

Supporting Information

Protecting group-Free Total Syntheses of (\pm)-Norascyronones A and B**

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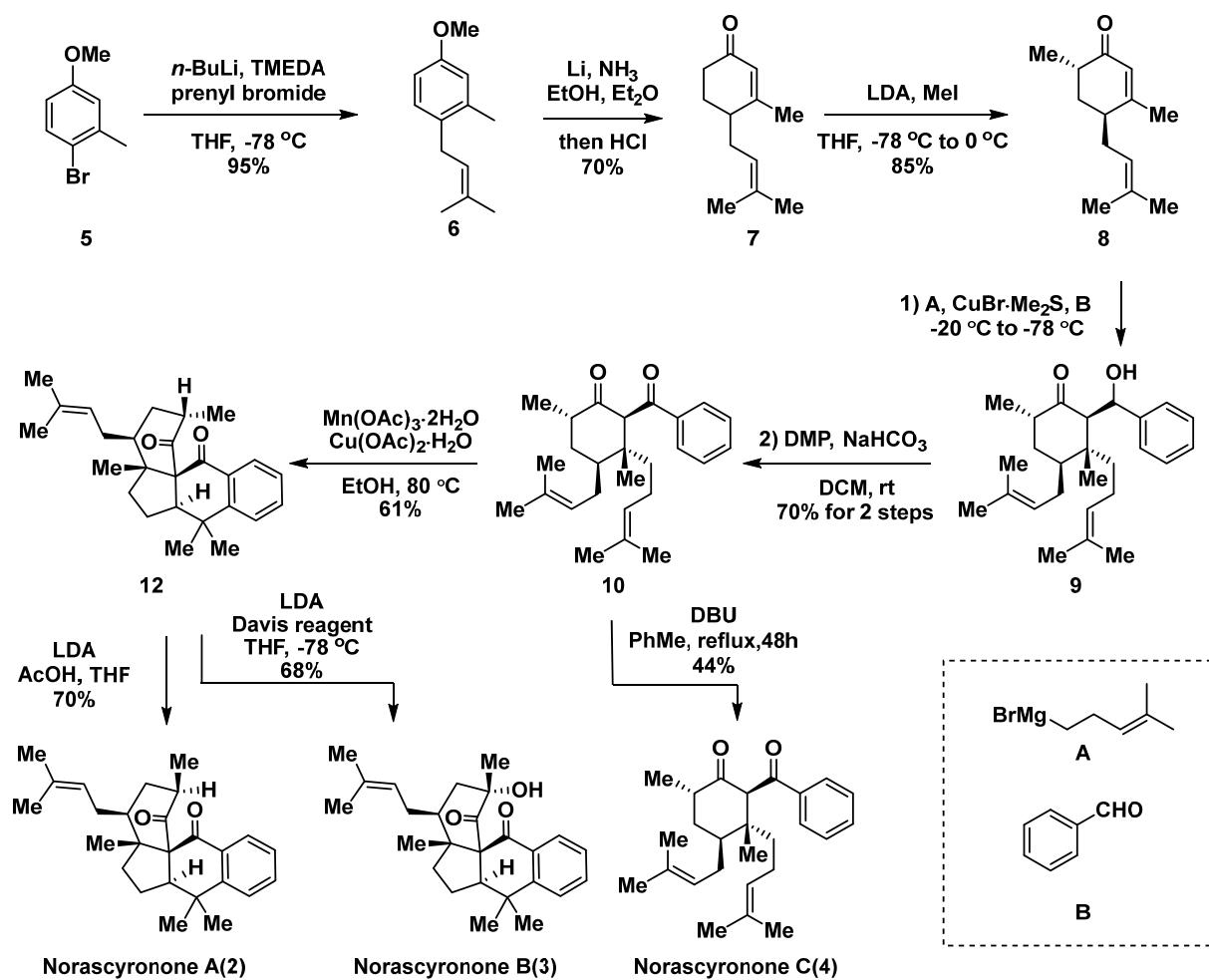
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I. General information

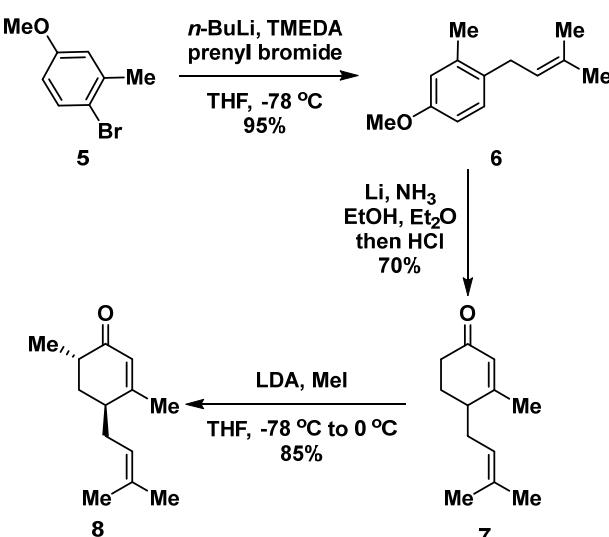
Unless otherwise noted, all reactions were carried out under an argon atmosphere with dry solvents. Reagents were purchased at the highest commercial quality and used without further purification. Solvents purification was conducted according to Purification of Laboratory Chemicals (Peerrin, D. D.; Armarego, W. L. and Perrins, D. R., Pergamon Press: Oxford, 1980). The reactions that require heating were maintained in oil bath. Yields refer to chromatographically and spectroscopically (¹H NMR) homogeneous materials. Reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm Tsingdao silica gel plates (GF-254) using UV light at 254 nm as visualizing agent and ethanolic solution of phosphomolybdic acid (PMA) and cerium sulfate or basic aqueous potassium permanganate (KMnO₄) solution as staining agent. Tsingdao silica gel (60, particle size 0.040–0.063 mm) was neutralized with PH = 7.0 buffer for flash column chromatography. NMR spectra were recorded on either a Brüker Advance III 400 (¹H: 400 MHz, ¹³C: 100 MHz), Brüker Advance 500 (¹H: 500 MHz, ¹³C: 125 MHz) or Brüker Advance 300 (¹H: 300 MHz, ¹³C: 75 MHz) and were calibrated using residual undeuterated solvent as an internal reference (CDCl₃: ¹H NMR = 7.26 ppm, ¹³C NMR = 77.16 ppm). The following abbreviations were used to designate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. IR spectra were recorded on an IR Prestige-21 FTIR spectrometer with a KBr disc. High resolution mass spectra (HRMS) data were recorded on ABI Qstar Elite mass with TOF analyzer.

II: Experimental Procedures and Spectroscopic Data of Synthesized Compounds



Scheme S1: An overview of the synthetic route.

Preparation of Compound 8:



Preparation of Compound 6:

To a solution of commercially available compound **5** (20 g, 100 mmol) in THF (200 mL) was added with *n*-BuLi (2.5 M, 60 mL, 150 mmol) at -78 °C, and the resultant mixture was stirred at the same temperature for 20 min. To this solution was added tetramethylethylenediamine (11.6 g, 100 mmol), and the mixture was stirred at the same temperature for an additional 20 min. To this solution was added prenyl bromide (5.24 g, 150 mmol) at -78 °C, and the resulting solution was stirred at 25 °C for 3 h. The reaction was quenched with water (100 mL), and the mixture was extracted with diethyl ether (3 x 100 mL). The combined extracts were dried over Na₂SO₄. The solvent was removed under vacuum, and the residue was purified by flash chromatography on a silica column (hexane/EtOAc = 100:1) to give product **6** (18 g, 95%) as a colorless oil.

Compound 6: R_f = 0.6 (silica gel, hexane/EtOAc = 20:1, UV).

IR (thin film, ν cm⁻¹): ν_{max} 1611, 1502, 1434, 1203, 940 cm⁻¹.

HRMS (APCI): m/z [M+H⁺] calcd for C₁₃H₁₉O⁺ [M+H⁺]: 191.1430; found: 191.1432.

¹H NMR (300 MHz, CDCl₃) δ 7.06 (d, J = 8.2 Hz, 1H), 6.70 (dd, J = 11.5, 3.3 Hz, 2H), 5.23 (t, J = 7.8 Hz, 1H), 3.79 (s, 3H), 3.25 (d, J = 7.1 Hz, 2H), 2.28 (s, 3H), 1.75 (s, 3H), 1.73 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ 157.8, 137.5, 132.3, 132.1, 129.6, 123.1, 116.0, 111.0, 55.3, 31.5, 25.9, 19.6, 18.0.

Preparation of Compound 7:

To a solution of **6** (10 g, 52.6 mmol) in THF (60 mL) and absolute EtOH (6 mL) was added freshly distilled anhydrous NH₃ (75 mL) at -78 °C. To this slurry was added small pieces of Li ribbon (5.0 g,

725 mmol) at -78 °C in portion-wise manner to keep the reaction slurry in blue color over a period of 3 h, and the reaction mixture was stirred at the same temperature for one hour. The reaction was worked up by addition of solid NH₄Cl (5.0 g), followed by addition of hexanes (50 mL). Ammonia in the reaction mixture was allowed to evaporate, and the mixture was slowly warmed up to room temperature. To this mixture was added hexanes (50 mL) and water (25 mL), and the formed organic layer was separated, and the aqueous layer was extracted with hexanes (2 x 5 mL). The combined organic extract was evaporated in vacuo to give a colorless oil, which was directly used in the next step.

To a solution of the crude product obtained above in THF (50 mL) was added aqueous HCl (1.0 M, 50 mL), and the resulting mixture was stirred at 23 °C for 20 h. The reaction was worked up by removal of the organic solvent under vacuum, and the resultant mixture was diluted with water (50 mL) and ether (50 mL), followed by addition of a saturated aqueous solution of NaHCO₃ slowly until gas evolution ceased. The resulting mixture was filtered off through a short silica gel pad, and the filtrate was extracted with EtOAc (3 x 50 mL). The combined extracts were dried over Na₂SO₄. The solvent was removed under vacuum, and residue was purified by a flash chromatography on silica gel (hexane:EtOAc = 50:1) to give product **7** (6.5 g, 70%) as a light-yellow oil.

Compound 7: R_f = 0.62 (silica gel, hexane/EtOAc = 10:1, UV);

IR (thin film, ν cm⁻¹): ν_{max} 2968, 2874, 1670, 1379, 857 cm⁻¹.

HRMS (ESI): m/z [M+H⁺] calcd for C₁₂H₁₉O⁺ [M+H⁺]: 179.1430; found: 179.1433.

¹H NMR (500 MHz, CDCl₃) δ 5.83 (s, 1H), 5.10 (s, 1H), 2.45–2.38 (m, 1H), 2.34 – 2.22 (m, 3H), 2.20 – 2.09 (m, 1H), 1.99 (d, J = 5.3 Hz, 1H), 1.96 (s, 3H), 1.90 – 1.76 (m, 1H), 1.71 (s, 3H), 1.62 (s, 3H).

¹³C NMR (125 MHz, CDCl₃) δ 199.4, 165.8, 134.0, 127.0, 122.0, 40.1, 34.2, 29.9, 26.6, 25.9, 23.2, 18.0.

Preparation of Compound 8:

To a solution of compound **7** (3.0 g, 16.82 mmol, 1.0 equiv.) in THF (200 mL) was added LDA (10 mL, 2.0 M solution in THF/hexane, 1.2 equiv.) at -78°C for 1 h, and the resultant mixture was then stirred at the same temperature for 1 h. To this solution was added MeI (1.5 mL, 25.23 mmol, 1.5 equiv.) at -78 °C slowly, and the resultant mixture was first stirred at -78°C for 30 min. and then stirred at 0°C for 2 h. The reaction mixture was quenched by addition of water (100 mL), and the resultant mixture was extracted with ethyl acetate (3 x 100 mL). The combined organic extracts were first washed with a saturated solution of NaCl (100 ml), and then dried over Na₂SO₄. The extract was filtrated off, and the

filtrate was concentrated under vacuum, and the residue was purified by a flash column chromatography (hexane:EtOAc = 10:1) on silica gel to give the desired product **8** (2.75 g, 85%) as a yellow oil.

Compound 8: R_f = 0.43 (silica gel, hexane/EtOAc = 5:1, UV).

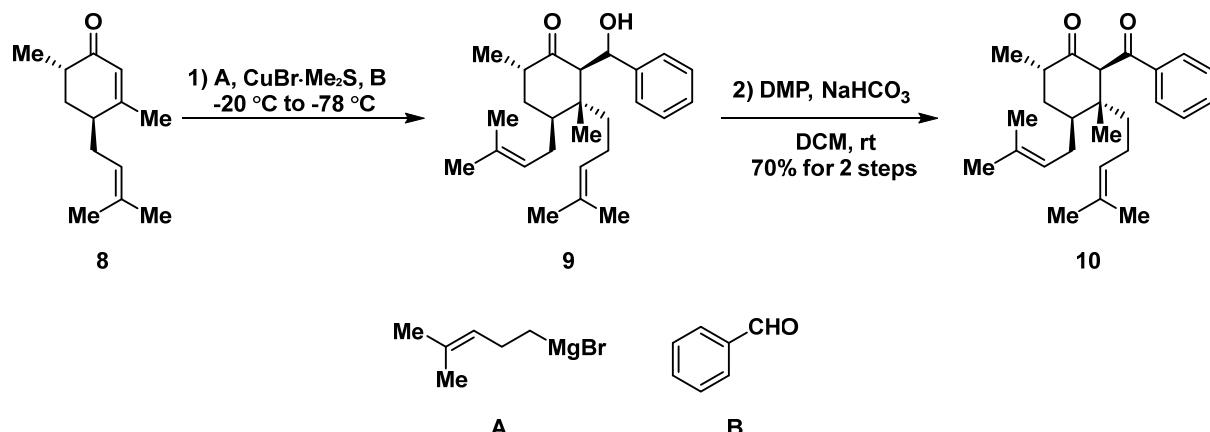
IR (thin film, ν cm⁻¹): ν_{max} 2968, 2930, 1627, 1379, 1217 cm⁻¹.

HRMS (ESI): m/z [M+H⁺] calcd for C₁₃H₂₁O⁺: 193.1587; found: 193.1591.

¹H NMR (300 MHz, CDCl₃) δ 5.78 (s, 1H), 5.13 (s, 1H), 2.50 – 2.37 (m, 1H), 2.33 – 2.09 (m, 3H), 1.94 (s, 4H), 1.72 (d, J = 1.4 Hz, 4H), 1.62 (s, 3H), 1.09 (d, J = 6.8 Hz, 3H).

¹³C NMR (75 MHz, CDCl₃) δ 201.0, 163.7, 132.8, 125.1, 121.3, 39.0, 35.1, 33.7, 28.6, 24.8, 21.9, 16.8, 14.4.

Preparation of Compound 10:



To a stirred suspension of mashed magnesium (749 mg, 31.20 mmol, 2.0 equiv.) and iodine (0.10 g) in THF (100 mL) was added a portion (1 mL) of a solution of 5-bromo-2-methyl-2-pentene (4.07 g, 24.96 mmol, 1.6 equiv.) in THF (15 mL) under argon, and the resultant mixture was first gently heated to initiate the Grignard reaction, and then added the rest of the THF solution of 5-bromo-2-methyl-2-pentene carefully. The resultant mixture was first heated under reflux for 1.5 h, and cooled to the room temperature. To this mixture was added to a solution of CuBr.Me₂S (160 mg, 0.78 mmol, 0.05 equiv) in THF (10 mL) at -20 °C slowly via a gas-tight syringe, and the resultant mixture was then stirred at the same temperature for 30 min. To this solution was added a solution of **8** (3.00 g, 15.60 mmol, 1.0 equiv.) in THF (10 mL) at -20 °C in a drop-wise manner, and the resultant mixture was first stirred at the same temperature for 20 min, and then cooled to -78 °C. To this solution was added a solution of **B** (1.99 g, 18.72 mmol, 1.2 equiv.) in THF (10 mL) at -78 °C slowly, and the resultant mixture was then stirred at the same temperature for 20 h. The reaction mixture was then quenched by addition of a saturated

solution of NH₄Cl, and the resultant mixture was extracted with ethyl acetate (3 x 100 mL). The combined organic extracts were first dried over MgSO₄, and then filtered off, and finally concentrated under vacuum.

To a solution of the crude product prepared above was added NaHCO₃ (2.62 g, 31.20 mmol, 2.0 equiv.) and DMP (9.92 g, 23.4 mmol, 1.5 equiv.) in DCM (50 mL) at 0 °C, and the resulting mixture was stirred at room temperature for 1 h. The reaction mixture was quenched by addition of a saturated solution of NaHCO₃ slowly, and the mixture was extracted with ethyl acetate (3 x 100 mL). The combined organic extracts were first dried over MgSO₄, and then filtered off, and finally concentrated under vacuum. The residue was purified by a flash column chromatography (hexane:EtOAc = 30:1) on silica gel to give the desired product **10** (4.20 g, 70% for 2 steps) as a colorless oil.

Compound 10: R_f = 0.38 (silica gel, hexane/EtOAc = 30:1, UV).

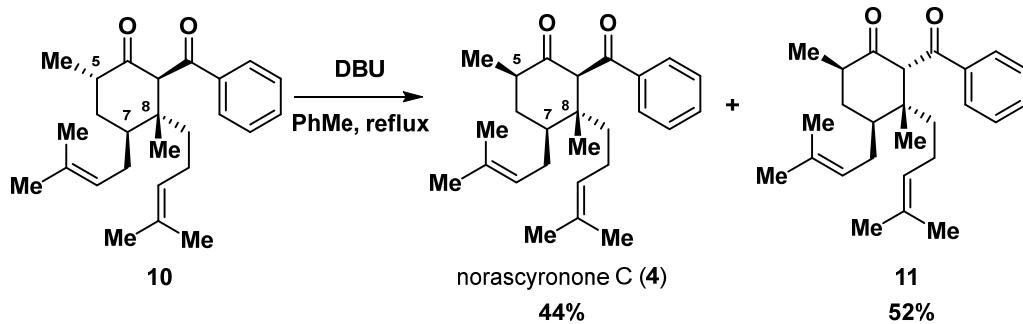
IR (thin film, ν cm⁻¹): ν_{max} 2972, 2877, 1687, 1349, 694 cm⁻¹.

HRMS (ESI): m/z [M+H⁺] calcd for C₂₆H₃₇O₂⁺: 381.2788; found: 381.2788.

¹H NMR 1H NMR (400 MHz, CDCl₃) δ 7.79 (d, J = 8.6 Hz, 2H), 7.52 (t, J = 7.4 Hz, 1H), 7.42 (t, J = 7.6 Hz, 2H), 5.14 – 5.07 (m, 1H), 4.88 (t, J = 7.2 Hz, 1H), 2.76 -2.70 (m, 1H), 2.18 (dd, J = 14.0, 4.4 Hz, 1H), 2.04 – 1.94 (m, 2H), 1.91 – 1.78 (m, 4H), 1.74 (s, 4H), 1.63 (s, 4H), 1.52 (s, 4H), 1.40 – 1.35 (m, 6H), 1.15 (s, 3H).

¹³C NMR (100MHz, CDCl₃) δ 212.7, 197.6, 138.8, 133.1, 132.9, 131.9, 128.8 (2C), 127.8 (2C), 123.8, 123.2, 60.5, 46.2, 43.9, 38.3, 37.6, 34.2, 27.1, 26.1, 25.7, 22.4, 18.3, 18.2, 18.1, 17.5.

Preparation of Compound Norascyonone C (4):



To a solution of compound **10** (400 mg, 1.05 mmol, 1.0 equiv) in PhMe (5 mL) was added DBU (1.6 g, 10.5 mmol, 10 equiv.), the resultant mixture was stirred at 130 °C for 48 h. After cooling to room temperature, the solvent of the reaction was removed under vacuum, and the residue was purified

by a flash column chromatography on silica gel (hexane:EtOAc = 10:1) to give Norascyronone C (**4**) (176 mg, 44%) as a colorless oil and compound **11** (208 mg, 52%) as a colorless oil.

Compound Norascyronone C(4): R_f = 0.44 (silica gel, hexane/EtOAc = 20:1, UV).

IR (thin film, ν cm⁻¹): ν_{max} 2968, 2861, 1682, 1379, 762 cm⁻¹.

HRMS (ESI): m/z [M+H⁺] calcd for C₂₆H₃₇O₂⁺: 381.2788; found: 381.2789.

¹H NMR (500 MHz, CDCl₃) δ 7.72 (d, J = 7.3 Hz, 2H), 7.45 (t, J = 7.4 Hz, 1H), 7.36 (t, J = 7.7 Hz, 2H), 5.10 (t, J = 7.2 Hz, 1H), 4.81 (t, J = 7.1 Hz, 1H), 4.55 (s, 1H), 2.59 – 2.51 (m, 1H), 2.16 – 2.10 (m, 2H), 1.98 – 1.93 (m, 1H), 1.91 (d, J = 3.6 Hz, 1H), 1.69 (s, 3H), 1.66 (d, J = 7.4 Hz, 2H), 1.57 (s, 3H), 1.53 – 1.47 (m, 2H), 1.45 (s, 3H), 1.28 (s, 3H), 1.26 (d, J = 13.5 Hz, 1H), 1.08 (s, 3H), 0.98 (d, J = 6.4 Hz, 3H).

¹³C NMR (125 MHz, CDCl₃) δ 209.6, 196.9, 138.6, 133.0, 132.8, 131.8, 128.7 (2C), 127.6 (2C), 123.7, 123.1, 63.5, 46.4, 45.5, 42.9, 37.3, 36.6, 27.1, 26.0, 25.6, 22.2, 18.0, 17.7, 17.4, 14.5.

Compound 11: R_f = 0.58 (silica gel, hexane/EtOAc = 40:1, UV).

IR (thin film, ν cm⁻¹): ν_{max} 2973, 2833, 1699, 1344, 765 cm⁻¹.

HRMS (ESI): m/z [M+H⁺] calcd for C₂₆H₃₇O₃⁺: 381.2788; found: 381.2781.

¹H NMR (400 MHz, CDCl₃) δ 8.05 (d, J = 7.4 Hz, 2H), 7.53 (t, J = 7.3 Hz, 1H), 7.43 (t, J = 7.6 Hz, 2H), 5.20 (t, J = 7.1 Hz, 1H), 4.86 (d, J = 6.7 Hz, 1H), 4.48 (s, 1H), 2.93 – 2.83 (m, 1H), 2.82 – 2.76 (m, 1H), 2.21 (d, J = 15.2 Hz, 1H), 2.16 – 2.10 (m, 1H), 1.82 – 1.74 (m, 1H), 1.73 (s, 3H), 1.67 (dd, J = 18.2, 6.5 Hz, 2H), 1.61 (s, 3H), 1.52 (s, 3H), 1.50 – 1.43 (m, 2H), 1.24 (s, 1H), 1.21 (s, 3H), 0.93 (d, J = 6.4 Hz, 3H), 0.89 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 209.1, 196.0, 138.0, 133.4 (2C), 132.5, 131.7, 128.8 (3C), 124.0, 123.9, 69.7, 46.4, 41.7, 41.4, 37.9 (2C), 28.2, 26.0, 25.7, 22.7, 19.0, 18.1, 17.3, 14.4.

Table 1. The profile for the oxidative cascade reaction of diketone **4^a**

entry	oxidant	equiv.	solvent	temp (°C)	time (h)	yield (%) ^a
						4 11 2
1	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	(Mn ^{III} /Cu ^{II} = 2/1)	EtOH ^b	80	48	30 trace
2	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	(Mn ^{III} /Cu ^{II} = 2/1)	AcOH ^b	80	16	25 10
3	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	(Mn ^{III} /Cu ^{II} = 2/1)	CF ₃ CH ₂ OH ^c	80	16	
4	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	(Mn ^{III} /Cu ^{II} = 2/1)	DMF ^c	130	16	
5	Mn(OAc) ₃ ·2H ₂ O	(2)	AcOH ^b	80	16	34 8
6	Mn(OAc) ₃ ·2H ₂ O (YbOTf) ₂ ·H ₂ O	(Mn ^{III} /Yb ^{II} = 2.2/1)	CF ₃ CH ₂ OH ^c	80	16	
7	CAN	(2)	MeCN ^c	70	12	
8	FeCl ₃	(2)	MeCN ^c	70	12	

^aIsolated yield. ^bThe starting material partially decomposed. ^cThe starting material decomposed.

Preparation of Compound **11**:

To a solution of Norascyonone C (**4**) (50 mg, 0.13 mmol, 1.0 equiv) in AcOH (1.0 ml) was added Mn(OAc)₃·2H₂O (70 mg, 0.26 mmol, 2.0 equiv) and Cu(OAc)₂·H₂O (26 mg, 0.13 mmol, 1.0 equiv), and the mixture was first cooled to -78 °C, and then degassed with Ar. The resultant mixture was then stirred at 80 °C for 16 h. Upon cooling to room temperature, the reaction mixture was purified by a flash column chromatography on silica gel (hexane:EtOAc = 40:1) to give product **11** (5 mg, 10%) as a colorless oil.

Compound 11: R_f = 0.58 (silica gel, hexane/EtOAc = 40:1, UV).

IR (thin film, ν cm⁻¹): ν_{max} 2973, 2833, 1699, 1344, 765 cm⁻¹.

HRMS (ESI): m/z [M+H⁺] calcd for C₂₆H₃₇O₃⁺: 381.2788; found: 381.2781.

¹H NMR (400 MHz, CDCl₃) δ 8.05 (d, J = 7.4 Hz, 2H), 7.53 (t, J = 7.3 Hz, 1H), 7.43 (t, J = 7.6 Hz, 2H), 5.20 (t, J = 7.1 Hz, 1H), 4.86 (d, J = 6.7 Hz, 1H), 4.48 (s, 1H), 2.93 – 2.83 (m, 1H), 2.82 – 2.76 (m, 1H), 2.21 (d, J = 15.2 Hz, 1H), 2.16 – 2.10 (m, 1H), 1.82 – 1.74 (m, 1H), 1.73 (s, 3H), 1.67 (dd, J = 18.2, 6.5 Hz, 2H), 1.61 (s, 3H), 1.52 (s, 3H), 1.50 – 1.43 (m, 2H), 1.24 (s, 1H), 1.21 (s, 3H), 0.93 (d, J = 6.4 Hz, 3H), 0.89 (s, 3H).

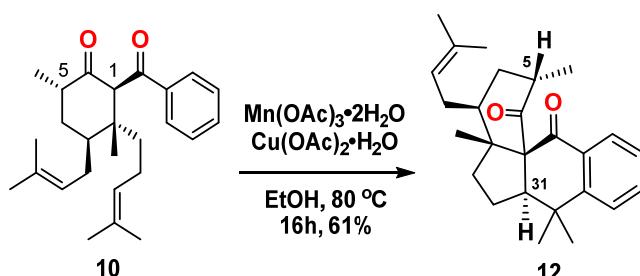
¹³C NMR (100 MHz, CDCl₃) δ 209.1, 196.0, 138.0, 133.4 (2C), 132.5, 131.7, 128.8 (3C), 124.0, 123.9, 69.7, 46.4, 41.7, 41.4, 37.9 (2C), 28.2, 26.0, 25.7, 22.7, 19.0, 18.1, 17.3, 14.4.

Table 2. Oxidative cyclization for the synthesis of 12.

entry	oxidant	equiv	solvent	temp (°C)	time (h)	yield (%) ^b		
						4	11	12
1	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	Mn ^{III} /Cu ^{II} = 2/1	AcOH	80	16	22	13	40
2	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	Mn ^{III} /Cu ^{II} = 2/1	EtOH	80	32			61
3	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	Mn ^{III} /Cu ^{II} = 2/1	MeCN	80	32			
4	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	Mn ^{III} /Cu ^{II} = 2/1	1,4-dioxane	80	32			5
5	Mn(OAc) ₃ ·2H ₂ O Cu(OAc) ₂ ·H ₂ O	Mn ^{III} /Cu ^{II} = 2/1	DMF	80	32			27
6	Mn(OAc) ₃ ·2H ₂ O	Mn ^{III} = 2	AcOH	80	16	25	10	18
7	Mn(OAc) ₃ ·2H ₂ O	Mn ^{III} = 2	AcOH/Ac ₂ O ^c	80	16	22	18	6
8	Mn(OAc) ₃ ·2H ₂ O	Mn ^{III} = 2	EtOH	80	16			4
9	Cu(OAc) ₂ ·H ₂ O	Cu ^{II} = 2	AcOH	80	16	64	14	

^aThe reactions were carried out under the conditions listed in the table. ^bIsolated yield. ^cThe ratio of AcOH/Ac₂O is 9/1.

Preparation of Compound 12:



To a solution of compound **10** (50 mg, 0.13 mmol, 1.0 equiv.) in EtOH (1 mL) was added Mn(OAc)₃·2H₂O (70 mg, 0.26 mmol, 2.0 equiv.) and Cu(OAc)₂·H₂O (26 mg, 0.13 mmol, 1.0 equiv.), and the resultant mixture was first cooled to -78 °C followed by degassed with Ar, and the resultant mixture was then stirred at 80 °C for 16 h. After cooling to room temperature, the reaction mixture was purified by a

flash chromatograph on silica gel (hexane:EtOAc = 40:1) to give product **12** (30 mg, 61%) as a colorless oil.

