

Electronic Supplementary Information

Zn(OTf)₂-mediated annulations of N-propargylated tetrahydrocarbolines: divergent synthesis of four distinct alkaloidal scaffolds

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General

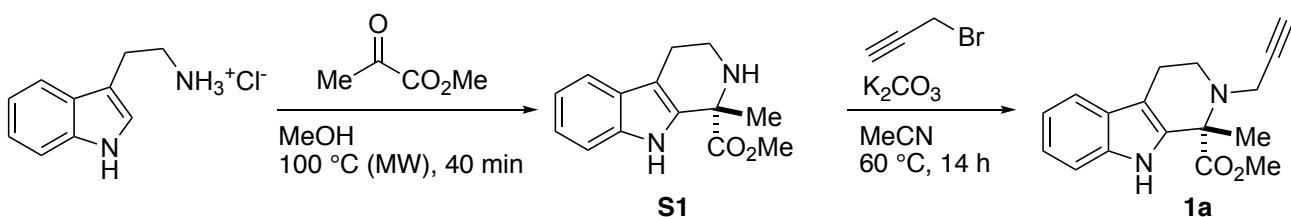
All reactions were performed under a nitrogen atmosphere unless otherwise noted. Microwave reactions were performed using a Biotage® Initiator. Reactions were monitored by thin layer chromatography using Merck Millipore TLC Silica gel F254 plates (0.25 mm), which were visualized using UV light, phosphomolybdic acid (PMA) stain, PMS stain and *p*-anisaldehyde strain. Flash column chromatography was performed using Kanto Silica Gel 60N and Wako Alumina, activated. The medium pressure liquid chromatography (MPLC) purifications were performed on a YAMAZEN YFLC-AI-580 and Biotage® Isolera. NMR spectra were recorded on JEOL ECA 500 (^1H /500 MHz, ^{13}C /125 MHz), ECA 400 (^1H /400 MHz, ^{13}C /100 MHz), and AL300 (^1H /300 MHz ^{13}C /75 MHz) spectrometers. Chemical Shifts (δ) were quoted in parts per million (ppm) from chloroform as an internal standard of 7.26 and 77.16 for ^1H and ^{13}C -NMR, respectively. Data for ^1H NMR were reported as follows: chemical shift (number of hydrogen, multiplicity, coupling constant). Multiplicity was abbreviated as follows: s (singlet), d (doublet), t (triplet), q (quartet), quin (quintet), m (multiplet), br (broad). ESI-Mass spectra were recorded on Bruker Daltonics microTOF-QII.

Materials

Solvents used for the $\text{Zn}(\text{OTf})_2$ -promoted reaction were dried and stored over activated molecular sieves 4A. $\text{Zn}(\text{OTf})_2$ was purchased from Tokyo Chemical Industry Co., Ltd. (TCI) and used as received.

Synthesis of starting materials (1)

Methyl 1-methyl-2-(prop-2-yn-1-yl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-1-carboxylate (**1a**):

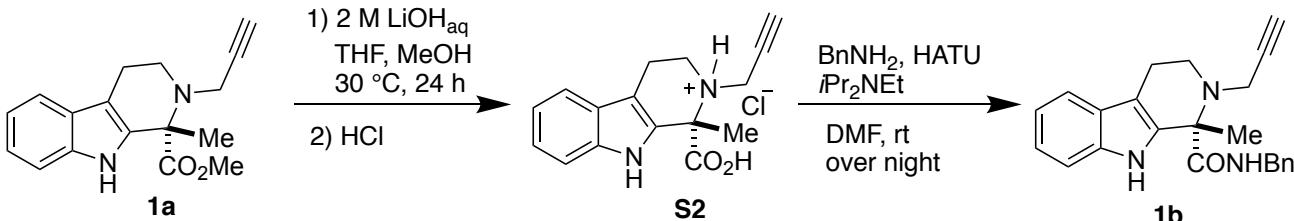


A Biotage microwave vial was charged with tryptamine hydrochloride (2.00 g, 10.2 mmol), MeOH (17 mL), and methyl pyruvate (1.12 mL, 12.2 mmol). The vial was sealed with a Teflon septum lined cap. The mixture was heated at 100 °C for 40 min under microwave irradiation. After cooling to room temperature, the mixture was diluted with EtOAc (100 mL) and then treated with a saturated aqueous solution of NaHCO_3 (50 mL). Organic layer was separated and washed with a saturated aqueous solution of NaHCO_3 (50 mL x 1). Aqueous layer was extracted with EtOAc (100 mL x 2). Combined organic extracts were washed with brine and dried over Na_2SO_4 . After filtration, the solvent was evaporated under reduced pressure to give **S1**, which was used for the following reaction without further purification.

The crude product **S1** was placed in a flask and dehydrated by azeotropic distillation with toluene. K₂CO₃ (4.23 g, 30.6 mmol), MeCN (34 mL), and propargyl bromide (0.919 mL, 12.1 mmol) were successively added to the resulting residue, and the mixture was stirred at 60 °C for 14 h. After cooling to room temperature, the mixture was passed through a pad of Celite, which was washed with toluene. The combined filtrate was concentrated and diluted with EtOAc (50 mL). A saturated aqueous solution of NaHCO₃ (10 mL) was added, and the layers were separated. The organic layer was washed with a saturated aqueous solution of NaHCO₃ (10 mL x 1). Combined aqueous layer was extracted with EtOAc (50 mL x 2). Combined organic extracts were washed with brine and dried over Na₂SO₄. After filtration and concentration under reduced pressure, the residue was purified by silica gel column chromatography (hexane/EtOAc) to give **1a** (2.65 g, 9.39 mmol, 92% in two steps) as a pale yellow powder.

1a: *R*_f = 0.27 (Hexane–EtOAc = 3 : 1); ¹H NMR (500 Hz, CDCl₃) δ 8.09 (1H, s), 7.53 (1H, d, *J* = 7.5 Hz), 7.33 (1H, d, *J* = 8.0 Hz), 7.21–7.16 (1H, m), 7.14–7.10 (1H, m), 3.74 (3H, s), 3.65 (1H, dd, *J* = 16.6, 2.3 Hz), 3.59 (1H, dd, *J* = 16.9, 2.3 Hz), 3.34 (1H, dt, *J* = 12.0, 6.0 Hz), 3.24 (1H, dt, *J* = 11.5, 6.0 Hz), 2.89 (2H, dd, *J* = 6.0, 6.0 Hz), 2.28 (1H, dd, *J* = 2.3, 2.3 Hz), 1.77 (3H, s); ¹³C NMR (125 MHz, CDCl₃) δ 174.2, 136.3, 133.1, 126.9, 122.3, 119.6, 118.7, 111.1, 109.7, 81.2, 72.1, 63.5, 52.6, 45.6, 40.7, 22.2, 21.3; HRMS (ESI, *m/z*): calcd for C₁₇H₁₉N₂O₂ [M+H]⁺ 283.1441, found 283.1481.

N-Benzyl-1-methyl-2-(prop-2-yn-1-yl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-1-carboxamide (1b):



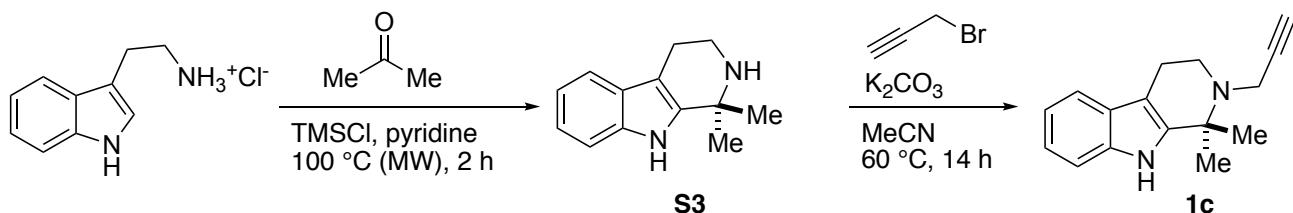
An aqueous solution of LiOH (2 M, 3.43 mL, 6.85 mmol) was added to a solution of **1a** (378 mg, 1.37 mmol) in a mixture of THF–MeOH (2.7 mL, 1:2, v/v) at 0 °C. The mixture was stirred at 30 °C for 24 h. The mixture was acidified to pH 2 by addition of 1 M HCl at 0 °C. The precipitates were collected by filtration, washed with hexane (3 mL x 3) and Et₂O (3 mL x 3), and dried *in vacuo*. After azeotropic dehydration with toluene, the carboxylic acid **S2** was obtained as a hydrochloride salt (354 mg, 1.16 mmol, 83%).

To a mixture of **S2** (345 mg, 1.13 mmol) and *N,N*-diisopropylethylamine (0.394 mL, 2.26 mmol) in DMF (7.5 mL), benzylamine (0.185 mL, 1.70 mmol) and HATU (473 mg, 1.24 mmol) were successively added at room temperature. After being stirred for overnight, the reaction was quenched with a saturated aqueous solution of NaHCO₃ (20 mL) at 0 °C. The resulting mixture was extracted with Et₂O (100 mL) and washed with H₂O (20 mL). The aqueous layers were extracted with Et₂O (100 mL x 2). Combined organic extracts were washed with brine (30 mL) and dried over Na₂SO₄. After filtration, the solvent was removed under reduced pressure. The crude residue was dissolved in CH₂Cl₂,

and resulting precipitate was collected by filtration. Further precipitate was obtained by treating the filtrate with hexane, and collected as well. Combined precipitates were dried *in vacuo* to give **1b** (388 mg, 1.09 mmol, 96%).

1b: R_f = 0.32 (Hexane-EtOAc = 3 : 1); ^1H NMR (500 Hz, CDCl_3) δ 8.73 (1H, s), 8.01 (1H, t, J = 6.0 Hz), 7.49 (1H, d, J = 8.0 Hz), 7.30 (1H, d, J = 8.0 Hz), 7.20–7.14 (4H, m), 7.12–7.06 (3H, m), 4.52 (1H, dd, J = 15.2, 6.6 Hz), 4.25 (1H, dd, J = 15.2, 5.4 Hz), 3.44 (1H, dd, J = 16.6, 2.3 Hz), 3.41–3.36 (1H, m), 3.27 (1H, dd, J = 16.6, 2.3 Hz), 2.96–2.76 (3H, m), 2.25 (1H, t, J = 2.3 Hz), 1.64 (3H, s); ^{13}C NMR (125 MHz, CDCl_3) δ 173.9, 138.1, 136.4, 134.7, 128.7, 127.3, 127.2, 126.6, 122.1, 119.4, 118.3, 111.4, 107.4, 80.7, 72.6, 64.4, 44.9, 43.4, 41.5, 21.6, 16.5; HRMS (ESI, m/z): calcd for $\text{C}_{23}\text{H}_{23}\text{N}_2\text{O}_2$ [M+H]⁺ 358.1914, found 358.1949.

1,1-Dimethyl-2-(prop-2-yn-1-yl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole (1c):



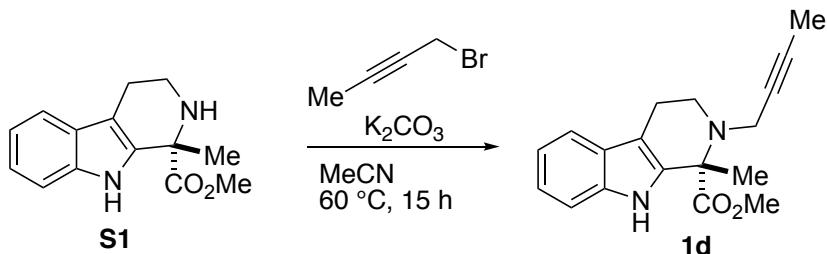
To a mixture of tryptamine hydrochloride (1.57 g, 8.00 mmol) and pyridine (8 mL) in a Biotage microwave vial, chlorotrimethylsilane (5.08 mL, 40.0 mmol) was slowly added. The vial was sealed with a Teflon septum lined cap. Acetone (0.884 mL, 12.0 mmol) was added via syringe to the mixture, which was then heated at 100 °C for 2 h under microwave irradiation. After cooling to 0 °C, the resulting mixture was treated with a saturated aqueous solution of NaHCO₃ (25 mL) and diluted with EtOAc (100 mL). After being stirred at room temperature for 1 h, the organic layer was separated, and the aqueous layer was extracted with EtOAc (100 mL x 2). Combined organic extracts were dried over Na₂SO₄. Filtration and concentration under reduced pressure afforded crude product **S3**, which was used for the following reaction without further purification.

The mixture of the crude product **S3**, K₂CO₃ (3.32 g, 24.0 mmol), and propargyl bromide (1.04 mL, 9.60 mmol) in MeCN (30 mL) was stirred at 60 °C for 14 h. After cooling to room temperature, insoluble materials were filtered off through a pad of Celite and washed with CH₂Cl₂. After concentration under reduced pressure, the residue was diluted with a saturated aqueous solution of NaHCO₃ (15 mL) and EtOAc (100 mL). The organic layer was separated, and the aqueous layer was extracted with EtOAc (100 mL x 2). Combined organic extracts were washed with brine (10 mL x 1) and dried over Na₂SO₄. After filtration and concentration under reduced pressure, the residue was purified by silica gel column chromatography (hexane/EtOAc) to give **1c** (1.26 g, 5.29 mmol, 66% in two steps) as an orange solid.

1c: $R_f = 0.29$ (Hexane-EtOAc = 3 : 1); ^1H NMR (500 Hz, CDCl_3) δ 7.63 (1H, s), 7.51 (1H, d, J = 8.0 Hz), 7.31 (1H, d, J = 8.0 Hz), 7.19–7.16 (1H, m), 7.14–7.11 (1H, m), 3.54 (2H, d, J = 2.8 Hz), 3.21 (2H, t, J = 5.7 Hz), 2.83 (2H, t, J = 5.7 Hz), 2.26 (1H, t, J = 2.8 Hz), 1.48 (6H, s); ^{13}C NMR (125 MHz,

CDCl_3) δ 139.6, 136.0, 127.3, 121.6, 119.4, 118.4, 110.7, 107.6, 82.1, 71.9, 55.3, 44.7, 38.6, 25.1, 21.0; HRMS (ESI, m/z): calcd for $\text{C}_{16}\text{H}_{19}\text{N}_2$ [$\text{M}+\text{H}$]⁺ 239.1543, found; 239.1582.

Methyl 2-(but-2-yn-1-yl)-1-methyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-1-carboxylate (1d**):**

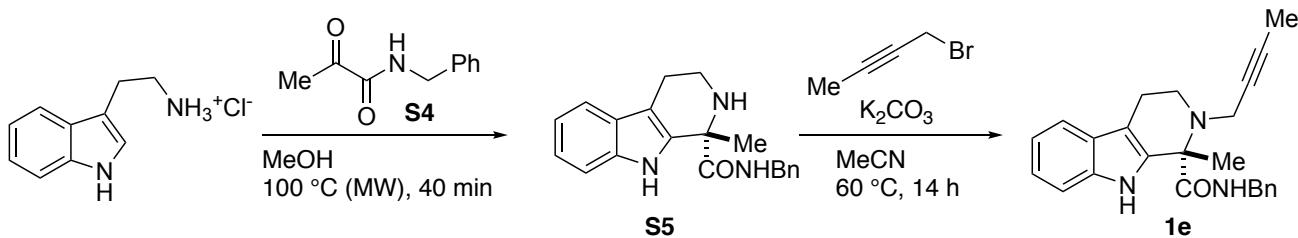


According to the essentially identical protocol as described for **1a**, compound **S1** was prepared from tryptamine hydrochloride (2.62 g, 13.3 mmol) and methyl pyruvate (1.47 mL, 16.0 mmol) and used for the following reaction without further purification.

The crude product **S1** was dried by azeotropic distillation with toluene and then treated with K_2CO_3 (5.51 g, 39.9 mmol), 1-bromo-2-butyne (1.33 mL, 14.6 mmol) in MeCN (44 mL) at 60°C for 15 h. After cooling to room temperature, insoluble materials were filtered off through a pad of Celite and washed with CH_2Cl_2 . After concentration under reduced pressure, the residue was diluted with a saturated aqueous solution of NaHCO_3 (20 mL) and EtOAc (100 mL). The organic layer was separated, and the aqueous layer was extracted with EtOAc (100 mL x 2). Combined organic extracts were washed with brine (10 mL x 1) and dried over Na_2SO_4 . After filtration and concentration *in vacuo*, the residue was treated with a mixture of hexane (3 mL) and EtOAc (10 ml). The resultant precipitates were collected by filtration and washed with hexane followed by CH_2Cl_2 . After concentration of the filtrate, the residue was subjected to reprecipitation once again as described above. Combined precipitates were dried *in vacuo* to give **1d** (2.58 g, 8.71 mmol, 65% in two steps) as a pale yellow powder.

1d: $R_f = 0.37$ (Hexane– EtOAc = 3 : 1); ^1H NMR (500 Hz, CDCl_3) δ 8.15 (1H, s), 7.52 (1H, d, $J = 7.2$ Hz), 7.32 (1H, d, $J = 7.6$ Hz), 7.18 (1H, dd, $J = 7.6, 7.1$ Hz), 7.11 (1H, dd, $J = 7.2, 7.1$ Hz), 3.74 (3H, s), 3.56–3.48 (2H, m), 3.34 (1H, ddd, $J = 12.0, 5.7, 5.7$ Hz), 3.18 (1H, ddd, $J = 12.0, 5.7, 5.7$ Hz), 2.92 (1H, ddd, $J = 16.0, 5.7, 5.7$ Hz), 2.86 (1H, ddd, $J = 16.0, 5.7, 5.7$ Hz), 1.86 (3H, t, $J = 2.4$ Hz), 1.74 (3H, s); ^{13}C NMR (125 MHz, CDCl_3) δ 174.5, 136.3, 133.2, 126.9, 122.2, 119.5, 118.7, 111.0, 109.5, 79.9, 75.9, 63.5, 52.6, 45.4, 41.2, 21.5, 21.2, 3.8; HRMS (ESI, m/z): calcd for $\text{C}_{18}\text{H}_{21}\text{N}_2\text{O}_2$ [$\text{M}+\text{H}$]⁺ 297.1598, found; 297.1623.

N-Benzyl-2-(but-2-yn-1-yl)-1-methyl-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-1-carboxamide (1e**)**



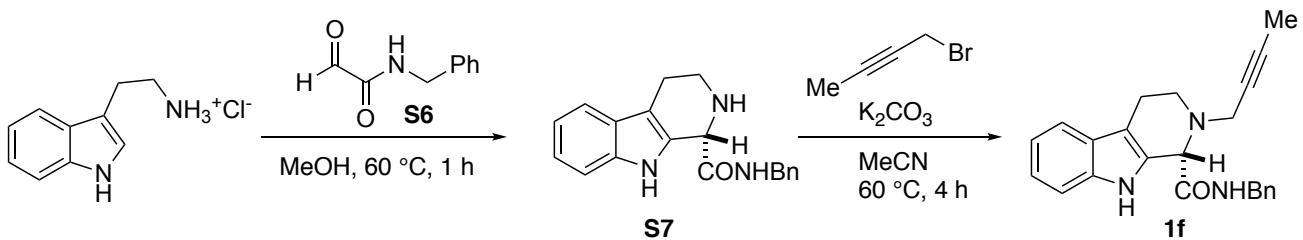
According to the literature procedure,¹ *N*-benzyl-2-oxopropanamide (**S4**) was prepared by condensation of pyruvic acid and benzylamine. A Biotage microwave vial was charged with **S4** (272 mg, 1.54 mmol), MeOH (3.5 mL), and tryptamine hydrochloride (275 mg, 1.41 mmol). The vial was sealed with a Teflon septum lined cap. The mixture was heated for 40 min at 100 °C under microwave irradiation. After cooling to room temperature, the mixture was diluted with EtOAc (10 mL) and treated with a saturated aqueous solution of NaHCO₃ at 0 °C. The organic layer was separated and washed with a saturated aqueous solution of NaHCO₃ (50 mL x 1). The aqueous layer was extracted with EtOAc (30 mL x 2). Combined organic extracts were washed with brine and dried over Na₂SO₄. After filtration, the solvent was evaporated under reduced pressure to give **S5** (431 mg), which was used for the following reaction without further purification.

The crude product **S5** (431 mg) was dehydrated by azeotropic distillation with toluene and then dissolved in MeCN (7 mL). The mixture was treated with K₂CO₃ (580 mg, 4.21 mmol) and 1-bromo-2-butyne (139 μL, 1.54 mmol) and heated to 60 °C for 14 h. After heating at 70 °C for 2 h, the mixture was cooled to room temperature. Resultant insoluble materials were filtered off through a pad of Celite and washed with CH₂Cl₂. The combined filtrates were concentrated under reduced pressure and then diluted with a saturated aqueous solution of EtOAc and NaHCO₃. After separating the organic layer, the aqueous layer was extracted with EtOAc. The combined organic extracts were washed with brine and dried over Na₂SO₄. After filtration and concentration under reduced pressure, the residue was purified by silica gel column chromatography (hexane/EtOAc) to give **1e** (876 mg, 2.36 mmol, 55% in two steps) as a pale yellow powder.

1e: $R_f = 0.41$ (Hexane–EtOAc = 3 : 1); ¹H NMR (400 Hz, CDCl₃) δ 9.14 (1H, s), 8.28 (1H, t, $J = 5.7$ Hz), 7.69 (1H, d, $J = 7.8$ Hz), 7.50 (1H, d, $J = 8.2$ Hz), 7.38–7.28 (7H, m), 4.72 (1H, dd, $J = 15.2, 6.9$ Hz), 4.45 (1H, dd, $J = 15.2, 5.3$ Hz), 3.61–3.56 (2H, m), 3.40 (1H, d, $J = 16.0$ Hz), 3.11–2.96 (3H, m), 2.01 (3H, s), 1.82 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 174.1, 138.2, 136.4, 134.9, 128.7, 127.2, 126.6, 121.9, 119.2, 118.2, 111.4, 107.4, 80.0, 75.9, 64.3, 44.8, 43.4, 41.9, 21.6, 16.2, 3.7; HRMS (ESI, *m/z*): calcd for C₂₄H₂₆N₃O [M+H]⁺ 372.2070, found; 372.2090.

¹ L. S. Konstantinova, O. I. Bol'shakov, N. V. Obruchnikova, S. P. Golova, Y. V. Nelyubina, K. A. Lyssenko, O. A. Rakitin, *Tetrahedron*, 2010, **66**, 4330–4338.

N-Benzyl-2-(but-2-yn-1-yl)-2,3,4,9-tetrahydro-1*H*-pyrido[3,4-*b*]indole-1-carboxamide (1f**)**



According to the literature procedure, *N*-benzyl-2-oxoacetamide (**S6**) was prepared from diisopropyl tartrate in two steps via ester-amide exchange reaction¹ with benzylamine followed by the oxidative cleavage of the resulting diols.² A mixture of **S6** (940 mg, 5.76 mmol) and tryptamine hydrochloride (1.03 g, 5.24 mmol) was suspended in MeOH (13.1 mL) in a Biotage microwave vial. The vial was sealed with a Teflon septum lined cap. The mixture was heated at 60 °C for 120 min under microwave irradiation. This reaction was conducted parallelly in two vials. After cooling to room temperature, the resulting reaction mixtures in the both vials were combined, diluted with EtOAc and treated with a saturated aqueous solution of NaHCO₃ at 0 °C. After separation of the organic layer, the aqueous layer was extracted with EtOAc. The combined organic extracts were washed with a saturated aqueous solution of NaHCO₃, brine and dried over Na₂SO₄. After filtration, the solvent was evaporated under reduced pressure to give **S7** (3.06 g, 10.0 mmol, 95%), which was used for the following reaction without further purification.

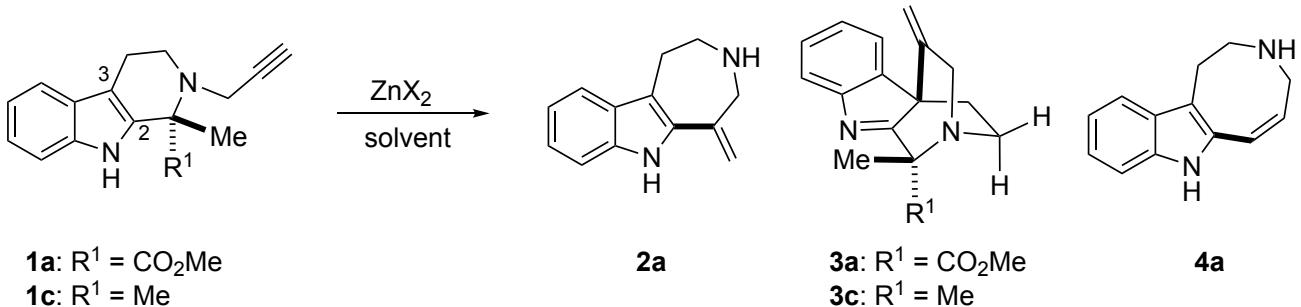
The crude product **S7** (2.40 g, 7.86 mmol) was dehydrated by azeotropic distillation with toluene and then dissolved in MeCN (26 mL). The mixture was treated with K₂CO₃ (5.43 g, 39.3 mmol) and 1-bromo-2-butyne (923 μL, 10.2 mmol) and then heated at 60 °C for 4 h. After cooling to room temperature, resultant insoluble materials were filtered off through a pad of Celite and washed with CH₂Cl₂. The combined filtrates were concentrated under reduced pressure and then diluted with EtOAc. The mixture was washed with a saturated aqueous solution of NaHCO₃ and then brine, and dried over Na₂SO₄. After filtration and concentration under reduced pressure, the residue was purified by silica gel column chromatography (hexane/EtOAc) to give **1f** (1.43 g, 4.00 mmol, 50%) as a pale yellow powder.

1f: *R*_f = 0.43 (Hexane–EtOAc = 2 : 1); ¹H NMR (500 Hz, CDCl₃) δ 9.04 (1H, s), 7.79 (1H, dd, *J* = 6.3, 5.6 Hz), 7.56 (1H, d, *J* = 7.5 Hz), 7.40 (1H, d, *J* = 8.0 Hz), 7.34–7.20 (6H, m), 7.16 (1H, ddd, *J* = 7.5, 7.5, 1.2 Hz), 4.64 (1H, s), 4.63 (1H, dd, *J* = 15.0, 6.3 Hz), 4.35 (1H, dd, *J* = 15.0, 5.6 Hz), 3.59 (1H, dq, *J* = 16.9, 2.3 Hz), 3.53 (1H, dq, *J* = 16.9, 2.3 Hz), 3.18 (1H, ddd, *J* = 12.0, 4.6, 4.6 Hz), 3.10 (1H, ddd, *J* = 12.0, 6.9, 6.3 Hz), 2.91–2.89 (2H, m), 1.87 (3H, t, *J* = 2.3 Hz); ¹³C NMR (125 MHz, CDCl₃) δ 171.3, 138.0, 136.5, 129.3, 129.1, 128.7, 127.4, 126.6, 121.9, 119.3, 118.1, 111.3, 108.1, 81.1, 73.6, 61.6, 48.3, 45.1, 43.1, 20.2, 3.55. HRMS (ESI, *m/z*): calcd for C₂₃H₂₄N₃O [M+H]⁺ 358.1914, found; 358.1927.

1 W. Wu, X. Yuan, J. Hu, X. Wu, Y. Wei, Z. Liu, J. Lu, J. Ye, *Org. Lett.*, 2013, **15**, 4524–4527.

2 S. Mukherjee, E. J. Corey, *Org. Lett.*, 2010, **12**, 1024–1027.

Zn(OTf)₂-mediated cyclizations of **1**



All reactions were carried out using the substrates **1** (1.00 mmol). A 0.2 M solution of Zn(OTf)₂ in various solvents tested was prepared prior to use as follows. Zn(OTf)₂ (436 mg, 1.20 mmol) was placed in a Biotage microwave vial, and then a solvent (6 mL) was added. The vial was sealed with a Teflon septum lined cap, and the mixture was then heated at 100 °C for 5 min to give a homogenous clear solution.

Finely powdered molecular sieves 4A (200 mg) were placed in a microwave vial and dried upon heating with a heat gun *in vacuo*. The solution of Zn(OTf)₂ (0.2 M, 5 mL, 1.00 mmol), prepared as described above, and compounds **1** (1.00 mmol) were successively added to the vial. After sealing the vial with a Teflon septum lined cap, the mixture was stirred for 1 h at room temperature and then heated at 60 °C for appropriate period of time as indicated in the Tables 1 and 2. After cooling to room temperature, the mixture was poured into a mixture of EtOAc and a saturated aqueous solution of the Rochelle salt at 0 °C, and vigorously stirred at 0 °C for 1 h. Resulting insoluble materials were filtered off and washed with EtOAc (50 mL) and H₂O (5 mL). The organic layer was separated and washed with a saturated aqueous solution of NaHCO₃ (10 mL). The aqueous layer was extracted with EtOAc (50 mL x 2). Combined organic extracts were washed with brine and dried over Na₂SO₄. Filtration and concentration under reduced pressure yielded a crude mixture of products.

To obtain the authentic sample for the NMR analysis, the compounds **2a** and **4a** were isolated from the crude mixture by alumina column chromatography (CH₂Cl₂/MeOH = 20/1) despite considerable decreases in their isolated yields. **2a:** R_f = 0.31 (EtOAc–MeOH = 1 : 1, 1% Et₃N); ¹H NMR (300 Hz, CDCl₃) δ 7.96 (1H, br s), 7.51 (1H, d, J = 7.5 Hz), 7.31 (1H, ddd, J = 8.1, 1.1, 1.1 Hz), 7.19 (1H, ddd, J = 8.1, 7.3, 1.1 Hz), 7.10 (1H, ddd, J = 7.5, 7.3, 1.1 Hz), 5.18 (1H, s), 5.11 (1H, s), 3.76 (2H, s), 3.27 (2H, t, J = 5.8 Hz), 3.02 (2H, t, J = 5.8 Hz), 1.75 (1H, s); ¹³C NMR (125 MHz, CDCl₃) δ 143.4, 135.9, 134.3, 129.1, 123.0, 119.6, 118.9, 114.5, 110.7, 110.1, 55.4, 49.5, 27.6; HRMS (ESI, m/z): calcd for C₁₃H₁₅N₂ [M+H]⁺ 199.1230, found; 199.1246. **4a:** R_f = 0.23 (EtOAc–MeOH = 1 : 1, one drop of Et₃N was added); ¹H NMR (400 MHz, CDCl₃) δ 7.92 (1H, s), 7.51 (1H, d, J = 7.4 Hz), 7.31 (1H, d, J = 8.1 Hz), 7.18 (1H, ddd, J = 8.1, 8.1, 1.4 Hz), 7.11 (1H, ddd, J = 8.1, 7.4, 0.9 Hz), 6.37 (1H, dt, J = 11.7, 1.8 Hz), 5.74 (1H, dt, J = 11.7, 5.0 Hz), 3.63 (2H, dd, J = 5.0, 1.8 Hz), 3.08–3.01 (4H, m), 1.99 (1H, br s); ¹³C NMR (125 MHz, CDCl₃) δ 136.3, 132.9, 131.4, 128.1, 122.4, 119.7, 119.6, 118.4, 111.8, 110.8, 48.0, 46.5, 24.6; HRMS (ESI, m/z): calcd. for C₁₃H₁₅N₂ [M+H]⁺ 199.1230, found; 199.1247.

The yields of **1**, **2a**, **3** and **4** shown in Tables 1 and 2 were determined based on ^1H NMR analysis of the crude mixture using pyrazine as an internal standard. Integral values for vinylic protons of these products were used for calculation in reference to that of pyrazine.

Time-course analysis of the cyclization of **1c**

$\text{Zn}(\text{OTf})_2$ -mediated reaction of **1c** was performed in 2-BuOH at 60 °C in several batches. In appropriate intervals, each reaction was quenched as described above. Yields of the products (**2a**, **3c** and **4a**) were calculated based on NMR analysis.

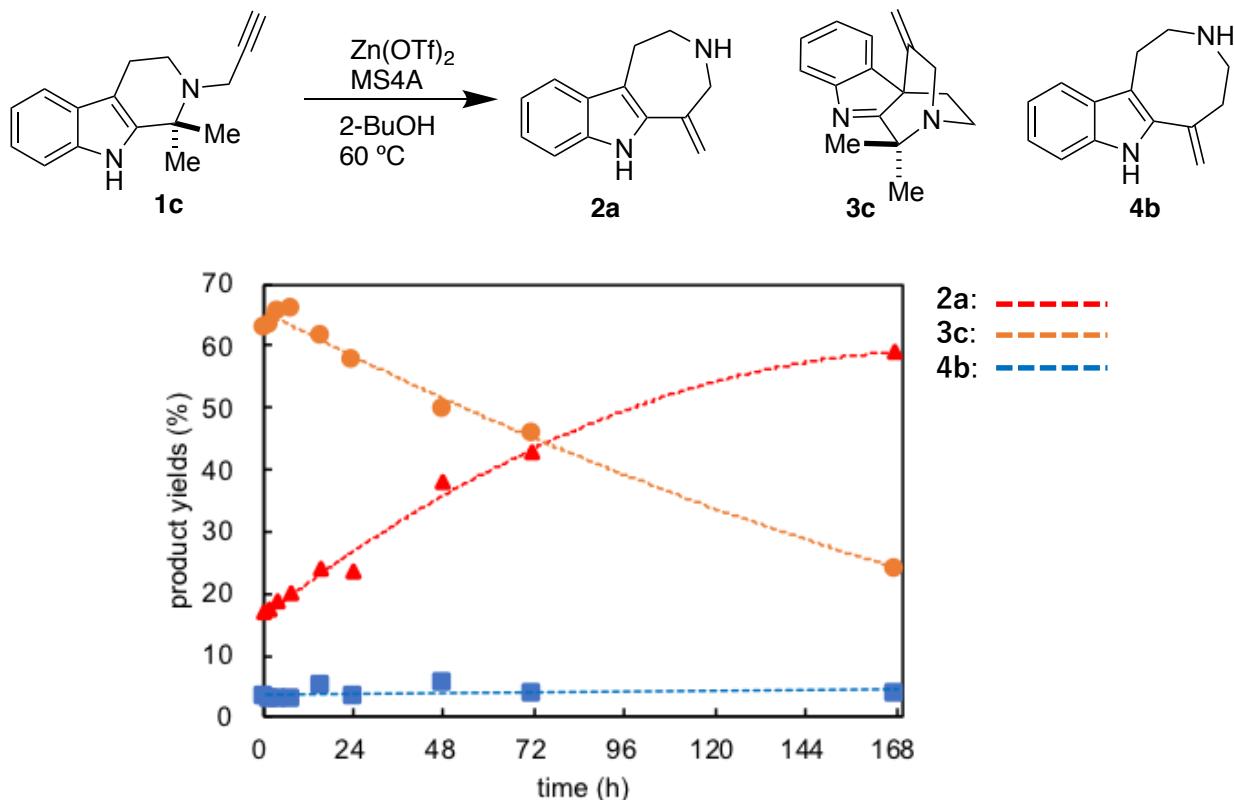


Figure S1. Plot of the yields of **2a** (▲), **3c** (●) and **4a** (■) in $\text{Zn}(\text{OTf})_2$ -mediated reaction with **1c** in 2-BuOH at 60 °C.

