Supporting Information

Mechanistic Study on Gold-Catalyzed Cycloisomerization of Dienediynes Involving Aliphatic C–H Functionalization and Inspiration for Developing a New Strategy to Access Polycarbocycles

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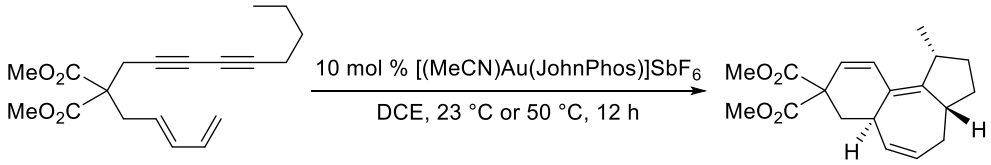
S1. General Information

All reactions were carried out in oven-dried glassware. All chemicals were used as received without further purification. DCE (with molecular sieves, water ≤30 ppm) was purchased from J&K. Flash column chromatographies were performed using silica gel (200−300 mesh) or neutral Al_2O_3 (200−300 mesh). Analytical thin layer chromatographies (TLCs) were performed with 0.2−0.3 mm silica gel HSGF254 plates. Melting points (uncorrected) were determined in open glass capillaries. Nuclear magnetic resonance (NMR) spectra were measured on Bruker AVANCE III 400 (^{1}H at 400 MHz; ^{13}C at 101 MHz), Bruker AVANCE III HD 400 (^{1}H at 400 MHz; ^{13}C at 101 MHz), and Bruker AVANCE NEO 600 (^{1}H at 600 MHz; ^{13}C at 151 MHz) NMR spectrometers. Data for ^{1}H NMR spectra are reported as follows: chemical shift δ (ppm) referenced to either tetramethylsilane (TMS, 0.00 ppm) or $CHDCl_2$ (5.32 ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets), coupling constant J (Hz), and integration. Data for ^{13}C{^{1}H} NMR spectra are reported in terms of chemical shift δ (ppm) referenced to either $CDCl_3$ (77.16 ppm) or CD_2Cl_2 (53.84 ppm). Distortionless enhancement by polarization transfer (DEPT) and heteronuclear singular quantum correlation (HSQC) experiments were used to distinguish carbon signals (CH_3, CH_2, CH, or C). High-resolution mass spectrometry (HRMS) data were recorded on Bruker Apex IV and Bruker Solarix XR fourier transform ion cyclotron resonance (FTICR) mass spectrometers (electrospray ionization, ESI).

S2. Reaction of Malonate-Tethered Substrate 7 under Gold Catalysis



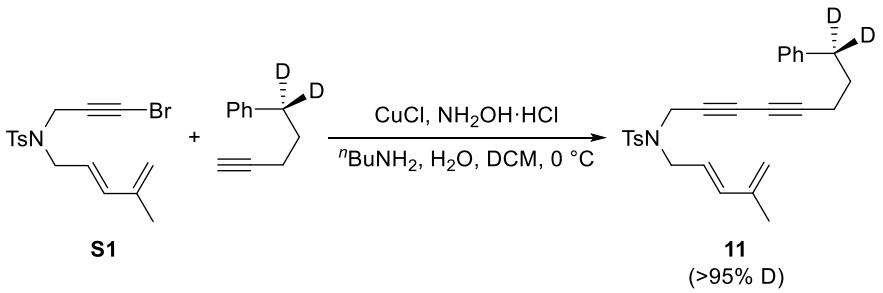
7 **8** (not detected)

Reaction at 23 °C. To a stirred solution of dienediyne **7**[1] (0.10 mmol, 1.0 equiv) in DCE (1.0 mL) was added a solution of [(MeCN)Au(JohnPhos)]SbF_6 (7.7 mg, 0.010 mmol, 10 mol %) in DCE (1.0 mL) under nitrogen atmosphere. The reaction mixture was stirred at 23 °C for 12 h, quenched by filtration through a pad of silica gel, and then concentrated by rotary evaporation. ^{1}H NMR (400 MHz, $CDCl_3$) analysis of the crude product indicated that tricyclic compound **8** was not obtained. Only the starting material **7** can be identified from the reaction mixture and it was recovered in 33% yield (estimated by ^{1}H NMR analysis; triphenylmethane was used as the internal standard).

Reaction at 50 °C. To a stirred solution of dienediyne **7**[1] (0.10 mmol, 1.0 equiv) in DCE (1.0 mL) was added a solution of [(MeCN)Au(JohnPhos)]SbF_6 (7.7 mg, 0.010 mmol, 10 mol %) in DCE (1.0 mL) under nitrogen atmosphere. The reaction mixture was stirred at 50 °C for 12 h, quenched by filtration through a pad of silica gel, and then concentrated by rotary evaporation. ^{1}H NMR (400 MHz, $CDCl_3$) analysis of the crude product indicated that the reaction gave a complex mixture (>95% conversion).

S3. Deuterium Labeling Experiments

The non-labeled analogues of **11**–**13** were synthesized and characterized in our previous work.[1] The deuterium content of **11**–**13** was determined by ^{1}H NMR and HRMS analyses.



(*E*)-4-Methyl-*N*-(4-methylpenta-2,4-dien-1-yl)-*N*-(8-phenylocta-2,4-diyn-1-yl-8,8-d_2)benzenesulfonamide (11)

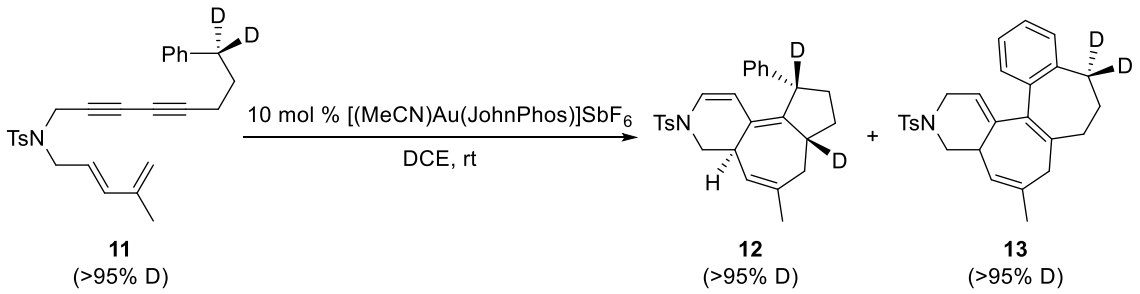
To a stirred solution of CuCl (43 mg, 0.43 mmol, 0.5 equiv) in 30% ^{n}BuNH$_2$/H$_2$O (3 mL) was added NH$_2$OH·HCl in small portions at 0 °C under argon atmosphere until the blue color disappeared. A solution of (pent-4-yn-1-yl-1,1-d_2)benzene[2] (>95% D, 1.9 mmol, 2.2 equiv) in DCM (3 mL) was then added dropwise. The reaction mixture was stirred at 0 °C for 5 min. Then, a solution of bromoalkyne **S1**[1] (318 mg, 0.863 mmol, 1.0 equiv) in DCM (3 mL) was added dropwise. The resulting mixture was stirred at 0 °C for 10 min, quenched with ammonia solution, and extracted with Et$_2$O. The combined organic phases were successively washed with water, saturated aqueous NH$_4$Cl solution, and brine, dried over MgSO$_4$, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 20:1 hexanes/EtOAc) afforded the title compound **11** (262 mg, 0.604 mmol, 70%) as a pink oil.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.5.

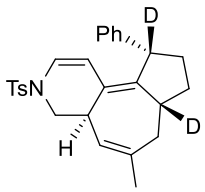
^{1}H NMR (400 MHz, CDCl$_3$, δ): 7.74 (d, J = 8.3 Hz, 2H), 7.34−7.26 (m, 4H), 7.23−7.15 (m, 3H), 6.29 (d, J = 15.6 Hz, 1H), 5.51 (dt, J = 15.6, 6.8 Hz, 1H), 5.00 (s, 1H), 4.97 (s, 1H), 4.13 (s, 2H), 3.86 (d, J = 6.8 Hz, 2H), 2.39 (s, 3H), 2.23 (t, J = 7.0 Hz, 2H), 1.81 (t, J = 7.0 Hz, 2H), 1.80 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$, δ): 143.8, 141.2, 141.1, 137.9, 135.9, 129.7, 128.6, 127.9, 126.2, 123.0, 117.8, 80.0, 70.7, 69.0, 64.9, 48.9, 36.8, 29.7, 21.7, 18.60, 18.58.

HRMS (ESI−FTICR, m/z): [M + H]$^+$ calculated for $C_{27}H_{28}D_2NO_2S^+$: 434.2117; found: 434.2127.



A solution of dienediyne **11** (227.5 mg, 0.525 mmol, 1.0 equiv) and [(MeCN)Au(JohnPhos)]SbF_6 (40.3 mg, 0.0522 mmol, 10 mol %) in DCE (10.6 mL) was stirred at room temperature for 6 h under argon atmosphere, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 20:1 hexanes/EtOAc) afforded the polycyclic products **12** (47.6 mg, 0.110 mmol, 21%, >20:1 dr) and **13** (139.9 mg, 0.323 mmol, 61%).



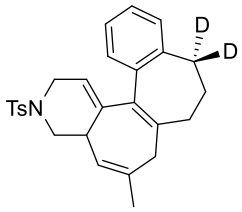
(4a*R*,7a*R*,10*S*)-6-Methyl-10-phenyl-3-tosyl-3,4,4a,7,7a,8,9,10-octahydroazuleno[5,4-*c*]pyridine-7a,10-d_2 (12)

TLC (10:1 petroleum ether/EtOAc, R_f): 0.5.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.61 (d, *J* = 8.2 Hz, 2H), 7.31−7.22 (m, 4H), 7.20−7.13 (m, 1H), 7.09−7.03 (m, 2H), 6.29 (d, *J* = 8.4 Hz, 1H), 5.12 (d, *J* = 8.4 Hz, 1H), 5.01 (s, 1H), 3.81 (dd, *J* = 11.2, 3.7 Hz, 1H), 3.40−3.32 (m, 1H), 2.73−2.58 (m, 2H), 2.41 (s, 3H), 2.05 (dd, *J* = 13.5, 1.1 Hz, 1H), 1.96−1.86 (m, 1H), 1.81 (s, 3H), 1.64 (dd, *J* = 11.7, 5.4 Hz, 1H), 1.56 (dd, *J* = 12.1, 5.5 Hz, 1H), 1.44−1.34 (m, 1H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 146.9, 143.9, 143.7, 142.3, 134.6, 129.9, 128.4, 127.8, 127.2, 125.8, 124.0, 123.4, 122.8, 111.4, 49.8, 37.0, 36.4, 34.8, 31.6, 25.7, 21.7.

HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{27}H_{28}D_2NO_2S^+$: 434.2117; found: 434.2120.



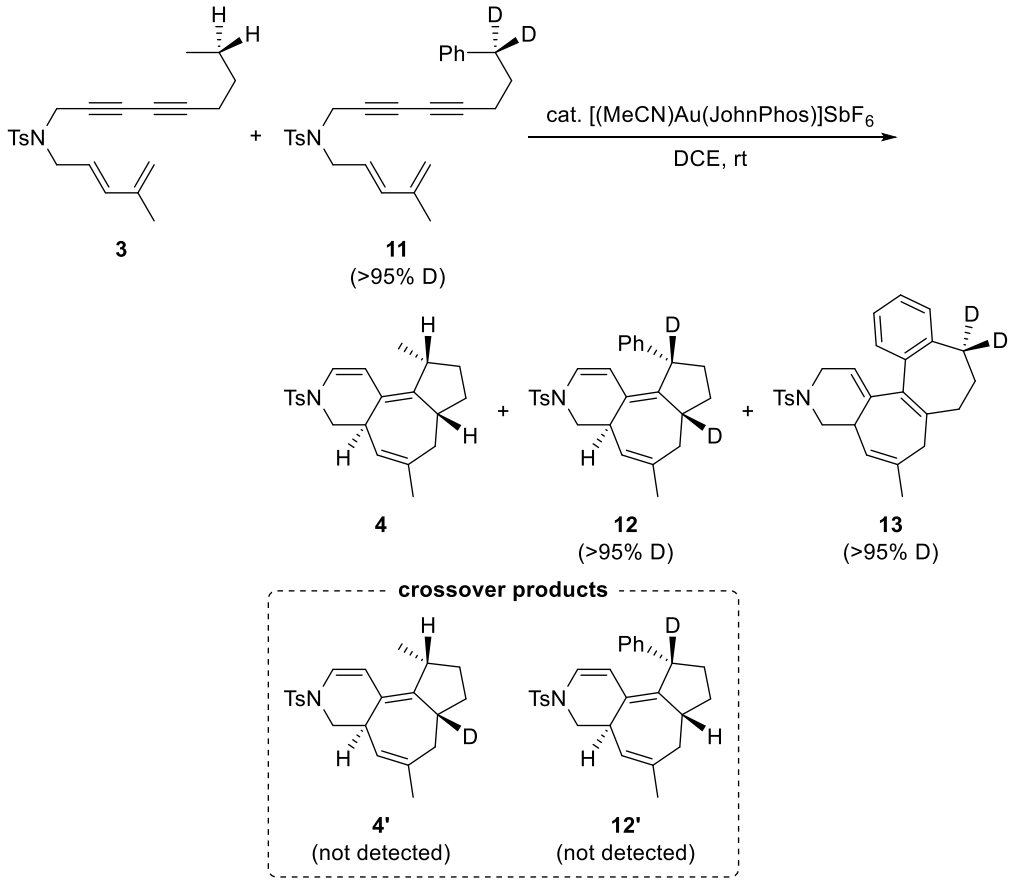
6-Methyl-3-tosyl-2,3,4,4a,7,8,9,10-octahydrobenzo[9,10]heptaleno[2,1-*c*]pyridine-10,10-d_2 (13)

TLC (10:1 petroleum ether/EtOAc, R_f): 0.4.

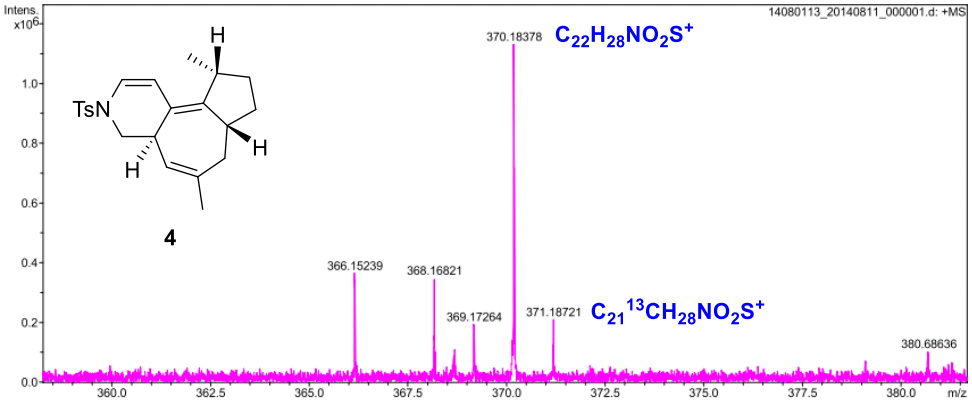
^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.68 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.14−7.06 (m, 3H), 7.03−6.97 (m, 1H), 5.75−5.71 (m, 1H), 5.02−4.98 (m, 1H), 3.89 (dd, *J* = 16.8, 4.3 Hz, 1H), 3.75 (d, *J* = 11.2 Hz, 1H), 3.60 (d, *J* = 19.9 Hz, 1H), 3.47−3.42 (m, 1H), 3.17 (dd, *J* = 16.8, 1.5 Hz, 1H), 2.73 (d, *J* = 19.9 Hz, 1H), 2.63 (dd, *J* = 11.2, 3.2 Hz, 1H), 2.44 (s, 3H), 2.11−2.04 (m, 1H), 1.95−1.87 (m, 1H), 1.81 (s, 3H), 1.76−1.71 (m, 2H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 143.7, 141.2, 136.9, 135.3, 135.1, 135.0, 133.1, 129.8, 129.5, 128.1, 127.9 (2C), 127.0, 126.8, 125.5, 118.6, 47.5, 45.2, 41.6, 38.6, 34.9, 32.5, 24.8, 21.7.

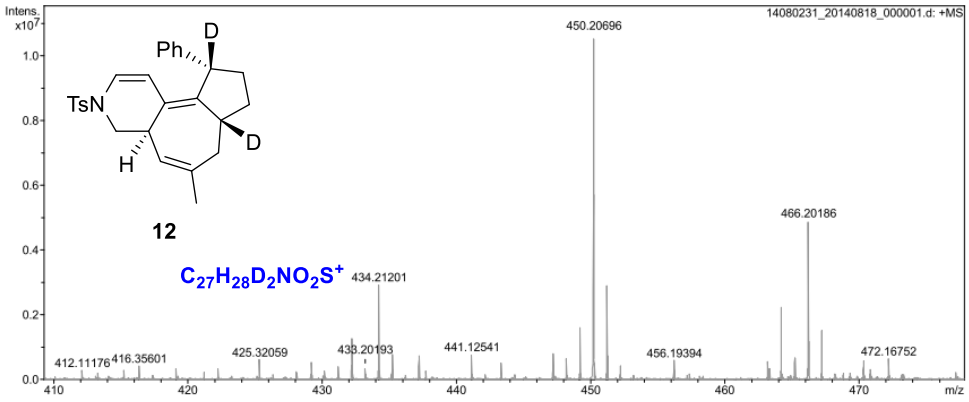
HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{27}H_{28}D_2NO_2S^+$: 434.2117; found: 434.2107.



Crossover Experiments. A solution of dienediynes **3**[1] (20.9 mg, 0.0566 mmol), **11** (89.2 mg, 0.206 mmol), and [(MeCN)Au(JohnPhos)]SbF_6 (21.0 mg, 0.0272 mmol) in DCE (5.1 mL) was stirred at room temperature for 16.5 h under argon atmosphere, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 20:1 petroleum ether/EtOAc) afforded the polycyclic products **4**[1] (20.9 mg, 0.0566 mmol, quantitative), **12** (26.1 mg, 0.0602 mmol, 29%), and **13** (56.0 mg, 0.129 mmol, 63%). HRMS analysis indicated that there were no crossover products.

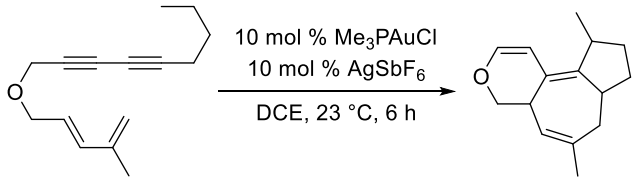


HRMS (ESI–FTICR, *m/z*): [M(**4**) + H]$^+$ calculated for $C_{22}H_{28}NO_2S^+$: 370.1835; found: 370.1838. [M(**4'**) + H]$^+$ calculated for $C_{22}H_{27}DNO_2S^+$: 371.1898; not detected.

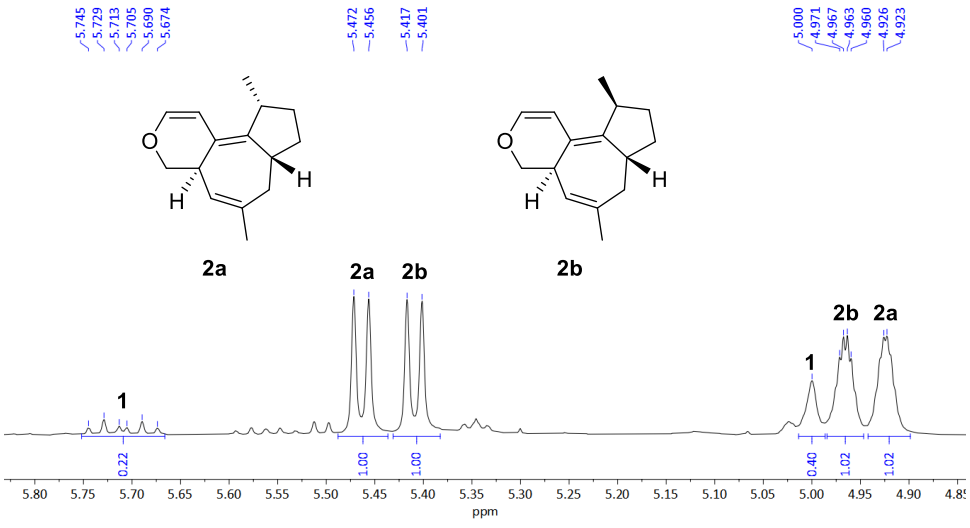


HRMS (ESI−FTICR, *m/z*): [M(**12**) + H]$^+$ calculated for $C_{27}H_{28}D_2NO_2S^+$: 434.2117; found: 434.2120. [M(**12'**) + H]$^+$ calculated for $C_{27}H_{29}DNO_2S^+$: 433.2055; not detected.

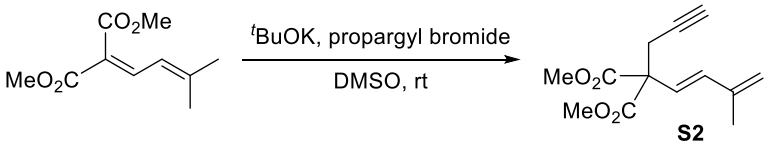
S4. Gold Catalysis with Trimethylphosphine as the Ligand



To a stirred solution of dienediyne **1**[1] (21.5 mg, 0.10 mmol, 1.0 equiv) and Me_3PAuCl (3.2 mg, 0.010 mmol, 10 mol %) in DCE (1.0 mL) was added a suspension of $AgSbF_6$ (3.4 mg, 0.010 mmol, 10 mol %) in DCE (1.0 mL) under nitrogen atmosphere. The reaction mixture was stirred at 23 °C for 6 h, quenched by filtration through a pad of silica gel, and then concentrated by rotary evaporation. ^{1}H NMR (400 MHz, $CDCl_3$) analysis of the crude product indicated that the tricyclic compound **2**[1] was obtained as a mixture of diastereomers (1:1 dr).



S5. Synthesis of Substrates



Dimethyl (*E*)-2-(3-methylbuta-1,3-dien-1-yl)-2-(prop-2-yn-1-yl)malonate (S2)

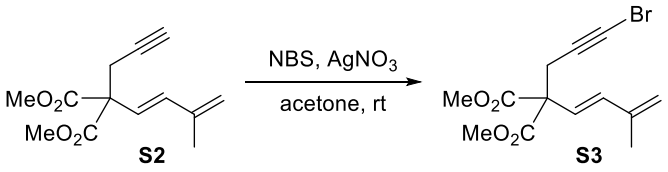
Following Grenning's procedure,[3] to a stirred solution of ^{t}BuOK (622 mg, 5.54 mmol, 1.2 equiv) in DMSO (10 mL) was added dropwise a solution of dimethyl 2-(3-methylbut-2-en-1-ylidene)malonate[3] (916 mg, 4.62 mmol, 1.0 equiv) in DMSO (5 mL) at room temperature under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 1 h. Then, propargyl bromide (80 wt% in toluene, 826 mg, 5.55 mmol, 1.2 equiv) was added dropwise. The resulting mixture was stirred at room temperature for 17 h, quenched with water (100 mL), and extracted with EtOAc (30 mL × 3). The combined organic phases were washed with brine (50 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 40:1 petroleum ether/EtOAc) afforded the title compound **S2** (842 mg, 3.56 mmol, 77%) as an off-white solid (mp: 35−37 °C).

TLC (5:1 petroleum ether/EtOAc, R_f): 0.5.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.25 (d, J = 16.4 Hz, 1H), 6.15 (d, J = 16.4 Hz, 1H), 5.06 (s, 1H), 5.02 (s, 1H), 3.78 (s, 6H), 2.98 (d, J = 2.6 Hz, 2H), 2.01 (t, J = 2.6 Hz, 1H), 1.90 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 169.8 (2C), 141.3 (C), 135.0 (CH), 124.8 (CH), 118.5 (CH_2), 78.9 (C), 71.4 (CH), 59.1 (C), 53.2 ($2CH_3$), 25.6 (CH_2), 18.5 (CH_3).

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{13}H_{17}O_4^+$: 237.1121; found: 237.1116.



Dimethyl (*E*)-2-(3-bromoprop-2-yn-1-yl)-2-(3-methylbuta-1,3-dien-1-yl)malonate (S3)

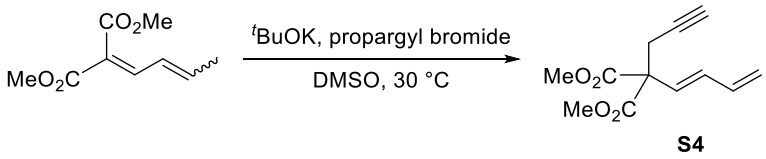
To a stirred solution of dienyne **S2** (438 mg, 1.85 mmol, 1.0 equiv) in acetone (9 mL) was added *N*-bromosuccinimide (NBS; 362 mg, 2.03 mmol, 1.1 equiv) in one portion at room temperature. Then, the reaction flask was wrapped with aluminum foil and $AgNO_3$ (31 mg, 0.18 mmol, 10 mol %) was added in one portion. The reaction mixture was stirred at room temperature for 4 h, quenched with semi-saturated aqueous $Na_2S_2O_3$ solution (30 mL), and extracted with Et_2O (30 mL × 2). The combined organic phases were washed with brine (50 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 40:1 petroleum ether/EtOAc) afforded the title compound **S3** (520 mg, 1.65 mmol, 89%) as a white solid (mp: 59−61 °C).

TLC (5:1 petroleum ether/EtOAc, R_f): 0.6.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.23 (d, J = 16.4 Hz, 1H), 6.12 (d, J = 16.4 Hz, 1H), 5.07 (s, 1H), 5.02 (s, 1H), 3.78 (s, 6H), 3.00 (s, 2H), 1.90 (s, 3H).

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$, δ): 169.7 (2C), 141.3 (C), 135.1 (CH), 124.7 (CH), 118.6 (CH_2), 75.0 (C), 59.0 (C), 53.3 ($2CH_3$), 41.6 (C), 26.9 (CH_2), 18.6 (CH_3).

HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{13}H_{16}BrO_4^+$: 315.0226; found: 315.0220.



S4

Dimethyl (*E*)-2-(buta-1,3-dien-1-yl)-2-(prop-2-yn-1-yl)malonate (S4)

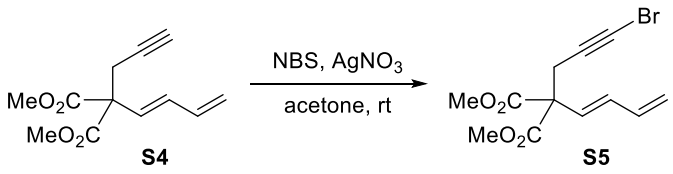
Following Grenning's procedure,[3] to a stirred solution of ^{t}BuOK (405 mg, 3.61 mmol, 1.2 equiv) in DMSO (7.5 mL) was added dropwise a solution of dimethyl 2-(but-2-en-1-ylidene)malonate[3] (*E*/*Z* mixture, 553 mg, 3.00 mmol, 1.0 equiv) in DMSO (7.5 mL) at 30 °C under nitrogen atmosphere. The reaction mixture was stirred at 30 °C for 1 h. Then, propargyl bromide (80 wt% in toluene, 535 mg, 3.60 mmol, 1.2 equiv) was added dropwise. The resulting mixture was stirred at 30 °C for 12 h, quenched with saturated aqueous NH_4Cl solution (30 mL) and water (100 mL), and extracted with Et_2O (50 mL × 2). The combined organic phases were washed with brine (50 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 40:1 petroleum ether/EtOAc) afforded the title compound **S4** (503 mg, 2.26 mmol, 75%) as a pale yellow oil.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.47−6.33 (m, 1H), 6.25−6.12 (m, 2H), 5.26 (dd, *J* = 17.0, 1.3 Hz, 1H), 5.18 (dd, *J* = 10.1, 1.3 Hz, 1H), 3.78 (s, 6H), 2.98 (d, *J* = 2.6 Hz, 2H), 2.01 (t, *J* = 2.6 Hz, 1H).

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$, δ): 169.6 (2C), 136.2 (CH), 133.1 (CH), 128.5 (CH), 119.2 (CH_2), 78.9 (C), 71.5 (CH), 59.1 (C), 53.3 ($2CH_3$), 25.4 (CH_2).

HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{12}H_{15}O_4^+$: 223.0965; found: 223.0968.



S4 **S5**

Dimethyl (*E*)-2-(3-bromoprop-2-yn-1-yl)-2-(buta-1,3-dien-1-yl)malonate (S5)

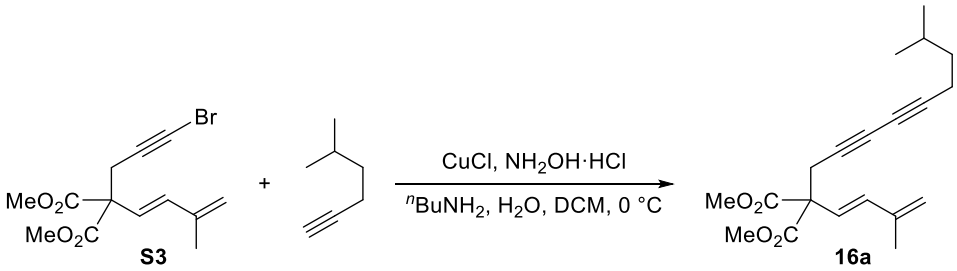
To a stirred solution of dienyne **S4** (493 mg, 2.22 mmol, 1.0 equiv) in acetone (11 mL) was added NBS (435 mg, 2.44 mmol, 1.1 equiv) in one portion at room temperature. Then, the reaction flask was wrapped with aluminum foil and $AgNO_3$ (38 mg, 0.22 mmol, 10 mol %) was added in one portion. The reaction mixture was stirred at room temperature for 4 h, quenched with semi-saturated aqueous $Na_2S_2O_3$ solution (30 mL), and extracted with Et_2O (30 mL × 2). The combined organic phases were washed with brine (50 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 40:1 petroleum ether/EtOAc) afforded the title compound **S5** (659 mg, 2.19 mmol, 99%) as a white solid (mp: 73−75 °C).

TLC (5:1 petroleum ether/EtOAc, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.46−6.34 (m, 1H), 6.23−6.09 (m, 2H), 5.27 (dd, J = 17.2, 1.2 Hz, 1H), 5.19 (dd, J = 10.1, 1.2 Hz, 1H), 3.78 (s, 6H), 2.99 (s, 2H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 169.5 (2C), 136.2 (CH), 133.1 (CH), 128.5 (CH), 119.2 (CH_2), 74.9 (C), 59.0 (C), 53.3 ($2CH_3$), 41.7 (C), 26.7 (CH_2).

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{12}H_{14}BrO_4^+$: 301.0070; found: 301.0070.



Dimethyl (*E*)-2-(3-methylbuta-1,3-dien-1-yl)-2-(8-methylnona-2,4-diyn-1-yl)malonate (16a)

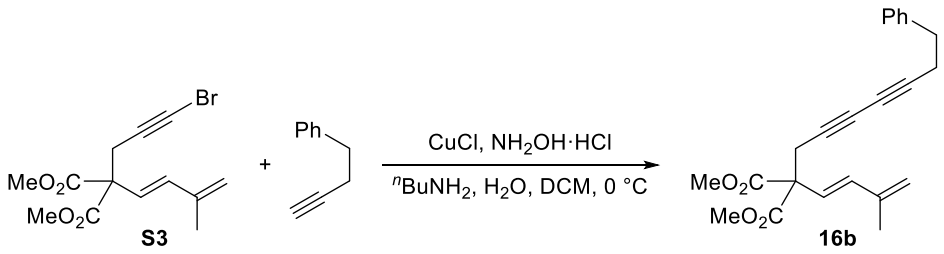
To a stirred solution of CuCl (99 mg, 1.0 mmol, 1.0 equiv) and $NH_2OH{\cdot}HCl$ (70 mg, 1.0 mmol, 1.0 equiv) in 30% ^{n}BuNH$_2$/H_2O (5 mL) was added dropwise a solution of 5-methylhex-1-yne (192 mg, 2.00 mmol, 2.0 equiv) in DCM (5 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred at 0 °C for 5 min. Then, a solution of bromoalkyne **S3** (315 mg, 1.00 mmol, 1.0 equiv) in DCM (5 mL) was added dropwise. The resulting mixture was stirred at 0 °C for 1 h, quenched with saturated aqueous NH_4Cl solution (30 mL), and extracted with EtOAc (30 mL × 2). The combined organic phases were successively washed with water (50 mL) and brine (50 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 30:1 petroleum ether/EtOAc) afforded the title compound **16a** (227 mg, 0.687 mmol, 69%) as a pale yellow oil.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.6.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.23 (d, J = 16.4 Hz, 1H), 6.12 (d, J = 16.4 Hz, 1H), 5.08−5.05 (m, 1H), 5.04−4.99 (m, 1H), 3.78 (s, 6H), 3.05 (s, 2H), 2.24 (t, J = 7.4 Hz, 2H), 1.93−1.88 (m, 3H), 1.66 (apparent nonet, J = 6.8 Hz, 1H), 1.40 (apparent q, J = 7.2 Hz, 2H), 0.88 (d, J = 6.6 Hz, 6H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 169.7 (2C), 141.3 (C), 135.1 (CH), 124.8 (CH), 118.5 (CH_2), 78.9 (C), 71.2 (C), 68.2 (C), 65.0 (C), 59.1 (C), 53.3 ($2CH_3$), 37.1 (CH_2), 27.3 (CH), 26.6 (CH_2), 22.2 ($2CH_3$), 18.6 (CH_3), 17.3 (CH_2).

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{20}H_{27}O_4^+$: 331.1904; found: 331.1908.



Dimethyl (*E*)-2-(3-methylbuta-1,3-dien-1-yl)-2-(7-phenylhepta-2,4-diyn-1-yl)malonate (16b)

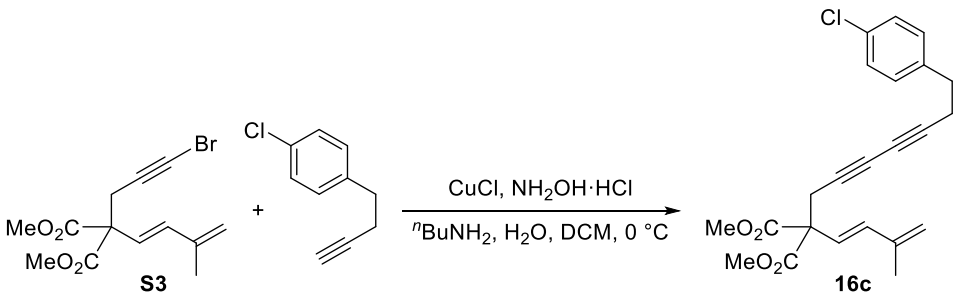
To a stirred solution of CuCl (99 mg, 1.0 mmol, 1.0 equiv) and $NH_2OH{\cdot}HCl$ (70 mg, 1.0 mmol, 1.0 equiv) in 30% $^nBuNH_2/H_2O$ (5 mL) was added dropwise a solution of but-3-yn-1-ylbenzene (260 mg, 2.00 mmol, 2.0 equiv) in DCM (1 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred at 0 °C for 5 min. Then, a solution of bromoalkyne **S3** (316 mg, 1.00 mmol, 1.0 equiv) in DCM (4 mL) was added dropwise. The resulting mixture was stirred at 0 °C for 1 h, quenched with saturated aqueous NH_4Cl solution (20 mL), and extracted with EtOAc (20 mL × 3). The combined organic phases were successively washed with water (50 mL) and brine (50 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 30:1 petroleum ether/EtOAc) afforded the title compound **16b** (326 mg, 0.895 mmol, 90%) as a pale yellow oil.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.33−7.26 (m, 2H), 7.24−7.16 (m, 3H), 6.23 (d, J = 16.4 Hz, 1H), 6.12 (d, J = 16.4 Hz, 1H), 5.08−5.05 (m, 1H), 5.04−5.00 (m, 1H), 3.78 (s, 6H), 3.05 (s, 2H), 2.82 (t, J = 7.6 Hz, 2H), 2.52 (t, J = 7.6 Hz, 2H), 1.93−1.88 (m, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 169.7 (2C), 141.3 (C), 140.2 (C), 135.2 (CH), 128.6 (2CH), 128.5 (2CH), 126.6 (CH), 124.8 (CH), 118.6 (CH_2), 77.7 (C), 71.8 (C), 68.1 (C), 65.8 (C), 59.1 (C), 53.3 ($2CH_3$), 34.7 (CH_2), 26.7 (CH_2), 21.6 (CH_2), 18.6 (CH_3).

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{23}H_{25}O_4^+$: 365.1747; found: 365.1744.



Dimethyl (*E*)-2-(7-(4-chlorophenyl)hepta-2,4-diyn-1-yl)-2-(3-methylbuta-1,3-dien-1-yl)malonate (16c)

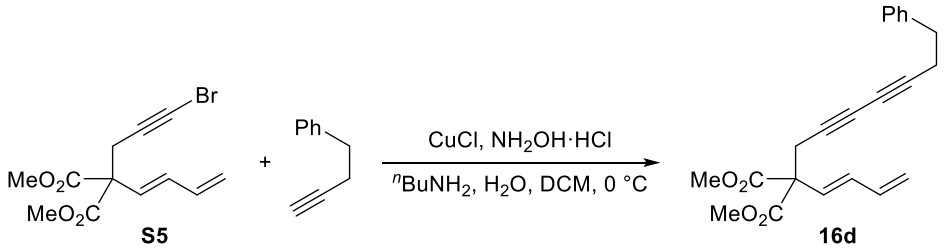
To a stirred solution of CuCl (99 mg, 1.0 mmol, 1.0 equiv) and $NH_2OH{\cdot}HCl$ (70 mg, 1.0 mmol, 1.0 equiv) in 30% $^nBuNH_2/H_2O$ (5 mL) was added dropwise a solution of 1-(but-3-yn-1-yl)-4-chlorobenzene[4] (165 mg, 1.00 mmol, 1.0 equiv) in DCM (2 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred at 0 °C for 5 min. Then, a solution of bromoalkyne **S3** (378 mg, 1.20 mmol, 1.2 equiv) in DCM (3 mL) was added dropwise. The resulting mixture was stirred at 0 °C for 1 h, quenched with saturated aqueous NH_4Cl solution (30 mL), and extracted with Et_2O (30 mL × 2). The combined organic phases were successively washed with water (50 mL) and brine (50 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 40:1 petroleum ether/EtOAc) afforded the title compound **16c** (311 mg, 0.780 mmol, 78%) as an off-white solid (mp: 59−61 °C).

TLC (5:1 petroleum ether/EtOAc, R_f): 0.5.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.26 (d, J = 8.3 Hz, 2H), 7.12 (d, J = 8.3 Hz, 2H), 6.23 (d, J = 16.4 Hz, 1H), 6.12 (d, J = 16.4 Hz, 1H), 5.07 (s, 1H), 5.02 (s, 1H), 3.78 (s, 6H), 3.05 (s, 2H), 2.78 (t, J = 7.4 Hz, 2H), 2.50 (t, J = 7.4 Hz, 2H), 1.90 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 169.7 (2C), 141.3 (C), 138.6 (C), 135.2 (CH), 132.4 (C), 129.9 (2CH), 128.7 (2CH), 124.7 (CH), 118.6 (CH_2), 77.2 (C), 72.0 (C), 68.0 (C), 66.2 (C), 59.1 (C), 53.3 ($2CH_3$), 33.9 (CH_2), 26.6 (CH_2), 21.5 (CH_2), 18.6 (CH_3).

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{23}H_{24}ClO_4^+$: 399.1358; found: 399.1363.



Dimethyl (*E*)-2-(buta-1,3-dien-1-yl)-2-(7-phenylhepta-2,4-diyn-1-yl)malonate (16d)

To a stirred solution of CuCl (99 mg, 1.0 mmol, 1.0 equiv) and $NH_2OH{\cdot}HCl$ (70 mg, 1.0 mmol, 1.0 equiv) in 30% ^{n}BuNH$_2$/H_2O (5 mL) was added dropwise a solution of but-3-yn-1-ylbenzene (130 mg, 1.00 mmol, 1.0 equiv) in DCM (2 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred at 0 °C for 5 min. Then, a solution of bromoalkyne **S5** (362 mg, 1.20 mmol, 1.2 equiv) in DCM (3 mL) was added dropwise. The resulting mixture was stirred at 0 °C for 1 h, quenched with saturated aqueous NH_4Cl solution (30 mL), and extracted with Et_2O (30 mL × 2). The combined organic phases were successively washed with water (50 mL) and brine (50 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation. Purification of the crude product by flash column chromatography (silica gel, 40:1 petroleum ether/EtOAc) afforded the title compound **16d** (275 mg, 0.785 mmol, 79%) as a pale yellow oil.

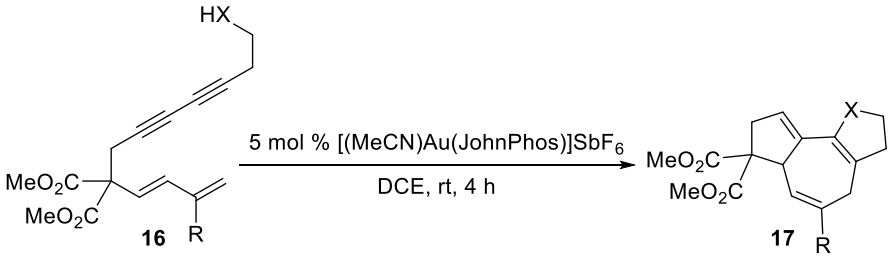
TLC (5:1 petroleum ether/EtOAc, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.32−7.26 (m, 2H), 7.24−7.16 (m, 3H), 6.46−6.33 (m, 1H), 6.23−6.09 (m, 2H), 5.26 (d, J = 16.8 Hz, 1H), 5.19 (d, J = 10.0 Hz, 1H), 3.77 (s, 6H), 3.04 (s, 2H), 2.82 (t, J = 7.6 Hz, 2H), 2.52 (t, J = 7.6 Hz, 2H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 169.5 (2C), 140.2 (C), 136.2 (CH), 133.2 (CH), 128.6 (2CH), 128.53 (CH), 128.47 (2CH), 126.6 (CH), 119.2 (CH_2), 77.8 (C), 71.7 (C), 68.2 (C), 65.8 (C), 59.2 (C), 53.3 ($2CH_3$), 34.7 (CH_2), 26.4 (CH_2), 21.5 (CH_2).

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{22}H_{23}O_4^+$: 351.1591; found: 351.1587.

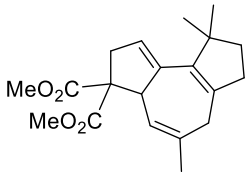
S6. General Procedure for the Gold-Catalyzed Cycloisomerization



To a stirred solution of dienediyne **16** (0.10 mmol, 1.0 equiv) in DCE (1.0 mL) was added a solution of [(MeCN)Au(JohnPhos)]SbF_6 (3.9 mg, 0.0051 mmol, 5 mol %) in DCE (1.0 mL) at room temperature under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 4 h, quenched with Et_3N (0.1 mL), and then directly loaded on neutral Al_2O_3. Purification by flash column chromatography (neutral Al_2O_3, DCM or 40:1 petroleum ether/EtOAc) afforded the polycyclic product **17**.

Notes: Polycyclic products **17a**−**17d** are fairly stable in dilute solutions. However, they slowly decomposed upon concentration.

S7. Characterization of Products



Dimethyl 5,9,9-trimethyl-2,3a,6,7,8,9-hexahydro-3*H*-cyclopenta[*e*]azulene-3,3-dicarboxylate (17a)

Following the general procedure with dienediyne **16a** on 0.10 mmol scale. Purification by flash column chromatography (neutral Al_2O_3, DCM) afforded the title compound **17a** as a yellow oil.

Run 1: dienediyne **16a** (33.3 mg) was converted into the title compound **17a** (30.7 mg, 92%).

Run 2: dienediyne **16a** (33.2 mg) was converted into the title compound **17a** (29.9 mg, 90%).