Compound 12: $R_f = 0.64$ (silica gel, hexane/EtOAc = 20:1, UV).

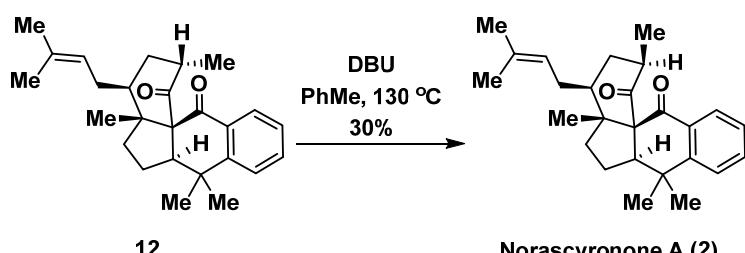
IR (thin film, ν cm $^{-1}$): ν_{max} 2964, 2689, 1674, 1456, 1238 cm $^{-1}$.

HRMS (ESI): m/z [M+H⁺] calcd for C₂₆H₃₅O₂⁺: 379.2632; found: 379.2632.

¹H NMR (400 MHz, CDCl₃) δ 7.69 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.53 – 7.46 (m, 1H), 7.32 – 7.28 (m, 2H), 5.02 (t, *J* = 7.1 Hz, 1H), 3.38 – 3.27 (m, 1H), 3.18 (dd, *J* = 12.0, 7.0 Hz, 1H), 2.47 – 2.38 (m, 1H), 1.92 (d, *J* = 11.5 Hz, 1H), 1.88 – 1.72 (m, 2H), 1.69 (s, 3H), 1.56 (s, 3H), 1.47 (s, 3H), 1.39 – 1.32 (m, 2H), 1.29 (dd, *J* = 8.0, 4.1 Hz, 1H), 1.16 (dd, *J* = 12.4, 6.0 Hz, 1H), 1.11 (d, *J* = 6.9 Hz, 4H), 1.06 (s, 3H), 0.78 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 214.2, 197.9, 150.2, 135.1, 133.2, 133.0, 127.5, 126.8, 124.5, 123.0, 72.7, 57.4, 51.9, 47.4, 42.3, 41.6, 36.2, 35.8, 32.4, 29.3, 28.5, 26.2, 25.9, 18.5, 18.0, 17.0

Preparation of Norascyronone A (2) through the base-mediated thermodynamic epimerization:



To a solution of compound **12** (100 mg, 0.26 mmol, 1.0 equiv.) in PhMe (3 mL) was added DBU (402 mg, 2.64 mmol, 10.0 equiv.), and the resultant mixture was then heated up gently to 130 °C with stirring for 48 h. Upon cooling to room temperature, the solvent of the mixture was concentrated under vacuum, and the residue was purified by a flash column chromatography on silica gel (hexane:EtOAc = 20:1) to give **norascyronone A (2)** (30 mg, 30%) as a colorless oil and compound **12** (67 mg, 67%) recycled as a colorless oil.

Compound Norascyronone A (2): $R_f = 0.31$ (silica gel, hexane/EtOAc = 40:1, UV).

IR (thin film, ν cm $^{-1}$): ν_{max} 2968, 2861, 1674, 1233, 767 cm $^{-1}$.

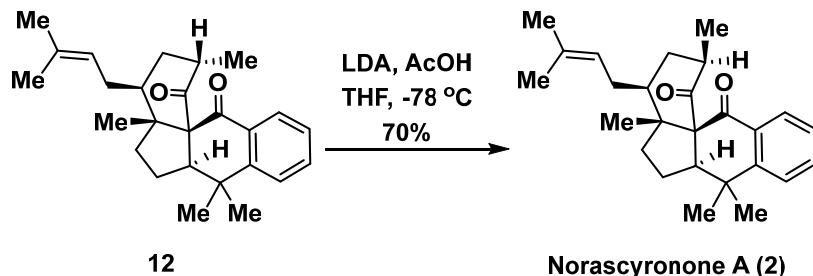
HRMS (ESI): m/z [M+H⁺] calcd for C₂₆H₃₅O₂⁺: 379.2632; found: 379.2629.

¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.44 - 7.40 (m, 1H), 7.25 (dd, *J* = 7.4, 1.9 Hz, 2H), 5.09 (t, *J* = 7.1 Hz, 1H), 3.12 (dd, *J* = 9.9, 8.1 Hz, 1H), 2.87-2.81 (m, 1H), 2.12 – 2.03 (m, 1H), 1.98 (dd, *J* = 13.7, 5.7 Hz, 1H), 1.95 – 1.90 (m, 1H), 1.84 (t, *J* = 11.4 Hz, 1H), 1.76 – 1.70 (m, 1H), 1.68

(s, 3H), 1.66 (d, J = 4.1 Hz, 1H), 1.56 (s, 3H), 1.50 – 1.40 (m, 1H), 1.37 (s, 3H), 1.32 – 1.24 (m, 1H), 1.07 (s, 3H), 1.06 (s, 2H), 1.04 (s, 2H), 0.96 (s, 3H).

¹³C NMR (125 MHz, CDCl₃) δ 213.3, 196.0, 148.9, 134.1, 133.2, 133.1, 127.9, 126.6, 125.1, 123.6, 73.4, 58.8, 54.8, 42.1, 41.8, 37.7, 37.4, 36.2, 33.6, 29.4, 27.6, 27.3, 25.9, 17.9, 17.0, 15.5.

Preparation of Norascyronone A (2) through the kinetic protonation:



To a solution of **12** (50 mg, 0.13 mmol, 1.0 equiv.) of THF (5 mL) was slowly added LDA (198 μ L, 2.0 M solution in THF/Hexane, 3.0 equiv.) at -78°C , and the resultant mixture was stirred at -78°C for 1 h. To this solution was added AcOH (0.10 mL, 1.75 mmol, 13.5 equiv.) at -78°C , the reaction mixture was then stirred for additional 5 min. The reaction mixture was addition of a solution of H_2O (10 mL), and extracted with EtOAc (3 x 50mL). The solvent of the extracts was concentrated under vacuum, and the residue was purified by a flash column chromatography on silica gel (hexane:EtOAc = 10:1) to norascyronone A (**2**) (35 mg, 70%) as a colorless oil and compound **12** (8 mg, 16%) recycled as a colorless oil.

Compound Norascyronone A (**2**): $R_f = 0.31$ (silica gel, hexane/EtOAc = 40:1, UV).

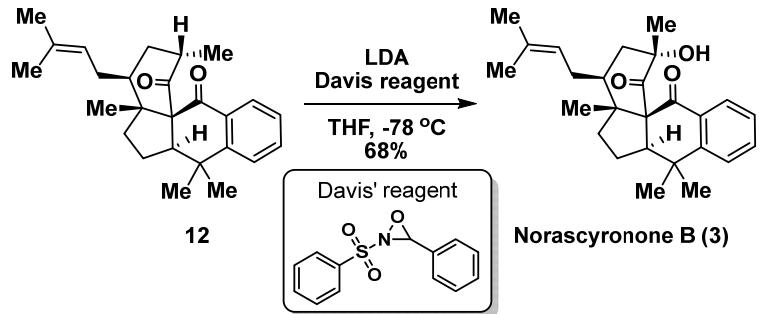
IR (thin film, ν cm $^{-1}$): ν_{max} 2968, 2861, 1674, 1233, 767 cm $^{-1}$.

HRMS (ESI): m/z [M+H⁺] calcd for C₂₆H₃₅O₂⁺: 379.2632; found: 379.2629.

¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.44 - 7.40 (m, 1H), 7.25 (dd, *J* = 7.4, 1.9 Hz, 2H), 5.09 (t, *J* = 7.1 Hz, 1H), 3.12 (dd, *J* = 9.9, 8.1 Hz, 1H), 2.87-2.81 (m, 1H), 2.12 – 2.03 (m, 1H), 1.98 (dd, *J* = 13.7, 5.7 Hz, 1H), 1.95 – 1.90 (m, 1H), 1.84 (t, *J* = 11.4 Hz, 1H), 1.76 – 1.70 (m, 1H), 1.68 (s, 3H), 1.66 (d, *J* = 4.1 Hz, 1H), 1.56 (s, 3H), 1.50 – 1.40 (m, 1H), 1.37 (s, 3H), 1.32 – 1.24 (m, 1H), 1.07 (s, 3H), 1.06 (s, 2H), 1.04 (s, 2H), 0.96 (s, 3H).

¹³C NMR (125 MHz, CDCl₃) δ 213.3, 196.0, 148.9, 134.1, 133.2, 133.1, 127.9, 126.6, 125.1, 123.6, 73.4, 58.8, 54.8, 42.1, 41.8, 37.7, 37.4, 36.2, 33.6, 29.4, 27.6, 27.3, 25.9, 17.9, 17.0, 15.5.

Preparation of Norascyronone B (3):



To a solution of **12** (30 mg, 0.079 mmol, 1.0 equiv.) of THF (5 mL) was slowly added LDA (119 μ L, 2.0 M solution in THF/hexane, 3.0 equiv.) at -78°C , and the resultant mixture was stirred at -78°C for 1 h. To this solution was added Davis reagent (68 mg, 0.26 mmol, 3.0 equiv.) at -78°C , the reaction mixture was then stirred for additional 3 h. The reaction mixture was quenched by addition of a solution of NH₄Cl (10 ml), and extracted with EtOAc (3 x 50 mL). The solvent of the extracts was concentrated under vacuum, and the residue was purified by a flash column chromatography on silica gel (hexane:EtOAc = 10:1) to give Norascyonone B (**3**) (21 mg, 68%) as a white foam.

Compound Norascyonone B (**3**): R_f = 0.25 (silica gel, hexane/EtOAc = 10:1, UV).

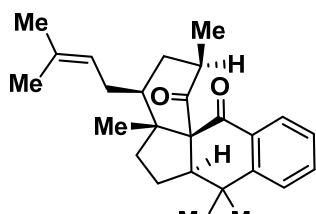
IR (thin film, ν cm⁻¹): ν_{max} 3525, 2933, 1700, 1598, 1062 cm⁻¹

HRMS (ESI): m/z [M+H⁺] calcd for C₂₆H₃₅O₃⁺: 395.2581; found: 395.2580.

¹H NMR (400 MHz, CDCl₃) δ 7.64 (d, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 8.3 Hz, 1H), 7.27 (d, *J* = 8.5 Hz, 1H), 7.24 (d, *J* = 8.7 Hz, 1H), 5.04 (t, *J* = 7.0 Hz, 1H), 2.99 (dd, *J* = 12.6, 6.8 Hz, 1H), 2.77 (s, 1H), 2.33 (t, *J* = 13.3 Hz, 1H), 1.91 (d, *J* = 14.3 Hz, 1H), 1.86 – 1.81 (m, 1H), 1.80 (d, *J* = 5.8 Hz, 1H), 1.70 – 1.65 (m, 2H), 1.64 (s, 3H), 1.52 (s, 3H), 1.51 (s, 3H), 1.43 (s, 3H), 1.31 (td, *J* = 12.4, 11.6, 5.4 Hz, 2H), 1.13 – 1.08 (m, 1H), 1.06 (s, 3H), 0.72 (s, 3H).

¹³C NMR (100MHz, CDCl₃) δ 217.7, 197.4, 159.5, 150.1, 134.4, 133.4, 132.8, 127.5, 126.8, 124.5, 122.8, 77.5, 72.6, 56.4, 53.0, 45.4, 41.9, 36.1, 36.0, 29.5, 28.9, 26.8, 26.3, 25.8, 18.8, 17.9.

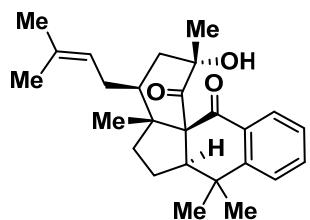
III: Comparison of NMR Spectra



Norascyronone A (2)

¹ H [δ H (ppm), mult, J (Hz)]			¹³ C		
Xu's work 600 MHz	Synthetic 500 MHz	Δδ ppm	Xu's work 600 MHz	Synthetic 125 MHz	Δδ ppm
2.84, m	2.85, dp (13.0, 6.6)	0.01	73.4	73.4	0
1.92, m	1.95–1.90, m	0.01	41.7	41.8	0.1
1.45, q (12.8)	1.50–1.40, m	0	36.2	36.2	0
1.84, brt (12.8)	1.84, t (11.4)	0	42.0	42.1	0.1
			58.8	58.8	0
			213.3	213.3	0
			195.9	196.0	0.1
			134.1	134.1	0
7.86, d (7.6)	7.86, dd (8.0, 1.4)	0	127.9	127.9	0
7.24, t (7.6)	7.27–7.22, m	0.01	126.6	126.6	0
7.42, t (7.6)	7.44–7.40, m	0	133.1	133.2	0.1
7.25, d (7.6)	7.25, dd (7.4, 1.9)	0	125.0	125.1	0.1
			148.8	148.9	0.1
1.05, d (6.6)	1.06, s	0.01	15.5	15.5	0
1.98, brd (13.6)	1.98, dd (13.7, 5.7)	0	29.4	29.4	0
1.65, overlap	1.66, d (4.1)	0.01	123.6	123.6	0
5.09, t (6.8)	5.09, t (7.1)	0	133.0	133.1	0.1
			16.9	17.0	0.1
1.68, s	1.68, s	0	25.9	25.9	0
1.55, s	1.56, s,	0.01	17.9	17.9	0
0.96, s	0.96, s	0	37.4	37.4	0
1.73, m	1.76–1.70, m	0			
1.03, overlap	1.04, s	0.01			
2.07, m	2.12–2.03, m	0.01	27.6	27.6	0
1.28, m	1.32–1.24, m	0	54.8	54.8	0
3.12, dd (9.9, 8.3)	3.12, dd (9.9, 8.1)	0	37.7	37.7	0
			33.5	33.6	0.1
1.06, s	1.07, s	0.01	27.3	27.3	0
1.37, s	1.37, s	0			

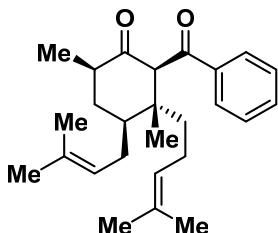
*(a) Spectrum measured in CDCl₃. (b) Δδ (ppm) = (Synthetic – Xu's work)



Norascyonone B(3)

¹ H [δ H (ppm), mult, J (Hz)]			¹³ C		
Xu's work 600 MHz	Synthetic 400 MHz	$\Delta\delta$ ppm	Xu's work 600 MHz	Synthetic 100 MHz	$\Delta\delta$ ppm
			72.6	72.6	0
			77.5	77.5	0
2.23, t (13.3)	2.33, t (13.3)	0	35.9	36.0	0.1
1.65, overlap	1.64, s	-0.01			
1.50, verlap			45.4	45.4	0
			56.4	56.4	0
			217.8	217.7	-0.1
			197.5	197.4	-0.1
			134.4	134.4	0
7.64, d (7.4)	7.64, d (7.4)	0	127.5	127.5	0
7.25, t (7.4)	7.24, d (8.7)	-0.01	126.8	126.8	0
7.45,t (7.4)	7.45, t (8.3)	0	133.4	133.4	0
7.26,d (7.4)	7.27, d (8.5)	0.01	124.5	124.5	0
			150.2	150.1	-0.1
1.51, s	1.51, s	0	26.8	26.8	0
1.91, m	1.91, d (14.3)	0	29.5	29.5	0
1.82, m	1.86–1.81, m				
5.03, t (7.0)	5.04, t (7.0)	0.01	122.8	122.8	0
			132.8	132.8	0
1.64, s	1.64, s	0	25.8	25.8	0
1.52, s	1.52, s	0	17.9	17.9	0
0.72, s	0.72, s	0	18.8	18.8	0
1.67, m	1.70–1.65, m		41.9	41.9	0
1.30, td (12.9,5.9)	1.31, td (12.4, 11.6, 5.4)	0.01			
1.80, m	1.80, d (5.8)	0	28.9	28.9	0
1.10, m	1.13-1.08, m				
2.99, dd (12.7,6.8)	2.99, dd (12.6, 6.8)	0	53.0	53.0	0
			36.1	36.1	0
1.06, s	1.06 , s	0	36.0	36.0	0
1.43, s	1.43, s	0	26.3	26.3	0
2.75, s	2.77, s	0.02			

*(a) Spectrum measured in CDCl₃. (b) $\Delta\delta$ (ppm) = (Synthetic – Xu's work)

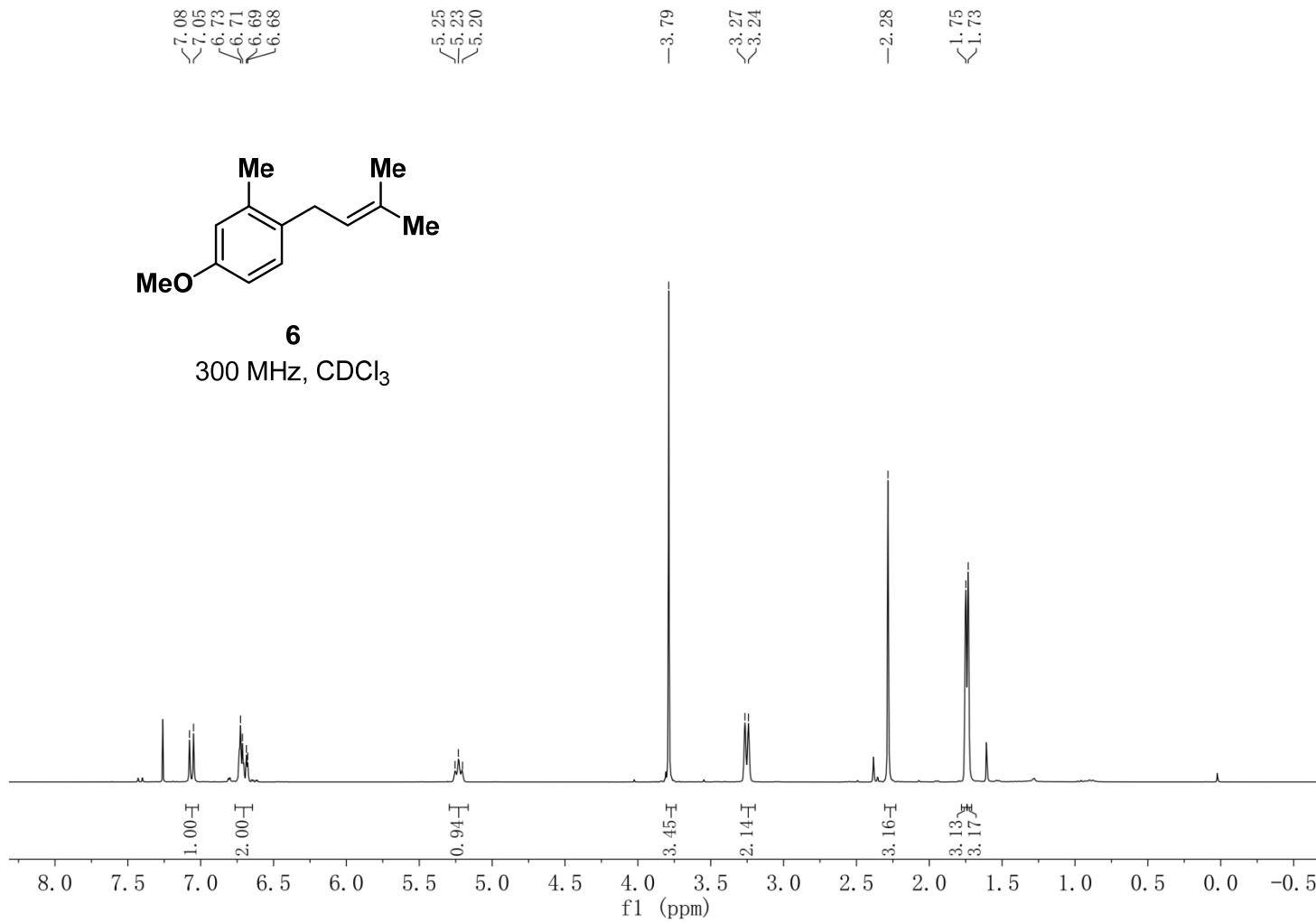


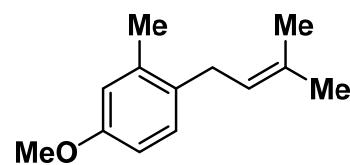
Norascyronone C(4)

¹ H [δ H (ppm), mult, J (Hz)]			¹³ C		
Xu's work 600 MHz	Synthetic 500 MHz	Δδ ppm	Xu's work 600 MHz	Synthetic 125 MHz	Δδ ppm
4.55, s	4.55, s	0	63.7	63.5	-0.2
2.55, m	2.59–2.51, m	0	45.4	45.5	0.1
2.13, m	2.16–2.10, m	0	37.1	37.3	0.2
1.25, q (12.3)	1.26, d (13.5)	0.01			
1.94, m	1.98–1.93, m	0.01	42.8	42.9	0.1
			46.3	46.4	0.1
			209.6	209.6	0.1
			196.8	196.9	0.1
			138.5	138.6	0.1
7.71, d (7.8)	7.72, d (7.3)	0.01	127.5	127.6	0.1
7.35, t (7.8)	7.36, t (7.7)	0.01	128.6	128.7	0.1
7.44, t (7.8)	7.45, t (7.4)	0.01	132.7	132.8	0.1
7.35, t (7.8)	7.36, t (7.7)	0.01	128.6	128.7	0.1
7.71, d (7.8)	7.72, d (7.3)	0.01	127.5	127.6	0.1
0.98, d (6.6)	0.98, d (6.4)		14.4	14.5	0.1
2.11, m	2.16–2.10, m	0.02	26.9	27.1	0.2
1.70, overlap	/				0.1
5.09, t (7.2)	5.10, t (7.2)	0.01	123.0	123.1	0.1
			132.9	132.8	-0.1
1.68, s	1.69, s	0.01	25.9	26.0	0.1
1.56, s	1.57, s	0.01	17.9	18.0	0.1
1.07, s	1.08, s	0.01	17.6	17.7	0.1
1.50, m	1.53–1.47, m	0	36.4	36.6	0.2
1.91, overlap	1.91, d (3.6)	0	22.0	22.2	0.2
1.65, m	1.66, d (7.4)	0.01			
4.80, t (7.0)	4.81, t (7.1)	0.01	123.6	123.7	0.1
			131.7	131.8	0.1
1.44, s	1.45, s	0.01	25.5	25.6	0.1
1.27, s	1.28, s	0.01	17.3	17.4	0.1

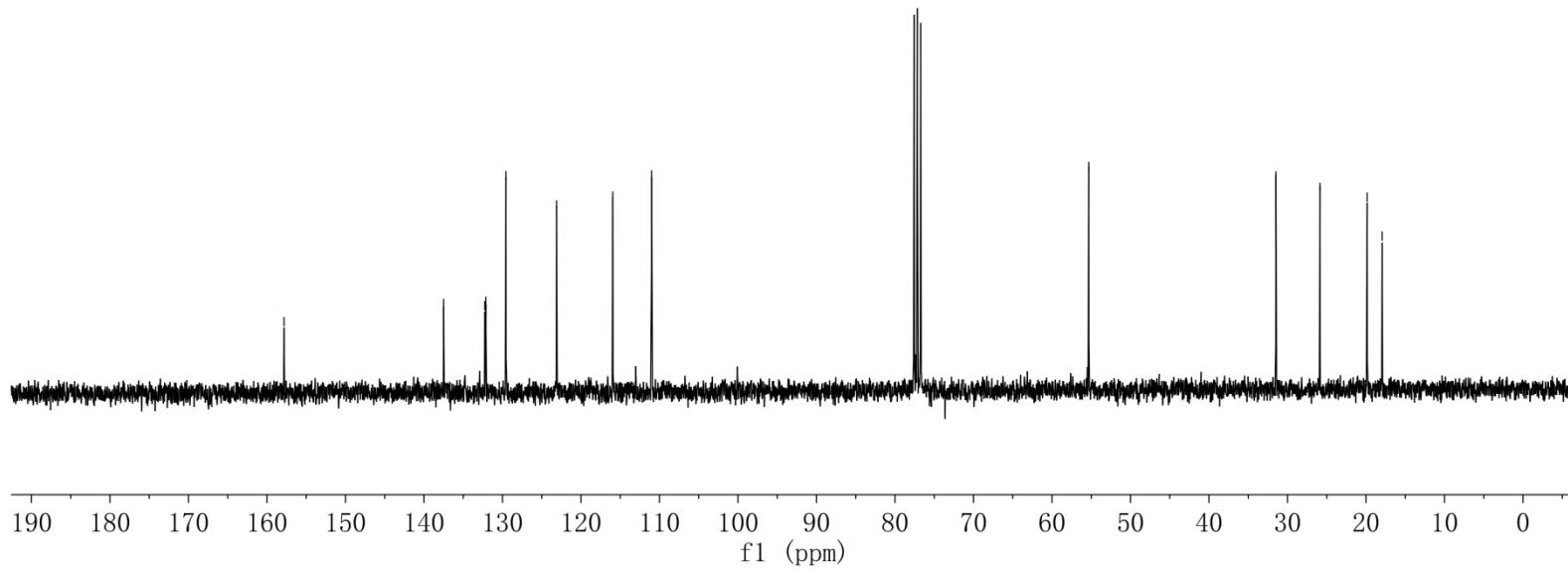
*(a) Spectrum measured in CDCl₃. (b) Δδ (ppm) = (Synthetic – Xu's work)

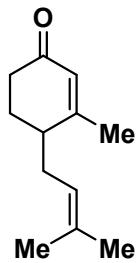
IV: NMR Spectra for the Synthesized Compounds



