

Supporting Information

Type-II Pauson-Khand Reaction of 1,8-enyne in the Attempt of Building 7/5 Ring of (-)-Caribenol A and DFT Understanding

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1. General information

All reagents were obtained from commercial suppliers unless otherwise stated. Toluene was distilled over sodium and tetrahydrofuran (THF) was distilled from potassium sodium alloys; Dichloromethane was distilled from calcium hydride. DMF was stirred with CaH₂ and distilled under reduced pressure. Flasks were flame-dried under vacuum and cooled under a stream of nitrogen or argon.

Visualization was achieved under a UV lamp (254 nm and 365 nm), and by developing the plates with phosphomolybdic acid or *p*-methoxybenzaldehyde in ethanol. Flash column chromatography was performed using silica gel (200-300 mesh) with solvents distilled prior to use.

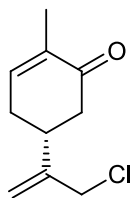
Nuclear magnetic resonance [¹H and ¹³C NMR] spectra were determined on Bruker AVIII-400 [¹H NMR (400 MHz), ¹³C NMR (100 MHz)] and AVIII-600 [¹H NMR (600 MHz), ¹³C NMR (150 MHz)] spectrometers. The following abbreviations are used for the multiplicities: s: singlet, d: doublet, t: triplet, q: quartet, quint: quintet, m: multiplet, br d: broad doublet, br s: broad singlet for proton spectra and carbon spectra. Coupling constants (*J*) are reported in Hertz (Hz).

High resolution mass spectral (HRMS) data were obtained with an ionization mode of ESI.

The following abbreviations are used: **FCC**: flash column chromatography; **PE**: petroleum ether; **EtOAc**: ethyl acetate; **DCM**: dichloromethane; **THF**: tetrahydrofuran; **DMF**: N,N-dimethylformamide; **TBS**: *tert*-butyldimethylsilyl; **TMS**: trimethylsilyl; **TBSOTf**: *tert*-butyldimethylsilyl triflate; **Tf**: trifluoromethanesulfonyl; **quant**: quantitative; **dppf**: 1,1'-bis(diphenylphosphino)ferrocene

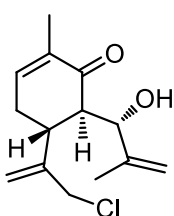
2. Experimental procedure

Compound 2



To a stirred solution of *R*-(-)-carvone (7.5 g, 50 mmol) in CH₂Cl₂/H₂O (500 mL, 1:1), CeCl₃ · 7H₂O (55.5 g, 150 mmol) was added. The mixture was vigorously stirred and diluted NaClO (64 mL, 10–13% available chlorine, 150 mmol) was added dropwise for 5 min. After 30 min, saturated aqueous Na₂SO₃ was added and the mixture was extracted with CH₂Cl₂. The combined organic layers were washed with brine, dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by FCC (PE-EtOAc, 10:1) to give **2** (6.5 g, 65%) as a yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 6.70 (m, 1H), 5.20 (s, 1H), 4.99 (s, 1H), 4.05 (d, *J* = 12.0 Hz, 1H), 4.02 (d, *J* = 12.0 Hz, 1H), 2.90 (m, 1H), 2.59 (ddd, *J* = 16.0, 4.0, 1.2 Hz, 1H), 2.50 (m, 1H), 2.31 (dd, *J* = 16.0, 13.0 Hz, 1H), 2.26 (m, 1H), 1.72 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 198.8, 146.6, 143.9, 135.6, 115.1, 46.9, 43.0, 37.8, 31.4, 15.6; HRMS(ESI) *m/z* calcd. for C₁₀H₁₄ClO (M+H)⁺ 185.0728, found 185.0733.

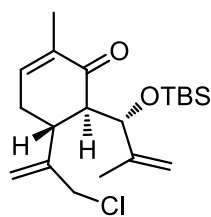
Compound 3



To a stirred solution of diisopropylamine (12.2 mL, 86.7 mmol) in THF (100 mL) *n*-BuLi (54.2 mL, 1.6 M in hexane, 86.7 mmol) was added dropwise at –78 °C. After 30 min, compound **2** (10.7 g, 57.8 mmol) was added dropwise. The reaction mixture was allowed to stir for 15 min after which methacrolein (8.1 g, 115.6 mmol) was added dropwise. The reaction mixture stirred at –78 °C for 4 h, the reaction was quenched with saturated aqueous NH₄Cl at –78 °C. After 20 min, the reaction mixture was allowed to warm to room temperature, then was diluted with ether and washed with water. The aqueous layer was extracted with ether. The combined organic layers were washed with brine, dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by FCC (PE-EtOAc, 8:1) to give **3** (13.2 g, 90%) as a white solid. ¹H NMR (400 MHz, CDCl₃) δ 6.67 (m, 1H), 5.29 (s, 1H), 5.04 (s, 1H), 5.02 (s, 1H), 5.00 (s, 1H), 4.25 (dd, *J* = 6.8, 6.0 Hz, 1H), 4.09 (d, *J* = 11.9 Hz, 1H), 4.05 (d, *J* = 11.8 Hz, 1H), 2.98 (dd, *J* = 10.2, 5.1

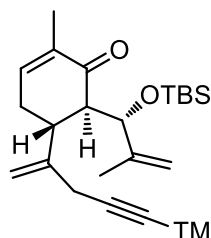
Hz, 1H), 2.69–2.62 (m, 2H), 2.57 (d, $J = 5.4$ Hz, 1H), 2.42 (m, 1H), 1.83–1.71 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 200.5, 145.7, 145.3, 142.8, 135.1, 117.0, 113.5, 75.2, 53.1, 47.5, 38.9, 28.4, 16.9, 15.8; HRMS(ESI) m/z calcd. for $\text{C}_{14}\text{H}_{20}\text{ClO}_2(\text{M}+\text{H})^+$ 255.1146, found 255.1139.

Compound 4



To a stirred solution of **3** (1.7 g, 6.6 mmol) in CH_2Cl_2 (15 mL), 2,6-lutidine (1.4 g, 13.2 mmol) was added. After 10 min, TBSOTf (2.6 g, 9.9 mmol) was added and the solution was stirred for 16 h at room temperature. The reaction was quenched with H_2O and extracted with CH_2Cl_2 three times. The combined organic layers were washed with brine, dried over Na_2SO_4 , filtered and concentrated in vacuo. The residue was purified by FCC (PE-EtOAc, 40:1) to give **4** (2.4 g, 98%.) as a white solid. ^1H NMR (400 MHz, CDCl_3) δ 6.56 (m, 1H), 5.17 (s, 1H), 4.99 (s, 1H), 4.98 (s, 1H), 4.95 (s, 1H), 4.41 (d, $J = 9.5$ Hz, 1H), 4.10 (d, $J = 11.9$ Hz, 1H), 4.01 (d, $J = 11.9$ Hz, 1H), 2.89 (m, 1H), 2.72–2.62 (m, 2H), 2.33 (dd, $J = 19.9, 4.7$ Hz, 1H), 1.76 (s, 3H), 1.74 (s, 3H), 0.84 (s, 9H), -0.05 (s, 3H), -0.06 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 198.6, 145.7, 145.5, 140.4, 134.8, 116.2, 114.1, 77.8, 54.0, 47.5, 37.3, 26.4, 25.6, 18.0, 16.1, 15.7, -4.8, -5.3; HRMS(ESI) m/z calcd. for $\text{C}_{20}\text{H}_{34}\text{ClO}_2\text{Si}(\text{M}+\text{H})^+$ 369.2011, found 369.2010.

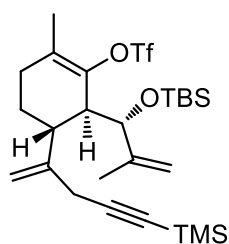
Compound 5



To a stirred solution of trimethylsilylacetylene (1.6 mL, 11.4 mmol) in dry DMF (28 mL) was sequentially added K_2CO_3 (1.9 g, 13.3 mmol), tetrabutylammonium iodide (280 mg, 0.8 mmol), and copper(I) iodide (72 mg, 0.4 mmol) at room temperature. After 15 min, compound **4** (1.4 g, 3.8 mmol) was added, and the reaction mixture was stirred for 12 h. Then the reaction was quenched with H_2O , extracted with Et_2O three times. The combined organic layers were washed with brine, dried over Na_2SO_4 , filtered and concentrated in vacuo. The residue was purified by FCC (PE- CH_2Cl_2 , 10:1) to give **5** (1.41 g, 87%) as a white solid. ^1H NMR (400 MHz, CDCl_3) δ 6.52 (m, 1H), 5.10 (s,

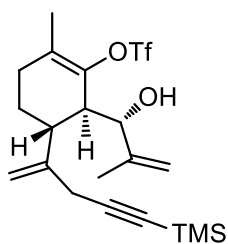
1H), 4.98 (s, 1H), 4.94 (s, 1H), 4.83 (s, 1H), 4.39 (d, $J = 9.6$ Hz, 1H), 2.98 (s, 2H), 2.72–2.60 (m, 3H), 2.32 (dd, $J = 19.7, 4.8$ Hz, 1H), 1.76 (s, 3H), 1.73 (s, 3H), 0.84 (s, 9H), 0.14 (s, 9H), -0.05 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 198.7, 146.0, 144.2, 140.5, 134.7, 113.8, 112.9, 103.5, 87.5, 77.8, 54.0, 39.9, 29.7, 26.6, 25.7, 18.1, 16.2, 16.0, 0.0, -4.9, -5.3; HRMS(ESI) m/z calcd. for $\text{C}_{25}\text{H}_{43}\text{O}_2\text{Si}_2(\text{M}+\text{H})^+$ 431.2796, found 431.2801.

Compound 9



To a stirred solution of compound **5** (2.0 g, 4.6 mmol) in 10 ml of THF at -78°C was added of L-Selectride (7 mL, 1 M solution in THF, 7.0 mmol). After stirring at -78°C for 1 h, comins reagent (5.5 g, 14.1 mmol) in 25 mL of THF was added. The resulting solution was then allowed to warm to room temperature. After stirring for overnight, the reaction was quenched with H_2O , extracted with Et_2O three times. The combined organic layers were washed with brine, dried over Na_2SO_4 , filtered and concentrated in vacuo. The residue was purified by FCC (PE- CH_2Cl_2 , 20:1) to give **9** (2.2 g, 85%) as a yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 5.25 (s, 1H), 5.02 (s, 1H), 4.96 (s, 1H), 4.90 (s, 1H), 4.22 (d, $J = 6.4$ Hz, 1H), 3.01 (d, $J = 19.4$ Hz, 1H), 2.96 (d, $J = 19.5$ Hz, 1H), 2.74 (m, 1H), 2.57 (m, 1H), 2.17 (m, 1H), 2.00 (dt, $J = 17.4, 4.4$ Hz, 1H), 1.77 (s, 3H), 1.72–1.66 (m, 4H), 1.60 (m, 1H), 0.87 (s, 9H), 0.15 (s, 9H), 0.01 (s, 3H), 0.00 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.3, 144.8, 143.4, 128.9, 118.4 (q, $J = 317.9$ Hz), 113.5, 112.1, 103.8, 87.4, 78.0, 46.0, 39.8, 28.3, 26.8, 25.7, 22.6, 18.2, 18.1, 17.4, 0.04, -4.9, -5.1; HRMS(ESI) m/z calcd. for $\text{C}_{26}\text{H}_{44}\text{F}_3\text{O}_4\text{Si}_2(\text{M}+\text{H})^+$ 565.2445, found 565.2452.

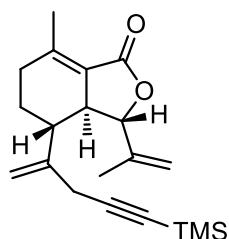
Compound 10



To a stirred solution of compound **9** (412 mg, 0.73 mmol) in THF (10 ml) was slowly added HF.pyridine (5 mL). After stirring for 1 h, saturated aqueous Na_2CO_3 (20mL) was added, then the mixture was diluted with ether and washed with water. The aqueous layer was

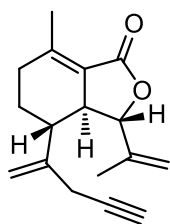
extracted with ether. The combined organic layers were washed with brine, dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by FCC (PE-EtOAc, 20:1) to give **10** (296 mg, 90%) as a yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 5.26 (s, 1H), 5.08 (s, 1H), 5.03 (s, 1H), 4.96 (s, 1H), 4.27 (dd, *J* = 4.4, 4.2 Hz, 1H), 3.03 (d, *J* = 19.24, 1H), 2.97 (d, *J* = 19.24, 1H), 2.86 (m, 1H), 2.58 (q, *J* = 4.4 Hz, 1H), 2.15 (m, 1H), 2.05 (dt, *J* = 17.5, 4.7 Hz, 1H), 1.79-1.77 (m, 4H), 1.72 (s, 3H), 1.67 (m, 1H), 1.59 (m, 1H), 0.15 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 145.4, 144.7, 143.0, 129.9, 118.4 (q, *J* = 317.7 Hz), 113.0, 112.6, 103.6, 87.6, 77.3, 44.9, 40.9, 28.5, 26.6, 23.2, 18.4, 17.4, 0.0; HRMS(ESI) *m/z* calcd. for C₂₀H₃₀F₃O₄SSi(M+H)⁺ 451.1581, found 451.1580.

Compound 11



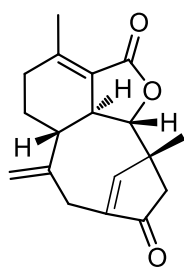
To a stirred solution of triflate **10** (45 mg, 0.1 mmol) in DMF (10 mL) at room temperature was sequentially added Et₃N (50.5 mg, 0.5 mmol), Pd(OAc)₂ (11.2 mg, 0.05 mmol), dppf (55.4 mg, 0.1 mmol) and LiCl (4.2 mg, 0.1 mmol). The resulting mixture was heated to 80 °C and stirred for 12 h under a CO atmosphere (1 atm) before it was quenched with NH₄Cl (10 mL, sat. aq.). The resulting mixture was extracted with ether and washed with water. The aqueous layer was extracted with ether. The combined organic layers were washed with brine, dried over Na₂SO₄, filtered and concentrated in vacuo. The residue was purified by FCC (PE-EtOAc, 30:1) to give **11** (16.5 mg, 50%) as a white solid. ¹H NMR (400 MHz, CDCl₃) δ 5.11 (s, 1H), 5.04 (s, 1H), 4.98 (m, 1H), 4.91 (s, 1H), 4.39 (d, *J* = 9.2 Hz, 1H), 2.88–2.79 (m, 3H), 2.39–2.21 (m, 2H), 2.15 (d, *J* = 2.3 Hz, 3H), 2.12 (m, 1H), 1.84 (m, 1H), 1.75 (s, 3H), 1.60 (m, 1H), 0.15 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 169.4, 149.2, 144.3, 141.0, 121.7, 117.3, 113.0, 103.3, 87.5, 86.9, 44.7, 43.4, 33.4, 29.6, 25.7, 18.0, 16.1, 0.0; HRMS(ESI) *m/z* calcd. for C₂₀H₂₉O₂Si (M+H)⁺ 329.1931, found 329.1936.

Compound 12



To a stirred solution of lactone **11** (50 mg, 0.15 mmol) in MeOH (5 mL) at room temperature was added K_2CO_3 (62 mg, 0.45 mmol). The resulting mixture was stirred for 1 h, then extracted with ether and washed with water. The aqueous layer was extracted with ether. The combined organic layers were washed with brine, dried over Na_2SO_4 , filtered and concentrated in vacuo. The residue was purified by FCC (PE-EtOAc, 8:1) to give **12** (25 mg, 65%) as a white solid. 1H NMR (400 MHz, $CDCl_3$) δ 5.16 (s, 1H), 5.04 (s, 1H), 5.00 (m, 1H), 4.95 (s, 1H), 4.40 (d, J = 9.4 Hz, 1H), 2.85–2.77 (m, 3H), 2.40–2.23 (m, 2H), 2.15–2.11 (m, 4H), 2.12 (t, J = 2.6 Hz, 1H), 1.83 (m, 1H), 1.75 (s, 3H), 1.62 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.3, 149.3, 144.0, 140.9, 121.7, 117.4, 113.1, 86.8, 80.7, 71.2, 44.9, 43.3, 33.4, 29.3, 23.9, 18.0, 16.1; HRMS(ESI) m/z calcd. for $C_{17}H_{21}O_2$ ($M+H$) $^+$ 257.1536, found 257.1538.