Computational investigations

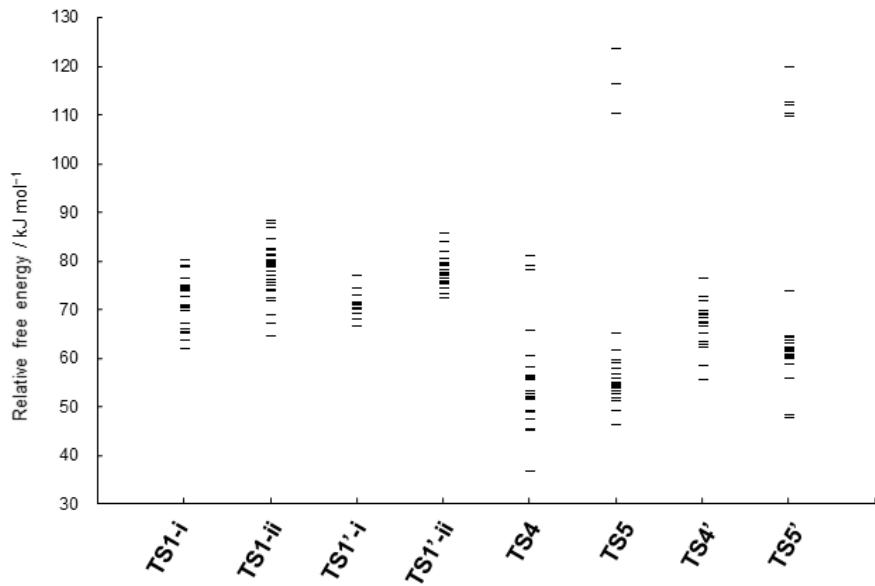


Figure S2. Energy distribution of TS structures with different conformations. Gibbs energies ($T = 333.15\text{ K}$) relative to the sum of Gibbs energies for separately calculated **1a** and $\text{Zn}(\text{OTf})_2$ are shown in kJ/mol . **TS4'** and **TS5'** correspond to **TS4** and **TS5** with *syn*-configuration, respectively.

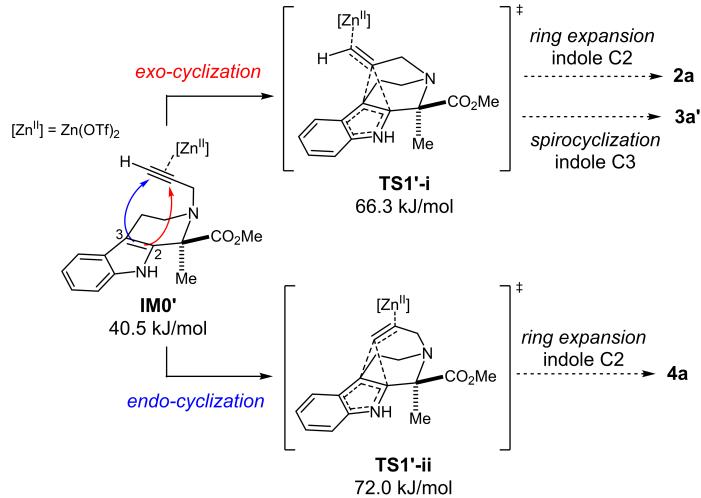
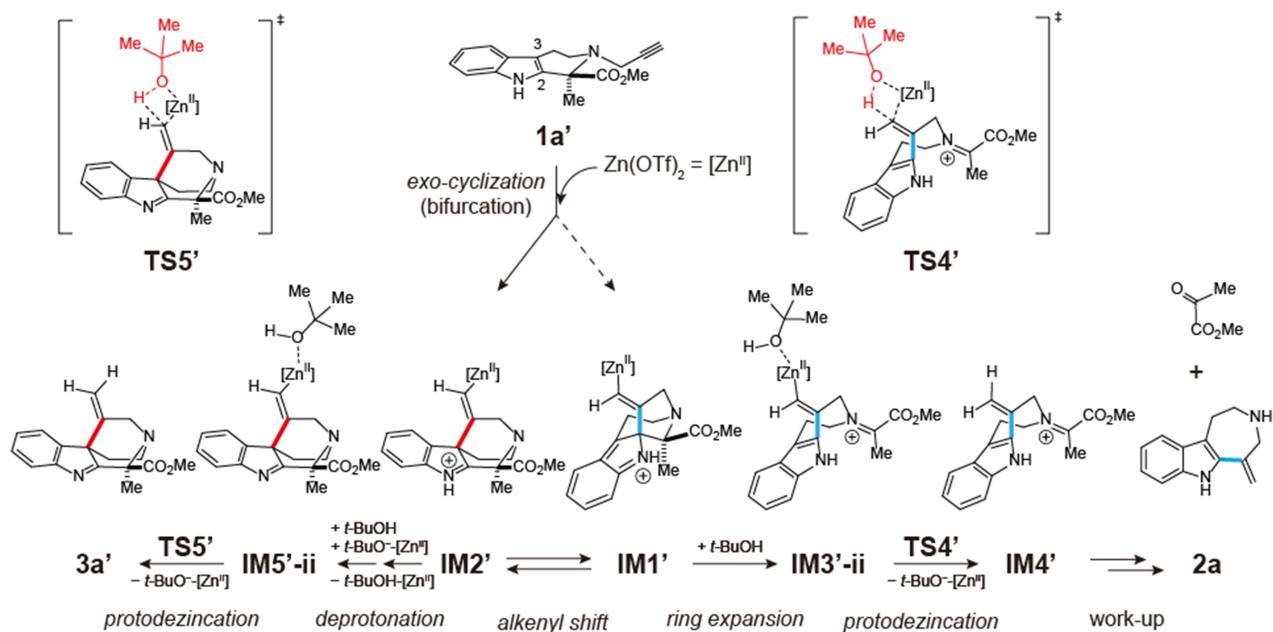


Figure S3. Two intramolecular cyclization pathways leading to *syn*-products. Gibbs energies ($T = 333.15\text{ K}$) relative to the sum of Gibbs energies for separately calculated **1a** and $\text{Zn}(\text{OTf})_2$ are shown in kJ/mol . **TS1'-i** and **TS1'-ii** correspond to **TS1-i** and **TS1-ii** with *syn*-configuration, respectively.

(a) Reaction mechanism



(b) Energy diagram

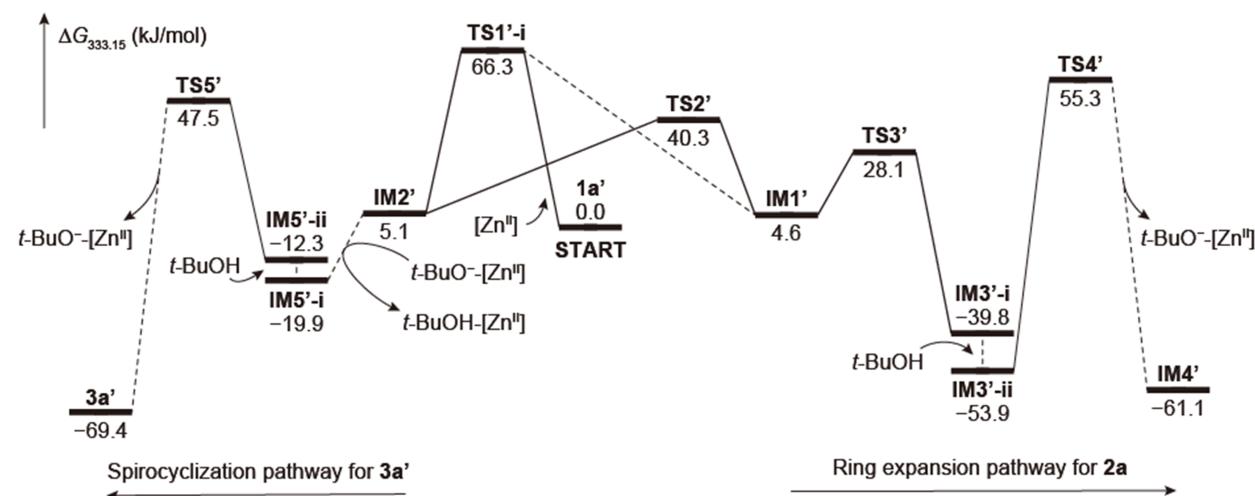


Figure S4. Zn(OTf)₂-mediated cyclization of **1a'** leading to *syn*-products: (a) mechanisms for generation of **2a** and **3a'**, (b) Gibbs energy profiles ($T = 333.15$ K). **IM** and **TS** stand for intermediate and transition state, respectively.

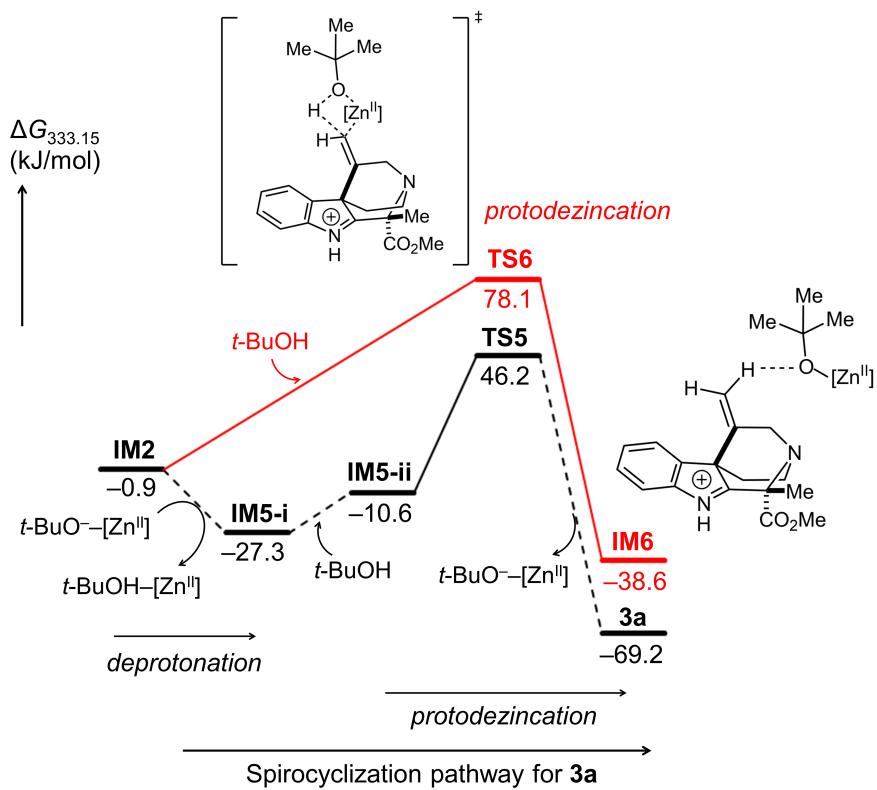


Figure S5. High barrier pathway for protodezinciation of **IM2** without deprotonation.

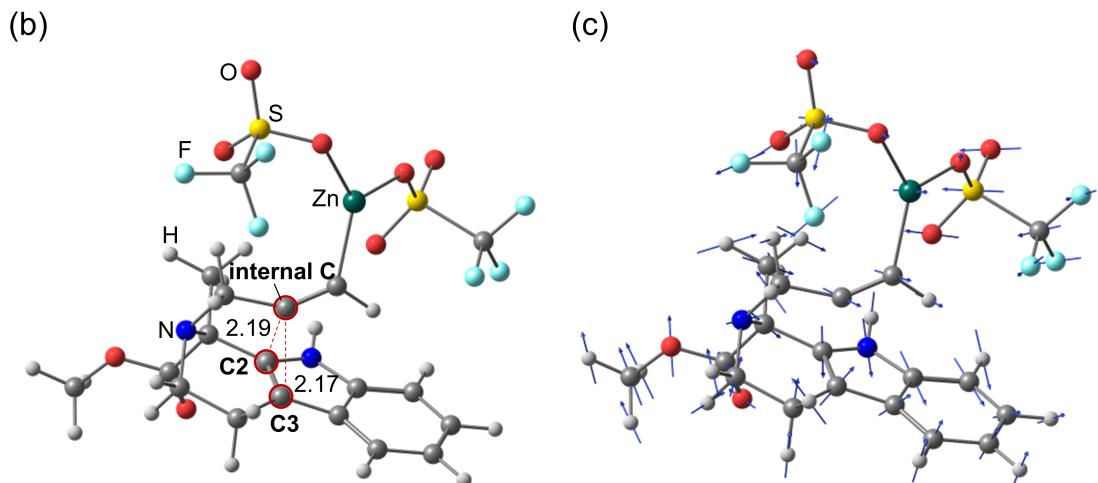
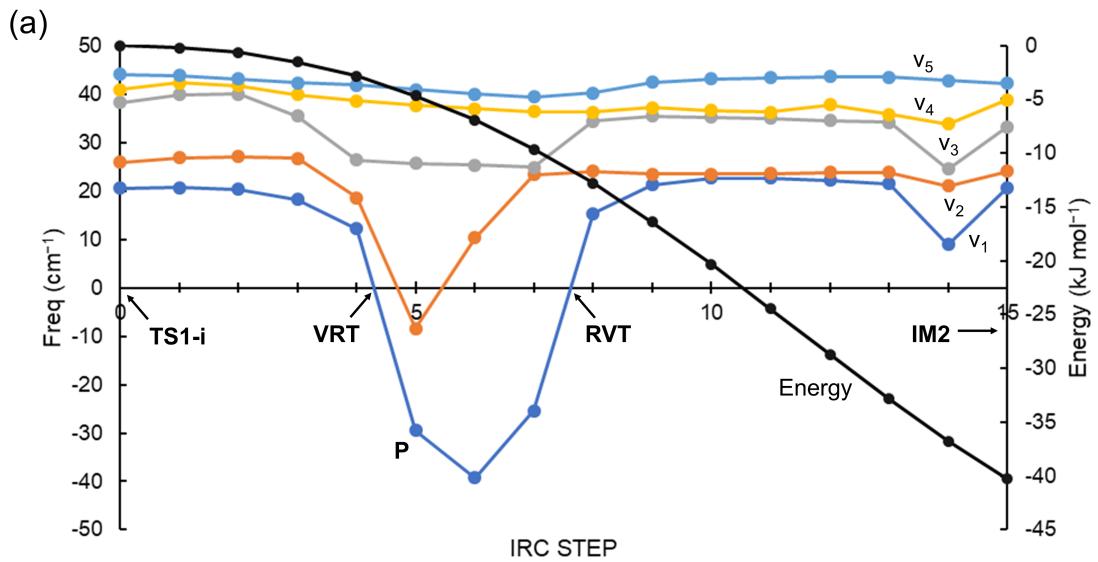


Figure S6. (a) Variations of energy and the five lowest vibrational frequency (v_{1-5}) values along the IRC path from **TS1-i** to **IM2**, where imaginary frequency values are multiplied by the imaginary unit i , (b) the molecular structure at **P** in (a), and (c) the imaginary frequency mode ($v_1 = 33.1i \text{ cm}^{-1}$) at **P**. To obtain v_{1-5} at each point, the normal mode analysis was performed in the coordinate subspace perpendicular to the (mass-weighted) gradient vector. The structure **P** exists on a ridge region of the potential energy surface, and around **P**, the dynamical path bifurcation can take place along the imaginary frequency v_1 mode shown in (c). The point at which v_1 changes from real to imaginary is called the valley-ridge transition (VRT) point, whereas the point at which v_1 changes from imaginary to real is the ridge-valley transition (RVT) point.

Kinetic simulation

The kinetic simulations have been performed using a simplified reaction mechanism shown in Figure S7. The simplified reaction mechanism was constructed from the original reaction profiles shown in Figure 6, where elementary steps that proceed in a very short timescale were omitted assuming a local thermal equilibrium. This simplification enabled to execute the simulation in the experimental timescale. The barrierless deprotonation step **IM2** → **IM5-i** was treated as an irreversible process.

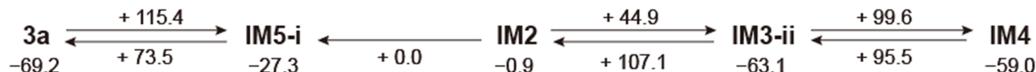


Figure S7. Simplified reaction mechanism adopted in the kinetic simulation. Activation free energy (kJ/mol) for each elementary step is shown on/below each arrow.

Kinetic equations for the simplified reaction mechanism in Figure S7 were solved by the fourth-order Runge-Kutta method.

When $[t\text{-BuO}^-\text{--Zn}^{II}] \leq [\mathbf{IM2}]$, the following equations were solved.

$$d[\mathbf{IM2}]/dt = k_{\mathbf{IM3-ii} \rightarrow \mathbf{IM2}}[\mathbf{IM3-ii}] - k_{\mathbf{IM2} \rightarrow \mathbf{IM3-ii}}[\mathbf{IM2}] - \min([\mathbf{IM2}], [t\text{-BuO}^-\text{--Zn}^{II}])$$

$$\begin{aligned}
 d[\mathbf{IM3-ii}]/dt &= k_{\mathbf{IM2} \rightarrow \mathbf{IM3-ii}}[\mathbf{IM2}] + k_{\mathbf{IM4} \rightarrow \mathbf{IM3-ii}}[\mathbf{IM4}][t\text{-BuO}^-\text{--Zn}^{II}] - k_{\mathbf{IM3-ii} \rightarrow \mathbf{IM2}}[\mathbf{IM3-ii}] \\
 &\quad - k_{\mathbf{IM3-ii} \rightarrow \mathbf{IM4}}[\mathbf{IM3-ii}]
 \end{aligned}$$

$$d[\mathbf{IM4}]/dt = k_{\mathbf{IM3-ii} \rightarrow \mathbf{IM4}}[\mathbf{IM3-ii}] - k_{\mathbf{IM4} \rightarrow \mathbf{IM3-ii}}[\mathbf{IM4}][t\text{-BuO}^-\text{--Zn}^{II}]$$

$$d[\mathbf{IM5-i}]/dt = k_{\mathbf{3a} \rightarrow \mathbf{IM5-i}}[\mathbf{3a}][t\text{-BuO}^-\text{--Zn}^{II}] + \min([\mathbf{IM2}], [t\text{-BuO}^-\text{--Zn}^{II}]) - k_{\mathbf{IM5-i} \rightarrow \mathbf{3a}}[\mathbf{IM5-i}]$$

$$d[\mathbf{3a}]/dt = k_{\mathbf{IM5-i} \rightarrow \mathbf{3a}}[\mathbf{IM5-i}] - k_{\mathbf{3a} \rightarrow \mathbf{IM5-i}}[\mathbf{3a}][t\text{-BuO}^-\text{--Zn}^{II}]$$

On the other hand, when $[t\text{-BuO}^-\text{--Zn}^{II}] > [\mathbf{IM2}]$, the following equations were solved.

$$d[\mathbf{IM2}]/dt = k_{\mathbf{IM3-ii} \rightarrow \mathbf{IM2}}[\mathbf{IM3-ii}] - \min([\mathbf{IM2}], [t\text{-BuO}^-\text{--Zn}^{II}])$$

$$d[\mathbf{IM3-ii}]/dt = k_{\mathbf{IM4} \rightarrow \mathbf{IM3-ii}}[\mathbf{IM4}][t\text{-BuO}^-\text{--Zn}^{II}] - k_{\mathbf{IM3-ii} \rightarrow \mathbf{IM2}}[\mathbf{IM3-ii}] - k_{\mathbf{IM3-ii} \rightarrow \mathbf{IM4}}[\mathbf{IM3-ii}]$$

$$d[\mathbf{IM4}]/dt = k_{\mathbf{IM3-ii} \rightarrow \mathbf{IM4}}[\mathbf{IM3-ii}] - k_{\mathbf{IM4} \rightarrow \mathbf{IM3-ii}}[\mathbf{IM4}][t\text{-BuO}^-\text{--Zn}^{II}]$$

$$d[\mathbf{IM5-i}]/dt = k_{\mathbf{3a} \rightarrow \mathbf{IM5-i}}[\mathbf{3a}][t\text{-BuO}^-\text{--Zn}^{II}] + \min([\mathbf{IM2}], [t\text{-BuO}^-\text{--Zn}^{II}]) - k_{\mathbf{IM5-i} \rightarrow \mathbf{3a}}[\mathbf{IM5-i}]$$

$$d[\mathbf{3a}]/dt = k_{\mathbf{IM5-i} \rightarrow \mathbf{3a}}[\mathbf{IM5-i}] - k_{\mathbf{3a} \rightarrow \mathbf{IM5-i}}[\mathbf{3a}][t\text{-BuO}^-\text{--Zn}^{II}]$$

The stepsize of time evolution was set to 10^{-9} s when $[t\text{-BuO}^-[\text{Zn}^{\text{II}}]] \leq [\text{IM2}]$, and it was changed to 10^{-6} s when $[t\text{-BuO}^-[\text{Zn}^{\text{II}}]] > [\text{IM2}]$. The simulation was terminated at 3600 s.

The rate constants listed in Table S1 were estimated by the standard transition state theory using the free-energy difference between the TS and the reactant, where the transmission coefficient was set to unity.

Table S1. Rate constants used.

Rate constant k	
$k_{3\text{a}\rightarrow\text{IM5-i}}$	1.53e^{-7}
$k_{\text{IM2}\rightarrow\text{IM3-ii}}$	6.33e^5
$k_{\text{IM3-ii}\rightarrow\text{IM4}}$	1.68e^{-3}
$k_{\text{IM4}\rightarrow\text{IM3-ii}}$	2.02e^{-4}
$k_{\text{IM3-ii}\rightarrow\text{IM2}}$	1.12e^{-4}
$k_{\text{IM5-1}\rightarrow\text{3a}}$	2.08e^1

Cartesian coordinate and electronic energy

1a				H	4.641717551113	3.079502934393	-0.692955348681
-917.616533986543				H	2.421431248790	4.443483073910	-0.562751694377
N 0.191951336860	-0.069404481951	2.698834155070		H	3.297054225128	4.161271042325	0.942416759779
N 1.302924491715	1.415155695199	-0.530177945429		Z	-0.936824328648	-0.573226950020	-0.591033581158
C 3.428212745451	2.919706337613	-2.867416587262		S	0.340102695240	-3.099043098825	0.972334028104
C 2.445087802543	2.786760995750	-2.174423510215		O	-0.624714771652	-2.395660814393	0.046231202382
C 1.244583483499	2.619446330487	-1.342564838512		O	-0.249175194827	-4.288404715180	1.559467868109
C 0.733408209432	1.542506477382	0.810217301508		O	1.061654709423	-2.181810516302	1.844135774673
C 0.632792327600	0.163686871359	1.416460405844		C	1.589824751874	-3.735759884596	-0.238308635176
C 1.003739318811	-1.009781839165	0.819146977822		F	1.003379663085	-4.536679633099	-1.115048565922
C 1.498599331744	-1.048372242520	-0.588794314454		F	2.151112699332	-2.727384442784	-0.891666739540
C 1.015408965584	0.208522018154	-1.301023446170		F	2.529340335893	-4.414401061515	0.399766168761
H -0.155658361478	0.633035675609	3.340794779963		S	-3.459843452035	1.330744272712	-0.520877572105
H 4.307410248091	3.042338308550	-3.478389967964		O	-2.680279322858	0.172043262773	-1.097054395591
H 1.154096756665	3.507374240955	-0.699574668496		O	-2.786472393142	1.934424531161	0.625792955488
H 0.354005010163	2.635594962334	-2.001405107651		O	-4.879696779498	1.052432322379	-0.421512607100
H 1.122169576549	-1.938108558569	-1.117203656991		C	-3.298519243805	2.575650036542	-1.883523850359
H 2.600671604191	-1.100396643156	-0.619288190098		F	-3.858919131740	3.715859719775	-1.514829017915
H -0.065723564890	0.116839237042	-1.525128712553		F	-2.016716442095	2.795215877936	-2.152562654304
H 1.536279718430	0.309751457625	-2.264708411137		F	-3.893007444398	2.135814622048	-2.980392111576
C 1.641340312625	2.412536471135	1.693986217463		C	5.408521354952	-0.257360203730	-0.854041900276
H 1.745641846304	3.429579122582	1.290396003017		C	4.455184405703	0.176446732509	0.085794291425
H 1.237397567575	2.502590085519	2.710785511261		C	5.921685216150	-1.542418663294	-0.745672807406
H 2.636003861206	1.949970248262	1.744761047131		H	6.659447199884	-1.893768255404	-1.471509238403
C -0.701570109717	2.123587507071	0.842344602139		C	4.049696389822	-0.713198903654	1.116451685104
O -1.154369338152	2.748998189675	1.771827438516		C	5.506322711465	-2.408660252565	0.288983125388
O -1.397208724065	1.822685705003	-0.244228825365		H	5.926950327756	-3.415808641642	0.346139362684
C -2.752006098531	2.262745947280	-0.292669299532		C	4.572832886348	-2.006928733482	1.233228887109
H -2.805585900896	3.359424611525	-0.240957926471		H	4.239622034104	-2.677351832321	2.027636326603
H -3.151958429319	1.913147613833	-1.250760030416		H	5.736622970087	0.407582663113	-1.657482775029
H -3.328178734391	1.828215258858	0.536377416835		C	0.586559532463	1.450298021128	2.365714052485
C 0.977666436036	-3.441164907609	1.794852062292		H	0.191286298128	0.743930694724	1.623191986732
C 0.791414981546	-2.047247868690	1.792915920485		H	0.824341633703	0.880115181112	3.274605276701
C 0.650979945644	-4.160169134399	2.935968137385		H	-0.189417974790	2.186497131506	2.615778049760
H 0.793188759251	-5.243614356788	2.953073348485		C	2.410384278764	2.933672265841	3.048769090990
C 0.274840549100	-1.414997491443	2.955810415769		O	3.232283476639	2.471868458190	3.802602677668
C 0.137283785288	-3.513856043259	4.080531176664		O	1.853361577230	4.122503692803	3.207240347140
H -0.111031155465	-4.106787895319	4.964561317696		C	2.286851035236	4.888782011176	4.327932196054
C -0.058332186575	-2.139717077174	4.107447357227		H	1.732148222905	5.832596190749	4.283874236291
H -0.457158332530	-1.639684321580	4.992809089203		H	2.064628625690	4.364090081902	5.268138098550
H 1.376031197107	-3.947066004186	0.911592620938		H	3.366901398544	5.084530732862	4.266146871810
IM0				C	0.907334383043	0.433668640698	-1.592965634956
-4618.369475790732				C	0.717768322527	1.452995165338	-0.949665157987
N 3.110699549039	-0.071122601151	1.878601386571		C	2.888767329479	1.176546250420	1.355722544152
N 1.532008177645	3.085793675099	0.750747995503		C	3.703233492565	1.387803016746	0.270444666535
C 0.497787749921	2.698492961591	-0.179358005588	TS1-i				
C 1.843466861089	2.158292081473	1.838622302149	-4618.355171225195				
C 3.642839058205	2.634763006594	-0.554164279814	N 3.352237509400	-0.057356114160	1.500069022658		
C 2.730848512089	3.657834204407	0.141512151115	N 1.347429821119	2.988411863878	1.373885647678		
H 2.572500591108	-0.510765563018	2.614639491166	C 0.586256606255	2.357910723463	0.309339049111		
H 1.240998497308	-0.364115694525	-2.244330693337	C 1.965157186771	1.971455351413	2.236881910028		
H 0.375465244047	3.507560158453	-0.915664846624	C 3.11254289119	3.220394811528	-0.182197061208		
H -0.480055143143	2.603039122393	0.317142611685	C 2.354171664747	3.901255858230	0.817677293520		
H 3.269015051169	2.403076148089	-1.567440534445	H 2.903544836222	-0.749281803235	2.097161904216		

H	1.976358247329	-0.711740010081	-1.001110423083	H	3.186915313894	-0.529028701765	2.715233219681
H	0.438972567531	3.081327224459	-0.504607887101	H	2.158331813410	-0.661866725988	-0.543201817551
H	-0.423303234573	2.059841721042	0.641302710294	H	-0.044584396784	3.014366063217	-0.427389928958
H	2.937835523545	3.309171848283	-1.214752264221	H	-0.600447669553	2.187188784023	1.013572917074
H	4.291106206397	3.722399105925	-0.164592523956	H	2.839659609375	2.456128193470	-1.547090925224
H	1.831728612114	4.740038714627	0.337288554220	H	4.236438368460	3.224040705340	-0.793089197256
H	2.922756041344	4.331949059963	1.654427255556	H	1.838578735900	4.295335621709	-0.387920574117
Z	-0.672522547628	-0.930215066248	-0.473012844833	H	2.983191812884	4.203467887955	0.945989918350
S	0.726256200010	-3.261019806021	1.348682520424	Z	-0.922450873718	-0.426291684959	-0.777213861505
O	0.279314013023	-4.334601662619	2.217863030331	S	0.045215501492	-3.011751784619	0.926225539240
O	1.720599209493	-2.332812335611	1.882199536037	O	-0.705384540932	-2.317331480544	-0.177863699127
O	-0.412102631277	-2.581211403786	0.648708689554	O	-0.715819189329	-4.100556850876	1.513505059565
C	1.584955192809	-4.111945492539	-0.057633146276	O	0.734465557752	-2.093536040357	1.826431493723
F	2.679883484722	-4.714607293119	0.379221942719	C	1.409648492157	-3.845957476143	-0.013422380877
F	0.783624026986	-5.014679614340	-0.600750393526	F	0.918328840042	-4.765886844167	-0.827135818881
F	1.927392374835	-3.233761051298	-0.995772117515	F	2.090431460266	-2.961658716460	-0.739952931098
S	-3.301554844188	0.929112594810	-0.425106448775	F	2.246000657628	-4.421500436079	0.836293385713
O	-2.584214142644	-0.391404935468	-0.502856200252	S	-3.642549502002	1.277905579632	-0.745494873297
O	-2.727764664111	1.834620895739	0.564987637112	O	-2.790080759250	0.135446841490	-1.237228362885
O	-4.743774555763	0.766612132194	-0.448017613163	O	-3.134295210351	1.882900219804	0.480578130161
C	-2.876696815072	1.691699327620	-2.061263789531	O	-5.061567371059	0.980756668899	-0.828155981648
F	-3.417086905672	2.896021889976	-2.150640282187	C	-3.341108983347	2.546226405233	-2.061030783614
F	-1.556721230270	1.805807905423	-2.188803624933	F	-3.941758094490	3.681543584851	-1.741056832200
F	-3.330030898267	0.940178204816	-3.052771178951	F	-2.036793102695	2.774151413724	-2.186766134237
C	4.999266547540	0.645086123096	-1.608945049303	F	-3.808936837277	2.125406540903	-3.226080723988
C	4.254037599608	0.736837705576	-0.421441721485	C	5.368096335922	0.064584832784	-1.179457310714
C	5.584735947321	-0.570210507953	-1.930758263888	C	4.511306894447	0.353151043806	-0.104261442613
H	6.166140063327	-0.664393775579	-2.850807073886	C	6.089192572592	-1.120002437747	-1.155159013962
C	4.124274092989	-0.401014037706	0.409200487186	H	6.764175748975	-1.361501848233	-1.979605473681
C	5.438699287692	-1.695644519888	-1.090781973008	C	4.404551585549	-0.564714936833	0.969822688506
H	5.907862319597	-2.639917880175	-1.377474461871	C	5.961270236934	-2.027489916316	-0.081840561152
C	4.711290607187	-1.631100614926	0.087995766587	H	6.535037810330	-2.957321763027	-0.097272830537
H	4.587102523917	-2.499979407529	0.735985854806	C	5.119925433240	-1.768060724041	0.990468652666
H	5.109140539163	1.511669557831	-2.265054358826	H	5.011439581774	-2.474878719147	1.815362209059
C	0.918505257853	1.053620475250	2.887707200877	H	5.461187939152	0.761839253336	-2.015630938836
H	1.392823702461	0.414192005649	3.646264489025	C	0.974854563218	1.251353288552	2.923481236433
H	0.151389426233	1.668944269450	3.375737274932	H	0.485543013879	0.464348523881	2.336093717707
H	0.439052913232	0.394898004335	2.153070476379	H	1.475105716768	0.767085255782	3.774666075180
C	2.730404193452	2.630105495301	3.395140724444	H	0.219126078112	1.942794899062	3.319261276642
O	3.839380636473	2.299466411067	3.734881760434	C	2.774467108754	2.905965613230	3.102545641156
O	2.004701729210	3.545804957678	4.010556580307	O	3.864717828718	2.625899844026	3.536886171511
C	2.588690360213	4.171718970039	5.151721666842	O	2.073984825938	3.960201903530	3.479878044461
H	1.846498240935	4.890240809029	5.515983360871	C	2.668057755494	4.817029624703	4.452159481136
H	2.806912192031	3.426419429663	5.929650354391	H	1.939400897220	5.613505397253	4.638908645522
H	3.515217315568	4.694070846609	4.874308868334	H	2.872616129440	4.267622920010	5.382057019288
C	1.153497417667	-0.035003656191	-0.748360628629	H	3.603956877954	5.245891217801	4.066387271941
C	1.219813090600	1.119152332454	-0.224963723072	C	1.574692134711	0.229318245943	-0.345092167146
C	2.929778824162	1.220308536346	1.351071294114	C	0.563256106978	0.967970966015	-0.275059470433
C	3.463240396148	1.775370322490	0.181795712715	C	3.004555965444	1.121033878849	1.401455980012
				C	3.585515614432	1.421745454291	0.173995088298