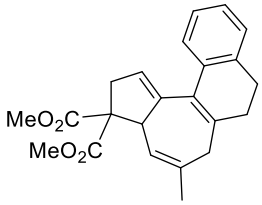
The average yield of two runs was 91%.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.7.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 5.33 (s, 1H), 5.31−5.27 (m, 1H), 4.32−4.27 (m, 1H), 3.75 (s, 3H), 3.73 (s, 3H), 3.44−3.32 (m, 2H), 2.86−2.78 (m, 1H), 2.42 (d, J = 18.6 Hz, 1H), 2.37−2.20 (m, 2H), 1.73−1.70 (m, 3H), 1.65−1.59 (m, 2H), 1.15 (s, 3H), 1.10 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, δ): 172.6 (C), 171.2 (C), 139.3 (C), 138.1 (C), 137.0 (C), 135.8 (C), 122.1 (CH), 116.4 (CH), 63.1 (C), 52.9 (CH_3), 52.7 (CH_3), 52.3 (CH), 48.1 (C), 40.3 (CH_2), 39.6 (CH_2), 36.6 (CH_2), 36.0 (CH_2), 27.6 (CH_3), 27.3 (CH_3), 25.8 (CH_3).

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{20}H_{27}O_4^+$: 331.1904; found: 331.1895.



Dimethyl 5-methyl-3a,6,7,8-tetrahydronaphtho[1,2-*e*]azulene-3,3(2*H*)-dicarboxylate (17b)

Following the general procedure with dienediyne **16b** on 0.10 mmol scale. Purification by flash column chromatography (neutral Al_2O_3, 40:1 petroleum ether/EtOAc) afforded the title compound **17b** as a pale yellow oil.

Run 1: dienediyne **16b** (36.1 mg) was converted into the title compound **17b** (33.1 mg, 92%).

Run 2: dienediyne **16b** (36.7 mg) was converted into the title compound **17b** (34.0 mg, 93%).

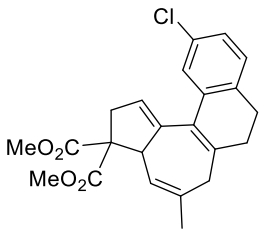
The average yield of two runs was 93%.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.6.

^{1}H NMR (400 MHz, CD_2Cl_2, δ): 7.20−7.16 (m, 1H), 7.13−7.03 (m, 3H), 5.51 (apparent q, J = 2.3 Hz, 1H), 5.38−5.34 (m, 1H), 4.22−4.17 (m, 1H), 3.77 (s, 3H), 3.68 (s, 3H), 3.35 (d, J = 16.0 Hz, 1H), 3.22 (apparent dt, J = 17.2, 2.2 Hz, 1H), 2.89−2.77 (m, 2H), 2.75−2.67 (m, 1H), 2.54−2.44 (m, 1H), 2.42 (d, J = 16.0 Hz, 1H), 2.29−2.20 (m, 1H), 1.78 (s, 3H).

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2, δ): 172.8 (C), 171.8 (C), 140.5 (C), 139.3 (C), 137.7 (C), 135.8 (C), 135.5 (C), 129.5 (C), 127.5 (CH), 126.5 (CH), 126.4 (CH), 125.3 (CH), 124.5 (CH), 122.6 (CH), 65.0 (C), 53.0 (CH_3), 52.8 (CH), 52.4 (CH_3), 39.20 (CH_2), 39.19 (CH_2), 31.6 (CH_2), 28.8 (CH_2), 27.3 (CH_3).

HRMS (ESI−FTICR, m/z): $[M + H]^+$ calculated for $C_{23}H_{25}O_4^+$: 365.1747; found: 365.1744.



Dimethyl 11-chloro-5-methyl-3a,6,7,8-tetrahydronaphtho[1,2-*e*]azulene-3,3(2*H*)-dicarboxylate (17c)

Following the general procedure with dienediyne **16c** on 0.10 mmol scale. Purification by flash column chromatography (neutral Al_2O_3, DCM) afforded the title compound **17c** as a pale yellow amorphous solid.

Run 1: dienediyne **16c** (40.0 mg) was converted into the title compound **17c** (37.2 mg, 93%).

Run 2: dienediyne **16c** (39.5 mg) was converted into the title compound **17c** (36.9 mg, 93%).

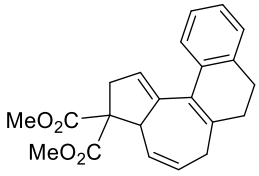
The average yield of two runs was 93%.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.6.

^{1}H NMR (600 MHz, $CDCl_3$, δ): 7.13 (d, J = 1.8 Hz, 1H), 7.03 (dd, J = 7.9, 1.8 Hz, 1H), 7.00 (d, J = 7.9 Hz, 1H), 5.59−5.55 (m, 1H), 5.41−5.37 (m, 1H), 4.23−4.20 (m, 1H), 3.82 (s, 3H), 3.69 (s, 3H), 3.40 (d, J = 15.8 Hz, 1H), 3.26 (apparent dt, J = 17.3, 2.1 Hz, 1H), 2.90 (apparent dt, J = 17.3, 2.2 Hz, 1H), 2.81−2.74 (m, 1H), 2.72−2.66 (m, 1H), 2.54−2.46 (m, 1H), 2.35 (d, J = 15.8 Hz, 1H), 2.28−2.21 (m, 1H), 1.77 (s, 3H).

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$, δ): 172.6 (C), 171.7 (C), 140.6 (C), 139.6 (C), 137.22 (C), 137.19 (C), 133.3 (C), 132.0 (C), 128.5 (CH, C), 125.8 (CH), 125.7 (CH), 124.2 (CH), 122.6 (CH), 64.7 (C), 52.9 (CH_3), 52.5 (CH), 52.3 (CH_3), 39.0 (CH_2), 38.9 (CH_2), 31.2 (CH_2), 27.9 (CH_2), 27.4 (CH_3).

HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{23}H_{24}ClO_4^+$: 399.1358; found: 399.1353.



Dimethyl 3a,6,7,8-tetrahydronaphtho[1,2-*e*]azulene-3,3(2*H*)-dicarboxylate (17d)

Following the general procedure with dienediyne **16d** on 0.10 mmol scale. Purification by flash column chromatography (neutral Al_2O_3, DCM) afforded the title compound **17d** as an off-white solid [mp: 88 °C (dec)].

Run 1: dienediyne **16d** (35.1 mg) was converted into the title compound **17d** (32.8 mg, 93%).

Run 2: dienediyne **16d** (34.9 mg) was converted into the title compound **17d** (33.1 mg, 95%).

The average yield of two runs was 94%.

TLC (5:1 petroleum ether/EtOAc, R_f): 0.6.

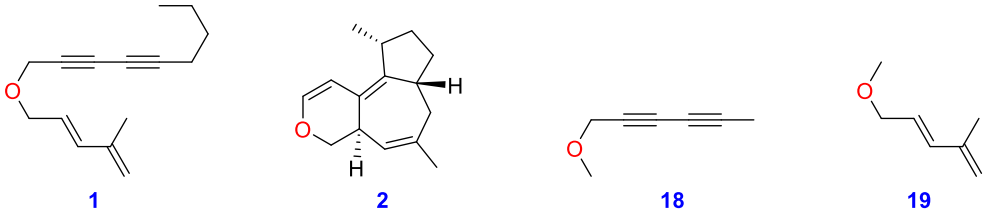
^1H NMR (600 MHz, $CDCl_3$, δ): 7.18 (d, J = 7.5 Hz, 1H), 7.14−7.06 (m, 3H), 5.85−5.79 (m, 1H), 5.59 (ddd, J = 11.1, 4.1, 2.6 Hz, 1H), 5.54 (apparent q, J = 2.2 Hz, 1H), 4.28−4.23 (m, 1H), 3.81 (s, 3H), 3.72 (s, 3H), 3.38 (d, J = 17.3 Hz, 1H), 3.31 (apparent dt, J = 17.4, 2.2 Hz, 1H), 2.89 (apparent dt, J = 17.4, 2.3 Hz, 1H), 2.87−2.80 (m, 1H), 2.72 (ddd, J = 15.2, 6.4, 4.3 Hz, 1H), 2.54−2.44 (m, 2H), 2.20 (ddd, J = 16.8, 6.7, 4.3 Hz, 1H).

$^{13}C\{^1H\}$ NMR (151 MHz, $CDCl_3$, δ): 172.6 (C), 171.4 (C), 140.4 (C), 139.1 (C), 135.8 (C), 135.0 (C), 129.6 (C), 128.9 (CH), 128.6 (CH), 127.3 (CH), 126.4 (CH), 126.2 (CH), 125.6 (CH), 124.4 (CH), 64.7 (C), 53.0 (CH_3), 52.4 (CH_3, CH), 39.2 (CH_2), 33.9 (CH_2), 31.0 (CH_2), 28.6 (CH_2).

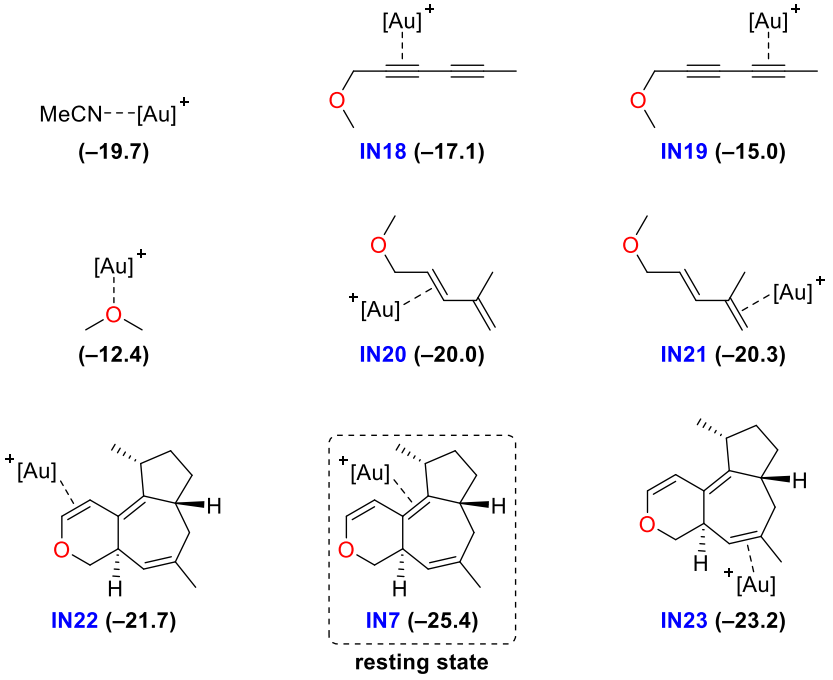
HRMS (ESI−FTICR, *m*/*z*): $[M + H]^+$ calculated for $C_{22}H_{23}O_4^+$: 351.1591; found: 351.1591.

S8. Additional Computational Results

Discussion on the Resting State of the Catalytic System. Cationic gold complexes may undergo facile intermolecular ligand exchange via an associative mechanism.[5] Therefore, to shed light on the resting state of the catalytic tricyclization of oxygen-tethered substrate **1**, we, in principle, have to consider all possible complexes of $[Au(PMe_3)]^+$ with MeCN, substrate **1**, and product **2**. For $[(MeCN)Au(PMe_3)]^+$ and gold−product complexes, we have located all the possible isomers. However, due to the conformational flexibility of the substrate, there are hundreds of gold−substrate complexes. To simplify the computations without sacrificing the understanding of the reaction mechanism, we used three model compounds, namely, dimethyl ether, 1-methoxyhexa-2,4-diyne (**18**), and (*E*)-5-methoxy-2-methylpenta-1,3-diene (**19**) to estimate the complexation ability of the ether, alkyne, and alkene moieties in substrate **1**, respectively. Among all these complexes, the most stable one, i.e., the resting state of the catalytic system, is gold−product complex **IN7**, in which the tetrasubstituted alkene coordinates to the gold center.



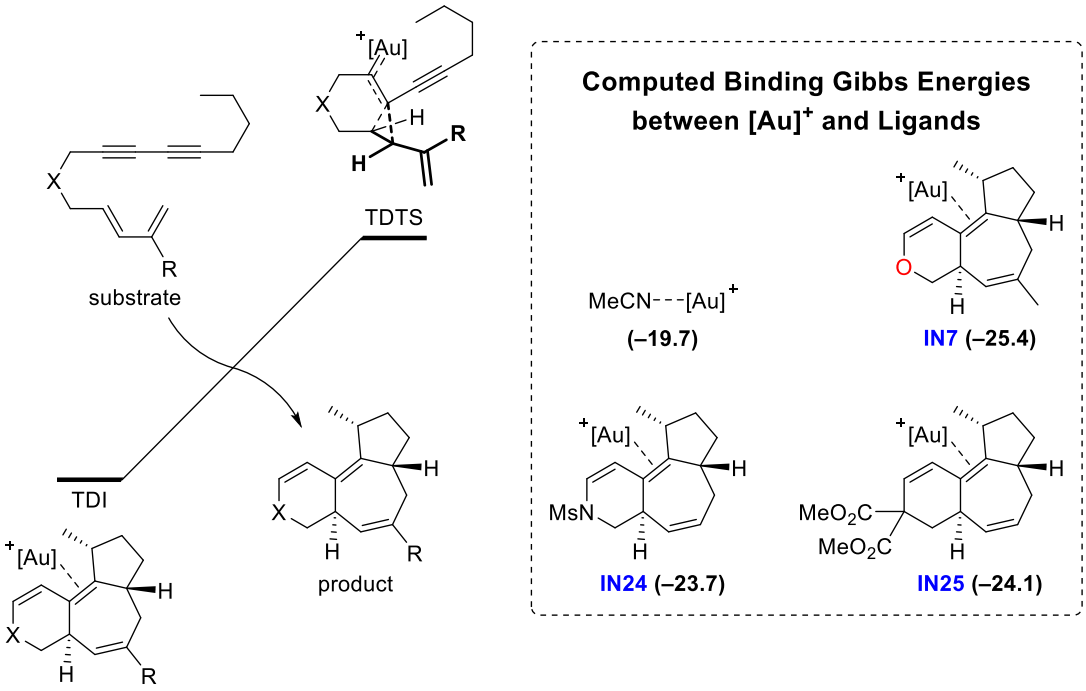
Computed Binding Gibbs Energies between $[Au]^+$ and Ligands



Computed at the SMD(DCE)/BMK-D3(BJ)/def2-TZVPP//SMD(DCE)/PBE0/SDD-6-311G(d,p) level. Relative Gibbs energies are reported in kcal/mol. [Au] = $[Au(PMe_3)]$.

Additional Discussion on the Tethering Effect. To shed more light on the tethering effect, we computed the overall activation Gibbs energies for the gold-catalyzed tricyclization of oxygen-tethered substrate **1**, model nitrogen-tethered substrate **14** (the *N*-mesyl analog of real substrate **5**), and malonate-tethered substrate **7** (Table S1). For nitrogen- and carbon-tethered substrates, we assumed that the TOF-determining transition state (TDTS; TOF = turnover frequency) and the TOF-determining intermediate (TDI) are similar to those of the oxygen-tethered substrate. DFT calculations suggested that the catalytic tricyclization of oxygen-, nitrogen-, and carbon-tethered substrates may all take place under mild conditions because the predicted overall activation Gibbs energies are not high (21–25 kcal/mol). Based on these results and the discussion in the main text (Table 1), we concluded that the undesired regioselectivity (5-*exo*-dig cyclization) of the cyclopropanation step, rather than the low reactivity, might be the reason why carbon-tethered substrate **7** failed to give the desired tricyclic product **8** under gold catalysis.

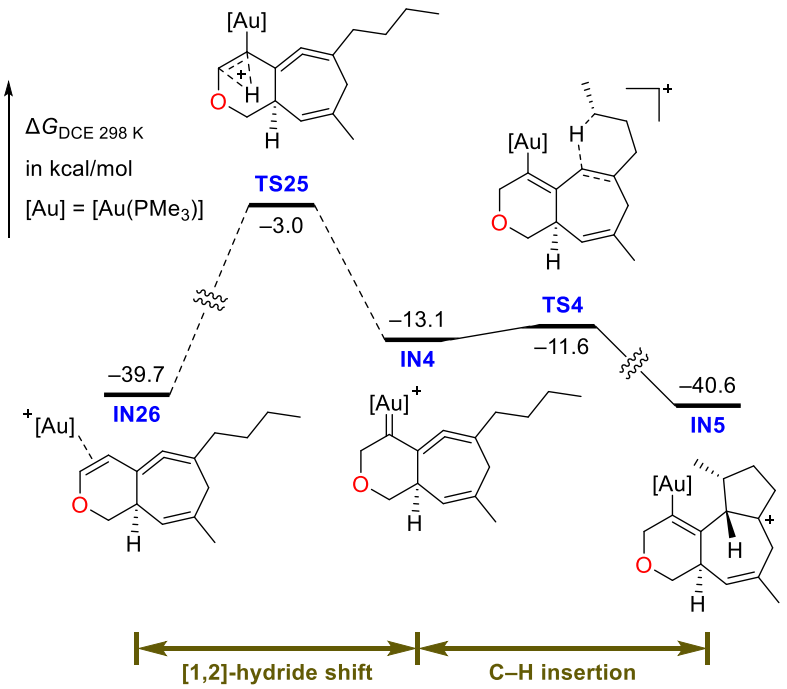
Table S1. Overall Activation Gibbs Energies for Gold-Catalyzed Tricyclization of Oxygen-, Nitrogen-, and Carbon-Tethered Substrates



entry	X	R	substrate	product	TDTS	TDI	ΔG_{rxn}	overall $\Delta G^{\ddagger}$
1	O	Me	**1**	**2**	**TS1**	**IN7**	−79.4	21.1
2	NMs	H	**14**	**20**	**TS16**	**IN24**	−77.5	22.1
3	$C(CO_2Me)_2$	H	**7**	**8**	**TS18**	**IN25**	−69.5	25.3

[a]Computed at the SMD(DCE)/BMK-D3(BJ)/def2-TZVPP//SMD(DCE)/PBE0/SDD-6-311G(d,p) level. Relative Gibbs energies are reported in kcal/mol. [Au] = [Au(PMe_3)]. ΔG_{rxn} = ΔG(product−substrate). Overall $\Delta G^{\ddagger}$ = ΔG(TDTS−TDI) + ΔG_{rxn}.

Discussion on the [1,2]-Hydride Shift of IN4. Other than aliphatic C–H insertion, gold carbene **IN4** may also undergo a [1,2]-hydride shift. DFT calculations suggested that the [1,2]-hydride shift transition state **TS25** is disfavored over the C–H insertion transition state **TS4** by 8.6 kcal/mol (computed at the SMD(DCE)/BMK-D3(BJ)/def2-TZVPP//SMD(DCE)/PBE0/SDD-6-311G(d,p) level). Thus the [1,2]-hydride shift of **IN4** may not take place.



S9. Computed Energies of the Stationary Points

Table S2. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs)

stationary point	solvent	TCG[a,b] (a.u.)	SPE[a] (a.u.)	SPE[c] (a.u.)	page
MeCN	DCE	0.021435	−132.634279	−132.731566	S20
Me_2O	DCE	0.054032	−154.884287	−154.994695	S20
propadiene	DCE	0.032287	−116.539114		S20
1	DCE	0.264062	−658.079410	−658.525238	S20
2	DCE	0.278394	−658.209589	−658.666162	S20
7	DCE	0.337279	−1038.312611	−1039.048733	S21
8	DCE	0.352160	−1038.428859	−1039.174394	S21
14	DCE	0.283645	−1186.576413	−1187.207235	S22
18	DCE	0.094186	−346.323694	−346.561775	S23
19	DCE	0.140177	−348.814876	−349.055220	S23
20	DCE	0.297731	−1186.703505	−1187.344787	S23

$[Au(PMe_3)]^+$	DCE	0.081607	−596.477673	−596.031280	S24
$[(MeCN)Au(PMe_3)]^+$	DCE	0.122931	−729.155364	−728.811127	S24
$[(Me_2O)Au(PMe_3)]^+$	DCE	0.157237	−751.394975	−751.064374	S24
IN1	DCE	0.369066	−1254.588312	−1254.602205	S24
IN2	DCE	0.372966	−1254.602053	−1254.616152	S25
IN3	DCE	0.373384	−1254.602991	−1254.616924	S26
IN4	DCE	0.376434	−1254.622318	−1254.636564	S26
IN5	DCE	0.379542	−1254.662672	−1254.683479	S27
IN6	DCE	0.381907	−1254.684589	−1254.705902	S27
IN7	DCE	0.384373	−1254.728808	−1254.759319	S28
IN8	DCE	0.381508	−1254.670792	−1254.692201	S29
IN9	DCE	0.376700	−1254.624411	−1254.638673	S29
IN10	DCE	0.376509	−1254.618292	−1254.636408	S30
IN11	DCE	0.379225	−1254.660217	−1254.681796	S31
IN12	DCE	0.375689	−1254.616128	−1254.634027	S31
IN13	DCE	0.380482	−1254.647431	−1254.670826	S32
IN14	DCE	0.374753	−1254.645798	−1254.660136	S33
IN15 (Table 2, entry 1)	DCM	0.382187	−1556.032254	−1556.275012	S33
IN15 (Table 2, entry 2)	DCM	0.304125	−1325.197365	−1325.276404	S34
IN15 (Table 2, entry 3)	DCM	0.342784	−1328.341698	−1328.409614	S34
IN15 (Table 2, entry 4)	DCM	0.264663	−1097.500089	−1097.408892	S35
IN16 (Table 2, entry 1)	DCM	0.384675	−1556.029344	−1556.279097	S36
IN16 (Table 2, entry 2)	DCM	0.307520	−1325.205912	−1325.290189	S36
IN16 (Table 2, entry 3)	DCM	0.346218	−1328.347765	−1328.420018	S37
IN16 (Table 2, entry 4)	DCM	0.268738	−1097.518012	−1097.427768	S37
IN17 (Table 2, entry 1)	DCM	0.382571	−1556.078280	−1556.319679	S38
IN17 (Table 2, entry 2)	DCM	0.305886	−1325.243521	−1325.323680	S39
IN17 (Table 2, entry 3)	DCM	0.344843	−1328.383971	−1328.452093	S39
IN17 (Table 2, entry 4)	DCM	0.266434	−1097.542725	−1097.452312	S40
IN18	DCE	0.197643	−942.835244	−942.639068	S40
IN19	DCE	0.197834	−942.832690	−942.635994	S41
IN20	DCE	0.245523	−945.333540	−945.139124	S41
IN21	DCE	0.245620	−945.335652	−945.139722	S41
IN22	DCE	0.384824	−1254.730645	−1254.753898	S42
IN23	DCE	0.385008	−1254.729519	−1254.756401	S42
IN24	DCE	0.403868	−1783.220376	−1783.435371	S43
IN25	DCE	0.458385	−1634.945715	−1635.265638	S44
IN26	DCE	0.377973	−1254.661755	−1254.680412	S45

TS1	DCE	0.370679	−1254.572510	−1254.585536	S45
TS2	DCE	0.373965	−1254.592597	−1254.604700	S46
TS3	DCE	0.374089	−1254.592822	−1254.605414	S46
TS4	DCE	0.376016	−1254.618118	−1254.633811	S47
TS4-JohnPhos	DCE	0.668018	−1912.634390	−1913.138020	S48
TS5	DCE	0.378068	−1254.660895	−1254.680639	S49
TS6	DCE	0.380613	−1254.666662	−1254.687438	S49
TS7	DCE	0.376161	−1254.618813	−1254.634946	S50
TS7-JohnPhos	DCE	0.668288	−1912.633834	−1913.135629	S51
TS8	DCE	0.375939	−1254.609957	−1254.623883	S52
TS9	DCE	0.376676	−1254.616959	−1254.631887	S52
TS10	DCE	0.377796	−1254.616913	−1254.636342	S53
TS11	DCE	0.376112	−1254.615840	−1254.633637	S54
TS12	DCE	0.378053	−1254.609462	−1254.629550	S54
TS13	DCE	0.374492	−1254.603294	−1254.619883	S55
TS14	DCE	0.376345	−1254.607213	−1254.623887	S56
TS15	DCE	0.369703	−1254.566574	−1254.578880	S56
TS16	DCE	0.390060	−1783.065968	−1783.262857	S57
TS17	DCE	0.390763	−1783.061302	−1783.261123	S58
TS18	DCE	0.444592	−1634.796872	−1635.100722	S58
TS19	DCE	0.444188	−1634.801803	−1635.105547	S59
TS20	DCE	0.415590	−1595.523595	−1595.797745	S60
TS21	DCE	0.415265	−1595.510048	−1595.784176	S60
TS22	DCE	0.371635	−1254.588501	−1254.599279	S61
TS23 (Table 2, entry 1)	DCM	0.382513	−1556.000203	−1556.248238	S62
TS23 (Table 2, entry 2)	DCM	0.305888	−1325.178019	−1325.259538	S63
TS23 (Table 2, entry 3)	DCM	0.344218	−1328.321914	−1328.394233	S63
TS23 (Table 2, entry 4)	DCM	0.267309	−1097.489116	−1097.398180	S64
TS24 (Table 2, entry 1)	DCM	0.379601	−1556.018999	−1556.258993	S64
TS24 (Table 2, entry 2)	DCM	0.302883	−1325.184986	−1325.261032	S65
TS24 (Table 2, entry 3)	DCM	0.340645	−1328.326250	−1328.390101	S65
TS24 (Table 2, entry 4)	DCM	0.263089	−1097.485280	−1097.390416	S66
TS25	DCE	0.374166	−1254.606442	−1254.618166	S67

[a]Computed at the SMD/PBE0/SDD-6-311G(d,p) level.

[b]A standard state at 1 atm and 298 K was used.

[c]Computed at the SMD/BMK-D3(BJ)/def2-TZVPP//SMD/PBE0/SDD-6-311G(d,p) level.

S10. Cartesian Coordinates of the Stationary Points

MeCN

N	1.427491	0.000015	−0.000078
C	0.275245	−0.000048	0.000178
C	−1.170030	0.000020	−0.000083
H	−1.541330	−0.061753	1.025263
H	−1.541285	−0.857224	−0.566129
H	−1.541107	0.919040	−0.459159

Me_2O

O	0.000000	−0.593746	0.000000
C	1.160648	0.195826	−0.000001
C	−1.160648	0.195826	0.000001
H	2.020980	−0.477190	0.000040
H	1.216190	0.838636	0.891879
H	1.216225	0.838585	−0.891914
H	−2.020980	−0.477190	−0.000059
H	−1.216181	0.838652	−0.891868
H	−1.216234	0.838569	0.891924

propadiene

C	0.000000	0.000000	1.302474
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	−1.302474
H	0.000000	0.930923	1.864598
H	0.000000	−0.930923	1.864598
H	−0.930923	0.000000	−1.864598
H	0.930923	0.000000	−1.864598

1

O	2.265947	−2.269479	0.872872
C	−7.136355	1.382296	1.339701
C	−6.520534	0.911841	0.030534
C	−5.081713	0.440701	0.194620
C	−4.478949	−0.042213	−1.130884
C	−3.113167	−0.511359	−0.998339
C	−1.972299	−0.900342	−0.866103
C	−0.689953	−1.342256	−0.723263
C	0.452613	−1.730377	−0.606557
C	1.823025	−2.215927	−0.465625
C	2.504866	−0.989865	1.452110
C	3.690859	−0.300417	0.860932
C	3.656313	0.942502	0.365334
C	4.793529	1.673300	−0.193181
C	4.612874	2.923365	−0.642658
C	6.132138	1.000193	−0.249273
H	−8.169698	1.713302	1.198231
H	−6.574179	2.221667	1.762996
H	−7.143395	0.579721	2.085075
H	−7.121624	0.094095	−0.386621
H	−6.552563	1.724750	−0.705750
H	−4.465884	1.255096	0.593071
H	−5.039117	−0.374913	0.925338
H	−5.093025	−0.853548	−1.541640
H	−4.505333	0.770714	−1.867525
H	2.486992	−1.594038	−1.083258
H	1.882552	−3.238402	−0.850192
H	2.679068	−1.200108	2.512187
H	1.610453	−0.356400	1.378216
H	4.619547	−0.869021	0.867075
H	2.707503	1.479667	0.370913
H	3.638485	3.401995	−0.595752
H	5.430661	3.498442	−1.066808
H	6.881776	1.657512	−0.694164
H	6.086959	0.079323	−0.840924
H	6.473776	0.717327	0.752469

2

O	−3.502223	−1.031197	0.066338
C	1.769887	−2.600252	0.915193
C	1.634858	−1.798986	−0.386067
C	2.989664	−1.186433	−0.775700
C	3.008768	0.140675	−0.025366
C	1.586319	0.666859	−0.231512
C	0.724605	−0.583644	−0.220166
C	−0.614304	−0.659153	−0.070323
C	−1.308048	−1.944049	−0.118912
C	−2.640042	−2.064668	−0.004072
C	−2.929781	0.204569	−0.345688
C	−1.564309	0.480837	0.284098
C	−1.197816	1.904767	−0.043286

C	−0.038165	2.520398	0.194369	C	−1.096430	−0.145661	1.184615
C	1.159548	1.779220	0.724104	C	−2.128265	−0.366073	0.057289
C	0.158301	3.971381	−0.120236	C	−2.063100	0.739644	−1.017020
H	2.416684	−3.470699	0.760077	C	−2.371041	2.105472	−0.498746
H	0.804995	−2.958983	1.281851	C	−1.522358	3.140464	−0.547999
H	2.214035	−1.990311	1.708288	C	−1.845371	4.473358	−0.072364
H	1.265084	−2.468719	−1.170124	C	−1.005605	5.511762	−0.126992
H	3.828916	−1.843125	−0.528084	H	−6.361673	−1.204268	−0.598329
H	3.022488	−0.995963	−1.854760	H	−6.137577	0.121461	0.580694
H	3.200155	−0.021997	1.042286	H	−5.851972	−1.569599	1.078063
H	3.764737	0.840027	−0.393748	H	−2.004466	−4.693988	0.630796
H	1.550984	1.080690	−1.251558	H	−0.810873	−4.152621	−0.587108
H	−0.744308	−2.863296	−0.214577	H	−2.539737	−4.256528	−1.019301
H	−3.147453	−3.023087	0.040232	H	9.725639	−0.099482	0.578682
H	−3.647603	0.974052	−0.058017	H	8.586158	−0.863480	1.691938
H	−2.837208	0.196856	−1.440752	H	8.547518	0.887143	1.451257
H	−1.717361	0.413666	1.375148	H	7.853854	0.535171	−0.945696
H	−2.008071	2.503343	−0.460631	H	7.887920	−1.203833	−0.703443
H	0.947041	1.347730	1.710908	H	6.081529	−1.002896	1.016752
H	1.992617	2.477716	0.856469	H	6.053308	0.740566	0.784530
H	−0.746143	4.428452	−0.529849	H	5.427931	0.406414	−1.625967
H	0.972863	4.107231	−0.842785	H	5.447989	−1.334451	−1.389589
H	0.448421	4.526854	0.780302	H	−1.292821	0.828313	1.645226
				H	−1.247606	−0.899134	1.962924
		7		H	−2.773753	0.472100	−1.805879
O	−3.769961	−0.129969	1.832437	H	−1.065620	0.717923	−1.463615
O	−1.578330	−1.886302	−1.758650	H	−3.363217	2.265951	−0.074283
O	−4.428280	−0.768185	−0.212521	H	−0.528563	2.995363	−0.972128
O	−2.035767	−2.706115	0.276208	H	−2.840112	4.609649	0.350816
C	−3.519389	−0.403994	0.688170	H	−0.005954	5.410113	−0.542694
C	−1.881106	−1.721761	−0.607288	H	−1.292393	6.491561	0.241389
C	−5.781053	−0.857331	0.254104				
C	−1.831589	−4.035811	−0.218400			**8**	
C	8.694046	−0.071826	0.942652	O	−2.465624	1.318551	1.670874
C	7.699824	−0.249889	−0.194802	O	−2.751938	−1.541328	−1.876887
C	6.253060	−0.211010	0.278809	O	−3.406479	−0.705698	1.485699
C	5.262047	−0.380741	−0.879642	O	−3.643367	0.453750	−1.380671
C	3.875588	−0.337410	−0.456082	C	−2.569207	0.259991	1.108477
C	2.723853	−0.294587	−0.079180	C	−2.763511	−0.534658	−1.218997
C	1.427139	−0.243729	0.341361	C	−4.220488	−0.420834	2.629349
C	0.276949	−0.197025	0.720709	C	−4.622587	0.260449	−2.408165

C	3.552931	−2.202497	1.261892
C	3.252167	−1.694239	−0.153118
C	4.550558	−1.395064	−0.915890
C	4.891107	0.028908	−0.495436
C	3.531975	0.736794	−0.493932
C	2.534860	−0.346776	−0.125779
C	1.218580	−0.197459	0.131454
C	0.382145	−1.385429	0.327007
C	−0.953447	−1.401151	0.238753
C	−1.764275	−0.184883	−0.117172
C	−0.859880	0.948711	−0.616526
C	0.413697	1.083785	0.239367
C	1.028454	2.437984	0.021465
C	2.291156	2.850157	0.122106
C	3.501611	2.002861	0.356140
H	−4.825843	−1.311288	2.787764
H	−4.860642	0.442075	2.435658
H	−3.596644	−0.226948	3.503988
H	−5.232308	1.162075	−2.406852
H	−5.238911	−0.613318	−2.187698
H	−4.139294	0.133039	−3.378647
H	4.082405	−3.160209	1.217052
H	2.639116	−2.348560	1.844181
H	4.182157	−1.496735	1.813157
H	2.660817	−2.450756	−0.676635
H	5.339418	−2.119192	−0.692261
H	4.365298	−1.426720	−1.995720
H	5.316840	0.039143	0.515111
H	5.608741	0.520123	−1.158158
H	3.313315	1.033431	−1.530428
H	0.876330	−2.327705	0.538066
H	−1.501179	−2.323923	0.396803
H	−1.421656	1.884374	−0.597711
H	−0.577694	0.746669	−1.655847
H	0.053457	1.114500	1.281302
H	0.277950	3.209658	−0.149705
H	2.466576	3.918805	0.011009
H	3.579551	1.726066	1.416578
H	4.396390	2.593295	0.130906

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S	2.982285	−2.118166	0.009679
O	2.921240	−2.844520	1.269889
O	4.225452	−2.088626	−0.746452
N	2.603044	−0.536790	0.360180
C	1.714241	−2.758219	−1.056467
C	−8.202585	0.241363	0.727274
C	−7.175708	0.038823	−0.376583
C	−5.747664	0.009988	0.151546
C	−4.720636	−0.193696	−0.969677
C	−3.353012	−0.219773	−0.489131
C	−2.217179	−0.237343	−0.065184
C	−0.939649	−0.255440	0.411487
C	0.197232	−0.283884	0.830597
C	1.560057	−0.292605	1.355378
C	2.730948	0.456836	−0.714524
C	3.211658	1.760956	−0.168656
C	2.570348	2.922403	−0.343889
C	3.059764	4.199242	0.143314
C	2.425652	5.360202	−0.046042
H	1.994593	−3.782449	−1.309748
H	1.664270	−2.148184	−1.959661
H	0.762790	−2.747714	−0.524445
H	−9.220730	0.258128	0.326769
H	−8.038201	1.187788	1.253609
H	−8.151633	−0.562802	1.469162
H	−7.384045	−0.899180	−0.906538
H	−7.269989	0.840700	−1.119641
H	−5.525784	0.947214	0.674453
H	−5.639467	−0.795401	0.886839
H	−4.928641	−1.133204	−1.497083
H	−4.819096	0.607888	−1.712520
H	1.655290	−1.039734	2.146574
H	1.771235	0.680504	1.811923
H	1.778167	0.587853	−1.243428
H	3.466802	0.068214	−1.423741
H	4.152389	1.732941	0.379910
H	1.626129	2.932019	−0.888892
H	4.001283	4.183037	0.690756
H	1.485571	5.409101	−0.590366
H	2.826857	6.293524	0.335806

18

O	2.928091	0.011153	−0.531784
C	2.996174	1.235346	0.167874
C	2.149446	−0.955094	0.130771
C	0.716528	−0.666311	0.112052
C	−0.470755	−0.425733	0.069807
C	−1.807529	−0.157802	0.030094
C	−2.994825	0.081097	−0.010319
C	−4.411144	0.366346	−0.058626
H	3.648737	1.894560	−0.406967
H	3.419941	1.098564	1.172746
H	2.010175	1.709423	0.261429
H	2.477418	−1.078106	1.174758
H	2.326727	−1.905795	−0.381560
H	−4.715254	0.651925	−1.070465
H	−4.667173	1.186289	0.619412
H	−4.992667	−0.513183	0.235001

19

O	2.144149	0.461355	−0.015842
C	3.549677	0.481545	0.011126
C	1.633926	−0.844038	−0.002951
C	0.145231	−0.842459	−0.002065
C	−0.615934	0.256704	−0.002584
C	−2.078138	0.273370	0.000635
C	−2.726584	1.447262	0.001279
C	−2.820945	−1.029970	0.003608
H	3.863492	1.527151	−0.000374
H	3.979929	−0.026615	−0.864231
H	3.944391	0.003552	0.919535
H	1.997358	−1.392769	0.884303
H	1.997603	−1.410797	−0.878650
H	−0.307451	−1.831892	0.000541
H	−0.124088	1.226682	−0.005070
H	−2.183443	2.388552	−0.000774
H	−3.811537	1.497050	0.003954
H	−3.900182	−0.864194	0.005641
H	−2.564543	−1.630021	0.883881
H	−2.568117	−1.632027	−0.876311

20

S	−3.677604	−0.187769	−0.043180
O	−4.254903	−1.518216	−0.147259
O	−4.258940	0.918357	−0.786064
N	−2.093082	−0.317551	−0.541860
C	−3.621561	0.260202	1.674212
C	2.982758	−2.316257	1.117490
C	2.887957	−1.638652	−0.255076
C	4.279069	−1.216545	−0.750608
C	4.478930	0.156959	−0.122427
C	3.108648	0.821800	−0.284273
C	2.116969	−0.322892	−0.185869
C	0.772565	−0.247890	−0.092002
C	−0.037277	−1.466161	−0.106570
C	−1.373395	−1.477978	−0.249051
C	−1.312575	0.881143	−0.836233
C	−0.089556	0.993321	0.087209
C	0.475797	2.381998	−0.029358
C	1.695260	2.831733	0.259712
C	2.877973	2.003866	0.652371
H	−4.652155	0.330208	2.027757
H	−3.123982	1.225706	1.773629
H	−3.084724	−0.515682	2.221393
H	3.540899	−3.255419	1.040096
H	1.996340	−2.544144	1.530215
H	3.499954	−1.677902	1.840728
H	2.418816	−2.336697	−0.955347
H	5.053557	−1.939887	−0.479251
H	4.276075	−1.124980	−1.842942
H	4.724171	0.060890	0.942163
H	5.275794	0.740323	−0.591712
H	3.053721	1.206695	−1.313750
H	0.445462	−2.429413	−0.004070
H	−1.957413	−2.389544	−0.219054
H	−1.955686	1.755092	−0.730889
H	−0.988910	0.829155	−1.881794
H	−0.495123	0.923083	1.112121
H	−0.269076	3.127890	−0.306006
H	1.855391	3.905511	0.182193
H	2.767902	1.633624	1.680840
H	3.773605	2.633638	0.647005

$[Au(PMe_3)]^+$

Au	0.940590	0.000020	0.000421
P	−1.304246	0.000025	0.000249
C	−1.982057	1.677313	0.019981
C	−1.985192	−0.857082	1.440700
C	−1.978045	−0.820475	−1.464168
H	−1.629949	2.206374	0.907695
H	−3.074893	1.624848	0.033988
H	−1.653164	2.215903	−0.870970
H	−1.643671	−1.894088	1.446283
H	−3.077909	−0.831766	1.391834
H	−1.647500	−0.364099	2.354381
H	−1.636903	−0.304202	−2.363613
H	−3.071144	−0.796593	−1.421144
H	−1.636044	−1.856851	−1.494508

$[(MeCN)Au(PMe_3)]^+$

Au	0.273511	0.006291	−0.006754
P	−2.001830	−0.004055	0.005022
N	2.342623	0.001363	−0.007334
C	3.490446	−0.005072	0.003454
C	4.926839	−0.014093	0.018202
C	−2.718887	1.657893	−0.107640
C	−2.690707	−0.740562	1.512973
C	−2.712104	−0.947247	−1.372092
H	5.280334	−1.001696	0.323794
H	5.287346	0.736803	0.725255
H	5.301794	0.214914	−0.982062
H	−2.378928	2.260924	0.737110
H	−3.810729	1.595279	−0.094093
H	−2.394106	2.135410	−1.034702
H	−2.340883	−1.770648	1.609498
H	−3.783388	−0.728851	1.469127
H	−2.355965	−0.173189	2.384240
H	−2.388694	−0.512740	−2.320493
H	−3.803962	−0.925868	−1.314801
H	−2.364577	−1.981587	−1.322709

$[(Me_2O)Au(PMe_3)]^+$

Au	−0.302243	−0.001650	−0.033236
P	1.950533	−0.000416	0.031287
O	−2.467426	0.000368	−0.208064
C	−3.185298	1.194516	0.117060
C	−3.191163	−1.187533	0.126753
C	2.661571	1.500707	−0.693010
C	2.668378	−1.387400	−0.888925
C	2.619533	−0.106984	1.711966
H	−2.589655	2.038538	−0.228721
H	−3.344534	1.262976	1.197607
H	−4.147080	1.184414	−0.403534
H	−2.599587	−2.037326	−0.211785
H	−4.152796	−1.176986	−0.394126
H	−3.350850	−1.246037	1.207823
H	2.344819	1.590787	−1.734102
H	3.753215	1.451155	−0.646180
H	2.313136	2.375626	−0.140082
H	2.334946	−2.330544	−0.451198
H	3.759997	−1.331899	−0.848685
H	2.339887	−1.343589	−1.929462
H	2.274928	0.748859	2.296316
H	3.712739	−0.106910	1.674625
H	2.271315	−1.025292	2.189326

IN1

Au	1.863307	0.075213	0.042456
P	3.921275	−0.968594	−0.070099
O	−0.729760	3.625916	0.850240
C	−5.434725	−4.683315	0.983960
C	−4.657378	−4.150680	−0.210291
C	−3.675815	−3.052453	0.175191
C	−2.884096	−2.539691	−1.035233
C	−1.971346	−1.470536	−0.701912
C	−1.228372	−0.562790	−0.392715
C	−0.424058	0.474994	−0.037690
C	0.200083	1.490794	0.299385
C	0.450413	2.885864	0.722955
C	−1.354136	3.986939	−0.373330
C	−2.685027	3.341037	−0.572301
C	−3.273275	2.509023	0.292769
C	−4.579759	1.877343	0.108462
C	−5.047648	1.041920	1.048106
C	−5.366635	2.179714	−1.132265