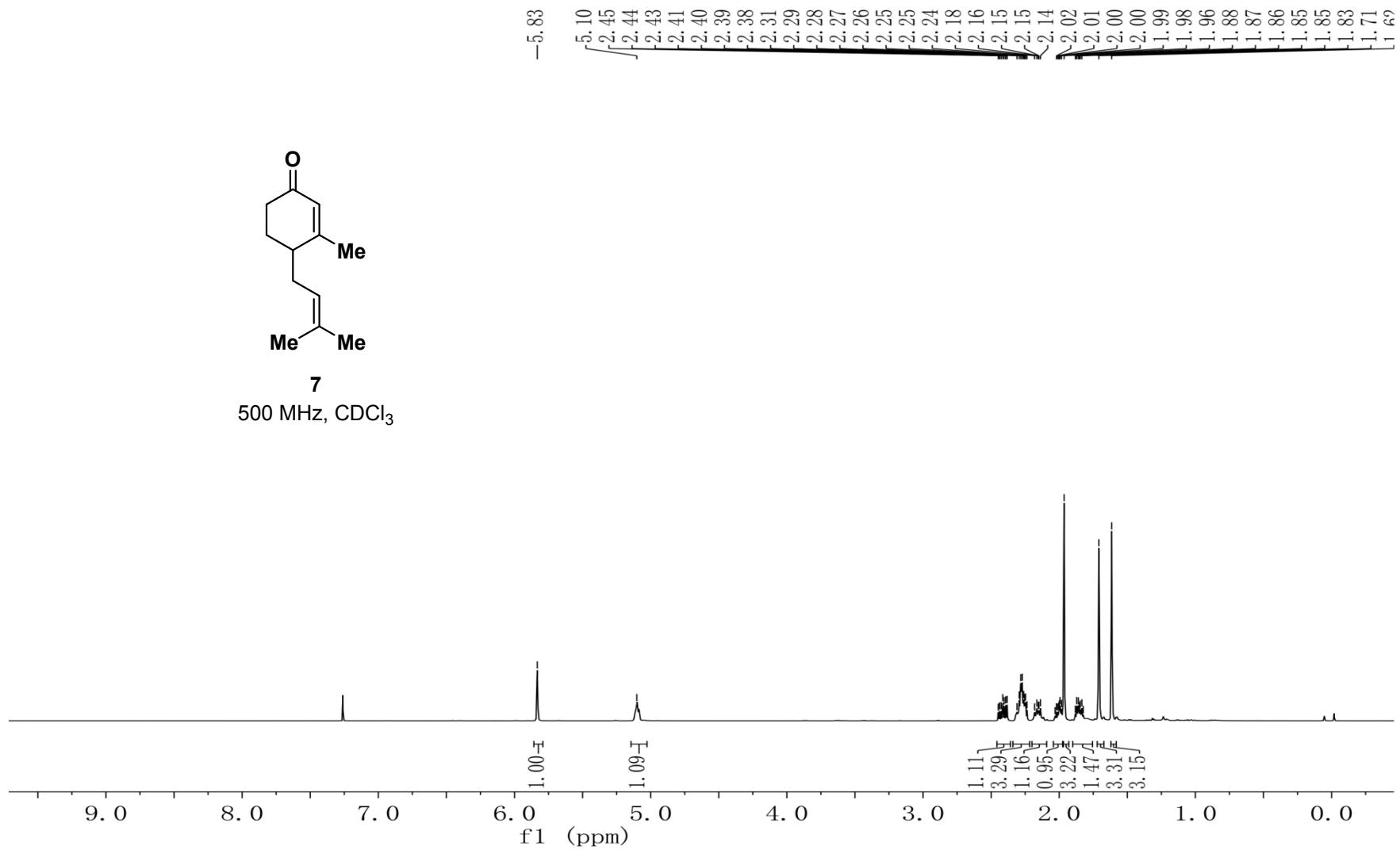


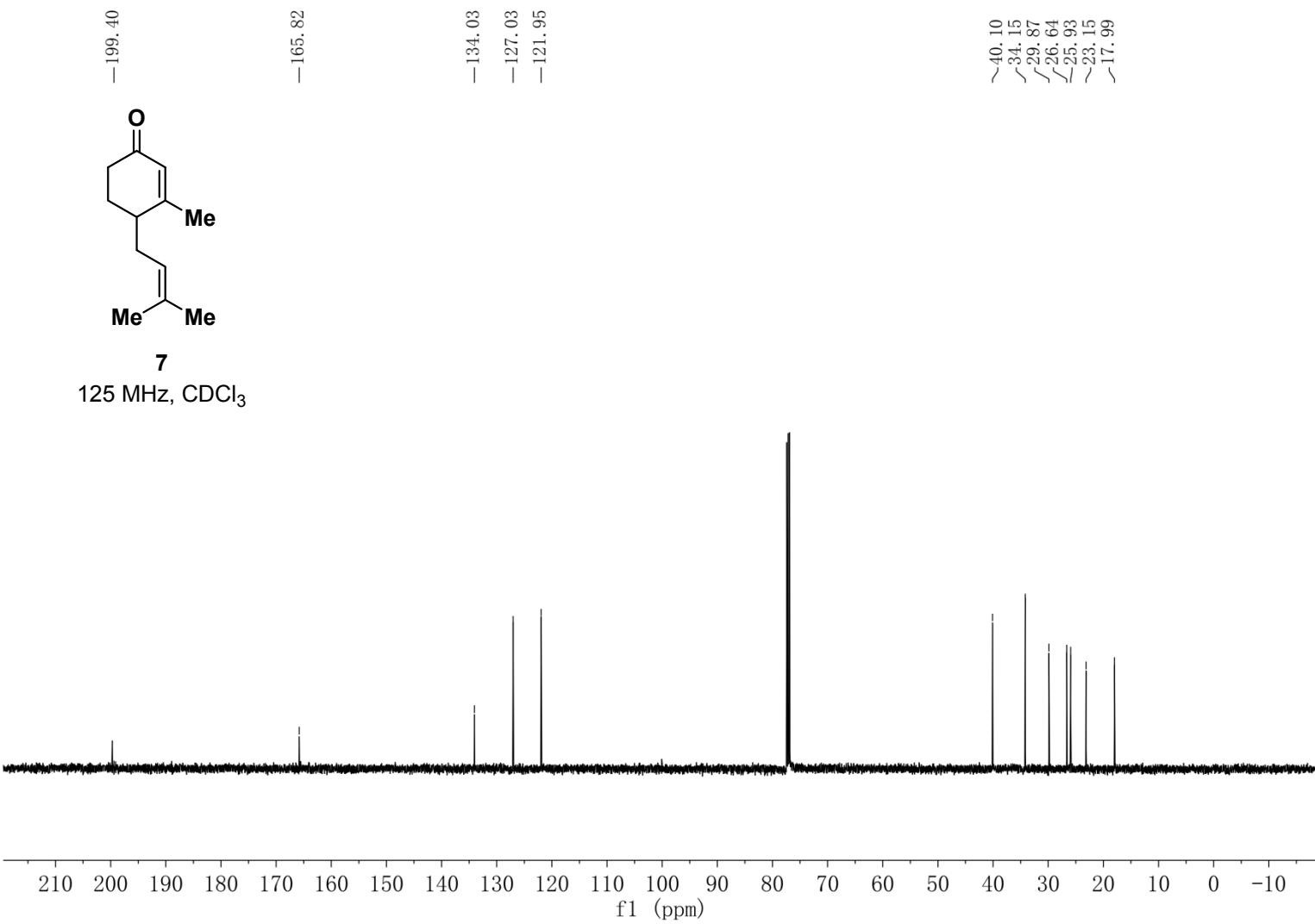
6
75 MHz, CDCl_3

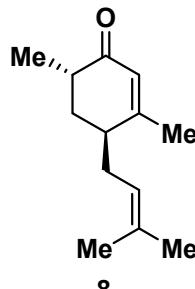




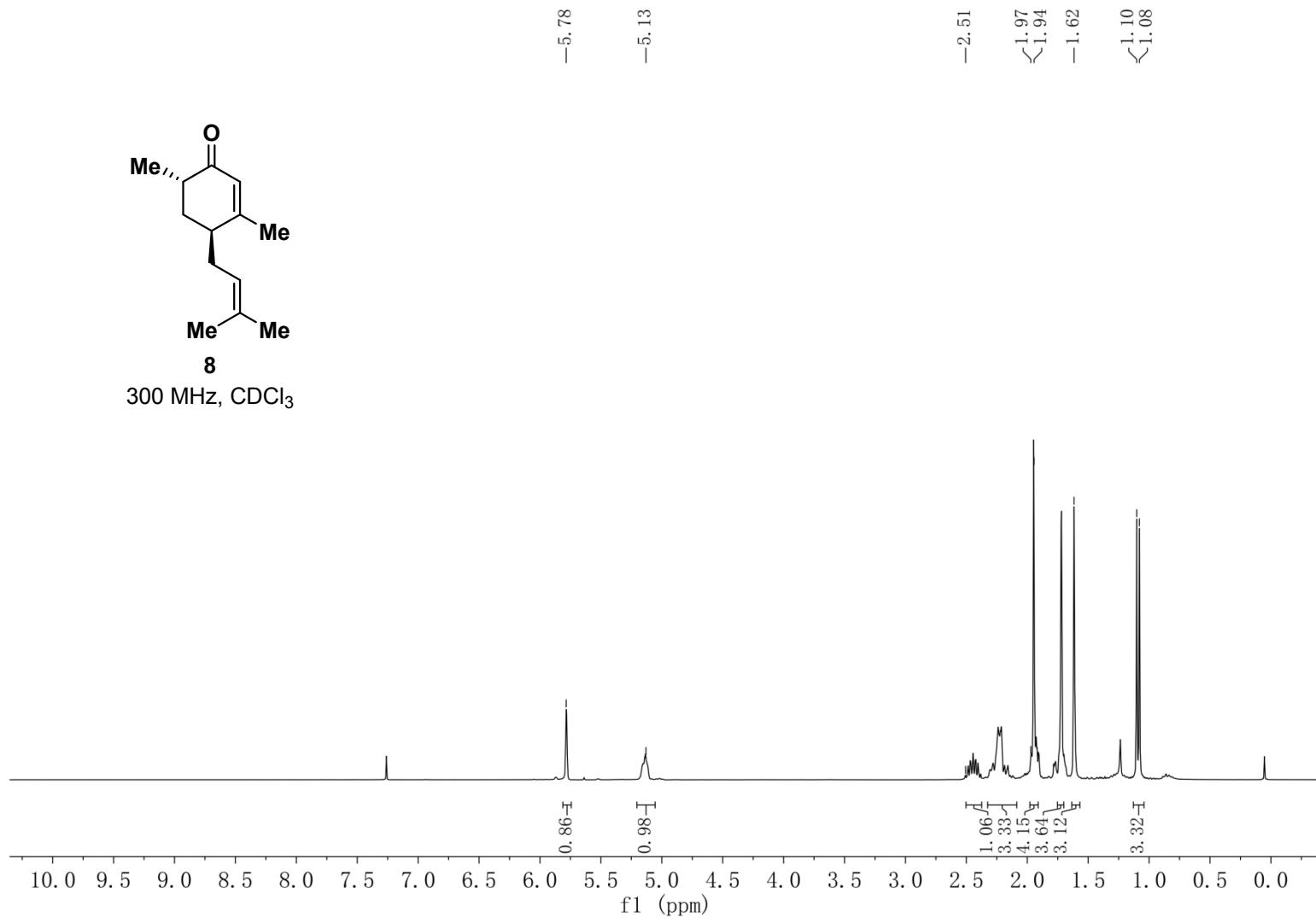
7
500 MHz, CDCl_3







300 MHz, CDCl₃



-200.99

-163.70

-158.53

-132.78

-125.06

-121.28

~39.00

~35.07

~33.67

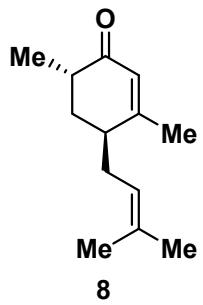
~28.60

~24.79

~21.90

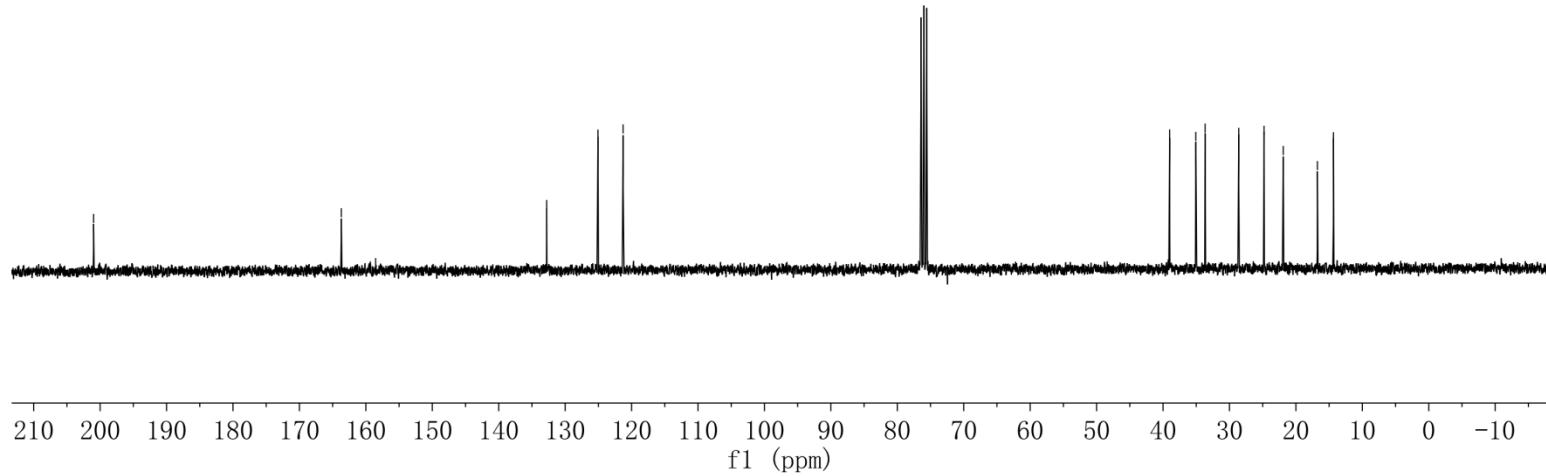
~16.76

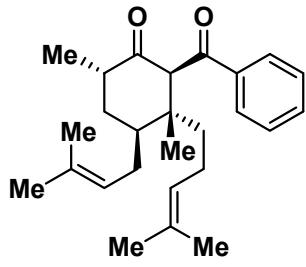
~14.35



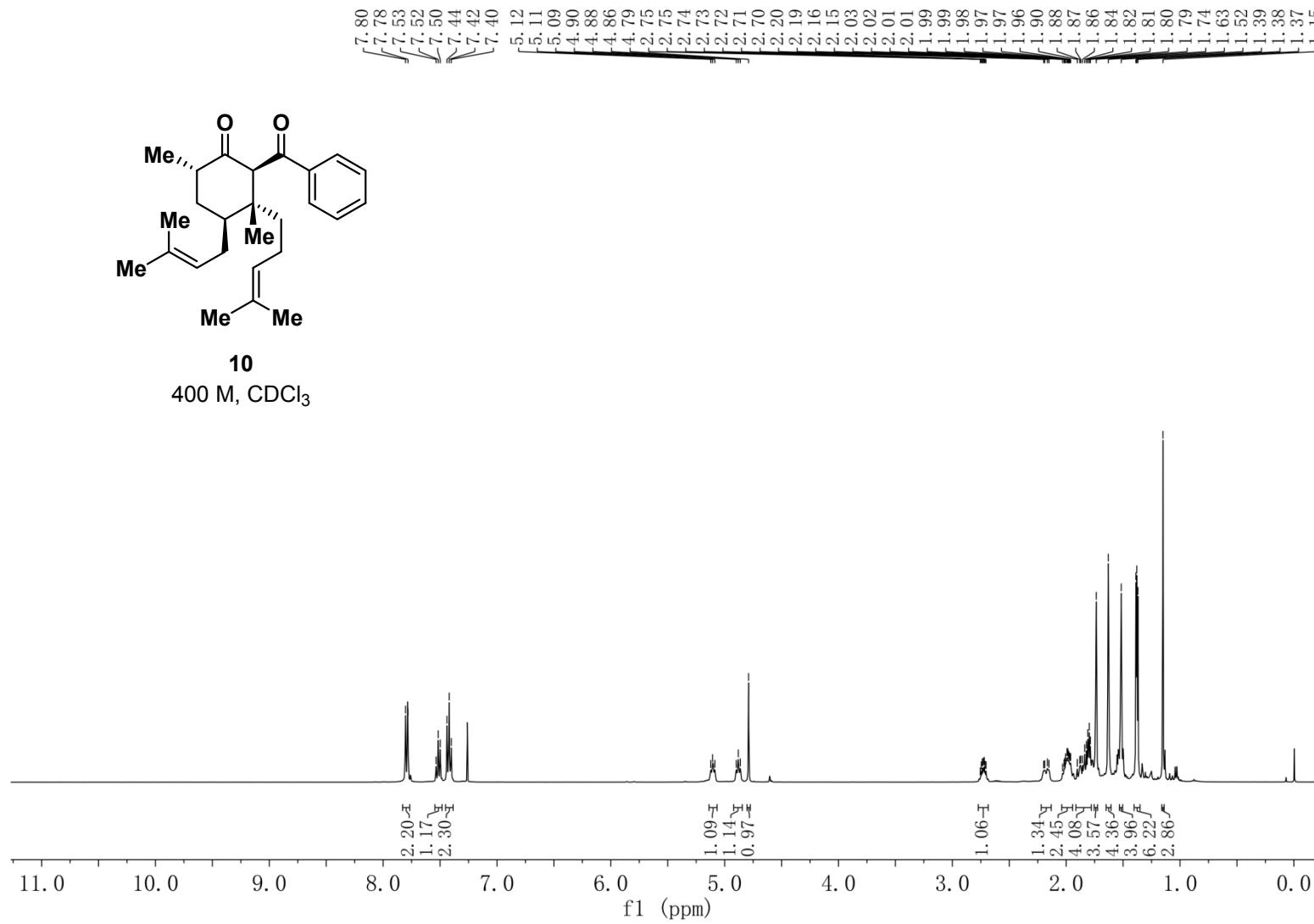
8

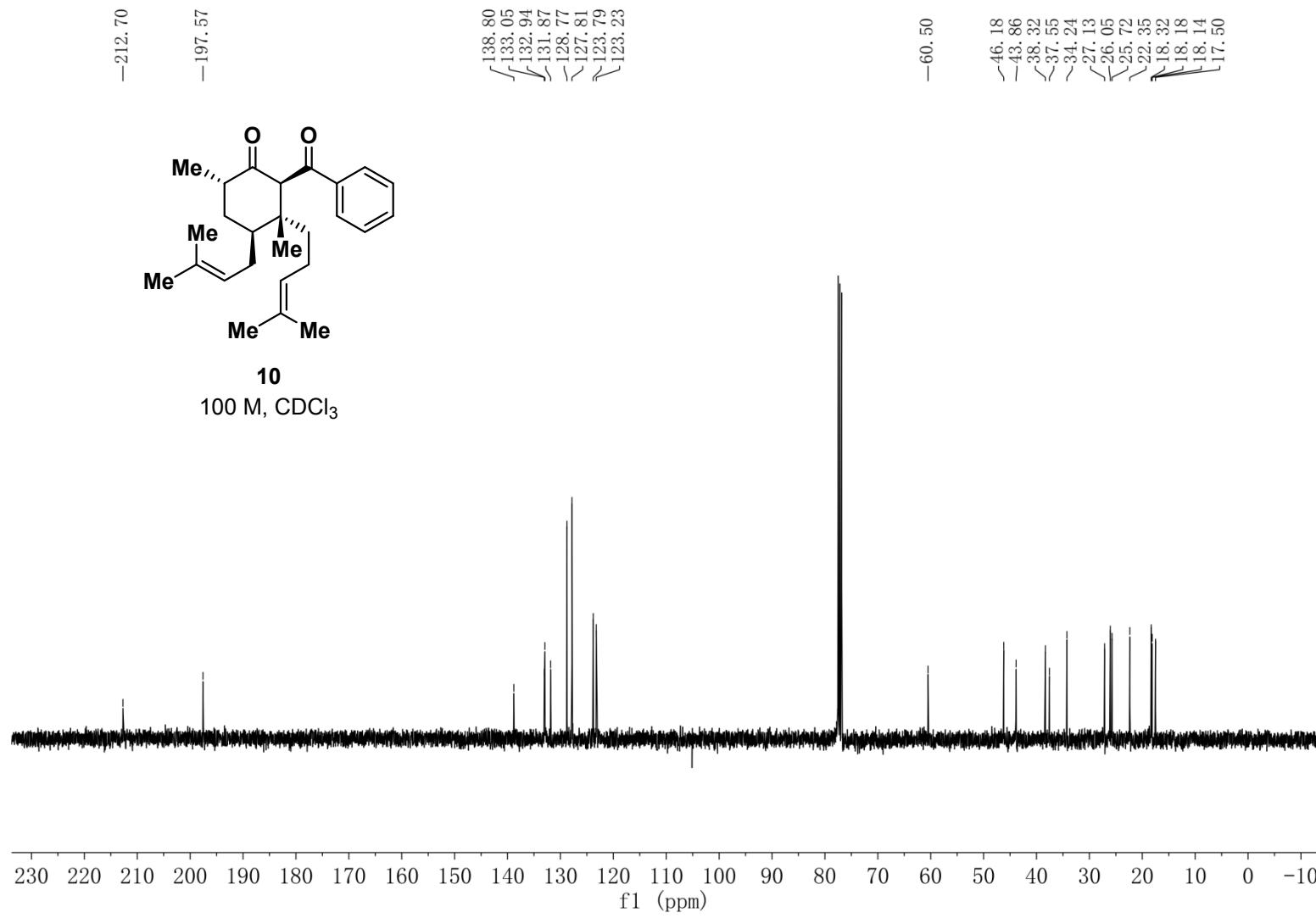
75 MHz, CDCl₃

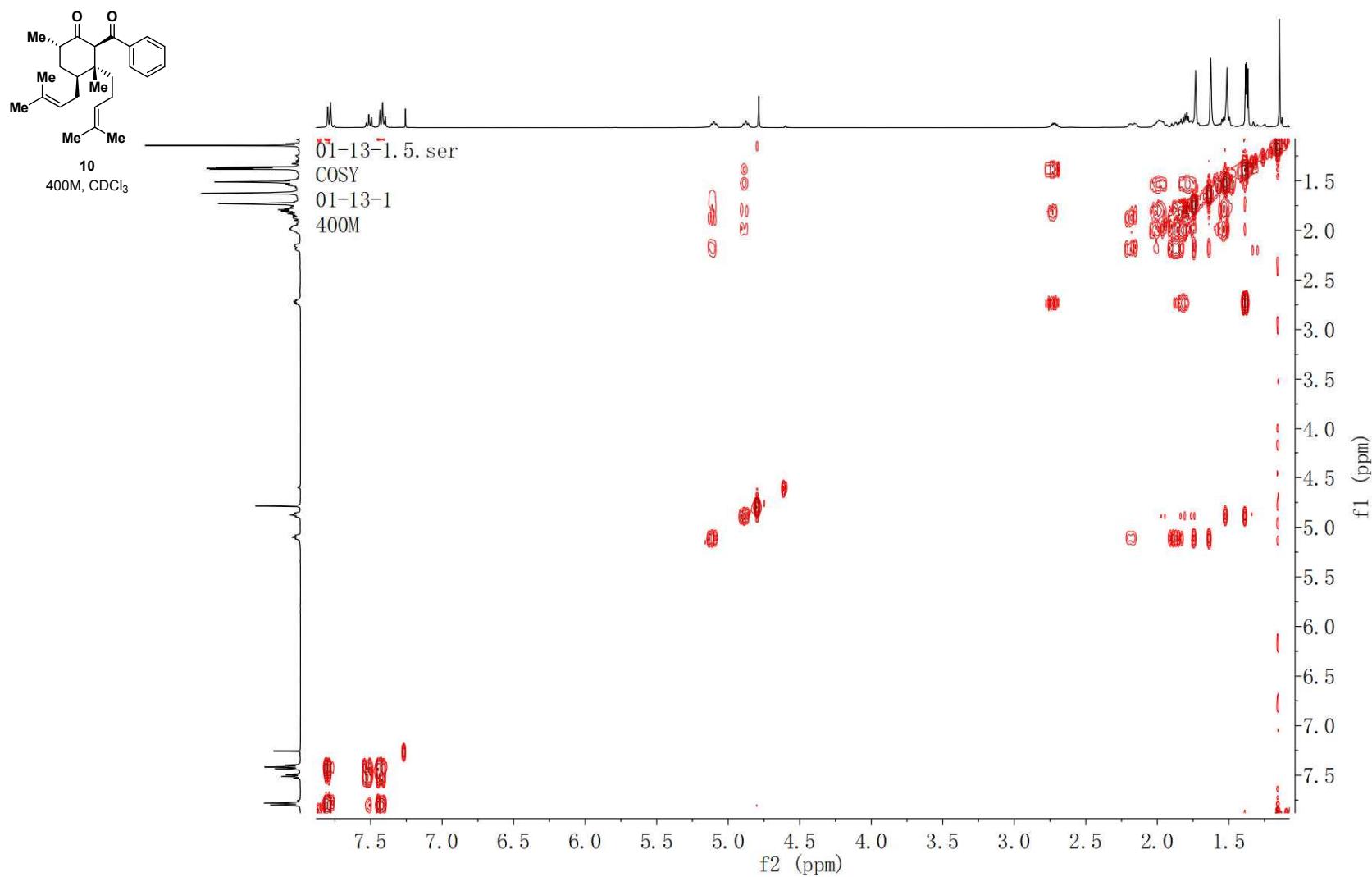


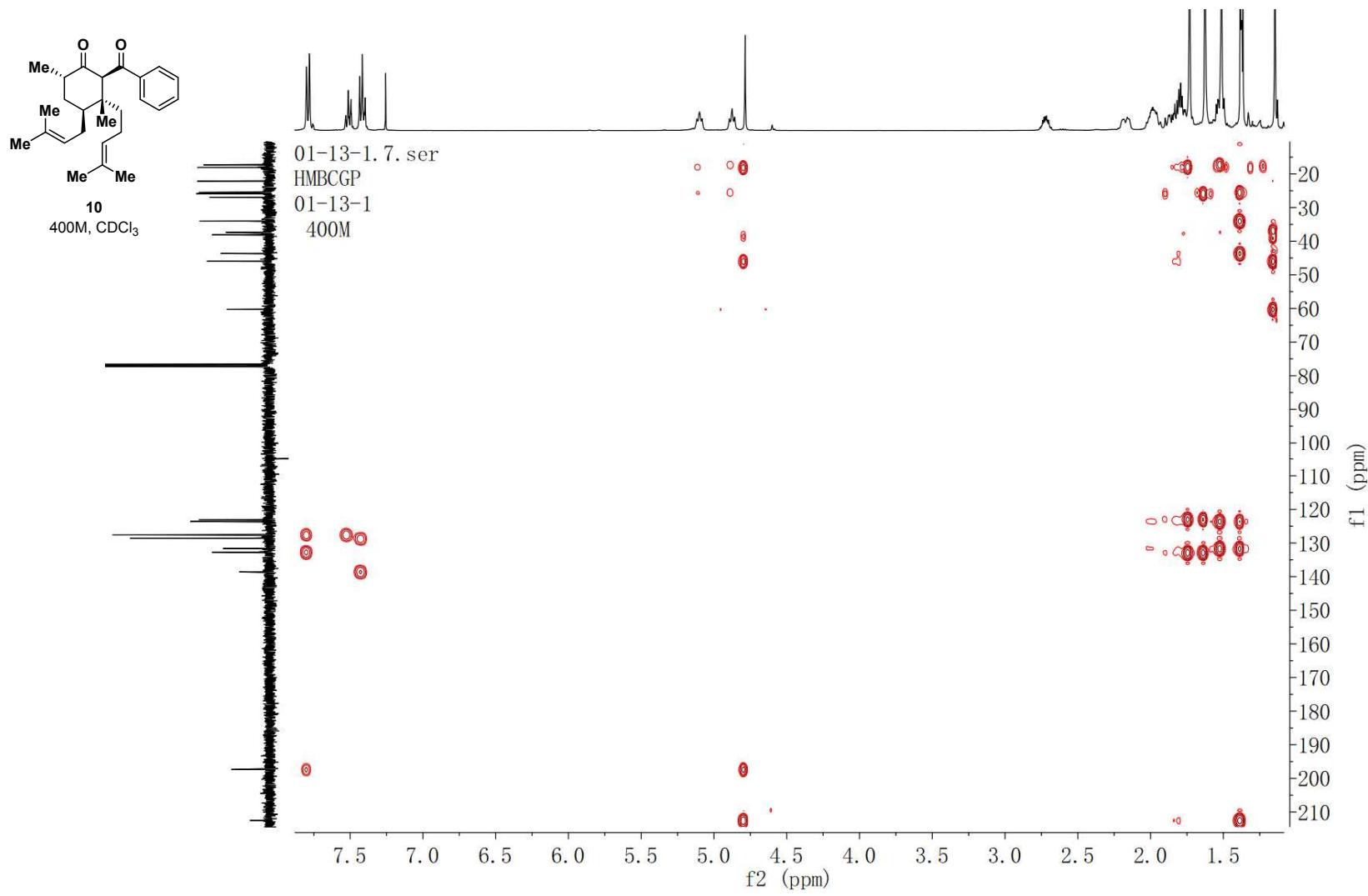


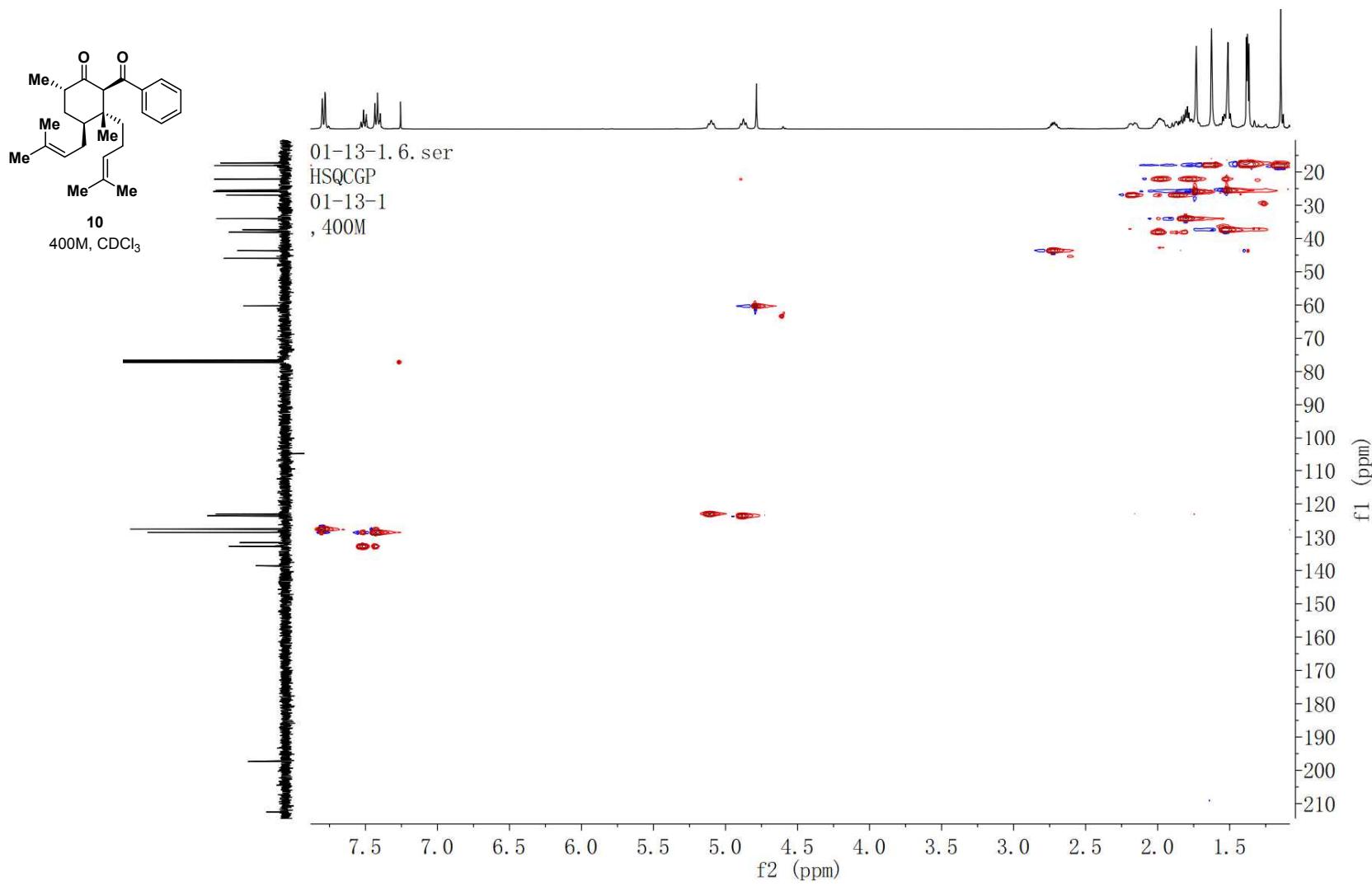
10
400 M, CDCl_3

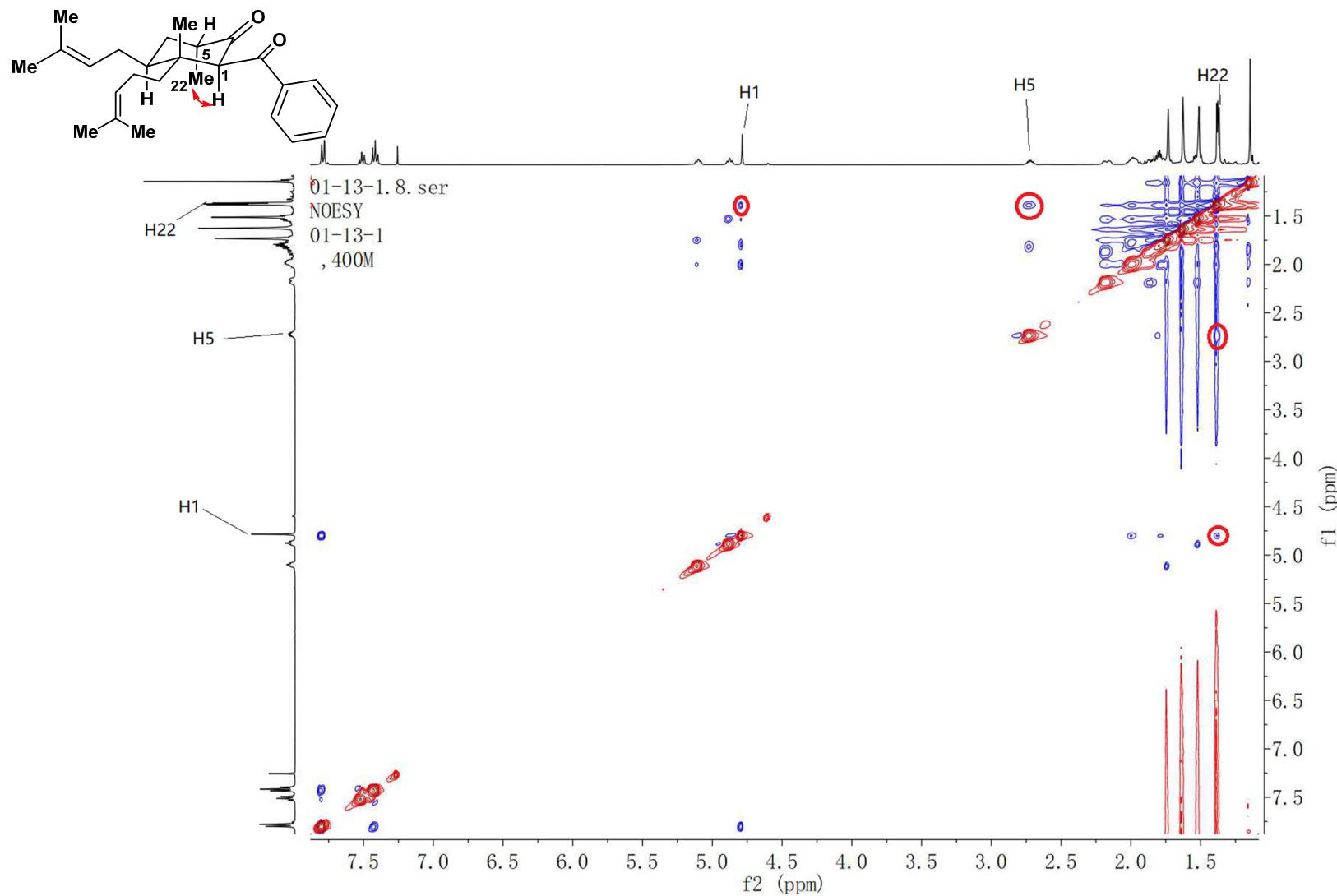


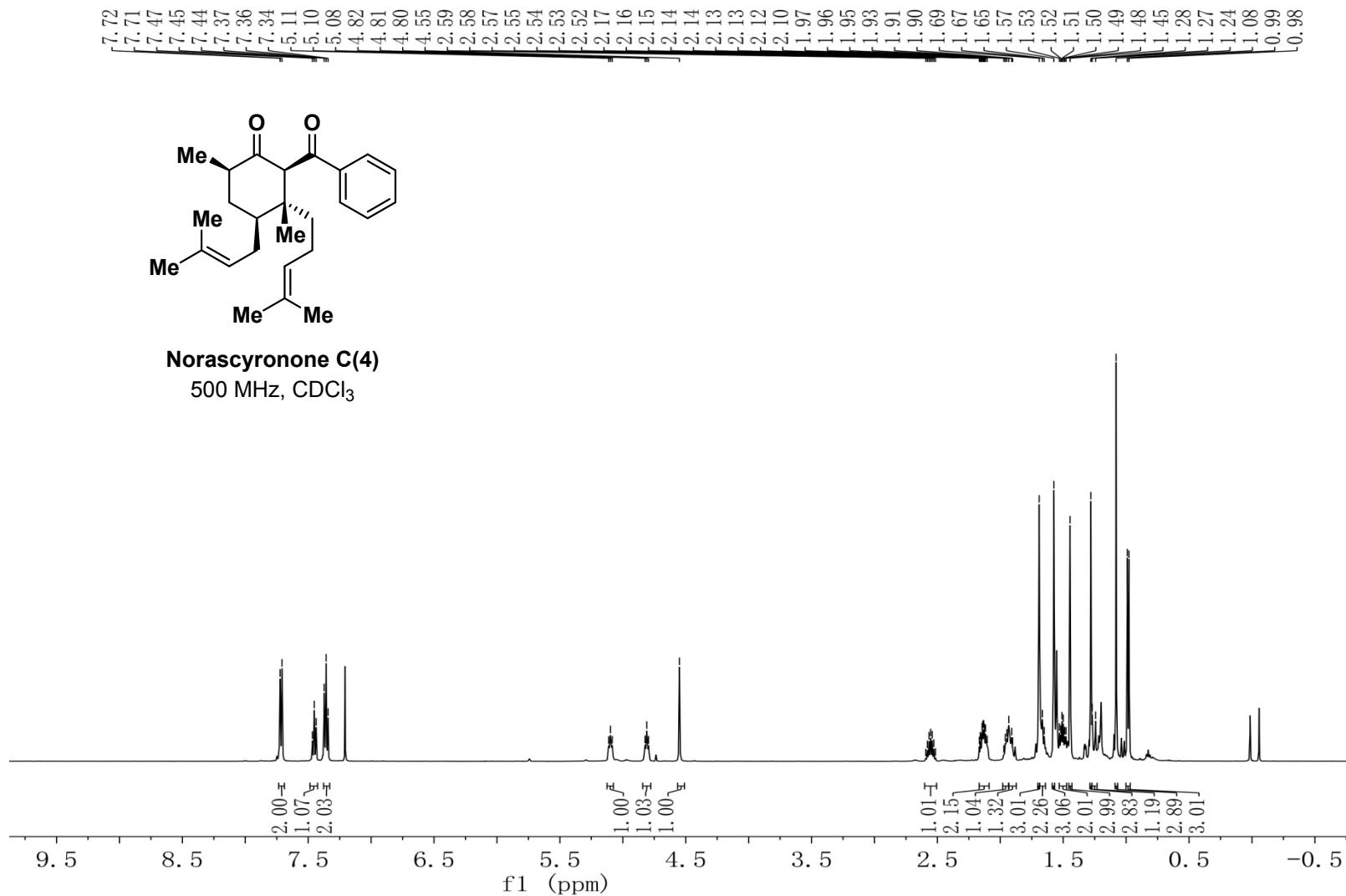