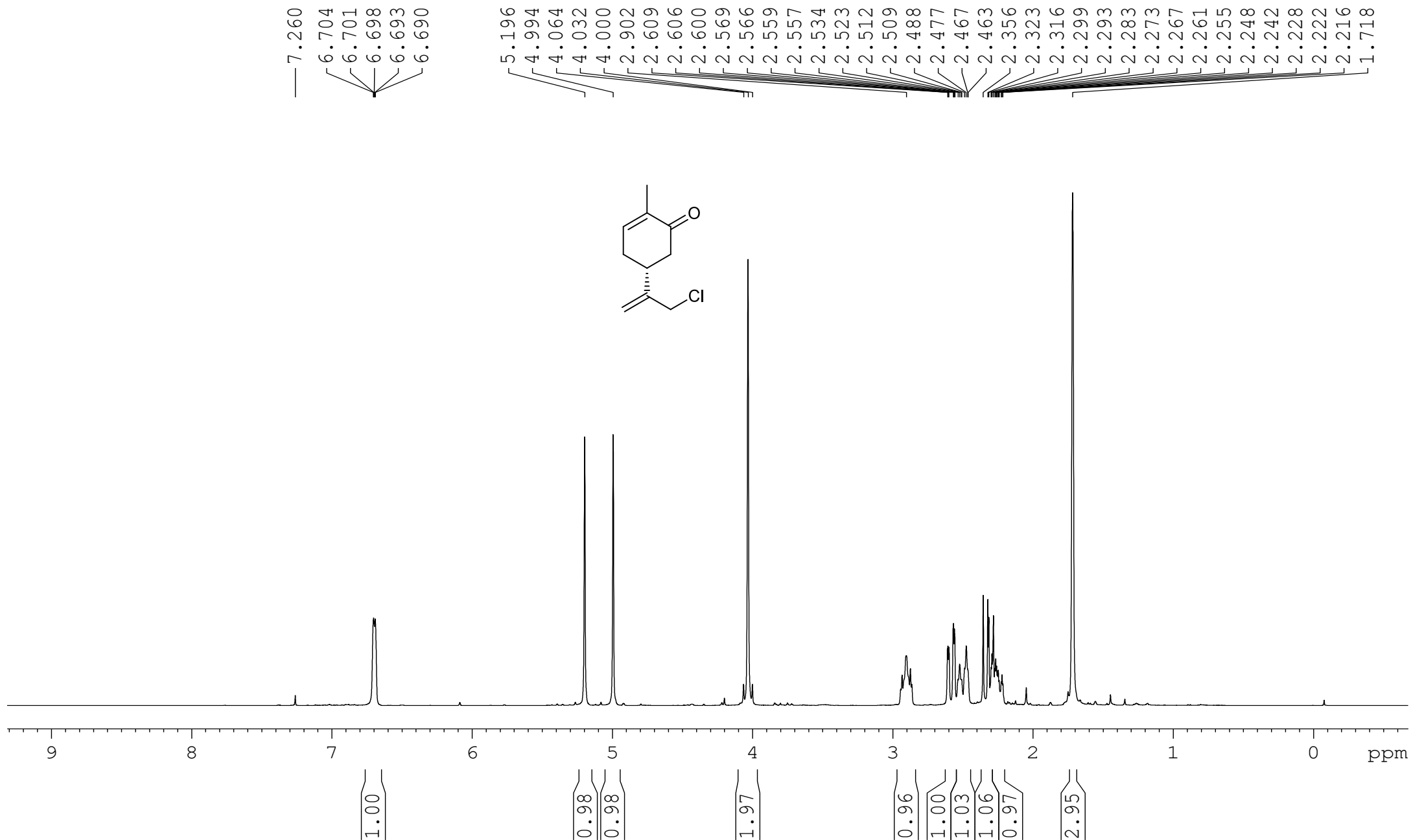
Compound 13



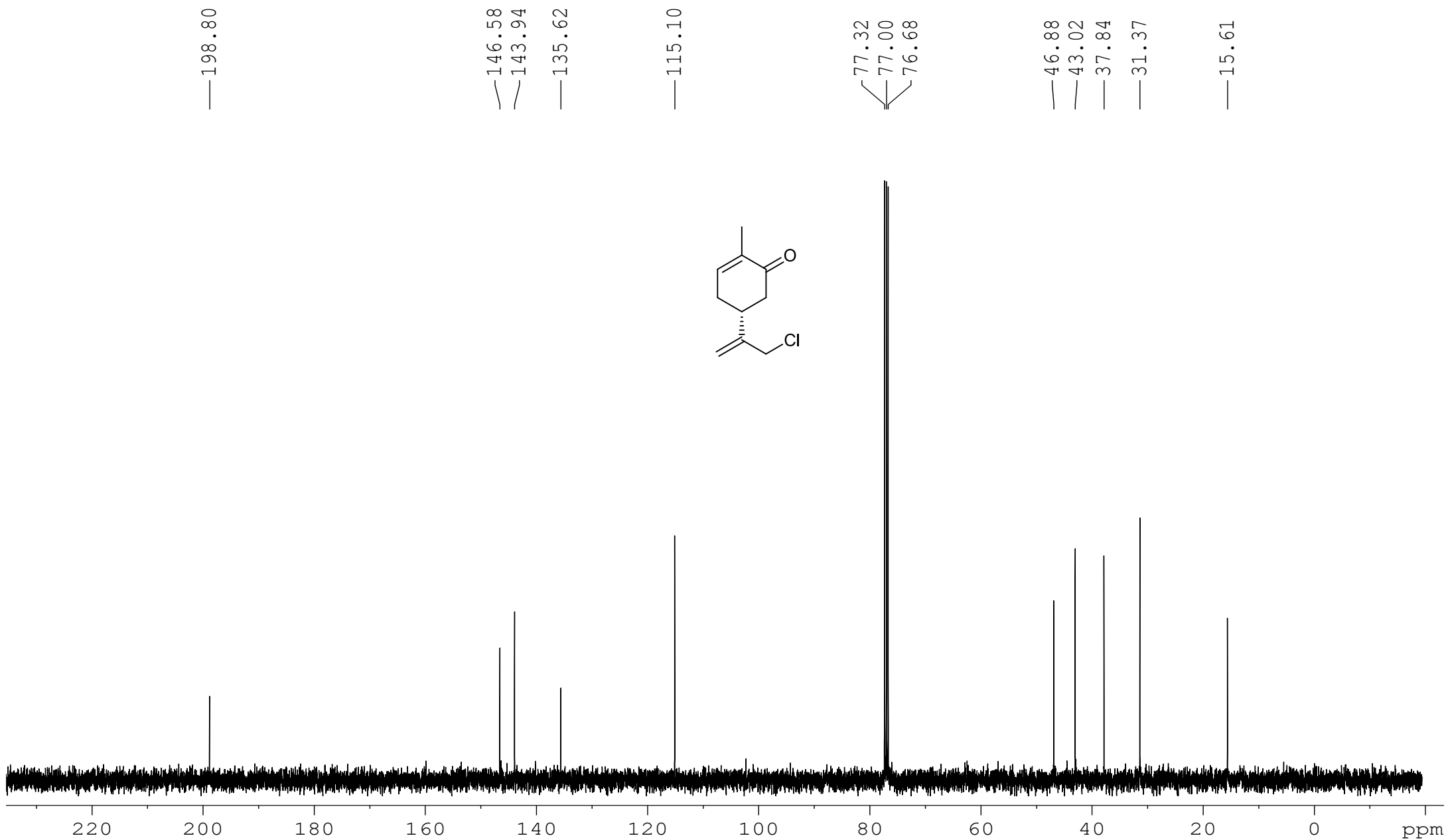
To a stirred solution of the compound **12** (12 mg, 0.05 mmol) in toluene (1 mL) was added $Co_2(CO)_8$ (21 mg, 0.06 mmol) under an argon atmosphere, the mixture was stirred at room temperature for 2 h. After the complete transformation of the starting material, the reaction mixture was heated to 110 °C and stirred overnight. The mixture was cooled down to room temperature and concentrated under reduced pressure, the residue was purified by FCC (PE-EtOAc, 8:1) to give **13** (7 mg, 54%) as a white solid. 1H NMR (600 MHz, $CDCl_3$) δ 7.06 (s, 1H), 5.00 (s, 1H), 4.93 (s, 1H), 3.85 (d, J = 10.4 Hz, 1H), 3.35 (d, J = 14.0 Hz, 1H), 3.02 (d, J = 14.0 Hz, 1H), 2.57 (d, J = 18.6 Hz, 1H), 2.23–2.14 (m, 6H), 2.05 (q, J = 5.8 Hz, 1H), 1.92 (m, 1H), 1.74 (m, 1H), 1.58–1.52 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 207.2, 168.6, 162.7, 153.2, 151.5, 145.6, 121.2, 112.7, 89.3, 48.9, 45.7, 41.1, 40.4, 35.1, 32.7, 28.9, 20.3, 19.2; HRMS(ESI) m/z calcd. for $C_{18}H_{21}O_3$ ($M+H$) $^+$ 285.1485, found 285.1493.

3. 1H and ^{13}C spectra of compounds (next page)

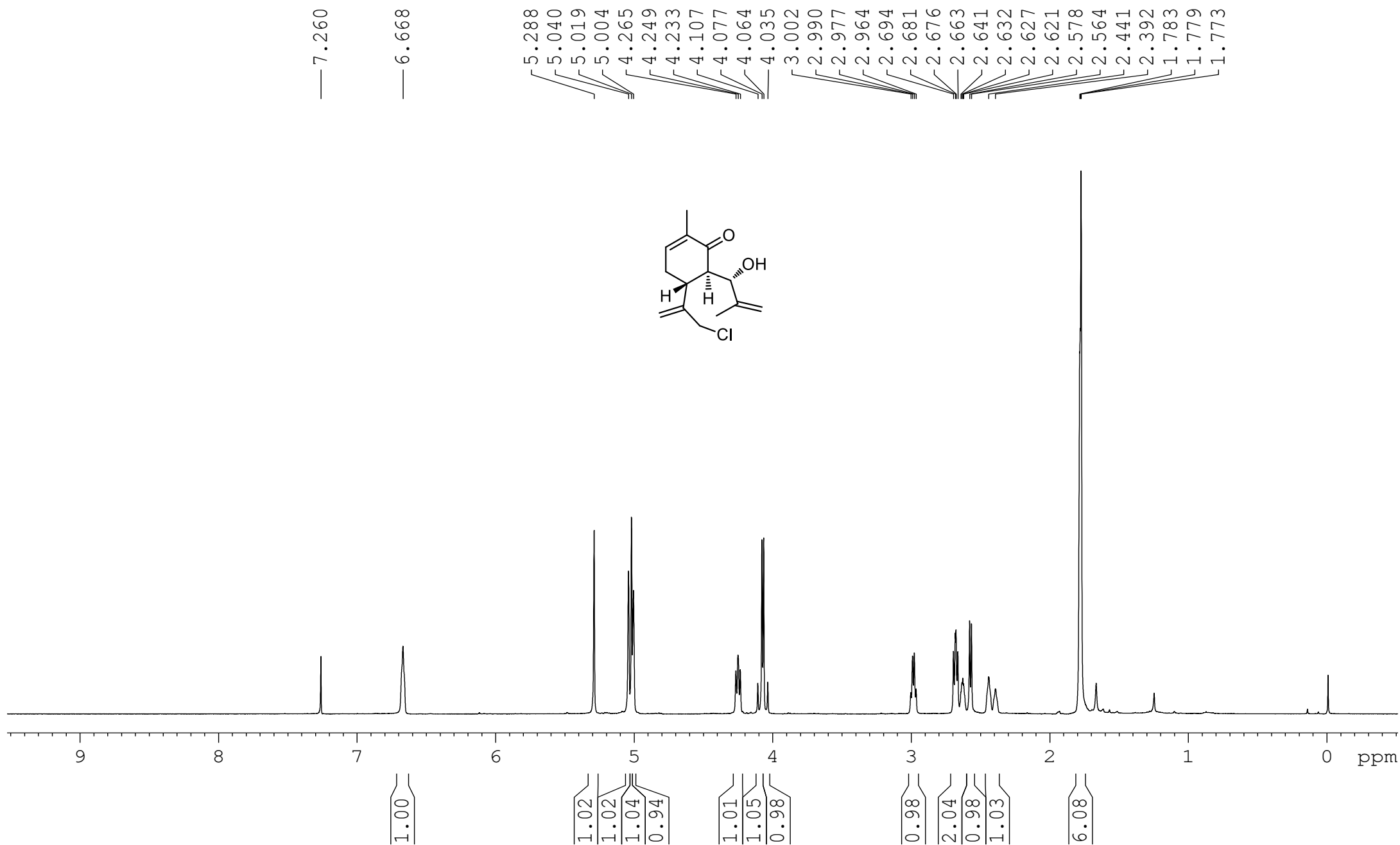
¹H NMR of compound 2 (CDCl₃, 400 MHz)



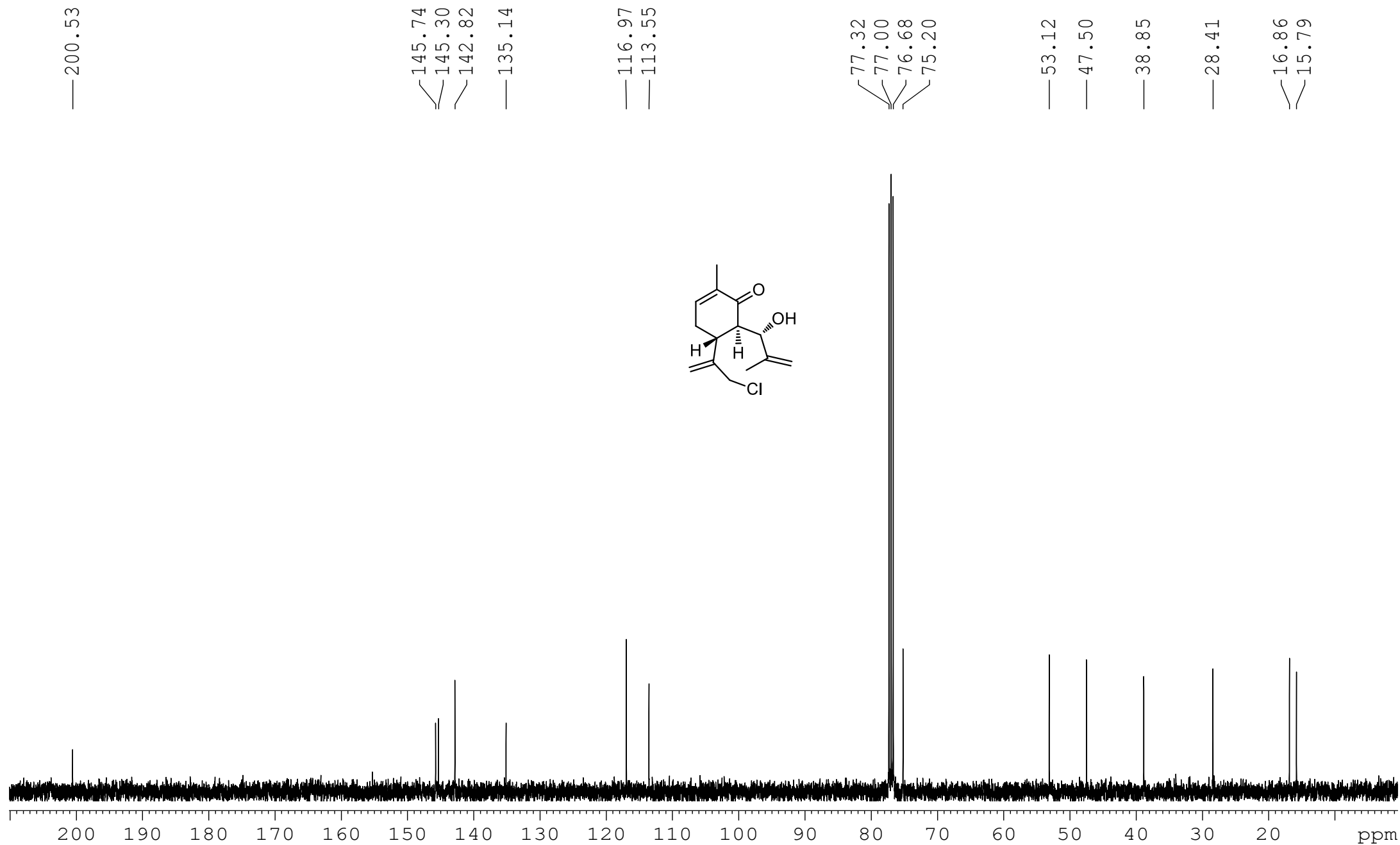
^{13}C NMR of compound 2 (CDCl_3 , 100 MHz)



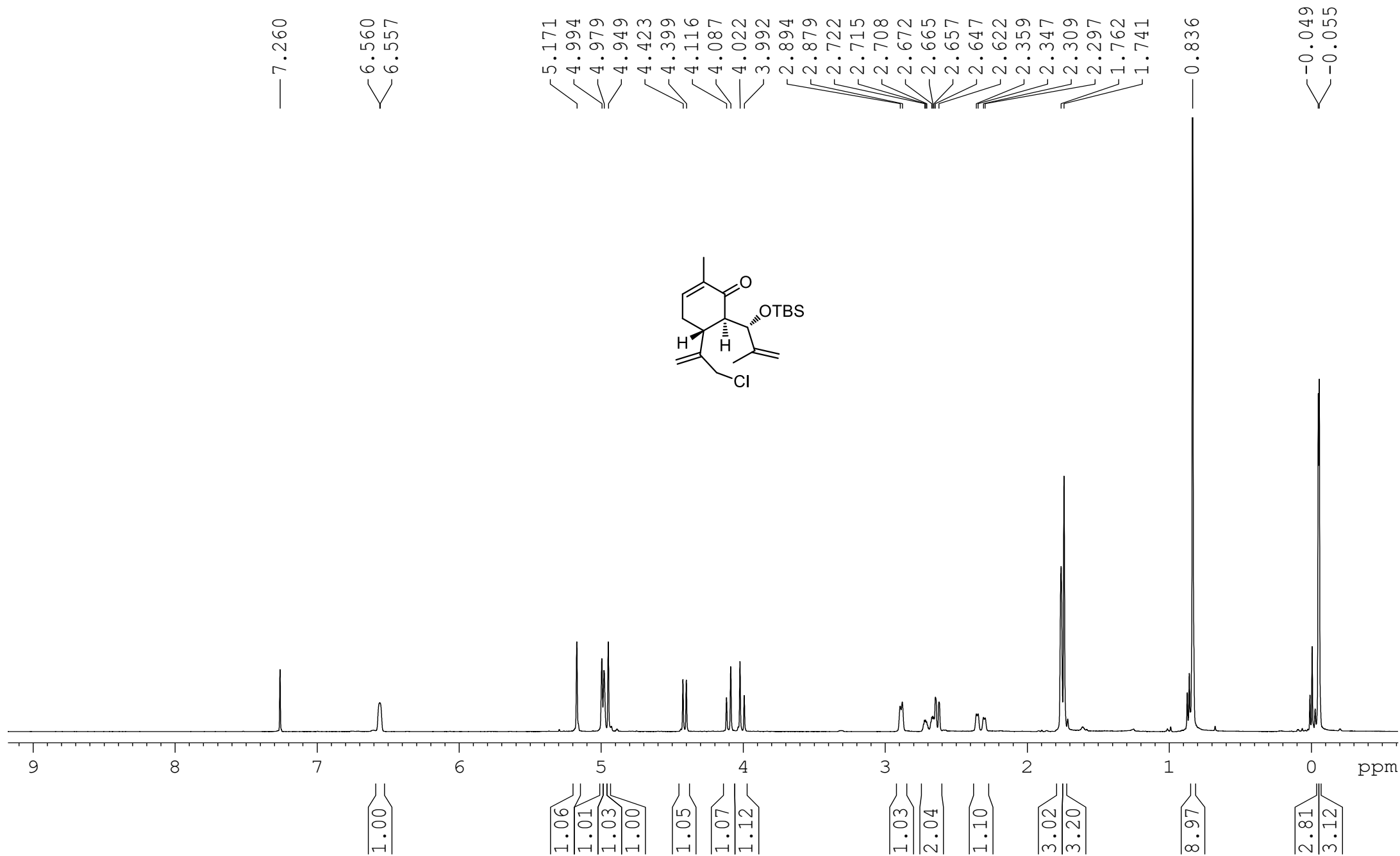
^1H NMR of compound 3 (CDCl_3 , 400 MHz)



