Supporting Information

Rhodium-Catalyzed [5 + 1 + 2] Cycloaddition of Yne-3-Acyloxy-1,4-Enynes (YACEs) and Carbon Monoxide: Reaction Development and Mechanism

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S1. General information

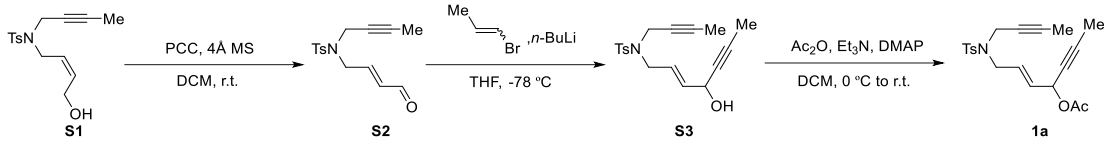
Unless otherwise noted, all reactions were carried out in an oven-dried glassware sealed with rubber septa, and under a positive pressure of inert gas, typically argon or nitrogen, and were stirred using Teflon-coated magnetic stir bars. Elevated temperatures were maintained using thermostat-controlled silicone oil baths. Analytical thin layer chromatography (TLC) was performed with 0.25 mm silica gel G plates with a 254 nm fluorescent indicator, and visualized by ultraviolet light and/or treatment with anisaldehyde followed by gentle heating. Flash chromatography on silica gel (200-300 mesh) was used for purification of products. Organic solutions were concentrated using an IKA, Büchi or Eyela rotary evaporator with a desktop vacuum pump. Chemicals were purchased from J&K, Energy, Acros, Aldrich or similar suppliers, and were used as received unless otherwise indicated. Super-dry solvents (water ≤ 30 ppm) were purchased from J&K. Tetrahydrofuran (THF) and toluene were distilled from sodium/benzophenone prior to use.

NMR spectra were measured on Bruker ARX 400 (^{1}H at 400 MHz, ^{13}C at 101 MHz), AVANCE III 500 (^{1}H at 500 MHz, ^{13}C at 126 MHz), and AVENCE NEO 600 (^{1}H at 600 MHz, ^{13}C at 151 MHz) nuclear magnetic resonance spectrometers. Data for ^{1}H-NMR spectra are reported as follows: chemical shift (ppm, referenced to residual solvent peak (CD_2Cl_2: 5.32 ppm, $CDCl_3$: 7.26 ppm); s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublets, ddt = doublet of doublet of triplets, dtd = doublet of triplet of doublets, dddd = doublet of doublet of doublet of doublets, m = multiplet), coupling constant (Hz), and integration. Data for ^{13}C-NMR are reported in terms of chemical shift (ppm) relative to residual solvent peak (CD_2Cl_2: 53.84 ppm, $CDCl_3$: 77.16 ppm). High-resolution mass spectra (HRMS) were recorded on a Bruker Apex IV FTMS mass spectrometer (m/z).

Abbreviations:

Ac = acetyl
Bn = benzyl
DCE = 1,2-dichloroethane
DCM = dichloromethane
DIAD = diisopropyl azodiformate
DMAP = 4-Dimethylaminopyridine
DMF = N, N-dimethylformamide
EA = ethyl acetate
LDA = lithium diisopropylamide
MP = melting point
MS = molecular sieve
PCC = pyridinium chlorochromate
PE = petroleum ether
r.t. = room temperature
TBAF = tetrabutylammonium fluoride
TBS = tertbutyldimethylsilyl
THF = tetrahydrofuran
Ts = tosyl

S2. Substrate Preparation

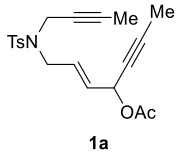


(E)-1-((N-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)hept-2-en-5-yn-4-yl acetate (1a)

To a suspension of PCC (2.42 g, 11.2 mmol, 1.5 eq.) and 4 Å MS (2.42 g) in CH_2Cl_2 (40 mL) was added a solution of **S1**[1] (2.15 g, 7.3 mmol, 1.0 eq. in 20 mL of DCM) at 0 °C. The mixture was stirred at room temperature for 12 h. Then silica gel (10 g) was added to the reaction solution to give turbid liquid, which was filtered through a pad of silica gel and washed with EA. The filtrate was concentrated under reduced pressure to yield the crude **S2** as a yellow viscous liquid for the next step without purification.

To a THF (10 mL) solution of 1-bromo-1-propene (950 μL, 11.2 mmol, 1.5 eq.) was added *n*-BuLi (2.4 M in hexane, 7.0 mL, 16.8 mmol, 2.2 eq.) under nitrogen atmosphere at -78 °C, and the mixture was stirred for 2 hours. After that, the solution of the entire **S2 (**in 5 mL of THF**)** in the first step was added and the resulting solution was stirred for 1 hour at room temperature. Ice-cold saturated NH_4Cl aq. was added to quench the reaction, followed by extraction with ethyl acetate. The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The crude product was purified by flash column chromatography (PE/EA = 2:1) to yield **S3** as a colorless viscous liquid (1.19 g, 3.6 mmol, 49%).

To the solution of alcohol **S3** (597 mg, 1.8 mmol in 15 mL of DCM), Et_3N (727 mg, 7.2 mmol, 4.0 eq.) and DMAP (22 mg, 0.18 mmol, 0.1 eq.) were added, followed by adding Ac_2O (364 mg, 3.6 mmol, 2.0 eq.) carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 11.5 h. The solution was concentrated under vacuum to yield crude product, then purified by flash column chromatography (PE/EA = 5:1) to yield **1a** as a yellow viscous liquid (410 mg, 1.1 mmol, 61%).

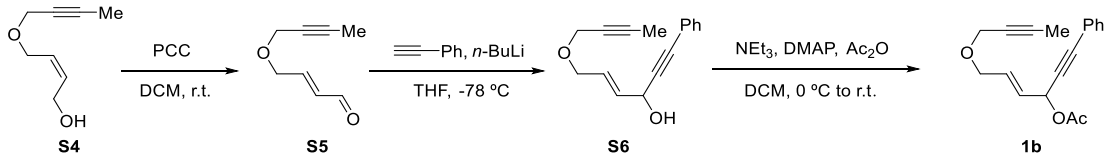


TLC (5:1 PE/EA, R_f): 0.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.9 Hz, 2H), 7.32 (d, J = 7.9 Hz, 2H), 5.96 – 5.87 (m, 1H), 5.86 – 5.81 (m, 1H), 5.77 (dd, J = 15.3, 5.3 Hz, 1H), 4.13 – 3.94 (m, 2H), 3.94 – 3.69 (m, 2H), 2.44 (s, 3H), 2.10 (s, 3H), 1.89 (s, 3H), 1.56 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 143.5, 136.2, 130.3, 129.4, 128.8, 128.0, 84.0, 81.9, 74.5, 71.6, 63.8, 47.5, 36.7, 21.6, 21.2, 3.8, 3.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{20}H_{24}NO_4S^+$: 374.1421, found: 374.1418.



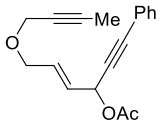
(E)-6-(but-2-yn-1-yloxy)-1-phenylhex-4-en-1-yn-3-yl acetate (1b)

To a suspension of PCC (3.24 g, 15 mmol, 1.5 eq.) and 4 Å MS (3.24 g) in CH_2Cl_2 (15 mL) was

added a solution of **S4**[2] (1.40 g, 10 mmol, 1.0 eq. in 35 mL of DCM) at 0 °C. The mixture was stirred at room temperature for 12 h. Then silica gel (6.48 g) was added to the reaction solution to give turbid liquid, which was filtered through a pad of silica gel and washed with EA. The filtrate was concentrated under reduced pressure to yield the crude **S5** as a yellow liquid for the next step without purification.

To a THF (30 mL) solution of ethynylbenzene (1.3 mL, 12 mmol, 1.2 eq.), *n*-BuLi (2.4 M in hexane, 4.6 mL, 11 mmol, 1.1 eq.) was added under nitrogen atmosphere at -78 °C. The mixture was stirred for 30 min. After that, the solution of **S5** (1.38 g, 10.0 mmol in 20 mL of THF) was added and the resulting solution was stirred for 1 hour at room temperature. The solution was stirred for 1 hour at room temperature. Ice-cold saturated NH_4Cl aq. was added to quench the reaction, followed by extraction with ethyl acetate. The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The crude product was purified by flash column chromatography (PE/EA = 5:1) to yield **S6** as a colorless viscous liquid (1.45 g, 6.0 mmol, 60%).

To the resolution of alcohol **S3** (0.481 g, 2.0 mmol in 50 mL of DCM), Et_3N (1.1 mL, 8.0 mmol, 4.0 eq.) and DMAP (24.4 mg, 0.2 mmol, 0.1 eq.) were added, followed by adding Ac_2O (0.38 mL, 4.0 mmol, 2.0 eq.) carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 14 h. The solution was concentrated under vacuum to yield crude product, then purified by flash column chromatography (PE/EA = 10:1) to yield **1b** as a yellow viscous liquid (323.2 mg, 1.1 mmol, 55%).



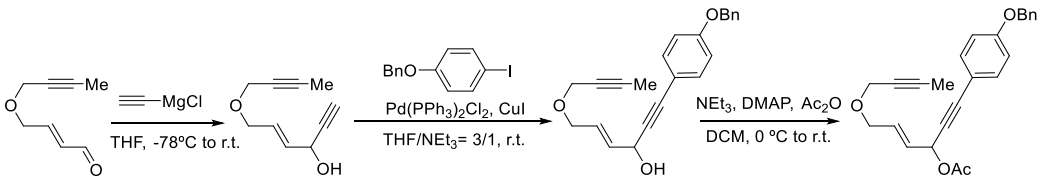
1b

TLC (5:1 PE/EA, R_f): 0.4.

^{1}H-NMR (400 MHz, CD_2Cl_2) δ 7.46 (dd, J = 7.5, 2.2 Hz, 2H), 7.39 – 7.30 (m, 3H), 6.16 – 6.08 (m, 2H), 5.88 (ddt, J = 15.5, 5.9, 1.6 Hz, 1H), 4.11 (q, J = 2.3 Hz, 2H), 4.08 (dt, J = 5.3, 1.4 Hz, 2H), 2.10 (s, 3H), 1.84 (t, J = 2.4 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.9, 132.2, 131.8, 129.3, 128.8, 127.4, 122.4, 86.9, 85.0, 82.9, 75.3, 68.9, 64.3, 58.4, 21.2, 3.6.

HRMS (m/z): $[M + H]^+$ calculated for $C_{18}H_{19}O_3^+$: 283.1329, found: 283.1327.



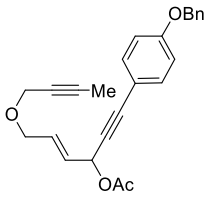
S5 **S7** **S8** **1c**

(E)-1-(4-(benzyloxy)phenyl)-6-(but-2-yn-1-yloxy)hex-4-en-1-yn-3-yl acetate (1c)

To a THF (30 mL) solution of **S5** (750 mg, 5.4 mmol, 1.2 eq.) was added the solution of ethynylmagnesium chloride (0.5 M in THF, 16 mL, 8 mmol, 1.5 eq.) dropwise under nitrogen atmosphere at -78 °C. The mixture was allowed to warm to r.t. and stirred for 65 min. Ice-cold saturated NH_4Cl aq. was added to quench the reaction, followed by extraction with EA. The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The crude product was purified by flash column chromatography (PE/EA = 3:1) to yield **S6** as a yellow liquid (613.8 mg, 3.7 mmol, 69%).

To the mixture of 1-(benzyloxy)-4-iodobenzene (1.27 g, 4.1 mmol, 1.1 eq.), $Pd(PPh_3)_2Cl_2$ (26.2 mg, 0.037 mmol, 0.01 eq.) and CuI (14.2 mg, 0.074 mmol, 0.02 eq.) were added the solution of alcohol **S6** (613.8 mg, 3.7 mmol) in THF (15 mL) under nitrogen atmosphere. Then the reaction mixture was added Et_3N (5 mL) and stirred for 12 h at room temperature. Then the mixture was concentrated under vacuum and purified by flash column chromatography (PE/EA = 5:1 to 3:1) to yield **S7** as an orange viscous liquid (945.3 mg, 2.7 mmol, 73%).

To the solution of alcohol **S8** (945.3 g, 2.6 mmol in 10 mL of DCM, 1.0 eq.), Et_3N (1.43 mL, 10.3 mmol, 4.0 eq.) and DMAP (31.7 mg, 0.26 mmol, 0.1 eq.) were added, followed by adding Ac_2O (491 μL, 5.2 mmol, 2.0 eq.) dropwise at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 18 h. The solution was concentrated under vacuum to yield crude product, then purified by flash column chromatography (PE/EA = 20:1) to yield **1c** as a red viscous liquid (819 mg, 2.1 mmol, 81%).



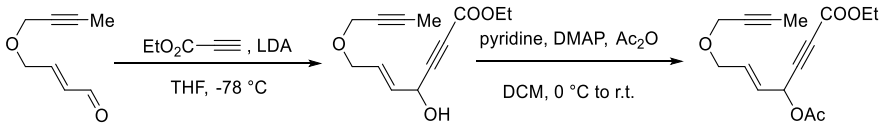
1c

TLC (5:1 PE/EA, R_f): 0.6.

^{1}H-NMR (400 MHz, CD_2Cl_2) δ 7.44 – 7.31 (m, 7H), 6.97 – 6.88 (m, 2H), 6.11 (m, 2H), 5.87 (ddt, J = 15.4, 5.9, 1.6 Hz, 1H), 5.06 (s, 2H), 4.10 (q, J = 2.3 Hz, 2H), 4.07 (dt, J = 5.3, 1.3 Hz, 2H), 2.09 (s, 3H), 1.84 (t, J = 2.3 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.9, 159.7, 137.1, 133.7, 131.6, 128.9, 128.5, 128.0, 127.7, 115.2, 114.6, 86.9, 83.8, 82.9, 75.3, 70.4, 68.9, 64.4, 58.4, 21.3, 3.6.

HRMS (m/z): $[M + H]^+$ calculated for $C_{25}H_{25}O_4^+$: 389.1747, found: 389.1750.



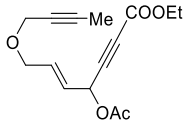
S5 **S9** **1d**

Ethyl (E)-4-acetoxy-7-((N-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)hept-5-en-2-ynoate (1d)

To a stirred solution of diisopropylamine (475 μL, 3.4 mmol, 1.7 eq.) in THF (10 mL) was added a solution of *n*-BuLi (2.4 M in hexanes, 1.42 mL, 3.4 mmol, 1.7 eq.) slowly at -78 °C. The mixture was stirred at 0 °C for 35 min, then cooled to -78 °C, and ethyl propiolate (307 μL, 3.0 mmol, 1.5 eq.) was added. After stirring for 40 min at -78 °C, a solution of aldehyde **S5** (276 mg, 2.0 mmol) in THF (5 mL) was added. After stirring at -78 °C for 3 h, the reaction mixture was added to an ice-cold saturated NH_4Cl aq. The aqueous phase was extracted with EA, and the combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure to yield crude **S9** (yellow viscous oil) for the next step without purification

To a solution of the entire **S9** (in CH_2Cl_2 15 mL) in the first step was added pyridine (480 μL, 6.0 mmol, 3.0 eq.), DMAP (12.2 mg, 0.1 mmol, 0.05 eq.) and Ac_2O (285 μL, 3 mmol, 1.5 eq.) at 0°C. After stirring for 13 h, the mixture was diluted with DCM and washed with a 10% copper sulfate aqueous solution, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (PE/EA = 10:1) to give **1d** as a yellow viscous liquid (305 mg, 1.1

mmol, 54% yield).



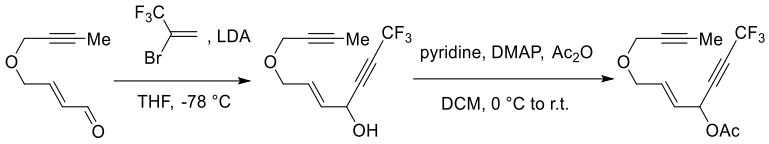
1d

TLC (5:1 PE/EA, R_f): 0.2.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 6.08 (dtd, *J* = 15.5, 5.1, 1.3 Hz, 1H), 5.99 – 5.93 (m, 1H), 5.81 (ddt, *J* = 15.5, 6.2, 1.7 Hz, 1H), 4.22 (q, *J* = 7.1 Hz, 2H), 4.10 (q, *J* = 2.3 Hz, 2H), 4.07 (dt, *J* = 5.1, 1.4 Hz, 2H), 2.09 (s, 3H), 1.85 (t, *J* = 2.4 Hz, 3H), 1.29 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.6, 153.1, 133.2, 125.2, 83.0, 82.1, 78.2, 75.1, 68.7, 63.1, 62.7, 58.5, 21.0, 14.1, 3.6.

HRMS (m/z): $[M + H]^+$ calculated for $C_{15}H_{19}O_5^+$: 279.1227, found: 279.1226.

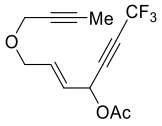


S5 **S10** **1e**

(E)-1-((N-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)-7,7,7-trifluorohept-2-en-5-yn-4-yl acetate (1e)

To a stirred solution of diisopropylamine (1.12 mL, 8.0 mmol, 2.0 eq.) in THF (10 mL) was added a solution of *n*-BuLi (2.4 M in hexanes, 3.33 mL, 8.0 mmol, 2.0 eq.) slowly at 0 °C. The mixture was stirred at 0°C for 30 min, then cooled to -78 °C and the solution of 2-bromo-3,3,3-trifluoroprop-1-ene (0.56 mL, 4 mmol, 1.0 eq. in 10 mL of THF) was added. After stirring for 30 min at -78 °C, a solution of aldehyde **S5** (553 mg, 4 mmol in 10 mL of THF) was added. After stirring at -78 °C for 3 h, the reaction mixture was added to an ice-cold saturated NH_4Cl aq. The aqueous phase was extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, then purified by flash column chromatography (PE/EA = 5:1) to yield **S9** as a dark red viscous oil (821 mg, 3.5 mmol, 88%).

To a solution of the above oil (410 mg, 1.8 mmol, in CH_2Cl_2 15 mL) was added pyridine (425 μL, 5.3 mmol, 3.0 eq.), DMAP (10.8 mg, 0.09 mmol, 0.05 eq.) and Ac_2O (250 μL, 2.7 mmol, 1.5 eq.) at 0 °C. After stirring overnight, the mixture was diluted with DCM and washed with a 10% copper sulfate aqueous solution, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (PE/EA = 20:1) to give **1e** as an orange viscous liquid (284 mg, 1.0 mmol, 59% yield).



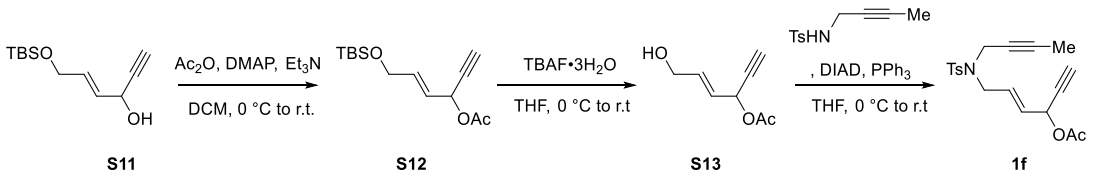
1e

TLC (10:1 PE/EA, R_f): 0.4.

^{1}H-NMR (400 MHz, CD_2Cl_2) δ 6.08 (dtd, J = 15.5, 5.0, 1.2 Hz, 1H), 5.99 – 5.93 (m, 1H), 5.81 (ddt, J = 15.5, 6.3, 1.8 Hz, 1H), 4.11 (q, J = 2.4 Hz, 2H), 4.07 (dt, J = 5.1, 1.3 Hz, 2H), 2.10 (s, 3H), 1.85 (t, J = 2.4 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.5, 133.7, 124.5, 112.6 (q, J = 257.5 Hz), 83.7 (q, J = 6.4 Hz), 83.1, 75.1, 73.2 (q, J = 53.1 Hz), 68.6, 62.5, 58.6, 20.9, 3.6.

HRMS (m/z): $[M + H]^+$ calculated for $C_{13}H_{14}F_3O_3^+$: 275.0890, found: 275.0889.



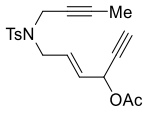
S11 **S12** **S13** **1f**

(E)-6-((N-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)hex-4-en-1-yn-3-yl acetate (1f)

To the solution of alcohol **S11**[3](452 mg, 2.0 mmol in 5 mL of DCM), both Et_3N (1.10 mL, 8.0 mmol, 4.0 eq.) and DMAP (24.4 mg, 0.2 mmol, 0.1 eq.) were added, followed by adding Ac_2O (380 μL, 4.0 mmol, 2.0 eq.) dropwise at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 5 h. The solution was concentrated under vacuum to yield crude product, then purified by flash column chromatography (PE/EA = 20:1) to yield **S12** as a colorless liquid (485 mg, 1.8 mmol, 90%).

To the solution of alcohol **S12** (485 mg, 1.8 mmol in 3 mL of THF), TBAF•$3H_2O$ (631 mL, 2.0 mmol, 1.1 eq.) was added at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 6 h. Then the reaction mixture was quenched with water. The aqueous phase was extracted with Et_2O. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, and then purified by flash column chromatography (PE/EA = 3:1) to yield **S13** as a yellow oil (149 mg, 0.97 mmol, 54%).

DIAD (209 mg, 1.03 mmol, 1.2 eq.) was added into the mixture of alcohol **S13** (146 mg, 0.95 mmol, 1.1 eq.), N-(but-2-yn-1-yl)-4-methylbenzenesulfonamide (192 mg, 0.86 mmol, 1.0 eq.), PPh_3 (271 mg, 1.03 mmol, 1.2 eq.) and THF (5 mL) at 0°C under an inert atmosphere. Then the reaction was warmed to room temperature and stirred for 5 h 20 min. DIAD (149 mg, 0.74 mmol, 0.86 eq.) was added to the reaction solution. Then the reaction was stirred for 18 h 40 min. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/EA/DCM = 6:1:1) to yield **1f** (90.4 mg, 0.25 mmol, 29%) as a yellow viscous oil.



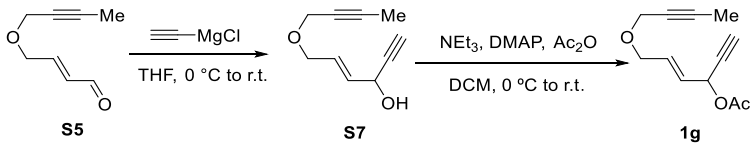
1f

TLC (3:1 PE/EA, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 5.94 (dt, J = 15.3, 6.3 Hz, 1H), 5.86 – 5.83 (m, 1H), 5.77 (dd, J = 15.3, 5.5 Hz, 1H), 4.07 – 3.94 (m, 2H), 3.94 – 3.77 (m, 2H), 2.56 (d, J = 2.2 Hz, 1H), 2.43 (s, 3H), 2.10 (s, 3H), 1.55 (t, J = 2.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 143.5, 136.1, 129.7, 129.5, 129.1, 128.0, 82.0, 79.0, 75.5, 71.6, 63.0, 47.4, 36.8, 21.6, 21.0, 3.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{19}H_{22}NO_4S$+: 360.1264, found: 360.1266.



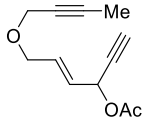
S5 **S7** **1g**

(E)-6-(but-2-yn-1-yloxy)hex-4-en-1-yn-3-yl acetate(1g)

To the solution of **S5** (829.2 mg, 6 mmol in 6 ml of THF) was added ethynylmagnesium chloride (0.5 M in THF, 18 mL, 9 mmol, 1.5 eq.) dropwise under nitrogen atmosphere at 0 °C. The mixture was allowed

to warm to r.t. and stirred for 3 h. Saturated NH_4Cl aq. was added to quench the reaction, followed by extraction with ethyl acetate. The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under a vacuum. The crude product was purified by flash column chromatography (PE/EA = 10:1 to 5:1) to yield **S7** as a yellow liquid (661.5 mg, 4.0 mmol, 67%).

To the solution of alcohol **S7** (240.3 mg, 1.46 mmol), both Et_3N (0.55 mL, 4 mmol, 2.7 eq.) and DMAP (12.2 mg, 0.1 mmol, 0.07 eq.) were added, followed by adding Ac_2O (0.19 mL, 2.0 mmol, 1.4 eq.) dropwise at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 16 h. The solution was concentrated under vacuum to yield crude product, then purified by flash column chromatography (PE/EA = 10:1) to yield **1g** as a yellow viscous oil(297.0 mg, 1.44 mmol, 98%).



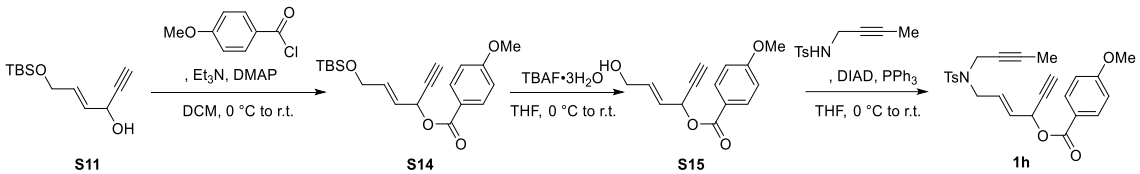
1g

TLC (3:1 PE/EA, R_f): 0.7.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.10 (dt, J = 15.2, 5.3 Hz, 1H), 5.90 – 5.86 (m, 1H), 5.82 (dt, J = 15.3, 5.9, 1H), 4.11 (q, J = 2.3 Hz, 2H), 4.08 (dt, J = 5.5, 1.3 Hz, 2H), 2.57 (d, J = 2.2 Hz, 1H), 2.09 (s, 3H), 1.85 (t, J = 2.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 131.7, 126.8, 82.9, 79.3, 75.3, 74.9, 68.7, 63.4, 58.3, 21.1, 3.7.

HRMS (m/z): $[M + H]^+$ calculated for $C_{12}H_{15}O_3^+$: 207.1016; found: 207.1016.



S11 **S14** **S15** **1h**

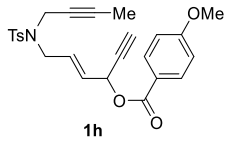
(E)-6-((N-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)hex-4-en-1-yn-3-yl 4-methoxybenzoate (1h)

To the alcohol solution of **S11**[3] (1.13 g, 5.0 mmol in 30 mL of DCM), both Et_3N (1.52 g, 15.0 mmol, 3.0 eq.) and DMAP (61.0 mg, 0.5 mmol, 0.1 eq.) were added, followed by adding 4-methoxybenzoyl chloride (1.71 g, 10.0 mmol, 2.0 eq.) dropwise at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 4.5 h. Then the reaction mixture was quenched with Saturated $NaHCO_3$ aq. The aqueous phase was extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, and then purified by flash column chromatography (PE/EA = 5:1) to yield **S14** as a yellow liquid (1.72 g, 4.8 mmol, 96%).

To the solution of alcohol **S14** (1.72 g, 4.8 mmol in 15 mL of THF), the solution of TBAF•$3H_2O$ (1.82 g, 5.8 mmol, 1.2 eq. in 15 mL of THF) was added at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 13 h. Then the reaction mixture was quenched with water. The aqueous phase was extracted with Et_2O. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, then purified by flash column chromatography (PE/EA = 5:1 to 2:1) to yield **S15** as a yellow liquid (0.74 g, 3.0 mmol, 63%).

DIAD (1.12 g, 5.5 mmol, 2.05 eq.) was added into the mixture of alcohol **S15** (0.74 g, 3.0 mmol, 1.1 eq.), N-(but-2-yn-1-yl)-4-methylbenzenesulfonamide (0.61 g, 2.7 mmol, 1.0 eq.), PPh_3 (0.87 g, 3.3 mmol, 1.2 eq.) and THF (15 mL) at 0°C under an inert atmosphere. Then the reaction was warmed to room temperature and stirred for 24 h. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/ EA = 7:1) to yield **1h** (90.4 mg, 0.25 mmol, 29%) as a

yellow viscous oil.



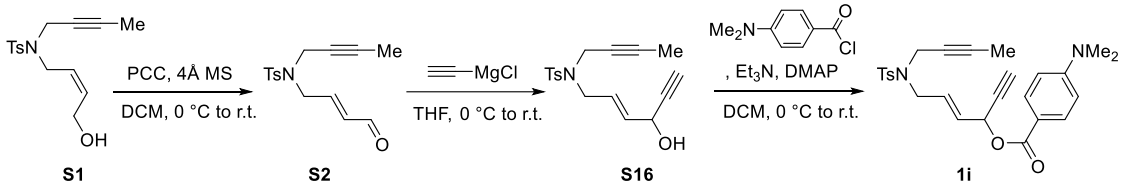
1h

TLC (3:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.9 Hz, 2H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.11 – 6.05 (m, 1H), 6.01 (dtd, *J* = 13.7, 6.2, 1.2 Hz, 1H), 5.92 – 5.84 (m, 1H), 4.02 (t, *J* = 2.7 Hz, 2H), 3.90 – 3.84 (m, 5H), 2.59 (d, *J* = 2.2 Hz, 1H), 2.40 (s, 3H), 1.53 (t, *J* = 2.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 163.9, 143.5, 136.2, 132.1, 129.5, 129.4, 129.4, 128.0, 121.9, 113.8, 82.0, 79.2, 75.5, 71.7, 63.2, 55.6, 47.6, 36.9, 21.6, 3.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{25}H_{26}NO_5S^+$: 452.1526, found: 452.1526.



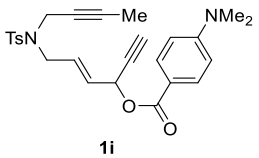
S1 S2 S16 1i

(E)-6-((N-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)hex-4-en-1-yn-3-yl 4-(dimethylamino) benzoate (1i)

To a mixture of PCC (2.0 g, 9.3 mmol, 1.5 eq.) and 4 Å MS (0.30 g) was added a solution of **S1** (1.80 g, 6.0 mmol, 1.0 eq. in 60 mL of DCM). The mixture was stirred at room temperature for 12 h. Then silica gel was added to the reaction solution to give turbid liquid, which was filtered through a pad of silica gel and washed with EA. The filtrate was concentrated under reduced pressure to yield the crude **S2** for the next step without purification.

To a THF (10 mL) solution of the entire crude **S2** in the first step was added ethynylmagnesium chloride (0.5 M in THF, 18 mL, 9 mmol, 1.5 eq.) dropwise under nitrogen atmosphere at -78 °C. The mixture was allowed to warm to r.t. and stirred for 1h. Saturated NH_4Cl aq. was added to quench the reaction, followed by extraction with ethyl acetate. The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under a vacuum to yield the crude **S16** for the next step without purification.

To **S16** (317 mg, 1.0 mmol in 10 mL of DCM), both Et_3N (0.55mL, 4.0 mmol, 4.0 eq.) and DMAP (11mg , 0.1 mmol, 0.1 eq.) were added, followed by adding 4-(dimethylamino)benzoyl chloride (200 mg, 1.1mmol, 1.1 eq.) carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 12 h. The solution was quenched with 50 mg MeOH and concentrated under a vacuum. The residue was purified by flash column chromatography (PE/ EA = 10:1 to 5:1) to yield **1i** (326.4 mg, 0.70 mmol, 70%) as a colorless oil.



1i

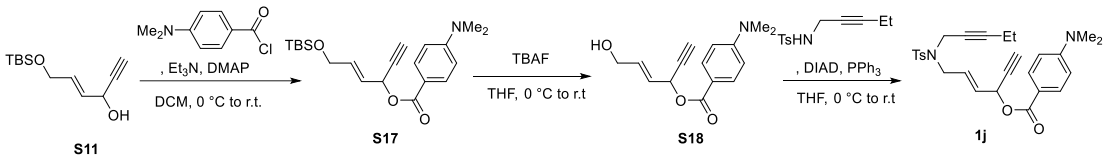
TLC (2:1 PE/EA, R_f): 0.7.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.87 (d, *J* = 9.1 Hz, 2H), 7.71 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz,

2H), 6.67 (d, *J* = 9.0 Hz, 2H), 6.05 (d, *J* = 5.2 Hz, 1H), 6.02 – 5.93 (m, 1H), 5.88 (dd, *J* = 15.3, 5.2 Hz, 1H), 4.00 (s,2H), 3.86 (d, *J* = 5.6 Hz, 2H), 3.04 (s, 6H), 2.63 (d, *J* = 2.1 Hz, 1H), 2.41 (s, 3H), 1.54 (t, *J* = 2.3 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 165.5, 154.1, 144.0, 136.4, 131.7, 130.1, 129.8, 129.2, 128.1, 116.1, 111.1, 82.3, 80.0, 75.1, 71.8, 62.8, 47.9, 40.2, 37.1, 21.6, 3.3.

HRMS (m/z): $[M + H]^+$ calculated for $C_{26}H_{29}N_2O_4S^+$: 465.1843; found: 465.1838.

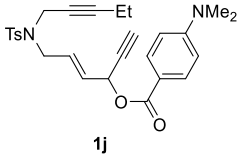


(E)-6-((4-methyl-N-(pent-2-yn-1-yl)phenyl)sulfonamido)hex-4-en-1-yn-3-yl 4-(dimethylamino) benzoate (1j)

To the solution of alcohol **S11**[3] (9.53 g, 42 mmol in 150 mL of DCM), both Et_3N (16.6 mL, 120 mmol, 2.9 eq.) and DMAP (0.51g, 4.2mmol, 0.1 eq.) were added, followed by adding the solution of 4-(dimethylamino)benzoyl chloride (9.18 g, 50mmol, 1.2 eq. in 60 mL of DCM) carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 5 h. The solution was quenched by saturated $NaHCO_3$ aq. and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum to yield the crude ester **S17** as yellow solid was used for the next step without further purification.

To the solution of the entire **S17** (in 50 mL of THF) in the first step, TBAF solution (1 M in THF, 50 mL, 50 mmol, 1.2 eq.) was added carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 1 h. The solution was quenched with water and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (PE/ EA/DCM = 5:1:1 to 2:1:1) to yield **S18** (9.97 g, 38 mmol, 92% for 2 steps) as a yellow solid.

DIAD (0.24 mL, 1.2 mmol, 1.2 eq.) was added into the mixture of alcohol **S18** (309 mg, 1.2 mmol, 1.2 eq.), 4-methyl-N-(pent-2-yn-1-yl)benzenesulfonamide (237.6 mg, 1 mmol), PPh_3 (331 mg, 1.2 mmol, 1.2 eq.) and THF (5 mL) at 0ºC under an inert atmosphere. Then the reaction was warmed to room temperature and stirred for 22 h 50 min. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE: EA:DCM = 8/1/1) to yield **1j** (403 mg, yield = 88%) as a colorless foam.

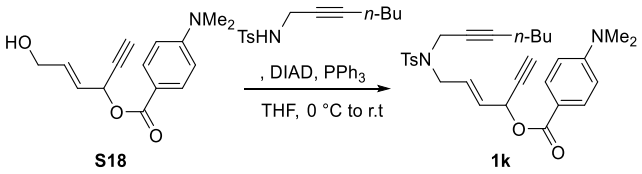


TLC (5:1 PE/EA, R_f): 0.6.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.87 (d, *J* = 9.0 Hz, 2H), 7.71 (d, *J* = 8.3 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 6.66 (d, *J* = 9.0 Hz, 2H), 6.08 – 6.04 (m, 1H), 6.03 – 5.94 (m, 1H), 5.89 (dd, *J* = 15.3, 5.3 Hz, 1H), 4.03 (s, 2H), 3.87 (d, *J* = 6.0 Hz, 2H), 3.04 (s, 6H), 2.63 (d, *J* = 2.2 Hz, 1H), 2.40 (s, 3H), 1.92 (qt, *J* = 7.5, 2.2 Hz, 2H), 0.89 (t, *J* = 7.5 Hz, 3H).

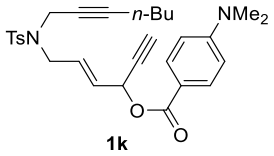
^{13}C NMR (101 MHz, CD_2Cl_2) δ 165.5, 154.1, 144.0, 136.5, 131.7, 130.1, 129.8, 129.2, 128.1, 116.1, 111.0, 88.2, 80.0, 75.1, 71.9, 62.8, 47.8, 40.2, 37.1, 21.6, 13.7, 12.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{27}H_{31}N_2O_4S^+$: 479.1999; found: 479.1996.



(E)-6-((N-(hept-2-yn-1-yl)-4-methylphenyl)sulfonamido)hex-4-en-1-yn-3-yl 4-(dimethylamino) benzoate (1k)

DIAD (0.24 mL, 1.2 mmol, 1.2eq.) was added into the mixture of alcohol **S18** (311 mg, 1.2 mmol, 1.2eq.), N-(hept-2-yn-1-yl)-4-methylbenzenesulfonamide (265 mg, 1 mmol), PPh_3 (331 mg, 1.2 mmol, 1.2eq.) and THF (5 mL) at 0 ºC under an inert atmosphere. Then the reaction was warmed to room temperature and stirred for 14 h. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/EA/DCM = 5:1:1) to yield **1k** (455 mg, 90%) as a colorless foam.

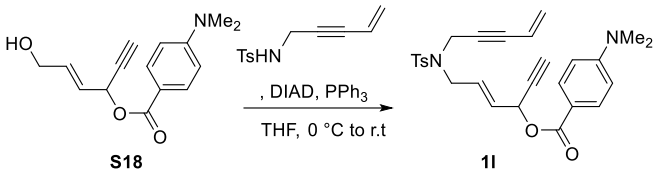


TLC (2:1 PE/EA, R_f): 0.7.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.87 (d, J = 9.0 Hz, 2H), 7.70 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 6.67 (d, J = 9.0 Hz, 2H), 6.08 – 6.04 (m, 1H), 6.03 – 5.94 (m, 1H), 5.88 (dd, J = 15.3, 5.4 Hz, 1H), 4.04 (s, 2H), 3.87 (d, J = 6.1 Hz, 2H), 3.04 (s, 6H), 2.63 (d, J = 2.2 Hz, 1H), 2.41 (s, 3H), 1.93 – 1.22 (m, 2H), 1.36 – 1.04 (m, 4H), 0.83 (t, J = 7.0 Hz, 3H).

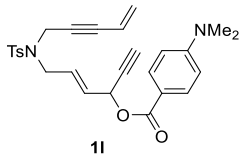
^{13}C NMR (101 MHz, CD_2Cl_2) δ 165.5, 154.0, 144.0, 136.5, 131.7, 130.2, 129.8, 129.2, 128.1, 116.2, 111.1, 86.9, 80.0, 75.1, 72.4, 62.8, 47.8, 40.3, 37.1, 30.8, 22.2, 21.6, 18.4, 13.7.

HRMS (m/z): $[M + H]^+$ calculated for $C_{29}H_{35}N_2O_4S^+$: 507.2312; found: 507.2310.



(E)-6-((4-methyl-N-(pent-4-en-2-yn-1-yl)phenyl)sulfonamido)hex-4-en-1-yn-3-yl 4-(dimethylamino)benzoate (1l)

DIAD (0.24 mL, 1.2 mmol, 1.2 eq.) was added into the mixture of alcohol **S18** (311 mg, 1.2 mmol, 1.2eq.), 4-methyl-N-(pent-4-en-2-yn-1-yl)benzenesulfonamide (235 mg, 1 mmol), PPh_3 (314 mg, 1.2 mmol, 1.2 eq.) and THF (5 mL) at 0 ºC under an inert atmosphere. Then the reaction was warmed to room temperature and stirred for 12 h. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/ EA/DCM = 20:1 to PE/ EA/DCM = 8:1:1) to yield **1l** (365.1 mg, 77%) as a colorless foam.

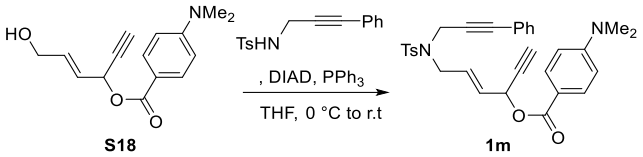


TLC (2:1 PE/EA, R_f): 0.5.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.83 (d, J = 9.1 Hz, 2H), 7.68 (d, J = 8.1 Hz, 2H), 7.27 (d, J = 8.1 Hz, 2H), 6.63 (d, J = 9.1 Hz, 2H), 6.05 – 6.00 (m, 1H), 6.00 – 5.91 (m, 1H), 5.86 (dd, J = 15.3, 5.3 Hz, 1H), 5.55 – 5.44 (m, 1H), 5.36 – 5.32 (m, 1H), 5.30 – 5.26 (m, 1H), 4.14 (s, 2H), 3.84 (d, J = 6.1 Hz, 2H), 3.00 (s, 6H), 2.59 (d, J = 2.2 Hz, 1H), 2.36 (s, 3H).

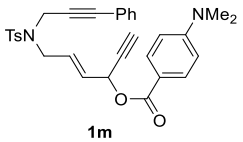
^{13}C NMR (101 MHz, CD_2Cl_2) δ 165.5, 154.1, 144.2, 136.2, 131.8, 130.4, 129.9, 129.0, 128.1, 127.7, 116.5, 116.1, 111.1, 84.7, 82.7, 80.0, 75.2, 62.8, 48.1, 40.2, 37.4, 21.6.

HRMS (m/z): $[M + H]^+$ calculated for $C_{27}H_{29}N_2O_4S^+$: 477.1843; found: 477.1857.



(E)-6-((4-methyl-N-(3-phenylprop-2-yn-1-yl)phenyl)sulfonamido)hex-4-en-1-yn-3-yl 4-(dimethylamino)benzoate (1m)

DIAD (0.24 mL, 1.2 mmol, 1.2 eq.) was added into the mixture of alcohol **S18** (311 mg, 1.2 mmol, 1.2eq.), 4-methyl-N-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (285 mg, 1 mmol, 1.0 eq.), PPh_3 (314 mg, 1.2 mmol) and THF (5 mL) at 0 °C under an inert atmosphere. Then the reaction was warmed to room temperature and stirred for 17 h. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/EA/DCM = 5:1:1) to yield **1m** (485 mg, 92%) as a white foam.

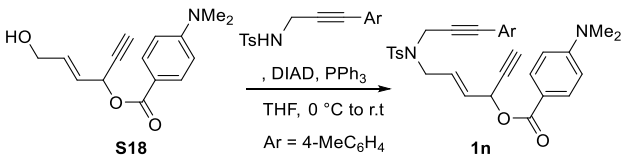


TLC (2:1 PE/EA, R_f): 0.5.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.87 (d, J = 9.0 Hz, 2H), 7.75 (d, J = 8.3 Hz, 2H), 7.34 – 7.19 (m, 5H), 7.10 – 7.06 (m, 2H), 6.65 (d, J = 9.0 Hz, 2H), 6.12 – 6.00 (m, 2H), 5.95 (dd, J = 15.1, 5.6 Hz, 1H), 4.30 (s, 2H), 3.96 (d, J = 6.7 Hz, 2H), 3.04 (s, 6H), 2.63 (d, J = 2.2 Hz, 1H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 165.5, 154.1, 144.3, 136.3, 131.9, 131.8, 130.5, 130.0, 129.0, 128.8, 128.5, 128.1, 122.5, 116.1, 111.1, 86.0, 82.0, 80.0, 75.2, 62.8, 48.2, 40.2, 37.5, 21.6.

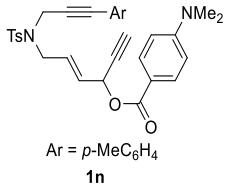
HRMS (m/z): $[M + H]^+$ calculated for $C_{31}H_{31}N_2O_4S^+$: 527.1999; found: 527.1999.



(E)-6-((4-methyl-N-(3-(p-tolyl)prop-2-yn-1-yl)phenyl)sulfonamido)hex-4-en-1-yn-3-yl 4-(dimethylamino)benzoate (1n)

DIAD (0.24 mL, 1.2 mmol, 1.2 eq.) was added into the mixture of alcohol **S18** (310.7 mg, 1.2 mmol, 1.2eq.), 4-methyl-N-(3-(*p*-tolyl)prop-2-yn-1-yl)benzenesulfonamide (299.1 mg, 1 mmol), PPh_3 (322.8 mg, 1.2 mmol, 1.2 eq.) and THF (5 mL) at 0 °C under an inert atmosphere. Then the reaction was warmed

to room temperature and stirred for 21 h. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/EA/DCM = 5:1:1) to yield **1n** (426.1 mg, 79%) as a white foam.

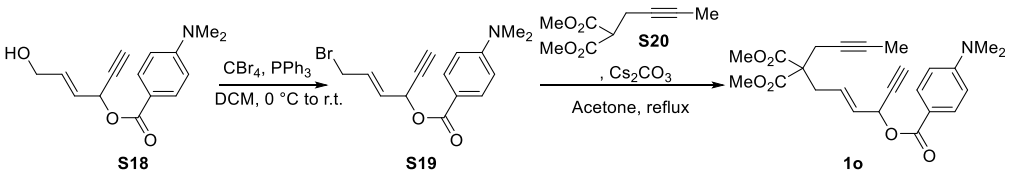


TLC (2:1 PE/EA, R_f): 0.6.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.87 (d, J = 9.0 Hz, 2H), 7.75 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 7.05 (d, J = 8.0 Hz, 2H), 6.97 (d, J = 8.2 Hz, 2H), 6.66 (d, J = 9.0 Hz, 2H), 6.11 – 5.99 (m, 2H), 5.94 (dd, J = 15.2, 5.5 Hz, 1H), 4.29 (s, 2H), 3.95 (d, J = 6.4 Hz, 2H), 3.04 (s, 6H), 2.62 (d, J = 2.1 Hz, 1H), 2.32 (s, 3H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 165.5, 154.0, 144.2, 139.2, 136.3, 131.8, 131.8, 130.4, 130.0, 129.2, 129.0, 128.1, 119.4, 116.1, 111.1, 86.2, 81.3, 80.0, 75.2, 62.8, 48.2, 40.3, 37.5, 21.6, 21.5.

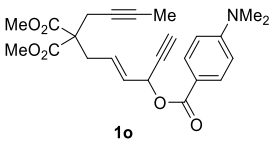
HRMS (m/z): $[M + H]^+$ calculated for $C_{32}H_{33}N_2O_4S^+$: 541.2156; found: 541.2160.



dimethyl (E)-2-(but-2-yn-1-yl)-2-(4-((4-(dimethylamino)benzoyl)oxy)hex-2-en-5-yn-1-yl)malonate (1o)

To the alcohol **S18** (1.04 g, 4.0 mmol, in 40 mL), both PPh_3 (1.26 g, 4.8 mmol, 1.2 eq.) and DCM (40 mL) were added, followed by adding CBr_4 powder (1.59g, 4.8mmol, 1.2 eq.) in batches at 0 °C. Then the reaction was warmed to room temperature, monitored by TLC, and stirred for 4 h. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/EA= 10:1) to yield **S19**, (1.18 g, 92%) as a colorless solid.

To a round-bottom flask, bromide **S19** (708 mg, 2.2 mmol, 1.1 eq.), **S20**[4] (368 mg, 2.0 mmol, 1.0 eq.), acetone (10 mL), and Cs_2CO_3 (717 mg, 2.2 mmol) were added. The reaction was then heated to 60 °C under an inert atmosphere. After being stirred for 19 h. The solution was quenched with water and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (PE/EA= 10:1 to PE/EA/DCM = 5:1:1) to yield **1o** (602.5 mg, 71%) as a yellow oil.



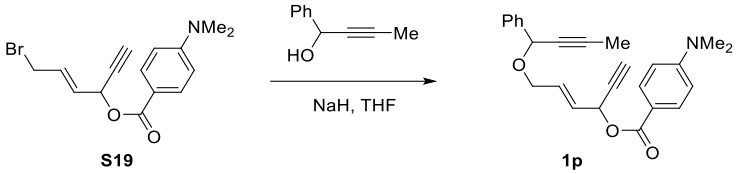
TLC (3:1 PE/EA, R_f): 0.5.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.86 (d, J = 9.0 Hz, 2H), 6.66 (d, J = 9.0 Hz, 2H), 6.07 – 5.94 (m, 1H), 5.95 – 5.86 (m, 1H), 5.78 (dd, J = 15.2, 6.1 Hz, 1H), 3.69 (s, 3H), 3.68 (s, 3H), 3.02 (s, 6H), 2.79 (d, J = 7.5 Hz, 2H), 2.71 (q, J = 2.6 Hz, 2H), 2.62 (d, J = 2.2 Hz, 1H), 1.74 (t, J = 2.6 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 170.5, 165.5, 153.9, 131.7, 130.3, 129.7, 116.5, 111.2, 80.4, 79.5, 74.9,

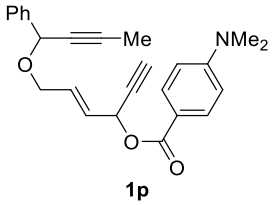
73.4, 63.3, 57.6, 54.2, 40.3, 35.3, 23.6, 3.5.

HRMS (m/z): $[M + H]^+$ calculated for $C_{24}H_{28}NO_6^+$: 426.1911; found: 426.1908.



(E)-6-((1-phenylbut-2-yn-1-yl)oxy)hex-4-en-1-yn-3-yl 4-(dimethylamino)benzoate (1p)

To a suspension of NaH (21 mg, 60% dispersion in mineral oil, 0.52 mmol, 1.3 eq. in 1.5mL of THF) was added 1-phenylbut-2-yn-1-ol (76.0 mg, 0.52 mmol, 1.3 eq.) under nitrogen atmosphere at 0 ºC. The resulting mixture was stirred for 30 min and then **S19** (129.0 mg, 0.4 mmol, 1.0 eq.) was added. After stirring for another 2 h at room temperature, the reaction solution was quenched by saturated NH_4Cl aq. and extracted with DCM. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography to yield **1p** (120.8 mg, 0.31 mmol, 78%) as a brown oil.

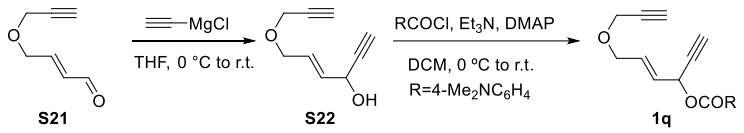


TLC (4:1:2 PE/EA/DCM, R_f): 0.7.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, J = 9.0 Hz, 2H), 7.51 (d, J = 7.0 Hz, 2H), 7.40 – 7.29 (m, 3H), 6.65 (d, J = 9.0 Hz, 2H), 6.20 (ddt, J = 15.5, 5.4, 1.6 Hz, 1H), 6.15 – 6.10 (m, 1H), 5.96 (dd, J = 15.5, 5.4 Hz, 1H), 5.17 (s, 1H), 4.22 (dd, J = 13.0, 5.1 Hz, 1H), 4.17 – 4.04 (m, 1H), 3.04 (s, 6H), 2.57 (d, J = 2.1 Hz, 1H), 1.91 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 153.6, 139.1, 131.8, 131.3, 131.2, 128.6, 128.4, 127.5, 116.5, 110.9, 96.4, 84.2, 80.0, 74.9, 71.4, 67.4, 63.1, 40.3, 4.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{25}H_{26}NO_3^+$: 388.1907; found: 388.1907.

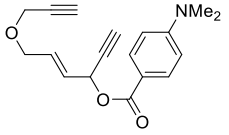


(E)-6-(prop-2-yn-1-yloxy)hex-4-en-1-yn-3-yl 4-(dimethylamino)benzoate (1q)

To a solution of **S21**[5] (0.765 g, 6.2 mmol, 1.0 eq. in 6.5 mL of THF) was added ethynylmagnesium chloride (0.5 M in THF, 18.5 mL, 9.3 mmol, 1.5 eq.) dropwise under nitrogen atmosphere at 0 °C. The mixture was allowed to warm to r.t. and stirred for 1 h. Saturated NH_4Cl aq. (20 mL) was added to quench the reaction, followed by extraction with ethyl acetate. The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under a vacuum. The crude product was purified by flash column chromatography (PE/EA = 6:1) to yield **S22** as a colorless liquid (756.2 mg, 5.0

mmol, 81%).

To the solution of alcohol **S22** (756.2 mg, 5.0 mmol in 12 mL of DCM), both Et_3N (2.5 mL, 18.5 mmol, 3.7 eq.) and DMAP (76 mg, 0.617 mmol, 0.12 eq.) were added, followed by adding 4-(dimethylamino)benzoyl chloride (1.38 g, 7.5 mmol, 1.5 eq.) dropwise at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 24 h. Saturated $NaHCO_3$ aq. was added to quench the reaction, followed by extraction with DCM. The combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under a vacuum to yield **1q** as a white solid (1.01 g, 3.4 mmol, 68%).



1q

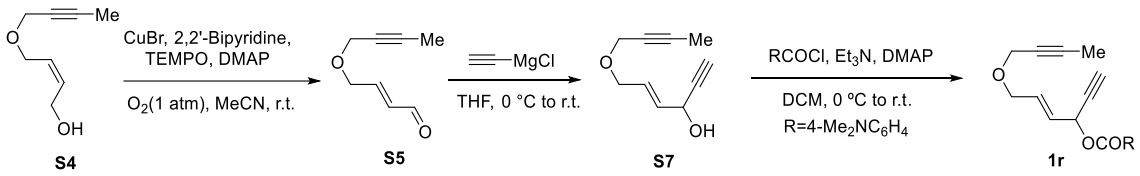
M.P. = 68.3-70.5 ºC

TLC (3:1 PE/EA, R_f): 0.5

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.88 (d, *J* = 9.0 Hz, 2H), 6.66 (d, *J* = 9.0 Hz, 2H), 6.14 (dtd, *J* = 15.7, 5.4, 1.3 Hz, 1H), 6.10 – 6.07 (m, 1H), 5.93 (ddt, *J* = 15.7, 5.6, 1.5 Hz, 1H), 4.16 (d, *J* = 2.4 Hz, 2H), 4.12 (d, *J* = 5.4 Hz, 2H), 3.04 (s, 6H), 2.65 (d, *J* = 2.2 Hz, 1H), 2.49 (t, *J* = 2.4 Hz, 1H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 165.6, 154.0, 131.7, 131.0, 128.0, 116.2, 111.0, 80.2, 80.0, 75.0, 74.7, 69.2, 63.1, 57.8, 40.2.

HRMS (m/z): $[M + H]^+$ calculated for $C_{18}H_{20}NO_3^+$: 298.1438; found: 298.1437.



S4 **S5** **S7** **1r**

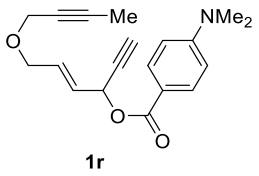
(E)-6-(but-2-yn-1-yloxy)hex-4-en-1-yn-3-yl 4-(dimethylamino)benzoate (1r)

To the solution of alcohol **S4** (1.22 g, 8.7 mmol in 15 mL of MeCN), the mixture of CuBr (12 mg, 0.1 mmol, 0.01 eq.), 2,2'-Bipyridine (13 mg, 0.1 mmol 0.01 eq.), TEMPO (13 mg, 0.1 mmol, 0.1 eq.) and DMAP (21 mg, 0.2 mmol, 0.2 eq.) was added, followed by switching the atmosphere to oxygen (balloon pressure, around 1 atm). Then the reaction was stirred for 19 h at room temperature. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/Et_2O = 1:1) to give aldehyde **S5** and put into the next step.

To a solution of the entire **S5** (in 15 mL of THF) in the first step, ethynylmagnesium chloride solution (25 mL, 0.5 M in THF) was added dropwise at -78 °C. The reaction was gradually allowed to warm to room temperature and stirred for 1 h. The solution was quenched with saturated NH_4Cl aq. and extracted with Et_2O. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (PE/ EA = 10:1 to 5:1) to yield **S7 (**1.30 g, 91% for 2 steps) as a yellow oil.

To the solution of alcohol **S7** (492 mg, 3.0 mmol in 15 mL of DCM), both Et_3N (1.25 mL, 9 mmol, 3.0 eq.) and DMAP (36 mg, 0.3 mmol, 0.1 eq.) were added, followed by adding 4-(dimethylamino)benzoyl chloride (661 mg, 3.6 mmol, 1.2 eq.) carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 12 h. The solution was quenched by Sat. $NaHCO_3$ aq. and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered,

and concentrated under vacuum. The residue was purified by flash column chromatography (PE: EA= 10/1) to yield **1r** (720.7 mg, 77%) as a yellow oil.



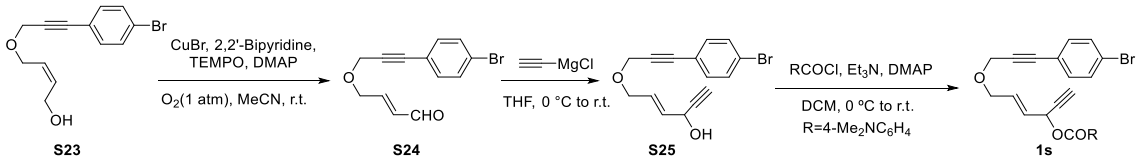
1r

TLC (5:1 PE/EA, R_f): 0.6.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.87 (d, J = 9.2 Hz, 2H), 6.65 (d, J = 9.2 Hz, 2H), 6.13 (dtd, J = 15.5, 5.7, 1.2 Hz, 1H), 6.11 – 6.05 (m, 1H), 5.91 (ddt, J = 15.5, 5.7, 1.5 Hz, 1H), 4.09 (q, J = 2.3 Hz, 2H), 4.08 – 4.06 (m, 2H), 3.02 (s, 6H), 2.64 (d, J = 2.2 Hz, 1H), 1.83 (t, J = 2.3 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 165.6, 154.0, 131.7, 131.4, 127.6, 116.3, 111.0, 82.9, 80.3, 75.3, 75.0, 68.9, 63.1, 58.4, 40.2, 3.6.

HRMS (m/z): $[M + H]^+$ calculated for $C_{19}H_{22}NO_3^+$: 312.1594; found: 312.1591.



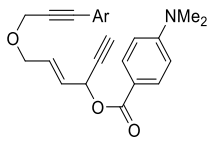
S23 **S24** **S25** **1s**

(E)-6-((3-(4-bromophenyl)prop-2-yn-1-yl)oxy)hex-4-en-1-yn-3-yl 4-(dimethylamino)benzoate (1s)

To the mixture of CuBr (4.3 mg, 0.03 mmol, 0.01 eq.), 2,2'-Bipyridine (4.9 mg, 0.03 mmol, 0.1 eq.), TEMPO (4.7 mg, 0.03 mmol, 0.01 eq.), DMAP (7.3 mg, 0.06 mmol, 0.02 eq.) and MeCN (1 mL) was added alcohol **S23**[2](845 mg, 3.0 mmol in 5mL of MeCN), followed by switching the atmosphere to oxygen (balloon pressure, around 1 atm). . Then the reaction was stirred for 22 h at room temperature. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (EA) to give aldehyde **S24** and put into the next step.

To the solution of aldehyde **S24** (in THF of 3 mL) in the first step solution, ethynylmagnesium chloride solution (9 mL, 0.5 M in THF, 4.5 mmol, 1.5 eq.) was added dropwise at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 1 h. The solution was quenched by saturated NH_4Cl aq. and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (EA) to give aldehyde **S25** and put into the next step.

To the solution of the entire alcohol **S25** (in 15 mL of DCM) in the second step, both Et_3N (1.25 mL, 9 mmol, 3.0 eq.) and DMAP (37 mg, 0.3 mmol, 0.1 eq.) were added, followed by adding 4-(dimethylamino)benzoyl chloride (661 mg, 3.6 mmol, 1.2 eq.) carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 19 h. After that, both Et_3N (0.4 mL, 3 mmol, 1.0 eq.) 4-(dimethylamino)benzoyl chloride (440.2 mg, 2.4 mmol, 0.8 eq.) were added to the reaction solution for a complete transformation. stirred for another 5 h, and quenched by saturated $NaHCO_3$ aq. and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (PE/ EA= 20:1 to 10:1) to yield **1s** (932.2 mg, 69% for 3 steps) as a white solid.



Ar = *p*-BrC_6H_4

1s

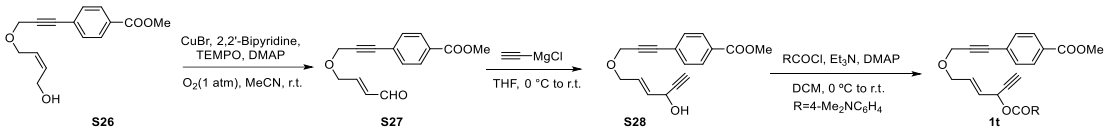
M.P. = 122.9-125 ºC

TLC (3:1 PE/EA, R_f): 0.8.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.88 (d, *J* = 9.0 Hz, 2H), 7.46 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 6.66 (d, *J* = 9.0 Hz, 2H), 6.18 (dtd, *J* = 15.5, 5.4, 1.2 Hz, 1H), 6.12 – 6.08 (m, 1H), 5.96 (ddt, *J* = 15.5, 5.4, 1.2 Hz, 1H), 4.37 (s, 2H), 4.17 (d, *J* = 5.4 Hz, 2H), 3.04 (s, 6H), 2.65 (d, *J* = 2.2 Hz, 1H).

^{13}C NMR (101 MHz, CD_2Cl_2) δf 165.6, 154.0, 133.6, 132.0, 131.7, 131.2, 128.0, 123.0, 122.0, 116.2, 111.1, 86.7, 85.4, 80.3, 75.0, 69.4, 63.1, 58.6, 40.3.

HRMS (m/z): $[M + H]^+$ calculated for $C_{24}H_{23}BrNO_3^+$: 452.0851; found: 452.0856.



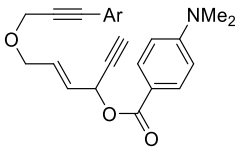
S26 **S27** **S28** **1t**

(E)-6-((3-(4-(methoxycarbonyl)phenyl)prop-2-yn-1-yl)oxy)hex-4-en-1-yn-3-yl 4-(dimethylamino) benzoate (1t)

To the solution of alcohol **S26**[2] (780 mg, 3.0 mmol, in 3mL MeCN), the mixture of CuBr (4.3 mg, 0.03 mmol, 0.01 eq.), 2,2'-Bipyridine (4.9 mg, 0.03 mmol, 0.1 eq.), TEMPO (4.7 mg, 0.03 mmol, 0.01 eq.), DMAP (7.3 mg, 0.06 mmol, 0.02 eq.) and MeCN (1 mL) was added, followed by switching the atmosphere to oxygen (balloon pressure, around 1 atm). Then the reaction was stirred for 12 h at room temperature. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (EA) to give aldehyde **S27** as a yellow solid and put into the next step.

To a solution of the entire aldehyde **S27** (in THF of 10 mL) in the first step, ethynylmagnesium chloride solution (6.6 mL, 0.5 M in THF, 3.3 mmol, 1.1 eq.) was added dropwise at -78 °C. The reaction was gradually allowed to warm to room temperature and stirred for 1 h. The solution was quenched by saturated NH_4Cl aq. and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (EA) to give aldehyde **S28** and put into the next step.

To a solution of entire alcohol **S28** (in 15 mL of DCM) in the second step, both Et_3N (2.1 mL,15 mmol, 5.0 eq.) and DMAP (37 mg, 0.3 mmol, 0.1eq.) were added, followed by adding 4-(dimethylamino)benzoyl chloride (1.10 mg, 3.6 mmol, 2.0 eq.) carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 12 h. The reaction was quenched by Sat. $NaHCO_3$ aq. and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (PE/ EA= 3:1) to yield **1t** (647.4 mg, 1.5 mmol, 50% for 3 steps) as a brown solid.



Ar = *p*-$MeO_2CC_6H_4$

1t

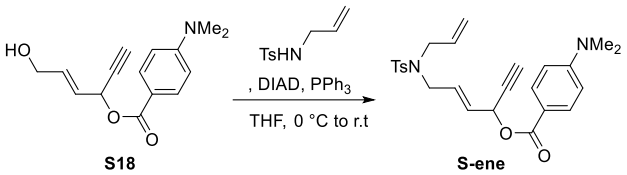
M.P. = 69.9-72.1 ºC

TLC (2:1 PE/EA, R_f): 0.8.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 72.96 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 9.0 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 6.67 (d, *J* = 9.0 Hz, 2H), 6.19 (dtd, *J* = 15.4, 5.4, 1.2 Hz, 1H), 6.13 – 6.07 (m, 1H), 5.97 (ddt, *J* = 15.5, 5.6, 1.5 Hz, 1H), 4.41 (s, 2H), 4.19 (d, *J* = 5.4 Hz, 2H), 3.89 (s, 3H), 3.04 (s, 6H), 2.65 (d, *J* = 2.2 Hz, 1H).

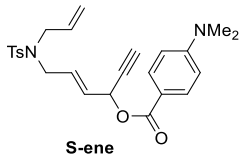
^{13}C NMR (101 MHz, CD_2Cl_2) δ 166.6, 165.6, 154.0, 132.0, 131.8, 131.2, 130.4, 129.8, 128.1, 127.6, 116.3, 111.1, 88.5, 85.7, 80.3, 75.1, 69.5, 63.1, 58.6, 52.5, 40.3.

HRMS (m/z): $[M + H]^+$ calculated for $C_{26}H_{26}NO_5^+$: 432.1805; found: 432.1808.



(E)-6-((N-allyl-4-methylphenyl)sulfonamido)hex-4-en-1-yn-3-yl 4-(dimethylamino)benzoate(S-ene)

DIAD (0.29 mL, 1.5 mmol, 1.5 eq.) was added into the mixture of alcohol **S3** (389 mg, 1.5 mmol), N-allyl-4-methylbenzenesulfonamide (211 mg, 1 mmol), PPh_3 (393 mg, 1.5 mmol) and THF (5 mL) at 0 ºC under an inert atmosphere. Then the reaction was warmed to room temperature and stirred for 14 h. After that, the solvent was removed under vacuum. The residue was purified by flash column chromatography (PE/ EA/DCM = 8:1:1) to yield **S-ene** (387.5 mg, 86%) as a yellow oil.

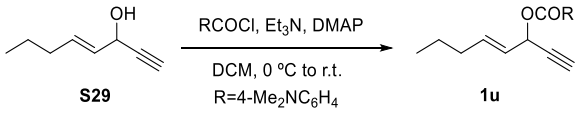


TLC (2:1 PE/EA, R_f): 0.5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 9.0 Hz, 2H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 6.64 (d, *J* = 9.0 Hz, 2H), 6.02 – 5.99 (m, 1H), 5.88 – 5.68 (m, 2H), 5.68 – 5.53 (m, 1H), 5.15 (d, *J* = 17.2 Hz, 1H), 5.15 (d, *J* = 11.1 Hz, 1H), 3.87 (d, *J* = 5.9 Hz, 2H), 3.81 (d, *J* = 6.4 Hz, 2H), 3.05 (s, 6H), 2.53 (d, *J* = 2.1 Hz, 1H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.5, 153.7, 143.4, 137.4, 132.7, 131.7, 129.9, 129.7, 129.1, 127.3, 119.5, 116.0, 110.8, 79.7, 75.0, 62.7, 49.8, 47.8, 40.2, 21.6.

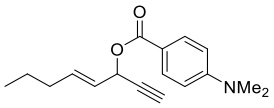
HRMS (m/z): $[M + H]^+$ calculated for $C_{25}H_{29}N_2O_4S^+$: 453.1842; found: 453.1839.



(E)-oct-4-en-1-yn-3-yl 4-(dimethylamino)benzoate (1u)

To a solution of **S29**[6] (659 mg, 5.3 mmol, in 20 mL of DCM), both Et_3N (2.2 mL, 15.9 mmol, 3.0 eq.) and DMAP (64 mg, 0.53 mmol, 0.1 eq.) were added, followed by adding 4-(dimethylamino)benzoyl chloride (1.19 g, 6.5 mmol, 1.2 eq.) carefully at 0 °C. The reaction was gradually allowed to warm to room temperature and stirred for 16 h 45min. The solution was quenched by sat. $NaHCO_3$ aq. and extracted with EA. The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4,

filtered, and concentrated under vacuum. The residue was purified by flash column chromatography (PE/EA= 10:1) to yield **1u** (1.26 g, 88%) as a yellow oil.



1u

TLC (5:1 PE/EA, R_f): 0.7.