TS1-ii

-4618.352032109727

N	3.499402034201	-0.056597365281	1.874448670773
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C	2.372834777625	3.590273683555	0.263610079994

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C	1.054519149012	0.548757906385	0.361647635079
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C	2.369676300879	1.202270426462	0.845660596376	C	2.410650522614	3.707279550795	0.821041001631
C	2.477382503969	2.549739876514	0.231541007504	H	3.285488484727	-0.633586327813	2.555892038781
C	1.375993074029	3.510404977020	0.432887240090	H	2.088241854156	-0.480588355640	-1.16984190304
C	0.719383956374	3.324810607339	1.832688475119	H	0.452739949537	3.018183334741	-0.595016262035
H	3.796691513529	-0.413438051988	0.695915316471	H	-0.264679136487	1.746798396952	0.394698567429
H	1.775150763286	-0.537021876440	-1.254971158001	H	3.418950276680	3.254658835134	-1.091227424212
H	-0.809934456773	1.609267159215	0.819195748294	H	4.465688568134	3.078155138924	0.333721661791
H	-0.473500481076	0.209798810657	1.854584723620	H	1.963600733206	4.528959191102	0.246109118112
H	0.616414726337	3.277862247025	-0.334320848833	H	2.900341910616	4.166876755876	1.690991296619
H	1.699278062957	4.545783178889	0.261938733375	Z	-0.545338173985	-0.598678643691	-1.298268105625
H	-0.308548274836	3.707006837151	1.793796471856	S	0.504828258001	-3.035227652466	0.592504870410
H	1.251584124670	3.932877529821	2.577944934219	O	-0.003934984172	-4.162423636174	1.360079596202
Z	-0.949918727868	-0.963972217885	-0.989119118865	O	1.313318197449	-2.050755481936	1.310800737080
S	-1.528831918647	-3.078131784778	1.356691500177	O	-0.528480857813	-2.439755530538	-0.311140502565
O	-2.529617527141	-4.038629419723	1.792155523094	C	1.697920834633	-3.803439443237	-0.602566578768
O	-1.058635367910	-2.097881759220	2.331883855076	F	2.700837471974	-4.362213053433	0.064074230055
O	-1.850507075279	-2.487840587159	0.013570531917	F	1.093484849405	-4.738355043740	-1.323140173806
C	-0.029053321366	-4.100027173687	0.975261480934	F	2.201827449792	-2.896607576791	-1.432347031705
F	0.344401643319	-4.774096730492	2.053746223597	S	-3.243902783797	0.437345309416	-0.031925831342
F	-0.288092776634	-4.961213622207	0.001472801949	O	-2.482469681794	-0.177223245347	-1.176809436094
F	0.980263316842	-3.322875026207	0.593833877889	O	-2.419518399668	0.649768724876	1.154605070753
S	-2.824968675927	1.538258661527	-1.871927024299	O	-4.560280924025	-0.150576089319	0.147355029432
O	-2.483920847059	0.078079952642	-1.819613135301	C	-3.565898364875	2.135239567363	-0.698895204555
O	-2.471416256011	2.271758126769	-0.659399911860	F	-4.218639062348	2.857494454902	0.199368316047
O	-4.140334085162	1.778015468132	-2.443515458461	F	-2.420101598038	2.743373136932	-0.983752614396
C	-1.637884011264	2.171100418689	-3.147866976677	F	-4.293407275364	2.065315210019	-1.803687818419
F	-1.833612744411	3.467728445737	-3.341851414438	C	4.731241130885	0.191597268890	-1.628757173255
F	-0.381252195916	1.989673789804	-2.752007180168	C	4.064831720816	0.398097285954	-0.429462387970
F	-1.811189082409	1.535749188095	-4.298354279090	C	5.500080998956	-0.968386229558	-1.765743208969
C	3.666031961018	2.617656479285	-0.467742990590	H	6.028948085682	-1.153343177274	-2.703242953485
C	4.330643534045	1.353476240366	-0.286380549201	C	4.192330784583	-0.542690195876	0.596705430892
C	4.276946549783	3.648505500559	-1.242957516961	C	5.594027062136	-1.904723988361	-0.730476015994
H	3.770804809654	4.606596327364	-1.374414588717	H	6.188751358010	-2.809192856312	-0.873687182382
C	5.592959132819	1.110937329693	-0.878684676156	C	4.935933133782	-1.705467135067	0.484610583426
C	5.497009779933	3.397073922464	-1.803805823956	H	4.992773740697	-2.429557176462	1.298276929949
H	6.100902717862	0.155217614966	-0.745647190084	H	4.643640063447	0.906053792996	-2.449600350896
H	5.998979680341	4.158970012558	-2.402510431343	C	0.681392605490	0.911163047318	2.734852120465
C	6.141114028543	2.130439167975	-1.617133921929	H	0.289951003357	0.255254418757	1.948769120391
H	7.115598082541	1.974367579174	-2.086772914452	H	1.058818378205	0.271712919243	3.545434847125
C	2.998012791415	2.270695089663	3.134612934664	H	-0.123722279219	1.548522912383	3.122257161015
O	4.057655710444	2.647655351822	2.697553066083	C	2.501625506705	2.424537751232	3.434944795132
O	2.557216396851	2.546529089596	4.349559500762	O	3.537278018969	2.003961054341	3.888615453048
C	3.390188736449	3.361149357006	5.172867210695	O	1.790727532542	3.400931315103	3.954455074775
H	3.548265757068	4.343379744089	4.705253099789	H	2.379723282174	3.256423613068	5.947930994735
H	2.856859856134	3.477772315987	6.122364269720	C	2.291428856557	4.004963668856	5.148239880235
H	4.360612846236	2.873580807139	5.341727282327	H	3.271734050029	4.465842268794	4.962554856700
C	2.039563727315	0.003394808522	3.084478769071	H	1.560660345986	4.771323450709	5.426770788981
H	1.502530748094	-0.760137310213	2.506825565274	C	2.814009054834	1.011031945743	1.418323072266
H	1.564733003970	0.097156276901	4.069961173027	C	3.082622392502	1.438625810753	0.013229631649
H	3.076507008726	-0.336082318806	3.221439072487	C	1.268972717446	0.155340296360	-1.261511258491
				C	1.632777672503	1.201875499370	-0.512362887928

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-4618.384651203000

N	3.414281382047	-0.100442457172	1.695484225053
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C	1.810902043220	1.814182710150	2.203313973217

IM3-i

-4618.396669915231

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C	1.585478556429	1.167019230082	2.508526682160	C	1.421699094524	2.689714796997	-1.622007252906
C	2.746457070837	1.454878033357	-0.684292980643	C	2.650415225043	-0.517585750782	-3.079883931325
C	3.124339603162	2.734386286455	-0.309923270662	C	3.108441048582	0.227829350825	-4.154521367681
C	2.206949590770	3.789432186642	0.236017995268	C	2.358352547224	1.310176701642	-4.875201058274
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H	3.847107853281	-0.188420724239	-1.457757514369	H	3.569800345877	-2.024793060568	-1.900461948584
H	1.726508072170	-0.631352340181	-2.017801357062	H	1.615914782109	-2.128142924674	-1.248586349263
H	-0.019061519839	2.385979247513	-0.044505663447	H	0.133361618732	0.681413921768	-3.795400627110
H	-0.326117198108	0.824448997614	0.697181373853	H	-0.347599375898	0.876170484630	-2.118037957016
H	1.416796080796	4.023837711537	-0.493141856341	H	1.482742469094	0.902249492689	-5.402706315589
H	2.756793289695	4.726932535498	0.397714884669	H	2.996773419814	1.744027875781	-5.657914990006
H	0.656030290132	3.992361681953	1.764944615712	H	1.226579556430	3.131907393491	-4.505302629704
H	2.271989377847	3.598229637070	2.398978240586	H	2.826930052102	3.062317701438	-3.715244000941
Z	-0.801217914991	-1.029815533294	-1.177589744860	C	0.842008948631	2.282088765347	-0.322173575433
S	-1.708096949525	-2.836750336892	1.309824813969	H	1.444088722669	1.449246278834	0.084049828125
O	-2.734251291199	-3.800275009222	1.669087257374	H	0.879194778711	3.113587686503	0.391626218468
O	-1.594473766893	-1.629962830562	2.126927347999	H	-0.193950833600	1.932656660433	-0.424090316815
O	-1.660161246721	-2.555716488565	-0.162041507933	C	2.301369810998	3.921972235764	-1.601071957247
C	-0.102844748723	-3.731854946768	1.568731866313	O	3.391610208206	3.898305321762	-1.097965208485
F	0.140260041759	-3.869453765022	2.864001771844	O	1.698684758670	4.954100775111	-2.140268923209
F	-0.147061782502	-4.930912271656	1.009318964286	C	2.414610021089	6.197255171775	-2.146631875592
F	0.900075743893	-3.049605307687	1.020744883882	H	1.754993914220	6.918101704959	-2.639628979892
S	-3.119135586569	1.148494934151	-1.595142069663	H	2.627321772896	6.513981957574	-1.116691654777
O	-2.562051264896	-0.231618682409	-1.777074653678	H	3.352934005370	6.088529050643	-2.707161763610
O	-2.681762408337	1.797590253768	-0.362355070250	S	1.246840233868	-0.508118592090	2.403266035728
O	-4.530925040856	1.224699355002	-1.935670772004	O	1.221595011497	0.142516268730	3.704327793917
C	-2.265312991038	2.091890484416	-2.943515317879	O	2.341876614133	-0.160074945138	1.497562764797
F	-2.743872439385	3.326912104008	-3.002900434575	O	-0.096409033546	-0.537228772580	1.745123748441
F	-0.957749321319	2.157326232501	-2.713504166488	C	1.534537357227	-2.300271608448	2.778250340583
F	-2.457144402604	1.502750278657	-4.115287981706	F	2.727579478369	-2.465371184955	3.331284466643
C	4.531909506508	2.841793848775	-0.576846242079	F	0.611756367349	-2.756491493186	3.616693694965
C	4.945020739465	1.594277461972	-1.112882180051	F	1.480711300708	-3.022671819750	1.663134113929
C	5.484725193883	3.864908415935	-0.411823159971	S	-2.977769807135	0.932700057938	-1.170255408093
H	5.191033921742	4.835459877487	-0.003278703027	O	-2.093570001092	0.335602188722	-0.119993748201
C	6.275163180987	1.343638562657	-1.476711452742	O	-3.454279103323	-0.029722098644	-2.159583669221
C	6.801282683377	3.619190607327	-0.770773742007	O	-2.476484297592	2.206252900875	-1.682934242675
H	6.574159218491	0.375815788603	-1.885251562394	C	-4.467439533561	1.384103190263	-0.168357175327
H	7.552457718030	4.40284548713	-0.644899446712	F	-5.389786566315	1.913614862695	-0.958737926072
C	7.192540574828	2.368563982128	-1.297867465422	F	-4.975198609561	0.308012607988	0.418055364585
H	8.238645114572	2.205435658372	-1.568617031371	F	-4.143626468049	2.266026404818	0.764306650189
C	2.467496548136	1.666831768049	3.633116264234	C	-2.773486192287	-3.349630384433	0.574260708309
O	3.658183652928	1.512078644857	3.595805819027	C	-3.943420144304	-3.048484509702	-0.354365459245
O	1.764109480316	2.196469350862	4.603032025080	H	-4.900630600724	-3.224360645416	0.158522269454
C	2.484247338574	2.656363465849	5.755972593385	H	-3.911667271552	-2.001933774479	-0.686848675386
H	3.192247211969	3.444684420569	5.467222078425	H	-3.913106490399	-3.694723971114	-1.246596541401
H	1.728466522630	3.052596432180	6.441241636081	C	-2.798603109634	-2.458727255269	1.806073600126
H	3.021880213423	1.819493944411	6.221737025750	H	-3.687744383711	-2.683183723940	2.412865441404
C	1.349469771279	-0.292385742559	2.490379704879	H	-1.905333464641	-2.623023416062	2.425326271314
H	0.434324129928	-0.575076771736	1.960501458753	H	-2.837864264456	-1.398141093723	1.519209488887
H	1.315739073130	-0.681977523720	3.516360215733	C	-2.714187616826	-4.824481526995	0.952767222643
H	2.215560933300	-0.752246355143	1.983751157187	H	-1.843526648889	-5.021667762882	1.596411932219
IM3-ii							
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N	1.289953856825	2.035028973740	-2.724098269106	C	-2.634373924738	-5.456079110848	0.053518361589
				C	5.409127010103	0.099046665174	-5.404522087809
				C	4.435740473721	-0.242762561730	-4.446571599551
				C	6.622985426977	-0.572247528808	-5.396446003033

H	7.387759553327	-0.315915610012	-6.133634599351	N	1.301484059187	2.855536706474	1.147355671168
C	4.723135892834	-1.267827050333	-3.508612107329	C	1.375701615368	0.016697384009	-1.258108055636
C	6.890537359695	-1.584540375268	-4.449072840399	C	1.705698470764	1.087777848167	-0.527104094460
H	7.857477447453	-2.093432158760	-4.467966819521	C	0.702648178917	2.075650082647	0.062445585515
C	5.949338255511	-1.946017801375	-3.496140740936	C	1.905585089668	1.970494527212	2.164926021995
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H	5.212125691303	0.881032325386	-6.142687518090	C	3.113088136282	1.433357294639	-0.017423007256
Z	-0.607800038605	-1.136380265901	-0.172650431323	C	3.398358243544	2.935359047584	-0.223341559902
C	0.943024844873	-1.272500390685	-1.419584578632	C	2.318649759075	3.734296596669	0.557741467336
O	-1.538951281072	-3.023006077921	-0.114334442508	H	2.210729228761	-0.615177965377	-1.591901384556
H	-1.488457063671	-3.503913247780	-0.952214743872	H	0.377134013972	2.792513314063	-0.706681697089
				H	-0.208026001315	1.562564733397	0.402773107168
				H	3.373326494648	3.165104726713	-1.298835436099
IM4				H	4.407486356840	3.170069896096	0.145421222237
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N	3.808370883833	-1.308798358958	-3.325941857269	H	2.782199611957	4.337011078303	1.352738921200
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C	2.158577027719	-1.124456685365	-0.900855519542	C	0.527335122803	0.272474295608	2.086273110825
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IM5-i

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IM5-ii

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H	-5.012843901227	5.090870811329	-1.764694420940	H	0.856930513832	2.456387902703	-2.675586204305	
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S	0.714870848348	-1.312826415315	2.215977917888	H	0.814061703594	5.539998533203	0.290137198413	
O	0.106063748267	-2.409845117944	2.956934905892	H	0.372030420916	4.696650504973	-2.491785606369	
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O	1.380785361297	-1.774909635159	0.954248406997	C	-0.954306955159	1.580883275625	-0.071498523645	
C	2.157280443294	-0.815796521095	3.272865736680	H	-1.204568514003	0.784525918652	-0.041264925821	
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C	1.968733120530	-2.942435262093	-3.711686140635	F	3.079267519005	0.460778133328	2.710215827385	
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C	4.268256178219	-2.027241163815	-4.131092561696	O	-2.840649928273	-1.524571700278	-0.788312527104	
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C	2.000706349408	-0.465897206159	-4.010141489314	H	2.288703696792	0.822473105252	-1.491146782564
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				H	2.760672963758	4.328101831175	1.618262125565
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O	-2.430662133443	5.179858023378	1.059248701822	C	4.789647175756	-1.683599510046	0.378588870931
O	-3.410174816616	4.567187519243	-0.849934730108	H	4.588534264516	-2.563815429370	0.990341040697
C	-4.373339326587	5.605751338153	-0.693573559494	H	5.462826742592	1.485934554257	-1.876265726943
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C	2.680775473197	2.507816695951	3.197174343367	H	7.872630325412	2.019418990988	-0.747657941637
O	3.861671701240	2.276043847532	3.277791795240	C	3.073223189346	2.269711756084	2.928396396442
O	2.019106407575	3.305810343908	4.014857857461	O	4.239533221512	1.984248732509	2.825379513157
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C	3.349947120278	1.640811263681	0.164418964840	C	1.99672613961	0.064165677482	2.773374739120
C	1.342759102477	0.002970829280	-0.962798226170	H	1.396131940049	-0.640938692731	2.191140842300
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				H	3.032888254170	-0.299351696593	2.823300382617
TS3				TS4			
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C	-0.050074326182	-4.120524288218	0.982552383636	O	1.214053919532	4.363146254159	-3.717555102394
F	0.343779147199	-4.702173397298	2.106735276220	C	1.918169377905	5.515831398824	-4.202736462027
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O	-2.572437212149	-0.075245698654	-1.966273056230	S	1.660379328651	-0.856680031524	2.236121339260
O	-2.899873692177	1.849611674277	-0.441268430414	O	1.849146175330	-0.200114854519	3.517939663856
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C	-2.026059893503	2.317222738393	-2.874012060331	O	0.230820686350	-1.220653238713	1.972856936028
F	-2.336726394642	3.600727941800	-2.763943858497	C	2.440157115423	-2.524974730558	2.432616955842
F	-0.751181960005	2.160548433640	-2.526152640584	F	3.741336638293	-2.386110053375	2.641364566215
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C	4.093851182310	2.636132493551	-0.195545997464	F	2.261817585893	-3.251751562821	1.335873750005
C	4.628507863387	1.317292290956	-0.143040729769	S	-2.626347699514	1.638773237017	0.055744569194
C	4.944816725420	3.737027886445	-0.4508664647489	O	-2.130368214682	0.395028049082	0.723934187763
H	4.537993486525	4.749417259594	-0.497863407179	O	-2.583663045148	1.579247527822	-1.406153513427
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H	6.409118798435	0.066332443693	-0.284375659657	F	-5.001047597832	2.715324450308	0.063187275441
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F	-5.020523078059	0.569941762065	-0.126700946905	H	-3.869748821110	6.050316538665	-1.023068437579
F	-4.596343330160	1.477728405206	1.781606090583	S	0.793007872860	-1.271135547997	2.590582984298
C	-3.051102844766	-2.870182363713	-1.238163515483	O	0.272060161222	-2.337292615193	3.431894309033
C	-3.207500203204	-1.762063282793	-2.281419075030	O	-0.040806834417	-0.094896803119	2.379951278369
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H	-3.014985409262	-5.040211873843	-1.150747869195	O	-2.544542616057	-1.673033778479	-0.652270769116
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H	7.611045716465	0.203214190589	-4.365342118464	C	1.824668434749	-0.155930030564	-4.041327534354
C	4.569160434243	-0.613907403518	-2.130801095317	H	1.703480376553	-0.339079880436	-5.120246541053
C	6.924916561180	-0.345510246822	-2.384522001991	H	0.829461252111	-0.176512321043	-3.577382708173
H	7.936509001707	-0.359751790846	-1.971114879817	H	2.249177077719	0.852630398218	-3.912710001726
C	5.850072752566	-0.644374409347	-1.561352944304	C	2.144771222860	-2.603615738263	-3.576641165226
H	5.988941879326	-0.892165594599	-0.506678065048	H	2.049758564428	-2.865981505433	-4.641812441888
H	5.336948890725	0.263539379736	-5.364500647934	H	2.789100969419	-3.355043628233	-3.093050123000
Z	-1.009099057157	-1.220842893709	0.396510989409	H	1.146240340909	-2.661337817786	-3.119920215745
C	0.467189914830	-1.691709040893	-1.288064368354	C	4.133285115138	-1.137389519175	-4.026917445762
O	-1.768785012478	-2.778519785069	-0.629958015126	H	4.799470926267	-1.878357268015	-3.557599918666
H	-0.814308939093	-2.325428574665	-1.210192810679	H	4.100337918138	-1.337343104499	-5.109631393689
TS5							
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N	-0.233364421491	3.086015677676	2.117036625057	C	2.013776123936	3.328118862435	1.500341120204
N	-0.685457544522	3.130752451954	-1.507183678895	C	1.105708508161	3.197744869640	2.566696049762
C	1.363074711812	2.035506631564	-0.649548853856	C	3.371640414288	3.470934778224	1.745516270141
C	0.289558545419	2.064708287709	-1.735418649970	H	4.085855639041	3.574863093012	0.924883791990
C	-1.299368202014	3.006172816563	-0.168671629764	C	1.537082629293	3.192889761611	3.887857103419
C	-0.181356478621	3.135391563196	0.840437959212	C	3.813251278566	3.470262690261	3.075029403012
C	1.207554639263	3.273150297131	0.239786797621	H	0.820666792569	3.081019362110	4.704103742427
C	1.196118392435	4.540694133966	-0.646678169883	H	4.879314842566	3.578079693981	3.289405663477
C	0.009227158678	4.416023237177	-1.640528570693	C	2.907418042617	3.328533539006	4.129658370763
H	2.962451569112	1.201942409280	0.348085914983	H	3.276078074163	3.322341818472	5.158522055666
H	0.757836278275	2.251198670902	-2.714173881561	C	2.262418873186	1.046697848394	-0.486155930292
H	-0.212105957081	1.092474782991	-1.814346534173	H	1.447717421306	-1.009631961969	-0.532702386000
H	2.159317933538	4.625640261235	-1.170883846639	O	2.870572652745	-0.952470642784	-2.010134584693
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TS6 (in ESI)							
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N	-0.157513964391	3.024703723203	2.074771085379	N	-0.711398934063	3.171218751969	-1.519203786265
N	-0.711398934063	3.171218751969	-1.519203786265	C	1.339777011406	2.072127256365	-0.676126335656
C	1.339777011406	2.072127256365	-0.676126335656	C	0.298307690638	2.143623150885	-1.792174854721
C	0.298307690638	2.143623150885	-1.792174854721	C	-1.307497635059	2.974789366490	-0.197521140333
H	-1.307497635059	2.974789366490	-0.197521140333	C	-0.183234781282	3.122438536832	0.788191743954
C	-0.183234781282	3.122438536832	0.788191743954	C	1.184907904155	3.325639089415	0.228481665637
C	1.184907904155	3.325639089415	0.228481665637	C	1.160259377897	4.588994274484	-0.668262387030
O	-3.280675210870	4.055351834266	-0.918800309193	C	-0.069530591511	4.488139326707	-1.607755113700
C	-4.299822529569	5.048781335382	-0.876509265541	H	2.868071170072	1.207025379697	0.400778725512
H	-4.988791524795	4.813147322352	-1.695197768357	H	0.783923623527	2.406457782980	-2.744094339037
H	-4.833303592461	5.018724670180	0.084279565654				

H	-0.183321648749	1.170601529883	-1.943369024684	H	2.684019079645	0.075292604676	-1.455764188952
H	2.103928692598	4.623724133964	-1.229623220652	H	-0.972845827117	2.835412809069	2.658788417602
H	1.111081438921	5.486825649047	-0.036943864929				
H	0.222855559414	4.651613480714	-2.653374836076				
H	-0.808161533570	5.264701313977	-1.363489814439	Zn(OTf) ₂			
C	-1.977177650990	1.593696553188	-0.045032047084	-3700.732570298083			
H	-1.239050241022	0.785417303926	-0.034705754838	Z	-1.765289752971	-2.005288604135	-1.989382501933
H	-2.539548103883	1.553010754625	0.898198461781	S	-0.172246249318	0.637952973210	-1.177143952833
H	-2.664343343235	1.438933089333	-0.886525430310	O	-0.541541093104	2.035860183085	-1.059957427083
C	-2.407796594990	4.004878591434	0.106622524521	O	-1.200516702482	-0.144998866475	-1.970185521975
O	-2.567274658288	4.491467926513	1.199097145536	O	0.282139844131	-0.075343900785	0.007436154859
O	-3.178153524014	4.218735837941	-0.936133832395	C	1.270385610447	0.607404124371	-2.339415794494
C	-4.290274716042	5.096918042338	-0.756354779612	F	0.968409342210	1.227426815829	-3.468994905778
H	-4.776629360622	5.171795649858	-1.734602682779	F	2.307236205662	1.209321827554	-1.779787886469
H	-4.990042950305	4.682615098270	-0.016955092136	F	1.600427389786	-0.648350277047	-2.615592377358
H	-3.948032289037	6.087990047525	-0.427294174555	S	-3.614877430819	-4.610650037978	-2.058225683344
S	0.812739100463	-1.053804691966	2.556715355891	O	-4.722101843751	-3.780897213591	-1.607713677453
O	0.198756116169	-2.003185359821	3.470614904993	O	-2.356489937564	-3.811474591336	-2.328262767204
O	0.151508374007	0.234662617309	2.368398505958	O	-3.851357136429	-5.597417057953	-3.095546394659
O	1.247688629977	-1.690551002685	1.267052609425	C	-3.100901621713	-5.583333334236	-0.568041477476
C	2.4434030765577	-0.642855135024	3.353681979998	F	-2.042339206259	-6.328498729047	-0.843741957364
F	2.215696219569	-0.071787856992	4.531457395799	F	-2.797887525244	-4.759559564542	0.427073550354
F	3.146216558391	-1.744475605231	3.540655987579	F	-4.094501236581	-6.369833070927	-0.186922896799
F	3.137403812522	0.193839443815	2.602779735682				
S	-1.737190215907	-1.920422475707	-1.716463714730				
O	-1.373753052563	-3.331527470656	-1.745390936927	t-BuOH			
O	-0.558333100499	-1.008476034242	-1.518196364817	-233.446665646230			
O	-2.898871264050	-1.534773253048	-0.928296560325	C	-1.412962408814	-0.797664363798	-0.218922296571
C	-2.185114282005	-1.493340274685	-3.462429151406	C	-0.730402278688	0.386476628318	0.468671298528
F	-2.397880442610	-0.188676518404	-3.577767480703	H	-0.828277488512	0.326912396416	1.563647663574
F	-1.210577316743	-1.839318107283	-4.293064116814	H	0.341388770325	0.411399650038	0.217500524881
F	-3.288783548050	-2.138209648866	-3.809526418185	H	-1.181657859818	1.337588669547	0.141344052540
C	2.748957039935	-1.269058857478	-3.280861916627	C	-0.758479220487	-2.111314932303	0.194615295111
C	1.877979696969	-0.210814705569	-3.960935440927	H	-0.857663806534	-2.276830153845	1.277642995238
H	1.802275836014	-0.397961025563	-5.042849691321	H	-1.229282745672	-2.957884017362	-0.328961232524
H	0.861249149832	-0.220142678790	-3.543433885977	H	0.313291751791	-2.104655570630	-0.057789169569
H	2.305637116472	0.794272872276	-3.818327859063	C	-2.909152294327	-0.814779002833	0.099320350718
C	2.140467284589	-2.658192227007	-3.459904842621	H	-3.403399522579	-1.651711356797	-0.418073688982
H	2.074265717962	-2.931649484954	-4.524025211793	H	-3.090388860646	-0.920936282030	1.180008768444
H	2.753653752550	-3.415063796511	-2.946077287869	H	-3.386685756039	0.122001217101	-0.232301878758
H	1.125203130560	-2.694052232939	-3.035955489480	O	-1.226567582600	-0.702255103495	-1.629482856219
C	4.172217684906	-1.226631638390	-3.835583370846	H	-1.635180964396	0.120604804676	-1.923685206410
H	4.805507375305	-1.968063734100	-3.324335004270				
H	4.187281562782	-1.443409206059	-4.915060945704	t-BuOH-[Zn ^{II}]			
H	4.618181422831	-0.231258147986	-3.680721448106	-3934.21053507901			
C	2.012049267070	3.372548616409	1.476871999537	Z	-1.879549442837	-1.856163947089	-1.947053845359
C	1.164890262618	3.166618358044	2.568507069949	S	-0.073003741704	0.606859168977	-0.854963092346
C	3.369794706578	3.557576042562	1.694341510833	O	-0.304331388609	1.996946476117	-0.506901399640
H	4.055889232067	3.719339545262	0.860795184753	O	-1.354336538641	-0.085202744819	-1.255207449909
C	1.601465479791	3.118192894309	3.881032800354	O	0.765475510947	-0.204339062586	0.014617299143
C	3.838715438007	3.520905756753	3.011308651465	C	0.832363747044	0.652046508749	-2.469645043162
H	0.911140076178	2.941081727468	4.706635860643	F	0.140513533700	1.331837846334	-3.373411317613
H	4.904001819110	3.662902808643	3.204939876402	F	2.014501751416	1.223365961090	-2.313727243677
C	2.970647013213	3.299348327885	4.085424234389	F	1.013178211716	-0.587907706832	-2.922051341052
H	3.368517605980	3.265626307425	5.101621278494	S	-3.701781247926	-4.512885254839	-1.669865306403
C	2.213222603942	1.072757714824	-0.470755835765	O	-4.722870623174	-3.735314909547	-0.980853656367
Zn	1.248381819265	-1.001707293143	-0.630724231255	O	-2.425985323262	-3.740294977612	-1.899167369736
O	2.819555680133	-1.010457429181	-1.879661934347	O	-4.095176074326	-5.290345783433	-2.835037978039

C	-3.112895373445	-5.758063154880	-0.433541352987	N	3.380868811170	0.033505805536	1.542233558367
F	-2.110291830511	-6.463771613281	-0.932779669170	N	1.274333797041	3.015298287069	1.214282492068
F	-2.700742504363	-5.145046438889	0.666912576349	C	0.592653766609	2.322110180774	0.131731485538
F	-4.104072238916	-6.578872937964	-0.121599001482	C	1.869494634837	2.040886873390	2.138795895140
C	-3.183007424996	-0.955957871465	-4.617447550430	C	3.315866450274	3.274655845703	-0.224237041886
C	-3.279778521918	0.537781266873	-4.335641329080	C	2.265347824754	3.954661761981	0.677879607512
H	-4.199616598553	0.953612984672	-4.772267479803	H	2.959443851695	-0.612319535448	2.201877403958
H	-3.289796048885	0.731716694766	-3.252579272802	H	2.134687481428	-0.751817853717	-1.080884534546
H	-2.423911042843	1.073519123353	-4.773900706874	H	0.458872381005	3.010076976332	-0.713477394725
C	-4.347396184348	-1.725618529925	-4.014528437866	H	-0.414414638504	1.997986678640	0.443608363877
H	-5.288070705836	-1.417317871185	-4.491477449408	H	3.005135513616	3.296200193261	-1.281495736178
H	-4.221286131729	-2.807715975744	-4.164466958403	H	4.269875654375	3.822654503359	-0.175827891822
H	-4.440161256757	-1.527214473766	-2.935046909458	H	1.725833593075	4.730670481719	0.117720335038
C	-3.039653909583	-1.243060826343	-6.105733415821	H	2.750892180792	4.463178506966	1.519443344303
H	-2.936303941875	-2.323585623099	-6.284007833730	C	2.514090063377	2.705945191071	3.367587794663
H	-3.924093358686	-0.881840474387	-6.650050062468	H	2.814855871947	1.931672121260	4.087027732673
H	-2.155428667583	-0.733248291006	-6.520295578067	H	3.414108322276	3.269473365784	3.091388076198
O	-1.984563471119	-1.467607574081	-3.961735831255	H	1.790666758204	3.381769807786	3.845061451650
H	-1.206836711412	-1.030280207156	-4.337101397068	C	0.808693093908	1.089412821528	2.716175780036
<i>t</i> -BuOH ⁻ -[Zn ^{II}] -3933.734783016550							
Zn	0.099257645117	0.043201899234	-0.010100716027	H	-2.261451311262	1.541696568986	3.566051582290
S	-2.978362673786	-0.586438086375	0.931441792306	H	-1.565044530065	0.000603185903	2.954733392350
O	-1.914829440409	0.122036200968	0.145809593897	H	-1.083254723550	0.620975451489	4.568829909249
O	-2.654619230215	-1.974516232502	1.241408444376	Z	-0.604918484389	-0.677596571463	-1.225935747382
O	-4.314264324449	-0.297881977043	0.431524454312	S	-0.832117247869	-3.480225464394	0.271362226889
C	-2.897588848628	0.281161564546	2.568133921017	O	-1.409131369504	-4.793574185464	0.041147387833
F	-1.676687196394	0.189779026887	3.086778973497	O	-1.335500093082	-2.684716192362	1.385058338760
F	-3.210184439913	1.560875110828	2.441054659330	O	-0.690213076457	-2.682777868351	-1.000998666010
F	-3.753416426742	-0.281453613881	3.412527056494	C	0.942401004759	-3.809781678790	0.695884463059
S	0.192660618420	3.167784147270	0.613666016773	F	1.014968473020	-4.550916479607	1.790944518061
O	0.410522542674	2.009754163053	-0.319842727547	F	1.549382712718	-4.446515560978	-0.294445212819
O	1.192390793845	4.212120715260	0.449021140181	F	1.582473485712	-2.664721681691	0.916645909899
O	-0.141555774875	2.748702233497	1.971204858500	S	-3.180734171362	1.228506493472	-0.655796074039
C	-1.363655904180	3.913842729872	-0.059874415713	O	-2.204265866613	0.453501602314	-1.498251061021
F	-1.686376134903	4.986613512190	0.652047641081	O	-2.653804182068	1.572009349456	0.661276479423
F	-1.184457694843	4.281145787973	-1.322233765119	O	-4.535270486052	0.709063734160	-0.728349584235
F	-2.364748374637	3.051787527849	-0.006771324171	C	-3.227535945606	2.824083576945	-1.593512545277
C	1.836938014145	-1.825505699440	1.184928928342	F	-4.037889731705	3.674935030501	-0.983278234291
C	0.766610651111	-2.407240197078	2.121170804568	F	-2.015167678405	3.361046433138	-1.657340901908
H	1.189009129062	-2.765722560989	3.074163799662	F	-3.667065513685	2.619785221677	-2.825610543863
H	0.004851837576	-1.645630123781	2.352004156417	C	5.280848635112	0.798755150386	-1.399670994981
H	0.251752271118	-3.248557233948	1.630822160612	C	4.412341648174	0.853901066639	-0.295737702070
C	2.540826497198	-0.646887425894	1.875354649451	C	5.981477168018	-0.374028240697	-1.633041301989
H	3.051628064248	-0.941297261982	2.806354105530	H	6.663369742643	-0.438531702734	-2.484057134639
H	3.286119453454	-0.203814644826	1.194940953839	C	4.275660791807	-0.278125039973	0.544648363932
H	1.810960067221	0.142805766392	2.129271353101	C	5.828643718263	-1.494219670209	-0.786237463875
C	2.867887618456	-2.911560037246	0.851529377424	H	6.391693291206	-2.405643492101	-1.001617586235
H	3.636197124845	-2.510241261126	0.171146658912	C	4.979407350234	-1.466800231766	0.309270351100
H	3.370323699290	-3.299848887934	1.751938636670	H	4.855415244883	-2.333512416579	0.960945230278
H	2.375768816912	-3.755029456548	0.340876696845	H	5.396318734435	1.662266897324	-2.058962324748
O	1.257041620288	-1.409985686224	-0.019429674566	C	1.325150037043	-0.040812233641	-0.894903995306