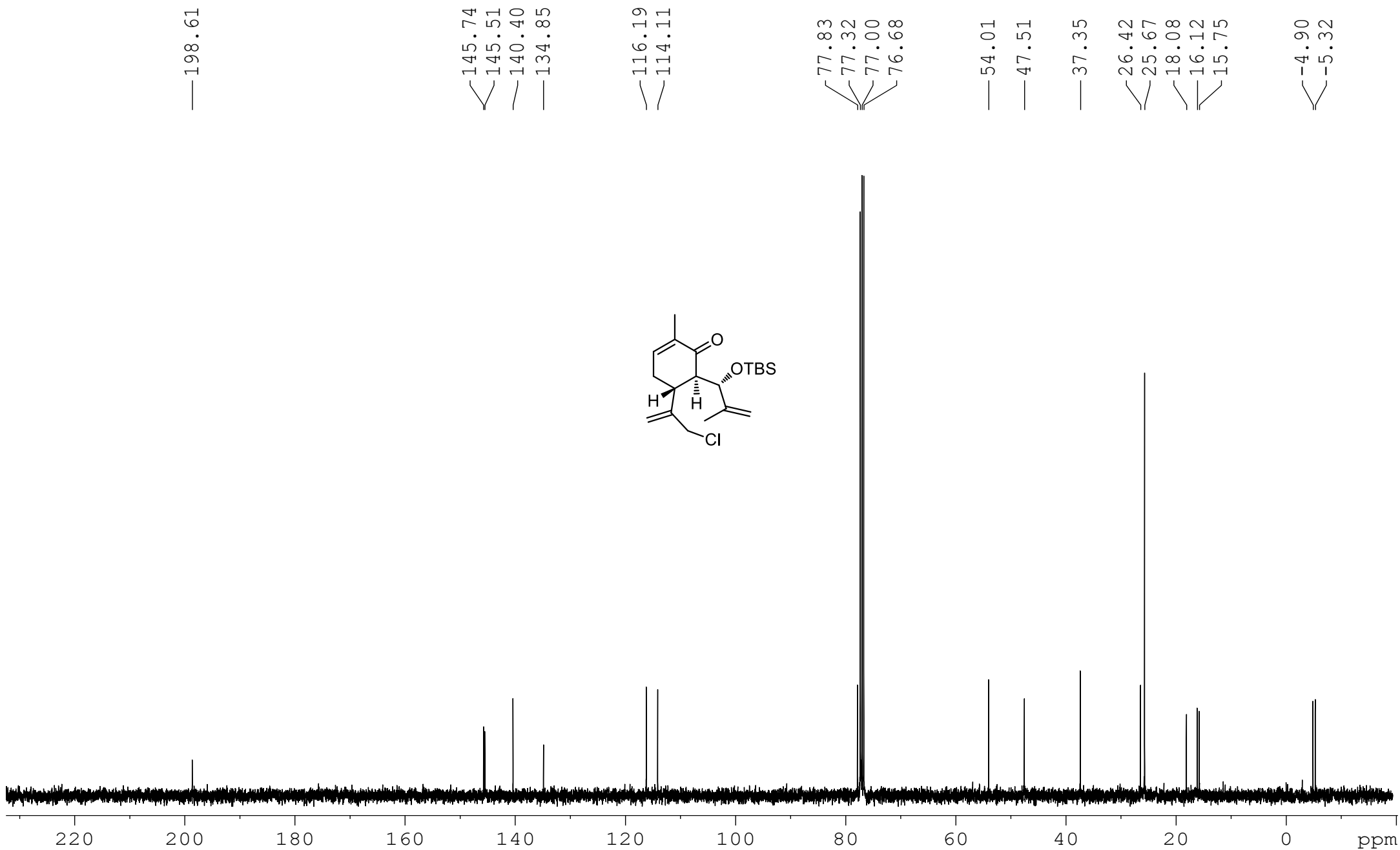
^{13}C NMR of compound 3 (CDCl_3 , 100 MHz)



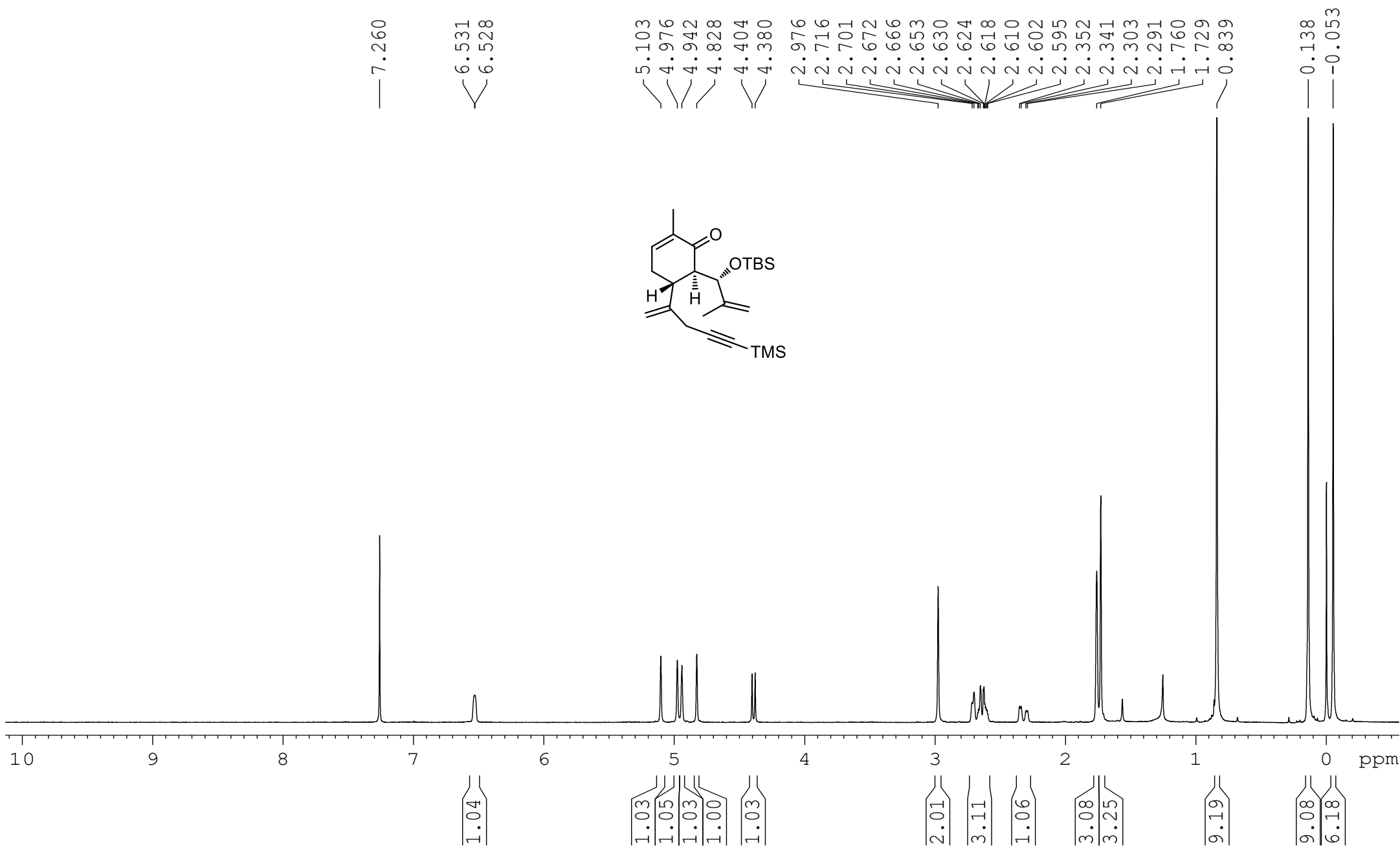
Chemical structure of compound 10: A bicyclic molecule featuring a ketone group, a vinyl group, a chlorine atom, and a tert-butyldimethylsilyl (OTBS) group.



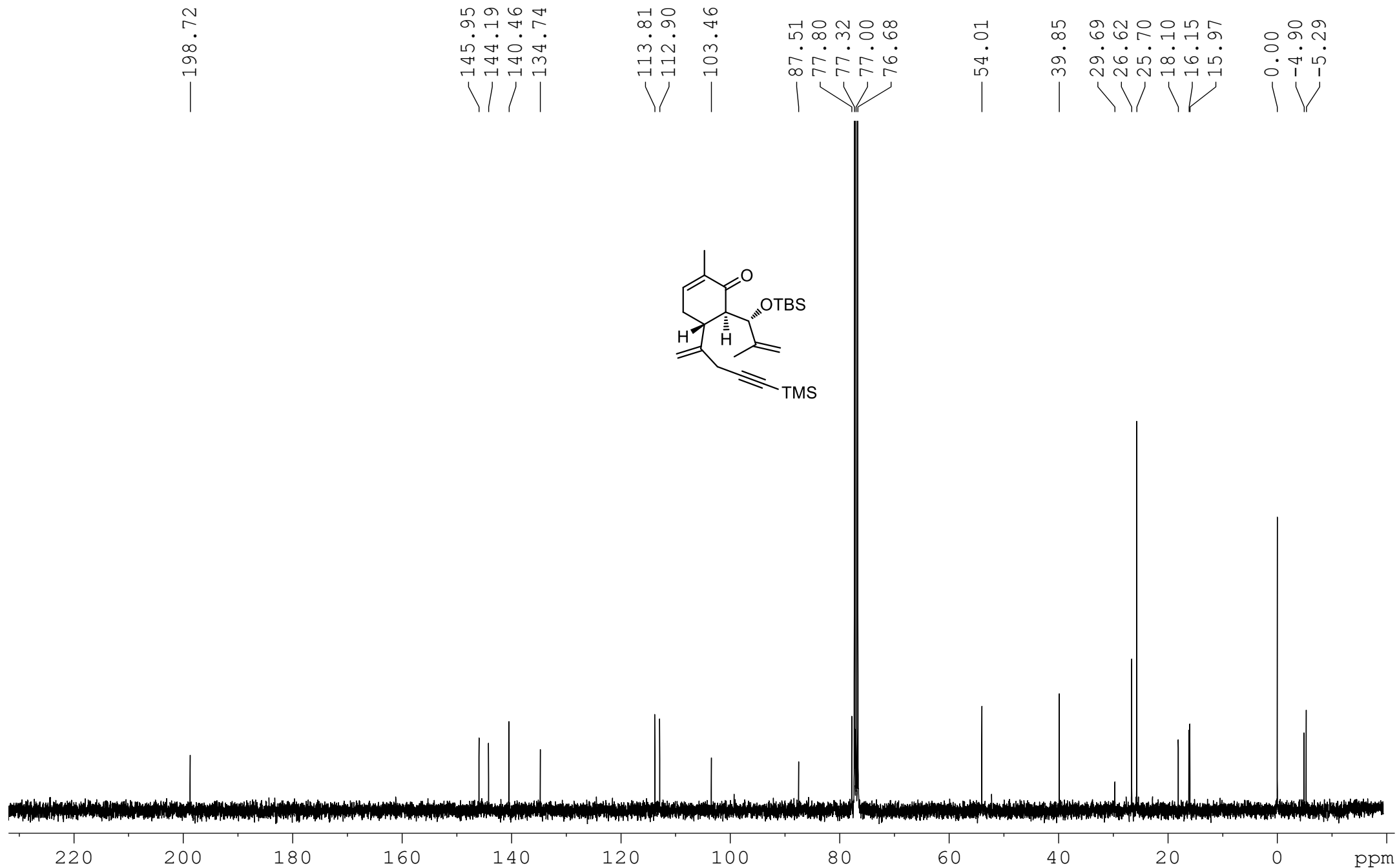
¹³C NMR of compound 4 (CDCl₃, 100 MHz)



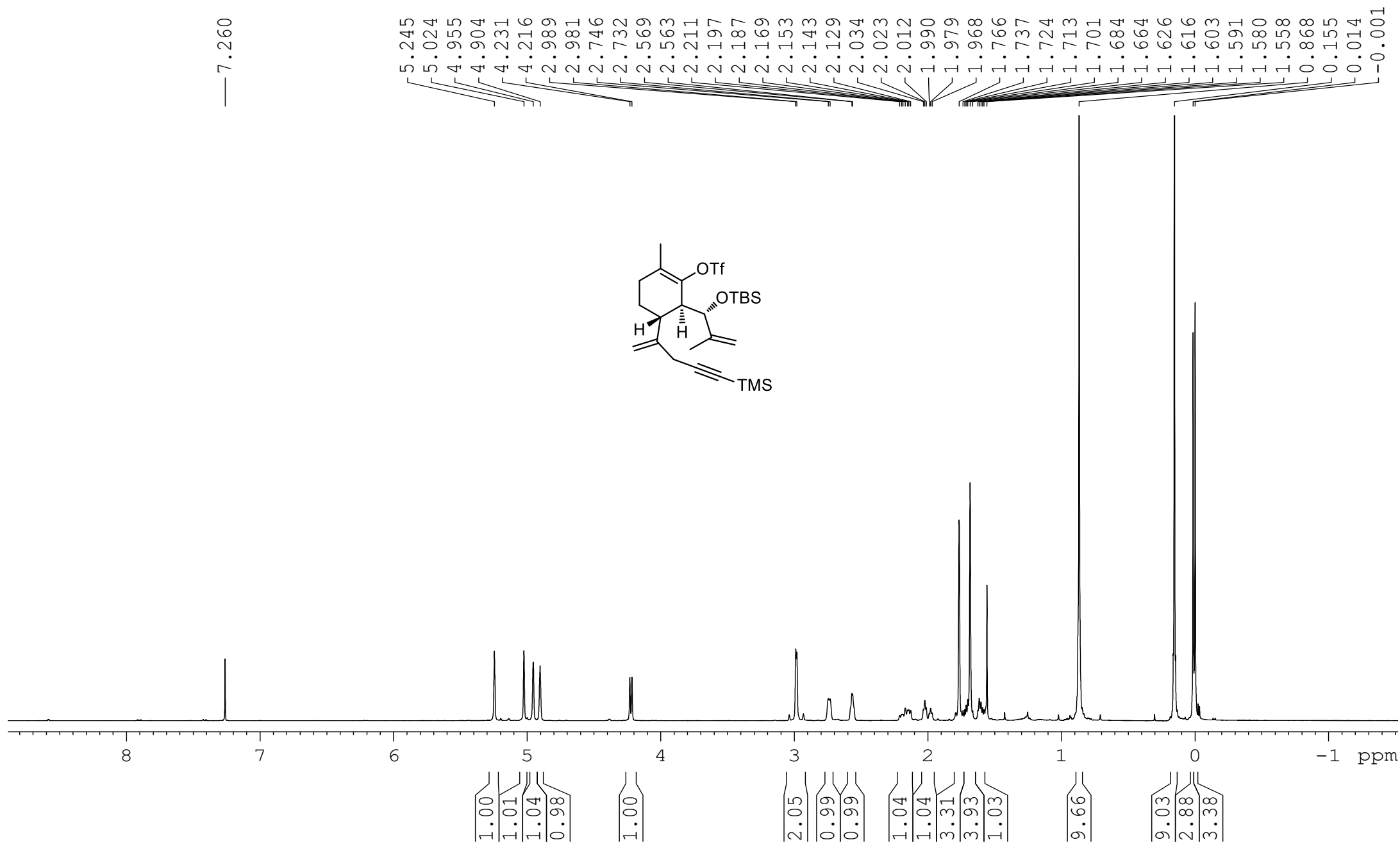
^1H NMR of compound 5 (CDCl_3 , 400 MHz)



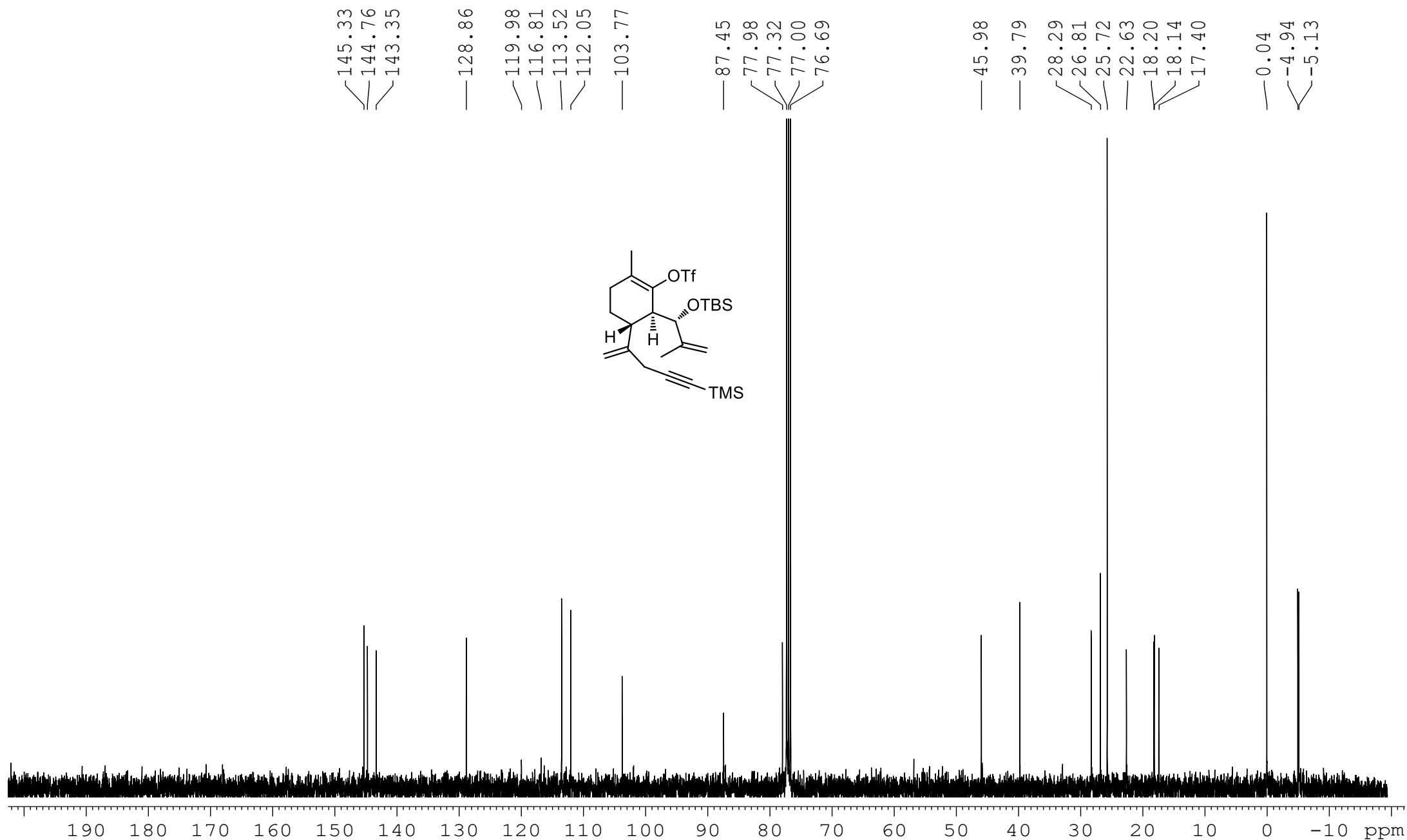
^{13}C NMR of compound 5 (CDCl_3 , 100 MHz)