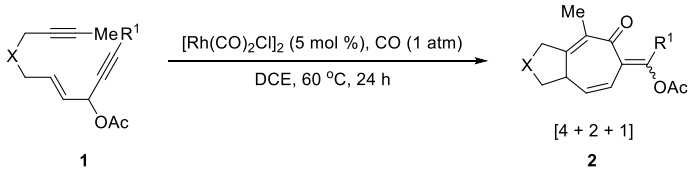
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 9.0 Hz, 2H), 6.62 (d, J = 8.9 Hz, 2H), 6.16 – 5.92 (m, 2H), 5.66 (dd, J = 15.7, 5.9 Hz, 1H), 3.01 (s, 6H), 2.57 (d, J = 2.1 Hz, 1H), 2.20 – 1.95 (m, 2H), 1.53 – 1.36 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 153.5, 136.2, 131.6, 125.2, 116.3, 110.7, 80.6, 74.4, 63.7, 40.1, 34.1, 21.9, 13.7.

HRMS (m/z): $[M + H]^+$ calculated for $C_{17}H_{22}NO_2^+$: 272.1645; found: 272.1645.

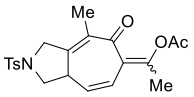
S3. [4 + 2 + 1] Cycloadditions

General procedure:



1 **2**

A solution of the substrate (**1**, 0.1 mmol in 4 mL of super-dried DCE) was added to the mixture of $[Rh(CO)_2Cl]_2$ (1.9 mg, 5 mol %). Then CO (1 atm) was bubbled into the solution for 5 min and the solution was stirred at 60 ºC under the balloon pressure (around 1 atm) of CO. (unless specially mentioned). After 12 h, the reaction mixture was concentrated and purified by flash column chromatography on silica gel, affording the cycloaddition product **2**. The yield reported for the [4 + 2 + 1]cycloaddition reaction is the average of two runs (**1a-1c**).



2a

1-(8-methyl-7-oxo-2-tosyl-2,3,3a,7-tetrahydrocyclohepta[c]pyrrol-6(1H)-ylidene)ethyl acetate (2a)

1a on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 5:1) afforded the title compound **2a** as a white solid.

Run 1: 1a (37.3 mg) was converted to the title compound **2a** (23.0 mg, 57%).

Run 2: 1a (37.3 mg) was converted to the title compound **2a** (22.7 mg, 57%).

The average yield of two runs was 57%.

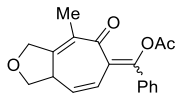
M.P. = 49.6-52.4 ºC

TLC (3:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 6.43 (d, *J* = 9.2 Hz, 1H), 5.39 (dd, *J* = 9.2, 4.6 Hz, 1H), 4.14 (d, *J* = 15.0 Hz, 1H), 3.79 (d, *J* = 9.5 Hz, 1H), 3.58 (d, *J* = 15.0 Hz, 1H), 3.23 (dd, *J* = 9.5, 7.0 Hz, 1H), 2.45 (s, 3H), 2.32 (s, 3H), 2.31 – 2.29 (m, 1H), 2.22 (s, 3H), 1.67 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.0, 168.9, 152.3, 144.4, 137.5, 131.6, 131.5, 130.0, 128.2, 127.2, 122.5, 121.0, 53.4, 51.1, 41.3, 30.4, 21.7, 20.9, 14.7.

HRMS (m/z): $[M + H]^+$ calculated for $C_{21}H_{24}NO_5S^+$: 402.1370; found: 402.1370.



2b

(8-methyl-7-oxo-1,3,3a,7-tetrahydro-6H-cyclohepta[c]furan-6-ylidene)(phenyl)methyl acetate (2b)

1b on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 5:1) afforded the title compound **2b** as a yellow oil.

Run 1: 1a (28.2 mg) was converted to the title compound **2b** (8.1 mg, 26%).

Run 2: 1a (28.2 mg) was converted to the title compound **2b** (8.4 mg, 27%).

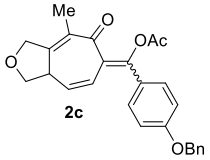
The average yield of two runs was 26%.

TLC (3:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.79 – 7.71 (m, 2H), 7.59 – 7.52 (m, 1H), 7.44 (dd, *J* = 8.3, 7.1 Hz, 2H), 6.46 (dd, *J* = 9.2, 1.9 Hz, 1H), 5.40 (dd, *J* = 9.2, 4.4 Hz, 1H), 4.58 – 4.37 (m, 2H), 4.31 – 4.16 (m, 2H), 2.66 (s, 1H), 1.69 (q, *J* = 1.3 Hz, 3H), 1.55 (s, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 196.7, 168.6, 152.2, 140.8, 138.2, 133.3, 130.0, 129.1, 128.9, 126.8, 123.8, 119.4, 74.8, 70.3, 43.3, 19.9, 14.9.

HRMS (m/z): $[M + H]^+$ calculated for $C_{19}H_{19}O_4^+$: 311.1278; found: 311.1275.



2c

(4-(benzyloxy)phenyl)(8-methyl-7-oxo-1,3,3a,7-tetrahydro-6H-cyclohepta[c]furan-6-ylidene) methyl acetate (2c)

1c on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 5:1) afforded the title compound **2c** as a yellow oil.

Run 1: 1a (38.8 mg) was converted to the title compound **2a** (14.0 mg, 34%).

Run 2: 1a (38.8 mg) was converted to the title compound **2a** (12.8 mg, 31%).

The average yield of two runs was 33%.

TLC (3:1 PE/EA, R_f): 0.4.

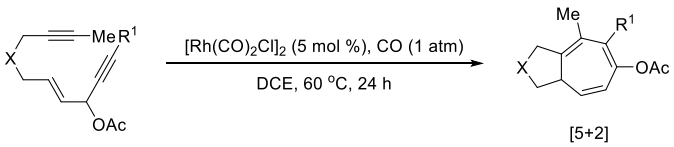
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.8 Hz, 2H), 7.50 – 7.30 (m, 5H), 7.08 – 6.82 (m, 2H), 6.42 (dd, *J* = 9.3, 1.8 Hz, 1H), 5.37 (dd, *J* = 9.3, 4.4 Hz, 1H), 5.13 (s, 2H), 4.64 – 4.35 (m, 2H), 4.33 – 4.18 (m, 2H), 2.67 (s, 1H), 1.70 (s, 3H), 1.66 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.1, 168.7, 162.8, 151.0, 139.6, 136.2, 131.5, 130.6, 130.0, 128.8, 128.4, 127.6, 126.4, 123.7, 119.0, 114.8, 74.7, 70.3, 70.2, 42.9, 20.2, 14.9.

HRMS (m/z): $[M + H]^+$ calculated for $C_{26}H_{25}NO_5^+$: 417.1697; found: 417.1696.

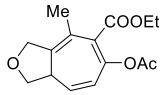
S4. [5 + 2] Cycloadditions

General procedure:



1 3

A solution of the substrate (**1**, 0.1 mmol in 4 mL of super-dried DCE) was added to the mixture of $[Rh(CO)_2Cl]_2$ (1.9 mg, 5 mol %). Then CO (1 atm) was bubbled into the solution for 5 minutes and the solution was stirred at 60 ºC under the balloon pressure (around 1 atm) of CO. After 12 h, the reaction mixture was concentrated and purified by flash column chromatography on silica gel, affording the cycloaddition product **3**. The yield reported for [5 + 2] cycloaddition reaction is the average of multiple runs



3d

ethyl 6-acetoxy-4-methyl-3,8a-dihydro-1H-cyclohepta[c]furan-5-carboxylate (3d)

1d on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 10:1 ~ 3:1) afforded the title compound **3d** as a yellow oil (some impurities cannot be removed with many efforts).

Run 1: 1a (27.8 mg) was converted to the title compound **3d** (6.8 mg, 24%).

Run 2: 1a (27.8 mg) was converted to the title compound **3d** (7.7 mg, 28%).

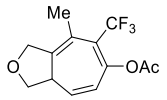
The average yield of two runs was 26%.

TLC (3:1 PE/EA, R_f): 0.4.

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.94 (dd, *J* = 9.6, 1.9 Hz, 1H), 5.55 (dd, *J* = 9.6, 4.7 Hz, 1H), 4.46 (d, *J* = 14.0 Hz, 1H), 4.38 – 4.32 (m, 1H), 4.29 (td, *J* = 7.1, 1.4 Hz, 2H), 4.24 – 4.17 (m, 2H), 2.64 (s, 1fH), 2.18 (s, 3H), 1.81 (d, *J* = 1.3 Hz, 3H), 1.34 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, CD_2Cl_2) δ 169.1, 166.8, 149.1, 138.8, 132.3, 130.3, 122.9, 118.1, 74.5, 70.2, 61.7, 42.9, 21.0, 17.0, 14.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{15}H_{19}O_5^+$: 279.1227; found: 279.1225.



3e

8-methyl-7-(trifluoromethyl)-3,3a-dihydro-1H-cyclohepta[c]furan-6-yl acetate (3e)

1e on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 10:1 ~ 3:1) afforded the title compound **3e** as a yellow oil.

Run 1: 1a (27.4 mg) was converted to the title compound **2a** (15.1 mg, 55%).

Run 2: 1a (27.4 mg) was converted to the title compound **2a** (15.5 mg, 56%).

The average yield of two runs was 56%.

TLC (3:1 PE/EA, R_f): 0.5.

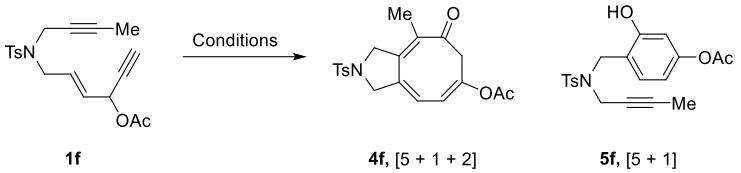
^{1}H NMR (400 MHz, CD_2Cl_2) δ 5.97 – 5.73 (m, 2H), 4.43 (d, *J* = 14.1 Hz, 1H), 4.32 – 4.24 (m, 1H), 4.22 (dd, *J* = 9.2, 1.6 Hz, 1H), 4.06 (dd, *J* = 9.2, 5.7 Hz, 1H), 2.57 – 2.50 (m, 1H), 2.20 (s, 3H), 1.87 – 1.79 (m, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.1, 151.9 (q, *J* = 3.5 Hz), 140.9, 137.4, 126.0 (q, *J* = 28.6 Hz), 124.4 (q, *J* = 276.0 Hz), 123.1, 116.9, 74.2, 69.7, 43.1, 20.8, 16.8 (q, *J* = 2.8 Hz).

HRMS (m/z): $[M + H]^+$ calculated for $C_{13}H_{14}F_3O_3^+$: 275.0886; found: 275.0890.

S5. [5 + 1 + 2] Cycloadditions

Table 1. Early Optimization of Reaction Conditions

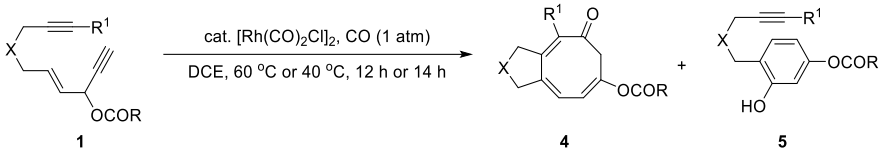


1f **4f,** [5 + 1 + 2] **5f,** [5 + 1]

entry	catalyst (mol %)	*p*(CO)	solvent[a]	temp.	time	[5+1+2]	[5+1]
1	$[Rh(CO)_2Cl]_2$ (10)	1 atm	DCE	60 °C	14 h	23%	10%
2	**$[Rh(CO)_2Cl]_2$ (10)**	**1 atm**	**DCE**	**40 °C**	**18 h**	**29%**	**11%**
3	$[Rh(CO)_2Cl]_2$ (10)	1 atm	THF	40 °C	42 h	17%	7%
4	$[Rh(CO)_2Cl]_2$ (10)	1 atm	Dioxane	40 °C	42 h	21%	trace
5	$[Rh(CO)_2Cl]_2$ (10)	0.2 atm	DCE	40 °C	18 h	26%	28%
6	$[Rh(CO)_2Cl]_2$ (10)	8 atm	DCE	40 °C	48 h	27%	
7	$[Rh(CO)_2Cl]_2$ (120)	1 atm	DCE	40 °C	12 h	33%	
8	$Rh(COD)_2SbF_6$ (5)	1 atm	DCE	60 °C	3 h	messy	
9	$[Rh(COD)Cl]_2$(5), $AgSbF_6$(10), PPh_2Cy(20)	1 atm	DCE	60 °C	24 h	17%	
10	$Co_2(CO)_8$ (20)	1 atm	DCE	80 °C	6 h	no reaction	
11	$Ir(CO)(PPh_3)_2Cl$ (10)	1 atm	DCE	80 °C	6 h	decomp.	

[a]The concentration is 0.05 M.

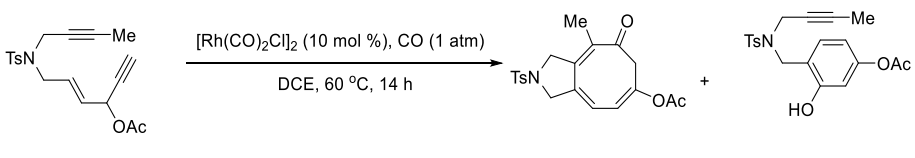
General procedure A:



1 **4** **5**

A solution of the substrate (**1**, 0.1 mmol in 2 mL of super-dried DCE) was added to the mixture of $[Rh(CO)_2Cl]_2$ (3.9 mg, 10 mol %; or 1.9 mg, 5 mol %). Then CO (1 atm) was bubbled into the solution for 5 minutes and the solution was stirred at 40 °C or 60 °C under the balloon pressure (around 1 atm) of CO. After 12 or 14 h, the reaction mixture was concentrated and purified by flash column chromatography on silica gel, affording the cycloaddition product **4** & **5**. The yield reported for [5 + 1 + 2] & [5 + 1] cycloaddition reaction is the average of multiple runs (**1f-1h**).

As mentioned, the [5 + 1 + 2] cycloaddition products **4** usually have low solubility in most solvents, $CHCl_3$ or DCM must be used to rinse or transfer the products.



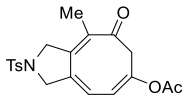
1f **4f** **5f**

1f on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA/DCM = 3:1:1) afforded the title compound **4f** as a yellow solid and **5f** as a yellow solid.

Run 1: 1f (35.6 mg) was converted to the title compound **4f** (10.6 mg, 28%) and **5f** (12.5 mg, 33%).

Run 2: 1f (36.1 mg) was converted to the title compound **4f** (9.2 mg, 24%) and **5f** (11.4 mg, 29%).

The average yield of four runs was 26% for **4f** and 31% for **5f**.



4f

(3aE,5E,9E)-9-methyl-8-oxo-2-tosyl-2,3,7,8-tetrahydro-1H-cycloocta[c]pyrrol-6-yl acetate (4f)

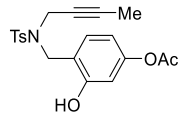
M.P. = 154.0-154.6 ℃

TLC (3:1 PE/EA, R_f): 0.2.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.75 – 7.68 (m, 2H), 7.39 – 7.31 (m, 2H), 6.47 (d, *J* = 6.2 Hz, 1H), 6.12 (d, *J* = 6.1 Hz, 1H), 4.28 – 4.26 (m, 2H), 4.25 (s, 2H), 2.86 (s, 2H), 2.41 (s, 3H), 2.16 (s, 3H), 1.95 (s, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2)) δ 186.0, 168.9, 145.1, 144.8, 144.3, 141.9, 133.5, 133.1, 130.3, 128.2, 126.3, 117.7, 57.8, 55.9, 44.9, 21.7, 21.2, 17.0.

HRMS (m/z): $[M + H]^+$ calculated for $C_{20}H_{22}NO_5S^+$: 388.1213; found: 388.1213.



5f

4-(((N-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)methyl)-3-hydroxyphenyl acetate (5f)

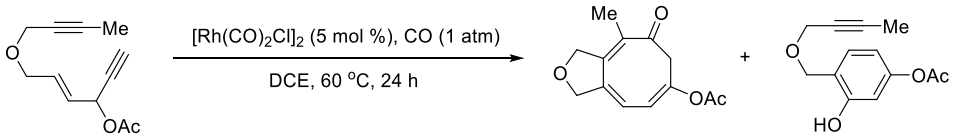
M.P. = 158.0-159.6 ℃

TLC (3:1 PE/EA, R_f): 0.1.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.83 (d, J = 8.4 Hz, 2H), 7.44 – 7.27 (m, 2H), 7.16 (s, 1H), 7.07 (d, J = 8.2 Hz, 1H), 6.67 (d, J = 2.3 Hz, 1H), 6.59 (dd, J = 8.2, 2.3 Hz, 1H), 4.25 (s, 2H), 3.95 (d, J = 2.4 Hz, 2H), 2.46 (s, 3H), 2.25 (s, 3H), 1.59 (s, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.5, 157.3, 152.8, 144.8, 135.2, 131.7, 130.0, 128.4, 117.9, 113.6, 111.1, 83.2, 71.2, 46.7, 36.6, 21.7, 21.3, 3.3.

HRMS (m/z): $[M + H]^+$ calculated for $C_{20}H_{22}NO_5S^+$: 388.1211; found: 388.1213.



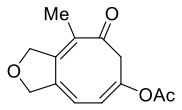
1g **4g** **5g**

1g on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 10:1 to 5:1) afforded the title compound **4g** as a yellow solid and **5g** as a yellow oil.

Run 1: 1g (20.6 mg) was converted to the title compound **4g** (11.3 mg, 48%) and **5g** (5.6 mg, 24%).

Run 2: 1g (20.6 mg) was converted to the title compound **4g** (12.0 mg, 51%) and **5g** (5.1 mg, 22%).

The average yield of two runs was 50% for **4g** and 23% for **5g**.



4g

(3aE,5E,9E)-9-methyl-8-oxo-1,3,7,8-tetrahydrocycloocta[c]furan-6-yl acetate (4g)

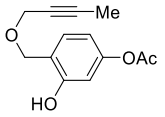
M.P. = 122.9-124.5 ℃

TLC (3:1 PE/EA, R_f): 0.2.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.55 (d, J = 6.3 Hz, 1H), 6.27 (d, J = 6.3 Hz, 1H), 4.81 (s, 2H), 4.76 (s, 2H), 3.07 (s, 2H), 2.22 (s, 3H), 2.00 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 186.0, 169.0, 147.1, 144.1, 139.8, 136.3, 124.0, 117.9, 75.2, 44.8, 29.8, 21.2, 16.5.

HRMS (m/z): $[M + NH_4]^+$ calculated for $C_{13}H_{15}NO_4^+$: 252.1230; found: 252.1230.



5g

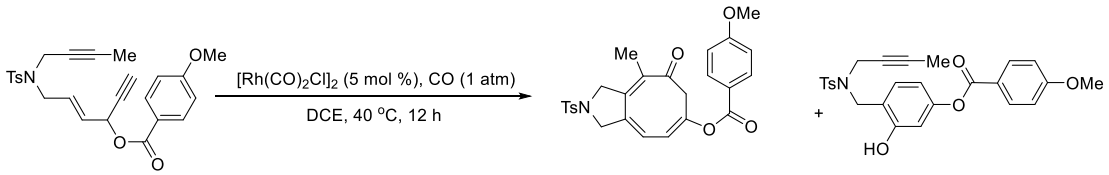
4-((but-2-yn-1-yloxy)methyl)-3-hydroxyphenyl acetate (5g)

TLC (3:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.29 (s, 1H), 7.10 – 7.03 (m, 1H), 6.62 – 6.55 (m, 2H), 4.74 (s, 2H), 4.21 (q, J = 2.3 Hz, 2H), 2.25 (s, 3H), 1.88 (t, J = 2.4 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.6, 157.5, 152.3, 129.4, 120.2, 113.5, 110.4, 84.4, 74.2, 70.3, 58.7, 22.0, 3.7.

HRMS (m/z): $[M + H]^+$ calculated for $C_{13}H_{15}O_4^+$: 235.0965; found: 235.0963.



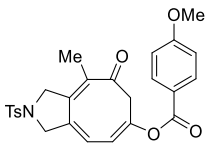
1h **4h** **5h**

1h on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA/DCM = 4:1:1) afforded the title compound **4h** as yellow solid and **5h** as a colorless oil.

Run 1: 1h (45.2 mg) was converted to the title compound **4h** (20.3 mg, 42%) and **5h** (11.1 mg, 23%).

Run 2: 1h (45.2 mg) was converted to the title compound **4h** (19.0 mg, 40%) and **5h** (8.3 mg, 17%).

The average yield of four runs was 41% for **4h** and 20% for **5h**.



4h

(3aE,5E,9E)-9-methyl-8-oxo-2-tosyl-2,3,7,8-tetrahydro-1H-cycloocta[c]pyrrol-6-yl 4-methoxy benzoate (4h)

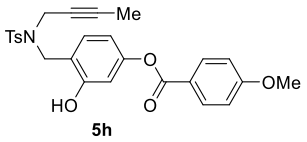
M.P. = 155.0-158.3 ℃

TLC (2:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.6 Hz, 2H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.34 (d, *J* = 7.9 Hz, 1H), 6.92 (d, *J* = 8.6 Hz, 2H), 6.53 (d, *J* = 6.0 Hz, 1H), 6.30 (d, *J* = 6.0 Hz, 1H), 4.30 (s, 2H), 4.28 (s, 2H), 3.86 (s, 3H), 3.02 (s, 2H), 2.43 (s, 3H), 2.00 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 185.9, 164.3, 164.3, 145.3, 144.4, 144.0, 141.8, 132.9, 132.8, 132.6, 130.1, 127.9, 126.4, 121.0, 117.5, 114.0, 57.6, 55.7, 55.6, 44.9, 21.7, 17.1.

HRMS (m/z): $[M + H]^+$ calculated for $C_{26}H_{26}NO_6S^+$: 480.1475; found: 480.1480.



5h

4-(((N-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)methyl)-3-hydroxyphenyl 4-methoxybenzoate (5h)

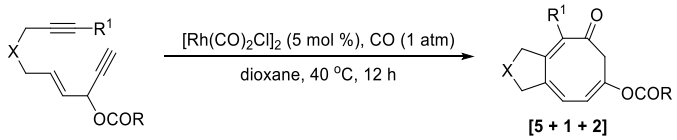
TLC (5:1 PE/EA, R_f): 0.4.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.12 (d, *J* = 8.9 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.19 (s, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 7.00 (d, *J* = 9.0 Hz, 2H), 6.80 (d, *J* = 2.3 Hz, 1H), 6.72 (dd, *J* = 8.2, 2.3 Hz, 1H), 4.29 (s, 2H), 3.98 (q, *J* = 2.4 Hz, 2H), 3.89 (s, 3H), 2.47 (s, 3H), 1.60 (t, *J* = 2.4 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 164.9, 164.4, 157.3, 153.1, 144.8, 135.2, 132.5, 131.7, 130.0, 128.4, 122.1, 117.9, 114.2, 113.8, 111.2, 83.2, 71.2, 56.0, 46.7, 36.6, 21.7, 3.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{26}H_{26}NO_6S^+$: 480.1475; found: 480.1476.

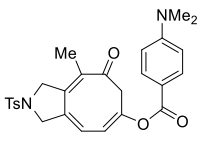
General procedure B:



1 **[5 + 1 + 2]** **4**

A solution of the substrate (**1**, 0.1 mmol in 4 mL of super-dried 1,4-dioxane) was added to the mixture of $[Rh(CO)_2Cl]_2$ (1.9 mg, 5 mol %). Then CO (1 atm) was bubbled into the solution for 5 minutes and the solution was stirred at 60 ºC under the balloon pressure (around 1 atm) of CO. After 12 h, the reaction mixture was concentrated and purified by flash column chromatography on silica gel, affording the cycloaddition product **4**. The yield reported for [5 + 1 + 2] cycloaddition reaction is the average of two runs (**1i-1t**).

We pointed out that, the [5 + 1 + 2] cycloaddition products **4** with NTs tether usually have low solubility in most solvents, $CHCl_3$ or DCM must be used for rinse or transfer the products.



4i

(3aE,5E,9E)-9-methyl-8-oxo-2-tosyl-2,3,7,8-tetrahydro-1H-cycloocta[c]pyrrol-6-yl 4-

(dimethylamino) benzoate (4i)

4i on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (DCM/MeOH = 300:1) afforded the title compound **4i** as a yellow solid.

Run 1: 1i (45.0 mg) was converted to the title compound **4i** (29.5 mg, 60%).

Run 2: 1i (45.0 mg) was converted to the title compound **4i** (29.2 mg, 59%).

The average yield of two runs was 60%.

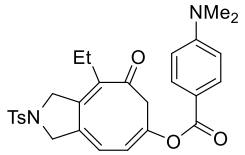
M.P. = 180.3-183.0 ℃

TLC (2:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.87 (d, J = 8.3 Hz, 2H), 7.73 (d, J = 7.4 Hz, 2H), 7.36 (d, J = 7.4 Hz, 2H), 6.66 (d, J = 8.3 Hz, 2H), 6.53 (d, J = 4.9 Hz, 1H), 6.27 (d, J = 5.4 Hz, 1H), 4.30 (s, 2H), 4.28 (s, 2H), 3.05 (s, 6H), 2.96 (s, 2H), 2.42 (s, 3H), 1.98 (s, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 185.9, 164.8, 154.4, 146.1, 144.8, 144.3, 141.7, 133.1, 132.8, 132.2, 130.3, 128.2, 126.7, 117.4, 115.0, 111.1, 57.9, 56.0, 45.2, 40.2, 21.7, 17.0.

HRMS (m/z): $[M + H]^+$ calculated for $C_{27}H_{29}N_2O_5S^+$: 493.1792; found: 493.1791.



4j

(3aE,5E,9E)-9-ethyl-8-oxo-2-tosyl-2,3,7,8-tetrahydro-1H-cycloocta[c]pyrrol-6-yl 4-(dimethylamino)benzoate (4j)

1j on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/$CHCl_3$ = 1:1) afforded the title compound **4j** as a yellow solid.

Run 1: 1j (47.9 mg) was converted to the title compound **4j** (33.6 mg, 66%).

Run 2: 1j (47.8 mg) was converted to the title compound **4j** (32.0 mg, 63%).

The average yield of two runs was 65%.

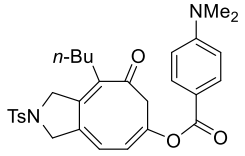
M.P. = 168.0-171.3 ℃

TLC (2:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, J = 9.0 Hz, 2H), 7.75 (d, J = 8.1 Hz, 2H), 7.34 (d, J = 8.1 Hz, 2H), 6.64 (d, J = 9.0 Hz, 2H), 6.52 (d, J = 6.3 Hz, 1H), 6.29 (d, J = 6.3 Hz, 1H), 4.38 (s, 2H), 4.27 (s, 2H), 3.05 (s, 6H), 3.00 (s, 2H), 2.44 (s, 3H), 2.43 (q, J = 7.5 Hz, 2H), 1.01 (t, J = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 185.0, 164.8, 154.0, 147.7, 146.1, 144.4, 143.2, 132.8, 132.3, 130.1, 128.0, 126.8, 117.1, 115.1, 110.9, 57.5, 54.7, 45.4, 40.2, 25.0, 21.7, 12.7.

HRMS (m/z): $[M + H]^+$ calculated for $C_{28}H_{31}N_2O_5S^+$: 507.1948; found: 507.1948.



4k

(3aE,5E,9E)-9-butyl-8-oxo-2-tosyl-2,3,7,8-tetrahydro-1H-cycloocta[c]pyrrol-6-yl 4-(dimethylamino)benzoate (4k)

1k on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography

(PE/$CHCl_3$ = 1:1) afforded the title compound **4k** as a yellow solid.

Run 1: 1k (50.7 mg) was converted to the title compound **4k** (35.8 mg, 68%).

Run 2: 1k (50.7 mg) was converted to the title compound **4k** (36.2 mg, 68%).

The average yield of two runs was 68%.

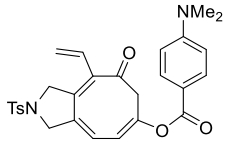
M.P. = 166.0-168.5 ℃

TLC (3:1 PE/EA, R_f): 0.3.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.87 (d, J = 9.0 Hz, 2H), 7.73 (d, J = 8.2 Hz, 2H), 7.36 (d, J = 8.2 Hz, 2H), 6.67 (d, J = 9.0 Hz, 2H), 6.51 (d, J = 6.2 Hz, 1H), 6.25 (d, J = 6.2 Hz, 1H), 4.37 (s, 2H), 4.26 (s, 2H), 3.05 (s, 6H), 2.95 (s, 2H), 2.42 (s, 3H), 2.40 – 2.33 (m, 2H), 1.47 – 1.14 (m, 4H), 0.92 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 185.2, 164.8, 154.0, 146.7, 146.1, 144.4, 143.3, 132.8, 132.3, 132.3, 130.1, 128.0, 126.7, 117.0, 115.0, 110.8, 57.6, 54.5, 45.3, 40.2, 31.6, 30.6, 23.3, 21.0, 14.1.

HRMS (m/z): $[M + H]^+$ calculated for $C_{30}H_{35}N_2O_5S^+$: 535.2261; found: 535.2254.



4l

(3aE,5E,9E)-8-oxo-2-tosyl-9-vinyl-2,3,7,8-tetrahydro-1H-cycloocta[c]pyrrol-6-yl 4-(dimethylamino)benzoate (4l)

1l on 0.10 mmol scale reacted under modified standard conditions (reaction time: 36 h). Purification by flash column chromatography (DCM/MeOH = 300:1) afforded the title compound **4l** as a yellow solid.

Run 1: 1l (47.0 mg) was converted to the title compound **4l** (16.9 mg, 34%).

Run 2: 1l (48.6 mg) was converted to the title compound **4l** (17.2 mg, 33%).

The average yield of two runs was 34%.

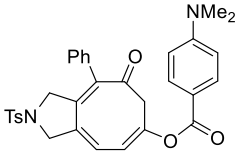
M.P. = 175.2-176.1℃

TLC (2:1 PE/EA, R_f): 0.4.

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.86 (d, J = 9.2 Hz, 2H), 7.67 (d, J = 8.1 Hz, 2H), 7.32 (d, J = 8.1 Hz, 2H), 6.66 (d, J = 9.2 Hz, 2H), 6.57 – 6.47 (m, 2H), 6.32 (d, J = 6.2 Hz, 1H), 5.57 (dd, J = 11.4, 1.5 Hz, 1H), 5.39 (dd, J = 17.7, 1.5 Hz, 1H), 4.43 (s, 2H), 4.34 (s, 2H), 3.05 (s, 6H), 2.85 (s, 2H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 185.7, 164.7, 154.4, 146.8, 144.9, 144.6, 143.1, 134.1, 134.0, 133.5, 132.3, 130.3, 128.1, 127.6, 123.0, 117.8, 115.0, 111.1, 57.0, 56.8, 45.7, 40.2, 21.6.

HRMS (m/z): $[M + H]^+$ calculated for $C_{28}H_{29}N_2O_5S^+$: 505.1792; found: 505.1796.



4m

(3aE,5E,9E)-8-oxo-9-phenyl-2-tosyl-2,3,7,8-tetrahydro-1H-cycloocta[c]pyrrol-6-yl 4-(dimethylamino)benzoate (4m)

1m on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (DCM/MeOH= 300:1) afforded the title compound **4j** as a yellow solid.

Run 1: 1m (52.7 mg) was converted to the title compound **4m** (34.8 mg, 63%).

Run 2: 1m (52.7 mg) was converted to the title compound **4m** (34.4 mg, 62%).

The average yield of two runs was 63%.

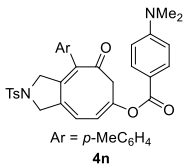
M.P. = 173.4-176.8 ℃

TLC (2:1 PE/EA, R_f): 0.3.

^{1}**H NMR** (400 MHz, CD_2Cl_2) δ 7.86 (d, J = 8.7 Hz, 2H), 7.60 (d, J = 8.0 Hz, 2H), 7.48 – 7.37 (m, 3H), 7.35 (d, J = 8.0 Hz, 2H), 6.99 (d, J = 7.2 Hz, 2H), 6.73 – 6.52 (m, 3H), 6.38 (d, J = 6.4 Hz, 1H), 4.37 (s, 2H), 3.98 (s, 2H), 3.03 (s, 6H), 3.02 (s, 2H), 2.43 (s, 3H).

^{13}**C NMR** (101 MHz, CD_2Cl_2) δ 185.7, 164.8, 154.4, 146.9, 146.8, 145.7, 144.8, 139.1, 133.6, 133.5, 132.3, 131.4, 130.3, 129.3, 128.9, 128.5, 128.1, 117.7, 114.9, 111.0, 57.4, 57.0, 45.7, 40.2, 21.7.

HRMS (m/z): $[M + H]^+$ calculated for $C_{32}H_{31}N_2O_5S^+$: 555.1948; found: 555.1952.



4n

(3aE,5E,9E)-8-oxo-9-(p-tolyl)-2-tosyl-2,3,7,8-tetrahydro-1H-cycloocta[c]pyrrol-6-yl 4-(dimethylamino)benzoate (4n)

1n on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/$CHCl_3$ = 1:1 to 2:3) afforded the title compound **4m** as a yellow solid.

Run 1: 1n (54.0 mg) was converted to the title compound **4n** (41.8 mg, 74%).

Run 2: 1n (54.0 mg) was converted to the title compound **4n** (42.3 mg, 74%).

The average yield of two runs was 74%.

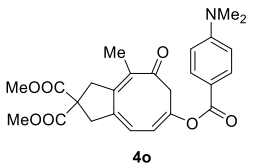
M.P. = 171.6-173.6 ℃

TLC (2:1 PE/EA, R_f): 0.6.

^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.87 (d, J = 8.8 Hz, 2H), 7.61 (d, J = 7.9 Hz, 2H), 7.31 (d, J = 7.9 Hz, 2H), 7.20 (d, J = 7.3 Hz, 2H), 6.88 (d, J = 7.7 Hz, 2H), 6.60 – 6.54 (m, 3H), 6.40 (d, J = 6.1 Hz, 1H), 4.37 (s, 2H), 4.05 (s, 2H), 3.02 (s, 6H), 2.99 (s, 2H), 2.43 (s, 3H), 2.39 (s, 3H).

^{13}**C NMR** (101 MHz, $CDCl_3$) δ 185.5, 164.9, 154.0, 147.0, 146.7, 145.2, 144.4, 138.3, 135.3, 133.4, 133.3, 132.4, 130.0, 129.5, 129.0, 127.9, 127.6, 117.5, 114.9, 110.8, 57.0, 45.4, 40.1, 29.8, 21.7, 21.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{33}H_{33}N_2O_5S^+$: 569.2105; found: 569.2106.



4o

dimethyl (3aZ,7E,9Z)-7-((4-(dimethylamino)benzoyl)oxy)-4-methyl-5-oxo-1,3,5,6-tetrahydro-2H-cyclopenta[8]annulene-2,2-dicarboxylate (4o)

1o on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 5:1 to 3:1) afforded the title compound **4o** as a yellow solid.

Run 1: 1o (41.9 mg) was converted to the title compound **4o** (22.6 mg, 51%).

Run 2: 1o (42.3 mg) was converted to the title compound **4o** (24.1 mg, 53%).

The average yield of two runs was 52%.

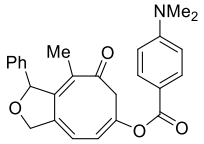
M.P. = 120.0-122.0 ℃

TLC (2:1 PE/EA, R_f): 0.3.

^{1}**H NMR** (400 MHz, CD_2Cl_2) δ 7.89 (d, J = 9.0 Hz, 2H), 6.70 (d, J = 9.0 Hz, 2H), 6.53 (d, J = 5.8 Hz, 1H), 6.23 (d, J = 5.8 Hz, 1H), 3.75 (s, 6H), 3.42 (s, 2H), 3.30 (s, 2H), 3.14 (s, 2H), 3.06 (s, 6H), 2.05 (s, 3H).

^{13}**C NMR** (101 MHz, CD_2Cl_2) δ 187.8, 171.7, 164.9, 154.2, 148.0, 145.6, 141.1, 137.6, 132.2, 126.6, 117.3, 115.7, 111.3, 55.2, 53.4, 46.3, 45.4, 43.8, 40.3, 17.2.

HRMS (m/z): $[M + H]^+$ calculated for $C_{25}H_{28}NO_7^+$: 454.1860; found: 454.1860.



4p

(3aE,5E,9E)-9-(4-(methoxycarbonyl)phenyl)-8-oxo-1,3,7,8-tetrahydrocycloocta[c]furan-6-yl 4-(dimethylamino)benzoate (4p)

1p on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 5:1) afforded the title compound **4p** as a yellow solid.

Run 1: 1p (39.0 mg) was converted to the title compound **4p** (23.7 mg, 57%).

Run 2: 1p (38.8 mg) was converted to the title compound **4p** (24.5 mg, 59%).

The average yield of two runs was 58%.

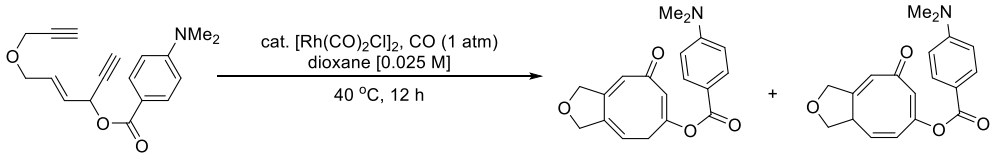
M.P. = 135.0-138.0 ℃

TLC (3:1 PE/EA, R_f): 0.3.

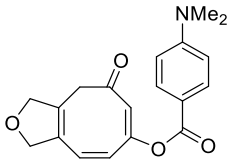
^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.97 (d, J = 9.0 Hz, 2H), 7.37 – 7.29 (m, 3H), 7.25 – 7.18 (m, 2H), 6.66 (d, J = 9.0 Hz, 2H), 6.62 (d, J = 6.1 Hz, 1H), 6.52 (d, J = 6.1 Hz, 1H), 5.95 (s, 1H), 4.80 (s, 2H), 3.48 (d, J = 11.5 Hz, 1H), 3.10 (d, J = 11.5 Hz, 1H), 3.06 (s, 6H), 1.91 (s, 3H).

^{13}**C NMR** (101 MHz, $CDCl_3$) δ 186.6, 165.1, 154.0, 147.9, 145.8, 141.6, 139.5, 136.5, 132.3, 128.9, 128.5, 127.8, 124.2, 117.9, 115.4, 111.0, 86.4, 74.7, 45.4, 40.2, 17.3.

HRMS (m/z): $[M + H]^+$ calculated for $C_{26}H_{26}NO_4^+$: 416.1856; found: 416.1846.



1q **4q** **4q'**



4q'

(4Z,6E,9E)-8-oxo-1,3,3a,8-tetrahydrocycloocta[c]furan-6-yl 4-(dimethylamino)benzoate (4q')

1q on a 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography ($CHCl_3$/PE/EA/ = 8:1:1) afforded the mixture of **4q** and **4q'**. We could only separate **4q'** sufficient for

characterization by preparative TLC. The structure of **4q** was proposed by the NMR spectra of the mixture of **4q** and **4q'** and the pure **4q'**. The ratio of **4q**/**4q'** is nearly 1/5, determined by crude NMR spectra.

Run 1: 1q (29.7 mg) was converted to the title compound **4q&4q'** (18.5 mg, 57%).

Run 2: 1q (29.7 mg) was converted to the title compound **4q&4q'** (19.3 mg, 60%).

The average yield of two runs was 59%.

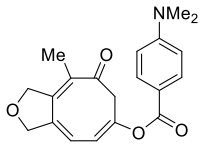
M.P. = 86.7-88.8 ℃

TLC (2:1 PE/EA, R_f): 0.4.

^{1}**H NMR** (400 MHz, CD_2Cl_2) δ 7.90 (d, J = 9.0 Hz, 2H), 6.68 (d, J = 9.0 Hz, 2H), 6.24 (s, 1H), 6.20 (s, 1H), 6.14 (dd, J = 10.6, 6.8 Hz, 1H), 6.07 (d, J = 10.6 Hz, 1H), 4.62 (d, J = 15.7 Hz, 1H), 4.36 (d, J = 15.7 Hz, 1H), 4.16 (d, J = 9.0 Hz, 1H), 4.10 – 4.03 (m, 1H), 4.00 (dd, J = 9.0, 5.0 Hz, 1H), 3.06 (s, 6H).

^{13}**C NMR** (101 MHz, CD_2Cl_2) δ 188.4, 165.1, 163.9, 155.2, 154.3, 141.5, 132.2, 124.8, 124.1, 123.5, 115.2, 111.1, 74.3, 71.9, 44.2, 40.2.

HRMS (m/z): $[M + H]^+$ calculated for $C_{19}H_{20}NO_4^+$: 326.1387; found: 326.1387.



4r

(3aE,5E,9E)-9-methyl-8-oxo-1,3,7,8-tetrahydrocycloocta[c]furan-6-yl 4-(dimethylamino)benzoate (4r)

1r on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 4:1) afforded the title compound **4r** as a yellow solid.

Run 1: 1r (32.0 mg) was converted to the title compound **4r** (23.2 mg, 67%).

Run 2: 1r (31.2 mg) was converted to the title compound **4r** (22.8 mg, 67%).

The average yield of two runs was 67%.

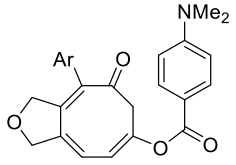
M.P. = 148.5-151.0 ℃

TLC (3:1 PE/EA, R_f): 0.2.

^{1}**H NMR** (400 MHz, CD_2Cl_2) δ 7.91 (d, J = 9.0 Hz, 2H), 6.68 (d, J = 9.0 Hz, 2H), 6.61 (d, J = 6.3 Hz, 1H), 6.39 (d, J = 6.3 Hz, 1H), 4.81 (s, 2H), 4.76 (s, 2H), 3.14 (s, 2H), 3.06 (s, 6H), 1.99 (s, 3H).

^{13}**C NMR** (101 MHz, CD_2Cl_2) δ 186.1, 165.0, 154.4, 147.4, 145.4, 139.6, 136.1, 132.2, 124.4, 117.7, 115.2, 111.1, 77.8, 75.4, 45.4, 40.2, 16.4.

HRMS (m/z): $[M + H]^+$ calculated for $C_{20}H_{22}NO_4^+$: 340.1543; found: 340.1540.



Ar = 4-BrC_6H_4

4s

(3aE,5E,9E)-9-(4-bromophenyl)-8-oxo-1,3,7,8-tetrahydrocycloocta[c]furan-6-yl 4-(dimethylamino)benzoate (4s)

1s on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography

(PE/EA = 10:1) afforded the title compound **4s** as a yellow solid.

Run 1: 1s (45.4 mg) was converted to the title compound **4s** (34.3 mg, 71%).

Run 2: 1s (45.3 mg) was converted to the title compound **4s** (32.0 mg, 66%).

The average yield of two runs was 69%

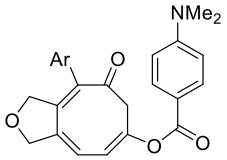
M.P. = 159.0-161.0 ℃

TLC (3:1 PE/EA, R_f): 0.3.

^{1}**H NMR** (400 MHz, CD_2Cl_2) δ 7.90 (d, J = 9.0 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 6.99 (d, J = 8.4 Hz, 2H), 6.73 (d, J = 6.4 Hz, 1H), 6.66 (d, J = 9.0 Hz, 2H), 6.53 (d, J = 6.4 Hz, 1H), 4.79 (s, 2H), 4.42 (s, 2H), 3.31 (s, 2H), 3.04 (s, 6H).

^{13}**C NMR** (101 MHz, CD_2Cl_2) δ 185.8, 164.9, 154.4, 149.3, 146.3, 143.9, 138.2, 136.5, 132.3, 131.9, 131.2, 126.5, 122.3, 118.2, 115.1, 111.1, 77.0, 75.8, 46.0, 40.2.

HRMS (m/z): $[M + H]^+$ calculated for $C_{25}H_{23}BrNO_4^+$: 480.0805; found: 480.0795.



Ar = 4-$MeO_2CC_6H_4$

4t

(3aE,5E,9E)-9-(4-(methoxycarbonyl)phenyl)-8-oxo-1,3,7,8-tetrahydrocycloocta[c]furan-6-yl 4-(dimethylamino)benzoate (4t)

1t on 0.10 mmol scale reacted under standard conditions. Purification by flash column chromatography (PE/EA = 5:1) afforded the title compound **4t** as a yellow solid.

Run 1: 1t (43.8 mg) was converted to the title compound **4t** (23.6 mg,51%).

Run 2: 1t (43.1 mg) was converted to the title compound **4t** (24.5 mg, 53%).

The average yield of two runs was 52%.

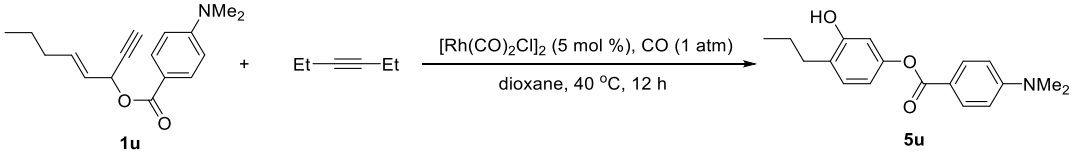
M.P. = 183.0-185.5 ℃

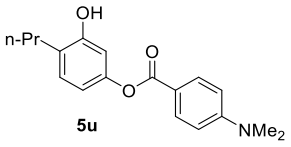
TLC (3:1 PE/EA, R_f): 0.3.

^{1}**H NMR** (400 MHz, CD_2Cl_2) δ 8.04 (d, J = 8.3 Hz, 2H), 7.90 (d, J = 9.0 Hz, 2H), 7.19 (d, J = 8.3 Hz, 2H), 6.75 (d, J = 6.4 Hz, 1H), 6.67 (d, J = 9.0 Hz, 2H), 6.54 (d, J = 6.4 Hz, 1H), 4.80 (s, 2H), 4.40 (s, 2H), 3.90 (s, 3H), 3.33 (s, 2H), 3.04 (s, 6H).

^{13}**C NMR** (101 MHz, CD_2Cl_2) δ 185.4, 166.6, 164.5, 154.0, 148.9, 145.9, 143.7, 136.1, 131.9, 131.7, 129.7, 129.5, 129.2, 126.3, 117.8, 114.8, 110.8, 76.7, 75.3, 52.0, 45.7, 39.8.

HRMS (m/z): $[M + H]^+$ calculated for $C_{27}H_{26}NO_6^+$: 460.1755; found: 460.1763.





3-hydroxy-4-propylphenyl 4-(dimethylamino)benzoate (5u)

1u on a 0.10 mmol scale (27.1 mg, 1.0 eq.) and hex-3-yne on a 1.5 mmol scale (57 μL, 5 eq.) reacted under standard conditions. Purification by flash column chromatography (PE/EA/ = 3:1) afforded the **5u.**

Run 1: 1u (27.1 mg) was converted to the title compound **5u** (4.4 mg, 13%).

Run 2: 1u (27.9 mg) was converted to the title compound **5u** (3.9 mg, 13%).

TLC (2:1 PE/EA, R_f): 0.4.

^{1}**H NMR** (400 MHz, $CDCl_3$) δ 8.04 (d, J = 9.0 Hz, 2H), 7.09 (d, J = 8.1 Hz, 1H), 6.69 (d, J = 9.0 Hz, 2H), 6.66 (dd, J = 8.1, 2.2 Hz, 1H), 6.63 (d, J = 2.2 Hz, 1H), 5.74 (brs, 1H), 3.07 (s, 6H), 2.57 – 2.45 (m, 2H), 1.67 – 1.52 (m, 2H), 0.96 (t, J = 7.3 Hz, 3H).

^{13}**C NMR** (101 MHz, $CDCl_3$) δ 166.3, 154.5, 153.9, 149.9, 132.2, 130.4, 126.2, 116.0, 113.4, 110.9, 109.4, 40.2, 31.8, 22.9, 14.2.

HRMS (m/z): $[M + H]^+$ calculated for $C_{18}H_{22}NO_3^+$: 300.1594; found: 300.1591.

S6. Computational Part

S6.1. Discussion on Other Competing 1,2- and 1,3-Acyloxy Migration Transition States

Except for 1,2-acyloxy and 1,3-acyloxy migration pathways shown in the main text, there are two kinds of other migration pathways featuring alkene coordination in the corresponding transition states (Figure S1). As for 1,2-acyloxy migration, both **TS1-S1** (with one CO coordination) and **TS1-S2** (with two CO coordination) are disfavored over **TS2** by 3.0 and 2.0 kcal/mol, respectively, which indicates that 1,2-acyloxy migration with alkene coordination can be ruled out. Similar results are also found for 1,3-acyloxy migration. Both **TS1'-S1** and **TS1'-S2** are highly disfavored over **TS1'**. As for all of the migration transition states, Rh atom has anionic characteristics, which means plane quadrilateral CO coordination on Rh can stabilize the formal anionic charge better.

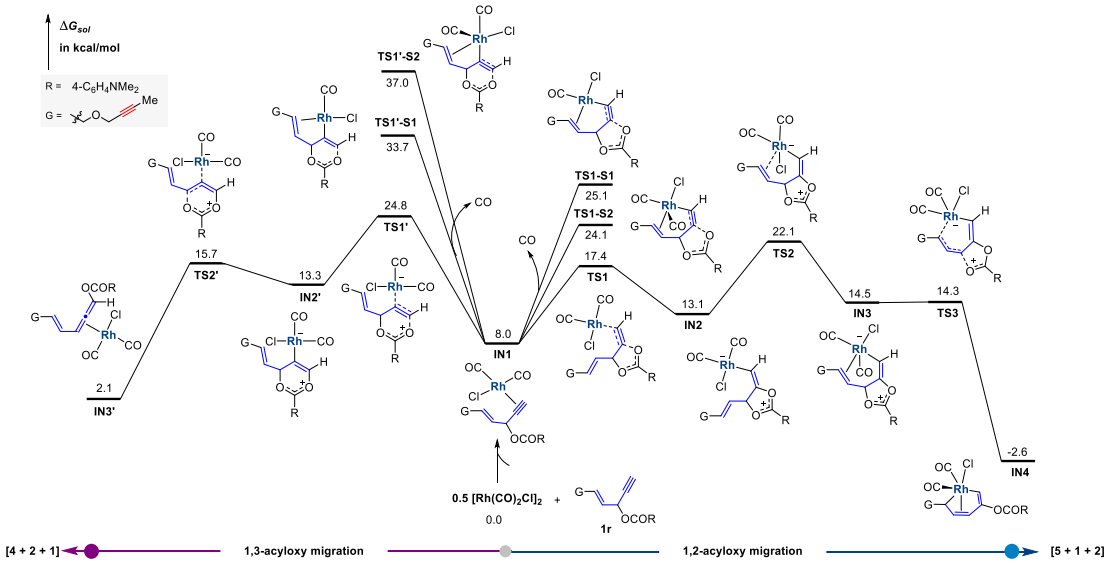


Figure S1. Other competing 1,2-acyloxy and 1,3-acyloxy migration pathways. Computed at the DLPNO-CCSD(T)/def2-TZVPP:SMD(1,4-dioxane)//SMD(1,4-dioxane)/BMK/def2-SVP level.

S6.2. [5 + 1] Cycloaddition Pathway via 6π Cyclization

After CO insertion to Rh carbene and catalyst transfer, ketene intermediate **IN4"** is generated. The process is exergonic by 21.7 kcal/mol. **IN4'** then undergoes 6π cyclization via **TS4"** to give **IN5"**, which has an activation free energy of only 12.8 kcal/mol. After tautomerization of **IN5"**, final product **5r** is then generated.

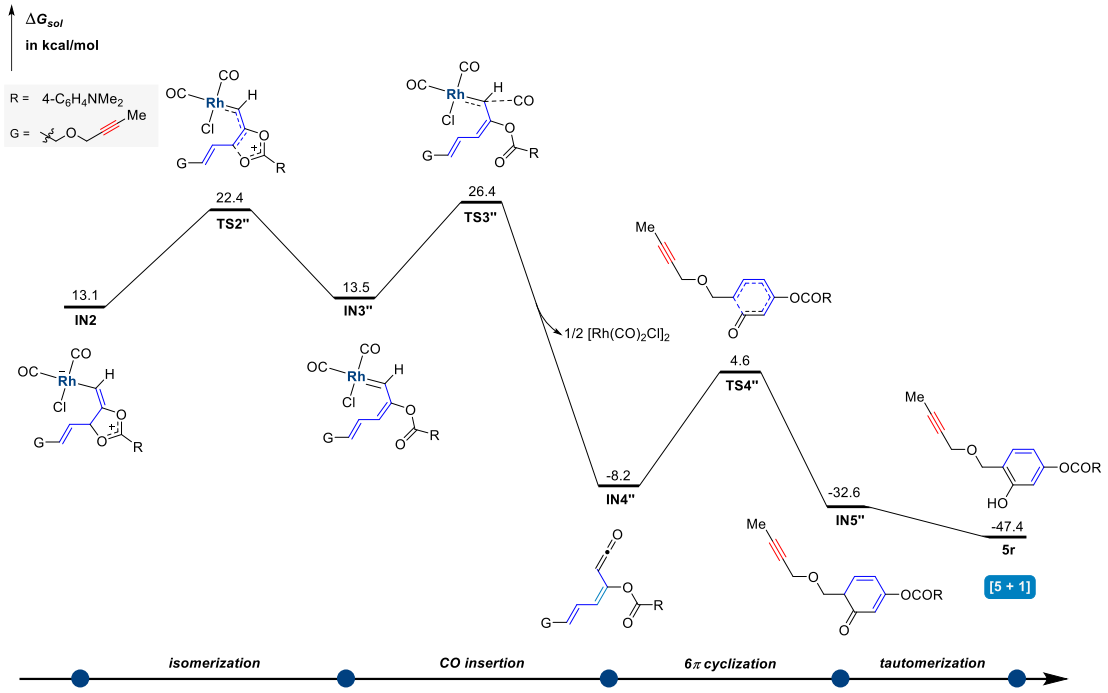


Figure S2. Gibbs energy profile of the [5 + 1] pathway via 6π cyclization. Computed at the DLPNO-CCSD(T)/def2-TZVPP:SMD(1,4-dioxane)//SMD(1,4-dioxane)/BMK/def2-SVP level.

S6.3. [5 + 1] Cycloaddition Pathway via Reductive Elimination

Except for 6π cyclization pathway to give [5 + 1] product, direct reductive elimination pathways were also considered. Compared to alkyne insertion transition state **TS5**, both possible transition states **TS5-S1** and **TS5-S2** are largely disfavored by 14.3 kcal/mol and 8.9 kcal/mol, respectively. Thus, these two pathways could be safely ruled out.

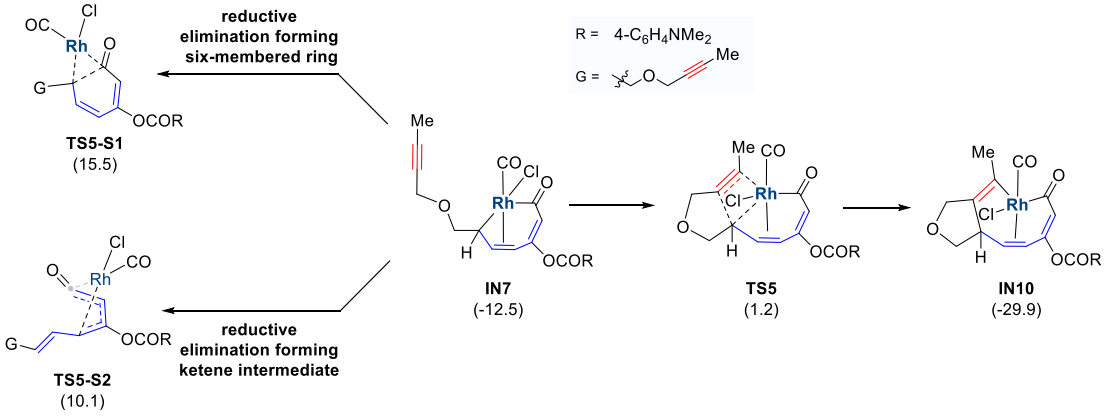


Figure S3. Gibbs energy profile of the [5 + 1] pathway via reductive elimination. Computed at the DLPNO-CCSD(T)/def2-TZVPP:SMD(1,4-dioxane)//SMD(1,4-dioxane)/BMK/def2-SVP level.

S6.4. [5 + 2] and [5+ 2 + 1] Pathways

In the main text, the [5 + 2] pathways are briefly discussed. Here, we give a full picture of both the [5 + 2] and [5 + 2 + 1] pathways. After ligand exchange between CO and alkyne of **IN4**, **IN5'** is then generated, which is endergonic by 9.7 kcal/mol. Subsequent coordination afford **IN6'**, which

then undergo alkyne insertion via **TS4'** with an activation free energy of 10.2 kcal/mol, affording an eight-membered rhodacycle **IN7'**. Then, there are two possible pathways. One is [5 + 2] pathways via a reductive elimination transition state **TS5'**, giving the Rh/[5 + 2] product complex **IN8'**, requiring an activation free energy of 3.8 kcal/mol. Another is the [5 + 2 + 1] pathway. After exergonic coordination of COs to **IN7'**, **IN9'** is formed. CO insertion via **TS6'** has an activation free energy of 11.5 kcal/mol, affording **IN10'**. Followed reductive elimination of **IN10'** is almost barrierless, generating the Rh/[5 + 2 + 1] product complex **IN11'**. The selectivity between [5 + 2] and [5 + 2 + 1] cycloaddition is determined by **TS5'** and **TS6'** and [5 + 2] pathway is favored by 4.2 kcal/mol. Thus, once alkyne insertion happens, the [5 + 2] product could be much favored.

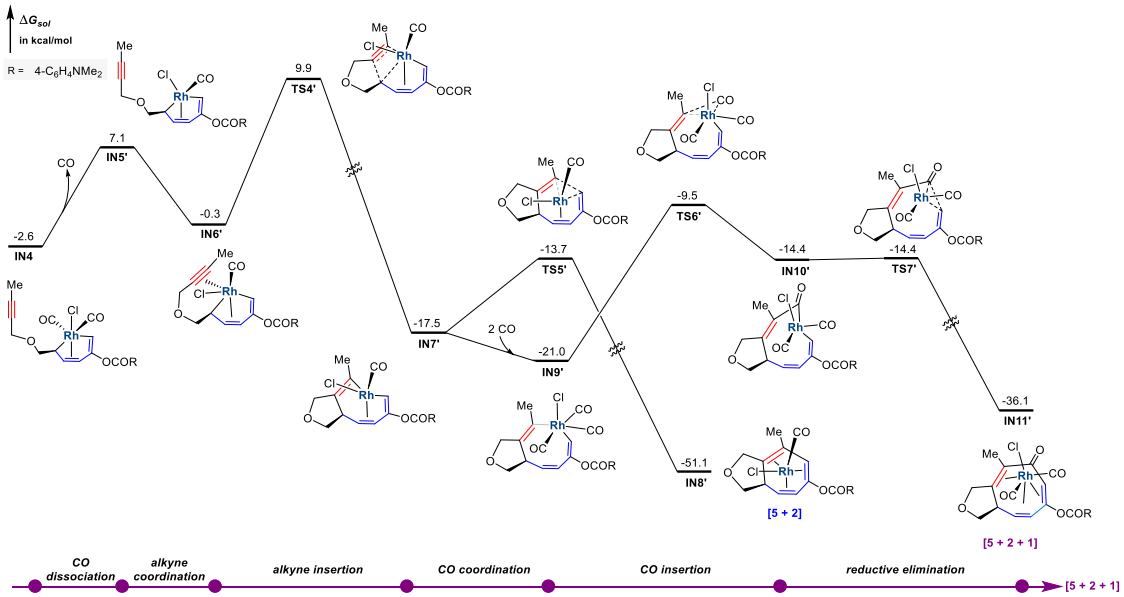


Figure S4. Gibbs energy profile for [5 + 2] and [5 + 2 + 1] pathways. Computed at the DLPNO-CCSD(T)/def2-TZVPP:SMD(1,4-dioxane)//SMD(1,4-dioxane)/BMK/def2-SVP level.

S6.5. Computed Energies of the Stationary Points

Table S1. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs)

Stationary point	solvent	TCG[a,b]	SPE[a]	SPE[c]	SPE[d]	SPE[e]
1r	dioxane	0.301907	-1015.511664		-1015.497784	-1015.186337
$[Rh(CO)_2Cl]_2$	dioxane	-0.007894	-1592.917252		-1592.916576	-1593.122371
CO	dioxane	-0.013859	-113.167803		-113.172745	-113.158166
CO	DCE	-0.013866	-113.167303		-113.172745	-113.158162
4r'	dioxane	0.324726	-1128.830598		-1128.813211	-1128.456382
4r	dioxane	0.325290	-1128.843805		-1128.827285	-1128.464134
5r	dioxane	0.317290	-1128.815208		-1128.797664	-1128.442631
IN1	dioxane	0.306499	-1811.957046		-1811.938330	-1811.737301
IN2	dioxane	0.313973	-1811.966233		-1811.944136	-1811.733259
IN2'	dioxane	0.312699	-1811.964868		-1811.943885	-1811.732767
IN3	dioxane	0.316826	-1811.966943		-1811.942116	-1811.731166
IN3'	dioxane	0.308920	-1811.978055		-1811.960460	-1811.750176
IN3''	dioxane	0.307296	-1811.959835		-1811.941067	-1811.729336

IN4	dioxane	0.314987	-1811.996684		-1811.977413	-1811.762097
IN4''	dioxane	0.308355	-1128.736254		-1128.719664	-1128.372124
IN5	dioxane	0.319158	-1812.000560		-1811.983205	-1811.766540
IN5'	dioxane	0.310056	-1698.792955		-1698.772534	-1698.571594
IN5''	dioxane	0.314314	-1128.788963		-1128.771083	-1128.415659
IN6	dioxane	0.318731	-1811.998423		-1811.976913	-1811.754478
IN6'	dioxane	0.314910	-1698.804580		-1698.785092	-1698.589194
IN7	dioxane	0.317074	-1812.021546		-1811.997030	-1811.774779
IN7'	dioxane	0.317570	-1698.844283		-1698.823055	-1698.617579
IN8	dioxane	0.316904	-1812.014731		-1811.991159	-1811.771237
IN8'	dioxane	0.318744	-1698.898127		-1698.877582	-1698.672967
IN9	dioxane	0.326616	-1812.035479		-1812.014844	-1811.793943
IN9'	dioxane	0.329863	-1925.225164		-1925.206204	-1924.975688
IN10	dioxane	0.327231	-1812.064305		-1812.042090	-1811.814920
IN10'	dioxane	0.332170	-1925.227161		-1925.205003	-1924.964296
IN11	dioxane	0.330191	-1812.096294		-1812.073498	-1811.842912
IN11'	dioxane	0.335702	-1925.266650		-1925.245502	-1925.003296
TS1	dioxane	0.309655	-1811.946438		-1811.926004	-1811.723736
TS1'	dioxane	0.308823	-1811.935411		-1811.917729	-1811.713891
TS1'-S1	dioxane	0.304241	-1698.735706		-1698.713774	-1698.521906
TS1-S1	dioxane	0.309797	-1698.752766		-1698.730539	-1698.540926
TS1'-S2	dioxane	0.311521	-1811.922207		-1811.902124	-1811.694680
TS1-S2	dioxane	0.313778	-1811.942884		-1811.921459	-1811.716246
TS2	dioxane	0.317746	-1811.952526		-1811.928063	-1811.720339
TS2'	dioxane	0.311586	-1811.959171		-1811.940663	-1811.730401
TS2''	dioxane	0.311503	-1811.947170		-1811.926578	-1811.717489
TS3	dioxane	0.315112	-1811.965363		-1811.942785	-1811.731993
TS3''	dioxane	0.311930	-1925.126586		-1925.107964	-1924.882499
TS4	dioxane	0.317415	-1811.991891		-1811.972993	-1811.752462
TS4'	dioxane	0.315513	-1698.792485		-1698.773679	-1698.574275
TS4''	dioxane	0.308627	-1128.718631		-1128.701516	-1128.351438
TS5	dioxane	0.325831	-1812.005539		-1811.983202	-1811.763908
TS5'	dioxane	0.317157	-1698.833021		-1698.813906	-1698.613087
TS5-S1	dioxane	0.317219	-1811.980833		-1811.956404	-1811.730351
TS5-S2	dioxane	0.313687	-1811.980273		-1811.958885	-1811.738496
TS6	dioxane	0.325836	-1812.053220		-1812.031988	-1811.804769
TS6'	dioxane	0.329163	-1925.213391		-1925.195023	-1924.957239
TS7	dioxane	0.318034	-1128.786960		-1128.769380	-1128.409424
TS7'	dioxane	0.332099	-1925.230795		-1925.212858	-1924.968378
TS-I (CF_3)	DCE	0.199707	-1823.386009		-1823.344580	-1823.271330
TS-II (CF_3)	DCE	0.191316	-1823.354499		-1823.328668	-1823.258604
TS-I (CO_2Me)	DCE	0.236552	-1714.306674		-1714.262293	-1714.142626
TS-II (CO_2Me)	DCE	0.229815	-1714.283199		-1714.252555	-1714.134050

TS-I (H)	DCE	0.200470	-1486.707062		-1486.667783	-1486.592673
TS-II (H)	DCE	0.190476	-1486.692827		-1486.665297	-1486.593421
TS-I (Me)	DCE	0.225220	-1525.965286		-1525.926417	-1525.838428
TS-II (Me)	DCE	0.216992	-1525.963411		-1525.934157	-1525.848026
TS-I (Ph)	DCE	0.274841	-1717.438403		-1717.392525	-1717.218723
TS-II (Ph)	DCE	0.265459	-1717.432387		-1717.400509	-1717.228128
TS-IV (CF_3)	DCE	0.198855	-1710.229600		-1710.203985	-1710.138753
TS-III (CF_3)	DCE	0.200520	-1823.411432		-1823.384486	-1823.294758
TS-IV (H)	DCE	0.196780	-1373.548380		-1373.523718	-1373.456960
TS-III (H)	DCE	0.199434	-1486.747435		-1486.721790	-1486.634014
TS-V (Me)	DCE	0.200470	-1486.707062	-1487.956560	-1486.667783	-1486.592673
TS-VI (Me)	DCE	0.195133	-1599.883403	-1601.268965	-1599.856902	-1599.764009
TS-V (R)[f]	DCE	0.317982	-1811.974412	-1813.577119	-1811.926598	-1811.717872
TS-VI (R)[f]	DCE	0.311576	-1925.142432	-1926.880651	-1925.106923	-1924.881220

[a]Computed at the SMD(solvent)/BMK/def2-SVP level.

[b]A standard state at 1 atm and 298.15 K was used.

[c]Computed at the SMD(solvent)/BMK/def2-TZVPP//SMD(solvent)/BMK/def2-SVP level.

[d]Computed at the BMK/def2-SVP//SMD(solvent)/BMK/def2-SVP level.

[e]Computed at the DLPNO-CCSD(T)/def2-TZVPP//SMD(solvent)/BMK/def2-SVP level.

[f]R = 4-$C_6H_4NMe_2$.