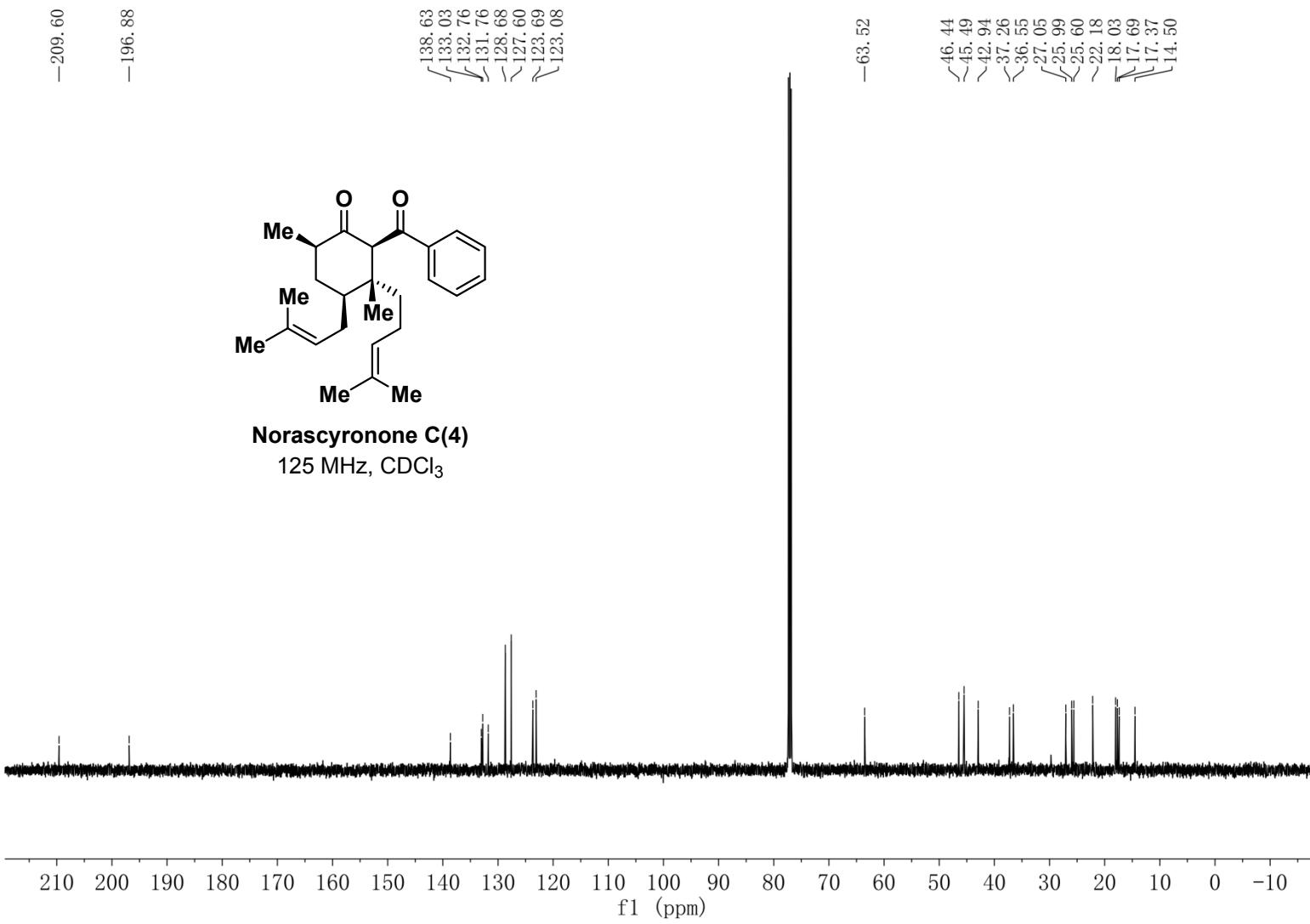


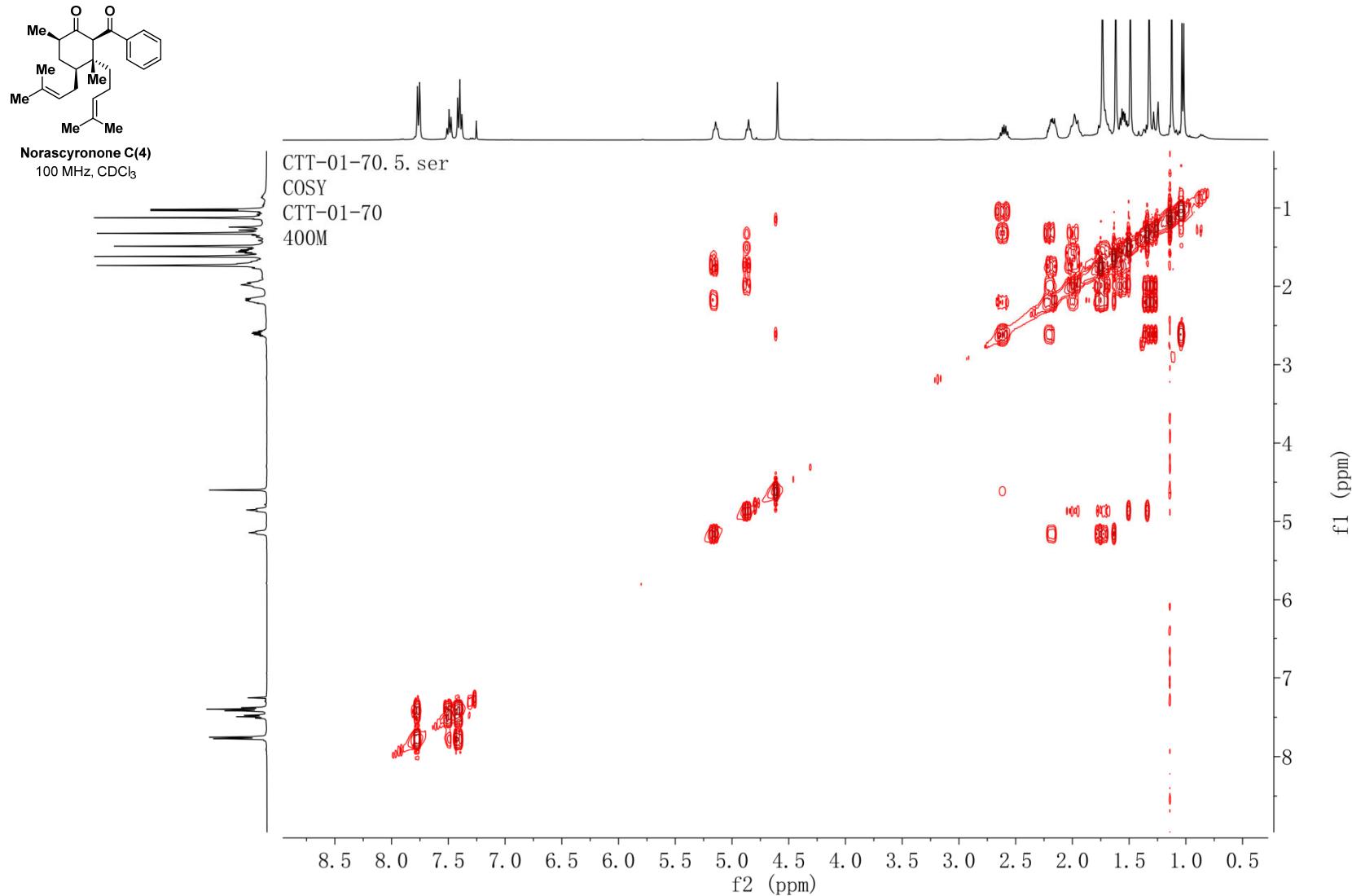


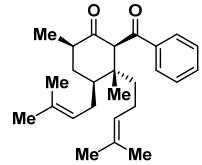




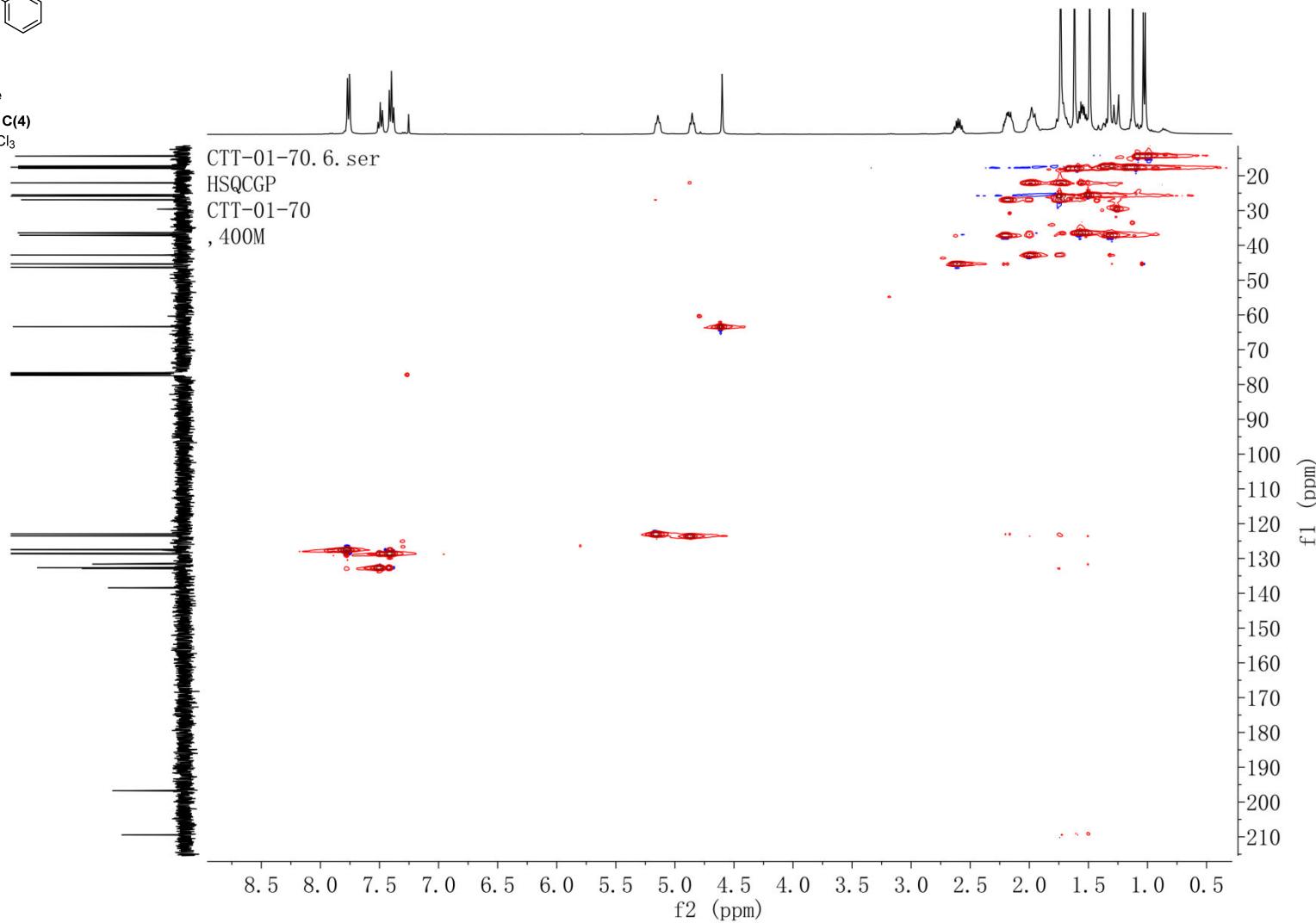


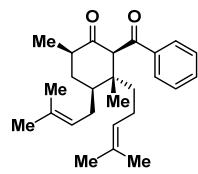




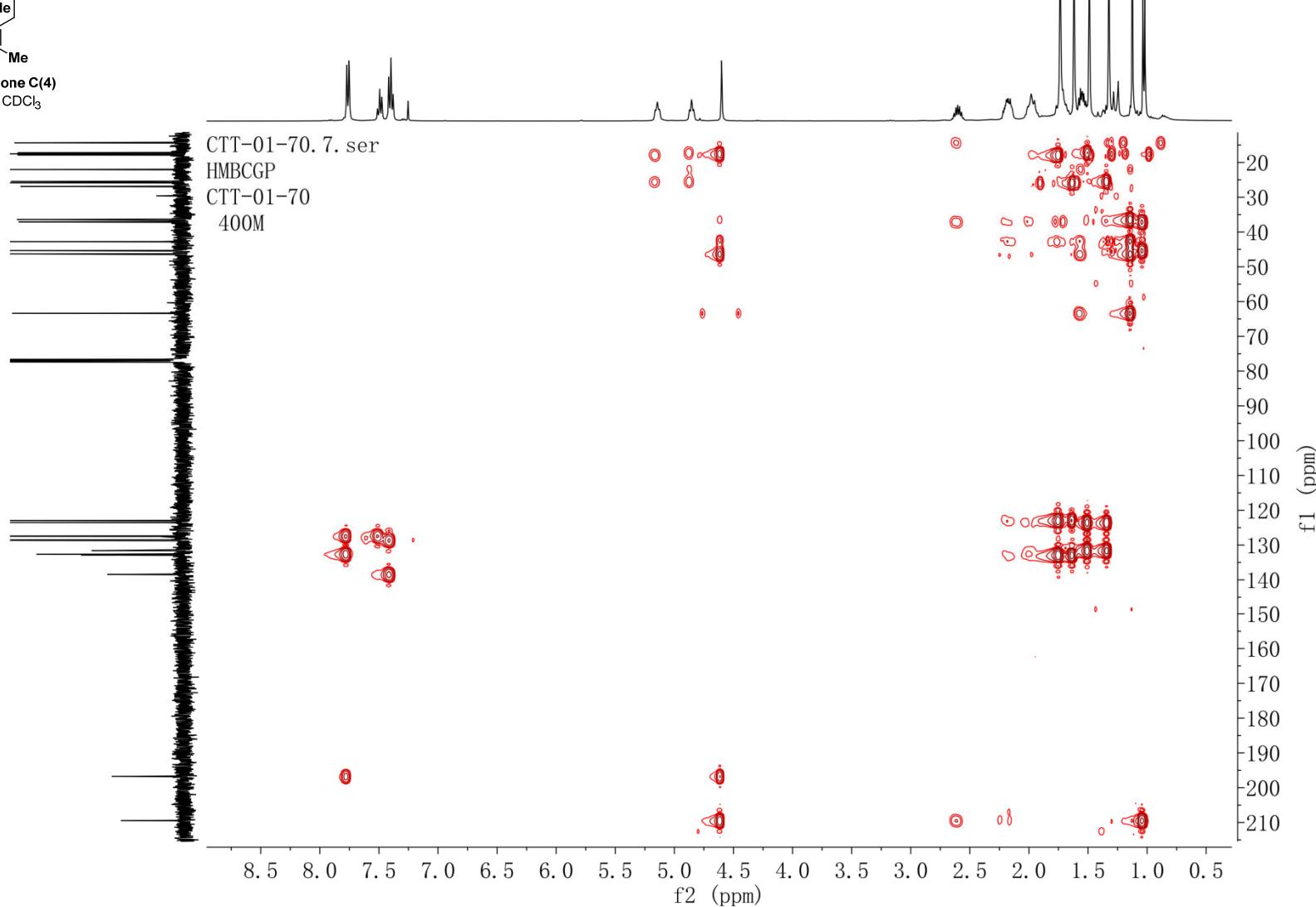


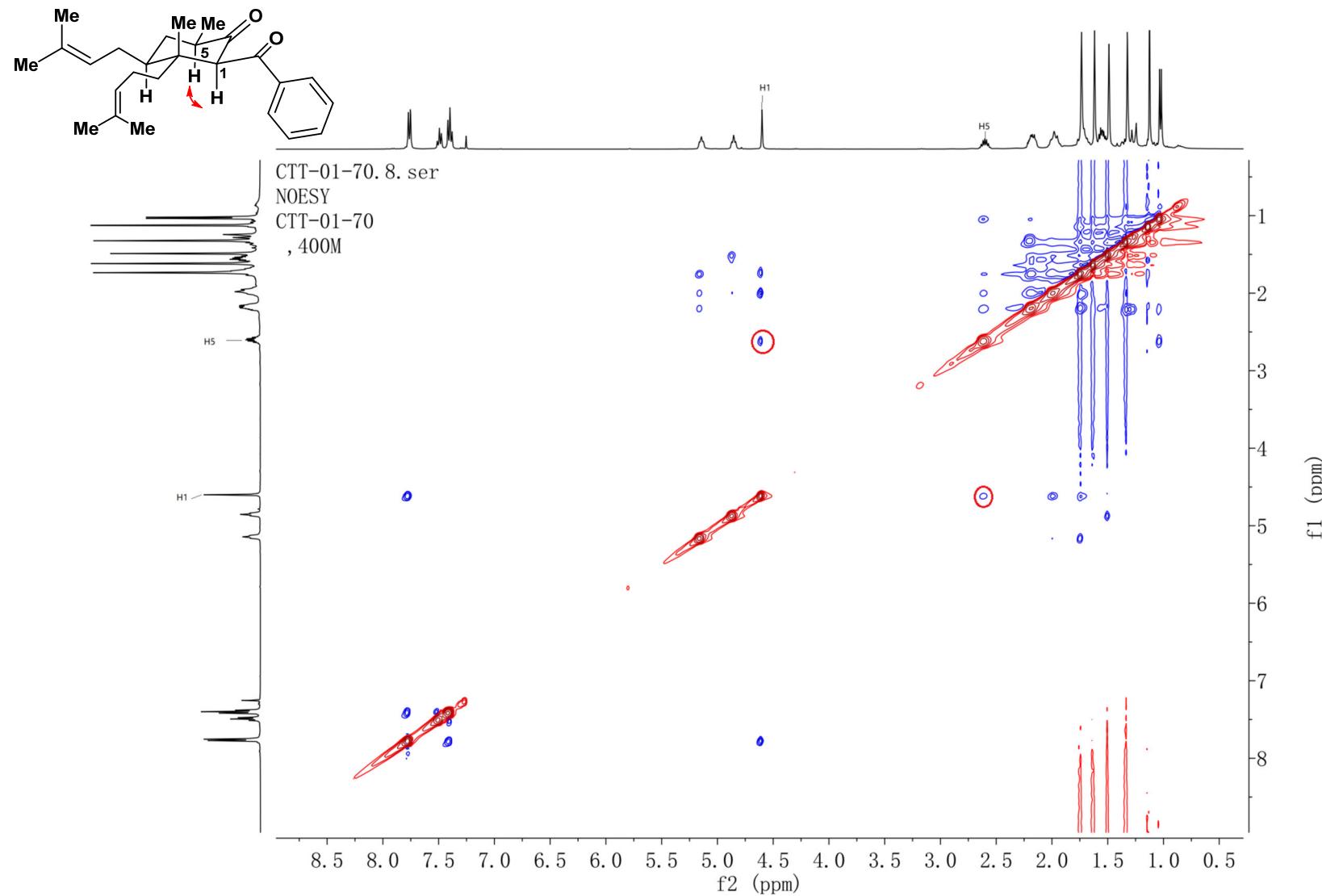
Norascyonone C(4)
100 MHz, CDCl₃

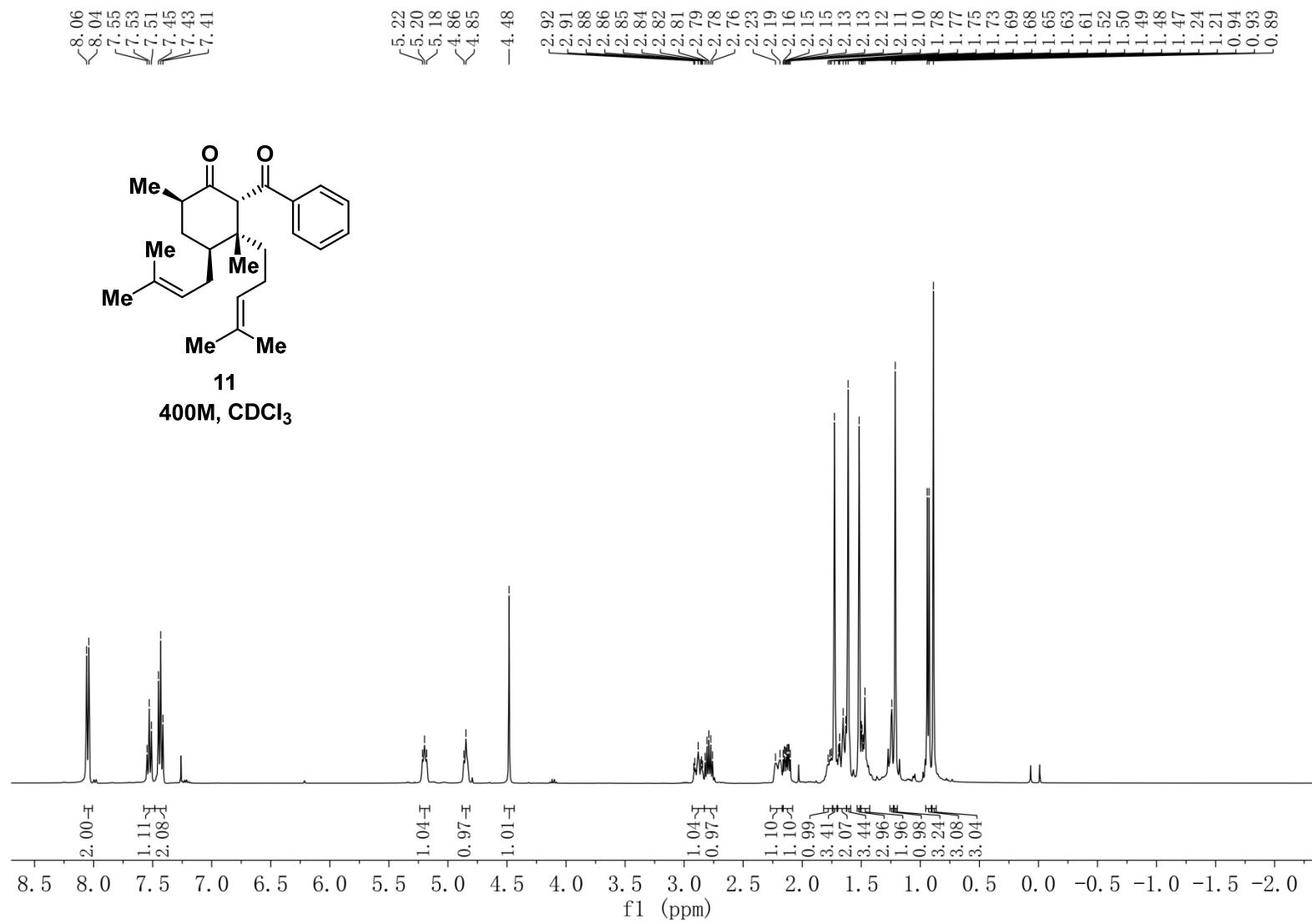


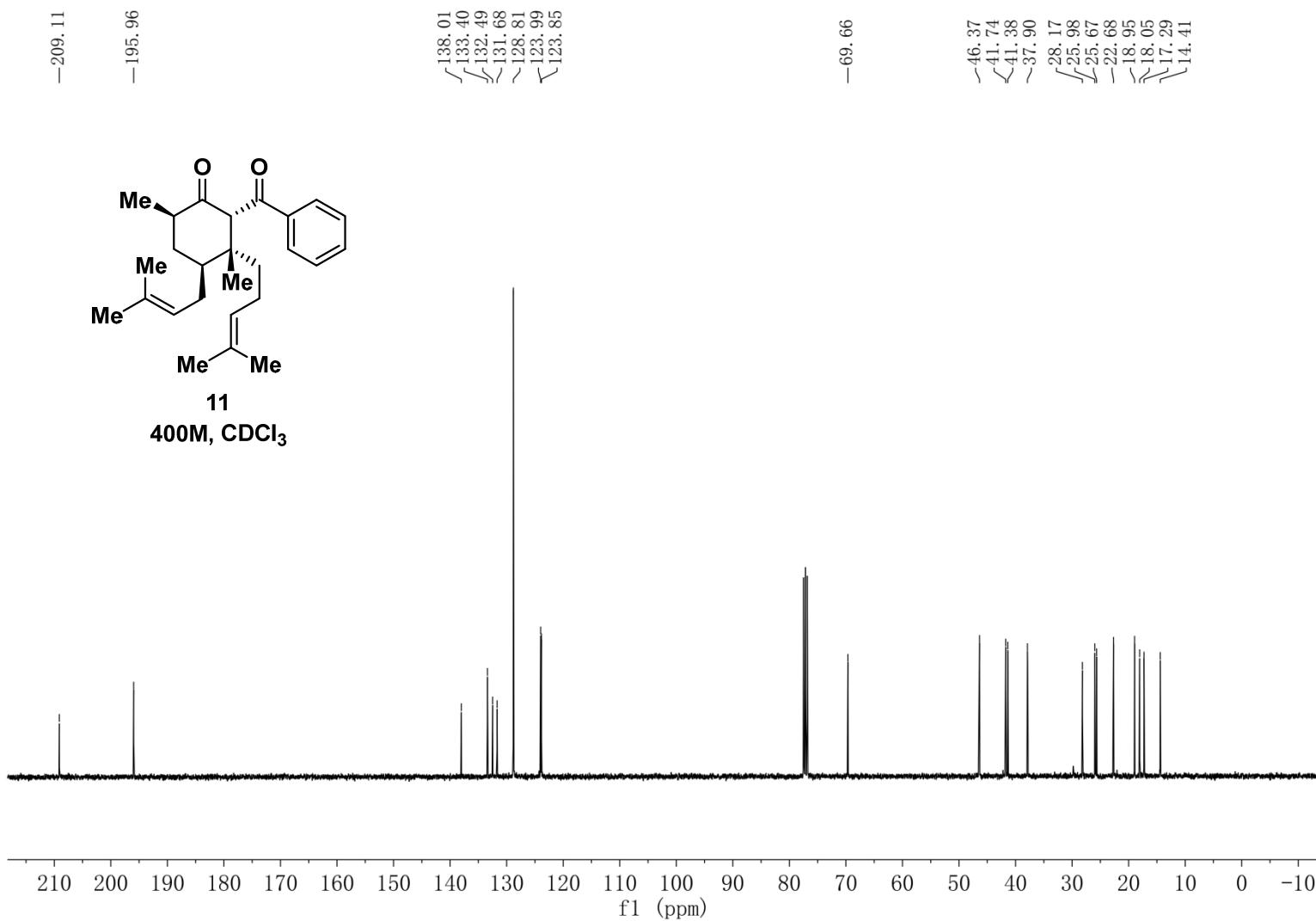


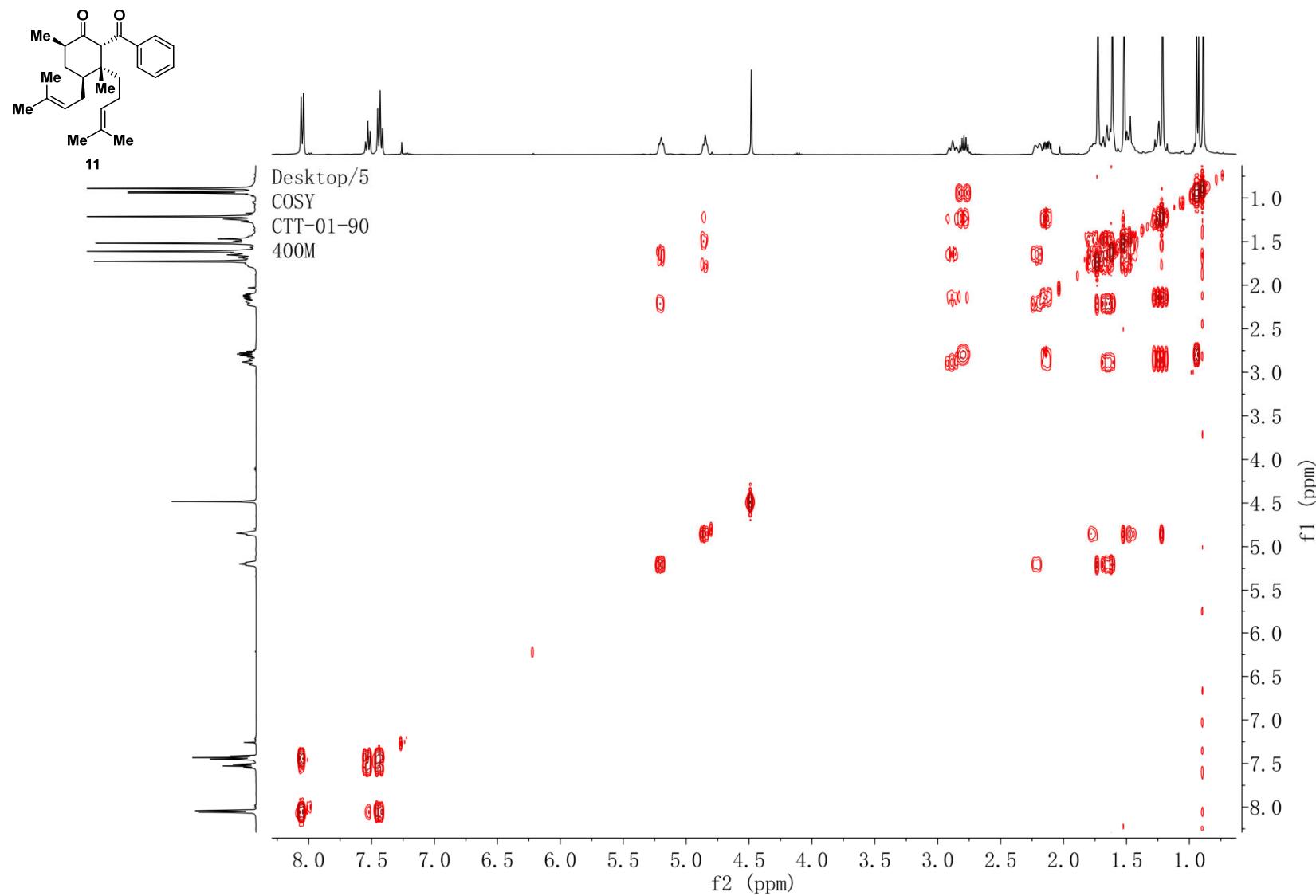
Norascyronone C(4)
100 MHz, CDCl_3

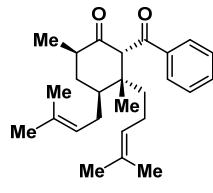






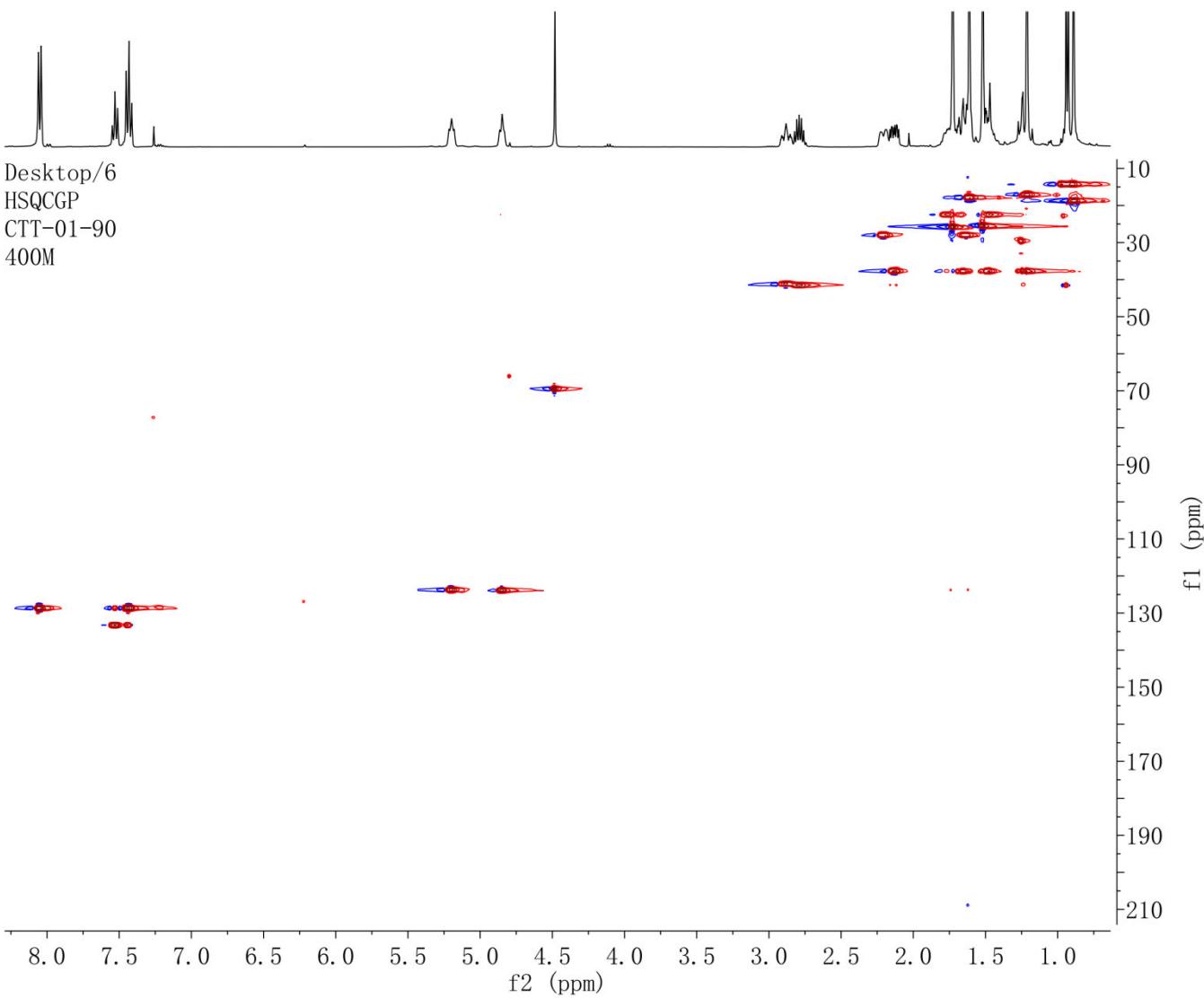


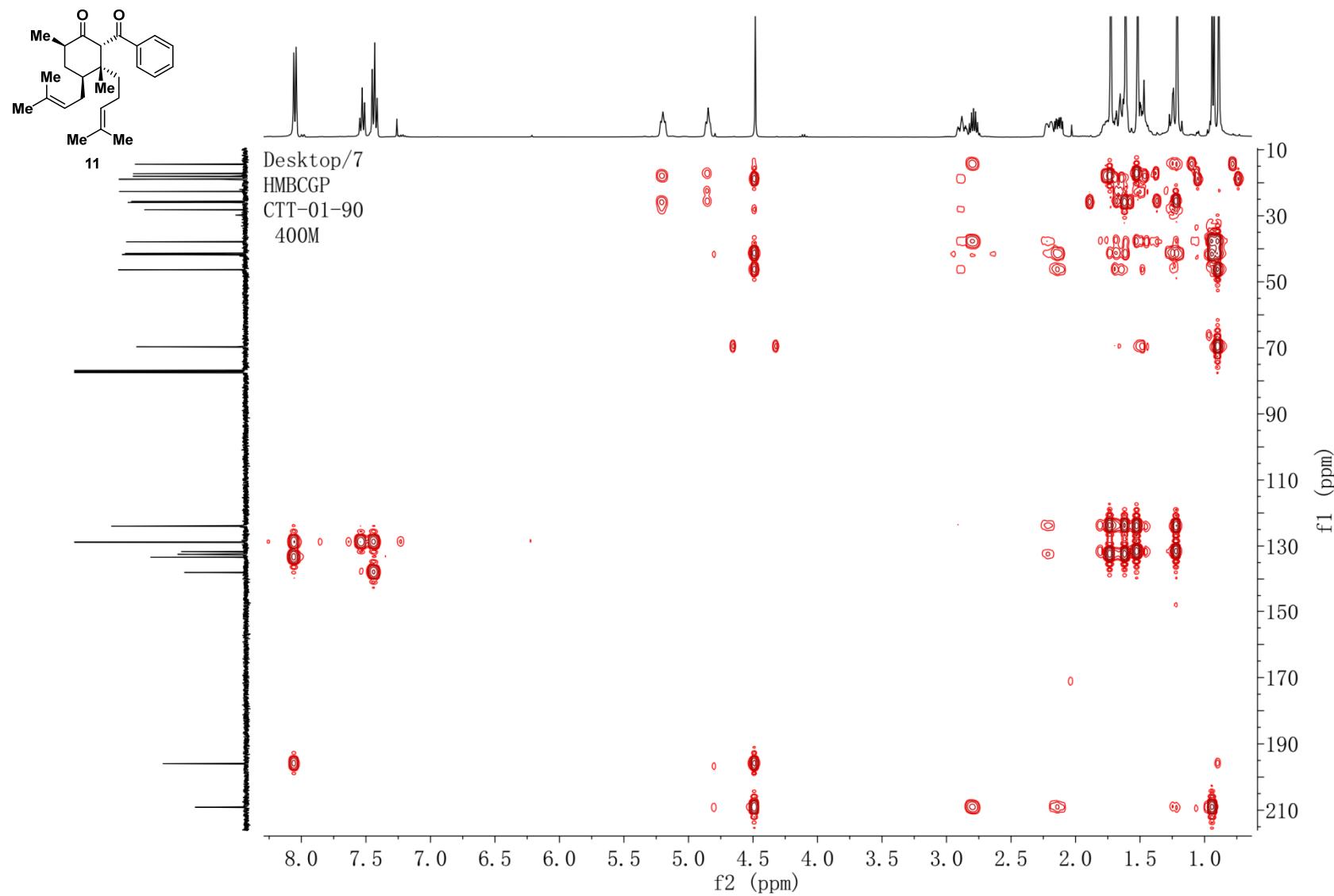


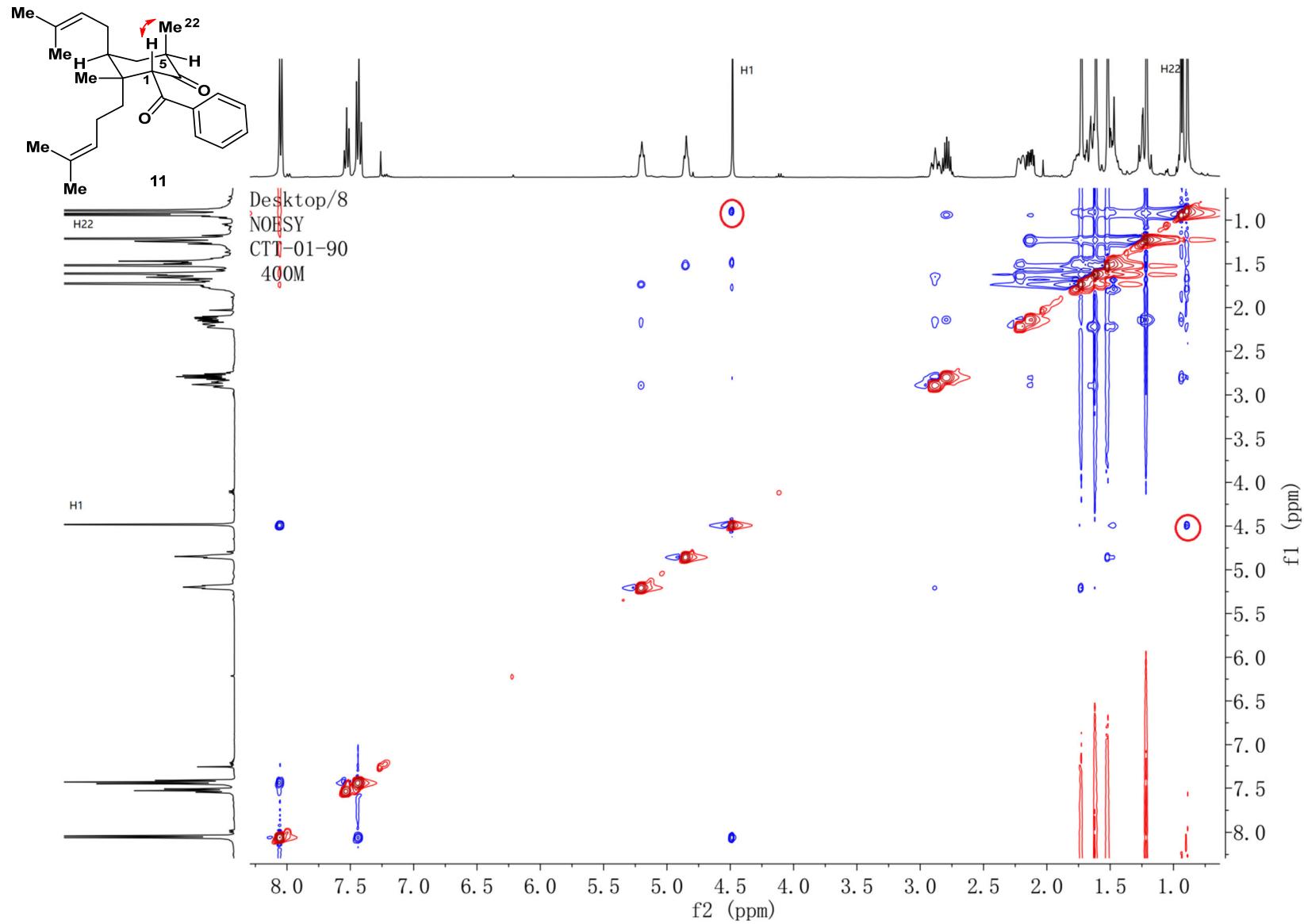


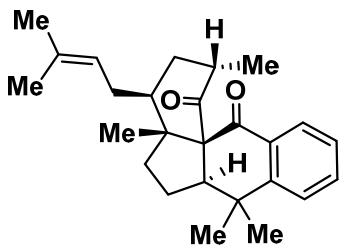
11

Desktop/6
HSQCGP
CTT-01-90
400M



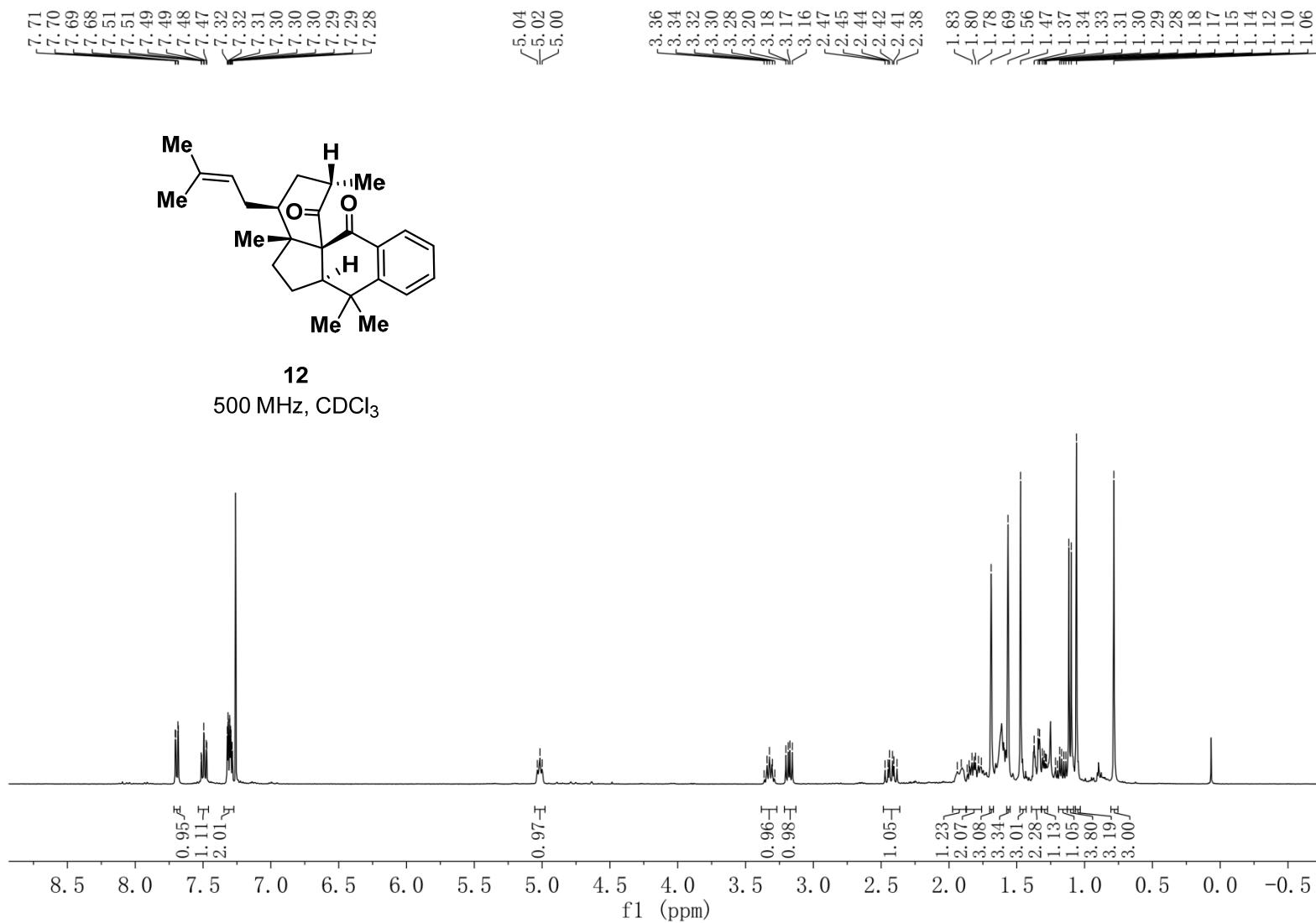