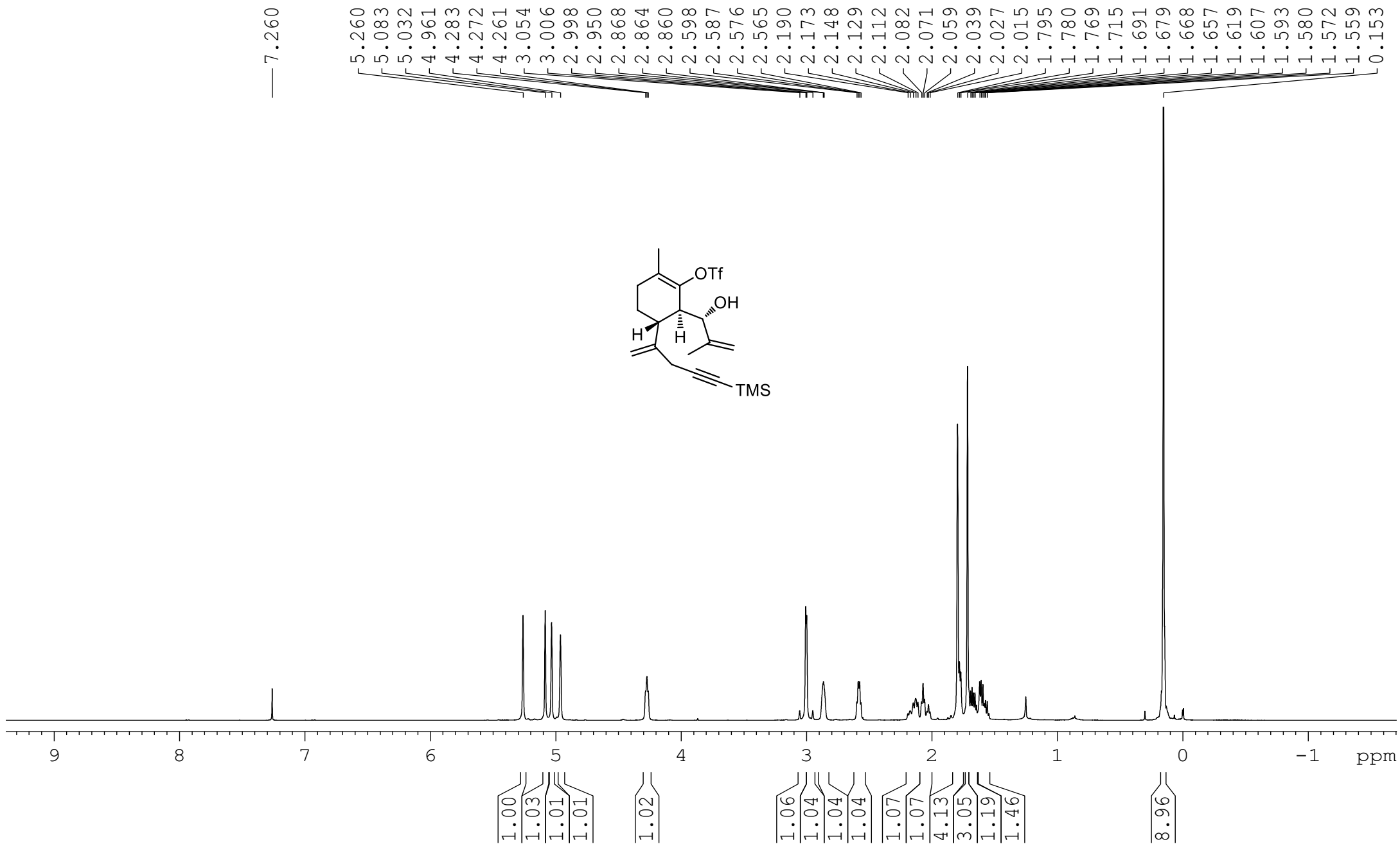
^1H NMR of compound 9 (CDCl_3 , 400 MHz)



^{13}C NMR of compound 9 (CDCl_3 , 100 MHz)



^1H NMR of compound 10 (CDCl_3 , 400 MHz)



^{13}C NMR of compound 10 (CDCl_3 , 100 MHz)

145.40
144.68
143.07

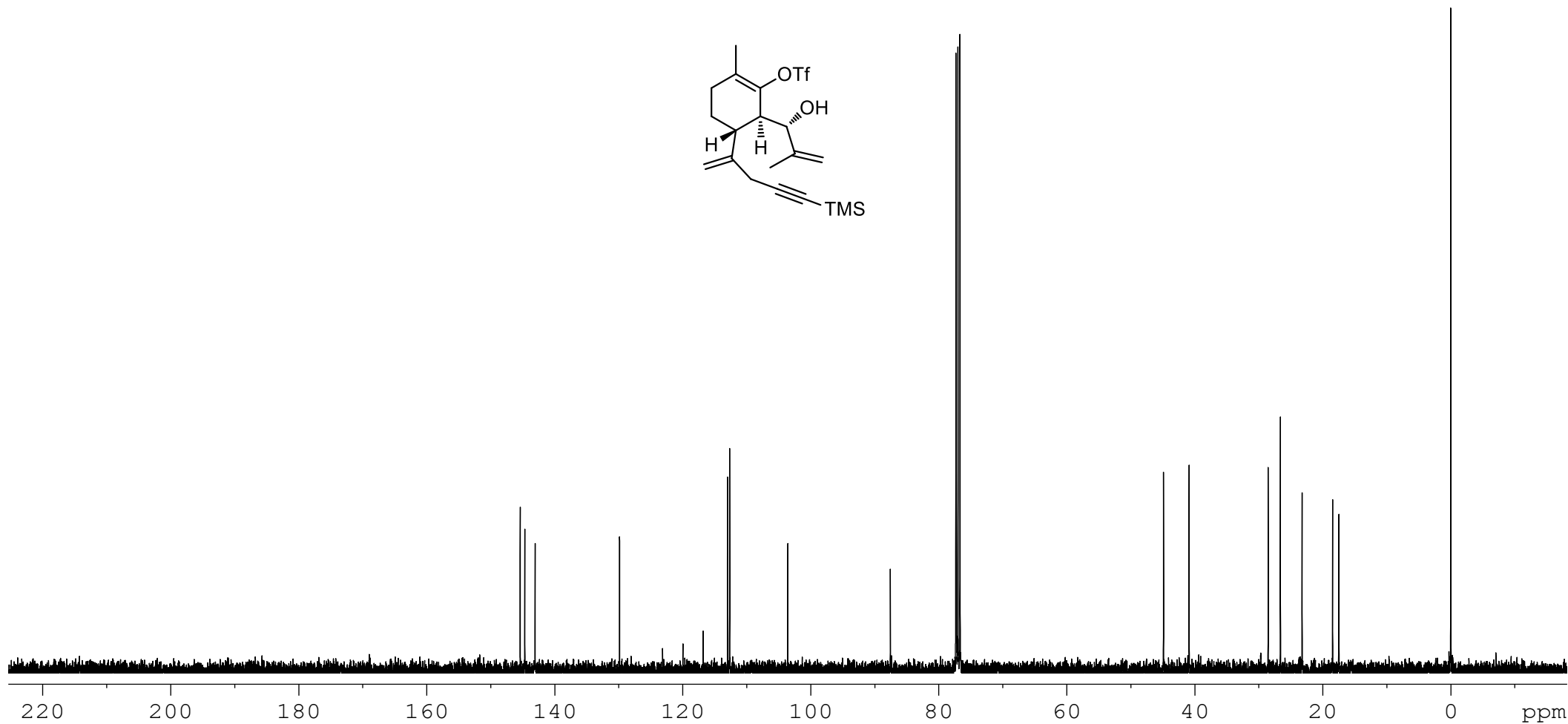
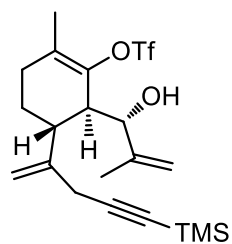
129.88
123.15
119.97
116.80
113.00
112.67
103.59

87.56
77.32
77.27
77.00
76.69

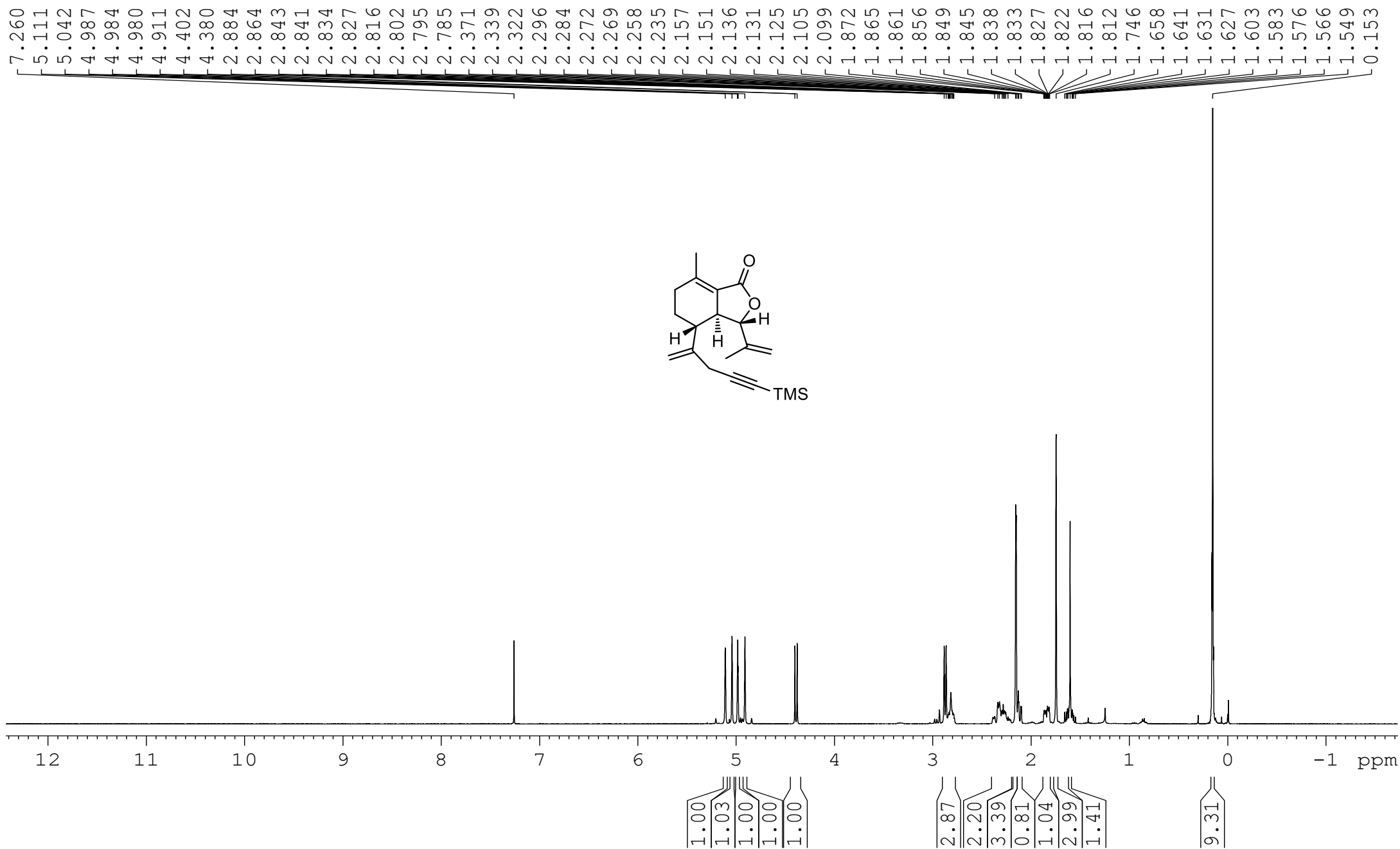
44.88
40.89

28.53
26.61
23.22
18.46
17.48

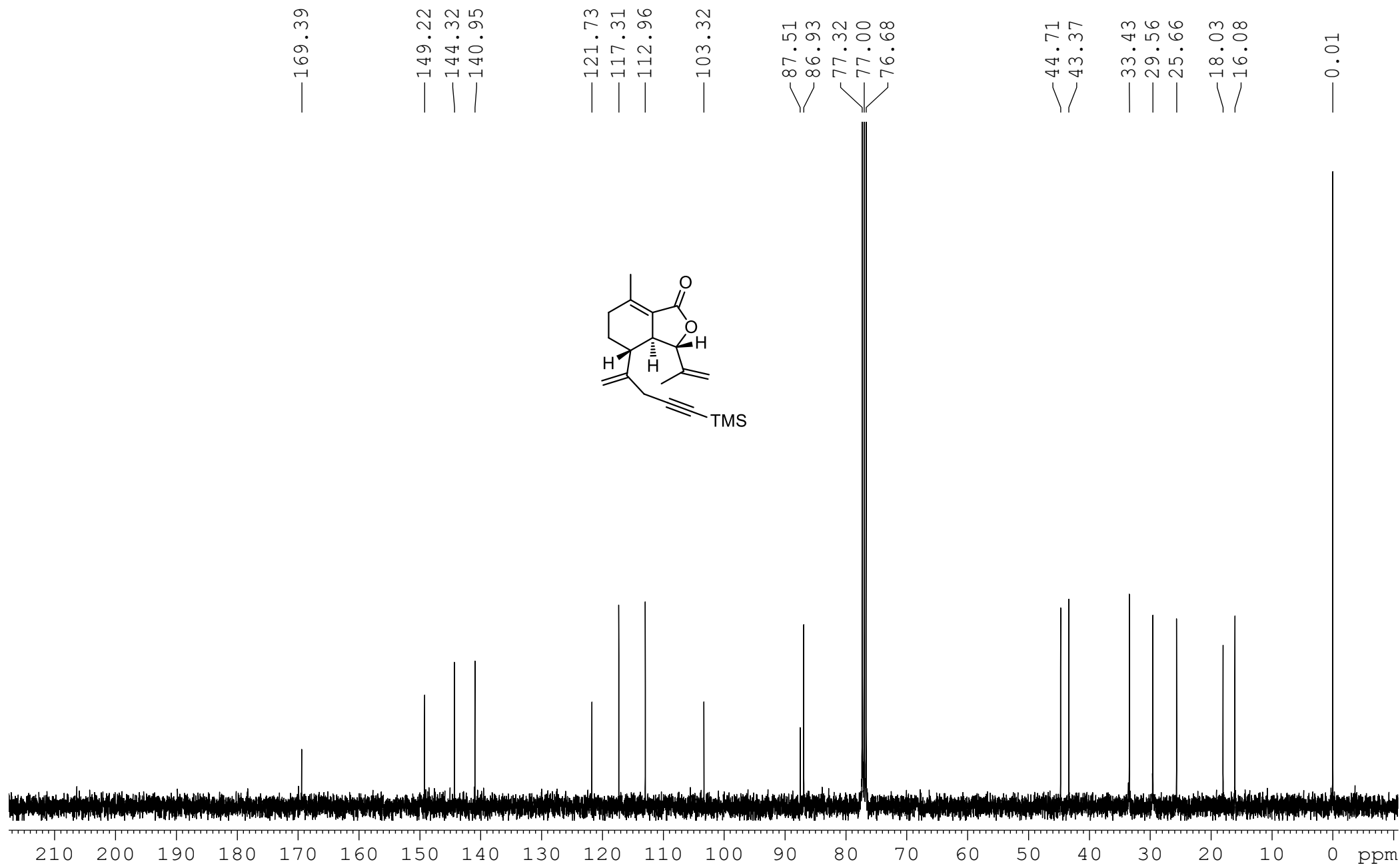
-0.01



^1H NMR of 11 (CDCl_3 , 400 MHz)

