 (C_{arom}-C), 128.37 (C_{arom}-H), 67.2 (OCH₂), 42.7 (CC=O), 35.7 (CHCH₂), 30.3 (COCH₃), 27.1 (3×C_{arom}-CH₃) 21.0 (CHCH₂). IR (ATR): 1715 (C=O st), 1691 (C=O st), 1176 (C-O st as) cm⁻¹. MS (EI) m/z (%): 336.2 (M⁺, 3), 157.1 (21), 143.1 (15), 142.1 (16), 141.1 (19), 128.1 (20), 115.1 (17), 91.1 (100), 77.0 (17). HRMS (ESI) m/z: [M+H]⁺ Calcd for: C₂₂H₂₅O₃ 336.1754; Found 336.1762.



(±)-**1o** **Ethyl (±)-cis-1-benzoyl-2-(p-tolyl)cyclopropane-1-carboxylate (1o)**. Following *GP-B*, **1o** (1.3 g, 4.2 mmol, 81%, dr > 20:1) was isolated by FC (petroleum ether/EtOAc, 9:1) on silica gel as white solid starting from ethyl benzoylacetate (1.0 g, 5.2 mmol, 1.0 eq.) and *p*-ABSA (1.5 g, 6.2 mmol, 1.2 eq.) in CH₃CN (37 mL) using Et₃N (1.1 mL, 7.8 mmol, 1.5 eq.). After dissolving the crude ethyl 2-diazo-3-oxo-3-phenylpropanoate (1.1 g, 5.2 mmol, 1.0 eq.) and 4-methylstyrene (3.4 mL, 26.0 mmol, 5.0 eq.) in toluene (5.2 mL), Rh₂(OAc)₄ (38 mg, 0.08 mmol, 2 mol%) was added. R_f = 0.50 (petroleum ether/EtOAc, 8:2). ¹H NMR (300 MHz, CDCl₃) δ 7.91 (dd, $J = 7.2, 1.0$ Hz, 2H, C_{arom}-H), 7.62-7.51 (m, 1H, C_{arom}-H), 7.50-7.40 (m, 2H, C_{arom}-H), 7.20 (d, $J = 7.9$ Hz, 2H, C_{arom}-H), 7.10 (d, $J = 7.9$ Hz, 2H, C_{arom}-H), 3.82-3.63 (m, 2H, OCH₂), 3.54 (app t, $J = 8.6$ Hz, 1H, CHCH₂), 2.42 (dd, $J = 8.1,$

4.7 Hz, 1H, CHCH_aH_b), 2.31 (s, 3H, C_{arom}-CH₃), 1.67 (dd, *J* = 9.1, 4.7 Hz, 1H, CHCH_aH_b), 0.69 (t, *J* = 7.1 Hz, 3H, CH₂CH₃). ¹³C NMR (75 MHz, CDCl₃) δ 195.2 (C_{arom}C=O), 168.6 (COO), 137.6 (C_{arom}-C), 136.9 (C_{arom}-C), 132.9 (C_{arom}-H), 131.8 (C_{arom}-C), 129.1 (2×C_{arom}-H), 128.9 (2×C_{arom}-H), 128.6 (2×C_{arom}-H), 128.3 (2×C_{arom}-H), 61.2 (OCH₂), 42.5 (CC=O), 30.6 (CHCH₂), 21.2 (C_{arom}-CH₃), 20.2 (CHCH₂), 13.6 (CH₂CH₃). **IR** (ATR): 1730 (C=O st), 1678 (C=O st), 1145 (C-O st as) cm⁻¹. **MS** (EI) *m/z* (%): 203.11 (M⁺ - C₇H₅O, 1), 105.0 (100), 77.0 (50). **HRMS** (ESI) *m/z*: [M+Na]⁺ Calcd for C₂₀H₂₀O₃Na 331.1210; Found 331.1322. **M.p.**: 56-59 °C (petroleum ether/EtOAc).

2.2 Synthesis of indoles 2a-q

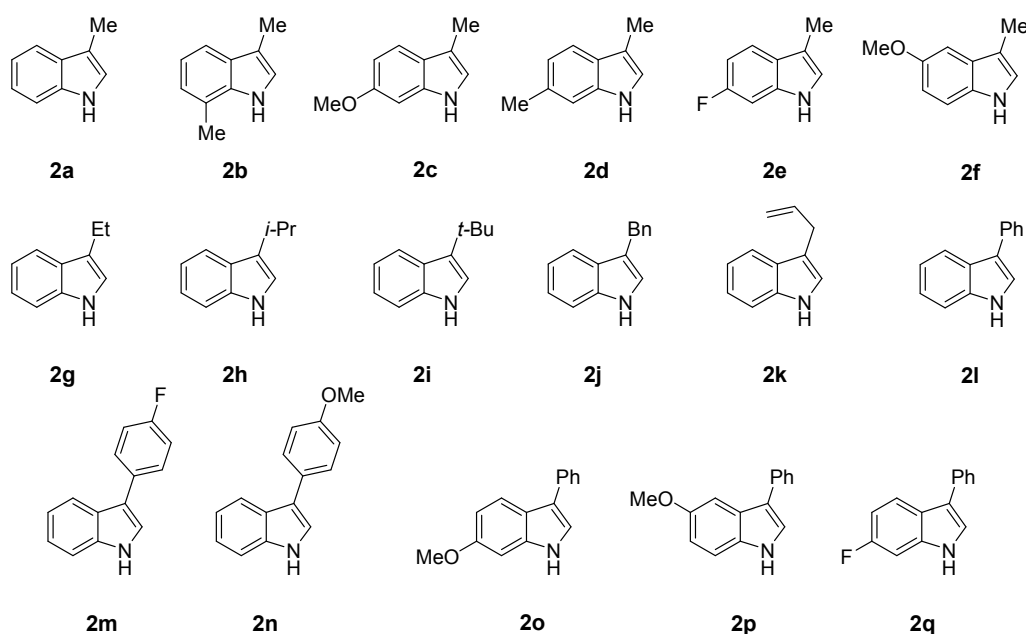


Figure S1. Employed indoles

Indole **2a** was obtained from commercial sources. Compounds **2b-d**¹⁵, **2f-g**¹⁴, **2o**¹⁴, **2e**¹⁶, **2k**¹⁵, **2h**¹⁷, **2i**¹⁸, **2j**¹⁹, **2l-n**²⁰, **2p**¹⁹, **2o**²¹, and **2q**²⁰ were reported compounds and they were prepared following procedures previously described in the literature.

¹⁵ Zhou, Z.; Li, Y.; Gong, L.; Meggers, E. *Org. Lett.* **2017**, *19*, 222.

¹⁶ Tomakinian, T.; Guillot, R.; Kouklovsky, C.; Vincent, G. *Angew. Chem. Int. Ed.* **2014**, *53*, 11881.

¹⁷ Zhang, Y.; Stephens, D.; Hernandez, G.; Mendoza, R.; Larionov, O. V. *Chem. Eur. J.* **2012**, *18*, 16612.

¹⁸ Zhu, X.; Ganesan, A. *J. Org. Chem.* **2002**, *67*, 2705.

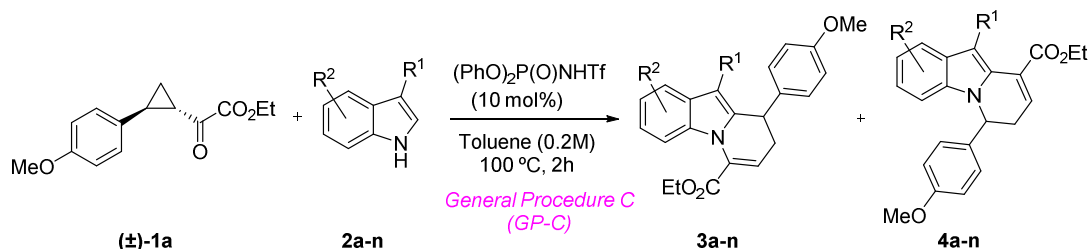
¹⁹ Cano, R.; Yus, M.; Ramón, D. J. *Tetrahedron Lett.* **2013**, *54*, 3394.

²⁰ O'Brien, C. J.; Droegge, D. G.; Jiu, A. Y.; Gandhi, S. S.; Paras, N. A.; Olson, S. H.; Conrad, J. *J. Org. Chem.* **2018**, *83*, 8926.

²¹ Gattu, R.; Bhattacharjee, S.; Mahato, K.; Khan, A. T. *Org. Biomol. Chem.* **2018**, *16*, 3760.

2.3 Cyclocondensation of 3-substituted indoles with donor-acceptor cyclopropanes

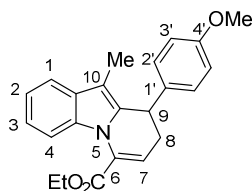
2.3.1 Synthesis of dihydropyridoindoles 3 and 4



Scheme S3. General Procedure C for the synthesis of dihydropyridoindoles (±)-3 and (±)-4

General Procedure C (GP-C) for the cyclocondensation: An oven-dried 5 mL screw-capped test tube containing a stirring bar was charged with the cyclopropane **1a** (1eq.) and the corresponding indole **2a-n** (1eq.) and dissolved in toluene (0.2 M) under Ar. After adding the diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate catalyst (10 mol%) the mixture was stirred at 100 °C in an oil bath. When the reaction was judged complete (monitored by TLC), it was warmed to room temperature, quenched by addition of aq. NaHCO₃ (sat) (3 mL) and diluted with EtOAc (3 mL). The phases were separated and the aqueous phase was extracted with EtOAc (3×3 mL). The combined organic layers were dried over Na₂SO₄, filtered and evaporated. The residue was purified by column chromatography on silica gel to afford the corresponding pure compounds **3a-n** and **4a-n**.

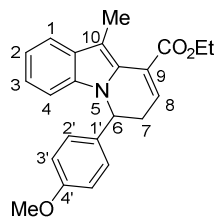
Ethyl (±)-9-(4-methoxyphenyl)-10-methyl-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3a) and ethyl (±)-6-(4-methoxyphenyl)-10-methyl-6,7-dihydropyrido[1,2-a]indole-9-carboxylate (4a). Following GP-C, (±)-**3a** (9 mg, 0.025 mmol, 50%) and (±)-**4a** (2 mg, 0.004 mmol, 9%) were isolated by FC (petroleum ether/EtOAc, from 25:1 to 19:1) on silica gel as white solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol) and indole **2a** (7 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h in an oil bath.



(±)-**3a**

¹H NMR (300 MHz, CDCl₃) δ 7.63-7.46 (m, 1H, H-1), 7.26-7.12 (m, 3H, H-2 + H-3 + H-4), 7.05 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.81 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.27 (dd, *J* = 6.6, 3.8 Hz, 1H, H-7), 4.46-4.05 (m, 3H, H-9 + OCH₂), 3.77 (s, 3H, OCH₃), 2.99-2.49 (m, 2H, H-8), 2.15 (s, 3H, C-10-CH₃), 1.37 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). ¹³C NMR (75 MHz, CDCl₃) δ 163.5 (COO), 158.4 (C_{arom}-O), 134.0 (C-4a + C-9a + C_{arom}-C), 131.3 (C-6), 129.9 (C-10a), 128.6 (2× C_{arom}-H), 122.0 (C-3), 120.3 (C-2), 119.9 (C-7), 118.5 (C-1), 114.0 (2× C_{arom}-H), 112.0 (C-4), 109.4 (C-10), 61.7 (OCH₂), 55.3 (OCH₃), 35.9 (C-9), 30.5 (C-8), 14.3 (OCH₂CH₃), 8.7 (C-10-CH₃). IR (ATR): 2987 (C-H st), 1727 (C=O st), 1260 (C-O st as) cm⁻¹. MS (EI) *m/z* (%): 362.2 (26), 361.2 (M⁺, 100), 289.1 (16), 288.1 (72), 287.1

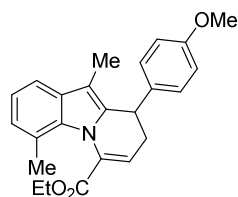
(23), 286.1 (20), 273.1 (19). **HRMS (ESI) m/z:** [M+H]⁺ Calcd for C₂₃H₂₄NO₃ 362.1756; Found 362.1758. **M.p.:** 126-129 °C (petroleum ether/EtOAc).



(±)-4a

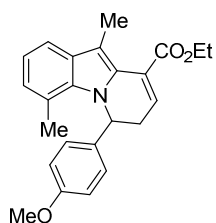
¹H NMR (300 MHz, CDCl₃) δ 7.73-7.52 (m, 1H, H-1), 7.18-6.98 (m, 3H, C_{arom}-H), 6.84 (d, *J* = 8.8 Hz, 2H, C_{arom}-H), 6.76 (d, *J* = 8.8 Hz, 2H, C_{arom}-H), 6.57 (dd, *J* = 7.1, 3.0 Hz, 1H, H-8), 5.63 (app d, *J* = 6.9 Hz, 1H, H-6), 4.45-4.25 (m, 2H, OCH₂CH₃), 3.73 (s, 3H, OCH₃), 3.13 (ddd, *J* = 17.1, 7.2, 3.0 Hz, 1H, H-7a), 2.82 (ddd, *J* = 17.1, 7.1, 1.8 Hz, 1H, H-7b), 2.40 (s, 3H, C-10-CH₃), 1.38 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 166.6 (COO), 158.9 (C_{arom}-O), 135.6 (C-4a), 133.2 (C_{arom}-C), 129.4 (C-8), 129.3 (C_{arom}-C), 128.6 (C_{arom}-C), 127.4 (C_{arom}-C), 126.9 (2×C_{arom}-H), 123.1 (C_{arom}-H), 119.5 (2×C_{arom}-H), 114.1 (2×C_{arom}-H), 109.9 (C-10), 109.1 (C_{arom}-H), 61.3 (OCH₂), 55.3 (OCH₃), 52.5 (C-6), 33.1 (C-7), 14.4 (OCH₂CH₃), 10.5 (C-10-CH₃). **IR** (ATR): 2937 (C-H st), 1721 (C=O st), 1250 (C-O st as) cm⁻¹. **MS** (EI) m/z (%): 362.2 (26), 361.2 (M⁺, 100), 288.1 (39), 287.1 (15), 286.1 (15), 273.1 (21), 121.0 (15). **HRMS (ESI) m/z:** [M+H]⁺ Calcd for C₂₃H₂₄NO₃ 362.1756; Found 362.1751. **M.p.:** 64-67 °C (petroleum ether/EtOAc).

Ethyl (±)-9-(4-methoxyphenyl)-4,10-dimethyl-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3b) and ethyl (±)-6-(4-methoxyphenyl)-4,10-dimethyl-6,7-dihydropyrido[1,2-a]indole-9-carboxylate (4b). Following *GP-C*, (±)-**3b** (10 mg, 0.026 mmol, 54%) and (±)-**4b** (1 mg, 0.002 mmol, 4%) were isolated by FC (petroleum ether/EtOAc, from 93:7 to 95:5) on silica gel as white solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol) and indole **2b** (7 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h.



(±)-3b

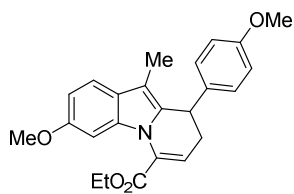
¹H NMR (300 MHz, CDCl₃) δ 7.35 (d, *J* = 7.7 Hz, 1H, H-1), 7.07 (app t, *J* = 7.5 Hz, 1H, H-2), 7.03-6.93 (m, 3H, C_{arom}-H + H-3), 6.79 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.32 (dd, *J* = 6.9, 4.8 Hz, 1H, H-7), 4.46-4.07 (m, 3H, H-9 + OCH₂), 3.77 (s, 3H, OCH₃), 2.84-2.61 (m, 2H, H-8), 2.43 (s, 3H, C-4-CH₃), 2.04 (s, 3H, C-10-CH₃), 1.27 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 164.6 (COO), 158.4 (C_{arom}-O), 135.9 (C-4a), 134.5 (C_{arom}-C), 133.6 (C-9a), 133.0 (C-6), 130.5 (C-10a), 128.8 (2×C_{arom}-H), 125.3 (C-2), 121.9 (C-4), 121.7 (C-3), 120.6 (C-7), 116.1 (C-1), 113.9 (2×C_{arom}-H), 109.2 (C-10), 61.5 (OCH₂), 55.3 (OCH₃), 37.9 (C-9), 31.1 (C-8), 19.4 (C-4-CH₃), 14.2 (OCH₂CH₃), 9.0 (C-10-CH₃). **IR** (ATR): 2958 (C-H st), 1725 (C=O st), 1259 (C-O st as) cm⁻¹. **MS** (EI) m/z (%): 376.2 (27), 375.2 (M⁺, 100), 302.1 (38), 287.1 (16). **HRMS (ESI) m/z:** [M+H]⁺ Calcd for C₂₄H₂₆NO₃ 376.1913; Found 376.1905. **M.p.:** 138-141 °C (petroleum ether/EtOAc).



(±)-4b

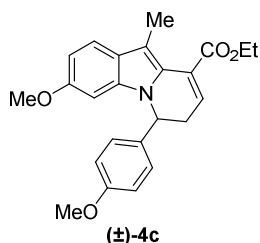
¹H NMR (300 MHz, CDCl₃) δ 7.46 (d, *J* = 7.8 Hz, 1H, H-1), 6.97 (app t, *J* = 7.4 Hz, 1H, H-2), 6.86 (d, *J* = 7.4 Hz, 1H, H-3), 6.82-6.69 (m, 4H, C_{arom}-H), 6.48 (dd, *J* = 7.3, 2.9 Hz, 1H, H-8), 6.16 (d, *J* = 6.8 Hz, 1H, H-6), 4.41-4.23 (m, 2H, OCH₂CH₃), 3.73 (s, 3H, OCH₃), 3.14 (ddd, *J* = 16.8, 6.8, 2.9 Hz, 1H, H-7a), 2.81 (dd, *J* = 16.8, 7.3 Hz, 1H, H-7b), 2.49 (s, 3H, C_{arom}-CH₃), 2.34 (s, 3H, C-10-CH₃), 1.36 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 166.8 (COO), 158.8 (C_{arom}-O), 134.6 (C_{arom}-C), 134.4 (C_{arom}-C), 129.7 (C_{arom}-C), 129.0 (C_{arom}-C), 128.8 (C-8), 127.9 (C_{arom}-C), 126.7 (2× C_{arom}-H), 126.1 (C_{arom}-H), 120.4 (C_{arom}-C), 119.4 (C_{arom}-H), 117.4 (C_{arom}-H), 114.1 (2× C_{arom}-H), 109.9 (C-10), 61.3 (OCH₂), 55.3 (OCH₃), 54.2 (C-6), 33.4 (C-7), 20.0 (C-4-CH₃), 14.4 (OCH₂CH₃), 10.5 (C-10-CH₃). **IR** (ATR): 2918 (C-H st), 1732 (C=O st), 1248 (C-O st as) cm⁻¹. **MS** (EI) *m/z* (%): 376.2 (27), 375.2 (M⁺, 100), 302.1 (48), 301.1 (17), 300.1 (15), 287.1 (28), 286.1 (15), 121.0 (18). **HRMS** (ESI) *m/z*: [M+H]⁺ Calcd for C₂₄H₂₆NO₃ 376.1913; Found 376.1909.

Ethyl (±)-3-methoxy-9-(4-methoxyphenyl)-10-methyl-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3c). Following *GP-C*, (±)-3c (12 mg, 0.030 mmol, 61%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as yellow solid, starting from cyclopropane **1a** (12 mg, 0.05 mmol) and indole **2c** (8 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h.



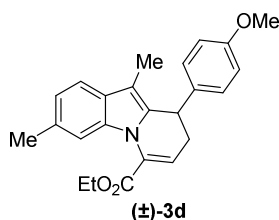
(±)-3c

¹H NMR (300 MHz, CDCl₃) δ 7.40 (d, *J* = 8.5 Hz, 1H, H-1), 7.05 (d, *J* = 8.5 Hz, 2H, C_{arom}-H), 6.92-6.76 (m, 3H, C_{arom}-H+ H-2), 6.73 (d, *J* = 2.2 Hz, 1H, H-4), 6.25 (dd, *J* = 6.7, 3.9 Hz, 1H, H-7), 4.63-4.28 (m, 3H, H-9 + OCH₂), 3.86 (s, 3H, OCH₃), 3.77 (s, 3H, OCH₃), 2.87-2.60 (m, 2H, H-8), 2.11 (s, 3H, C-10-CH₃), 1.38 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 163.5 (COO), 158.3 (C_{arom}-O), 156.3 (C-O), 134.8 (C-4a), 134.2 (C_{arom}-C), 132.9 (C-9a), 131.3 (C-6), 128.5 (2× C_{arom}-H), 124.3 (C-10a), 120.0 (C-7), 118.8 (C-1), 113.9 (2× C_{arom}-H), 109.2 (C-2 + C-10), 97.0 (C-4), 61.7 (OCH₂), 55.9 (OCH₃), 55.3 (OCH₃), 35.9 (C-9), 30.6 (C-8), 14.4 (OCH₂CH₃), 8.7 (C-10-CH₃). **IR** (ATR): 2936 (C-H st), 1724 (C=O st), 1247 (C-O st as) cm⁻¹. **MS** (EI) *m/z* (%): 392.2 (26), 391.2 (M⁺, 100), 318.1 (35), 302.1 (13). **HRMS** (ESI) *m/z*: [M+H]⁺ Calcd for C₂₄H₂₆NO₄ 392.1862; Found 392.1855. **M.p.**: 100-104 °C (petroleum ether/EtOAc).

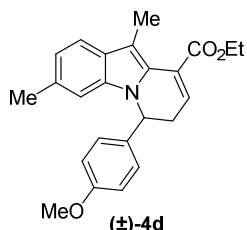


¹H NMR (300 MHz, CDCl₃) δ 7.47 (d, *J* = 8.6, 1H, H-1), 6.86 (d, *J* = 8.6, 2H, C_{arom}-H), 6.80-6.69 (m, 3H, C_{arom}-H + H-2), 6.52-6.46 (m, 2H, H-4 + H-8), 5.54 (app d, *J* = 6.6 Hz, 1H, H-6), 4.40-4.24 (m, 2H, OCH₂CH₃), 3.76 (s, 3H, OCH₃), 3.73 (s, 3H, OCH₃), 3.11 (ddd, *J* = 17.0, 7.0, 3.1 Hz, 1H, H-7a), 2.80 (ddd, *J* = 17.0, 7.1, 1.8 Hz, 1H, H-7b), 2.36 (s, 3H, C-10-CH₃), 1.37 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 166.7 (COO), 158.9 (C-3), 157.4 (C_{arom}-O), 136.5 (C-4a), 133.2 (C_{arom}-C), 128.6 (C_{arom}-C), 128.0 (C-8), 127.0 (2× C_{arom}-H), 126.6 (C_{arom}-C), 123.9 (C_{arom}-C), 120.2 (C_{arom}-H), 114.1 (2× C_{arom}-H), 110.0 (C-10), 109.2 (C_{arom}-H), 92.8 (C_{arom}-H), 61.2 (OCH₂), 55.7 (OCH₃), 55.7 (OCH₃), 52.5 (C-6), 33.1 (C-7), 14.3 (OCH₂CH₃), 10.5 (C-10-CH₃). **IR** (ATR): 2934 (C-H st), 1721 (C=O st), 1249 (C-O st as) cm⁻¹. **MS** (EI) *m/z* (%): 392.2 (27), 391.2 (M⁺, 100), 318.1 (23), 303.1 (13). **HRMS (ESI) *m/z***: [M+H]⁺ Calcd for C₂₄H₂₆NO₄ 392.1862; Found 392.1866. **M.p.**: 65-68 °C (petroleum ether/EtOAc).

Ethyl (±)-9-(4-methoxyphenyl)-3,10-dimethyl-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3d) and ethyl (±)-6-(4-methoxyphenyl)-3,10-dimethyl-6,7-dihydropyrido[1,2-a]indole-9-carboxylate (4d). Following *GP-C*, (±)-**3d** (10 mg, 0.026 mmol, 52%) and (±)-**4d** (2 mg, 0.004 mmol, 8%) were isolated by FC (petroleum ether/EtOAc, from 25:1 to 19:1) on silica gel as yellow solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol) and indole **2d** (7 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h in an oil bath.

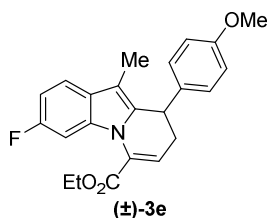


¹H NMR (300 MHz, CDCl₃) δ 7.40 (d, *J* = 7.9 Hz, 1H, H-1), 7.10-6.89 (m, 4H, C_{arom}-H + H-4 + H-2), 6.79 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.22 (dd, *J* = 6.6, 3.9 Hz, 1H, H-7), 4.49-4.39 (m, 3H, H-9 + OCH₂), 3.76 (s, 3H, OCH₃), 2.85-2.59 (m, 2H, H-8), 2.47 (s, 3H, CH₃), 2.11 (s, 3H, CH₃), 1.37 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 163.7 (COO), 158.4 (C_{arom}-O), 134.4 (C-4a), 134.2 (C_{arom}-C), 133.3 (C-9a), 131.7 (C-3), 131.4 (C-6), 128.6 (2× C_{arom}-H), 127.7 (C-10a), 121.9 (C-2), 119.6 (C-9), 118.2 (C-1), 113.9 (2× C_{arom}-H), 112.1 (C-4), 109.2 (C-10), 61.6 (OCH₂), 55.3 (OCH₃), 35.9 (C-9), 30.5 (C-8), 22.1 (C-3-CH₃), 14.3 (OCH₂CH₃), 8.7 (C-10-CH₃). **MS** (EI) *m/z* (%): 376.2 (26), 375.2 (M⁺, 100), 302.2 (56), 301.1 (16), 287.1 (19). **IR** (ATR): 2925 (C-H st), 1725 (C=O st), 1245 (C-O st as) cm⁻¹. **HRMS (ESI) *m/z***: [M+H]⁺ Calcd for C₂₄H₂₆NO₃ 376.1913; Found 376.1911. **M.p.**: 76-79 °C (petroleum ether/EtOAc).

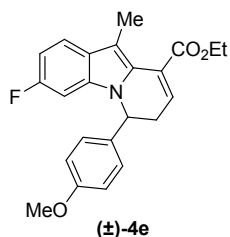


¹H NMR (300 MHz, CDCl₃) δ 7.48 (d, *J* = 7.9 Hz, 1H, H-1), 7.02-6.81 (m, 4H, C_{arom}-H + H-4 + H-2), 6.76 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.52 (dd, *J* = 7.2, 3.0 Hz, 1H, H-8), 5.70-5.52 (m, 1H, H-6), 4.50-4.12 (m, 2H, OCH₂CH₃), 3.73 (s, 3H, OCH₃), 3.11 (ddd, *J* = 17.0, 7.2, 3.0 Hz, 1H, H-7a), 2.80 (ddd, *J* = 17.0, 7.2, 1.6 Hz, 1H, H-7b), 2.39 (s, 3H, C_{arom}-CH₃), 2.37 (s, 3H, C_{arom}-CH₃), 1.37 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 166.6 (COO), 158.9 (C_{arom}-O), 136.1 (C-4a), 133.4 (C_{arom}-C), 133.1 (C_{arom}-C), 128.7 (C-8 + C_{arom}-C), 127.5 (C_{arom}-C), 127.3 (C_{arom}-C), 126.9 (2× C_{arom}-H), 121.3 (C_{arom}-H), 119.2 (C_{arom}-H), 114.1 (2× C_{arom}-H), 109.9 (C-10), 108.9 (C_{arom}-H), 61.3 (OCH₂), 55.3 (OCH₃), 52.3 (C-6), 33.1 (C-7), 22.1 (C-3-CH₃), 14.4 (OCH₂CH₃), 10.5 (C-10-CH₃). **IR** (ATR): 2925 (C-H st), 1721 (C=O st), 1250 (C-O st as) cm⁻¹. **MS** (EI) *m/z* (%): 375.2 (M⁺, 36), 281.0 (17), 208.0 (23), 207.0 (100), 96.0 (15). **HRMS (ESI) *m/z***: [M+H]⁺ Calcd for C₂₄H₂₆NO₃ 376.1913; Found 376.1908. **M.p.**: 85-88 °C (petroleum ether/EtOAc).

Ethyl (±)-3-fluoro-9-(4-methoxyphenyl)-10-methyl-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3e) and ethyl (±)-3-fluoro-6-(4-methoxyphenyl)-10-methyl-6,7-dihydropyrido[1,2-a]indole-9-carboxylate (4e). Following *GP-C*, (±)-**3e** (11 mg, 0.030 mmol, 60%) and (±)-**4e** (1 mg, 0.003 mmol, 5%) were isolated by FC (petroleum ether/EtOAc, from 25:1 to 19:1) on silica gel as yellow solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2e** (7 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h.

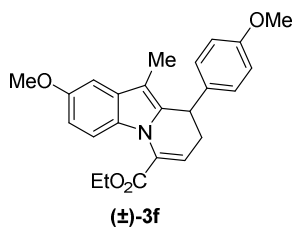


¹H NMR (300 MHz, CDCl₃) δ 7.49-7.32 (m, 1H, H-1), 7.03 (d, *J* = 7.9 Hz, 2H, C_{arom}-H), 6.97-6.86 (m, 2H, H-2 + H-4), 6.80 (d, *J* = 8.0 Hz, 2H, C_{arom}-H), 6.41-6.21 (m, 1H, H-7), 4.63-4.07 (m, 3H, H-9 + OCH₂), 3.77 (s, 3H, OCH₃), 2.91-2.54 (m, 2H, H-8), 2.11 (s, 3H, C-10-CH₃), 1.38 (t, *J* = 7.0 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 163.1 (COO), 159.8 (d, ¹*J*_{C-F} = 237.1 Hz, C-3), 158.3 (C_{arom}-O), 134.3 (d, ⁴*J*_{C-F} = 3.6 Hz, C-4a), 134.1 (d, ³*J*_{C-F} = 12.3 Hz, C-4a), 133.8 (C-9a + C_{arom}-C), 131.0 (C-6), 128.5 (2× C_{arom}-H), 126.4 (C-10a), 120.9 (C-7), 118.9 (d, ³*J*_{C-F} = 10.0 Hz, C-1), 114.0 (2× C_{arom}-H), 109.3 (C-10), 108.6 (d, ²*J*_{C-F} = 24.3 Hz, C-4), 99.2 (d, ²*J*_{C-F} = 27.7 Hz, C-2), 61.8 (OCH₂), 55.3 (OCH₃), 35.9 (C-9), 30.5 (C-8), 14.3 (OCH₂CH₃), 8.7 (C-10-CH₃). **IR** (ATR): 2933 (C-H st), 1722 (C=O st), 1247 (C-O st as), 1147 (C-F st) cm⁻¹. **MS** (EI) *m/z* (%): 380.2 (26), 379.2 (M⁺, 100), 307.2 (17), 306.2 (79), 305.2 (29), 304.2 (22), 291.1 (22), 198.1 (22). **HRMS (ESI) *m/z***: [M+H]⁺ Calcd for C₂₃H₂₃NO₃F 380.1662; Found 380.1668. **M.p.**: 123-126 °C (petroleum ether/EtOAc).

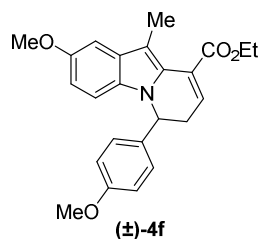


¹H NMR (300 MHz, CDCl₃) δ 7.50 (dd, *J* = 8.6, 5.3 Hz, 1H, H-1), 6.90-6.80 (m, 3H, C_{arom}-H + H-2), 6.80-6.67 (m, 3H, C_{arom}-H + H-4), 6.56 (dd, *J* = 7.1, 3.1 Hz, 1H, H-8), 5.51 (app d, *J* = 7.1 Hz, 1H, H-6), 4.42-4.22 (m, 2H, OCH₂CH₃), 3.74 (s, 3H, OCH₃), 3.13 (ddd, *J* = 17.2, 7.1, 3.1 Hz, 1H, H-7a), 2.81 (ddd, *J* = 17.2, 7.1, 1.9 Hz, 1H, H-7b), 2.36 (s, 3H, C-10-CH₃), 1.37 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 166.4 (COO), 160.7 (d, ¹*J*_{C-F} = 239.2 Hz, C-3), 159.1 (C_{arom}-O), 135.8 (d, ³*J*_{C-F} = 12.4 Hz, C-4a), 132.8 (C_{arom}-C), 129.2 (C-8), 128.5 (C_{arom}-C), 127.9 (d, ⁴*J*_{C-F} = 4.2 Hz, C-10a), 126.9 (2× C_{arom}-H), 126.0 (C_{arom}-C), 120.4 (d, ³*J*_{C-F} = 10.3 Hz, C-1), 114.2 (2× C_{arom}-H), 110.0 (C-10), 108.2 (d, ²*J*_{C-F} = 24.7 Hz, C_{arom}-H), 95.6 (d, ²*J*_{C-F} = 26.5 Hz, C_{arom}-H), 61.4 (OCH₂), 55.4 (OCH₃), 52.8 (C-6), 33.1 (C-7), 14.4 (OCH₂CH₃), 10.5 (C-10-CH₃). **IR** (ATR): 2930 (C-H st), 1728 (C=O st), 1242 (C-O st as), 1179 (C-F st) cm⁻¹. **MS** (EI) *m/z* (%): 380.2 (26), 379.2 (M⁺, 100), 306.2 (29). **HRMS (ESI) *m/z***: [M+H]⁺ Calcd for C₂₃H₂₃NO₃F 380.1662; Found 380.1653.

Ethyl (±)-2-methoxy-9-(4-methoxyphenyl)-10-methyl-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3f) and ethyl (±)-2-methoxy-6-(4-methoxyphenyl)-10-methyl-6,7-dihydropyrido[1,2-a]indole-9-carboxylate (4f). Following *GP-C*, (±)-**3f** (8 mg, 0.021 mmol, 42%) and (±)-**4f** (2 mg, 0.004 mmol, 8%) were isolated by FC (petroleum ether/EtOAc, from 25:1 to 19:1) on silica gel as yellow solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2f** (7 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h.

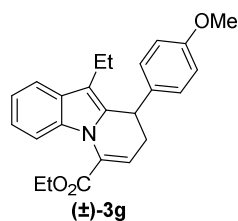


¹H NMR (300 MHz, CDCl₃) δ 7.17-6.92 (m, 4H, C_{arom}-H), 6.91-6.69 (m, 3H, C_{arom}-H), 6.22 (dd, *J* = 6.8, 3.8 Hz, 1H, H-7), 4.55-4.18 (m, 3H, H-9 + OCH₂), 3.88 (s, 3H, OCH₃), 3.76 (s, 3H, OCH₃), 2.84-2.60 (m, 2H, H-8), 2.10 (s, 3H, C-10-CH₃), 1.36 (t, *J* = 7.2 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 163.5 (COO), 158.4 (C_{arom}-O), 154.7 (C-2), 134.7 (C_{arom}-C), 134.0 (C-9a), 131.3 (C-6), 130.5 (C-10a), 129.2 (C-4a), 128.6 (2× C_{arom}-H), 119.3 (C-7), 114.0 (2× C_{arom}-H), 112.7 (C-4), 111.3 (C-3), 109.1 (C-10), 101.0 (C-1), 61.7 (OCH₂), 55.9 (OCH₃), 55.3 (OCH₃), 35.9 (C-9), 30.6 (C-8), 14.4 (OCH₂CH₃), 8.7 (C-10-CH₃). **IR** (ATR): 2926 (C-H st), 1728 (C=O st), 1258 (C-O st as) cm⁻¹. **MS** (EI) *m/z* (%): 392.2 (27), 391.2 (M⁺, 100), 318.1 (22). **HRMS (ESI) *m/z***: [M+H]⁺ Calcd for C₂₄H₂₆NO₄ 392.1862; Found 392.1857. **M.p.**: 98-101 °C (petroleum ether/EtOAc).

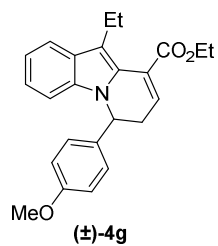


¹H NMR (300 MHz, CDCl₃) δ 7.03 (d, *J* = 2.3 Hz, 1H, H-1), 6.95 (d, *J* = 8.9, 1H, H-3), 6.86-6.70 (m, 5H, C_{arom}-H + H-4), 6.54 (dd, *J* = 7.0, 3.1 Hz, 1H, H-8), 5.56 (d, *J* = 7.1 Hz, 1H, H-6), 4.42-4.18 (m, 2H, OCH₂CH₃), 3.36 (s, 3H, OCH₃), 3.73 (s, 3H, OCH₃), 3.21-3.01 (m, 1H, H-7a), 2.88-2.71 (m, 1H, H-7b), 2.36 (s, 3H, C-10-CH₃), 1.37 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 166.6 (COO), 158.9 (C_{arom}-O), 154.1 (C-2-OCH₃), 133.3 (C_{arom}-C), 131.0 (C_{arom}-C), 129.5 (C_{arom}-C), 129.0 (C-8), 128.7 (C_{arom}-C), 128.0 (C_{arom}-C), 126.9 (2× C_{arom}-H), 114.0 (2× C_{arom}-H), 113.4 (C_{arom}-H), 109.9 (C_{arom}-H), 109.4 (C-10), 101.1 (C_{arom}-H), 61.3 (OCH₂), 56.1 (OCH₃), 55.3 (OCH₃), 52.7 (C-6), 33.1 (C-7), 14.4 (OCH₂CH₃), 10.6 (C-10-CH₃). **IR** (ATR): 2918 (C-H st), 1724 (C=O st), 1249 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₂₄H₂₆NO₄ 392.1862; Found 392.1866.

Ethyl (±)-10-ethyl-9-(4-methoxyphenyl)-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3g) and ethyl (±)-10-ethyl-6-(4-methoxyphenyl)-6,7-dihydropyrido[1,2-a]indole-9-carboxylate (4g). Following *GP-C*, (±)-**3g** (9 mg, 0.023 mmol, 46%) and (±)-**4g** (2 mg, 0.005 mmol, 10%) were isolated by FC (petroleum ether/EtOAc, from 25:1 to 19:1) on silica gel as white solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2g** (7 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h in an oil bath.

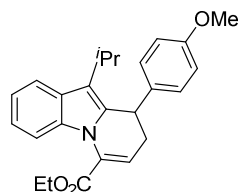


¹H NMR (300 MHz, CDCl₃) δ 7.63-7.53 (m, 1H, H-1), 7.22-7.10 (m, 3H, H-2 + H-3 + H-4), 7.02 (d, *J* = 8.6 Hz, 2H, C_{arom}-H), 6.78 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.23 (dd, *J* = 7.0, 3.6 Hz, 1H, H-7), 4.58-4.28 (m, 3H, H-9 + OCH₂), 3.76 (s, 3H, OCH₃), 2.91-2.50 (m, 4H, C-10-CH₂ + H-8), 1.36 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃), 1.09 (t, *J* = 7.5 Hz, 3H, C-10-CH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 163.5 (COO), 158.3 (C_{arom}-O), 134.3 (C-4a + C_{arom}-C), 133.5 (C-9a), 131.4 (C-6), 128.9 (C-10a), 128.5 (2× C_{arom}-H), 121.9 (C-3), 120.3 (C-2), 119.9 (C-7), 118.7 (C-1), 115.9 (C-10), 113.9 (2× C_{arom}-H), 112.1 (C-4), 61.7 (OCH₂), 55.3 (OCH₃), 35.6 (C-9), 30.6 (C-8), 17.5 (C-10-CH₂), 15.3 (C-10-CH₂CH₃), 14.4 (OCH₂CH₃). **IR** (ATR): 2933 (C-H st), 1724 (C=O st), 1246 (C-O st as) cm⁻¹. **MS** (EI) m/z (%): 376.2 (27), 375.2 (M⁺, 100), 360.2 (25), 302.1 (40), 286.1 (26), 273.1 (18), 239.1 (16). **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₂₄H₂₆NO₃ 376.1913; Found 376.1902. **M.p.**: 50-53 °C (petroleum ether/EtOAc).



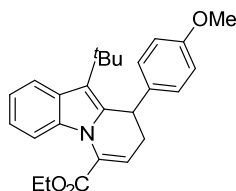
(±)-4g $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.65 (d, $J = 7.6$ Hz, 1H, H-1), 7.19-7.01 (m, 3H, H-2 + H-3 + H-4), 6.84 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.76 (d, $J = 8.8$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.53 (dd, $J = 7.1, 3.0$ Hz, 1H, H-8), 5.63 (app d, $J = 7.0$ Hz, 1H, H-6), 4.53-4.19 (m, 2H, OCH_2CH_3), 3.73 (s, 3H, OCH_3), 3.13 (ddd, $J = 17.1, 7.1, 3.0$ Hz, 1H, H-7a), 2.85 (m, 3H, C-10- CH_2CH_3 + H-7b), 1.48-1.17 (m, 6H, C-10- CH_2CH_3 + OCH_2CH_3). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 166.8 (COO), 158.9 ($\text{C}_{\text{arom-O}}$), 135.8 (C-4a), 133.3 ($\text{C}_{\text{arom-C}}$), 129.3 ($\text{C}_{\text{arom-C}}$), 129.2 (C-8), 128.9 ($\text{C}_{\text{arom-C}}$), 128.4 ($\text{C}_{\text{arom-C}}$), 126.9 ($2\times \text{C}_{\text{arom-H}}$), 126.6 ($\text{C}_{\text{arom-C}}$), 123.0 ($\text{C}_{\text{arom-H}}$), 119.8 ($\text{C}_{\text{arom-H}}$), 119.4 ($\text{C}_{\text{arom-H}}$), 116.7 (C-10), 114.1 ($2\times \text{C}_{\text{arom-H}}$), 109.2 ($\text{C}_{\text{arom-H}}$), 61.3 (OCH_2), 55.3 (OCH_3), 52.4 (C-6), 33.0 (C-7), 18.5 (C-10- CH_2CH_3), 15.0 (CH_2CH_3), 14.3 (CH_2CH_3). **IR** (ATR): 2923 (C-H st), 1722 (C=O st), 1249 (C-O st as) cm^{-1} . **MS** (EI) m/z (%): 376.2 (26), 375.2 (M^+ , 100), 360.2 (29), 273.1 (22). **HRMS (ESI) m/z :** [$\text{M}+\text{H}$] $^+$ Calcd for $\text{C}_{24}\text{H}_{26}\text{NO}_3$ 376.1913; Found 376.1902. **M.p.:** 48-51 °C (petroleum ether/EtOAc).

Ethyl (±)-10-isopropyl-9-(4-methoxyphenyl)-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3h). Following *GP-C*, (±)-**3h** (4.9 mg, 0.012 mmol, 25%) was isolated by FC (petroleum ether/EtOAc 19:1) on silica gel as white solid, starting from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2h** (8 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h.



(±)-3h $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.79-7.60 (m, 1H, H-1), 7.21-7.03 (m, 3H, H-2 + H-3 + H-4), 6.98 (d, $J = 8.5$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.76 (d, $J = 8.5$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.20 (ddd, $J = 7.2, 3.4, 0.8$ Hz, 1H, H-7), 4.63-4.54 (m, 1H, H-9), 4.49-4.24 (m, 2H, OCH_2), 3.75 (s, 3H, OCH_3), 3.21-3.04 (m, 1H, $\text{CH}(\text{CH}_3)_2$), 2.87-2.57 (m, 2H, H-8), 1.43-1.14 (m, 9H, $\text{CH}(\text{CH}_3)_2$ + OCH_2CH_3). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 163.5 (COO), 158.3 ($\text{C}_{\text{arom-O}}$), 134.5 (C-4a), 134.2 (C-9- C_{arom}), 132.6 (C-9a), 131.4 (C-6), 128.4 ($2\times \text{C}_{\text{arom-H}}$), 127.8 (C-10a), 121.6 (C-3), 120.1 (C-2), 120.0 (C-1), 119.9 (C-7), 119.6 (C-10), 113.8 ($2\times \text{C}_{\text{arom-H}}$), 112.1 (C-4), 61.7 (OCH_2), 55.3 (OCH_3), 35.8 (C-9), 30.6 (C-8), 26.0 ($\text{CH}(\text{CH}_3)_2$), 22.9 ($\text{CH}(\text{CH}_3)_2$), 22.7 ($\text{CH}(\text{CH}_3)_2$), 14.3 (OCH_2CH_3). **IR** (ATR): 2927 (C-H st), 1725 (C=O st), 1246 (C-O st as) cm^{-1} . **HRMS (ESI) m/z :** [$\text{M}+\text{H}$] $^+$ Calcd for $\text{C}_{25}\text{H}_{28}\text{NO}_3$ 390.2069; Found 390.2066. **M.p.:** 59-62 °C (petroleum ether/EtOAc).

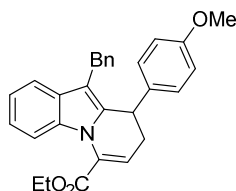
Ethyl (±)-10-(tert-butyl)-9-(4-methoxyphenyl)-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3i). Following *GP-C*, (±)-**3i** (3 mg, 0.007 mmol, 14%) was isolated by FC (petroleum ether/EtOAc 19:1) on silica gel as white solid, starting from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2i** (9 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h in an oil bath.



(±)-**3i**

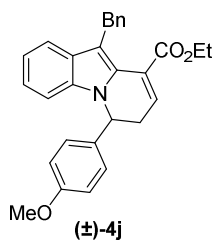
¹H NMR (300 MHz, CDCl₃) δ 7.95-7.86 (m, 1H, H-1), 7.23-7.06 (m, 3H, H-2 + H-3 + H-4), 6.95 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.78 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.39-6.07 (m, 1H, H-7), 4.99 (d, *J* = 4.6 Hz, 1H, H-9), 4.56-4.12 (m, 2H, OCH₂), 3.77 (s, 3H, OCH₃), 2.80 (ddd, *J* = 16.1, 5.5, 3.4 Hz, 1H, H-8a), 2.66 (ddd, *J* = 16.1, 7.5, 2.3 Hz, 1H, H-8b), 1.49 (s, 9H, C(CH₃)₃), 1.35 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 163.7 (COO), 158.2 (C_{arom}-O), 134.6 (C-4a), 134.5 (C-9-C_{arom}), 132.4 (C-9a), 131.2 (C-6), 128.6 (2×C_{arom}-H), 128.0 (C-10a), 122.1 (C-3), 121.5 (C-10), 121.4 (C-2), 120.6 (C-7), 119.7 (C-1), 113.8 (2×C_{arom}-H), 111.9 (C-4), 61.6 (OCH₂), 55.3 (OCH₃), 37.4 (C-9), 33.7 (C(CH₃)₃), 31.8 (C(CH₃)₃), 30.9 (C-8), 14.3 (OCH₂CH₃). **IR** (ATR): 2926 (C-H st), 1725 (C=O st), 1246 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₂₆H₃₀NO₃ 404.2226; Found 404.2224. **M.p.**: 61-64 °C (petroleum ether/EtOAc).

Ethyl (±)-10-benzyl-9-(4-methoxyphenyl)-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3j) and ethyl (±)-10-benzyl-6-(4-methoxyphenyl)-6,7-dihydropyrido[1,2-a]indole-9-carboxylate (4j). Following *GP-C*, (±)-**3j** (10 mg, 0.024 mmol, 47%) and (±)-**4j** (3 mg, 0.006 mmol, 13%) were isolated by FC (petroleum ether/EtOAc, from 25:1 to 19:1) on silica gel as white solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2j** (10 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h in an oil bath.



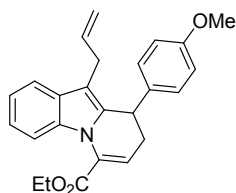
(±)-**3j**

¹H NMR (300 MHz, CDCl₃) δ 7.42 (d, *J* = 7.5 Hz, 1H, H-1), 7.22-7.02 (m, 8H, C_{arom}-H + H-2 + H-3 + H-4), 6.99 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.75 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.27 (dd, *J* = 6.6, 3.8 Hz, 1H, H-7), 4.62-4.26 (m, 3H, H-9 + OCH₂), 4.0 (s, 2H, C-10-CH₂), 3.76 (s, 3H, OCH₃), 2.86-2.58 (m, 2H, H-8), 1.37 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 163.5 (COO), 158.4 (C_{arom}-O), 140.5 (C_{arom}-C), 134.9 (C-4a), 134.4 (C_{arom}-C), 133.8 (C-9a), 131.4 (C-6), 129.2 (C-10a), 128.6 (2×C_{arom}-H), 128.5 (2×C_{arom}-H), 128.3 (2×C_{arom}-H), 125.9 (C_{arom}-H), 122.1 (C-3), 120.5 (C-2), 120.2 (C-7), 119.2 (C-1), 113.9 (2×C_{arom}-H), 112.4 (C-4), 112.0 (C-10), 61.7 (OCH₂), 55.4 (OCH₃), 35.7 (C-9), 30.6 (C-8), 30.3 (C-10-CH₂), 14.4 (OCH₂CH₃). **IR** (ATR): 2903 (C-H st), 1724 (C=O st), 1247 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₂₉H₂₈NO₃ 438.2069; Found 438.2065. **M.p.**: 54-57 °C (petroleum ether/EtOAc).

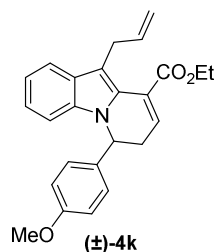


(±)-4j $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.45 (d, $J = 7.8$, 1H, H-1), 7.25-7.09 (m, 7H, $\text{C}_{\text{arom}}\text{-H} + \text{H-2} + \text{H-3}$), 7.04-6.95 (m, 1H, H-4), 6.88 (d, $J = 8.8$ Hz, 2H, $\text{C}_{\text{arom}}\text{-H}$), 6.78 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom}}\text{-H}$), 6.57 (dd, $J = 7.2$, 3.0 Hz, 1H, H-8), 5.67 (app d, $J = 7.3$ Hz, 1H, H-6), 4.30 (s, 2H, C-10- CH_2), 4.23-4.14 (m, 1H, OCH_aCH_3), 4.13-4.03 (m, 1H, OCH_bCH_3), 3.74 (s, 3H, OCH_3), 3.16 (ddd, $J = 17.1$, 7.3, 3.0 Hz, 1H, H-7a), 2.84 (ddd, $J = 17.1$, 7.2, 1.7 Hz, 1H, H-7b), 1.16 (t, $J = 7.1$ Hz, 3H, OCH_2CH_3). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 166.4 (COO), 159.0 ($\text{C}_{\text{arom}}\text{-O}$), 141.7 ($\text{C}_{\text{arom}}\text{-C}$), 135.9 (C-4a), 133.1 ($\text{C}_{\text{arom}}\text{-C}$), 130.1 (C-8), 129.0 ($\text{C}_{\text{arom}}\text{-C}$), 128.8 ($\text{C}_{\text{arom}}\text{-C}$), 128.6 ($2 \times \text{C}_{\text{arom}}\text{-H}$), 128.3 ($2 \times \text{C}_{\text{arom}}\text{-H}$), 127.9 ($\text{C}_{\text{arom}}\text{-C}$), 126.9 ($2 \times \text{C}_{\text{arom}}\text{-H}$), 125.7 ($\text{C}_{\text{arom}}\text{-H}$), 123.1 ($\text{C}_{\text{arom}}\text{-H}$), 120.1 ($\text{C}_{\text{arom}}\text{-H}$), 119.7 ($\text{C}_{\text{arom}}\text{-H}$), 114.1 ($2 \times \text{C}_{\text{arom}}\text{-H}$), 112.8 (C-10), 109.2 ($\text{C}_{\text{arom}}\text{-H}$), 61.3 (OCH_2), 55.4 (OCH_3), 52.4 (C-6), 33.0 (C-7), 31.0 (C-10- CH_2), 14.1 (OCH_2CH_3). **IR** (ATR): 2927 (C-H st), 1720 (C=O st), 1250 (C-O st as) cm^{-1} . **MS** (EI) m/z (%): 438.2 (32), 437.2 (M^+ , 100), 364.2 (20), 273.1 (34). **HRMS (ESI) m/z** : [$\text{M}+\text{H}$] $^+$ Calcd for $\text{C}_{29}\text{H}_{28}\text{NO}_3$ 438.2069; Found 438.2068. **M.p.**: 47-50 $^\circ\text{C}$ (petroleum ether/EtOAc).

Ethyl (±)-10-allyl-9-(4-methoxyphenyl)-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3k) and ethyl (±)-10-allyl-6-(4-methoxyphenyl)-6,7-dihydropyrido[1,2-a]indole-9-carboxylate (4k). Following *GP-C*, (±)-**3k** (8 mg, 0.020 mmol, 36%) and (±)-**4k** (2 mg, 0.005 mmol, 22%) were isolated by FC (petroleum ether/EtOAc, from 25:1 to 19:1) on silica gel as orange solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2k** (8 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 $^\circ\text{C}$ for 2 h in an oil bath.

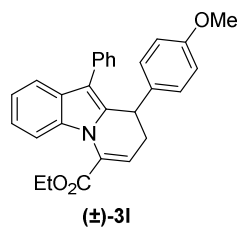


(±)-3k $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.56 (d, $J = 6.7$ Hz, 1H, H-1), 7.22-7.11 (m, 3H, H-2 + H-3 + H-4), 7.02 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom}}\text{-H}$), 6.78 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom}}\text{-H}$), 6.26 (dd, $J = 6.9$, 3.7 Hz, 1H, H-7), 5.82 (ddt, $J = 16.4$, 10.0, 6.2 Hz, 1H, $\text{CH}=\text{CH}_2$), 5.01 (dd, $J = 16.4$, 1.7 Hz, 1H, $\text{CH}=\text{CH}_a\text{H}_b$), 4.93 (dd, $J = 10.0$, 1.7 Hz, 1H, $\text{CH}=\text{CH}_a\text{H}_b$), 4.51 (dd, $J = 6.0$, 2.9 Hz, 1H, H-9), 4.47-4.32 (m, 2H, OCH_2), 3.76 (s, 3H, OCH_3), 3.38 (d, $J = 6.2$ Hz, 1H, C-10- CH_2), 2.84-2.60 (m, 2H, H-8), 1.36 (t, $J = 7.1$ Hz, 3H, OCH_2CH_3). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 163.4 (COO), 158.4 ($\text{C}_{\text{arom}}\text{-O}$), 136.5 ($\text{CH}=\text{CH}_2$), 134.5 (C-4a), 134.3 ($\text{C}_{\text{arom}}\text{-C}$), 133.9 (C-9a), 131.4 (C-6), 129.1 (C-10a), 128.5 ($2 \times \text{C}_{\text{arom}}\text{-H}$), 122.0 (C-3), 120.4 (C-2), 120.1 (C-7), 118.9 (C1), 115.2 ($\text{CH}=\text{CH}_2$), 113.9 ($2 \times \text{C}_{\text{arom}}\text{-H}$), 112.1 (C-4), 111.3 (C-10), 61.7 (OCH_2), 55.3 (OCH_3), 35.6 (C-9), 30.5 (C-8), 28.7 (C-10- CH_2), 14.3 (OCH_2CH_3). **IR** (ATR): 2930 (C-H st), 1724 (C=O st), 1246 (C-O st as) cm^{-1} . **MS** (EI) m/z (%): 388.1 (27), 387.2 (M^+ , 93), 314.1 (38), 312.1 (22), 298.0 (20), 273.1 (30), 272.1 (21), 254.0 (25), 242.1 (24), 241.0 (26), 228.0 (20), 206.1 (26), 205.1 (20), 204.0 (55), 180.0 (34), 167.1 (21), 127.9 (22), 127.0 (23), 121.0 (41), 115.1 (25), 108.0 (100), 78.1 (38), 77.0 (36), 65.0 (25). **HRMS (ESI) m/z** : [$\text{M}+\text{Na}$] $^+$ Calcd for $\text{C}_{25}\text{H}_{25}\text{NO}_3\text{Na}$ 410.1732 [$\text{M}+\text{Na}$] $^+$; found: 410.1734. **M.p.**: 79-82 $^\circ\text{C}$ (petroleum ether/EtOAc).

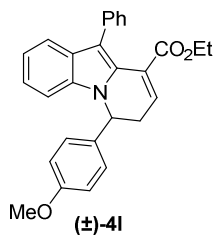


¹H NMR (300 MHz, CDCl₃) δ 7.64 (d, *J* = 7.7 Hz, 1H, H-1), 7.19-6.93 (m, 3H, H-2 + H-3 + H-4), 6.84 (d, *J* = 8.4 Hz, 2H, C_{arom}-H), 6.76 (d, *J* = 8.5 Hz, 2H, C_{arom}-H), 6.59 (d, *J* = 5.9 Hz, 1H, H-8), 6.34-5.76 (m, 1H, CH=CH₂), 5.65 (app d, *J* = 7.1 Hz, 1H, H-6), 5.31-4.69 (m, 2H, CH=CH₂), 4.49-4.10 (m, 2H, OCH₂), 3.73 (s, 3H, OCH₃), 3.66 (d, *J* = 6.2 Hz, 2H, C-10-CH₂), 3.28-2.97 (m, 1H, H-7a), 2.83 (dd, *J* = 17.2, 7.1 Hz, 1H, H-7b), 1.35 (t, *J* = 7.2 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 166.3 (COO), 158.8 (C_{arom}-O), 138.0 (C-8), 135.8 (C-4a), 133.1 (C_{arom}-C), 130.0 (C_{arom}-H), 128.8 (C_{arom}-C), 128.7 (C_{arom}-C), 127.4 (C_{arom}-C), 126.9 (2× C_{arom}-H), 123.1 (C_{arom}-H), 120.0 (C_{arom}-H), 119.6 (C_{arom}-H), 114.8 (CH=CH₂), 114.1 (2× C_{arom}-H), 112.0 (C-10), 109.2 (C_{arom}-H), 61.3 (OCH₂), 55.3 (OCH₃), 52.4 (C-6), 33.0 (C-7), 29.6 (C-10-CH₂), 14.3 (OCH₂CH₃). **IR** (ATR): 2945 (C-H st), 1729 (C=O st), 1248 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₂₅H₂₅NO₃Na 410.1732; Found 410.1729. **M.p.**: 85-88 °C (petroleum ether/EtOAc).

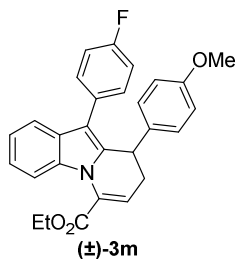
Ethyl (±)-9-(4-methoxyphenyl)-10-phenyl-8,9-dihydropyrindo[1,2-a]indole-6-carboxylate (3l) and ethyl (±)-6-(4-methoxyphenyl)-10-phenyl-6,7-dihydropyrindo[1,2-a]indole-9-carboxylate (4l). Following *GP-C*, (±)-**3l** (13 mg, 0.031 mmol, 62%) and (±)-**4l** (2 mg, 0.004 mmol, 7%) were isolated by FC (petroleum ether/EtOAc, from 25:1 to 19:1) on silica gel as white solids, starting from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2l** (10 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h in an oil bath.



¹H NMR (300 MHz, CDCl₃) δ 7.87 (d, *J* = 7.5 Hz, 1H, H-1), 7.53-7.20 (m, 8H, C_{arom}-H + H-2 + H-3 + H-4), 7.14 (d, *J* = 8.1 Hz, 2H, C_{arom}-H), 6.89 (d, *J* = 8.3 Hz, 2H, C_{arom}-H), 6.41 (dd, *J* = 7.0, 3.6 Hz, 1H, H-7), 4.76-4.29 (m, 3H, H-9 + OCH₂), 3.83 (s, 3H, OCH₃), 3.12-2.57 (m, 2H, H-8), 1.45 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 163.2 (COO), 158.3 (C_{arom}-O), 134.5 (C-4a + C_{arom}-C + C-10-C_{arom}), 134.1 (C-9a), 131.2 (C-6), 129.4 (2×C_{arom}-H), 128.5 (4×C_{arom}-H), 127.9 (C-10a), 126.5 (C_{arom}-H), 122.4 (C-3), 122.2 (C-2), 121.1 (C-7), 119.5 (C-1), 115.9 (C-10), 114.1 (2× C_{arom}-H), 112.1 (C-4), 61.7 (OCH₂), 55.2 (OCH₃), 35.6 (C-9), 30.9 (C-8), 14.3 (OCH₂CH₃). **IR** (ATR): 2981 (C-H st), 1724 (C=O st), 1246 (C-O st as) cm⁻¹. **MS** (EI) m/z (%): 424.2 (30), 423.2 (M⁺, 100), 351.2 (17), 350.2 (64), 349.2 (24), 348.2 (22). **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₂₈H₂₆NO₃ 424.1913; Found 424.1894. **M.p.**: 80-83 °C (petroleum ether/EtOAc).



(±)-4l $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.79 (d, $J = 7.8$ Hz, 1H, H-1), 7.63-7.39 (m, 4H, $\text{C}_{\text{arom-H}}$), 7.38-7.28 (m, 1H, $\text{C}_{\text{arom-H}}$), 7.24-7.07 (m, 3H, $\text{C}_{\text{arom-H}}$), 6.93 (d, $J = 8.3$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.80 (d, $J = 8.4$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.64 (dd, $J = 7.2, 2.8$ Hz, 1H, H-8), 5.72 (app d, $J = 7.1$ Hz, 1H, H-6), 3.82-3.66 (m, 4H, $\text{OCH}_3 + \text{OCH}_a\text{H}_b\text{CH}_3$), 3.35-3.16 (m, 2H, H-7a + $\text{OCH}_a\text{H}_b\text{CH}_3$), 2.90 (dd, $J = 17.0, 7.1$ Hz, 1H, H-7b), 0.85 (t, $J = 7.1$ Hz, 3H, OCH_2CH_3). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 166.8 (COO), 159.1 ($\text{C}_{\text{arom-O}}$), 136.0 (C-4a), 135.7 ($\text{C}_{\text{arom-C}}$), 132.7 ($\text{C}_{\text{arom-C}}$), 130.7 (C-8), 129.6 ($2 \times \text{C}_{\text{arom-H}}$), 129.1 ($\text{C}_{\text{arom-C}}$), 128.6 ($2 \times \text{C}_{\text{arom-H}}$), 127.8 ($\text{C}_{\text{arom-C}}$), 127.6 ($\text{C}_{\text{arom-C}}$), 127.1 ($2 \times \text{C}_{\text{arom-H}}$), 126.4 ($\text{C}_{\text{arom-H}}$), 123.4 ($\text{C}_{\text{arom-H}}$), 120.5 ($\text{C}_{\text{arom-H}}$), 120.2 ($\text{C}_{\text{arom-H}}$), 116.1 (C-10), 114.2 ($2 \times \text{C}_{\text{arom-H}}$), 109.5 ($\text{C}_{\text{arom-H}}$), 61.1 (OCH_2), 55.4 (OCH_3), 52.7 (C-6), 33.1 (C-7), 13.7 (OCH_2CH_3). **IR** (ATR): 2939 (C-H st), 1726 (C=O st), 1243 (C-O st as) cm^{-1} . **HRMS (ESI) m/z**: $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{28}\text{H}_{26}\text{NO}_3$ 424.1913; Found 424.1915. **M.p.**: 56-59 °C (petroleum ether/EtOAc).

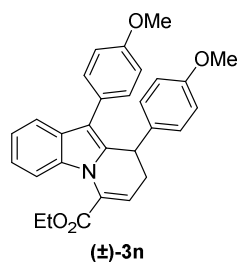


(±)-3m **Ethyl (±)-10-(4-fluorophenyl)-9-(4-methoxyphenyl)-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3m)**. Following *GP-C*, **(±)-3m** (15 mg, 0.033 mmol, 73%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2m** (11 mg, 0.05 mmol) and employing diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h in an oil bath. $R_f = 0.70$ (petroleum ether/EtOAc, 9:1).

$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.62 (d, $J = 6.8$ Hz, 1H, H-1), 7.38-7.18 (m, 5H, $\text{C}_{\text{arom-H}}$), 7.17-6.97 (m, 4H, $\text{C}_{\text{arom-H}}$), 6.83 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.35 (dd, $J = 7.0, 3.4$ Hz, 1H, H-7), 4.73-4.23 (m, 3H, H-9 + OCH_2), 3.79 (s, 3H, OCH_3), 2.93-2.56 (m, 2H, H-8), 1.39 (t, $J = 7.1$ Hz, 3H, OCH_2CH_3). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 163.4 (COO), 161.8 (d, $^1J_{\text{C-F}} = 245.5$ Hz, $\text{C}_{\text{arom-F}}$), 158.4 ($\text{C}_{\text{arom-O}}$), 134.5 (C-4a), 134.4 ($\text{C}_{\text{arom-C}}$), 134.3 (C-9a), 131.3 (C-6), 130.9 (d, $^3J_{\text{C-F}} = 7.9$ Hz, $2 \times \text{C}_{\text{arom-H}}$), 130.1 (d, $^4J_{\text{C-F}} = 3.3$ Hz, $\text{C}_{\text{arom-C}}$), 128.6 ($2 \times \text{C}_{\text{arom-H}}$), 127.9 (C-10a), 122.5 (C-3), 122.1 (C-2), 121.3 (C-7), 119.3 (C-1), 115.5 (d, $^2J_{\text{C-F}} = 21.3$ Hz, $2 \times \text{C}_{\text{arom-H}}$), 115.1 (C-10), 114.2 ($2 \times \text{C}_{\text{arom-H}}$), 112.2 (C-4), 61.8 (OCH_2), 55.3 (OCH_3), 35.7 (C-9), 30.9 (C-8), 14.4 (OCH_2CH_3). **IR** (ATR): 2935 (C-H st), 1724 (C=O st), 1243 (C-O st as), 1225 (C-F st) cm^{-1} . **MS** (EI) m/z (%): 442.2 (30), 441.2 (M^+ , 100), 369.1 (18), 368.1 (73), 367.2 (35), 366.1 (33), 324.1 (22), 322.1 (25), 261.0 (34), 260.0 (22), 259.0 (34). **HRMS (ESI) m/z**: $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{28}\text{H}_{25}\text{NO}_3\text{F}$ 442.1818; Found 442.1814. **M.p.**: 90-93 °C (petroleum ether/EtOAc).

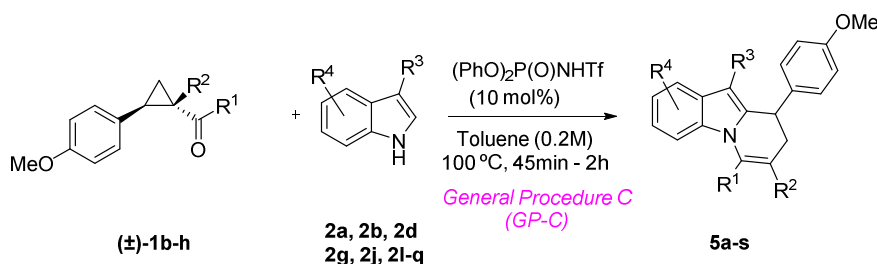
Ethyl (±)-9,10-bis(4-methoxyphenyl)-8,9-dihydropyrido[1,2-a]indole-6-carboxylate (3n). Following *GP-C*, **(±)-3n** (18 mg, 0.040 mmol, 79%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1a** (12 mg, 0.05 mmol), indole **2n** (11 mg, 0.05 mmol)

and employing diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) as catalyst in toluene (0.25 mL) at 100 °C for 2 h in an oil bath. $R_f = 0.70$ (petroleum ether/EtOAc, 9:1).



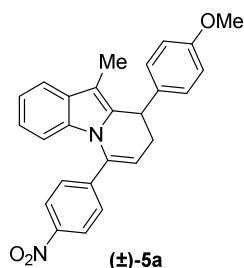
$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.76 (d, $J = 6.9$ Hz, 1H, H-1), 7.39-7.17 (m, 5H, $\text{C}_{\text{arom-H}}$), 7.07 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.92 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.83 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.33 (dd, $J = 7.0, 3.4$ Hz, 1H, H-7), 4.86-4.28 (m, 3H, H-9 + OCH_2), 3.83 (s, 3H, OCH_3), 3.80 (s, 3H, OCH_3), 2.89-2.47 (m, 2H, H-8), 1.39 (t, $J = 7.1$ Hz, 3H, OCH_2CH_3). **$^{13}\text{C NMR}$** (75 MHz, CDCl_3) δ 163.4 (COO), 158.4 ($\text{C}_{\text{arom-O}}$), 158.3 ($\text{C}_{\text{arom-O}}$), 134.6 (C-4a), 134.5 ($\text{C}_{\text{arom-C}}$), 134.0 (C-9a), 131.3 (C-6), 129.5 ($2\times\text{C}_{\text{arom-H}}$), 128.6 ($2\times\text{C}_{\text{arom-H}}$), 128.2 ($\text{C}_{\text{arom-C}}$), 126.5 (C-10a), 122.4 (C-3), 122.0 (C-2), 121.1 (C-7), 119.5 (C-1), 115.6 (C-10), 114.1 ($2\times\text{C}_{\text{arom-H}}$), 114.0 ($2\times\text{C}_{\text{arom-H}}$), 112.1 (C-4), 61.8 (OCH_2), 55.4 (OCH_3), 55.3 (OCH_3), 35.7 (C-9), 31.0 (C-8), 14.4 (OCH_2CH_3). **IR** (ATR): 2959 (C-H st), 1724 (C=O st), 1245 (C-O st as) cm^{-1} . **MS** (EI) m/z (%): 454.2 (27), 453.2 (M^+ , 100), 379.2 (17), 380.2 (69). **HRMS (ESI) m/z** : [$\text{M}+\text{H}$] $^+$ Calcd for $\text{C}_{29}\text{H}_{28}\text{NO}_4$ 454.2018; Found 454.2016. **M.p.**: 84-87 °C (petroleum ether/EtOAc).

2.3.2 Synthesis of dihydropyridoindoles 5

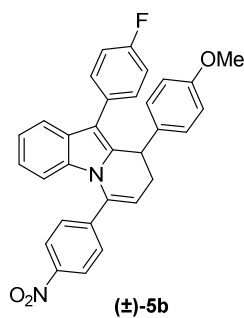


Scheme S4. General Procedure C for the synthesis of dihydropyridoindoles (±)-5a-s

General Procedure C (GP-C) for the cyclocondensation: An oven-dried 5 mL screw-capped test tube containing a stirring bar was charged with the cyclopropane **1b-h** (1eq.) and the corresponding indole **2** (1eq.) and dissolved in toluene (0.2 M) under Ar. After adding the diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate catalyst (10 mol%) the mixture was stirred at 100 °C in an oil bath. When the reaction was judged complete (monitored by TLC), it was warmed to room temperature, quenched by addition of aq. NaHCO_3 (sat) (3 mL) and diluted with EtOAc (3 mL). The phases were separated and the aqueous phase was extracted with EtOAc (3 \times 3 mL). The combined organic layers were dried over Na_2SO_4 , filtered and evaporated. The residue was purified by column chromatography on silica gel to afford the corresponding pure compounds **5a-s**.