S7. Cartesian Coordinates of the Stationary Points

1r

C	-2.705891	-1.379919	0.403243
C	-3.637962	-0.974985	-0.465545
H	-3.662571	-1.396951	-1.480259
C	-1.930722	-4.552669	1.701331
H	-2.049796	-5.404501	2.350961
C	-1.790520	-3.598758	0.970716
H	-2.653917	-0.961612	1.417423
C	-1.668565	-2.433839	0.075943
O	-0.354444	-1.903334	0.241084
C	0.192658	-1.273158	-0.812768
O	-0.365237	-1.179809	-1.878139
C	1.539023	-0.728351	-0.510243
C	2.154734	-0.859365	0.748366
C	2.237366	-0.050943	-1.526700
C	3.419607	-0.333651	0.988475
H	1.630571	-1.383715	1.551173
C	3.502032	0.480406	-1.306242
H	1.765266	0.053743	-2.507836
C	4.135221	0.355754	-0.034285
H	3.857616	-0.460199	1.979074
H	4.000868	0.996424	-2.127031
N	5.377388	0.876021	0.196258
C	6.085280	1.565342	-0.861820
H	5.535422	2.458881	-1.212362
H	7.063684	1.897205	-0.489076
H	6.261040	0.909280	-1.734564
C	5.989039	0.742136	1.501346
H	5.378846	1.216953	2.292163
H	6.141739	-0.317624	1.779146
H	6.971557	1.233036	1.495163
H	-1.793916	-2.759616	-0.970247
C	-4.713918	0.034103	-0.141856
H	-5.692073	-0.477001	-0.107416
H	-4.532819	0.477644	0.857935
O	-4.844319	1.025944	-1.123566
C	-3.749697	1.889300	-1.248237
H	-3.952255	2.521401	-2.128600
H	-2.815751	1.328810	-1.454356
C	-3.530531	2.757456	-0.069687
C	-3.335855	3.469479	0.892655
C	-3.101290	4.338086	2.049320
H	-3.954559	4.295251	2.747187
H	-2.193940	4.032670	2.597137
H	-2.974793	5.386818	1.731489

[Rh(CO)$_2$Cl]$_2$

C	2.768408	-1.360996	-0.545657
O	3.426380	-2.194888	-0.944543
C	2.818992	1.329489	-0.465581
O	3.514916	2.162840	-0.795099
Rh	1.632740	-0.012060	0.105435
Cl	-0.012486	-1.670541	0.896504
Cl	0.012442	1.670467	0.896702
Rh	-1.632729	0.012098	0.105253
C	-2.768415	1.361135	-0.545626
C	-2.818944	-1.329577	-0.465561
O	-3.514862	-2.163065	-0.794743
O	-3.426430	2.195013	-0.944476

CO (in dioxane)

C	0.000000	0.000000	-0.643286
O	0.000000	0.000000	0.482464

CO (in DCE)

C	0.000000	0.000000	-0.643219
O	0.000000	0.000000	0.482414

4r'

C	-4.485648	-0.234681	-0.063760
C	-3.334170	-1.214817	0.133911
C	-2.576495	-0.960370	1.412168
C	-1.539359	-0.116038	1.502268
C	-4.455487	1.112334	-0.178408
H	-2.631201	-1.144111	-0.715444
H	-2.889342	-1.515482	2.305391
C	-1.074461	0.699383	0.372249
C	-1.808154	1.482987	-0.443908
H	-1.244793	2.065118	-1.182080
O	0.294356	0.750033	0.220577
C	0.945914	-0.381152	-0.154279
O	0.358023	-1.372273	-0.498026
C	-5.743340	-1.090987	-0.135932
H	-6.245219	-1.123529	0.858286

H	-6.473507	-0.733359	-0.877863	O	-0.697650	-2.515397	-0.485221
C	-4.075230	-2.577847	0.131038	C	5.696032	0.837821	-0.811168
O	-5.291878	-2.356991	-0.521499	H	5.736136	0.691979	-1.914786
H	-3.524173	-3.367912	-0.400767	H	6.028948	1.864324	-0.591040
H	-4.247031	-2.915059	1.175861	C	5.833160	-1.244239	0.078964
C	-5.731622	1.922788	-0.280341	O	6.534456	-0.055841	-0.140114
H	-6.628717	1.315492	-0.096677	H	6.179241	-1.694377	1.025400
H	-5.714154	2.743467	0.455037	H	6.016228	-1.979081	-0.734428
H	-5.819085	2.400010	-1.271630	C	3.556410	2.804787	-1.065486
H	-0.966766	-0.029114	2.433521	H	4.225607	2.678205	-1.929357
C	2.416556	-0.224671	-0.107950	H	2.595009	3.206710	-1.419054
C	3.221435	-1.310410	-0.502803	H	3.994210	3.569918	-0.396385
C	3.052787	0.959414	0.311070	H	1.451835	-2.675402	-0.206512
C	4.607403	-1.229005	-0.481906	C	-2.362357	-0.877475	-0.005000
H	2.734919	-2.233173	-0.831852	C	-3.416510	-1.648287	-0.533168
C	4.438983	1.059850	0.337993	C	-2.656103	0.413829	0.475877
H	2.449495	1.816881	0.619437	C	-4.716697	-1.163657	-0.576113
C	5.263342	-0.034793	-0.057922	H	-3.196923	-2.649856	-0.913916
H	5.186217	-2.097249	-0.798017	C	-3.951221	0.916291	0.437583
H	4.886822	1.997180	0.669172	H	-1.853418	1.040046	0.871540
N	6.624935	0.056792	-0.032656	C	-5.026718	0.141035	-0.088246
C	7.262755	1.286875	0.387928	H	-5.498244	-1.800313	-0.991674
H	7.003593	1.549167	1.430650	H	-4.129483	1.923760	0.814430
H	8.353237	1.169349	0.331164	N	-6.300775	0.628376	-0.126176
H	6.979838	2.138531	-0.258334	C	-6.586175	1.956863	0.374683
C	7.437299	-1.072231	-0.435660	H	-6.028183	2.734473	-0.179420
H	7.260886	-1.351832	-1.491220	H	-7.658448	2.166318	0.261519
H	8.499168	-0.813200	-0.328236	H	-6.333675	2.054661	1.446852
H	7.241258	-1.962456	0.190166	C	-7.370654	-0.177598	-0.676224
C	-3.226571	1.965046	-0.334440	H	-7.505488	-1.120931	-0.114990
O	-3.380702	3.159692	-0.508037	H	-8.313256	0.383257	-0.622992
				H	-7.188711	-0.434351	-1.736432
4r				C	2.041608	1.489735	0.447404
C	4.286797	0.542583	-0.288726	O	1.210683	2.364324	0.322998
C	4.349418	-0.864091	0.114135	H	2.771304	0.065157	1.934642
C	3.409277	-1.850236	0.228843				
C	1.965435	-1.806119	0.202974	**5r**			
C	3.310548	1.502779	-0.331575	C	2.693466	0.410321	-0.022969
H	3.820308	-2.869676	0.260948	C	3.194729	-0.863856	0.254875
C	1.226029	-0.787129	0.718541	C	0.897283	-1.689630	0.430730
C	1.826271	0.368358	1.463265	H	0.198217	-2.511779	0.598819
H	1.113603	0.731587	2.217107	C	0.426641	-0.401019	0.143521
O	-0.122003	-0.650992	0.651797	H	3.401622	1.223297	-0.196481
C	-1.002060	-1.458881	0.001119	O	-0.910799	-0.096127	0.148299

C	-1.839377	-0.860962	-0.472363	H	-1.945517	1.402708	-1.093436
O	-1.567184	-1.851266	-1.097524	C	-0.542945	-3.039669	0.303775
C	1.314651	0.652999	-0.083205	H	-0.374634	-4.092290	0.492109
C	-3.207899	-0.320842	-0.286595	C	-0.458619	-1.832728	0.076729
C	-3.486481	0.837274	0.463822	H	-0.716137	0.566024	1.627920
C	-4.285078	-0.999061	-0.888027	O	1.838554	-1.280730	-1.862592
C	-4.788091	1.302696	0.613554	C	2.170843	-0.676943	-0.876022
H	-2.666896	1.382504	0.937840	O	1.270365	-0.205107	0.014716
C	-5.591955	-0.548993	-0.750703	C	-0.101940	-0.425323	-0.263356
H	-4.077363	-1.898931	-1.474114	C	-4.612200	-2.399257	-0.045221
C	-5.885708	0.621637	0.009722	O	-5.731456	-2.439132	-0.205760
H	-4.953828	2.204404	1.203804	C	3.567148	-0.362499	-0.493599
H	-6.392707	-1.107962	-1.236026	C	4.607547	-0.798001	-1.336144
N	-7.166944	1.071669	0.153244	C	3.906858	0.354781	0.668956
C	-8.260567	0.362235	-0.476493	C	5.938131	-0.533412	-1.039163
H	-8.342306	-0.677922	-0.109508	H	4.351473	-1.355284	-2.241860
H	-9.205316	0.874455	-0.249409	C	5.233337	0.628630	0.983220
H	-8.150000	0.327900	-1.576393	H	3.117457	0.706292	1.337524
C	-7.435814	2.261107	0.933455	C	6.294362	0.192788	0.135967
H	-6.930788	3.151596	0.514654	H	6.707900	-0.892279	-1.723050
H	-8.516327	2.457663	0.937267	H	5.448143	1.189327	1.893377
H	-7.108616	2.146492	1.983721	N	7.599041	0.460133	0.436853
H	0.920727	1.648928	-0.299072	C	7.931841	1.193337	1.639986
C	4.673161	-1.169602	0.321655	H	7.579060	0.672074	2.549297
H	4.916324	-1.601802	1.317381	H	9.022925	1.295625	1.713764
H	4.919229	-1.959862	-0.421602	H	7.494930	2.209552	1.638384
O	5.417634	-0.016139	0.085807	C	8.654209	0.019545	-0.451354
C	6.794928	-0.243370	0.126011	H	8.545740	0.450950	-1.463790
H	7.096569	-0.651596	1.114966	H	9.624807	0.341589	-0.050862
H	7.090076	-1.000396	-0.632535	H	8.676846	-1.081774	-0.550719
C	7.533866	1.002291	-0.125275	H	-0.302655	-0.305046	-1.341981
C	8.160395	2.018814	-0.330847	C	-2.622266	2.377186	0.776544
C	8.912976	3.251094	-0.579144	H	-3.680132	2.029086	0.762620
H	8.386171	4.120959	-0.151908	H	-2.301785	2.397830	1.840150
H	9.912819	3.197118	-0.116303	O	-2.523093	3.641050	0.191112
H	9.043355	3.424753	-1.660517	C	-3.354493	4.586817	0.797322
C	2.278895	-1.913223	0.478589	H	-4.418262	4.269000	0.737820
O	2.801322	-3.127954	0.741610	H	-3.113455	4.687289	1.877960
H	2.099734	-3.779084	0.855292	C	-3.206741	5.897578	0.149787
				C	-3.096680	6.984615	-0.373842
IN1				C	-2.957290	8.294732	-1.014303
C	-0.900879	0.569897	0.545539	H	-2.573453	9.044149	-0.301836
C	-1.781207	1.410226	-0.007729	H	-2.252700	8.235082	-1.860982
Rh	-2.694393	-2.347518	0.143581	H	-3.927186	8.649922	-1.401191

C	-2.753938	-2.471642	2.024444
O	-2.763296	-2.527908	3.160872
Cl	-2.654592	-2.078340	-2.209194

IN2

C	0.734431	0.825659	-0.515653
C	1.956862	1.229797	-0.152980
Rh	2.276577	-2.590872	0.103023
H	2.315762	1.032373	0.865728
C	0.203274	-2.447021	-0.189174
H	-0.398977	-3.320344	-0.488591
C	-0.519123	-1.348041	-0.009399
H	0.361930	0.973419	-1.538530
O	-1.950968	-1.317268	-0.167367
C	-2.391313	-0.148399	0.121294
O	-1.485282	0.703145	0.463486
C	-0.160420	0.069330	0.421044
C	4.162423	-2.734721	0.457591
O	5.271548	-2.803408	0.701752
C	-3.778441	0.190987	0.069565
C	-4.744562	-0.779534	-0.297228
C	-4.210887	1.502408	0.390288
C	-6.085991	-0.458809	-0.343021
H	-4.423034	-1.795459	-0.543207
C	-5.549921	1.834705	0.348522
H	-3.474431	2.259523	0.673827
C	-6.538642	0.862969	-0.019055
H	-6.799639	-1.232412	-0.625801
H	-5.844132	2.853737	0.599545
N	-7.850739	1.180956	-0.057594
C	-8.291975	2.517879	0.300026
H	-7.873224	3.279220	-0.381954
H	-9.386313	2.567406	0.235090
H	-7.999064	2.775969	1.333033
C	-8.836328	0.186841	-0.445992
H	-8.849360	-0.666942	0.255002
H	-9.833434	0.645464	-0.443714
H	-8.640533	-0.199066	-1.461868
H	0.244622	0.076537	1.444504
C	2.934504	1.878044	-1.089879
H	3.756855	1.156731	-1.296664
H	2.451948	2.108412	-2.063953
O	3.442960	3.033820	-0.490269
C	4.469915	3.621606	-1.232466
H	5.313897	2.910491	-1.366305
H	4.116419	3.889238	-2.252193
C	4.964643	4.833411	-0.563666
C	5.386605	5.832094	-0.022679
C	5.893469	7.035697	0.641222
H	6.963222	6.928946	0.887990
H	5.774131	7.923052	-0.002978
H	5.343223	7.217609	1.579870
C	2.365176	-3.369319	-1.565060
O	2.387849	-3.843292	-2.607794
Cl	2.134018	-1.532872	2.314119

IN2'

C	-1.006738	0.728997	0.068751
C	-1.530331	1.804116	-0.531800
Rh	-2.607420	-2.253993	0.006271
H	-1.433969	1.936393	-1.618477
C	0.426076	-2.559597	-0.011403
H	0.397243	-3.604656	0.295391
C	-0.591219	-1.740582	-0.270309
H	-1.129819	0.552705	1.144119
O	1.785683	-2.138130	-0.057979
C	2.083644	-0.906955	-0.257642
O	1.198974	-0.028343	-0.538918
C	-0.267467	-0.335332	-0.695708
C	3.466516	-0.505201	-0.157947
C	3.844776	0.840595	-0.382979
C	4.472047	-1.445073	0.175612
C	5.164698	1.236004	-0.278263
H	3.081593	1.579059	-0.641410
C	5.796112	-1.063646	0.280331
H	4.198039	-2.487676	0.356346
C	6.190756	0.295666	0.059977
H	5.412304	2.281452	-0.461571
H	6.537139	-1.818576	0.542880
N	7.484591	0.677335	0.168578
C	8.512818	-0.298999	0.480340
H	8.350897	-0.759030	1.471848
H	8.547442	-1.104459	-0.274612
H	9.492204	0.196500	0.490726
C	7.857725	2.067056	-0.024015
H	7.323445	2.729326	0.680010
H	8.934419	2.181482	0.156126
H	7.644359	2.408776	-1.053062

H	-0.436466	-0.205191	-1.778552
C	-2.268945	2.895680	0.187764
H	-2.522511	2.576224	1.219428
H	-1.613856	3.790672	0.269321
O	-3.423953	3.208173	-0.540537
C	-4.216696	4.200349	0.035872
H	-5.155633	4.230164	-0.541641
H	-4.482374	3.936468	1.081215
C	-3.603150	5.548595	0.027280
C	-3.113319	6.658189	0.028354
C	-2.529634	8.002312	0.022881
H	-3.315879	8.766838	-0.096625
H	-1.992461	8.206806	0.964301
H	-1.817272	8.114668	-0.811862
C	-2.681075	-2.757283	-1.767922
O	-2.690401	-3.068512	-2.870524
C	-4.451520	-2.662476	0.376746
O	-5.536717	-2.886851	0.630683
Cl	-2.416247	-1.619105	2.350973

IN3

C	-0.781555	-0.549600	-1.362518
C	-1.352075	0.563384	-0.606423
Rh	-2.198130	-1.204988	0.106465
H	-0.727561	1.032642	0.164693
C	-0.514441	-1.339673	1.315933
H	-0.423088	-1.365490	2.408764
C	0.562046	-1.301888	0.543098
H	-1.047362	-0.672178	-2.419016
O	1.929937	-1.120632	0.889406
C	2.521861	-0.576442	-0.127669
O	1.815275	-0.465602	-1.190732
C	0.487132	-1.202566	-0.943874
Cl	-2.408524	-3.700540	-0.060716
C	-3.708938	-1.205460	-1.156561
O	-4.570340	-1.285299	-1.886778
C	3.878717	-0.124581	-0.043168
C	4.601259	-0.229483	1.171197
C	4.521530	0.434230	-1.175108
C	5.909817	0.202815	1.255918
H	4.115924	-0.658383	2.052232
C	5.829255	0.871979	-1.102569
H	3.973909	0.518220	-2.117996
C	6.573470	0.770419	0.118836
H	6.430016	0.104815	2.208417
H	6.288313	1.295051	-1.995778
N	7.855054	1.193907	0.195030
C	8.505852	1.774156	-0.966701
H	7.975742	2.677296	-1.317929
H	9.530595	2.063783	-0.701216
H	8.559837	1.054376	-1.802980
C	8.596087	1.072957	1.438548
H	8.670712	0.020253	1.764224
H	9.614215	1.455794	1.292265
H	8.125526	1.656265	2.250074
H	0.643591	-2.156711	-1.475578
C	-2.221324	1.561557	-1.340973
H	-1.593415	2.405944	-1.706399
H	-2.671983	1.091404	-2.243503
O	-3.222784	2.053649	-0.495946
C	-3.995384	3.050729	-1.095362
H	-3.359916	3.908293	-1.407221
H	-4.484561	2.669091	-2.018227
C	-5.030530	3.534535	-0.170577
C	-5.890295	3.941015	0.580284
C	-6.928034	4.421026	1.496426
H	-7.929382	4.322972	1.044336
H	-6.916751	3.834260	2.430500
H	-6.768285	5.481077	1.756101
C	-3.265911	-0.832042	1.684360
O	-3.817331	-0.555226	2.638013

IN3'

C	-1.525600	0.987631	-0.607417
C	-2.197842	1.717640	-1.517443
Rh	-2.269545	-1.983915	0.040691
H	-2.341528	1.318915	-2.530976
C	0.755518	-1.561635	0.655363
H	0.636502	-2.391923	1.357079
C	-0.252410	-1.104531	-0.071091
H	-1.351186	1.379943	0.400676
O	2.055598	-1.151419	0.593067
C	2.409971	0.125044	0.289179
O	1.606218	1.002670	0.125576
C	-0.969111	-0.329322	-0.935164
C	3.879888	0.280316	0.209358
C	4.405230	1.556031	-0.072602
C	4.781426	-0.784824	0.398587

C	5.773895	1.770633	-0.165210
H	3.712279	2.389316	-0.220519
C	6.154681	-0.589074	0.310119
H	4.397756	-1.784257	0.617202
C	6.696563	0.698790	0.023701
H	6.131286	2.776921	-0.385461
H	6.814169	-1.443899	0.462454
N	8.043745	0.897922	-0.066552
C	8.957211	-0.206396	0.139532
H	8.845844	-0.648501	1.146984
H	8.806745	-1.010765	-0.604667
H	9.990363	0.153291	0.042927
C	8.565001	2.213810	-0.372452
H	9.661436	2.169452	-0.418110
H	8.200288	2.583086	-1.348897
H	8.287092	2.956615	0.398483
H	-1.041996	-0.663117	-1.980155
C	-2.753597	3.096808	-1.264814
H	-2.133429	3.832320	-1.811263
H	-3.771124	3.167893	-1.702496
O	-2.753149	3.475558	0.077495
C	-3.823826	2.978723	0.833570
H	-3.912044	1.877832	0.731535
H	-3.586193	3.190910	1.889065
C	-5.126352	3.592759	0.495638
C	-6.200899	4.084065	0.222319
C	-7.497558	4.685906	-0.099060
H	-7.360267	5.629207	-0.654139
H	-8.108328	4.007733	-0.718356
H	-8.060716	4.912447	0.821986
C	-2.420428	-1.092868	1.697717
O	-2.487981	-0.581412	2.711531
C	-3.664882	-3.270958	0.458493
O	-4.436324	-4.070536	0.669611
Cl	-2.091166	-3.170757	-2.002751

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C	-0.288602	1.279642	-0.470266
C	0.464456	0.187211	-0.079088
C	-0.025550	-1.112307	0.186517
Rh	-1.867541	-1.955220	0.231186
C	-2.016577	-2.240178	-1.599971
O	-2.093830	-2.404653	-2.727398
Cl	-1.355563	-1.420449	2.542223
C	-3.575212	-2.775539	0.638419
O	-4.566962	-3.246934	0.926012
H	0.278416	2.203890	-0.642688
C	-1.710503	1.355992	-0.641124
C	-2.285165	2.525457	-1.016760
H	0.763408	-1.780043	0.567395
H	-2.331392	0.470706	-0.469246
H	-1.664564	3.418617	-1.169425
C	-3.747480	2.716975	-1.243440
H	-4.106223	3.505935	-0.544060
H	-3.894106	3.132590	-2.267477
O	-4.442963	1.529006	-1.074248
C	-5.825984	1.629080	-1.264989
H	-6.051985	2.042943	-2.269905
H	-6.219156	0.600068	-1.237148
C	-6.515678	2.443353	-0.241619
C	-7.089804	3.108460	0.594163
C	-7.788026	3.896412	1.612753
H	-7.940881	4.935877	1.277405
H	-8.775191	3.456323	1.833045
H	-7.208263	3.917016	2.550874
O	1.813589	0.456517	0.092014
C	2.705323	-0.282877	-0.612424
O	2.355822	-1.144881	-1.377324
C	4.104709	0.103316	-0.333520
C	5.138151	-0.556332	-1.026225
C	4.454824	1.101312	0.596258
C	6.471941	-0.236495	-0.810416
H	4.874568	-1.335603	-1.747162
C	5.784336	1.433710	0.826901
H	3.668917	1.621747	1.149168
C	6.838699	0.774774	0.127337
H	7.235584	-0.775083	-1.372183
H	6.008652	2.209946	1.559013
N	8.145700	1.099263	0.347055
C	8.486437	2.132376	1.302694
H	8.140393	1.880051	2.322281
H	9.577655	2.250814	1.337276
H	8.048446	3.109289	1.025467
C	9.196929	0.411350	-0.373394
H	9.188979	-0.675978	-0.172217
H	9.109602	0.556896	-1.466234
H	10.172556	0.805099	-0.058029

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C	1.609998	0.836111	0.559723
C	2.192394	0.640324	-0.754180
Rh	2.082226	-1.294064	0.092040
H	1.498803	0.633772	-1.605311
C	0.246284	-1.403283	-0.800009
H	-0.150936	-2.033346	-1.594980
C	-0.426604	-0.544260	-0.026970
H	2.210398	1.323301	1.337337
O	-1.739663	-0.174227	0.073759
C	-2.681906	-0.608607	-0.792031
O	-2.431448	-1.314753	-1.733200
C	0.472025	0.124360	0.959958
C	-4.033672	-0.104051	-0.446897
C	-4.295572	0.727209	0.658340
C	-5.114142	-0.476112	-1.269248
C	-5.583693	1.172590	0.935778
H	-3.475687	1.030529	1.313529
C	-6.407212	-0.041494	-1.008595
H	-4.920040	-1.123518	-2.129119
C	-6.683736	0.800561	0.108665
H	-5.738053	1.814353	1.803835
H	-7.210339	-0.359054	-1.674326
N	-7.951889	1.232184	0.375282
C	-9.048378	0.838378	-0.484011
H	-8.900244	1.183706	-1.524228
H	-9.181203	-0.259494	-0.505569
H	-9.980712	1.283662	-0.111441
C	-8.204846	2.077011	1.522872
H	-7.654411	3.034402	1.459367
H	-9.277357	2.307890	1.575565
H	-7.917911	1.581547	2.469217
H	0.173422	0.164682	2.014550
C	3.508845	1.318002	-1.074422
H	3.946369	0.867059	-1.989229
H	3.322753	2.389682	-1.298983
O	4.394889	1.200750	0.003908
C	5.618826	1.860628	-0.168991
H	6.265016	1.548485	0.667816
H	6.109848	1.529681	-1.107401
C	5.509551	3.334818	-0.176799
C	5.435636	4.545203	-0.188851
C	5.351094	6.007725	-0.200634
H	5.306211	6.409884	0.825264
H	6.231714	6.442500	-0.702820
H	4.450410	6.342491	-0.742214
C	2.845744	-2.352187	-1.320284
O	3.239256	-2.973788	-2.178255
C	3.771626	-1.212440	1.262634
O	4.650846	-1.290271	1.962673
Cl	1.614728	-3.254660	1.526060

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C	2.629807	0.905311	-0.322262
C	3.629749	0.191154	-0.874226
H	3.410674	-0.739444	-1.414464
C	0.206639	2.666933	0.452127
H	-0.441703	3.024881	1.258403
C	0.175215	1.259114	0.014153
H	2.878255	1.824548	0.224446
O	-1.072895	0.694158	-0.116672
C	-1.955688	0.702706	0.907122
O	-1.677122	1.129408	1.998409
C	1.228953	0.507041	-0.382013
C	-3.264520	0.127889	0.521708
C	-3.552928	-0.327309	-0.779041
C	-4.271703	0.029560	1.500670
C	-4.797732	-0.858551	-1.096226
H	-2.786759	-0.262560	-1.555470
C	-5.520654	-0.499751	1.203106
H	-4.055607	0.379774	2.514125
C	-5.824741	-0.961878	-0.112078
H	-4.972956	-1.197676	-2.117480
H	-6.268412	-0.555477	1.994784
N	-7.049714	-1.481999	-0.415577
C	-8.067135	-1.589981	0.609038
H	-8.343512	-0.601520	1.021000
H	-8.971404	-2.040044	0.177732
H	-7.737987	-2.229609	1.448978
C	-7.333923	-1.935107	-1.761012
H	-6.666759	-2.762419	-2.067623
H	-8.368356	-2.300487	-1.811165
H	-7.227349	-1.119115	-2.499683
H	0.998358	-0.488666	-0.776385
C	5.073786	0.597178	-0.829175
H	5.405904	0.901320	-1.848659
H	5.206044	1.482933	-0.171590
O	5.845761	-0.482539	-0.384074

C	7.215479	-0.212734	-0.408146
H	7.546946	0.048178	-1.437266
H	7.456894	0.663406	0.232501
C	7.982645	-1.374597	0.063258
C	8.630737	-2.321803	0.451816
C	9.406672	-3.471758	0.922900
H	10.093448	-3.832982	0.138984
H	10.004677	-3.207326	1.811226
H	8.735006	-4.302382	1.198217
C	0.984852	3.568380	-0.135976
O	1.654198	4.368708	-0.633417

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C	-1.129017	-2.386647	1.782519
C	-2.304826	-1.467562	1.682352
Rh	-2.752191	-0.663841	-0.193701
H	-3.193807	-1.929565	2.137457
C	-0.751565	-0.444330	-0.498156
H	-0.448424	0.301328	-1.246430
C	0.225817	-1.094093	0.164582
H	-1.214402	-3.262729	2.437338
O	1.553250	-0.815624	-0.138963
C	2.284674	-0.173113	0.791825
O	1.808496	0.234731	1.822635
C	0.040539	-2.171467	1.145732
C	3.705781	-0.024528	0.396448
C	4.219188	-0.516967	-0.818252
C	4.586441	0.637714	1.271950
C	5.559913	-0.356997	-1.150432
H	3.553670	-1.032935	-1.514711
C	5.929152	0.806660	0.957997
H	4.195325	1.023459	2.217801
C	6.460124	0.312491	-0.270250
H	5.912029	-0.753949	-2.103044
H	6.570923	1.325976	1.670284
N	7.777925	0.474065	-0.590881
C	8.669144	1.157453	0.322564
H	8.345341	2.198014	0.511324
H	9.678092	1.192012	-0.110024
H	8.735797	0.639714	1.297774
C	8.288507	-0.039610	-1.844278
H	8.173046	-1.137235	-1.917839
H	9.359174	0.192138	-1.923315
H	7.778261	0.415380	-2.713626
H	0.901440	-2.824401	1.326379
C	-2.041260	-0.074925	2.292977
H	-2.464828	0.070729	3.303400
H	-0.961061	0.148589	2.311387
O	-2.693920	0.838907	1.382769
C	-2.116667	2.139101	1.329923
H	-1.104375	2.073062	0.885756
H	-2.012423	2.504764	2.368686
C	-2.968475	3.041033	0.556373
C	-3.665958	3.777137	-0.105316
C	-4.500839	4.632665	-0.948632
H	-5.420386	4.939124	-0.422906
H	-4.783935	4.088909	-1.865656
H	-3.950584	5.541844	-1.243835
Cl	-3.317607	0.633748	-2.227313
C	-4.801785	-0.743413	0.033237
O	-5.925495	-0.740261	0.093130
C	-2.525508	-2.203024	-1.242220
O	-2.345670	-3.115132	-1.883920

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C	1.727844	0.589168	0.911091
C	2.250482	0.602093	-0.406225
Rh	2.228710	-1.468429	0.316442
H	1.569124	0.514822	-1.261573
C	0.440830	-1.603024	-0.574894
H	0.202426	-2.140671	-1.492555
C	-0.263833	-0.824861	0.249485
H	2.347749	1.009706	1.711758
O	-1.555670	-0.400996	0.303625
C	-2.465634	-0.784940	-0.624499
O	-2.188344	-1.515540	-1.538433
C	0.679087	-0.303151	1.291115
C	-3.801854	-0.198252	-0.371504
C	-4.081148	0.655949	0.712307
C	-4.847397	-0.504195	-1.263668
C	-5.352013	1.187003	0.901880
H	-3.287486	0.910124	1.418872
C	-6.122795	0.017332	-1.091378
H	-4.640088	-1.167254	-2.108488
C	-6.416778	0.885368	0.002174
H	-5.518889	1.844360	1.755574
H	-6.896912	-0.250601	-1.810902
N	-7.665890	1.406890	0.179473

C	-8.725216	1.092590	-0.756483
H	-8.476014	1.417966	-1.783611
H	-8.941837	0.008395	-0.785084
H	-9.644102	1.611959	-0.453059
C	-7.935573	2.281419	1.301374
H	-7.313416	3.195451	1.270064
H	-8.989368	2.589846	1.277290
H	-7.752340	1.777221	2.268456
H	0.413948	-0.374021	2.352502
C	3.560281	1.287721	-0.707519
H	4.052555	0.756274	-1.547127
H	3.377202	2.333346	-1.036132
O	4.370660	1.266007	0.432491
C	5.655650	1.781973	0.242118
H	6.228627	1.547551	1.154537
H	6.159034	1.270797	-0.604124
C	5.687986	3.243351	0.011579
C	5.728056	4.439945	-0.181651
C	5.781170	5.885712	-0.413748
H	5.792317	6.440406	0.539483
H	6.689005	6.155278	-0.979441
H	4.905934	6.219814	-0.996055
C	1.873043	-3.246894	1.057052
O	1.620954	-4.278560	1.442494
Cl	3.816346	-2.288990	-1.249392

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C	2.568949	0.414096	0.344030
C	3.273566	-0.905482	0.467715
H	3.626466	-0.982790	1.518860
C	0.926370	-1.956262	0.205325
H	0.316186	-2.853151	0.137186
C	0.395345	-0.701408	0.188366
H	3.193273	1.312789	0.371084
O	-0.916448	-0.370760	0.119240
C	-1.970006	-1.233418	0.036161
O	-1.844729	-2.426346	-0.005405
C	1.233456	0.505167	0.231183
C	-3.260365	-0.510285	0.003736
C	-3.374470	0.892295	0.066620
C	-4.443707	-1.269521	-0.092069
C	-4.616247	1.515548	0.036745
H	-2.475307	1.507465	0.141723
C	-5.692487	-0.665016	-0.123914
H	-4.366314	-2.359370	-0.141741
C	-5.819421	0.755061	-0.058813
H	-4.654116	2.603991	0.088964
H	-6.576947	-1.298233	-0.198910
N	-7.040980	1.360920	-0.086017
C	-8.246724	0.563958	-0.181262
H	-8.350277	-0.128166	0.674927
H	-9.121956	1.227351	-0.185760
H	-8.271098	-0.035295	-1.110300
C	-7.137750	2.804125	-0.015891
H	-6.623354	3.292521	-0.864346
H	-8.194723	3.100280	-0.047813
H	-6.703056	3.199939	0.920706
H	0.722499	1.469031	0.162791
C	4.532099	-0.985317	-0.409517
H	5.006125	-1.973686	-0.256747
H	4.246411	-0.912744	-1.481363
O	5.390499	0.055260	-0.052098
C	6.563465	0.077432	-0.813999
H	7.111690	-0.883759	-0.714239
H	6.326656	0.197832	-1.893066
C	7.439007	1.177886	-0.386714
C	8.176939	2.077883	-0.049640
C	9.067300	3.165526	0.363563
H	8.924671	3.398436	1.432280
H	10.123147	2.883090	0.214505
H	8.870513	4.082023	-0.217654
C	2.386130	-2.140567	0.251896
O	2.889137	-3.241179	0.147003

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C	1.101528	-2.038016	-2.042976
C	2.248217	-1.116821	-1.859719
Rh	2.721505	-0.657180	0.143072
H	3.107809	-1.466937	-2.449248
C	0.689147	-1.198462	0.922195
H	0.406174	-0.710137	1.861024
C	-0.241874	-1.267034	-0.094056
H	1.161884	-2.778854	-2.851719
O	-1.473298	-0.791023	0.190278
C	-2.188065	-0.064290	-0.732396
O	-1.656252	0.423592	-1.692397
C	-0.060780	-1.990128	-1.344360
H	-0.933555	-2.557656	-1.689021

C	1.919698	0.349415	-2.218272
H	2.148249	0.599325	-3.273376
H	0.850041	0.563558	-2.032930
O	2.725211	1.143523	-1.352223
C	2.300105	2.486491	-1.236604
H	1.270052	2.519304	-0.826746
H	2.273531	2.946532	-2.244369
C	3.208673	3.233998	-0.365260
C	3.947947	3.840321	0.378023
C	4.835833	4.541148	1.306672
H	5.044314	3.901552	2.180788
H	4.366472	5.472398	1.665869
H	5.793750	4.799210	0.825206
Cl	3.189541	0.335280	2.321556
C	4.548026	-1.150586	-0.113592
O	5.619592	-1.502187	-0.205758
C	1.919092	-2.142224	0.974089
O	2.056932	-3.224765	1.420264
C	-3.606559	0.053805	-0.362908
C	-4.456492	0.817264	-1.189469
C	-4.159139	-0.562597	0.778413
C	-5.804641	0.962117	-0.899470
H	-4.035810	1.301596	-2.075436
C	-5.506184	-0.427360	1.084723
H	-3.518853	-1.156332	1.435556
C	-6.376337	0.341189	0.253314
H	-6.420955	1.563353	-1.568235
H	-5.888900	-0.921933	1.977769
N	-7.698439	0.477182	0.548266
C	-8.248139	-0.148073	1.734390
H	-7.751671	0.212702	2.653748
H	-9.316214	0.094871	1.810688
H	-8.150626	-1.248983	1.701244
C	-8.563842	1.251339	-0.318820
H	-8.250348	2.310308	-0.373992
H	-8.581492	0.844911	-1.346609
H	-9.589461	1.222157	0.072404

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C	3.950101	-0.297818	1.543522
C	2.149520	-1.747694	0.002399
C	1.544819	-1.247924	-1.191393
C	0.646100	-0.156681	-1.140402
C	4.123130	0.922974	1.419175
Rh	2.574968	0.372245	-0.146480
Cl	4.382089	0.190909	-1.841972
H	1.500216	-1.811759	0.884012
H	1.978436	-1.500952	-2.164968
C	-0.015098	0.252951	0.141338
C	0.917654	0.598419	1.030403
H	0.755333	0.952300	2.054933
O	-1.378835	0.343085	0.260232
C	-2.149921	-0.708578	-0.100893
O	-1.682207	-1.765327	-0.438679
C	4.036322	-1.726779	1.950891
H	4.898791	-1.812238	2.633598
H	3.128938	-1.990493	2.530137
C	3.265320	-2.764568	-0.078796
O	4.276085	-2.597905	0.900869
H	2.836940	-3.780158	0.038377
H	3.754571	-2.705504	-1.064652
C	2.523837	2.264117	-0.677279
O	2.488090	3.337182	-1.029940
C	4.671561	2.282495	1.582337
H	5.419850	2.282914	2.392083
H	5.166407	2.603655	0.650657
H	3.879198	3.006376	1.832907
H	0.313980	0.278477	-2.091530
C	-3.596448	-0.400921	-0.020785
C	-4.519178	-1.409922	-0.355933
C	-4.096210	0.854671	0.373788
C	-5.888547	-1.184868	-0.304206
H	-4.138830	-2.388430	-0.663101
C	-5.463729	1.098940	0.432125
H	-3.398359	1.652431	0.640026
C	-6.406550	0.083754	0.093211
H	-6.562396	-1.998439	-0.574057
H	-5.803149	2.087301	0.743455
N	-7.750842	0.316129	0.147146
C	-8.248555	1.611925	0.558733
H	-7.904114	2.417990	-0.115601
H	-9.346682	1.602984	0.539005
H	-7.929985	1.867845	1.586545
C	-8.684887	-0.734896	-0.198593
H	-8.581696	-1.612997	0.465976
H	-9.710954	-0.356192	-0.099320
H	-8.550164	-1.078358	-1.241089

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C	1.318677	0.823937	-0.457975
C	2.055777	0.180659	-1.485550
Rh	2.283798	-0.846405	0.449364
H	1.549188	-0.532787	-2.147723
C	-0.126697	-2.087864	-0.615006
H	-0.739948	-2.869930	-1.058380
C	-0.583973	-0.881739	-0.193687
H	1.734739	1.752558	-0.044959
O	-1.853570	-0.433936	-0.174978
C	-2.951465	-1.116340	-0.634014
O	-2.870538	-2.174066	-1.193358
C	0.352290	0.144463	0.349010
H	-0.037296	0.698177	1.210129
C	3.233809	0.881098	-2.127925
H	3.883282	0.125807	-2.618331
H	2.871239	1.559503	-2.932643
O	3.940389	1.601841	-1.164680
C	5.016664	2.328215	-1.692913
H	4.658645	3.054826	-2.452736
H	5.727928	1.648887	-2.208754
C	5.723019	3.049337	-0.626412
C	6.319486	3.647991	0.241916
C	7.036913	4.367975	1.296721
H	6.552474	4.201213	2.273574
H	7.044472	5.452905	1.098521
H	8.081464	4.021621	1.369515
Cl	2.147235	-1.739846	2.646676
C	4.050446	-1.733971	0.149096
O	5.042839	-2.237752	-0.030406
C	1.315265	-2.332630	-0.427326
O	1.899806	-3.325810	-0.752356
C	-4.198567	-0.376350	-0.359603
C	-4.238356	0.863347	0.309316
C	-5.417025	-0.943251	-0.785639
C	-5.442250	1.514930	0.544848
H	-3.309931	1.325012	0.652382
C	-6.628714	-0.306913	-0.559131
H	-5.397356	-1.906515	-1.303396
C	-6.680413	0.949834	0.116343
H	-5.421417	2.471624	1.067267
H	-7.545551	-0.785763	-0.904306
N	-7.865742	1.583131	0.342639
C	-7.892342	2.848264	1.047560
H	-8.931713	3.189160	1.144272
H	-7.468106	2.759452	2.064787
H	-7.326894	3.630875	0.508374
C	-9.106321	0.986942	-0.109011
H	-9.110390	0.831893	-1.203479
H	-9.295127	0.010858	0.375595
H	-9.942146	1.654495	0.139479

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C	3.044795	1.647908	-0.713770
C	1.821471	1.937490	0.138910
C	1.627444	0.947045	1.256336
C	0.723208	-0.082733	1.242895
C	3.554883	0.426539	-0.893152
Rh	2.669210	-1.023114	0.178927
Cl	4.373483	-1.190552	1.925835
H	0.916329	1.945863	-0.493292
H	2.158784	1.141830	2.197093
C	0.073219	-0.562159	-0.016350
C	0.963255	-1.033507	-0.904206
H	0.683545	-1.455790	-1.876298
O	-1.289760	-0.634246	-0.119267
C	-2.027647	0.484269	0.098786
O	-1.518110	1.557494	0.294585
C	3.582821	3.004322	-1.164514
H	4.636216	3.132838	-0.839937
H	3.539469	3.151518	-2.258184
C	2.150346	3.378030	0.580074
O	2.743008	3.954180	-0.552883
H	1.262625	3.969649	0.851464
H	2.850435	3.363191	1.443326
C	3.536445	-2.358139	-0.846480
O	4.025543	-3.188866	-1.435833
C	4.780477	0.128645	-1.717466
H	5.232042	1.060900	-2.099680
H	5.545756	-0.397585	-1.120709
H	4.536989	-0.500372	-2.592924
H	0.505346	-0.610408	2.182938
C	-3.481066	0.221530	0.044865
C	-4.367397	1.301088	0.226306
C	-4.025195	-1.056184	-0.189356
C	-5.743180	1.123196	0.176996
H	-3.953041	2.297041	0.407418
C	-5.399847	-1.253341	-0.243660

H	-3.357786	-1.909399	-0.333308
C	-6.305882	-0.166117	-0.063764
H	-6.388774	1.989796	0.321949
H	-5.774431	-2.260631	-0.427426
N	-7.656314	-0.350420	-0.120940
C	-8.200098	-1.664955	-0.391953
H	-7.924767	-2.394812	0.392191
H	-9.296139	-1.605451	-0.427629
H	-7.850956	-2.060135	-1.363844
C	-8.552037	0.769902	0.079228
H	-8.412730	1.552361	-0.690061
H	-9.591261	0.419862	0.020308
H	-8.408653	1.236727	1.071121

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C	-1.464670	0.181948	-0.980605
C	-2.358563	0.611028	0.007041
Rh	-2.564406	-1.595186	-0.442209
H	-2.066054	0.585693	1.064558
C	-0.400533	-1.558700	1.596889
H	0.055709	-1.667614	2.579372
C	0.212423	-1.098566	0.478470
H	-1.673602	0.464150	-2.022116
O	1.489871	-0.731092	0.300019
C	2.486564	-0.808130	1.245148
O	2.282925	-1.181650	2.365530
C	-0.577025	-0.947168	-0.780690
C	3.781674	-0.383792	0.682930
C	3.940726	0.054339	-0.647552
C	4.920839	-0.422545	1.512741
C	5.182965	0.435755	-1.135832
H	3.073181	0.097373	-1.309584
C	6.170289	-0.046487	1.041461
H	4.809112	-0.758623	2.547692
C	6.343321	0.394807	-0.305829
H	5.254399	0.767683	-2.171742
H	7.021801	-0.094833	1.720588
N	7.566382	0.761399	-0.780299
C	8.728910	0.706081	0.082849
H	8.910622	-0.317436	0.458834
H	9.616466	1.019386	-0.482850
H	8.625892	1.378456	0.954634
C	7.711498	1.210004	-2.150395
H	7.102863	2.110276	-2.353768
H	8.762681	1.464544	-2.340251
H	7.416242	0.426202	-2.872300
H	-0.030260	-1.272663	-1.674249
C	-3.491725	1.552884	-0.314990
H	-3.788398	1.451744	-1.380415
H	-4.375707	1.271723	0.292554
O	-3.079457	2.859232	-0.027998
C	-4.121296	3.786897	-0.136950
H	-4.577454	3.747307	-1.149786
H	-4.932623	3.551481	0.584817
C	-3.630295	5.149212	0.113568
C	-3.245266	6.280258	0.315321
C	-2.773971	7.645519	0.560953
H	-2.962912	8.291402	-0.313004
H	-3.283125	8.087706	1.433774
H	-1.689056	7.648539	0.760445
C	-2.428435	-3.504599	-0.781930
O	-2.336504	-4.612799	-0.978585
Cl	-4.955535	-1.619388	-0.628574
C	-1.813433	-1.916901	1.391802
O	-2.561344	-2.358740	2.210240

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C	-3.443679	1.572661	0.796839
C	-3.368255	1.699371	-0.708996
C	-2.533470	0.702937	-1.489766
C	-1.152046	0.533387	-1.362811
C	-2.532689	1.013475	1.616959
Rh	-1.923241	-1.147937	-0.213616
Cl	-3.365249	-2.684963	-1.288237
H	-2.996239	2.716043	-0.951953
H	-2.936664	0.458992	-2.480528
C	-0.532197	0.435510	-0.065835
C	-1.278341	0.364470	1.154580
H	-0.634313	0.046149	1.984222
O	0.816863	0.188632	0.003218
C	1.659701	1.171589	-0.426797
O	1.246048	2.205483	-0.878705
C	-4.817589	2.099893	1.190286
H	-5.382353	1.322754	1.746715
H	-4.774960	3.005101	1.822615
C	-4.872092	1.675711	-1.044753
O	-5.462049	2.423538	-0.016552
H	-5.116316	2.147683	-2.009362

H	-5.239599	0.627040	-1.056903
C	-1.107203	-2.595108	0.754692
O	-0.586409	-3.442970	1.298115
C	-2.757425	0.904231	3.110563
H	-1.965025	1.441632	3.661964
H	-3.726177	1.321139	3.422492
H	-2.720301	-0.151594	3.434016
H	-0.534841	0.236630	-2.218011
C	3.080627	0.804254	-0.263492
C	4.061474	1.731241	-0.667727
C	3.506569	-0.423750	0.279217
C	5.415214	1.453468	-0.540244
H	3.739405	2.687583	-1.089722
C	4.857511	-0.718847	0.415709
H	2.766500	-1.160659	0.600002
C	5.858954	0.212728	0.008731
H	6.135320	2.204068	-0.867015
H	5.138885	-1.682913	0.840017
N	7.186309	-0.070734	0.139261
C	7.607683	-1.331195	0.715139
H	7.254212	-2.193775	0.120250
H	8.704785	-1.368741	0.744877
H	7.236381	-1.454205	1.749441
C	8.181585	0.888371	-0.294252
H	8.111915	1.838023	0.268328
H	9.184131	0.471371	-0.129573
H	8.084543	1.120516	-1.370804

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C	-1.149573	-1.501477	-0.301937
C	-1.908928	-1.218473	-1.447612
Rh	-2.569414	-0.012781	0.382242
H	-1.618799	-0.404512	-2.122877
C	-0.391473	1.648371	-0.810772
H	0.082669	2.457868	-1.363315
C	0.264356	0.632228	-0.205853
H	-1.326046	-2.453982	0.208961
O	1.591685	0.403997	-0.117301
C	2.573184	1.241958	-0.575040
O	2.336751	2.289839	-1.108428
C	-0.497367	-0.469390	0.466986
C	3.918061	0.684784	-0.324576
C	4.144035	-0.557650	0.300634
C	5.037417	1.435621	-0.736837
C	5.432042	-1.035347	0.507687
H	3.295839	-1.161889	0.629827
C	6.331015	0.974853	-0.538124
H	4.873335	2.401346	-1.223493
C	6.571423	-0.282525	0.093830
H	5.554886	-2.002584	0.995621
H	7.163529	1.593055	-0.875103
N	7.838176	-0.744763	0.293113
C	8.975450	0.041665	-0.138960
H	9.012162	1.023720	0.368000
H	9.902075	-0.496673	0.100651
H	8.959929	0.220234	-1.229968
C	8.053032	-2.022955	0.939834
H	7.597723	-2.853534	0.369100
H	9.131438	-2.216710	1.014910
H	7.633384	-2.040738	1.962668
H	-0.055724	-0.802392	1.414003
C	-2.804167	-2.280487	-2.051055
H	-2.321878	-2.688264	-2.955930
H	-2.943024	-3.110531	-1.330116
O	-4.042690	-1.778948	-2.468302
C	-4.918693	-1.473905	-1.432978
H	-5.918741	-1.352385	-1.881270
H	-4.962727	-2.289478	-0.683689
C	-4.625720	-0.218534	-0.690392
C	-4.754469	0.825418	-0.047224
C	-5.206755	2.081499	0.566730
H	-6.171556	2.374447	0.119919
H	-5.347633	1.961740	1.653867
H	-4.474607	2.879528	0.368410
C	-2.597865	1.047602	1.998579
O	-2.567488	1.613011	2.976867
Cl	-3.451318	-1.881386	1.808288
C	-1.869367	1.595600	-0.677397
O	-2.579664	2.452182	-1.146197

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C	-2.983971	2.076240	-0.037794
C	-1.505083	2.449191	0.044022
C	-0.858465	2.224714	-1.297795
C	-0.084298	1.167030	-1.591007
C	-3.559778	0.863390	-0.048569
H	-0.966164	1.878901	0.813772
H	-1.041418	2.989056	-2.064346

C	0.218128	0.096175	-0.622800
C	-0.618876	-0.635736	0.129460
H	-0.115696	-1.363522	0.780507
O	1.583326	-0.176933	-0.530479
C	2.344970	0.661145	0.202505
O	1.878657	1.557375	0.858239
C	-3.728369	3.417404	-0.158616
H	-4.407187	3.467208	-1.025982
H	-4.329841	3.603629	0.758193
C	-1.603521	3.951014	0.377045
O	-2.739338	4.395510	-0.314884
H	-1.722049	4.089421	1.472331
H	-0.731076	4.535176	0.045570
C	-5.076954	0.770745	-0.162422
H	-5.554886	1.756187	-0.285475
H	-5.385661	0.157078	-1.029052
H	-5.526697	0.314778	0.739120
H	0.418579	1.105518	-2.564587
C	3.790496	0.334823	0.117759
C	4.698036	1.094637	0.879007
C	4.301385	-0.701096	-0.686295
C	6.062979	0.837092	0.849519
H	4.309488	1.902382	1.505768
C	5.665228	-0.971086	-0.732754
H	3.617980	-1.307664	-1.285399
C	6.591688	-0.209856	0.038159
H	6.724919	1.452858	1.459153
H	6.012839	-1.784481	-1.370303
N	7.932187	-0.473250	0.003376
C	8.442338	-1.536374	-0.836181
H	8.204566	-1.367146	-1.902826
H	9.535603	-1.583873	-0.740848
H	8.033978	-2.523527	-0.548663
C	8.842707	0.291713	0.828583
H	8.604814	0.193465	1.904388
H	9.867287	-0.073607	0.676983
H	8.826677	1.367772	0.573689
Rh	-2.649270	-1.027794	0.126760
C	-2.546340	-0.610219	2.041591
O	-2.436434	-0.310130	3.120689
C	-2.456043	-1.059171	-1.827363
O	-2.323196	-1.064835	-2.944820
Cl	-2.007729	-3.411281	0.410695
C	-4.472764	-2.015110	0.184332
O	-5.379735	-2.680279	0.215760

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C	-1.327401	0.935380	-1.118218
C	-1.600261	2.122973	-0.244570
Rh	-2.793099	-0.810463	-0.386491
H	-0.838064	2.189947	0.551368
C	-0.701473	-0.707733	1.655716
H	-0.252185	-0.879613	2.639211
C	0.039625	-0.337439	0.592489
H	-1.672390	0.984898	-2.161538
O	1.386252	-0.297378	0.702574
C	2.132314	0.668509	0.079839
O	1.623097	1.650042	-0.389824
C	-0.577255	-0.153421	-0.754805
C	3.569566	0.351317	0.101563
C	4.087236	-0.839705	0.650209
C	4.472715	1.278114	-0.457414
C	5.450680	-1.100640	0.640417
H	3.407663	-1.573015	1.091138
C	5.837929	1.033834	-0.476025
H	4.080349	2.205821	-0.883978
C	6.373733	-0.171033	0.073082
H	5.804528	-2.035340	1.075887
H	6.495472	1.781703	-0.919525
N	7.711914	-0.424063	0.056103
C	8.628057	0.535499	-0.526575
H	8.596132	1.506751	0.001067
H	9.653001	0.147354	-0.457988
H	8.404941	0.717999	-1.593874
C	8.227454	-1.653072	0.624747
H	7.817358	-2.544120	0.114613
H	9.319753	-1.674173	0.514699
H	7.993026	-1.736860	1.702037
H	-0.279297	-0.882952	-1.518068
C	-1.718479	3.495916	-0.933505
H	-0.752613	3.997445	-1.096259
H	-2.236645	3.390998	-1.911462
O	-2.471700	4.260641	-0.027923
C	-3.460783	3.449198	0.570414
H	-3.536551	3.720577	1.639513
H	-4.452103	3.620799	0.104547
C	-2.989283	2.017305	0.346657
C	-3.636684	0.844239	0.476877

C	-4.991762	0.756002	1.143761
H	-5.313619	1.718869	1.577393
H	-5.776887	0.424893	0.439477
H	-4.955521	0.017458	1.965864
C	-4.322396	-1.930701	0.018725
O	-5.177323	-2.631817	0.236652
Cl	-2.248531	-2.654223	-1.915525
C	-2.140146	-1.027988	1.477436
O	-2.822270	-1.473699	2.359052

IN10'

C	2.814887	1.980372	-0.184255
C	1.341834	2.230850	0.132966
C	0.867124	1.660312	1.455806
C	0.062835	0.591186	1.579996
C	3.416914	1.135935	-1.060919
H	0.677400	1.901329	-0.677734
H	1.141785	2.232630	2.351081
C	-0.297540	-0.277373	0.437845
C	0.581365	-0.905415	-0.358609
H	0.135405	-1.483002	-1.181725
O	-1.662215	-0.473794	0.264118
C	-2.407112	0.568315	-0.162493
O	-1.917313	1.606881	-0.528049
C	3.576262	3.137579	0.459366
H	4.264235	2.804754	1.257612
H	4.180644	3.660209	-0.311359
C	1.415485	3.770956	0.276512
O	2.601096	3.984962	0.999777
H	1.457009	4.250411	-0.722955
H	0.570459	4.195655	0.838927
C	4.892922	1.266346	-1.398302
H	5.500872	1.484232	-0.507557
H	5.287044	0.345064	-1.849917
H	5.014774	2.088190	-2.127990
H	-0.362059	0.339023	2.561417
C	-3.859679	0.274885	-0.135036
C	-4.760078	1.273394	-0.551054
C	-4.384700	-0.957943	0.296014
C	-6.132802	1.061606	-0.537171
H	-4.359885	2.233920	-0.888219
C	-5.755535	-1.190317	0.313609
H	-3.702972	-1.747541	0.621785
C	-6.676162	-0.183521	-0.101717
H	-6.789376	1.867441	-0.866351
H	-6.115105	-2.162149	0.653209
N	-8.024067	-0.401958	-0.082451
C	-8.547818	-1.673648	0.369526
H	-8.259663	-1.889055	1.415439
H	-9.644869	-1.653526	0.319778
H	-8.195233	-2.511461	-0.260595
C	-8.935355	0.641395	-0.503081
H	-8.759341	0.942513	-1.552431
H	-9.967665	0.274452	-0.426886
H	-8.848657	1.544523	0.129822
Rh	2.612302	-1.009466	-0.040551
C	2.367240	-1.533149	2.062729
O	2.292306	-1.939000	3.109165
C	2.758090	-0.037719	-1.750561
O	2.521018	-0.226292	-2.896905
Cl	4.985760	-1.473434	0.463064
C	2.566750	-2.710263	-0.836006
O	2.565433	-3.724290	-1.332663

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C	3.220920	-1.148932	0.103707
C	2.116686	-1.909569	-0.646504
C	1.407042	-0.722785	-1.247655
C	0.506014	0.036226	-0.518225
C	3.100459	-0.529071	1.370222
Rh	2.581551	0.874563	-0.222500
Cl	1.934302	2.746220	-1.523525
H	1.455152	-2.513007	-0.005016
H	1.557626	-0.493711	-2.309639
C	-0.097365	-0.379813	0.766710
C	0.501194	-0.781425	1.909099
H	-0.158683	-1.056689	2.737649
O	-1.459338	-0.261592	0.804376
C	-2.221556	-0.938719	-0.104145
O	-1.745433	-1.770215	-0.829720
C	4.520640	-1.573909	-0.580085
H	5.259806	-0.770450	-0.712381
H	4.986004	-2.386363	0.023271
C	2.929343	-2.743856	-1.653363
O	4.131250	-2.043769	-1.837294
C	1.931157	-0.759842	2.313328
O	2.173246	-0.907593	3.494162
C	4.373557	-0.205052	2.141995

H	4.600065	-1.023867	2.844771
H	5.239383	-0.073604	1.476990
H	4.247268	0.708479	2.745643
H	-0.048836	0.818348	-1.048424
C	-3.641221	-0.543044	-0.044701
C	-4.556256	-1.188466	-0.899698
C	-4.127465	0.449955	0.828525
C	-5.904903	-0.861935	-0.892255
H	-4.186759	-1.961163	-1.580071
C	-5.474375	0.788784	0.850938
H	-3.434915	0.963722	1.499963
C	-6.409535	0.142000	-0.011477
H	-6.574633	-1.389817	-1.571555
H	-5.805205	1.564709	1.541739
N	-7.732664	0.469755	0.005176
C	-8.220608	1.476543	0.925282
H	-7.763547	2.465417	0.734563
H	-9.307986	1.579276	0.810336
H	-8.015811	1.202453	1.976617
C	-8.655691	-0.186410	-0.897943
H	-8.709687	-1.275439	-0.712752
H	-9.661838	0.230323	-0.756678
H	-8.371552	-0.032998	-1.955288
C	4.279213	1.810662	-0.090202
O	5.244710	2.400565	-0.100071
H	2.431273	-2.861744	-2.627871
H	3.119601	-3.750444	-1.228620

IN11’

C	-3.477685	0.550253	-0.467818
C	-3.203881	1.321041	-1.756637
C	-1.901189	2.012726	-2.025835
C	-0.730744	1.853353	-1.397988
C	-3.309703	0.962401	0.854907
H	-3.994595	2.097265	-1.773810
H	-1.925527	2.709677	-2.872095
C	-0.420328	1.007794	-0.207931
C	-0.923416	1.286283	1.128455
H	-0.220795	1.357941	1.966796
O	0.924360	0.579576	-0.236156
C	1.902873	1.481826	0.033927
O	1.660734	2.624929	0.320697
C	-4.607402	-0.387571	-0.883602
H	-4.659013	-1.303190	-0.274724
H	-5.578567	0.147645	-0.802499
C	-3.560356	0.269524	-2.845114
O	-4.327884	-0.730360	-2.214980
H	-4.123507	0.728009	-3.678227
H	-2.644926	-0.185902	-3.266192
C	-4.301734	0.610227	1.940892
H	-4.872839	-0.298279	1.715398
H	-3.804273	0.479163	2.913612
H	-4.993835	1.468266	2.029596
H	0.129062	2.423020	-1.768058
C	3.257966	0.891540	-0.057074
C	4.363943	1.702462	0.263891
C	3.500113	-0.439827	-0.445862
C	5.661502	1.211351	0.211484
H	4.185792	2.739322	0.563220
C	4.792077	-0.949436	-0.504895
H	2.662433	-1.088642	-0.712094
C	5.917569	-0.138997	-0.172037
H	6.484445	1.877367	0.472631
H	4.929349	-1.986317	-0.812678
N	7.187915	-0.634613	-0.218253
C	7.416268	-2.014064	-0.594913
H	7.069723	-2.223278	-1.624210
H	8.492003	-2.230758	-0.551125
H	6.901969	-2.715692	0.087701
C	8.311732	0.215810	0.115316
H	8.253093	0.585889	1.155852
H	9.244163	-0.355325	0.012732
H	8.376448	1.092360	-0.555706
Rh	-1.655050	-0.572607	0.379682
C	-2.248207	1.936630	1.335563
O	-2.480089	2.886697	2.033355
C	-1.824852	-1.884888	-1.202082
O	-1.810713	-2.712921	-1.966919
C	-0.164154	-1.500586	1.214662
O	0.656453	-2.059988	1.750502
Cl	-2.907882	-2.341148	1.617653

TS1

C	-0.798749	0.660586	-0.435796
C	-1.794244	1.060057	-1.233416
Rh	-2.770450	-1.924436	0.301127
H	-1.872609	0.673979	-2.257868
C	-0.675302	-2.549099	0.412471

H	-0.449355	-3.537364	0.814925	Cl	-2.917940	-2.855565	-1.906219
C	0.025227	-1.647338	-0.124051				
H	-0.726061	1.015180	0.597536	**TS1'**			
O	2.013452	-1.976280	-0.245227	C	-1.069442	0.844220	-0.109496
C	2.412372	-0.822288	-0.358675	C	-1.765918	1.845160	-0.657910
O	1.531025	0.131585	-0.627116	Rh	-2.250865	-2.466238	0.205444
C	0.213498	-0.364153	-0.870379	H	-1.729379	2.021286	-1.741871
C	-4.634998	-1.602057	0.182329	C	0.210793	-2.523555	-1.030580
O	-5.754854	-1.433577	0.077119	H	0.594034	-3.527979	-1.155527
C	3.801574	-0.392273	-0.213055	C	-0.534889	-1.549912	-0.736686
C	4.190161	0.953766	-0.378953	H	-1.110010	0.628761	0.965318
C	4.790930	-1.348082	0.099229	O	1.956402	-1.621907	-1.652889
C	5.515396	1.336006	-0.236275	C	2.143300	-0.606450	-0.986289
H	3.437999	1.708105	-0.624276	O	1.155677	0.171661	-0.571505
C	6.119702	-0.982271	0.243481	C	-0.210541	-0.082676	-0.925497
H	4.497450	-2.393762	0.228602	C	3.479021	-0.148427	-0.574120
C	6.527083	0.378110	0.081573	C	3.677503	1.041551	0.155795
H	5.772658	2.386226	-0.374481	C	4.607887	-0.917970	-0.921712
H	6.851721	-1.752957	0.485628	C	4.950364	1.449561	0.528335
N	7.828341	0.745992	0.224404	H	2.815685	1.652539	0.435121
C	8.838130	-0.249398	0.526475	C	5.887328	-0.524280	-0.558858
H	9.821703	0.235517	0.581331	H	4.464670	-1.842608	-1.487619
H	8.648239	-0.745213	1.496169	C	6.101127	0.677996	0.181873
H	8.887898	-1.029784	-0.254620	H	5.055544	2.375657	1.093790
C	8.215154	2.134873	0.073600	H	6.729276	-1.153697	-0.847697
H	7.691716	2.784704	0.798294	N	7.352981	1.073603	0.543054
H	9.294115	2.232760	0.251970	C	8.505041	0.279683	0.165890
H	8.002547	2.512430	-0.943560	H	8.467489	-0.734213	0.605510
H	0.122324	-0.573241	-1.952381	H	8.586726	0.174287	-0.931488
C	-2.895270	1.984085	-0.807733	H	9.418844	0.770820	0.525750
H	-2.904633	2.873137	-1.474646	C	7.539393	2.289335	1.309398
H	-3.866412	1.462721	-0.966437	H	7.005464	2.248464	2.276445
O	-2.743190	2.354945	0.525765	H	8.608293	2.426633	1.520429
C	-3.730792	3.220192	1.004250	H	7.183986	3.180156	0.759082
H	-4.741461	2.791147	0.840671	H	-0.327383	0.133540	-2.003541
H	-3.580101	3.297288	2.093622	C	-2.627168	2.796844	0.122100
C	-3.684677	4.574806	0.410284	H	-2.726794	2.458240	1.173956
C	-3.659588	5.686823	-0.072937	H	-2.141828	3.796697	0.140185
C	-3.625685	7.033726	-0.648761	O	-3.879928	2.879460	-0.500363
H	-2.591276	7.325555	-0.896804	C	-4.771846	3.757044	0.117031
H	-4.229655	7.087275	-1.570073	H	-5.750824	3.604817	-0.367185
H	-4.025139	7.771726	0.067205	H	-4.894174	3.505237	1.191668
C	-2.627065	-1.195253	2.014722	C	-4.394877	5.184692	0.003500
O	-2.509179	-0.755177	3.061092	C	-4.096688	6.357306	-0.080856

C	-3.745012	7.775654	-0.189192
H	-4.653369	8.401590	-0.191622
H	-3.111223	8.093935	0.655531
H	-3.195381	7.970945	-1.125447
C	-2.940222	-2.964725	-1.455678
O	-3.338730	-3.259641	-2.483008
C	-3.745390	-3.163315	1.177611
O	-4.614939	-3.551737	1.794589
Cl	-1.346943	-1.798161	2.327077

TS1'-S1

C	-0.828781	-0.531444	-1.418768
C	-1.293468	0.488391	-0.540761
Rh	-2.338542	-1.311716	-0.189695
H	-0.739225	0.691282	0.386770
C	0.266309	-2.459362	1.393119
C	-0.356024	-1.967685	0.421261
H	-0.990427	-0.479961	-2.501438
O	2.265116	-2.342187	0.746637
C	2.434852	-1.339875	0.060240
O	1.500020	-0.845937	-0.743460
C	0.227629	-1.475525	-0.891894
C	3.689843	-0.569157	0.058457
C	4.736291	-0.962743	0.917487
C	3.894505	0.547763	-0.777438
C	5.938572	-0.272121	0.952703
H	4.590309	-1.830495	1.566738
C	5.091405	1.250237	-0.755638
H	3.100559	0.868973	-1.455919
C	6.155520	0.863539	0.114432
H	6.718699	-0.612541	1.634104
H	5.204623	2.107382	-1.419768
N	7.331103	1.549569	0.143435
C	7.525283	2.700168	-0.715543
H	6.788858	3.497609	-0.505144
H	8.528620	3.113648	-0.547559
H	7.443572	2.431832	-1.784953
C	8.393680	1.134310	1.036820
H	8.736608	0.106635	0.816353
H	9.251655	1.809400	0.919381
H	8.076201	1.169995	2.095183
H	0.347131	-2.351497	-1.552336
C	-2.042325	1.683509	-1.081574
H	-1.332973	2.531395	-1.210923
H	-2.454616	1.454503	-2.089186
O	-3.062801	2.042757	-0.198293
C	-3.767691	3.178530	-0.610235
H	-3.077820	4.040335	-0.740402
H	-4.248970	3.004957	-1.597087
C	-4.798844	3.534258	0.373685
C	-5.653261	3.839681	1.176508
C	-6.686115	4.193568	2.153142
H	-6.417878	5.113779	2.698853
H	-7.657526	4.356099	1.656587
H	-6.811026	3.381712	2.889437
H	0.525771	-2.906833	2.343569
C	-3.909336	-0.711832	-1.075725
O	-4.853984	-0.393628	-1.619020
Cl	-3.680033	-2.926546	0.923613

TS1-S1

C	-0.837069	-0.579826	-1.330854
C	-1.350464	0.442089	-0.470246
Rh	-2.368107	-1.351513	-0.096212
H	-0.801791	0.693983	0.447052
C	-0.788245	-1.974804	1.300847
H	-0.907103	-2.283837	2.336370
C	0.141561	-1.820285	0.454785
H	-1.052794	-0.546607	-2.405415
O	2.010781	-1.839261	0.839678
C	2.428579	-1.024637	0.009536
O	1.627329	-0.660728	-0.976865
C	0.384493	-1.381610	-0.942725
Cl	-3.884803	-2.809816	1.032025
C	-3.827651	-0.905911	-1.238223
O	-4.723197	-0.682694	-1.899643
C	3.753700	-0.417215	0.040216
C	4.637257	-0.726287	1.096469
C	4.186240	0.473736	-0.965408
C	5.904539	-0.169771	1.155197
H	4.309624	-1.415982	1.879604
C	5.451179	1.038022	-0.921325
H	3.516026	0.722361	-1.792437
C	6.355334	0.734722	0.143686
H	6.552538	-0.434715	1.990881
H	5.747970	1.721023	-1.717401
N	7.596095	1.286160	0.190466
C	8.025319	2.202656	-0.847880

H	7.373029	3.093350	-0.900888
H	9.046414	2.543463	-0.631818
H	8.031161	1.720165	-1.842431
C	8.499033	0.964203	1.278503
H	8.725966	-0.116923	1.314634
H	9.444742	1.503483	1.136327
H	8.081197	1.261441	2.257626
H	0.502833	-2.252284	-1.611660
C	-2.109567	1.608667	-1.060178
H	-1.403304	2.454787	-1.219834
H	-2.511940	1.339393	-2.061654
O	-3.138738	2.000132	-0.202644
C	-3.851854	3.103035	-0.682506
H	-3.169707	3.962784	-0.860106
H	-4.326196	2.866973	-1.659846
C	-4.892835	3.507361	0.271674
C	-5.757176	3.853486	1.046854
C	-6.801617	4.258797	1.990592
H	-7.801868	4.168237	1.534684
H	-6.776320	3.618057	2.888151
H	-6.660612	5.304551	2.311762