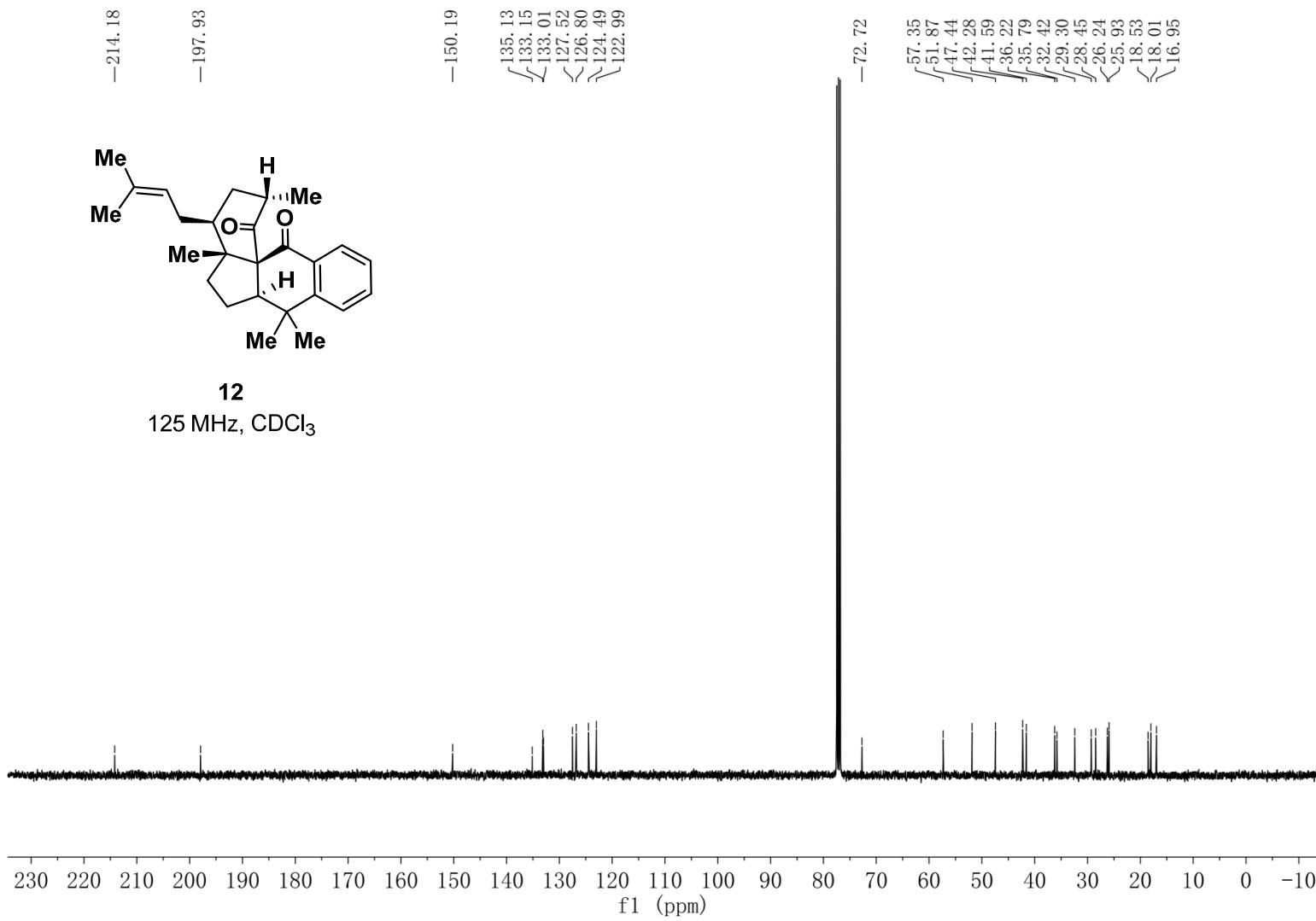


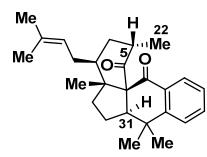


12

500 MHz, CDCl₃



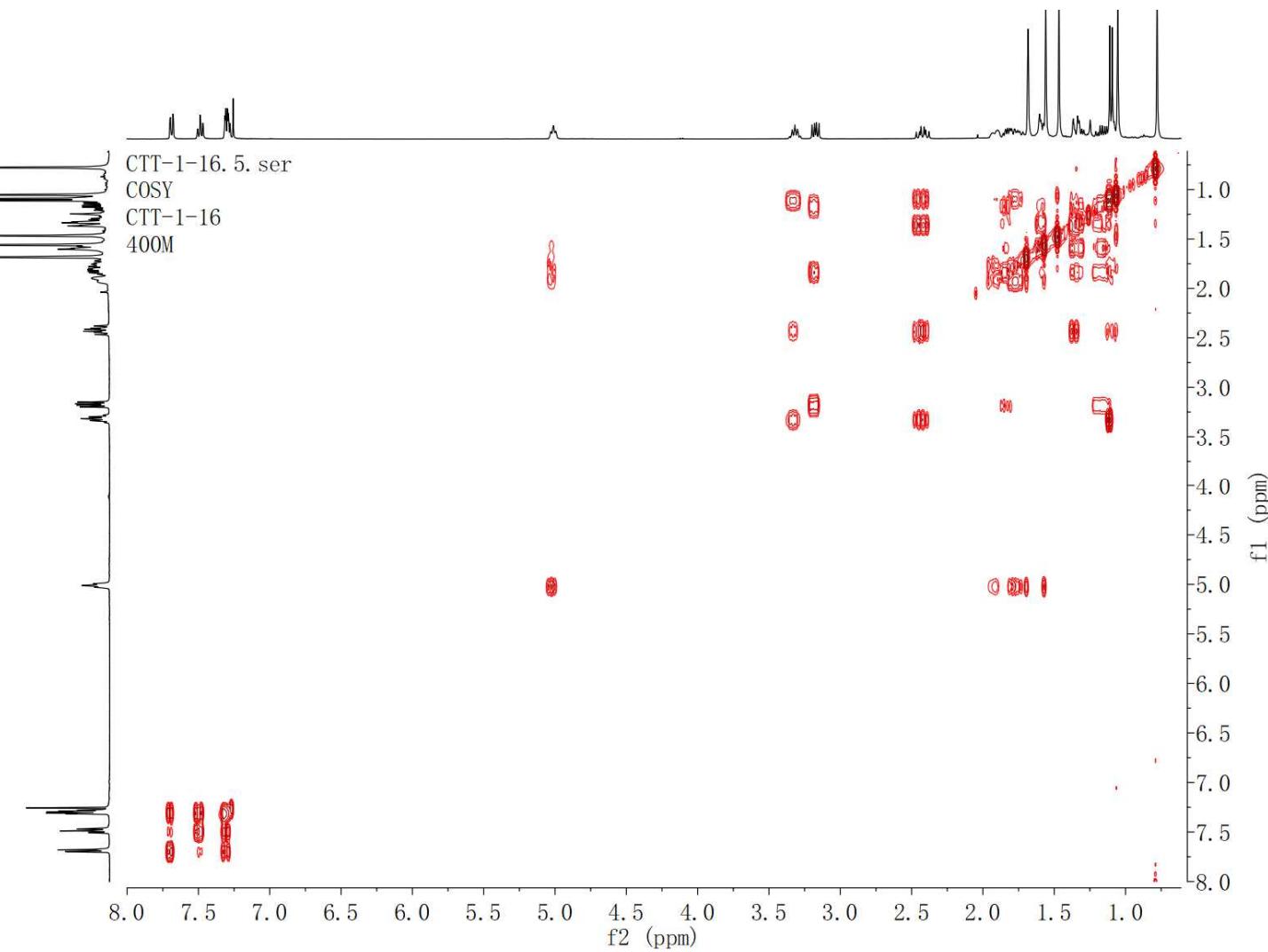


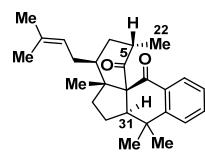


12

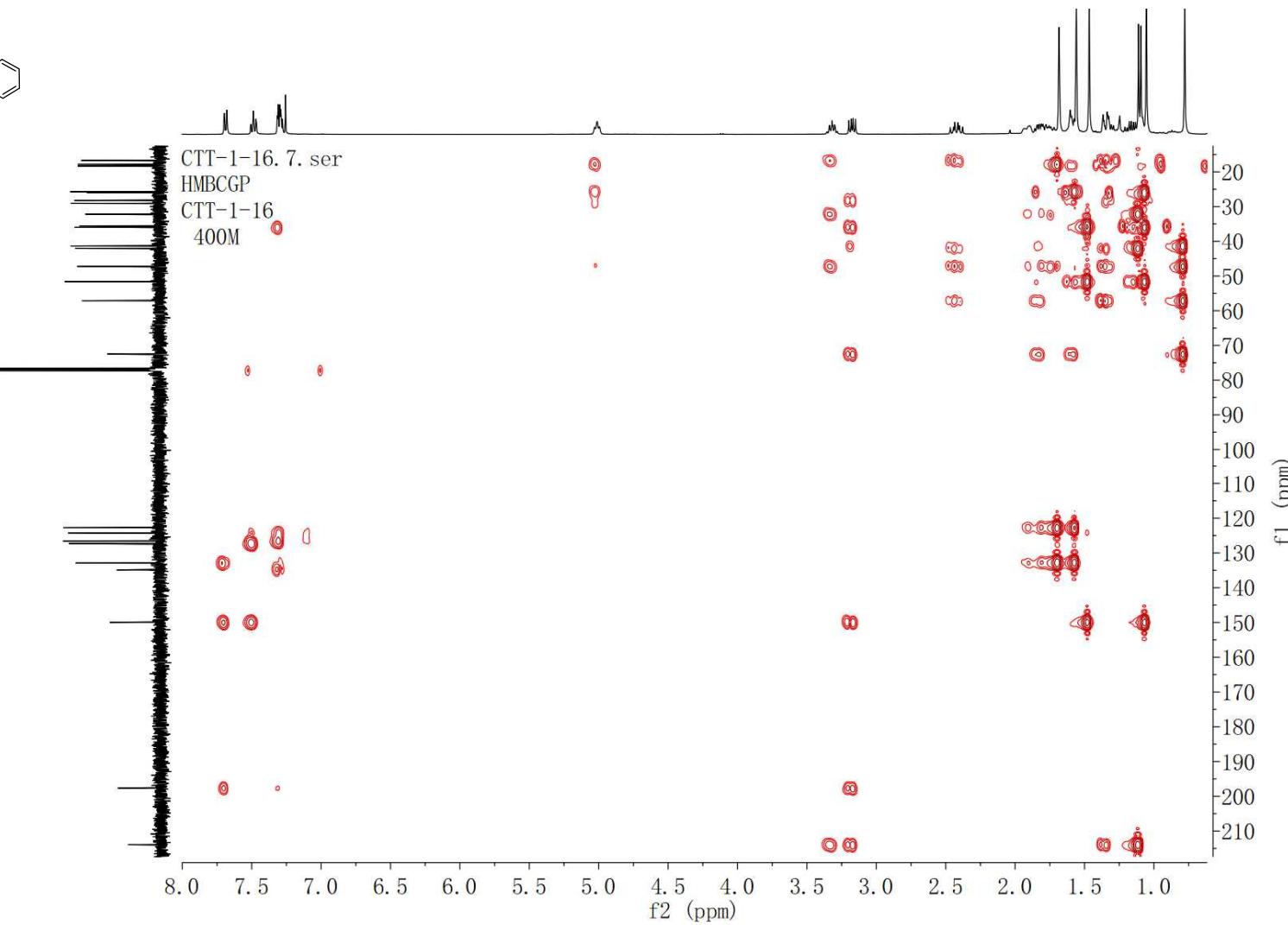
125 MHz, CDCl₃

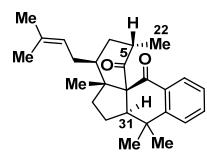
CTT-1-16.5.ser
COSY
CTT-1-16
400M



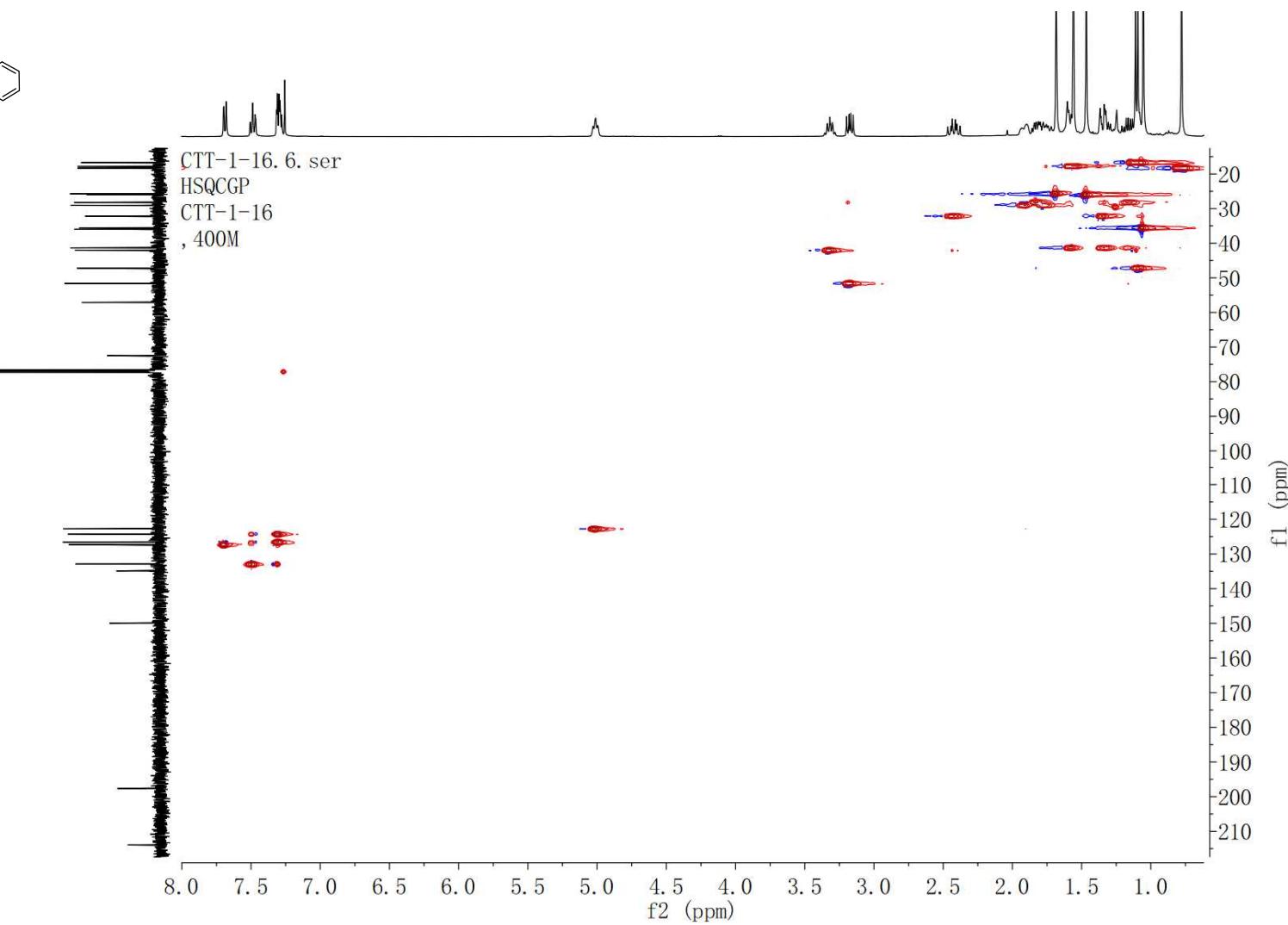


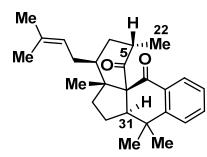
12
125 MHz, CDCl_3



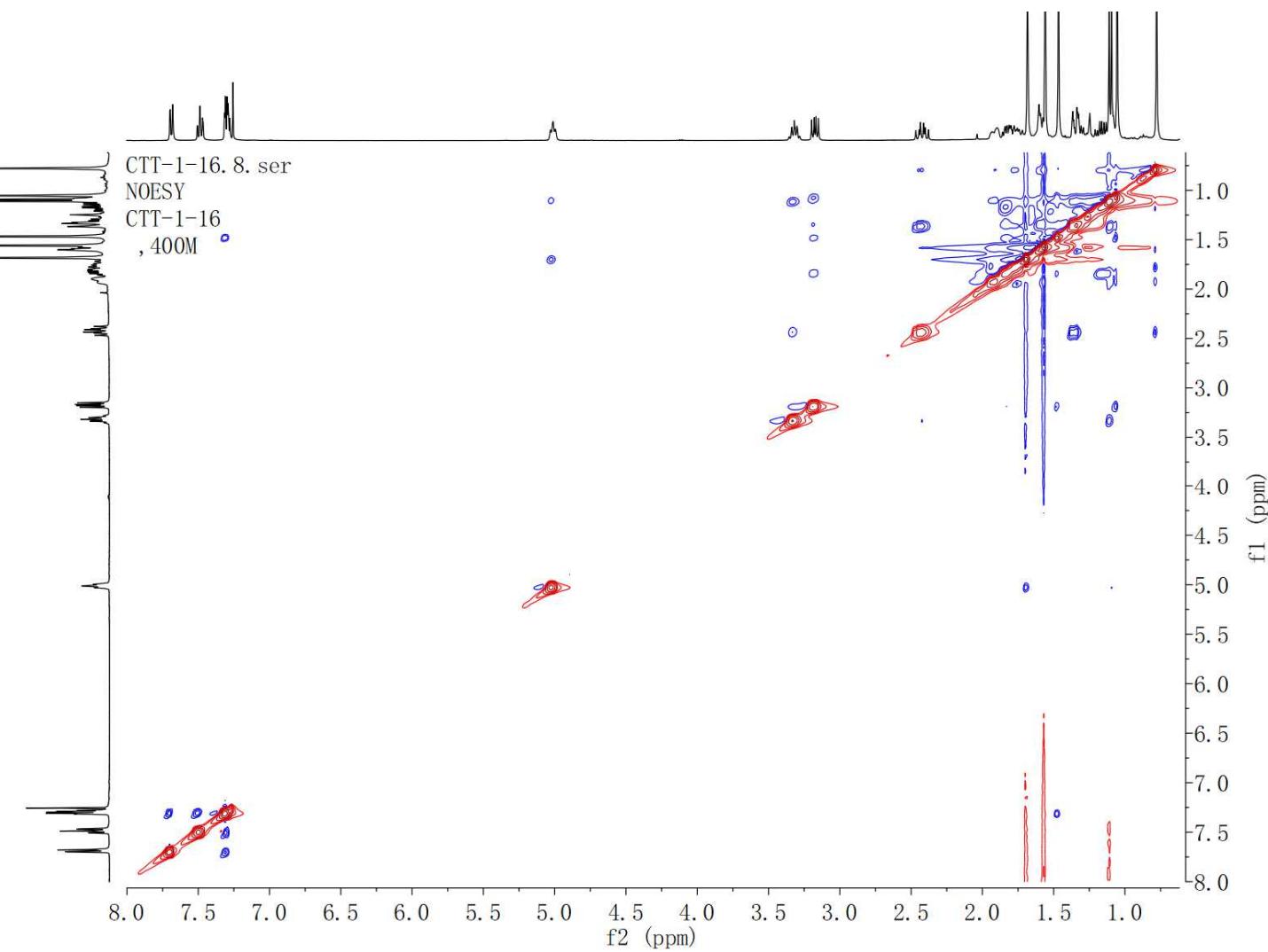


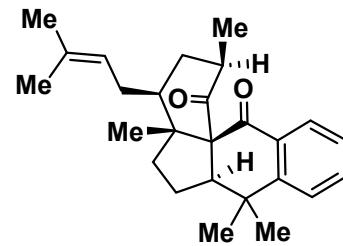
12
125 MHz, CDCl₃





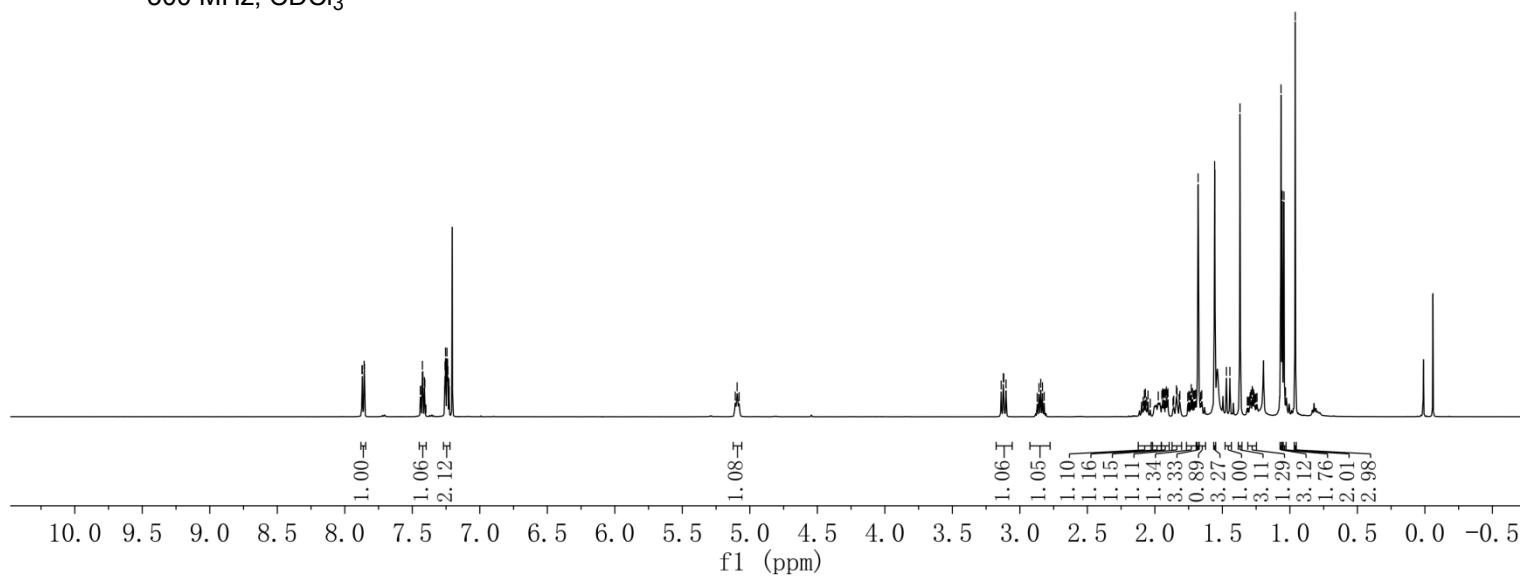
12

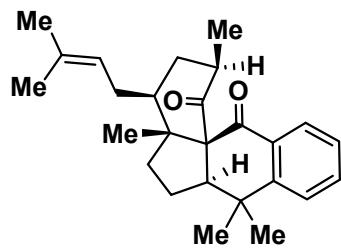
125 MHz, CDCl₃CTT-1-16. 8. ser
NOESY
CTT-1-16
, 400M



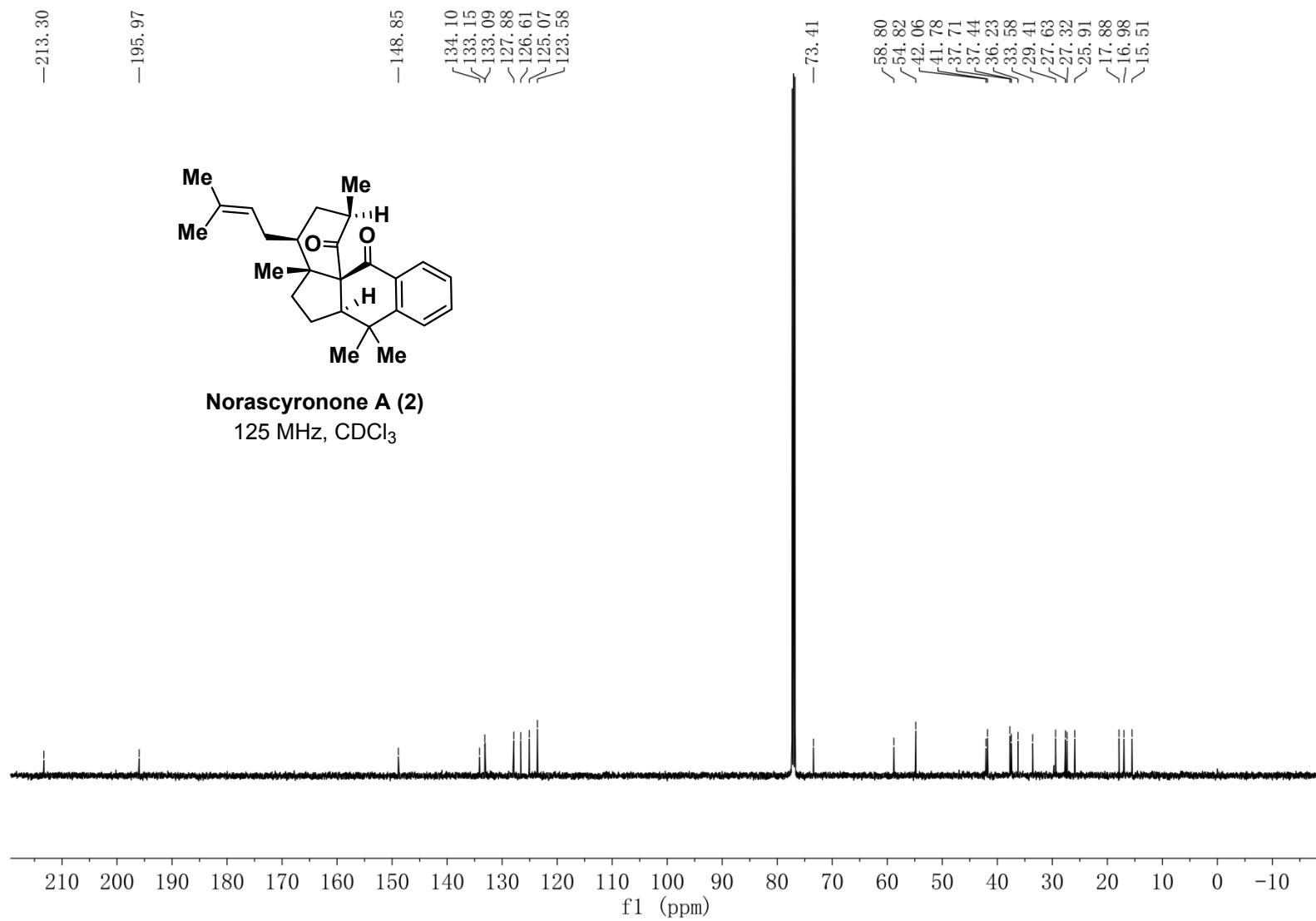
Norascyronone A (2)

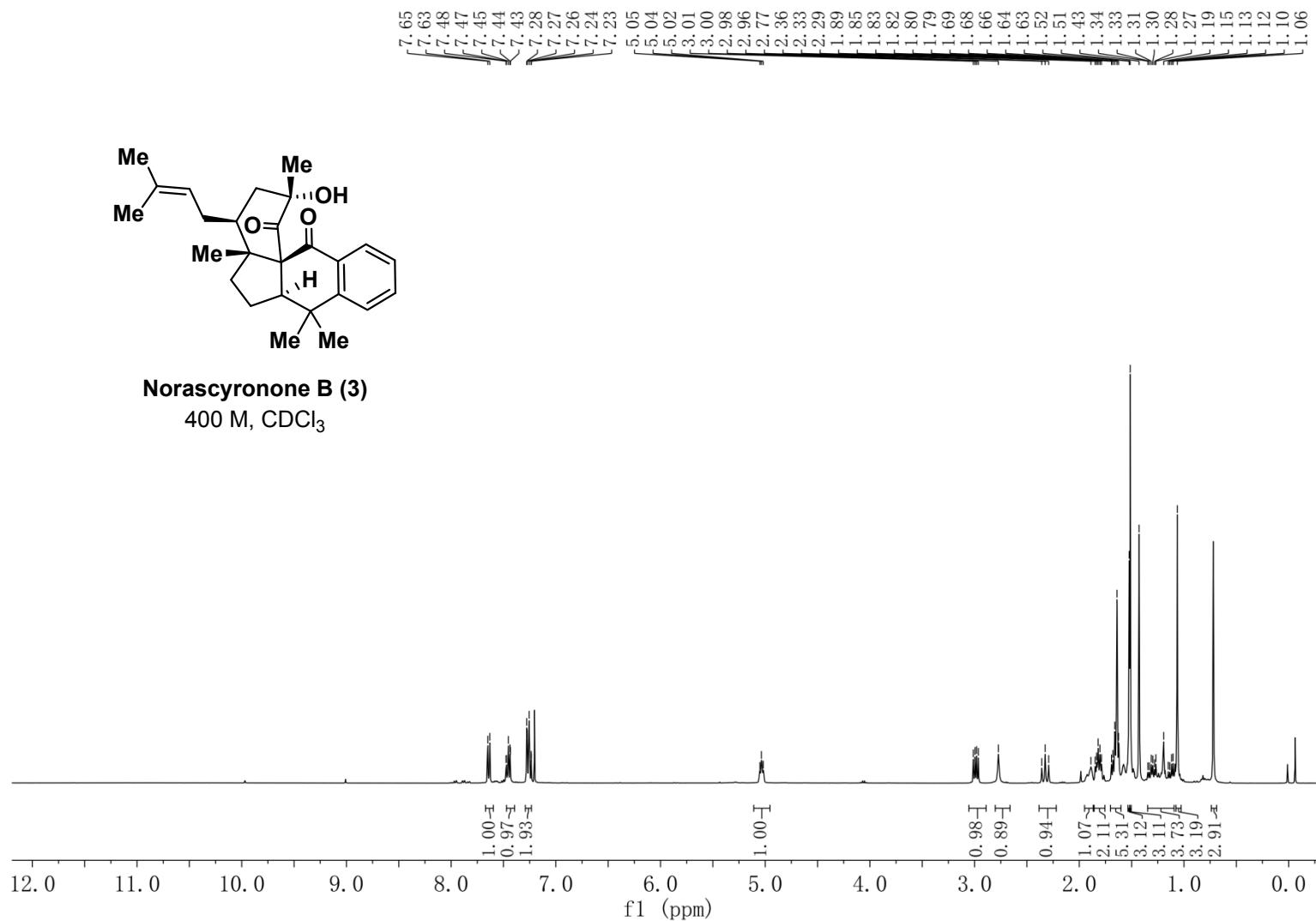