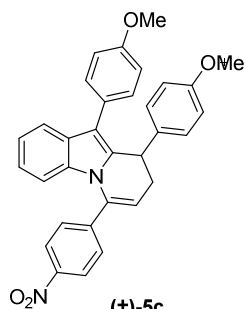


(±)-**9-(4-Methoxyphenyl)-10-methyl-6-(4-nitrophenyl)-8,9-dihydropyrido[1,2-a]indole (5a)**. Following *GP-C*, (±)-**5a** (13 mg, 0.031 mmol, 80%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1b** (15 mg, 0.05 mmol) and indole **2a** (7 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 2 h in an oil bath. $R_f = 0.70$ (petroleum ether/EtOAc, 9:1). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.26 (d, $J = 8.7$ Hz, 2H, H-3''), 7.64-7.46 (m, 3H, H-2'' + H-1), 7.17-7.03 (m, 3H, H-2' + H-2), 6.92 (app t, $J = 7.7$ Hz, 1H, H-3), 6.81 (d, $J = 8.7$ Hz, 2H, H-3'), 6.25 (d, $J = 8.3$ Hz, 1H, H-4), 5.48 (dd, $J = 6.5, 3.9$ Hz, 1H, H-7), 4.76-4.41 (m, 1H, H-9), 3.76 (s, 3H, OCH_3), 3.04-2.46 (m, 2H, H-8), 2.21 (s, 3H, CCH_3). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 158.4 ($\text{C}_{\text{arom-O}}$), 147.8 ($\text{C}_{\text{arom-N}}$), 142.9 ($\text{C}_{\text{arom-C}}$), 137.4 (C-4a), 135.0 ($\text{C}_{\text{arom-C}}$), 134.2 (C-9a), 133.9 (C-6), 130.2 (C-10a), 128.4 ($4 \times \text{C}_{\text{arom-H}}$), 123.9 ($2 \times \text{C}_{\text{arom-H}}$), 121.7 (C-3), 120.2 (C-2), 118.8 (C-1), 114.0 ($2 \times \text{C}_{\text{arom-H}}$), 113.5 (C-7), 112.5 (C-4), 109.6 (C-10), 55.3 (OCH_3), 36.2 (C-9), 30.2 (C-8), 8.7 (C-10- CH_3). **IR** (ATR): 2930 (C-H st), 1510 (NO_2 st as), 1344 (NO_2 st sim) cm^{-1} . **MS** (EI) m/z (%): 411.2 (28), 410.2 (M^+ , 100), 409.2 (20), 289.1 (14). **HRMS (ESI) m/z** : [$\text{M}+\text{H}$] $^+$ Calcd for $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}_3$ 411.1709; Found 411.1704. **M.p.**: 110-113 °C (petroleum ether/EtOAc).

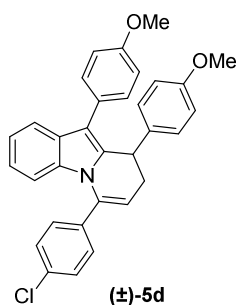


(±)-**10-(4-Fluorophenyl)-9-(4-methoxyphenyl)-6-(4-nitrophenyl)-8,9-dihydropyrido[1,2-a]indole (5b)**. Following *GP-C*, (±)-**5b** (18 mg, 0.040 mmol, 80%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1b** (15 mg, 0.05 mmol) and indole **2m** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 2 h in an oil bath. $R_f = 0.70$ (petroleum ether/EtOAc, 9:1). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.30 (d, $J = 8.6$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 7.74 (d, $J = 7.9$ Hz, 1H, H-1), 7.64 (d, $J = 7.6$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 7.33 (dd, $J = 8.6, 5.5$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 7.23-6.92 (m, 6H, $\text{C}_{\text{arom-H}}$), 6.83 (d, $J = 8.7$ Hz, 2H, $\text{C}_{\text{arom-H}}$), 6.38 (d, $J = 8.4$ Hz, 1H, H-4), 5.58 (dd, $J = 6.8, 3.6$ Hz, 1H, H-7), 4.51 (dd, $J = 5.3, 2.5$ Hz, 1H, H-9), 3.78 (s, 3H, OCH_3), 2.96-2.67 (m, 2H, H-8). $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 161.9 (d, $^1J_{\text{C-F}} = 246.0$ Hz, $\text{C}_{\text{arom-C}}$), 158.5 ($\text{C}_{\text{arom-C}}$), 147.9 ($\text{C}_{\text{arom-C}}$), 142.6 (C-6), 137.4 ($\text{C}_{\text{arom-C}}$), 135.4 ($\text{C}_{\text{arom-C}}$), 134.6 ($2 \times \text{C}_{\text{arom-C}}$), 134.4 ($\text{C}_{\text{arom-C}}$), 130.9 (d, $^3J_{\text{C-F}} = 7.9$ Hz, $2 \times \text{C}_{\text{arom-H}}$), 130.0 (d, $^4J_{\text{C-F}} = 3.2$ Hz, $\text{C}_{\text{arom-C}}$), 128.3 ($3 \times \text{C}_{\text{arom-H}}$), 128.2 ($\text{C}_{\text{arom-H}}$), 124.1 ($2 \times \text{C}_{\text{arom-H}}$), 122.3 (C-3), 121.2 (C-2), 119.6 (C-1), 115.5 (d, $^2J_{\text{C-F}} = 21.5$ Hz, $2 \times \text{C}_{\text{arom-H}}$), 115.4 (C-7), 115.3 (C-10), 114.2 ($2 \times$

C_{arom}-H), 112.8 (C-4), 55.3 (OCH₃), 36.1 (C-9), 30.8 (C-8). **IR** (ATR): 2951 (C-H st), 1505 (NO₂ st as), 1340 (NO₂ st sim), 1221 (C-F st) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₁H₂₄N₂O₃F 491.1771; Found 491.1771. **M.p.**: 237-240 °C (petroleum ether/EtOAc).

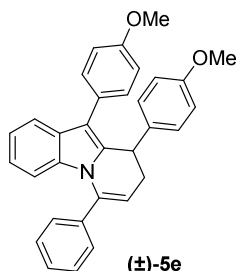


(±)-9,10-Bis(4-methoxyphenyl)-6-(4-nitrophenyl)-8,9-dihydropyrido[1,2-a]indole (5c). Following *GP-C*, (±)-**5c** (23 mg, 0.046 mmol, 92%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1b** (15 mg, 0.05 mmol) and indole **2n** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 2 h in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 8.30 (d, *J* = 8.3 Hz, 2H, C_{arom}-H), 7.79 (d, *J* = 7.8 Hz, 1H, H-1), 7.64 (d, *J* = 8.3 Hz, 2H, C_{arom}-H), 7.33 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 7.21-7.09 (m, 3H, C_{arom}-H), 7.06-6.92 (m, 3H, C_{arom}-H), 6.85 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.39 (d, *J* = 8.3 Hz, 1H, H-4), 5.57 (dd, *J* = 6.7, 3.4 Hz, 1H, H-7), 4.55 (dd, *J* = 5.2, 2.4 Hz, 1H, H-9), 3.85 (s, 3H, OCH₃), 3.79 (s, 3H, OCH₃), 2.96-2.66 (m, 2H, H-8). **¹³C NMR** (75 MHz, CDCl₃) δ 158.5 (C_{arom}-C), 158.4 (C_{arom}-C), 147.8 (C_{arom}-C), 142.7 (C-6), 137.4 (C_{arom}-C), 134.93 (C_{arom}-C), 134.85 (C_{arom}-C), 134.4 (C_{arom}-C), 130.5 (2×C_{arom}-H), 128.5 (C_{arom}-C), 128.3 (2×C_{arom}-H), 128.2 (2×C_{arom}-H), 126.4 (C-10a), 124.0 (2×C_{arom}-H), 122.1 (C-3), 120.9 (C-2), 119.8 (C-1), 115.9 (C-10), 115.3 (C-7), 114.1 (4×C_{arom}-H), 112.7 (C-4), 55.4 (OCH₃), 55.3 (OCH₃), 36.1 (C-9), 30.8 (C-8). **IR** (ATR): 2940 (C-H st), 1509 (NO₂ st as), 1343 (NO₂ st sim) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₂H₂₇N₂O₄ 503.1971; Found 503.1962. **M.p.**: 122-125 °C (petroleum ether/EtOAc).



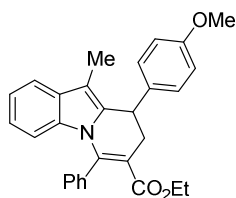
(±)-6-(4-Chlorophenyl)-9,10-bis(4-methoxyphenyl)-8,9-dihydropyrido[1,2-a]indole (5d). Following *GP-C*, (±)-**5d** (22 mg, 0.045 mmol, 90%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1c** (14 mg, 0.05 mmol) and indole **2n** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 2 h in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.76 (d, *J* = 7.9 Hz, 1H, H-1), 7.46-7.35 (m, 4H, C_{arom}-H), 7.31 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 7.18-7.05 (m, 3H, C_{arom}-H), 7.05-6.88 (m, 3H, C_{arom}-H), 6.83 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.45 (d, *J* = 8.3 Hz, 1H, H-4), 5.37 (dd, *J* = 7.2, 3.1 Hz, 1H, H-7), 4.66-4.40 (m, 1H, H-9), 3.84 (s, 3H, OCH₃), 3.78 (s, 3H, OCH₃), 2.78 (ddd, *J* = 15.8, 5.5, 3.1 Hz, 1H, H-8a), 2.67 (ddd, *J* = 15.8, 7.2, 2.2 Hz, 1H, H-8b). **¹³C NMR** (75 MHz, CDCl₃) δ 158.4 (C_{arom}-C), 158.3 (C_{arom}-C), 138.1 (C-6), 135.3 (C_{arom}-Cl), 135.2 (C_{arom}-C), 135.0 (C_{arom}-C), 134.7 (C_{arom}-C), 134.5 (C_{arom}-C), 130.6 (2×C_{arom}-H), 129.0 (4×C_{arom}-H), 128.5

(2×C_{arom}-H), 128.4 (C_{arom}-C), 126.7 (C-10a), 121.8 (C-3), 120.6 (C-2), 119.5 (C-1), 115.5 (C-10), 114.1 (2× C_{arom}-H), 114.0 (2× C_{arom}-H), 113.1 (C-7), 112.0 (C-4), 55.4 (OCH₃), 55.3 (OCH₃), 36.2 (C-9), 30.5 (C-8). **IR** (ATR): 2947 (C-H st), 1645 (arC-C), 1608 (arC-C), 1034 (C-Cl st) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₂H₂₇ClNO₂ 492.1725; Found 492.1729. **M.p.**: 100-103 °C (petroleum ether/EtOAc).



(±)-5e **(±)-9,10-Bis(4-methoxyphenyl)-6-phenyl-8,9-dihydropyrido[1,2-a]indole (5e).**

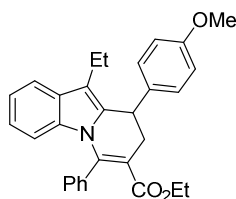
Following *GP-C*, (±)-**5e** (19 mg, 0.043 mmol, 85%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1d** (13 mg, 0.05 mmol) and indole **2n** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 2 h in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.75 (d, *J* = 7.9 Hz, 1H, H-1), 7.57-7.36 (m, 5H, C_{arom}-H), 7.32 (d, *J* = 8.6 Hz, 2H, C_{arom}-H), 7.21-7.07 (m, 3H, C_{arom}-H), 6.99-6.90 (m, 3H, C_{arom}-H), 6.83 (d, *J* = 8.6 Hz, 2H, C_{arom}-H), 6.41 (d, *J* = 8.4 Hz, 1H, H-4), 5.36 (dd, *J* = 7.3, 3.0 Hz, 1H, H-7), 4.51 (app d, *J* = 5.2 Hz, 1H, H-9), 3.85 (s, 3H, OCH₃), 3.78 (s, 3H, OCH₃), 2.80 (ddd, *J* = 15.8, 5.5, 3.1 Hz, 1H, H-8a), 2.66 (ddd, *J* = 15.8, 7.3, 2.1 Hz, 1H, H-8b). **¹³C NMR** (75 MHz, CDCl₃) δ 158.4 (C_{arom}-O), 158.2 (C_{arom}-O), 139.1 (C-6), 136.7 (C_{arom}-C), 135.5 (C_{arom}-C), 135.3 (C_{arom}-C), 134.8 (C_{arom}-C), 130.6 (2×C_{arom}-H), 128.6 (5×C_{arom}-H), 128.4 (C_{arom}-C), 127.8 (2×C_{arom}-H), 126.9 (C-10a), 121.6 (C-3), 120.5 (C-2), 119.4 (C-1), 115.3 (C-10), 114.1 (2× C_{arom}-H), 114.0 (2× C_{arom}-H), 113.3 (C-7), 111.2 (C-4), 55.4 (OCH₃), 55.3 (OCH₃), 36.2 (C-9), 30.5 (C-8). **IR** (ATR): 2950 (C-H st), 1645 (arC-C), 1608 (arC-C) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₂H₂₈NO₂ 458.2120; Found 458.2100. **M.p.**: 89-92 °C (petroleum ether/EtOAc).



(±)-5f **Ethyl (±)-9-(4-methoxyphenyl)-10-methyl-6-phenyl-8,9-dihydropyrido[1,2-**

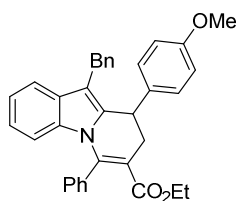
a]indole-7-carboxylate (5f). Following *GP-C*, (±)-**5f** (21 mg, 0.047 mmol, 94%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2a** (7 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.59-7.33 (m, 5H, C_{arom}-H), 7.25-7.02 (m, 4H, C_{arom}-H + H-2), 6.92-6.63 (m, 3H, H-3 + C_{arom}-H), 5.70 (d, *J* = 8.5 Hz, 1H, H-4), 4.53 (app t, *J* = 4.7 Hz, 1H, H-9), 4.02-3.77 (m, 2H, OCH₂), 3.79 (s, 3H, OCH₃), 3.27 (dd, *J* = 15.5, 3.9 Hz, 1H, H-8a), 3.03 (dd, *J* = 15.5, 5.4 Hz, 1H, H-8b), 2.13 (s, 3H, C-10-CH₃), 0.87 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 168.0 (COO), 158.4 (C_{arom}-O), 146.1 (C-6), 136.0 (C_{arom}-C), 135.5 (C_{arom}-C), 135.2 (C_{arom}-C), 133.6 (C_{arom}-C), 131.3 (C-10a), 129.2 (2× C_{arom}-H), 128.5 (5×C_{arom}-H), 122.3 (C-3), 121.1 (C-2), 118.4 (C-1), 114.0 (2× C_{arom}-H), 113.6 (C-4), 111.1 (C-10), 109.1 (C-7), 60.0 (OCH₂), 55.4 (OCH₃), 36.2 (C-9), 31.0 (C-8), 13.8 (OCH₂CH₃), 8.7 (C-10-CH₃). **IR** (ATR): 2980 (C-H st), 1683 (C=O st), 1239 (C-O st as)

cm⁻¹. **MS** (EI) m/z (%): 438.2 (23), 437.2 (M⁺, 74), 365.2 (23), 364.1 (100), 257.1 (19), 256.1 (50), 254.1 (27), 241.1 (21), 204.0 (24), 135.0 (35) 115.0 (52), 108.0 (38), 78.0 (23), 77.0 (48), 21.0 (65). **HRMS** (ESI) m/z: [M+Na]⁺ Calcd for C₂₉H₂₇NO₃Na 460.1889; Found 460.1889. **M.p.**: 121-123 °C (petroleum ether/EtOAc).



(±)-**5g** **Ethyl** (±)-10-ethyl-9-(4-methoxyphenyl)-6-phenyl-8,9-dihydropyrido[1,2-

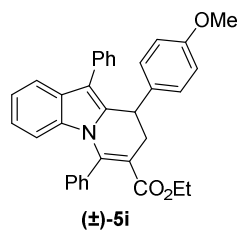
a]indole-7-carboxylate (5g). Following *GP-C*, (±)-**5g** (21 mg, 0.046 mmol, 92%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2g** (7 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R*_f = 0.70 (petroleum ether/EtOAc, 9:1). ¹H NMR (300 MHz, CDCl₃) δ 7.59-7.34 (m, 5H, C_{arom}-H), 7.26-7.17 (m, 1H, C_{arom}-H), 7.17-6.99 (m, 3H, H-2 + C_{arom}-H), 6.88-6.69 (m, 3H, H-3 + C_{arom}-H), 5.72 (d, *J* = 8.4 Hz, 1H, H-4), 4.55 (dd, *J* = 5.4, 3.2 Hz, 1H, H-9), 4.02-3.59 (m, 2H, OCH₂), 3.78 (s, 3H, OCH₃), 3.27 (dd, *J* = 15.4, 3.2 Hz, 1H, H-8a), 3.02 (dd, *J* = 15.4, 5.4 Hz, 1H, H-8b), 2.65 (m, 2H, C-10-CH₂), 1.12 (t, *J* = 7.5 Hz, 3H, CH₂CH₃), 0.85 (t, *J* = 7.1 Hz, 3H, CH₂CH₃). ¹³C NMR (75 MHz, CDCl₃) δ 168.0 (COO), 158.3 (C_{arom}-O), 146.1 (C-6), 136.0 (C-4a), 135.8 (C_{arom}-C), 134.6 (C_{arom}-C), 133.9 (C-9a), 130.3 (C-10a), 129.2 (2× C_{arom}-H), 128.4 (5× C_{arom}-H), 122.2 (C-3), 121.1 (C-2), 118.7 (C-1), 117.3 (C-10), 113.9 (2× C_{arom}-H), 113.7 (C-4), 109.1 (C-7), 60.0 (OCH₂), 55.4 (OCH₃), 35.9 (C-9), 31.1 (C-8), 17.3 (C-10-CH₂), 14.8 (CH₂CH₃), 13.8 (CH₂CH₃). **MS** (EI) m/z (%): 452.2 (30), 451.2 (M⁺, 100), 379.1 (31), 378.2 (86), 362.0 (19), 349.1 (24), 330.1 (20), 300.1 (26), 270.1 (31), 256.1 (34), 255.1 (19), 254.1 (43), 241.0 (33), 217.9 (29), 204.0 (36), 121.0 (50), 115.0 (84), 108.0 (87), 92.0 (21), 89.0 (23), 65.0 (29). **IR** (ATR): 2965 (C-H st), 1683 (C=O st), 1246 (C-O st as) cm⁻¹. **HRMS** (ESI) m/z: [M+Na]⁺ Calcd for C₃₀H₂₉NO₃Na 474.2045; Found 474.2053. **M.p.**: 123-125 °C (petroleum ether/EtOAc).



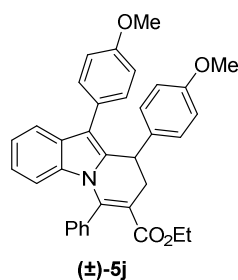
(±)-**5h** **Ethyl** (±)-10-benzyl-9-(4-methoxyphenyl)-6-phenyl-8,9-dihydropyrido[1,2-

a]indole-7-carboxylate (5h). Following *GP-C*, (±)-**5h** (21 mg, 0.040 mmol, 81%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2j** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R*_f = 0.70 (petroleum ether/EtOAc, 9:1). ¹H NMR (300 MHz, CDCl₃) δ 7.57-7.39 (m, 4H, C_{arom}-H), 7.34 (d, *J* = 7.6 Hz, 1H, H-1), 7.23-7.05 (m, 8H, C_{arom}-H), 6.98 (app t, *J* = 7.5 Hz, 1H, H-2), 6.83-6.70 (m, 3H, H-3 + C_{arom}-H), 5.73 (d, *J* = 8.5 Hz, 1H, H-4), 4.57 (dd, *J* = 5.5, 3.3 Hz, 1H, H-9), 3.99 (s, 1H, C-10-CH₂), 3.93-3.76 (m, 2H, OCH₂), 3.78 (s, 3H, OCH₃), 3.26 (dd, *J* = 15.5, 3.3 Hz, 1H, H-8a), 3.04 (dd, *J* = 15.5, 5.5 Hz, 1H, H-8b), 0.86 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). ¹³C NMR (75 MHz, CDCl₃) δ 167.9 (COO), 158.4 (C_{arom}-O), 145.9 (C-6), 140.1 (C_{arom}-C), 136.1 (C_{arom}-C), 135.9 (C_{arom}-C), 135.8 (C-9a), 133.5 (C_{arom}-C), 130.5 (C-10a), 130.2

(C_{arom}-H), 129.3 (C_{arom}-H), 129.0 (C_{arom}-H), 128.5 (5×C_{arom}-H), 128.4 (2×C_{arom}-H), 126.0 (C_{arom}-H), 122.3 (C-3), 121.3 (C-2), 119.2 (C-1), 114.0 (3×C_{arom}-H), 113.7 (C-4), 109.5 (C-7 + C-10), 60.0 (OCH₂), 55.4 (OCH₃), 36.1 (C-9), 31.3 (C-8), 30.1 (C-10-CH₂-C_{arom}), 13.7 (OCH₂CH₃). **IR** (ATR): 2977 (C-H st), 1683 (C=O st), 1245 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₅H₃₁NO₃Na 536.2202; Found 536.2202. **M.p.**: 135-138 °C (petroleum ether/EtOAc).

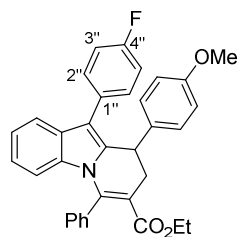


Ethyl (±)-9-(4-methoxyphenyl)-6,10-diphenyl-8,9-dihydropyrido[1,2-a]indole-7-carboxylate (5i). Following *GP-C*, (±)-**5i** (22 mg, 0.045 mmol, 90%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f= 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.71 (d, *J* = 7.9 Hz, 1H, H-1), 7.61-7.29 (m, 10H, C_{arom}-H), 7.22-7.04 (m, 3H, H-2 + C_{arom}-H), 6.93-6.80 (m, 3H, H-3 + C_{arom}-H), 5.86 (d, *J* = 8.5 Hz, 1H, H-4), 4.58 (dd, *J* = 5.3, 2.4 Hz, 1H, H-9), 4.06-3.76 (m, 2H, OCH₂), 3.82 (s, 3H, OCH₃), 3.29 (dd, *J* = 15.5, 2.4 Hz, 1H, H-8a), 3.0 (dd, *J* = 15.5, 5.3 Hz, 1H, H-8b), 0.88 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.8 (COO), 158.3 (C_{arom}-O), 145.6 (C-6), 136.0 (C-4a), 135.8 (C_{arom}-C), 135.4 (C_{arom}-C), 134.1 (C-9a), 133.6 (C_{arom}-C), 129.5 (3×C_{arom}-H), 129.4 (C_{arom}-H), 128.6 (7×C_{arom}-H + C-10a), 126.9 (C_{arom}-H), 122.7 (C-3), 121.7 (C-2), 119.6 (C-1), 117.2 (C_{arom}-C), 114.1 (2× C_{arom}-H), 113.7 (C-4), 111.0 (C-7), 60.1 (OCH₂), 55.4 (OCH₃), 35.7 (C-9), 31.5 (C-8), 13.8 (OCH₂CH₃). **IR** (ATR): 2926 (C-H st), 1686 (C=O st), 1239 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₄H₃₀NO₃ 500.2226; Found 500.2226. **M.p.**: 179-182 °C (petroleum ether/EtOAc).



Ethyl (±)-9,10-bis(4-methoxyphenyl)-6-phenyl-8,9-dihydropyrido[1,2-a]indole-7-carboxylate (5j). Following *GP-C*, (±)-**5j** (23 mg, 0.043 mmol, 86%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2n** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f= 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.64 (d, *J* = 7.8 Hz, 1H, H-1), 7.56-7.23 (m, 7H, C_{arom}-H), 7.19-7.04 (m, 3H, H-2 + C_{arom}-H), 6.93 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.88-6.77 (m, 3H, H-3 + C_{arom}-H), 5.81 (d, *J* = 8.5 Hz, 1H, H-4), 4.52 (dd, *J* = 5.2, 2.5 Hz, 1H, H-9), 4.06-3.64 (m, 8H, OCH₂ + 2×OCH₃), 3.25 (dd, *J* = 15.5, 2.5 Hz, 1H, H-8a), 2.97 (dd, *J* = 15.5, 5.2 Hz, 1H, H-8b), 0.84 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.8 (COO), 158.7 (C_{arom}-C), 158.3 (C_{arom}-O), 145.7 (C-6), 135.9 (C_{arom}-C), 135.8 (C_{arom}-C), 135.0 (C_{arom}-C), 134.2 (C-9a), 130.5 (3×C_{arom}-H), 129.7 (C_{arom}-C), 129.4 (C_{arom}-H), 128.5 (5×C_{arom}-H), 125.9 (C-10a), 122.6 (C-3), 121.6 (C-1), 119.5 (C-2), 116.9 (C-10), 114.1 (2× C_{arom}-H),

114.0 (2× C_{arom}-H), 113.7 (C-4), 110.7 (C-7), 60.1 (OCH₂), 55.4 (OCH₃), 55.3 (OCH₃), 35.7 (C-9), 31.5 (C-8), 13.7 (OCH₂CH₃). **IR** (ATR): 2955 (C-H st), 1685 (C=O st), 1263 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₅H₃₂NO₄ 530.2331; Found 530.2325. **M.p.**: 197-200 °C (petroleum ether/EtOAc).

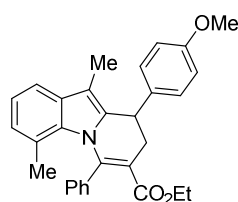


(±)-**5k**

Ethyl

(±)-**10-(4-fluorophenyl)-9-(4-methoxyphenyl)-6-phenyl-8,9-**

dihydropyrido[1,2-a]indole-7-carboxylate (5k). Following *GP-C*, (±)-**5k** (21 mg, 0.041 mmol, 82%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2m** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.60 (d, *J* = 7.9 Hz, 1H, H-1), 7.57-7.38 (m, 4H, C_{arom}-H), 7.39-7.20 (m, 3H, C_{arom}-H), 7.19-7.00 (m, 5H, C_{arom}-H), 6.92-6.73 (m, 3H, C_{arom}-H), 5.83 (d, *J* = 8.5 Hz, 1H, H-4), 4.49 (dd, *J* = 5.4, 2.6 Hz, 1H, H-9), 3.95-3.69 (m, 2H, OCH₂), 3.80 (s, 3H, OCH₃), 3.24 (dd, *J* = 15.5, 2.6 Hz, 1H, H-8a), 2.98 (dd, *J* = 15.5, 5.4 Hz, 1H, H-8b), 0.85 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.7 (COO), 162.0 (d, ¹*J*_{C-F} = 246.2 Hz, C_{arom}-F), 158.4 (C_{arom}-O), 145.5 (C-6), 135.9 (C_{arom}-C), 135.7 (C-4a), 135.4 (C_{arom}-C), 133.9 (C_{arom}-C), 131.2 (d, ³*J*_{C-F} = 8.0 Hz, 2× C_{arom}-H), 129.6 (C-10a + C_{arom}-C), 129.4 (2× C_{arom}-H), 128.5 (5× C_{arom}-H), 122.7 (C-3), 121.8 (C-1), 119.3 (C-2), 116.2 (C-10), 115.6 (d, ²*J*_{C-F} = 21.4 Hz, 2× C_{arom}-H), 114.1 (2× C_{arom}-H), 113.7 (C-4), 111.0 (C-7), 60.1 (OCH₂), 55.4 (OCH₃), 35.7 (C-9), 31.5 (C-8), 13.7 (OCH₂CH₃). **IR** (ATR): 2980 (C-H st), 1685 (C=O st), 1239 (C-O st as), 1221 (C-F st) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₄H₂₉NO₃F 518.2131; Found 518.2139. **M.p.**: 175-178 °C (petroleum ether/EtOAc).

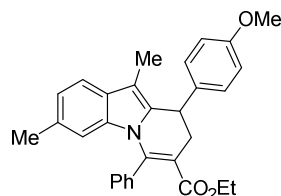


(±)-**5l**

Ethyl (±)-9-(4-methoxyphenyl)-4,10-dimethyl-6-phenyl-8,9-dihydropyrido[1,2-

a]indole-7-carboxylate (5l). Following *GP-C*, (±)-**5l** (12 mg, 0.027 mmol, 54%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2b** (7 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.38-7.28 (m, 2H, C_{arom}-H), 7.26-7.19 (m, 2H, C_{arom}-H), 7.15-7.00 (m, 5H, C_{arom}-H), 6.87-6.67 (m, 3H, C_{arom}-H), 4.42 (app t, *J* = 5.2 Hz, 1H, H-9), 3.84 (m, 2H, OCH₂), 3.75 (s, 3H, OCH₃), 3.22-2.79 (m, 2H, H-8), 2.00 (s, 3H, C_{arom}-CH₃), 1.43 (s, 3H, C_{arom}-CH₃), 0.86 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 169.0 (COO), 158.4 (C_{arom}-O), 144.7 (C-6), 139.1 (C_{arom}-C), 136.4 (C_{arom}-C), 135.6 (C_{arom}-C), 133.3 (C_{arom}-C), 132.6 (C-10a), 129.9 (2× C_{arom}-H), 129.0 (C_{arom}-H), 128.9 (2× C_{arom}-H), 127.6 (2× C_{arom}-H), 125.7 (C-2), 124.5 (C-4), 121.8 (C-3), 115.9 (C-

1), 113.9 (C_{arom}-H), 113.0 (C-10), 110.9 (C-7), 60.2 (OCH₂), 55.3 (OCH₃), 40.5 (C-9), 34.1 (C-8), 20.6 (C_{arom}-CH₃), 13.8 (OCH₂CH₃), 9.2 (C-10-CH₃). **MS** (EI) m/z (%): 452.1 (27), 451.2 (M⁺, 74), 379.1 (22), 378.2 (100), 363.2 (21), 270.0 (44), 254.9 (17), 253.9 (25), 248.0 (17), 218.1 (25), 216.9 (18), 204.1 (23), 135.0 (52), 121.0 (31), 115.9 (18), 115.0 (90), 108.0 (50), 78.0 (24), 77.0 (36). **IR** (ATR): 2926 (C-H st), 1692 (C=O st), 1247 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₀H₂₉NO₃Na 474.2045; Found 474.2041. **M.p.**: 132-135 °C (petroleum ether/EtOAc).

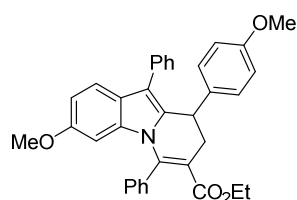


(±)-5m

Ethyl

(±)-9-(4-methoxyphenyl)-3,10-dimethyl-6-phenyl-8,9-

dihydropyrido[1,2-a]indole-7-carboxylate (5m). Following *GP-C*, (±)-5m (21 mg, 0.047 mmol, 93%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2d** (7 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.56-7.36 (m, 4H, C_{arom}-H), 7.32 (d, *J* = 7.9 Hz, 1H, H-1), 7.25-7.15 (m, 1H, C_{arom}-H), 7.10 (d, *J* = 8.3 Hz, 2H, C_{arom}-H), 6.89 (d, 1H, *J* = 8.0 Hz, H-2), 6.82 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 5.42 (s, 1H, H-4), 4.50 (app t, *J* = 4.7 Hz, 1H, H-9), 4.10-3.64 (m, 2H, OCH₂), 3.78 (s, 3H, OCH₃), 3.25 (dd, *J* = 15.4, 3.9 Hz, 1H, H-8a), 3.01 (dd, *J* = 15.4, 5.4 Hz, 1H, H-8b), 2.10 (s, 3H, CH₃), 2.07 (s, 3H, CH₃), 0.86 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 168.1 (COO), 158.4 (C_{arom}-O), 146.3 (C-6), 136.2 (C_{arom}-C), 135.9 (C_{arom}-C), 134.5 (C_{arom}-C), 133.8 (C_{arom}-C), 131.8 (C-10a), 130.2 (C_{arom}-H), 129.1 (3×C_{arom}-H), 128.5 (3×C_{arom}-H+ C-3), 122.5 (C-2), 118.0 (C-1), 114.1 (C-4), 114.0 (2×C_{arom}-H), 111.0 (C-10), 108.6 (C-7), 60.0 (OCH₂), 55.4 (OCH₃), 36.2 (C-9), 31.0 (C-8), 21.9 (C-3-CH₃), 13.8 (OCH₂CH₃), 8.7 (C-10-CH₃). **IR** (ATR): 2980 (C-H st), 1683 (C=O st), 1244 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₀H₂₉NO₃Na 474.2045; Found 474.2047. **M.p.**: 111-114 °C (petroleum ether/EtOAc).



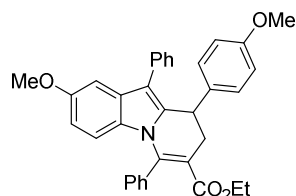
(±)-5n

Ethyl

(±)-3-methoxy-9-(4-methoxyphenyl)-6,10-diphenyl-8,9-

dihydropyrido[1,2-a]indole-7-carboxylate (5n). Following *GP-C*, (±)-5n (21 mg, 0.040 mmol, 79%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2o** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.61-7.44 (m, 5H, C_{arom}-H), 7.44-7.28 (m, 6H, C_{arom}-H), 7.12 (d, *J* = 8.6 Hz, 2H, C_{arom}-H), 6.85 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.73 (dd, *J* = 8.7, 2.3 Hz, 1H, H-2), 5.40 (d, *J* = 2.3 Hz, 1H, H-4), 4.52 (dd, *J* = 5.3, 2.5 Hz, 1H, H-9), 4.13-3.74 (m, 2H, OCH₂), 3.80 (s, 3H, OCH₃), 3.35 (s, 1H, OCH₃), 3.27 (dd, *J* = 15.5, 2.5 Hz, 1H, H-8a), 2.96 (dd, *J* = 15.5, 5.3 Hz, 1H, H-8b), 0.86 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.7 (COO), 158.3 (C_{arom}-O), 156.2 (C-3), 145.7 (C-6), 136.7 (C_{arom}-C), 136.0 (C_{arom}-

C), 134.3 (C_{arom}-C), 133.9 (C_{arom}-C), 133.7 (C_{arom}-C), 129.3 (5×C_{arom}-H), 128.6 (6×C_{arom}-H), 126.8 (C_{arom}-H), 123.3 (C-10a), 119.9 (C-1), 117.0 (C-10), 114.0 (2×C_{arom}-H), 111.4 (C-2), 110.8 (C-7), 97.8 (C-4), 60.1 (OCH₂), 55.3 (OCH₃), 55.2 (OCH₃), 35.6 (C-9), 31.5 (C-8), 13.7 (OCH₂CH₃). **IR** (ATR): 2984 (C-H st), 1685 (C=O st), 1246 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₅H₃₁NO₄Na 552.2151; Found 552.2148. **M.p.**: 152-155 °C (petroleum ether/EtOAc).

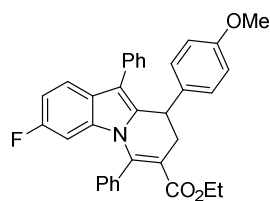


(±)-5o

Ethyl

(±)-2-methoxy-9-(4-methoxyphenyl)-6,10-diphenyl-8,9-

dihydropyrido[1,2-a]indole-7-carboxylate (5o). Following *GP-C*, (±)-5o (19 mg, 0.035 mmol, 71%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2p** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.61-7.27 (m, 10H, C_{arom}-H), 7.15-7.05 (m, 3H, H-1 + C_{arom}-H), 6.83 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.46 (dd, *J* = 9.2, 2.6 Hz, 1H, H-4), 5.67 (d, *J* = 9.2 Hz, 1H, H-3), 4.51 (dd, *J* = 5.2, 2.5 Hz, 1H, H-9), 3.98-3.67 (m, 2H, OCH₂), 3.79 (s, 3H, OCH₃), 3.76 (s, 3H, (OCH₃)), 3.24 (dd, *J* = 15.5, 2.5 Hz, 1H, H-8a), 2.96 (dd, *J* = 15.5, 5.2 Hz, 1H, H-8b), 0.84 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.8 (COO), 158.3 (C_{arom}-O), 155.5 (C-2), 145.7 (C-6), 136.1 (C_{arom}-C), 135.8 (C_{arom}-C), 134.1 (C_{arom}-C), 133.7 (C_{arom}-C), 130.8 (C_{arom}-C), 130.3 (C_{arom}-C), 129.4 (4×C_{arom}-H), 128.6 (7×C_{arom}-H), 126.9 (C_{arom}-H), 117.1 (C-10), 114.4 (C-4), 114.1 (2×C_{arom}-H), 111.6 (C-3), 110.2 (C-7), 102.1 (C-1), 60.1 (OCH₂), 55.9 (OCH₃), 55.3 (OCH₃), 35.7 (C-9), 31.4 (C-8), 13.7 (OCH₂CH₃). **IR** (ATR): 2951 (C-H st), 1684 (C=O st), 1248 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₅H₃₁NO₄Na 552.2151; Found 552.2147. **M.p.**: 157-160 °C (petroleum ether/EtOAc).



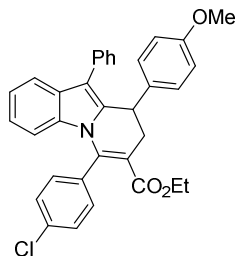
(±)-5p

Ethyl

(±)-3-fluoro-9-(4-methoxyphenyl)-6,10-diphenyl-8,9-

dihydropyrido[1,2-a]indole-7-carboxylate (5p). Following *GP-C*, (±)-5p (23 mg, 0.044 mmol, 87%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1e** (16 mg, 0.05 mmol) and indole **2q** (11 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.67-7.29 (m, 11H, C_{arom}-H), 7.11 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.85 (d, *J* = 8.7 Hz, 3H, H-2 + C_{arom}-H), 5.47 (dd, *J* = 11.4, 2.3 Hz, 1H, H-4), 4.53 (dd, *J* = 5.2, 2.5 Hz, 1H, H-9), 3.94-3.69 (m, 2H, OCH₂), 3.80 (s, 3H, OCH₃), 3.25 (dd, *J* = 15.6, 2.5 Hz, 1H, H-8a), 2.98 (dd, *J* = 15.6, 5.2 Hz, 1H, H-8b), 0.85 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.6 (COO), 159.5 (d, ¹J_{C-F} = 238.2 Hz, C-3), 158.4 (C_{arom}-O), 145.2 (C-6), 135.9 (d, ³J_{C-F} = 12.3 Hz, C-4a), 135.6 (d, ⁴J_{C-F} = 4.0 Hz, C-10a), 135.2 (C_{arom}-C), 134.0 (C_{arom}-C), 133.3 (C_{arom}-C), 129.7 (C_{arom}-H), 129.4 (2×C_{arom}-H), 128.5 (8×C_{arom}-H), 127.1 (C_{arom}-H), 125.8

(C-9a), 120.0 (d, $^3J_{C-F} = 9.9$ Hz, C-1), 117.0 (C-10), 114.1 ($2 \times C_{\text{arom-H}}$), 111.5 (C-7), 109.9 (d, $^2J_{C-F} = 24.4$ Hz, C-4), 100.85 (d, $^2J_{C-F} = 29.2$ Hz, C-2), 60.2 (OCH₂), 55.3 (OCH₃), 35.7 (C-9), 31.5 (C-8), 13.7 (OCH₂CH₃). **IR** (ATR): 2980 (C-H st), 1688 (C=O st), 1244 (C-O st as), 1143 (C-F st) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₄H₂₈NO₃FNa 540.1951; Found 540.1955. **M.p.**: 178-181 °C (petroleum ether/EtOAc).



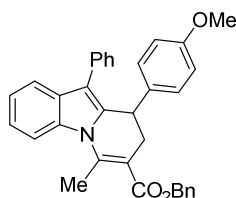
(±)-5q

Ethyl

(±)-6-(4-chlorophenyl)-9-(4-methoxyphenyl)-10-phenyl-8,9-

dihydropyrido[1,2-a]indole-7-carboxylate (5q). Following *GP-C*, (±)-5q (24 mg, 0.045 mmol, 90%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1f** (18 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R*_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.69 (d, *J* = 7.9 Hz, 1H, H-1), 7.54-7.28 (m, 9H, C_{arom-H}), 7.17-7.02 (m, 3H, H-2 + C_{arom-H}), 6.90 (ddd, *J* = 8.5, 7.1, 1.3 Hz, 1H, H-3), 6.84 (d, *J* = 8.7 Hz, 2H, C_{arom-H}), 5.95 (d, *J* = 8.5 Hz, 1H, H-4), 4.55 (dd, *J* = 5.3, 2.5 Hz, 1H, H-9), 4.14-3.66 (m, 2H, OCH₂), 3.80 (s, 3H, OCH₃), 3.28 (dd, *J* = 15.5, 2.5 Hz, 1H, H-8a), 2.95 (dd, *J* = 15.5, 5.3 Hz, 1H, H-8b), 0.93 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.4 (COO), 158.4 (C_{arom-O}), 144.4 (C-6), 135.6 (C_{arom-C}), 135.5 (C_{arom-C}), 135.3 (C_{arom-C}), 134.1 (C-9a), 133.8 (C_{arom-C}), 133.4 (C-Cl), 129.5 (C_{arom-C}), 129.4 ($3 \times C_{\text{arom-H}}$), 128.6 ($5 \times C_{\text{arom-H}}$), 128.4 ($2 \times C_{\text{arom-H}}$), 127.0 (C_{arom-H}), 122.9 (C-3), 121.9 (C-2), 119.7 (C-1), 117.4 (C-10), 114.1 ($2 \times C_{\text{arom-H}}$), 113.5 (C-4), 111.6 (C-7), 60.3 (OCH₂), 55.3 (OCH₃), 35.6 (C-9), 31.4 (C-8), 13.8 (OCH₂CH₃). **IR** (ATR): 2980 (C-H st), 1686 (C=O st), 1242 (C-O st as), 1088 (C-Cl st) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₄H₂₉NO₃Cl 534.1836; Found 534.1828. **M.p.**: 175-178 °C (petroleum ether/EtOAc).

The reaction was carried out in a bigger scale: Following *GP-C*, (±)-5q (443 mg, 0.83 mmol, 83%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1f** (360 mg, 1.00 mmol) and indole **2l** (200 mg, 1.00 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (40 mg, 0.10 mmol) in toluene (0.25 mL) at 100 °C for 90 min in an oil bath.



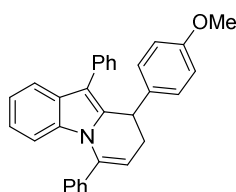
(±)-5r

Benzyl

(±)-9-(4-methoxyphenyl)-6-methyl-10-phenyl-8,9-dihydropyrido[1,2-

a]indole-7-carboxylate (5r). Following *GP-C*, (±)-5r (21 mg, 0.042 mmol, 83%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1g** (16 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R*_f = 0.70 (petroleum ether/EtOAc,

9:1). ¹H NMR (300 MHz, CDCl₃) δ 7.92-7.63 (m, 2H, H-1 + H-4), 7.48-7.09 (m, 12H, C_{arom}-H), 6.95 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.77 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 5.22 (d, *J* = 12.8 Hz, 1H, OCH_aH_b), 5.09 (d, *J* = 12.8 Hz, 1H, OCH_aH_b), 4.44 (dd, *J* = 5.1, 2.6 Hz, 1H, H-9), 3.79 (s, 3H, OCH₃), 3.33 (dd, *J* = 15.7, 2.6 Hz, 1H, H-8a), 3.01 (d, *J* = 2.1 Hz, 3H, C-6-CH₃), 2.75-2.63 (m, 1H, H-8b). ¹³C NMR (75 MHz, CDCl₃) δ 167.5 (COO), 158.3 (C_{arom}-O), 146.4 (C-6), 136.6 (C_{arom}-C), 136.0 (C_{arom}-C), 135.2 (C_{arom}-C), 133.9 (C_{arom}-C), 133.7 (C_{arom}-C), 129.6 (C_{arom}-C), 129.5 (2×C_{arom}-H), 128.6 (4×C_{arom}-H), 128.5 (2×C_{arom}-H), 128.0 (C_{arom}-H), 127.6 (2×C_{arom}-H), 126.8 (C_{arom}-H), 123.0 (C-3), 121.9 (C-2), 120.1 (C-1), 116.3 (C-10), 114.0 (2×C_{arom}-H), 113.7 (C-4), 110.5 (C-7), 66.0 (OCH₂), 55.3 (OCH₃), 35.6 (C-9), 30.5 (C-8), 19.7 (C-6-CH₃). IR (ATR): 2976 (C-H st), 1698 (C=O st), 1247 (C-O st as) cm⁻¹. MS (EI) *m/z* (%): 438.2 (27), 437.1 (100), 365.1 (27), 364.1 (M⁺-C₈H₇O₂, 86), 363.1 (20), 349.2 (33), 337.1 (24), 329.1 (18), 301.1 (19). HRMS (ESI) *m/z*: [M+Na]⁺ Calcd for C₃₄H₂₉NO₃Na 522.2045; Found 522.2047. M.p.: 60-63 °C (petroleum ether/EtOAc).

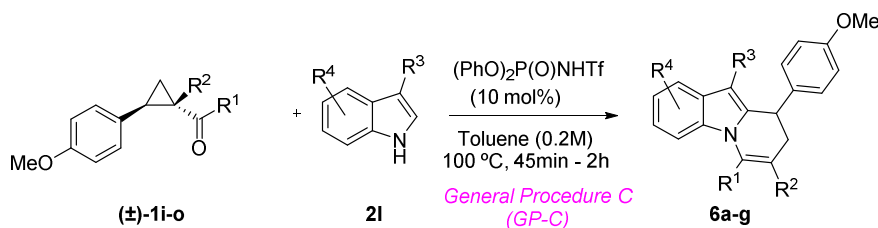


(±)-5s

(±)-9-(4-Methoxyphenyl)-6,10-diphenyl-8,9-dihydropyrido[1,2-a]indole (5s).

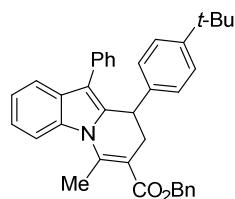
Following GP-C, (±)-5s (15 mg, 0.036 mmol, 72%) was isolated by FC (petroleum ether/EtOAc, 99:1) on silica gel as a white solid, from cyclopropane **1h** (18 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. R_f = 0.60 (petroleum ether/EtOAc, 19:1). ¹H NMR (300 MHz, CDCl₃) δ 7.79 (d, *J* = 8.0 Hz, 1H, H-1), 7.57-7.28 (m, 10H, C_{arom}-H), 7.21-7.06 (m, 3H, C_{arom}-H), 6.95 (ddd, *J* = 8.3, 7.1, 1.2 Hz, 1H, H-3), 6.83 (d, *J* = 8.7 Hz, 2H, C_{arom}-H), 6.42 (d, *J* = 8.4 Hz, 1H, H-4), 5.38 (dd, *J* = 7.2, 3.0 Hz, 1H, H-7), 4.53 (app d, *J* = 5.2 Hz, 1H, H-9), 3.78 (s, 3H, OCH₃), 2.80 (ddd, *J* = 15.9, 5.5, 3.1 Hz, 1H, H-8a), 2.673 (ddd, *J* = 15.9, 7.3, 2.1 Hz, 1H, H-8b). ¹³C NMR (75 MHz, CDCl₃) δ 158.2 (C_{arom}-O), 139.1 (C-6), 136.6 (C_{arom}-C), 135.7 (C_{arom}-C), 135.3 (C_{arom}-C), 134.9 (C_{arom}-C), 129.5 (2×C_{arom}-H), 128.6 (8×C_{arom}-H), 128.2 (C_{arom}-C), 127.8 (2×C_{arom}-H), 126.4 (C_{arom}-C), 121.7 (C-3), 120.6 (C-2), 119.4 (C-1), 115.7 (C-10), 114.0 (2×C_{arom}-H), 113.3 (C-7), 111.5 (C-4), 55.3 (OCH₃), 36.2 (C-9), 30.5 (C-8). IR (ATR): 2955 (C-H st), 1650 (arC-C), 1608 (arC-C) cm⁻¹. IR (ATR): 2955 (C-H st), 1650 (arC-C), 1608 (arC-C) cm⁻¹. HRMS (ESI) *m/z*: [M+H]⁺ Calcd for C₃₁H₂₆NO 428.2014; Found 428.2004. M.p.: 239-242 °C (petroleum ether/EtOAc).

2.3.3 Synthesis of dihydropyridoindoles **6**



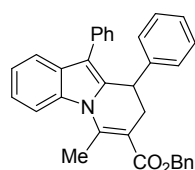
Scheme S5. General Procedure C for the synthesis of dihydropyridoindoles (±)-6a-g

General Procedure C (GP-C) for the cyclocondensation: An oven-dried 5 mL screw-capped test tube containing a stirring bar was charged with cyclopropane **1i-o** (1eq.) and corresponding indole **2I** (1eq.) and dissolved in toluene (0.2 M) under Ar. After adding the diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate catalyst (10 mol%) the mixture was stirred at 100 °C in an oil bath. When the reaction was judged complete (monitored by TLC), it was warmed to room temperature, quenched by addition of aq. NaHCO₃ (sat) (3 mL) and diluted with EtOAc (3 mL). The phases were separated and the aqueous phase was extracted with EtOAc (3×3 mL). The combined organic layers were dried over Na₂SO₄, filtered and evaporated. The residue was purified by column chromatography on silica gel to afford the corresponding pure compounds **6a-g**.



(±)-**6a**

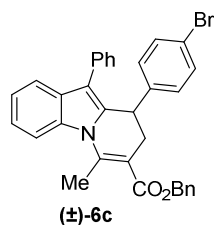
Benzyl (±)-9-(4-(tert-butyl)phenyl)-6-methyl-10-phenyl-8,9-dihydropyrido[1,2-a]indole-7-carboxylate (6a). Following *GP-C*, (±)-**6a** (20 mg, 0.038 mmol, 76%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1i** (17 mg, 0.05 mmol) and indole **2I** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. $R_f = 0.70$ (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.87-7.61 (m, 2H, H-1 + H-4), 7.41-7.13 (m, 14H, C_{arom}-H), 6.96 (d, $J = 8.3$ Hz, 2H, C_{arom}-H), 5.22 (d, $J = 12.8$ Hz, 1H, OCH_aH_b), 5.11 (d, $J = 12.8$ Hz, 1H, OCH_aH_b), 4.47 (dd, $J = 5.2, 2.9$ Hz, 1H, H-9), 3.36 (dd, $J = 15.8, 2.9$ Hz, 1H, H-8a), 3.03 (d, $J = 2.0$ Hz, 3H, C-6-CH₃), 2.74 (dd, $J = 15.8, 5.2$ Hz, 1H, H-8b), 1.30 (s, 9H, C(CH₃)₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.6 (COO), 149.2 (C_{arom}-O), 146.5 (C-6), 138.4 (C_{arom}-C), 136.6 (C_{arom}-C), 136.0 (C_{arom}-C), 135.2 (C_{arom}-C), 133.7 (C_{arom}-C), 129.7 (C_{arom}-C), 129.5 (2×C_{arom}-H), 128.6 (4×C_{arom}-H), 128.0 (C_{arom}-H), 127.7 (2×C_{arom}-H), 127.1 (2×C_{arom}-H), 126.8 (C_{arom}-H), 125.4 (2×C_{arom}-H), 123.0 (C-3), 121.8 (C-2), 120.1 (C-1), 116.5 (C-10), 113.7 (C-4), 110.5 (C-7), 66.0 (OCH₂), 35.9 (C-9), 34.5 (C(CH₃)₃), 31.5 (C(CH₃)₃), 30.2 (C-8), 19.7 (C-6-CH₃). **IR** (ATR): 2961 (C-H st), 1698 (C=O st), 1243 (C-O st as) cm⁻¹. **HRMS (ESI) m/z:** [M+Na]⁺ Calcd for C₃₇H₃₅NO₂Na 548.2565; Found 548.2569. **M.p.:** 82-85 °C (petroleum ether/EtOAc).



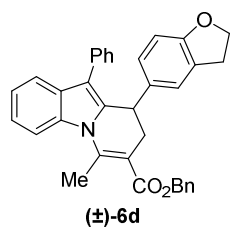
(±)-**6b**

Benzyl (±)-6-methyl-9,10-diphenyl-8,9-dihydropyrido[1,2-a]indole-7-carboxylate (6b). Following *GP-C*, (±)-**6b** (17 mg, 0.036 mmol, 72%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1j** (15 mg, 0.05 mmol) and indole **2I** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. $R_f = 0.70$ (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 8.00-7.57 (m, 2H, H-1 + H-4), 7.46-7.13 (m, 15H, C_{arom}-H), 7.04 (dd, $J = 7.5, 2.0$ Hz, 2H, C_{arom}-H), 5.20 (d, $J = 12.8$ Hz, 1H, OCH_aH_b), 5.08 (d, $J = 12.8$ Hz, 1H, OCH_aH_b), 4.49 (dd, $J = 5.1, 2.5$ Hz, 1H, H-9), 3.36 (dd, $J = 15.7, 2.6$ Hz, 1H, H-8a), 3.01 (d, $J = 2.2$ Hz, 3H, C-6-CH₃), 2.82-2.65 (m, 1H, H-8b). **¹³C NMR** (75 MHz, CDCl₃) δ 167.4 (COO), 146.5 (C-6), 141.8 (C_{arom}-C), 136.6 (C_{arom}-C),

135.6 (C_{arom}-C), 135.3 (C_{arom}-C), 133.6 (C_{arom}-C), 129.6 (C-10a), 129.5 (2×C_{arom}-H), 128.6 (6×C_{arom}-H), 128.0 (C_{arom}-H), 127.6 (2×C_{arom}-H), 127.5 (2×C_{arom}-H), 126.9 (C_{arom}-H), 126.6 (C_{arom}-H), 123.1 (C-3), 121.9 (C-2), 120.1 (C-1), 116.5 (C-10), 113.8 (C-4), 110.4 (C-7), 66.0 (OCH₂), 36.4 (C-9), 30.5 (C-8), 19.7 (C-6-CH₃). **IR** (ATR): 2956 (C-H st), 1698 (C=O st), 1248 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₃H₂₇NO₂Na 492.1939; Found 492.1944. **M.p.**: 67-70 °C (petroleum ether/EtOAc).

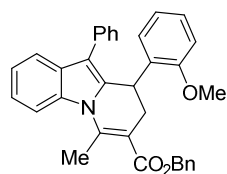


Benzyl (±)-9-(4-bromophenyl)-6-methyl-10-phenyl-8,9-dihydropyrido[1,2-a]indole-7-carboxylate (6c). Following *GP-C*, (±)-**6c** (15 mg, 0.031 mmol, 62%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1k** (19 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R_f* = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.78-7.53 (m, 2H, H-1 + H-4), 7.40-6.98 (m, 14H, C_{arom}-H), 6.81 (d, *J* = 8.4 Hz, 2H, C_{arom}-H), 5.13 (d, *J* = 12.7 Hz, 1H, OCH_aCH_b), 4.98 (d, *J* = 12.7 Hz, 1H, OCH_aCH_b), 4.33 (dd, *J* = 5.2, 2.6 Hz, 1H, H-9), 3.21 (dd, *J* = 15.7, 2.6 Hz, 1H, H-8a), 2.90 (d, *J* = 2.1 Hz, 3H, CH₃), 2.63 (ddd, *J* = 15.7, 5.2, 2.2 Hz, 1H, H-8b). **¹³C NMR** (75 MHz, CDCl₃) δ 167.3 (COO), 146.4 (C-6), 140.9 (C_{arom}-C), 136.5 (C_{arom}-C), 135.2 (C_{arom}-C), 134.8 (C_{arom}-C), 133.4 (C_{arom}-C), 131.7 (2×C_{arom}-H), 129.5 (C_{arom}-C), 129.4 (2×C_{arom}-H), 129.3 (2×C_{arom}-H), 128.7 (4×C_{arom}-H), 128.1 (C_{arom}-H), 127.6 (2×C_{arom}-H), 127.0 (C_{arom}-H), 123.3 (C-3), 122.0 (C-2), 120.6 (C-Br), 120.2 (C-1), 116.8 (C-10), 113.8 (C-4), 110.1 (C-7), 66.1 (OCH₂), 36.0 (C-9), 30.4 (C-8), 19.6 (C-6-CH₃). **IR** (ATR): 2942 (C-H st), 1698 (C=O st), 1265 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₃H₂₇BrNO₂ 548.1225; Found 548.1219. **M.p.**: 152-155 °C (petroleum ether/EtOAc).



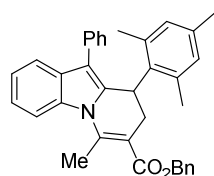
Benzyl (±)-9-(2,3-dihydrobenzofuran-5-yl)-6-methyl-10-phenyl-8,9-dihydropyrido[1,2-a]indole-7-carboxylate (6d). Following *GP-C*, (±)-**6d** (24 mg, 0.046 mmol, 92%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1l** (17 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R_f* = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.80-7.75 (m, 2H, H-1 + H-4), 7.52-7.17 (m, 12H, C_{arom}-H), 6.96-6.70 (m, 2H, C_{arom}-H), 6.66 (d, *J* = 8.2 Hz, 1H, C_{arom}-H), 5.24 (d, *J* = 12.8 Hz, 1H, OCH_aH_b), 5.10 (d, *J* = 12.8 Hz, 1H, OCH_aH_b), 4.54 (t, *J* = 8.9 Hz, 2H, OCH₂CH₂), 4.42 (dd, *J* = 5.1, 2.7 Hz, 1H, H-9), 3.31 (dd, *J* = 15.7, 2.7 Hz, 1H, H-8a), 3.17-2.87 (m, 2H, OCH₂CH₂), 3.02 (d, *J* = 2.1 Hz, 3H, CH₃), 2.79-2.56 (m, 1H, H-8b). **¹³C NMR** (75 MHz, CDCl₃) δ 167.5 (COO), 158.8 (C_{arom}-OCH₂), 146.4 (C-6), 136.6 (C_{arom}-C), 136.1 (C_{arom}-C), 135.2 (C_{arom}-C), 133.8 (C_{arom}-C), 133.7 (C_{arom}-C), 129.6 (C_{arom}-C), 129.4 (2×C_{arom}-H), 128.6 (4×C_{arom}-H), 128.0 (C_{arom}-H), 127.6 (2×C_{arom}-H), 127.2 (C_{arom}-C + C_{arom}-H), 126.8 (C_{arom}-H), 123.9 (C_{arom}-H), 123.0 (C-3), 121.9 (C-2), 120.1

(C-1), 116.2 (C-10), 113.7 (C-4), 110.6 (C-7), 109.1 (C_{arom}-H), 71.3 (OCH₂CH₂), 66.0 (OCH₂C_{arom}), 35.9 (C-9), 30.7 (C-8), 29.9 (OCH₂CH₂), 19.7 (C-6-CH₃). **IR** (ATR): 2957 (C-H st), 1698 (C=O st), 1242 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₅H₂₉NO₃Na 534.2045; Found 534.2054. **M.p.**: 85-88 °C (petroleum ether/EtOAc).



(±)-**6e**

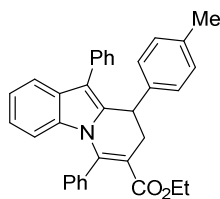
Benzyl (±)-9-(2-methoxyphenyl)-6-methyl-10-phenyl-8,9-dihydropyrido[1,2-a]indole-7-carboxylate (6e). Following *GP-C*, (±)-**6e** (20 mg, 0.040 mmol, 80%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1m** (16 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R*_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.79 (m, 2H, H-1 + H-4), 7.49-7.05 (m, 13H, C_{arom}-H), 6.88 (dd, *J* = 8.2, 1.1 Hz, 1H, C_{arom}-H), 6.75 (app td, *J* = 7.5, 1.1 Hz, 1H, C_{arom}-H), 6.56 (dd, *J* = 7.6, 1.7 Hz, 1H, C_{arom}-H), 5.17 (d, *J* = 12.9 Hz, 1H, OCH_aH_b), 5.03 (d, *J* = 12.9 Hz, 1H, OCH_aH_b), 4.76 (dd, *J* = 5.5, 2.5 Hz, 1H, H-9), 3.76 (s, 3H, OCH₃), 3.41 (dd, *J* = 15.8, 2.5 Hz, 1H, H-8a), 3.03 (d, *J* = 2.1 Hz, 3H, C-6-CH₃), 2.58 (dd, *J* = 15.8, 5.5 Hz, 1H, H-8b). **¹³C NMR** (75 MHz, CDCl₃) δ 167.7 (COO), 156.5 (C_{arom}-OCH₃), 145.8 (C-6), 136.7 (C_{arom}-C), 136.4 (C_{arom}-C), 135.3 (C_{arom}-C), 133.8 (C_{arom}-C), 130.0 (C_{arom}-C), 129.7 (C-10a), 129.4 (2×C_{arom}-H), 128.8 (C_{arom}-H), 128.5 (2×C_{arom}-H), 128.4 (2×C_{arom}-H), 127.9 (2×C_{arom}-H), 127.5 (2×C_{arom}-H), 126.6 (C_{arom}-H), 122.9 (C-3), 121.8 (C-2), 120.4 (C_{arom}-H), 120.1 (C-1), 115.9 (C-10), 113.7 (C_{arom}-H), 111.3 (C-4), 110.7 (C-7), 65.8 (OCH₂), 55.4 (OCH₃), 31.6 (C-9), 28.3 (C-8), 19.6 (C-6-CH₃). **IR** (ATR): 2934 (C-H st), 1698 (C=O st), 1241 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₄H₂₉NO₃Na 522.2045; Found 522.2046. **M.p.**: 74-77 °C (petroleum ether/EtOAc).



(±)-**6f**

Benzyl (±)-9-mesityl-6-methyl-10-phenyl-8,9-dihydropyrido[1,2-a]indole-7-carboxylate (6f). Following *GP-C*, (±)-**6f** (16 mg, 0.031 mmol, 42%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1n** (17 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl] phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R*_f = 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.74 (d, *J* = 8.2 Hz, 1H, H-1), 7.52 (d, *J* = 7.4 Hz, 1H, H-4), 7.41-7.28 (m, 5H, C_{arom}-H), 7.25-7.12 (m, 2H, C_{arom}-H), 7.08-6.98 (m, 5H, C_{arom}-H), 6.65 (s, 1H, C_{arom}-H), 6.33 (s, 1H, C_{arom}-H), 5.33-5.07 (m, 2H, OCH₂), 4.71 (dd, *J* = 11.3, 6.7 Hz, 1H, H-9), 3.06 (s, 3H, C-6-CH₃), 3.00-2.72 (m, 2H, H-8), 2.34 (s, 3H, CH₃), 2.07 (s, 3H, CH₃), 1.82 (s, 3H, CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.7 (COO), 146.6 (C-6), 136.5 (C_{arom}-C), 136.0 (2×C_{arom}-C), 135.8 (C_{arom}-C), 135.0 (C_{arom}-C), 133.8 (C_{arom}-C), 133.4 (C_{arom}-C), 130.6 (2×C_{arom}-C), 129.2 (3×C_{arom}-H), 129.0 (C_{arom}-H), 128.7 (3×C_{arom}-H), 128.2 (C_{arom}-H), 128.1 (2×C_{arom}-H), 127.4 (C_{arom}-H), 126.1 (C_{arom}-H), 122.7 (C-3), 121.7 (C-2), 119.8 (C-1), 117.3 (C-10), 114.3 (C-4), 111.0 (C-7), 66.3 (OCH₂), 35.5 (C-9), 28.1 (C-8), 20.6 (CH₃), 19.8

(3×CH₃). **IR** (ATR): 2920 (C-H st), 1699 (C=O st), 1243 (C-O st as) cm⁻¹. **HRMS (ESI) m/z**: [M+Na]⁺ Calcd for C₃₆H₃₃NO₂Na 534.2409; Found 534.2408. **M.p.**: 197-200 °C (petroleum ether/EtOAc).



(±)-**6g**

Ethyl

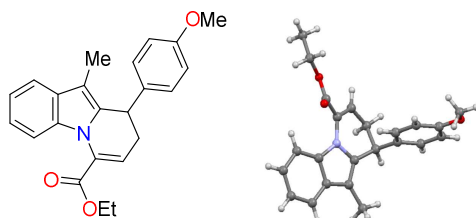
(±)-**6,10-diphenyl-9-(p-tolyl)-8,9-dihydropyrido[1,2-a]indole-7-**

carboxylate (6g). Following *GP-C*, (±)-**6g** (19 mg, 0.039 mmol, 78%) was isolated by FC (petroleum ether/EtOAc, 25:1) on silica gel as a white solid, from cyclopropane **1o** (15 mg, 0.05 mmol) and indole **2l** (10 mg, 0.05 mmol) under diphenyl [(trifluoromethyl)sulfonyl]phosphoramidate (2 mg, 0.005 mmol) in toluene (0.25 mL) at 100 °C for 45 min in an oil bath. *R_f*= 0.70 (petroleum ether/EtOAc, 9:1). **¹H NMR** (300 MHz, CDCl₃) δ 7.69 (d, *J* = 7.9 Hz, 1H, H-1), 7.56-7.24 (m, 10H, C_{arom}-H), 7.17-7.01 (m, 5H, C_{arom}-H), 6.84 (ddd, *J* = 8.4, 7.1, 1.3 Hz, 1H, H-3), 5.83 (d, *J* = 8.5 Hz, 1H, H-4), 4.57 (dd, *J* = 5.3, 2.4 Hz, 1H, H-9) 4.07-3.67 (m, 2H, OCH₂), 3.28 (dd, *J* = 15.5, 2.4 Hz, 1H, H-8a), 2.99 (dd, *J* = 15.5, 5.3 Hz, 1H, H-8b), 2.33 (s, 3H, C_{arom}-CH₃), 0.86 (t, *J* = 7.1 Hz, 3H, OCH₂CH₃). **¹³C NMR** (75 MHz, CDCl₃) δ 167.7 (COO), 145.6 (C-6), 138.9 (C_{arom}-C), 136.2 (C_{arom}-C), 136.0 (C_{arom}-C), 135.8 (C_{arom}-C), 135.3 (C_{arom}-C), 133.6 (C_{arom}-C), 129.4 (6×C_{arom}-H + C-10a), 128.6 (5×C_{arom}-H), 127.3 (2×C_{arom}-H), 126.9 (C_{arom}-H), 122.7 (C-3), 121.7 (C-2), 119.6 (C-1), 117.3 (C-10), 113.7 (C-4), 111.0 (C-7), 60.1 (OCH₂), 36.0 (C-9), 31.4 (C-8), 21.2 (C_{arom}-CH₃), 13.7 (OCH₂CH₃). **IR** (ATR): 2984 (C-H st), 1692 (C=O st), 1237 (C-O st as) cm⁻¹. **MS** (EI) *m/z* (%): 410.2 (M⁺-C₃H₅O, 3), 207.0 (21). **HRMS (ESI) m/z**: [M+H]⁺ Calcd for C₃₄H₃₀NO₂ 484.2277; Found 484.2279. **M.p.**: 182-185 °C (petroleum ether/EtOAc).

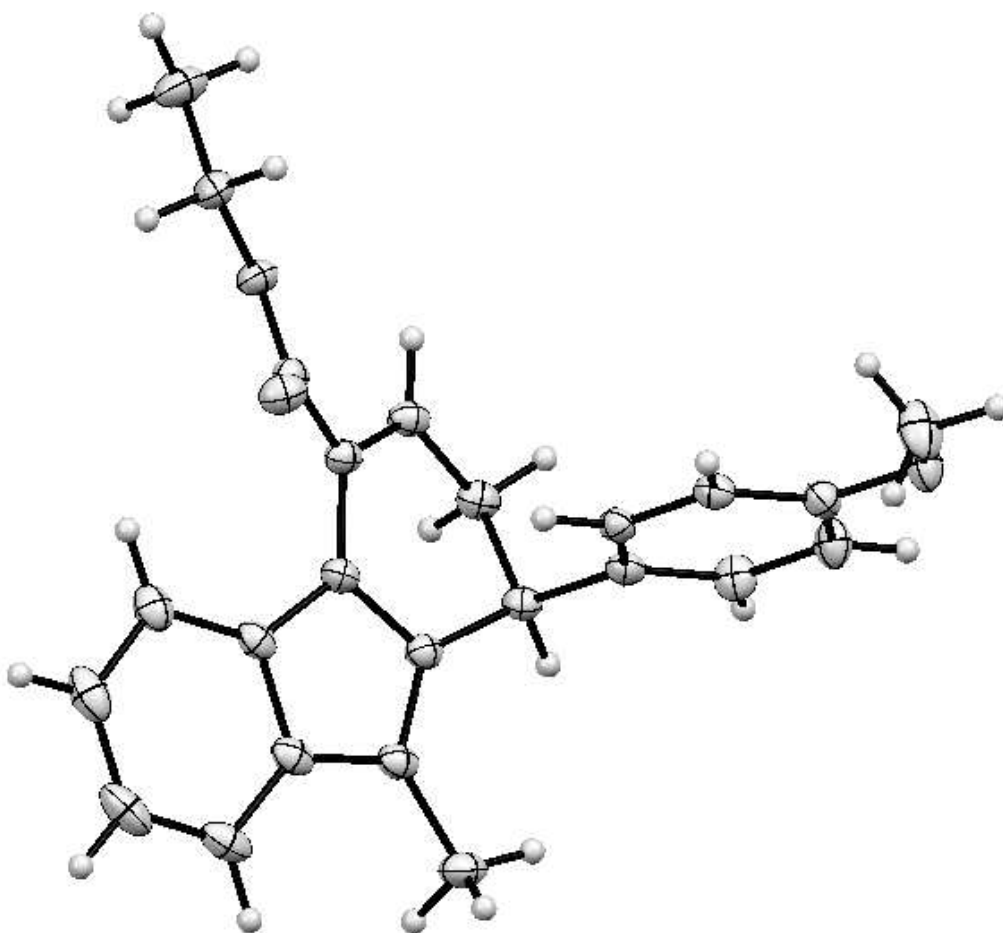
3 X-Ray Analysis

3.1 Compound 3a

Suitable crystal for X-ray analysis were obtained by liquid/liquid diffusion at room temperature using CH_2Cl_2 as the first solvent and hexane as the solvent for perform the diffusion (aprox. 7 days). Compound **3a** is completely soluble in the first one but insoluble in the second one.



3a



ORTEP for **3a**

Figure S2. Crystal structure determination of **3a** and ORTEP plot at 50% probability

Crystal Data for $C_{23}H_{23}NO_3$ ($M = 361.42$ g/mol): monoclinic, space group P2₁/n (no. 14), $a = 8.87178(12)$ Å, $b = 11.07423(15)$ Å, $c = 19.5230(3)$ Å, $\beta = 92.1583(13)^\circ$, $V = 1916.73(5)$ Å³, $Z = 4$, $T = 293(2)$ K, $\mu(\text{CuK}\alpha) = 0.661$ mm⁻¹, $D_{\text{calc}} = 1.252$ g/cm³, 23713 reflections measured ($9.06^\circ \leq 2\Theta \leq 152.9^\circ$), 3972 unique ($R_{\text{int}} = 0.0329$, $R_{\text{sigma}} = 0.0191$) which were used in all calculations. The final R_1 was 0.0541 ($>2\sigma(I)$) and wR_2 was 0.1614 (all data).

Instrumentation: Intensity data were collected on an Agilent Technologies Super-Nova diffractometer, which was equipped with monochromated Cu $k\alpha$ radiation ($\lambda = 1.54184$ Å) and Atlas CCD detector. Measurement was carried out at 150.01(10) K with the help of an Oxford Cryostream 700 PLUS temperature device.