TS1'-i				TS1'-ii			
-4618.354134529219							

IM1'			
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N 3.454592550517	-0.051772985036	1.697843212230	-4618.382760806757
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C 0.285908148265	2.409416048756	0.000851236728	N 0.766231191491
C 1.820707236925	1.935497245633	1.891032281899	C 0.878202983106
C 3.305729635884	2.823156241580	-0.602246332230	C 1.087660151727
C 2.359609167105	3.673112726605	0.261557427928	C 0.041707072329
H 3.024914838030	-0.615715947052	2.423513113590	C 2.062828963590
H 2.128161887313	-0.650326368362	-0.722393921621	C 2.419818184493
H 0.189345243516	3.119598387031	-0.831613662456	C 2.627368444292
H -0.697975200747	2.374824118505	0.484117594748	C 1.568059283277
H 2.850342599831	2.628884064820	-1.587664878838	C 0.850234195550
H 4.238662557641	3.375233175607	-0.797467121042	H 3.793916234798
H 1.883353084757	4.453710125705	-0.347481449616	H 1.755492936523
H 2.936409380562	4.197399264764	1.035486807125	H -0.743788186021
C 2.433593364770	2.652857092518	3.115317936856	H -0.452253233370
H 2.735040571967	1.912060093673	3.869264222568	H 0.822937745789
H 3.327359950341	3.222840033771	2.831479132649	H 1.951205436830
H 1.691950935877	3.335873934965	3.552867970683	H -0.166327459863
C 0.726480799220	1.044698598995	2.499047234837	H 1.369417069994
O 0.923930152538	-0.093398116066	2.855547611642	C 3.108085607978
O -0.410775866140	1.683920101896	2.687731262931	H 4.028964085173
C -1.477465518564	0.955567711751	3.299542274193	H 3.370021531846
H -2.334858871633	1.636262613804	3.315184840443	H 2.728563275330
H -1.713017082232	0.056259411690	2.714236775714	C 1.954132305005
H -1.203818682137	0.665979204918	4.323896041491	O 2.624777092959
Z -1.047587687422	-0.189214959559	-1.194164356722	O 1.113188394380
S -1.184399160483	-2.969140755730	0.256742116376	C 0.972685869997
O -1.990041778184	-4.162052656205	0.066103644800	H 0.229901509577
O -1.460997544363	-2.118900901458	1.408993918256	H 0.613375346158
O -1.013179298622	-2.177612305275	-1.016953776923	H 1.931174709597
C 0.535360456285	-3.606034627003	0.527513805276	Z -0.973232840647
F 0.548102994385	-4.426810013978	1.566025212303	S -1.623531838259
F 0.959313148842	-4.259815430762	-0.543266606187	O -2.598618975220
F 1.371741917189	-2.602682454466	0.770233520963	O -1.297109415281
S -3.636628389781	1.658226442263	-1.102999668400	O -1.867613269881
O -5.057546488555	1.427631896968	-1.289438150758	C -0.043367517794
O -2.788458544124	0.591644601953	-1.749075209047	F 0.309013770527
O -3.164777869027	2.023201802556	0.229403082966	F -0.200051279095
C -3.242381402956	3.119841073022	-2.170965410522	F 0.936888648061
F -3.791066170892	4.211445668884	-1.661870663697	S -3.049712960995
F -1.927348601357	3.296566719211	-2.243682177702	O -2.521890370921
F -3.710426181499	2.932472811266	-3.394957934976	O -2.827891808955
C 5.640352313191	0.424469962282	-1.100578656542	O -4.367505527060
C 4.632429986912	0.561969149991	-0.129793810321	C -1.918619982863
C 6.473812631726	-0.681492602394	-1.041129156389	F -2.220633478967
H 7.263949599289	-0.805522937925	-1.785464940362	F -0.652660754662
C 4.496041306282	-0.422086122089	0.882109694354	F -2.032364515537
C 6.315471944591	-1.658145221804	-0.033231405463	C 3.881142550770
H 6.986466725411	-2.520546660599	-0.017126224239	C 4.478214598607
C 5.329950621789	-1.546993214688	0.936491718482	C 4.606447709944
H 5.206319303103	-2.302569839016	1.714948928838	H 4.148228193547
H 5.760160352305	1.176016971331	-1.884835194893	C 5.793221702366
C 1.545893293242	0.246669984337	-0.544549530999	C 5.870174060594
C 0.577390078187	1.043248086685	-0.570269529791	H 6.252333206493
C 2.891673167195	1.097687927581	1.212671218261	H 6.458029436868
C 3.597754754085	1.533934279060	0.096971115164	C 6.450982718888
			H 7.466097530929
			1.856189330453
			-1.595344494347

IM2'							
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N	1.233448009175	2.874096614003	1.124512984759	IM3'-i			
C	0.690426187015	2.092211355791	0.0085865953392	-4618.39539023313			
C	1.787843567223	1.984619985328	2.144478502013	N	3.848319040585	0.678290723202	-0.762079941765
C	3.419340760960	2.998893967101	-0.100013298028	N	1.166563040434	1.850228450684	1.945936202455
C	2.253551204642	3.777456399697	0.573213874361	C	1.020004295350	-0.455397743905	-0.981292117579
H	3.203520189557	-0.443682526784	2.686619982764	C	1.414861445804	0.552532929891	-0.185062452795
H	2.351942746192	-0.517016320948	-1.635514814820	C	0.470590062602	1.083699113284	0.891981333294
H	0.368047808519	2.803338043467	-0.764715688952	C	1.702047395793	1.269426631860	2.961449713055
H	-0.208496821402	1.542817386315	0.318824428233	C	2.690294843473	1.270197709775	-0.323585725107
H	3.502274849317	3.238000033031	-1.168893422259	C	2.908396463746	2.619295298564	-0.117640697718
H	4.383770758907	3.233467857220	0.372229300632	C	1.836638348737	3.581603998888	0.300703697715
H	1.746111431003	4.417832858953	-0.159610441800	C	1.296731213058	3.300223824567	1.709178879207
H	2.627756591799	4.442543604247	1.360021722513	H	3.958919588455	-0.314986018600	-0.930100544018
C	2.483337345458	2.752804976223	3.289294863605	H	1.734732775511	-0.738576825446	-1.767596483507
H	2.760472089842	2.053258029445	4.088301220269	H	-0.293420904430	1.749447292888	0.467234690506
H	3.395137753935	3.255905925361	2.943788210193	H	-0.069133140515	0.253799488154	1.367130086805
H	1.781412395899	3.500989193201	3.683200303083	H	1.008655805506	3.560943050535	-0.424433498121
C	0.748693844614	1.073552285915	2.824796406030	H	2.217331636421	4.612280280353	0.302904579960
O	1.090260904561	0.078862498618	3.419618540716	H	0.300705996884	3.743917503308	1.851107623554
O	-0.481038316839	1.514831527605	2.736178748029	H	1.971879774576	3.712589231914	2.463068875116
C	-1.504191952498	0.698517652656	3.315461536568	C	2.446234889544	1.967534013801	4.041924202509
H	-2.448035478785	1.218287895967	3.124022696105	H	3.373904636853	2.395612816466	3.628243055045
H	-1.508364869142	-0.289727618765	2.836126310892	H	1.844817487591	2.784643074222	4.465459950553
H	-1.338937814498	0.588460808421	4.396012582431	H	2.707579557291	1.263336253026	4.840030658049
Z	-0.328017153554	-0.613836954626	-1.672489265573	C	1.687060050026	-0.242896034175	3.053156881034
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O	-0.741952927382	-4.232430100011	0.743341981623	O	0.788060020006	-0.659722338273	3.906975952811
O	0.436988610050	-2.067524505402	1.144083876999	C	0.768785243728	-2.060439512189	4.224776490468
O	-0.607078804998	-2.546782661292	-1.046767840866	H	-0.231488317773	-2.273768233183	4.611464910350
C	1.585005609985	-3.845983936178	-0.406519262446	H	0.976176476887	-2.656760075287	3.331367061357
F	2.258915206107	-4.364562206496	0.612541488592	H	1.529550747365	-2.258878540839	4.992502800739
F	1.338028117286	-4.805961834066	-1.286820198032	Z	-0.832877527475	-1.137508617989	-1.017721626647
F	2.349582267217	-2.928829956040	-0.987928870981	S	-1.991216044159	-3.139427985381	1.195375504479
S	-3.134148503881	0.755403226225	-1.271366936243	O	-3.110152843767	-4.036334252685	1.427801997192
O	-2.205395759330	-0.096067139794	-2.092727808847	O	-1.712921239503	-2.116377941915	2.200162205815
O	-2.642656995387	0.988070330438	0.083967951234	O	-1.955459953100	-2.607452386979	-0.208926289845
O	-4.528856702618	0.384986489200	-1.436853995063	C	-0.492939427205	-4.230442729765	1.207169593670
C	-2.974279792337	2.392713396616	-2.123476574185	F	-0.350247164267	-4.803800180239	2.394551455307
F	-3.595085492979	3.330028907511	-1.423670835952	F	-0.599778865575	-5.177067970642	0.287126501636
F	-1.694064880938	2.728808351792	-2.244997087361	F	0.597814387467	-3.512385156855	0.948807430844
F	-3.509917252136	2.335516090973	-3.333691735295	S	-2.936042159051	1.226096863839	-1.595189601519
C	4.978532421911	0.265551601009	-1.407121097748	O	-2.395200608552	-0.147064363753	-1.855158153744
C	4.202558293339	0.483844740530	-0.277714573363	O	-2.627306655297	1.725875165688	-0.256458738898
C	5.824629233139	-0.847871708820	-1.422934505505	O	-4.295297492100	1.397019529843	-2.082043097349
H	6.444580336742	-1.038298130684	-2.301655688539	C	-1.900998309455	2.275013925256	-2.718736511505
C	4.293822164147	-0.403629580663	0.800202438015	F	-2.244007437191	3.549174663170	-2.587998669722
C	5.884942085152	-1.729574923284	-0.338489788903	F	-0.612558086712	2.152580296088	-2.414455213143
H	6.549519665261	-2.594898776725	-0.383628745574	F	-2.071521149317	1.913495935374	-3.982013950666
C	5.111328076439	-1.521422291150	0.805142846641	C	4.285037906696	2.866513914157	-0.446249661596
H	5.144487666724	-2.202451893740	1.656796088564	C	4.840576123263	1.619916643194	-0.842506679040
H	4.922379467550	0.938398129074	-2.265114588060	C	5.101494393724	4.013224767529	-0.456885902910
C	2.800971450884	1.127064353453	1.441145341853	H	4.696196246730	4.985595206659	-0.165148310317
C	3.141251008554	1.492382902763	0.038718798627	C	6.181263077641	1.491981992213	-1.229168860460
C	1.483781445734	0.077734743099	-1.326750762771	C	6.427457205263	3.888728850208	-0.844181358362
				H	6.591369691207	0.524682669167	-1.527765728186
				H	7.072561831402	4.770826939579	-0.857330656485

C	6.962425454495	2.638808960822	-1.225099242775	C	-2.893554414668	-4.879303968462	0.036372124315				
H	8.011436440502	2.573662402959	-1.524495827452	H	-2.038679706166	-5.239739045253	0.627867329848				
IM3'-ii											
	-4851.874587727582			H	-3.805160049667	-5.380323670228	0.394027098815				
N	3.185092043667	-0.805578168622	-2.897649565066	H	-2.737672590065	-5.166512283445	-1.016181191676				
N	1.305251794855	2.652682428962	-1.402929680147	C	4.489768023914	1.314141051034	-5.458390646898				
C	1.185746992217	0.177430664294	-1.773601498525	C	3.726609213505	0.768575832108	-4.409001620171				
C	0.425613533988	1.480495056246	-1.616261654094	C	5.565733944562	0.590887531677	-5.951165407998				
C	1.614332616300	3.049498855167	-0.217955929656	H	6.166480406109	1.001868626096	-6.766252793612				
C	2.280091409936	0.220516102786	-2.755118817969	C	4.076736662339	-0.505138719725	-3.890953374641				
C	2.579076559081	1.217847427947	-3.668808783625	C	5.900204305959	-0.672996802781	-5.417818476546				
C	1.843877726487	2.513782120658	-3.851247718191	H	6.754446985344	-1.217240471348	-5.828085352288				
C	1.809878089151	3.373719581483	-2.594894518994	C	5.165229407322	-1.236897707736	-4.384907178968				
H	3.214637811131	-1.635225750382	-2.317641110979	H	5.420149227086	-2.214717663794	-3.970491866470				
H	1.386144533064	-1.827065375485	-1.299333699102	H	4.23823707958	2.291003266022	-5.879649311263				
H	-0.175922859457	1.708641928910	-2.504631377312	C	0.815248646548	-0.912430251762	-1.072782618895				
H	-0.270675414913	1.419488558573	-0.772973004780	H	-1.586085480159	-3.054391690214	-1.170377172178				
H	0.825293210611	2.349240149486	-4.235488668550	IM4'							
H	2.350894582877	3.121065733024	-4.614715077142		-918.112586098048						
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H	2.824074120482	3.718976640024	-2.361467913073	N	0.688471653000	1.736908233000	-2.366693452000				
C	2.460408477366	4.237680545395	0.057204922897	C	2.172569065000	-1.086527320000	-0.868090580000				
H	3.487662237576	4.045306375245	-0.295496470731	C	1.923871504000	-0.382292598000	-1.980864843000				
H	2.076014363870	5.118541540245	-0.477889404578	C	0.576539063000	0.277137049000	-2.153503570000				
H	2.490791761503	4.449450396499	1.132326095335	C	0.647307786000	2.578114759000	-1.391993136000				
C	1.186560742370	2.237986039513	0.988336061653	C	2.892623397000	-0.259536488000	-3.080614382000				
O	1.851322544146	1.310997387645	1.365162735191	C	3.090117828000	0.761012765000	-3.995645022000				
O	0.119750010261	2.737730433719	1.552663732363	C	2.425606848000	2.102749154000	-4.101220292000				
C	-0.327343418919	2.131286246601	2.777990429220	C	0.943890536000	2.159305218000	-3.756400420000				
H	0.389163999483	2.364862313578	3.577542727675	H	3.829830588000	-2.151057569000	-2.830901403000				
H	-1.301427724026	2.582091215634	2.988495611265	H	3.127141629000	-1.593816409000	-0.704563432000				
H	-0.427686993937	1.046449496235	2.658377929720	H	0.056777384000	-0.126062284000	-3.032284633000				
S	0.213366142608	-2.418766218933	3.027454240456	H	-0.057714756000	0.091242532000	-1.280674398000				
O	0.414859320733	-3.636799035984	2.246614506903	H	2.512432830000	2.463778009000	-5.136860618000				
O	-0.302337689647	-2.559544709074	4.381235877279	H	2.964392793000	2.839433604000	-3.481031740000				
O	-0.474911750874	-1.328827348120	2.260540595064	H	0.359490150000	1.490003758000	-4.400080261000				
C	1.916454315133	-1.724403668538	3.238318319093	H	0.556899693000	3.174855452000	-3.889864937000				
F	2.660250596621	-2.567291549997	3.944643425259	C	0.806341300000	4.045994846000	-1.552446881000				
F	2.490283565759	-1.546102901793	2.055794391568	H	1.746776031000	4.275937899000	-2.074328286000				
F	1.872710346857	-0.564102522564	3.877252796057	H	-0.026042989000	4.446345182000	-2.153467093000				
S	-3.239467867158	1.166723020707	0.411807871588	H	0.805125083000	4.542786065000	-0.575580016000				
O	-4.350434617895	0.303611524083	0.798614359762	C	0.368399076000	2.077511141000	0.012473297000				
O	-1.893463210592	0.552612161960	0.604859410238	O	-0.751376136000	1.913497134000	0.415215855000				
O	-3.287875578074	2.552794752526	0.858469581604	O	1.484274397000	1.929425319000	0.679498073000				
C	-3.356194555424	1.276801609178	-1.443744264769	C	1.382975657000	1.502689054000	2.046237642000				
F	-2.672314879685	2.325146083243	-1.888027738894	H	0.825002238000	0.559068626000	2.109766117000				
F	-2.856113455677	0.181444297374	-2.010578302329	H	2.411620657000	1.363545884000	2.392523368000				
F	-4.619016117469	1.408127521096	-1.817088582551	H	0.879810864000	2.276153404000	2.642011854000				
C	-3.025065075092	-3.366619970972	0.171140705530	H	1.417600270000	-1.181559385000	-0.083479337000				
C	-4.139065318261	-2.813039886165	-0.710266380020	C	4.881704443000	0.960880976000	-5.891076815000				
H	-5.104247901793	-3.269284789452	-0.444114055787	C	4.205927771000	0.359952440000	-4.812268132000				
H	-4.224957453917	-1.726448106274	-0.576391492126	C	5.937238797000	0.282113410000	-6.479432458000				
H	-3.942356027614	-3.029393583965	-1.772585467305	H	6.470271210000	0.733454035000	-7.319673203000				
C	-3.214536601250	-2.955306907393	1.622691758745	C	4.629275882000	-0.910179413000	-4.350809722000				
H	-4.176596990082	-3.338372170135	1.992958643251	C	6.336954258000	-0.989488480000	-6.011353781000				
H	-2.415175628100	-3.364708417415	2.255409153239	H	7.172912445000	-1.499101636000	-6.496958282000				
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C	5.692909413000	-1.602667691000	-4.947546111000	C	5.662174072795	-1.046245600521	0.868063223313
H	6.002280306000	-2.584456623000	-4.582633275000	H	5.961259917693	-1.514461069169	1.808274116666
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N	1.280105859744	2.799919916697	1.163660965354	N	-1.293921855819	2.812392459051	-1.392158580496
C	1.351829463601	-0.012837763745	-1.280464623466	C	0.823502692122	1.920204273135	-0.443883514010
C	1.686654051467	1.053575481168	-0.543817090620	C	-0.287674974777	1.744460146831	-1.480148738539
C	0.689686531235	2.043846183032	0.051015911041	C	-1.835003554421	2.904526908161	-0.012864469015
C	1.876288805688	1.890014284739	2.160043103479	C	-0.668254080631	3.233945698497	0.890531177852
C	2.984230297726	1.131770451828	1.457863336816	C	0.680247995649	3.301459007614	0.199712070968
C	3.085284723017	1.397653515993	-0.033189659446	C	0.580209123722	4.393214238384	-0.892577503186
C	3.362582585768	2.910271159605	-0.214973783699	C	-0.642125525426	4.064262304961	-1.791884222136
C	2.291066147819	3.694777284079	0.590289671324	H	2.388282871804	1.241271517670	0.712106527604
H	2.187465578093	-0.640327079092	-1.622585755352	H	0.128215681515	1.776359229641	-2.499890065327
H	0.384599735249	2.777899531909	-0.710086805665	H	-0.762004190873	0.756101227511	-1.377545247014
H	-0.231785077283	1.536575451509	0.368602909706	H	1.517458206557	4.412337294992	-1.468668897862
H	3.328277101451	3.154121019583	-1.287367385636	H	0.465619054237	5.377540520914	-0.414090710662
H	4.376690016106	3.139927947581	0.144263234588	H	-0.334327320318	3.948542547981	-2.840692129573
H	1.765770367556	4.410705231676	-0.057114734639	H	-1.375160348991	4.880610725492	-1.771880570955
H	2.756945261989	4.283066990609	1.390745942705	C	-2.941736519728	3.952964399649	0.115078708708
C	2.412453524700	2.637272850192	3.392282247810	H	-3.393797551197	3.888526973467	1.114891965168
H	2.753924873246	1.909574344300	4.140920312842	H	-2.548361266883	4.970716027866	-0.006629862345
H	3.268930640581	3.274176816219	3.134316709670	H	-3.716921785889	3.769859611040	-0.641356152261
H	1.618236242481	3.261010448449	3.826466313368	C	-2.458562166781	1.528177555058	0.299678799288
C	0.832644379866	0.900946065579	2.715230069957	O	-3.522499549797	1.173407292700	-0.145985957787
O	1.109736167267	-0.195741351122	3.129986477368	O	-1.688330377750	0.780680901530	1.065184426563
O	-0.386508762320	1.414538143390	2.758376826719	C	-2.082747833599	-0.568718860414	1.298618842924
C	-1.418586045873	0.556292825443	3.242669436982	H	-2.345273550707	-1.062514710916	0.356355339591
H	-2.355694648429	1.110253352097	3.124332760262	H	-1.214332032256	-1.057335061465	1.750390494971
H	-1.450923625633	-0.374232388882	2.658946426104	H	-2.940186577690	-0.600072905492	1.986931376020
H	-1.253043693796	0.317369811766	4.303162750092	S	1.822602949324	-1.373084467970	2.513681964593
Z	-0.497639830400	-0.638046179782	-1.563799798355	O	0.902406780459	-0.330386582551	2.958172966507
S	-0.966998183179	-3.368564949331	0.212422581657	O	3.249388347658	-1.067257178877	2.584603389931
O	-1.390068948342	-4.745198730015	-0.007142143746	O	1.419324458484	-2.052242318849	1.240051115159
O	-1.461272332680	-2.697780378836	1.410219589365	C	1.567483721350	-2.746923402374	3.726185600664
O	-1.064114602015	-2.540034634092	-1.029011182211	F	1.872499854782	-2.329190622656	4.949002715049
C	0.867957518978	-3.490113493934	0.471508646998	F	0.301340302393	-3.143702011823	3.719532172683
F	1.130679839729	-4.408896726492	1.392537379037	F	2.338838996975	-3.785310413672	3.430687819115
F	1.474229736675	-3.838660516153	-0.658306861278	S	-0.813964000480	-3.205864707526	-1.195420697048
F	1.367341580470	-2.331703826319	0.877273621223	O	0.152289768863	-4.272536575712	-1.438324178142
S	-3.283507680000	0.866828284723	-1.258650247872	O	-0.218751978147	-1.831543245846	-1.234072758535
O	-2.357983567381	-0.017818490964	-2.044850240494	O	-1.765761814276	-3.416063064630	-0.112532682179
O	-2.843470582850	1.080492231894	0.117262331348	C	-1.862723898246	-3.145350811584	-2.719948918424
O	-4.686090170013	0.558412393307	-1.484699124400	F	-2.769584068248	-2.182458557564	-2.617728091786
C	-3.023292696396	2.501917061823	-2.091432950701	F	-1.117537978533	-2.911254306894	-3.794376066514
F	-3.629719938776	3.462503648959	-1.409111345434	F	-2.487710579583	-4.303226606932	-2.883652790780
F	-1.726652416841	2.785305825242	-2.163360404699	C	2.849661868087	-1.470989172726	-3.411635086781
F	-3.515639737975	2.477412924325	-3.322056999555	C	1.752683513846	-0.470967549140	-3.767257732749
C	4.862313104493	0.177272993159	-1.560100078056	H	1.558113343119	-0.478638664357	-4.850329257530
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C	5.912175958153	-0.749394556469	-1.534397482583	H	2.051962901426	0.549345300183	-3.479122952656
H	6.428809042270	-1.006539770347	-2.462372778276	C	2.403168275876	-2.901838365810	-3.663501986981
C	4.618772265643	-0.127461042280	0.834874621575	H	2.128236067763	-3.035974148995	-4.719864321408
C	6.304485242423	-1.352526797093	-0.335737505755	H	3.211974052331	-3.607613326660	-3.420626276525
H	7.122603724808	-2.077147649583	-0.339829570436	H	1.533047179688	-3.153987185301	-3.043819876046

C	4.145151414168	-1.156480366309	-4.150850042995	C	2.474691543992	3.203541748113	4.340500691886
H	4.946818790266	-1.841146875221	-3.834994250283	H	2.807771506508	3.148850550320	5.379927277052
H	4.003195514574	-1.265997302641	-5.235984704371		TS2'		
H	4.469708613780	-0.121395137795	-3.954483420571		-4618.36321816893		
C	1.539910116160	3.628424368005	1.380694674962	N	3.236221602121	0.013275621170	1.620876179615
C	0.684710246969	3.716784525438	2.494453121445	N	1.225055930963	3.061880486492	1.107808758115
C	2.903783615157	3.838248397455	1.521665496532	C	0.655802006631	2.230714425276	0.048450317454
H	3.575993852988	3.769760739749	0.662627041141	C	1.782102954791	2.118447185246	2.076307575603
C	1.177493240175	4.005413059515	3.762179607379	C	3.304506194068	3.173096175911	-0.299410609040
C	3.407286615273	4.128642534226	2.796178974012	C	2.245333975212	3.941874107338	0.529999917868
H	0.503379260776	4.063939987132	4.619519862614	H	2.760883086621	-0.638478986588	2.238659892838
H	4.479586561592	4.289611416007	2.931223712379	H	2.324682736187	-0.732976990683	-0.892930753958
C	2.553948943224	4.209060383447	3.900393427328	H	0.537772821310	2.821300933309	-0.868584466441
H	2.969509484219	4.430765914546	4.886604408592	H	-0.339745381309	1.850636124507	0.322856627364
C	1.674981599456	0.954623808216	-0.075430767595	H	3.085948727842	3.223287190459	-1.376230210409
Zn	1.511002060642	-0.968844883280	-0.575738231772	H	4.305309411070	3.612739876086	-0.168150071973
O	3.119310733455	-1.387201144707	-1.987761315787	H	1.732262565976	4.671925400659	-0.109752256405
H	3.669226316539	-0.606216098753	-1.828147670170	H	2.722563000682	4.514428074408	1.333754634521
3a'				C	2.615893391603	2.760251284066	3.188038707912
	-917.645848363606			H	2.898999503693	1.994508772063	3.922229816918
N	-0.600640135499	3.089332133596	2.214490092352	H	3.538956764683	3.204684602315	2.794164009739
N	-0.946958728153	3.522301985977	-1.395779217020	H	2.023639791486	3.537446139703	3.691649010263
C	2.048768759864	1.408468730254	-0.654229334533	C	0.692805180880	1.285201874610	2.768978689924
C	1.098476012217	2.342482008199	-0.656800746503	O	0.926319504597	0.191235271883	3.229019013508
C	0.014237080953	2.467508079614	-1.725526536293	O	-0.471539356844	1.889498862636	2.849167129366
C	-1.598727706197	3.233884718073	-0.101196302081	C	-1.535956191078	1.155588262250	3.458380413317
C	-0.505902176214	3.201265209858	0.943666753778	H	-2.433707005013	1.770976328595	3.339595454556
C	0.898452503988	3.408505473690	0.404038781055	H	-1.668807765600	0.188386484446	2.955092672526
C	0.894229614588	4.798590410144	-0.287138728043	H	-1.325321480257	0.990943309241	4.524509050016
C	-0.223460982335	4.797266653492	-1.364653373201	Z	-0.263219408239	-0.726395087241	-1.598498798721
H	2.799823415440	1.346648080408	0.137318507590	S	-0.035864354177	-3.328201409610	0.180255674628
H	0.465382246998	2.708342702669	-2.700320075435	O	-0.832748467553	-4.451196836786	0.646999132709
H	-0.506456374154	1.505990305810	-1.858151686543	O	0.473120710088	-2.389934384485	1.176727925588
H	1.885614318080	4.983582349286	-0.725507791197	O	-0.633489043758	-2.652690713611	-1.021475552660
H	0.716872533839	5.573487519410	0.473222051626	C	1.488748216347	-4.106872073802	-0.533175196246
H	0.202463333120	4.951365234738	-2.365800459063	F	2.197807271137	-4.675821231952	0.432287288510
H	-0.932733352239	5.617850959102	-1.198458053619	F	1.166259782129	-5.029877187306	-1.427588059176
C	-2.670002498349	4.270456758827	0.266960878424	F	2.251290201923	-3.194314197917	-1.129807142327
H	-3.204009001262	3.939191529430	1.168752335241	S	-3.062793281073	0.726905998934	-1.257746931268
H	-2.218853587542	5.246307467270	0.489531540327	O	-2.096302252819	-0.082402669717	-2.081149611850
H	-3.386863306152	4.382377350498	-0.557639528578	O	-2.600246628919	0.944510387146	0.110564463108
C	-2.308544694812	1.870812288571	-0.190665270936	O	-4.444105289893	0.323618908272	-1.454179319565
O	-2.186214570248	0.975378382394	0.606453608337	C	-2.932829875028	2.385815051599	-2.073768854882
O	-3.105512570038	1.813654019778	-1.246791615128	F	-3.579574364021	3.292207600347	-1.357089739786
C	-3.808305772505	0.592870334799	-1.458230358649	F	-1.660151731105	2.753783897384	-2.177739955968
H	-4.371594227239	0.723813644152	-2.388685260539	F	-3.458867695111	2.343776628790	-3.288433906441
H	-3.103819319941	-0.244895731336	-1.561186697850	C	5.344117157433	0.667586069615	-1.216955821379
H	-4.497787424532	0.388741607225	-0.626648715978	C	4.381477804241	0.747695237752	-0.200069452208
H	2.100943381718	0.666296529614	-1.457354586080	C	6.121847744957	-0.475739909690	-1.29321824352
C	1.670220179824	3.339537876366	1.686535337814	H	6.879808527854	-0.568491365870	-2.073643124214
C	0.725020433983	3.165249638742	2.714095143214	C	4.221610788591	-0.312740069676	0.723031340569
C	3.020607564930	3.459886597510	1.982985487761	C	5.937601394751	-1.536072749233	-0.378448396591
H	3.762133835766	3.608235232421	1.194108092450	H	6.556411936159	-2.431351221416	-0.475837005093
C	1.111798684676	3.093755769666	4.047523710153	C	4.993437874458	-1.479411209980	0.634103695886
C	3.417026386314	3.385455978588	3.324441968244	H	4.846119946087	-2.305959019556	1.330691270298
H	0.367919579787	2.958934569917	4.835586475518	H	5.465759164041	1.483094386314	-1.933044771432
H	4.475970296825	3.473162513810	3.579066675452	C	2.634158246182	1.185775302522	1.212841936247

C	3.385091811475	1.736650563250	0.123339367168	H	6.470805956550	0.020787327319	-0.417828850617
C	1.456915728995	-0.059202606435	-0.865681167646	H	7.106710878696	4.284884008040	-0.811017876353
C	1.594376134483	1.056720496718	-0.158866611744	C	6.903409814908	2.129803998218	-0.634178315335
H							
TS3'							
-4618.372394002							
N	3.693964713272	0.438047035597	0.024598218593	-4851.830261777723			
N	0.968879042580	2.057982909194	1.981946621121	N	3.405590834304	-0.973593773244	-2.052834535106
C	0.836738086204	-0.408472340603	-0.766389908068	N	0.588715539837	1.849516440997	-2.432297464010
C	1.165283432089	0.558290235017	0.095172802151	C	0.942506741448	-0.586784480001	-1.966385546191
C	0.181486147929	1.217232448629	1.071385778276	C	-0.055951053873	0.529231664866	-2.247452709253
C	2.181122847246	1.477611538275	2.232099606493	C	0.917793930654	2.605579896658	-1.442197694699
C	2.528153111871	1.144704995054	0.272746683904	C	2.269630498251	-0.391244775753	-2.560172849267
C	2.820555710223	2.532434972204	0.060975084340	C	2.588486128053	0.328697851501	-3.698830083112
C	1.794197983905	3.582009161514	0.211845759506	C	1.593158400470	1.052016367839	-4.557161841454
C	1.029314081647	3.444417103421	1.582140003391	C	0.898408718834	2.210687059370	-3.829944937469
H	3.786892666729	-0.561099101670	0.171832038797	H	3.448231732789	-1.492028165231	-1.182835102064
H	1.651201085031	-0.772401871166	-1.408894776113	H	1.383542748963	-2.421176406203	-1.120929558815
H	-0.563168940881	1.837937627824	0.557065241105	H	-0.616265213840	0.334821109969	-3.171912302672
H	-0.367350951737	0.446309687456	1.627628916785	H	-0.797956677961	0.614518313348	-1.445825360920
H	1.045617645816	3.461426815559	-0.586470449483	H	0.840742655281	0.346044371140	-4.941243537272
H	2.229100995641	4.585945046706	0.122429285684	H	2.086373638331	1.480806221608	-5.440293858282
H	0.009736366182	3.828614491697	1.468307736497	H	-0.050657836555	2.475114199434	-4.318655396224
H	1.524752738626	4.034685806037	2.360288547615	H	1.544573405064	3.091691935019	-3.824600044614
C	3.301820917395	2.211545950696	2.914179713987	C	1.556440750699	3.939311820276	-1.588310714183
H	4.241528690862	1.674493897388	2.721584377818	H	2.557177109733	3.821707597895	-2.035028156759
H	3.422619133029	3.251331601588	2.595445939062	H	0.956861063107	4.586142064755	-2.245335697616
H	3.122635747137	2.189223747499	4.001868431402	H	1.661784041563	4.420266311525	-0.609873368437
C	2.173322292199	0.021913634726	2.722340101900	C	0.779036401241	2.094303041319	-0.019811147573
O	3.101669280384	-0.730247388734	2.570081147430	O	1.453025794702	1.176792924654	0.366969292646
O	1.086693592432	-0.256468752541	3.410196787760	O	-0.028672224177	2.834789334219	0.687881381832
C	1.002854476404	-1.562848709600	3.987751533057	C	-0.114785309757	2.546796920549	2.093629704646
H	0.013538638716	-1.625146663886	4.450685835822	H	0.833047645410	2.822221765059	2.575971873330
H	1.107443832818	-2.330882093228	3.211705591586	H	-0.933188866789	3.163758236787	2.473707166156
H	1.787897765133	-1.689469234329	4.746382306423	H	-0.329401326966	1.484610869692	2.255213275737
Z	-1.027411006094	-1.054140020125	-0.997210410884	S	0.658730045609	-2.149837677704	3.135710363503
S	-1.878804098802	-3.282886061444	1.068029620793	O	0.824895833489	-3.481238008368	2.565393170952
O	-2.904127700789	-4.283080566978	1.315259581977	O	0.474138638178	-2.031261456258	4.572863091526
O	-1.675649509633	-2.244994351216	2.075032573471	O	-0.314408905510	-1.294405547013	2.367525017665
O	-1.925042717194	-2.741371865461	-0.332794414342	C	2.270736123152	-1.301047212076	2.799901962685
C	-0.289722814196	-4.2366668683244	1.054074876928	F	3.238623069275	-1.902800957387	3.479333307678
F	-0.090475469422	-4.803486155747	2.236160260615	F	2.565383471954	-1.362066030153	1.506777970957
F	-0.324875643750	-5.182379923027	0.126673508376	F	2.220880351375	-0.030061238919	3.170336044077
F	0.735154908068	-3.429253804778	0.794676692670	S	-3.279663568914	0.861779846017	1.171481913317
S	-3.146872861321	1.288737756296	-1.603854896240	O	-4.347642921458	-0.095661199509	0.912547860430
O	-2.596135949691	-0.090284756189	-1.820848217245	O	-1.947209194196	0.443277480985	0.613250817900
O	-2.900679603359	1.809264203696	-0.261717504421	O	-3.193516814383	1.424088153441	2.510617720739
O	-4.481471223005	1.448602986746	-2.157900959017	C	-3.670657176931	2.303116494526	0.069967772066
C	-2.060160286155	2.316234620098	-2.698310691967	F	-2.901412549352	3.341761551823	0.358484921236
F	-2.385266942496	3.596055994658	-2.584705009222	F	-3.481970714585	1.979571187110	-1.205185273822
F	-0.783382062682	2.173414140712	-2.351333684172	F	-4.937138269335	2.651527580057	0.236403295968
F	-2.194374553545	1.950759536396	-3.964550617181	C	-2.862689488801	-2.913317815932	-1.404507013885
C	4.203849443134	2.627605563403	-0.204780053397	C	-3.149219428091	-1.592465392165	-2.124404202748
C	4.715121449042	1.298443152173	-0.212082053819	H	-4.086261886803	-1.644368327077	-2.700500839819
C	5.074734272497	3.721999210741	-0.422920806237	H	-3.248383336709	-0.774570672279	-1.397402534584
H	4.687484773313	4.743214252662	-0.425369701170	H	-2.334481525459	-1.348452952310	-2.825235854417
C	6.082985242222	1.040617481581	-0.421543980948	C	-3.976511929618	-3.233603684767	-0.409771677695
C	6.409739223333	3.462785262737	-0.636405852115	H	-4.947858833319	-3.342718312187	-0.917278990133