500 MHz, CDCl₃

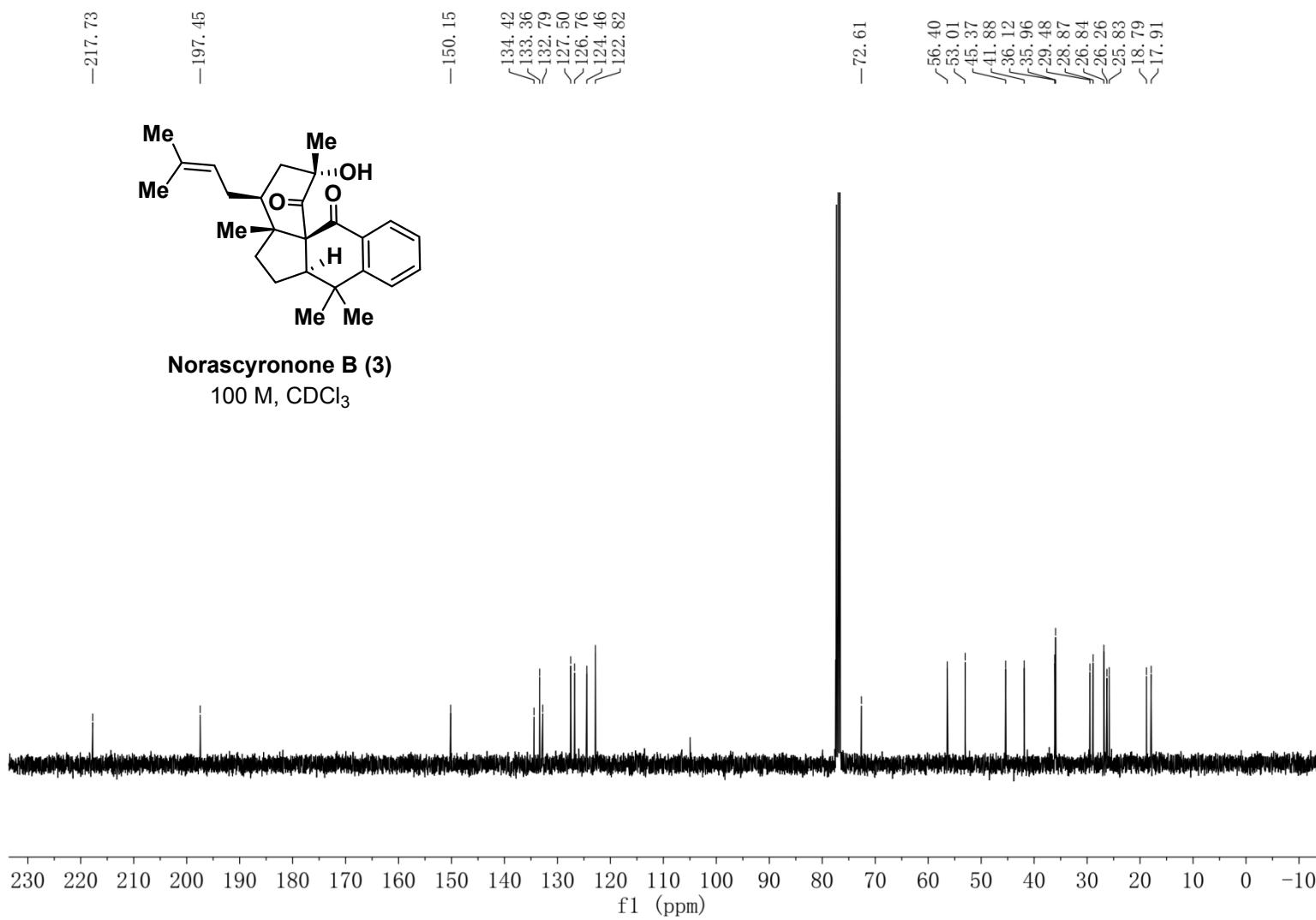




Norascyronone A (2)
125 MHz, CDCl₃







V: Computational Results

1. Complete Reference for Gaussian 09

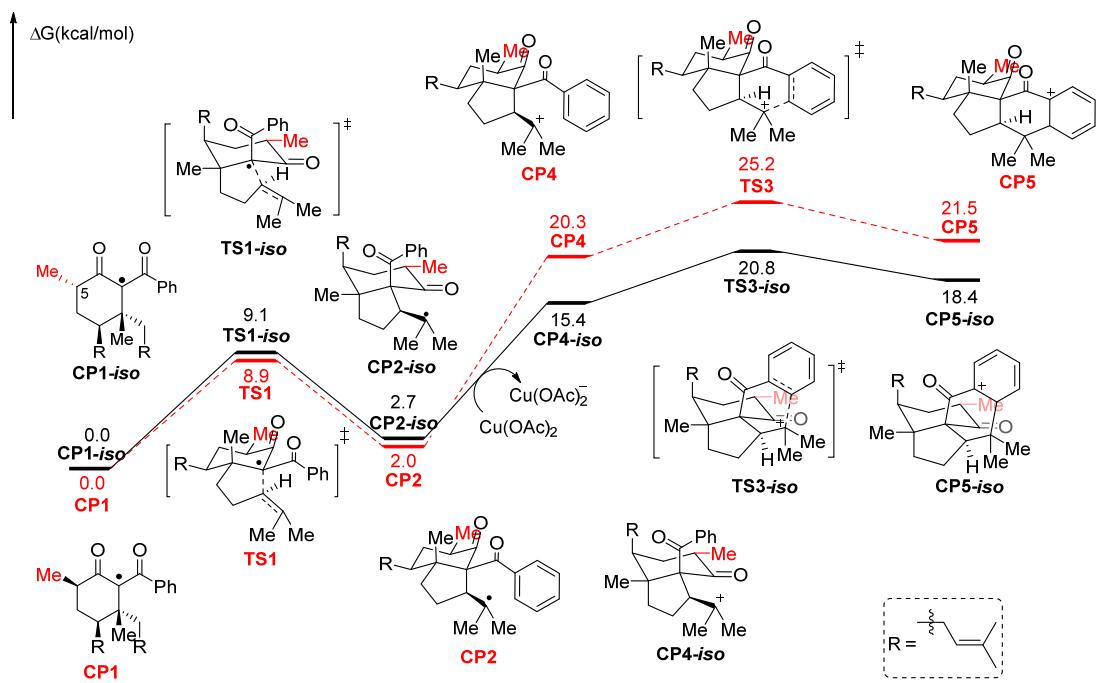
Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

2. Computational Methods

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. Density functional theory B3LYP¹ with a standard 6-31G(d) (SDD for Cu) basis set was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. M06-2x² functional with the SMD³ solvation model is used to calculate the single point energies in solvent. The larger basis set 6-311+G(d,p) (SDD for Cu) is used in the single point calculations in solvent. The energies given in this paper are M06 calculated Gibbs free energies and enthalpies.