Table S1. Crystal data and structure refinement for 3a

Identification code	a2015395_AL170
Empirical formula	$C_{23}H_{23}NO_3$
Formula weight	361.42
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2 ₁ /n
$a/\text{Å}$	8.87178(12)
$b/\text{Å}$	11.07423(15)
$c/\text{Å}$	19.5230(3)
$\alpha/^\circ$	90
$\beta/^\circ$	92.1583(13)
$\gamma/^\circ$	90
Volume/Å ³	1916.73(5)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.252
μ/mm^{-1}	0.661
$F(000)$	768.0
Crystal size/mm ³	$0.29 \times 0.1786 \times 0.1548$
Radiation	CuK α ($\lambda = 1.54184$)
2Θ range for data collection/ $^\circ$	9.06 to 152.9
Index ranges	$-11 \leq h \leq 10, -13 \leq k \leq 13, -24 \leq l \leq 24$
Reflections collected	23713
Independent reflections	3972 [$R_{\text{int}} = 0.0329, R_{\text{sigma}} = 0.0451$]
Data/restraints/parameters	3972/0/248
Goodness-of-fit on F^2	1.040
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0330, wR_2 = 0.0817$
Final R indexes [all data]	$R_1 = 0.0370, wR_2 = 0.0846$

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
O1	1787.3(9)	6795.9(7)	994.2(4)	25.72(18)
O2	350.5(8)	8212.1(7)	462.4(4)	22.58(17)
O3	-1751.1(9)	6778.8(7)	4423.1(4)	27.96(19)
N1	3081.9(9)	8700.8(8)	1837.1(4)	19.97(19)
C1	1694.7(11)	8783.1(9)	1464.9(5)	19.8(2)
C2	653.2(11)	9576.9(9)	1654.5(5)	21.2(2)
C3	937.9(12)	10410.3(9)	2250.5(5)	22.3(2)
C4	1939.1(11)	9789.1(9)	2816.1(5)	19.8(2)
C5	3271.4(11)	9214.7(9)	2494.6(5)	19.5(2)
C6	4730.0(12)	9076.9(9)	2726.2(5)	21.4(2)
C7	5510.2(12)	8465.6(9)	2194.7(6)	22.2(2)
C8	7009.9(12)	8090.2(10)	2147.4(7)	28.2(2)
C9	7438.3(13)	7533.6(10)	1552.8(7)	33.1(3)
C10	6405.6(14)	7369.5(10)	1000.4(7)	32.4(3)
C11	4915.2(13)	7735.6(10)	1028.6(6)	26.0(2)
C12	4472.1(12)	8258.0(9)	1640.5(6)	21.1(2)
C13	1321.1(11)	7818.2(9)	954.6(5)	20.5(2)
C14	-170.4(12)	7287.3(10)	-22.6(5)	24.6(2)
C15	-1228.5(15)	7889.3(12)	-535.9(6)	34.5(3)
C16	1018.7(11)	8915.0(9)	3234.3(5)	19.3(2)
C17	826.7(11)	7701.2(9)	3072.3(5)	19.3(2)
C18	-68.9(11)	6941.9(9)	3460.1(5)	20.2(2)
C19	-805.9(11)	7417.4(9)	4016.3(5)	21.5(2)
C20	-617.0(13)	8629.3(10)	4190.0(6)	26.9(2)
C21	286.7(13)	9363.3(10)	3803.6(6)	25.2(2)
C22	-1869.9(16)	5519.8(11)	4310.6(7)	37.8(3)
C23	5443.9(13)	9476.4(11)	3393.7(6)	28.2(2)

Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 22a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	28.9(4)	20.6(4)	27.2(4)	1.5(3)	-5.1(3)	-0.4(3)
O2	24.5(4)	24.1(4)	18.8(4)	0.7(3)	-4.3(3)	-0.8(3)
O3	30.3(4)	23.2(4)	31.2(4)	-0.8(3)	11.3(3)	-3.1(3)
N1	16.7(4)	21.9(4)	21.2(4)	-0.1(3)	-0.7(3)	-0.2(3)
C1	19.3(5)	20.3(5)	19.6(5)	4.3(4)	-2.2(4)	-2.9(4)
C2	19.4(5)	20.2(5)	23.8(5)	4.5(4)	-3.4(4)	-1.3(4)
C3	21.7(5)	18.4(5)	26.7(5)	1.7(4)	-1.6(4)	0.7(4)
C4	18.7(5)	19.0(5)	21.6(5)	-1.0(4)	-1.4(4)	-1.3(4)
C5	19.5(5)	18.8(5)	20.0(5)	2.4(4)	-0.9(4)	-2.8(4)
C6	18.8(5)	20.4(5)	24.9(5)	5.0(4)	-1.8(4)	-3.5(4)
C7	18.6(5)	18.9(5)	29.2(5)	5.9(4)	0.4(4)	-2.4(4)
C8	18.0(5)	23.3(5)	43.2(7)	7.6(5)	-0.6(4)	-2.0(4)
C9	19.2(5)	23.5(6)	57.1(8)	3.9(5)	10.1(5)	0.9(4)
C10	29.6(6)	22.8(5)	45.9(7)	-3.1(5)	15.0(5)	-3.1(4)
C11	26.2(6)	21.0(5)	31.1(6)	-0.3(4)	6.6(4)	-4.1(4)
C12	18.2(5)	18.2(5)	27.2(5)	3.2(4)	3.0(4)	-1.9(4)
C13	19.0(5)	23.0(5)	19.4(5)	3.8(4)	-0.7(4)	-2.5(4)
C14	24.9(5)	28.2(5)	20.3(5)	-3.2(4)	-2.1(4)	-1.7(4)
C15	40.4(7)	35.2(6)	26.7(6)	2.9(5)	-12.2(5)	-4.1(5)
C16	16.8(5)	19.4(5)	21.4(5)	0.4(4)	-1.8(4)	1.1(4)
C17	16.2(5)	21.4(5)	20.1(5)	-2.3(4)	-0.2(4)	2.7(4)
C18	18.8(5)	17.7(5)	23.8(5)	-2.4(4)	-1.1(4)	0.7(4)
C19	19.1(5)	22.4(5)	23.1(5)	1.8(4)	1.7(4)	-0.3(4)
C20	30.8(6)	23.8(5)	26.8(5)	-3.9(4)	8.5(4)	2.5(4)
C21	29.8(6)	17.9(5)	28.2(6)	-3.1(4)	3.1(4)	0.1(4)
C22	44.8(7)	26.6(6)	43.0(7)	-4.5(5)	16.2(6)	-12.9(5)
C23	23.6(5)	31.7(6)	28.8(6)	2.7(5)	-7.0(4)	-4.6(4)

4 NMR spectra

4.1 Acyl-substituted donor-acceptor cyclopropanes (1a-d)

1a

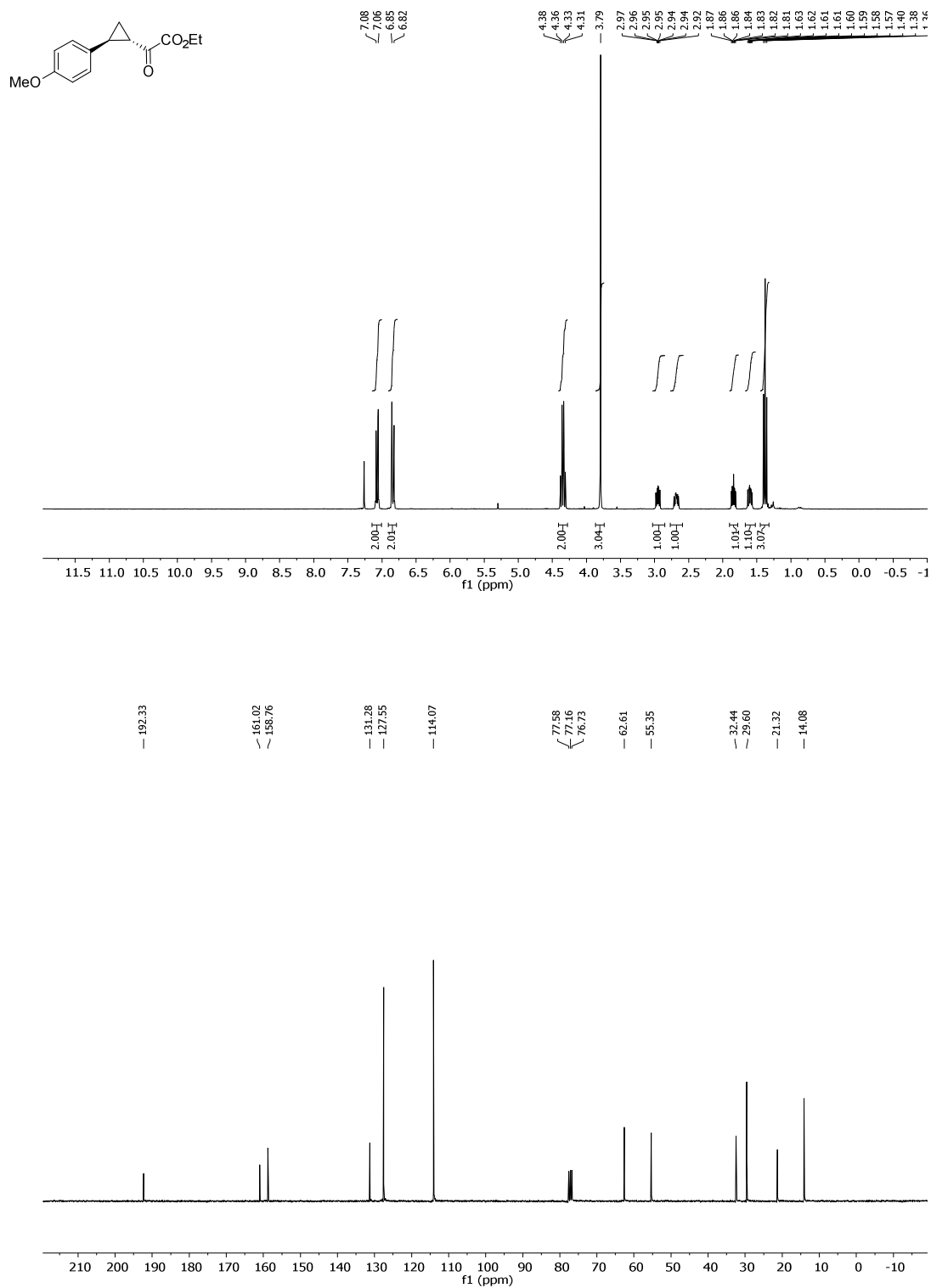


Figure S3. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1a

1b

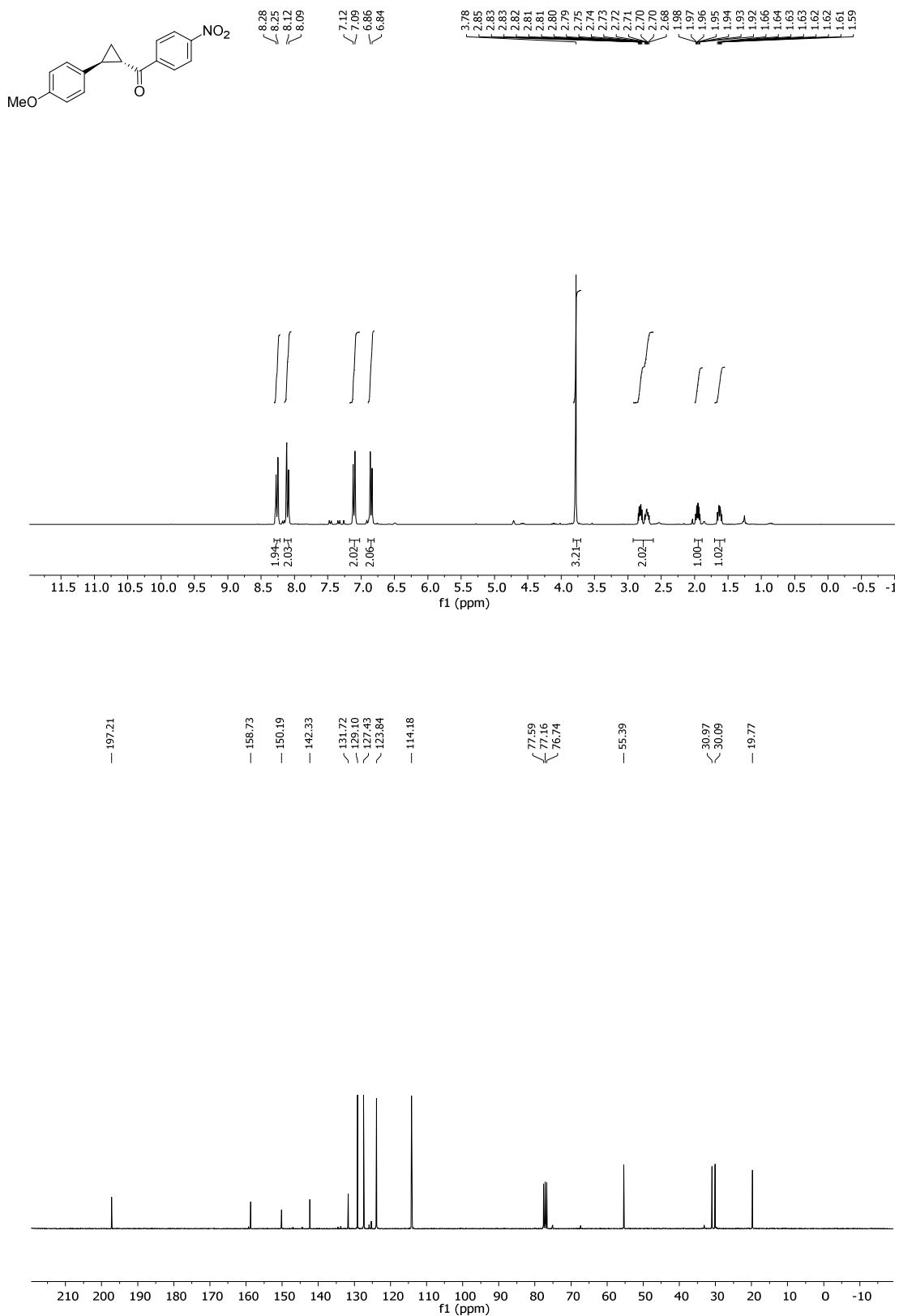


Figure S4. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1b

1c

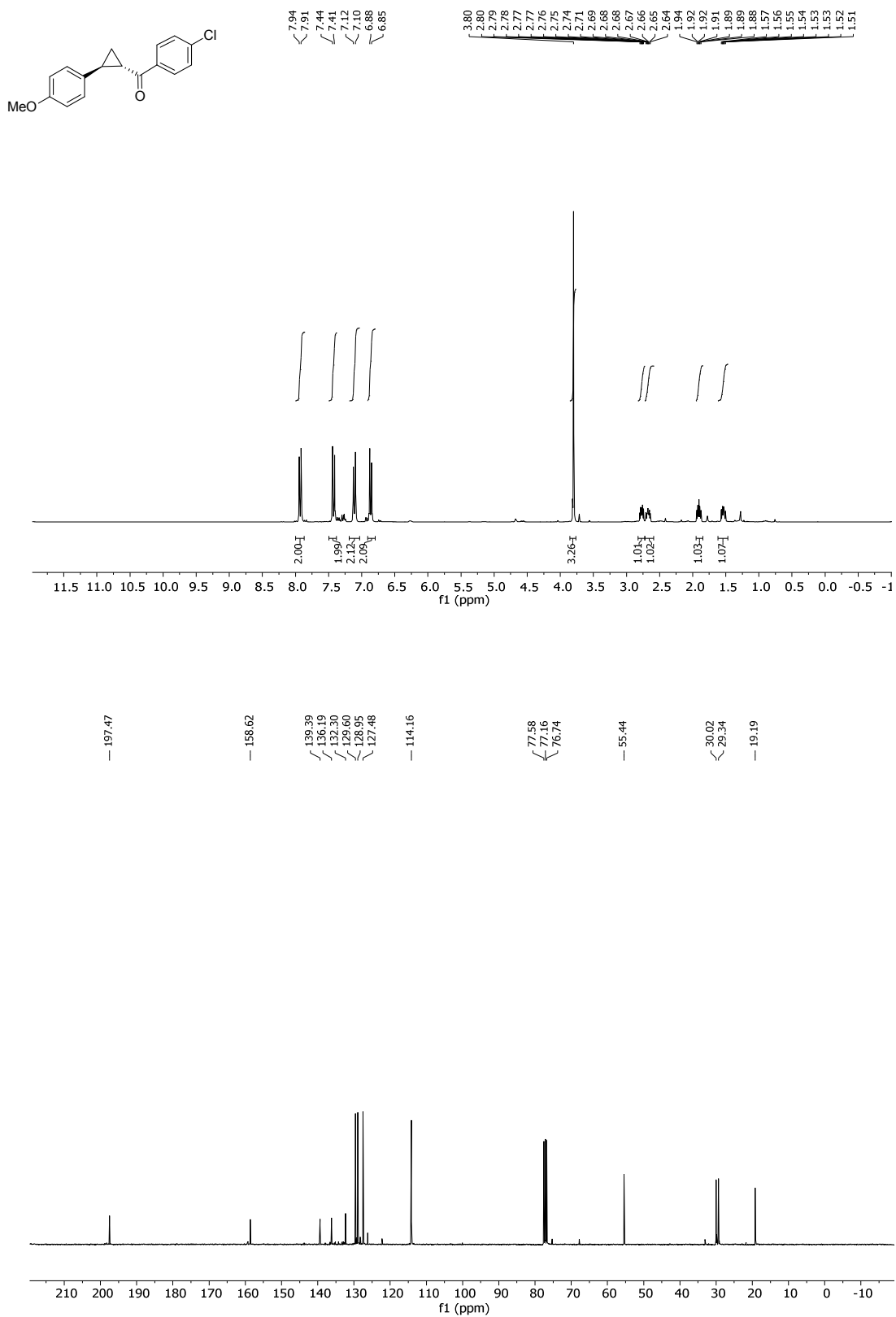


Figure S5. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1c

1d

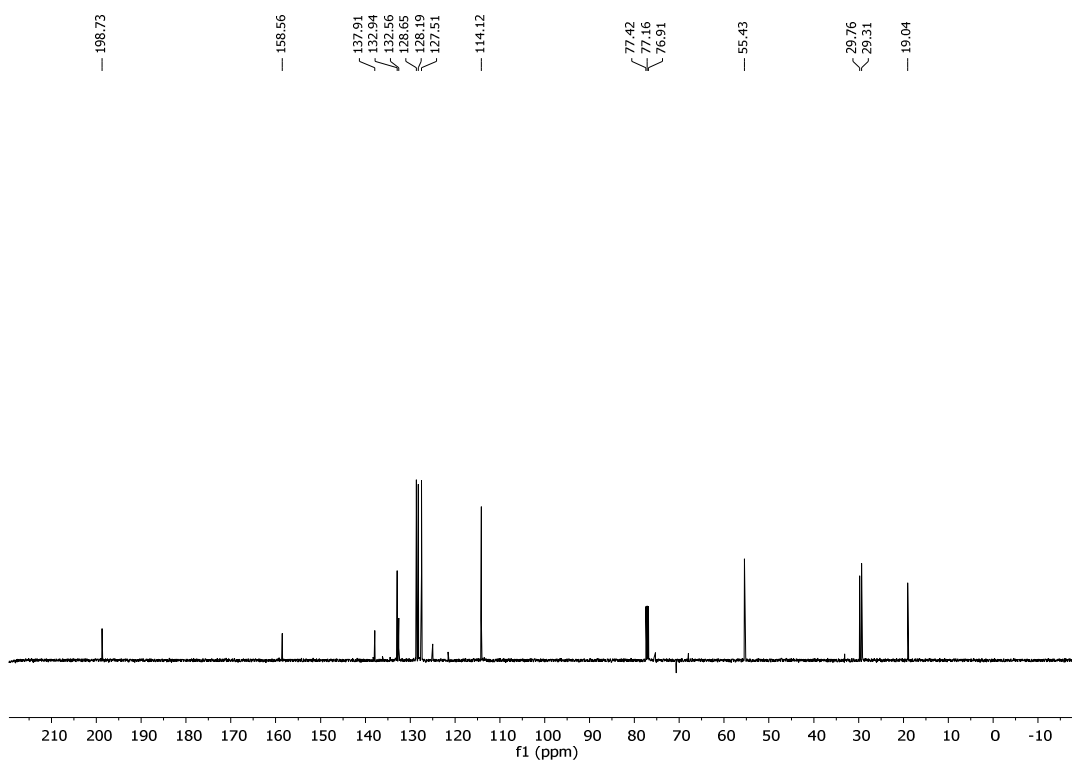
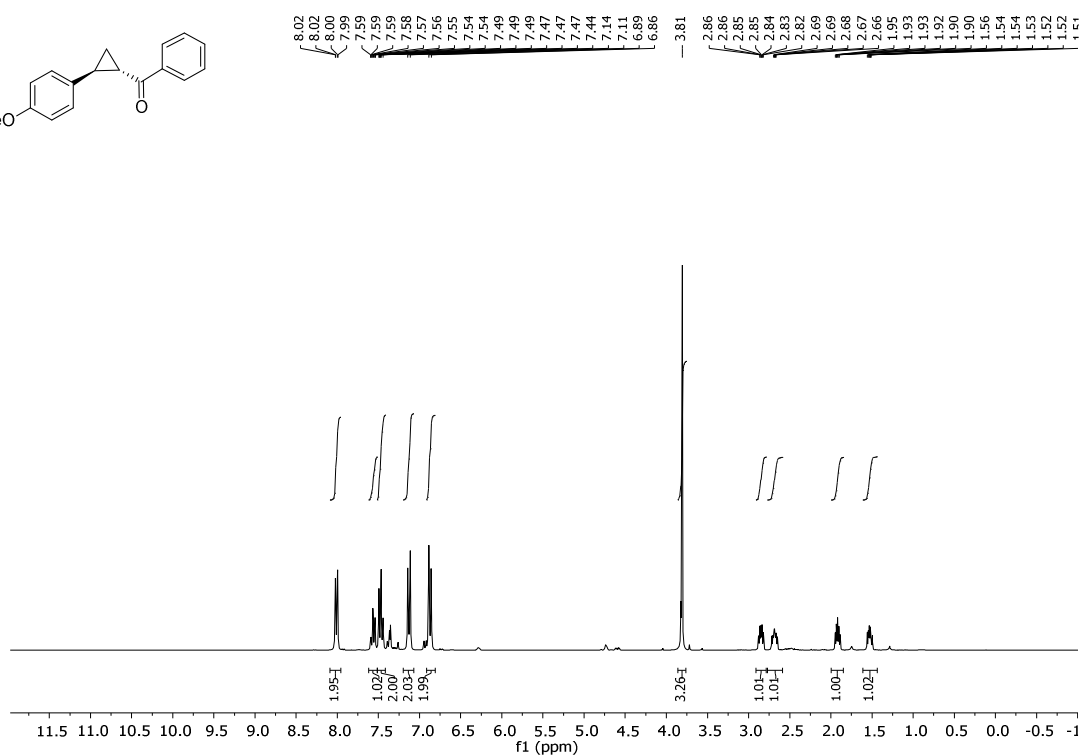
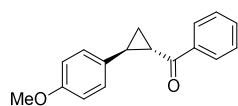


Figure S6. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1d

4.2 Cyclopropanes derived from β -ketoesters (1e-o)

1e

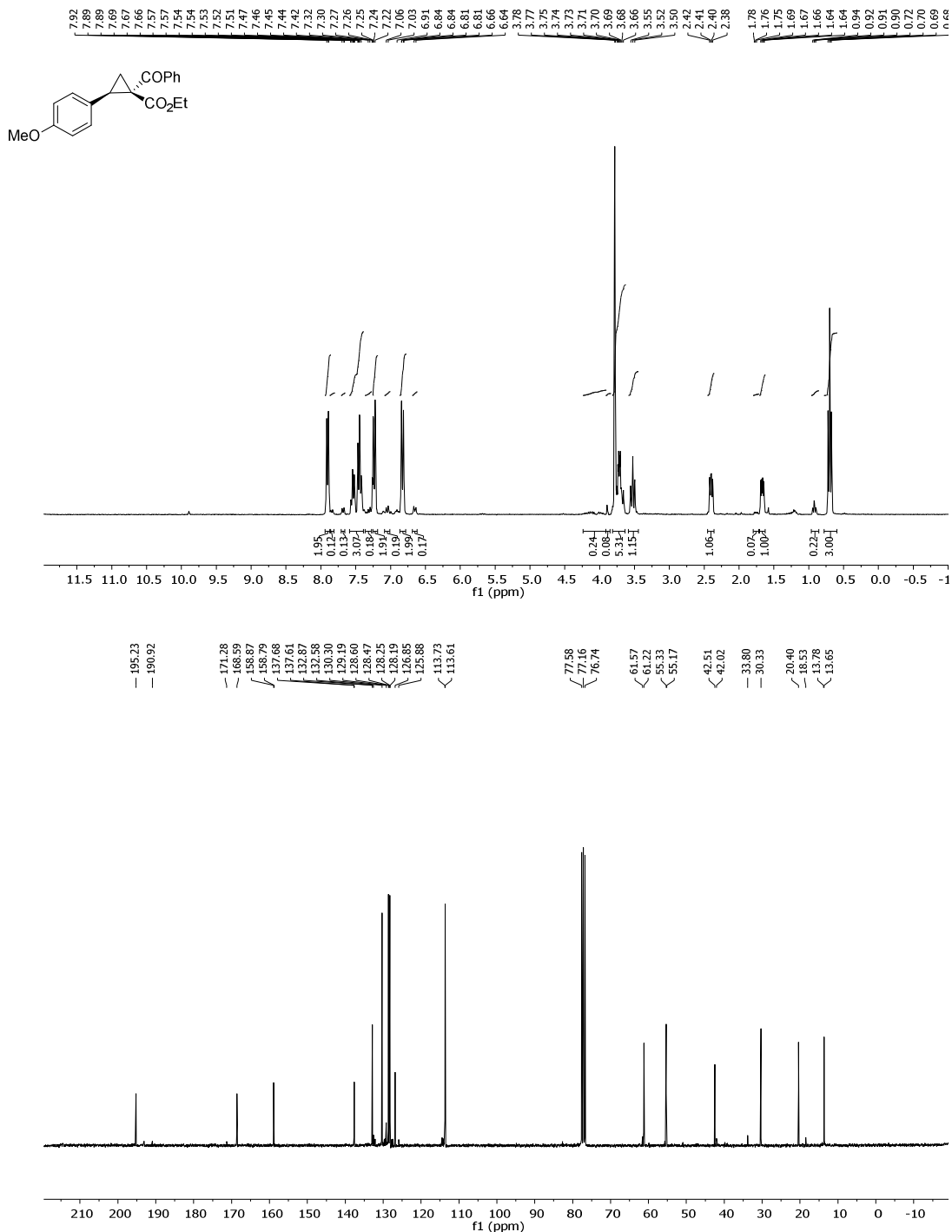


Figure S7. $^1\text{H-NMR}$ (300 MHz, CDCl_3) and $^{13}\text{C-NMR}$ (75 MHz, CDCl_3) spectra of compound 1e

1f

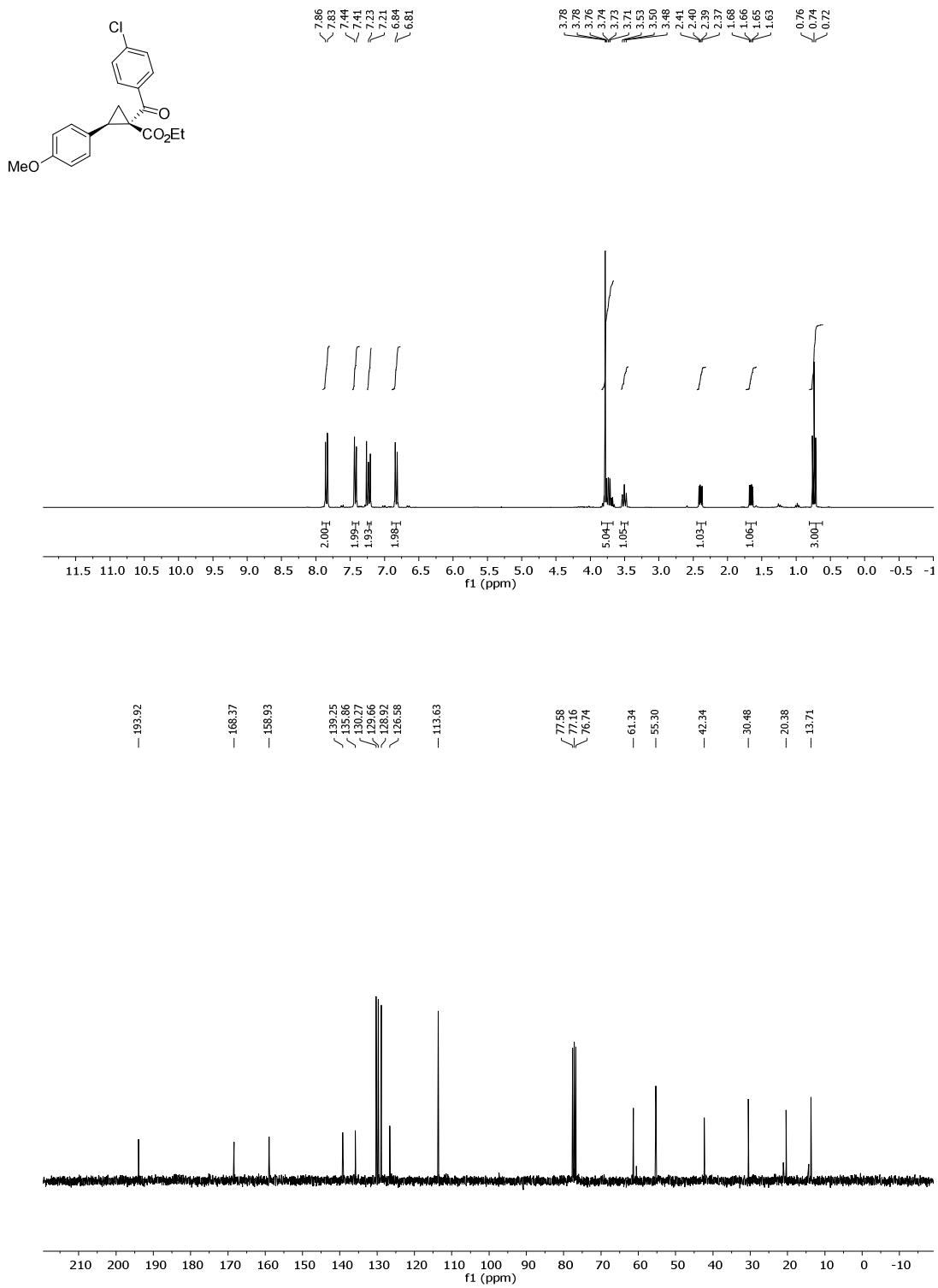


Figure S8. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1f

1g

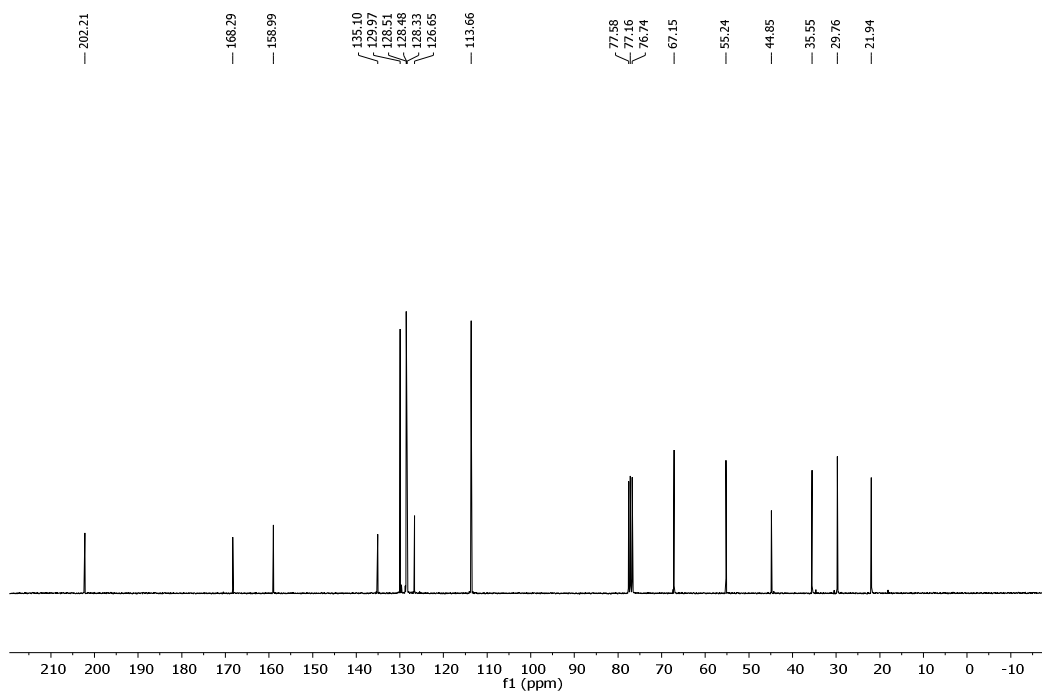
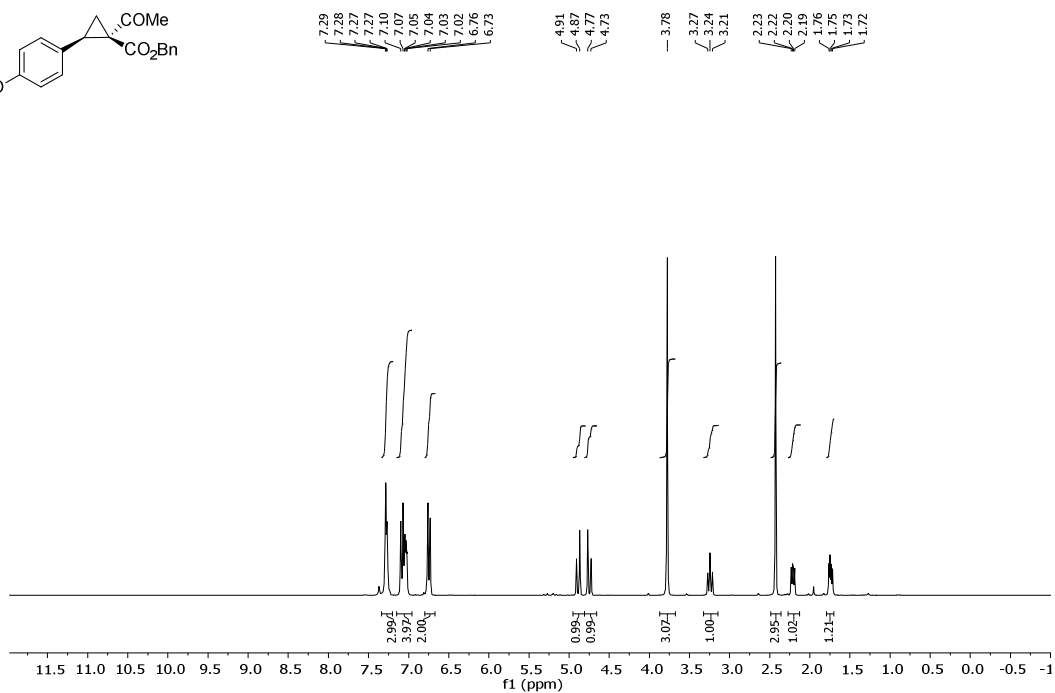
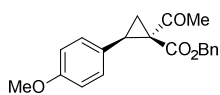


Figure S9. $^1\text{H-NMR}$ (300 MHz, CDCl_3) and $^{13}\text{C-NMR}$ (75 MHz, CDCl_3) spectra of compound **1g**

1h

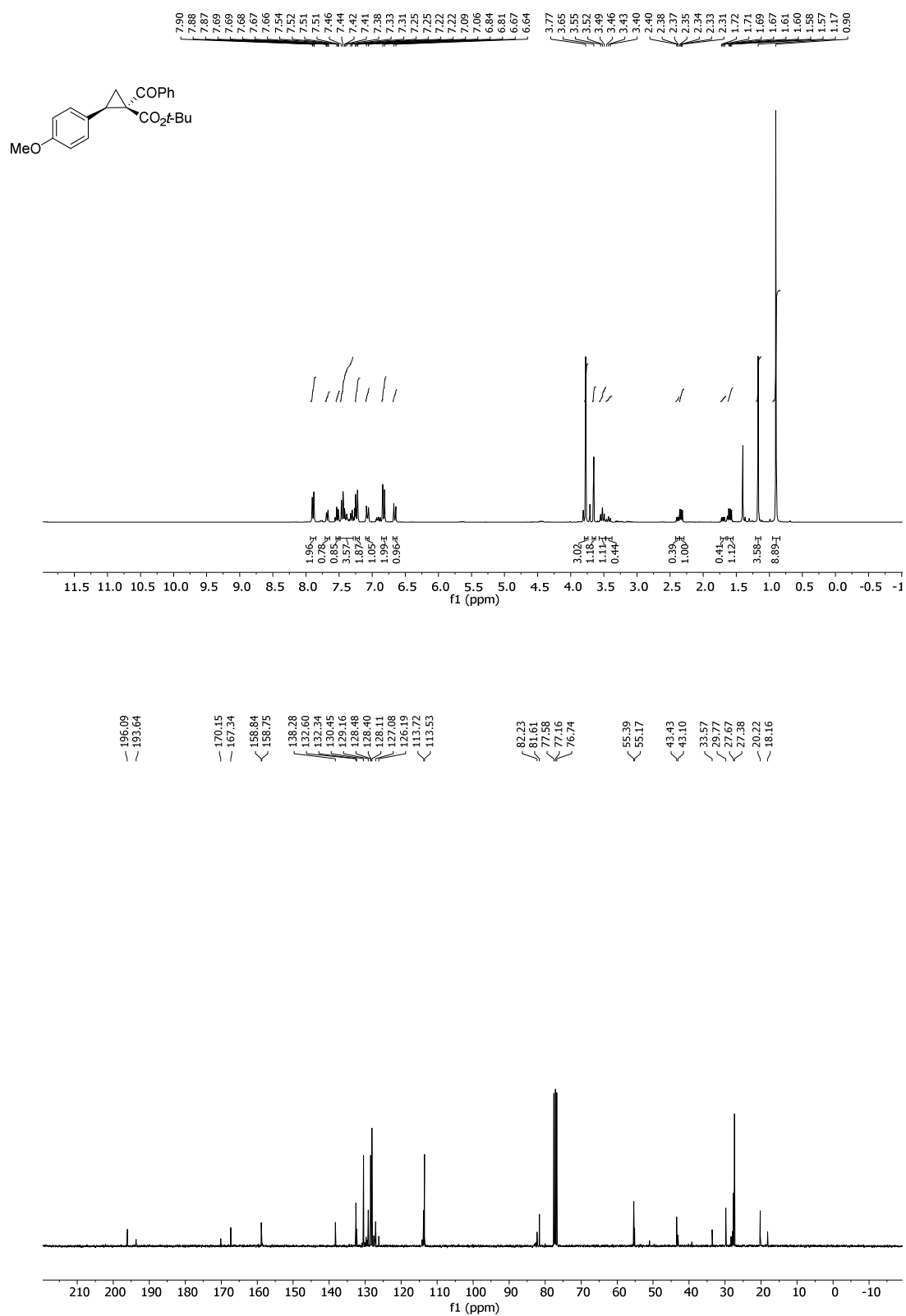


Figure S10. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1h

1i

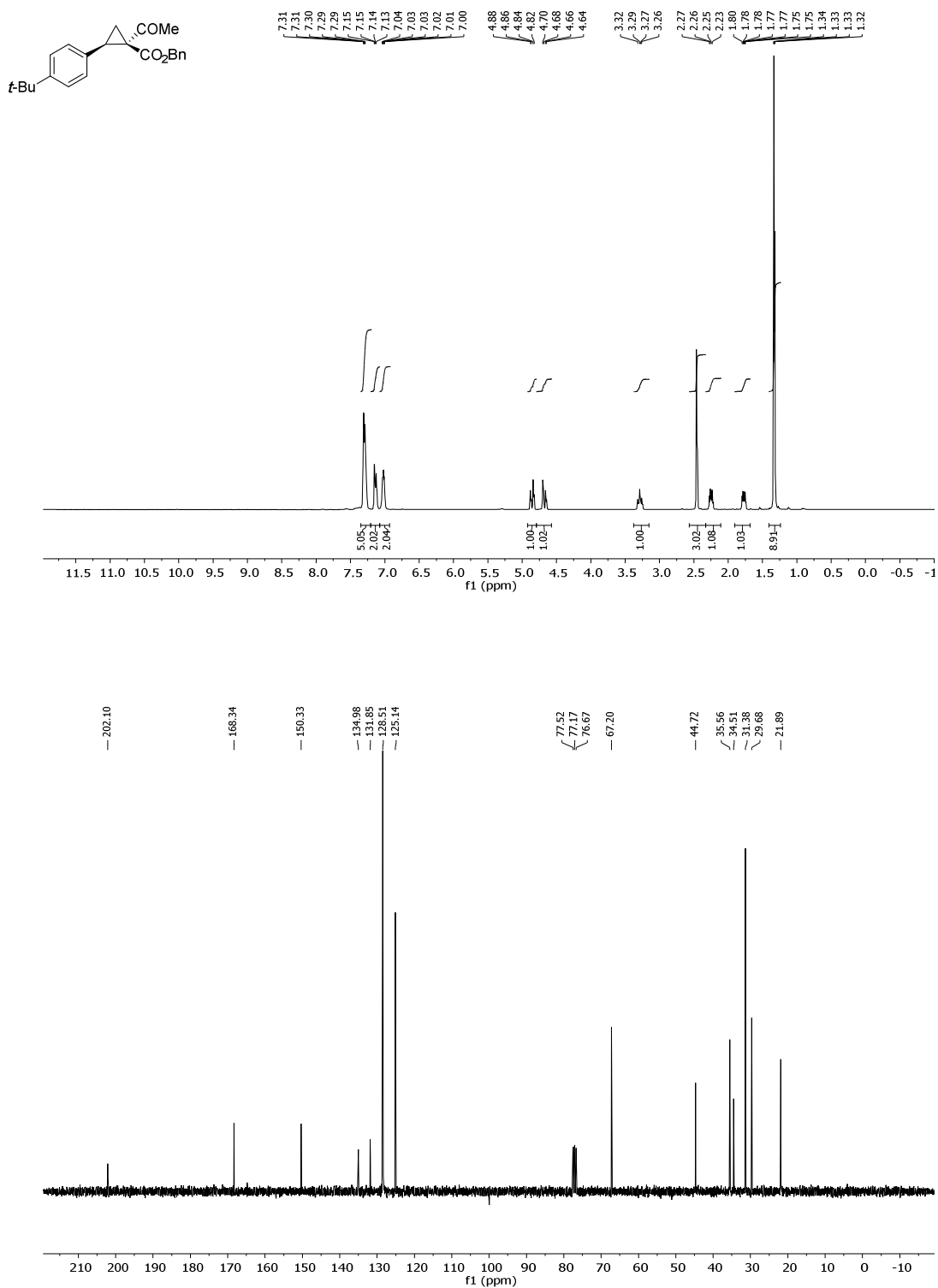


Figure S11. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1i

1j

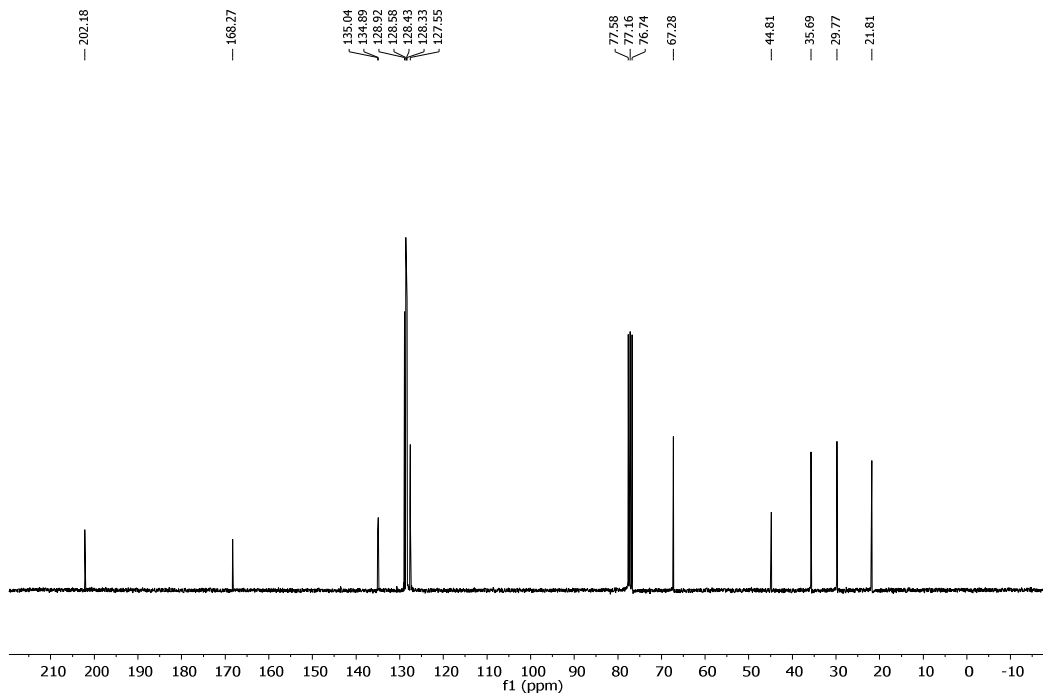
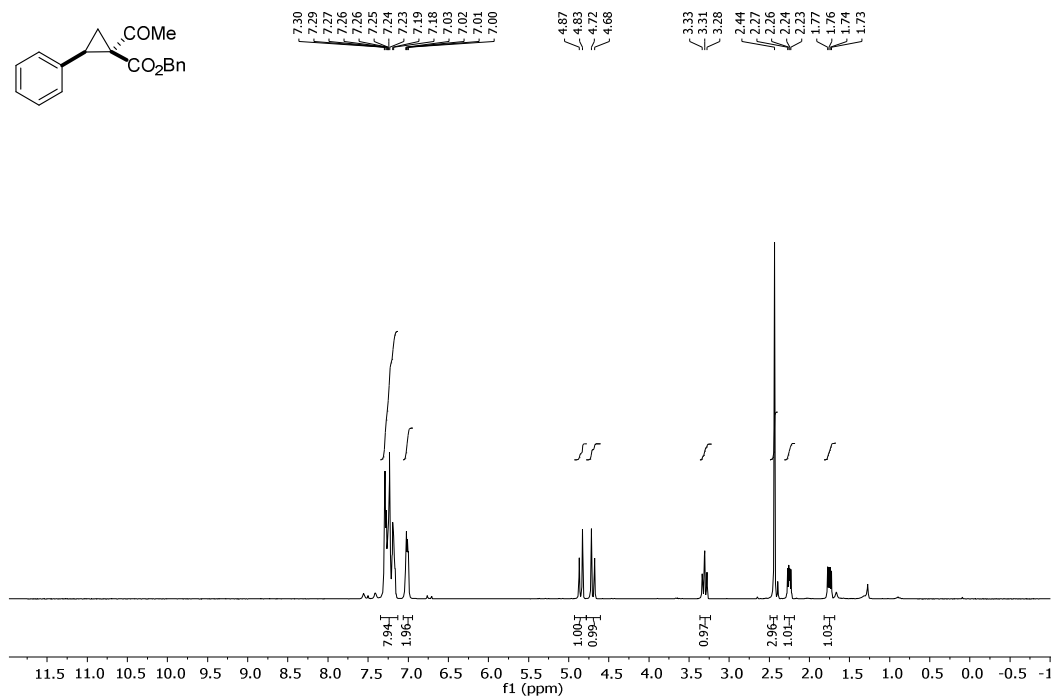
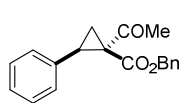


Figure S12. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1j

1k

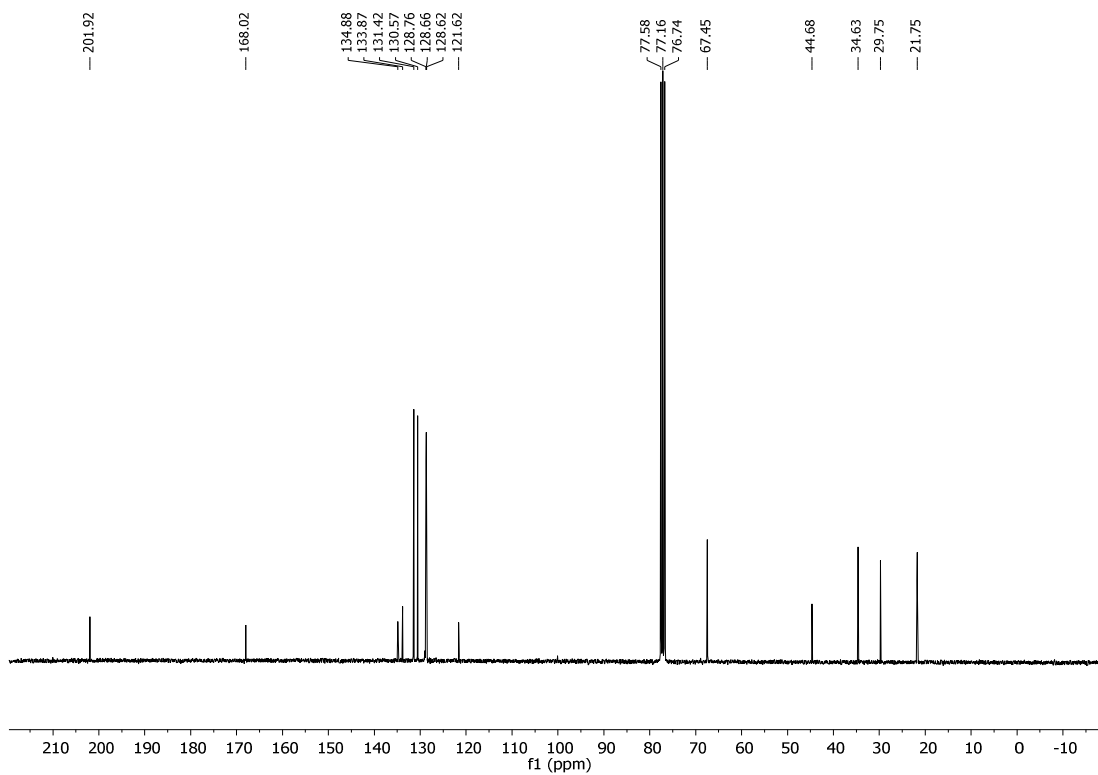
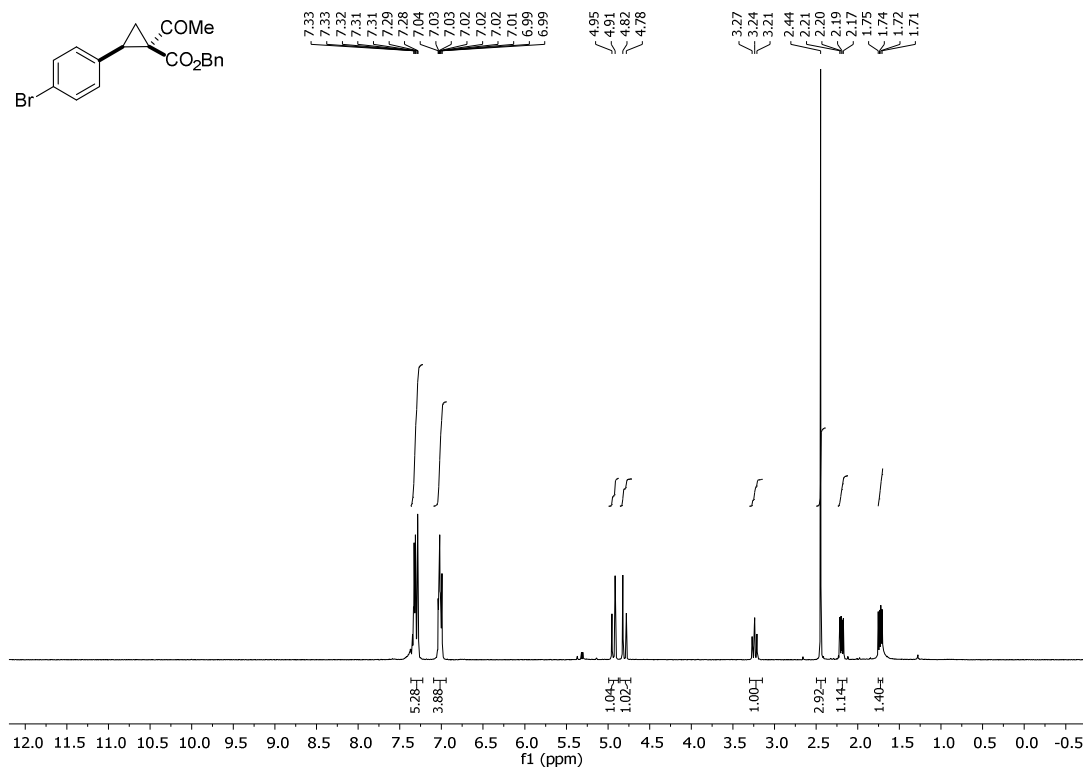
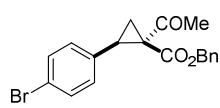


Figure S13. $^1\text{H-NMR}$ (300 MHz, CDCl_3) and $^{13}\text{C-NMR}$ (75 MHz, CDCl_3) spectra of compound 1k

11

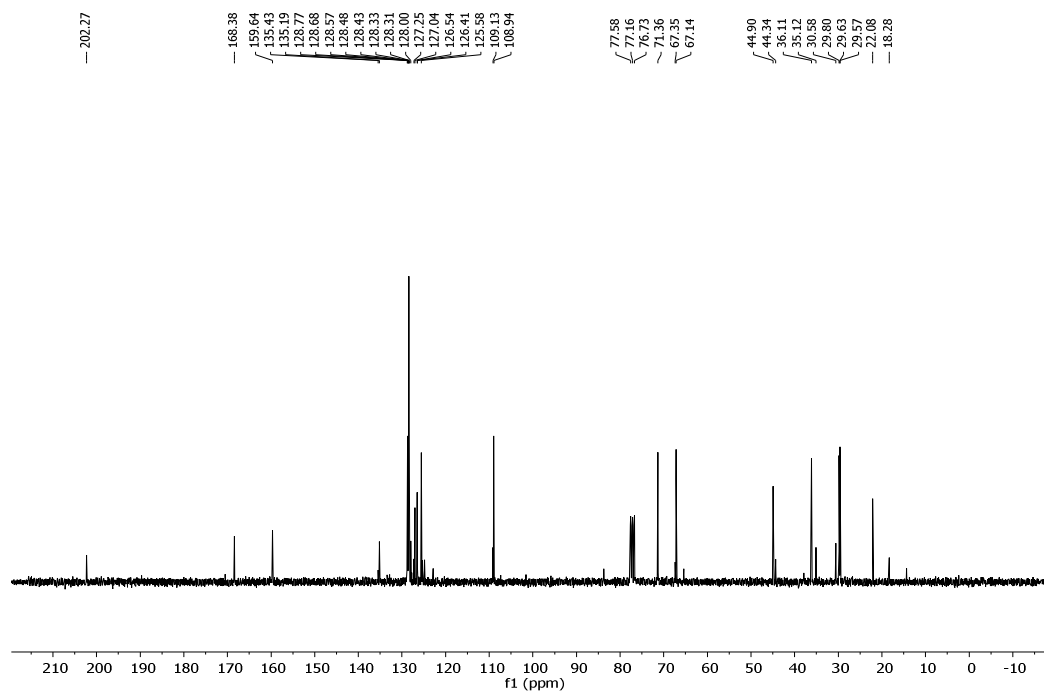
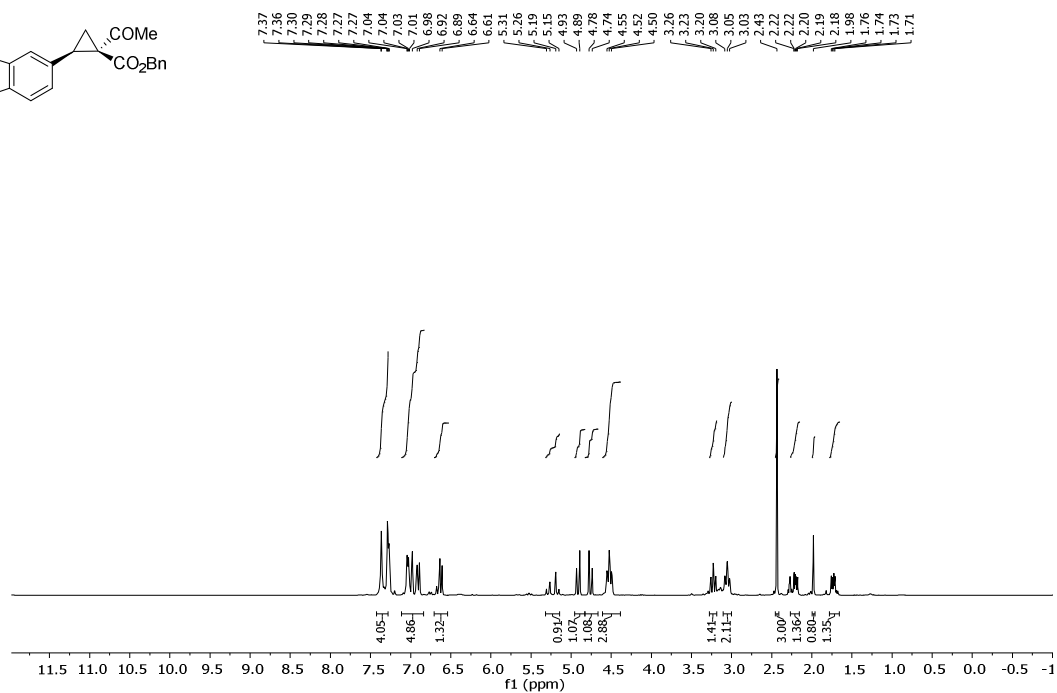
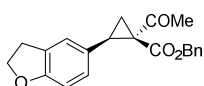


Figure S14. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 11

1m

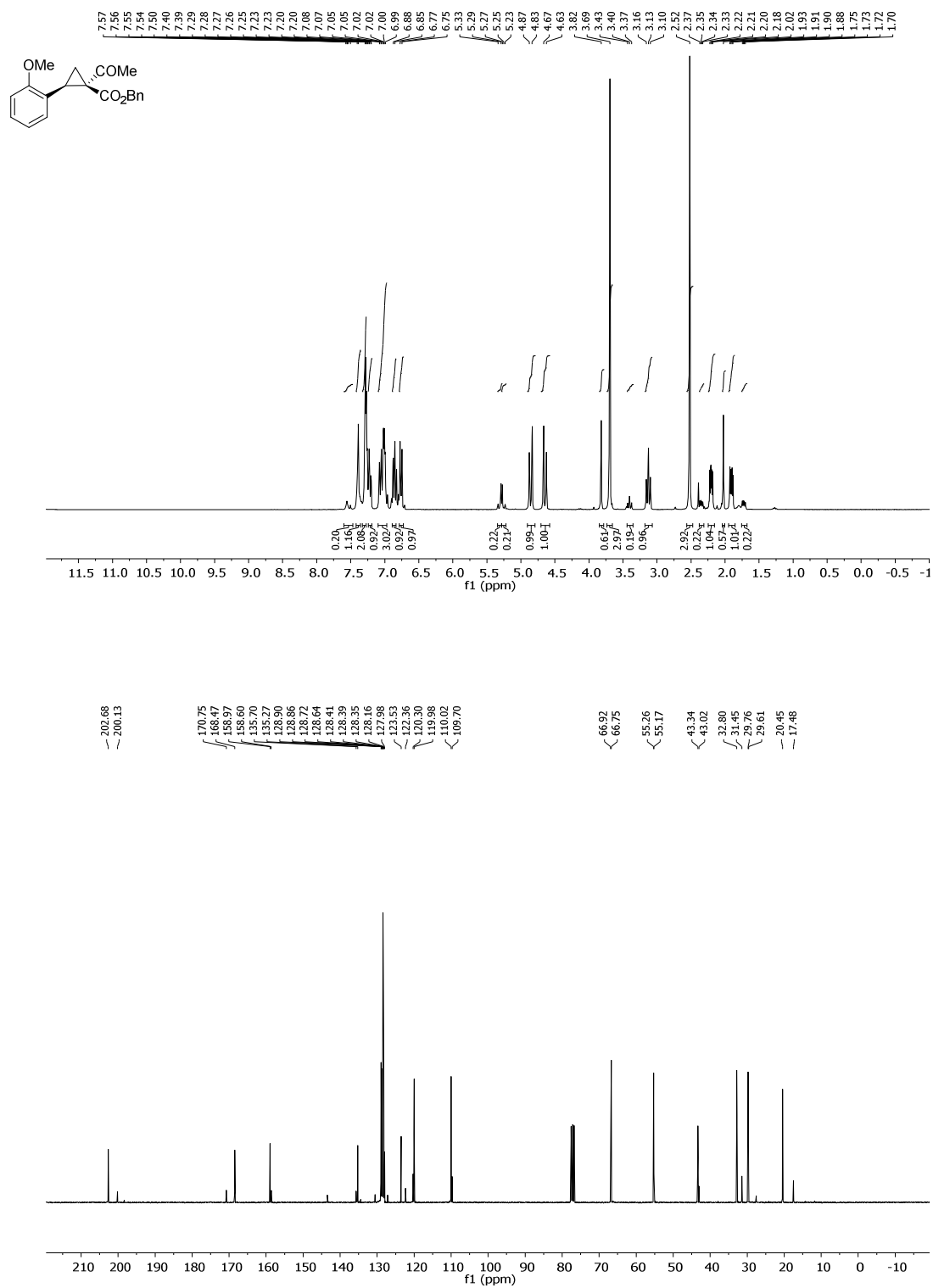


Figure S15. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1m

1n

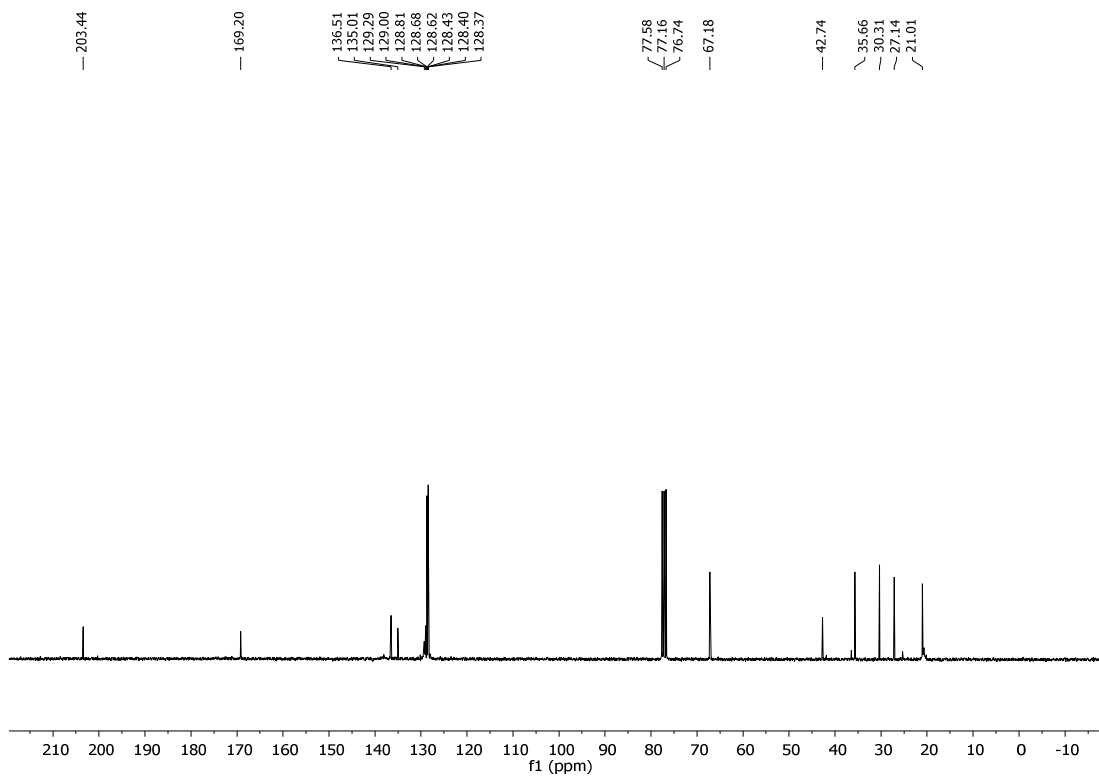
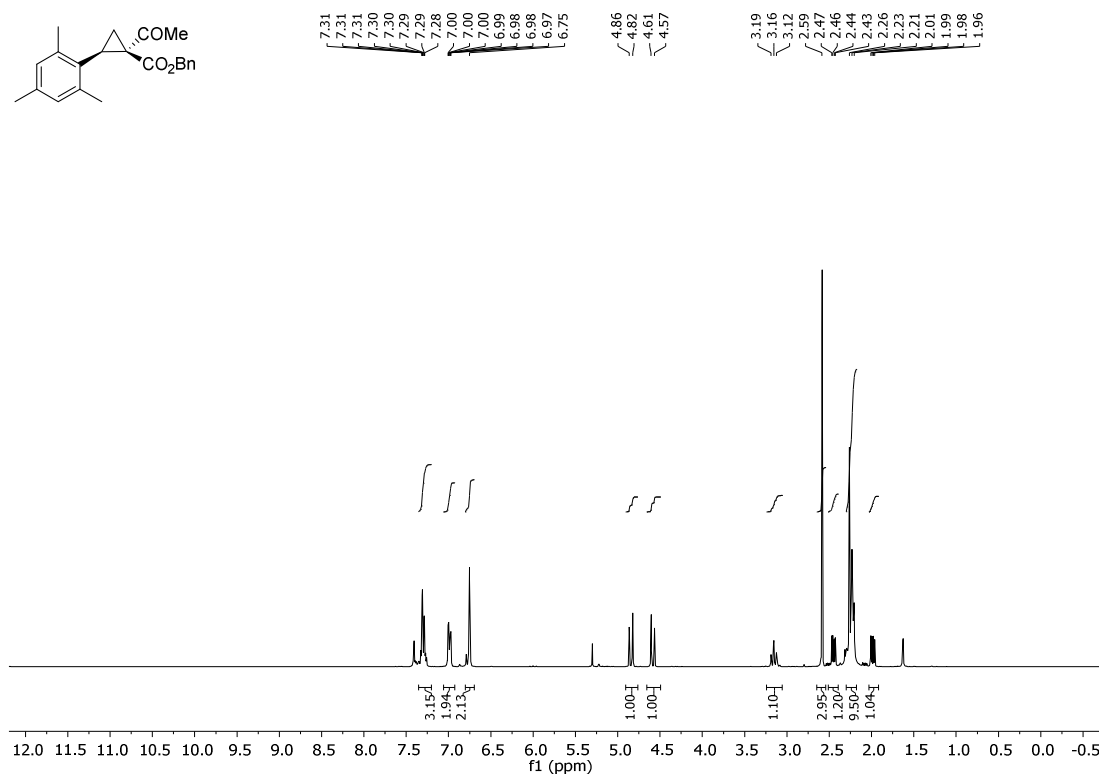
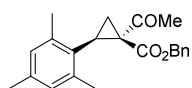


Figure S16. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1n

1o

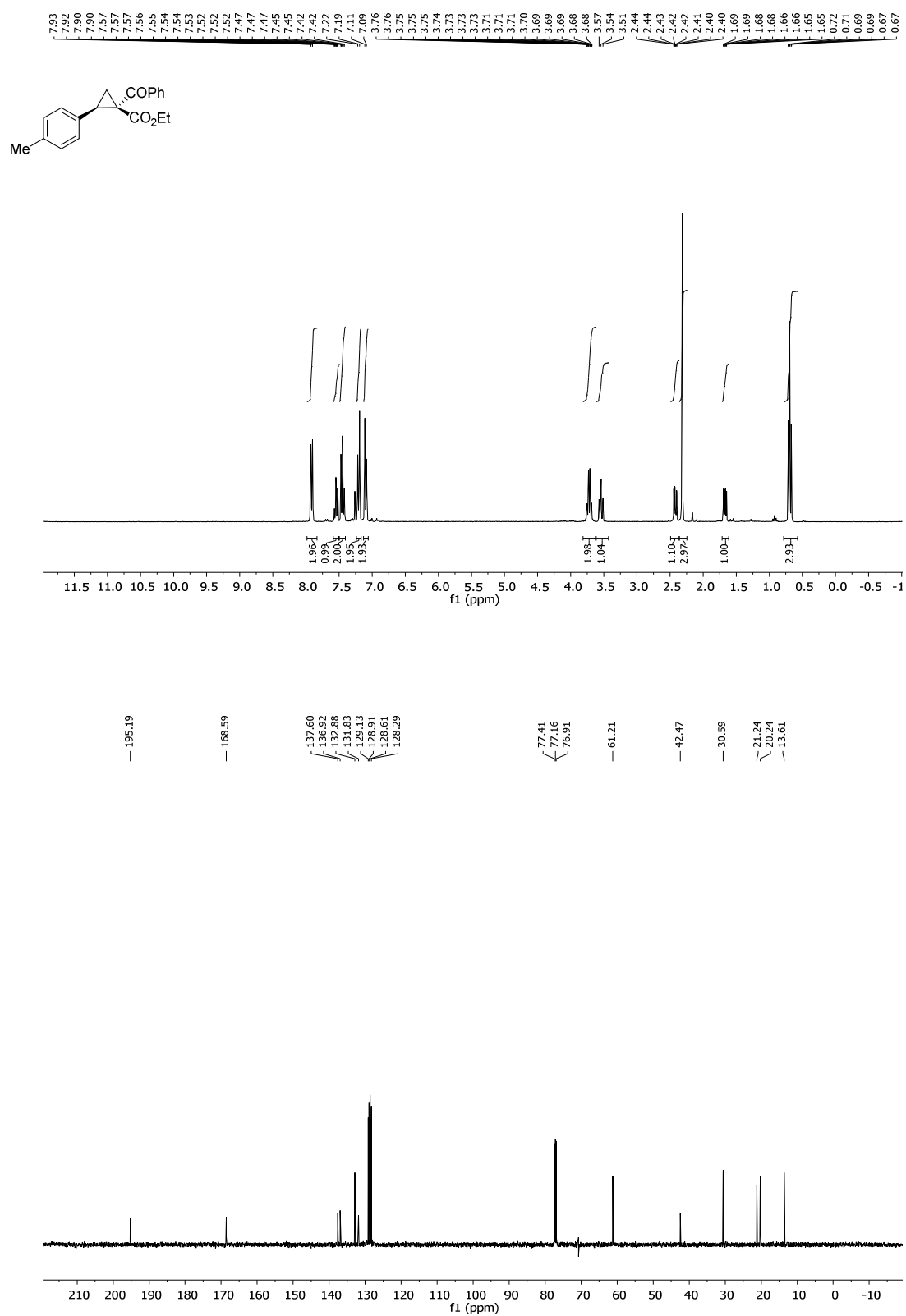


Figure S17. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 1o

4.3 Dihydropyridindoindoles 3 and 4

3a

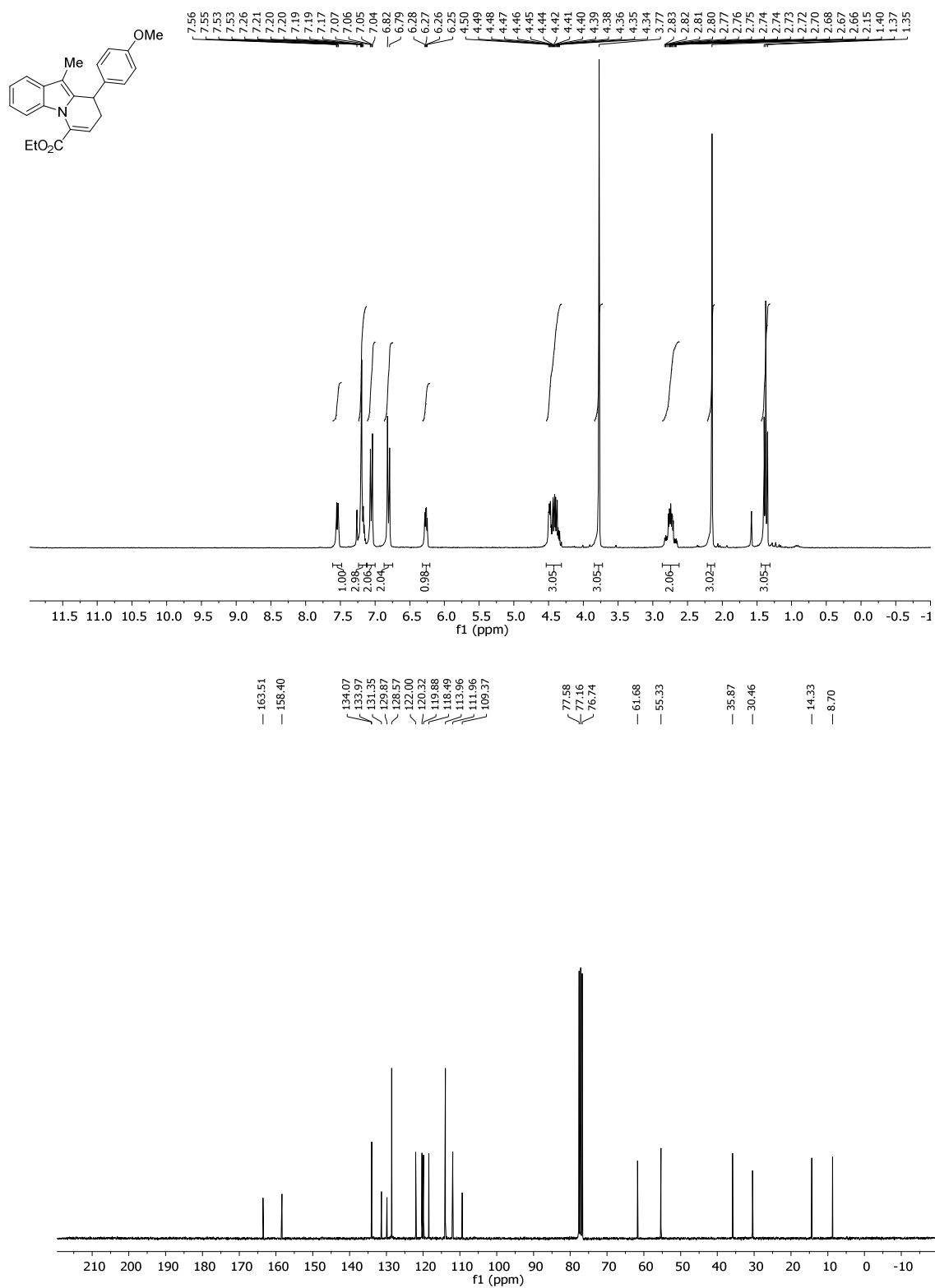


Figure S18. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3a

4a

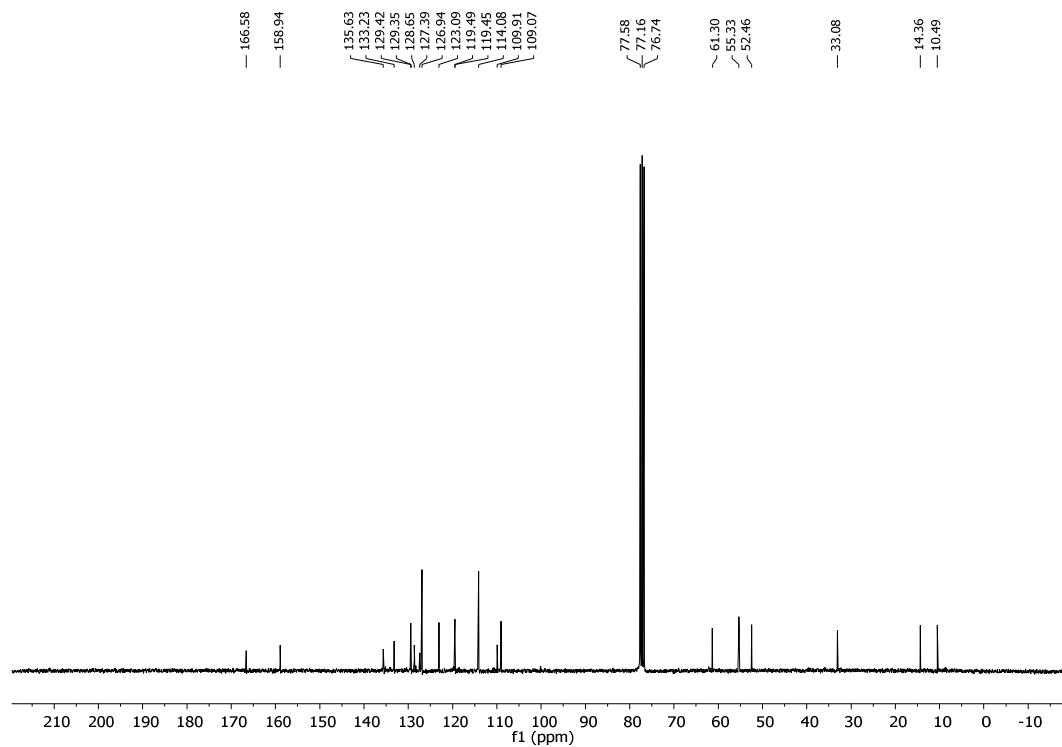
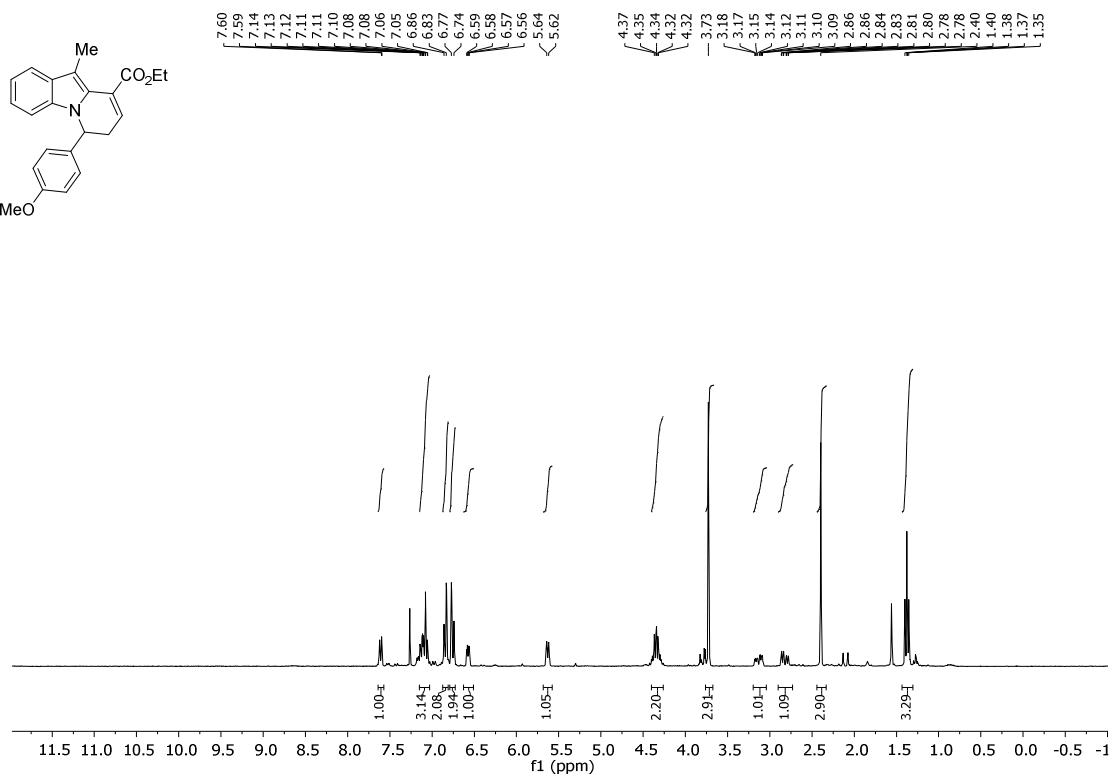
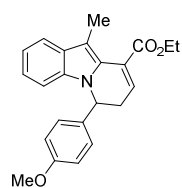