H	-3.755408406286	-4.173744363637	0.119576055006	S	-0.915924223164	-3.302798892383	-1.253141918419
H	-4.067946139603	-2.425839587385	0.331539800229	O	0.122213104333	-4.301213899145	-1.480854369507
C	-2.706608580694	-4.045633924204	-2.421175192505	O	-0.390698579080	-1.895898003989	-1.200250845284
H	-2.457406137202	-4.987723236090	-1.908552960795	O	-1.908220007955	-3.594840361561	-0.228094424013
H	-3.633932814812	-4.198577502612	-2.995052820138	C	-1.886166585968	-3.227905652324	-2.827009893833
H	-1.895967596895	-3.817416934361	-3.131738588414	F	-2.825398629569	-2.296400169457	-2.74333348571
C	4.915660809409	0.650951301443	-4.856611570609	F	-1.093346311380	-2.942269682672	-3.852401785094
C	4.003160229548	0.178789546529	-3.893296125435	F	-2.463494950160	-4.399583972591	-3.050866196929
C	6.253966463492	0.312650556574	-4.732751020230	C	2.765194155239	-1.183636542858	-3.330833486652
H	6.974427174871	0.672395483883	-5.471334568900	C	1.564769554976	-0.440033292284	-3.924656212944
C	4.477824345226	-0.638892458679	-2.833491710706	H	1.458431675377	-0.642735569093	-5.001653977002
C	6.707321166805	-0.493317101805	-3.664230071656	H	0.633140740410	-0.752080856579	-3.428288217530
H	7.769531483176	-0.740093339188	-3.593723002025	H	1.682368915967	0.647438476786	-3.794541421640
C	5.832152726596	-0.978101224889	-2.704538705984	C	2.600915074844	-2.690229670635	-3.525347234697
H	6.178503047314	-1.604684455231	-1.879779979855	H	2.543230575218	-2.953436756587	-4.593179530327
H	4.573925764736	1.275121801618	-5.686348129012	H	3.453827221198	-3.227282723470	-3.081066482958
C	0.589152697807	-1.669320303625	-1.242931078924	H	1.683263605570	-3.044773433641	-3.033386822781
Z	-0.935027876541	-1.309445789537	0.463995966158	C	4.061388810269	-0.696152869715	-3.980495534602
O	-1.647255426716	-2.814102700032	-0.678732608648	H	4.927674294684	-1.209593710409	-3.534787040356
H	-0.639282058446	-2.291960394892	-1.174895694043	H	4.066419078969	-0.884650731451	-5.065720059887
				H	4.188037777638	0.386410366836	-3.819428227059
TS5'				C	1.655168745043	3.400757446391	1.418355784273
-4851.359597775067				C	0.806052258784	3.421800883181	2.539027623734
N	-0.549002232411	3.195335169979	2.186424488073	C	3.018483357606	3.612501833069	1.560928126755
N	-1.196545847810	2.795851394874	-1.387734060790	H	3.684884346915	3.603211903774	0.694977967143
C	0.970561906675	1.880059990589	-0.587618260503	C	1.304805659098	3.638250447396	3.818214557057
C	-0.187350462225	1.750880815136	-1.579605197648	C	3.527855295431	3.829877660404	2.847253811074
C	-1.727664066887	2.766212936643	-0.003319619120	H	0.635905433635	3.644379203248	4.681404999907
C	-0.557779787816	3.020430533208	0.919036331517	H	4.599898581501	3.989957722159	2.984507388267
C	0.784450426607	3.153947089271	0.226493355148	C	2.681045495427	3.840347748192	3.959161020865
C	0.649472031685	4.351888658699	-0.752992219665	H	3.102010546154	4.007040735544	4.953830182412
C	-0.557988180648	4.081233261853	-1.689325383089	C	1.970474417595	0.990455712272	-0.446044888923
H	2.694780750833	1.228496863057	0.346995316542	Zn	1.333480561350	-1.090036483842	-0.574182837359
H	0.191166615363	1.836695165333	-2.609291562137	O	2.853663936276	-0.933447615293	-1.937422047254
H	-0.653794388286	0.758078632798	-1.509887069656	H	2.513902671582	0.143291028422	-1.446903321497
H	1.588975800471	4.461545096476	-1.314188262572				
H	0.502329465715	5.272529058765	-0.169334443494				
H	-0.235304003679	4.043117500522	-2.739079620330				
H	-1.299229063912	4.887032214797	-1.620506744879				
C	-2.833911849101	3.800686852146	0.220271837840				
H	-3.279224394934	3.652701326389	1.214178624667				
H	-2.440005115104	4.824648463484	0.183129881411				
H	-3.613283898029	3.680801718168	-0.544261789772				
C	-2.359820841946	1.376310445105	0.216263913953				
O	-3.414043185077	1.049252185306	-0.269144604188				
O	-1.621809373075	0.597347062247	0.984924984449				
C	-2.117702565324	-0.705308121801	1.286234886213				
H	-2.393991121152	-1.238018809813	0.370039816178				
H	-1.299367877305	-1.225499814474	1.793191362820				
H	-2.989353803773	-0.628659062622	1.952473272103				
S	1.808076784429	-1.105876520477	2.523882301808				
O	0.960696380117	-0.000413873594	2.951220711632				
O	3.247838113875	-0.879123179219	2.489504261111				
O	1.289694613827	-1.828931556217	1.307530632214				
C	1.552498416254	-2.416467389314	3.804985595740				
F	1.962273910026	-1.968046547093	4.984265385549				
F	0.267797293133	-2.733152418272	3.894806405329				
F	2.240933466475	-3.507696715529	3.502463394864				

¹H and ¹³C NMR spectra of 1–4 and 18

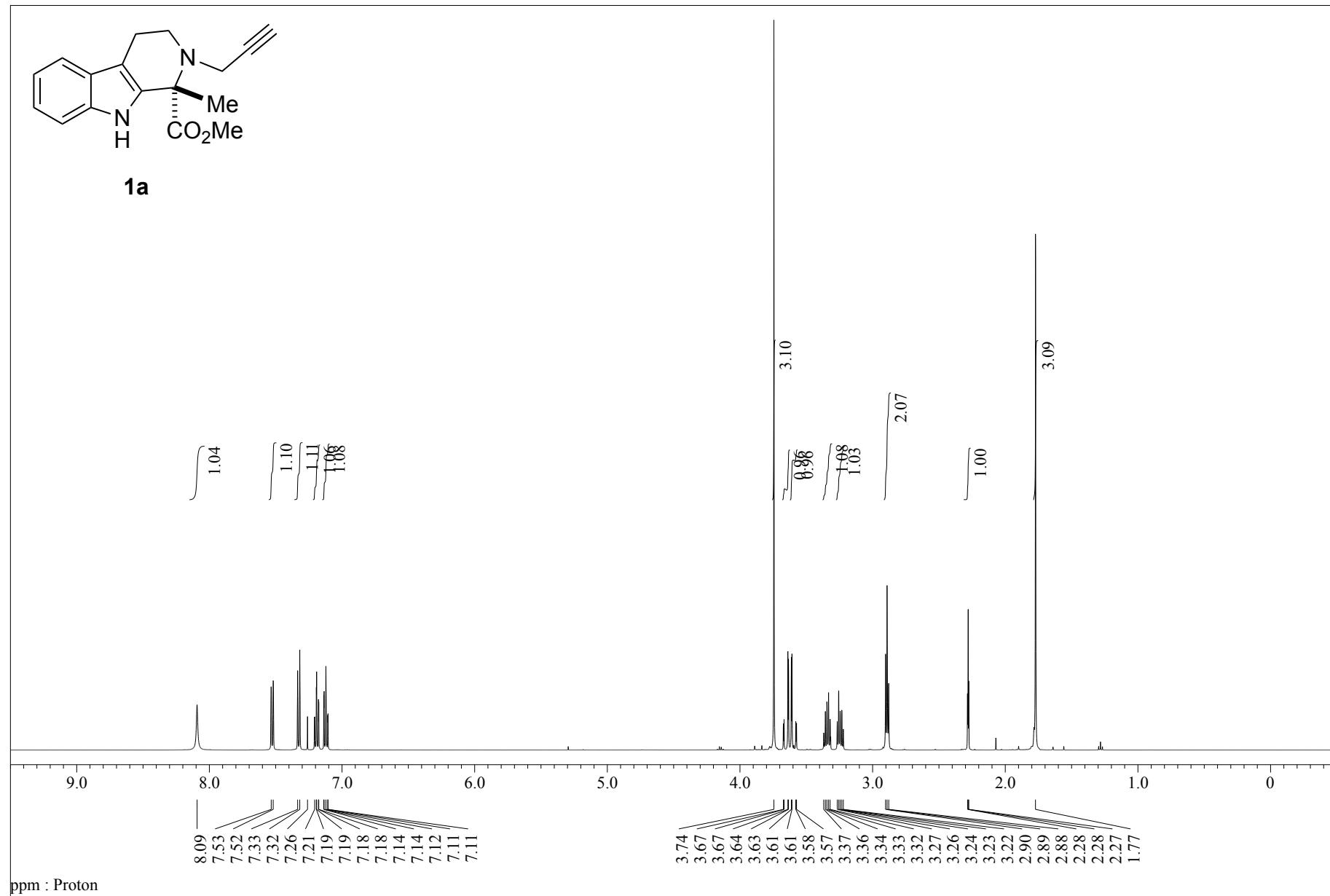


Figure S7. ¹H NMR spectrum (500 MHz, CDCl₃) of **1a**.

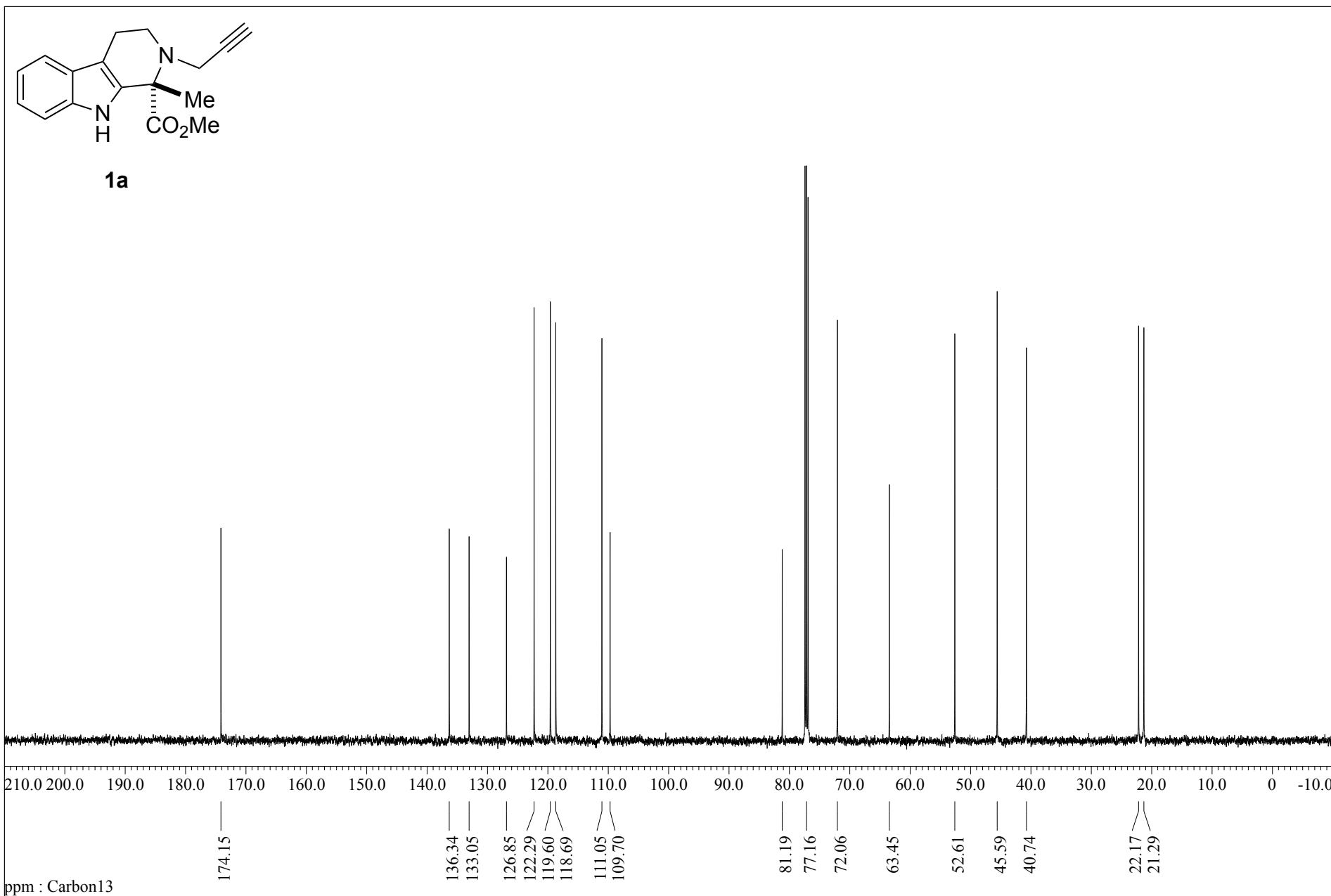


Figure S8. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **1a**.

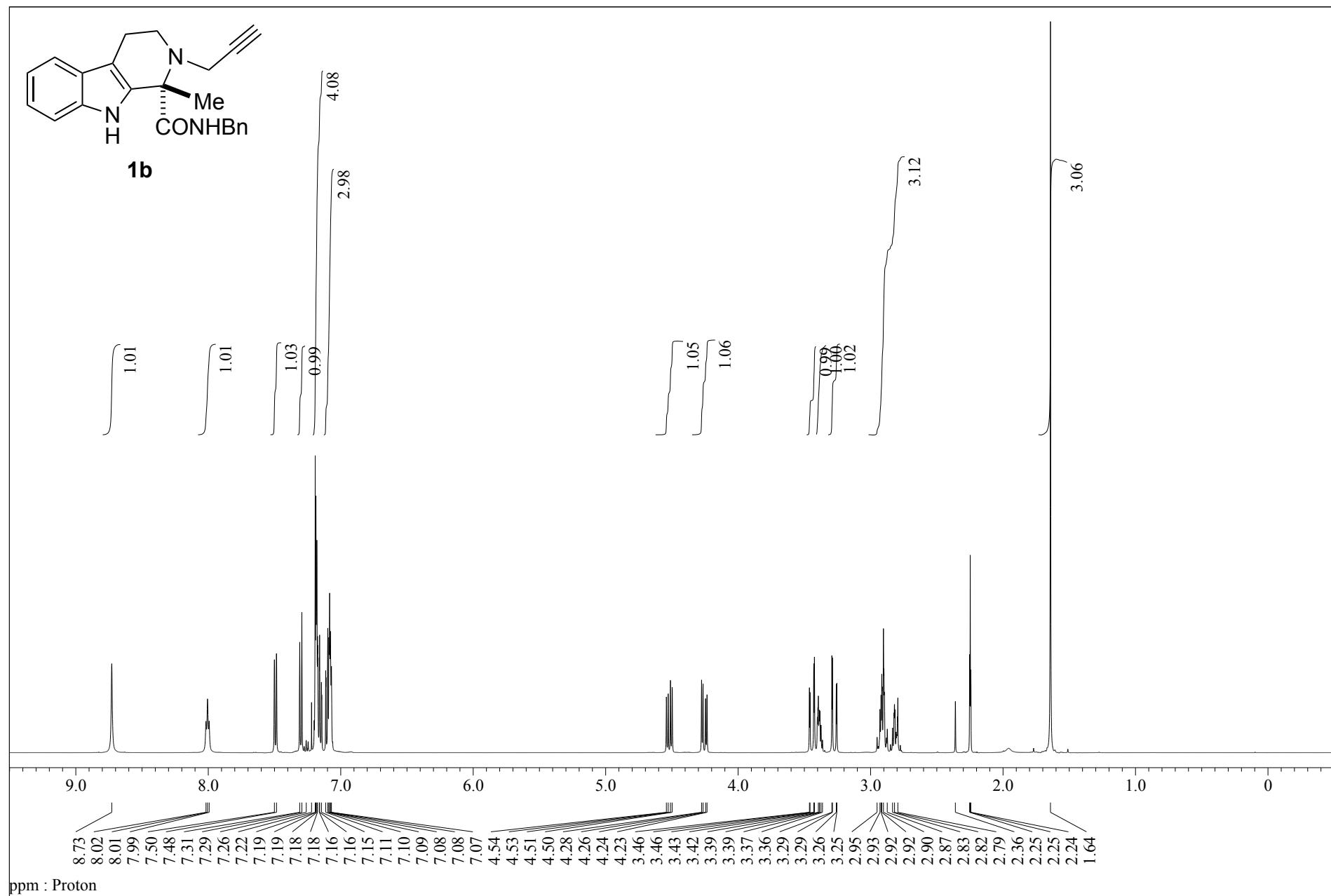


Figure S9. ^1H NMR spectrum (500 MHz, CDCl_3) of **1b**.

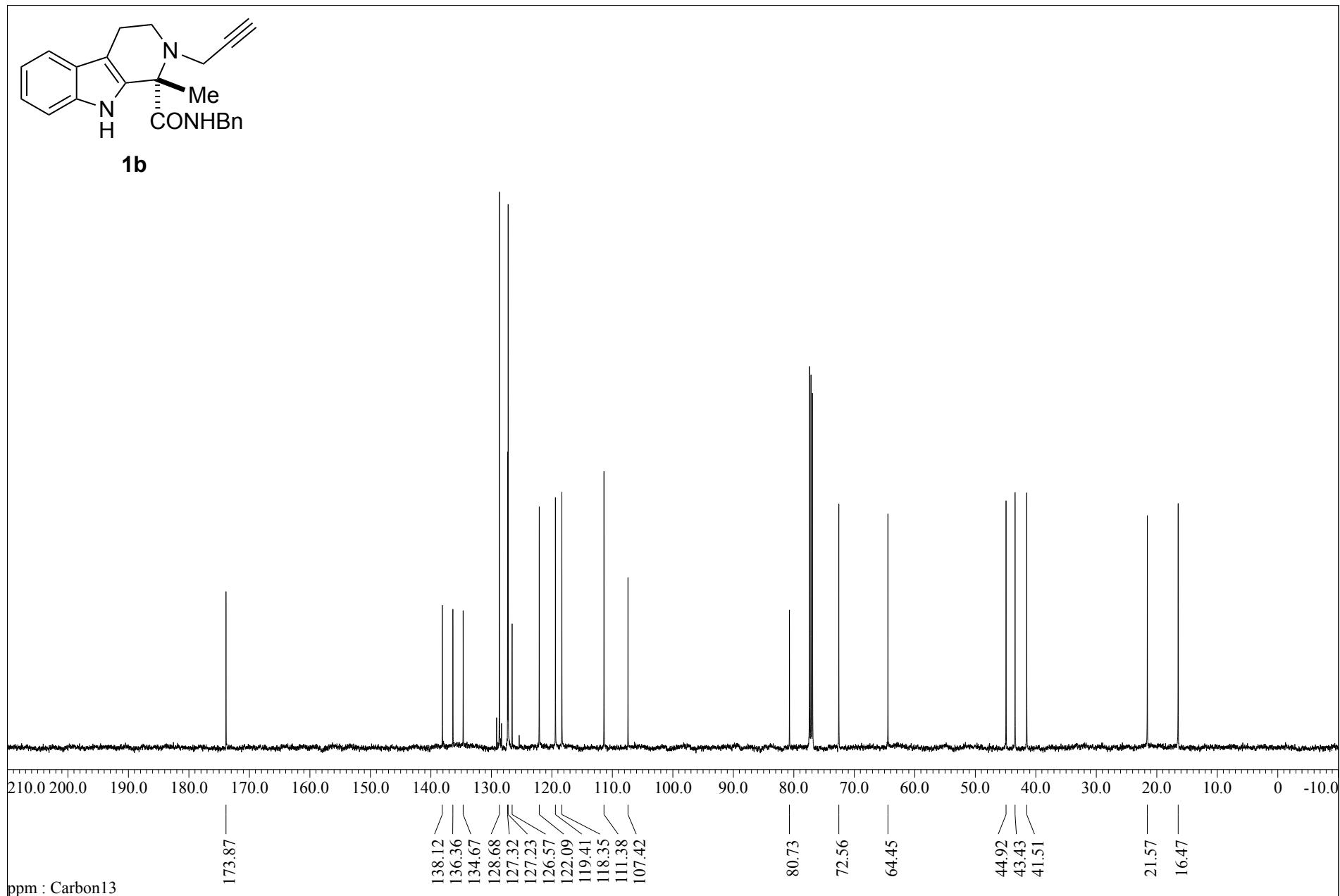


Figure S10. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **1b**.

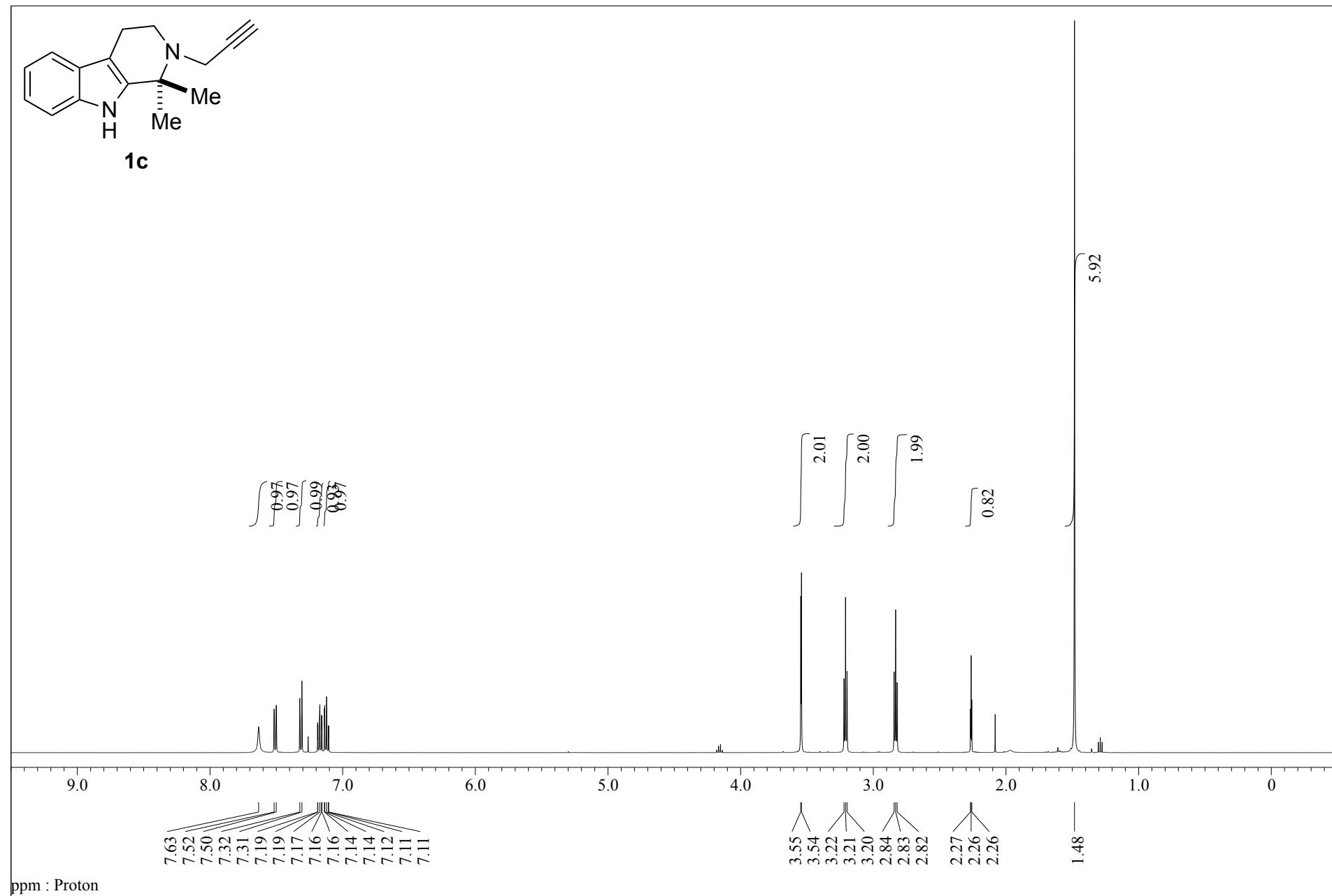


Figure S11. ^1H NMR spectrum (500 MHz, CDCl_3) of **1c**.

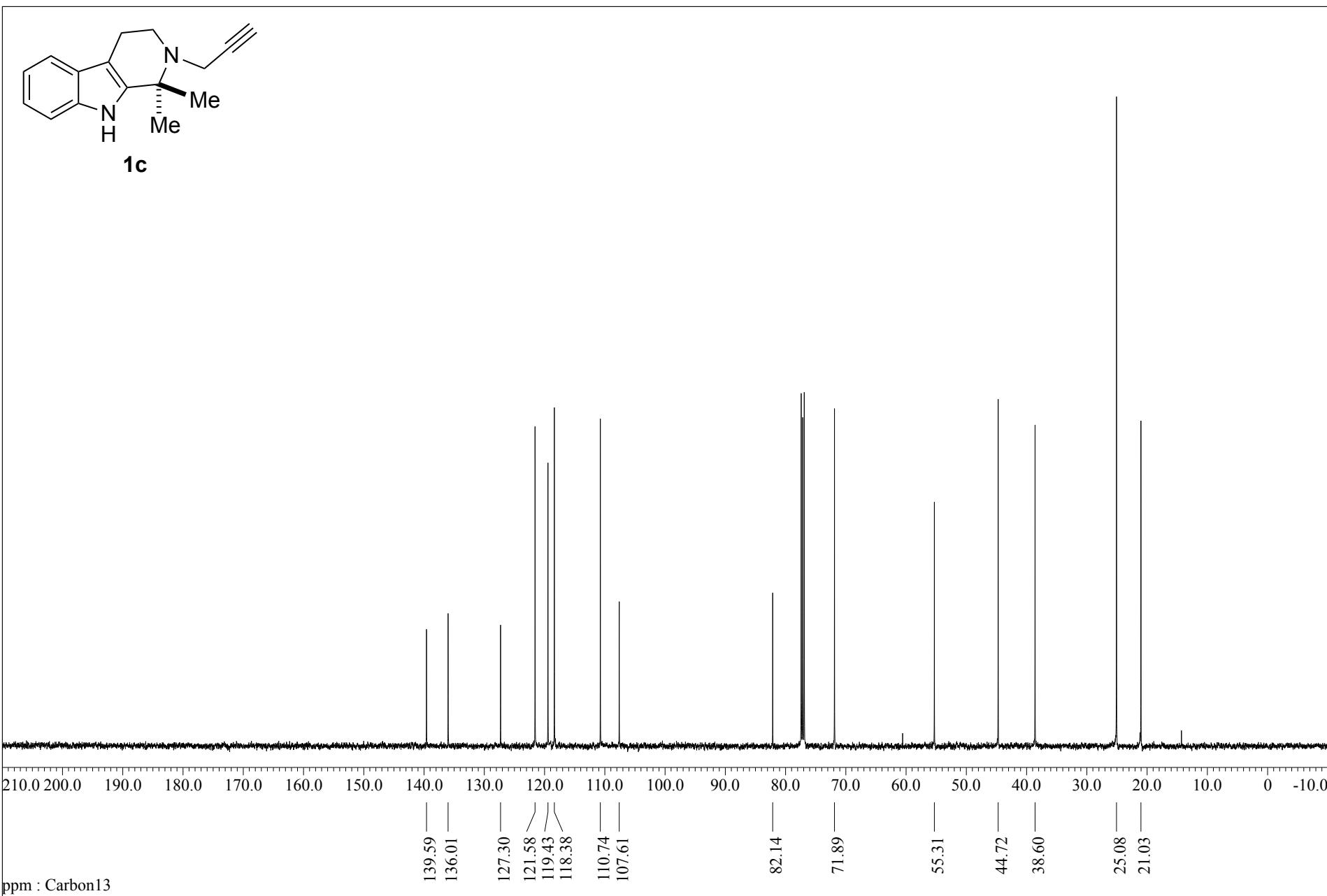


Figure S12. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **1c**.

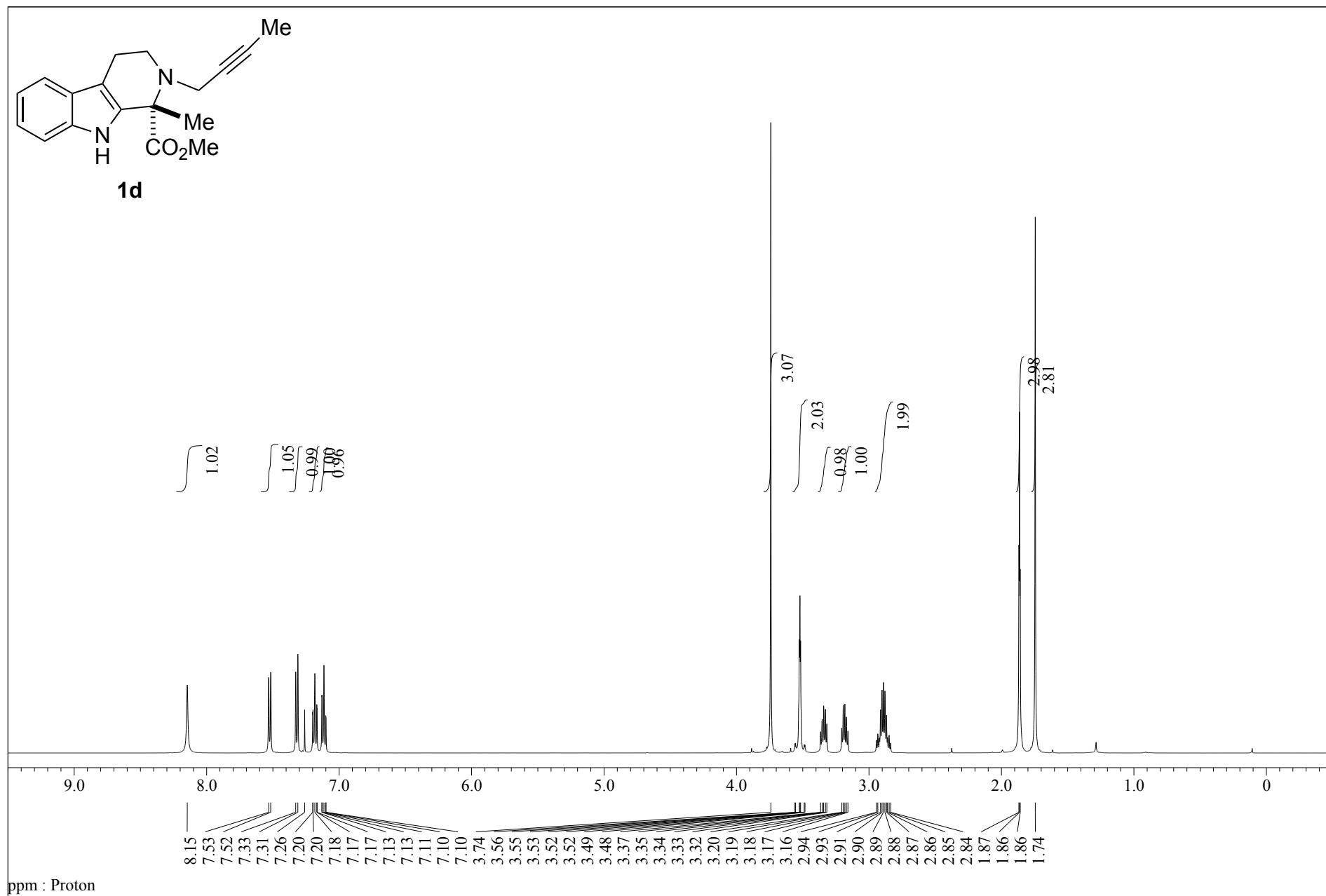


Figure S13. ^1H NMR spectrum (500 MHz, CDCl_3) of **1d**.