C	5.259715	0.188305	−0.471901	C	1.089291	2.181632	−0.899267
C	3.991903	−2.263708	−1.338672	C	1.538602	1.085628	−0.663795
C	4.409016	−1.766641	1.483522	C	2.073110	−0.219055	−0.418757
H	−6.137208	−5.466621	0.683930	C	1.224073	−1.317782	−0.215417
H	−6.011328	−3.888069	1.468398	C	1.786889	−2.683938	−0.214644
H	−4.762736	−5.110497	1.735984	C	3.749533	−1.959920	−1.269174
H	−4.111227	−4.971688	−0.691198	C	3.549653	−0.532451	−0.821537
H	−5.355569	−3.762292	−0.962097	C	3.451829	−0.274183	0.596611
H	−4.213912	−2.212613	0.628961	C	3.826252	0.982124	1.268737
H	−2.973947	−3.426335	0.928983	C	3.628122	1.062991	2.589718
H	−2.310943	−3.358622	−1.488391	C	4.493562	2.067650	0.481465
H	−3.571765	−2.176869	−1.809783	C	−3.989425	−0.353090	−1.226079
H	1.152612	3.351798	0.019042	C	−3.597701	0.161624	1.585879
H	0.929242	2.873714	1.705546	C	−3.925305	−2.544805	0.646000
H	−0.696529	3.758651	−1.223640	H	−2.788802	6.589377	0.072369
H	−1.480135	5.078184	−0.367390	H	−2.105744	5.607934	1.373141
H	−3.180622	3.619977	−1.500466	H	−3.216044	4.880246	0.205715
H	−2.750268	2.267276	1.215543	H	−1.530636	5.261924	−1.626338
H	−4.474488	0.827908	1.946209	H	−0.428082	5.985735	−0.467063
H	−6.013001	0.555063	0.944817	H	−0.319379	3.820110	0.785491
H	−6.316666	1.641702	−1.132860	H	−1.428681	3.096442	−0.373147
H	−4.811210	1.895422	−2.032957	H	0.218451	3.544580	−2.218455
H	−5.579545	3.251224	−1.214339	H	1.328752	4.245989	−1.053148
H	5.065243	0.653280	−1.440837	H	1.259747	−3.195374	−1.043521
H	6.212136	−0.347955	−0.509596	H	1.473827	−3.213623	0.692827
H	5.311119	0.968405	0.290626	H	3.317715	−2.101957	−2.269144
H	3.270152	−3.048562	−1.102893	H	4.815869	−2.191292	−1.311765
H	4.997595	−2.692319	−1.372766	H	3.969310	0.240134	−1.458704
H	3.744788	−1.836174	−2.312608	H	3.374804	−1.142430	1.241052
H	4.449927	−1.019874	2.279494	H	3.165047	0.251819	3.143830
H	5.391023	−2.234449	1.370562	H	3.927549	1.943717	3.149337
H	3.671797	−2.526606	1.751068	H	4.712535	2.923344	1.122713
				H	3.870497	2.410638	−0.349250
		IN2		H	5.435711	1.707237	0.053604
Au	−0.797231	−1.142994	−0.029856	H	−3.614180	0.638855	−1.488255
P	−3.114695	−0.967529	0.244629	H	−5.064160	−0.296229	−1.032000
O	3.179532	−2.849482	−0.334582	H	−3.808422	−1.026812	−2.066838
C	−2.395911	5.598013	0.317036	H	−3.171937	−0.188487	2.529047
C	−1.218895	5.232725	−0.574625	H	−4.687096	0.202513	1.672699
C	−0.646839	3.857011	−0.260075	H	−3.211742	1.162474	1.379817
C	0.534129	3.498337	−1.168840	H	−3.758180	−3.257603	−0.164802

H	−4.999992	−2.395377	0.783085
H	−3.497104	−2.953624	1.564129

IN3

Au	−1.460158	−0.395200	−0.023215
P	−3.134698	1.222476	0.210500
O	0.606562	−4.211684	−0.204216
C	3.390260	5.557144	0.491565
C	3.190266	4.625669	−0.694533
C	2.723881	3.236736	−0.279265
C	2.521275	2.309583	−1.482890
C	2.095241	0.968843	−1.114910
C	1.741020	−0.139009	−0.789453
C	1.349302	−1.471074	−0.442421
C	0.005243	−1.799149	−0.192281
C	−0.388528	−3.220681	−0.127641
C	1.596913	−3.918130	−1.166710
C	2.317863	−2.643535	−0.803314
C	2.404797	−2.291585	0.594120
C	3.433006	−1.444047	1.225064
C	4.652548	−1.335964	0.691771
C	3.026998	−0.779833	2.503195
C	−2.520958	2.926275	0.053680
C	−3.976795	1.169924	1.821087
C	−4.468278	1.086546	−1.017032
H	3.727768	6.546943	0.169626
H	4.139524	5.160567	1.185282
H	2.458630	5.690579	1.052026
H	2.457902	5.060709	−1.386285
H	4.128840	4.537174	−1.255858
H	3.457452	2.786965	0.399903
H	1.782776	3.312651	0.278242
H	1.779280	2.744126	−2.164160
H	3.456073	2.237181	−2.052288
H	−1.117119	−3.327717	−0.956584
H	−0.965970	−3.410514	0.784352
H	1.160239	−3.827111	−2.170410
H	2.294410	−4.758169	−1.163549
H	3.105490	−2.317122	−1.475397
H	1.828002	−2.904708	1.280598
H	4.926820	−1.840484	−0.228882
H	5.423207	−0.752398	1.186305
H	3.859299	−0.229668	2.945540
H	2.670383	−1.518457	3.229439
H	2.202221	−0.079853	2.326657
H	−1.758671	3.111866	0.814030
H	−3.339915	3.640261	0.178276
H	−2.069622	3.061137	−0.932234
H	−4.438416	0.189511	1.959764
H	−4.748057	1.943783	1.870560
H	−3.250256	1.329605	2.621143
H	−4.051626	1.168305	−2.023503
H	−5.204689	1.880760	−0.864545
H	−4.957866	0.114911	−0.918061

IN4

Au	−1.396885	−0.664257	−0.093879
P	−3.474319	0.222470	0.522997
O	1.797797	−3.408384	−1.154941
C	0.762067	5.541709	−1.580208
C	1.742042	4.926214	−0.592604
C	1.601552	3.413289	−0.485604
C	2.582069	2.804592	0.505914
C	2.495922	1.317529	0.639692
C	1.747236	0.489258	−0.015365
C	1.588531	−0.695967	−0.636850
C	0.409779	−1.447927	−0.595209
C	0.513337	−2.861987	−1.009068
C	2.669358	−2.552289	−1.869418
C	2.932415	−1.270093	−1.092224
C	3.792561	−1.509012	0.133806
C	3.962348	−0.781035	1.250598
C	3.410906	0.583116	1.618433
C	4.851273	−1.310165	2.342585
C	−4.346123	−0.770857	1.771562
C	−4.642212	0.362142	−0.863175
C	−3.384262	1.894532	1.231271
H	0.881116	6.627813	−1.635539
H	−0.274409	5.336086	−1.291455
H	0.910463	5.139898	−2.588376
H	2.768376	5.173061	−0.891611
H	1.595142	5.372670	0.398904

H	0.577082	3.160726	−0.183025
H	1.756638	2.961299	−1.473659
H	3.615314	3.042468	0.221076
H	2.442795	3.236944	1.505814
H	−0.069320	−2.937726	−1.951014
H	−0.025071	−3.488323	−0.289203
H	2.236104	−2.305050	−2.849383
H	3.593302	−3.111701	−2.029257
H	3.408421	−0.551585	−1.769834
H	4.341491	−2.449311	0.101187
H	4.275591	1.250276	1.740249
H	2.943474	0.531006	2.609301
H	5.275873	−2.280665	2.078437
H	4.290825	−1.423158	3.278314
H	5.675751	−0.617989	2.550616
H	−4.500079	−1.782992	1.390382
H	−5.314010	−0.319580	2.007147
H	−3.742406	−0.828502	2.680371
H	−4.226708	1.024205	−1.626518
H	−5.597957	0.764487	−0.515518
H	−4.803426	−0.623401	−1.306145
H	−2.749405	1.882845	2.120336
H	−4.383354	2.245398	1.504943
H	−2.948076	2.578799	0.499620

IN5

Au	−1.416544	−0.438991	−0.010931
P	−3.575912	0.324581	0.474344
O	1.896763	−3.158992	−0.742220
C	1.658315	1.771577	−2.640186
C	1.024832	2.016790	−1.277923
C	1.373655	3.384835	−0.682546
C	2.719380	3.138497	−0.003777
C	2.717963	1.729342	0.395384
C	1.570259	1.053014	−0.181180
C	1.590875	−0.420792	−0.431930
C	0.468454	−1.161540	−0.417419
C	0.579533	−2.631031	−0.715307
C	2.775745	−2.323473	−1.460699
C	2.959381	−1.003294	−0.727506
C	3.754383	−1.184797	0.541753
C	4.068704	−0.248487	1.438483
C	3.705778	1.208384	1.333555
C	4.866292	−0.564399	2.668260
C	−4.338577	1.334110	−0.835432
C	−3.692038	1.362412	1.966382
C	−4.770143	−1.018206	0.765521
H	1.227907	2.455542	−3.377405
H	1.469708	0.750705	−2.982891
H	2.741711	1.931816	−2.630426
H	−0.055309	1.869292	−1.352510
H	1.423630	4.177738	−1.430296
H	0.633637	3.669993	0.072290
H	3.535684	3.165869	−0.752698
H	3.034340	3.822514	0.789014
H	0.890839	1.249084	0.694597
H	0.077921	−2.838261	−1.677415
H	0.047397	−3.210506	0.045079
H	2.388570	−2.137691	−2.474020
H	3.722533	−2.862939	−1.550044
H	3.493871	−0.306925	−1.393363
H	4.081587	−2.202324	0.750782
H	4.603742	1.840434	1.298291
H	3.244506	1.523806	2.295903
H	5.153758	−1.617183	2.691738
H	4.292887	−0.342982	3.576694
H	5.779079	0.041923	2.715216
H	−3.717096	2.211746	−1.028864
H	−5.340355	1.658458	−0.539137
H	−4.405048	0.747773	−1.755110
H	−3.310091	0.808801	2.827388
H	−4.730173	1.650937	2.154381
H	−3.085394	2.261562	1.833794
H	−4.817304	−1.662857	−0.115429
H	−5.764702	−0.611628	0.970330
H	−4.443058	−1.618806	1.617659

IN6

Au	1.455992	−0.341999	0.027860
P	3.617047	0.348875	−0.539367
O	−1.520205	−3.156748	1.241942
C	−0.572336	1.730680	2.206297

C	−0.805353	1.864586	0.689957	H	5.420291	1.658827	0.423417
C	−1.402907	3.235696	0.348411	H	4.484002	0.791463	1.669625
C	−2.900970	3.010432	0.494128	H	3.287308	0.786816	−2.890399
C	−3.076671	1.622847	−0.125773	H	4.738785	1.620029	−2.274028
C	−1.838025	0.862687	0.249038	H	3.112347	2.263225	−1.920768
C	−1.674235	−0.523988	0.283254				
C	−0.404041	−1.095884	0.467763			**IN7**	
C	−0.322824	−2.511139	0.904646	Au	0.771131	−0.095170	−0.196885
C	−2.482451	−2.907982	0.243451	P	3.038982	−0.246448	0.176114
C	−2.909300	−1.448884	0.249213	O	−1.350143	3.655970	−0.860599
C	−3.851945	−1.210024	−0.896588	C	−2.870958	−1.168403	−2.564626
C	−4.626283	−0.128377	−0.992208	C	−1.569585	−1.471128	−1.808865
C	−4.456548	0.980008	0.009472	C	−1.587840	−2.904869	−1.267288
C	−5.594223	0.088845	−2.109007	C	−2.401611	−2.784477	0.016502
C	4.765053	−1.030627	−0.829199	C	−1.869069	−1.499507	0.659792
C	4.416312	1.363331	0.741160	C	−1.463965	−0.621220	−0.536085
C	3.701630	1.352812	−2.052930	C	−1.354342	0.766344	−0.561999
H	0.126289	2.507840	2.528770	C	−1.174463	1.484135	−1.824632
H	−0.151234	0.753080	2.450546	C	−1.239860	2.825294	−1.903034
H	−1.501169	1.854616	2.771320	C	−1.062967	3.045573	0.395054
H	0.154105	1.676467	0.188811	C	−1.747773	1.698515	0.581183
H	−1.008950	4.021199	0.996762	C	−1.512325	1.240449	1.994242
H	−1.169148	3.503924	−0.687704	C	−2.028341	0.132448	2.530760
H	−3.201560	2.995177	1.547501	C	−2.798268	−0.839237	1.678126
H	−3.509076	3.758235	−0.019002	C	−1.799827	−0.246947	3.958732
H	−2.894813	1.767261	−1.210779	C	4.011334	1.006463	−0.706839
H	0.331732	−2.544264	1.785848	C	3.739141	−1.844747	−0.324489
H	0.218444	−3.073076	0.119668	C	3.476806	−0.054068	1.926880
H	−3.340266	−3.551256	0.448481	H	−2.941966	−1.815241	−3.444563
H	−2.077214	−3.179931	−0.744562	H	−2.923445	−0.132103	−2.904503
H	−3.449607	−1.278316	1.189945	H	−3.749926	−1.353995	−1.940726
H	−3.914255	−1.987702	−1.656799	H	−0.725428	−1.302035	−2.483443
H	−4.596400	0.616646	1.034485	H	−2.010180	−3.611709	−1.986320
H	−5.204471	1.760546	−0.154208	H	−0.568477	−3.232138	−1.031551
H	−5.600244	−0.749145	−2.810006	H	−3.468357	−2.683727	−0.211201
H	−5.352189	1.003624	−2.664196	H	−2.288854	−3.641371	0.684942
H	−6.610419	0.222665	−1.718954	H	−0.951109	−1.778071	1.194650
H	4.827683	−1.649416	0.068981	H	−1.041234	0.937363	−2.748560
H	5.760162	−0.651484	−1.078497	H	−1.217992	3.354638	−2.850151
H	4.395870	−1.646432	−1.652514	H	−1.395833	3.753255	1.154235
H	3.817272	2.258049	0.925752	H	0.025926	2.921489	0.473029

H	−2.829123	1.861322	0.438362
H	−0.917474	1.904211	2.620857
H	−3.621342	−0.336127	1.154612
H	−3.244311	−1.617327	2.305165
H	−1.194062	0.492665	4.487725
H	−1.298609	−1.220443	4.028063
H	−2.755304	−0.353749	4.486087
H	3.843720	0.910862	−1.781887
H	5.074922	0.872077	−0.489862
H	3.698733	2.004119	−0.390301
H	3.254636	−2.648170	0.234793
H	4.814428	−1.858170	−0.124867
H	3.565653	−2.004545	−1.390990
H	3.141176	0.921870	2.284731
H	4.560265	−0.133611	2.053405
H	2.984067	−0.831639	2.514785

IN8

Au	−1.462068	−0.421126	−0.002106
P	−3.587973	0.491880	0.358073
O	1.807940	−3.248337	−0.134892
C	1.084206	2.058602	−2.624343
C	2.092946	1.878452	−1.507740
C	2.429531	3.158764	−0.733874
C	3.031802	2.669058	0.590089
C	2.470194	1.309575	0.773296
C	1.616551	0.942138	−0.376716
C	1.518215	−0.544952	−0.556250
C	0.393173	−1.248060	−0.335316
C	0.491316	−2.749617	−0.318773
C	2.681772	−2.694496	−1.080931
C	2.845594	−1.179026	−0.875870
C	3.945077	−0.817777	0.066524
C	3.929252	−0.107695	1.217097
C	2.647857	0.420347	1.894385
C	5.195527	0.279800	1.913247
C	−4.465341	−0.185585	1.802388
C	−4.745811	0.251017	−1.027032
C	−3.589407	2.292244	0.636023
H	0.139672	2.455554	−2.235895
H	0.869799	1.109837	−3.125160
H	1.457875	2.757001	−3.379271
H	0.616878	1.301088	−0.043201
H	3.023786	1.465955	−1.918903
H	3.106829	3.818296	−1.279122
H	1.506515	3.715347	−0.536610
H	4.126761	2.610236	0.544741
H	2.806246	3.290462	1.463927
H	0.058418	−3.168285	−1.244798
H	−0.091098	−3.153592	0.513491
H	2.298315	−2.867661	−2.097500
H	3.639672	−3.210869	−0.984947
H	3.195950	−0.797786	−1.850197
H	4.931651	−1.148945	−0.258661
H	2.900187	0.899176	2.837846
H	1.875418	−0.340249	1.987359
H	6.071806	−0.090168	1.377659
H	5.201359	−0.122092	2.931814
H	5.283161	1.368759	2.003093
H	−4.595479	−1.263304	1.678013
H	−5.445636	0.286707	1.913886
H	−3.874343	−0.010577	2.704518
H	−4.337863	0.713960	−1.928713
H	−5.717037	0.698932	−0.797684
H	−4.875685	−0.817536	−1.214301
H	−2.983834	2.527960	1.514487
H	−4.609120	2.655952	0.792119
H	−3.155450	2.796568	−0.230795

IN9

Au	−1.438231	−0.646327	−0.077927
P	−3.448272	0.339341	0.606989
O	1.539068	−3.189939	−1.954090
C	0.968900	5.222842	−2.013660
C	1.844408	4.690280	−0.889043
C	1.655640	3.197588	−0.651802
C	2.516280	2.670407	0.486388
C	2.372221	1.208030	0.748373
C	1.675510	0.321909	0.117245
C	1.555867	−0.874938	−0.493795
C	0.311613	−1.489967	−0.679299
C	0.314625	−2.779856	−1.396544

C	2.611728	−3.010066	−1.053202	P	3.420568	0.252239	−0.579041
C	2.886261	−1.517924	−0.846302	O	−1.870191	−3.257265	1.161603
C	3.969367	−1.351411	0.195959	C	0.461561	2.046957	2.545635
C	4.123167	−0.577762	1.284618	C	−0.188555	2.353934	1.239512
C	3.215235	0.513037	1.823685	C	−1.232489	3.409899	1.147694
C	5.343900	−0.754929	2.143521	C	−2.091514	3.229977	−0.097107
C	−4.935296	−0.552396	0.060062	C	−2.398148	1.778213	−0.322346
C	−3.666206	2.035550	−0.009730	C	−1.715183	0.825862	0.278599
C	−3.618282	0.476053	2.412056	C	−1.715959	−0.600340	0.416339
H	1.128618	6.293723	−2.170592	C	−0.569544	−1.329918	0.360562
H	−0.093875	5.074501	−1.793318	C	−0.650875	−2.803864	0.605975
H	1.184947	4.713946	−2.959262	C	−2.970088	−2.722374	0.470973
H	2.898719	4.889149	−1.118037	C	−3.082401	−1.209220	0.685941
H	1.622880	5.233945	0.038038	C	−4.242036	−0.724735	−0.143667
H	0.600513	2.991993	−0.430020	C	−4.420180	0.300396	−0.984720
H	1.895041	2.647642	−1.570668	C	−3.458935	1.412720	−1.327441
H	3.580690	2.853505	0.287006	C	−5.721706	0.433972	−1.725207
H	2.295387	3.199696	1.422970	C	4.738354	−1.002065	−0.554351
H	−0.423568	−2.750362	−2.206795	C	4.018196	1.560238	0.537865
H	−0.070708	−3.530416	−0.677775	C	3.525165	0.990266	−2.239444
H	3.483400	−3.502730	−1.488033	H	1.149776	2.875198	2.763589
H	2.386413	−3.490972	−0.089053	H	1.055892	1.131182	2.494096
H	3.248074	−1.119614	−1.804008	H	−0.262534	1.981688	3.360018
H	4.795433	−2.039304	0.011593	H	0.478379	2.294713	0.377585
H	3.835988	1.288814	2.285254	H	−0.864329	1.272195	1.075199
H	2.576911	0.118140	2.621124	H	−1.849235	3.398754	2.050821
H	5.972761	−1.575566	1.791928	H	−0.716643	4.377944	1.107153
H	5.060602	−0.961817	3.182567	H	−3.024136	3.792451	−0.000749
H	5.944043	0.162759	2.159785	H	−1.587334	3.617734	−0.991994
H	−4.948796	−0.602331	−1.031253	H	0.131532	−3.107828	1.307960
H	−5.836304	−0.041658	0.411111	H	−0.441138	−3.330855	−0.342749
H	−4.917385	−1.570742	0.455146	H	−3.864371	−3.222161	0.851536
H	−2.841401	2.661772	0.338292	H	−2.889110	−2.934386	−0.607146
H	−4.612938	2.450520	0.347596	H	−3.335518	−1.050220	1.745293
H	−3.663136	2.031212	−1.102313	H	−5.103065	−1.387249	−0.040559
H	−3.576700	−0.519386	2.859993	H	−4.050818	2.312231	−1.525428
H	−4.568699	0.951890	2.669665	H	−2.963761	1.178881	−2.281250
H	−2.794800	1.072226	2.811989	H	−6.388712	−0.407167	−1.525446
				H	−5.549031	0.484116	−2.807224
		IN10		H	−6.238085	1.360551	−1.446652
Au	1.293851	−0.571811	−0.056511	H	4.819655	−1.428648	0.448254

H	5.695609	−0.554531	−0.836248
H	4.493523	−1.804535	−1.253995
H	3.327607	2.406624	0.517025
H	5.011156	1.900556	0.229649
H	4.071411	1.175895	1.559180
H	3.266293	0.237933	−2.988158
H	4.536356	1.359891	−2.431925
H	2.815441	1.817144	−2.319529

IN11

Au	1.300038	−0.449925	−0.029748
P	3.487051	0.257034	−0.462899
O	−1.814958	−3.300267	0.768128
C	−0.657718	1.610585	2.897253
C	−0.747885	1.814621	1.399238
C	−1.115710	3.232341	0.955922
C	−1.644914	3.034470	−0.464945
C	−2.230770	1.701972	−0.470225
C	−1.839238	0.961785	0.716393
C	−1.746866	−0.543240	0.544562
C	−0.594297	−1.196400	0.314765
C	−0.630181	−2.704241	0.269671
C	−2.945780	−2.700499	0.192484
C	−3.084491	−1.246737	0.650838
C	−4.229680	−0.634774	−0.107996
C	−4.268575	0.322490	−1.038797
C	−3.076736	1.149355	−1.515133
C	−5.542272	0.691389	−1.737945
C	4.659620	−1.112283	−0.713808
C	4.236937	1.258845	0.860038
C	3.665667	1.281004	−1.958339
H	0.119993	2.247597	3.328962
H	−0.410934	0.572886	3.139098
H	−1.606344	1.858808	3.385952
H	0.210728	1.539995	0.936559
H	−2.773097	1.163383	1.308345
H	−1.917355	3.630326	1.588595
H	−0.275352	3.926492	0.995787
H	−2.283591	3.804365	−0.904568
H	−0.794674	2.912651	−1.169807
H	0.179802	−3.111876	0.881019
H	−0.447985	−3.043794	−0.765672
H	−3.817464	−3.286425	0.494916
H	−2.877292	−2.732491	−0.907134
H	−3.382356	−1.263078	1.712217
H	−5.185740	−1.110108	0.112898
H	−3.390596	1.927631	−2.211985
H	−2.385063	0.486513	−2.071187
H	−6.376410	0.081105	−1.385721
H	−5.445509	0.548816	−2.820869
H	−5.790179	1.747458	−1.579099
H	4.673172	−1.749403	0.173785
H	5.666548	−0.726649	−0.897680
H	4.341897	−1.714347	−1.568394
H	3.634449	2.155098	1.026274
H	5.255629	1.552664	0.590949
H	4.260369	0.680170	1.786645
H	3.294056	0.729421	−2.825183
H	4.714682	1.544477	−2.121255
H	3.076855	2.194920	−1.848805

IN12

Au	−1.335349	−0.529107	−0.021691
P	−3.464906	0.281200	0.520312
O	1.762702	−3.334107	−1.142807
C	−0.530690	2.808749	−1.201666
C	0.818026	2.470745	−1.749847
C	1.987259	3.324302	−1.370080
C	2.420382	3.097715	0.077579
C	2.407020	1.635076	0.387695
C	1.730722	0.755511	−0.315491
C	1.676255	−0.657224	−0.469939
C	0.499178	−1.347288	−0.426005
C	0.538573	−2.822602	−0.655304
C	2.853098	−2.820607	−0.416964
C	3.027595	−1.321009	−0.682313
C	4.187322	−0.831010	0.146614
C	4.307184	0.119234	1.083203
C	3.218307	1.073187	1.537183
C	5.611776	0.314016	1.798796
C	−4.669018	−1.054257	0.799039
C	−4.235586	1.332798	−0.750018

C	−3.528894	1.280055	2.040156	C	1.750565	−0.560102	−0.688135
H	−0.497170	3.057338	−0.138512	C	0.581266	−1.204018	−0.509129
H	−1.244561	1.995758	−1.360461	C	0.600576	−2.711341	−0.536461
H	−0.898312	3.687025	−1.748009	C	2.896416	−2.756794	−0.320122
H	1.089558	1.333972	−1.289882	C	3.090713	−1.276532	−0.663111
H	0.803517	2.154535	−2.795958	C	4.089281	−0.721330	0.324311
H	2.827493	3.108015	−2.033812	C	3.960648	0.176250	1.306907
H	1.706399	4.374710	−1.514558	C	2.688486	0.990160	1.604676
H	3.427660	3.494026	0.231077	C	5.087267	0.495700	2.241228
H	1.773224	3.618445	0.794747	C	−3.853176	1.929138	−0.075553
H	−0.223541	−3.098729	−1.391404	C	−3.729028	0.378237	2.341810
H	0.255577	−3.327572	0.286055	C	−4.758478	−0.798691	−0.073954
H	3.741751	−3.368759	−0.738484	H	−0.646994	2.292584	−0.903385
H	2.713284	−2.991293	0.661939	H	−0.659984	1.061133	−2.174067
H	3.313561	−1.217930	−1.740069	H	−0.508889	2.770864	−2.602003
H	5.092747	−1.404904	−0.056199	H	1.668034	1.684971	−2.818960
H	3.677283	1.905502	2.076351	H	2.931414	3.379381	−1.741208
H	2.550310	0.570982	2.246331	H	1.333054	4.129960	−1.610986
H	6.364320	−0.407843	1.473854	H	2.772589	3.707161	0.714749
H	5.478461	0.206773	2.882290	H	1.063773	3.299327	0.681353
H	6.002369	1.325043	1.631024	H	3.021694	1.080146	−1.065824
H	−4.759787	−1.658236	−0.106889	H	−0.186513	−3.072449	−1.204996
H	−5.647715	−0.640565	1.058270	H	0.369228	−3.106358	0.468743
H	−4.321109	−1.696303	1.611555	H	3.780519	−3.337344	−0.595334
H	−3.639515	2.237646	−0.889346	H	2.742602	−2.862597	0.765964
H	−5.248972	1.614042	−0.449229	H	3.554994	−1.216909	−1.660611
H	−4.278451	0.790420	−1.697437	H	5.068739	−1.194269	0.249354
H	−3.145959	0.693325	2.878362	H	2.879486	1.707710	2.401965
H	−4.556689	1.587404	2.252849	H	1.895041	0.299865	1.927561
H	−2.902290	2.167169	1.921124	H	5.973098	−0.098660	2.007756
				H	4.799035	0.291657	3.279184
		IN13		H	5.353763	1.557808	2.189885
Au	−1.283877	−0.456538	−0.046073	H	−3.174815	2.671271	0.352117
P	−3.424895	0.272569	0.549432	H	−4.881787	2.186485	0.193460
O	1.801141	−3.292442	−1.014097	H	−3.750567	1.948011	−1.163117
C	−0.216054	2.011489	−1.869495	H	−3.600146	−0.608557	2.792812
C	1.300394	1.937513	−1.821998	H	−4.743753	0.736785	2.537115
C	1.924141	3.257798	−1.329900	H	−3.009522	1.063904	2.795540
C	2.035624	3.094048	0.190588	H	−4.715849	−0.836158	−1.165174
C	2.201265	1.659899	0.400891	H	−5.735322	−0.417577	0.237629
C	1.920593	0.933727	−0.804557	H	−4.625356	−1.811523	0.313576

IN14

Au	1.468657	−0.277088	−0.370038
P	3.129714	1.124185	0.421689
O	0.575206	−3.384873	−0.310930
C	−3.387664	5.726740	−0.874141
C	−3.521237	4.684958	0.226631
C	−2.922743	3.338930	−0.159572
C	−3.056973	2.299784	0.958764
C	−2.492666	1.003518	0.610171
C	−2.023509	−0.068960	0.310998
C	−1.453046	−1.334596	−0.056445
C	−0.374888	−1.320959	−1.085959
C	0.491909	−2.388619	−1.178272
C	−0.004049	−3.180756	0.990240
C	−1.304944	−2.427996	0.979256
C	−2.337703	−2.611560	−0.072189
C	−3.798536	−2.518709	0.188798
C	−4.326304	−2.712153	1.397581
C	−4.628863	−2.197117	−1.016686
C	2.647623	1.991421	1.942276
C	3.582004	2.429520	−0.756840
C	4.678550	0.267175	0.823919
H	−3.830421	6.681758	−0.575524
H	−3.890040	5.400881	−1.791244
H	−2.336349	5.912134	−1.119950
H	−3.033090	5.048640	1.139685
H	−4.580535	4.548901	0.478210
H	−3.415362	2.959778	−1.062573
H	−1.862004	3.463726	−0.408589
H	−2.569158	2.673842	1.867524
H	−4.116428	2.167583	1.210324
H	−0.527823	−0.741668	−1.994219
H	1.097637	−2.559313	−2.063612
H	0.730554	−2.621849	1.582628
H	−0.112270	−4.180616	1.411559
H	−1.654278	−2.178136	1.975997
H	−2.077297	−3.270243	−0.899316
H	−3.715532	−2.956193	2.261318
H	−5.398310	−2.638151	1.556461
H	−4.478970	−2.945027	−1.804258
H	−4.334999	−1.229234	−1.439131
H	−5.692738	−2.160601	−0.773289
H	1.745187	2.578646	1.758377
H	3.454274	2.655654	2.265239
H	2.439003	1.263788	2.729697
H	3.939584	1.978660	−1.685125
H	4.367441	3.060834	−0.331841
H	2.704472	3.041035	−0.978776
H	4.487759	−0.500188	1.577333
H	5.411373	0.981643	1.209836
H	5.075283	−0.213875	−0.072857

IN15 (Table 2, entry 1)

Au	2.218380	−0.096005	0.241376
P	3.957834	−0.145098	−1.327713
O	−0.477747	−1.064416	3.510678
O	−4.743015	2.102540	−0.761393
O	−5.205606	0.284606	−1.980788
C	0.012713	4.203598	−0.944788
C	−0.114163	3.041094	−0.088013
C	−0.213634	2.072169	0.624343
C	−0.338560	0.940384	1.493946
C	0.659535	−0.053127	1.548455
C	0.618504	−1.054095	2.630967
C	−0.883120	0.233010	3.892351
C	−1.333298	1.015620	2.683449
C	−1.890823	0.265604	1.571828
C	−2.835767	0.841250	0.627374
C	−3.538758	0.130731	−0.277705
C	−4.582131	0.823853	−1.099541
C	−5.706413	2.832398	−1.528481
C	−3.344447	−1.309628	−0.546157
C	−2.070886	−1.804104	−0.843358
C	−1.878540	−3.158253	−1.090872
C	−2.955790	−4.035485	−1.038357
C	−4.227819	−3.551181	−0.746859
C	−4.425108	−2.197455	−0.511896
C	3.519477	0.673424	−2.891057
C	4.488192	−1.820109	−1.794745
C	5.471047	0.691034	−0.763843
H	−0.006431	5.126803	−0.358031
H	−0.805622	4.243440	−1.669992

H	0.955252	4.173546	−1.499517
H	1.566145	−0.884518	3.181542
H	0.710901	−2.063602	2.213442
H	−0.071815	0.768339	4.403694
H	−1.714010	0.107604	4.589441
H	−1.695901	2.024856	2.854110
H	−1.842150	−0.814877	1.635326
H	−3.020491	1.906343	0.708160
H	−5.682229	3.848543	−1.139310
H	−6.702004	2.402610	−1.400603
H	−5.438977	2.825461	−2.586959
H	−1.231878	−1.117918	−0.903475
H	−0.886114	−3.525504	−1.332043
H	−2.807471	−5.093128	−1.230892
H	−5.072312	−4.231533	−0.707897
H	−5.419869	−1.825990	−0.292831
H	2.651941	0.178306	−3.333566
H	4.356878	0.632782	−3.593420
H	3.262715	1.716766	−2.692799
H	4.849756	−2.347122	−0.908708
H	5.285953	−1.773467	−2.541463
H	3.639382	−2.371084	−2.206375
H	5.247316	1.735841	−0.536526
H	6.242014	0.645212	−1.538279
H	5.839132	0.206946	0.143735

IN15 (Table 2, entry 2)

Au	−1.749706	0.201415	−0.179772
P	−3.522303	−1.318906	−0.356553
O	0.839169	3.629904	−0.822064
O	5.638373	−1.635074	−1.592631
O	5.425529	−1.469488	0.636174
C	0.963063	−1.769328	3.502867
C	0.953300	−0.700334	2.523895
C	0.942113	0.186750	1.706199
C	0.939896	1.256184	0.751986
C	−0.179410	1.491385	−0.076295
C	−0.255794	2.750025	−0.839997
C	1.407421	3.763181	0.463695
C	1.937139	2.434092	0.939983
C	2.384040	1.490139	−0.070058
C	3.385325	0.462869	0.183723
C	4.056749	−0.140190	−0.801227
C	5.099919	−1.137097	−0.479084
C	6.654811	−2.624365	−1.400793
C	−3.049040	−3.029706	0.033349
C	−4.248006	−1.397608	−2.021702
C	−4.915560	−0.946777	0.750718
H	1.794020	−2.456560	3.318419
H	0.032261	−2.342540	3.457888
H	1.068238	−1.371802	4.516607
H	−1.165321	3.240413	−0.436170
H	−0.491293	2.540737	−1.889859
H	0.675649	4.155267	1.182705
H	2.225590	4.480393	0.371743
H	2.422389	2.412687	1.910851
H	2.217454	1.759973	−1.107009
H	3.612509	0.205312	1.214215
H	3.868130	0.077474	−1.847591
H	6.970190	−2.920948	−2.399389
H	6.255203	−3.484197	−0.859103
H	7.497420	−2.205758	−0.846657
H	−2.259006	−3.354197	−0.647823
H	−3.910653	−3.695622	−0.067137
H	−2.668961	−3.079229	1.056391
H	−4.631851	−0.413785	−2.301100
H	−5.063179	−2.126241	−2.046619
H	−3.479303	−1.689619	−2.740861
H	−4.570673	−0.955123	1.787218
H	−5.709183	−1.689175	0.626598
H	−5.308716	0.046286	0.521609

IN15 (Table 2, entry 3)

Au	−1.719149	−0.114851	−0.406409
P	−3.642281	−1.268633	0.257859
O	1.617063	1.396502	−2.753738
C	−0.858041	2.797799	3.552979
C	−0.319348	2.420733	2.260871
C	0.122564	2.101816	1.183492
C	0.646496	1.755705	−0.100723
C	−0.025023	0.879739	−0.958841
C	0.437445	0.734500	−2.357305

C	1.727593	2.691917	−2.206722
C	1.784054	2.620048	−0.698340
C	2.394924	1.440202	−0.117814
C	2.964893	1.380412	1.207004
C	3.808536	0.428390	1.657272
C	4.397858	−0.703280	0.944306
C	4.625235	−1.888581	1.660073
C	5.169128	−3.001928	1.037255
C	5.525383	−2.944478	−0.307397
C	5.342375	−1.763762	−1.019825
C	4.786623	−0.651130	−0.402093
C	−3.617564	−1.752412	2.010885
C	−3.938204	−2.815489	−0.651223
C	−5.172582	−0.307701	0.054554
H	−1.243828	3.821430	3.534386
H	−0.086838	2.740761	4.327233
H	−1.676185	2.131078	3.841236
H	−0.421650	1.070630	−2.969137
H	0.569130	−0.325864	−2.600317
H	0.886166	3.327432	−2.514360
H	2.652171	3.120168	−2.599250
H	1.906937	3.562830	−0.172559
H	2.592681	0.621706	−0.799107
H	2.673352	2.165325	1.897976
H	4.089707	0.498675	2.706353
H	4.358146	−1.931603	2.711760
H	5.326298	−3.914158	1.603539
H	5.962987	−3.810820	−0.792626
H	5.648505	−1.702676	−2.059160
H	4.701750	0.277071	−0.956414
H	−2.767249	−2.413525	2.194194
H	−4.543180	−2.269940	2.278259
H	−3.506410	−0.861921	2.633765
H	−4.043331	−2.599189	−1.716916
H	−4.848447	−3.301264	−0.288312
H	−3.089468	−3.489316	−0.514159
H	−5.103037	0.618646	0.629295
H	−6.033870	−0.885593	0.401606
H	−5.307938	−0.054154	−0.999393

IN15 (Table 2, entry 4)

Au	−0.871966	−0.385258	0.017412
P	−3.145033	0.146881	0.196085
O	2.854641	−2.600192	−0.270444
C	1.098498	4.025159	−1.204810
C	1.445971	2.648738	−0.909508
C	1.727851	1.501121	−0.663941
C	2.084258	0.139668	−0.400137
C	1.107659	−0.837669	−0.154663
C	1.495508	−2.262598	−0.131822
C	3.511650	−1.811913	−1.239143
C	3.497875	−0.360384	−0.826959
C	3.467709	−0.062243	0.588434
C	3.973194	1.170705	1.179560
C	4.211058	1.268251	2.488343
C	−3.934849	−0.439124	1.725078
C	−4.153826	−0.547962	−1.148120
C	−3.471284	1.935446	0.152059
H	1.687876	4.714927	−0.593294
H	0.040234	4.210144	−0.997549
H	1.284919	4.259674	−2.257165
H	0.893010	−2.722113	−0.939566
H	1.137562	−2.730866	0.792665
H	3.044816	−1.924560	−2.227126
H	4.539572	−2.175835	−1.293785
H	3.996006	0.344186	−1.486676
H	3.331922	−0.900116	1.263818
H	4.194051	1.997137	0.510592
H	3.994660	0.447790	3.167262
H	4.641924	2.168730	2.913699
H	−3.853274	−1.526919	1.784071
H	−4.990369	−0.153537	1.740526
H	−3.427902	−0.004154	2.589449
H	−3.780145	−0.189441	−2.109974
H	−5.199466	−0.249438	−1.031305
H	−4.084985	−1.638143	−1.130746
H	−2.957497	2.421713	0.984572
H	−4.545319	2.129088	0.224696
H	−3.091535	2.352266	−0.783665

IN16 (Table 2, entry 1)

Au	2.364367	0.277067	−0.134839
P	3.905305	−1.484020	−0.246086
O	0.346755	3.940773	1.027062
O	−1.511821	−2.020696	0.931358
O	−2.481485	−0.854746	2.576575
C	−2.193949	−1.106860	−2.127409
C	−1.864976	−0.205828	−0.982977
C	−0.854523	0.594511	−0.903326
C	−0.260001	1.744031	−0.541413
C	1.021499	1.792732	0.023887
C	1.380018	3.039234	0.728740
C	−0.516990	4.159591	−0.071605
C	−1.265217	2.886291	−0.441848
C	−2.308344	2.499466	0.588428
C	−2.851443	1.314592	0.892413
C	−2.754216	−0.090154	0.292749
C	−2.238314	−1.016283	1.410645
C	−1.013623	−2.951635	1.903852
C	−4.176647	−0.528730	−0.095160
C	−4.617172	−1.837583	0.103421
C	−5.900362	−2.215186	−0.277966
C	−6.753299	−1.295820	−0.875448
C	−6.316460	0.007721	−1.087175
C	−5.039013	0.389219	−0.697754
C	3.200066	−3.090804	0.231720
C	5.346544	−1.259611	0.839139
C	4.595861	−1.746424	−1.907617
H	−2.277049	−2.138113	−1.772859
H	−1.416094	−1.056370	−2.890189
H	−3.151106	−0.822954	−2.571395
H	2.164701	3.511215	0.099512
H	1.879476	2.795325	1.672497
H	0.058183	4.508884	−0.941060
H	−1.209444	4.948846	0.227367
H	−1.738339	3.040364	−1.419047
H	−2.649823	3.330645	1.203756
H	−3.543957	1.313106	1.729489
H	−0.465941	−3.701256	1.335930
H	−1.838475	−3.415244	2.447684
H	−0.349534	−2.445174	2.606354
H	−3.967991	−2.579121	0.556980
H	−6.229596	−3.234730	−0.105522
H	−7.754239	−1.591647	−1.172134
H	−6.974499	0.734788	−1.551950
H	−4.710389	1.410717	−0.858280
H	2.821254	−3.032858	1.254888
H	3.960756	−3.874244	0.170902
H	2.370237	−3.337394	−0.434766
H	5.872971	−0.342889	0.563629
H	6.028233	−2.110014	0.748196
H	5.012140	−1.172470	1.875554
H	3.787799	−1.975176	−2.606267
H	5.311988	−2.573000	−1.895693
H	5.099984	−0.836668	−2.241752

IN16 (Table 2, entry 2)

Au	1.409150	0.521360	0.009241
P	3.352534	−0.781485	−0.054234
O	−1.630908	3.418938	1.122747
O	−2.213035	−1.660231	1.739453
O	−2.933680	−3.300859	0.390116
C	−2.481554	−1.785094	−2.650169
C	−2.424092	−0.908340	−1.447081
C	−1.650638	0.098683	−1.197161
C	−1.435342	1.316757	−0.673813
C	−0.295352	1.621640	0.086592
C	−0.375922	2.818146	0.944451
C	−2.352429	3.536529	−0.088231
C	−2.704179	2.165360	−0.648971
C	−3.747399	1.448959	0.185465
C	−3.989794	0.143461	0.352602
C	−3.417163	−1.102495	−0.285596
C	−2.789937	−2.028134	0.749403
C	−2.335870	−4.270380	1.262556
C	3.022362	−2.569627	−0.029326
C	4.486358	−0.489504	1.336396
C	4.356632	−0.509246	−1.545466
H	−2.337923	−2.828580	−2.353183
H	−1.718601	−1.511889	−3.379137
H	−3.469677	−1.704656	−3.113366
H	0.359423	3.531659	0.515449

H	0.013549	2.573830	1.939248
H	−1.759798	4.091529	−0.829806
H	−3.252862	4.110733	0.138135
H	−3.068045	2.299757	−1.674513
H	−4.389057	2.118663	0.755843
H	−4.781368	−0.105071	1.056634
H	−4.255582	−1.645241	−0.738700
H	−2.579171	−5.240039	0.832738
H	−2.752246	−4.185498	2.267778
H	−1.253464	−4.132819	1.299803
H	2.486881	−2.830459	0.886639
H	3.960594	−3.129714	−0.074292
H	2.399531	−2.836805	−0.886306
H	4.801378	0.556530	1.336680
H	5.366209	−1.133195	1.250295
H	3.973121	−0.699787	2.277611
H	3.761416	−0.731705	−2.434071
H	5.241529	−1.151845	−1.530470
H	4.670176	0.536353	−1.587965

IN16 (Table 2, entry 3)

Au	2.171658	0.131366	0.000124
P	3.779775	−1.572025	0.059693
O	0.056992	3.875090	0.610179
C	−2.458272	−1.657269	−1.600356
C	−2.126204	−0.577439	−0.623812
C	−1.104040	0.212299	−0.672135
C	−0.525489	1.419389	−0.521171
C	0.767096	1.599344	−0.016262
C	1.107740	2.957109	0.455261
C	−0.821545	3.877961	−0.498617
C	−1.551353	2.547671	−0.621427
C	−2.590462	2.346013	0.465177
C	−3.130269	1.224337	0.960566
C	−3.019497	−0.248750	0.604963
C	−4.407393	−0.831401	0.395037
C	−4.739347	−2.055615	0.974344
C	−6.001686	−2.608092	0.784103
C	−6.943365	−1.943184	0.006957
C	−6.618521	−0.721565	−0.575846
C	−5.358703	−0.168363	−0.382408
C	5.483399	−0.965361	0.247246
C	3.809277	−2.604704	−1.436248
C	3.539743	−2.735668	1.436239
H	−2.524440	−2.619284	−1.082468
H	−1.698037	−1.725360	−2.379377
H	−3.430401	−1.463874	−2.060606
H	1.877388	3.335366	−0.249559
H	1.617326	2.883106	1.422330
H	−0.261031	4.072463	−1.424434
H	−1.524776	4.697872	−0.338977
H	−2.024137	2.509620	−1.609883
H	−2.924115	3.270783	0.933479
H	−3.826133	1.367212	1.785145
H	−2.589446	−0.767339	1.471132
H	−4.005479	−2.574367	1.584475
H	−6.249575	−3.557493	1.247879
H	−7.929074	−2.372468	−0.140499
H	−7.351023	−0.195583	−1.179828
H	−5.112861	0.788530	−0.833064
H	5.731143	−0.306521	−0.588200
H	6.186633	−1.802829	0.268902
H	5.569038	−0.396988	1.176345
H	2.832064	−3.072716	−1.576477
H	4.574686	−3.381401	−1.351116
H	4.024603	−1.979053	−2.305639
H	3.576928	−2.192743	2.383459
H	4.319302	−3.502696	1.425900
H	2.561225	−3.212761	1.344779

IN16 (Table 2, entry 4)