TS1'-S2

C	-0.675713	-0.463638	-1.357657
C	-1.119383	0.620368	-0.500748
Rh	-2.198468	-1.144078	-0.085920
H	-0.492288	0.891784	0.359210
C	0.296887	-2.183355	1.631999
H	0.558044	-2.583405	2.602683
C	-0.242247	-1.740658	0.595821
H	-0.784141	-0.434827	-2.447045
O	2.399530	-2.205554	0.909505
C	2.581530	-1.244808	0.176351
O	1.646769	-0.769853	-0.644507
C	0.363582	-1.377825	-0.756824
C	3.849978	-0.492805	0.119428
C	4.906413	-0.867500	0.973305
C	4.056966	0.582016	-0.768214
C	6.122556	-0.199683	0.952523
H	4.758355	-1.703652	1.662439
C	5.267497	1.261441	-0.803215
H	3.253080	0.885804	-1.443214
C	6.343634	0.891648	0.058813
H	6.909968	-0.527008	1.631814
H	5.381787	2.085146	-1.508141
N	7.535199	1.551889	0.028495
C	7.735409	2.651843	-0.892801
H	7.020513	3.475270	-0.709957
H	8.750175	3.051977	-0.766062
H	7.625909	2.331145	-1.945396
C	8.613072	1.148555	0.908534
H	8.923224	0.103147	0.725319
H	9.484230	1.794367	0.735713
H	8.329284	1.239638	1.973223
H	0.459313	-2.319673	-1.323767
C	-1.855214	1.794929	-1.108216
H	-1.157163	2.652613	-1.226175
H	-2.215702	1.533540	-2.128037
O	-2.933069	2.168645	-0.294404
C	-3.596890	3.308941	-0.760356
H	-2.902032	4.174801	-0.809058
H	-3.975802	3.147737	-1.792985
C	-4.724849	3.646372	0.118718
C	-5.659893	3.933936	0.833728
C	-6.788762	4.273742	1.703512
H	-7.748819	4.124789	1.181374
H	-6.786362	3.635966	2.603566
H	-6.732074	5.325732	2.030157
C	-3.153884	-1.015079	1.657852
O	-3.627677	-0.886689	2.678647
C	-3.703755	-0.623926	-1.148854
O	-4.594341	-0.379684	-1.802433
Cl	-2.782715	-3.476859	-0.724433

TS1-S2

C	-0.677873	-0.533575	-1.272600
C	-1.158408	0.561190	-0.441604
Rh	-2.241279	-1.164500	0.031677
H	-0.541735	0.863040	0.415198
C	-0.670465	-1.740958	1.444904
H	-0.751836	-1.974415	2.503319
C	0.232155	-1.677933	0.561835
H	-0.888989	-0.540602	-2.347876
O	2.177453	-1.729016	0.972360
C	2.589316	-0.972308	0.092340
O	1.787539	-0.654240	-0.911870
C	0.525972	-1.336598	-0.848773
Cl	-2.816734	-3.554779	-0.424154

C	-3.618072	-0.831802	-1.270870	H	-0.192066	-2.506394	1.629498
O	-4.439937	-0.701630	-2.037082	C	0.515833	-1.281819	0.102789
C	3.921610	-0.369716	0.072950	H	-1.267514	0.840248	-1.947493
C	4.817316	-0.633482	1.130259	O	1.924201	-1.345731	0.362801
C	4.344568	0.472194	-0.976897	C	2.497396	-0.380347	-0.268496
C	6.087337	-0.078853	1.148338	O	1.727554	0.303558	-1.042759
H	4.497706	-1.286868	1.947082	C	0.392320	-0.357411	-1.080991
C	5.611627	1.035525	-0.973413	Cl	-1.978649	-2.259953	-2.139974
H	3.664990	0.684487	-1.806308	C	-4.056711	-0.717754	-0.640228
C	6.527041	0.779013	0.093313	O	-5.053521	-0.520575	-1.147730
H	6.747778	-0.308037	1.984962	C	3.886343	-0.080368	-0.106173
H	5.899534	1.680813	-1.803579	C	4.685747	-0.826669	0.795538
N	7.769820	1.330808	0.103656	C	4.486157	0.969636	-0.845035
C	8.189647	2.200903	-0.977026	C	6.026081	-0.538782	0.957198
H	7.538017	3.089730	-1.062586	H	4.234646	-1.640568	1.369975
H	9.213174	2.549429	-0.786002	C	5.825280	1.267887	-0.690990
H	8.184965	1.676344	-1.950163	H	3.879679	1.549158	-1.546718
C	8.681861	1.053279	1.195718	C	6.646429	0.522587	0.218410
H	8.908973	-0.025645	1.275113	H	6.606219	-1.136761	1.659823
H	9.626849	1.585150	1.023149	H	6.249113	2.082616	-1.277701
H	8.273258	1.390910	2.165780	N	7.957816	0.809853	0.372921
H	0.615253	-2.253442	-1.457521	C	8.568260	1.887181	-0.386693
C	-1.881333	1.716830	-1.101457	H	8.495659	1.707314	-1.474058
H	-1.175178	2.565241	-1.239266	H	8.095399	2.859834	-0.161920
H	-2.226057	1.424343	-2.118365	H	9.631620	1.957222	-0.124439
O	-2.969420	2.126548	-0.320884	C	8.773656	0.045296	1.300379
C	-3.604169	3.263057	-0.833985	H	8.397393	0.129559	2.335412
H	-2.900552	4.122517	-0.870715	H	8.804626	-1.024193	1.026317
H	-3.941798	3.085239	-1.878183	H	9.801074	0.430422	1.280265
C	-4.765726	3.626931	-0.011098	H	0.363998	-0.905366	-2.036524
C	-5.730092	3.938753	0.652943	C	-2.302882	2.165469	0.244953
C	-6.894487	4.306890	1.462185	H	-2.929951	1.955376	1.133586
H	-7.819178	4.272427	0.861902	H	-1.831099	3.161287	0.413833
H	-7.010208	3.608985	2.308561	O	-3.066671	2.179648	-0.919709
H	-6.785368	5.325453	1.871100	C	-4.121283	3.097767	-0.914344
C	-3.395625	-0.799100	1.583950	H	-3.742119	4.127671	-0.744887
O	-4.001823	-0.528973	2.502210	H	-4.563431	3.071381	-1.923675
				C	-5.170586	2.802633	0.085247
TS2				C	-6.033440	2.560907	0.902224
C	-0.773032	0.587388	-1.007147	C	-7.084992	2.258984	1.876413
C	-1.210399	1.134090	0.157557	H	-8.012569	2.800272	1.624525
Rh	-2.344214	-1.209296	0.117696	H	-7.310742	1.179440	1.881894
H	-0.670167	0.955722	1.093852	H	-6.780796	2.553455	2.894806
C	-0.464106	-1.849324	0.792334	C	-2.982500	-1.432319	1.840742

O	-3.338868	-1.615569	2.917936

TS2’

C	-0.909260	1.085970	-0.325869
C	-1.313525	2.025661	-1.203239
Rh	-2.533084	-2.041511	0.074778
H	-1.293601	1.802747	-2.278883
C	0.525672	-1.888196	0.739581
H	0.478399	-2.743505	1.415673
C	-0.513715	-1.361595	0.089920
H	-0.915505	1.281773	0.752014
O	1.839643	-1.442426	0.662394
C	2.243292	-0.508842	-0.178594
O	1.488711	0.055880	-0.972283
C	-0.474199	-0.229979	-0.781551
C	3.674063	-0.194959	-0.089914
C	4.210270	0.830494	-0.896187
C	4.540631	-0.885924	0.783198
C	5.554409	1.164402	-0.835152
H	3.547551	1.369981	-1.578391
C	5.888162	-0.566121	0.855009
H	4.145314	-1.686482	1.413238
C	6.440714	0.475525	0.048543
H	5.924839	1.964871	-1.475890
H	6.522524	-1.125398	1.543157
N	7.760043	0.799210	0.121068
C	8.637410	0.078121	1.021347
H	8.321032	0.185663	2.075197
H	8.672319	-1.000386	0.781644
H	9.656797	0.475991	0.932215
C	8.293988	1.869725	-0.697186
H	9.364319	1.991927	-0.484067
H	8.184680	1.654949	-1.776194
H	7.793607	2.832547	-0.486220
H	-0.579748	-0.441140	-1.852628
C	-1.789339	3.401358	-0.823127
H	-1.042380	4.132640	-1.188236
H	-2.727516	3.626791	-1.372478
O	-1.937044	3.595615	0.547042
C	-3.162104	3.157435	1.077773
H	-3.376154	2.110394	0.782261
H	-3.048987	3.171636	2.174266
C	-4.309065	4.007445	0.694719
C	-5.260693	4.691446	0.383049
C	-6.411436	5.521499	0.018094
H	-6.077637	6.467212	-0.441210
H	-7.063944	5.000302	-0.702325
H	-7.011224	5.769544	0.909980
C	-2.553462	-1.746891	1.904249
O	-2.528746	-1.551063	3.030289
C	-4.337723	-2.695778	-0.007347
O	-5.397730	-3.095903	-0.087816
Cl	-2.433495	-2.379421	-2.320972

TS2”

C	-1.305724	0.789021	-0.660609
C	-1.953222	1.602830	-1.526480
Rh	-2.329626	-2.257283	0.301596
H	-1.562313	1.745934	-2.542310
C	-0.272286	-1.996237	0.291063
H	0.385135	-2.774712	0.716204
C	0.424001	-1.034463	-0.348080
H	-1.691693	0.626830	0.349079
O	1.827214	-1.049957	-0.417436
C	2.334507	0.174814	-0.400520
O	1.571035	1.132649	-0.544766
C	-0.110967	0.106676	-1.070476
C	-4.229672	-2.576450	0.175334
O	-5.343655	-2.766707	0.050132
C	3.777093	0.280927	-0.214847
C	4.588849	-0.857713	-0.020681
C	4.388353	1.552957	-0.225115
C	5.958128	-0.735001	0.154626
H	4.133208	-1.851147	-0.007671
C	5.755275	1.692492	-0.048033
H	3.766903	2.440333	-0.375461
C	6.589205	0.547668	0.148205
H	6.548080	-1.639852	0.301655
H	6.184732	2.694373	-0.063997
N	7.931027	0.673544	0.321933
C	8.546412	1.986298	0.327376
H	8.129156	2.627923	1.124579
H	9.624378	1.881487	0.507802
H	8.411220	2.506169	-0.638872
C	8.756765	-0.504180	0.504748
H	8.682175	-1.191863	-0.357108
H	9.806948	-0.199453	0.603150
H	8.477236	-1.063258	1.416551

H	0.221421	0.262662	-2.103861
C	-3.220582	2.322584	-1.216586
H	-3.061167	3.409212	-1.400254
H	-3.987821	1.997255	-1.956581
O	-3.630598	2.075133	0.084958
C	-4.841568	2.678020	0.442723
H	-5.645908	2.390390	-0.265620
H	-5.112877	2.269959	1.429876
C	-4.775036	4.153203	0.525491
C	-4.735410	5.363160	0.597565
C	-4.688450	6.823726	0.701815
H	-5.113594	7.301070	-0.196918
H	-5.261570	7.168412	1.579032
H	-3.648007	7.171192	0.817725
C	-2.290733	-2.193584	2.149206
O	-2.244884	-2.147082	3.292349
Cl	-2.327775	-2.348399	-2.129682

TS3

C	-0.806261	-0.383547	-1.450260
C	-1.455729	0.662681	-0.651658
Rh	-2.144660	-1.139080	0.100801
H	-0.836802	1.183245	0.090478
C	-0.434784	-1.148999	1.257763
H	-0.312225	-1.174311	2.347286
C	0.615379	-1.085078	0.445736
H	-1.104467	-0.536989	-2.493048
O	1.972783	-0.934219	0.757081
C	2.595521	-0.394680	-0.263811
O	1.937082	-0.238360	-1.320234
C	0.410201	-1.040251	-1.025487
Cl	-2.272968	-3.639648	0.040122
C	-3.718132	-1.276000	-1.126832
O	-4.599901	-1.436681	-1.814904
C	3.982470	-0.015996	-0.111680
C	4.654048	-0.166506	1.123629
C	4.692750	0.516376	-1.212012
C	5.981482	0.199138	1.258949
H	4.117754	-0.576011	1.983880
C	6.020318	0.885424	-1.091390
H	4.181574	0.635032	-2.171532
C	6.712895	0.738324	0.152879
H	6.463957	0.068534	2.227647
H	6.533138	1.290643	-1.963812
N	8.014212	1.096210	0.279050
C	8.736951	1.638758	-0.856268
H	8.284888	2.581254	-1.214820
H	9.772353	1.850497	-0.559371
H	8.764553	0.924866	-1.699010
C	8.694196	0.945376	1.552088
H	8.718445	-0.109939	1.878556
H	9.730708	1.292997	1.452869
H	8.209771	1.542519	2.345522
H	0.659313	-1.947563	-1.594351
C	-2.426959	1.585656	-1.359786
H	-1.891749	2.496299	-1.710954
H	-2.837947	1.090275	-2.268049
O	-3.464697	1.950451	-0.494232
C	-4.340416	2.882638	-1.058251
H	-3.801481	3.817196	-1.326305
H	-4.779063	2.489127	-2.001125
C	-5.427420	3.206179	-0.123502
C	-6.331624	3.481250	0.634732
C	-7.420487	3.806008	1.559582
H	-8.396387	3.506404	1.141914
H	-7.281453	3.276515	2.517275
H	-7.451454	4.888569	1.768742
C	-3.179068	-0.740412	1.678595
O	-3.723364	-0.454699	2.632119

TS3”

C	-0.293669	1.398740	-0.557612
C	0.465428	0.399020	-0.004264
C	-0.038963	-0.848281	0.509667
Rh	-1.651787	-2.005280	0.015324
C	-1.296190	-1.633159	-1.776903
O	-1.094127	-1.405334	-2.876076
Cl	-2.222218	-2.453388	2.321776
C	-2.982022	-3.357116	-0.408592
O	-3.729992	-4.184056	-0.613510
C	-0.691739	-0.107169	2.585519
O	-1.234970	0.650279	3.222673
H	0.256132	2.275972	-0.921597
C	-1.732437	1.434829	-0.658893
C	-2.361667	2.473986	-1.254382
H	0.737396	-1.430858	1.027334
H	-2.324376	0.608564	-0.252654
H	-1.780117	3.313915	-1.657033

C	-3.843516	2.578349	-1.421206	H	-1.123311	-2.982900	2.688518
H	-4.190491	3.514203	-0.928547	O	1.562745	-0.729800	-0.120636
H	-4.070140	2.704732	-2.505270	C	2.294463	-0.026497	0.782783
O	-4.482040	1.461759	-0.899415	O	1.796197	0.448310	1.770833
C	-5.872216	1.453888	-1.053012	C	0.107538	-1.968506	1.322513
H	-6.146797	1.545054	-2.124887	C	3.713860	0.088830	0.391589
H	-6.217605	0.466038	-0.707434	C	4.237429	-0.492471	-0.779725
C	-6.570003	2.509612	-0.287776	C	4.588093	0.809798	1.227987
C	-7.156048	3.372258	0.331081	C	5.581728	-0.363300	-1.106241
C	-7.868022	4.403000	1.090584	H	3.576974	-1.054094	-1.445219
H	-8.206050	5.220550	0.431969	C	5.934373	0.947354	0.919238
H	-8.752599	3.975092	1.591635	H	4.188955	1.266577	2.138187
H	-7.213193	4.833560	1.866812	C	6.476876	0.361481	-0.263997
O	1.816665	0.672938	0.109883	H	5.942396	-0.829676	-2.023368
C	2.684280	-0.216570	-0.434877	H	6.569723	1.515508	1.599049
O	2.301501	-1.206969	-1.003865	N	7.798083	0.488599	-0.577861
C	4.095579	0.180465	-0.253639	C	8.689436	1.215077	0.302813
C	5.101971	-0.642490	-0.796014	H	8.394710	2.276300	0.403956
C	4.484908	1.346525	0.433741	H	9.708413	1.185203	-0.105694
C	6.445928	-0.320677	-0.666248	H	8.717179	0.770521	1.314785
H	4.808120	-1.550981	-1.329639	C	8.316569	-0.103886	-1.793509
C	5.825542	1.684740	0.573873	H	8.202376	-1.203967	-1.797325
H	3.722782	1.998516	0.867392	H	9.387139	0.124606	-1.881189
C	6.852139	0.860350	0.024373	H	7.810548	0.295219	-2.691846
H	7.189726	-0.987069	-1.104062	H	0.989463	-2.556738	1.598482
H	6.078984	2.595302	1.117601	C	-2.060481	0.152175	2.261146
N	8.170151	1.187039	0.152653	H	-2.393233	0.346489	3.298251
C	8.555653	2.404104	0.835995	H	-0.998189	0.439879	2.166665
H	8.236638	2.401545	1.894969	O	-2.849516	0.941428	1.357471
H	9.649192	2.502919	0.813254	C	-2.390244	2.274736	1.194712
H	8.124991	3.300004	0.351510	H	-1.397028	2.265157	0.702583
C	9.190413	0.320708	-0.400630	H	-2.268966	2.727133	2.197715
H	9.143580	-0.695268	0.032843	C	-3.345544	3.050377	0.403794
H	9.101081	0.227615	-1.499142	C	-4.124277	3.683674	-0.273364
H	10.181419	0.736941	-0.175625	C	-5.058074	4.416586	-1.128783
				H	-6.000611	4.632347	-0.598616
TS4				H	-5.289052	3.820987	-2.028014
C	-1.070217	-2.159296	1.964644	H	-4.616936	5.373809	-1.453907
C	-2.272494	-1.303759	1.798500	Cl	-3.335192	0.423363	-2.265794
Rh	-2.749382	-0.706322	-0.159747	C	-4.687929	-1.112452	0.043306
H	-3.132455	-1.751996	2.317064	O	-5.784242	-1.373946	0.085911
C	-0.722948	-0.643163	-0.643970	C	-1.928104	-2.074133	-1.124880
H	-0.430741	-0.049114	-1.519026	O	-1.637660	-2.988043	-1.756556
C	0.269331	-1.057240	0.197261				

TS4'

C	-3.688585	0.764514	1.285742
C	-2.300006	1.732375	0.116727
C	-1.728642	1.356897	-1.198189
C	-0.666721	0.472651	-1.357913
C	-3.741621	-0.517514	1.350717
Rh	-2.614215	-0.462171	-0.349240
Cl	-4.550935	-0.199664	-1.876941
H	-1.558010	1.751691	0.927211
H	-2.223695	1.745023	-2.094925
C	0.019242	-0.125806	-0.175683
C	-0.855914	-0.679809	0.676939
H	-0.622554	-1.186922	1.613609
O	1.380147	0.012370	-0.200886
C	2.194505	-0.560333	0.714302
O	1.786504	-1.202146	1.646179
C	-4.461418	2.009701	1.642318
H	-5.420858	1.971646	1.085271
H	-4.679299	2.002163	2.722835
C	-3.169304	2.982779	0.079571
O	-3.755184	3.160608	1.328700
H	-2.536421	3.862261	-0.121797
H	-3.927893	2.894004	-0.725743
C	-2.626275	-2.317496	-0.790474
O	-2.659808	-3.419903	-1.045734
C	-4.337874	-1.663289	2.087707
H	-4.898921	-1.324605	2.974038
H	-5.021982	-2.217464	1.422164
H	-3.549302	-2.362104	2.414153
H	-0.289249	0.280446	-2.370003
C	3.624927	-0.296415	0.424273
C	4.594642	-0.842396	1.286585
C	4.066300	0.471382	-0.670127
C	5.951768	-0.638063	1.073757
H	4.261520	-1.440379	2.139691
C	5.420595	0.688748	-0.898821
H	3.334373	0.907293	-1.354143
C	6.409987	0.138305	-0.031753
H	6.662148	-1.083975	1.770351
H	5.713523	1.291220	-1.759308
N	7.741709	0.345771	-0.250482
C	8.177890	1.142516	-1.377639
H	7.792661	2.177906	-1.323897
H	9.275127	1.191957	-1.385095
H	7.852332	0.706719	-2.340582
C	8.723322	-0.228441	0.645610
H	8.663793	-1.332586	0.668031
H	9.730683	0.047548	0.306259
H	8.601437	0.140475	1.681101

TS4"

C	-2.416438	-0.465372	1.630492
C	-3.271269	-0.454001	0.554828
H	-3.062763	0.258320	-0.258058
C	-0.842570	-1.059400	-0.838476
H	-0.126866	-1.562943	-1.498368
C	-0.341339	-0.431880	0.350526
H	-2.788041	-0.792443	2.612368
O	0.989299	-0.109893	0.350273
C	1.957700	-1.047804	0.169360
O	1.713731	-2.222516	0.110343
C	-1.031339	-0.156625	1.512011
C	3.303904	-0.440638	0.081386
C	3.528779	0.948689	0.126096
C	4.416643	-1.292593	-0.056465
C	4.813335	1.472322	0.037384
H	2.680330	1.629368	0.231637
C	5.706975	-0.787914	-0.145285
H	4.250375	-2.373095	-0.093509
C	5.947286	0.617940	-0.099943
H	4.937813	2.554788	0.075610
H	6.536120	-1.487791	-0.251641
N	7.211898	1.123680	-0.184387
C	8.343994	0.230395	-0.317214
H	8.287469	-0.371988	-1.243084
H	9.270079	0.819423	-0.354175
H	8.419507	-0.465976	0.538449
C	7.426693	2.555170	-0.144099
H	7.068605	2.998148	0.803875
H	8.501444	2.765013	-0.229145
H	6.913876	3.071358	-0.976955
H	-0.442331	0.134211	2.385631
C	-4.677924	-0.972276	0.590886
H	-4.788288	-1.781746	-0.165352
H	-4.892256	-1.423541	1.583785
O	-5.566810	0.071365	0.305484
C	-6.886696	-0.365156	0.165703
H	-6.969343	-1.109871	-0.655500

H	-7.233922	-0.874301	1.091140
C	-7.779741	0.767131	-0.119298
C	-8.529837	1.689303	-0.354174
C	-9.430156	2.809334	-0.639651
H	-8.860090	3.750223	-0.721041
H	-9.966607	2.651637	-1.590455
H	-10.177283	2.930545	0.162710
C	-2.142393	-1.398147	-1.105448
O	-2.963065	-1.800953	-1.834715

TS5

C	-1.222678	0.987292	-0.833313
C	-2.079597	1.621508	0.186598
Rh	-2.611534	-0.573311	-0.278629
H	-1.688796	1.579837	1.212646
C	-0.411825	-0.829912	1.748284
H	0.067413	-1.048995	2.708339
C	0.294713	-0.426549	0.675486
H	-1.396558	1.293937	-1.870118
O	1.654359	-0.436547	0.713096
C	2.363507	0.670099	0.337458
O	1.827421	1.730520	0.160582
C	-0.321347	-0.055382	-0.628692
C	3.806035	0.390170	0.212812
C	4.363443	-0.888391	0.412781
C	4.669536	1.449857	-0.129126
C	5.728226	-1.106257	0.274284
H	3.713536	-1.724927	0.681424
C	6.035236	1.250960	-0.272070
H	4.245465	2.446236	-0.283711
C	6.611111	-0.040831	-0.075573
H	6.114310	-2.112808	0.437083
H	6.662309	2.102637	-0.536933
N	7.950762	-0.248326	-0.216340
C	8.823026	0.849143	-0.581551
H	8.813119	1.653382	0.177558
H	9.853562	0.480326	-0.669857
H	8.537327	1.292367	-1.553140
C	8.510326	-1.565897	0.005728
H	8.097934	-2.311634	-0.698948
H	9.597963	-1.528625	-0.141366
H	8.319195	-1.924324	1.034062
H	0.223676	-0.405965	-1.514006
C	-2.525545	3.035379	-0.195765
H	-1.672148	3.720962	-0.073580
H	-2.855056	3.053854	-1.255312
O	-3.534340	3.436680	0.667451
C	-4.545391	2.492900	0.596012
H	-5.210082	2.602729	1.468195
H	-5.143221	2.623053	-0.329901
C	-3.977341	1.089837	0.585482
C	-4.383310	-0.132805	0.618067
C	-5.518466	-1.005291	1.010790
H	-6.326907	-0.426791	1.487166
H	-5.920254	-1.524137	0.123920
H	-5.154656	-1.763832	1.723803
C	-2.878163	-2.435888	-0.576152
O	-3.062546	-3.532515	-0.787098
Cl	-3.548246	-0.311070	-2.586503
C	-1.882153	-0.994342	1.590204
O	-2.566180	-1.371314	2.511649

TS5'

C	2.778096	1.697230	-0.879725
C	1.974022	2.078753	0.338138
C	1.881280	0.962648	1.352444
C	0.889138	0.002636	1.263668
C	2.885869	0.423856	-1.308683
Rh	2.717124	-0.932548	0.195283
Cl	3.824285	-1.858406	2.120107
H	0.946086	2.342393	0.015311
H	2.448183	1.044711	2.287555
C	0.228579	-0.258454	-0.038440
C	1.129836	-0.588036	-1.000200
H	0.858033	-0.931741	-2.003398
O	-1.123607	-0.365395	-0.174736
C	-1.922812	0.600813	0.353859
O	-1.472405	1.585271	0.879677
C	3.431004	2.971508	-1.390740
H	4.534611	2.861986	-1.431347
H	3.082498	3.263644	-2.398691
C	2.717841	3.360457	0.753182
O	3.050239	3.967479	-0.471073
H	2.101995	4.063876	1.333869
H	3.624730	3.105912	1.342379
C	3.556347	-2.358281	-0.772061
O	4.034197	-3.237689	-1.300266
C	3.570391	0.041416	-2.601264

H	3.606379	0.892017	-3.303538
H	4.606647	-0.296475	-2.421241
H	3.037777	-0.781710	-3.107682
H	0.603567	-0.587196	2.145232
C	-3.357983	0.293958	0.187892
C	-4.303439	1.221672	0.667275
C	-3.829221	-0.879807	-0.432146
C	-5.666785	0.997103	0.536760
H	-3.945752	2.135350	1.150655
C	-5.190449	-1.121155	-0.572735
H	-3.114177	-1.614759	-0.809922
C	-6.156047	-0.186949	-0.092334
H	-6.359659	1.744959	0.923296
H	-5.509152	-2.043634	-1.059030
N	-7.493695	-0.415594	-0.228923
C	-7.963104	-1.620163	-0.881466
H	-7.639772	-2.532038	-0.345708
H	-9.061035	-1.615733	-0.906463
H	-7.600916	-1.689482	-1.923900
C	-8.451598	0.544870	0.278793
H	-8.344046	1.531128	-0.209692
H	-9.469133	0.181083	0.083145
H	-8.347650	0.690624	1.369944

TS5-S1

C	-1.705024	0.220044	-0.948069
C	-2.587498	0.211688	0.233347
Rh	-1.523640	-1.725194	-0.191020
H	-2.397522	1.093790	0.878947
C	-0.431511	-0.200549	1.792475
H	0.060766	-0.231773	2.768421
C	0.266273	0.104475	0.649360
H	-2.087578	0.383391	-1.960063
O	1.599457	0.272740	0.758604
C	2.239716	1.288903	0.085807
O	1.623715	2.193387	-0.405222
C	-0.321706	0.079214	-0.696914
C	3.701146	1.117981	0.091512
C	4.345209	-0.010843	0.637554
C	4.496186	2.125147	-0.492690
C	5.727478	-0.135094	0.600632
H	3.751512	-0.806617	1.093868
C	5.878246	2.018447	-0.536377
H	4.004456	3.004062	-0.919612
C	6.541883	0.877508	0.009622
H	6.180885	-1.028037	1.031404
H	6.449736	2.822824	-0.999947
N	7.898154	0.759131	-0.033914
C	8.700697	1.798022	-0.647330
H	8.564019	2.771713	-0.142186
H	9.762706	1.527737	-0.575850
H	8.454211	1.929673	-1.717325
C	8.543520	-0.418166	0.510963
H	8.210741	-1.341205	0.001256
H	9.629958	-0.331939	0.377275
H	8.342748	-0.532318	1.592106
H	0.372016	0.068308	-1.540396
C	-4.085665	0.048023	0.054434
H	-4.300512	-0.553697	-0.852892
H	-4.488946	-0.499788	0.931527
O	-4.645080	1.323367	-0.039362
C	-6.042170	1.300254	-0.140561
H	-6.358952	0.737619	-1.044803
H	-6.486825	0.777923	0.733340
C	-6.575091	2.667209	-0.210556
C	-7.030095	3.788621	-0.267940
C	-7.572284	5.147777	-0.335373
H	-8.273755	5.333919	0.495168
H	-6.758618	5.889663	-0.268859
H	-8.108636	5.312337	-1.284976
C	-1.838319	-0.607477	1.675084
O	-2.597177	-0.929332	2.545737
Cl	-0.411258	-3.238013	-1.602171
C	-2.813872	-3.129001	0.110177
O	-3.590540	-3.949497	0.193103

TS5-S2

C	-2.133854	-1.349856	-0.288908
C	-2.811968	-2.240809	0.455525
Rh	-1.009161	1.444433	0.343577
H	-2.427611	-2.534404	1.441983
C	-0.423416	0.882538	-1.720712
H	0.258638	1.535686	-2.274831
C	0.059827	-0.002956	-0.648123
H	-2.538102	-1.101223	-1.277010
O	1.378182	-0.289738	-0.494883
C	2.390968	0.606998	-0.704014
O	2.188971	1.733323	-1.069099

C	-0.875913	-0.721547	0.157551	C	-0.589378	-0.239455	-0.772442
H	-0.395141	-1.221120	1.007682	C	-3.331039	0.691330	0.919155
C	-4.088409	-2.920121	0.014741	Rh	-2.742160	-0.867052	-0.372224
H	-3.870614	-3.978679	-0.222090	Cl	-2.521979	-2.347593	-2.233268
H	-4.809358	-2.937501	0.858172	H	-0.728227	2.258594	0.221069
O	-4.662941	-2.355645	-1.125788	H	-1.703095	0.793973	-2.269667
C	-5.471343	-1.234571	-0.882581	C	0.024626	-0.221539	0.583066
H	-4.941731	-0.485114	-0.260718	C	-0.729480	-0.281655	1.693364
H	-5.665900	-0.767712	-1.862018	H	-0.276539	-0.302823	2.689847
C	-6.760791	-1.565160	-0.237920	O	1.382168	-0.273997	0.669357
C	-7.819333	-1.820954	0.295726	C	2.139296	0.662164	0.028327
C	-9.104211	-2.123367	0.931939	O	1.643229	1.636783	-0.473520
H	-9.721137	-2.772446	0.288034	C	-3.514542	3.233026	0.534191
H	-8.955637	-2.635609	1.897427	H	-4.539509	3.172302	0.109140
H	-9.668202	-1.194647	1.122677	H	-3.601967	3.616344	1.567276
C	-0.985821	1.333461	2.268654	C	-2.014007	3.317431	-1.168670
O	-0.973621	1.229657	3.396323	O	-2.695443	4.089957	-0.216153
Cl	-1.565039	3.734679	0.413605	H	-1.150591	3.889795	-1.538484
C	-1.763880	1.156331	-1.824714	H	-2.670267	3.060363	-2.027987
O	-2.822186	1.388500	-2.231270	C	-2.192426	-0.592273	1.605433
C	3.710835	0.008435	-0.434103	O	-2.726229	-1.213994	2.501359
C	3.889005	-1.330675	-0.032104	C	-4.658675	0.655325	1.646651
C	4.855336	0.817009	-0.588916	H	-4.742150	1.483614	2.372217
C	5.156056	-1.846257	0.206982	H	-5.492701	0.747258	0.927734
H	3.018917	-1.979421	0.092764	H	-4.776300	-0.282904	2.207679
C	6.128398	0.319343	-0.353050	H	-0.239830	-1.005769	-1.474327
H	4.727485	1.857852	-0.899870	C	3.576834	0.339385	0.064573
C	6.321094	-1.035734	0.054402	C	4.486155	1.247901	-0.512786
H	5.243429	-2.888165	0.515648	C	4.087139	-0.836007	0.651068
H	6.981752	0.984996	-0.484676	C	5.851709	1.002377	-0.510622
N	7.566875	-1.535114	0.288045	H	4.098541	2.163005	-0.969758
C	8.731997	-0.687950	0.131951	C	5.450830	-1.098440	0.661930
H	8.701474	0.181317	0.814563	H	3.401864	-1.555378	1.106138
H	9.636104	-1.266792	0.363278	C	6.380548	-0.185593	0.079336
H	8.827379	-0.308616	-0.902067	H	6.514859	1.736138	-0.969306
C	7.732284	-2.913578	0.701981	H	5.799797	-2.020468	1.127325
H	7.335430	-3.618002	-0.052178	N	7.719713	-0.438292	0.086629
H	8.801074	-3.128140	0.834392	C	8.227745	-1.651702	0.693632
H	7.223150	-3.117726	1.662173	H	7.818380	-2.555759	0.206411
				H	9.320669	-1.679269	0.590910
TS6				H	7.986444	-1.704812	1.771538
C	-2.841250	1.873868	0.469149	C	8.643481	0.508634	-0.503906
C	-1.617206	2.038943	-0.397976	H	8.596772	1.494375	-0.004961
C	-1.375199	0.798934	-1.222180	H	9.668439	0.127739	-0.402158

H	8.443745	0.659938	-1.580777
C	-4.251896	-1.999632	0.103298
O	-5.105606	-2.698737	0.341687

TS6’

C	3.028543	2.107787	-0.061521
C	1.562818	2.504738	0.051599
C	0.945306	2.021981	1.345775
C	0.101341	0.980698	1.444624
C	3.606847	0.946543	-0.442433
H	0.991291	2.125559	-0.807590
H	1.195407	2.602213	2.243474
C	-0.265480	0.157113	0.269778
C	0.573752	-0.480475	-0.560018
H	0.082022	-0.954064	-1.422944
O	-1.626464	0.175938	-0.032613
C	-2.469735	-0.492053	0.779586
O	-2.081381	-1.162741	1.702837
C	3.822345	3.351924	0.328552
H	4.557849	3.162440	1.129205
H	4.379282	3.721449	-0.561817
C	1.700048	4.044696	0.055309
O	2.882808	4.289130	0.767401
H	1.774446	4.421886	-0.986035
H	0.866983	4.559119	0.558251
C	5.125301	0.875585	-0.521393
H	5.562584	0.710305	0.478629
H	5.473741	0.044954	-1.150499
H	5.536601	1.814736	-0.930964
H	-0.382467	0.749442	2.401263
C	-3.891274	-0.302493	0.402928
C	-4.881903	-0.971101	1.146421
C	-4.301126	0.525782	-0.658822
C	-6.231306	-0.824834	0.850764
H	-4.571711	-1.617047	1.972895
C	-5.647170	0.686376	-0.968831
H	-3.550087	1.055358	-1.250069
C	-6.658263	0.015171	-0.220163
H	-6.961419	-1.365347	1.453976
H	-5.916522	1.341336	-1.798026
N	-7.982483	0.170925	-0.515584
C	-8.385977	1.019670	-1.616657
H	-7.969268	0.670358	-2.579763
H	-9.480979	1.010820	-1.701509
H	-8.066119	2.067983	-1.467384
C	-8.987076	-0.514157	0.270250
H	-8.936289	-0.230471	1.337843
H	-9.985419	-0.246527	-0.101221
H	-8.883978	-1.613573	0.204569
Rh	2.560056	-0.990710	-0.279757
C	2.341434	-1.177146	1.768132
O	2.324911	-1.295286	2.886674
C	2.934415	-0.052259	-1.884188
O	3.010849	0.314762	-2.974089
Cl	4.671197	-2.228474	0.124223
C	1.975493	-2.820816	-0.719971
O	1.684100	-3.869022	-1.011994

TS7

C	4.572142	0.280478	-0.155521
C	3.867325	-0.985796	0.224715
C	2.939595	-1.570992	-0.706641
C	1.673016	-1.060270	-0.948310
C	4.054713	1.527481	-0.164546
H	3.179723	-2.553505	-1.133872
C	1.124068	-0.139894	-0.035746
C	1.890331	0.577234	0.927318
H	1.283526	0.902919	1.784304
O	-0.228014	-0.012247	0.070964
C	-1.088125	-1.075199	0.128629
O	-0.710989	-2.208419	0.240212
C	6.020421	-0.105149	-0.413373
H	6.325814	0.078753	-1.459673
H	6.689333	0.489294	0.243877
C	5.035523	-1.867917	0.671633
O	6.120586	-1.477080	-0.137721
H	5.256905	-1.701411	1.746337
H	4.848770	-2.943225	0.521260
C	4.834165	2.757083	-0.556604
H	5.775511	2.501085	-1.066353
H	4.234387	3.391756	-1.230304
H	5.068182	3.374102	0.328660
H	1.007786	-1.575136	-1.643925
C	-2.497237	-0.633393	0.067371
C	-3.510776	-1.608227	0.149526
C	-2.877796	0.715894	-0.071149
C	-4.853648	-1.260989	0.094721
H	-3.223630	-2.658103	0.258285

C	-4.216961	1.081983	-0.128183
H	-2.108796	1.489766	-0.133485
C	-5.250931	0.102583	-0.046582
H	-5.602316	-2.050743	0.162190
H	-4.463648	2.138552	-0.235636
N	-6.567462	0.455142	-0.100662
C	-6.941605	1.846751	-0.245252
H	-6.546135	2.283293	-1.181114
H	-8.036436	1.928422	-0.271557
H	-6.575700	2.460523	0.598737
C	-7.596121	-0.560317	-0.011527
H	-7.538617	-1.120141	0.940330
H	-8.584053	-0.083261	-0.062813
H	-7.528033	-1.289115	-0.840574
C	2.733720	1.758927	0.460896
O	2.331162	2.881281	0.685544
H	2.936785	-0.399728	1.059719

TS7'

C	-2.984373	1.140893	0.143010
C	-1.926090	2.260561	-0.086825
C	-1.051221	2.098893	-1.296955
C	-0.001376	1.258768	-1.322994
C	-3.034578	0.515445	1.477235
H	-1.268144	2.327682	0.794678
H	-1.232360	2.749416	-2.161261
C	0.297846	0.282951	-0.269633
C	-0.586408	-0.490428	0.431726
H	-0.070394	-1.225417	1.063495
O	1.630830	-0.004222	-0.109474
C	2.508183	0.998214	0.178432
O	2.137029	2.101962	0.474231
C	-4.285538	1.743489	-0.441513
H	-4.722841	1.127521	-1.239483
H	-5.051449	1.860168	0.351488
C	-2.860757	3.476297	-0.217122
O	-3.934603	2.996965	-0.971491
H	-3.189427	3.816673	0.788093
H	-2.404206	4.330396	-0.741899
C	-4.260943	0.409111	2.372979
H	-5.115639	0.040115	1.786186
H	-4.087010	-0.295971	3.200596
H	-4.507705	1.396288	2.801356
H	0.701348	1.275698	-2.165050
C	3.914965	0.550230	0.107499
C	4.929938	1.477304	0.414905
C	4.293245	-0.757585	-0.252990
C	6.271349	1.124651	0.362963
H	4.644670	2.494617	0.697938
C	5.631241	-1.129406	-0.309500
H	3.524435	-1.496648	-0.491357
C	6.666780	-0.196608	-0.004416
H	7.020271	1.878240	0.607708
H	5.875253	-2.154322	-0.590247
N	7.982377	-0.552298	-0.061528
C	8.355651	-1.896289	-0.450846
H	7.986225	-2.146702	-1.462470
H	9.450446	-1.981702	-0.462277
H	7.963349	-2.653549	0.253425
C	9.011188	0.412675	0.267370
H	8.908734	0.784855	1.303545
H	9.997668	-0.061401	0.176812
H	8.990186	1.284555	-0.412675
Rh	-2.565469	-0.881097	-0.080919
C	-1.826325	0.091514	2.061778
O	-1.248817	-0.239145	3.016940
C	-2.234398	-1.006649	-2.004740
O	-2.102264	-1.055873	-3.125930
C	-2.395570	-2.861481	0.408403
O	-2.364296	-3.962221	0.653039
Cl	-4.904930	-1.502945	-0.525747

TS-I (CF_3)

C	-0.250081	1.857582	0.315043
C	0.345994	1.508331	-0.855885
Rh	0.266127	-0.696131	0.593840
H	-0.245782	1.117202	-1.691767
C	-1.733059	-0.770243	-0.103926
C	-2.314202	0.421537	-0.027941
H	0.329541	2.341315	1.104440
O	-3.568547	0.838403	-0.558852
C	-3.594553	2.119857	-0.583811
O	-2.593777	2.701601	-0.060685
C	-1.715161	1.669084	0.571511
Cl	-0.510046	-0.197491	2.938572
C	2.023076	-0.575404	1.380327
O	3.011950	-0.519625	1.934674
H	-1.926639	1.748644	1.649614

C	1.787972	1.786931	-1.175121
H	2.212995	0.920317	-1.718964
H	1.825297	2.651765	-1.875355
O	2.505355	2.061768	-0.011758
C	3.855301	2.375804	-0.218061
H	3.953678	3.227267	-0.921980
H	4.253662	2.703018	0.756085
C	4.662344	1.240878	-0.719824
C	5.332455	0.316728	-1.132970
C	6.147789	-0.798674	-1.623046
H	7.220163	-0.584833	-1.477205
H	5.906859	-1.726633	-1.077683
H	5.974512	-0.973247	-2.698173
C	0.806868	-2.016672	-0.605644
O	1.168972	-2.844817	-1.311025
C	-4.727635	2.858209	-1.169128
H	-4.422061	3.885874	-1.407073
H	-5.102134	2.323890	-2.054705
H	-5.531077	2.882548	-0.408656
C	-2.421660	-1.955321	-0.710476
F	-3.720404	-1.781892	-0.983618
F	-1.839909	-2.303684	-1.867109
F	-2.348384	-3.021566	0.090485

TS-II (CF_3)

C	-1.302755	0.954707	0.274373
C	-2.456796	0.890783	-0.399300
Rh	1.130306	-1.547618	0.117209
H	-2.514942	1.248882	-1.436652
C	2.360600	0.908628	-0.397021
C	1.149419	0.594780	-0.279331
H	-1.212174	0.585581	1.303063
O	2.320090	2.990584	-0.448411
C	1.386022	3.394205	0.228505
O	0.245827	2.745544	0.359336
C	-0.048882	1.520704	-0.331973
H	-0.205689	1.760110	-1.399661
C	-3.733995	0.356545	0.183588
H	-3.550271	-0.098908	1.177717
H	-4.444112	1.198592	0.329943
O	-4.272654	-0.584623	-0.707211
C	-5.472447	-1.160381	-0.278073
H	-5.690183	-1.991769	-0.968886
H	-5.359963	-1.594162	0.737030
C	-6.620949	-0.223890	-0.271252
C	-7.568228	0.535464	-0.257545
C	-8.717009	1.446444	-0.240966
H	-9.016511	1.723175	-1.265751
H	-9.580376	0.968779	0.252452
H	-8.476453	2.370583	0.311150
C	1.402617	-1.946995	-1.690542
O	1.570223	-2.169857	-2.795036
C	0.953849	-3.389933	0.587186
O	0.827511	-4.469571	0.913050
Cl	0.772059	-1.015427	2.456821
C	1.427891	4.664173	1.025345
H	0.500162	5.236748	0.873847
H	1.495520	4.396034	2.094346
H	2.307902	5.253735	0.736752
C	3.851166	0.831913	-0.496543
F	4.437705	1.379211	0.554323
F	4.291911	1.447865	-1.578818
F	4.222309	-0.439501	-0.564197

TS-I (CO_2Me)

C	0.221791	-1.934900	0.003750
C	-0.333945	-1.326127	-1.078949
Rh	-0.244407	0.524364	0.756235
H	0.289974	-0.795063	-1.807095
C	1.779712	0.683526	0.139111
C	2.317754	-0.522140	0.014175
H	-0.394214	-2.553605	0.659950
O	3.576973	-0.845636	-0.582640
C	3.577370	-2.091036	-0.875511
O	2.556120	-2.748176	-0.496809
C	1.684553	-1.851665	0.327725
Cl	0.424645	-0.487930	2.972663
C	-2.033163	0.303332	1.446560
O	-3.043347	0.171129	1.947327
H	1.861855	-2.168331	1.367688
C	-1.773627	-1.497367	-1.479721
H	-2.164520	-0.531778	-1.856370
H	-1.813266	-2.212529	-2.332091
O	-2.528112	-1.969257	-0.405699
C	-3.879167	-2.200094	-0.694796
H	-3.980635	-2.897404	-1.551315
H	-4.308683	-2.697474	0.190054
C	-4.647613	-0.968378	-0.983892

C	-5.287775	0.034656	-1.224539
C	-6.065113	1.245267	-1.505898
H	-6.996822	1.255589	-0.915542
H	-5.484717	2.145876	-1.243501
H	-6.330884	1.305531	-2.574618
C	-0.684533	2.109400	-0.116234
O	-0.984820	3.098047	-0.613793
C	4.703615	-2.724417	-1.585827
H	4.341062	-3.591130	-2.156323
H	5.204610	-1.988606	-2.230122
H	5.418225	-3.076984	-0.818466
C	2.555716	1.909686	-0.190020
O	3.503962	2.317467	0.433547
O	2.046467	2.546119	-1.241942
C	2.652050	3.775311	-1.609112
H	2.096304	4.145305	-2.480942
H	2.585890	4.503211	-0.784790
H	3.711517	3.627929	-1.873210

TS-II (CO_2Me)

C	-1.260908	0.942678	0.350371
C	-2.409590	0.943755	-0.335652
Rh	0.989969	-1.595316	0.142922
H	-2.444288	1.346156	-1.357765
C	2.412382	0.858898	-0.372824
C	1.192425	0.549135	-0.208454
H	-1.192668	0.531296	1.364634
O	2.327545	2.944095	-0.435118
C	1.455656	3.341030	0.321315
O	0.324247	2.692943	0.516615
C	0.012867	1.502682	-0.220812
H	-0.132083	1.784010	-1.280787
C	-3.710546	0.427868	0.209422
H	-3.555869	-0.069756	1.188125
H	-4.396868	1.285588	0.377131
O	-4.264852	-0.462220	-0.723732
C	-5.504201	-0.989240	-0.348110
H	-5.732197	-1.801425	-1.058214
H	-5.450397	-1.440224	0.664228
C	-6.609773	-0.002451	-0.372784
C	-7.526715	0.793154	-0.388747
C	-8.636579	1.751146	-0.409035
H	-8.895585	2.033748	-1.443221
H	-9.532654	1.313326	0.062505
H	-8.372918	2.667990	0.144725
C	1.246471	-1.948532	-1.672011
O	1.421568	-2.140568	-2.781885
C	0.634567	-3.420143	0.549964
O	0.398303	-4.493070	0.838378
Cl	0.738383	-1.123531	2.516314
C	1.569572	4.587956	1.147494
H	0.632968	5.163731	1.099170
H	1.735425	4.289445	2.197657
H	2.420353	5.187082	0.797412
C	3.850296	0.568006	-0.572536
O	4.213294	-0.569982	-0.718508
O	4.621480	1.622527	-0.570623
C	6.015210	1.393661	-0.765372
H	6.487165	2.383956	-0.751627
H	6.417305	0.767391	0.046088
H	6.191706	0.899518	-1.733297

TS-I (H), TS-V (H)

C	0.936396	1.129160	-0.746766
C	0.212609	1.425690	0.366000
Rh	-0.025143	-1.165391	0.086836
H	0.672956	1.386516	1.359847
C	1.870575	-1.193228	0.988121
H	2.252875	-1.770065	1.841558
C	2.660878	-0.271678	0.456674
H	0.501493	1.276002	-1.737895
O	3.950355	0.155163	0.932573
C	4.205126	1.300205	0.430137
O	3.363849	1.733970	-0.422251
C	2.360049	0.655545	-0.692029
Cl	0.920360	-1.888747	-2.143021
C	-1.720839	-1.190456	-0.849622
O	-2.676109	-1.277656	-1.457949
H	2.659703	0.239879	-1.667001
C	-1.168792	2.019140	0.333130
H	-1.776743	1.571074	1.143546
H	-1.083436	3.105438	0.562409
O	-1.761064	1.825809	-0.914600
C	-3.026592	2.408711	-1.056314
H	-2.981658	3.495193	-0.837348
H	-3.307908	2.295533	-2.115964
C	-4.069057	1.791416	-0.205428
C	-4.931663	1.296633	0.490854

C	-5.978409	0.698943	1.325274
H	-5.730165	0.793528	2.395793
H	-6.943969	1.203385	1.151296
H	-6.103178	-0.371679	1.091516
C	-0.735547	-1.755221	1.693388
O	-1.125045	-2.146954	2.700828
C	5.411113	2.065913	0.801075
H	5.240012	3.137043	0.625534
H	5.679563	1.859936	1.846906
H	6.234797	1.722219	0.147736

TS-II (H)

C	0.699550	1.068317	-0.222412
C	1.873051	0.870689	0.388599
Rh	-1.900199	-1.240010	0.019880
H	2.012406	1.180864	1.433675
C	-2.914104	1.314120	0.625973
H	-3.992536	1.343786	0.735664
C	-1.740349	0.885851	0.441784
H	0.525622	0.744543	-1.256022
O	-2.698512	3.342829	0.750441
C	-1.771100	3.707538	0.042398
O	-0.690189	2.986844	-0.169289
C	-0.471632	1.713344	0.467433
H	-0.234324	1.906932	1.529242
C	3.062974	0.233857	-0.271218
H	2.796719	-0.140818	-1.280263
H	3.860397	0.996974	-0.398798
O	3.518493	-0.812577	0.546844
C	4.635618	-1.488685	0.047688
H	4.770801	-2.385186	0.675494
H	4.454853	-1.836219	-0.990524
C	5.884023	-0.690260	0.072702
C	6.914797	-0.048902	0.086920
C	8.161258	0.722955	0.106750
H	8.517865	0.922412	-0.917777
H	8.007895	1.691567	0.611972
H	8.951677	0.176390	0.648250
C	-2.190043	-1.593793	1.825157
O	-2.378880	-1.781240	2.934416
C	-1.900799	-3.090182	-0.456695
O	-1.873037	-4.176986	-0.785046
Cl	-1.575989	-0.758537	-2.345816
C	-1.762821	5.008327	-0.706703
H	-0.791395	5.510816	-0.583557
H	-1.901131	4.787815	-1.779776
H	-2.583605	5.645698	-0.352466

TS-I (Me)

C	-0.769777	1.409031	0.605146
C	-0.077752	1.477104	-0.560241
Rh	0.076059	-1.078019	0.197465
H	-0.572059	1.261429	-1.514632
C	-1.850207	-1.193263	-0.660328
C	-2.567736	-0.140079	-0.278241
H	-0.298746	1.712310	1.542719
O	-3.864834	0.241821	-0.783977
C	-4.074345	1.460069	-0.478893
O	-3.190709	2.009468	0.258589
C	-2.202515	0.965253	0.677752
Cl	-0.852481	-1.310606	2.534722
C	1.793743	-0.973143	1.089548
O	2.762917	-0.961326	1.682213
H	-2.470842	0.733669	1.720604
C	1.327244	1.999523	-0.674013
H	1.888304	1.375357	-1.397380
H	1.283462	3.025042	-1.105422
O	1.950302	2.016520	0.573665
C	3.248374	2.541566	0.572314
H	3.253323	3.567555	0.150658
H	3.558121	2.615771	1.627471
C	4.228961	1.714894	-0.167157
C	5.043085	1.050103	-0.774569
C	6.029850	0.243714	-1.499300
H	6.080064	0.538199	-2.560978
H	7.032697	0.371169	-1.057768
H	5.768345	-0.826679	-1.448822
C	0.753907	-1.994137	-1.264154
O	1.151866	-2.603712	-2.153868
C	-5.274463	2.190954	-0.933425
H	-5.014001	3.243548	-1.118788
H	-5.694071	1.711803	-1.828081
H	-6.016808	2.154436	-0.114613
C	-2.388793	-2.219178	-1.626756
H	-3.445162	-2.057921	-1.903446
H	-1.785655	-2.220751	-2.552737
H	-2.291248	-3.230410	-1.194057

TS-II (Me)

C	-0.780782	1.008585	0.254346
C	-1.952693	0.865053	-0.375087
Rh	1.621729	-1.368822	0.015722
H	-2.065589	1.194537	-1.417468
C	2.860256	1.208639	-0.493899
C	1.671635	0.767279	-0.341489
H	-0.636829	0.665608	1.286274
O	2.678710	3.182919	-0.597215
C	1.728291	3.594627	0.059274
O	0.629782	2.906545	0.236484
C	0.423406	1.625973	-0.404728
H	0.211450	1.830880	-1.469766
C	-3.177590	0.272826	0.261599
H	-2.938123	-0.138794	1.262977
H	-3.935623	1.072758	0.403404
O	-3.682822	-0.728763	-0.583104
C	-4.846585	-1.344180	-0.112623
H	-5.028723	-2.217441	-0.760901
H	-4.702602	-1.723507	0.920187
C	-6.041261	-0.467265	-0.136109
C	-7.022466	0.247742	-0.148007
C	-8.211493	1.105524	-0.165688
H	-8.529664	1.360395	0.859202
H	-8.002565	2.045102	-0.704680
H	-9.050486	0.600054	-0.672984
C	1.917401	-1.652108	-1.794796
O	2.119717	-1.793403	-2.910053
C	1.486730	-3.228375	0.412089
O	1.389035	-4.326129	0.690885
Cl	1.337364	-0.961137	2.406329
C	1.732702	4.917813	0.765081
H	0.765087	5.424129	0.631291
H	1.876103	4.727300	1.843505
H	2.558820	5.536241	0.390017
C	4.316962	1.135390	-0.607819
H	4.588354	0.065710	-0.613222
H	4.661881	1.594892	-1.547834
H	4.813071	1.623957	0.246086

TS-I (Ph)

C	0.410636	2.095470	0.058820
C	0.825222	1.457178	-1.066097
Rh	0.389619	-0.448365	0.735348
H	0.099150	1.079003	-1.794902
C	-1.644034	-0.212744	0.126867
C	-1.919077	1.090316	0.050062
H	1.141861	2.552619	0.729480
O	-3.125310	1.707219	-0.437430
C	-2.892860	2.943330	-0.652646
O	-1.738264	3.358293	-0.311455
C	-1.035728	2.254950	0.418886
Cl	-0.053437	0.560686	3.007011
C	2.197237	-0.608855	1.396166
O	3.223564	-0.696626	1.875182
H	-1.130790	2.535322	1.479876
C	2.263443	1.360886	-1.491111
H	2.452965	0.348854	-1.900297
H	2.428256	2.077956	-2.326791
O	3.113070	1.644911	-0.422490
C	4.477756	1.604437	-0.734984
H	4.706451	2.294047	-1.573140
H	5.014561	1.973771	0.154030
C	4.972753	0.251851	-1.077770
C	5.388072	-0.852226	-1.364669
C	5.896960	-2.183950	-1.706227
H	6.977987	-2.139167	-1.921555
H	5.741840	-2.889210	-0.872609
H	5.385894	-2.583617	-2.598196
C	0.496050	-2.006185	-0.271245
O	0.542455	-2.981696	-0.874635
C	-3.908108	3.841731	-1.236244
H	-3.412210	4.667364	-1.765891
H	-4.580570	3.276757	-1.896572
H	-4.496203	4.260075	-0.397928
C	-2.619951	-1.275486	-0.229390
C	-2.643880	-2.467940	0.526933
C	-3.515157	-1.163478	-1.317505
C	-3.550626	-3.492490	0.233297
H	-1.936684	-2.580715	1.354973
C	-4.406737	-2.198626	-1.625019
H	-3.502177	-0.266904	-1.942639
C	-4.435832	-3.363735	-0.846278
H	-3.556907	-4.401390	0.843379
H	-5.082402	-2.093409	-2.480079
H	-5.136386	-4.169978	-1.085438

TS-II (Ph)

C	1.524583	0.970591	-0.315555	H	-7.372358	-0.010320	0.140089
C	2.702629	0.940220	0.318028				
Rh	-0.711857	-1.535860	0.009229	**TS-IV (CF_3)**			
H	2.789760	1.331127	1.341473	C	2.160321	-0.282026	1.165433
C	-2.130045	0.981228	0.344431	C	1.219911	-1.794444	0.081017
C	-0.907013	0.606710	0.270733	C	0.605150	-1.776435	-1.264134
H	1.406242	0.569008	-1.329710	C	-0.694146	-1.361827	-1.524225
O	-2.079204	2.950477	0.406819	C	1.741470	0.928958	1.120250
C	-1.137658	3.406720	-0.235993	Rh	0.757906	0.334853	-0.573198
O	0.005873	2.787809	-0.367643	Cl	2.708754	0.740852	-2.040908
C	0.281943	1.540385	0.315280	H	0.505470	-1.992169	0.891860
H	0.472401	1.793066	1.374327	H	1.233972	-2.066065	-2.113615
C	3.967081	0.398830	-0.285144	C	-1.599471	-0.924283	-0.426600
H	3.761408	-0.080845	-1.263462	C	-1.010761	-0.038428	0.387563
H	4.670378	1.239413	-0.468135	O	-2.852833	-1.468116	-0.387458
O	4.533122	-0.519655	0.613505	C	-3.939549	-0.689352	-0.644255
C	5.743839	-1.071501	0.184550	O	-3.846278	0.454174	-0.980513
H	5.979218	-1.897364	0.876280	C	3.301556	-1.150598	1.628527
H	5.640644	-1.508936	-0.829922	H	4.201949	-0.846244	1.055689
C	6.873112	-0.111578	0.177474	H	3.481006	-0.958023	2.698858
C	7.806891	0.664338	0.166340	C	2.467231	-2.662869	0.181363
C	8.935937	1.599799	0.154180	O	3.031772	-2.498765	1.443336
H	8.578534	2.638369	0.257119	H	2.175354	-3.720421	0.077536
H	9.629724	1.391581	0.985941	H	3.180967	-2.407468	-0.628312
H	9.497200	1.523631	-0.792338	C	0.147756	2.057011	-1.158558
C	-0.743401	-1.761356	1.854289	O	-0.157259	3.090462	-1.500360
O	-0.763678	-1.871444	2.990563	C	1.829823	2.273012	1.749406
C	-0.422990	-3.388539	-0.327406	H	2.436510	2.239774	2.668814
O	-0.228118	-4.481606	-0.571735	H	2.285261	2.986767	1.041512
Cl	-0.679728	-1.183702	-2.403336	H	0.822031	2.645393	1.996805
C	-1.213235	4.708378	-0.975565	H	-1.080493	-1.428899	-2.548697
H	-0.269717	5.263998	-0.870830	C	-5.208000	-1.470737	-0.447259
H	-1.364232	4.479048	-2.045592	H	-6.068157	-0.859942	-0.750812
H	-2.064816	5.295721	-0.607278	H	-5.169015	-2.403868	-1.031596
C	-3.556574	0.757071	0.287436	H	-5.295104	-1.743252	0.618111
C	-4.431791	1.358480	1.215468	C	-1.612129	0.639154	1.570975
C	-4.062324	-0.111352	-0.705036	F	-1.679157	1.965818	1.389985
C	-5.799735	1.084089	1.153772	F	-2.850790	0.227929	1.864961
H	-4.031965	2.041799	1.969325	F	-0.883669	0.449221	2.677958
C	-5.431917	-0.391607	-0.744680				
H	-3.369961	-0.558259	-1.425979	**TS-III (CF_3)**			
C	-6.300144	0.205826	0.179726	C	-1.210384	-2.247228	-1.908451
H	-6.479913	1.552409	1.871462	C	0.154045	-1.679588	-1.872886
H	-5.822684	-1.071825	-1.507392	Rh	0.816013	-0.997603	-0.009688

H	0.869717	-2.384865	-2.317622
C	-1.170494	-0.346478	0.512845
C	-2.219187	-0.595577	-0.349944
H	-1.376490	-3.152909	-2.506118
O	-3.395738	0.094346	-0.299555
C	-3.441108	1.408582	-0.650849
O	-2.478440	1.987004	-1.064220
C	-2.287091	-1.694095	-1.298122
H	-3.296393	-2.068345	-1.500422
C	0.300625	-0.287510	-2.518417
H	0.640289	-0.318941	-3.569472
H	-0.647443	0.274730	-2.461642
O	1.290078	0.384664	-1.720265
C	1.131323	1.800720	-1.708416
H	0.199804	2.057038	-1.165797
H	1.024618	2.144990	-2.754314
C	2.292300	2.449403	-1.094612
C	3.240359	3.016696	-0.594692
C	4.378370	3.688884	0.036321
H	5.245161	3.727174	-0.644262
H	4.676574	3.154149	0.953828
H	4.109212	4.722048	0.313778
Cl	2.091446	-0.004294	1.865905
C	2.475001	-2.038709	-0.176317
O	3.419018	-2.654347	-0.200398
C	-0.364138	-1.928822	1.101662
O	-0.856677	-2.684967	1.819159
C	-1.272771	0.701888	1.607609
F	-2.522281	1.113704	1.864334
F	-0.811895	0.225881	2.762553
F	-0.575843	1.799207	1.316447
C	-4.820332	1.964629	-0.454581
H	-4.855596	2.998957	-0.820166
H	-5.554430	1.338934	-0.987211
H	-5.065052	1.932667	0.620335

TS-IV (H)

C	-1.705537	0.915402	1.146092
C	-0.537652	1.688187	-0.385286
C	0.012335	1.042917	-1.598535
C	1.187049	0.300142	-1.613875
C	-1.551420	-0.288769	1.564237
Rh	-0.559451	-0.576479	-0.198490
Cl	-2.629363	-1.060880	-1.502820
H	0.235607	2.021065	0.320965
H	-0.571237	1.114124	-2.523113
C	2.003707	0.138081	-0.377301
C	1.266800	-0.267783	0.667011
H	1.619302	-0.461500	1.681052
O	3.331919	0.436663	-0.553011
C	4.256927	0.289883	0.415664
O	3.999494	-0.081669	1.526441
C	-2.625914	2.106372	1.221560
H	-3.597864	1.801331	0.781094
H	-2.785123	2.369227	2.280115
C	-1.577114	2.765420	-0.662569
O	-2.104962	3.203834	0.550223
H	-1.086006	3.625294	-1.146036
H	-2.364737	2.376247	-1.339908
C	-0.319552	-2.469853	-0.098957
O	-0.211315	-3.594646	-0.027447
C	-1.895281	-1.247019	2.648601
H	-2.445920	-0.747762	3.462515
H	-2.516113	-2.064002	2.242297
H	-0.979082	-1.700944	3.062579
H	1.544383	-0.107116	-2.567950
C	5.624845	0.657986	-0.099328
H	6.363614	0.539184	0.704143
H	5.884650	0.011493	-0.953792
H	5.616743	1.700596	-0.457526

TS-III (H)

C	1.799275	-1.222493	1.896548
C	0.353241	-0.885102	1.867571
Rh	-0.596563	-0.882175	-0.001899
H	-0.192022	-1.491784	2.604577
C	1.167638	-0.240927	-0.903158
H	1.097366	0.215396	-1.898903
C	2.365083	-0.137767	-0.254450
H	2.160306	-1.840914	2.728675
O	3.394150	0.493853	-0.912184
C	3.993439	1.563417	-0.338014
O	3.580778	2.066625	0.668679
C	2.718441	-0.786906	0.999342
H	3.785011	-0.974400	1.165687
C	0.068589	0.615018	2.087060
H	-0.142903	0.882760	3.138676
H	0.909148	1.230447	1.720797

O	-1.094751	0.884449	1.286598
C	-1.232793	2.244126	0.903108
H	-0.442514	2.506579	0.172295
H	-1.090596	2.876393	1.799719
C	-2.561984	2.485174	0.334074
C	-3.655508	2.707386	-0.140824
C	-4.970161	2.961550	-0.734761
H	-5.766669	2.901259	0.025515
H	-5.183733	2.222202	-1.524928
H	-4.999735	3.966950	-1.187658
Cl	-1.857672	-0.453072	-2.085740
C	-2.195172	-1.875194	0.691724
O	-3.091412	-2.472229	1.024249
C	0.518186	-2.060483	-0.921348
O	1.028221	-2.928656	-1.474667
C	5.185933	2.006457	-1.139534
H	4.881636	2.193832	-2.182111
H	5.612657	2.914988	-0.695107
H	5.936684	1.198535	-1.149595

TS-VI (H)

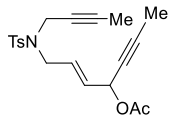
C	-0.752281	-2.189567	-0.340846
C	-1.833314	-1.553168	0.224400
C	-1.873465	-0.176690	0.622842
Rh	-0.914699	1.489360	-0.115332
C	-1.261905	0.841753	-1.826240
O	-1.461912	0.446329	-2.877841
Cl	-0.359182	2.366655	2.094409
C	-0.287076	3.197134	-0.783894
O	0.047114	4.223761	-1.132530
C	-0.818985	-0.386512	2.616880
O	0.090128	-0.820487	3.128017
H	-0.888928	-3.247136	-0.600791
C	0.551140	-1.620690	-0.563495
C	1.541735	-2.357423	-1.123166
H	-2.795123	0.075432	1.168885
H	0.741853	-0.581543	-0.275340
H	1.360145	-3.403490	-1.403012
C	2.917056	-1.847266	-1.396216
H	3.639093	-2.482148	-0.835243
H	3.148898	-2.006433	-2.473628
O	3.033833	-0.505586	-1.046199
C	4.308713	0.040395	-1.244866
H	4.655633	-0.143851	-2.282002
H	4.206960	1.130526	-1.118538
C	5.326690	-0.466046	-0.296553
C	6.167644	-0.873119	0.478528
C	7.182744	-1.355881	1.419544
H	7.699200	-0.509858	1.903477
H	6.716001	-1.968120	2.209604
H	7.937149	-1.974154	0.904694
O	-2.932653	-2.362161	0.478381
C	-4.123490	-1.993705	-0.041253
O	-4.255558	-1.003312	-0.706275
C	-5.203184	-2.976000	0.320272
H	-5.270604	-3.060060	1.417314
H	-6.161493	-2.640736	-0.097191
H	-4.940983	-3.970413	-0.077287

TS-V (R)

C	-0.782935	0.490320	-1.041511
C	-1.160290	1.114493	0.104782
Rh	-2.335420	-1.244028	0.150154
H	-0.585138	0.978000	1.027972
C	-0.452282	-1.899620	0.799472
H	-0.169018	-2.525059	1.657719
C	0.525574	-1.351845	0.088226
H	-1.300096	0.708248	-1.978454
O	1.924145	-1.397600	0.349860
C	2.493741	-0.432576	-0.299112
O	1.708412	0.221504	-1.091065
C	0.391595	-0.448853	-1.111805
Cl	-2.067405	-2.340390	-2.119180
C	-4.052535	-0.688896	-0.554343
O	-5.057562	-0.449683	-1.027778
C	3.867867	-0.108653	-0.135152
C	4.674428	-0.822701	0.792236
C	4.456531	0.943396	-0.887884
C	6.003715	-0.502998	0.965695
H	4.235290	-1.635662	1.377613
C	5.784510	1.273217	-0.722804
H	3.848193	1.498904	-1.607560
C	6.611593	0.562187	0.214518
H	6.587797	-1.074543	1.687013
H	6.199139	2.087203	-1.317424
N	7.907461	0.882703	0.382643
C	8.509302	1.956937	-0.393174
H	8.448153	1.751730	-1.476057