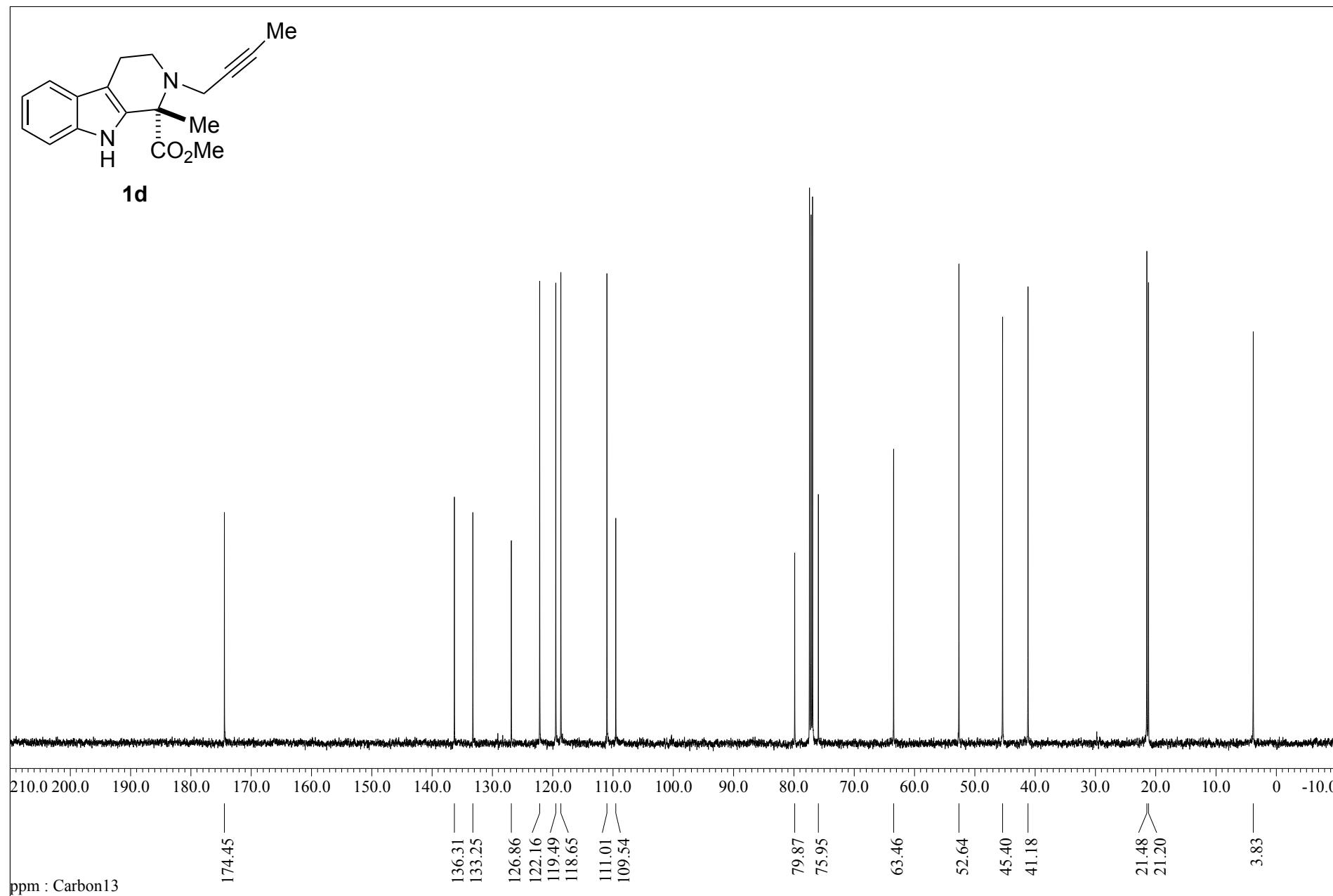


Figure S14. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **1d**.

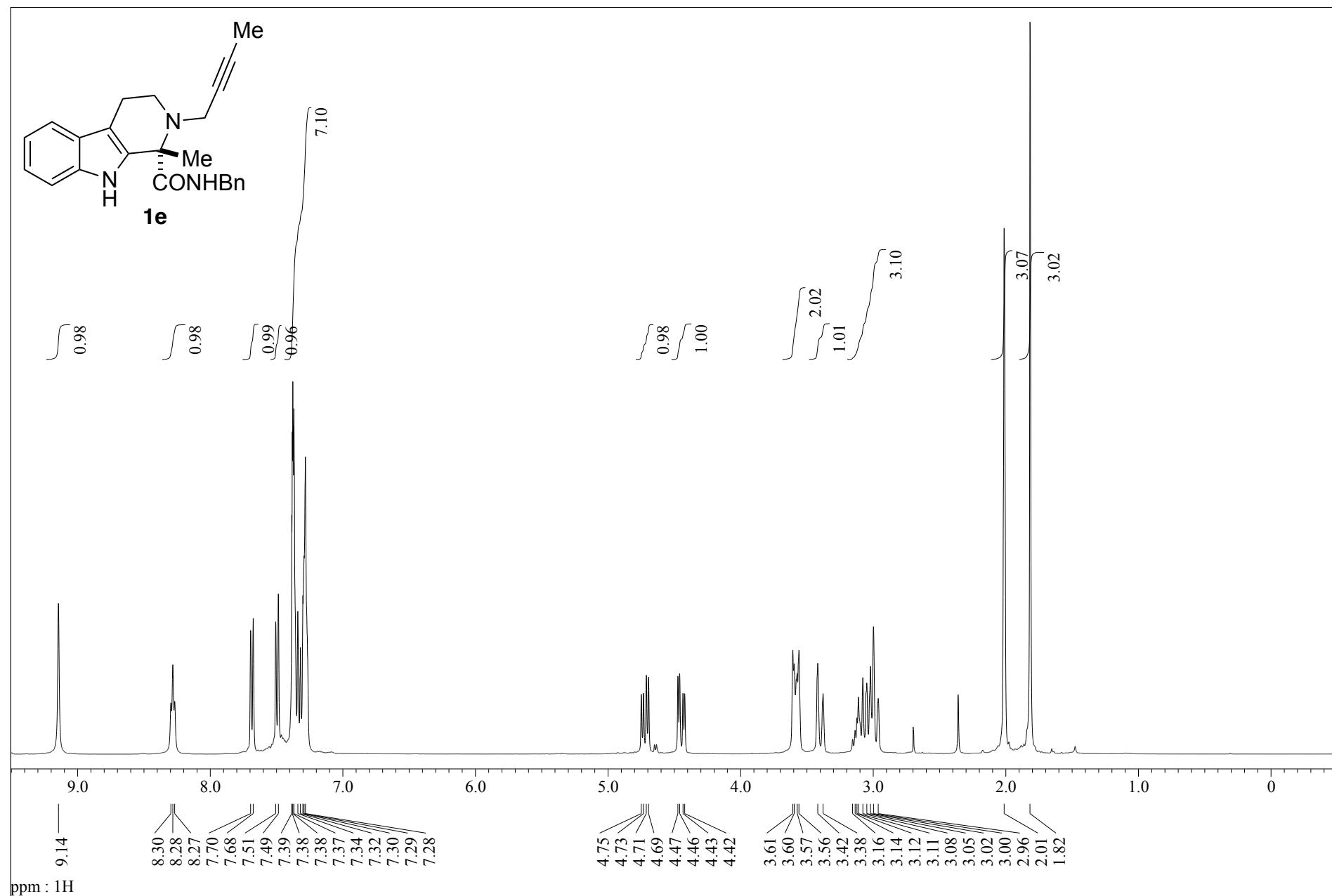


Figure S15. ^1H NMR spectrum (400 MHz, CDCl_3) of **1e**.

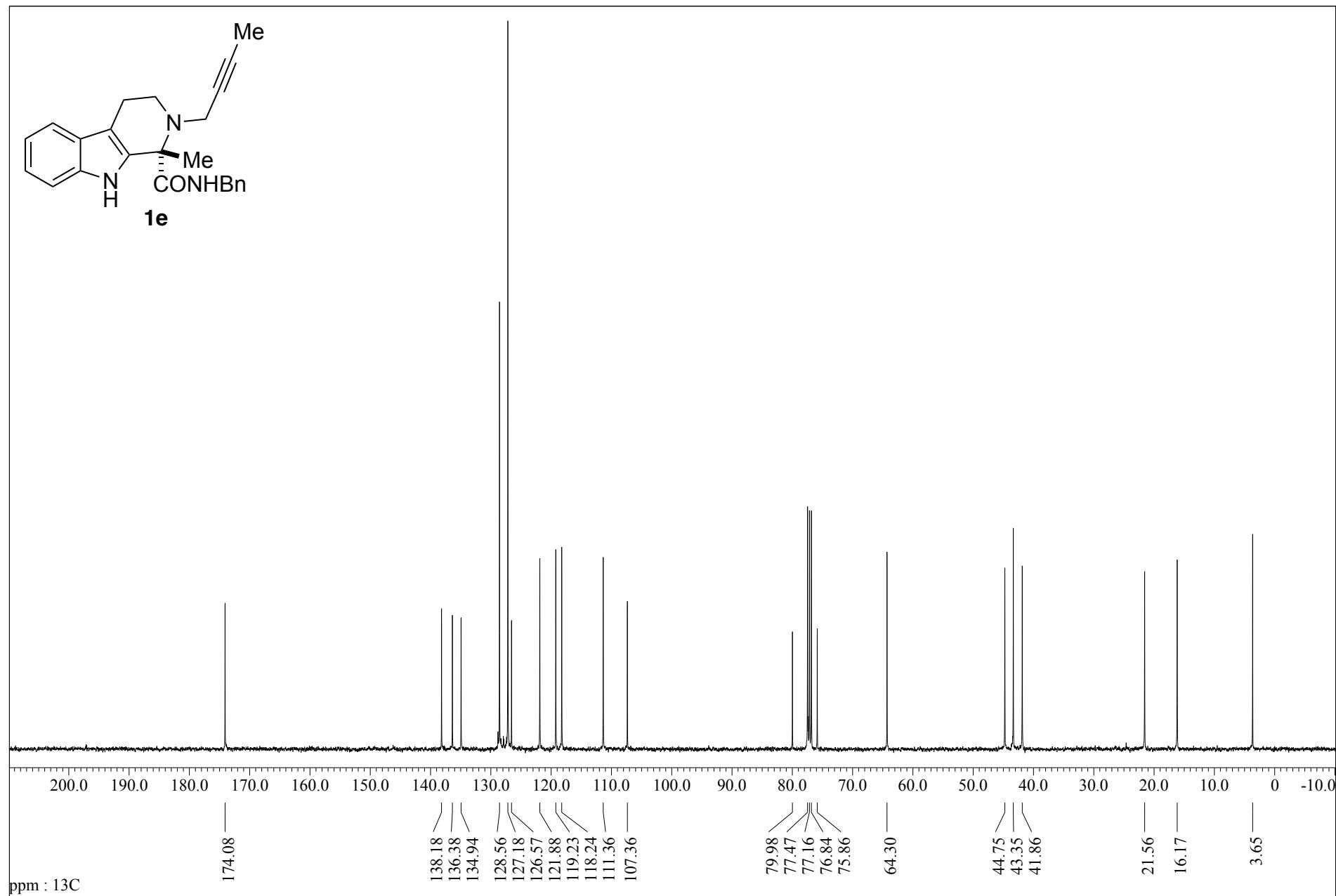


Figure S16. ^{13}C NMR spectrum (100 MHz, CDCl_3) of **1e**.

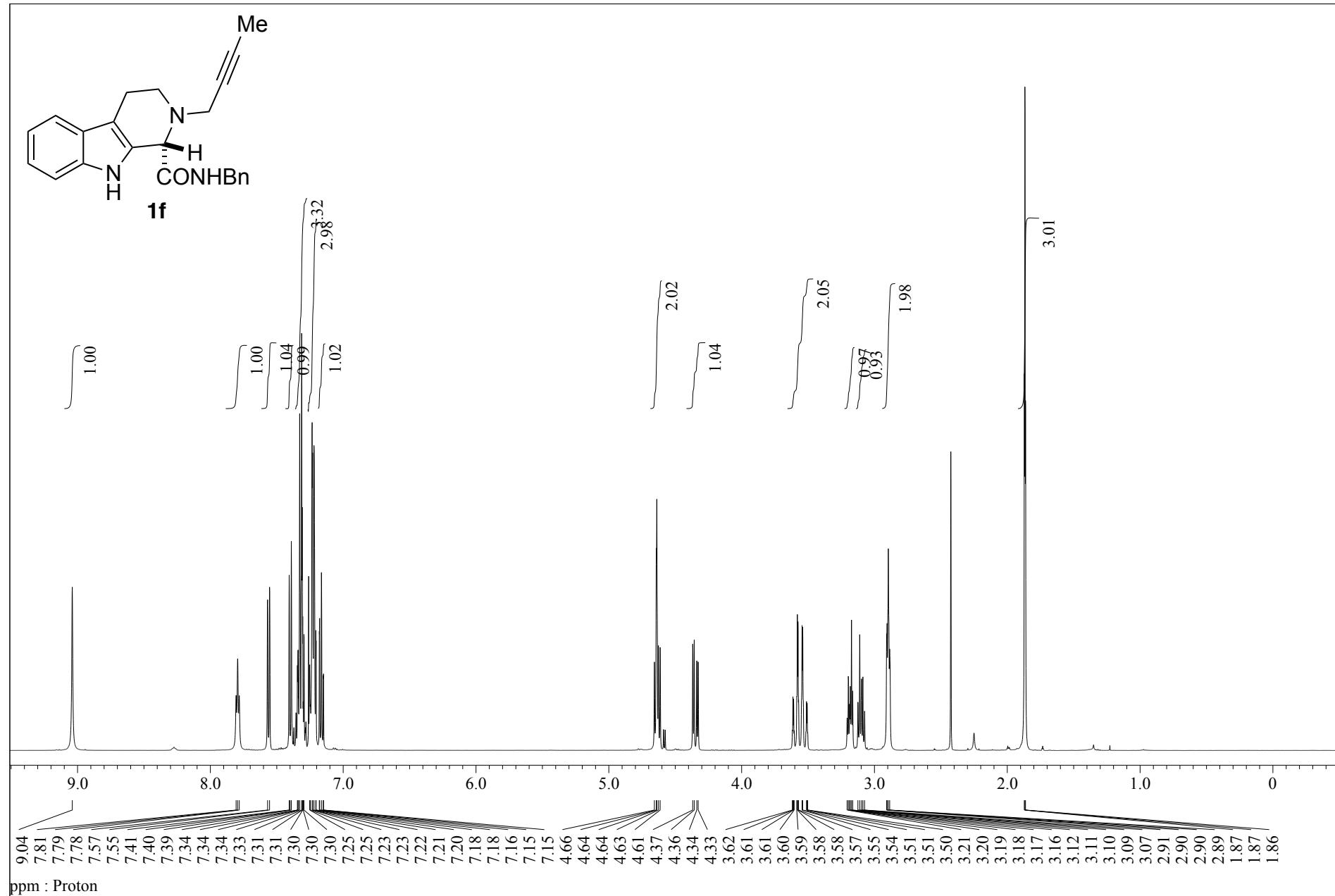


Figure S17. ¹H NMR spectrum (500 MHz, CDCl₃) of **1f**.

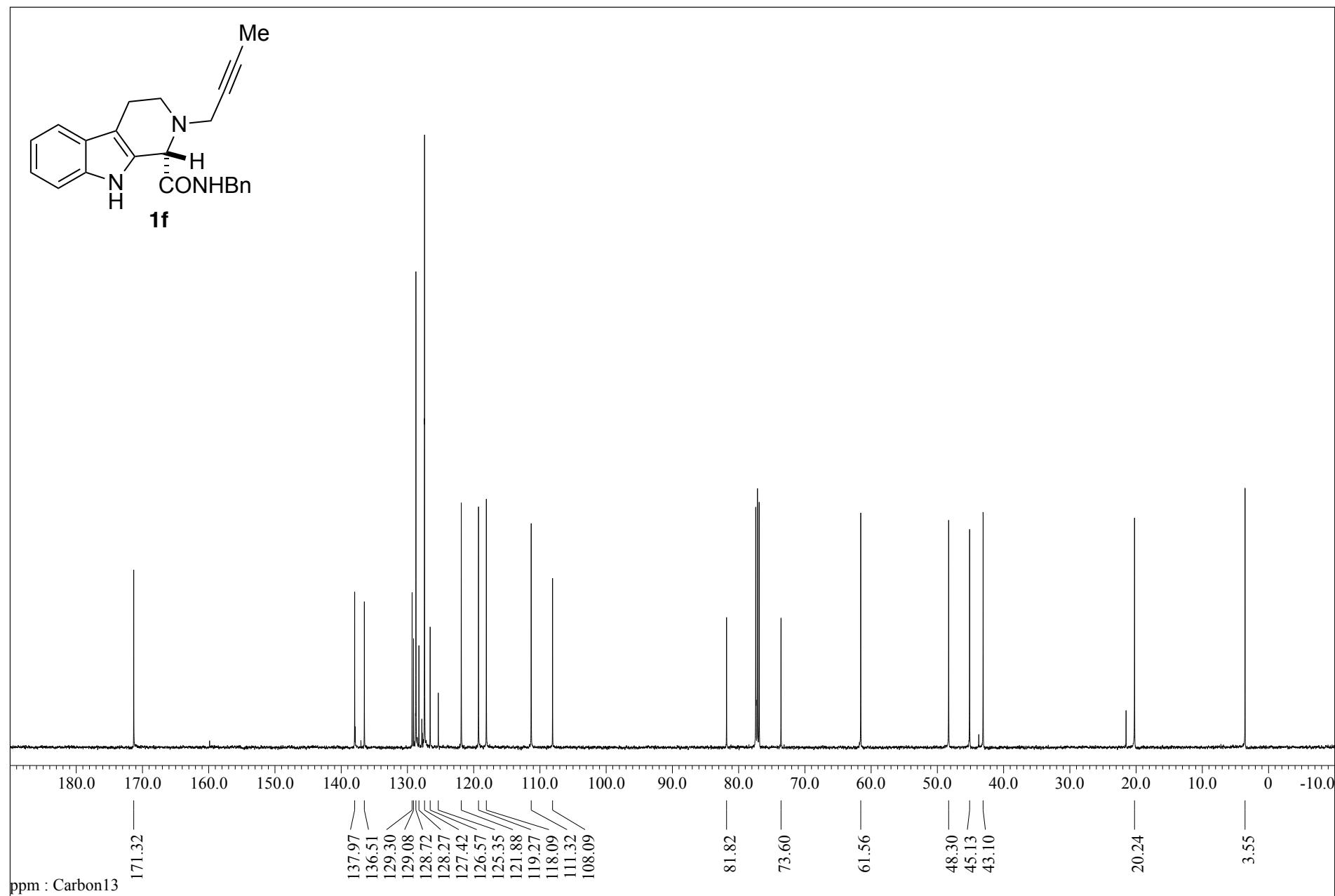


Figure S18. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **1f**.

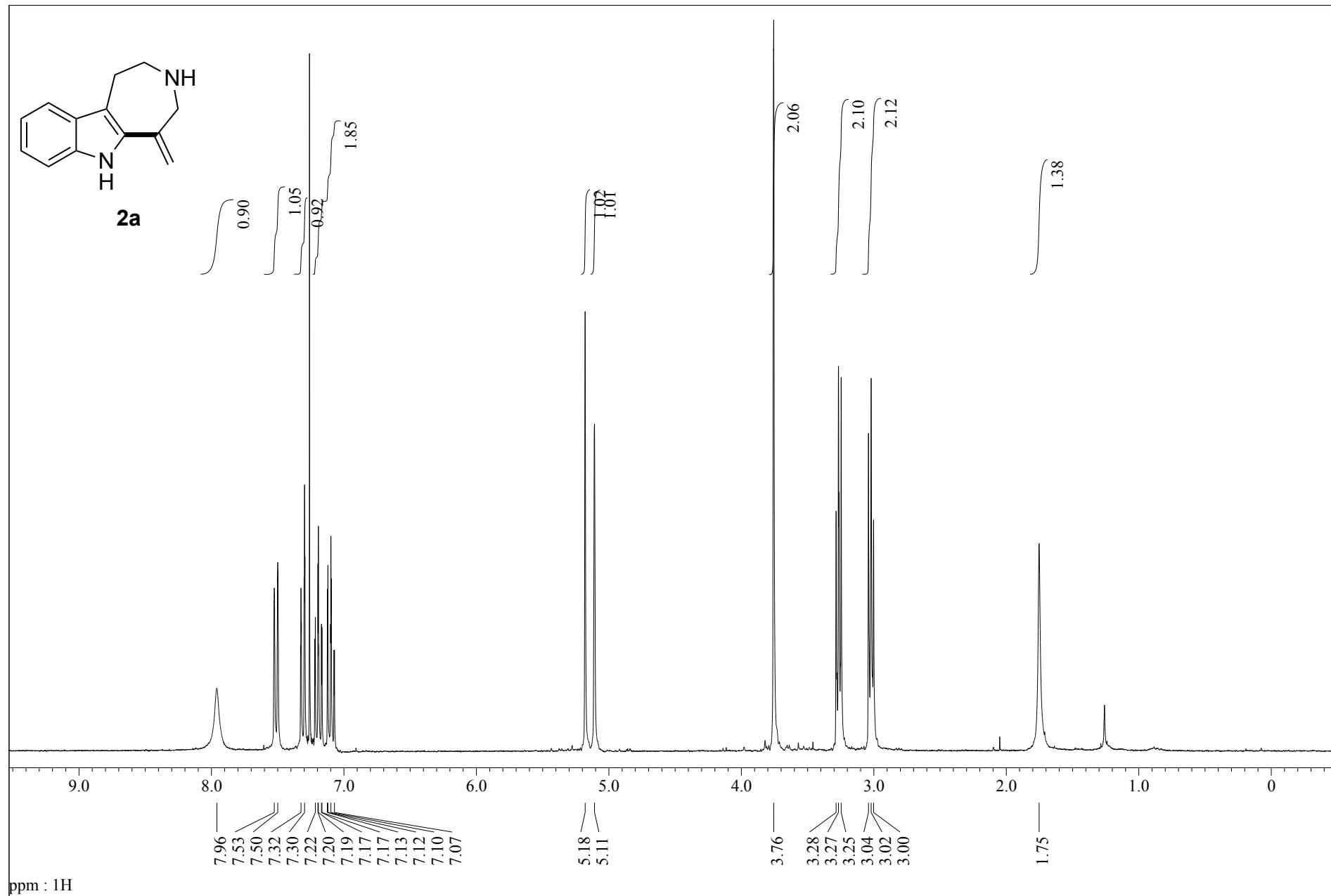


Figure S19. ^1H NMR spectrum (300 MHz, CDCl_3) of **2a**.

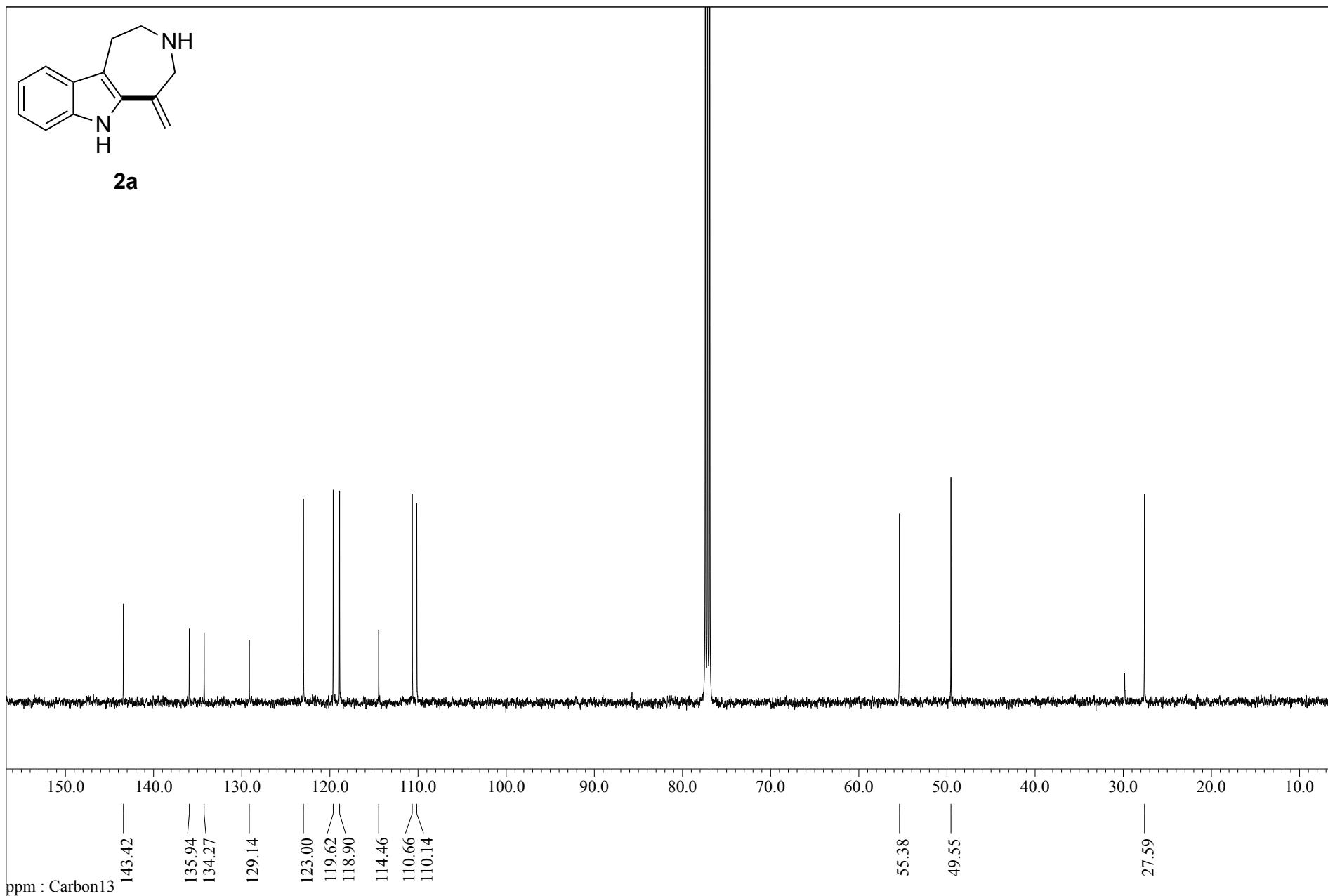


Figure S20. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **2a**.

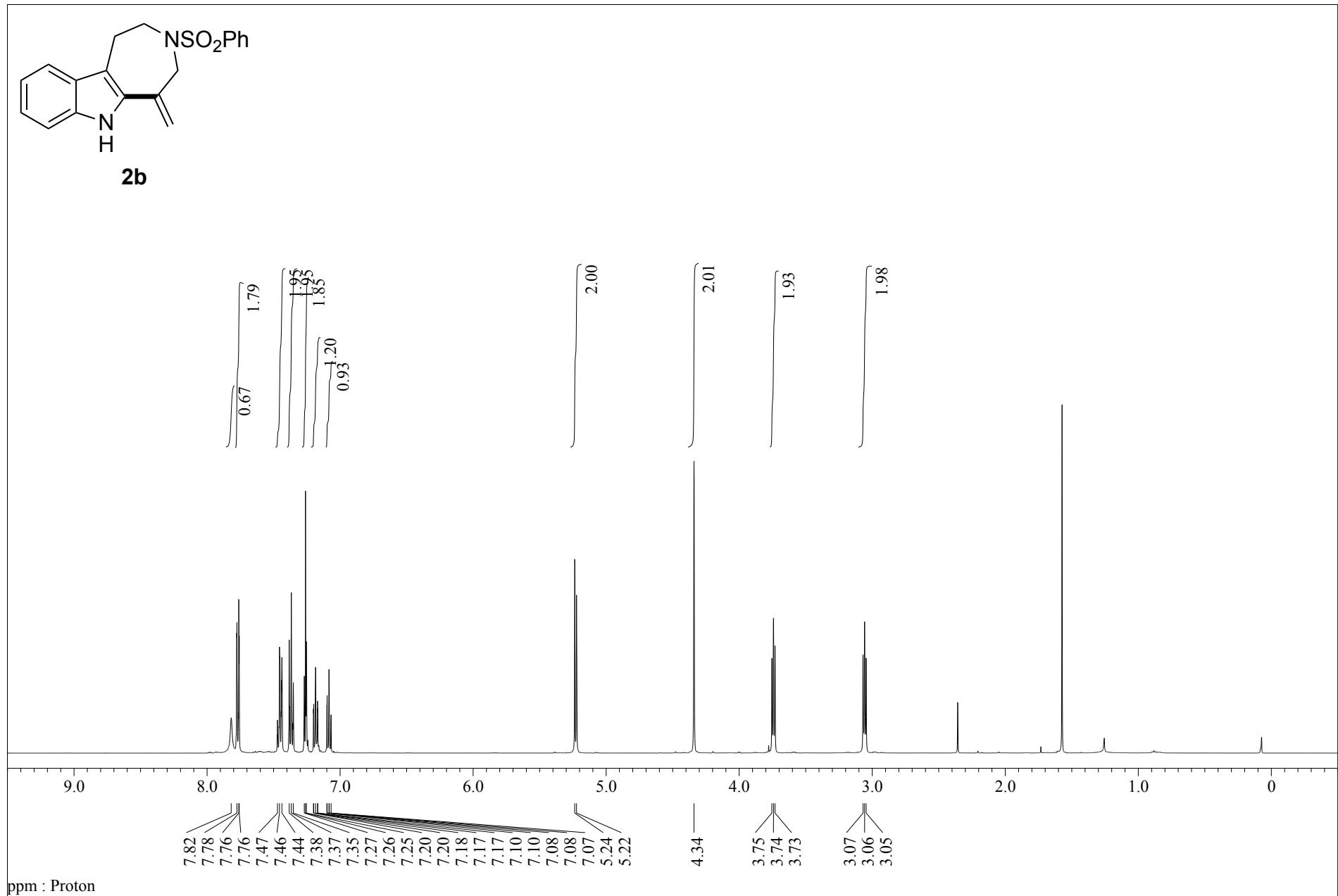


Figure S21. ^1H NMR spectrum (500 MHz, CDCl_3) of **2b**.

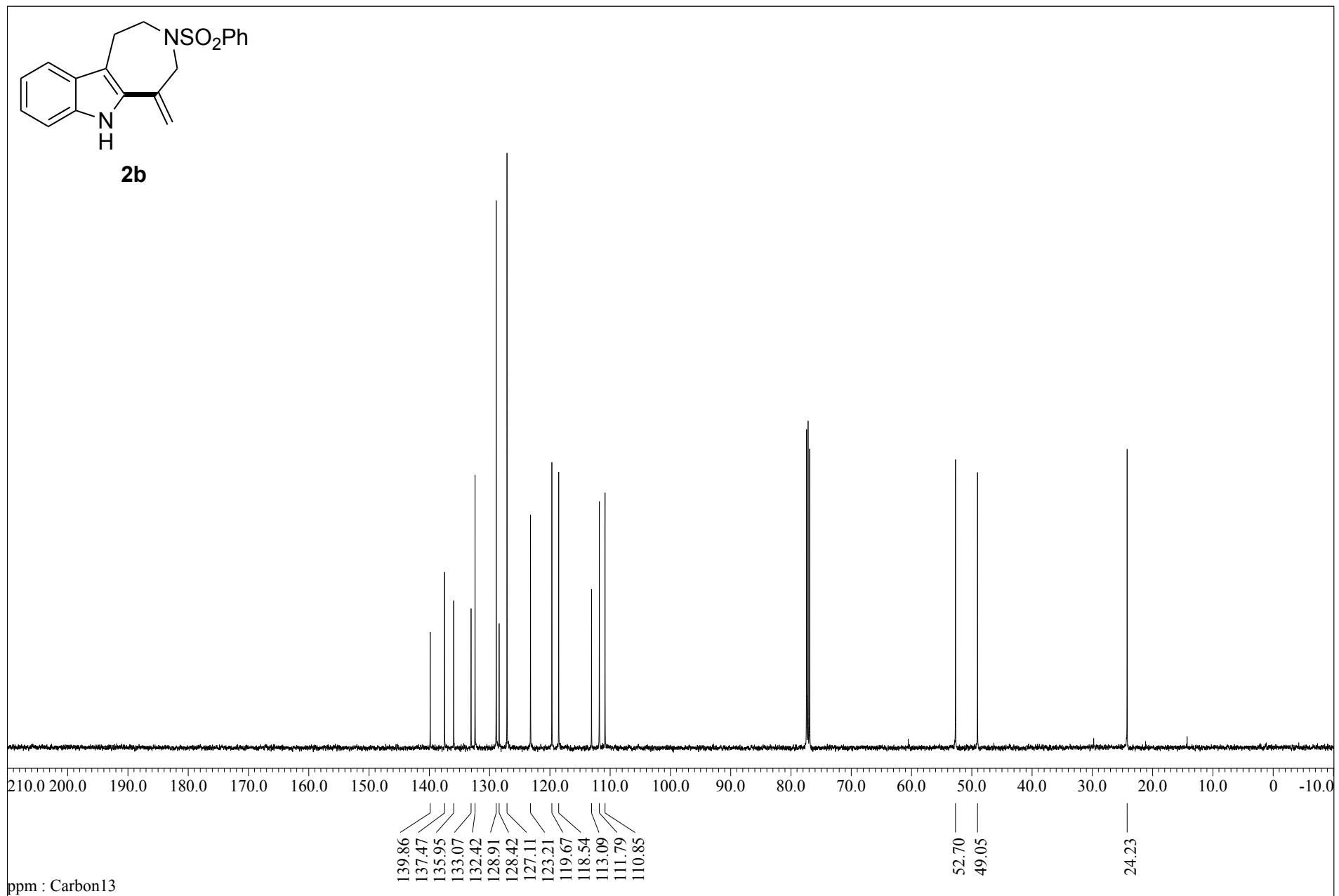


Figure S22. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **2b**.