Au	−1.007055	−0.358868	−0.031940
P	−3.222814	0.385706	0.108406
O	2.589015	−2.768153	0.291956
C	2.375333	3.579830	−1.012862
C	2.491923	2.314354	−0.233005
C	1.940760	1.167255	−0.468298
C	1.991630	−0.178745	−0.493523
C	0.920287	−0.998892	−0.120100
C	1.237902	−2.414253	0.158644
C	3.395349	−2.209353	−0.728102
C	3.429147	−0.691230	−0.624822

C	4.217183	−0.208696	0.577718	C	−0.575422	0.221368	1.606612
C	4.167957	0.960521	1.230058	C	−1.707043	−0.044042	0.657574
C	3.410077	2.240491	0.985925	C	−2.853905	0.858919	0.642891
C	−4.440801	−0.841421	−0.454176	C	−4.112313	0.538198	0.294085
C	−3.555790	1.872281	−0.885030	C	−5.121086	1.629409	0.426126
C	−3.740393	0.822728	1.795323	C	−7.360699	2.234762	0.114044
H	2.021006	4.383931	−0.359617	C	−4.519612	−0.799236	−0.203474
H	1.689163	3.477001	−1.853625	C	−3.971868	−1.309154	−1.383797
H	3.362884	3.869099	−1.385342	C	−4.331639	−2.571113	−1.845703
H	0.744484	−2.990298	−0.652473	C	−5.241979	−3.341829	−1.132044
H	0.729424	−2.724195	1.078167	C	−5.794348	−2.841899	0.043942
H	3.012048	−2.502406	−1.716161	C	−5.440429	−1.579825	0.502287
H	4.393502	−2.633879	−0.604192	C	5.646179	0.710927	−1.586801
H	3.861190	−0.293402	−1.550435	C	5.959632	−1.149506	0.605934
H	4.912579	−0.945014	0.977111	C	5.202395	1.592293	1.129931
H	4.817429	1.043472	2.099703	H	0.422614	4.942559	−0.573679
H	4.154836	3.031465	0.823263	H	−0.917163	4.621659	−1.686279
H	2.871112	2.533626	1.895301	H	0.746521	4.279183	−2.182427
H	−4.248724	−1.093048	−1.499822	H	0.496378	−0.664767	−1.597806
H	−5.454618	−0.442779	−0.357477	H	1.032723	−2.701183	−0.358897
H	−4.348745	−1.749911	0.145382	H	1.165686	−0.512910	2.591048
H	−2.908806	2.686673	−0.550703	H	−0.342679	−1.282759	3.141917
H	−4.601819	2.174206	−0.781305	H	−0.665634	1.108875	2.225102
H	−3.341099	1.665304	−1.936026	H	−1.904581	−1.081350	0.407900
H	−3.648577	−0.051295	2.444072	H	−2.680149	1.881670	0.969112
H	−4.778000	1.168302	1.795247	H	−8.267040	1.749706	−0.244242
H	−3.095253	1.614129	2.183959	H	−7.129125	3.104229	−0.504837
				H	−7.486274	2.551179	1.151570
	IN17 (Table 2, entry 1)			H	−3.269905	−0.704370	−1.949681
Au	2.679704	−0.371310	−0.183506	H	−3.902407	−2.949351	−2.768218
P	4.914895	0.204111	−0.004109	H	−5.524640	−4.326304	−1.491034
O	0.424187	−2.029523	1.430330	H	−6.506696	−3.437404	0.606188
O	−6.329050	1.250526	0.007763	H	−5.878215	−1.195136	1.417610
O	−4.886072	2.736905	0.852886	H	5.566021	−0.105480	−2.307908
C	0.051909	4.252533	−1.337551	H	6.699694	0.968721	−1.445404
C	−0.068225	2.905666	−0.810871	H	5.108246	1.578861	−1.975026
C	−0.180565	1.788156	−0.368760	H	5.608505	−1.471525	1.588826
C	−0.316588	0.454399	0.146899	H	6.997659	−0.813091	0.681578
C	0.483447	−0.618596	−0.511066	H	5.900793	−1.994963	−0.083210
C	0.710562	−1.802243	0.159131	H	4.646172	2.467116	0.785886
C	0.185869	−0.889304	2.273345	H	6.269224	1.830591	1.165308

H	4.856041	1.325492	2.130948

IN17 (Table 2, entry 2)

Au	−1.960545	0.270419	−0.329524
P	−4.065144	−0.499644	0.240200
O	0.055993	2.725688	0.315980
O	6.205978	−1.149958	0.734095
O	7.181700	0.442467	−0.510641
C	1.268317	−4.027741	−0.015231
C	1.216846	−2.577409	−0.014881
C	1.185511	−1.370785	−0.013827
C	1.138379	0.064863	−0.039914
C	0.141282	0.691843	−0.955048
C	−0.249670	1.996868	−0.743577
C	0.533051	2.039312	1.486156
C	1.425271	0.865924	1.196462
C	2.453373	0.890705	0.102332
C	3.726624	0.202557	0.299325
C	4.893364	0.613865	−0.205840
C	6.127167	−0.140616	0.071205
C	8.440972	−0.198595	−0.296198
C	−4.981818	−1.162133	−1.180609
C	−5.131014	0.789179	0.947672
C	−4.036846	−1.835524	1.468954
H	0.775892	−4.441545	0.869767
H	2.304544	−4.378292	−0.021691
H	0.771101	−4.433466	−0.901361
H	−0.745292	2.578373	−1.515569
H	0.070423	0.322684	−1.975794
H	−0.349029	1.690628	2.036239
H	1.040412	2.802486	2.076912
H	1.687155	0.299117	2.084503
H	2.481454	1.775372	−0.527775
H	3.718478	−0.700637	0.906914
H	4.977320	1.505635	−0.818534
H	9.173606	0.400636	−0.834234
H	8.427012	−1.218074	−0.687695
H	8.684236	−0.223862	0.768347
H	−5.105290	−0.379440	−1.932465
H	−5.965267	−1.517754	−0.860266
H	−4.423349	−1.989715	−1.623730
H	−4.671573	1.188151	1.854755
H	−6.111492	0.369700	1.190585
H	−5.251254	1.601602	0.227724
H	−3.483245	−2.688676	1.070512
H	−5.058978	−2.143331	1.707202
H	−3.540831	−1.487525	2.377675

IN17 (Table 2, entry 3)

Au	−1.979389	−0.409994	0.316820
P	−4.264650	−0.299271	−0.021797
O	0.644921	−1.983584	−0.738527
C	−0.387549	4.739648	0.190329
C	0.045101	3.359780	0.063044
C	0.410054	2.214124	−0.047296
C	0.836956	0.848130	−0.166400
C	0.197196	−0.146772	0.741906
C	0.232337	−1.486393	0.417183
C	0.712704	−1.080608	−1.855027
C	1.227619	0.288144	−1.507726
C	2.318877	0.511012	−0.503140
C	3.294274	1.594430	−0.681546
C	4.618327	1.533826	−0.475567
C	5.433473	0.373366	−0.092017
C	6.532065	0.570218	0.756395
C	7.330172	−0.494009	1.153277
C	7.059971	−1.779910	0.694246
C	5.992399	−1.987115	−0.173020
C	5.189199	−0.922915	−0.565391
C	−4.941021	1.344985	0.345752
C	−5.205689	−1.454727	1.014777
C	−4.763921	−0.660029	−1.729619
H	−0.830149	5.101805	−0.742391
H	0.454280	5.391808	0.441523
H	−1.137077	4.839888	0.981104
H	0.113799	0.093049	1.799786
H	0.041842	−2.259896	1.155278
H	−0.303701	−0.991349	−2.258321
H	1.343162	−1.582371	−2.589590
H	1.193248	0.982059	−2.342010
H	2.673722	−0.371859	0.019452
H	2.876465	2.555201	−0.975637

H	5.170883	2.466502	−0.573867
H	6.751726	1.572737	1.112426
H	8.169715	−0.318685	1.818612
H	7.686463	−2.612136	0.998652
H	5.789561	−2.982169	−0.556732
H	4.385226	−1.095456	−1.272833
H	−4.735908	1.601283	1.387606
H	−6.021410	1.351200	0.175566
H	−4.467011	2.088321	−0.299113
H	−4.903572	−2.479579	0.788149
H	−6.276392	−1.341045	0.822068
H	−5.002161	−1.251084	2.068363
H	−4.288685	0.051134	−2.408860
H	−5.850665	−0.582902	−1.825938
H	−4.446549	−1.670266	−1.997856

IN17 (Table 2, entry 4)

Au	−0.903470	−0.278712	0.342535
P	−3.047615	0.321301	−0.287901
O	1.256645	−2.603060	−0.239949
C	2.026848	4.221357	−0.054880
C	2.077310	2.770757	−0.029484
C	2.126077	1.564582	−0.007059
C	2.173743	0.130022	0.053275
C	1.219781	−0.538059	0.984510
C	0.910536	−1.870143	0.805718
C	1.674620	−1.908253	−1.428154
C	2.506249	−0.683616	−1.169305
C	3.533379	−0.614417	−0.082979
C	4.779857	0.137339	−0.288222
C	5.939139	−0.178446	0.284620
C	−3.292603	2.120293	−0.310462
C	−4.328105	−0.330881	0.821712
C	−3.503880	−0.258282	−1.946876
H	1.507208	4.585075	−0.946352
H	3.035235	4.645659	−0.053897
H	1.501206	4.606262	0.824183
H	1.123634	−0.149753	1.996088
H	0.457810	−2.464087	1.594406
H	0.764260	−1.619242	−1.967185
H	2.213723	−2.651303	−2.016729
H	2.725095	−0.120043	−2.071382
H	3.612504	−1.478338	0.571954
H	4.723394	0.994482	−0.956902
H	6.030932	−1.027394	0.957504
H	6.835868	0.402482	0.093480
H	−3.106472	2.526140	0.686384
H	−4.317489	2.354279	−0.611912
H	−2.592099	2.576888	−1.013030
H	−4.288702	−1.422566	0.825127
H	−5.316425	−0.004405	0.485285
H	−4.152577	0.031180	1.837157
H	−2.805568	0.146774	−2.682674
H	−4.519437	0.066691	−2.190504
H	−3.454584	−1.349060	−1.977661

IN18

Au	−0.125759	−0.048900	−0.144392
P	−2.303572	−0.770956	0.097386
O	0.488457	3.330407	−0.030202
C	0.944314	3.524113	1.296134
C	1.422180	2.678751	−0.839260
C	1.648012	1.261218	−0.486619
C	2.168333	0.162305	−0.259944
C	2.891699	−0.968326	−0.021736
C	3.535423	−1.974762	0.180730
C	4.311076	−3.166433	0.414317
C	−3.381310	0.535874	0.745110
C	−2.466783	−2.168233	1.243491
C	−3.057944	−1.314090	−1.459505
H	0.180778	4.107551	1.811835
H	1.891941	4.077805	1.310838
H	1.078441	2.570082	1.822620
H	2.404596	3.174712	−0.803771
H	1.054580	2.729180	−1.867539
H	3.655106	−4.006551	0.662861
H	5.010207	−3.016905	1.242386
H	4.883406	−3.430958	−0.480164
H	−3.010582	0.869527	1.716742
H	−4.401096	0.155739	0.853574
H	−3.380171	1.384163	0.057060
H	−1.888830	−3.016941	0.871692

H	−3.518912	−2.454515	1.329369
H	−2.084736	−1.882209	2.225732
H	−3.041043	−0.494219	−2.180948
H	−4.092149	−1.623852	−1.284785
H	−2.489253	−2.153473	−1.865834

IN19

Au	−0.698087	0.412850	0.003852
P	−2.414448	−1.127180	−0.057301
O	4.957285	−1.691938	−0.255728
C	5.697433	−0.778998	−1.041859
C	4.444605	−1.113962	0.915245
C	3.327351	−0.204754	0.672051
C	2.397287	0.539717	0.454507
C	1.355329	1.390238	0.217221
C	0.544550	2.298710	0.008846
C	−0.129220	3.568348	−0.206096
C	−2.099593	−2.494537	−1.205446
C	−3.993845	−0.396722	−0.568755
C	−2.718761	−1.895037	1.557109
H	6.097697	−1.340085	−1.887276
H	6.529770	−0.346993	−0.470307
H	5.068806	0.035652	−1.424661
H	5.224461	−0.571663	1.472112
H	4.095457	−1.932172	1.552802
H	−0.859864	3.757496	0.584465
H	−0.649633	3.576266	−1.166872
H	0.614910	4.370861	−0.199799
H	−1.967059	−2.101142	−2.215559
H	−2.940591	−3.193798	−1.193080
H	−1.188162	−3.017560	−0.907857
H	−4.264821	0.408363	0.117447
H	−4.775057	−1.162090	−0.559871
H	−3.897532	0.014048	−1.576153
H	−1.813064	−2.402535	1.896287
H	−3.533943	−2.620107	1.478628
H	−2.984878	−1.124528	2.283792

IN20

Au	−0.163740	−0.073023	−0.081980
P	−2.460110	0.147874	0.076036
O	2.223703	2.122602	0.462553
C	2.605274	3.480176	0.515078
C	2.333820	1.590665	−0.826533
C	1.997247	0.134167	−0.826985
C	2.033129	−0.654238	0.300743
C	2.057868	−2.123507	0.310718
C	2.264066	−2.743440	1.480598
C	1.899185	−2.866095	−0.979103
C	−3.105685	−0.297218	1.712900
C	−3.361976	−0.893575	−1.104767
C	−3.032087	1.842623	−0.231413
H	2.489019	3.810714	1.548373
H	1.970587	4.100973	−0.131813
H	3.653129	3.613399	0.214282
H	3.367626	1.687077	−1.203313
H	1.689848	2.129102	−1.538359
H	1.976093	−0.328497	−1.811425
H	2.235154	−0.163809	1.250865
H	2.386250	−2.181359	2.402034
H	2.326460	−3.825524	1.541682
H	1.921891	−3.943958	−0.810491
H	2.701074	−2.611408	−1.680750
H	0.951853	−2.613802	−1.469296
H	−2.863550	−1.339580	1.931558
H	−4.191012	−0.163343	1.732259
H	−2.646638	0.338377	2.473165
H	−3.068791	−0.632180	−2.123922
H	−4.438738	−0.742106	−0.987026
H	−3.121338	−1.943850	−0.926222
H	−2.585397	2.519149	0.500479
H	−4.121931	1.886458	−0.151233
H	−2.729153	2.156682	−1.232775

IN21

Au	0.765583	−0.481880	−0.267768
P	2.415312	1.053677	0.238245
O	−4.187553	1.323728	−0.440060
C	−5.191511	2.304409	−0.562845
C	−4.220911	0.684604	0.803676
C	−3.161957	−0.350118	0.905559
C	−2.327759	−0.675333	−0.088835

C	−1.304850	−1.715177	−0.000456
C	−0.569503	−2.042168	−1.125231
C	−1.174770	−2.522346	1.255372
C	3.730426	1.110644	−1.012020
C	3.252409	0.708412	1.811168
C	1.798645	2.755716	0.377150
H	−5.090148	2.752383	−1.552785
H	−5.081838	3.091759	0.196324
H	−6.196035	1.868031	−0.471397
H	−5.201530	0.206825	0.977848
H	−4.089514	1.410586	1.625201
H	−3.107055	−0.852277	1.868344
H	−2.414499	−0.158885	−1.040486
H	−0.831111	−1.610743	−2.088740
H	0.044976	−2.938029	−1.130076
H	−0.328337	−3.207573	1.197326
H	−2.086936	−3.113561	1.394073
H	−1.061487	−1.888407	2.138175
H	4.192654	0.125537	−1.105190
H	4.488543	1.842814	−0.720111
H	3.305234	1.392680	−1.977710
H	2.525257	0.741809	2.625542
H	4.034995	1.451207	1.990237
H	3.697024	−0.288517	1.777877
H	1.341054	3.057539	−0.567529
H	2.622973	3.433334	0.616899
H	1.044147	2.805184	1.165407

IN22

Au	−1.480756	−0.105154	−0.380281
P	−3.264389	0.296703	1.024483
O	0.063663	−2.561517	−1.700461
C	2.082769	2.660368	−2.040910
C	1.662791	2.279698	−0.614531
C	2.387478	3.177962	0.401079
C	3.709776	2.454003	0.632048
C	3.277165	0.989602	0.736816
C	2.119021	0.875054	−0.234456
C	1.564301	−0.258013	−0.706919
C	0.400124	−0.193691	−1.610790
C	−0.206104	−1.331381	−2.106120
C	0.843090	−2.629724	−0.499728
C	2.046235	−1.688011	−0.512644
C	2.908647	−2.043345	0.671203
C	3.973476	−1.381409	1.128900
C	4.387646	−0.045904	0.572236
C	4.783037	−1.903937	2.275060
C	−2.879291	1.490393	2.337983
C	−3.859491	−1.190521	1.878399
C	−4.711600	0.977166	0.165378
H	1.733654	3.671278	−2.274996
H	1.678382	1.983374	−2.797515
H	3.171797	2.650439	−2.146588
H	0.574281	2.375780	−0.531859
H	2.504824	4.201891	0.035834
H	1.824582	3.220832	1.340699
H	4.381481	2.591648	−0.223285
H	4.240314	2.789632	1.526844
H	2.856174	0.861124	1.746034
H	0.201315	0.711346	−2.175926
H	−0.887256	−1.302330	−2.950973
H	1.157364	−3.669536	−0.420460
H	0.175560	−2.383870	0.338487
H	2.608682	−1.939964	−1.428609
H	2.662779	−2.991592	1.148750
H	4.654884	−0.130807	−0.488765
H	5.282689	0.305193	1.095271
H	4.402871	−2.858983	2.645818
H	4.788919	−1.186071	3.104621
H	5.829900	−2.040624	1.977553
H	−2.056216	1.111869	2.947932
H	−3.759220	1.645477	2.968665
H	−2.579431	2.441374	1.892171
H	−4.186648	−1.927617	1.141793
H	−4.697056	−0.934760	2.533767
H	−3.050426	−1.621354	2.472213
H	−4.439705	1.915439	−0.323283
H	−5.519154	1.159407	0.880258
H	−5.053465	0.270264	−0.593869

IN23

Au	1.240585	0.098388	0.372656

P	3.014702	−0.244964	−1.069222	H	3.543845	0.132979	−3.397334
O	−2.037876	3.646897	−0.361915	H	2.466837	1.399114	−2.747059
C	−4.865259	−1.250733	−0.804576	H	3.765032	−2.386348	−0.250429
C	−3.426705	−1.262783	−1.335586	H	4.319679	−2.093435	−1.921041
C	−2.894411	−2.701318	−1.423283	H	2.627943	−2.564979	−1.604064
C	−2.323912	−2.956644	−0.033363	H	4.333931	1.692664	−0.506122
C	−1.609520	−1.641324	0.291607	H	5.330811	0.425109	−1.268924
C	−2.459212	−0.578365	−0.375031	H	4.828016	0.270091	0.435979
C	−2.381410	0.757378	−0.216946				
C	−3.201252	1.668873	−1.014855			**IN24**	
C	−3.026369	2.999582	−1.011700	Au	−1.146603	−0.525702	−0.085727
C	−1.004573	2.787870	0.101795	S	4.648576	−0.379844	−0.146507
C	−1.555474	1.536010	0.789905	P	−2.074793	−2.631668	0.024668
C	−0.455678	0.918609	1.614523	O	5.235821	−0.083144	1.146807
C	−0.366442	−0.352188	2.136734	O	5.274909	0.091445	−1.368462
C	−1.290899	−1.474974	1.768808	N	3.107014	0.283670	−0.123308
C	0.504152	−0.612110	3.331387	C	4.405843	−2.131627	−0.269158
C	2.677490	0.327346	−2.758639	C	−0.699527	3.369835	−2.242885
C	3.479176	−1.993017	−1.228360	C	−1.484492	2.198317	−1.636721
C	4.525790	0.618434	−0.554286	C	−2.908541	2.638271	−1.280141
H	−5.536722	−1.739142	−1.518646	C	−2.735136	3.327708	0.067812
H	−5.231945	−0.234668	−0.637906	C	−1.771286	2.404950	0.821033
H	−4.940684	−1.786689	0.146951	C	−0.895197	1.788056	−0.281107
H	−3.416215	−0.778875	−2.317802	C	0.374130	1.225863	−0.152980
H	−3.671467	−3.413978	−1.713464	C	1.146474	0.882211	−1.350686
H	−2.091757	−2.762994	−2.167312	C	2.432950	0.489297	−1.312269
H	−3.130952	−3.132433	0.687829	C	2.288355	0.149336	1.073622
H	−1.648076	−3.814896	0.011396	C	1.223892	1.245086	1.117542
H	−0.647040	−1.665825	−0.247008	C	0.525616	1.162189	2.448468
H	−4.010407	1.285104	−1.622457	C	−0.418642	2.003684	2.860866
H	−3.675584	3.684314	−1.547170	C	−1.015451	3.055694	1.979959
H	−0.408605	3.384907	0.793887	C	−0.991535	−3.938428	−0.619387
H	−0.376870	2.498697	−0.752612	C	−3.610892	−2.768028	−0.931312
H	−2.270171	1.912882	1.543100	C	−2.503734	−3.145799	1.711002
H	0.126158	1.673760	2.147976	H	5.395285	−2.592584	−0.289902
H	−2.221460	−1.317121	2.333093	H	3.866924	−2.351213	−1.191690
H	−0.861106	−2.409852	2.143148	H	3.851455	−2.475119	0.604995
H	1.156368	0.231229	3.565591	H	−1.170398	3.675805	−3.182159
H	1.107071	−1.514483	3.197873	H	0.339611	3.111098	−2.455871
H	−0.149795	−0.794290	4.194062	H	−0.690758	4.235082	−1.574383
H	1.806481	−0.198100	−3.156526	H	−1.485062	1.368583	−2.349343

H	−3.343238	3.283826	−2.047564	C	0.172755	1.100347	−0.089641
H	−3.558206	1.762362	−1.168641	C	0.868830	0.666369	−1.314958
H	−2.291511	4.321249	−0.059112	C	2.067513	0.075767	−1.345734
H	−3.672461	3.455091	0.614832	C	2.844031	−0.266604	−0.108457
H	−2.381744	1.598809	1.248740	C	1.924037	−0.267266	1.113983
H	0.696350	0.999670	−2.326809	C	0.996477	0.948444	1.187292
H	3.009178	0.342532	−2.217926	C	0.253725	0.905489	2.498999
H	2.932928	0.235930	1.947871	C	−0.567778	1.854842	2.939263
H	1.798249	−0.834936	1.083130	C	−0.975241	3.025704	2.101411
H	1.755752	2.209247	1.069907	C	−1.784339	−3.780959	−0.763372
H	0.883593	0.391647	3.128470	C	−4.268105	−2.325158	−1.061925
H	−0.824938	1.884330	3.862598	C	−3.247944	−2.924860	1.577362
H	−0.238899	3.722106	1.581685	H	6.486180	1.372634	−1.875822
H	−1.711066	3.678318	2.548884	H	6.567717	1.340128	−0.089263
H	−0.759466	−3.738509	−1.667744	H	5.609272	2.599894	−0.914808
H	−1.491305	−4.907631	−0.534722	H	5.761983	−3.136230	1.424420
H	−0.060456	−3.960707	−0.048725	H	5.500262	−3.331441	−0.334132
H	−4.346914	−2.057732	−0.548432	H	4.282552	−3.941618	0.820782
H	−4.008374	−3.783819	−0.850567	H	−0.938280	3.862457	−3.048386
H	−3.411304	−2.538756	−1.980312	H	0.453873	3.028920	−2.344797
H	−1.604628	−3.159418	2.331084	H	−0.384555	4.274000	−1.420377
H	−2.947567	−4.145243	1.691792	H	−1.619896	1.601062	−2.304469
H	−3.216634	−2.438824	2.140867	H	−3.159116	3.769865	−1.949801
				H	−3.620011	2.271378	−1.128927
		IN25		H	−1.985389	4.559701	0.086216
Au	−1.562590	−0.415664	−0.102631	H	−3.495256	3.897378	0.714725
P	−2.741301	−2.397086	−0.082774	H	−2.522185	1.826870	1.263886
O	4.139832	1.472076	0.998238	H	0.369123	0.843946	−2.259871
O	3.071834	−2.489812	−1.050893	H	2.514602	−0.183592	−2.299165
O	4.809542	0.677869	−0.987790	H	2.529252	−0.304149	2.021662
O	4.394278	−1.867577	0.648819	H	1.309744	−1.175373	1.084477
C	3.994632	0.731428	0.061833	H	1.636900	1.843995	1.200366
C	3.441249	−1.666118	−0.255135	H	0.475188	0.055470	3.141393
C	5.939107	1.560144	−0.954008	H	−1.016957	1.748094	3.924105
C	5.018549	−3.158550	0.630051	H	−0.096563	3.585771	1.755038
C	−0.529837	3.447768	−2.121853	H	−1.587112	3.718878	2.684620
C	−1.497883	2.395114	−1.563061	H	−1.509032	−3.560759	−1.797130
C	−2.840929	3.038894	−1.202133	H	−2.378178	−4.698917	−0.732113
C	−2.581912	3.644882	0.171097	H	−0.871786	−3.916470	−0.178661
C	−1.786230	2.554284	0.894905	H	−4.922892	−1.546986	−0.663514
C	−0.989560	1.859146	−0.217004	H	−4.782637	−3.289355	−1.018976

H	−4.026766	−2.086933	−2.100177
H	−2.364250	−3.054223	2.205934
H	−3.791822	−3.871774	1.516381
H	−3.890606	−2.163929	2.025394

IN26

Au	−1.465308	−0.271640	−0.621688
P	−3.077126	1.332176	−0.265620
O	−0.654092	−3.203659	0.336992
C	7.208745	0.690757	−1.896208
C	6.389409	1.258073	−0.746609
C	4.974651	0.694861	−0.690313
C	4.150446	1.279109	0.446292
C	2.755618	0.743850	0.559850
C	2.216914	−0.215708	−0.156482
C	1.381606	−1.233344	−0.136035
C	0.345485	−1.562778	−1.105266
C	−0.600189	−2.525682	−0.804571
C	0.563326	−3.245916	1.115060
C	1.288753	−1.915732	1.220385
C	0.643175	−0.930652	2.176869
C	0.863272	0.388505	2.336370
C	1.855746	1.305569	1.643987
C	0.075795	1.129227	3.382907
C	−4.443055	1.246070	−1.458445
C	−2.434184	3.025384	−0.389013
C	−3.857827	1.219125	1.368776
H	8.222047	1.103778	−1.908901
H	6.746019	0.918038	−2.862765
H	7.296503	−0.398586	−1.820811
H	6.898518	1.052337	0.203619
H	6.339170	2.350808	−0.836486
H	4.465694	0.888085	−1.643522
H	5.020470	−0.396419	−0.582354
H	4.655896	1.101060	1.406197
H	4.095056	2.373232	0.349885
H	0.437640	−1.240256	−2.138711
H	−1.326448	−2.866472	−1.536839
H	1.216761	−3.979895	0.634478
H	0.261498	−3.624627	2.091514
H	2.300500	−2.158932	1.562554
H	−0.101503	−1.371395	2.840290
H	2.513582	1.698896	2.432650
H	1.313293	2.190811	1.282537
H	−0.644219	0.479379	3.885088
H	−0.466043	1.974316	2.941870
H	0.743195	1.552887	4.143043
H	−4.053275	1.356071	−2.472658
H	−5.163851	2.043652	−1.256896
H	−4.940681	0.277406	−1.374025
H	−1.638087	3.172444	0.344025
H	−3.237996	3.743283	−0.202734
H	−2.024882	3.187762	−1.388667
H	−4.351533	0.249937	1.469305
H	−4.596506	2.017219	1.486350
H	−3.098012	1.307042	2.148391

TS1

Au	−1.791497	−0.173274	0.026855
P	−3.500209	1.389004	0.092256
O	0.330567	−4.000976	0.320727
C	5.210068	4.607146	0.817084
C	4.474139	4.008216	−0.371855
C	3.698875	2.748858	−0.008919
C	2.972296	2.154292	−1.221523
C	2.203521	0.968814	−0.913531
C	1.550127	−0.014408	−0.628979
C	0.822412	−1.124985	−0.303159
C	−0.302597	−1.656431	0.026606
C	−0.712124	−3.059592	0.323012
C	1.113694	−3.923931	−0.848394
C	2.194431	−2.888866	−0.726656
C	2.750614	−2.552760	0.470550
C	3.962234	−1.770603	0.647581
C	4.308918	−1.416831	1.896345
C	4.806744	−1.431858	−0.544464
C	−2.958847	3.064624	−0.354599
C	−4.261222	1.557476	1.733347
C	−4.873781	1.010057	−1.034456
H	5.755023	5.512199	0.532526
H	5.936026	3.899800	1.231976
H	4.514827	4.876642	1.619395

H	3.780924	4.749824	−0.788320
H	5.190254	3.773984	−1.169373
H	4.379486	1.995934	0.404874
H	2.964911	2.975336	0.772511
H	2.291558	2.899759	−1.653291
H	3.693533	1.909254	−2.011940
H	−1.484914	−3.341091	−0.408443
H	−1.173486	−3.100748	1.312981
H	0.489456	−3.729751	−1.730494
H	1.581488	−4.904300	−0.991208
H	2.675711	−2.586176	−1.653892
H	2.266485	−2.911716	1.375806
H	3.692014	−1.688858	2.747970
H	5.215041	−0.852507	2.094696
H	5.675383	−0.840590	−0.248715
H	4.242649	−0.866062	−1.291550
H	5.163509	−2.343388	−1.036783
H	−2.175778	3.390737	0.333540
H	−3.801117	3.760678	−0.303056
H	−2.554942	3.059792	−1.369431
H	−4.687928	0.599380	2.038525
H	−5.049425	2.315406	1.708122
H	−3.500219	1.849464	2.460380
H	−4.500328	0.953329	−2.059364
H	−5.642607	1.785460	−0.970583
H	−5.307671	0.044262	−0.765973

TS2

Au	−0.644203	−1.216135	−0.019996
P	−2.947648	−1.366707	0.372303
O	3.501479	−2.319330	−0.662954
C	−3.017650	5.421552	0.443263
C	−2.043655	5.027085	−0.656794
C	−1.189735	3.823370	−0.281328
C	−0.206546	3.437607	−1.392392
C	0.606799	2.278078	−1.062483
C	1.280854	1.327728	−0.745063
C	2.043810	0.142797	−0.473870
C	1.363418	−1.093957	−0.316963
C	2.112198	−2.353503	−0.463591
C	3.901967	−1.284064	−1.536109
C	3.520470	0.059196	−0.966509
C	3.372920	0.181518	0.476622
C	3.790456	1.340874	1.311359
C	3.204210	2.532873	1.397307
C	5.028103	1.003995	2.097503
C	−3.962564	−0.536634	−0.886979
C	−3.447177	−0.617444	1.951106
C	−3.580408	−3.069212	0.438524
H	−3.625280	6.282592	0.148904
H	−2.488592	5.689442	1.364085
H	−3.701553	4.599607	0.681427
H	−2.597512	4.803562	−1.577328
H	−1.388412	5.875503	−0.890536
H	−0.629354	4.038251	0.636009
H	−1.836215	2.965635	−0.060675
H	−0.757120	3.235318	−2.319406
H	0.457334	4.283909	−1.607995
H	1.601973	−2.841368	−1.320217
H	1.914263	−3.013658	0.388950
H	3.453685	−1.410743	−2.531090
H	4.987221	−1.359170	−1.629838
H	3.815551	0.941500	−1.525177
H	3.480777	−0.761429	1.005835
H	2.305463	2.788035	0.852601
H	3.630040	3.291488	2.047263
H	5.359455	1.865688	2.680068
H	5.845628	0.697298	1.435326
H	4.841007	0.169321	2.782341
H	−3.697738	0.522143	−0.931544
H	−5.024132	−0.635105	−0.642876
H	−3.773144	−0.986330	−1.864465
H	−2.926333	−1.114718	2.772594
H	−4.527024	−0.715265	2.093679
H	−3.175367	0.440672	1.954991
H	−3.392715	−3.568090	−0.515089
H	−4.655463	−3.065451	0.639692
H	−3.066335	−3.619907	1.229641

TS3

Au	−1.243881	−0.862281	−0.053396
P	−3.377929	−0.026938	0.399390

O	2.111097	−3.542203	−0.819314	H	−4.581536	−2.098405	0.693927
C	−0.135436	6.149467	−0.979007	H	−3.089730	2.244527	−0.370133
C	1.019346	5.419070	−0.310396	H	−4.815223	1.795078	−0.314578
C	0.958159	3.911797	−0.521667	H	−3.773635	1.209963	−1.638773
C	2.142123	3.192863	0.136626	H	−3.452385	−0.374064	2.788676
C	2.068729	1.748090	−0.032342	H	−4.636916	0.858364	2.277346
C	1.749619	0.601968	−0.338942	H	−2.903002	1.263282	2.383979
C	1.727047	−0.777020	−0.571614				
C	0.637070	−1.587196	−0.427643			**TS4**	
C	0.793380	−3.048670	−0.674789	Au	−1.345393	−0.558851	0.018465
C	2.907181	−2.711106	−1.633055	P	−3.501116	0.199260	0.525978
C	3.116009	−1.365652	−0.959376	O	2.005797	−3.204328	−0.764453
C	3.666605	−1.466660	0.402169	C	1.102249	2.857413	−2.679207
C	4.078940	−0.392668	1.165622	C	0.460896	2.753541	−1.314624
C	4.144165	0.867121	0.565251	C	1.013885	3.648215	−0.232257
C	4.286866	−0.531643	2.647532	C	2.419985	3.229902	0.184289
C	−4.720862	−1.210365	0.072986	C	2.506505	1.752381	0.426814
C	−3.810440	1.448778	−0.573349	C	1.728521	0.846179	−0.099726
C	−3.621305	0.480450	2.129421	C	1.649367	−0.472377	−0.501064
H	−0.076607	7.228324	−0.806898	C	0.525973	−1.260854	−0.400464
H	−1.100537	5.805018	−0.592053	C	0.688797	−2.713067	−0.673417
H	−0.134701	5.985355	−2.061851	C	2.823963	−2.375008	−1.564180
H	1.971435	5.800056	−0.700176	C	3.022794	−1.016524	−0.908268
H	1.018019	5.632820	0.765705	C	3.895152	−1.096286	0.323917
H	0.022924	3.516564	−0.108685	C	4.106716	−0.177575	1.277438
H	0.953318	3.684736	−1.593680	C	3.602897	1.244464	1.347178
H	3.083322	3.554774	−0.294381	C	4.993730	−0.506142	2.445392
H	2.173676	3.430024	1.206925	C	−3.546856	1.518629	1.777772
H	0.195907	−3.294265	−1.570979	C	−4.583246	−1.103225	1.189547
H	0.346234	−3.609741	0.151587	C	−4.407189	0.874889	−0.900192
H	2.440894	−2.557197	−2.616148	H	0.887332	3.837788	−3.118340
H	3.859054	−3.226842	−1.776516	H	0.708849	2.097853	−3.360323
H	3.642607	−0.668256	−1.614804	H	2.188954	2.742878	−2.633981
H	3.550839	−2.435089	0.885387	H	−0.630767	2.814195	−1.376284
H	4.341989	0.969253	−0.493909	H	0.601011	1.680887	−0.914574
H	4.350175	1.741720	1.176878	H	1.037032	4.687770	−0.578210
H	4.301247	−1.582867	2.941504	H	0.355318	3.610541	0.641032
H	3.475993	−0.039572	3.195465	H	3.152256	3.482392	−0.593033
H	5.226731	−0.071921	2.963385	H	2.736172	3.757204	1.089322
H	−4.694834	−1.512501	−0.976497	H	0.121686	−2.936518	−1.597519
H	−5.691655	−0.759012	0.296669	H	0.195984	−3.282303	0.122048

H	2.373483	−2.240789	−2.558621	C	1.845845	3.327954	−0.402550
H	3.777032	−2.895180	−1.683394	C	3.297226	1.067359	1.776681
H	3.457465	−0.336115	−1.650094	C	2.306834	1.831519	2.665007
H	4.392645	−2.055374	0.463068	C	4.581091	1.890140	1.684396
H	4.462162	1.900080	1.144210	C	3.587024	−0.282987	2.439798
H	3.314831	1.473373	2.381615	C	3.431134	−0.678068	−0.648614
H	5.423489	−1.505514	2.351899	C	4.802280	−0.452283	−0.844864
H	4.431549	−0.459001	3.385827	C	5.647904	−1.434691	−1.336562
H	5.814751	0.215227	2.533487	C	5.134818	−2.687902	−1.641613
H	−3.066711	1.167944	2.694275	C	3.781925	−2.929705	−1.463502
H	−4.580491	1.801934	1.995616	C	2.909779	−1.945204	−0.980640
H	−3.001789	2.391664	1.411052	C	1.480260	−2.356474	−0.885588
H	−4.674400	−1.910247	0.458872	C	0.556525	−1.961377	−1.856998
H	−5.575434	−0.699141	1.409668	C	−0.740780	−2.462935	−1.843633
H	−4.146281	−1.509674	2.104694	C	−1.134515	−3.362862	−0.858996
H	−3.859208	1.726459	−1.310591	C	−0.221299	−3.762867	0.110922
H	−5.407578	1.198717	−0.599206	C	1.078766	−3.268574	0.094337
H	−4.490762	0.108804	−1.674584	H	−3.287216	5.091031	−0.372773
				H	−3.037263	4.030403	1.016094

TS4-JohnPhos

Au	0.184843	0.143404	0.667899	H	−4.321173	3.672948	−0.151679
P	2.435873	0.669437	0.125050	H	−1.286342	3.604966	−0.724301
O	−3.108068	−1.532963	2.905287	H	−2.223670	2.176505	−0.411530
C	−3.298641	4.045478	−0.045456	H	−2.866791	3.965951	−2.807950
C	−2.311475	3.248310	−0.862935	H	−1.781167	2.574940	−2.818896
C	−2.647127	3.013046	−2.313170	H	−4.779279	2.598529	−2.215570
C	−3.843298	2.080477	−2.460798	H	−3.948636	1.730275	−3.492287
C	−3.735977	0.895395	−1.549480	H	−1.386315	−0.473737	3.377253
C	−2.991844	0.826136	−0.475342	H	−1.189704	−1.953277	2.449772
C	−2.887553	0.210581	0.761079	H	−3.786159	0.352968	3.418544
C	−1.713517	−0.242734	1.317462	H	−5.007964	−0.922770	3.215734
C	−1.825371	−1.067951	2.552716	H	−4.850346	0.846427	1.354576
C	−4.080633	−0.513668	2.808094	H	−5.397008	−1.948484	1.123840
C	−4.265091	−0.081132	1.361657	H	−5.482611	0.077412	−2.360110
C	−4.948882	−1.147870	0.536219	H	−4.076076	−0.897177	−2.661267
C	−5.050132	−1.269450	−0.794870	H	−6.154244	−3.113474	−0.603561
C	−4.581287	−0.321948	−1.873703	H	−5.071976	−3.049046	−2.007346
C	−5.754419	−2.460597	−1.382095	H	−6.583377	−2.149959	−2.029280
C	2.449868	2.108347	−1.101907	H	1.455822	2.498752	−2.969939
C	1.534016	1.674693	−2.251341	H	0.527959	1.426644	−1.898916
C	3.812152	2.477819	−1.687619	H	1.937583	0.808029	−2.783711
C	1.845845	3.327954	−0.402550	H	3.674812	3.351039	−2.335904

H	4.221265	1.676278	−2.306189	C	4.188196	1.215182	0.649443
H	4.548262	2.745569	−0.927409	C	4.963729	−0.274650	2.553628
H	1.662520	4.107890	−1.150474	C	−4.841083	−0.989018	0.441831
H	2.522913	3.743130	0.348077	C	−4.196561	1.604727	−0.617638
H	0.892756	3.091187	0.081180	C	−3.709607	1.023037	2.157346
H	2.778009	1.992335	3.641634	H	0.245681	2.625818	−2.934458
H	1.383735	1.266416	2.823391	H	0.671482	0.912409	−2.825793
H	2.044622	2.810356	2.259152	H	1.941693	2.146185	−2.780620
H	4.953744	2.051310	2.702752	H	−0.257587	1.751723	−0.670661
H	4.407284	2.873697	1.241917	H	0.985138	4.178023	−1.028466
H	5.376266	1.388115	1.131747	H	0.721640	3.521184	0.593960
H	3.940295	−0.100863	3.460906	H	3.291427	3.390628	−1.047798
H	4.358615	−0.848500	1.912160	H	3.144562	3.791632	0.660000
H	2.686498	−0.903588	2.505523	H	1.667195	1.253942	0.903695
H	5.228503	0.511405	−0.603965	H	0.055725	−2.883562	−1.571509
H	6.702182	−1.218426	−1.473890	H	−0.049245	−3.137472	0.168549
H	5.780975	−3.472559	−2.021606	H	2.401286	−2.395214	−2.350485
H	3.372150	−3.902890	−1.714310	H	3.679898	−3.097495	−1.336635
H	0.863441	−1.274712	−2.638805	H	3.569451	−0.539459	−1.404902
H	−1.441868	−2.154761	−2.612876	H	3.769473	−2.204110	1.093006
H	−2.146433	−3.754720	−0.849705	H	4.880430	1.292696	−0.210291
H	−0.517912	−4.470239	0.878976	H	4.563833	1.957745	1.359737
H	1.793477	−3.597912	0.842367	H	5.000396	−1.308202	2.904431
				H	4.467708	0.333581	3.319660
		TS5		H	5.992412	0.097760	2.474163
Au	−1.404140	−0.432420	−0.017245	H	−4.899711	−1.407513	−0.565800
P	−3.563228	0.306199	0.490020	H	−5.814719	−0.574952	0.718997
O	1.822728	−3.241064	−0.554191	H	−4.577324	−1.790698	1.135496
C	0.921900	1.910569	−2.458253	H	−3.529679	2.469774	−0.586941
C	0.773270	1.994168	−0.942461	H	−5.201943	1.912125	−0.315436
C	1.216260	3.342475	−0.366461	H	−4.227003	1.227732	−1.642734
C	2.717401	3.174797	−0.132834	H	−3.429719	0.273194	2.901049
C	2.911548	1.719990	0.097652	H	−4.735142	1.353623	2.345191
C	1.734405	1.004783	−0.266154	H	−3.031921	1.874881	2.251670
C	1.650480	−0.464907	−0.462773				
C	0.488675	−1.150395	−0.412164			**TS6**	
C	0.539934	−2.641695	−0.608283	Au	1.530131	−0.385624	−0.049210
C	2.757102	−2.511908	−1.315410	P	3.685802	0.342870	0.431374
C	2.989817	−1.145601	−0.693382	O	−1.501876	−3.251069	−0.988724
C	3.724678	−1.226405	0.616402	C	−0.290195	2.512781	0.368477
C	4.252890	−0.173363	1.240925	C	−0.895882	1.828297	−0.864855