3. Free energy profiles for Friedel–Crafts reaction involved pathway of the radical

cyclization.



4. Absolute Calculation Energies, Isohalpies, and Free Energies

Geometry	$E_{(\text{elec-M06})}$ ¹	$E_{(\text{elec-B3LYP})}$ ²	$G_{(\text{corr-B3LYP})}$ ³	$H_{(\text{corr-B3LYP})}$ ⁴	IF ⁵
CP1	-1162.041345	-1162.21368	0.485457	0.582061	-
CP2	-1162.044226	-1162.200187	0.491453	0.582612	-
CP3	-1162.058105	-1162.20985	0.498422	0.583831	-
CP4	-1161.868323	-1161.971545	0.494955	0.583501	-
CP5	-1161.87081	-1161.981124	0.499388	0.584592	-
CP1-iso	-1162.040332	-1162.211539	0.485966	0.582254	-
CP2-iso	-1162.042558	-1162.201695	0.492539	0.58312	-
CP3-iso	-1162.064573	-1162.219409	0.500042	0.584134	-
CP4-iso	-1161.876196	-1161.981716	0.496672	0.584013	-
CP5-iso	-1161.875043	-1161.98828	0.500223	0.584302	-
TS1	-1162.031398	-1162.192757	0.489681	0.580767	-425.51
TS2	-1162.029971	-1162.184961	0.495897	0.581815	-432.88
TS3	-1161.864032	-1161.970715	0.49858	0.583333	-103.93
TS1-iso	-1162.02987	-1162.189755	0.489949	0.58101	-421.33

TS2-iso	-1162.032967	-1162.191693	0.497295	0.582107	-345.20
TS3-iso	-1161.871375	-1161.980939	0.500341	0.583782	-115.99

¹The electronic energy calculated by M06-2x in solviso.²The electronic energy calculated by B3LYP in gas phase. ³The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ⁴The thermal correction to isohalpy calculated by B3LYP in gas phase. ⁵The B3LYP calculated imaginary frequencies for the transition states.

5. B3LYP Geometries for All the Optimized Compounds and Transition State

CP1					
C	-8.33152500	-2.34812000	1.76252600	C	-11.57722600
C	-6.79015500	-2.50018000	1.50163100	H	-10.88424100
C	-6.12949400	-1.12837300	1.62106600	C	-11.38016500
C	-6.62726000	-0.08054600	2.51098900	H	-11.87734600
C	-8.09138300	-0.09677300	2.94401600	H	-10.33007900
C	-8.62440500	-1.53264700	3.03192400	H	-11.84015600
H	-8.73864900	-1.77114800	0.91933400	C	-13.02236700
H	-8.19264600	-2.02996000	3.91157500	H	-13.59521200
H	-9.70758900	-1.50557000	3.19737900	H	-13.51091400
C	-6.49894300	-3.14604800	0.11074500	H	-13.12064000
C	-7.05426300	-2.42102800	-1.13430400	C	-6.13221600
H	-6.88729400	-4.17171600	0.12294300	H	-6.54875200
H	-5.41520800	-3.24702000	0.00065400	H	-5.05552200
H	-8.14544700	-2.31800200	-1.04639300	H	-5.47579300
H	-6.65354100	-1.40330300	-1.18377400	H	-6.29639800
C	-6.75116300	-3.18658100	-2.39670000	O	-5.85451700
C	-5.97904100	-2.82827300	-3.43461500	C	-4.75488100
H	-7.22386800	-4.17006800	-2.44468800	O	-3.88154900
C	-5.23664100	-1.51926400	-3.55411700	C	-4.46125700
H	-5.56462600	-0.96928600	-4.44767500	C	-3.12327900
H	-5.36330000	-0.86206800	-2.69131000	C	-5.46418300
H	-4.15989900	-1.69866100	-3.68038400	C	-2.79416600
C	-5.79475300	-3.75791700	-4.61193600	H	-2.35907600
H	-6.12764200	-3.28437100	-5.54664200	C	-6.50418300
H	-4.73436200	-4.01075100	-4.75364000	H	-3.79989500
H	-6.35218300	-4.69186600	-4.48785300	C	-5.13535500
C	-9.10198500	-3.69507600	1.79898700	H	-2.27268200
H	-8.75487900	-4.33641200	0.97809200	H	-6.50418300
H	-8.86508400	-4.22919300	2.72471600	H	-1.75483400
C	-10.59020000	-3.51037700	1.64585900	H	-2.91963600
				H	-3.54335800
				C	-3.38251600
				H	-1.41119700
				C	-8.31445300
				H	-1.98123200
				C	-0.71299200
				H	-4.22454500
				C	-7.93044400
				H	-1.73030100
				H	-4.11720000
				C	-9.38279400
				H	-0.76026600
				H	-4.46360900

H	-7.79478800	0.25222300	5.07268600	H	-6.27494800	-4.05408200	2.28893500				
H	-8.63631500	0.40131300	2.12259400	H	-4.92888600	-2.92401800	2.16719000				
CP2											
C	-8.34696900	-2.27007200	1.63733100	O	-6.14284600	0.19685600	3.55223800				
C	-6.79732100	-2.16701400	1.33760200	C	-4.80642100	-0.43249300	1.21294400				
C	-6.34438500	-0.61754400	1.31090900	O	-4.11715600	-1.33085900	0.74379000				
C	-6.88791600	-0.01581700	2.60815800	C	-4.11821400	0.86175500	1.57506500				
C	-8.39767800	0.03835500	2.78325400	C	-2.71526200	0.82029500	1.64148100				
C	-8.81866400	-1.44911200	2.84987600	C	-4.76049900	2.09258700	1.78307700				
H	-8.86937300	-1.87245600	0.75611000	C	-1.97653900	1.96719200	1.92010400				
H	-8.40810100	-1.87758300	3.77519300	H	-2.22137400	-0.12940800	1.46822200				
H	-9.90984500	-1.51991300	2.93235400	C	-4.02131300	3.24549200	2.04300100				
C	-6.55832600	-2.62039100	-0.13072000	H	-5.83920700	2.16544200	1.73785700				
C	-6.66654800	-1.36031800	-1.02172300	C	-2.62809000	3.18654800	2.11861200				
H	-7.28830200	-3.38213300	-0.42378300	H	-0.89286200	1.91097600	1.97884300				
H	-5.56700700	-3.06567400	-0.22414500	H	-4.53621400	4.19012100	2.19613700				
H	-5.72566100	-1.20131600	-1.55368400	H	-2.05507400	4.08510900	2.33217100				
H	-7.44892200	-1.44478000	-1.78438900	H	-8.86262600	0.48530700	1.89558900				
C	-6.97054800	-0.15087500	-0.09122700	C	-8.81763300	0.82067100	4.02840100				
C	-6.60598500	1.19452300	-0.65810200	H	-8.51839800	1.87199100	3.95756100				
H	-8.05076900	-0.12975900	0.07861100	H	-9.90573500	0.78201700	4.15271600				
C	-5.41447500	1.39922700	-1.54817300	H	-8.34669300	0.40598900	4.92402800				
H	-5.00462000	2.41006500	-1.42595000								
H	-4.60457400	0.69000600	-1.35490300	CP3							
H	-5.68232900	1.29842100	-2.61553300	C	-8.29241000	-2.38267300	1.62179500				
C	-7.58935100	2.32629600	-0.58003900	C	-6.75799000	-2.46160100	1.26709600				
H	-7.09327700	3.28042300	-0.34923900	C	-6.15113300	-0.98924000	1.18314000				
H	-8.10971500	2.48393500	-1.54234600	C	-6.53079300	-0.23029800	2.47116600				
H	-8.36526900	2.16055700	0.17638200	C	-8.01276500	-0.12389200	2.81555300				
C	-8.83695700	-3.73729800	1.79524100	C	-8.56948000	-1.56161900	2.89138800				
H	-8.33666500	-4.37037500	1.04930800	H	-8.79846900	-1.86858500	0.79333100				
H	-8.53124100	-4.12147600	2.77300900	H	-8.13121300	-2.06193900	3.76634100				
C	-10.32572800	-3.87212700	1.60142700	H	-9.65075700	-1.52069400	3.06884500				
C	-11.24896200	-4.34812300	2.45267400	C	-6.58627400	-2.90926100	-0.20098700				
H	-10.67909300	-3.54020100	0.62226200	C	-6.96835600	-1.68663500	-1.06236100				
C	-10.96343000	-4.86079600	3.84392300	H	-7.18255300	-3.79426100	-0.44806600				
H	-11.25324200	-5.91723500	3.93342300	H	-5.53684900	-3.17489700	-0.36361700				
H	-9.91269700	-4.77807200	4.13035600	H	-6.35749300	-1.65163300	-1.96495700				
H	-11.55911200	-4.31327400	4.58752500	H	-8.00884900	-1.74973500	-1.40033800				
C	-12.70415000	-4.41915600	2.05068100	C	-6.77971100	-0.42141100	-0.15901200				
H	-13.07526800	-5.45318400	2.08973900	C	-6.06448900	0.82832400	-0.81829800				
H	-13.33441100	-3.83836600	2.73906700	H	-7.77847300	-0.06412900	0.10341300				
H	-12.86859300	-4.03935500	1.03717000	C	-5.20639000	0.48629100	-2.05367300				
C	-5.99923600	-2.99697000	2.35888200	H	-4.64133200	1.37176400	-2.36474200				

H	-4.48486700	-0.31244500	-1.85571900	C	-8.33917400	-2.27639600	1.69998800
H	-5.82961700	0.18111700	-2.90075700	C	-6.78333200	-2.21276500	1.43127900
C	-7.15743000	1.82487000	-1.25568100	C	-6.29494700	-0.68557700	1.52730000
H	-6.73839600	2.66874500	-1.81456300	C	-6.83087100	-0.14822800	2.87252200
H	-7.88439300	1.33010900	-1.91108300	C	-8.32543400	-0.11128500	3.10023100
H	-7.70533600	2.22717700	-0.39381600	C	-8.76691800	-1.59457600	3.01082700
C	-8.97345000	-3.77425700	1.74520600	H	-8.83869700	-1.72965200	0.88673000
H	-8.59346300	-4.43607000	0.95480900	H	-8.35236900	-2.13217100	3.87334100
H	-8.68804900	-4.23861800	2.69380000	H	-9.85678000	-1.64997100	3.10285900
C	-10.47256300	-3.69301400	1.60995600	C	-6.49782900	-2.52236600	-0.05089500
C	-11.42161800	-4.03586700	2.49617500	C	-6.97054800	-1.28765000	-0.83689100
H	-10.81197900	-3.30051500	0.64839500	H	-7.00916500	-3.42403900	-0.40019200
C	-11.15993900	-4.59896500	3.87245500	H	-5.42581000	-2.68056400	-0.18940500
H	-11.60539700	-5.59875600	3.97250900	H	-6.38059400	-1.13737400	-1.74306800
H	-10.09766200	-4.68163300	4.11280500	H	-8.01306900	-1.36963100	-1.15621200
H	-11.63137800	-3.97260400	4.64257800	C	-6.88893000	-0.05593700	0.16961900
C	-12.88599500	-3.88505800	2.15371900	C	-6.19615300	1.08073000	-0.49138200
H	-13.40629400	-4.85205900	2.20626000	H	-7.89876000	0.28438600	0.40589700
H	-13.39401700	-3.22154900	2.86796700	C	-4.97073100	0.92131900	-1.31767400
H	-13.03153500	-3.47690700	1.14840700	H	-4.31150900	1.78827000	-1.20650500
C	-6.03477000	-3.38665100	2.26378500	H	-4.41955500	-0.00042800	-1.13277400
H	-6.45795000	-4.39557600	2.21816800	H	-5.29437100	0.92896500	-2.37287700
H	-4.97304000	-3.44503900	2.03472800	C	-6.96026300	2.34086000	-0.68609600
H	-6.13304800	-3.03234700	3.29655500	H	-6.32801400	3.19259200	-0.94434400
O	-5.67166800	0.16471900	3.24283000	H	-7.62453300	2.15317900	-1.55082200
C	-4.61048700	-0.89293700	1.04491400	H	-7.61567600	2.57954400	0.15501600
O	-3.83624200	-1.84255300	1.14487400	C	-8.91154600	-3.72145400	1.65596000
C	-4.12274200	0.45604400	0.71561700	H	-8.45163800	-4.27298400	0.82366900
C	-2.76182600	0.71466400	0.71794800	H	-8.62530700	-4.25406800	2.56695800
C	-5.12968700	1.48763000	0.27808700	C	-10.40792200	-3.73738000	1.47000900
C	-2.25652400	1.96344600	0.34284800	C	-11.34418500	-4.29070800	2.25917800
H	-2.09450700	-0.08825000	1.01698100	H	-10.75253100	-3.24677100	0.55680000
C	-4.49360100	2.78842500	-0.12649900	C	-11.07142400	-5.02885100	3.54721700
H	-5.80186800	1.72403800	1.12343700	H	-11.41239500	-6.06988700	3.46974600
C	-3.14830800	2.99469900	-0.07999100	H	-10.01670300	-5.04624600	3.83171100
H	-1.18719600	2.15001700	0.36818100	H	-11.63728700	-4.58049500	4.37471800
H	-5.15318500	3.59755000	-0.42800800	C	-12.80441400	-4.22525400	1.87719900
H	-2.73987500	3.96228200	-0.36237700	H	-13.22314600	-5.23382600	1.75937100
C	-8.24735900	0.66886900	4.10276100	H	-13.39562600	-3.73486800	2.66246400
H	-7.85925200	1.68882100	4.01912900	H	-12.96173200	-3.68172200	0.94044400
H	-9.31945900	0.72252400	4.32362500	C	-6.02971400	-3.14688800	2.39732200
H	-7.74052600	0.19661500	4.94982900	H	-6.38901700	-4.17171200	2.27182300
H	-8.52426700	0.38338300	1.98499400	H	-4.95885500	-3.14048000	2.20135900
				H	-6.18436900	-2.86691400	3.44426300

O	-6.02245500	0.01627800	3.76936100	H	-7.52648400	1.15453400	-2.38571700				
C	-4.75671500	-0.45453300	1.51189800	H	-7.46877400	2.32533000	-1.06235100				
O	-3.97325300	-1.35517100	1.27394700	C	-9.05076000	-3.74989800	1.67414600				
C	-4.23522100	0.95857700	1.61115000	H	-8.76387300	-4.34136000	0.79377800				
C	-2.86205000	1.13534200	1.37006500	H	-8.69167600	-4.30654600	2.54431400				
C	-5.03924200	2.10178700	1.80434600	C	-10.55382000	-3.62559400	1.69690100				
C	-2.30967900	2.41057800	1.31117900	C	-11.41705700	-4.05931800	2.63066000				
H	-2.24673100	0.25447700	1.22360600	H	-10.97567500	-3.12880200	0.82037300				
C	-4.48242400	3.38535100	1.73369600	C	-11.03488800	-4.78320700	3.89910000				
H	-6.07799700	2.01313900	2.09608000	H	-11.47238800	-5.79051000	3.91104300				
C	-3.12237400	3.54289800	1.48065800	H	-9.95633200	-4.88856200	4.03820200				
H	-1.24468100	2.52995100	1.13574100	H	-11.43941000	-4.26180100	4.77695400				
H	-5.11079200	4.25445200	1.90475400	C	-12.90420400	-3.86118000	2.45183900				
H	-2.68675000	4.53657100	1.43564500	H	-13.42824400	-4.82645700	2.43691100				
H	-8.81353300	0.43073300	2.27660900	H	-13.33011300	-3.29118200	3.28886700				
C	-8.70006700	0.54153900	4.43247600	H	-13.14088200	-3.33316500	1.52295900				
H	-8.38389300	1.58914100	4.47000100	C	-6.05783600	-3.41799000	2.00286800				
H	-9.78469100	0.50619200	4.57496500	H	-6.52924800	-4.40336300	1.95908100				
H	-8.22149500	0.02297700	5.26754300	H	-5.03179200	-3.52611400	1.65638200				
CP5											
C	-8.35084600	-2.36364400	1.61673400	H	-6.02477700	-3.11788200	3.05641400				
C	-6.85388000	-2.42359900	1.13462000	O	-5.74397600	0.55032500	2.89357500				
C	-6.26000600	-0.95007300	1.11415900	C	-4.73434100	-0.82527700	1.03260600				
C	-6.62275200	-0.12857200	2.36487100	O	-3.90992100	-1.71512300	0.99829600				
C	-8.03101400	-0.18112300	2.91285400	C	-4.23423000	0.59446100	0.87055200				
C	-8.50022200	-1.64908700	2.96647900	C	-2.92300400	0.90580500	1.18508000				
H	-8.91326500	-1.76762500	0.88379600	C	-5.10465500	1.54521000	0.14132200				
H	-7.94378400	-2.17926000	3.75027300	C	-2.41169200	2.15611800	0.82802800				
H	-9.55266800	-1.66779500	3.26800600	H	-2.29997100	0.16753100	1.67830000				
C	-6.78820900	-2.77363100	-0.37024700	C	-4.45776700	2.81616000	-0.25291300				
C	-7.27723400	-1.51749100	-1.10854700	H	-5.87882800	1.87698700	0.86097600				
H	-7.37797100	-3.65872000	-0.62434800	C	-3.17332400	3.11383900	0.10803600				
H	-5.74986800	-2.99808600	-0.64135000	H	-1.38392800	2.39690200	1.08930700				
H	-6.88138000	-1.46945900	-2.12447500	H	-5.05554800	3.54223600	-0.79536400				
H	-8.36650400	-1.52344100	-1.20716600	H	-2.72550100	4.06657000	-0.15467100				
C	-6.84249100	-0.29850900	-0.23433400	C	-8.16563300	0.55649600	4.24803500				
C	-5.93134000	0.75120200	-0.97751900	H	-7.85332600	1.60122200	4.16619100				
H	-7.73815000	0.25888700	0.05919700	H	-9.20819600	0.53171800	4.57960100				
C	-4.91659000	0.13963800	-1.97283000	H	-7.54933400	0.08547700	5.02038200				
H	-4.18666500	0.89716800	-2.27919600	H	-8.66194600	0.32481500	2.16158500				
H	-4.36588500	-0.71161000	-1.56189100	CP1-iso							
H	-5.41848000	-0.19959900	-2.88213100	C	-8.35098200	-2.28026200	1.76276600				
C	-6.85016500	1.72372100	-1.73913300	C	-6.80217000	-2.42314800	1.55051800				
H	-6.28382500	2.40025300	-2.38761300	C	-6.16518600	-1.04086400	1.66958200				
				C	-6.70458900	0.01609600	2.51057500				

C	-8.13223500	-0.06603000	3.04430600	H	-9.13455400	0.60301700	1.20146800
C	-8.67970500	-1.50196600	3.04781700	O	-6.00325100	1.00576600	2.77915100
H	-8.72958900	-1.68898800	0.91754800	C	-4.77772500	-0.79957200	1.13149100
H	-8.08346700	0.31075100	4.07338400	O	-3.88760800	-1.58835100	1.44030400
H	-8.27987200	-2.04483300	3.91368300	C	-4.49139600	0.34657200	0.21556600
H	-9.76746900	-1.47684700	3.18189800	C	-3.15524200	0.57120900	-0.15243400
C	-6.46084100	-3.08521500	0.17858500	C	-5.49599800	1.16531100	-0.32247200
C	-7.03704300	-2.42522400	-1.09270200	C	-2.82956300	1.59943600	-1.03200400
H	-6.79593000	-4.12907000	0.21342800	H	-2.38999200	-0.07351900	0.26679100
H	-5.37163500	-3.13536800	0.08370700	C	-5.17024400	2.18917800	-1.21098700
H	-8.13276700	-2.37223000	-1.01598000	H	-6.53294600	1.00494700	-0.04728200
H	-6.68420500	-1.39191000	-1.17208300	C	-3.83698400	2.41009400	-1.56446400
C	-6.68690100	-3.21721100	-2.32633700	H	-1.79193600	1.77063100	-1.30531800
C	-5.95608700	-2.84621000	-3.38928100	H	-5.95524500	2.81717100	-1.62294600
H	-7.08426400	-4.23469300	-2.32742500	H	-3.58333400	3.21182000	-2.25296400
C	-5.31874300	-1.49065700	-3.57638000	CP2-iso			
H	-5.69847900	-1.00920600	-4.48881400	C	-2.20359000	0.43046200	0.36328800
H	-5.48690000	-0.80653100	-2.74213000	C	-0.89801400	1.25864300	0.06975600
H	-4.23273500	-1.59158200	-3.71026700	C	0.50922900	0.53373700	0.34410400
C	-5.71491100	-3.80928800	-4.52892600	C	0.34080000	-0.32172200	1.65314100
H	-6.09437200	-3.40335300	-5.47755100	C	-0.83049100	-1.28534700	1.67899800
H	-4.63999900	-3.98637700	-4.67603300	C	-2.09583000	-0.39776600	1.65704300
H	-6.19737900	-4.77680500	-4.35711700	H	-2.97922900	1.19056200	0.53865300
C	-9.11911200	-3.62865700	1.74355200	H	-0.81316200	-1.87346000	0.75151400
H	-8.75743200	-4.24258500	0.90796800	H	-2.07471900	0.25445800	2.53959200
H	-8.89599000	-4.19174400	2.65554300	H	-2.98439600	-1.02751300	1.77183700
C	-10.60518700	-3.44217400	1.57250900	C	-0.99420200	1.89152000	-1.33760900
C	-11.60559000	-3.84556200	2.37242300	H	-1.95568700	2.41408300	-1.42438100
H	-10.88468500	-2.91276100	0.65866500	H	-0.21248700	2.63468600	-1.50509700
C	-11.42958100	-4.59581600	3.67080900	C	-2.74782200	-0.43725200	-0.81349500
H	-11.92184400	-5.57719500	3.62000500	H	-2.02541300	-1.21698100	-1.07066400
H	-10.38368400	-4.76127100	3.93888000	H	-2.82622200	0.18924200	-1.70450900
H	-11.90738800	-4.05329600	4.49839100	C	-4.08651400	-1.07425100	-0.52151100
C	-13.04523000	-3.57362300	2.00126800	C	-5.30704200	-0.59392700	-0.81212500
H	-13.61219100	-4.51024300	1.90284700	H	-4.04975200	-2.04265500	-0.02046100
H	-13.55116400	-2.98628500	2.78061000	C	-5.56647500	0.72157700	-1.50653500
H	-13.12838300	-3.02716300	1.05637300	H	-6.15642700	0.56852900	-2.42122300
C	-6.16147100	-3.32655100	2.65116500	H	-4.65137500	1.25132600	-1.78190200
H	-6.58375700	-4.33639500	2.60285600	H	-6.15980800	1.38837400	-0.86491300
H	-5.08328200	-3.38700400	2.49528500	C	-6.55323700	-1.36925000	-0.45408200
H	-6.33076600	-2.93181300	3.65762600	H	-7.14690500	-1.60104900	-1.34998800
C	-9.01920900	0.91430800	2.24676300	H	-7.20838500	-0.78532500	0.20821900
H	-10.01961500	0.96696800	2.69093800	H	-6.31718500	-2.31250900	0.04896000
H	-8.58111800	1.91724000	2.25843400	C	-0.78291200	2.43152900	1.08450300

H	-1.54439300	3.19621100	0.89039200	H	-2.11572700	0.71540700	2.35955000
H	-0.93846100	2.07617600	2.11018700	H	-3.28720900	-0.45052200	1.78462600
C	-0.78531900	-2.22415200	2.88523400	C	-0.73341300	1.44873500	-1.68098100
H	0.13442600	-2.81777600	2.89333900	H	-1.56343900	2.09906900	-1.98410600
H	-1.63915600	-2.91032300	2.86070100	H	0.19235400	1.97374600	-1.93153400
H	-0.82026800	-1.65984900	3.82225900	C	-2.89606300	-0.35035200	-0.88580100
O	1.06261300	-0.18164300	2.62403500	H	-2.23398200	-1.20030400	-1.07231300
C	0.96631700	-0.46933800	-0.74610200	H	-2.95089800	0.19463500	-1.83176200
O	0.21201100	-0.76969900	-1.66372800	C	-4.27073300	-0.85430800	-0.51478700
C	2.31662300	-1.13812200	-0.69168200	C	-5.45927200	-0.31450800	-0.83211300
C	2.67956700	-1.90014400	-1.81785400	H	-4.29194600	-1.77178400	0.07545900
C	3.20352400	-1.08209200	0.39753400	C	-5.63564000	0.94868800	-1.64046000
C	3.89447700	-2.57624000	-1.86226200	H	-6.23972500	0.75589400	-2.53840700
H	1.98624700	-1.94696300	-2.65030800	H	-4.68863000	1.39003800	-1.96044500
C	4.41561800	-1.77223400	0.35563000	H	-6.17951600	1.70742500	-1.06013900
H	2.95051300	-0.52569600	1.28993200	C	-6.75126000	-0.96134600	-0.39084300
C	4.76768200	-2.51502700	-0.77233100	H	-7.37686200	-1.22692300	-1.25518100
H	4.16057100	-3.15363900	-2.74356900	H	-7.35023900	-0.27507500	0.22492200
H	5.08589100	-1.72658500	1.20953900	H	-6.57435000	-1.87182700	0.19080200
H	5.71581900	-3.04568600	-0.80179600	C	-0.61858300	2.49374800	0.58851100
H	-0.92840700	1.15345600	-2.13466600	H	-1.22737600	3.29589800	0.15481200
C	1.54147200	1.70508100	0.64950500	H	-0.92390200	2.39070200	1.63792200
C	0.64638900	2.96324800	0.93400500	C	-1.39732000	-1.95850000	3.04057500
H	0.99260600	3.48974200	1.82930300	H	-0.62362200	-2.72623900	3.13373800
H	0.70830200	3.67637900	0.10574000	H	-2.37769600	-2.44742400	3.06393500
H	2.00076300	1.43431700	1.60272000	H	-1.31762000	-1.30541200	3.91629600
C	2.67333000	1.97754400	-0.30977400	O	0.96318300	-0.62879800	2.51955100
C	3.96606600	2.46661800	0.27756200	C	0.89480300	-0.81092200	-0.60268400
C	2.47284300	2.21601600	-1.77763600	O	0.07399100	-1.46431600	-1.25501900
H	4.15087900	2.04747800	1.27376900	C	2.32486800	-1.12676600	-0.64138100
H	4.82027100	2.21090800	-0.36368000	C	2.75754800	-2.13689200	-1.49443500
H	3.98448800	3.56714700	0.38855400	C	3.29489500	-0.32703600	0.19063500
H	1.72247900	1.55887100	-2.22705100	C	4.11117500	-2.43889000	-1.64297700
H	2.15355900	3.25287200	-1.99392500	H	2.00359800	-2.67523000	-2.06087800
H	3.41310500	2.06724900	-2.32338500	C	4.72750700	-0.69557000	-0.07064200
CP3-iso				H	3.09906900	-0.55138800	1.25741700
C	-2.25771400	0.58864000	0.18379700	C	5.09249200	-1.69308700	-0.92129700
C	-0.83330000	1.15361700	-0.16778200	H	4.42192100	-3.23204800	-2.31641100
C	0.43050500	0.32062600	0.34669600	H	5.48980700	-0.16298900	0.49044900
C	0.12496400	-0.50708900	1.64168200	H	6.14404100	-1.93647800	-1.05325300
C	-1.23814200	-1.16248900	1.74409000	H	-0.77251800	0.54018100	-2.28234300
C	-2.28973300	-0.04468200	1.58567600	C	1.54678100	1.39109800	0.69813400
H	-2.91399800	1.47121100	0.22101200	C	0.88393200	2.77597600	0.51299800
H	-1.33199000	-1.83840600	0.88313800	H	1.21008100	3.48362500	1.28270600