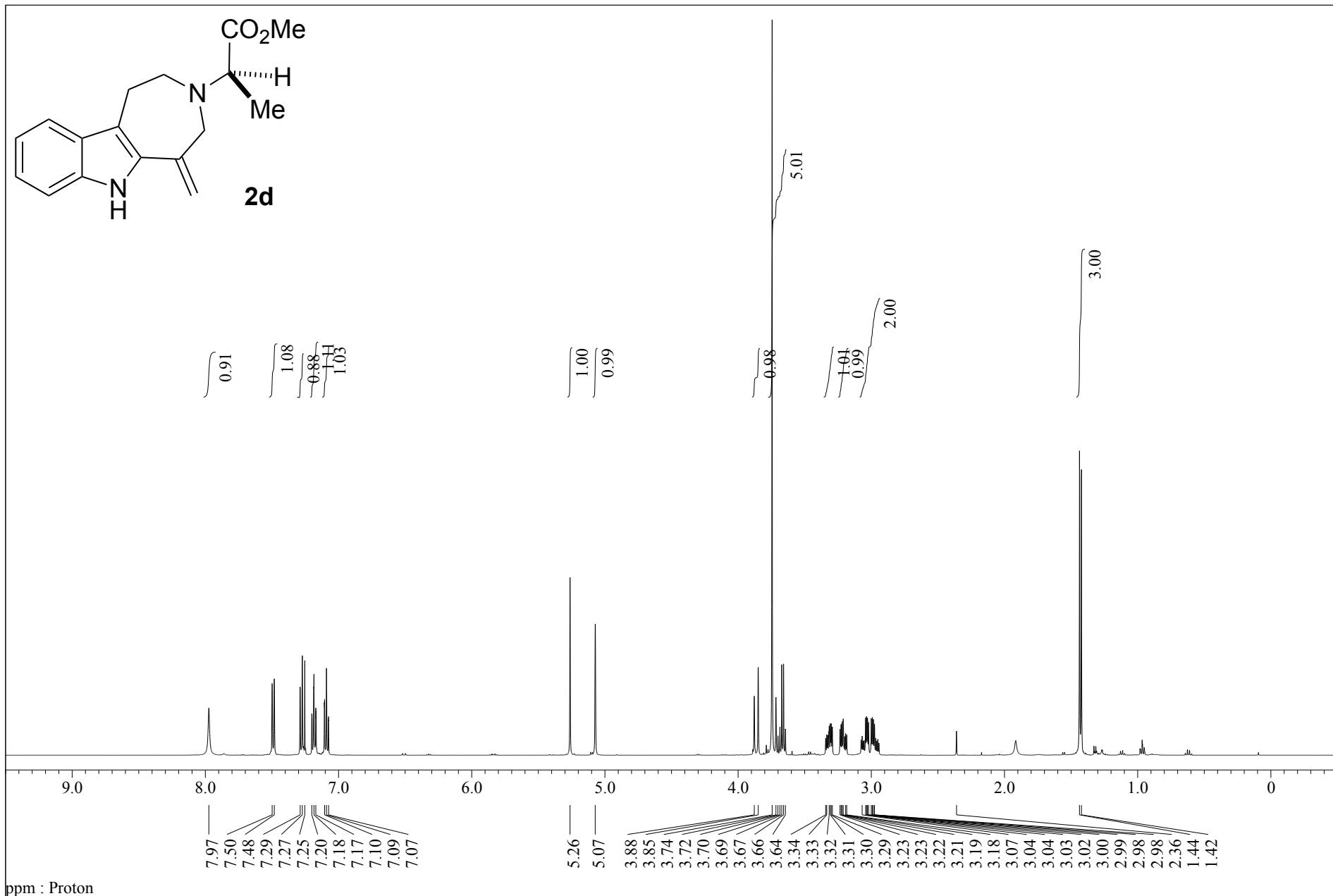


Figure S23. ^1H NMR spectrum (500 MHz, CDCl_3) of **2d**.

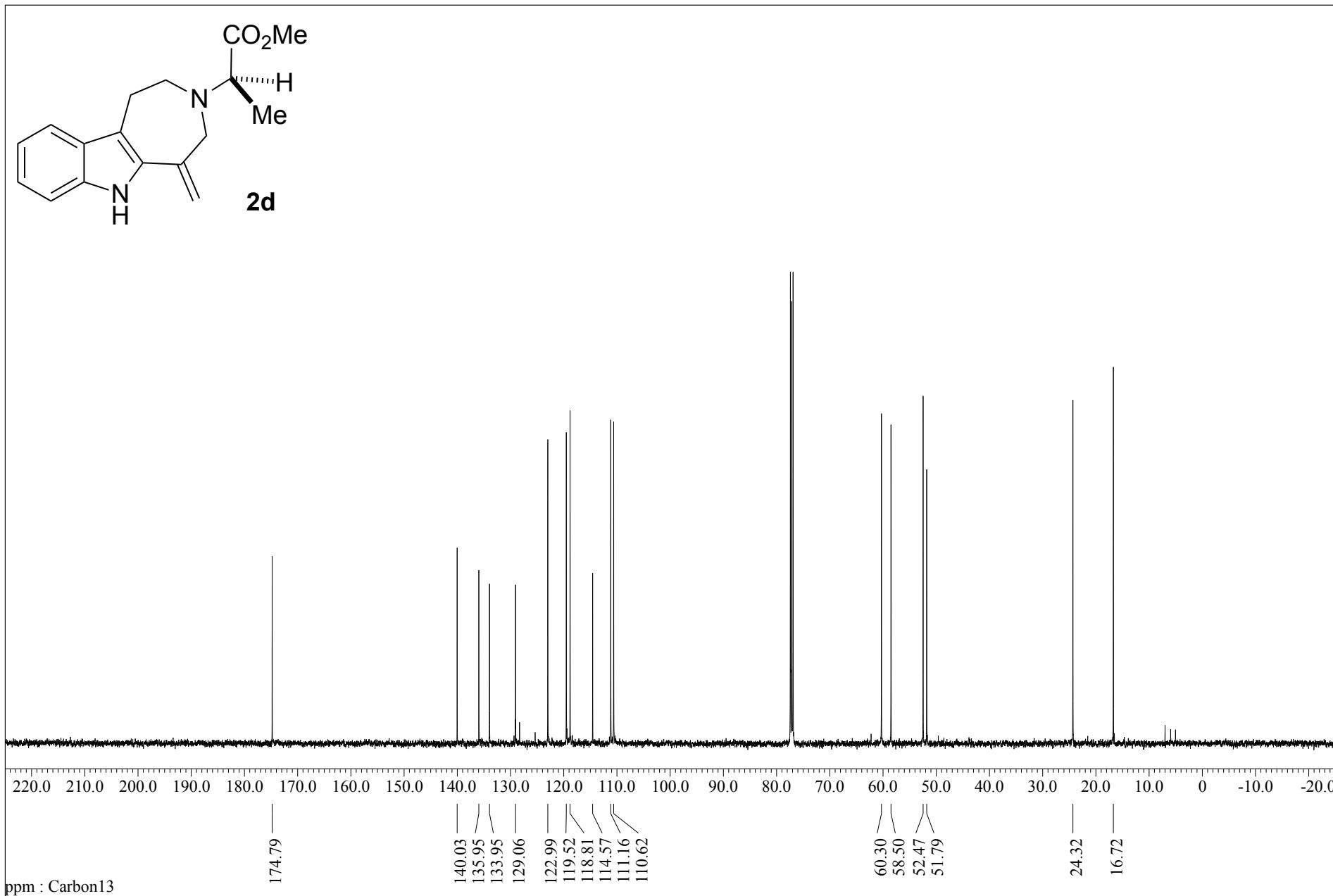


Figure S24. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **2d**.

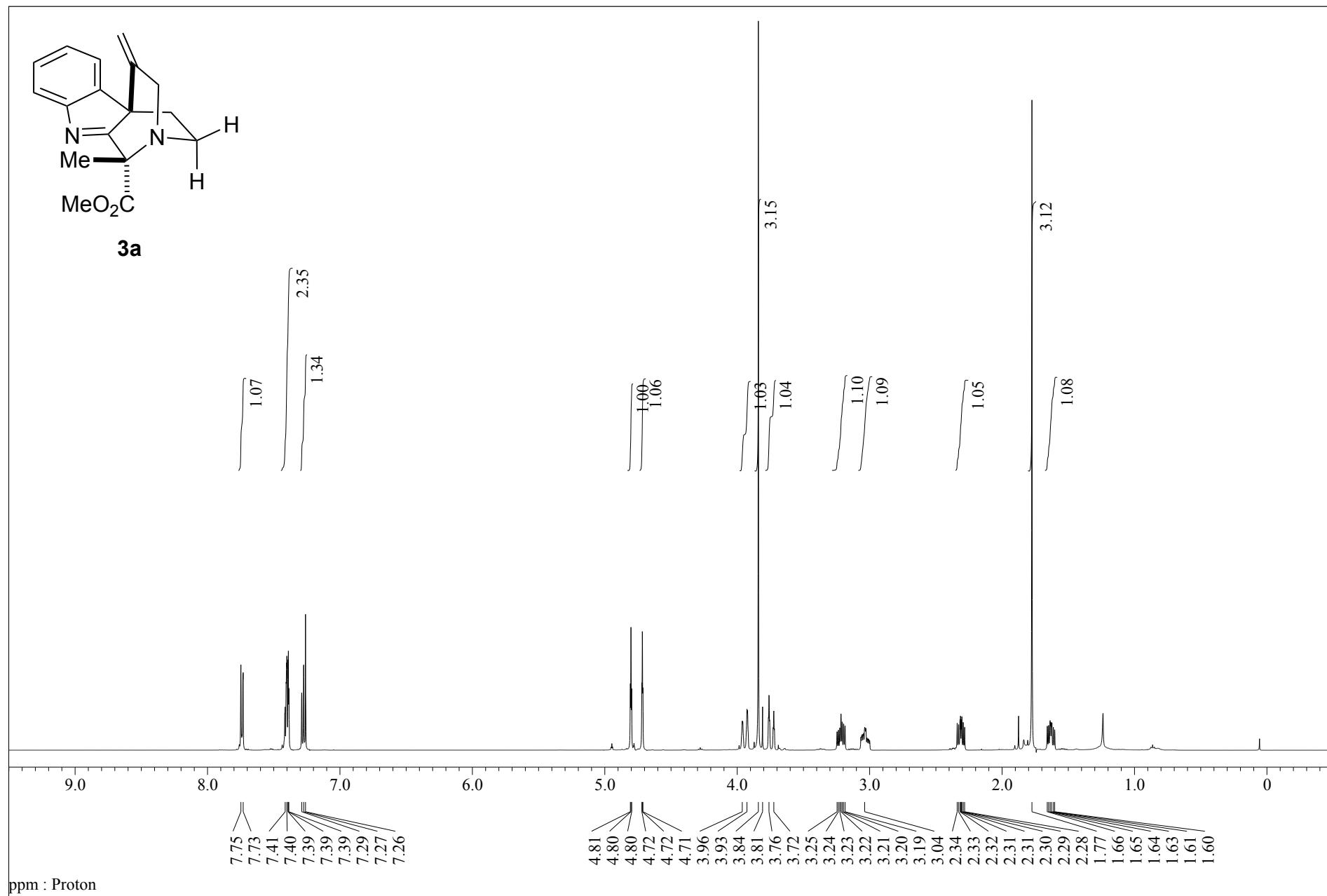


Figure S25. ¹H NMR spectrum (500 MHz, CDCl₃) of **3a**.

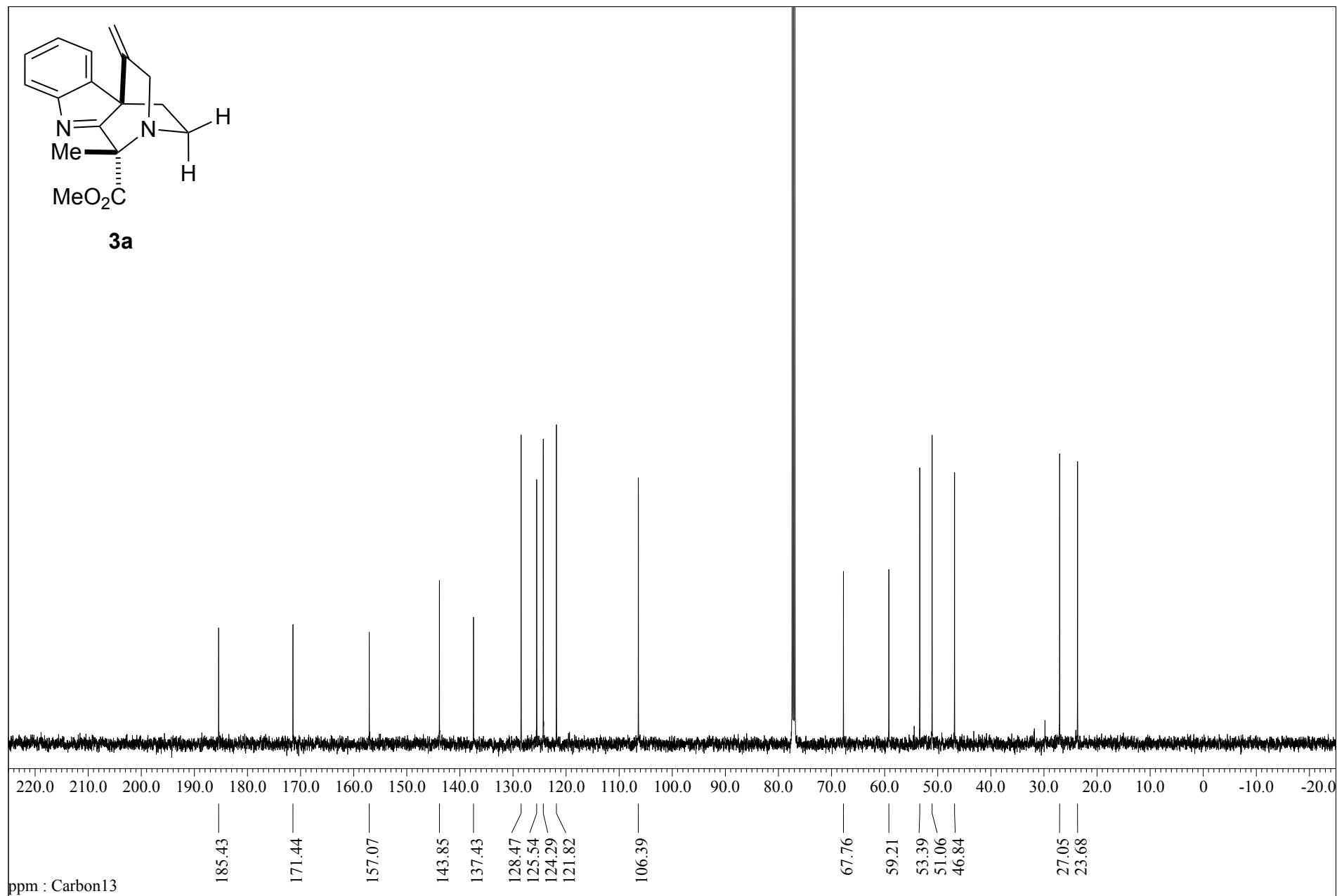


Figure S26. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **3a**.

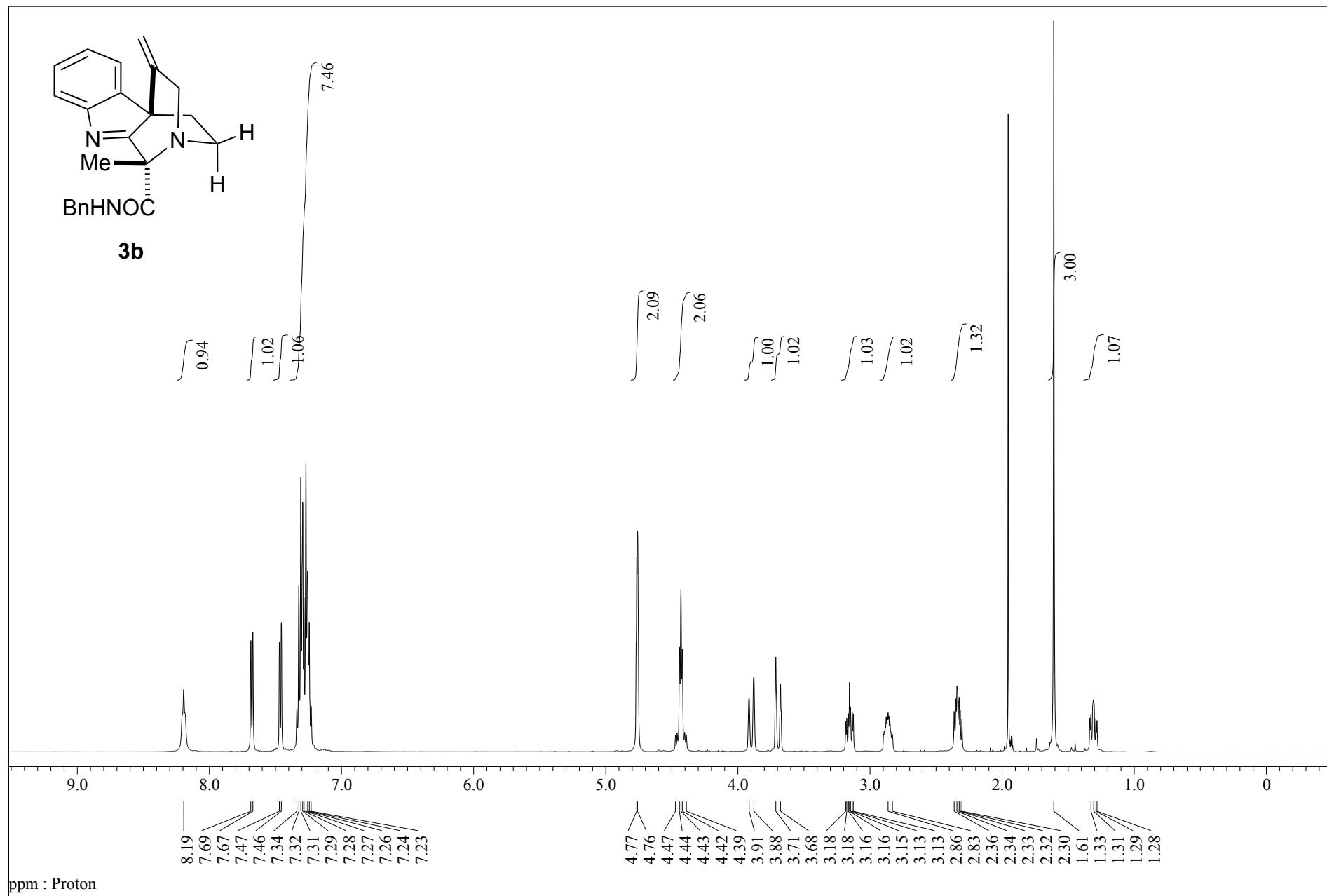


Figure S27. ^1H NMR spectrum (500 MHz, CD_3CN) of **3b**.

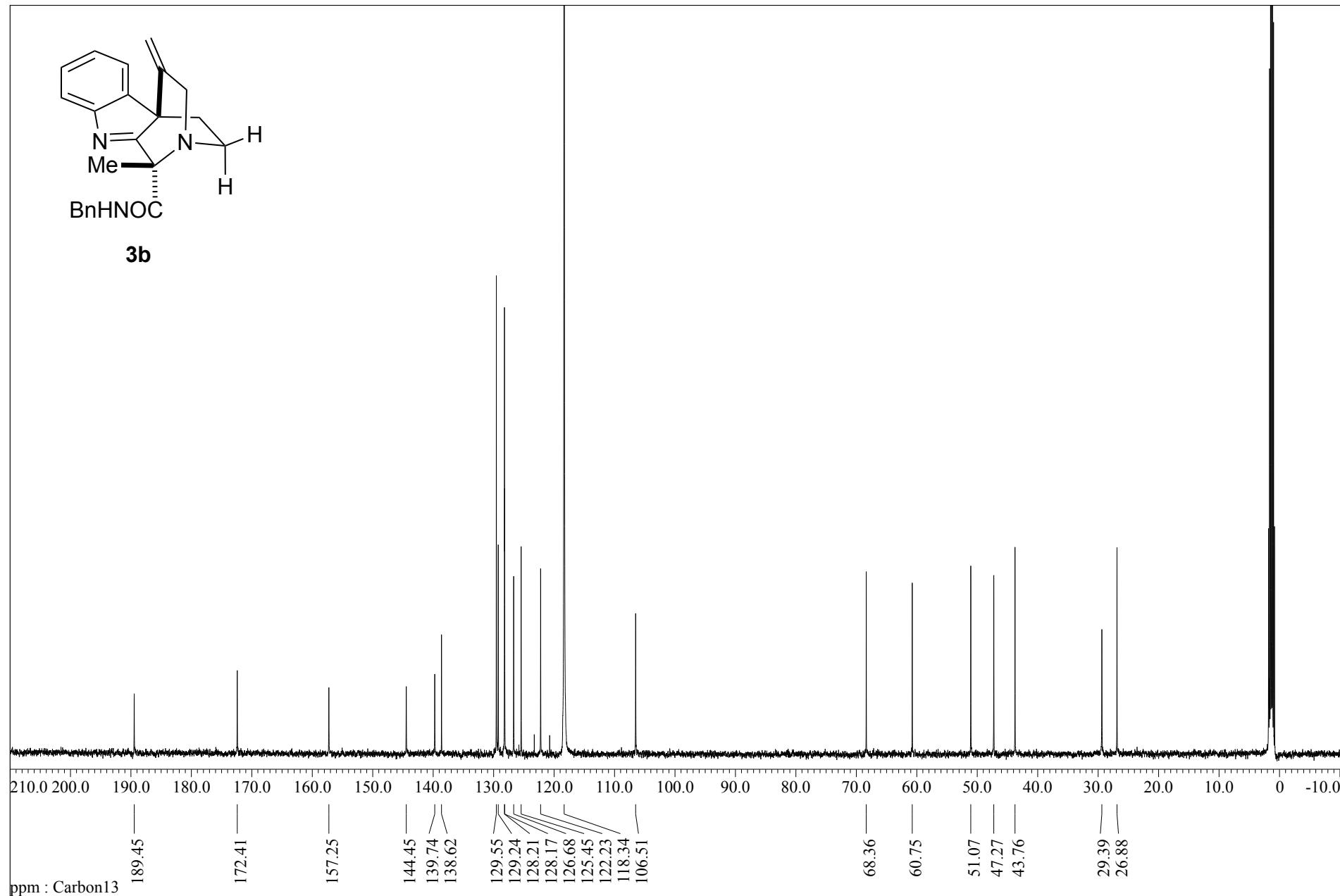


Figure S28. ^{13}C NMR spectrum (125 MHz, CD_3CN) of **3b**.

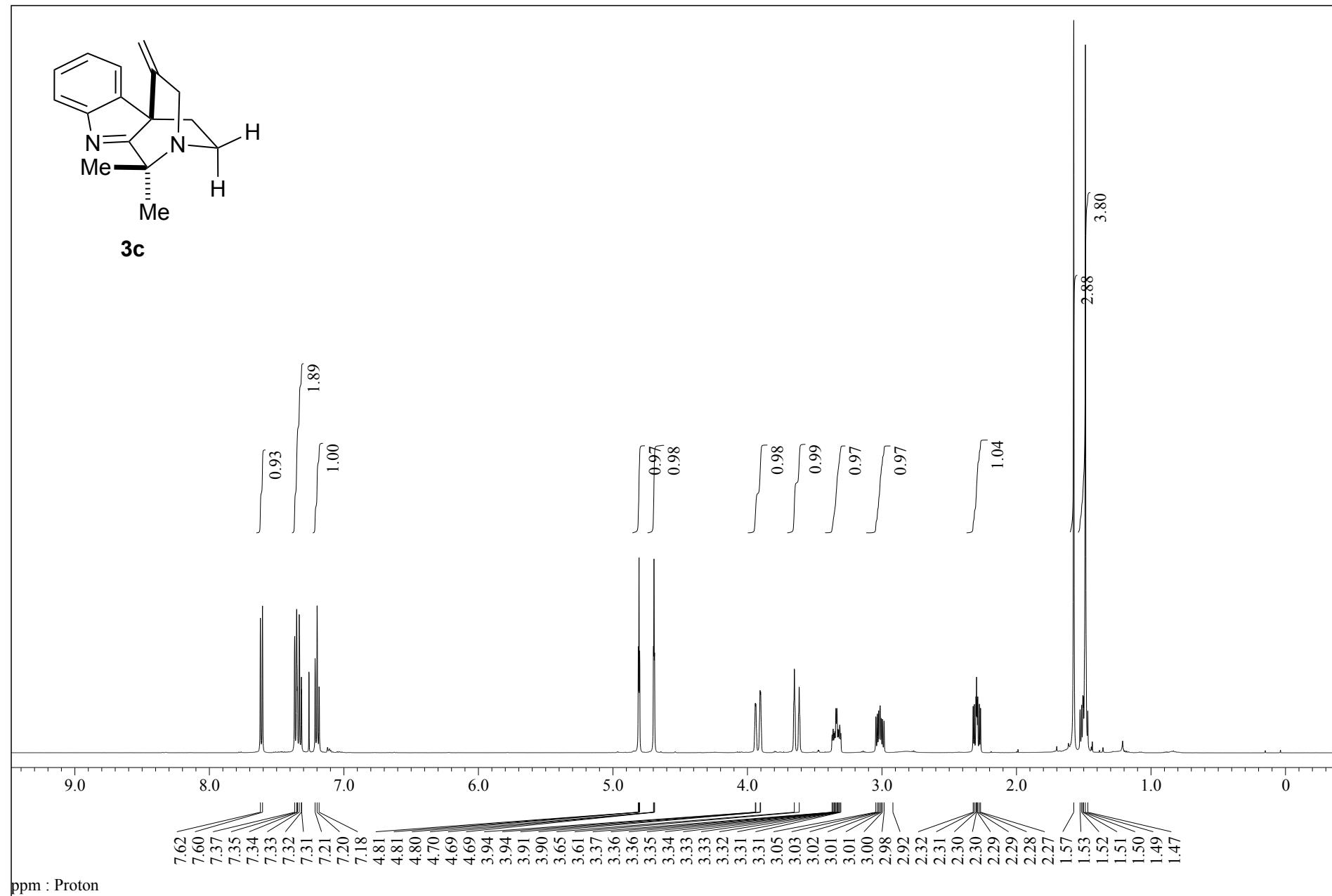


Figure S29. ¹H NMR spectrum (500 MHz, CDCl₃) of **3c**.

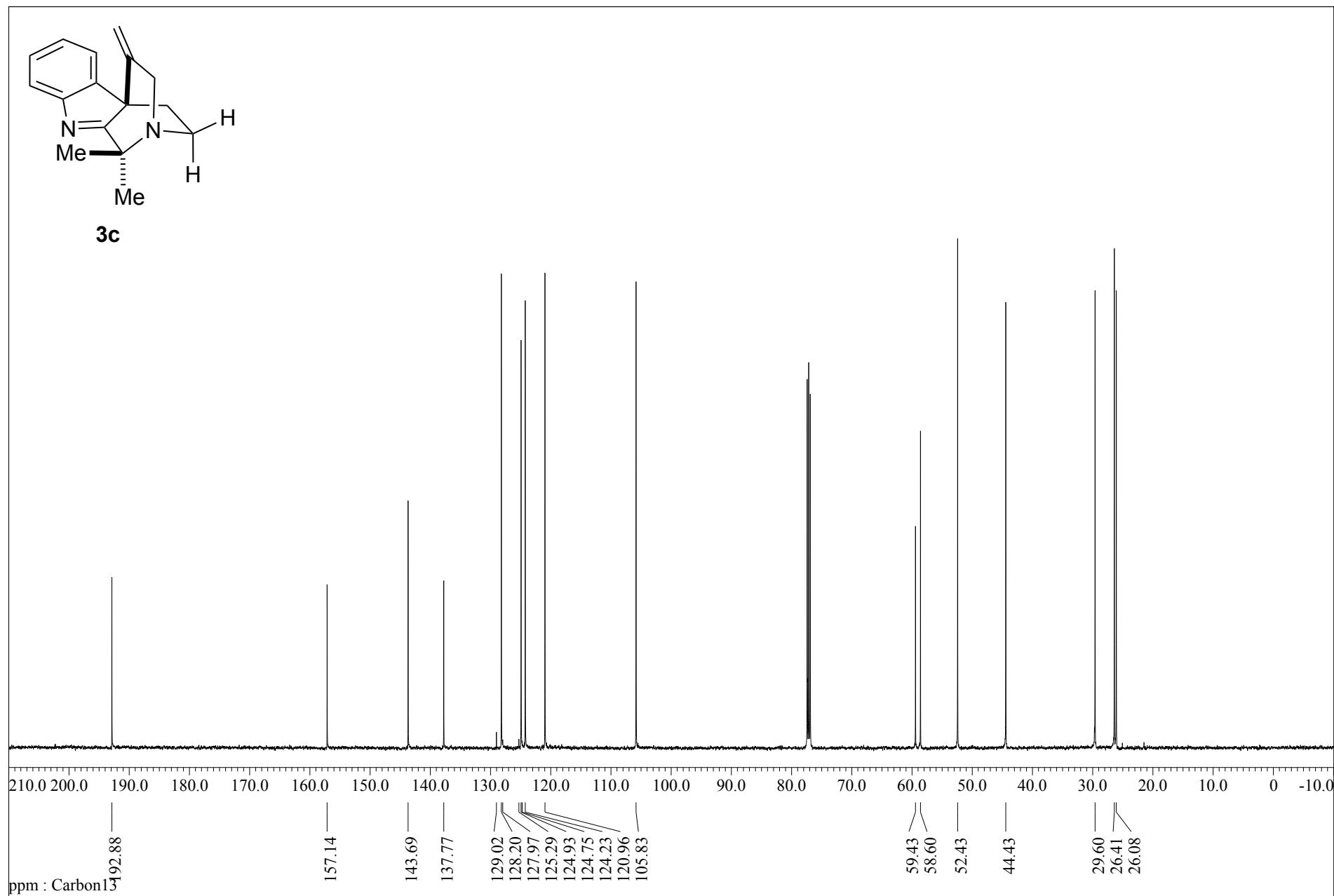


Figure S30. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **3c**.

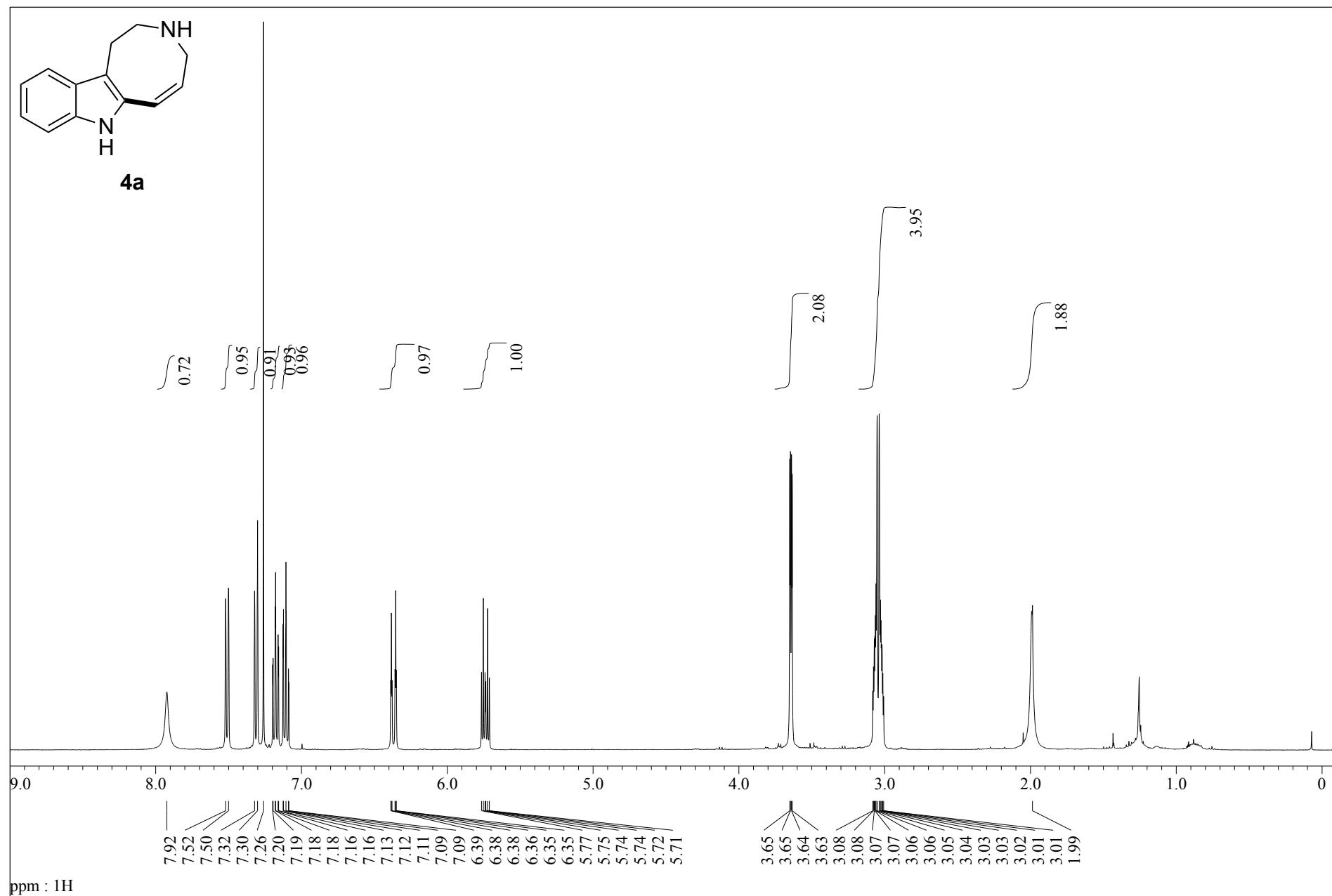


Figure S31. ^1H NMR spectrum (400 MHz, CDCl_3) of **4a**.