C	−1.738426	2.812658	−1.686848	H	3.388875	0.815488	2.780517
C	−3.060840	2.865258	−0.929533	H	4.501900	0.765263	−1.801456
C	−3.289295	1.415317	−0.478806	H	5.444340	1.668608	−0.585411
C	−1.910835	0.792732	−0.428129	H	3.821442	2.230731	−1.066829
C	−1.672743	−0.509055	−0.146634				
C	−0.372512	−1.131290	−0.388248			**TS7**	
C	−0.412155	−2.469134	−0.864647	Au	−1.257310	−0.588167	−0.034583
C	−2.767697	−2.604433	−0.806757	P	−3.430129	0.064292	0.550436
C	−2.684944	−1.549610	0.296536	O	2.140326	−3.137022	−0.902897
C	−4.059156	−1.223227	0.804112	C	−0.884581	2.960598	−1.801634
C	−4.678558	−0.070995	1.074444	C	0.574341	2.825859	−1.430821
C	−4.134250	1.297893	0.785717	C	1.066217	3.704550	−0.310075
C	−6.034147	−0.079955	1.719467	C	2.456756	3.286593	0.146081
C	4.859167	−1.016036	0.715284	C	2.550162	1.805520	0.369576
C	3.788150	1.369735	1.928087	C	1.789986	0.899884	−0.184069
C	4.440522	1.350116	−0.880695	C	1.733992	−0.414815	−0.600612
H	0.400854	3.301435	0.053505	C	0.625810	−1.225683	−0.501096
H	0.265361	1.795488	0.980754	C	0.815425	−2.670750	−0.797186
H	−1.057144	2.969875	1.000307	C	2.941034	−2.280779	−1.691753
H	−0.087842	1.389504	−1.453863	C	3.115390	−0.929331	−1.015520
H	−1.252874	3.787238	−1.786753	C	3.988278	−1.012585	0.216799
H	−1.899182	2.413430	−2.694645	C	4.174310	−0.113049	1.193830
H	−2.977742	3.519703	−0.055009	C	3.632066	1.292619	1.302753
H	−3.891330	3.236692	−1.534533	C	5.069846	−0.448573	2.353618
H	−3.826312	0.889505	−1.281564	C	−4.429476	−1.302246	1.216676
H	0.501307	−3.057083	−0.908134	C	−4.409092	0.718693	−0.837065
H	−0.240842	−1.654363	−1.771883	C	−3.501732	1.356897	1.828653
H	−3.463760	−3.402871	−0.546245	H	−1.527746	2.851540	−0.923878
H	−3.080201	−2.156324	−1.757229	H	−1.180175	2.217447	−2.546666
H	−2.209398	−2.078455	1.140565	H	−1.067489	3.952453	−2.231275
H	−4.598898	−2.132678	1.070705	H	0.709085	1.748890	−1.042773
H	−3.559966	1.663634	1.647272	H	1.227379	2.884228	−2.307694
H	−4.981465	1.986476	0.683546	H	1.095124	4.750208	−0.636170
H	−6.370634	−1.092012	1.955960	H	0.367298	3.645779	0.532162
H	−6.779328	0.391808	1.067539	H	3.206915	3.554091	−0.609783
H	−6.022702	0.502664	2.648941	H	2.746083	3.801479	1.067184
H	4.524426	−1.616405	1.564360	H	0.247726	−2.887743	−1.722732
H	5.856473	−0.618683	0.924052	H	0.337324	−3.263306	−0.010083
H	4.901919	−1.655034	−0.169791	H	2.485784	−2.139818	−2.683117
H	3.195198	2.276942	1.791152	H	3.903277	−2.781250	−1.821075
H	4.827903	1.642934	2.129078	H	3.540123	−0.231158	−1.746642

H	4.513034	−1.960202	0.332793
H	4.480074	1.975553	1.147883
H	3.311625	1.476111	2.336796
H	5.524668	−1.434087	2.235007
H	4.507312	−0.439622	3.295018
H	5.872836	0.290448	2.459924
H	−4.499785	−2.098363	0.471799
H	−5.434143	−0.953686	1.471956
H	−3.947730	−1.704051	2.111122
H	−3.918848	1.604611	−1.247292
H	−5.416175	0.984236	−0.503398
H	−4.474926	−0.037666	−1.622725
H	−2.996966	1.003956	2.731037
H	−4.540918	1.600942	2.066533
H	−2.991446	2.255218	1.473235

TS7-JohnPhos

Au	−0.008673	0.198196	−0.394358
P	−2.053666	−1.002832	−0.518692
O	3.245101	2.532856	−2.001915
C	1.081216	−0.055315	3.901630
C	2.401657	−0.461014	3.297246
C	2.741870	−1.925639	3.291360
C	3.962198	−2.184748	2.420296
C	3.881132	−1.447815	1.117547
C	3.105259	−0.421695	0.873897
C	2.988248	0.695397	0.058663
C	1.835100	1.054058	−0.600519
C	1.947678	2.140661	−1.614012
C	4.100812	2.691219	−0.889946
C	4.339857	1.355922	−0.201222
C	5.199000	0.436282	−1.042043
C	5.359782	−0.893752	−0.991328
C	4.786046	−1.893884	−0.013070
C	6.255213	−1.570024	−1.992896
C	−2.380618	−1.254795	−2.366826
C	−2.365102	0.148201	−2.983019
C	−3.711001	−1.916589	−2.722665
C	−1.223336	−2.069500	−2.949153
C	−1.854587	−2.633433	0.444945
C	−0.389944	−3.072440	0.319975
C	−2.733139	−3.800914	−0.004912
C	−2.135461	−2.309809	1.915155
C	−3.566852	−0.186300	0.148697
C	−4.760192	−0.924581	0.169858
C	−5.934108	−0.412486	0.700150
C	−5.941002	0.869659	1.232232
C	−4.775131	1.618467	1.214712
C	−3.581048	1.119566	0.677417
C	−2.432479	2.071163	0.715030
C	−2.147326	2.882112	−0.386919
C	−1.195236	3.891659	−0.293486
C	−0.511703	4.102452	0.899786
C	−0.784159	3.295878	1.999378
C	−1.741481	2.290205	1.909724
H	0.248440	−0.603790	3.454244
H	0.900211	1.015638	3.784949
H	1.093283	−0.274788	4.976090
H	2.324285	−0.185646	2.160019
H	3.231342	0.151331	3.663494
H	2.945270	−2.264717	4.313256
H	1.884913	−2.499386	2.921378
H	4.876924	−1.849028	2.926975
H	4.095163	−3.252415	2.218911
H	1.382092	3.004000	−1.214594
H	1.428382	1.840049	−2.529552
H	3.665662	3.403174	−0.172625
H	5.035551	3.111365	−1.268646
H	4.825262	1.555341	0.762578
H	5.752916	0.949388	−1.827746
H	5.638384	−2.389620	0.471120
H	4.283929	−2.694141	−0.574040
H	6.687277	−0.853266	−2.694246
H	5.700216	−2.320447	−2.568731
H	7.075229	−2.100693	−1.494425
H	−2.532481	0.058589	−4.062569
H	−1.405614	0.651059	−2.827289
H	−3.159805	0.779618	−2.574934
H	−3.745831	−2.036759	−3.811771
H	−4.563825	−1.295606	−2.439798
H	−3.834015	−2.906251	−2.280774
H	−1.309078	−2.067899	−4.041680

H	−1.242913	−3.110620	−2.618020	C	−4.407148	0.953210	−0.900124
H	−0.252009	−1.637293	−2.686879	C	−3.263760	1.800406	1.605089
H	−0.254323	−3.988130	0.907396	H	1.513457	6.649013	−1.653113
H	0.296296	−2.313614	0.706174	H	0.230935	5.456958	−1.416834
H	−0.105465	−3.294645	−0.710783	H	1.493356	5.170440	−2.620621
H	−2.517706	−4.654137	0.649161	H	3.208368	5.041355	−0.779292
H	−2.509850	−4.112695	−1.027377	H	1.952086	5.321661	0.414605
H	−3.802314	−3.600806	0.077868	H	0.812851	3.203317	−0.293562
H	−1.850877	−3.175815	2.523602	H	2.086404	2.921431	−1.474634
H	−3.191708	−2.101324	2.099792	H	3.781814	2.842523	0.385414
H	−1.550560	−1.452149	2.263384	H	2.512299	3.115358	1.559199
H	−4.779617	−1.926822	−0.234604	H	−0.481745	−3.198363	−1.514564
H	−6.835358	−1.016504	0.697498	H	0.539145	−3.353689	−0.097926
H	−6.848277	1.288321	1.655458	H	2.999648	−2.333837	−2.922813
H	−4.777153	2.625287	1.619814	H	3.484306	−3.426535	−1.617833
H	−2.694412	2.738256	−1.312910	H	3.599768	−0.742605	−1.467770
H	−0.996441	4.522983	−1.153871	H	3.841542	−2.824238	0.478720
H	0.224017	4.896951	0.974456	H	4.175236	0.933343	1.879467
H	−0.262144	3.459121	2.937112	H	2.694047	0.500721	2.697784
H	−1.970897	1.681665	2.779028	H	4.468815	−2.701291	2.586717
				H	3.395022	−1.682992	3.565495
		TS8		H	4.996706	−1.098202	3.130147
Au	−1.386756	−0.595556	−0.115930	H	−4.759906	−1.643673	0.765618
P	−3.431873	0.356114	0.513543	H	−5.470289	−0.276719	1.666487
O	1.471776	−3.238828	−1.968314	H	−4.045014	−1.136181	2.309147
C	1.300436	5.576326	−1.621769	H	−3.837321	1.709741	−1.444599
C	2.144746	4.874323	−0.568684	H	−5.348661	1.388688	−0.553486
C	1.877037	3.376630	−0.498128	H	−4.619969	0.122348	−1.576658
C	2.711159	2.683491	0.569514	H	−2.749606	1.507468	2.523476
C	2.496231	1.207247	0.665280	H	−4.248158	2.206081	1.854612
C	1.774420	0.435204	−0.080869	H	−2.671401	2.569395	1.103749
C	1.592626	−0.738443	−0.715587				
C	0.373655	−1.423675	−0.694266			**TS9**	
C	0.457901	−2.841300	−1.084463	Au	1.351210	−0.562340	−0.021702
C	2.764698	−2.649546	−1.902473	P	3.445920	0.313604	−0.589533
C	2.921321	−1.443232	−0.971311	O	−1.786208	−3.215435	1.363736
C	3.477867	−1.800758	0.398258	C	−0.208654	2.505002	2.878694
C	3.570660	−1.057382	1.514578	C	−0.573469	2.570810	1.417579
C	3.222993	0.401072	1.742169	C	−1.752990	3.428983	1.045083
C	4.140424	−1.674826	2.761447	C	−2.279713	3.102982	−0.348054
C	−4.537950	−0.782700	1.400481	C	−2.326004	1.626131	−0.588365

C	−1.681022	0.716757	0.086766	H	4.844512	−1.539770	0.073098
C	−1.651190	−0.632329	0.426556				
C	−0.477027	−1.350447	0.445245			**TS10**	
C	−0.551177	−2.783151	0.835118	Au	1.299624	−0.504558	−0.040210
C	−2.868369	−2.757976	0.587444	P	3.456621	0.251429	−0.545712
C	−3.017527	−1.236644	0.709159	O	−1.811407	−3.293184	1.038392
C	−4.155637	−0.797620	−0.178176	C	0.168748	1.967200	2.591348
C	−4.265416	0.089575	−1.177824	C	−0.429097	2.227372	1.245566
C	−3.196010	1.034980	−1.690831	C	−1.312091	3.416445	1.028330
C	−5.563839	0.219841	−1.920700	C	−2.129180	3.182432	−0.237875
C	3.629616	2.092236	−0.251085	C	−2.407758	1.721587	−0.353908
C	3.847246	0.135537	−2.354923	C	−1.777878	0.879665	0.470257
C	4.837425	−0.467615	0.282894	C	−1.720445	−0.583175	0.491503
H	0.136991	3.490727	3.212469	C	−0.565615	−1.272653	0.371446
H	0.600231	1.792383	3.059650	C	−0.609894	−2.769237	0.502962
H	−1.068184	2.225102	3.493879	C	−2.928597	−2.741955	0.388926
H	0.294117	2.755759	0.776217	C	−3.070839	−1.249080	0.700003
H	−0.867670	1.481523	1.115704	C	−4.242924	−0.732520	−0.093022
H	−2.551979	3.281190	1.779552	C	−4.365813	0.236884	−1.005966
H	−1.464054	4.485504	1.087446	C	−3.274220	1.192072	−1.451078
H	−3.284411	3.512303	−0.486732	C	−5.672353	0.456598	−1.710635
H	−1.656742	3.550546	−1.134064	C	4.641045	−1.102778	−0.819871
H	0.206806	−2.996297	1.596370	C	4.228772	1.274674	0.747728
H	−0.270083	−3.383184	−0.050789	C	3.571258	1.264822	−2.053846
H	−3.765707	−3.257028	0.959695	H	0.971068	2.704756	2.719445
H	−2.730387	−3.035792	−0.468914	H	0.622140	0.974734	2.642221
H	−3.301205	−1.026329	1.750483	H	−0.549905	2.098216	3.403040
H	−5.065144	−1.358310	0.041700	H	0.244392	1.988341	0.422906
H	−3.679427	1.865288	−2.212948	H	−1.484324	1.332540	1.495932
H	−2.563925	0.529544	−2.429396	H	−1.959718	3.554595	1.899116
H	−6.305583	−0.500438	−1.568921	H	−0.678275	4.304118	0.936178
H	−5.413349	0.059934	−2.995298	H	−3.050660	3.770665	−0.264564
H	−5.976845	1.229766	−1.809704	H	−1.551109	3.466908	−1.128201
H	2.895793	2.653134	−0.834591	H	0.185302	−3.105821	1.174850
H	4.635404	2.428792	−0.518595	H	−0.403741	−3.224423	−0.482282
H	3.454687	2.282850	0.810438	H	−3.808332	−3.289145	0.736942
H	3.853788	−0.923867	−2.621589	H	−2.846165	−2.881330	−0.700907
H	4.827640	0.570107	−2.569504	H	−3.339505	−1.164762	1.765052
H	3.086961	0.640760	−2.955087	H	−5.148169	−1.308816	0.104502
H	4.720403	−0.324444	1.359668	H	−3.732655	2.033000	−1.976989
H	5.785134	−0.027761	−0.040178	H	−2.625532	0.691746	−2.184887

H	−6.428373	−0.266124	−1.396154
H	−5.545370	0.369557	−2.796803
H	−6.055477	1.466697	−1.521426
H	4.691533	−1.730675	0.072888
H	5.635793	−0.704486	−1.039280
H	4.305194	−1.717479	−1.658312
H	3.616448	2.161452	0.928507
H	5.232748	1.586041	0.445175
H	4.292733	0.701471	1.675817
H	3.179207	0.700088	−2.902956
H	4.610717	1.540963	−2.252611
H	2.972992	2.171143	−1.933297

TS11

Au	−1.334942	−0.554777	−0.031512
P	−3.441275	0.291200	0.545923
O	1.793441	−3.322155	−1.186449
C	−0.527270	2.870974	−1.287830
C	0.825705	2.470811	−1.811756
C	2.003200	3.316749	−1.405089
C	2.395899	3.095383	0.053804
C	2.360542	1.641054	0.398099
C	1.715633	0.715477	−0.259850
C	1.674572	−0.665072	−0.475090
C	0.493993	−1.368887	−0.450581
C	0.555218	−2.831257	−0.719355
C	2.866037	−2.813384	−0.428984
C	3.036647	−1.309738	−0.675429
C	4.164974	−0.810065	0.192056
C	4.253080	0.137268	1.137254
C	3.153734	1.087628	1.575140
C	5.540777	0.336613	1.882448
C	−4.666992	−1.009515	0.887852
C	−4.219887	1.338532	−0.721722
C	−3.425972	1.319545	2.046776
H	−0.514911	3.044468	−0.208296
H	−1.280163	2.109861	−1.510018
H	−0.838442	3.801407	−1.777340
H	1.051895	1.391025	−1.382216
H	0.811002	2.243274	−2.881550
H	2.859203	3.074681	−2.040822
H	1.762627	4.374237	−1.564995
H	3.402888	3.479352	0.238861
H	1.734937	3.628479	0.749464
H	−0.190558	−3.092411	−1.478056
H	0.248039	−3.356801	0.203575
H	3.763952	−3.352962	−0.737955
H	2.702513	−2.998274	0.643963
H	3.344432	−1.193245	−1.724857
H	5.082423	−1.371664	0.011424
H	3.600834	1.931004	2.107513
H	2.478214	0.591860	2.280301
H	6.303460	−0.381660	1.573839
H	5.384066	0.228115	2.962601
H	5.930016	1.349577	1.723642
H	−4.801089	−1.626667	−0.003664
H	−5.625884	−0.565741	1.170165
H	−4.308535	−1.644976	1.700887
H	−3.594637	2.215411	−0.905877
H	−5.210395	1.664756	−0.391778
H	−4.316012	0.775918	−1.653330
H	−3.037511	0.736070	2.884719
H	−4.435695	1.666413	2.284007
H	−2.774007	2.182415	1.891563

TS12

Au	−1.321178	−0.503492	−0.060637
P	−3.438396	0.286152	0.550128
O	1.761079	−3.320535	−1.136020
C	−0.362378	2.520925	−1.322349
C	1.041726	2.400252	−1.788027
C	2.074746	3.380917	−1.325566
C	2.415480	3.094992	0.135945
C	2.372084	1.622795	0.326127
C	1.846100	0.851951	−0.638874
C	1.699611	−0.614995	−0.613336
C	0.529779	−1.279966	−0.506197
C	0.555435	−2.778885	−0.628185
C	2.858321	−2.810555	−0.423140
C	3.051097	−1.313090	−0.690322
C	4.113492	−0.829839	0.268281
C	4.076248	0.072070	1.256099

C	2.882553	0.966654	1.568070	C	1.044242	2.794822	−1.376830
C	5.259226	0.290023	2.150879	C	2.181969	3.188773	−0.437046
C	−4.648131	−1.031372	0.889135	C	2.629900	1.862908	0.067912
C	−4.244690	1.330967	−0.704690	C	1.802131	0.901661	−0.311677
C	−3.444165	1.306841	2.058245	C	1.765401	−0.473635	−0.541212
H	−0.442475	2.767564	−0.263019	C	0.679208	−1.286131	−0.356443
H	−0.940536	1.621183	−1.544283	C	0.900650	−2.756290	−0.472154
H	−0.796896	3.342622	−1.910527	C	3.021982	−2.432455	−1.390816
H	1.984528	1.230889	−1.704677	C	3.161920	−0.998559	−0.900886
H	1.109160	2.112931	−2.840737	C	4.075977	−0.888172	0.300099
H	2.968711	3.293956	−1.946967	C	4.358001	0.180897	1.057366
H	1.668928	4.390119	−1.447393	C	3.852150	1.595828	0.883741
H	3.381701	3.511903	0.433815	C	5.316698	0.056206	2.206906
H	1.665729	3.536896	0.805565	C	−4.568709	−1.437377	0.639038
H	−0.229538	−3.102052	−1.318573	C	−4.218955	0.979248	−0.884618
H	0.321146	−3.232518	0.351288	C	−3.660790	0.958735	1.945199
H	3.742544	−3.371705	−0.736202	H	−1.888248	4.023302	0.053243
H	2.715721	−2.971725	0.657533	H	−0.329379	3.858580	0.859894
H	3.455450	−1.206314	−1.709333	H	−1.198093	2.413408	0.319889
H	5.051803	−1.374850	0.154986	H	−0.940149	3.148570	−2.077916
H	3.171963	1.722980	2.300073	H	−0.051346	4.568072	−1.550691
H	2.075633	0.372517	2.014749	H	0.793170	1.658118	−1.017812
H	6.084797	−0.380375	1.901117	H	1.390863	2.644831	−2.400273
H	4.986379	0.121325	3.199848	H	2.974002	3.713000	−0.981226
H	5.618219	1.324325	2.084319	H	1.864338	3.844618	0.380247
H	−4.774528	−1.648188	−0.003752	H	0.362202	−3.104592	−1.373908
H	−5.613111	−0.602517	1.174085	H	0.424793	−3.258841	0.376086
H	−4.280000	−1.664766	1.699565	H	2.565646	−2.436833	−2.391750
H	−3.631533	2.215097	−0.895851	H	3.996945	−2.921275	−1.455202
H	−5.234961	1.648185	−0.365125	H	3.548468	−0.391546	−1.728618
H	−4.345283	0.769753	−1.636771	H	4.559239	−1.821695	0.585496
H	−3.039317	0.727657	2.891487	H	4.661447	2.187362	0.429653
H	−4.460567	1.629364	2.301655	H	3.711936	2.047910	1.875181
H	−2.812454	2.185527	1.907125	H	5.735685	−0.949787	2.274531
				H	4.819032	0.287895	3.156279
		TS13		H	6.145064	0.767781	2.104974
Au	−1.233357	−0.652526	−0.005091	H	−4.573462	−2.040153	−0.272194
P	−3.447733	−0.020161	0.426447	H	−5.584851	−1.091519	0.849168
O	2.240839	−3.194906	−0.495170	H	−4.220343	−2.059985	1.466234
C	−0.956963	3.450974	0.062325	H	−3.651588	1.901713	−1.026956
C	−0.273486	3.520385	−1.294010	H	−5.250634	1.227138	−0.618990

H	−4.212346	0.416943	−1.821396
H	−3.281537	0.392496	2.799126
H	−4.718158	1.188374	2.105041
H	−3.096164	1.890436	1.867321

TS14

Au	−1.343145	−0.577396	0.015836
P	−3.485308	0.241654	0.483240
O	1.989227	−3.269236	−0.699536
C	0.345207	2.114549	−1.834909
C	1.079235	3.422243	−1.838729
C	1.308470	3.920670	−0.411418
C	2.452026	3.214761	0.296654
C	2.456805	1.713647	0.382672
C	1.683903	0.836751	−0.218400
C	1.641909	−0.531629	−0.534238
C	0.524277	−1.305584	−0.399285
C	0.670931	−2.774136	−0.613056
C	2.786597	−2.472033	−1.549005
C	2.998727	−1.086962	−0.953122
C	3.936059	−1.117316	0.229461
C	4.118118	−0.207198	1.193664
C	3.483893	1.153379	1.351212
C	5.101880	−0.478658	2.298096
C	−3.928103	1.730861	−0.465130
C	−3.743601	0.716668	2.220211
C	−4.815862	−0.946788	0.124935
H	0.626975	1.483904	−0.866461
H	0.538813	1.434578	−2.663191
H	−0.725163	2.197558	−1.620213
H	2.037797	3.326147	−2.358147
H	0.480860	4.150369	−2.397383
H	1.547566	4.987402	−0.428639
H	0.381778	3.815359	0.165114
H	3.404250	3.491165	−0.176978
H	2.525040	3.583409	1.326992
H	0.097507	−3.040488	−1.520796
H	0.192941	−3.308553	0.214308
H	2.313189	−2.378819	−2.537967
H	3.738694	−2.994116	−1.670511
H	3.407832	−0.442357	−1.742026
H	4.532565	−2.025712	0.306775
H	4.304496	1.884659	1.354985
H	3.052928	1.223761	2.360247
H	5.573131	−1.456618	2.180928
H	4.608120	−0.450053	3.276764
H	5.890127	0.283173	2.320261
H	−3.231741	2.538465	−0.227147
H	−4.945200	2.049752	−0.219356
H	−3.866649	1.517463	−1.534846
H	−3.574494	−0.148794	2.864998
H	−4.762521	1.085643	2.367542
H	−3.031835	1.498686	2.494721
H	−4.784347	−1.222738	−0.931653
H	−5.791627	−0.510556	0.356753
H	−4.669597	−1.848667	0.723894

TS15

Au	−1.550366	0.031758	0.081822
P	−3.621145	1.040494	0.095364
O	−0.047869	−3.866434	−1.426142
C	4.532708	5.210691	−1.363352
C	4.278720	4.348026	−0.136205
C	3.305925	3.209224	−0.412208
C	3.064550	2.341645	0.830143
C	2.140601	1.250226	0.588566
C	1.402003	0.315643	0.362259
C	0.474077	−0.686501	0.116477
C	0.395812	−1.937545	−0.129826
C	−0.461603	−3.132579	−0.311708
C	1.304777	−4.235007	−1.204456
C	2.136795	−3.046446	−0.800223
C	2.781530	−3.032872	0.404829
C	3.880861	−2.172361	0.789263
C	4.320207	−2.253136	2.058358
C	4.539610	−1.295064	−0.231611
C	−4.868363	0.163259	−0.891212
C	−3.580797	2.728380	−0.572127
C	−4.336538	1.193919	1.757547
H	5.229239	6.024645	−1.141168
H	3.604166	5.660450	−1.730910
H	4.961363	4.620827	−2.180568

H	5.227614	3.932408	0.225385	C	1.105180	−0.315223	0.102420
H	3.885116	4.969794	0.677579	C	−0.055771	−0.852001	−0.020522
H	2.348097	3.613878	−0.758929	C	−0.548907	−2.235264	−0.246183
H	3.693520	2.578509	−1.220536	C	1.635918	−2.855560	−1.181716
H	4.017905	1.931313	1.186412	C	2.592015	−1.938260	−0.475807
H	2.670590	2.965101	1.642705	C	2.868927	−2.042307	0.852922
H	−1.487449	−2.798821	−0.480545	C	3.935285	−1.333465	1.513035
H	−0.437577	−3.744252	0.603760	C	4.178550	−1.469394	2.823203
H	1.674430	−4.657432	−2.140769	C	−2.613553	3.964783	−0.090759
H	1.353329	−5.005538	−0.422488	C	−4.174853	2.217400	1.598609
H	2.453891	−2.369482	−1.589650	C	−4.402303	2.031721	−1.276001
H	2.467857	−3.762179	1.150928	H	−0.936167	−6.323551	−1.624193
H	3.847477	−2.918423	2.774985	H	0.025865	−5.106476	−2.513227
H	5.160742	−1.659959	2.405334	H	−1.575082	−4.664783	−1.821870
H	5.348184	−0.718824	0.221640	H	5.322064	6.676918	−1.454317
H	3.828234	−0.597398	−0.680772	H	3.700698	6.202104	−1.971950
H	4.961474	−1.898436	−1.042410	H	5.103373	5.249532	−2.472603
H	−4.531413	0.098103	−1.928147	H	5.515773	4.604089	−0.074092
H	−5.821610	0.698051	−0.850906	H	4.126299	5.554189	0.425934
H	−5.001363	−0.847681	−0.499689	H	2.627752	4.084389	−0.939205
H	−2.904728	3.342683	0.026735	H	4.020260	3.131088	−1.439398
H	−4.583812	3.163831	−0.548646	H	4.474235	2.533175	0.957910
H	−3.216910	2.705581	−1.601668	H	3.092986	3.489068	1.465297
H	−4.454187	0.201952	2.199221	H	−1.134686	−2.229628	−1.177887
H	−5.311596	1.686121	1.700917	H	−1.227864	−2.506635	0.564784
H	−3.668789	1.783361	2.389860	H	1.261547	−2.386882	−2.099641
				H	2.180045	−3.759579	−1.471734

TS16

Au	−1.497817	0.681634	0.026181	H	3.233840	−1.332661	−1.111783
S	0.110263	−4.814273	−0.165897	H	2.257621	−2.706816	1.460323
P	−3.199353	2.252801	0.066822	H	4.565980	−0.690911	0.903469
O	−0.881487	−4.886089	0.896013	H	3.564442	−2.114661	3.445918
O	1.351754	−5.562952	−0.056575	H	4.999744	−0.947322	3.303377
N	0.531117	−3.212415	−0.301660	H	−1.940421	4.198188	0.737134
C	−0.674417	−5.266066	−1.692037	H	−3.460547	4.656906	−0.077222
C	4.671597	5.817459	−1.641641	H	−2.067121	4.078937	−1.029712
C	4.527249	4.952002	−0.398873	H	−4.622096	1.228737	1.724352
C	3.622680	3.748252	−0.625898	H	−4.965030	2.972743	1.561098
C	3.485774	2.886939	0.636034	H	−3.521410	2.417719	2.450658
C	2.632953	1.732965	0.459454	H	−3.893528	2.111577	−2.239217
C	1.898622	0.780406	0.290253	H	−5.182922	2.795376	−1.213640
C	1.105180	−0.315223	0.102420	H	−4.856855	1.041448	−1.199031

TS17

Au	−0.084084	1.358130	0.237447
S	−3.799963	−1.441201	−0.792141
P	−0.373856	3.643861	0.232307
O	−4.166195	−0.087436	−0.401482
O	−4.828514	−2.415710	−1.114476
N	−2.962779	−2.073426	0.505562
C	−2.700760	−1.338773	−2.184037
C	7.643755	−0.665371	−0.184292
C	6.528018	−1.141053	−1.102403
C	5.145330	−0.933095	−0.499007
C	4.027090	−1.424548	−1.429033
C	2.703856	−1.203317	−0.877479
C	1.608954	−1.032842	−0.385150
C	0.366134	−0.738505	0.158426
C	−0.672995	−1.315480	0.625218
C	−2.028408	−1.219602	1.214274
C	−2.429850	−3.439288	0.413743
C	−0.940712	−3.430729	0.176836
C	−0.077535	−3.813725	1.163965
C	1.325591	−4.074568	0.988614
C	2.108748	−4.435204	2.014667
C	−2.068994	4.162717	−0.159608
C	0.681673	4.483458	−0.983105
C	0.014951	4.414527	1.828928
H	−3.281522	−0.930241	−3.013691
H	−2.348603	−2.339544	−2.436607
H	−1.869681	−0.675638	−1.942127
H	8.626696	−0.820451	−0.639264
H	7.631018	−1.205234	0.768589
H	7.546808	0.402758	0.038009
H	6.587627	−0.609377	−2.060313
H	6.667278	−2.205080	−1.330687
H	5.073101	−1.463269	0.457544
H	4.990723	0.130275	−0.283725
H	4.098269	−0.908249	−2.394527
H	4.160214	−2.493938	−1.634459
H	−2.364486	−0.181614	1.184351
H	−2.003416	−1.537587	2.261986
H	−2.952589	−3.984589	−0.373964
H	−2.649151	−3.937089	1.362441
H	−0.579967	−3.368165	−0.847583
H	−0.477913	−3.956629	2.168137
H	1.733436	−3.995643	−0.015195
H	1.713210	−4.518565	3.023454
H	3.160790	−4.659043	1.871336
H	−2.345361	3.789861	−1.148488
H	−2.136793	5.254403	−0.149343
H	−2.760610	3.748161	0.577178
H	1.730926	4.276766	−0.760927
H	0.507256	5.562669	−0.948923
H	0.453330	4.110446	−1.983936
H	−0.633531	3.997547	2.602662
H	−0.137394	5.496149	1.771627
H	1.054485	4.206456	2.091846

TS18

Au	1.404356	−1.110182	−0.338753
P	3.452475	−2.153207	−0.040603
O	−2.653603	−0.188437	2.077783
O	−3.829073	−2.794508	−1.455331
O	−1.978170	−2.257387	1.540986
O	−4.882899	−1.981151	0.348236
C	−2.489036	−1.059900	1.264953
C	−3.887090	−2.028048	−0.530305
C	−1.627559	−2.492316	2.911274
C	−5.933638	−2.942066	0.170163
C	1.078327	7.961521	1.145598
C	1.774241	6.616322	1.286168
C	0.929824	5.463334	0.759485
C	1.648369	4.115179	0.911007
C	0.873192	2.994043	0.421581
C	0.237057	2.044008	0.014582
C	−0.496960	0.971272	−0.429090
C	−0.494918	−0.293954	−0.691396
C	−1.605570	−1.204441	−1.094625
C	−2.842569	−0.955810	−0.217771
C	−3.462748	0.410858	−0.536331
C	−2.572220	1.621716	−0.438113
C	−2.301864	2.377193	−1.549520
C	−1.817416	3.729912	−1.528513
C	−1.583332	4.415493	−2.656603

C	4.791122	−1.019932	0.435017	O	4.399109	−1.543627	−1.621566
C	4.045566	−2.987551	−1.541732	O	3.108049	0.148106	1.215498
C	3.439364	−3.438921	1.243705	O	4.860045	−2.315378	0.433697
H	−1.285045	−3.524429	2.953119	C	2.581600	−1.068023	1.335383
H	−2.497451	−2.353954	3.555544	C	4.051689	−1.851574	−0.511724
H	−0.828180	−1.816136	3.220256	C	3.125375	0.949827	2.405552
H	−6.642418	−2.749918	0.973093	C	6.244796	−2.437922	0.076117
H	−5.536639	−3.955812	0.248890	C	−7.888682	−2.037153	−0.069393
H	−6.414110	−2.807804	−0.800529	C	−6.823040	−1.751908	0.978030
H	1.703769	8.774078	1.527108	C	−5.446386	−1.522189	0.368744
H	0.135088	7.980741	1.701881	C	−4.386931	−1.225494	1.438594
H	0.850118	8.182946	0.097457	C	−3.067758	−0.990398	0.880982
H	2.730441	6.637128	0.748610	C	−1.970903	−0.824747	0.391889
H	2.016137	6.434173	2.340575	C	−0.718693	−0.532161	−0.136194
H	−0.023904	5.426360	1.298035	C	0.336175	−1.130799	−0.539939
H	0.695104	5.627673	−0.297919	C	1.722405	−1.081918	−1.020078
H	2.601321	4.144083	0.367861	C	2.616938	−1.800368	−0.005914
H	1.891659	3.942865	1.966776	C	2.056459	−3.230931	0.139717
H	−1.299458	−2.246311	−1.023118	C	0.555160	−3.219049	0.139807
H	−1.876990	−1.021694	−2.140583	C	−0.164582	−3.599470	−0.955907
H	−4.305978	0.575306	0.140705	C	−1.587428	−3.827267	−0.978562
H	−3.861379	0.351864	−1.554100	C	−2.229498	−4.203501	−2.091966
H	−2.472800	2.079431	0.542733	C	0.926308	4.497875	1.071991
H	−2.492090	1.940487	−2.529737	C	−1.596657	4.744192	−0.313989
H	−1.678158	4.201592	−0.559949	C	0.849582	4.436182	−1.816376
H	−1.729840	3.960279	−3.632646	H	3.669556	1.854491	2.141870
H	−1.249832	5.447734	−2.633336	H	3.638073	0.423195	3.211970
H	4.904683	−0.247894	−0.329308	H	2.105945	1.193880	2.710821
H	5.731446	−1.568808	0.539697	H	6.747468	−2.796769	0.971789
H	4.542484	−0.538786	1.383704	H	6.645520	−1.467947	−0.222999
H	3.312998	−3.733614	−1.857645	H	6.363687	−3.154325	−0.738691
H	5.004421	−3.477982	−1.350625	H	−8.867989	−2.195487	0.392192
H	4.165250	−2.255110	−2.343288	H	−7.646600	−2.934218	−0.649347
H	3.139712	−2.999562	2.197806	H	−7.985027	−1.203624	−0.773456
H	4.434333	−3.882038	1.344075	H	−7.109320	−0.868965	1.563159
H	2.721277	−4.216771	0.974819	H	−6.769104	−2.587058	1.687579
				H	−5.140869	−2.404717	−0.205029
		TS19		H	−5.487596	−0.685191	−0.337666
Au	−0.287919	1.558190	−0.270995	H	−4.690432	−0.347484	2.022147
P	−0.018931	3.845566	−0.335247	H	−4.331582	−2.064566	2.143359
O	2.129166	−1.517390	2.354503	H	2.012162	−0.036483	−1.146414

H	1.815519	−1.574457	−1.992548
H	2.432229	−3.682289	1.059416
H	2.413673	−3.822987	−0.707530
H	0.046103	−3.094082	1.092228
H	0.371790	−3.785981	−1.886487
H	−2.130056	−3.708990	−0.044893
H	−1.702024	−4.325327	−3.034481
H	−3.296250	−4.402638	−2.088862
H	0.407677	4.255719	2.002362
H	1.031399	5.583103	0.985438
H	1.916596	4.037248	1.092656
H	−2.187368	4.465735	−1.189675
H	−1.413940	5.822527	−0.326197
H	−2.156881	4.480232	0.585766
H	1.854271	4.008511	−1.847591
H	0.920268	5.527556	−1.799763
H	0.305355	4.120894	−2.709357

TS20

Au	1.277735	−1.527516	−0.165776
P	3.138145	−2.911447	−0.082370
O	−2.545426	−1.492215	1.848438
O	−4.573564	0.647179	−1.653403
O	−4.051766	0.164673	1.944206
O	−4.675326	−1.357140	−0.655566
C	−3.108754	−0.555783	1.348431
C	−4.136988	−0.164942	−0.884338
C	−4.418729	−0.241772	3.270849
C	−5.873091	−1.660578	−1.387498
C	3.735437	6.979406	−0.398498
C	3.186198	6.121462	0.731290
C	2.418067	4.908670	0.224025
C	1.878407	4.047640	1.372627
C	1.120946	2.899205	0.930958
C	0.500959	1.930905	0.536009
C	−0.253947	0.891207	0.083811
C	−0.419910	−0.339009	−0.285417
C	−1.740660	−0.862514	−0.737615
C	−2.847461	−0.014179	−0.062429
C	−2.414162	1.423173	0.021889
C	−2.045914	2.140133	−1.080280
C	−1.755441	3.548855	−1.044145
C	−1.371565	4.218278	−2.138872
C	4.715677	−2.016739	−0.207386
C	3.185241	−4.140460	−1.420615
C	3.260342	−3.873691	1.454762
H	−5.200716	0.447958	3.581357
H	−3.560773	−0.170453	3.941650
H	−4.796290	−1.265672	3.261145
H	−6.158219	−2.663604	−1.076773
H	−5.677533	−1.635886	−2.460818
H	−6.659212	−0.946370	−1.137150
H	4.282856	7.844124	−0.011790
H	2.929971	7.355973	−1.038205
H	4.421902	6.407969	−1.032392
H	4.010086	5.784479	1.372655
H	2.527747	6.725842	1.367643
H	1.579948	5.233312	−0.403173
H	3.067469	4.293537	−0.408824
H	2.706110	3.691700	2.000161
H	1.238889	4.650684	2.030498
H	−1.880153	−1.913005	−0.485352
H	−1.795962	−0.779274	−1.829917
H	−2.576196	1.949172	0.958067
H	−1.965400	1.642951	−2.044150
H	−1.873723	4.063749	−0.094246
H	−1.255459	3.714219	−3.094563
H	−1.173713	5.284783	−2.109445
H	4.750940	−1.467683	−1.151013
H	5.552796	−2.719274	−0.163012
H	4.795733	−1.303388	0.616119
H	2.288795	−4.763087	−1.378040
H	4.072778	−4.772031	−1.324054
H	3.208756	−3.625895	−2.383918
H	3.307408	−3.192516	2.307397
H	4.156849	−4.500152	1.440172
H	2.375732	−4.505657	1.561068

TS21

Au	1.323450	−1.460762	−0.084119
P	2.430632	−3.480243	−0.286107
O	−3.329562	0.273002	2.394731

O	−4.285644	0.307247	−2.102161	H	−2.173081	2.010129	1.228495
O	−4.176801	−1.353859	1.102384	H	−2.052917	2.068671	−1.867130
O	−5.260191	1.155444	−0.266678	H	−0.895198	3.984068	0.289794
C	−3.531559	−0.215084	1.315058	H	−0.915442	3.979228	−2.795605
C	−4.268282	0.584641	−0.932354	H	−0.190966	5.276096	−1.682998
C	−4.697620	−2.011423	2.268018	H	0.557637	−4.971572	0.013378
C	−6.444877	1.456204	−1.022574	H	1.913479	−5.788406	−0.809161
C	4.736638	6.371698	−0.212915	H	0.869266	−4.652560	−1.705105
C	4.332103	5.379954	0.867376	H	3.979783	−3.249397	1.547713
C	3.368039	4.317168	0.357353	H	3.769162	−4.960537	1.088127
C	2.962408	3.329833	1.459670	H	2.513745	−4.120185	2.038592
C	2.044644	2.305822	0.994451	H	3.301241	−3.197108	−2.518407
C	1.260418	1.478158	0.582573	H	4.206213	−4.447047	−1.622404
C	0.433068	0.452157	0.128953	H	4.487206	−2.716840	−1.288140
C	−0.801929	0.345082	−0.217287				
C	−1.952616	−0.476724	−0.653143			**TS22**	
C	−3.068101	0.370548	−0.013425	Au	−0.572224	−1.221140	−0.113545
C	−2.275119	1.650467	0.208478	P	−2.836573	−1.368055	0.398323
C	−1.832848	2.396352	−0.851133	O	3.541576	−2.288761	−0.964231
C	−1.100023	3.626557	−0.715649	C	−3.462588	4.910567	−0.217942
C	−0.712552	4.330509	−1.787464	C	−2.029864	4.953641	−0.727741
C	1.339586	−4.859713	−0.741124	C	−1.287110	3.643582	−0.502730
C	3.254915	−4.007907	1.244089	C	0.154728	3.693664	−1.019320
C	3.734302	−3.462961	−1.551574	C	0.883034	2.451650	−0.807041
H	−5.188328	−2.910411	1.901170	C	1.470386	1.413211	−0.619077
H	−5.417362	−1.365286	2.773244	C	2.186863	0.187193	−0.408949
H	−3.887534	−2.270997	2.951419	C	1.452427	−1.082984	−0.498668
H	−7.135561	1.906471	−0.312924	C	2.207893	−2.226542	−0.817219
H	−6.869477	0.541096	−1.438097	C	4.209684	−1.084325	−1.364316
H	−6.212070	2.157188	−1.825720	C	3.685549	0.143211	−0.677210
H	5.428814	7.124481	0.176290	C	3.272470	0.120659	0.736752
H	3.864531	6.898931	−0.614342	C	3.406744	1.269934	1.668551
H	5.232570	5.866837	−1.048955	C	4.298382	2.240883	1.471058
H	5.226829	4.890676	1.272280	C	2.480019	1.238863	2.844952
H	3.867918	5.915444	1.705062	C	−3.314434	−2.953374	1.148739
H	2.467244	4.794053	−0.045731	C	−3.923280	−1.188718	−1.048352
H	3.828934	3.763742	−0.468862	C	−3.399990	−0.102109	1.574726
H	3.858234	2.850734	1.873636	H	−3.975400	5.862780	−0.383893
H	2.491972	3.877316	2.285983	H	−3.493718	4.700979	0.856811
H	−1.892896	−1.509266	−0.301875	H	−4.040766	4.130210	−0.724859
H	−2.063410	−0.478242	−1.742465	H	−2.025631	5.191882	−1.798834

H	−1.485813	5.765883	−0.229651	C	−2.511536	−0.377721	−1.719771
H	−1.275894	3.403626	0.567108	C	−2.985707	0.504390	−0.687754
H	−1.818742	2.826200	−1.004731	C	−3.311740	1.887217	−1.231481
H	0.153925	3.933804	−2.089609	C	−4.607694	3.814350	−0.948978
H	0.695143	4.507760	−0.520891	C	−3.933307	−0.069217	0.328268
H	1.556001	−1.725898	−1.774136	C	−3.941775	0.230024	1.692898
H	1.767707	−3.216427	−0.729952	C	−4.906934	−0.311322	2.531027
H	4.094031	−0.975950	−2.448502	C	−5.894493	−1.148851	2.023512
H	5.263452	−1.251185	−1.138551	C	−5.904827	−1.445633	0.666943
H	4.096276	1.071032	−1.062444	C	−4.931847	−0.917120	−0.171975
H	3.280129	−0.850435	1.229619	C	4.096729	2.821358	−0.001588
H	4.970981	2.242899	0.619125	C	5.813181	0.631389	−0.754758
H	4.387087	3.064945	2.173041	C	5.096338	1.016311	2.011015
H	2.608867	0.312929	3.417153	H	−2.486589	2.767209	1.453624
H	1.435398	1.264616	2.513475	H	−1.369893	3.290169	0.179650
H	2.652909	2.085413	3.512234	H	−0.734903	2.753243	1.742012
H	−3.073209	−3.770232	0.464638	H	1.726558	−3.418119	0.038237
H	−4.387082	−2.963652	1.361639	H	1.777507	−2.893684	−1.636835
H	−2.758881	−3.099846	2.077883	H	−0.712144	−3.804136	0.857741
H	−3.742368	−0.223997	−1.527976	H	−1.834331	−4.223026	−0.457660
H	−4.971688	−1.250715	−0.743368	H	−2.304644	−1.950248	0.637285
H	−3.706600	−1.982572	−1.766802	H	−1.604123	−2.173868	−2.333669
H	−2.833873	−0.188769	2.504791	H	−2.502795	0.014607	−2.731024
H	−4.465651	−0.229693	1.785190	H	−5.350928	4.159853	−0.233651
H	−3.230393	0.891346	1.153248	H	−5.039489	3.756517	−1.949512
				H	−3.745866	4.484184	−0.957786
	TS23 (Table 2, entry 1)			H	−3.179106	0.863024	2.124934
Au	2.544319	−0.313146	0.027474	H	−4.882963	−0.076925	3.590166
P	4.413728	1.060184	0.324951	H	−6.648095	−1.567428	2.682405
O	0.001037	−3.670779	−1.087171	H	−6.669545	−2.094959	0.253456
O	−4.222780	2.506309	−0.499681	H	−4.954941	−1.151172	−1.229949
O	−2.799547	2.340357	−2.222846	H	3.743344	2.945317	−1.027880
C	−1.514730	2.576551	0.996595	H	5.010340	3.405449	0.141223
C	−1.372011	1.203951	0.502967	H	3.323932	3.186519	0.678950
C	−0.739670	0.134814	0.432824	H	6.123649	−0.397411	−0.557861
C	−0.363464	−1.140538	0.050728	H	6.655682	1.305113	−0.574204
C	0.917564	−1.513002	−0.279580	H	5.504828	0.707348	−1.800127
C	1.139252	−2.907489	−0.747675	H	4.337470	1.353247	2.721091
C	−1.046518	−3.531037	−0.152745	H	5.974577	1.664075	2.084497
C	−1.559361	−2.102391	−0.144820	H	5.379546	−0.007940	2.264479
C	−1.966430	−1.600753	−1.483436				