Figure S19. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4a

3b

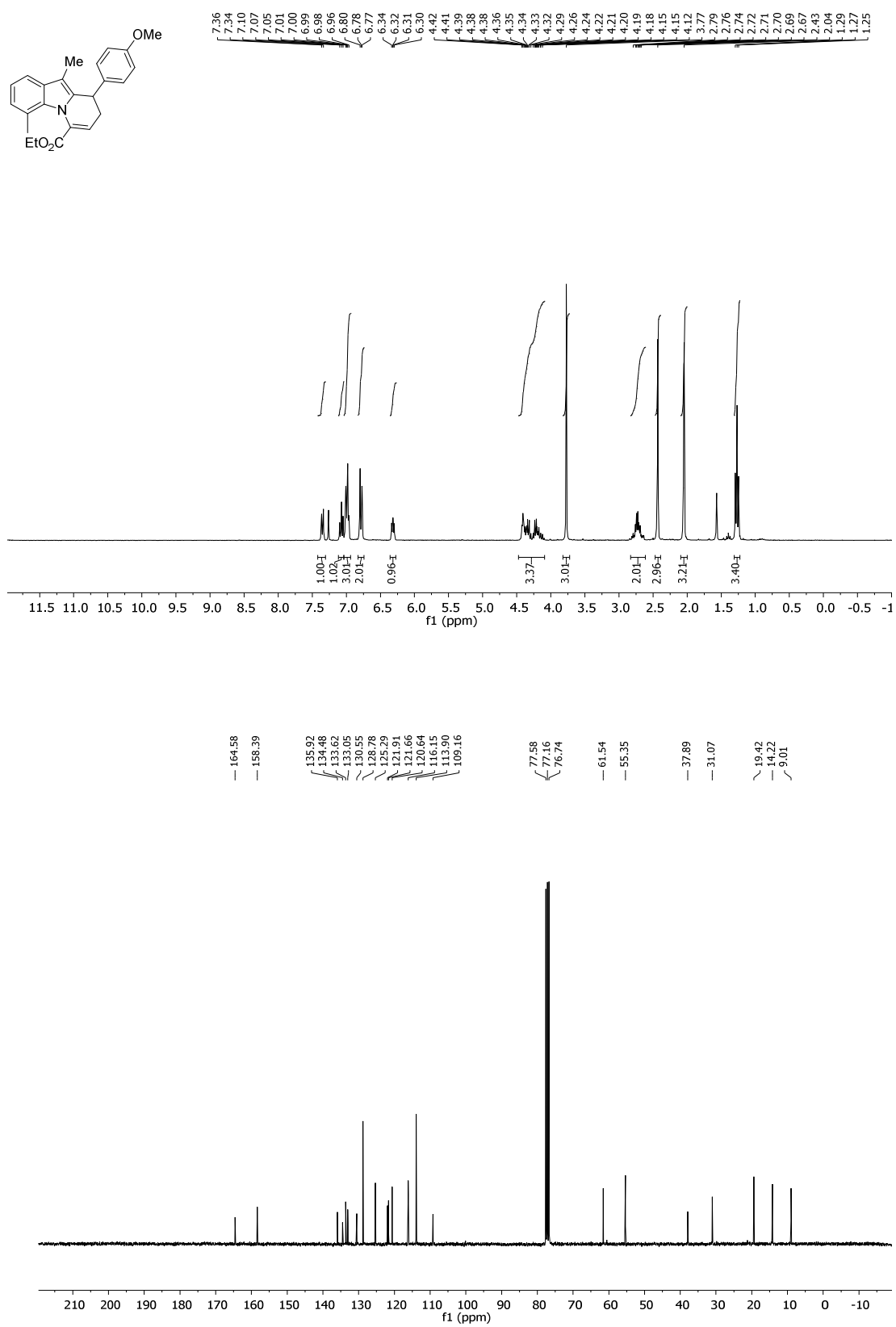


Figure S20. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3b

4b

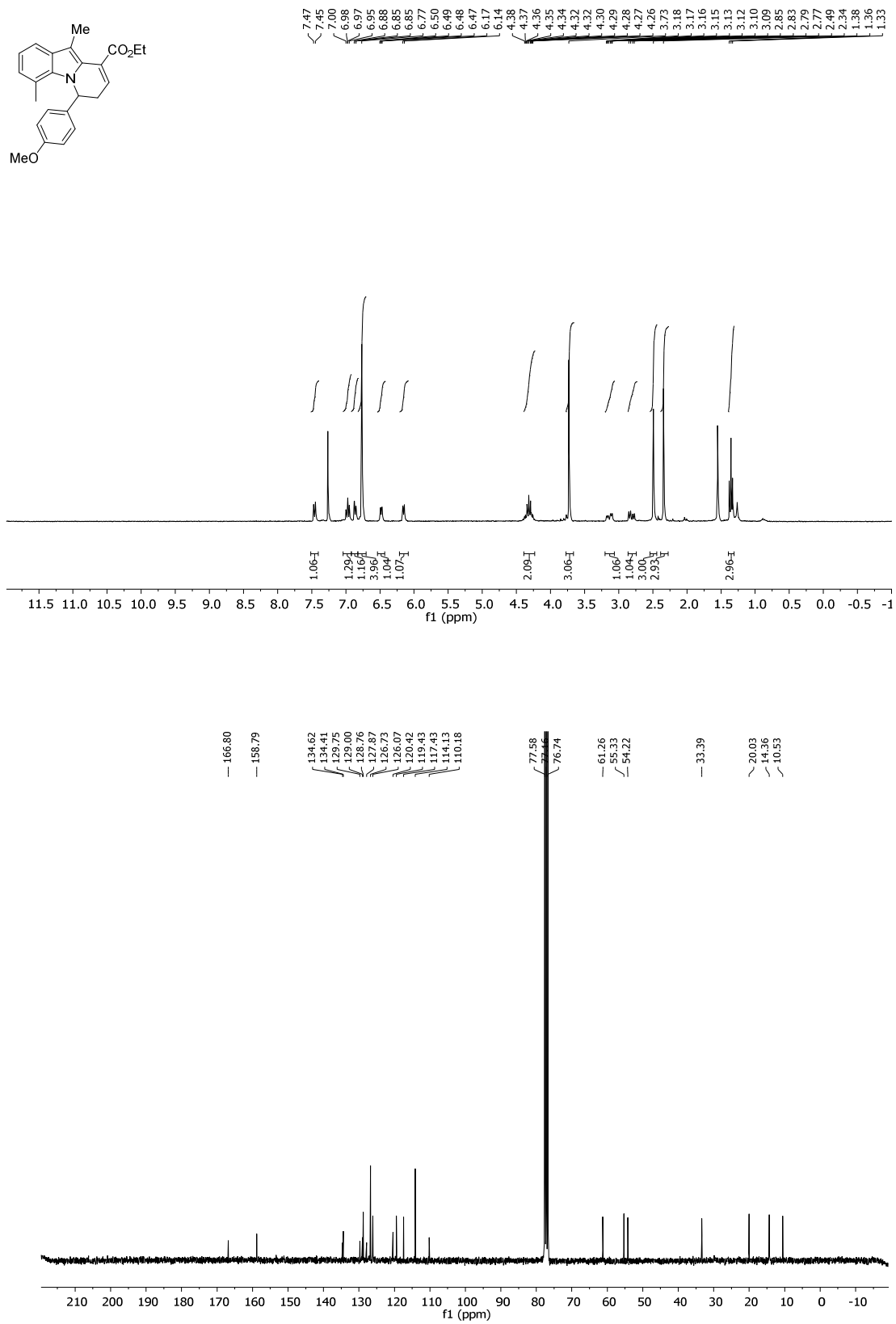


Figure S21. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4b

3c

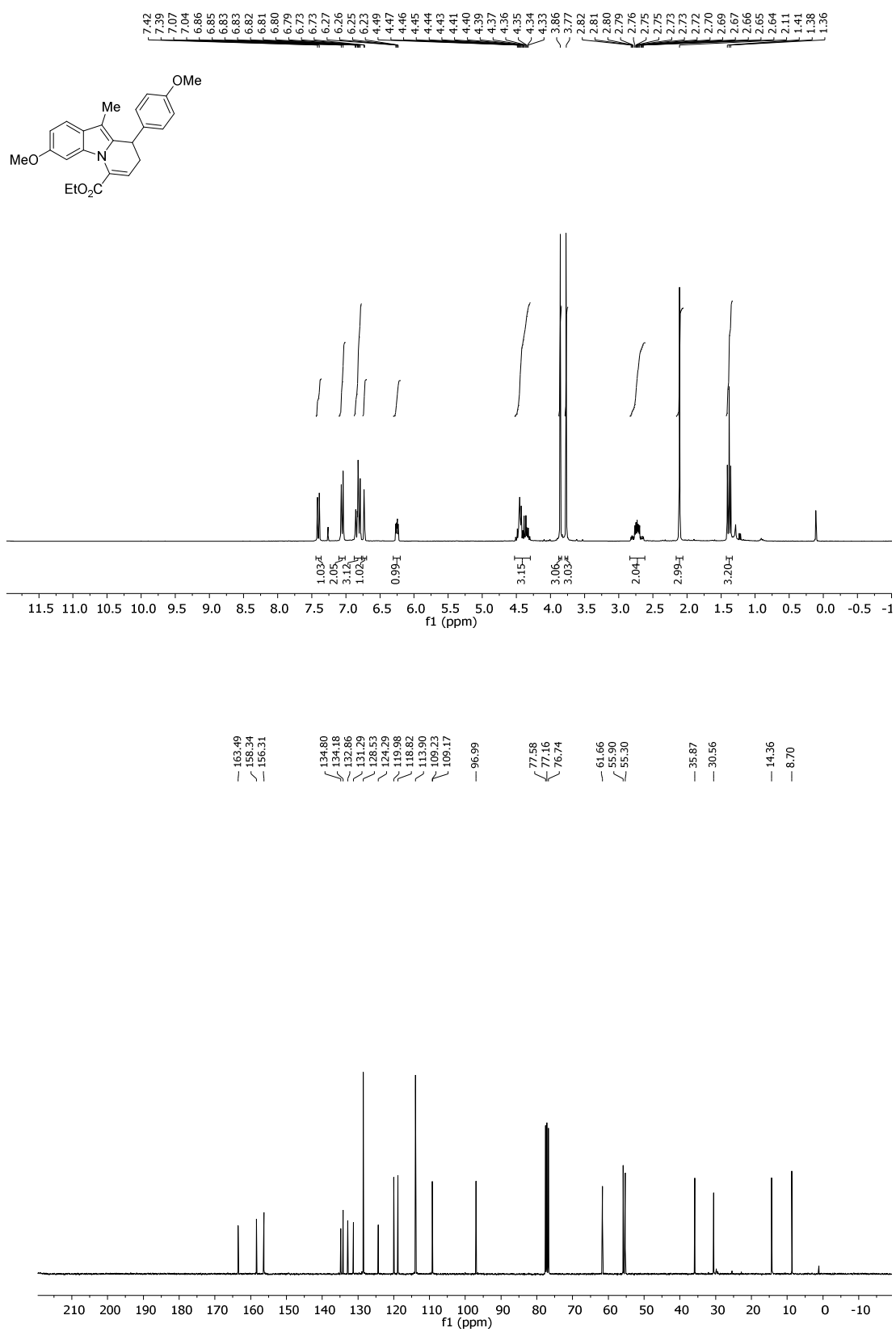


Figure S22. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3c

4c

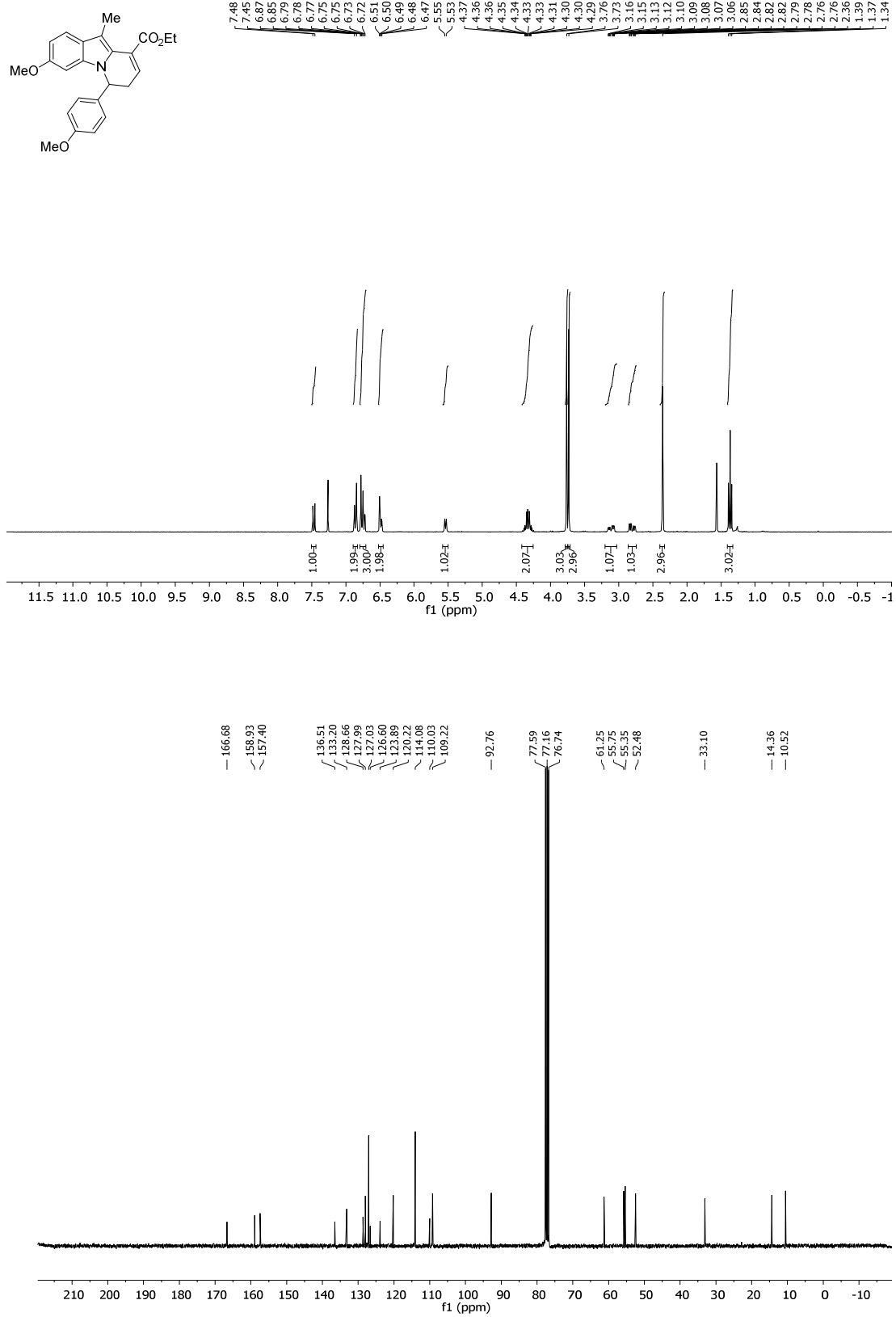


Figure S23. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4c

3d

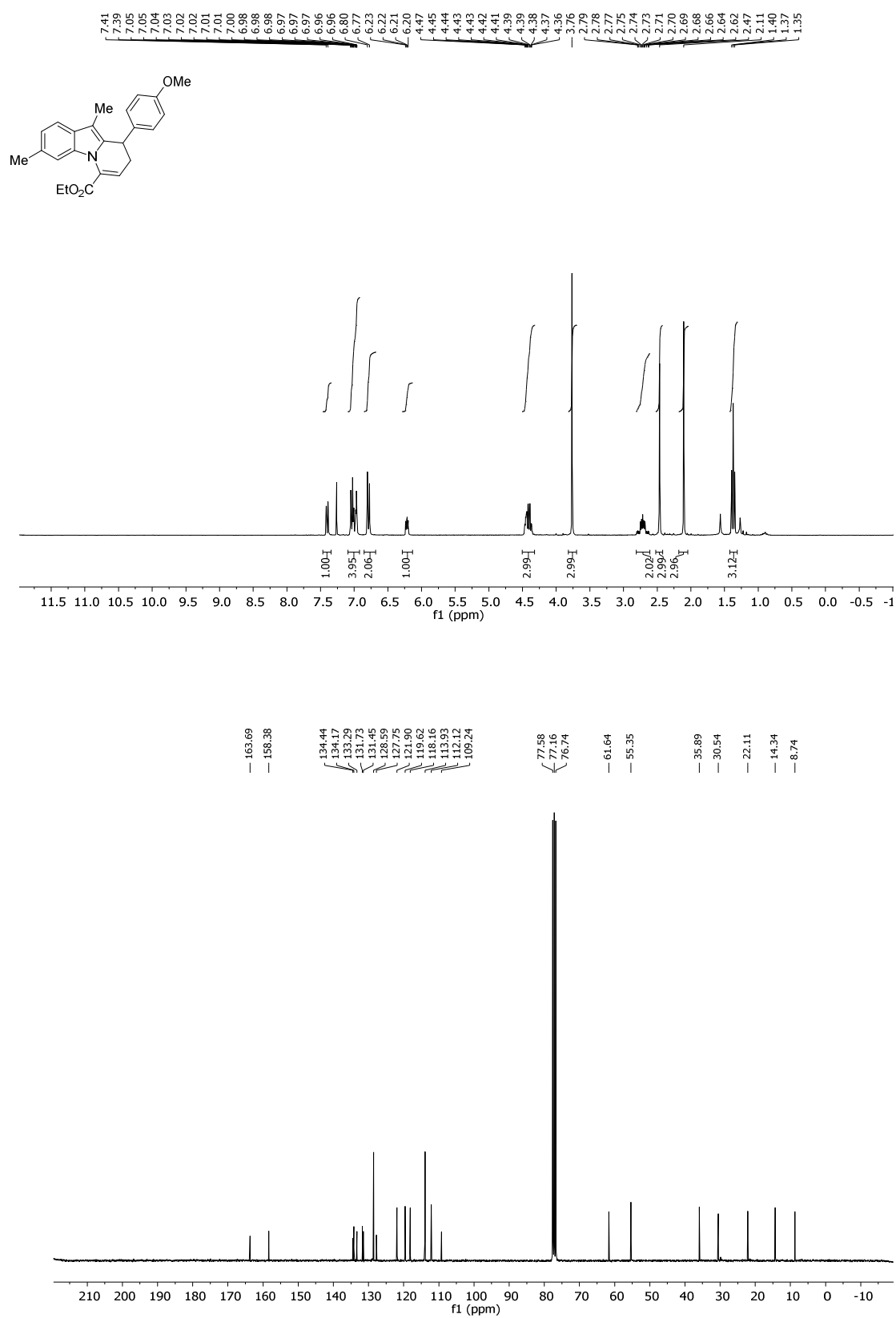


Figure S24. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3d

4d

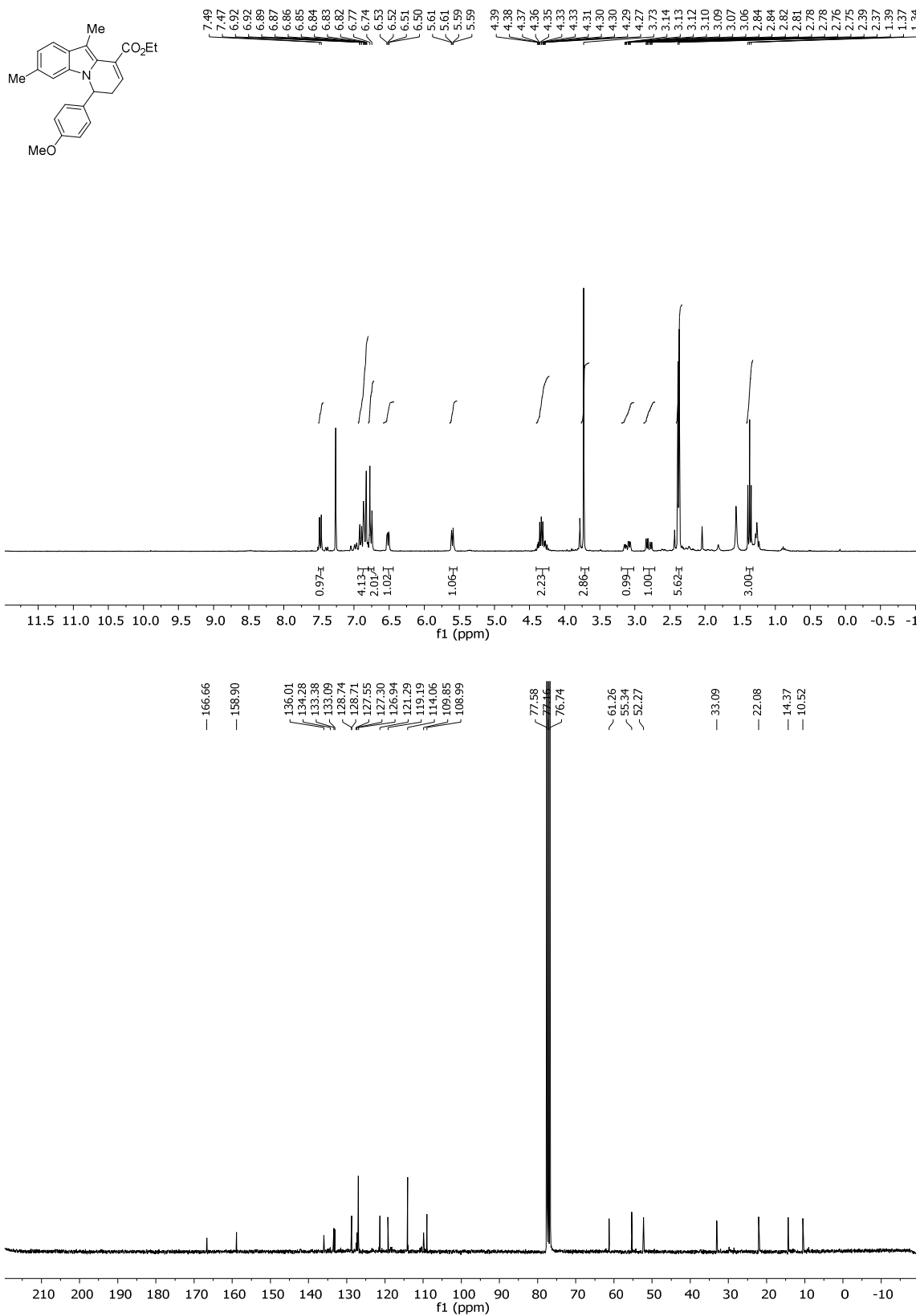


Figure S25. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4d

3e

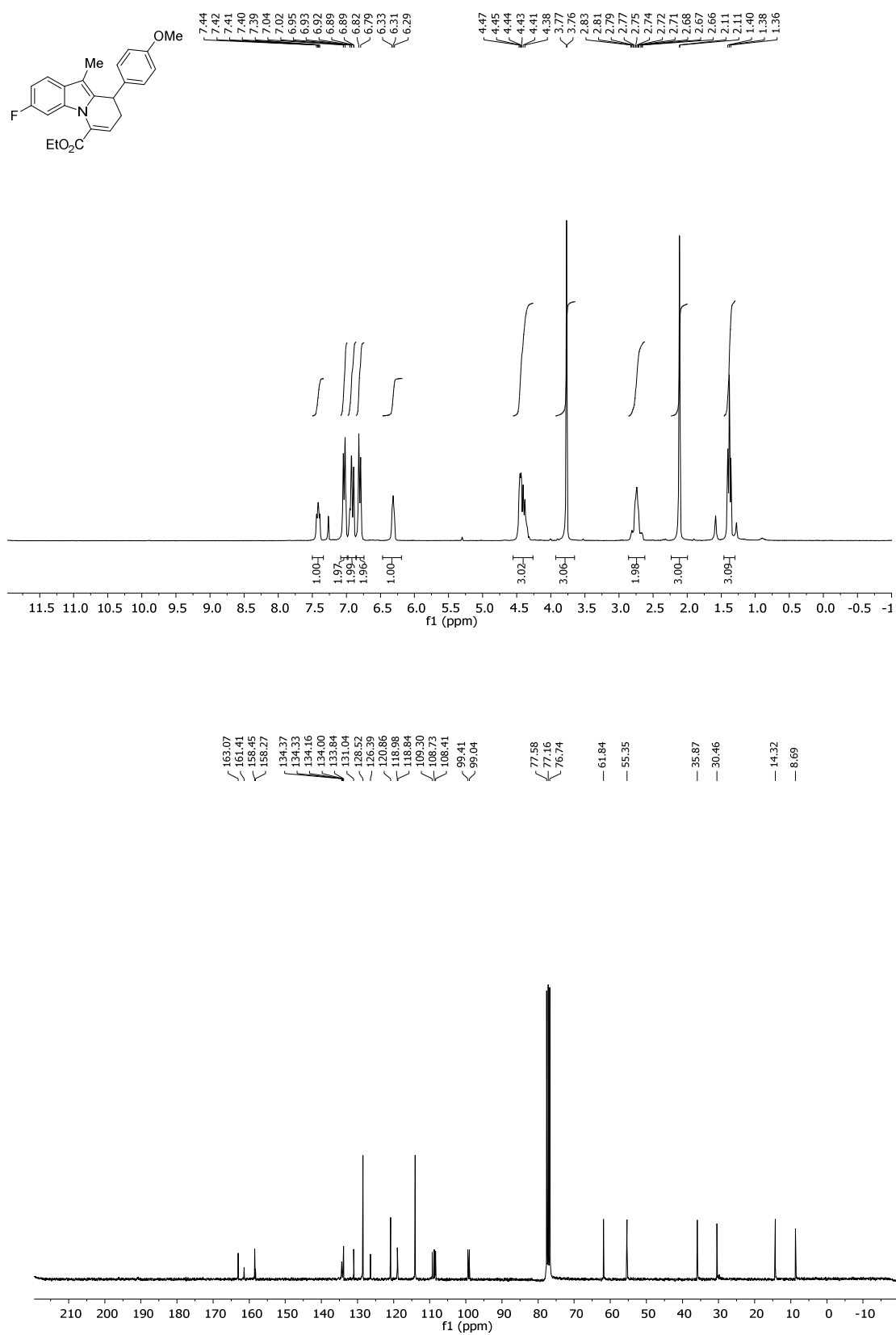


Figure S26. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3e

4e

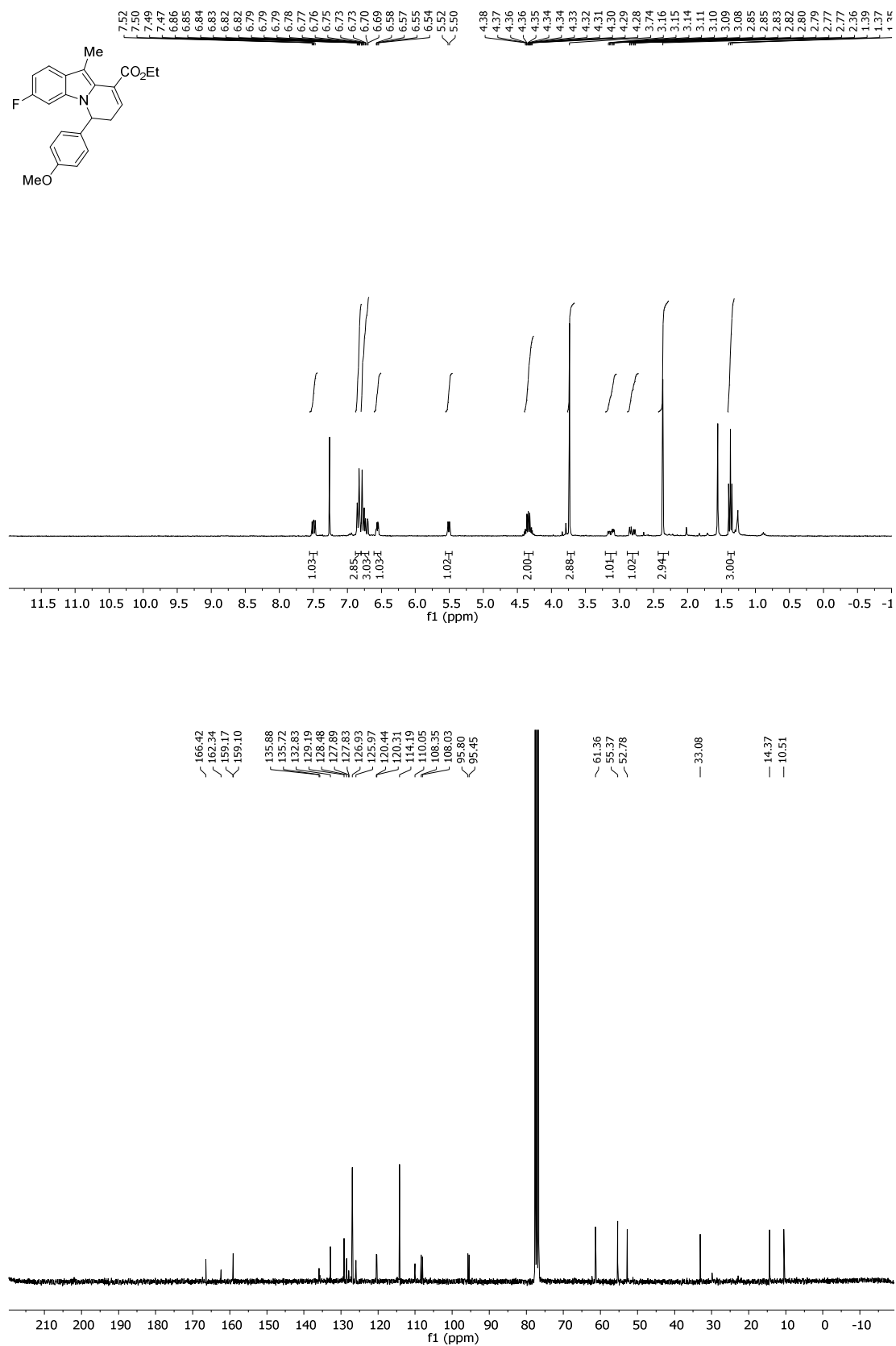


Figure S27. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4e

3f

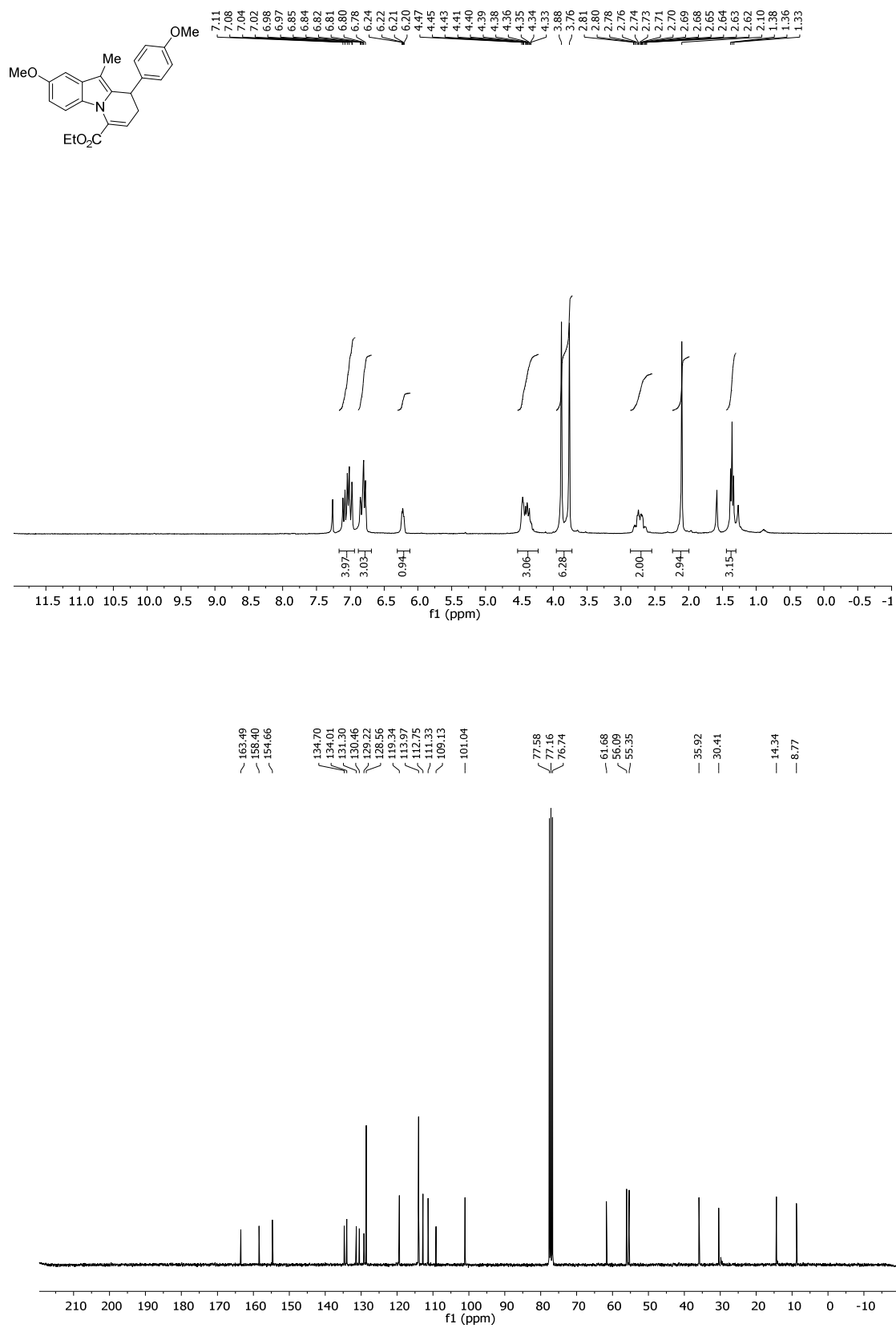


Figure S28. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3f

4f

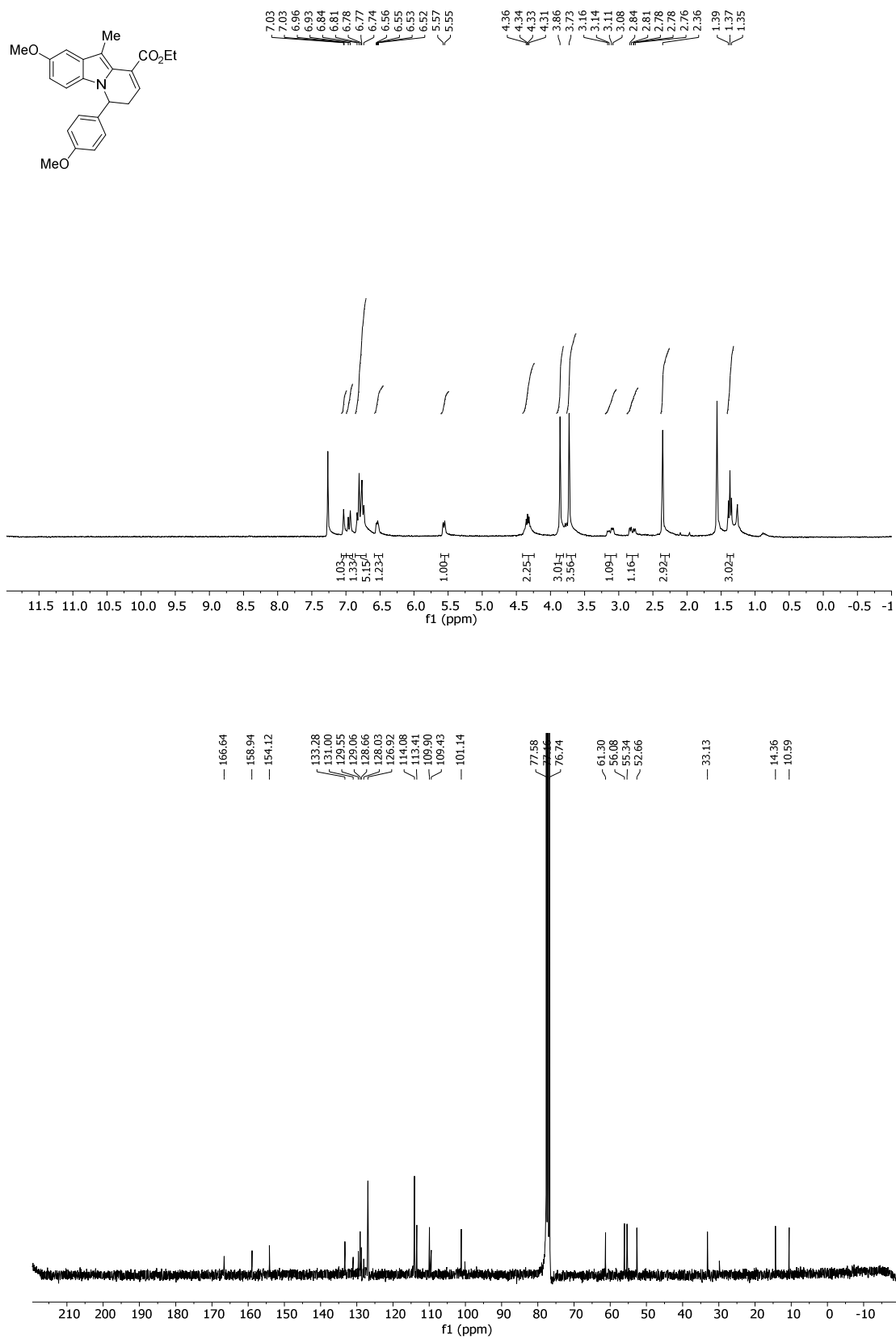


Figure S29. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4f

3g

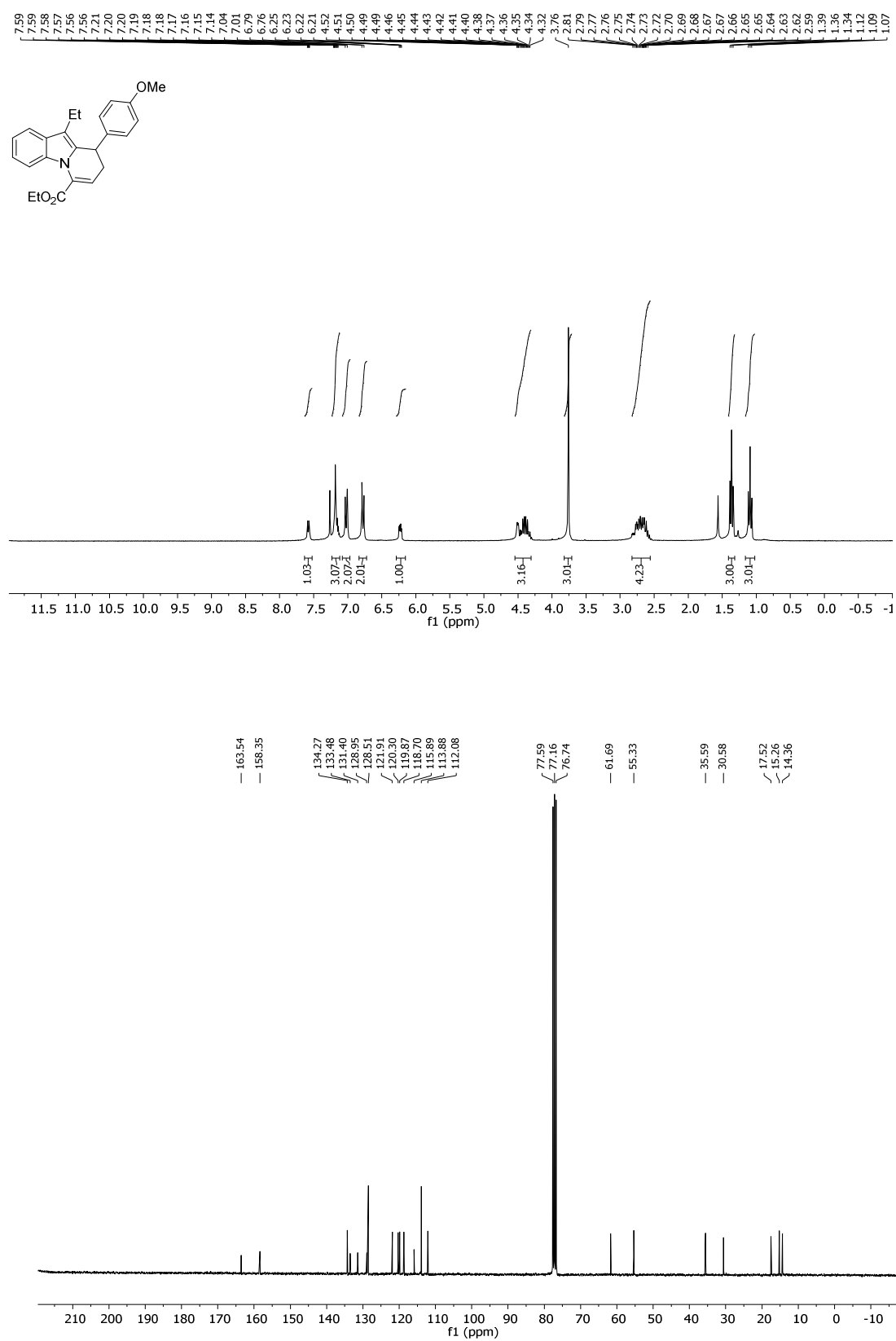


Figure S30. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3g

4g

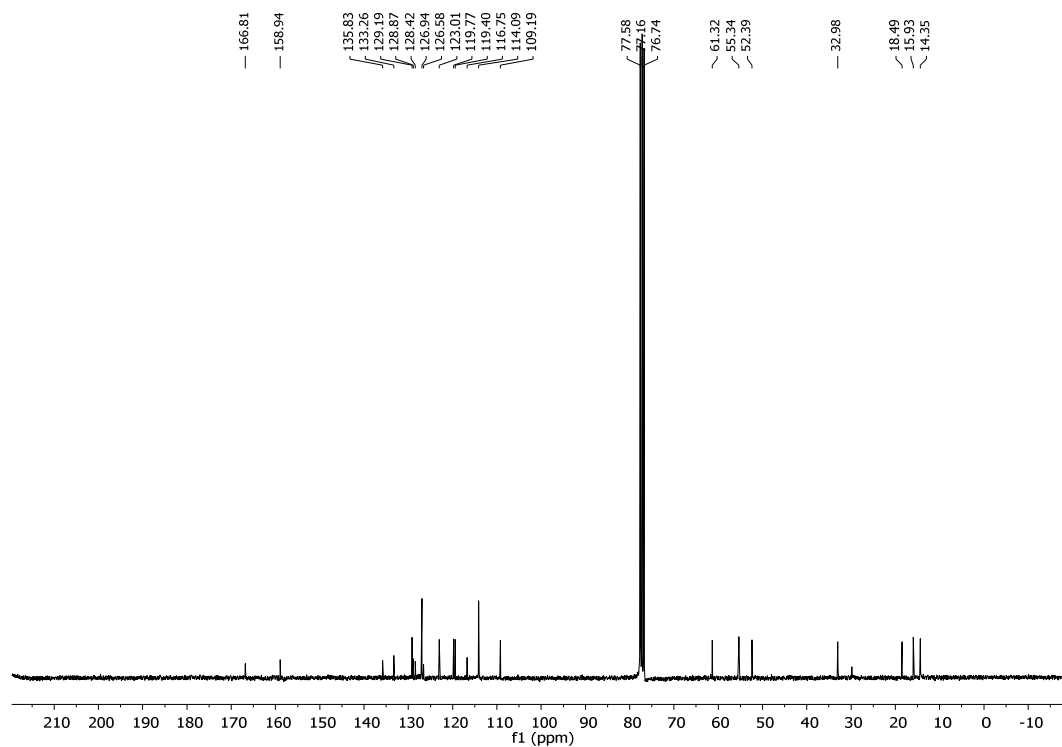
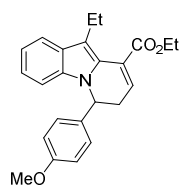
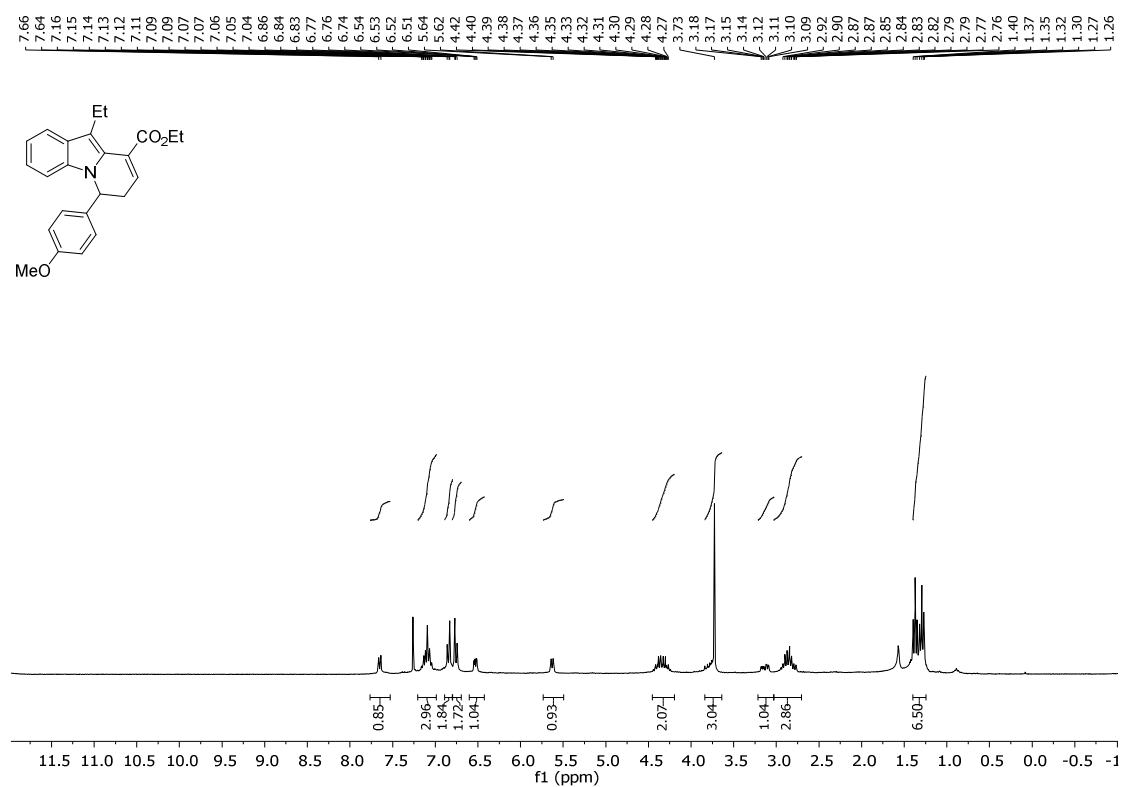