H	8.013839	2.923064	-0.192693	H	0.729830	-1.384874	1.057890
H	9.567803	2.048110	-0.119408	H	-2.305527	0.609347	-0.286702
C	8.728227	0.161858	1.344295	H	-1.769307	3.290049	-1.748590
H	8.317448	0.248527	2.365218	C	-3.831174	2.565168	-1.483893
H	8.801345	-0.909327	1.087243	H	-4.167049	3.508063	-0.997130
H	9.739644	0.586705	1.342899	H	-4.065288	2.683698	-2.566113
H	0.356953	-1.014679	-2.056650	O	-4.473110	1.453489	-0.946728
C	-2.239231	2.159569	0.179128	C	-5.866902	1.460391	-1.084960
H	-2.832460	2.005756	1.102116	H	-6.153334	1.609676	-2.146027
H	-1.751700	3.155873	0.276559	H	-6.217286	0.459351	-0.785210
O	-3.047637	2.118108	-0.956983	C	-6.543558	2.482335	-0.254435
C	-4.051794	3.092738	-0.995563	C	-7.107244	3.319175	0.420495
H	-3.615067	4.107346	-0.892716	C	-7.794352	4.321267	1.240708
H	-4.512184	3.030470	-1.995162	H	-7.696973	5.327660	0.800124
C	-5.100052	2.916335	0.035181	H	-8.868512	4.082737	1.319943
C	-5.966465	2.786318	0.875573	H	-7.373726	4.346430	2.260022
C	-7.019511	2.622022	1.882242	O	1.825509	0.675739	0.068476
H	-7.982193	3.002171	1.500670	C	2.695691	-0.232210	-0.434736
H	-7.149924	1.556435	2.135752	O	2.315972	-1.243812	-0.972748
H	-6.773837	3.170238	2.807186	C	4.104804	0.165857	-0.252080
C	-2.954384	-1.517086	1.872938	C	5.117578	-0.686338	-0.739288
O	-3.297612	-1.735766	2.948614	C	4.490425	1.362299	0.387681
				C	6.461176	-0.367555	-0.599602
TS-VI (R)				H	4.830839	-1.617546	-1.237055
C	-0.282571	1.392910	-0.625129	C	5.830119	1.699260	0.536912
C	0.472341	0.403100	-0.039965	H	3.726798	2.041196	0.775800
C	-0.040542	-0.816503	0.515745	C	6.863714	0.842395	0.046935
Rh	-1.670273	-1.978558	0.030786	H	7.209500	-1.057138	-0.992213
C	-1.317521	-1.611792	-1.759338	H	6.080646	2.634547	1.038982
O	-1.100681	-1.393137	-2.858153	N	8.177319	1.163837	0.189245
Cl	-2.179860	-2.480899	2.362738	C	8.559831	2.400719	0.843328
C	-2.990404	-3.331907	-0.398820	H	8.200957	2.438641	1.888215
O	-3.731317	-4.165528	-0.607081	H	9.654897	2.479366	0.856004
C	-0.770484	-0.004506	2.497101	H	8.159128	3.284013	0.312893
O	-1.441545	0.775447	2.963878	C	9.204444	0.272154	-0.315014
H	0.266557	2.257880	-1.018521	H	9.148893	-0.724091	0.160570
C	-1.719094	1.428403	-0.715355	H	9.124262	0.132743	-1.408773
C	-2.350847	2.459572	-1.327101	H	10.192157	0.699057	-0.097013

S8. Copies of NMR Spectra



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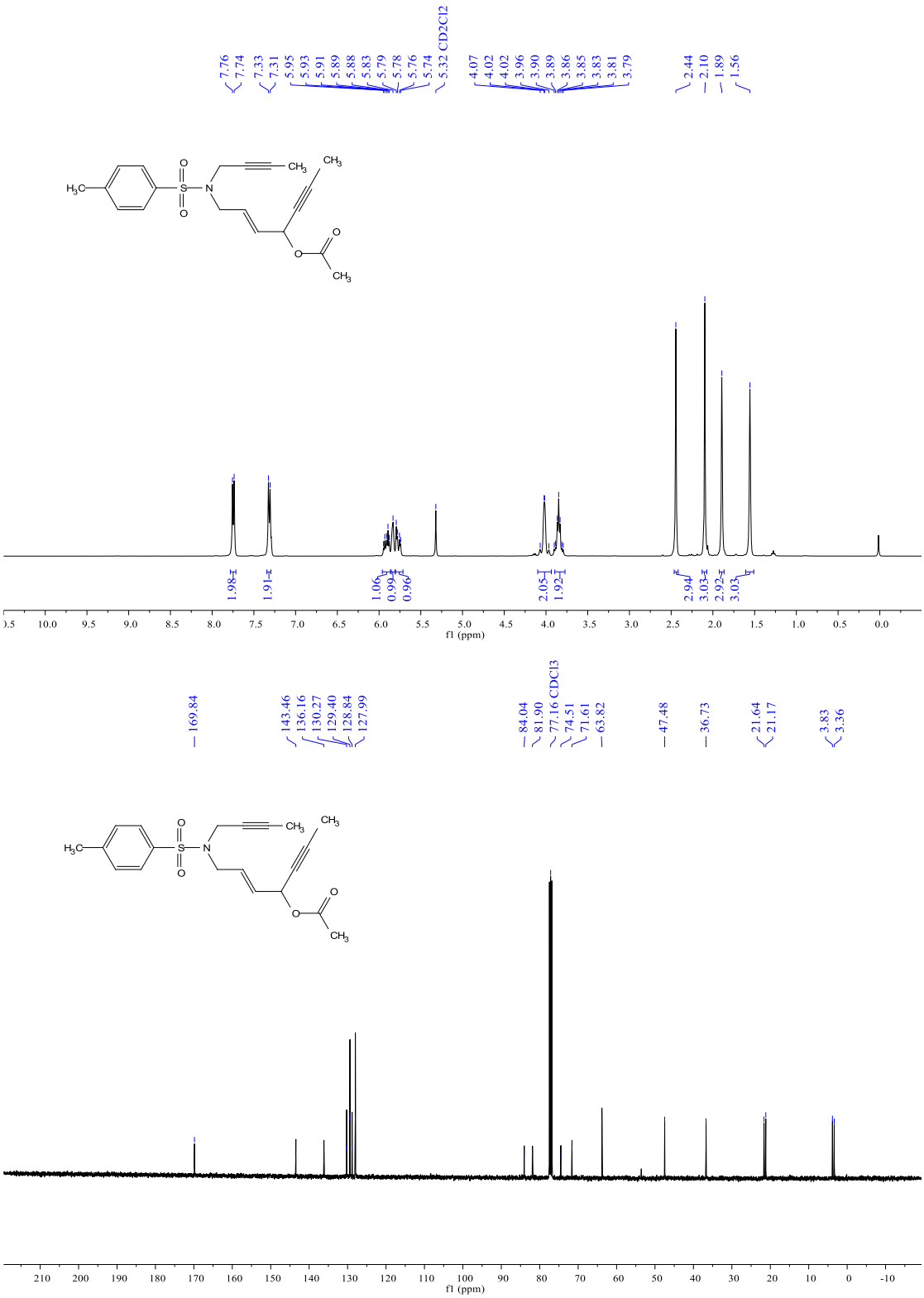

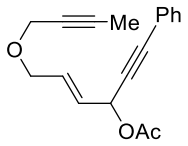
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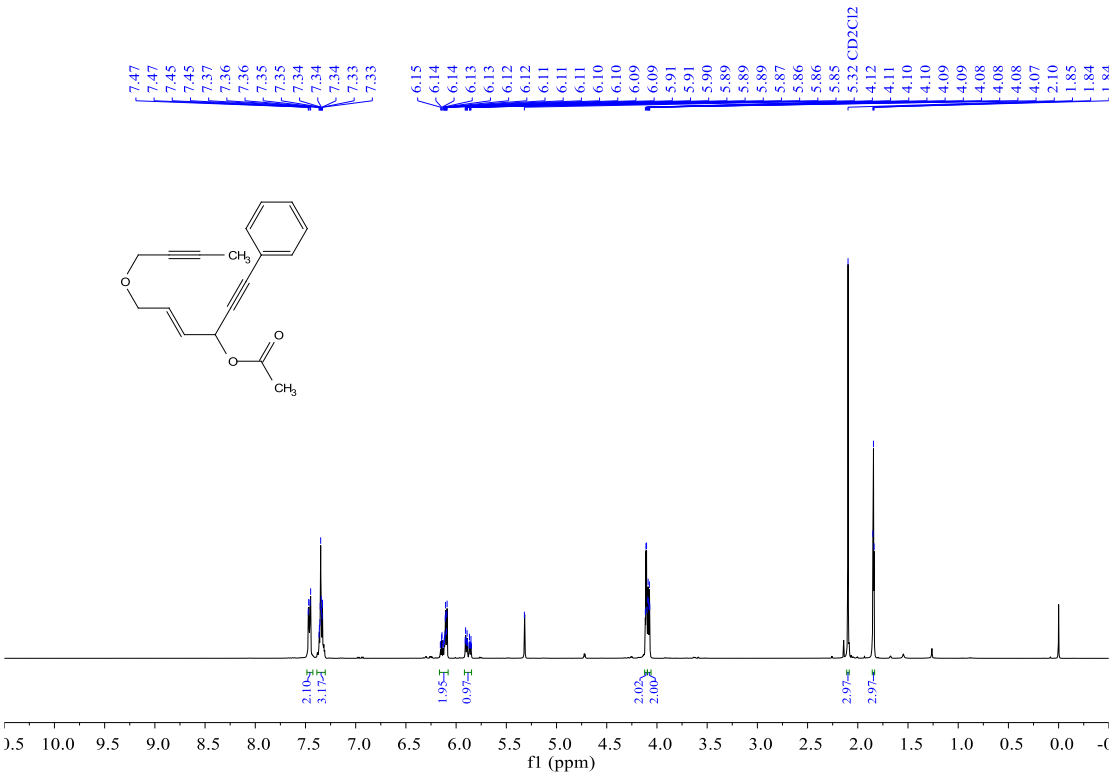
Ph
O
OAc

1b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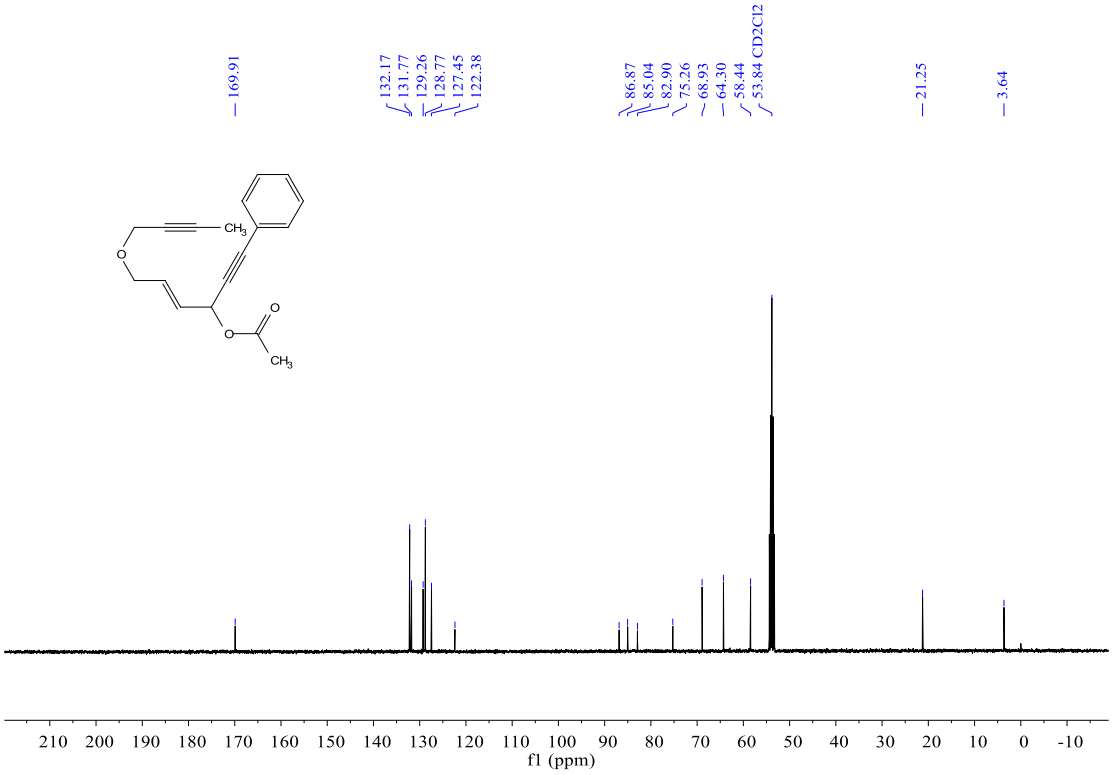
7.33
6.15
6.14
6.14
6.13
6.13
6.12
6.12
6.11
6.11
6.11
6.10
6.10
6.09
6.09
5.91
5.90
5.89
5.89
5.87
5.86
5.86
5.85
5.85
5.32 CD2Cl2
4.12
4.11
4.10
4.10
4.09
4.09
4.08
4.08
4.08
4.07
2.10
1.85
1.84
CH3
O
O
O
CH3
2.10
3.17
1.95
0.97
2.02
2.00
2.97
2.97
f1 (ppm)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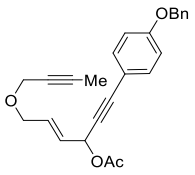
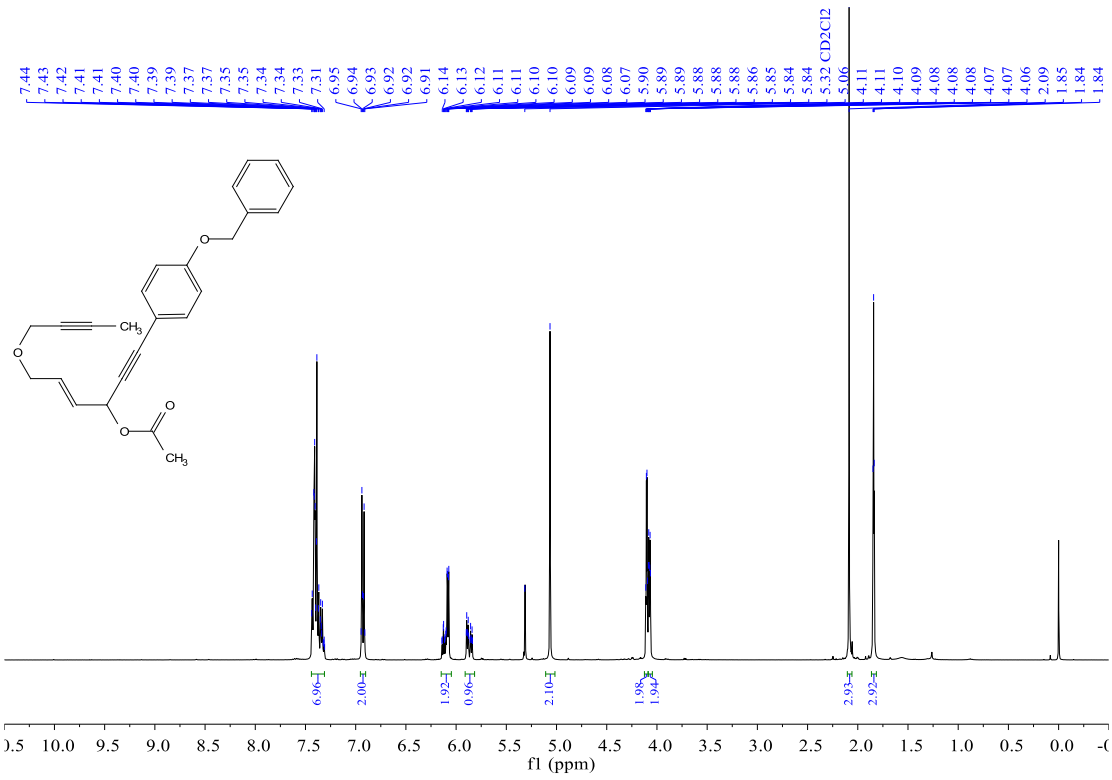
128.77
127.45
122.38
86.87
85.04
82.90
75.26
68.93
64.30
58.44
53.84 CD2Cl2
21.25
3.64
CH3
O
O
O
CH3
f1 (ppm)


OBn
Me
O
OAc

1c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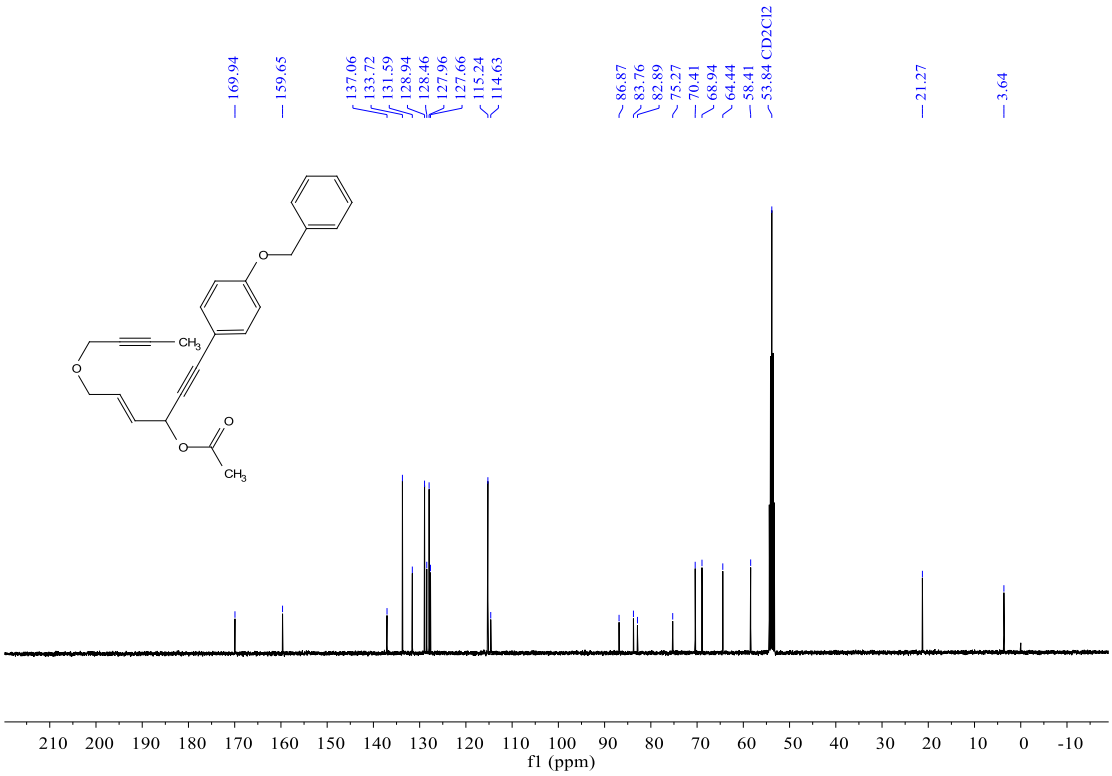
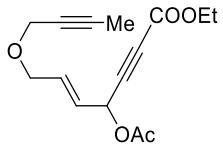
6.96 2.00 1.92 0.96 2.10 1.98 1.94 2.93 2.92
fl (ppm)


169.94 159.65 137.06 133.72 131.59 128.94 128.46 127.96 127.66 115.24 114.63 86.87 83.76 82.89 75.27 70.41 68.94 64.44 58.41 53.84 CD2Cl2 21.27 3.64
fl (ppm)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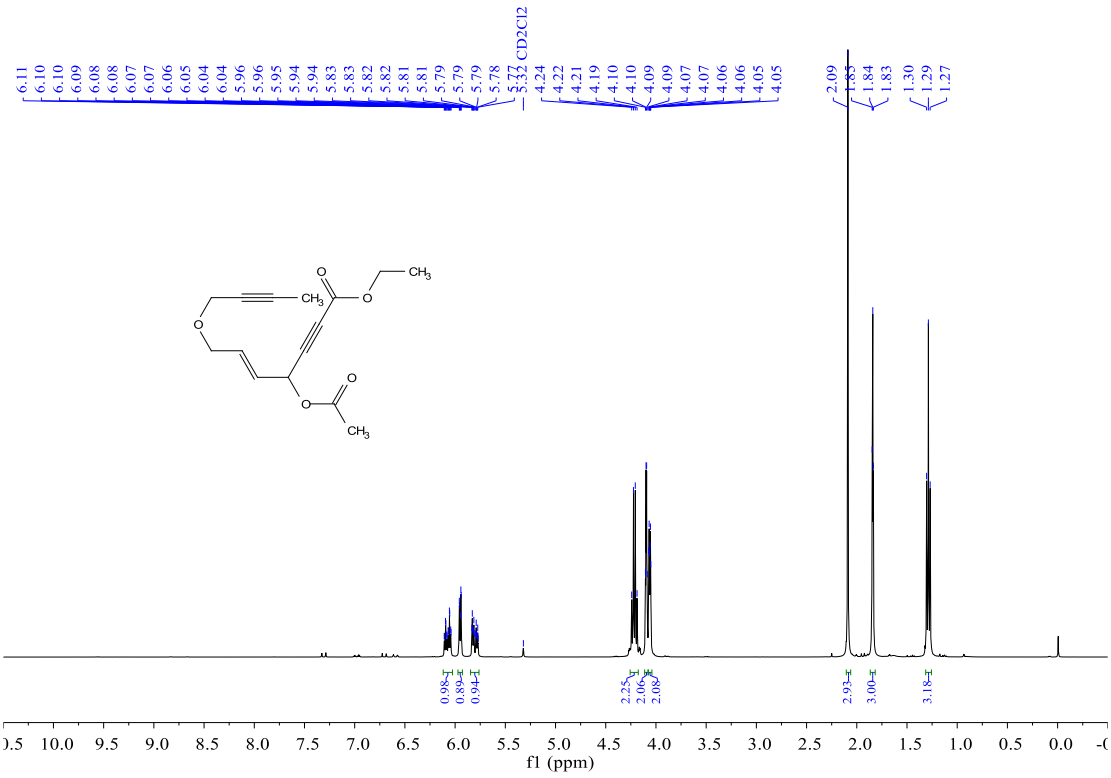
COOEt
O
OAc

1d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6.08
6.07
6.07
6.06
6.05
6.04
6.04
5.96
5.96
5.95
5.94
5.94
5.83
5.83
5.82
5.82
5.81
5.81
5.79
5.79
5.79
5.78
5.77
5.32 CD2Cl2
4.24
4.22
4.21
4.19
4.10
4.10
4.09
4.09
4.07
4.07
4.06
4.06
4.05
4.05
2.09
1.85
1.84
1.83
1.30
1.29
1.27
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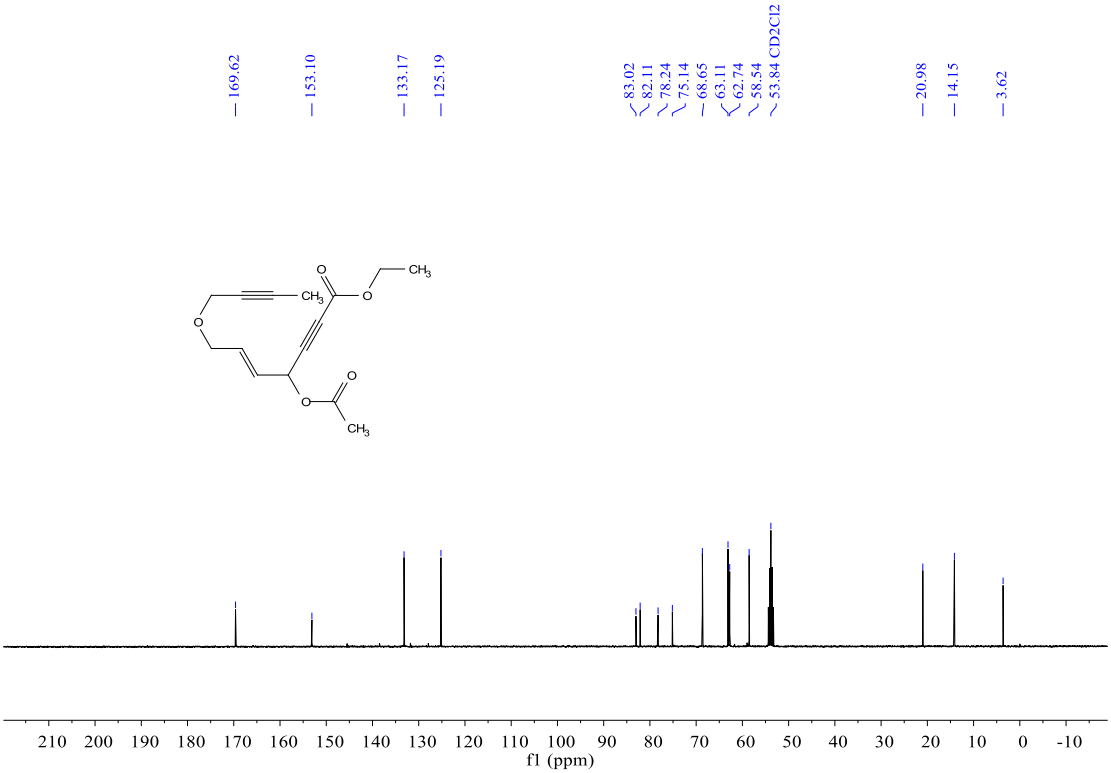
0.89
0.94
2.25
2.06
2.02
2.93
3.00
3.18
f1 (ppm)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153.10
133.17
125.19
83.02
82.11
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75.14
68.65
63.11
62.74
58.54
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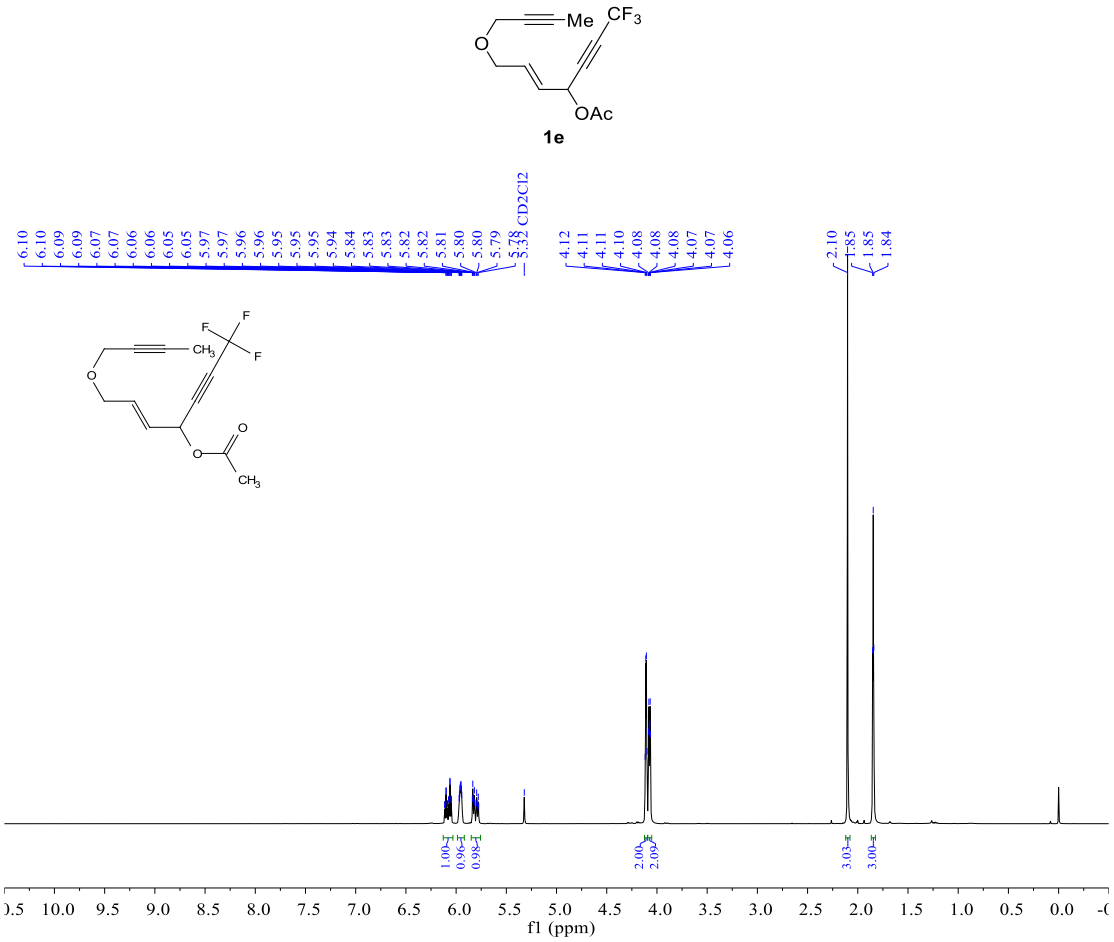
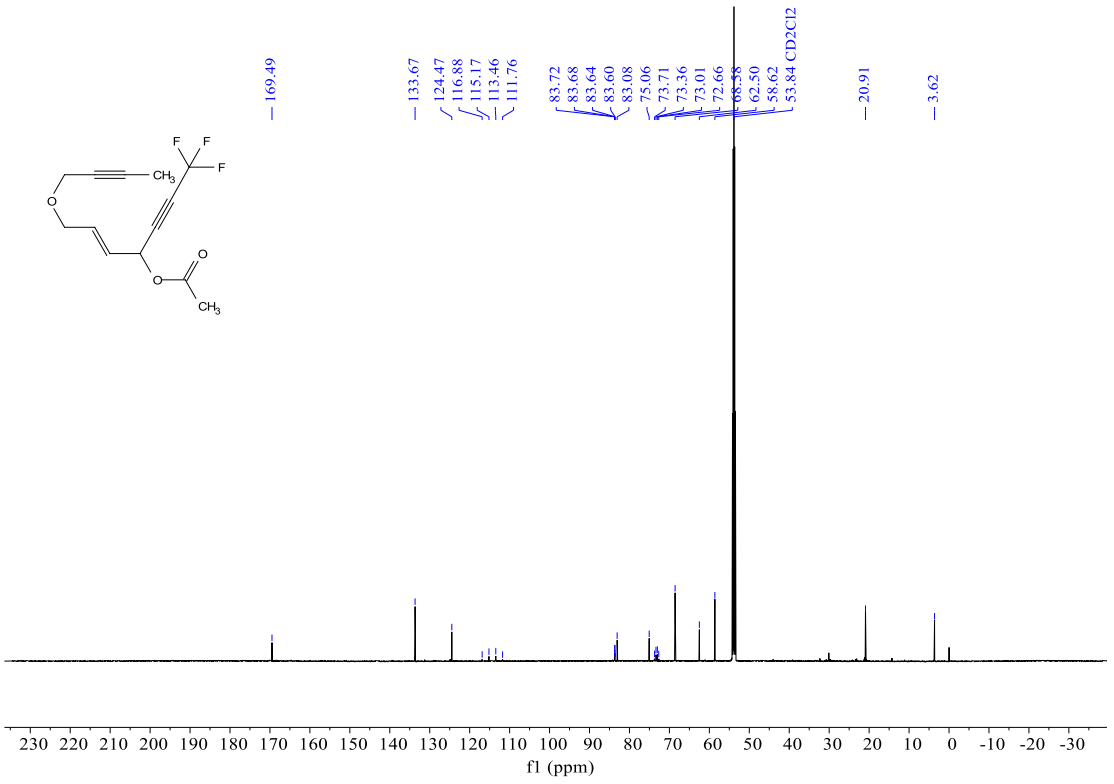
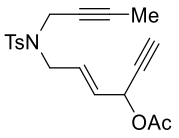
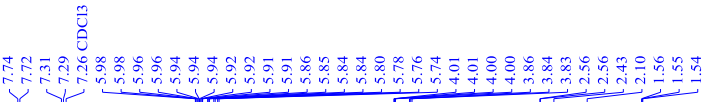
20.98
14.15
3.62
f1 (ppm)


Me
CF3
O
OAc
1e
CD2Cl2
f1 (ppm)


CD2Cl2
f1 (ppm)


Me
TsN
OAc

1f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7.72
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7.29
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5.98
5.98
5.96
5.96
5.94
5.94
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5.92
5.92
5.91
5.91
5.86
5.85
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5.84
5.80
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5.76
5.74
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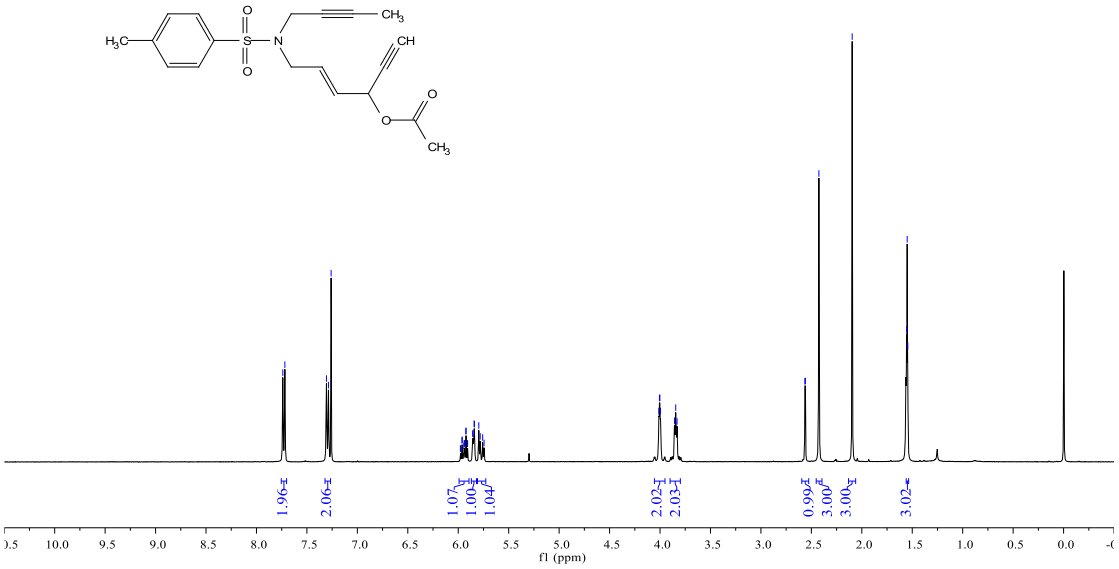
1.56
1.55
1.54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O
CH3
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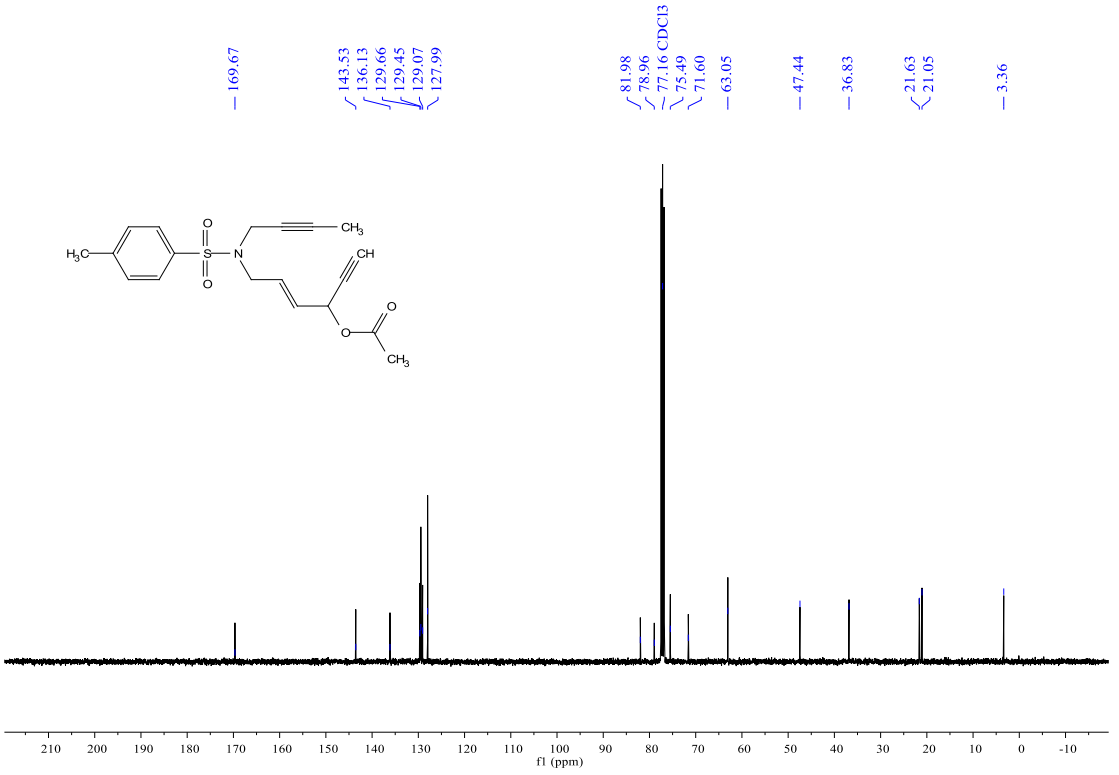
1.04
2.02
2.03
0.99
3.00
3.00
3.02
f1 (ppm)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129.45
129.07
127.99
81.98
78.96
77.16 CDCl3
75.49
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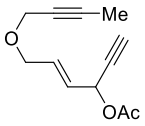
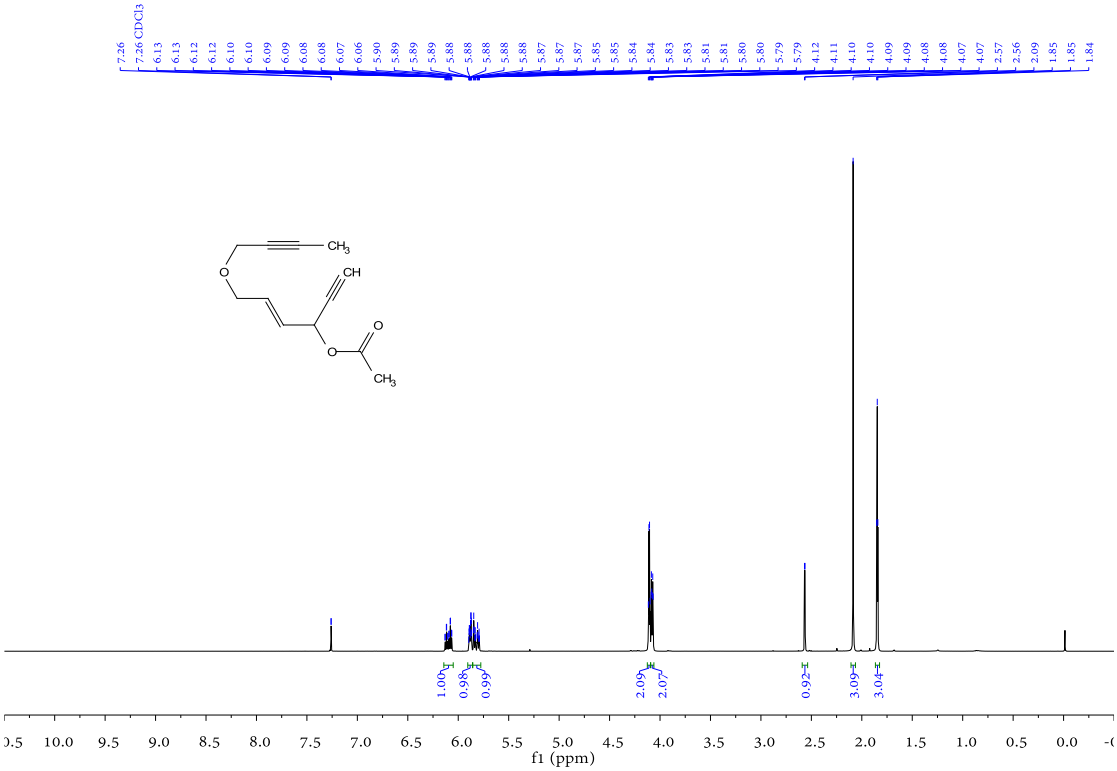
47.44
36.83
21.63
21.05
3.36
CH3
CH
O
O
CH3
f1 (ppm)


Me
O
OAc

1g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6.12
6.12
6.10
6.10
6.09
6.09
6.08
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6.08
6.07
6.06
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5.84
5.83
5.83
5.81
5.81
5.80
5.80
5.79
5.79
4.12
4.11
4.10
4.10
4.09
4.09
4.08
4.08
4.07
4.07
2.57
2.56
2.09
1.85
1.85
1.84
CH3
CH
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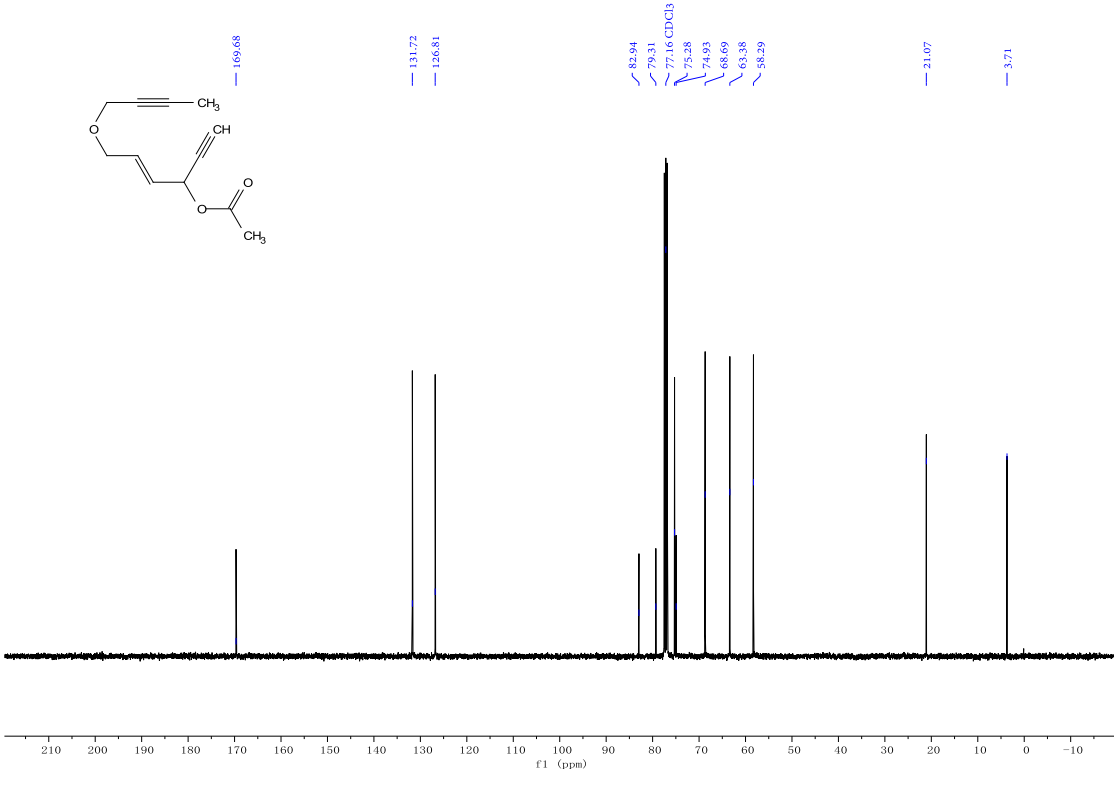
O
O
CH3
1.00
0.98
0.99
2.09
2.07
0.92
3.09
3.04
f1 (ppm)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79.31
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58.29
21.07
3.71
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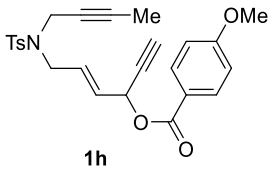
CH
O
O
O
CH3
f1 (ppm)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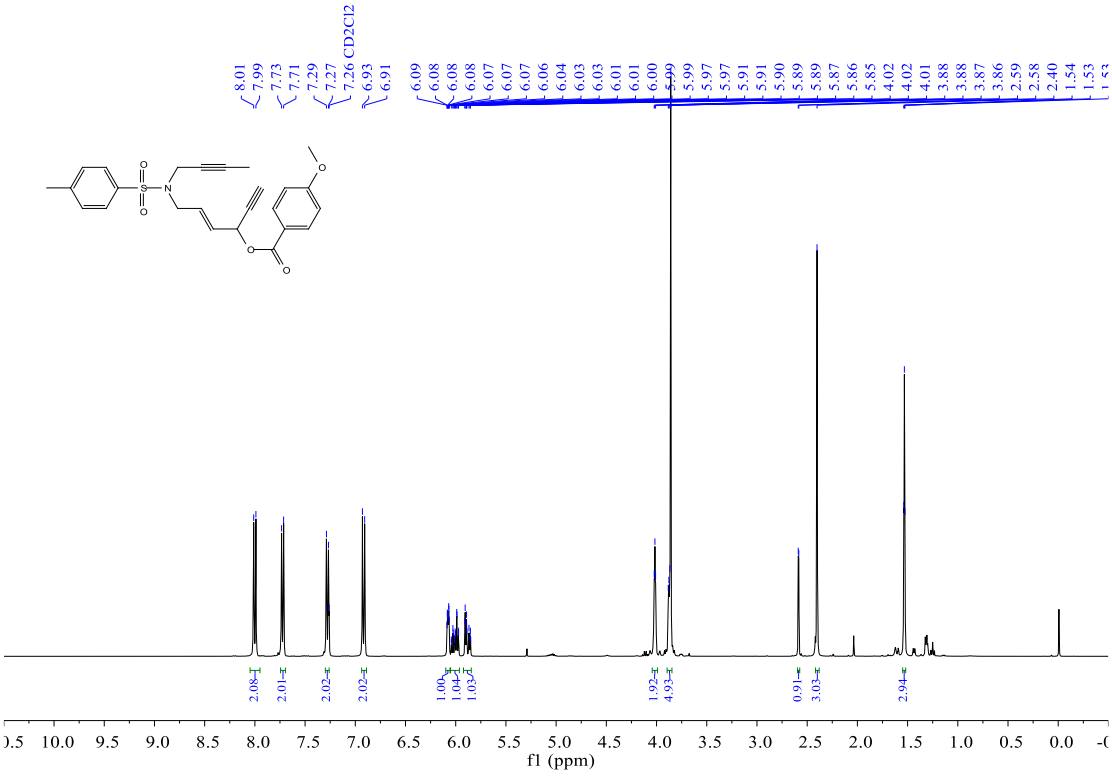
OMe
TsN
O
O

1h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6.09
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6.07
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5.91
5.90
5.89
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5.87
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5.85
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4.02
4.01
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3.88
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2.58
2.40
1.54
1.53
2.08
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1.03
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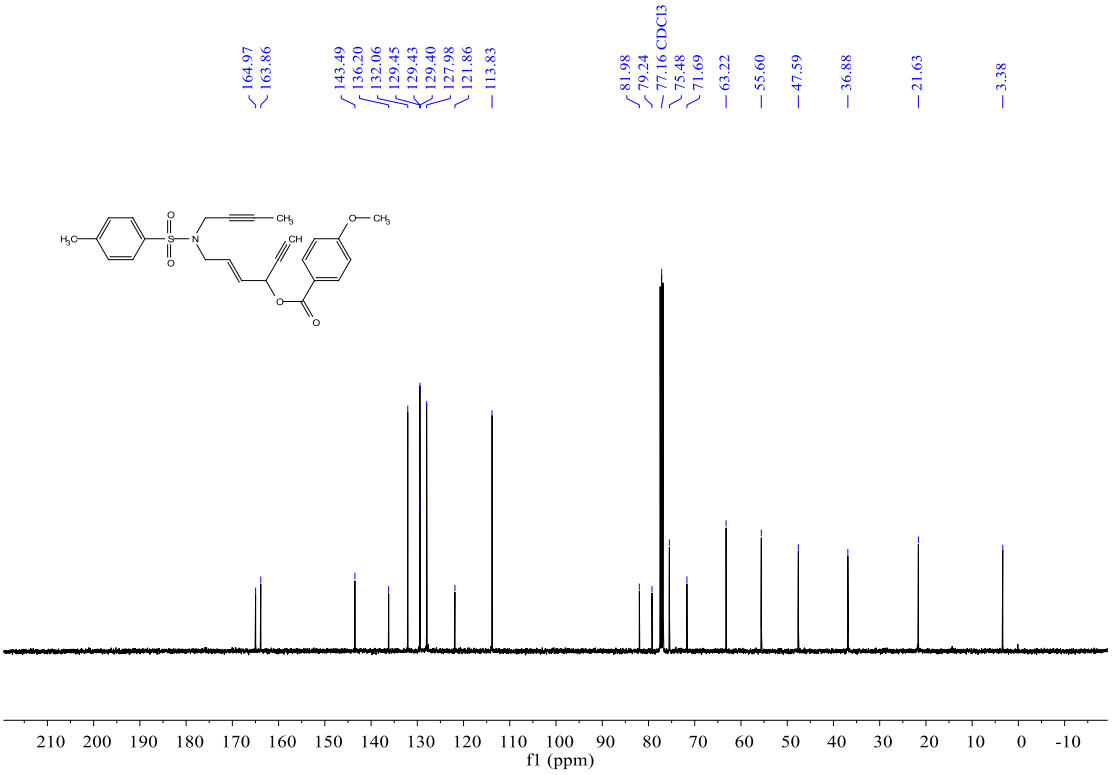
f1 (ppm)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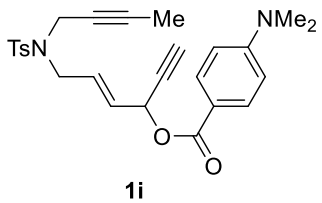
f1 (ppm)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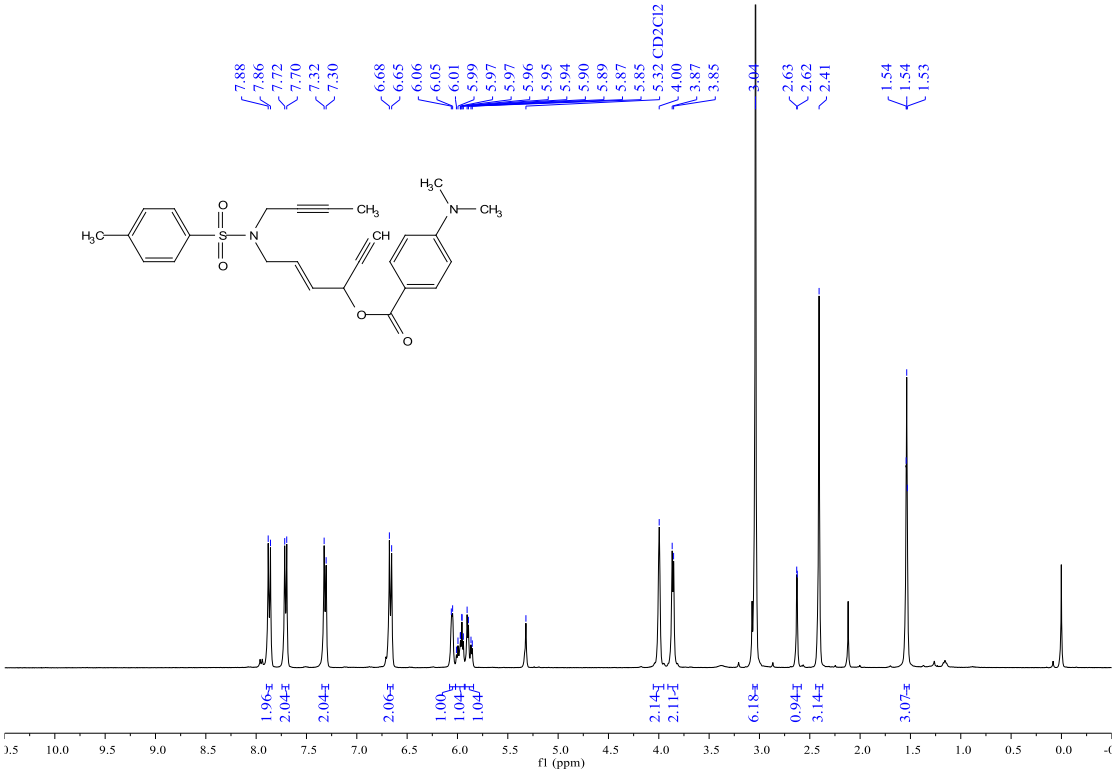
NMe2
TsN
O
O

1i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6.05
6.01
5.99
5.97
5.97
5.96
5.95
5.94
5.90
5.89
5.87
5.85
5.32 CD2Cl2
4.00
3.87
3.85
3.04
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2.62
2.41
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1.54
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1.96
2.04
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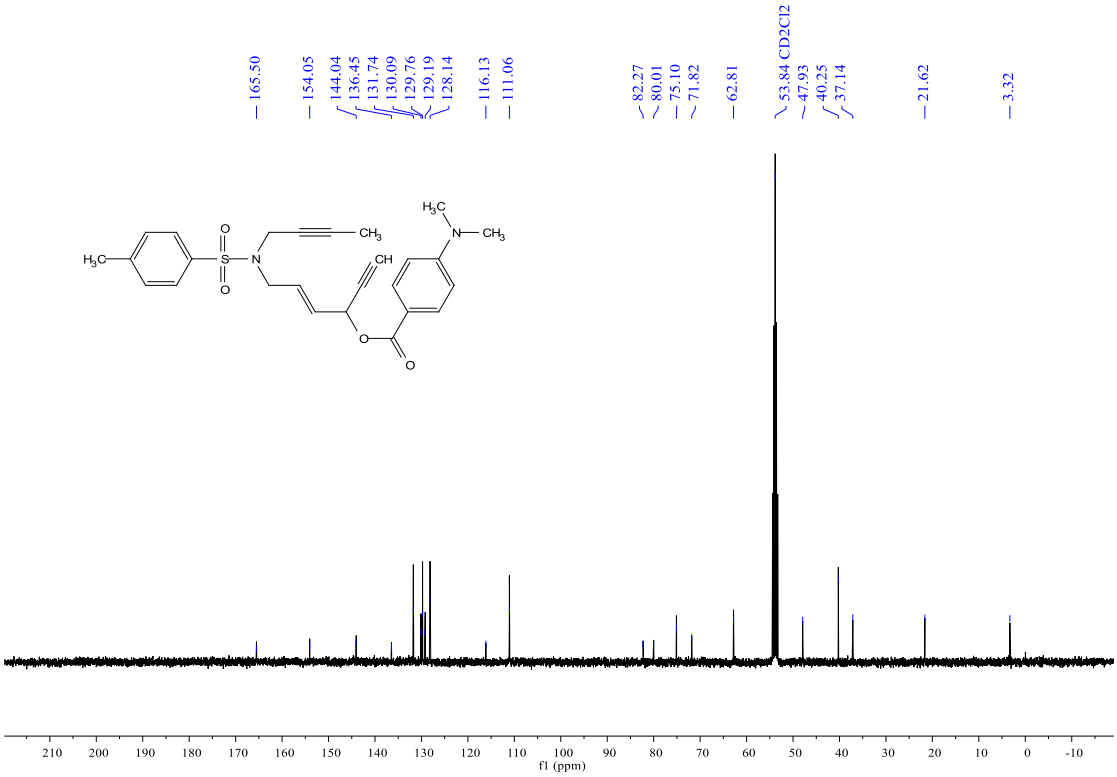
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116.13
111.06
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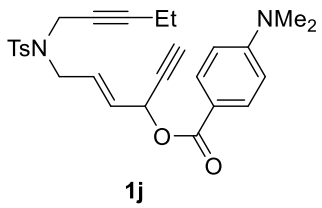
40.25
37.14
21.62
3.32
f1 (ppm)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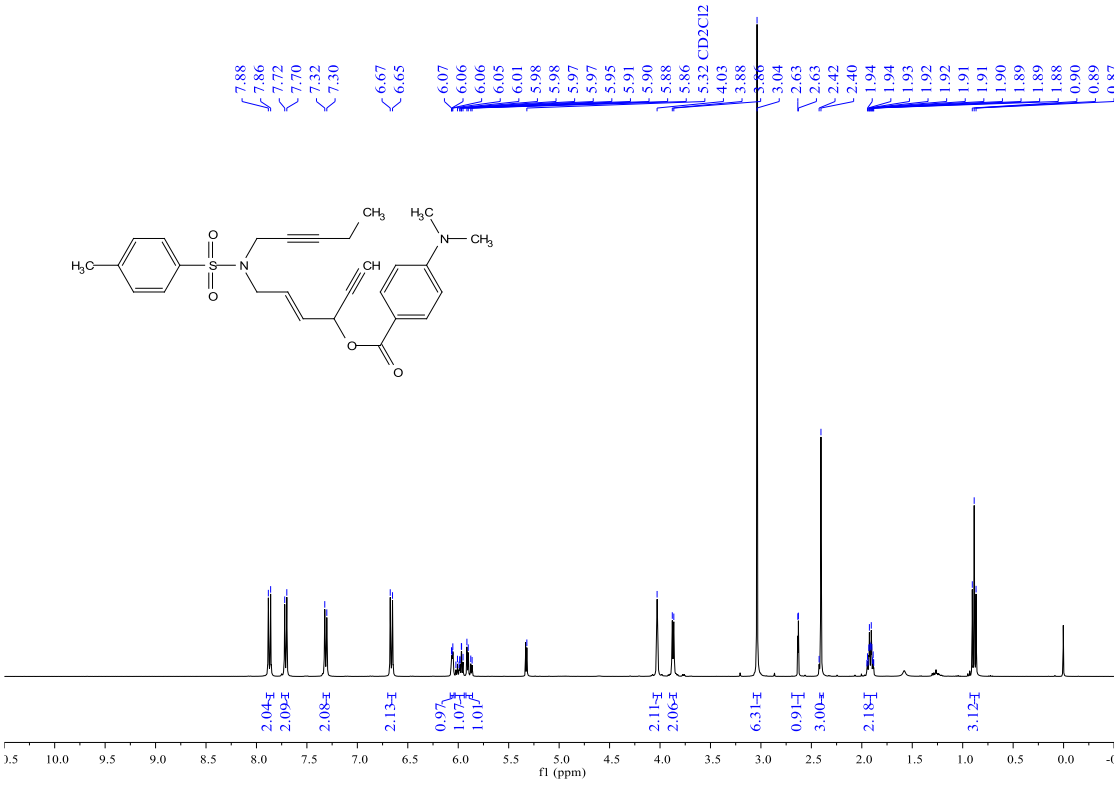
TsN
O
O

1j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6.06
6.05
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2.40
1.94
1.94
1.93
1.92
1.91
1.91
1.90
1.89
1.89
1.88
0.90
0.89
2.04
2.09
2.08
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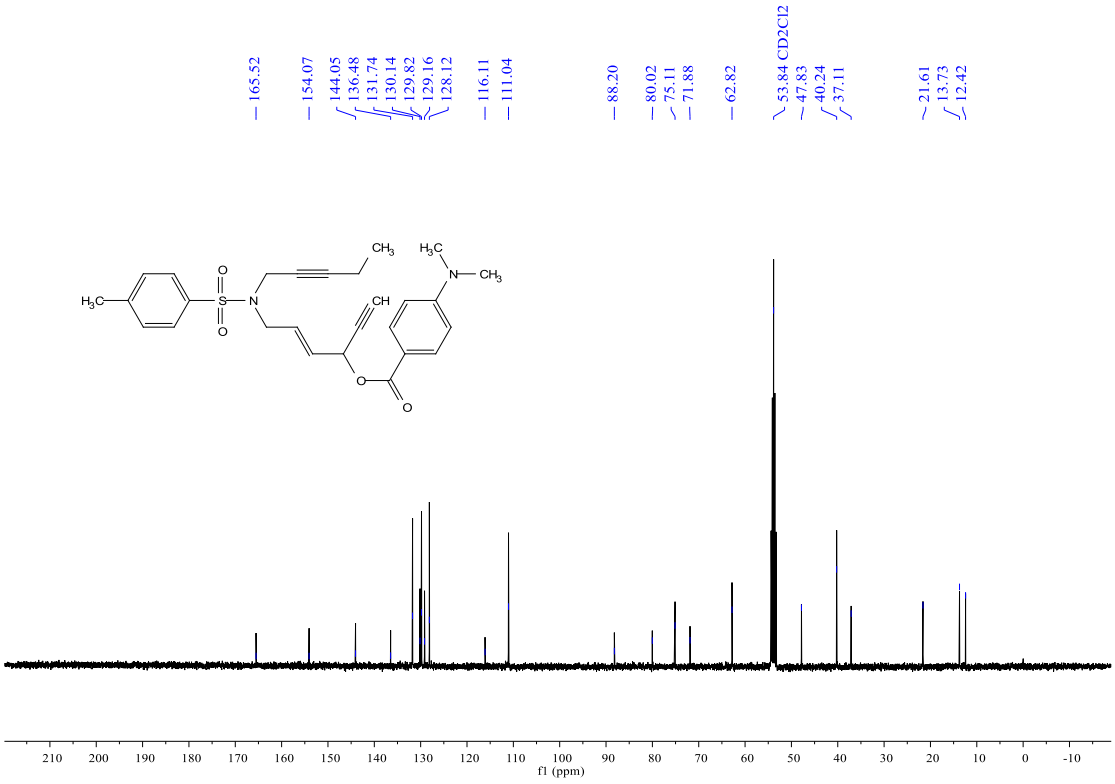
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53.84 CD2Cl2
47.83
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21.61
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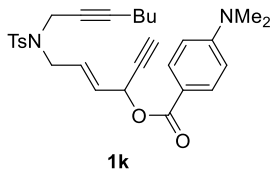
Bu
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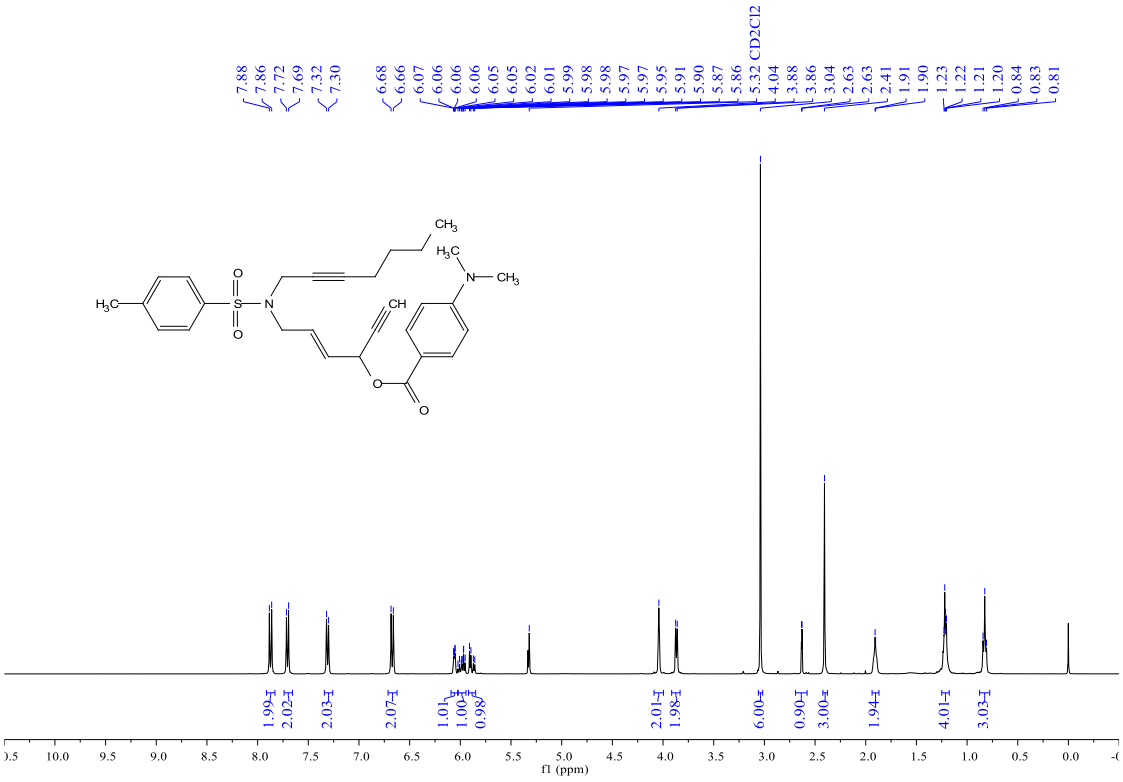
O
O

1k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1.90
1.23
1.22
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0.83
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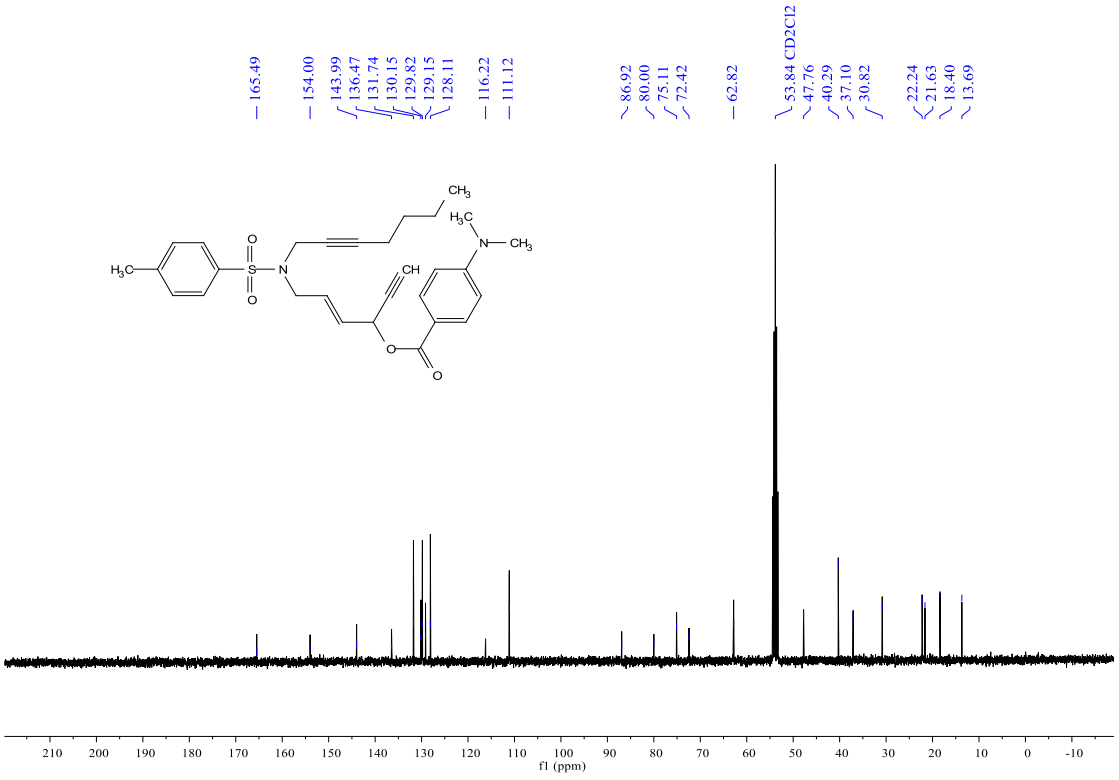
f1 (ppm)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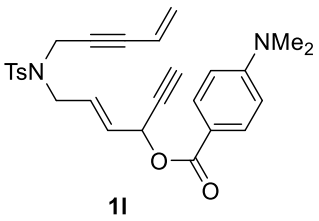
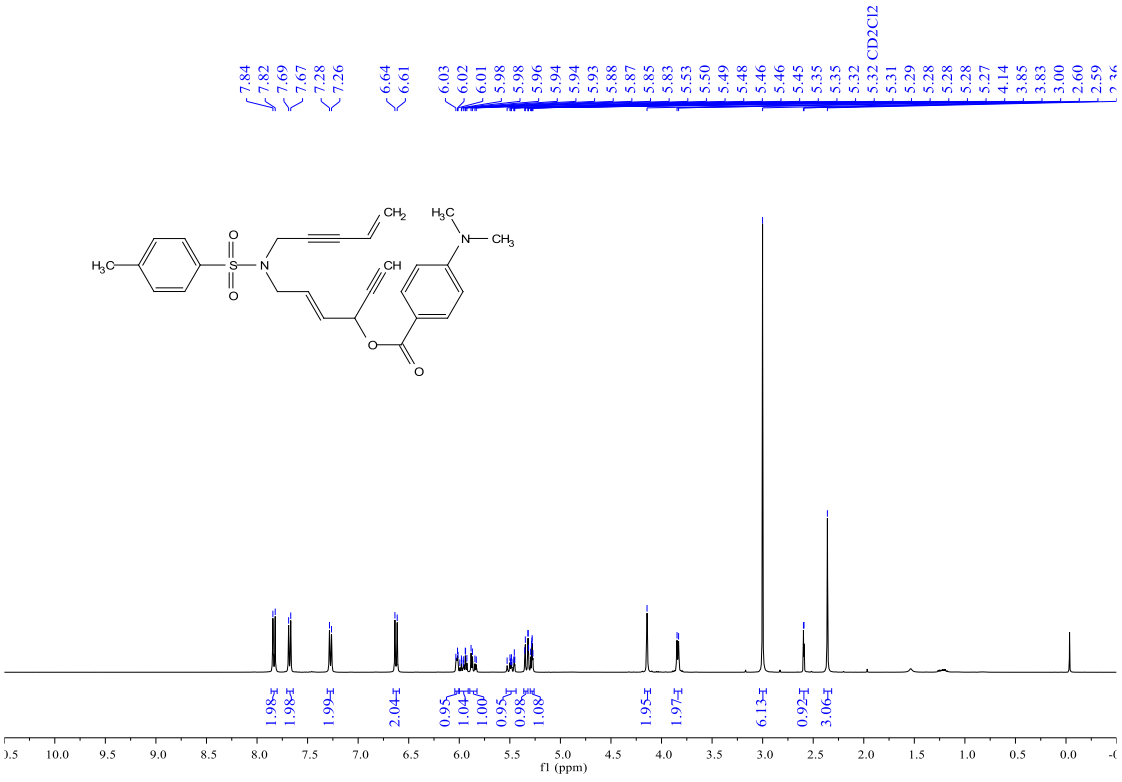
128.11
116.22
111.12
86.92
80.00
75.11
72.42
62.82
53.84 CD2Cl2
47.76
40.29
37.10
30.82
22.24
21.63
18.40
13.69
f1 (ppm)