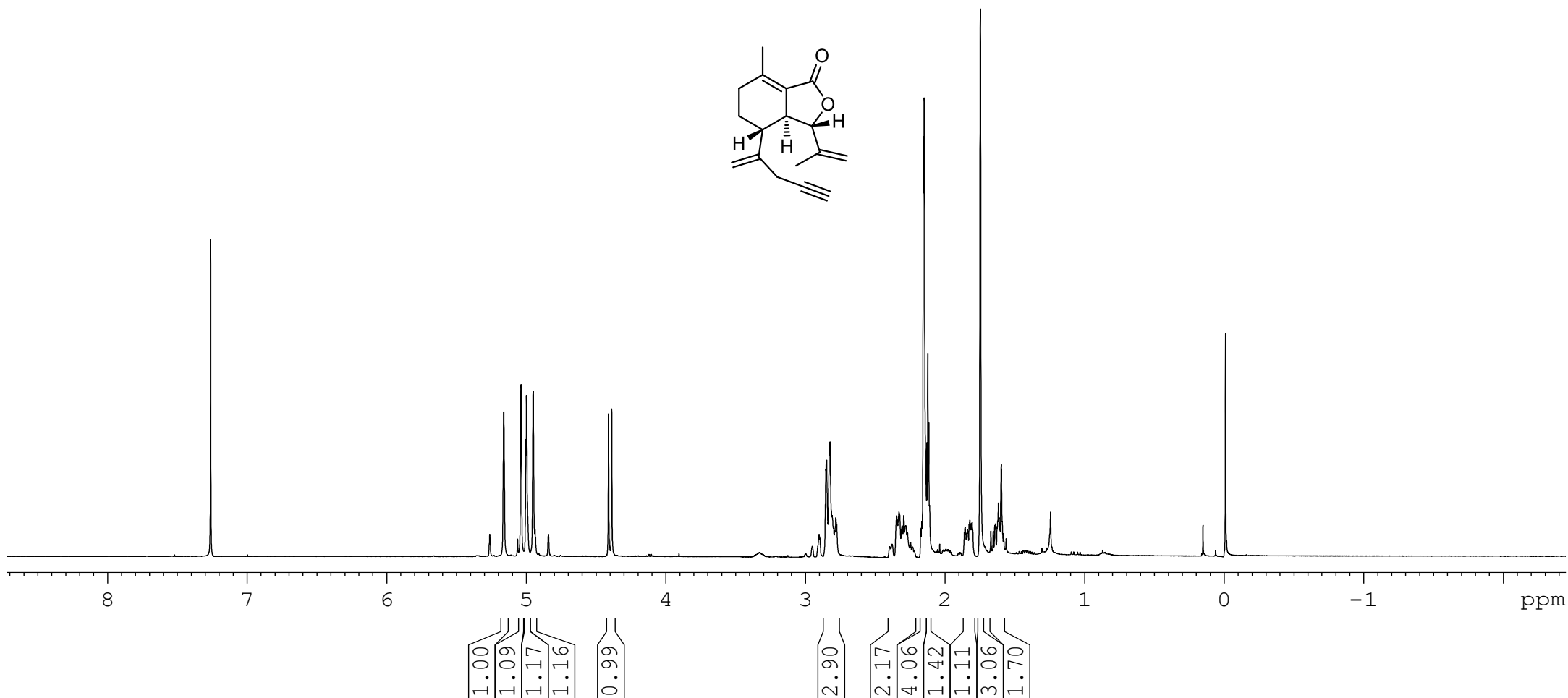


^{13}C NMR of compound 11(CDCl₃, 100 MHz)

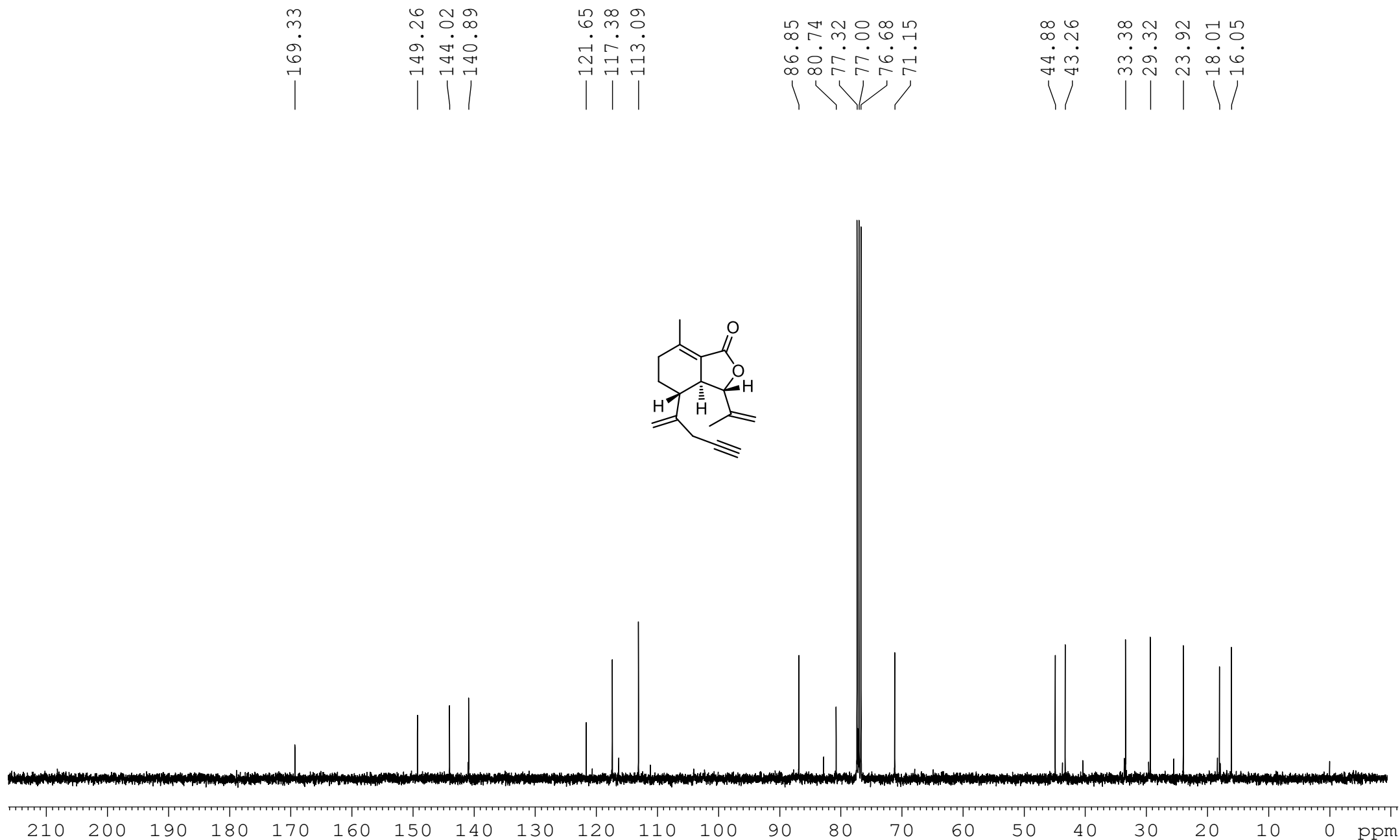


^1H NMR of compound 12 (CDCl_3 , 400 MHz)

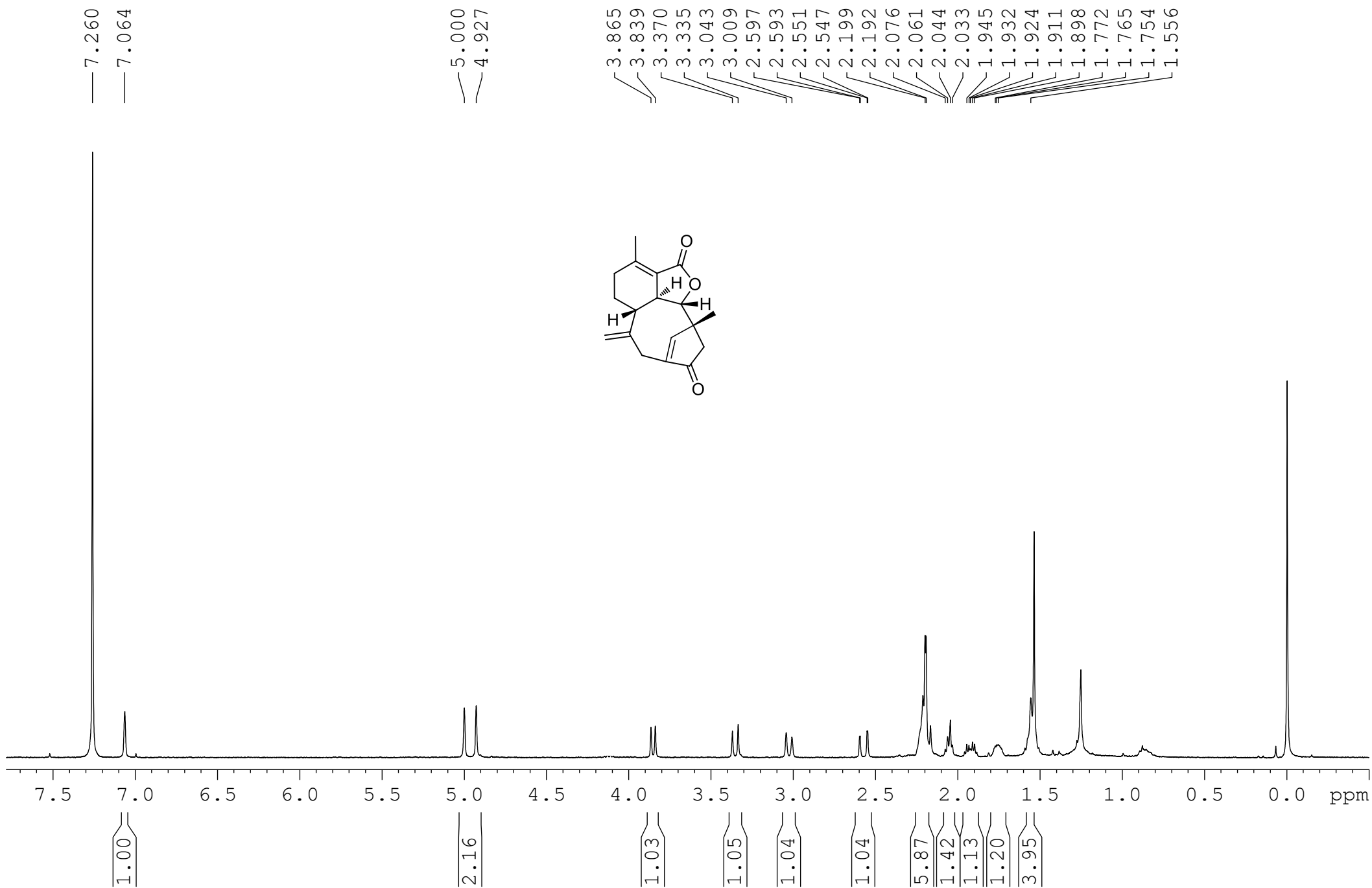
7.260
5.160
5.036
5.001
4.998
4.994
4.949
4.410
4.387
2.853
2.850
2.847
2.829
2.826
2.823
2.781
2.775
2.395
2.378
2.346
2.329
2.306
2.294
2.279
2.269
2.246
2.233
2.173
2.166
2.154
2.148
2.128
2.122
2.115
1.856
1.844
1.837
1.826
1.821
1.815
1.811
1.804
1.746
1.670
1.653
1.643
1.639
1.617
1.612
1.605
1.596
1.578
1.561



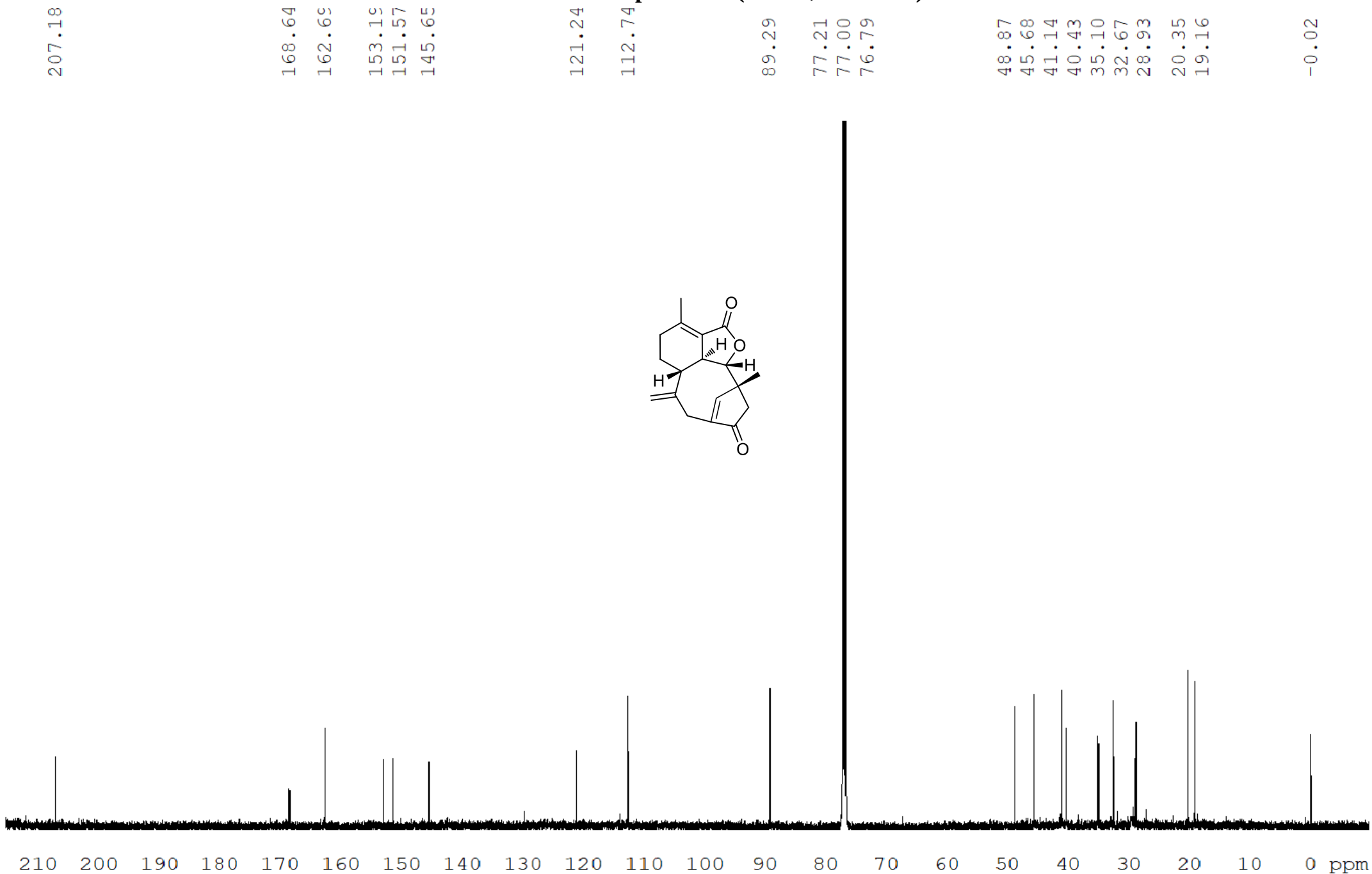
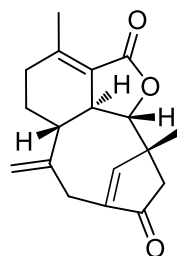
^{13}C NMR of compound 12 (CDCl_3 , 100 MHz)



^1H NMR of compound 13 (CDCl_3 , 400 MHz)



¹³C NMR of compound 13 (CDCl₃, 150 MHz)



4. DFT results about regiochemistry and reaction process of the Pauson-Khand reaction

4.1 Computational method

DFT calculations were performed with Gaussian 09.¹ Geometry optimizations of the stationary points were carried out at the B3LYP level, 6-31G(d)² basis set was used for other atoms except Co, which used LANL2DZ basis set and pseudopotential. Unscaled harmonic frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and thermal corrections at 298 K. To improve the calculation accuracy, single-point energy calculations were carried out using the B3LYP functional with the SDD² basis set for Co and the 6-311+G(d)² basis set for the other atoms. Gibbs free energies in solutions were obtained from sums of the large basis set gas-phase single-point energies, solvation energies (ΔG_{solv}) and the gas-phase Gibbs free energy corrections, which were carried out at the SMD(toluene)/ B3LYP /6-311+G(d)(SDD basis set for Co) level.² All discussed energy differences were based on Gibbs energies in toluene at 298 K. Standard state concentrations of 18.98 and 1.0 mol/L were used for toluene and all the other species, respectively. The keyword “5D” was used to specify that five d-type orbitals were used for CO in the calculations.

4.2 Gibbs energy profile for four competing pathways of Pauson-Khand reaction and the whole reaction process

The computed Gibbs energy profile for the regioselective Pauson-Khand reaction of the enyne **12** catalyzed by $\text{Co}_2(\text{CO})_8$ in toluene is shown in **Figure S1**.³ According to the previous computational studies, the regioselectivity of the PK reaction is plausibly controlled by the rate-determining alkene insertion step.⁴ We also analyze the different pathways of alkene regioselective insertion progress (**TS6** and **TS7**). All these pathways are disfavored compared to the type-II PK reaction pathway with an overall Gibbs energy of activation to **TS1** is 32.7 kcal/mol.

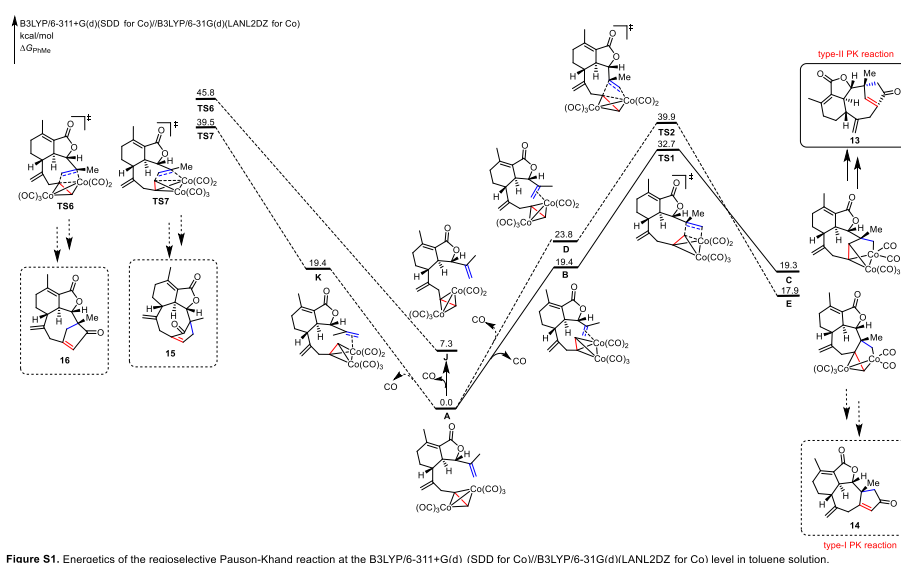


Figure S1. Energetics of the regioselective Pauson-Khand reaction at the B3LYP/6-311+G(d) (SDD for Co)/B3LYP/6-31G(d)(LANL2DZ for Co) level in toluene solution.