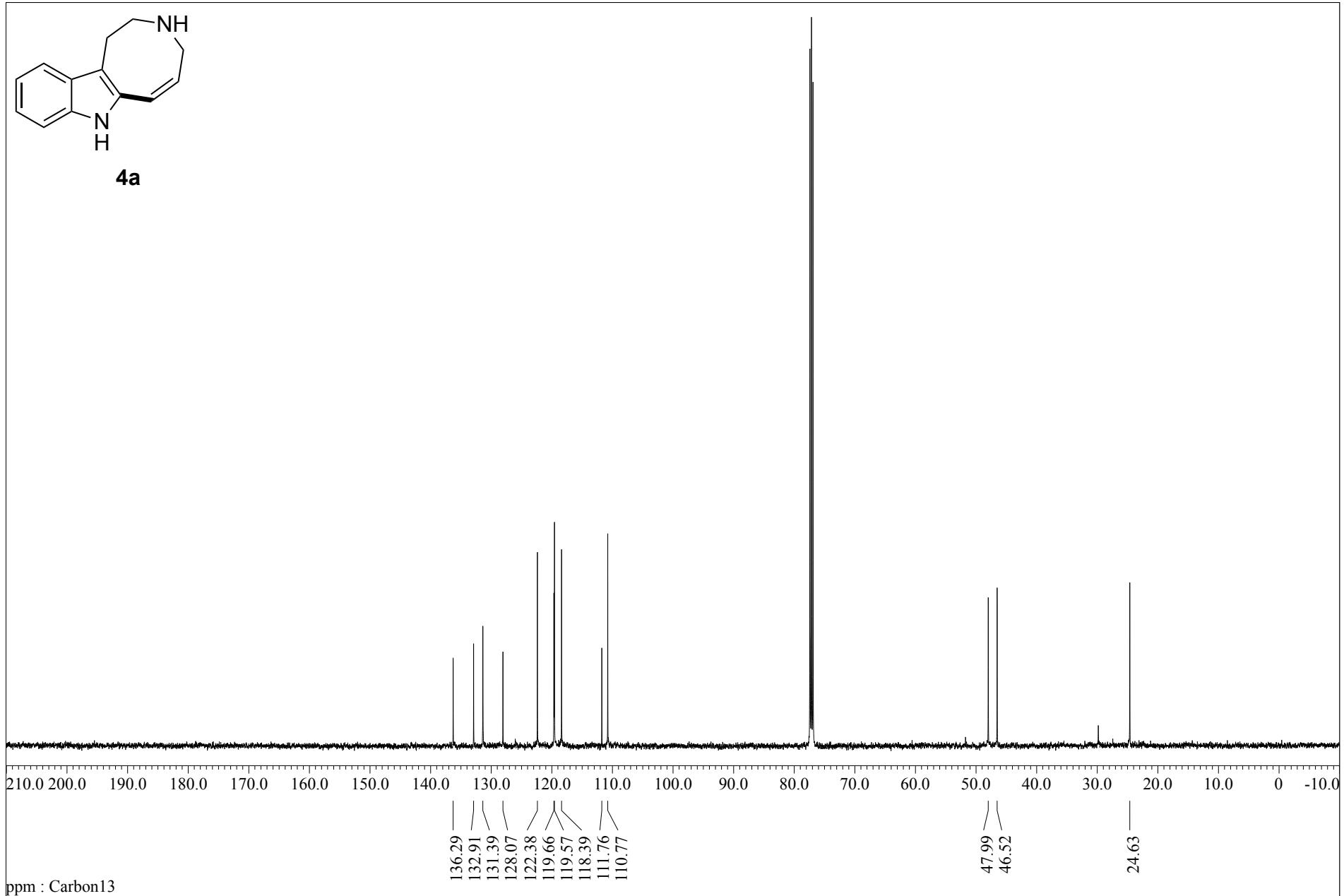


Figure S32. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **4a**.

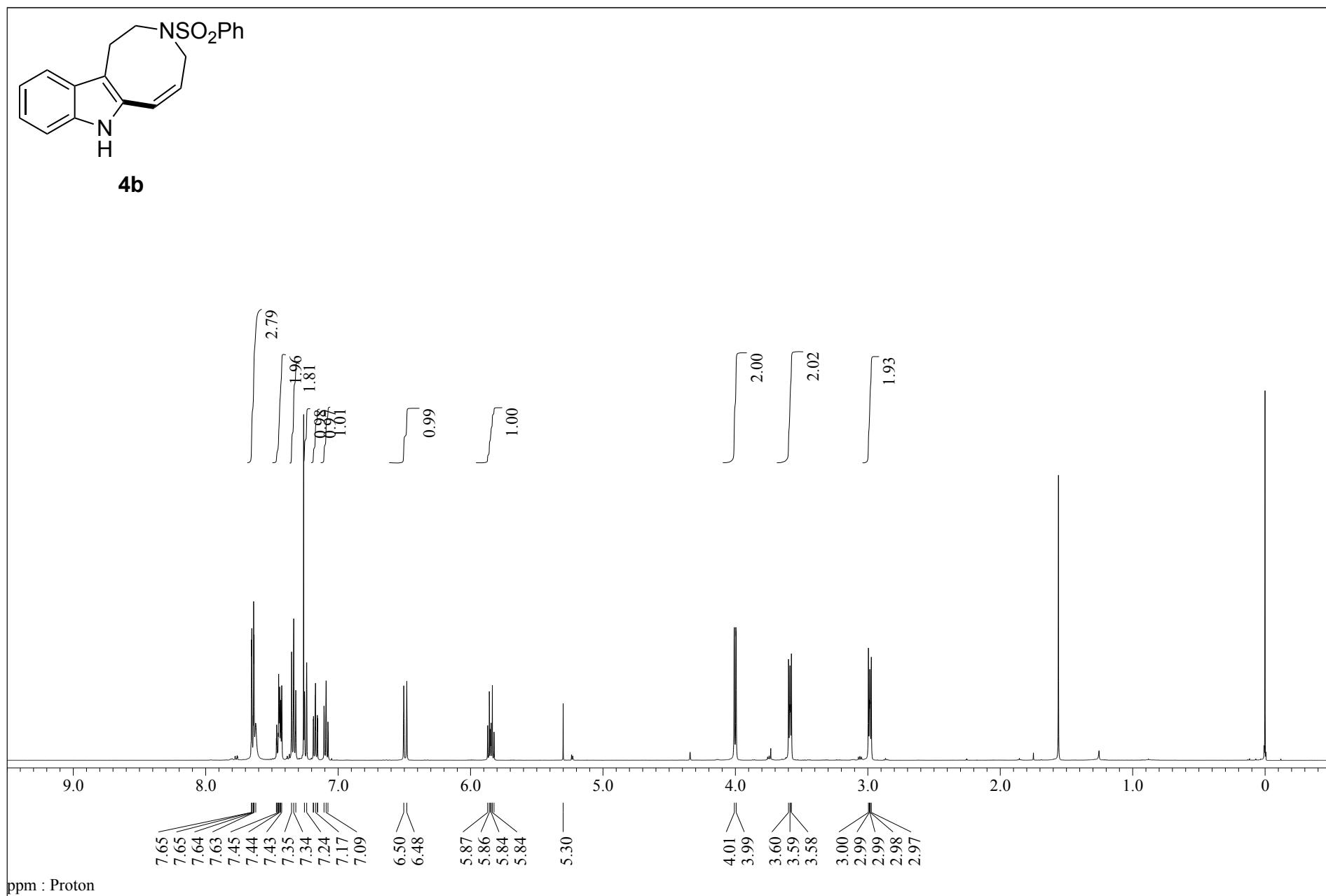


Figure S33. ^1H NMR spectrum (500 MHz, CDCl_3) of **4b**.

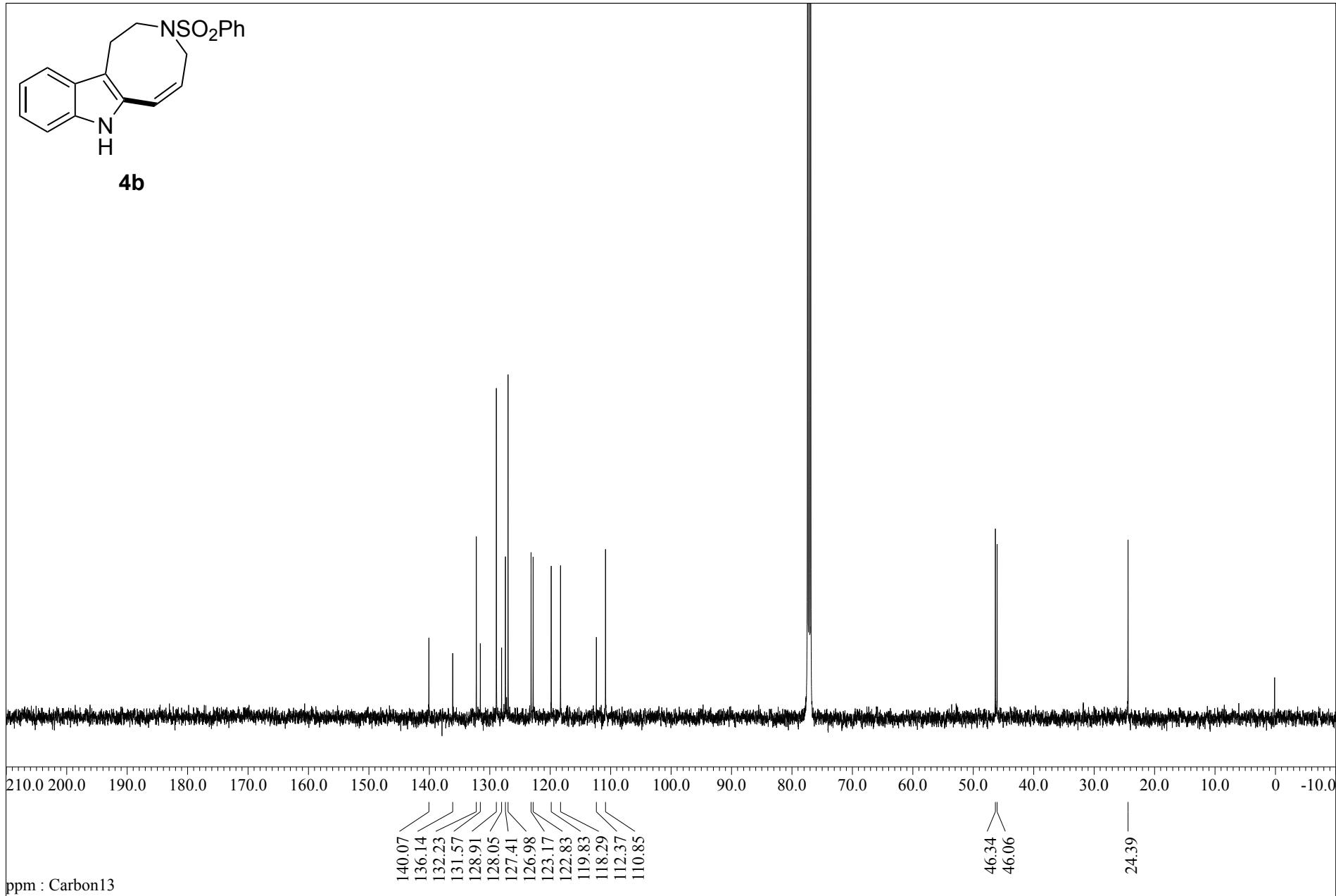


Figure S34. ^{13}C NMR spectrum (125 MHz, CDCl_3) of **4b**.

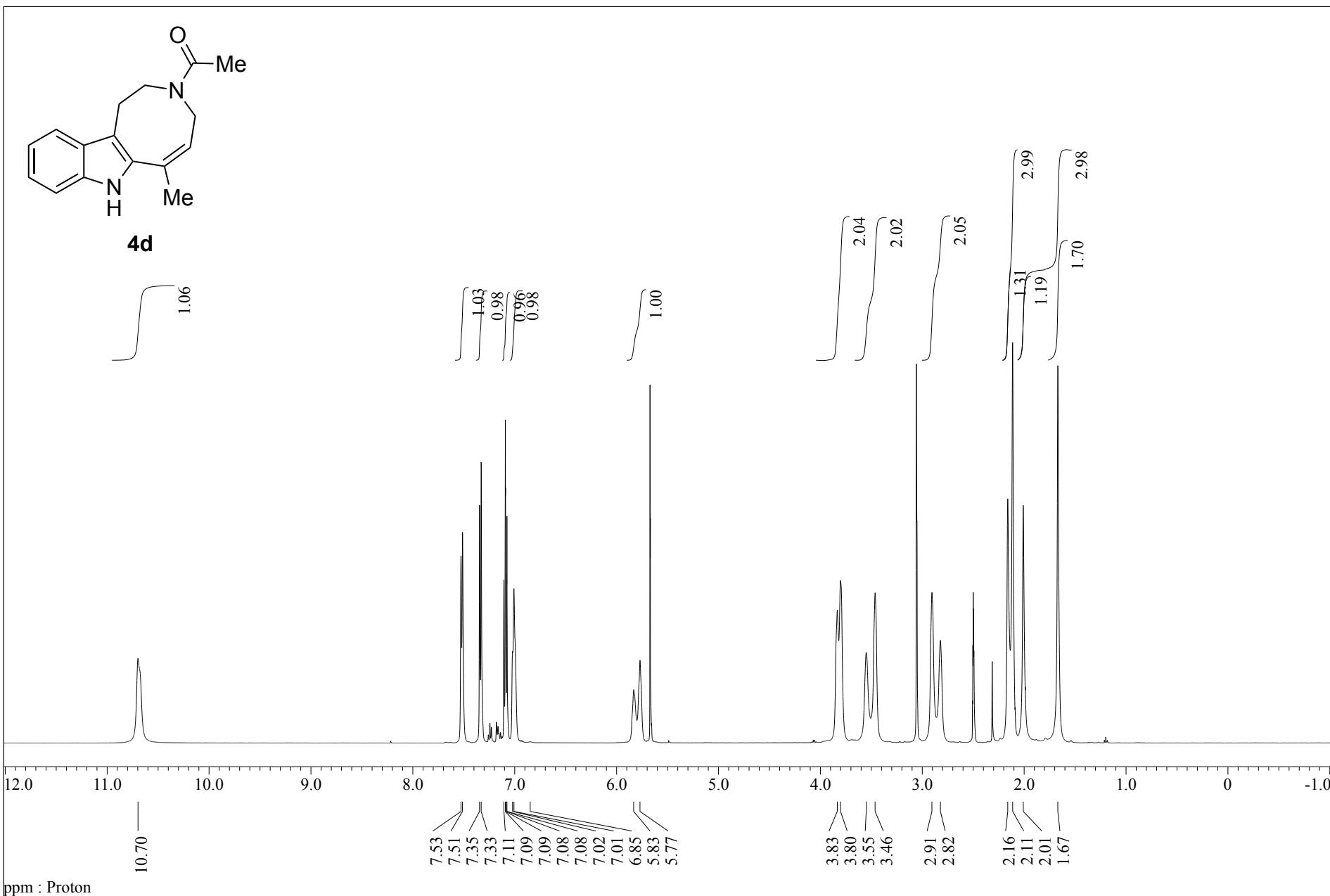


Figure S35. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$, 90 °C) of **4d**.

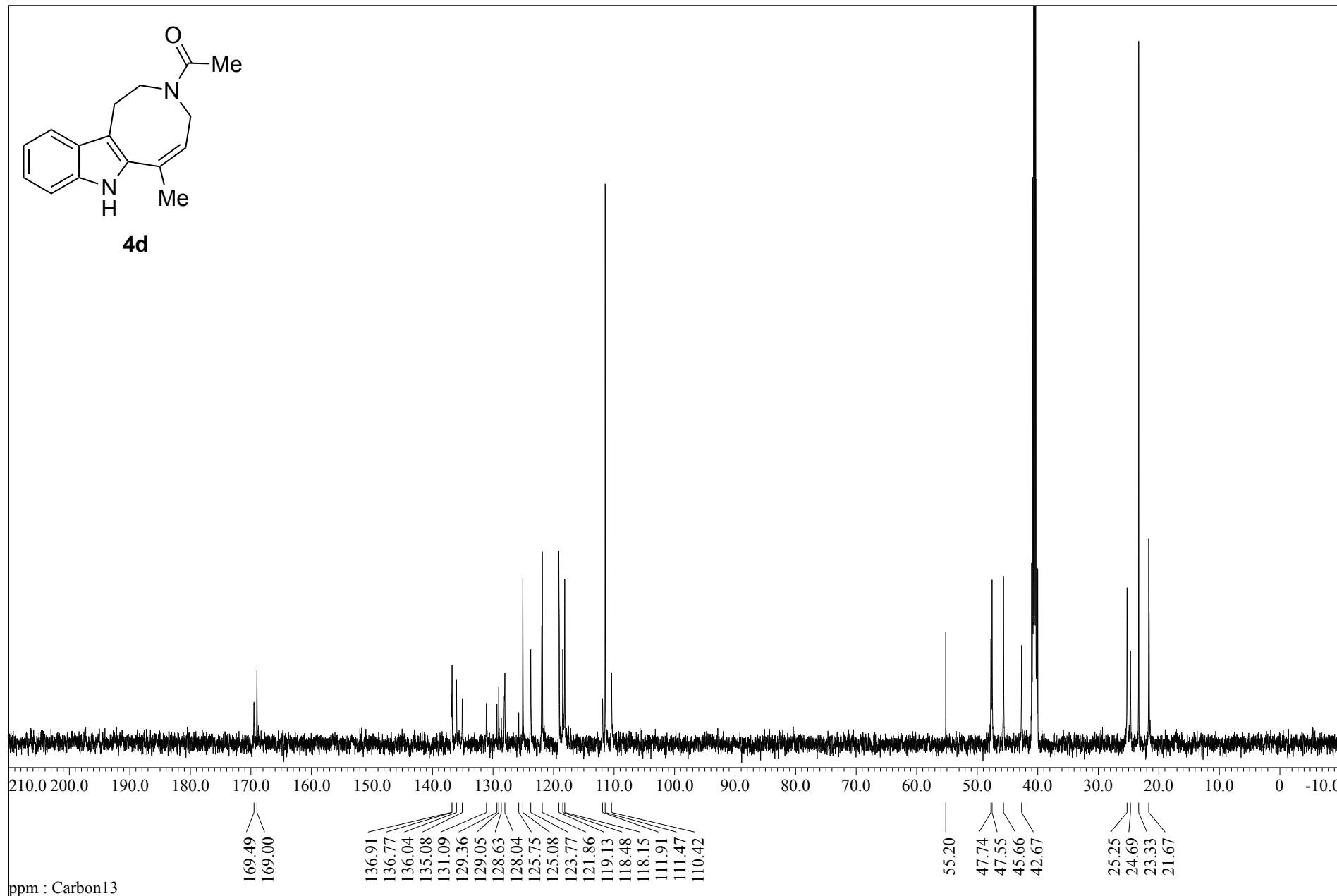


Figure S36. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$, 90 °C) of **4d**.

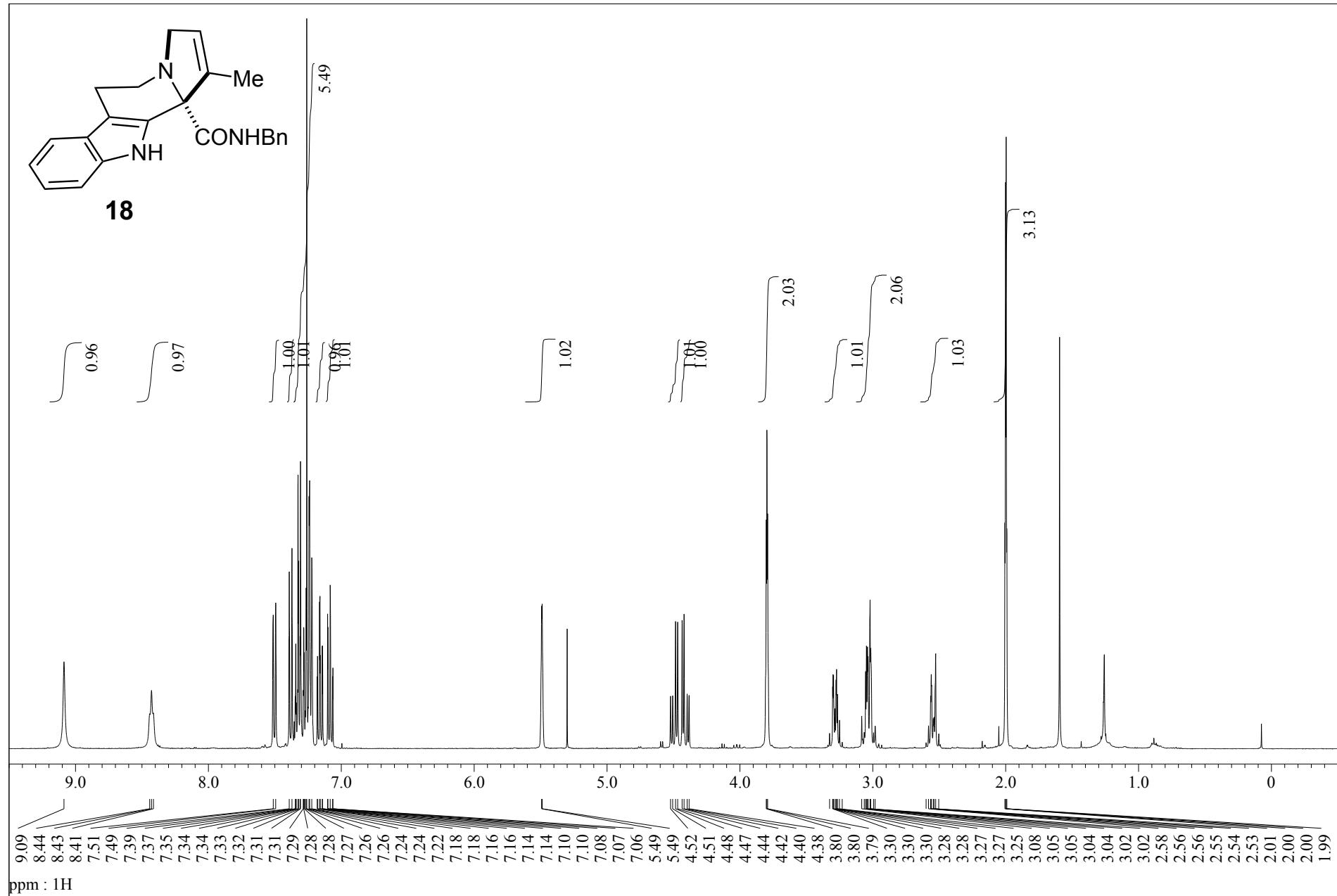


Figure S37. ^1H NMR spectrum (400 MHz, CDCl_3) of **18**.

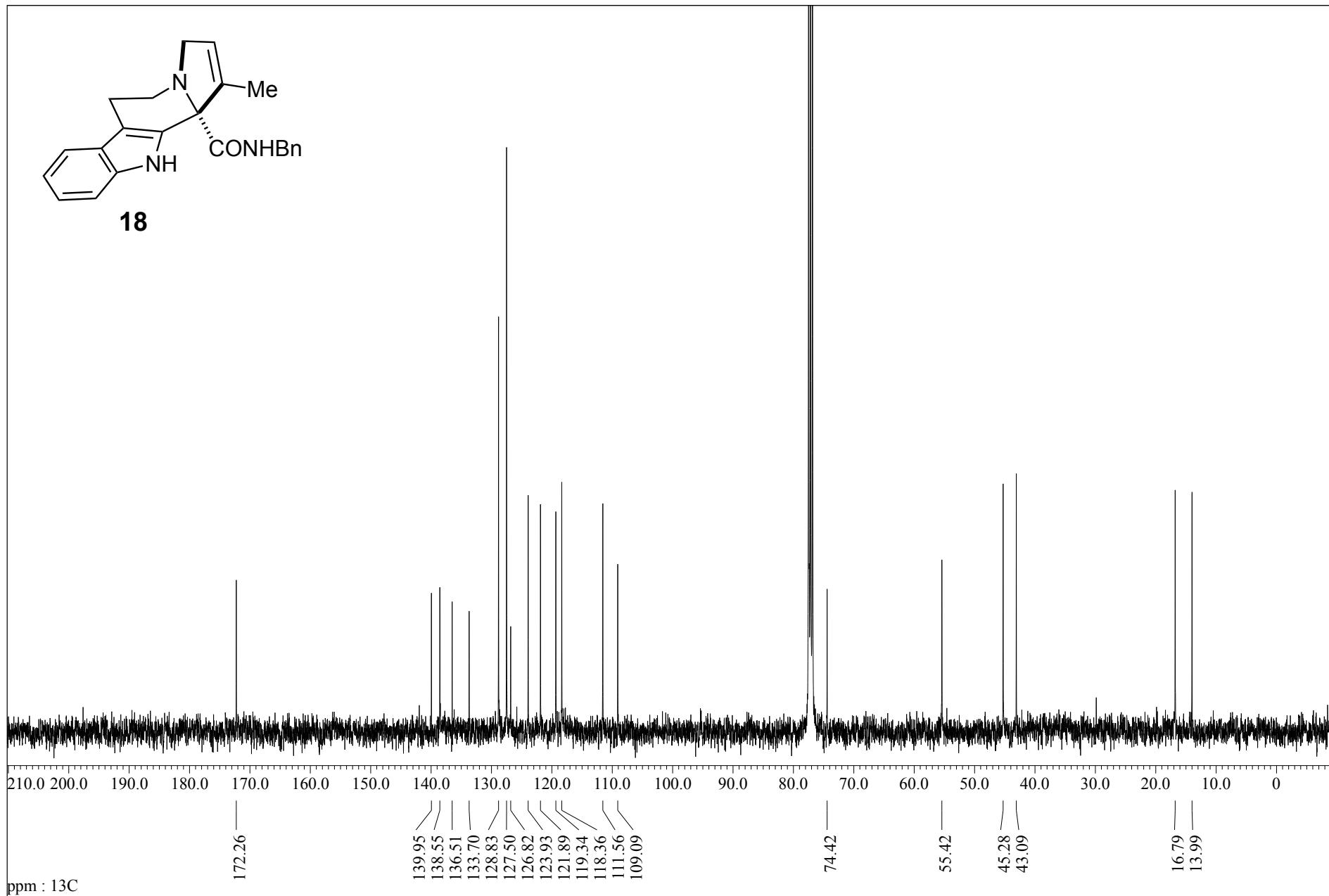


Figure S38. ^{13}C NMR spectrum (100 MHz, CDCl_3) of **18**.

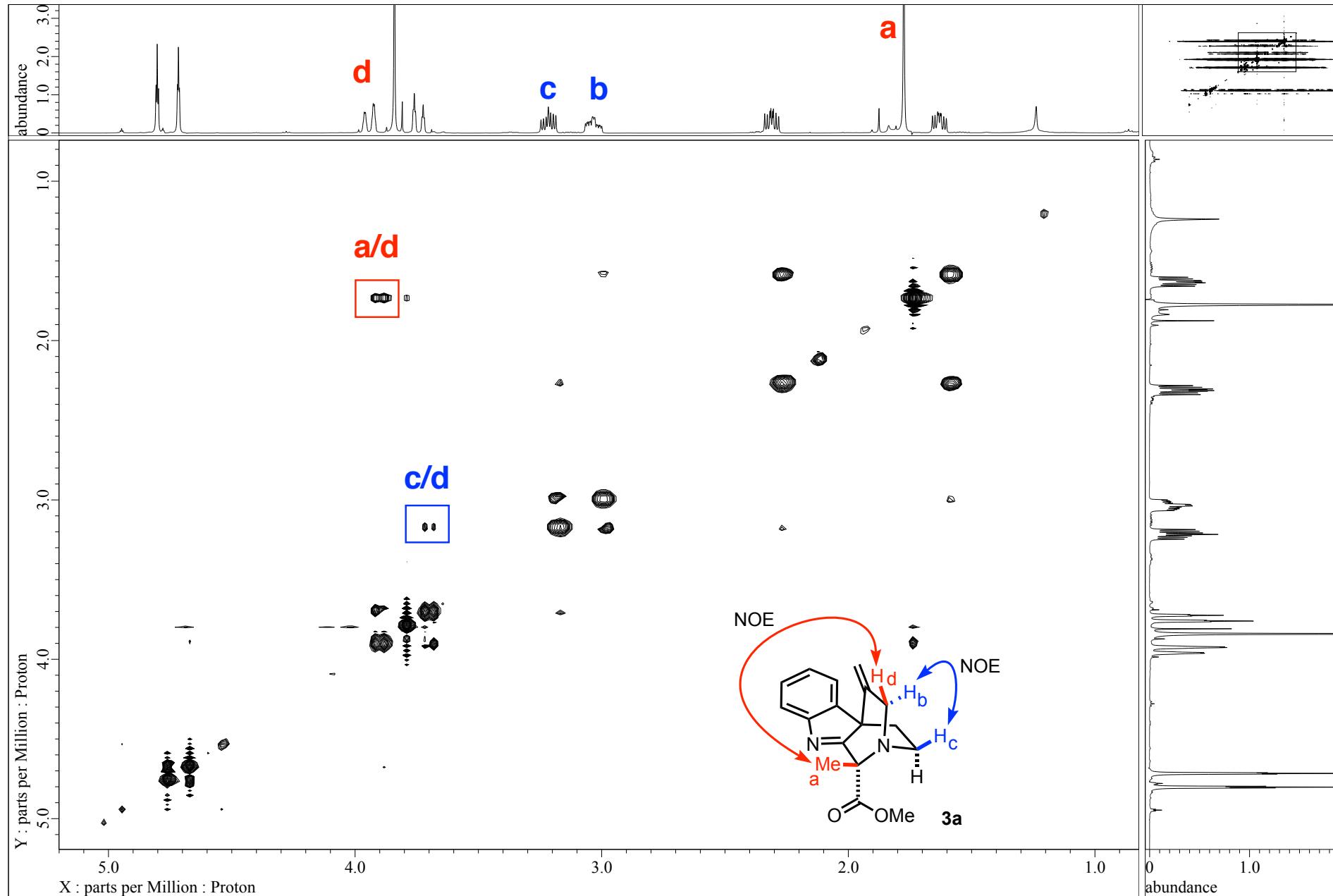


Figure S39. NOESY spectrum (500 MHz, CDCl_3) of **3a**.

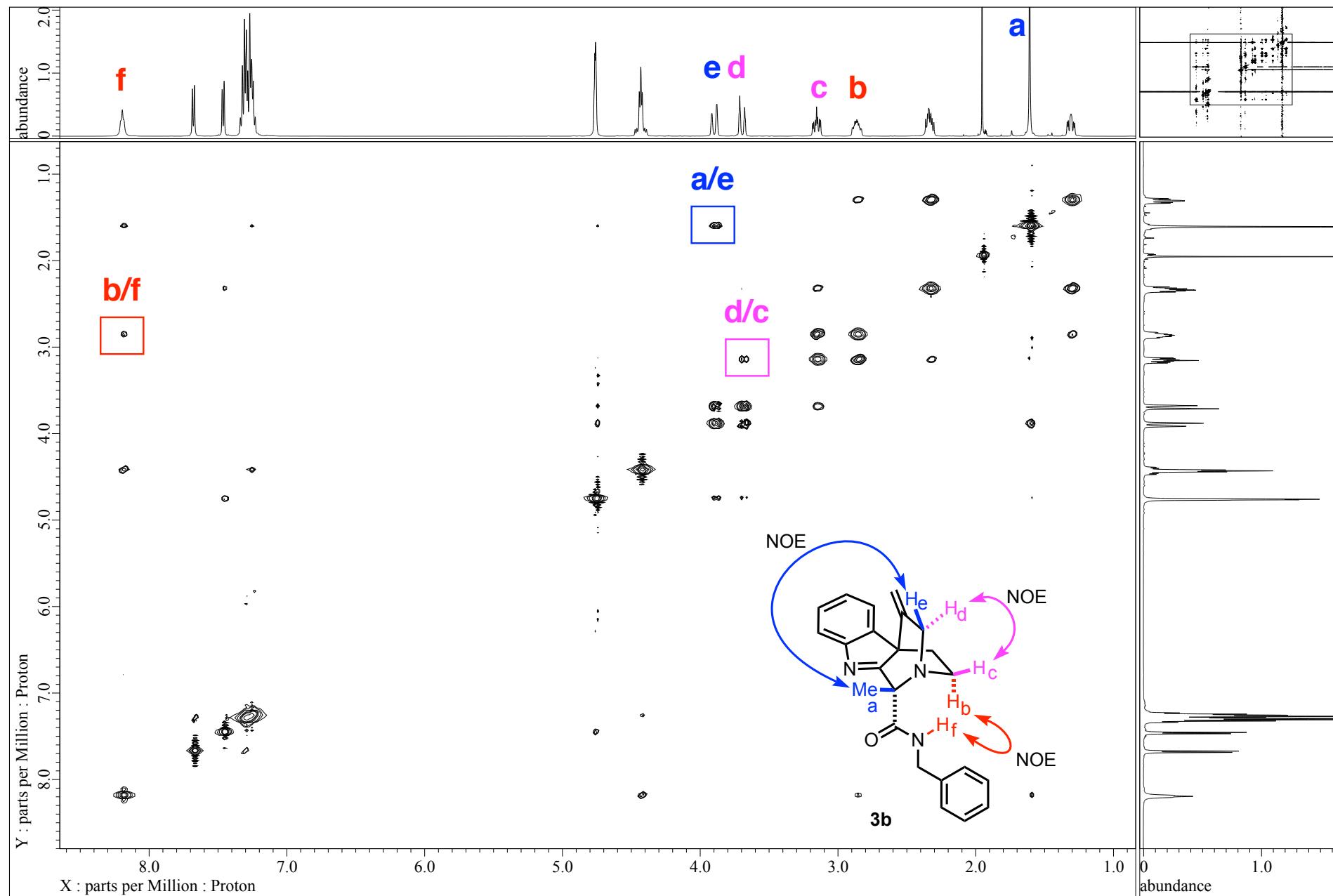


Figure S40. NOESY spectrum (500 MHz, CDCl_3) of **3b**.