NMe2
TsN
O
O

1l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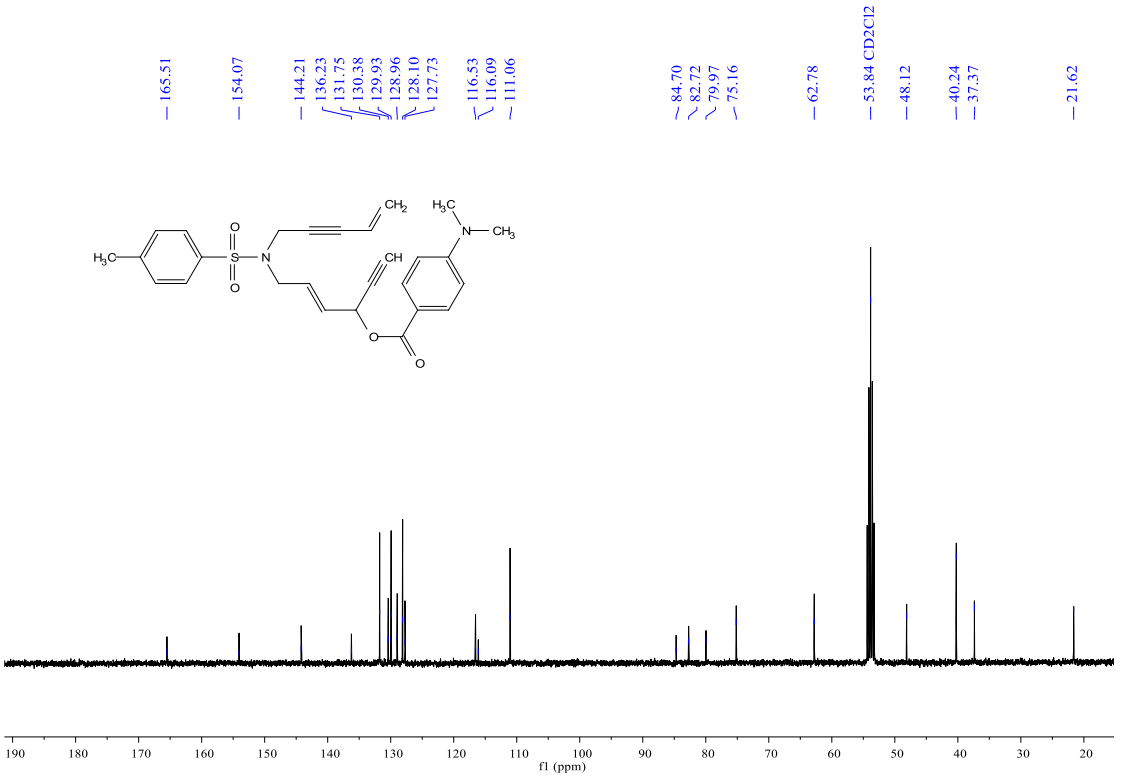
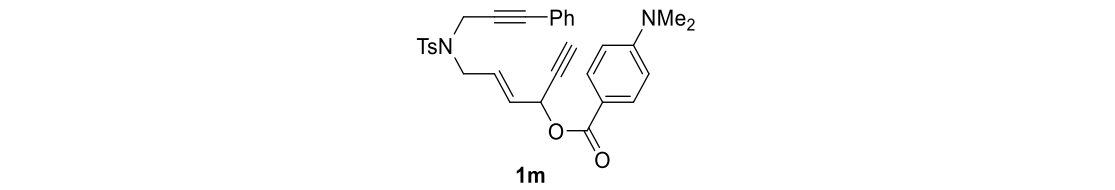
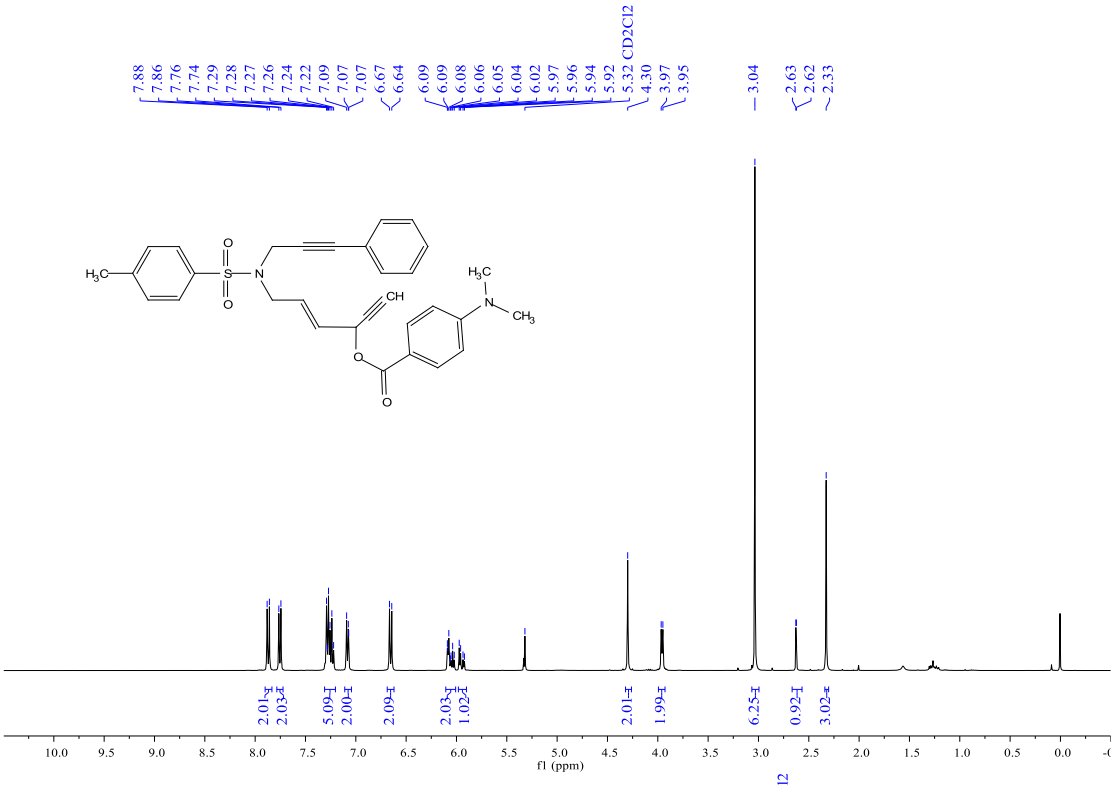
7.82
7.69
7.67
7.28
7.26
6.64
6.61
6.03
6.02
6.01
5.98
5.98
5.96
5.94
5.94
5.93
5.88
5.87
5.85
5.83
5.53
5.50
5.49
5.48
5.46
5.46
5.45
5.35
5.35
5.32
5.32 CD2Cl2
5.31
5.29
5.28
5.28
5.28
5.27
4.14
3.85
3.83
3.00
2.60
2.59
1.98
1.98
1.99
2.04
0.95
1.04
1.00
0.95
0.98
1.08
1.95
1.97
6.13
0.92
3.06
f1 (ppm)


165.51
154.07
144.21
136.23
131.75
130.38
129.93
128.96
128.10
127.73
116.53
116.09
111.06
84.70
82.72
79.97
75.16
62.78
53.84 CD2Cl2
48.12
40.24
37.37
21.62
f1 (ppm)


Ph
NMe2
TsN
O
O

1m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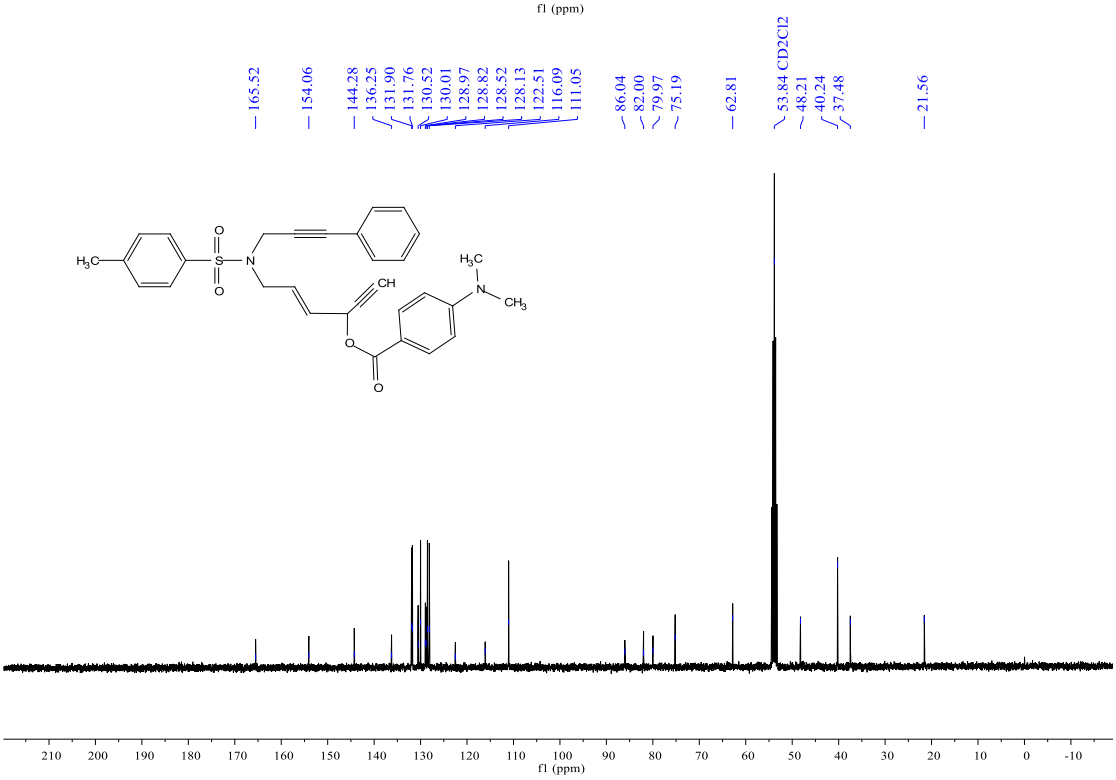
7.86
7.76
7.74
7.29
7.28
7.27
7.26
7.24
7.22
7.09
7.07
7.07
6.67
6.64
6.09
6.09
6.08
6.06
6.05
6.04
6.02
5.97
5.96
5.94
5.92
5.32 CD2Cl2
4.30
3.97
3.95
3.04
2.63
2.62
2.33
2.01
2.03
5.09
2.00
2.09
2.03
1.02
2.01
1.99
6.25
0.92
3.02
f1 (ppm)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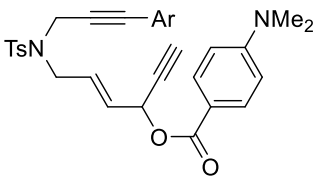
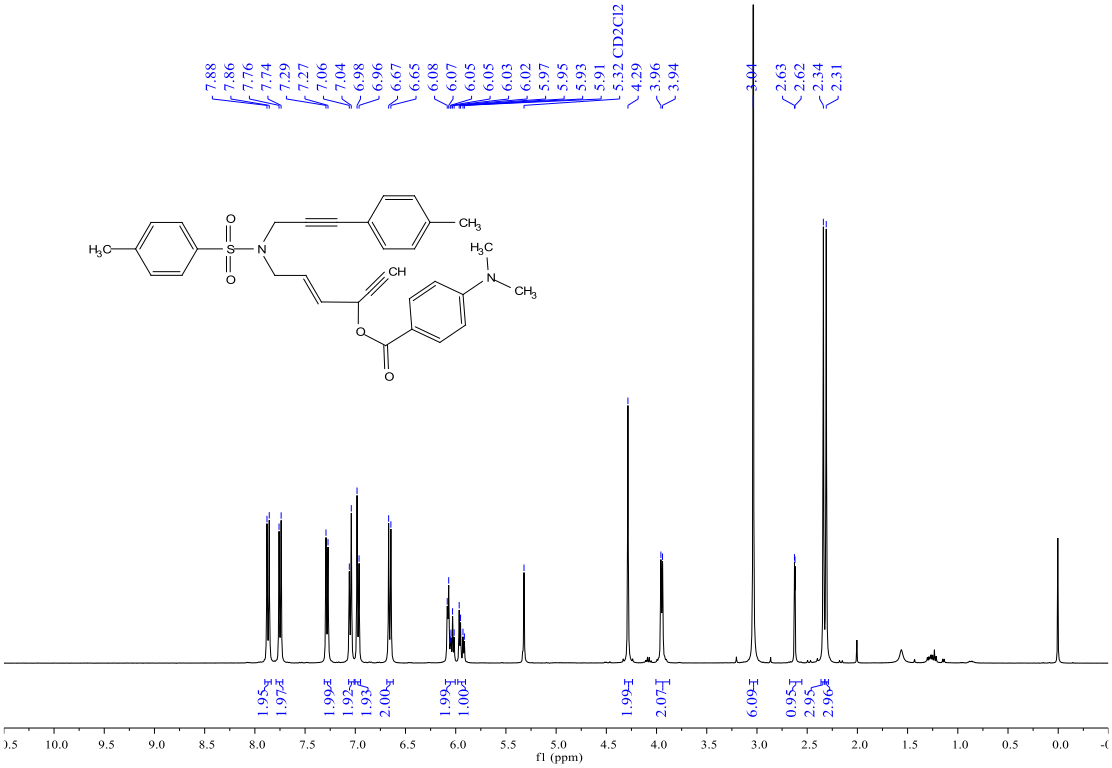
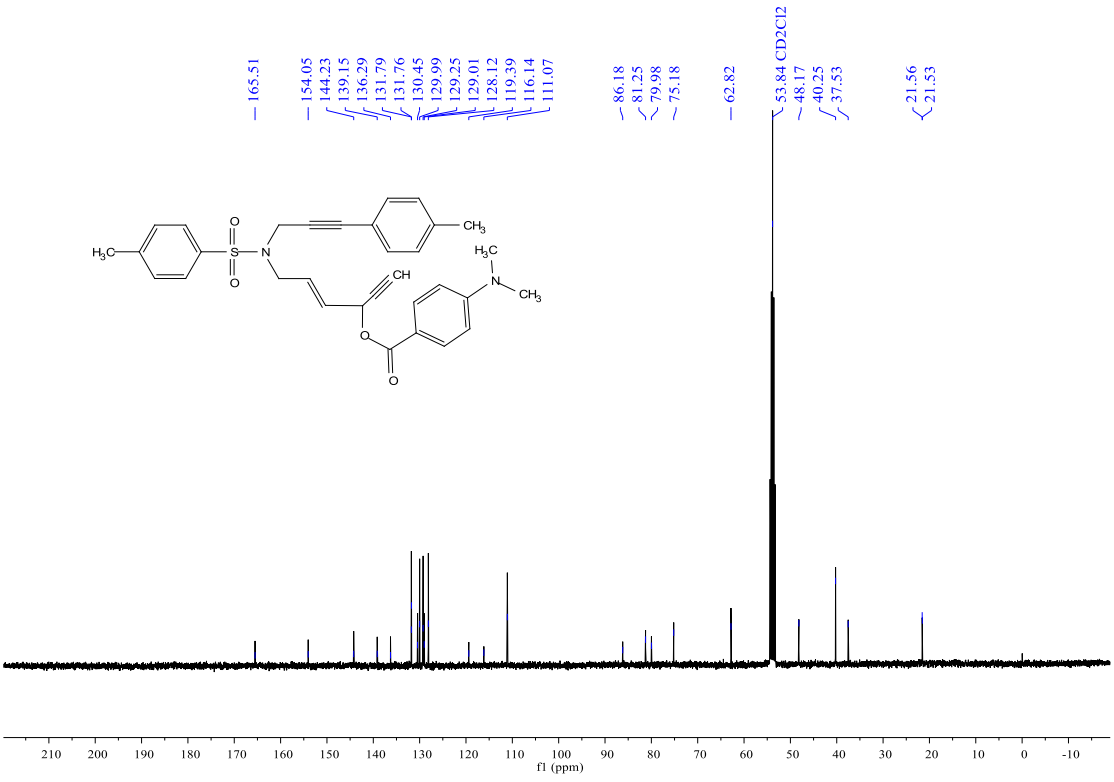
154.06
144.28
136.25
131.90
131.76
130.52
130.01
128.97
128.82
128.52
128.13
122.51
116.09
111.05
86.04
82.00
79.97
75.19
62.81
53.84 CD2Cl2
48.21
40.24
37.48
21.56
f1 (ppm)

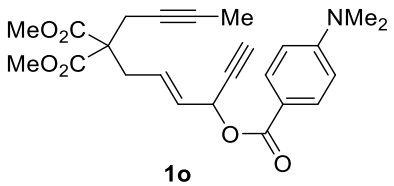


Ar = p-MeC$_6$H$_4$

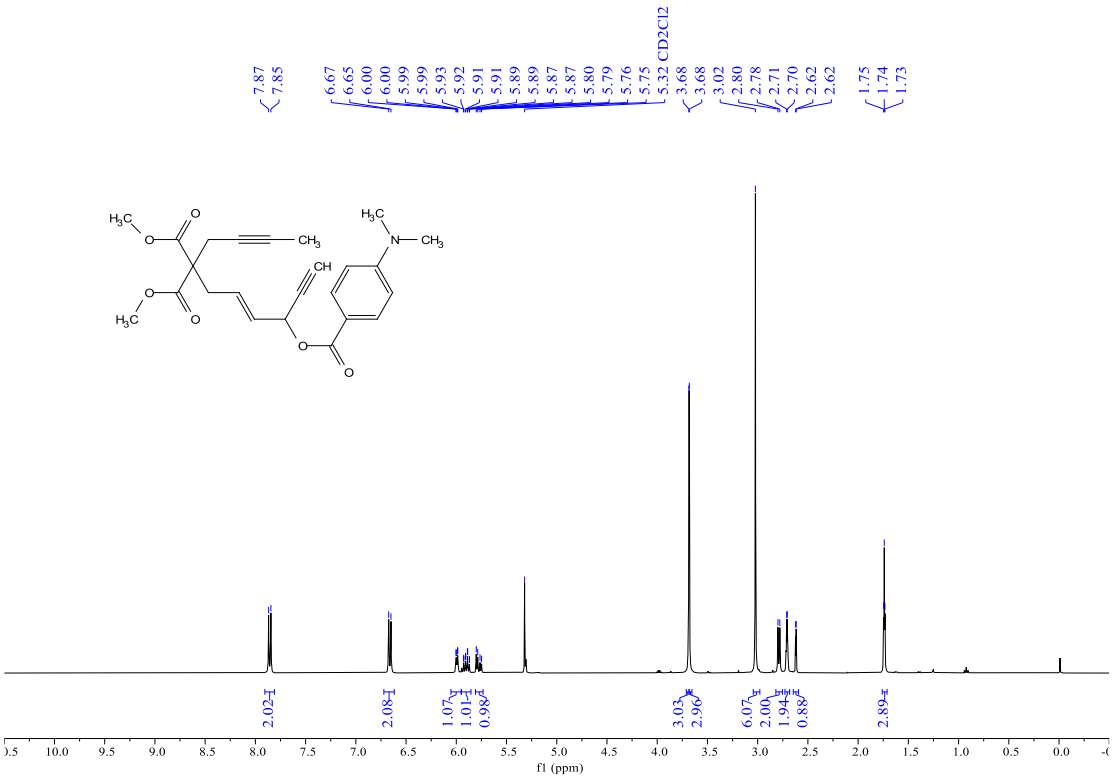
1n

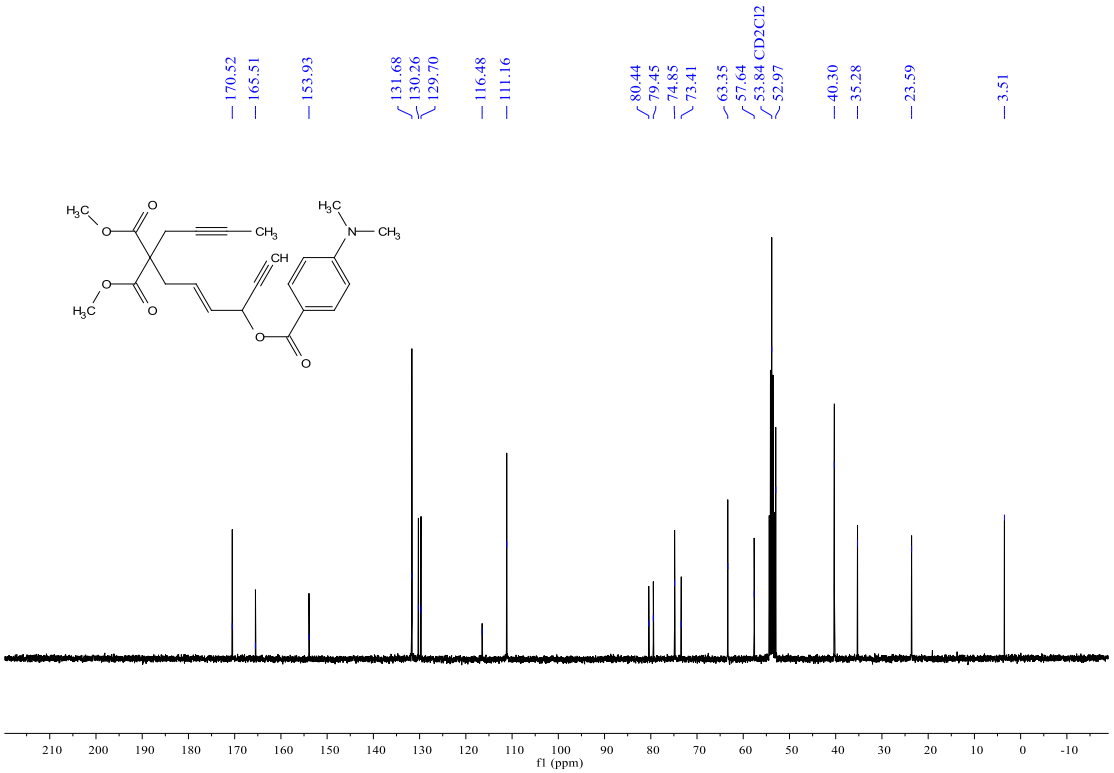


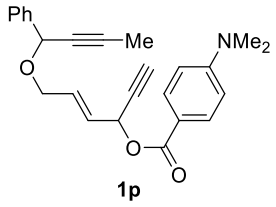


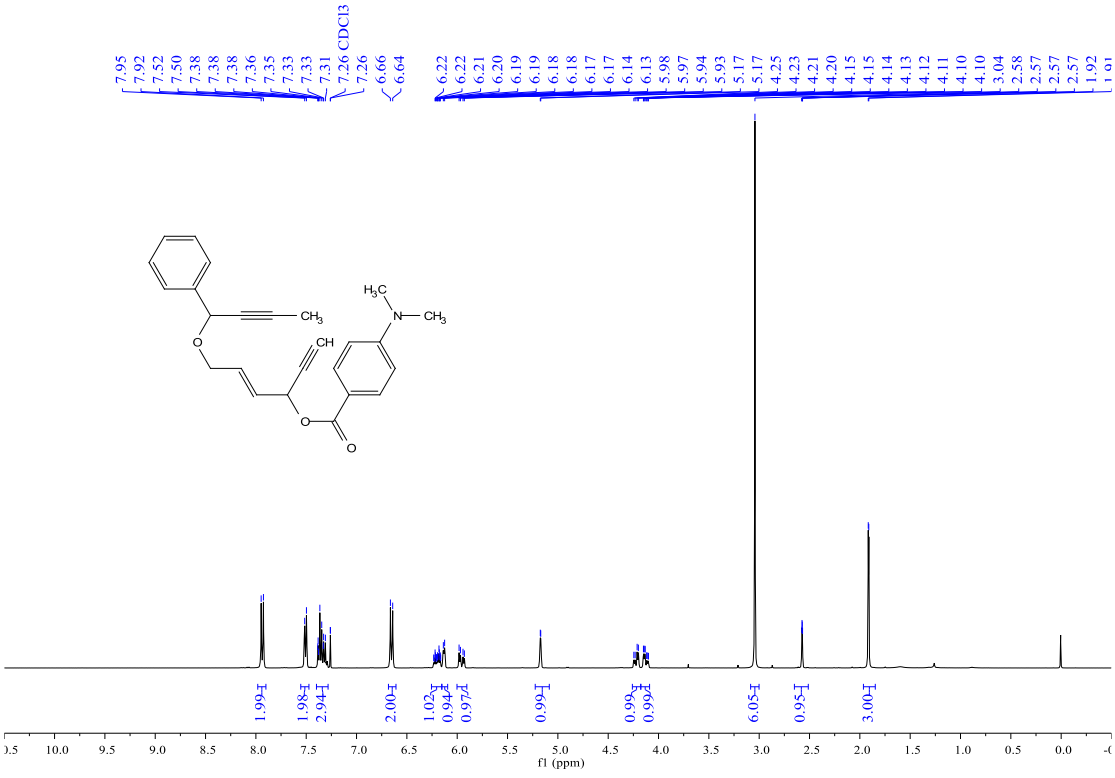

MeO2C
MeO2C
Me
NMe2
O
O

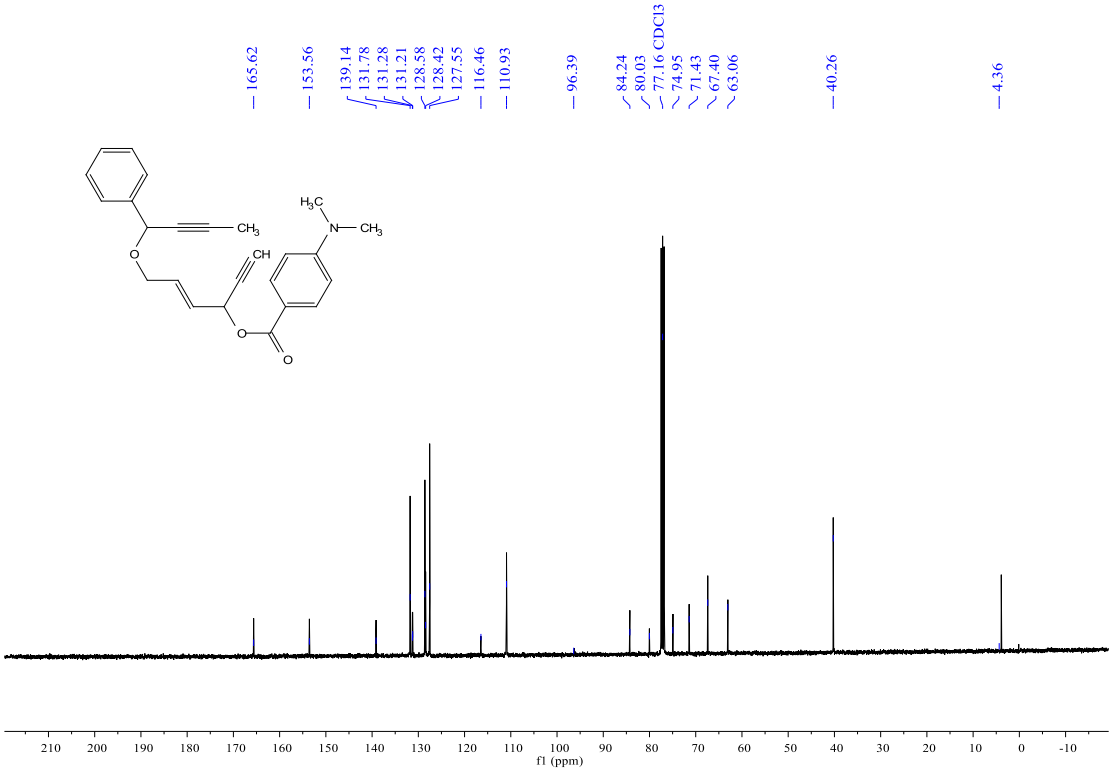
1o

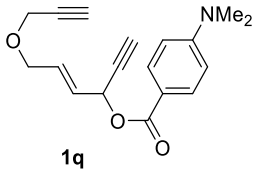

7.87
7.85
6.67
6.65
6.00
6.00
5.99
5.99
5.93
5.92
5.91
5.91
5.89
5.89
5.87
5.87
5.80
5.79
5.76
5.75
5.32 CD2Cl2
3.68
3.68
3.02
2.80
2.78
2.71
2.70
2.62
2.62
1.75
1.74
1.73
2.02
2.08
1.07
1.01
0.98
3.03
2.96
6.07
2.00
1.94
0.88
2.89
f1 (ppm)


170.52
165.51
153.93
131.68
130.26
129.70
116.48
111.16
80.44
79.45
74.85
73.41
63.35
57.64
53.84 CD2Cl2
52.97
40.30
35.28
23.59
3.51
f1 (ppm)

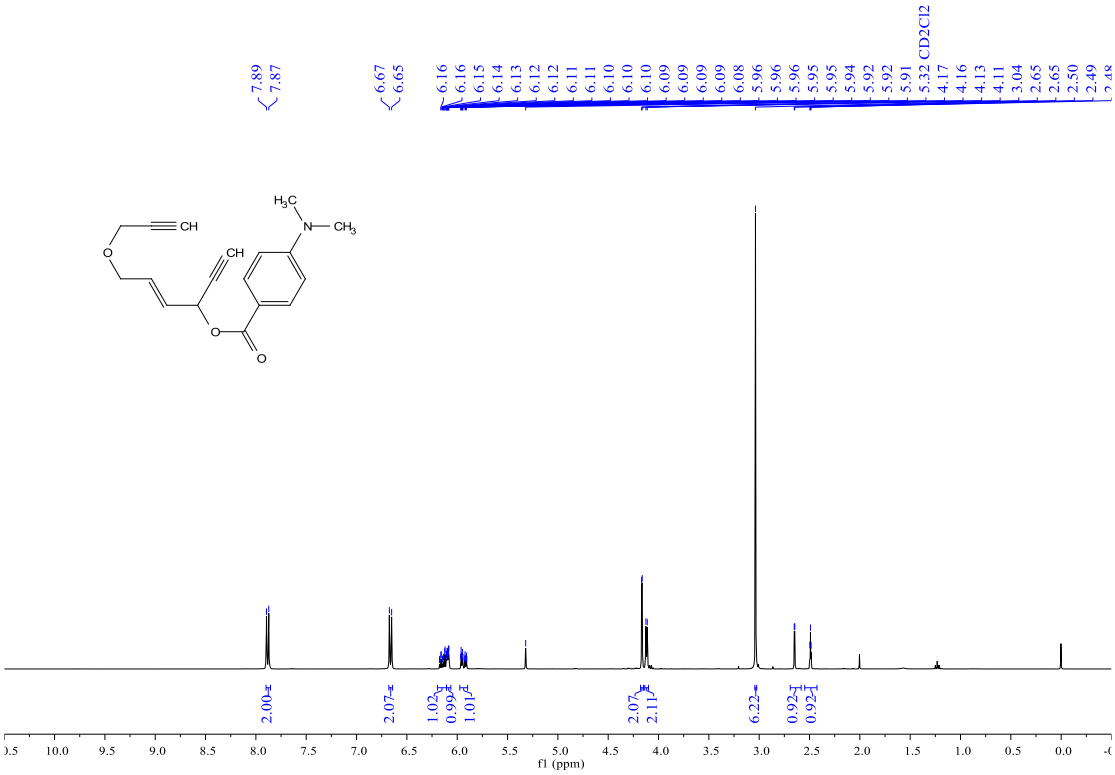

Ph
Me
NMe2
O
O
O
1p


7.95
7.92
7.52
7.50
7.38
7.38
7.38
7.36
7.35
7.33
7.33
7.31
7.26 CDCl3
7.26
6.66
6.64
6.22
6.22
6.21
6.20
6.19
6.19
6.18
6.18
6.17
6.17
6.14
6.13
5.98
5.97
5.94
5.93
5.17
5.17
4.25
4.23
4.21
4.20
4.15
4.15
4.14
4.13
4.12
4.11
4.10
4.10
3.04
2.58
2.57
2.57
1.92
H3C
N
CH3
CH3
CH
O
O
O
1.99
1.98
2.94
2.00
1.02
0.94
0.97
0.99
0.99
0.99
6.05
0.95
3.00
f1 (ppm)


165.62
153.56
139.14
131.78
131.28
131.21
128.58
128.42
127.55
116.46
110.93
96.39
84.24
80.03
77.16 CDCl3
74.95
71.43
67.40
63.06
40.26
4.36
H3C
N
CH3
CH3
CH
O
O
O
f1 (ppm)


NMe2
O
O
O

1q


7.89
7.87
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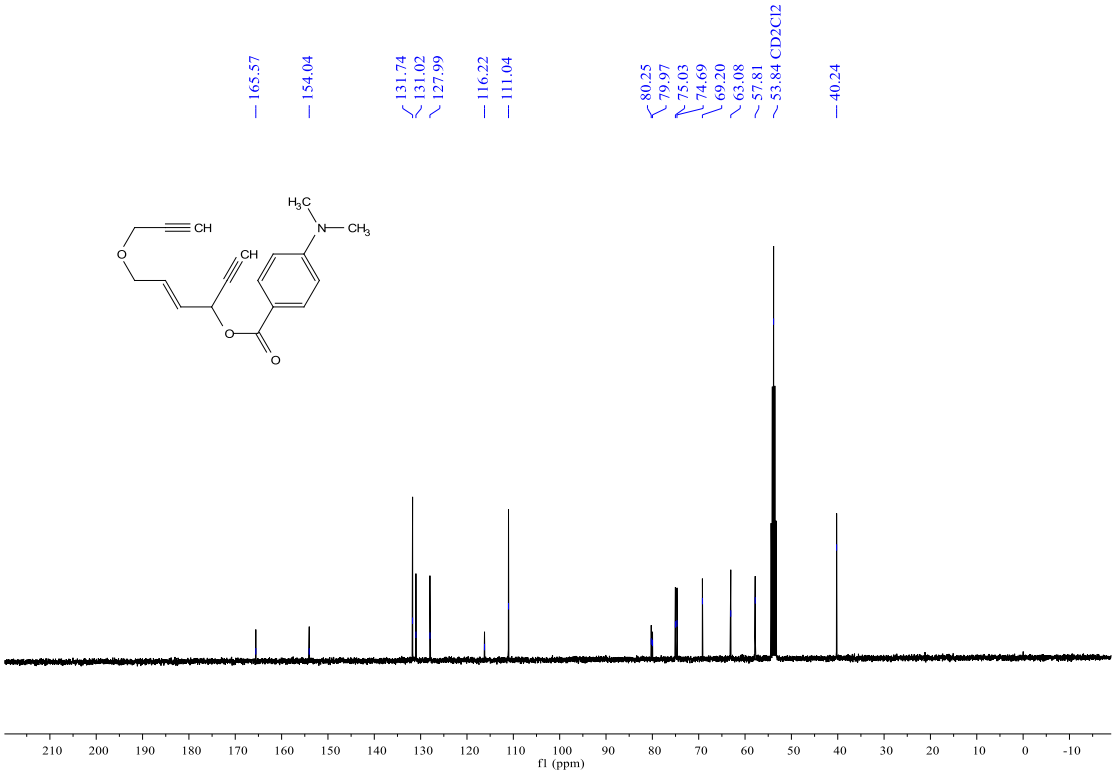
6.65
6.16
6.16
6.15
6.14
6.13
6.12
6.12
6.11
6.11
6.10
6.10
6.10
6.09
6.09
6.09
6.09
6.08
5.96
5.96
5.95
5.95
5.94
5.92
5.92
5.91
5.32 CD2Cl2
4.17
4.16
4.13
4.11
3.04
2.65
2.50
2.49
H3C
N
CH3
CH
CH
O
O
O
2.00
2.07
1.02
0.99
1.01
2.07
2.11
6.22
0.92
0.92
f1 (ppm)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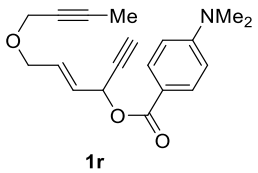
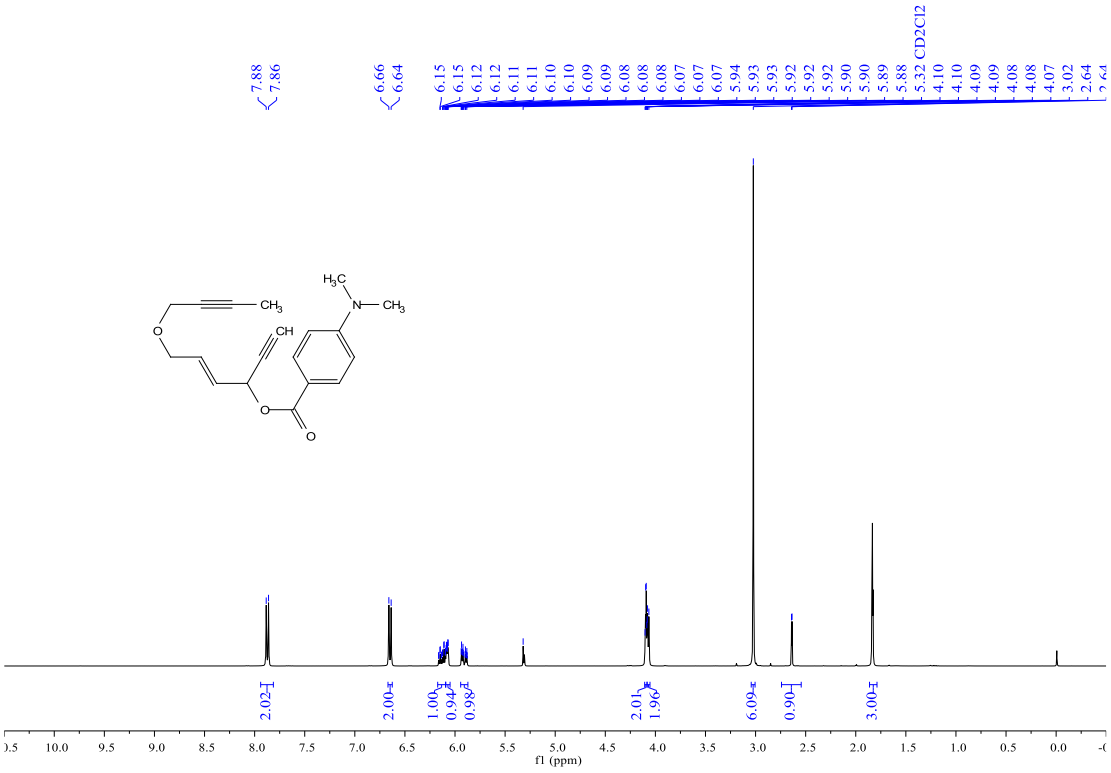
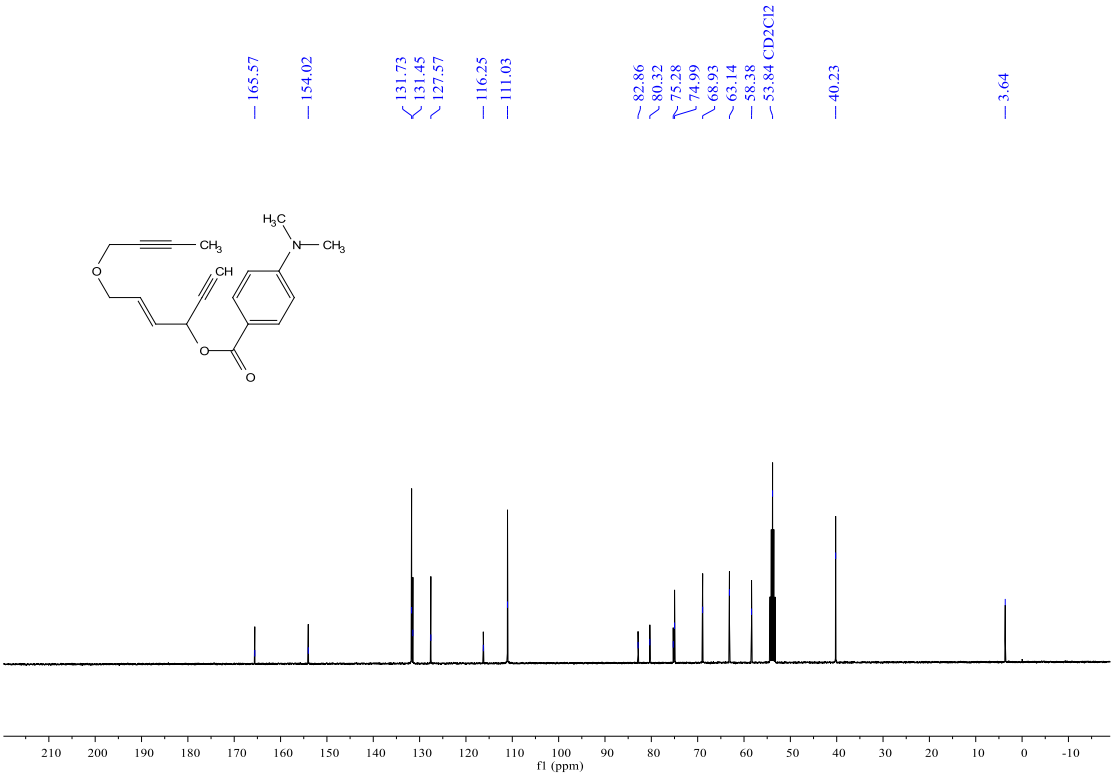
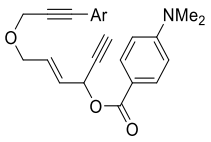
154.04
131.74
131.02
127.99
116.22
111.04
80.25
79.97
75.03
74.69
69.20
63.08
57.81
53.84 CD2Cl2
40.24
H3C
N
CH3
CH
CH
O
O
O
f1 (ppm)


Me
NMe2
O
O
O

1r

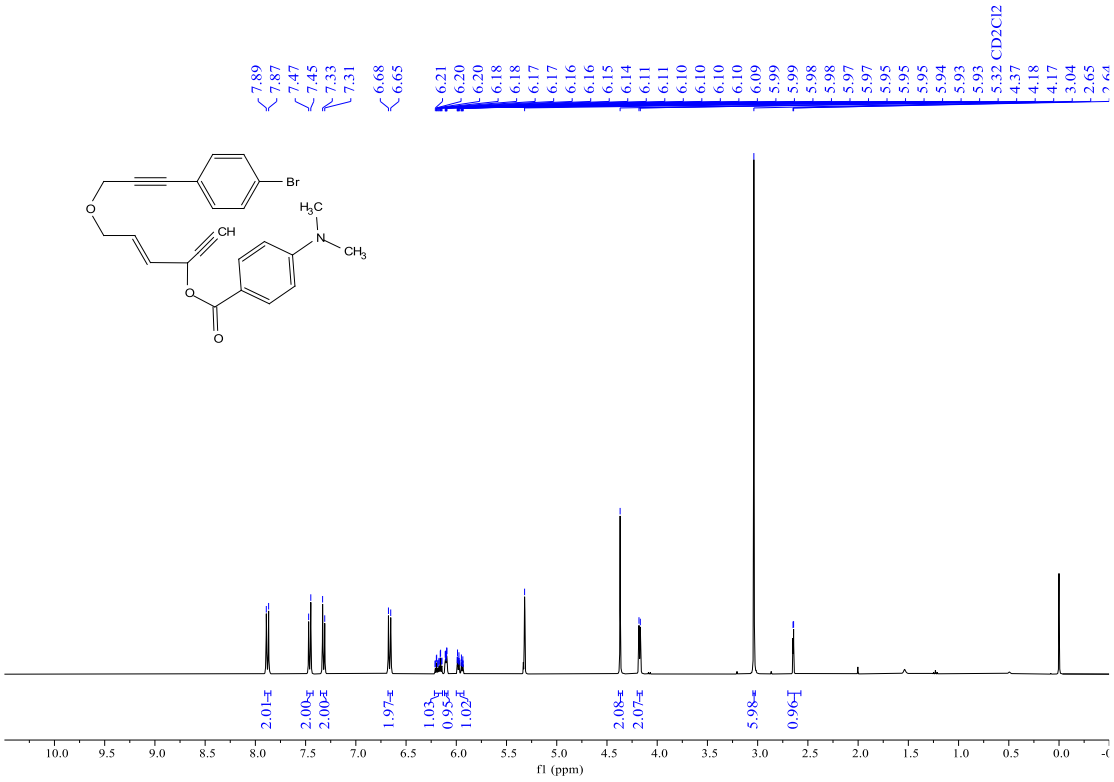

7.88
7.86
6.66
6.64
6.15
6.15
6.12
6.12
6.11
6.11
6.10
6.10
6.09
6.09
6.08
6.08
6.08
6.07
6.07
6.07
5.94
5.93
5.93
5.92
5.92
5.92
5.90
5.90
5.89
5.88
5.32 CD2Cl2
4.10
4.10
4.09
4.09
4.08
4.08
4.07
3.02
2.64
H3C
N
CH3
CH3
CH
O
O
O
2.02
2.00
1.00
0.94
0.98
2.01
1.96
6.09
0.90
3.00
f1 (ppm)

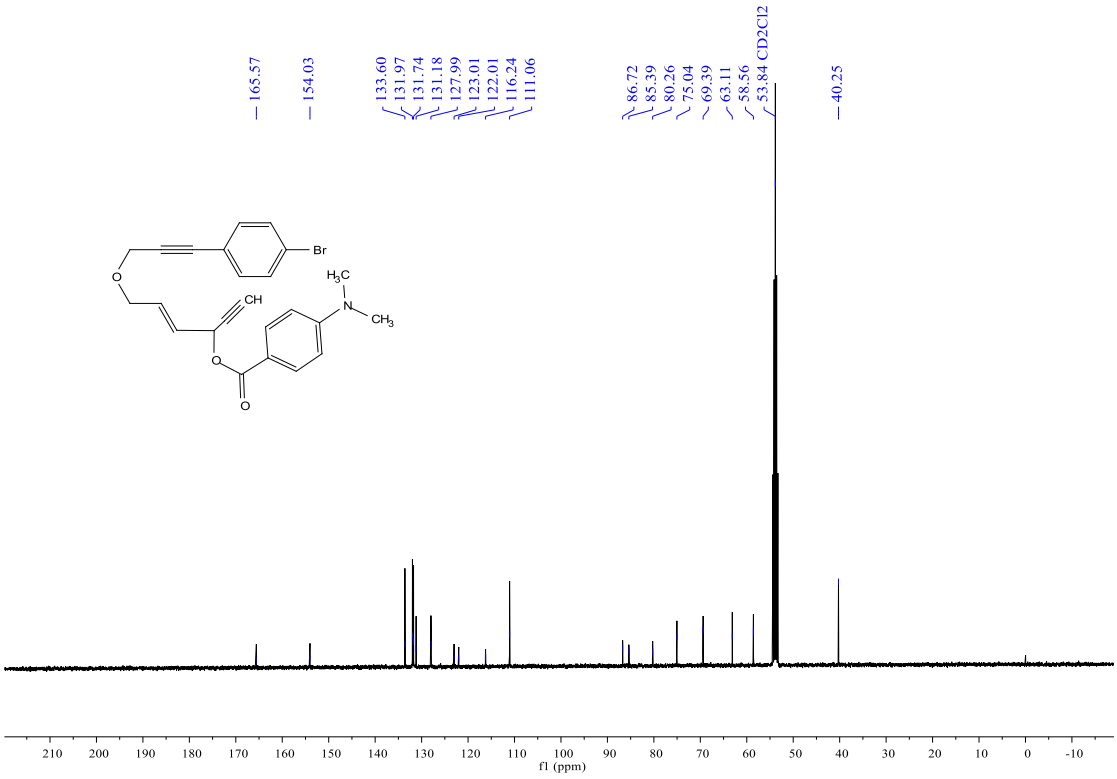

165.57
154.02
131.73
131.45
127.57
116.25
111.03
82.86
80.32
75.28
74.99
68.93
63.14
58.38
53.84 CD2Cl2
40.23
3.64
H3C
N
CH3
CH3
CH
O
O
O
f1 (ppm)

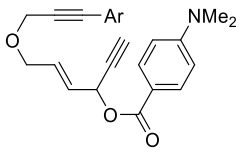


Ar = *p*-BrC_6H_4

1s

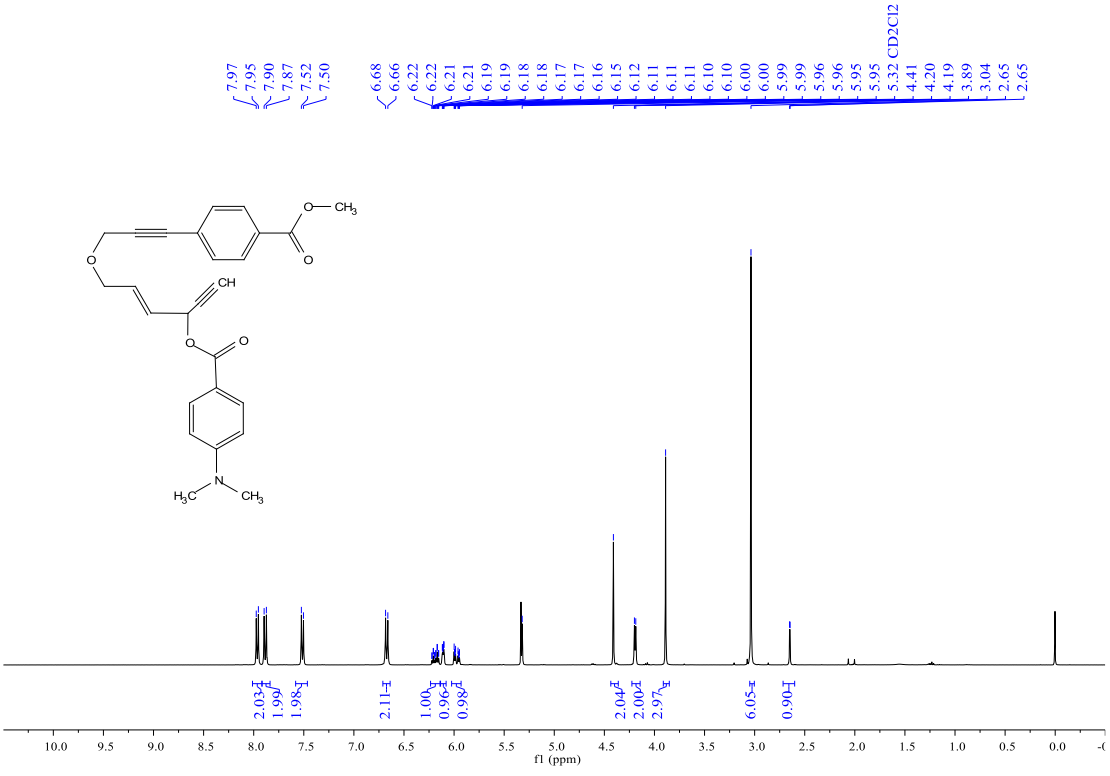


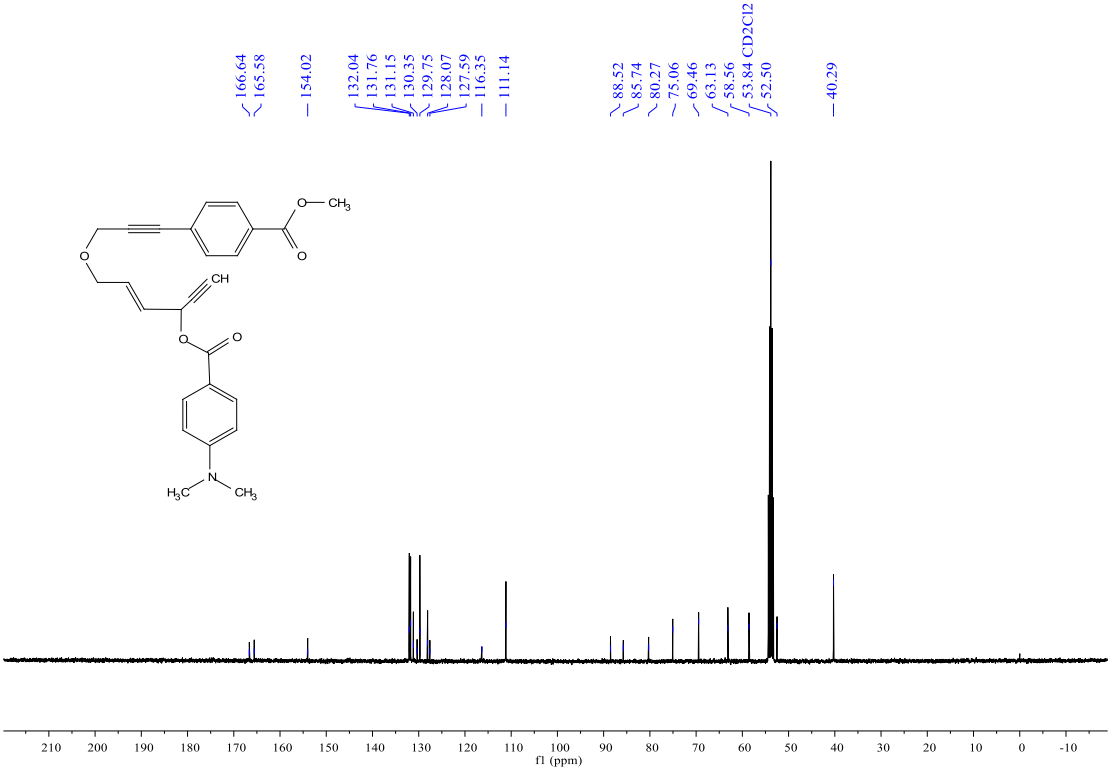


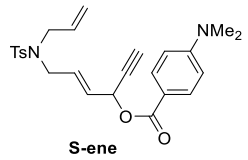


Ar = *p*-$MeO_2CC_6H_4$

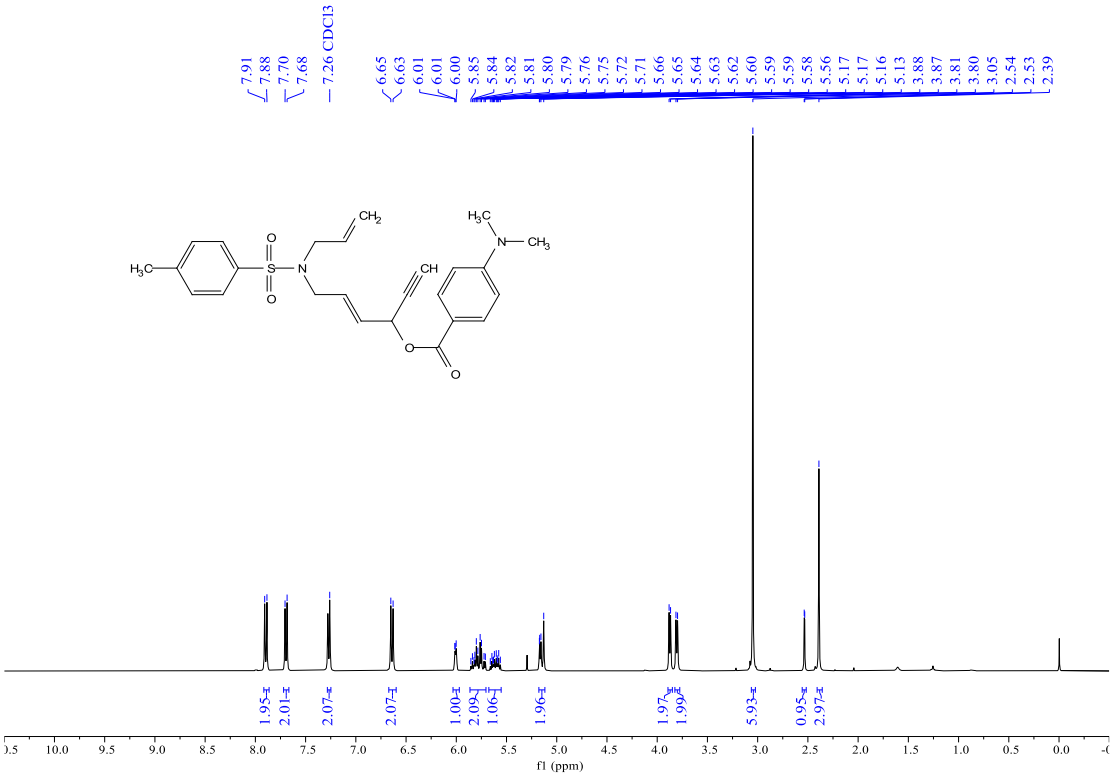
1t

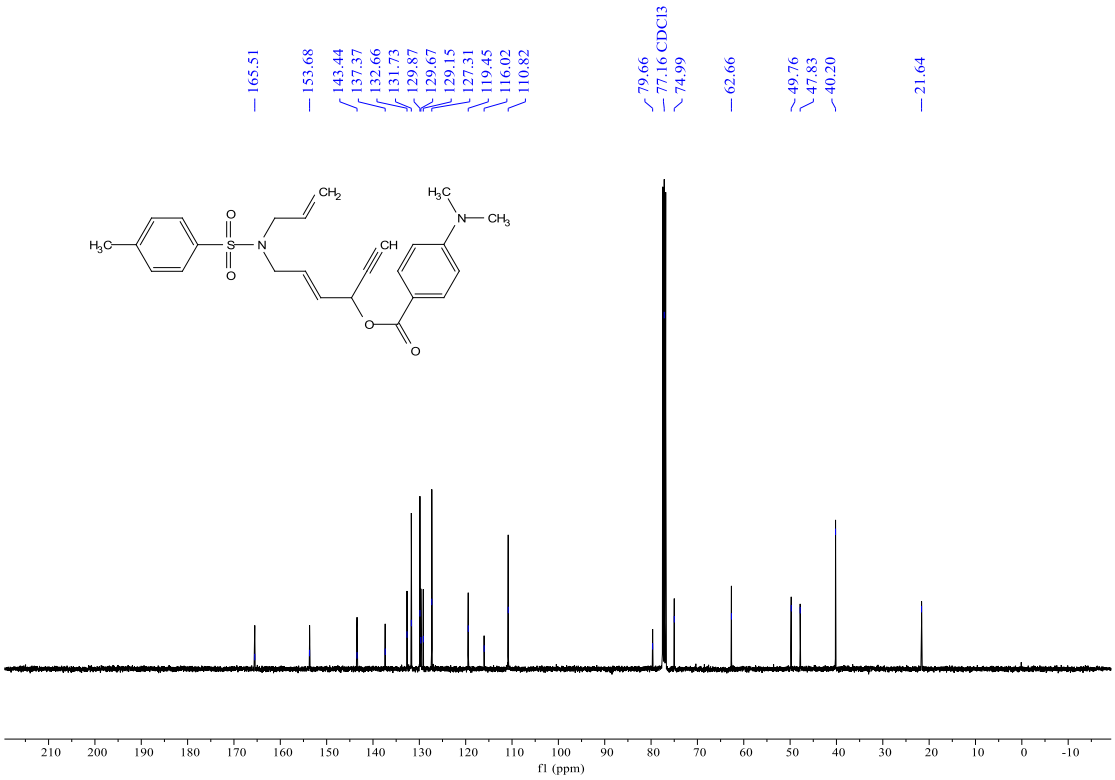


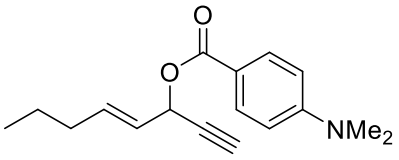



TsN
NMe2
O
O

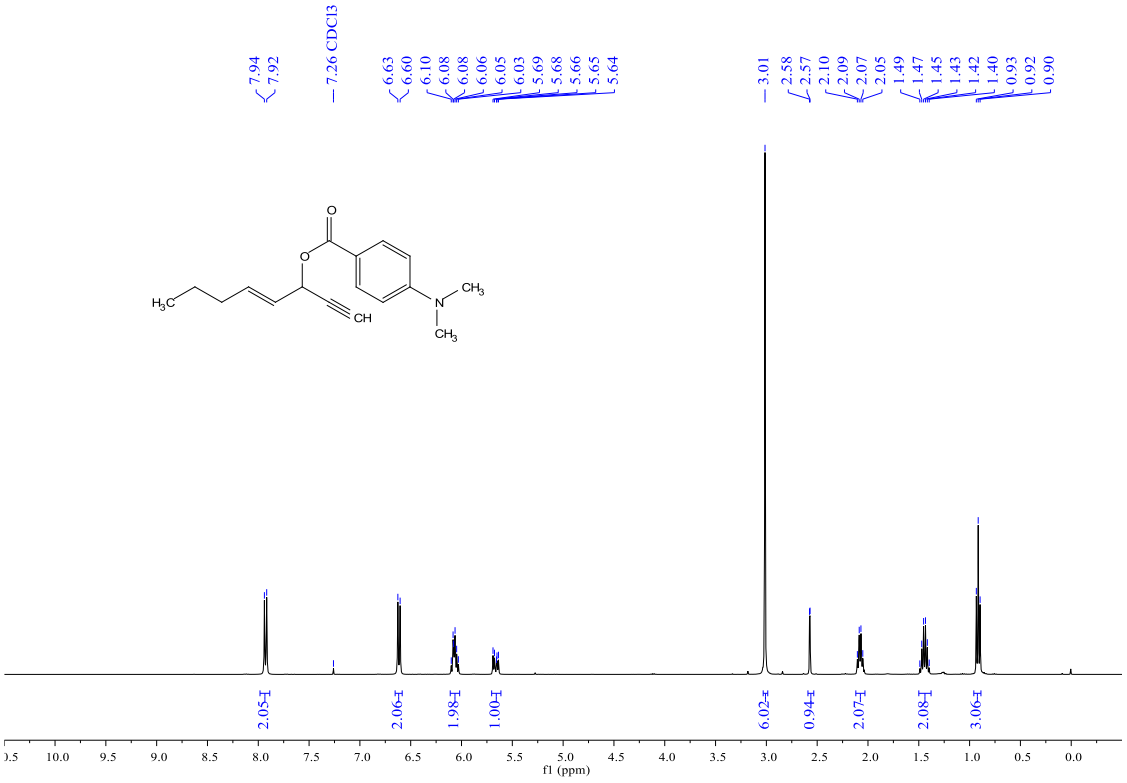
S-ene

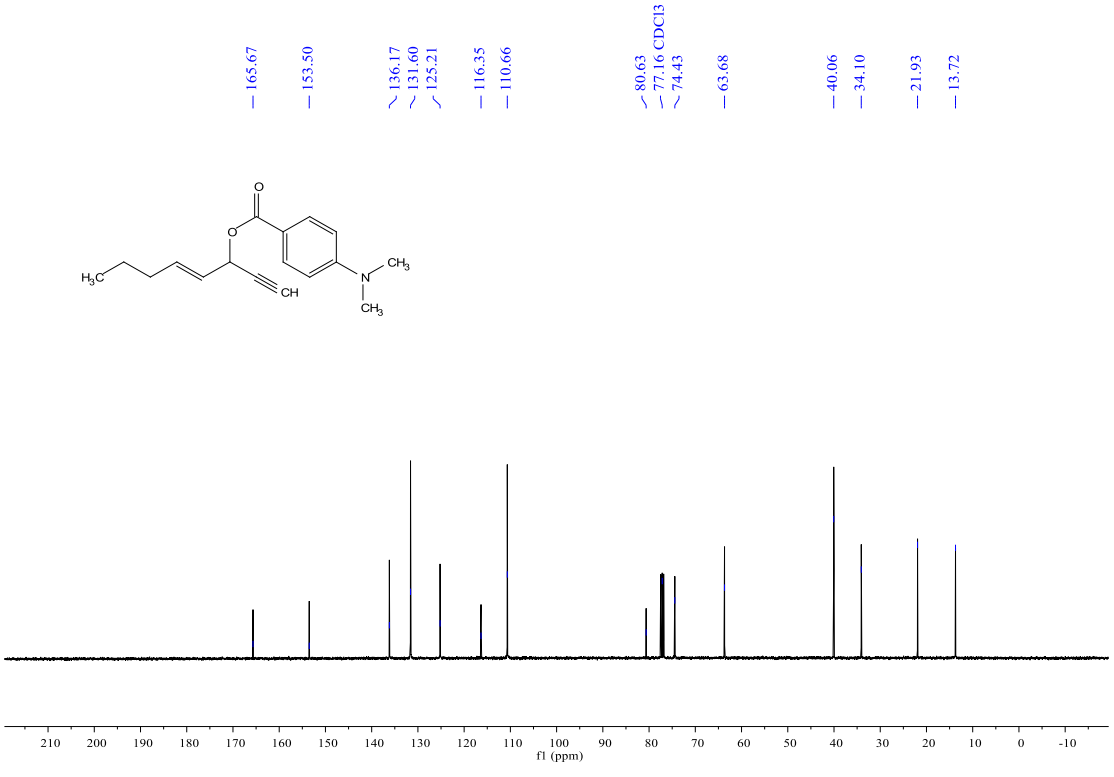

7.91
7.88
7.70
7.68
7.26 CDCl3
6.65
6.63
6.01
6.00
5.85
5.84
5.82
5.81
5.80
5.79
5.76
5.75
5.72
5.71
5.66
5.65
5.64
5.63
5.62
5.60
5.59
5.59
5.58
5.56
5.17
5.17
5.16
5.13
3.88
3.87
3.81
3.80
3.05
2.54
2.53
2.39
CH2
H3C
N
CH3
S
O
CH
O
O
1.95
2.01
2.07
2.07
1.00
2.09
1.06
1.96
1.97
1.99
5.93
0.95
2.97
f1 (ppm)

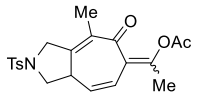

165.51
153.68
143.44
137.37
132.66
131.73
129.87
129.67
129.15
127.31
119.45
116.02
110.82
79.66
77.16 CDCl3
74.99
62.66
49.76
47.83
40.20
21.64
CH2
H3C
N
CH3
S
O
CH
O
O
f1 (ppm)