The full energy profile is given in **Figure S2** to better understand the type-II Pauson-Khand reaction. The catalytic cycle starts with the formation of Co₂/acetylene complex **A**, loss of CO, which is then followed by coordination with ethylene giving the intermediate **B**. The subsequent insertion of alkene into Co-metallocycle process delivers the complex **C** through the transition state **TS1**. The activation energy from intermediate **A** to **TS1** is 32.7 kcal/mol. After that, exothermic coordination of CO with **C** delivers a more stable species **F**. The migratory insertion of CO on the CH₂ side leads to the intermediate **G** via **TS3**. The subsequent CO coordination and reductive elimination reaction affords the unexpected complex **I** via transition state **TS5**. Finally, a dissociation process of intermediate **I** releases the type-II PK product **13**. We have also considered another pathway involving CO migratory insertion into the Co-(alkynyl) carbon (via **TS4**), which is disfavored than **TS3** in the above discussed type-II PK pathway (20.5 kcal/mol vs 36.0 kcal/mol).³

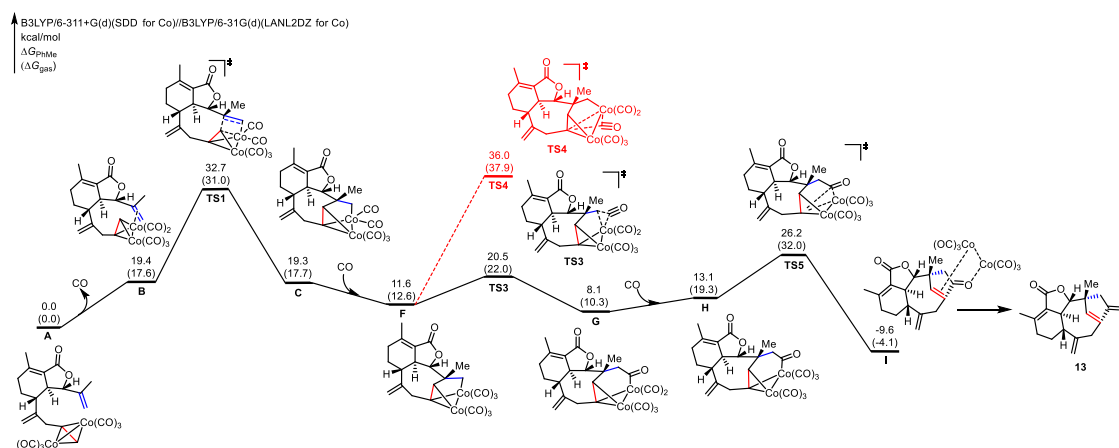


Figure S2. Energetics of the unusual Pauson-Khand reaction in the gas phase and toluene solution.

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

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2. (a) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, **1986**. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (c) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378. (d) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866. (e) Schwerdtfeger, P.; Dolg, M.; Schwarz, W. H. E.; Bowmaker, G. A.; Boyd, P. D. W. *J. Chem. Phys.* **1989**, *91*, 1762.
 3. (a) Yamanaka, M.; Nakamura, E. *J. Am. Chem. Soc.* **2001**, *123*, 1703. (b) Robert, F.; Milet, A.; Gimbet, Y.; Konya, D.; Greene, A. E. *J. Am. Chem. Soc.* **2001**, *123*, 5396. (c) Bruin, T. J. M.; Milet, A.; Robet, F.; Gimbet, Y.; Greene, A. E. *J. Am. Chem. Soc.* **2001**, *123*, 7184.
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5. Calculation data

	<i>TCG</i> ^b	<i>SPE</i> ^c	<i>SPE</i> _{gas} ^d	<i>SPE</i> _{solv} ^e
A	0.309695	-1780.412916	-1782.37860495	-1782.39375022
B	0.308219	-1667.0612132	-1668.98612775	-1669.0028282
C	0.314778	-1667.0698675	-1668.99259769	-1669.00955086
D	0.308131	-1667.0532598	-1668.97867431	-1668.9957389
E	0.313126	-1667.0714604	-1668.99371408	-1669.0102329
F	0.322122	-1780.4102403	-1782.37562379	-1782.38771063
G	0.323076	-1780.4174817	-1895.71045863	-1782.3942155
H	0.329625	-1893.7348586	-1895.7307242	-1895.75132048
I	0.328983	-1893.776446	-1895.76743469	-1895.78680164
J	0.302153	-1667.0739334	-1669.00050448	-1669.01614215
K	0.309515	-1667.0613392	-1668.98676138	-1669.00415918
TS1	0.311701	-1667.0440459	-1668.96831619	-1668.98517615
TS2	0.311531	-1667.0325834	-1668.95644289	-1668.97355682
TS3	0.323511	-1780.3990812	-1782.35736816	-1782.37490204
TS4	0.324067	-1780.3748837	-1782.33259422	-1782.35067049
TS5	0.329555	-1893.7168335	-1895.71045863	-1895.73022336
TS6	0.313215	-1667.0238229	-1668.94845858	-1668.96584741
TS7	0.313318	-1667.0332427	-1668.95820652	-1668.97590323
CO	-0.014102	-113.3069138	-113.348826609	-113.344379056

^a in a.u.

^b thermal correction to Gibbs free energies at the level of B3LYP/6-31G(d) (LANL2DZ for Co)

^c single-point energies at the level of B3LYP/6-31G(d) (LANL2DZ for Co) in the gas phase

^d single-point energies at the level of B3LYP/6-311+G(d) (SDD for Co) in the gas phase

^e single-point energies at the level of B3LYP/6-311+G(d) (SDD for Co) in toluene solution

6. Cartesian coordinates of all stationary points

A

O	4.77951000	1.73628900	-0.67302000
O	6.70580900	0.87797300	0.11602700
C	6.34200200	-2.20018200	0.39989000
C	4.93271100	-1.68395100	0.32355200
C	3.80756700	-2.69552200	0.27888800
C	2.68176500	-2.20228300	-0.64436200
C	2.07118800	-0.85788100	-0.15620500
C	3.19693100	0.17046400	0.14382200
C	4.60215200	-0.38403400	0.21646000
C	5.51838800	0.74832800	-0.07116500
C	3.40088900	1.30033300	-0.88499200
C	2.52230100	2.53133900	-0.83241000
C	2.83506400	3.56921900	-1.88250400
C	1.55266800	2.69616300	0.07327500
C	-1.19905000	-0.59635200	0.13828800
C	-1.29566600	0.53901700	-0.55967900
C	-0.25319000	-1.65932700	0.62263600
C	1.12472600	-1.13437000	1.01068300
C	1.45701600	-1.02391400	2.30280200
H	6.54703100	-2.87776300	-0.44043500
H	6.47056200	-2.79551500	1.31487700
H	7.07425600	-1.39251600	0.40039800
H	3.40910100	-2.88355300	1.28651000
H	4.19363900	-3.65671600	-0.08175300
H	1.89888700	-2.96497900	-0.72511500
H	3.09046100	-2.06286100	-1.65328000
H	1.45777300	-0.45987500	-0.97587200
H	2.98645000	0.65976800	1.10290700
H	3.36081500	0.87809700	-1.90211400
H	3.87040100	3.91463000	-1.78217000
H	2.16907600	4.43318200	-1.80175200
H	2.73718600	3.15148600	-2.89393500
H	1.33297800	1.96464800	0.84335700
H	0.94450100	3.59757900	0.08114100
H	-0.70542100	1.27907700	-1.08060000
H	-0.14883700	-2.39711600	-0.18501200
H	-0.70371900	-2.19413100	1.46432400
H	0.75555900	-1.29148800	3.08929500
H	2.42966200	-0.67084200	2.63315500

Co	-2.46370900	0.64181300	1.01783200
C	-3.56250200	2.04893900	0.64284000
C	-3.36021900	-0.44781200	2.16542000
O	-3.89960300	-1.14782000	2.89866400
O	-4.23682700	2.94496000	0.39868600
Co	-2.78124000	-0.63584300	-1.06003900
C	-2.03206200	-1.43489000	-2.46338700
C	-3.93254600	0.48954700	-1.92154300
C	-3.78482500	-2.00434400	-0.40708100
O	-4.63604000	1.20434700	-2.47910100
O	-1.52212100	-1.94226500	-3.35938400
O	-4.40434700	-2.87928600	0.00413900
C	-1.36840800	1.45289000	2.16488900
O	-0.67365100	1.99073200	2.90460500

B

O	3.02868100	2.11214900	-0.69096900
O	5.25233600	2.16307400	-1.00800100
C	6.49405900	-0.65700900	-0.62215300
C	5.06002800	-0.83196500	-0.21615800
C	4.58865600	-2.20199500	0.21676600
C	3.23132300	-2.52618200	-0.43853300
C	2.10979200	-1.47466500	-0.15304600
C	2.70107300	-0.07813300	0.22693100
C	4.12284700	0.13386600	-0.23893900
C	4.27263800	1.53304500	-0.68291200
C	1.97419100	1.15593800	-0.37694800
C	0.95440900	1.94025200	0.45437800
C	0.67035100	3.32650000	-0.08218100
C	0.55547200	1.56481700	1.70711200
C	-0.94755600	-0.94807600	-0.10207600
C	-0.96159300	-0.02113100	-1.06802300
C	-0.30478700	-2.22151600	0.36184700
C	1.10352700	-1.98451400	0.87604800
C	1.41823400	-2.23167700	2.15323600
H	6.73823600	-1.33766100	-1.44967100
H	7.15480900	-0.93562900	0.21071900
H	6.71204200	0.36815300	-0.92153300
H	4.50117600	-2.24096300	1.31300500
H	5.32548800	-2.96543100	-0.05867200

H	2.89086500	-3.51631700	-0.11957300	C	0.44695000	0.20403700	0.90523100
H	3.39646700	-2.57938600	-1.52111800	C	0.10558100	-2.29699300	-0.04485600
H	1.56629500	-1.34266100	-1.09442300	C	-1.35345700	-2.24253000	-0.45958900
H	2.69372200	0.00495600	1.32063500	C	-1.75232400	-2.79490900	-1.61081500
H	1.52513300	0.88173400	-1.33845500	H	-7.01668400	-0.44777000	1.05563700
H	1.60100200	3.90268800	-0.08939200	H	-7.07865000	-0.35504400	-0.69921100
H	-0.06224700	3.85175800	0.53328700	H	-6.61919200	1.08924100	0.23808900
H	0.30687000	3.29760000	-1.11523900	H	-4.67206200	-2.19282900	-1.06128400
H	0.93548200	0.66924000	2.18401900	H	-5.68597600	-2.49122200	0.33609500
H	0.06364000	2.28606500	2.35205200	H	-3.38724100	-3.38367400	0.73624700
H	-0.48443400	0.26264600	-1.99606900	H	-3.84477600	-2.13198700	1.88523200
H	-0.27273400	-2.93185400	-0.48031200	H	-1.74159500	-1.43730000	1.46263600
H	-0.91102200	-2.68329300	1.14752100	H	-2.33463700	-0.01689100	-1.03294100
H	0.68247400	-2.61334000	2.85642300	H	-1.85029500	0.87681000	1.84404000
H	2.41887500	-2.07268500	2.54866900	H	-0.69191400	3.56923800	0.90914800
Co	-1.34567300	0.79077100	0.66148700	H	1.01022400	3.06438100	0.79056900
C	-2.23294200	2.35308800	0.41160200	H	0.03555800	2.57775300	2.18436900
C	-1.81486200	0.22128500	2.30879100	H	-1.10516200	1.27917100	-1.77128900
O	-2.10855300	-0.20366000	3.33780300	H	-0.04062800	2.68584400	-1.47021700
O	-2.88313900	3.28970900	0.25343500	H	0.33181600	0.18628700	1.98910900
Co	-2.81933900	-0.58141100	-0.73855300	H	0.17532400	-2.81789500	0.92418400
C	-2.97156900	-1.96551500	-1.84740600	H	0.68672900	-2.88712800	-0.76060600
C	-3.68967800	0.69868500	-1.71006600	H	-1.04669500	-3.28694700	-2.27515400
C	-3.92750100	-1.13235600	0.58723000	H	-2.78725500	-2.78458900	-1.94014700
O	-4.20782900	1.49504500	-2.35489200	Co	1.26341100	0.52008300	-1.01757500
O	-3.04278300	-2.86355300	-2.56227100	C	2.48178100	1.82545600	-1.35698600
O	-4.63414800	-1.47711700	1.42563300	C	1.00598200	-0.32272700	-2.51790100
C				O	0.90547400	-0.90069300	-3.50743200
O	-2.73134400	2.24202000	0.58259000	O	3.30174100	2.58068200	-1.62506100
O	-4.92849000	2.65674500	0.31879900	Co	2.49008000	-0.45522400	0.80010700
C	-6.52811300	0.00465800	0.18132900	C	2.58758300	-1.57247800	2.19545900
C	-5.09600700	-0.43862800	0.10314400	C	3.43432100	0.96448300	1.42454600
C	-4.81399600	-1.92013200	-0.00552900	C	3.52332800	-1.23111300	-0.43530900
C	-3.58462100	-2.31141100	0.83488400	O	3.99271300	1.86544500	1.87023200
C	-2.28532400	-1.52012700	0.51420900	O	2.69639200	-2.30793600	3.07459700
C	-2.59294100	-0.06371100	0.03151700	O	4.21065800	-1.76035000	-1.19518400
C	-4.03195100	0.38205800	0.15477800	D			
C	-4.02796400	1.85104300	0.34417900	C	5.05958700	0.36183900	-0.51377600
C	-1.87010800	1.09156300	0.76470000	C	4.94088700	1.82895800	-0.84821300
C	-0.43098600	1.48914700	0.34174600	C	3.51684100	2.40466600	-0.78791700
C	0.00901700	2.75337700	1.10226000	C	2.63987100	1.76550700	0.30969800
C	-0.30121400	1.67625100	-1.15673800	C	2.56983400	0.24222500	0.02005300
C	0.71651000	-0.93165700	0.12247900	C	3.97259600	-0.32442400	-0.11284100

C	3.99122000	-1.67254900	0.50223200
O	2.85908100	-1.80560800	1.25461400
C	1.96829700	-0.65980800	1.13598600
O	4.81006100	-2.56117100	0.45790800
C	1.29275700	2.45169600	0.48553700
C	0.21582600	1.71000100	1.26382600
C	-0.58833900	0.78280400	0.36509400
C	0.59058200	-1.34004800	1.01440900
C	1.00391800	3.66724300	0.00412700
C	0.44524200	-2.24949100	-0.05433300
C	-0.84013900	0.75806900	-0.95642400
C	-0.02418800	-1.62189800	2.36839000
H	5.59397500	2.36820400	-0.14394600
H	5.37902800	2.01864300	-1.83851400
H	3.59212900	3.48447700	-0.63003100
H	3.01309500	2.26555000	-1.75343000
H	3.17243500	1.86327400	1.27186000
H	2.00834700	0.08381000	-0.91115000
H	2.03743800	-0.14575800	2.09860000
H	0.60742200	1.20237900	2.14818200
H	-0.49098300	2.44523600	1.65900400
H	1.69367300	4.25167600	-0.59425800
H	0.03866100	4.12858200	0.19680100
H	1.20346800	-2.25564400	-0.83300800
H	0.01509300	-3.22726900	0.14526800
H	-0.55246800	1.32258100	-1.83208800
H	-0.33105900	-0.70543400	2.88435300
H	0.72472300	-2.11852500	3.00223700
H	-0.89629700	-2.27457000	2.29739700
C	6.44750400	-0.21490700	-0.58761200
H	7.14301400	0.39041700	0.00954000
H	6.81076700	-0.17240000	-1.62384900
H	6.48219400	-1.24973200	-0.24938100
Co	-1.15783500	-1.08700500	-0.54013800
C	-1.10566800	-1.49978600	-2.26595800
C	-2.38376700	-2.25081900	0.09919800
O	-1.01852800	-1.75208700	-3.38664600
O	-3.19365400	-3.01551400	0.39220800
Co	-2.52290000	0.81790000	0.10291400
C	-3.16013800	0.28605100	1.71728800
C	-3.72767300	0.34444000	-1.15798100
C	-2.77156900	2.57783300	0.15987400
O	-3.55532800	-0.03852200	2.74730500
O	-2.89733000	3.72144800	0.18411200

E

O	-4.46596400	0.06756100	-1.99419600
C	-4.92646800	-0.08656000	0.29411400
C	-5.04763900	1.27305600	0.94694700
C	-3.71672900	1.99323600	1.22463100
C	-2.68199000	1.79032100	0.10209700
C	-2.43204600	0.27065500	-0.02729900
C	-3.72446700	-0.50773100	-0.13937100
C	-3.44397100	-1.70823800	-0.96671100
O	-2.22479200	-1.52148100	-1.57649300
C	-1.70391400	-0.19754400	-1.30217600
O	-4.08713000	-2.71424300	-1.15409600
C	-1.40496600	2.60700100	0.26034800
C	-0.28183300	2.31961600	-0.72908800
C	0.34269000	0.93819800	-0.47049900
C	-0.13485300	-0.23863200	-1.32117800
C	-1.23045200	3.53873100	1.20558600
C	0.42704000	-1.54118500	-0.69713900
C	0.85825000	0.62307600	0.77794100
C	0.26501700	-0.17330300	-2.81399300
H	-5.67923400	1.89177700	0.28958800
H	-5.62018100	1.17882800	1.88060100
H	-3.92017200	3.05964300	1.36664400
H	-3.28644900	1.62763100	2.16629800
H	-3.14677200	2.10697300	-0.84819000
H	-1.87284200	-0.07139300	0.85558000
H	-2.03157600	0.44050800	-2.13388200
H	-0.65687200	2.37334900	-1.75969100
H	0.47291400	3.10379100	-0.63814600
H	-1.97955800	3.77088000	1.95532800
H	-0.31205100	4.11832100	1.25642900
H	-0.34666200	-2.25961300	-0.42922200
H	1.14354700	-2.02744300	-1.35938100
H	0.73626700	1.29886700	1.62460200
H	-0.02240000	0.78760700	-3.25754000
H	-0.24635300	-0.96617300	-3.37107700
H	1.34097800	-0.29313600	-2.94767700
C	-6.20782900	-0.85448200	0.11867900
H	-6.95354900	-0.23880000	-0.40270100
H	-6.63614800	-1.09385500	1.10188700
H	-6.05624600	-1.78428800	-0.42919200
Co	1.53464300	-1.13431500	0.92116300
C	0.25281700	-1.75472700	2.00226700