TS23 (Table 2, entry 2)

Au	−1.750944	0.231570	−0.038129
P	−3.484687	−1.336976	−0.093112
O	0.633294	3.842763	−0.595548
O	5.455529	−1.703008	0.697228
O	4.302429	−1.815731	−1.227276
C	2.587821	−2.058881	2.041473
C	2.163318	−0.878604	1.297614
C	1.418204	0.072575	1.019713
C	1.011365	1.303153	0.537113
C	−0.214428	1.580550	−0.027460
C	−0.464502	2.958660	−0.521430
C	1.483063	3.758631	0.527932
C	2.124650	2.383693	0.589715
C	2.775818	1.977239	−0.673635
C	3.495360	0.824226	−0.845854
C	3.844059	−0.028646	0.219976
C	4.623694	−1.270653	−0.062064
C	5.044750	−2.987135	−1.597570
C	−2.912213	−3.055707	−0.252689
C	−4.643888	−1.101038	−1.474435
C	−4.524013	−1.325735	1.399790
H	2.758134	−2.912913	1.380281
H	1.800033	−2.325463	2.751331
H	3.506977	−1.862156	2.599118
H	−1.256313	3.381754	0.124459
H	−0.895133	2.911850	−1.527083
H	0.928944	3.945379	1.457936
H	2.238794	4.537746	0.409392
H	2.737308	2.254709	1.485237
H	2.505201	2.552933	−1.555507
H	3.723093	0.499335	−1.855401
H	4.075534	0.402400	1.187430
H	4.656625	−3.282362	−2.570103
H	4.886840	−3.783069	−0.867440
H	6.109163	−2.755933	−1.665849
H	−2.338841	−3.164907	−1.176297
H	−3.762652	−3.743301	−0.271208
H	−2.263632	−3.304492	0.590519
H	−5.102211	−0.112090	−1.400781
H	−5.425495	−1.865782	−1.452238
H	−4.101673	−1.164596	−2.420756
H	−3.906404	−1.543533	2.274323
H	−5.317445	−2.074534	1.321200
H	−4.970333	−0.336494	1.525940

TS23 (Table 2, entry 3)

Au	2.126836	0.231417	−0.078731
P	4.014812	−1.145399	−0.056151
O	−0.483488	3.718410	0.088624
C	−1.903920	−2.891338	0.064547
C	−1.714970	−1.448960	0.164963
C	−1.161580	−0.368545	−0.065980
C	−0.801892	0.974441	−0.158501
C	0.475903	1.444026	−0.085237
C	0.670735	2.924450	−0.110612
C	−1.575012	3.276069	−0.686533
C	−2.028532	1.900363	−0.227577
C	−2.503887	1.870206	1.188438
C	−2.952431	0.782186	1.847165
C	−3.296476	−0.524279	1.319977
C	−4.431779	−0.760873	0.427888
C	−4.992485	−2.050029	0.394185
C	−6.116392	−2.317200	−0.371276
C	−6.707897	−1.299709	−1.113006
C	−6.185415	−0.008950	−1.062996
C	−5.067035	0.263029	−0.293379
C	5.589903	−0.242118	−0.179316
C	4.067897	−2.347961	−1.421301
C	4.176531	−2.151280	1.452354
H	−2.047323	−3.346462	1.048329
H	−1.006545	−3.324692	−0.385686
H	−2.757624	−3.141092	−0.569602
H	1.155274	3.187323	−1.068308
H	1.373259	3.211571	0.677502
H	−1.304245	3.232579	−1.751193
H	−2.370988	4.014192	−0.562676
H	−2.746614	1.485075	−0.938454
H	−2.263650	2.749036	1.782798
H	−2.988279	0.832447	2.933689
H	−3.159875	−1.321514	2.049223
H	−4.549943	−2.838438	0.993417

H	−6.538333	−3.316359	−0.380367
H	−7.589712	−1.505341	−1.710944
H	−6.666940	0.793060	−1.612089
H	−4.708912	1.282270	−0.221838
H	5.612111	0.327913	−1.111057
H	6.432442	−0.939248	−0.160108
H	5.676998	0.454965	0.657497
H	3.188560	−2.994613	−1.374678
H	4.972537	−2.959463	−1.359334
H	4.056209	−1.813966	−2.374413
H	4.230457	−1.494678	2.323908
H	5.078601	−2.768066	1.407503
H	3.300644	−2.795910	1.557047

TS23 (Table 2, entry 4)

Au	−0.988258	−0.359102	−0.010956
P	−3.211607	0.350566	0.099955
O	2.605867	−2.824302	0.090429
C	2.082614	3.911262	−0.634520
C	2.123916	2.474306	−0.424348
C	1.910363	1.263838	−0.463639
C	2.003746	−0.125858	−0.359612
C	0.965969	−0.972969	−0.090222
C	1.248982	−2.431252	0.029522
C	3.404526	−2.141334	−0.849117
C	3.457780	−0.662247	−0.509109
C	3.906674	−0.384126	0.866520
C	4.153585	0.878447	1.347063
C	4.142938	1.994168	0.507493
C	−4.415370	−0.890719	−0.465557
C	−3.557025	1.824765	−0.909947
C	−3.764425	0.799676	1.773880
H	2.000946	4.450545	0.313244
H	1.212368	4.160632	−1.248724
H	2.979834	4.256347	−1.156389
H	0.744626	−2.931537	−0.816749
H	0.776790	−2.820951	0.936717
H	3.012090	−2.267771	−1.867629
H	4.400133	−2.587449	−0.801772
H	3.982016	−0.089996	−1.278640
H	3.855372	−1.215238	1.566223
H	4.226428	1.028613	2.419484
H	4.449860	1.906458	−0.527968
H	4.213232	2.986011	0.944259
H	−4.209438	−1.150066	−1.506726
H	−5.434026	−0.501017	−0.383602
H	−4.322090	−1.793894	0.141958
H	−2.921986	2.650113	−0.579421
H	−4.607295	2.115787	−0.817879
H	−3.331472	1.610464	−1.957272
H	−3.671869	−0.065448	2.434436
H	−4.806156	1.132325	1.754545
H	−3.135463	1.603287	2.164209

TS24 (Table 2, entry 1)

Au	−2.136376	−0.096419	0.224361
P	−3.664671	0.913306	−1.209548
O	0.211045	−1.114071	3.727801
O	4.783453	−1.221850	−1.595523
O	4.989180	0.988787	−1.869979
C	−0.051224	−3.660649	−2.648555
C	0.112446	−2.966492	−1.385297
C	0.246598	−2.388820	−0.334345
C	0.411379	−1.722957	0.926715
C	−0.709980	−0.933712	1.457802
C	−0.737575	−0.738818	2.852058
C	1.020781	−2.238877	3.364617
C	1.433277	−2.229854	1.920663
C	1.771146	−0.962031	1.226023
C	2.783436	−0.930283	0.170642
C	3.397273	0.175065	−0.289845
C	4.464898	0.046710	−1.325169
C	5.783756	−1.407427	−2.600965
C	3.074647	1.552891	0.148888
C	1.761175	2.027861	0.090804
C	1.453462	3.316067	0.514641
C	2.454892	4.147956	1.002169
C	3.767064	3.686888	1.057139
C	4.076701	2.403364	0.627508
C	−3.029655	1.129161	−2.898970
C	−4.179520	2.573966	−0.680237
C	−5.210267	−0.025109	−1.401294

H	0.312244	−4.690207	−2.579259
H	0.502297	−3.157488	−3.446891
H	−1.105969	−3.694151	−2.937461
H	−1.503752	−1.641393	2.437174
H	−1.429736	−0.025503	3.292102
H	0.452816	−3.152464	3.574363
H	1.883184	−2.200756	4.030339
H	1.973021	−3.118037	1.606364
H	1.627837	−0.041916	1.783255
H	3.069379	−1.887783	−0.252298
H	5.934017	−2.483427	−2.670444
H	6.714194	−0.914384	−2.312375
H	5.444301	−1.010686	−3.560122
H	0.978613	1.388523	−0.306613
H	0.429460	3.671523	0.456268
H	2.216223	5.153999	1.331812
H	4.554953	4.332016	1.432615
H	5.102688	2.053935	0.667401
H	−2.127713	1.745123	−2.877155
H	−3.782654	1.609388	−3.530058
H	−2.773089	0.153824	−3.318944
H	−4.639158	2.516253	0.309060
H	−4.897103	2.994150	−1.390577
H	−3.304899	3.226054	−0.621360
H	−4.986358	−1.020780	−1.790952
H	−5.884860	0.490910	−2.090314
H	−5.697324	−0.132387	−0.429380

TS24 (Table 2, entry 2)

Au	−1.741681	0.195685	−0.239158
P	−3.385074	−1.449558	−0.311473
O	0.696523	3.709316	−1.003948
O	5.345660	−1.523334	0.736215
O	5.596722	−1.835386	−1.472724
C	0.664937	−1.092302	3.919251
C	0.770419	−0.211554	2.771441
C	0.856701	0.519158	1.815086
C	0.961929	1.399042	0.684850
C	−0.226900	1.595311	−0.162745
C	−0.275204	2.784490	−0.913815
C	1.578132	3.828741	0.119507
C	1.997937	2.501946	0.682204
C	2.261352	1.345640	−0.214226
C	3.291018	0.360744	0.109744
C	3.984988	−0.311822	−0.811852
C	5.029348	−1.269348	−0.403070
C	6.629834	−2.785914	−1.200116
C	−3.834556	−1.970365	−1.994045
C	−4.949668	−0.955323	0.472051
C	−2.890346	−2.975673	0.543262
H	1.472237	−1.830849	3.917546
H	−0.286031	−1.633234	3.905872
H	0.721752	−0.528717	4.855208
H	−0.959365	2.797294	0.141071
H	−1.030313	2.915603	−1.685050
H	1.067951	4.410419	0.895803
H	2.434009	4.398864	−0.242970
H	2.597661	2.567387	1.584513
H	2.063321	1.489208	−1.272809
H	3.508539	0.182479	1.160517
H	3.813199	−0.178127	−1.875133
H	6.976786	−3.131357	−2.172499
H	6.238797	−3.624392	−0.619695
H	7.449631	−2.316671	−0.651957
H	−4.215307	−1.112175	−2.552583
H	−4.600548	−2.750298	−1.959379
H	−2.948225	−2.353809	−2.504742
H	−4.766957	−0.703028	1.519186
H	−5.677572	−1.769811	0.416978
H	−5.351877	−0.075150	−0.034951
H	−1.985146	−3.376629	0.081357
H	−3.687829	−3.722068	0.486667
H	−2.676549	−2.752044	1.591108

TS24 (Table 2, entry 3)

Au	−1.693386	−0.114073	−0.450873
P	−3.463405	−1.460240	0.227732
O	1.477959	1.744070	−2.759379
C	−1.248872	3.060936	3.404490
C	−0.564609	2.623986	2.201898
C	0.000188	2.259812	1.199336
C	0.672829	1.844846	0.001137

C	−0.079030	1.057258	−0.987744
C	0.377260	1.112942	−2.317813
C	1.939530	2.861616	−1.989471
C	1.862227	2.632990	−0.507313
C	2.160026	1.304493	0.087756
C	2.771189	1.167746	1.414045
C	3.670152	0.247345	1.793838
C	4.310925	−0.802950	0.991587
C	4.578028	−2.039352	1.596080
C	5.180167	−3.067931	0.884823
C	5.548892	−2.876271	−0.443649
C	5.317899	−1.645393	−1.048712
C	4.708587	−0.617191	−0.339234
C	−2.932640	−3.010590	1.014433
C	−4.575796	−1.969669	−1.116664
C	−4.540631	−0.655550	1.451650
H	−1.270794	4.152796	3.469737
H	−0.750669	2.677173	4.299779
H	−2.282204	2.701198	3.413213
H	−0.623754	1.836069	−2.055556
H	−0.019729	0.428542	−3.063051
H	1.332811	3.734433	−2.256473
H	2.964942	3.034508	−2.317963
H	2.118917	3.503269	0.088815
H	2.349032	0.497852	−0.613437
H	2.422802	1.872016	2.165723
H	3.952002	0.251874	2.845109
H	4.299639	−2.191111	2.634990
H	5.369154	−4.019829	1.370903
H	6.027325	−3.676628	−0.998745
H	5.625661	−1.478642	−2.076203
H	4.575865	0.349558	−0.812793
H	−2.332248	−3.591745	0.310776
H	−3.803326	−3.597806	1.319874
H	−2.320827	−2.784771	1.890800
H	−4.998758	−1.084951	−1.598135
H	−5.385519	−2.589978	−0.722132
H	−4.013990	−2.537723	−1.861739
H	−3.954238	−0.387193	2.333430
H	−5.352459	−1.327240	1.744759
H	−4.962636	0.256697	1.023534

TS24 (Table 2, entry 4)

Au	−0.865232	−0.407589	−0.090783
P	−3.094631	0.134939	0.284260
O	2.850152	−2.612171	−0.479422
C	1.181443	3.962866	−1.570372
C	1.525766	2.622099	−1.135320
C	1.811775	1.507128	−0.772392
C	2.173651	0.180919	−0.357829
C	1.135322	−0.859230	−0.335055
C	1.575233	−2.191598	−0.443038
C	3.826790	−1.687773	−0.976129
C	3.610831	−0.282737	−0.493325
C	3.137107	−0.004541	0.883851
C	3.574347	1.181428	1.631788
C	3.659601	1.212006	2.959815
C	−4.258826	−1.211094	−0.088610
C	−3.678269	1.550503	−0.694764
C	−3.433074	0.588270	2.012050
H	1.623761	4.712325	−0.907204
H	0.096983	4.107711	−1.563845
H	1.542034	4.152868	−2.585606
H	1.114863	−1.684305	−1.502632
H	0.886702	−3.012703	−0.261636
H	3.790806	−1.708956	−2.071336
H	4.789578	−2.081476	−0.648917
H	4.282890	0.446584	−0.935048
H	2.881643	−0.866848	1.494902
H	3.849247	2.055355	1.045324
H	3.392698	0.351496	3.568085
H	4.007859	2.099251	3.478774
H	−4.179368	−1.482283	−1.143901
H	−5.284032	−0.898150	0.128635
H	−4.011827	−2.086274	0.516823
H	−3.070183	2.428442	−0.464387
H	−4.726131	1.764783	−0.466013
H	−3.577775	1.326780	−1.759318
H	−3.183075	−0.250199	2.666208
H	−4.489014	0.843682	2.138097
H	−2.816300	1.445237	2.292337

TS25

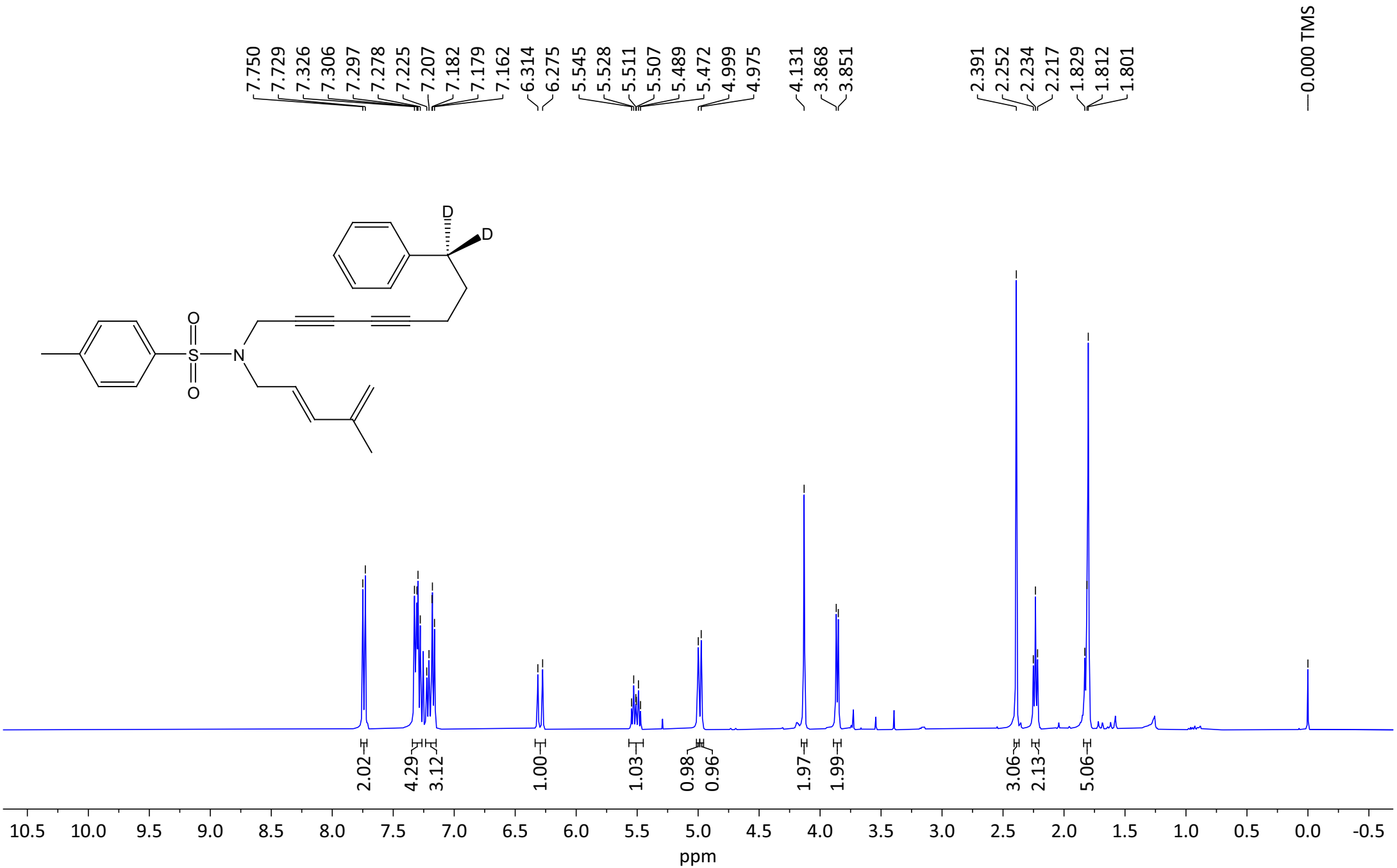
Au	−1.490868	−0.495435	−0.193454
P	−3.413007	0.585055	0.539519
O	1.363272	−3.515072	−1.462085
C	2.130313	5.482114	−1.626248
C	2.741433	4.691655	−0.478982
C	2.303749	3.232349	−0.463580
C	2.922127	2.444092	0.680913
C	2.527165	1.001983	0.740500
C	1.760642	0.355433	−0.098650
C	1.541166	−0.773392	−0.750959
C	0.255139	−1.439427	−0.768992
C	0.274275	−2.795154	−1.163567
C	2.508825	−2.761974	−1.894494
C	2.812129	−1.579656	−0.992301
C	3.348552	−2.002091	0.363785
C	3.431773	−1.325200	1.523630
C	3.092894	0.120449	1.839154
C	3.973754	−2.031936	2.735796
C	−4.957801	−0.245362	0.059338
C	−3.578926	2.286577	−0.077836
C	−3.499011	0.736095	2.348986
H	2.455207	6.526829	−1.609983
H	1.036005	5.474685	−1.575556
H	2.419049	5.061023	−2.595348
H	3.835828	4.739649	−0.542543
H	2.469358	5.159234	0.475829
H	1.209596	3.179685	−0.391634
H	2.574009	2.760069	−1.416811
H	4.018193	2.483930	0.618455
H	2.669875	2.908654	1.644687
H	−0.087901	−1.945542	−2.042884
H	−0.610578	−3.415388	−1.051606
H	2.306440	−2.409328	−2.912222
H	3.329714	−3.478279	−1.923611
H	3.543228	−0.960965	−1.524164
H	3.705931	−3.031484	0.394434
H	4.030577	0.595708	2.160016
H	2.453204	0.145041	2.731607
H	4.258022	−3.061565	2.509085
H	3.227324	−2.050622	3.538897
H	4.852198	−1.511409	3.134944
H	−5.018617	−0.299679	−1.030054
H	−5.821443	0.304450	0.443749
H	−4.965958	−1.261606	0.460129
H	−2.710164	2.873109	0.230324
H	−4.487915	2.748328	0.317929
H	−3.621975	2.277899	−1.169488
H	−3.487928	−0.258690	2.800068
H	−4.412852	1.259441	2.644171
H	−2.630093	1.291608	2.709359

S11. Copies of NMR Spectra

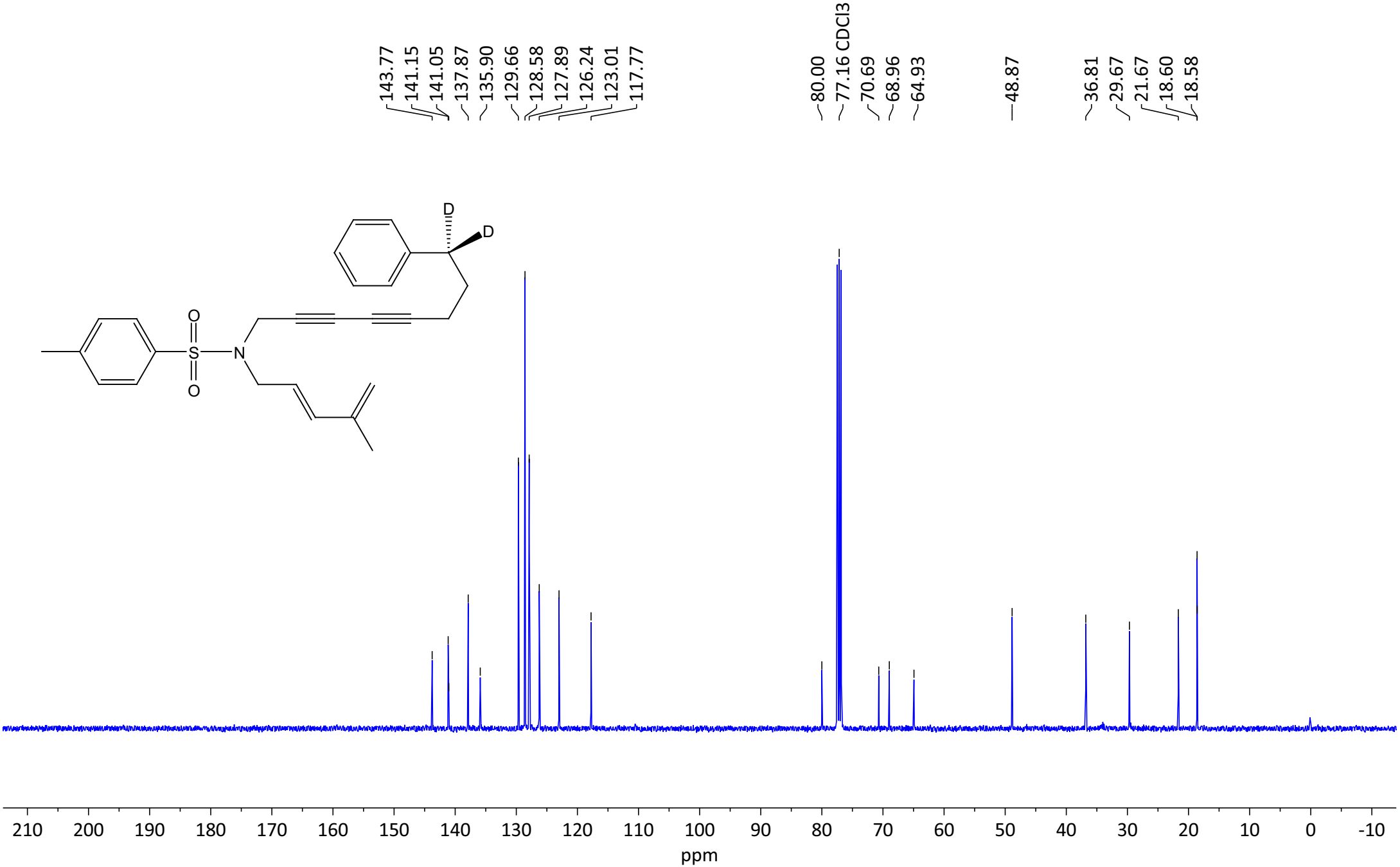
Table S3. Summary of NMR Spectra

compound	^{1}H NMR	page	^{13}C{^{1}H} NMR	page
11	400 MHz, $CDCl_3$	S69	101 MHz, $CDCl_3$	S70
12	400 MHz, $CDCl_3$	S71	101 MHz, $CDCl_3$	S72
13	400 MHz, $CDCl_3$	S73	101 MHz, $CDCl_3$	S74
S2	400 MHz, $CDCl_3$	S75	101 MHz, $CDCl_3$	S76
S3	400 MHz, $CDCl_3$	S77	101 MHz, $CDCl_3$	S78
S4	400 MHz, $CDCl_3$	S79	101 MHz, $CDCl_3$	S80
S5	400 MHz, $CDCl_3$	S81	101 MHz, $CDCl_3$	S82
16a	400 MHz, $CDCl_3$	S83	101 MHz, $CDCl_3$	S84
16b	400 MHz, $CDCl_3$	S85	101 MHz, $CDCl_3$	S86
16c	400 MHz, $CDCl_3$	S87	101 MHz, $CDCl_3$	S88
16d	400 MHz, $CDCl_3$	S89	101 MHz, $CDCl_3$	S90
17a	400 MHz, $CDCl_3$	S91	101 MHz, $CDCl_3$	S92
17b	400 MHz, CD_2Cl_2	S93	101 MHz, CD_2Cl_2	S94
17c	600 MHz, $CDCl_3$	S95	151 MHz, $CDCl_3$	S96
17d	600 MHz, $CDCl_3$	S97	151 MHz, $CDCl_3$	S98

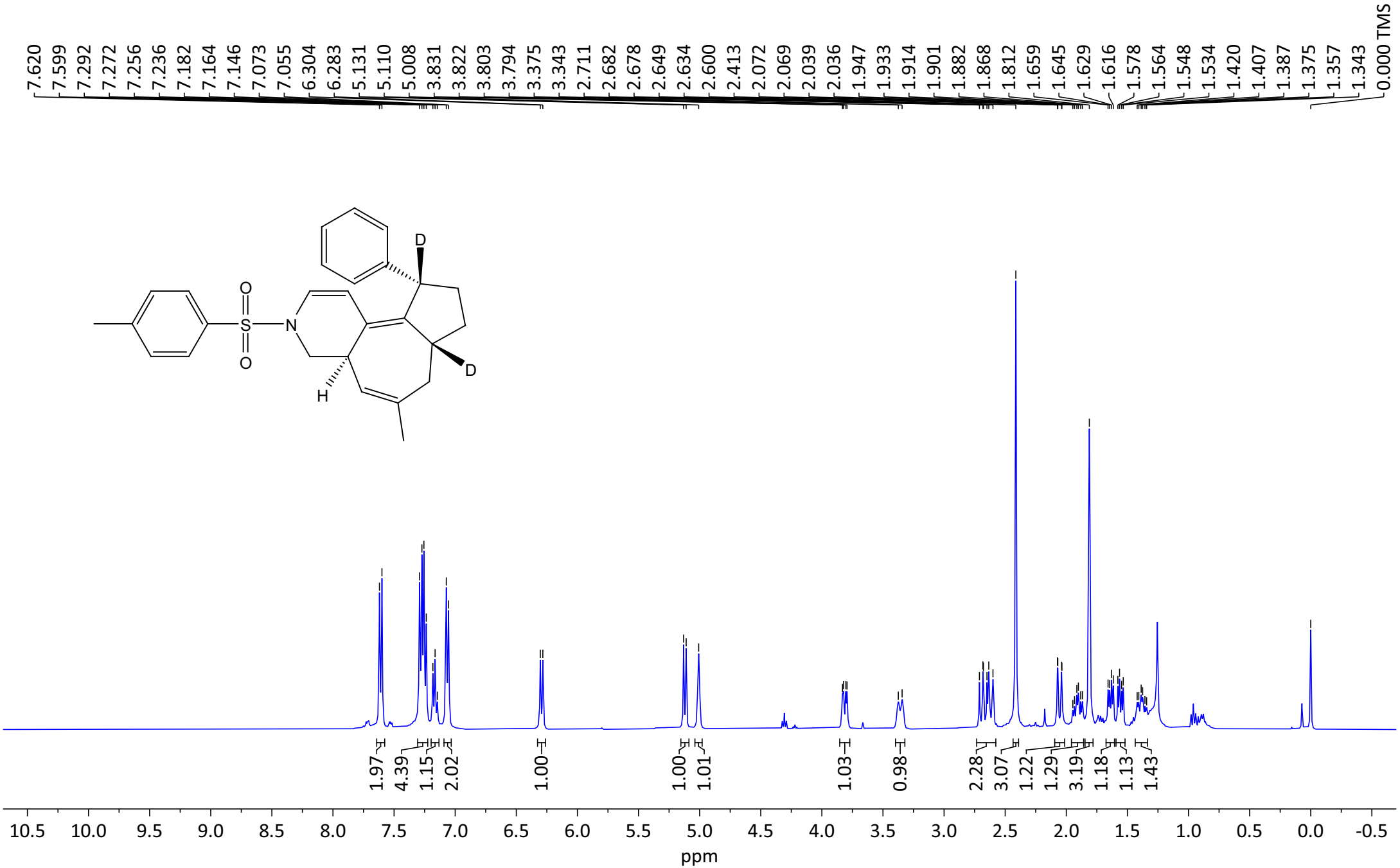
Compound **11**: ^{1}H NMR (400 MHz, $CDCl_3$)



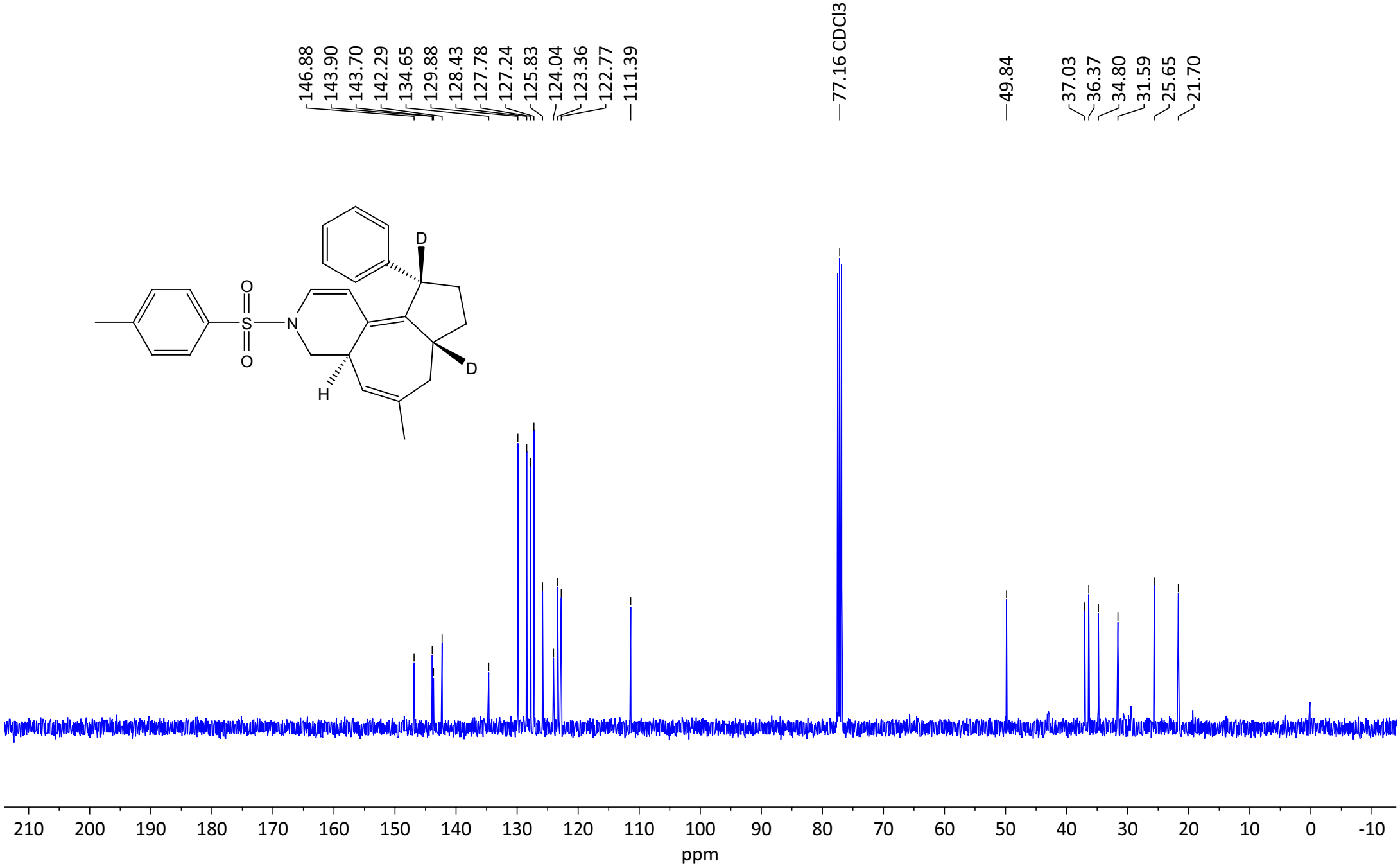
Compound **11**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



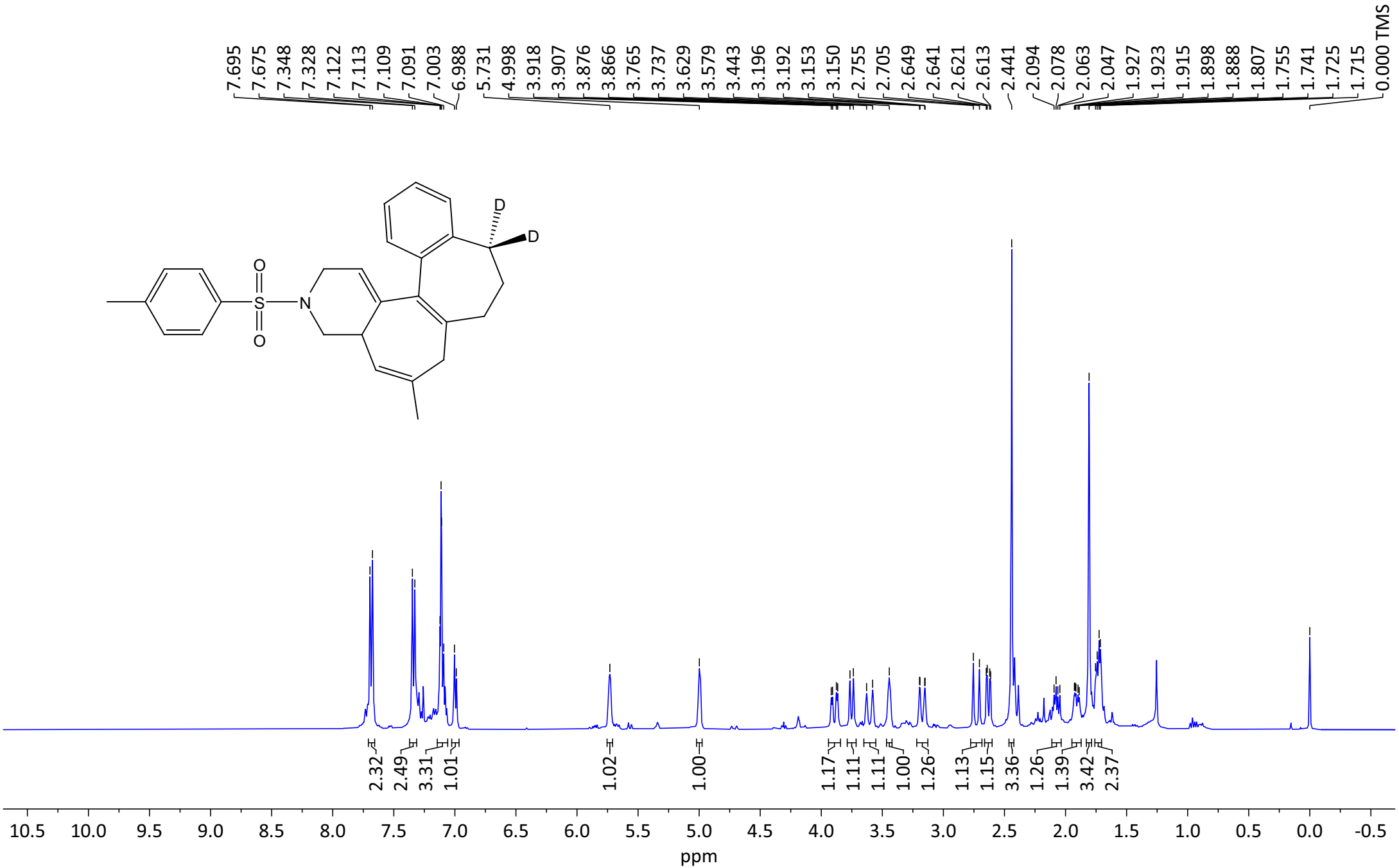
Compound **12**: ^{1}H NMR (400 MHz, $CDCl_3$)



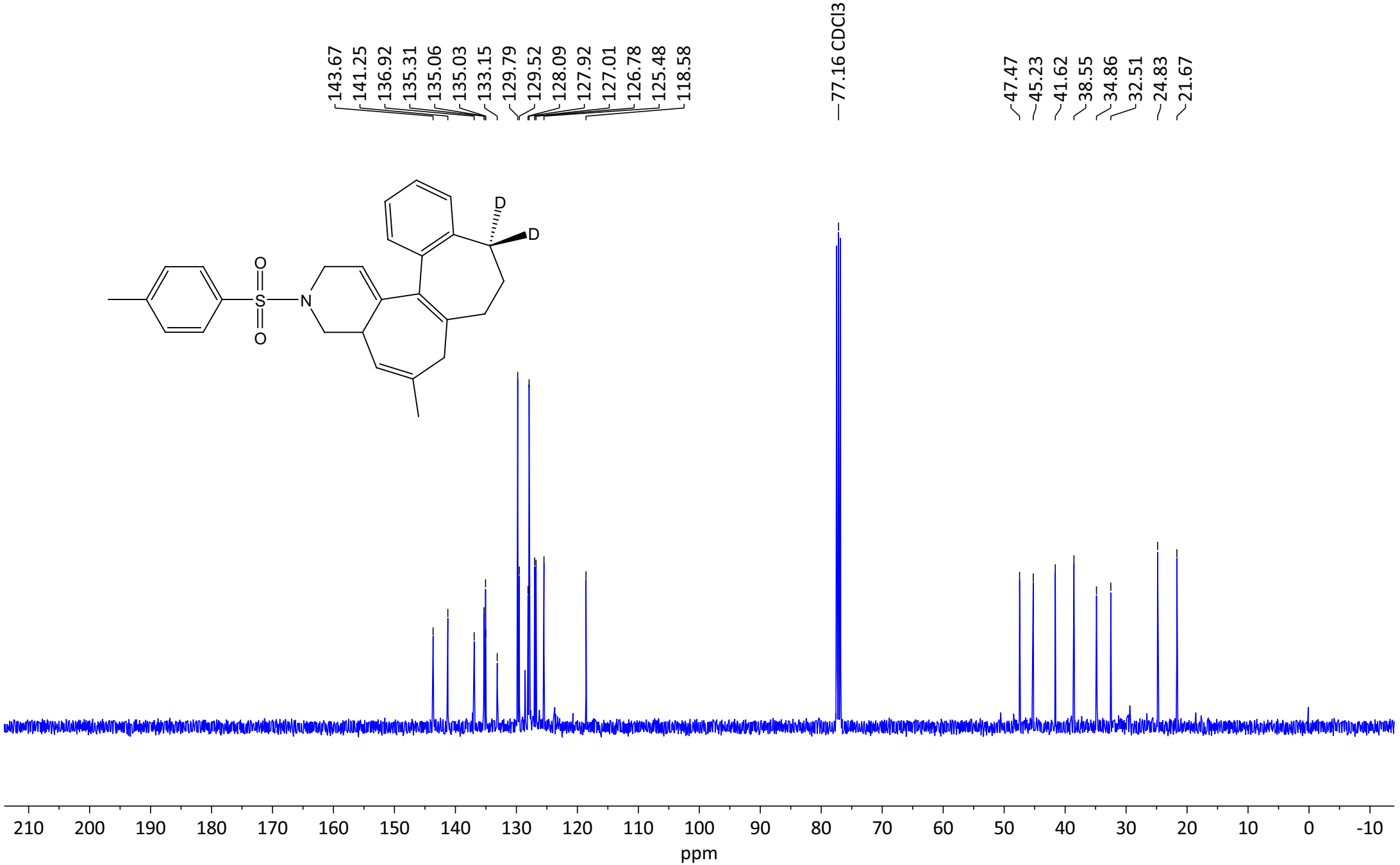
Compound **12**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



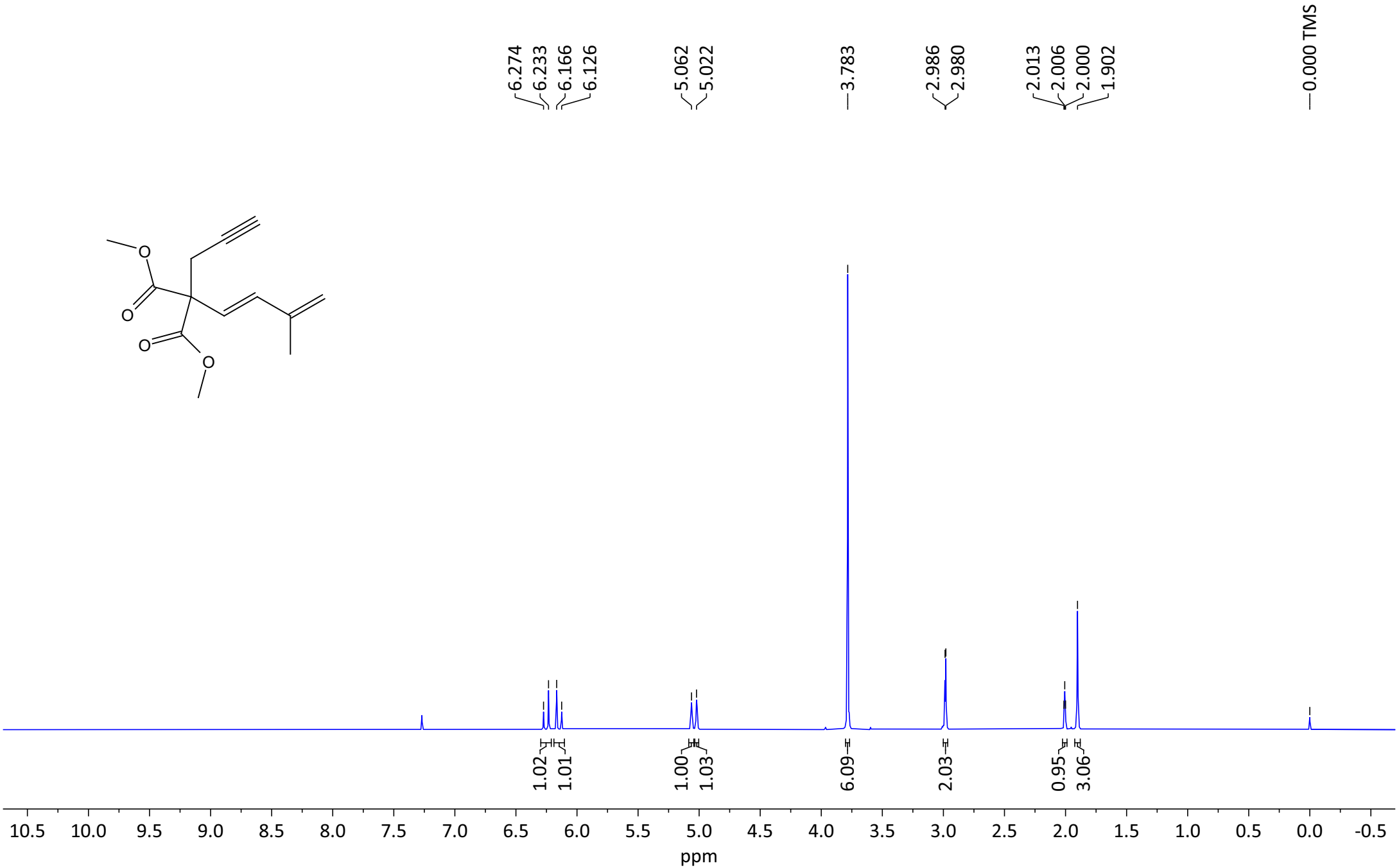
Compound **13**: ^{1}H NMR (400 MHz, $CDCl_3$)