O
O
NMe2

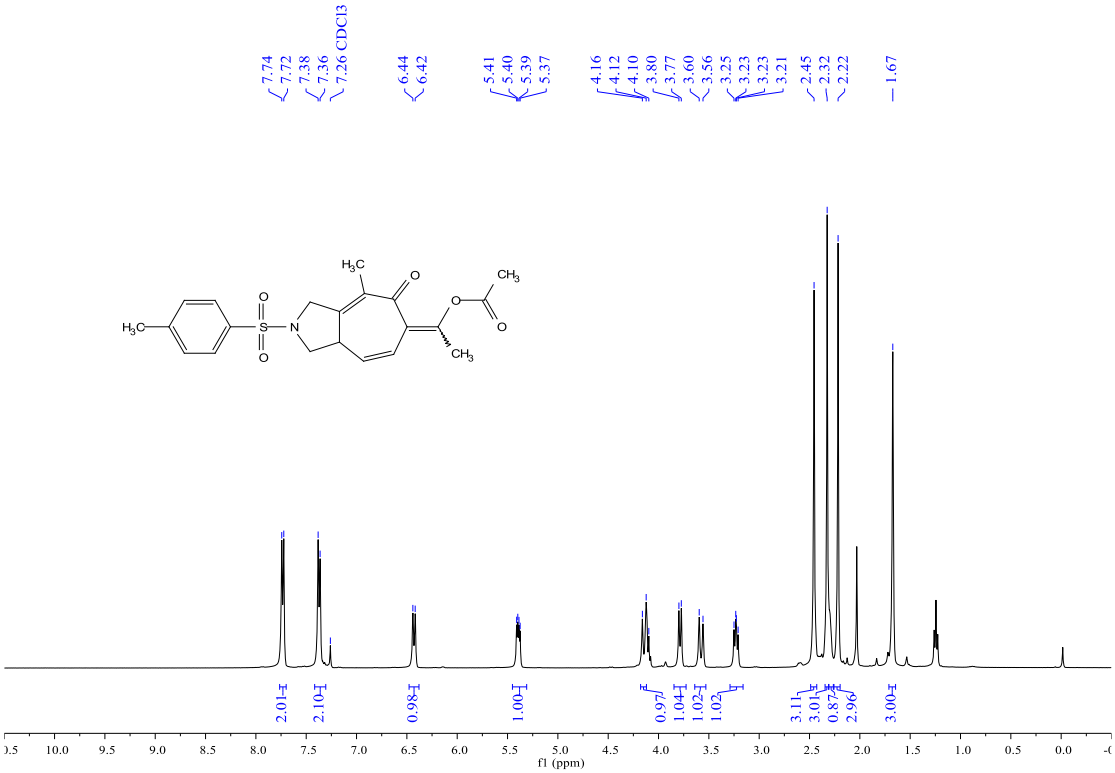
1u

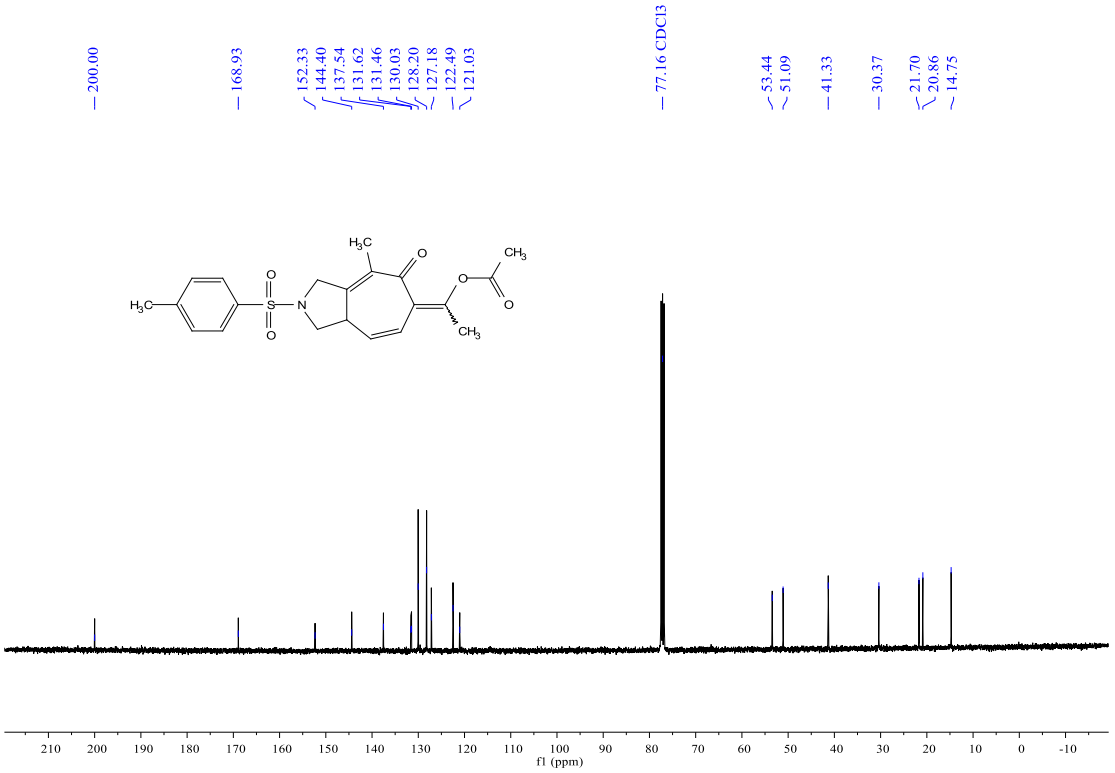

7.94
7.92
7.26 CDCl3
6.63
6.60
6.10
6.08
6.08
6.06
6.05
6.03
5.69
5.68
5.66
5.65
5.64
3.01
2.58
2.57
2.10
2.09
2.07
2.05
1.49
1.47
1.45
1.43
1.42
1.40
0.93
0.92
0.90
2.05
2.06
1.98
1.00
6.02
0.94
2.07
2.08
3.06
f1 (ppm)

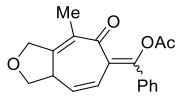

165.67
153.50
136.17
131.60
125.21
116.35
110.66
80.63
77.16 CDCl3
74.43
63.68
40.06
34.10
21.93
13.72
f1 (ppm)


Me
O
OAc
TsN
Me

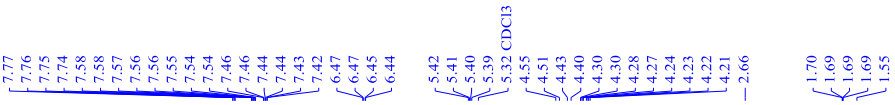
2a

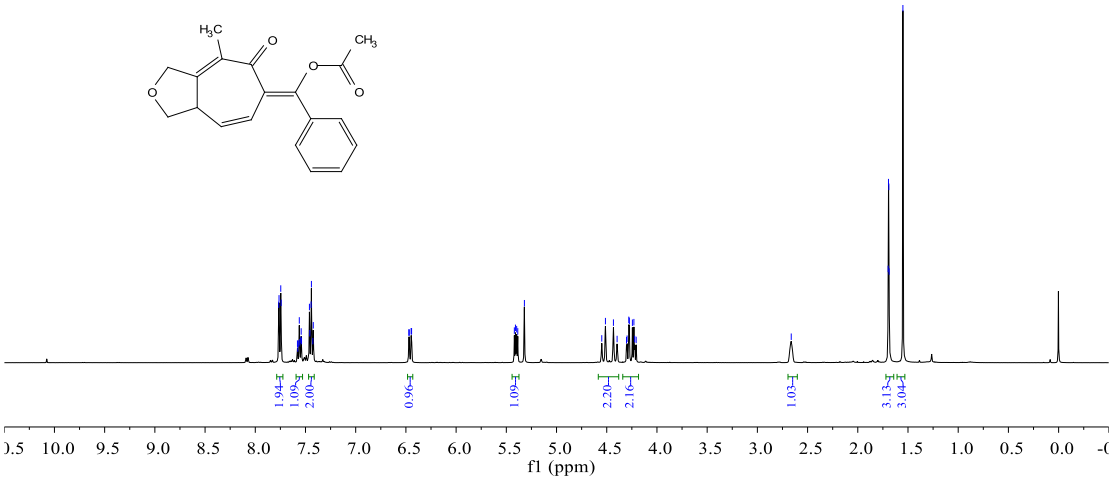

7.74
7.72
7.38
7.36
7.26 CDCl3
6.44
6.42
5.41
5.40
5.39
5.37
4.16
4.12
4.10
3.80
3.77
3.60
3.56
3.25
3.23
3.23
3.21
2.45
2.32
2.22
1.67
2.01
2.10
0.98
1.00
0.97
1.04
1.02
1.02
3.11
3.01
0.87
2.96
3.00
f1 (ppm)

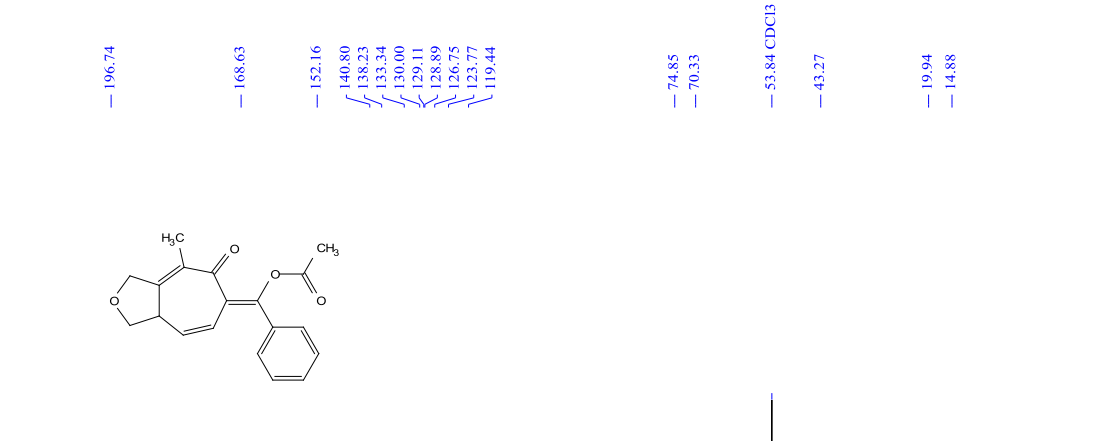

200.00
168.93
152.33
144.40
137.54
131.62
131.46
130.03
128.20
127.18
122.49
121.03
77.16 CDCl3
53.44
51.09
41.33
30.37
21.70
20.86
14.75
f1 (ppm)

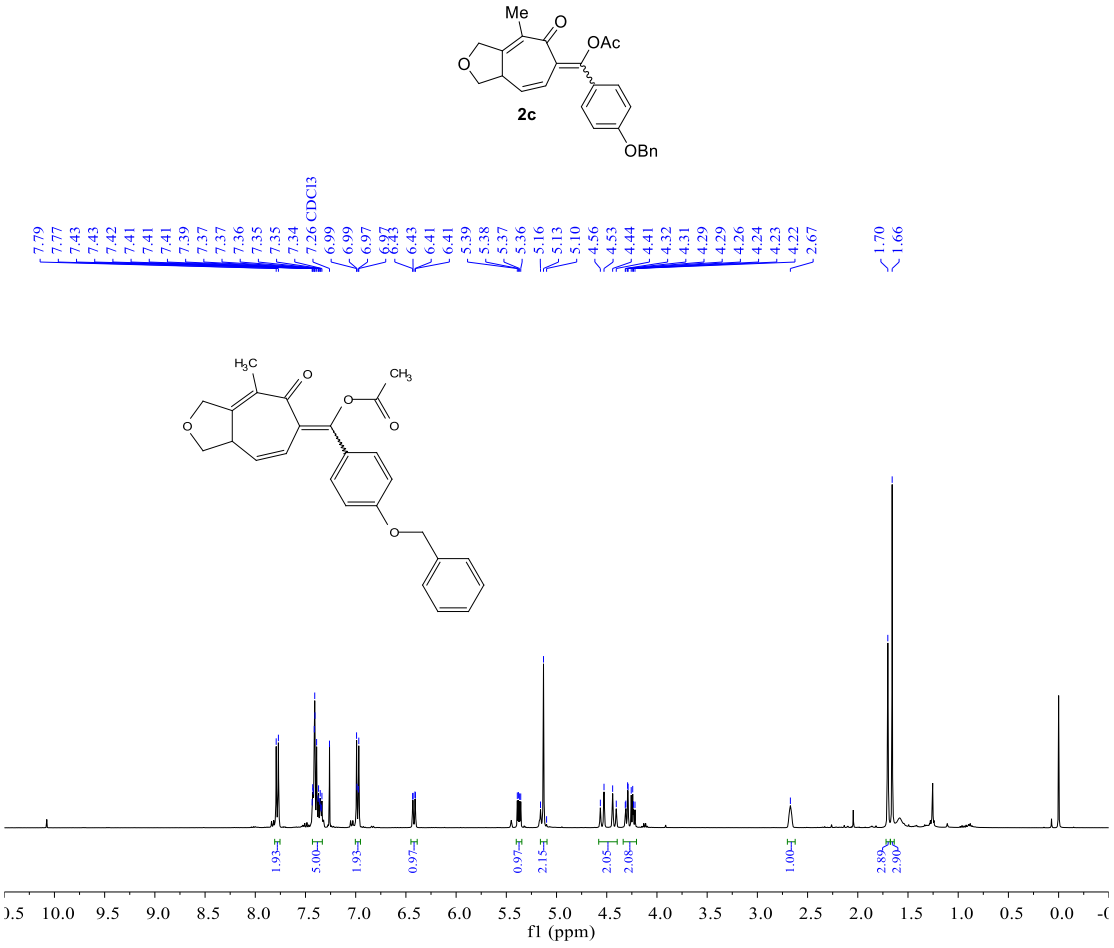

Me
O
OAc
O
Ph

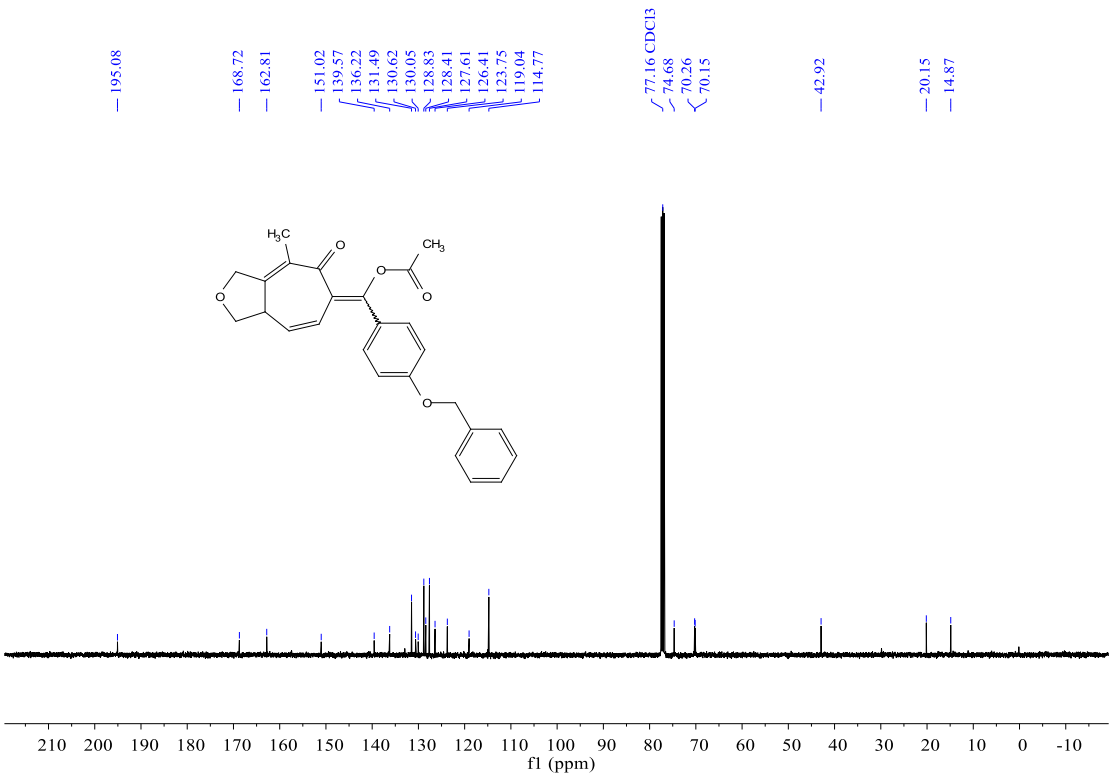
2b

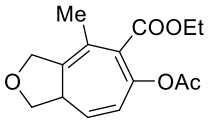

7.77
7.76
7.75
7.74
7.58
7.58
7.57
7.56
7.56
7.55
7.54
7.54
7.46
7.46
7.44
7.44
7.43
7.42
6.47
6.47
6.45
6.44
5.42
5.41
5.40
5.39
5.32 CDCl3
4.55
4.51
4.43
4.40
4.30
4.28
4.27
4.24
4.23
4.22
4.21
2.66
1.70
1.69
1.69
1.69
1.55


H3C
O
CH3
O
O
O
1.94
1.09
2.00
0.96
1.09
2.20
2.16
1.03
3.13
3.04
f1 (ppm)

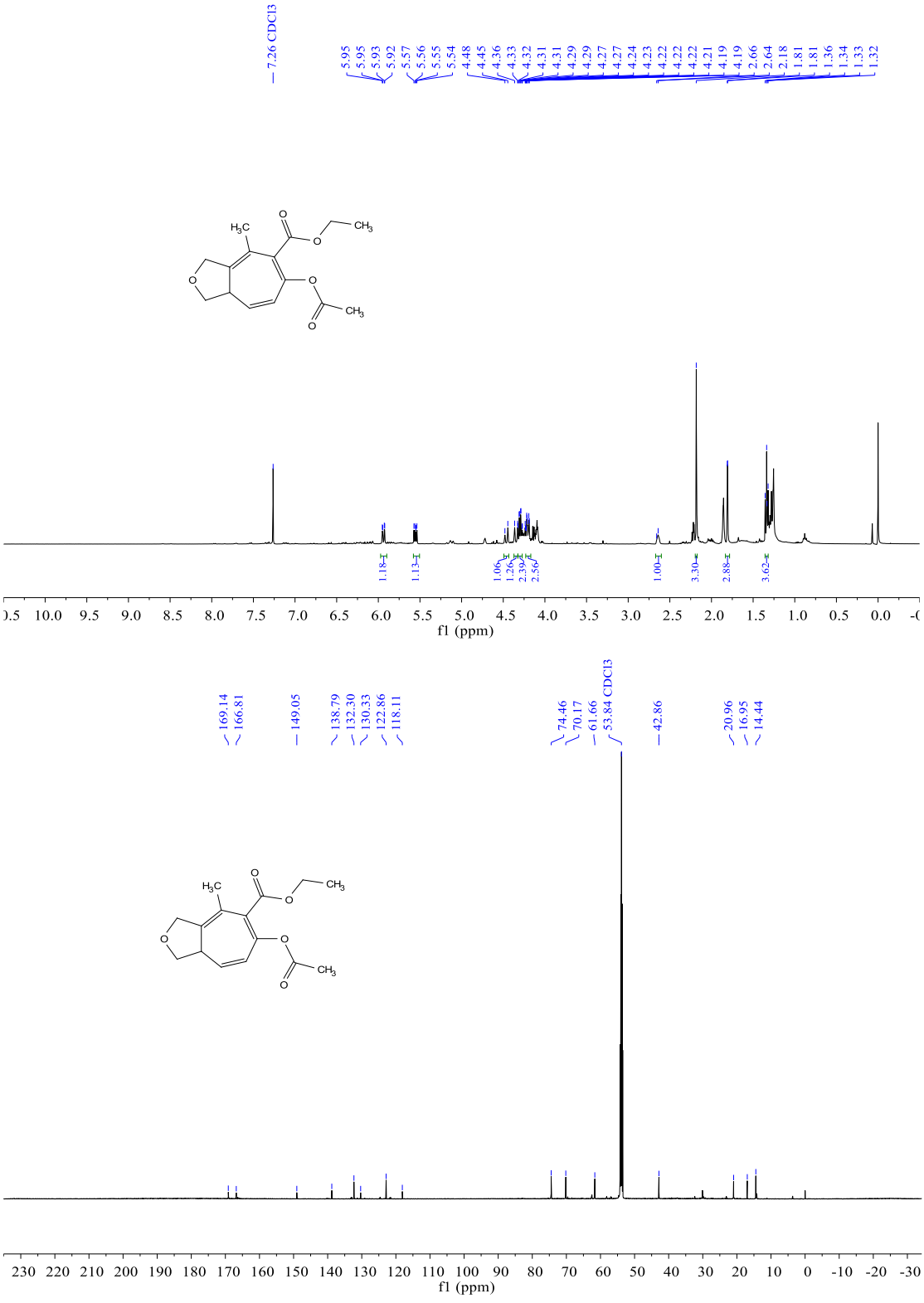

196.74
168.63
152.16
140.80
138.23
133.34
130.00
129.11
128.89
126.75
123.77
119.44
74.85
70.33
53.84 CDCl3
43.27
19.94
14.88
H3C
O
CH3
O
O
O
f1 (ppm)

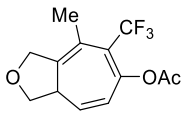

Me
O
OAc
O
2c
OBn
7.79
7.77
7.43
7.43
7.42
7.41
7.41
7.41
7.39
7.37
7.37
7.36
7.35
7.35
7.34
7.26 CDCl3
6.99
6.99
6.97
6.97
6.43
6.41
6.41
5.39
5.38
5.37
5.36
5.16
5.13
5.10
4.56
4.53
4.44
4.41
4.32
4.31
4.29
4.29
4.26
4.24
4.23
4.22
2.67
1.70
1.66
H3C
O
O
CH3
O
O
1.93
5.00
1.93
0.97
0.97
2.15
2.05
2.08
1.00
2.89
2.90
f1 (ppm)


195.08
168.72
162.81
151.02
139.57
136.22
131.49
130.62
130.05
128.83
128.41
127.61
126.41
123.75
119.04
114.77
77.16 CDCl3
74.68
70.26
70.15
42.92
20.15
14.87
H3C
O
O
CH3
O
O
f1 (ppm)

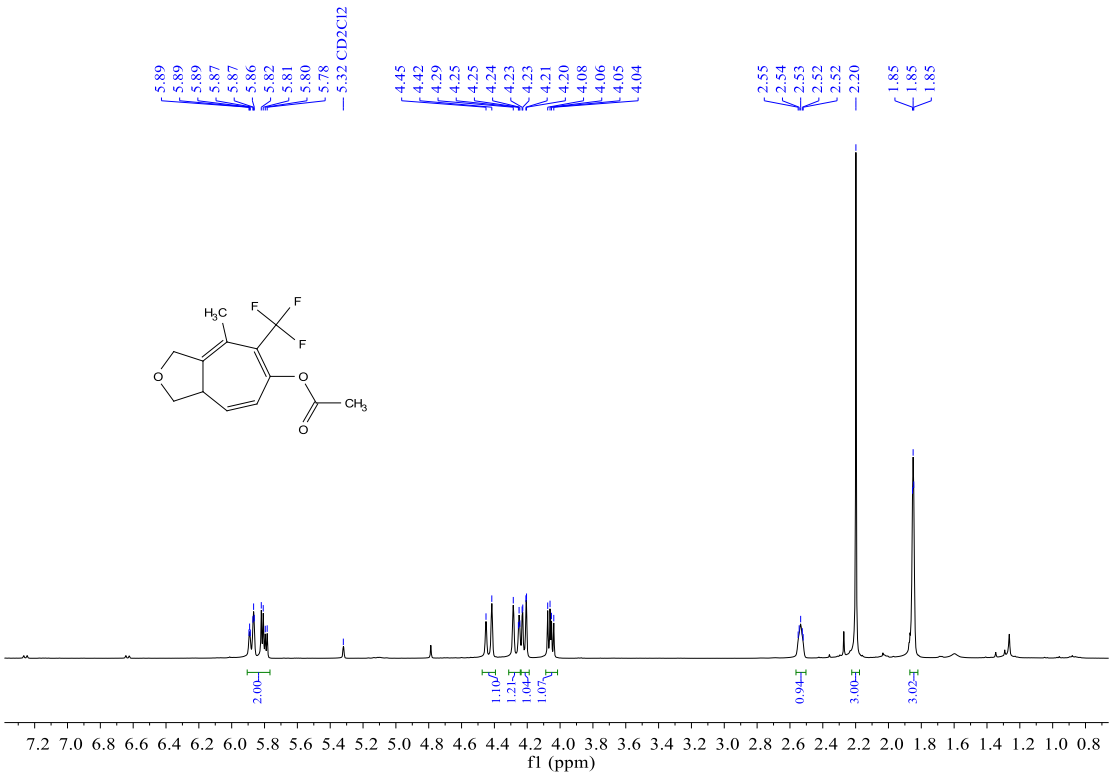

Me
COOEt
O
OAc

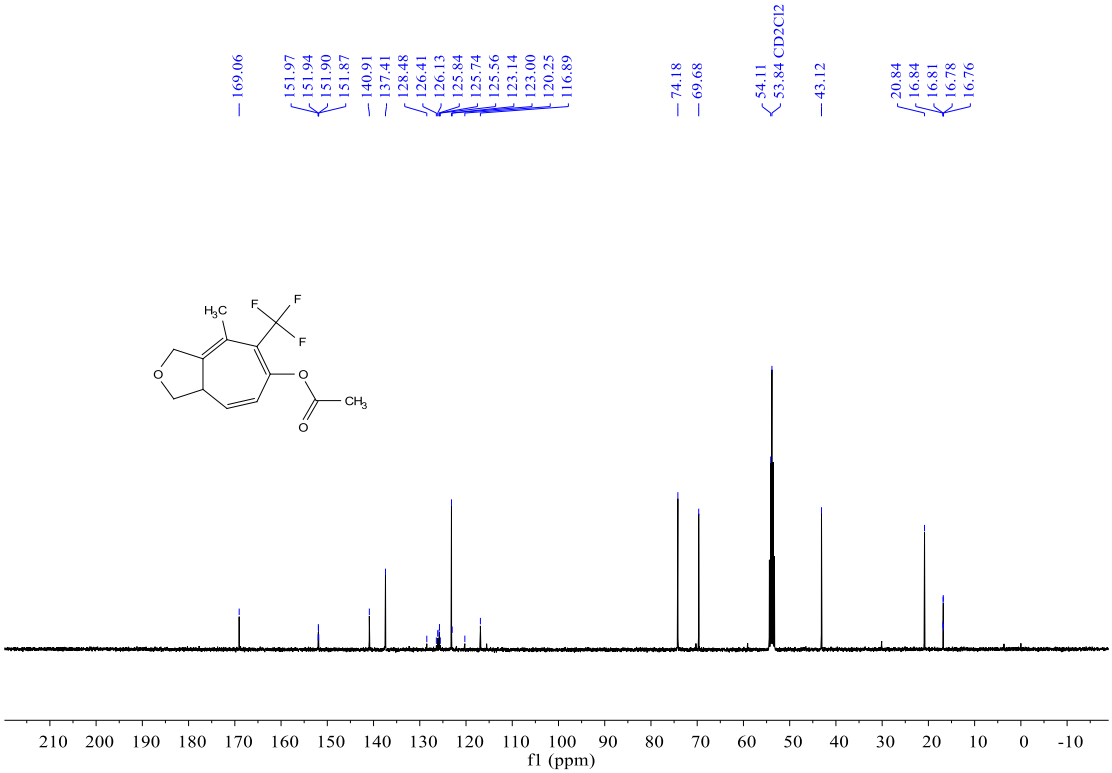
3d

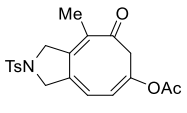

7.26 CDCl3
5.95
5.95
5.93
5.92
5.57
5.56
5.55
5.54
4.48
4.45
4.36
4.33
4.32
4.31
4.31
4.29
4.29
4.27
4.27
4.24
4.23
4.22
4.22
4.22
4.21
4.19
4.19
2.66
2.64
2.18
1.81
1.81
1.36
1.34
1.33
1.32
1.18
1.13
1.05
1.26
2.39
2.56
1.00
3.30
2.88
3.62
f1 (ppm)
169.14
166.81
149.05
138.79
132.30
130.33
122.86
118.11
74.46
70.17
61.66
53.84 CDCl3
42.86
20.96
16.95
14.44
f1 (ppm)


Me
CF3
O
OAc

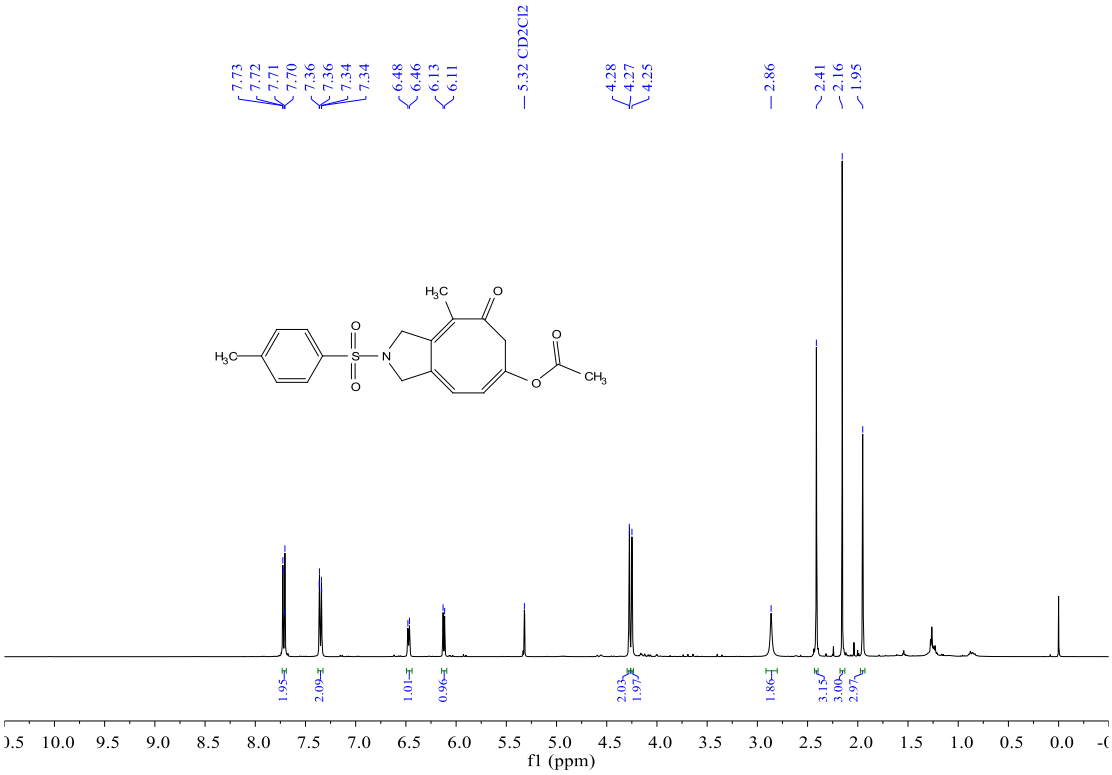
3e

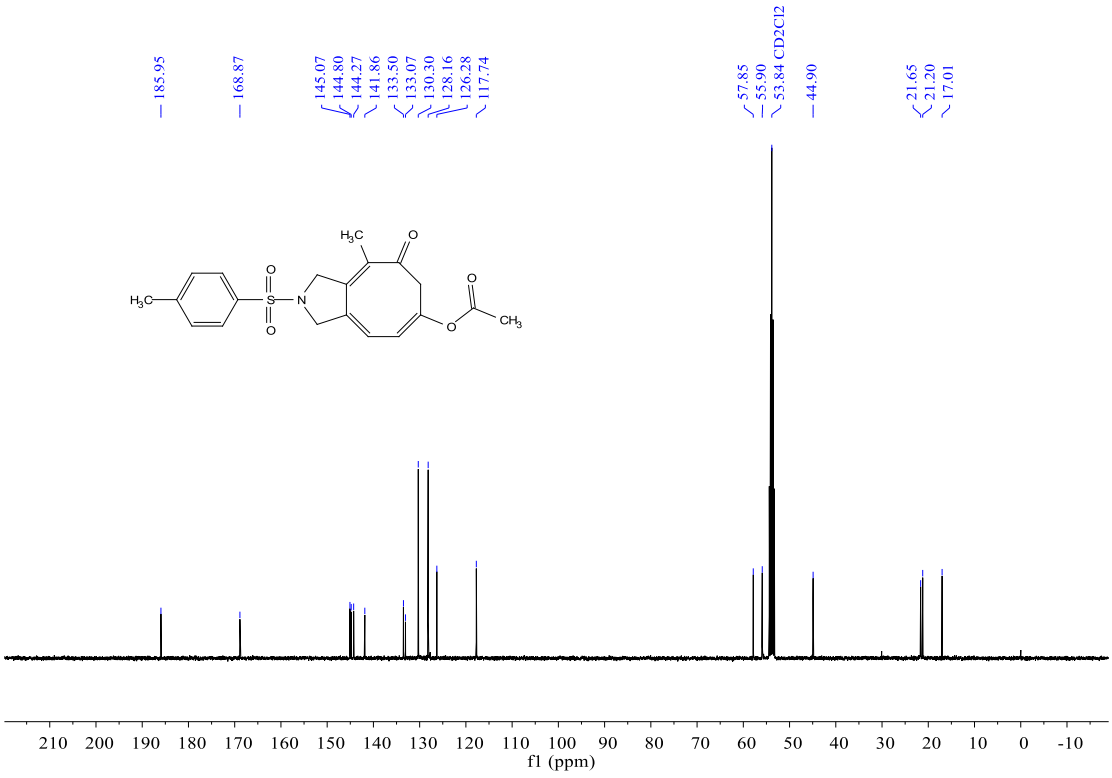

5.89
5.89
5.89
5.87
5.87
5.86
5.82
5.81
5.80
5.78
5.32 CD2Cl2
4.45
4.42
4.29
4.25
4.25
4.24
4.23
4.23
4.21
4.20
4.08
4.06
4.05
4.04
2.55
2.54
2.53
2.52
2.52
2.20
1.85
1.85
1.85
H3C
F
F
F
O
O
O
CH3
2.00
1.10
1.21
1.04
1.07
0.94
3.00
3.02
7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
f1 (ppm)

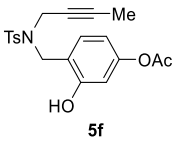

169.06
151.97
151.94
151.90
151.87
140.91
137.41
128.48
126.41
126.13
125.84
125.74
125.56
123.14
123.00
120.25
116.89
74.18
69.68
54.11
53.84 CD2Cl2
43.12
20.84
16.84
16.81
16.78
16.76
H3C
F
F
F
O
O
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Me
O
TsN
OAc

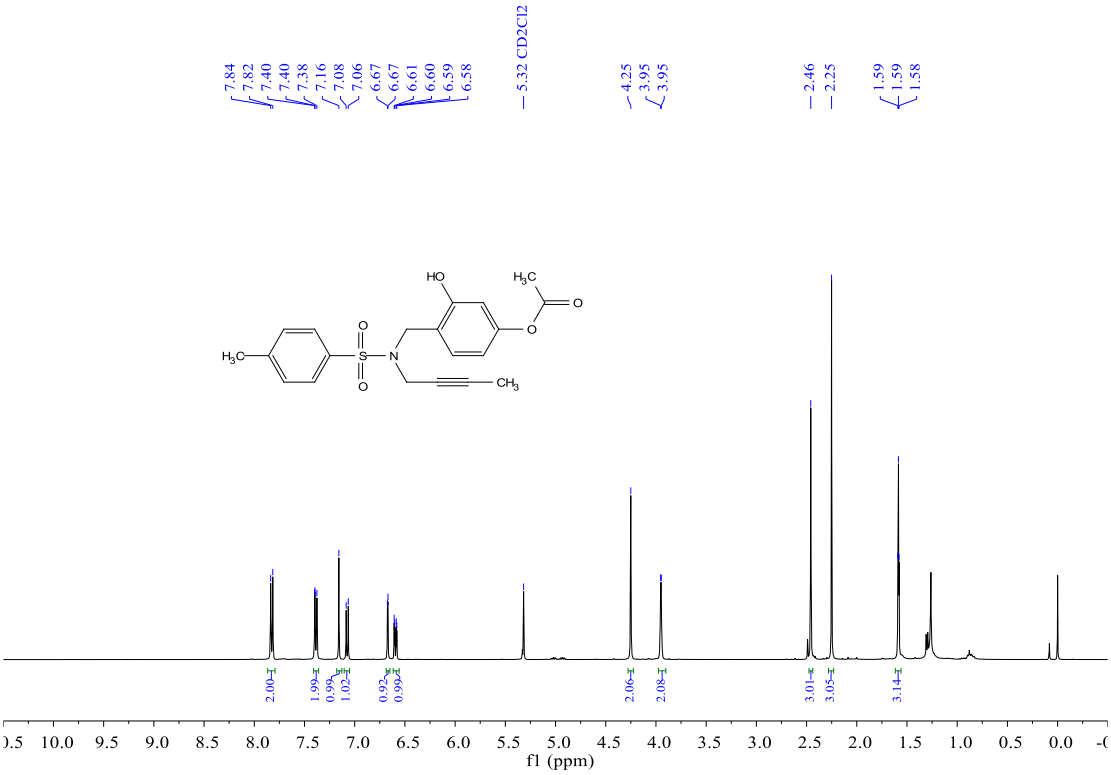
4f

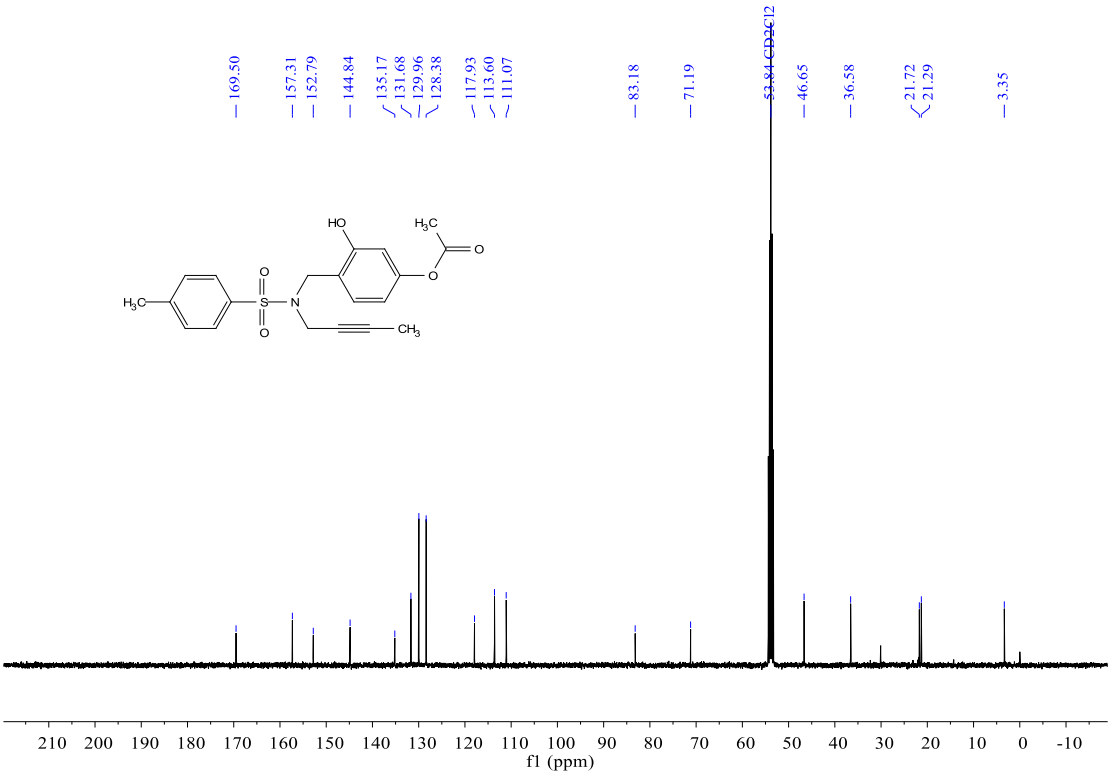

7.73
7.72
7.71
7.70
7.36
7.36
7.34
7.34
6.48
6.46
6.13
6.11
5.32 CD2Cl2
4.28
4.27
4.25
2.86
2.41
2.16
1.95
1.95
2.09
1.01
0.96
2.03
1.97
1.86
3.15
3.00
2.97
f1 (ppm)

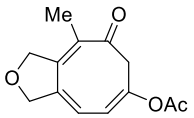

185.95
168.87
145.07
144.80
144.27
141.86
133.50
133.07
130.30
128.16
126.28
117.74
57.85
55.90
53.84 CD2Cl2
44.90
21.65
21.20
17.01
f1 (ppm)


Me
TsN
OAc
HO

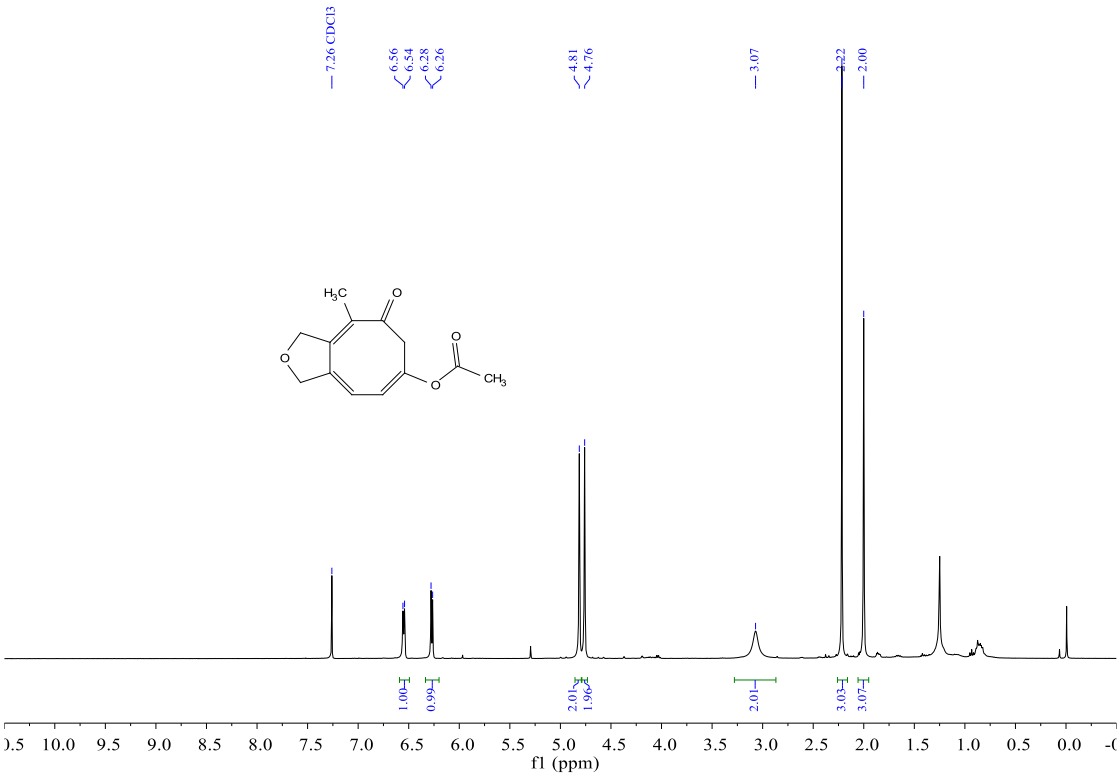
5f

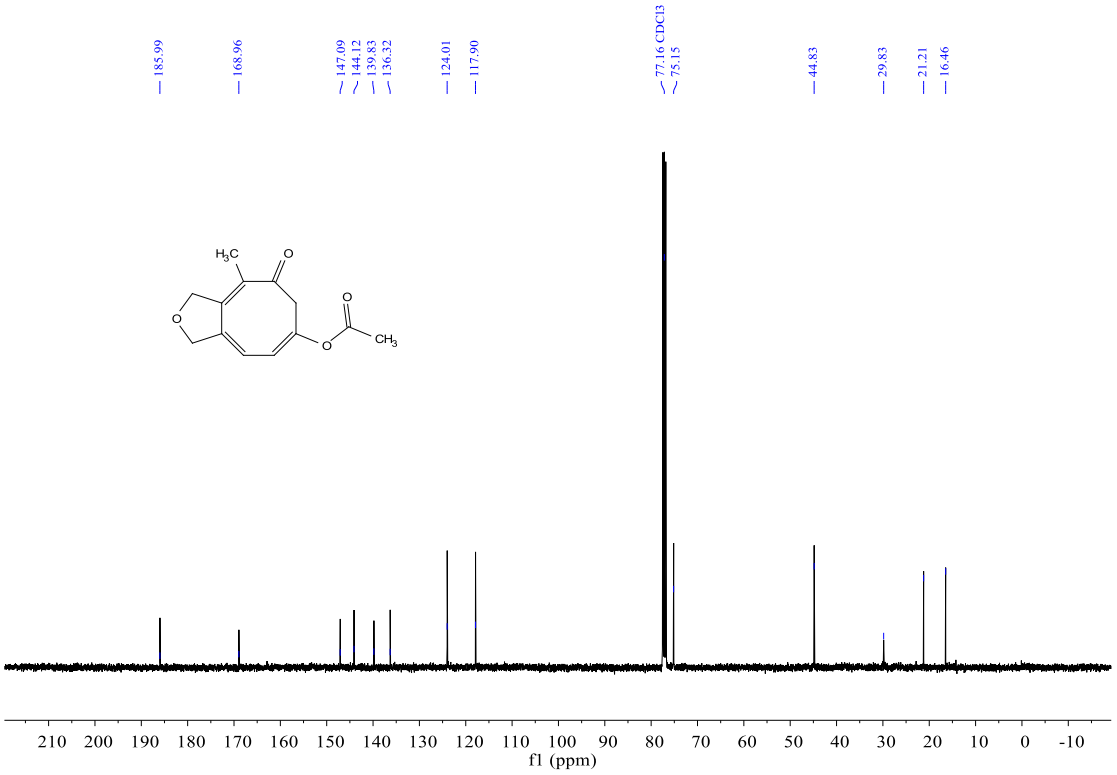

7.84
7.82
7.40
7.40
7.38
7.16
7.08
7.06
6.67
6.67
6.61
6.60
6.59
6.58
5.32 CD2Cl2
4.25
3.95
3.95
2.46
2.25
1.59
1.59
1.58
HO
H3C
O
O
H3C
S
N
O
O
CH3
2.00
1.99
0.90
1.02
0.92
0.99
2.06
2.08
3.01
3.05
3.14
f1 (ppm)

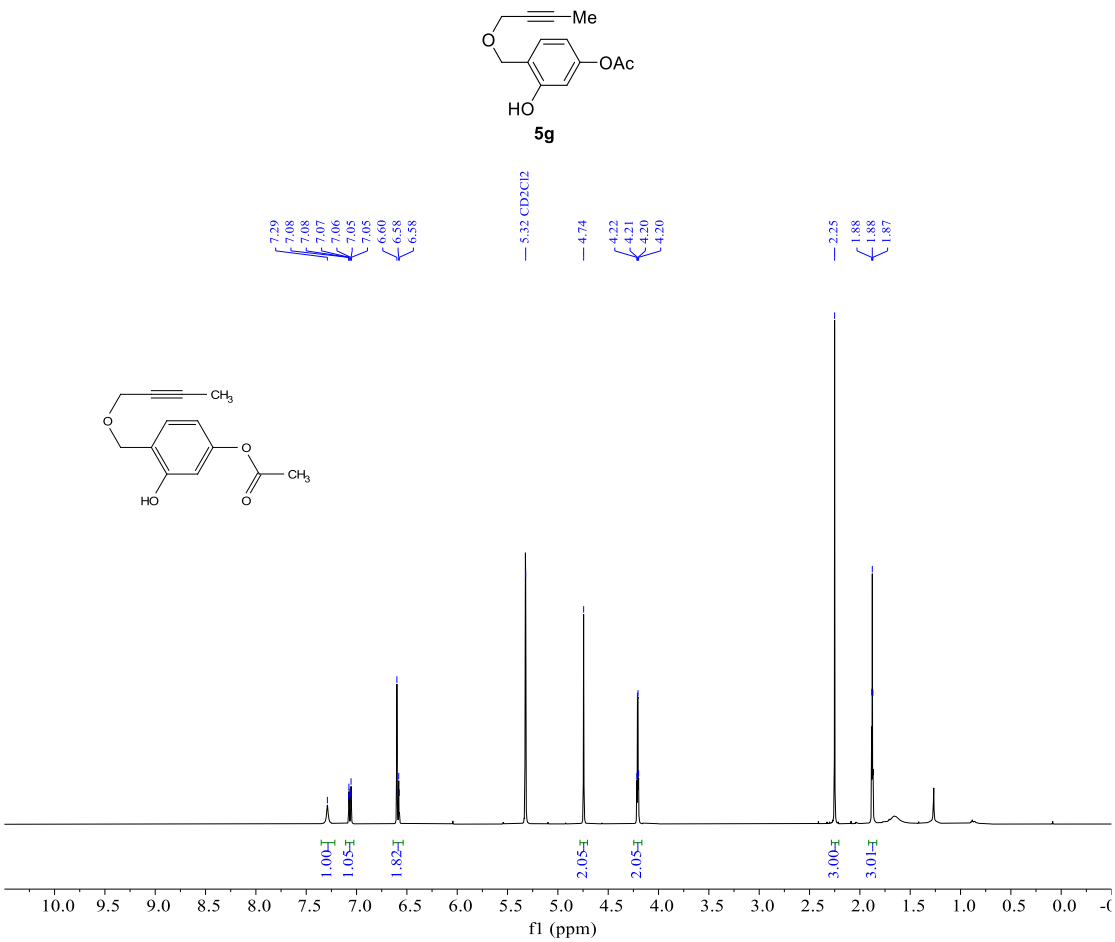

169.50
157.31
152.79
144.84
135.17
131.68
129.96
128.38
117.93
113.60
111.07
83.18
71.19
53.84 CD2Cl2
46.65
36.58
21.72
21.29
3.35
HO
H3C
O
O
H3C
S
N
O
O
CH3
f1 (ppm)

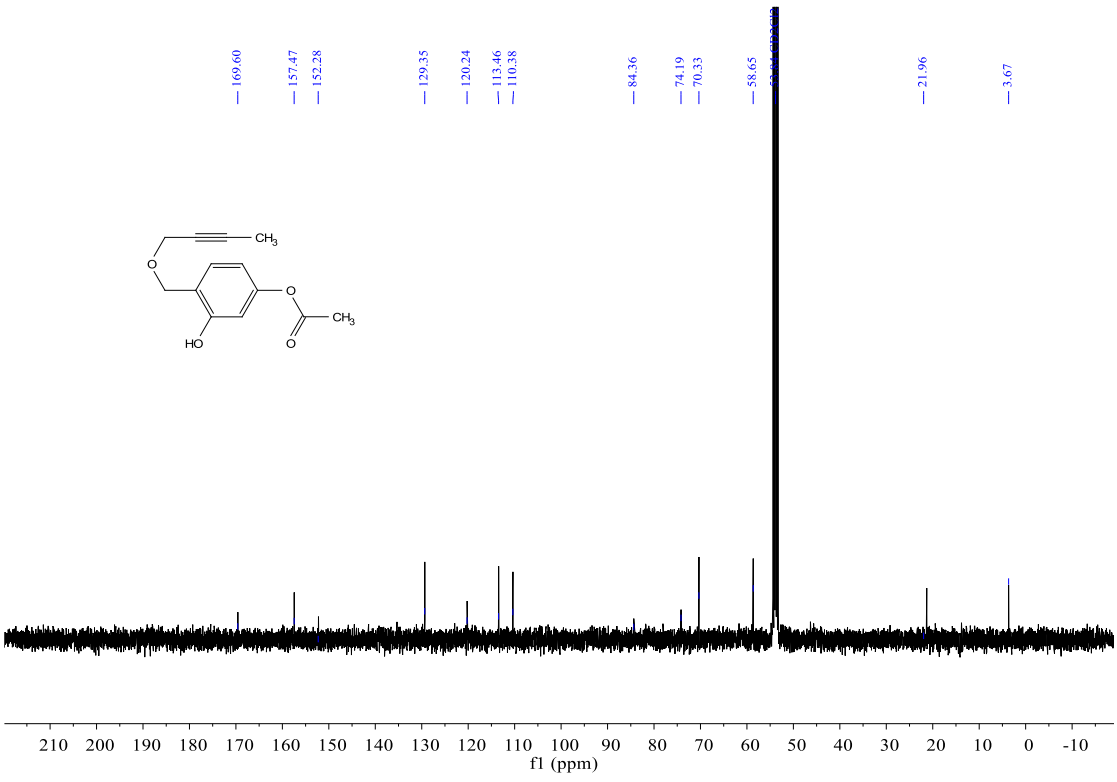

Me
O
O
OAc

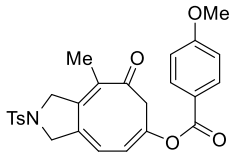
4g


7.26 CDCl3
6.56
6.54
6.28
6.26
4.81
4.76
3.07
2.22
2.00
1.00
0.99
2.01
1.96
2.01
3.03
3.07
f1 (ppm)

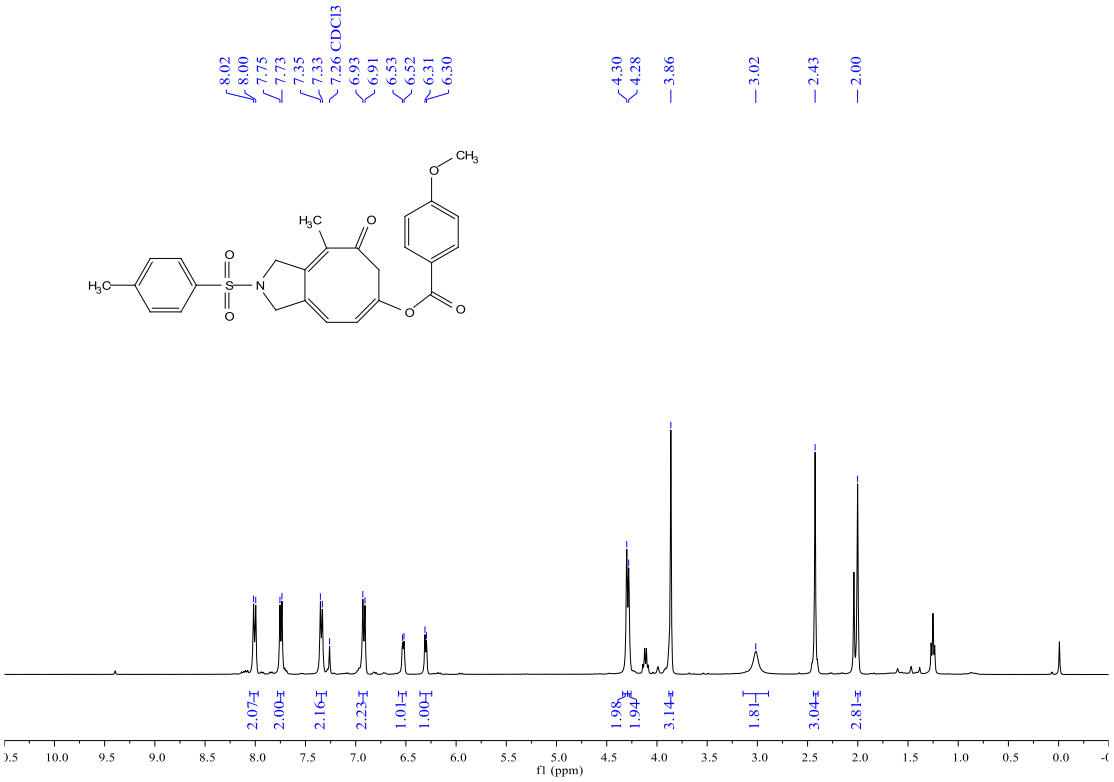

185.99
168.96
147.09
144.12
139.83
136.32
124.01
117.90
77.16 CDCl3
75.15
44.83
29.83
21.21
16.46
f1 (ppm)

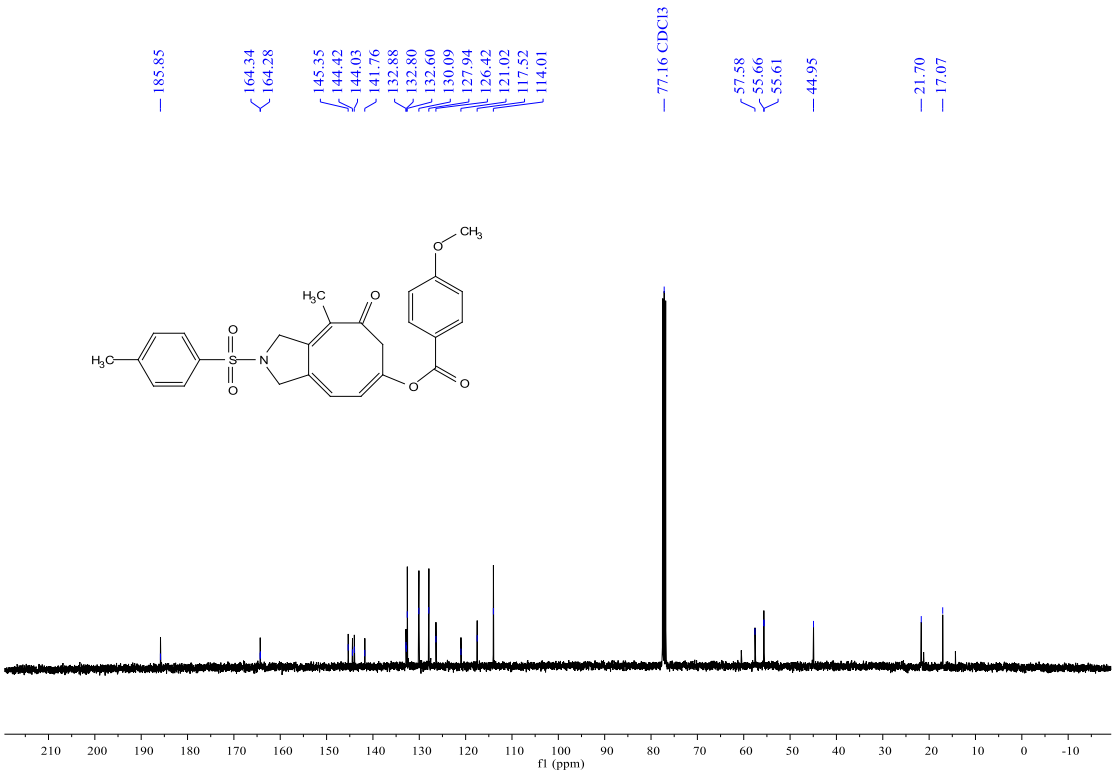

Me
O
OAc
HO
5g
7.29
7.08
7.08
7.07
7.06
7.05
7.05
6.60
6.58
6.58
5.32 CD2Cl2
4.74
4.22
4.21
4.20
4.20
2.25
1.88
1.88
1.87
CH3
O
O
CH3
HO
O
1.00
1.05
1.82
2.05
2.05
3.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

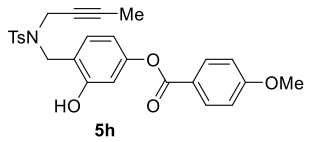

169.60
157.47
152.28
129.35
120.24
113.46
110.38
84.36
74.19
70.33
58.65
21.96
3.67
CH3
O
O
CH3
HO
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OMe
Me
O
TsN
O
O

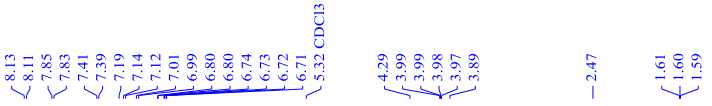
4h

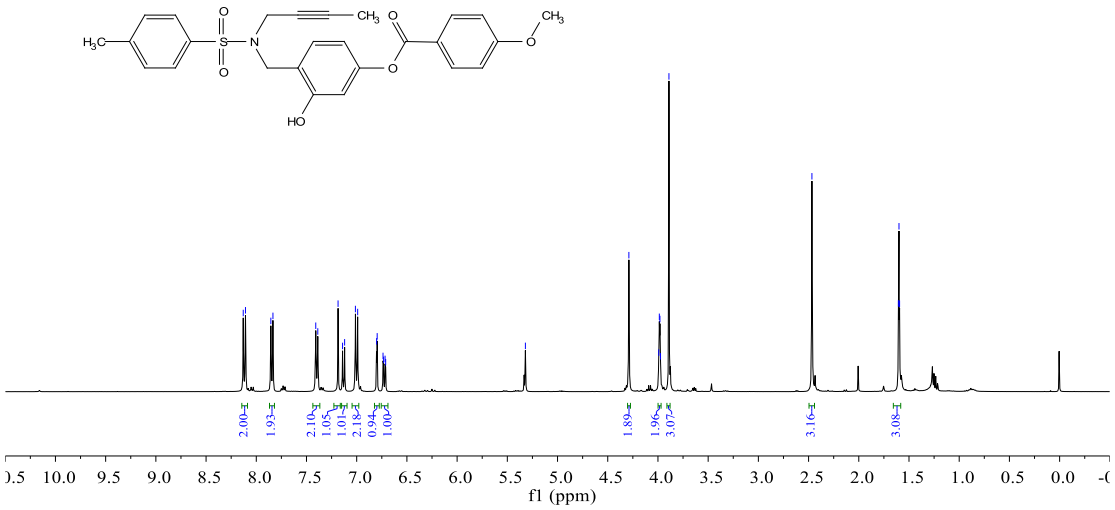

8.02
8.00
7.75
7.73
7.35
7.33
7.26 CDCl3
6.93
6.91
6.53
6.52
6.31
6.30
4.30
4.28
3.86
3.02
2.43
2.00
2.07
2.00
2.16
2.23
1.01
1.00
1.98
1.94
3.14
1.81
3.04
2.81
f1 (ppm)

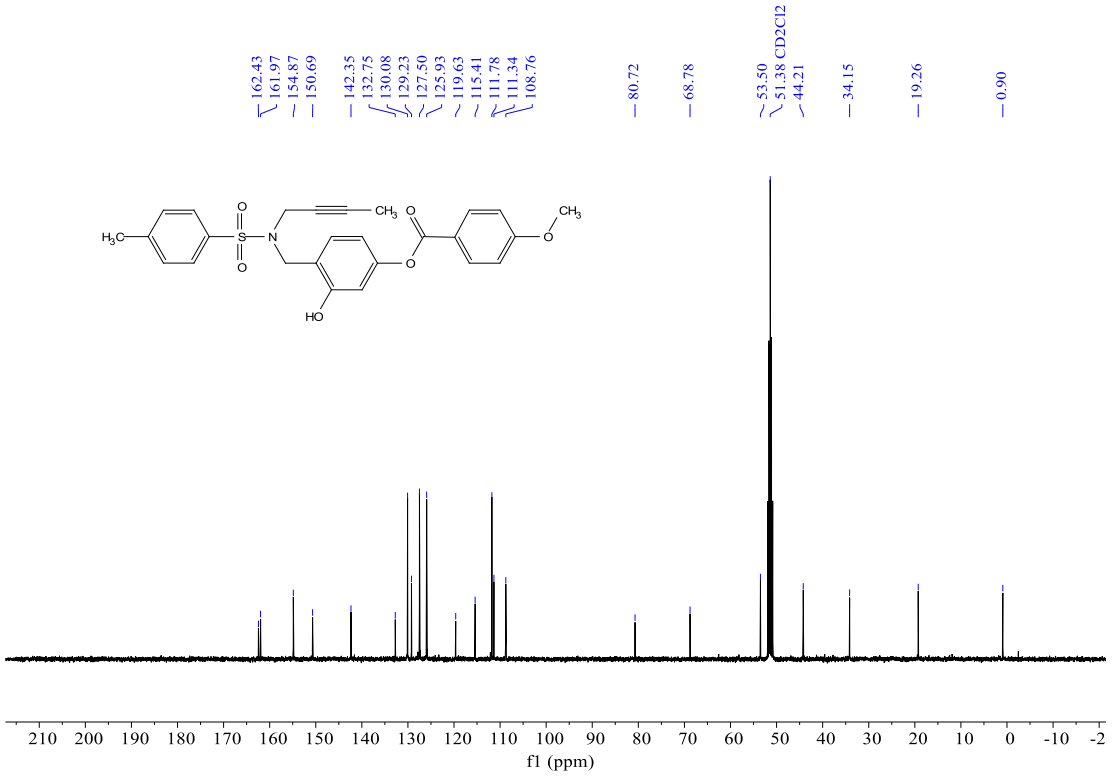

185.85
164.34
164.28
145.35
144.42
144.03
141.76
132.88
132.80
132.60
130.09
127.94
126.42
121.02
117.52
114.01
77.16 CDCl3
57.58
55.66
55.61
44.95
21.70
17.07
f1 (ppm)

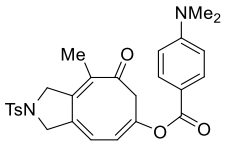

Me
TsN
O
OMe
HO
O

5h

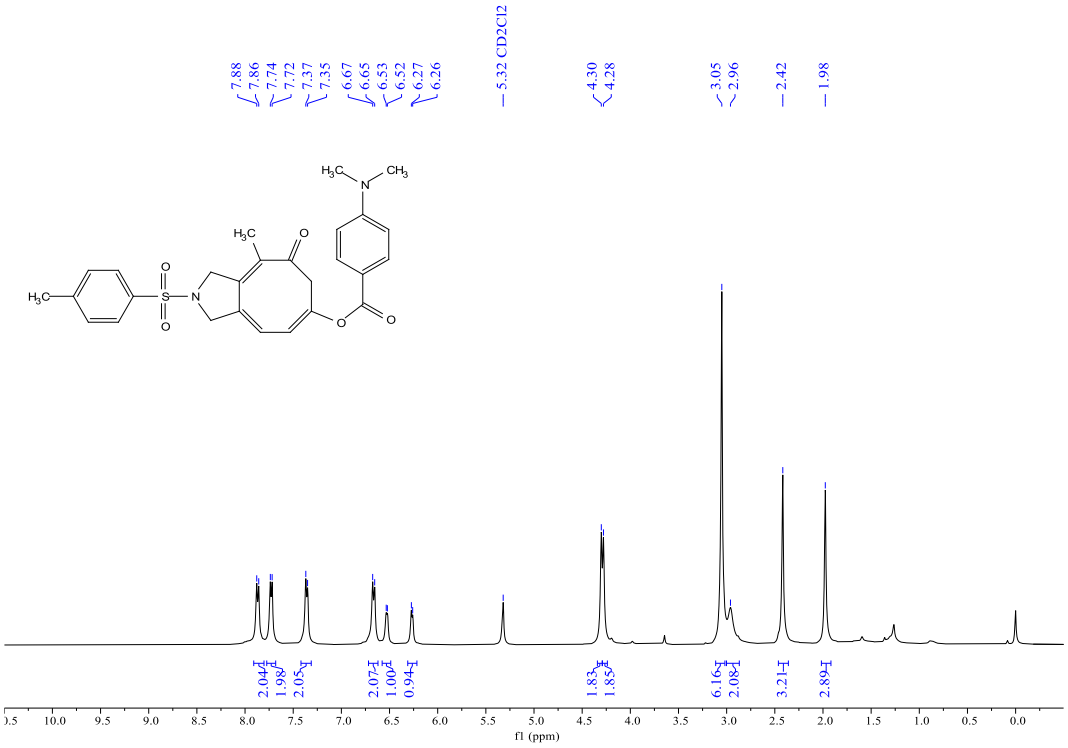

8.13
8.11
7.85
7.83
7.41
7.39
7.19
7.14
7.12
7.01
6.99
6.80
6.80
6.74
6.73
6.72
6.71
5.32 CDCl3
4.29
3.99
3.99
3.98
3.97
3.89
2.47
1.61
1.60
1.59

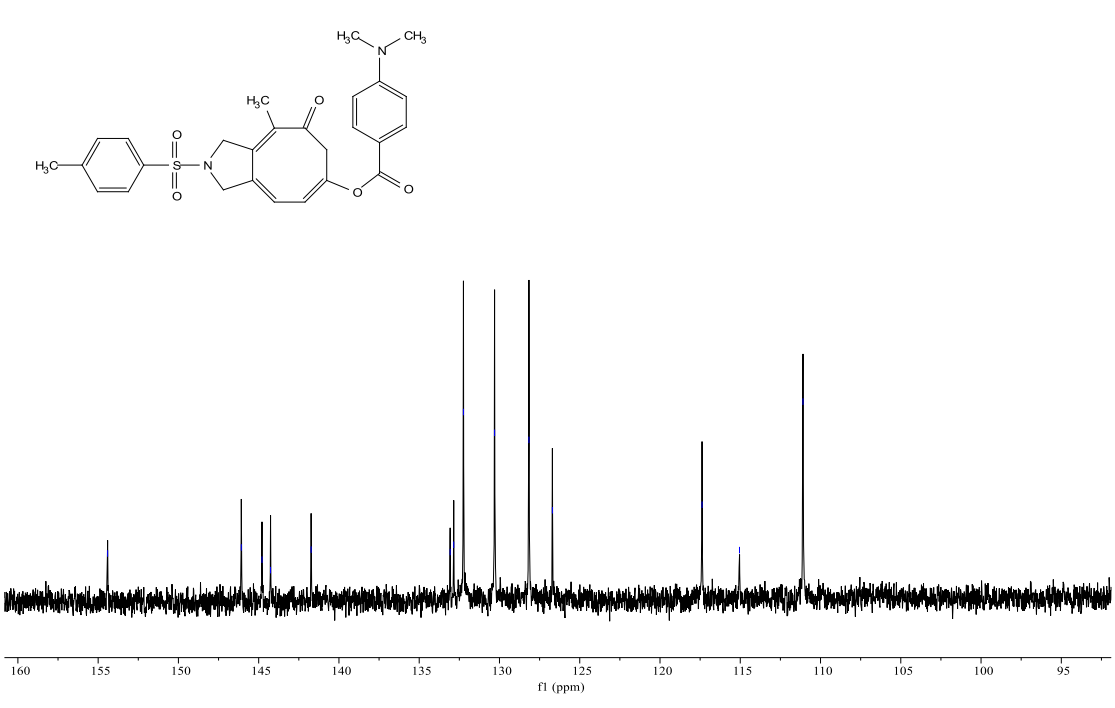

H3C
O
S
O
N
CH3
O
O
HO
O
CH3
2.00
1.93
2.10
1.05
1.01
2.18
0.94
1.00
1.89
1.96
3.07
3.16
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