Figure S31. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4g

3h

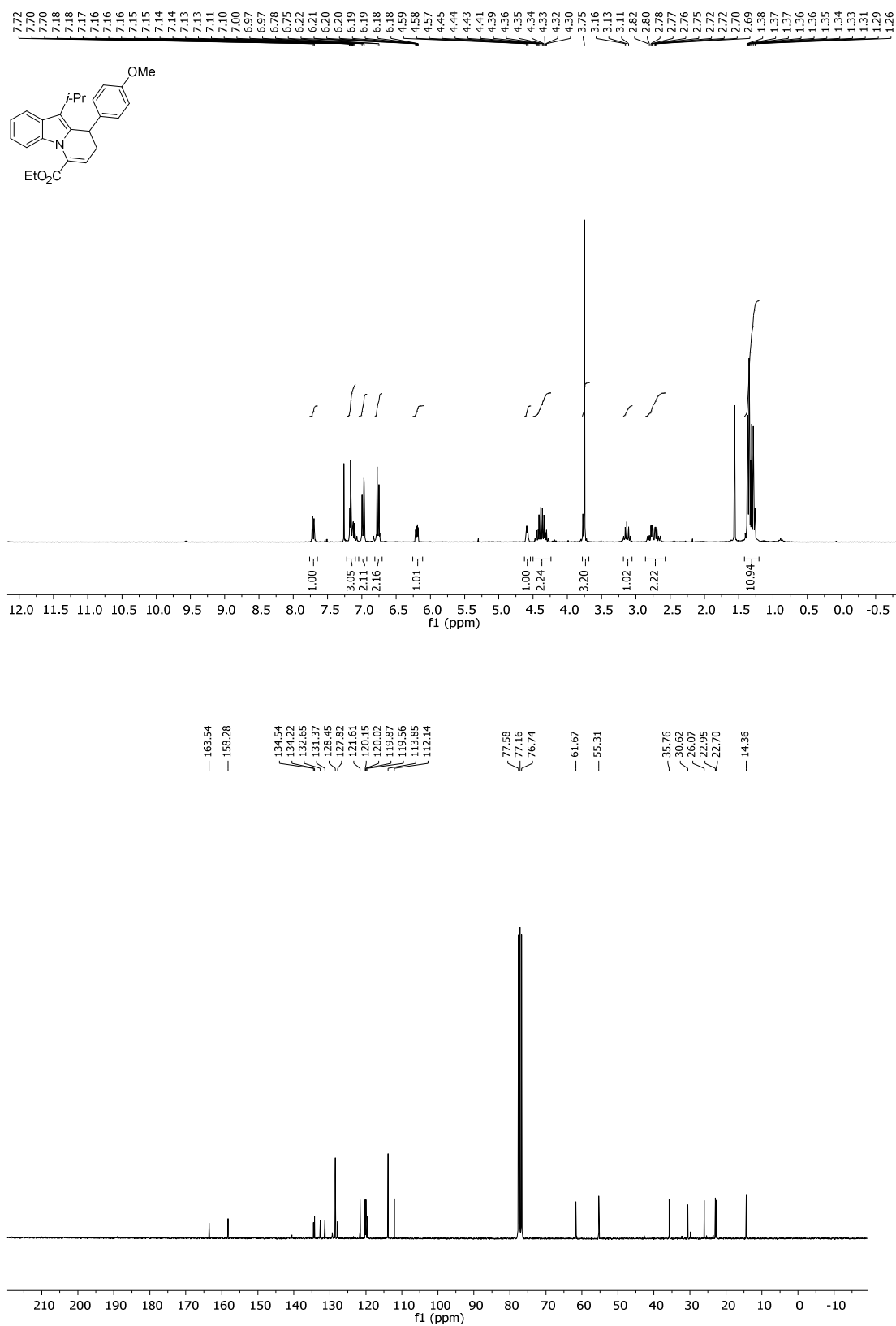


Figure S32. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3h

3i

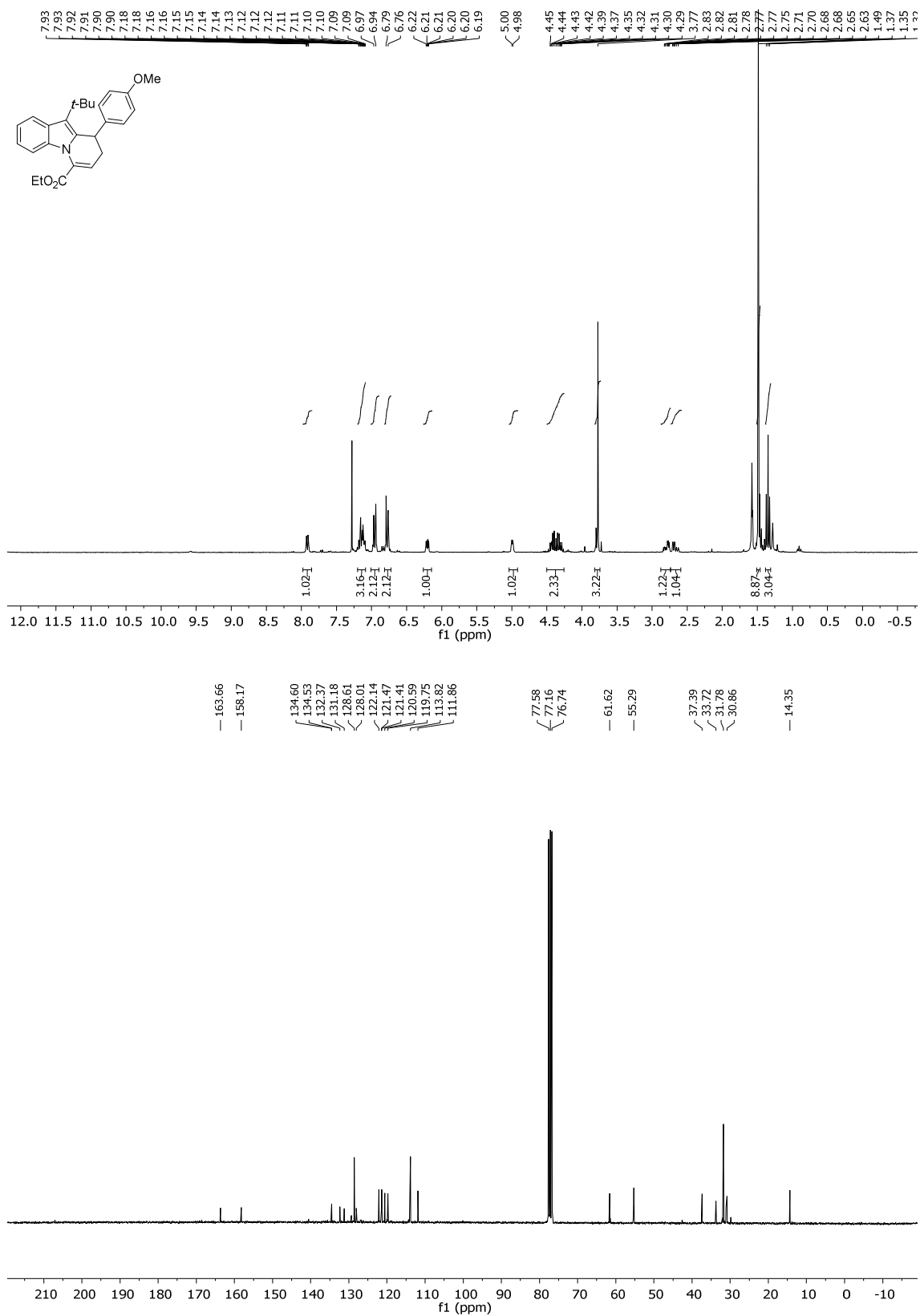


Figure S33. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3i

3j

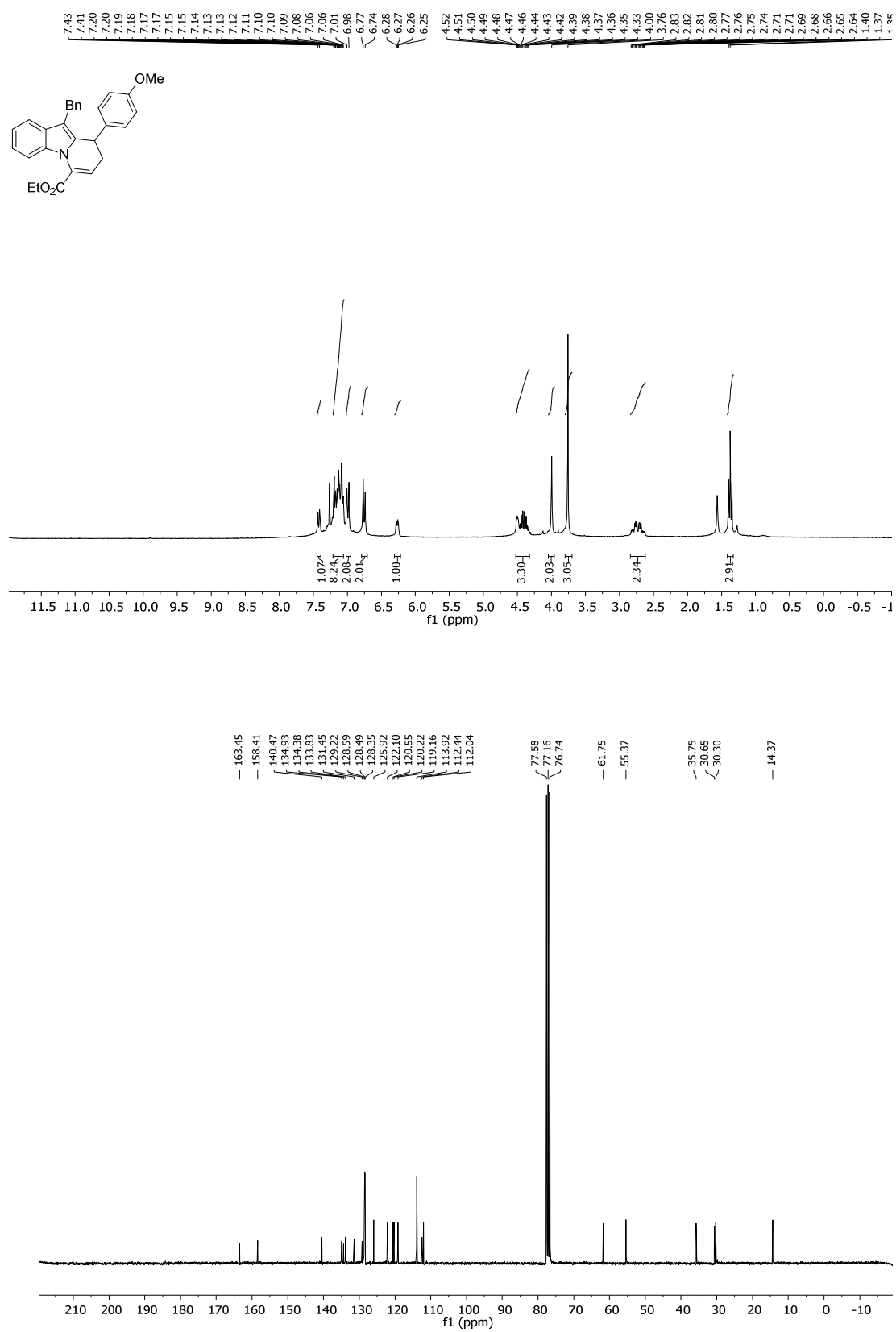


Figure S34. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3j

4j

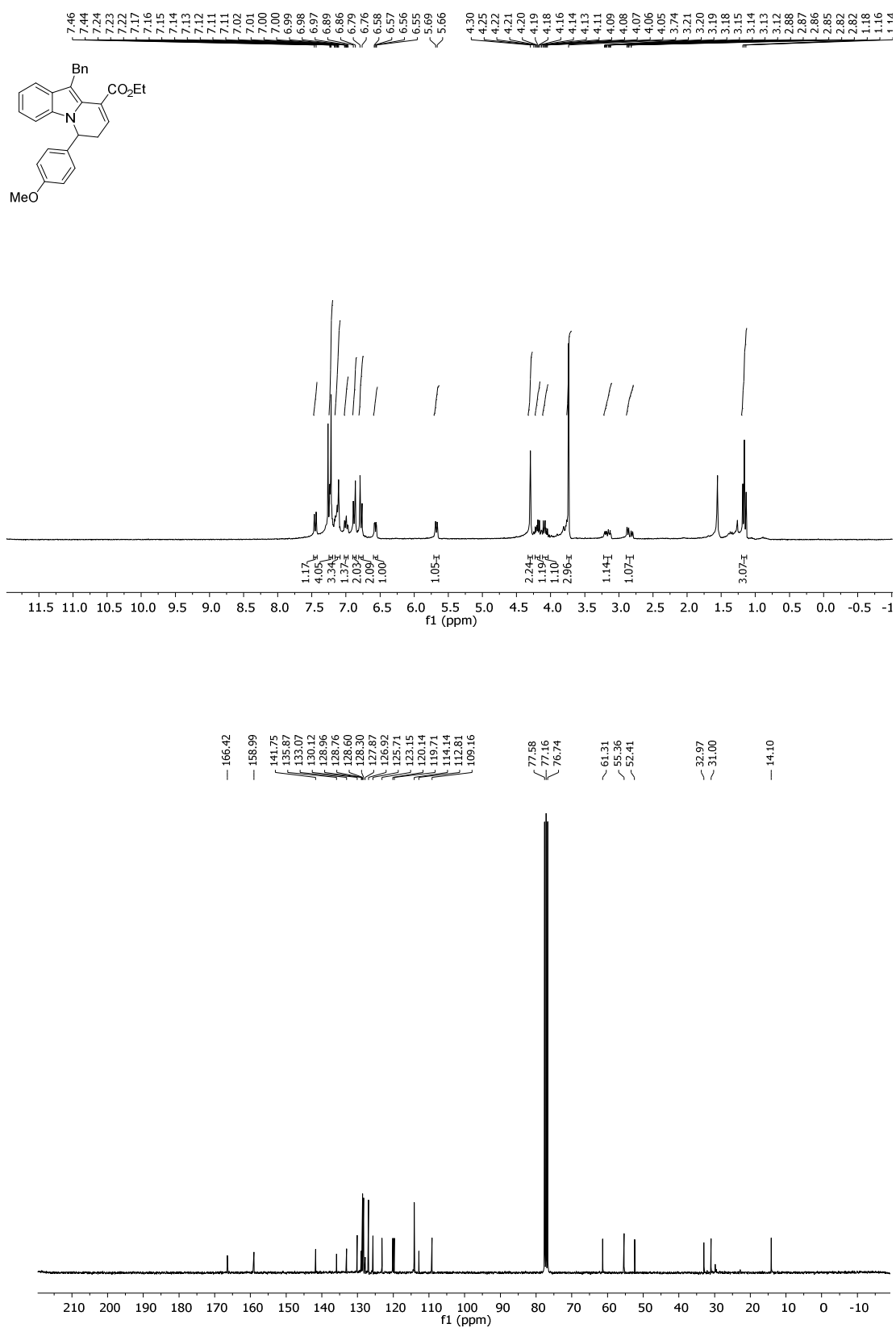


Figure S35. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4j

3k

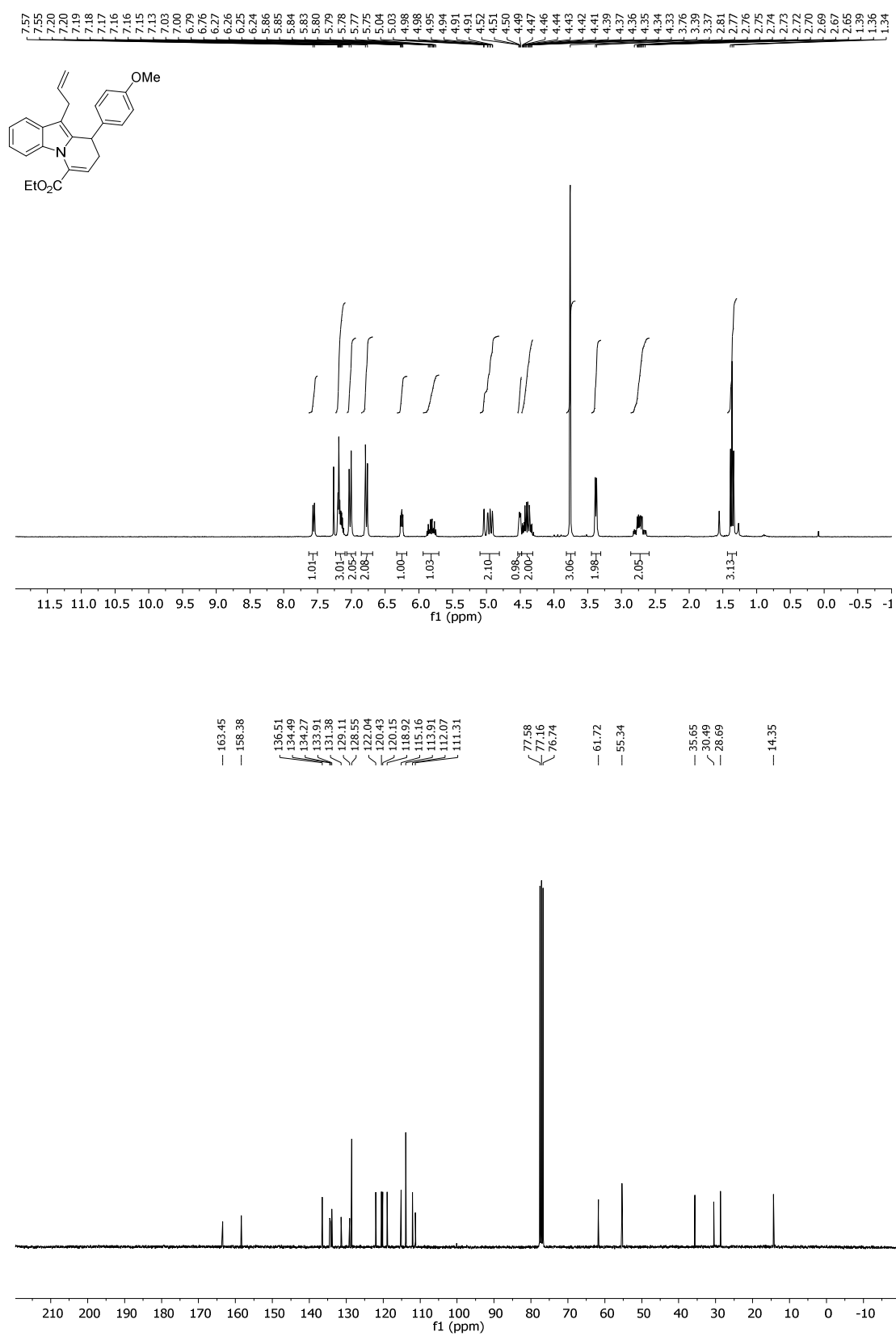


Figure S36. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3k

4k

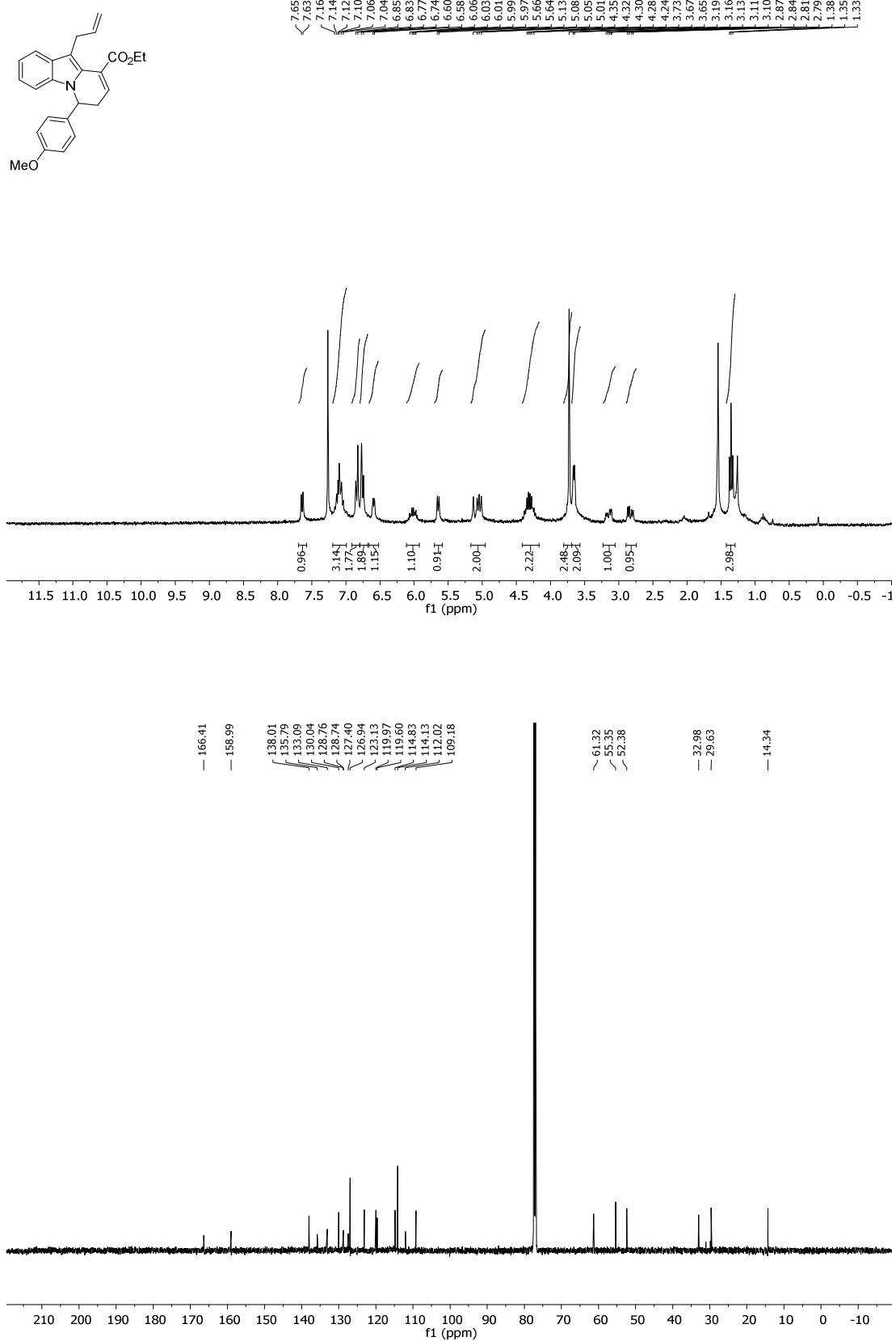


Figure S37. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4k

3l

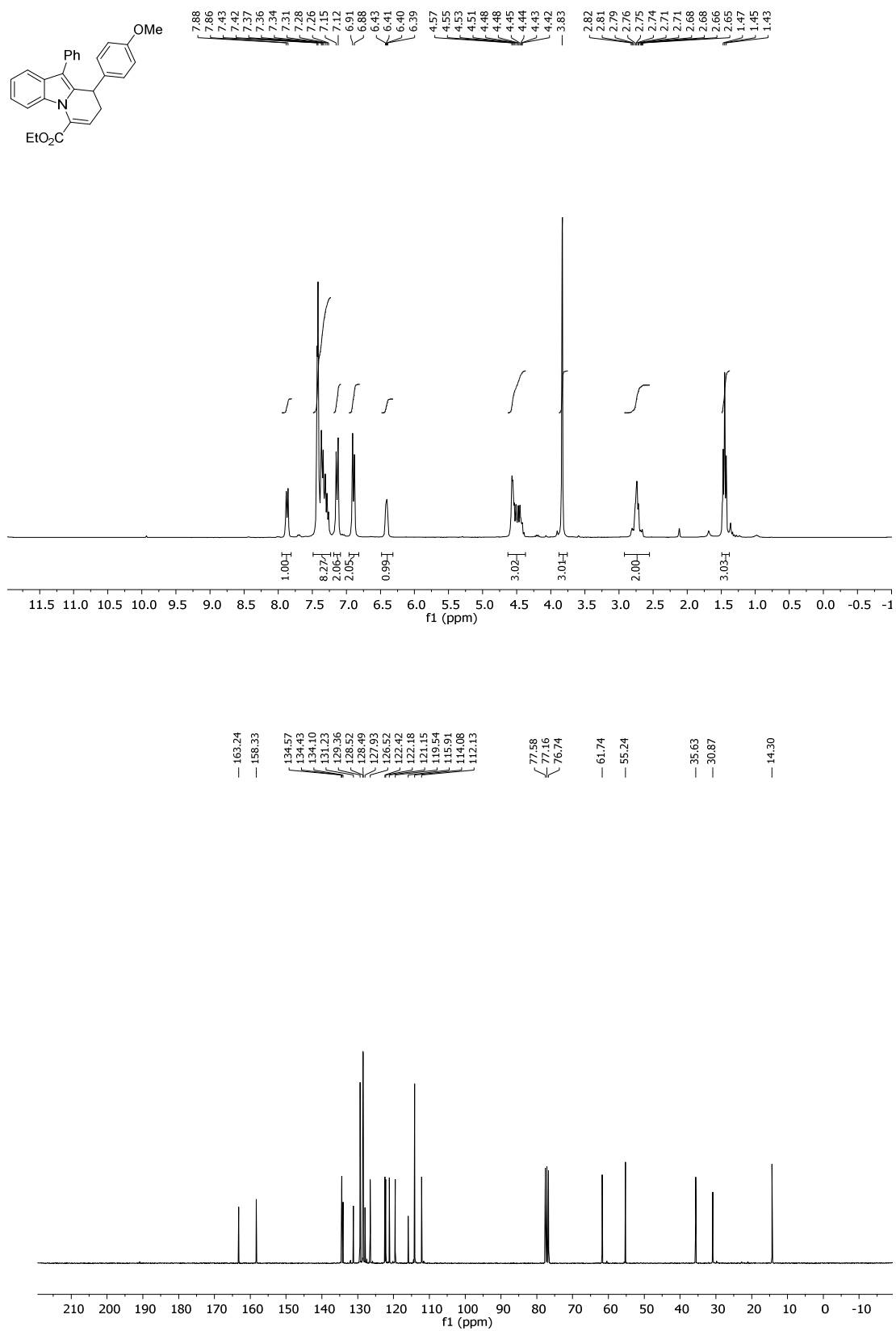


Figure S38. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3l

4l

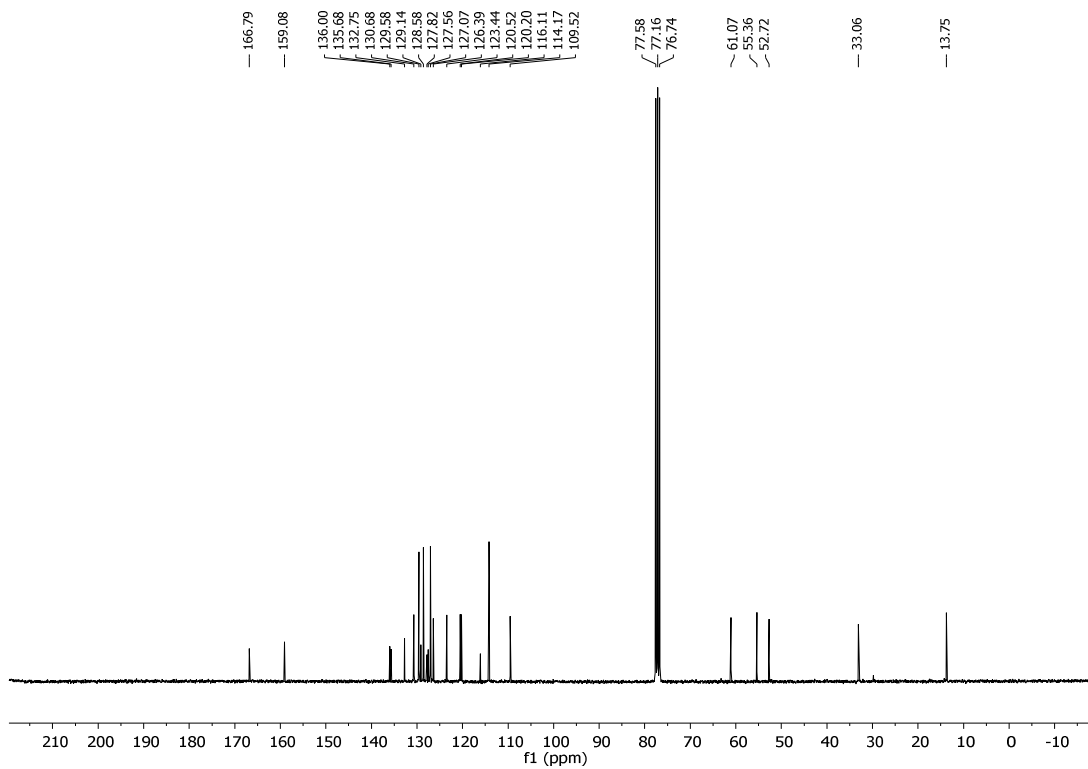
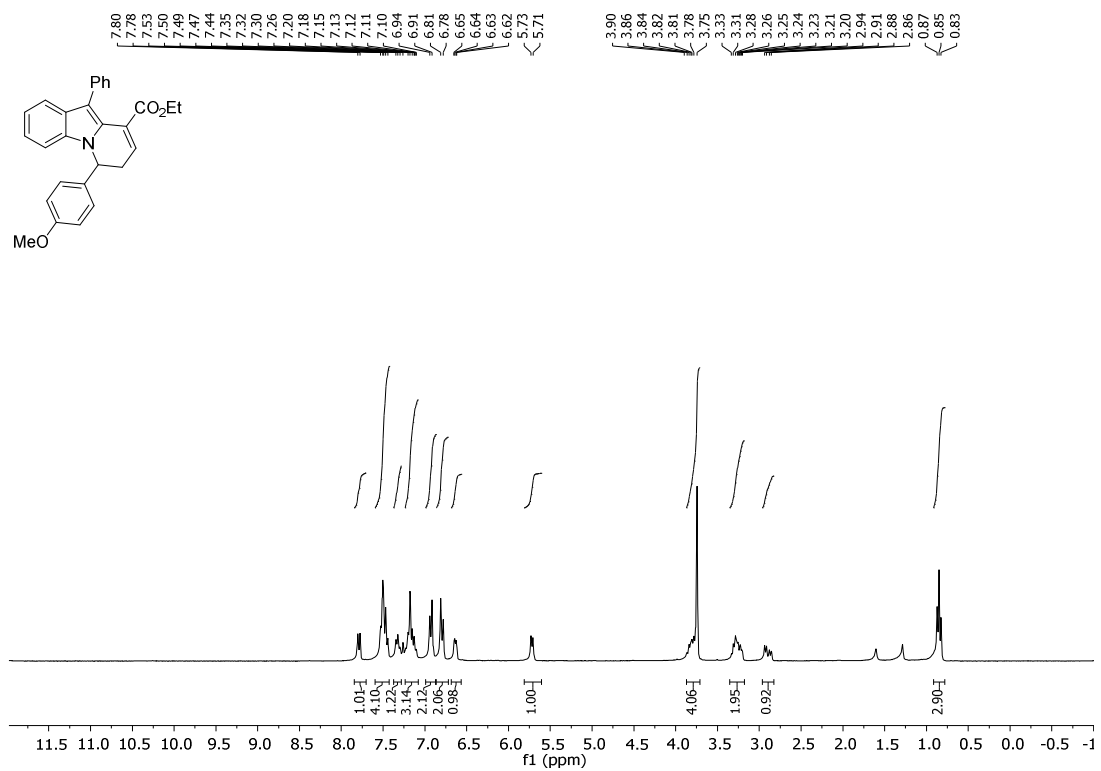


Figure S39. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 4l

3m

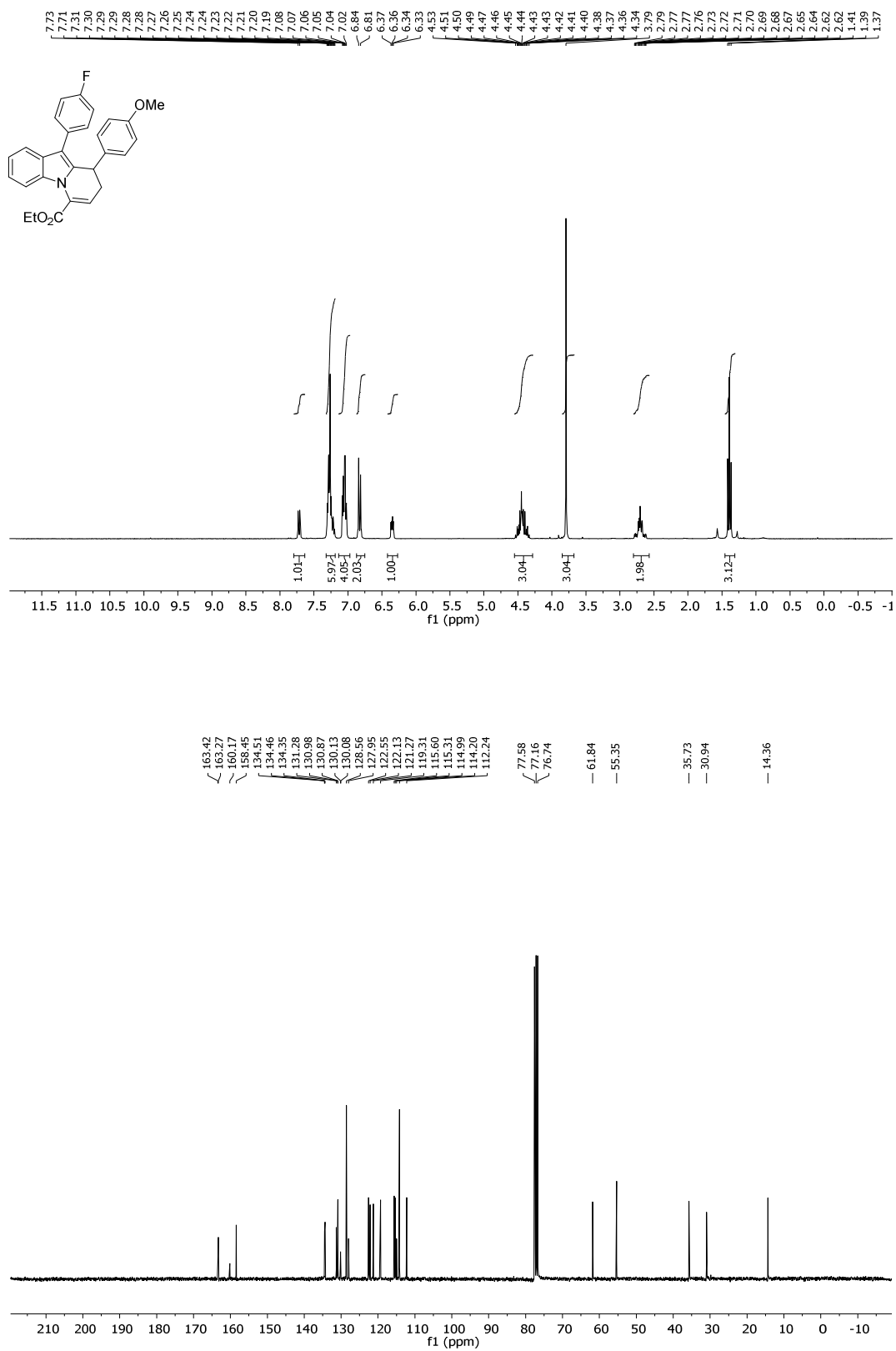


Figure S40. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3m

3n

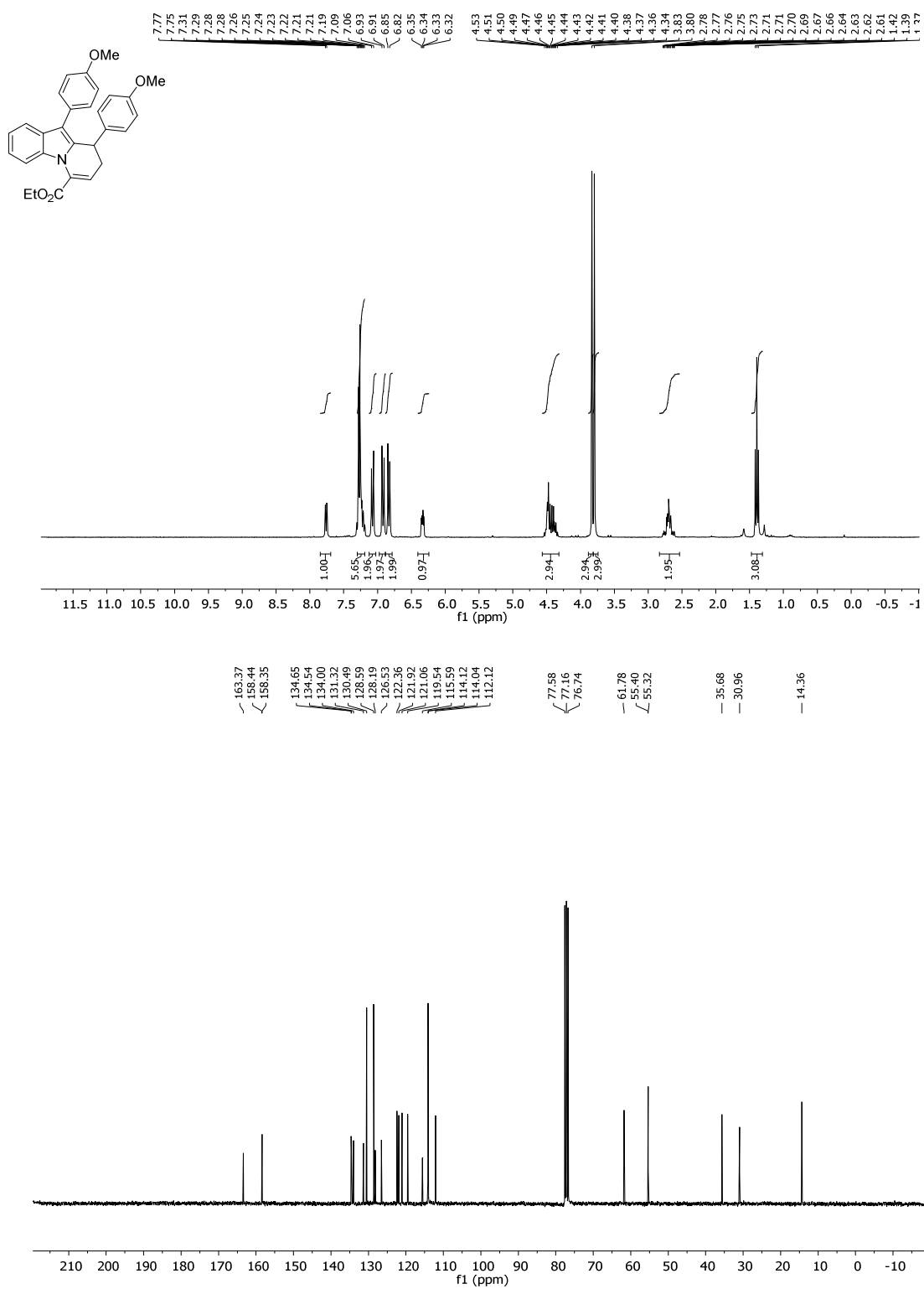


Figure S41. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 3n

4.4 Dihydropyridindoindoles 5a-s

5a

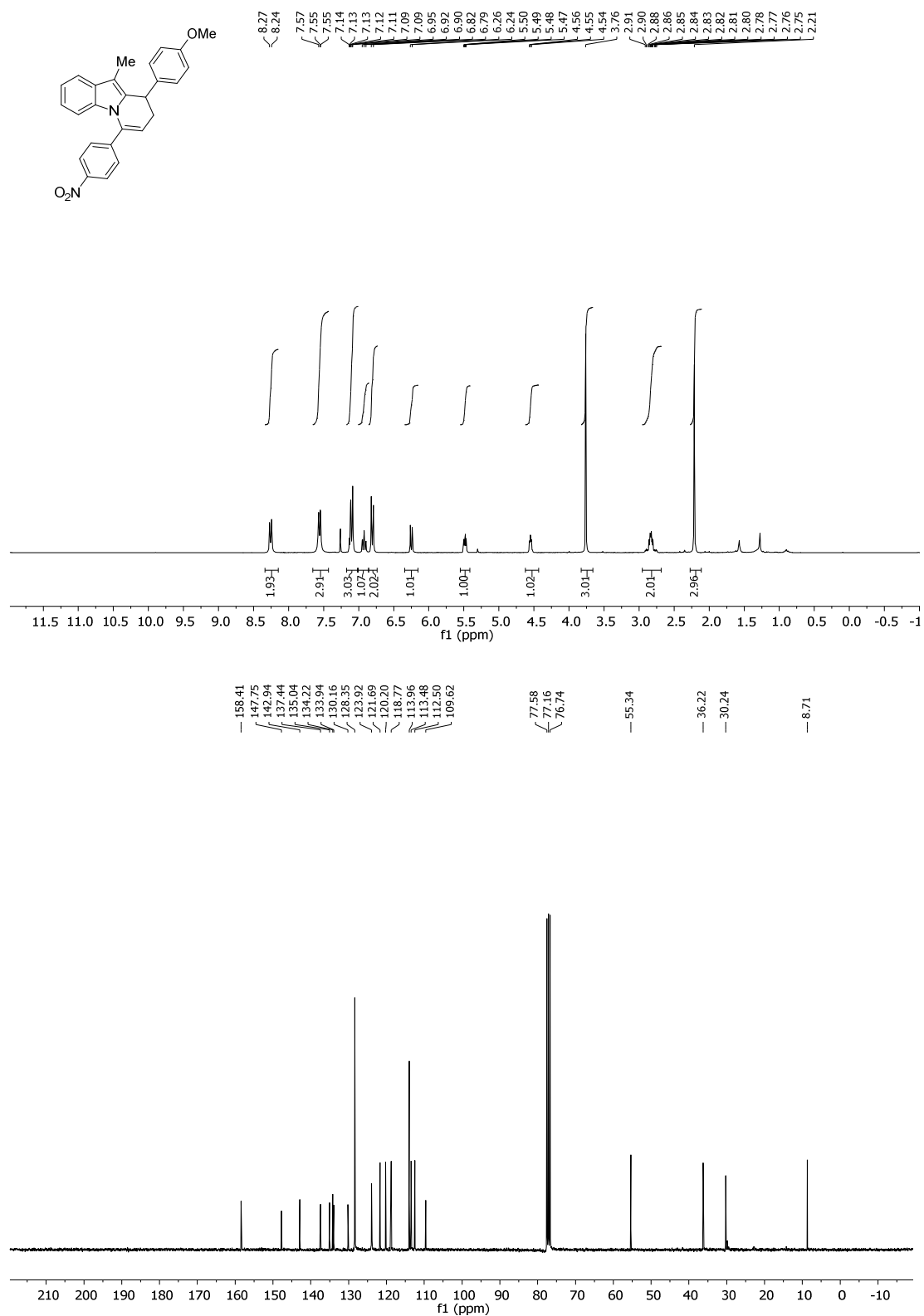


Figure S42. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5a

5b

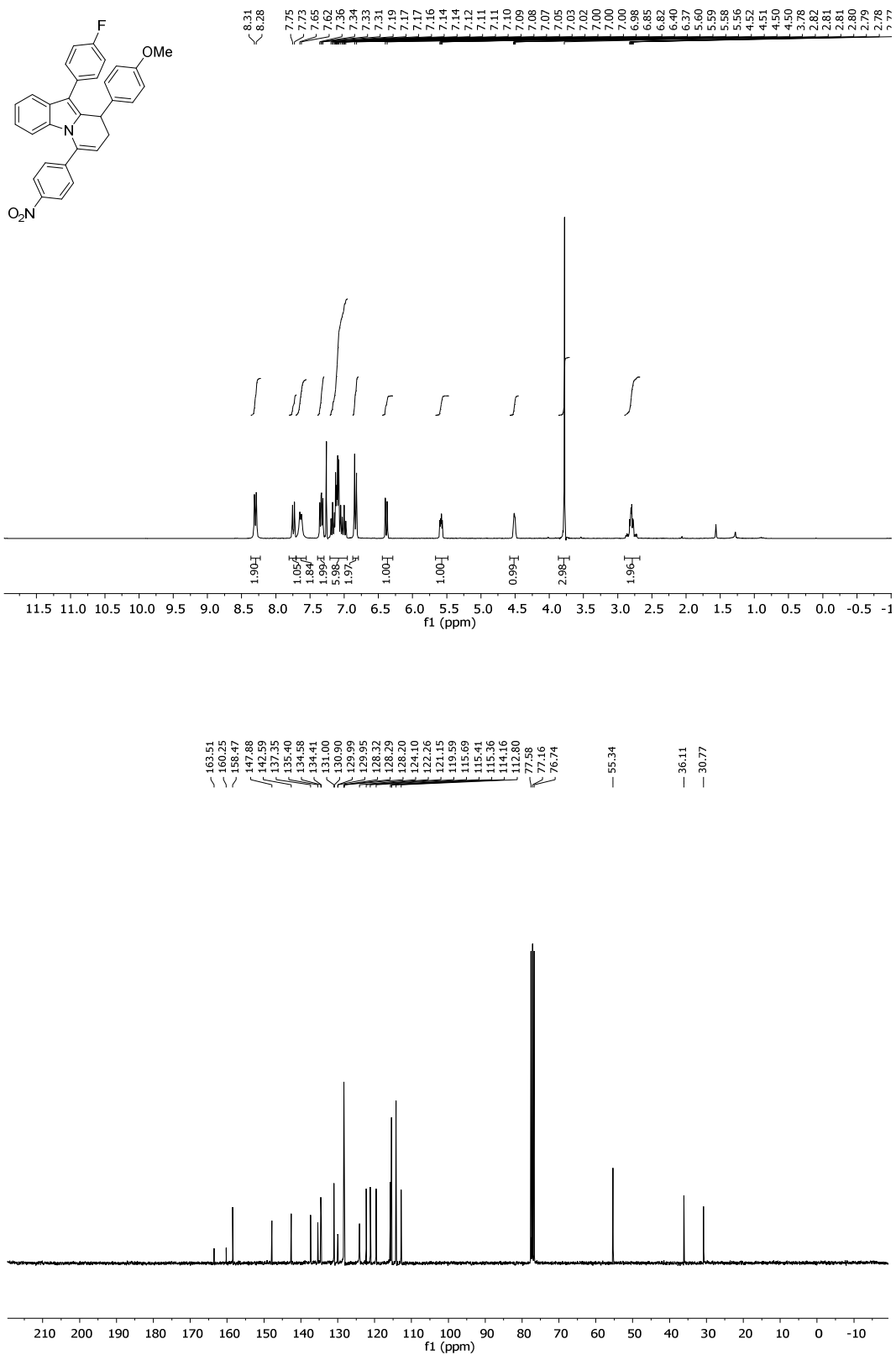


Figure S43. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5b

5c

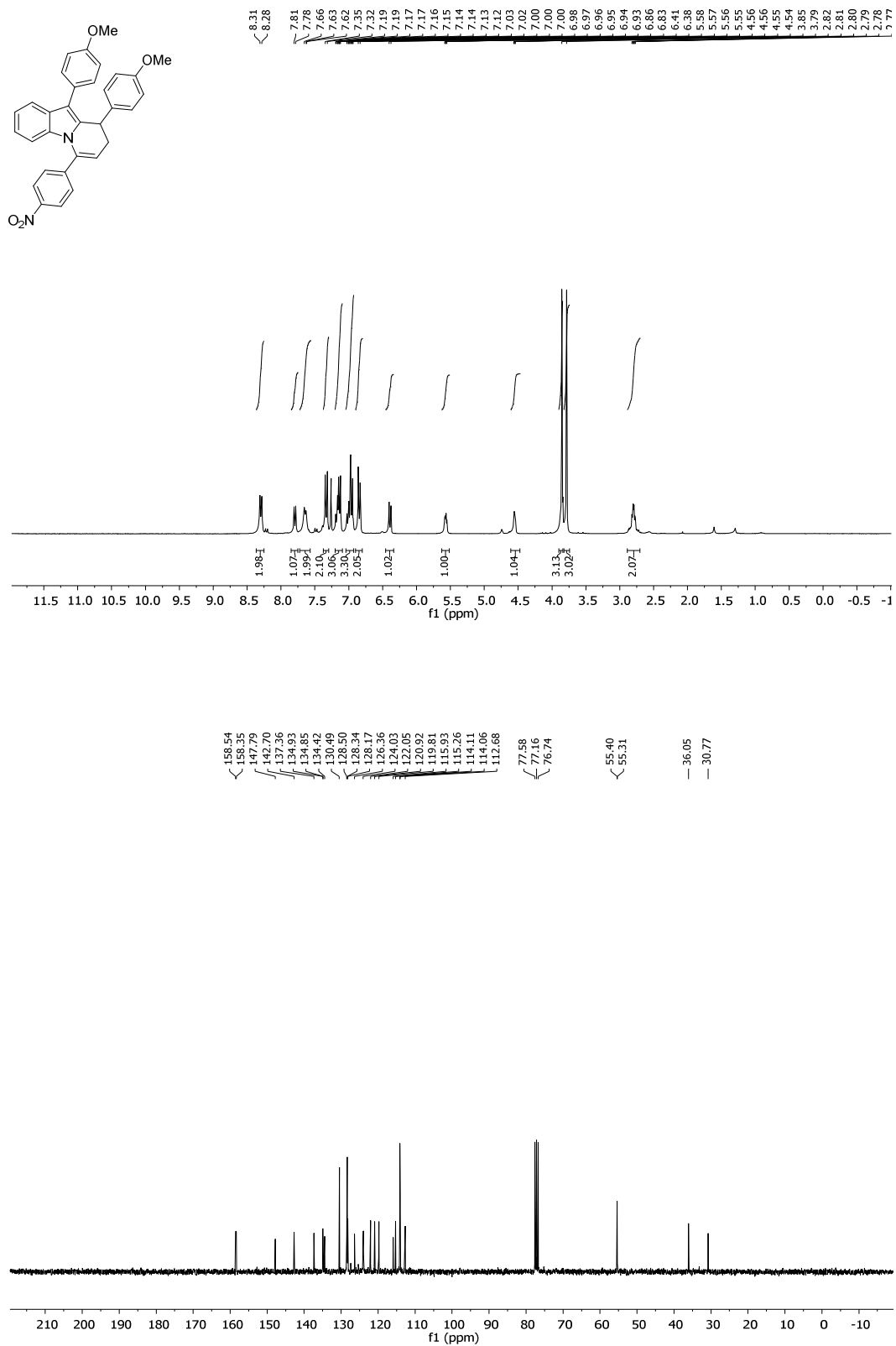


Figure S44. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5c

5d

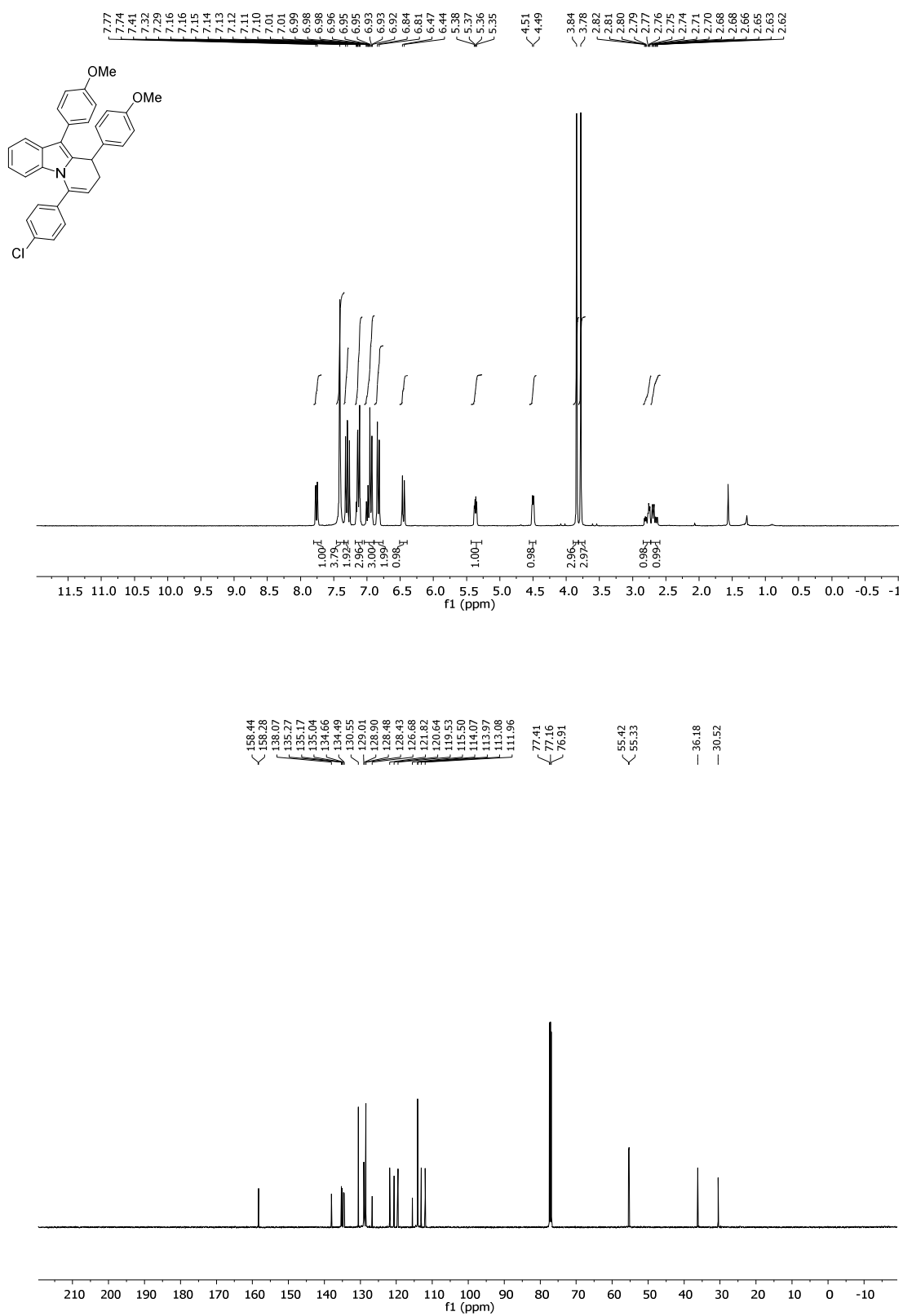


Figure S45. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5d

5e

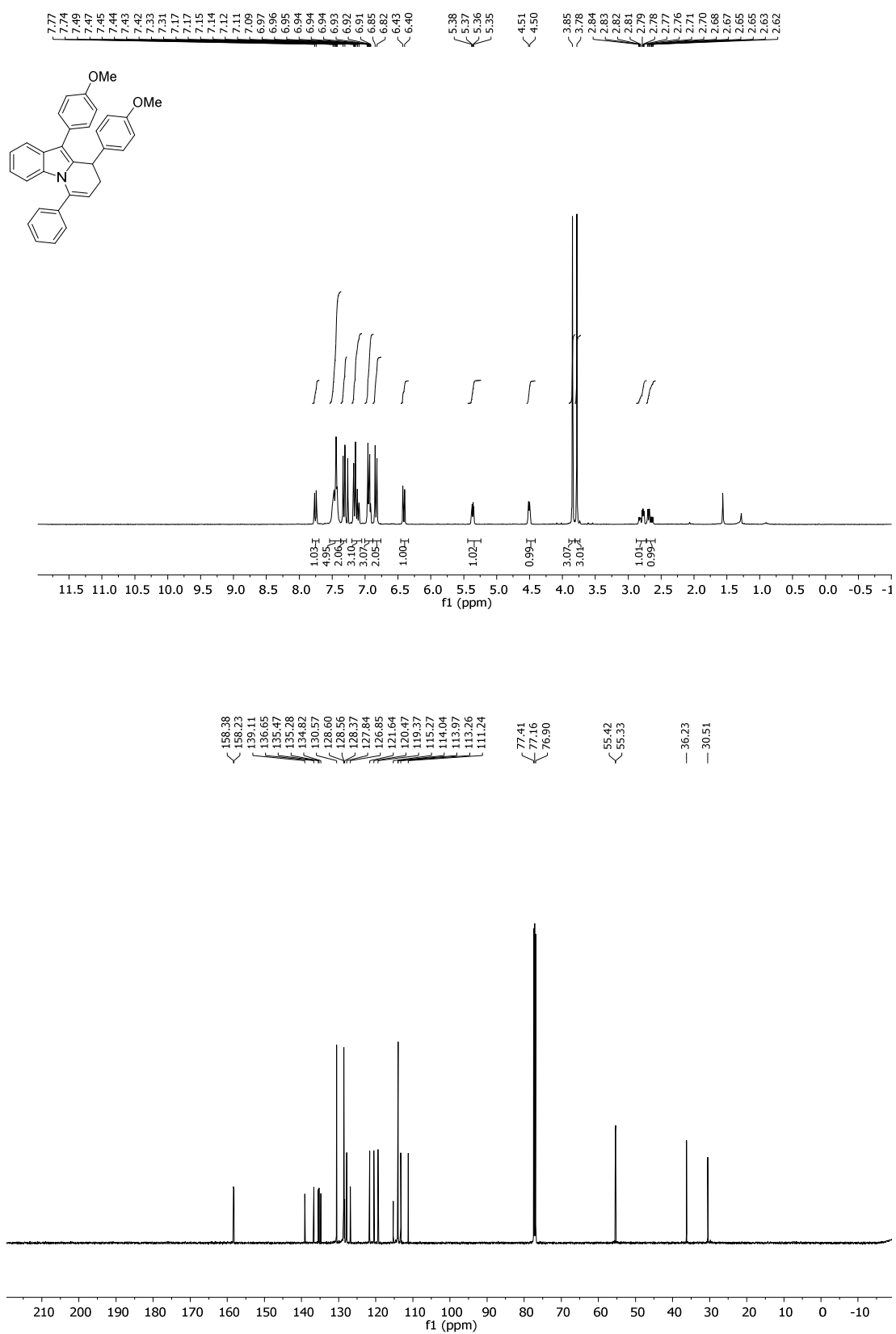


Figure S46. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5e

5f

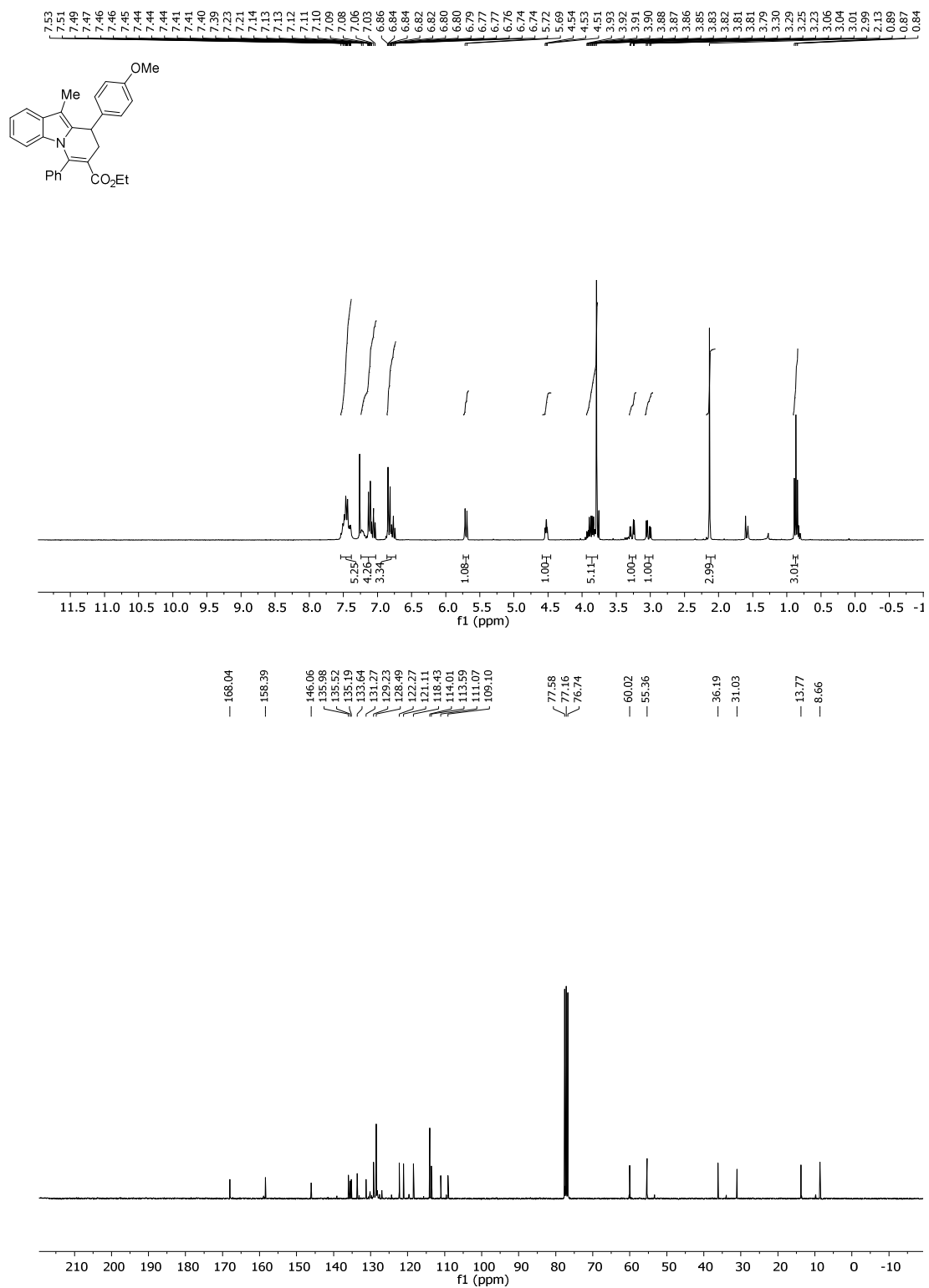


Figure S47. $^1\text{H-NMR}$ (300 MHz, CDCl_3) and $^{13}\text{C-NMR}$ (75 MHz, CDCl_3) spectra of compound 5f

5g

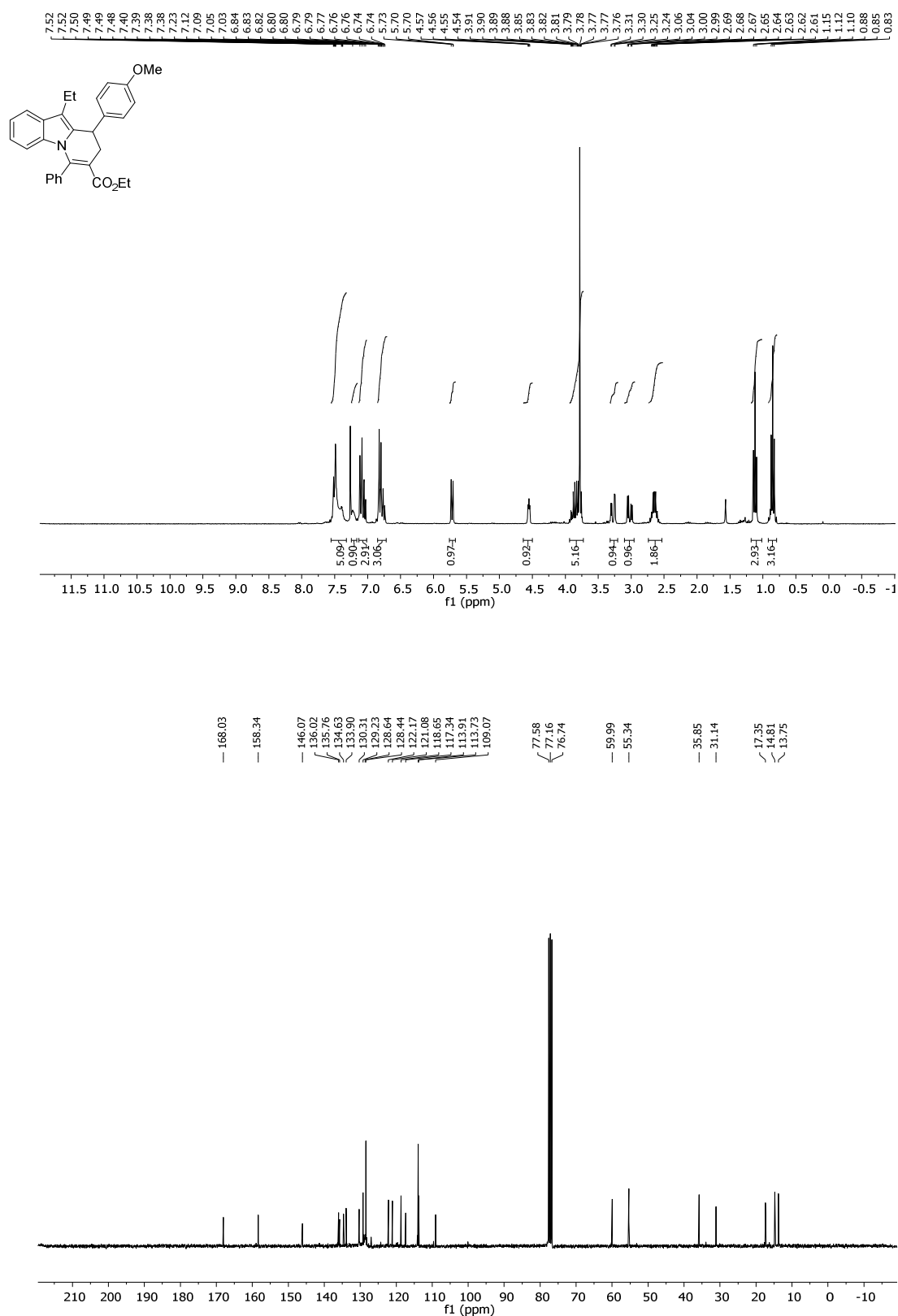


Figure S48. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5g

5h

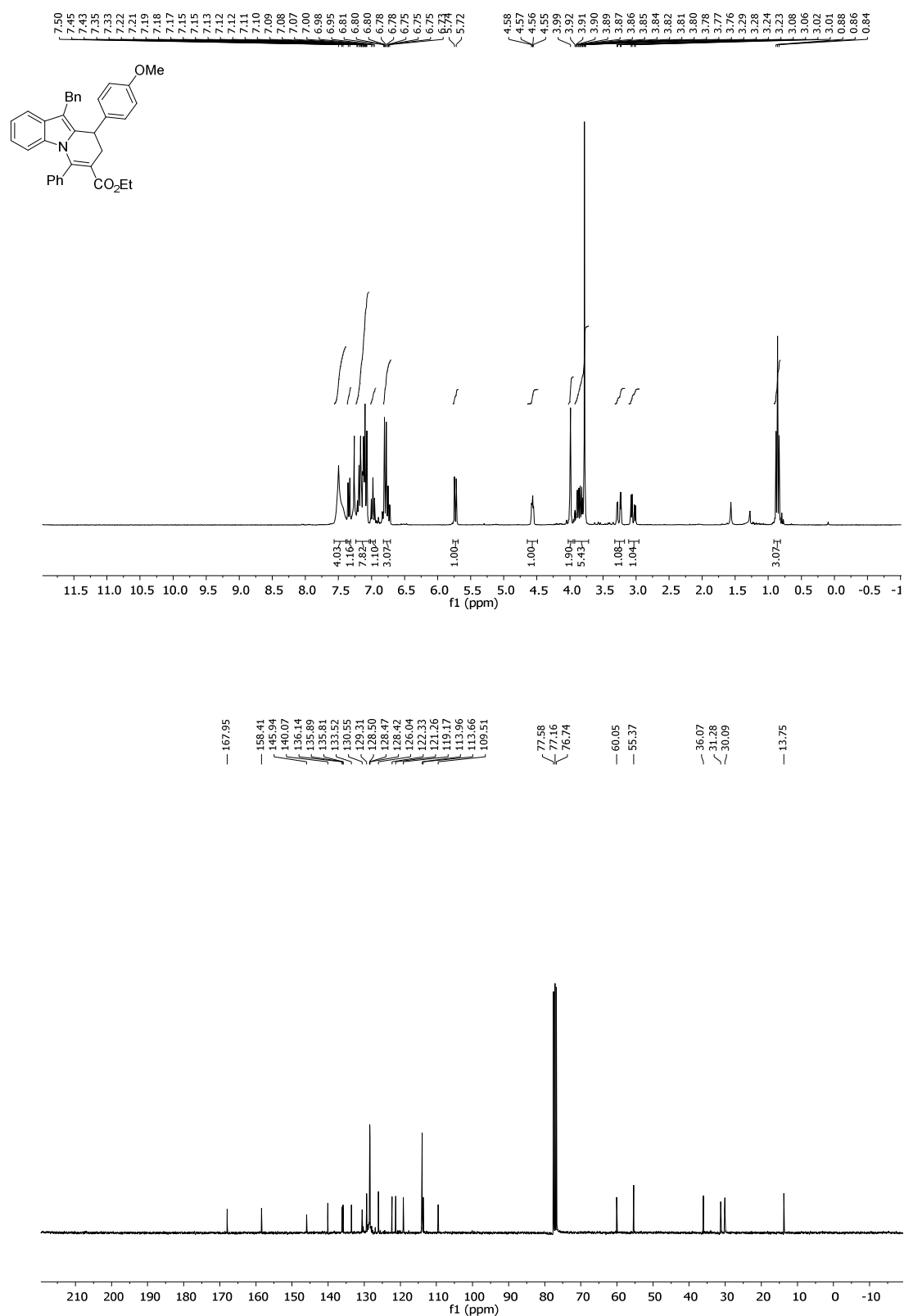


Figure S49. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5h

5i

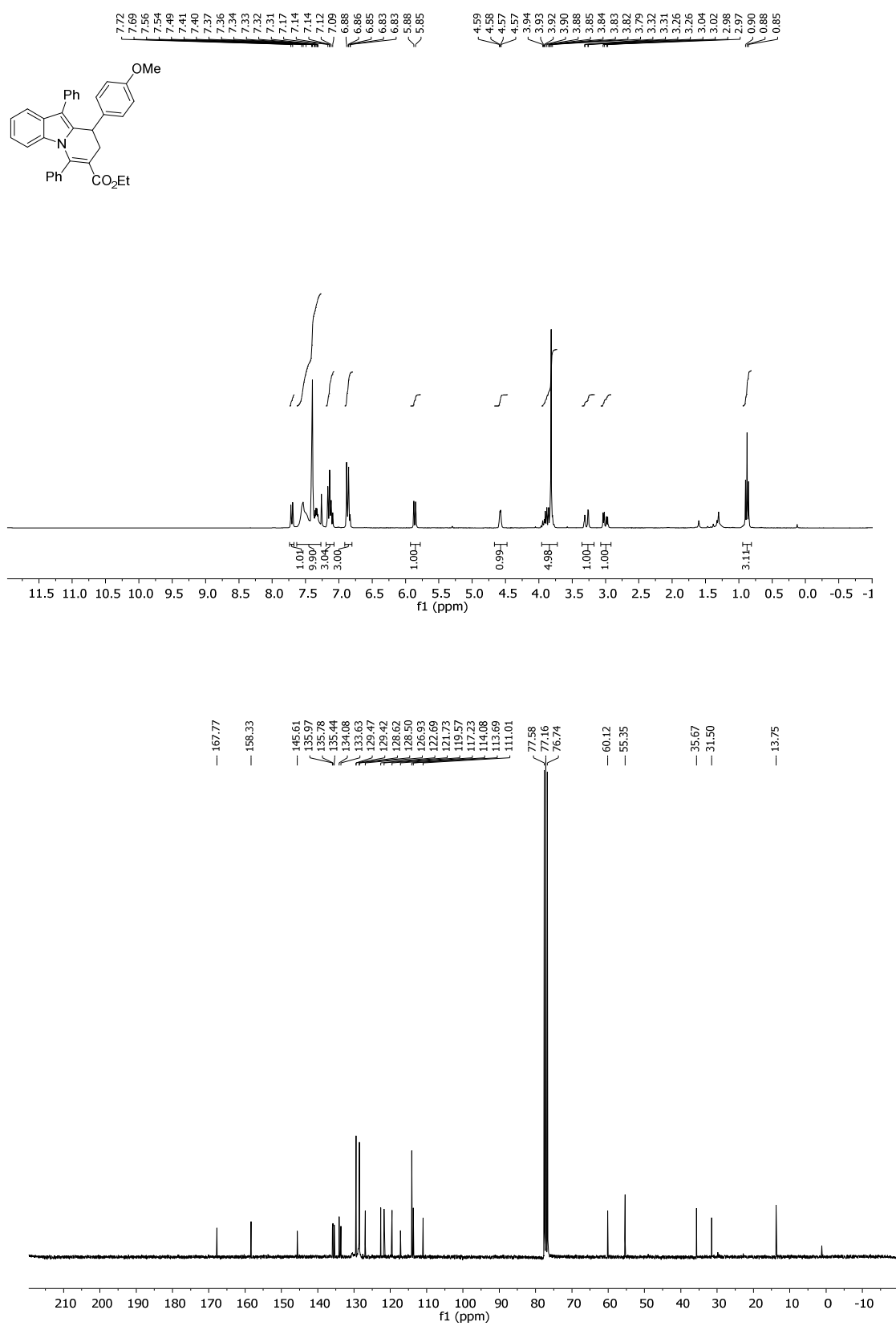


Figure S50. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5i

5j

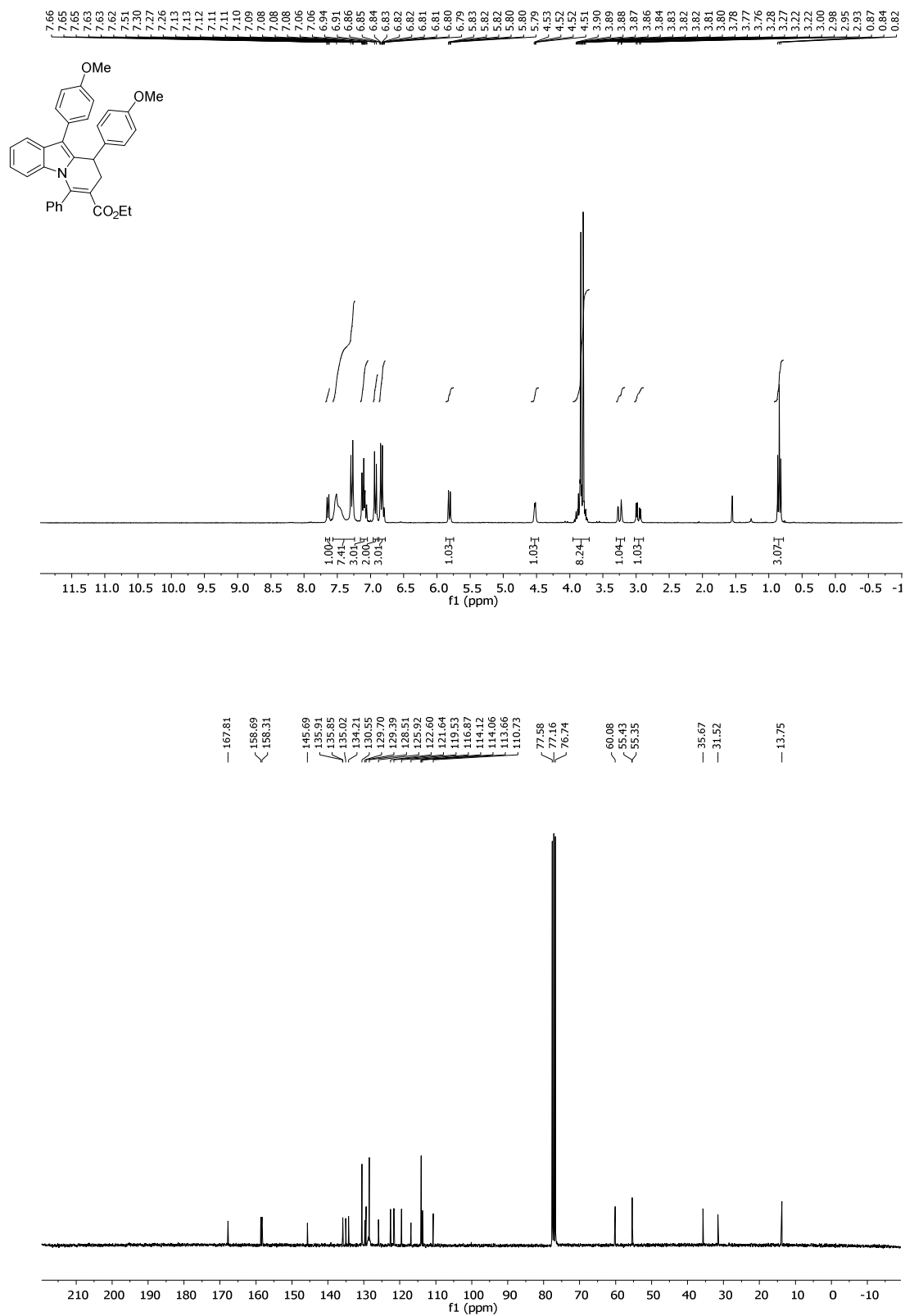


Figure S51. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5j

5k

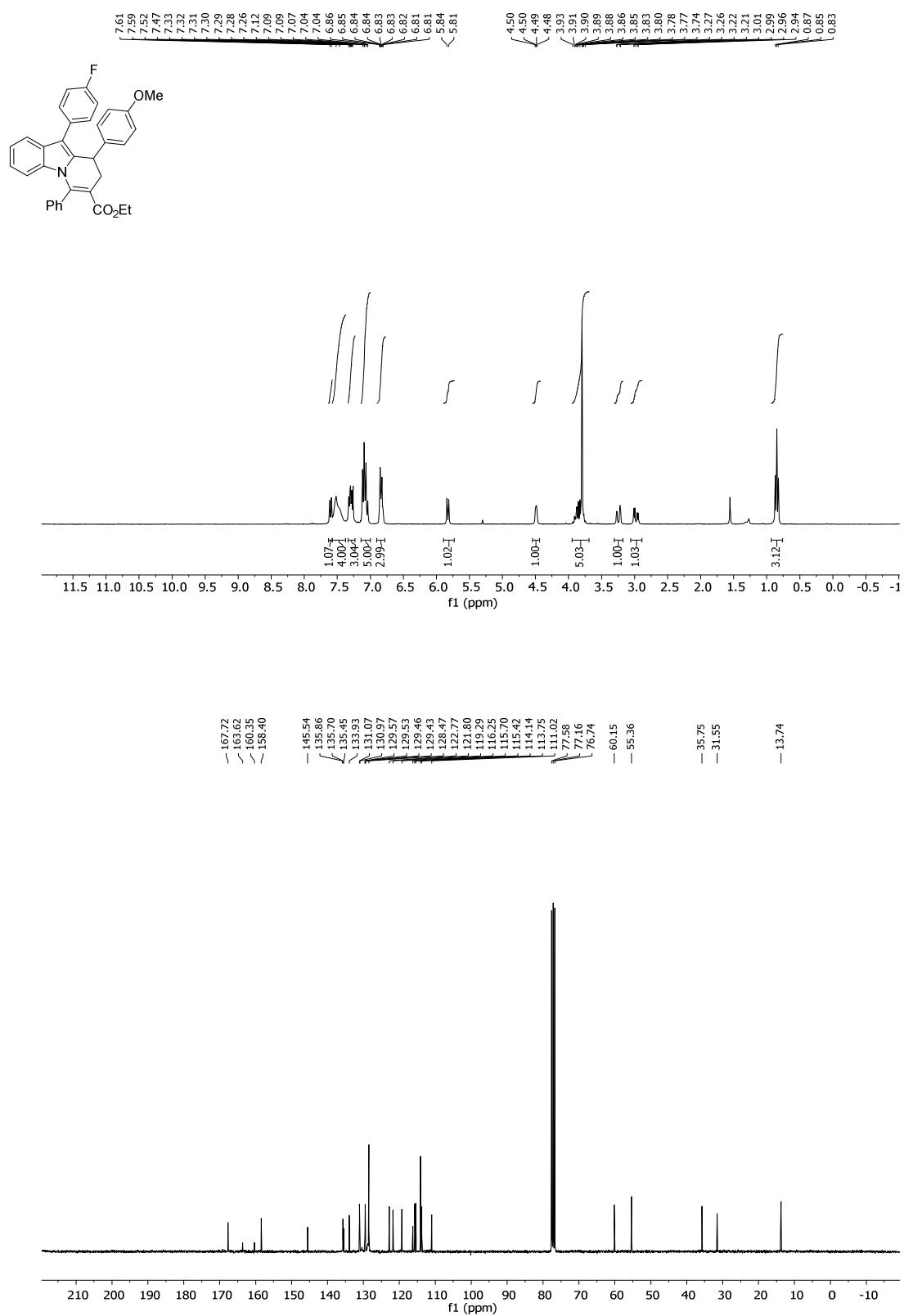


Figure S52. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5k

51

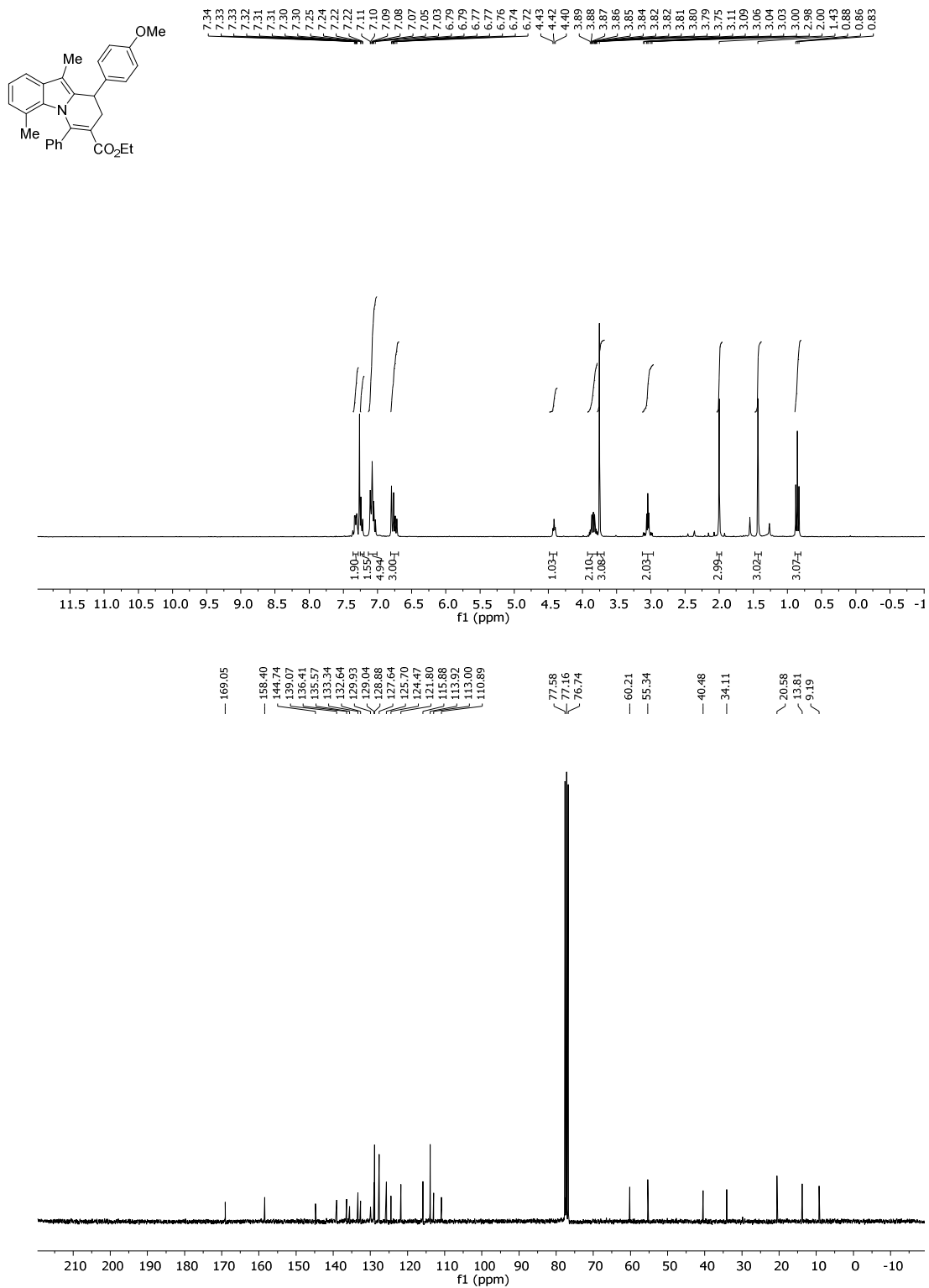


Figure S53. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 51

5m

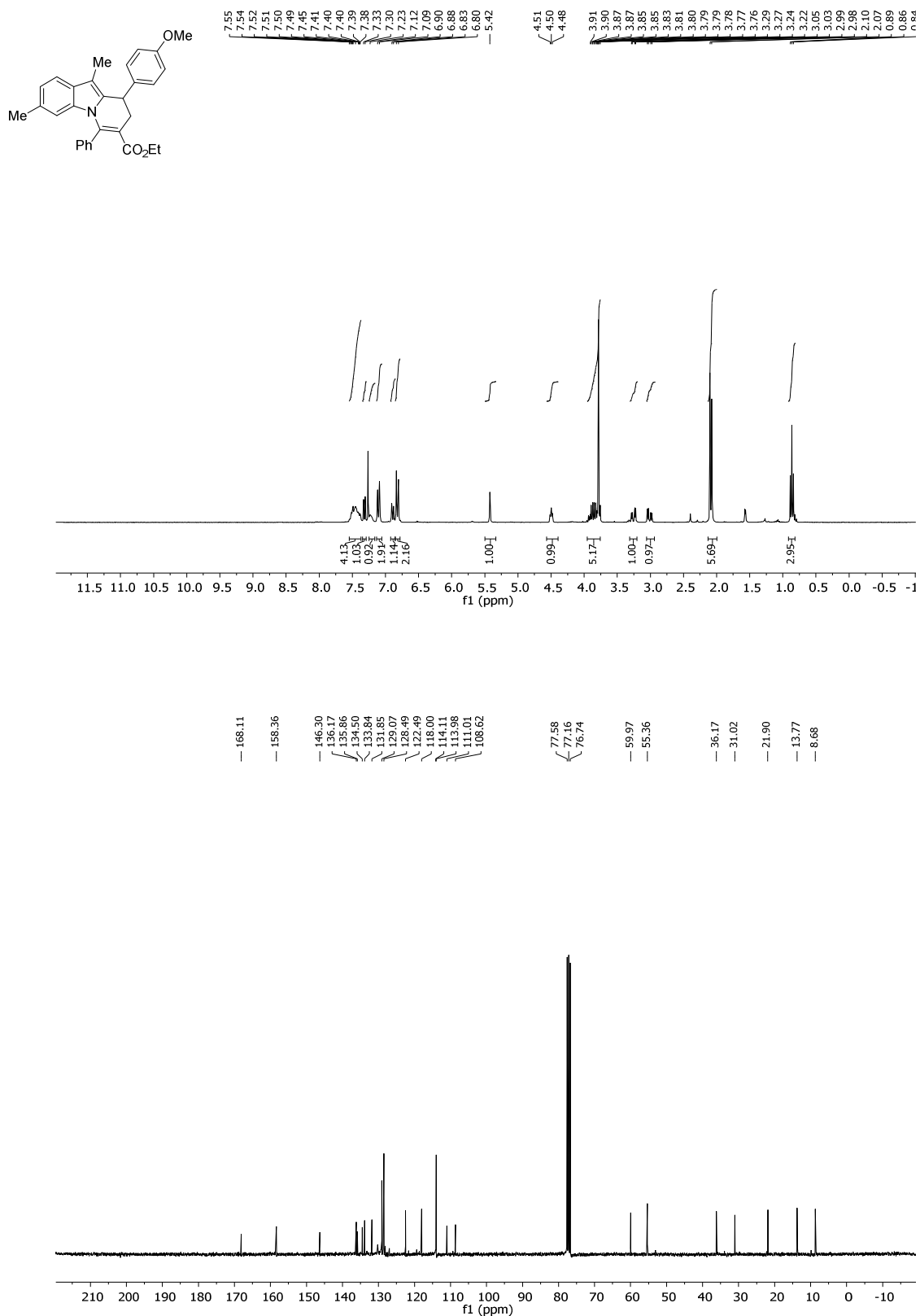


Figure S54. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5m

5n

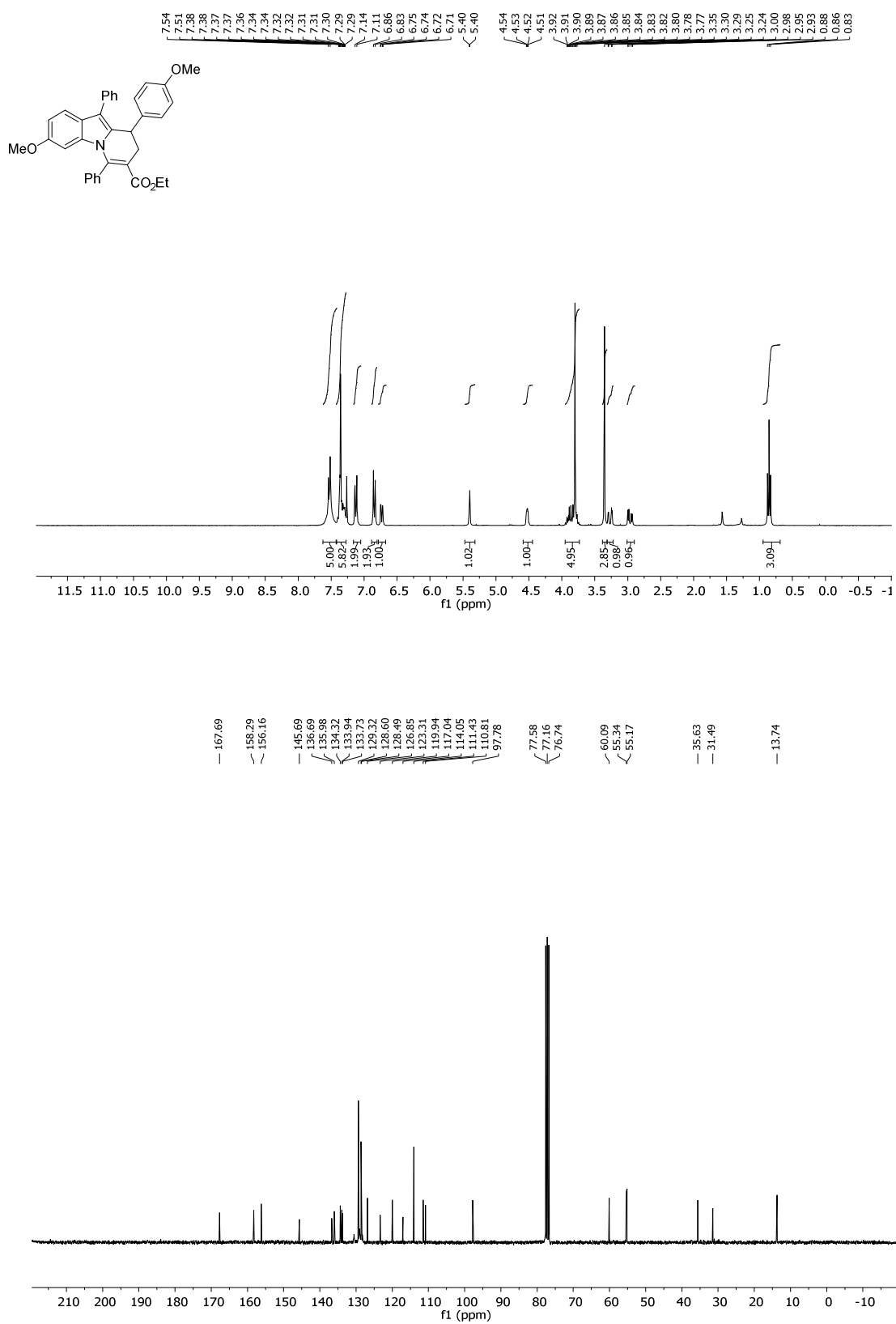


Figure S55. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5n

50

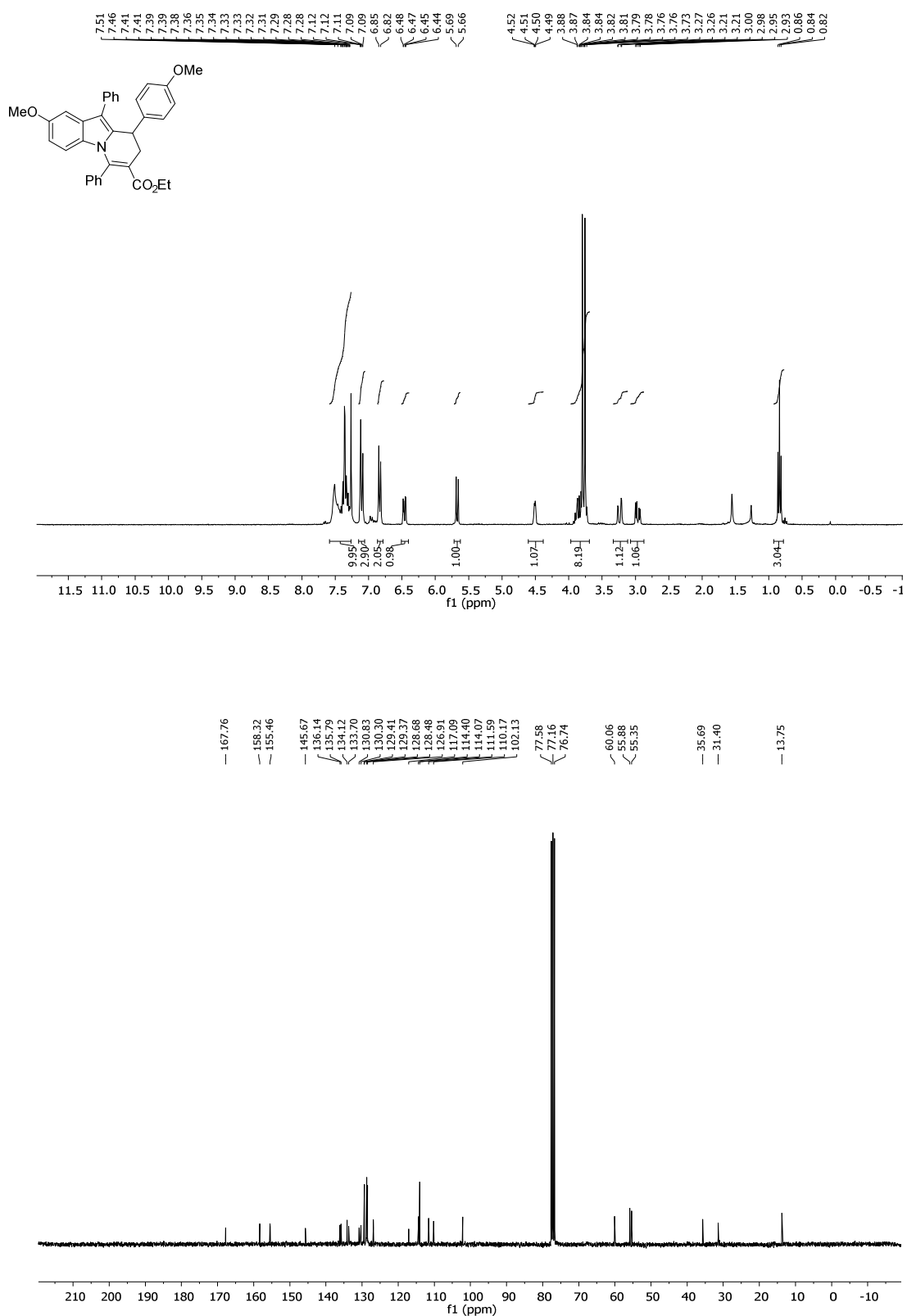


Figure S56. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 50

5p

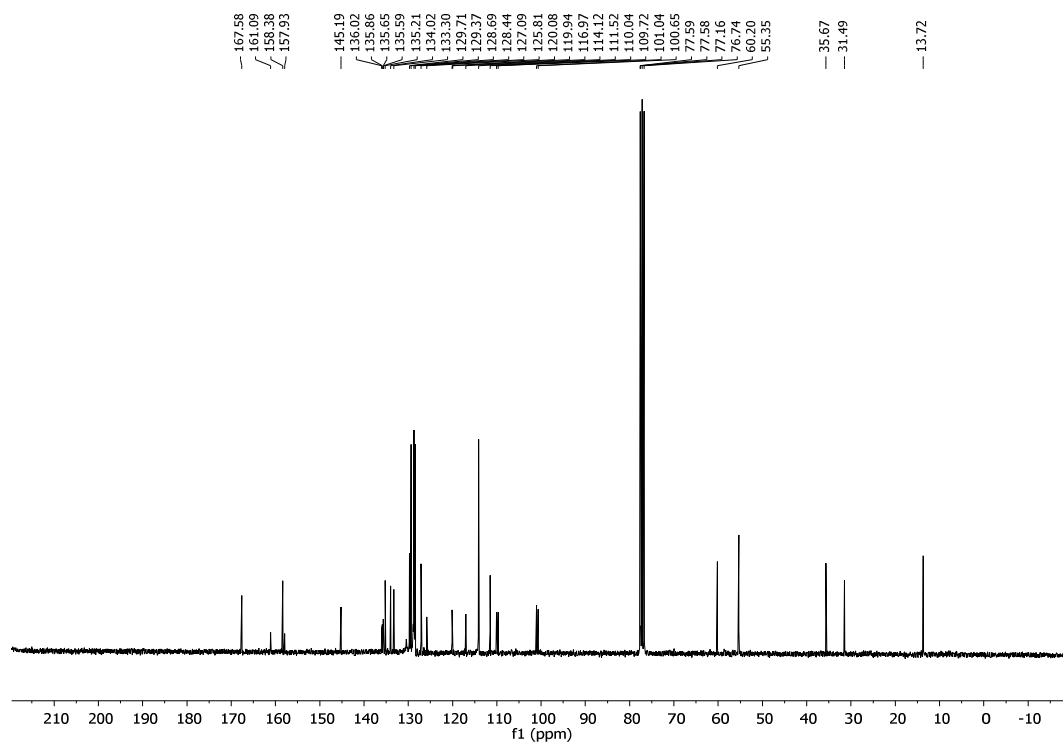
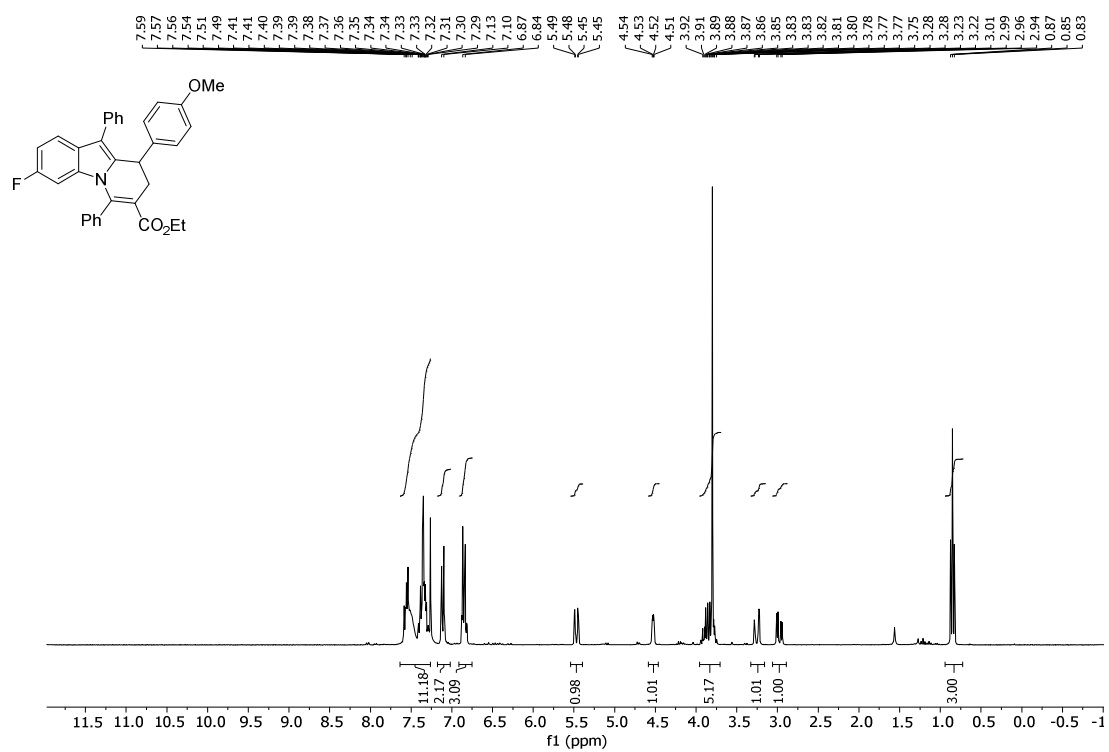