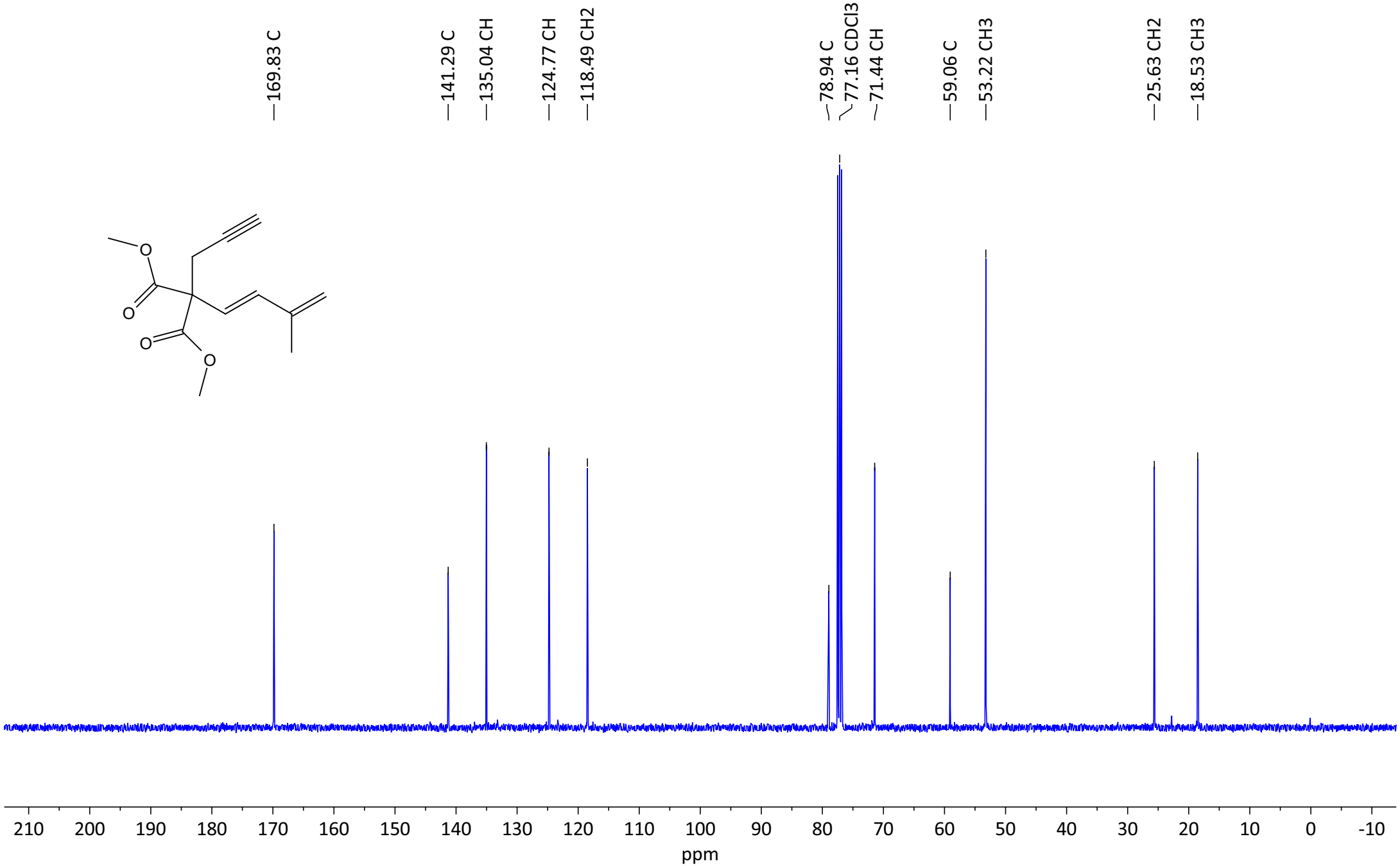
Compound **13**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



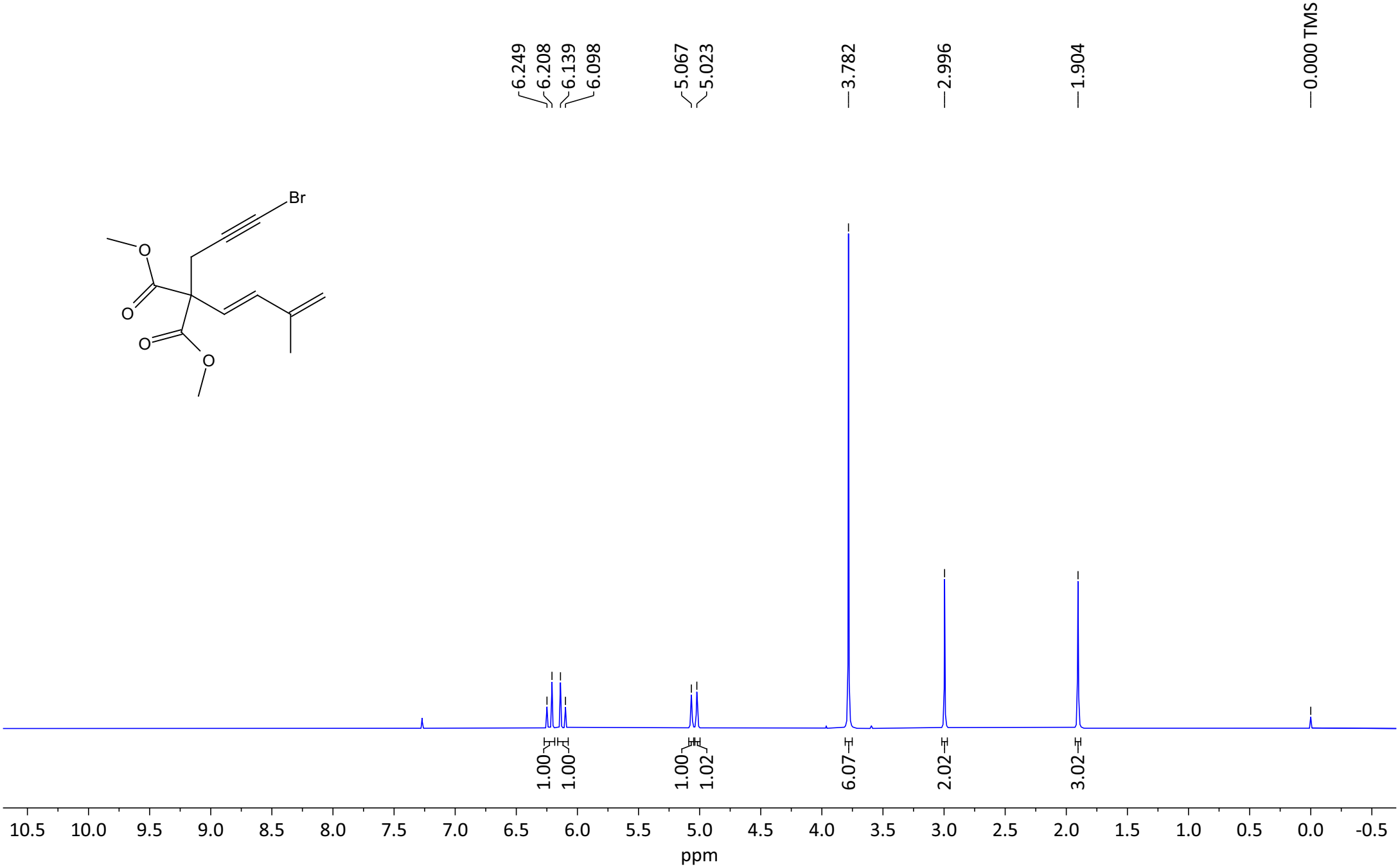
Compound **S2**: ^{1}H NMR (400 MHz, $CDCl_3$)



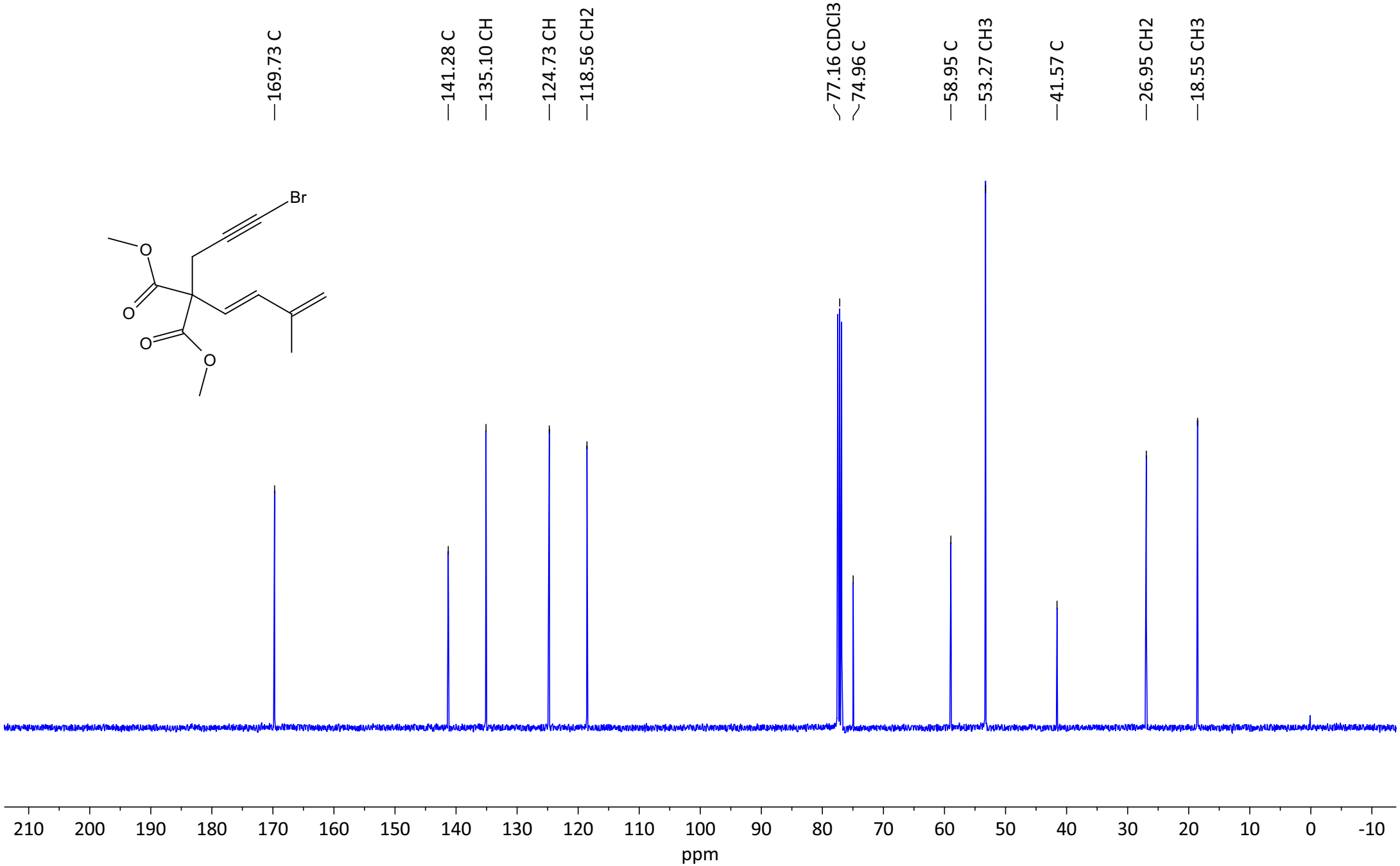
Compound **S2**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



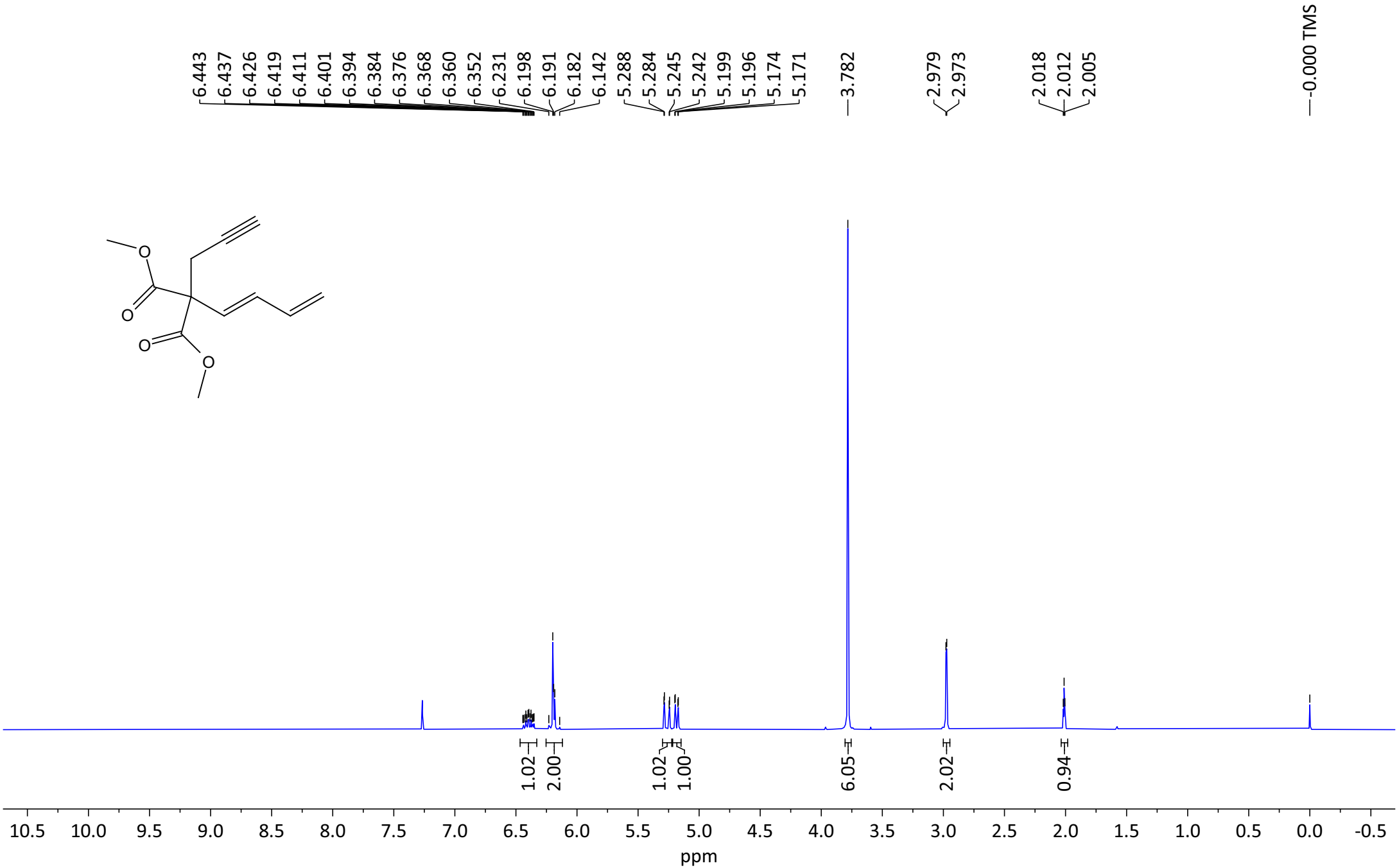
Compound **S3**: ^{1}H NMR (400 MHz, $CDCl_3$)



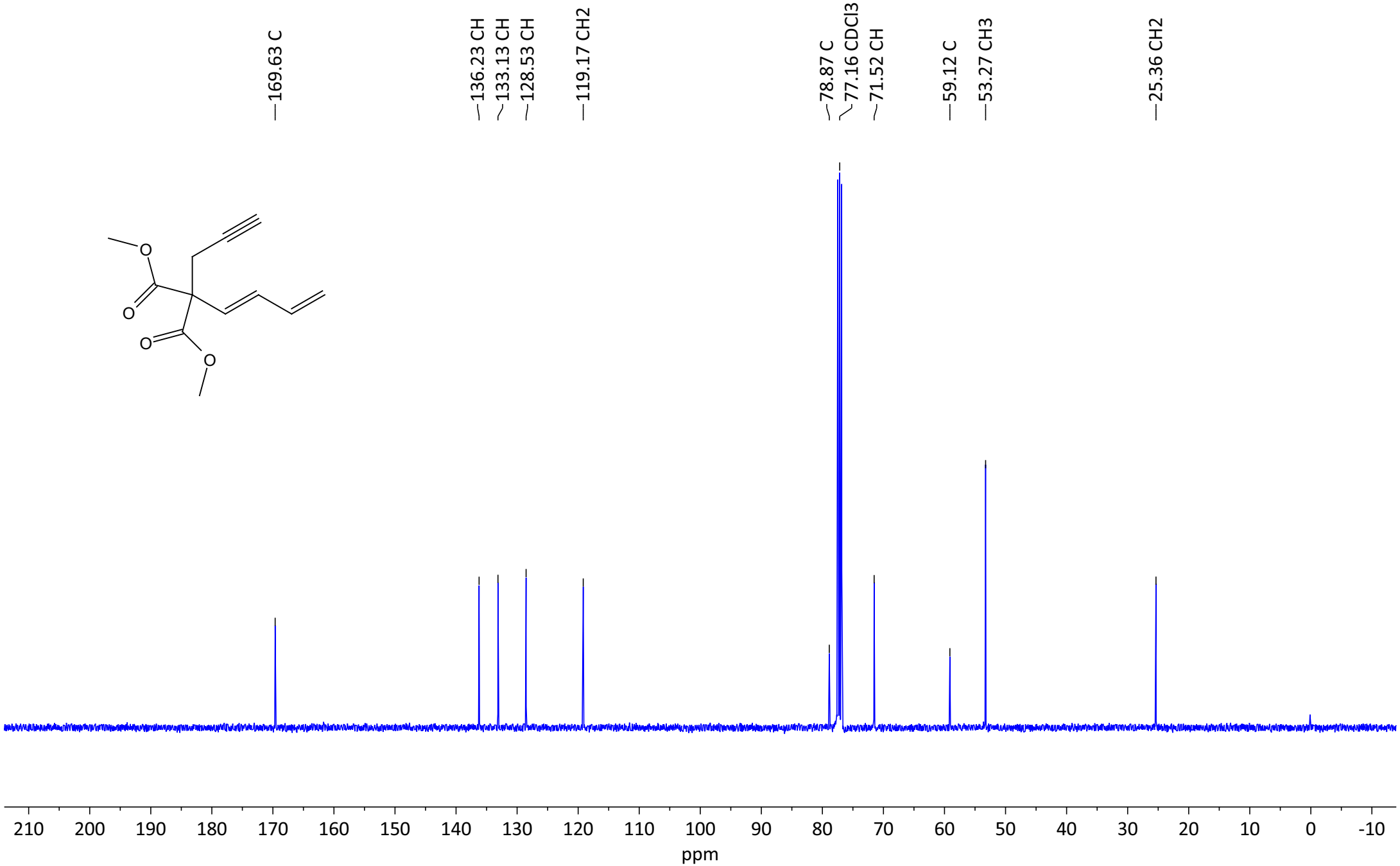
Compound **S3**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



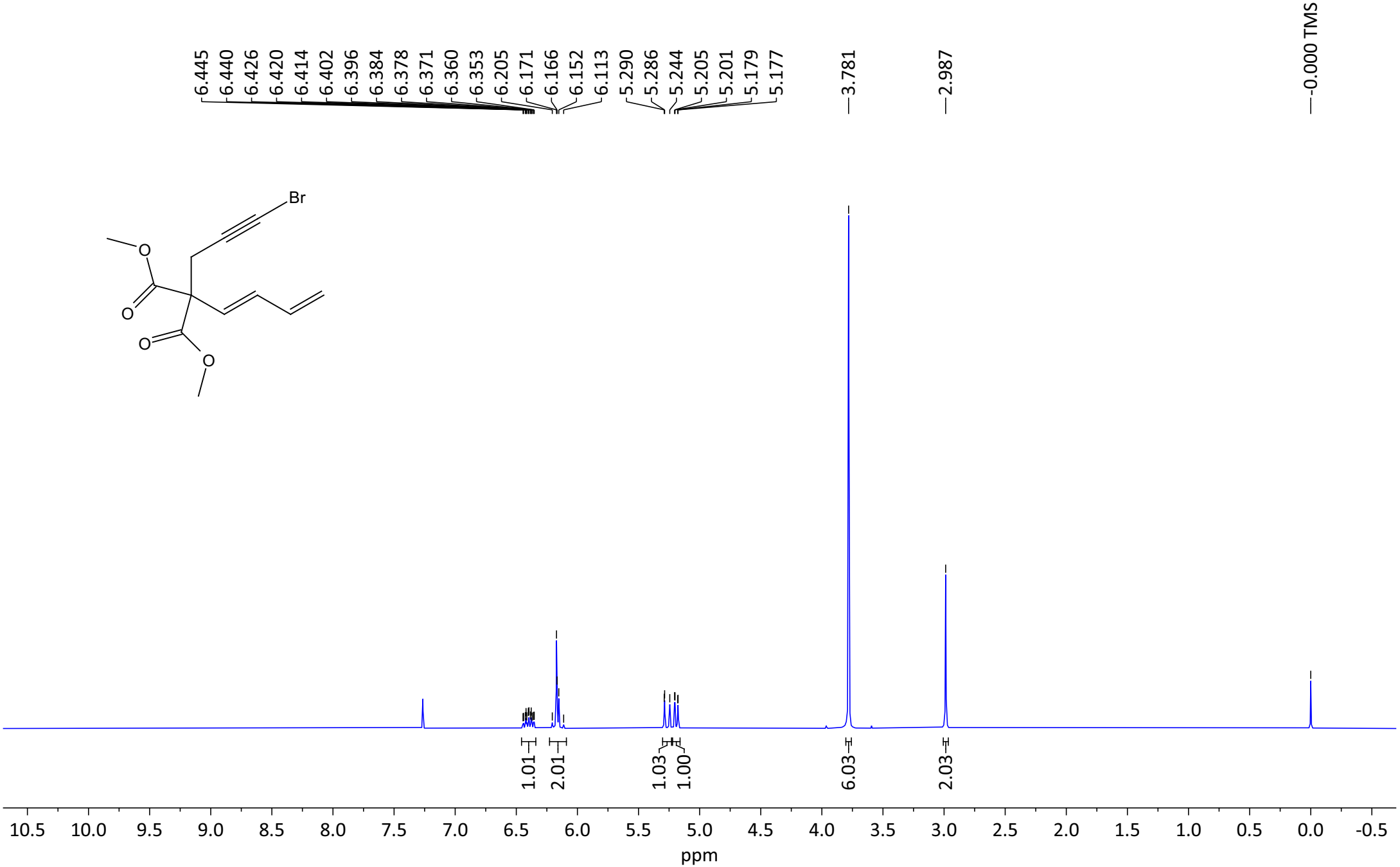
Compound **S4**: ^{1}H NMR (400 MHz, $CDCl_3$)



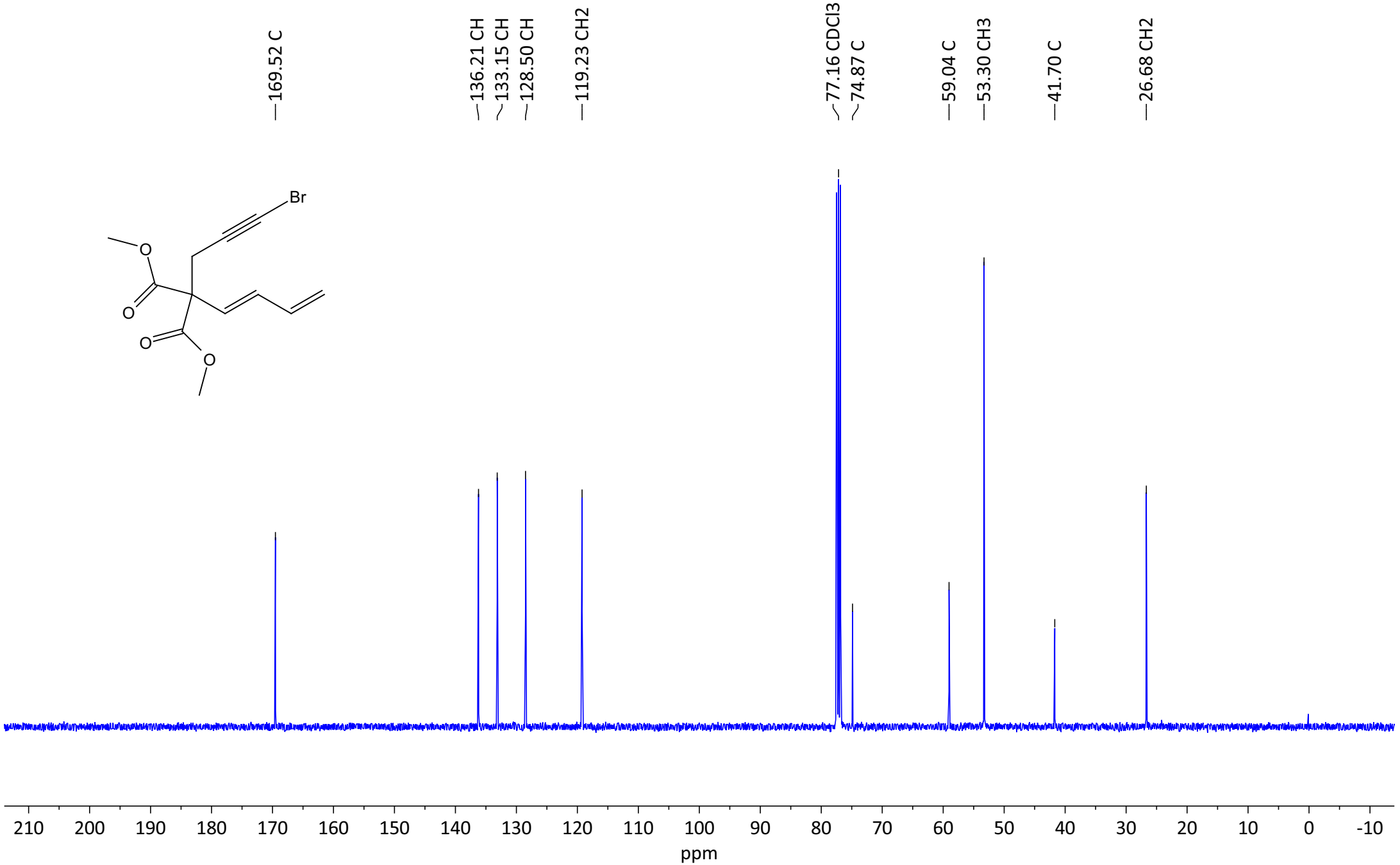
Compound **S4**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



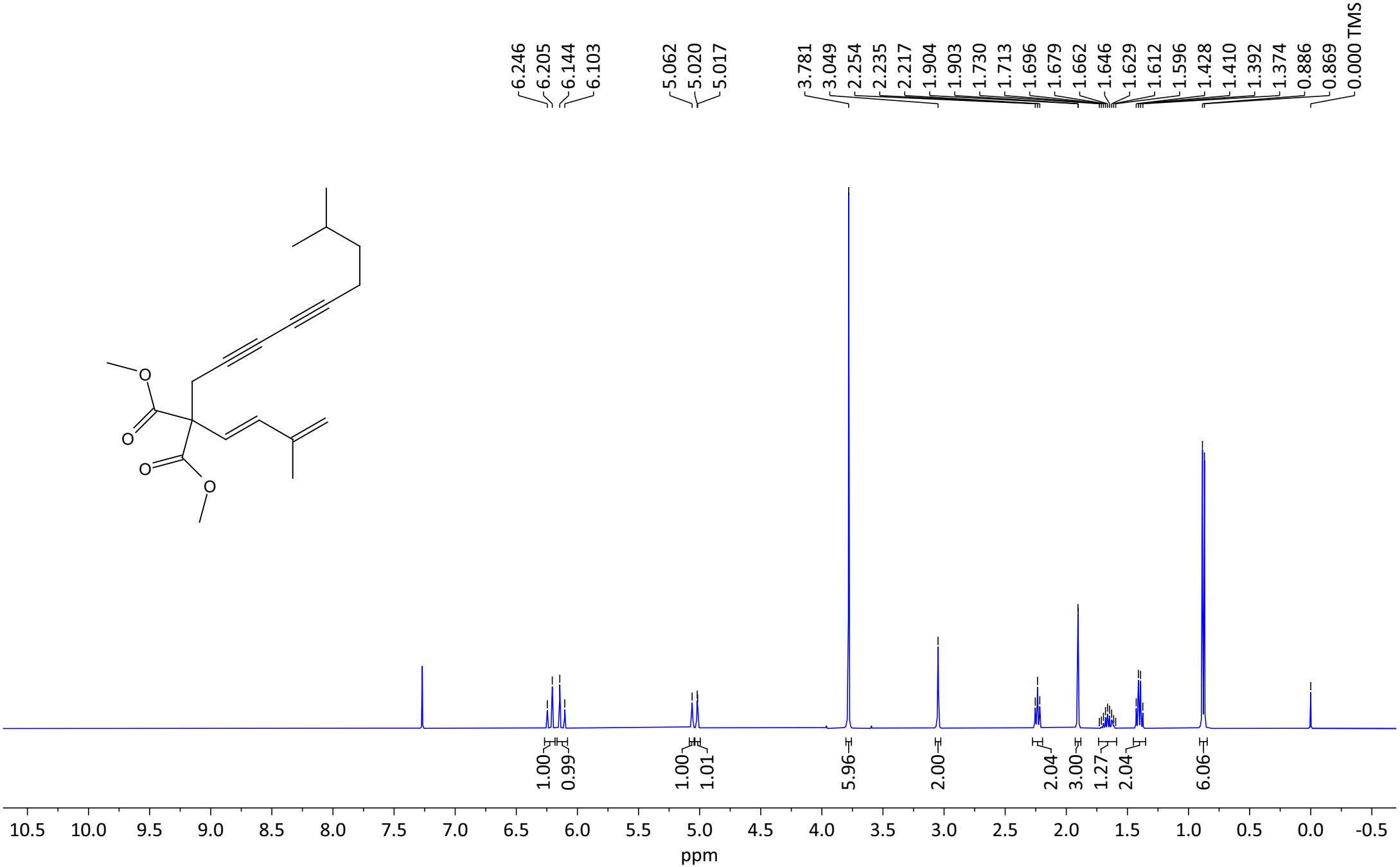
Compound **S5**: ^{1}H NMR (400 MHz, $CDCl_3$)



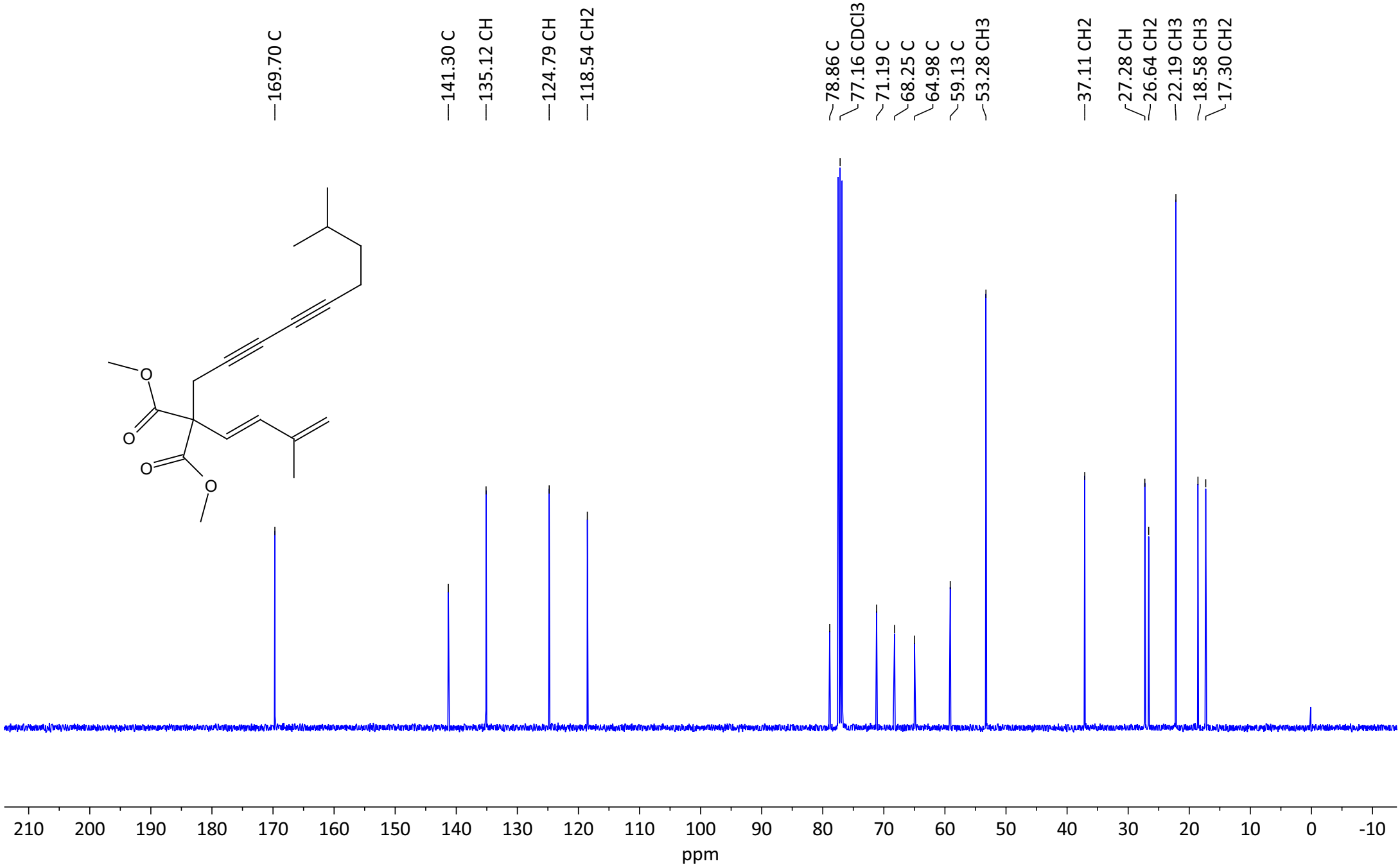
Compound **S5**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



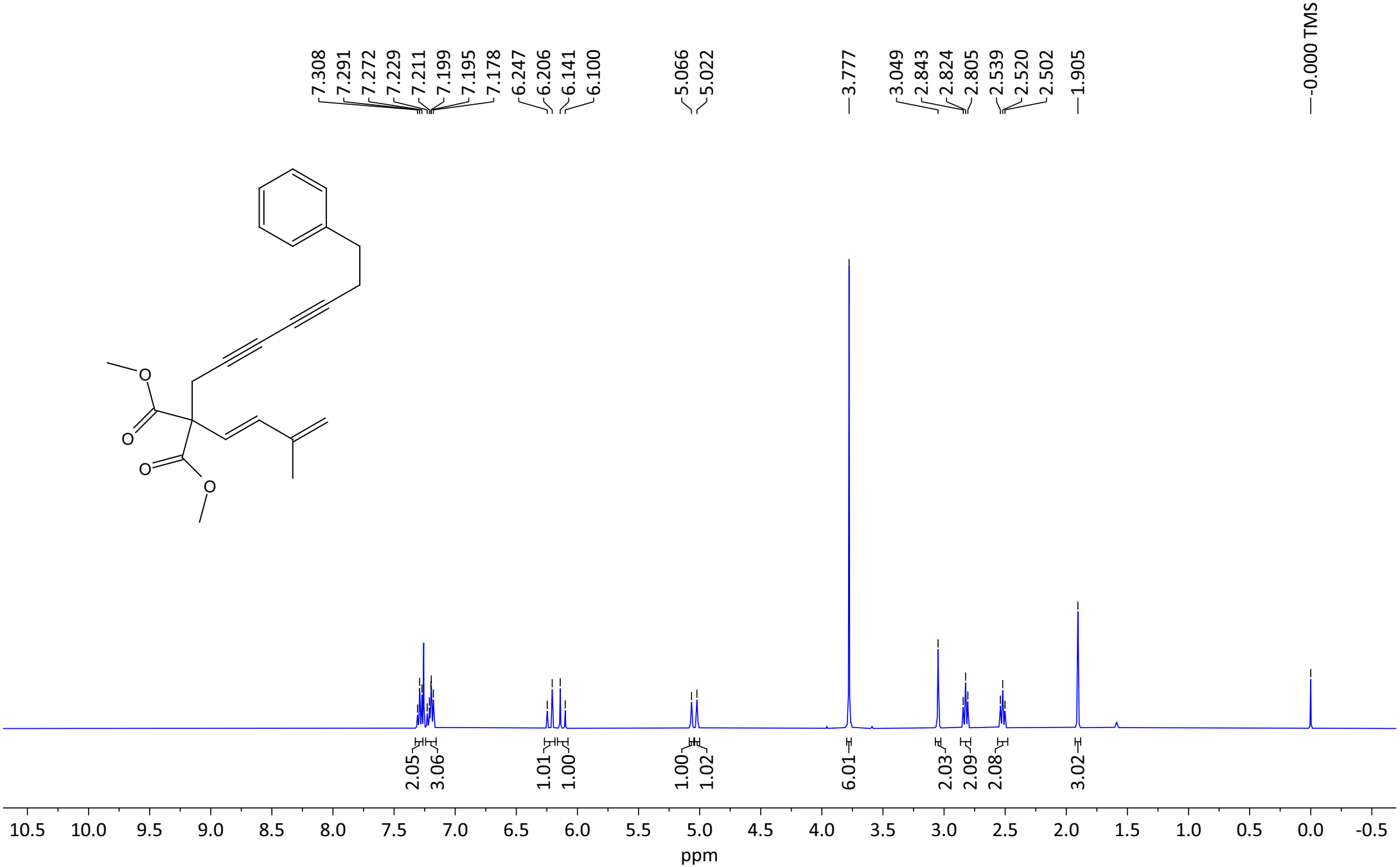
Compound **16a**: ^{1}H NMR (400 MHz, $CDCl_3$)



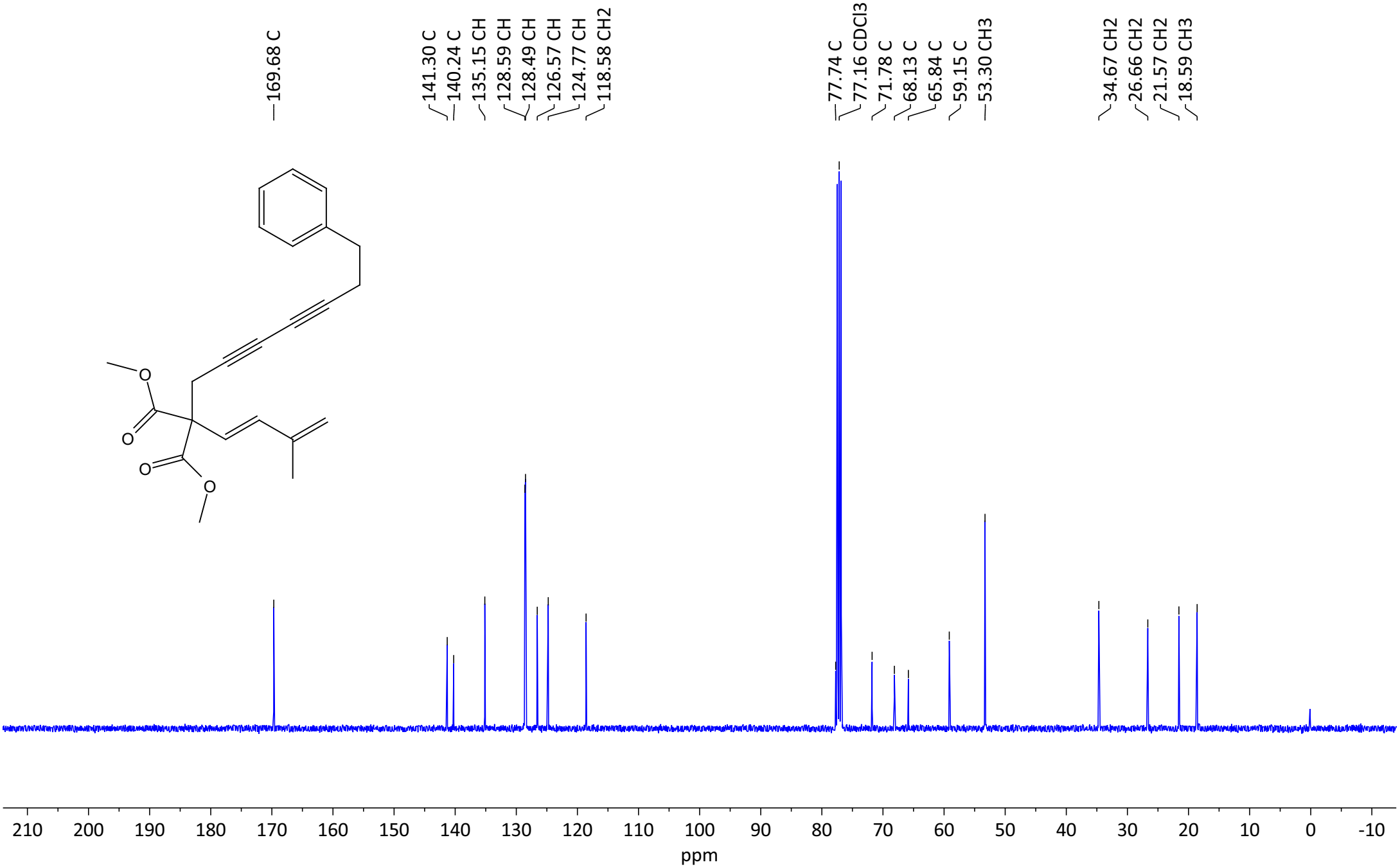
Compound **16a**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