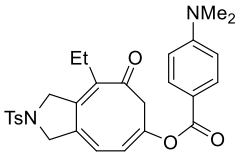

162.43
161.97
154.87
150.69
142.35
132.75
130.08
129.23
127.50
125.93
119.63
115.41
111.78
111.34
108.76
80.72
68.78
53.50
51.38 CD2Cl2
44.21
34.15
19.26
0.90
H3C
O
S
O
N
CH3
O
O
HO
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)


NMe2
Me
O
TsN
O
O

4i

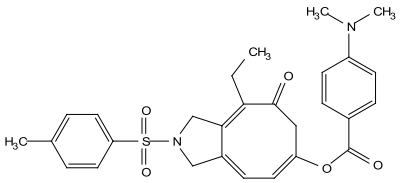

7.88
7.86
7.74
7.72
7.37
7.35
6.67
6.65
6.53
6.52
6.27
6.26
5.32 CD2Cl2
4.30
4.28
3.05
2.96
2.42
1.98
2.04
1.98
2.05
2.07
1.00
0.94
1.83
1.85
6.16
2.08
3.21
2.89
f1 (ppm)

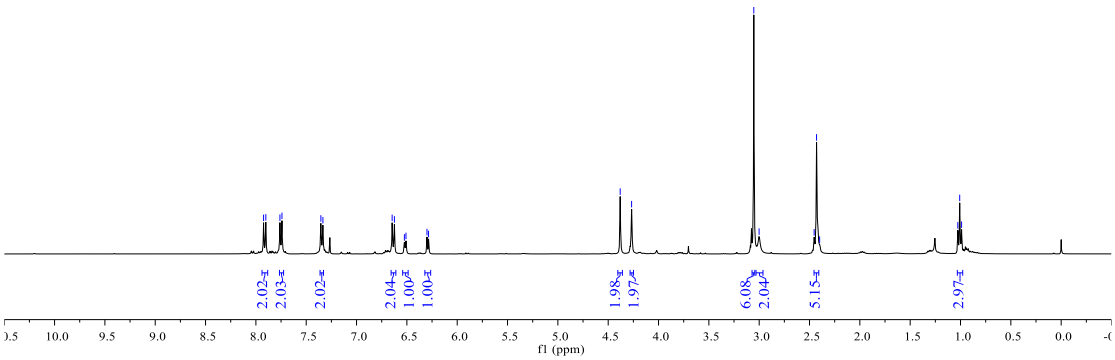

154.41
146.08
144.79
144.26
141.73
133.07
132.85
132.24
130.30
128.16
126.70
117.38
115.05
111.09
f1 (ppm)



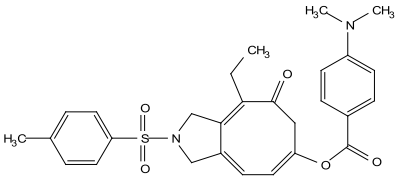
4j

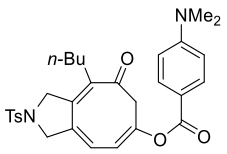
7.92
7.90
7.76
7.74
7.35
7.33
6.65
6.62
6.52
6.51
6.30
6.28
4.38
4.27
3.05
3.00
2.45
2.43
2.40
1.03
1.01
0.99



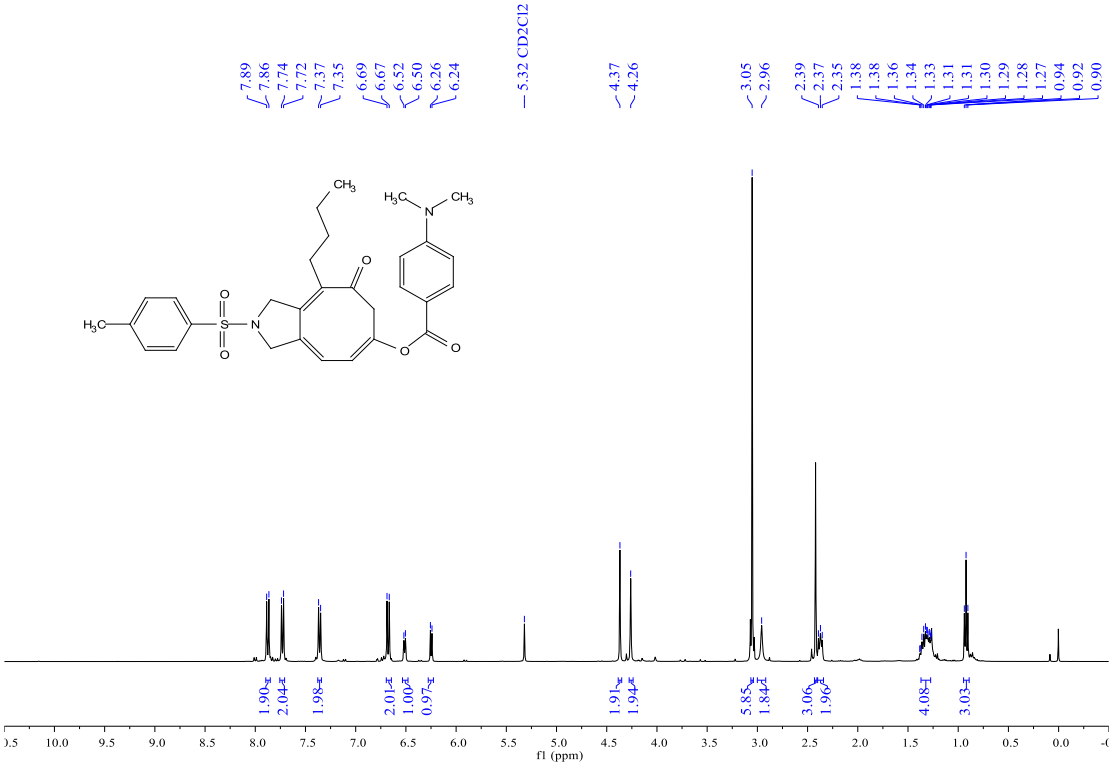


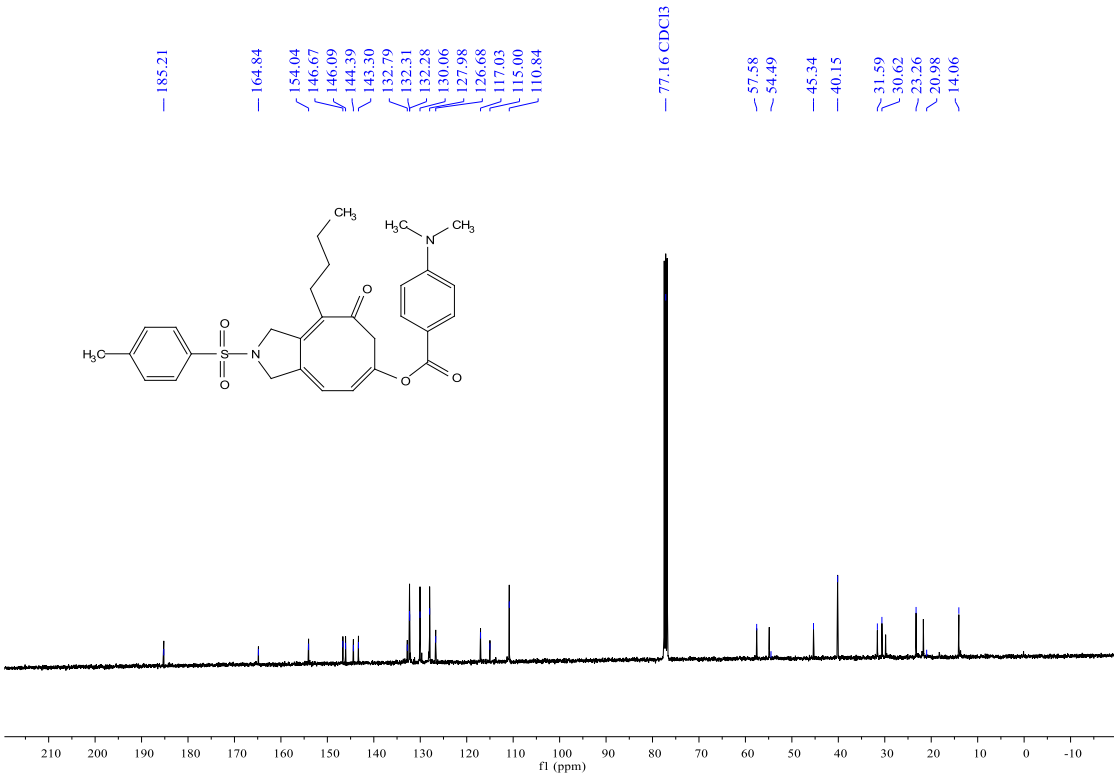
185.04
164.83
154.02
147.68
146.06
144.39
143.23
132.79
132.31
130.06
127.98
126.76
117.06
115.07
110.89
77.16 CDCl3
57.52
54.71
45.38
40.17
24.97
21.69
12.74




NMe2
n-Bu
O
TsN
O
O

4k


7.89
7.86
7.74
7.72
7.37
7.35
6.69
6.67
6.52
6.50
6.26
6.24
5.32 CD2Cl2
4.37
4.26
3.05
2.96
2.39
2.37
2.35
1.38
1.38
1.36
1.34
1.33
1.31
1.31
1.30
1.29
1.28
1.27
0.94
0.92
0.90
1.90
2.04
1.98
2.01
1.00
0.97
1.91
1.94
5.85
1.84
3.06
1.96
4.08
3.03
f1 (ppm)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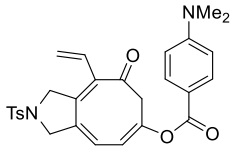
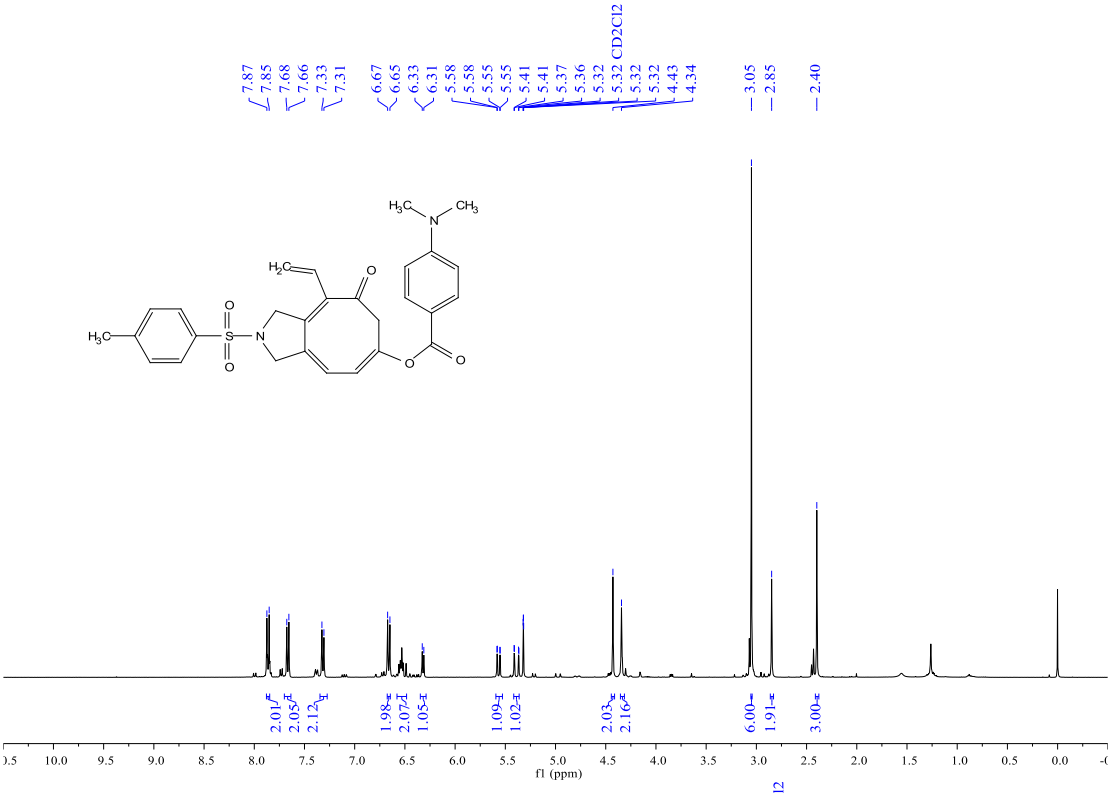
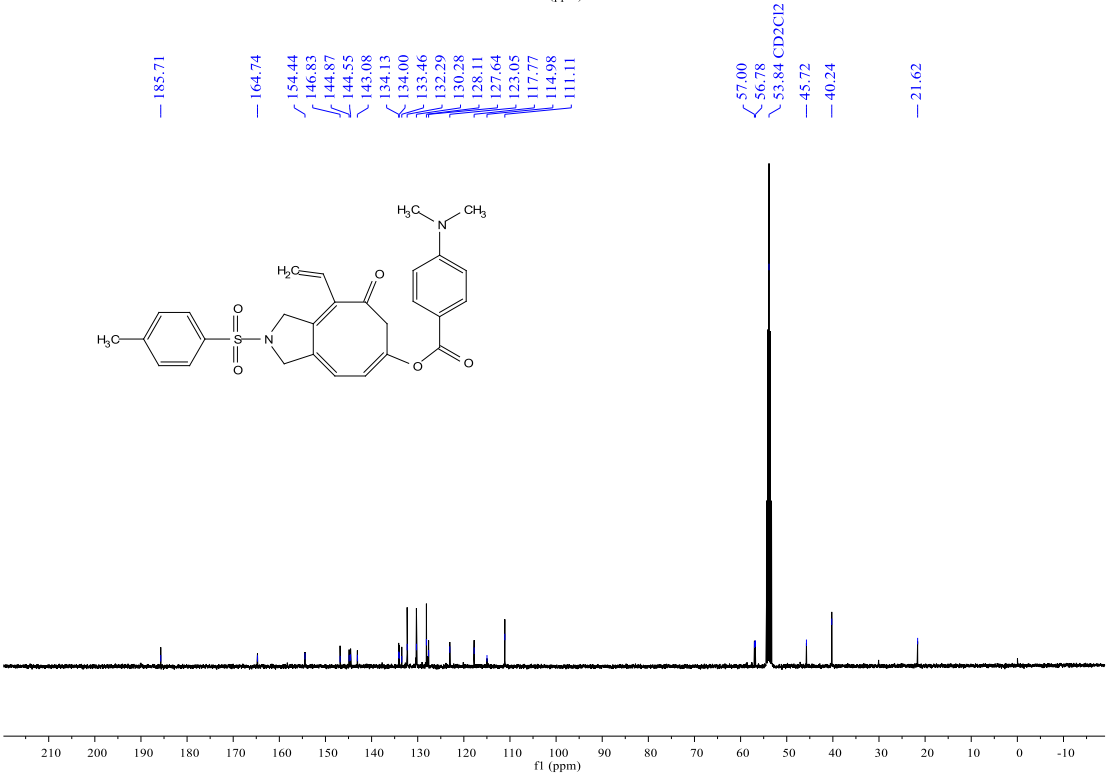
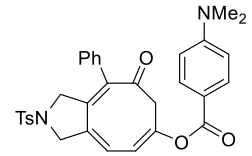
164.84
154.04
146.67
146.09
144.39
143.30
132.79
132.31
132.28
130.06
127.98
126.68
117.03
115.00
110.84
77.16 CDCl3
57.58
54.49
45.34
40.15
31.59
30.62
23.26
20.98
14.06
f1 (ppm)


NMe2
O
TsN
O
O

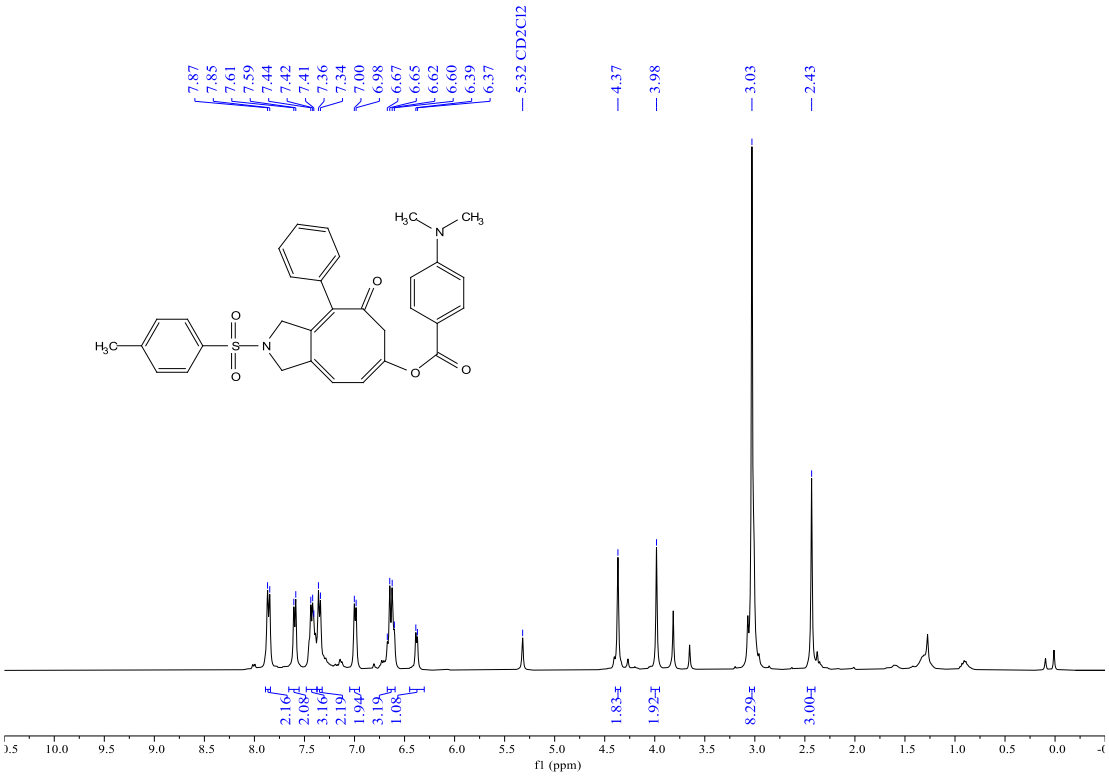
4l

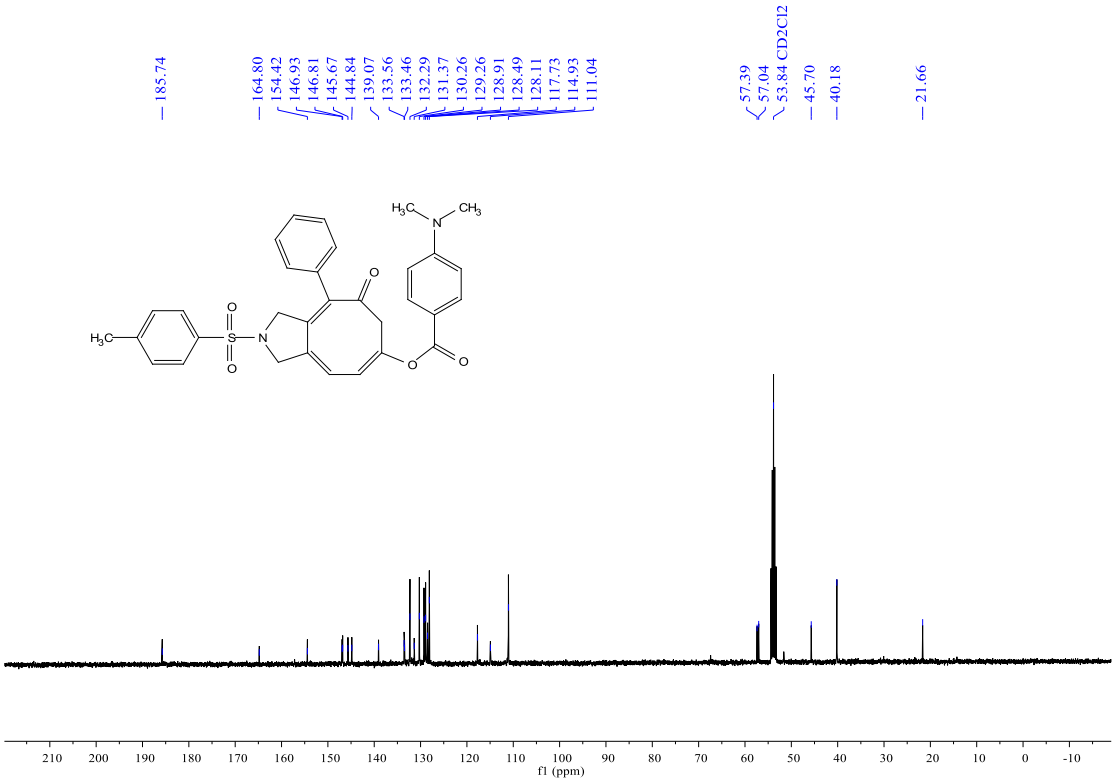

7.87
7.85
7.68
7.66
7.33
7.31
6.67
6.65
6.33
6.31
5.58
5.58
5.55
5.55
5.55
5.41
5.41
5.37
5.36
5.32
5.32 CD2Cl2
5.32
5.32
4.43
4.34
3.05
2.85
2.40
2.01
2.05
2.12
1.98
2.07
1.05
1.09
1.02
2.03
2.16
6.00
1.91
3.00
f1 (ppm)

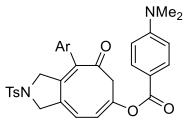

185.71
164.74
154.44
146.83
144.87
144.55
143.08
134.13
134.00
133.46
132.29
130.28
128.11
127.64
123.05
117.77
114.98
111.11
57.00
56.78
53.84 CD2Cl2
45.72
40.24
21.62
f1 (ppm)


NMe2
Ph
O
TsN
O
O

4m

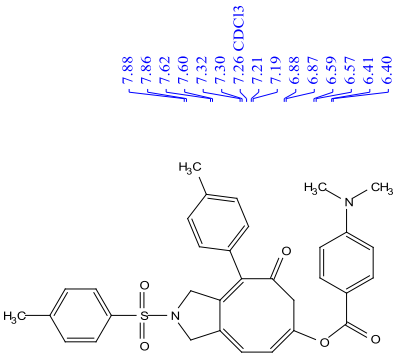

7.87
7.85
7.61
7.59
7.44
7.42
7.41
7.36
7.34
7.00
6.98
6.67
6.65
6.62
6.60
6.39
6.37
5.32 CD2Cl2
4.37
3.98
3.03
2.43
2.16
2.08
3.16
2.19
1.94
3.19
1.08
1.83
1.92
8.29
3.00
f1 (ppm)

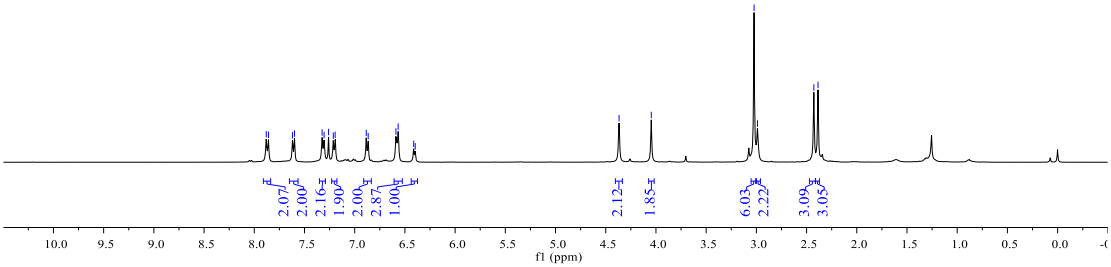

185.74
164.80
154.42
146.93
146.81
145.67
144.84
139.07
133.56
133.46
132.29
131.37
130.26
129.26
128.91
128.49
128.11
117.73
114.93
111.04
57.39
57.04
53.84 CD2Cl2
45.70
40.18
21.66
f1 (ppm)

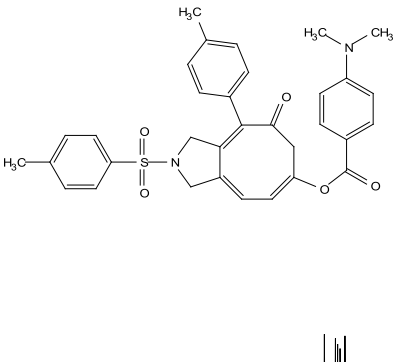


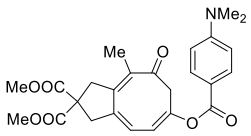
Ar = p-MeC$_6$H$_4$

4n

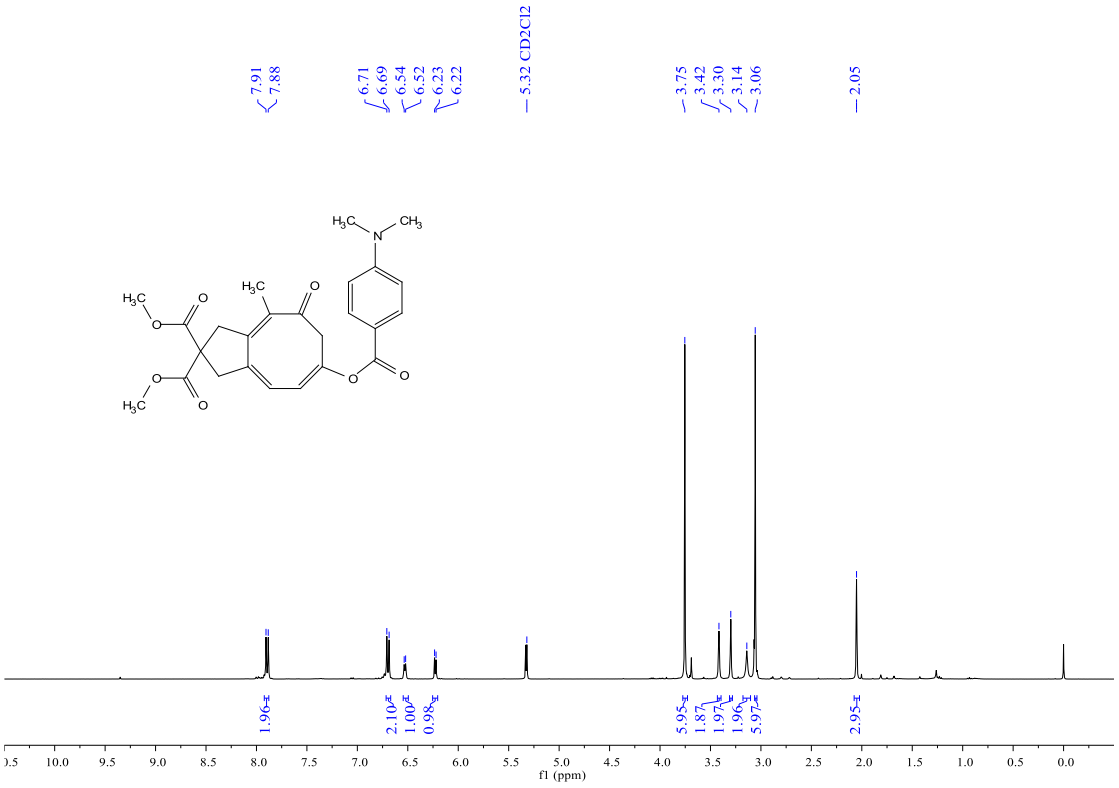


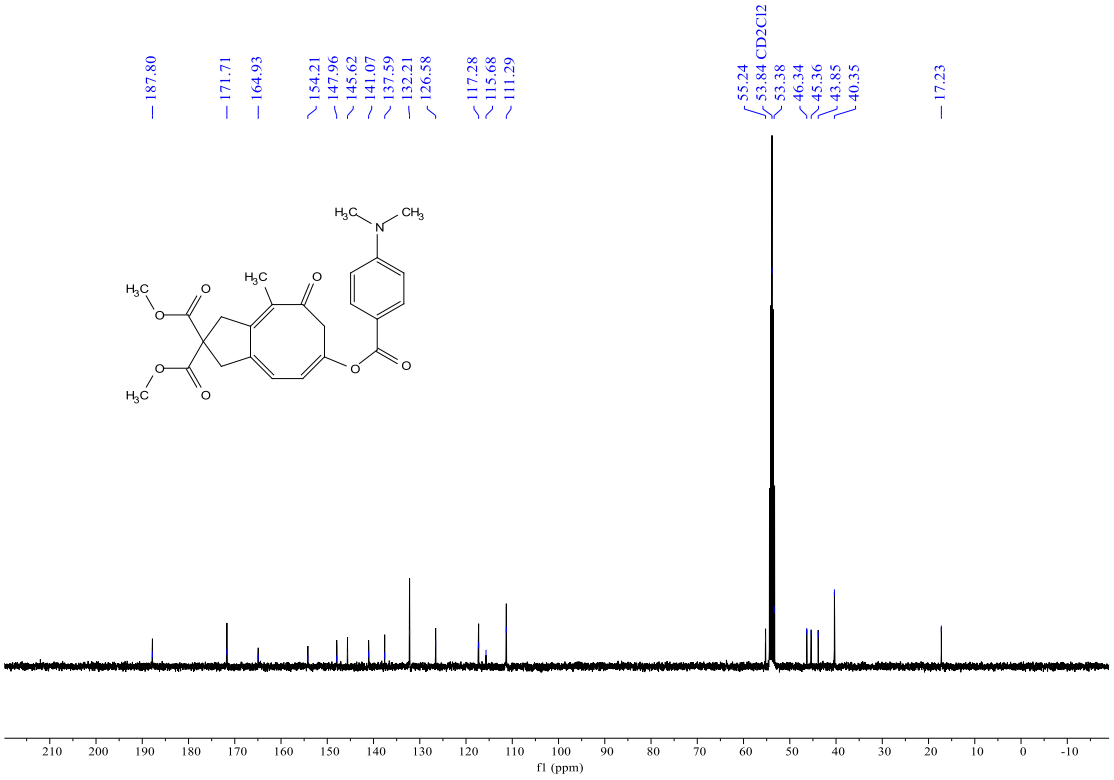


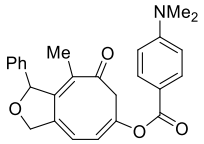



NMe2
Me
O
MeOOC
MeOOC
O
O

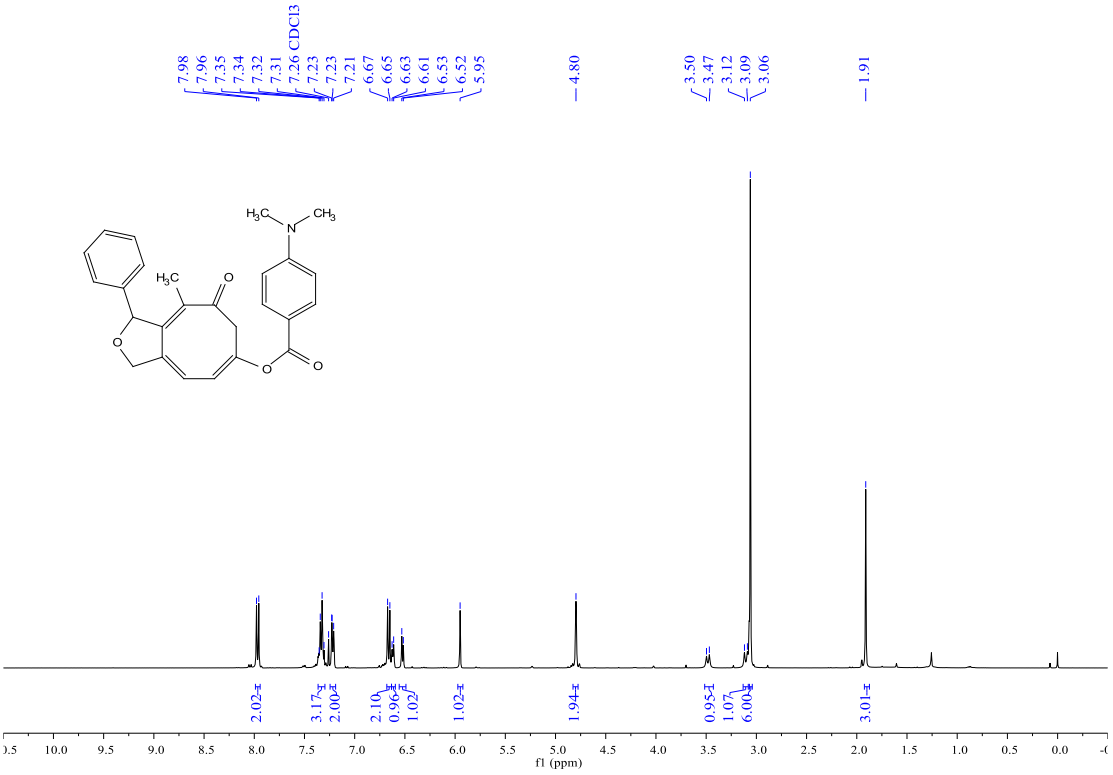
4o

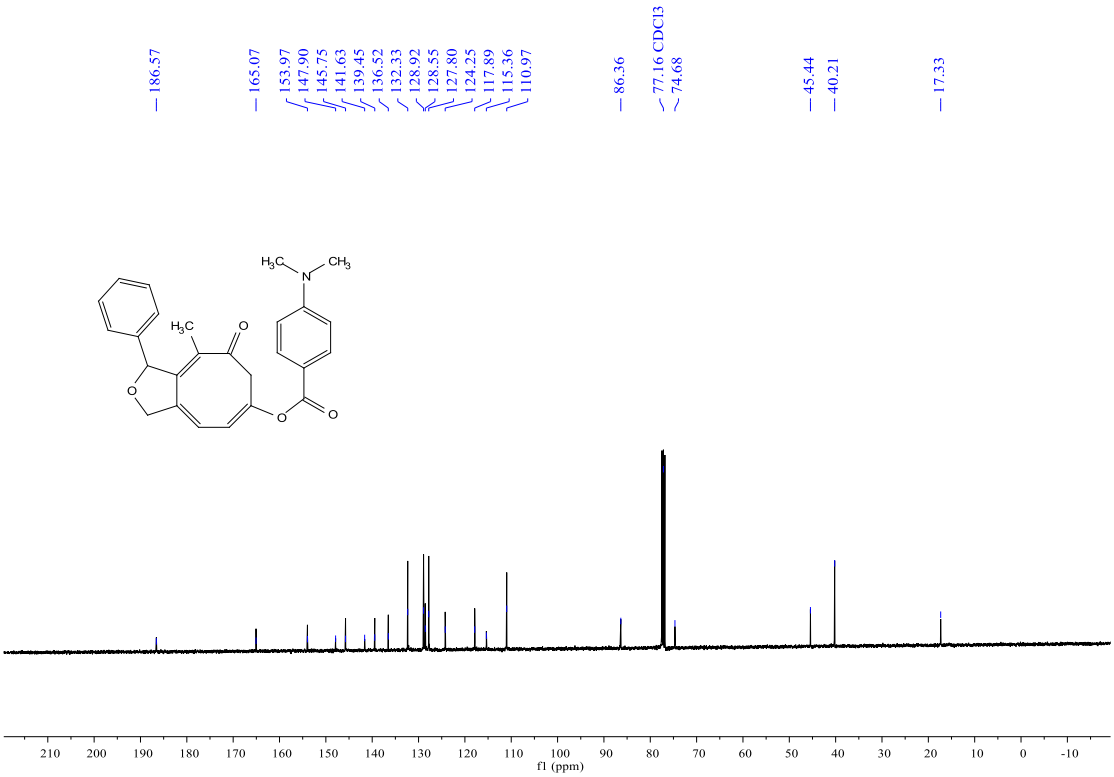

7.91
7.88
6.71
6.69
6.54
6.52
6.23
6.22
5.32 CD2Cl2
3.75
3.42
3.30
3.14
3.06
2.05
1.96
2.10
1.00
0.98
5.95
1.87
1.97
1.96
5.97
2.95
f1 (ppm)


187.80
171.71
164.93
154.21
147.96
145.62
141.07
137.59
132.21
126.58
117.28
115.68
111.29
55.24
53.84 CD2Cl2
53.38
46.34
45.36
43.85
40.35
17.23
f1 (ppm)

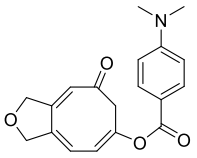

NMe2
Ph
Me
O
O
O
O

4p


7.98
7.96
7.35
7.34
7.32
7.31
7.26 CDCl3
7.23
7.23
7.21
6.67
6.65
6.63
6.61
6.53
6.52
5.95
4.80
3.50
3.47
3.12
3.09
3.06
1.91
H3C
N
CH3
H3C
O
O
O
O
2.02
3.17
2.00
2.10
0.96
1.02
1.02
1.94
0.95
1.07
6.00
3.01
f1 (ppm)

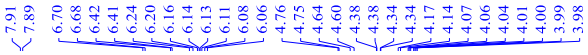

186.57
165.07
153.97
147.90
145.75
141.63
139.45
136.52
132.33
128.92
128.55
127.80
124.25
117.89
115.36
110.97
86.36
77.16 CDCl3
74.68
45.44
40.21
17.33
H3C
N
CH3
H3C
O
O
O
O
f1 (ppm)

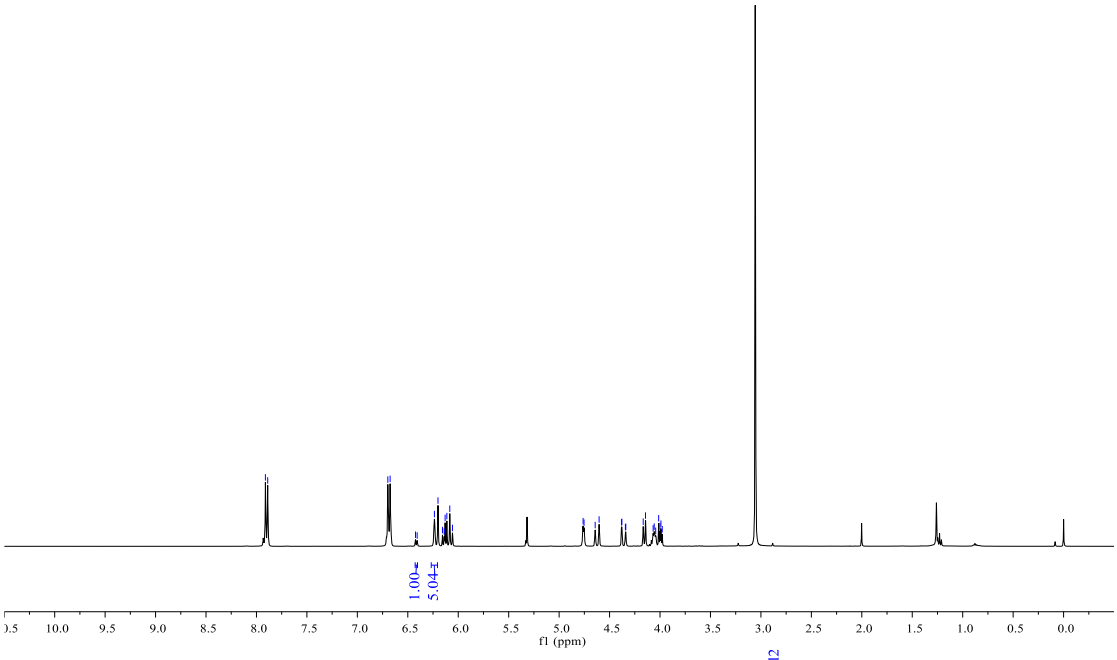
4q : 4q' = 1 : 5

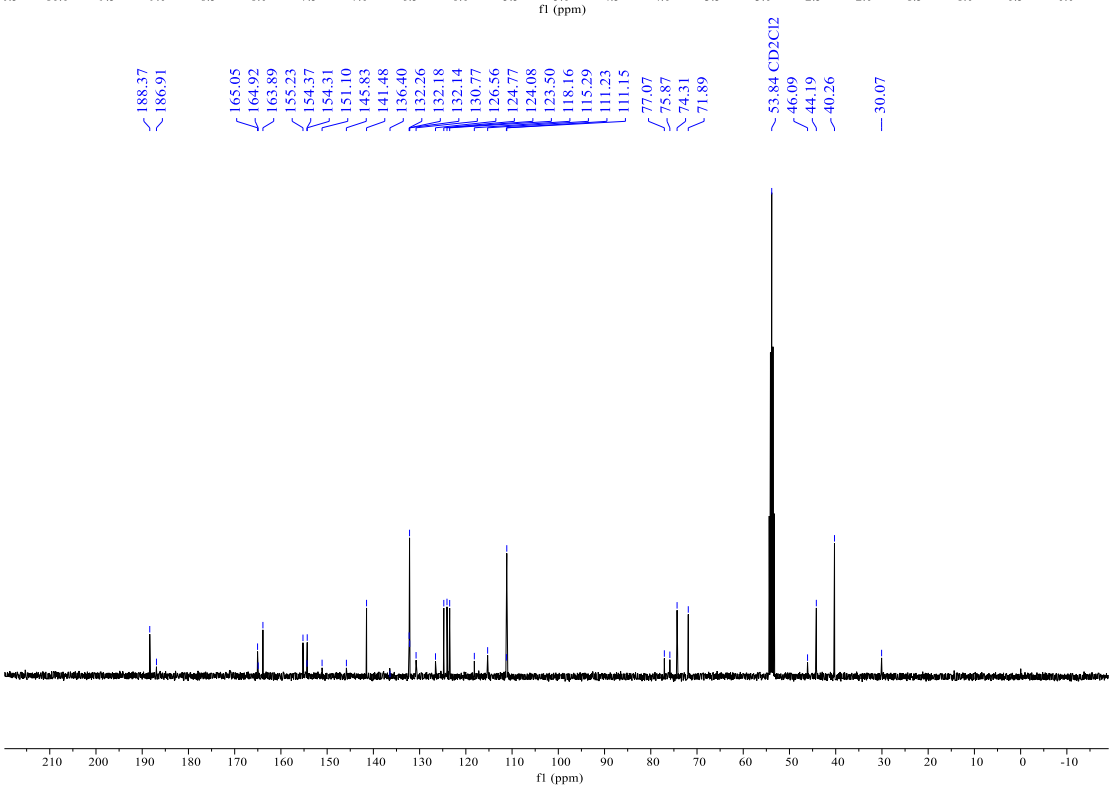


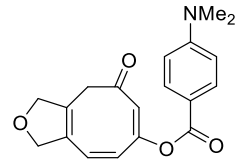
4q

4q'

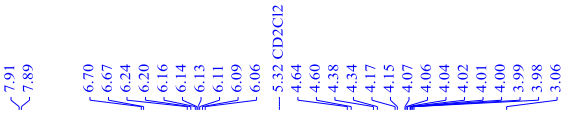

7.91
7.89
6.70
6.68
6.42
6.41
6.24
6.20
6.16
6.14
6.13
6.11
6.08
6.06
4.76
4.75
4.64
4.60
4.38
4.38
4.34
4.34
4.17
4.14
4.07
4.06
4.04
4.01
4.00
3.99
3.98


1.00
5.04
f1 (ppm)


188.37
186.91
165.05
164.92
163.89
155.23
154.37
154.31
151.10
145.83
141.48
136.40
132.26
132.18
132.14
130.77
126.56
124.77
124.08
123.50
118.16
115.29
111.23
111.15
77.07
75.87
74.31
71.89
53.84 CD2Cl2
46.09
44.19
40.26
30.07
f1 (ppm)


NMe2
O
O
O
O

4q'


7.91
7.89
6.70
6.67
6.24
6.20
6.16
6.14
6.13
6.11
6.09
6.06
5.32 CD2Cl2
4.64
4.60
4.38
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4.07
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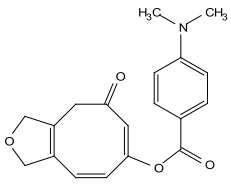
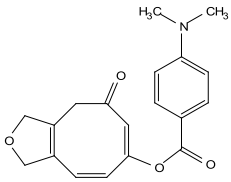
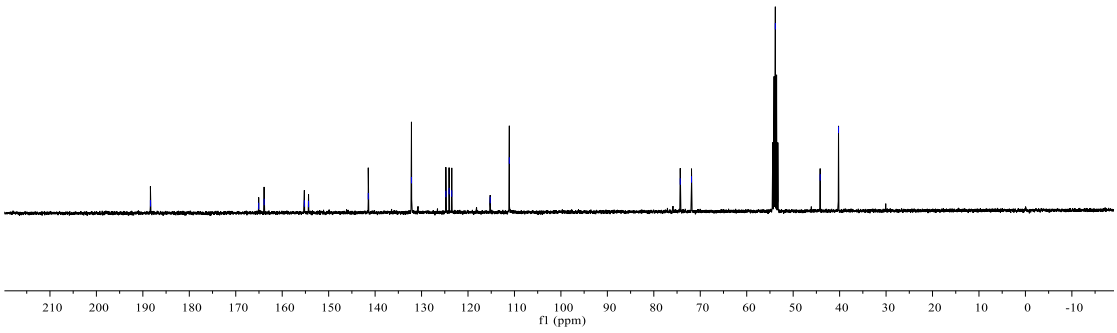
4.04
4.02
4.01
4.00
3.99
3.98
3.06

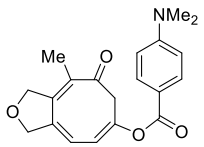

H3C
N
CH3
O
O
O
O

2.00
2.07
0.97
0.92
1.05
0.90
0.99
0.99
0.99
1.02
0.97
6.06
f1 (ppm)

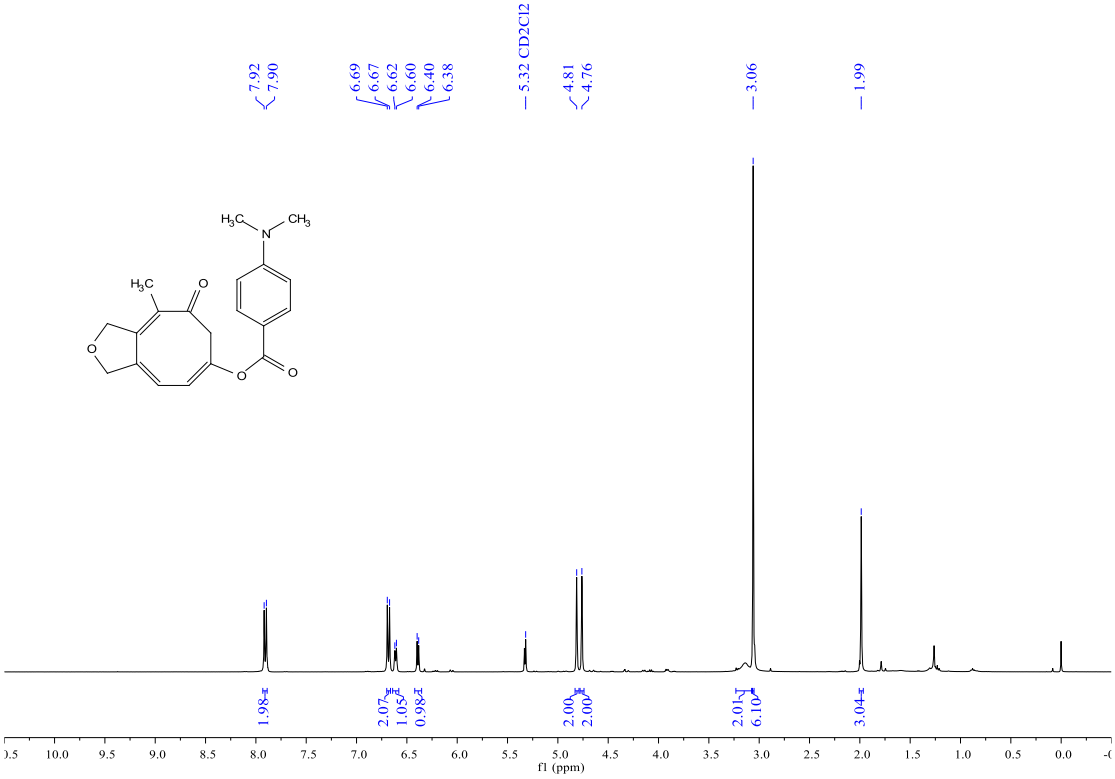

188.37
165.06
163.90
155.23
154.33
141.48
132.18
124.77
124.07
123.49
115.23
111.11
74.31
71.89
53.84 CD2Cl2
44.19
40.23

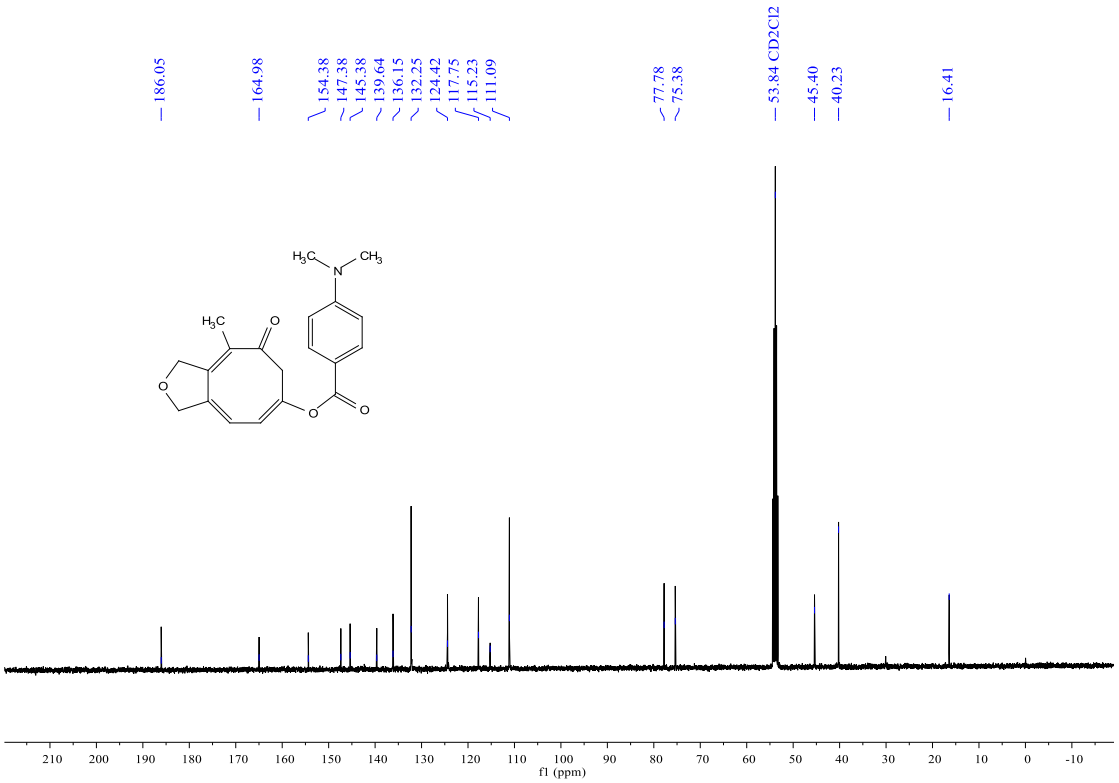

H3C
N
CH3
O
O
O
O

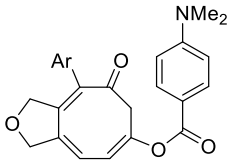

f1 (ppm)


NMe2
Me
O
O
O
O

4r

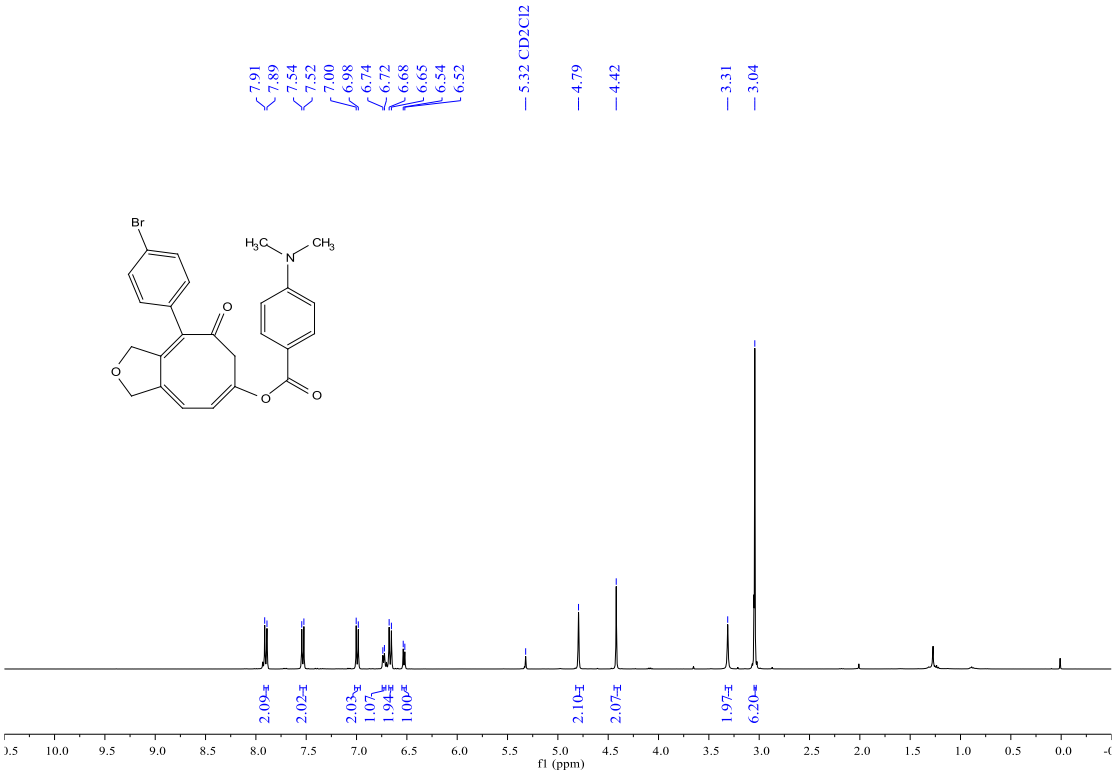

7.92
7.90
6.69
6.67
6.62
6.60
6.40
6.38
5.32 CD2Cl2
4.81
4.76
3.06
1.99
1.98
2.07
1.05
0.98
2.00
2.00
2.01
6.10
3.04
f1 (ppm)

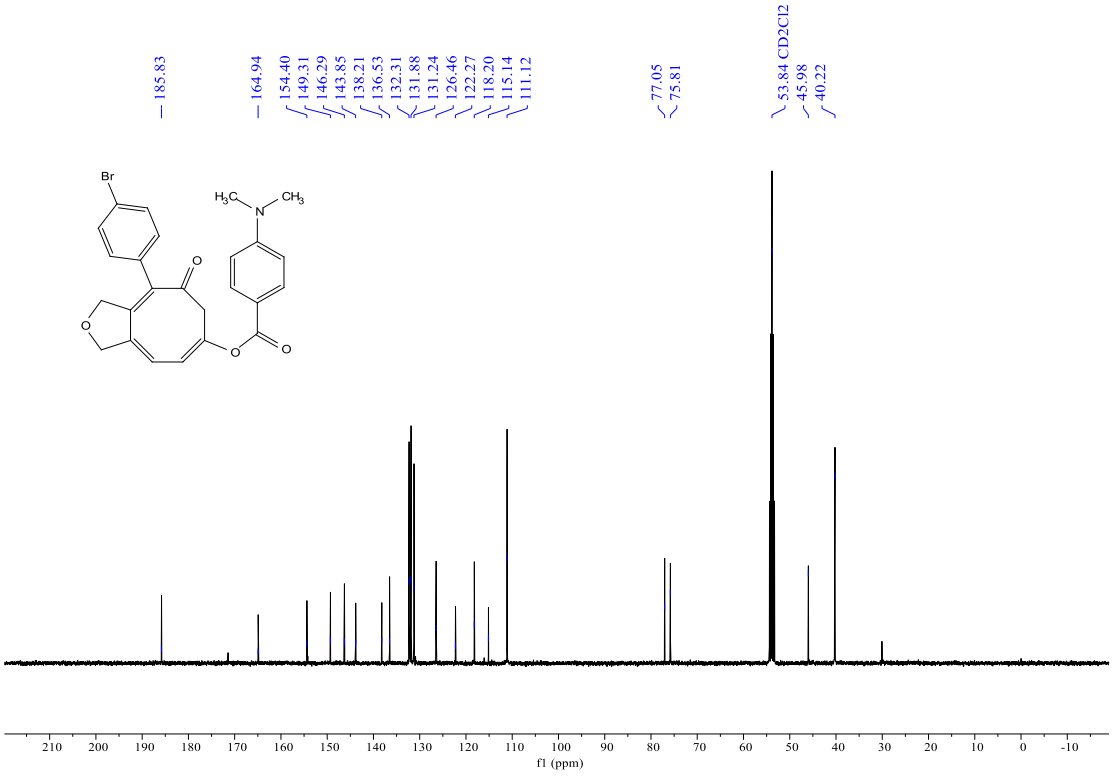

186.05
164.98
154.38
147.38
145.38
139.64
136.15
132.25
124.42
117.75
115.23
111.09
77.78
75.38
53.84 CD2Cl2
45.40
40.23
16.41
f1 (ppm)

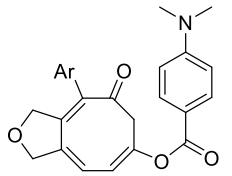


Ar = 4-BrC_6H_4

4s

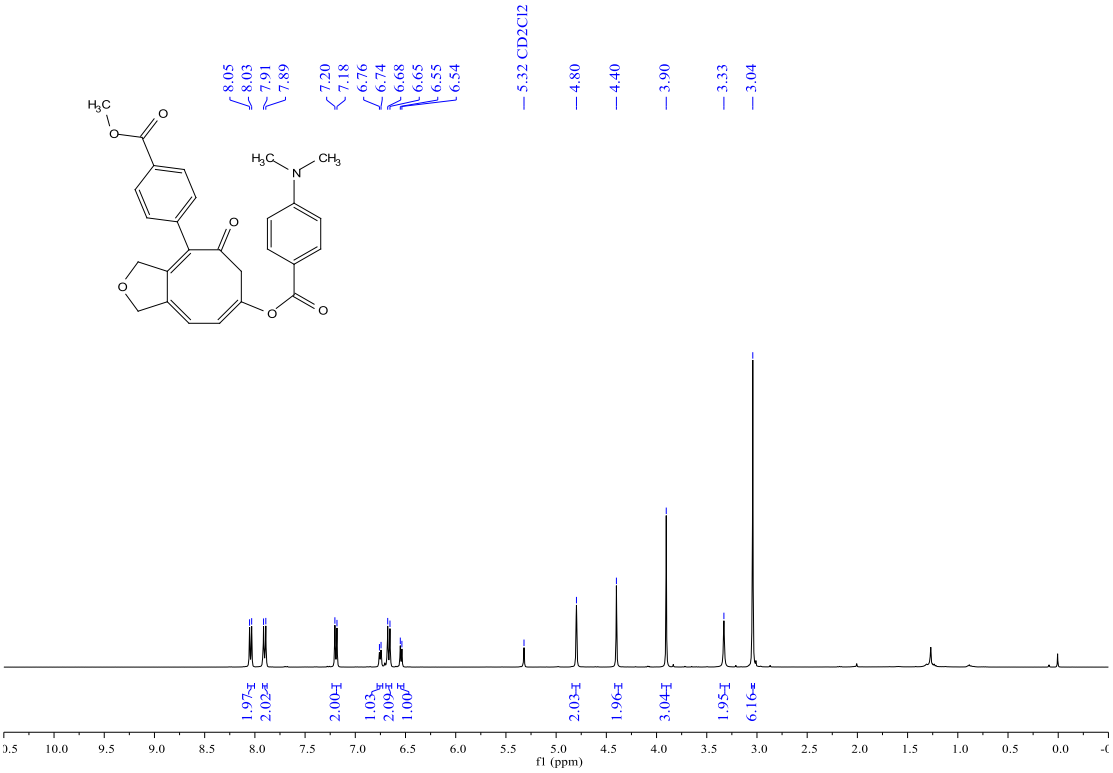


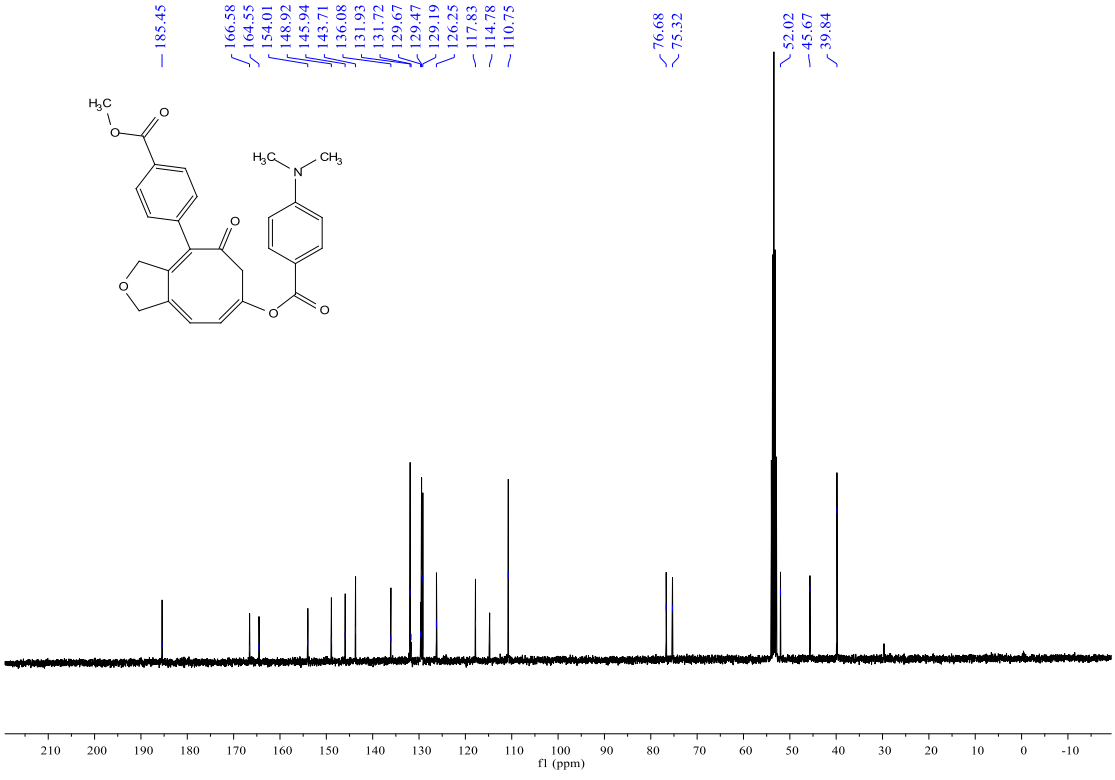


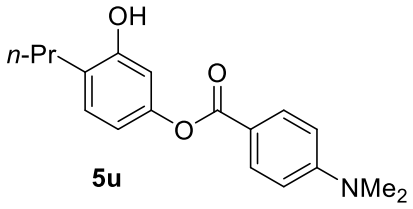


Ar = 4-$MeO_2CC_6H_4$

4t

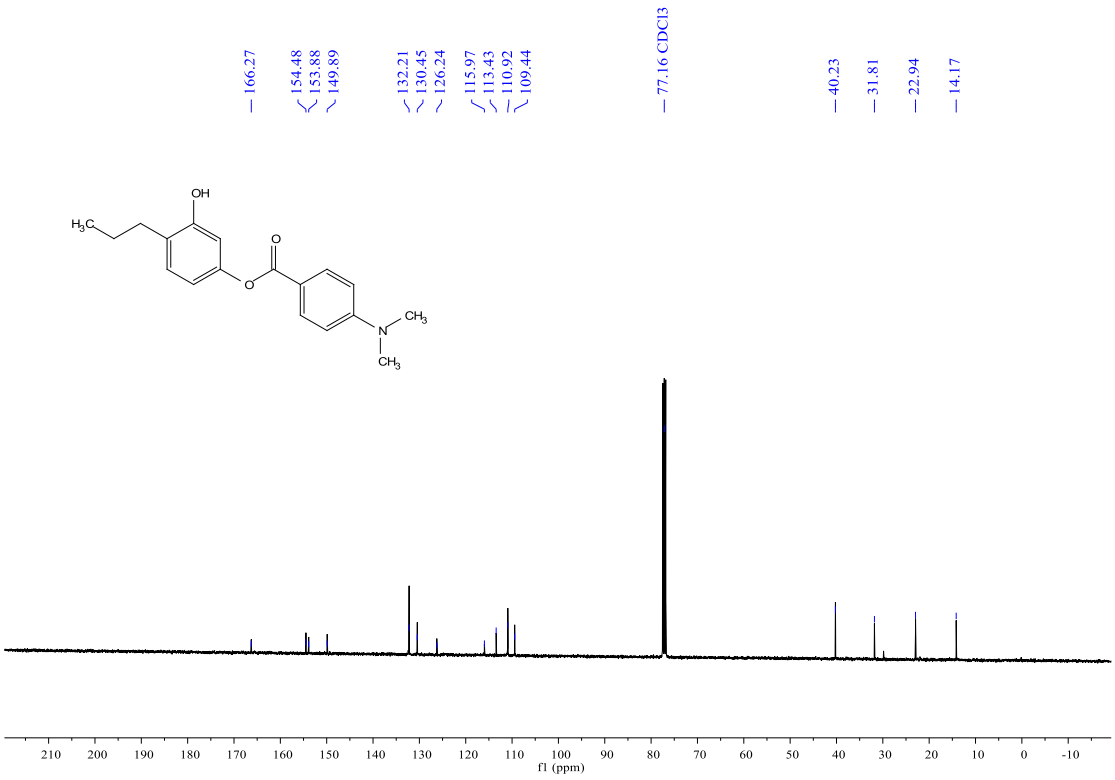





OH
n-Pr
O
O
NMe2

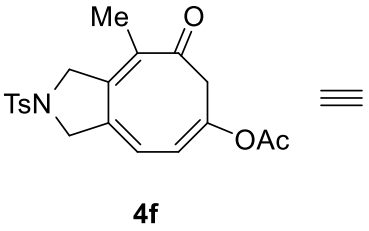
5u


8.05
8.03
7.26 CDCl3
7.10
7.08
6.70
6.68
6.67
6.65
6.65
6.63
6.62
5.74
3.07
2.54
2.52
2.50
1.65
1.63
1.61
1.59
1.58
1.56
0.98
0.96
0.94
OH
H3C
O
O
N
CH3
CH3
2.07
1.00
2.16
1.03
0.95
0.95
6.27
1.96
2.11
3.02
f1 (ppm)


166.27
154.48
153.88
149.89
132.21
130.45
126.24
115.97
113.43
110.92
109.44
77.16 CDCl3
40.23
31.81
22.94
14.17
OH
H3C
O
O
N
CH3
CH3
f1 (ppm)

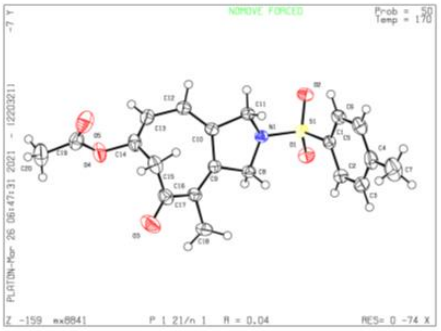
S9. X-Ray Data

X-ray diffraction of compound 4f



4f

CCDC: 2325937



Crystal data

Chemical formula	$C_{20}H_{21}NO_5S$
M_r	387.44
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	170
a, b, c (Å)	13.9338 (4), 5.3680 (1), 26.0420 (7)
β (°)	104.617 (3)
V (Å^3)	1884.81 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.32 × 0.25 × 0.03

Data collection

Diffractometer	XtaLAB AFC10 (RCD3): fixed-chi single
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.39.45i (Rigaku Oxford Diffraction, 2018) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.750, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14584, 5063, 4469
R_{int}	0.015
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.716

Refinement

$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.104, 1.04
No. of reflections	5063
No. of parameters	247

H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.28

S10. References

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