Figure S57. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5p

5q

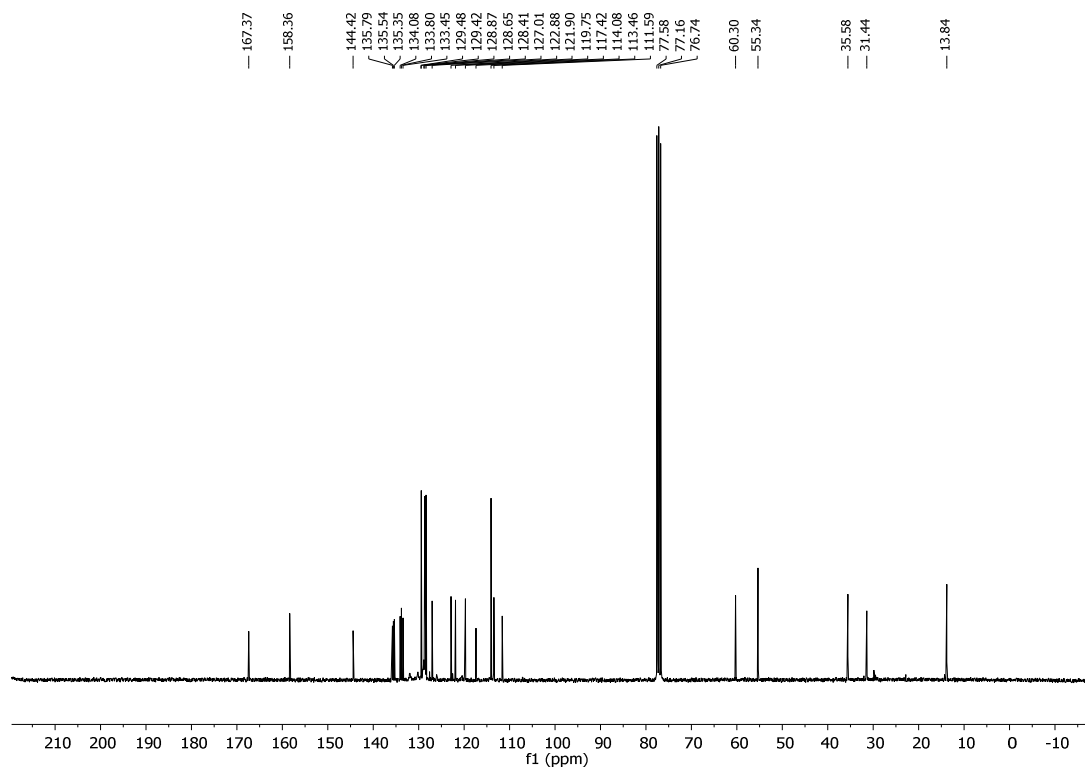
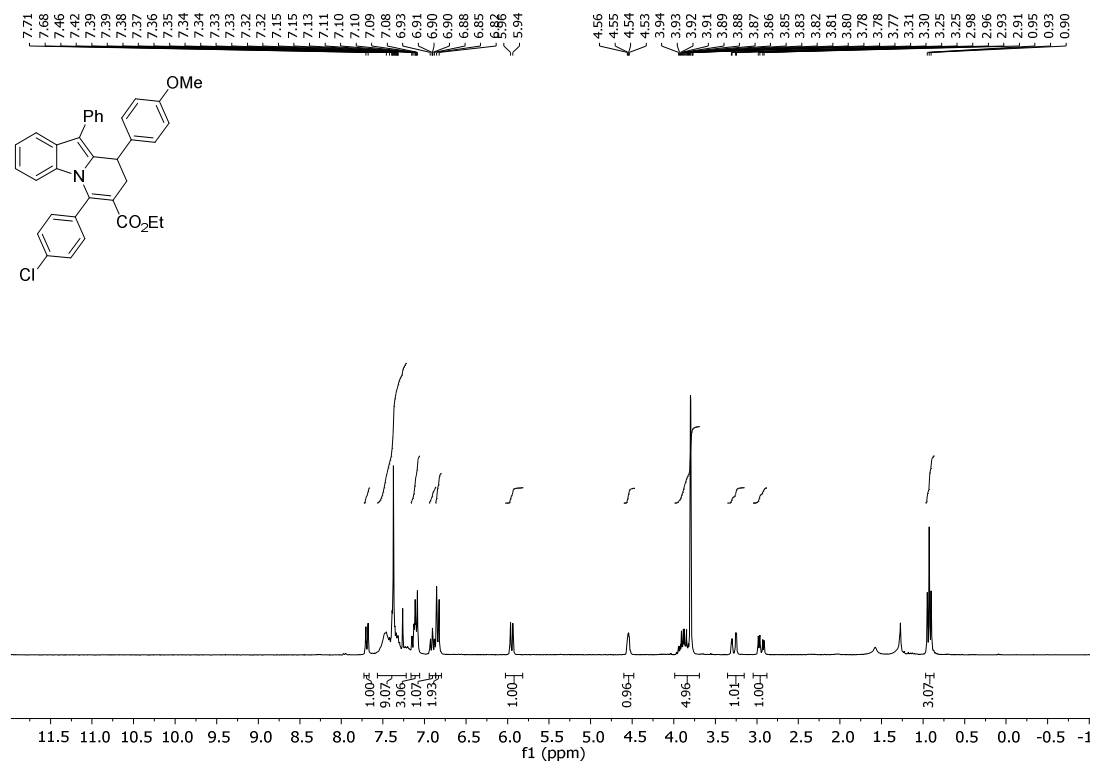


Figure S58. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5q

5r

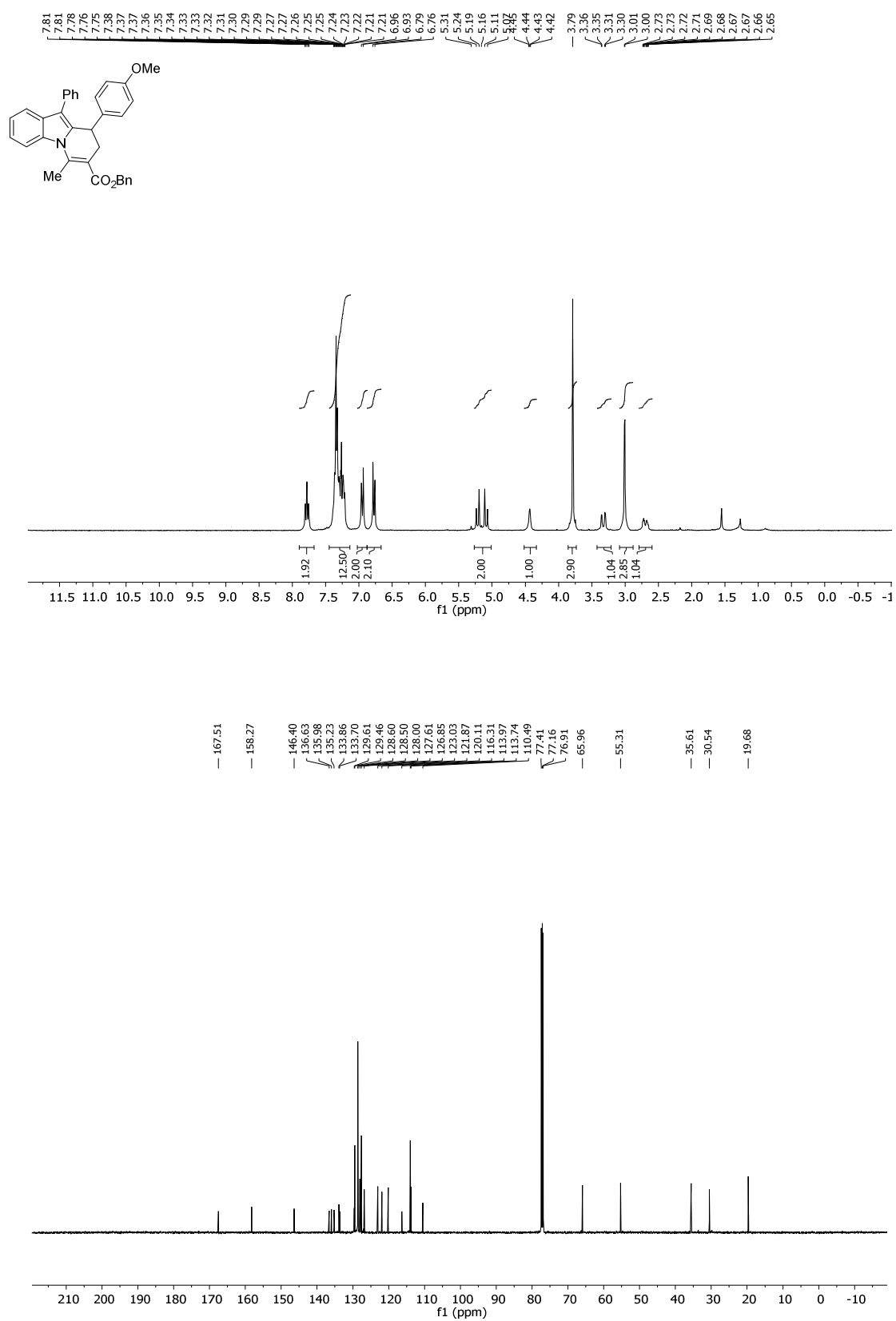


Figure S59. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5r

5s

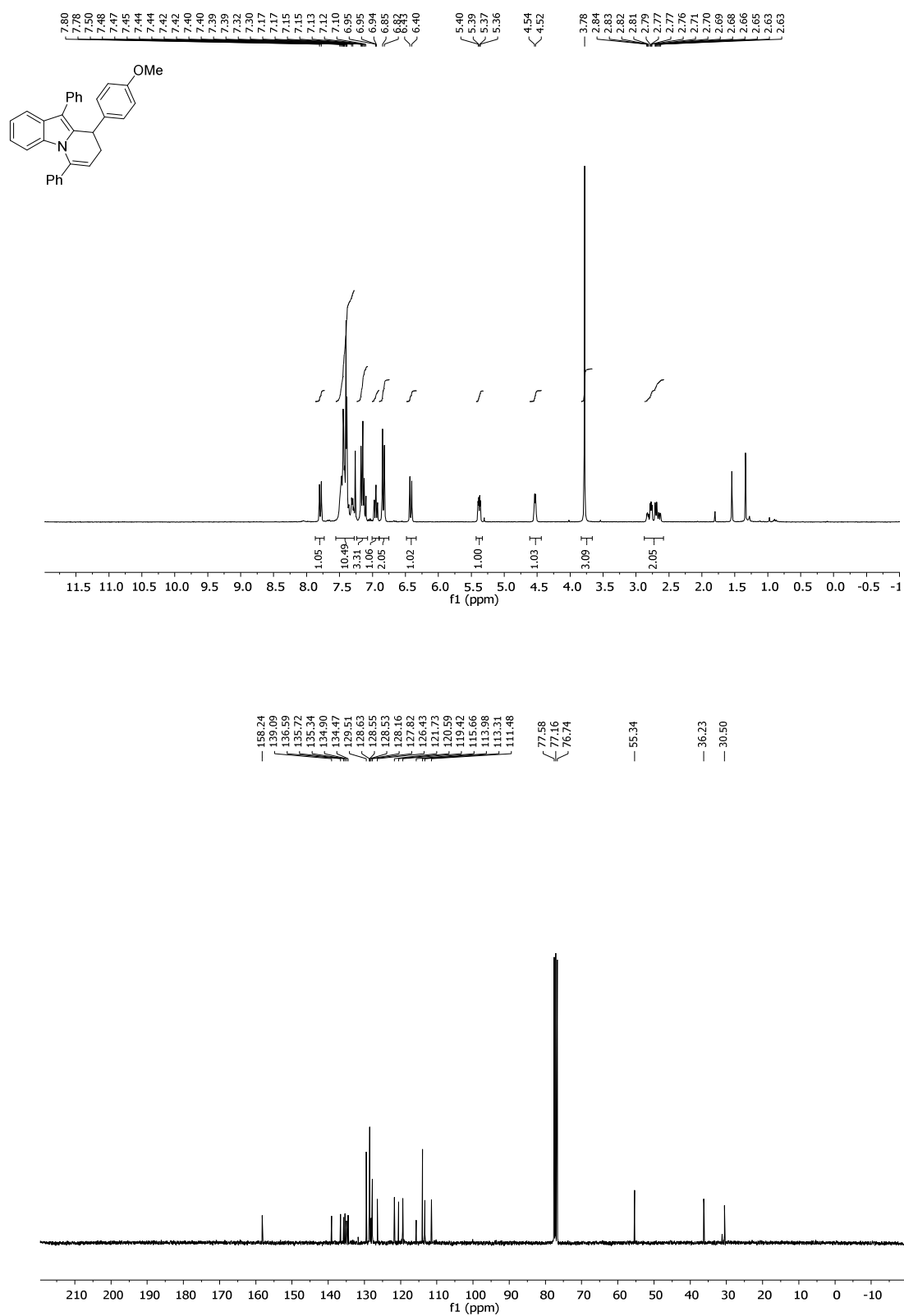


Figure S60. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 5s

4.5 Dihydropyridindoindoles 6a-g

6a

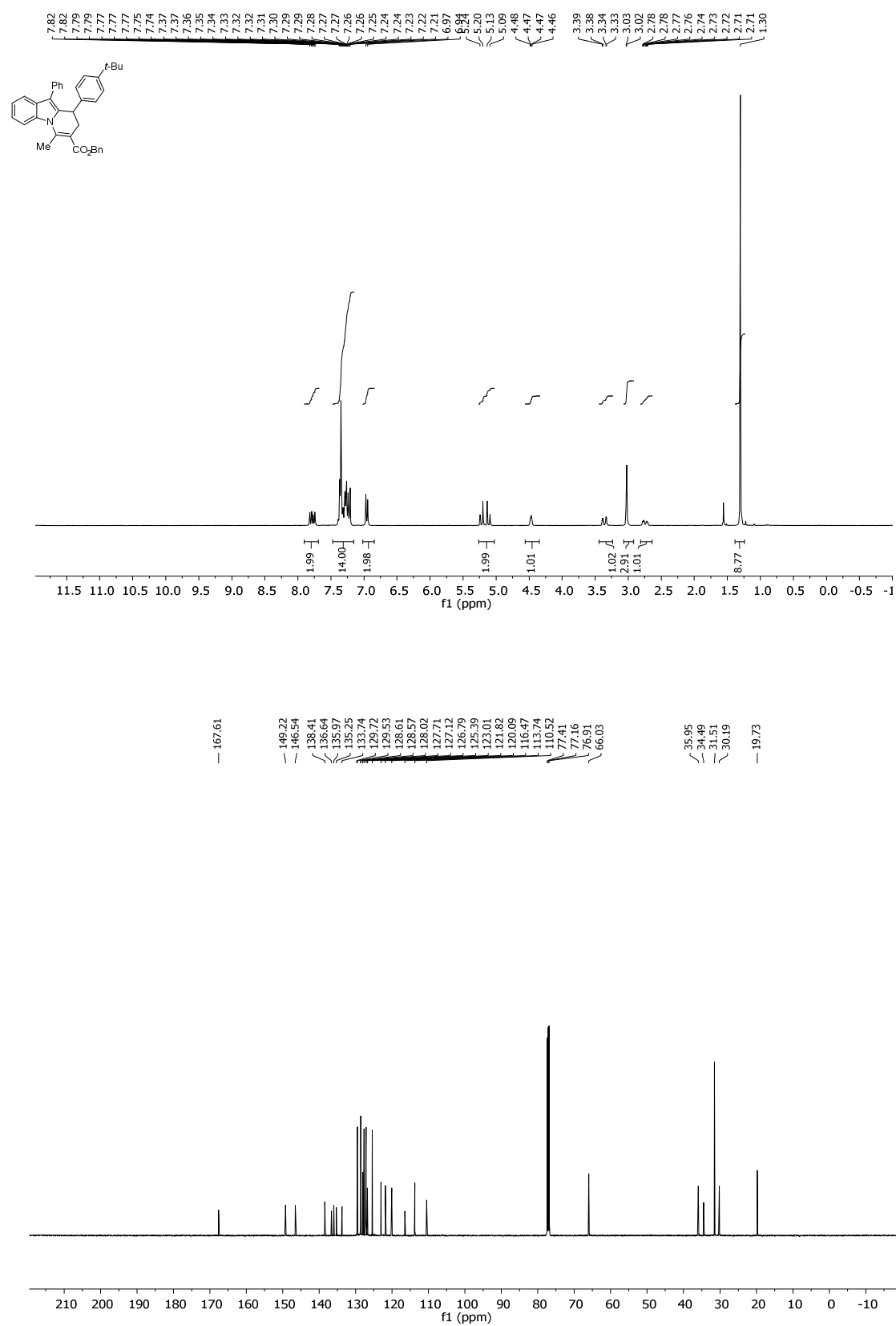


Figure S61. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 6a

6b

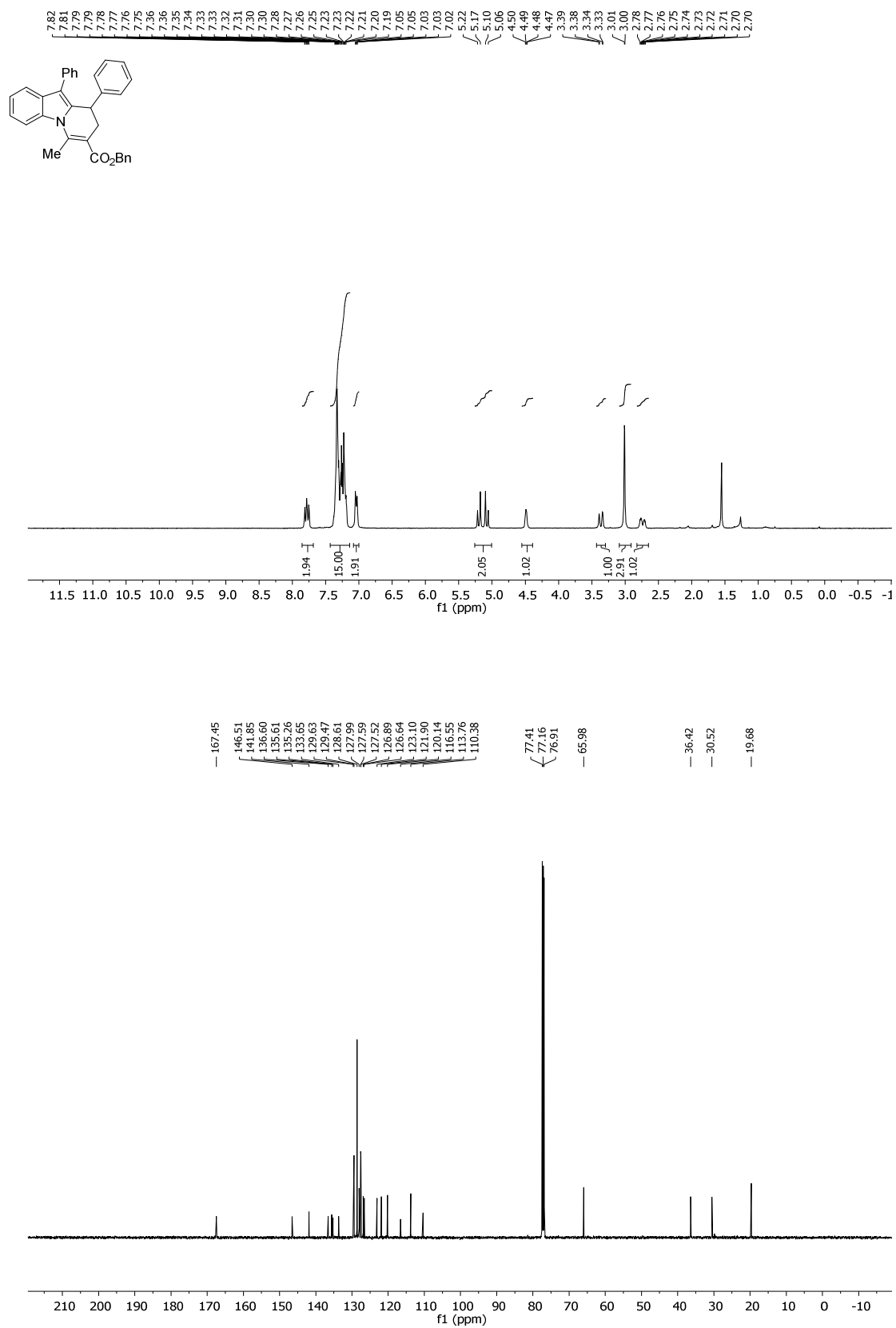


Figure S62. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 6b

6c

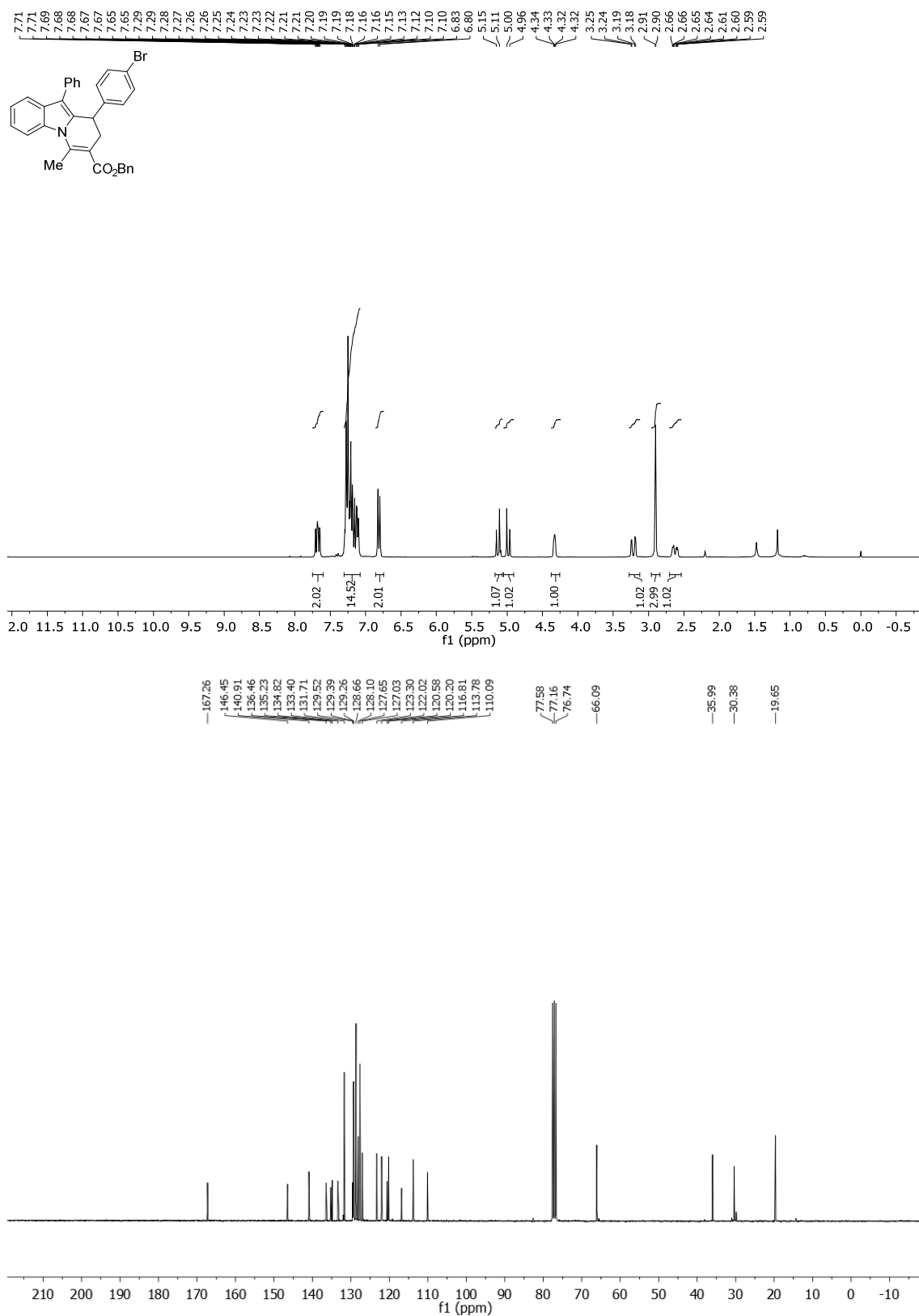


Figure S63. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 6c

6d

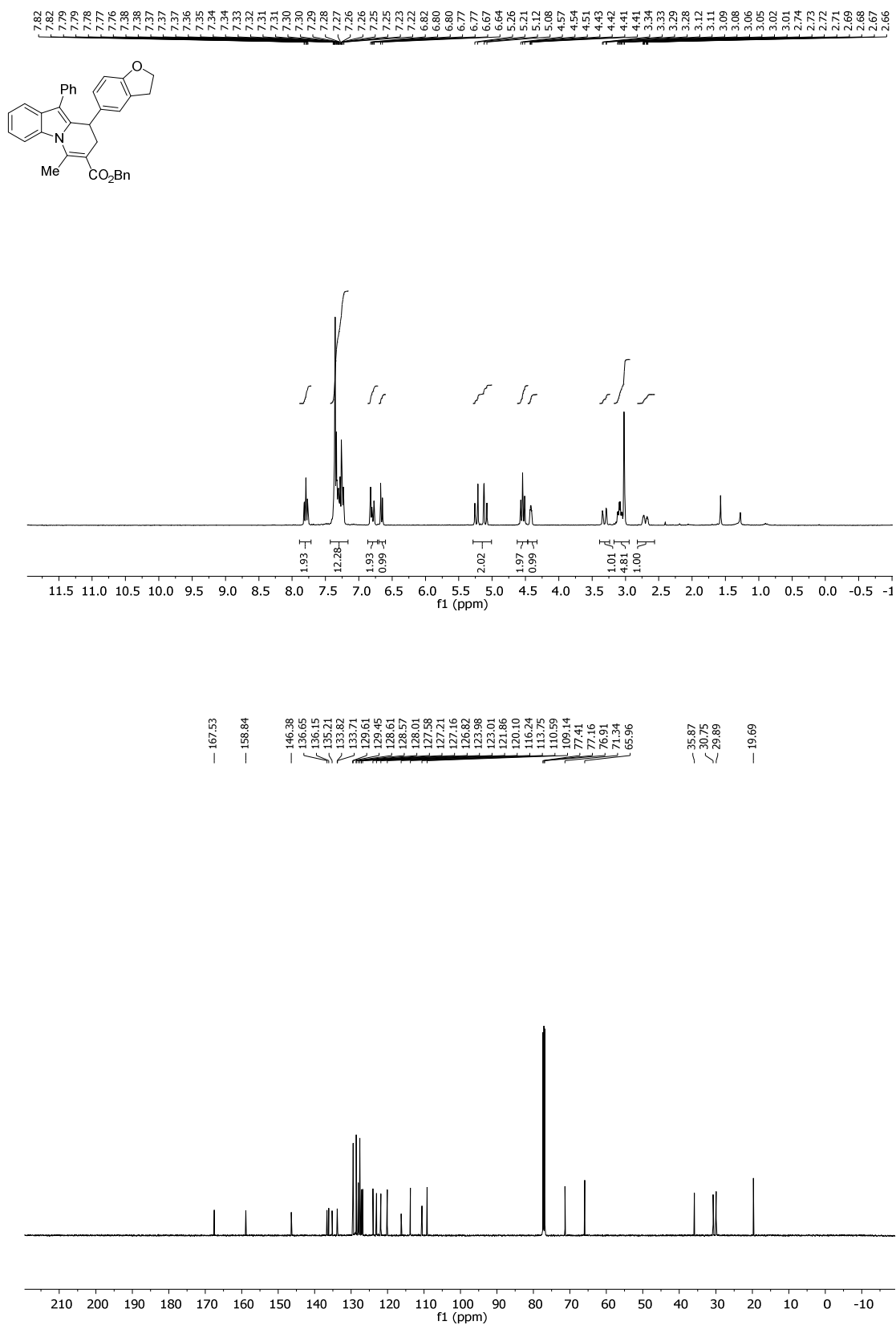


Figure S64. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 6d

6e

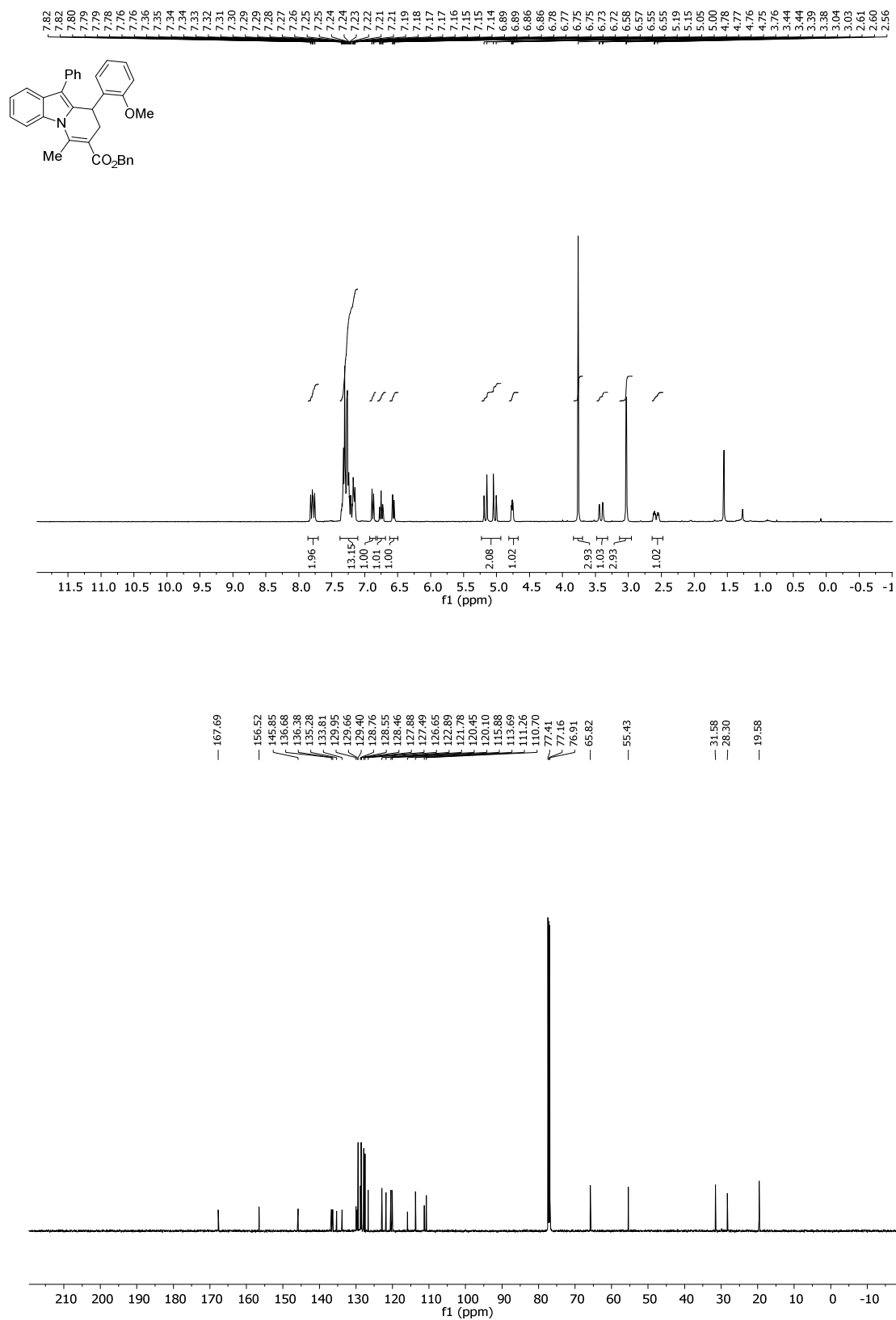


Figure S65. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 6e

6f

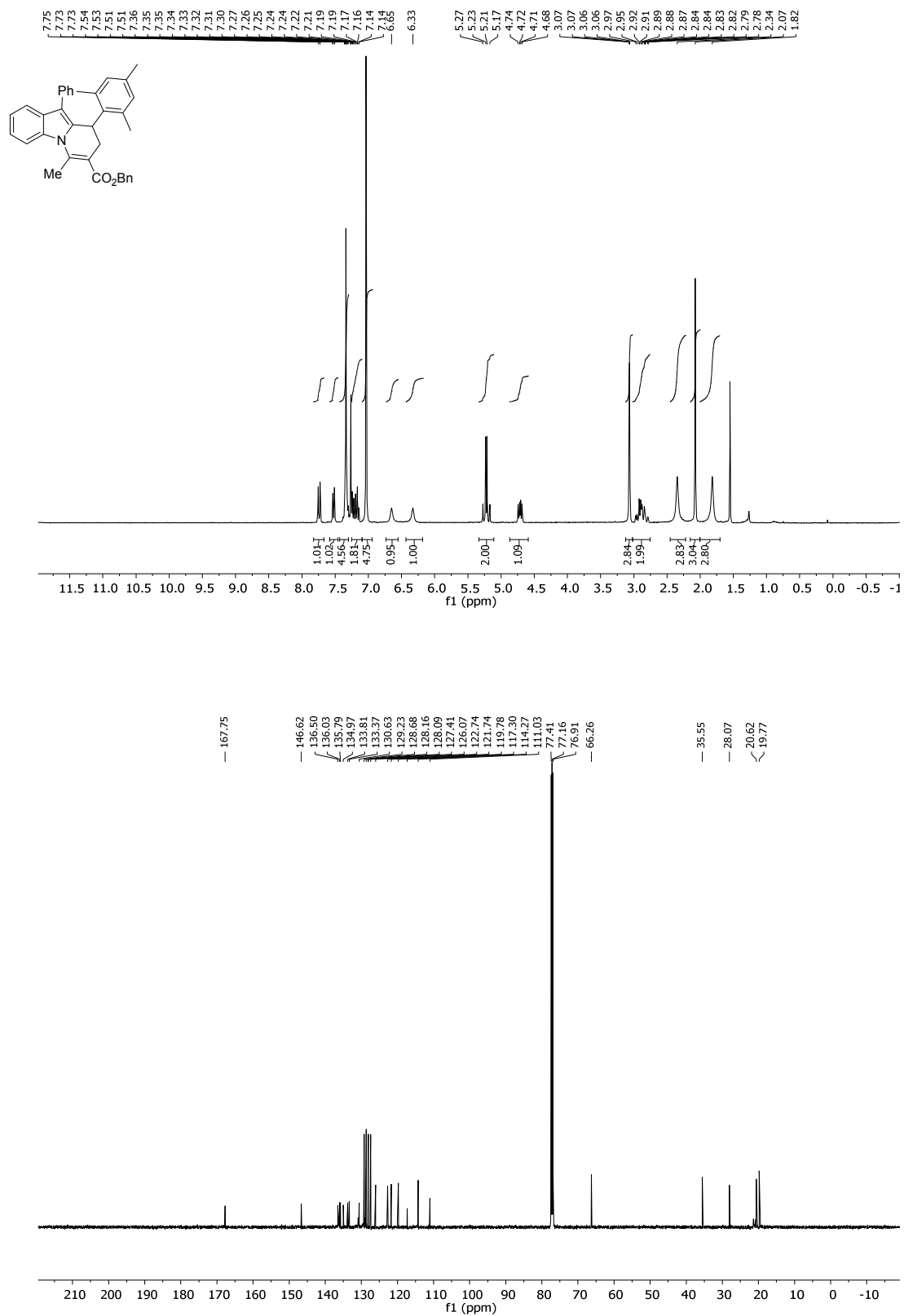


Figure S66. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 6f

6g

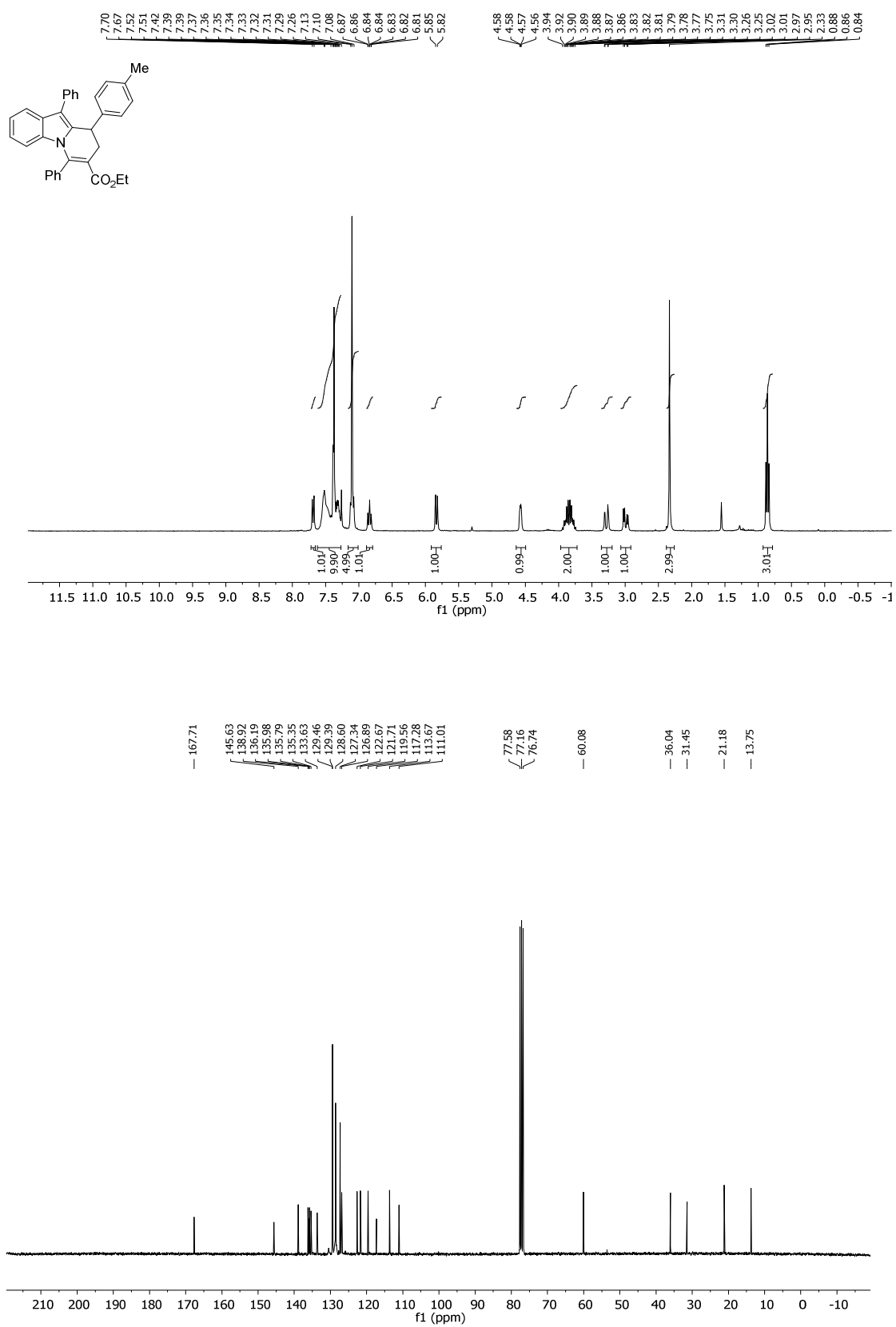


Figure S67. ¹H-NMR (300 MHz, CDCl₃) and ¹³C-NMR (75 MHz, CDCl₃) spectra of compound 6g

5. Computational Studies

5.1. Computational Methods

All of the calculations were performed using the Gaussian09 program.²² Computations were done using B3LYP functional²³ in conjunction with Grimme's dispersion correction²⁴ and standard basis set def2SVP.²⁵ Geometry full optimizations were made at b3lyp-d3bj/def2SVP level. Solvent effects (toluene) were considered using the PCM model.²⁶ The nature of stationary points was defined on the basis of calculations of normal vibrational frequencies (force constant Hessian matrix). The optimizations were carried out using the Berny analytical gradient optimization method.²⁷ Minimum energy pathways for the reactions studied were found by gradient descent of transition states in the forward and backward direction of the transition vector (IRC analysis),²⁸ using the Hratchian-Schlegel algorithm.²⁹ Analytical second derivatives of the energy were calculated to classify the nature of every stationary point, to determine the harmonic vibrational frequencies, and to provide zero-point vibrational energy corrections. The thermal and entropic contributions to the free energies were also obtained from the vibrational frequency calculations, using the unscaled frequencies. Structural representations were generated using CYLView.³⁰

²² Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT,; 2009.

²³ (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789.

²⁴ (a) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104-154119. (b) Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.* **2011**, *32*, 1456-1465.

²⁵ (a) Weigend, F. *Phys. Chem. Chem. Phys.* **2006**, *8*, 227-236. (b) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

²⁶ (a) J. Tomasi and M. Persico, *Chem. Rev.*, 1994, **94**, 2027-2094. (b) M. Cossi, G. Scalmani, N. Rega and V. Barone, *J. Chem. Phys.*, 2002, **117**, 43-54.

²⁷ (a) Schlegel, H. B. *J. Comput. Chem.* **1982**, *3*, 214218. (b) Schlegel, H. B. In *Modern Electronic Structure Theory*; Yarkony, D. R., Ed.; World Scientific Publishing: Singapore, 1994.

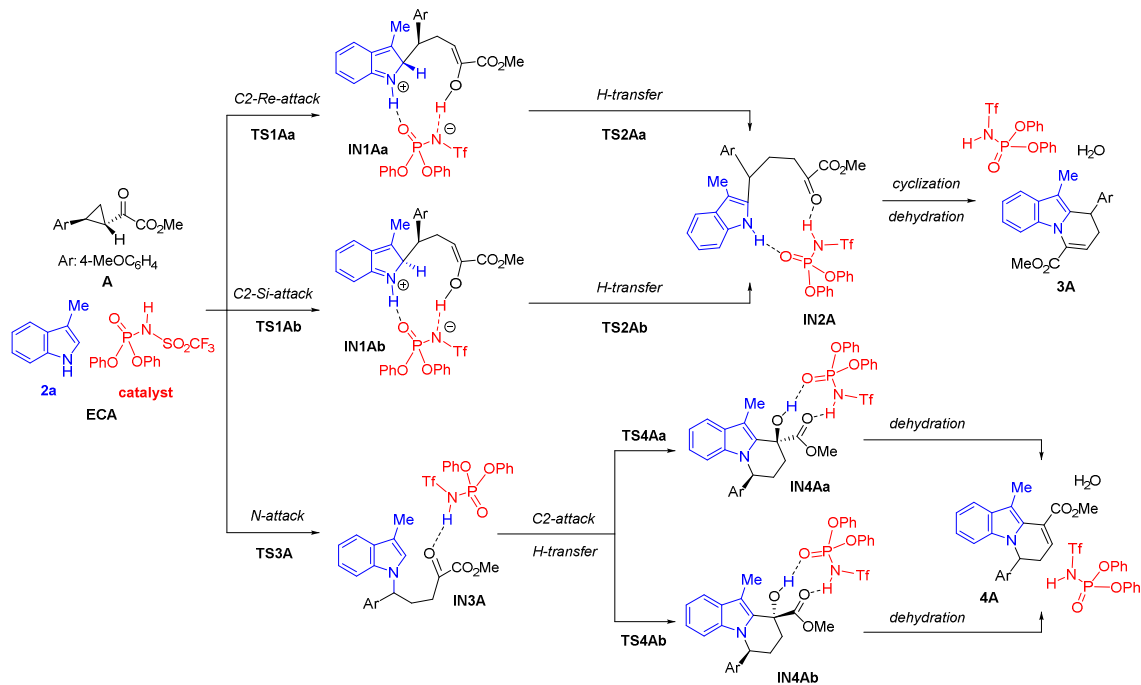
²⁸ (a) Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363-368. (b) Fukui, K. *J. Phys. Chem.* **1970**, *74*, 4161-4163.

²⁹ Hratchian, H. P.; Schlegel, H. B. *J. Phys. Chem. A* **2002**, *106*, 165-169.

³⁰ C. Y. Legault, *Université de Sherbrooke*, 2009, <http://www.cylview.org>.

5.2. Reaction of cyclopropane **A** with indole **2a**

During the reaction of cyclopropane **A** with indole **2a**, diastereomers can be formed. **a** and **b** series correspond to the more and less favoured pathways, respectively. In the main manuscript only the favoured **a** series is shown.



Scheme S6. Reaction of cyclopropane **A** with indole **2a**

5.2.1. Energy Profiles

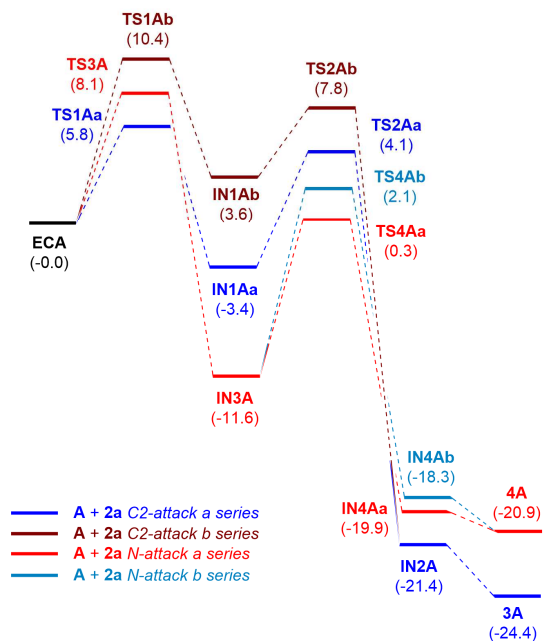


Figure S68. Energy profile (free relative energies given in kcal/mol) for the reaction of cyclopropane **A** with indole **2a**

5.2.2. Energy values

Table S4. Total energy and zero-point vibrational energy (hartrees); absolute (hartrees) and relative (kcal/mol) energies (b3lyp-gd3bj/def2svp/pcm=toluene) for the reaction of cyclopropane **A** with indole **2a**.

	E	ZPVE	E ₀	ΔE ₀ ^b	G	ΔG ^b	im. freq ^c
A	-804.136659	0.247877	-803.888782		-803.935601		
2a	-402.887911	0.157466	-402.730445		-402.762883		
(PhO)₂P(O)NHTf	-1970.887857	0.238259	-1970.649598		-1970.705829		
H₂O	-76.358890	0.021227	-76.337663		-76.355327		
ECA^a	-3177.992997	0.647542	-3177.345455	0.0	-3177.432973	0.0	
TS1Aa	-3177.984896	0.647568	-3177.337328	5.1	-3177.423772	5.8	-249.6
TS1Ab	-3177.977210	0.647789	-3177.329421	10.1	-3177.416409	10.4	-215.9
IN1Aa	-3177.999129	0.649241	-3177.349888	-2.8	-3177.438386	-3.4	
IN1Ab	-3177.987086	0.648915	-3177.338171	4.6	-3177.427253	3.6	
TS2Aa	-3177.989128	0.645838	-3177.343290	1.4	-3177.426360	4.1	-788.5
TS2Ab	-3177.981755	0.644684	-3177.337071	5.3	-3177.420488	7.8	-1347.9
IN2A	-3178.030531	0.650798	-3177.379733	-21.5	-3177.467035	-21.4	
3A	-3178.032854	0.648961	-3177.383893	-24.1	-3177.471792	-24.4	
TS3A	-3177.981802	0.648155	-3177.333647	7.4	-3177.420067	8.1	-147.5
IN3a	-3178.013123	0.649770	-3177.363353	-11.2	-3177.451409	-11.6	
TS4Aa	-3178.001903	0.649796	-3177.352107	-4.2	-3177.432540	0.3	-171.7
TS4Ab	-3177.995834	0.649555	-3177.346279	-0.5	-3177.429566	2.1	-298.3
IN4Aa	-3178.032773	0.652039	-3177.380734	-22.1	-3177.464657	-19.9	
IN4Ab	-3178.024747	0.651364	-3177.373383	-17.5	-3177.462083	-18.3	
4A	-3178.019465	0.648653	-3177.380812	-22.2	-3177.466317	-20.9	

^a encounter complex formed by the two reagents and the catalyst. ^b referred to **ECA**. ^cAll minima have no imaginary frequencies and transition structures presented one imaginary frequency that is listed in the table.

5.2.3. Optimized geometries

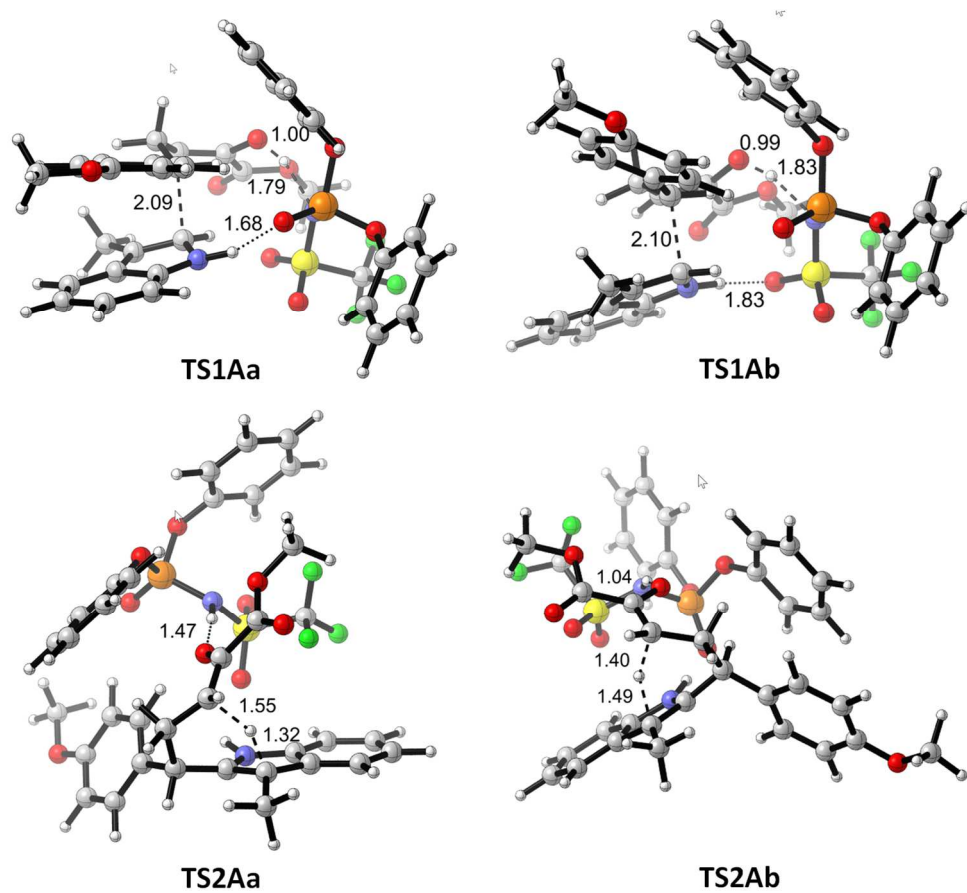


Figure S69. Optimized (b3lyp-gd3bj/def2svp/pcm=toluene) geometries of the located transition structures for the C2-attack.

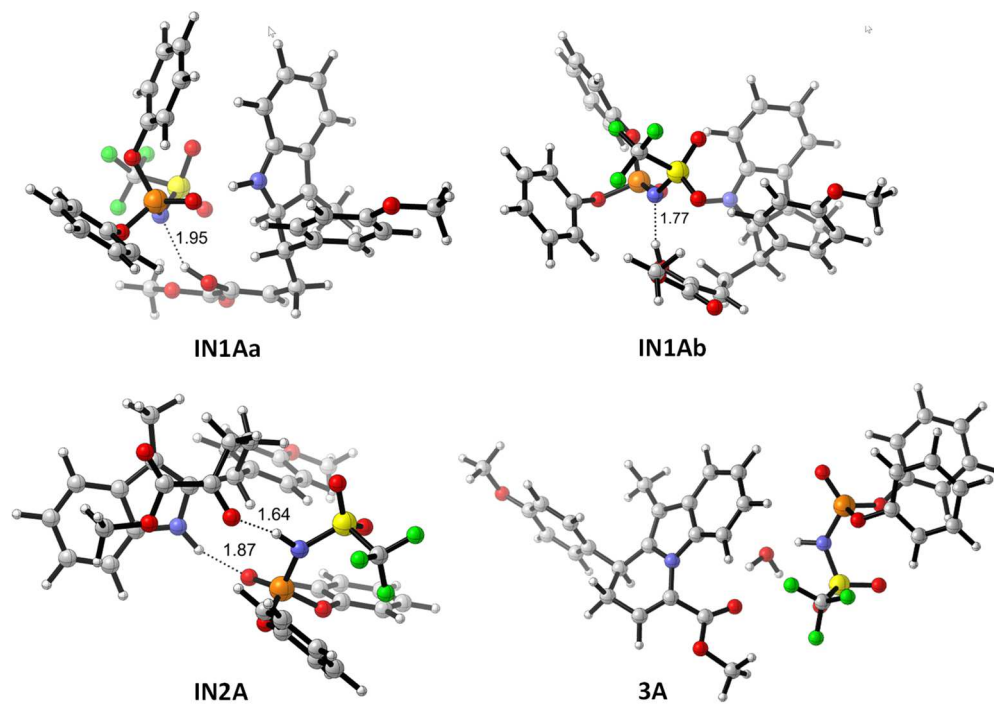


Figure S70. Optimized (b3lyp-gd3bj/def2svp/pcm=toluene) geometries of the located minima for the C2-attack.

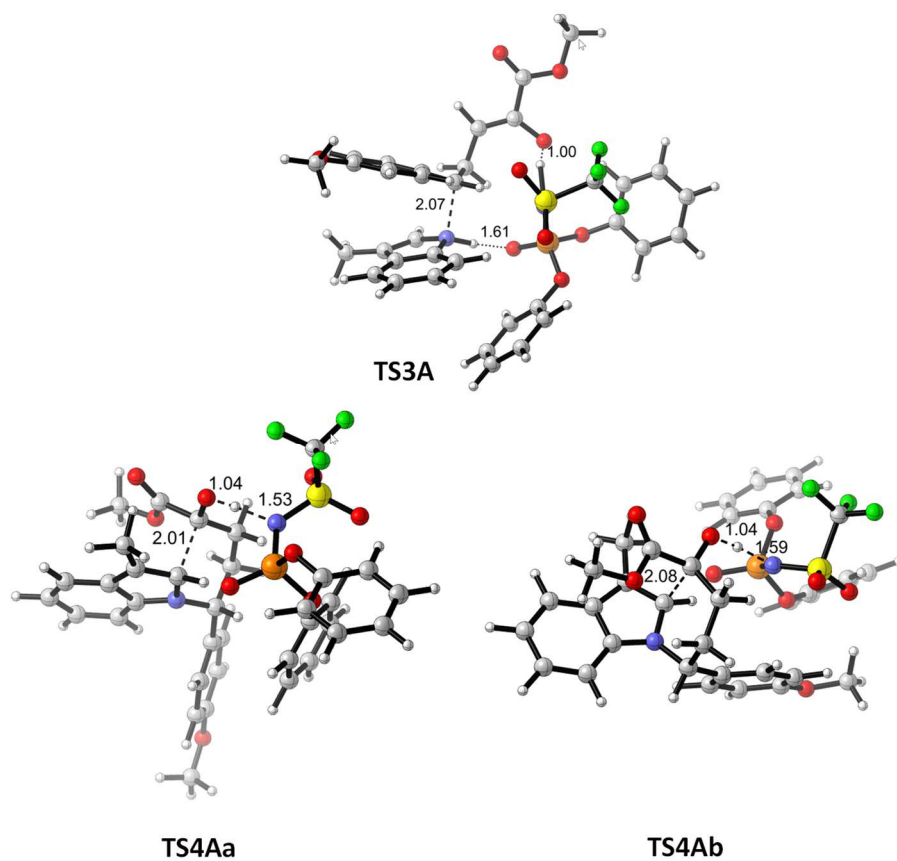


Figure S71. Optimized (b3lyp-gd3bj/def2svp/pcm=toluene) geometries of the located transition structures for the *N*-attack.

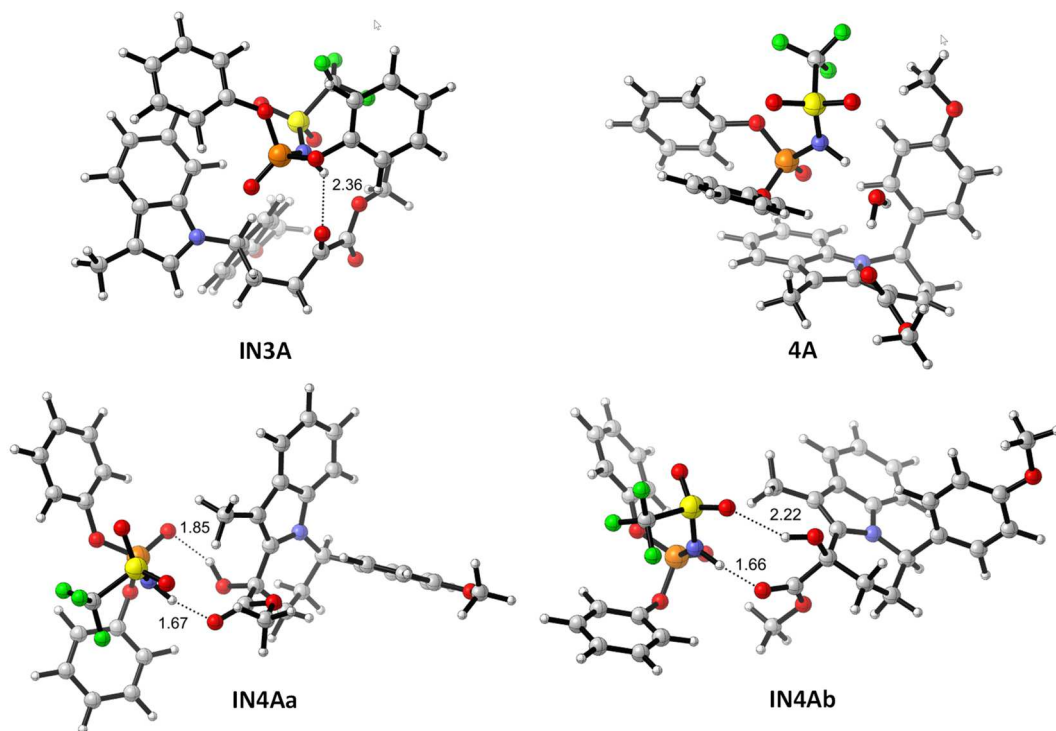
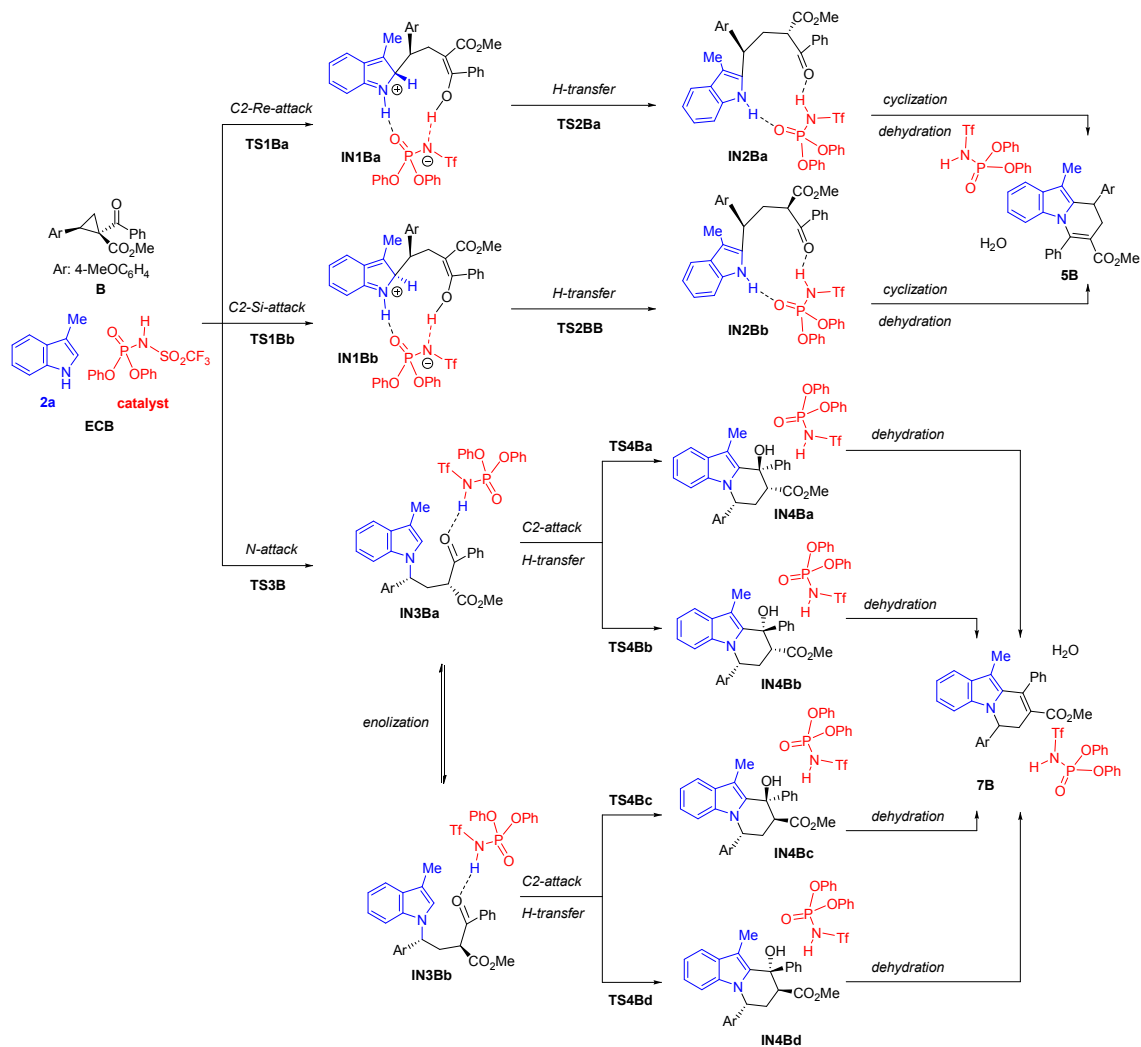


Figure S72. Optimized (b3lyp-gd3bj/def2svp/pcm=toluene) geometries of the located minima for the *N*-attack.

5.3. Reaction of cyclopropane **B** with indole **2a**

During the reaction of cyclopropane **B** with indole **2a**, diastereomers can be formed. **a** and **b** series correspond to the more and less favoured pathways, respectively. In the main manuscript only the favoured **a** series is shown. Although two intermediates **IN3Ba** and **IN3Bb** can be formed, only one **TS3B** is possible due to the required coordination between the reagent and the catalyst.