H	1.13652700	3.22506100	-0.45212700	H	-2.20548300	-2.82877900	2.80506700
H	1.72493700	1.25972100	1.76904400	H	-1.24626600	-1.70832900	3.79240800
C	2.95772400	1.21126500	0.05767300	O	0.93906300	-0.60186900	2.57159000
C	3.95663000	2.05242400	0.87829700	C	0.94077600	-0.67637500	-0.68577100
C	3.05958600	1.63788100	-1.41976500	O	0.16772400	-1.15230200	-1.49905900
H	4.03019100	1.69291200	1.91198700	C	2.38871500	-1.08300700	-0.72721900
H	4.95907200	2.03573100	0.43720200	C	2.88106200	-1.53026000	-1.96484300
H	3.63691500	3.09992800	0.91124800	C	3.26244400	-1.02334600	0.38071500
H	2.31507000	1.14645100	-2.05297800	C	4.22370600	-1.86828100	-2.10798400
H	2.93851700	2.72037700	-1.53232500	H	2.19737900	-1.59811200	-2.80451400
H	4.04834300	1.37737300	-1.81522900	C	4.60850000	-1.39044700	0.23285000
CP4-iso				H	2.87987100	-0.80363000	1.37121400
C	-2.26117700	0.49516700	0.25493500	C	5.09422300	-1.79136800	-1.00892900
C	-0.86897900	1.17761900	-0.02546500	H	4.59630800	-2.20348700	-3.07142500
C	0.44011800	0.33571700	0.37441800	H	5.26491100	-1.37953400	1.09806100
C	0.15043100	-0.57454100	1.64525900	H	6.13792900	-2.06832900	-1.12369200
C	-1.14520600	-1.34518700	1.64615800	H	-0.78799300	0.88147400	-2.20893100
C	-2.26895500	-0.28302600	1.58138800	C	1.51950400	1.39191500	0.83089100
H	-2.95784000	1.33645600	0.37905800	C	0.77515200	2.80384200	0.85886500
H	-1.18754300	-1.93257400	0.71888500	H	1.10923400	3.37881300	1.72601300
H	-2.16766000	0.39031800	2.44268000	H	0.98195800	3.39669500	-0.03596200
H	-3.23561000	-0.77979000	1.70402600	H	1.77686100	1.15184900	1.86378800
C	-0.82183100	1.69172300	-1.48110300	C	2.77222200	1.62928400	0.09360900
H	-1.72109100	2.28502900	-1.68007700	C	3.95641700	2.06715400	0.88397900
H	0.02956600	2.35392300	-1.66637700	C	2.86599300	1.83853100	-1.37415000
C	-2.85665000	-0.35499000	-0.90967300	H	4.00661900	1.60188200	1.87004600
H	-2.18164100	-1.17821700	-1.15963600	H	4.89592300	1.93634800	0.34171400
H	-2.90639700	0.26759100	-1.80622000	H	3.83372100	3.15307700	1.04650100
C	-4.22868900	-0.91263000	-0.60474000	H	1.97321900	1.55944200	-1.92976400
C	-5.41871400	-0.35190400	-0.87876300	H	3.07801200	2.90667600	-1.54450300
H	-4.24303100	-1.89043500	-0.12243300	H	3.73569300	1.30492500	-1.77540100
C	-5.60005200	0.98624900	-1.55344400	CP5-iso			
H	-6.19745800	0.87901100	-2.46873600	C	-2.27748500	0.60932200	0.22272200
H	-4.65731500	1.46936200	-1.82397600	C	-0.89135400	1.23070000	-0.16312400
H	-6.15600500	1.67453600	-0.90230600	C	0.39851600	0.35807800	0.20980700
C	-6.70708600	-1.05567200	-0.52573700	C	0.18086200	-0.68709800	1.37610300
H	-7.31359000	-1.23640500	-1.42366300	C	-1.20081200	-1.23886400	1.62834300
H	-7.32248600	-0.44096900	0.14538700	C	-2.22325900	-0.08578300	1.59275100
H	-6.52857600	-2.01883300	-0.03790600	H	-2.95355200	1.46853200	0.33479600
C	-0.70252500	2.39878300	0.91662900	H	-1.40829400	-1.88935300	0.76274100
H	-1.34951200	3.22962800	0.61613700	H	-1.98531900	0.62736800	2.39199000
H	-0.96235800	2.13640500	1.94796900	H	-3.21140600	-0.48798600	1.83429700
C	-1.26317000	-2.27448300	2.85600400	C	-0.87538300	1.65195800	-1.65068300
H	-0.44102500	-2.99545600	2.88905400	H	-1.70125800	2.34854400	-1.83299300

H	0.04850000	2.17498500	-1.91915600	C	3.18856100	1.83612200	-1.20182500
C	-2.93709500	-0.29675800	-0.86166500	H	3.90815500	1.39134500	2.17651700
H	-2.25720300	-1.10967500	-1.14144000	H	4.94391300	1.92106900	0.82800500
H	-3.06868900	0.29671900	-1.76975400	H	3.61315800	2.93447200	1.36977500
C	-4.26500000	-0.88290000	-0.44114100	H	2.43385100	1.51981600	-1.93001200
C	-5.48959900	-0.37962700	-0.67087400	H	3.17107400	2.92882600	-1.15867400
H	-4.21356700	-1.82885500	0.09972900	H	4.17169700	1.54358700	-1.58652400
C	-5.76221700	0.90919100	-1.40783200	TS1			
H	-6.40788300	0.72711200	-2.27740200	C	-8.30200400	-1.99985000	1.52350300
H	-4.85713700	1.41013800	-1.76107200	C	-6.84444700	-1.75007900	1.00185400
H	-6.30561400	1.61345400	-0.76335500	C	-6.56405900	-0.22145300	0.89031000
C	-6.72648900	-1.10368500	-0.19560600	C	-7.34582600	0.78969800	1.64015900
H	-7.38062300	-1.35775700	-1.04080600	C	-8.64791500	0.38128400	2.33783800
H	-7.32132600	-0.47048700	0.47678900	C	-8.64369800	-1.10173100	2.72031700
H	-6.48285300	-2.02951500	0.33473500	H	-8.98847000	-1.71584200	0.71232100
C	-0.63833300	2.51075500	0.68272000	H	-7.92821300	-1.27253400	3.53863200
H	-1.25159000	3.34380200	0.32536400	H	-9.62858000	-1.38094300	3.11356600
H	-0.90519700	2.34115700	1.73296100	C	-6.67272800	-2.30773600	-0.43354000
C	-1.26280300	-2.07647300	2.90940300	C	-7.44482600	-1.42191800	-1.42504900
H	-0.53258300	-2.88978000	2.89621600	H	-6.99400500	-3.35446800	-0.49651100
H	-2.26213000	-2.50899100	3.01639500	H	-5.61032700	-2.28086000	-0.68900900
H	-1.06223900	-1.46042600	3.79234500	H	-7.02183100	-1.53146600	-2.42785900
O	1.15376400	-1.05500900	2.02287500	H	-8.48822000	-1.75350700	-1.49732100
C	0.88866100	-0.59024200	-0.88750100	C	-7.44524100	0.04247200	-0.98869800
O	0.16448200	-1.11687700	-1.71403000	C	-6.82633700	1.06401100	-1.74156900
C	2.34564200	-0.98595600	-0.85091000	H	-8.39664100	0.36081400	-0.56394000
C	2.80212200	-1.97414000	-1.69852800	C	-5.75606700	0.82841100	-2.76748500
C	3.22638700	-0.34261800	0.12291700	H	-4.86787700	1.43453200	-2.54513400
C	4.14775100	-2.37576200	-1.62700100	H	-5.43120700	-0.21017300	-2.82530400
H	2.11570100	-2.43383700	-2.40203400	H	-6.11009800	1.14607900	-3.76106300
C	4.61121100	-0.79879200	0.12906800	C	-7.18471500	2.50392500	-1.50624500
H	2.77619500	-0.67245300	1.11946900	H	-6.36868700	3.02966400	-0.98986500
C	5.04820100	-1.80253900	-0.70870500	H	-7.34209100	3.02543700	-2.46170300
H	4.50006900	-3.15854600	-2.29420600	H	-8.07951900	2.62062800	-0.88958300
H	5.30037800	-0.34916400	0.83725500	C	-8.60193700	-3.48700000	1.85404800
H	6.07641100	-2.14759000	-0.67282800	H	-8.16751300	-4.12759200	1.07378100
H	-0.98877700	0.81088100	-2.33282600	H	-8.10223100	-3.76298000	2.78793400
C	1.49517200	1.39470900	0.73090900	C	-10.07979500	-3.77359500	1.92594000
C	0.86133400	2.79078600	0.57559600	C	-10.79895000	-4.25102100	2.95476600
H	1.21381500	3.47801300	1.35084400	H	-10.62004400	-3.56213800	1.00020700
H	1.09809200	3.24653500	-0.38922700	C	-10.24051600	-4.60924000	4.31118600
H	1.57354600	1.20910000	1.80588700	H	-10.40375300	-5.67448700	4.52727400
C	2.95085400	1.23939100	0.20100100	H	-9.17091100	-4.40969500	4.40746500
C	3.91567400	1.89589800	1.20329600	H	-10.75937800	-4.05071600	5.10265300

C	-12.28522100	-4.48574800	2.81312300	C	-6.29226300	0.85607200	-0.77431500
H	-12.53820000	-5.54033200	2.99306800	H	-7.81044600	-0.40084700	-0.03331700
H	-12.85114000	-3.90159600	3.55261300	C	-5.49493600	0.84602100	-2.05680300
H	-12.64960700	-4.21623400	1.81665000	H	-5.20288300	1.86461400	-2.33207600
C	-5.81183300	-2.44473400	1.92575700	H	-4.58222000	0.24785300	-1.98198300
H	-5.93687700	-3.53182600	1.89033700	H	-6.08960700	0.43798200	-2.88950900
H	-4.78900700	-2.22750000	1.60511900	C	-7.36057000	1.92837300	-0.73808400
H	-5.90762000	-2.13174900	2.97069500	H	-6.96003200	2.90611600	-1.02815200
O	-7.00274200	1.97259200	1.61835400	H	-8.17353500	1.69022000	-1.44401400
C	-5.09667900	0.12511600	0.70489800	H	-7.81944500	2.03036300	0.25290000
O	-4.50566500	-0.20675700	-0.32008400	C	-8.95581600	-3.77721300	1.80382900
C	-4.29406100	0.78963900	1.79463900	H	-8.51982200	-4.47613400	1.07646200
C	-3.06861900	1.36735400	1.42431000	H	-8.70309700	-4.17121000	2.79230600
C	-4.64786400	0.77718900	3.15195800	C	-10.44864500	-3.74998900	1.59622900
C	-2.23238900	1.93927900	2.37923100	C	-11.42710700	-4.08839300	2.45163600
H	-2.78873900	1.35311000	0.37641600	H	-10.75450600	-3.40858900	0.60432000
C	-3.80237100	1.33082500	4.11200700	C	-11.21365000	-4.58727900	3.86064200
H	-5.58142800	0.32580700	3.46926900	H	-11.64092100	-5.59240900	3.98360400
C	-2.59632200	1.92079200	3.72831800	H	-10.16151900	-4.63513000	4.15000600
H	-1.29412300	2.39478600	2.07373500	H	-11.73241500	-3.94111800	4.58247200
H	-4.08798700	1.30546800	5.16016200	C	-12.87772500	-3.99961900	2.03664700
H	-1.94280700	2.36135100	4.47674900	H	-13.36834400	-4.98138900	2.09992400
H	-9.44028800	0.52246200	1.58179500	H	-13.44011200	-3.32964000	2.70245900
C	-8.96141100	1.31250000	3.51512000	H	-12.98889000	-3.63160700	1.01165500
H	-9.95240000	1.08992300	3.92654500	C	-6.08053200	-3.28809700	2.45184400
H	-8.22606800	1.18887800	4.31964300	H	-6.47265000	-4.30995800	2.42516300
H	-8.93262400	2.35733300	3.19824600	H	-5.00472600	-3.33070000	2.30031600
TS2				H	-6.26468300	-2.88785900	3.45561000
C	-8.30834500	-2.37584300	1.62111300	O	-5.82407700	0.18962200	3.33991000
C	-6.75233700	-2.43302000	1.35894100	C	-4.61476000	-0.87682900	1.14559400
C	-6.16213400	-0.94812300	1.25417600	O	-3.89332400	-1.86875100	1.19715600
C	-6.62536000	-0.17546600	2.49415900	C	-4.03954500	0.44210800	0.78376800
C	-8.12855200	-0.04616300	2.71337200	C	-2.70786800	0.48531600	0.35391700
C	-8.68734600	-1.48322200	2.81478400	C	-4.85662700	1.61186800	0.67209800
H	-8.78018600	-1.94476000	0.72767300	C	-2.14779600	1.66230700	-0.13792800
H	-8.31902600	-1.93251300	3.74755300	H	-2.12932200	-0.43139000	0.40793800
H	-9.77933900	-1.44122700	2.90397700	C	-4.24640000	2.81901000	0.21999300
C	-6.48766400	-2.97275800	-0.07412300	H	-5.71346500	1.72336200	1.32468600
C	-6.47144800	-1.75245500	-1.03164300	C	-2.93021600	2.83174100	-0.20716600
H	-7.24458900	-3.70699300	-0.36824900	H	-1.11050500	1.68035500	-0.45983600
H	-5.52114500	-3.48211100	-0.09794200	H	-4.82736500	3.73749700	0.21887200
H	-5.49859400	-1.68568000	-1.52471900	H	-2.48631400	3.75658000	-0.56768600
H	-7.21991900	-1.83040000	-1.82805300	C	-8.46194900	0.79920500	3.94387300
C	-6.72798700	-0.48637500	-0.16511000	H	-8.07242300	1.81771500	3.84617300

H	-9.54756100	0.85590400	4.08238700	C	-6.05459700	-3.33662900	2.22035700				
H	-8.01733100	0.36617400	4.84490300	H	-6.49400400	-4.33747100	2.20216200				
H	-8.57333000	0.41934000	1.82278000	H	-5.00467000	-3.42540700	1.94957100				
TS3											
C	-8.34687700	-2.36944900	1.63095400	O	-5.76112600	0.16626200	3.24218100				
C	-6.81646200	-2.41791900	1.24696200	C	-4.70895300	-0.77766300	1.09933800				
C	-6.24730100	-0.92394200	1.18519700	O	-3.92625400	-1.70569700	1.06998900				
C	-6.65130100	-0.19458700	2.48900800	C	-4.17938200	0.62106300	0.86760000				
C	-8.11763000	-0.12073300	2.85519600	C	-2.81826400	0.75803200	0.58862700				
C	-8.61856400	-1.58340800	2.92255400	C	-5.03651400	1.74273400	0.70284000				
H	-8.87746700	-1.83848300	0.82756800	C	-2.30524600	1.98604900	0.17156900				
H	-8.14669900	-2.07844300	3.78133200	H	-2.17922100	-0.11313800	0.68491200				
H	-9.69598100	-1.58046100	3.11858500	C	-4.50006000	2.98398400	0.28121700				
C	-6.65752400	-2.84113800	-0.22865000	H	-6.01494200	1.75933400	1.16606800				
C	-7.14127100	-1.64035700	-1.05887500	C	-3.14891100	3.10025100	-0.00180000				
H	-7.21802700	-3.74741400	-0.47590600	H	-1.24208100	2.08224100	-0.02962000				
H	-5.60274700	-3.05120500	-0.43299300	H	-5.15188300	3.84917800	0.20398100				
H	-6.65352000	-1.60350000	-2.03466000	H	-2.73384600	4.04971500	-0.32518800				
H	-8.21604800	-1.68523200	-1.25406900	C	-8.35506300	0.65533300	4.15251800				
C	-6.86019600	-0.35642200	-0.17070500	H	-8.00249300	1.68851000	4.07411700				
C	-6.09516600	0.66872600	-0.99205800	H	-9.42426100	0.67316400	4.38601200				
H	-7.81474800	0.11065600	0.08184300	H	-7.82497600	0.19005900	4.98838800				
C	-4.97061200	0.26963600	-1.90617800	H	-8.66081100	0.37029400	2.03249300				
H	-4.24510500	1.08185200	-2.01273500	TS1-iso							
H	-4.45547600	-0.64382200	-1.60746900	C	-8.34333700	-1.99753900	1.52401600				
H	-5.39969200	0.11480200	-2.90697400	C	-6.89144200	-1.75118400	0.98550300				
C	-6.91959100	1.81814400	-1.50082800	C	-6.61955700	-0.21950100	0.86867400				
H	-6.32407200	2.56988700	-2.02272700	C	-7.42543300	0.78203300	1.61272500				
H	-7.62183200	1.38592800	-2.23379100	C	-8.62162500	0.35854600	2.47356100				
H	-7.52746600	2.28958100	-0.72470700	C	-8.63781000	-1.14718200	2.76887800				
C	-9.00929500	-3.77271900	1.72737200	H	-9.03884000	-1.67369800	0.73726000				
H	-8.64132700	-4.41015600	0.91140700	H	-8.48881600	0.91115000	3.41371200				
H	-8.69770700	-4.25856900	2.65611000	H	-7.90015800	-1.38144400	3.54877000				
C	-10.51291100	-3.69852600	1.63478500	H	-9.61403200	-1.43151100	3.17988000				
C	-11.42867900	-4.08507800	2.53876800	C	-6.73481300	-2.30670200	-0.45314700				
H	-10.88457200	-3.28590900	0.69402800	C	-7.52840300	-1.42385000	-1.42645600				
C	-11.11901900	-4.69348900	3.88507600	H	-7.04501400	-3.35659900	-0.51693300				
H	-11.53928600	-5.70589600	3.95240500	H	-5.67595800	-2.26529200	-0.72176800				
H	-10.05057600	-4.76286000	4.10242700	H	-7.16945200	-1.57779100	-2.44892200				
H	-11.58989100	-4.11095500	4.68825300	H	-8.58570300	-1.71527800	-1.42934000				
C	-12.90383400	-3.94779400	2.24279000	C	-7.43733500	0.04844400	-1.02938500				
H	-13.40198200	-4.92621700	2.27439600	C	-6.72497400	0.99456400	-1.80275100				
H	-13.40105000	-3.32322200	2.99745800	H	-8.37079900	0.45397800	-0.64449700				
H	-13.08741900	-3.50607900	1.25843100	C	-5.66311200	0.63786700	-2.80233000				

H	-4.73423800	1.18354500	-2.59138000	C	-2.25690700	0.54021900	0.16603100
H	-5.41748900	-0.42411400	-2.81689200	C	-0.84706400	1.12389800	-0.21821200
H	-5.98134100	0.94054800	-3.81273000	C	0.45027000	0.36278700	0.34205300
C	-6.96400100	2.46516300	-1.61383100	C	0.15424700	-0.35084900	1.70684800
H	-6.13329700	2.92544700	-1.05905000	C	-1.17689400	-1.06601800	1.83739100
H	-7.01810000	2.97720200	-2.58531800	C	-2.27584100	-0.00853000	1.60332900
H	-7.87477100	2.67480000	-1.04811200	H	-2.93288600	1.40831400	0.15184900
C	-8.66351300	-3.49036000	1.80677600	H	-1.23400100	-1.79823700	1.02087400
H	-8.24894600	-4.11160800	1.00083700	H	-2.14411100	0.80234800	2.33253300
H	-8.15722900	-3.80557600	2.72478200	H	-3.25591300	-0.44694400	1.81884200
C	-10.14504400	-3.75549400	1.88697700	C	-0.75854700	1.34600200	-1.74497000
C	-10.85896900	-4.26652200	2.90317900	H	-1.60147600	1.96743700	-2.07259000
H	-10.69372000	-3.49403000	0.97911600	H	0.15647600	1.87405400	-2.02670600
C	-10.28915000	-4.69454700	4.23426900	C	-2.88209400	-0.47276900	-0.84084300
H	-10.46252000	-5.76685000	4.40240300	H	-2.22751600	-1.34104400	-0.94898400
H	-9.21614300	-4.51193000	4.32596600	H	-2.91382000	-0.00366300	-1.82746400
H	-10.79179100	-4.16785200	5.05738300	C	-4.26954700	-0.93099700	-0.45642500
C	-12.35074800	-4.46984400	2.77118600	C	-5.44463500	-0.39362700	-0.82404800
H	-12.61955600	-5.52745300	2.90474500	H	-4.31379100	-1.80762600	0.19161100
H	-12.89685700	-3.91195700	3.54507300	C	-5.58904900	0.81674400	-1.71536500
H	-12.72326600	-4.14741000	1.79363900	H	-6.19002200	0.57699500	-2.60399900
C	-5.84683300	-2.44754900	1.89421700	H	-4.63092200	1.21726200	-2.05547700
H	-5.98931500	-3.53312500	1.87888100	H	-6.12183600	1.62286600	-1.19134500
H	-4.83055200	-2.25081400	1.54172100	C	-6.75303900	-0.98799100	-0.35817300
H	-5.90833300	-2.11827000	2.93671400	H	-7.37384100	-1.29709200	-1.21138700
C	-9.93753500	0.87137500	1.85276900	H	-7.34583100	-0.25308600	0.20523700
H	-10.76703400	0.73344500	2.55555100	H	-6.59942000	-1.86233100	0.28250400
H	-9.85095000	1.93668000	1.62000900	C	-0.68449800	2.51050800	0.46406600
H	-10.19514400	0.33711500	0.93058500	H	-1.33308400	3.25963500	-0.00535700
O	-7.17399400	1.98162200	1.49617900	H	-0.97332000	2.45282500	1.52147600
C	-5.15308900	0.14122000	0.72083900	C	-1.31376600	-1.78416800	3.18097400
O	-4.51260700	-0.23822200	-0.25720000	H	-0.51003200	-2.51190000	3.32735900
C	-4.40960600	0.89041200	1.79726600	H	-2.27308700	-2.31152100	3.22867800
C	-3.21137200	1.52296200	1.42819200	H	-1.26865500	-1.07430300	4.01361900
C	-4.78791900	0.90253700	3.14773600	O	0.96100800	-0.33414100	2.62165700
C	-2.42887200	2.17592400	2.37662600	C	0.90430300	-0.83982000	-0.53650600
H	-2.90920100	1.48709200	0.38693900	O	0.07722500	-1.46672200	-1.19785800
C	-3.99450500	1.53708100	4.10253600	C	2.33057700	-1.22278700	-0.56017300
H	-5.69789800	0.40437900	3.46539800	C	2.78094300	-2.00120400	-1.63767100
C	-2.81787500	2.18351400	3.71891700	C	3.27066900	-0.70388200	0.38241000
H	-1.51236200	2.67416200	2.07184400	C	4.13291100	-2.28541000	-1.79898800
H	-4.29744500	1.52939300	5.14609400	H	2.04513500	-2.35862300	-2.35116200
H	-2.20571700	2.68731900	4.46235200	C	4.64032200	-1.05662000	0.22855300
				H	2.92794100	-0.43088000	1.37446000

TS2-iso

C	5.06469100	-1.79955800	-0.86006600	H	-6.13914300	1.89938000	-0.70179300
H	4.46848200	-2.88348100	-2.64134900	C	-6.76430500	-0.83758700	-0.60005800
H	5.35553000	-0.73661100	0.98126800	H	-7.38438900	-0.90554300	-1.50432800
H	6.11912600	-2.03899400	-0.97497800	H	-7.35472900	-0.27923600	0.13930900
H	-0.78513800	0.40969900	-2.30118300	H	-6.61010600	-1.85139200	-0.21795000
C	1.53486300	1.50738300	0.61531600	C	-0.64533200	2.29012200	1.09426300
C	0.79957700	2.85379100	0.35281000	H	-1.24550800	3.16930600	0.83857800
H	1.11201300	3.61641000	1.07427300	H	-0.95146800	1.96833900	2.09632900
H	1.02847200	3.24827400	-0.64219700	C	-1.42505900	-2.55191200	2.59932400
H	1.71873500	1.45428600	1.69122000	H	-0.65862800	-3.33001200	2.54293600
C	2.90741200	1.44526300	-0.03226800	H	-2.40742600	-3.02771800	2.52046000
C	4.00410800	2.12106500	0.75411200	H	-1.34954800	-2.08192600	3.58515000
C	3.04770500	1.58155200	-1.52631000	O	0.95421300	-1.14845900	2.32926900
H	3.98608900	1.83707300	1.81284200	C	0.90371900	-0.66069200	-0.76526000
H	4.99318900	1.88057500	0.34748800	O	0.13564900	-1.13538200	-1.58357600
H	3.89831900	3.21810600	0.71199900	C	2.37118300	-0.96911300	-0.88397500
H	2.29006500	1.02027900	-2.07925900	C	2.87137800	-1.28143600	-2.14888800
H	2.96573400	2.63649800	-1.83439400	C	3.26055600	-0.85848100	0.22066300
H	4.03323700	1.23040700	-1.85394200	C	4.24303700	-1.47357500	-2.32801700
				H	2.18174300	-1.35785900	-2.98295000
				C	4.64328100	-1.10082000	0.02343700

TS3-iso

C	-2.27020200	0.50711900	0.28342100	H	2.85924600	-0.91870500	1.22926800
C	-0.85088500	1.14791300	0.06321500	C	5.13442400	-1.37458200	-1.24378900
C	0.41705400	0.22197300	0.39685000	H	4.62609300	-1.70705800	-3.31741600
C	0.09964400	-0.87026200	1.50750700	H	5.31364000	-1.08396300	0.87765500
C	-1.26050200	-1.51944100	1.48140700	H	6.19533700	-1.54493600	-1.39830200
C	-2.30903800	-0.38542600	1.53518400	H	-0.78785700	1.00855700	-2.13857400
H	-2.93090600	1.36178100	0.48704000	C	1.51505400	1.18675300	1.00666400
H	-1.35797200	-2.01552000	0.50491400	C	0.85269000	2.60703300	1.09558800
H	-2.15087200	0.20147300	2.44943500	H	1.17974100	3.12936000	1.99911100
H	-3.30489200	-0.82700400	1.63328400	H	1.11372700	3.23589000	0.24033600
C	-0.75378100	1.76138100	-1.35116800	H	1.67779000	0.84221900	2.02936900
H	-1.59487500	2.44595900	-1.50586300	C	2.88578900	1.32004700	0.38979100
H	0.15821300	2.35157600	-1.48768400	C	3.97590900	1.69066600	1.35911800
C	-2.89898900	-0.20740800	-0.95207100	C	3.08536000	1.86261000	-0.99536600
H	-2.24827700	-1.01901100	-1.29105600	H	3.97526800	1.07093700	2.25876800
H	-2.93925000	0.50422800	-1.78055700	H	4.96671700	1.69230100	0.90033100
C	-4.28331700	-0.75647100	-0.69120200	H	3.76182600	2.72261300	1.68131600
C	-5.45889100	-0.13788800	-0.89363500	H	2.23968600	1.69830300	-1.66242200
H	-4.32108200	-1.77705800	-0.30892700	H	3.24753000	2.94629400	-0.89966600
C	-5.60679800	1.26717100	-1.42545400	H	3.99494700	1.46105200	-1.45286000
H	-6.21265100	1.27157500	-2.34151200				
H	-4.65270100	1.75037000	-1.65256300				

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