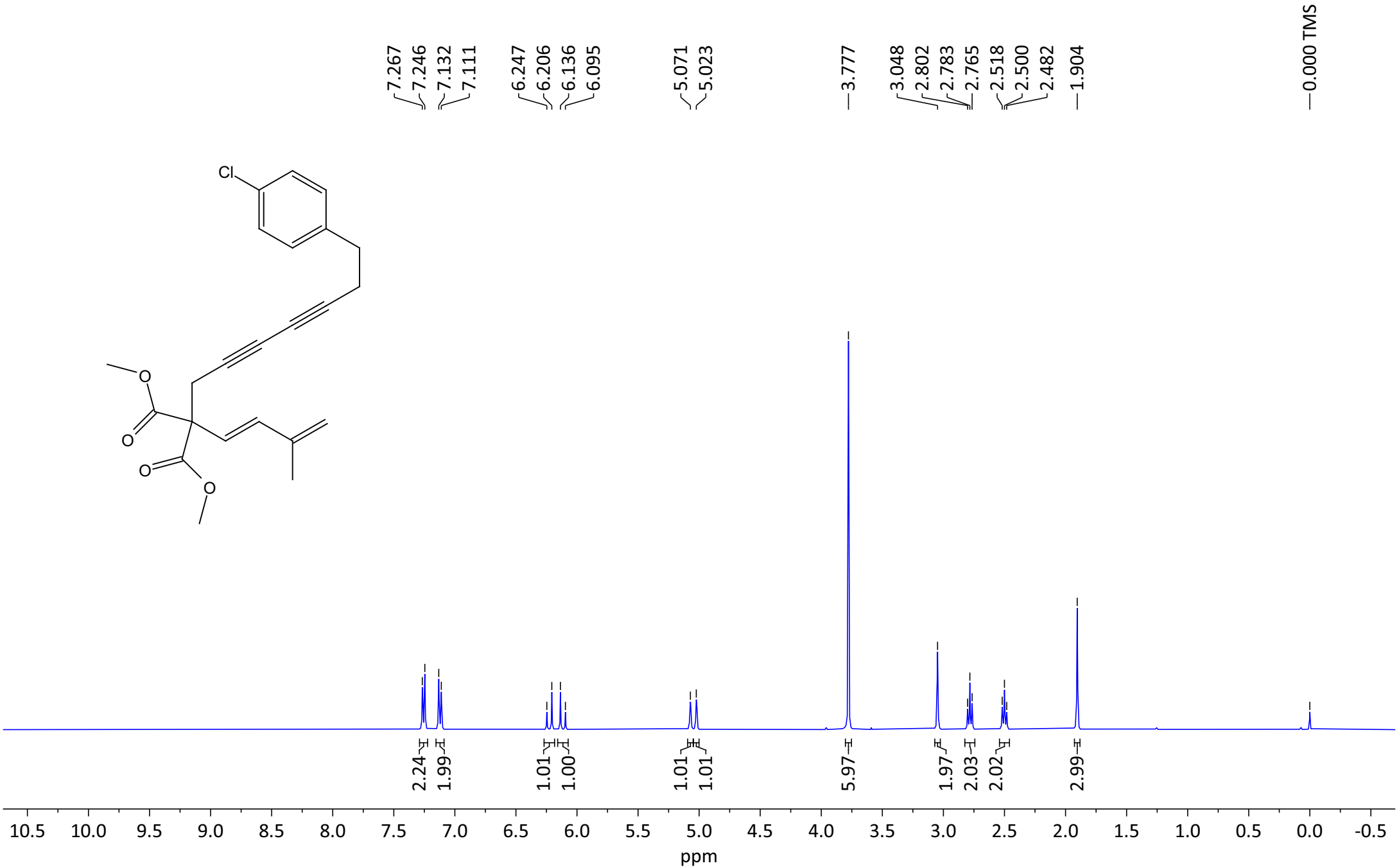
Compound **16b**: ^{1}H NMR (400 MHz, $CDCl_3$)



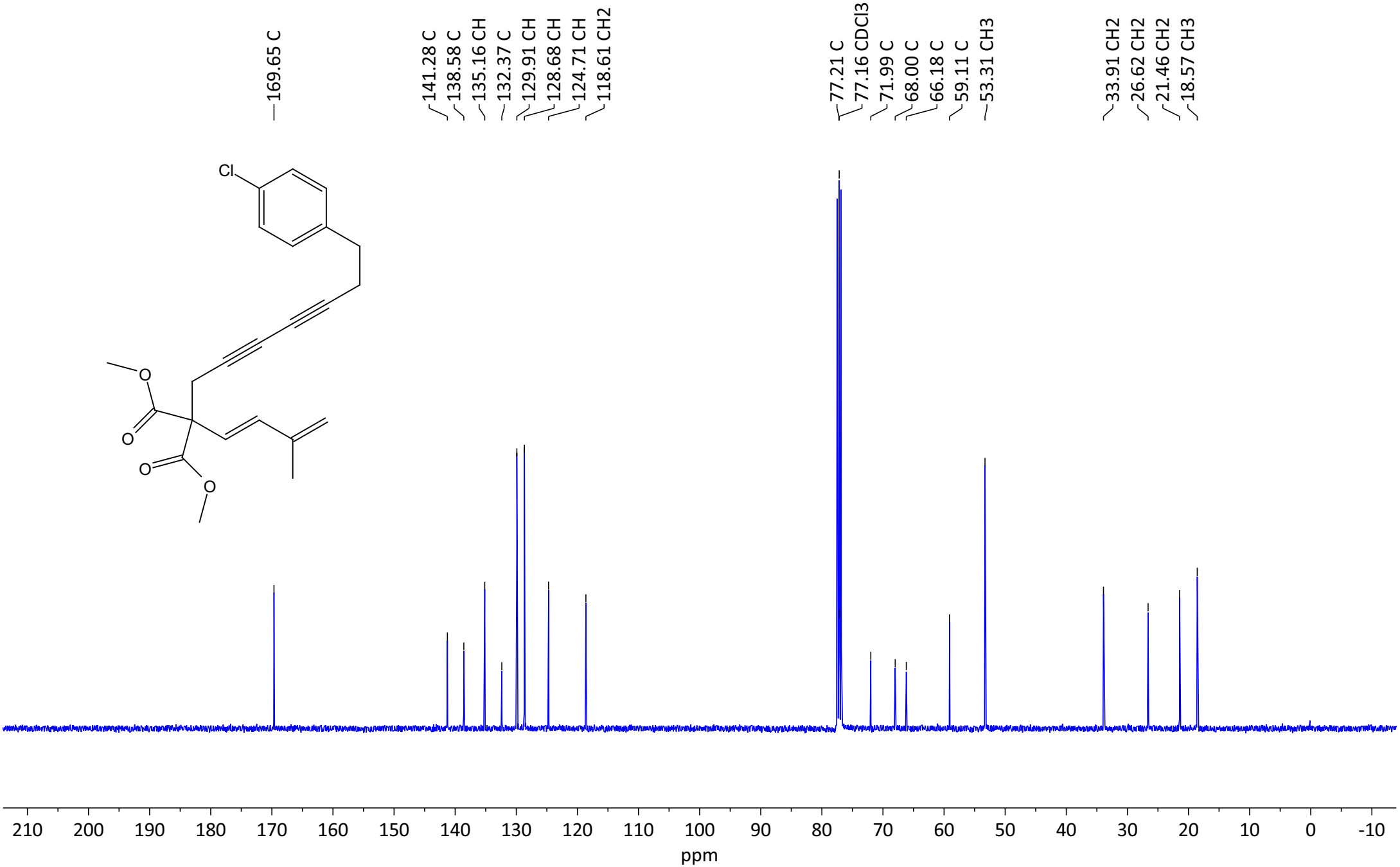
Compound **16b**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



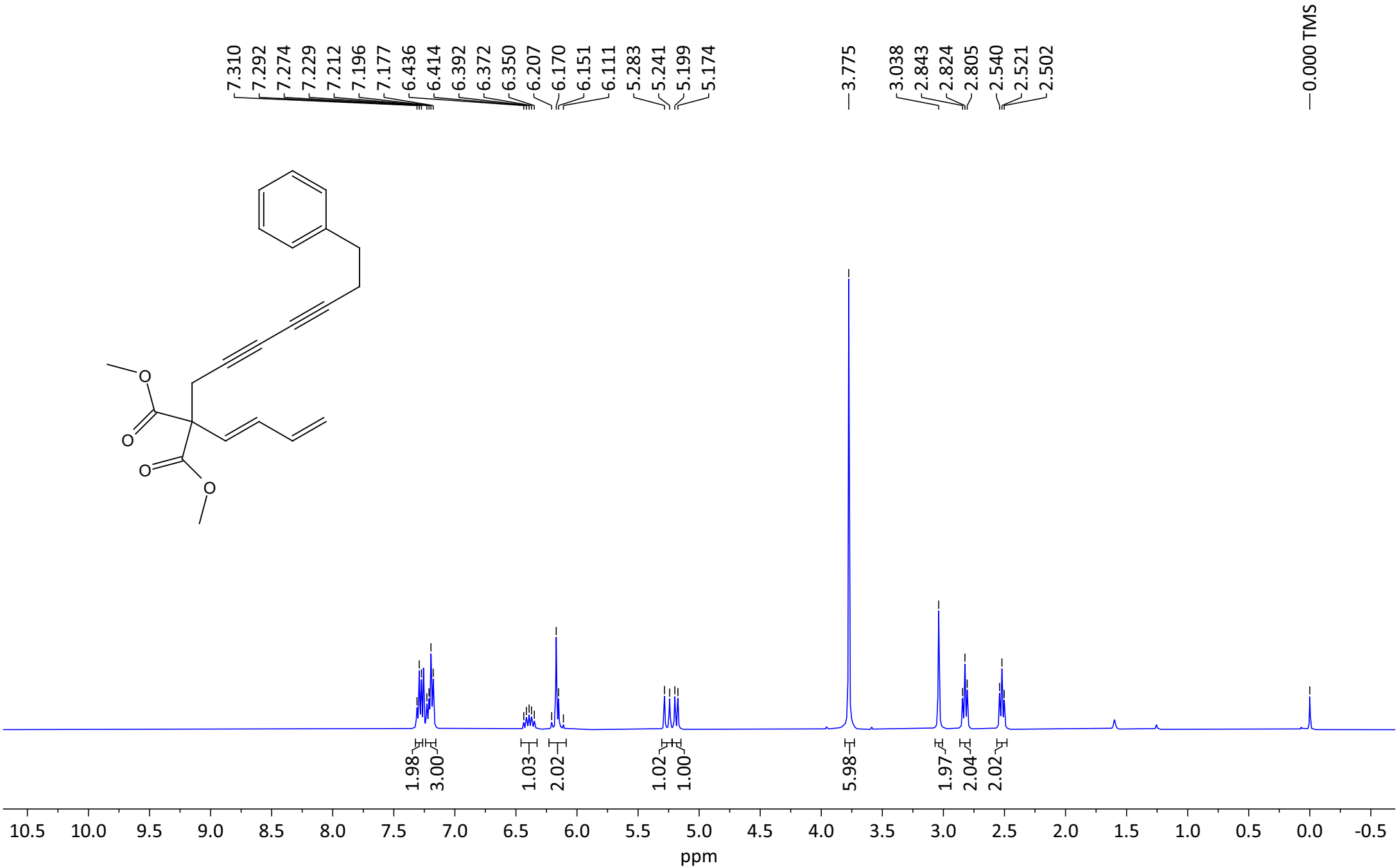
Compound **16c**: ^{1}H NMR (400 MHz, $CDCl_3$)



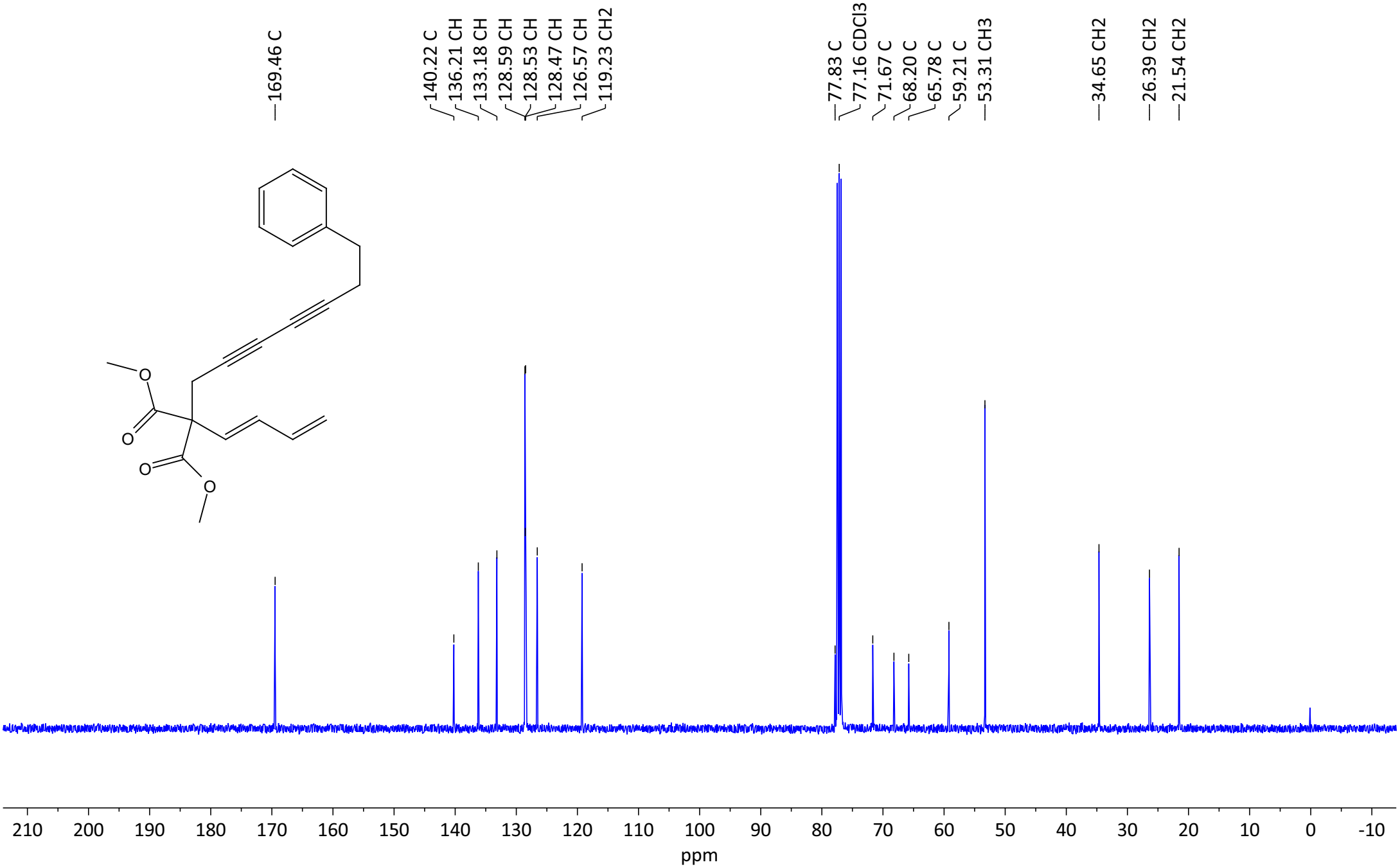
Compound **16c**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



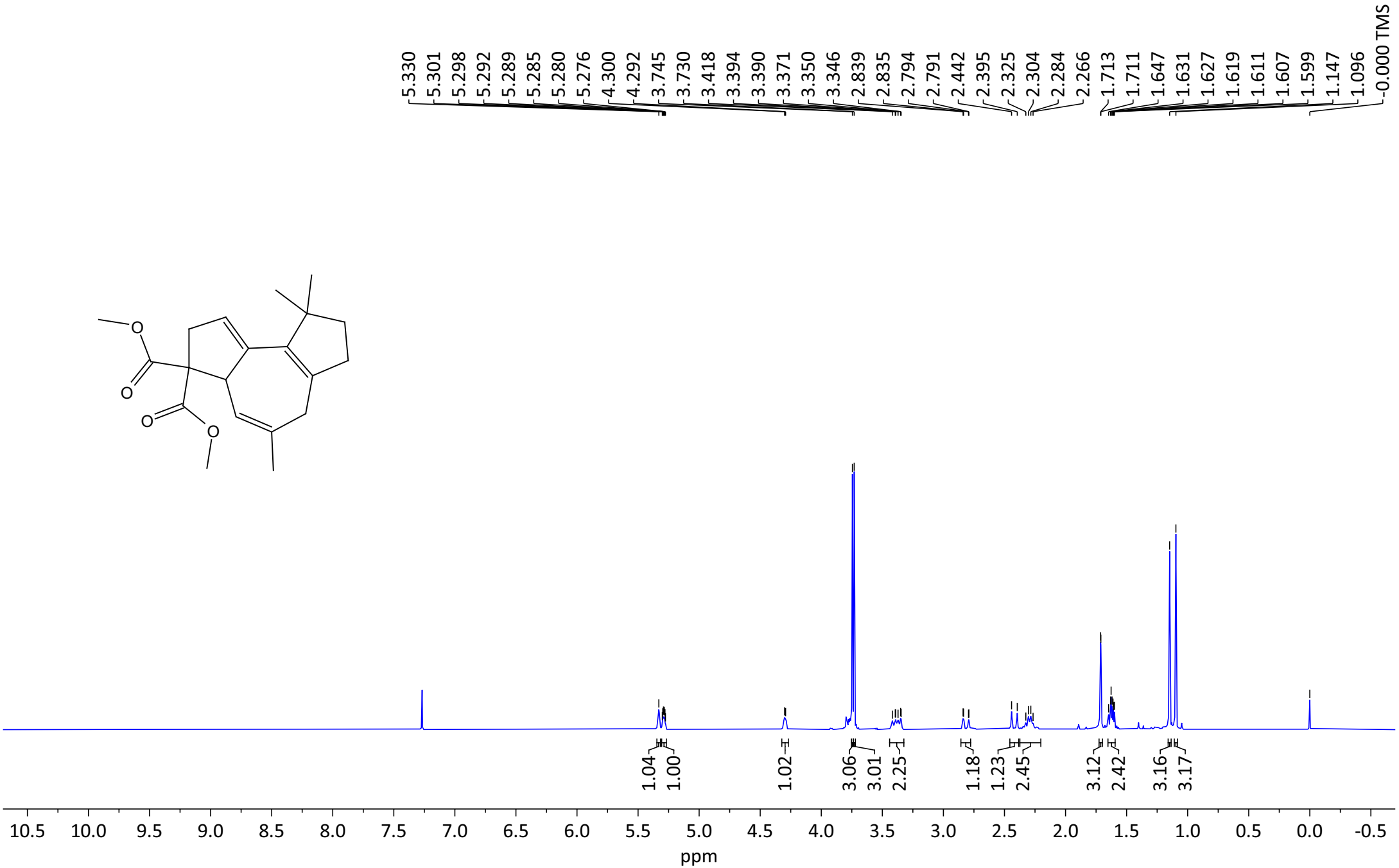
Compound **16d**: ^{1}H NMR (400 MHz, $CDCl_3$)



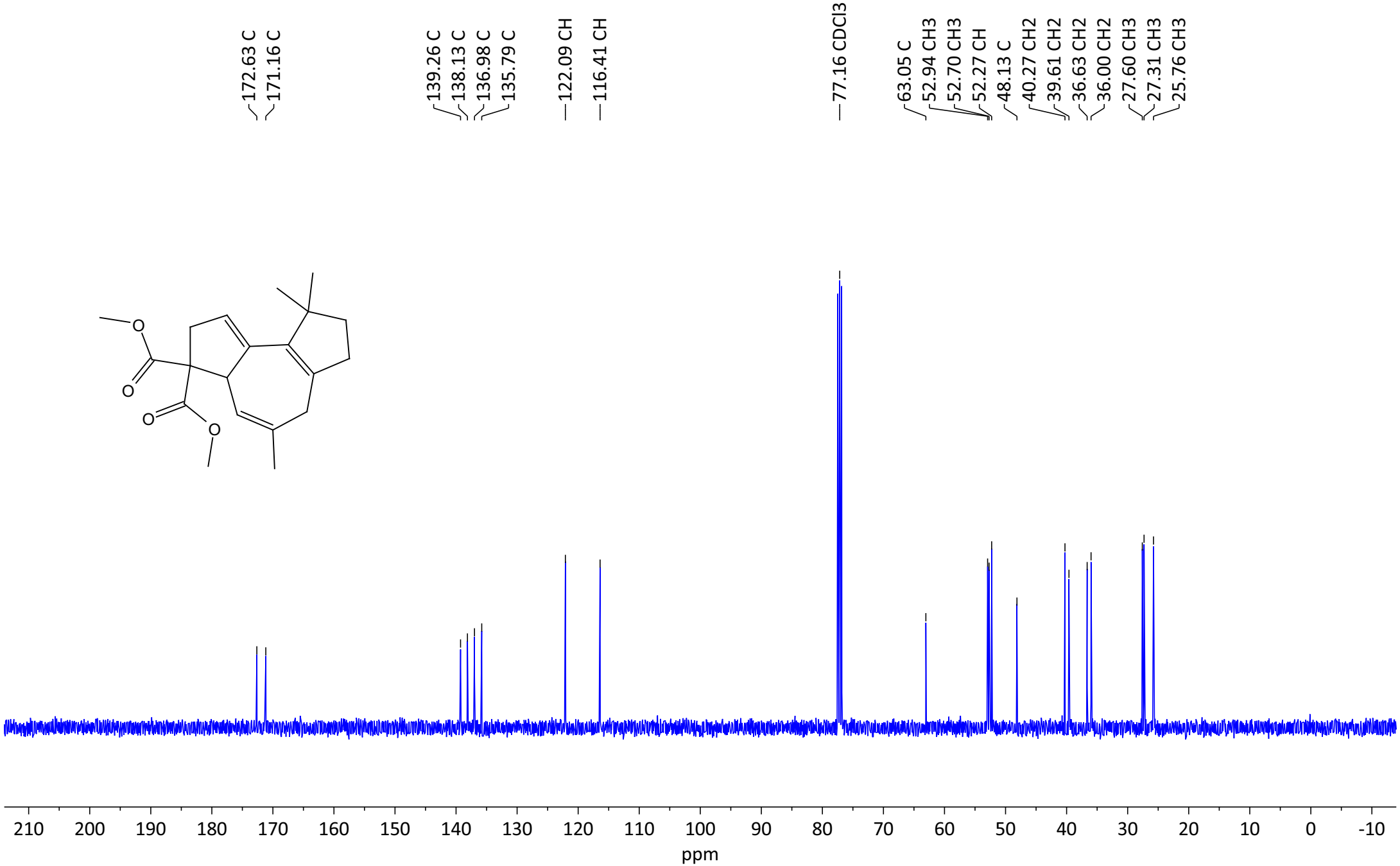
Compound **16d**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



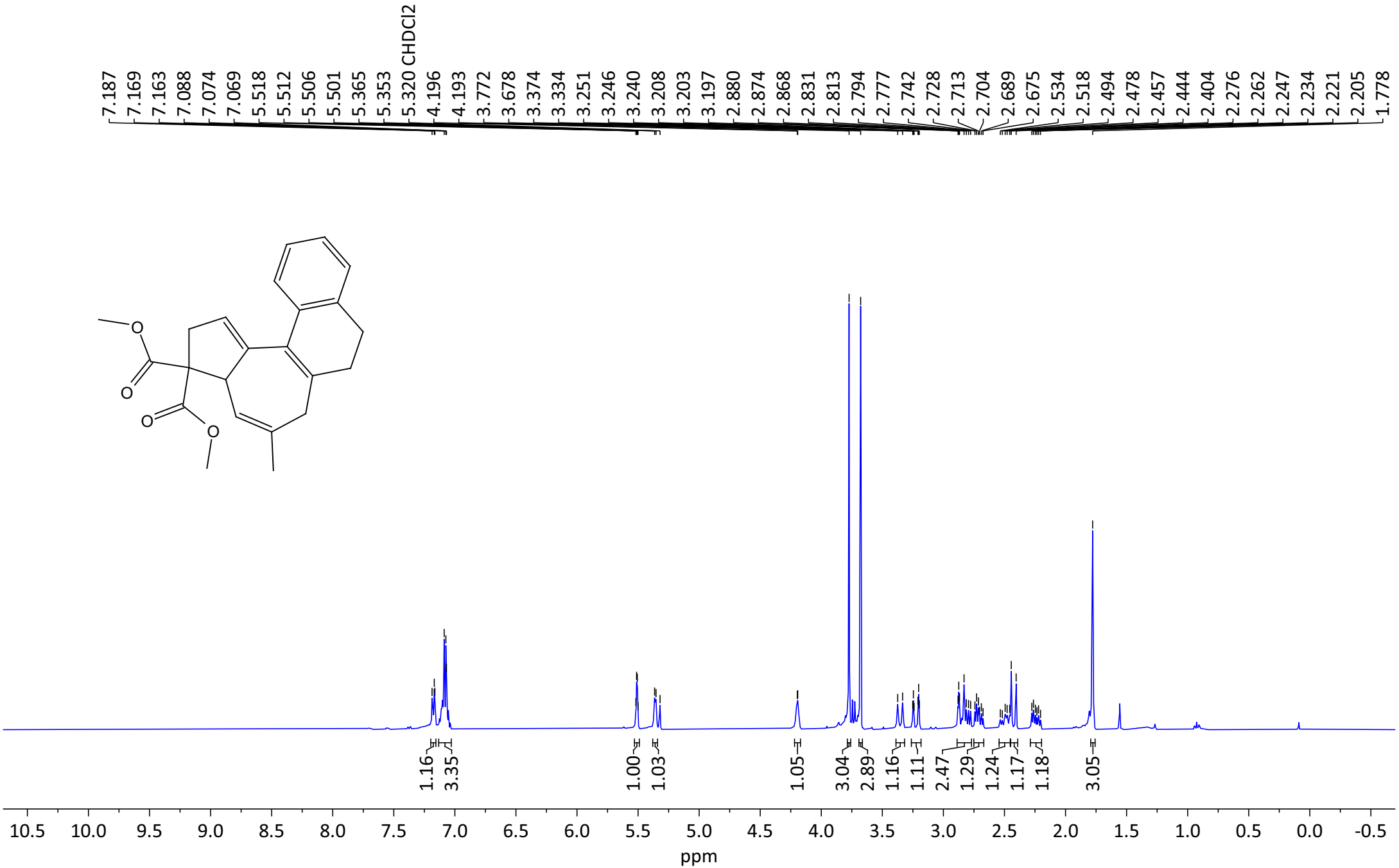
Compound **17a**: ^{1}H NMR (400 MHz, $CDCl_3$)



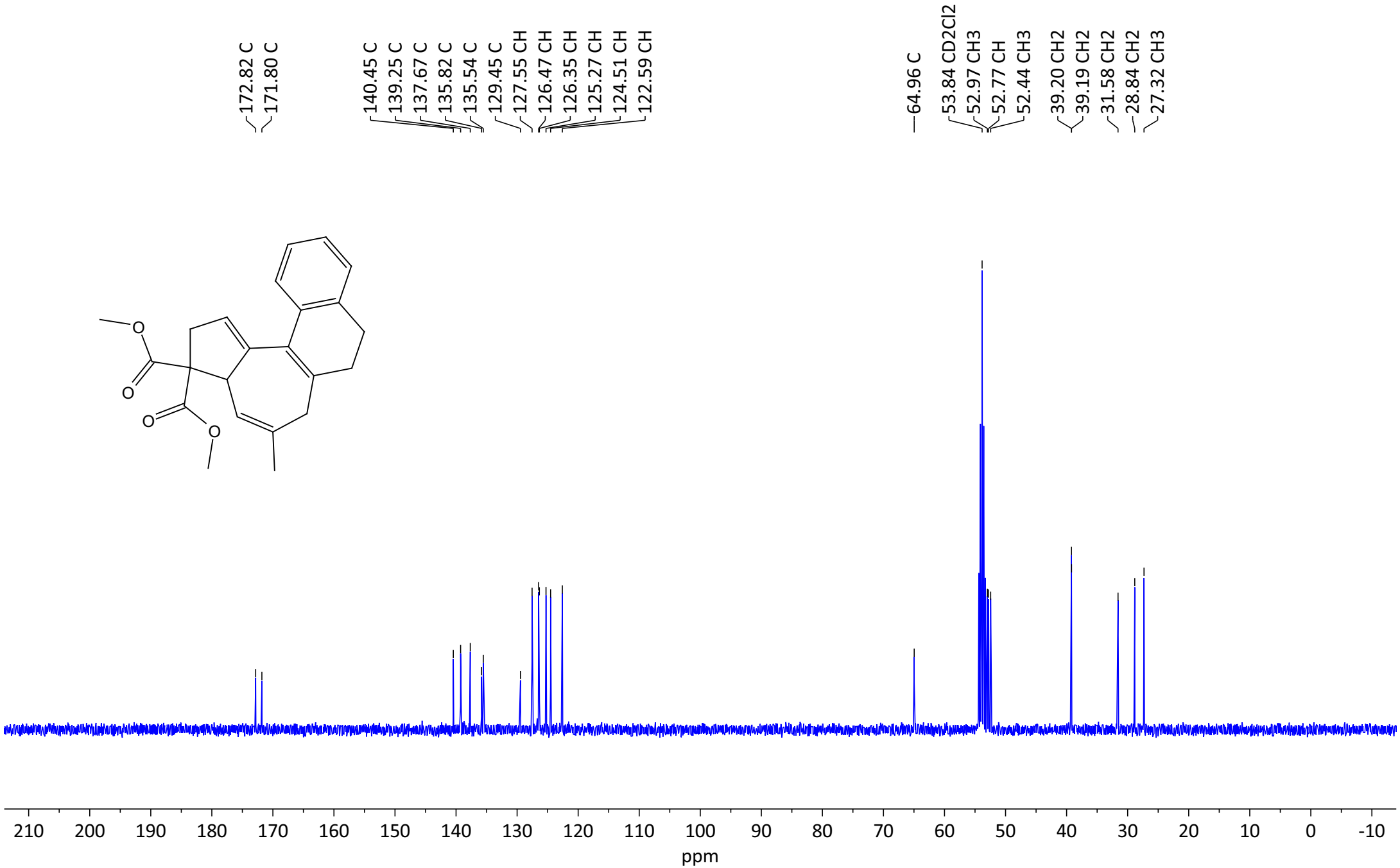
Compound **17a**: $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



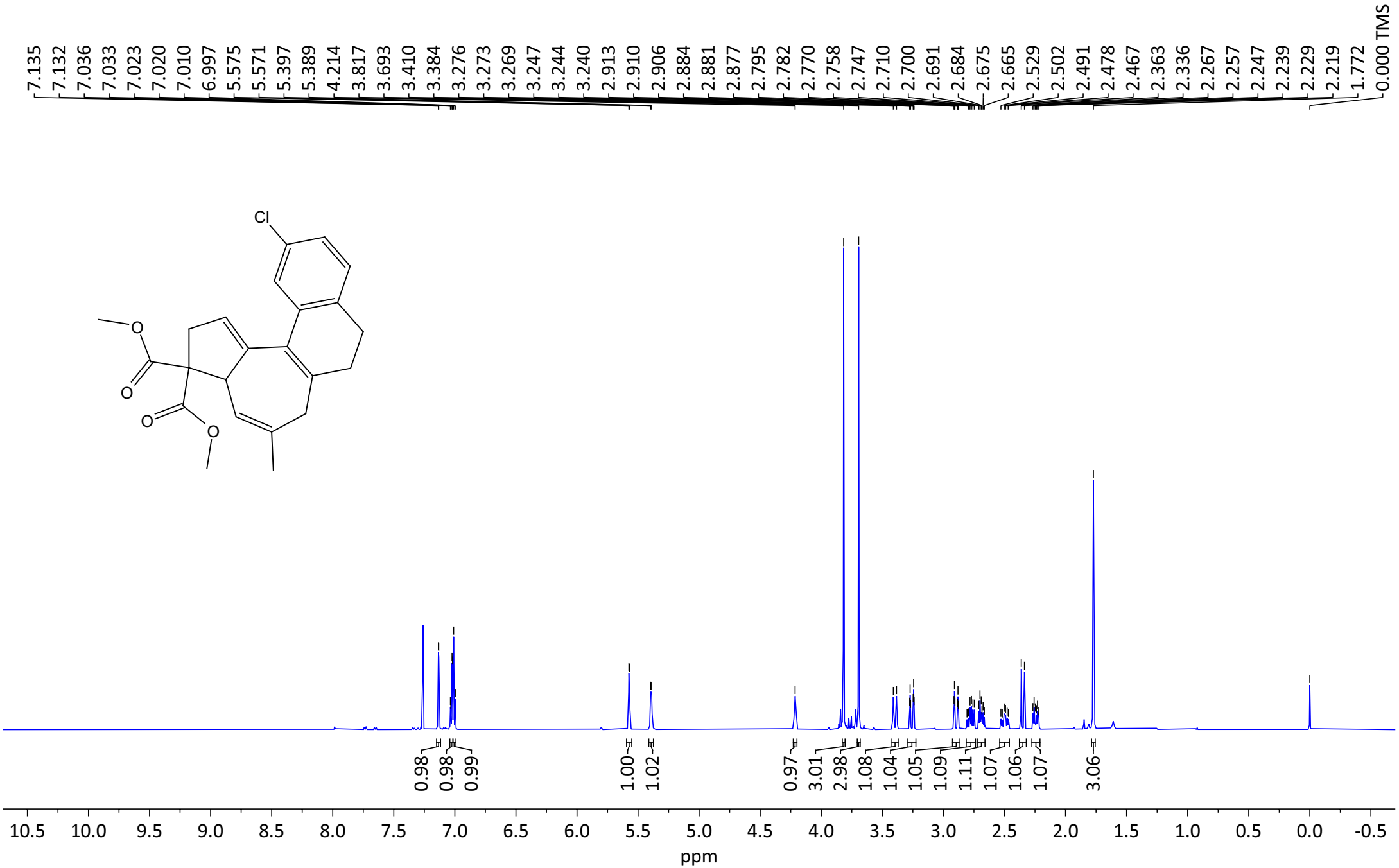
Compound **17b**: ^{1}H NMR (400 MHz, CD_2Cl_2)



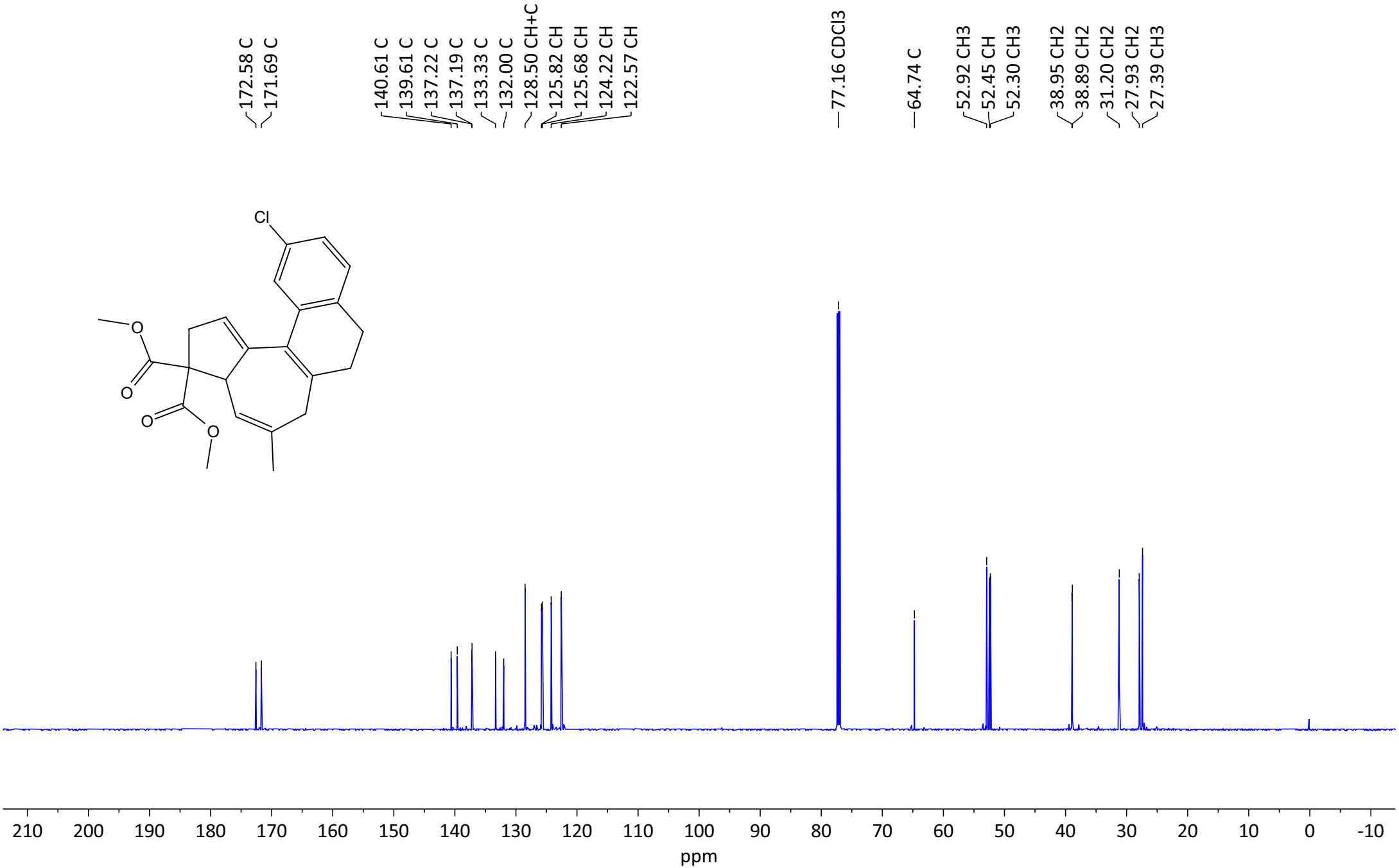
Compound **17b**: $^{13}C\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2)



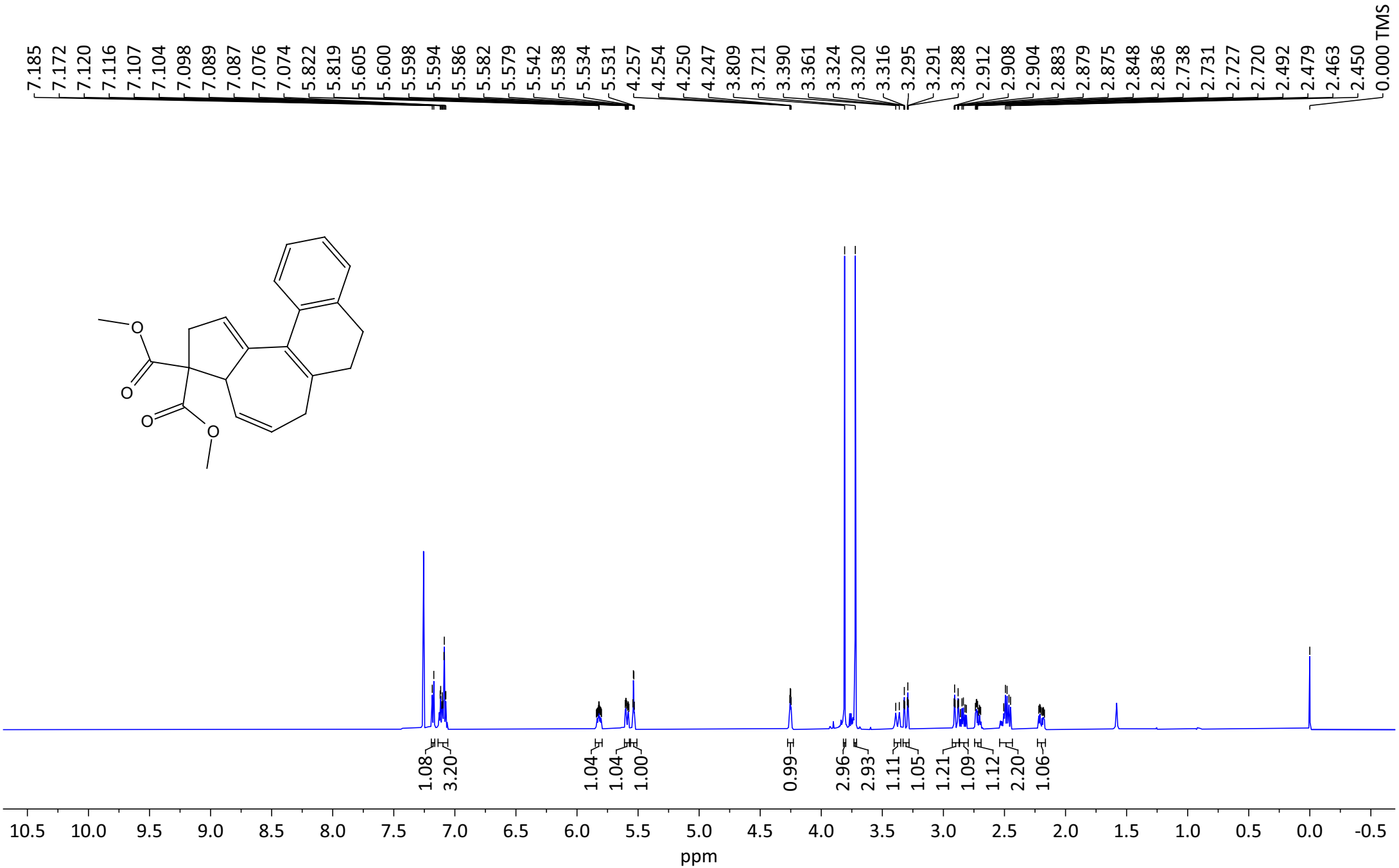
Compound **17c**: ^{1}H NMR (600 MHz, $CDCl_3$)



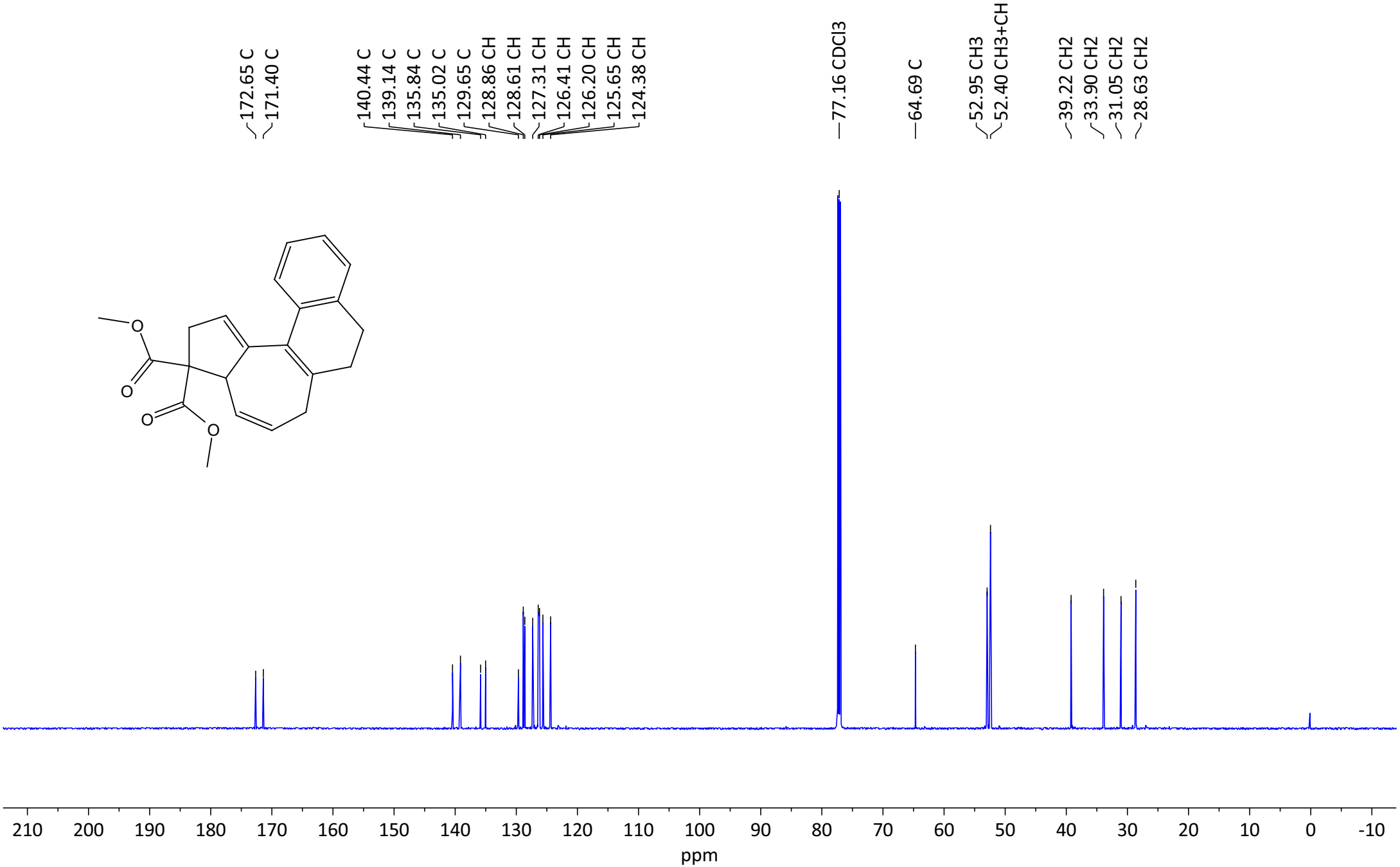
Compound **17c**: $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$)



Compound **17d**: ^{1}H NMR (600 MHz, $CDCl_3$)



Compound **17d**: $^{13}C\{^{1}H\}$ NMR (151 MHz, $CDCl_3$)



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