Scheme S7. Reaction of cyclopropane **B** with indole **2a**

5.3.1. Energy Profiles

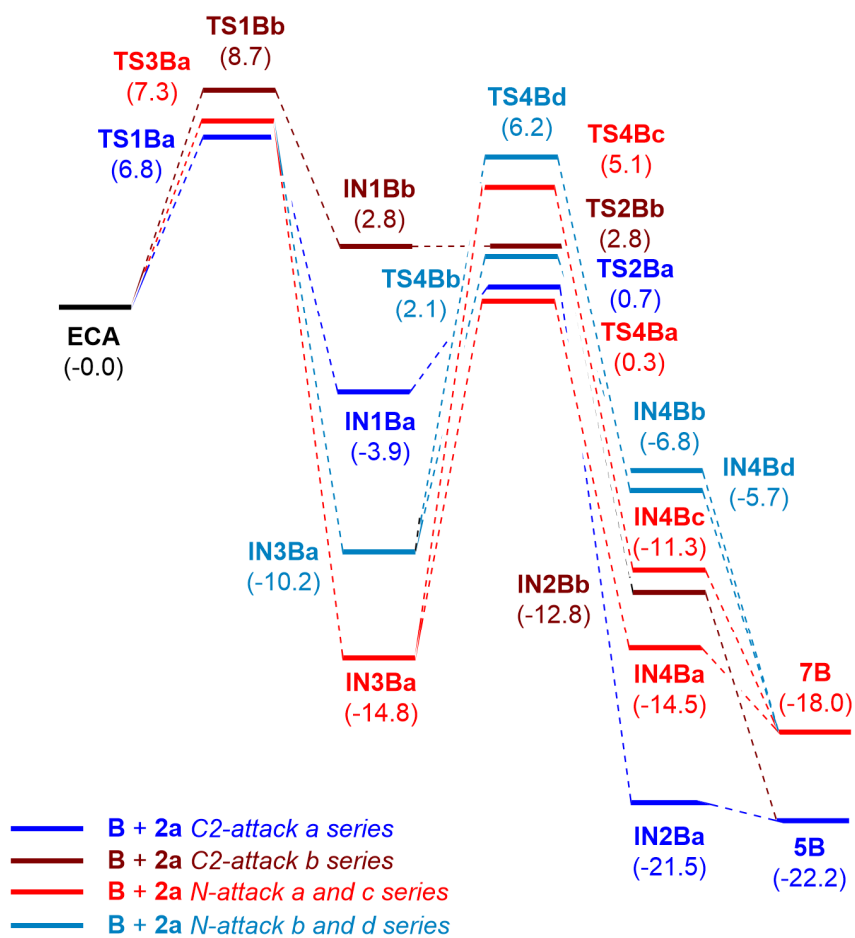


Figure S72. Energy profile (free relative energies given in kcal/mol) for the reaction of cyclopropane **B** with indole **2a**

5.3.2. Energy values

Table S5. Total energy and zero-point vibrational energy (hartrees); absolute (hartrees) and relative (kcal/mol) energies (b3lyp-gd3bj/def2svp/pcm=toluene) for the reaction of cyclopropane **B** with indole **2a**.

	E	ZPVE	E ₀	ΔE ₀ ^b	G	ΔG ^b	im. freq ^c
B	-1035.069736	0.329060	-1034.740676		-1034.793930		
2a	-402.887911	0.157466	-402.730445		-402.762883		
(PhO)₂P(O)NHTf	-1970.887857	0.238259	-1970.649598		-1970.705829		
H₂O	-76.358890	0.021227	-76.337663		-76.355327		
ECB^a	-3408.917001	0.728241	-3408.188760	0.0	-3408.283475	0.0	
TS1Ba	-3408.910452	0.729495	-3408.180957	4.9	-3408.272711	6.8	-352.6
TS1Bb	-3408.905479	0.728517	-3408.176962	7.4	-3408.269565	8.7	-136.6
IN1Ba	-3408.926049	0.730252	-3408.195797	-4.4	-3408.289761	-3.9	
IN1Bb	-3408.917315	0.731029	-3408.186286	1.6	-3408.279017	2.8	
TS2Ba	-3408.918701	0.726374	-3408.192327	-2.2	-3408.282311	0.7	-800.5
TS2Bb	-3408.912052	0.724731	-3408.187321	0.9	-3408.279045	2.8	-1466.3
IN2Ba	-3408.955075	0.731390	-3408.223685	-21.9	-3408.317674	-21.5	
IN2Bb	-3408.937882	0.730660	-3408.207222	-11.6	-3408.303951	-12.8	
5B	-3408.958833	0.730555	-3408.228278	-24.8	-3408.318820	-22.2	
TS3Ba	-3408.910994	0.729872	-3408.181122	4.8	-3408.271765	7.3	-188.6
IN3Ba	-3408.941242	0.731425	-3408.209817	-13.2	-3408.307074	-14.8	
IN3Bb	-3408.937014	0.731003	-3408.206011	-10.8	-3408.299777	-10.2	
TS4Ba	-3408.917736	0.731593	-3408.186143	1.6	-3408.279254	2.6	-298.9
TS4Bb	-3408.925095	0.731981	-3408.193114	-2.7	-3408.279558	2.5	-336.8
TS4Bc	-3408.912783	0.730736	-3408.182047	4.2	-3408.275322	5.1	-319.6
TS4Bd	-3408.913640	0.730913	-3408.182727	3.8	-3408.273572	6.2	-348.7
IN4Ba	-3408.951888	0.733931	-3408.217957	-18.3	-3408.306630	-14.5	
IN4Bb	-3408.936018	0.733543	-3408.202475	-8.6	-3408.294330	-6.8	
IN4Bc	-3408.945866	0.732914	-3408.212952	-15.2	-3408.301439	-11.3	
IN4Bd	-3408.936720	0.733356	-3408.203364	-9.2	-3408.292500	-5.7	
7B	-3408.950035	0.729934	-3408.220101	-19.7	-3408.312212	-18.0	

^a encounter complex formed by the two reagents and the catalyst. ^b referred to **ECB**. ^cAll minima have no imaginary frequencies and transition structures presented one imaginary frequency that is listed in the table.

5.3.3. Optimized geometries

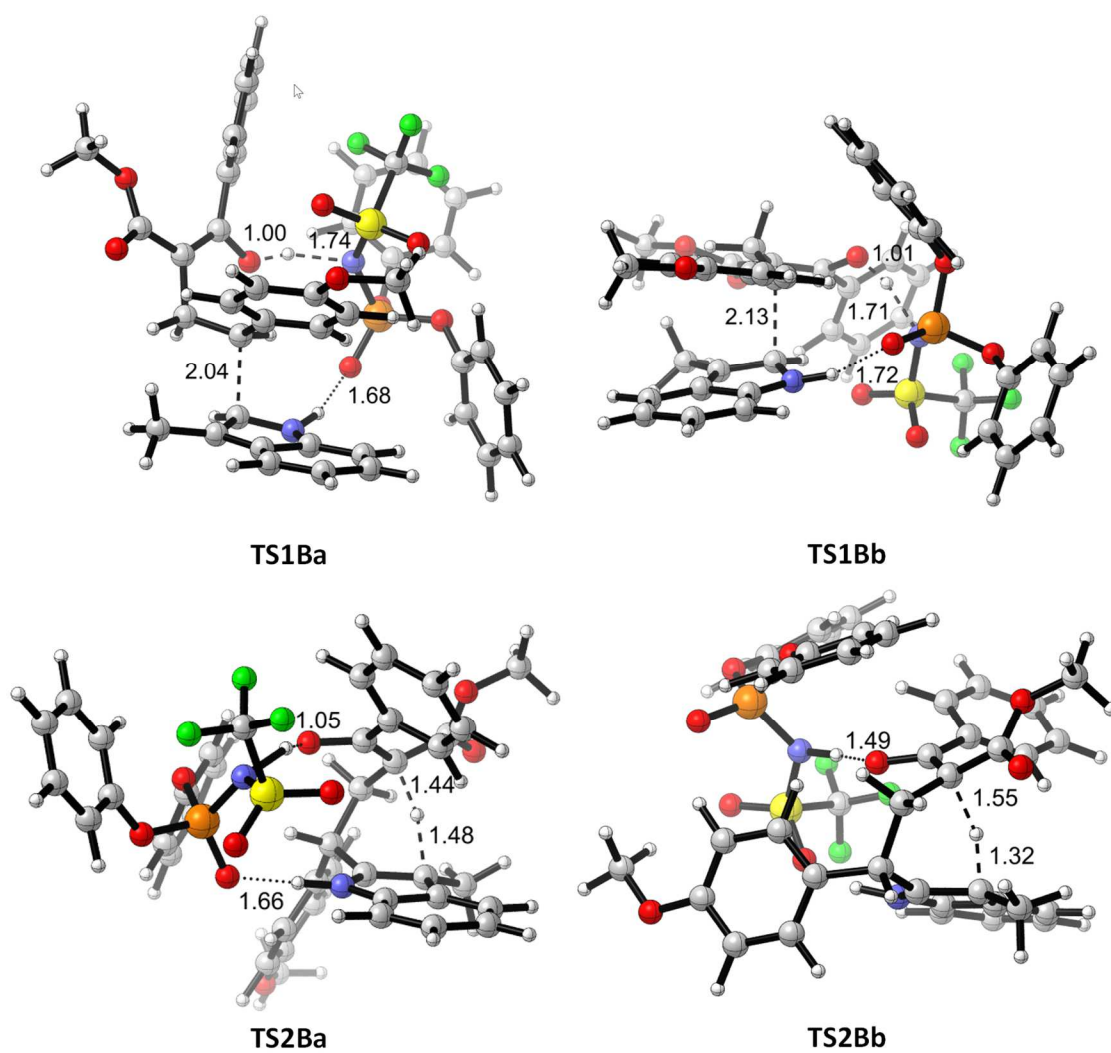


Figure S73. Optimized (b3lyp-gd3bj/def2svp/pcm=toluene) geometries of the located transition structures for the C2-attack.

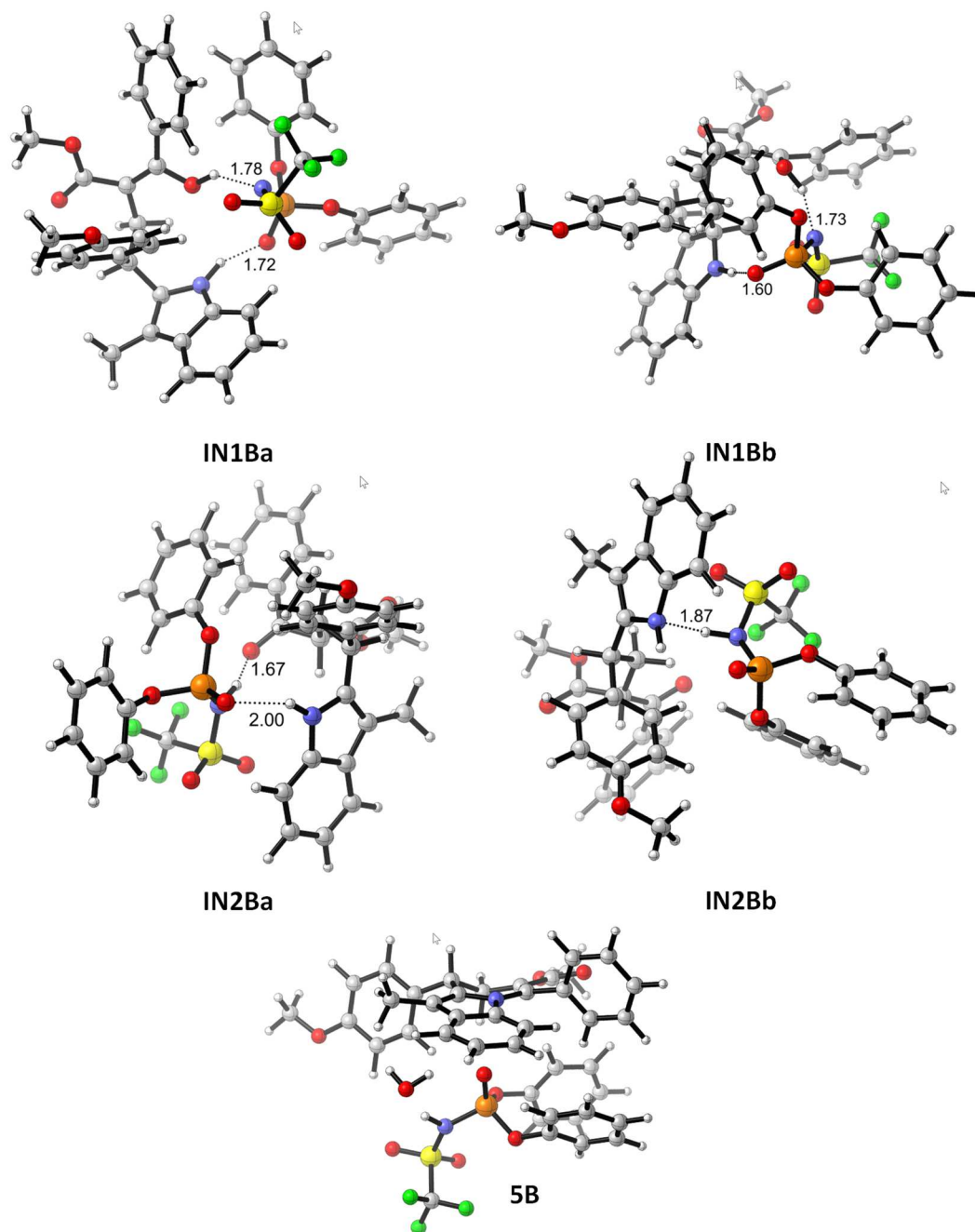


Figure S74. Optimized (b3lyp-gd3bj/def2svp/pcm=toluene) geometries of the located minima for the C2-attack.

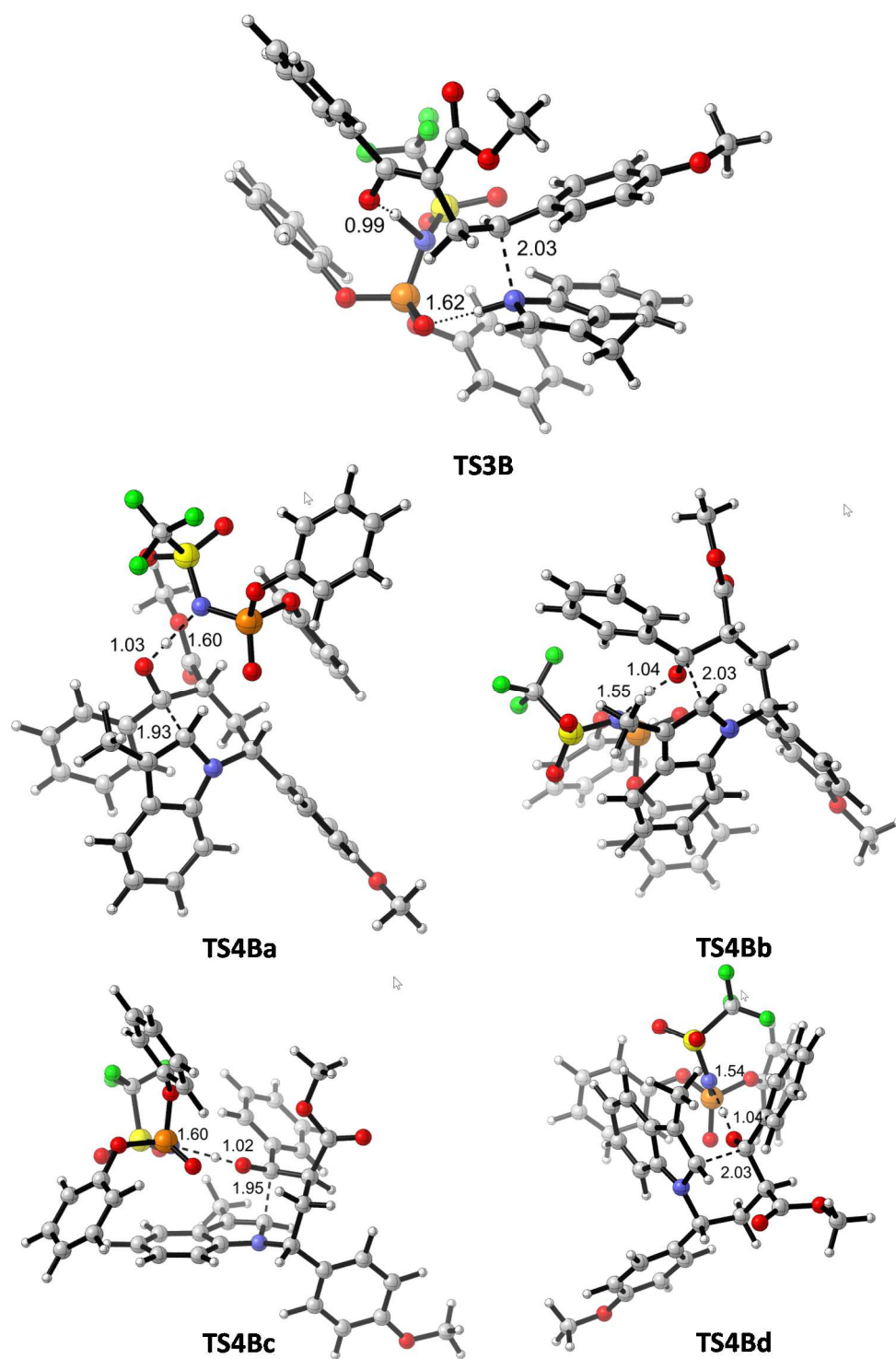


Figure S75. Optimized (b3lyp-gd3bj/def2svp/pcm=toluene) geometries of the located transition structures for the N-attack.

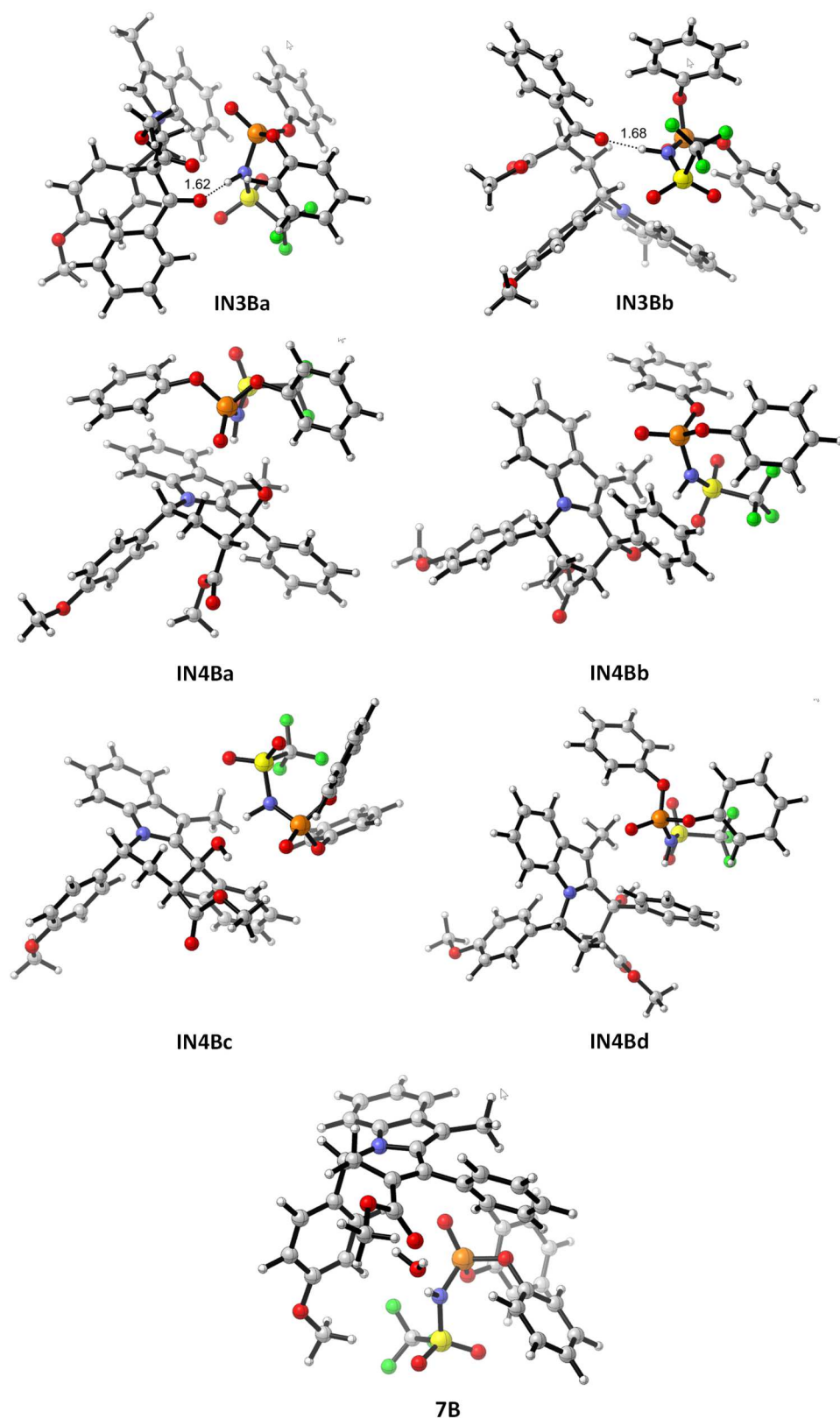


Figure S76. Optimized (b3lyp-gd3bj/def2svp/pcm=toluene) geometries of the located minima for the *N*-attack.

6. Cartesian coordinates

A

C	-1.3222217147	0.4016606166	0.6773899001
O	-1.3321141213	0.4112803075	1.8876542841
C	-1.8313590800	-0.7459788769	-0.1084007771
C	-1.1166241715	-1.2885867522	-1.3660337002
C	-2.4604041293	-0.6512742121	-1.4847145783
H	-0.2882822362	-0.6696656518	-1.7138469595
H	-2.5024366259	0.3314659838	-1.9553104487
H	-3.3275530298	-1.2939387816	-1.6574108528
C	-0.8907783748	-2.7544725753	-1.4983091793
C	0.3529196332	-3.2250905691	-1.9331830450
C	-1.8803261406	-3.7097683919	-1.1984937391
C	0.6190036233	-4.5913588815	-2.0725598475
H	1.1408949742	-2.5065880505	-2.1736832488
C	-1.6333187462	-5.0701272847	-1.3281329272
H	-2.8667828108	-3.3889998206	-0.8543612331
C	-0.3786548208	-5.5267395394	-1.7678659951
H	1.6026520084	-4.9092841752	-2.4169306025
H	-2.4003456325	-5.8108271534	-1.0949935321
O	-0.2303394116	-6.8718682784	-1.8652517354
C	1.0059205226	-7.3906383029	-2.2957527895
H	1.2606675439	-7.0519883487	-3.3164617272
H	0.9046469700	-8.4840223948	-2.2983596925
H	1.8293030113	-7.1085933228	-1.6147007848
H	-2.2270373084	-1.5155831950	0.5594315529
C	-0.7493443943	1.6229773787	-0.0840653992
O	-0.5905315832	1.6741078598	-1.2831130256
O	-0.4477580508	2.6111765420	0.7512866296
C	0.0994323178	3.7908937125	0.1605714763
H	1.0388468853	3.5607913765	-0.3642311283
H	-0.6064947758	4.2248799299	-0.5635122576
H	0.2812431789	4.4885843917	0.9861049033

B

C	0.2984437238	0.5198054288	0.2935278737
O	1.2784994640	0.3475603561	0.9937167094
C	-0.1000786949	-0.5022443556	-0.7468650635
C	0.8134496447	-1.7275822414	-0.8816086430
C	0.8115780058	-0.6861747421	-1.9467445363
H	1.6371855613	-1.6671717953	-0.1632398403
H	1.6732616181	-0.0186704371	-2.0152113025
H	0.2905931438	-0.8918916561	-2.8845836998
C	0.2046802951	-3.0806210464	-1.0491027442
C	0.0585173082	-3.6970998382	-2.2927444521
C	-0.2714265648	-3.7605167980	0.0876903377
C	-0.5387369068	-4.9563214268	-2.4193637489
H	0.4161253457	-3.1903844293	-3.1911920205
C	-0.8694404244	-5.0089145279	-0.0196306501
H	-0.1774126275	-3.2886816635	1.0690834073

C	-1.0094070274	-5.6197888581	-1.2786971989
H	-0.6334675529	-5.4025444141	-3.4087603292
H	-1.2420043684	-5.5406187824	0.8578682263
O	-1.6073508774	-6.8379983591	-1.2893325434
C	-1.7813270620	-7.4999443652	-2.5199315459
H	-2.4141316745	-6.9174814204	-3.2138955568
H	-2.2800348576	-8.4525748856	-2.2970645331
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C	3.3186096155	-2.1549809452	-0.4780320225
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H	-2.4112591583	3.5591997169	-3.5014042225
H	-3.3068018718	1.5633684522	-4.7001550761
C	4.6288395760	-0.0920017831	1.0877238222
F	4.8163060343	1.2209979259	1.0159276362
F	5.1669463078	-0.5504548520	2.2156409324
F	5.2365596315	-0.6731117978	0.0536118860

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C	-1.2725041752	-2.1026417488	1.9561518986
C	0.5235285207	-3.8314767289	-2.0656101213
C	0.8337978031	-5.1659752715	-2.4359303936
C	-0.1337886610	-6.1363834200	-2.2708507031
C	-1.4133304154	-5.8150085986	-1.7297044480
C	-1.7562159036	-4.5269964457	-1.3573382852
C	-0.7803296946	-3.5285865024	-1.5448965242
C	1.2546239677	-2.6211638853	-2.0821038284
C	0.4164890318	-1.6270627624	-1.4771066477
N	-0.8304612547	-2.2059199513	-1.2579515969
H	0.4703430734	-0.5425847190	-1.6072809318
H	1.8175776428	-5.4144222887	-2.8403378305
H	0.0779679199	-7.1712145289	-2.5476923926
H	-2.1425223912	-6.6175815702	-1.5957596003
H	-2.7174700527	-4.2867704759	-0.9010375961
H	-1.6641844452	-1.7300934273	-0.8867204164
C	2.6364916112	-2.4205184623	-2.5876192548
H	2.8814481025	-1.3584015484	-2.7070684070
H	2.7661181991	-2.9276656269	-3.5566705594
H	3.3779512484	-2.8504241846	-1.8910402627
O	-0.8700555258	-0.8654975813	2.3179548797
C	-0.4208131929	-3.0301278832	1.4863506062
C	1.3691197650	-1.5422025700	0.3948827855
C	1.0263562089	-2.7972715234	1.1638474583
H	-0.8398239661	-4.0176553290	1.2988922089
H	0.7162049082	-0.6946728827	0.5951595524
H	1.4356394326	-3.6844593115	0.6564203049
H	1.6033243594	-2.7100057921	2.1064944028
C	2.7651064447	-1.1657426676	0.2201666998
C	3.0909385728	0.1415382102	-0.2201941670
C	3.8262342730	-2.0485095429	0.5062049525
C	4.4075230713	0.5366864047	-0.3557617176
H	2.2807598040	0.8388351673	-0.4426582831
C	5.1570990251	-1.6513337746	0.3928168505
H	3.6180782763	-3.0634263002	0.8478712403
C	5.4571314778	-0.3485682257	-0.0414577144
H	4.6617087666	1.5464748125	-0.6795980613
H	5.9480334066	-2.3564822811	0.6452182164
C	-2.7257719110	-2.4572665080	2.0531465900
O	-3.2027288691	-3.4983158289	1.6573652036
O	-3.4366878693	-1.4723685478	2.6111508074
C	-4.8522944612	-1.6470677783	2.6010577063
H	-5.1332453187	-2.5643258450	3.1390358107
H	-5.2725388909	-0.7627791886	3.0920297803
H	-5.2116097897	-1.7146608740	1.5641894096
O	6.7065171280	0.1376702491	-0.1779142554
C	7.8108246776	-0.6885521159	0.1254945102
H	7.8402540372	-1.5823148430	-0.5221446459
H	8.7099872401	-0.0857147684	-0.0546701720
H	7.7984987373	-1.0117477652	1.1811530739
H	-1.4910794465	-0.1747686141	1.9682598401
N	-1.9682403378	1.0133893281	0.6635230902
P	-0.6800172419	1.9423602901	0.2812013706
S	-2.9549335037	0.5261212043	-0.4816485158

O	0.3529247516	1.4162519554	-0.6656185221
O	-1.2920785085	3.3825535446	-0.1672360001
O	-0.0701278243	2.2387826895	1.7638442905
O	-2.6510523530	1.0163415251	-1.8327855232
O	-3.2184950671	-0.9269233517	-0.3376523687
C	-0.7067448025	4.1831928725	-1.1345481704
C	-0.7536796069	3.8012037109	-2.4767105824
C	-0.1102329746	5.3810535264	-0.7384327477
C	-0.1833273039	4.6416138542	-3.4346461315
H	-1.2407251217	2.8612456351	-2.7391289926
C	0.4545631320	6.2143699363	-1.7087797008
H	-0.1085780175	5.6481865828	0.3200188055
C	0.4225343241	5.8452339634	-3.0565320319
H	-0.2156829429	4.3536528638	-4.4882576822
H	0.9194250933	7.1563188089	-1.4076977969
H	0.8646467762	6.4974240946	-3.8131954691
C	1.2815507886	2.1560176507	2.0519938603
C	1.7243333314	1.1047375218	2.8570971432
C	2.1704182804	3.1190207044	1.5680651401
C	3.0794678863	1.0261739518	3.1881904952
H	0.9990666307	0.3618097979	3.1913451206
C	3.5221893360	3.0284048072	1.9070937435
H	1.8004555305	3.9210599411	0.9271959507
C	3.9806916858	1.9844090680	2.7164571267
H	3.4331990259	0.2024686894	3.8128633159
H	4.2222942263	3.7772611724	1.5291095853
H	5.0406204782	1.9141464112	2.9701918752
C	-4.5691066825	1.3426978207	-0.0194083658
F	-4.4515498298	2.6557971339	-0.1698188121
F	-5.5370274641	0.8914516998	-0.8129812260
F	-4.8899451928	1.0779442415	1.2461777538

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C	-0.6039931626	-0.9026314863	2.0587724730
C	-2.4834472587	-3.6235588625	-0.1001687516
C	-2.1434301510	-4.9801043053	-0.0764779183
C	-1.4318243709	-5.5072811119	-1.1557837790
C	-1.0639159245	-4.6999215377	-2.2485838872
C	-1.4038405320	-3.3483356875	-2.2973306280
C	-2.1126908302	-2.8345066447	-1.2112710234
C	-3.1717368506	-2.7347755677	0.8516453188
C	-3.2496501169	-1.4624259083	0.1747412867
N	-2.5856584391	-1.5390255909	-0.9874128200
H	-2.2981808144	-2.1914070230	1.6772433623
H	-2.4208163863	-5.6122654091	0.7698529127
H	-1.1523360569	-6.5632174551	-1.1528757259
H	-0.4986616387	-5.1380771851	-3.0740042547
H	-1.1064324254	-2.7083776431	-3.1270854596
H	-2.2599407088	-0.7286258314	-1.5145950728
O	-0.4093448883	-0.1529357618	1.0655863379
C	-1.8742921206	-1.0548110877	2.6343911585
C	-3.6966749288	-0.2152428480	0.8455947795

C	-2.9132232610	-0.0311580735	2.2495624589
H	-4.7477601295	-0.3898433270	1.1247122866
H	-3.6752659394	0.0391595689	3.0371491271
H	-2.4271672839	0.9492999056	2.1745222183
C	-3.6531085306	1.0064304336	-0.0545943817
C	-4.8372135393	1.5931817872	-0.5307335208
C	-2.4358928823	1.5614685485	-0.4712024333
C	-4.8033571069	2.6872654689	-1.3906904798
H	-5.8053498775	1.1865356542	-0.2236300474
C	-2.3801312073	2.6487819663	-1.3445533918
H	-1.5087052454	1.1337360151	-0.1005075523
C	-3.5720821773	3.2216660198	-1.8105545366
H	-5.7218598688	3.1475843032	-1.7594321627
H	-1.3993777322	3.0219291690	-1.6400133444
O	-3.6263734838	4.2788385955	-2.6549793091
C	-2.4108941580	4.8346030154	-3.1135698029
H	-1.7954110716	5.2180395590	-2.2811064302
H	-2.6791610454	5.6663944670	-3.7780290832
H	-1.8110838642	4.0981135413	-3.6759943025
H	0.7476911453	0.1931443547	0.2352205855
N	1.4032500148	0.5625573558	-0.5605710513
S	1.1514931311	-0.2371884715	-1.9696982880
O	0.9562201050	3.1269843896	-1.3137281362
O	2.0498921607	0.2621221627	-3.0025988374
O	-0.2707958484	-0.4331922449	-2.2555851200
P	1.7968478134	2.2132204644	-0.5124564324
O	1.8358505047	2.4536197653	1.0902006203
O	3.3582667473	2.3062354290	-0.8738790713
C	0.7389538848	2.6239198382	1.9288423063
C	4.3222396028	1.3883572376	-0.4655062442
C	0.7689932692	1.9424564278	3.1454831144
C	-0.3246331777	3.4574598007	1.5846144896
C	4.7248749899	1.3333159683	0.8696960466
C	4.8854375379	0.5574647042	-1.4326324144
C	-0.2934949801	2.0957921843	4.0358316939
C	-1.3867493935	3.5941898598	2.4826289596
H	-0.3199749933	3.9707454186	0.6241170028
C	5.7143775884	0.4179674283	1.2384607183
C	5.8742514867	-0.3513044529	-1.0501392311
C	-1.3749004315	2.9210665610	3.7067670510
H	-0.2821318017	1.5579245499	4.9864501486
H	-2.2322471651	4.2305273698	2.2126424857
C	6.2897439493	-0.4259240238	0.2828322717
H	6.0399145219	0.3696104817	2.2804040225
H	6.3171514786	-1.0106051961	-1.8001276448
H	-2.2099445939	3.0324602292	4.4016520765
H	7.0638717486	-1.1383890688	0.5765209401
H	4.5194286331	0.6186328471	-2.4573079587
C	1.7777345515	-1.9411721350	-1.4658554722
F	1.0051157853	-2.4538088022	-0.5123061727
F	3.0254194342	-1.8726604478	-1.0219375176
F	1.7349208672	-2.7255621894	-2.5378167290
H	4.2619294983	1.9993836330	1.5972307586
H	1.6092713878	1.2810573545	3.3583672982
C	-4.2143994601	-3.2385598582	1.8288030103

H	-5.0949053467	-3.6368772708	1.3008434095
H	-3.7971858512	-4.0438482371	2.4517968778
H	-4.5495142850	-2.4409025872	2.5073797467
H	-1.9460199896	-1.5862757408	3.5854357986
C	0.5587779073	-1.7312817480	2.5812057284
O	0.4628609638	-2.6720620197	3.3317124411
O	1.7150147483	-1.2763358569	2.0767970907
C	2.8944419821	-2.0198100108	2.3776381473
H	3.7163474651	-1.4965185895	1.8757608385
H	3.0618197670	-2.0624028628	3.4643231408
H	2.8033756553	-3.0474626721	1.9951238804

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C	-0.1752145955	1.3974641043	2.1916855559
C	-1.2705469304	3.4696527420	-1.2002806336
C	-0.9413385105	4.7886230308	-1.5388111416
C	0.1100534414	4.9990102706	-2.4305414761
C	0.8310885318	3.9196333532	-2.9791720129
C	0.5138073850	2.5992737894	-2.6661605763
C	-0.5478334872	2.4018536037	-1.7827642259
C	-2.2585234412	2.8746354384	-0.3008658987
C	-2.1106338413	1.4568341343	-0.4663019469
N	-1.0831822563	1.2116674825	-1.2931348322
H	-1.5370968015	2.5404710240	0.9651091850
H	-1.4864836066	5.6315108130	-1.1082674109
H	0.3888972614	6.0195852338	-2.7025636254
H	1.6630447353	4.1207920357	-3.6574869342
H	1.0899797261	1.7604257269	-3.0561525844
H	-0.6627535343	0.2660850551	-1.4582026226
O	0.0843050273	0.1800216947	1.8243986173
C	-1.4898817205	1.8593611192	2.1897047624
C	-2.6857869600	0.3980706690	0.4290349280
C	-2.6226130820	0.8837446290	1.9165665647
H	-2.0144527081	-0.4685261849	0.3442598878
H	-3.5669963413	1.3740974609	2.1849438603
H	-2.5244476790	-0.0083329584	2.5519391001
C	-4.0628837379	-0.0775252802	-0.0161409903
C	-4.3101803677	-0.2846733607	-1.3852865769
C	-5.0733670535	-0.4193115263	0.8846726111
C	-5.5160722927	-0.8079942805	-1.8329682927
H	-3.5340586497	-0.0429938874	-2.1150838498
C	-6.2958104459	-0.9480665662	0.4525696871
H	-4.9182741297	-0.3017780288	1.9573664461
C	-6.5253778392	-1.1469590804	-0.9151005213
H	-5.7057664050	-0.9679621130	-2.8957837294
H	-7.0540517714	-1.2020009696	1.1926936714
O	-7.6691816429	-1.6516051080	-1.4387078395
C	-8.7132771764	-2.0203046358	-0.5679835900
H	-9.0842104330	-1.1587429832	0.0161209956
H	-9.5280283731	-2.4012909666	-1.1976128019
H	-8.4007820550	-2.8148254935	0.1337016012
H	0.9936432815	-0.0135293373	1.3604376047

N	1.9261101575	-0.4819933962	0.1758639181
S	2.7428650991	0.7522990569	-0.4613284385
O	0.0652085679	-1.1753398101	-1.6584755269
O	3.0095934620	0.6022364640	-1.8967066174
O	2.2164776266	2.0222954340	0.0537644952
P	1.1805859236	-1.6119695877	-0.7594873342
O	0.6889158707	-2.7015024861	0.3525861735
O	2.2617910480	-2.4531236627	-1.6041077339
C	-0.6132324512	-2.8558890092	0.8011882191
C	3.5702321321	-2.7254305696	-1.2373620876
C	-0.8291746537	-2.8177182527	2.1795219932
C	-1.6714422591	-3.0694589553	-0.0883214509
C	4.5455403344	-2.5662573397	-2.2214130437
C	3.8979222783	-3.1636853163	0.0470611703
C	-2.1235126548	-2.9933386104	2.6743584589
C	-2.9630328021	-3.2293186808	0.4194091672
H	-1.4803825759	-3.0747432313	-1.1604263685
C	5.8745068411	-2.8588027001	-1.9143311631
C	5.2350053724	-3.4406613420	0.3437394910
C	-3.1938448723	-3.1938686340	1.7972808810
H	-2.2949250486	-2.9645159846	3.7532054379
H	-3.7974901418	-3.3653547442	-0.2714955671
C	6.2241104666	-3.2935507445	-0.6319002598
H	6.6438575729	-2.7331152344	-2.6797005018
H	5.5010273243	-3.7777736256	1.3483557738
H	-4.2079760003	-3.3139690859	2.1831649455
H	7.2669351203	-3.5131637066	-0.3927180586
H	3.1160826633	-3.2833723777	0.7972473035
C	4.4303987119	0.5859555001	0.3702402362
F	5.2343828224	-0.1770665902	-0.3540271548
F	4.3141632876	0.0604137750	1.5899544931
F	4.9709070296	1.8005741583	0.4790862982
H	0.0173016183	-2.6345964679	2.8419661387
H	4.2454948839	-2.1979522225	-3.2028353204
C	-3.4874496674	3.5940657262	0.1918251679
H	-4.0718133269	3.9734189009	-0.6617596464
H	-4.1458603065	2.9345339136	0.7716790759
H	-3.2199380468	4.4579077850	0.8206708818
H	-1.6794823456	2.7389461837	2.8120024705
C	0.9271848969	2.3411408553	2.6023341193
O	0.7654600001	3.5329126162	2.6967943191
O	2.0479850379	1.6832945042	2.8885986268
C	3.1898477726	2.4973232285	3.1773887732
H	3.9917390734	1.8051254723	3.4523274543
H	3.4662486631	3.0645901092	2.2780391111
H	2.9669289727	3.1936900349	3.9980317137

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C	1.1812714914	3.2912273040	-1.0762786488
C	-3.9651484815	-1.2277331009	-0.8248508941
C	-4.8880442286	-1.7162154152	0.1044047662
C	-4.4041905820	-2.2307953865	1.3119179377

C	-3.0281715841	-2.2553373938	1.5883522987
C	-2.0929810581	-1.7516584359	0.6771383434
C	-2.5862969200	-1.2473575448	-0.5196042779
C	-4.1018882397	-0.6536466206	-2.1623117189
C	-2.8426971452	-0.3559275388	-2.5896306394
N	-1.8968981107	-0.5980611154	-1.5699188560
H	-2.5141563588	0.0653513519	-3.5365863966
H	-5.9590895608	-1.7022278046	-0.1094327120
H	-5.1064258981	-2.6267975165	2.0493385701
H	-2.6685134513	-2.6714912694	2.5312201281
H	-1.0330571242	-1.7587004454	0.9242175984
H	-0.9202141880	-0.9006686125	-1.8417770113
C	-5.3909660435	-0.4416435780	-2.8797209146
H	-5.9570188258	-1.3833506956	-2.9706072937
H	-5.2339230669	-0.0343314704	-3.8886993234
H	-6.0275183630	0.2643642388	-2.3185527965
O	2.1014176856	2.3228420079	-1.0279122111
C	-0.1049769948	3.1802166635	-1.4766097565
C	-1.3885240282	1.2560309119	-0.7997874188
C	-0.7391833174	1.9106252652	-1.9809069018
H	-0.7181481065	4.0790506311	-1.4049456989
H	0.0209476379	1.2323300939	-2.3955870035
H	-1.4686619274	2.1465013304	-2.7694105734
C	1.6706104378	4.6594454320	-0.6795203062
O	0.9930607104	5.6615392287	-0.7069278248
O	2.9508520195	4.6397530850	-0.2889451031
C	3.4955785186	5.8941813934	0.1090315233
H	2.9387408894	6.3082202218	0.9635003393
H	4.5374990675	5.6996762955	0.3908390961
H	3.4501211038	6.6209758949	-0.7165406188
P	1.6535784573	-1.3100856050	-1.2151344102
O	0.5896248859	-1.2344440093	-2.2743674773
O	3.0925975278	-1.1361592812	-1.9134280776
O	1.7856903028	-2.7858259991	-0.5445184339
N	1.5188181896	-0.1519640111	-0.0767720975
S	1.2832514257	-0.1799455813	1.4972511041
O	0.4575314290	0.9759983668	1.8764456767
O	0.9340357964	-1.4987286316	2.0431128168
H	1.7549208828	1.4407857019	-0.7234194500
C	-2.6239297394	1.6806346243	-0.2012754468
C	-3.6788676651	2.2673768175	-0.9410067904
C	-2.8461181651	1.3762705518	1.1610114656
C	-4.9069457691	2.5082270917	-0.3517953646
H	-3.5299547030	2.5242693956	-1.9901998618
C	-4.0751950740	1.6103325829	1.7599808325
H	-2.0214499188	0.9623653875	1.7434098645
C	-5.1238515735	2.1598270198	0.9980191940
H	-5.7318644916	2.9565384117	-0.9074603281
H	-4.2141943177	1.3579229303	2.8097614901
O	-6.3581053553	2.3977683950	1.4747833865
C	-6.6663220883	2.0511674818	2.8114238557
H	-6.5290384892	0.9705119385	2.9880244168
H	-6.0466936573	2.6152467222	3.5292353630
H	-7.7211048439	2.3123973989	2.9636576781
H	-0.6719597431	0.8405195532	-0.0934850308

C	2.9638649803	0.1953487509	2.2245491065
F	3.4388558719	1.3342882005	1.7335434194
F	2.8470923585	0.3047008244	3.5455285735
F	3.8073034720	-0.7945428471	1.9445355739
C	4.2786541457	-0.9449882200	-1.2075407633
C	4.7430167848	0.3539750850	-1.0054381094
C	4.9816215944	-2.0567188156	-0.7433110142
C	5.9458965865	0.5361019712	-0.3187751713
H	4.1530867502	1.2019207918	-1.3547760676
C	6.1842618308	-1.8585587294	-0.0620002127
H	4.5745029616	-3.0541169846	-0.9131402395
C	6.6680408266	-0.5641190535	0.1516026053
H	6.3118431715	1.5502211299	-0.1433174153
H	6.7426664999	-2.7215743077	0.3081519262
H	7.6065231704	-0.4136184648	0.6900429530
C	0.7319897773	-3.6626870552	-0.3053847433
C	0.6377498405	-4.2225030281	0.9692776783
C	-0.1785633648	-3.9955258146	-1.3121622664
C	-0.3993280702	-5.1151829231	1.2437760200
H	1.3562952164	-3.9201153162	1.7287689004
C	-1.2178781443	-4.8823625357	-1.0177282802
H	-0.0757017461	-3.5483037710	-2.2997185218
C	-1.3354410279	-5.4410993681	0.2567999531
H	-0.4815663671	-5.5496864287	2.2429016682
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H	-2.1531075153	-6.1295303457	0.4810263903

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C	4.7858422064	-1.4086462463	0.6811135995
C	5.6135335548	-2.2678158763	1.3826758630
C	5.1338863309	-3.1229170536	2.4148774883
C	3.7965342993	-3.1312231668	2.7519323032
C	1.5123709555	-2.0911695685	2.1254630033
C	1.1773218807	-1.1604826998	1.1001924535
H	5.1790536414	-0.7719540575	-0.1075087853
H	6.6774853692	-2.2910177791	1.1340747015
H	5.8363803588	-3.7778403873	2.9340254720
H	3.4135643283	-3.7920509395	3.5320395101
N	2.3671748137	-0.6778800551	0.5284917250
C	2.2549484514	0.1862887760	-0.6538848710
H	1.4593803531	0.9009451022	-0.3935696163
C	0.5043742690	-2.7566135093	2.9836806564
H	-0.0493064514	-3.4930692768	2.3728063278
H	-0.2348522042	-2.0225812089	3.3384588348
H	0.9622954278	-3.2801514754	3.8338685856
C	1.7452713837	-0.6425055030	-1.8371690586
H	2.5133951365	-1.3572733010	-2.1567192336
H	1.5510550112	0.0460602326	-2.6728065492
C	0.3529088296	-2.3076865822	-0.3243344058
C	0.4301483126	-1.3518461615	-1.5154746186

H	0.0997314987	-1.9513747399	-2.3812408777
H	-0.3632973347	-0.6080829206	-1.3718818102
C	3.5111260152	0.9936485842	-0.8922554371
C	4.2231421325	0.9633661063	-2.0989702922
C	3.9825680569	1.8254311097	0.1298813711
C	5.3708349123	1.7323409539	-2.2744306078
H	3.8872302689	0.3306417587	-2.9209921348
C	5.1326009658	2.5993640368	-0.0253136551
H	3.4414715276	1.8630277253	1.0780061113
C	5.8390739936	2.5568879588	-1.2391877148
H	5.9278788666	1.7131341326	-3.2126938032
H	5.4670935810	3.2294624103	0.7980829605
O	6.9623009437	3.2661212241	-1.4966918644
C	7.4770609979	4.1221226845	-0.5009922420
H	6.7550759252	4.9121105652	-0.2274526398
H	8.3749223147	4.5904882035	-0.9245867233
H	7.7583716086	3.5663479059	0.4113629981
O	-0.8383744547	-2.6214225388	0.1055457083
C	1.2631732520	-3.5345727436	-0.2823332349
O	0.9718986929	-4.5674199628	0.2595560754
O	2.4273180134	-3.3185313742	-0.9126700109
C	3.3805542077	-4.3855041766	-0.8589701829
H	2.9709203519	-5.2892935075	-1.3318523151
H	3.6389677825	-4.6096264365	0.1851113675
H	4.2628473819	-4.0275314617	-1.4010366013
N	-2.4534692285	-0.6251322830	-0.1021793800
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S	-3.4073661862	-0.6106272971	-1.4015983888
O	-1.3224665499	0.2065398665	2.0736724516
O	-3.9027409909	0.5876667486	1.6998891004
O	-2.2950391061	1.9916648726	0.4410139092
O	-2.7163874048	-1.2887389014	-2.5003633916
O	-4.0692420872	0.6784931172	-1.6449003563
C	-4.7880654325	-1.7778624545	-0.9153874526
H	0.3173069569	-0.4869987363	1.2007679550
H	-1.5184079158	-1.8360990388	0.0003657026
C	-1.1593294377	2.4111142162	-0.2185453500
C	-1.0698388970	2.2535022229	-1.6048107756
C	-0.1301541319	3.0202430637	0.5067726056
C	0.0682885781	2.7233160881	-2.2688152117
H	-1.8982234274	1.7859996757	-2.1376758331
C	0.9933221730	3.4976845381	-0.1723053596
H	-0.2337533914	3.1117243259	1.5886977211
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H	0.1414656119	2.6065977610	-3.3527732617
H	1.7981764962	3.9810087139	0.3851405393
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H	-5.4274871801	1.9020328029	0.0537197951
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H	-5.1467667414	3.8366883314	4.6423208062
H	-6.6134205549	4.9158644805	2.9387764671
F	-4.2787762270	-2.9339928553	-0.4953311510
F	-5.5226020718	-1.2477409333	0.0576957619
F	-5.5626367424	-2.0017885858	-1.9733564429

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C	5.8753794294	0.5702391520	1.8474385783
C	6.9502752209	1.3901912273	1.5455904542
C	6.8738471350	2.4052469150	0.5508865890
C	5.7096682815	2.6073359303	-0.1644725388
C	3.2923574040	1.7018399991	-0.4552053970
C	2.6423697790	0.6164245861	0.1955415332
H	5.9547142039	-0.2035914980	2.6118908372
H	7.8881544473	1.2570009087	2.0902732686
H	7.7512543674	3.0253464995	0.3570618961
H	5.6476753011	3.3797913129	-0.9337833493
N	3.4787817940	0.1414129286	1.2143753275
C	3.1444376958	-1.0985046353	1.9207195573
H	3.8682057555	-1.1925803142	2.7461451056
C	2.6808241425	2.5056541680	-1.5421170816
H	1.6162449664	2.6753827076	-1.3263207952
H	3.2024256024	3.4623341318	-1.6862046813
H	2.7334115072	1.9390780380	-2.4896113752
C	3.3754238360	-2.2571881317	0.9374171997
H	4.4447156011	-2.2913692983	0.6944097727
H	3.1259838696	-3.2093749492	1.4274008647
C	2.6261443002	-0.9101359975	-1.2223388510
C	2.5376236245	-2.1460139662	-0.3380143084
H	2.8095996804	-2.9762066756	-1.0159105822
H	1.4772307601	-2.3017941778	-0.1162653479
C	1.7340883633	-0.9972780047	2.4900014759
C	1.3101949610	0.2055721270	3.0845585130
C	0.8113382285	-2.0436516435	2.4122669941
C	0.0122230520	0.3643196041	3.5468719503
H	2.0035297399	1.0472528031	3.1526768644
C	-0.4994754049	-1.9008649313	2.8722872990
H	1.0777153767	-2.9959707215	1.9553193009
C	-0.9167612997	-0.6844513609	3.4266636388
H	-0.3253868193	1.3083496169	3.9771196512
H	-1.1966674737	-2.7241900274	2.7350404533
O	-2.1707235132	-0.4302974059	3.8506491602
C	-3.1675692959	-1.4145444695	3.6394354620
H	-2.9876585712	-2.3050266631	4.2686446560
H	-4.1211062321	-0.9544769958	3.9278176236
H	-3.2109335884	-1.7186145384	2.5830145181
O	1.5977626863	-0.6432015274	-1.9730602230
C	3.9335322091	-0.5996563486	-1.9357239051
O	4.0092406125	-0.0547137073	-3.0055303351

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H	6.4292019578	-1.2471427905	-2.7137845787
H	6.3740908893	0.3650872513	-1.9350951951
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N	-0.6511271982	-0.9364251209	-0.6609326876
P	-1.2470798752	0.5458415478	-0.3023429229
S	-1.3928639027	-2.3580391839	-0.5749607764
O	-0.1718706851	1.5618793834	-0.1087707476
O	-2.2686192729	0.8801158584	-1.5318612594
O	-2.2257719491	0.3997170686	0.9837566274
O	-0.3754137876	-3.4140293699	-0.5344598854
O	-2.5285754896	-2.4293244724	0.3519591072
C	-2.1807746474	-2.5421055176	-2.2679431533
H	1.5580059041	0.5841831636	0.3228520431
H	0.7010504299	-0.8526433776	-1.4951369000
C	-2.9693576834	2.0620943244	-1.7161584316
C	-2.4064322076	3.3141548932	-1.4544230097
C	-4.2755065133	1.9438163203	-2.1948598931
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H	-1.3865550568	3.3757470824	-1.0759822548
C	-5.0351919367	3.0952291166	-2.4005024249
H	-4.6762212433	0.9469693737	-2.3798734810
C	-4.4938279914	4.3567199886	-2.1317309354
H	-2.7496956243	5.4402014692	-1.4539795945
H	-6.0608193291	3.0041668424	-2.7657928853
H	-5.0930804000	5.2563293057	-2.2885813452
C	-3.5346809124	0.8477491315	1.0672742559
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C	-5.0958719361	2.5798315938	1.6571712552
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H	-4.3328046655	-0.9709008917	0.2586876795
C	-6.1518945611	1.7629996981	1.2410084081
H	-5.2959185622	3.5824513737	2.0418200200
H	-6.7096590159	-0.1588291288	0.4187764944
H	-7.1803868755	2.1258566934	1.3015389629
F	-2.5604139186	-3.8048617230	-2.4410318412
F	-1.3104719394	-2.2147283537	-3.2202951614
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C	-2.0717381030	0.6857877857	-0.2551718619
C	-3.2660430102	0.7305694305	-1.1250660745
H	-1.4208089316	1.5597249622	-0.2856131275
H	-4.1544919411	0.1829803879	-0.8128877300
H	-3.4552597178	1.6637983910	-1.6548175271
C	-1.9919018462	-0.1166582209	0.9969272193
C	-0.7574029555	-0.2454556553	1.6441722961

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C	-0.6009714296	-1.0542938436	2.7688878206
H	0.1058879833	0.2862811778	1.2465306230
C	-2.9469779949	-1.6357747949	2.6432517888
H	-4.0706245039	-0.7261708147	1.0632845334
C	-1.6971272874	-1.7740222128	3.2668435355
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H	-3.7953791656	-2.1878456635	3.0511112337
O	-1.6404368338	-2.6132350212	4.3309244980
C	-0.3883973255	-2.8620592278	4.9279914741
H	0.3343277209	-3.2706492631	4.1993737842
H	-0.5587967915	-3.6030958851	5.7200781332
H	0.0419103570	-1.9494482015	5.3786703741
C	-3.2548683746	-2.4062131640	-1.5735548095
C	-4.3639090842	-2.0147842246	-2.3407430181
C	-3.2734498553	-3.6398627634	-0.8997078113
C	-5.4791574585	-2.8485790763	-2.4310531669
H	-4.3441623742	-1.0679132960	-2.8821208625
C	-4.3969904679	-4.4587481793	-0.9736211399
H	-2.3958038696	-3.9260049644	-0.3181219089
C	-5.5003814597	-4.0642155640	-1.7402369788
H	-6.3352900528	-2.5492378771	-3.0396677230
H	-4.4156576443	-5.4098267942	-0.4367996391
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C	-1.2600324969	0.5504852859	-2.6965520468
O	-1.2957345104	1.7337331997	-2.9583708535
O	-0.4853436939	-0.3312130384	-3.3362751720
C	0.3422393657	0.1572058475	-4.4036853055
H	0.6361911337	-0.7293253870	-4.9779533940
H	1.2392826928	0.6388191986	-3.9907357394
H	-0.2200439308	0.8624351954	-5.0306098828
N	1.5792763324	-1.3413775901	-1.0040960211
S	2.3552119961	-2.7948438040	-0.8389166567
O	2.9780435653	0.5010807708	-2.4663744285
O	3.7925843252	-2.5725825894	-0.9215955354
O	1.6608977817	-3.8152653490	-1.5998876319
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C	1.4129943137	2.4699362727	-0.5291839110
C	4.7485765244	0.4099360455	0.0737125422
C	2.0656802273	2.9319008768	0.6161911618
C	0.9735867985	3.3442245872	-1.5225382866
C	5.2414127696	1.5628918669	-0.5372335316
C	5.5889303435	-0.4871370260	0.7307638980
C	2.2812119659	4.3038936341	0.7685457576
C	1.1913698152	4.7154067409	-1.3549057678
H	0.4438566797	2.9497462621	-2.3890728818
C	6.6139684841	1.8185722525	-0.4787919219
C	6.9568556194	-0.2145100217	0.7868002867
C	1.8444310978	5.1989879084	-0.2147995614
H	2.7915226805	4.6734692566	1.6606307514
H	0.8464846735	5.4094890336	-2.1245886953
C	7.4727453234	0.9370341208	0.1835960752
H	7.0115444530	2.7160293676	-0.9582870807

H	7.6237459525	-0.9124687344	1.2981445503
H	2.0137914338	6.2709746518	-0.0930673202
H	8.5443272177	1.1441289473	0.2251518053
H	5.1583865964	-1.3857815217	1.1708419920
H	0.5421230223	-1.4502723597	-1.1750386968
C	-2.4871737611	3.8655358048	0.7155264901
C	-1.0026587525	3.3653925992	2.3294120327
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C	-3.1561056350	3.1028817589	1.7201849800
H	-0.0265425637	3.3560206127	2.8087395317
N	-1.1788882423	4.0068269175	1.1158138707
C	-4.5150413469	2.7859917062	1.5438678076
H	-5.0439671095	2.1935945480	2.2945276956
C	-3.1435497145	4.3126091285	-0.4382349127
H	-2.6133733722	4.8799790221	-1.2059525387
C	-5.1715133720	3.2349370901	0.4014439810
C	-4.4920248050	3.9928015098	-0.5781413588
H	-6.2283193240	2.9987861858	0.2549413544
H	-5.0320595657	4.3278426332	-1.4670192886
H	-0.4529933773	4.4885699756	0.6010880466
C	1.9954672774	-3.1963145646	0.9586824759
F	2.6589579606	-4.2986552228	1.2881786645
F	2.3952795627	-2.1970980049	1.7464912408
F	0.6952214730	-3.3954490565	1.1329264872
H	4.5638117503	2.2370397899	-1.0605961197
H	2.3960091948	2.2169834354	1.3697016095
C	-2.4260121250	1.9957827430	3.9826386465
H	-3.2067081602	2.4516573549	4.6154729870
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C	-5.8445000038	-0.0928962970	-1.6893969805
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H	-3.7998473243	-2.7930417052	-2.0716348098
C	-7.0389385676	-0.7550180016	-1.3973015867
H	-5.7893254574	0.9947700737	-1.7292658241
C	-7.0819197329	-2.1518772643	-1.3499673200
H	-5.9494393917	-3.9840665464	-1.5578195426
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C	0.2879824258	-1.6625116491	-1.6098279882
C	-0.0120304277	-3.1892509352	0.2402018697
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H	0.7106166354	-0.7488809584	-2.0245151752
C	-0.9155515456	-3.9343326760	-0.5185901683
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H	-0.8732870742	-2.0770999560	-3.3777322049
H	-1.3945849839	-4.8124053822	-0.0797051725
H	-1.9079802604	-4.1458334362	-2.4307113997
C	2.9945819063	-3.4657996811	0.7620575282
O	3.0917598037	-3.8820416343	1.8875061153
O	2.8083122184	-4.2744111613	-0.3048117752
C	2.6617463632	-5.6618506642	-0.0231774919
H	1.7565583589	-5.8395327826	0.5778290833
H	2.5741346660	-6.1650770807	-0.9938338415
H	3.5294005327	-6.0438188680	0.5347727750

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C	-1.2713972338	-1.7378359415	4.9596849599
C	-0.2534801487	-2.3744931139	4.2544786542
C	0.5253786450	-3.0708483303	1.8779318601
C	-0.0616730558	-2.8817886364	0.6498288683
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C	-0.2448757039	-2.2349712433	-1.7615463535
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H	-3.4748430181	0.4015042868	-0.2369508126
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O	0.1107020552	0.1526618824	0.7591518215
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O	2.8598772713	3.3488885288	-1.1958038236
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H	3.0259390123	-1.2404851947	1.7115323467
H	1.6183898347	-0.7413450629	2.0438875529
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F	3.8403033047	3.1930110683	2.4628958536
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C	-1.9774000119	2.0846170473	1.9523524418
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H	-1.3651059399	1.3578450894	2.4849339815
C	-3.5459734257	3.9129462746	0.5173117599
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C	2.5882464807	-1.9003701952	-0.6945616740
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H	4.4747016507	-0.8356526645	-0.6541790309
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H	6.6553325289	-4.2486932403	-2.5297260724
H	-7.2801671095	-1.0085783486	1.2081508398
H	0.2601834912	-1.2567414658	-1.7133703016
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C	3.9121521909	0.9744986906	4.9061130456
C	3.5249000483	1.8457428511	3.8956412209
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H	4.7606063610	-1.8115185955	3.0730491651
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H	3.8674832130	1.2969402455	5.9488207484
H	3.1723418042	2.8520435432	4.1333205386
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H	5.2596250992	-1.7162561146	0.7147704975
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H	5.8094246283	-0.2774058742	-1.0998278858
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C	3.5642102172	-3.5651212434	-0.4708195200
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H	-0.0065545617	-2.8263034085	0.8350637555
H	2.7857450611	-5.4945573307	-1.0794281898
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O	0.0908281213	0.5415931728	1.3917307440
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O	-3.0177421259	-2.4280298814	-1.4210622488
O	0.3939433944	-0.7453254634	-1.7574827756
H	1.0897604377	-1.1602823348	-1.2237631458
H	0.8654552860	-0.3847520276	-2.5389399393
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C	-3.0149739581	1.1935530020	2.8514101137
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C	-2.8020941883	2.9708449345	4.4507883323
H	-1.1137117867	1.9050324480	3.5760974605
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C	2.4276420173	2.1185182400	-1.7335186051
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C	0.4052933316	3.4534115739	-1.8144725237
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C	2.1806253626	3.8660258980	-3.4045416416
H	3.9312226225	2.6142347033	-3.2031558005
C	0.9120570985	4.1707986439	-2.9020636286
H	-0.5796728165	3.6908242868	-1.4114949749
H	2.5872065656	4.4286218045	-4.2484082217
H	0.3208931496	4.9712100044	-3.3536319930
C	3.3856962574	-0.2511443003	-3.2317956353
O	2.2608486122	-0.0944494532	-3.6845244475
O	4.3669004836	-0.7989727895	-3.9718997928
C	4.0098579184	-1.2127862034	-5.2900665685
H	3.2005153049	-1.9575861536	-5.2584962023
H	3.6681534196	-0.3551226676	-5.8882197455
H	4.9157923868	-1.6485885315	-5.7282539762
C	2.7665180593	3.4399328964	1.1914258808
H	2.9799606932	3.8810651250	0.2109568574
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C	6.0618650944	-0.5776219369	0.3077916100
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C	4.5322423784	1.0862659769	-0.6616158861
C	3.9820691726	0.0421777660	-1.4371686876
C	3.6725629188	-2.1003499421	-2.1894919047
C	2.6352450033	-1.2430367234	-2.6726163518
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H	2.0631307354	-1.4113213453	-3.5852927365
H	5.9162832866	-2.6212437508	-0.3586240060
H	6.8718707556	-0.7801541510	1.0114907826
H	5.9974213411	1.5375057655	0.8226724869
H	4.1375581334	2.1001128973	-0.7232140476
H	2.2391430723	0.8274314398	-2.3313137784
C	3.7538477920	-3.5721694014	-2.3816142365
H	3.2313233395	-3.9011680432	-3.2902263165
H	3.2926934338	-4.0930782555	-1.5220450863
H	4.8000369691	-3.9089630915	-2.4364657326
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H	2.5895758909	0.5520579020	2.3440244775
H	2.4918157373	-3.7644299684	2.5277381749
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O	-1.0455149582	-0.6839536924	1.5969418424
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F	-2.8601540068	2.6449945212	1.6553579663
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C	2.0254955173	3.6285847356	1.2175005843
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H	3.7991364515	3.9165856964	2.4086914896
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C	-2.7560834162	3.0022713800	-1.6569204028
C	-3.7201104729	2.0041050522	-1.7971802120
C	-3.0638729860	4.2338224905	-1.0803813529
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C	-5.3458942847	3.4766946909	-0.7687748637
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O	-0.0325994415	-5.2721387470	-0.6184926207
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H	-1.8502010264	-6.3131060390	0.9998562890
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C	-3.0993030725	-2.2294460013	-0.3407883038

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C	-4.2838097033	-2.6126093435	1.7388736731
H	-2.1800997916	-3.0005068709	1.4509730309
C	-5.4606025516	-1.6819359546	-0.1586626265
H	-4.2699913498	-1.3690632739	-1.9359911311
C	-5.4636491482	-2.1252333816	1.1656280681
H	-4.2759188704	-2.9346554495	2.7828610405
H	-6.3774395683	-1.2965696270	-0.6114028429
H	-6.3815714124	-2.0798965278	1.7568585617

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C	-1.7478326599	-2.3035128400	1.1461417817
C	2.4907389479	-1.7164327232	-2.4582766552
C	3.6713365742	-2.2542426829	-3.0312235013
C	4.7063742493	-1.3965977159	-3.3381755166
C	4.5919555487	0.0057920755	-3.1009183268
C	3.4462318253	0.5728995285	-2.5756906053
C	2.3830825905	-0.2943372421	-2.2513612749
C	1.3067433098	-2.2971987646	-1.9547869240
C	0.5553208451	-1.2354287757	-1.3716651808
N	1.1778557384	-0.0300953075	-1.6959238110
H	-0.5183814994	-1.2531993790	-1.1830930175
H	3.7600840071	-3.3289532625	-3.2049409584
H	5.6306127697	-1.7857608225	-3.7706712976
H	5.4385121836	0.6508528467	-3.3483468219
H	3.3666587073	1.6447240168	-2.3909807461
H	0.8793024840	0.8738231909	-1.2802829220
C	0.9276153602	-3.7362451934	-1.9890893754
H	-0.1606234865	-3.8652723167	-1.9173489526
H	1.3751042972	-4.2983927655	-1.1527772075
H	1.2765600843	-4.2043996599	-2.9220133171
O	-1.4386596237	-1.1201858375	1.7016878432
C	-0.7008033391	-3.1731512460	0.9529256181
C	1.1934536389	-1.4023279827	0.6578049128
C	0.7190376674	-2.7084407051	1.2336242927
H	0.5394758871	-0.5640928851	0.8830866505
H	1.4160594447	-3.5168658914	0.9972452369
H	0.8353734051	-2.5428766106	2.3258504050
C	2.5950744243	-1.0521225288	0.6466267882
C	2.9677458026	0.3098206665	0.7817093074
C	3.6224304831	-1.9950054087	0.4290949205
C	4.2924986744	0.6982528626	0.7227062539
H	2.1909092721	1.0626070807	0.9142439767
C	4.9551517615	-1.6136203257	0.3470445348
H	3.3697328632	-3.0479245517	0.2963562387
C	5.2994955866	-0.2547599686	0.4826665432
H	4.5795634373	1.7447989066	0.8312998119
H	5.7158292742	-2.3682221995	0.1542087166
O	6.5576084771	0.2168449478	0.3928009033
C	7.6100801679	-0.6703153079	0.0756436702
H	7.4425221697	-1.1598803978	-0.8996743899

H	8.5233644211	-0.0640234860	0.0236180027
H	7.7371683611	-1.4463810323	0.8503046171
H	-1.9203936252	-0.3592701539	1.2513136884
N	-2.0647672832	0.9676851394	0.1865565783
P	-0.9706551020	2.1347205037	0.4984717816
S	-2.5849591883	0.7499084880	-1.3198844345
O	0.3891960847	2.0631773645	-0.1385971742
O	-1.7163469384	3.5526098109	0.2450192164
O	-0.8654983803	2.0579216029	2.1258700729
O	-2.0406358159	1.7231409544	-2.2774310831
O	-2.5533110806	-0.6763026172	-1.6698771734
C	-1.0451976724	4.6740842197	-0.2206941955
C	-0.7397958933	4.7757490096	-1.5785438918
C	-0.7179144038	5.6869526554	0.6810083447
C	-0.0902870372	5.9240949029	-2.0357126262
H	-1.0219262329	3.9559073349	-2.2408464743
C	-0.0683446345	6.8318005900	0.2090797690
H	-0.9847154490	5.5692928553	1.7329445723
C	0.2481869286	6.9512416495	-1.1472389638
H	0.1521505516	6.0175563133	-3.0970934889
H	0.1883497648	7.6333349766	0.9059311799
H	0.7549416086	7.8470385169	-1.5134443232
C	0.3422723905	1.9229759862	2.7892955709
C	0.5766803439	0.7433745007	3.4985594580
C	1.2951434283	2.9443988216	2.7514727007
C	1.7868832866	0.5867709835	4.1790201524
H	-0.1841050642	-0.0372561673	3.4822053211
C	2.5023105522	2.7729291324	3.4329890160
H	1.0943392742	3.8493567913	2.1761772043
C	2.7530776117	1.5962064341	4.1459224042
H	1.9781387040	-0.3369870103	4.7303076581
H	3.2537790279	3.5654147107	3.4012327912
H	3.7017702440	1.4654040008	4.6707566179
C	-4.3991087714	1.1619076866	-1.1630784774
F	-4.5398056188	2.4301330952	-0.7908263007
F	-4.9926663940	0.9824846185	-2.3404158579
F	-4.9750847828	0.3746128933	-0.2601687128
C	-0.9203037350	-4.6033794731	0.6744503023
O	-1.9536112820	-5.1536345514	0.3622993458
O	0.2312620399	-5.3287346674	0.8220476729
C	0.1085445395	-6.7259421885	0.5859429197
H	-0.2242393385	-6.9242637207	-0.4447283025
H	1.1050257762	-7.1541742103	0.7540738468
H	-0.6224484746	-7.1790061325	1.2722012083
C	-3.1929234126	-2.4965312562	0.8894311660
C	-4.0974763558	-2.0203432285	1.8551178415
C	-3.6926580713	-3.0431751087	-0.3018454970
C	-5.4730094407	-2.1204377613	1.6495129905
H	-3.7118455573	-1.5749399368	2.7738109465
C	-5.0659268140	-3.1211893437	-0.5147340049
H	-3.0019735108	-3.3768131239	-1.0717085181
C	-5.9598187357	-2.6694117290	0.4614230843
H	-6.1647817847	-1.7575648994	2.4131231317
H	-5.4429385991	-3.5305724790	-1.4545435974
H	-7.0370088105	-2.7353670898	0.2894063184