C	2.69462000	-2.57258200	0.71399500
O	-0.59860000	-2.09030400	2.69443200
O	3.39341300	-3.46507900	0.55836000
Co	2.64819600	0.69679000	-0.15478600
C	3.33930400	-0.35772200	-1.42385800
C	3.68183600	0.62119100	1.28782400
C	3.04621300	2.32045100	-0.77348900
O	3.88411300	-1.03203000	-2.18736600
O	3.27060000	3.37486400	-1.17917400
O	4.40151400	0.56986200	2.19056400

F

O	2.48829400	2.36989800	-0.00411400
O	4.54811000	2.61292300	0.86873500
C	6.25644400	0.09176000	0.31942400
C	4.86387900	-0.33583500	-0.04703900
C	4.66268400	-1.74692400	-0.55019300
C	3.61534100	-1.78219500	-1.67959900
C	2.22544600	-1.19461400	-1.31223000
C	2.36135100	0.01832300	-0.31782600
C	3.77597600	0.45285800	0.00313000
C	3.72312700	1.89206600	0.35646800
C	1.73718500	1.37284200	-0.74060500
C	0.21368000	1.64215000	-0.53447500
C	-0.07108400	3.04356200	-1.11995500
C	-0.23270300	1.56037600	0.93866300
C	-0.73058400	-0.67509400	-0.58019600
C	-0.47086600	0.52403000	-1.28133400
C	-0.24734500	-1.99824000	-1.13032400
C	1.22603800	-2.24285100	-0.80812100
C	1.57598300	-3.34772900	-0.13918700
H	6.92459600	-0.01012400	-0.54720400
H	6.65748600	-0.57276700	1.09761500
H	6.28773400	1.11923600	0.68152600
H	4.36512800	-2.39505900	0.28653400
H	5.61350100	-2.14937100	-0.92120500
H	3.48912300	-2.80501700	-2.04899800
H	4.02363900	-1.19516900	-2.51130700
H	1.80862100	-0.79910300	-2.24782000
H	1.90590600	-0.28104300	0.62851300
H	1.95609400	1.53455200	-1.80709600
H	0.51553200	3.80392000	-0.59685900
H	-1.12924300	3.29942400	-1.02795500
H	0.19380200	3.08470200	-2.18458300

H	0.60025700	1.72184800	1.62733200
H	-0.96612000	2.33905200	1.14989400
H	-0.23316000	0.45925700	-2.34825000
H	-0.35877800	-1.97339800	-2.22767400
H	-0.84180900	-2.84294600	-0.76912900
H	0.82880200	-4.06349500	0.19502000
H	2.60628600	-3.59735800	0.09240300
Co	-1.20175400	-0.26306400	1.28337400
C	-2.31791900	0.64994300	2.41446500
C	-1.94184700	-1.92597700	1.51595700
C	0.22167800	-0.62701400	2.29323000
O	1.10865200	-0.81903600	2.99641900
O	-2.34562100	-2.98587400	1.67106500
O	-2.99050600	1.27400800	3.10127000
Co	-2.49516100	0.17964100	-0.86090800
C	-2.81964800	0.13510000	-2.60702900
C	-3.17283600	1.80832200	-0.37261400
C	-3.80617100	-0.97752500	-0.43190900
O	-3.67432000	2.80015700	-0.07851300
O	-2.99188400	0.12605500	-3.74416300
O	-4.68241800	-1.68421900	-0.19314400

G

O	2.52364100	-2.36473300	-0.48455600
O	4.52465500	-2.32237600	-1.51018500
C	6.19016900	0.07175000	-0.50434100
C	4.81000600	0.36141300	0.01227400
C	4.61470800	1.59148500	0.86748800
C	3.64730700	1.28365200	2.02669400
C	2.23933600	0.80292400	1.58714600
C	2.32842600	-0.11455100	0.30395400
C	3.73251200	-0.42115000	-0.17972700
C	3.71036800	-1.75650700	-0.81940600
C	1.75120600	-1.55235300	0.43002400
C	0.23226400	-1.81225100	0.15931400
C	-0.06377500	-3.27263900	0.56473400
C	-0.10940500	-1.65653000	-1.33417100
C	-0.74194900	0.51948100	0.75931800
C	-0.48682000	-0.82929800	1.07087400
C	-0.24300900	1.60932600	1.68741200
C	1.22627300	1.94506700	1.43821400
C	1.56579100	3.20812000	1.15440000
H	6.89641700	-0.01942700	0.33267600
H	6.54201600	0.91596200	-1.11379900

H	6.22246300	-0.83646800	-1.10562700	C	3.85510600	-1.65691700	-0.81096200
H	4.24139500	2.41899800	0.24791000	C	1.89263700	-1.62091200	0.44674500
H	5.58009900	1.92233000	1.26955800	C	0.38746300	-1.94755300	0.15575400
H	3.54443500	2.15440400	2.68169000	C	0.14905600	-3.41323700	0.57626000
H	4.10978500	0.49124500	2.62763400	C	0.03760400	-1.81340200	-1.33242800
H	1.86420400	0.17128600	2.40377200	C	-0.10062400	-0.40468600	-1.87877000
H	1.81201400	0.40519400	-0.51172300	C	-0.69906000	0.35624200	0.78675800
H	1.96644800	-1.92107300	1.44315900	C	-0.36225200	-0.98017300	1.04749500
H	0.54835800	-3.97144800	-0.01331200	C	-0.27145100	1.37804200	1.82411200
H	-1.11888000	-3.51301500	0.40450900	C	1.18800700	1.79922900	1.64309800
H	0.15821100	-3.42688700	1.62737700	C	1.46627300	3.09992800	1.49436600
H	0.65343500	-2.15070700	-1.94292800	H	6.94293000	0.21745600	0.38854400
H	-1.06730700	-2.14554700	-1.53224700	H	6.51551100	1.19830800	-1.00744000
H	-0.24178200	-1.03592500	2.11880800	H	6.30170100	-0.56871600	-1.08164000
H	-0.34544200	1.25128400	2.72618500	H	4.13819400	2.49000100	0.45375700
H	-0.84062100	2.52339500	1.60770100	H	5.52106200	2.02748100	1.43292800
H	0.81214300	3.98696600	1.07133500	H	3.50594400	2.04398700	2.88795700
H	2.59094600	3.52877700	1.00343700	H	4.15531600	0.42050800	2.71592000
Co	-1.49597200	0.85401900	-0.96523400	H	1.91992400	0.00832800	2.50402900
C	-2.79892600	0.75696700	-2.26539500	H	1.83700500	0.37746700	-0.39881100
C	-0.62748300	2.35759300	-1.49325300	H	2.12228400	-2.01984900	1.44539100
C	-0.23498800	-0.23331600	-1.88581400	H	0.81576300	-4.08368500	0.02538700
O	0.34534200	0.15559700	-2.85847000	H	-0.88491300	-3.71193700	0.37709300
O	-0.16249700	3.35325500	-1.81193100	H	0.34001400	-3.55010400	1.64760900
O	-3.60137000	0.66114300	-3.07687500	H	0.78740800	-2.32538000	-1.94227300
Co	-2.52960700	-0.39585800	0.82226000	H	-0.92760100	-2.30388600	-1.50052800
C	-2.91783500	-0.95717900	2.47834300	H	-0.13955700	-1.18852700	2.10028600
C	-3.22016900	-1.70813800	-0.19419900	H	-0.37425400	0.92292900	2.82347100
C	-3.65339400	0.98763900	0.70732800	H	-0.90244600	2.27200900	1.81201700
O	-3.70794200	-2.53410900	-0.83463100	H	0.67332100	3.84334700	1.46704200
O	-3.13171200	-1.33509400	3.54317700	H	2.47534800	3.48721000	1.40523600
O	-4.40778800	1.86022400	0.66933300	Co	-1.34384300	0.93487500	-0.99134900
H				Co	-2.44862300	-0.63704000	0.75032800
O	2.71075100	-2.34976800	-0.49368200	C	-0.09043800	2.14990400	-1.46700300
O	4.69874600	-2.14458700	-1.52518900	C	-2.32805900	0.68522200	-2.52981100
O	0.48868100	-0.06443600	-2.87720300	C	-2.49499600	2.25995800	-0.33512100
C	6.22254300	0.30600800	-0.43662600	O	0.67212500	2.92231600	-1.82632400
C	4.83346500	0.48639200	0.10467000	O	-2.91207600	0.54845000	-3.50485400
C	4.57321700	1.65713200	1.02370600	O	-3.18063500	3.12092700	-0.02097500
C	3.64327400	1.22532200	2.17478200	C	-2.68480300	-1.96715300	1.88802100
C	2.25717300	0.69974000	1.71949400	C	-3.55375600	0.51420200	1.61976300
C	2.38802200	-0.14773400	0.38921400	C	-3.23415000	-1.42706800	-0.65563200
C	3.80274300	-0.34954400	-0.11611100	O	-2.82230000	-2.83035200	2.63672700
				O	-4.30116000	1.14171000	2.22918000

O	-3.81517300	-1.96077900	-1.49756000
I			
O	3.16494200	2.17941400	0.66695400
O	5.10006500	2.09159700	1.81308900
O	-0.76986100	-0.97503600	1.51292300
C	6.69523700	-0.44096700	1.03312500
C	5.33511100	-0.68509700	0.44405800
C	5.11132900	-1.97459300	-0.31114100
C	4.19853100	-1.74806200	-1.53127300
C	2.81354300	-1.12279300	-1.21578200
C	2.91339200	-0.07417600	-0.04223300
C	4.30326600	0.17490000	0.50742300
C	4.30525300	1.53811800	1.09033300
C	2.46011600	1.38803000	-0.31774800
C	0.94383800	1.74562300	-0.24755100
C	0.77119000	3.25276200	-0.46930800
C	0.30589000	1.21502400	1.06279600
C	-0.31493400	-0.12776700	0.66048000
C	-0.04876900	-0.39263900	-0.74293400
C	0.31150300	0.84895000	-1.30750100
C	0.27804100	-1.74707400	-1.31732300
C	1.70874600	-2.15580200	-0.95766900
C	1.92979800	-3.37826700	-0.46322200
H	7.45832900	-0.45496700	0.24245900
H	6.95289700	-1.25564300	1.72441800
H	6.74688300	0.50658300	1.56895900
H	4.68661300	-2.72662400	0.36894700
H	6.07420300	-2.37989300	-0.64606300
H	4.05447700	-2.68578100	-2.07745900
H	4.73233700	-1.06954600	-2.20800200
H	2.51955600	-0.57285300	-2.12000900
H	2.31749800	-0.46411900	0.79408000
H	2.83238800	1.69551300	-1.30698600
H	1.29715300	3.82186100	0.30195300
H	-0.28645300	3.52872000	-0.44796500
H	1.17822600	3.55058300	-1.44385800
H	1.04549000	1.03336800	1.85204400
H	-0.42080800	1.91274400	1.48418900
H	0.66878300	0.92211600	-2.33188300
H	0.18074100	-1.69677800	-2.41113100
H	-0.41841300	-2.51170100	-0.96306000
H	1.10950200	-4.06775600	-0.28169000
H	2.92125200	-3.74982400	-0.22690700

Co	-2.68910000	-0.64847600	1.21715700
Co	-1.82202200	0.62149600	-1.17265800
C	-2.89817600	-2.46468400	1.11899900
C	-2.71210200	0.33694300	2.76079500
C	-4.37004700	-0.25690400	0.76650000
O	-2.95841900	-3.60808800	1.16708500
O	-2.68626700	0.84565800	3.78741900
O	-5.45943300	-0.01828800	0.50091500
C	-1.94048100	1.40935100	-2.74694900
C	-2.73913500	-0.84178800	-1.66449500
C	-2.49400200	1.95383100	-0.17554300
O	-2.01950700	1.94187900	-3.76489300
O	-3.29724400	-1.74318300	-2.12383300
O	-2.95592100	2.87041900	0.35577800

J			
C	5.29232500	1.62665900	0.04214400
C	4.42161600	2.75137400	-0.47682700
C	3.10640100	2.29585300	-1.12610500
C	2.41637000	1.15387300	-0.34062800
C	3.39290200	-0.03358500	-0.29077400
C	4.79342200	0.37885900	0.10527400
C	5.43017600	-0.81520800	0.72024800
O	4.44090000	-1.72660100	0.98822100
C	3.12269000	-1.14672000	0.75190800
O	6.58800600	-1.04801300	0.98017900
C	1.04963300	0.81215500	-0.93514000
C	-0.10995000	1.03213100	0.02388800
C	0.90817300	0.39171800	-2.19485000
C	-2.32450200	0.68774000	-1.46407900
C	1.13497800	-2.52772900	1.19507100
H	4.21478300	3.42834800	0.36765000
H	4.99709600	3.35645100	-1.19168800
H	2.42378600	3.14816800	-1.22196200
H	3.30524900	1.94344300	-2.14577900
H	2.26859700	1.50299100	0.69248500
H	3.42581600	-0.49970100	-1.28587900
H	2.79998300	-0.68601700	1.69524300
H	0.05906200	0.43533000	0.93084100
H	-0.08206700	2.07619800	0.37791300
H	1.76425400	0.25755800	-2.85093700
H	-0.06042000	0.16210600	-2.62309100
H	-2.44377200	0.91850800	-2.51350600
H	0.96046300	-1.96898800	2.11179000

H	0.43443500	-3.32922100	0.97604900
C	6.66861300	2.01247300	0.51088800
H	6.60688900	2.82459500	1.24840100
H	7.25481600	2.40327400	-0.33238200
H	7.20503200	1.16784600	0.94301400
Co	-2.58818500	-1.01542500	-0.50940800
C	-1.70490800	-2.15187900	-1.51644400
C	-3.22989200	-2.17102700	0.69319800
O	-1.12076500	-2.88370100	-2.18784500
O	-3.63067700	-2.91083200	1.47681400
Co	-3.30152000	1.06884900	0.26252600
C	-3.04622500	0.76433900	2.01265700
C	-4.94449800	0.43233100	-0.10714100
C	-3.51029200	2.86079600	0.21039900
O	-2.86255400	0.56713700	3.13076900
O	-3.63683100	4.00147200	0.16463300
O	-5.99697100	0.03261100	-0.34609300
C	2.16893700	-2.25962100	0.38882200
C	2.46261300	-3.05987700	-0.85435500
H	2.35578300	-2.45095700	-1.76075800
H	3.49057900	-3.43982200	-0.83285300
H	1.78015100	-3.90964600	-0.94400800
C	-1.49647400	0.79209500	-0.45284800

K

O	2.86514200	2.03567700	-0.93540500
O	5.08556400	2.17819000	-1.26400300
C	6.47609600	-0.53472400	-0.64981000
C	5.05100400	-0.74930900	-0.23170200
C	4.64509100	-2.10025500	0.31301600
C	3.31677800	-2.55824000	-0.32528000
C	2.13864100	-1.53926600	-0.17803700
C	2.65554100	-0.09864000	0.14336700
C	4.06487200	0.16125100	-0.32981800
C	4.13775300	1.52776400	-0.88620900
C	1.85993200	1.05581700	-0.52102200
C	0.85081500	1.86793100	0.28443800
C	1.31290000	2.37910100	1.63459700
C	-0.08777400	2.58180400	-0.44544200
C	-0.95084800	-0.95892300	-0.22853000
C	-1.12183500	-0.17133400	-1.28419900
C	-0.31702900	-2.20740300	0.31559900
C	1.09403000	-2.00248300	0.83279400
C	1.38536400	-2.24686300	2.11545200

H	6.75921000	-1.26660300	-1.41925900
H	7.14694900	-0.70985800	0.20299000
H	6.64124600	0.47279100	-1.03178600
H	4.54244600	-2.04534500	1.40756100
H	5.42517100	-2.84481700	0.11594400
H	3.01834700	-3.52378800	0.09430900
H	3.50863300	-2.72093900	-1.39230400
H	1.64735300	-1.48898500	-1.15633900
H	2.62718400	0.02300600	1.23327200
H	1.38795100	0.69955300	-1.44122500
H	1.54644100	1.57526200	2.33883500
H	0.55282800	3.01869300	2.09174800
H	2.22366100	2.97723100	1.49917800
H	-0.31006600	-2.96355600	-0.48601300
H	-0.93670500	-2.60773000	1.12348600
H	0.62848800	-2.57930400	2.82039400
H	2.38930800	-2.12592300	2.51537900
Co	-1.21885600	0.89538900	0.37607400
C	-2.50071300	2.12824000	0.47714100
C	-1.02604300	0.46361500	2.12224100
O	-0.92810400	0.15645400	3.22701900
O	-3.33086900	2.92004900	0.59942100
Co	-2.90946800	-0.59681100	-0.59651200
C	-3.26640900	-2.13704200	-1.41283000
C	-3.89225100	0.54612500	-1.63808400
C	-3.75469900	-0.87353600	0.98154100
O	-4.48086700	1.24035200	-2.33770800
O	-3.48920900	-3.13240800	-1.94336400
O	-4.26520700	-1.04263200	1.99729300
H	-0.15921800	2.47135300	-1.52233900
H	-0.49985300	3.50144800	-0.04263600
H	-0.75352300	0.02864300	-2.28072600

TS1

O	2.63184500	2.25148500	-0.59563300
O	4.82859400	2.64097600	-0.31982500
C	6.39684000	-0.01729600	-0.18442000
C	4.96109000	-0.44987100	-0.10064500
C	4.66965800	-1.92918300	0.00210300
C	3.43367500	-2.30251500	-0.83698200
C	2.13887700	-1.50507600	-0.50305300
C	2.45712300	-0.05228500	-0.00464000
C	3.90214000	0.37914100	-0.14459400
C	3.91927700	1.84488400	-0.34387200