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C	-1.6586558505	-0.5858903372	0.8508378545
C	-3.4818631848	-0.3770462031	-2.4833199630
C	-4.0786892794	-1.4695263327	-3.1214130773
C	-3.3312067000	-2.1823427321	-4.0601845344
C	-2.0077333465	-1.8138254074	-4.3701815274
C	-1.3992484696	-0.7172998362	-3.7597702966
C	-2.1588577725	-0.0129466457	-2.8242596015
C	-3.9143280894	0.5337669060	-1.4101159749
C	-2.8362573051	1.4815483040	-1.2755760341
N	-1.8196842312	1.1057331183	-2.0659627697
H	-3.4744970143	0.0259517672	-0.2702518653
H	-5.1034602861	-1.7645369817	-2.8844349336
H	-3.7780051212	-3.0416832303	-4.5652231352
H	-1.4472749702	-2.3949905644	-5.1057296791
H	-0.3793339683	-0.4176348786	-3.9985510260
H	-0.8641203565	1.4662565993	-1.9852433458
O	-0.6261149358	0.1055372709	0.6731274243
C	-2.8883144623	0.0970886789	1.1672224836
C	-2.6915448446	2.4269496692	-0.1362268319
C	-2.7984616045	1.6119807176	1.2407511285
H	-3.5810368144	3.0770355787	-0.1593931578
H	-3.6887024386	1.9725754973	1.7666272540
H	-1.9247619849	1.8880064202	1.8400500491
C	-1.4565634275	3.2991489806	-0.3237638317
C	-1.4770865925	4.2798928043	-1.3341577527
C	-0.2492556989	3.0844764624	0.3437307883
C	-0.3286034156	4.9734864771	-1.6969531398
H	-2.4098325001	4.4803661604	-1.8702483133
C	0.9158531750	3.7708896294	-0.0051608602
H	-0.1867950138	2.3277703343	1.1198540218
C	0.8911360430	4.6972963822	-1.0534422407
H	-0.3412498236	5.7153272756	-2.4975507849
H	1.8373255319	3.5277336730	0.5202610234
O	1.9863944950	5.3480138989	-1.5088426601
C	3.2510149647	4.9348483945	-1.0242658009
H	3.3667954845	5.1452261108	0.0531146882
H	4.0010902529	5.5078180213	-1.5850871533
H	3.4123502113	3.8555620091	-1.1878271531
H	0.8078390604	-0.0091620010	0.2777505252
N	1.8639556458	0.1357889777	0.0800716792
S	2.1808752511	0.5097837381	-1.4857320879
O	3.0859660142	2.0769216790	1.5557472636
O	3.5449462868	1.0028981111	-1.6181477928
O	1.0466153889	1.1977446535	-2.1046413523
P	2.8092150668	0.6346867333	1.4065537272
O	1.9870944069	-0.0847564280	2.6065685285
O	4.1552399208	-0.2322209087	1.3555258471
C	0.8897275715	0.4304396780	3.3001208067
C	4.3280845688	-1.5469108280	0.9486164341
C	-0.0934770416	-0.4848003595	3.6753542534

C	0.7783087436	1.7858118753	3.6123726002
C	3.5267689134	-2.5801959110	1.4369771811
C	5.3710449249	-1.7941420854	0.0566377921
C	-1.2306515753	-0.0305141397	4.3424810080
C	-0.3664721459	2.2253147184	4.2853173654
H	1.5656324920	2.4779285801	3.3169004681
C	3.7749860041	-3.8859930689	1.0043187839
C	5.6109321971	-3.1036731367	-0.3613101964
C	-1.3739833261	1.3272903763	4.6455705418
H	-2.0160693748	-0.7423631086	4.6017112230
H	-0.4677924539	3.2870951575	4.5208267057
C	4.8116744748	-4.1519210572	0.1057180286
H	3.1578576356	-4.7024657995	1.3868482170
H	6.4230740061	-3.3040400469	-1.0637903498
H	-2.2709089648	1.6833644991	5.1563845002
H	5.0001098118	-5.1750804409	-0.2262778446
C	-3.9738315402	-0.4940614685	1.9689211700
O	-5.0487525356	0.0388358551	2.1740994786
O	-3.6715786812	-1.7037310885	2.5006403783
C	-4.7207990608	-2.3626768297	3.1995296541
H	-5.5947536146	-2.5160218255	2.5476982548
H	-5.0436274276	-1.7743640622	4.0717672783
H	-4.3127316454	-3.3294614405	3.5198975482
C	-1.5640603352	-2.0460383133	0.5520913309
C	-0.3255024382	-2.6851220562	0.7222690914
C	-2.6259142273	-2.7684563212	-0.0139494926
C	-0.1558011195	-4.0192624810	0.3559016597
H	0.5117766989	-2.1226580266	1.1329990317
C	-2.4532666396	-4.0976469421	-0.3963672414
H	-3.5849108686	-2.2815852431	-0.1849611190
C	-1.2199161591	-4.7294645345	-0.2068943344
H	0.8166486755	-4.4970337544	0.4910518114
H	-3.2823008105	-4.6400388242	-0.8563942495
H	-1.0858318598	-5.7708128832	-0.5093803899
H	5.9616273991	-0.9527293820	-0.3076403363
C	2.1135619089	-1.1917881055	-2.2827004373
F	0.9913908553	-1.8045109459	-1.9187994914
F	3.1537373174	-1.9276412367	-1.9322008229
F	2.1142121174	-1.0271834189	-3.6038325692
H	2.7373923589	-2.3605542262	2.1548540436
H	0.0198221229	-1.5357269928	3.4095849501
C	-5.3649710395	0.8295853604	-1.0932677982
H	-5.8320533649	1.4279992868	-1.8913134082
H	-5.9309085520	-0.1086635880	-0.9964623142
H	-5.4707116931	1.3556970392	-0.1353858047

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C	-0.0906823553	-1.4472837818	-1.5091633170
C	-1.6071317719	-2.2371604124	2.1898584459
C	-1.7300751764	-3.4839836444	2.8177457405
C	-0.6991295435	-3.9062813306	3.6578783146
C	0.4400015285	-3.1055864392	3.8777014538

C	0.5766289622	-1.8555634196	3.2765199126
C	-0.4640970613	-1.4398214257	2.4445094577
C	-2.4309924616	-1.5106241348	1.2196980703
C	-1.7543716469	-0.2635480799	1.0193015240
N	-0.5968063396	-0.2702606891	1.7030650802
H	-1.8040753125	-1.7673279800	-0.0980620454
H	-2.6080186732	-4.1118776364	2.6490600424
H	-0.7717957687	-4.8770165880	4.1539315069
H	1.2365562296	-3.4740555868	4.5275467008
H	1.4682933058	-1.2442161133	3.4165442841
H	0.0928401168	0.5111750684	1.6367789529
O	0.4797536280	-0.2805840258	-1.5956364601
C	-1.5167256344	-1.4567692983	-1.4759157627
C	-1.9792027555	0.6984762725	-0.1111191690
C	-2.2252687568	-0.1030651758	-1.4274286073
H	-1.0342603752	1.2414699507	-0.2297429075
H	-3.2922238263	-0.3165695734	-1.5492600435
H	-1.9168081388	0.5371911333	-2.2653910932
C	-3.0260551141	1.7585739967	0.2057634004
C	-2.7838610871	2.6097204814	1.3004599312
C	-4.1720495972	1.9826417067	-0.5555100957
C	-3.6586934700	3.6364429132	1.6229362951
H	-1.8732520438	2.4755725122	1.8893055990
C	-5.0636182890	3.0194429136	-0.2482754446
H	-4.3913697101	1.3596546281	-1.4228974427
C	-4.8103599458	3.8546064023	0.8461672757
H	-3.4695333382	4.2998097169	2.4687875612
H	-5.9448943514	3.1615242595	-0.8729919943
O	-5.6036831551	4.8878056429	1.2266707253
C	-6.7709997235	5.1569033973	0.4870440089
H	-7.4710682460	4.3019124643	0.4984650506
H	-7.2544194149	6.0197539631	0.9640572086
H	-6.5421660171	5.4103199892	-0.5642497176
H	1.4137741259	-0.1801045489	-1.1355076994
N	2.5185153074	0.3655924639	-0.1640640332
S	3.2805189554	-0.6522256665	0.8377035275
O	0.9163164581	1.9215538755	1.3520592891
O	3.7404220313	-0.0016917658	2.0707548804
O	2.5721515183	-1.9284814513	0.9253319700
P	2.0225947213	1.8495376163	0.3442962629
O	1.6050751682	2.5170790738	-1.0868363821
O	3.2631123502	2.7473375054	0.8474007673
C	0.4132288113	3.1764571397	-1.3430666172
C	4.5597843916	2.7093698845	0.3573402034
C	-0.2682131926	2.8268515950	-2.5109507720
C	-0.0849982393	4.1600684100	-0.4858012943
C	5.5883538780	2.6959979765	1.2990023567
C	4.8279256333	2.7104836970	-1.0129044738
C	-1.4703683725	3.4672326039	-2.8183219793
C	-1.2930129574	4.7865681715	-0.8025290966
H	0.4551368486	4.4108598894	0.4268854660
C	6.9118744635	2.6938653641	0.8587292810
C	6.1589251192	2.6965341013	-1.4388980687
C	-1.9899118717	4.4432963866	-1.9627846410
H	-2.0099925966	3.1910603683	-3.7274123176

H	-1.6988102859	5.5393505652	-0.1242061791
C	7.2018278275	2.6919469959	-0.5095564798
H	7.7224135542	2.6799939133	1.5911002092
H	6.3778086914	2.6924816140	-2.5093313517
H	-2.9416847512	4.9256300049	-2.1921821498
H	8.2395542502	2.6819865947	-0.8501374780
C	-2.3099906757	-2.5399867355	-2.1374217847
O	-3.5221532594	-2.5617973251	-2.1536381870
O	-1.5618533322	-3.4862212946	-2.7251694073
C	-2.2641181610	-4.5824304326	-3.3064665966
H	-2.8682155713	-5.1046139620	-2.5492720333
H	-2.9338246624	-4.2364625051	-4.1076420240
H	-1.4956604237	-5.2524905182	-3.7100379021
C	0.7663288977	-2.6261494245	-1.3605246547
C	2.0079482427	-2.6586798478	-2.0173139706
C	0.4083191854	-3.6790437756	-0.5006716277
C	2.8707793560	-3.7346635982	-1.8288398166
H	2.2936645877	-1.8365114096	-2.6748771985
C	1.2842132226	-4.7388223922	-0.2966188703
H	-0.5300235639	-3.6383267729	0.0516367730
C	2.5136733197	-4.7713491823	-0.9632169449
H	3.8361789175	-3.7510224066	-2.3378550436
H	1.0167639357	-5.5328184290	0.4034606761
H	3.2033389939	-5.6016588400	-0.7944308841
H	4.0058633942	2.7221280179	-1.7288857593
C	4.8410890457	-1.0660852976	-0.1427669990
F	5.8120969148	-0.2084719383	0.1364090823
F	4.6047282203	-1.0360998530	-1.4564882056
F	5.2358563888	-2.2926603603	0.1904578276
H	0.1486366320	2.0456442862	-3.1468137900
H	5.3294346529	2.6660279700	2.3574842776
C	-3.8995899576	-1.7753300267	0.9985154687
H	-4.4503287649	-1.6335559555	1.9425673615
H	-4.3303155316	-1.0988203245	0.2514066785
H	-4.0748449015	-2.8036403617	0.6514007422

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C	1.3047054914	2.7499780210	-0.7789036390
C	-3.9437100500	-1.7278823701	-1.0622002944
C	-4.9031541635	-2.3793012938	-0.2831038242
C	-4.4708321537	-3.0940087292	0.8399891033
C	-3.1117228578	-3.1508324999	1.1811903561
C	-2.1424052681	-2.4873676668	0.4205867008
C	-2.5820382983	-1.7924582242	-0.6961749713
C	-4.0259847751	-0.9159707736	-2.2759202898
C	-2.7558485766	-0.5314982756	-2.5768310818
N	-1.8482676074	-0.9525902386	-1.5729549777
H	-2.3905511501	0.0585780466	-3.4131823553
H	-5.9626380032	-2.3339838195	-0.5445203530
H	-5.2026342279	-3.6170300341	1.4602465390
H	-2.7938739508	-3.7144204502	2.0600274352
H	-1.1001621151	-2.4893072308	0.7268760902

H	-0.8743278306	-1.2313564189	-1.8838578968
O	2.0289845708	1.6433571277	-0.9751088503
C	-0.0627775368	2.7632280358	-0.9054635234
C	-1.3632941885	0.6927115699	-0.4876705944
C	-0.7880039003	1.5910229562	-1.5477698381
H	-0.0777404043	1.0102014005	-2.1530378068
H	-1.5713010692	1.9827455726	-2.2081375467
P	1.6783390944	-1.7554313833	-1.3642349249
O	0.6281941699	-1.5273553802	-2.4155352413
O	3.1323915866	-1.4061277244	-1.9583865323
O	1.8666483613	-3.3266470730	-0.9841157283
N	1.4055559910	-0.8609312947	-0.0274614037
S	1.5218926704	-1.2284647354	1.5244413530
O	0.1946025174	-1.2121792634	2.1657348872
O	2.4326458582	-2.3292865097	1.8539792233
H	1.5988126354	0.8085505662	-0.6598789395
C	-2.5806928580	0.9563650760	0.2373113028
C	-3.6980374781	1.6059252537	-0.3418151564
C	-2.7185277722	0.4095499050	1.5327763706
C	-4.8979006831	1.6896921329	0.3406898756
H	-3.6125556786	2.0430273512	-1.3339179857
C	-3.9188060937	0.4915358363	2.2257947013
H	-1.8586618095	-0.0869774158	1.9869156747
C	-5.0251565140	1.1186238723	1.6240636665
H	-5.7699150875	2.1822011465	-0.0924815689
H	-3.9903577276	0.0554523093	3.2207226992
O	-6.2370365998	1.2270244492	2.1983446040
C	-6.4557978325	0.6508513929	3.4713398458
H	-6.2794075100	-0.4384417216	3.4553544693
H	-5.8100118807	1.1085688015	4.2401816978
H	-7.5063614988	0.8439787394	3.7227608154
H	-0.6031417882	0.1653156950	0.0911889018
C	2.3305945461	0.3152279718	2.2052938426
F	3.5195385144	0.5234416874	1.6477721940
F	1.5525289120	1.3756940606	1.9742033109
F	2.4836187426	0.1699873265	3.5162159861
C	4.2290183244	-1.0392799899	-1.1798112121
C	4.7777900319	0.2248227043	-1.3927396326
C	4.7573715907	-1.9152793530	-0.2326272148
C	5.8852580717	0.6173966970	-0.6397861381
H	4.3109065643	0.8903415691	-2.1177308672
C	5.8616915758	-1.5062507570	0.5192104012
H	4.2953327838	-2.8894331379	-0.0768983131
C	6.4284807862	-0.2451598700	0.3180796805
H	6.3140607483	1.6103357659	-0.7940784207
H	6.2736441765	-2.1806705872	1.2731913316
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C	0.7009278732	-4.7034838012	0.5884561877
C	-0.1449610364	-4.4699175750	-1.6850229175
C	-0.3530933209	-5.5737662683	0.8791566167
H	1.4382620220	-4.4138821751	1.3367388511
C	-1.1961636878	-5.3352928552	-1.3749686647
H	-0.0447944145	-4.0193384752	-2.6723548977
C	-1.3027362499	-5.8900905664	-0.0966324610

H	-0.4335022453	-6.0003891515	1.8818139401
H	-1.9392114892	-5.5730565511	-2.1395651098
H	-2.1298822459	-6.5625944705	0.1403581965
C	2.1719026173	3.9254196972	-0.5313851061
C	3.3470677793	3.7546207913	0.2201649448
C	1.9010115813	5.1811913781	-1.0977203497
C	4.2097131109	4.8299614128	0.4340332236
H	3.5748965236	2.7744931812	0.6363746639
C	2.7685992255	6.2511663991	-0.8910441113
H	1.0157803058	5.3125226250	-1.7213015881
C	3.9221164660	6.0811051075	-0.1178562352
H	5.1132114097	4.6882307064	1.0318629310
H	2.5490675636	7.2220769252	-1.3412361590
H	4.6007425626	6.9220643310	0.0448378105
C	-0.8651135740	3.8990575252	-0.4074968557
O	-0.5732078632	4.6637155415	0.4827387442
O	-2.0545219803	3.9964815100	-1.0665885203
C	-2.9471983993	4.9923351182	-0.5803304815
H	-3.2117570239	4.7999730120	0.4704298144
H	-2.4944127514	5.9927975112	-0.6465908180
H	-3.8435108478	4.9369296046	-1.2112010498
C	-5.2826780492	-0.5878910555	-3.0074713300
H	-5.9636276236	-0.0124632003	-2.3568463858
H	-5.0853345853	0.0072107947	-3.9104431296
H	-5.8205104157	-1.5028706560	-3.3059190729

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C	3.5952476377	-0.5905248416	1.4183196332
C	4.9390890826	-0.2443774116	1.1368887888
C	5.9305143506	-0.9835768113	1.7537023362
C	5.6471022759	-2.0624911456	2.6412813866
C	4.3461280788	-2.4126258717	2.9245693624
C	1.8954191728	-1.8269909101	2.3590572030
C	1.3581448983	-0.8873458733	1.4235690045
H	5.1853006046	0.5684043797	0.4581523675
H	6.9746808650	-0.7330187367	1.5505643411
H	6.4757634444	-2.6122222513	3.0916869498
H	4.1186233916	-3.2422277121	3.5967031488
N	2.4225563162	-0.0836286978	0.9609905018
C	2.1122008906	0.9029933190	-0.0877325160
H	1.1761341044	1.3704261080	0.2551899407
C	1.0822566011	-2.8084376511	3.1171541536
H	0.2610605480	-3.1771754162	2.4821908353
H	0.6088814788	-2.3265265027	3.9901996114
H	1.6830769120	-3.6567405888	3.4726648665
C	1.7896631011	0.1538807511	-1.3784350781
H	2.6744849647	-0.3255796766	-1.8125030854
H	1.4435386260	0.8829863402	-2.1212132772
C	0.7859383555	-1.9492055653	-0.0876292289
C	0.6569067512	-0.8498578573	-1.1797605199
H	-0.2387498559	-0.2875380942	-0.9021744875

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C	3.9332395865	2.1884847073	-1.3509637404
C	3.3797516547	2.8262100856	0.8996287644
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H	3.7848877596	1.5614813082	-2.2307522964
C	4.3525353458	3.8264100713	0.8740335876
H	2.7817153364	2.6887655219	1.8042364507
C	5.1285240277	4.0100063035	-0.2823288561
H	5.5084263475	3.3471769832	-2.2905540265
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O	6.0961006524	4.9469253273	-0.4144702478
C	6.3620593374	5.8155877342	0.6642139224
H	5.4786565442	6.4245671650	0.9265931638
H	7.1706557273	6.4821237869	0.3372073397
H	6.6925741664	5.2636931582	1.5623601996
O	-0.3754651054	-2.4528231593	0.3103938290
N	-2.4160319400	-0.7971278197	0.1781268335
P	-2.2658243058	0.7576109740	0.6651255522
S	-3.7262749557	-1.4371226884	-0.5125819793
O	-0.9193334932	1.0192457742	1.2642699843
O	-3.5256239745	1.0691625440	1.6260835490
O	-2.5983714733	1.7965675683	-0.5524433419
O	-3.3768756780	-2.7254350347	-1.1099661160
O	-4.5241635039	-0.4688560092	-1.2804009877
C	-4.8248404271	-1.9227664941	0.9411004752
H	0.4000664177	-0.3653850296	1.5470675353
H	-1.1674711419	-1.8039766424	0.2344125028
C	-1.7420897115	1.9458943156	-1.6254807048
C	-1.9307301172	1.1598733863	-2.7650742812
C	-0.7165208642	2.8929620846	-1.5573630499
C	-1.0734622536	1.3345774791	-3.8546492599
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C	0.1254039899	3.0665321487	-2.6590481169
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C	-0.0496527388	2.2873608065	-3.8080833301
H	-1.2075795894	0.7217085514	-4.7488052717
H	0.9301025085	3.8038803288	-2.6120863401
H	0.6149660202	2.4171940909	-4.6648580986
C	-4.3186552995	2.2089648969	1.6174721724
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C	-6.1878352710	3.4316759880	0.7379445998
H	-5.5135141493	1.4992760058	-0.0209973835
C	-4.8995839174	4.3360877244	2.5776166849
H	-3.2352687231	3.0954238986	3.2470383583
C	-5.9585804226	4.4480961636	1.6723218661
H	-7.0124972709	3.5180289043	0.0264352378
H	-4.7156475797	5.1272555086	3.3085258019
H	-6.6057286506	5.3279341528	1.6937586977
F	-4.0819342005	-2.3833594062	1.9462184844
F	-5.5454724224	-0.8915672813	1.3720844473
F	-5.6537877765	-2.8839220655	0.5410652267
C	1.8156634425	-3.0278614051	-0.2827723898
C	1.4496407314	-4.3559432668	0.0022146099
C	3.1291268820	-2.7756160896	-0.7134226684

C	2.3745949368	-5.3920083213	-0.1173262040
H	0.4240177306	-4.5624063982	0.3039464235
C	4.0556082274	-3.8134843641	-0.8227998574
H	3.4505246639	-1.7723374602	-0.9656073375
C	3.6859924348	-5.1247258867	-0.5212721792
H	2.0661348294	-6.4171941723	0.1010175395
H	5.0730616327	-3.5886829312	-1.1497692939
H	4.4118273540	-5.9363428077	-0.6109669132
C	0.3319591421	-1.5425780618	-2.5039508068
O	1.1072470252	-1.6819531122	-3.4182310461
O	-0.9279709442	-1.9641170789	-2.4980228288
C	-1.4083640053	-2.6857465591	-3.6316804188
H	-2.4243455180	-2.9915813444	-3.3617055689
H	-1.4086979614	-2.0390365067	-4.5223657208
H	-0.7692647983	-3.5588858900	-3.8285807931

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C	-6.0329127914	-3.5552247975	-1.2896507328
C	-4.9297704939	-3.0346695203	-1.9335210361
C	-2.7220093958	-1.7454278980	-1.5019390304
C	-2.1968787679	-1.2019747281	-0.2900913178
H	-5.3228543288	-2.7916115107	2.0001279839
H	-7.0478341371	-3.8896063278	0.6017082746
H	-6.8236111719	-4.0431956341	-1.8626321130
H	-4.8298909446	-3.0965945528	-3.0189412399
N	-2.9942535848	-1.6669420054	0.7743235037
C	-2.7524163157	-1.1697563768	2.1312877594
H	-3.4431449921	-1.7127491647	2.7953699711
C	-2.0982956981	-1.5415623063	-2.8287112080
H	-1.0099295540	-1.6855167873	-2.7552410109
H	-2.5301289142	-2.1988392060	-3.5958078030
H	-2.2489409351	-0.4930449859	-3.1450089104
C	-3.1189852934	0.3191247138	2.1467394553
H	-4.2032434432	0.4409542274	2.0357597984
H	-2.8862106733	0.7546389763	3.1251537372
C	-2.4829955614	0.7476903452	-0.4007866339
C	-2.3497541077	1.1194831545	1.0932993593
H	-1.2805055580	0.9996680312	1.3125948517
C	-1.3094391982	-1.4648331072	2.5334886444
C	-0.7246130294	-2.6947343407	2.1812220588
C	-0.5078467198	-0.5294841895	3.1937203085
C	0.6108271294	-2.9611381902	2.4470684840
H	-1.3196769846	-3.4444021088	1.6539901801
C	0.8396259756	-0.7782075747	3.4614060498
H	-0.8974633572	0.4460351789	3.4808550469
C	1.4168688371	-1.9924625412	3.0713199727
H	1.0711789598	-3.9034470012	2.1460671960
H	1.4360190961	0.0072587760	3.9205995337

O	2.7185648956	-2.3032264707	3.2349578819
C	3.5977611853	-1.2984150297	3.7116464011
H	3.3943172379	-1.0618559553	4.7714664502
H	4.6114381105	-1.7079275102	3.6189268964
H	3.5176336081	-0.3793593169	3.1111985344
O	-1.4605032094	1.1367378226	-1.1490695685
N	0.8142181276	0.8667732212	0.2281132408
P	1.6291385973	-0.3397578016	-0.5129958598
S	1.3998772123	1.9611530469	1.2403395241
O	0.7270330697	-1.3439137494	-1.1469798525
O	2.6125488134	0.4392400968	-1.5597748202
O	2.6426365099	-0.9928054851	0.5711449365
O	0.3146631694	2.4801674695	2.0823863514
O	2.6790014688	1.6169024702	1.8727175704
C	1.8208866052	3.4057794040	0.1134599596
H	-1.1177404715	-1.1393228395	-0.1361838785
H	-0.5970379281	1.1411184878	-0.6203404064
C	3.4399136990	-0.0993138772	-2.5251761292
C	3.3334389813	-1.4180396979	-2.9753524789
C	4.4128142479	0.7611261642	-3.0404733070
C	4.2315109869	-1.8736582221	-3.9447737013
H	2.5567063053	-2.0679884557	-2.5724381605
C	5.2970523572	0.2926603786	-4.0119752340
H	4.4602284928	1.7820013462	-2.6586244012
C	5.2134890408	-1.0279167885	-4.4660136241
H	4.1567126959	-2.9062210727	-4.2945313025
H	6.0607076930	0.9637677957	-4.4125444910
H	5.9107070837	-1.3947915969	-5.2223763976
C	3.9912524579	-1.2587762478	0.4175854956
C	4.3938089083	-2.5904563186	0.3219046884
C	4.9164372921	-0.2142353263	0.4091264729
C	5.7539550395	-2.8810342707	0.1997094473
H	3.6358571256	-3.3737347551	0.3498062984
C	6.2728709592	-0.5187197284	0.2776270180
H	4.5594290341	0.8098821305	0.5101382783
C	6.6956067889	-1.8473238097	0.1710483434
H	6.0787646066	-3.9213674991	0.1224762199
H	7.0049092877	0.2921082963	0.2610108129
H	7.7583952478	-2.0775758700	0.0682054220
F	1.9413264061	4.5122765300	0.8444322283
F	0.8571542891	3.5937817281	-0.7900046962
F	2.9693041137	3.1827145502	-0.5239010855
C	-3.7943300839	0.9729603268	-1.0907844855
C	-3.7838369440	1.6042127393	-2.3483920799
C	-5.0316462006	0.5831396359	-0.5485018666
C	-4.9713049867	1.8243513705	-3.0454216112
H	-2.8305201592	1.9366650198	-2.7564574671
C	-6.2168354637	0.7965125373	-1.2529023201
H	-5.0885318511	0.0997015174	0.4202457318
C	-6.1931250233	1.4150325742	-2.5044889267
H	-4.9414814562	2.3243737063	-4.0163851813
H	-7.1643818573	0.4750620702	-0.8152231056
H	-7.1230298708	1.5846762056	-3.0522368039
C	-2.5738577223	2.6194598849	1.3095450118
O	-3.1611377497	3.0769323496	2.2580115747

O	-1.9833806141	3.3505151241	0.3643617343
C	-1.8744131158	4.7524322015	0.6087322976
H	-1.2008087439	4.9221627672	1.4616727500
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H	-2.8585279398	5.1917415661	0.8250477077

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C	-0.9694225893	-1.3055544616	2.0777194130
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C	-0.5442996028	-2.9549424847	0.2751966417
C	0.5500485858	-3.3749797760	1.0061678981
C	0.8939946305	-2.8064407775	2.2689001803
C	0.1531074757	-1.7831944566	2.8074358198
C	-1.8555627193	-0.2441731648	2.3032640941
C	-2.6860290435	-0.1575436408	1.1346077302
H	-0.7588904411	-3.3789152705	-0.7050421268
H	1.1963893839	-4.1526505045	0.5957130388
H	1.7864881550	-3.1654227293	2.7795327151
H	0.4443775612	-1.3014533198	3.7401170392
N	-2.4596603071	-1.3228160497	0.3585230626
C	-3.0662982512	-1.4627254765	-0.9663879151
H	-2.7177074583	-2.4283942250	-1.3625608743
C	-1.8546906360	0.7007122299	3.4481376988
H	-0.9374402067	1.3123319448	3.4096896918
H	-2.7307354485	1.3606212243	3.4428259567
H	-1.8230313054	0.1490960864	4.4012929745
C	-2.5460325401	-0.3533971171	-1.8907933838
H	-1.4836342574	-0.5342615106	-2.1017238171
H	-3.0909615221	-0.3703647119	-2.8427200833
C	-1.7604768853	1.1257622904	-0.0046628752
C	-2.6774037766	1.0344941607	-1.2362782754
H	-3.7208881600	1.2082463448	-0.9453502757
C	-4.5845859952	-1.5259904346	-0.8211593504
C	-5.1385471407	-2.3740962401	0.1562808911
C	-5.4634927304	-0.7946639587	-1.6245433636
C	-6.5112492359	-2.4880591298	0.3212154219
H	-4.4724861162	-2.9502982513	0.8030147918
C	-6.8521202135	-0.8964457230	-1.4700969734
H	-5.0861756651	-0.1171421671	-2.3916195592
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H	-6.3915479499	-3.3377060140	1.2685059992
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P	0.6477414756	1.3980479370	0.1547675457
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H	1.6183898347	-0.7413450629	2.0438875529
C	3.5320302511	3.8372288889	1.3429103490
F	3.8403033047	3.1930110683	2.4628958536
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H	-1.3651059399	1.3578450894	2.4849339815
C	-3.5459734257	3.9129462746	0.5173117599
H	-1.7235768830	4.3465893399	-0.5927328981
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C	2.6915629326	-4.2341856586	-1.2302163451
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C	3.2883423573	-2.3198658432	0.1213872256
C	1.9968382824	-2.0849540565	0.5992401806
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O	-2.4656143429	0.2271511292	2.0177314202
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O	-3.0177421259	-2.4280298814	-1.4210622488
O	0.3939433944	-0.7453254634	-1.7574827756
H	1.0897604377	-1.1602823348	-1.2237631458
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H	2.5872065656	4.4286218045	-4.2484082217
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C	3.9820691726	0.0421777660	-1.4371686876
C	3.6725629188	-2.1003499421	-2.1894919047
C	2.6352450033	-1.2430367234	-2.6726163518
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H	2.0631307354	-1.4113213453	-3.5852927365
H	5.9162832866	-2.6212437508	-0.3586240060
H	6.8718707556	-0.7801541510	1.0114907826
H	5.9974213411	1.5375057655	0.8226724869
H	4.1375581334	2.1001128973	-0.7232140476
H	2.2391430723	0.8274314398	-2.3313137784
C	3.7538477920	-3.5721694014	-2.3816142365
H	3.2313233395	-3.9011680432	-3.2902263165
H	3.2926934338	-4.0930782555	-1.5220450863
H	4.8000369691	-3.9089630915	-2.4364657326
O	-1.6628921413	-1.0448930457	-1.8300771361
C	-0.9052507774	-3.1634638089	-1.2865916400
C	1.0975735483	-1.6512566322	-1.3999937548
C	0.3878493457	-2.8339765645	-2.0195890731
H	0.1600418242	-2.5903881412	-3.0691394827
H	1.0144404397	-3.7326792308	-2.0064180711
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C	1.9092855635	-0.4635768676	0.5918608726
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H	2.5895758909	0.5520579020	2.3440244775
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H	2.4112765122	0.1255521856	4.6220171914
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N	-1.0768986851	1.0427855777	-0.2256005150
S	-1.0393721315	0.7574996300	1.3457283596
O	-1.0455149582	-0.6839536924	1.5969418424
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C	2.0254955173	3.6285847356	1.2175005843
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H	3.7991364515	3.9165856964	2.4086914896
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C	-2.7560834162	3.0022713800	-1.6569204028
C	-3.7201104729	2.0041050522	-1.7971802120
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C	-2.3882924785	-6.2549529810	0.0411125343
H	-1.8502010264	-6.3131060390	0.9998562890
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H	-1.9881551033	-7.0326662589	-0.6269617147
C	-3.0993030725	-2.2294460013	-0.3407883038

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C	-5.4636491482	-2.1252333816	1.1656280681
H	-4.2759188704	-2.9346554495	2.7828610405
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C	3.4462318253	0.5728995285	-2.5756906053
C	2.3830825905	-0.2943372421	-2.2513612749
C	1.3067433098	-2.2971987646	-1.9547869240
C	0.5553208451	-1.2354287757	-1.3716651808
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H	-0.1606234865	-3.8652723167	-1.9173489526
H	1.3751042972	-4.2983927655	-1.1527772075
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C	0.7190376674	-2.7084407051	1.2336242927
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H	0.8353734051	-2.5428766106	2.3258504050
C	2.5950744243	-1.0521225288	0.6466267882
C	2.9677458026	0.3098206665	0.7817093074
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H	3.3697328632	-3.0479245517	0.2963562387
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P	-0.9706551020	2.1347205037	0.4984717816
S	-2.5849591883	0.7499084880	-1.3198844345
O	0.3891960847	2.0631773645	-0.1385971742
O	-1.7163469384	3.5526098109	0.2450192164
O	-0.8654983803	2.0579216029	2.1258700729
O	-2.0406358159	1.7231409544	-2.2774310831
O	-2.5533110806	-0.6763026172	-1.6698771734
C	-1.0451976724	4.6740842197	-0.2206941955
C	-0.7397958933	4.7757490096	-1.5785438918
C	-0.7179144038	5.6869526554	0.6810083447
C	-0.0902870372	5.9240949029	-2.0357126262
H	-1.0219262329	3.9559073349	-2.2408464743
C	-0.0683446345	6.8318005900	0.2090797690
H	-0.9847154490	5.5692928553	1.7329445723
C	0.2481869286	6.9512416495	-1.1472389638
H	0.1521505516	6.0175563133	-3.0970934889
H	0.1883497648	7.6333349766	0.9059311799
H	0.7549416086	7.8470385169	-1.5134443232
C	0.3422723905	1.9229759862	2.7892955709
C	0.5766803439	0.7433745007	3.4985594580
C	1.2951434283	2.9443988216	2.7514727007
C	1.7868832866	0.5867709835	4.1790201524
H	-0.1841050642	-0.0372561673	3.4822053211
C	2.5023105522	2.7729291324	3.4329890160
H	1.0943392742	3.8493567913	2.1761772043
C	2.7530776117	1.5962064341	4.1459224042
H	1.9781387040	-0.3369870103	4.7303076581
H	3.2537790279	3.5654147107	3.4012327912
H	3.7017702440	1.4654040008	4.6707566179
C	-4.3991087714	1.1619076866	-1.1630784774
F	-4.5398056188	2.4301330952	-0.7908263007
F	-4.9926663940	0.9824846185	-2.3404158579
F	-4.9750847828	0.3746128933	-0.2601687128
C	-0.9203037350	-4.6033794731	0.6744503023
O	-1.9536112820	-5.1536345514	0.3622993458
O	0.2312620399	-5.3287346674	0.8220476729
C	0.1085445395	-6.7259421885	0.5859429197
H	-0.2242393385	-6.9242637207	-0.4447283025
H	1.1050257762	-7.1541742103	0.7540738468
H	-0.6224484746	-7.1790061325	1.2722012083
C	-3.1929234126	-2.4965312562	0.8894311660
C	-4.0974763558	-2.0203432285	1.8551178415
C	-3.6926580713	-3.0431751087	-0.3018454970
C	-5.4730094407	-2.1204377613	1.6495129905
H	-3.7118455573	-1.5749399368	2.7738109465
C	-5.0659268140	-3.1211893437	-0.5147340049
H	-3.0019735108	-3.3768131239	-1.0717085181
C	-5.9598187357	-2.6694117290	0.4614230843
H	-6.1647817847	-1.7575648994	2.4131231317
H	-5.4429385991	-3.5305724790	-1.4545435974
H	-7.0370088105	-2.7353670898	0.2894063184

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C	-1.6586558505	-0.5858903372	0.8508378545
C	-3.4818631848	-0.3770462031	-2.4833199630
C	-4.0786892794	-1.4695263327	-3.1214130773
C	-3.3312067000	-2.1823427321	-4.0601845344
C	-2.0077333465	-1.8138254074	-4.3701815274
C	-1.3992484696	-0.7172998362	-3.7597702966
C	-2.1588577725	-0.0129466457	-2.8242596015
C	-3.9143280894	0.5337669060	-1.4101159749
C	-2.8362573051	1.4815483040	-1.2755760341
N	-1.8196842312	1.1057331183	-2.0659627697
H	-3.4744970143	0.0259517672	-0.2702518653
H	-5.1034602861	-1.7645369817	-2.8844349336
H	-3.7780051212	-3.0416832303	-4.5652231352
H	-1.4472749702	-2.3949905644	-5.1057296791
H	-0.3793339683	-0.4176348786	-3.9985510260
H	-0.8641203565	1.4662565993	-1.9852433458
O	-0.6261149358	0.1055372709	0.6731274243
C	-2.8883144623	0.0970886789	1.1672224836
C	-2.6915448446	2.4269496692	-0.1362268319
C	-2.7984616045	1.6119807176	1.2407511285
H	-3.5810368144	3.0770355787	-0.1593931578
H	-3.6887024386	1.9725754973	1.7666272540
H	-1.9247619849	1.8880064202	1.8400500491
C	-1.4565634275	3.2991489806	-0.3237638317
C	-1.4770865925	4.2798928043	-1.3341577527
C	-0.2492556989	3.0844764624	0.3437307883
C	-0.3286034156	4.9734864771	-1.6969531398
H	-2.4098325001	4.4803661604	-1.8702483133
C	0.9158531750	3.7708896294	-0.0051608602
H	-0.1867950138	2.3277703343	1.1198540218
C	0.8911360430	4.6972963822	-1.0534422407
H	-0.3412498236	5.7153272756	-2.4975507849
H	1.8373255319	3.5277336730	0.5202610234
O	1.9863944950	5.3480138989	-1.5088426601
C	3.2510149647	4.9348483945	-1.0242658009
H	3.3667954845	5.1452261108	0.0531146882
H	4.0010902529	5.5078180213	-1.5850871533
H	3.4123502113	3.8555620091	-1.1878271531
H	0.8078390604	-0.0091620010	0.2777505252
N	1.8639556458	0.1357889777	0.0800716792
S	2.1808752511	0.5097837381	-1.4857320879
O	3.0859660142	2.0769216790	1.5557472636
O	3.5449462868	1.0028981111	-1.6181477928
O	1.0466153889	1.1977446535	-2.1046413523
P	2.8092150668	0.6346867333	1.4065537272
O	1.9870944069	-0.0847564280	2.6065685285
O	4.1552399208	-0.2322209087	1.3555258471
C	0.8897275715	0.4304396780	3.3001208067
C	4.3280845688	-1.5469108280	0.9486164341
C	-0.0934770416	-0.4848003595	3.6753542534

C	0.7783087436	1.7858118753	3.6123726002
C	3.5267689134	-2.5801959110	1.4369771811
C	5.3710449249	-1.7941420854	0.0566377921
C	-1.2306515753	-0.0305141397	4.3424810080
C	-0.3664721459	2.2253147184	4.2853173654
H	1.5656324920	2.4779285801	3.3169004681
C	3.7749860041	-3.8859930689	1.0043187839
C	5.6109321971	-3.1036731367	-0.3613101964
C	-1.3739833261	1.3272903763	4.6455705418
H	-2.0160693748	-0.7423631086	4.6017112230
H	-0.4677924539	3.2870951575	4.5208267057
C	4.8116744748	-4.1519210572	0.1057180286
H	3.1578576356	-4.7024657995	1.3868482170
H	6.4230740061	-3.3040400469	-1.0637903498
H	-2.2709089648	1.6833644991	5.1563845002
H	5.0001098118	-5.1750804409	-0.2262778446
C	-3.9738315402	-0.4940614685	1.9689211700
O	-5.0487525356	0.0388358551	2.1740994786
O	-3.6715786812	-1.7037310885	2.5006403783
C	-4.7207990608	-2.3626768297	3.1995296541
H	-5.5947536146	-2.5160218255	2.5476982548
H	-5.0436274276	-1.7743640622	4.0717672783
H	-4.3127316454	-3.3294614405	3.5198975482
C	-1.5640603352	-2.0460383133	0.5520913309
C	-0.3255024382	-2.6851220562	0.7222690914
C	-2.6259142273	-2.7684563212	-0.0139494926
C	-0.1558011195	-4.0192624810	0.3559016597
H	0.5117766989	-2.1226580266	1.1329990317
C	-2.4532666396	-4.0976469421	-0.3963672414
H	-3.5849108686	-2.2815852431	-0.1849611190
C	-1.2199161591	-4.7294645345	-0.2068943344
H	0.8166486755	-4.4970337544	0.4910518114
H	-3.2823008105	-4.6400388242	-0.8563942495
H	-1.0858318598	-5.7708128832	-0.5093803899
H	5.9616273991	-0.9527293820	-0.3076403363
C	2.1135619089	-1.1917881055	-2.2827004373
F	0.9913908553	-1.8045109459	-1.9187994914
F	3.1537373174	-1.9276412367	-1.9322008229
F	2.1142121174	-1.0271834189	-3.6038325692
H	2.7373923589	-2.3605542262	2.1548540436
H	0.0198221229	-1.5357269928	3.4095849501
C	-5.3649710395	0.8295853604	-1.0932677982
H	-5.8320533649	1.4279992868	-1.8913134082
H	-5.9309085520	-0.1086635880	-0.9964623142
H	-5.4707116931	1.3556970392	-0.1353858047

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C	-0.0906823553	-1.4472837818	-1.5091633170
C	-1.6071317719	-2.2371604124	2.1898584459
C	-1.7300751764	-3.4839836444	2.8177457405
C	-0.6991295435	-3.9062813306	3.6578783146
C	0.4400015285	-3.1055864392	3.8777014538

C	0.5766289622	-1.8555634196	3.2765199126
C	-0.4640970613	-1.4398214257	2.4445094577
C	-2.4309924616	-1.5106241348	1.2196980703
C	-1.7543716469	-0.2635480799	1.0193015240
N	-0.5968063396	-0.2702606891	1.7030650802
H	-1.8040753125	-1.7673279800	-0.0980620454
H	-2.6080186732	-4.1118776364	2.6490600424
H	-0.7717957687	-4.8770165880	4.1539315069
H	1.2365562296	-3.4740555868	4.5275467008
H	1.4682933058	-1.2442161133	3.4165442841
H	0.0928401168	0.5111750684	1.6367789529
O	0.4797536280	-0.2805840258	-1.5956364601
C	-1.5167256344	-1.4567692983	-1.4759157627
C	-1.9792027555	0.6984762725	-0.1111191690
C	-2.2252687568	-0.1030651758	-1.4274286073
H	-1.0342603752	1.2414699507	-0.2297429075
H	-3.2922238263	-0.3165695734	-1.5492600435
H	-1.9168081388	0.5371911333	-2.2653910932
C	-3.0260551141	1.7585739967	0.2057634004
C	-2.7838610871	2.6097204814	1.3004599312
C	-4.1720495972	1.9826417067	-0.5555100957
C	-3.6586934700	3.6364429132	1.6229362951
H	-1.8732520438	2.4755725122	1.8893055990
C	-5.0636182890	3.0194429136	-0.2482754446
H	-4.3913697101	1.3596546281	-1.4228974427
C	-4.8103599458	3.8546064023	0.8461672757
H	-3.4695333382	4.2998097169	2.4687875612
H	-5.9448943514	3.1615242595	-0.8729919943
O	-5.6036831551	4.8878056429	1.2266707253
C	-6.7709997235	5.1569033973	0.4870440089
H	-7.4710682460	4.3019124643	0.4984650506
H	-7.2544194149	6.0197539631	0.9640572086
H	-6.5421660171	5.4103199892	-0.5642497176
H	1.4137741259	-0.1801045489	-1.1355076994
N	2.5185153074	0.3655924639	-0.1640640332
S	3.2805189554	-0.6522256665	0.8377035275
O	0.9163164581	1.9215538755	1.3520592891
O	3.7404220313	-0.0016917658	2.0707548804
O	2.5721515183	-1.9284814513	0.9253319700
P	2.0225947213	1.8495376163	0.3442962629
O	1.6050751682	2.5170790738	-1.0868363821
O	3.2631123502	2.7473375054	0.8474007673
C	0.4132288113	3.1764571397	-1.3430666172
C	4.5597843916	2.7093698845	0.3573402034
C	-0.2682131926	2.8268515950	-2.5109507720
C	-0.0849982393	4.1600684100	-0.4858012943
C	5.5883538780	2.6959979765	1.2990023567
C	4.8279256333	2.7104836970	-1.0129044738
C	-1.4703683725	3.4672326039	-2.8183219793
C	-1.2930129574	4.7865681715	-0.8025290966
H	0.4551368486	4.4108598894	0.4268854660
C	6.9118744635	2.6938653641	0.8587292810
C	6.1589251192	2.6965341013	-1.4388980687
C	-1.9899118717	4.4432963866	-1.9627846410
H	-2.0099925966	3.1910603683	-3.7274123176

H	-1.6988102859	5.5393505652	-0.1242061791
C	7.2018278275	2.6919469959	-0.5095564798
H	7.7224135542	2.6799939133	1.5911002092
H	6.3778086914	2.6924816140	-2.5093313517
H	-2.9416847512	4.9256300049	-2.1921821498
H	8.2395542502	2.6819865947	-0.8501374780
C	-2.3099906757	-2.5399867355	-2.1374217847
O	-3.5221532594	-2.5617973251	-2.1536381870
O	-1.5618533322	-3.4862212946	-2.7251694073
C	-2.2641181610	-4.5824304326	-3.3064665966
H	-2.8682155713	-5.1046139620	-2.5492720333
H	-2.9338246624	-4.2364625051	-4.1076420240
H	-1.4956604237	-5.2524905182	-3.7100379021
C	0.7663288977	-2.6261494245	-1.3605246547
C	2.0079482427	-2.6586798478	-2.0173139706
C	0.4083191854	-3.6790437756	-0.5006716277
C	2.8707793560	-3.7346635982	-1.8288398166
H	2.2936645877	-1.8365114096	-2.6748771985
C	1.2842132226	-4.7388223922	-0.2966188703
H	-0.5300235639	-3.6383267729	0.0516367730
C	2.5136733197	-4.7713491823	-0.9632169449
H	3.8361789175	-3.7510224066	-2.3378550436
H	1.0167639357	-5.5328184290	0.4034606761
H	3.2033389939	-5.6016588400	-0.7944308841
H	4.0058633942	2.7221280179	-1.7288857593
C	4.8410890457	-1.0660852976	-0.1427669990
F	5.8120969148	-0.2084719383	0.1364090823
F	4.6047282203	-1.0360998530	-1.4564882056
F	5.2358563888	-2.2926603603	0.1904578276
H	0.1486366320	2.0456442862	-3.1468137900
H	5.3294346529	2.6660279700	2.3574842776
C	-3.8995899576	-1.7753300267	0.9985154687
H	-4.4503287649	-1.6335559555	1.9425673615
H	-4.3303155316	-1.0988203245	0.2514066785
H	-4.0748449015	-2.8036403617	0.6514007422

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C	1.3047054914	2.7499780210	-0.7789036390
C	-3.9437100500	-1.7278823701	-1.0622002944
C	-4.9031541635	-2.3793012938	-0.2831038242
C	-4.4708321537	-3.0940087292	0.8399891033
C	-3.1117228578	-3.1508324999	1.1811903561
C	-2.1424052681	-2.4873676668	0.4205867008
C	-2.5820382983	-1.7924582242	-0.6961749713
C	-4.0259847751	-0.9159707736	-2.2759202898
C	-2.7558485766	-0.5314982756	-2.5768310818
N	-1.8482676074	-0.9525902386	-1.5729549777
H	-2.3905511501	0.0585780466	-3.4131823553
H	-5.9626380032	-2.3339838195	-0.5445203530
H	-5.2026342279	-3.6170300341	1.4602465390
H	-2.7938739508	-3.7144204502	2.0600274352
H	-1.1001621151	-2.4893072308	0.7268760902

H	-0.8743278306	-1.2313564189	-1.8838578968
O	2.0289845708	1.6433571277	-0.9751088503
C	-0.0627775368	2.7632280358	-0.9054635234
C	-1.3632941885	0.6927115699	-0.4876705944
C	-0.7880039003	1.5910229562	-1.5477698381
H	-0.0777404043	1.0102014005	-2.1530378068
H	-1.5713010692	1.9827455726	-2.2081375467
P	1.6783390944	-1.7554313833	-1.3642349249
O	0.6281941699	-1.5273553802	-2.4155352413
O	3.1323915866	-1.4061277244	-1.9583865323
O	1.8666483613	-3.3266470730	-0.9841157283
N	1.4055559910	-0.8609312947	-0.0274614037
S	1.5218926704	-1.2284647354	1.5244413530
O	0.1946025174	-1.2121792634	2.1657348872
O	2.4326458582	-2.3292865097	1.8539792233
H	1.5988126354	0.8085505662	-0.6598789395
C	-2.5806928580	0.9563650760	0.2373113028
C	-3.6980374781	1.6059252537	-0.3418151564
C	-2.7185277722	0.4095499050	1.5327763706
C	-4.8979006831	1.6896921329	0.3406898756
H	-3.6125556786	2.0430273512	-1.3339179857
C	-3.9188060937	0.4915358363	2.2257947013
H	-1.8586618095	-0.0869774158	1.9869156747
C	-5.0251565140	1.1186238723	1.6240636665
H	-5.7699150875	2.1822011465	-0.0924815689
H	-3.9903577276	0.0554523093	3.2207226992
O	-6.2370365998	1.2270244492	2.1983446040
C	-6.4557978325	0.6508513929	3.4713398458
H	-6.2794075100	-0.4384417216	3.4553544693
H	-5.8100118807	1.1085688015	4.2401816978
H	-7.5063614988	0.8439787394	3.7227608154
H	-0.6031417882	0.1653156950	0.0911889018
C	2.3305945461	0.3152279718	2.2052938426
F	3.5195385144	0.5234416874	1.6477721940
F	1.5525289120	1.3756940606	1.9742033109
F	2.4836187426	0.1699873265	3.5162159861
C	4.2290183244	-1.0392799899	-1.1798112121
C	4.7777900319	0.2248227043	-1.3927396326
C	4.7573715907	-1.9152793530	-0.2326272148
C	5.8852580717	0.6173966970	-0.6397861381
H	4.3109065643	0.8903415691	-2.1177308672
C	5.8616915758	-1.5062507570	0.5192104012
H	4.2953327838	-2.8894331379	-0.0768983131
C	6.4284807862	-0.2451598700	0.3180796805
H	6.3140607483	1.6103357659	-0.7940784207
H	6.2736441765	-2.1806705872	1.2731913316
H	7.2896200843	0.0688903445	0.9123032219
C	0.7929573031	-4.1629095336	-0.6953068396
C	0.7009278732	-4.7034838012	0.5884561877
C	-0.1449610364	-4.4699175750	-1.6850229175
C	-0.3530933209	-5.5737662683	0.8791566167
H	1.4382620220	-4.4138821751	1.3367388511
C	-1.1961636878	-5.3352928552	-1.3749686647
H	-0.0447944145	-4.0193384752	-2.6723548977
C	-1.3027362499	-5.8900905664	-0.0966324610

H	-0.4335022453	-6.0003891515	1.8818139401
H	-1.9392114892	-5.5730565511	-2.1395651098
H	-2.1298822459	-6.5625944705	0.1403581965
C	2.1719026173	3.9254196972	-0.5313851061
C	3.3470677793	3.7546207913	0.2201649448
C	1.9010115813	5.1811913781	-1.0977203497
C	4.2097131109	4.8299614128	0.4340332236
H	3.5748965236	2.7744931812	0.6363746639
C	2.7685992255	6.2511663991	-0.8910441113
H	1.0157803058	5.3125226250	-1.7213015881
C	3.9221164660	6.0811051075	-0.1178562352
H	5.1132114097	4.6882307064	1.0318629310
H	2.5490675636	7.2220769252	-1.3412361590
H	4.6007425626	6.9220643310	0.0448378105
C	-0.8651135740	3.8990575252	-0.4074968557
O	-0.5732078632	4.6637155415	0.4827387442
O	-2.0545219803	3.9964815100	-1.0665885203
C	-2.9471983993	4.9923351182	-0.5803304815
H	-3.2117570239	4.7999730120	0.4704298144
H	-2.4944127514	5.9927975112	-0.6465908180
H	-3.8435108478	4.9369296046	-1.2112010498
C	-5.2826780492	-0.5878910555	-3.0074713300
H	-5.9636276236	-0.0124632003	-2.3568463858
H	-5.0853345853	0.0072107947	-3.9104431296
H	-5.8205104157	-1.5028706560	-3.3059190729

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C	3.2919862070	-1.6820026285	2.3161736574
C	3.5952476377	-0.5905248416	1.4183196332
C	4.9390890826	-0.2443774116	1.1368887888
C	5.9305143506	-0.9835768113	1.7537023362
C	5.6471022759	-2.0624911456	2.6412813866
C	4.3461280788	-2.4126258717	2.9245693624
C	1.8954191728	-1.8269909101	2.3590572030
C	1.3581448983	-0.8873458733	1.4235690045
H	5.1853006046	0.5684043797	0.4581523675
H	6.9746808650	-0.7330187367	1.5505643411
H	6.4757634444	-2.6122222513	3.0916869498
H	4.1186233916	-3.2422277121	3.5967031488
N	2.4225563162	-0.0836286978	0.9609905018
C	2.1122008906	0.9029933190	-0.0877325160
H	1.1761341044	1.3704261080	0.2551899407
C	1.0822566011	-2.8084376511	3.1171541536
H	0.2610605480	-3.1771754162	2.4821908353
H	0.6088814788	-2.3265265027	3.9901996114
H	1.6830769120	-3.6567405888	3.4726648665
C	1.7896631011	0.1538807511	-1.3784350781
H	2.6744849647	-0.3255796766	-1.8125030854
H	1.4435386260	0.8829863402	-2.1212132772
C	0.7859383555	-1.9492055653	-0.0876292289
C	0.6569067512	-0.8498578573	-1.1797605199
H	-0.2387498559	-0.2875380942	-0.9021744875

C	3.1606124217	1.9859547001	-0.1978378632
C	3.9332395865	2.1884847073	-1.3509637404
C	3.3797516547	2.8262100856	0.8996287644
C	4.9045924743	3.1844749527	-1.3961501623
H	3.7848877596	1.5614813082	-2.2307522964
C	4.3525353458	3.8264100713	0.8740335876
H	2.7817153364	2.6887655219	1.8042364507
C	5.1285240277	4.0100063035	-0.2823288561
H	5.5084263475	3.3471769832	-2.2905540265
H	4.4937160917	4.4561397886	1.7517380813
O	6.0961006524	4.9469253273	-0.4144702478
C	6.3620593374	5.8155877342	0.6642139224
H	5.4786565442	6.4245671650	0.9265931638
H	7.1706557273	6.4821237869	0.3372073397
H	6.6925741664	5.2636931582	1.5623601996
O	-0.3754651054	-2.4528231593	0.3103938290
N	-2.4160319400	-0.7971278197	0.1781268335
P	-2.2658243058	0.7576109740	0.6651255522
S	-3.7262749557	-1.4371226884	-0.5125819793
O	-0.9193334932	1.0192457742	1.2642699843
O	-3.5256239745	1.0691625440	1.6260835490
O	-2.5983714733	1.7965675683	-0.5524433419
O	-3.3768756780	-2.7254350347	-1.1099661160
O	-4.5241635039	-0.4688560092	-1.2804009877
C	-4.8248404271	-1.9227664941	0.9411004752
H	0.4000664177	-0.3653850296	1.5470675353
H	-1.1674711419	-1.8039766424	0.2344125028
C	-1.7420897115	1.9458943156	-1.6254807048
C	-1.9307301172	1.1598733863	-2.7650742812
C	-0.7165208642	2.8929620846	-1.5573630499
C	-1.0734622536	1.3345774791	-3.8546492599
H	-2.7430262541	0.4328331329	-2.7690410962
C	0.1254039899	3.0665321487	-2.6590481169
H	-0.5979424406	3.4775386934	-0.6442203366
C	-0.0496527388	2.2873608065	-3.8080833301
H	-1.2075795894	0.7217085514	-4.7488052717
H	0.9301025085	3.8038803288	-2.6120863401
H	0.6149660202	2.4171940909	-4.6648580986
C	-4.3186552995	2.2089648969	1.6174721724
C	-5.3678105168	2.3025929093	0.7022156594
C	-4.0696098501	3.2114130080	2.5531534380
C	-6.1878352710	3.4316759880	0.7379445998
H	-5.5135141493	1.4992760058	-0.0209973835
C	-4.8995839174	4.3360877244	2.5776166849
H	-3.2352687231	3.0954238986	3.2470383583
C	-5.9585804226	4.4480961636	1.6723218661
H	-7.0124972709	3.5180289043	0.0264352378
H	-4.7156475797	5.1272555086	3.3085258019
H	-6.6057286506	5.3279341528	1.6937586977
F	-4.0819342005	-2.3833594062	1.9462184844
F	-5.5454724224	-0.8915672813	1.3720844473
F	-5.6537877765	-2.8839220655	0.5410652267
C	1.8156634425	-3.0278614051	-0.2827723898
C	1.4496407314	-4.3559432668	0.0022146099
C	3.1291268820	-2.7756160896	-0.7134226684

C	2.3745949368	-5.3920083213	-0.1173262040
H	0.4240177306	-4.5624063982	0.3039464235
C	4.0556082274	-3.8134843641	-0.8227998574
H	3.4505246639	-1.7723374602	-0.9656073375
C	3.6859924348	-5.1247258867	-0.5212721792
H	2.0661348294	-6.4171941723	0.1010175395
H	5.0730616327	-3.5886829312	-1.1497692939
H	4.4118273540	-5.9363428077	-0.6109669132
C	0.3319591421	-1.5425780618	-2.5039508068
O	1.1072470252	-1.6819531122	-3.4182310461
O	-0.9279709442	-1.9641170789	-2.4980228288
C	-1.4083640053	-2.6857465591	-3.6316804188
H	-2.4243455180	-2.9915813444	-3.3617055689
H	-1.4086979614	-2.0390365067	-4.5223657208
H	-0.7692647983	-3.5588858900	-3.8285807931

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C	-1.0810437705	-0.5589705082	-2.6469393673
C	-0.4675895402	-1.6622927656	-1.9470572476
C	0.9388606656	-1.8111787013	-2.0003055151
C	1.6626304896	-0.8689961972	-2.7064034187
C	1.0662894462	0.2460002809	-3.3561268031
C	-0.2968763863	0.4011810813	-3.3393469199
C	-2.4702376725	-0.6683389779	-2.5026976779
C	-2.6949327707	-1.7753395919	-1.6320022113
H	1.4557631403	-2.6327500465	-1.5211937598
H	2.7473788144	-0.9796345798	-2.7458201087
H	1.7022701217	0.9854811913	-3.8437418447
H	-0.7798966798	1.2588521853	-3.8061426964
N	-1.4639659453	-2.4226471205	-1.3892049783
C	-1.4186078202	-3.5375073433	-0.4135860615
H	-1.9976682666	-4.3491653269	-0.8867373614
C	-3.4984902568	0.2368681759	-3.0761801225
H	-3.5279828008	1.1679614292	-2.4855284531
H	-4.4981763345	-0.2141420943	-3.0803697842
H	-3.2284284211	0.5244847622	-4.1035175295
C	-2.0985926393	-3.1926804243	0.9341470639
H	-1.3891034151	-2.6896203976	1.5965609976
H	-2.3591382203	-4.1480803973	1.4133042825
C	-2.9667382473	-0.9526446584	0.2014372639
C	-3.3299259036	-2.2927398098	0.8780479887
H	-4.1758642591	-2.7532748731	0.3540220514
C	-0.0137449187	-4.0487539404	-0.1693590460
C	0.8443621286	-3.4119128470	0.7473199349
C	0.4806472713	-5.1310880294	-0.8997222452
C	2.1508575726	-3.8486808139	0.9132489712
H	0.5334115324	-2.5144948358	1.2853150416
C	1.8018834630	-5.5705043816	-0.7563079471
H	-0.1681457905	-5.6368952958	-1.6201866754
C	2.6493093740	-4.9205762600	0.1534143415
H	2.8198219100	-3.3510073581	1.6164217486
H	2.1537961391	-6.4100408736	-1.3547233087

O	3.9491873023	-5.2434085447	0.3592631447
C	4.5247873935	-6.2842332336	-0.3981227096
H	4.0223920615	-7.2503685201	-0.2129747872
H	5.5727718694	-6.3603430431	-0.0805095447
H	4.4915216773	-6.0672066062	-1.4807498240
O	-1.7768714258	-0.5698547507	0.5741772012
N	-0.2574822956	1.3879756337	-0.0662795651
P	1.1619728367	1.0071204774	0.6606150973
S	-0.5421627581	2.7110629347	-0.9312574915
O	1.1424835324	-0.2518185846	1.4494170831
O	1.5223183752	2.3561409565	1.5208594775
O	2.3089152620	1.0537066255	-0.5043322663
O	-1.8021990413	2.5203063169	-1.6627857916
O	0.6223669675	3.2632967119	-1.6247042888
C	-0.9924713286	4.0409449437	0.3448037738
H	-3.5919037253	-2.3912413926	-1.6798228571
H	-1.3268692766	0.3063962901	0.2292020978
C	3.5609041110	0.4737859889	-0.4595364362
C	4.6344500224	1.2359486584	-0.9241655307
C	3.7478478732	-0.8437615519	-0.0323585682
C	5.9102312330	0.6690624052	-0.9570226672
H	4.4515642102	2.2633364517	-1.2398185073
C	5.0273982095	-1.4016862581	-0.0752941948
H	2.8937370592	-1.4073550247	0.3303229357
C	6.1131387331	-0.6493477519	-0.5348173574
H	6.7530679610	1.2664971928	-1.3129758615
H	5.1641217891	-2.4378689823	0.2459591646
H	7.1133653913	-1.0875675981	-0.5653164771
C	2.8361770622	2.7299824060	1.7467212773
C	3.3111143349	3.8799131231	1.1147665616
C	3.6618494245	1.9512287976	2.5597103982
C	4.6414089604	4.2574666108	1.3089137616
H	2.6354211025	4.4357169919	0.4640951712
C	4.9931145930	2.3347919314	2.7372417222
H	3.2558871399	1.0487184603	3.0194207343
C	5.4853822627	3.4857783722	2.1149718939
H	5.0243636062	5.1544167974	0.8159475367
H	5.6504497807	1.7244557943	3.3607981310
H	6.5280858929	3.7797905351	2.2548741569
F	-1.5460850286	3.4963953272	1.4338926283
F	0.0741099803	4.7399117553	0.7115980244
F	-1.8809806735	4.8719904441	-0.2019607203
C	-3.8117962554	-1.9861239795	2.2982055078
O	-3.1007661385	-1.8528926076	3.2590000129
O	-5.1488056013	-1.8644826240	2.3293608562
C	-5.7147287231	-1.4568228602	3.5770255446
H	-5.3165235033	-0.4757445167	3.8753125415
H	-6.7972819976	-1.3965853356	3.4148088857
H	-5.4814530481	-2.1860250454	4.3667041977
C	-4.0512924338	0.0604528267	0.0573672670
C	-3.7916877705	1.3883198912	0.4195627158
C	-5.3378265732	-0.2853185462	-0.3903425190
C	-4.7846881680	2.3626078816	0.3053147564
H	-2.8137114030	1.6598766946	0.8056061232
C	-6.3302041482	0.6845872424	-0.4985010325

H	-5.5670602895	-1.3166172423	-0.6640482517
C	-6.0539859120	2.0153739241	-0.1577618138
H	-4.5510310362	3.3945531125	0.5742798218
H	-7.3248548171	0.4054283291	-0.8534729788
H	-6.8320166489	2.7764631068	-0.2521347635

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C	-0.9694225893	-1.3055544616	2.0777194130
C	-1.3307014308	-1.9213508780	0.8241041525
C	-0.5442996028	-2.9549424847	0.2751966417
C	0.5500485858	-3.3749797760	1.0061678981
C	0.8939946305	-2.8064407775	2.2689001803
C	0.1531074757	-1.7831944566	2.8074358198
C	-1.8555627193	-0.2441731648	2.3032640941
C	-2.6860290435	-0.1575436408	1.1346077302
H	-0.7588904411	-3.3789152705	-0.7050421268
H	1.1963893839	-4.1526505045	0.5957130388
H	1.7864881550	-3.1654227293	2.7795327151
H	0.4443775612	-1.3014533198	3.7401170392
N	-2.4596603071	-1.3228160497	0.3585230626
C	-3.0662982512	-1.4627254765	-0.9663879151
H	-2.7177074583	-2.4283942250	-1.3625608743
C	-1.8546906360	0.7007122299	3.4481376988
H	-0.9374402067	1.3123319448	3.4096896918
H	-2.7307354485	1.3606212243	3.4428259567
H	-1.8230313054	0.1490960864	4.4012929745
C	-2.5460325401	-0.3533971171	-1.8907933838
H	-1.4836342574	-0.5342615106	-2.1017238171
H	-3.0909615221	-0.3703647119	-2.8427200833
C	-1.7604768853	1.1257622904	-0.0046628752
C	-2.6774037766	1.0344941607	-1.2362782754
H	-3.7208881600	1.2082463448	-0.9453502757
C	-4.5845859952	-1.5259904346	-0.8211593504
C	-5.1385471407	-2.3740962401	0.1562808911
C	-5.4634927304	-0.7946639587	-1.6245433636
C	-6.5112492359	-2.4880591298	0.3212154219
H	-4.4724861162	-2.9502982513	0.8030147918
C	-6.8521202135	-0.8964457230	-1.4700969734
H	-5.0861756651	-0.1171421671	-2.3916195592
C	-7.3863514634	-1.7468183147	-0.4940930921
H	-6.9410138252	-3.1471910650	1.0775563439
H	-7.4987017957	-0.3047064084	-2.1170028552
O	-8.7087663871	-1.9168318327	-0.2619688127
C	-9.6381374407	-1.2071956813	-1.0501005269
H	-9.5467233296	-1.4640064878	-2.1205823223
H	-10.6357889595	-1.4983410687	-0.6965483675
H	-9.5211924451	-0.1145623207	-0.9362530024
O	-0.6091989821	0.5631684226	-0.2906531793
N	1.7251626550	0.3040370020	0.7230110736
P	2.4317099248	-0.3627520925	-0.5985199137
S	2.3328198830	0.6222972900	2.1596851548
O	1.5148413387	-1.1140120794	-1.4967331739

O	3.1602905341	0.9336974525	-1.2731569045
O	3.7670007127	-1.1976106394	-0.1593650479
O	1.2569566183	1.1572362678	3.0076074470
O	3.2191724137	-0.4030286650	2.7163856175
C	3.4561463592	2.1038855266	1.8984014654
H	-3.7036730370	0.2316367528	1.1678004085
H	0.2041769633	0.6031954119	0.3264328434
C	3.9919113595	0.8533444553	-2.3737870665
C	3.6028567355	0.1834777366	-3.5381904788
C	5.2271359819	1.4997288319	-2.2914202119
C	4.4734489254	0.1672166782	-4.6314289058
H	2.6324611042	-0.3133931517	-3.5651095826
C	6.0827100413	1.4814249601	-3.3944656874
H	5.4936528618	2.0001284741	-1.3595739828
C	5.7107599764	0.8146280040	-4.5665864988
H	4.1769900285	-0.3558121631	-5.5441230889
H	7.0499171900	1.9864012226	-3.3343557345
H	6.3844556375	0.7988950924	-5.4262841186
C	3.8054645533	-2.5674283701	0.0172080476
C	3.4967165651	-3.4351777724	-1.0346299326
C	4.1975807773	-3.0544813326	1.2659412046
C	3.5758764598	-4.8136951732	-0.8213863894
H	3.1805218218	-3.0221981963	-1.9915850639
C	4.2759335124	-4.4351103018	1.4629825995
H	4.4018608853	-2.3352594619	2.0586884135
C	3.9618867291	-5.3191201483	0.4247044287
H	3.3340394106	-5.4976119282	-1.6387552895
H	4.5804037558	-4.8223396132	2.4385321847
H	4.0231995172	-6.3980652470	0.5844117718
F	3.8498613962	2.5729218622	3.0794427443
F	2.8049780341	3.0761120478	1.2497582825
F	4.5309130525	1.7617519930	1.1906589225
C	-1.7771687080	2.4146166300	0.7547452283
C	-0.5681332836	3.0114042499	1.1340067473
C	-2.9859913384	3.0518303100	1.0785491670
C	-0.5664179085	4.2112922532	1.8458336017
H	0.3780753085	2.5457021799	0.8718644409
C	-2.9829814962	4.2538126350	1.7854164829
H	-3.9402300540	2.6066831086	0.7879183287
C	-1.7712487741	4.8348503834	2.1766753897
H	0.3884923970	4.6504595959	2.1414823969
H	-3.9297179014	4.7386434738	2.0344259989
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O	-1.1902518231	2.6586639694	-2.1712427699
C	-0.8325922395	3.6453903466	-3.1401676354
H	-0.8608671532	3.2180826840	-4.1531168118
H	-1.5268011174	4.4975655521	-3.0960211238
H	0.1849636604	3.9622802604	-2.8847969167

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C	1.1538709528	0.5956368301	-2.3362888732
C	0.9345764759	1.6751712199	-1.4026943845
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C	3.0177936538	0.8910636550	-1.0872318787
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H	-2.3468013643	2.2040511956	-2.0245885978
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H	0.2702493250	-0.6813322294	-3.8669773891
N	2.1177646900	1.9323898174	-0.7680848629
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H	1.2483310918	1.6768189336	1.8801837264
H	2.6479225412	2.5627470495	2.5381379470
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C	1.5819649606	4.0468580529	0.3942860517
C	0.6264971522	4.3548659400	1.3739086533
C	1.7562339865	4.9476510485	-0.6618609721
C	-0.1348101753	5.5165652503	1.2913460239
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C	0.9977597734	6.1144383637	-0.7643353946
H	2.4905884045	4.7230695070	-1.4398238734
C	0.0386338720	6.4058924797	0.2190080850
H	-0.8843458988	5.7563406272	2.0473196773
H	1.1597735564	6.7840680214	-1.6082454819
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C	-0.6395647339	8.4267245926	-0.8447675282
H	0.3694852237	8.8738910482	-0.8947868641
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O	1.2753204719	-0.2617112839	0.5739329804
N	-0.6709179837	-1.5603149134	-0.3920087045
P	-1.8607340676	-0.9771916518	0.5777009512
S	-0.7454544664	-2.6170526414	-1.5859838310
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O	-3.3088511774	-1.1270298790	-0.1613025541
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O	-1.8765091046	-2.4546457744	-2.5023372926
C	-1.0784614727	-4.2729132148	-0.7604964866
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H	0.6574236486	-0.8963415691	0.0303815755
C	-3.9471500104	-0.1156106918	-0.8532818944
C	-4.2758287703	-0.3488303418	-2.1900425955
C	-4.2847164050	1.0846041312	-0.2213139202
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H	-3.9639476134	-1.2907413663	-2.6409472741
C	-4.9574956280	2.0677053121	-0.9512157768
H	-3.9971773100	1.2401659910	0.8176739184

C	-5.2918355158	1.8528756179	-2.2924918914
H	-5.2103516174	0.4668186099	-3.9530009943
H	-5.2209948292	3.0102713333	-0.4650768404
H	-5.8185964255	2.6254756001	-2.8572878592
C	-3.0159105635	-2.2141078907	2.6262927084
C	-3.7420775428	-3.3995901597	2.7576347339
C	-3.2682254685	-1.1161397576	3.4547303435
C	-4.7312787424	-3.4892635787	3.7386881801
H	-3.5193460099	-4.2266375084	2.0825028317
C	-4.2672157237	-1.2181971802	4.4266908427
H	-2.6826502643	-0.2057092018	3.3221620033
C	-4.9989798700	-2.4000594940	4.5745661814
H	-5.3014306626	-4.4153504079	3.8454067774
H	-4.4711514785	-0.3635399838	5.0766093030
H	-5.7765814034	-2.4725330515	5.3382956679
F	-0.2433079468	-4.4711680319	0.2661393776
F	-2.3300548171	-4.3305634151	-0.3100695963
F	-0.8950805915	-5.2472183694	-1.6477664954
C	4.5958540893	0.8383027970	1.6954140041
O	5.2369008834	1.5411635558	0.9426012670
O	5.1517432434	0.1452928177	2.6932831017
C	6.5742015333	0.2217964886	2.8125846867
H	6.8343430552	-0.3498434919	3.7107693570
H	7.0549312763	-0.2207170812	1.9271819675
H	6.9014447993	1.2670853553	2.9071658524
C	3.2688198068	-1.5875617218	0.2820357298
C	2.5167186141	-2.7663059115	0.3927395783
C	4.6402684400	-1.6804214576	-0.0144374208
C	3.1178569348	-4.0112502352	0.2008261003
H	1.4563458130	-2.7160155390	0.6296051406
C	5.2392171781	-2.9249404661	-0.1971378830
H	5.2409216893	-0.7798720289	-0.1423228657
C	4.4791869855	-4.0958012073	-0.0921867763
H	2.5060238315	-4.9121475139	0.2749663389
H	6.3034892518	-2.9822718050	-0.4372433498
H	4.9494862769	-5.0697029521	-0.2462396296
C	3.1250056135	-0.9844482233	-2.8890770348
H	4.2154986323	-0.9735338142	-2.7697088918
H	2.7298822970	-1.9417160764	-2.5097681963
H	2.8802105501	-0.9495988556	-3.9618030297