C	1.72613200	1.11933300	-0.71152600	C	-4.82714000	1.79319600	0.87070800
C	0.36840600	1.65069400	-0.19769300	C	-3.40614400	2.38211200	0.82025700
C	-0.12281600	2.82743300	-1.03465400	C	-2.52805400	1.75910400	-0.28322500
C	0.24509900	1.78200600	1.24131300	C	-2.45688400	0.23947400	-0.00675000
C	-0.88051000	-0.97897900	-0.11864400	C	-3.84904600	-0.34638400	0.11129800
C	-0.72175900	0.11871800	-0.92614900	C	-3.83579100	-1.69440500	-0.50483200
C	-0.24580000	-2.32761400	0.05946800	O	-2.67269800	-1.81849900	-1.22033000
C	1.21373500	-2.24019100	0.46872100	C	-1.83690800	-0.63030200	-1.12411600
C	1.62206900	-2.78548400	1.62000400	O	-4.64832000	-2.58936100	-0.48203300
H	6.87868300	-0.47347300	-1.06044700	C	-1.17370000	2.43128200	-0.45678100
H	6.94670900	-0.38264700	0.69422600	C	-0.11559400	1.68904800	-1.26146000
H	6.49715900	1.06637600	-0.24032600	C	0.59853900	0.61647200	-0.42528700
H	4.52979600	-2.20780800	1.05637700	C	-0.39482500	-1.17554800	-0.99086200
H	5.53557400	-2.50487800	-0.34705400	C	-0.87283700	3.63640100	0.04286100
H	3.22754400	-3.37373200	-0.74669500	C	-0.27072800	-2.17274900	0.07001100
H	3.69153100	-2.11600300	-1.88665100	C	0.92678700	0.66829300	0.90679400
H	1.59127300	-1.41098600	-1.44793600	C	0.16407500	-1.54954000	-2.35654400
H	2.21283300	-0.02023000	1.06376000	H	-5.48238200	2.33667000	0.17171800
H	1.64416800	0.90129700	-1.78511600	H	-5.26825600	1.96893500	1.86224700
H	0.61201300	3.63732900	-0.98172500	H	-3.48907400	3.46357400	0.67637300
H	-1.08306500	3.20058800	-0.67180800	H	-2.90299400	2.23397900	1.78477400
H	-0.24265300	2.55474900	-2.08904900	H	-3.06075300	1.86628300	-1.24432900
H	1.01709100	1.34429100	1.86741400	H	-1.89935000	0.07533000	0.92634300
H	-0.10973700	2.73868400	1.61704800	H	-1.94349700	-0.12531100	-2.08887700
H	-0.33183000	0.24664800	-1.92695200	H	-0.51905200	1.27732300	-2.19061700
H	-0.31508300	-2.86200200	-0.90231400	H	0.64000300	2.40973800	-1.57804700
H	-0.80632200	-2.91989400	0.78952300	H	-1.55950900	4.21570300	0.65031200
H	0.92452500	-3.28866700	2.28431900	H	0.09450600	4.09480500	-0.14486100
H	2.65598000	-2.75643000	1.95108000	H	-1.05222800	-2.18361000	0.82659000
Co	-1.31720500	0.56191000	0.97625800	H	0.01727200	-3.17588700	-0.23743600
C	-2.56131600	1.83445700	1.32579300	H	0.61064300	1.27116800	1.74760600
C	-1.15522100	-0.30687800	2.49889800	H	0.37860000	-0.66643900	-2.96772100
O	-1.04802700	-0.87349300	3.49544700	H	-0.58054100	-2.15278300	-2.89264900
O	-3.38338500	2.57892800	1.62723700	H	1.08339700	-2.13322600	-2.28107800
Co	-2.64532300	-0.44302600	-0.78939900	C	-6.32405900	-0.25833300	0.58922500
C	-2.76133000	-1.54615600	-2.18510000	H	-7.02387400	0.34622600	-0.00363900
C	-3.55009900	0.99912700	-1.42671900	H	-6.68825300	-0.22679300	1.62551500
C	-3.70404100	-1.21557600	0.44489600	H	-6.35075400	-1.29067000	0.24207300
O	-4.10301500	1.90901200	-1.86018400	Co	1.32921800	-1.15741600	0.58589500
O	-2.83998400	-2.27113200	-3.07546800	C	1.21634000	-1.55117700	2.28934400
O	-4.36044300	-1.73267400	1.23618800	C	2.53691700	-2.33332900	-0.08701600
TS2				O	1.12742700	-1.80695000	3.40817000
C	-4.94031300	0.32775500	0.51981100	O	3.34948400	-3.08077500	-0.40551700
				Co	2.60858500	0.77556000	-0.09354200

C	3.27715500	0.25662300	-1.69702500
C	3.80876600	0.31328500	1.16616100
C	2.84695100	2.54200000	-0.12576400
O	3.68854400	-0.04818100	-2.72739600
O	3.01363700	3.68123600	-0.13284100
O	4.56872600	0.04320900	1.98761500

TS3

O	-2.50733400	-2.33069300	-0.25747600
O	-4.56094900	-2.63950000	0.60970000
C	-6.24101800	-0.05624600	0.33765000
C	-4.84538400	0.39298800	0.01165200
C	-4.63259800	1.84464000	-0.34970800
C	-3.58976400	1.98049700	-1.47544500
C	-2.20353000	1.35090800	-1.17088800
C	-2.34654700	0.04510500	-0.30328400
C	-3.76487900	-0.40738400	-0.02137200
C	-3.73272100	-1.87557700	0.17304400
C	-1.74393400	-1.26624800	-0.87449000
C	-0.22619600	-1.59025400	-0.70496100
C	0.05104700	-2.89302100	-1.49417100
C	0.17438900	-1.82957000	0.75670300
C	0.77142300	0.74142700	-0.48772600
C	0.50001500	-0.39461200	-1.28898700
C	0.27339500	2.10988300	-0.89852700
C	-1.19874000	2.33532000	-0.56125400
C	-1.54448900	3.37696800	0.20402400
H	-6.91011200	0.13966900	-0.51184700
H	-6.63248700	0.53079500	1.18023600
H	-6.28267200	-1.11444100	0.59475800
H	-4.32530400	2.40322700	0.54582500
H	-5.58118700	2.29040100	-0.67376600
H	-3.45705300	3.03292500	-1.74588700
H	-4.00607800	1.47946200	-2.35799100
H	-1.78792000	1.05052000	-2.14176700
H	-1.88477600	0.24985000	0.66593300
H	-1.95983200	-1.29988600	-1.95270900
H	-0.55820100	-3.71746800	-1.11309000
H	1.10506100	-3.17314500	-1.42523300
H	-0.19109100	-2.75409500	-2.55494700
H	-0.57754500	-2.42120200	1.27906900
H	1.11661400	-2.36814500	0.83135300
H	0.24214300	-0.21383500	-2.33739700
H	0.38731700	2.18714400	-1.99279600

H	0.87432400	2.91389600	-0.46326200
H	-0.79413000	4.04784100	0.61415000
H	-2.57451900	3.61528900	0.44766000
Co	1.28564900	0.08785300	1.27958600
C	2.67175700	-0.65750900	2.24991300
C	1.36659900	1.73774300	1.91896500
C	-0.13140400	-0.48967400	2.11745500
O	-1.00454600	-0.60040400	2.88474100
O	1.41578100	2.80426700	2.33772600
O	3.53577700	-1.08728300	2.86777200
Co	2.52209300	-0.03813300	-0.90921900
C	2.86047700	0.27453200	-2.63091400
C	3.25012400	-1.68159300	-0.64465900
C	3.67158000	1.15062800	-0.22079200
O	3.75036400	-2.70848300	-0.49605600
O	3.04657600	0.45951500	-3.75091300
O	4.40568400	1.92571500	0.21181000

TS4

O	2.50122800	-2.10148800	0.95878700
O	4.55471500	-2.76318600	0.31395900
C	6.33117600	-0.30056900	-0.30515200
C	4.94793800	0.27526900	-0.19925300
C	4.78174000	1.76611800	-0.38619500
C	3.71623900	2.31737500	0.57952100
C	2.30888500	1.67887800	0.43845200
C	2.43010700	0.12953900	0.14074000
C	3.83920600	-0.42821900	0.08979800
C	3.74963000	-1.86914000	0.43174700
C	1.78768300	-0.85871700	1.15253600
C	0.24839700	-1.13227100	1.13857400
C	-0.09202000	-1.89397700	2.43774700
C	-0.25682100	-1.92902500	-0.08215900
C	-0.64935800	0.89798700	-0.12342100
C	-0.35412300	0.25180500	1.11254400
C	-0.13225900	2.32073500	-0.35000100
C	1.38850000	2.42606500	-0.54490100
C	1.84492800	3.23386100	-1.50840900
H	6.99493300	0.16686500	0.43553400
H	6.75623700	-0.06647500	-1.29129300
H	6.33724100	-1.38142400	-0.16520000
H	4.51738800	1.97939700	-1.43187700
H	5.73835400	2.27168900	-0.20469600
H	3.63502100	3.40452000	0.48377100

H	4.07536000	2.12015300	1.59697300
H	1.84328900	1.77933500	1.42688000
H	2.00696600	-0.06296200	-0.84710600
H	2.03241800	-0.50270100	2.16515100
H	0.48130700	-2.82454900	2.49373700
H	-1.15716200	-2.13701000	2.47471900
H	0.14739300	-1.29011300	3.32214100
H	0.55003600	-2.24237600	-0.74842200
H	-0.79420600	-2.82492800	0.23234600
H	0.01569000	0.90878500	1.90108400
H	-0.39936800	2.88134900	0.55647000
H	-0.64272300	2.81890900	-1.18024000
H	1.16268300	3.74767600	-2.18095400
H	2.89952800	3.42558000	-1.67261900
Co	-1.62774100	-0.73567900	-1.13427400
C	-1.81111200	-2.24404400	-2.03986600
C	-2.94144100	0.19491100	-2.03575900
C	-0.22364600	0.11797400	-1.74654600
O	0.55808900	0.43407200	-2.55046100
O	-3.75114100	0.73947500	-2.63087900
O	-1.89635000	-3.23018700	-2.61614500
Co	-2.36506000	0.49676300	0.92107700
C	-3.49416400	1.80036500	0.38745600
C	-2.54246100	0.71827700	2.65953300
C	-3.10472600	-1.13206500	0.73362900
O	-2.64065000	0.87303700	3.79771800
O	-4.21227700	2.66454000	0.13251700
O	-3.74218400	-2.08723600	0.90778500

TS5

O	2.99276200	2.10875200	0.93637900
O	5.13206900	2.01588700	1.63351400
O	0.52383800	-1.41420500	1.85831700
C	6.63964900	-0.31053200	0.23438100
C	5.20286200	-0.53656700	-0.13888100
C	4.86676300	-1.73409300	-0.99776800
C	3.76578200	-1.39117000	-2.01949900
C	2.44306600	-0.83492700	-1.41673700
C	2.72208200	-0.00699900	-0.10704100
C	4.17798700	0.25949600	0.21327500
C	4.23358500	1.51188300	1.00240100
C	2.15399300	1.43678100	-0.02787400
C	0.65639300	1.66783700	0.35457100
C	0.39019400	3.18169800	0.36663700

C	0.30885600	0.99566500	1.69206300
C	-0.06565700	-0.45949400	1.41276900
C	-0.59224100	-0.39807100	-0.48756700
C	-0.08476700	0.89518700	-0.72325600
C	-0.09989200	-1.49920600	-1.43399200
C	1.35965800	-1.90689500	-1.21652100
C	1.63686500	-3.18144800	-0.92233800
H	7.25301100	-0.19557600	-0.67022500
H	7.03070600	-1.19174700	0.76201700
H	6.76522900	0.56622200	0.86957000
H	4.55886200	-2.56908300	-0.35143800
H	5.76293000	-2.07699500	-1.52947700
H	3.54158300	-2.26322000	-2.64147200
H	4.18016600	-0.62705200	-2.68838400
H	2.05316500	-0.13510000	-2.16697200
H	2.32757300	-0.58204000	0.73544900
H	2.31689100	1.93380600	-0.99677500
H	1.04442100	3.68212700	1.08569600
H	-0.64946100	3.38880400	0.63506200
H	0.57955100	3.61747900	-0.62202000
H	1.14799300	1.01606300	2.39354500
H	-0.53685000	1.50603700	2.15912000
H	0.32574300	1.06920400	-1.71882600
H	-0.18634800	-1.09864700	-2.45607800
H	-0.73321700	-2.38734400	-1.39128700
H	0.84602500	-3.91320900	-0.78084100
H	2.64984500	-3.55172200	-0.80127500
Co	-2.07349300	-0.89392100	0.85157200
Co	-2.19797100	0.89299500	-0.93681800
C	-1.80147300	-2.67720800	1.09268300
C	-2.53275800	-0.26397700	2.51778700
C	-3.73035100	-1.17924300	0.23387100
O	-1.64589000	-3.79757300	1.27171400
O	-2.87221600	0.00418700	3.58132000
O	-4.82776900	-1.42258600	-0.01608000
C	-2.09563700	2.29594400	-2.01066200
C	-2.95926800	-0.17397000	-2.20057000
C	-2.95798900	1.79928100	0.39626100
O	-2.01242000	3.20828200	-2.70554800
O	-3.41420100	-0.80564100	-3.04771700
O	-3.47298500	2.46504500	1.18713800

TS6

C	4.90781300	0.49731300	-0.06999000
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C	4.85077600	1.88944100	0.50848500
C	3.53603100	2.59006100	0.18221500
C	2.26303800	1.79907500	0.57783100
C	2.33421600	0.35706500	-0.03907000
C	3.75198100	-0.12765300	-0.35326000
C	3.62396700	-1.58061700	-0.63754000
O	2.46565600	-1.99721000	-0.03012500
C	1.92779800	-0.91393100	0.77742300
O	4.33450600	-2.34350200	-1.24646000
C	1.01312800	2.61213700	0.17944200
C	-0.33391800	2.36827600	0.85403800
C	1.04253000	3.56253100	-0.76605300
C	-1.02421100	0.62665100	-0.90770500
C	-0.23264400	-0.22423600	1.80491200
H	5.01049900	1.82549400	1.59702500
H	5.68855300	2.48718200	0.12449600
H	3.50111500	3.57695200	0.65562500
H	3.52713200	2.75629400	-0.90035600
H	2.27012800	1.70344600	1.67535500
H	1.75322400	0.34803100	-0.97062600
H	2.52739500	-0.88671200	1.70614200
H	-0.26064600	2.41925500	1.94755500
H	-1.00603300	3.18151800	0.56156900
H	1.92822900	3.83284500	-1.32793900
H	0.14484300	4.12179800	-1.01692200
H	-0.64030800	1.03490300	-1.83323400
H	0.34990200	0.62362900	2.13899900
H	-1.00755200	-0.47964200	2.52377800
C	6.27083000	-0.11679000	-0.23498500
H	6.83156600	-0.05251900	0.70762000
H	6.84715300	0.45151800	-0.97797500
H	6.22302500	-1.15585700	-0.56128600
Co	-1.01701900	-1.04221400	-0.05090000
C	-0.38433600	-1.82000300	-1.49508100
C	-2.14646200	-2.29919300	0.60846200
O	0.00292200	-2.31913500	-2.45591700
O	-2.90844400	-3.11675900	0.87873400
Co	-2.83961700	0.64904800	-0.19273300
C	-3.65367900	0.35928200	1.40420800
C	-3.69880600	-0.35444200	-1.42128200
C	-3.39200800	2.28266100	-0.65922900
O	-4.12961800	0.20395600	2.43979200
O	-3.73966900	3.33983600	-0.95059500
O	-4.21435200	-0.98773500	-2.23049800

C	0.52508900	-1.30848000	1.21558900
C	0.52850700	-2.66775500	1.90997500
H	0.70956700	-3.48507400	1.20772000
H	1.33343000	-2.70261600	2.65985300
H	-0.41475600	-2.85254200	2.43183200
C	-0.98886100	1.07394000	0.39318700

TS7

O	2.88369500	2.15860000	-0.26978100
O	4.99960400	2.22724900	0.50067700
C	6.29693400	-0.58269000	0.10687800
C	4.82576300	-0.84919700	-0.05148500
C	4.40229400	-2.26822400	-0.36312900
C	3.12141700	-2.31327400	-1.21300900
C	1.92608700	-1.49618400	-0.65309700
C	2.38123400	-0.11690000	-0.09546900
C	3.87225700	0.09615700	0.02650400
C	4.05558000	1.56450600	0.14083200
C	1.98604100	1.17217300	-0.84740900
C	0.54679800	1.73003400	-0.85611000
C	0.51755400	3.25242600	-0.72961900
C	-0.32839000	1.15037800	-1.87349600
C	-1.05613500	-1.06329700	-0.26052600
C	-1.41890200	-0.40160600	-1.40976900
C	-0.39205400	-2.37342300	0.08759900
C	1.09082200	-2.24140000	0.38888000
C	1.58043000	-2.71849500	1.53876400
H	6.83546700	-0.85886000	-0.81025200
H	6.70644200	-1.21436600	0.90762700
H	6.50066600	0.46151400	0.34477700
H	4.27782300	-2.84116800	0.56597800
H	5.21214400	-2.77206900	-0.90687000
H	2.80817500	-3.35217800	-1.36495800
H	3.37155100	-1.91001000	-2.20327900
H	1.26612100	-1.31635200	-1.50935900
H	1.97078800	-0.01017100	0.91329300
H	2.29174400	1.06341000	-1.90229900
H	0.79826000	3.59116800	0.27055100
H	-0.47272800	3.64757200	-0.97138400
H	1.23745800	3.70263800	-1.42621400
H	-0.53889800	-3.06064400	-0.76263100
H	-0.88937600	-2.82696300	0.94983900
H	0.93867500	-3.21722500	2.26058800
H	2.62327800	-2.61905500	1.82181500

Co	-0.97664300	0.81751700	0.18343200
C	-2.01597500	2.28758600	0.50458000
C	-0.24143000	0.63462600	1.77032300
O	0.18689100	0.53504300	2.83418100
O	-2.69474600	3.15190500	0.83832900
Co	-2.96437000	-0.56940900	-0.16623200
C	-3.67202700	-2.10411100	-0.73460900
C	-4.13296200	0.62527300	-0.87752600
C	-3.27348500	-0.63580000	1.60954900
O	-4.85996500	1.36560800	-1.37335800
O	-4.13269900	-3.09738700	-1.08881300
O	-3.45344100	-0.69825700	2.74436100
H	0.18315000	0.50661900	-2.58536600
H	-1.02871500	1.82494300	-2.36155000
H	-1.55048300	-0.73113200	-2.43143200

CO

C	-1.26558594	0.84788029	0.00000000
O	-0.15018594	0.84788029	0.00000000